Figure 18 (continued)

```
REMARK   3   NON-BONDED CONTACTS REFINED ATOMS (A):  2631 ; 0.200 ; 0.200
REMARK   3   NON-BONDED TORSION REFINED ATOMS  (A):  4496 ; 0.292 ; 0.200
REMARK   3   H-BOND (X...Y) REFINED ATOMS      (A):   321 ; 0.173 ; 0.200
REMARK   3   SYMMETRY VDW REFINED ATOMS        (A):   124 ; 0.333 ; 0.200
REMARK   3   SYMMETRY H-BOND REFINED ATOMS     (A):    17 ; 0.205 ; 0.200
REMARK   3
REMARK   3  ISOTROPIC THERMAL FACTOR RESTRAINTS.      COUNT   RMS     WEIGHT
REMARK   3   MAIN-CHAIN BOND REFINED ATOMS  (A**2):  4221 ; 0.728 ; 1.500
REMARK   3   MAIN-CHAIN ANGLE REFINED ATOMS (A**2):  6577 ; 1.124 ; 2.000
REMARK   3   SIDE-CHAIN BOND REFINED ATOMS  (A**2):  2920 ; 2.095 ; 3.000
REMARK   3   SIDE-CHAIN ANGLE REFINED ATOMS (A**2):  2539 ; 3.232 ; 4.500
REMARK   3
REMARK   3  NCS RESTRAINTS STATISTICS
REMARK   3   NUMBER OF DIFFERENT NCS GROUPS :   1
REMARK   3
REMARK   3  NCS GROUP NUMBER                  :   1
REMARK   3     CHAIN NAMES                    : B D E A
REMARK   3     NUMBER OF COMPONENTS NCS GROUP :    9
REMARK   3       COMPONENT C  SSSEQI  TO  C   SSSEQI    CODE
REMARK   3           1     B    323       B     330      1
REMARK   3           1     D    323       D     330      1
REMARK   3           1     E    323       E     330      1
REMARK   3           1     A    323       A     330      1
REMARK   3           2     B    333       B     340      1
REMARK   3           2     D    333       D     340      1
REMARK   3           2     E    333       E     340      1
REMARK   3           2     A    333       A     340      1
REMARK   3           3     B    350       B     368      1
REMARK   3           3     D    350       D     368      1
REMARK   3           3     E    350       E     368      1
REMARK   3           3     A    350       A     368      1
REMARK   3           4     B    370       B     389      1
REMARK   3           4     D    370       D     389      1
REMARK   3           4     E    370       E     389      1
REMARK   3           4     A    370       A     389      1
REMARK   3           5     B    393       B     407      1
REMARK   3           5     D    393       D     407      1
REMARK   3           5     E    393       E     407      1
REMARK   3           5     A    393       A     407      1
REMARK   3           6     B    411       B     420      1
REMARK   3           6     D    411       D     420      1
REMARK   3           6     E    411       E     420      1
REMARK   3           6     A    411       A     420      1
REMARK   3           7     B    428       B     434      1
REMARK   3           7     D    428       D     434      1
REMARK   3           7     E    428       E     434      1
REMARK   3           7     A    428       A     434      1
REMARK   3           8     B    443       B     451      1
REMARK   3           8     D    443       D     451      1
REMARK   3           8     E    443       E     451      1
REMARK   3           8     A    443       A     451      1
REMARK   3           9     B    455       B     482      1
REMARK   3           9     D    455       D     482      1
REMARK   3           9     E    455       E     482      1
REMARK   3           9     A    455       A     482      1
REMARK   3                    GROUP CHAIN          COUNT   RMS     WEIGHT
REMARK   3   TIGHT POSITIONAL   1     B     (A):    965 ; 0.05 ; 0.05
REMARK   3   TIGHT POSITIONAL   1     D     (A):    965 ; 0.04 ; 0.05
REMARK   3   TIGHT POSITIONAL   1     E     (A):    965 ; 0.05 ; 0.05
REMARK   3   TIGHT POSITIONAL   1     A     (A):    965 ; 0.06 ; 0.05
REMARK   3   TIGHT THERMAL      1     B (A**2):    965 ; 1.46 ; 5.00
REMARK   3   TIGHT THERMAL      1     D (A**2):    965 ; 1.42 ; 5.00
REMARK   3   TIGHT THERMAL      1     E (A**2):    965 ; 1.17 ; 5.00
REMARK   3   TIGHT THERMAL      1     A (A**2):    965 ; 1.46 ; 5.00
REMARK   3
REMARK   3
REMARK   3  TLS DETAILS
REMARK   3   NUMBER OF TLS GROUPS  :    5
REMARK   3   ATOM RECORD CONTAINS SUM OF TLS AND RESIDUAL B FACTORS
REMARK   3   ANISOU RECORD CONTAINS SUM OF TLS AND RESIDUAL U FACTORS
REMARK   3
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Figure 18 (continued)

```
REMARK   3   TLS GROUP :      1
REMARK   3    NUMBER OF COMPONENTS GROUP :     2
REMARK   3    COMPONENTS         C SSSEQI   TO  C SSSEQI
REMARK   3    RESIDUE RANGE :    A   320        A   483
REMARK   3    RESIDUE RANGE :    A     1        A     1
REMARK   3    ORIGIN FOR THE GROUP (A):  35.1410  19.8550 -23.4970
REMARK   3    T TENSOR
REMARK   3      T11:  -0.1550 T22:  -0.1929
REMARK   3      T33:  -0.1067 T12:   0.0176
REMARK   3      T13:  -0.0298 T23:   0.0184
REMARK   3    L TENSOR
REMARK   3      L11:   2.3533 L22:   1.7075
REMARK   3      L33:   2.2571 L12:   0.0348
REMARK   3      L13:  -0.0773 L23:   0.5035
REMARK   3    S TENSOR
REMARK   3      S11:   0.0055 S12:   0.1725 S13:   0.1938
REMARK   3      S21:  -0.0821 S22:   0.0154 S23:  -0.0549
REMARK   3      S31:   0.0216 S32:   0.1221 S33:  -0.0208
REMARK   3
REMARK   3   TLS GROUP :      2
REMARK   3    NUMBER OF COMPONENTS GROUP :     2
REMARK   3    COMPONENTS         C SSSEQI   TO  C SSSEQI
REMARK   3    RESIDUE RANGE :    B   320        B   483
REMARK   3    RESIDUE RANGE :    B     1        B     1
REMARK   3    ORIGIN FOR THE GROUP (A):  12.4750  -3.5580 -19.4120
REMARK   3    T TENSOR
REMARK   3      T11:  -0.1896 T22:  -0.1182
REMARK   3      T33:  -0.0978 T12:  -0.0381
REMARK   3      T13:  -0.0171 T23:  -0.0637
REMARK   3    L TENSOR
REMARK   3      L11:   1.9172 L22:   2.6126
REMARK   3      L33:   3.6260 L12:   0.0348
REMARK   3      L13:  -0.2423 L23:  -0.1860
REMARK   3    S TENSOR
REMARK   3      S11:  -0.0729 S12:   0.1999 S13:  -0.0806
REMARK   3      S21:  -0.0771 S22:   0.0269 S23:   0.2153
REMARK   3      S31:   0.1325 S32:  -0.3438 S33:   0.0460
REMARK   3
REMARK   3   TLS GROUP :      3
REMARK   3    NUMBER OF COMPONENTS GROUP :     2
REMARK   3    COMPONENTS         C SSSEQI   TO  C SSSEQI
REMARK   3    RESIDUE RANGE :    D   319        D   483
REMARK   3    RESIDUE RANGE :    D     1        D     1
REMARK   3    ORIGIN FOR THE GROUP (A):  58.8840  -3.4260 -19.4800
REMARK   3    T TENSOR
REMARK   3      T11:  -0.2007 T22:  -0.1084
REMARK   3      T33:  -0.1629 T12:   0.0008
REMARK   3      T13:   0.0350 T23:  -0.0105
REMARK   3    L TENSOR
REMARK   3      L11:   2.5312 L22:   3.5830
REMARK   3      L33:   2.7686 L12:  -0.2516
REMARK   3      L13:  -0.0723 L23:   0.1658
REMARK   3    S TENSOR
REMARK   3      S11:   0.0281 S12:   0.3485 S13:  -0.0276
REMARK   3      S21:  -0.3438 S22:  -0.1013 S23:  -0.1815
REMARK   3      S31:   0.0548 S32:  -0.1509 S33:   0.0732
REMARK   3
REMARK   3   TLS GROUP :      4
REMARK   3    NUMBER OF COMPONENTS GROUP :     2
REMARK   3    COMPONENTS         C SSSEQI   TO  C SSSEQI
REMARK   3    RESIDUE RANGE :    E   320        E   483
REMARK   3    RESIDUE RANGE :    E     1        E     1
REMARK   3    ORIGIN FOR THE GROUP (A):  35.6570 -25.9320 -15.2800
REMARK   3    T TENSOR
REMARK   3      T11:  -0.0768 T22:  -0.2139
REMARK   3      T33:  -0.0804 T12:  -0.0233
REMARK   3      T13:   0.0636 T23:  -0.0476
REMARK   3    L TENSOR
REMARK   3      L11:   3.7194 L22:   2.4929
REMARK   3      L33:   2.9822 L12:   0.6274
REMARK   3      L13:   0.2948 L23:   1.0025
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Figure 18 (continued)

```
REMARK   3     S TENSOR
REMARK   3       S11:  -0.0484 S12:   0.3196 S13:  -0.2371
REMARK   3       S21:  -0.1986 S22:   0.0864 S23:  -0.0561
REMARK   3       S31:   0.1208 S32:   0.1243 S33:  -0.0380
REMARK   3
REMARK   3    TLS GROUP :      5
REMARK   3     NUMBER OF COMPONENTS GROUP :     2
REMARK   3     COMPONENTS         C SSSEQI    TO  C SSSEQI
REMARK   3     RESIDUE RANGE :    F   322         F   483
REMARK   3     RESIDUE RANGE :    F     1         F     1
REMARK   3     ORIGIN FOR THE GROUP (A):  29.6550  -7.6170 -50.4960
REMARK   3     T TENSOR
REMARK   3       T11:   0.0277 T22:   0.2406
REMARK   3       T33:  -0.1217 T12:   0.0164
REMARK   3       T13:  -0.0146 T23:  -0.0766
REMARK   3     L TENSOR
REMARK   3       L11:   2.4339 L22:   4.7601
REMARK   3       L33:   4.8718 L12:   0.4947
REMARK   3       L13:  -0.0699 L23:   1.5231
REMARK   3     S TENSOR
REMARK   3       S11:  -0.0489 S12:   0.5805 S13:  -0.1649
REMARK   3       S21:  -0.2269 S22:   0.0375 S23:  -0.0293
REMARK   3       S31:   0.2872 S32:   0.3181 S33:   0.0114
REMARK   3
REMARK   3
REMARK   3  BULK SOLVENT MODELLING.
REMARK   3   METHOD USED :  MASK
REMARK   3   PARAMETERS FOR MASK CALCULATION
REMARK   3   VDW PROBE RADIUS    :   1.40
REMARK   3   ION PROBE RADIUS    :   0.80
REMARK   3   SHRINKAGE RADIUS    :   0.80
REMARK   3
REMARK   3  OTHER REFINEMENT REMARKS:
REMARK   3  HYDROGENS HAVE BEEN ADDED IN THE RIDING POSITIONS
REMARK   3
LINK              VAL B 421                      ALA B 424                 gap
LINK              ASN E 422                      ARG E 427                 gap
LINK              ASN F 422                      ASN F 425                 gap
CRYST1   92.200   94.440  220.400  90.00  90.00  90.00 C 2 2 21
SCALE1      0.010846  0.000000  0.000000        0.00000
SCALE2      0.000000  0.010589  0.000000        0.00000
SCALE3      0.000000  0.000000  0.004537        0.00000
ATOM      1  N   SER A 320      54.724  26.969 -16.114  1.00 49.27           N
ANISOU    1  N   SER A 320     4119   7020   7581   -643   -576   -957       N
ATOM      2  CA  SER A 320      53.387  26.747 -16.772  1.00 47.48           C
ANISOU    2  CA  SER A 320     4127   6616   7296   -583   -499   -811       C
ATOM      3  CB  SER A 320      52.263  27.451 -15.989  1.00 46.88           C
ANISOU    3  CB  SER A 320     4227   6364   7221   -625   -539   -825       C
ATOM      4  OG  SER A 320      51.912  26.737 -14.806  1.00 47.95           O
ANISOU    4  OG  SER A 320     4428   6550   7242   -485   -673   -881       O
ATOM      5  C   SER A 320      53.375  27.229 -18.230  1.00 47.12           C
ANISOU    5  C   SER A 320     4085   6503   7314   -693   -330   -697       C
ATOM      6  O   SER A 320      54.163  28.116 -18.614  1.00 48.38           O
ANISOU    6  O   SER A 320     4111   6684   7588   -870   -256   -724       O
ATOM      7  N   SER A 321      52.500  26.617 -19.034  1.00 44.78           N
ANISOU    7  N   SER A 321     3940   6137   6937   -592   -270   -571       N
ATOM      8  CA  SER A 321      52.188  27.123 -20.378  1.00 43.99           C
ANISOU    8  CA  SER A 321     3899   5951   6864   -686   -122   -442       C
ATOM      9  CB  SER A 321      52.645  26.139 -21.481  1.00 44.33           C
ANISOU    9  CB  SER A 321     3883   6132   6831   -594    -42   -388       C
ATOM     10  OG  SER A 321      51.642  25.165 -21.790  1.00 44.54           O
ANISOU   10  OG  SER A 321     4074   6110   6740   -434    -58   -318       O
ATOM     11  C   SER A 321      50.674  27.446 -20.489  1.00 41.02           C
ANISOU   11  C   SER A 321     3753   5371   6461   -667   -116   -344       C
ATOM     12  O   SER A 321      49.828  26.667 -20.050  1.00 38.76           O
ANISOU   12  O   SER A 321     3585   5058   6085   -525   -186   -338       O
ATOM     13  N   SER A 322      50.365  28.608 -21.063  1.00 39.94           N
ANISOU   13  N   SER A 322     3672   5093   6409   -814    -31   -267       N
ATOM     14  CA  SER A 322      48.990  29.066 -21.192  1.00 37.50           C
ANISOU   14  CA  SER A 322     3558   4592   6098   -798    -28   -177       C
ATOM     15  CB  SER A 322      48.780  30.408 -20.502  1.00 38.36           C
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Figure 18 (continued)

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ANISOU   15  CB  SER A 322     3699   4533   6342   -928    -45   -227       C
ATOM     16  OG  SER A 322      48.807  30.236 -19.105  1.00 41.26           O
ANISOU   16  OG  SER A 322     4040   4932   6704   -882   -161   -379       O
ATOM     17  C   SER A 322      48.540  29.176 -22.627  1.00 35.90           C
ANISOU   17  C   SER A 322     3439   4343   5858   -813     81    -11       C
ATOM     18  O   SER A 322      49.323  29.452 -23.543  1.00 36.92           O
ANISOU   18  O   SER A 322     3488   4535   6006   -912    183     47       O
ATOM     19  N   PHE A 323      47.261  28.915 -22.811  1.00 32.90           N
ANISOU   19  N   PHE A 323     3216   3870   5414   -714     56     62       N
ATOM     20  CA  PHE A 323      46.611  29.195 -24.077  1.00 31.70           C
ANISOU   20  CA  PHE A 323     3167   3652   5224   -726    134    223       C
ATOM     21  CB  PHE A 323      46.730  28.032 -25.092  1.00 30.07           C
ANISOU   21  CB  PHE A 323     2953   3600   4872   -634    177    274       C
ATOM     22  CG  PHE A 323      46.322  26.714 -24.552  1.00 27.72           C
ANISOU   22  CG  PHE A 323     2678   3371   4481   -474     93    196       C
ATOM     23  CD1 PHE A 323      45.030  26.271 -24.707  1.00 25.75           C
ANISOU   23  CD1 PHE A 323     2566   3057   4162   -378     53    245       C
ATOM     24  CE1 PHE A 323      44.642  25.070 -24.196  1.00 24.05           C
ANISOU   24  CE1 PHE A 323     2380   2888   3871   -251    -15    180       C
ATOM     25  CZ  PHE A 323      45.541  24.275 -23.524  1.00 24.93           C
ANISOU   25  CZ  PHE A 323     2397   3105   3969   -195    -52     76       C
ATOM     26  CE2 PHE A 323      46.840  24.686 -23.357  1.00 25.71           C
ANISOU   26  CE2 PHE A 323     2350   3285   4133   -269    -26     23       C
ATOM     27  CD2 PHE A 323      47.234  25.908 -23.874  1.00 28.00           C
ANISOU   27  CD2 PHE A 323     2597   3536   4504   -418     51     77       C
ATOM     28  C   PHE A 323      45.163  29.568 -23.830  1.00 29.89           C
ANISOU   28  C   PHE A 323     3093   3256   5008   -667     82    270       C
ATOM     29  O   PHE A 323      44.616  29.366 -22.743  1.00 29.10           O
ANISOU   29  O   PHE A 323     3023   3117   4917   -600     -3    175       O
ATOM     30  N   SER A 324      44.553  30.095 -24.867  1.00 29.85           N
ANISOU   30  N   SER A 324     3182   3167   4994   -688    135    420       N
ATOM     31  CA  SER A 324      43.159  30.471 -24.844  1.00 30.29           C
ANISOU   31  CA  SER A 324     3369   3076   5062   -621     90    481       C
ATOM     32  CB  SER A 324      43.035  31.897 -25.367  1.00 32.34           C
ANISOU   32  CB  SER A 324     3691   3160   5436   -725    143    602       C
ATOM     33  OG  SER A 324      41.869  32.520 -24.855  1.00 36.69           O
ANISOU   33  OG  SER A 324     4337   3538   6064   -667     84    602       O
ATOM     34  C   SER A 324      42.357  29.507 -25.724  1.00 28.87           C
ANISOU   34  C   SER A 324     3257   2982   4731   -505     81    560       C
ATOM     35  O   SER A 324      42.760  29.221 -26.855  1.00 29.40           O
ANISOU   35  O   SER A 324     3315   3147   4709   -524    146    648       O
ATOM     36  N   PHE A 325      41.252  28.971 -25.199  1.00 26.88           N
ANISOU   36  N   PHE A 325     3064   2706   4445   -394      5    517       N
ATOM     37  CA  PHE A 325      40.371  28.148 -25.992  1.00 25.57           C
ANISOU   37  CA  PHE A 325     2960   2603   4153   -299    -13    580       C
ATOM     38  CB  PHE A 325      40.776  26.659 -25.905  1.00 24.87           C
ANISOU   38  CB  PHE A 325     2828   2671   3952   -233    -24    493       C
ATOM     39  CG  PHE A 325      39.944  25.733 -26.769  1.00 23.25           C
ANISOU   39  CG  PHE A 325     2684   2533   3617   -152    -40    535       C
ATOM     40  CD1 PHE A 325      40.003  25.815 -28.165  1.00 25.46           C
ANISOU   40  CD1 PHE A 325     2990   2876   3809   -171     12    645       C
ATOM     41  CE1 PHE A 325      39.243  24.954 -28.976  1.00 23.62           C
ANISOU   41  CE1 PHE A 325     2810   2717   3447   -102    -11    664       C
ATOM     42  CZ  PHE A 325      38.430  23.990 -28.377  1.00 23.09           C
ANISOU   42  CZ  PHE A 325     2768   2648   3358    -24    -79    576       C
ATOM     43  CE2 PHE A 325      38.359  23.916 -26.980  1.00 19.84           C
ANISOU   43  CE2 PHE A 325     2336   2168   3036     -9   -119    485       C
ATOM     44  CD2 PHE A 325      39.118  24.773 -26.195  1.00 20.21           C
ANISOU   44  CD2 PHE A 325     2332   2156   3190    -67   -102    463       C
ATOM     45  C   PHE A 325      38.945  28.342 -25.493  1.00 25.59           C
ANISOU   45  C   PHE A 325     3035   2502   4189   -224    -81    574       C
ATOM     46  O   PHE A 325      38.673  28.189 -24.307  1.00 24.95           O
ANISOU   46  O   PHE A 325     2941   2388   4150   -195   -126    462       O
ATOM     47  N   GLY A 326      38.032  28.646 -26.416  1.00 25.94           N
ANISOU   47  N   GLY A 326     3147   2510   4200   -188    -90    693       N
ATOM     48  CA  GLY A 326      36.612  28.725 -26.111  1.00 25.17           C
ANISOU   48  CA  GLY A 326     3096   2344   4125   -103   -155    690       C
ATOM     49  C   GLY A 326      36.229  29.790 -25.105  1.00 26.10           C
ANISOU   49  C   GLY A 326     3221   2299   4397   -108   -174    641       C
ATOM     50  O   GLY A 326      35.223  29.646 -24.422  1.00 25.44           O
ANISOU   50  O   GLY A 326     3144   2187   4334    -38   -220    574       O
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Figure 18 (continued)

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ATOM     51  N   GLY A 327      37.027  30.862 -25.017  1.00 27.43           N
ANISOU   51  N   GLY A 327    3385   2361   4675   -198   -132    664        N
ATOM     52  CA  GLY A 327      36.814  31.912 -24.021  1.00 27.22           C
ANISOU   52  CA  GLY A 327    3367   2168   4806   -214   -145    590        C
ATOM     53  C   GLY A 327      37.405  31.621 -22.645  1.00 26.92           C
ANISOU   53  C   GLY A 327    3269   2165   4793   -247   -155    409        C
ATOM     54  O   GLY A 327      37.162  32.382 -21.694  1.00 27.56           O
ANISOU   54  O   GLY A 327    3357   2128   4986   -254   -170    314        O
ATOM     55  N   PHE A 328      38.164  30.521 -22.524  1.00 25.21           N
ANISOU   55  N   PHE A 328    2998   2113   4470   -258   -153    357        N
ATOM     56  CA  PHE A 328      38.854  30.196 -21.271  1.00 24.27           C
ANISOU   56  CA  PHE A 328    2818   2049   4354   -284   -175    202        C
ATOM     57  CB  PHE A 328      38.420  28.823 -20.748  1.00 21.36           C
ANISOU   57  CB  PHE A 328    2450   1807   3859   -193   -216    141        C
ATOM     58  CG  PHE A 328      37.002  28.783 -20.278  1.00 21.75           C
ANISOU   58  CG  PHE A 328    2552   1805   3906   -115   -245    118        C
ATOM     59  CD1 PHE A 328      36.703  28.945 -18.927  1.00 20.12           C
ANISOU   59  CD1 PHE A 328    2344   1576   3724   -103   -269    -11        C
ATOM     60  CE1 PHE A 328      35.409  28.928 -18.474  1.00 18.66           C
ANISOU   60  CE1 PHE A 328    2192   1359   3539    -36   -280    -42        C
ATOM     61  CZ  PHE A 328      34.350  28.706 -19.370  1.00 19.24           C
ANISOU   61  CZ  PHE A 328    2291   1424   3594     24   -280     54        C
ATOM     62  CE2 PHE A 328      34.621  28.534 -20.739  1.00 19.65           C
ANISOU   62  CE2 PHE A 328    2351   1500   3614     16   -271    184        C
ATOM     63  CD2 PHE A 328      35.943  28.578 -21.186  1.00 20.82           C
ANISOU   63  CD2 PHE A 328    2476   1679   3755    -53   -247    216        C
ATOM     64  C   PHE A 328      40.359  30.228 -21.450  1.00 24.86           C
ANISOU   64  C   PHE A 328    2812   2194   4438   -383   -140    189        C
ATOM     65  O   PHE A 328      40.866  29.801 -22.489  1.00 25.40           O
ANISOU   65  O   PHE A 328    2860   2349   4442   -398    -98    278        O
ATOM     66  N   THR A 329      41.061  30.721 -20.433  1.00 25.87           N
ANISOU   66  N   THR A 329    2885   2302   4643   -451   -157     64        N
ATOM     67  CA  THR A 329      42.516  30.587 -20.320  1.00 26.02           C
ANISOU   67  CA  THR A 329    2793   2427   4668   -537   -143      9        C
ATOM     68  CB  THR A 329      43.119  31.743 -19.510  1.00 27.28           C
ANISOU   68  CB  THR A 329    2908   2490   4967   -657   -149   -100        C
ATOM     69  OG1 THR A 329      42.778  32.984 -20.135  1.00 28.71           O
ANISOU   69  OG1 THR A 329    3154   2479   5276   -731    -95     -9        O
ATOM     70  CG2 THR A 329      44.634  31.634 -19.423  1.00 28.51           C
ANISOU   70  CG2 THR A 329    2923   2773   5137   -755   -139   -164        C
ATOM     71  C   THR A 329      42.803  29.250 -19.623  1.00 25.30           C
ANISOU   71  C   THR A 329    2656   2504   4453   -448   -202    -77        C
ATOM     72  O   THR A 329      42.381  29.020 -18.481  1.00 24.62           O
ANISOU   72  O   THR A 329    2591   2422   4339   -397   -263   -177        O
ATOM     73  N   PHE A 330      43.508  28.370 -20.328  1.00 25.13           N
ANISOU   73  N   PHE A 330    2578   2617   4353   -425   -178    -34        N
ATOM     74  CA  PHE A 330      44.004  27.109 -19.781  1.00 23.76           C
ANISOU   74  CA  PHE A 330    2354   2594   4080   -338   -231   -105        C
ATOM     75  CB  PHE A 330      44.025  26.057 -20.885  1.00 22.27           C
ANISOU   75  CB  PHE A 330    2176   2492   3794   -266   -193    -21        C
ATOM     76  CG  PHE A 330      42.680  25.488 -21.239  1.00 20.53           C
ANISOU   76  CG  PHE A 330    2078   2221   3502   -181   -200     43        C
ATOM     77  CD1 PHE A 330      42.392  24.145 -20.983  1.00 19.04           C
ANISOU   77  CD1 PHE A 330    1924   2097   3213    -73   -240     19        C
ATOM     78  CE1 PHE A 330      41.140  23.599 -21.356  1.00 18.69           C
ANISOU   78  CE1 PHE A 330    1982   2010   3110    -15   -244     70        C
ATOM     79  CZ  PHE A 330      40.183  24.409 -21.969  1.00 16.45           C
ANISOU   79  CZ  PHE A 330    1753   1636   2861    -47   -219    144        C
ATOM     80  CE2 PHE A 330      40.483  25.735 -22.229  1.00 17.52           C
ANISOU   80  CE2 PHE A 330    1861   1702   3092   -134   -185    180        C
ATOM     81  CD2 PHE A 330      41.712  26.267 -21.870  1.00 18.89           C
ANISOU   81  CD2 PHE A 330    1947   1901   3330   -209   -170    131        C
ATOM     82  C   PHE A 330      45.442  27.334 -19.342  1.00 25.60           C
ANISOU   82  C   PHE A 330    2443   2923   4362   -411   -244   -196        C
ATOM     83  O   PHE A 330      46.220  27.886 -20.103  1.00 26.69           O
ANISOU   83  O   PHE A 330    2504   3075   4562   -509   -176   -160        O
ATOM     84  N   LYS A 331      45.798  26.952 -18.116  1.00 26.58           N
ANISOU   84  N   LYS A 331    2524   3119   4455   -370   -331   -311        N
ATOM     85  CA  LYS A 331      47.198  26.814 -17.729  1.00 28.34           C
ANISOU   85  CA  LYS A 331    2589   3483   4695   -400   -366   -401        C
ATOM     86  CB  LYS A 331      47.576  27.791 -16.597  1.00 29.96           C
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Figure 18 (continued)

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ANISOU   86  CB  LYS A 331     2740   3665   4978   -499   -424   -533  C
ATOM     87  CG  LYS A 331      46.950  29.141 -16.805  1.00 33.02      C
ANISOU   87  CG  LYS A 331     3199   3864   5484   -618   -366   -514  C
ATOM     88  CD  LYS A 331      47.691  30.310 -16.166  1.00 36.96      C
ANISOU   88  CD  LYS A 331     3609   4328   6108   -772   -384   -641  C
ATOM     89  CE  LYS A 331      46.932  31.614 -16.487  1.00 38.10      C
ANISOU   89  CE  LYS A 331     3856   4240   6381   -869   -318   -602  C
ATOM     90  NZ  LYS A 331      45.453  31.490 -16.098  1.00 35.18      N
ANISOU   90  NZ  LYS A 331     3643   3766   5958   -754   -340   -582  N
ATOM     91  C   LYS A 331      47.426  25.382 -17.285  1.00 27.41      C
ANISOU   91  C   LYS A 331     2461   3496   4457   -247   -438   -423  C
ATOM     92  O   LYS A 331      46.686  24.886 -16.436  1.00 26.89      O
ANISOU   92  O   LYS A 331     2493   3409   4316   -163   -502   -440  O
ATOM     93  N   ARG A 332      48.430  24.719 -17.857  1.00 27.61      N
ANISOU   93  N   ARG A 332     2371   3651   4467   -207   -422   -419  N
ATOM     94  CA  ARG A 332      48.758  23.355 -17.455  1.00 27.40      C
ANISOU   94  CA  ARG A 332     2331   3735   4345    -47   -494   -440  C
ATOM     95  CB  ARG A 332      49.602  22.651 -18.535  1.00 28.32      C
ANISOU   95  CB  ARG A 332     2347   3958   4456      6   -433   -413  C
ATOM     96  CG  ARG A 332      49.838  21.151 -18.250  1.00 27.07      C
ANISOU   96  CG  ARG A 332     2199   3876   4209    196   -503   -424  C
ATOM     97  CD  ARG A 332      50.442  20.434 -19.426  1.00 28.72      C
ANISOU   97  CD  ARG A 332     2338   4163   4411    261   -425   -404  C
ATOM     98  NE  ARG A 332      51.692  21.044 -19.875  1.00 33.91      N
ANISOU   98  NE  ARG A 332     2788   4950   5147    174   -371   -457  N
ATOM     99  CZ  ARG A 332      52.274  20.789 -21.043  1.00 34.89      C
ANISOU   99  CZ  ARG A 332     2824   5156   5276    178   -265   -445  C
ATOM    100  NH1 ARG A 332      51.722  19.917 -21.900  1.00 36.69      N
ANISOU  100  NH1 ARG A 332     3162   5348   5430    273   -212   -393  N
ATOM    101  NH2 ARG A 332      53.401  21.404 -21.362  1.00 33.49      N
ANISOU  101  NH2 ARG A 332     2447   5104   5173     80   -208   -495  N
ATOM    102  C   ARG A 332      49.478  23.325 -16.100  1.00 28.09      C
ANISOU  102  C   ARG A 332     2332   3923   4419    -22   -617   -552  C
ATOM    103  O   ARG A 332      50.525  23.979 -15.940  1.00 29.61      O
ANISOU  103  O   ARG A 332     2361   4203   4686   -112   -631   -634  O
ATOM    104  N   THR A 333      48.919  22.570 -15.143  1.00 26.95      N
ANISOU  104  N   THR A 333     2293   3774   4172     91   -705   -554  N
ATOM    105  CA  THR A 333      49.474  22.450 -13.787  1.00 27.54      C
ANISOU  105  CA  THR A 333     2315   3954   4195    133   -836   -647  C
ATOM    106  CB  THR A 333      48.388  22.724 -12.718  1.00 27.54      C
ANISOU  106  CB  THR A 333     2466   3874   4125    122   -877   -663  C
ATOM    107  OG1 THR A 333      47.269  21.862 -12.950  1.00 25.80      O
ANISOU  107  OG1 THR A 333     2413   3561   3829    209   -841   -558  O
ATOM    108  CG2 THR A 333      47.898  24.155 -12.811  1.00 27.45      C
ANISOU  108  CG2 THR A 333     2468   3750   4212    -40   -814   -706  C
ATOM    109  C   THR A 333      50.166  21.106 -13.487  1.00 28.06      C
ANISOU  109  C   THR A 333     2339   4142   4179    311   -925   -636  C
ATOM    110  O   THR A 333      50.964  21.028 -12.549  1.00 29.37      O
ANISOU  110  O   THR A 333     2410   4438   4313    352  -1042   -713  O
ATOM    111  N   SER A 334      49.860  20.070 -14.277  1.00 27.10      N
ANISOU  111  N   SER A 334     2292   3978   4028    420   -875   -547  N
ATOM    112  CA  SER A 334      50.480  18.728 -14.162  1.00 27.68      C
ANISOU  112  CA  SER A 334     2343   4130   4045    606   -945   -529  C
ATOM    113  CB  SER A 334      49.626  17.789 -13.327  1.00 26.96      C
ANISOU  113  CB  SER A 334     2442   3966   3835    718  -1011   -462  C
ATOM    114  OG  SER A 334      50.099  17.727 -12.010  1.00 30.72      O
ANISOU  114  OG  SER A 334     2890   4542   4239    772  -1148   -505  O
ATOM    115  C   SER A 334      50.552  18.102 -15.525  1.00 26.76      C
ANISOU  115  C   SER A 334     2220   3985   3963    656   -843   -480  C
ATOM    116  O   SER A 334      49.729  18.424 -16.392  1.00 25.27      O
ANISOU  116  O   SER A 334     2118   3691   3794    573   -735   -429  O
ATOM    117  N   GLY A 335      51.514  17.201 -15.702  1.00 27.29      N
ANISOU  117  N   GLY A 335     2187   4150   4033    801   -881   -502  N
ATOM    118  CA  GLY A 335      51.543  16.328 -16.851  1.00 27.54      C
ANISOU  118  CA  GLY A 335     2237   4152   4073    890   -798   -470  C
ATOM    119  C   GLY A 335      52.108  16.996 -18.081  1.00 28.17      C
ANISOU  119  C   GLY A 335     2172   4300   4230    785   -672   -502  C
ATOM    120  O   GLY A 335      52.658  18.070 -18.002  1.00 28.84      O
ANISOU  120  O   GLY A 335     2118   4461   4377    651   -657   -549  O
ATOM    121  N   SER A 336      51.966  16.334 -19.225  1.00 29.01      N
ANISOU  121  N   SER A 336     2317   4378   4327    841   -577   -478  N
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Figure 18 (continued)

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ATOM    122  CA  SER A 336      52.594  16.734 -20.488  1.00 29.82           C
ANISOU  122  CA  SER A 336    2284   4572   4476    770   -446   -503       C
ATOM    123  CB  SER A 336      54.095  16.434 -20.467  1.00 31.95           C
ANISOU  123  CB  SER A 336    2316   5026   4798    861   -468   -597       C
ATOM    124  OG  SER A 336      54.337  15.074 -20.142  1.00 33.68           O
ANISOU  124  OG  SER A 336    2566   5243   4988   1088   -549   -616       O
ATOM    125  C   SER A 336      51.901  15.920 -21.579  1.00 29.25           C
ANISOU  125  C   SER A 336    2348   4417   4348    830   -360   -463       C
ATOM    126  O   SER A 336      51.086  15.038 -21.269  1.00 29.76           O
ANISOU  126  O   SER A 336    2585   4361   4362    927   -411   -428       O
ATOM    127  N   SER A 337      52.166  16.233 -22.844  1.00 28.72           N
ANISOU  127  N   SER A 337    2213   4414   4284    760   -226   -467       N
ATOM    128  CA  SER A 337      51.555  15.491 -23.941  1.00 27.37           C
ANISOU  128  CA  SER A 337    2163   4189   4047    811   -146   -447       C
ATOM    129  CB  SER A 337      50.107  15.923 -24.208  1.00 25.82           C
ANISOU  129  CB  SER A 337    2159   3849   3801    703   -126   -356       C
ATOM    130  OG  SER A 337      49.993  17.233 -24.736  1.00 25.02           O
ANISOU  130  OG  SER A 337    2022   3769   3717    524    -47   -301       O
ATOM    131  C   SER A 337      52.380  15.600 -25.197  1.00 28.77           C
ANISOU  131  C   SER A 337    2201   4511   4219    786     -9   -489       C
ATOM    132  O   SER A 337      53.165  16.538 -25.354  1.00 29.57           O
ANISOU  132  O   SER A 337    2138   4728   4370    669     48   -499       O
ATOM    133  N   ILE A 338      52.232  14.601 -26.062  1.00 28.60           N
ANISOU  133  N   ILE A 338    2243   4486   4138    894     46   -524       N
ATOM    134  CA  ILE A 338      52.744  14.661 -27.433  1.00 29.37           C
ANISOU  134  CA  ILE A 338    2253   4715   4191    862    197   -558       C
ATOM    135  CB  ILE A 338      53.684  13.470 -27.745  1.00 30.62           C
ANISOU  135  CB  ILE A 338    2306   4969   4358   1060    220   -684       C
ATOM    136  CG1 ILE A 338      52.951  12.126 -27.567  1.00 28.62           C
ANISOU  136  CG1 ILE A 338    2242   4558   4076   1227    144   -711       C
ATOM    137  CD1 ILE A 338      53.801  10.890 -27.901  1.00 31.84           C
ANISOU  137  CD1 ILE A 338    2573   5023   4504   1443    164   -841       C
ATOM    138  CG2 ILE A 338      54.936  13.557 -26.869  1.00 29.51           C
ANISOU  138  CG2 ILE A 338    1946   4947   4320   1128    157   -748       C
ATOM    139  C   ILE A 338      51.544  14.715 -28.383  1.00 29.43           C
ANISOU  139  C   ILE A 338    2448   4638   4097    787    257   -490       C
ATOM    140  O   ILE A 338      50.421  14.456 -27.965  1.00 27.50           O
ANISOU  140  O   ILE A 338    2379   4237   3831    796    177   -443       O
ATOM    141  N   LYS A 339      51.768  15.077 -29.643  1.00 32.18           N
ANISOU  141  N   LYS A 339    2753   5101   4374    708    395   -484       N
ATOM    142  CA  LYS A 339      50.659  15.264 -30.588  1.00 32.96           C
ANISOU  142  CA  LYS A 339    3017   5146   4361    628    443   -410       C
ATOM    143  CB  LYS A 339      50.689  16.636 -31.277  1.00 33.66           C
ANISOU  143  CB  LYS A 339    3068   5303   4417    436    542   -299       C
ATOM    144  CG  LYS A 339      50.626  17.879 -30.433  1.00 35.13           C
ANISOU  144  CG  LYS A 339    3225   5418   4704    302    495   -209       C
ATOM    145  CD  LYS A 339      50.839  19.070 -31.356  1.00 39.41           C
ANISOU  145  CD  LYS A 339    3730   6034   5211    126    622   -105       C
ATOM    146  CE  LYS A 339      51.214  20.330 -30.602  1.00 43.35           C
ANISOU  146  CE  LYS A 339    4145   6489   5837    -18    608    -49       C
ATOM    147  NZ  LYS A 339      51.747  21.354 -31.562  1.00 47.40           N
ANISOU  147  NZ  LYS A 339    4590   7093   6327   -188    758     41       N
ATOM    148  C   LYS A 339      50.829  14.249 -31.693  1.00 34.82           C
ANISOU  148  C   LYS A 339    3269   5464   4496    730    526   -506       C
ATOM    149  O   LYS A 339      51.942  13.867 -32.033  1.00 35.45           O
ANISOU  149  O   LYS A 339    3198   5686   4586    804    603   -605       O
ATOM    150  N   ARG A 340      49.708  13.859 -32.287  1.00 34.88           N
ANISOU  150  N   ARG A 340    3453   5392   4405    727    514   -488       N
ATOM    151  CA  ARG A 340      49.725  12.999 -33.446  1.00 37.31           C
ANISOU  151  CA  ARG A 340    3799   5779   4597    798    594   -585       C
ATOM    152  CB  ARG A 340      49.722  11.545 -32.981  1.00 37.81           C
ANISOU  152  CB  ARG A 340    3918   5738   4710    985    522   -715       C
ATOM    153  CG  ARG A 340      49.740  10.518 -34.090  1.00 41.11           C
ANISOU  153  CG  ARG A 340    4385   6209   5025   1077    596   -851       C
ATOM    154  CD  ARG A 340      49.106   9.264 -33.574  1.00 44.08           C
ANISOU  154  CD  ARG A 340    4906   6391   5449   1202    493   -927       C
ATOM    155  NE  ARG A 340      49.351   8.129 -34.448  1.00 49.69           N
ANISOU  155  NE  ARG A 340    5647   7130   6103   1325    557  -1096       N
ATOM    156  CZ  ARG A 340      48.735   6.956 -34.322  1.00 52.03           C
ANISOU  156  CZ  ARG A 340    6093   7254   6423   1418    492  -1183       C
ATOM    157  NH1 ARG A 340      47.836   6.774 -33.353  1.00 51.49           N
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Figure 18 (continued)

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ANISOU  157  NH1 ARG A 340     6152   6986   6426   1395    368  -1102       N
ATOM    158  NH2 ARG A 340      49.013   5.967 -35.163  1.00 53.54           N
ANISOU  158  NH2 ARG A 340     6308   7469   6565   1528    558  -1356       N
ATOM    159  C   ARG A 340      48.494  13.280 -34.318  1.00 36.74           C
ANISOU  159  C   ARG A 340     3889   5680   4391    701    601   -510       C
ATOM    160  O   ARG A 340      47.381  13.418 -33.808  1.00 35.04           O
ANISOU  160  O   ARG A 340     3799   5317   4196    663    499   -439       O
ATOM    161  N   GLU A 341      48.689  13.298 -35.631  1.00 38.65           N
ANISOU  161  N   GLU A 341     4121   6076   4488    670    720   -537       N
ATOM    162  CA  GLU A 341      47.613  13.581 -36.585  1.00 38.96           C
ANISOU  162  CA  GLU A 341     4300   6129   4373    584    724   -467       C
ATOM    163  CB  GLU A 341      48.207  14.150 -37.884  1.00 41.11           C
ANISOU  163  CB  GLU A 341     4510   6619   4490    505    881   -436       C
ATOM    164  CG  GLU A 341      47.223  14.984 -38.717  1.00 44.93           C
ANISOU  164  CG  GLU A 341     5114   7131   4828    380    878   -285       C
ATOM    165  CD  GLU A 341      47.713  16.411 -38.966  1.00 50.98           C
ANISOU  165  CD  GLU A 341     5809   7976   5584    232    968   -111       C
ATOM    166  OE1 GLU A 341      48.843  16.587 -39.478  1.00 53.24           O
ANISOU  166  OE1 GLU A 341     5969   8430   5831    202   1115   -135       O
ATOM    167  OE2 GLU A 341      46.961  17.362 -38.638  1.00 52.85           O
ANISOU  167  OE2 GLU A 341     6117   8101   5863    142    896     49       O
ATOM    168  C   GLU A 341      46.793  12.331 -36.867  1.00 38.09           C
ANISOU  168  C   GLU A 341     4327   5941   4204    678    662   -589       C
ATOM    169  O   GLU A 341      47.339  11.310 -37.253  1.00 39.85           O
ANISOU  169  O   GLU A 341     4528   6213   4402    792    712   -749       O
ATOM    170  N   GLU A 342      45.486  12.415 -36.661  1.00 36.22           N
ANISOU  170  N   GLU A 342     4225   5579   3958    630    556   -523       N
ATOM    171  CA  GLU A 342      44.583  11.283 -36.867  1.00 35.81           C
ANISOU  171  CA  GLU A 342     4305   5437   3866    688    488   -634       C
ATOM    172  CB  GLU A 342      44.147  10.658 -35.531  1.00 34.01           C
ANISOU  172  CB  GLU A 342     4129   4994   3799    747    372   -653       C
ATOM    173  CG  GLU A 342      45.206   9.806 -34.803  1.00 36.13           C
ANISOU  173  CG  GLU A 342     4330   5210   4188    889    381   -758       C
ATOM    174  CD  GLU A 342      44.743   9.377 -33.407  1.00 35.59           C
ANISOU  174  CD  GLU A 342     4326   4936   4262    929    264   -729       C
ATOM    175  OE1 GLU A 342      45.588   9.256 -32.489  1.00 36.85           O
ANISOU  175  OE1 GLU A 342     4407   5063   4532   1012    245   -731       O
ATOM    176  OE2 GLU A 342      43.515   9.182 -33.211  1.00 38.13           O
ANISOU  176  OE2 GLU A 342     4771   5140   4578    874    190   -700       O
ATOM    177  C   GLU A 342      43.348  11.764 -37.613  1.00 34.67           C
ANISOU  177  C   GLU A 342     4264   5320   3589    586    446   -553       C
ATOM    178  O   GLU A 342      42.952  12.925 -37.477  1.00 33.00           O
ANISOU  178  O   GLU A 342     4047   5109   3382    490    423   -388       O
ATOM    179  N   GLU A 343      42.744  10.866 -38.396  1.00 34.97           N
ANISOU  179  N   GLU A 343     4394   5378   3515    612    430   -675       N
ATOM    180  CA  GLU A 343      41.458  11.149 -39.027  1.00 34.95           C
ANISOU  180  CA  GLU A 343     4487   5398   3393    529    359   -621       C
ATOM    181  CB  GLU A 343      41.400  10.673 -40.480  1.00 36.90           C
ANISOU  181  CB  GLU A 343     4778   5818   3423    531    413   -733       C
ATOM    182  CG  GLU A 343      42.297  11.448 -41.402  1.00 40.28           C
ANISOU  182  CG  GLU A 343     5137   6463   3706    499    544   -666       C
ATOM    183  CD  GLU A 343      42.120  11.051 -42.851  1.00 46.55           C
ANISOU  183  CD  GLU A 343     5988   7449   4252    492    592   -767       C
ATOM    184  OE1 GLU A 343      42.201   9.829 -43.156  1.00 49.23           O
ANISOU  184  OE1 GLU A 343     6363   7781   4562    569    603   -985       O
ATOM    185  OE2 GLU A 343      41.906  11.965 -43.686  1.00 47.82           O
ANISOU  185  OE2 GLU A 343     6164   7764   4241    412    616   -627       O
ATOM    186  C   GLU A 343      40.331  10.521 -38.238  1.00 33.33           C
ANISOU  186  C   GLU A 343     4367   5004   3293    529    234   -656       C
ATOM    187  O   GLU A 343      40.314   9.306 -37.987  1.00 33.83           O
ANISOU  187  O   GLU A 343     4478   4963   3412    597    215   -808       O
ATOM    188  N   VAL A 344      39.377  11.366 -37.868  1.00 31.66           N
ANISOU  188  N   VAL A 344     4174   4745   3110    451    153   -512       N
ATOM    189  CA  VAL A 344      38.220  10.946 -37.086  1.00 29.70           C
ANISOU  189  CA  VAL A 344     3988   4336   2960    430     43   -524       C
ATOM    190  CB  VAL A 344      38.219  11.619 -35.676  1.00 27.60           C
ANISOU  190  CB  VAL A 344     3682   3937   2866    420      8   -403       C
ATOM    191  CG1 VAL A 344      39.536  11.354 -34.968  1.00 27.04           C
ANISOU  191  CG1 VAL A 344     3551   3828   2895    497     68   -437       C
ATOM    192  CG2 VAL A 344      38.006  13.082 -35.781  1.00 26.27           C
ANISOU  192  CG2 VAL A 344     3472   3829   2680    354      3   -231       C
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Figure 18 (continued)

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ATOM    193  C   VAL A 344      36.924  11.195 -37.880  1.00 29.93           C
ANISOU  193  C   VAL A 344    4067   4436   2869    358    -34   -498       C
ATOM    194  O   VAL A 344      36.926  11.910 -38.891  1.00 30.08           O
ANISOU  194  O   VAL A 344    4076   4615   2736    327    -12   -427       O
ATOM    195  N   LEU A 345      35.842  10.556 -37.454  1.00 29.10           N
ANISOU  195  N   LEU A 345    4013   4220   2824    331   -122   -559       N
ATOM    196  CA  LEU A 345      34.564  10.639 -38.170  1.00 29.46           C
ANISOU  196  CA  LEU A 345    4088   4339   2767    267   -210   -564       C
ATOM    197  CB  LEU A 345      34.148   9.271 -38.665  1.00 30.37           C
ANISOU  197  CB  LEU A 345    4269   4435   2834    260   -234   -769       C
ATOM    198  CG  LEU A 345      34.852   8.751 -39.913  1.00 33.75           C
ANISOU  198  CG  LEU A 345    4723   5011   3089    297   -167   -900       C
ATOM    199  CD1 LEU A 345      35.036   7.242 -39.784  1.00 35.77           C
ANISOU  199  CD1 LEU A 345    5045   5139   3408    333   -149  -1117       C
ATOM    200  CD2 LEU A 345      34.081   9.105 -41.171  1.00 33.10           C
ANISOU  200  CD2 LEU A 345    4653   5125   2797    243   -226   -900       C
ATOM    201  C   LEU A 345      33.486  11.170 -37.248  1.00 27.67           C
ANISOU  201  C   LEU A 345    3841   4009   2661    219   -296   -463       C
ATOM    202  O   LEU A 345      33.301  10.630 -36.166  1.00 27.33           O
ANISOU  202  O   LEU A 345    3812   3808   2766    218   -308   -498       O
ATOM    203  N   THR A 346      32.793  12.229 -37.663  1.00 27.06           N
ANISOU  203  N   THR A 346    3734   4024   2522    186   -351   -335       N
ATOM    204  CA  THR A 346      31.706  12.815 -36.857  1.00 25.51           C
ANISOU  204  CA  THR A 346    3504   3749   2440    153   -431   -248       C
ATOM    205  CB  THR A 346      31.306  14.244 -37.367  1.00 25.70           C
ANISOU  205  CB  THR A 346    3492   3871   2401    152   -474    -71       C
ATOM    206  OG1 THR A 346      30.535  14.151 -38.575  1.00 27.06           O
ANISOU  206  OG1 THR A 346    3676   4199   2405    136   -550    -97       O
ATOM    207  CG2 THR A 346      32.515  15.135 -37.609  1.00 24.02           C
ANISOU  207  CG2 THR A 346    3273   3699   2154    177   -384     49       C
ATOM    208  C   THR A 346      30.457  11.896 -36.816  1.00 26.38           C
ANISOU  208  C   THR A 346    3628   3829   2568    101   -515   -371       C
ATOM    209  O   THR A 346      30.402  10.882 -37.518  1.00 27.44           O
ANISOU  209  O   THR A 346    3805   4004   2616     84   -521   -521       O
ATOM    210  N   GLY A 347      29.450  12.255 -36.016  1.00 25.61           N
ANISOU  210  N   GLY A 347    3486   3661   2583     68   -575   -320       N
ATOM    211  CA  GLY A 347      28.142  11.586 -36.109  1.00 25.17           C
ANISOU  211  CA  GLY A 347    3414   3613   2535      0   -659   -421       C
ATOM    212  C   GLY A 347      27.442  11.653 -37.467  1.00 26.55           C
ANISOU  212  C   GLY A 347    3572   3975   2541    -19   -747   -458       C
ATOM    213  O   GLY A 347      26.559  10.833 -37.753  1.00 27.47           O
ANISOU  213  O   GLY A 347    3681   4117   2641    -85   -811   -591       O
ATOM    214  N   ASN A 348      27.812  12.630 -38.302  1.00 26.51           N
ANISOU  214  N   ASN A 348    3561   4103   2408     31   -754   -337       N
ATOM    215  CA  ASN A 348      27.340  12.690 -39.715  1.00 27.47           C
ANISOU  215  CA  ASN A 348    3685   4430   2323     26   -835   -360       C
ATOM    216  CB  ASN A 348      27.036  14.128 -40.155  1.00 27.65           C
ANISOU  216  CB  ASN A 348    3670   4556   2281     75   -894   -155       C
ATOM    217  CG  ASN A 348      25.936  14.197 -41.212  1.00 30.51           C
ANISOU  217  CG  ASN A 348    3999   5108   2487     66 -1036   -172       C
ATOM    218  OD1 ASN A 348      25.056  13.330 -41.277  1.00 32.90           O
ANISOU  218  OD1 ASN A 348    4267   5438   2795      8 -1112   -331       O
ATOM    219  ND2 ASN A 348      26.001  15.206 -42.070  1.00 30.49           N
ANISOU  219  ND2 ASN A 348    4008   5240   2337    120 -1076     -9       N
ATOM    220  C   ASN A 348      28.300  12.039 -40.715  1.00 28.41           C
ANISOU  220  C   ASN A 348    3879   4646   2270     37   -769   -462       C
ATOM    221  O   ASN A 348      28.092  12.120 -41.927  1.00 29.94           O
ANISOU  221  O   ASN A 348    4087   5027   2260     37   -821   -478       O
ATOM    222  N   LEU A 349      29.339  11.376 -40.203  1.00 27.99           N
ANISOU  222  N   LEU A 349    3869   4473   2293     53   -657   -538       N
ATOM    223  CA  LEU A 349      30.311  10.650 -41.043  1.00 29.00           C
ANISOU  223  CA  LEU A 349    4058   4676   2284     77   -577   -664       C
ATOM    224  CB  LEU A 349      29.602   9.567 -41.884  1.00 30.71           C
ANISOU  224  CB  LEU A 349    4309   4973   2386     27   -646   -875       C
ATOM    225  CG  LEU A 349      28.751   8.531 -41.136  1.00 30.08           C
ANISOU  225  CG  LEU A 349    4234   4731   2466    -42   -696  -1020       C
ATOM    226  CD1 LEU A 349      28.022   7.598 -42.085  1.00 30.19           C
ANISOU  226  CD1 LEU A 349    4274   4842   2357   -109   -773  -1229       C
ATOM    227  CD2 LEU A 349      29.637   7.731 -40.222  1.00 29.27           C
ANISOU  227  CD2 LEU A 349    4181   4417   2521    -10   -593  -1087       C
ATOM    228  C   LEU A 349      31.195  11.574 -41.914  1.00 29.53           C
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Figure 18 (continued)

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ANISOU  228  C   LEU A 349     4130   4907   2185    121   -512   -535       C
ATOM    229  O   LEU A 349      31.589  11.202 -43.025  1.00 31.24           O
ANISOU  229  O   LEU A 349     4386   5279   2206    128   -480   -624       O
ATOM    230  N   GLN A 350      31.500  12.768 -41.395  1.00 28.82           N
ANISOU  230  N   GLN A 350     4003   4776   2171    141   -485   -330       N
ATOM    231  CA  GLN A 350      32.430  13.729 -42.020  1.00 30.27           C
ANISOU  231  CA  GLN A 350     4189   5072   2238    164   -402   -180       C
ATOM    232  CB  GLN A 350      31.967  15.164 -41.722  1.00 29.66           C
ANISOU  232  CB  GLN A 350     4082   4968   2219    164   -454     54       C
ATOM    233  CG  GLN A 350      32.811  16.292 -42.325  1.00 30.58           C
ANISOU  233  CG  GLN A 350     4211   5174   2234    167   -373    242       C
ATOM    234  CD  GLN A 350      32.356  17.682 -41.883  1.00 30.94           C
ANISOU  234  CD  GLN A 350     4238   5137   2382    172   -423    464       C
ATOM    235  OE1 GLN A 350      31.407  17.830 -41.095  1.00 28.70           O
ANISOU  235  OE1 GLN A 350     3920   4739   2246    182   -518    470       O
ATOM    236  NE2 GLN A 350      33.032  18.708 -42.394  1.00 31.65           N
ANISOU  236  NE2 GLN A 350     4350   5278   2397    161   -353    643       N
ATOM    237  C   GLN A 350      33.826  13.515 -41.457  1.00 29.30           C
ANISOU  237  C   GLN A 350     4053   4868   2210    193   -262   -209       C
ATOM    238  O   GLN A 350      33.975  13.375 -40.257  1.00 27.88           O
ANISOU  238  O   GLN A 350     3848   4515   2231    203   -253   -217       O
ATOM    239  N   THR A 351      34.832  13.499 -42.315  1.00 30.89           N
ANISOU  239  N   THR A 351     4265   5208   2262    207   -156   -226       N
ATOM    240  CA  THR A 351      36.226  13.364 -41.880  1.00 31.43           C
ANISOU  240  CA  THR A 351     4295   5233   2412    241    -21   -254       C
ATOM    241  CB  THR A 351      37.120  12.811 -43.019  1.00 33.11           C
ANISOU  241  CB  THR A 351     4522   5629   2431    264     91   -373       C
ATOM    242  OG1 THR A 351      36.598  11.543 -43.428  1.00 32.96           O
ANISOU  242  OG1 THR A 351     4555   5620   2346    282     42   -592       O
ATOM    243  CG2 THR A 351      38.567  12.622 -42.553  1.00 34.11           C
ANISOU  243  CG2 THR A 351     4582   5723   2657    309    229   -418       C
ATOM    244  C   THR A 351      36.792  14.669 -41.370  1.00 31.33           C
ANISOU  244  C   THR A 351     4233   5181   2492    220     30    -48       C
ATOM    245  O   THR A 351      36.719  15.702 -42.065  1.00 32.56           O
ANISOU  245  O   THR A 351     4400   5442   2531    184     38    119       O
ATOM    246  N   LEU A 352      37.338  14.623 -40.153  1.00 30.61           N
ANISOU  246  N   LEU A 352     4091   4933   2605    240     57    -57       N
ATOM    247  CA  LEU A 352      38.103  15.732 -39.588  1.00 30.88           C
ANISOU  247  CA  LEU A 352     4065   4923   2744    215    120     94       C
ATOM    248  CB  LEU A 352      37.467  16.248 -38.296  1.00 28.81           C
ANISOU  248  CB  LEU A 352     3790   4476   2680    205     35    169       C
ATOM    249  CG  LEU A 352      36.033  16.805 -38.295  1.00 28.66           C
ANISOU  249  CG  LEU A 352     3809   4417   2663    183    -86    262       C
ATOM    250  CD1 LEU A 352      35.625  17.143 -36.864  1.00 26.74           C
ANISOU  250  CD1 LEU A 352     3538   3992   2629    184   -138    291       C
ATOM    251  CD2 LEU A 352      35.847  18.027 -39.226  1.00 29.78           C
ANISOU  251  CD2 LEU A 352     3972   4656   2686    149    -86    449       C
ATOM    252  C   LEU A 352      39.550  15.297 -39.350  1.00 32.06           C
ANISOU  252  C   LEU A 352     4145   5094   2942    250    241      5       C
ATOM    253  O   LEU A 352      39.807  14.219 -38.805  1.00 31.91           O
ANISOU  253  O   LEU A 352     4119   5002   3003    313    237   -151       O
ATOM    254  N   LYS A 353      40.489  16.127 -39.790  1.00 33.85           N
ANISOU  254  N   LYS A 353     4320   5423   3120    208    350    105       N
ATOM    255  CA  LYS A 353      41.898  15.963 -39.470  1.00 34.96           C
ANISOU  255  CA  LYS A 353     4358   5594   3332    230    465     43       C
ATOM    256  CB  LYS A 353      42.735  16.484 -40.626  1.00 37.50           C
ANISOU  256  CB  LYS A 353     4644   6115   3488    179    606    104       C
ATOM    257  CG  LYS A 353      44.133  15.905 -40.717  1.00 41.91           C
ANISOU  257  CG  LYS A 353     5091   6777   4055    224    740    -29       C
ATOM    258  CD  LYS A 353      44.876  16.499 -41.917  1.00 48.11           C
ANISOU  258  CD  LYS A 353     5841   7780   4658    151    894     45       C
ATOM    259  CE  LYS A 353      45.805  15.477 -42.553  1.00 51.72           C
ANISOU  259  CE  LYS A 353     6232   8401   5018    228   1016   -154       C
ATOM    260  NZ  LYS A 353      46.301  15.930 -43.897  1.00 55.83           N
ANISOU  260  NZ  LYS A 353     6745   9164   5305    155   1168    -93       N
ATOM    261  C   LYS A 353      42.176  16.775 -38.212  1.00 33.47           C
ANISOU  261  C   LYS A 353     4107   5260   3349    199    442    138       C
ATOM    262  O   LYS A 353      42.115  18.008 -38.238  1.00 33.44           O
ANISOU  262  O   LYS A 353     4099   5242   3365    118    453    305       O
ATOM    263  N   ILE A 354      42.447  16.075 -37.110  1.00 32.36           N
ANISOU  263  N   ILE A 354     3930   5007   3360    266    404     30       N
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Figure 18 (continued)

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ATOM    264  CA  ILE A 354      42.806  16.720 -35.842  1.00 31.37           C
ANISOU  264  CA  ILE A 354    3738   4762   3418    245    377     87       C
ATOM    265  CB  ILE A 354      41.737  16.490 -34.731  1.00 29.39           C
ANISOU  265  CB  ILE A 354    3552   4334   3280    270    247     81       C
ATOM    266  CG1 ILE A 354      41.620  15.001 -34.379  1.00 28.30           C
ANISOU  266  CG1 ILE A 354    3451   4143   3159    368    206    -78       C
ATOM    267  CD1 ILE A 354      40.879  14.705 -33.055  1.00 28.35           C
ANISOU  267  CD1 ILE A 354    3501   3978   3294    389    104    -86       C
ATOM    268  CG2 ILE A 354      40.373  17.085 -35.158  1.00 29.30           C
ANISOU  268  CG2 ILE A 354    3629   4293   3209    219    176    185       C
ATOM    269  C   ILE A 354      44.170  16.257 -35.328  1.00 31.76           C
ANISOU  269  C   ILE A 354    3668   4847   3552    301    442    -15       C
ATOM    270  O   ILE A 354      44.603  15.135 -35.611  1.00 32.13           O
ANISOU  270  O   ILE A 354    3703   4946   3559    394    471   -157       O
ATOM    271  N   ARG A 355      44.834  17.127 -34.571  1.00 31.99           N
ANISOU  271  N   ARG A 355    3606   4847   3703    249    457     49       N
ATOM    272  CA  ARG A 355      46.027  16.753 -33.847  1.00 32.46           C
ANISOU  272  CA  ARG A 355    3536   4929   3866    306    483    -44       C
ATOM    273  CB  ARG A 355      46.987  17.948 -33.720  1.00 34.26           C
ANISOU  273  CB  ARG A 355    3637   5219   4163    198    559     35       C
ATOM    274  CG  ARG A 355      47.656  18.288 -35.032  1.00 39.00           C
ANISOU  274  CG  ARG A 355    4181   5997   4639    132    708     67       C
ATOM    275  CD  ARG A 355      48.600  19.431 -34.872  1.00 45.77           C
ANISOU  275  CD  ARG A 355    4910   6902   5578      6    790    144       C
ATOM    276  NE  ARG A 355      48.574  20.333 -36.023  1.00 52.25           N
ANISOU  276  NE  ARG A 355    5764   7806   6284   -123    901    284       N
ATOM    277  CZ  ARG A 355      49.146  21.539 -36.057  1.00 56.14           C
ANISOU  277  CZ  ARG A 355    6188   8307   6837   -272    980    398       C
ATOM    278  NH1 ARG A 355      49.801  22.023 -34.996  1.00 55.45           N
ANISOU  278  NH1 ARG A 355    5982   8157   6928   -320    956    369       N
ATOM    279  NH2 ARG A 355      49.061  22.269 -37.166  1.00 58.73           N
ANISOU  279  NH2 ARG A 355    6571   8703   7040   -381   1083    542       N
ATOM    280  C   ARG A 355      45.608  16.213 -32.488  1.00 29.93           C
ANISOU  280  C   ARG A 355    3252   4453   3666    379    359    -91       C
ATOM    281  O   ARG A 355      45.187  16.959 -31.616  1.00 28.02           O
ANISOU  281  O   ARG A 355    3025   4108   3513    324    295    -17       O
ATOM    282  N   VAL A 356      45.705  14.897 -32.339  1.00 28.99           N
ANISOU  282  N   VAL A 356    3158   4313   3543    504    331   -216       N
ATOM    283  CA  VAL A 356      45.350  14.233 -31.098  1.00 27.31           C
ANISOU  283  CA  VAL A 356    2994   3955   3426    581    223   -254       C
ATOM    284  CB  VAL A 356      45.003  12.746 -31.341  1.00 27.54           C
ANISOU  284  CB  VAL A 356    3118   3930   3417    695    198   -368       C
ATOM    285  CG1 VAL A 356      44.842  11.989 -30.014  1.00 27.23           C
ANISOU  285  CG1 VAL A 356    3128   3741   3479    780     99   -394       C
ATOM    286  CG2 VAL A 356      43.732  12.634 -32.157  1.00 26.35           C
ANISOU  286  CG2 VAL A 356    3094   3753   3164    637    186   -350       C
ATOM    287  C   VAL A 356      46.460  14.367 -30.058  1.00 26.67           C
ANISOU  287  C   VAL A 356    2786   3889   3460    624    204   -279       C
ATOM    288  O   VAL A 356      47.604  14.038 -30.324  1.00 28.57           O
ANISOU  288  O   VAL A 356    2907   4239   3708    689    263   -354       O
ATOM    289  N   HIS A 357      46.128  14.879 -28.884  1.00 25.43           N
ANISOU  289  N   HIS A 357    2642   3635   3385    590    121   -224       N
ATOM    290  CA  HIS A 357      47.107  14.993 -27.808  1.00 25.05           C
ANISOU  290  CA  HIS A 357    2478   3607   3433    631     79   -254       C
ATOM    291  CB  HIS A 357      46.849  16.229 -26.954  1.00 23.90           C
ANISOU  291  CB  HIS A 357    2315   3412   3353    517     36   -177       C
ATOM    292  CG  HIS A 357      47.266  17.509 -27.615  1.00 24.64           C
ANISOU  292  CG  HIS A 357    2322   3585   3457    380    123   -117       C
ATOM    293  ND1 HIS A 357      48.390  18.216 -27.235  1.00 25.54           N
ANISOU  293  ND1 HIS A 357    2277   3779   3648    325    146   -136       N
ATOM    294  CE1 HIS A 357      48.507  19.290 -27.995  1.00 24.49           C
ANISOU  294  CE1 HIS A 357    2110   3684   3511    188    235    -62       C
ATOM    295  NE2 HIS A 357      47.505  19.300 -28.857  1.00 25.00           N
ANISOU  295  NE2 HIS A 357    2307   3703   3488    167    263      9       N
ATOM    296  CD2 HIS A 357      46.725  18.191 -28.652  1.00 22.30           C
ANISOU  296  CD2 HIS A 357    2077   3296   3100    282    192    -34       C
ATOM    297  C   HIS A 357      47.122  13.716 -26.984  1.00 25.08           C
ANISOU  297  C   HIS A 357    2536   3529   3463    781     -5   -319       C
ATOM    298  O   HIS A 357      46.079  13.215 -26.573  1.00 24.14           O
ANISOU  298  O   HIS A 357    2561   3280   3330    795    -66   -297       O
ATOM    299  N   GLU A 358      48.322  13.175 -26.778  1.00 25.97           N
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Figure 18 (continued)

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ANISOU  299  N   GLU A 358     2530   3722   3616    895     -6   -397    N
ATOM    300  CA  GLU A 358      48.492  11.913 -26.065  1.00 25.43        C
ANISOU  300  CA  GLU A 358     2512   3575   3577   1062    -86   -451    C
ATOM    301  CB  GLU A 358      49.224  10.905 -26.939  1.00 26.70        C
ANISOU  301  CB  GLU A 358     2626   3796   3722   1198    -23   -558    C
ATOM    302  CG  GLU A 358      48.506  10.641 -28.264  1.00 26.20        C
ANISOU  302  CG  GLU A 358     2661   3726   3567   1151     64   -583    C
ATOM    303  CD  GLU A 358      49.340   9.852 -29.243  1.00 28.06        C
ANISOU  303  CD  GLU A 358     2826   4059   3777   1267    151   -709    C
ATOM    304  OE1 GLU A 358      50.595   9.994 -29.261  1.00 27.40        O
ANISOU  304  OE1 GLU A 358     2558   4117   3735   1329    192   -763    O
ATOM    305  OE2 GLU A 358      48.730   9.082 -30.014  1.00 28.42        O
ANISOU  305  OE2 GLU A 358     2993   4046   3760   1295    181   -767    O
ATOM    306  C   GLU A 358      49.233  12.107 -24.751  1.00 25.42        C
ANISOU  306  C   GLU A 358     2416   3596   3646   1113   -180   -446    C
ATOM    307  O   GLU A 358      50.317  12.638 -24.734  1.00 25.81        O
ANISOU  307  O   GLU A 358     2285   3785   3737   1107   -159   -481    O
ATOM    308  N   GLY A 359      48.608  11.697 -23.651  1.00 24.36        N
ANISOU  308  N   GLY A 359     2405   3335   3518   1152   -283   -403    N
ATOM    309  CA  GLY A 359      49.203  11.836 -22.335  1.00 23.73        C
ANISOU  309  CA  GLY A 359     2258   3280   3476   1204   -388   -394    C
ATOM    310  C   GLY A 359      48.271  12.445 -21.311  1.00 22.21        C
ANISOU  310  C   GLY A 359     2168   3005   3267   1103   -452   -318    C
ATOM    311  O   GLY A 359      47.324  13.163 -21.653  1.00 21.39        O
ANISOU  311  O   GLY A 359     2131   2854   3144    965   -404   -274    O
ATOM    312  N   TYR A 360      48.535  12.139 -20.049  1.00 22.42        N
ANISOU  312  N   TYR A 360     2206   3018   3293   1183   -562   -305    N
ATOM    313  CA  TYR A 360      47.836  12.761 -18.939  1.00 22.10        C
ANISOU  313  CA  TYR A 360     2238   2934   3226   1096   -623   -252    C
ATOM    314  CB  TYR A 360      48.072  11.966 -17.646  1.00 23.09        C
ANISOU  314  CB  TYR A 360     2423   3034   3318   1228   -745   -227    C
ATOM    315  CG  TYR A 360      47.620  12.724 -16.422  1.00 22.63        C
ANISOU  315  CG  TYR A 360     2399   2981   3217   1141   -809   -196    C
ATOM    316  CD1 TYR A 360      46.261  12.802 -16.094  1.00 21.89        C
ANISOU  316  CD1 TYR A 360     2469   2771   3076   1053   -784   -137    C
ATOM    317  CE1 TYR A 360      45.826  13.516 -14.980  1.00 22.60        C
ANISOU  317  CE1 TYR A 360     2589   2877   3121    976   -829   -125    C
ATOM    318  CZ  TYR A 360      46.759  14.181 -14.201  1.00 23.69        C
ANISOU  318  CZ  TYR A 360     2599   3145   3259    979   -908   -177    C
ATOM    319  OH  TYR A 360      46.326  14.889 -13.103  1.00 24.72        O
ANISOU  319  OH  TYR A 360     2764   3296   3335    903   -950   -184    O
ATOM    320  CE2 TYR A 360      48.122  14.118 -14.506  1.00 23.39        C
ANISOU  320  CE2 TYR A 360     2391   3226   3272   1057   -943   -234    C
ATOM    321  CD2 TYR A 360      48.543  13.397 -15.617  1.00 21.33        C
ANISOU  321  CD2 TYR A 360     2094   2952   3059   1140   -889   -241    C
ATOM    322  C   TYR A 360      48.232  14.229 -18.731  1.00 21.86        C
ANISOU  322  C   TYR A 360     2068   3007   3231    959   -615   -276    C
ATOM    323  O   TYR A 360      49.413  14.553 -18.673  1.00 23.34        O
ANISOU  323  O   TYR A 360     2082   3326   3462    981   -634   -333    O
ATOM    324  N   GLU A 361      47.237  15.100 -18.598  1.00 21.04        N
ANISOU  324  N   GLU A 361     2037   2837   3118    821   -587   -239    N
ATOM    325  CA  GLU A 361      47.450  16.524 -18.288  1.00 21.68        C
ANISOU  325  CA  GLU A 361     2021   2973   3244    684   -582   -262    C
ATOM    326  CB  GLU A 361      47.406  17.391 -19.552  1.00 20.98        C
ANISOU  326  CB  GLU A 361     1876   2893   3201    564   -469   -250    C
ATOM    327  CG  GLU A 361      48.599  17.217 -20.468  1.00 24.43        C
ANISOU  327  CG  GLU A 361     2161   3450   3670    596   -412   -291    C
ATOM    328  CD  GLU A 361      48.413  17.894 -21.813  1.00 22.96        C
ANISOU  328  CD  GLU A 361     1960   3269   3496    484   -289   -254    C
ATOM    329  OE1 GLU A 361      47.351  17.715 -22.440  1.00 20.90        O
ANISOU  329  OE1 GLU A 361     1833   2919   3188    469   -249   -198    O
ATOM    330  OE2 GLU A 361      49.338  18.607 -22.238  1.00 26.07        O
ANISOU  330  OE2 GLU A 361     2204   3762   3940    408   -232   -278    O
ATOM    331  C   GLU A 361      46.384  17.031 -17.332  1.00 20.41        C
ANISOU  331  C   GLU A 361     1975   2727   3053    614   -618   -235    C
ATOM    332  O   GLU A 361      45.240  16.587 -17.379  1.00 19.53        O
ANISOU  332  O   GLU A 361     2009   2512   2900    617   -599   -184    O
ATOM    333  N   GLU A 362      46.774  17.961 -16.476  1.00 21.16        N
ANISOU  333  N   GLU A 362     1994   2876   3172    547   -666   -282    N
ATOM    334  CA  GLU A 362      45.841  18.688 -15.628  1.00 22.46        C
ANISOU  334  CA  GLU A 362     2243   2974   3317    465   -683   -283    C
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Figure 18 (continued)

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ATOM    335  CB  GLU A 362      46.105  18.430 -14.141  1.00 22.93           C
ANISOU  335  CB  GLU A 362    2317   3092   3304    522   -796   -319       C
ATOM    336  CG  GLU A 362      45.054  19.016 -13.191  1.00 23.73           C
ANISOU  336  CG  GLU A 362    2522   3135   3361    454   -803   -328       C
ATOM    337  CD  GLU A 362      45.445  18.797 -11.736  1.00 26.51           C
ANISOU  337  CD  GLU A 362    2881   3575   3616    507   -916   -369       C
ATOM    338  OE1 GLU A 362      44.878  17.909 -11.080  1.00 31.01           O
ANISOU  338  OE1 GLU A 362    3579   4121   4081    581   -946   -311       O
ATOM    339  OE2 GLU A 362      46.357  19.496 -11.254  1.00 32.87           O
ANISOU  339  OE2 GLU A 362    3562   4482   4446    471   -977   -458       O
ATOM    340  C   GLU A 362      45.923  20.184 -15.927  1.00 22.18           C
ANISOU  340  C   GLU A 362    2128   2929   3372    317   -633   -319       C
ATOM    341  O   GLU A 362      47.018  20.735 -16.087  1.00 23.04           O
ANISOU  341  O   GLU A 362    2089   3123   3544    271   -636   -371       O
ATOM    342  N   PHE A 363      44.759  20.825 -15.996  1.00 21.18           N
ANISOU  342  N   PHE A 363    2095   2693   3259    243   -588   -290       N
ATOM    343  CA  PHE A 363      44.646  22.260 -16.286  1.00 21.78           C
ANISOU  343  CA  PHE A 363    2129   2714   3431    111   -538   -309       C
ATOM    344  CB  PHE A 363      44.028  22.491 -17.691  1.00 20.64           C
ANISOU  344  CB  PHE A 363    2025   2495   3323     74   -443   -220       C
ATOM    345  CG  PHE A 363      44.832  21.911 -18.837  1.00 21.21           C
ANISOU  345  CG  PHE A 363    2029   2642   3388    104   -397   -186       C
ATOM    346  CD1 PHE A 363      45.831  22.663 -19.453  1.00 20.96           C
ANISOU  346  CD1 PHE A 363    1874   2663   3429     19   -346   -195       C
ATOM    347  CE1 PHE A 363      46.570  22.150 -20.514  1.00 21.38           C
ANISOU  347  CE1 PHE A 363    1855   2803   3465     45   -287   -172       C
ATOM    348  CZ  PHE A 363      46.313  20.885 -20.998  1.00 18.73           C
ANISOU  348  CZ  PHE A 363    1579   2489   3048    163   -284   -150       C
ATOM    349  CE2 PHE A 363      45.316  20.123 -20.407  1.00 20.47           C
ANISOU  349  CE2 PHE A 363    1932   2638   3209    242   -340   -139       C
ATOM    350  CD2 PHE A 363      44.570  20.637 -19.319  1.00 18.91           C
ANISOU  350  CD2 PHE A 363    1799   2365   3021    209   -392   -151       C
ATOM    351  C   PHE A 363      43.738  22.994 -15.315  1.00 21.72           C
ANISOU  351  C   PHE A 363    2196   2632   3426     65   -558   -349       C
ATOM    352  O   PHE A 363      42.737  22.439 -14.830  1.00 20.51           O
ANISOU  352  O   PHE A 363    2152   2441   3199    117   -569   -326       O
ATOM    353  N   THR A 364      44.060  24.266 -15.070  1.00 22.89           N
ANISOU  353  N   THR A 364    2282   2752   3664    -41   -553   -414       N
ATOM    354  CA  THR A 364      43.032  25.177 -14.615  1.00 23.63           C
ANISOU  354  CA  THR A 364    2449   2733   3796    -93   -534   -443       C
ATOM    355  CB  THR A 364      43.500  26.176 -13.539  1.00 25.43           C
ANISOU  355  CB  THR A 364    2624   2968   4069   -171   -580   -577       C
ATOM    356  OG1 THR A 364      44.450  27.087 -14.102  1.00 29.67           O
ANISOU  356  OG1 THR A 364    3054   3489   4730   -281   -554   -601       O
ATOM    357  CG2 THR A 364      44.117  25.466 -12.315  1.00 24.74           C
ANISOU  357  CG2 THR A 364    2509   3025   3866   -111   -682   -657       C
ATOM    358  C   THR A 364      42.480  25.903 -15.855  1.00 23.68           C
ANISOU  358  C   THR A 364    2479   2620   3896   -148   -448   -357       C
ATOM    359  O   THR A 364      43.224  26.192 -16.803  1.00 23.87           O
ANISOU  359  O   THR A 364    2436   2655   3980   -201   -406   -313       O
ATOM    360  N   MSE A 365      41.172  26.145 -15.860  1.00 22.96           N
ANISOU  360  N   MSE A 365    2483   2430   3811   -130   -423   -327       N
ATOM    361  CA  MSE A 365      40.493  26.940 -16.879  1.00 23.90           C
ANISOU  361  CA  MSE A 365    2637   2429   4017   -165   -361   -246       C
ATOM    362  CB  MSE A 365      39.333  26.162 -17.525  1.00 22.98           C
ANISOU  362  CB  MSE A 365    2597   2301   3833    -88   -343   -155       C
ATOM    363  CG  MSE A 365      39.696  24.837 -18.242  1.00 23.11           C
ANISOU  363  CG  MSE A 365    2611   2416   3753    -32   -341    -95       C
ATOM    364  SE  MSE A 365      38.160  23.718 -18.667  0.90 26.48          SE
ANISOU  364  SE  MSE A 365    3137   2833   4091     49   -336    -31       SE
ATOM    365  CE  MSE A 365      37.026  25.011 -19.510  1.00 21.85           C
ANISOU  365  CE  MSE A 365    2574   2128   3599     18   -301     38       C
ATOM    366  C   MSE A 365      39.916  28.149 -16.156  1.00 23.45           C
ANISOU  366  C   MSE A 365    2605   2254   4051   -209   -361   -322       C
ATOM    367  O   MSE A 365      39.223  27.994 -15.148  1.00 23.44           O
ANISOU  367  O   MSE A 365    2645   2258   4002   -167   -386   -396       O
ATOM    368  N   VAL A 366      40.215  29.346 -16.654  1.00 23.42           N
ANISOU  368  N   VAL A 366    2581   2139   4177   -293   -326   -306       N
ATOM    369  CA  VAL A 366      39.691  30.586 -16.090  1.00 23.54           C
ANISOU  369  CA  VAL A 366    2629   2009   4308   -331   -319   -382       C
ATOM    370  CB  VAL A 366      40.833  31.452 -15.443  1.00 25.39           C
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Figure 18 (continued)

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ANISOU  370  CB  VAL A 366     2793   2224   4631   -448   -336   -505       C
ATOM    371  CG1 VAL A 366      40.312  32.803 -14.943  1.00 25.44           C
ANISOU  371  CG1 VAL A 366     2842   2047   4776   -492   -323   -594       C
ATOM    372  CG2 VAL A 366      41.533  30.678 -14.298  1.00 25.91           C
ANISOU  372  CG2 VAL A 366     2801   2461   4582   -433   -406   -628       C
ATOM    373  C   VAL A 366      38.916  31.393 -17.163  1.00 24.02           C
ANISOU  373  C   VAL A 366     2745   1911   4469   -329   -270   -260       C
ATOM    374  O   VAL A 366      39.498  31.895 -18.140  1.00 24.09           O
ANISOU  374  O   VAL A 366     2741   1868   4545   -398   -232   -164       O
ATOM    375  N   GLY A 367      37.609  31.524 -16.962  1.00 23.61           N
ANISOU  375  N   GLY A 367     2753   1792   4425   -248   -271   -262       N
ATOM    376  CA  GLY A 367      36.782  32.410 -17.779  1.00 25.53           C
ANISOU  376  CA  GLY A 367     3047   1876   4776   -223   -244   -164       C
ATOM    377  C   GLY A 367      36.277  33.660 -17.044  1.00 27.40           C
ANISOU  377  C   GLY A 367     3313   1940   5157   -225   -240   -269       C
ATOM    378  O   GLY A 367      36.620  33.896 -15.876  1.00 28.05           O
ANISOU  378  O   GLY A 367     3375   2032   5251   -261   -254   -435       O
ATOM    379  N   LYS A 368      35.459  34.461 -17.728  1.00 28.02           N
ANISOU  379  N   LYS A 368     3442   1863   5342   -177   -225   -178       N
ATOM    380  CA  LYS A 368      34.815  35.621 -17.111  1.00 30.01           C
ANISOU  380  CA  LYS A 368     3727   1931   5744   -146   -219   -276       C
ATOM    381  CB  LYS A 368      34.065  36.473 -18.152  1.00 31.76           C
ANISOU  381  CB  LYS A 368     4007   1974   6086    -83   -211   -125       C
ATOM    382  CG  LYS A 368      34.947  37.212 -19.147  1.00 36.76           C
ANISOU  382  CG  LYS A 368     4677   2481   6808   -185   -185     20       C
ATOM    383  CD  LYS A 368      34.052  37.959 -20.123  1.00 43.28           C
ANISOU  383  CD  LYS A 368     5574   3141   7729    -94   -190    186       C
ATOM    384  CE  LYS A 368      34.692  38.098 -21.504  1.00 48.10           C
ANISOU  384  CE  LYS A 368     6224   3733   8319   -165   -165    410       C
ATOM    385  NZ  LYS A 368      33.990  39.150 -22.301  1.00 50.85           N
ANISOU  385  NZ  LYS A 368     6662   3864   8792    -92   -174    569       N
ATOM    386  C   LYS A 368      33.837  35.243 -15.977  1.00 28.59           C
ANISOU  386  C   LYS A 368     3533   1823   5507    -54   -230   -427       C
ATOM    387  O   LYS A 368      33.803  35.912 -14.963  1.00 28.78           O
ANISOU  387  O   LYS A 368     3561   1774   5601    -66   -224   -594       O
ATOM    388  N   ARG A 369      33.047  34.184 -16.141  1.00 26.59           N
ANISOU  388  N   ARG A 369     3264   1712   5126     28   -239   -377       N
ATOM    389  CA  ARG A 369      32.032  33.851 -15.117  1.00 25.86           C
ANISOU  389  CA  ARG A 369     3155   1690   4982    105   -231   -507       C
ATOM    390  CB  ARG A 369      30.615  34.105 -15.636  1.00 26.07           C
ANISOU  390  CB  ARG A 369     3177   1657   5072    225   -227   -447       C
ATOM    391  CG  ARG A 369      30.370  35.495 -16.189  1.00 28.17           C
ANISOU  391  CG  ARG A 369     3477   1696   5532    264   -228   -403       C
ATOM    392  CD  ARG A 369      28.865  35.741 -16.363  1.00 30.60           C
ANISOU  392  CD  ARG A 369     3757   1968   5902    411   -232   -393       C
ATOM    393  NE  ARG A 369      28.465  36.887 -15.535  1.00 37.04           N
ANISOU  393  NE  ARG A 369     4580   2621   6871    463   -207   -550       N
ATOM    394  CZ  ARG A 369      27.527  36.892 -14.591  1.00 37.12           C
ANISOU  394  CZ  ARG A 369     4542   2678   6882    543   -176   -709       C
ATOM    395  NH1 ARG A 369      26.793  35.818 -14.317  1.00 34.10           N
ANISOU  395  NH1 ARG A 369     4097   2499   6360    575   -163   -727       N
ATOM    396  NH2 ARG A 369      27.296  38.024 -13.941  1.00 43.52           N
ANISOU  396  NH2 ARG A 369     5369   3322   7847    590   -151   -856       N
ATOM    397  C   ARG A 369      32.135  32.449 -14.526  1.00 23.85           C
ANISOU  397  C   ARG A 369     2878   1646   4537     96   -238   -539       C
ATOM    398  O   ARG A 369      31.300  32.046 -13.716  1.00 22.65           O
ANISOU  398  O   ARG A 369     2714   1571   4319    145   -220   -626       O
ATOM    399  N   ALA A 370      33.158  31.705 -14.934  1.00 23.31           N
ANISOU  399  N   ALA A 370     2805   1669   4383     35   -258   -466       N
ATOM    400  CA  ALA A 370      33.390  30.376 -14.395  1.00 22.66           C
ANISOU  400  CA  ALA A 370     2715   1763   4132     32   -271   -485       C
ATOM    401  CB  ALA A 370      32.551  29.299 -15.160  1.00 21.26           C
ANISOU  401  CB  ALA A 370     2543   1663   3872     89   -268   -369       C
ATOM    402  C   ALA A 370      34.875  30.034 -14.427  1.00 22.52           C
ANISOU  402  C   ALA A 370     2679   1811   4069    -42   -299   -476       C
ATOM    403  O   ALA A 370      35.619  30.550 -15.262  1.00 23.04           O
ANISOU  403  O   ALA A 370     2730   1812   4213    -93   -297   -408       O
ATOM    404  N   THR A 371      35.290  29.169 -13.503  1.00 22.37           N
ANISOU  404  N   THR A 371     2656   1925   3920    -44   -324   -542       N
ATOM    405  CA  THR A 371      36.622  28.573 -13.512  1.00 22.86           C
ANISOU  405  CA  THR A 371     2686   2083   3918    -84   -362   -529       C
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Figure 18 (continued)

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ATOM    406  CB  THR A 371      37.577  29.196 -12.446  1.00 24.26           C
ANISOU  406  CB  THR A 371    2826   2283   4108   -147   -400   -676         C
ATOM    407  OG1 THR A 371      37.179  28.782 -11.144  1.00 27.06           O
ANISOU  407  OG1 THR A 371    3210   2727   4343   -114   -419   -776         O
ATOM    408  CG2 THR A 371      37.597  30.704 -12.518  1.00 22.87           C
ANISOU  408  CG2 THR A 371    2640   1949   4099   -210   -377   -743         C
ATOM    409  C   THR A 371      36.510  27.054 -13.335  1.00 21.90           C
ANISOU  409  C   THR A 371    2588   2092   3640    -29   -380   -480         C
ATOM    410  O   THR A 371      35.451  26.546 -12.967  1.00 22.77           O
ANISOU  410  O   THR A 371    2742   2223   3688     15   -360   -478         O
ATOM    411  N   ALA A 372      37.576  26.312 -13.616  1.00 21.17           N
ANISOU  411  N   ALA A 372    2467   2082   3493    -32   -413   -439         N
ATOM    412  CA  ALA A 372      37.495  24.865 -13.505  1.00 19.77           C
ANISOU  412  CA  ALA A 372    2327   1997   3186     28   -430   -386         C
ATOM    413  CB  ALA A 372      36.796  24.241 -14.737  1.00 18.33           C
ANISOU  413  CB  ALA A 372    2174   1784   3006     59   -394   -271         C
ATOM    414  C   ALA A 372      38.835  24.237 -13.308  1.00 19.97           C
ANISOU  414  C   ALA A 372    2310   2121   3156     39   -484   -393         C
ATOM    415  O   ALA A 372      39.853  24.849 -13.608  1.00 20.79           O
ANISOU  415  O   ALA A 372    2337   2231   3330     -8   -497   -419         O
ATOM    416  N   ILE A 373      38.816  23.010 -12.789  1.00 19.57           N
ANISOU  416  N   ILE A 373    2308   2144   2983    102   -514   -368         N
ATOM    417  CA  ILE A 373      39.963  22.112 -12.831  1.00 19.72           C
ANISOU  417  CA  ILE A 373    2295   2249   2948    151   -568   -345         C
ATOM    418  CB  ILE A 373      40.416  21.607 -11.444  1.00 20.88           C
ANISOU  418  CB  ILE A 373    2464   2493   2978    193   -643   -394         C
ATOM    419  CG1 ILE A 373      40.502  22.762 -10.432  1.00 22.57           C
ANISOU  419  CG1 ILE A 373    2645   2729   3201    130   -667   -517         C
ATOM    420  CD1 ILE A 373      40.936  22.348  -8.989  1.00 22.21           C
ANISOU  420  CD1 ILE A 373    2624   2805   3011    169   -752   -574         C
ATOM    421  CG2 ILE A 373      41.764  20.932 -11.585  1.00 18.66           C
ANISOU  421  CG2 ILE A 373    2115   2300   2676    252   -710   -381         C
ATOM    422  C   ILE A 373      39.645  20.919 -13.691  1.00 18.62           C
ANISOU  422  C   ILE A 373    2207   2092   2774    209   -544   -246         C
ATOM    423  O   ILE A 373      38.635  20.253 -13.476  1.00 18.19           O
ANISOU  423  O   ILE A 373    2241   2007   2662    231   -522   -209         O
ATOM    424  N   LEU A 374      40.530  20.643 -14.656  1.00 18.68           N
ANISOU  424  N   LEU A 374    2154   2125   2818    229   -542   -216         N
ATOM    425  CA  LEU A 374      40.328  19.586 -15.652  1.00 16.99           C
ANISOU  425  CA  LEU A 374    1981   1892   2582    281   -514   -144         C
ATOM    426  CB  LEU A 374      40.251  20.197 -17.064  1.00 15.29           C
ANISOU  426  CB  LEU A 374    1724   1644   2441    233   -453   -108         C
ATOM    427  CG  LEU A 374      40.219  19.251 -18.265  1.00 15.44           C
ANISOU  427  CG  LEU A 374    1766   1665   2434    277   -421    -57         C
ATOM    428  CD1 LEU A 374      38.992  18.305 -18.302  1.00 14.91           C
ANISOU  428  CD1 LEU A 374    1810   1543   2313    303   -413    -24         C
ATOM    429  CD2 LEU A 374      40.303  20.021 -19.573  1.00 16.74           C
ANISOU  429  CD2 LEU A 374    1884   1827   2651    222   -365    -20         C
ATOM    430  C   LEU A 374      41.486  18.592 -15.607  1.00 17.53           C
ANISOU  430  C   LEU A 374    2018   2033   2611    368   -562   -144         C
ATOM    431  O   LEU A 374      42.663  19.008 -15.663  1.00 18.31           O
ANISOU  431  O   LEU A 374    2004   2204   2748    365   -586   -185         O
ATOM    432  N   ARG A 375      41.161  17.302 -15.495  1.00 16.74           N
ANISOU  432  N   ARG A 375    2010   1906   2444    445   -575   -102         N
ATOM    433  CA  ARG A 375      42.128  16.231 -15.749  1.00 17.32           C
ANISOU  433  CA  ARG A 375    2066   2016   2497    550   -609    -93         C
ATOM    434  CB  ARG A 375      42.224  15.233 -14.612  1.00 17.75           C
ANISOU  434  CB  ARG A 375    2205   2070   2469    639   -680    -69         C
ATOM    435  CG  ARG A 375      43.006  15.772 -13.443  1.00 18.20           C
ANISOU  435  CG  ARG A 375    2196   2225   2493    651   -761   -113         C
ATOM    436  CD  ARG A 375      42.926  14.833 -12.281  1.00 20.67           C
ANISOU  436  CD  ARG A 375    2618   2538   2698    734   -831    -66         C
ATOM    437  NE  ARG A 375      43.721  15.319 -11.164  1.00 22.34           N
ANISOU  437  NE  ARG A 375    2762   2868   2856    753   -925   -115         N
ATOM    438  CZ  ARG A 375      43.603  14.892  -9.911  1.00 24.36           C
ANISOU  438  CZ  ARG A 375    3108   3157   2992    799   -993    -83         C
ATOM    439  NH1 ARG A 375      42.718  13.955  -9.595  1.00 26.04           N
ANISOU  439  NH1 ARG A 375    3486   3280   3130    822   -967     10         N
ATOM    440  NH2 ARG A 375      44.383  15.409  -8.971  1.00 27.64           N
ANISOU  440  NH2 ARG A 375    3448   3702   3353    812  -1089   -144         N
ATOM    441  C   ARG A 375      41.742  15.522 -17.009  1.00 17.19           C
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Figure 18 (continued)

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ANISOU  441  C   ARG A 375     2092   1945   2495    569   -551    -62       C
ATOM    442  O   ARG A 375      40.566  15.227 -17.252  1.00 16.68           O
ANISOU  442  O   ARG A 375     2122   1802   2414    533   -514    -29       O
ATOM    443  N   LYS A 376      42.743  15.264 -17.830  1.00 17.94           N
ANISOU  443  N   LYS A 376     2106   2093   2619    621   -540    -83       N
ATOM    444  CA  LYS A 376      42.484  14.748 -19.154  1.00 18.80           C
ANISOU  444  CA  LYS A 376     2238   2172   2732    630   -477    -75       C
ATOM    445  CB  LYS A 376      42.485  15.948 -20.089  1.00 19.04           C
ANISOU  445  CB  LYS A 376     2186   2243   2804    530   -415    -73       C
ATOM    446  CG  LYS A 376      42.472  15.657 -21.514  1.00 22.12           C
ANISOU  446  CG  LYS A 376     2573   2649   3183    532   -351    -70       C
ATOM    447  CD  LYS A 376      43.216  16.738 -22.249  1.00 25.06           C
ANISOU  447  CD  LYS A 376     2826   3105   3592    464   -298    -68       C
ATOM    448  CE  LYS A 376      43.015  16.490 -23.721  1.00 26.93           C
ANISOU  448  CE  LYS A 376     3079   3367   3787    456   -227    -54       C
ATOM    449  NZ  LYS A 376      43.691  15.264 -24.120  1.00 27.50           N
ANISOU  449  NZ  LYS A 376     3143   3478   3828    566   -218   -111       N
ATOM    450  C   LYS A 376      43.569  13.729 -19.486  1.00 19.24           C
ANISOU  450  C   LYS A 376     2256   2266   2787    756   -493   -106       C
ATOM    451  O   LYS A 376      44.650  13.770 -18.915  1.00 20.06           O
ANISOU  451  O   LYS A 376     2269   2448   2907    818   -543   -135       O
ATOM    452  N   ALA A 377      43.257  12.766 -20.348  1.00 19.46           N
ANISOU  452  N   ALA A 377     2354   2239   2799    802   -456   -112       N
ATOM    453  CA  ALA A 377      44.251  11.822 -20.856  1.00 20.59           C
ANISOU  453  CA  ALA A 377     2459   2411   2953    930   -454   -160       C
ATOM    454  CB  ALA A 377      44.120  10.473 -20.155  1.00 20.90           C
ANISOU  454  CB  ALA A 377     2623   2340   2977   1047   -512   -144       C
ATOM    455  C   ALA A 377      44.003  11.728 -22.371  1.00 20.76           C
ANISOU  455  C   ALA A 377     2480   2447   2962    897   -367   -192       C
ATOM    456  O   ALA A 377      43.249  12.533 -22.902  1.00 20.64           O
ANISOU  456  O   ALA A 377     2473   2438   2933    780   -325   -163       O
ATOM    457  N   THR A 378      44.622  10.780 -23.061  1.00 22.11           N
ANISOU  457  N   THR A 378     2642   2627   3133   1005   -342   -253       N
ATOM    458  CA  THR A 378      44.428  10.601 -24.505  1.00 22.78           C
ANISOU  458  CA  THR A 378     2731   2741   3183    981   -260   -299       C
ATOM    459  CB  THR A 378      45.231   9.415 -25.017  1.00 23.45           C
ANISOU  459  CB  THR A 378     2808   2825   3277   1131   -241   -389       C
ATOM    460  OG1 THR A 378      46.575   9.539 -24.551  1.00 23.66           O
ANISOU  460  OG1 THR A 378     2689   2950   3349   1227   -263   -415       O
ATOM    461  CG2 THR A 378      45.203   9.355 -26.561  1.00 23.42           C
ANISOU  461  CG2 THR A 378     2787   2895   3216   1103   -145   -456       C
ATOM    462  C   THR A 378      42.959  10.423 -24.902  1.00 22.92           C
ANISOU  462  C   THR A 378     2886   2662   3160    891   -249   -274       C
ATOM    463  O   THR A 378      42.361   9.373 -24.664  1.00 23.13           O
ANISOU  463  O   THR A 378     3038   2563   3187    929   -277   -288       O
ATOM    464  N   ARG A 379      42.395  11.464 -25.505  1.00 23.07           N
ANISOU  464  N   ARG A 379     2878   2739   3150    770   -213   -235       N
ATOM    465  CA  ARG A 379      41.001  11.461 -25.957  1.00 23.17           C
ANISOU  465  CA  ARG A 379     2988   2693   3123    683   -211   -213       C
ATOM    466  CB  ARG A 379      40.838  10.623 -27.240  1.00 23.76           C
ANISOU  466  CB  ARG A 379     3108   2781   3137    707   -169   -291       C
ATOM    467  CG  ARG A 379      41.771  11.029 -28.390  1.00 23.77           C
ANISOU  467  CG  ARG A 379     3011   2933   3089    720    -95   -325       C
ATOM    468  CD  ARG A 379      41.330  10.371 -29.694  1.00 25.40           C
ANISOU  468  CD  ARG A 379     3277   3169   3207    718    -57   -401       C
ATOM    469  NE  ARG A 379      40.022  10.902 -30.106  1.00 24.50           N
ANISOU  469  NE  ARG A 379     3216   3051   3041    606    -80   -347       N
ATOM    470  CZ  ARG A 379      39.252  10.392 -31.059  1.00 24.10           C
ANISOU  470  CZ  ARG A 379     3232   3014   2911    577    -79   -404       C
ATOM    471  NH1 ARG A 379      39.641   9.323 -31.758  1.00 25.54           N
ANISOU  471  NH1 ARG A 379     3449   3204   3050    644    -47   -530       N
ATOM    472  NH2 ARG A 379      38.099  10.974 -31.317  1.00 22.39           N
ANISOU  472  NH2 ARG A 379     3041   2808   2658    485   -115   -345       N
ATOM    473  C   ARG A 379      40.061  10.981 -24.854  1.00 23.18           C
ANISOU  473  C   ARG A 379     3094   2563   3150    668   -268   -182       C
ATOM    474  O   ARG A 379      39.189  10.137 -25.092  1.00 24.70           O
ANISOU  474  O   ARG A 379     3388   2671   3327    652   -272   -208       O
ATOM    475  N   ARG A 380      40.242  11.534 -23.654  1.00 22.60           N
ANISOU  475  N   ARG A 380     2994   2481   3113    663   -306   -133       N
ATOM    476  CA  ARG A 380      39.482  11.149 -22.465  1.00 22.87           C
ANISOU  476  CA  ARG A 380     3120   2413   3156    648   -350    -96       C
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Figure 18 (continued)

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ATOM    477  CB  ARG A 380      40.063   9.888 -21.829  1.00 23.67           C
ANISOU  477  CB  ARG A 380    3291   2436   3267    763   -386   -109       C
ATOM    478  CG  ARG A 380      39.313   9.349 -20.612  1.00 25.57           C
ANISOU  478  CG  ARG A 380    3648   2566   3499    747   -421    -54       C
ATOM    479  CD  ARG A 380      40.092   8.171 -20.021  1.00 30.01           C
ANISOU  479  CD  ARG A 380    4280   3051   4071    882   -464    -48       C
ATOM    480  NE  ARG A 380      39.887   8.025 -18.572  1.00 39.22           N
ANISOU  480  NE  ARG A 380    5520   4172   5211    888   -512     30       N
ATOM    481  CZ  ARG A 380      40.796   7.522 -17.733  1.00 40.49           C
ANISOU  481  CZ  ARG A 380    5699   4323   5363   1013   -577     62       C
ATOM    482  NH1 ARG A 380      41.968   7.110 -18.193  1.00 43.42           N
ANISOU  482  NH1 ARG A 380    6006   4723   5768   1149   -600     15       N
ATOM    483  NH2 ARG A 380      40.537   7.434 -16.435  1.00 42.81           N
ANISOU  483  NH2 ARG A 380    6069   4590   5607   1008   -619    141       N
ATOM    484  C   ARG A 380      39.490  12.279 -21.455  1.00 21.00           C
ANISOU  484  C   ARG A 380    2828   2214   2937    601   -375    -50       C
ATOM    485  O   ARG A 380      40.551  12.775 -21.067  1.00 20.79           O
ANISOU  485  O   ARG A 380    2713   2256   2929    638   -393    -57       O
ATOM    486  N   LEU A 381      38.288  12.705 -21.066  1.00 19.70           N
ANISOU  486  N   LEU A 381    2706   2009   2769    514   -373    -18       N
ATOM    487  CA  LEU A 381      38.090  13.567 -19.904  1.00 18.41           C
ANISOU  487  CA  LEU A 381    2522   1857   2616    475   -396      9       C
ATOM    488  CB  LEU A 381      36.745  14.289 -19.985  1.00 16.88           C
ANISOU  488  CB  LEU A 381    2337   1645   2433    380   -372     26       C
ATOM    489  CG  LEU A 381      36.469  15.343 -18.928  1.00 17.01           C
ANISOU  489  CG  LEU A 381    2323   1675   2467    338   -382     32       C
ATOM    490  CD1 LEU A 381      35.655  16.492 -19.499  1.00 12.78           C
ANISOU  490  CD1 LEU A 381    1738   1145   1973    273   -356     41       C
ATOM    491  CD2 LEU A 381      35.764  14.667 -17.749  1.00 15.08           C
ANISOU  491  CD2 LEU A 381    2164   1384   2181    330   -388     44       C
ATOM    492  C   LEU A 381      38.123  12.638 -18.694  1.00 18.24           C
ANISOU  492  C   LEU A 381    2589   1780   2564    525   -433     27       C
ATOM    493  O   LEU A 381      37.296  11.748 -18.564  1.00 17.60           O
ANISOU  493  O   LEU A 381    2610   1616   2464    509   -422     44       O
ATOM    494  N   VAL A 382      39.085  12.854 -17.814  1.00 18.87           N
ANISOU  494  N   VAL A 382    2628   1907   2635    580   -480     26       N
ATOM    495  CA  VAL A 382      39.212  12.031 -16.604  1.00 19.46           C
ANISOU  495  CA  VAL A 382    2791   1944   2660    640   -528     61       C
ATOM    496  CB  VAL A 382      40.671  11.956 -16.074  1.00 19.74           C
ANISOU  496  CB  VAL A 382    2760   2052   2688    749   -598     48       C
ATOM    497  CG1 VAL A 382      40.736  11.203 -14.743  1.00 20.37           C
ANISOU  497  CG1 VAL A 382    2942   2102   2697    814   -661    104       C
ATOM    498  CG2 VAL A 382      41.561  11.303 -17.093  1.00 19.70           C
ANISOU  498  CG2 VAL A 382    2711   2051   2723    843   -593     16       C
ATOM    499  C   VAL A 382      38.274  12.584 -15.548  1.00 19.47           C
ANISOU  499  C   VAL A 382    2832   1944   2622    558   -521     84       C
ATOM    500  O   VAL A 382      37.472  11.840 -14.971  1.00 19.89           O
ANISOU  500  O   VAL A 382    2999   1928   2631    538   -507    128       O
ATOM    501  N   GLN A 383      38.362  13.885 -15.307  1.00 18.92           N
ANISOU  501  N   GLN A 383    2671   1946   2571    507   -521     49       N
ATOM    502  CA  GLN A 383      37.483  14.517 -14.335  1.00 20.00           C
ANISOU  502  CA  GLN A 383    2833   2091   2675    436   -506     46       C
ATOM    503  CB  GLN A 383      37.874  14.122 -12.908  1.00 21.18           C
ANISOU  503  CB  GLN A 383    3042   2275   2732    481   -560     66       C
ATOM    504  CG  GLN A 383      36.899  14.605 -11.894  1.00 28.38           C
ANISOU  504  CG  GLN A 383    3993   3203   3587    409   -528     59       C
ATOM    505  CD  GLN A 383      36.981  13.887 -10.544  1.00 37.43           C
ANISOU  505  CD  GLN A 383    5244   4372   4605    445   -564    109       C
ATOM    506  OE1 GLN A 383      38.033  13.320 -10.146  1.00 36.64           O
ANISOU  506  OE1 GLN A 383    5163   4301   4457    540   -643    139       O
ATOM    507  NE2 GLN A 383      35.848  13.911  -9.823  1.00 39.52           N
ANISOU  507  NE2 GLN A 383    5575   4633   4808    372   -503    122       N
ATOM    508  C   GLN A 383      37.476  16.041 -14.523  1.00 18.54           C
ANISOU  508  C   GLN A 383    2542   1952   2551    374   -491     -8       C
ATOM    509  O   GLN A 383      38.482  16.611 -14.934  1.00 18.67           O
ANISOU  509  O   GLN A 383    2468   2013   2613    390   -513    -37       O
ATOM    510  N   LEU A 384      36.330  16.663 -14.252  1.00 16.78           N
ANISOU  510  N   LEU A 384    2330   1708   2337    305   -448    -21       N
ATOM    511  CA  LEU A 384      36.156  18.111 -14.349  1.00 16.11           C
ANISOU  511  CA  LEU A 384    2165   1634   2321    254   -431    -70       C
ATOM    512  CB  LEU A 384      35.379  18.478 -15.633  1.00 14.20           C
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Figure 18 (continued)

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ANISOU  512  CB  LEU A 384     1897   1346   2153    221   -387    -47  C
ATOM    513  CG  LEU A 384      35.100  19.947 -15.893  1.00 15.78      C
ANISOU  513  CG  LEU A 384     2031   1526   2439    180   -369    -75  C
ATOM    514  CD1 LEU A 384      36.401  20.725 -16.207  1.00 10.81      C
ANISOU  514  CD1 LEU A 384     1330    915   1863    174   -391    -92  C
ATOM    515  CD2 LEU A 384      34.054  20.107 -16.999  1.00 14.91      C
ANISOU  515  CD2 LEU A 384     1914   1378   2373    164   -338    -36  C
ATOM    516  C   LEU A 384      35.367  18.584 -13.150  1.00 16.11      C
ANISOU  516  C   LEU A 384     2191   1646   2283    219   -413   -111  C
ATOM    517  O   LEU A 384      34.264  18.059 -12.911  1.00 16.54      O
ANISOU  517  O   LEU A 384     2303   1680   2301    197   -371    -89  O
ATOM    518  N   ILE A 385      35.903  19.575 -12.422  1.00 16.23      N
ANISOU  518  N   ILE A 385     2159   1700   2309    206   -439   -182  N
ATOM    519  CA  ILE A 385      35.136  20.337 -11.409  1.00 17.22      C
ANISOU  519  CA  ILE A 385     2291   1838   2415    170   -411   -252  C
ATOM    520  CB  ILE A 385      35.776  20.285  -9.974  1.00 19.18      C
ANISOU  520  CB  ILE A 385     2565   2173   2549    183   -460   -306  C
ATOM    521  CG1 ILE A 385      36.149  18.859  -9.636  1.00 21.06      C
ANISOU  521  CG1 ILE A 385     2884   2446   2673    236   -496   -222  C
ATOM    522  CD1 ILE A 385      37.060  18.725  -8.443  1.00 25.03      C
ANISOU  522  CD1 ILE A 385     3405   3048   3060    273   -575   -251  C
ATOM    523  CG2 ILE A 385      34.780  20.792  -8.871  1.00 18.63      C
ANISOU  523  CG2 ILE A 385     2525   2131   2421    148   -410   -379  C
ATOM    524  C   ILE A 385      35.022  21.812 -11.817  1.00 17.38      C
ANISOU  524  C   ILE A 385     2235   1809   2560    134   -392   -315  C
ATOM    525  O   ILE A 385      36.038  22.477 -12.052  1.00 16.35      O
ANISOU  525  O   ILE A 385     2047   1678   2489    122   -428   -346  O
ATOM    526  N   VAL A 386      33.788  22.308 -11.888  1.00 17.59      N
ANISOU  526  N   VAL A 386     2260   1791   2632    116   -336   -334  N
ATOM    527  CA  VAL A 386      33.497  23.673 -12.328  1.00 17.46      C
ANISOU  527  CA  VAL A 386     2187   1700   2747     99   -317   -379  C
ATOM    528  CB  VAL A 386      32.501  23.721 -13.521  1.00 17.32      C
ANISOU  528  CB  VAL A 386     2153   1623   2805    111   -285   -308  C
ATOM    529  CG1 VAL A 386      32.435  25.126 -14.121  1.00 14.48      C
ANISOU  529  CG1 VAL A 386     1746   1168   2586    108   -281   -322  C
ATOM    530  CG2 VAL A 386      32.875  22.722 -14.622  1.00 14.00      C
ANISOU  530  CG2 VAL A 386     1747   1216   2356    121   -303   -206  C
ATOM    531  C   VAL A 386      32.924  24.512 -11.181  1.00 19.48      C
ANISOU  531  C   VAL A 386     2439   1958   3003     89   -289   -498  C
ATOM    532  O   VAL A 386      32.052  24.065 -10.400  1.00 19.17      O
ANISOU  532  O   VAL A 386     2432   1971   2882     93   -248   -524  O
ATOM    533  N   SER A 387      33.434  25.741 -11.087  1.00 20.06      N
ANISOU  533  N   SER A 387     2475   1975   3174     69   -304   -576  N
ATOM    534  CA  SER A 387      32.894  26.762 -10.198  1.00 20.65      C
ANISOU  534  CA  SER A 387     2541   2021   3286     64   -273   -709  C
ATOM    535  CB  SER A 387      34.004  27.197  -9.236  1.00 21.25      C
ANISOU  535  CB  SER A 387     2612   2141   3321     26   -322   -822  C
ATOM    536  OG  SER A 387      33.536  28.081  -8.225  1.00 25.92      O
ANISOU  536  OG  SER A 387     3205   2723   3922     20   -293   -979  O
ATOM    537  C   SER A 387      32.403  27.938 -11.076  1.00 20.74      C
ANISOU  537  C   SER A 387     2515   1887   3478     75   -250   -705  C
ATOM    538  O   SER A 387      33.153  28.448 -11.920  1.00 20.93      O
ANISOU  538  O   SER A 387     2521   1834   3597     50   -277   -654  O
ATOM    539  N   GLY A 388      31.171  28.394 -10.876  1.00 20.37      N
ANISOU  539  N   GLY A 388     2457   1802   3480    115   -199   -755  N
ATOM    540  CA  GLY A 388      30.607  29.375 -11.771  1.00 20.03      C
ANISOU  540  CA  GLY A 388     2385   1621   3603    151   -188   -725  C
ATOM    541  C   GLY A 388      29.641  30.315 -11.094  1.00 21.29      C
ANISOU  541  C   GLY A 388     2524   1722   3843    198   -142   -856  C
ATOM    542  O   GLY A 388      29.139  30.030 -10.008  1.00 20.82      O
ANISOU  542  O   GLY A 388     2464   1757   3689    204   -100   -961  O
ATOM    543  N   LYS A 389      29.391  31.447 -11.743  1.00 22.34      N
ANISOU  543  N   LYS A 389     2643   1697   4149    235   -144   -847  N
ATOM    544  CA  LYS A 389      28.404  32.440 -11.252  1.00 23.74      C
ANISOU  544  CA  LYS A 389     2793   1788   4438    308   -101   -972  C
ATOM    545  CB  LYS A 389      28.635  33.761 -11.940  1.00 24.80      C
ANISOU  545  CB  LYS A 389     2942   1708   4771    330   -123   -951  C
ATOM    546  CG  LYS A 389      29.884  34.437 -11.447  1.00 28.40      C
ANISOU  546  CG  LYS A 389     3437   2087   5267    239   -141  -1042  C
ATOM    547  CD  LYS A 389      30.035  35.791 -12.096  1.00 35.05      C
ANISOU  547  CD  LYS A 389     4306   2688   6324    250   -150  -1019  C
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Figure 18 (continued)

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ATOM    548  CE  LYS A 389      31.177  36.562 -11.441  1.00 41.60           C
ANISOU  548  CE  LYS A 389    5164   3432   7212    145   -160  -1153        C
ATOM    549  NZ  LYS A 389      31.822  37.562 -12.391  1.00 47.46           N
ANISOU  549  NZ  LYS A 389    5944   3955   8136     93   -174  -1054        N
ATOM    550  C   LYS A 389      26.964  32.018 -11.437  1.00 23.29           C
ANISOU  550  C   LYS A 389    2680   1796   4372    389    -64   -947        C
ATOM    551  O   LYS A 389      26.103  32.459 -10.703  1.00 24.56           O
ANISOU  551  O   LYS A 389    2804   1962   4567    446    -11  -1079        O
ATOM    552  N   ASP A 390      26.725  31.102 -12.371  1.00 22.47           N
ANISOU  552  N   ASP A 390    2563   1759   4214    388    -89   -794        N
ATOM    553  CA  ASP A 390      25.370  30.703 -12.704  1.00 23.07           C
ANISOU  553  CA  ASP A 390    2569   1900   4296    454    -66   -765        C
ATOM    554  CB  ASP A 390      24.663  31.853 -13.445  1.00 24.00           C
ANISOU  554  CB  ASP A 390    2644   1876   4601    562    -88   -743        C
ATOM    555  CG  ASP A 390      25.432  32.299 -14.704  1.00 24.13           C
ANISOU  555  CG  ASP A 390    2712   1766   4691    555   -157   -587        C
ATOM    556  OD1 ASP A 390      25.404  31.534 -15.677  1.00 25.37           O
ANISOU  556  OD1 ASP A 390    2865   1991   4783    541   -195   -449        O
ATOM    557  OD2 ASP A 390      26.078  33.378 -14.716  1.00 18.12           O
ANISOU  557  OD2 ASP A 390    1997    842   4045    553   -168   -605        O
ATOM    558  C   ASP A 390      25.431  29.453 -13.563  1.00 21.82           C
ANISOU  558  C   ASP A 390    2416   1838   4036    412    -98   -618        C
ATOM    559  O   ASP A 390      26.473  29.107 -14.095  1.00 21.61           O
ANISOU  559  O   ASP A 390    2445   1800   3967    359   -140   -529        O
ATOM    560  N   GLU A 391      24.289  28.816 -13.752  1.00 22.29           N
ANISOU  560  N   GLU A 391    2410   1991   4069    437    -77   -602        N
ATOM    561  CA  GLU A 391      24.220  27.543 -14.442  1.00 21.52           C
ANISOU  561  CA  GLU A 391    2317   1987   3871    387    -99   -494        C
ATOM    562  CB  GLU A 391      22.839  26.928 -14.190  1.00 22.15           C
ANISOU  562  CB  GLU A 391    2309   2181   3927    393    -50   -536        C
ATOM    563  CG  GLU A 391      22.286  26.000 -15.243  1.00 24.99           C
ANISOU  563  CG  GLU A 391    2632   2607   4255    372    -88   -439        C
ATOM    564  CD  GLU A 391      20.751  25.986 -15.206  1.00 33.67           C
ANISOU  564  CD  GLU A 391    3596   3789   5407    410    -56   -495        C
ATOM    565  OE1 GLU A 391      20.154  25.746 -14.111  1.00 34.20           O
ANISOU  565  OE1 GLU A 391    3622   3935   5438    379     35   -596        O
ATOM    566  OE2 GLU A 391      20.138  26.247 -16.270  1.00 38.52           O
ANISOU  566  OE2 GLU A 391    4139   4401   6095    472   -121   -439        O
ATOM    567  C   GLU A 391      24.611  27.602 -15.922  1.00 20.48           C
ANISOU  567  C   GLU A 391    2204   1800   3778    403   -176   -352        C
ATOM    568  O   GLU A 391      25.229  26.686 -16.401  1.00 19.95           O
ANISOU  568  O   GLU A 391    2183   1778   3619    346   -199   -277        O
ATOM    569  N   GLN A 392      24.288  28.689 -16.609  1.00 21.46           N
ANISOU  569  N   GLN A 392    2299   1824   4031    484   -212   -317        N
ATOM    570  CA  GLN A 392      24.666  28.910 -18.002  1.00 23.52           C
ANISOU  570  CA  GLN A 392    2587   2032   4318    502   -281   -172        C
ATOM    571  CB  GLN A 392      23.926  30.147 -18.557  1.00 24.65           C
ANISOU  571  CB  GLN A 392    2688   2067   4610    617   -317   -138        C
ATOM    572  CG  GLN A 392      24.537  30.860 -19.769  1.00 28.63           C
ANISOU  572  CG  GLN A 392    3252   2461   5164    639   -376     13        C
ATOM    573  CD  GLN A 392      24.305  32.416 -19.753  1.00 30.83           C
ANISOU  573  CD  GLN A 392    3540   2551   5624    735   -387     15        C
ATOM    574  OE1 GLN A 392      25.010  33.190 -19.035  1.00 34.80           O
ANISOU  574  OE1 GLN A 392    4092   2924   6205    705   -349    -58        O
ATOM    575  NE2 GLN A 392      23.321  32.867 -20.548  1.00 33.14           N
ANISOU  575  NE2 GLN A 392    3784   2821   5985    853   -447     94        N
ATOM    576  C   GLN A 392      26.188  29.017 -18.189  1.00 22.62           C
ANISOU  576  C   GLN A 392    2561   1858   4175    433   -289   -120        C
ATOM    577  O   GLN A 392      26.726  28.443 -19.125  1.00 21.91           O
ANISOU  577  O   GLN A 392    2503   1807   4016    398   -319    -17        O
ATOM    578  N   SER A 393      26.877  29.730 -17.295  1.00 22.81           N
ANISOU  578  N   SER A 393    2615   1801   4249    409   -260   -206        N
ATOM    579  CA  SER A 393      28.347  29.794 -17.315  1.00 21.99           C
ANISOU  579  CA  SER A 393    2570   1664   4121    331   -264   -183        C
ATOM    580  CB  SER A 393      28.857  30.874 -16.346  1.00 23.44           C
ANISOU  580  CB  SER A 393    2770   1738   4397    313   -242   -300        C
ATOM    581  OG  SER A 393      28.140  32.078 -16.569  1.00 25.29           O
ANISOU  581  OG  SER A 393    2992   1830   4786    390   -243   -305        O
ATOM    582  C   SER A 393      29.011  28.464 -16.993  1.00 20.66           C
ANISOU  582  C   SER A 393    2422   1626   3801    265   -259   -189        C
ATOM    583  O   SER A 393      30.049  28.132 -17.552  1.00 19.87           O
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Figure 18 (continued)

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ANISOU  583  O   SER A 393     2350   1542   3659    219   -276   -122      O
ATOM    584  N   ILE A 394      28.422  27.713 -16.073  1.00 20.77           N
ANISOU  584  N   ILE A 394     2422   1732   3737    263   -230   -268      N
ATOM    585  CA  ILE A 394      28.889  26.369 -15.747  1.00 19.11           C
ANISOU  585  CA  ILE A 394     2244   1630   3386    214   -227   -260      C
ATOM    586  CB  ILE A 394      28.139  25.782 -14.497  1.00 19.85           C
ANISOU  586  CB  ILE A 394     2333   1806   3402    206   -179   -352      C
ATOM    587  CG1 ILE A 394      28.509  26.606 -13.259  1.00 20.43           C
ANISOU  587  CG1 ILE A 394     2415   1856   3490    201   -158   -477      C
ATOM    588  CD1 ILE A 394      27.499  26.518 -12.109  1.00 22.75           C
ANISOU  588  CD1 ILE A 394     2688   2218   3738    210    -93   -583      C
ATOM    589  CG2 ILE A 394      28.435  24.278 -14.274  1.00 15.59           C
ANISOU  589  CG2 ILE A 394     1843   1358   2723    163   -177   -313      C
ATOM    590  C   ILE A 394      28.784  25.474 -16.977  1.00 18.68           C
ANISOU  590  C   ILE A 394     2195   1619   3284    212   -254   -148      C
ATOM    591  O   ILE A 394      29.760  24.825 -17.311  1.00 17.57           O
ANISOU  591  O   ILE A 394     2090   1507   3080    182   -270   -104      O
ATOM    592  N   ALA A 395      27.630  25.500 -17.663  1.00 19.22           N
ANISOU  592  N   ALA A 395     2220   1695   3386    250   -262   -113      N
ATOM    593  CA  ALA A 395      27.401  24.738 -18.901  1.00 19.01           C
ANISOU  593  CA  ALA A 395     2194   1718   3313    248   -295    -23      C
ATOM    594  CB  ALA A 395      25.980  24.956 -19.419  1.00 18.56           C
ANISOU  594  CB  ALA A 395     2065   1683   3305    297   -314    -13      C
ATOM    595  C   ALA A 395      28.416  25.074 -19.990  1.00 19.20           C
ANISOU  595  C   ALA A 395     2250   1706   3340    245   -327     70      C
ATOM    596  O   ALA A 395      28.898  24.171 -20.671  1.00 18.93           O
ANISOU  596  O   ALA A 395     2244   1727   3223    220   -339    115      O
ATOM    597  N   GLU A 396      28.719  26.364 -20.157  1.00 20.22           N
ANISOU  597  N   GLU A 396     2377   1739   3567    267   -332     96      N
ATOM    598  CA  GLU A 396      29.710  26.818 -21.142  1.00 21.09           C
ANISOU  598  CA  GLU A 396     2517   1810   3684    247   -345    193      C
ATOM    599  CB  GLU A 396      29.807  28.341 -21.147  1.00 22.89           C
ANISOU  599  CB  GLU A 396     2749   1899   4047    266   -343    216      C
ATOM    600  CG  GLU A 396      28.607  29.009 -21.787  1.00 27.44           C
ANISOU  600  CG  GLU A 396     3306   2429   4693    349   -378    278      C
ATOM    601  CD  GLU A 396      28.571  30.513 -21.606  1.00 31.59           C
ANISOU  601  CD  GLU A 396     3844   2785   5373    385   -375    287      C
ATOM    602  OE1 GLU A 396      29.466  31.075 -20.945  1.00 37.15           O
ANISOU  602  OE1 GLU A 396     4573   3406   6136    328   -342    230      O
ATOM    603  OE2 GLU A 396      27.632  31.141 -22.145  1.00 34.90           O
ANISOU  603  OE2 GLU A 396     4250   3151   5862    473   -412    349      O
ATOM    604  C   GLU A 396      31.090  26.181 -20.894  1.00 19.62           C
ANISOU  604  C   GLU A 396     2357   1667   3430    186   -325    174      C
ATOM    605  O   GLU A 396      31.755  25.774 -21.820  1.00 19.19           O
ANISOU  605  O   GLU A 396     2317   1657   3319    166   -327    242      O
ATOM    606  N   ALA A 397      31.480  26.093 -19.631  1.00 18.63           N
ANISOU  606  N   ALA A 397     2231   1543   3306    164   -309     75      N
ATOM    607  CA  ALA A 397      32.722  25.456 -19.210  1.00 18.01           C
ANISOU  607  CA  ALA A 397     2163   1517   3164    125   -305     44      C
ATOM    608  CB  ALA A 397      32.994  25.795 -17.741  1.00 17.36           C
ANISOU  608  CB  ALA A 397     2076   1422   3099    108   -300    -69      C
ATOM    609  C   ALA A 397      32.768  23.936 -19.457  1.00 16.96           C
ANISOU  609  C   ALA A 397     2052   1477   2914    133   -311     60      C
ATOM    610  O   ALA A 397      33.775  23.398 -19.924  1.00 17.05           O
ANISOU  610  O   ALA A 397     2067   1532   2880    123   -313     85      O
ATOM    611  N   ILE A 398      31.668  23.250 -19.152  1.00 17.13           N
ANISOU  611  N   ILE A 398     2086   1526   2898    151   -309     38      N
ATOM    612  CA  ILE A 398      31.536  21.827 -19.422  1.00 15.91           C
ANISOU  612  CA  ILE A 398     1963   1430   2651    150   -312     51      C
ATOM    613  CB  ILE A 398      30.199  21.264 -18.834  1.00 17.18           C
ANISOU  613  CB  ILE A 398     2128   1608   2792    144   -297     15      C
ATOM    614  CG1 ILE A 398      30.119  21.527 -17.326  1.00 16.13           C
ANISOU  614  CG1 ILE A 398     2000   1471   2657    136   -271    -57      C
ATOM    615  CD1 ILE A 398      28.779  21.236 -16.716  1.00 16.58           C
ANISOU  615  CD1 ILE A 398     2043   1553   2705    121   -235    -95      C
ATOM    616  CG2 ILE A 398      30.022  19.747 -19.155  1.00 13.67           C
ANISOU  616  CG2 ILE A 398     1729   1199   2267    127   -297     27      C
ATOM    617  C   ILE A 398      31.671  21.562 -20.922  1.00 16.07           C
ANISOU  617  C   ILE A 398     1985   1475   2647    156   -326    121      C
ATOM    618  O   ILE A 398      32.434  20.686 -21.326  1.00 16.26           O
ANISOU  618  O   ILE A 398     2034   1535   2609    157   -326    128      O
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Figure 18 (continued)

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ATOM    619  N   ILE A 399      30.963  22.335 -21.741  1.00 16.42           N
ANISOU  619  N   ILE A 399    2003   1502   2734    169   -339    169       N
ATOM    620  CA  ILE A 399      31.042  22.212 -23.210  1.00 16.68           C
ANISOU  620  CA  ILE A 399    2040   1574   2722    175   -356    243       C
ATOM    621  CB  ILE A 399      30.128  23.237 -23.951  1.00 17.23           C
ANISOU  621  CB  ILE A 399    2083   1621   2843    205   -385    310       C
ATOM    622  CG1 ILE A 399      28.652  22.926 -23.683  1.00 16.60           C
ANISOU  622  CG1 ILE A 399    1968   1565   2776    225   -410    268       C
ATOM    623  CD1 ILE A 399      27.669  24.079 -24.032  1.00 17.54           C
ANISOU  623  CD1 ILE A 399    2040   1648   2976    281   -446    315       C
ATOM    624  CG2 ILE A 399      30.379  23.228 -25.492  1.00 18.27           C
ANISOU  624  CG2 ILE A 399    2231   1807   2903    209   -404    401       C
ATOM    625  C   ILE A 399      32.467  22.321 -23.722  1.00 17.17           C
ANISOU  625  C   ILE A 399    2111   1650   2761    159   -335    277       C
ATOM    626  O   ILE A 399      32.926  21.437 -24.454  1.00 17.83           O
ANISOU  626  O   ILE A 399    2214   1798   2764    160   -329    282       O
ATOM    627  N   VAL A 400      33.152  23.398 -23.336  1.00 16.69           N
ANISOU  627  N   VAL A 400    2033   1534   2776    141   -318    289       N
ATOM    628  CA  VAL A 400      34.542  23.641 -23.732  1.00 16.70           C
ANISOU  628  CA  VAL A 400    2020   1553   2773    109   -288    316       C
ATOM    629  CB  VAL A 400      35.026  25.034 -23.221  1.00 16.70           C
ANISOU  629  CB  VAL A 400    1997   1463   2887     69   -273    321       C
ATOM    630  CG1 VAL A 400      36.523  25.234 -23.427  1.00 15.47           C
ANISOU  630  CG1 VAL A 400    1803   1337   2737     16   -236    327       C
ATOM    631  CG2 VAL A 400      34.216  26.116 -23.893  1.00 16.90           C
ANISOU  631  CG2 VAL A 400    2039   1410   2973     79   -281    410       C
ATOM    632  C   VAL A 400      35.510  22.529 -23.314  1.00 15.98           C
ANISOU  632  C   VAL A 400    1922   1527   2623    114   -279    252       C
ATOM    633  O   VAL A 400      36.327  22.104 -24.112  1.00 17.42           O
ANISOU  633  O   VAL A 400    2094   1773   2753    112   -256    272       O
ATOM    634  N   ALA A 401      35.406  22.061 -22.079  1.00 16.30           N
ANISOU  634  N   ALA A 401    1971   1556   2666    128   -297    178       N
ATOM    635  CA  ALA A 401      36.199  20.909 -21.593  1.00 16.28           C
ANISOU  635  CA  ALA A 401    1976   1604   2606    155   -305    128       C
ATOM    636  CB  ALA A 401      35.953  20.689 -20.091  1.00 14.87           C
ANISOU  636  CB  ALA A 401    1817   1404   2428    165   -328     68       C
ATOM    637  C   ALA A 401      35.896  19.628 -22.378  1.00 16.82           C
ANISOU  637  C   ALA A 401    2088   1709   2596    188   -304    136       C
ATOM    638  O   ALA A 401      36.802  18.869 -22.684  1.00 18.03           O
ANISOU  638  O   ALA A 401    2236   1907   2709    218   -296    118       O
ATOM    639  N   MSE A 402      34.624  19.373 -22.681  1.00 17.03           N
ANISOU  639  N   MSE A 402    2147   1717   2604    183   -313    147       N
ATOM    640  CA  MSE A 402      34.253  18.142 -23.412  1.00 17.44           C
ANISOU  640  CA  MSE A 402    2244   1796   2588    199   -316    135       C
ATOM    641  CB  MSE A 402      32.737  17.935 -23.431  1.00 16.42           C
ANISOU  641  CB  MSE A 402    2133   1649   2458    176   -333    130       C
ATOM    642  CG  MSE A 402      32.140  17.462 -22.125  1.00 16.29           C
ANISOU  642  CG  MSE A 402    2144   1590   2456    163   -332     92       C
ATOM    643  SE  MSE A 402      30.183  17.395 -22.251  0.90 20.12          SE
ANISOU  643  SE  MSE A 402    2609   2079   2958    119   -340     80       SE
ATOM    644  CE  MSE A 402      29.774  16.578 -20.532  1.00 14.21           C
ANISOU  644  CE  MSE A 402    1909   1287   2202     87   -307     39       C
ATOM    645  C   MSE A 402      34.797  18.137 -24.843  1.00 17.04           C
ANISOU  645  C   MSE A 402    2179   1807   2487    205   -298    163       C
ATOM    646  O   MSE A 402      35.297  17.114 -25.295  1.00 17.79           O
ANISOU  646  O   MSE A 402    2299   1933   2528    233   -288    126       O
ATOM    647  N   VAL A 403      34.697  19.277 -25.541  1.00 17.61           N
ANISOU  647  N   VAL A 403    2220   1894   2576    182   -292    230       N
ATOM    648  CA  VAL A 403      35.335  19.465 -26.866  1.00 17.49           C
ANISOU  648  CA  VAL A 403    2194   1951   2500    177   -261    275       C
ATOM    649  CB  VAL A 403      34.977  20.843 -27.538  1.00 18.05           C
ANISOU  649  CB  VAL A 403    2252   2014   2593    149   -261    380       C
ATOM    650  CG1 VAL A 403      35.759  21.042 -28.835  1.00 15.38           C
ANISOU  650  CG1 VAL A 403    1909   1761   2174    132   -215    441       C
ATOM    651  CG2 VAL A 403      33.475  20.963 -27.819  1.00 18.29           C
ANISOU  651  CG2 VAL A 403    2302   2033   2616    162   -316    405       C
ATOM    652  C   VAL A 403      36.880  19.322 -26.774  1.00 18.33           C
ANISOU  652  C   VAL A 403    2259   2096   2607    184   -216    250       C
ATOM    653  O   VAL A 403      37.496  18.607 -27.563  1.00 18.16           O
ANISOU  653  O   VAL A 403    2238   2149   2515    185   -207    224       O
ATOM    654  N   PHE A 404      37.482  20.014 -25.804  1.00 18.22           N
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Figure 18 (continued)

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ANISOU  654  N   PHE A 404     2203   2042   2676    166   -213    246       N
ATOM    655  CA  PHE A 404      38.935  20.002 -25.606  1.00 18.45           C
ANISOU  655  CA  PHE A 404     2167   2120   2724    167   -180    215       C
ATOM    656  CB  PHE A 404      39.279  20.946 -24.451  1.00 18.40           C
ANISOU  656  CB  PHE A 404     2118   2060   2815    130   -197    203       C
ATOM    657  CG  PHE A 404      40.743  21.047 -24.167  1.00 16.27           C
ANISOU  657  CG  PHE A 404     1758   1850   2576    119   -176    163       C
ATOM    658  CD1 PHE A 404      41.538  21.926 -24.884  1.00 17.08           C
ANISOU  658  CD1 PHE A 404     1794   1990   2708     49   -116    207       C
ATOM    659  CE1 PHE A 404      42.921  22.016 -24.616  1.00 21.24           C
ANISOU  659  CE1 PHE A 404     2210   2589   3271     29    -94    157       C
ATOM    660  CZ  PHE A 404      43.501  21.222 -23.619  1.00 19.15           C
ANISOU  660  CZ  PHE A 404     1905   2364   3009     98   -148     68       C
ATOM    661  CE2 PHE A 404      42.718  20.351 -22.893  1.00 18.17           C
ANISOU  661  CE2 PHE A 404     1866   2192   2846    176   -211     40       C
ATOM    662  CD2 PHE A 404      41.325  20.260 -23.180  1.00 17.63           C
ANISOU  662  CD2 PHE A 404     1906   2047   2745    177   -217     86       C
ATOM    663  C   PHE A 404      39.518  18.593 -25.332  1.00 18.68           C
ANISOU  663  C   PHE A 404     2200   2187   2710    241   -190    135       C
ATOM    664  O   PHE A 404      40.673  18.296 -25.683  1.00 18.92           O
ANISOU  664  O   PHE A 404     2170   2292   2727    266   -154    105       O
ATOM    665  N   SER A 405      38.712  17.745 -24.692  1.00 18.21           N
ANISOU  665  N   SER A 405     2210   2070   2638    277   -233    102       N
ATOM    666  CA  SER A 405      39.091  16.363 -24.380  1.00 18.68           C
ANISOU  666  CA  SER A 405     2304   2127   2668    352   -249     41       C
ATOM    667  CB  SER A 405      38.012  15.723 -23.496  1.00 18.57           C
ANISOU  667  CB  SER A 405     2375   2027   2653    356   -290     32       C
ATOM    668  OG  SER A 405      36.849  15.381 -24.246  1.00 16.66           O
ANISOU  668  OG  SER A 405     2188   1765   2376    326   -287     37       O
ATOM    669  C   SER A 405      39.340  15.491 -25.619  1.00 20.09           C
ANISOU  669  C   SER A 405     2498   2356   2779    391   -214      8       C
ATOM    670  O   SER A 405      40.066  14.496 -25.533  1.00 21.25           O
ANISOU  670  O   SER A 405     2648   2509   2916    468   -213    -50       O
ATOM    671  N   GLN A 406      38.723  15.866 -26.758  1.00 20.26           N
ANISOU  671  N   GLN A 406     2533   2414   2751    345   -190     41       N
ATOM    672  CA  GLN A 406      38.832  15.162 -28.048  1.00 20.05           C
ANISOU  672  CA  GLN A 406     2527   2454   2636    368   -155      2       C
ATOM    673  CB  GLN A 406      40.290  15.095 -28.531  1.00 19.99           C
ANISOU  673  CB  GLN A 406     2441   2542   2612    409    -93    -31       C
ATOM    674  CG  GLN A 406      40.906  16.472 -28.726  1.00 20.76           C
ANISOU  674  CG  GLN A 406     2452   2702   2734    342    -49     46       C
ATOM    675  CD  GLN A 406      42.332  16.414 -29.196  1.00 20.39           C
ANISOU  675  CD  GLN A 406     2306   2766   2674    366     24      9       C
ATOM    676  OE1 GLN A 406      43.147  15.693 -28.645  1.00 19.25           O
ANISOU  676  OE1 GLN A 406     2117   2630   2566    444     17    -66       O
ATOM    677  NE2 GLN A 406      42.640  17.179 -30.233  1.00 22.01           N
ANISOU  677  NE2 GLN A 406     2474   3065   2824    301     97     68       N
ATOM    678  C   GLN A 406      38.164  13.777 -28.045  1.00 20.64           C
ANISOU  678  C   GLN A 406     2691   2466   2684    406   -184    -74       C
ATOM    679  O   GLN A 406      38.465  12.937 -28.887  1.00 22.16           O
ANISOU  679  O   GLN A 406     2906   2696   2817    445   -157   -144       O
ATOM    680  N   GLU A 407      37.248  13.554 -27.111  1.00 20.37           N
ANISOU  680  N   GLU A 407     2710   2337   2695    385   -231    -65       N
ATOM    681  CA  GLU A 407      36.556  12.268 -26.951  1.00 21.29           C
ANISOU  681  CA  GLU A 407     2916   2369   2805    396   -254   -125       C
ATOM    682  CB  GLU A 407      35.638  12.293 -25.718  1.00 19.97           C
ANISOU  682  CB  GLU A 407     2786   2110   2691    355   -289    -92       C
ATOM    683  CG  GLU A 407      36.371  12.188 -24.373  1.00 21.49           C
ANISOU  683  CG  GLU A 407     2982   2253   2931    404   -301    -73       C
ATOM    684  CD  GLU A 407      35.649  11.292 -23.352  1.00 21.16           C
ANISOU  684  CD  GLU A 407     3033   2101   2906    391   -321    -72       C
ATOM    685  OE1 GLU A 407      34.688  10.585 -23.711  1.00 21.26           O
ANISOU  685  OE1 GLU A 407     3107   2062   2909    342   -319   -101       O
ATOM    686  OE2 GLU A 407      36.071  11.267 -22.189  1.00 20.34           O
ANISOU  686  OE2 GLU A 407     2943   1965   2820    424   -339    -43       O
ATOM    687  C   GLU A 407      35.725  11.866 -28.158  1.00 22.08           C
ANISOU  687  C   GLU A 407     3052   2504   2835    357   -256   -169       C
ATOM    688  O   GLU A 407      35.066  12.694 -28.765  1.00 20.70           O
ANISOU  688  O   GLU A 407     2846   2394   2624    267   -267   -123       O
ATOM    689  N   ASP A 408      35.720  10.573 -28.461  1.00 23.34           N
ANISOU  689  N   ASP A 408     3280   2611   2976    386   -253   -261       N
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Figure 18 (continued)

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ATOM    690  CA  ASP A 408      34.928  10.035 -29.544  1.00 24.61           C
ANISOU  690  CA  ASP A 408    3481   2801   3068    344   -263   -332       C
ATOM    691  CB  ASP A 408      35.160   8.530 -29.658  1.00 25.59           C
ANISOU  691  CB  ASP A 408    3692   2830   3202    388   -253   -449       C
ATOM    692  CG  ASP A 408      34.396   7.913 -30.801  1.00 27.72           C
ANISOU  692  CG  ASP A 408    4003   3131   3397    336   -265   -551       C
ATOM    693  OD1 ASP A 408      34.710   8.279 -31.958  1.00 31.59           O
ANISOU  693  OD1 ASP A 408    4457   3762   3786    347   -246   -579       O
ATOM    694  OD2 ASP A 408      33.492   7.066 -30.549  1.00 28.73           O
ANISOU  694  OD2 ASP A 408    4201   3151   3564    276   -293   -607       O
ATOM    695  C   ASP A 408      33.427  10.347 -29.389  1.00 24.65           C
ANISOU  695  C   ASP A 408    3488   2793   3084    249   -310   -301       C
ATOM    696  O   ASP A 408      32.784  10.796 -30.342  1.00 24.93           O
ANISOU  696  O   ASP A 408    3495   2927   3051    207   -333   -299       O
ATOM    697  N  ACYS A 409      32.869  10.126 -28.205  0.70 24.72           N
ANISOU  697  N  ACYS A 409    3524   2697   3172    218   -325   -276       N
ATOM    698  N  BCYS A 409      32.906  10.105 -28.182  0.30 24.11           N
ANISOU  698  N  BCYS A 409    3448   2617   3096    220   -324   -276       N
ATOM    699  CA ACYS A 409      31.430  10.317 -28.021  0.70 25.22           C
ANISOU  699  CA ACYS A 409    3572   2756   3254    128   -359   -264       C
ATOM    700  CA BCYS A 409      31.506  10.359 -27.816  0.30 23.92           C
ANISOU  700  CA BCYS A 409    3408   2580   3101    132   -355   -254       C
ATOM    701  CB ACYS A 409      30.961   9.730 -26.681  0.70 25.40           C
ANISOU  701  CB ACYS A 409    3644   2652   3353     91   -351   -253       C
ATOM    702  CB BCYS A 409      31.313  10.176 -26.307  0.30 23.45           C
ANISOU  702  CB BCYS A 409    3378   2413   3118    117   -345   -213       C
ATOM    703  SG ACYS A 409      31.124  10.858 -25.325  0.70 28.09           S
ANISOU  703  SG ACYS A 409    3936   2990   3746    108   -341   -150       S
ATOM    704  SG BCYS A 409      31.533   8.502 -25.712  0.30 24.62           S
ANISOU  704  SG BCYS A 409    3655   2400   3300    125   -326   -269       S
ATOM    705  C  ACYS A 409      31.016  11.792 -28.173  0.70 23.86           C
ANISOU  705  C  ACYS A 409    3310   2680   3076    114   -379   -177       C
ATOM    706  C  BCYS A 409      31.060  11.762 -28.191  0.30 23.24           C
ANISOU  706  C  BCYS A 409    3233   2600   2995    116   -378   -179       C
ATOM    707  O  ACYS A 409      29.841  12.089 -28.420  0.70 23.73           O
ANISOU  707  O  ACYS A 409    3255   2703   3058     58   -417   -174       O
ATOM    708  O  BCYS A 409      29.914  11.985 -28.591  0.30 23.42           O
ANISOU  708  O  BCYS A 409    3222   2670   3007     61   -417   -184       O
ATOM    709  N   MSE A 410      31.991  12.696 -28.033  1.00 22.71           N
ANISOU  709  N   MSE A 410    3128   2566   2936    166   -357   -110       N
ATOM    710  CA  MSE A 410      31.811  14.092 -28.382  1.00 21.64           C
ANISOU  710  CA  MSE A 410    2925   2503   2796    162   -370    -25       C
ATOM    711  CB  MSE A 410      32.941  14.929 -27.770  1.00 21.38           C
ANISOU  711  CB  MSE A 410    2860   2456   2807    198   -336     34       C
ATOM    712  CG  MSE A 410      32.895  16.431 -28.071  1.00 19.41           C
ANISOU  712  CG  MSE A 410    2554   2246   2573    190   -339    129       C
ATOM    713  SE  MSE A 410      33.826  17.055 -29.687  0.90 23.28          SE
ANISOU  713  SE  MSE A 410    3027   2856   2961    199   -303    190       SE
ATOM    714  CE  MSE A 410      35.627  16.334 -29.341  1.00 17.42           C
ANISOU  714  CE  MSE A 410    2275   2120   2226    242   -234    125       C
ATOM    715  C   MSE A 410      31.762  14.285 -29.903  1.00 22.99           C
ANISOU  715  C   MSE A 410    3085   2788   2861    162   -383    -21       C
ATOM    716  O   MSE A 410      30.839  14.974 -30.405  1.00 23.49           O
ANISOU  716  O   MSE A 410    3115   2908   2904    140   -429     26       O
ATOM    717  N   ILE A 411      32.750  13.711 -30.616  1.00 22.18           N
ANISOU  717  N   ILE A 411    3009   2728   2689    195   -345    -69       N
ATOM    718  CA  ILE A 411      32.822  13.744 -32.071  1.00 23.23           C
ANISOU  718  CA  ILE A 411    3145   2987   2693    196   -344    -80       C
ATOM    719  CB  ILE A 411      34.201  13.201 -32.577  1.00 24.59           C
ANISOU  719  CB  ILE A 411    3332   3203   2809    246   -273   -138       C
ATOM    720  CG1 ILE A 411      35.271  14.295 -32.388  1.00 26.32           C
ANISOU  720  CG1 ILE A 411    3493   3453   3056    263   -219    -38       C
ATOM    721  CD1 ILE A 411      36.666  13.790 -32.234  1.00 28.71           C
ANISOU  721  CD1 ILE A 411    3775   3761   3371    318   -151    -95       C
ATOM    722  CG2 ILE A 411      34.171  12.852 -34.050  1.00 25.93           C
ANISOU  722  CG2 ILE A 411    3524   3504   2824    243   -266   -195       C
ATOM    723  C   ILE A 411      31.610  13.049 -32.705  1.00 23.32           C
ANISOU  723  C   ILE A 411    3181   3033   2646    153   -406   -158       C
ATOM    724  O   ILE A 411      31.080  13.526 -33.698  1.00 23.80           O
ANISOU  724  O   ILE A 411    3225   3207   2611    139   -447   -126       O
ATOM    725  N   LYS A 412      31.150  11.948 -32.095  1.00 22.39           N
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Figure 18 (continued)

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ANISOU  725  N   LYS A 412     3103   2816   2587    126   -417   -254    N
ATOM    726  CA  LYS A 412      30.008  11.189 -32.619  1.00 22.44        C
ANISOU  726  CA  LYS A 412     3126   2844   2557     64   -473   -349    C
ATOM    727  CB  LYS A 412      30.065   9.720 -32.145  1.00 22.70        C
ANISOU  727  CB  LYS A 412     3236   2744   2644     43   -450   -472    C
ATOM    728  CG  LYS A 412      31.201   8.920 -32.768  1.00 22.92        C
ANISOU  728  CG  LYS A 412     3324   2769   2614    105   -401   -564    C
ATOM    729  CD  LYS A 412      31.025   8.761 -34.293  1.00 21.99        C
ANISOU  729  CD  LYS A 412     3210   2800   2346     92   -424   -649    C
ATOM    730  CE  LYS A 412      32.028   7.811 -34.909  1.00 25.65        C
ANISOU  730  CE  LYS A 412     3734   3256   2754    152   -367   -778    C
ATOM    731  NZ  LYS A 412      33.428   8.304 -34.688  1.00 27.17        N
ANISOU  731  NZ  LYS A 412     3899   3468   2955    246   -293   -708    N
ATOM    732  C   LYS A 412      28.666  11.875 -32.299  1.00 21.94        C
ANISOU  732  C   LYS A 412     2995   2803   2540     14   -538   -292    C
ATOM    733  O   LYS A 412      27.630  11.557 -32.849  1.00 22.69        O
ANISOU  733  O   LYS A 412     3067   2958   2597    -40   -599   -352    O
ATOM    734  N   ALA A 413      28.709  12.869 -31.427  1.00 21.22        N
ANISOU  734  N   ALA A 413     2860   2671   2530     36   -525   -183    N
ATOM    735  CA  ALA A 413      27.536  13.650 -31.085  1.00 20.92        C
ANISOU  735  CA  ALA A 413     2747   2655   2548     13   -576   -129    C
ATOM    736  CB  ALA A 413      27.649  14.219 -29.668  1.00 18.88        C
ANISOU  736  CB  ALA A 413     2470   2294   2409     26   -537    -70    C
ATOM    737  C   ALA A 413      27.248  14.752 -32.097  1.00 21.86        C
ANISOU  737  C   ALA A 413     2818   2897   2593     49   -633    -41    C
ATOM    738  O   ALA A 413      26.187  15.379 -32.051  1.00 22.85        O
ANISOU  738  O   ALA A 413     2871   3058   2752     48   -693     -4    O
ATOM    739  N   VAL A 414      28.175  14.991 -33.014  1.00 22.39        N
ANISOU  739  N   VAL A 414     2922   3032   2556     85   -611     -4    N
ATOM    740  CA  VAL A 414      27.955  15.974 -34.070  1.00 23.35        C
ANISOU  740  CA  VAL A 414     3019   3272   2581    117   -662     98    C
ATOM    741  CB  VAL A 414      29.231  16.231 -34.885  1.00 23.82        C
ANISOU  741  CB  VAL A 414     3127   3392   2531    144   -600    150    C
ATOM    742  CG1 VAL A 414      28.916  17.030 -36.162  1.00 23.49        C
ANISOU  742  CG1 VAL A 414     3084   3492   2348    165   -656    255    C
ATOM    743  CG2 VAL A 414      30.269  16.960 -34.029  1.00 21.14        C
ANISOU  743  CG2 VAL A 414     2786   2952   2296    164   -520    231    C
ATOM    744  C   VAL A 414      26.807  15.533 -34.993  1.00 25.52        C
ANISOU  744  C   VAL A 414     3267   3670   2760     90   -761     34    C
ATOM    745  O   VAL A 414      26.724  14.372 -35.386  1.00 26.20        O
ANISOU  745  O   VAL A 414     3384   3785   2785     46   -766   -102    O
ATOM    746  N   ARG A 415      25.914  16.474 -35.297  1.00 26.58        N
ANISOU  746  N   ARG A 415     3339   3868   2891    121   -844    127    N
ATOM    747  CA  ARG A 415      24.812  16.243 -36.203  1.00 29.14        C
ANISOU  747  CA  ARG A 415     3617   4335   3118    109   -958     83    C
ATOM    748  CB  ARG A 415      23.449  16.436 -35.494  1.00 29.44        C
ANISOU  748  CB  ARG A 415     3545   4355   3286     99  -1027     62    C
ATOM    749  CG  ARG A 415      23.141  15.430 -34.381  1.00 29.25        C
ANISOU  749  CG  ARG A 415     3504   4222   3388     18   -974    -70    C
ATOM    750  CD  ARG A 415      23.007  14.000 -34.895  1.00 29.56        C
ANISOU  750  CD  ARG A 415     3579   4300   3352    -70   -985   -236    C
ATOM    751  NE  ARG A 415      22.856  13.082 -33.769  1.00 29.80        N
ANISOU  751  NE  ARG A 415     3621   4194   3510   -150   -917   -331    N
ATOM    752  CZ  ARG A 415      23.825  12.317 -33.266  1.00 28.42        C
ANISOU  752  CZ  ARG A 415     3546   3892   3360   -167   -824   -374    C
ATOM    753  NH1 ARG A 415      25.038  12.351 -33.797  1.00 29.21        N
ANISOU  753  NH1 ARG A 415     3727   3996   3374   -111   -782   -347    N
ATOM    754  NH2 ARG A 415      23.574  11.513 -32.230  1.00 25.27        N
ANISOU  754  NH2 ARG A 415     3164   3367   3070   -239   -772   -438    N
ATOM    755  C   ARG A 415      24.940  17.199 -37.386  1.00 30.32        C
ANISOU  755  C   ARG A 415     3784   4614   3121    172  -1013    223    C
ATOM    756  O   ARG A 415      25.119  18.400 -37.205  1.00 30.57        O
ANISOU  756  O   ARG A 415     3812   4599   3205    231  -1007    381    O
ATOM    757  N   GLY A 416      24.846  16.660 -38.592  1.00 31.60        N
ANISOU  757  N   GLY A 416     3973   4936   3096    156  -1066    164    N
ATOM    758  CA  GLY A 416      25.049  17.449 -39.795  1.00 32.75        C
ANISOU  758  CA  GLY A 416     4156   5224   3063    209  -1110    301    C
ATOM    759  C   GLY A 416      26.516  17.725 -40.084  1.00 32.51        C
ANISOU  759  C   GLY A 416     4216   5174   2960    216   -984    379    C
ATOM    760  O   GLY A 416      27.397  17.335 -39.318  1.00 30.64        O
ANISOU  760  O   GLY A 416     4002   4814   2824    191   -871    323    O
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Figure 18 (continued)

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ATOM    761  N   ASP A 417      26.766  18.388 -41.211  1.00 34.28           N
ANISOU  761  N   ASP A 417    4487   5534   3002    249  -1005    511        N
ATOM    762  CA  ASP A 417      28.113  18.751 -41.645  1.00 35.22           C
ANISOU  762  CA  ASP A 417    4682   5669   3032    244   -879    601        C
ATOM    763  CB  ASP A 417      28.165  18.916 -43.173  1.00 37.33           C
ANISOU  763  CB  ASP A 417    5008   6157   3018    256   -915    671        C
ATOM    764  CG  ASP A 417      28.224  17.574 -43.905  1.00 40.79           C
ANISOU  764  CG  ASP A 417    5468   6743   3286    216   -916    453        C
ATOM    765  OD1 ASP A 417      28.476  16.530 -43.243  1.00 40.15           O
ANISOU  765  OD1 ASP A 417    5373   6567   3315    180   -861    264        O
ATOM    766  OD2 ASP A 417      28.023  17.556 -45.146  1.00 44.28           O
ANISOU  766  OD2 ASP A 417    5951   7394   3481    223   -973    470        O
ATOM    767  C   ASP A 417      28.588  20.023 -40.949  1.00 34.37           C
ANISOU  767  C   ASP A 417    4575   5408   3075    269   -821    788        C
ATOM    768  O   ASP A 417      27.782  20.865 -40.553  1.00 33.70           O
ANISOU  768  O   ASP A 417    4453   5250   3100    314   -901    893        O
ATOM    769  N   LEU A 418      29.902  20.142 -40.795  1.00 34.15           N
ANISOU  769  N   LEU A 418    4581   5331   3061    239   -680    814        N
ATOM    770  CA  LEU A 418      30.506  21.331 -40.188  1.00 34.32           C
ANISOU  770  CA  LEU A 418    4607   5210   3223    240   -613    976        C
ATOM    771  CB  LEU A 418      31.439  20.937 -39.032  1.00 32.56           C
ANISOU  771  CB  LEU A 418    4354   4852   3167    206   -504    872        C
ATOM    772  CG  LEU A 418      30.818  20.136 -37.877  1.00 32.15           C
ANISOU  772  CG  LEU A 418    4251   4695   3270    212   -546    713        C
ATOM    773  CD1 LEU A 418      31.869  19.758 -36.847  1.00 32.10           C
ANISOU  773  CD1 LEU A 418    4227   4578   3390    188   -444    632        C
ATOM    774  CD2 LEU A 418      29.674  20.910 -37.221  1.00 32.15           C
ANISOU  774  CD2 LEU A 418    4210   4598   3407    247   -640    782        C
ATOM    775  C   LEU A 418      31.217  22.207 -41.237  1.00 36.42           C
ANISOU  775  C   LEU A 418    4940   5563   3335    227   -553   1165        C
ATOM    776  O   LEU A 418      32.148  21.768 -41.919  1.00 36.22           O
ANISOU  776  O   LEU A 418    4945   5656   3162    188   -454   1130        O
ATOM    777  N   ASN A 419      30.740  23.444 -41.374  1.00 38.22           N
ANISOU  777  N   ASN A 419    5193   5731   3598    263   -611   1367        N
ATOM    778  CA  ASN A 419      31.215  24.360 -42.413  1.00 40.94           C
ANISOU  778  CA  ASN A 419    5619   6147   3791    250   -570   1584        C
ATOM    779  CB  ASN A 419      30.272  24.322 -43.627  1.00 42.84           C
ANISOU  779  CB  ASN A 419    5901   6577   3800    306   -702   1654        C
ATOM    780  CG  ASN A 419      30.365  23.011 -44.413  1.00 43.28           C
ANISOU  780  CG  ASN A 419    5958   6853   3634    281   -699   1469        C
ATOM    781  OD1 ASN A 419      31.429  22.652 -44.933  1.00 42.07           O
ANISOU  781  OD1 ASN A 419    5839   6798   3349    224   -567   1436        O
ATOM    782  ND2 ASN A 419      29.243  22.307 -44.522  1.00 41.71           N
ANISOU  782  ND2 ASN A 419    5716   6735   3396    320   -841   1339        N
ATOM    783  C   ASN A 419      31.355  25.811 -41.928  1.00 41.80           C
ANISOU  783  C   ASN A 419    5754   6059   4070    255   -549   1788        C
ATOM    784  O   ASN A 419      31.184  26.739 -42.727  1.00 43.13           O
ANISOU  784  O   ASN A 419    5997   6247   4142    277   -579   2006        O
ATOM    785  N   PHE A 420      30.717  26.787 -37.763  1.00 38.53           N
ANISOU  785  N   PHE A 420    5167   5033   4438    296   -567   1596        N
ATOM    786  CA  PHE A 420      31.813  27.317 -40.017  1.00 41.44           C
ANISOU  786  CA  PHE A 420    5674   5609   4463    231   -477   1867        C
ATOM    787  CB  PHE A 420      31.969  27.229 -38.484  1.00 38.75           C
ANISOU  787  CB  PHE A 420    5258   5093   4371    217   -448   1720        C
ATOM    788  CG  PHE A 420      30.638  25.508 -37.189  1.00 35.77           C
ANISOU  788  CG  PHE A 420    4757   4741   4094    283   -566   1382        C
ATOM    789  CD1 PHE A 420      29.480  25.098 -36.517  1.00 35.30           C
ANISOU  789  CD1 PHE A 420    4636   4656   4121    336   -660   1273        C
ATOM    790  CE1 PHE A 420      28.390  25.961 -36.410  1.00 36.31           C
ANISOU  790  CE1 PHE A 420    4745   4716   4335    416   -759   1362        C
ATOM    791  CZ  PHE A 420      28.453  27.236 -36.976  1.00 37.91           C
ANISOU  791  CZ  PHE A 420    5009   4854   4542    452   -773   1570        C
ATOM    792  CE2 PHE A 420      29.615  27.647 -37.648  1.00 38.57           C
ANISOU  792  CE2 PHE A 420    5173   4948   4536    385   -676   1694        C
ATOM    793  CD2 PHE A 420      32.985  28.099 -40.621  1.00 43.58           C
ANISOU  793  CD2 PHE A 420    6013   5871   4673    144   -345   2038        C
ATOM    794  C   PHE A 420      34.016  27.544 -40.971  1.00 43.69           O
ANISOU  794  C   PHE A 420    6017   6000   4582     67   -227   1979        O
ATOM    795  O   PHE A 420      32.815  29.402 -40.734  1.00 46.01           N
ATOM    796  N   VAL A 421
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Figure 18 (continued)

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ANISOU  796  N   VAL A 421     6388   6035   5060    155   -361   2250    N
ATOM    797  CA  VAL A 421      33.827  30.281 -41.275  1.00 48.42        C
ANISOU  797  CA  VAL A 421     6767   6301   5331     58   -235   2439    C
ATOM    798  CB  VAL A 421      33.415  30.657 -42.715  1.00 50.72        C
ANISOU  798  CB  VAL A 421     7168   6727   5375     95   -285   2662    C
ATOM    799  CG1 VAL A 421      33.405  32.139 -42.946  1.00 53.63        C
ANISOU  799  CG1 VAL A 421     7644   6908   5824     89   -278   2939    C
ATOM    800  CG2 VAL A 421      34.260  29.882 -43.738  1.00 50.83        C
ANISOU  800  CG2 VAL A 421     7196   6999   5117     16   -175   2634    C
ATOM    801  C   VAL A 421      33.969  31.474 -40.304  1.00 49.05        C
ANISOU  801  C   VAL A 421     6856   6092   5690     35   -213   2513    C
ATOM    802  O   VAL A 421      33.147  31.634 -39.405  1.00 48.40        O
ANISOU  802  O   VAL A 421     6734   5873   5784    117   -308   2435    O
ATOM    803  N   ASN A 422      35.019  32.281 -40.431  1.00 50.78        N
ANISOU  803  N   ASN A 422     7118   6220   5956    -86    -79   2641    N
ATOM    804  CA  ASN A 422      35.104  33.500 -39.619  1.00 51.41        C
ANISOU  804  CA  ASN A 422     7224   6012   6298   -114    -65   2718    C
ATOM    805  CB  ASN A 422      36.417  33.548 -38.825  1.00 50.54        C
ANISOU  805  CB  ASN A 422     7039   5832   6330   -263     80   2603    C
ATOM    806  CG  ASN A 422      37.651  33.599 -39.710  1.00 53.01        C
ANISOU  806  CG  ASN A 422     7370   6272   6500   -410    242   2706    C
ATOM    807  OD1 ASN A 422      38.708  33.120 -39.316  1.00 54.15        O
ANISOU  807  OD1 ASN A 422     7415   6486   6672   -510    351   2564    O
ATOM    808  ND2 ASN A 422      37.536  34.195 -40.891  1.00 54.93        N
ANISOU  808  ND2 ASN A 422     7734   6550   6586   -424    260   2956    N
ATOM    809  C   ASN A 422      34.855  34.791 -40.412  1.00 54.51        C
ANISOU  809  C   ASN A 422     7760   6272   6679   -107    -77   3020    C
ATOM    810  O   ASN A 422      34.565  34.742 -41.619  1.00 55.83        O
ANISOU  810  O   ASN A 422     8008   6590   6613    -71   -108   3185    O
ATOM    811  N   ARG A 423      34.971  35.936 -39.726  1.00 55.63        N
ANISOU  811  N   ARG A 423     7940   6128   7070   -139    -56   3090    N
ATOM    812  CA  ARG A 423      34.778  37.275 -40.329  1.00 58.60        C
ANISOU  812  CA  ARG A 423     8467   6310   7489   -134    -63   3384    C
ATOM    813  CB  ARG A 423      35.154  38.368 -39.309  1.00 59.00        C
ANISOU  813  CB  ARG A 423     8531   6029   7855   -205    -10   3374    C
ATOM    814  CG  ARG A 423      35.137  39.808 -39.824  1.00 63.01        C
ANISOU  814  CG  ARG A 423     9207   6282   8454   -228      9   3672    C
ATOM    815  CD  ARG A 423      35.119  40.813 -38.669  1.00 63.11        C
ANISOU  815  CD  ARG A 423     9229   5943   8808   -243     11   3608    C
ATOM    816  NE  ARG A 423      35.372  42.173 -39.147  1.00 69.55        N
ANISOU  816  NE  ARG A 423    10211   6488   9728   -310     65   3886    N
ATOM    817  CZ  ARG A 423      35.212  43.291 -38.432  1.00 71.04        C
ANISOU  817  CZ  ARG A 423    10463   6323  10208   -303     54   3903    C
ATOM    818  NH1 ARG A 423      34.780  43.251 -37.173  1.00 69.69        N
ANISOU  818  NH1 ARG A 423    10195   6035  10247   -226     -8   3649    N
ATOM    819  NH2 ARG A 423      35.491  44.463 -38.983  1.00 73.29        N
ANISOU  819  NH2 ARG A 423    10914   6362  10570   -377    112   4175    N
ATOM    820  C   ARG A 423      35.554  37.441 -41.644  1.00 60.66        C
ANISOU  820  C   ARG A 423     8824   6708   7516   -250     52   3610    C
ATOM    821  O   ARG A 423      34.991  37.878 -42.656  1.00 63.13        O
ANISOU  821  O   ARG A 423     9263   7049   7676   -176    -13   3852    O
ATOM    822  N   ALA A 424      36.833  37.059 -41.619  1.00 60.09        N
ANISOU  822  N   ALA A 424     8685   6740   7406   -424    220   3525    N
ATOM    823  CA  ALA A 424      37.733  37.087 -42.782  1.00 61.86        C
ANISOU  823  CA  ALA A 424     8968   7132   7403   -560    366   3695    C
ATOM    824  CB  ALA A 424      39.184  37.099 -42.313  1.00 61.84        C
ANISOU  824  CB  ALA A 424     8869   7119   7507   -766    558   3590    C
ATOM    825  C   ALA A 424      37.525  35.953 -43.803  1.00 61.47        C
ANISOU  825  C   ALA A 424     8907   7435   7014   -498    342   3661    C
ATOM    826  O   ALA A 424      38.302  35.834 -44.758  1.00 63.06        O
ANISOU  826  O   ALA A 424     9142   7818   7001   -608    476   3765    O
ATOM    827  N   ASN A 425      36.503  35.117 -43.583  1.00 59.19        N
ANISOU  827  N   ASN A 425     8565   7245   6681   -334    181   3501    N
ATOM    828  CA  ASN A 425      36.066  34.070 -44.533  1.00 58.70        C
ANISOU  828  CA  ASN A 425     8501   7493   6310   -257    119   3455    C
ATOM    829  CB  ASN A 425      35.834  34.650 -45.946  1.00 61.60        C
ANISOU  829  CB  ASN A 425     9027   7961   6417   -245    108   3760    C
ATOM    830  CG  ASN A 425      35.025  33.719 -46.851  1.00 61.89        C
ANISOU  830  CG  ASN A 425     9073   8290   6153   -127    -18   3714    C
ATOM    831  OD1 ASN A 425      34.099  33.032 -46.410  1.00 60.11        O
ANISOU  831  OD1 ASN A 425     8770   8100   5969     -2   -169   3531    O
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Figure 18 (continued)

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ATOM    832  ND2 ASN A 425      35.377  33.700 -48.125  1.00 65.09           N
ANISOU  832  ND2 ASN A 425     9572   8911   6249   -176     49   3875       N
ATOM    833  C   ASN A 425      36.992  32.848 -44.543  1.00 56.85           C
ANISOU  833  C   ASN A 425     8150   7489   5962   -338    240   3221       C
ATOM    834  O   ASN A 425      37.088  32.101 -45.516  1.00 57.64           O
ANISOU  834  O   ASN A 425     8263   7855   5782   -333    263   3202       O
ATOM    835  N   GLN A 426      37.662  32.653 -43.424  1.00 54.65           N
ANISOU  835  N   GLN A 426     7757   7103   5906   -403    310   3033       N
ATOM    836  CA  GLN A 426      38.574  31.539 -43.259  1.00 52.90           C
ANISOU  836  CA  GLN A 426     7412   7061   5626   -461    416   2803       C
ATOM    837  CB  GLN A 426      39.823  31.999 -42.501  1.00 53.02           C
ANISOU  837  CB  GLN A 426     7345   6954   5845   -609    567   2761       C
ATOM    838  CG  GLN A 426      40.496  33.214 -43.170  1.00 57.14           C
ANISOU  838  CG  GLN A 426     7957   7403   6350   -755    700   3030       C
ATOM    839  CD  GLN A 426      41.953  33.340 -42.795  1.00 59.04           C
ANISOU  839  CD  GLN A 426     8085   7648   6699   -930    886   2958       C
ATOM    840  OE1 GLN A 426      42.294  33.478 -41.614  1.00 58.44           O
ANISOU  840  OE1 GLN A 426     7913   7417   6874   -964    882   2816       O
ATOM    841  NE2 GLN A 426      42.825  33.277 -43.793  1.00 60.49           N
ANISOU  841  NE2 GLN A 426     8269   8028   6687  -1044   1051   3047       N
ATOM    842  C   GLN A 426      37.859  30.413 -42.543  1.00 49.11           C
ANISOU  842  C   GLN A 426     6847   6621   5192   -339    290   2547       C
ATOM    843  O   GLN A 426      37.235  30.626 -41.508  1.00 47.36           O
ANISOU  843  O   GLN A 426     6597   6214   5183   -278    192   2479       O
ATOM    844  N   ARG A 427      37.920  29.226 -43.133  1.00 48.00           N
ANISOU  844  N   ARG A 427     6674   6721   4843   -307    298   2408       N
ATOM    845  CA  ARG A 427      37.341  28.025 -42.550  1.00 45.29           C
ANISOU  845  CA  ARG A 427     6256   6425   4525   -212    198   2160       C
ATOM    846  CB  ARG A 427      37.621  26.831 -43.471  1.00 45.82           C
ANISOU  846  CB  ARG A 427     6312   6763   4335   -202    242   2034       C
ATOM    847  CG  ARG A 427      37.173  25.507 -42.909  1.00 43.52           C
ANISOU  847  CG  ARG A 427     5952   6510   4074   -124    162   1771       C
ATOM    848  CD  ARG A 427      37.185  24.344 -43.919  1.00 44.50           C
ANISOU  848  CD  ARG A 427     6088   6884   3937    -97    174   1641       C
ATOM    849  NE  ARG A 427      36.589  23.168 -43.281  1.00 42.09           N
ANISOU  849  NE  ARG A 427     5732   6558   3701    -26     80   1406       N
ATOM    850  CZ  ARG A 427      35.305  22.813 -43.382  1.00 41.80           C
ANISOU  850  CZ  ARG A 427     5721   6535   3625     43    -78   1366       C
ATOM    851  NH1 ARG A 427      34.472  23.522 -44.138  1.00 40.53           N
ANISOU  851  NH1 ARG A 427     5630   6425   3343     70   -173   1541       N
ATOM    852  NH2 ARG A 427      34.859  21.734 -42.737  1.00 38.54           N
ANISOU  852  NH2 ARG A 427     5262   6088   3294     83   -141   1153       N
ATOM    853  C   ARG A 427      37.941  27.795 -41.156  1.00 42.92           C
ANISOU  853  C   ARG A 427     5846   5984   4476   -242    239   1985       C
ATOM    854  O   ARG A 427      39.158  27.682 -41.033  1.00 43.19           O
ANISOU  854  O   ARG A 427     5815   6060   4536   -330    378   1932       O
ATOM    855  N   LEU A 428      37.109  27.762 -40.111  1.00 40.68           N
ANISOU  855  N   LEU A 428     5537   5548   4373   -169    120   1900       N
ATOM    856  CA  LEU A 428      37.620  27.491 -38.771  1.00 38.47           C
ANISOU  856  CA  LEU A 428     5162   5153   4302   -189    146   1733       C
ATOM    857  CB  LEU A 428      36.507  27.485 -37.706  1.00 37.16           C
ANISOU  857  CB  LEU A 428     4983   4836   4300   -103     12   1656       C
ATOM    858  CG  LEU A 428      35.520  28.644 -37.563  1.00 38.47           C
ANISOU  858  CG  LEU A 428     5210   4834   4572    -57    -80   1807       C
ATOM    859  CD1 LEU A 428      34.640  28.465 -36.331  1.00 36.49           C
ANISOU  859  CD1 LEU A 428     4911   4461   4493     17   -177   1674       C
ATOM    860  CD2 LEU A 428      36.231  29.983 -37.520  1.00 40.33           C
ANISOU  860  CD2 LEU A 428     5484   4917   4922   -147      4   1968       C
ATOM    861  C   LEU A 428      38.327  26.130 -38.791  1.00 37.36           C
ANISOU  861  C   LEU A 428     4947   5175   4073   -187    206   1533       C
ATOM    862  O   LEU A 428      37.927  25.217 -39.528  1.00 37.44           O
ANISOU  862  O   LEU A 428     4980   5342   3905   -134    173   1466       O
ATOM    863  N   ASN A 429      39.393  26.000 -38.005  1.00 36.22           N
ANISOU  863  N   ASN A 429     4713   4996   4055   -240    291   1432       N
ATOM    864  CA  ASN A 429      40.027  24.699 -37.838  1.00 35.15           C
ANISOU  864  CA  ASN A 429     4501   4981   3874   -209    331   1232       C
ATOM    865  CB  ASN A 429      41.422  24.797 -37.154  1.00 35.29           C
ANISOU  865  CB  ASN A 429     4406   4986   4018   -278    438   1162       C
ATOM    866  CG  ASN A 429      41.376  25.137 -35.654  1.00 34.45           C
ANISOU  866  CG  ASN A 429     4253   4696   4142   -277    377   1100       C
ATOM    867  OD1 ASN A 429      40.351  25.025 -34.971  1.00 33.81           O
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Figure 18 (continued)

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ANISOU  867  OD1 ASN A 429     4210   4506   4130   -211    263   1066      O
ATOM    868  ND2 ASN A 429      42.531  25.532 -35.132  1.00 32.90           N
ANISOU  868  ND2 ASN A 429     3961   4484   4057   -356    458   1073      N
ATOM    869  C   ASN A 429      39.062  23.680 -37.199  1.00 32.57           C
ANISOU  869  C   ASN A 429     4181   4618   3577   -107    207   1081      C
ATOM    870  O   ASN A 429      38.051  24.074 -36.619  1.00 31.85           O
ANISOU  870  O   ASN A 429     4121   4399   3582    -74    105   1113      O
ATOM    871  N   PRO A 430      39.325  22.378 -37.376  1.00 31.96           N
ANISOU  871  N   PRO A 430     4076   4654   3413    -60    223    919      N
ATOM    872  CA  PRO A 430      38.489  21.306 -36.827  1.00 30.42           C
ANISOU  872  CA  PRO A 430     3895   4422   3243     19    122    773      C
ATOM    873  CB  PRO A 430      39.374  20.073 -36.998  1.00 30.52           C
ANISOU  873  CB  PRO A 430     3865   4539   3194     51    191    608      C
ATOM    874  CG  PRO A 430      40.115  20.354 -38.256  1.00 32.63           C
ANISOU  874  CG  PRO A 430     4130   4972   3296      8    302    673      C
ATOM    875  CD  PRO A 430      40.439  21.822 -38.174  1.00 33.57           C
ANISOU  875  CD  PRO A 430     4239   5029   3487    -78    346    859      C
ATOM    876  C   PRO A 430      38.030  21.452 -35.362  1.00 28.84           C
ANISOU  876  C   PRO A 430     3672   4045   3243     38     48    733      C
ATOM    877  O   PRO A 430      36.844  21.250 -35.072  1.00 28.54           O
ANISOU  877  O   PRO A 430     3669   3949   3226     76    -51    715      O
ATOM    878  N   MSE A 431      38.938  21.798 -34.454  1.00 27.42           N
ANISOU  878  N   MSE A 431     3425   3793   3198      8     97    713      N
ATOM    879  CA  MSE A 431      38.573  21.963 -33.044  1.00 25.88           C
ANISOU  879  CA  MSE A 431     3213   3450   3172     23     33    670      C
ATOM    880  CB  MSE A 431      39.832  22.116 -32.159  1.00 25.62           C
ANISOU  880  CB  MSE A 431     3094   3390   3252     -8     89    615      C
ATOM    881  CG  MSE A 431      40.705  20.833 -32.079  1.00 26.44           C
ANISOU  881  CG  MSE A 431     3147   3586   3315     45    124    475      C
ATOM    882  SE  MSE A 431      39.842  19.246 -31.234  0.90 30.28          SE
ANISOU  882  SE  MSE A 431     3685   4010   3809    150     26    327      SE
ATOM    883  CE  MSE A 431      39.652  20.084 -29.473  1.00 25.02           C
ANISOU  883  CE  MSE A 431     2993   3190   3324    126    -33    340      C
ATOM    884  C   MSE A 431      37.575  23.100 -32.781  1.00 25.36           C
ANISOU  884  C   MSE A 431     3187   3264   3186      9    -30    783      C
ATOM    885  O   MSE A 431      36.673  22.960 -31.939  1.00 24.38           O
ANISOU  885  O   MSE A 431     3073   3052   3140     47   -107    735      O
ATOM    886  N   HIS A 432      37.743  24.212 -33.483  1.00 26.43           N
ANISOU  886  N   HIS A 432     3345   3391   3306    -42      7    933      N
ATOM    887  CA  HIS A 432      36.804  25.342 -33.406  1.00 27.85           C
ANISOU  887  CA  HIS A 432     3573   3450   3560    -37    -53   1055      C
ATOM    888  CB  HIS A 432      37.483  26.636 -33.864  1.00 29.15           C
ANISOU  888  CB  HIS A 432     3755   3560   3759   -119     20   1213      C
ATOM    889  CG  HIS A 432      38.458  27.164 -32.859  1.00 31.05           C
ANISOU  889  CG  HIS A 432     3933   3702   4163   -191     77   1164      C
ATOM    890  ND1 HIS A 432      39.711  26.614 -32.671  1.00 31.07           N
ANISOU  890  ND1 HIS A 432     3853   3795   4157   -238    156   1070      N
ATOM    891  CE1 HIS A 432      40.338  27.277 -31.714  1.00 33.02           C
ANISOU  891  CE1 HIS A 432     4046   3937   4562   -300    177   1035      C
ATOM    892  NE2 HIS A 432      39.529  28.221 -31.255  1.00 32.01           N
ANISOU  892  NE2 HIS A 432     3972   3642   4547   -295    121   1094      N
ATOM    893  CD2 HIS A 432      38.348  28.170 -31.956  1.00 32.70           C
ANISOU  893  CD2 HIS A 432     4141   3736   4548   -220     58   1179      C
ATOM    894  C   HIS A 432      35.510  25.078 -34.165  1.00 27.83           C
ANISOU  894  C   HIS A 432     3625   3502   3447     29   -143   1098      C
ATOM    895  O   HIS A 432      34.466  25.587 -33.800  1.00 28.93           O
ANISOU  895  O   HIS A 432     3780   3549   3665     73   -223   1134      O
ATOM    896  N   GLN A 433      35.608  24.283 -35.217  1.00 28.16           N
ANISOU  896  N   GLN A 433     3686   3705   3308     38   -128   1081      N
ATOM    897  CA  GLN A 433      34.467  23.712 -35.940  1.00 29.30           C
ANISOU  897  CA  GLN A 433     3866   3942   3324     95   -220   1070      C
ATOM    898  CB  GLN A 433      35.053  22.746 -36.985  1.00 30.36           C
ANISOU  898  CB  GLN A 433     4014   4260   3263     84   -165   1008      C
ATOM    899  CG  GLN A 433      34.400  22.595 -38.320  1.00 34.65           C
ANISOU  899  CG  GLN A 433     4611   4954   3599    106   -217   1065      C
ATOM    900  CD  GLN A 433      34.134  23.881 -39.054  1.00 37.03           C
ANISOU  900  CD  GLN A 433     4967   5253   3848    101   -235   1288      C
ATOM    901  OE1 GLN A 433      32.987  24.307 -39.137  1.00 38.30           O
ANISOU  901  OE1 GLN A 433     5148   5383   4022    154   -351   1359      O
ATOM    902  NE2 GLN A 433      35.176  24.486 -39.632  1.00 38.30           N
ANISOU  902  NE2 GLN A 433     5153   5454   3945     38   -121   1405      N
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Figure 18 (continued)

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ATOM    903  C   GLN A 433      33.551  22.973 -34.938  1.00 27.21           C
ANISOU  903  C   GLN A 433    3569   3614   3155    140   -301    930       C
ATOM    904  O   GLN A 433      32.367  23.270 -34.843  1.00 26.79           O
ANISOU  904  O   GLN A 433    3518   3526   3136    182   -393    960       O
ATOM    905  N   LEU A 434      34.134  22.047 -34.166  1.00 25.47           N
ANISOU  905  N   LEU A 434    3317   3379   2983    132   -261    785       N
ATOM    906  CA  LEU A 434      33.444  21.324 -33.076  1.00 23.90           C
ANISOU  906  CA  LEU A 434    3095   3107   2877    157   -313    662       C
ATOM    907  CB  LEU A 434      34.364  20.255 -32.466  1.00 21.96           C
ANISOU  907  CB  LEU A 434    2834   2862   2649    154   -258    530       C
ATOM    908  CG  LEU A 434      34.764  19.139 -33.439  1.00 23.59           C
ANISOU  908  CG  LEU A 434    3064   3192   2709    164   -230    450       C
ATOM    909  CD1 LEU A 434      35.976  18.335 -32.918  1.00 20.60           C
ANISOU  909  CD1 LEU A 434    2659   2806   2361    179   -162    347       C
ATOM    910  CD2 LEU A 434      33.550  18.247 -33.779  1.00 19.71           C
ANISOU  910  CD2 LEU A 434    2602   2734   2153    179   -308    372       C
ATOM    911  C   LEU A 434      32.955  22.243 -31.952  1.00 23.68           C
ANISOU  911  C   LEU A 434    3044   2938   3017    164   -342    696       C
ATOM    912  O   LEU A 434      31.826  22.090 -31.488  1.00 22.82           O
ANISOU  912  O   LEU A 434    2922   2795   2954    191   -409    658       O
ATOM    913  N   LEU A 435      33.830  23.153 -31.512  1.00 23.88           N
ANISOU  913  N   LEU A 435    3056   2886   3130    132   -286    752       N
ATOM    914  CA  LEU A 435      33.499  24.163 -30.507  1.00 25.30           C
ANISOU  914  CA  LEU A 435    3221   2926   3468    134   -304    776       C
ATOM    915  CB  LEU A 435      34.675  25.123 -30.289  1.00 25.47           C
ANISOU  915  CB  LEU A 435    3231   2880   3567     76   -233    832       C
ATOM    916  CG  LEU A 435      34.639  26.078 -29.094  1.00 25.12           C
ANISOU  916  CG  LEU A 435    3169   2684   3693     62   -237    814       C
ATOM    917  CD1 LEU A 435      34.703  25.341 -27.754  1.00 24.17           C
ANISOU  917  CD1 LEU A 435    3012   2549   3622     73   -247    664       C
ATOM    918  CD2 LEU A 435      35.784  27.023 -29.203  1.00 25.51           C
ANISOU  918  CD2 LEU A 435    3211   2680   3803    -15   -167    880       C
ATOM    919  C   LEU A 435      32.245  24.976 -30.853  1.00 27.05           C
ANISOU  919  C   LEU A 435    3458   3104   3717    181   -377    868       C
ATOM    920  O   LEU A 435      31.290  25.013 -30.067  1.00 27.13           O
ANISOU  920  O   LEU A 435    3441   3056   3810    219   -426    813       O
ATOM    921  N   ARG A 436      32.256  25.645 -32.008  1.00 29.13           N
ANISOU  921  N   ARG A 436    3760   3400   3908    183   -382   1011       N
ATOM    922  CA  ARG A 436      31.117  26.464 -32.400  1.00 30.76           C
ANISOU  922  CA  ARG A 436    3982   3566   4140    248   -463   1117       C
ATOM    923  CB  ARG A 436      31.376  27.299 -33.659  1.00 33.08           C
ANISOU  923  CB  ARG A 436    4340   3883   4346    244   -457   1307       C
ATOM    924  CG  ARG A 436      32.474  28.404 -33.560  1.00 40.00           C
ANISOU  924  CG  ARG A 436    5252   4636   5311    174   -367   1413       C
ATOM    925  CD  ARG A 436      32.607  29.153 -32.189  1.00 47.23           C
ANISOU  925  CD  ARG A 436    6140   5358   6447    160   -347   1351       C
ATOM    926  NE  ARG A 436      34.019  29.442 -31.860  1.00 51.94           N
ANISOU  926  NE  ARG A 436    6729   5911   7097     53   -242   1339       N
ATOM    927  CZ  ARG A 436      34.460  30.070 -30.761  1.00 55.22           C
ANISOU  927  CZ  ARG A 436    7119   6181   7681     10   -211   1275       C
ATOM    928  NH1 ARG A 436      33.623  30.495 -29.823  1.00 56.84           N
ANISOU  928  NH1 ARG A 436    7313   6263   8019     70   -265   1212       N
ATOM    929  NH2 ARG A 436      35.766  30.280 -30.592  1.00 56.92           N
ANISOU  929  NH2 ARG A 436    7311   6387   7930    -96   -122   1262       N
ATOM    930  C   ARG A 436      29.860  25.608 -32.560  1.00 29.85           C
ANISOU  930  C   ARG A 436    3833   3546   3961    304   -554   1040       C
ATOM    931  O   ARG A 436      28.781  26.041 -32.179  1.00 29.79           O
ANISOU  931  O   ARG A 436    3791   3486   4041    365   -622   1042       O
ATOM    932  N   HIS A 437      30.000  24.397 -33.106  1.00 28.56           N
ANISOU  932  N   HIS A 437    3672   3522   3657    280   -551    961       N
ATOM    933  CA  HIS A 437      28.855  23.524 -33.256  1.00 27.62           C
ANISOU  933  CA  HIS A 437    3517   3491   3485    308   -633    872       C
ATOM    934  CB  HIS A 437      29.238  22.173 -33.872  1.00 26.97           C
ANISOU  934  CB  HIS A 437    3455   3538   3253    269   -613    771       C
ATOM    935  CG  HIS A 437      28.094  21.203 -33.939  1.00 24.96           C
ANISOU  935  CG  HIS A 437    3163   3358   2963    273   -691    657       C
ATOM    936  ND1 HIS A 437      27.096  21.289 -34.889  1.00 23.43           N
ANISOU  936  ND1 HIS A 437    2950   3277   2675    305   -793    694       N
ATOM    937  CE1 HIS A 437      26.222  20.315 -34.704  1.00 23.02           C
ANISOU  937  CE1 HIS A 437    2852   3273   2623    283   -843    560       C
ATOM    938  NE2 HIS A 437      26.611  19.602 -33.660  1.00 24.74           N
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Figure 18 (continued)

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ANISOU  938  NE2 HIS A 437     3071   3399   2929    238   -771    453       N
ATOM    939  CD2 HIS A 437      27.787  20.134 -33.169  1.00 22.63           C
ANISOU  939  CD2 HIS A 437     2844   3039   2717    240   -683    510       C
ATOM    940  C   HIS A 437      28.175  23.327 -31.894  1.00 26.83           C
ANISOU  940  C   HIS A 437     3359   3302   3534    317   -643    763       C
ATOM    941  O   HIS A 437      26.971  23.545 -31.765  1.00 27.43           O
ANISOU  941  O   HIS A 437     3383   3382   3658    363   -717    757       O
ATOM    942  N   PHE A 438      28.958  22.972 -30.878  1.00 25.29           N
ANISOU  942  N   PHE A 438     3167   3035   3407    276   -569    682       N
ATOM    943  CA  PHE A 438      28.394  22.684 -29.559  1.00 24.57           C
ANISOU  943  CA  PHE A 438     3034   2877   3426    274   -566    579       C
ATOM    944  CB  PHE A 438      29.261  21.668 -28.812  1.00 22.50           C
ANISOU  944  CB  PHE A 438     2794   2601   3155    227   -502    477       C
ATOM    945  CG  PHE A 438      29.231  20.302 -29.427  1.00 20.80           C
ANISOU  945  CG  PHE A 438     2601   2477   2826    203   -510    405       C
ATOM    946  CD1 PHE A 438      28.021  19.574 -29.486  1.00 20.00           C
ANISOU  946  CD1 PHE A 438     2472   2420   2708    192   -562    337       C
ATOM    947  CE1 PHE A 438      27.970  18.314 -30.056  1.00 18.22           C
ANISOU  947  CE1 PHE A 438     2274   2260   2389    160   -571    256       C
ATOM    948  CZ  PHE A 438      29.155  17.745 -30.605  1.00 20.73           C
ANISOU  948  CZ  PHE A 438     2649   2605   2624    156   -525    238       C
ATOM    949  CE2 PHE A 438      30.357  18.468 -30.569  1.00 17.04           C
ANISOU  949  CE2 PHE A 438     2194   2113   2167    174   -469    308       C
ATOM    950  CD2 PHE A 438      30.383  19.739 -29.965  1.00 19.46           C
ANISOU  950  CD2 PHE A 438     2473   2349   2573    188   -464    392       C
ATOM    951  C   PHE A 438      28.046  23.929 -28.731  1.00 25.24           C
ANISOU  951  C   PHE A 438     3090   2842   3658    311   -567    615       C
ATOM    952  O   PHE A 438      27.189  23.875 -27.871  1.00 24.41           O
ANISOU  952  O   PHE A 438     2936   2710   3630    328   -580    543       O
ATOM    953  N   GLN A 439      28.691  25.057 -29.040  1.00 27.21           N
ANISOU  953  N   GLN A 439     3372   3021   3947    320   -548    723       N
ATOM    954  CA  GLN A 439      28.316  26.353 -28.476  1.00 28.57           C
ANISOU  954  CA  GLN A 439     3530   3062   4264    365   -557    766       C
ATOM    955  CB  GLN A 439      29.395  27.400 -28.724  1.00 29.66           C
ANISOU  955  CB  GLN A 439     3721   3102   4446    335   -509    870       C
ATOM    956  CG  GLN A 439      30.531  27.306 -27.690  1.00 30.49           C
ANISOU  956  CG  GLN A 439     3826   3151   4608    264   -433    781       C
ATOM    957  CD  GLN A 439      31.679  28.234 -27.997  1.00 34.96           C
ANISOU  957  CD  GLN A 439     4429   3638   5214    207   -379    871       C
ATOM    958  OE1 GLN A 439      31.762  28.782 -29.090  1.00 38.23           O
ANISOU  958  OE1 GLN A 439     4884   4053   5587    208   -383   1013       O
ATOM    959  NE2 GLN A 439      32.570  28.423 -27.029  1.00 35.77           N
ANISOU  959  NE2 GLN A 439     4515   3679   5395    149   -329    791       N
ATOM    960  C   GLN A 439      26.934  26.813 -28.925  1.00 29.99           C
ANISOU  960  C   GLN A 439     3669   3257   4470    454   -644    815       C
ATOM    961  O   GLN A 439      26.223  27.399 -28.120  1.00 30.12           O
ANISOU  961  O   GLN A 439     3639   3192   4612    505   -655    772       O
ATOM    962  N   LYS A 440      26.528  26.494 -30.162  1.00 31.18           N
ANISOU  962  N   LYS A 440     3825   3525   4496    477   -708    887       N
ATOM    963  CA  LYS A 440      25.142  26.739 -30.603  1.00 33.51           C
ANISOU  963  CA  LYS A 440     4058   3873   4799    568   -811    916       C
ATOM    964  CB  LYS A 440      24.983  26.655 -32.140  1.00 35.28           C
ANISOU  964  CB  LYS A 440     4316   4227   4864    593   -887   1034       C
ATOM    965  CG  LYS A 440      25.813  27.704 -32.903  1.00 37.77           C
ANISOU  965  CG  LYS A 440     4728   4471   5152    603   -867   1220       C
ATOM    966  CD  LYS A 440      25.401  27.909 -34.364  1.00 39.08           C
ANISOU  966  CD  LYS A 440     4927   4756   5164    659   -961   1367       C
ATOM    967  CE  LYS A 440      26.117  29.152 -34.913  1.00 43.76           C
ANISOU  967  CE  LYS A 440     5623   5235   5768    670   -931   1574       C
ATOM    968  NZ  LYS A 440      25.782  29.513 -36.329  1.00 47.40           N
ANISOU  968  NZ  LYS A 440     6140   5801   6067    730  -1019   1756       N
ATOM    969  C   LYS A 440      24.114  25.822 -29.905  1.00 32.70           C
ANISOU  969  C   LYS A 440     3858   3844   4721    562   -831    761       C
ATOM    970  O   LYS A 440      23.029  26.285 -29.495  1.00 33.55           O
ANISOU  970  O   LYS A 440     3882   3936   4931    635   -876    735       O
ATOM    971  N   ASP A 441      24.440  24.539 -29.780  1.00 30.72           N
ANISOU  971  N   ASP A 441     3617   3671   4384    475   -794    659       N
ATOM    972  CA  ASP A 441      23.533  23.580 -29.155  1.00 30.83           C
ANISOU  972  CA  ASP A 441     3554   3747   4415    443   -800    522       C
ATOM    973  CB  ASP A 441      22.400  23.160 -30.119  1.00 33.58           C
ANISOU  973  CB  ASP A 441     3830   4241   4688    466   -905    515       C
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Figure 18 (continued)

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ATOM    974  CG  ASP A 441      21.496  22.044 -29.536  1.00 36.33           C
ANISOU  974  CG  ASP A 441    4094   4658   5053    398   -900    365       C
ATOM    975  OD1 ASP A 441      20.945  22.224 -28.422  1.00 37.04           O
ANISOU  975  OD1 ASP A 441    4116   4697   5259    402   -859    301       O
ATOM    976  OD2 ASP A 441      21.344  20.987 -30.206  1.00 39.15           O
ANISOU  976  OD2 ASP A 441    4455   5117   5303    335   -932    308       O
ATOM    977  C   ASP A 441      24.280  22.357 -28.620  1.00 28.33           C
ANISOU  977  C   ASP A 441    3285   3430   4047    345   -724    424       C
ATOM    978  O   ASP A 441      24.976  21.649 -29.360  1.00 27.35           O
ANISOU  978  O   ASP A 441    3222   3360   3809    305   -718    428       O
ATOM    979  N   ALA A 442      24.125  22.122 -27.320  1.00 26.96           N
ANISOU  979  N   ALA A 442    3088   3198   3956    316   -666    338       N
ATOM    980  CA  ALA A 442      24.818  21.037 -26.645  1.00 24.82           C
ANISOU  980  CA  ALA A 442    2872   2908   3650    240   -598    261       C
ATOM    981  CB  ALA A 442      25.668  21.599 -25.523  1.00 23.21           C
ANISOU  981  CB  ALA A 442    2703   2600   3517    243   -531    259       C
ATOM    982  C   ALA A 442      23.960  19.870 -26.145  1.00 24.67           C
ANISOU  982  C   ALA A 442    2817   2932   3624    175   -587    156       C
ATOM    983  O   ALA A 442      24.488  19.030 -25.378  1.00 25.14           O
ANISOU  983  O   ALA A 442    2932   2949   3670    120   -527    105       O
ATOM    984  N   LYS A 443      22.691  19.779 -26.585  1.00 24.95           N
ANISOU  984  N   LYS A 443    2761   3052   3668    177   -646    129       N
ATOM    985  CA  LYS A 443      21.742  18.689 -26.217  1.00 25.03           C
ANISOU  985  CA  LYS A 443    2718   3111   3680     93   -634     28       C
ATOM    986  CB  LYS A 443      20.371  18.874 -26.875  1.00 27.31           C
ANISOU  986  CB  LYS A 443    2874   3514   3986    110   -718      6       C
ATOM    987  CG  LYS A 443      19.531  19.967 -26.291  1.00 31.52           C
ANISOU  987  CG  LYS A 443    3294   4049   4632    188   -724     14       C
ATOM    988  CD  LYS A 443      18.276  20.175 -27.156  1.00 38.16           C
ANISOU  988  CD  LYS A 443    3995   5022   5481    230   -832      4       C
ATOM    989  CE  LYS A 443      17.658  21.570 -26.901  1.00 44.11           C
ANISOU  989  CE  LYS A 443    4650   5761   6348    365   -863     48       C
ATOM    990  NZ  LYS A 443      16.692  21.975 -27.987  1.00 44.43           N
ANISOU  990  NZ  LYS A 443    4575   5926   6381    450  -1000     80       N
ATOM    991  C   LYS A 443      22.191  17.276 -26.526  1.00 23.86           C
ANISOU  991  C   LYS A 443    2652   2965   3449      5   -617    -26       C
ATOM    992  O   LYS A 443      22.087  16.413 -25.659  1.00 22.54           O
ANISOU  992  O   LYS A 443    2510   2753   3301    -71   -554    -86       O
ATOM    993  N   VAL A 444      22.654  17.043 -27.761  1.00 23.85           N
ANISOU  993  N   VAL A 444    2695   3013   3353     17   -669     -5       N
ATOM    994  CA  VAL A 444      23.079  15.707 -28.183  1.00 23.44           C
ANISOU  994  CA  VAL A 444    2724   2958   3226    -53   -656    -74       C
ATOM    995  CB  VAL A 444      23.278  15.593 -29.728  1.00 24.08           C
ANISOU  995  CB  VAL A 444    2823   3139   3186    -33   -728    -69       C
ATOM    996  CG1 VAL A 444      23.640  14.169 -30.129  1.00 23.87           C
ANISOU  996  CG1 VAL A 444    2877   3100   3093   -104   -710   -171       C
ATOM    997  CG2 VAL A 444      22.026  16.031 -30.447  1.00 24.33           C
ANISOU  997  CG2 VAL A 444    2743   3297   3206    -20   -828    -70       C
ATOM    998  C   VAL A 444      24.327  15.306 -27.408  1.00 22.67           C
ANISOU  998  C   VAL A 444    2733   2748   3133    -54   -574    -66       C
ATOM    999  O   VAL A 444      24.445  14.151 -26.968  1.00 24.02           O
ANISOU  999  O   VAL A 444    2963   2860   3303   -117   -534   -131       O
ATOM   1000  N   LEU A 445      25.228  16.270 -27.203  1.00 20.80           N
ANISOU 1000  N   LEU A 445    2516   2477   2910     16   -553     14       N
ATOM   1001  CA  LEU A 445      26.470  16.029 -26.491  1.00 19.22           C
ANISOU 1001  CA  LEU A 445    2395   2194   2715     28   -491     22       C
ATOM   1002  CB  LEU A 445      27.355  17.284 -26.540  1.00 18.43           C
ANISOU 1002  CB  LEU A 445    2290   2081   2632     92   -482    107       C
ATOM   1003  CG  LEU A 445      28.698  17.335 -25.788  1.00 16.91           C
ANISOU 1003  CG  LEU A 445    2147   1823   2456    111   -430    119       C
ATOM   1004  CD1 LEU A 445      29.714  16.292 -26.272  1.00 15.64           C
ANISOU 1004  CD1 LEU A 445    2050   1668   2225    114   -410     86       C
ATOM   1005  CD2 LEU A 445      29.301  18.716 -25.861  1.00 17.13           C
ANISOU 1005  CD2 LEU A 445    2149   1839   2522    148   -425    195       C
ATOM   1006  C   LEU A 445      26.221  15.634 -25.038  1.00 19.21           C
ANISOU 1006  C   LEU A 445    2405   2118   2774    -10   -439    -11       C
ATOM   1007  O   LEU A 445      26.803  14.665 -24.554  1.00 20.41           O
ANISOU 1007  O   LEU A 445    2635   2211   2909    -32   -404    -39       O
ATOM   1008  N   PHE A 446      25.386  16.416 -24.350  1.00 18.58           N
ANISOU 1008  N   PHE A 446    2252   2045   2761     -8   -434     -3       N
ATOM   1009  CA  PHE A 446      25.072  16.215 -22.948  1.00 17.93           C
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Figure 18 (continued)

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ANISOU 1009  CA  PHE A 446     2174   1919   2722    -43   -376    -31       C
ATOM   1010  CB  PHE A 446      24.302  17.424 -22.372  1.00 18.01           C
ANISOU 1010  CB  PHE A 446     2089   1949   2806    -10   -370    -27       C
ATOM   1011  CG  PHE A 446      25.186  18.610 -21.966  1.00 17.40           C
ANISOU 1011  CG  PHE A 446     2025   1826   2762     59   -363     15       C
ATOM   1012  CD1 PHE A 446      26.531  18.664 -22.307  1.00 16.25           C
ANISOU 1012  CD1 PHE A 446     1946   1647   2580     85   -369     55       C
ATOM   1013  CE1 PHE A 446      27.333  19.740 -21.958  1.00 16.45           C
ANISOU 1013  CE1 PHE A 446     1974   1630   2646    127   -361     84       C
ATOM   1014  CZ  PHE A 446      26.800  20.806 -21.285  1.00 17.43           C
ANISOU 1014  CZ  PHE A 446     2046   1728   2849    153   -350     69       C
ATOM   1015  CE2 PHE A 446      25.447  20.791 -20.941  1.00 21.09           C
ANISOU 1015  CE2 PHE A 446     2441   2224   3346    147   -342     25       C
ATOM   1016  CD2 PHE A 446      24.639  19.701 -21.302  1.00 18.75           C
ANISOU 1016  CD2 PHE A 446     2128   1987   3008     97   -348      2       C
ATOM   1017  C   PHE A 446      24.270  14.927 -22.727  1.00 18.39           C
ANISOU 1017  C   PHE A 446     2246   1974   2768   -139   -353    -89       C
ATOM   1018  O   PHE A 446      24.607  14.160 -21.843  1.00 18.65           O
ANISOU 1018  O   PHE A 446     2357   1942   2788   -177   -302    -95       O
ATOM   1019  N   GLN A 447      23.240  14.694 -23.545  1.00 18.81           N
ANISOU 1019  N   GLN A 447     2227   2095   2824   -180   -394   -128       N
ATOM   1020  CA  GLN A 447      22.379  13.508 -23.457  1.00 19.67           C
ANISOU 1020  CA  GLN A 447     2333   2203   2937   -294   -374   -195       C
ATOM   1021  CB  GLN A 447      21.108  13.676 -24.326  1.00 19.41           C
ANISOU 1021  CB  GLN A 447     2168   2284   2922   -326   -437   -243       C
ATOM   1022  CG  GLN A 447      20.183  14.825 -23.916  1.00 20.98           C
ANISOU 1022  CG  GLN A 447     2223   2556   3190   -282   -442   -234       C
ATOM   1023  CD  GLN A 447      19.493  14.638 -22.559  1.00 23.91           C
ANISOU 1023  CD  GLN A 447     2554   2915   3616   -353   -348   -267       C
ATOM   1024  OE1 GLN A 447      19.925  13.841 -21.725  1.00 20.75           O
ANISOU 1024  OE1 GLN A 447     2258   2433   3195   -418   -273   -264       O
ATOM   1025  NE2 GLN A 447      18.419  15.397 -22.335  1.00 26.39           N
ANISOU 1025  NE2 GLN A 447     2715   3316   3997   -331   -350   -295       N
ATOM   1026  C   GLN A 447      23.084  12.169 -23.771  1.00 20.15           C
ANISOU 1026  C   GLN A 447     2524   2184   2950   -339   -364   -221       C
ATOM   1027  O   GLN A 447      22.659  11.125 -23.307  1.00 21.51           O
ANISOU 1027  O   GLN A 447     2739   2297   3136   -437   -322   -259       O
ATOM   1028  N   ASN A 448      24.170  12.210 -24.531  1.00 20.43           N
ANISOU 1028  N   ASN A 448     2621   2207   2934   -265   -396   -202       N
ATOM   1029  CA  ASN A 448      24.872  11.006 -24.958  1.00 22.00           C
ANISOU 1029  CA  ASN A 448     2933   2333   3092   -282   -391   -242       C
ATOM   1030  CB  ASN A 448      25.032  10.974 -26.496  1.00 22.08           C
ANISOU 1030  CB  ASN A 448     2930   2422   3036   -256   -453   -284       C
ATOM   1031  CG  ASN A 448      23.720  10.673 -27.209  1.00 23.31           C
ANISOU 1031  CG  ASN A 448     3009   2660   3190   -343   -504   -359       C
ATOM   1032  OD1 ASN A 448      23.280   9.533 -27.269  1.00 24.47           O
ANISOU 1032  OD1 ASN A 448     3195   2755   3349   -439   -495   -443       O
ATOM   1033  ND2 ASN A 448      23.088  11.703 -27.735  1.00 23.68           N
ANISOU 1033  ND2 ASN A 448     2941   2828   3226   -310   -563   -330       N
ATOM   1034  C   ASN A 448      26.213  10.800 -24.295  1.00 21.90           C
ANISOU 1034  C   ASN A 448     3021   2230   3070   -213   -353   -198       C
ATOM   1035  O   ASN A 448      26.856   9.772 -24.513  1.00 23.82           O
ANISOU 1035  O   ASN A 448     3361   2395   3293   -206   -344   -230       O
ATOM   1036  N   TRP A 449      26.606  11.740 -23.448  1.00 22.09           N
ANISOU 1036  N   TRP A 449     3019   2260   3112   -160   -334   -133       N
ATOM   1037  CA  TRP A 449      27.908  11.699 -22.745  1.00 22.12           C
ANISOU 1037  CA  TRP A 449     3095   2205   3105    -89   -313    -92       C
ATOM   1038  CB  TRP A 449      28.184  13.060 -22.066  1.00 21.28           C
ANISOU 1038  CB  TRP A 449     2925   2138   3020    -41   -308    -42       C
ATOM   1039  CG  TRP A 449      29.534  13.158 -21.367  1.00 21.14           C
ANISOU 1039  CG  TRP A 449     2955   2087   2990     28   -301    -10       C
ATOM   1040  CD1 TRP A 449      29.786  12.971 -20.040  1.00 20.23           C
ANISOU 1040  CD1 TRP A 449     2886   1931   2868     31   -278     10       C
ATOM   1041  NE1 TRP A 449      31.129  13.124 -19.779  1.00 19.99           N
ANISOU 1041  NE1 TRP A 449     2874   1899   2823    107   -295     28       N
ATOM   1042  CE2 TRP A 449      31.780  13.406 -20.950  1.00 20.43           C
ANISOU 1042  CE2 TRP A 449     2892   1990   2881    146   -314     19       C
ATOM   1043  CD2 TRP A 449      30.800  13.453 -21.976  1.00 19.62           C
ANISOU 1043  CD2 TRP A 449     2757   1916   2781    100   -319      1       C
ATOM   1044  CE3 TRP A 449      31.205  13.729 -23.288  1.00 18.99           C
ANISOU 1044  CE3 TRP A 449     2646   1890   2681    125   -335     -3       C
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Figure 18 (continued)

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ATOM   1045  CZ3 TRP A 449      32.565  13.992 -23.531  1.00 20.81           C
ANISOU 1045  CZ3 TRP A 449    2865   2143   2899    187   -331     10          C
ATOM   1046  CH2 TRP A 449      33.515  13.972 -22.478  1.00 18.26           C
ANISOU 1046  CH2 TRP A 449    2554   1793   2591    230   -327     19          C
ATOM   1047  CZ2 TRP A 449      33.141  13.677 -21.188  1.00 18.76           C
ANISOU 1047  CZ2 TRP A 449    2659   1805   2663    215   -327     25          C
ATOM   1048  C   TRP A 449      28.112  10.540 -21.757  1.00 22.76           C
ANISOU 1048  C   TRP A 449    3285   2175   3186   -114   -275    -87          C
ATOM   1049  O   TRP A 449      29.253  10.071 -21.571  1.00 24.65           O
ANISOU 1049  O   TRP A 449    3599   2358   3407    -44   -278    -71          O
ATOM   1050  N   GLY A 450      27.057  10.056 -21.115  1.00 22.54           N
ANISOU 1050  N   GLY A 450    3270   2117   3179   -211   -240    -94          N
ATOM   1051  CA  GLY A 450      27.269   9.021 -20.083  1.00 21.83           C
ANISOU 1051  CA  GLY A 450    3301   1913   3081   -237   -199    -61          C
ATOM   1052  C   GLY A 450      26.923   9.581 -18.715  1.00 21.43           C
ANISOU 1052  C   GLY A 450    3233   1890   3018   -259   -155    -11          C
ATOM   1053  O   GLY A 450      27.192  10.758 -18.436  1.00 20.21           O
ANISOU 1053  O   GLY A 450    3005   1815   2860   -202   -167      1          O
ATOM   1054  N   ILE A 451      26.284   8.751 -17.889  1.00 21.10           N
ANISOU 1054  N   ILE A 451    3262   1784   2970   -352    -98     14          N
ATOM   1055  CA  ILE A 451      25.818   9.147 -16.578  1.00 20.69           C
ANISOU 1055  CA  ILE A 451    3202   1772   2887   -392    -39     54          C
ATOM   1056  CB  ILE A 451      24.237   9.164 -16.503  1.00 21.84           C
ANISOU 1056  CB  ILE A 451    3255   1973   3069   -531     24     13          C
ATOM   1057  CG1 ILE A 451      23.720  10.086 -15.389  1.00 20.59           C
ANISOU 1057  CG1 ILE A 451    3025   1914   2885   -542     83     19          C
ATOM   1058  CD1 ILE A 451      23.706  11.556 -15.790  1.00 19.64           C
ANISOU 1058  CD1 ILE A 451    2765   1897   2800   -456     40    -28          C
ATOM   1059  CG2 ILE A 451      23.649   7.766 -16.361  1.00 22.44           C
ANISOU 1059  CG2 ILE A 451    3427   1942   3156   -663     78     26          C
ATOM   1060  C   ILE A 451      26.458   8.155 -15.621  1.00 22.07           C
ANISOU 1060  C   ILE A 451    3539   1838   3008   -382    -18    134          C
ATOM   1061  O   ILE A 451      26.781   7.044 -16.013  1.00 22.36           O
ANISOU 1061  O   ILE A 451    3682   1753   3060   -385    -30    146          O
ATOM   1062  N   GLU A 452      26.683   8.553 -14.378  1.00 22.05           N
ANISOU 1062  N   GLU A 452    3565   1877   2938   -359      8    187          N
ATOM   1063  CA  GLU A 452      27.397   7.691 -13.451  1.00 23.30           C
ANISOU 1063  CA  GLU A 452    3882   1946   3025   -326     10    280          C
ATOM   1064  CB  GLU A 452      28.909   8.005 -13.455  1.00 22.10           C
ANISOU 1064  CB  GLU A 452    3748   1802   2846   -164    -79    296          C
ATOM   1065  CG  GLU A 452      29.322   9.401 -12.931  1.00 21.20           C
ANISOU 1065  CG  GLU A 452    3532   1826   2696   -103   -103    268          C
ATOM   1066  CD  GLU A 452      30.841   9.593 -12.871  1.00 22.68           C
ANISOU 1066  CD  GLU A 452    3732   2026   2861     37   -190    281          C
ATOM   1067  OE1 GLU A 452      31.592   8.596 -12.982  1.00 27.30           O
ANISOU 1067  OE1 GLU A 452    4414   2519   3440    105   -229    328          O
ATOM   1068  OE2 GLU A 452      31.303  10.728 -12.689  1.00 23.21           O
ANISOU 1068  OE2 GLU A 452    3706   2189   2922     81   -220    240          O
ATOM   1069  C   GLU A 452      26.827   7.884 -12.057  1.00 24.23           C
ANISOU 1069  C   GLU A 452    4026   2124   3057   -392     85    331          C
ATOM   1070  O   GLU A 452      26.298   8.943 -11.755  1.00 22.41           O
ANISOU 1070  O   GLU A 452    3678   2018   2819   -412    115    279          O
ATOM   1071  N   HIS A 453      26.937   6.859 -11.220  1.00 26.35           N
ANISOU 1071  N   HIS A 453    4453   2300   3257   -423    117    434          N
ATOM   1072  CA  HIS A 453      26.636   7.037  -9.814  1.00 29.05           C
ANISOU 1072  CA  HIS A 453    4843   2716   3480   -466    183    497          C
ATOM   1073  CB  HIS A 453      26.420   5.688  -9.121  1.00 31.54           C
ANISOU 1073  CB  HIS A 453    5346   2900   3737   -546    242    627          C
ATOM   1074  CG  HIS A 453      25.586   5.793  -7.881  1.00 37.83           C
ANISOU 1074  CG  HIS A 453    6167   3786   4420   -660    356    679          C
ATOM   1075  ND1 HIS A 453      26.069   5.479  -6.623  1.00 42.46           N
ANISOU 1075  ND1 HIS A 453    6901   4383   4849   -627    364    804          N
ATOM   1076  CE1 HIS A 453      25.122   5.697  -5.727  1.00 45.28           C
ANISOU 1076  CE1 HIS A 453    7243   4847   5115   -752    487    817          C
ATOM   1077  NE2 HIS A 453      24.054   6.168  -6.351  1.00 44.67           N
ANISOU 1077  NE2 HIS A 453    6999   4830   5145   -855    557    700          N
ATOM   1078  CD2 HIS A 453      24.320   6.241  -7.697  1.00 40.72           C
ANISOU 1078  CD2 HIS A 453    6418   4258   4796   -798    469    618          C
ATOM   1079  C   HIS A 453      27.767   7.838  -9.144  1.00 28.67           C
ANISOU 1079  C   HIS A 453    4790   2760   3345   -324    106    504          C
ATOM   1080  O   HIS A 453      28.940   7.782  -9.559  1.00 28.14           O
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Figure 18 (continued)

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ANISOU 1080  O   HIS A 453     4741   2654   3297   -194      5    509      O
ATOM   1081  N   ILE A 454      27.423   8.618  -8.132  1.00 29.08           N
ANISOU 1081  N   ILE A 454     4802   2945   3304   -350    154    488      N
ATOM   1082  CA  ILE A 454      28.448   9.403  -7.440  1.00 28.83           C
ANISOU 1082  CA  ILE A 454     4760   3009   3183   -232     78    475      C
ATOM   1083  CB  ILE A 454      28.400  10.945  -7.822  1.00 27.51           C
ANISOU 1083  CB  ILE A 454     4412   2956   3086   -201     60    334      C
ATOM   1084  CG1 ILE A 454      27.220  11.666  -7.174  1.00 27.31           C
ANISOU 1084  CG1 ILE A 454     4309   3040   3029   -292    168    268      C
ATOM   1085  CD1 ILE A 454      27.215  13.162  -7.375  1.00 25.56           C
ANISOU 1085  CD1 ILE A 454     3937   2905   2872   -246    148    138      C
ATOM   1086  CG2 ILE A 454      28.360  11.131  -9.313  1.00 26.45           C
ANISOU 1086  CG2 ILE A 454     4180   2762   3106   -186     25    277      C
ATOM   1087  C   ILE A 454      28.381   9.208  -5.937  1.00 30.68           C
ANISOU 1087  C   ILE A 454     5104   3314   3238   -258    123    553      C
ATOM   1088  O   ILE A 454      27.341   8.876  -5.395  1.00 32.05           O
ANISOU 1088  O   ILE A 454     5312   3505   3359   -381    239    587      O
ATOM   1089  N   ASP A 455      29.506   9.410  -5.269  1.00 32.23           N
ANISOU 1089  N   ASP A 455     5348   3565   3333   -144     29    580      N
ATOM   1090  CA  ASP A 455      29.570   9.458  -3.811  1.00 34.84           C
ANISOU 1090  CA  ASP A 455     5769   4006   3465   -149     49    635      C
ATOM   1091  CB  ASP A 455      30.984   9.101  -3.357  1.00 36.54           C
ANISOU 1091  CB  ASP A 455     6075   4220   3587     -3    -92    712      C
ATOM   1092  CG  ASP A 455      31.449   7.732  -3.876  1.00 40.61           C
ANISOU 1092  CG  ASP A 455     6722   4552   4157     51   -140    845      C
ATOM   1093  OD1 ASP A 455      30.664   6.746  -3.860  1.00 45.61           O
ANISOU 1093  OD1 ASP A 455     7471   5067   4792    -46    -50    945      O
ATOM   1094  OD2 ASP A 455      32.617   7.641  -4.302  1.00 44.13           O
ANISOU 1094  OD2 ASP A 455     7150   4967   4651    190   -265    841      O
ATOM   1095  C   ASP A 455      29.193  10.845  -3.264  1.00 34.43           C
ANISOU 1095  C   ASP A 455     5588   4124   3368   -173     89    493      C
ATOM   1096  O   ASP A 455      29.396  11.863  -3.913  1.00 33.12           O
ANISOU 1096  O   ASP A 455     5280   3987   3318   -134     49    366      O
ATOM   1097  N   ASN A 456      28.616  10.872  -2.073  1.00 36.47           N
ANISOU 1097  N   ASN A 456     5907   4491   3459   -241    178    516      N
ATOM   1098  CA  ASN A 456      28.410  12.114  -1.357  1.00 36.78           C
ANISOU 1098  CA  ASN A 456     5852   4697   3426   -245    209    376      C
ATOM   1099  CB  ASN A 456      27.498  11.878  -0.155  1.00 38.76           C
ANISOU 1099  CB  ASN A 456     6179   5058   3489   -349    349    415      C
ATOM   1100  CG  ASN A 456      26.107  11.425  -0.555  1.00 39.81           C
ANISOU 1100  CG  ASN A 456     6277   5142   3709   -491    505    433      C
ATOM   1101  OD1 ASN A 456      25.486  11.995  -1.468  1.00 37.31           O
ANISOU 1101  OD1 ASN A 456     5803   4798   3573   -513    535    321      O
ATOM   1102  ND2 ASN A 456      25.598  10.397   0.136  1.00 39.68           N
ANISOU 1102  ND2 ASN A 456     6402   5117   3558   -591    604    578      N
ATOM   1103  C   ASN A 456      29.751  12.683  -0.903  1.00 36.67           C
ANISOU 1103  C   ASN A 456     5840   4760   3333   -121     63    333      C
ATOM   1104  O   ASN A 456      30.413  12.110  -0.036  1.00 37.97           O
ANISOU 1104  O   ASN A 456     6134   4970   3323    -74      2    435      O
ATOM   1105  N   VAL A 457      30.161  13.779  -1.535  1.00 35.06           N
ANISOU 1105  N   VAL A 457     5490   4565   3266    -71      2    190      N
ATOM   1106  CA  VAL A 457      31.320  14.556  -1.101  1.00 34.96           C
ANISOU 1106  CA  VAL A 457     5441   4642   3201     18   -121    106      C
ATOM   1107  CB  VAL A 457      32.418  14.572  -2.196  1.00 33.72           C
ANISOU 1107  CB  VAL A 457     5219   4392   3202    106   -247    107      C
ATOM   1108  CG1 VAL A 457      33.621  15.370  -1.740  1.00 33.63           C
ANISOU 1108  CG1 VAL A 457     5151   4481   3146    179   -372     14      C
ATOM   1109  CG2 VAL A 457      32.816  13.127  -2.554  1.00 35.71           C
ANISOU 1109  CG2 VAL A 457     5589   4533   3446    151   -290    281      C
ATOM   1110  C   VAL A 457      30.848  15.978  -0.779  1.00 34.15           C
ANISOU 1110  C   VAL A 457     5219   4633   3121    -16    -68    -85      C
ATOM   1111  O   VAL A 457      30.251  16.622  -1.639  1.00 32.78           O
ANISOU 1111  O   VAL A 457     4932   4395   3126    -42    -17   -167      O
ATOM   1112  N   MSE A 458      31.088  16.452   0.451  1.00 35.25           N
ANISOU 1112  N   MSE A 458     5390   4923   3079    -11    -81   -157      N
ATOM   1113  CA  MSE A 458      30.699  17.815   0.846  1.00 34.91           C
ANISOU 1113  CA  MSE A 458     5246   4964   3055    -34    -32   -361      C
ATOM   1114  CB  MSE A 458      30.871  18.047   2.353  1.00 37.58           C
ANISOU 1114  CB  MSE A 458     5655   5487   3136    -39    -39   -424      C
ATOM   1115  CG  MSE A 458      30.252  19.378   2.825  1.00 36.62           C
ANISOU 1115  CG  MSE A 458     5440   5445   3030    -71     49   -651      C
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Figure 18 (continued)

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ATOM   1116 SE   MSE A 458      30.457  19.706   4.676  0.90 40.81          SE
ANISOU 1116 SE   MSE A 458    6058   6227   3221    -80     51   -762       SE
ATOM   1117  CE  MSE A 458      29.473  21.279   4.926  1.00 43.27           C
ANISOU 1117  CE  MSE A 458    6238   6576   3626   -113    185  -1053       C
ATOM   1118  C   MSE A 458      31.466  18.877   0.071  1.00 33.44           C
ANISOU 1118  C   MSE A 458    4933   4714   3057     13   -127   -485       C
ATOM   1119  O   MSE A 458      32.657  18.724  -0.155  1.00 34.08           O
ANISOU 1119  O   MSE A 458    5016   4783   3152     71   -259   -451       O
ATOM   1120  N   GLY A 459      30.783  19.943  -0.342  1.00 32.49           N
ANISOU 1120  N   GLY A 459    4703   4553   3090    -12    -57   -623       N
ATOM   1121  CA  GLY A 459      31.402  21.007  -1.139  1.00 31.36           C
ANISOU 1121  CA  GLY A 459    4449   4324   3141     18   -129   -728       C
ATOM   1122  C   GLY A 459      31.266  20.849  -2.641  1.00 30.19           C
ANISOU 1122  C   GLY A 459    4243   4025   3204     28   -132   -646       C
ATOM   1123  O   GLY A 459      31.810  21.635  -3.395  1.00 28.91           O
ANISOU 1123  O   GLY A 459    4001   3786   3198     47   -186   -701       O
ATOM   1124  N   MSE A 460      30.504  19.844  -3.079  1.00 30.67           N
ANISOU 1124  N   MSE A 460    4344   4046   3265      4    -68   -519       N
ATOM   1125  CA  MSE A 460      30.479  19.418  -4.475  1.00 30.71           C
ANISOU 1125  CA  MSE A 460    4316   3927   3427     14    -86   -427       C
ATOM   1126  CB  MSE A 460      31.612  18.422  -4.661  1.00 30.18           C
ANISOU 1126  CB  MSE A 460    4321   3842   3305     58   -185   -308       C
ATOM   1127  CG  MSE A 460      32.091  18.176  -6.021  1.00 31.46           C
ANISOU 1127  CG  MSE A 460    4442   3899   3611     88   -234   -249       C
ATOM   1128 SE   MSE A 460      33.476  16.771  -5.852  0.90 37.35          SE
ANISOU 1128 SE   MSE A 460    5293   4649   4248    165   -348   -114       SE
ATOM   1129  CE  MSE A 460      34.825  17.837  -4.917  1.00 35.43           C
ANISOU 1129  CE  MSE A 460    4991   4531   3939    209   -461   -235       C
ATOM   1130  C   MSE A 460      29.152  18.715  -4.753  1.00 28.46           C
ANISOU 1130  C   MSE A 460    4042   3618   3154    -41     24   -362       C
ATOM   1131  O   MSE A 460      28.575  18.079  -3.850  1.00 28.50           O
ANISOU 1131  O   MSE A 460    4120   3694   3015    -88     97   -325       O
ATOM   1132  N   VAL A 461      28.671  18.840  -5.989  1.00 25.91           N
ANISOU 1132  N   VAL A 461    3643   3204   2995    -44      34   -348       N
ATOM   1133  CA  VAL A 461      27.446  18.159  -6.436  1.00 25.77           C
ANISOU 1133  CA  VAL A 461    3614   3165   3014   -103    121   -296       C
ATOM   1134  CB  VAL A 461      26.129  19.057  -6.389  1.00 26.21           C
ANISOU 1134  CB  VAL A 461    3552   3258   3149   -125    217   -406       C
ATOM   1135  CG1 VAL A 461      25.667  19.320  -4.974  1.00 28.85           C
ANISOU 1135  CG1 VAL A 461    3904   3710   3347   -154    306   -485       C
ATOM   1136  CG2 VAL A 461      26.293  20.405  -7.139  1.00 25.60           C
ANISOU 1136  CG2 VAL A 461    3368   3122   3236    -60    167   -496       C
ATOM   1137  C   VAL A 461      27.621  17.605  -7.849  1.00 24.27           C
ANISOU 1137  C   VAL A 461    3411   2873   2939    -92     69   -216       C
ATOM   1138  O   VAL A 461      28.436  18.099  -8.633  1.00 22.83           O
ANISOU 1138  O   VAL A 461    3191   2640   2843    -37    -10   -224       O
ATOM   1139  N   GLY A 462      26.837  16.583  -8.174  1.00 23.87           N
ANISOU 1139  N   GLY A 462    3388   2795   2886   -154    122   -147       N
ATOM   1140  CA  GLY A 462      26.661  16.169  -9.564  1.00 21.99           C
ANISOU 1140  CA  GLY A 462    3116   2478   2763   -158     90   -107       C
ATOM   1141  C   GLY A 462      25.731  17.096 -10.366  1.00 21.21           C
ANISOU 1141  C   GLY A 462    2876   2387   2797   -156    109   -179       C
ATOM   1142  O   GLY A 462      25.023  17.917  -9.803  1.00 21.23           O
ANISOU 1142  O   GLY A 462    2805   2448   2813   -158    166   -260       O
ATOM   1143  N   VAL A 463      25.746  16.937 -11.686  1.00 19.62           N
ANISOU 1143  N   VAL A 463    2639   2130   2686   -142     58   -151       N
ATOM   1144  CA  VAL A 463      24.947  17.731 -12.581  1.00 19.75           C
ANISOU 1144  CA  VAL A 463    2533   2153   2820   -125     52   -195       C
ATOM   1145  CB  VAL A 463      25.767  18.971 -13.157  1.00 19.50           C
ANISOU 1145  CB  VAL A 463    2461   2085   2865    -37    -19   -215       C
ATOM   1146  CG1 VAL A 463      26.906  18.526 -14.079  1.00 18.45           C
ANISOU 1146  CG1 VAL A 463    2382   1899   2729    -11    -93   -148       C
ATOM   1147  CG2 VAL A 463      24.903  19.884 -13.892  1.00 20.87           C
ANISOU 1147  CG2 VAL A 463    2520   2259   3151     -5    -26   -248       C
ATOM   1148  C   VAL A 463      24.402  16.803 -13.675  1.00 19.21           C
ANISOU 1148  C   VAL A 463    2454   2061   2785   -173     38   -153       C
ATOM   1149  O   VAL A 463      25.117  15.975 -14.245  1.00 17.34           O
ANISOU 1149  O   VAL A 463    2295   1770   2523   -173     -6    -98       O
ATOM   1150  N   LEU A 464      23.113  16.938 -13.952  1.00 20.10           N
ANISOU 1150  N   LEU A 464    2460   2221   2955   -211     75   -193       N
ATOM   1151  CA  LEU A 464      22.451  16.147 -14.993  1.00 20.06           C
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Figure 18 (continued)

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ANISOU 1151  CA  LEU A 464     2423   2214   2986   -267     55   -179       C
ATOM   1152  CB  LEU A 464      20.978  15.896 -14.611  1.00 20.50           C
ANISOU 1152  CB  LEU A 464     2379   2345   3065   -356    136   -228       C
ATOM   1153  CG  LEU A 464      20.640  15.224 -13.271  1.00 20.46           C
ANISOU 1153  CG  LEU A 464     2432   2366   2978   -451    249   -224       C
ATOM   1154  CD1 LEU A 464      19.137  15.006 -13.119  1.00 21.72           C
ANISOU 1154  CD1 LEU A 464     2461   2614   3178   -551    334   -280       C
ATOM   1155  CD2 LEU A 464      21.359  13.932 -13.071  1.00 18.35           C
ANISOU 1155  CD2 LEU A 464     2330   2012   2629   -510    252   -143       C
ATOM   1156  C   LEU A 464      22.547  16.908 -16.326  1.00 19.95           C
ANISOU 1156  C   LEU A 464     2335   2196   3048   -190    -34   -178       C
ATOM   1157  O   LEU A 464      22.865  18.083 -16.323  1.00 19.98           O
ANISOU 1157  O   LEU A 464     2302   2195   3096   -107    -60   -189       O
ATOM   1158  N   PRO A 465      22.308  16.229 -17.470  1.00 20.59           N
ANISOU 1158  N   PRO A 465     2409   2275   3140   -222    -82   -163       N
ATOM   1159  CA  PRO A 465      22.309  16.897 -18.783  1.00 21.07           C
ANISOU 1159  CA  PRO A 465     2405   2352   3247   -154   -167   -151       C
ATOM   1160  CB  PRO A 465      21.839  15.803 -19.740  1.00 21.49           C
ANISOU 1160  CB  PRO A 465     2459   2425   3283   -226   -198   -161       C
ATOM   1161  CG  PRO A 465      22.268  14.552 -19.122  1.00 20.52           C
ANISOU 1161  CG  PRO A 465     2456   2236   3104   -304   -147   -152       C
ATOM   1162  CD  PRO A 465      22.139  14.772 -17.616  1.00 21.10           C
ANISOU 1162  CD  PRO A 465     2542   2310   3163   -323    -62   -154       C
ATOM   1163  C   PRO A 465      21.445  18.147 -18.919  1.00 22.58           C
ANISOU 1163  C   PRO A 465     2460   2598   3522    -89   -184   -180       C
ATOM   1164  O   PRO A 465      21.848  19.088 -19.645  1.00 22.93           O
ANISOU 1164  O   PRO A 465     2489   2623   3600     -1   -247   -143       O
ATOM   1165  N   ASP A 466      20.288  18.182 -18.246  1.00 23.41           N
ANISOU 1165  N   ASP A 466     2467   2765   3663   -127   -125   -240       N
ATOM   1166  CA  ASP A 466      19.484  19.423 -18.181  1.00 24.48           C
ANISOU 1166  CA  ASP A 466     2467   2944   3890    -41   -132   -280       C
ATOM   1167  CB  ASP A 466      17.987  19.137 -17.935  1.00 25.77           C
ANISOU 1167  CB  ASP A 466     2481   3214   4096    -97    -86   -353       C
ATOM   1168  CG  ASP A 466      17.711  18.432 -16.596  1.00 27.78           C
ANISOU 1168  CG  ASP A 466     2762   3494   4300   -205     43   -396       C
ATOM   1169  OD1 ASP A 466      18.616  18.350 -15.739  1.00 29.82           O
ANISOU 1169  OD1 ASP A 466     3148   3692   4490   -212     88   -374       O
ATOM   1170  OD2 ASP A 466      16.564  17.962 -16.383  1.00 29.01           O
ANISOU 1170  OD2 ASP A 466     2805   3739   4477   -288    100   -451       O
ATOM   1171  C   ASP A 466      20.026  20.476 -17.185  1.00 24.43           C
ANISOU 1171  C   ASP A 466     2490   2886   3906     30    -90   -302       C
ATOM   1172  O   ASP A 466      19.377  21.498 -16.948  1.00 24.93           O
ANISOU 1172  O   ASP A 466     2453   2967   4054    106    -80   -352       O
ATOM   1173  N   MSE A 467      21.206  20.210 -16.610  1.00 24.00           N
ANISOU 1173  N   MSE A 467     2568   2770   3780      9    -70   -275       N
ATOM   1174  CA  MSE A 467      21.905  21.152 -15.710  1.00 24.32           C
ANISOU 1174  CA  MSE A 467     2648   2764   3829     63    -45   -305       C
ATOM   1175  CB  MSE A 467      22.058  22.557 -16.331  1.00 24.10           C
ANISOU 1175  CB  MSE A 467     2574   2675   3907    171   -105   -297       C
ATOM   1176  CG  MSE A 467      23.071  22.602 -17.472  1.00 23.28           C
ANISOU 1176  CG  MSE A 467     2537   2512   3797    191   -185   -203       C
ATOM   1177  SE  MSE A 467      24.823  21.862 -16.977  0.90 26.00          SE
ANISOU 1177  SE  MSE A 467     3030   2817   4031    137   -179   -170       SE
ATOM   1178  CE  MSE A 467      25.294  23.125 -15.564  1.00 22.62           C
ANISOU 1178  CE  MSE A 467     2609   2344   3643    172   -138   -259       C
ATOM   1179  C   MSE A 467      21.320  21.226 -14.313  1.00 25.38           C
ANISOU 1179  C   MSE A 467     2754   2951   3936     34     55   -390       C
ATOM   1180  O   MSE A 467      21.736  22.059 -13.507  1.00 26.95           O
ANISOU 1180  O   MSE A 467     2972   3126   4141     78     79   -444       O
ATOM   1181  N   THR A 468      20.388  20.320 -14.021  1.00 25.59           N
ANISOU 1181  N   THR A 468     2740   3056   3927    -51    119   -408       N
ATOM   1182  CA  THR A 468      19.830  20.146 -12.684  1.00 25.97           C
ANISOU 1182  CA  THR A 468     2773   3176   3917   -106    235   -475       C
ATOM   1183  CB  THR A 468      18.559  19.255 -12.705  1.00 27.06           C
ANISOU 1183  CB  THR A 468     2822   3405   4054   -209    304   -491       C
ATOM   1184  OG1 THR A 468      17.500  19.937 -13.395  1.00 30.40           O
ANISOU 1184  OG1 THR A 468     3070   3880   4602   -149    278   -546       O
ATOM   1185  CG2 THR A 468      18.066  18.937 -11.284  1.00 30.00           C
ANISOU 1185  CG2 THR A 468     3200   3861   4340   -288    444   -541       C
ATOM   1186  C   THR A 468      20.882  19.520 -11.783  1.00 24.91           C
ANISOU 1186  C   THR A 468     2799   3016   3650   -153    260   -435       C
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Figure 18 (continued)

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ATOM   1187  O   THR A 468      21.500  18.510 -12.160  1.00 23.50           O
ANISOU 1187  O   THR A 468    2721   2793   3415   -201    223   -351       O
ATOM   1188  N   PRO A 469      21.109  20.120 -10.592  1.00 25.19           N
ANISOU 1188  N   PRO A 469    2858   3082   3631   -131    315   -501       N
ATOM   1189  CA  PRO A 469      22.089  19.534  -9.669  1.00 24.77           C
ANISOU 1189  CA  PRO A 469    2952   3026   3434   -167    326   -461       C
ATOM   1190  CB  PRO A 469      22.210  20.588  -8.551  1.00 24.83           C
ANISOU 1190  CB  PRO A 469    2946   3078   3409   -120    369   -571       C
ATOM   1191  CG  PRO A 469      20.960  21.302  -8.583  1.00 26.70           C
ANISOU 1191  CG  PRO A 469    3035   3365   3743    -94    434   -668       C
ATOM   1192  CD  PRO A 469      20.505  21.340 -10.031  1.00 25.78           C
ANISOU 1192  CD  PRO A 469    2830   3197   3768    -64    364   -622       C
ATOM   1193  C   PRO A 469      21.549  18.221  -9.098  1.00 25.27           C
ANISOU 1193  C   PRO A 469    3071   3142   3390   -285    412   -407       C
ATOM   1194  O   PRO A 469      20.345  18.033  -8.949  1.00 25.16           O
ANISOU 1194  O   PRO A 469    2965   3199   3396   -348    501   -444       O
ATOM   1195  N   SER A 470      22.455  17.313  -8.793  1.00 24.98           N
ANISOU 1195  N   SER A 470    3182   3064   3245   -314    385   -316       N
ATOM   1196  CA  SER A 470      22.073  16.051  -8.215  1.00 25.82           C
ANISOU 1196  CA  SER A 470    3375   3189   3248   -425    463   -243       C
ATOM   1197  CB  SER A 470      21.885  14.999  -9.301  1.00 25.56           C
ANISOU 1197  CB  SER A 470    3359   3073   3278   -482    430   -169       C
ATOM   1198  OG  SER A 470      21.558  13.741  -8.711  1.00 26.57           O
ANISOU 1198  OG  SER A 470    3590   3189   3315   -600    509    -90       O
ATOM   1199  C   SER A 470      23.142  15.585  -7.255  1.00 25.97           C
ANISOU 1199  C   SER A 470    3556   3199   3112   -413    444   -175       C
ATOM   1200  O   SER A 470      24.333  15.726  -7.510  1.00 24.16           O
ANISOU 1200  O   SER A 470    3385   2915   2880   -333    339   -148       O
ATOM   1201  N   THR A 471      22.695  15.018  -6.149  1.00 27.91           N
ANISOU 1201  N   THR A 471    3869   3513   3224   -495    547   -143       N
ATOM   1202  CA  THR A 471      23.597  14.451  -5.161  1.00 29.38           C
ANISOU 1202  CA  THR A 471    4221   3704   3238   -487    529    -57       C
ATOM   1203  CB  THR A 471      23.171  14.821  -3.704  1.00 30.73           C
ANISOU 1203  CB  THR A 471    4408   4020   3246   -523    638   -106       C
ATOM   1204  OG1 THR A 471      21.791  14.497  -3.513  1.00 33.75           O
ANISOU 1204  OG1 THR A 471    4724   4465   3636   -644    787   -120       O
ATOM   1205  CG2 THR A 471      23.366  16.340  -3.446  1.00 32.23           C
ANISOU 1205  CG2 THR A 471    4493   4284   3469   -432    612   -268       C
ATOM   1206  C   THR A 471      23.718  12.925  -5.361  1.00 29.30           C
ANISOU 1206  C   THR A 471    4350   3591   3193   -555    530     94       C
ATOM   1207  O   THR A 471      24.416  12.246  -4.615  1.00 30.80           O
ANISOU 1207  O   THR A 471    4695   3763   3244   -545    509    197       O
ATOM   1208  N   GLU A 472      23.057  12.397  -6.388  1.00 28.16           N
ANISOU 1208  N   GLU A 472    4152   3371   3176   -619    544    105       N
ATOM   1209  CA  GLU A 472      22.982  10.945  -6.598  1.00 28.80           C
ANISOU 1209  CA  GLU A 472    4360   3336   3246   -706    563    226       C
ATOM   1210  CB  GLU A 472      21.524  10.456  -6.513  1.00 30.19           C
ANISOU 1210  CB  GLU A 472    4475   3546   3451   -873    704    218       C
ATOM   1211  CG  GLU A 472      20.831  10.674  -5.152  1.00 34.77           C
ANISOU 1211  CG  GLU A 472    5053   4266   3892   -953    848    212       C
ATOM   1212  CD  GLU A 472      19.477  11.392  -5.276  1.00 40.82           C
ANISOU 1212  CD  GLU A 472    5606   5160   4744  -1019    952     79       C
ATOM   1213  OE1 GLU A 472      18.438  10.760  -5.008  1.00 43.43           O
ANISOU 1213  OE1 GLU A 472    5909   5526   5067  -1176   1085     99       O
ATOM   1214  OE2 GLU A 472      19.441  12.599  -5.641  1.00 42.85           O
ANISOU 1214  OE2 GLU A 472    5717   5482   5083   -914    904    -45       O
ATOM   1215  C   GLU A 472      23.616  10.535  -7.934  1.00 26.87           C
ANISOU 1215  C   GLU A 472    4128   2959   3124   -647    448    242       C
ATOM   1216  O   GLU A 472      24.293   9.534  -8.021  1.00 26.79           O
ANISOU 1216  O   GLU A 472    4261   2832   3087   -633    404    339       O
ATOM   1217  N   MSE A 473      23.414  11.334  -8.971  1.00 25.30           N
ANISOU 1217  N   MSE A 473    3780   2780   3052   -603    399    145       N
ATOM   1218  CA  MSE A 473      23.895  10.993 -10.300  1.00 23.42           C
ANISOU 1218  CA  MSE A 473    3540   2442   2915   -559    305    147       C
ATOM   1219  CB  MSE A 473      22.729  10.564 -11.227  1.00 24.39           C
ANISOU 1219  CB  MSE A 473    3575   2550   3143   -667    341    105       C
ATOM   1220  CG  MSE A 473      21.879   9.393 -10.755  1.00 22.32           C
ANISOU 1220  CG  MSE A 473    3383   2245   2854   -828    445    157       C
ATOM   1221  SE  MSE A 473      22.758   7.582 -10.747  0.90 27.95          SE
ANISOU 1221  SE  MSE A 473    4356   2738   3528   -855    419    296       SE
ATOM   1222  CE  MSE A 473      23.101   7.399 -12.636  1.00 20.44           C
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Figure 18 (continued)

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ANISOU 1222  CE  MSE A 473     3347   1704   2713   -798    301    216       C
ATOM   1223  C   MSE A 473      24.575  12.199 -10.916  1.00 22.43           C
ANISOU 1223  C   MSE A 473     3320   2354   2848   -433    214     81       C
ATOM   1224  O   MSE A 473      24.300  13.376 -10.550  1.00 22.03           O
ANISOU 1224  O   MSE A 473     3168   2395   2807   -401    232      9       O
ATOM   1225  N   SER A 474      25.430  11.929 -11.891  1.00 20.89           N
ANISOU 1225  N   SER A 474     3156   2083   2699   -366    125     99       N
ATOM   1226  CA  SER A 474      26.072  13.028 -12.627  1.00 19.23           C
ANISOU 1226  CA  SER A 474     2857   1900   2551   -266     47     49       C
ATOM   1227  CB  SER A 474      27.291  13.535 -11.840  1.00 18.96           C
ANISOU 1227  CB  SER A 474     2868   1886   2448   -177      2     61       C
ATOM   1228  OG  SER A 474      27.784  14.746 -12.377  1.00 16.50           O
ANISOU 1228  OG  SER A 474     2462   1603   2203   -107    -50      7       O
ATOM   1229  C   SER A 474      26.509  12.576 -14.024  1.00 18.90           C
ANISOU 1229  C   SER A 474     2818   1792   2572   -236    -19     56       C
ATOM   1230  O   SER A 474      26.803  11.396 -14.234  1.00 17.99           O
ANISOU 1230  O   SER A 474     2805   1592   2438   -253    -27     99       O
ATOM   1231  N   MSE A 475      26.581  13.518 -14.969  1.00 18.62           N
ANISOU 1231  N   MSE A 475     2681   1790   2605   -186    -65     13       N
ATOM   1232  CA  MSE A 475      27.294  13.281 -16.212  1.00 19.11           C
ANISOU 1232  CA  MSE A 475     2751   1815   2697   -138   -129     20       C
ATOM   1233  CB  MSE A 475      27.395  14.576 -17.035  1.00 19.24           C
ANISOU 1233  CB  MSE A 475     2658   1880   2771    -84   -169     -7       C
ATOM   1234  CG  MSE A 475      26.060  14.982 -17.637  1.00 19.93           C
ANISOU 1234  CG  MSE A 475     2644   2015   2915   -127   -159    -41       C
ATOM   1235  SE  MSE A 475      26.115  16.409 -18.957  0.90 21.44          SE
ANISOU 1235  SE  MSE A 475     2727   2246   3173    -52   -225    -41       SE
ATOM   1236  CE  MSE A 475      26.632  17.884 -17.856  1.00 18.53           C
ANISOU 1236  CE  MSE A 475     2330   1873   2838      6   -208    -53       C
ATOM   1237  C   MSE A 475      28.676  12.781 -15.867  1.00 18.97           C
ANISOU 1237  C   MSE A 475     2830   1750   2629    -68   -163     61       C
ATOM   1238  O   MSE A 475      29.338  13.335 -14.995  1.00 18.37           O
ANISOU 1238  O   MSE A 475     2759   1703   2518    -23   -174     68       O
ATOM   1239  N   ARG A 476      29.102  11.717 -16.541  1.00 19.82           N
ANISOU 1239  N   ARG A 476     3007   1787   2736    -55   -185     76       N
ATOM   1240  CA  ARG A 476      30.380  11.052 -16.273  1.00 20.30           C
ANISOU 1240  CA  ARG A 476     3158   1796   2760     27   -221    112       C
ATOM   1241  CB  ARG A 476      30.630  10.005 -17.344  1.00 20.86           C
ANISOU 1241  CB  ARG A 476     3281   1790   2855     42   -238     98       C
ATOM   1242  CG  ARG A 476      32.003   9.337 -17.254  1.00 24.78           C
ANISOU 1242  CG  ARG A 476     3849   2233   3333    153   -279    122       C
ATOM   1243  CD  ARG A 476      32.373   8.494 -18.498  1.00 24.21           C
ANISOU 1243  CD  ARG A 476     3807   2100   3292    190   -293     77       C
ATOM   1244  NE  ARG A 476      31.927   9.009 -19.813  1.00 28.63           N
ANISOU 1244  NE  ARG A 476     4278   2724   3877    152   -291     14       N
ATOM   1245  CZ  ARG A 476      32.680   9.734 -20.648  1.00 28.25           C
ANISOU 1245  CZ  ARG A 476     4147   2758   3829    211   -311    -11       C
ATOM   1246  NH1 ARG A 476      33.921  10.119 -20.292  1.00 26.44           N
ANISOU 1246  NH1 ARG A 476     3889   2565   3593    303   -333      8       N
ATOM   1247  NH2 ARG A 476      32.181  10.089 -21.830  1.00 24.34           N
ANISOU 1247  NH2 ARG A 476     3593   2320   3336    173   -310    -52       N
ATOM   1248  C   ARG A 476      31.621  11.984 -16.096  1.00 19.03           C
ANISOU 1248  C   ARG A 476     2942   1696   2591    121   -269    108       C
ATOM   1249  O   ARG A 476      32.010  12.709 -17.012  1.00 16.62           O
ANISOU 1249  O   ARG A 476     2556   1432   2328    149   -291     79       O
ATOM   1250  N   GLY A 477      32.221  11.942 -14.899  1.00 18.74           N
ANISOU 1250  N   GLY A 477     2952   1671   2495    159   -285    140       N
ATOM   1251  CA  GLY A 477      33.429  12.703 -14.578  1.00 17.97           C
ANISOU 1251  CA  GLY A 477     2803   1637   2389    236   -337    126       C
ATOM   1252  C   GLY A 477      33.226  14.205 -14.333  1.00 17.20           C
ANISOU 1252  C   GLY A 477     2603   1614   2317    207   -329     77       C
ATOM   1253  O   GLY A 477      34.210  14.931 -14.151  1.00 15.87           O
ANISOU 1253  O   GLY A 477     2380   1495   2157    250   -370     52       O
ATOM   1254  N   ILE A 478      31.964  14.675 -14.355  1.00 16.13           N
ANISOU 1254  N   ILE A 478     2436   1485   2208    135   -277     56       N
ATOM   1255  CA  ILE A 478      31.645  16.097 -14.197  1.00 15.15           C
ANISOU 1255  CA  ILE A 478     2221   1406   2129    118   -266      4       C
ATOM   1256  CB  ILE A 478      30.602  16.635 -15.259  1.00 15.06           C
ANISOU 1256  CB  ILE A 478     2137   1385   2200     83   -240    -12       C
ATOM   1257  CG1 ILE A 478      30.870  16.165 -16.718  1.00 12.67           C
ANISOU 1257  CG1 ILE A 478     1829   1058   1927     99   -266     15       C
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Figure 18 (continued)

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ATOM   1258  CD1 ILE A 478      32.254  16.479 -17.326  1.00  8.92           C
ANISOU 1258  CD1 ILE A 478    1332    591   1465    154   -306     24       C
ATOM   1259  CG2 ILE A 478      30.433  18.171 -15.129  1.00 15.73           C
ANISOU 1259  CG2 ILE A 478    2137   1489   2350     90   -237    -59       C
ATOM   1260  C   ILE A 478      31.087  16.390 -12.800  1.00 16.26           C
ANISOU 1260  C   ILE A 478    2381   1587   2209     87   -228    -24       C
ATOM   1261  O   ILE A 478      30.163  15.703 -12.334  1.00 16.78           O
ANISOU 1261  O   ILE A 478    2496   1650   2231     35   -175     -4       O
ATOM   1262  N   ARG A 479      31.657  17.401 -12.128  1.00 16.30           N
ANISOU 1262  N   ARG A 479    2348   1635   2210    108   -251    -77       N
ATOM   1263  CA  ARG A 479      31.158  17.854 -10.825  1.00 16.29           C
ANISOU 1263  CA  ARG A 479    2357   1689   2145     82   -213   -129       C
ATOM   1264  CB  ARG A 479      32.041  17.347  -9.667  1.00 17.20           C
ANISOU 1264  CB  ARG A 479    2549   1855   2130    110   -254   -112       C
ATOM   1265  CG  ARG A 479      32.242  15.837  -9.578  1.00 17.87           C
ANISOU 1265  CG  ARG A 479    2744   1910   2135    125   -266     -8       C
ATOM   1266  CD  ARG A 479      30.940  15.106  -9.170  1.00 19.88           C
ANISOU 1266  CD  ARG A 479    3064   2151   2338     51   -176     33       C
ATOM   1267  NE  ARG A 479      31.198  13.695  -8.923  1.00 22.90           N
ANISOU 1267  NE  ARG A 479    3575   2483   2644     61   -187    138       N
ATOM   1268  CZ  ARG A 479      31.224  12.743  -9.866  1.00 24.84           C
ANISOU 1268  CZ  ARG A 479    3860   2631   2948     66   -195    193       C
ATOM   1269  NH1 ARG A 479      30.991  13.014 -11.161  1.00 21.80           N
ANISOU 1269  NH1 ARG A 479    3392   2208   2681     57   -195    153       N
ATOM   1270  NH2 ARG A 479      31.452  11.491  -9.507  1.00 27.04           N
ANISOU 1270  NH2 ARG A 479    4270   2843   3162     80   -203    287       N
ATOM   1271  C   ARG A 479      31.081  19.369 -10.792  1.00 16.55           C
ANISOU 1271  C   ARG A 479    2300   1729   2259     85   -209   -222       C
ATOM   1272  O   ARG A 479      31.858  20.053 -11.462  1.00 16.48           O
ANISOU 1272  O   ARG A 479    2240   1691   2330    108   -255   -234       O
ATOM   1273  N   VAL A 480      30.163  19.894  -9.992  1.00 17.45           N
ANISOU 1273  N   VAL A 480    2396   1878   2356     59   -149   -289       N
ATOM   1274  CA  VAL A 480      30.056  21.335  -9.776  1.00 17.94           C
ANISOU 1274  CA  VAL A 480    2387   1932   2497     69   -142   -394       C
ATOM   1275  CB  VAL A 480      28.637  21.841 -10.120  1.00 17.22           C
ANISOU 1275  CB  VAL A 480    2229   1821   2494     62    -74   -429       C
ATOM   1276  CG1 VAL A 480      28.491  23.277  -9.739  1.00 18.86           C
ANISOU 1276  CG1 VAL A 480    2378   2004   2783     87    -61   -546       C
ATOM   1277  CG2 VAL A 480      28.341  21.649 -11.590  1.00 16.12           C
ANISOU 1277  CG2 VAL A 480    2051   1622   2451     72    -96   -352       C
ATOM   1278  C   VAL A 480      30.431  21.686  -8.330  1.00 19.46           C
ANISOU 1278  C   VAL A 480    2611   2200   2583     64   -140   -483       C
ATOM   1279  O   VAL A 480      29.897  21.106  -7.379  1.00 20.11           O
ANISOU 1279  O   VAL A 480    2745   2355   2539     41    -90   -485       O
ATOM   1280  N   SER A 481      31.353  22.635  -8.168  1.00 20.47           N
ANISOU 1280  N   SER A 481    2707   2315   2754     77   -194   -558       N
ATOM   1281  CA  SER A 481      31.759  23.081  -6.858  1.00 22.30           C
ANISOU 1281  CA  SER A 481    2960   2626   2887     70   -207   -666       C
ATOM   1282  CB  SER A 481      33.078  23.835  -6.956  1.00 22.36           C
ANISOU 1282  CB  SER A 481    2929   2614   2953     72   -292   -723       C
ATOM   1283  OG  SER A 481      33.419  24.393  -5.699  1.00 24.36           O
ANISOU 1283  OG  SER A 481    3192   2948   3117     58   -312   -855       O
ATOM   1284  C   SER A 481      30.670  23.933  -6.189  1.00 24.56           C
ANISOU 1284  C   SER A 481    3218   2926   3189     60   -123   -791       C
ATOM   1285  O   SER A 481      30.019  24.767  -6.836  1.00 23.76           O
ANISOU 1285  O   SER A 481    3052   2737   3240     74    -89   -829       O
ATOM   1286  N   LYS A 482      30.448  23.692  -4.903  1.00 27.48           N
ANISOU 1286  N   LYS A 482    3637   3408   3395     45    -89   -850       N
ATOM   1287  CA  LYS A 482      29.583  24.554  -4.094  1.00 31.02           C
ANISOU 1287  CA  LYS A 482    4056   3893   3836     41     -6  -1002       C
ATOM   1288  CB  LYS A 482      28.838  23.725  -3.047  1.00 32.27           C
ANISOU 1288  CB  LYS A 482    4275   4186   3798     12     78   -988       C
ATOM   1289  CG  LYS A 482      27.735  22.854  -3.618  1.00 32.74           C
ANISOU 1289  CG  LYS A 482    4325   4232   3881    -11    159   -873       C
ATOM   1290  CD  LYS A 482      27.113  22.055  -2.499  1.00 40.38           C
ANISOU 1290  CD  LYS A 482    5361   5334   4646    -60    252   -853       C
ATOM   1291  CE  LYS A 482      25.586  22.137  -2.501  1.00 43.54           C
ANISOU 1291  CE  LYS A 482    5686   5766   5094    -88    391   -897       C
ATOM   1292  NZ  LYS A 482      25.001  21.133  -1.548  1.00 47.71           N
ANISOU 1292  NZ  LYS A 482    6289   6419   5421   -161    493   -835       N
ATOM   1293  C   LYS A 482      30.357  25.666  -3.391  1.00 33.07           C
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Figure 18 (continued)

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ANISOU 1293  C   LYS A 482     4304   4164   4099     42    -55  -1167      C
ATOM   1294  O   LYS A 482       29.775  26.460  -2.686  1.00 34.72          O
ANISOU 1294  O   LYS A 482     4492   4396   4304     45      7  -1320      O
ATOM   1295  N   MSE A 483       31.670  25.718  -3.556  1.00 34.66          N
ANISOU 1295  N   MSE A 483     4509   4352   4306     37   -163  -1151      N
ATOM   1296  CA  MSE A 483       32.448  26.793  -2.918  1.00 37.65          C
ANISOU 1296  CA  MSE A 483     4866   4739   4700     19   -216  -1322      C
ATOM   1297  CB  MSE A 483       33.914  26.410  -2.812  1.00 37.80          C
ANISOU 1297  CB  MSE A 483     4893   4819   4650      7   -340  -1286      C
ATOM   1298  CG  MSE A 483       34.138  25.073  -2.119  1.00 39.83          C
ANISOU 1298  CG  MSE A 483     5231   5224   4679     26   -372  -1178      C
ATOM   1299 SE   MSE A 483       33.330  25.128  -0.344  0.90 47.98         SE
ANISOU 1299 SE   MSE A 483     6338   6432   5460     13   -299  -1311     SE
ATOM   1300  CE  MSE A 483       34.165  26.683   0.484  1.00 37.03          C
ANISOU 1300  CE  MSE A 483     4897   5079   4093    -21   -371  -1592      C
ATOM   1301  C   MSE A 483       32.325  28.052  -3.738  1.00 38.73          C
ANISOU 1301  C   MSE A 483     4933   4704   5077     19   -203  -1393      C
ATOM   1302  O   MSE A 483       32.588  27.979  -4.960  1.00 38.53          O
ANISOU 1302  O   MSE A 483     4879   4574   5187     23   -229  -1272      O
ATOM   1303  OXT MSE A 483       31.982  29.121  -3.192  1.00 40.68          O
ANISOU 1303  OXT MSE A 483     5163   4914   5380     17   -166  -1568      O
ATOM   1304  N   SER B 320        6.053  17.488 -14.523  1.00 52.35          N
ANISOU 1304  N   SER B 320     7545   5144   7203   2251    154   -336      N
ATOM   1305  CA  SER B 320        6.175  16.006 -14.678  1.00 50.09          C
ANISOU 1305  CA  SER B 320     6969   5155   6909   2037    116   -339      C
ATOM   1306  CB  SER B 320        5.622  15.284 -13.442  1.00 49.98          C
ANISOU 1306  CB  SER B 320     6809   5295   6886   2058    243   -458      C
ATOM   1307  OG  SER B 320        6.227  14.008 -13.284  1.00 47.08          O
ANISOU 1307  OG  SER B 320     6311   5089   6488   1786    217   -488      O
ATOM   1308  C   SER B 320        5.493  15.472 -15.958  1.00 50.02          C
ANISOU 1308  C   SER B 320     6692   5379   6934   2091     11   -208      C
ATOM   1309  O   SER B 320        4.593  16.118 -16.530  1.00 52.10          O
ANISOU 1309  O   SER B 320     6909   5650   7236   2351    -17   -120      O
ATOM   1310  N   SER B 321        5.933  14.292 -16.391  1.00 47.01          N
ANISOU 1310  N   SER B 321     6145   5184   6533   1852    -52   -200      N
ATOM   1311  CA  SER B 321        5.467  13.682 -17.637  1.00 46.52          C
ANISOU 1311  CA  SER B 321     5861   5338   6476   1841   -166    -97      C
ATOM   1312  CB  SER B 321        6.558  13.805 -18.715  1.00 45.54          C
ANISOU 1312  CB  SER B 321     5887   5120   6297   1664   -270    -17      C
ATOM   1313  OG  SER B 321        6.312  12.943 -19.816  1.00 45.99          O
ANISOU 1313  OG  SER B 321     5744   5402   6326   1586   -373     48      O
ATOM   1314  C   SER B 321        5.048  12.212 -17.426  1.00 44.12          C
ANISOU 1314  C   SER B 321     5267   5313   6185   1707   -153   -150      C
ATOM   1315  O   SER B 321        5.732  11.476 -16.721  1.00 42.89          O
ANISOU 1315  O   SER B 321     5134   5155   6007   1511   -100   -235      O
ATOM   1316  N   SER B 322        3.928  11.813 -18.037  1.00 43.82          N
ANISOU 1316  N   SER B 322     4963   5507   6179   1810   -209    -96      N
ATOM   1317  CA  SER B 322        3.371  10.454 -17.924  1.00 42.09          C
ANISOU 1317  CA  SER B 322     4461   5551   5981   1676   -201   -140      C
ATOM   1318  CB  SER B 322        2.114  10.463 -17.059  1.00 43.94          C
ANISOU 1318  CB  SER B 322     4489   5924   6284   1855    -88   -176      C
ATOM   1319  OG  SER B 322        2.445  10.678 -15.713  1.00 46.56          O
ANISOU 1319  OG  SER B 322     4969   6115   6605   1864     69   -271      O
ATOM   1320  C   SER B 322        2.996   9.800 -19.256  1.00 40.57          C
ANISOU 1320  C   SER B 322     4083   5563   5770   1602   -354    -68      C
ATOM   1321  O   SER B 322        2.599  10.477 -20.210  1.00 42.21          O
ANISOU 1321  O   SER B 322     4284   5791   5965   1754   -465     32      O
ATOM   1322  N   PHE B 323        3.081   8.475 -19.284  1.00 36.89          N
ANISOU 1322  N   PHE B 323     3479   5243   5295   1374   -362   -122      N
ATOM   1323  CA  PHE B 323        2.551   7.663 -20.374  1.00 36.10          C
ANISOU 1323  CA  PHE B 323     3178   5364   5176   1279   -495    -90      C
ATOM   1324  CB  PHE B 323        3.513   7.627 -21.574  1.00 34.59          C
ANISOU 1324  CB  PHE B 323     3153   5104   4888   1159   -613    -44      C
ATOM   1325  CG  PHE B 323        4.919   7.274 -21.200  1.00 30.95          C
ANISOU 1325  CG  PHE B 323     2900   4468   4391    973   -541   -102      C
ATOM   1326  CD1 PHE B 323        5.340   5.953 -21.231  1.00 26.79          C
ANISOU 1326  CD1 PHE B 323     2326   4009   3845    748   -533   -173      C
ATOM   1327  CE1 PHE B 323        6.630   5.629 -20.870  1.00 28.42          C
ANISOU 1327  CE1 PHE B 323     2700   4071   4027    608   -472   -218      C
ATOM   1328  CZ  PHE B 323        7.524   6.648 -20.464  1.00 28.42          C
ANISOU 1328  CZ  PHE B 323     2907   3870   4021    662   -426   -198      C
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Figure 18 (continued)

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ATOM   1329  CE2 PHE B 323       7.088   7.988 -20.442  1.00 27.51           C
ANISOU 1329  CE2 PHE B 323    2862   3668   3922    862   -434   -134          C
ATOM   1330  CD2 PHE B 323       5.813   8.277 -20.801  1.00 27.06           C
ANISOU 1330  CD2 PHE B 323    2650   3742   3890   1028   -486    -86          C
ATOM   1331  C   PHE B 323       2.265   6.253 -19.873  1.00 35.08           C
ANISOU 1331  C   PHE B 323    2870   5383   5074   1071   -439   -175          C
ATOM   1332  O   PHE B 323       2.618   5.888 -18.744  1.00 33.74           O
ANISOU 1332  O   PHE B 323    2759   5134   4925    997   -303   -245          O
ATOM   1333  N   SER B 324       1.618   5.474 -20.725  1.00 35.51           N
ANISOU 1333  N   SER B 324    2724   5647   5120    971   -553   -167          N
ATOM   1334  CA  SER B 324       1.270   4.093 -20.446  1.00 35.61           C
ANISOU 1334  CA  SER B 324    2576   5797   5160    747   -521   -240          C
ATOM   1335  CB  SER B 324      -0.200   3.869 -20.791  1.00 38.02           C
ANISOU 1335  CB  SER B 324    2544   6381   5520    785   -594   -217          C
ATOM   1336  OG  SER B 324      -0.802   2.894 -19.960  1.00 41.46           O
ANISOU 1336  OG  SER B 324    2800   6931   6024    634   -483   -279          O
ATOM   1337  C   SER B 324       2.182   3.210 -21.320  1.00 33.97           C
ANISOU 1337  C   SER B 324    2498   5542   4866    521   -606   -273          C
ATOM   1338  O   SER B 324       2.389   3.498 -22.500  1.00 34.44           O
ANISOU 1338  O   SER B 324    2615   5622   4850    539   -742   -227          O
ATOM   1339  N   PHE B 325       2.760   2.167 -20.734  1.00 31.78           N
ANISOU 1339  N   PHE B 325    2289   5194   4592    327   -518   -348          N
ATOM   1340  CA  PHE B 325       3.513   1.176 -21.491  1.00 29.85           C
ANISOU 1340  CA  PHE B 325    2148   4915   4278    124   -577   -395          C
ATOM   1341  CB  PHE B 325       4.972   1.610 -21.693  1.00 28.12           C
ANISOU 1341  CB  PHE B 325    2192   4498   3995    143   -561   -383          C
ATOM   1342  CG  PHE B 325       5.770   0.673 -22.571  1.00 26.86           C
ANISOU 1342  CG  PHE B 325    2137   4311   3757    -27   -608   -429          C
ATOM   1343  CD1 PHE B 325       5.458   0.518 -23.931  1.00 28.72           C
ANISOU 1343  CD1 PHE B 325    2340   4663   3908    -68   -746   -422          C
ATOM   1344  CE1 PHE B 325       6.190  -0.356 -24.743  1.00 28.43           C
ANISOU 1344  CE1 PHE B 325    2420   4597   3784   -214   -772   -481          C
ATOM   1345  CZ  PHE B 325       7.263  -1.082 -24.196  1.00 26.96           C
ANISOU 1345  CZ  PHE B 325    2368   4261   3612   -302   -660   -539          C
ATOM   1346  CE2 PHE B 325       7.581  -0.933 -22.850  1.00 23.52           C
ANISOU 1346  CE2 PHE B 325    1951   3720   3265   -259   -543   -533          C
ATOM   1347  CD2 PHE B 325       6.831  -0.057 -22.045  1.00 25.04           C
ANISOU 1347  CD2 PHE B 325    2043   3944   3527   -131   -518   -483          C
ATOM   1348  C   PHE B 325       3.456  -0.162 -20.770  1.00 29.26           C
ANISOU 1348  C   PHE B 325    2036   4838   4242    -75   -486   -471          C
ATOM   1349  O   PHE B 325       3.759  -0.239 -19.586  1.00 27.73           O
ANISOU 1349  O   PHE B 325    1904   4545   4086    -67   -351   -485          O
ATOM   1350  N   GLY B 326       3.028  -1.202 -21.487  1.00 30.19           N
ANISOU 1350  N   GLY B 326    2067   5063   4339   -256   -565   -518          N
ATOM   1351  CA  GLY B 326       2.970  -2.562 -20.950  1.00 30.07           C
ANISOU 1351  CA  GLY B 326    2049   5020   4356   -471   -488   -587          C
ATOM   1352  C   GLY B 326       2.057  -2.782 -19.754  1.00 31.33           C
ANISOU 1352  C   GLY B 326    2041   5253   4609   -494   -364   -580          C
ATOM   1353  O   GLY B 326       2.288  -3.706 -18.964  1.00 30.80           O
ANISOU 1353  O   GLY B 326    2046   5095   4563   -612   -253   -612          O
ATOM   1354  N   GLY B 327       1.029  -1.938 -19.624  1.00 32.09           N
ANISOU 1354  N   GLY B 327    1922   5515   4756   -348   -374   -531          N
ATOM   1355  CA  GLY B 327       0.118  -1.987 -18.486  1.00 33.34           C
ANISOU 1355  CA  GLY B 327    1900   5769   4998   -337   -231   -519          C
ATOM   1356  C   GLY B 327       0.542  -1.183 -17.265  1.00 31.95           C
ANISOU 1356  C   GLY B 327    1846   5467   4829   -154    -76   -495          C
ATOM   1357  O   GLY B 327      -0.117  -1.257 -16.216  1.00 33.59           O
ANISOU 1357  O   GLY B 327    1940   5738   5083   -142     73   -490          O
ATOM   1358  N   PHE B 328       1.609  -0.399 -17.411  1.00 29.32           N
ANISOU 1358  N   PHE B 328    1738   4962   4439   -107   -107   -482          N
ATOM   1359  CA  PHE B 328       2.156   0.428 -16.338  1.00 28.13           C
ANISOU 1359  CA  PHE B 328    1744   4669   4277    135     12   -473          C
ATOM   1360  CB  PHE B 328       3.628   0.057 -16.050  1.00 25.60           C
ANISOU 1360  CB  PHE B 328    1698   4135   3894     50    27   -499          C
ATOM   1361  CG  PHE B 328       3.793  -1.258 -15.358  1.00 25.59           C
ANISOU 1361  CG  PHE B 328    1733   4099   3890   -141    113   -529          C
ATOM   1362  CD1 PHE B 328       3.840  -1.329 -13.968  1.00 25.50           C
ANISOU 1362  CD1 PHE B 328    1790   4033   3866   -125    261   -531          C
ATOM   1363  CE1 PHE B 328       3.965  -2.559 -13.319  1.00 24.09           C
ANISOU 1363  CE1 PHE B 328    1665   3812   3675   -297    342   -539          C
ATOM   1364  CZ  PHE B 328       4.054  -3.706 -14.047  1.00 24.40           C
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Figure 18 (continued)

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ANISOU 1364  CZ  PHE B 328     1699   3843   3728   -482    279   -556  C
ATOM   1365  CE2 PHE B 328       4.005  -3.655 -15.450  1.00 25.53      C
ANISOU 1365  CE2 PHE B 328     1777   4043   3882   -505    132   -574  C
ATOM   1366  CD2 PHE B 328       3.876  -2.433 -16.092  1.00 24.35      C
ANISOU 1366  CD2 PHE B 328     1565   3954   3731   -335     49   -556  C
ATOM   1367  C   PHE B 328       2.093   1.894 -16.718  1.00 28.62      C
ANISOU 1367  C   PHE B 328     1826   4711   4336    382    -44   -429  C
ATOM   1368  O   PHE B 328       2.399   2.262 -17.854  1.00 28.17      O
ANISOU 1368  O   PHE B 328     1811   4646   4248    412   -185   -399  O
ATOM   1369  N   THR B 329       1.690   2.727 -15.760  1.00 29.74      N
ANISOU 1369  N   THR B 329     1959   4837   4502    563     74   -425  N
ATOM   1370  CA  THR B 329       1.801   4.169 -15.900  1.00 29.75      C
ANISOU 1370  CA  THR B 329     2059   4747   4498    808     49   -391  C
ATOM   1371  CB  THR B 329       0.751   4.914 -15.031  1.00 32.29      C
ANISOU 1371  CB  THR B 329     2253   5145   4871   1029    182   -390  C
ATOM   1372  OG1 THR B 329      -0.576   4.482 -15.374  1.00 31.53      O
ANISOU 1372  OG1 THR B 329     1818   5316   4846   1033    168   -364  O
ATOM   1373  CG2 THR B 329       0.846   6.411 -15.230  1.00 31.75      C
ANISOU 1373  CG2 THR B 329     2316   4948   4799   1297    153   -356  C
ATOM   1374  C   THR B 329       3.223   4.532 -15.485  1.00 28.41      C
ANISOU 1374  C   THR B 329     2200   4331   4263    781     67   -416  C
ATOM   1375  O   THR B 329       3.629   4.259 -14.350  1.00 29.14      O
ANISOU 1375  O   THR B 329     2399   4343   4330    729    183   -463  O
ATOM   1376  N   PHE B 330       3.995   5.073 -16.429  1.00 27.40      N
ANISOU 1376  N   PHE B 330     2210   4099   4102    796    -52   -380  N
ATOM   1377  CA  PHE B 330       5.301   5.664 -16.167  1.00 25.35      C
ANISOU 1377  CA  PHE B 330     2219   3620   3794    784    -48   -393  C
ATOM   1378  CB  PHE B 330       6.178   5.570 -17.410  1.00 24.18      C
ANISOU 1378  CB  PHE B 330     2153   3429   3605    684   -174   -355  C
ATOM   1379  CG  PHE B 330       6.737   4.194 -17.671  1.00 21.46      C
ANISOU 1379  CG  PHE B 330     1782   3132   3238    468   -193   -390  C
ATOM   1380  CD1 PHE B 330       8.110   3.963 -17.574  1.00 18.03      C
ANISOU 1380  CD1 PHE B 330     1514   2572   2767    358   -191   -410  C
ATOM   1381  CE1 PHE B 330       8.642   2.682 -17.836  1.00 18.22      C
ANISOU 1381  CE1 PHE B 330     1523   2625   2773    192   -201   -442  C
ATOM   1382  CZ  PHE B 330       7.787   1.630 -18.182  1.00 18.84      C
ANISOU 1382  CZ  PHE B 330     1451   2841   2869    110   -215   -462  C
ATOM   1383  CE2 PHE B 330       6.396   1.859 -18.267  1.00 18.39      C
ANISOU 1383  CE2 PHE B 330     1214   2923   2849    186   -226   -444  C
ATOM   1384  CD2 PHE B 330       5.895   3.134 -18.019  1.00 20.38      C
ANISOU 1384  CD2 PHE B 330     1457   3165   3123    377   -214   -404  C
ATOM   1385  C   PHE B 330       5.142   7.118 -15.831  1.00 27.08      C
ANISOU 1385  C   PHE B 330     2554   3714   4019   1002    -15   -376  C
ATOM   1386  O   PHE B 330       4.443   7.841 -16.532  1.00 28.76      O
ANISOU 1386  O   PHE B 330     2699   3969   4258   1167    -72   -316  O
ATOM   1387  N   LYS B 331       5.795   7.544 -14.756  1.00 27.03      N
ANISOU 1387  N   LYS B 331     2738   3549   3983   1008     70   -432  N
ATOM   1388  CA  LYS B 331       5.856   8.956 -14.420  1.00 29.58      C
ANISOU 1388  CA  LYS B 331     3242   3697   4301   1189    100   -435  C
ATOM   1389  CB  LYS B 331       5.064   9.247 -13.135  1.00 30.49      C
ANISOU 1389  CB  LYS B 331     3344   3823   4419   1336    253   -500  C
ATOM   1390  CG  LYS B 331       5.276  10.638 -12.593  1.00 34.42      C
ANISOU 1390  CG  LYS B 331     4088   4096   4893   1503    301   -536  C
ATOM   1391  CD  LYS B 331       4.335  10.970 -11.437  1.00 37.48      C
ANISOU 1391  CD  LYS B 331     4452   4511   5276   1692    469   -604  C
ATOM   1392  CE  LYS B 331       4.357  12.470 -11.157  1.00 44.58      C
ANISOU 1392  CE  LYS B 331     5601   5174   6164   1907    508   -635  C
ATOM   1393  NZ  LYS B 331       3.272  12.887 -10.223  1.00 50.24      N
ANISOU 1393  NZ  LYS B 331     6274   5932   6884   2152    684   -696  N
ATOM   1394  C   LYS B 331       7.324   9.355 -14.298  1.00 28.10      C
ANISOU 1394  C   LYS B 331     3311   3304   4062   1062     61   -456  C
ATOM   1395  O   LYS B 331       8.037   8.798 -13.466  1.00 27.89      O
ANISOU 1395  O   LYS B 331     3352   3249   3997    924     98   -517  O
ATOM   1396  N   ARG B 332       7.787  10.293 -15.132  1.00 28.13      N
ANISOU 1396  N   ARG B 332     3451   3172   4064   1099    -16   -397  N
ATOM   1397  CA  ARG B 332       9.184  10.755 -15.057  1.00 27.45      C
ANISOU 1397  CA  ARG B 332     3590   2899   3940    958    -50   -412  C
ATOM   1398  CB  ARG B 332       9.671  11.403 -16.367  1.00 27.67      C
ANISOU 1398  CB  ARG B 332     3703   2846   3966    939   -143   -313  C
ATOM   1399  CG  ARG B 332      11.213  11.679 -16.389  1.00 27.23      C
ANISOU 1399  CG  ARG B 332     3826   2642   3879    736   -173   -321  C
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Figure 18 (continued)

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ATOM   1400  CD  ARG B 332      11.712  12.014 -17.789  1.00 28.39           C
ANISOU 1400  CD  ARG B 332    4015   2763   4011    677   -245   -212       C
ATOM   1401  NE  ARG B 332      11.084  13.243 -18.288  1.00 31.78           N
ANISOU 1401  NE  ARG B 332    4571   3058   4448    859   -260   -132       N
ATOM   1402  CZ  ARG B 332      11.095  13.644 -19.557  1.00 31.92           C
ANISOU 1402  CZ  ARG B 332    4626   3063   4438    881   -322    -10       C
ATOM   1403  NH1 ARG B 332      11.702  12.900 -20.497  1.00 29.06           N
ANISOU 1403  NH1 ARG B 332    4180   2829   4034    723   -365     33       N
ATOM   1404  NH2 ARG B 332      10.480  14.783 -19.881  1.00 27.89           N
ANISOU 1404  NH2 ARG B 332    4251   2412   3935   1075   -335     69       N
ATOM   1405  C   ARG B 332       9.449  11.702 -13.890  1.00 28.06           C
ANISOU 1405  C   ARG B 332    3890   2780   3993   1015     19   -492       C
ATOM   1406  O   ARG B 332       8.854  12.786 -13.811  1.00 29.26           O
ANISOU 1406  O   ARG B 332    4150   2809   4160   1208     53   -486       O
ATOM   1407  N   THR B 333      10.387  11.304 -13.020  1.00 26.57           N
ANISOU 1407  N   THR B 333    3782   2555   3757    850     30   -566       N
ATOM   1408  CA  THR B 333      10.701  12.072 -11.806  1.00 27.14           C
ANISOU 1408  CA  THR B 333    4076   2459   3779    868     83   -664       C
ATOM   1409  CB  THR B 333      10.605  11.185 -10.551  1.00 26.57           C
ANISOU 1409  CB  THR B 333    3954   2494   3648    824    153   -747       C
ATOM   1410  OG1 THR B 333      11.447  10.029 -10.706  1.00 26.24           O
ANISOU 1410  OG1 THR B 333    3808   2566   3597    626     88   -725       O
ATOM   1411  CG2 THR B 333       9.165  10.725 -10.341  1.00 27.09           C
ANISOU 1411  CG2 THR B 333    3835   2720   3738    992    259   -741       C
ATOM   1412  C   THR B 333      12.062  12.825 -11.844  1.00 26.96           C
ANISOU 1412  C   THR B 333    4273   2240   3731    703      8   -680       C
ATOM   1413  O   THR B 333      12.273  13.724 -11.056  1.00 27.63           O
ANISOU 1413  O   THR B 333    4577   2144   3775    722     33   -758       O
ATOM   1414  N   SER B 334      12.957  12.454 -12.768  1.00 25.38           N
ANISOU 1414  N   SER B 334    4008   2081   3552    536    -76   -610       N
ATOM   1415  CA  SER B 334      14.274  13.108 -12.964  1.00 25.51           C
ANISOU 1415  CA  SER B 334    4182   1950   3561    351   -143   -605       C
ATOM   1416  CB  SER B 334      15.373  12.428 -12.171  1.00 24.37           C
ANISOU 1416  CB  SER B 334    4014   1868   3377    157   -184   -671       C
ATOM   1417  OG  SER B 334      15.537  13.002 -10.926  1.00 29.53           O
ANISOU 1417  OG  SER B 334    4850   2400   3971    145   -173   -780       O
ATOM   1418  C   SER B 334      14.705  12.915 -14.375  1.00 24.24           C
ANISOU 1418  C   SER B 334    3928   1847   3436    271   -195   -492       C
ATOM   1419  O   SER B 334      14.323  11.934 -15.016  1.00 22.59           O
ANISOU 1419  O   SER B 334    3521   1822   3240    295   -199   -445       O
ATOM   1420  N   GLY B 335      15.562  13.811 -14.833  1.00 24.97           N
ANISOU 1420  N   GLY B 335    4172   1782   3533    151   -230   -453       N
ATOM   1421  CA  GLY B 335      16.223  13.648 -16.116  1.00 24.84           C
ANISOU 1421  CA  GLY B 335    4086   1821   3529     33   -264   -347       C
ATOM   1422  C   GLY B 335      15.352  14.058 -17.286  1.00 25.60           C
ANISOU 1422  C   GLY B 335    4192   1905   3631    188   -262   -234       C
ATOM   1423  O   GLY B 335      14.281  14.625 -17.106  1.00 27.00           O
ANISOU 1423  O   GLY B 335    4436   2007   3818    395   -241   -231       O
ATOM   1424  N   SER B 336      15.838  13.762 -18.487  1.00 25.43           N
ANISOU 1424  N   SER B 336    4099   1967   3594     95   -285   -138       N
ATOM   1425  CA  SER B 336      15.225  14.169 -19.749  1.00 26.34           C
ANISOU 1425  CA  SER B 336    4242   2078   3686    207   -303    -11       C
ATOM   1426  CB  SER B 336      15.484  15.656 -20.048  1.00 28.83           C
ANISOU 1426  CB  SER B 336    4827   2128   3998    202   -299     68       C
ATOM   1427  OG  SER B 336      16.856  16.025 -19.901  1.00 30.57           O
ANISOU 1427  OG  SER B 336    5147   2245   4224    -53   -286     57       O
ATOM   1428  C   SER B 336      15.816  13.280 -20.832  1.00 25.42           C
ANISOU 1428  C   SER B 336    3985   2145   3531     81   -316     46       C
ATOM   1429  O   SER B 336      16.779  12.541 -20.571  1.00 23.98           O
ANISOU 1429  O   SER B 336    3706   2050   3355    -85   -301     -9       O
ATOM   1430  N   SER B 337      15.231  13.301 -22.031  1.00 25.43           N
ANISOU 1430  N   SER B 337    3968   2213   3481    171   -346    151       N
ATOM   1431  CA  SER B 337      15.828  12.576 -23.140  1.00 24.60           C
ANISOU 1431  CA  SER B 337    3774   2261   3312     52   -346    201       C
ATOM   1432  CB  SER B 337      15.457  11.084 -23.140  1.00 23.13           C
ANISOU 1432  CB  SER B 337    3365   2304   3120     64   -359    122       C
ATOM   1433  OG  SER B 337      14.075  10.828 -23.373  1.00 25.51           O
ANISOU 1433  OG  SER B 337    3581   2702   3411    240   -413    131       O
ATOM   1434  C   SER B 337      15.505  13.216 -24.460  1.00 26.16           C
ANISOU 1434  C   SER B 337    4078   2434   3427    115   -376    348       C
ATOM   1435  O   SER B 337      14.583  14.017 -24.556  1.00 27.15                O
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Figure 18 (continued)

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ANISOU 1435  O   SER B 337     4301   2463   3552    294   -417    413      O
ATOM   1436  N   ILE B 338      16.325  12.882 -25.455  1.00 26.35           N
ANISOU 1436  N   ILE B 338     4093   2544   3376    -27   -349    404      N
ATOM   1437  CA  ILE B 338      16.075  13.222 -26.849  1.00 27.55           C
ANISOU 1437  CA  ILE B 338     4332   2727   3410     14   -377    545      C
ATOM   1438  CB  ILE B 338      17.191  14.129 -27.454  1.00 28.81           C
ANISOU 1438  CB  ILE B 338     4678   2747   3523   -152   -306    660      C
ATOM   1439  CG1 ILE B 338      18.579  13.472 -27.383  1.00 26.68           C
ANISOU 1439  CG1 ILE B 338     4302   2568   3268   -384   -214    597      C
ATOM   1440  CD1 ILE B 338      19.665  14.286 -28.122  1.00 28.93           C
ANISOU 1440  CD1 ILE B 338     4733   2760   3499   -571   -128    723      C
ATOM   1441  CG2 ILE B 338      17.170  15.486 -26.777  1.00 29.60           C
ANISOU 1441  CG2 ILE B 338     4987   2564   3694   -128   -302    701      C
ATOM   1442  C   ILE B 338      15.884  11.899 -27.586  1.00 26.88           C
ANISOU 1442  C   ILE B 338     4074   2894   3245      3   -398    501      C
ATOM   1443  O   ILE B 338      16.186  10.856 -27.040  1.00 24.81           O
ANISOU 1443  O   ILE B 338     3658   2737   3031    -63   -370    378      O
ATOM   1444  N   LYS B 339      15.351  11.936 -28.800  1.00 29.34           N
ANISOU 1444  N   LYS B 339     4428   3294   3428     73   -455    600      N
ATOM   1445  CA  LYS B 339      15.109  10.715 -29.550  1.00 29.97           C
ANISOU 1445  CA  LYS B 339     4375   3601   3413     56   -486    546      C
ATOM   1446  CB  LYS B 339      13.657  10.595 -30.002  1.00 31.00           C
ANISOU 1446  CB  LYS B 339     4446   3844   3489    232   -625    574      C
ATOM   1447  CG  LYS B 339      12.575  10.731 -28.976  1.00 33.08           C
ANISOU 1447  CG  LYS B 339     4606   4083   3882    388   -683    524      C
ATOM   1448  CD  LYS B 339      11.246  10.804 -29.743  1.00 39.25           C
ANISOU 1448  CD  LYS B 339     5331   4998   4584    558   -828    596      C
ATOM   1449  CE  LYS B 339      10.060  11.092 -28.864  1.00 42.38           C
ANISOU 1449  CE  LYS B 339     5609   5391   5103    748   -881    574      C
ATOM   1450  NZ  LYS B 339       8.914  11.502 -29.728  1.00 47.09           N
ANISOU 1450  NZ  LYS B 339     6177   6097   5618    936  -1030    689      N
ATOM   1451  C   LYS B 339      15.927  10.747 -30.817  1.00 31.76           C
ANISOU 1451  C   LYS B 339     4705   3878   3485    -58   -431    632      C
ATOM   1452  O   LYS B 339      16.135  11.812 -31.422  1.00 33.75           O
ANISOU 1452  O   LYS B 339     5140   4018   3664    -59   -419    782      O
ATOM   1453  N   ARG B 340      16.350   9.566 -31.237  1.00 31.26           N
ANISOU 1453  N   ARG B 340     4539   3977   3361   -146   -389    540      N
ATOM   1454  CA  ARG B 340      16.998   9.401 -32.494  1.00 33.42           C
ANISOU 1454  CA  ARG B 340     4895   4340   3462   -234   -327    598      C
ATOM   1455  CB  ARG B 340      18.495   9.339 -32.275  1.00 33.24           C
ANISOU 1455  CB  ARG B 340     4857   4283   3488   -401   -164    576      C
ATOM   1456  CG  ARG B 340      19.324   9.305 -33.537  1.00 37.60           C
ANISOU 1456  CG  ARG B 340     5499   4922   3866   -502    -54    648      C
ATOM   1457  CD  ARG B 340      20.659   8.729 -33.170  1.00 40.36           C
ANISOU 1457  CD  ARG B 340     5728   5314   4294   -636    100    564      C
ATOM   1458  NE  ARG B 340      21.646   8.866 -34.226  1.00 47.19           N
ANISOU 1458  NE  ARG B 340     6660   6250   5019   -750    249    643      N
ATOM   1459  CZ  ARG B 340      22.821   8.236 -34.223  1.00 50.98           C
ANISOU 1459  CZ  ARG B 340     7018   6824   5528   -847    401    575      C
ATOM   1460  NH1 ARG B 340      23.142   7.436 -33.197  1.00 49.64           N
ANISOU 1460  NH1 ARG B 340     6666   6673   5521   -835    403    436      N
ATOM   1461  NH2 ARG B 340      23.677   8.409 -35.235  1.00 52.82           N
ANISOU 1461  NH2 ARG B 340     7309   7137   5623   -947    557    654      N
ATOM   1462  C   ARG B 340      16.484   8.111 -33.093  1.00 33.37           C
ANISOU 1462  C   ARG B 340     4794   4530   3355   -214   -380    492      C
ATOM   1463  O   ARG B 340      16.559   7.042 -32.483  1.00 31.57           O
ANISOU 1463  O   ARG B 340     4424   4358   3211   -242   -359    344      O
ATOM   1464  N   GLU B 341      15.934   8.230 -34.287  1.00 35.28           N
ANISOU 1464  N   GLU B 341     5133   4866   3405   -168   -458    572      N
ATOM   1465  CA  GLU B 341      15.436   7.081 -34.986  1.00 35.48           C
ANISOU 1465  CA  GLU B 341     5103   5074   3304   -171   -522    469      C
ATOM   1466  CB  GLU B 341      14.512   7.527 -36.105  1.00 37.67           C
ANISOU 1466  CB  GLU B 341     5486   5442   3384    -83   -672    584      C
ATOM   1467  CG  GLU B 341      14.003   6.403 -36.917  1.00 39.18           C
ANISOU 1467  CG  GLU B 341     5645   5825   3415   -110   -756    475      C
ATOM   1468  CD  GLU B 341      12.728   6.772 -37.589  1.00 43.97           C
ANISOU 1468  CD  GLU B 341     6272   6540   3896      5   -971    563      C
ATOM   1469  OE1 GLU B 341      12.775   7.040 -38.814  1.00 45.83           O
ANISOU 1469  OE1 GLU B 341     6670   6857   3888      4  -1010    659      O
ATOM   1470  OE2 GLU B 341      11.690   6.807 -36.876  1.00 44.98           O
ANISOU 1470  OE2 GLU B 341     6245   6681   4165    102  -1097    541      O
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Figure 18 (continued)

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ATOM   1471  C   GLU B 341      16.615   6.290 -35.516  1.00 35.17           C
ANISOU 1471  C   GLU B 341    5086   5099   3177   -298   -363    393       C
ATOM   1472  O   GLU B 341      17.472   6.835 -36.209  1.00 37.32           O
ANISOU 1472  O   GLU B 341    5483   5357   3339   -362   -251    492       O
ATOM   1473  N   GLU B 342      16.644   5.013 -35.154  1.00 33.75           N
ANISOU 1473  N   GLU B 342    4787   4983   3052   -329   -342    219       N
ATOM   1474  CA  GLU B 342      17.705   4.076 -35.501  1.00 33.58           C
ANISOU 1474  CA  GLU B 342    4763   5018   2979   -412   -187    115       C
ATOM   1475  CB  GLU B 342      18.534   3.739 -34.259  1.00 32.29           C
ANISOU 1475  CB  GLU B 342    4466   4768   3036   -442    -80     40       C
ATOM   1476  CG  GLU B 342      19.606   4.754 -33.977  1.00 34.89           C
ANISOU 1476  CG  GLU B 342    4812   5012   3434   -500     36    153       C
ATOM   1477  CD  GLU B 342      20.496   4.362 -32.851  1.00 37.32           C
ANISOU 1477  CD  GLU B 342    4979   5269   3931   -536    124     77       C
ATOM   1478  OE1 GLU B 342      20.843   5.278 -32.069  1.00 41.51           O
ANISOU 1478  OE1 GLU B 342    5491   5694   4587   -569    129    148       O
ATOM   1479  OE2 GLU B 342      20.843   3.159 -32.724  1.00 37.32           O
ANISOU 1479  OE2 GLU B 342    4900   5327   3954   -527    180    -53       O
ATOM   1480  C   GLU B 342      17.091   2.790 -35.997  1.00 33.24           C
ANISOU 1480  C   GLU B 342    4709   5088   2833   -414   -253    -36       C
ATOM   1481  O   GLU B 342      15.936   2.497 -35.709  1.00 32.03           O
ANISOU 1481  O   GLU B 342    4490   4961   2718   -376   -409    -82       O
ATOM   1482  N   GLU B 343      17.874   2.026 -36.750  1.00 33.79           N
ANISOU 1482  N   GLU B 343    4844   5224   2771   -463   -125   -118       N
ATOM   1483  CA  GLU B 343      17.505   0.666 -37.091  1.00 33.29           C
ANISOU 1483  CA  GLU B 343    4790   5227   2632   -481   -154   -296       C
ATOM   1484  CB  GLU B 343      17.416   0.491 -38.604  1.00 36.07           C
ANISOU 1484  CB  GLU B 343    5318   5705   2683   -507   -163   -306       C
ATOM   1485  CG  GLU B 343      16.227   1.164 -39.223  1.00 38.05           C
ANISOU 1485  CG  GLU B 343    5629   6034   2792   -482   -375   -205       C
ATOM   1486  CD  GLU B 343      16.323   1.206 -40.720  1.00 44.38           C
ANISOU 1486  CD  GLU B 343    6631   6962   3270   -507   -371   -179       C
ATOM   1487  OE1 GLU B 343      17.386   1.640 -41.255  1.00 46.93           O
ANISOU 1487  OE1 GLU B 343    7056   7285   3489   -524   -186   -100       O
ATOM   1488  OE2 GLU B 343      15.327   0.808 -41.360  1.00 46.73           O
ANISOU 1488  OE2 GLU B 343    6979   7369   3409   -518   -553   -236       O
ATOM   1489  C   GLU B 343      18.493  -0.319 -36.484  1.00 31.64           C
ANISOU 1489  C   GLU B 343    4511   4962   2549   -492     10   -426       C
ATOM   1490  O   GLU B 343      19.706  -0.165 -36.609  1.00 31.47           O
ANISOU 1490  O   GLU B 343    4491   4938   2528   -499    188   -397       O
ATOM   1491  N   VAL B 344      17.937  -1.331 -35.831  1.00 30.29           N
ANISOU 1491  N   VAL B 344    4273   4751   2484   -492    -54   -560       N
ATOM   1492  CA  VAL B 344      18.689  -2.310 -35.054  1.00 28.25           C
ANISOU 1492  CA  VAL B 344    3947   4413   2372   -477     67   -673       C
ATOM   1493  CB  VAL B 344      18.436  -2.166 -33.514  1.00 26.46           C
ANISOU 1493  CB  VAL B 344    3570   4085   2396   -456     14   -647       C
ATOM   1494  CG1 VAL B 344      18.841  -0.786 -33.009  1.00 25.57           C
ANISOU 1494  CG1 VAL B 344    3398   3945   2372   -442     27   -489       C
ATOM   1495  CG2 VAL B 344      16.977  -2.489 -33.150  1.00 24.38           C
ANISOU 1495  CG2 VAL B 344    3272   3821   2170   -479   -160   -691       C
ATOM   1496  C   VAL B 344      18.313  -3.718 -35.484  1.00 28.72           C
ANISOU 1496  C   VAL B 344    4091   4473   2347   -501     54   -854       C
ATOM   1497  O   VAL B 344      17.259  -3.928 -36.106  1.00 29.90           O
ANISOU 1497  O   VAL B 344    4309   4683   2368   -553    -89   -899       O
ATOM   1498  N   LEU B 345      19.158  -4.685 -35.122  1.00 27.67           N
ANISOU 1498  N   LEU B 345    3954   4268   2292   -464    195   -959       N
ATOM   1499  CA  LEU B 345      19.009  -6.054 -35.598  1.00 28.06           C
ANISOU 1499  CA  LEU B 345    4127   4281   2253   -479    220  -1141       C
ATOM   1500  CB  LEU B 345      20.251  -6.481 -36.379  1.00 28.98           C
ANISOU 1500  CB  LEU B 345    4335   4421   2254   -413    431  -1204       C
ATOM   1501  CG  LEU B 345      20.407  -5.803 -37.751  1.00 30.75           C
ANISOU 1501  CG  LEU B 345    4677   4787   2220   -439    469  -1154       C
ATOM   1502  CD1 LEU B 345      21.733  -6.157 -38.415  1.00 30.52           C
ANISOU 1502  CD1 LEU B 345    4708   4796   2093   -363    717  -1205       C
ATOM   1503  CD2 LEU B 345      19.278  -6.215 -38.670  1.00 32.27           C
ANISOU 1503  CD2 LEU B 345    5033   5030   2199   -522    316  -1251       C
ATOM   1504  C   LEU B 345      18.720  -6.985 -34.436  1.00 27.04           C
ANISOU 1504  C   LEU B 345    3939   4015   2320   -476    193  -1220       C
ATOM   1505  O   LEU B 345      19.387  -6.910 -33.389  1.00 25.76           O
ANISOU 1505  O   LEU B 345    3661   3784   2342   -410    262  -1167       O
ATOM   1506  N   THR B 346      17.695  -7.823 -34.588  1.00 26.96           N
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Figure 18 (continued)

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ANISOU 1506  N   THR B 346     4007   3970   2268   -562     81  -1336       N
ATOM   1507  CA  THR B 346      17.350  -8.749 -33.512  1.00 26.28           C
ANISOU 1507  CA  THR B 346     3888   3741   2355   -582     62  -1403       C
ATOM   1508  CB  THR B 346      15.887  -9.268 -33.635  1.00 26.91           C
ANISOU 1508  CB  THR B 346     4000   3826   2400   -731   -111  -1483       C
ATOM   1509  OG1 THR B 346      15.764 -10.147 -34.762  1.00 25.20           O
ANISOU 1509  OG1 THR B 346     3979   3603   1992   -799   -110  -1646       O
ATOM   1510  CG2 THR B 346      14.906  -8.098 -33.746  1.00 25.10           C
ANISOU 1510  CG2 THR B 346     3644   3748   2145   -775   -277  -1361       C
ATOM   1511  C   THR B 346      18.348  -9.919 -33.460  1.00 27.87           C
ANISOU 1511  C   THR B 346     4198   3808   2581   -499    229  -1520       C
ATOM   1512  O   THR B 346      19.239 -10.033 -34.325  1.00 29.40           O
ANISOU 1512  O   THR B 346     4483   4038   2650   -427    363  -1567       O
ATOM   1513  N   GLY B 347      18.192 -10.779 -32.459  1.00 27.20           N
ANISOU 1513  N   GLY B 347     4111   3571   2653   -499    231  -1563       N
ATOM   1514  CA  GLY B 347      18.936 -12.031 -32.387  1.00 29.00           C
ANISOU 1514  CA  GLY B 347     4473   3639   2908   -413    367  -1680       C
ATOM   1515  C   GLY B 347      18.678 -12.996 -33.546  1.00 32.22           C
ANISOU 1515  C   GLY B 347     5117   3994   3132   -473    386  -1868       C
ATOM   1516  O   GLY B 347      19.373 -14.017 -33.671  1.00 33.15           O
ANISOU 1516  O   GLY B 347     5381   3967   3245   -376    523  -1981       O
ATOM   1517  N   ASN B 348      17.675 -12.677 -34.381  1.00 32.97           N
ANISOU 1517  N   ASN B 348     5255   4201   3069   -625    248  -1904       N
ATOM   1518  CA  ASN B 348      17.405 -13.400 -35.631  1.00 35.54           C
ANISOU 1518  CA  ASN B 348     5814   4519   3172   -705    242  -2083       C
ATOM   1519  CB  ASN B 348      15.971 -13.938 -35.629  1.00 36.61           C
ANISOU 1519  CB  ASN B 348     5999   4622   3290   -925     51  -2171       C
ATOM   1520  CG  ASN B 348      15.795 -15.108 -36.571  1.00 39.61           C
ANISOU 1520  CG  ASN B 348     6662   4895   3493  -1018     63  -2399       C
ATOM   1521  OD1 ASN B 348      16.626 -16.016 -36.596  1.00 43.16           O
ANISOU 1521  OD1 ASN B 348     7285   5163   3950   -910    232  -2509       O
ATOM   1522  ND2 ASN B 348      14.725 -15.085 -37.373  1.00 40.71           N
ANISOU 1522  ND2 ASN B 348     6855   5147   3464  -1211   -120  -2476       N
ATOM   1523  C   ASN B 348      17.667 -12.572 -36.916  1.00 36.61           C
ANISOU 1523  C   ASN B 348     5990   4852   3067   -687    255  -2062       C
ATOM   1524  O   ASN B 348      17.122 -12.874 -37.983  1.00 38.05           O
ANISOU 1524  O   ASN B 348     6341   5088   3030   -793    181  -2183       O
ATOM   1525  N   LEU B 349      18.513 -11.541 -36.785  1.00 35.54           N
ANISOU 1525  N   LEU B 349     5710   4822   2971   -566    347  -1905       N
ATOM   1526  CA  LEU B 349      18.816 -10.526 -37.819  1.00 36.28           C
ANISOU 1526  CA  LEU B 349     5813   5105   2868   -550    371  -1824       C
ATOM   1527  CB  LEU B 349      19.731 -11.063 -38.920  1.00 38.60           C
ANISOU 1527  CB  LEU B 349     6300   5411   2954   -470    564  -1949       C
ATOM   1528  CG  LEU B 349      21.223 -11.340 -38.716  1.00 39.26           C
ANISOU 1528  CG  LEU B 349     6348   5448   3121   -285    826  -1953       C
ATOM   1529  CD1 LEU B 349      21.879 -11.427 -40.098  1.00 42.73           C
ANISOU 1529  CD1 LEU B 349     6964   5987   3283   -234    995  -2038       C
ATOM   1530  CD2 LEU B 349      21.941 -10.323 -37.866  1.00 36.33           C
ANISOU 1530  CD2 LEU B 349     5719   5139   2944   -211    877  -1751       C
ATOM   1531  C   LEU B 349      17.624  -9.803 -38.446  1.00 36.73           C
ANISOU 1531  C   LEU B 349     5872   5311   2775   -684    152  -1771       C
ATOM   1532  O   LEU B 349      17.698  -9.335 -39.579  1.00 38.72           O
ANISOU 1532  O   LEU B 349     6228   5696   2787   -694    154  -1759       O
ATOM   1533  N   GLN B 350      16.522  -9.716 -37.721  1.00 35.55           N
ANISOU 1533  N   GLN B 350     5604   5147   2756   -777    -33  -1735       N
ATOM   1534  CA  GLN B 350      15.386  -8.965 -38.230  1.00 36.17           C
ANISOU 1534  CA  GLN B 350     5639   5385   2719   -874   -250  -1664       C
ATOM   1535  CB  GLN B 350      14.078  -9.409 -37.570  1.00 35.38           C
ANISOU 1535  CB  GLN B 350     5441   5259   2744  -1005   -437  -1706       C
ATOM   1536  CG  GLN B 350      12.839  -8.730 -38.162  1.00 37.56           C
ANISOU 1536  CG  GLN B 350     5649   5725   2896  -1094   -678  -1646       C
ATOM   1537  CD  GLN B 350      11.541  -9.112 -37.450  1.00 37.75           C
ANISOU 1537  CD  GLN B 350     5522   5756   3067  -1225   -850  -1674       C
ATOM   1538  OE1 GLN B 350      11.541  -9.925 -36.534  1.00 37.89           O
ANISOU 1538  OE1 GLN B 350     5514   5620   3264  -1269   -784  -1742       O
ATOM   1539  NE2 GLN B 350      10.433  -8.514 -37.872  1.00 38.46           N
ANISOU 1539  NE2 GLN B 350     5505   6031   3077  -1284  -1067  -1612       N
ATOM   1540  C   GLN B 350      15.641  -7.495 -37.930  1.00 34.39           C
ANISOU 1540  C   GLN B 350     5259   5249   2560   -786   -250  -1441       C
ATOM   1541  O   GLN B 350      15.987  -7.132 -36.801  1.00 32.10           O
ANISOU 1541  O   GLN B 350     4817   4883   2495   -722   -194  -1348       O
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Figure 18 (continued)

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ATOM   1542  N   THR B 351      15.480  -6.654 -38.937  1.00 35.51           N
ANISOU 1542  N   THR B 351    5460   5538   2492   -786   -314  -1357          N
ATOM   1543  CA  THR B 351      15.638  -5.218 -38.753  1.00 35.15           C
ANISOU 1543  CA  THR B 351    5308   5556   2491   -715   -325  -1141          C
ATOM   1544  CB  THR B 351      15.876  -4.493 -40.090  1.00 36.33           C
ANISOU 1544  CB  THR B 351    5605   5840   2357   -703   -319  -1061          C
ATOM   1545  OG1 THR B 351      17.037  -5.035 -40.720  1.00 36.38           O
ANISOU 1545  OG1 THR B 351    5755   5831   2237   -677    -97  -1150          O
ATOM   1546  CG2 THR B 351      16.109  -3.013 -39.855  1.00 35.19           C
ANISOU 1546  CG2 THR B 351    5379   5719   2273   -636   -312   -830          C
ATOM   1547  C   THR B 351      14.428  -4.602 -38.066  1.00 34.79           C
ANISOU 1547  C   THR B 351    5095   5543   2579   -732   -530  -1043          C
ATOM   1548  O   THR B 351      13.297  -4.781 -38.513  1.00 36.32           O
ANISOU 1548  O   THR B 351    5289   5835   2677   -804   -723  -1083          O
ATOM   1549  N   LEU B 352      14.669  -3.878 -36.979  1.00 33.75           N
ANISOU 1549  N   LEU B 352    4817   5341   2667   -663   -487   -922          N
ATOM   1550  CA  LEU B 352      13.622  -3.070 -36.344  1.00 34.12           C
ANISOU 1550  CA  LEU B 352    4710   5420   2832   -640   -648   -808          C
ATOM   1551  CB  LEU B 352      13.362  -3.513 -34.889  1.00 32.44           C
ANISOU 1551  CB  LEU B 352    4345   5100   2881   -645   -632   -847          C
ATOM   1552  CG  LEU B 352      12.886  -4.942 -34.597  1.00 32.96           C
ANISOU 1552  CG  LEU B 352    4408   5119   2994   -749   -654  -1020          C
ATOM   1553  CD1 LEU B 352      12.818  -5.103 -33.090  1.00 32.72           C
ANISOU 1553  CD1 LEU B 352    4242   4977   3214   -731   -607  -1006          C
ATOM   1554  CD2 LEU B 352      11.534  -5.282 -35.237  1.00 34.08           C
ANISOU 1554  CD2 LEU B 352    4529   5392   3028   -855   -857  -1081          C
ATOM   1555  C   LEU B 352      13.996  -1.589 -36.370  1.00 33.77           C
ANISOU 1555  C   LEU B 352    4660   5383   2790   -547   -626   -610          C
ATOM   1556  O   LEU B 352      15.095  -1.217 -35.983  1.00 33.03           O
ANISOU 1556  O   LEU B 352    4572   5204   2773   -512   -465   -558          O
ATOM   1557  N   LYS B 353      13.074  -0.753 -36.832  1.00 35.44           N
ANISOU 1557  N   LYS B 353    4859   5692   2916   -511   -793   -499          N
ATOM   1558  CA  LYS B 353      13.235   0.694 -36.758  1.00 35.60           C
ANISOU 1558  CA  LYS B 353    4887   5683   2957   -416   -792   -303          C
ATOM   1559  CB  LYS B 353      12.510   1.355 -37.917  1.00 37.98           C
ANISOU 1559  CB  LYS B 353    5277   6118   3036   -378   -955   -195          C
ATOM   1560  CG  LYS B 353      12.989   2.760 -38.252  1.00 40.38           C
ANISOU 1560  CG  LYS B 353    5690   6373   3280   -298   -911     12          C
ATOM   1561  CD  LYS B 353      12.251   3.271 -39.513  1.00 47.52           C
ANISOU 1561  CD  LYS B 353    6709   7420   3925   -254  -1086    121          C
ATOM   1562  CE  LYS B 353      13.174   4.063 -40.450  1.00 51.30           C
ANISOU 1562  CE  LYS B 353    7408   7878   4205   -253   -970    266          C
ATOM   1563  NZ  LYS B 353      12.550   4.327 -41.795  1.00 55.38           N
ANISOU 1563  NZ  LYS B 353    8074   8553   4416   -224  -1134    354          N
ATOM   1564  C   LYS B 353      12.636   1.177 -35.441  1.00 34.34           C
ANISOU 1564  C   LYS B 353    4557   5448   3042   -351   -841   -254          C
ATOM   1565  O   LYS B 353      11.425   1.077 -35.231  1.00 34.90           O
ANISOU 1565  O   LYS B 353    4510   5595   3155   -331   -997   -267          O
ATOM   1566  N   ILE B 354      13.478   1.693 -34.559  1.00 32.69           N
ANISOU 1566  N   ILE B 354    4329   5103   2987   -322   -706   -204          N
ATOM   1567  CA  ILE B 354      13.045   2.177 -33.262  1.00 31.87           C
ANISOU 1567  CA  ILE B 354    4097   4914   3098   -258   -726   -169          C
ATOM   1568  CB  ILE B 354      13.522   1.253 -32.057  1.00 29.83           C
ANISOU 1568  CB  ILE B 354    3748   4568   3018   -309   -619   -293          C
ATOM   1569  CG1 ILE B 354      15.045   1.231 -31.936  1.00 29.97           C
ANISOU 1569  CG1 ILE B 354    3830   4502   3055   -342   -447   -296          C
ATOM   1570  CD1 ILE B 354      15.560   0.674 -30.576  1.00 28.39           C
ANISOU 1570  CD1 ILE B 354    3540   4204   3043   -353   -362   -368          C
ATOM   1571  CG2 ILE B 354      12.948  -0.182 -32.167  1.00 28.73           C
ANISOU 1571  CG2 ILE B 354    3563   4495   2859   -389   -663   -447          C
ATOM   1572  C   ILE B 354      13.526   3.621 -33.042  1.00 32.17           C
ANISOU 1572  C   ILE B 354    4202   4845   3176   -186   -681    -10          C
ATOM   1573  O   ILE B 354      14.521   4.069 -33.643  1.00 32.57           O
ANISOU 1573  O   ILE B 354    4377   4863   3134   -221   -582     57          O
ATOM   1574  N   ARG B 355      12.815   4.352 -32.186  1.00 31.65           N
ANISOU 1574  N   ARG B 355    4061   4720   3243    -91   -742     48          N
ATOM   1575  CA  ARG B 355      13.288   5.641 -31.749  1.00 32.09           C
ANISOU 1575  CA  ARG B 355    4195   4629   3367    -34   -689    170          C
ATOM   1576  CB  ARG B 355      12.149   6.642 -31.605  1.00 34.12           C
ANISOU 1576  CB  ARG B 355    4439   4870   3656    122   -811    276          C
ATOM   1577  CG  ARG B 355      11.544   7.019 -32.964  1.00 40.68           C
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Figure 18 (continued)

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ANISOU 1577  CG  ARG B 355     5351   5813   4294    184   -940    384    C
ATOM   1578  CD  ARG B 355      10.425   7.984 -32.784  1.00 49.99           C
ANISOU 1578  CD  ARG B 355     6500   6978   5518    372  -1063    495    C
ATOM   1579  NE  ARG B 355       9.347   7.782 -33.751  1.00 57.85           N
ANISOU 1579  NE  ARG B 355     7438   8169   6374    442  -1246    533    N
ATOM   1580  CZ  ARG B 355       8.140   8.351 -33.661  1.00 61.98           C
ANISOU 1580  CZ  ARG B 355     7861   8751   6936    624  -1388    610    C
ATOM   1581  NH1 ARG B 355       7.842   9.147 -32.628  1.00 61.47           N
ANISOU 1581  NH1 ARG B 355     7761   8550   7045    765  -1346    648    N
ATOM   1582  NH2 ARG B 355       7.220   8.116 -34.599  1.00 64.39           N
ANISOU 1582  NH2 ARG B 355     8099   9264   7103    672  -1573    644    N
ATOM   1583  C   ARG B 355      14.040   5.442 -30.452  1.00 29.39           C
ANISOU 1583  C   ARG B 355     3795   4172   3199    -82   -573     96    C
ATOM   1584  O   ARG B 355      13.448   5.166 -29.416  1.00 29.13           O
ANISOU 1584  O   ARG B 355     3651   4123   3296    -44   -595     33    O
ATOM   1585  N   VAL B 356      15.361   5.534 -30.531  1.00 27.06           N
ANISOU 1585  N   VAL B 356     3568   3818   2896   -173   -448    106    N
ATOM   1586  CA  VAL B 356      16.203   5.352 -29.374  1.00 24.71           C
ANISOU 1586  CA  VAL B 356     3213   3431   2745   -225   -354     44    C
ATOM   1587  CB  VAL B 356      17.660   4.989 -29.781  1.00 24.66           C
ANISOU 1587  CB  VAL B 356     3228   3443   2701   -334   -221     27    C
ATOM   1588  CG1 VAL B 356      18.584   4.978 -28.570  1.00 22.93           C
ANISOU 1588  CG1 VAL B 356     2938   3141   2632   -383   -149    -14    C
ATOM   1589  CG2 VAL B 356      17.691   3.637 -30.499  1.00 24.39           C
ANISOU 1589  CG2 VAL B 356     3163   3532   2572   -358   -198    -77    C
ATOM   1590  C   VAL B 356      16.195   6.627 -28.548  1.00 24.03           C
ANISOU 1590  C   VAL B 356     3178   3194   2758   -182   -360    122    C
ATOM   1591  O   VAL B 356      16.500   7.679 -29.070  1.00 25.01           O
ANISOU 1591  O   VAL B 356     3429   3245   2830   -189   -348    238    O
ATOM   1592  N   HIS B 357      15.853   6.512 -27.266  1.00 21.94           N
ANISOU 1592  N   HIS B 357     2836   2873   2626   -144   -371     56    N
ATOM   1593  CA  HIS B 357      15.871   7.643 -26.336  1.00 21.71           C
ANISOU 1593  CA  HIS B 357     2873   2687   2689   -106   -368     97    C
ATOM   1594  CB  HIS B 357      14.798   7.476 -25.251  1.00 20.79           C
ANISOU 1594  CB  HIS B 357     2672   2563   2663      2   -412     33    C
ATOM   1595  CG  HIS B 357      13.410   7.756 -25.737  1.00 21.75           C
ANISOU 1595  CG  HIS B 357     2767   2747   2751    144   -503     82    C
ATOM   1596  ND1 HIS B 357      12.706   8.884 -25.371  1.00 23.54           N
ANISOU 1596  ND1 HIS B 357     3056   2871   3017    287   -534    145    N
ATOM   1597  CE1 HIS B 357      11.530   8.882 -25.974  1.00 22.53           C
ANISOU 1597  CE1 HIS B 357     2858   2853   2849    411   -626    188    C
ATOM   1598  NE2 HIS B 357      11.450   7.797 -26.723  1.00 23.39           N
ANISOU 1598  NE2 HIS B 357     2873   3128   2886    329   -662    148    N
ATOM   1599  CD2 HIS B 357      12.613   7.077 -26.595  1.00 22.62           C
ANISOU 1599  CD2 HIS B 357     2792   3016   2786    170   -577     78    C
ATOM   1600  C   HIS B 357      17.247   7.801 -25.708  1.00 20.95           C
ANISOU 1600  C   HIS B 357     2796   2511   2655   -232   -283     74    C
ATOM   1601  O   HIS B 357      17.824   6.843 -25.188  1.00 18.76           O
ANISOU 1601  O   HIS B 357     2417   2290   2421   -290   -244    -15    O
ATOM   1602  N   GLU B 358      17.764   9.024 -25.773  1.00 21.60           N
ANISOU 1602  N   GLU B 358     3009   2459   2740   -276   -262    161    N
ATOM   1603  CA  GLU B 358      19.132   9.306 -25.328  1.00 21.12           C
ANISOU 1603  CA  GLU B 358     2957   2337   2730   -429   -192    153    C
ATOM   1604  CB  GLU B 358      19.907   9.942 -26.477  1.00 22.08           C
ANISOU 1604  CB  GLU B 358     3175   2446   2769   -535   -131    268    C
ATOM   1605  CG  GLU B 358      20.023   9.004 -27.665  1.00 22.15           C
ANISOU 1605  CG  GLU B 358     3121   2631   2664   -539    -93    272    C
ATOM   1606  CD  GLU B 358      20.615   9.629 -28.884  1.00 24.08           C
ANISOU 1606  CD  GLU B 358     3477   2879   2794   -626    -23    397    C
ATOM   1607  OE1 GLU B 358      20.524  10.875 -29.048  1.00 23.87           O
ANISOU 1607  OE1 GLU B 358     3613   2702   2753   -643    -34    513    O
ATOM   1608  OE2 GLU B 358      21.157   8.845 -29.705  1.00 25.65           O
ANISOU 1608  OE2 GLU B 358     3616   3224   2907   -671     52    379    O
ATOM   1609  C   GLU B 358      19.112  10.217 -24.111  1.00 21.14           C
ANISOU 1609  C   GLU B 358     3040   2167   2824   -430   -215    132    C
ATOM   1610  O   GLU B 358      18.544  11.303 -24.159  1.00 21.17           O
ANISOU 1610  O   GLU B 358     3194   2027   2822   -362   -242    198    O
ATOM   1611  N   GLY B 359      19.685   9.752 -23.008  1.00 20.16           N
ANISOU 1611  N   GLY B 359     2830   2055   2773   -490   -208     36    N
ATOM   1612  CA  GLY B 359      19.778  10.572 -21.819  1.00 20.57           C
ANISOU 1612  CA  GLY B 359     2974   1953   2890   -512   -231    -3    C
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Figure 18 (continued)

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ATOM   1613  C   GLY B 359      19.326   9.821 -20.596  1.00 19.73           C
ANISOU 1613  C   GLY B 359    2783   1889   2826   -437   -258   -113         C
ATOM   1614  O   GLY B 359      18.499   8.922 -20.689  1.00 19.63           O
ANISOU 1614  O   GLY B 359    2676   1982   2800   -330   -265   -142         O
ATOM   1615  N   TYR B 360      19.863  10.218 -19.445  1.00 19.73           N
ANISOU 1615  N   TYR B 360    2828   1801   2865   -508   -274   -174         N
ATOM   1616  CA  TYR B 360      19.483   9.673 -18.153  1.00 18.62           C
ANISOU 1616  CA  TYR B 360    2650   1681   2744   -445   -296   -271         C
ATOM   1617  CB  TYR B 360      20.482  10.115 -17.053  1.00 19.15           C
ANISOU 1617  CB  TYR B 360    2770   1677   2830   -579   -329   -331         C
ATOM   1618  CG  TYR B 360      19.942   9.873 -15.646  1.00 18.18           C
ANISOU 1618  CG  TYR B 360    2679   1534   2694   -499   -350   -425         C
ATOM   1619  CD1 TYR B 360      19.945   8.585 -15.104  1.00 16.45           C
ANISOU 1619  CD1 TYR B 360    2326   1457   2469   -465   -354   -465         C
ATOM   1620  CE1 TYR B 360      19.438   8.342 -13.850  1.00 19.36           C
ANISOU 1620  CE1 TYR B 360    2735   1814   2805   -398   -359   -536         C
ATOM   1621  CZ  TYR B 360      18.885   9.395 -13.126  1.00 19.45           C
ANISOU 1621  CZ  TYR B 360    2920   1679   2790   -350   -353   -585         C
ATOM   1622  OH  TYR B 360      18.382   9.138 -11.873  1.00 18.88           O
ANISOU 1622  OH  TYR B 360    2897   1608   2666   -282   -339   -658         O
ATOM   1623  CE2 TYR B 360      18.840  10.677 -13.657  1.00 18.02           C
ANISOU 1623  CE2 TYR B 360    2881   1343   2625   -365   -349   -557         C
ATOM   1624  CD2 TYR B 360      19.353  10.902 -14.916  1.00 17.40           C
ANISOU 1624  CD2 TYR B 360    2762   1269   2579   -442   -351   -469         C
ATOM   1625  C   TYR B 360      18.049  10.089 -17.759  1.00 19.14           C
ANISOU 1625  C   TYR B 360    2798   1672   2803   -267   -294   -288         C
ATOM   1626  O   TYR B 360      17.680  11.247 -17.870  1.00 21.05           O
ANISOU 1626  O   TYR B 360    3194   1761   3044   -218   -294   -255         O
ATOM   1627  N   GLU B 361      17.263   9.137 -17.275  1.00 18.20           N
ANISOU 1627  N   GLU B 361    2574   1657   2683   -169   -284   -337         N
ATOM   1628  CA  GLU B 361      15.899   9.416 -16.844  1.00 19.16           C
ANISOU 1628  CA  GLU B 361    2724   1749   2806      0   -265   -357         C
ATOM   1629  CB  GLU B 361      14.901   9.154 -17.981  1.00 18.69           C
ANISOU 1629  CB  GLU B 361    2575   1784   2741    107   -272   -291         C
ATOM   1630  CG  GLU B 361      14.816  10.226 -19.056  1.00 20.04           C
ANISOU 1630  CG  GLU B 361    2852   1865   2895    146   -296   -193         C
ATOM   1631  CD  GLU B 361      13.917   9.795 -20.203  1.00 22.31           C
ANISOU 1631  CD  GLU B 361    3033   2288   3154    236   -330   -129         C
ATOM   1632  OE1 GLU B 361      14.066   8.623 -20.652  1.00 20.60           O
ANISOU 1632  OE1 GLU B 361    2685   2224   2919    163   -336   -149         O
ATOM   1633  OE2 GLU B 361      13.064  10.618 -20.659  1.00 23.98           O
ANISOU 1633  OE2 GLU B 361    3300   2452   3359    383   -357    -61         O
ATOM   1634  C   GLU B 361      15.557   8.512 -15.689  1.00 17.64           C
ANISOU 1634  C   GLU B 361    2458   1633   2612     27   -240   -437         C
ATOM   1635  O   GLU B 361      15.996   7.369 -15.651  1.00 17.76           O
ANISOU 1635  O   GLU B 361    2363   1760   2626    -43   -244   -451         O
ATOM   1636  N   GLU B 362      14.776   9.020 -14.758  1.00 18.34           N
ANISOU 1636  N   GLU B 362    2620   1655   2692    137   -205   -484         N
ATOM   1637  CA  GLU B 362      14.217   8.208 -13.690  1.00 18.97           C
ANISOU 1637  CA  GLU B 362    2638   1816   2755    180   -158   -546         C
ATOM   1638  CB  GLU B 362      14.698   8.683 -12.317  1.00 18.78           C
ANISOU 1638  CB  GLU B 362    2764   1691   2682    150   -150   -626         C
ATOM   1639  CG  GLU B 362      13.769   7.780 -11.129  1.00 19.81           C
ANISOU 1639  CG  GLU B 362    2854   1908   2765    175    -96   -679         C
ATOM   1640  CD  GLU B 362      14.658   8.416  -9.769  1.00 23.89           C
ANISOU 1640  CD  GLU B 362    3556   2321   3202    160    -92   -765         C
ATOM   1641  OE1 GLU B 362      15.700   8.061  -9.173  1.00 27.64           O
ANISOU 1641  OE1 GLU B 362    4065   2806   3630     38   -156   -790         O
ATOM   1642  OE2 GLU B 362      13.946   9.338  -9.332  1.00 31.97           O
ANISOU 1642  OE2 GLU B 362    4699   3247   4203    278    -32   -811         O
ATOM   1643  C   GLU B 362      12.692   8.261 -13.751  1.00 19.33           C
ANISOU 1643  C   GLU B 362    2608   1916   2818    350   -102   -537         C
ATOM   1644  O   GLU B 362      12.130   9.347 -13.924  1.00 21.05           O
ANISOU 1644  O   GLU B 362    2908   2040   3049    476    -89   -521         O
ATOM   1645  N   PHE B 363      12.053   7.096 -13.591  1.00 18.10           N
ANISOU 1645  N   PHE B 363    2298   1909   2669    352    -67   -544         N
ATOM   1646  CA  PHE B 363      10.603   6.935 -13.598  1.00 19.56           C
ANISOU 1646  CA  PHE B 363    2355   2196   2881    481    -10   -536         C
ATOM   1647  CB  PHE B 363      10.160   6.097 -14.830  1.00 18.76           C
ANISOU 1647  CB  PHE B 363    2078   2239   2813    443    -60   -483         C
ATOM   1648  CG  PHE B 363      10.538   6.710 -16.149  1.00 20.16                C
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Figure 18 (continued)

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ANISOU 1648  CG  PHE B 363     2290   2378   2990    445   -145   -419      C
ATOM   1649  CD1 PHE B 363       9.671   7.585 -16.786  1.00 20.57          C
ANISOU 1649  CD1 PHE B 363     2324   2434   3060    595   -170   -365      C
ATOM   1650  CE1 PHE B 363      10.005   8.145 -17.991  1.00 22.34          C
ANISOU 1650  CE1 PHE B 363     2603   2620   3264    598   -247   -290      C
ATOM   1651  CZ  PHE B 363      11.229   7.855 -18.587  1.00 17.85          C
ANISOU 1651  CZ  PHE B 363     2100   2021   2662    440   -280   -275      C
ATOM   1652  CE2 PHE B 363      12.100   6.988 -17.975  1.00 18.88          C
ANISOU 1652  CE2 PHE B 363     2224   2160   2789    301   -251   -336      C
ATOM   1653  CD2 PHE B 363      11.761   6.407 -16.760  1.00 18.78          C
ANISOU 1653  CD2 PHE B 363     2166   2175   2793    306   -193   -403      C
ATOM   1654  C   PHE B 363      10.104   6.182 -12.366  1.00 19.99          C
ANISOU 1654  C   PHE B 363     2365   2319   2910    480     83   -588      C
ATOM   1655  O   PHE B 363      10.813   5.318 -11.820  1.00 19.21          O
ANISOU 1655  O   PHE B 363     2290   2232   2778    360     82   -608      O
ATOM   1656  N   THR B 364       8.874   6.490 -11.950  1.00 21.40          N
ANISOU 1656  N   THR B 364     2475   2551   3103    622    169   -600      N
ATOM   1657  CA  THR B 364       8.094   5.540 -11.194  1.00 22.37          C
ANISOU 1657  CA  THR B 364     2478   2803   3219    605    268   -619      C
ATOM   1658  CB  THR B 364       7.228   6.189 -10.082  1.00 24.65          C
ANISOU 1658  CB  THR B 364     2799   3088   3478    761    405   -666      C
ATOM   1659  OG1 THR B 364       6.244   7.069 -10.672  1.00 29.54          O
ANISOU 1659  OG1 THR B 364     3325   3737   4161    950    417   -641      O
ATOM   1660  CG2 THR B 364       8.077   6.917  -9.090  1.00 20.46          C
ANISOU 1660  CG2 THR B 364     2522   2392   2860    769    420   -732      C
ATOM   1661  C   THR B 364       7.200   4.826 -12.190  1.00 23.57          C
ANISOU 1661  C   THR B 364     2398   3119   3440    586    242   -570      C
ATOM   1662  O   THR B 364       6.734   5.447 -13.162  1.00 24.92          O
ANISOU 1662  O   THR B 364     2497   3317   3654    681    180   -530      O
ATOM   1663  N   MSE B 365       6.990   3.527 -11.962  1.00 23.51          N
ANISOU 1663  N   MSE B 365     2289   3210   3433    455    278   -570      N
ATOM   1664  CA  MSE B 365       6.070   2.707 -12.758  1.00 25.28          C
ANISOU 1664  CA  MSE B 365     2293   3596   3716    395    258   -541      C
ATOM   1665  CB  MSE B 365       6.777   1.479 -13.354  1.00 23.17          C
ANISOU 1665  CB  MSE B 365     2037   3323   3443    205    188   -537      C
ATOM   1666  CG  MSE B 365       7.959   1.767 -14.260  1.00 23.72          C
ANISOU 1666  CG  MSE B 365     2224   3295   3494    180     74   -527      C
ATOM   1667 SE   MSE B 365       9.006   0.180 -14.677  0.90 24.85         SE
ANISOU 1667 SE   MSE B 365     2418   3405   3619    -17     33   -540     SE
ATOM   1668  CE  MSE B 365       7.640  -1.058 -15.246  1.00 20.54          C
ANISOU 1668  CE  MSE B 365     1672   3014   3117   -135     41   -548      C
ATOM   1669  C   MSE B 365       4.961   2.217 -11.835  1.00 26.07          C
ANISOU 1669  C   MSE B 365     2259   3817   3829    397    400   -552      C
ATOM   1670  O   MSE B 365       5.252   1.610 -10.808  1.00 25.95          O
ANISOU 1670  O   MSE B 365     2332   3765   3763    319    488   -569      O
ATOM   1671  N   VAL B 366       3.699   2.486 -12.183  1.00 27.59          N
ANISOU 1671  N   VAL B 366     2234   4164   4084    489    424   -533      N
ATOM   1672  CA  VAL B 366       2.565   2.042 -11.348  1.00 29.18          C
ANISOU 1672  CA  VAL B 366     2265   4513   4308    484    578   -537      C
ATOM   1673  CB  VAL B 366       1.807   3.257 -10.708  1.00 31.18          C
ANISOU 1673  CB  VAL B 366     2482   4797   4568    737    692   -550      C
ATOM   1674  CG1 VAL B 366       0.547   2.816  -9.890  1.00 31.65          C
ANISOU 1674  CG1 VAL B 366     2322   5048   4655    741    877   -550      C
ATOM   1675  CG2 VAL B 366       2.757   4.071  -9.830  1.00 29.76          C
ANISOU 1675  CG2 VAL B 366     2601   4409   4296    827    734   -597      C
ATOM   1676  C   VAL B 366       1.630   1.113 -12.138  1.00 30.40          C
ANISOU 1676  C   VAL B 366     2151   4861   4538    349    536   -511      C
ATOM   1677  O   VAL B 366       1.042   1.529 -13.138  1.00 31.27          O
ANISOU 1677  O   VAL B 366     2097   5082   4703    424    432   -486      O
ATOM   1678  N   GLY B 367       1.533  -0.147 -11.709  1.00 30.76          N
ANISOU 1678  N   GLY B 367     2170   4939   4578    139    604   -513      N
ATOM   1679  CA  GLY B 367       0.588  -1.110 -12.303  1.00 32.91          C
ANISOU 1679  CA  GLY B 367     2196   5388   4921    -34    581   -500      C
ATOM   1680  C   GLY B 367      -0.498  -1.517 -11.325  1.00 35.94          C
ANISOU 1680  C   GLY B 367     2401   5920   5333    -85    771   -488      C
ATOM   1681  O   GLY B 367      -0.558  -0.986 -10.220  1.00 37.15          O
ANISOU 1681  O   GLY B 367     2625   6048   5442     44    925   -491      O
ATOM   1682  N   LYS B 368      -1.356  -2.458 -11.722  1.00 37.73          N
ANISOU 1682  N   LYS B 368     2403   6306   5626   -285    766   -478      N
ATOM   1683  CA  LYS B 368      -2.392  -2.977 -10.842  1.00 40.82          C
ANISOU 1683  CA  LYS B 368     2606   6852   6051   -385    959   -457      C
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Figure 18 (continued)

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ATOM   1684  CB  LYS B 368      -3.379  -3.863 -11.614  1.00 43.14           C
ANISOU 1684  CB  LYS B 368     2608   7343   6439   -618    896   -451       C
ATOM   1685  CG  LYS B 368      -4.224  -3.164 -12.650  1.00 46.39           C
ANISOU 1685  CG  LYS B 368     2718   7976   6933   -496    753   -448       C
ATOM   1686  CD  LYS B 368      -5.098  -4.196 -13.325  1.00 53.87           C
ANISOU 1686  CD  LYS B 368     3403   9110   7957   -784    679   -454       C
ATOM   1687  CE  LYS B 368      -5.442  -3.835 -14.770  1.00 56.62           C
ANISOU 1687  CE  LYS B 368     3572   9602   8340   -740    427   -464       C
ATOM   1688  NZ  LYS B 368      -6.644  -4.642 -15.228  1.00 62.56           N
ANISOU 1688  NZ  LYS B 368     3968  10621   9180   -997    377   -470       N
ATOM   1689  C   LYS B 368      -1.811  -3.784  -9.679  1.00 40.22           C
ANISOU 1689  C   LYS B 368     2770   6621   5891   -521   1112   -444       C
ATOM   1690  O   LYS B 368      -2.325  -3.708  -8.559  1.00 41.54           O
ANISOU 1690  O   LYS B 368     2901   6854   6028   -488   1318   -424       O
ATOM   1691  N   ARG B 369      -0.739  -4.539  -9.950  1.00 38.40           N
ANISOU 1691  N   ARG B 369     2787   6190   5615   -656   1015   -452       N
ATOM   1692  CA  ARG B 369      -0.231  -5.556  -9.020  1.00 38.59           C
ANISOU 1692  CA  ARG B 369     3028   6068   5567   -815   1127   -423       C
ATOM   1693  CB  ARG B 369      -0.483  -6.952  -9.606  1.00 39.39           C
ANISOU 1693  CB  ARG B 369     3090   6155   5723  -1113   1085   -417       C
ATOM   1694  CG  ARG B 369      -1.889  -7.506  -9.367  1.00 43.61           C
ANISOU 1694  CG  ARG B 369     3344   6893   6331  -1301   1219   -390       C
ATOM   1695  CD  ARG B 369      -2.166  -8.798 -10.162  1.00 45.50           C
ANISOU 1695  CD  ARG B 369     3542   7112   6635  -1617   1138   -405       C
ATOM   1696  NE  ARG B 369      -2.734  -8.513 -11.485  1.00 50.50           N
ANISOU 1696  NE  ARG B 369     3925   7913   7351  -1634    956   -457       N
ATOM   1697  CZ  ARG B 369      -2.076  -8.625 -12.642  1.00 51.55           C
ANISOU 1697  CZ  ARG B 369     4162   7949   7474  -1642    750   -512       C
ATOM   1698  NH1 ARG B 369      -0.809  -9.053 -12.673  1.00 49.87           N
ANISOU 1698  NH1 ARG B 369     4281   7475   7191  -1634    707   -525       N
ATOM   1699  NH2 ARG B 369      -2.696  -8.327 -13.783  1.00 52.31           N
ANISOU 1699  NH2 ARG B 369     4025   8226   7624  -1654    588   -550       N
ATOM   1700  C   ARG B 369       1.251  -5.377  -8.622  1.00 35.98           C
ANISOU 1700  C   ARG B 369     3036   5502   5132   -717   1074   -428       C
ATOM   1701  O   ARG B 369       1.835  -6.216  -7.915  1.00 36.25           O
ANISOU 1701  O   ARG B 369     3277   5399   5097   -821   1132   -395       O
ATOM   1702  N   ALA B 370       1.852  -4.282  -9.083  1.00 33.63           N
ANISOU 1702  N   ALA B 370     2790   5164   4825   -519    958   -462       N
ATOM   1703  CA  ALA B 370       3.242  -3.951  -8.791  1.00 31.07           C
ANISOU 1703  CA  ALA B 370     2741   4650   4415   -426    890   -472       C
ATOM   1704  CB  ALA B 370       4.209  -4.861  -9.590  1.00 29.47           C
ANISOU 1704  CB  ALA B 370     2663   4314   4222   -553    754   -475       C
ATOM   1705  C   ALA B 370       3.536  -2.485  -9.087  1.00 30.13           C
ANISOU 1705  C   ALA B 370     2633   4522   4291   -205    816   -506       C
ATOM   1706  O   ALA B 370       2.837  -1.834  -9.869  1.00 30.45           O
ANISOU 1706  O   ALA B 370     2489   4676   4403   -120    767   -516       O
ATOM   1707  N   THR B 371       4.577  -1.968  -8.447  1.00 29.21           N
ANISOU 1707  N   THR B 371     2743   4267   4088   -115    802   -520       N
ATOM   1708  CA  THR B 371       5.070  -0.623  -8.712  1.00 28.42           C
ANISOU 1708  CA  THR B 371     2713   4108   3978     60    723   -553       C
ATOM   1709  CB  THR B 371       4.594   0.442  -7.657  1.00 29.87           C
ANISOU 1709  CB  THR B 371     2940   4307   4103    233    854   -584       C
ATOM   1710  OG1 THR B 371       5.182   0.139  -6.396  1.00 31.90           O
ANISOU 1710  OG1 THR B 371     3400   4485   4238    197    929   -590       O
ATOM   1711  CG2 THR B 371       3.077   0.486  -7.506  1.00 29.41           C
ANISOU 1711  CG2 THR B 371     2640   4434   4101    284    995   -575       C
ATOM   1712  C   THR B 371       6.587  -0.709  -8.730  1.00 26.74           C
ANISOU 1712  C   THR B 371     2715   3734   3710     26    611   -559       C
ATOM   1713  O   THR B 371       7.167  -1.696  -8.278  1.00 27.73           O
ANISOU 1713  O   THR B 371     2942   3802   3791    -84    618   -537       O
ATOM   1714  N   ALA B 372       7.245   0.306  -9.262  1.00 24.71           N
ANISOU 1714  N   ALA B 372     2524   3405   3458    120    509   -581       N
ATOM   1715  CA  ALA B 372       8.691   0.260  -9.366  1.00 22.74           C
ANISOU 1715  CA  ALA B 372     2435   3033   3172     78    402   -584       C
ATOM   1716  CB  ALA B 372       9.123  -0.612 -10.575  1.00 20.88           C
ANISOU 1716  CB  ALA B 372     2138   2802   2995   -29    305   -563       C
ATOM   1717  C   ALA B 372       9.313   1.651  -9.455  1.00 21.47           C
ANISOU 1717  C   ALA B 372     2381   2784   2993    183    354   -614       C
ATOM   1718  O   ALA B 372       8.644   2.637  -9.767  1.00 22.51           O
ANISOU 1718  O   ALA B 372     2465   2931   3157    299    353   -625       O
ATOM   1719  N   ILE B 373      10.596   1.712  -9.160  1.00 20.23           N
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Figure 18 (continued)

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ANISOU 1719  N   ILE B 373     2368   2532   2787    140    265   -623       N
ATOM   1720  CA  ILE B 373      11.406   2.858  -9.509  1.00 20.10           C
ANISOU 1720  CA  ILE B 373     2445   2422   2770    176    179   -644       C
ATOM   1721  CB  ILE B 373      12.105   3.494  -8.281  1.00 20.66           C
ANISOU 1721  CB  ILE B 373     2702   2404   2743    188    175   -692       C
ATOM   1722  CG1 ILE B 373      11.114   3.705  -7.131  1.00 21.48           C
ANISOU 1722  CG1 ILE B 373     2853   2532   2776    274    308   -730       C
ATOM   1723  CD1 ILE B 373      11.724   4.339  -5.870  1.00 23.57           C
ANISOU 1723  CD1 ILE B 373     3331   2712   2913    284    306   -794       C
ATOM   1724  CG2 ILE B 373      12.777   4.814  -8.687  1.00 20.73           C
ANISOU 1724  CG2 ILE B 373     2810   2302   2764    207     96   -719       C
ATOM   1725  C   ILE B 373      12.440   2.357 -10.494  1.00 18.98           C
ANISOU 1725  C   ILE B 373     2275   2270   2668     84     75   -613       C
ATOM   1726  O   ILE B 373      13.084   1.346 -10.229  1.00 18.45           O
ANISOU 1726  O   ILE B 373     2219   2210   2582      9     57   -599       O
ATOM   1727  N   LEU B 374      12.551   3.049 -11.633  1.00 19.11           N
ANISOU 1727  N   LEU B 374     2259   2268   2733    102     18   -597       N
ATOM   1728  CA  LEU B 374      13.487   2.723 -12.716  1.00 17.96           C
ANISOU 1728  CA  LEU B 374     2084   2123   2617     26    -60   -569       C
ATOM   1729  CB  LEU B 374      12.712   2.403 -14.002  1.00 17.80           C
ANISOU 1729  CB  LEU B 374     1942   2182   2641     33    -70   -541       C
ATOM   1730  CG  LEU B 374      13.468   2.237 -15.313  1.00 17.37           C
ANISOU 1730  CG  LEU B 374     1867   2137   2597    -24   -132   -516       C
ATOM   1731  CD1 LEU B 374      14.387   1.025 -15.269  1.00 16.31           C
ANISOU 1731  CD1 LEU B 374     1730   2011   2458   -107   -135   -527       C
ATOM   1732  CD2 LEU B 374      12.488   2.104 -16.488  1.00 19.06           C
ANISOU 1732  CD2 LEU B 374     1980   2438   2824     -4   -153   -495       C
ATOM   1733  C   LEU B 374      14.409   3.901 -12.991  1.00 18.14           C
ANISOU 1733  C   LEU B 374     2200   2055   2636     17   -119   -567       C
ATOM   1734  O   LEU B 374      13.919   5.035 -13.178  1.00 17.76           O
ANISOU 1734  O   LEU B 374     2202   1951   2595     91   -114   -565       O
ATOM   1735  N   ARG B 375      15.721   3.625 -12.989  1.00 16.95           N
ANISOU 1735  N   ARG B 375     2072   1891   2478    -71   -171   -564       N
ATOM   1736  CA  ARG B 375      16.705   4.489 -13.602  1.00 17.47           C
ANISOU 1736  CA  ARG B 375     2179   1903   2558   -127   -225   -546       C
ATOM   1737  CB  ARG B 375      17.892   4.764 -12.677  1.00 18.12           C
ANISOU 1737  CB  ARG B 375     2329   1943   2611   -204   -277   -574       C
ATOM   1738  CG  ARG B 375      17.604   5.831 -11.648  1.00 18.30           C
ANISOU 1738  CG  ARG B 375     2500   1865   2590   -178   -276   -625       C
ATOM   1739  CD  ARG B 375      18.705   5.872 -10.626  1.00 17.52           C
ANISOU 1739  CD  ARG B 375     2459   1755   2442   -267   -347   -663       C
ATOM   1740  NE  ARG B 375      18.396   6.839  -9.574  1.00 20.93           N
ANISOU 1740  NE  ARG B 375     3063   2084   2807   -248   -345   -733       N
ATOM   1741  CZ  ARG B 375      18.996   6.901  -8.392  1.00 22.13           C
ANISOU 1741  CZ  ARG B 375     3304   2227   2876   -303   -404   -787       C
ATOM   1742  NH1 ARG B 375      19.955   6.037  -8.075  1.00 23.45           N
ANISOU 1742  NH1 ARG B 375     3389   2494   3028   -370   -480   -765       N
ATOM   1743  NH2 ARG B 375      18.629   7.827  -7.528  1.00 24.29           N
ANISOU 1743  NH2 ARG B 375     3760   2394   3076   -279   -390   -865       N
ATOM   1744  C   ARG B 375      17.209   3.921 -14.913  1.00 17.41           C
ANISOU 1744  C   ARG B 375     2079   1958   2578   -175   -238   -505       C
ATOM   1745  O   ARG B 375      17.554   2.747 -15.016  1.00 17.68           O
ANISOU 1745  O   ARG B 375     2043   2057   2618   -198   -232   -507       O
ATOM   1746  N   LYS B 376      17.327   4.788 -15.899  1.00 17.92           N
ANISOU 1746  N   LYS B 376     2167   1990   2651   -187   -251   -466       N
ATOM   1747  CA  LYS B 376      17.635   4.368 -17.233  1.00 18.44           C
ANISOU 1747  CA  LYS B 376     2166   2121   2718   -219   -249   -427       C
ATOM   1748  CB  LYS B 376      16.313   4.249 -17.956  1.00 19.30           C
ANISOU 1748  CB  LYS B 376     2242   2274   2816   -141   -242   -411       C
ATOM   1749  CG  LYS B 376      16.410   4.111 -19.385  1.00 24.35           C
ANISOU 1749  CG  LYS B 376     2854   2971   3426   -163   -251   -371       C
ATOM   1750  CD  LYS B 376      15.233   4.725 -20.053  1.00 25.52           C
ANISOU 1750  CD  LYS B 376     3010   3132   3554    -79   -279   -330       C
ATOM   1751  CE  LYS B 376      15.262   4.220 -21.479  1.00 24.91           C
ANISOU 1751  CE  LYS B 376     2899   3145   3419   -111   -296   -304       C
ATOM   1752  NZ  LYS B 376      16.403   4.826 -22.153  1.00 24.23           N
ANISOU 1752  NZ  LYS B 376     2885   3021   3302   -176   -279   -252       N
ATOM   1753  C   LYS B 376      18.551   5.421 -17.892  1.00 18.68           C
ANISOU 1753  C   LYS B 376     2253   2098   2746   -262   -380       C
ATOM   1754  O   LYS B 376      18.550   6.582 -17.503  1.00 19.26           O
ANISOU 1754  O   LYS B 376     2432   2063   2823   -300   -277   -372       O
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Figure 18 (continued)

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ATOM   1755  N   ALA B 377      19.344   5.004 -18.873  1.00 18.41           N
ANISOU 1755  N   ALA B 377    2158   2132   2704   -354   -244   -351       N
ATOM   1756  CA  ALA B 377      20.187   5.927 -19.633  1.00 19.30           C
ANISOU 1756  CA  ALA B 377    2313   2213   2809   -443   -234   -292       C
ATOM   1757  CB  ALA B 377      21.642   5.877 -19.139  1.00 18.88           C
ANISOU 1757  CB  ALA B 377    2200   2184   2791   -557   -236   -304       C
ATOM   1758  C   ALA B 377      20.043   5.447 -21.070  1.00 19.24           C
ANISOU 1758  C   ALA B 377    2269   2292   2751   -429   -199   -253       C
ATOM   1759  O   ALA B 377      19.145   4.641 -21.328  1.00 18.97           O
ANISOU 1759  O   ALA B 377    2199   2314   2694   -354   -205   -280       O
ATOM   1760  N   THR B 378      20.885   5.930 -21.991  1.00 19.58           N
ANISOU 1760  N   THR B 378    2326   2348   2766   -514   -160   -192       N
ATOM   1761  CA  THR B 378      20.812   5.546 -23.409  1.00 19.32           C
ANISOU 1761  CA  THR B 378    2285   2401   2653   -506   -118   -155       C
ATOM   1762  CB  THR B 378      21.861   6.284 -24.233  1.00 20.34           C
ANISOU 1762  CB  THR B 378    2444   2534   2751   -620    -56    -76       C
ATOM   1763  OG1 THR B 378      21.768   7.684 -23.973  1.00 20.74           O
ANISOU 1763  OG1 THR B 378    2618   2442   2819   -665    -85    -11       O
ATOM   1764  CG2 THR B 378      21.664   6.025 -25.717  1.00 20.00           C
ANISOU 1764  CG2 THR B 378    2433   2574   2591   -603    -11    -31       C
ATOM   1765  C   THR B 378      21.001   4.033 -23.613  1.00 19.30           C
ANISOU 1765  C   THR B 378    2178   2513   2641   -474    -84   -227       C
ATOM   1766  O   THR B 378      22.120   3.502 -23.476  1.00 19.32           O
ANISOU 1766  O   THR B 378    2096   2570   2676   -516    -33   -250       O
ATOM   1767  N   ARG B 379      19.914   3.359 -23.968  1.00 18.79           N
ANISOU 1767  N   ARG B 379    2122   2483   2535   -401   -113   -261       N
ATOM   1768  CA  ARG B 379      19.921   1.918 -24.208  1.00 19.22           C
ANISOU 1768  CA  ARG B 379    2121   2610   2572   -377    -84   -338       C
ATOM   1769  CB  ARG B 379      20.587   1.584 -25.568  1.00 20.01           C
ANISOU 1769  CB  ARG B 379    2232   2791   2579   -405    -10   -331       C
ATOM   1770  CG  ARG B 379      19.959   2.282 -26.762  1.00 21.05           C
ANISOU 1770  CG  ARG B 379    2454   2950   2595   -411    -34   -267       C
ATOM   1771  CD  ARG B 379      20.376   1.641 -28.060  1.00 20.86           C
ANISOU 1771  CD  ARG B 379    2459   3018   2448   -427     38   -291       C
ATOM   1772  NE  ARG B 379      19.805   0.291 -28.188  1.00 21.07           N
ANISOU 1772  NE  ARG B 379    2478   3077   2449   -392     21   -402       N
ATOM   1773  CZ  ARG B 379      20.169  -0.608 -29.110  1.00 21.75           C
ANISOU 1773  CZ  ARG B 379    2601   3225   2438   -392     91   -469       C
ATOM   1774  NH1 ARG B 379      21.092  -0.337 -30.021  1.00 20.29           N
ANISOU 1774  NH1 ARG B 379    2446   3100   2163   -415    195   -434       N
ATOM   1775  NH2 ARG B 379      19.594  -1.797 -29.126  1.00 22.67           N
ANISOU 1775  NH2 ARG B 379    2735   3336   2542   -377     67   -576       N
ATOM   1776  C   ARG B 379      20.589   1.159 -23.045  1.00 19.24           C
ANISOU 1776  C   ARG B 379    2052   2596   2663   -368    -69   -390       C
ATOM   1777  O   ARG B 379      21.432   0.291 -23.257  1.00 18.60           O
ANISOU 1777  O   ARG B 379    1921   2560   2586   -362    -11   -424       O
ATOM   1778  N   ARG B 380      20.187   1.503 -21.816  1.00 20.13           N
ANISOU 1778  N   ARG B 380    2170   2643   2835   -353   -120   -395       N
ATOM   1779  CA  ARG B 380      20.790   0.946 -20.598  1.00 20.31           C
ANISOU 1779  CA  ARG B 380    2146   2650   2921   -343   -125   -427       C
ATOM   1780  CB  ARG B 380      22.100   1.697 -20.262  1.00 21.34           C
ANISOU 1780  CB  ARG B 380    2237   2785   3086   -409   -126   -393       C
ATOM   1781  CG  ARG B 380      22.872   1.156 -19.087  1.00 24.13           C
ANISOU 1781  CG  ARG B 380    2528   3150   3490   -396   -155   -417       C
ATOM   1782  CD  ARG B 380      24.060   2.071 -18.796  1.00 33.52           C
ANISOU 1782  CD  ARG B 380    3664   4360   4713   -492   -179   -385       C
ATOM   1783  NE  ARG B 380      24.427   2.050 -17.376  1.00 40.26           N
ANISOU 1783  NE  ARG B 380    4504   5201   5593   -496   -257   -405       N
ATOM   1784  CZ  ARG B 380      25.066   3.030 -16.744  1.00 41.26           C
ANISOU 1784  CZ  ARG B 380    4631   5311   5736   -597   -318   -398       C
ATOM   1785  NH1 ARG B 380      25.427   4.118 -17.419  1.00 44.00           N
ANISOU 1785  NH1 ARG B 380    4992   5636   6088   -711   -298   -363       N
ATOM   1786  NH2 ARG B 380      25.345   2.919 -15.441  1.00 40.13           N
ANISOU 1786  NH2 ARG B 380    4489   5166   5591   -596   -403   -425       N
ATOM   1787  C   ARG B 380      19.822   1.058 -19.448  1.00 18.92           C
ANISOU 1787  C   ARG B 380    2007   2415   2767   -309   -171   -445       C
ATOM   1788  O   ARG B 380      19.320   2.129 -19.164  1.00 19.53           O
ANISOU 1788  O   ARG B 380    2136   2442   2844   -309   -199   -423       O
ATOM   1789  N   LEU B 381      19.535  -0.060 -18.802  1.00 19.03           N
ANISOU 1789  N   LEU B 381    2006   2427   2796   -274   -165   -485       N
ATOM   1790  CA  LEU B 381      18.844  -0.036 -17.509  1.00 18.96           C
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Figure 18 (continued)

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ANISOU 1790  CA  LEU B 381     2029   2373   2800   -249   -186   -498      C
ATOM   1791  CB  LEU B 381      18.117  -1.356 -17.258  1.00 18.22          C
ANISOU 1791  CB  LEU B 381     1933   2281   2708   -229   -160   -529      C
ATOM   1792  CG  LEU B 381      17.277  -1.567 -16.000  1.00 18.70          C
ANISOU 1792  CG  LEU B 381     2025   2311   2770   -212   -152   -535      C
ATOM   1793  CD1 LEU B 381      16.073  -2.493 -16.303  1.00 16.19          C
ANISOU 1793  CD1 LEU B 381     1688   2009   2454   -232   -118   -558      C
ATOM   1794  CD2 LEU B 381      18.121  -2.129 -14.860  1.00 18.01          C
ANISOU 1794  CD2 LEU B 381     1969   2193   2680   -196   -161   -527      C
ATOM   1795  C   LEU B 381      19.942   0.175 -16.476  1.00 18.78          C
ANISOU 1795  C   LEU B 381     2006   2334   2794   -262   -216   -491      C
ATOM   1796  O   LEU B 381      20.876  -0.627 -16.374  1.00 18.28          O
ANISOU 1796  O   LEU B 381     1898   2301   2747   -252   -214   -491      O
ATOM   1797  N   VAL B 382      19.839   1.265 -15.730  1.00 19.29          N
ANISOU 1797  N   VAL B 382     2125   2353   2851   -279   -250   -489      N
ATOM   1798  CA  VAL B 382      20.836   1.563 -14.675  1.00 19.54          C
ANISOU 1798  CA  VAL B 382     2167   2377   2881   -314   -304   -493      C
ATOM   1799  CB  VAL B 382      20.934   3.093 -14.380  1.00 20.23          C
ANISOU 1799  CB  VAL B 382     2332   2395   2958   -372   -341   -498      C
ATOM   1800  CG1 VAL B 382      21.928   3.397 -13.238  1.00 19.44          C
ANISOU 1800  CG1 VAL B 382     2249   2295   2842   -433   -418   -518      C
ATOM   1801  CG2 VAL B 382      21.319   3.844 -15.652  1.00 20.85          C
ANISOU 1801  CG2 VAL B 382     2392   2472   3060   -431   -323   -459      C
ATOM   1802  C   VAL B 382      20.465   0.761 -13.431  1.00 19.16          C
ANISOU 1802  C   VAL B 382     2157   2320   2803   -264   -312   -511      C
ATOM   1803  O   VAL B 382      21.273   0.005 -12.911  1.00 20.08          O
ANISOU 1803  O   VAL B 382     2241   2469   2918   -251   -343   -500      O
ATOM   1804  N   GLN B 383      19.221   0.890 -12.992  1.00 18.96          N
ANISOU 1804  N   GLN B 383     2195   2258   2752   -228   -275   -528      N
ATOM   1805  CA  GLN B 383      18.755   0.178 -11.818  1.00 19.44          C
ANISOU 1805  CA  GLN B 383     2306   2311   2769   -193   -258   -534      C
ATOM   1806  CB  GLN B 383      19.339   0.796 -10.539  1.00 20.96          C
ANISOU 1806  CB  GLN B 383     2581   2483   2901   -208   -319   -552      C
ATOM   1807  CG  GLN B 383      18.988   0.003  -9.318  1.00 28.70          C
ANISOU 1807  CG  GLN B 383     3630   3464   3810   -172   -301   -545      C
ATOM   1808  CD  GLN B 383      19.917   0.256  -8.142  1.00 38.33          C
ANISOU 1808  CD  GLN B 383     4920   4691   4951   -190   -395   -552      C
ATOM   1809  OE1 GLN B 383      20.549   1.348  -8.009  1.00 37.76          O
ANISOU 1809  OE1 GLN B 383     4873   4607   4867   -246   -467   -588      O
ATOM   1810  NE2 GLN B 383      20.021  -0.768  -7.272  1.00 39.52          N
ANISOU 1810  NE2 GLN B 383     5116   4861   5041   -153   -403   -515      N
ATOM   1811  C   GLN B 383      17.247   0.146 -11.767  1.00 17.86          C
ANISOU 1811  C   GLN B 383     2121   2104   2562   -158   -184   -546      C
ATOM   1812  O   GLN B 383      16.598   1.075 -12.243  1.00 16.03          O
ANISOU 1812  O   GLN B 383     1886   1860   2344   -140   -169   -556      O
ATOM   1813  N   LEU B 384      16.709  -0.958 -11.236  1.00 17.13          N
ANISOU 1813  N   LEU B 384     2036   2020   2452   -149   -135   -536      N
ATOM   1814  CA  LEU B 384      15.291  -1.124 -11.035  1.00 17.71          C
ANISOU 1814  CA  LEU B 384     2096   2111   2521   -135    -54   -542      C
ATOM   1815  CB  LEU B 384      14.719  -2.032 -12.141  1.00 17.64          C
ANISOU 1815  CB  LEU B 384     2001   2134   2568   -172    -28   -537      C
ATOM   1816  CG  LEU B 384      13.218  -2.392 -12.135  1.00 17.32          C
ANISOU 1816  CG  LEU B 384     1897   2141   2542   -192     47   -541      C
ATOM   1817  CD1 LEU B 384      12.346  -1.239 -12.603  1.00 13.70          C
ANISOU 1817  CD1 LEU B 384     1367   1735   2105   -139     48   -553      C
ATOM   1818  CD2 LEU B 384      12.974  -3.626 -12.969  1.00 18.57          C
ANISOU 1818  CD2 LEU B 384     2013   2307   2737   -267     54   -544      C
ATOM   1819  C   LEU B 384      14.984  -1.751  -9.669  1.00 18.33          C
ANISOU 1819  C   LEU B 384     2251   2179   2533   -132     -1   -529      C
ATOM   1820  O   LEU B 384      15.530  -2.822  -9.331  1.00 18.89          O
ANISOU 1820  O   LEU B 384     2361   2229   2587   -149    -12   -496      O
ATOM   1821  N   ILE B 385      14.075  -1.135  -8.921  1.00 18.21          N
ANISOU 1821  N   ILE B 385     2267   2178   2475    -99     66   -548      N
ATOM   1822  CA  ILE B 385      13.525  -1.725  -7.689  1.00 19.18          C
ANISOU 1822  CA  ILE B 385     2460   2308   2520   -101    151   -530      C
ATOM   1823  CB  ILE B 385      13.787  -0.844  -6.427  1.00 20.69          C
ANISOU 1823  CB  ILE B 385     2787   2478   2597    -54    150   -561      C
ATOM   1824  CG1 ILE B 385      15.258  -0.466  -6.346  1.00 21.44          C
ANISOU 1824  CG1 ILE B 385     2946   2535   2668    -67     10   -570      C
ATOM   1825  CD1 ILE B 385      15.488   0.659  -5.362  1.00 26.55          C
ANISOU 1825  CD1 ILE B 385     3726   3152   3211    -43   -15   -628      C
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Figure 18 (continued)

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ATOM   1826  CG2 ILE B 385      13.366  -1.580  -5.128  1.00 19.88           C
ANISOU 1826  CG2 ILE B 385    2782   2389   2383    -62    240   -529       C
ATOM   1827  C   ILE B 385      12.005  -1.915  -7.850  1.00 19.64           C
ANISOU 1827  C   ILE B 385    2419   2430   2616   -108    271   -529       C
ATOM   1828  O   ILE B 385      11.281  -0.951  -8.157  1.00 18.63           O
ANISOU 1828  O   ILE B 385    2224   2339   2517    -49    299   -561       O
ATOM   1829  N   VAL B 386      11.540  -3.146  -7.645  1.00 20.36           N
ANISOU 1829  N   VAL B 386    2497   2531   2708   -181    338   -489       N
ATOM   1830  CA  VAL B 386      10.150  -3.524  -7.836  1.00 21.66           C
ANISOU 1830  CA  VAL B 386    2538   2772   2919   -229    446   -483       C
ATOM   1831  CB  VAL B 386       9.994  -4.733  -8.805  1.00 21.60           C
ANISOU 1831  CB  VAL B 386    2463   2755   2991   -344    426   -466       C
ATOM   1832  CG1 VAL B 386       8.493  -5.016  -9.111  1.00 20.69           C
ANISOU 1832  CG1 VAL B 386    2180   2746   2934   -422    516   -468       C
ATOM   1833  CG2 VAL B 386      10.748  -4.499 -10.055  1.00 20.40           C
ANISOU 1833  CG2 VAL B 386    2279   2580   2894   -326    304   -494       C
ATOM   1834  C   VAL B 386       9.522  -3.950  -6.522  1.00 24.28           C
ANISOU 1834  C   VAL B 386    2935   3125   3166   -253    584   -450       C
ATOM   1835  O   VAL B 386      10.124  -4.709  -5.755  1.00 24.69           O
ANISOU 1835  O   VAL B 386    3130   3109   3141   -286    588   -403       O
ATOM   1836  N   SER B 387       8.292  -3.476  -6.306  1.00 26.04           N
ANISOU 1836  N   SER B 387    3043   3448   3401   -229    700   -466       N
ATOM   1837  CA  SER B 387       7.460  -3.856  -5.191  1.00 28.34           C
ANISOU 1837  CA  SER B 387    3353   3793   3620   -262    868   -434       C
ATOM   1838  CB  SER B 387       7.142  -2.619  -4.362  1.00 28.84           C
ANISOU 1838  CB  SER B 387    3457   3899   3602   -119    947   -482       C
ATOM   1839  OG  SER B 387       6.509  -2.975  -3.165  1.00 32.36           O
ANISOU 1839  OG  SER B 387    3957   4394   3942   -143   1122   -451       O
ATOM   1840  C   SER B 387       6.204  -4.454  -5.815  1.00 30.08           C
ANISOU 1840  C   SER B 387    3358   4122   3947   -367    949   -418       C
ATOM   1841  O   SER B 387       5.597  -3.846  -6.691  1.00 30.62           O
ANISOU 1841  O   SER B 387    3245   4280   4109   -323    915   -454       O
ATOM   1842  N   GLY B 388       5.827  -5.658  -5.406  1.00 31.67           N
ANISOU 1842  N   GLY B 388    3582   4316   4136   -517   1043   -359       N
ATOM   1843  CA  GLY B 388       4.716  -6.338  -6.053  1.00 33.63           C
ANISOU 1843  CA  GLY B 388    3625   4660   4491   -666   1099   -348       C
ATOM   1844  C   GLY B 388       3.996  -7.304  -5.157  1.00 36.39           C
ANISOU 1844  C   GLY B 388    3994   5032   4800   -818   1277   -279       C
ATOM   1845  O   GLY B 388       4.534  -7.712  -4.131  1.00 36.83           O
ANISOU 1845  O   GLY B 388    4267   4991   4736   -821   1336   -224       O
ATOM   1846  N   LYS B 389       2.775  -7.660  -5.557  1.00 39.31           N
ANISOU 1846  N   LYS B 389    4131   5538   5266   -952   1358   -276       N
ATOM   1847  CA  LYS B 389       1.905  -8.546  -4.799  1.00 42.59           C
ANISOU 1847  CA  LYS B 389    4517   6004   5664  -1134   1549   -207       C
ATOM   1848  CB  LYS B 389       0.455  -8.392  -5.270  1.00 45.19           C
ANISOU 1848  CB  LYS B 389    4495   6563   6111  -1219   1629   -227       C
ATOM   1849  CG  LYS B 389      -0.202  -7.040  -4.873  1.00 47.63           C
ANISOU 1849  CG  LYS B 389    4629   7059   6410   -998   1722   -262       C
ATOM   1850  CD  LYS B 389      -1.671  -6.960  -5.309  1.00 49.06           C
ANISOU 1850  CD  LYS B 389    4426   7496   6718  -1071   1803   -268       C
ATOM   1851  CE  LYS B 389      -2.366  -5.751  -4.683  1.00 52.41           C
ANISOU 1851  CE  LYS B 389    4699   8096   7120   -834   1950   -290       C
ATOM   1852  NZ  LYS B 389      -3.530  -5.319  -5.518  1.00 55.24           N
ANISOU 1852  NZ  LYS B 389    4659   8702   7629   -803   1926   -313       N
ATOM   1853  C   LYS B 389       2.346 -10.017  -4.832  1.00 42.90           C
ANISOU 1853  C   LYS B 389    4742   5859   5697  -1341   1534   -147       C
ATOM   1854  O   LYS B 389       2.093 -10.748  -3.870  1.00 44.63           O
ANISOU 1854  O   LYS B 389    5079   6036   5842  -1458   1691    -62       O
ATOM   1855  N   ASP B 390       3.002 -10.448  -5.926  1.00 41.86           N
ANISOU 1855  N   ASP B 390    4658   5610   5637  -1378   1356   -187       N
ATOM   1856  CA  ASP B 390       3.552 -11.836  -6.076  1.00 42.33           C
ANISOU 1856  CA  ASP B 390    4930   5455   5698  -1538   1326   -145       C
ATOM   1857  CB  ASP B 390       2.436 -12.859  -6.342  1.00 44.76           C
ANISOU 1857  CB  ASP B 390    5124   5793   6090  -1829   1420   -127       C
ATOM   1858  CG  ASP B 390       1.592 -12.508  -7.561  1.00 44.57           C
ANISOU 1858  CG  ASP B 390    4794   5948   6194  -1903   1333   -218       C
ATOM   1859  OD1 ASP B 390       2.129 -11.946  -8.525  1.00 43.20           O
ANISOU 1859  OD1 ASP B 390    4586   5778   6050  -1774   1162   -293       O
ATOM   1860  OD2 ASP B 390       0.384 -12.797  -7.556  1.00 46.53           O
ANISOU 1860  OD2 ASP B 390    4828   6344   6507  -2095   1432   -208       O
ATOM   1861  C   ASP B 390       4.666 -11.971  -7.140  1.00 40.43           C
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Figure 18 (continued)

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ANISOU 1861  C   ASP B 390     4791   5075   5495  -1464   1126   -205  C
ATOM   1862  O   ASP B 390       4.998 -10.988  -7.788  1.00 39.18      O
ANISOU 1862  O   ASP B 390     4534   4994   5360  -1312   1011   -272  O
ATOM   1863  N   GLU B 391       5.221 -13.178  -7.325  1.00 40.63      N
ANISOU 1863  N   GLU B 391     5020   4893   5525  -1566   1099   -179  N
ATOM   1864  CA  GLU B 391       6.313 -13.425  -8.304  1.00 39.14      C
ANISOU 1864  CA  GLU B 391     4939   4566   5365  -1487    939   -236  C
ATOM   1865  CB  GLU B 391       6.913 -14.847  -8.174  1.00 40.09      C
ANISOU 1865  CB  GLU B 391     5332   4428   5474  -1569    953   -186  C
ATOM   1866  CG  GLU B 391       8.099 -14.930  -7.176  1.00 40.49      C
ANISOU 1866  CG  GLU B 391     5615   4348   5420  -1384    945    -95  C
ATOM   1867  CD  GLU B 391       8.475 -16.353  -6.733  1.00 43.04      C
ANISOU 1867  CD  GLU B 391     6221   4416   5717  -1454    995     -5  C
ATOM   1868  OE1 GLU B 391       8.222 -17.326  -7.492  1.00 45.74      O
ANISOU 1868  OE1 GLU B 391     6626   4619   6135  -1610    998    -44  O
ATOM   1869  OE2 GLU B 391       9.052 -16.495  -5.615  1.00 44.91      O
ANISOU 1869  OE2 GLU B 391     6636   4581   5848  -1347   1025    106  O
ATOM   1870  C   GLU B 391       5.964 -13.106  -9.762  1.00 38.03      C
ANISOU 1870  C   GLU B 391     4609   4525   5316  -1529    824   -347  C
ATOM   1871  O   GLU B 391       6.794 -12.544 -10.477  1.00 36.08      O
ANISOU 1871  O   GLU B 391     4365   4273   5069  -1380    701   -400  O
ATOM   1872  N   GLN B 392       4.750 -13.463 -10.192  1.00 39.60      N
ANISOU 1872  N   GLN B 392     4640   4822   5583  -1740    863   -375  N
ATOM   1873  CA  GLN B 392       4.252 -13.121 -11.535  1.00 38.76      C
ANISOU 1873  CA  GLN B 392     4333   4849   5544  -1791    743   -474  C
ATOM   1874  CB  GLN B 392       2.892 -13.797 -11.814  1.00 42.01      C
ANISOU 1874  CB  GLN B 392     4577   5357   6027  -2076    791   -493  C
ATOM   1875  CG  GLN B 392       2.290 -13.588 -13.235  1.00 44.80      C
ANISOU 1875  CG  GLN B 392     4722   5861   6437  -2162    643   -595  C
ATOM   1876  CD  GLN B 392       3.258 -13.942 -14.391  1.00 51.20      C
ANISOU 1876  CD  GLN B 392     5712   6521   7222  -2125    497   -682  C
ATOM   1877  OE1 GLN B 392       4.031 -14.910 -14.311  1.00 53.93      O
ANISOU 1877  OE1 GLN B 392     6326   6621   7545  -2163    520   -686  O
ATOM   1878  NE2 GLN B 392       3.209 -13.147 -15.476  1.00 51.38      N
ANISOU 1878  NE2 GLN B 392     5589   6692   7241  -2037    355   -747  N
ATOM   1879  C   GLN B 392       4.181 -11.602 -11.782  1.00 36.21      C
ANISOU 1879  C   GLN B 392     3816   4724   5219  -1585    678   -496  C
ATOM   1880  O   GLN B 392       4.634 -11.118 -12.828  1.00 34.96      O
ANISOU 1880  O   GLN B 392     3629   4588   5067  -1495    542   -558  O
ATOM   1881  N   SER B 393       3.649 -10.860 -10.813  1.00 34.95      N
ANISOU 1881  N   SER B 393     3549   4690   5041  -1504    785   -445  N
ATOM   1882  CA  SER B 393       3.519  -9.411 -10.941  1.00 33.17      C
ANISOU 1882  CA  SER B 393     3168   4622   4815  -1299    742   -464  C
ATOM   1883  CB  SER B 393       2.667  -8.847  -9.825  1.00 34.13      C
ANISOU 1883  CB  SER B 393     3167   4880   4919  -1250    901   -417  C
ATOM   1884  OG  SER B 393       1.467  -9.579  -9.745  1.00 38.87      O
ANISOU 1884  OG  SER B 393     3599   5590   5579  -1467    999   -399  O
ATOM   1885  C   SER B 393       4.865  -8.711 -10.949  1.00 30.03      C
ANISOU 1885  C   SER B 393     2939   4115   4358  -1091    657   -471  C
ATOM   1886  O   SER B 393       5.056  -7.742 -11.689  1.00 28.60      O
ANISOU 1886  O   SER B 393     2679   3999   4189   -962    554   -508  O
ATOM   1887  N   ILE B 394       5.786  -9.209 -10.124  1.00 28.74      N
ANISOU 1887  N   ILE B 394     3005   3789   4128  -1066    696   -428  N
ATOM   1888  CA  ILE B 394       7.140  -8.694 -10.082  1.00 26.95      C
ANISOU 1888  CA  ILE B 394     2927   3464   3849   -898    609   -432  C
ATOM   1889  CB  ILE B 394       7.945  -9.231  -8.866  1.00 27.07      C
ANISOU 1889  CB  ILE B 394     3165   3341   3778   -867    665   -365  C
ATOM   1890  CG1 ILE B 394       7.375  -8.668  -7.560  1.00 27.49      C
ANISOU 1890  CG1 ILE B 394     3213   3475   3757   -823    791   -323  C
ATOM   1891  CD1 ILE B 394       7.721  -9.498  -6.320  1.00 30.31      C
ANISOU 1891  CD1 ILE B 394     3780   3722   4015   -857    877   -236  C
ATOM   1892  CG2 ILE B 394       9.424  -8.817  -8.994  1.00 25.51      C
ANISOU 1892  CG2 ILE B 394     3088   3060   3545   -716    547   -374  C
ATOM   1893  C   ILE B 394       7.863  -8.944 -11.412  1.00 25.54      C
ANISOU 1893  C   ILE B 394     2774   3223   3709   -900    476   -486  C
ATOM   1894  O   ILE B 394       8.505  -8.056 -11.939  1.00 24.61      O
ANISOU 1894  O   ILE B 394     2639   3128   3585   -774    387   -513  O
ATOM   1895  N   ALA B 395       7.737 -10.156 -11.945  1.00 26.28      N
ANISOU 1895  N   ALA B 395     2921   3231   3834  -1051    474   -504  N
ATOM   1896  CA  ALA B 395       8.278 -10.524 -13.247  1.00 25.51      C
ANISOU 1896  CA  ALA B 395     2857   3077   3758  -1069    369   -571  C
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Figure 18 (continued)

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ATOM   1897  CB  ALA B 395       8.021 -12.026 -13.536  1.00 26.45           C
ANISOU 1897  CB  ALA B 395    3085   3062   3901  -1258    400   -593           C
ATOM   1898  C   ALA B 395       7.733  -9.662 -14.399  1.00 24.95           C
ANISOU 1898  C   ALA B 395    2600   3169   3712  -1056    277   -628           C
ATOM   1899  O   ALA B 395       8.500  -9.203 -15.243  1.00 22.82           O
ANISOU 1899  O   ALA B 395    2354   2893   3424   -962    190   -660           O
ATOM   1900  N   GLU B 396       6.413  -9.463 -14.442  1.00 26.63           N
ANISOU 1900  N   GLU B 396    2622   3534   3962  -1148    299   -631           N
ATOM   1901  CA  GLU B 396       5.790  -8.559 -15.438  1.00 27.37           C
ANISOU 1901  CA  GLU B 396    2521   3803   4073  -1108    201   -664           C
ATOM   1902  CB  GLU B 396       4.277  -8.475 -15.213  1.00 29.22           C
ANISOU 1902  CB  GLU B 396    2520   4221   4361  -1205    245   -652           C
ATOM   1903  CG  GLU B 396       3.527  -9.794 -15.523  1.00 32.18           C
ANISOU 1903  CG  GLU B 396    2860   4592   4773  -1475    256   -688           C
ATOM   1904  CD  GLU B 396       2.066  -9.807 -15.029  1.00 35.39           C
ANISOU 1904  CD  GLU B 396    3014   5189   5242  -1595    335   -660           C
ATOM   1905  OE1 GLU B 396       1.642  -8.836 -14.337  1.00 37.14           O
ANISOU 1905  OE1 GLU B 396    3100   5536   5475  -1443    406   -611           O
ATOM   1906  OE2 GLU B 396       1.350 -10.800 -15.323  1.00 36.33           O
ANISOU 1906  OE2 GLU B 396    3073   5331   5402  -1846    335   -690           O
ATOM   1907  C   GLU B 396       6.422  -7.145 -15.460  1.00 25.68           C
ANISOU 1907  C   GLU B 396    2306   3621   3832   -885    157   -642           C
ATOM   1908  O   GLU B 396       6.720  -6.591 -16.526  1.00 25.72           O
ANISOU 1908  O   GLU B 396    2290   3663   3819   -824     51   -666           O
ATOM   1909  N   ALA B 397       6.661  -6.577 -14.284  1.00 24.70           N
ANISOU 1909  N   ALA B 397    2225   3468   3690   -776    239   -596           N
ATOM   1910  CA  ALA B 397       7.333  -5.290 -14.153  1.00 22.65           C
ANISOU 1910  CA  ALA B 397    2004   3200   3402   -591    205   -582           C
ATOM   1911  CB  ALA B 397       7.298  -4.867 -12.714  1.00 23.05           C
ANISOU 1911  CB  ALA B 397    2103   3231   3422   -516    311   -548           C
ATOM   1912  C   ALA B 397       8.789  -5.313 -14.662  1.00 21.56           C
ANISOU 1912  C   ALA B 397    2019   2943   3231   -547    131   -594           C
ATOM   1913  O   ALA B 397       9.232  -4.375 -15.328  1.00 21.06           O
ANISOU 1913  O   ALA B 397    1949   2897   3156   -455     60   -597           O
ATOM   1914  N   ILE B 398       9.536  -6.365 -14.321  1.00 20.90           N
ANISOU 1914  N   ILE B 398    2071   2737   3132   -604    158   -592           N
ATOM   1915  CA  ILE B 398      10.913  -6.523 -14.788  1.00 20.40           C
ANISOU 1915  CA  ILE B 398    2124   2579   3048   -554    103   -603           C
ATOM   1916  CB  ILE B 398      11.619  -7.735 -14.116  1.00 20.53           C
ANISOU 1916  CB  ILE B 398    2288   2459   3053   -583    148   -585           C
ATOM   1917  CG1 ILE B 398      11.713  -7.536 -12.597  1.00 20.53           C
ANISOU 1917  CG1 ILE B 398    2348   2434   3017   -534    206   -527           C
ATOM   1918  CD1 ILE B 398      12.047  -8.805 -11.842  1.00 22.94           C
ANISOU 1918  CD1 ILE B 398    2798   2613   3304   -574    257   -485           C
ATOM   1919  CG2 ILE B 398      13.040  -7.930 -14.677  1.00 20.38           C
ANISOU 1919  CG2 ILE B 398    2352   2365   3024   -509     97   -598           C
ATOM   1920  C   ILE B 398      10.967  -6.589 -16.325  1.00 20.24           C
ANISOU 1920  C   ILE B 398    2065   2595   3029   -586     28   -652           C
ATOM   1921  O   ILE B 398      11.740  -5.886 -16.951  1.00 20.94           O
ANISOU 1921  O   ILE B 398    2167   2693   3098   -509    -23   -654           O
ATOM   1922  N   ILE B 399      10.109  -7.406 -16.920  1.00 21.51           N
ANISOU 1922  N   ILE B 399    2184   2784   3204   -714     22   -692           N
ATOM   1923  CA  ILE B 399      10.015  -7.555 -18.364  1.00 20.76           C
ANISOU 1923  CA  ILE B 399    2067   2736   3085   -764    -55   -750           C
ATOM   1924  CB  ILE B 399       8.910  -8.566 -18.768  1.00 21.63           C
ANISOU 1924  CB  ILE B 399    2131   2876   3211   -946    -65   -802           C
ATOM   1925  CG1 ILE B 399       9.288  -9.984 -18.311  1.00 22.66           C
ANISOU 1925  CG1 ILE B 399    2424   2832   3354  -1040      7   -825           C
ATOM   1926  CD1 ILE B 399       8.135 -11.012 -18.342  1.00 22.92           C
ANISOU 1926  CD1 ILE B 399    2427   2865   3418  -1259     24   -864           C
ATOM   1927  CG2 ILE B 399       8.658  -8.506 -20.279  1.00 19.65           C
ANISOU 1927  CG2 ILE B 399    1844   2714   2910   -995   -171   -865           C
ATOM   1928  C   ILE B 399       9.770  -6.221 -19.068  1.00 21.46           C
ANISOU 1928  C   ILE B 399    2050   2953   3152   -676   -131   -730           C
ATOM   1929  O   ILE B 399      10.477  -5.901 -20.019  1.00 21.12           O
ANISOU 1929  O   ILE B 399    2054   2908   3061   -632   -180   -743           O
ATOM   1930  N   VAL B 400       8.760  -5.470 -18.605  1.00 22.28           N
ANISOU 1930  N   VAL B 400    2017   3161   3287   -643   -129   -693           N
ATOM   1931  CA  VAL B 400       8.423  -4.134 -19.122  1.00 21.58           C
ANISOU 1931  CA  VAL B 400    1838   3175   3186   -529   -194   -658           C
ATOM   1932  CB  VAL B 400       7.122  -3.570 -18.448  1.00 22.39           C
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Figure 18 (continued)

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ANISOU 1932  CB  VAL B 400     1773   3394   3339   -487   -166   -626       C
ATOM   1933  CG1 VAL B 400       6.830  -2.142 -18.873  1.00 21.87           C
ANISOU 1933  CG1 VAL B 400     1642   3400   3267   -328   -226   -580       C
ATOM   1934  CG2 VAL B 400       5.918  -4.465 -18.794  1.00 22.46           C
ANISOU 1934  CG2 VAL B 400     1633   3525   3378   -639   -188   -659       C
ATOM   1935  C   VAL B 400       9.588  -3.144 -19.029  1.00 20.81           C
ANISOU 1935  C   VAL B 400     1846   2997   3063   -403   -194   -622       C
ATOM   1936  O   VAL B 400       9.846  -2.400 -19.974  1.00 21.60           O
ANISOU 1936  O   VAL B 400     1956   3127   3125   -349   -261   -603       O
ATOM   1937  N   ALA B 401      10.301  -3.154 -17.909  1.00 20.61           N
ANISOU 1937  N   ALA B 401     1904   2873   3052   -370   -125   -610       N
ATOM   1938  CA  ALA B 401      11.458  -2.262 -17.687  1.00 19.84           C
ANISOU 1938  CA  ALA B 401     1899   2702   2937   -283   -131   -583       C
ATOM   1939  CB  ALA B 401      11.879  -2.301 -16.225  1.00 19.17           C
ANISOU 1939  CB  ALA B 401     1879   2544   2860   -259    -68   -573       C
ATOM   1940  C   ALA B 401      12.637  -2.629 -18.608  1.00 19.90           C
ANISOU 1940  C   ALA B 401     1979   2670   2913   -310   -158   -597       C
ATOM   1941  O   ALA B 401      13.278  -1.758 -19.177  1.00 18.35           O
ANISOU 1941  O   ALA B 401     1809   2471   2693   -267   -189   -571       O
ATOM   1942  N   MSE B 402      12.894  -3.931 -18.781  1.00 20.40           N
ANISOU 1942  N   MSE B 402     2079   2699   2974   -381   -136   -638       N
ATOM   1943  CA  MSE B 402      13.954  -4.385 -19.707  1.00 20.55           C
ANISOU 1943  CA  MSE B 402     2161   2687   2958   -388   -140   -664       C
ATOM   1944  CB  MSE B 402      14.214  -5.888 -19.546  1.00 21.32           C
ANISOU 1944  CB  MSE B 402     2329   2705   3066   -438    -96   -712       C
ATOM   1945  CG  MSE B 402      14.859  -6.269 -18.205  1.00 19.84           C
ANISOU 1945  CG  MSE B 402     2193   2430   2916   -395    -51   -679       C
ATOM   1946  SE  MSE B 402      15.005  -8.198 -18.086  0.90 23.84          SE
ANISOU 1946  SE  MSE B 402     2821   2801   3435   -446       4   -723      SE
ATOM   1947  CE  MSE B 402      16.111  -8.378 -16.488  1.00 20.10           C
ANISOU 1947  CE  MSE B 402     2411   2243   2983   -338      29   -648       C
ATOM   1948  C   MSE B 402      13.680  -4.012 -21.179  1.00 20.87           C
ANISOU 1948  C   MSE B 402     2183   2810   2939   -405   -194   -677       C
ATOM   1949  O   MSE B 402      14.567  -3.492 -21.882  1.00 21.13           O
ANISOU 1949  O   MSE B 402     2248   2848   2930   -371   -196   -660       O
ATOM   1950  N   VAL B 403      12.449  -4.240 -21.642  1.00 20.78           N
ANISOU 1950  N   VAL B 403     2109   2873   2913   -463   -241   -701       N
ATOM   1951  CA  VAL B 403      12.053  -3.857 -22.988  1.00 19.97           C
ANISOU 1951  CA  VAL B 403     1987   2866   2733   -475   -317   -705       C
ATOM   1952  CB  VAL B 403      10.621  -4.369 -23.365  1.00 21.28           C
ANISOU 1952  CB  VAL B 403     2060   3133   2892   -566   -386   -744       C
ATOM   1953  CG1 VAL B 403      10.175  -3.778 -24.723  1.00 21.74           C
ANISOU 1953  CG1 VAL B 403     2093   3315   2853   -556   -494   -730       C
ATOM   1954  CG2 VAL B 403      10.574  -5.860 -23.429  1.00 19.64           C
ANISOU 1954  CG2 VAL B 403     1912   2867   2684   -694   -358   -835       C
ATOM   1955  C   VAL B 403      12.131  -2.338 -23.143  1.00 19.26           C
ANISOU 1955  C   VAL B 403     1877   2811   2630   -375   -351   -621       C
ATOM   1956  O   VAL B 403      12.691  -1.835 -24.114  1.00 18.91           O
ANISOU 1956  O   VAL B 403     1888   2786   2512   -354   -371   -595       O
ATOM   1957  N   PHE B 404      11.588  -1.610 -22.163  1.00 18.84           N
ANISOU 1957  N   PHE B 404     1763   2752   2642   -312   -343   -577       N
ATOM   1958  CA  PHE B 404      11.582  -0.161 -22.194  1.00 18.40           C
ANISOU 1958  CA  PHE B 404     1716   2693   2584   -208   -369   -502       C
ATOM   1959  CB  PHE B 404      10.817   0.351 -20.968  1.00 18.31           C
ANISOU 1959  CB  PHE B 404     1642   2669   2645   -138   -339   -486       C
ATOM   1960  CG  PHE B 404      10.743   1.833 -20.875  1.00 18.13           C
ANISOU 1960  CG  PHE B 404     1654   2608   2627    -16   -355   -420       C
ATOM   1961  CD1 PHE B 404       9.712   2.526 -21.510  1.00 21.57           C
ANISOU 1961  CD1 PHE B 404     2019   3125   3050     75   -424   -372       C
ATOM   1962  CE1 PHE B 404       9.623   3.911 -21.415  1.00 19.89           C
ANISOU 1962  CE1 PHE B 404     1867   2845   2845    209   -433   -306       C
ATOM   1963  CZ  PHE B 404      10.559   4.622 -20.695  1.00 19.02           C
ANISOU 1963  CZ  PHE B 404     1892   2583   2751    222   -377   -301       C
ATOM   1964  CE2 PHE B 404      11.600   3.964 -20.055  1.00 17.62           C
ANISOU 1964  CE2 PHE B 404     1765   2349   2583    115   -323   -353       C
ATOM   1965  CD2 PHE B 404      11.686   2.554 -20.149  1.00 18.96           C
ANISOU 1965  CD2 PHE B 404     1868   2590   2748     11   -311   -406       C
ATOM   1966  C   PHE B 404      13.000   0.452 -22.282  1.00 17.86           C
ANISOU 1966  C   PHE B 404     1756   2534   2495   -193   -334   -470       C
ATOM   1967  O   PHE B 404      13.187   1.520 -22.880  1.00 18.45           O
ANISOU 1967  O   PHE B 404     1877   2601   2533   -147   -362   -406       O
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Figure 18 (continued)

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ATOM   1968  N   SER B 405     13.981  -0.215 -21.670  1.00 17.56           N
ANISOU 1968  N   SER B 405   1754   2433   2485   -234   -273   -506       N
ATOM   1969  CA  SER B 405     15.373   0.264 -21.614  1.00 17.50           C
ANISOU 1969  CA  SER B 405   1807   2365   2476   -236   -240   -480       C
ATOM   1970  CB  SER B 405     16.229  -0.605 -20.689  1.00 17.20           C
ANISOU 1970  CB  SER B 405   1772   2280   2483   -256   -192   -518       C
ATOM   1971  OG  SER B 405     16.462  -1.911 -21.262  1.00 20.67           O
ANISOU 1971  OG  SER B 405   2216   2738   2901   -289   -164   -571       O
ATOM   1972  C   SER B 405     16.025   0.316 -22.998  1.00 17.94           C
ANISOU 1972  C   SER B 405   1898   2462   2456   -265   -235   -464       C
ATOM   1973  O   SER B 405     16.989   1.044 -23.203  1.00 18.90           O
ANISOU 1973  O   SER B 405   2055   2558   2568   -275   -210   -418       O
ATOM   1974  N   GLN B 406     15.494  -0.461 -23.935  1.00 18.28           N
ANISOU 1974  N   GLN B 406   1937   2573   2437   -291   -256   -504       N
ATOM   1975  CA  GLN B 406     16.000  -0.549 -25.304  1.00 19.28           C
ANISOU 1975  CA  GLN B 406   2116   2752   2458   -318   -243   -503       C
ATOM   1976  CB  GLN B 406     15.955   0.817 -25.999  1.00 19.35           C
ANISOU 1976  CB  GLN B 406   2167   2777   2406   -291   -278   -404       C
ATOM   1977  CG  GLN B 406     14.532   1.352 -26.113  1.00 20.49           C
ANISOU 1977  CG  GLN B 406   2281   2965   2539   -240   -379   -367       C
ATOM   1978  CD  GLN B 406     14.456   2.710 -26.785  1.00 22.34           C
ANISOU 1978  CD  GLN B 406   2584   3192   2713   -188   -418   -254       C
ATOM   1979  OE1 GLN B 406     15.224   3.623 -26.471  1.00 20.91           O
ANISOU 1979  OE1 GLN B 406   2462   2918   2562   -184   -372   -193       O
ATOM   1980  NE2 GLN B 406     13.519   2.849 -27.714  1.00 20.46           N
ANISOU 1980  NE2 GLN B 406   2345   3047   2383   -154   -512   -221       N
ATOM   1981  C   GLN B 406     17.374  -1.207 -25.426  1.00 19.38           C
ANISOU 1981  C   GLN B 406   2150   2743   2469   -335   -149   -539       C
ATOM   1982  O   GLN B 406     18.039  -1.028 -26.432  1.00 21.03           O
ANISOU 1982  O   GLN B 406   2400   2994   2595   -348   -107   -522       O
ATOM   1983  N   GLU B 407     17.781  -1.976 -24.415  1.00 18.80           N
ANISOU 1983  N   GLU B 407   2049   2614   2481   -325   -113   -581       N
ATOM   1984  CA  GLU B 407     19.109  -2.576 -24.370  1.00 19.09           C
ANISOU 1984  CA  GLU B 407   2080   2636   2537   -307    -30   -605       C
ATOM   1985  CB  GLU B 407     19.365  -3.321 -23.048  1.00 18.52           C
ANISOU 1985  CB  GLU B 407   1981   2495   2561   -275    -21   -629       C
ATOM   1986  CG  GLU B 407     19.622  -2.433 -21.859  1.00 18.23           C
ANISOU 1986  CG  GLU B 407   1904   2432   2593   -268    -55   -571       C
ATOM   1987  CD  GLU B 407     20.657  -2.959 -20.879  1.00 20.08           C
ANISOU 1987  CD  GLU B 407   2101   2638   2890   -228    -36   -571       C
ATOM   1988  OE1 GLU B 407     21.347  -3.968 -21.157  1.00 24.36           O
ANISOU 1988  OE1 GLU B 407   2638   3181   3437   -183     17   -605       O
ATOM   1989  OE2 GLU B 407     20.803  -2.340 -19.816  1.00 15.98           O
ANISOU 1989  OE2 GLU B 407   1565   2098   2410   -232    -77   -538       O
ATOM   1990  C   GLU B 407     19.347  -3.519 -25.533  1.00 20.61           C
ANISOU 1990  C   GLU B 407   2328   2862   2643   -309     25   -675       C
ATOM   1991  O   GLU B 407     18.464  -4.263 -25.933  1.00 20.40           O
ANISOU 1991  O   GLU B 407   2351   2831   2570   -338     -7   -741       O
ATOM   1992  N   ASP B 408     20.557  -3.455 -26.078  1.00 21.85           N
ANISOU 1992  N   ASP B 408   2473   3056   2773   -287    113   -666       N
ATOM   1993  CA  ASP B 408     20.990  -4.385 -27.121  1.00 23.75           C
ANISOU 1993  CA  ASP B 408   2775   3323   2925   -264    199   -744       C
ATOM   1994  CB  ASP B 408     22.417  -4.035 -27.600  1.00 24.31           C
ANISOU 1994  CB  ASP B 408   2792   3464   2982   -234    316   -708       C
ATOM   1995  CG  ASP B 408     22.868  -4.897 -28.750  1.00 28.24           C
ANISOU 1995  CG  ASP B 408   3363   3999   3369   -193    429   -792       C
ATOM   1996  OD1 ASP B 408     22.218  -4.835 -29.818  1.00 30.42           O
ANISOU 1996  OD1 ASP B 408   3745   4314   3501   -240    412   -821       O
ATOM   1997  OD2 ASP B 408     23.858  -5.658 -28.585  1.00 29.98           O
ANISOU 1997  OD2 ASP B 408   3540   4212   3639   -103    531   -834       O
ATOM   1998  C   ASP B 408     20.919  -5.851 -26.691  1.00 23.93           C
ANISOU 1998  C   ASP B 408   2843   3258   2993   -209    222   -841       C
ATOM   1999  O   ASP B 408     20.644  -6.717 -27.523  1.00 26.33           O
ANISOU 1999  O   ASP B 408   3249   3545   3209   -226    252   -934       O
ATOM   2000  N   ACYS B 409     21.157  -6.152 -25.422  0.50 23.03           N
ANISOU 2000  N   ACYS B 409   2677   3074   2999   -178    208   -820       N
ATOM   2001  N   BCYS B 409     21.192  -6.118 -25.410  0.50 23.70           N
ANISOU 2001  N   BCYS B 409   2758   3161   3085   -177    209   -817       N
ATOM   2002  CA  ACYS B 409     21.117  -7.552 -25.013  0.50 23.05           C
ANISOU 2002  CA  ACYS B 409   2751   2969   3040   -130    237   -894       C
ATOM   2003  CA  BCYS B 409     21.114  -7.471 -24.832  0.50 24.45           C
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Figure 18 (continued)

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ANISOU 2003  CA BCYS B 409     2916   3144   3231   -129    228   -883       C
ATOM   2004  CB ACYS B 409      21.870  -7.779 -23.708  0.50 22.54           C
ANISOU 2004  CB ACYS B 409     2619   2853   3090    -46    240   -844       C
ATOM   2005  CB BCYS B 409      21.537  -7.471 -23.355  0.50 23.66           C
ANISOU 2005  CB BCYS B 409     2747   2996   3247    -76    201   -820       C
ATOM   2006  SG ACYS B 409      20.881  -7.846 -22.247  0.50 20.66           S
ANISOU 2006  SG ACYS B 409     2393   2533   2922    -91    150   -805       S
ATOM   2007  SG BCYS B 409      23.267  -7.970 -23.032  0.50 30.51           S
ANISOU 2007  SG BCYS B 409     3537   3875   4180     76    284   -802       S
ATOM   2008  C  ACYS B 409      19.678  -8.084 -24.950  0.50 23.04           C
ANISOU 2008  C  ACYS B 409     2832   2904   3018   -222    165   -946       C
ATOM   2009  C  BCYS B 409      19.704  -8.048 -24.956  0.50 23.79           C
ANISOU 2009  C  BCYS B 409     2924   3003   3114   -220    166   -944       C
ATOM   2010  O  ACYS B 409      19.462  -9.292 -25.088  0.50 23.63           O
ANISOU 2010  O  ACYS B 409     3015   2881   3084   -225    195  -1031       O
ATOM   2011  O  BCYS B 409      19.535  -9.243 -25.224  0.50 24.43           O
ANISOU 2011  O  BCYS B 409     3115   2992   3174   -221    200  -1033       O
ATOM   2012  N   MSE B 410      18.715  -7.174 -24.763  1.00 22.13           N
ANISOU 2012  N   MSE B 410     2663   2845   2900   -296     77   -895       N
ATOM   2013  CA  MSE B 410      17.291  -7.506 -24.815  1.00 22.65           C
ANISOU 2013  CA  MSE B 410     2756   2901   2947   -395      4   -935       C
ATOM   2014  CB  MSE B 410      16.469  -6.363 -24.180  1.00 22.12           C
ANISOU 2014  CB  MSE B 410     2589   2896   2920   -418    -73   -851       C
ATOM   2015  CG  MSE B 410      14.919  -6.489 -24.305  1.00 23.37           C
ANISOU 2015  CG  MSE B 410     2717   3098   3064   -513   -154   -876       C
ATOM   2016  SE  MSE B 410      14.089  -5.800 -25.963  0.90 26.60          SE
ANISOU 2016  SE  MSE B 410     3114   3662   3331   -562   -257   -885      SE
ATOM   2017  CE  MSE B 410      14.915  -4.026 -25.917  1.00 18.43           C
ANISOU 2017  CE  MSE B 410     2040   2665   2297   -451   -245   -752       C
ATOM   2018  C   MSE B 410      16.832  -7.795 -26.261  1.00 24.21           C
ANISOU 2018  C   MSE B 410     3030   3154   3015   -459    -18  -1015       C
ATOM   2019  O   MSE B 410      16.097  -8.758 -26.507  1.00 26.05           O
ANISOU 2019  O   MSE B 410     3337   3340   3223   -543    -42  -1103       O
ATOM   2020  N   ILE B 411      17.279  -6.966 -27.209  1.00 23.73           N
ANISOU 2020  N   ILE B 411     2964   3190   2862   -434    -10   -984       N
ATOM   2021  CA  ILE B 411      16.968  -7.127 -28.621  1.00 24.58           C
ANISOU 2021  CA  ILE B 411     3159   3368   2813   -484    -31  -1049       C
ATOM   2022  CB  ILE B 411      17.364  -5.833 -29.388  1.00 25.91           C
ANISOU 2022  CB  ILE B 411     3303   3651   2892   -455    -32   -956       C
ATOM   2023  CG1 ILE B 411      16.275  -4.775 -29.197  1.00 25.08           C
ANISOU 2023  CG1 ILE B 411     3119   3612   2799   -483   -161   -866       C
ATOM   2024  CD1 ILE B 411      16.743  -3.369 -29.342  1.00 27.19           C
ANISOU 2024  CD1 ILE B 411     3355   3923   3051   -438   -154   -740       C
ATOM   2025  CG2 ILE B 411      17.488  -6.094 -30.859  1.00 27.26           C
ANISOU 2025  CG2 ILE B 411     3593   3891   2874   -479     -9  -1022       C
ATOM   2026  C   ILE B 411      17.630  -8.389 -29.207  1.00 25.31           C
ANISOU 2026  C   ILE B 411     3387   3383   2845   -464     69  -1174       C
ATOM   2027  O   ILE B 411      17.036  -9.078 -30.020  1.00 25.74           O
ANISOU 2027  O   ILE B 411     3553   3436   2793   -541     34  -1280       O
ATOM   2028  N   LYS B 412      18.851  -8.695 -28.771  1.00 24.46           N
ANISOU 2028  N   LYS B 412     3273   3215   2808   -354    188  -1167       N
ATOM   2029  CA  LYS B 412      19.531  -9.938 -29.166  1.00 25.83           C
ANISOU 2029  CA  LYS B 412     3574   3291   2950   -290    300  -1283       C
ATOM   2030  CB  LYS B 412      21.037  -9.850 -28.886  1.00 25.21           C
ANISOU 2030  CB  LYS B 412     3423   3220   2935   -138    430  -1237       C
ATOM   2031  CG  LYS B 412      21.773  -8.806 -29.742  1.00 23.92           C
ANISOU 2031  CG  LYS B 412     3193   3213   2684   -119    493  -1176       C
ATOM   2032  CD  LYS B 412      21.678  -9.165 -31.220  1.00 22.65           C
ANISOU 2032  CD  LYS B 412     3183   3097   2327   -142    550  -1280       C
ATOM   2033  CE  LYS B 412      22.511  -8.236 -32.094  1.00 20.84           C
ANISOU 2033  CE  LYS B 412     2906   3018   1995   -121    647  -1213       C
ATOM   2034  NZ  LYS B 412      21.948  -6.857 -32.071  1.00 20.43           N
ANISOU 2034  NZ  LYS B 412     2781   3055   1928   -215    534  -1081       N
ATOM   2035  C   LYS B 412      18.949 -11.213 -28.536  1.00 26.84           C
ANISOU 2035  C   LYS B 412     3802   3249   3147   -329    281  -1365       C
ATOM   2036  O   LYS B 412      19.226 -12.299 -29.012  1.00 28.99           O
ANISOU 2036  O   LYS B 412     4229   3413   3371   -300    355  -1482       O
ATOM   2037  N   ALA B 413      18.131 -11.068 -27.497  1.00 26.02           N
ANISOU 2037  N   ALA B 413     3625   3115   3145   -398    193  -1304       N
ATOM   2038  CA  ALA B 413      17.459 -12.202 -26.858  1.00 27.44           C
ANISOU 2038  CA  ALA B 413     3899   3138   3389   -471    177  -1361       C
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Figure 18 (continued)

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ATOM   2039  CB  ALA B 413      17.107 -11.851 -25.376  1.00 25.11           C
ANISOU 2039  CB  ALA B 413    3488   2823   3229   -476    137  -1246          C
ATOM   2040  C   ALA B 413      16.215 -12.670 -27.635  1.00 29.24           C
ANISOU 2040  C   ALA B 413    4212   3372   3526   -653     93  -1466          C
ATOM   2041  O   ALA B 413      15.635 -13.725 -27.336  1.00 30.83           O
ANISOU 2041  O   ALA B 413    4521   3433   3761   -753     87  -1536          O
ATOM   2042  N   VAL B 414      15.801 -11.893 -28.634  1.00 30.33           N
ANISOU 2042  N   VAL B 414    4307   3674   3544   -707     19  -1472          N
ATOM   2043  CA  VAL B 414      14.651 -12.269 -29.456  1.00 31.87           C
ANISOU 2043  CA  VAL B 414    4563   3912   3634   -882    -88  -1572          C
ATOM   2044  CB  VAL B 414      14.201 -11.126 -30.389  1.00 31.88           C
ANISOU 2044  CB  VAL B 414    4477   4127   3508   -905   -194  -1526          C
ATOM   2045  CG1 VAL B 414      13.206 -11.626 -31.408  1.00 31.91           C
ANISOU 2045  CG1 VAL B 414    4563   4190   3369  -1074   -313  -1646          C
ATOM   2046  CG2 VAL B 414      13.590 -10.006 -29.588  1.00 28.46           C
ANISOU 2046  CG2 VAL B 414    3837   3799   3177   -893   -273  -1380          C
ATOM   2047  C   VAL B 414      14.958 -13.532 -30.257  1.00 35.11           C
ANISOU 2047  C   VAL B 414    5209   4187   3946   -914    -25  -1742          C
ATOM   2048  O   VAL B 414      16.029 -13.670 -30.835  1.00 35.73           O
ANISOU 2048  O   VAL B 414    5385   4238   3952   -784     89  -1784          O
ATOM   2049  N   ARG B 415      14.009 -14.465 -30.261  1.00 37.91           N
ANISOU 2049  N   ARG B 415    5655   4449   4300  -1095    -89  -1844          N
ATOM   2050  CA  ARG B 415      14.141 -15.699 -31.006  1.00 40.89           C
ANISOU 2050  CA  ARG B 415    6289   4669   4580  -1157    -43  -2026          C
ATOM   2051  CB  ARG B 415      14.084 -16.913 -30.063  1.00 42.00           C
ANISOU 2051  CB  ARG B 415    6555   4547   4856  -1201     23  -2063          C
ATOM   2052  CG  ARG B 415      15.271 -17.043 -29.108  1.00 41.66           C
ANISOU 2052  CG  ARG B 415    6513   4373   4942   -969    167  -1969          C
ATOM   2053  CD  ARG B 415      16.615 -17.211 -29.848  1.00 43.44           C
ANISOU 2053  CD  ARG B 415    6857   4564   5085   -754    304  -2032          C
ATOM   2054  NE  ARG B 415      17.736 -17.257 -28.906  1.00 44.27           N
ANISOU 2054  NE  ARG B 415    6911   4587   5323   -528    418  -1927          N
ATOM   2055  CZ  ARG B 415      18.535 -16.226 -28.622  1.00 44.39           C
ANISOU 2055  CZ  ARG B 415    6727   4761   5378   -377    446  -1798          C
ATOM   2056  NH1 ARG B 415      18.363 -15.052 -29.226  1.00 42.41           N
ANISOU 2056  NH1 ARG B 415    6333   4736   5045   -419    386  -1752          N
ATOM   2057  NH2 ARG B 415      19.524 -16.371 -27.736  1.00 42.84           N
ANISOU 2057  NH2 ARG B 415    6481   4495   5301   -187    528  -1712          N
ATOM   2058  C   ARG B 415      13.024 -15.753 -32.047  1.00 42.87           C
ANISOU 2058  C   ARG B 415    6576   5039   4676  -1373   -200  -2134          C
ATOM   2059  O   ARG B 415      11.836 -15.538 -31.722  1.00 43.41           O
ANISOU 2059  O   ARG B 415    6496   5203   4795  -1543   -339  -2096          O
ATOM   2060  N   GLY B 416      13.414 -16.003 -33.295  1.00 43.58           N
ANISOU 2060  N   GLY B 416    6847   5143   4569  -1359   -179  -2265          C
ATOM   2061  CA  GLY B 416      12.471 -16.015 -34.399  1.00 44.83           C
ANISOU 2061  CA  GLY B 416    7057   5437   4540  -1552   -342  -2373          C
ATOM   2062  C   GLY B 416      12.035 -14.620 -34.801  1.00 43.68           C
ANISOU 2062  C   GLY B 416    6698   5579   4320  -1531   -474  -2238          C
ATOM   2063  O   GLY B 416      12.426 -13.636 -34.182  1.00 40.62           O
ANISOU 2063  O   GLY B 416    6131   5266   4039  -1383   -433  -2066          O
ATOM   2064  N   ASP B 417      11.220 -14.550 -35.849  1.00 45.98           N
ANISOU 2064  N   ASP B 417    7025   6022   4422  -1682   -641  -2318          N
ATOM   2065  CA  ASP B 417      10.713 -13.285 -36.381  1.00 46.13           C
ANISOU 2065  CA  ASP B 417    6873   6313   4341  -1660   -791  -2193          C
ATOM   2066  CB  ASP B 417      10.301 -13.462 -37.856  1.00 49.03           C
ANISOU 2066  CB  ASP B 417    7403   6811   4417  -1778   -927  -2325          C
ATOM   2067  CG  ASP B 417      11.490 -13.487 -38.803  1.00 49.91           C
ANISOU 2067  CG  ASP B 417    7750   6890   4322  -1638   -771  -2389          C
ATOM   2068  OD1 ASP B 417      12.611 -13.144 -38.380  1.00 49.40           O
ANISOU 2068  OD1 ASP B 417    7671   6752   4348  -1440   -575  -2299          O
ATOM   2069  OD2 ASP B 417      11.303 -13.843 -39.981  1.00 54.40           O
ANISOU 2069  OD2 ASP B 417    8515   7522   4632  -1731   -844  -2530          O
ATOM   2070  C   ASP B 417       9.534 -12.731 -35.573  1.00 45.38           C
ANISOU 2070  C   ASP B 417    6492   6343   4409  -1743   -943  -2070          C
ATOM   2071  O   ASP B 417       8.746 -13.487 -34.982  1.00 46.51           O
ANISOU 2071  O   ASP B 417    6586   6417   4670  -1916   -994  -2131          O
ATOM   2072  N   LEU B 418       9.403 -11.409 -35.575  1.00 44.04           N
ANISOU 2072  N   LEU B 418    6141   6353   4239  -1621  -1007  -1897          N
ATOM   2073  CA  LEU B 418       8.293 -10.755 -34.905  1.00 43.53           C
ANISOU 2073  CA  LEU B 418    5799   6428   4311  -1656  -1143  -1777          C
ATOM   2074  CB  LEU B 418       8.810  -9.653 -33.980  1.00 40.59           C
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Figure 18 (continued)

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ANISOU 2074  CB  LEU B 418     5283   6046   4093  -1450  -1042  -1589  C
ATOM   2075  CG  LEU B 418       9.808 -10.051 -32.878  1.00 38.75      C
ANISOU 2075  CG  LEU B 418     5100   5593   4029  -1362   -833  -1577  C
ATOM   2076  CD1 LEU B 418      10.306  -8.834 -32.112  1.00 35.47      C
ANISOU 2076  CD1 LEU B 418     4554   5196   3728  -1178   -766  -1401  C
ATOM   2077  CD2 LEU B 418       9.250 -11.068 -31.915  1.00 39.40      C
ANISOU 2077  CD2 LEU B 418     5149   5552   4270  -1500   -811  -1642  C
ATOM   2078  C   LEU B 418       7.241 -10.235 -35.898  1.00 45.84      C
ANISOU 2078  C   LEU B 418     6001   6978   4439  -1735  -1384  -1763  C
ATOM   2079  O   LEU B 418       7.535  -9.394 -36.757  1.00 46.01      O
ANISOU 2079  O   LEU B 418     6071   7120   4290  -1621  -1431  -1691  O
ATOM   2080  N   ASN B 419       6.020 -10.759 -35.773  1.00 47.64      N
ANISOU 2080  N   ASN B 419     6094   7293   4714  -1936  -1539  -1827  N
ATOM   2081  CA  ASN B 419       4.923 -10.448 -36.687  1.00 50.61      C
ANISOU 2081  CA  ASN B 419     6358   7932   4940  -2038  -1799  -1833  C
ATOM   2082  CB  ASN B 419       4.793 -11.549 -37.747  1.00 53.52      C
ANISOU 2082  CB  ASN B 419     6955   8284   5095  -2259  -1891  -2052  C
ATOM   2083  CG  ASN B 419       5.967 -11.586 -38.713  1.00 54.69      C
ANISOU 2083  CG  ASN B 419     7420   8348   5013  -2152  -1783  -2116  C
ATOM   2084  OD1 ASN B 419       6.257 -10.605 -39.409  1.00 55.78      O
ANISOU 2084  OD1 ASN B 419     7577   8623   4994  -1997  -1823  -2005  O
ATOM   2085  ND2 ASN B 419       6.645 -12.728 -38.767  1.00 55.63      N
ANISOU 2085  ND2 ASN B 419     7797   8235   5105  -2228  -1634  -2293  N
ATOM   2086  C   ASN B 419       3.565 -10.242 -35.997  1.00 51.57      C
ANISOU 2086  C   ASN B 419     6141   8219   5233  -2130  -1940  -1764  C
ATOM   2087  O   ASN B 419       2.515 -10.554 -36.574  1.00 54.24      O
ANISOU 2087  O   ASN B 419     6375   8743   5492  -2316  -2156  -1834  O
ATOM   2088  N   PHE B 420       3.590  -9.705 -34.776  1.00 49.62      N
ANISOU 2088  N   PHE B 420     5719   7922   5214  -1998  -1820  -1630  N
ATOM   2089  CA  PHE B 420       2.373  -9.504 -33.976  1.00 50.02      C
ANISOU 2089  CA  PHE B 420     5439   8121   5445  -2058  -1900  -1560  C
ATOM   2090  CB  PHE B 420       2.712  -9.101 -32.538  1.00 47.52      C
ANISOU 2090  CB  PHE B 420     5026   7673   5357  -1910  -1701  -1445  C
ATOM   2091  CG  PHE B 420       3.276 -10.218 -31.721  1.00 47.20      C
ANISOU 2091  CG  PHE B 420     5137   7373   5425  -2025  -1514  -1537  C
ATOM   2092  CD1 PHE B 420       4.620 -10.241 -31.399  1.00 44.34      C
ANISOU 2092  CD1 PHE B 420     4992   6786   5070  -1880  -1326  -1527  C
ATOM   2093  CE1 PHE B 420       5.152 -11.271 -30.647  1.00 43.10      C
ANISOU 2093  CE1 PHE B 420     4980   6389   5008  -1957  -1165  -1597  C
ATOM   2094  CZ  PHE B 420       4.344 -12.302 -30.207  1.00 45.97      C
ANISOU 2094  CZ  PHE B 420     5299   6709   5458  -2199  -1177  -1678  C
ATOM   2095  CE2 PHE B 420       2.993 -12.306 -30.516  1.00 48.22      C
ANISOU 2095  CE2 PHE B 420     5362   7217   5743  -2379  -1352  -1696  C
ATOM   2096  CD2 PHE B 420       2.461 -11.261 -31.273  1.00 49.98      C
ANISOU 2096  CD2 PHE B 420     5411   7705   5873  -2283  -1527  -1627  C
ATOM   2097  C   PHE B 420       1.406  -8.507 -34.584  1.00 51.27      C
ANISOU 2097  C   PHE B 420     5363   8585   5534  -1978  -2129  -1452  C
ATOM   2098  O   PHE B 420       1.809  -7.486 -35.147  1.00 50.92      O
ANISOU 2098  O   PHE B 420     5373   8599   5374  -1767  -2166  -1341  O
ATOM   2099  N   VAL B 421       0.124  -8.817 -34.417  1.00 53.07      N
ANISOU 2099  N   VAL B 421     5320   9003   5842  -2148  -2275  -1475  N
ATOM   2100  CA  VAL B 421      -0.949  -8.217 -35.197  1.00 55.35      C
ANISOU 2100  CA  VAL B 421     5378   9617   6037  -2138  -2546  -1417  C
ATOM   2101  CB  VAL B 421      -1.320  -9.170 -36.362  1.00 58.38      C
ANISOU 2101  CB  VAL B 421     5876  10095   6212  -2420  -2749  -1597  C
ATOM   2102  CG1 VAL B 421      -2.801  -9.548 -36.346  1.00 62.13      C
ANISOU 2102  CG1 VAL B 421     6005  10842   6760  -2651  -2962  -1635  C
ATOM   2103  CG2 VAL B 421      -0.857  -8.594 -37.696  1.00 59.48      C
ANISOU 2103  CG2 VAL B 421     6222  10317   6062  -2293  -2882  -1575  C
ATOM   2104  C   VAL B 421      -2.181  -7.818 -34.375  1.00 55.75      C
ANISOU 2104  C   VAL B 421     5010   9876   6297  -2121  -2603  -1318  C
ATOM   2105  O   VAL B 421      -2.233  -7.998 -33.161  1.00 53.74      O
ANISOU 2105  O   VAL B 421     4650   9514   6255  -2128  -2419  -1295  O
ATOM   2106  N   ALA B 424      -8.330  -7.054 -34.316  1.00 83.41      N
ANISOU 2106  N   ALA B 424     6624  14886  10180  -2373  -3433  -1118  N
ATOM   2107  CA  ALA B 424      -8.109  -5.823 -35.078  1.00 83.39      C
ANISOU 2107  CA  ALA B 424     6684  14974  10028  -2016  -3575   -972  C
ATOM   2108  CB  ALA B 424      -7.502  -4.750 -34.179  1.00 80.03      C
ANISOU 2108  CB  ALA B 424     6321  14356   9729  -1638  -3328   -816  C
ATOM   2109  C   ALA B 424      -7.235  -6.044 -36.325  1.00 83.09      C
ANISOU 2109  C   ALA B 424     7065  14815   9689  -2072  -3692  -1054  C
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Figure 18 (continued)

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ATOM   2110  O   ALA B 424      -7.422  -5.385 -37.357  1.00 84.69           O
ANISOU 2110  O   ALA B 424    7275  15205   9698  -1925  -3931   -976        O
ATOM   2111  N   ASN B 425      -6.283  -6.973 -36.206  1.00 81.03           N
ANISOU 2111  N   ASN B 425    7157  14244   9387  -2271  -3512  -1204        N
ATOM   2112  CA  ASN B 425      -5.300  -7.305 -37.262  1.00 80.26           C
ANISOU 2112  CA  ASN B 425    7495  13986   9016  -2326  -3549  -1305        C
ATOM   2113  CB  ASN B 425      -5.987  -7.797 -38.555  1.00 84.45           C
ANISOU 2113  CB  ASN B 425    8001  14775   9309  -2559  -3886  -1417        C
ATOM   2114  CG  ASN B 425      -5.041  -8.595 -39.454  1.00 84.90           C
ANISOU 2114  CG  ASN B 425    8524  14628   9108  -2728  -3870  -1597        C
ATOM   2115  OD1 ASN B 425      -4.463  -9.623 -39.028  1.00 84.50           O
ANISOU 2115  OD1 ASN B 425    8690  14300   9116  -2930  -3673  -1754        O
ATOM   2116  ND2 ASN B 425      -4.880  -8.118 -40.700  1.00 86.24           N
ANISOU 2116  ND2 ASN B 425    8858  14929   8980  -2630  -4069  -1569        N
ATOM   2117  C   ASN B 425      -4.251  -6.211 -37.547  1.00 77.13           C
ANISOU 2117  C   ASN B 425    7357  13442   8505  -1975  -3451  -1163        C
ATOM   2118  O   ASN B 425      -3.579  -6.224 -38.607  1.00 77.12           O
ANISOU 2118  O   ASN B 425    7668  13393   8242  -1971  -3519  -1205        O
ATOM   2119  N   GLN B 426      -4.098  -5.287 -36.579  1.00 74.28           N
ANISOU 2119  N   GLN B 426    6881  13003   8337  -1698  -3278  -1003        N
ATOM   2120  CA  GLN B 426      -3.150  -4.184 -36.730  1.00 71.77           C
ANISOU 2120  CA  GLN B 426    6789  12536   7944  -1383  -3177   -858        C
ATOM   2121  CB  GLN B 426      -3.642  -2.945 -35.979  1.00 71.41           C
ANISOU 2121  CB  GLN B 426    6489  12565   8078  -1069  -3143   -660        C
ATOM   2122  CG  GLN B 426      -4.259  -1.900 -36.902  1.00 75.93           C
ANISOU 2122  CG  GLN B 426    6956  13384   8510   -844  -3402   -501        C
ATOM   2123  CD  GLN B 426      -5.489  -1.238 -36.301  1.00 79.00           C
ANISOU 2123  CD  GLN B 426    6914  14008   9093   -664  -3487   -379        C
ATOM   2124  OE1 GLN B 426      -5.395  -0.480 -35.325  1.00 77.23           O
ANISOU 2124  OE1 GLN B 426    6622  13667   9055   -431  -3303   -275        O
ATOM   2125  NE2 GLN B 426      -6.657  -1.526 -36.882  1.00 82.04           N
ANISOU 2125  NE2 GLN B 426    7000  14737   9434   -772  -3766   -397        N
ATOM   2126  C   GLN B 426      -1.744  -4.552 -36.272  1.00 67.70           C
ANISOU 2126  C   GLN B 426    6612  11664   7446  -1398  -2889   -925        C
ATOM   2127  O   GLN B 426      -1.531  -4.823 -35.079  1.00 65.90           O
ANISOU 2127  O   GLN B 426    6334  11273   7433  -1414  -2675   -943        O
ATOM   2128  N   ARG B 427      -0.793  -4.546 -37.212  1.00 66.20           N
ANISOU 2128  N   ARG B 427    6756  11371   7026  -1382  -2882   -954        N
ATOM   2129  CA  ARG B 427       0.612  -4.844 -36.900  1.00 62.42           C
ANISOU 2129  CA  ARG B 427    6586  10583   6550  -1372  -2617  -1008        C
ATOM   2130  CB  ARG B 427       1.461  -4.982 -38.166  1.00 63.31           C
ANISOU 2130  CB  ARG B 427    7032  10653   6369  -1395  -2643  -1064        C
ATOM   2131  CG  ARG B 427       2.893  -5.323 -37.824  1.00 60.44           C
ANISOU 2131  CG  ARG B 427    6941   9997   6027  -1376  -2363  -1121        C
ATOM   2132  CD  ARG B 427       3.839  -5.274 -38.987  1.00 62.17           C
ANISOU 2132  CD  ARG B 427    7475  10176   5972  -1350  -2335  -1148        C
ATOM   2133  NE  ARG B 427       5.192  -5.498 -38.488  1.00 60.41           N
ANISOU 2133  NE  ARG B 427    7440   9693   5819  -1299  -2053  -1179        N
ATOM   2134  CZ  ARG B 427       5.789  -6.686 -38.435  1.00 61.00           C
ANISOU 2134  CZ  ARG B 427    7681   9608   5886  -1440  -1921  -1360        C
ATOM   2135  NH1 ARG B 427       5.165  -7.770 -38.880  1.00 62.69           N
ANISOU 2135  NH1 ARG B 427    7932   9872   6017  -1663  -2042  -1538        N
ATOM   2136  NH2 ARG B 427       7.015  -6.789 -37.940  1.00 59.05           N
ANISOU 2136  NH2 ARG B 427    7568   9150   5718  -1357  -1675  -1364        N
ATOM   2137  C   ARG B 427       1.276  -3.851 -35.925  1.00 58.46           C
ANISOU 2137  C   ARG B 427    6084   9911   6216  -1119  -2409   -857        C
ATOM   2138  O   ARG B 427       1.461  -2.673 -36.244  1.00 58.25           O
ANISOU 2138  O   ARG B 427    6093   9913   6128   -892  -2441   -697        O
ATOM   2139  N   LEU B 428       1.661  -4.365 -34.758  1.00 55.08           N
ANISOU 2139  N   LEU B 428    5646   9295   5987  -1171  -2200   -912        N
ATOM   2140  CA  LEU B 428       2.179  -3.563 -33.637  1.00 51.23           C
ANISOU 2140  CA  LEU B 428    5136   8653   5678   -972  -2010   -796        C
ATOM   2141  CB  LEU B 428       2.409  -4.453 -32.403  1.00 49.31           C
ANISOU 2141  CB  LEU B 428    4870   8241  5623  -1094  -1820   -888        C
ATOM   2142  CG  LEU B 428       1.337  -5.465 -31.970  1.00 49.76           C
ANISOU 2142  CG  LEU B 428    4722   8398  5786  -1320  -1873   -988        C
ATOM   2143  CD1 LEU B 428       1.713  -6.150 -30.667  1.00 44.96           C
ANISOU 2143  CD1 LEU B 428    4138   7589  5355  -1393  -1657  -1034        C
ATOM   2144  CD2 LEU B 428      -0.032  -4.799 -31.836  1.00 52.31           C
ANISOU 2144  CD2 LEU B 428    4701   8986  6189  -1248  -2023   -893        C
ATOM   2145  C   LEU B 428       3.472  -2.848 -33.998  1.00 48.96           C
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Figure 18 (continued)

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ANISOU 2145  C   LEU B 428     5109   8206   5286   -819  -1897   -722       C
ATOM   2146  O   LEU B 428       4.238  -3.337 -34.840  1.00 49.40           O
ANISOU 2146  O   LEU B 428     5395   8205   5171   -902  -1877   -801       O
ATOM   2147  N   ASN B 429       3.711  -1.694 -33.375  1.00 46.41           N
ANISOU 2147  N   ASN B 429     4755   7813   5065   -605  -1817   -577       N
ATOM   2148  CA  ASN B 429       4.977  -1.001 -33.559  1.00 43.84           C
ANISOU 2148  CA  ASN B 429     4661   7322   4674   -490  -1689   -503       C
ATOM   2149  CB  ASN B 429       4.911   0.478 -33.085  1.00 43.47           C
ANISOU 2149  CB  ASN B 429     4569   7235   4712   -252  -1670   -326       C
ATOM   2150  CG  ASN B 429       4.794   0.641 -31.557  1.00 42.88           C
ANISOU 2150  CG  ASN B 429     4363   7053   4876   -193  -1534   -322       C
ATOM   2151  OD1 ASN B 429       4.994  -0.294 -30.774  1.00 42.00           O
ANISOU 2151  OD1 ASN B 429     4224   6868   4867   -321  -1425   -433       O
ATOM   2152  ND2 ASN B 429       4.489   1.865 -31.133  1.00 43.80           N
ANISOU 2152  ND2 ASN B 429     4425   7149   5068     13  -1537   -190       N
ATOM   2153  C   ASN B 429       6.117  -1.831 -32.934  1.00 40.62           C
ANISOU 2153  C   ASN B 429     4391   6708   4334   -590  -1479   -612       C
ATOM   2154  O   ASN B 429       5.847  -2.720 -32.118  1.00 40.12           O
ANISOU 2154  O   ASN B 429     4238   6603   4402   -701  -1423   -708       O
ATOM   2155  N   PRO B 430       7.376  -1.594 -33.358  1.00 38.69           N
ANISOU 2155  N   PRO B 430     4362   6345   3995   -554  -1365   -592       N
ATOM   2156  CA  PRO B 430       8.524  -2.378 -32.884  1.00 36.44           C
ANISOU 2156  CA  PRO B 430     4197   5886   3762   -622  -1177   -688       C
ATOM   2157  CB  PRO B 430       9.721  -1.573 -33.388  1.00 36.11           C
ANISOU 2157  CB  PRO B 430     4322   5772   3625   -531  -1078   -599       C
ATOM   2158  CG  PRO B 430       9.217  -1.000 -34.683  1.00 38.86           C
ANISOU 2158  CG  PRO B 430     4726   6273   3765   -501  -1232   -528       C
ATOM   2159  CD  PRO B 430       7.784  -0.603 -34.373  1.00 39.49           C
ANISOU 2159  CD  PRO B 430     4600   6481   3923   -451  -1407   -472       C
ATOM   2160  C   PRO B 430       8.614  -2.593 -31.371  1.00 34.07           C
ANISOU 2160  C   PRO B 430     3795   5462   3688   -612  -1058   -701       C
ATOM   2161  O   PRO B 430       8.953  -3.700 -30.951  1.00 33.84           O
ANISOU 2161  O   PRO B 430     3804   5342   3711   -716   -973   -815       O
ATOM   2162  N   MSE B 431       8.323  -1.571 -30.566  1.00 32.32           N
ANISOU 2162  N   MSE B 431     3467   5227   3587   -484  -1051   -588       N
ATOM   2163  CA  MSE B 431       8.460  -1.693 -29.110  1.00 30.33           C
ANISOU 2163  CA  MSE B 431     3144   4860   3520   -467   -933   -597       C
ATOM   2164  CB  MSE B 431       8.410  -0.314 -28.423  1.00 30.13           C
ANISOU 2164  CB  MSE B 431     3074   4793   3580   -299   -911   -470       C
ATOM   2165  CG  MSE B 431       9.687   0.570 -28.662  1.00 28.94           C
ANISOU 2165  CG  MSE B 431     3090   4524   3381   -227   -832   -394       C
ATOM   2166 SE   MSE B 431      11.365  -0.168 -27.993  0.90 30.04          SE
ANISOU 2166 SE   MSE B 431     3345   4495   3575   -303   -647   -469       SE
ATOM   2167  CE  MSE B 431      10.912  -0.117 -26.095  1.00 24.52           C
ANISOU 2167  CE  MSE B 431     2526   3717   3074   -261   -588   -475       C
ATOM   2168  C   MSE B 431       7.432  -2.651 -28.519  1.00 30.68           C
ANISOU 2168  C   MSE B 431     3039   4964   3655   -580   -963   -679       C
ATOM   2169  O   MSE B 431       7.735  -3.405 -27.597  1.00 29.00           O
ANISOU 2169  O   MSE B 431     2836   4642   3540   -644   -854   -738       O
ATOM   2170  N   HIS B 432       6.223  -2.634 -29.071  1.00 32.59           N
ANISOU 2170  N   HIS B 432     3139   5384   3859   -612  -1115   -677       N
ATOM   2171  CA  HIS B 432       5.147  -3.532 -28.631  1.00 33.91           C
ANISOU 2171  CA  HIS B 432     3137   5640   4109   -754  -1154   -751       C
ATOM   2172  CB  HIS B 432       3.767  -2.933 -28.954  1.00 36.00           C
ANISOU 2172  CB  HIS B 432     3166   6133   4378   -703  -1318   -688       C
ATOM   2173  CG  HIS B 432       3.389  -1.817 -28.034  1.00 37.73           C
ANISOU 2173  CG  HIS B 432     3252   6360   4722   -503  -1267   -573       C
ATOM   2174  ND1 HIS B 432       3.912  -0.546 -28.149  1.00 38.20           N
ANISOU 2174  ND1 HIS B 432     3408   6352   4753   -297  -1254   -461       N
ATOM   2175  CE1 HIS B 432       3.416   0.220 -27.191  1.00 39.33           C
ANISOU 2175  CE1 HIS B 432     3427   6494   5023   -146  -1198   -394       C
ATOM   2176  NE2 HIS B 432       2.611  -0.513 -26.443  1.00 40.30           N
ANISOU 2176  NE2 HIS B 432     3363   6697   5252   -246  -1161   -453       N
ATOM   2177  CD2 HIS B 432       2.578  -1.793 -26.950  1.00 40.85           C
ANISOU 2177  CD2 HIS B 432     3447   6806   5268   -481  -1207   -560       C
ATOM   2178  C   HIS B 432       5.320  -4.919 -29.218  1.00 33.99           C
ANISOU 2178  C   HIS B 432     3258   5618   4040   -966  -1169   -895       C
ATOM   2179  O   HIS B 432       4.875  -5.903 -28.645  1.00 34.07           O
ANISOU 2179  O   HIS B 432     3212   5601   4134  -1120  -1134   -973       O
ATOM   2180  N   GLN B 433       5.985  -4.971 -30.363  1.00 34.16           N
ANISOU 2180  N   GLN B 433     3456   5630   3893   -972  -1208   -928       N
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Figure 18 (continued)

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ATOM   2181  CA  GLN B 433      6.441  -6.214 -30.990  1.00 35.06           C
ANISOU 2181  CA  GLN B 433    3747   5667   3907  -1135  -1189  -1076        C
ATOM   2182  CB  GLN B 433      7.210  -5.810 -32.268  1.00 35.84           C
ANISOU 2182  CB  GLN B 433    4029   5789   3799  -1070  -1217  -1069        C
ATOM   2183  CG  GLN B 433      7.217  -6.698 -33.462  1.00 39.05           C
ANISOU 2183  CG  GLN B 433    4591   6231   4014  -1213  -1290  -1208        C
ATOM   2184  CD  GLN B 433      5.848  -7.071 -33.976  1.00 42.97           C
ANISOU 2184  CD  GLN B 433    4958   6913   4453  -1371  -1501  -1267        C
ATOM   2185  OE1 GLN B 433      5.439  -8.218 -33.828  1.00 44.60           O
ANISOU 2185  OE1 GLN B 433    5176   7077   4694  -1566  -1513  -1404        O
ATOM   2186  NE2 GLN B 433      5.138  -6.124 -34.603  1.00 44.73           N
ANISOU 2186  NE2 GLN B 433    5063   7344   4587  -1294  -1676  -1164        N
ATOM   2187  C   GLN B 433      7.344  -6.960 -29.970  1.00 32.64           C
ANISOU 2187  C   GLN B 433    3545   5136   3721  -1150   -995  -1123        C
ATOM   2188  O   GLN B 433      7.122  -8.135 -29.653  1.00 33.52           O
ANISOU 2188  O   GLN B 433    3691   5166   3879  -1305   -963  -1228        O
ATOM   2189  N   LEU B 434      8.341  -6.245 -29.452  1.00 30.05           N
ANISOU 2189  N   LEU B 434    3268   4710   3441   -990   -877  -1037        N
ATOM   2190  CA  LEU B 434      9.293  -6.738 -28.427  1.00 28.11           C
ANISOU 2190  CA  LEU B 434    3102   4275   3305   -960   -710  -1051        C
ATOM   2191  CB  LEU B 434     10.386  -5.685 -28.177  1.00 24.78           C
ANISOU 2191  CB  LEU B 434    2718   3801   2896   -791   -627   -949        C
ATOM   2192  CG  LEU B 434     11.320  -5.482 -29.364  1.00 25.69           C
ANISOU 2192  CG  LEU B 434    2976   3925   2859   -752   -609   -959        C
ATOM   2193  CD1 LEU B 434     12.113  -4.184 -29.212  1.00 22.35           C
ANISOU 2193  CD1 LEU B 434    2551   3492   2449   -617   -559   -833        C
ATOM   2194  CD2 LEU B 434     12.245  -6.705 -29.605  1.00 21.91           C
ANISOU 2194  CD2 LEU B 434    2655   3326   2345   -797   -500  -1079        C
ATOM   2195  C   LEU B 434      8.644  -7.100 -27.082  1.00 27.61           C
ANISOU 2195  C   LEU B 434    2919   4169   3404  -1009   -667  -1038        C
ATOM   2196  O   LEU B 434      8.945  -8.142 -26.504  1.00 27.00           O
ANISOU 2196  O   LEU B 434    2924   3952   3382  -1083   -579  -1101        O
ATOM   2197  N   LEU B 435      7.790  -6.207 -26.587  1.00 27.73           N
ANISOU 2197  N   LEU B 435    2752   4297   3485   -949   -716   -950        N
ATOM   2198  CA  LEU B 435      7.020  -6.426 -25.375  1.00 28.98           C
ANISOU 2198  CA  LEU B 435    2775   4458   3779   -991   -669   -930        C
ATOM   2199  CB  LEU B 435      6.102  -5.222 -25.124  1.00 28.92           C
ANISOU 2199  CB  LEU B 435    2567   4606   3816   -876   -730   -833        C
ATOM   2200  CG  LEU B 435      5.273  -5.249 -23.842  1.00 32.08           C
ANISOU 2200  CG  LEU B 435    2806   5035   4346   -886   -657   -802        C
ATOM   2201  CD1 LEU B 435      6.159  -5.150 -22.588  1.00 31.09           C
ANISOU 2201  CD1 LEU B 435    2790   4739   4284   -805   -505   -770        C
ATOM   2202  CD2 LEU B 435      4.251  -4.124 -23.876  1.00 32.55           C
ANISOU 2202  CD2 LEU B 435    2657   5276   4437   -759   -732   -723        C
ATOM   2203  C   LEU B 435      6.201  -7.743 -25.431  1.00 30.18           C
ANISOU 2203  C   LEU B 435    2897   4620   3949  -1216   -695  -1029        C
ATOM   2204  O   LEU B 435      6.344  -8.595 -24.548  1.00 29.89           O
ANISOU 2204  O   LEU B 435    2917   4450   3988  -1295   -589  -1055        O
ATOM   2205  N   ARG B 436      5.363  -7.905 -26.462  1.00 31.87           N
ANISOU 2205  N   ARG B 436    3035   4987   4086  -1327   -841  -1079        N
ATOM   2206  CA  ARG B 436      4.545  -9.104 -26.599  1.00 34.36           C
ANISOU 2206  CA  ARG B 436    3319   5321   4414  -1575   -884  -1182        C
ATOM   2207  CB  ARG B 436      3.584  -9.014 -27.800  1.00 37.45           C
ANISOU 2207  CB  ARG B 436    3591   5932   4704  -1679  -1087  -1225        C
ATOM   2208  CG  ARG B 436      2.381  -8.053 -27.651  1.00 42.59           C
ANISOU 2208  CG  ARG B 436    3929   6839   5416  -1610  -1192  -1127        C
ATOM   2209  CD  ARG B 436      1.953  -7.793 -26.187  1.00 48.03           C
ANISOU 2209  CD  ARG B 436    4449   7521   6280  -1555  -1056  -1045        C
ATOM   2210  NE  ARG B 436      0.516  -8.001 -26.006  1.00 55.04           N
ANISOU 2210  NE  ARG B 436    5043   8622   7247  -1697  -1128  -1046        N
ATOM   2211  CZ  ARG B 436     -0.097  -8.150 -24.827  1.00 58.20           C
ANISOU 2211  CZ  ARG B 436    5280   9046   7789  -1739  -1005  -1006        C
ATOM   2212  NH1 ARG B 436      0.594  -8.108 -23.690  1.00 57.05           N
ANISOU 2212  NH1 ARG B 436    5256   8713   7706  -1645   -815   -964        N
ATOM   2213  NH2 ARG B 436     -1.419  -8.336 -24.784  1.00 60.68           N
ANISOU 2213  NH2 ARG B 436    5297   9587   8172  -1880  -1073  -1007        N
ATOM   2214  C   ARG B 436      5.378 -10.388 -26.679  1.00 33.35           C
ANISOU 2214  C   ARG B 436    3452   4963   4256  -1688   -796  -1293        C
ATOM   2215  O   ARG B 436      4.996 -11.405 -26.118  1.00 33.93           O
ANISOU 2215  O   ARG B 436    3548   4941   4401  -1862   -742  -1344        O
ATOM   2216  N   HIS B 437      6.510 -10.333 -27.376  1.00 31.27           N
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Figure 18 (continued)

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ANISOU 2216  N   HIS B 437     3388   4606   3887  -1584   -771  -1325     N
ATOM   2217  CA  HIS B 437       7.375 -11.493 -27.486  1.00 30.46          C
ANISOU 2217  CA  HIS B 437     3535   4282   3755  -1640   -676  -1429     C
ATOM   2218  CB  HIS B 437       8.585 -11.176 -28.355  1.00 29.42          C
ANISOU 2218  CB  HIS B 437     3569   4112   3499  -1490   -645  -1449     C
ATOM   2219  CG  HIS B 437       9.604 -12.270 -28.367  1.00 29.25          C
ANISOU 2219  CG  HIS B 437     3789   3861   3463  -1483   -520  -1543     C
ATOM   2220  ND1 HIS B 437       9.469 -13.411 -29.135  1.00 30.43          N
ANISOU 2220  ND1 HIS B 437     4121   3919   3524  -1636   -540  -1701     N
ATOM   2221  CE1 HIS B 437      10.511 -14.195 -28.937  1.00 30.95          C
ANISOU 2221  CE1 HIS B 437     4388   3767   3605  -1556   -401  -1752     C
ATOM   2222  NE2 HIS B 437      11.318 -13.608 -28.068  1.00 28.06          N
ANISOU 2222  NE2 HIS B 437     3956   3372   3333  -1368   -306  -1628     N
ATOM   2223  CD2 HIS B 437      10.769 -12.407 -27.692  1.00 28.33          C
ANISOU 2223  CD2 HIS B 437     3765   3589   3411  -1332   -377  -1504     C
ATOM   2224  C   HIS B 437       7.870 -11.985 -26.129  1.00 28.91          C
ANISOU 2224  C   HIS B 437     3395   3896   3694  -1603   -520  -1385     C
ATOM   2225  O   HIS B 437       7.863 -13.189 -25.851  1.00 29.06          O
ANISOU 2225  O   HIS B 437     3551   3745   3744  -1735   -462  -1459     O
ATOM   2226  N   PHE B 438       8.358 -11.040 -25.329  1.00 26.73          N
ANISOU 2226  N   PHE B 438     3039   3636   3480  -1419   -459  -1264     N
ATOM   2227  CA  PHE B 438       8.937 -11.304 -24.028  1.00 25.80          C
ANISOU 2227  CA  PHE B 438     2974   3366   3465  -1349   -329  -1204     C
ATOM   2228  CB  PHE B 438       9.963 -10.216 -23.649  1.00 23.35          C
ANISOU 2228  CB  PHE B 438     2648   3063   3161  -1126   -284  -1110     C
ATOM   2229  CG  PHE B 438      11.265 -10.342 -24.421  1.00 22.62          C
ANISOU 2229  CG  PHE B 438     2709   2894   2992  -1025   -250  -1151     C
ATOM   2230  CD1 PHE B 438      11.950 -11.575 -24.458  1.00 24.84          C
ANISOU 2230  CD1 PHE B 438     3175   2995   3269  -1043   -173  -1228     C
ATOM   2231  CE1 PHE B 438      13.122 -11.730 -25.196  1.00 23.69          C
ANISOU 2231  CE1 PHE B 438     3151   2795   3054   -935   -123  -1274     C
ATOM   2232  CZ  PHE B 438      13.623 -10.638 -25.892  1.00 23.06          C
ANISOU 2232  CZ  PHE B 438     3011   2846   2905   -836   -146  -1233     C
ATOM   2233  CE2 PHE B 438      12.934  -9.427 -25.889  1.00 20.07          C
ANISOU 2233  CE2 PHE B 438     2476   2627   2525   -836   -232  -1152     C
ATOM   2234  CD2 PHE B 438      11.757  -9.288 -25.168  1.00 20.56          C
ANISOU 2234  CD2 PHE B 438     2415   2738   2659   -917   -286  -1115     C
ATOM   2235  C   PHE B 438       7.911 -11.559 -22.925  1.00 27.49          C
ANISOU 2235  C   PHE B 438     3066   3597   3782  -1462   -296  -1158     C
ATOM   2236  O   PHE B 438       8.232 -12.211 -21.936  1.00 27.88          O
ANISOU 2236  O   PHE B 438     3210   3490   3892  -1471   -192  -1132     O
ATOM   2237  N   GLN B 439       6.680 -11.078 -23.096  1.00 29.49          N
ANISOU 2237  N   GLN B 439     3108   4045   4051  -1546   -381  -1143     N
ATOM   2238  CA  GLN B 439       5.604 -11.431 -22.158  1.00 31.31          C
ANISOU 2238  CA  GLN B 439     3202   4318   4377  -1685   -336  -1111     C
ATOM   2239  CB  GLN B 439       4.397 -10.507 -22.312  1.00 31.66          C
ANISOU 2239  CB  GLN B 439     2958   4625   4445  -1684   -425  -1067     C
ATOM   2240  CG  GLN B 439       4.664  -9.127 -21.740  1.00 31.16          C
ANISOU 2240  CG  GLN B 439     2805   4631   4404  -1437   -393   -961     C
ATOM   2241  CD  GLN B 439       3.554  -8.135 -21.987  1.00 35.12          C
ANISOU 2241  CD  GLN B 439     3041   5378   4926  -1380   -482   -914     C
ATOM   2242  OE1 GLN B 439       2.791  -8.271 -22.941  1.00 39.50          O
ANISOU 2242  OE1 GLN B 439     3478   6083   5446  -1486   -616   -957     O
ATOM   2243  NE2 GLN B 439       3.451  -7.121 -21.115  1.00 33.78          N
ANISOU 2243  NE2 GLN B 439     2777   5251   4808  -1202   -413   -827     N
ATOM   2244  C   GLN B 439       5.233 -12.903 -22.334  1.00 33.82          C
ANISOU 2244  C   GLN B 439     3637   4511   4701  -1941   -324  -1206     C
ATOM   2245  O   GLN B 439       4.854 -13.575 -21.370  1.00 33.96          O
ANISOU 2245  O   GLN B 439     3667   4441   4794  -2059   -225  -1176     O
ATOM   2246  N   LYS B 440       5.402 -13.399 -23.562  1.00 35.41          N
ANISOU 2246  N   LYS B 440     3956   4685   4812  -2025   -415  -1321     N
ATOM   2247  CA  LYS B 440       5.169 -14.800 -23.882  1.00 38.51          C
ANISOU 2247  CA  LYS B 440     4517   4922   5193  -2267   -412  -1437     C
ATOM   2248  CB  LYS B 440       5.054 -14.997 -25.392  1.00 40.39          C
ANISOU 2248  CB  LYS B 440     4818   5225   5302  -2360   -556  -1571     C
ATOM   2249  CG  LYS B 440       3.714 -14.593 -25.976  1.00 42.28          C
ANISOU 2249  CG  LYS B 440     4794   5744   5525  -2519   -721  -1588     C
ATOM   2250  CD  LYS B 440       3.577 -15.162 -27.360  1.00 46.14          C
ANISOU 2250  CD  LYS B 440     5410   6249   5872  -2677   -861  -1746     C
ATOM   2251  CE  LYS B 440       3.177 -16.611 -27.299  1.00 48.55          C
ANISOU 2251  CE  LYS B 440     5873   6370   6205  -2981   -837  -1868     C
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Figure 18 (continued)

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ATOM   2252  NZ  LYS B 440      3.494 -17.274 -28.574  1.00 52.80           N
ANISOU 2252  NZ  LYS B 440    6658   6823   6582  -3080   -924  -2045       N
ATOM   2253  C   LYS B 440      6.248 -15.714 -23.330  1.00 38.27           C
ANISOU 2253  C   LYS B 440    4773   4586   5181  -2209   -273  -1446       C
ATOM   2254  O   LYS B 440      5.963 -16.802 -22.818  1.00 39.92           O
ANISOU 2254  O   LYS B 440    5104   4621   5443  -2385   -203  -1469       O
ATOM   2255  N   ASP B 441      7.490 -15.259 -23.433  1.00 37.00           N
ANISOU 2255  N   ASP B 441    4716   4363   4979  -1961   -233  -1420       N
ATOM   2256  CA  ASP B 441      8.646 -16.065 -23.061  1.00 36.98           C
ANISOU 2256  CA  ASP B 441    4970   4096   4985  -1856   -118  -1430       C
ATOM   2257  CB  ASP B 441      9.051 -17.038 -24.186  1.00 39.34           C
ANISOU 2257  CB  ASP B 441    5510   4241   5196  -1921   -132  -1587       C
ATOM   2258  CG  ASP B 441     10.054 -18.065 -23.712  1.00 41.85           C
ANISOU 2258  CG  ASP B 441    6096   4260   5544  -1824     -5  -1598       C
ATOM   2259  OD1 ASP B 441     10.678 -17.827 -22.647  1.00 45.44           O
ANISOU 2259  OD1 ASP B 441    6535   4664   6067  -1657     74  -1472       O
ATOM   2260  OD2 ASP B 441     10.223 -19.107 -24.371  1.00 44.75           O
ANISOU 2260  OD2 ASP B 441    6700   4440   5864  -1905     13  -1729       O
ATOM   2261  C   ASP B 441      9.820 -15.187 -22.699  1.00 33.68           C
ANISOU 2261  C   ASP B 441    4532   3698   4566  -1573    -72  -1339       C
ATOM   2262  O   ASP B 441     10.467 -14.624 -23.570  1.00 33.22           O
ANISOU 2262  O   ASP B 441    4476   3713   4433  -1450   -108  -1370       O
ATOM   2263  N   ALA B 442     10.076 -15.111 -21.398  1.00 31.93           N
ANISOU 2263  N   ALA B 442    4298   3412   4421  -1490      9  -1227       N
ATOM   2264  CA  ALA B 442     11.092 -14.273 -20.794  1.00 29.34           C
ANISOU 2264  CA  ALA B 442    3931   3110   4105  -1256     44  -1131       C
ATOM   2265  CB  ALA B 442     10.565 -13.725 -19.499  1.00 28.01           C
ANISOU 2265  CB  ALA B 442    3635   3010   3996  -1252     75  -1017       C
ATOM   2266  C   ALA B 442     12.362 -15.072 -20.530  1.00 29.14           C
ANISOU 2266  C   ALA B 442    4112   2874   4085  -1118    122  -1131       C
ATOM   2267  O   ALA B 442     13.360 -14.523 -20.065  1.00 28.18           O
ANISOU 2267  O   ALA B 442    3967   2766   3973   -928    144  -1060       O
ATOM   2268  N   LYS B 443     12.312 -16.375 -20.791  1.00 30.53           N
ANISOU 2268  N   LYS B 443    4490   2851   4260  -1214    161  -1209       N
ATOM   2269  CA  LYS B 443     13.417 -17.281 -20.437  1.00 30.65           C
ANISOU 2269  CA  LYS B 443    4716   2636   4292  -1068    243  -1199       C
ATOM   2270  CB  LYS B 443     13.107 -18.727 -20.819  1.00 32.70           C
ANISOU 2270  CB  LYS B 443    5223   2653   4549  -1211    284  -1301       C
ATOM   2271  CG  LYS B 443     12.149 -19.457 -19.915  1.00 34.47           C
ANISOU 2271  CG  LYS B 443    5515   2754   4829  -1415    319  -1250       C
ATOM   2272  CD  LYS B 443     11.797 -20.833 -20.531  1.00 39.27           C
ANISOU 2272  CD  LYS B 443    6384   3113   5426  -1597    346  -1379       C
ATOM   2273  CE  LYS B 443     10.531 -21.410 -19.929  1.00 42.83           C
ANISOU 2273  CE  LYS B 443    6847   3503   5925  -1897    362  -1351       C
ATOM   2274  NZ  LYS B 443      9.967 -22.468 -20.802  1.00 49.83           N
ANISOU 2274  NZ  LYS B 443    7928   4218   6787  -2143    348  -1509       N
ATOM   2275  C   LYS B 443     14.752 -16.877 -21.049  1.00 29.07           C
ANISOU 2275  C   LYS B 443    4516   2473   4056   -835    255  -1220       C
ATOM   2276  O   LYS B 443     15.765 -16.817 -20.355  1.00 28.19           O
ANISOU 2276  O   LYS B 443    4414   2317   3978   -643    293  -1137       O
ATOM   2277  N   VAL B 444     14.760 -16.582 -22.341  1.00 28.47           N
ANISOU 2277  N   VAL B 444    4419   2495   3904   -857    219  -1324       N
ATOM   2278  CA  VAL B 444     15.989 -16.171 -23.001  1.00 27.62           C
ANISOU 2278  CA  VAL B 444    4298   2443   3753   -657    251  -1342       C
ATOM   2279  CB  VAL B 444     15.844 -16.164 -24.546  1.00 29.10           C
ANISOU 2279  CB  VAL B 444    4535   2697   3822   -721    229  -1480       C
ATOM   2280  CG1 VAL B 444     17.165 -15.772 -25.210  1.00 27.34           C
ANISOU 2280  CG1 VAL B 444    4300   2538   3551   -514    294  -1491       C
ATOM   2281  CG2 VAL B 444     15.361 -17.547 -25.079  1.00 29.33           C
ANISOU 2281  CG2 VAL B 444    4809   2521   3814   -859    251  -1625       C
ATOM   2282  C   VAL B 444     16.469 -14.798 -22.492  1.00 26.53           C
ANISOU 2282  C   VAL B 444    3944   2494   3640   -540    221  -1220       C
ATOM   2283  O   VAL B 444     17.678 -14.605 -22.233  1.00 26.44           O
ANISOU 2283  O   VAL B 444    3908   2485   3653   -353    265  -1171       O
ATOM   2284  N   LEU B 445     15.527 -13.866 -22.343  1.00 24.58           N
ANISOU 2284  N   LEU B 445    3544   2404   3392   -651    144  -1177       N
ATOM   2285  CA  LEU B 445     15.783 -12.541 -21.821  1.00 23.69           C
ANISOU 2285  CA  LEU B 445    3257   2443   3302   -569    112  -1072       C
ATOM   2286  CB  LEU B 445     14.471 -11.724 -21.792  1.00 22.83           C
ANISOU 2286  CB  LEU B 445    3011   2476   3188   -699     34  -1048       C
ATOM   2287  CG  LEU B 445     14.528 -10.302 -21.202  1.00 20.40           C
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Figure 18 (continued)

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ANISOU 2287  CG  LEU B 445     2549   2300   2903   -624      1   -949       C
ATOM   2288  CD1 LEU B 445      15.452  -9.445 -22.022  1.00 20.80           C
ANISOU 2288  CD1 LEU B 445     2565   2433   2905   -525     -8   -942       C
ATOM   2289  CD2 LEU B 445      13.139  -9.660 -21.107  1.00 21.01           C
ANISOU 2289  CD2 LEU B 445     2499   2498   2987   -724    -59   -929       C
ATOM   2290  C   LEU B 445      16.386 -12.568 -20.405  1.00 23.63           C
ANISOU 2290  C   LEU B 445     3244   2369   3367   -464    143   -970       C
ATOM   2291  O   LEU B 445      17.378 -11.894 -20.145  1.00 23.04           O
ANISOU 2291  O   LEU B 445     3098   2354   3304   -332    144   -914       O
ATOM   2292  N   PHE B 446      15.749 -13.322 -19.503  1.00 24.55           N
ANISOU 2292  N   PHE B 446     3434   2372   3522   -540    163   -944       N
ATOM   2293  CA  PHE B 446      16.165 -13.405 -18.103  1.00 24.13           C
ANISOU 2293  CA  PHE B 446     3400   2257   3510   -456    185   -840       C
ATOM   2294  CB  PHE B 446      15.065 -14.052 -17.240  1.00 24.76           C
ANISOU 2294  CB  PHE B 446     3545   2251   3610   -600    213   -806       C
ATOM   2295  CG  PHE B 446      13.941 -13.121 -16.834  1.00 24.29           C
ANISOU 2295  CG  PHE B 446     3329   2348   3552   -706    187   -774       C
ATOM   2296  CD1 PHE B 446      13.834 -11.833 -17.342  1.00 23.90           C
ANISOU 2296  CD1 PHE B 446     3118   2476   3486   -675    130   -782       C
ATOM   2297  CE1 PHE B 446      12.781 -10.995 -16.975  1.00 24.51           C
ANISOU 2297  CE1 PHE B 446     3058   2686   3570   -740    113   -754       C
ATOM   2298  CZ  PHE B 446      11.834 -11.441 -16.088  1.00 25.45           C
ANISOU 2298  CZ  PHE B 446     3177   2782   3710   -847    166   -718       C
ATOM   2299  CE2 PHE B 446      11.922 -12.724 -15.582  1.00 26.97           C
ANISOU 2299  CE2 PHE B 446     3531   2804   3914   -908    228   -704       C
ATOM   2300  CD2 PHE B 446      12.973 -13.555 -15.954  1.00 26.27           C
ANISOU 2300  CD2 PHE B 446     3601   2560   3821   -831    232   -730       C
ATOM   2301  C   PHE B 446      17.483 -14.179 -17.956  1.00 24.88           C
ANISOU 2301  C   PHE B 446     3609   2223   3621   -283    225   -826       C
ATOM   2302  O   PHE B 446      18.356 -13.744 -17.220  1.00 24.61           O
ANISOU 2302  O   PHE B 446     3518   2231   3603   -148    207   -746       O
ATOM   2303  N   GLN B 447      17.622 -15.313 -18.650  1.00 26.27           N
ANISOU 2303  N   GLN B 447     3944   2245   3792   -281    275   -907       N
ATOM   2304  CA  GLN B 447      18.836 -16.149 -18.568  1.00 27.60           C
ANISOU 2304  CA  GLN B 447     4228   2275   3983    -85    326   -899       C
ATOM   2305  CB  GLN B 447      18.612 -17.566 -19.132  1.00 29.38           C
ANISOU 2305  CB  GLN B 447     4694   2267   4204   -123    392   -993       C
ATOM   2306  CG  GLN B 447      17.510 -18.396 -18.464  1.00 30.32           C
ANISOU 2306  CG  GLN B 447     4963   2215   4340   -306    406   -972       C
ATOM   2307  CD  GLN B 447      17.823 -18.852 -17.033  1.00 33.13           C
ANISOU 2307  CD  GLN B 447     5407   2450   4733   -211    422   -829       C
ATOM   2308  OE1 GLN B 447      18.625 -18.249 -16.326  1.00 34.35           O
ANISOU 2308  OE1 GLN B 447     5450   2708   4895    -47    387   -731       O
ATOM   2309  NE2 GLN B 447      17.167 -19.921 -16.603  1.00 33.37           N
ANISOU 2309  NE2 GLN B 447     5644   2258   4776   -332    469   -814       N
ATOM   2310  C   GLN B 447      20.092 -15.516 -19.196  1.00 27.69           C
ANISOU 2310  C   GLN B 447     4114   2418   3988     88    332   -910       C
ATOM   2311  O   GLN B 447      21.206 -15.860 -18.819  1.00 28.70           O
ANISOU 2311  O   GLN B 447     4248   2505   4150    282    355   -863       O
ATOM   2312  N   ASN B 448      19.912 -14.574 -20.117  1.00 28.11           N
ANISOU 2312  N   ASN B 448     4044   2639   3997     20    310   -961       N
ATOM   2313  CA  ASN B 448      21.036 -13.924 -20.791  1.00 28.81           C
ANISOU 2313  CA  ASN B 448     4012   2863   4073    147    333   -967       C
ATOM   2314  CB  ASN B 448      20.855 -13.960 -22.313  1.00 30.00           C
ANISOU 2314  CB  ASN B 448     4206   3050   4141     92    375  -1087       C
ATOM   2315  CG  ASN B 448      21.087 -15.348 -22.884  1.00 33.62           C
ANISOU 2315  CG  ASN B 448     4871   3323   4581    157    462  -1194       C
ATOM   2316  OD1 ASN B 448      22.214 -15.833 -22.902  1.00 36.46           O
ANISOU 2316  OD1 ASN B 448     5249   3635   4969    354    538  -1194       O
ATOM   2317  ND2 ASN B 448      20.022 -16.002 -23.324  1.00 35.23           N
ANISOU 2317  ND2 ASN B 448     5229   3417   4739     -5    449  -1287       N
ATOM   2318  C   ASN B 448      21.345 -12.521 -20.310  1.00 27.59           C
ANISOU 2318  C   ASN B 448     3659   2892   3933    147    269   -877       C
ATOM   2319  O   ASN B 448      22.364 -11.957 -20.700  1.00 28.46           O
ANISOU 2319  O   ASN B 448     3654   3115   4046    238    290   -863       O
ATOM   2320  N   TRP B 449      20.496 -11.979 -19.431  1.00 27.14           N
ANISOU 2320  N   TRP B 449     3567   2857   3886     45    203   -819       N
ATOM   2321  CA  TRP B 449      20.598 -10.569 -18.976  1.00 25.11           C
ANISOU 2321  CA  TRP B 449     3159   2749   3634     23    140   -751       C
ATOM   2322  CB  TRP B 449      19.384 -10.193 -18.115  1.00 23.06           C
ANISOU 2322  CB  TRP B 449     2904   2486   3374    -89     95   -715       C
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Figure 18 (continued)

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ATOM   2323  CG  TRP B 449      19.356  -8.762 -17.660  1.00 22.27           C
ANISOU 2323  CG  TRP B 449    2686   2504   3269   -109     39   -663       C
ATOM   2324  CD1 TRP B 449      19.742  -8.290 -16.438  1.00 20.41           C
ANISOU 2324  CD1 TRP B 449    2424   2285   3047    -68     -1   -596       C
ATOM   2325  NE1 TRP B 449      19.559  -6.921 -16.377  1.00 20.85           N
ANISOU 2325  NE1 TRP B 449    2400   2431   3090   -109    -42   -580       N
ATOM   2326  CE2 TRP B 449      19.051  -6.475 -17.580  1.00 20.31           C
ANISOU 2326  CE2 TRP B 449    2300   2412   3004   -163    -32   -620       C
ATOM   2327  CD2 TRP B 449      18.911  -7.599 -18.423  1.00 20.86           C
ANISOU 2327  CD2 TRP B 449    2430   2431   3064   -171     12   -676       C
ATOM   2328  CE3 TRP B 449      18.388  -7.415 -19.723  1.00 22.46           C
ANISOU 2328  CE3 TRP B 449    2627   2683   3225   -229     16   -727       C
ATOM   2329  CZ3 TRP B 449      18.032  -6.099 -20.146  1.00 19.45           C
ANISOU 2329  CZ3 TRP B 449    2176   2397   2819   -261    -26   -701       C
ATOM   2330  CH2 TRP B 449      18.184  -5.005 -19.271  1.00 20.17           C
ANISOU 2330  CH2 TRP B 449    2218   2512   2935   -242    -59   -641       C
ATOM   2331  CZ2 TRP B 449      18.683  -5.166 -17.992  1.00 19.60           C
ANISOU 2331  CZ2 TRP B 449    2154   2396   2896   -202    -64   -609       C
ATOM   2332  C   TRP B 449      21.897 -10.183 -18.247  1.00 25.56           C
ANISOU 2332  C   TRP B 449    3119   2864   3729    148    117   -678       C
ATOM   2333  O   TRP B 449      22.382  -9.027 -18.344  1.00 25.79           O
ANISOU 2333  O   TRP B 449    3020   3020   3758    135     84   -649       O
ATOM   2334  N   GLY B 450      22.478 -11.120 -17.510  1.00 25.38           N
ANISOU 2334  N   GLY B 450    3157   2749   3739    265    124   -642       N
ATOM   2335  CA  GLY B 450      23.632 -10.745 -16.694  1.00 23.99           C
ANISOU 2335  CA  GLY B 450    2870   2652   3595    375     71   -565       C
ATOM   2336  C   GLY B 450      23.294 -10.879 -15.215  1.00 22.88           C
ANISOU 2336  C   GLY B 450    2794   2456   3443    373      4   -488       C
ATOM   2337  O   GLY B 450      22.203 -10.500 -14.778  1.00 21.96           O
ANISOU 2337  O   GLY B 450    2726   2323   3294    250    -10   -485       O
ATOM   2338  N   ILE B 451      24.230 -11.444 -14.467  1.00 23.43           N
ANISOU 2338  N   ILE B 451    2862   2506   3532    521    -32   -423       N
ATOM   2339  CA  ILE B 451      24.085 -11.705 -13.026  1.00 23.62           C
ANISOU 2339  CA  ILE B 451    2972   2480   3523    547    -99   -335       C
ATOM   2340  CB  ILE B 451      24.108 -13.262 -12.731  1.00 25.59           C
ANISOU 2340  CB  ILE B 451    3405   2536   3781    668    -54   -296       C
ATOM   2341  CG1 ILE B 451      23.397 -13.628 -11.415  1.00 23.95           C
ANISOU 2341  CG1 ILE B 451    3355   2232   3512    625    -81   -211       C
ATOM   2342  CD1 ILE B 451      21.902 -13.753 -11.539  1.00 21.00           C
ANISOU 2342  CD1 ILE B 451    3094   1771   3115    435     -5   -253       C
ATOM   2343  CG2 ILE B 451      25.512 -13.822 -12.743  1.00 26.15           C
ANISOU 2343  CG2 ILE B 451    3411   2625   3899    895    -78   -254       C
ATOM   2344  C   ILE B 451      25.203 -10.957 -12.295  1.00 23.68           C
ANISOU 2344  C   ILE B 451    2829   2639   3529    616   -211   -274       C
ATOM   2345  O   ILE B 451      26.284 -10.721 -12.867  1.00 24.64           O
ANISOU 2345  O   ILE B 451    2790   2871   3701    694   -221   -284       O
ATOM   2346  N   GLU B 452      24.948 -10.545 -11.062  1.00 22.87           N
ANISOU 2346  N   GLU B 452    2770   2558   3363    573   -294   -217       N
ATOM   2347  CA  GLU B 452      25.953  -9.818 -10.284  1.00 23.14           C
ANISOU 2347  CA  GLU B 452    2678   2738   3377    610   -425   -170       C
ATOM   2348  CB  GLU B 452      25.784  -8.289 -10.406  1.00 22.01           C
ANISOU 2348  CB  GLU B 452    2434   2709   3218    450   -462   -223       C
ATOM   2349  CG  GLU B 452      24.512  -7.724  -9.739  1.00 20.85           C
ANISOU 2349  CG  GLU B 452    2420   2510   2993    324   -449   -239       C
ATOM   2350  CD  GLU B 452      24.217  -6.272 -10.076  1.00 22.01           C
ANISOU 2350  CD  GLU B 452    2499   2725   3137    190   -457   -300       C
ATOM   2351  OE1 GLU B 452      25.104  -5.613 -10.663  1.00 27.18           O
ANISOU 2351  OE1 GLU B 452    3010   3475   3841    169   -493   -317       O
ATOM   2352  OE2 GLU B 452      23.097  -5.773  -9.748  1.00 23.75           O
ANISOU 2352  OE2 GLU B 452    2812   2904   3310    108   -421   -326       O
ATOM   2353  C   GLU B 452      25.850 -10.194  -8.828  1.00 24.13           C
ANISOU 2353  C   GLU B 452    2934   2823   3413    655   -507    -83       C
ATOM   2354  O   GLU B 452      24.765 -10.560  -8.354  1.00 23.91           O
ANISOU 2354  O   GLU B 452    3081   2678   3325    593   -450    -69       O
ATOM   2355  N  AHIS B 453      26.975 -10.085  -8.119  0.50 25.47           N
ANISOU 2355  N  AHIS B 453    3010   3104   3564    753   -642    -21       N
ATOM   2356  N  BHIS B 453      26.985 -10.127  -8.136  0.50 25.61           N
ANISOU 2356  N  BHIS B 453    3029   3119   3584    758   -640    -20       N
ATOM   2357  CA AHIS B 453      27.020 -10.189  -6.668  0.50 26.91           C
ANISOU 2357  CA AHIS B 453    3303   3295   3629    785   -756     64       C
ATOM   2358  CA BHIS B 453      27.023 -10.168  -6.690  0.50 27.08           C
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Figure 18 (continued)

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ANISOU 2358  CA BHIS B 453     3319   3317   3651    783   -755     61      C
ATOM   2359  CB AHIS B 453      28.450 -10.463  -6.189  0.50 28.79          C
ANISOU 2359  CB AHIS B 453     3408   3656   3874    952   -909    143      C
ATOM   2360  CB BHIS B 453      28.476 -10.182  -6.188  0.50 29.00          C
ANISOU 2360  CB BHIS B 453     3408   3713   3899    919   -922    129      C
ATOM   2361  CG AHIS B 453      28.526 -10.925  -4.767  0.50 30.03          C
ANISOU 2361  CG AHIS B 453     3716   3797   3897   1033  -1027    254      C
ATOM   2362  CG BHIS B 453      29.316 -11.302  -6.740  0.50 30.90          C
ANISOU 2362  CG BHIS B 453     3578   3926   4237   1140   -898    180      C
ATOM   2363  ND1AHIS B 453      29.035 -10.142  -3.753  0.50 30.65          N
ANISOU 2363  ND1AHIS B 453     3748   4029   3869    987  -1204    274      N
ATOM   2364  ND1BHIS B 453      29.448 -12.521  -6.107  0.50 32.82          N
ANISOU 2364  ND1BHIS B 453     3973   4053   4444   1327   -921    290      N
ATOM   2365  CE1AHIS B 453      28.956 -10.802  -2.613  0.50 31.81          C
ANISOU 2365  CE1AHIS B 453     4076   4127   3883   1080  -1278    384      C
ATOM   2366  CE1BHIS B 453      30.259 -13.295  -6.810  0.50 33.79          C
ANISOU 2366  CE1BHIS B 453     3997   4166   4676   1525   -885    307      C
ATOM   2367  NE2AHIS B 453      28.403 -11.980  -2.849  0.50 31.22          N
ANISOU 2367  NE2AHIS B 453     4168   3857   3836   1177  -1145    441      N
ATOM   2368  NE2BHIS B 453      30.665 -12.623  -7.871  0.50 32.37          N
ANISOU 2368  NE2BHIS B 453     3598   4108   4594   1462   -832    212      N
ATOM   2369  CD2AHIS B 453      28.125 -12.081  -4.187  0.50 29.97          C
ANISOU 2369  CD2AHIS B 453     3930   3629   3828   1144   -992    352      C
ATOM   2370  CD2BHIS B 453      30.092 -11.374  -7.852  0.50 31.63          C
ANISOU 2370  CD2BHIS B 453     3473   4089   4457   1217   -845    138      C
ATOM   2371  C  AHIS B 453      26.479  -8.902  -6.033  0.50 26.48          C
ANISOU 2371  C  AHIS B 453     3268   3310   3482    609   -804     15      C
ATOM   2372  C  BHIS B 453      26.269  -8.928  -6.168  0.50 26.24          C
ANISOU 2372  C  BHIS B 453     3253   3258   3458    595   -774      5      C
ATOM   2373  O  AHIS B 453      26.801  -7.795  -6.474  0.50 26.15          O
ANISOU 2373  O  AHIS B 453     3082   3376   3477    510   -837    -54      O
ATOM   2374  O  BHIS B 453      26.205  -7.888  -6.829  0.50 25.07          O
ANISOU 2374  O  BHIS B 453     2993   3176   3357    478   -757    -78      O
ATOM   2375  N   ILE B 454      25.653  -9.052  -5.003  1.00 27.27          N
ANISOU 2375  N   ILE B 454     3565   3340   3458    574   -794     52      N
ATOM   2376  CA  ILE B 454      24.998  -7.895  -4.372  1.00 27.11          C
ANISOU 2376  CA  ILE B 454     3599   3362   3338    428   -809     -5      C
ATOM   2377  CB  ILE B 454      23.458  -7.972  -4.438  1.00 26.13          C
ANISOU 2377  CB  ILE B 454     3614   3124   3189    336   -643    -36      C
ATOM   2378  CG1 ILE B 454      22.894  -9.039  -3.497  1.00 26.52          C
ANISOU 2378  CG1 ILE B 454     3869   3071   3135    383   -593     61      C
ATOM   2379  CD1 ILE B 454      21.346  -8.995  -3.430  1.00 25.42          C
ANISOU 2379  CD1 ILE B 454     3835   2857   2966    266   -427     30      C
ATOM   2380  CG2 ILE B 454      22.973  -8.138  -5.878  1.00 24.81          C
ANISOU 2380  CG2 ILE B 454     3361   2901   3162    300   -521    -96      C
ATOM   2381  C   ILE B 454      25.494  -7.622  -2.952  1.00 29.39          C
ANISOU 2381  C   ILE B 454     3966   3732   3468    447   -963     45      C
ATOM   2382  O   ILE B 454      26.002  -8.522  -2.286  1.00 30.77          O
ANISOU 2382  O   ILE B 454     4208   3900   3584    574  -1039    150      O
ATOM   2383  N   ASP B 455      25.404  -6.364  -2.524  1.00 30.94          N
ANISOU 2383  N   ASP B 455     4162   4002   3593    326  -1021    -33      N
ATOM   2384  CA  ASP B 455      25.620  -6.005  -1.121  1.00 33.96          C
ANISOU 2384  CA  ASP B 455     4670   4448   3787    311  -1152    -13      C
ATOM   2385  CB  ASP B 455      25.973  -4.520  -0.989  1.00 35.01          C
ANISOU 2385  CB  ASP B 455     4741   4672   3890    174  -1250   -124      C
ATOM   2386  CG  ASP B 455      27.250  -4.149  -1.740  1.00 38.55          C
ANISOU 2386  CG  ASP B 455     4937   5236   4473    156  -1370   -141      C
ATOM   2387  OD1 ASP B 455      28.218  -4.942  -1.722  1.00 41.76          O
ANISOU 2387  OD1 ASP B 455     5228   5723   4918    276  -1471    -55      O
ATOM   2388  OD2 ASP B 455      27.285  -3.060  -2.363  1.00 42.88          O
ANISOU 2388  OD2 ASP B 455     5401   5798   5094     27  -1354   -234      O
ATOM   2389  C   ASP B 455      24.357  -6.303  -0.319  1.00 33.96          C
ANISOU 2389  C   ASP B 455     4908   4349   3646    293  -1024     10      C
ATOM   2390  O   ASP B 455      23.262  -6.210  -0.836  1.00 32.87          O
ANISOU 2390  O   ASP B 455     4798   4127   3563    235   -851    -36      O
ATOM   2391  N   ASN B 456      24.516  -6.670   0.945  1.00 36.21          N
ANISOU 2391  N   ASN B 456     5355   4657   3744    343  -1109     87      N
ATOM   2392  CA  ASN B 456      23.386  -6.753   1.864  1.00 36.87          C
ANISOU 2392  CA  ASN B 456     5670   4678   3659    306   -986    102      C
ATOM   2393  CB  ASN B 456      23.798  -7.463   3.160  1.00 39.34          C
ANISOU 2393  CB  ASN B 456     6165   5017   3764    394  -1096    229      C
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Figure 18 (continued)

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ATOM   2394  CG  ASN B 456      24.239  -8.874   2.934  1.00 41.30           C
ANISOU 2394  CG  ASN B 456    6415   5195   4082    538  -1111    377       C
ATOM   2395  OD1 ASN B 456      23.568  -9.643   2.250  1.00 44.21           O
ANISOU 2395  OD1 ASN B 456    6797   5430   4570    545   -942    407       O
ATOM   2396  ND2 ASN B 456      25.373  -9.238   3.516  1.00 45.13           N
ANISOU 2396  ND2 ASN B 456    6893   5765   4491    658  -1320    471       N
ATOM   2397  C   ASN B 456      22.849  -5.350   2.191  1.00 35.93           C
ANISOU 2397  C   ASN B 456    5597   4597   3458    185   -957    -37       C
ATOM   2398  O   ASN B 456      23.527  -4.564   2.854  1.00 36.85           O
ANISOU 2398  O   ASN B 456    5741   4804   3458    149  -1118    -88       O
ATOM   2399  N   VAL B 457      21.652  -5.044   1.700  1.00 34.16           N
ANISOU 2399  N   VAL B 457    5380   4302   3299    127   -759   -100       N
ATOM   2400  CA  VAL B 457      20.941  -3.805   2.045  1.00 33.91           C
ANISOU 2400  CA  VAL B 457    5421   4277   3188     49   -691   -223       C
ATOM   2401  CB  VAL B 457      20.748  -2.905   0.801  1.00 32.48           C
ANISOU 2401  CB  VAL B 457    5070   4073   3197     -6   -646   -327       C
ATOM   2402  CG1 VAL B 457      20.040  -1.606   1.166  1.00 32.79           C
ANISOU 2402  CG1 VAL B 457    5203   4095   3159    -56   -577   -451       C
ATOM   2403  CG2 VAL B 457      22.108  -2.600   0.143  1.00 33.09           C
ANISOU 2403  CG2 VAL B 457    4980   4206   3385    -23   -828   -340       C
ATOM   2404  C   VAL B 457      19.575  -4.186   2.625  1.00 33.78           C
ANISOU 2404  C   VAL B 457    5553   4211   3070     49   -478   -196       C
ATOM   2405  O   VAL B 457      18.791  -4.831   1.940  1.00 32.79           O
ANISOU 2405  O   VAL B 457    5360   4029   3068     45   -328   -158       O
ATOM   2406  N   MSE B 458      19.303  -3.798   3.876  1.00 34.81           N
ANISOU 2406  N   MSE B 458    5882   4374   2971     43   -464   -218       N
ATOM   2407  CA  MSE B 458      18.039  -4.135   4.545  1.00 35.03           C
ANISOU 2407  CA  MSE B 458    6051   4379   2879     40   -244   -187       C
ATOM   2408  CB  MSE B 458      18.056  -3.708   6.020  1.00 37.27           C
ANISOU 2408  CB  MSE B 458    6581   4716   2866     45   -267   -210       C
ATOM   2409  CG  MSE B 458      16.872  -4.222   6.828  1.00 37.38           C
ANISOU 2409  CG  MSE B 458    6752   4723   2726     45    -30   -149       C
ATOM   2410  SE  MSE B 458      16.820  -3.511   8.603  0.90 41.33          SE
ANISOU 2410  SE  MSE B 458    7579   5297   2828     55    -30   -211       SE
ATOM   2411  CE  MSE B 458      15.420  -4.680   9.317  1.00 44.38           C
ANISOU 2411  CE  MSE B 458    8103   5675   3084     45    298    -58       C
ATOM   2412  C   MSE B 458      16.868  -3.480   3.818  1.00 33.79           C
ANISOU 2412  C   MSE B 458    5784   4197   2856     10    -53   -282       C
ATOM   2413  O   MSE B 458      16.995  -2.362   3.336  1.00 32.16           O
ANISOU 2413  O   MSE B 458    5505   3991   2722     -1    -98   -401       O
ATOM   2414  N   GLY B 459      15.744  -4.194   3.715  1.00 34.01           N
ANISOU 2414  N   GLY B 459    5796   4205   2922     -6    153   -221       N
ATOM   2415  CA  GLY B 459      14.570  -3.680   2.991  1.00 33.33           C
ANISOU 2415  CA  GLY B 459    5569   4123   2974    -25    328   -296       C
ATOM   2416  C   GLY B 459      14.548  -4.009   1.501  1.00 31.85           C
ANISOU 2416  C   GLY B 459    5161   3902   3041    -49    307   -289       C
ATOM   2417  O   GLY B 459      13.682  -3.523   0.781  1.00 30.68           O
ANISOU 2417  O   GLY B 459    4875   3768   3012    -57    409   -348       O
ATOM   2418  N   MSE B 460      15.478  -4.860   1.057  1.00 31.24           N
ANISOU 2418  N   MSE B 460    5054   3784   3033    -50    177   -214       N
ATOM   2419  CA  MSE B 460      15.677  -5.150  -0.354  1.00 31.07           C
ANISOU 2419  CA  MSE B 460    4850   3729   3225    -65    137   -221       C
ATOM   2420  CB  MSE B 460      16.629  -4.100  -0.868  1.00 30.09           C
ANISOU 2420  CB  MSE B 460    4650   3629   3156    -42    -20   -303       C
ATOM   2421  CG  MSE B 460      16.615  -3.833  -2.309  1.00 32.45           C
ANISOU 2421  CG  MSE B 460    4767   3917   3643    -59    -30   -347       C
ATOM   2422  SE  MSE B 460      17.913  -2.375  -2.609  0.90 34.00          SE
ANISOU 2422  SE  MSE B 460    4919   4140   3859    -59   -219   -436       SE
ATOM   2423  CE  MSE B 460      16.991  -0.929  -1.707  1.00 33.99           C
ANISOU 2423  CE  MSE B 460    5050   4135   3729    -54   -133   -542       C
ATOM   2424  C   MSE B 460      16.331  -6.512  -0.539  1.00 28.84           C
ANISOU 2424  C   MSE B 460    4594   3383   2980    -52     79   -112       C
ATOM   2425  O   MSE B 460      17.138  -6.910   0.282  1.00 30.15           O
ANISOU 2425  O   MSE B 460    4884   3544   3026     -3    -19    -42       O
ATOM   2426  N   VAL B 461      16.008  -7.206  -1.624  1.00 27.09           N
ANISOU 2426  N   VAL B 461    4265   3111   2918    -87    131   -100       N
ATOM   2427  CA  VAL B 461      16.671  -8.480  -1.957  1.00 26.80           C
ANISOU 2427  CA  VAL B 461    4263   2984   2937    -58     81    -14       C
ATOM   2428  CB  VAL B 461      15.830  -9.766  -1.561  1.00 27.65           C
ANISOU 2428  CB  VAL B 461    4497   2994   3014    -121    226     84       C
ATOM   2429  CG1 VAL B 461      15.820  -9.957  -0.084  1.00 30.27           C
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Figure 18 (continued)

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ANISOU 2429  CG1 VAL B 461     5027   3330   3145    -99    248    174       C
ATOM   2430  CG2 VAL B 461      14.394  -9.726  -2.097  1.00 27.50           C
ANISOU 2430  CG2 VAL B 461     4380   2992   3077   -246    392     36       C
ATOM   2431  C   VAL B 461      17.010  -8.528  -3.436  1.00 24.89           C
ANISOU 2431  C   VAL B 461     3858   2724   2874    -57     39    -71       C
ATOM   2432  O   VAL B 461      16.458  -7.760  -4.216  1.00 22.95           O
ANISOU 2432  O   VAL B 461     3485   2528   2709   -103     75   -156       O
ATOM   2433  N   GLY B 462      17.912  -9.440  -3.809  1.00 24.45           N
ANISOU 2433  N   GLY B 462     3821   2599   2872     11    -31    -19       N
ATOM   2434  CA  GLY B 462      18.142  -9.764  -5.208  1.00 23.12           C
ANISOU 2434  CA  GLY B 462     3536   2394   2854     12    -34    -67       C
ATOM   2435  C   GLY B 462      17.109 -10.760  -5.728  1.00 23.17           C
ANISOU 2435  C   GLY B 462     3586   2297   2922    -82     97    -61       C
ATOM   2436  O   GLY B 462      16.340 -11.359  -4.962  1.00 23.84           O
ANISOU 2436  O   GLY B 462     3793   2324   2942   -146    191      2       O
ATOM   2437  N   VAL B 463      17.080 -10.925  -7.043  1.00 22.89           N
ANISOU 2437  N   VAL B 463     3453   2241   3003   -108    105   -129       N
ATOM   2438  CA  VAL B 463      16.154 -11.866  -7.677  1.00 23.22           C
ANISOU 2438  CA  VAL B 463     3530   2185   3106   -220    206   -145       C
ATOM   2439  CB  VAL B 463      14.824 -11.131  -8.120  1.00 22.55           C
ANISOU 2439  CB  VAL B 463     3313   2204   3052   -353    274   -216       C
ATOM   2440  CG1 VAL B 463      15.089 -10.058  -9.145  1.00 20.58           C
ANISOU 2440  CG1 VAL B 463     2902   2062   2857   -321    205   -302       C
ATOM   2441  CG2 VAL B 463      13.796 -12.107  -8.634  1.00 23.79           C
ANISOU 2441  CG2 VAL B 463     3493   2283   3263   -503    366   -230       C
ATOM   2442  C   VAL B 463      16.893 -12.591  -8.810  1.00 22.85           C
ANISOU 2442  C   VAL B 463     3485   2051   3146   -163    174   -184       C
ATOM   2443  O   VAL B 463      17.576 -11.960  -9.618  1.00 21.88           O
ANISOU 2443  O   VAL B 463     3242   2006   3066   -101    110   -243       O
ATOM   2444  N   LEU B 464      16.772 -13.917  -8.835  1.00 24.48           N
ANISOU 2444  N   LEU B 464     3847   2086   3370   -184    230   -147       N
ATOM   2445  CA  LEU B 464      17.398 -14.757  -9.860  1.00 24.70           C
ANISOU 2445  CA  LEU B 464     3920   1996   3469   -121    225   -193       C
ATOM   2446  CB  LEU B 464      16.692 -16.167  -9.278  1.00 26.50           C
ANISOU 2446  CB  LEU B 464     4383   2003   3684    -60    262   -101       C
ATOM   2447  CG  LEU B 464      18.614 -16.282  -8.045  1.00 27.20           C
ANISOU 2447  CG  LEU B 464     4556   2079   3698    112    196     31       C
ATOM   2448  CD1 LEU B 464      18.909 -17.751  -7.716  1.00 26.95           C
ANISOU 2448  CD1 LEU B 464     4774   1800   3666    194    234    122       C
ATOM   2449  CD2 LEU B 464      19.925 -15.482  -8.186  1.00 25.91           C
ANISOU 2449  CD2 LEU B 464     4231   2069   3545    291     74     17       C
ATOM   2450  C   LEU B 464      16.470 -14.848 -11.075  1.00 24.29           C
ANISOU 2450  C   LEU B 464     3811   1943   3475   -279    275   -305       C
ATOM   2451  O   LEU B 464      15.296 -14.566 -10.935  1.00 23.51           O
ANISOU 2451  O   LEU B 464     3661   1902   3369   -438    321   -317       O
ATOM   2452  N   PRO B 465      16.996 -15.222 -12.270  1.00 25.25           N
ANISOU 2452  N   PRO B 465     3932   2015   3645   -232    265   -388       N
ATOM   2453  CA  PRO B 465      16.120 -15.432 -13.438  1.00 25.68           C
ANISOU 2453  CA  PRO B 465     3964   2062   3731   -391    297   -499       C
ATOM   2454  CB  PRO B 465      17.050 -16.084 -14.460  1.00 25.85           C
ANISOU 2454  CB  PRO B 465     4061   1984   3778   -277    298   -570       C
ATOM   2455  CG  PRO B 465      18.388 -15.510 -14.133  1.00 24.55           C
ANISOU 2455  CG  PRO B 465     3812   1904   3610    -63    245   -516       C
ATOM   2456  CD  PRO B 465      18.421 -15.441 -12.622  1.00 25.27           C
ANISOU 2456  CD  PRO B 465     3945   1989   3669    -26    225   -389       C
ATOM   2457  C   PRO B 465      14.846 -16.281 -13.209  1.00 28.21           C
ANISOU 2457  C   PRO B 465     4391   2269   4059   -603    369   -498       C
ATOM   2458  O   PRO B 465      13.803 -15.960 -13.790  1.00 27.91           O
ANISOU 2458  O   PRO B 465     4244   2328   4033   -771    372   -565       O
ATOM   2459  N   ASP B 466      14.925 -17.337 -12.388  1.00 30.80           N
ANISOU 2459  N   ASP B 466     4922   2403   4379   -599    424   -415       N
ATOM   2460  CA  ASP B 466      13.752 -18.159 -12.058  1.00 33.52           C
ANISOU 2460  CA  ASP B 466     5376   2631   4730   -825    507   -396       C
ATOM   2461  CB  ASP B 466      14.126 -19.605 -11.623  1.00 35.98           C
ANISOU 2461  CB  ASP B 466     5985   2643   5044   -799    566   -329       C
ATOM   2462  CG  ASP B 466      14.980 -19.668 -10.343  1.00 37.63           C
ANISOU 2462  CG  ASP B 466     6297   2804   5198   -600    556   -174       C
ATOM   2463  OD1 ASP B 466      15.185 -18.631  -9.683  1.00 38.27           O
ANISOU 2463  OD1 ASP B 466     6230   3080   5230   -519    509   -123       O
ATOM   2464  OD2 ASP B 466      15.460 -20.776  -9.985  1.00 41.34           O
ANISOU 2464  OD2 ASP B 466     7013   3029   5664   -519    587   -101       O
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Figure 18 (continued)

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ATOM   2465  C   ASP B 466      12.853 -17.487 -11.009  1.00 33.70           C
ANISOU 2465  C   ASP B 466    5289   2800   4716   -926    547   -316       C
ATOM   2466  O   ASP B 466      11.911 -18.095 -10.495  1.00 35.21           O
ANISOU 2466  O   ASP B 466    5552   2920   4904  -1111    636   -270       O
ATOM   2467  N   MSE B 467      13.146 -16.229 -10.700  1.00 32.05           N
ANISOU 2467  N   MSE B 467    4911   2790   4475   -810    493   -302       N
ATOM   2468  CA  MSE B 467      12.363 -15.426  -9.749  1.00 32.32           C
ANISOU 2468  CA  MSE B 467    4839   2978   4464   -867    537   -247       C
ATOM   2469  CB  MSE B 467      10.852 -15.367 -10.098  1.00 33.45           C
ANISOU 2469  CB  MSE B 467    4846   3217   4648  -1096    603   -295       C
ATOM   2470  CG  MSE B 467      10.480 -14.569 -11.341  1.00 34.23           C
ANISOU 2470  CG  MSE B 467    4734   3476   4798  -1122    530   -411       C
ATOM   2471  SE  MSE B 467      11.051 -12.703 -11.393  0.90 35.66          SE
ANISOU 2471  SE  MSE B 467    4726   3873   4950   -913    438   -429      SE
ATOM   2472  CE  MSE B 467      10.370 -12.081  -9.735  1.00 33.79           C
ANISOU 2472  CE  MSE B 467    4462   3731   4645   -908    538   -336       C
ATOM   2473  C   MSE B 467      12.545 -15.812  -8.285  1.00 32.77           C
ANISOU 2473  C   MSE B 467    5059   2956   4437   -824    593   -111       C
ATOM   2474  O   MSE B 467      11.814 -15.332  -7.424  1.00 33.07           O
ANISOU 2474  O   MSE B 467    5047   3099   4420   -886    661    -63       O
ATOM   2475  N   THR B 468      13.511 -16.674  -8.005  1.00 33.28           N
ANISOU 2475  N   THR B 468    5323   2840   4482   -705    569    -45       N
ATOM   2476  CA  THR B 468      13.885 -16.983  -6.629  1.00 33.89           C
ANISOU 2476  CA  THR B 468    5568   2851   4457   -623    589     98       C
ATOM   2477  CB  THR B 468      14.768 -18.251  -6.562  1.00 35.34           C
ANISOU 2477  CB  THR B 468    5996   2785   4646   -509    572    172       C
ATOM   2478  OG1 THR B 468      13.977 -19.388  -6.930  1.00 37.79           O
ANISOU 2478  OG1 THR B 468    6452   2897   5009   -697    675    166       O
ATOM   2479  CG2 THR B 468      15.313 -18.475  -5.164  1.00 36.57           C
ANISOU 2479  CG2 THR B 468    6321   2896   4679   -382    556    334       C
ATOM   2480  C   THR B 468      14.591 -15.751  -6.022  1.00 32.35           C
ANISOU 2480  C   THR B 468    5263   2840   4187   -460    495    111       C
ATOM   2481  O   THR B 468      15.453 -15.146  -6.652  1.00 30.75           O
ANISOU 2481  O   THR B 468    4946   2713   4024   -334    390     46       O
ATOM   2482  N   PRO B 469      14.192 -15.361  -4.801  1.00 32.67           N
ANISOU 2482  N   PRO B 469    5345   2955   4113   -481    542    189       N
ATOM   2483  CA  PRO B 469      14.887 -14.289  -4.133  1.00 31.19           C
ANISOU 2483  CA  PRO B 469    5102   2914   3836   -342    447    195       C
ATOM   2484  CB  PRO B 469      13.971 -13.957  -2.953  1.00 32.02           C
ANISOU 2484  CB  PRO B 469    5259   3094   3815   -428    558    252       C
ATOM   2485  CG  PRO B 469      13.209 -15.162  -2.692  1.00 35.33           C
ANISOU 2485  CG  PRO B 469    5828   3365   4231   -568    694    337       C
ATOM   2486  CD  PRO B 469      13.071 -15.891  -4.001  1.00 34.33           C
ANISOU 2486  CD  PRO B 469    5660   3121   4262   -648    695    268       C
ATOM   2487  C   PRO B 469      16.256 -14.732  -3.650  1.00 31.84           C
ANISOU 2487  C   PRO B 469    5312   2920   3863   -153    327    282       C
ATOM   2488  O   PRO B 469      16.421 -15.890  -3.258  1.00 34.25           O
ANISOU 2488  O   PRO B 469    5817   3054   4141   -128    356    388       O
ATOM   2489  N   SER B 470      17.223 -13.819  -3.690  1.00 30.20           N
ANISOU 2489  N   SER B 470    4990   2841   3645    -24    191    241       N
ATOM   2490  CA  SER B 470      18.571 -14.100  -3.234  1.00 30.87           C
ANISOU 2490  CA  SER B 470    5139   2908   3684    161     53    318       C
ATOM   2491  CB  SER B 470      19.482 -14.433  -4.402  1.00 29.68           C
ANISOU 2491  CB  SER B 470    4890   2716   3672    269    -11    267       C
ATOM   2492  OG  SER B 470      20.792 -14.608  -3.929  1.00 30.33           O
ANISOU 2492  OG  SER B 470    4987   2820   3717    461   -149    343       O
ATOM   2493  C   SER B 470      19.131 -12.899  -2.510  1.00 30.64           C
ANISOU 2493  C   SER B 470    5033   3057   3553    216    -65    302       C
ATOM   2494  O   SER B 470      18.928 -11.761  -2.930  1.00 29.05           O
ANISOU 2494  O   SER B 470    4674   2979   3385    159    -76    194       O
ATOM   2495  N   THR B 471      19.865 -13.168  -1.437  1.00 32.50           N
ANISOU 2495  N   THR B 471    5393   3296   3659    329    -164    411       N
ATOM   2496  CA  THR B 471      20.614 -12.129  -0.716  1.00 32.89           C
ANISOU 2496  CA  THR B 471    5386   3515   3599    395   -315    395       C
ATOM   2497  CB  THR B 471      20.490 -12.340   0.813  1.00 34.91           C
ANISOU 2497  CB  THR B 471    5860   3771   3632    403   -333    511       C
ATOM   2498  OG1 THR B 471      20.876 -13.675   1.140  1.00 37.72           O
ANISOU 2498  OG1 THR B 471    6384   3985   3961    514   -348    662       O
ATOM   2499  CG2 THR B 471      19.028 -12.160   1.273  1.00 34.90           C
ANISOU 2499  CG2 THR B 471    5958   3753   3549    246   -138    495       C
ATOM   2500  C   THR B 471      22.099 -12.082  -1.145  1.00 32.75           C
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Figure 18 (continued)

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ANISOU 2500  C   THR B 471     5227   3559   3656    534   -494    396       C
ATOM   2501  O   THR B 471      22.890 -11.337  -0.583  1.00 34.16           O
ANISOU 2501  O   THR B 471     5345   3877   3756    575   -648    389       O
ATOM   2502  N   GLU B 472      22.465 -12.869  -2.157  1.00 31.92           N
ANISOU 2502  N   GLU B 472     5064   3360   3702    609   -467    396       N
ATOM   2503  CA  GLU B 472      23.861 -12.976  -2.589  1.00 31.44           C
ANISOU 2503  CA  GLU B 472     4859   3365   3724    773   -605    407       C
ATOM   2504  CB  GLU B 472      24.370 -14.411  -2.376  1.00 33.51           C
ANISOU 2504  CB  GLU B 472     5266   3476   3992    956   -618    540       C
ATOM   2505  CG  GLU B 472      24.422 -14.846  -0.927  1.00 37.90           C
ANISOU 2505  CG  GLU B 472     6031   4005   4363   1022   -691    691       C
ATOM   2506  CD  GLU B 472      23.763 -16.204  -0.707  1.00 44.50           C
ANISOU 2506  CD  GLU B 472     7139   4591   5179   1042   -560    804       C
ATOM   2507  OE1 GLU B 472      24.485 -17.177  -0.350  1.00 46.85           O
ANISOU 2507  OE1 GLU B 472     7556   4788   5457   1242   -630    939       O
ATOM   2508  OE2 GLU B 472      22.521 -16.302  -0.892  1.00 44.38           O
ANISOU 2508  OE2 GLU B 472     7216   4477   5169    856   -389    762       O
ATOM   2509  C   GLU B 472      24.062 -12.542  -4.036  1.00 28.34           C
ANISOU 2509  C   GLU B 472     4255   3014   3498    741   -565    283       C
ATOM   2510  O   GLU B 472      25.024 -11.859  -4.337  1.00 27.47           O
ANISOU 2510  O   GLU B 472     3954   3050   3434    785   -672    244       O
ATOM   2511  N   MSE B 473      23.145 -12.942  -4.916  1.00 26.75           N
ANISOU 2511  N   MSE B 473     4093   2693   3379    652   -412    224       N
ATOM   2512  CA  MSE B 473      23.244 -12.649  -6.358  1.00 25.55           C
ANISOU 2512  CA  MSE B 473     3777   2567   3364    621   -362    111       C
ATOM   2513  CB  MSE B 473      23.499 -13.920  -7.189  1.00 25.85           C
ANISOU 2513  CB  MSE B 473     3877   2448   3495    728   -290    117       C
ATOM   2514  CG  MSE B 473      24.655 -14.796  -6.777  1.00 28.02           C
ANISOU 2514  CG  MSE B 473     4194   2678   3776    959   -368    220       C
ATOM   2515 SE   MSE B 473      26.394 -14.027  -6.988  0.90 30.87          SE
ANISOU 2515 SE   MSE B 473     4253   3284   4190   1120   -526    214       SE
ATOM   2516  CE  MSE B 473      26.496 -13.771  -8.933  1.00 22.35           C
ANISOU 2516  CE  MSE B 473     2999   2234   3260   1079   -399     59       C
ATOM   2517  C   MSE B 473      21.954 -12.044  -6.864  1.00 23.67           C
ANISOU 2517  C   MSE B 473     3524   2330   3138    431   -255     20       C
ATOM   2518  O   MSE B 473      20.913 -12.197  -6.250  1.00 23.75           O
ANISOU 2518  O   MSE B 473     3657   2283   3082    333   -183     45       O
ATOM   2519  N   SER B 474      22.018 -11.384  -8.012  1.00 23.00           N
ANISOU 2519  N   SER B 474     3283   2317   3138    384   -240    -79       N
ATOM   2520  CA  SER B 474      20.815 -10.819  -8.621  1.00 21.94           C
ANISOU 2520  CA  SER B 474     3118   2194   3023    228   -154   -159       C
ATOM   2521  CB  SER B 474      20.425  -9.496  -7.949  1.00 20.28           C
ANISOU 2521  CB  SER B 474     2863   2099   2745    152   -190   -179       C
ATOM   2522  OG  SER B 474      19.094  -9.121  -8.284  1.00 20.72           O
ANISOU 2522  OG  SER B 474     2910   2154   2809     30    -97   -231       O
ATOM   2523  C   SER B 474      21.036 -10.602 -10.103  1.00 22.22           C
ANISOU 2523  C   SER B 474     3031   2262   3151    217   -130   -246       C
ATOM   2524  O   SER B 474      22.178 -10.392 -10.544  1.00 22.87           O
ANISOU 2524  O   SER B 474     3006   2412   3273    308   -185   -253       O
ATOM   2525  N   MSE B 475      19.942 -10.646 -10.871  1.00 22.60           N
ANISOU 2525  N   MSE B 475     3085   2278   3225    101    -49   -308       N
ATOM   2526  CA  MSE B 475      19.951 -10.117 -12.224  1.00 22.94           C
ANISOU 2526  CA  MSE B 475     3014   2384   3318     64    -37   -391       C
ATOM   2527  CB  MSE B 475      18.539 -10.126 -12.829  1.00 21.81           C
ANISOU 2527  CB  MSE B 475     2880   2226   3181    -76    -26   -446       C
ATOM   2528  CG  MSE B 475      18.108 -11.548 -13.200  1.00 24.19           C
ANISOU 2528  CG  MSE B 475     3308   2381   3504   -112     93   -465       C
ATOM   2529 SE   MSE B 475      16.546 -11.727 -14.313  0.90 27.36          SE
ANISOU 2529 SE   MSE B 475     3688   2786   3921   -305    143   -557       SE
ATOM   2530  CE  MSE B 475      15.247 -11.070 -13.061  1.00 18.34           C
ANISOU 2530  CE  MSE B 475     2500   1718   2750   -406    169   -500       C
ATOM   2531  C   MSE B 475      20.526  -8.725 -12.161  1.00 22.17           C
ANISOU 2531  C   MSE B 475     2788   2424   3212     70   -108   -396       C
ATOM   2532  O   MSE B 475      20.131  -7.953 -11.287  1.00 21.81           O
ANISOU 2532  O   MSE B 475     2749   2419   3118     30   -137   -377       O
ATOM   2533  N   ARG B 476      21.484  -8.425 -13.055  1.00 22.25           N
ANISOU 2533  N   ARG B 476     2693   2497   3264    116   -116   -422       N
ATOM   2534  CA  ARG B 476      22.159  -7.132 -13.117  1.00 22.50           C
ANISOU 2534  CA  ARG B 476     2605   2648   3297     98   -188   -424       C
ATOM   2535  CB  ARG B 476      23.037  -7.065 -14.384  1.00 22.64           C
ANISOU 2535  CB  ARG B 476     2515   2725   3361    130   -162   -454       C
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Figure 18 (continued)

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ATOM   2536  CG  ARG B 476      23.641  -5.664 -14.657  1.00 24.65           C
ANISOU 2536  CG  ARG B 476    2649   3092   3623     68   -205   -454       C
ATOM   2537  CD  ARG B 476      24.241  -5.462 -16.092  1.00 25.76           C
ANISOU 2537  CD  ARG B 476    2697   3299   3792     63   -145   -481       C
ATOM   2538  NE  ARG B 476      23.541  -6.128 -17.231  1.00 27.18           N
ANISOU 2538  NE  ARG B 476    2943   3428   3957     63    -58   -533       N
ATOM   2539  CZ  ARG B 476      22.619  -5.553 -18.020  1.00 27.94           C
ANISOU 2539  CZ  ARG B 476    3071   3528   4018    -25    -39   -562       C
ATOM   2540  NH1 ARG B 476      22.175  -4.295 -17.792  1.00 26.67           N
ANISOU 2540  NH1 ARG B 476    2896   3395   3843   -102    -85   -540       N
ATOM   2541  NH2 ARG B 476      22.108  -6.250 -19.027  1.00 19.87           N
ANISOU 2541  NH2 ARG B 476    2107   2475   2969    -28     19   -615       N
ATOM   2542  C   ARG B 476      21.228  -5.892 -12.998  1.00 21.11           C
ANISOU 2542  C   ARG B 476    2425   2504   3091     -6   -197   -447       C
ATOM   2543  O   ARG B 476      20.346  -5.675 -13.836  1.00 20.87           O
ANISOU 2543  O   ARG B 476    2391   2470   3068    -64   -149   -485       O
ATOM   2544  N   GLY B 477      21.432  -5.093 -11.949  1.00 21.59           N
ANISOU 2544  N   GLY B 477    2495   2597   3111    -19   -262   -426       N
ATOM   2545  CA  GLY B 477      20.682  -3.845 -11.726  1.00 20.28           C
ANISOU 2545  CA  GLY B 477    2344   2444   2916    -89   -267   -452       C
ATOM   2546  C   GLY B 477      19.265  -4.001 -11.186  1.00 19.95           C
ANISOU 2546  C   GLY B 477    2384   2360   2837   -110   -204   -459       C
ATOM   2547  O   GLY B 477      18.600  -2.995 -10.954  1.00 20.31           O
ANISOU 2547  O   GLY B 477    2442   2415   2859   -137   -196   -482       O
ATOM   2548  N   ILE B 478      18.805  -5.242 -10.986  1.00 19.45           N
ANISOU 2548  N   ILE B 478    2374   2245   2770    -98   -152   -437       N
ATOM   2549  CA  ILE B 478      17.425  -5.543 -10.523  1.00 17.96           C
ANISOU 2549  CA  ILE B 478    2239   2031   2556   -143    -73   -436       C
ATOM   2550  CB  ILE B 478      16.747  -6.700 -11.323  1.00 18.46           C
ANISOU 2550  CB  ILE B 478    2303   2046   2665   -189     -7   -446       C
ATOM   2551  CG1 ILE B 478      17.035  -6.649 -12.849  1.00 16.97           C
ANISOU 2551  CG1 ILE B 478    2037   1879   2532   -198    -24   -493       C
ATOM   2552  CD1 ILE B 478      16.569  -5.382 -13.592  1.00 12.97           C
ANISOU 2552  CD1 ILE B 478    1440   1453   2034   -221    -43   -526       C
ATOM   2553  CG2 ILE B 478      15.216  -6.762 -11.010  1.00 18.15           C
ANISOU 2553  CG2 ILE B 478    2259   2020   2616   -267     75   -451       C
ATOM   2554  C   ILE B 478      17.351  -5.901  -9.018  1.00 18.54           C
ANISOU 2554  C   ILE B 478    2425   2075   2545   -124    -62   -387       C
ATOM   2555  O   ILE B 478      18.093  -6.760  -8.523  1.00 18.41           O
ANISOU 2555  O   ILE B 478    2476   2015   2504    -76    -93   -336       O
ATOM   2556  N   ARG B 479      16.435  -5.252  -8.299  1.00 18.71           N
ANISOU 2556  N   ARG B 479    2473   2124   2512   -148    -11   -398       N
ATOM   2557  CA  ARG B 479      16.205  -5.537  -6.881  1.00 19.06           C
ANISOU 2557  CA  ARG B 479    2640   2153   2450   -139     24   -354       C
ATOM   2558  CB  ARG B 479      16.835  -4.454  -5.980  1.00 19.31           C
ANISOU 2558  CB  ARG B 479    2727   2220   2388   -100    -54   -375       C
ATOM   2559  CG  ARG B 479      18.364  -4.281  -6.108  1.00 17.90           C
ANISOU 2559  CG  ARG B 479    2524   2056   2221    -65   -199   -368       C
ATOM   2560  CD  ARG B 479      19.159  -5.504  -5.595  1.00 20.83           C
ANISOU 2560  CD  ARG B 479    2956   2400   2558    -12   -249   -287       C
ATOM   2561  NE  ARG B 479      20.603  -5.259  -5.641  1.00 22.94           N
ANISOU 2561  NE  ARG B 479    3160   2718   2838     31   -392   -279       N
ATOM   2562  CZ  ARG B 479      21.370  -5.399  -6.728  1.00 22.88           C
ANISOU 2562  CZ  ARG B 479    3022   2729   2941     52   -425   -288       C
ATOM   2563  NH1 ARG B 479      20.850  -5.826  -7.888  1.00 18.51           N
ANISOU 2563  NH1 ARG B 479    2416   2135   2482     38   -335   -309       N
ATOM   2564  NH2 ARG B 479      22.673  -5.109  -6.657  1.00 21.36           N
ANISOU 2564  NH2 ARG B 479    2746   2610   2759     82   -549   -278       N
ATOM   2565  C   ARG B 479      14.714  -5.617  -6.625  1.00 19.99           C
ANISOU 2565  C   ARG B 479    2751   2287   2555   -193    157   -358       C
ATOM   2566  O   ARG B 479      13.908  -5.004  -7.352  1.00 19.57           O
ANISOU 2566  O   ARG B 479    2588   2283   2564   -214    195   -407       O
ATOM   2567  N   VAL B 480      14.344  -6.383  -5.600  1.00 20.85           N
ANISOU 2567  N   VAL B 480    2971   2367   2583   -214    231   -299       N
ATOM   2568  CA  VAL B 480      12.969  -6.481  -5.147  1.00 21.50           C
ANISOU 2568  CA  VAL B 480    3043   2486   2640   -275    379   -291       C
ATOM   2569  CB  VAL B 480      12.437  -7.952  -5.221  1.00 22.40           C
ANISOU 2569  CB  VAL B 480    3194   2531   2785   -375    465   -227       C
ATOM   2570  CG1 VAL B 480      11.090  -8.086  -4.576  1.00 22.44           C
ANISOU 2570  CG1 VAL B 480    3183   2592   2754   -458    630   -204       C
ATOM   2571  CG2 VAL B 480      12.380  -8.430  -6.680  1.00 20.69           C
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Figure 18 (continued)

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ANISOU 2571  CG2 VAL B 480     2869   2287   2705   -430    428   -266    C
ATOM   2572  C   VAL B 480      12.858  -5.880  -3.738  1.00 23.73        C
ANISOU 2572  C   VAL B 480     3442   2803   2771   -231    424   -282    C
ATOM   2573  O   VAL B 480      13.635  -6.213  -2.833  1.00 23.83        O
ANISOU 2573  O   VAL B 480     3604   2779   2670   -198    372   -230    O
ATOM   2574  N   SER B 481      11.899  -4.968  -3.571  1.00 24.34        N
ANISOU 2574  N   SER B 481     3455   2956   2838   -217    517   -336    N
ATOM   2575  CA  SER B 481      11.641  -4.340  -2.293  1.00 26.50        C
ANISOU 2575  CA  SER B 481     3846   3264   2958   -169    590   -350    C
ATOM   2576  CB  SER B 481      10.803  -3.087  -2.498  1.00 26.56        C
ANISOU 2576  CB  SER B 481     3755   3338   2998   -108    659   -436    C
ATOM   2577  OG  SER B 481      10.413  -2.542  -1.251  1.00 29.55        O
ANISOU 2577  OG  SER B 481     4258   3749   3221    -56    765   -461    O
ATOM   2578  C   SER B 481      10.922  -5.271  -1.311  1.00 29.41        C
ANISOU 2578  C   SER B 481     4304   3643   3226   -230    745   -270    C
ATOM   2579  O   SER B 481      10.009  -6.006  -1.679  1.00 29.10        O
ANISOU 2579  O   SER B 481     4167   3623   3266   -319    857   -233    O
ATOM   2580  N   LYS B 482      11.350  -5.230  -0.054  1.00 32.28        N
ANISOU 2580  N   LYS B 482     4862   3998   3405   -194    747   -241    N
ATOM   2581  CA  LYS B 482      10.679  -5.956   1.007  1.00 36.48        C
ANISOU 2581  CA  LYS B 482     5512   4545   3803   -246    910   -159    C
ATOM   2582  CB  LYS B 482      11.708  -6.552   1.973  1.00 37.56        C
ANISOU 2582  CB  LYS B 482     5882   4620   3770   -223    813    -72    C
ATOM   2583  CG  LYS B 482      12.493  -7.739   1.427  1.00 39.17        C
ANISOU 2583  CG  LYS B 482     6106   4718   4059   -250    700     19    C
ATOM   2584  CD  LYS B 482      13.494  -8.227   2.457  1.00 46.13        C
ANISOU 2584  CD  LYS B 482     7211   5556   4762   -192    592    114    C
ATOM   2585  CE  LYS B 482      13.409  -9.749   2.690  1.00 50.34        C
ANISOU 2585  CE  LYS B 482     7871   5976   5278   -245    653    267    C
ATOM   2586  NZ  LYS B 482      14.542 -10.223   3.564  1.00 55.51        N
ANISOU 2586  NZ  LYS B 482     8732   6587   5770   -151    505    373    N
ATOM   2587  C   LYS B 482       9.701  -5.045   1.766  1.00 39.13        C
ANISOU 2587  C   LYS B 482     5851   4981   4035   -202   1082   -221    C
ATOM   2588  O   LYS B 482       9.060  -5.500   2.711  1.00 41.48        O
ANISOU 2588  O   LYS B 482     6242   5315   4202   -242   1250   -160    O
ATOM   2589  N   MSE B 483       9.603  -3.764   1.371  1.00 39.66        N
ANISOU 2589  N   MSE B 483     5832   5082   4154   -113   1050   -338    N
ATOM   2590  CA  MSE B 483       8.689  -2.788   2.016  1.00 42.78        C
ANISOU 2590  CA  MSE B 483     6232   5558   4464    -32   1217   -416    C
ATOM   2591  CB  MSE B 483       9.114  -1.322   1.779  1.00 42.34        C
ANISOU 2591  CB  MSE B 483     6198   5470   4417     85   1113   -544    C
ATOM   2592  CG  MSE B 483      10.519  -0.958   2.191  1.00 42.80        C
ANISOU 2592  CG  MSE B 483     6451   5447   4363     95    911   -575    C
ATOM   2593  SE  MSE B 483      10.790  -1.343   4.076  0.90 53.78       SE
ANISOU 2593  SE  MSE B 483     8155   6858   5420     89    969   -539    SE
ATOM   2594  CE  MSE B 483       9.681  -0.017   5.008  1.00 43.83        C
ANISOU 2594  CE  MSE B 483     6998   5650   4003    213   1203   -680    C
ATOM   2595  C   MSE B 483       7.253  -2.929   1.531  1.00 44.09        C
ANISOU 2595  C   MSE B 483     6165   5828   4760    -57   1407   -409    C
ATOM   2596  O   MSE B 483       7.028  -2.888   0.312  1.00 43.61        O
ANISOU 2596  O   MSE B 483     5899   5777   4893    -73   1342   -423    O
ATOM   2597  OXT MSE B 483       6.311  -3.041   2.339  1.00 46.48        O
ANISOU 2597  OXT MSE B 483     6471   6220   4971    -61   1623   -390    O
ATOM   2598  N   ILE D 319      63.442 -23.655 -17.970  1.00 53.76        N
ANISOU 2598  N   ILE D 319     7685   4667   8075    274    727   -949    N
ATOM   2599  CA  ILE D 319      62.501 -23.137 -16.919  1.00 52.62        C
ANISOU 2599  CA  ILE D 319     7506   4623   7863     88    628   -790    C
ATOM   2600  CB  ILE D 319      62.826 -23.727 -15.487  1.00 53.65        C
ANISOU 2600  CB  ILE D 319     7709   4559   8116    134    561   -578    C
ATOM   2601  CG1 ILE D 319      61.736 -23.378 -14.463  1.00 53.18        C
ANISOU 2601  CG1 ILE D 319     7660   4578   7969    -75    499   -438    C
ATOM   2602  CD1 ILE D 319      61.719 -24.322 -13.234  1.00 55.09        C
ANISOU 2602  CD1 ILE D 319     8066   4566   8299    -89    460   -258    C
ATOM   2603  CG2 ILE D 319      64.206 -23.306 -14.994  1.00 52.60        C
ANISOU 2603  CG2 ILE D 319     7451   4467   8067    373    525   -452    C
ATOM   2604  C   ILE D 319      62.352 -21.605 -16.916  1.00 49.28        C
ANISOU 2604  C   ILE D 319     6892   4530   7301     56    600   -732    C
ATOM   2605  O   ILE D 319      61.237 -21.097 -16.682  1.00 48.90        O
ANISOU 2605  O   ILE D 319     6817   4614   7147   -127    555   -712    O
ATOM   2606  N   SER D 320      63.458 -20.898 -17.210  1.00 47.45        N
ANISOU 2606  N   SER D 320     6524   4418   7087    232    634   -713    N
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Figure 18 (continued)

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ATOM   2607  CA  SER D 320      63.576 -19.403 -17.245  1.00 43.82           C
ANISOU 2607  CA  SER D 320    5886   4238   6528    231    618   -650       C
ATOM   2608  CB  SER D 320      62.853 -18.783 -18.463  1.00 43.61           C
ANISOU 2608  CB  SER D 320    5846   4391   6332    139    666   -791       C
ATOM   2609  OG  SER D 320      62.411 -19.771 -19.397  1.00 46.63           O
ANISOU 2609  OG  SER D 320    6378   4652   6686     96    715   -975       O
ATOM   2610  C   SER D 320      63.164 -18.674 -15.938  1.00 40.81           C
ANISOU 2610  C   SER D 320    5444   3950   6114    147    509   -475       C
ATOM   2611  O   SER D 320      62.342 -17.737 -15.963  1.00 39.35           O
ANISOU 2611  O   SER D 320    5199   3949   5803     29    485   -470       O
ATOM   2612  N   SER D 321      63.744 -19.096 -14.810  1.00 38.96           N
ANISOU 2612  N   SER D 321    5233   3587   5982    223    441   -336       N
ATOM   2613  CA  SER D 321      63.435 -18.492 -13.514  1.00 35.41           C
ANISOU 2613  CA  SER D 321    4761   3214   5478    159    341   -177       C
ATOM   2614  CB  SER D 321      63.252 -19.571 -12.458  1.00 37.05           C
ANISOU 2614  CB  SER D 321    5133   3209   5736    139    291    -64       C
ATOM   2615  OG  SER D 321      64.485 -20.151 -12.113  1.00 39.50           O
ANISOU 2615  OG  SER D 321    5449   3370   6187    334    243      7       O
ATOM   2616  C   SER D 321      64.454 -17.445 -13.030  1.00 33.02           C
ANISOU 2616  C   SER D 321    4299   3045   5202    275    271    -86       C
ATOM   2617  O   SER D 321      64.263 -16.842 -11.978  1.00 31.66           O
ANISOU 2617  O   SER D 321    4115   2947   4966    231    181     25       O
ATOM   2618  N   SER D 322      65.501 -17.202 -13.829  1.00 31.16           N
ANISOU 2618  N   SER D 322    3939   2845   5057    410    324   -145       N
ATOM   2619  CA  SER D 322      66.656 -16.427 -13.420  1.00 28.20           C
ANISOU 2619  CA  SER D 322    3392   2555   4768    525    259    -67       C
ATOM   2620  CB  SER D 322      67.515 -17.350 -12.575  1.00 30.48           C
ANISOU 2620  CB  SER D 322    3710   2670   5202    669    164     29       C
ATOM   2621  OG  SER D 322      68.312 -16.682 -11.683  1.00 28.82           O
ANISOU 2621  OG  SER D 322    3373   2534   5042    733     26    137       O
ATOM   2622  C   SER D 322      67.425 -16.050 -14.688  1.00 27.21           C
ANISOU 2622  C   SER D 322    3127   2506   4706    610    390    -168       C
ATOM   2623  O   SER D 322      67.831 -16.930 -15.437  1.00 28.51           O
ANISOU 2623  O   SER D 322    3324   2557   4949    708    491    -255       O
ATOM   2624  N   PHE D 323      67.651 -14.758 -14.921  1.00 24.48           N
ANISOU 2624  N   PHE D 323    2638   2339   4326    576    402    -155       N
ATOM   2625  CA  PHE D 323      68.250 -14.299 -16.169  1.00 24.11           C
ANISOU 2625  CA  PHE D 323    2478   2379   4303    627    556    -233       C
ATOM   2626  CB  PHE D 323      67.335 -14.608 -17.378  1.00 23.01           C
ANISOU 2626  CB  PHE D 323    2478   2256   4010    561    682    -365       C
ATOM   2627  CG  PHE D 323      65.905 -14.146 -17.190  1.00 21.13           C
ANISOU 2627  CG  PHE D 323    2340   2096   3593    393    614    -364       C
ATOM   2628  CD1 PHE D 323      65.509 -12.883 -17.609  1.00 18.06           C
ANISOU 2628  CD1 PHE D 323    1896   1878   3090    321    629    -351       C
ATOM   2629  CE1 PHE D 323      64.229 -12.463 -17.415  1.00 18.85           C
ANISOU 2629  CE1 PHE D 323    2060   2050   3052    195    564    -350       C
ATOM   2630  CZ  PHE D 323      63.312 -13.289 -16.768  1.00 18.75           C
ANISOU 2630  CZ  PHE D 323    2157   1953   3016    115    496    -360       C
ATOM   2631  CE2 PHE D 323      63.706 -14.538 -16.339  1.00 19.68           C
ANISOU 2631  CE2 PHE D 323    2346   1892   3241    165    489    -361       C
ATOM   2632  CD2 PHE D 323      64.977 -14.960 -16.567  1.00 18.81           C
ANISOU 2632  CD2 PHE D 323    2185   1700   3264    312    540    -365       C
ATOM   2633  C   PHE D 323      68.551 -12.810 -16.119  1.00 23.35           C
ANISOU 2633  C   PHE D 323    2228   2449   4195    574    541    -174       C
ATOM   2634  O   PHE D 323      68.114 -12.092 -15.213  1.00 22.75           O
ANISOU 2634  O   PHE D 323    2155   2426   4064    488    412    -101       O
ATOM   2635  N   SER D 324      69.271 -12.361 -17.128  1.00 24.41           N
ANISOU 2635  N   SER D 324    2245   2654   4374    623    689    -212       N
ATOM   2636  CA  SER D 324      69.624 -10.980 -17.324  1.00 25.05           C
ANISOU 2636  CA  SER D 324    2189   2868   4460    566    717    -160       C
ATOM   2637  CB  SER D 324      71.102 -10.908 -17.645  1.00 26.25           C
ANISOU 2637  CB  SER D 324    2123   3028   4822    674    816    -146       C
ATOM   2638  OG  SER D 324      71.632  -9.664 -17.257  1.00 30.85           O
ANISOU 2638  OG  SER D 324    2540   3694   5489    607    763     -65       O
ATOM   2639  C   SER D 324      68.774 -10.395 -18.480  1.00 24.43           C
ANISOU 2639  C   SER D 324    2213   2890   4180    485    840    -211       C
ATOM   2640  O   SER D 324      68.616 -11.018 -19.533  1.00 26.03           O
ANISOU 2640  O   SER D 324    2506   3084   4301    525    976    -305       O
ATOM   2641  N   PHE D 325      68.185  -9.219 -18.275  1.00 22.46           N
ANISOU 2641  N   PHE D 325    1967   2727   3838    380    779    -155       N
ATOM   2642  CA  PHE D 325      67.496  -8.549 -19.370  1.00 21.87           C
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Figure 18 (continued)

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ANISOU 2642  CA  PHE D 325     1975   2750   3586    326    877   -178      C
ATOM   2643  CB  PHE D 325      66.033  -9.046 -19.505  1.00 20.62           C
ANISOU 2643  CB  PHE D 325     1995   2598   3243    268    813   -247      C
ATOM   2644  CG  PHE D 325      65.292  -8.433 -20.664  1.00 20.13           C
ANISOU 2644  CG  PHE D 325     2019   2644   2985    231    879   -274      C
ATOM   2645  CD1 PHE D 325      65.624  -8.761 -21.981  1.00 21.66           C
ANISOU 2645  CD1 PHE D 325     2270   2870   3090    285   1038   -341      C
ATOM   2646  CE1 PHE D 325      64.947  -8.172 -23.059  1.00 22.94           C
ANISOU 2646  CE1 PHE D 325     2536   3141   3041    260   1079   -353      C
ATOM   2647  CZ  PHE D 325      63.902  -7.259 -22.812  1.00 21.18           C
ANISOU 2647  CZ  PHE D 325     2337   2986   2723    190    953   -296      C
ATOM   2648  CE2 PHE D 325      63.581  -6.933 -21.498  1.00 16.68           C
ANISOU 2648  CE2 PHE D 325     1694   2379   2264    142    816   -240      C
ATOM   2649  CD2 PHE D 325      64.266  -7.516 -20.443  1.00 17.35           C
ANISOU 2649  CD2 PHE D 325     1699   2364   2528    156    782   -231      C
ATOM   2650  C   PHE D 325      67.564  -7.047 -19.143  1.00 21.28           C
ANISOU 2650  C   PHE D 325     1823   2743   3519    255    845    -83      C
ATOM   2651  O   PHE D 325      67.193  -6.571 -18.081  1.00 20.40           O
ANISOU 2651  O   PHE D 325     1704   2620   3427    202    694    -41      O
ATOM   2652  N   GLY D 326      68.068  -6.315 -20.129  1.00 22.68           N
ANISOU 2652  N   GLY D 326     1956   2980   3681    255    996    -51      N
ATOM   2653  CA  GLY D 326      68.092  -4.857 -20.077  1.00 21.89           C
ANISOU 2653  CA  GLY D 326     1812   2918   3589    180    986     43      C
ATOM   2654  C   GLY D 326      68.926  -4.267 -18.972  1.00 21.89           C
ANISOU 2654  C   GLY D 326     1648   2871   3799    145    884    102      C
ATOM   2655  O   GLY D 326      68.699  -3.141 -18.549  1.00 22.59           O
ANISOU 2655  O   GLY D 326     1733   2957   3894     70    809    157      O
ATOM   2656  N   GLY D 327      69.900  -5.022 -18.502  1.00 23.39           N
ANISOU 2656  N   GLY D 327     1704   3016   4166    204    868     84      N
ATOM   2657  CA  GLY D 327      70.839  -4.538 -17.493  1.00 23.14           C
ANISOU 2657  CA  GLY D 327     1492   2951   4348    176    749    131      C
ATOM   2658  C   GLY D 327      70.329  -4.854 -16.096  1.00 21.75           C
ANISOU 2658  C   GLY D 327     1381   2731   4150    171    514    118      C
ATOM   2659  O   GLY D 327      70.892  -4.379 -15.118  1.00 22.68           O
ANISOU 2659  O   GLY D 327     1397   2828   4394    138    366    145      O
ATOM   2660  N   PHE D 328      69.279  -5.678 -16.009  1.00 19.65           N
ANISOU 2660  N   PHE D 328     1290   2454   3722    196    483     75      N
ATOM   2661  CA  PHE D 328      68.706  -6.111 -14.734  1.00 17.83           C
ANISOU 2661  CA  PHE D 328     1149   2184   3442    190    299     73      C
ATOM   2662  CB  PHE D 328      67.233  -5.642 -14.619  1.00 15.94           C
ANISOU 2662  CB  PHE D 328     1072   1982   3001    117    271     59      C
ATOM   2663  CG  PHE D 328      67.092  -4.187 -14.431  1.00 14.33           C
ANISOU 2663  CG  PHE D 328     847   1811   2787     46    236     88      C
ATOM   2664  CD1 PHE D 328      67.017  -3.642 -13.141  1.00 16.78           C
ANISOU 2664  CD1 PHE D 328     1171   2101   3102      9     76     98      C
ATOM   2665  CE1 PHE D 328      66.918  -2.239 -12.944  1.00 15.67           C
ANISOU 2665  CE1 PHE D 328     1024   1962   2966    -54     42    109      C
ATOM   2666  CZ  PHE D 328      66.886  -1.387 -14.054  1.00 15.40           C
ANISOU 2666  CZ  PHE D 328     971   1944   2938    -80    169    134      C
ATOM   2667  CE2 PHE D 328      66.986  -1.913 -15.341  1.00 14.72           C
ANISOU 2667  CE2 PHE D 328     873   1892   2828    -43    329    144      C
ATOM   2668  CD2 PHE D 328      67.088  -3.328 -15.522  1.00 15.45           C
ANISOU 2668  CD2 PHE D 328     971   1989   2910     21    362    108      C
ATOM   2669  C   PHE D 328      68.769  -7.623 -14.575  1.00 18.64           C
ANISOU 2669  C   PHE D 328     1303   2216   3563    279    290     46      C
ATOM   2670  O   PHE D 328      68.507  -8.386 -15.522  1.00 20.76           O
ANISOU 2670  O   PHE D 328     1636   2471   3780    318    422     -9      O
ATOM   2671  N   THR D 329      69.112  -8.074 -13.376  1.00 18.73           N
ANISOU 2671  N   THR D 329     1307   2172   3639    313    128     82      N
ATOM   2672  CA  THR D 329      69.005  -9.486 -13.040  1.00 18.53           C
ANISOU 2672  CA  THR D 329     1375   2049   3615    390     97     78      C
ATOM   2673  CB  THR D 329      70.023  -9.885 -11.931  1.00 20.11           C
ANISOU 2673  CB  THR D 329     1490   2190   3961    478    -77    142      C
ATOM   2674  OG1 THR D 329      71.364  -9.562 -12.341  1.00 19.13           O
ANISOU 2674  OG1 THR D 329     1128   2092   4050    544    -48    144      O
ATOM   2675  CG2 THR D 329      69.932 -11.382 -11.615  1.00 18.59           C
ANISOU 2675  CG2 THR D 329     1418   1867   3778    573   -104    159      C
ATOM   2676  C   THR D 329      67.566  -9.736 -12.566  1.00 17.59           C
ANISOU 2676  C   THR D 329     1460   1922   3302    307     61     73      C
ATOM   2677  O   THR D 329      67.134  -9.147 -11.597  1.00 17.15           O
ANISOU 2677  O   THR D 329     1450   1898   3166    247    -52    110      O
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Figure 18 (continued)

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ATOM   2678  N   PHE D 330      66.827 -10.592 -13.275  1.00 17.78           N
ANISOU 2678  N   PHE D 330    1597   1907   3254    299    165     17        NNC
ATOM   2679  CA  PHE D 330      65.483 -11.015 -12.896  1.00 16.15           C
ANISOU 2679  CA  PHE D 330    1553   1684   2900    211    149      7        CCC
ATOM   2680  CB  PHE D 330      64.639 -11.297 -14.140  1.00 15.29           C
ANISOU 2680  CB  PHE D 330    1503   1600   2706    164    276    -89        CCC
ATOM   2681  CG  PHE D 330      64.137 -10.053 -14.865  1.00 14.68           C
ANISOU 2681  CG  PHE D 330    1379   1664   2533    108    322   -115        CCC
ATOM   2682  CD1 PHE D 330      62.776  -9.790 -14.933  1.00 13.44           C
ANISOU 2682  CD1 PHE D 330    1289   1576   2242     15    315   -144        CCC
ATOM   2683  CE1 PHE D 330      62.297  -8.658 -15.616  1.00 12.28           C
ANISOU 2683  CE1 PHE D 330    1106   1548   2011    -11    342   -157        CCC
ATOM   2684  CZ  PHE D 330      63.203  -7.777 -16.224  1.00 10.41           C
ANISOU 2684  CZ  PHE D 330     787   1349   1819     38    392   -129        CCC
ATOM   2685  CE2 PHE D 330      64.553  -8.017 -16.140  1.00 10.15           C
ANISOU 2685  CE2 PHE D 330     674   1255   1926    107    417   -102        CCC
ATOM   2686  CD2 PHE D 330      65.026  -9.161 -15.481  1.00 11.56           C
ANISOU 2686  CD2 PHE D 330     868   1328   2197    152    376   -101        CCC
ATOM   2687  C   PHE D 330      65.588 -12.317 -12.123  1.00 18.49           C
ANISOU 2687  C   PHE D 330    1952   1835   3239    255     88     51        CCO
ATOM   2688  O   PHE D 330      66.310 -13.222 -12.529  1.00 19.07           O
ANISOU 2688  O   PHE D 330    2014   1802   3429    356    126     32        OON
ATOM   2689  N   LYS D 331      64.871 -12.417 -11.004  1.00 18.87           N
ANISOU 2689  N   LYS D 331    2112   1869   3190    188      7    114        NNC
ATOM   2690  CA  LYS D 331      64.775 -13.663 -10.273  1.00 19.84           C
ANISOU 2690  CA  LYS D 331    2374   1841   3323    209    -35    177        CCC
ATOM   2691  CB  LYS D 331      65.564 -13.571  -8.961  1.00 21.52           C
ANISOU 2691  CB  LYS D 331    2594   2030   3554    282   -199    293        CCC
ATOM   2692  CG  LYS D 331      67.070 -13.465  -9.152  1.00 23.54           C
ANISOU 2692  CG  LYS D 331    2684   2273   3989    429   -270    302        CCC
ATOM   2693  CD  LYS D 331      67.817 -13.640  -7.837  1.00 30.28           C
ANISOU 2693  CD  LYS D 331    3560   3083   4861    514   -470    419        CCC
ATOM   2694  CE  LYS D 331      69.326 -13.743  -8.063  1.00 32.87           C
ANISOU 2694  CE  LYS D 331    3692   3387   5410    673   -546    426        CCC
ATOM   2695  NZ  LYS D 331      70.045 -13.890  -6.766  1.00 36.55           N
ANISOU 2695  NZ  LYS D 331    4174   3826   5889    762   -782    540        NNC
ATOM   2696  C   LYS D 331      63.317 -13.898  -9.984  1.00 19.36           C
ANISOU 2696  C   LYS D 331    2445   1788   3123     64     15    174        CCC
ATOM   2697  O   LYS D 331      62.675 -13.085  -9.342  1.00 18.88           O
ANISOU 2697  O   LYS D 331    2391   1836   2946    -11    -10    198        OON
ATOM   2698  N   ARG D 332      62.778 -15.009 -10.461  1.00 19.97           N
ANISOU 2698  N   ARG D 332    2620   1747   3223     20     93    133        NNC
ATOM   2699  CA  ARG D 332      61.355 -15.290 -10.281  1.00 19.72           C
ANISOU 2699  CA  ARG D 332    2679   1723   3091   -141    152    120        CCC
ATOM   2700  CB  ARG D 332      60.867 -16.358 -11.279  1.00 20.07           C
ANISOU 2700  CB  ARG D 332    2784   1649   3191   -199    239     17        CCC
ATOM   2701  CG  ARG D 332      59.346 -16.450 -11.354  1.00 20.01           C
ANISOU 2701  CG  ARG D 332    2804   1695   3106   -388    297    -30        CCC
ATOM   2702  CD  ARG D 332      58.875 -17.327 -12.504  1.00 20.70           C
ANISOU 2702  CD  ARG D 332    2929   1692   3243   -458    356   -169        CCC
ATOM   2703  NE  ARG D 332      59.269 -18.715 -12.316  1.00 22.45           N
ANISOU 2703  NE  ARG D 332    3301   1656   3571   -438    369   -145        NNC
ATOM   2704  CZ  ARG D 332      59.397 -19.590 -13.307  1.00 25.52           C
ANISOU 2704  CZ  ARG D 332    3753   1907   4035   -430    408   -274        CCN
ATOM   2705  NH1 ARG D 332      59.137 -19.233 -14.566  1.00 25.47           N
ANISOU 2705  NH1 ARG D 332    3678   2016   3984   -447    433   -436        NNN
ATOM   2706  NH2 ARG D 332      59.748 -20.829 -13.035  1.00 27.36           N
ANISOU 2706  NH2 ARG D 332    4137   1879   4378   -401    419   -243        NNC
ATOM   2707  C   ARG D 332      61.108 -15.726  -8.841  1.00 20.88           C
ANISOU 2707  C   ARG D 332    2961   1796   3175   -177    105    260        CCO
ATOM   2708  O   ARG D 332      61.801 -16.602  -8.331  1.00 21.02           O
ANISOU 2708  O   ARG D 332    3078   1652   3257    -95     52    348        OON
ATOM   2709  N   THR D 333      60.149 -15.078  -8.180  1.00 20.24           N
ANISOU 2709  N   THR D 333    2890   1838   2964   -284    127    286        NNC
ATOM   2710  CA  THR D 333      59.820 -15.426  -6.778  1.00 21.32           C
ANISOU 2710  CA  THR D 333    3176   1927   2997   -328    111    423        CCC
ATOM   2711  CB  THR D 333      59.888 -14.174  -5.876  1.00 20.56           C
ANISOU 2711  CB  THR D 333    3051   1993   2767   -301     47    456        CCC
ATOM   2712  OG1 THR D 333      59.095 -13.132  -6.468  1.00 19.68           O
ANISOU 2712  OG1 THR D 333    2807   2049   2621   -363    113    346        OOC
ATOM   2713  CG2 THR D 333      61.342 -13.644  -5.770  1.00 21.41
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Figure 18 (continued)

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ANISOU 2713  CG2 THR D 333     3092   2109   2933   -143   -107    471       C
ATOM   2714  C   THR D 333      58.450 -16.124  -6.612  1.00 22.28           C
ANISOU 2714  C   THR D 333     3381   2007   3077   -508    241    434       C
ATOM   2715  O   THR D 333      58.187 -16.719  -5.565  1.00 24.07           O
ANISOU 2715  O   THR D 333     3763   2148   3232   -557    263    564       O
ATOM   2716  N   SER D 334      57.595 -16.054  -7.636  1.00 21.08           N
ANISOU 2716  N   SER D 334     3124   1916   2968   -609    321    305       N
ATOM   2717  CA  SER D 334      56.275 -16.727  -7.644  1.00 22.78           C
ANISOU 2717  CA  SER D 334     3368   2099   3187   -801    437    290       C
ATOM   2718  CB  SER D 334      55.169 -15.774  -7.203  1.00 22.34           C
ANISOU 2718  CB  SER D 334     3214   2251   3025   -891    506    277       C
ATOM   2719  OG  SER D 334      54.919 -15.851  -5.848  1.00 26.42           O
ANISOU 2719  OG  SER D 334     3849   2761   3430   -928    557    413       O
ATOM   2720  C   SER D 334      55.889 -17.081  -9.055  1.00 21.71           C
ANISOU 2720  C   SER D 334     3148   1948   3153   -862    459    131       C
ATOM   2721  O   SER D 334      56.317 -16.426  -9.985  1.00 20.94           O
ANISOU 2721  O   SER D 334     2944   1944   3068   -771    412     32       O
ATOM   2722  N   GLY D 335      55.021 -18.077  -9.193  1.00 23.23           N
ANISOU 2722  N   GLY D 335     3391   2027   3407  -1030    533    108       N
ATOM   2723  CA  GLY D 335      54.375 -18.411 -10.458  1.00 21.87           C
ANISOU 2723  CA  GLY D 335     3139   1860   3310  -1132    543    -62       C
ATOM   2724  C   GLY D 335      55.276 -19.178 -11.397  1.00 22.97           C
ANISOU 2724  C   GLY D 335     3362   1826   3539  -1040    501   -149       C
ATOM   2725  O   GLY D 335      56.339 -19.683 -10.997  1.00 21.77           O
ANISOU 2725  O   GLY D 335     3331   1510   3430   -910    477    -63       O
ATOM   2726  N   SER D 336      54.833 -19.252 -12.651  1.00 23.39           N
ANISOU 2726  N   SER D 336     3346   1924   3615  -1097    487   -326       N
ATOM   2727  CA  SER D 336      55.445 -20.058 -13.689  1.00 25.47           C
ANISOU 2727  CA  SER D 336     3699   2029   3950  -1039    472   -454       C
ATOM   2728  CB  SER D 336      55.193 -21.560 -13.460  1.00 28.08           C
ANISOU 2728  CB  SER D 336     4201   2067   4403  -1165    513   -454       C
ATOM   2729  OG  SER D 336      53.803 -21.892 -13.365  1.00 31.54           O
ANISOU 2729  OG  SER D 336     4597   2519   4869  -1418    545   -493       O
ATOM   2730  C   SER D 336      54.844 -19.634 -15.019  1.00 25.72           C
ANISOU 2730  C   SER D 336     3625   2220   3926  -1088    437   -644       C
ATOM   2731  O   SER D 336      53.847 -18.912 -15.056  1.00 25.59           O
ANISOU 2731  O   SER D 336     3468   2403   3851  -1187    417   -664       O
ATOM   2732  N   SER D 337      55.464 -20.046 -16.117  1.00 26.46           N
ANISOU 2732  N   SER D 337     3787   2238   4029  -1003    427   -783       N
ATOM   2733  CA  SER D 337      54.928 -19.730 -17.429  1.00 27.34           C
ANISOU 2733  CA  SER D 337     3839   2495   4056  -1043    381   -965       C
ATOM   2734  CB  SER D 337      55.383 -18.344 -17.922  1.00 25.38           C
ANISOU 2734  CB  SER D 337     3476   2488   3680   -890    361   -946       C
ATOM   2735  OG  SER D 337      56.780 -18.297 -18.126  1.00 26.90           O
ANISOU 2735  OG  SER D 337     3722   2614   3884   -694    409   -919       O
ATOM   2736  C   SER D 337      55.239 -20.809 -18.446  1.00 29.10           C
ANISOU 2736  C   SER D 337     4212   2533   4312  -1040    389  -1148       C
ATOM   2737  O   SER D 337      56.117 -21.653 -18.247  1.00 29.85           O
ANISOU 2737  O   SER D 337     4444   2396   4503   -947    441  -1131       O
ATOM   2738  N   ILE D 338      54.459 -20.799 -19.515  1.00 30.44           N
ANISOU 2738  N   ILE D 338     4360   2804   4402  -1139    325  -1328       N
ATOM   2739  CA  ILE D 338      54.760 -21.558 -20.713  1.00 32.19           C
ANISOU 2739  CA  ILE D 338     4726   2912   4591  -1113    322  -1541       C
ATOM   2740  CB  ILE D 338      53.644 -22.589 -21.052  1.00 34.45           C
ANISOU 2740  CB  ILE D 338     5075   3071   4942  -1359    255  -1712       C
ATOM   2741  CG1 ILE D 338      52.280 -21.909 -21.249  1.00 34.10           C
ANISOU 2741  CG1 ILE D 338     4845   3281   4832  -1530    140  -1749       C
ATOM   2742  CD1 ILE D 338      51.154 -22.880 -21.685  1.00 36.18           C
ANISOU 2742  CD1 ILE D 338     5133   3442   5171  -1794     50  -1941       C
ATOM   2743  CG2 ILE D 338      53.582 -23.654 -19.966  1.00 35.56           C
ANISOU 2743  CG2 ILE D 338     5308   2920   5282  -1470    315  -1615       C
ATOM   2744  C   ILE D 338      55.002 -20.549 -21.828  1.00 31.93           C
ANISOU 2744  C   ILE D 338     4641   3126  4363  -988    294  -1615       C
ATOM   2745  O   ILE D 338      54.712 -19.381 -21.647  1.00 30.28           O
ANISOU 2745  O   ILE D 338     4282   3147  4075  -964    258  -1510       O
ATOM   2746  N   LYS D 339      55.566 -20.983 -22.950  1.00 35.00           N
ANISOU 2746  N   LYS D 339     5170   3459  4671  -897    324  -1788       N
ATOM   2747  CA  LYS D 339      55.850 -20.096 -24.079  1.00 36.41           C
ANISOU 2747  CA  LYS D 339     5338   3859  4637  -776    321  -1851       C
ATOM   2748  CB  LYS D 339      57.326 -20.142 -24.495  1.00 36.95           C
ANISOU 2748  CB  LYS D 339     5494   3859  4687  -549    472  -1853       C
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Figure 18 (continued)

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ATOM   2749  CG  LYS D 339      58.378 -19.987 -23.447  1.00 37.74           C
ANISOU 2749  CG  LYS D 339     5523   3868   4948   -415    568  -1657       C
ATOM   2750  CD  LYS D 339      59.724 -20.262 -24.109  1.00 42.28           C
ANISOU 2750  CD  LYS D 339     6178   4366   5520   -206    718  -1721       C
ATOM   2751  CE  LYS D 339      60.861 -20.353 -23.116  1.00 43.49           C
ANISOU 2751  CE  LYS D 339     6261   4395   5869    -62    795  -1556       C
ATOM   2752  NZ  LYS D 339      62.013 -21.010 -23.793  1.00 46.57           N
ANISOU 2752  NZ  LYS D 339     6738   4653   6302    127    942  -1667       N
ATOM   2753  C   LYS D 339      55.092 -20.560 -25.307  1.00 39.56           C
ANISOU 2753  C   LYS D 339     5843   4294   4893   -881    222  -2099       C
ATOM   2754  O   LYS D 339      54.885 -21.757 -25.525  1.00 41.85           O
ANISOU 2754  O   LYS D 339     6273   4373   5255   -979    208  -2268       O
ATOM   2755  N   ARG D 340      54.750 -19.599 -26.148  1.00 40.34           N
ANISOU 2755  N   ARG D 340     5894   4653   4779   -847    148  -2123       N
ATOM   2756  CA  ARG D 340      54.128 -19.873 -27.426  1.00 43.61           C
ANISOU 2756  CA  ARG D 340     6421   5149   5002   -912     32  -2354       C
ATOM   2757  CB  ARG D 340      52.616 -19.731 -27.273  1.00 44.40           C
ANISOU 2757  CB  ARG D 340     6374   5372   5123  -1124   -171  -2385       C
ATOM   2758  CG  ARG D 340      51.801 -20.062 -28.490  1.00 48.83           C
ANISOU 2758  CG  ARG D 340     7023   6024   5507  -1227   -350  -2632       C
ATOM   2759  CD  ARG D 340      50.478 -19.350 -28.366  1.00 52.29           C
ANISOU 2759  CD  ARG D 340     7237   6693   5939  -1353   -548  -2586       C
ATOM   2760  NE  ARG D 340      49.496 -19.823 -29.329  1.00 58.76           N
ANISOU 2760  NE  ARG D 340     8095   7584   6649  -1504   -768  -2830       N
ATOM   2761  CZ  ARG D 340      48.306 -19.252 -29.509  1.00 62.04           C
ANISOU 2761  CZ  ARG D 340     8317   8227   7030  -1600   -982  -2837       C
ATOM   2762  NH1 ARG D 340      47.964 -18.181 -28.792  1.00 60.08           N
ANISOU 2762  NH1 ARG D 340     7836   8142   6848  -1546   -980  -2613       N
ATOM   2763  NH2 ARG D 340      47.457 -19.748 -30.409  1.00 66.38           N
ANISOU 2763  NH2 ARG D 340     8900   8838   7483  -1742  -1208  -3077       N
ATOM   2764  C   ARG D 340      54.699 -18.825 -28.379  1.00 43.42           C
ANISOU 2764  C   ARG D 340     6432   5344   4723   -731     75  -2320       C
ATOM   2765  O   ARG D 340      54.666 -17.628 -28.079  1.00 41.49           O
ANISOU 2765  O   ARG D 340     6042   5281   4442   -669     66  -2130       O
ATOM   2766  N   GLU D 341      55.293 -19.272 -29.480  1.00 45.77           N
ANISOU 2766  N   GLU D 341     6935   5607   4850   -638    147  -2495       N
ATOM   2767  CA  GLU D 341      55.826 -18.341 -30.477  1.00 46.72           C
ANISOU 2767  CA  GLU D 341     7119   5932   4699   -477    212  -2464       C
ATOM   2768  CB  GLU D 341      56.762 -19.062 -31.453  1.00 49.50           C
ANISOU 2768  CB  GLU D 341     7709   6182   4915   -352    375  -2651       C
ATOM   2769  CG  GLU D 341      57.526 -18.146 -32.413  1.00 51.74           C
ANISOU 2769  CG  GLU D 341     8071   6657   4932   -174    514  -2591       C
ATOM   2770  CD  GLU D 341      58.919 -18.672 -32.742  1.00 55.51           C
ANISOU 2770  CD  GLU D 341     8666   6998   5426      1    793  -2654       C
ATOM   2771  OE1 GLU D 341      59.022 -19.726 -33.415  1.00 59.55           O
ANISOU 2771  OE1 GLU D 341     9387   7379   5861     12    832  -2909       O
ATOM   2772  OE2 GLU D 341      59.911 -18.027 -32.326  1.00 54.92           O
ANISOU 2772  OE2 GLU D 341     8468   6945   5454    128    973  -2457       O
ATOM   2773  C   GLU D 341      54.668 -17.653 -31.202  1.00 47.34           C
ANISOU 2773  C   GLU D 341     7175   6260   4552   -555    -12  -2501       C
ATOM   2774  O   GLU D 341      53.755 -18.308 -31.666  1.00 49.11           O
ANISOU 2774  O   GLU D 341     7462   6479   4718   -696   -188  -2701       O
ATOM   2775  N   GLU D 342      54.698 -16.327 -31.260  1.00 46.37           N
ANISOU 2775  N   GLU D 342     6952   6343   4322   -463    -17  -2304       N
ATOM   2776  CA  GLU D 342      53.581 -15.557 -31.814  1.00 48.18           C
ANISOU 2776  CA  GLU D 342     7130   6809   4367   -510   -246  -2296       C
ATOM   2777  CB  GLU D 342      52.718 -14.978 -30.691  1.00 45.85           C
ANISOU 2777  CB  GLU D 342     6568   6567   4287   -600   -362  -2136       C
ATOM   2778  CG  GLU D 342      51.598 -15.878 -30.201  1.00 49.03           C
ANISOU 2778  CG  GLU D 342     6868   6895   4866   -815   -524  -2272       C
ATOM   2779  CD  GLU D 342      50.813 -15.233 -29.079  1.00 48.12           C
ANISOU 2779  CD  GLU D 342     6483   6849   4951   -882   -591  -2102       C
ATOM   2780  OE1 GLU D 342      50.844 -15.791 -27.956  1.00 52.42           O
ANISOU 2780  OE1 GLU D 342     6943   7228   5746   -975   -507  -2058       O
ATOM   2781  OE2 GLU D 342      50.194 -14.158 -29.301  1.00 51.11           O
ANISOU 2781  OE2 GLU D 342     6748   7440   5233   -829   -716  -2007       O
ATOM   2782  C   GLU D 342      54.051 -14.407 -32.683  1.00 47.55           C
ANISOU 2782  C   GLU D 342     7135   6921   4011   -343   -190  -2174       C
ATOM   2783  O   GLU D 342      55.108 -13.831 -32.436  1.00 45.79           O
ANISOU 2783  O   GLU D 342     6900   6671   3827   -217     22  -2008       O
ATOM   2784  N   GLU D 343      53.237 -14.060 -33.674  1.00 49.19           N
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Figure 18 (continued)

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ANISOU 2784  N   GLU D 343     7421   7319   3949   -350   -391  -2247       N
ATOM   2785  CA  GLU D 343      53.517 -12.924 -34.539  1.00 49.57           C
ANISOU 2785  CA  GLU D 343     7571   7555   3708   -200   -366  -2109       C
ATOM   2786  CB  GLU D 343      53.181 -13.255 -35.991  1.00 53.34           C
ANISOU 2786  CB  GLU D 343     8304   8158   3805   -185   -494  -2308       C
ATOM   2787  CG  GLU D 343      53.423 -14.707 -36.327  1.00 57.34           C
ANISOU 2787  CG  GLU D 343     8979   8503   4305   -258   -446  -2603       C
ATOM   2788  CD  GLU D 343      54.110 -14.904 -37.652  1.00 62.14           C
ANISOU 2788  CD  GLU D 343     9908   9165   4538   -141   -320  -2734       C
ATOM   2789  OE1 GLU D 343      53.678 -14.282 -38.648  1.00 66.06           O
ANISOU 2789  OE1 GLU D 343    10542   9875   4684    -85   -464  -2723       O
ATOM   2790  OE2 GLU D 343      55.074 -15.699 -37.694  1.00 62.92           O
ANISOU 2790  OE2 GLU D 343    10127   9092   4688    -95    -77  -2850       O
ATOM   2791  C   GLU D 343      52.733 -11.701 -34.073  1.00 47.50           C
ANISOU 2791  C   GLU D 343     7105   7439   3503   -187   -523  -1896       C
ATOM   2792  O   GLU D 343      51.494 -11.696 -34.101  1.00 48.59           O
ANISOU 2792  O   GLU D 343     7137   7683   3642   -274   -791  -1960       O
ATOM   2793  N   VAL D 344      53.461 -10.674 -33.637  1.00 44.51           N
ANISOU 2793  N   VAL D 344     6664   7057   3190    -77   -355  -1653       N
ATOM   2794  CA  VAL D 344      52.851  -9.406 -33.207  1.00 42.32           C
ANISOU 2794  CA  VAL D 344     6222   6892   2967    -33   -471  -1441       C
ATOM   2795  CB  VAL D 344      53.315  -8.974 -31.787  1.00 38.72           C
ANISOU 2795  CB  VAL D 344     5564   6310   2839    -38   -329  -1273       C
ATOM   2796  CG1 VAL D 344      52.789  -9.950 -30.744  1.00 37.84           C
ANISOU 2796  CG1 VAL D 344     5295   6085   2998   -187   -384  -1388       C
ATOM   2797  CG2 VAL D 344      54.852  -8.867 -31.698  1.00 37.43           C
ANISOU 2797  CG2 VAL D 344     5480   6029   2712     42    -33  -1181       C
ATOM   2798  C   VAL D 344      53.142  -8.313 -34.227  1.00 43.10           C
ANISOU 2798  C   VAL D 344     6482   7128   2765    114   -449  -1292       C
ATOM   2799  O   VAL D 344      54.177  -8.360 -34.880  1.00 43.50           O
ANISOU 2799  O   VAL D 344     6721   7153   2653    187   -238  -1280       O
ATOM   2800  N   LEU D 345      52.223  -7.349 -34.352  1.00 43.51           N
ANISOU 2800  N   LEU D 345     6459   7320   2751    163   -657  -1172       N
ATOM   2801  CA  LEU D 345      52.330  -6.227 -35.300  1.00 45.05           C
ANISOU 2801  CA  LEU D 345     6817   7642   2659    308   -675   -998       C
ATOM   2802  CB  LEU D 345      51.020  -6.033 -36.060  1.00 47.61           C
ANISOU 2802  CB  LEU D 345     7160   8159   2770    333  -1020  -1052       C
ATOM   2803  CG  LEU D 345      50.743  -6.475 -37.488  1.00 51.69           C
ANISOU 2803  CG  LEU D 345     7938   8822   2881    358  -1172  -1200       C
ATOM   2804  CD1 LEU D 345      49.400  -5.893 -37.870  1.00 52.98           C
ANISOU 2804  CD1 LEU D 345     8021   9173   2935    408  -1542  -1167       C
ATOM   2805  CD2 LEU D 345      51.809  -6.018 -38.456  1.00 52.76           C
ANISOU 2805  CD2 LEU D 345     8377   8975   2694    479   -945  -1081       C
ATOM   2806  C   LEU D 345      52.638  -4.914 -34.591  1.00 43.02           C
ANISOU 2806  C   LEU D 345     6443   7334   2567    390   -577   -726       C
ATOM   2807  O   LEU D 345      51.867  -4.483 -33.736  1.00 41.31           O
ANISOU 2807  O   LEU D 345     6010   7119   2567    375   -711   -671       O
ATOM   2808  N   THR D 346      53.739  -4.270 -34.977  1.00 43.51           N
ANISOU 2808  N   THR D 346     6654   7353   2525    471   -339   -564       N
ATOM   2809  CA  THR D 346      54.144  -3.000 -34.387  1.00 42.63           C
ANISOU 2809  CA  THR D 346     6463   7169   2566    535   -233   -311       C
ATOM   2810  CB  THR D 346      55.658  -2.699 -34.549  1.00 42.01           C
ANISOU 2810  CB  THR D 346     6490   6988   2482    557    105   -189       C
ATOM   2811  OG1 THR D 346      55.892  -2.121 -35.833  1.00 44.89           O
ANISOU 2811  OG1 THR D 346     7110   7447   2499    650    159    -72       O
ATOM   2812  CG2 THR D 346      56.495  -3.942 -34.379  1.00 40.99           C
ANISOU 2812  CG2 THR D 346     6357   6779   2440    484    289   -371       C
ATOM   2813  C   THR D 346      53.350  -1.816 -34.938  1.00 44.91           C
ANISOU 2813  C   THR D 346     6813   7567   2686    654   -424   -137       C
ATOM   2814  O   THR D 346      52.564  -1.953 -35.884  1.00 47.19           O
ANISOU 2814  O   THR D 346     7219   8008   2701    699   -638   -198       O
ATOM   2815  N   GLY D 347      53.580  -0.657 -34.312  1.00 44.77           N
ANISOU 2815  N   GLY D 347     6714   7455   2839    706   -353     76       N
ATOM   2816  CA  GLY D 347      52.914   0.595 -34.643  1.00 47.06           C
ANISOU 2816  CA  GLY D 347     7049   7795   3037    837   -509    273       C
ATOM   2817  C   GLY D 347      53.311   1.122 -35.999  1.00 50.85           C
ANISOU 2817  C   GLY D 347     7832   8341   3149    933   -452    421       C
ATOM   2818  O   GLY D 347      52.763   2.128 -36.458  1.00 53.05           O
ANISOU 2818  O   GLY D 347     8198   8660   3297   1060   -596    601       O
ATOM   2819  N   ASN D 348      54.272   0.453 -36.638  1.00 51.99           N
ANISOU 2819  N   ASN D 348     8144   8489   3120    885   -232    354       N
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Figure 18 (continued)

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ATOM   2820  CA  ASN D 348      54.607   0.740 -38.029  1.00 55.74           C
ANISOU 2820  CA  ASN D 348    8937   9058   3184    967   -164    458       C
ATOM   2821  CB  ASN D 348      56.043   1.273 -38.165  1.00 56.17           C
ANISOU 2821  CB  ASN D 348    9099   8991   3252    953    220    639       C
ATOM   2822  CG  ASN D 348      56.246   2.063 -39.453  1.00 61.46           C
ANISOU 2822  CG  ASN D 348   10094   9733   3527   1057    289    857       C
ATOM   2823  OD1 ASN D 348      55.428   2.921 -39.808  1.00 64.89           O
ANISOU 2823  OD1 ASN D 348   10617  10214   3824   1167     67   1018       O
ATOM   2824  ND2 ASN D 348      57.326   1.760 -40.175  1.00 64.62           N
ANISOU 2824  ND2 ASN D 348   10677  10143   3734   1033    603    867       N
ATOM   2825  C   ASN D 348      54.350  -0.455 -38.966  1.00 57.47           C
ANISOU 2825  C   ASN D 348    9315   9429   3090    945   -253    215       C
ATOM   2826  O   ASN D 348      54.970  -0.582 -40.028  1.00 59.79           O
ANISOU 2826  O   ASN D 348    9882   9784   3050    980    -93    233       O
ATOM   2827  N   LEU D 349      53.412  -1.315 -38.557  1.00 56.20           N
ANISOU 2827  N   LEU D 349    8987   9325   3042    880   -504    -17       N
ATOM   2828  CA  LEU D 349      52.992  -2.499 -39.333  1.00 57.58           C
ANISOU 2828  CA  LEU D 349    9285   9625   2966    836   -647   -288       C
ATOM   2829  CB  LEU D 349      52.211  -2.097 -40.591  1.00 61.54           C
ANISOU 2829  CB  LEU D 349   10023  10324   3035    950   -912   -241       C
ATOM   2830  CG  LEU D 349      50.920  -1.293 -40.393  1.00 62.61           C
ANISOU 2830  CG  LEU D 349   10006  10547   3235   1033  -1273   -131       C
ATOM   2831  CD1 LEU D 349      50.097  -1.301 -41.692  1.00 66.68           C
ANISOU 2831  CD1 LEU D 349   10749  11283   3304   1126  -1593   -171       C
ATOM   2832  CD2 LEU D 349      50.089  -1.802 -39.206  1.00 59.33           C
ANISOU 2832  CD2 LEU D 349    9218  10095   3228    926  -1441   -291       C
ATOM   2833  C   LEU D 349      54.118  -3.484 -39.668  1.00 56.92           C
ANISOU 2833  C   LEU D 349    9346   9481   2800    775   -347   -445       C
ATOM   2834  O   LEU D 349      54.078  -4.191 -40.669  1.00 59.54           O
ANISOU 2834  O   LEU D 349    9905   9914   2802    781   -383   -615       O
ATOM   2835  N   GLN D 350      55.114  -3.533 -38.799  1.00 53.58           N
ANISOU 2835  N   GLN D 350    8781   8890   2685    724    -60   -398       N
ATOM   2836  CA  GLN D 350      56.191  -4.499 -38.940  1.00 52.62           C
ANISOU 2836  CA  GLN D 350    8734   8692   2566    681    227   -551       C
ATOM   2837  CB  GLN D 350      57.506  -3.890 -38.472  1.00 51.26           C
ANISOU 2837  CB  GLN D 350    8493   8390   2594    694    581   -356       C
ATOM   2838  CG  GLN D 350      58.701  -4.803 -38.614  1.00 50.19           C
ANISOU 2838  CG  GLN D 350    8402   8179   2489    677    898   -492       C
ATOM   2839  CD  GLN D 350      59.992  -4.205 -38.068  1.00 48.94           C
ANISOU 2839  CD  GLN D 350    8115   7899   2580    676   1225   -304       C
ATOM   2840  OE1 GLN D 350      60.012  -3.105 -37.519  1.00 43.94           O
ANISOU 2840  OE1 GLN D 350    7366   7218   2111    672   1213    -78       O
ATOM   2841  NE2 GLN D 350      61.086  -4.936 -38.238  1.00 49.94           N
ANISOU 2841  NE2 GLN D 350    8258   7972   2745    684   1516   -409       N
ATOM   2842  C   GLN D 350      55.865  -5.750 -38.123  1.00 50.95           C
ANISOU 2842  C   GLN D 350    8341   8395   2625    565    135   -811       C
ATOM   2843  O   GLN D 350      55.432  -5.662 -36.975  1.00 47.85           O
ANISOU 2843  O   GLN D 350    7690   7924   2565    503     31   -786       O
ATOM   2844  N   THR D 351      56.049  -6.915 -38.728  1.00 52.61           N
ANISOU 2844  N   THR D 351    8702   8610   2676    537    178  -1062       N
ATOM   2845  CA  THR D 351      55.779  -8.175 -38.044  1.00 51.53           C
ANISOU 2845  CA  THR D 351    8435   8362   2782    422    105  -1310       C
ATOM   2846  CB  THR D 351      55.468  -9.299 -39.050  1.00 54.66           C
ANISOU 2846  CB  THR D 351    9064   8813   2891    395     11  -1608       C
ATOM   2847  OG1 THR D 351      54.324  -8.936 -39.833  1.00 58.05           O
ANISOU 2847  OG1 THR D 351    9596   9433   3026    407   -315  -1629       O
ATOM   2848  CG2 THR D 351      55.210 -10.608 -38.356  1.00 53.78           C
ANISOU 2848  CG2 THR D 351    8837   8552   3047    266    -52  -1856       C
ATOM   2849  C   THR D 351      56.988  -8.559 -37.210  1.00 49.24           C
ANISOU 2849  C   THR D 351    8023   7884   2800    411    412  -1292       C
ATOM   2850  O   THR D 351      58.117  -8.534 -37.699  1.00 50.66           O
ANISOU 2850  O   THR D 351    8325   8042   2884    486    705  -1256       O
ATOM   2851  N   LEU D 352      56.742  -8.897 -35.949  1.00 46.43           N
ANISOU 2851  N   LEU D 352    7422   7404   2813    322    345  -1309       N
ATOM   2852  CA  LEU D 352      57.770  -9.440 -35.074  1.00 44.39           C
ANISOU 2852  CA  LEU D 352    7042   6963   2860    309    574  -1318       C
ATOM   2853  CB  LEU D 352      58.010  -8.535 -33.873  1.00 41.23           C
ANISOU 2853  CB  LEU D 352    6404   6502   2761    301    608  -1090       C
ATOM   2854  CG  LEU D 352      58.524  -7.106 -34.038  1.00 41.08           C
ANISOU 2854  CG  LEU D 352    6381   6541   2689    379    724   -827       C
ATOM   2855  CD1 LEU D 352      58.549  -6.426 -32.663  1.00 36.89           C
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Figure 18 (continued)

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ANISOU 2855  CD1 LEU D 352     5605   5920   2491    342    695   -670  C
ATOM   2856  CD2 LEU D 352      59.892  -7.044 -34.742  1.00 42.81      C
ANISOU 2856  CD2 LEU D 352     6718   6745   2804    456   1049   -782  C
ATOM   2857  C   LEU D 352      57.361 -10.814 -34.566  1.00 44.29      C
ANISOU 2857  C   LEU D 352     6985   6825   3018    206    476  -1554  C
ATOM   2858  O   LEU D 352      56.238 -11.002 -34.099  1.00 43.77      O
ANISOU 2858  O   LEU D 352     6813   6774   3042    103    230  -1608  O
ATOM   2859  N   LYS D 353      58.278 -11.768 -34.669  1.00 44.79      N
ANISOU 2859  N   LYS D 353     7127   6756   3136    236    681  -1689  N
ATOM   2860  CA  LYS D 353      58.073 -13.104 -34.159  1.00 45.15      C
ANISOU 2860  CA  LYS D 353     7153   6632   3369    151    628  -1896  C
ATOM   2861  CB  LYS D 353      58.797 -14.122 -35.043  1.00 47.86      C
ANISOU 2861  CB  LYS D 353     7721   6897   3567    219    805  -2118  C
ATOM   2862  CG  LYS D 353      58.258 -15.538 -34.984  1.00 49.96      C
ANISOU 2862  CG  LYS D 353     8068   7007   3906    117    685  -2393  C
ATOM   2863  CD  LYS D 353      59.022 -16.428 -35.977  1.00 54.00      C
ANISOU 2863  CD  LYS D 353     8834   7446   4239    215    880  -2623  C
ATOM   2864  CE  LYS D 353      58.155 -17.546 -36.539  1.00 59.44      C
ANISOU 2864  CE  LYS D 353     9711   8070   4806    104    687  -2938  C
ATOM   2865  NZ  LYS D 353      58.831 -18.247 -37.687  1.00 64.80      N
ANISOU 2865  NZ  LYS D 353    10681   8712   5227    217    872  -3177  N
ATOM   2866  C   LYS D 353      58.643 -13.117 -32.754  1.00 42.12      C
ANISOU 2866  C   LYS D 353     6545   6092   3366    139    721  -1761  C
ATOM   2867  O   LYS D 353      59.852 -13.025 -32.567  1.00 41.20      O
ANISOU 2867  O   LYS D 353     6392   5905   3356    236    956  -1680  O
ATOM   2868  N   ILE D 354      57.766 -13.202 -31.758  1.00 40.54      N
ANISOU 2868  N   ILE D 354     6187   5851   3365     21    534  -1732  N
ATOM   2869  CA  ILE D 354      58.192 -13.268 -30.366  1.00 38.30      C
ANISOU 2869  CA  ILE D 354     5716   5424   3411      2    591  -1611  C
ATOM   2870  CB  ILE D 354      57.745 -12.007 -29.553  1.00 36.18      C
ANISOU 2870  CB  ILE D 354     5261   5254   3233    -19    498  -1388  C
ATOM   2871  CG1 ILE D 354      56.211 -11.875 -29.518  1.00 36.29      C
ANISOU 2871  CG1 ILE D 354     5222   5374   3193   -132    243  -1432  C
ATOM   2872  CD1 ILE D 354      55.700 -10.892 -28.478  1.00 34.52      C
ANISOU 2872  CD1 ILE D 354     4800   5199   3117   -155    163  -1250  C
ATOM   2873  CG2 ILE D 354      58.399 -10.725 -30.109  1.00 35.98      C
ANISOU 2873  CG2 ILE D 354     5252   5350   3070     93    613  -1218  C
ATOM   2874  C   ILE D 354      57.669 -14.549 -29.696  1.00 38.61      C
ANISOU 2874  C   ILE D 354     5744   5289   3636   -119    500  -1757  C
ATOM   2875  O   ILE D 354      56.645 -15.128 -30.109  1.00 40.64      O
ANISOU 2875  O   ILE D 354     6070   5566   3808   -231    333  -1922  O
ATOM   2876  N   ARG D 355      58.383 -15.004 -28.679  1.00 36.91      N
ANISOU 2876  N   ARG D 355     5447   4900   3678    -99    603  -1695  N
ATOM   2877  CA  ARG D 355      57.871 -16.064 -27.832  1.00 37.02      C
ANISOU 2877  CA  ARG D 355     5439   4735   3891   -219    522  -1768  C
ATOM   2878  CB  ARG D 355      58.994 -16.964 -27.340  1.00 37.88      C
ANISOU 2878  CB  ARG D 355     5582   4617   4194   -134    680  -1782  C
ATOM   2879  CG  ARG D 355      59.574 -17.833 -28.449  1.00 45.02      C
ANISOU 2879  CG  ARG D 355     6685   5434   4986    -48    798  -1993  C
ATOM   2880  CD  ARG D 355      60.668 -18.706 -27.904  1.00 52.28      C
ANISOU 2880  CD  ARG D 355     7615   6120   6130     61    947  -1997  C
ATOM   2881  NE  ARG D 355      61.771 -18.840 -28.849  1.00 59.10      N
ANISOU 2881  NE  ARG D 355     8572   6983   6901    238   1156  -2087  N
ATOM   2882  CZ  ARG D 355      62.978 -19.295 -28.524  1.00 61.64      C
ANISOU 2882  CZ  ARG D 355     8855   7157   7409    394   1324  -2061  C
ATOM   2883  NH1 ARG D 355      63.241 -19.653 -27.265  1.00 59.91      N
ANISOU 2883  NH1 ARG D 355     8522   6776   7463    396   1281  -1939  N
ATOM   2884  NH2 ARG D 355      63.920 -19.396 -29.461  1.00 64.91      N
ANISOU 2884  NH2 ARG D 355     9340   7592   7731    555   1536  -2157  N
ATOM   2885  C   ARG D 355      57.115 -15.449 -26.673  1.00 33.46      C
ANISOU 2885  C   ARG D 355     4803   4335   3576   -315    404  -1608  C
ATOM   2886  O   ARG D 355      57.717 -14.849 -25.782  1.00 30.78      O
ANISOU 2886  O   ARG D 355     4346   3982   3366   -256    470  -1430  O
ATOM   2887  N   VAL D 356      55.792 -15.577 -26.725  1.00 33.25      N
ANISOU 2887  N   VAL D 356     4744   4375   3512   -463    229  -1682  N
ATOM   2888  CA  VAL D 356      54.908 -14.994 -25.724  1.00 31.29      C
ANISOU 2888  CA  VAL D 356     4314   4199   3375   -555    127  -1554  C
ATOM   2889  CB  VAL D 356      53.495 -14.774 -26.281  1.00 32.47      C
ANISOU 2889  CB  VAL D 356     4410   4515   3413   -668    -69  -1643  C
ATOM   2890  CG1 VAL D 356      52.532 -14.347 -25.167  1.00 31.15      C
ANISOU 2890  CG1 VAL D 356     4036   4403   3395   -768   -146  -1532  C
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Figure 18 (continued)

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ATOM   2891  CG2 VAL D 356      53.522 -13.735 -27.416  1.00 32.66           C
ANISOU 2891  CG2 VAL D 356    4479   4746   3184   -550   -115  -1624       C
ATOM   2892  C   VAL D 356      54.883 -15.895 -24.485  1.00 30.33           C
ANISOU 2892  C   VAL D 356    4157   3876   3491   -651    160  -1525       C
ATOM   2893  O   VAL D 356      54.610 -17.084 -24.580  1.00 31.63           O
ANISOU 2893  O   VAL D 356    4413   3886   3719   -754    142  -1666       O
ATOM   2894  N   HIS D 357      55.229 -15.330 -23.330  1.00 27.89           N
ANISOU 2894  N   HIS D 357    3738   3555   3304   -612    211  -1339       N
ATOM   2895  CA  HIS D 357      55.108 -16.067 -22.055  1.00 27.09           C
ANISOU 2895  CA  HIS D 357    3613   3286   3396   -703    233  -1277       C
ATOM   2896  CB  HIS D 357      56.157 -15.624 -21.051  1.00 24.13           C
ANISOU 2896  CB  HIS D 357    3198   2855   3116   -585    320  -1100       C
ATOM   2897  CG  HIS D 357      57.530 -16.091 -21.397  1.00 23.18           C
ANISOU 2897  CG  HIS D 357    3173   2605   3030   -441    426  -1120       C
ATOM   2898  ND1 HIS D 357      58.182 -17.076 -20.684  1.00 23.15           N
ANISOU 2898  ND1 HIS D 357    3234   2380   3180   -414    478  -1092       N
ATOM   2899  CE1 HIS D 357      59.360 -17.313 -21.233  1.00 21.17           C
ANISOU 2899  CE1 HIS D 357    3036   2061   2946   -261    573  -1129       C
ATOM   2900  NE2 HIS D 357      59.496 -16.511 -22.275  1.00 25.10           N
ANISOU 2900  NE2 HIS D 357    3515   2730   3291   -203    603  -1175       N
ATOM   2901  CD2 HIS D 357      58.363 -15.742 -22.405  1.00 21.56           C
ANISOU 2901  CD2 HIS D 357    3005   2457   2728   -310    501  -1165       C
ATOM   2902  C   HIS D 357      53.706 -15.975 -21.470  1.00 27.09           C
ANISOU 2902  C   HIS D 357    3488   3362   3441   -872    137  -1264       C
ATOM   2903  O   HIS D 357      53.151 -14.887 -21.336  1.00 26.76           O
ANISOU 2903  O   HIS D 357    3314   3507   3346   -858     85  -1189       O
ATOM   2904  N   GLU D 358      53.130 -17.135 -21.179  1.00 28.20           N
ANISOU 2904  N   GLU D 358    3673   3353   3691  -1033    123  -1343       N
ATOM   2905  CA  GLU D 358      51.766 -17.230 -20.704  1.00 28.28           C
ANISOU 2905  CA  GLU D 358    3553   3425   3768  -1223     54  -1351       C
ATOM   2906  CB  GLU D 358      50.984 -18.208 -21.581  1.00 31.17           C
ANISOU 2906  CB  GLU D 358    3968   3736   4138  -1389    -39  -1564       C
ATOM   2907  CG  GLU D 358      50.973 -17.773 -23.047  1.00 32.95           C
ANISOU 2907  CG  GLU D 358    4233   4120   4167  -1309   -143  -1709       C
ATOM   2908  CD  GLU D 358      50.303 -18.740 -23.964  1.00 39.33           C
ANISOU 2908  CD  GLU D 358    5118   4872   4954  -1465   -257  -1944       C
ATOM   2909  OE1 GLU D 358      50.379 -19.974 -23.732  1.00 41.30           O
ANISOU 2909  OE1 GLU D 358    5483   4874   5336  -1583   -213  -2029       O
ATOM   2910  OE2 GLU D 358      49.688 -18.254 -24.939  1.00 42.18           O
ANISOU 2910  OE2 GLU D 358    5432   5432   5161  -1467   -405  -2049       O
ATOM   2911  C   GLU D 358      51.790 -17.669 -19.252  1.00 27.36           C
ANISOU 2911  C   GLU D 358    3429   3163   3804  -1292    145  -1208       C
ATOM   2912  O   GLU D 358      52.383 -18.677 -18.925  1.00 29.08           O
ANISOU 2912  O   GLU D 358    3791   3148   4112  -1304    210  -1203       O
ATOM   2913  N   GLY D 359      51.167 -16.892 -18.380  1.00 25.52           N
ANISOU 2913  N   GLY D 359    3044   3064   3587  -1322    155  -1086       N
ATOM   2914  CA  GLY D 359      51.052 -17.255 -16.979  1.00 24.48           C
ANISOU 2914  CA  GLY D 359    2916   2823   3560  -1399    247   -946       C
ATOM   2915  C   GLY D 359      51.467 -16.139 -16.057  1.00 22.50           C
ANISOU 2915  C   GLY D 359    2608   2681   3262  -1265    290   -781       C
ATOM   2916  O   GLY D 359      52.317 -15.309 -16.401  1.00 21.03           O
ANISOU 2916  O   GLY D 359    2431   2564   2997  -1090    271   -754       O
ATOM   2917  N   TYR D 360      50.879 -16.137 -14.865  1.00 22.56           N
ANISOU 2917  N   TYR D 360    2564   2692   3315  -1355    359   -674       N
ATOM   2918  CA  TYR D 360      51.277 -15.220 -13.807  1.00 20.82           C
ANISOU 2918  CA  TYR D 360    2328   2542   3042  -1243    405   -527       C
ATOM   2919  CB  TYR D 360      50.251 -15.243 -12.659  1.00 21.78           C
ANISOU 2919  CB  TYR D 360    2374   2709   3191  -1377    496   -447       C
ATOM   2920  CG  TYR D 360      50.774 -14.552 -11.417  1.00 21.58           C
ANISOU 2920  CG  TYR D 360    2399   2706   3092  -1269    551   -301       C
ATOM   2921  CD1 TYR D 360      50.769 -13.146 -11.321  1.00 18.96           C
ANISOU 2921  CD1 TYR D 360    1967   2554   2682  -1140    525   -292       C
ATOM   2922  CE1 TYR D 360      51.265 -12.515 -10.199  1.00 20.05           C
ANISOU 2922  CE1 TYR D 360    2168   2704   2746  -1049    560   -185       C
ATOM   2923  CZ  TYR D 360      51.801 -13.280  -9.164  1.00 20.65           C
ANISOU 2923  CZ  TYR D 360    2411   2630   2805  -1074    608    -71       C
ATOM   2924  OH  TYR D 360      52.295 -12.687  -8.034  1.00 19.63           O
ANISOU 2924  OH  TYR D 360    2362   2519   2577   -986    619     26       O
ATOM   2925  CE2 TYR D 360      51.829 -14.661  -9.238  1.00 22.70           C
ANISOU 2925  CE2 TYR D 360    2775   2709   3141  -1186    635    -54       C
ATOM   2926  CD2 TYR D 360      51.320 -15.292 -10.365  1.00 21.83           C
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Figure 18 (continued)

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ANISOU 2926  CD2 TYR D 360     2601   2570   3125  -1287    613   -175       C
ATOM   2927  C   TYR D 360      52.662 -15.527 -13.249  1.00 19.75           C
ANISOU 2927  C   TYR D 360     2358   2241   2906  -1119    426   -426       C
ATOM   2928  O   TYR D 360      52.983 -16.691 -12.914  1.00 20.71           O
ANISOU 2928  O   TYR D 360     2617   2153   3097  -1174    460   -393       O
ATOM   2929  N   GLU D 361      53.461 -14.477 -13.117  1.00 17.95           N
ANISOU 2929  N   GLU D 361     2109   2098   2614   -955    398   -371       N
ATOM   2930  CA  GLU D 361      54.818 -14.564 -12.568  1.00 18.25           C
ANISOU 2930  CA  GLU D 361     2255   2018   2660   -823    391   -276       C
ATOM   2931  CB  GLU D 361      55.857 -14.727 -13.665  1.00 17.09           C
ANISOU 2931  CB  GLU D 361     2139   1814   2541   -707    361   -349       C
ATOM   2932  CG  GLU D 361      55.906 -16.074 -14.343  1.00 20.73           C
ANISOU 2932  CG  GLU D 361     2703   2101   3074   -760    379   -440       C
ATOM   2933  CD  GLU D 361      56.874 -16.096 -15.496  1.00 21.89           C
ANISOU 2933  CD  GLU D 361     2870   2225   3221   -630    377   -530       C
ATOM   2934  OE1 GLU D 361      56.789 -15.177 -16.334  1.00 21.96           O
ANISOU 2934  OE1 GLU D 361     2796   2400   3148   -588    360   -586       O
ATOM   2935  OE2 GLU D 361      57.713 -17.035 -15.572  1.00 26.64           O
ANISOU 2935  OE2 GLU D 361     3576   2639   3905   -563    403   -540       O
ATOM   2936  C   GLU D 361      55.166 -13.305 -11.787  1.00 17.71           C
ANISOU 2936  C   GLU D 361     2137   2068   2522   -724    371   -189       C
ATOM   2937  O   GLU D 361      54.783 -12.180 -12.189  1.00 17.20           O
ANISOU 2937  O   GLU D 361     1959   2166   2408   -690    352   -229       O
ATOM   2938  N   GLU D 362      55.904 -13.489 -10.694  1.00 18.09           N
ANISOU 2938  N   GLU D 362     2281   2027   2567   -671    363    -75       N
ATOM   2939  CA  GLU D 362      56.464 -12.367  -9.950  1.00 19.15           C
ANISOU 2939  CA  GLU D 362     2393   2245   2638   -572    319    -10       C
ATOM   2940  CB  GLU D 362      55.949 -12.359  -8.507  1.00 19.27           C
ANISOU 2940  CB  GLU D 362     2482   2271   2569   -627    354     85       C
ATOM   2941  CG  GLU D 362      56.310 -11.107  -7.717  1.00 21.42           C
ANISOU 2941  CG  GLU D 362     2741   2644   2753   -541    306    118       C
ATOM   2942  CD  GLU D 362      55.912 -11.248  -6.250  1.00 24.81           C
ANISOU 2942  CD  GLU D 362     3289   3073   3065   -584    348    211       C
ATOM   2943  OE1 GLU D 362      54.919 -10.639  -5.837  1.00 34.00           O
ANISOU 2943  OE1 GLU D 362     4411   4356   4153   -632    428    187       O
ATOM   2944  OE2 GLU D 362      56.557 -12.014  -5.516  1.00 32.91           O
ANISOU 2944  OE2 GLU D 362     4457   3979   4069   -565    309    311       O
ATOM   2945  C   GLU D 362      57.976 -12.433  -9.968  1.00 17.74           C
ANISOU 2945  C   GLU D 362     2250   1975   2515   -438    247     30       C
ATOM   2946  O   GLU D 362      58.543 -13.501  -9.839  1.00 19.01           O
ANISOU 2946  O   GLU D 362     2502   1982   2740   -416    238     69       O
ATOM   2947  N   PHE D 363      58.617 -11.277 -10.154  1.00 17.84           N
ANISOU 2947  N   PHE D 363     2179   2078   2521   -348    198     20       N
ATOM   2948  CA  PHE D 363      60.073 -11.175 -10.225  1.00 17.84           C
ANISOU 2948  CA  PHE D 363     2159   2019   2600   -229    133     50       C
ATOM   2949  CB  PHE D 363      60.525 -10.817 -11.655  1.00 17.34           C
ANISOU 2949  CB  PHE D 363     1999   1994   2594   -179    169    -29       C
ATOM   2950  CG  PHE D 363      60.204 -11.851 -12.684  1.00 18.26           C
ANISOU 2950  CG  PHE D 363     2152   2047   2738   -208    236   -108       C
ATOM   2951  CD1 PHE D 363      61.094 -12.897 -12.951  1.00 19.62           C
ANISOU 2951  CD1 PHE D 363     2369   2076   3010   -138    249   -114       C
ATOM   2952  CE1 PHE D 363      60.784 -13.856 -13.898  1.00 20.76           C
ANISOU 2952  CE1 PHE D 363     2571   2145   3172   -165    312   -211       C
ATOM   2953  CZ  PHE D 363      59.597 -13.776 -14.610  1.00 18.79           C
ANISOU 2953  CZ  PHE D 363     2323   1978   2839   -274    341   -302       C
ATOM   2954  CE2 PHE D 363      58.711 -12.738 -14.363  1.00 20.21           C
ANISOU 2954  CE2 PHE D 363     2433   2315   2932   -338    317   -284       C
ATOM   2955  CD2 PHE D 363      59.020 -11.769 -13.412  1.00 17.87           C
ANISOU 2955  CD2 PHE D 363     2089   2080   2620   -298    276   -189       C
ATOM   2956  C   PHE D 363      60.584 -10.065  -9.329  1.00 17.94           C
ANISOU 2956  C   PHE D 363     2144   2096   2575   -182     50     99       C
ATOM   2957  O   PHE D 363      59.915  -9.014  -9.174  1.00 17.61           O
ANISOU 2957  O   PHE D 363     2069   2165   2459   -214     62     73       O
ATOM   2958  N   THR D 364      61.774 -10.269  -8.775  1.00 17.84           N
ANISOU 2958  N   THR D 364     2142   2012   2625   -100    -43    160       N
ATOM   2959  CA  THR D 364      62.589  -9.144  -8.386  1.00 18.22           C
ANISOU 2959  CA  THR D 364     2116   2116   2692    -50   -138    169       C
ATOM   2960  CB  THR D 364      63.421  -9.390  -7.113  1.00 18.94           C
ANISOU 2960  CB  THR D 364     2269   2152   2775    -284    251           C
ATOM   2961  OG1 THR D 364      64.333 -10.460  -7.344  1.00 22.11           O
ANISOU 2961  OG1 THR D 364     2655   2441   3304     89   -317    293       O
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Figure 18 (continued)

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ATOM   2962  CG2 THR D 364      62.554  -9.703  -5.942  1.00 18.12           C
ANISOU 2962  CG2 THR D 364    2332   2049   2504    -49   -289    306       C
ATOM   2963  C   THR D 364      63.528  -8.805  -9.555  1.00 18.43           C
ANISOU 2963  C   THR D 364    1999   2147   2858      8   -112    128       C
ATOM   2964  O   THR D 364      63.977  -9.703 -10.275  1.00 19.45           O
ANISOU 2964  O   THR D 364    2108   2205   3076     54    -61    116       O
ATOM   2965  N   MSE D 365      63.759  -7.504  -9.770  1.00 17.63           N
ANISOU 2965  N   MSE D 365    1808   2119   2769      0   -126    104       N
ATOM   2966  CA  MSE D 365      64.730  -7.023 -10.747  1.00 18.41           C
ANISOU 2966  CA  MSE D 365    1769   2226   2998     40    -88     87       C
ATOM   2967  CB  MSE D 365      64.077  -6.068 -11.759  1.00 17.25           C
ANISOU 2967  CB  MSE D 365    1596   2157   2801      0     10     46       C
ATOM   2968  CG  MSE D 365      62.868  -6.645 -12.487  1.00 16.17           C
ANISOU 2968  CG  MSE D 365    1532   2052   2561    -32    102      1       C
ATOM   2969  SE  MSE D 365      61.845  -5.313 -13.450  0.90 20.72          SE
ANISOU 2969  SE  MSE D 365    2093   2738   3041    -63    163    -30       SE
ATOM   2970  CE  MSE D 365      63.243  -4.311 -14.263  1.00 11.76           C
ANISOU 2970  CE  MSE D 365     852   1592   2023    -26    207      8       C
ATOM   2971  C   MSE D 365      65.810  -6.262  -9.991  1.00 17.87           C
ANISOU 2971  C   MSE D 365    1615   2153   3021     59   -218    116       C
ATOM   2972  O   MSE D 365      65.495  -5.340  -9.241  1.00 17.57           O
ANISOU 2972  O   MSE D 365    1614   2147   2913     15   -292    109       O
ATOM   2973  N   VAL D 366      67.068  -6.639 -10.196  1.00 18.01           N
ANISOU 2973  N   VAL D 366    1510   2130   3203    125   -245    137       N
ATOM   2974  CA  VAL D 366      68.202  -5.950  -9.570  1.00 18.86           C
ANISOU 2974  CA  VAL D 366    1492   2239   3436    133   -384    156       C
ATOM   2975  CB  VAL D 366      68.942  -6.864  -8.537  1.00 20.54           C
ANISOU 2975  CB  VAL D 366    1707   2397   3701    214   -553    207       C
ATOM   2976  CG1 VAL D 366      70.186  -6.172  -7.928  1.00 20.97           C
ANISOU 2976  CG1 VAL D 366    1598   2466   3905    220   -731    215       C
ATOM   2977  CG2 VAL D 366      67.976  -7.296  -7.406  1.00 21.86           C
ANISOU 2977  CG2 VAL D 366    2095   2550   3660    195   -633    237       C
ATOM   2978  C   VAL D 366      69.171  -5.358 -10.585  1.00 19.08           C
ANISOU 2978  C   VAL D 366    1324   2284   3643    133   -294    147       C
ATOM   2979  O   VAL D 366      69.843  -6.084 -11.309  1.00 19.34           O
ANISOU 2979  O   VAL D 366    1258   2296   3796    205   -204    151       O
ATOM   2980  N   GLY D 367      69.241  -4.027 -10.623  1.00 19.12           N
ANISOU 2980  N   GLY D 367    1279   2316   3670     51   -305    134       N
ATOM   2981  CA  GLY D 367      70.244  -3.316 -11.436  1.00 20.13           C
ANISOU 2981  CA  GLY D 367    1215   2451   3984     23   -221    144       C
ATOM   2982  C   GLY D 367      71.337  -2.617 -10.640  1.00 21.77           C
ANISOU 2982  C   GLY D 367    1266   2642   4363    -22   -391    146       C
ATOM   2983  O   GLY D 367      71.408  -2.757  -9.417  1.00 21.83           O
ANISOU 2983  O   GLY D 367    1322   2639   4334    -13   -599    136       O
ATOM   2984  N   LYS D 368      72.214  -1.887 -11.335  1.00 22.99           N
ANISOU 2984  N   LYS D 368    1233   2797   4706    -78   -304    160       N
ATOM   2985  CA  LYS D 368      73.258  -1.124 -10.655  1.00 25.77           C
ANISOU 2985  CA  LYS D 368    1410   3130   5252   -153   -467    150       C
ATOM   2986  CB  LYS D 368      74.267  -0.536 -11.644  1.00 27.60           C
ANISOU 2986  CB  LYS D 368    1403   3363   5721   -218   -307    181       C
ATOM   2987  CG  LYS D 368      75.163  -1.558 -12.320  1.00 33.38           C
ANISOU 2987  CG  LYS D 368    1937   4132   6613   -110   -181    206       C
ATOM   2988  CD  LYS D 368      76.116  -0.834 -13.239  1.00 40.97           C
ANISOU 2988  CD  LYS D 368    2663   5104   7802   -196      4    241       C
ATOM   2989  CE  LYS D 368      76.457  -1.646 -14.479  1.00 44.55           C
ANISOU 2989  CE  LYS D 368    3032   5601   8293    -92    283    264       C
ATOM   2990  NZ  LYS D 368      77.644  -1.037 -15.172  1.00 45.91           N
ANISOU 2990  NZ  LYS D 368    2915   5795   8735   -172    454    304       N
ATOM   2991  C   LYS D 368      72.654   0.026  -9.845  1.00 24.40           C
ANISOU 2991  C   LYS D 368    1379   2920   4973   -257   -603    106       C
ATOM   2992  O   LYS D 368      73.146   0.344  -8.779  1.00 25.32           O
ANISOU 2992  O   LYS D 368    1457   3020   5142   -295   -829     68       O
ATOM   2993  N   ARG D 369      71.581   0.624 -10.361  1.00 22.61           N
ANISOU 2993  N   ARG D 369    1320   2680   4592   -289   -471    106       N
ATOM   2994  CA  ARG D 369      71.084   1.898  -9.820  1.00 22.72           C
ANISOU 2994  CA  ARG D 369    1450   2637   4547   -381   -553     61       C
ATOM   2995  CB  ARG D 369      71.284   3.026 -10.839  1.00 23.23           C
ANISOU 2995  CB  ARG D 369    1454   2643   4728   -474   -393     99       C
ATOM   2996  CG  ARG D 369      72.739   3.461 -11.079  1.00 25.22           C
ANISOU 2996  CG  ARG D 369    1448   2862   5272   -572   -395    123       C
ATOM   2997  CD  ARG D 369      72.724   4.978 -11.254  1.00 27.02           C
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Figure 18 (continued)

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ANISOU 2997  CD  ARG D 369     1710   2974   5581   -711   -368    125  C
ATOM   2998  NE  ARG D 369      73.878   5.516 -10.578  1.00 30.88      N
ANISOU 2998  NE  ARG D 369     2013   3410   6311   -834   -535     79  N
ATOM   2999  CZ  ARG D 369      73.901   6.588  -9.811  1.00 32.41      C
ANISOU 2999  CZ  ARG D 369     2268   3495   6550   -948   -695      3  C
ATOM   3000  NH1 ARG D 369      72.814   7.329  -9.581  1.00 27.48      N
ANISOU 3000  NH1 ARG D 369     1898   2792   5751   -941   -698    -36  N
ATOM   3001  NH2 ARG D 369      75.066   6.923  -9.282  1.00 37.95      N
ANISOU 3001  NH2 ARG D 369     2761   4164   7495  -1068   -857    -43  N
ATOM   3002  C   ARG D 369      69.625   1.847  -9.399  1.00 21.13      C
ANISOU 3002  C   ARG D 369     1494   2450   4083   -335   -554     28  C
ATOM   3003  O   ARG D 369      69.083   2.830  -8.934  1.00 21.50      O
ANISOU 3003  O   ARG D 369     1657   2450   4063   -381   -605    -21  O
ATOM   3004  N   ALA D 370      68.982   0.695  -9.556  1.00 20.31      N
ANISOU 3004  N   ALA D 370     1467   2407   3845   -245   -491     48  N
ATOM   3005  CA  ALA D 370      67.568   0.560  -9.210  1.00 19.37      C
ANISOU 3005  CA  ALA D 370     1545   2315   3499   -211   -469     22  C
ATOM   3006  CB  ALA D 370      66.677   1.149 -10.287  1.00 17.08      C
ANISOU 3006  CB  ALA D 370     1309   2033   3150   -214   -301     37  C
ATOM   3007  C   ALA D 370      67.248  -0.884  -9.014  1.00 19.29      C
ANISOU 3007  C   ALA D 370     1584   2348   3395   -138   -463     43  C
ATOM   3008  O   ALA D 370      67.922  -1.742  -9.573  1.00 19.71      O
ANISOU 3008  O   ALA D 370     1534   2404   3548    -97   -417     79  O
ATOM   3009  N   THR D 371      66.236  -1.151  -8.200  1.00 19.16      N
ANISOU 3009  N   THR D 371     1728   2356   3196   -124   -499     19  N
ATOM   3010  CA  THR D 371      65.719  -2.493  -8.036  1.00 20.02      C
ANISOU 3010  CA  THR D 371     1913   2488   3207    -77   -468     48  C
ATOM   3011  CB  THR D 371      66.139  -3.157  -6.702  1.00 20.97      C
ANISOU 3011  CB  THR D 371     2102   2591   3274    -49   -635     69  C
ATOM   3012  OG1 THR D 371      65.494  -2.487  -5.624  1.00 23.31      O
ANISOU 3012  OG1 THR D 371     2538   2908   3410    -79   -706     26  O
ATOM   3013  CG2 THR D 371      67.641  -3.122  -6.488  1.00 21.86      C
ANISOU 3013  CG2 THR D 371     2068   2673   3565    -30   -782     86  C
ATOM   3014  C   THR D 371      64.184  -2.423  -8.121  1.00 19.54      C
ANISOU 3014  C   THR D 371     1975   2472   2979    -89   -363     23  C
ATOM   3015  O   THR D 371      63.586  -1.359  -8.003  1.00 19.86      O
ANISOU 3015  O   THR D 371     2053   2526   2966   -111   -349    -18  O
ATOM   3016  N   ALA D 372      63.528  -3.552  -8.324  1.00 19.12      N
ANISOU 3016  N   ALA D 372     1973   2435   2858    -76   -288     43  N
ATOM   3017  CA  ALA D 372      62.076  -3.489  -8.455  1.00 17.32      C
ANISOU 3017  CA  ALA D 372     1816   2263   2502    -99   -191     15  C
ATOM   3018  CB  ALA D 372      61.686  -3.097  -9.920  1.00 17.05      C
ANISOU 3018  CB  ALA D 372     1709   2262   2508    -97    -82     -3  C
ATOM   3019  C   ALA D 372      61.442  -4.786  -8.072  1.00 16.39      C
ANISOU 3019  C   ALA D 372     1780   2143   2304   -114   -155     40  C
ATOM   3020  O   ALA D 372      62.117  -5.809  -7.986  1.00 17.78      O
ANISOU 3020  O   ALA D 372     1965   2259   2533    -92   -189     83  O
ATOM   3021  N   ILE D 373      60.138  -4.749  -7.838  1.00 16.26      N
ANISOU 3021  N   ILE D 373     1816   2184   2177   -149    -81     16  N
ATOM   3022  CA  ILE D 373      59.332  -5.958  -7.815  1.00 14.85      C
ANISOU 3022  CA  ILE D 373     1687   2003   1950   -195     -6     35  C
ATOM   3023  CB  ILE D 373      58.647  -6.199  -6.451  1.00 17.21      C
ANISOU 3023  CB  ILE D 373     2106   2321   2113   -231      8     63  C
ATOM   3024  CG1 ILE D 373      59.646  -6.124  -5.278  1.00 14.71      C
ANISOU 3024  CG1 ILE D 373     1885   1957   1748   -191   -121    110  C
ATOM   3025  CD1 ILE D 373      58.992  -6.294  -3.900  1.00 16.18      C
ANISOU 3025  CD1 ILE D 373     2225   2170   1751   -219    -97    142  C
ATOM   3026  CG2 ILE D 373      57.892  -7.565  -6.465  1.00 14.20      C
ANISOU 3026  CG2 ILE D 373     1774   1909   1713   -304     99    100  C
ATOM   3027  C   ILE D 373      58.275  -5.853  -8.918  1.00 15.49      C
ANISOU 3027  C   ILE D 373     1695   2153   2037   -225     90    -18  C
ATOM   3028  O   ILE D 373      57.564  -4.846  -9.013  1.00 14.66      O
ANISOU 3028  O   ILE D 373     1549   2123   1896   -214    114    -57  O
ATOM   3029  N   LEU D 374      58.168  -6.910  -9.725  1.00 15.28      N
ANISOU 3029  N   LEU D 374     1656   2094   2054   -255    132    -25  N
ATOM   3030  CA  LEU D 374      57.294  -6.952 -10.890  1.00 14.84      C
ANISOU 3030  CA  LEU D 374     1534   2103   2000   -285    188    -85  C
ATOM   3031  CB  LEU D 374      58.116  -7.089 -12.188  1.00 13.81      C
ANISOU 3031  CB  LEU D 374     1370   1943   1933   -240    188   -107  C
ATOM   3032  CG  LEU D 374      57.391  -7.325 -13.533  1.00 16.12      C
ANISOU 3032  CG  LEU D 374     1628   2295   2201   -265    224   -176  C
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Figure 18 (continued)

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ATOM   3033  CD1 LEU D 374      56.508  -6.147 -13.943  1.00 14.16           C
ANISOU 3033  CD1 LEU D 374    1315   2168   1897   -246    213   -194       C
ATOM   3034  CD2 LEU D 374      58.355  -7.620 -14.697  1.00 15.29           C
ANISOU 3034  CD2 LEU D 374    1528   2150   2131   -214    248   -197       C
ATOM   3035  C   LEU D 374      56.317  -8.127 -10.796  1.00 15.20           C
ANISOU 3035  C   LEU D 374    1607   2138   2030   -383    243   -101       C
ATOM   3036  O   LEU D 374      56.725  -9.266 -10.606  1.00 15.35           O
ANISOU 3036  O   LEU D 374    1699   2048   2084   -411    248    -74       O
ATOM   3037  N   ARG D 375      55.028  -7.827 -10.911  1.00 15.31           N
ANISOU 3037  N   ARG D 375    1554   2256   2009   -434    284   -144       N
ATOM   3038  CA  ARG D 375      54.040  -8.841 -11.218  1.00 16.30           C
ANISOU 3038  CA  ARG D 375    1656   2386   2152   -547    331   -184       C
ATOM   3039  CB  ARG D 375      52.876  -8.773 -10.272  1.00 17.01           C
ANISOU 3039  CB  ARG D 375    1708   2548   2207   -621    404   -172       C
ATOM   3040  CG  ARG D 375      53.151  -9.446  -8.924  1.00 16.88           C
ANISOU 3040  CG  ARG D 375    1823   2439   2152   -666    454    -83       C
ATOM   3041  CD  ARG D 375      52.036  -9.111  -7.966  1.00 17.47           C
ANISOU 3041  CD  ARG D 375    1859   2613   2166   -719    557    -71       C
ATOM   3042  NE  ARG D 375      52.301  -9.670  -6.649  1.00 20.64           N
ANISOU 3042  NE  ARG D 375    2417   2937   2488   -755    610      28       N
ATOM   3043  CZ  ARG D 375      51.689  -9.306  -5.525  1.00 21.86           C
ANISOU 3043  CZ  ARG D 375    2602   3163   2540   -771    710      60       C
ATOM   3044  NH1 ARG D 375      50.773  -8.327  -5.513  1.00 20.93           N
ANISOU 3044  NH1 ARG D 375    2351   3193   2408   -742    774     -10       N
ATOM   3045  NH2 ARG D 375      52.012  -9.927  -4.411  1.00 23.29           N
ANISOU 3045  NH2 ARG D 375    2960   3266   2625   -803    749     164       N
ATOM   3046  C   ARG D 375      53.565  -8.716 -12.664  1.00 17.05           C
ANISOU 3046  C   ARG D 375    1663   2555   2260   -548    300    -271       C
ATOM   3047  O   ARG D 375      53.246  -7.633 -13.155  1.00 16.83           O
ANISOU 3047  O   ARG D 375    1557   2634   2204   -481    270    -291       O
ATOM   3048  N   LYS D 376      53.476  -9.856 -13.325  1.00 18.24           N
ANISOU 3048  N   LYS D 376    1844   2640   2446   -624    301    -323       N
ATOM   3049  CA  LYS D 376      53.192  -9.905 -14.723  1.00 18.60           C
ANISOU 3049  CA  LYS D 376    1849   2743   2477   -625    256    -416       C
ATOM   3050  CB  LYS D 376      54.542 -10.061 -15.399  1.00 19.02           C
ANISOU 3050  CB  LYS D 376    1990   2707   2528   -534    251    -415       C
ATOM   3051  CG  LYS D 376      54.498 -10.388 -16.778  1.00 22.27           C
ANISOU 3051  CG  LYS D 376    2419   3141   2901   -532    226    -511       C
ATOM   3052  CD  LYS D 376      55.680 -11.228 -17.131  1.00 21.43           C
ANISOU 3052  CD  LYS D 376    2420   2893   2831   -488    267    -529       C
ATOM   3053  CE  LYS D 376      55.706 -11.320 -18.640  1.00 23.94           C
ANISOU 3053  CE  LYS D 376    2773   3260   3065   -460    255    -635       C
ATOM   3054  NZ  LYS D 376      54.576 -12.148 -19.074  1.00 23.78           N
ANISOU 3054  NZ  LYS D 376    2758   3250   3028   -589    205    -754       N
ATOM   3055  C   LYS D 376      52.271 -11.109 -14.980  1.00 20.06           C
ANISOU 3055  C   LYS D 376    2022   2897   2704   -780    261    -496       C
ATOM   3056  O   LYS D 376      52.290 -12.068 -14.216  1.00 21.47           O
ANISOU 3056  O   LYS D 376    2269   2952   2938   -868    315    -463       O
ATOM   3057  N   ALA D 377      51.449 -11.038 -16.025  1.00 20.56           N
ANISOU 3057  N   ALA D 377    2002   3067   2743   -817    196    -596       N
ATOM   3058  CA  ALA D 377      50.654 -12.164 -16.502  1.00 22.62           C
ANISOU 3058  CA  ALA D 377    2249   3295   3051   -974    171    -703       C
ATOM   3059  CB  ALA D 377      49.141 -12.016 -16.103  1.00 22.84           C
ANISOU 3059  CB  ALA D 377    2091   3455   3132  -1095    166    -725       C
ATOM   3060  C   ALA D 377      50.830 -12.200 -18.012  1.00 23.29           C
ANISOU 3060  C   ALA D 377    2371   3421   3056   -931     81    -817       C
ATOM   3061  O   ALA D 377      51.732 -11.531 -18.538  1.00 22.97           O
ANISOU 3061  O   ALA D 377    2392   3399   2935   -785     78   -786       O
ATOM   3062  N   THR D 378      49.995 -12.969 -18.713  1.00 24.81           N
ANISOU 3062  N   THR D 378    2534   3628   3263  -1062     10   -949       N
ATOM   3063  CA  THR D 378      50.084 -13.071 -20.188  1.00 25.87           C
ANISOU 3063  CA  THR D 378    2732   3812   3286  -1028    -90  -1078       C
ATOM   3064  CB  THR D 378      49.044 -14.046 -20.745  1.00 27.81           C
ANISOU 3064  CB  THR D 378    2938   4058   3571  -1214   -185  -1242       C
ATOM   3065  OG1 THR D 378      49.107 -15.264 -19.991  1.00 28.15           O
ANISOU 3065  OG1 THR D 378    3047   3892   3755  -1360    -97  -1250       O
ATOM   3066  CG2 THR D 378      49.290 -14.336 -22.254  1.00 28.26           C
ANISOU 3066  CG2 THR D 378    3122   4136   3481  -1179   -287  -1397       C
ATOM   3067  C   THR D 378      51.709 -13.709 -20.898  1.00 25.13           C
ANISOU 3067  C   THR D 378    2574   3913   3059   -881   -169  -1044       C
ATOM   3068  O   THR D 378      48.904 -11.120 -20.958  1.00 26.17           O
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Figure 18 (continued)

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ANISOU 3068  O   THR D 378     2548   4203   3193   -898   -259  -1050    O
ATOM   3069  N   ARG D 379      51.091 -11.219 -21.423  1.00 24.75        N
ANISOU 3069  N   ARG D 379     2648   3846   2911   -733   -128   -998    N
ATOM   3070  CA  ARG D 379      51.137  -9.937 -22.140  1.00 24.06        C
ANISOU 3070  CA  ARG D 379     2543   3907   2692   -591   -183   -941    C
ATOM   3071  CB  ARG D 379      50.530 -10.069 -23.546  1.00 25.58        C
ANISOU 3071  CB  ARG D 379     2771   4219   2730   -599   -324  -1065    C
ATOM   3072  CG  ARG D 379      51.184 -11.136 -24.401  1.00 26.56        C
ANISOU 3072  CG  ARG D 379     3077   4242   2772   -629   -295  -1197    C
ATOM   3073  CD  ARG D 379      50.803 -11.005 -25.880  1.00 28.25        C
ANISOU 3073  CD  ARG D 379     3373   4594   2766   -594   -431  -1303    C
ATOM   3074  NE  ARG D 379      51.357  -9.774 -26.432  1.00 26.17        N
ANISOU 3074  NE  ARG D 379     3166   4426   2352   -423   -403  -1173    N
ATOM   3075  CZ  ARG D 379      51.005  -9.218 -27.587  1.00 26.90        C
ANISOU 3075  CZ  ARG D 379     3324   4670   2228   -349   -523  -1189    C
ATOM   3076  NH1 ARG D 379      50.097  -9.774 -28.377  1.00 26.03        N
ANISOU 3076  NH1 ARG D 379     3225   4654   2011   -425   -705  -1348    N
ATOM   3077  NH2 ARG D 379      51.574  -8.084 -27.945  1.00 25.85        N
ANISOU 3077  NH2 ARG D 379     3250   4588   1983   -203   -467  -1038    N
ATOM   3078  C   ARG D 379      50.451  -8.817 -21.339  1.00 23.81        C
ANISOU 3078  C   ARG D 379     2351   3979   2718   -548   -204   -834    C
ATOM   3079  O   ARG D 379      49.654  -8.062 -21.877  1.00 24.12        O
ANISOU 3079  O   ARG D 379     2303   4167   2693   -496   -315   -835    O
ATOM   3080  N   ARG D 380      50.796  -8.719 -20.055  1.00 23.74        N
ANISOU 3080  N   ARG D 380     2316   3884   2821   -555   -101   -746    N
ATOM   3081  CA  ARG D 380      50.201  -7.776 -19.126  1.00 24.65        C
ANISOU 3081  CA  ARG D 380     2301   4071   2994   -517    -90   -664    C
ATOM   3082  CB  ARG D 380      48.866  -8.319 -18.591  1.00 25.94        C
ANISOU 3082  CB  ARG D 380     2307   4296   3251   -653   -110   -725    C
ATOM   3083  CG  ARG D 380      48.090  -7.378 -17.662  1.00 27.73        C
ANISOU 3083  CG  ARG D 380     2381   4618   3538   -606    -79   -663    C
ATOM   3084  CD  ARG D 380      46.845  -8.116 -17.110  1.00 32.70        C
ANISOU 3084  CD  ARG D 380     2844   5302   4279   -768    -57   -724    C
ATOM   3085  NE  ARG D 380      46.470  -7.643 -15.763  1.00 41.53        N
ANISOU 3085  NE  ARG D 380     3880   6440   5461   -757     67   -655    N
ATOM   3086  CZ  ARG D 380      45.818  -8.377 -14.862  1.00 44.62        C
ANISOU 3086  CZ  ARG D 380     4194   6818   5941   -906    173   -660    C
ATOM   3087  NH1 ARG D 380      45.450  -9.626 -15.147  1.00 47.78        N
ANISOU 3087  NH1 ARG D 380     4579   7169   6405  -1093    162   -728    N
ATOM   3088  NH2 ARG D 380      45.534  -7.858 -13.668  1.00 46.02        N
ANISOU 3088  NH2 ARG D 380     4324   7025   6138   -874    301   -598    N
ATOM   3089  C   ARG D 380      51.163  -7.516 -17.970  1.00 22.17        C
ANISOU 3089  C   ARG D 380     2048   3640   2735   -477     23   -562    C
ATOM   3090  O   ARG D 380      51.649  -8.448 -17.344  1.00 22.38        O
ANISOU 3090  O   ARG D 380     2142   3543   2819   -550     89   -560    O
ATOM   3091  N   LEU D 381      51.447  -6.242 -17.712  1.00 20.15        N
ANISOU 3091  N   LEU D 381     1778   3415   2461   -357     30   -478    N
ATOM   3092  CA  LEU D 381      52.122  -5.824 -16.482  1.00 18.33        C
ANISOU 3092  CA  LEU D 381     1581   3101   2282   -326    104   -398    C
ATOM   3093  CB  LEU D 381      52.866  -4.501 -16.698  1.00 16.65        C
ANISOU 3093  CB  LEU D 381     1404   2880   2041   -197     98   -324    C
ATOM   3094  CG  LEU D 381      53.665  -3.909 -15.562  1.00 16.21        C
ANISOU 3094  CG  LEU D 381     1388   2738   2032   -163    142   -259    C
ATOM   3095  CD1 LEU D 381      54.864  -3.126 -16.123  1.00 15.32        C
ANISOU 3095  CD1 LEU D 381     1337   2566   1918    -87    146   -198    C
ATOM   3096  CD2 LEU D 381      52.771  -3.029 -14.664  1.00 13.19        C
ANISOU 3096  CD2 LEU D 381     938   2411   1663   -126    146   -254    C
ATOM   3097  C   LEU D 381      51.003  -5.675 -15.465  1.00 18.54        C
ANISOU 3097  C   LEU D 381     1498   3193   2353   -368    130   -404    C
ATOM   3098  O   LEU D 381      50.041  -4.942 -15.713  1.00 18.05        O
ANISOU 3098  O   LEU D 381     1322   3249   2289   -319     87   -421    O
ATOM   3099  N   VAL D 382      51.092  -6.417 -14.358  1.00 18.79        N
ANISOU 3099  N   VAL D 382     1564   3152   2425   -454    205   -387    N
ATOM   3100  CA  VAL D 382      50.030  -6.373 -13.333  1.00 19.66        C
ANISOU 3100  CA  VAL D 382     1578   3326   2564   -508    270   -388    C
ATOM   3101  CB  VAL D 382      49.864  -7.734 -12.561  1.00 20.30        C
ANISOU 3101  CB  VAL D 382     1704   3327   2682   -664    351   -380    C
ATOM   3102  CG1 VAL D 382      48.932  -7.592 -11.345  1.00 21.28        C
ANISOU 3102  CG1 VAL D 382     1755   3516   2814   -713    462   -358    C
ATOM   3103  CG2 VAL D 382      49.384  -8.852 -13.492  1.00 18.12        C
ANISOU 3103  CG2 VAL D 382     1390   3040   2452   -790    311   -458    C
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Figure 18 (continued)

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ATOM   3104  C   VAL D 382      50.355  -5.218 -12.398  1.00 20.00           C
ANISOU 3104  C   VAL D 382    1654   3367   2580   -399    305   -336       C
ATOM   3105  O   VAL D 382      49.503  -4.363 -12.132  1.00 20.34           O
ANISOU 3105  O   VAL D 382    1594   3506   2628   -338    324   -353       O
ATOM   3106  N   GLN D 383      51.602  -5.188 -11.930  1.00 20.10           N
ANISOU 3106  N   GLN D 383    1804   3265   2570   -368    305   -282       N
ATOM   3107  CA  GLN D 383      52.076  -4.128 -11.044  1.00 20.46           C
ANISOU 3107  CA  GLN D 383    1903   3285   2586   -280    314   -249       C
ATOM   3108  CB  GLN D 383      51.440  -4.281  -9.645  1.00 22.14           C
ANISOU 3108  CB  GLN D 383    2130   3523   2758   -323    407   -245       C
ATOM   3109  CG  GLN D 383      51.782  -3.166  -8.701  1.00 27.86           C
ANISOU 3109  CG  GLN D 383    2924   4230   3430   -231    413   -242       C
ATOM   3110  CD  GLN D 383      50.784  -2.962  -7.567  1.00 35.94           C
ANISOU 3110  CD  GLN D 383    3931   5330   4396   -236    530   -267       C
ATOM   3111  OE1 GLN D 383      50.146  -3.921  -7.057  1.00 37.23           O
ANISOU 3111  OE1 GLN D 383    4080   5526   4539   -341    628   -250       O
ATOM   3112  NE2 GLN D 383      50.628  -1.688  -7.167  1.00 36.75           N
ANISOU 3112  NE2 GLN D 383    4039   5450   4475   -122    537   -310       N
ATOM   3113  C   GLN D 383      53.600  -4.104 -10.977  1.00 18.47           C
ANISOU 3113  C   GLN D 383    1765   2914   2337   -249    266   -202       C
ATOM   3114  O   GLN D 383      54.256  -5.122 -11.078  1.00 18.25           O
ANISOU 3114  O   GLN D 383    1793   2812   2329   -299    259   -182       O
ATOM   3115  N   LEU D 384      54.153  -2.908 -10.828  1.00 18.23           N
ANISOU 3115  N   LEU D 384    1759   2860   2309   -163    230   -190       N
ATOM   3116  CA  LEU D 384      55.575  -2.690 -10.666  1.00 16.87           C
ANISOU 3116  CA  LEU D 384    1658   2587   2165   -139    179   -151       C
ATOM   3117  CB  LEU D 384      56.164  -2.192 -11.983  1.00 16.08           C
ANISOU 3117  CB  LEU D 384    1525   2473   2113    -96    154   -135       C
ATOM   3118  CG  LEU D 384      57.662  -1.872 -12.075  1.00 16.83           C
ANISOU 3118  CG  LEU D 384    1646   2475   2275    -79    119    -94       C
ATOM   3119  CD1 LEU D 384      58.510  -3.146 -12.068  1.00 11.98           C
ANISOU 3119  CD1 LEU D 384    1046   1808   1697   -114    119    -78       C
ATOM   3120  CD2 LEU D 384      57.896  -1.065 -13.332  1.00 12.84           C
ANISOU 3120  CD2 LEU D 384    1111   1973   1792    -36    133    -69       C
ATOM   3121  C   LEU D 384      55.832  -1.650  -9.567  1.00 17.39           C
ANISOU 3121  C   LEU D 384    1779   2622   2207    -96    154   -158       C
ATOM   3122  O   LEU D 384      55.240  -0.552  -9.591  1.00 18.03           O
ANISOU 3122  O   LEU D 384    1836   2732   2282    -36    164   -189       O
ATOM   3123  N   ILE D 385      56.704  -1.988  -8.617  1.00 16.14           N
ANISOU 3123  N   ILE D 385    1702   2399   2032   -119    109   -136       N
ATOM   3124  CA  ILE D 385      57.217  -1.037  -7.649  1.00 16.77           C
ANISOU 3124  CA  ILE D 385    1850   2434   2086    -88     49   -157       C
ATOM   3125  CB  ILE D 385      56.942  -1.448  -6.168  1.00 17.93           C
ANISOU 3125  CB  ILE D 385    2109   2597   2105   -110     57   -164       C
ATOM   3126  CG1 ILE D 385      55.479  -1.806  -6.000  1.00 19.43           C
ANISOU 3126  CG1 ILE D 385    2275   2882   2226   -129    188   -183       C
ATOM   3127  CD1 ILE D 385      55.134  -2.472  -4.673  1.00 20.09           C
ANISOU 3127  CD1 ILE D 385    2475   2988   2170   -170    242   -163       C
ATOM   3128  CG2 ILE D 385      57.252  -0.256  -5.217  1.00 17.45           C
ANISOU 3128  CG2 ILE D 385    2135   2503   1991    -68     -6   -224       C
ATOM   3129  C   ILE D 385      58.712  -0.916  -7.838  1.00 16.33           C
ANISOU 3129  C   ILE D 385    1790   2292   2123    -90    -48   -125       C
ATOM   3130  O   ILE D 385      59.401  -1.917  -7.778  1.00 15.60           O
ANISOU 3130  O   ILE D 385    1701   2171   2056   -114    -80    -82       O
ATOM   3131  N   VAL D 386      59.193   0.302  -8.082  1.00 16.79           N
ANISOU 3131  N   VAL D 386    1830   2302   2249    -66    -89   -145       N
ATOM   3132  CA  VAL D 386      60.628   0.573  -8.316  1.00 16.53           C
ANISOU 3132  CA  VAL D 386    1754   2189   2338    -85   -170   -117       C
ATOM   3133  CB  VAL D 386      60.864   1.322  -9.646  1.00 16.12           C
ANISOU 3133  CB  VAL D 386    1628   2110   2389    -76   -119    -88       C
ATOM   3134  CG1 VAL D 386      62.343   1.365  -9.984  1.00 15.54           C
ANISOU 3134  CG1 VAL D 386    1475   1971   2459   -111   -161    -48       C
ATOM   3135  CG2 VAL D 386      60.077   0.665 -10.776  1.00 15.17           C
ANISOU 3135  CG2 VAL D 386    1471   2064   2228    -55    -21    -62       C
ATOM   3136  C   VAL D 386      61.267   1.429  -7.207  1.00 18.00           C
ANISOU 3136  C   VAL D 386    2001   2310   2527    -99   -288   -165       C
ATOM   3137  O   VAL D 386      60.688   2.436  -6.757  1.00 17.63           O
ANISOU 3137  O   VAL D 386    2022   2246   2432    -78   -286   -229       O
ATOM   3138  N   SER D 387      62.475   1.024  -6.818  1.00 17.98           N
ANISOU 3138  N   SER D 387    1968   2271   2593   -128   -398   -143       N
ATOM   3139  CA  SER D 387      63.295   1.740  -5.874  1.00 19.91           C
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Figure 18 (continued)

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ANISOU 3139  CA  SER D 387     2246   2456   2863   -157   -549   -194      C
ATOM   3140  CB  SER D 387      63.525   0.862  -4.642  1.00 20.75           C
ANISOU 3140  CB  SER D 387     2441   2593   2848   -148   -662   -190      C
ATOM   3141  OG  SER D 387      64.138   1.637  -3.629  1.00 26.41           O
ANISOU 3141  OG  SER D 387     3222   3268   3545   -174   -828   -263      O
ATOM   3142  C   SER D 387      64.614   2.081  -6.601  1.00 19.75           C
ANISOU 3142  C   SER D 387     2073   2372   3058   -200   -595   -160      C
ATOM   3143  O   SER D 387      65.205   1.226  -7.243  1.00 19.61           O
ANISOU 3143  O   SER D 387     1949   2374   3129   -192   -563    -95      O
ATOM   3144  N   GLY D 388      65.045   3.336  -6.558  1.00 20.44           N
ANISOU 3144  N   GLY D 388     2147   2377   3242   -249   -648   -207      N
ATOM   3145  CA  GLY D 388      66.169   3.760  -7.373  1.00 20.71           C
ANISOU 3145  CA  GLY D 388     2024   2350   3495   -310   -644   -164      C
ATOM   3146  C   GLY D 388      66.910   4.945  -6.819  1.00 22.28           C
ANISOU 3146  C   GLY D 388     2212   2442   3810   -396   -776   -233      C
ATOM   3147  O   GLY D 388      66.412   5.643  -5.960  1.00 22.74           O
ANISOU 3147  O   GLY D 388     2413   2458   3769   -398   -850   -326      O
ATOM   3148  N   LYS D 389      68.118   5.162  -7.318  1.00 23.01           N
ANISOU 3148  N   LYS D 389     2130   2489   4124   -474   -798   -195      N
ATOM   3149  CA  LYS D 389      68.973   6.226  -6.823  1.00 25.51           C
ANISOU 3149  CA  LYS D 389     2401   2696   4597   -588   -939   -262      C
ATOM   3150  CB  LYS D 389      70.436   5.931  -7.166  1.00 27.03           C
ANISOU 3150  CB  LYS D 389     2339   2893   5036   -662   -988   -213      C
ATOM   3151  CG  LYS D 389      71.016   4.768  -6.405  1.00 29.16           C
ANISOU 3151  CG  LYS D 389     2536   3261   5282   -606  -1149   -218      C
ATOM   3152  CD  LYS D 389      72.475   4.525  -6.778  1.00 33.37           C
ANISOU 3152  CD  LYS D 389     2779   3803   6095   -662  -1193   -174      C
ATOM   3153  CE  LYS D 389      73.170   3.650  -5.740  1.00 38.88           C
ANISOU 3153  CE  LYS D 389     3409   4571   6792   -609  -1439   -199      C
ATOM   3154  NZ  LYS D 389      74.315   2.871  -6.313  1.00 42.89           N
ANISOU 3154  NZ  LYS D 389     3629   5130   7536   -578  -1414   -125      N
ATOM   3155  C   LYS D 389      68.574   7.622  -7.336  1.00 25.27           C
ANISOU 3155  C   LYS D 389     2446   2528   4627   -643   -846   -275      C
ATOM   3156  O   LYS D 389      68.815   8.616  -6.671  1.00 27.52           O
ANISOU 3156  O   LYS D 389     2792   2696   4970   -722   -969   -371      O
ATOM   3157  N   ASP D 390      67.957   7.673  -8.502  1.00 23.52           N
ANISOU 3157  N   ASP D 390     2238   2314   4385   -594   -643   -180      N
ATOM   3158  CA  ASP D 390      67.627   8.899  -9.203  1.00 24.41           C
ANISOU 3158  CA  ASP D 390     2418   2292   4565   -626   -538   -147      C
ATOM   3159  CB  ASP D 390      68.851   9.494  -9.933  1.00 25.90           C
ANISOU 3159  CB  ASP D 390     2446   2380   5014   -767   -487    -72      C
ATOM   3160  CG  ASP D 390      69.523   8.504 -10.892  1.00 26.86           C
ANISOU 3160  CG  ASP D 390     2382   2621   5204   -760   -358     41      C
ATOM   3161  OD1 ASP D 390      69.057   8.339 -12.046  1.00 26.07           O
ANISOU 3161  OD1 ASP D 390     2311   2561   5035   -701   -169    145      O
ATOM   3162  OD2 ASP D 390      70.541   7.906 -10.494  1.00 27.91           O
ANISOU 3162  OD2 ASP D 390     2341   2805   5458   -807   -451     19      O
ATOM   3163  C   ASP D 390      66.538   8.541 -10.190  1.00 23.04           C
ANISOU 3163  C   ASP D 390     2310   2197   4248   -508   -363    -61      C
ATOM   3164  O   ASP D 390      66.326   7.369 -10.478  1.00 20.52           O
ANISOU 3164  O   ASP D 390     1944   2019   3834   -443   -313    -25      O
ATOM   3165  N   GLU D 391      65.854   9.559 -10.695  1.00 24.31           N
ANISOU 3165  N   GLU D 391     2582   2254   4399   -480   -285    -32      N
ATOM   3166  CA  GLU D 391      64.698   9.375 -11.545  1.00 25.09           C
ANISOU 3166  CA  GLU D 391     2753   2426   4353   -357   -161     37      C
ATOM   3167  CB  GLU D 391      63.893  10.685 -11.645  1.00 25.59           C
ANISOU 3167  CB  GLU D 391     2964   2345   4414   -303   -142     33      C
ATOM   3168  CG  GLU D 391      63.654  11.247 -13.044  1.00 29.26           C
ANISOU 3168  CG  GLU D 391     3463   2757   4898   -269     -8    185      C
ATOM   3169  CD  GLU D 391      63.469  12.790 -13.016  1.00 31.73           C
ANISOU 3169  CD  GLU D 391     3910   2836   5312   -270    -16    194      C
ATOM   3170  OE1 GLU D 391      63.085  13.318 -11.941  1.00 37.16           O
ANISOU 3170  OE1 GLU D 391     4684   3437   5996   -243   -114     56      O
ATOM   3171  OE2 GLU D 391      63.683  13.469 -14.057  1.00 34.98           O
ANISOU 3171  OE2 GLU D 391     4359   3140   5793   -292     83    339      O
ATOM   3172  C   GLU D 391      65.058   8.781 -12.903  1.00 24.24           C
ANISOU 3172  C   GLU D 391     2553   2399   4260   -360    -18    171      C
ATOM   3173  O   GLU D 391      64.273   8.010 -13.468  1.00 22.69           O
ANISOU 3173  O   GLU D 391     2374   2332   3915   -266     47    200      O
ATOM   3174  N   GLN D 392      66.247   9.114 -13.408  1.00 24.93           N
ANISOU 3174  N   GLN D 392     2538   2412   4524   -473     36    242      N
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Figure 18 (continued)

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ATOM   3175  CA  GLN D 392      66.743   8.484 -14.629  1.00 25.44           C
ANISOU 3175  CA  GLN D 392    2508   2561   4595   -478    192    356       C
ATOM   3176  CB  GLN D 392      68.044   9.130 -15.089  1.00 27.83           C
ANISOU 3176  CB  GLN D 392    2695   2758   5122   -620    273    435       C
ATOM   3177  CG  GLN D 392      68.528   8.613 -16.433  1.00 30.48           C
ANISOU 3177  CG  GLN D 392    2956   3178   5449   -617    479    558       C
ATOM   3178  CD  GLN D 392      69.873   9.190 -16.862  1.00 32.38           C
ANISOU 3178  CD  GLN D 392    3046   3328   5929   -770    593    641       C
ATOM   3179  OE1 GLN D 392      70.866   9.160 -16.120  1.00 34.05           O
ANISOU 3179  OE1 GLN D 392    3083   3509   6346   -874    503    579       O
ATOM   3180  NE2 GLN D 392      69.915   9.682 -18.098  1.00 36.39           N
ANISOU 3180  NE2 GLN D 392    3617   3803   6407   -787    796    790       N
ATOM   3181  C   GLN D 392      66.861   6.952 -14.515  1.00 23.36           C
ANISOU 3181  C   GLN D 392    2153   2465   4257   -425    183    315       C
ATOM   3182  O   GLN D 392      66.428   6.241 -15.420  1.00 22.71           O
ANISOU 3182  O   GLN D 392    2091   2487   4051   -353    291    361       O
ATOM   3183  N   SER D 393      67.396   6.449 -13.399  1.00 22.65           N
ANISOU 3183  N   SER D 393    1984   2391   4230   -455     43    226       N
ATOM   3184  CA  SER D 393      67.491   5.002 -13.124  1.00 21.47           C
ANISOU 3184  CA  SER D 393    1772   2367   4020   -396     13    192       C
ATOM   3185  CB  SER D 393      68.327   4.756 -11.883  1.00 21.62           C
ANISOU 3185  CB  SER D 393    1702   2368   4143   -443   -165    121       C
ATOM   3186  OG  SER D 393      69.540   5.423 -12.049  1.00 27.86           O
ANISOU 3186  OG  SER D 393    2342   3083   5162   -552   -165    148       O
ATOM   3187  C   SER D 393      66.148   4.332 -12.909  1.00 19.41           C
ANISOU 3187  C   SER D 393    1642   2192   3542   -296     -2    151       C
ATOM   3188  O   SER D 393      65.985   3.151 -13.253  1.00 18.62           O
ANISOU 3188  O   SER D 393    1522   2183   3368   -242     46    156       O
ATOM   3189  N   ILE D 394      65.218   5.075 -12.314  1.00 18.26           N
ANISOU 3189  N   ILE D 394    1621   2007   3310   -275    -63    103       N
ATOM   3190  CA  ILE D 394      63.857   4.613 -12.104  1.00 17.01           C
ANISOU 3190  CA  ILE D 394    1563   1931   2968   -189    -60     64       C
ATOM   3191  CB  ILE D 394      63.049   5.528 -11.111  1.00 17.01           C
ANISOU 3191  CB  ILE D 394    1678   1876   2909   -165   -137    -15       C
ATOM   3192  CG1 ILE D 394      63.665   5.443  -9.702  1.00 17.08           C
ANISOU 3192  CG1 ILE D 394    1698   1854   2938   -213   -281    -98       C
ATOM   3193  CD1 ILE D 394      63.245   6.554  -8.715  1.00 19.53           C
ANISOU 3193  CD1 ILE D 394    2130   2075   3217   -209   -359   -197       C
ATOM   3194  CG2 ILE D 394      61.591   5.140 -11.069  1.00 15.94           C
ANISOU 3194  CG2 ILE D 394    1608   1838   2612    -76    -97    -43       C
ATOM   3195  C   ILE D 394      63.185   4.408 -13.442  1.00 16.42           C
ANISOU 3195  C   ILE D 394    1505   1922   2813   -134     66    130       C
ATOM   3196  O   ILE D 394      62.597   3.330 -13.682  1.00 17.30           O
ANISOU 3196  O   ILE D 394    1618   2138   2819    -93     94    116       O
ATOM   3197  N   ALA D 395      63.298   5.400 -14.315  1.00 16.91           N
ANISOU 3197  N   ALA D 395    1588   1917   2920   -141    135    204       N
ATOM   3198  CA  ALA D 395      62.780   5.347 -15.687  1.00 17.37           C
ANISOU 3198  CA  ALA D 395    1681   2033   2883    -86    242    282       C
ATOM   3199  CB  ALA D 395      63.094   6.656 -16.431  1.00 18.96           C
ANISOU 3199  CB  ALA D 395    1932   2120   3153   -106    307    386       C
ATOM   3200  C   ALA D 395      63.322   4.179 -16.485  1.00 17.20           C
ANISOU 3200  C   ALA D 395    1596   2104   2837    -93    329    304       C
ATOM   3201  O   ALA D 395      62.559   3.518 -17.161  1.00 17.12           O
ANISOU 3201  O   ALA D 395    1624   2193   2688    -37    361    297       O
ATOM   3202  N   GLU D 396      64.642   3.945 -16.431  1.00 18.24           N
ANISOU 3202  N   GLU D 396    1621   2199   3109   -159    365    321       N
ATOM   3203  CA  GLU D 396      65.268   2.754 -17.052  1.00 19.05           C
ANISOU 3203  CA  GLU D 396    1650   2376   3211   -147    455    320       C
ATOM   3204  CB  GLU D 396      66.786   2.709 -16.793  1.00 19.83           C
ANISOU 3204  CB  GLU D 396    1592   2423   3518   -212    479    336       C
ATOM   3205  CG  GLU D 396      67.552   3.855 -17.468  1.00 25.11           C
ANISOU 3205  CG  GLU D 396    2219   3017   4306   -286    591    433       C
ATOM   3206  CD  GLU D 396      69.015   4.000 -17.021  1.00 27.94           C
ANISOU 3206  CD  GLU D 396    2381   3319   4915   -376    586    439       C
ATOM   3207  OE1 GLU D 396      69.468   3.298 -16.076  1.00 34.31           O
ANISOU 3207  OE1 GLU D 396    3089   4143   5805   -369    459    366       O
ATOM   3208  OE2 GLU D 396      69.726   4.828 -17.643  1.00 32.70           O
ANISOU 3208  OE2 GLU D 396    2925   3862   5638   -458    709    525       O
ATOM   3209  C   GLU D 396      64.601   1.433 -16.628  1.00 16.89           C
ANISOU 3209  C   GLU D 396    1399   2181   2836    -97     -97    236       C
ATOM   3210  O   GLU D 396      64.337   0.594 -17.467  1.00 17.29           O
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Figure 18 (continued)

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ANISOU 3210  O   GLU D 396     1477   2301   2790    -57    470    225       O
ATOM   3211  N   ALA D 397      64.318   1.260 -15.340  1.00 16.42           N
ANISOU 3211  N   ALA D 397     1346   2104   2788   -105    265    178       N
ATOM   3212  CA  ALA D 397      63.635   0.071 -14.829  1.00 15.26           C
ANISOU 3212  CA  ALA D 397     1236   2012   2549    -75    218    117       C
ATOM   3213  CB  ALA D 397      63.668   0.033 -13.291  1.00 15.13           C
ANISOU 3213  CB  ALA D 397     1230   1961   2557    -95     85     78       C
ATOM   3214  C   ALA D 397      62.215  -0.057 -15.320  1.00 15.97           C
ANISOU 3214  C   ALA D 397     1408   2176   2484    -43    238     95       C
ATOM   3215  O   ALA D 397      61.786  -1.172 -15.654  1.00 16.45           O
ANISOU 3215  O   ALA D 397     1487   2289   2476    -32    262     58       O
ATOM   3216  N   ILE D 398      61.462   1.059 -15.321  1.00 16.01           N
ANISOU 3216  N   ILE D 398     1457   2178   2446    -26    217    108       N
ATOM   3217  CA  ILE D 398      60.095   1.065 -15.859  1.00 16.25           C
ANISOU 3217  CA  ILE D 398     1533   2291   2348     19    219     92       C
ATOM   3218  CB  ILE D 398      59.352   2.440 -15.637  1.00 16.90           C
ANISOU 3218  CB  ILE D 398     1654   2346   2422     64    182    109       C
ATOM   3219  CG1 ILE D 398      59.198   2.757 -14.154  1.00 16.25           C
ANISOU 3219  CG1 ILE D 398     1581   2218   2376     53    117     51       C
ATOM   3220  CD1 ILE D 398      58.939   4.211 -13.831  1.00 17.39           C
ANISOU 3220  CD1 ILE D 398     1771   2278   2557     94     91     55       C
ATOM   3221  CG2 ILE D 398      57.975   2.398 -16.248  1.00 15.79           C
ANISOU 3221  CG2 ILE D 398     1524   2306   2169    127    170     95       C
ATOM   3222  C   ILE D 398      60.089   0.658 -17.357  1.00 16.35           C
ANISOU 3222  C   ILE D 398     1563   2365   2282     40    294    120       C
ATOM   3223  O   ILE D 398      59.343  -0.227 -17.770  1.00 16.18           O
ANISOU 3223  O   ILE D 398     1555   2424   2169     47    288     69       O
ATOM   3224  N   ILE D 399      60.961   1.269 -18.152  1.00 16.83           N
ANISOU 3224  N   ILE D 399     1632   2386   2379     41    371    196       N
ATOM   3225  CA  ILE D 399      61.094   0.870 -19.567  1.00 16.97           C
ANISOU 3225  CA  ILE D 399     1691   2465   2293     64    463    222       C
ATOM   3226  CB  ILE D 399      62.227   1.668 -20.302  1.00 18.12           C
ANISOU 3226  CB  ILE D 399     1838   2552   2495     49    584    328       C
ATOM   3227  CG1 ILE D 399      61.855   3.147 -20.442  1.00 16.73           C
ANISOU 3227  CG1 ILE D 399     1724   2317   2315     67    562    423       C
ATOM   3228  CD1 ILE D 399      63.062   4.110 -20.649  1.00 18.57           C
ANISOU 3228  CD1 ILE D 399     1936   2437   2683      8    667    531       C
ATOM   3229  CG2 ILE D 399      62.537   1.045 -21.698  1.00 17.41           C
ANISOU 3229  CG2 ILE D 399     1800   2535   2278     75    713    340       C
ATOM   3230  C   ILE D 399      61.312  -0.653 -19.738  1.00 16.98           C
ANISOU 3230  C   ILE D 399     1675   2507   2269     53    495    138       C
ATOM   3231  O   ILE D 399      60.592  -1.306 -20.497  1.00 17.78           O
ANISOU 3231  O   ILE D 399     1832   2687   2237     73    491     87       O
ATOM   3232  N   VAL D 400      62.307  -1.207 -19.045  1.00 16.61           N
ANISOU 3232  N   VAL D 400     1556   2398   2359     26    512    120       N
ATOM   3233  CA  VAL D 400      62.608  -2.659 -19.102  1.00 15.36           C
ANISOU 3233  CA  VAL D 400     1388   2241   2209     32    541     46       C
ATOM   3234  CB  VAL D 400      63.878  -2.999 -18.262  1.00 16.29           C
ANISOU 3234  CB  VAL D 400     1403   2277   2508     26    542     57       C
ATOM   3235  CG1 VAL D 400      64.115  -4.500 -18.195  1.00 13.50           C
ANISOU 3235  CG1 VAL D 400     1055   1897   2178     53    557    -12       C
ATOM   3236  CG2 VAL D 400      65.116  -2.244 -18.837  1.00 13.64           C
ANISOU 3236  CG2 VAL D 400     986   1920   2278     24    654    130       C
ATOM   3237  C   VAL D 400      61.412  -3.538 -18.702  1.00 15.40           C
ANISOU 3237  C   VAL D 400     1440   2279   2133     16    456    -35       C
ATOM   3238  O   VAL D 400      61.069  -4.500 -19.408  1.00 16.47           O
ANISOU 3238  O   VAL D 400     1626   2443   2188     19    485   -105       O
ATOM   3239  N   ALA D 401      60.759  -3.208 -17.597  1.00 14.49           N
ANISOU 3239  N   ALA D 401     1311   2156   2037    -10    363    -33       N
ATOM   3240  CA  ALA D 401      59.557  -3.930 -17.183  1.00 14.67           C
ANISOU 3240  CA  ALA D 401     1359   2218   1996    -43    305    -97       C
ATOM   3241  CB  ALA D 401      59.103  -3.452 -15.809  1.00 13.69           C
ANISOU 3241  CB  ALA D 401     1219   2081   1904    -63    238    -82       C
ATOM   3242  C   ALA D 401      58.398  -3.848 -18.208  1.00 15.39           C
ANISOU 3242  C   ALA D 401     1478   2411   1958    -37    291   -135       C
ATOM   3243  O   ALA D 401      57.713  -4.818 -18.452  1.00 16.06           O
ANISOU 3243  O   ALA D 401     1579   2526   1997    -76    274   -209       O
ATOM   3244  N   MSE D 402      58.174  -2.688 -18.801  1.00 16.28           N
ANISOU 3244  N   MSE D 402     1597   2569   2018    -10    301    -82       N
ATOM   3245  CA  MSE D 402      57.144  -2.553 -19.841  1.00 18.26           C
ANISOU 3245  CA  MSE D 402     1875   2926   2137     36    243   -106       C
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Figure 18 (continued)

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ATOM   3246  CB  MSE D 402      56.928  -1.071 -20.204  1.00 18.49           C
ANISOU 3246  CB  MSE D 402    1919   2974   2132    108    222    -14        C
ATOM   3247  CG  MSE D 402      56.199  -0.248 -19.135  1.00 17.60           C
ANISOU 3247  CG  MSE D 402    1749   2850   2087    130    160     -1        C
ATOM   3248  SE  MSE D 402      56.146   1.624 -19.687  0.90 22.98          SE
ANISOU 3248  SE  MSE D 402    2485   3496   2753    237    146    125       SE
ATOM   3249  CE  MSE D 402      55.076   2.410 -18.255  1.00 21.33           C
ANISOU 3249  CE  MSE D 402    2203   3271   2632    282     78     86        C
ATOM   3250  C   MSE D 402      57.429  -3.401 -21.105  1.00 17.59           C
ANISOU 3250  C   MSE D 402    1861   2875   1947     35    288   -158        C
ATOM   3251  O   MSE D 402      56.527  -4.090 -21.622  1.00 17.86           O
ANISOU 3251  O   MSE D 402    1912   2982   1891      9    226   -245        O
ATOM   3252  N   VAL D 403      58.675  -3.365 -21.578  1.00 17.04           N
ANISOU 3252  N   VAL D 403    1828   2753   1894     59    399   -117        N
ATOM   3253  CA  VAL D 403      59.106  -4.194 -22.698  1.00 17.23           C
ANISOU 3253  CA  VAL D 403    1930   2797   1818     71    477   -179        C
ATOM   3254  CB  VAL D 403      60.556  -3.848 -23.174  1.00 18.02           C
ANISOU 3254  CB  VAL D 403    2039   2850   1958    109    637   -106        C
ATOM   3255  CG1 VAL D 403      61.044  -4.814 -24.226  1.00 17.77           C
ANISOU 3255  CG1 VAL D 403    2091   2834   1828    135    747   -191        C
ATOM   3256  CG2 VAL D 403      60.625  -2.412 -23.711  1.00 17.84           C
ANISOU 3256  CG2 VAL D 403    2047   2857   1873    143    665     26        C
ATOM   3257  C   VAL D 403      58.943  -5.683 -22.346  1.00 17.40           C
ANISOU 3257  C   VAL D 403    1955   2774   1884     20    460   -304        C
ATOM   3258  O   VAL D 403      58.320  -6.447 -23.087  1.00 17.38           O
ANISOU 3258  O   VAL D 403    2019   2816   1768     -1    427   -409        O
ATOM   3259  N   PHE D 404      59.463  -6.068 -21.187  1.00 16.85           N
ANISOU 3259  N   PHE D 404    1821   2605   1975     -4    468   -290        N
ATOM   3260  CA  PHE D 404      59.430  -7.453 -20.709  1.00 16.94           C
ANISOU 3260  CA  PHE D 404    1850   2535   2053    -47    459   -377        C
ATOM   3261  CB  PHE D 404      60.112  -7.514 -19.346  1.00 15.89           C
ANISOU 3261  CB  PHE D 404    1652   2303   2081    -48    451   -311        C
ATOM   3262  CG  PHE D 404      60.205  -8.886 -18.770  1.00 14.98           C
ANISOU 3262  CG  PHE D 404    1571   2077   2043    -77    445   -364        C
ATOM   3263  CD1 PHE D 404      61.249  -9.757 -19.143  1.00 15.77           C
ANISOU 3263  CD1 PHE D 404    1698   2082   2212    -16    525   -400        C
ATOM   3264  CE1 PHE D 404      61.321 -11.039 -18.585  1.00 17.63           C
ANISOU 3264  CE1 PHE D 404    1984   2185   2531    -30    513   -438        C
ATOM   3265  CZ  PHE D 404      60.388 -11.449 -17.653  1.00 16.05           C
ANISOU 3265  CZ  PHE D 404    1812   1951   2336   -121    435   -426        C
ATOM   3266  CE2 PHE D 404      59.342 -10.569 -17.262  1.00 17.50           C
ANISOU 3266  CE2 PHE D 404    1951   2250   2448   -190    374   -393        C
ATOM   3267  CD2 PHE D 404      59.283  -9.297 -17.818  1.00 13.88           C
ANISOU 3267  CD2 PHE D 404    1438   1917   1919   -156    374   -367        C
ATOM   3268  C   PHE D 404      58.010  -8.031 -20.605  1.00 17.76           C
ANISOU 3268  C   PHE D 404    1967   2679   2102   -130    361   -459        C
ATOM   3269  O   PHE D 404      57.797  -9.247 -20.769  1.00 17.49           O
ANISOU 3269  O   PHE D 404    1986   2584   2073   -180    361   -559        O
ATOM   3270  N   SER D 405      57.052  -7.151 -20.315  1.00 18.09           N
ANISOU 3270  N   SER D 405    1951   2814   2110   -146    283   -420        N
ATOM   3271  CA  SER D 405      55.637  -7.523 -20.129  1.00 19.11           C
ANISOU 3271  CA  SER D 405    2039   3005   2216   -228    193   -487        C
ATOM   3272  CB  SER D 405      54.863  -6.332 -19.573  1.00 18.78           C
ANISOU 3272  CB  SER D 405    1906   3051   2179   -203    138   -418        C
ATOM   3273  OG  SER D 405      54.618  -5.349 -20.582  1.00 21.57           O
ANISOU 3273  OG  SER D 405    2269   3504   2423   -125     96   -388        O
ATOM   3274  C   SER D 405      54.985  -8.034 -21.418  1.00 20.52           C
ANISOU 3274  C   SER D 405    2267   3260   2268   -254    138   -600        C
ATOM   3275  O   SER D 405      54.015  -8.769 -21.350  1.00 21.91           O
ANISOU 3275  O   SER D 405    2413   3456   2458   -351     72   -689        O
ATOM   3276  N   GLN D 406      55.571  -7.670 -22.566  1.00 21.23           N
ANISOU 3276  N   GLN D 406    2441   3390   2236   -175    172   -596        N
ATOM   3277  CA  GLN D 406      55.127  -8.012 -23.897  1.00 22.62           C
ANISOU 3277  CA  GLN D 406    2703   3650   2242   -175    117   -699        C
ATOM   3278  CB  GLN D 406      55.211  -9.513 -24.125  1.00 23.49           C
ANISOU 3278  CB  GLN D 406    2891   3667   2369   -252    136   -852        C
ATOM   3279  CG  GLN D 406      56.607 -10.072 -23.936  1.00 22.07           C
ANISOU 3279  CG  GLN D 406    2774   3339   2271   -202    291   -842        C
ATOM   3280  CD  GLN D 406      56.648 -11.573 -24.102  1.00 23.20           C
ANISOU 3280  CD  GLN D 406    3007   3356   2451   -264    309   -996        C
ATOM   3281  OE1 GLN D 406      55.795 -12.289 -23.567  1.00 21.91           O
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Figure 18 (continued)

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ANISOU 3281  OE1 GLN D 406     2815   3144   2366   -382    229  -1058    O
ATOM   3282  NE2 GLN D 406      57.631 -12.062 -24.863  1.00 22.17        N
ANISOU 3282  NE2 GLN D 406     2989   3163   2270   -186    426  -1061    N
ATOM   3283  C   GLN D 406      53.732  -7.462 -24.252  1.00 24.34        C
ANISOU 3283  C   GLN D 406     2853   4022   2375   -190    -45   -716    C
ATOM   3284  O   GLN D 406      53.072  -8.002 -25.126  1.00 26.35        O
ANISOU 3284  O   GLN D 406     3151   4349   2512   -230   -144   -835    O
ATOM   3285  N   GLU D 407      53.301  -6.400 -23.576  1.00 23.86        N
ANISOU 3285  N   GLU D 407     2683   4006   2376   -150    -80   -607    N
ATOM   3286  CA  GLU D 407      51.981  -5.796 -23.788  1.00 25.52        C
ANISOU 3286  CA  GLU D 407     2793   4360   2543   -134   -232   -609    C
ATOM   3287  CB  GLU D 407      51.717  -4.639 -22.799  1.00 24.44        C
ANISOU 3287  CB  GLU D 407     2544   4227   2515    -71   -223   -490    C
ATOM   3288  CG  GLU D 407      51.472  -5.060 -21.360  1.00 25.08        C
ANISOU 3288  CG  GLU D 407     2519   4243   2767   -157   -170   -504    C
ATOM   3289  CD  GLU D 407      50.431  -4.211 -20.650  1.00 25.93        C
ANISOU 3289  CD  GLU D 407     2476   4430   2946   -117   -219   -468    C
ATOM   3290  OE1 GLU D 407      49.823  -3.328 -21.282  1.00 30.67        O
ANISOU 3290  OE1 GLU D 407     3037   5131   3485    -17   -316   -436    O
ATOM   3291  OE2 GLU D 407      50.193  -4.445 -19.455  1.00 24.61        O
ANISOU 3291  OE2 GLU D 407     2235   4224   2892   -177   -157   -471    O
ATOM   3292  C   GLU D 407      51.805  -5.244 -25.195  1.00 26.98        C
ANISOU 3292  C   GLU D 407     3072   4661   2517    -44   -322   -598    C
ATOM   3293  O   GLU D 407      52.719  -4.653 -25.768  1.00 26.51        O
ANISOU 3293  O   GLU D 407     3136   4577   2359     43   -236   -508    O
ATOM   3294  N   ASP D 408      50.596  -5.404 -25.710  1.00 29.10        N
ANISOU 3294  N   ASP D 408     3273   5062   2720    -68   -498   -681    N
ATOM   3295  CA  ASP D 408      50.199  -4.853 -27.013  1.00 31.78        C
ANISOU 3295  CA  ASP D 408     3697   5539   2839     27   -637   -666    C
ATOM   3296  CB  ASP D 408      48.762  -5.265 -27.372  1.00 34.18        C
ANISOU 3296  CB  ASP D 408     3873   5992   3124    -31   -866   -792    C
ATOM   3297  CG  ASP D 408      48.348  -4.814 -28.781  1.00 39.52        C
ANISOU 3297  CG  ASP D 408     4655   6821   3538     70  -1048   -789    C
ATOM   3298  OD1 ASP D 408      49.101  -5.101 -29.741  1.00 40.65        O
ANISOU 3298  OD1 ASP D 408     5022   6953   3469     91   -999   -816    O
ATOM   3299  OD2 ASP D 408      47.267  -4.173 -28.920  1.00 42.45        O
ANISOU 3299  OD2 ASP D 408     4889   7328   3911    139  -1240   -758    O
ATOM   3300  C   ASP D 408      50.353  -3.342 -27.114  1.00 30.90        C
ANISOU 3300  C   ASP D 408     3607   5449   2686    185   -631   -478    C
ATOM   3301  O   ASP D 408      50.746  -2.852 -28.164  1.00 32.78        O
ANISOU 3301  O   ASP D 408     4008   5725   2721    275   -638   -408    O
ATOM   3302  N  ACYS D 409      50.067  -2.594 -26.052  0.50 29.14        N
ANISOU 3302  N  ACYS D 409     3243   5189   2642    219   -609   -394    N
ATOM   3303  N  BCYS D 409      50.023  -2.637 -26.028  0.50 29.40        N
ANISOU 3303  N  BCYS D 409     3268   5224   2679    214   -613   -401    N
ATOM   3304  CA ACYS D 409      50.211  -1.138 -26.143  0.50 29.02        C
ANISOU 3304  CA ACYS D 409     3266   5159   2603    370   -605   -222    C
ATOM   3305  CA BCYS D 409      50.202  -1.188 -25.910  0.50 29.33        C
ANISOU 3305  CA BCYS D 409     3279   5184   2680    356   -592   -230    C
ATOM   3306  CB ACYS D 409      49.420  -0.405 -25.050  0.50 28.83        C
ANISOU 3306  CB ACYS D 409     3056   5130   2766    418   -640   -186    C
ATOM   3307  CB BCYS D 409      49.874  -0.714 -24.481  0.50 28.22        C
ANISOU 3307  CB BCYS D 409     2976   4982   2765    357   -546   -204    C
ATOM   3308  SG ACYS D 409      50.276  -0.105 -23.502  0.50 27.27        S
ANISOU 3308  SG ACYS D 409     2828   4756   2776    378   -445   -139    S
ATOM   3309  SG BCYS D 409      48.105  -0.436 -24.090  0.50 33.35        S
ANISOU 3309  SG BCYS D 409     3379   5779   3515    404   -720   -257    S
ATOM   3310  C  ACYS D 409      51.667  -0.658 -26.204  0.50 27.74        C
ANISOU 3310  C  ACYS D 409     3260   4860   2420    395   -416   -104    C
ATOM   3311  C  BCYS D 409      51.624  -0.756 -26.258  0.50 28.09        C
ANISOU 3311  C  BCYS D 409     3304   4913   2455    389   -423   -117    C
ATOM   3312  O  ACYS D 409      51.933   0.433 -26.730  0.50 28.22        O
ANISOU 3312  O  ACYS D 409     3420   4902   2398    505   -407     42    O
ATOM   3313  O  BCYS D 409      51.824   0.197 -27.026  0.50 28.90        O
ANISOU 3313  O  BCYS D 409     3525   5025   2431    499   -434     14    O
ATOM   3314  N   MSE D 410      52.594  -1.466 -25.672  1.00 25.88        N
ANISOU 3314  N   MSE D 410     3037   4523   2272    295   -268   -161    N
ATOM   3315  CA  MSE D 410      54.024  -1.213 -25.835  1.00 24.44        C
ANISOU 3315  CA  MSE D 410     2971   4231   2082    304    -88    -74    C
ATOM   3316  CB  MSE D 410      54.833  -2.065 -24.854  1.00 22.88        C
ANISOU 3316  CB  MSE D 410     2718   3922   2054    208    -32   -139    C
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Figure 18 (continued)

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ATOM   3317  CG  MSE D 410      56.350  -1.955 -24.998  1.00 21.58           C
ANISOU 3317  CG  MSE D 410    2626   3656   1917    211    213    -70       C
ATOM   3318  SE  MSE D 410      57.152  -3.307 -26.167  0.90 25.86          SE
ANISOU 3318  SE  MSE D 410    3301   4215   2311    188    331   -187      SE
ATOM   3319  CE  MSE D 410      56.323  -4.892 -25.393  1.00 24.10           C
ANISOU 3319  CE  MSE D 410    2993   3974   2189     79    226   -383       C
ATOM   3320  C   MSE D 410      54.468  -1.456 -27.290  1.00 26.13           C
ANISOU 3320  C   MSE D 410    3363   4505   2058    335    -51    -73       C
ATOM   3321  O   MSE D 410      55.180  -0.626 -27.871  1.00 26.11           O
ANISOU 3321  O   MSE D 410    3474   4473   1973    398     47     65       O
ATOM   3322  N   ILE D 411      54.017  -2.573 -27.865  1.00 26.59           N
ANISOU 3322  N   ILE D 411    3456   4644   2004    284   -125   -229       N
ATOM   3323  CA  ILE D 411      54.312  -2.938 -29.242  1.00 28.85           C
ANISOU 3323  CA  ILE D 411    3929   5002   2031    313   -103   -269       C
ATOM   3324  CB  ILE D 411      53.870  -4.398 -29.528  1.00 29.45           C
ANISOU 3324  CB  ILE D 411    4020   5117   2054    221   -180   -493       C
ATOM   3325  CG1 ILE D 411      54.922  -5.354 -28.950  1.00 30.86           C
ANISOU 3325  CG1 ILE D 411    4192   5151   2384    152      9   -568       C
ATOM   3326  CD1 ILE D 411      54.414  -6.711 -28.627  1.00 33.71           C
ANISOU 3326  CD1 ILE D 411    4508   5477   2824     40    -62   -761       C
ATOM   3327  CG2 ILE D 411      53.748  -4.648 -31.007  1.00 32.12           C
ANISOU 3327  CG2 ILE D 411    4558   5571   2076    263   -237   -560       C
ATOM   3328  C   ILE D 411      53.726  -1.918 -30.235  1.00 30.57           C
ANISOU 3328  C   ILE D 411    4252   5336   2025    427   -227   -151       C
ATOM   3329  O   ILE D 411      54.376  -1.536 -31.219  1.00 31.47           O
ANISOU 3329  O   ILE D 411    4553   5470   1935    489   -128    -62       O
ATOM   3330  N   LYS D 412      52.501  -1.477 -29.956  1.00 30.42           N
ANISOU 3330  N   LYS D 412    4112   5395   2052    462   -436   -143       N
ATOM   3331  CA  LYS D 412      51.861  -0.437 -30.741  1.00 32.14           C
ANISOU 3331  CA  LYS D 412    4405   5709   2097    595   -584    -13       C
ATOM   3332  CB  LYS D 412      50.356  -0.417 -30.473  1.00 32.55           C
ANISOU 3332  CB  LYS D 412    4273   5878   2215    618   -846    -83       C
ATOM   3333  CG  LYS D 412      49.618  -1.672 -30.980  1.00 35.49           C
ANISOU 3333  CG  LYS D 412    4615   6379   2489    522  -1011   -302       C
ATOM   3334  CD  LYS D 412      49.784  -1.869 -32.495  1.00 37.96           C
ANISOU 3334  CD  LYS D 412    5179   6799   2444    570  -1080   -323       C
ATOM   3335  CE  LYS D 412      48.933  -3.010 -33.017  1.00 41.23           C
ANISOU 3335  CE  LYS D 412    5565   7342   2760    474  -1290   -557       C
ATOM   3336  NZ  LYS D 412      49.410  -4.347 -32.577  1.00 40.94           N
ANISOU 3336  NZ  LYS D 412    5511   7204   2841    307  -1155   -748       N
ATOM   3337  C   LYS D 412      52.488   0.954 -30.564  1.00 31.37           C
ANISOU 3337  C   LYS D 412    4368   5501   2052    689   -464    219       C
ATOM   3338  O   LYS D 412      52.263   1.832 -31.384  1.00 34.17           O
ANISOU 3338  O   LYS D 412    4853   5899   2228    808   -535    364       O
ATOM   3339  N   ALA D 413      53.283   1.145 -29.513  1.00 28.83           N
ANISOU 3339  N   ALA D 413    3961   5027   1966    633   -291    254       N
ATOM   3340  CA  ALA D 413      54.009   2.413 -29.275  1.00 28.38           C
ANISOU 3340  CA  ALA D 413    3958   4834   1993    687   -162    453       C
ATOM   3341  CB  ALA D 413      54.311   2.582 -27.805  1.00 25.93           C
ANISOU 3341  CB  ALA D 413    3482   4390   1981    626    -91    433       C
ATOM   3342  C   ALA D 413      55.295   2.553 -30.097  1.00 29.23           C
ANISOU 3342  C   ALA D 413    4248   4891   1969    672     54    557       C
ATOM   3343  O   ALA D 413      55.935   3.610 -30.084  1.00 29.28           O
ANISOU 3343  O   ALA D 413    4316   4781   2026    698    170    734       O
ATOM   3344  N   VAL D 414      55.681   1.491 -30.803  1.00 29.64           N
ANISOU 3344  N   VAL D 414    4382   5018   1860    624    122    442       N
ATOM   3345  CA  VAL D 414      56.838   1.555 -31.696  1.00 31.53           C
ANISOU 3345  CA  VAL D 414    4796   5239   1947    622    349    527       C
ATOM   3346  CB  VAL D 414      57.244   0.153 -32.204  1.00 31.72           C
ANISOU 3346  CB  VAL D 414    4872   5330   1851    568    433    337       C
ATOM   3347  CG1 VAL D 414      58.299   0.242 -33.322  1.00 32.64           C
ANISOU 3347  CG1 VAL D 414    5189   5463   1751    592    677    419       C
ATOM   3348  CG2 VAL D 414      57.755  -0.679 -31.067  1.00 26.96           C
ANISOU 3348  CG2 VAL D 414    4084   4628   1532    474    509    207       C
ATOM   3349  C   VAL D 414      56.567   2.486 -32.871  1.00 34.97           C
ANISOU 3349  C   VAL D 414    5447   5737   2103    730    311    706       C
ATOM   3350  O   VAL D 414      55.529   2.404 -33.514  1.00 37.43           O
ANISOU 3350  O   VAL D 414    5833   6183   2206    804     94    673       O
ATOM   3351  N   ARG D 415      57.504   3.384 -33.133  1.00 37.13           N
ANISOU 3351  N   ARG D 415    5819   5909   2380    735    517    905       N
ATOM   3352  CA  ARG D 415      57.422   4.265 -34.293  1.00 41.20           C
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Figure 18 (continued)

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ANISOU 3352  CA  ARG D 415     6579   6461   2613    830    529   1110       C
ATOM   3353  CB  ARG D 415      57.470   5.732 -33.856  1.00 41.42           C
ANISOU 3353  CB  ARG D 415     6605   6324   2807    867    539   1341       C
ATOM   3354  CG  ARG D 415      56.268   6.184 -33.006  1.00 40.12           C
ANISOU 3354  CG  ARG D 415     6292   6136   2814    940    267   1312       C
ATOM   3355  CD  ARG D 415      54.948   6.139 -33.791  1.00 40.78           C
ANISOU 3355  CD  ARG D 415     6465   6391   2638   1079    -17   1301       C
ATOM   3356  NE  ARG D 415      53.810   6.480 -32.938  1.00 40.08           N
ANISOU 3356  NE  ARG D 415     6189   6295   2746   1151   -253   1252       N
ATOM   3357  CZ  ARG D 415      53.013   5.596 -32.344  1.00 38.46           C
ANISOU 3357  CZ  ARG D 415     5779   6195   2639   1117   -410   1034       C
ATOM   3358  NH1 ARG D 415      53.202   4.298 -32.529  1.00 38.97           N
ANISOU 3358  NH1 ARG D 415     5819   6364   2626   1012   -379    843       N
ATOM   3359  NH2 ARG D 415      52.011   6.011 -31.573  1.00 36.41           N
ANISOU 3359  NH2 ARG D 415     5342   5928   2563   1190   -586   1008       N
ATOM   3360  C   ARG D 415      58.551   3.952 -35.281  1.00 43.98           C
ANISOU 3360  C   ARG D 415     7110   6845   2756    796    815   1153       C
ATOM   3361  O   ARG D 415      59.724   3.892 -34.899  1.00 43.78           O
ANISOU 3361  O   ARG D 415     6999   6716   2919    706   1074   1170       O
ATOM   3362  N   GLY D 416      58.191   3.744 -36.545  1.00 47.07           N
ANISOU 3362  N   GLY D 416     7743   7387   2756    874    766   1163       N
ATOM   3363  CA  GLY D 416      59.167   3.367 -37.555  1.00 50.12           C
ANISOU 3363  CA  GLY D 416     8322   7829   2894    856   1047   1180       C
ATOM   3364  C   GLY D 416      59.585   1.904 -37.482  1.00 49.71           C
ANISOU 3364  C   GLY D 416     8192   7833   2861    793   1140    902       C
ATOM   3365  O   GLY D 416      59.098   1.128 -36.639  1.00 47.48           O
ANISOU 3365  O   GLY D 416     7713   7542   2783    750    976    701       O
ATOM   3366  N   ASP D 417      60.483   1.527 -38.386  1.00 52.34           N
ANISOU 3366  N   ASP D 417     8692   8219   2976    793   1417    896       N
ATOM   3367  CA  ASP D 417      60.963   0.150 -38.487  1.00 52.48           C
ANISOU 3367  CA  ASP D 417     8681   8279   2981    761   1539    635       C
ATOM   3368  CB  ASP D 417      61.397  -0.171 -39.931  1.00 56.31           C
ANISOU 3368  CB  ASP D 417     9473   8894   3029    820   1741    619       C
ATOM   3369  CG  ASP D 417      60.213  -0.435 -40.865  1.00 59.32           C
ANISOU 3369  CG  ASP D 417    10103   9446   2990    899   1447    528       C
ATOM   3370  OD1 ASP D 417      59.072  -0.585 -40.386  1.00 59.62           O
ANISOU 3370  OD1 ASP D 417    10036   9508   3109    898   1092    434       O
ATOM   3371  OD2 ASP D 417      60.426  -0.508 -42.095  1.00 65.27           O
ANISOU 3371  OD2 ASP D 417    11157  10319   3324    961   1571    544       O
ATOM   3372  C   ASP D 417      62.098  -0.116 -37.495  1.00 49.99           C
ANISOU 3372  C   ASP D 417     8103   7818   3073    676   1773    604       C
ATOM   3373  O   ASP D 417      62.852   0.793 -37.130  1.00 49.00           O
ANISOU 3373  O   ASP D 417     7885   7587   3145    634   1948    804       O
ATOM   3374  N   LEU D 418      62.205  -1.370 -37.064  1.00 48.76           N
ANISOU 3374  N   LEU D 418     7831   7652   3045    649   1760    353       N
ATOM   3375  CA  LEU D 418      63.263  -1.792 -36.159  1.00 47.10           C
ANISOU 3375  CA  LEU D 418     7377   7317   3201    592   1951    302       C
ATOM   3376  CB  LEU D 418      62.671  -2.523 -34.951  1.00 43.74           C
ANISOU 3376  CB  LEU D 418     6747   6820   3051    545   1712    135       C
ATOM   3377  CG  LEU D 418      61.641  -1.770 -34.088  1.00 41.30           C
ANISOU 3377  CG  LEU D 418     6331   6480   2881    518   1426    222       C
ATOM   3378  CD1 LEU D 418      61.103  -2.653 -32.963  1.00 38.43           C
ANISOU 3378  CD1 LEU D 418     5787   6060   2756    466   1240     45       C
ATOM   3379  CD2 LEU D 418      62.198  -0.471 -33.502  1.00 40.54           C
ANISOU 3379  CD2 LEU D 418     6125   6279   2999    488   1516    456       C
ATOM   3380  C   LEU D 418      64.314  -2.643 -36.873  1.00 49.82           C
ANISOU 3380  C   LEU D 418     7792   7692   3447    625   2264    186       C
ATOM   3381  O   LEU D 418      64.020  -3.727 -37.397  1.00 50.62           O
ANISOU 3381  O   LEU D 418     8020   7854   3358    665   2228    -37       O
ATOM   3382  N   ASN D 419      65.543  -2.131 -36.890  1.00 51.58           N
ANISOU 3382  N   ASN D 419     7923   7863   3811    605   2578    331       N
ATOM   3383  CA  ASN D 419      66.641  -2.741 -37.637  1.00 55.38           C
ANISOU 3383  CA  ASN D 419     8453   8383   4204    650   2935    258       C
ATOM   3384  CB  ASN D 419      66.810  -2.036 -38.993  1.00 59.00           C
ANISOU 3384  CB  ASN D 419     9195   8957   4265    688   3148    420       C
ATOM   3385  CG  ASN D 419      65.665  -2.308 -39.945  1.00 61.70           C
ANISOU 3385  CG  ASN D 419     9864   9436   4145    756   2933    329       C
ATOM   3386  OD1 ASN D 419      65.411  -3.454 -40.327  1.00 65.31           O
ANISOU 3386  OD1 ASN D 419    10428   9949   4440    806   2887     70       O
ATOM   3387  ND2 ASN D 419      64.978  -1.249 -40.352  1.00 63.31           N
ANISOU 3387  ND2 ASN D 419    10234   9687   4135    763   2791    539       N
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Figure 18 (continued)

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ATOM   3388  C   ASN D 419      67.967  -2.719 -36.875  1.00 55.20           C
ANISOU 3388  C   ASN D 419    8127   8253   4594    607   3178    304       C
ATOM   3389  O   ASN D 419      69.023  -2.657 -37.482  1.00 57.94           O
ANISOU 3389  O   ASN D 419    8467   8629   4917    625   3529    357       O
ATOM   3390  N   PHE D 420      67.907  -2.779 -35.544  1.00 53.13           N
ANISOU 3390  N   PHE D 420    7606   7875   4704    552   2988    281       N
ATOM   3391  CA  PHE D 420      69.109  -2.716 -34.699  1.00 52.97           C
ANISOU 3391  CA  PHE D 420    7276   7755   5095    508   3151    324       C
ATOM   3392  CB  PHE D 420      68.768  -2.606 -33.210  1.00 49.23           C
ANISOU 3392  CB  PHE D 420    6582   7166   4956    444   2866    319       C
ATOM   3393  CG  PHE D 420      68.193  -1.287 -32.813  1.00 47.59           C
ANISOU 3393  CG  PHE D 420    6385   6920   4777    366   2702    511       C
ATOM   3394  CD1 PHE D 420      66.832  -1.155 -32.549  1.00 44.55           C
ANISOU 3394  CD1 PHE D 420    6113   6548   4267    372   2390    485       C
ATOM   3395  CE1 PHE D 420      66.292   0.070 -32.189  1.00 42.45           C
ANISOU 3395  CE1 PHE D 420    5858   6235   4036    326   2247    653       C
ATOM   3396  CZ  PHE D 420      67.108   1.173 -32.079  1.00 44.31           C
ANISOU 3396  CZ  PHE D 420    6013   6391   4434    255   2405    848       C
ATOM   3397  CE2 PHE D 420      68.467   1.060 -32.333  1.00 47.66           C
ANISOU 3397  CE2 PHE D 420    6314   6802   4991    223   2712    881       C
ATOM   3398  CD2 PHE D 420      69.007  -0.170 -32.699  1.00 48.65           C
ANISOU 3398  CD2 PHE D 420    6408   6994   5082    287   2863    713       C
ATOM   3399  C   PHE D 420      70.044  -3.885 -34.897  1.00 55.24           C
ANISOU 3399  C   PHE D 420    7475   8045   5470    588   3382    148       C
ATOM   3400  O   PHE D 420      69.616  -5.017 -35.139  1.00 55.65           O
ANISOU 3400  O   PHE D 420    7645   8113   5387    664   3310    -68       O
ATOM   3401  N   VAL D 421      71.326  -3.572 -34.740  1.00 57.63           N
ANISOU 3401  N   VAL D 421    7549   8317   6030    565   3651    242       N
ATOM   3402  CA  VAL D 421      72.446  -4.448 -35.036  1.00 60.77           C
ANISOU 3402  CA  VAL D 421    7821   8726   6542    654   3948    120       C
ATOM   3403  CB  VAL D 421      73.166  -3.930 -36.322  1.00 64.47           C
ANISOU 3403  CB  VAL D 421    8404   9304   6788    666   4360    236       C
ATOM   3404  CG1 VAL D 421      74.630  -4.300 -36.367  1.00 67.05           C
ANISOU 3404  CG1 VAL D 421    8458   9632   7386    714   4721    208       C
ATOM   3405  CG2 VAL D 421      72.428  -4.388 -37.580  1.00 66.03           C
ANISOU 3405  CG2 VAL D 421    8997   9617   6475    754   4400    126       C
ATOM   3406  C   VAL D 421      73.361  -4.471 -33.799  1.00 60.35           C
ANISOU 3406  C   VAL D 421    7378   8567   6985    619   3924    144       C
ATOM   3407  O   VAL D 421      73.403  -3.496 -33.045  1.00 58.87           O
ANISOU 3407  O   VAL D 421    7042   8323   7003    501   3800    305       O
ATOM   3408  N   ASN D 422      74.043  -5.593 -33.555  1.00 62.10           N
ANISOU 3408  N   ASN D 422    7446   8752   7397    728   4012     -23       N
ATOM   3409  CA  ASN D 422      75.069  -5.636 -32.502  1.00 62.56           C
ANISOU 3409  CA  ASN D 422    7120   8730   7918    718   4012      6       C
ATOM   3410  CB  ASN D 422      75.045  -6.970 -31.720  1.00 61.54           C
ANISOU 3410  CB  ASN D 422    6907   8505   7969    834   3835   -189       C
ATOM   3411  CG  ASN D 422      75.460  -8.203 -32.559  1.00 64.42           C
ANISOU 3411  CG  ASN D 422    7361   8885   8231   1012   4080   -391       C
ATOM   3412  OD1 ASN D 422      75.195  -9.336 -32.147  1.00 63.87           O
ANISOU 3412  OD1 ASN D 422    7329   8720   8219   1110   3933   -561       O
ATOM   3413  ND2 ASN D 422      76.118  -7.995 -33.700  1.00 67.10           N
ANISOU 3413  ND2 ASN D 422    7740   9330   8425   1055   4460   -372       N
ATOM   3414  C   ASN D 422      76.469  -5.287 -33.033  1.00 66.36           C
ANISOU 3414  C   ASN D 422    7376   9270   8567    724   4415     91       C
ATOM   3415  O   ASN D 422      76.626  -4.987 -34.223  1.00 69.23           O
ANISOU 3415  O   ASN D 422    7905   9734   8666    733   4718    140       O
ATOM   3416  N   ARG D 423      77.475  -5.324 -32.158  1.00 67.11           N
ANISOU 3416  N   ARG D 423    7093   9311   9095    719   4419    113       N
ATOM   3417  CA  ARG D 423      78.878  -5.054 -32.539  1.00 71.12           C
ANISOU 3417  CA  ARG D 423    7306   9875   9840    720   4794    183       C
ATOM   3418  CB  ARG D 423      79.805  -5.272 -31.338  1.00 70.83           C
ANISOU 3418  CB  ARG D 423    6839   9769  10305    731   4668    172       C
ATOM   3419  CG  ARG D 423      81.105  -4.524 -31.468  1.00 75.85           C
ANISOU 3419  CG  ARG D 423    7115  10456  11248    641   4957    306       C
ATOM   3420  CD  ARG D 423      82.094  -4.875 -30.379  1.00 78.88           C
ANISOU 3420  CD  ARG D 423    7053  10793  12126    681   4832    269       C
ATOM   3421  NE  ARG D 423      83.449  -4.480 -30.778  1.00 83.39           N
ANISOU 3421  NE  ARG D 423    7254  11442  12987    644   5197    346       N
ATOM   3422  CZ  ARG D 423      84.346  -3.929 -29.962  1.00 85.30           C
ANISOU 3422  CZ  ARG D 423    7077  11667  13667    531   5116    429       C
ATOM   3423  NH1 ARG D 423      84.039  -3.684 -28.689  1.00 83.30           N
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Figure 18 (continued)

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ANISOU 3423  NH1 ARG D 423     6747  11320  13584    452   4676    442       N
ATOM   3424  NH2 ARG D 423       85.547  -3.606 -30.420  1.00 88.44           N
ANISOU 3424  NH2 ARG D 423     7128  12146  14328    490   5478    494       N
ATOM   3425  C   ARG D 423       79.401  -5.843 -33.761  1.00 74.67           C
ANISOU 3425  C   ARG D 423     7845  10417  10109    882   5200     61       C
ATOM   3426  O   ARG D 423       80.280  -5.369 -34.493  1.00 78.15           O
ANISOU 3426  O   ARG D 423     8167  10945  10580    855   5588    155       O
ATOM   3427  N   ALA D 424       78.849  -7.036 -33.971  1.00 74.34           N
ANISOU 3427  N   ALA D 424     8018  10348   9879   1042   5120   -153       N
ATOM   3428  CA  ALA D 424       79.275  -7.945 -35.036  1.00 77.50           C
ANISOU 3428  CA  ALA D 424     8532  10811  10104   1222   5468   -322       C
ATOM   3429  CB  ALA D 424       79.327  -9.375 -34.497  1.00 77.08           C
ANISOU 3429  CB  ALA D 424     8426  10642  10219   1410   5328   -554       C
ATOM   3430  C   ALA D 424       78.429  -7.881 -36.329  1.00 78.58           C
ANISOU 3430  C   ALA D 424     9131  11043   9682   1227   5589   -362       C
ATOM   3431  O   ALA D 424       78.708  -8.612 -37.287  1.00 81.61           O
ANISOU 3431  O   ALA D 424     9666  11484   9858   1375   5881   -520       O
ATOM   3432  N   ASN D 425       77.396  -7.032 -36.340  1.00 76.24           N
ANISOU 3432  N   ASN D 425     9062  10762   9143   1081   5352   -230       N
ATOM   3433  CA  ASN D 425       76.541  -6.773 -37.531  1.00 77.06           C
ANISOU 3433  CA  ASN D 425     9601  10971   8708   1070   5413   -224       C
ATOM   3434  CB  ASN D 425       77.382  -6.619 -38.817  1.00 81.53           C
ANISOU 3434  CB  ASN D 425    10245  11670   9062   1128   5927   -191       C
ATOM   3435  CG  ASN D 425       76.892  -5.487 -39.721  1.00 82.66           C
ANISOU 3435  CG  ASN D 425    10683  11919   8803   1017   6017     23       C
ATOM   3436  OD1 ASN D 425       75.842  -4.884 -39.484  1.00 79.73           O
ANISOU 3436  OD1 ASN D 425    10484  11524   8284    921   5681    122       O
ATOM   3437  ND2 ASN D 425       77.670  -5.189 -40.763  1.00 87.19           N
ANISOU 3437  ND2 ASN D 425    11314  12609   9204   1038   6484    104       N
ATOM   3438  C   ASN D 425       75.343  -7.727 -37.759  1.00 75.53           C
ANISOU 3438  C   ASN D 425     9745  10754   8199   1149   5142   -450       C
ATOM   3439  O   ASN D 425       74.857  -7.888 -38.889  1.00 77.60           O
ANISOU 3439  O   ASN D 425    10357  11113   8012   1196   5244   -527       O
ATOM   3440  N   GLN D 426       74.866  -8.349 -36.685  1.00 72.05           N
ANISOU 3440  N   GLN D 426     9203  10184   7987   1153   4795   -555       N
ATOM   3441  CA  GLN D 426       73.650  -9.164 -36.756  1.00 70.27           C
ANISOU 3441  CA  GLN D 426     9262   9919   7517   1181   4501   -748       C
ATOM   3442  CB  GLN D 426       73.803 -10.451 -35.941  1.00 69.42           C
ANISOU 3442  CB  GLN D 426     9024   9655   7697   1280   4372   -950       C
ATOM   3443  CG  GLN D 426       74.946 -11.353 -36.387  1.00 73.99           C
ANISOU 3443  CG  GLN D 426     9510  10209   8392   1461   4723  -1107       C
ATOM   3444  CD  GLN D 426       75.603 -12.085 -35.226  1.00 74.03           C
ANISOU 3444  CD  GLN D 426     9200  10055   8872   1543   4632  -1157       C
ATOM   3445  OE1 GLN D 426       75.551 -11.640 -34.081  1.00 71.79           O
ANISOU 3445  OE1 GLN D 426     8697   9713   8868   1449   4387  -1016       O
ATOM   3446  NE2 GLN D 426       76.238 -13.210 -35.525  1.00 76.73           N
ANISOU 3446  NE2 GLN D 426     9532  10324   9297   1733   4831  -1361       N
ATOM   3447  C   GLN D 426       72.469  -8.361 -36.228  1.00 66.34           C
ANISOU 3447  C   GLN D 426     8844   9421   6942   1033   4126   -613       C
ATOM   3448  O   GLN D 426       72.648  -7.428 -35.444  1.00 64.20           O
ANISOU 3448  O   GLN D 426     8361   9122   6912    930   4038   -414       O
ATOM   3449  N   ARG D 427       71.267  -8.715 -36.673  1.00 65.24           N
ANISOU 3449  N   ARG D 427     9004   9310   6472   1027   4027   -733       N
ATOM   3450  CA  ARG D 427       70.051  -8.191 -36.069  1.00 61.55           C
ANISOU 3450  CA  ARG D 427     8583   8831   5972    913   3523   -653       C
ATOM   3451  CB  ARG D 427       68.814  -8.575 -36.886  1.00 62.29           C
ANISOU 3451  CB  ARG D 427     9018   9000   5650    917   3336   -797       C
ATOM   3452  CG  ARG D 427       68.261  -7.481 -37.795  1.00 64.44           C
ANISOU 3452  CG  ARG D 427     9512   9421   5551    879   3327   -631       C
ATOM   3453  CD  ARG D 427       66.962  -7.945 -38.473  1.00 65.91           C
ANISOU 3453  CD  ARG D 427    10000   9683   5358    883   3067   -794       C
ATOM   3454  NE  ARG D 427       65.923  -8.303 -37.500  1.00 66.69           N
ANISOU 3454  NE  ARG D 427    10003   9701   5634    809   2687   -872       N
ATOM   3455  CZ  ARG D 427       64.760  -7.663 -37.349  1.00 67.25           C
ANISOU 3455  CZ  ARG D 427    10120   9829   5603    741   2381   -785       C
ATOM   3456  NH1 ARG D 427       64.467  -6.631 -38.135  1.00 69.18           N
ANISOU 3456  NH1 ARG D 427    10527  10201   5557    750   2385   -613       N
ATOM   3457  NH2 ARG D 427       63.886  -8.059 -36.414  1.00 63.74           N
ANISOU 3457  NH2 ARG D 427     9559   9311   5349    671   2080   -864       N
ATOM   3458  C   ARG D 427       69.909  -8.721 -34.642  1.00 57.19           C
ANISOU 3458  C   ARG D 427     7803   8128   5798    883   3273   -704       C
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Figure 18 (continued)

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ATOM   3459  O   ARG D 427      70.103  -9.914 -34.377  1.00 57.69           O
ANISOU 3459  O   ARG D 427    7840   8092   5987    959   3269   -894        O
ATOM   3460  N   LEU D 428      69.595  -7.815 -33.724  1.00 52.80           N
ANISOU 3460  N   LEU D 428    7098   7547   5418    778   3076   -527        N
ATOM   3461  CA  LEU D 428      69.144  -8.185 -32.399  1.00 48.04           C
ANISOU 3461  CA  LEU D 428    6348   6827   5079    732   2792   -559        C
ATOM   3462  CB  LEU D 428      68.918  -6.930 -31.545  1.00 45.72           C
ANISOU 3462  CB  LEU D 428    5911   6527   4933    622   2636   -347        C
ATOM   3463  CG  LEU D 428      70.023  -5.875 -31.426  1.00 45.49           C
ANISOU 3463  CG  LEU D 428    5686   6505   5093    586   2834   -153        C
ATOM   3464  CD1 LEU D 428      69.597  -4.802 -30.425  1.00 41.45           C
ANISOU 3464  CD1 LEU D 428    5066   5948   4733    475   2612      4        C
ATOM   3465  CD2 LEU D 428      71.353  -6.491 -31.016  1.00 45.37           C
ANISOU 3465  CD2 LEU D 428    5422   6426   5391    651   3013   -200        C
ATOM   3466  C   LEU D 428      67.846  -8.982 -32.525  1.00 46.17           C
ANISOU 3466  C   LEU D 428    6321   6580   4642    717   2547   -732        C
ATOM   3467  O   LEU D 428      67.099  -8.802 -33.495  1.00 46.00           O
ANISOU 3467  O   LEU D 428    6533   6665   4279    710   2512   -766        O
ATOM   3468  N   ASN D 429      67.587  -9.863 -31.556  1.00 43.68           N
ANISOU 3468  N   ASN D 429    5922   6137   4538    708   2374   -834        N
ATOM   3469  CA  ASN D 429      66.288 -10.534 -31.500  1.00 42.36           C
ANISOU 3469  CA  ASN D 429    5910   5947   4237    654   2121   -976        C
ATOM   3470  CB  ASN D 429      66.290 -11.755 -30.550  1.00 41.80           C
ANISOU 3470  CB  ASN D 429    5766   5699   4415    662   2019  -1102        C
ATOM   3471  CG  ASN D 429      66.394 -11.396 -29.062  1.00 40.02           C
ANISOU 3471  CG  ASN D 429    5314   5396   4495    608   1878   -956        C
ATOM   3472  OD1 ASN D 429      66.177 -10.270 -28.644  1.00 40.08           O
ANISOU 3472  OD1 ASN D 429    5232   5473   4524    542   1798   -792        O
ATOM   3473  ND2 ASN D 429      66.713 -12.395 -28.251  1.00 41.75           N
ANISOU 3473  ND2 ASN D 429    5463   5458   4943    644   1840  -1024        N
ATOM   3474  C   ASN D 429      65.147  -9.524 -31.230  1.00 39.73           C
ANISOU 3474  C   ASN D 429    5590   5701   3805    548   1883   -849        C
ATOM   3475  O   ASN D 429      65.412  -8.410 -30.755  1.00 37.87           O
ANISOU 3475  O   ASN D 429    5221   5490   3678    516   1887   -655        O
ATOM   3476  N   PRO D 430      63.894  -9.878 -31.600  1.00 39.17           N
ANISOU 3476  N   PRO D 430    5679   5677   3529    497   1681   -965        N
ATOM   3477  CA  PRO D 430      62.734  -8.984 -31.432  1.00 37.02           C
ANISOU 3477  CA  PRO D 430    5410   5497   3159    420   1451   -863        C
ATOM   3478  CB  PRO D 430      61.553  -9.913 -31.669  1.00 37.39           C
ANISOU 3478  CB  PRO D 430    5577   5550   3079    364   1242  -1062        C
ATOM   3479  CG  PRO D 430      62.081 -10.877 -32.687  1.00 40.79           C
ANISOU 3479  CG  PRO D 430    6190   5964   3346    432   1404  -1251        C
ATOM   3480  CD  PRO D 430      63.507 -11.136 -32.276  1.00 40.91           C
ANISOU 3480  CD  PRO D 430    6084   5865   3594    513   1659  -1213        C
ATOM   3481  C   PRO D 430      62.622  -8.261 -30.087  1.00 33.75           C
ANISOU 3481  C   PRO D 430    4783   5029   3011    363   1338   -704        C
ATOM   3482  O   PRO D 430      62.364  -7.059 -30.075  1.00 33.39           O
ANISOU 3482  O   PRO D 430    4712   5054   2922    350   1292   -543        O
ATOM   3483  N   MSE D 431      62.848  -8.958 -28.971  1.00 31.86           N
ANISOU 3483  N   MSE D 431    4412   4658   3035    338   1298   -746        N
ATOM   3484  CA  MSE D 431      62.743  -8.348 -27.632  1.00 28.73           C
ANISOU 3484  CA  MSE D 431    3838   4212   2866    286   1187   -615        C
ATOM   3485  CB  MSE D 431      62.750  -9.420 -26.522  1.00 27.66           C
ANISOU 3485  CB  MSE D 431    3625   3936   2949    257   1113   -693        C
ATOM   3486  CG  MSE D 431      61.493 -10.315 -26.470  1.00 27.35           C
ANISOU 3486  CG  MSE D 431    3673   3880   2840    179    946   -835        C
ATOM   3487  SE  MSE D 431      59.849  -9.332 -26.102  0.90 31.03          SE
ANISOU 3487  SE  MSE D 431    4095   4475   3220     81    709   -763        SE
ATOM   3488  CE  MSE D 431      60.279  -8.893 -24.268  1.00 22.81           C
ANISOU 3488  CE  MSE D 431    2865   3332   2469     58    684   -614        C
ATOM   3489  C   MSE D 431      63.805  -7.287 -27.358  1.00 28.34           C
ANISOU 3489  C   MSE D 431    3663   4159   2948    313   1319   -441        C
ATOM   3490  O   MSE D 431      63.527  -6.285 -26.719  1.00 26.80           O
ANISOU 3490  O   MSE D 431    3388   3975   2822    271   1226   -314        O
ATOM   3491  N   HIS D 432      65.023  -7.514 -27.840  1.00 30.47           N
ANISOU 3491  N   HIS D 432    3907   4407   3264    380   1540   -445        N
ATOM   3492  CA  HIS D 432      66.103  -6.525 -27.751  1.00 31.28           C
ANISOU 3492  CA  HIS D 432    3877   4513   3497    388   1692   -287        C
ATOM   3493  CB  HIS D 432      67.466  -7.225 -27.838  1.00 32.69           C
ANISOU 3493  CB  HIS D 432    3946   4634   3841    464   1905   -335        C
ATOM   3494  CG  HIS D 432      67.822  -7.950 -26.579  1.00 33.74           C
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Figure 18 (continued)

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ANISOU 3494  CG  HIS D 432     3924   4646   4251    475   1799   -373       C
ATOM   3495  ND1 HIS D 432      67.295  -9.184 -26.261  1.00 34.66           N
ANISOU 3495  ND1 HIS D 432     4117   4682   4371    496   1690   -514       N
ATOM   3496  CE1 HIS D 432      67.748  -9.561 -25.077  1.00 34.47           C
ANISOU 3496  CE1 HIS D 432     3947   4553   4597    508   1603   -490       C
ATOM   3497  NE2 HIS D 432      68.534  -8.608 -24.606  1.00 33.88           N
ANISOU 3497  NE2 HIS D 432     3695   4499   4680    491   1632   -354       N
ATOM   3498  CD2 HIS D 432      68.587  -7.583 -25.521  1.00 33.50           C
ANISOU 3498  CD2 HIS D 432     3682   4555   4490    461   1760   -279       C
ATOM   3499  C   HIS D 432      65.961  -5.388 -28.772  1.00 32.02           C
ANISOU 3499  C   HIS D 432     4081   4712   3373    380   1782   -166       C
ATOM   3500  O   HIS D 432      66.410  -4.265 -28.541  1.00 31.60           O
ANISOU 3500  O   HIS D 432     3939   4650   3418    343   1831     -4       O
ATOM   3501  N   GLN D 433      65.317  -5.703 -29.889  1.00 33.25           N
ANISOU 3501  N   GLN D 433     4447   4957   3229    412   1790   -247       N
ATOM   3502  CA  GLN D 433      64.893  -4.737 -30.897  1.00 34.81           C
ANISOU 3502  CA  GLN D 433     4806   5264   3155    417   1816   -136       C
ATOM   3503  CB  GLN D 433      64.124  -5.526 -31.969  1.00 37.14           C
ANISOU 3503  CB  GLN D 433     5332   5652   3127    458   1766   -297       C
ATOM   3504  CG  GLN D 433      64.229  -5.159 -33.425  1.00 40.17           C
ANISOU 3504  CG  GLN D 433     5942   6157   3166    513   1917   -256       C
ATOM   3505  CD  GLN D 433      65.636  -4.990 -33.941  1.00 42.73           C
ANISOU 3505  CD  GLN D 433     6242   6477   3518    553   2269   -184       C
ATOM   3506  OE1 GLN D 433      66.081  -3.868 -34.122  1.00 42.34           O
ANISOU 3506  OE1 GLN D 433     6173   6441   3473    532   2393     22       O
ATOM   3507  NE2 GLN D 433      66.331  -6.095 -34.227  1.00 44.78           N
ANISOU 3507  NE2 GLN D 433     6506   6712   3797    612   2445   -355       N
ATOM   3508  C   GLN D 433      63.985  -3.705 -30.188  1.00 33.00           C
ANISOU 3508  C   GLN D 433     4532   5029   2979    363   1591    -12       C
ATOM   3509  O   GLN D 433      64.238  -2.508 -30.244  1.00 33.66           O
ANISOU 3509  O   GLN D 433     4602   5106   3081    347   1644    167       O
ATOM   3510  N   LEU D 434      62.956  -4.188 -29.488  1.00 30.54           N
ANISOU 3510  N   LEU D 434     4191   4705   2709    334   1355   -111       N
ATOM   3511  CA  LEU D 434      62.019  -3.349 -28.723  1.00 28.54           C
ANISOU 3511  CA  LEU D 434     3877   4447   2519    298   1147    -27       C
ATOM   3512  CB  LEU D 434      60.860  -4.193 -28.170  1.00 26.57           C
ANISOU 3512  CB  LEU D 434     3605   4209   2281    263    932   -173       C
ATOM   3513  CG  LEU D 434      59.960  -4.841 -29.225  1.00 28.19           C
ANISOU 3513  CG  LEU D 434     3969   4522   2219    278    838   -304       C
ATOM   3514  CD1 LEU D 434      59.179  -6.004 -28.622  1.00 25.09           C
ANISOU 3514  CD1 LEU D 434     3526   4099   1908    213    690   -476       C
ATOM   3515  CD2 LEU D 434      59.035  -3.808 -29.879  1.00 26.55           C
ANISOU 3515  CD2 LEU D 434     3849   4430   1809    316    706   -203       C
ATOM   3516  C   LEU D 434      62.664  -2.581 -27.568  1.00 27.04           C
ANISOU 3516  C   LEU D 434     3514   4152   2609    258   1167     91       C
ATOM   3517  O   LEU D 434      62.423  -1.387 -27.390  1.00 25.53           O
ANISOU 3517  O   LEU D 434     3318   3948   2436    251   1119    227       O
ATOM   3518  N   LEU D 435      63.462  -3.285 -26.775  1.00 26.54           N
ANISOU 3518  N   LEU D 435     3318   4005   2760    239   1220     31       N
ATOM   3519  CA  LEU D 435      64.256  -2.688 -25.702  1.00 26.16           C
ANISOU 3519  CA  LEU D 435     3103   3862   2975    200   1234    119       C
ATOM   3520  CB  LEU D 435      65.092  -3.789 -25.043  1.00 25.47           C
ANISOU 3520  CB  LEU D 435     2895   3705   3077    208   1276     27       C
ATOM   3521  CG  LEU D 435      65.725  -3.556 -23.679  1.00 24.89           C
ANISOU 3521  CG  LEU D 435     2647   3540   3271    171   1207     70       C
ATOM   3522  CD1 LEU D 435      64.682  -3.442 -22.582  1.00 20.95           C
ANISOU 3522  CD1 LEU D 435     2152   3019   2787    132    993     52       C
ATOM   3523  CD2 LEU D 435      66.673  -4.719 -23.380  1.00 26.46           C
ANISOU 3523  CD2 LEU D 435     2748   3683   3624    217   1274     -9       C
ATOM   3524  C   LEU D 435      65.136  -1.488 -26.142  1.00 27.72           C
ANISOU 3524  C   LEU D 435     3277   4043   3215    183   1392    280       C
ATOM   3525  O   LEU D 435      65.062  -0.432 -25.523  1.00 27.64           O
ANISOU 3525  O   LEU D 435     3216   3976   3311    140   1321    381       O
ATOM   3526  N   ARG D 436      65.954  -1.635 -27.191  1.00 30.12           N
ANISOU 3526  N   ARG D 436     3621   4384   3438    211   1617    302       N
ATOM   3527  CA  ARG D 436      66.820  -0.532 -27.661  1.00 32.34           C
ANISOU 3527  CA  ARG D 436     3877   4644   3766    175   1803    469       C
ATOM   3528  CB  ARG D 436      67.825  -0.970 -28.749  1.00 34.74           C
ANISOU 3528  CB  ARG D 436     4200   5003   3997    211   2095    466       C
ATOM   3529  CG  ARG D 436      68.788  -2.119 -28.428  1.00 38.82           C
ANISOU 3529  CG  ARG D 436     4552   5499   4700    249   2201    339       C
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Figure 18 (continued)

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ATOM   3530  CD  ARG D 436      69.651  -1.978 -27.166  1.00 45.47           C
ANISOU 3530  CD  ARG D 436    5125   6244   5908    197   2148    361       C
ATOM   3531  NE  ARG D 436      70.087  -3.302 -26.682  1.00 50.46           N
ANISOU 3531  NE  ARG D 436    5647   6850   6677    269   2131    214       N
ATOM   3532  CZ  ARG D 436      70.128  -3.695 -25.402  1.00 51.20           C
ANISOU 3532  CZ  ARG D 436    5607   6868   6978    261   1938    168       C
ATOM   3533  NH1 ARG D 436      69.776  -2.873 -24.420  1.00 50.06           N
ANISOU 3533  NH1 ARG D 436    5415   6676   6930    180   1748    238       N
ATOM   3534  NH2 ARG D 436      70.533  -4.928 -25.097  1.00 53.27           N
ANISOU 3534  NH2 ARG D 436    5801   7095   7346    344   1938     52       N
ATOM   3535  C   ARG D 436      66.028   0.663 -28.204  1.00 32.58           C
ANISOU 3535  C   ARG D 436    4070   4692   3616    169   1749    610       C
ATOM   3536  O   ARG D 436      66.482   1.801 -28.113  1.00 33.26           O
ANISOU 3536  O   ARG D 436    4125   4705   3810    112   1815    763       O
ATOM   3537  N   HIS D 437      64.874   0.396 -28.813  1.00 32.38           N
ANISOU 3537  N   HIS D 437    4222   4757   3325    230   1627    560       N
ATOM   3538  CA  HIS D 437      63.992   1.447 -29.316  1.00 32.23           C
ANISOU 3538  CA  HIS D 437    4358   4760   3127    257   1533    689       C
ATOM   3539  CB  HIS D 437      62.776   0.835 -29.996  1.00 32.33           C
ANISOU 3539  CB  HIS D 437    4528   4902   2856    329   1377    588       C
ATOM   3540  CG  HIS D 437      61.792   1.845 -30.505  1.00 32.58           C
ANISOU 3540  CG  HIS D 437    4705   4969   2705    384   1241    716       C
ATOM   3541  ND1 HIS D 437      62.005   2.587 -31.652  1.00 33.44           N
ANISOU 3541  ND1 HIS D 437    5004   5109   2594    423   1364    882       N
ATOM   3542  CE1 HIS D 437      60.975   3.389 -31.850  1.00 32.84           C
ANISOU 3542  CE1 HIS D 437    5028   5050   2399    489   1178    978       C
ATOM   3543  NE2 HIS D 437      60.100   3.192 -30.877  1.00 31.03           N
ANISOU 3543  NE2 HIS D 437    4663   4812   2316    493    955    869       N
ATOM   3544  CD2 HIS D 437      60.589   2.233 -30.023  1.00 28.67           C
ANISOU 3544  CD2 HIS D 437    4193   4482   2217    419    996    711       C
ATOM   3545  C   HIS D 437      63.529   2.367 -28.191  1.00 31.00           C
ANISOU 3545  C   HIS D 437    4111   4501   3166    224   1360    750       C
ATOM   3546  O   HIS D 437      63.642   3.606 -28.303  1.00 31.79           O
ANISOU 3546  O   HIS D 437    4259   4524   3297    208   1393    917       O
ATOM   3547  N   PHE D 438      63.015   1.763 -27.119  1.00 28.21           N
ANISOU 3547  N   PHE D 438    3643   4136   2938    213   1191    616       N
ATOM   3548  CA  PHE D 438      62.438   2.523 -26.020  1.00 27.04           C
ANISOU 3548  CA  PHE D 438    3427   3908   2940    198   1026    640       C
ATOM   3549  CB  PHE D 438      61.377   1.704 -25.284  1.00 24.52           C
ANISOU 3549  CB  PHE D 438    3057   3643   2616    215    836    490       C
ATOM   3550  CG  PHE D 438      60.176   1.379 -26.140  1.00 23.90           C
ANISOU 3550  CG  PHE D 438    3093   3692   2294    282    727    446       C
ATOM   3551  CD1 PHE D 438      59.391   2.399 -26.676  1.00 23.65           C
ANISOU 3551  CD1 PHE D 438    3161   3687   2138    351    643    555       C
ATOM   3552  CE1 PHE D 438      58.280   2.110 -27.459  1.00 24.54           C
ANISOU 3552  CE1 PHE D 438    3360   3932   2032    417    509    512       C
ATOM   3553  CZ  PHE D 438      57.941   0.772 -27.715  1.00 25.28           C
ANISOU 3553  CZ  PHE D 438    3448   4125   2034    392    465    343       C
ATOM   3554  CE2 PHE D 438      58.734  -0.261 -27.196  1.00 23.25           C
ANISOU 3554  CE2 PHE D 438    3113   3818   1903    320    569    233       C
ATOM   3555  CD2 PHE D 438      59.836   0.052 -26.416  1.00 22.04           C
ANISOU 3555  CD2 PHE D 438    2868   3543   1964    276    694    292       C
ATOM   3556  C   PHE D 438      63.462   3.158 -25.072  1.00 27.33           C
ANISOU 3556  C   PHE D 438    3326   3806   3251    116   1082    694       C
ATOM   3557  O   PHE D 438      63.182   4.188 -24.467  1.00 27.54           O
ANISOU 3557  O   PHE D 438    3351   3740   3375    103    998    758       O
ATOM   3558  N   GLN D 439      64.639   2.551 -24.975  1.00 27.93           N
ANISOU 3558  N   GLN D 439    3289   3867   3455     69   1218    661       N
ATOM   3559  CA  GLN D 439      65.790   3.129 -24.318  1.00 28.89           C
ANISOU 3559  CA  GLN D 439    3266   3877   3835    -18   1287    717       C
ATOM   3560  CB  GLN D 439      66.920   2.062 -24.200  1.00 29.69           C
ANISOU 3560  CB  GLN D 439    3213   4002   4067    -32   1401    637       C
ATOM   3561  CG  GLN D 439      66.621   0.950 -23.141  1.00 26.15           C
ANISOU 3561  CG  GLN D 439    2686   3563   3686     -6   1239    487       C
ATOM   3562  CD  GLN D 439      67.662  -0.160 -23.094  1.00 28.79           C
ANISOU 3562  CD  GLN D 439    2888   3909   4142     14   1338    414       C
ATOM   3563  OE1 GLN D 439      68.317  -0.497 -24.104  1.00 32.54           O
ANISOU 3563  OE1 GLN D 439    3363   4430   4572     44   1542    425       O
ATOM   3564  NE2 GLN D 439      67.822  -0.748 -21.912  1.00 28.30           N
ANISOU 3564  NE2 GLN D 439    2720   3805   4230     12   1198    340       N
ATOM   3565  C   GLN D 439      66.284   4.385 -25.045  1.00 31.94           C
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Figure 18 (continued)

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ANISOU 3565  C   GLN D 439     3715   4193   4229    -65   1434    895    C
ATOM   3566  O   GLN D 439      66.781   5.320 -24.410  1.00 32.63           O
ANISOU 3566  O   GLN D 439     3727   4152   4519   -149   1421    959    O
ATOM   3567  N   LYS D 440      66.162   4.415 -26.374  1.00 34.31           N
ANISOU 3567  N   LYS D 440     4167   4567   4301    -18   1575    976    N
ATOM   3568  CA  LYS D 440      66.529   5.601 -27.135  1.00 37.03           C
ANISOU 3568  CA  LYS D 440     4613   4841   4618    -60   1725   1173    C
ATOM   3569  CB  LYS D 440      66.617   5.319 -28.642  1.00 39.69           C
ANISOU 3569  CB  LYS D 440     5117   5293   4672     -5   1921   1245    C
ATOM   3570  CG  LYS D 440      67.882   4.548 -29.032  1.00 43.01           C
ANISOU 3570  CG  LYS D 440     5411   5768   5163    -42   2176   1205    C
ATOM   3571  CD  LYS D 440      68.388   4.877 -30.420  1.00 49.43           C
ANISOU 3571  CD  LYS D 440     6372   6631   5777    -42   2461   1354    C
ATOM   3572  CE  LYS D 440      69.683   4.104 -30.681  1.00 52.40           C
ANISOU 3572  CE  LYS D 440     6580   7061   6271    -70   2732   1294    C
ATOM   3573  NZ  LYS D 440      70.294   4.407 -32.006  1.00 56.62           N
ANISOU 3573  NZ  LYS D 440     7243   7651   6617    -78   3064   1439    N
ATOM   3574  C   LYS D 440      65.556   6.741 -26.849  1.00 36.89           C
ANISOU 3574  C   LYS D 440     4715   4726   4575    -33   1555   1259    C
ATOM   3575  O   LYS D 440      65.993   7.846 -26.543  1.00 37.86           O
ANISOU 3575  O   LYS D 440     4824   4692   4869   -113   1589   1372    O
ATOM   3576  N   ASP D 441      64.250   6.442 -26.917  1.00 35.37           N
ANISOU 3576  N   ASP D 441     4626   4620   4192     79   1370   1193    N
ATOM   3577  CA  ASP D 441      63.183   7.396 -26.655  1.00 34.86           C
ANISOU 3577  CA  ASP D 441     4660   4486   4100    145   1196   1252    C
ATOM   3578  CB  ASP D 441      62.914   8.221 -27.913  1.00 37.92           C
ANISOU 3578  CB  ASP D 441     5267   4866   4275    207   1267   1450    C
ATOM   3579  CG  ASP D 441      61.804   9.261 -27.730  1.00 40.30           C
ANISOU 3579  CG  ASP D 441     5676   5081   4554    307   1084   1529    C
ATOM   3580  OD1 ASP D 441      61.425   9.618 -26.576  1.00 39.22           O
ANISOU 3580  OD1 ASP D 441     5443   4850   4609    306    947   1449    O
ATOM   3581  OD2 ASP D 441      61.301   9.721 -28.784  1.00 45.16           O
ANISOU 3581  OD2 ASP D 441     6486   5729   4944    401   1080   1674    O
ATOM   3582  C   ASP D 441      61.900   6.717 -26.136  1.00 32.31           C
ANISOU 3582  C   ASP D 441     4311   4270   3697    235    971   1096    C
ATOM   3583  O   ASP D 441      61.199   6.013 -26.871  1.00 32.02           O
ANISOU 3583  O   ASP D 441     4348   4382   3436    310    920   1048    O
ATOM   3584  N   ALA D 442      61.576   6.945 -24.867  1.00 29.74           N
ANISOU 3584  N   ALA D 442     3881   3867   3552    220    839   1014    N
ATOM   3585  CA  ALA D 442      60.377   6.300 -24.287  1.00 27.57           C
ANISOU 3585  CA  ALA D 442     3558   3693   3225    289    658    871    C
ATOM   3586  CB  ALA D 442      60.695   5.663 -22.929  1.00 24.90           C
ANISOU 3586  CB  ALA D 442     3063   3329   3068    217    615    728    C
ATOM   3587  C   ALA D 442      59.104   7.154 -24.217  1.00 27.63           C
ANISOU 3587  C   ALA D 442     3630   3685   3182    404    506    909    C
ATOM   3588  O   ALA D 442      58.109   6.710 -23.648  1.00 27.53           O
ANISOU 3588  O   ALA D 442     3547   3753   3160    452    372    793    O
ATOM   3589  N   LYS D 443      59.122   8.344 -24.818  1.00 29.38           N
ANISOU 3589  N   LYS D 443     3983   3804   3377    452    535   1077    N
ATOM   3590  CA  LYS D 443      57.985   9.293 -24.817  1.00 30.50           C
ANISOU 3590  CA  LYS D 443     4196   3903   3492    591    395   1137    C
ATOM   3591  CB  LYS D 443      58.290  10.528 -25.671  1.00 33.67           C
ANISOU 3591  CB  LYS D 443     4779   4162   3853    630    465   1361    C
ATOM   3592  CG  LYS D 443      59.229  11.526 -25.065  1.00 36.65           C
ANISOU 3592  CG  LYS D 443     5167   4298   4461    529    567   1432    C
ATOM   3593  CD  LYS D 443      59.650  12.550 -26.133  1.00 45.40           C
ANISOU 3593  CD  LYS D 443     6473   5274   5503    538    680   1678    C
ATOM   3594  CE  LYS D 443      60.962  13.265 -25.747  1.00 47.82           C
ANISOU 3594  CE  LYS D 443     6766   5359   6046    363    843   1750    C
ATOM   3595  NZ  LYS D 443      61.530  14.054 -26.889  1.00 50.87           N
ANISOU 3595  NZ  LYS D 443     7337   5634   6356    332   1010   2003    N
ATOM   3596  C   LYS D 443      56.646   8.725 -25.307  1.00 30.23           C
ANISOU 3596  C   LYS D 443     4154   4060   3271    716    235   1077    C
ATOM   3597  O   LYS D 443      55.631   8.934 -24.669  1.00 29.75           O
ANISOU 3597  O   LYS D 443     4018   4015   3270    802    100   1008    O
ATOM   3598  N   VAL D 444      56.638   8.041 -26.453  1.00 30.26           N
ANISOU 3598  N   VAL D 444     4234   4210   3051    726    252   1098    N
ATOM   3599  CA  VAL D 444      55.407   7.466 -26.998  1.00 29.10           C
ANISOU 3599  CA  VAL D 444     4078   4254   2725    825     78   1029    C
ATOM   3600  CB  VAL D 444      55.585   6.963 -28.484  1.00 31.06           C
ANISOU 3600  CB  VAL D 444     4485   4636   2681    840    109   1084    C
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Figure 18 (continued)

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ATOM   3601  CG1 VAL D 444      54.288   6.421 -29.035  1.00 29.96           C
ANISOU 3601  CG1 VAL D 444    4330   4691   2363    934   -109    999       C
ATOM   3602  CG2 VAL D 444      56.115   8.078 -29.394  1.00 30.95           C
ANISOU 3602  CG2 VAL D 444    4684   4520   2557    891    208   1324       C
ATOM   3603  C   VAL D 444      54.875   6.360 -26.079  1.00 27.62           C
ANISOU 3603  C   VAL D 444    3699   4166   2629    768      3    815       C
ATOM   3604  O   VAL D 444      53.680   6.285 -25.819  1.00 27.97           O
ANISOU 3604  O   VAL D 444    3650   4300   2679    844   -156    743       O
ATOM   3605  N   LEU D 445      55.788   5.542 -25.567  1.00 25.93           N
ANISOU 3605  N   LEU D 445    3422   3927   2503    636    126    725       N
ATOM   3606  CA  LEU D 445      55.501   4.447 -24.647  1.00 23.92           C
ANISOU 3606  CA  LEU D 445    3016   3731   2341    563     89    546       C
ATOM   3607  CB  LEU D 445      56.804   3.645 -24.334  1.00 21.91           C
ANISOU 3607  CB  LEU D 445    2738   3423   2166    439    243    496       C
ATOM   3608  CG  LEU D 445      56.751   2.511 -23.313  1.00 20.89           C
ANISOU 3608  CG  LEU D 445    2483   3313   2143    358    226    342       C
ATOM   3609  CD1 LEU D 445      55.801   1.381 -23.778  1.00 20.54           C
ANISOU 3609  CD1 LEU D 445    2418   3414   1973    353    132    220       C
ATOM   3610  CD2 LEU D 445      58.144   1.953 -22.982  1.00 18.80           C
ANISOU 3610  CD2 LEU D 445    2194   2968   1982    270    365    327       C
ATOM   3611  C   LEU D 445      54.862   4.932 -23.354  1.00 23.22           C
ANISOU 3611  C   LEU D 445    2811   3585   2427    587     19    499       C
ATOM   3612  O   LEU D 445      53.820   4.424 -22.965  1.00 24.32           O
ANISOU 3612  O   LEU D 445    2843   3827   2571    605    -83    395       O
ATOM   3613  N   PHE D 446      55.525   5.867 -22.678  1.00 22.66           N
ANISOU 3613  N   PHE D 446    2760   3351   2500    576     85    565       N
ATOM   3614  CA  PHE D 446      55.043   6.489 -21.438  1.00 21.33           C
ANISOU 3614  CA  PHE D 446    2518   3103   2482    609     39    517       C
ATOM   3615  CB  PHE D 446      56.138   7.400 -20.838  1.00 20.56           C
ANISOU 3615  CB  PHE D 446    2473   2806   2534    555    124    577       C
ATOM   3616  CG  PHE D 446      57.229   6.646 -20.076  1.00 19.42           C
ANISOU 3616  CG  PHE D 446    2266   2630   2484    414    198    502       C
ATOM   3617  CD1 PHE D 446      57.332   5.253 -20.143  1.00 17.40           C
ANISOU 3617  CD1 PHE D 446    1945   2496   2168    352    213    418       C
ATOM   3618  CE1 PHE D 446      58.339   4.559 -19.453  1.00 20.22           C
ANISOU 3618  CE1 PHE D 446    2246   2816   2619    249    265    363       C
ATOM   3619  CZ  PHE D 446      59.301   5.271 -18.691  1.00 19.91           C
ANISOU 3619  CZ  PHE D 446    2198   2633   2733    192    291    386       C
ATOM   3620  CE2 PHE D 446      59.217   6.678 -18.646  1.00 19.69           C
ANISOU 3620  CE2 PHE D 446    2236   2480   2765    229    279    458       C
ATOM   3621  CD2 PHE D 446      58.186   7.346 -19.330  1.00 18.60           C
ANISOU 3621  CD2 PHE D 446    2170   2362   2535    345    240    519       C
ATOM   3622  C   PHE D 446      53.719   7.274 -21.629  1.00 22.61           C
ANISOU 3622  C   PHE D 446    2672   3302   2617    769    -82    546       C
ATOM   3623  O   PHE D 446      52.788   7.129 -20.834  1.00 21.26           O
ANISOU 3623  O   PHE D 446    2384   3189   2505    810   -143    444       O
ATOM   3624  N   GLN D 447      53.634   8.092 -22.683  1.00 24.31           N
ANISOU 3624  N   GLN D 447    3009   3485   2743    868   -111    691       N
ATOM   3625  CA  GLN D 447      52.434   8.923 -22.930  1.00 26.58           C
ANISOU 3625  CA  GLN D 447    3294   3792   3015   1051   -242    741       C
ATOM   3626  CB  GLN D 447      52.727  10.052 -23.948  1.00 28.74           C
ANISOU 3626  CB  GLN D 447    3759   3946   3215   1147   -240    948       C
ATOM   3627  CG  GLN D 447      53.822  11.037 -23.521  1.00 28.97           C
ANISOU 3627  CG  GLN D 447    3898   3721   3387   1085   -109   1039       C
ATOM   3628  CD  GLN D 447      53.417  11.958 -22.367  1.00 31.94           C
ANISOU 3628  CD  GLN D 447    4237   3939   3959   1160   -136    984       C
ATOM   3629  OE1 GLN D 447      52.467  11.685 -21.632  1.00 31.98           O
ANISOU 3629  OE1 GLN D 447    4103   4036   4012   1229   -210    849       O
ATOM   3630  NE2 GLN D 447      54.147  13.060 -22.209  1.00 32.72           N
ANISOU 3630  NE2 GLN D 447    4465   3791   4174   1139    -64   1083       N
ATOM   3631  C   GLN D 447      51.172   8.138 -23.353  1.00 27.31           C
ANISOU 3631  C   GLN D 447    3261   4112   3003   1115   -388    657       C
ATOM   3632  O   GLN D 447      50.059   8.620 -23.205  1.00 28.77           O
ANISOU 3632  O   GLN D 447    3359   4341   3230   1259   -502    646       O
ATOM   3633  N   ASN D 448      51.353   6.919 -23.839  1.00 27.07           N
ANISOU 3633  N   ASN D 448    3210   4218   2855   1005   -385    585       N
ATOM   3634  CA  ASN D 448      50.262   6.088 -24.336  1.00 27.76           C
ANISOU 3634  CA  ASN D 448    3189   4515   2844   1027   -531    492       C
ATOM   3635  CB  ASN D 448      50.574   5.642 -25.776  1.00 28.82           C
ANISOU 3635  CB  ASN D 448    3470   4742   2740   1014   -568    545       C
ATOM   3636  CG  ASN D 448      50.346   6.749 -26.784  1.00 28.94           C
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Figure 18 (continued)

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ANISOU 3636  CG  ASN D 448     3635   4738   2623   1181   -656    726  C
ATOM   3637  OD1 ASN D 448      49.218   7.083 -27.082  1.00 31.76       O
ANISOU 3637  OD1 ASN D 448     3924   5192   2950   1320   -840    738  O
ATOM   3638  ND2 ASN D 448      51.414   7.321 -27.300  1.00 26.91       N
ANISOU 3638  ND2 ASN D 448     3577   4353   2295   1168   -523    876  N
ATOM   3639  C   ASN D 448      49.972   4.866 -23.458  1.00 27.61       C
ANISOU 3639  C   ASN D 448     3000   4579   2912    892   -508    312  C
ATOM   3640  O   ASN D 448      49.042   4.091 -23.740  1.00 28.34       O
ANISOU 3640  O   ASN D 448     2973   4834   2960    874   -623    214  O
ATOM   3641  N   TRP D 449      50.740   4.720 -22.378  1.00 26.08       N
ANISOU 3641  N   TRP D 449     2795   4267   2845    793   -369    274  N
ATOM   3642  CA  TRP D 449      50.617   3.569 -21.487  1.00 26.10       C
ANISOU 3642  CA  TRP D 449     2678   4318   2922    661   -326    133  C
ATOM   3643  CB  TRP D 449      51.844   3.464 -20.552  1.00 22.77       C
ANISOU 3643  CB  TRP D 449     2311   3748   2592    562   -183    131  C
ATOM   3644  CG  TRP D 449      51.796   2.288 -19.626  1.00 22.86       C
ANISOU 3644  CG  TRP D 449     2234   3788   2662    436   -140     15  C
ATOM   3645  CD1 TRP D 449      51.346   2.273 -18.330  1.00 19.13       C
ANISOU 3645  CD1 TRP D 449     1674   3305   2290    418   -109    -46  C
ATOM   3646  NE1 TRP D 449      51.479   1.021 -17.799  1.00 18.46       N
ANISOU 3646  NE1 TRP D 449     1555   3239   2218    288    -65   -120  N
ATOM   3647  CE2 TRP D 449      52.025   0.180 -18.738  1.00 19.96       C
ANISOU 3647  CE2 TRP D 449     1806   3444   2335    226    -70   -126  C
ATOM   3648  CD2 TRP D 449      52.254   0.945 -19.905  1.00 22.60       C
ANISOU 3648  CD2 TRP D 449     2219   3784   2585    316   -109    -47  C
ATOM   3649  CE3 TRP D 449      52.810   0.315 -21.036  1.00 22.07       C
ANISOU 3649  CE3 TRP D 449     2239   3740   2407    283   -102    -46  C
ATOM   3650  CZ3 TRP D 449      53.121  -1.038 -20.960  1.00 20.32       C
ANISOU 3650  CZ3 TRP D 449     2018   3518   2186    172    -64   -135  C
ATOM   3651  CH2 TRP D 449      52.904  -1.767 -19.775  1.00 19.50       C
ANISOU 3651  CH2 TRP D 449     1836   3385   2187     86    -36   -201  C
ATOM   3652  CZ2 TRP D 449      52.368  -1.173 -18.652  1.00 19.23       C
ANISOU 3652  CZ2 TRP D 449     1723   3343   2240    108    -34   -191  C
ATOM   3653  C   TRP D 449      49.301   3.488 -20.696  1.00 26.80       C
ANISOU 3653  C   TRP D 449     2575   4500   3107    694   -385     42  C
ATOM   3654  O   TRP D 449      48.820   2.383 -20.387  1.00 28.17       O
ANISOU 3654  O   TRP D 449     2636   4768   3300    585   -389    -67  O
ATOM   3655  N   GLY D 450      48.724   4.626 -20.338  1.00 27.01       N
ANISOU 3655  N   GLY D 450     2562   4494   3209    413    -84    413  N
ATOM   3656  CA  GLY D 450      47.550   4.564 -19.465  1.00 26.85       C
ANISOU 3656  CA  GLY D 450     2343   4561   3298    873   -423    -10  C
ATOM   3657  C   GLY D 450      47.850   5.155 -18.104  1.00 26.36       C
ANISOU 3657  C   GLY D 450     2299   4371   3347    887   -298    -33  C
ATOM   3658  O   GLY D 450      48.936   4.913 -17.524  1.00 24.35       O
ANISOU 3658  O   GLY D 450     2156   4003   3095    777   -201    -34  O
ATOM   3659  N   ILE D 451      46.877   5.919 -17.597  1.00 26.86       N
ANISOU 3659  N   ILE D 451     2250   4457   3500   1030   -308    -60  N
ATOM   3660  CA  ILE D 451      47.001   6.664 -16.348  1.00 26.37       C
ANISOU 3660  CA  ILE D 451     2221   4274   3526   1082   -198    -98  C
ATOM   3661  CB  ILE D 451      46.969   8.237 -16.581  1.00 27.89       C
ANISOU 3661  CB  ILE D 451     2507   4318   3770   1289   -238    -20  C
ATOM   3662  CG1 ILE D 451      47.657   9.008 -15.440  1.00 25.93       C
ANISOU 3662  CG1 ILE D 451     2392   3875   3584   1293   -129    -57  C
ATOM   3663  CD1 ILE D 451      49.176   9.125 -15.584  1.00 21.81       C
ANISOU 3663  CD1 ILE D 451     2069   3187   3030   1167   -106     13  C
ATOM   3664  CG2 ILE D 451      45.544   8.748 -16.801  1.00 27.64       C
ANISOU 3664  CG2 ILE D 451     2298   4397   3809   1490   -315    -36  C
ATOM   3665  C   ILE D 451      45.874   6.181 -15.432  1.00 27.18       C
ANISOU 3665  C   ILE D 451     2116   4514   3696   1077   -132   -215  C
ATOM   3666  O   ILE D 451      44.791   5.803 -15.904  1.00 28.28       O
ANISOU 3666  O   ILE D 451     2060   4822   3862   1110   -204   -243  O
ATOM   3667  N   GLU D 452      46.130   6.140 -14.131  1.00 26.29       N
ANISOU 3667  N   GLU D 452     2042   4341   3606   1022      4   -283  N
ATOM   3668  CA  GLU D 452      45.061   5.692 -13.194  1.00 27.65       C
ANISOU 3668  CA  GLU D 452     2028   4647   3830   1011    109   -385  C
ATOM   3669  CB  GLU D 452      45.256   4.198 -12.798  1.00 26.19       C
ANISOU 3669  CB  GLU D 452     1818   4538   3597    781    176   -418  C
ATOM   3670  CG  GLU D 452      46.647   3.878 -12.149  1.00 24.41       C
ANISOU 3670  CG  GLU D 452     1815   4166   3293    656    231   -398  C
ATOM   3671  CD  GLU D 452      46.830   2.423 -11.743  1.00 24.76       C
ANISOU 3671  CD  GLU D 452     1852   4259   3296    455    291   -414  C
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Figure 18 (continued)

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ATOM   3672  OE1 GLU D 452      45.888   1.618 -11.901  1.00 31.91           O
ANISOU 3672  OE1 GLU D 452    2587   5300   4236    384    309   -448       O
ATOM   3673  OE2 GLU D 452      47.908   2.057 -11.253  1.00 23.36           O
ANISOU 3673  OE2 GLU D 452    1834   3978   3064    366    315   -392       O
ATOM   3674  C   GLU D 452      45.042   6.574 -11.949  1.00 27.37           C
ANISOU 3674  C   GLU D 452    2061   4513   3825   1111    234   -449       C
ATOM   3675  O   GLU D 452      46.052   7.169 -11.604  1.00 26.55           O
ANISOU 3675  O   GLU D 452    2164   4236   3690   1111    242   -433       O
ATOM   3676  N  AHIS D 453      43.898   6.648 -11.278  0.50 29.37           N
ANISOU 3676  N  AHIS D 453    2137   4881   4142   1189    336   -532       N
ATOM   3677  N  BHIS D 453      43.885   6.656 -11.308  0.50 29.06           N
ANISOU 3677  N  BHIS D 453    2095   4843   4104   1192    332   -531       N
ATOM   3678  CA AHIS D 453      43.836   7.247  -9.942  0.50 30.28           C
ANISOU 3678  CA AHIS D 453    2326   4928   4250   1259    493   -622       C
ATOM   3679  CA BHIS D 453      43.774   7.182  -9.955  0.50 29.69           C
ANISOU 3679  CA BHIS D 453    2237   4868   4178   1254    495   -623       C
ATOM   3680  CB AHIS D 453      42.418   7.692  -9.572  0.50 32.76           C
ANISOU 3680  CB AHIS D 453    2411   5367   4670   1432    592   -703       C
ATOM   3681  CB BHIS D 453      42.302   7.269  -9.541  0.50 31.70           C
ANISOU 3681  CB BHIS D 453    2229   5287   4527   1371    609   -705       C
ATOM   3682  CG AHIS D 453      42.349   8.492  -8.302  0.50 34.48           C
ANISOU 3682  CG AHIS D 453    2734   5498   4869   1546    757   -810       C
ATOM   3683  CG BHIS D 453      41.496   8.296 -10.288  0.50 33.06           C
ANISOU 3683  CG BHIS D 453    2263   5469   4828   1622    512   -693       C
ATOM   3684  ND1AHIS D 453      41.699   8.043  -7.170  0.50 37.07           N
ANISOU 3684  ND1AHIS D 453    2974   5946   5164   1508    969   -904       N
ATOM   3685  ND1BHIS D 453      40.830   8.013 -11.463  0.50 33.68           N
ANISOU 3685  ND1BHIS D 453    2135   5683   4978   1653    357   -636       N
ATOM   3686  CE1AHIS D 453      41.803   8.950  -6.214  0.50 37.81           C
ANISOU 3686  CE1AHIS D 453    3219   5928   5219   1638   1082  -1002       C
ATOM   3687  CE1BHIS D 453      40.176   9.092 -11.868  0.50 34.95           C
ANISOU 3687  CE1BHIS D 453    2210   5823   5246   1913    285   -627       C
ATOM   3688  NE2AHIS D 453      42.505   9.967  -6.682  0.50 37.40           N
ANISOU 3688  NE2AHIS D 453    3344   5671   5195   1747    942   -976       N
ATOM   3689  NE2BHIS D 453      40.397  10.065 -11.001  0.50 33.44           N
ANISOU 3689  NE2BHIS D 453    2168   5472   5067   2049    403   -686       N
ATOM   3690  CD2AHIS D 453      42.863   9.704  -7.982  0.50 34.66           C
ANISOU 3690  CD2AHIS D 453    2960   5318   4892   1690    748   -845       C
ATOM   3691  CD2BHIS D 453      41.208   9.589  -9.998  0.50 33.77           C
ANISOU 3691  CD2BHIS D 453    2392   5449   4990   1865    542   -736       C
ATOM   3692  C  AHIS D 453      44.368   6.267  -8.900  0.50 29.31           C
ANISOU 3692  C  AHIS D 453    2300   4818   4018   1058    615   -655       C
ATOM   3693  C  BHIS D 453      44.521   6.231  -8.998  0.50 28.61           C
ANISOU 3693  C  BHIS D 453    2231   4715   3923   1044    596   -643       C
ATOM   3694  O  AHIS D 453      44.077   5.067  -8.933  0.50 29.41           O
ANISOU 3694  O  AHIS D 453    2203   4957   4013    899    649   -643       O
ATOM   3695  O  BHIS D 453      44.536   5.005  -9.196  0.50 27.91           O
ANISOU 3695  O  BHIS D 453    2079   4722   3805    868    596   -612       O
ATOM   3696  N    ILE D 454      45.164   6.783  -7.978  1.00 28.76           N
ANISOU 3696  N    ILE D 454    2449   4605   3874   1063    667   -695       N
ATOM   3697  CA   ILE D 454      45.777   5.937  -6.964  1.00 28.13           C
ANISOU 3697  CA   ILE D 454    2498   4524   3669    893    751   -712       C
ATOM   3698  CB   ILE D 454      47.332   5.999  -7.018  1.00 26.26           C
ANISOU 3698  CB   ILE D 454    2490   4116   3371    803    634   -662       C
ATOM   3699  CG1  ILE D 454      47.890   7.250  -6.344  1.00 24.68           C
ANISOU 3699  CG1  ILE D 454    2478   3746   3152    906    625   -733       C
ATOM   3700  CD1  ILE D 454      49.392   7.303  -6.398  1.00 25.66           C
ANISOU 3700  CD1  ILE D 454    2783   3717   3249    801    503   -689       C
ATOM   3701  CG2  ILE D 454      47.826   5.855  -8.457  1.00 23.15           C
ANISOU 3701  CG2  ILE D 454    2062   3692   3042    772    483   -559       C
ATOM   3702  C    ILE D 454      45.222   6.230  -5.576  1.00 30.71           C
ANISOU 3702  C    ILE D 454    2860   4884   3925    953    938   -822       C
ATOM   3703  O    ILE D 454      44.661   7.306  -5.345  1.00 32.07           O
ANISOU 3703  O    ILE D 454    3011   5025   4150   1141    991   -901       O
ATOM   3704  N    ASP D 455      45.333   5.234  -4.691  1.00 32.26           N
ANISOU 3704  N    ASP D 455    3111   5146   4000   1047   1047   -821       N
ATOM   3705  CA   ASP D 455      45.106   5.380  -3.250  1.00 34.47           C
ANISOU 3705  CA   ASP D 455    3507   5446   4142    822   1227   -911       C
ATOM   3706  CB   ASP D 455      44.729   4.030  -2.628  1.00 35.56           C
ANISOU 3706  CB   ASP D 455    3602   5719   4189    648   1374   -865       C
ATOM   3707  CG   ASP D 455      43.446   3.430  -3.228  1.00 39.76           C
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Figure 18 (continued)

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ANISOU 3707  CG  ASP D 455     3816   6426   4866    618   1465   -844       C
ATOM   3708  OD1 ASP D 455      42.493   4.181  -3.532  1.00 42.46           O
ANISOU 3708  OD1 ASP D 455     3961   6837   5333    779   1511   -908       O
ATOM   3709  OD2 ASP D 455      43.394   2.189  -3.401  1.00 44.22           O
ANISOU 3709  OD2 ASP D 455     4320   7051   5432    431   1479   -765       O
ATOM   3710  C   ASP D 455      46.372   5.899  -2.568  1.00 34.03           C
ANISOU 3710  C   ASP D 455     3751   5221   3959    814   1139   -945       C
ATOM   3711  O   ASP D 455      47.494   5.599  -2.992  1.00 31.59           O
ANISOU 3711  O   ASP D 455     3543   4815   3646    712    975   -870       O
ATOM   3712  N   ASN D 456      46.191   6.679  -1.505  1.00 36.31           N
ANISOU 3712  N   ASN D 456     4174   5475   4146    921   1248  -1069       N
ATOM   3713  CA  ASN D 456      47.306   7.068  -0.637  1.00 36.72           C
ANISOU 3713  CA  ASN D 456     4519   5389   4046    891   1168  -1127       C
ATOM   3714  CB  ASN D 456      46.871   8.172   0.341  1.00 39.40           C
ANISOU 3714  CB  ASN D 456     4986   5683   4301   1056   1292  -1302       C
ATOM   3715  CG  ASN D 456      46.475   9.447  -0.357  1.00 40.47           C
ANISOU 3715  CG  ASN D 456     5043   5708   4625   1250   1255  -1367       C
ATOM   3716  OD1 ASN D 456      47.200   9.934  -1.227  1.00 42.70           O
ANISOU 3716  OD1 ASN D 456     5348   5842   5034   1246   1067  -1312       O
ATOM   3717  ND2 ASN D 456      45.322   9.995   0.010  1.00 40.50           N
ANISOU 3717  ND2 ASN D 456     4954   5779   4655   1427   1445  -1475       N
ATOM   3718  C   ASN D 456      47.813   5.870   0.159  1.00 36.38           C
ANISOU 3718  C   ASN D 456     4600   5409   3814    717   1191  -1062       C
ATOM   3719  O   ASN D 456      47.117   5.374   1.047  1.00 39.46           O
ANISOU 3719  O   ASN D 456     5005   5924   4065    698   1387  -1084       O
ATOM   3720  N   VAL D 457      49.004   5.398  -0.170  1.00 34.18           N
ANISOU 3720  N   VAL D 457     4405   5046   3536    597   1001   -974       N
ATOM   3721  CA  VAL D 457      49.676   4.338   0.582  1.00 33.74           C
ANISOU 3721  CA  VAL D 457     4497   5014   3310    455    975   -903       C
ATOM   3722  CB  VAL D 457      49.883   3.059  -0.286  1.00 32.28           C
ANISOU 3722  CB  VAL D 457     4179   4866   3220    319    921   -748       C
ATOM   3723  CG1 VAL D 457      50.617   1.967   0.500  1.00 32.61           C
ANISOU 3723  CG1 VAL D 457     4387   4904   3098    195    883   -661       C
ATOM   3724  CG2 VAL D 457      48.541   2.522  -0.807  1.00 33.51           C
ANISOU 3724  CG2 VAL D 457     4097   5162   3471    308   1091   -717       C
ATOM   3725  C   VAL D 457      51.031   4.904   1.032  1.00 32.68           C
ANISOU 3725  C   VAL D 457     4580   4731   3105    444    773   -949       C
ATOM   3726  O   VAL D 457      51.822   5.334   0.185  1.00 30.77           O
ANISOU 3726  O   VAL D 457     4297   4375   3018    437    604   -926       O
ATOM   3727  N   MSE D 458      51.279   4.935   2.348  1.00 33.57           N
ANISOU 3727  N   MSE D 458     4921   4852   2984    440    792  -1018       N
ATOM   3728  CA  MSE D 458      52.542   5.460   2.892  1.00 33.03           C
ANISOU 3728  CA  MSE D 458     5058   4656   2837    420    576  -1082       C
ATOM   3729  CB  MSE D 458      52.509   5.541   4.421  1.00 35.52           C
ANISOU 3729  CB  MSE D 458     5638   5013   2845    439    627  -1182       C
ATOM   3730  CG  MSE D 458      53.711   6.288   5.016  1.00 34.66           C
ANISOU 3730  CG  MSE D 458     5739   4772   2659    428    383  -1294       C
ATOM   3731  SE  MSE D 458      53.851   6.197   6.940  0.90 39.03          SE
ANISOU 3731  SE  MSE D 458     6670   5394   2765    437    388  -1406       SE
ATOM   3732  CE  MSE D 458      55.169   7.548   7.238  1.00 40.64           C
ANISOU 3732  CE  MSE D 458     7044   5395   3003    434     59  -1605       C
ATOM   3733  C   MSE D 458      53.711   4.597   2.449  1.00 31.60           C
ANISOU 3733  C   MSE D 458     4852   4434   2721    297    378   -943       C
ATOM   3734  O   MSE D 458      53.591   3.367   2.390  1.00 31.80           O
ANISOU 3734  O   MSE D 458     4832   4541   2711    221    428   -811       O
ATOM   3735  N   GLY D 459      54.833   5.231   2.119  1.00 30.97           N
ANISOU 3735  N   GLY D 459     4791   4220   2755    277    165   -973       N
ATOM   3736  CA  GLY D 459      56.032   4.514   1.643  1.00 29.96           C
ANISOU 3736  CA  GLY D 459     4609   4050   2725    178    -21   -853       C
ATOM   3737  C   GLY D 459      56.149   4.354   0.118  1.00 28.53           C
ANISOU 3737  C   GLY D 459     4203   3839   2800    157   -25   -754       C
ATOM   3738  O   GLY D 459      57.067   3.695  -0.379  1.00 27.21           O
ANISOU 3738  O   GLY D 459     3968   3645   2726     88   -141   -656       O
ATOM   3739  N   MSE D 460      55.240   4.983  -0.620  1.00 28.31           N
ANISOU 3739  N   MSE D 460     4064   3815   2879    230    96   -784       N
ATOM   3740  CA  MSE D 460      55.042   4.734  -2.044  1.00 28.35           C
ANISOU 3740  CA  MSE D 460     3874   3830   3069    225    124   -688       C
ATOM   3741  CB  MSE D 460      54.078   3.573  -2.174  1.00 27.77           C
ANISOU 3741  CB  MSE D 460     3709   3898   2944    200    267   -617       C
ATOM   3742  CG  MSE D 460      54.112   2.810  -3.436  1.00 30.07           C
ANISOU 3742  CG  MSE D 460     3842   4216   3368    152    259   -511       C
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Figure 18 (continued)

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ATOM   3743 SE   MSE D 460      52.689   1.457  -3.282  0.90 33.52          SE
ANISOU 3743 SE   MSE D 460    4185   4819   3732    100    451   -464      SE
ATOM   3744  CE  MSE D 460      53.605   0.285  -1.992  1.00 34.15           C
ANISOU 3744  CE  MSE D 460    4467   4874   3636     -1    401   -395      C
ATOM   3745  C   MSE D 460      54.378   5.961  -2.667  1.00 26.69           C
ANISOU 3745  C   MSE D 460    3605   3566   2972    333    177   -750      C
ATOM   3746  O   MSE D 460      53.553   6.615  -2.027  1.00 27.88           O
ANISOU 3746  O   MSE D 460    3813   3730   3051    427    275   -855      O
ATOM   3747  N   VAL D 461      54.750   6.277  -3.901  1.00 24.21           N
ANISOU 3747  N   VAL D 461    3187   3185   2826    331    120   -682      N
ATOM   3748  CA  VAL D 461      54.111   7.350  -4.657  1.00 23.60           C
ANISOU 3748  CA  VAL D 461    3055   3051   2861    443    159   -701      C
ATOM   3749  CB  VAL D 461      54.973   8.683  -4.716  1.00 24.29           C
ANISOU 3749  CB  VAL D 461    3246   2931   3053    454     54   -748      C
ATOM   3750  CG1 VAL D 461      54.919   9.441  -3.418  1.00 26.49           C
ANISOU 3750  CG1 VAL D 461    3693   3135   3236    497     49   -907      C
ATOM   3751  CG2 VAL D 461      56.409   8.417  -5.145  1.00 21.55           C
ANISOU 3751  CG2 VAL D 461    2887   2510   2790    322    -73   -669      C
ATOM   3752  C   VAL D 461      53.857   6.895  -6.082  1.00 21.54           C
ANISOU 3752  C   VAL D 461    2635   2848   2701    440    169   -582      C
ATOM   3753  O   VAL D 461      54.504   5.950  -6.569  1.00 20.30           O
ANISOU 3753  O   VAL D 461    2431   2727   2556    340    127   -497      O
ATOM   3754  N   GLY D 462      52.960   7.610  -6.757  1.00 21.64           N
ANISOU 3754  N   GLY D 462    2577   2862   2782    561    213   -581      N
ATOM   3755  CA  GLY D 462      52.766   7.470  -8.213  1.00 20.05           C
ANISOU 3755  CA  GLY D 462    2259   2696   2664    580    191   -472      C
ATOM   3756  C   GLY D 462      53.780   8.244  -9.042  1.00 19.20           C
ANISOU 3756  C   GLY D 462    2210   2429   2656    563    109   -399      C
ATOM   3757  O   GLY D 462      54.540   9.061  -8.544  1.00 19.52           O
ANISOU 3757  O   GLY D 462    2363   2313   2739    543     65   -439      O
ATOM   3758  N   VAL D 463      53.780   8.004 -10.337  1.00 18.47           N
ANISOU 3758  N   VAL D 463    2045   2375   2599    563     93   -292      N
ATOM   3759  CA  VAL D 463      54.761   8.620 -11.196  1.00 18.33           C
ANISOU 3759  CA  VAL D 463    2080   2223   2662    531     49   -199      C
ATOM   3760  CB  VAL D 463      56.088   7.738 -11.343  1.00 18.13           C
ANISOU 3760  CB  VAL D 463    2045   2200   2645    374     27   -152      C
ATOM   3761  CG1 VAL D 463      55.844   6.407 -12.051  1.00 15.46           C
ANISOU 3761  CG1 VAL D 463    1612   2021   2239    337     52   -108      C
ATOM   3762  CG2 VAL D 463      57.144   8.490 -12.103  1.00 18.20           C
ANISOU 3762  CG2 VAL D 463    2096   2063   2755    329     12    -63      C
ATOM   3763  C   VAL D 463      54.076   8.889 -12.517  1.00 18.79           C
ANISOU 3763  C   VAL D 463    2091   2324   2726    630     47   -103      C
ATOM   3764  O   VAL D 463      53.343   8.039 -13.061  1.00 18.59           O
ANISOU 3764  O   VAL D 463    1963   2463   2636    645     53    -87      O
ATOM   3765  N   LEU D 464      54.245  10.107 -12.999  1.00 19.85           N
ANISOU 3765  N   LEU D 464    2307   2300   2934    701     29    -42      N
ATOM   3766  CA  LEU D 464      53.639  10.532 -14.258  1.00 20.22           C
ANISOU 3766  CA  LEU D 464    2344   2365   2972    816      9     71      C
ATOM   3767  CB  LEU D 464      53.298  12.015 -14.196  1.00 21.24           C
ANISOU 3767  CB  LEU D 464    2572   2308   3190    958     -6     86      C
ATOM   3768  CG  LEU D 464      52.392  12.555 -13.082  1.00 21.78           C
ANISOU 3768  CG  LEU D 464    2634   2349   3293   1085     11    -55      C
ATOM   3769  CD1 LEU D 464      52.192  14.033 -13.307  1.00 21.48           C
ANISOU 3769  CD1 LEU D 464    2714   2089   3357   1234     -8    -13      C
ATOM   3770  CD2 LEU D 464      51.033  11.835 -13.039  1.00 19.48           C
ANISOU 3770  CD2 LEU D 464    2173   2290   2938   1184     22   -109      C
ATOM   3771  C   LEU D 464      54.600  10.221 -15.434  1.00 20.13           C
ANISOU 3771  C   LEU D 464    2363   2346   2938    720     16    205      C
ATOM   3772  O   LEU D 464      55.774   9.957 -15.215  1.00 19.34           O
ANISOU 3772  O   LEU D 464    2286   2186   2877    580     42    209      O
ATOM   3773  N   PRO D 465      54.096  10.203 -16.684  1.00 21.70           N
ANISOU 3773  N   PRO D 465    2556   2622   3065    799     -8    311      N
ATOM   3774  CA  PRO D 465      54.985   9.992 -17.845  1.00 22.57           C
ANISOU 3774  CA  PRO D 465    2723   2726   3126    722     25    440      C
ATOM   3775  CB  PRO D 465      54.069  10.254 -19.037  1.00 23.86           C
ANISOU 3775  CB  PRO D 465    2910   2970   3187    865     -34    540      C
ATOM   3776  CG  PRO D 465      52.699   9.890 -18.550  1.00 23.05           C
ANISOU 3776  CG  PRO D 465    2677   3013   3067    968   -105    429      C
ATOM   3777  CD  PRO D 465      52.675  10.307 -17.092  1.00 22.87           C
ANISOU 3777  CD  PRO D 465    2637   2889   3164    965    -71    311      C
ATOM   3778  C   PRO D 465      56.248  10.874 -17.928  1.00 25.04           C
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Figure 18 (continued)

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ANISOU 3778  C   PRO D 465     3145   2825   3544    637     84    529    C
ATOM   3779  O   PRO D 465      57.278  10.395 -18.414  1.00 25.30         O
ANISOU 3779  O   PRO D 465     3176   2867   3570    517    149    583    O
ATOM   3780  N   ASP D 466      56.170  12.133 -17.480  1.00 26.78         N
ANISOU 3780  N   ASP D 466     3452   2849   3874    696     69    538    N
ATOM   3781  CA  ASP D 466      57.344  13.009 -17.382  1.00 28.69         C
ANISOU 3781  CA  ASP D 466     3786   2862   4253    586    117    599    C
ATOM   3782  CB  ASP D 466      56.953  14.498 -17.491  1.00 31.09         C
ANISOU 3782  CB  ASP D 466     4230   2938   4643    702     98    670    C
ATOM   3783  CG  ASP D 466      56.078  14.998 -16.330  1.00 32.24         C
ANISOU 3783  CG  ASP D 466     4380   3024   4845    822     37    512    C
ATOM   3784  OD1 ASP D 466      55.823  14.292 -15.330  1.00 30.53         O
ANISOU 3784  OD1 ASP D 466     4070   2932   4599    800     19    349    O
ATOM   3785  OD2 ASP D 466      55.642  16.161 -16.413  1.00 38.19         O
ANISOU 3785  OD2 ASP D 466     5248   3591   5673    948     19    556    O
ATOM   3786  C   ASP D 466      58.190  12.757 -16.130  1.00 28.75         C
ANISOU 3786  C   ASP D 466     3742   2819   4363    442    111    460    C
ATOM   3787  O   ASP D 466      59.120  13.523 -15.851  1.00 29.86         O
ANISOU 3787  O   ASP D 466     3937   2764   4644    338    125    475    O
ATOM   3788  N   MSE D 467      57.871  11.674 -15.404  1.00 27.82         N
ANISOU 3788  N   MSE D 467     3523   2874   4173    430     82    334    N
ATOM   3789  CA  MSE D 467      58.653  11.191 -14.238  1.00 27.18         C
ANISOU 3789  CA  MSE D 467     3395   2788   4144    304     55    213    C
ATOM   3790  CB  MSE D 467      60.143  11.016 -14.581  1.00 27.16         C
ANISOU 3790  CB  MSE D 467     3352   2728   4238    142     90    280    C
ATOM   3791  CG  MSE D 467      60.473   9.801 -15.486  1.00 26.75         C
ANISOU 3791  CG  MSE D 467     3210   2847   4106    108    154    349    C
ATOM   3792  SE  MSE D 467      59.696   8.138 -14.902  0.90 30.05        SE
ANISOU 3792  SE  MSE D 467     3540   3499   4378    144    116    232    SE
ATOM   3793  CE  MSE D 467      60.578   8.025 -13.137  1.00 28.88         C
ANISOU 3793  CE  MSE D 467     3369   3279   4325     39     26    100    C
ATOM   3794  C   MSE D 467      58.470  12.021 -12.971  1.00 27.94         C
ANISOU 3794  C   MSE D 467     3565   2749   4304    327     -1     81    C
ATOM   3795  O   MSE D 467      59.154  11.804 -11.978  1.00 28.10         O
ANISOU 3795  O   MSE D 467     3577   2745   4357    227    -48    -18    O
ATOM   3796  N   THR D 468      57.548  12.977 -13.020  1.00 28.97         N
ANISOU 3796  N   THR D 468     3776   2788   4443    470     -3     77    N
ATOM   3797  CA  THR D 468      57.137  13.732 -11.838  1.00 30.36         C
ANISOU 3797  CA  THR D 468     4035   2848   4652    533    -37    -73    C
ATOM   3798  CB  THR D 468      56.270  14.949 -12.237  1.00 32.44         C
ANISOU 3798  CB  THR D 468     4395   2963   4969    710    -26    -37    C
ATOM   3799  OG1 THR D 468      57.079  15.883 -12.965  1.00 35.37         O
ANISOU 3799  OG1 THR D 468     4863   3109   5468    645    -20     91    O
ATOM   3800  CG2 THR D 468      55.697  15.678 -11.014  1.00 36.00         C
ANISOU 3800  CG2 THR D 468     4932   3304   5441    809    -40   -217    C
ATOM   3801  C   THR D 468      56.377  12.807 -10.868  1.00 28.96         C
ANISOU 3801  C   THR D 468     3791   2867   4345    575    -35   -208    C
ATOM   3802  O   THR D 468      55.453  12.082 -11.295  1.00 27.88         O
ANISOU 3802  O   THR D 468     3558   2917   4118    657     -2   -178    O
ATOM   3803  N   PRO D 469      56.760  12.819  -9.568  1.00 28.78         N
ANISOU 3803  N   PRO D 469     3824   2804   4307    512    -72   -354    N
ATOM   3804  CA  PRO D 469      56.011  12.034  -8.581  1.00 28.00         C
ANISOU 3804  CA  PRO D 469     3694   2876   4068    554    -47   -469    C
ATOM   3805  CB  PRO D 469      56.847  12.161  -7.306  1.00 28.47         C
ANISOU 3805  CB  PRO D 469     3854   2854   4107    451   -118   -600    C
ATOM   3806  CG  PRO D 469      57.615  13.422  -7.471  1.00 30.60         C
ANISOU 3806  CG  PRO D 469     4223   2871   4532    407   -176   -605    C
ATOM   3807  CD  PRO D 469      57.864  13.578  -8.946  1.00 30.30         C
ANISOU 3807  CD  PRO D 469     4118   2793   4602    395   -144   -421    C
ATOM   3808  C   PRO D 469      54.628  12.624  -8.344  1.00 28.95         C
ANISOU 3808  C   PRO D 469     3830   3009   4161     18   -541    C
ATOM   3809  O   PRO D 469      54.422  13.821  -8.471  1.00 31.03         O
ANISOU 3809  O   PRO D 469     4181   3092   4515    846     15   -558    O
ATOM   3810  N   SER D 470      53.680  11.773  -8.007  1.00 28.12         N
ANISOU 3810  N   SER D 470     3630   3107   3946    799     84   -579    N
ATOM   3811  CA  SER D 470      52.325  12.211  -7.789  1.00 28.32         C
ANISOU 3811  CA  SER D 470     3619   3181   3962    984    162   -647    C
ATOM   3812  CB  SER D 470      51.519  12.098  -9.070  1.00 27.33         C
ANISOU 3812  CB  SER D 470     3351   3150   3883   1084    164   -524    C
ATOM   3813  OG  SER D 470      50.209  12.579  -8.834  1.00 30.16         O
ANISOU 3813  OG  SER D 470     3644   3556   4261   1280    230   -595    O
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Figure 18 (continued)

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ATOM   3814  C   SER D 470      51.727  11.317  -6.739  1.00 28.11           C
ANISOU 3814  C   SER D 470    3546   3336   3798    967    247   -746        C
ATOM   3815  O   SER D 470      51.955  10.097  -6.738  1.00 26.67           O
ANISOU 3815  O   SER D 470    3294   3298   3541    842    249   -697        O
ATOM   3816  N   THR D 471      50.970  11.922  -5.847  1.00 29.88           N
ANISOU 3816  N   THR D 471    3821   3542   3989   1095    330   -882        N
ATOM   3817  CA  THR D 471      50.235  11.190  -4.825  1.00 31.76           C
ANISOU 3817  CA  THR D 471    4022   3958   4090   1099    454   -973        C
ATOM   3818  CB  THR D 471      50.322  11.895  -3.438  1.00 34.06           C
ANISOU 3818  CB  THR D 471    4508   4151   4283   1147    504  -1155        C
ATOM   3819  OG1 THR D 471      49.928  13.268  -3.563  1.00 36.80           O
ANISOU 3819  OG1 THR D 471    4916   4323   4743   1327    515  -1233        O
ATOM   3820  CG2 THR D 471      51.762  11.842  -2.895  1.00 34.68           C
ANISOU 3820  CG2 THR D 471    4765   4112   4299    980    369  -1177        C
ATOM   3821  C   THR D 471      48.769  10.996  -5.221  1.00 32.22           C
ANISOU 3821  C   THR D 471    3872   4182   4189   1237    567   -962        C
ATOM   3822  O   THR D 471      47.976  10.500  -4.422  1.00 33.96           O
ANISOU 3822  O   THR D 471    4032   4552   4321   1256    707  -1035        O
ATOM   3823  N   GLU D 472      48.430  11.356  -6.463  1.00 31.70           N
ANISOU 3823  N   GLU D 472    3692   4098   4254   1325    502   -862        N
ATOM   3824  CA  GLU D 472      47.035  11.363  -6.926  1.00 32.30           C
ANISOU 3824  CA  GLU D 472    3552   4318   4400   1483    566   -856        C
ATOM   3825  CB  GLU D 472      46.564  12.792  -7.215  1.00 34.20           C
ANISOU 3825  CB  GLU D 472    3825   4402   4768   1721    548   -885        C
ATOM   3826  CG  GLU D 472      46.472  13.710  -6.001  1.00 39.23           C
ANISOU 3826  CG  GLU D 472    4619   4902   5385   1834    650  -1059        C
ATOM   3827  CD  GLU D 472      47.149  15.074  -6.249  1.00 44.76           C
ANISOU 3827  CD  GLU D 472    5528   5294   6185   1917    554  -1063        C
ATOM   3828  OE1 GLU D 472      46.462  16.121  -6.201  1.00 47.87           O
ANISOU 3828  OE1 GLU D 472    5937   5570   6681   2147    593  -1130        O
ATOM   3829  OE2 GLU D 472      48.384  15.090  -6.500  1.00 45.99           O
ANISOU 3829  OE2 GLU D 472    5826   5316   6333   1749    444   -998        O
ATOM   3830  C   GLU D 472      46.839  10.501  -8.164  1.00 29.96           C
ANISOU 3830  C   GLU D 472    3083   4165   4136   1413    484   -717        C
ATOM   3831  O   GLU D 472      45.842   9.804  -8.275  1.00 29.57           O
ANISOU 3831  O   GLU D 472    2827   4313   4094   1424    541   -722        O
ATOM   3832  N   MSE D 473      47.796  10.559  -9.100  1.00 28.19           N
ANISOU 3832  N   MSE D 473    2943   3839   3930   1336    355   -601        N
ATOM   3833  CA  MSE D 473      47.703   9.800 -10.341  1.00 26.31           C
ANISOU 3833  CA  MSE D 473    2581   3719   3695   1276    272   -481        C
ATOM   3834  CB  MSE D 473      47.452  10.726 -11.552  1.00 27.81           C
ANISOU 3834  CB  MSE D 473    2766   3834   3967   1434    167   -380        C
ATOM   3835  CG  MSE D 473      46.264  11.657 -11.443  1.00 26.21           C
ANISOU 3835  CG  MSE D 473    2472   3630   3858   1680    188   -429        C
ATOM   3836 SE   MSE D 473      44.516  10.785 -11.482  0.90 29.78          SE
ANISOU 3836 SE   MSE D 473    2569   4404   4342   1752    231   -487        SE
ATOM   3837  CE  MSE D 473      44.552  10.081 -13.324  1.00 24.55           C
ANISOU 3837  CE  MSE D 473    1821   3865   3642   1686     30   -325        C
ATOM   3838  C   MSE D 473      48.978   9.045 -10.570  1.00 24.24           C
ANISOU 3838  C   MSE D 473    2418   3421   3371   1074    225   -417        C
ATOM   3839  O   MSE D 473      50.039   9.420 -10.051  1.00 23.22           O
ANISOU 3839  O   MSE D 473    2450   3138   3233   1006    216   -432        O
ATOM   3840  N   SER D 474      48.890   8.004 -11.387  1.00 22.74           N
ANISOU 3840  N   SER D 474    2125   3368   3148    983    187   -352        N
ATOM   3841  CA  SER D 474      50.092   7.287 -11.803  1.00 20.80           C
ANISOU 3841  CA  SER D 474    1959   3086   2859    820    146   -285        C
ATOM   3842  CB  SER D 474      50.489   6.264 -10.751  1.00 19.28           C
ANISOU 3842  CB  SER D 474    1787   2935   2604    675    208   -343        C
ATOM   3843  OG  SER D 474      51.820   5.854 -10.984  1.00 16.43           O
ANISOU 3843  OG  SER D 474    1518   2493   2230    553    164   -287        O
ATOM   3844  C   SER D 474      49.928   6.603 -13.137  1.00 20.73           C
ANISOU 3844  C   SER D 474    1868   3182   2825    789     81   -205        C
ATOM   3845  O   SER D 474      48.821   6.295 -13.530  1.00 21.95           O
ANISOU 3845  O   SER D 474    1877   3482   2983    843     62   -221        O
ATOM   3846  N   MSE D 475      51.037   6.376 -13.838  1.00 20.98           N
ANISOU 3846  N   MSE D 475    1989   3147   2833    702     46   -127        N
ATOM   3847  CA  MSE D 475      51.056   5.443 -14.964  1.00 21.48           C
ANISOU 3847  CA  MSE D 475    2006   3317   2838    639      5    -80        C
ATOM   3848  CB  MSE D 475      52.472   5.270 -15.530  1.00 19.83           C
ANISOU 3848  CB  MSE D 475    1910   3013   2612    548     10     -6        C
ATOM   3849  CG  MSE D 475      52.894   6.455 -16.381  1.00 20.37           C
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Figure 18 (continued)

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ANISOU 3849  CG  MSE D 475     2076   2969   2696    631    -15    102   C
ATOM   3850 SE   MSE D 475      54.525   6.239 -17.395  0.90 22.90        SE
ANISOU 3850 SE   MSE D 475     2500   3209   2992    523     29    211   SE
ATOM   3851  CE  MSE D 475      55.763   6.073 -15.923  1.00 15.43         C
ANISOU 3851  CE  MSE D 475     1566   2140   2155    395     75    144   C
ATOM   3852  C   MSE D 475      50.505   4.108 -14.458  1.00 21.28         C
ANISOU 3852  C   MSE D 475     1873   3425   2786    535     40   -159   C
ATOM   3853  O   MSE D 475      50.898   3.647 -13.399  1.00 20.98         O
ANISOU 3853  O   MSE D 475     1867   3355   2749    451    102   -203   O
ATOM   3854  N   ARG D 476      49.570   3.531 -15.206  1.00 22.47         N
ANISOU 3854  N   ARG D 476     1904   3721   2914    539     -9   -173   N
ATOM   3855  CA  ARG D 476      48.834   2.320 -14.818  1.00 22.84         C
ANISOU 3855  CA  ARG D 476     1826   3891   2961    432     23   -248   C
ATOM   3856  CB  ARG D 476      47.933   1.869 -15.985  1.00 23.67         C
ANISOU 3856  CB  ARG D 476     1807   4140   3046    439    -79   -261   C
ATOM   3857  CG  ARG D 476      47.287   0.475 -15.783  1.00 27.51         C
ANISOU 3857  CG  ARG D 476     2172   4732   3549    284    -56   -339   C
ATOM   3858  CD  ARG D 476      46.787  -0.218 -17.071  1.00 27.82         C
ANISOU 3858  CD  ARG D 476     2140   4882   3546    238   -183   -369   C
ATOM   3859  NE  ARG D 476      47.530   0.020 -18.335  1.00 32.26         N
ANISOU 3859  NE  ARG D 476     2845   5411   4002    288   -273   -313   N
ATOM   3860  CZ  ARG D 476      48.407  -0.822 -18.879  1.00 31.84         C
ANISOU 3860  CZ  ARG D 476     2916   5306   3876    190   -263   -319   C
ATOM   3861  NH1 ARG D 476      48.759  -1.946 -18.240  1.00 32.87         N
ANISOU 3861  NH1 ARG D 476     3064   5384   4042     43   -180   -370   N
ATOM   3862  NH2 ARG D 476      48.962  -0.521 -20.040  1.00 28.92         N
ANISOU 3862  NH2 ARG D 476     2666   4927   3395    249   -323   -268   N
ATOM   3863  C   ARG D 476      49.715   1.168 -14.282  1.00 20.44         C
ANISOU 3863  C   ARG D 476     1601   3533   2632    271     84   -261   C
ATOM   3864  O   ARG D 476      50.603   0.659 -14.985  1.00 19.53         O
ANISOU 3864  O   ARG D 476     1567   3372   2481    213     57   -227   O
ATOM   3865  N   GLY D 477      49.476   0.777 -13.028  1.00 20.13         N
ANISOU 3865  N   GLY D 477     1544   3497   2606    212    174   -303   N
ATOM   3866  CA  GLY D 477      50.241  -0.307 -12.377  1.00 19.10         C
ANISOU 3866  CA  GLY D 477     1500   3308   2451     77    223   -300   C
ATOM   3867  C   GLY D 477      51.654   0.032 -11.943  1.00 18.37         C
ANISOU 3867  C   GLY D 477     1558   3076   2345     81    215   -259   C
ATOM   3868  O   GLY D 477      52.351  -0.837 -11.447  1.00 18.98         O
ANISOU 3868  O   GLY D 477     1702   3100   2407     -7    233   -246   O
ATOM   3869  N   ILE D 478      52.094   1.285 -12.110  1.00 18.42         N
ANISOU 3869  N   ILE D 478     1614   3013   2371    179    180   -235   N
ATOM   3870  CA  ILE D 478      53.467   1.698 -11.747  1.00 17.40         C
ANISOU 3870  CA  ILE D 478     1602   2752   2259    167    158   -203   C
ATOM   3871  CB  ILE D 478      54.167   2.509 -12.862  1.00 17.64         C
ANISOU 3871  CB  ILE D 478     1662   2712   2328    215    115   -140   C
ATOM   3872  CG1 ILE D 478      53.884   1.926 -14.282  1.00 18.18         C
ANISOU 3872  CG1 ILE D 478     1682   2862   2363    211     98   -108   C
ATOM   3873  CD1 ILE D 478      54.456   0.525 -14.545  1.00 17.82         C
ANISOU 3873  CD1 ILE D 478     1642   2831   2299    109    115   -115   C
ATOM   3874  CG2 ILE D 478      55.699   2.688 -12.556  1.00 16.84         C
ANISOU 3874  CG2 ILE D 478     1638   2484   2276    163     98   -107   C
ATOM   3875  C   ILE D 478      53.516   2.522 -10.450  1.00 18.27         C
ANISOU 3875  C   ILE D 478     1780   2801   2362    205   -248   C
ATOM   3876  O   ILE D 478      52.759   3.501 -10.278  1.00 19.57         O
ANISOU 3876  O   ILE D 478     1928   2971   2538    304    192   -284   O
ATOM   3877  N   ARG D 479      54.407   2.131  -9.538  1.00 17.66         N
ANISOU 3877  N   ARG D 479     1785   2662   2261    138    160   -252   N
ATOM   3878  CA  ARG D 479      54.620   2.867  -8.297  1.00 18.17         C
ANISOU 3878  CA  ARG D 479     1947   2665   2291    163    152   -308   C
ATOM   3879  CB  ARG D 479      53.947   2.147  -7.108  1.00 19.25         C
ANISOU 3879  CB  ARG D 479     2115   2880   2318    131    225   -348   C
ATOM   3880  CG  ARG D 479      52.436   1.937  -7.217  1.00 19.34         C
ANISOU 3880  CG  ARG D 479     2015   3018   2313    163    334   -376   C
ATOM   3881  CD  ARG D 479      51.652   3.264  -7.152  1.00 22.05         C
ANISOU 3881  CD  ARG D 479     2332   3364   2683    298    368   -442   C
ATOM   3882  NE  ARG D 479      50.213   3.019  -7.118  1.00 23.03         N
ANISOU 3882  NE  ARG D 479     2316   3626   2807    332    477   -475   N
ATOM   3883  CZ  ARG D 479      49.448   2.766  -8.182  1.00 24.23         C
ANISOU 3883  CZ  ARG D 479     2306   3868   3033    347    466   -451   C
ATOM   3884  NH1 ARG D 479      49.944   2.768  -9.423  1.00 22.96         N
ANISOU 3884  NH1 ARG D 479     2127   3672   2923    344    360   -392   N
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Figure 18 (continued)

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ATOM   3885  NH2 ARG D 479      48.161   2.542  -7.998  1.00 26.72           N
ANISOU 3885  NH2 ARG D 479    2471   4316   3365    367    563   -491       N
ATOM   3886  C   ARG D 479      56.113   3.010  -8.047  1.00 18.00           C
ANISOU 3886  C   ARG D 479    2000   2531   2310    111     60   -286       C
ATOM   3887  O   ARG D 479      56.893   2.152  -8.450  1.00 17.43           O
ANISOU 3887  O   ARG D 479    1902   2452   2268     49     31   -230       O
ATOM   3888  N   VAL D 480      56.506   4.091  -7.376  1.00 18.88           N
ANISOU 3888  N   VAL D 480    2194   2547   2431    138     13   -340       N
ATOM   3889  CA  VAL D 480      57.872   4.288  -6.941  1.00 18.12           C
ANISOU 3889  CA  VAL D 480    2153   2351   2382     77    -95   -341       C
ATOM   3890  CB  VAL D 480      58.424   5.658  -7.477  1.00 19.53           C
ANISOU 3890  CB  VAL D 480    2339   2392   2689     91   -137   -344       C
ATOM   3891  CG1 VAL D 480      59.811   6.004  -6.914  1.00 16.90           C
ANISOU 3891  CG1 VAL D 480    2041   1951   2430      9   -261   -368       C
ATOM   3892  CG2 VAL D 480      58.462   5.665  -8.979  1.00 16.55           C
ANISOU 3892  CG2 VAL D 480    1871   2019   2398    100    -88   -246       C
ATOM   3893  C   VAL D 480      57.914   4.199  -5.402  1.00 20.38           C
ANISOU 3893  C   VAL D 480    2561   2642   2541     65   -138   -419       C
ATOM   3894  O   VAL D 480      57.129   4.864  -4.687  1.00 20.96           O
ANISOU 3894  O   VAL D 480    2713   2720   2531    126    -92   -507       O
ATOM   3895  N   SER D 481      58.821   3.365  -4.894  1.00 20.39           N
ANISOU 3895  N   SER D 481    2584   2645   2517      1   -225   -387       N
ATOM   3896  CA  SER D 481      59.058   3.257  -3.454  1.00 22.99           C
ANISOU 3896  CA  SER D 481    3052   2978   2703    -11   -302   -444       C
ATOM   3897  CB  SER D 481      59.874   1.996  -3.174  1.00 22.03           C
ANISOU 3897  CB  SER D 481    2928   2881   2562    -61   -385   -362       C
ATOM   3898  OG  SER D 481      60.138   1.858  -1.810  1.00 21.23           O
ANISOU 3898  OG  SER D 481    2978   2789   2300    -66   -480   -399       O
ATOM   3899  C   SER D 481      59.757   4.490  -2.835  1.00 25.71           C
ANISOU 3899  C   SER D 481    3483   3214   3072    -19   -429   -546       C
ATOM   3900  O   SER D 481      60.658   5.061  -3.420  1.00 25.93           O
ANISOU 3900  O   SER D 481    3439   3147   3265    -59   -511   -535       O
ATOM   3901  N   LYS D 482      59.321   4.900  -1.655  1.00 29.14           N
ANISOU 3901  N   LYS D 482    4076   3658   3339     13   -436   -651       N
ATOM   3902  CA  LYS D 482      60.019   5.935  -0.899  1.00 33.36           C
ANISOU 3902  CA  LYS D 482    4723   4086   3866     -7   -583   -772       C
ATOM   3903  CB  LYS D 482      59.022   6.840  -0.155  1.00 34.30           C
ANISOU 3903  CB  LYS D 482    4994   4191   3848     75   -492   -915       C
ATOM   3904  CG  LYS D 482      58.218   7.746  -1.062  1.00 35.12           C
ANISOU 3904  CG  LYS D 482    5025   4233   4086    151   -361   -933       C
ATOM   3905  CD  LYS D 482      57.186   8.541  -0.242  1.00 38.57           C
ANISOU 3905  CD  LYS D 482    5604   4663   4387    260   -254  -1083       C
ATOM   3906  CE  LYS D 482      57.252  10.056  -0.537  1.00 45.10           C
ANISOU 3906  CE  LYS D 482    6478   5298   5359    308   -284  -1185       C
ATOM   3907  NZ  LYS D 482      56.099  10.810   0.069  1.00 47.81           N
ANISOU 3907  NZ  LYS D 482    6933   5632   5603    453   -143  -1329       N
ATOM   3908  C   LYS D 482      61.038   5.332   0.072  1.00 35.24           C
ANISOU 3908  C   LYS D 482    5039   4343   4008    -65   -774   -772       C
ATOM   3909  O   LYS D 482      61.727   6.074   0.758  1.00 37.45           O
ANISOU 3909  O   LYS D 482    5410   4546   4275    -99   -937   -880       O
ATOM   3910  N   MSE D 483      61.139   3.993   0.102  1.00 35.93           N
ANISOU 3910  N   MSE D 483    5093   4523   4037    -74   -766   -651       N
ATOM   3911  CA  MSE D 483      62.049   3.244   0.994  1.00 38.63           C
ANISOU 3911  CA  MSE D 483    5507   4890   4278   -103   -953   -617       C
ATOM   3912  CB  MSE D 483      61.526   1.809   1.265  1.00 38.49           C
ANISOU 3912  CB  MSE D 483    5539   4971   4113    -80   -858   -492       C
ATOM   3913  CG  MSE D 483      60.174   1.672   1.929  1.00 38.95           C
ANISOU 3913  CG  MSE D 483    5746   5112   3940    -43   -667   -517       C
ATOM   3914  SE  MSE D 483      60.058   2.796   3.498  0.90 48.19          SE
ANISOU 3914  SE  MSE D 483    7190   6282   4839    -11   -748   -705       SE
ATOM   3915  CE  MSE D 483      61.347   1.963   4.722  1.00 38.88           C
ANISOU 3915  CE  MSE D 483    6178   5122   3472    -35  -1049   -643       C
ATOM   3916  C   MSE D 483      63.440   3.077   0.385  1.00 39.71           C
ANISOU 3916  C   MSE D 483    5470   4969   4647   -156  -1120   -557       C
ATOM   3917  O   MSE D 483      63.582   2.646  -0.783  1.00 39.13           O
ANISOU 3917  O   MSE D 483    5221   4891   4756   -163  -1031   -463       O
ATOM   3918  OXT MSE D 483      64.451   3.268   1.060  1.00 42.00           O
ANISOU 3918  OXT MSE D 483    5786   5231   4942   -190  -1344   -601       O
ATOM   3919  N   SER E 320      17.288 -30.979 -15.413  1.00 45.14           N
ANISOU 3919  N   SER E 320    4874   5333   6943  -1348    253  -1314       N
ATOM   3920  CA  SER E 320      18.777 -31.109 -15.580  1.00 43.13           C
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Figure 18 (continued)

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ANISOU 3920  CA  SER E 320     4877   4914   6598  -1261    271  -1210  C
ATOM   3921  CB  SER E 320      19.237 -30.250 -16.770  1.00 42.79      C
ANISOU 3921  CB  SER E 320     4873   4954   6429  -1088    116  -1208  C
ATOM   3922  OG  SER E 320      20.570 -30.562 -17.153  1.00 42.94      O
ANISOU 3922  OG  SER E 320     5102   4848   6364  -1042    136  -1161  O
ATOM   3923  C   SER E 320      19.579 -30.728 -14.308  1.00 40.67      C
ANISOU 3923  C   SER E 320     4675   4506   6270  -1199    402  -1051  C
ATOM   3924  O   SER E 320      20.651 -30.104 -14.400  1.00 38.93      O
ANISOU 3924  O   SER E 320     4584   4241   5966  -1052    384   -962  O
ATOM   3925  N   SER E 321      19.089 -31.107 -13.126  1.00 39.80      N
ANISOU 3925  N   SER E 321     4515   4379   6227  -1326    537  -1019  N
ATOM   3926  CA  SER E 321      19.714 -30.590 -11.897  1.00 37.65      C
ANISOU 3926  CA  SER E 321     4321   4074   5908  -1264    645   -884  C
ATOM   3927  CB  SER E 321      18.684 -29.870 -11.033  1.00 38.56      C
ANISOU 3927  CB  SER E 321     4239   4357   6053  -1282    719   -919  C
ATOM   3928  OG  SER E 321      17.883 -30.781 -10.335  1.00 42.51      O
ANISOU 3928  OG  SER E 321     4667   4871   6613  -1506    844   -940  O
ATOM   3929  C   SER E 321      20.577 -31.528 -11.043  1.00 35.74      C
ANISOU 3929  C   SER E 321     4273   3651   5656  -1347    751   -758  C
ATOM   3930  O   SER E 321      20.985 -31.157  -9.954  1.00 35.15      O
ANISOU 3930  O   SER E 321     4249   3580   5525  -1318    835   -651  O
ATOM   3931  N   SER E 322      20.888 -32.716 -11.566  1.00 34.84      N
ANISOU 3931  N   SER E 322     4269   3374   5595  -1437    733   -776  N
ATOM   3932  CA  SER E 322      21.599 -33.753 -10.828  1.00 33.04      C
ANISOU 3932  CA  SER E 322     4224   2938   5393  -1514    809   -653  C
ATOM   3933  CB  SER E 322      20.570 -34.509  -9.996  1.00 35.56      C
ANISOU 3933  CB  SER E 322     4485   3245   5779  -1754    925   -626  C
ATOM   3934  OG  SER E 322      21.115 -35.024  -8.821  1.00 37.24      O
ANISOU 3934  OG  SER E 322     4855   3332   5961  -1811   1016   -441  O
ATOM   3935  C   SER E 322      22.235 -34.682 -11.863  1.00 31.91      C
ANISOU 3935  C   SER E 322     4198   2615   5311  -1502    734   -725  C
ATOM   3936  O   SER E 322      21.534 -35.240 -12.700  1.00 32.42      O
ANISOU 3936  O   SER E 322     4194   2677   5448  -1608    693   -870  O
ATOM   3937  N   PHE E 323      23.554 -34.840 -11.834  1.00 29.63      N
ANISOU 3937  N   PHE E 323     4068   2192   4996  -1371    715   -650  N
ATOM   3938  CA  PHE E 323      24.244 -35.599 -12.891  1.00 29.75      C
ANISOU 3938  CA  PHE E 323     4174   2063   5065  -1325    650   -758  C
ATOM   3939  CB  PHE E 323      24.149 -34.903 -14.263  1.00 28.38      C
ANISOU 3939  CB  PHE E 323     3911   2061   4813  -1241    558   -915  C
ATOM   3940  CG  PHE E 323      24.548 -33.447 -14.229  1.00 26.56      C
ANISOU 3940  CG  PHE E 323     3636   2007   4449  -1083    532   -845  C
ATOM   3941  CD1 PHE E 323      25.862 -33.076 -14.466  1.00 22.90      C
ANISOU 3941  CD1 PHE E 323     3264   1521   3918   -932    519   -808  C
ATOM   3942  CE1 PHE E 323      26.235 -31.770 -14.412  1.00 24.39      C
ANISOU 3942  CE1 PHE E 323     3422   1843   4002   -815    501   -741  C
ATOM   3943  CZ  PHE E 323      25.292 -30.792 -14.111  1.00 23.48      C
ANISOU 3943  CZ  PHE E 323     3191   1869   3862   -821    488   -715  C
ATOM   3944  CE2 PHE E 323      23.978 -31.148 -13.862  1.00 24.40      C
ANISOU 3944  CE2 PHE E 323     3199   2025   4048   -947    500   -764  C
ATOM   3945  CD2 PHE E 323      23.615 -32.469 -13.928  1.00 24.02      C
ANISOU 3945  CD2 PHE E 323     3176   1861   4091  -1090    526   -826  C
ATOM   3946  C   PHE E 323      25.685 -35.852 -12.537  1.00 29.09      C
ANISOU 3946  C   PHE E 323     4245   1828   4982  -1184    651   -658  C
ATOM   3947  O   PHE E 323      26.186 -35.304 -11.578  1.00 27.33      O
ANISOU 3947  O   PHE E 323     4053   1639   4692  -1113    681   -508  O
ATOM   3948  N   SER E 324      26.322 -36.718 -13.318  1.00 31.14      N
ANISOU 3948  N   SER E 324     4586   1925   5321  -1147    614   -765  N
ATOM   3949  CA  SER E 324      27.734 -37.036 -13.197  1.00 31.70      C
ANISOU 3949  CA  SER E 324     4771   1855   5418   -989    600   -719  C
ATOM   3950  CB  SER E 324      27.870 -38.553 -13.286  1.00 34.12      C
ANISOU 3950  CB  SER E 324     5192   1860   5913  -1047    596   -770  C
ATOM   3951  OG  SER E 324      29.065 -38.980 -12.669  1.00 38.99      O
ANISOU 3951  OG  SER E 324     5921   2300   6591   -905    581   -655  O
ATOM   3952  C   SER E 324      28.506 -36.359 -14.344  1.00 30.11      C
ANISOU 3952  C   SER E 324     4525   1797   5118   -844    560   -855  C
ATOM   3953  O   SER E 324      28.106 -36.436 -15.500  1.00 31.59      O
ANISOU 3953  O   SER E 324     4663   2058   5282   -883    530  -1033  O
ATOM   3954  N   PHE E 325      29.598 -35.683 -14.036  1.00 28.89      N
ANISOU 3954  N   PHE E 325     4383   1701   4891   -694    561   -773  N
ATOM   3955  CA  PHE E 325      30.474 -35.145 -15.073  1.00 27.03      C
ANISOU 3955  CA  PHE E 325     4117   1587   4568   -576    545   -888  C
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Figure 18 (continued)

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ATOM   3956  CB  PHE E 325      30.028 -33.721 -15.485  1.00 25.71           C
ANISOU 3956  CB  PHE E 325    3861   1671   4236   -581    531   -870        C
ATOM   3957  CG  PHE E 325      30.847 -33.123 -16.611  1.00 24.39           C
ANISOU 3957  CG  PHE E 325    3676   1643   3950   -499    524   -964        C
ATOM   3958  CD1 PHE E 325      30.800 -33.667 -17.896  1.00 26.53           C
ANISOU 3958  CD1 PHE E 325    3946   1946   4189   -527    510  -1154        C
ATOM   3959  CE1 PHE E 325      31.557 -33.143 -18.941  1.00 26.12           C
ANISOU 3959  CE1 PHE E 325    3882   2048   3996   -474    523  -1236        C
ATOM   3960  CZ  PHE E 325      32.370 -32.062 -18.716  1.00 25.88           C
ANISOU 3960  CZ  PHE E 325    3837   2119   3876   -402    549  -1121        C
ATOM   3961  CE2 PHE E 325      32.432 -31.495 -17.417  1.00 23.76           C
ANISOU 3961  CE2 PHE E 325    3565   1800   3661   -371    553   -942        C
ATOM   3962  CD2 PHE E 325      31.668 -32.040 -16.383  1.00 22.30           C
ANISOU 3962  CD2 PHE E 325    3395   1484   3596   -415    540   -870        C
ATOM   3963  C   PHE E 325      31.902 -35.144 -14.575  1.00 26.40           C
ANISOU 3963  C   PHE E 325    4074   1446   4509   -425    553   -823        C
ATOM   3964  O   PHE E 325      32.194 -34.540 -13.538  1.00 26.23           O
ANISOU 3964  O   PHE E 325    4054   1463   4449   -387    556   -660        O
ATOM   3965  N   GLY E 326      32.796 -35.792 -15.322  1.00 27.37           N
ANISOU 3965  N   GLY E 326    4212   1496   4692   -336    554   -970        N
ATOM   3966  CA  GLY E 326      34.235 -35.778 -15.041  1.00 26.54           C
ANISOU 3966  CA  GLY E 326    4100   1366   4617   -174    556   -952        C
ATOM   3967  C   GLY E 326      34.617 -36.415 -13.719  1.00 27.28           C
ANISOU 3967  C   GLY E 326    4264   1264   4837   -114    519   -785        C
ATOM   3968  O   GLY E 326      35.626 -36.061 -13.130  1.00 26.73           O
ANISOU 3968  O   GLY E 326    4170   1232   4755      5    500   -704        O
ATOM   3969  N   GLY E 327      33.802 -37.361 -13.255  1.00 28.74           N
ANISOU 3969  N   GLY E 327    4538   1245   5136   -209    504   -726        N
ATOM   3970  CA  GLY E 327      34.068 -38.077 -12.017  1.00 29.31           C
ANISOU 3970  CA  GLY E 327    4711   1111   5316   -173    461   -535        C
ATOM   3971  C   GLY E 327      33.462 -37.392 -10.811  1.00 28.45           C
ANISOU 3971  C   GLY E 327    4617   1109   5084   -268    472   -313        C
ATOM   3972  O   GLY E 327      33.702 -37.801  -9.695  1.00 29.85           O
ANISOU 3972  O   GLY E 327    4879   1173   5289   -249    436   -125        O
ATOM   3973  N   PHE E 328      32.672 -36.346 -11.040  1.00 27.12           N
ANISOU 3973  N   PHE E 328    4367   1164   4775   -365    519   -340        N
ATOM   3974  CA  PHE E 328      32.019 -35.572  -9.968  1.00 26.05           C
ANISOU 3974  CA  PHE E 328    4218   1162   4519   -453    548   -181        C
ATOM   3975  CB  PHE E 328      32.455 -34.102 -10.014  1.00 23.69           C
ANISOU 3975  CB  PHE E 328    3822   1103   4075   -380    554   -197        C
ATOM   3976  CG  PHE E 328      33.877 -33.872  -9.572  1.00 23.60           C
ANISOU 3976  CG  PHE E 328    3813   1108   4048   -226    510   -147        C
ATOM   3977  CD1 PHE E 328      34.167 -33.591  -8.245  1.00 22.43           C
ANISOU 3977  CD1 PHE E 328    3694   1000   3828   -211    488     14        C
ATOM   3978  CE1 PHE E 328      35.475 -33.394  -7.831  1.00 23.44           C
ANISOU 3978  CE1 PHE E 328    3804   1160   3943    -72    429     48        C
ATOM   3979  CZ  PHE E 328      36.506 -33.431  -8.745  1.00 21.73           C
ANISOU 3979  CZ  PHE E 328    3523    942   3793     50    409    -84        C
ATOM   3980  CE2 PHE E 328      36.228 -33.706 -10.080  1.00 22.34           C
ANISOU 3980  CE2 PHE E 328    3575    984   3929     31    451   -248        C
ATOM   3981  CD2 PHE E 328      34.921 -33.932 -10.485  1.00 21.48           C
ANISOU 3981  CD2 PHE E 328    3500    839   3823   -105    492   -276        C
ATOM   3982  C   PHE E 328      30.497 -35.621 -10.086  1.00 26.19           C
ANISOU 3982  C   PHE E 328    4206   1214   4532   -642    600   -207        C
ATOM   3983  O   PHE E 328      29.950 -35.431 -11.172  1.00 26.07           O
ANISOU 3983  O   PHE E 328    4118   1269   4517   -682    603   -365        O
ATOM   3984  N   THR E 329      29.819 -35.857  -8.968  1.00 26.51           N
ANISOU 3984  N   THR E 329    4290   1228   4553   -764    638    -54        N
ATOM   3985  CA  THR E 329      28.360 -35.708  -8.900  1.00 26.59           C
ANISOU 3985  CA  THR E 329    4228   1329   4544   -949    705    -80        C
ATOM   3986  CB  THR E 329      27.755 -36.554  -7.740  1.00 28.57           C
ANISOU 3986  CB  THR E 329    4571   1463   4820  -1117    762     93        C
ATOM   3987  OG1 THR E 329      28.147 -37.920  -7.876  1.00 29.01           O
ANISOU 3987  OG1 THR E 329    4767   1221   5033  -1129    723    133        O
ATOM   3988  CG2 THR E 329      26.239 -36.497  -7.744  1.00 28.98           C
ANISOU 3988  CG2 THR E 329    4518   1619   4875  -1326    845     36        C
ATOM   3989  C   THR E 329      28.025 -34.221  -8.688  1.00 25.15           C
ANISOU 3989  C   THR E 329    3921   1415   4220   -919    731   -98        C
ATOM   3990  O   THR E 329      28.444 -33.613  -7.696  1.00 24.93           O
ANISOU 3990  O   THR E 329    3907   1473   4091   -873    746     12        O
ATOM   3991  N   PHE E 330      27.315 -33.629  -9.642  1.00 24.51           N
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Figure 18 (continued)

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ANISOU 3991  N   PHE E 330     3721   1458   4135   -936    723   -244    N
ATOM   3992  CA  PHE E 330      26.858 -32.240  -9.556  1.00 23.01        C
ANISOU 3992  CA  PHE E 330     3410   1483   3850   -900    734   -274    C
ATOM   3993  CB  PHE E 330      26.817 -31.604 -10.941  1.00 21.72        C
ANISOU 3993  CB  PHE E 330     3173   1403   3676   -825    666   -409    C
ATOM   3994  CG  PHE E 330      28.177 -31.190 -11.498  1.00 21.21        C
ANISOU 3994  CG  PHE E 330     3166   1329   3566   -677    621   -415    C
ATOM   3995  CD1 PHE E 330      28.458 -29.852 -11.723  1.00 15.46        C
ANISOU 3995  CD1 PHE E 330     2388    729   2756   -587    599   -415    C
ATOM   3996  CE1 PHE E 330      29.657 -29.480 -12.246  1.00 17.14        C
ANISOU 3996  CE1 PHE E 330     2641    946   2926   -487    576   -422    C
ATOM   3997  CZ  PHE E 330      30.629 -30.427 -12.567  1.00 16.73        C
ANISOU 3997  CZ  PHE E 330     2657    787   2913   -450    574   -450    C
ATOM   3998  CE2 PHE E 330      30.376 -31.764 -12.358  1.00 17.20        C
ANISOU 3998  CE2 PHE E 330     2768    698   3069   -508    583   -460    C
ATOM   3999  CD2 PHE E 330      29.154 -32.149 -11.835  1.00 21.06        C
ANISOU 3999  CD2 PHE E 330     3238   1164   3598   -632    606   -432    C
ATOM   4000  C   PHE E 330      25.453 -32.252  -9.007  1.00 24.29        C
ANISOU 4000  C   PHE E 330     3474   1732   4023  -1056    804   -281    C
ATOM   4001  O   PHE E 330      24.630 -33.022  -9.465  1.00 26.43        O
ANISOU 4001  O   PHE E 330     3710   1954   4378  -1183    811   -348    O
ATOM   4002  N   LYS E 331      25.180 -31.429  -7.999  1.00 24.67        N
ANISOU 4002  N   LYS E 331     3469   1917   3990  -1057    863   -230    N
ATOM   4003  CA  LYS E 331      23.812 -31.224  -7.513  1.00 26.44        C
ANISOU 4003  CA  LYS E 331     3552   2275   4217  -1188    945   -275    C
ATOM   4004  CB  LYS E 331      23.617 -31.802  -6.093  1.00 27.86        C
ANISOU 4004  CB  LYS E 331     3795   2455   4336  -1333   1061   -141    C
ATOM   4005  CG  LYS E 331      23.960 -33.297  -5.951  1.00 31.24        C
ANISOU 4005  CG  LYS E 331     4390   2659   4822  -1444   1064    -17    C
ATOM   4006  CD  LYS E 331      23.547 -33.844  -4.584  1.00 33.05        C
ANISOU 4006  CD  LYS E 331     4681   2905   4972  -1626   1184    138    C
ATOM   4007  CE  LYS E 331      23.640 -35.361  -4.566  1.00 38.36        C
ANISOU 4007  CE  LYS E 331     5513   3318   5742  -1762   1182    262    C
ATOM   4008  NZ  LYS E 331      22.905 -35.921  -3.365  1.00 42.80        N
ANISOU 4008  NZ  LYS E 331     6117   3916   6230  -2004   1321    413    N
ATOM   4009  C   LYS E 331      23.523 -29.732  -7.509  1.00 25.02        C
ANISOU 4009  C   LYS E 331     3240   2275   3994  -1072    934   -357    C
ATOM   4010  O   LYS E 331      24.129 -28.997  -6.727  1.00 24.10        O
ANISOU 4010  O   LYS E 331     3157   2208   3793   -994    956   -308    O
ATOM   4011  N   ARG E 332      22.604 -29.291  -8.370  1.00 25.04        N
ANISOU 4011  N   ARG E 332     3089   2363   4061  -1059    886   -484    N
ATOM   4012  CA  ARG E 332      22.229 -27.881  -8.446  1.00 24.35        C
ANISOU 4012  CA  ARG E 332     2874   2411   3969   -932    855   -562    C
ATOM   4013  CB  ARG E 332      21.285 -27.616  -9.610  1.00 25.25        C
ANISOU 4013  CB  ARG E 332     2839   2593   4163   -905    757   -680    C
ATOM   4014  CG  ARG E 332      21.014 -26.115  -9.816  1.00 21.87        C
ANISOU 4014  CG  ARG E 332     2303   2255   3752   -736    689   -736    C
ATOM   4015  CD  ARG E 332      20.462 -25.836 -11.209  1.00 20.39        C
ANISOU 4015  CD  ARG E 332     2030   2105   3611   -667    535   -801    C
ATOM   4016  NE  ARG E 332      19.065 -26.242 -11.251  1.00 24.14        N
ANISOU 4016  NE  ARG E 332     2301   2699   4172   -764    543   -916    N
ATOM   4017  CZ  ARG E 332      18.397 -26.578 -12.351  1.00 23.40        C
ANISOU 4017  CZ  ARG E 332     2117   2660   4116   -788    424   -991    C
ATOM   4018  NH1 ARG E 332      18.988 -26.571 -13.538  1.00 21.11        N
ANISOU 4018  NH1 ARG E 332     1938   2320   3762   -722    293   -959    N
ATOM   4019  NH2 ARG E 332      17.126 -26.891 -12.252  1.00 20.98        N
ANISOU 4019  NH2 ARG E 332     1594   2479   3898   -885    440  -1109    N
ATOM   4020  C   ARG E 332      21.525 -27.438  -7.198  1.00 26.32        C
ANISOU 4020  C   ARG E 332     3014   2794   4193   -986    977   -590    C
ATOM   4021  O   ARG E 332      20.536 -28.054  -6.779  1.00 27.98        O
ANISOU 4021  O   ARG E 332     3124   3075   4432  -1144   1068   -625    O
ATOM   4022  N   THR E 333      22.010 -26.355  -6.605  1.00 25.21        N
ANISOU 4022  N   THR E 333     2884   2698   3998   -869    988   -593    N
ATOM   4023  CA  THR E 333      21.397 -25.862  -5.375  1.00 26.76        C
ANISOU 4023  CA  THR E 333     2975   3042   4151   -911   1115   -652    C
ATOM   4024  CB  THR E 333      22.430 -25.785  -4.254  1.00 26.26        C
ANISOU 4024  CB  THR E 333     3060   2971   3947   -914   1174   -557    C
ATOM   4025  OG1 THR E 333      23.540 -25.025  -4.725  1.00 26.60        O
ANISOU 4025  OG1 THR E 333     3196   2922   3989   -755   1066   -537    O
ATOM   4026  CG2 THR E 333      22.913 -27.195  -3.863  1.00 26.22        C
ANISOU 4026  CG2 THR E 333     3215   2876   3869  -1058   1210   -394    C
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Figure 18 (continued)

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ATOM   4027  C   THR E 333      20.663 -24.526  -5.541  1.00 26.87           C
ANISOU 4027  C   THR E 333    2805   3156   4249   -774   1087   -809       C
ATOM   4028  O   THR E 333      19.854 -24.162  -4.697  1.00 28.07           O
ANISOU 4028  O   THR E 333    2810   3455   4401   -809   1199   -916       O
ATOM   4029  N   SER E 334      20.951 -23.808  -6.627  1.00 26.17           N
ANISOU 4029  N   SER E 334    2727   2986   4232   -617    940   -820       N
ATOM   4030  CA  SER E 334      20.279 -22.542  -6.963  1.00 27.33           C
ANISOU 4030  CA  SER E 334    2719   3177   4488   -459    871   -942       C
ATOM   4031  CB  SER E 334      21.102 -21.370  -6.495  1.00 26.24           C
ANISOU 4031  CB  SER E 334    2660   2977   4331   -331    863   -947       C
ATOM   4032  OG  SER E 334      20.687 -20.972  -5.253  1.00 30.33           O
ANISOU 4032  OG  SER E 334    3084   3610   4830   -352    996  -1061       O
ATOM   4033  C   SER E 334      20.227 -22.353  -8.446  1.00 27.14           C
ANISOU 4033  C   SER E 334    2699   3081   4532   -363    695   -914       C
ATOM   4034  O   SER E 334      21.097 -22.860  -9.148  1.00 24.82           O
ANISOU 4034  O   SER E 334    2565   2688   4175   -384    635   -806       O
ATOM   4035  N   GLY E 335      19.259 -21.545  -8.895  1.00 28.15           N
ANISOU 4035  N   GLY E 335    2651   3264   4780   -243    609  -1014       N
ATOM   4036  CA  GLY E 335      19.198 -21.137 -10.292  1.00 27.93           C
ANISOU 4036  CA  GLY E 335    2635   3180   4796   -127    415   -971       C
ATOM   4037  C   GLY E 335      18.565 -22.157 -11.198  1.00 28.12           C
ANISOU 4037  C   GLY E 335    2593   3273   4817   -224    346   -983       C
ATOM   4038  O   GLY E 335      17.901 -23.072 -10.736  1.00 29.23           O
ANISOU 4038  O   GLY E 335    2627   3506   4972   -375    446  -1053       O
ATOM   4039  N   SER E 336      18.775 -21.971 -12.500  1.00 28.38           N
ANISOU 4039  N   SER E 336    2694   3267   4823   -150    176   -918       N
ATOM   4040  CA  SER E 336      18.131 -22.753 -13.569  1.00 29.07           C
ANISOU 4040  CA  SER E 336    2710   3437   4900   -217     65   -954       C
ATOM   4041  CB  SER E 336      16.621 -22.473 -13.635  1.00 31.46           C
ANISOU 4041  CB  SER E 336    2727   3891   5336   -168     -9  -1092       C
ATOM   4042  OG  SER E 336      16.347 -21.090 -13.798  1.00 31.69           O
ANISOU 4042  OG  SER E 336    2690   3901   5451     54   -132  -1084       O
ATOM   4043  C   SER E 336      18.788 -22.347 -14.882  1.00 28.45           C
ANISOU 4043  C   SER E 336    2781   3302   4725   -127   -102   -846       C
ATOM   4044  O   SER E 336      19.493 -21.345 -14.949  1.00 28.13           O
ANISOU 4044  O   SER E 336    2857   3166   4665     -7   -138   -747       O
ATOM   4045  N   SER E 337      18.584 -23.140 -15.920  1.00 28.83           N
ANISOU 4045  N   SER E 337    2834   3415   4705   -205   -194   -868       N
ATOM   4046  CA  SER E 337      19.123 -22.804 -17.221  1.00 28.54           C
ANISOU 4046  CA  SER E 337    2932   3371   4540   -140   -346   -774       C
ATOM   4047  CB  SER E 337      20.569 -23.278 -17.364  1.00 26.18           C
ANISOU 4047  CB  SER E 337    2866   2970   4113   -211   -249   -695       C
ATOM   4048  OG  SER E 337      20.653 -24.681 -17.263  1.00 28.38           O
ANISOU 4048  OG  SER E 337    3156   3248   4378   -372   -156   -782       O
ATOM   4049  C   SER E 337      18.249 -23.305 -18.353  1.00 29.78           C
ANISOU 4049  C   SER E 337    2982   3676   4656   -176   -510   -851       C
ATOM   4050  O   SER E 337      17.378 -24.160 -18.157  1.00 30.45           O
ANISOU 4050  O   SER E 337    2905   3849   4814   -290   -483   -990       O
ATOM   4051  N   ILE E 338      18.476 -22.729 -19.525  1.00 30.64           N
ANISOU 4051  N   ILE E 338    3181   3820   4639    -89   -681   -757       N
ATOM   4052  CA  ILE E 338      17.938 -23.221 -20.783  1.00 31.77           C
ANISOU 4052  CA  ILE E 338    3281   4120   4670   -132   -851   -814       C
ATOM   4053  CB  ILE E 338      17.005 -22.176 -21.446  1.00 33.98           C
ANISOU 4053  CB  ILE E 338    3438   4503   4968     41  -1101   -760       C
ATOM   4054  CG1 ILE E 338      17.737 -20.850 -21.743  1.00 32.53           C
ANISOU 4054  CG1 ILE E 338    3435   4204   4721    199  -1175   -540       C
ATOM   4055  CD1 ILE E 338      16.899 -19.806 -22.508  1.00 34.27           C
ANISOU 4055  CD1 ILE E 338    3577   4492   4952    387  -1453   -443       C
ATOM   4056  CG2 ILE E 338      15.748 -21.966 -20.580  1.00 34.20           C
ANISOU 4056  CG2 ILE E 338    3181   4582   5232    103  -1106   -883       C
ATOM   4057  C   ILE E 338      19.151 -23.626 -21.656  1.00 31.96           C
ANISOU 4057  C   ILE E 338    3543   4122   4476   -205   -826   -751       C
ATOM   4058  O   ILE E 338      20.274 -23.333 -21.307  1.00 29.56           O
ANISOU 4058  O   ILE E 338    3404   3692   4137   -193   -705   -650       O
ATOM   4059  N   LYS E 339      18.931 -24.339 -22.747  1.00 35.06           N
ANISOU 4059  N   LYS E 339    3939   4655   4729   -290   -928   -838       N
ATOM   4060  CA  LYS E 339      20.029 -24.773 -23.631  1.00 36.58           C
ANISOU 4060  CA  LYS E 339    4335   4861   4705   -363   -892   -821       C
ATOM   4061  CB  LYS E 339      20.084 -26.290 -23.805  1.00 36.71           C
ANISOU 4061  CB  LYS E 339    4342   4894   4712   -536   -805  -1027       C
ATOM   4062  CG  LYS E 339      20.066 -27.164 -22.598  1.00 37.43           C
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Figure 18 (continued)

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ANISOU 4062  CG  LYS E 339     4380   4835   5006   -627   -622  -1118    C
ATOM   4063  CD  LYS E 339      19.853 -28.608 -23.095  1.00 40.71        C
ANISOU 4063  CD  LYS E 339     4778   5276   5414   -797   -606  -1331    C
ATOM   4064  CE  LYS E 339      19.579 -29.601 -21.976  1.00 42.52        C
ANISOU 4064  CE  LYS E 339     4945   5354   5856   -921   -452  -1418    C
ATOM   4065  NZ  LYS E 339      19.132 -30.907 -22.530  1.00 45.89        N
ANISOU 4065  NZ  LYS E 339     5332   5798   6308  -1093   -469  -1635    N
ATOM   4066  C   LYS E 339      19.787 -24.253 -25.032  1.00 39.73        C
ANISOU 4066  C   LYS E 339     4775   5437   4882   -315  -1112   -753    C
ATOM   4067  O   LYS E 339      18.632 -24.092 -25.473  1.00 41.88        O
ANISOU 4067  O   LYS E 339     4892   5855   5167   -273  -1310   -795    O
ATOM   4068  N   ARG E 340      20.885 -24.049 -25.745  1.00 40.42        N
ANISOU 4068  N   ARG E 340     5065   5535   4757   -334  -1077   -656    N
ATOM   4069  CA  ARG E 340      20.863 -23.611 -27.123  1.00 43.90        C
ANISOU 4069  CA  ARG E 340     5594   6160   4925   -320  -1258   -568    C
ATOM   4070  CB  ARG E 340      20.961 -22.081 -27.170  1.00 44.64        C
ANISOU 4070  CB  ARG E 340     5770   6188   5002   -170  -1365   -292    C
ATOM   4071  CG  ARG E 340      20.849 -21.453 -28.545  1.00 49.08        C
ANISOU 4071  CG  ARG E 340     6441   6929   5279   -142  -1581   -134    C
ATOM   4072  CD  ARG E 340      21.496 -20.082 -28.498  1.00 51.89        C
ANISOU 4072  CD  ARG E 340     6964   7138   5614    -49  -1589    158    C
ATOM   4073  NE  ARG E 340      21.220 -19.278 -29.683  1.00 56.36        N
ANISOU 4073  NE  ARG E 340     7638   7837   5940      5  -1831    373    N
ATOM   4074  CZ  ARG E 340      21.825 -18.121 -29.947  1.00 59.39        C
ANISOU 4074  CZ  ARG E 340     8212   8114   6241     48  -1858    658    C
ATOM   4075  NH1 ARG E 340      22.748 -17.647 -29.115  1.00 56.32        N
ANISOU 4075  NH1 ARG E 340     7907   7494   5997     38  -1655    729    N
ATOM   4076  NH2 ARG E 340      21.514 -17.438 -31.051  1.00 63.84        N
ANISOU 4076  NH2 ARG E 340     8887   8799   6569     90  -2097    878    N
ATOM   4077  C   ARG E 340      22.067 -24.271 -27.797  1.00 44.15        C
ANISOU 4077  C   ARG E 340     5797   6240   4738   -444  -1118   -630    C
ATOM   4078  O   ARG E 340      23.203 -24.110 -27.355  1.00 42.69        O
ANISOU 4078  O   ARG E 340     5728   5923   4568   -452   -937   -561    O
ATOM   4079  N   GLU E 341      21.819 -25.062 -28.834  1.00 46.84        N
ANISOU 4079  N   GLU E 341     6132   6780   4884   -542  -1197   -791    N
ATOM   4080  CA  GLU E 341      22.906 -25.647 -29.629  1.00 47.97        C
ANISOU 4080  CA  GLU E 341     6424   7010   4792   -651  -1074   -881    C
ATOM   4081  CB  GLU E 341      22.392 -26.781 -30.528  1.00 50.34        C
ANISOU 4081  CB  GLU E 341     6666   7504   4956   -770  -1150  -1154    C
ATOM   4082  CG  GLU E 341      23.492 -27.439 -31.354  1.00 53.33        C
ANISOU 4082  CG  GLU E 341     7181   7984   5099   -876  -1010  -1297    C
ATOM   4083  CD  GLU E 341      23.258 -28.925 -31.594  1.00 57.92        C
ANISOU 4083  CD  GLU E 341     7691   8590   5726   -998   -966  -1652    C
ATOM   4084  OE1 GLU E 341      22.554 -29.280 -32.578  1.00 60.51        O
ANISOU 4084  OE1 GLU E 341     7977   9149   5864  -1070  -1129  -1802    O
ATOM   4085  OE2 GLU E 341      23.805 -29.734 -30.804  1.00 56.96        O
ANISOU 4085  OE2 GLU E 341     7564   8249   5831  -1021   -776  -1779    O
ATOM   4086  C   GLU E 341      23.631 -24.578 -30.459  1.00 48.77        C
ANISOU 4086  C   GLU E 341     6704   7214   4614   -626  -1112   -642    C
ATOM   4087  O   GLU E 341      22.992 -23.827 -31.186  1.00 51.13        O
ANISOU 4087  O   GLU E 341     7019   7655   4752   -576  -1330   -491    O
ATOM   4088  N   GLU E 342      24.961 -24.539 -30.346  1.00 47.41        N
ANISOU 4088  N   GLU E 342     6657   6969   4389   -668   -901   -607    N
ATOM   4089  CA  GLU E 342      25.803 -23.487 -30.926  1.00 48.38        C
ANISOU 4089  CA  GLU E 342     6949   7146   4286   -674   -880   -363    C
ATOM   4090  CB  GLU E 342      26.214 -22.470 -29.845  1.00 46.46        C
ANISOU 4090  CB  GLU E 342     6731   6650   4270   -584   -806   -148    C
ATOM   4091  CG  GLU E 342      25.137 -21.435 -29.509  1.00 48.29        C
ANISOU 4091  CG  GLU E 342     6913   6795   4640   -445  -1019     45    C
ATOM   4092  CD  GLU E 342      25.495 -20.511 -28.349  1.00 45.94        C
ANISOU 4092  CD  GLU E 342     6626   6233   4596   -356   -937    198    C
ATOM   4093  OE1 GLU E 342      24.616 -20.290 -27.494  1.00 46.26        O
ANISOU 4093  OE1 GLU E 342     6536   6152   4889   -245  -1012    183    O
ATOM   4094  OE2 GLU E 342      26.637 -19.996 -28.287  1.00 46.95        O
ANISOU 4094  OE2 GLU E 342     6881   6288   4671   -406   -794    315    O
ATOM   4095  C   GLU E 342      27.072 -24.059 -31.538  1.00 48.22        C
ANISOU 4095  C   GLU E 342     7028   7239   4056   -797   -676   -486    C
ATOM   4096  O   GLU E 342      27.501 -25.153 -31.181  1.00 47.12        O
ANISOU 4096  O   GLU E 342     6828   7042   4033   -837   -521   -734    O
ATOM   4097  N   GLU E 343      27.682 -23.303 -32.446  1.00 49.43        N
ANISOU 4097  N   GLU E 343     7330   7543   3907   -857   -673   -307    N
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Figure 18 (continued)

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ATOM   4098  CA  GLU E 343      28.980 -23.660 -32.998  1.00 49.39           C
ANISOU 4098  CA  GLU E 343    7407   7663   3698   -977   -452   -405       C
ATOM   4099  CB  GLU E 343      28.974 -23.575 -34.524  1.00 53.28           C
ANISOU 4099  CB  GLU E 343    8011   8493   3737  -1090   -528   -387       C
ATOM   4100  CG  GLU E 343      28.356 -24.787 -35.191  1.00 55.60           C
ANISOU 4100  CG  GLU E 343    8229   8984   3914  -1138   -598   -712       C
ATOM   4101  CD  GLU E 343      28.384 -24.690 -36.695  1.00 61.06           C
ANISOU 4101  CD  GLU E 343    9037  10045   4118  -1260   -671   -706       C
ATOM   4102  OE1 GLU E 343      29.354 -24.119 -37.237  1.00 63.45           O
ANISOU 4102  OE1 GLU E 343    9471  10471   4165  -1353   -536   -563       O
ATOM   4103  OE2 GLU E 343      27.437 -25.188 -37.339  1.00 64.46           O
ANISOU 4103  OE2 GLU E 343    9423  10659   4409  -1277   -862   -848       O
ATOM   4104  C   GLU E 343      30.096 -22.797 -32.435  1.00 47.41           C
ANISOU 4104  C   GLU E 343    7226   7262   3525   -983   -284   -209       C
ATOM   4105  O   GLU E 343      30.107 -21.573 -32.600  1.00 47.73           O
ANISOU 4105  O   GLU E 343    7377   7275   3484   -980   -360     94       O
ATOM   4106  N   VAL E 344      31.046 -23.454 -31.778  1.00 44.90           N
ANISOU 4106  N   VAL E 344    6843   6842   3375   -993    -63   -387       N
ATOM   4107  CA  VAL E 344      32.197 -22.761 -31.209  1.00 43.05           C
ANISOU 4107  CA  VAL E 344    6643   6486   3226  -1012    109   -252       C
ATOM   4108  CB  VAL E 344      32.331 -23.057 -29.702  1.00 39.90           C
ANISOU 4108  CB  VAL E 344    6131   5809   3220   -906    177   -321       C
ATOM   4109  CG1 VAL E 344      31.101 -22.518 -28.950  1.00 38.32           C
ANISOU 4109  CG1 VAL E 344    5899   5435   3226   -792    -14   -182       C
ATOM   4110  CG2 VAL E 344      32.487 -24.553 -29.465  1.00 38.73           C
ANISOU 4110  CG2 VAL E 344    5876   5650   3188   -889    269   -644       C
ATOM   4111  C   VAL E 344      33.490 -23.102 -31.963  1.00 44.32           C
ANISOU 4111  C   VAL E 344    6833   6849   3159  -1141    328   -377       C
ATOM   4112  O   VAL E 344      33.591 -24.158 -32.616  1.00 44.99           O
ANISOU 4112  O   VAL E 344    6878   7105   3111  -1182    386   -649       O
ATOM   4113  N   LEU E 345      34.471 -22.206 -31.883  1.00 43.87           N
ANISOU 4113  N   LEU E 345    6834   6773   3060  -1212    457   -199       N
ATOM   4114  CA  LEU E 345      35.747 -22.449 -32.550  1.00 45.58           C
ANISOU 4114  CA  LEU E 345    7050   7199   3071  -1345    689   -320       C
ATOM   4115  CB  LEU E 345      36.032 -21.390 -33.626  1.00 48.71           C
ANISOU 4115  CB  LEU E 345    7610   7796   3101  -1510    700    -58       C
ATOM   4116  CG  LEU E 345      35.431 -21.671 -35.017  1.00 53.49           C
ANISOU 4116  CG  LEU E 345    8310   8712   3302  -1592    600    -90       C
ATOM   4117  CD1 LEU E 345      35.111 -20.382 -35.775  1.00 57.03           C
ANISOU 4117  CD1 LEU E 345    8960   9243   3466  -1690    468    304       C
ATOM   4118  CD2 LEU E 345      36.333 -22.561 -35.889  1.00 56.50           C
ANISOU 4118  CD2 LEU E 345    8642   9402   3424  -1714    825   -394       C
ATOM   4119  C   LEU E 345      36.896 -22.595 -31.559  1.00 43.09           C
ANISOU 4119  C   LEU E 345    6618   6736   3019  -1317    884   -414       C
ATOM   4120  O   LEU E 345      37.045 -21.789 -30.628  1.00 41.78           O
ANISOU 4120  O   LEU E 345    6453   6357   3066  -1279    869   -231       O
ATOM   4121  N   THR E 346      37.683 -23.651 -31.742  1.00 42.92           N
ANISOU 4121  N   THR E 346    6486   6827   2994  -1323   1054   -721       N
ATOM   4122  CA  THR E 346      38.811 -23.942 -30.852  1.00 41.13           C
ANISOU 4122  CA  THR E 346    6122   6488   3017  -1274   1224   -845       C
ATOM   4123  CB  THR E 346      39.287 -25.407 -30.977  1.00 40.99           C
ANISOU 4123  CB  THR E 346    5972   6534   3070  -1207   1337  -1229       C
ATOM   4124  OG1 THR E 346      39.774 -25.630 -32.308  1.00 42.56           O
ANISOU 4124  OG1 THR E 346    6186   7057   2929  -1338   1471  -1380       O
ATOM   4125  CG2 THR E 346      38.155 -26.375 -30.640  1.00 38.07           C
ANISOU 4125  CG2 THR E 346    5595   6009   2863  -1084   1175  -1361       C
ATOM   4126  C   THR E 346      39.986 -23.035 -31.189  1.00 43.36           C
ANISOU 4126  C   THR E 346    6415   6908   3153  -1428   1402   -722       C
ATOM   4127  O   THR E 346      40.054 -22.483 -32.302  1.00 45.98           O
ANISOU 4127  O   THR E 346    6857   7467   3144  -1588   1441   -607       O
ATOM   4128  N   GLY E 347      40.919 -22.907 -30.244  1.00 42.34           N
ANISOU 4128  N   GLY E 347    6167   6654   3267  -1393   1511   -749       N
ATOM   4129  CA  GLY E 347      42.178 -22.198 -30.484  1.00 44.62           C
ANISOU 4129  CA  GLY E 347    6414   7080   3459  -1551   1710   -693       C
ATOM   4130  C   GLY E 347      42.936 -22.690 -31.716  1.00 48.49           C
ANISOU 4130  C   GLY E 347    6856   7916   3651  -1680   1913   -899       C
ATOM   4131  O   GLY E 347      43.950 -22.101 -32.104  1.00 50.47           O
ANISOU 4131  O   GLY E 347    7071   8338   3766  -1851   2101   -856       O
ATOM   4132  N   ASN E 348      42.442 -23.772 -32.316  1.00 49.38           N
ANISOU 4132  N   ASN E 348    6961   8138   3665  -1611   1882  -1139       N
ATOM   4133  CA  ASN E 348      43.017 -24.343 -33.522  1.00 53.66           C
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Figure 18 (continued)

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ANISOU 4133  CA  ASN E 348     7459   9021   3906  -1720   2064  -1385      C
ATOM   4134  CB  ASN E 348      43.303 -25.835 -33.302  1.00 53.90          C
ANISOU 4134  CB  ASN E 348     7316   9024   4141  -1548   2123  -1804      C
ATOM   4135  CG  ASN E 348      44.284 -26.389 -34.308  1.00 57.89          C
ANISOU 4135  CG  ASN E 348     7705   9868   4422  -1639   2373  -2119      C
ATOM   4136  OD1 ASN E 348      45.044 -25.643 -34.912  1.00 61.94          O
ANISOU 4136  OD1 ASN E 348     8216  10630   4689  -1832   2550  -2031      O
ATOM   4137  ND2 ASN E 348      44.272 -27.699 -34.497  1.00 59.86          N
ANISOU 4137  ND2 ASN E 348     7856  10127   4760  -1508   2399  -2498      N
ATOM   4138  C   ASN E 348      42.113 -24.173 -34.739  1.00 55.81          C
ANISOU 4138  C   ASN E 348     7918   9505   3784  -1834   1968  -1293      C
ATOM   4139  O   ASN E 348      42.448 -24.620 -35.833  1.00 59.14          O
ANISOU 4139  O   ASN E 348     8330  10245   3896  -1941   2104  -1495      O
ATOM   4140  N   LEU E 349      40.962 -23.532 -34.544  1.00 54.75          N
ANISOU 4140  N   LEU E 349     7942   9207   3654  -1805   1726  -1000      N
ATOM   4141  CA  LEU E 349      39.927 -23.424 -35.585  1.00 56.68          C
ANISOU 4141  CA  LEU E 349     8352   9623   3560  -1871   1566   -904      C
ATOM   4142  CB  LEU E 349      40.470 -22.725 -36.850  1.00 60.70          C
ANISOU 4142  CB  LEU E 349     8981  10485   3599  -2117   1702   -766      C
ATOM   4143  CG  LEU E 349      41.305 -21.440 -36.688  1.00 61.95          C
ANISOU 4143  CG  LEU E 349     9196  10613   3728  -2277   1827   -450      C
ATOM   4144  CD1 LEU E 349      42.160 -21.185 -37.940  1.00 65.27          C
ANISOU 4144  CD1 LEU E 349     9667  11441   3693  -2540   2062   -454      C
ATOM   4145  CD2 LEU E 349      40.447 -20.215 -36.321  1.00 60.69          C
ANISOU 4145  CD2 LEU E 349     9223  10201   3636  -2262   1587     -7      C
ATOM   4146  C   LEU E 349      39.218 -24.767 -35.944  1.00 56.66          C
ANISOU 4146  C   LEU E 349     8297   9686   3545  -1769   1484  -1246      C
ATOM   4147  O   LEU E 349      38.866 -24.994 -37.106  1.00 59.07          O
ANISOU 4147  O   LEU E 349     8682  10278   3484  -1869   1460  -1327      O
ATOM   4148  N   GLN E 350      39.005 -25.636 -34.947  1.00 53.61          N
ANISOU 4148  N   GLN E 350     7787   9033   3550  -1586   1436  -1439      N
ATOM   4149  CA  GLN E 350      38.133 -26.811 -35.108  1.00 53.10          C
ANISOU 4149  CA  GLN E 350     7691   8940   3543  -1494   1316  -1711      C
ATOM   4150  CB  GLN E 350      38.663 -28.028 -34.332  1.00 51.62          C
ANISOU 4150  CB  GLN E 350     7339   8560   3716  -1348   1419  -2042      C
ATOM   4151  CG  GLN E 350      37.873 -29.328 -34.565  1.00 52.67          C
ANISOU 4151  CG  GLN E 350     7445   8647   3921  -1280   1324  -2357      C
ATOM   4152  CD  GLN E 350      38.338 -30.499 -33.702  1.00 50.84          C
ANISOU 4152  CD  GLN E 350     7077   8154   4087  -1123   1397  -2632      C
ATOM   4153  OE1 GLN E 350      39.291 -30.387 -32.937  1.00 49.10          O
ANISOU 4153  OE1 GLN E 350     6767   7811   4078  -1049   1513  -2603      O
ATOM   4154  NE2 GLN E 350      37.658 -31.631 -33.831  1.00 50.04          N
ANISOU 4154  NE2 GLN E 350     6962   7961   4090  -1076   1317  -2896      N
ATOM   4155  C   GLN E 350      36.738 -26.435 -34.620  1.00 51.00          C
ANISOU 4155  C   GLN E 350     7502   8477   3398  -1419   1039  -1482      C
ATOM   4156  O   GLN E 350      36.586 -25.851 -33.553  1.00 48.42          O
ANISOU 4156  O   GLN E 350     7168   7889   3341  -1337    973  -1266      O
ATOM   4157  N   THR E 351      35.720 -26.751 -35.413  1.00 52.50          N
ANISOU 4157  N   THR E 351     7754   8813   3381  -1451    877  -1545      N
ATOM   4158  CA  THR E 351      34.345 -26.457 -35.043  1.00 51.35          C
ANISOU 4158  CA  THR E 351     7647   8521   3345  -1378    610  -1367      C
ATOM   4159  CB  THR E 351      33.426 -26.373 -36.272  1.00 54.37          C
ANISOU 4159  CB  THR E 351     8122   9185   3350  -1464    430  -1351      C
ATOM   4160  OG1 THR E 351      33.904 -25.359 -37.160  1.00 57.38          O
ANISOU 4160  OG1 THR E 351     8642   9811   3347  -1597    470  -1106      O
ATOM   4161  CG2 THR E 351      31.995 -26.030 -35.851  1.00 54.10          C
ANISOU 4161  CG2 THR E 351     8091   9006   3461  -1372    144  -1173      C
ATOM   4162  C   THR E 351      33.814 -27.529 -34.107  1.00 48.97          C
ANISOU 4162  C   THR E 351     7225   7955   3425  -1251    560  -1586      C
ATOM   4163  O   THR E 351      33.904 -28.716 -34.421  1.00 49.72          O
ANISOU 4163  O   THR E 351     7258   8093   3539  -1254    623  -1930      O
ATOM   4164  N   LEU E 352      33.273 -27.098 -32.966  1.00 45.92          N
ANISOU 4164  N   LEU E 352     6814   7296   3339  -1150    455  -1389      N
ATOM   4165  CA  LEU E 352      32.556 -27.983 -32.059  1.00 44.43          C
ANISOU 4165  CA  LEU E 352     6531   6865   3485  -1055    383  -1532      C
ATOM   4166  CB  LEU E 352      33.221 -28.020 -30.676  1.00 41.32          C
ANISOU 4166  CB  LEU E 352     6073   6188   3439   -957    494  -1483      C
ATOM   4167  CG  LEU E 352      34.668 -28.498 -30.506  1.00 41.46          C
ANISOU 4167  CG  LEU E 352     6040   6188   3524   -941    718  -1642      C
ATOM   4168  CD1 LEU E 352      35.062 -28.343 -29.037  1.00 38.52          C
ANISOU 4168  CD1 LEU E 352     5612   5540   3485   -837    755  -1527      C
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Figure 18 (continued)

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ATOM   4169  CD2 LEU E 352      34.921 -29.937 -30.990  1.00 42.58           C
ANISOU 4169  CD2 LEU E 352    6127   6363   3689   -938    799  -2023          C
ATOM   4170  C   LEU E 352      31.099 -27.545 -31.923  1.00 44.26           C
ANISOU 4170  C   LEU E 352    6514   6808   3497  -1026    139  -1372          C
ATOM   4171  O   LEU E 352      30.819 -26.372 -31.696  1.00 43.64           O
ANISOU 4171  O   LEU E 352    6483   6697   3400   -997     47  -1074          O
ATOM   4172  N   LYS E 353      30.182 -28.496 -32.077  1.00 45.32           N
ANISOU 4172  N   LYS E 353    6585   6943   3691  -1035     36  -1586          N
ATOM   4173  CA  LYS E 353      28.773 -28.271 -31.800  1.00 45.51           C
ANISOU 4173  CA  LYS E 353    6559   6921   3812  -1002   -182  -1491          C
ATOM   4174  CB  LYS E 353      27.921 -29.158 -32.701  1.00 47.91           C
ANISOU 4174  CB  LYS E 353    6823   7400   3979  -1081   -305  -1748          C
ATOM   4175  CG  LYS E 353      26.524 -28.628 -33.009  1.00 50.14           C
ANISOU 4175  CG  LYS E 353    7063   7798   4190  -1071   -572  -1626          C
ATOM   4176  CD  LYS E 353      25.789 -29.583 -33.964  1.00 53.59           C
ANISOU 4176  CD  LYS E 353    7450   8440   4472  -1172   -688  -1924          C
ATOM   4177  CE  LYS E 353      24.859 -28.824 -34.921  1.00 59.05           C
ANISOU 4177  CE  LYS E 353    8155   9414   4866  -1182   -955  -1782          C
ATOM   4178  NZ  LYS E 353      24.338 -29.667 -36.045  1.00 61.33           N
ANISOU 4178  NZ  LYS E 353    8416   9973   4912  -1300  -1066  -2081          N
ATOM   4179  C   LYS E 353      28.524 -28.604 -30.336  1.00 42.55           C
ANISOU 4179  C   LYS E 353    6095   6234   3837   -922   -146  -1482          C
ATOM   4180  O   LYS E 353      28.662 -29.747 -29.922  1.00 42.17           O
ANISOU 4180  O   LYS E 353    5995   6049   3977   -931    -59  -1705          O
ATOM   4181  N   ILE E 354      28.186 -27.597 -29.545  1.00 41.27           N
ANISOU 4181  N   ILE E 354    5923   5956   3801   -845   -209  -1222          N
ATOM   4182  CA  ILE E 354      27.891 -27.795 -28.136  1.00 39.35           C
ANISOU 4182  CA  ILE E 354    5599   5456   3897   -780   -175  -1195          C
ATOM   4183  CB  ILE E 354      28.992 -27.170 -27.205  1.00 37.50           C
ANISOU 4183  CB  ILE E 354    5404   5064   3781   -718    -28  -1037          C
ATOM   4184  CG1 ILE E 354      29.069 -25.650 -27.368  1.00 37.51           C
ANISOU 4184  CG1 ILE E 354    5473   5114   3665   -685    -92   -761          C
ATOM   4185  CD1 ILE E 354      29.800 -24.918 -26.225  1.00 35.25           C
ANISOU 4185  CD1 ILE E 354    5197   4643   3554   -625     11   -607          C
ATOM   4186  CG2 ILE E 354      30.370 -27.816 -27.461  1.00 36.99           C
ANISOU 4186  CG2 ILE E 354    5377   5012   3665   -747    157  -1184          C
ATOM   4187  C   ILE E 354      26.513 -27.229 -27.775  1.00 39.58           C
ANISOU 4187  C   ILE E 354    5544   5471   4023   -734   -358  -1077          C
ATOM   4188  O   ILE E 354      26.029 -26.280 -28.412  1.00 40.69           O
ANISOU 4188  O   ILE E 354    5712   5749   4001   -707   -510   -920          O
ATOM   4189  N   ARG E 355      25.880 -27.817 -26.764  1.00 38.29           N
ANISOU 4189  N   ARG E 355    5277   5147   4124   -726   -345  -1150          N
ATOM   4190  CA  ARG E 355      24.674 -27.225 -26.217  1.00 38.79           C
ANISOU 4190  CA  ARG E 355    5231   5189   4318   -672   -479  -1049          C
ATOM   4191  CB  ARG E 355      23.713 -28.293 -25.719  1.00 39.53           C
ANISOU 4191  CB  ARG E 355    5192   5223   4605   -741   -490  -1232          C
ATOM   4192  CG  ARG E 355      23.039 -29.024 -26.844  1.00 45.52           C
ANISOU 4192  CG  ARG E 355    5905   6160   5230   -836   -612  -1430          C
ATOM   4193  CD  ARG E 355      22.085 -30.055 -26.303  1.00 53.44           C
ANISOU 4193  CD  ARG E 355    6770   7084   6450   -932   -613  -1609          C
ATOM   4194  NE  ARG E 355      22.114 -31.290 -27.088  1.00 59.58           N
ANISOU 4194  NE  ARG E 355    7564   7903   7169  -1061   -606  -1876          N
ATOM   4195  CZ  ARG E 355      21.599 -32.454 -26.686  1.00 62.66           C
ANISOU 4195  CZ  ARG E 355    7882   8169   7757  -1181   -561  -2064          C
ATOM   4196  NH1 ARG E 355      21.011 -32.555 -25.495  1.00 61.48           N
ANISOU 4196  NH1 ARG E 355    7637   7868   7853  -1201   -510  -1999          N
ATOM   4197  NH2 ARG E 355      21.672 -33.527 -27.477  1.00 65.58           N
ANISOU 4197  NH2 ARG E 355    8278   8563   8076  -1295   -561  -2326          N
ATOM   4198  C   ARG E 355      25.064 -26.273 -25.116  1.00 36.09           C
ANISOU 4198  C   ARG E 355    4905   4689   4118   -577   -408   -850          C
ATOM   4199  O   ARG E 355      25.478 -26.709 -24.035  1.00 34.96           O
ANISOU 4199  O   ARG E 355    4749   4377   4156   -577   -270   -877          O
ATOM   4200  N   VAL E 356      24.969 -24.977 -25.411  1.00 35.53           N
ANISOU 4200  N   VAL E 356    4875   4668   3958   -499   -510   -651          N
ATOM   4201  CA  VAL E 356      25.331 -23.934 -24.460  1.00 32.64           C
ANISOU 4201  CA  VAL E 356    4532   4149   3721   -411   -457   -475          C
ATOM   4202  CB  VAL E 356      25.631 -22.604 -25.178  1.00 33.72           C
ANISOU 4202  CB  VAL E 356    4781   4333   3698   -360   -549   -256          C
ATOM   4203  CG1 VAL E 356      25.785 -21.456 -24.168  1.00 31.57           C
ANISOU 4203  CG1 VAL E 356    4517   3879   3601   -265   -523    -99          C
ATOM   4204  CG2 VAL E 356      26.875 -22.756 -26.040  1.00 33.21           C
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Figure 18 (continued)

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ANISOU 4204  CG2 VAL E 356     4859   4358   3403   -450   -446   -246       C
ATOM   4205  C   VAL E 356      24.208 -23.765 -23.447  1.00 31.55           C
ANISOU 4205  C   VAL E 356     4242   3932   3814   -346   -509   -488       C
ATOM   4206  O   VAL E 356      23.059 -23.558 -23.834  1.00 32.82           O
ANISOU 4206  O   VAL E 356     4300   4190   3980   -309   -675   -500       O
ATOM   4207  N   HIS E 357      24.545 -23.882 -22.160  1.00 28.73           N
ANISOU 4207  N   HIS E 357     3860   3421   3635   -336   -366   -497       N
ATOM   4208  CA  HIS E 357      23.592 -23.583 -21.092  1.00 27.88           C
ANISOU 4208  CA  HIS E 357     3613   3252   3728   -280   -380   -505       C
ATOM   4209  CB  HIS E 357      23.842 -24.457 -19.864  1.00 26.86           C
ANISOU 4209  CB  HIS E 357     3453   3014   3739   -344   -211   -589       C
ATOM   4210  CG  HIS E 357      23.454 -25.890 -20.068  1.00 25.78           C
ANISOU 4210  CG  HIS E 357     3270   2906   3619   -465   -186   -748       C
ATOM   4211  ND1 HIS E 357      22.343 -26.453 -19.475  1.00 27.87           N
ANISOU 4211  ND1 HIS E 357     3387   3180   4021   -525   -182   -843       N
ATOM   4212  CE1 HIS E 357      22.243 -27.719 -19.843  1.00 27.26           C
ANISOU 4212  CE1 HIS E 357     3312   3100   3943   -648   -160   -977       C
ATOM   4213  NE2 HIS E 357      23.247 -27.995 -20.658  1.00 28.04           N
ANISOU 4213  NE2 HIS E 357     3549   3196   3910   -650   -149   -990       N
ATOM   4214  CD2 HIS E 357      24.014 -26.867 -20.820  1.00 26.06           C
ANISOU 4214  CD2 HIS E 357     3383   2956   3561   -544   -159   -844       C
ATOM   4215  C   HIS E 357      23.597 -22.112 -20.736  1.00 27.57           C
ANISOU 4215  C   HIS E 357     3590   3142   3745   -155   -429   -350       C
ATOM   4216  O   HIS E 357      24.660 -21.522 -20.518  1.00 26.56           O
ANISOU 4216  O   HIS E 357     3583   2922   3587   -140   -349   -249       O
ATOM   4217  N   GLU E 358      22.399 -21.527 -20.715  1.00 28.31           N
ANISOU 4217  N   GLU E 358     3550   3275   3930    -63   -567   -348       N
ATOM   4218  CA  GLU E 358      22.216 -20.116 -20.449  1.00 28.24           C
ANISOU 4218  CA  GLU E 358     3543   3178   4010     80   -644   -222       C
ATOM   4219  CB  GLU E 358      21.452 -19.463 -21.593  1.00 30.21           C
ANISOU 4219  CB  GLU E 358     3775   3519   4186    174   -884   -133       C
ATOM   4220  CG  GLU E 358      22.112 -19.703 -22.953  1.00 31.27           C
ANISOU 4220  CG  GLU E 358     4073   3757   4051     94   -943    -48       C
ATOM   4221  CD  GLU E 358      21.291 -19.234 -24.129  1.00 35.58           C
ANISOU 4221  CD  GLU E 358     4604   4435   4480    170  -1200     41       C
ATOM   4222  OE1 GLU E 358      20.044 -19.336 -24.097  1.00 36.53           O
ANISOU 4222  OE1 GLU E 358     4532   4641   4708    242  -1341    -49       O
ATOM   4223  OE2 GLU E 358      21.915 -18.767 -25.108  1.00 40.00           O
ANISOU 4223  OE2 GLU E 358     5342   5029   4827    150  -1264    206       O
ATOM   4224  C   GLU E 358      21.481 -19.944 -19.121  1.00 28.03           C
ANISOU 4224  C   GLU E 358     3350   3095   4206    136   -577   -318       C
ATOM   4225  O   GLU E 358      20.399 -20.505 -18.923  1.00 28.19           O
ANISOU 4225  O   GLU E 358     3188   3214   4310    121   -606   -448       O
ATOM   4226  N   GLY E 359      22.095 -19.173 -18.223  1.00 26.47           N
ANISOU 4226  N   GLY E 359     3210   2755   4092    185   -480   -269       N
ATOM   4227  CA  GLY E 359      21.487 -18.828 -16.971  1.00 25.81           C
ANISOU 4227  CA  GLY E 359     2985   2630   4193    246   -409   -364       C
ATOM   4228  C   GLY E 359      22.386 -19.086 -15.810  1.00 23.40           C
ANISOU 4228  C   GLY E 359     2743   2248   3898    169   -211   -393       C
ATOM   4229  O   GLY E 359      23.253 -19.970 -15.866  1.00 23.25           O
ANISOU 4229  O   GLY E 359     2827   2236   3772     53   -119   -381       O
ATOM   4230  N   TYR E 360      22.143 -18.340 -14.742  1.00 23.60           N
ANISOU 4230  N   TYR E 360     2697   2212   4057    243   -154   -447       N
ATOM   4231  CA  TYR E 360      22.840 -18.486 -13.476  1.00 22.59           C
ANISOU 4231  CA  TYR E 360     2606   2041   3936    180     21   -491       C
ATOM   4232  CB  TYR E 360      22.563 -17.303 -12.523  1.00 24.19           C
ANISOU 4232  CB  TYR E 360     2742   2170   4279    292     47   -560       C
ATOM   4233  CG  TYR E 360      23.051 -17.586 -11.112  1.00 23.41           C
ANISOU 4233  CG  TYR E 360     2647   2087   4160    212    225   -639       C
ATOM   4234  CD1 TYR E 360      24.414 -17.521 -10.793  1.00 22.30           C
ANISOU 4234  CD1 TYR E 360     2665   1873   3936    153    290   -572       C
ATOM   4235  CE1 TYR E 360      24.866 -17.828  -9.505  1.00 23.08           C
ANISOU 4235  CE1 TYR E 360     2769   2011   3991     82    427   -634       C
ATOM   4236  CZ  TYR E 360      23.948 -18.220  -8.543  1.00 23.76           C
ANISOU 4236  CZ  TYR E 360     2717   2212   4098     51    519   -752       C
ATOM   4237  OH  TYR E 360      24.387 -18.506  -7.272  1.00 25.07           O
ANISOU 4237  OH  TYR E 360     2903   2436   4185    -28    647   -795       O
ATOM   4238  CE2 TYR E 360      22.593 -18.299  -8.837  1.00 23.70           C
ANISOU 4238  CE2 TYR E 360     2542   2282   4181     91    483   -829       C
ATOM   4239  CD2 TYR E 360      22.156 -17.984 -10.118  1.00 24.20           C
ANISOU 4239  CD2 TYR E 360     2586   2303   4305    179    326   -777       C
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Figure 18 (continued)

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ATOM   4240  C   TYR E 360      22.448 -19.792 -12.804  1.00 22.00           C
ANISOU 4240  C   TYR E 360    2446   2074   3840     52    139   -585       C
ATOM   4241  O   TYR E 360      21.253 -20.113 -12.717  1.00 23.47           O
ANISOU 4241  O   TYR E 360    2461   2361   4097     47    124   -681       O
ATOM   4242  N   GLU E 361      23.457 -20.544 -12.352  1.00 20.15           N
ANISOU 4242  N   GLU E 361    2328   1813   3516    -52    249   -550       N
ATOM   4243  CA  GLU E 361      23.240 -21.781 -11.604  1.00 20.24           C
ANISOU 4243  CA  GLU E 361    2302   1881   3506   -182    365   -600       C
ATOM   4244  CB  GLU E 361      23.280 -23.001 -12.533  1.00 20.04           C
ANISOU 4244  CB  GLU E 361    2319   1870   3425   -274    330   -587       C
ATOM   4245  CG  GLU E 361      22.084 -23.147 -13.487  1.00 20.79           C
ANISOU 4245  CG  GLU E 361    2284   2055   3561   -270    215   -651       C
ATOM   4246  CD  GLU E 361      22.262 -24.295 -14.477  1.00 22.54           C
ANISOU 4246  CD  GLU E 361    2567   2285   3713   -366    176   -664       C
ATOM   4247  OE1 GLU E 361      23.309 -24.332 -15.160  1.00 21.63           O
ANISOU 4247  OE1 GLU E 361    2597   2118   3502   -350    153   -602       O
ATOM   4248  OE2 GLU E 361      21.336 -25.150 -14.592  1.00 25.55           O
ANISOU 4248  OE2 GLU E 361    2839   2731   4140   -464    173   -754       O
ATOM   4249  C   GLU E 361      24.332 -21.935 -10.561  1.00 19.23           C
ANISOU 4249  C   GLU E 361    2283   1704   3319   -225    479   -560       C
ATOM   4250  O   GLU E 361      25.489 -21.586 -10.802  1.00 18.49           O
ANISOU 4250  O   GLU E 361    2312   1537   3174   -195    463   -490       O
ATOM   4251  N   GLU E 362      23.965 -22.487  -9.413  1.00 19.76           N
ANISOU 4251  N   GLU E 362    2298   1827   3381   -307    593   -601       N
ATOM   4252  CA  GLU E 362      24.937 -22.899  -8.402  1.00 19.50           C
ANISOU 4252  CA  GLU E 362    2372   1771   3266   -364    684   -547       C
ATOM   4253  CB  GLU E 362      24.684 -22.172  -7.076  1.00 19.25           C
ANISOU 4253  CB  GLU E 362    2279   1811   3225   -354    772   -615       C
ATOM   4254  CG  GLU E 362      25.760 -22.371  -6.025  1.00 21.30           C
ANISOU 4254  CG  GLU E 362    2650   2069   3375   -395    835   -559       C
ATOM   4255  CD  GLU E 362      25.377 -21.770  -4.703  1.00 25.48           C
ANISOU 4255  CD  GLU E 362    3112   2708   3863   -409    932   -651       C
ATOM   4256  OE1 GLU E 362      25.884 -20.702  -4.358  1.00 29.65           O
ANISOU 4256  OE1 GLU E 362    3651   3221   4393   -334    920   -709       O
ATOM   4257  OE2 GLU E 362      24.528 -22.338  -4.008  1.00 33.55           O
ANISOU 4257  OE2 GLU E 362    4062   3839   4848   -507   1030   -680       O
ATOM   4258  C   GLU E 362      24.871 -24.422  -8.213  1.00 19.37           C
ANISOU 4258  C   GLU E 362    2397   1748   3215   -498    738   -502       C
ATOM   4259  O   GLU E 362      23.795 -24.978  -8.171  1.00 20.68           O
ANISOU 4259  O   GLU E 362    2465   1971   3423   -582    771   -549       O
ATOM   4260  N   PHE E 363      26.034 -25.068  -8.098  1.00 19.27           N
ANISOU 4260  N   PHE E 363    2522   1656   3143   -514    741   -414       N
ATOM   4261  CA  PHE E 363      26.136 -26.509  -7.875  1.00 20.25           C
ANISOU 4261  CA  PHE E 363    2717   1722   3257   -621    778   -353       C
ATOM   4262  CB  PHE E 363      26.740 -27.207  -9.116  1.00 19.58           C
ANISOU 4262  CB  PHE E 363    2705   1534   3201   -599    705   -347       C
ATOM   4263  CG  PHE E 363      25.919 -27.074 -10.368  1.00 19.78           C
ANISOU 4263  CG  PHE E 363    2651   1593   3274   -596    638   -432       C
ATOM   4264  CD1 PHE E 363      24.935 -28.007 -10.676  1.00 22.26           C
ANISOU 4264  CD1 PHE E 363    2909   1905   3645   -708    644   -486       C
ATOM   4265  CE1 PHE E 363      24.176 -27.899 -11.843  1.00 22.61           C
ANISOU 4265  CE1 PHE E 363    2868   2006   3717   -706    560   -575       C
ATOM   4266  CZ  PHE E 363      24.434 -26.853 -12.731  1.00 21.83           C
ANISOU 4266  CZ  PHE E 363    2762   1956   3576   -585    467   -582       C
ATOM   4267  CE2 PHE E 363      25.409 -25.906 -12.425  1.00 21.29           C
ANISOU 4267  CE2 PHE E 363    2764   1866   3461   -485    474   -512       C
ATOM   4268  CD2 PHE E 363      26.145 -26.028 -11.248  1.00 21.29           C
ANISOU 4268  CD2 PHE E 363    2826   1817   3445   -493    560   -452       C
ATOM   4269  C   PHE E 363      27.072 -26.809  -6.708  1.00 20.24           C
ANISOU 4269  C   PHE E 363    2818   1699   3172   -634    823   -258       C
ATOM   4270  O   PHE E 363      28.019 -26.078  -6.466  1.00 18.19           O
ANISOU 4270  O   PHE E 363    2595   1448   2868   -549    797   -245       O
ATOM   4271  N   THR E 364      26.798 -27.908  -6.012  1.00 21.35           N
ANISOU 4271  N   THR E 364    3007   1811   3294   -749    880   -184       N
ATOM   4272  CA  THR E 364      27.846 -28.619  -5.311  1.00 21.53           C
ANISOU 4272  CA  THR E 364    3165   1757   3258   -747    870    -57       C
ATOM   4273  CB  THR E 364      27.360 -29.262  -3.994  1.00 23.12           C
ANISOU 4273  CB  THR E 364    3410   2001   3374   -884    958     47       C
ATOM   4274  OG1 THR E 364      26.505 -30.365  -4.288  1.00 23.16           O
ANISOU 4274  OG1 THR E 364    3422   1920   3459  -1022    996     71       O
ATOM   4275  CG2 THR E 364      26.661 -28.251  -3.101  1.00 21.80           C
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Figure 18 (continued)

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ANISOU 4275  CG2 THR E 364     3139   2030   3113   -919   1046    -24       C
ATOM   4276  C   THR E 364      28.359 -29.730  -6.241  1.00 21.92           C
ANISOU 4276  C   THR E 364     3296   1633   3398   -732    808    -30       C
ATOM   4277  O   THR E 364      27.586 -30.289  -7.010  1.00 21.17           O
ANISOU 4277  O   THR E 364     3168   1488   3387   -800    812    -88       O
ATOM   4278  N   MSE E 365      29.664 -30.009  -6.154  1.00 21.90           N
ANISOU 4278  N   MSE E 365     3384   1553   3386   -638    750     34       N
ATOM   4279  CA  MSE E 365      30.337 -31.060  -6.894  1.00 23.37           C
ANISOU 4279  CA  MSE E 365     3644   1570   3666   -594    695     41       C
ATOM   4280  CB  MSE E 365      31.472 -30.506  -7.757  1.00 21.74           C
ANISOU 4280  CB  MSE E 365     3414   1378   3470   -454    639    -36       C
ATOM   4281  CG  MSE E 365      31.045 -29.545  -8.842  1.00 23.13           C
ANISOU 4281  CG  MSE E 365     3502   1647   3639   -443    640   -154       C
ATOM   4282  SE  MSE E 365      32.526 -28.585  -9.625  0.90 23.40          SE
ANISOU 4282  SE  MSE E 365     3512   1739   3638   -313    602   -208      SE
ATOM   4283  CE  MSE E 365      33.771 -30.022  -9.974  1.00 18.37           C
ANISOU 4283  CE  MSE E 365     2937    958   3086   -233    569   -221       C
ATOM   4284  C   MSE E 365      30.960 -31.945  -5.849  1.00 24.00           C
ANISOU 4284  C   MSE E 365     3840   1550   3729   -592    674    197       C
ATOM   4285  O   MSE E 365      31.712 -31.448  -5.007  1.00 24.02           O
ANISOU 4285  O   MSE E 365     3857   1634   3635   -529    647    264       O
ATOM   4286  N   VAL E 366      30.647 -33.239  -5.897  1.00 24.70           N
ANISOU 4286  N   VAL E 366     4015   1459   3911   -665    674    257       N
ATOM   4287  CA  VAL E 366      31.225 -34.211  -4.985  1.00 26.44           C
ANISOU 4287  CA  VAL E 366     4372   1538   4136   -656    631    436       C
ATOM   4288  CB  VAL E 366      30.132 -34.805  -4.045  1.00 28.13           C
ANISOU 4288  CB  VAL E 366     4654   1731   4302   -858    710    576       C
ATOM   4289  CG1 VAL E 366      30.702 -35.906  -3.156  1.00 29.65           C
ANISOU 4289  CG1 VAL E 366     5023   1742   4502   -858    650    802       C
ATOM   4290  CG2 VAL E 366      29.493 -33.697  -3.201  1.00 27.64           C
ANISOU 4290  CG2 VAL E 366     4506   1933   4062   -936    796    572       C
ATOM   4291  C   VAL E 366      31.984 -35.333  -5.738  1.00 27.40           C
ANISOU 4291  C   VAL E 366     4567   1412   4432   -557    553    413       C
ATOM   4292  O   VAL E 366      31.382 -36.089  -6.501  1.00 27.59           O
ANISOU 4292  O   VAL E 366     4608   1292   4584   -633    575    335       O
ATOM   4293  N   GLY E 367      33.293 -35.428  -5.493  1.00 28.19           N
ANISOU 4293  N   GLY E 367     4697   1473   4542   -388    461    462       N
ATOM   4294  CA  GLY E 367      34.123 -36.526  -5.992  1.00 30.20           C
ANISOU 4294  CA  GLY E 367     5014   1486   4973   -261    380    446       C
ATOM   4295  C   GLY E 367      34.685 -37.405  -4.894  1.00 33.69           C
ANISOU 4295  C   GLY E 367     5595   1766   5439   -206    286    673       C
ATOM   4296  O   GLY E 367      34.376 -37.209  -3.720  1.00 34.80           O
ANISOU 4296  O   GLY E 367     5797   1996   5427   -292    292    858       O
ATOM   4297  N   LYS E 368      35.498 -38.390  -5.273  1.00 35.94           N
ANISOU 4297  N   LYS E 368     5932   1812   5911    -57    196    658       N
ATOM   4298  CA  LYS E 368      36.162 -39.264  -4.312  1.00 38.97           C
ANISOU 4298  CA  LYS E 368     6451   2010   6347     42     69    884       C
ATOM   4299  CB  LYS E 368      36.914 -40.385  -5.031  1.00 41.21           C
ANISOU 4299  CB  LYS E 368     6767   1990   6901    219    -19    796       C
ATOM   4300  CG  LYS E 368      36.054 -41.402  -5.755  1.00 44.82           C
ANISOU 4300  CG  LYS E 368     7315   2166   7548     97     41    717       C
ATOM   4301  CD  LYS E 368      36.966 -42.427  -6.402  1.00 52.13           C
ANISOU 4301  CD  LYS E 368     8260   2799   8749    311    -54    600       C
ATOM   4302  CE  LYS E 368      36.378 -43.018  -7.678  1.00 55.25           C
ANISOU 4302  CE  LYS E 368     8645   3030   9319    233     28    339       C
ATOM   4303  NZ  LYS E 368      37.081 -44.304  -8.039  1.00 58.01           N
ANISOU 4303  NZ  LYS E 368     9071   2998   9973    415    -68    265       N
ATOM   4304  C   LYS E 368      37.163 -38.513  -3.429  1.00 38.51           C
ANISOU 4304  C   LYS E 368     6337   2165   6130    175    -25    979       C
ATOM   4305  O   LYS E 368      37.330 -38.848  -2.254  1.00 40.15           O
ANISOU 4305  O   LYS E 368     6662   2346   6248    176   -113   1226       O
ATOM   4306  N   ARG E 369      37.827 -37.509  -4.010  1.00 36.39           N
ANISOU 4306  N   ARG E 369     5893   2111   5823    272    -10    786       N
ATOM   4307  CA  ARG E 369      39.003 -36.893  -3.397  1.00 36.20           C
ANISOU 4307  CA  ARG E 369     5782   2263   5708    423   -115    816       C
ATOM   4308  CB  ARG E 369      40.271 -37.288  -4.170  1.00 37.98           C
ANISOU 4308  CB  ARG E 369     5899   2401   6129    655   -198    665       C
ATOM   4309  CG  ARG E 369      40.565 -38.794  -4.243  1.00 41.98           C
ANISOU 4309  CG  ARG E 369     6520   2561   6871    788   -303    738       C
ATOM   4310  CD  ARG E 369      42.027 -39.098  -3.979  1.00 47.29           C
ANISOU 4310  CD  ARG E 369     7105   3211   7651   1057   -473    743       C
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Figure 18 (continued)

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ATOM   4311  NE  ARG E 369      42.155 -39.943  -2.787  1.00 54.15           N
ANISOU 4311  NE  ARG E 369    8144   3905   8525   1121   -641   1046        N
ATOM   4312  CZ  ARG E 369      42.934 -39.702  -1.733  1.00 55.72           C
ANISOU 4312  CZ  ARG E 369    8323   4243   8606   1231   -801   1209        C
ATOM   4313  NH1 ARG E 369      43.718 -38.625  -1.680  1.00 54.95           N
ANISOU 4313  NH1 ARG E 369    8026   4461   8393   1288   -814   1079        N
ATOM   4314  NH2 ARG E 369      42.930 -40.558  -0.724  1.00 58.26           N
ANISOU 4314  NH2 ARG E 369    8832   4383   8920   1274   -956   1510        N
ATOM   4315  C   ARG E 369      38.934 -35.380  -3.308  1.00 33.75           C
ANISOU 4315  C   ARG E 369    5345   2273   5207    348    -39    717        C
ATOM   4316  O   ARG E 369      39.914 -34.725  -2.945  1.00 34.16           O
ANISOU 4316  O   ARG E 369    5295   2491   5191    450   -111    692        O
ATOM   4317  N   ALA E 370      37.792 -34.814  -3.675  1.00 31.33           N
ANISOU 4317  N   ALA E 370    5030   2041   4833    176     99    647        N
ATOM   4318  CA  ALA E 370      37.559 -33.400  -3.527  1.00 28.93           C
ANISOU 4318  CA  ALA E 370    4628   1995   4370    100    169    566        C
ATOM   4319  CB  ALA E 370      38.363 -32.620  -4.535  1.00 27.23           C
ANISOU 4319  CB  ALA E 370    4264   1875   4207    190    183    368        C
ATOM   4320  C   ALA E 370      36.067 -33.095  -3.648  1.00 28.11           C
ANISOU 4320  C   ALA E 370    4547   1924   4208    -87    299    547        C
ATOM   4321  O   ALA E 370      35.301 -33.902  -4.202  1.00 28.06           O
ANISOU 4321  O   ALA E 370    4597   1757   4307   -159    342    541        O
ATOM   4322  N   THR E 371      35.662 -31.950  -3.090  1.00 27.19           N
ANISOU 4322  N   THR E 371    4377   2016   3936   -165    354    524        N
ATOM   4323  CA  THR E 371      34.304 -31.425  -3.247  1.00 26.56           C
ANISOU 4323  CA  THR E 371    4270   2009   3814   -313    474    464        C
ATOM   4324  CB  THR E 371      33.385 -31.679  -2.005  1.00 28.20           C
ANISOU 4324  CB  THR E 371    4554   2275   3886   -460    531    605        C
ATOM   4325  OG1 THR E 371      33.794 -30.847  -0.909  1.00 29.59           O
ANISOU 4325  OG1 THR E 371    4714   2648   3883   -451    514    632        O
ATOM   4326  CG2 THR E 371      33.393 -33.154  -1.572  1.00 28.40           C
ANISOU 4326  CG2 THR E 371    4730   2103   3955   -493    486    799        C
ATOM   4327  C   THR E 371      34.395 -29.935  -3.534  1.00 25.42           C
ANISOU 4327  C   THR E 371    4005   2038   3615   -293    508    318        C
ATOM   4328  O   THR E 371      35.432 -29.303  -3.270  1.00 26.43           O
ANISOU 4328  O   THR E 371    4090   2253   3699   -209    452    292        O
ATOM   4329  N   ALA E 372      33.332 -29.363  -4.091  1.00 23.65           N
ANISOU 4329  N   ALA E 372    3723   1856   3408   -370    590    222        N
ATOM   4330  CA  ALA E 372      33.374 -27.962  -4.454  1.00 21.68           C
ANISOU 4330  CA  ALA E 372    3378   1723   3137   -344    611     98        C
ATOM   4331  CB  ALA E 372      34.062 -27.763  -5.828  1.00 20.08           C
ANISOU 4331  CB  ALA E 372    3135   1466   3029   -263    579     10        C
ATOM   4332  C   ALA E 372      32.005 -27.314  -4.448  1.00 20.75           C
ANISOU 4332  C   ALA E 372    3202   1678   3005   -430    691     32        C
ATOM   4333  O   ALA E 372      30.976 -28.000  -4.439  1.00 20.60           O
ANISOU 4333  O   ALA E 372    3192   1627   3010   -519    740     58        O
ATOM   4334  N   ILE E 373      32.007 -25.988  -4.420  1.00 19.68           N
ANISOU 4334  N   ILE E 373    2997   1635   2845   -402    704    -60        N
ATOM   4335  CA  ILE E 373      30.801 -25.212  -4.699  1.00 20.41           C
ANISOU 4335  CA  ILE E 373    3008   1776   2971   -434    756   -152        C
ATOM   4336  CB  ILE E 373      30.356 -24.310  -3.515  1.00 21.75           C
ANISOU 4336  CB  ILE E 373    3130   2078   3058   -463    816   -213        C
ATOM   4337  CG1 ILE E 373      30.315 -25.102  -2.203  1.00 22.01           C
ANISOU 4337  CG1 ILE E 373    3221   2184   2956   -546    858   -120        C
ATOM   4338  CD1 ILE E 373      29.912 -24.273  -0.985  1.00 23.87           C
ANISOU 4338  CD1 ILE E 373    3410   2587   3072   -587    931   -202        C
ATOM   4339  CG2 ILE E 373      28.992 -23.701  -3.819  1.00 22.34           C
ANISOU 4339  CG2 ILE E 373    3098   2190   3199   -479    868   -317        C
ATOM   4340  C   ILE E 373      31.126 -24.332  -5.891  1.00 19.23           C
ANISOU 4340  C   ILE E 373    2823   1587   2896   -361    711   -221        C
ATOM   4341  O   ILE E 373      32.156 -23.665  -5.899  1.00 18.51           O
ANISOU 4341  O   ILE E 373    2742   1500   2792   -313    680   -234        O
ATOM   4342  N   LEU E 374      30.252 -24.362  -6.898  1.00 18.79           N
ANISOU 4342  N   LEU E 374    2728   1502   2910   -368    705   -257        N
ATOM   4343  CA  LEU E 374      30.467 -23.673  -8.176  1.00 17.10           C
ANISOU 4343  CA  LEU E 374    2503   1253   2742   -312    653   -288        C
ATOM   4344  CB  LEU E 374      30.623 -24.697  -9.314  1.00 17.63           C
ANISOU 4344  CB  LEU E 374    2605   1264   2828   -322    623   -275        C
ATOM   4345  CG  LEU E 374      30.560 -24.218 -10.764  1.00 17.47           C
ANISOU 4345  CG  LEU E 374    2579   1243   2816   -294    572   -302        C
ATOM   4346  CD1 LEU E 374      31.820 -23.383 -11.076  1.00 17.18           C
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Figure 18 (continued)

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ANISOU 4346  CD1 LEU E 374     2575   1203   2747   -255    564   -283       C
ATOM   4347  CD2 LEU E 374      30.469 -25.360 -11.696  1.00 17.08           C
ANISOU 4347  CD2 LEU E 374     2553   1165   2772   -323    556   -327       C
ATOM   4348  C   LEU E 374      29.286 -22.786  -8.498  1.00 16.92           C
ANISOU 4348  C   LEU E 374     2401   1258   2770   -295    642   -348       C
ATOM   4349  O   LEU E 374      28.126 -23.249  -8.481  1.00 15.98           O
ANISOU 4349  O   LEU E 374     2218   1172   2681   -335    659   -377       O
ATOM   4350  N   ARG E 375      29.570 -21.498  -8.726  1.00 16.55           N
ANISOU 4350  N   ARG E 375     2349   1192   2748   -236    611   -368       N
ATOM   4351  CA  ARG E 375      28.615 -20.620  -9.352  1.00 17.49           C
ANISOU 4351  CA  ARG E 375     2408   1298   2938   -184    562   -403       C
ATOM   4352  CB  ARG E 375      28.483 -19.295  -8.633  1.00 18.68           C
ANISOU 4352  CB  ARG E 375     2524   1428   3145   -130    572   -466       C
ATOM   4353  CG  ARG E 375      27.717 -19.389  -7.371  1.00 20.56           C
ANISOU 4353  CG  ARG E 375     2678   1751   3384   -149    650   -557       C
ATOM   4354  CD  ARG E 375      27.873 -18.091  -6.582  1.00 21.88           C
ANISOU 4354  CD  ARG E 375     2826   1893   3596    -98    670   -652       C
ATOM   4355  NE  ARG E 375      27.046 -18.192  -5.379  1.00 25.86           N
ANISOU 4355  NE  ARG E 375     3235   2515   4078   -123    763   -765       N
ATOM   4356  CZ  ARG E 375      27.146 -17.421  -4.310  1.00 26.86           C
ANISOU 4356  CZ  ARG E 375     3334   2677   4193   -112    819   -885       C
ATOM   4357  NH1 ARG E 375      28.046 -16.437  -4.266  1.00 25.55           N
ANISOU 4357  NH1 ARG E 375     3231   2415   4060    -78    782   -912       N
ATOM   4358  NH2 ARG E 375      26.320 -17.641  -3.296  1.00 29.10           N
ANISOU 4358  NH2 ARG E 375     3524   3103   4428   -151    921   -990       N
ATOM   4359  C   ARG E 375      29.014 -20.386 -10.800  1.00 18.25           C
ANISOU 4359  C   ARG E 375     2561   1348   3024   -160    485   -343       C
ATOM   4360  O   ARG E 375      30.185 -20.109 -11.131  1.00 17.38           O
ANISOU 4360  O   ARG E 375     2525   1203   2875   -168    486   -298       O
ATOM   4361  N   LYS E 376      28.012 -20.433 -11.660  1.00 18.54           N
ANISOU 4361  N   LYS E 376     2552   1405   3088   -138    418   -348       N
ATOM   4362  CA  LYS E 376      28.255 -20.335 -13.071  1.00 19.40           C
ANISOU 4362  CA  LYS E 376     2719   1506   3147   -130    341   -288       C
ATOM   4363  CB  LYS E 376      28.315 -21.771 -13.583  1.00 20.73           C
ANISOU 4363  CB  LYS E 376     2900   1723   3255   -198    357   -310       C
ATOM   4364  CG  LYS E 376      28.136 -21.939 -15.015  1.00 24.60           C
ANISOU 4364  CG  LYS E 376     3416   2255   3675   -204    277   -295       C
ATOM   4365  CD  LYS E 376      27.437 -23.258 -15.295  1.00 25.85           C
ANISOU 4365  CD  LYS E 376     3527   2461   3833   -265    272   -374       C
ATOM   4366  CE  LYS E 376      27.641 -23.566 -16.743  1.00 24.77           C
ANISOU 4366  CE  LYS E 376     3442   2383   3587   -287    210   -382       C
ATOM   4367  NZ  LYS E 376      26.874 -22.594 -17.523  1.00 26.75           N
ANISOU 4367  NZ  LYS E 376     3667   2688   3807   -233     84   -331       N
ATOM   4368  C   LYS E 376      27.119 -19.526 -13.719  1.00 19.69           C
ANISOU 4368  C   LYS E 376     2697   1543   3240    -55    230   -279       C
ATOM   4369  O   LYS E 376      26.022 -19.438 -13.178  1.00 19.19           O
ANISOU 4369  O   LYS E 376     2517   1510   3263    -17    221   -351       O
ATOM   4370  N   ALA E 377      27.402 -18.913 -14.861  1.00 19.87           N
ANISOU 4370  N   ALA E 377     2797   1542   3209    -31    144   -188       N
ATOM   4371  CA  ALA E 377      26.369 -18.220 -15.644  1.00 21.63           C
ANISOU 4371  CA  ALA E 377     2981   1768   3469     54      0   -149       C
ATOM   4372  CB  ALA E 377      26.452 -16.693 -15.458  1.00 21.14           C
ANISOU 4372  CB  ALA E 377     2959   1567   3505    144    -50    -82       C
ATOM   4373  C   ALA E 377      26.594 -18.616 -17.102  1.00 21.95           C
ANISOU 4373  C   ALA E 377     3102   1884   3355      9    -75    -74       C
ATOM   4374  O   ALA E 377      27.330 -19.549 -17.351  1.00 21.69           O
ANISOU 4374  O   ALA E 377     3116   1904   3222    -80      1   -102       O
ATOM   4375  N   THR E 378      25.972 -17.923 -18.050  1.00 23.90           N
ANISOU 4375  N   THR E 378     3362   2140   3578     76   -228      13       N
ATOM   4376  CA  THR E 378      26.139 -18.227 -19.483  1.00 25.60           C
ANISOU 4376  CA  THR E 378     3662   2460   3605     26   -310      87       C
ATOM   4377  CB  THR E 378      25.299 -17.275 -20.380  1.00 27.85           C
ANISOU 4377  CB  THR E 378     3960   2747   3875    127   -515    214       C
ATOM   4378  OG1 THR E 378      23.947 -17.261 -19.926  1.00 29.57           O
ANISOU 4378  OG1 THR E 378     4001   2984   4250    234   -608    120       O
ATOM   4379  CG2 THR E 378      25.304 -17.743 -21.851  1.00 30.08           C
ANISOU 4379  CG2 THR E 378     4315   3193   3920     64   -612    270       C
ATOM   4380  C   THR E 378      27.615 -18.190 -19.933  1.00 25.01           C
ANISOU 4380  C   THR E 378     3737   2377   3386    -74   -208    164       C
ATOM   4381  O   THR E 378      28.215 -17.115 -20.060  1.00 25.04           O
ANISOU 4381  O   THR E 378     3843   2284   3387    -70   -212    297       O
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Figure 18 (continued)

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ATOM   4382  N   ARG E 379      28.184 -19.373 -20.172  1.00 24.99           N
ANISOU 4382  N   ARG E 379    3740   2472   3282   -166   -114     69       N
ATOM   4383  CA  ARG E 379      29.589 -19.500 -20.611  1.00 25.62           C
ANISOU 4383  CA  ARG E 379    3921   2580   3232   -258     -1     97       C
ATOM   4384  CB  ARG E 379      29.750 -19.126 -22.102  1.00 27.18           C
ANISOU 4384  CB  ARG E 379    4227   2889   3212   -308    -73    210       C
ATOM   4385  CG  ARG E 379      28.814 -19.879 -23.053  1.00 28.80           C
ANISOU 4385  CG  ARG E 379    4399   3250   3295   -310   -189    143       C
ATOM   4386  CD  ARG E 379      29.241 -19.684 -24.521  1.00 29.35           C
ANISOU 4386  CD  ARG E 379    4591   3475   3087   -391   -225    235       C
ATOM   4387  NE  ARG E 379      30.539 -20.308 -24.733  1.00 29.26           N
ANISOU 4387  NE  ARG E 379    4615   3531   2972   -495    -44    147       N
ATOM   4388  CZ  ARG E 379      31.290 -20.180 -25.826  1.00 30.78           C
ANISOU 4388  CZ  ARG E 379    4907   3869   2920   -596      5    198       C
ATOM   4389  NH1 ARG E 379      30.879 -19.451 -26.857  1.00 32.74           N
ANISOU 4389  NH1 ARG E 379    5258   4210   2972   -620   -124    368       N
ATOM   4390  NH2 ARG E 379      32.460 -20.789 -25.883  1.00 28.70           N
ANISOU 4390  NH2 ARG E 379    4634   3667   2604   -672    184     78       N
ATOM   4391  C   ARG E 379      30.531 -18.661 -19.737  1.00 25.30           C
ANISOU 4391  C   ARG E 379    3915   2410   3286   -262     92     154      C
ATOM   4392  O   ARG E 379      31.356 -17.912 -20.253  1.00 26.75           O
ANISOU 4392  O   ARG E 379    4194   2579   3389   -319    119     264      O
ATOM   4393  N   ARG E 380      30.394 -18.803 -18.417  1.00 25.10           N
ANISOU 4393  N   ARG E 380    3810   2304   3421   -220    143      73       N
ATOM   4394  CA  ARG E 380      31.158 -18.022 -17.438  1.00 25.31           C
ANISOU 4394  CA  ARG E 380    3851   2220   3547   -222    216      92       C
ATOM   4395  CB  ARG E 380      30.500 -16.655 -17.212  1.00 26.33           C
ANISOU 4395  CB  ARG E 380    3995   2220   3788   -147    126     171      C
ATOM   4396  CG  ARG E 380      31.262 -15.682 -16.289  1.00 27.56           C
ANISOU 4396  CG  ARG E 380    4176   2243   4052   -160    190     176      C
ATOM   4397  CD  ARG E 380      30.391 -14.433 -16.058  1.00 30.89           C
ANISOU 4397  CD  ARG E 380    4602   2511   4622    -58     88     218      C
ATOM   4398  NE  ARG E 380      30.622 -13.828 -14.744  1.00 38.11           N
ANISOU 4398  NE  ARG E 380    5478   3322   5681    -38    149     120      N
ATOM   4399  CZ  ARG E 380      29.754 -13.045 -14.114  1.00 42.71           C
ANISOU 4399  CZ  ARG E 380    6009   3793   6425     71     96      61      C
ATOM   4400  NH1 ARG E 380      28.579 -12.763 -14.675  1.00 45.06           N
ANISOU 4400  NH1 ARG E 380    6275   4064   6780    186    -32     102      N
ATOM   4401  NH2 ARG E 380      30.059 -12.552 -12.914  1.00 44.78           N
ANISOU 4401  NH2 ARG E 380    6238   3985   6791     72    166     -57      N
ATOM   4402  C   ARG E 380      31.203 -18.783 -16.134  1.00 23.46           C
ANISOU 4402  C   ARG E 380    3532   1980   3404   -208    293     -29      C
ATOM   4403  O   ARG E 380      30.167 -19.189 -15.617  1.00 24.09           O
ANISOU 4403  O   ARG E 380    3534   2067   3551   -163    264     -91      O
ATOM   4404  N   LEU E 381      32.405 -19.005 -15.619  1.00 22.65           N
ANISOU 4404  N   LEU E 381    3438   1877   3293   -254    389     -57      N
ATOM   4405  CA  LEU E 381      32.583 -19.406 -14.222  1.00 21.63           C
ANISOU 4405  CA  LEU E 381    3250   1728   3240   -238    446    -133      C
ATOM   4406  CB  LEU E 381      33.941 -20.107 -14.030  1.00 21.33           C
ANISOU 4406  CB  LEU E 381    3212   1732   3162   -278    523    -167      C
ATOM   4407  CG  LEU E 381      34.244 -20.753 -12.662  1.00 19.23           C
ANISOU 4407  CG  LEU E 381    2900   1465   2942   -259    560    -221      C
ATOM   4408  CD1 LEU E 381      35.081 -21.997 -12.834  1.00 13.40           C
ANISOU 4408  CD1 LEU E 381    2152    765   2174   -259    593    -258      C
ATOM   4409  CD2 LEU E 381      34.922 -19.699 -11.796  1.00 17.93           C
ANISOU 4409  CD2 LEU E 381    2726   1273   2813   -272    577    -225      C
ATOM   4410  C   LEU E 381      32.513 -18.135 -13.379  1.00 21.99           C
ANISOU 4410  C   LEU E 381    3292   1685   3378   -213    439    -126      C
ATOM   4411  O   LEU E 381      33.301 -17.199 -13.572  1.00 23.59           O
ANISOU 4411  O   LEU E 381    3544   1833   3586   -250    450     -79      O
ATOM   4412  N   VAL E 382      31.546 -18.064 -12.477  1.00 21.86           N
ANISOU 4412  N   VAL E 382    3214   1654   3439   -161    427    -184      N
ATOM   4413  CA  VAL E 382      31.417 -16.882 -11.602  1.00 21.55           C
ANISOU 4413  CA  VAL E 382    3160   1532   3496   -127    428    -223      C
ATOM   4414  CB  VAL E 382      29.957 -16.691 -11.098  1.00 21.88           C
ANISOU 4414  CB  VAL E 382    3114   1573   3625    -48    398    -294      C
ATOM   4415  CG1 VAL E 382      29.859 -15.541 -10.076  1.00 22.19           C
ANISOU 4415  CG1 VAL E 382    3128   1534   3770     -6    417    -382      C
ATOM   4416  CG2 VAL E 382      29.020 -16.449 -12.269  1.00 20.93           C
ANISOU 4416  CG2 VAL E 382    2990   1431   3530     11    293    -231      C
ATOM   4417  C   VAL E 382      32.403 -17.045 -10.441  1.00 20.98           C
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Figure 18 (continued)

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ANISOU 4417  C   VAL E 382     3076   1491   3404   -172    502   -285    C
ATOM   4418  O   VAL E 382      33.214 -16.165 -10.189  1.00 21.61        O
ANISOU 4418  O   VAL E 382     3184   1514   3514   -203    515   -294    O
ATOM   4419  N   GLN E 383      32.352 -18.188  -9.762  1.00 20.35        N
ANISOU 4419  N   GLN E 383     2959   1500   3272   -184    541   -319    N
ATOM   4420  CA  GLN E 383      33.239 -18.459  -8.653  1.00 20.51        C
ANISOU 4420  CA  GLN E 383     2970   1571   3251   -214    585   -358    C
ATOM   4421  CB  GLN E 383      32.825 -17.601  -7.432  1.00 22.63        C
ANISOU 4421  CB  GLN E 383     3202   1840   3555   -201    605   -454    C
ATOM   4422  CG  GLN E 383      33.753 -17.779  -6.252  1.00 28.07        C
ANISOU 4422  CG  GLN E 383     3885   2608   4173   -239    631   -498    C
ATOM   4423  CD  GLN E 383      33.698 -16.625  -5.265  1.00 36.66        C
ANISOU 4423  CD  GLN E 383     4948   3689   5291   -243    647   -622    C
ATOM   4424  OE1 GLN E 383      32.636 -15.998  -5.049  1.00 36.66        O
ANISOU 4424  OE1 GLN E 383     4916   3654   5358   -202    662   -698    O
ATOM   4425  NE2 GLN E 383      34.860 -16.332  -4.649  1.00 38.02        N
ANISOU 4425  NE2 GLN E 383     5121   3901   5423   -289    640   -665    N
ATOM   4426  C   GLN E 383      33.243 -19.938  -8.326  1.00 19.34        C
ANISOU 4426  C   GLN E 383     2817   1492   3040   -225    604   -337    C
ATOM   4427  O   GLN E 383      32.239 -20.609  -8.509  1.00 18.92        O
ANISOU 4427  O   GLN E 383     2748   1449   2993   -222    605   -329    O
ATOM   4428  N   LEU E 384      34.387 -20.445  -7.868  1.00 18.66        N
ANISOU 4428  N   LEU E 384     2739   1443   2907   -238    610   -326    N
ATOM   4429  CA  LEU E 384      34.544 -21.825  -7.460  1.00 18.10        C
ANISOU 4429  CA  LEU E 384     2681   1403   2795   -235    612   -288    C
ATOM   4430  CB  LEU E 384      35.331 -22.585  -8.546  1.00 18.49        C
ANISOU 4430  CB  LEU E 384     2743   1425   2855   -217    599   -264    C
ATOM   4431  CG  LEU E 384      35.671 -24.077  -8.334  1.00 18.11        C
ANISOU 4431  CG  LEU E 384     2716   1358   2806   -190    586   -231    C
ATOM   4432  CD1 LEU E 384      34.428 -24.981  -8.395  1.00 15.62        C
ANISOU 4432  CD1 LEU E 384     2432    995   2509   -217    597   -207    C
ATOM   4433  CD2 LEU E 384      36.728 -24.517  -9.342  1.00 17.92        C
ANISOU 4433  CD2 LEU E 384     2677   1325   2807   -156    583   -260    C
ATOM   4434  C   LEU E 384      35.349 -21.856  -6.147  1.00 19.39        C
ANISOU 4434  C   LEU E 384     2837   1632   2899   -236    602   -293    C
ATOM   4435  O   LEU E 384      36.373 -21.166  -6.044  1.00 19.75        O
ANISOU 4435  O   LEU E 384     2857   1702   2944   -238    586   -328    O
ATOM   4436  N   ILE E 385      34.898 -22.664  -5.175  1.00 19.03        N
ANISOU 4436  N   ILE E 385     2812   1624   2793   -249    609   -252    N
ATOM   4437  CA  ILE E 385      35.659 -22.991  -3.966  1.00 19.96        C
ANISOU 4437  CA  ILE E 385     2941   1820   2821   -245    576   -221    C
ATOM   4438  CB  ILE E 385      34.993 -22.480  -2.627  1.00 21.28        C
ANISOU 4438  CB  ILE E 385     3107   2094   2884   -296    612   -260    C
ATOM   4439  CG1 ILE E 385      34.558 -21.029  -2.788  1.00 21.71        C
ANISOU 4439  CG1 ILE E 385     3111   2146   2993   -305    650   -390    C
ATOM   4440  CD1 ILE E 385      33.762 -20.478  -1.643  1.00 22.98        C
ANISOU 4440  CD1 ILE E 385     3249   2408   3075   -344    707   -479    C
ATOM   4441  CG2 ILE E 385      36.012 -22.510  -1.462  1.00 21.32        C
ANISOU 4441  CG2 ILE E 385     3118   2212   2770   -293    553   -247    C
ATOM   4442  C   ILE E 385      35.839 -24.504  -3.882  1.00 20.24        C
ANISOU 4442  C   ILE E 385     3032   1811   2849   -222    542   -109    C
ATOM   4443  O   ILE E 385      34.856 -25.249  -3.881  1.00 19.69        O
ANISOU 4443  O   ILE E 385     3003   1695   2782   -261    578    -57    O
ATOM   4444  N   VAL E 386      37.097 -24.943  -3.810  1.00 19.46        N
ANISOU 4444  N   VAL E 386     2924   1714   2754   -158    472    -79    N
ATOM   4445  CA  VAL E 386      37.410 -26.350  -3.752  1.00 20.14        C
ANISOU 4445  CA  VAL E 386     3063   1721   2866   -106    420     23    C
ATOM   4446  CB  VAL E 386      38.383 -26.761  -4.859  1.00 20.24        C
ANISOU 4446  CB  VAL E 386     3030   1666   2993    -20    390    -23    C
ATOM   4447  CG1 VAL E 386      38.441 -28.280  -4.958  1.00 19.96        C
ANISOU 4447  CG1 VAL E 386     3061   1495   3030     41    346     60    C
ATOM   4448  CG2 VAL E 386      37.960 -26.147  -6.192  1.00 19.11        C
ANISOU 4448  CG2 VAL E 386     2855   1498   2906    -57    463   -116    C
ATOM   4449  C   VAL E 386      37.999 -26.643  -2.420  1.00 21.41        C
ANISOU 4449  C   VAL E 386     3261   1950   2925    -78    336    123    C
ATOM   4450  O   VAL E 386      38.857 -26.159  -1.871  1.00 19.90        O
ANISOU 4450  O   VAL E 386     3012   1873   2674    -54    282     81    O
ATOM   4451  N   SER E 387      37.500 -27.932  -1.919  1.00 23.78        N
ANISOU 4451  N   SER E 387     3661   2176   3199    -93    320    261    N
ATOM   4452  CA  SER E 387      38.069 -28.605  -0.755  1.00 26.40        C
ANISOU 4452  CA  SER E 387     4058   2542   3430    -55    216    407    C
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Figure 18 (continued)

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ATOM   4453  CB  SER E 387      36.995 -28.748   0.300  1.00 26.98           C
ANISOU 4453  CB  SER E 387    4226   2682   3345   -183    274    511       C
ATOM   4454  OG  SER E 387      37.539 -29.206   1.517  1.00 32.13           O
ANISOU 4454  OG  SER E 387    4952   3411   3846   -163    169    663       O
ATOM   4455  C   SER E 387      38.555 -29.968  -1.228  1.00 27.98           C
ANISOU 4455  C   SER E 387    4311   2549   3769     49    138    502       C
ATOM   4456  O   SER E 387      37.824 -30.693  -1.905  1.00 28.28           O
ANISOU 4456  O   SER E 387    4407   2428   3912     14    195    518       O
ATOM   4457  N   GLY E 388      39.787 -30.324  -0.904  1.00 30.49           N
ANISOU 4457  N   GLY E 388    4601   2877   4108    182      2    545       N
ATOM   4458  CA  GLY E 388      40.414 -31.510  -1.506  1.00 31.87           C
ANISOU 4458  CA  GLY E 388    4792   2855   4464    322    -77    582       C
ATOM   4459  C   GLY E 388      41.481 -32.119  -0.645  1.00 35.20           C
ANISOU 4459  C   GLY E 388    5224   3281   4870    465   -259    711       C
ATOM   4460  O   GLY E 388      42.053 -31.431   0.193  1.00 35.40           O
ANISOU 4460  O   GLY E 388    5192   3507   4752    473   -333    715       O
ATOM   4461  N   LYS E 389      41.744 -33.416  -0.854  1.00 37.79           N
ANISOU 4461  N   LYS E 389    5625   3381   5354    584   -343    808       N
ATOM   4462  CA  LYS E 389      42.695 -34.177  -0.038  1.00 41.58           C
ANISOU 4462  CA  LYS E 389    6134   3817   5846    751   -547    967       C
ATOM   4463  CB  LYS E 389      42.453 -35.683  -0.179  1.00 43.32           C
ANISOU 4463  CB  LYS E 389    6511   3710   6238    824   -607   1121      C
ATOM   4464  CG  LYS E 389      41.149 -36.173   0.475  1.00 45.67           C
ANISOU 4464  CG  LYS E 389    7029   3907   6418    632   -541   1336      C
ATOM   4465  CD  LYS E 389      40.990 -37.698   0.334  1.00 48.65           C
ANISOU 4465  CD  LYS E 389    7573   3918   6995    695   -610   1495      C
ATOM   4466  CE  LYS E 389      39.920 -38.253   1.282  1.00 53.15           C
ANISOU 4466  CE  LYS E 389    8371   4404   7418    499   -579   1774      C
ATOM   4467  NZ  LYS E 389      39.307 -39.499   0.737  1.00 55.21           N
ANISOU 4467  NZ  LYS E 389    8779   4293   7904    458   -545   1839      N
ATOM   4468  C   LYS E 389      44.154 -33.830  -0.362  1.00 41.93           C
ANISOU 4468  C   LYS E 389    5968   3976   5988    934   -650    813       C
ATOM   4469  O   LYS E 389      45.009 -33.920   0.510  1.00 43.82           O
ANISOU 4469  O   LYS E 389    6171   4312   6166   1049   -828    906       O
ATOM   4470  N   ASP E 390      44.426 -33.440  -1.615  1.00 40.64           N
ANISOU 4470  N   ASP E 390    5659   3817   5965    951   -538    578       N
ATOM   4471  CA  ASP E 390      45.777 -33.057  -2.081  1.00 40.81           C
ANISOU 4471  CA  ASP E 390    5452   3968   6088   1091   -589    396       C
ATOM   4472  CB  ASP E 390      46.690 -34.296  -2.287  1.00 43.89           C
ANISOU 4472  CB  ASP E 390    5794   4180   6703   1343   -735    406       C
ATOM   4473  CG  ASP E 390      46.218 -35.219  -3.405  1.00 44.30           C
ANISOU 4473  CG  ASP E 390    5913   3965   6955   1376   -637    329       C
ATOM   4474  OD1 ASP E 390      45.353 -34.826  -4.203  1.00 44.98           O
ANISOU 4474  OD1 ASP E 390    6038   4044   7009   1213   -458    233       O
ATOM   4475  OD2 ASP E 390      46.724 -36.355  -3.504  1.00 48.47           O
ANISOU 4475  OD2 ASP E 390    6450   4282   7682   1574   -751    352       O
ATOM   4476  C   ASP E 390      45.746 -32.154  -3.336  1.00 38.51           C
ANISOU 4476  C   ASP E 390    5031   3767   5836    995   -404    157       C
ATOM   4477  O   ASP E 390      44.671 -31.829  -3.839  1.00 36.33           O
ANISOU 4477  O   ASP E 390    4845   3447   5510    841   -259    138       O
ATOM   4478  N   GLU E 391      46.925 -31.763  -3.828  1.00 38.93           N
ANISOU 4478  N   GLU E 391    4869   3952   5972   1081   -414    -16      N
ATOM   4479  CA  GLU E 391      47.081 -30.789  -4.922  1.00 37.97           C
ANISOU 4479  CA  GLU E 391    4618   3953   5855    972   -246   -219      C
ATOM   4480  CB  GLU E 391      48.560 -30.441  -5.133  1.00 38.98           C
ANISOU 4480  CB  GLU E 391    4490   4258   6064   1066   -286   -380      C
ATOM   4481  CG  GLU E 391      48.856 -28.960  -4.994  1.00 40.24           C
ANISOU 4481  CG  GLU E 391    4543   4643   6104    900   -222   -461      C
ATOM   4482  CD  GLU E 391      50.336 -28.644  -4.975  1.00 43.40           C
ANISOU 4482  CD  GLU E 391    4675   5236   6579    973   -281   -608      C
ATOM   4483  OE1 GLU E 391      50.699 -27.575  -4.425  1.00 48.91           O
ANISOU 4483  OE1 GLU E 391    5289   6112   7182    857   -298   -644      O
ATOM   4484  OE2 GLU E 391      51.139 -29.445  -5.512  1.00 49.31           O
ANISOU 4484  OE2 GLU E 391    5283   5963   7491   1142   -308   -707      O
ATOM   4485  C   GLU E 391      46.489 -31.257  -6.243  1.00 36.17           C
ANISOU 4485  C   GLU E 391    4442   3579   5722    947   -104   -312      C
ATOM   4486  O   GLU E 391      45.845 -30.480  -6.927  1.00 34.25           O
ANISOU 4486  O   GLU E 391    4226   3383   5403    790     37   -371      O
ATOM   4487  N   GLN E 392      46.733 -32.515  -6.596  1.00 36.79           N
ANISOU 4487  N   GLN E 392    4532   3478   5968   1108   -154    -333      N
ATOM   4488  CA  GLN E 392      46.180 -33.135  -7.801  1.00 36.36           C
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Figure 18 (continued)

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ANISOU 4488  CA  GLN E 392     4533   3272   6008   1095    -38   -442    C
ATOM   4489  CB  GLN E 392      46.833 -34.495  -8.032  1.00 39.07        C
ANISOU 4489  CB  GLN E 392     4841   3428   6575   1320   -124   -506    C
ATOM   4490  CG  GLN E 392      46.093 -35.431  -8.959  1.00 42.17        C
ANISOU 4490  CG  GLN E 392     5347   3596   7078   1314    -46   -586    C
ATOM   4491  CD  GLN E 392      46.480 -36.877  -8.682  1.00 51.76        C
ANISOU 4491  CD  GLN E 392     6607   4534   8524   1534   -183   -558    C
ATOM   4492  OE1 GLN E 392      46.212 -37.410  -7.595  1.00 55.83        O
ANISOU 4492  OE1 GLN E 392     7265   4895   9053   1576   -325   -322    O
ATOM   4493  NE2 GLN E 392      47.145 -37.513  -9.647  1.00 54.63        N
ANISOU 4493  NE2 GLN E 392     6850   4836   9072   1680   -143   -798    N
ATOM   4494  C   GLN E 392      44.645 -33.273  -7.800  1.00 33.83        C
ANISOU 4494  C   GLN E 392     4427   2818   5610    940     22   -326    C
ATOM   4495  O   GLN E 392      44.020 -33.044  -8.836  1.00 31.93        O
ANISOU 4495  O   GLN E 392     4205   2580   5345    834    152   -432    O
ATOM   4496  N   SER E 393      44.058 -33.650  -6.657  1.00 32.93        N
ANISOU 4496  N   SER E 393     4460   2605   5446    923    -72   -113    N
ATOM   4497  CA  SER E 393      42.611 -33.725  -6.519  1.00 31.18        C
ANISOU 4497  CA  SER E 393     4411   2291   5146    759     -8     -5    C
ATOM   4498  CB  SER E 393      42.242 -34.366  -5.185  1.00 33.05        C
ANISOU 4498  CB  SER E 393     4797   2419   5340    763   -120    238    C
ATOM   4499  OG  SER E 393      42.910 -35.606  -5.020  1.00 36.61        O
ANISOU 4499  OG  SER E 393     5282   2665   5964    946   -249    295    O
ATOM   4500  C   SER E 393      41.941 -32.337  -6.624  1.00 28.79        C
ANISOU 4500  C   SER E 393     4086   2181   4671    581    102    -36    C
ATOM   4501  O   SER E 393      40.854 -32.192  -7.202  1.00 27.10        O
ANISOU 4501  O   SER E 393     3935   1933   4428    456    198    -62    O
ATOM   4502  N   ILE E 394      42.586 -31.323  -6.062  1.00 27.47        N
ANISOU 4502  N   ILE E 394     3824   2208   4405    574     76    -41    N
ATOM   4503  CA  ILE E 394      42.091 -29.953  -6.192  1.00 26.15        C
ANISOU 4503  CA  ILE E 394     3629   2193   4112    427    170    -88    C
ATOM   4504  CB  ILE E 394      42.826 -28.959  -5.223  1.00 26.34        C
ANISOU 4504  CB  ILE E 394     3570   2404   4034    417    111    -78    C
ATOM   4505  CG1 ILE E 394      42.490 -29.298  -3.766  1.00 28.07        C
ANISOU 4505  CG1 ILE E 394     3891   2627   4148    416     14     91    C
ATOM   4506  CD1 ILE E 394      43.465 -28.723  -2.752  1.00 28.88        C
ANISOU 4506  CD1 ILE E 394     3905   2906   4162    452    -94     95    C
ATOM   4507  CG2 ILE E 394      42.405 -27.519  -5.487  1.00 24.76        C
ANISOU 4507  CG2 ILE E 394     3340   2317   3749    276    210   -152    C
ATOM   4508  C   ILE E 394      42.142 -29.511  -7.661  1.00 24.62        C
ANISOU 4508  C   ILE E 394     3365   2030   3959    387    283   -247    C
ATOM   4509  O   ILE E 394      41.175 -28.957  -8.182  1.00 22.84        O
ANISOU 4509  O   ILE E 394     3189   1810   3678    272    366   -261    O
ATOM   4510  N   ALA E 395      43.257 -29.804  -8.328  1.00 25.55        N
ANISOU 4510  N   ALA E 395     3364   2176   4169    487    282   -366    N
ATOM   4511  CA  ALA E 395      43.459 -29.462  -9.732  1.00 25.07        C
ANISOU 4511  CA  ALA E 395     3232   2174   4119    445    397   -519    C
ATOM   4512  CB  ALA E 395      44.872 -29.811 -10.162  1.00 27.09        C
ANISOU 4512  CB  ALA E 395     3321   2497   4473    567    394   -657    C
ATOM   4513  C   ALA E 395      42.439 -30.156 -10.642  1.00 25.59        C
ANISOU 4513  C   ALA E 395     3403   2112   4209    408    454   -551    C
ATOM   4514  O   ALA E 395      41.894 -29.517 -11.549  1.00 23.95        O
ANISOU 4514  O   ALA E 395     3210   1966   3923    300    540   -600    O
ATOM   4515  N   GLU E 396      42.193 -31.454 -10.389  1.00 27.00        N
ANISOU 4515  N   GLU E 396     3657   2108   4496    495    393   -519    N
ATOM   4516  CA  GLU E 396      41.166 -32.229 -11.086  1.00 27.69        C
ANISOU 4516  CA  GLU E 396     3848   2051   4623    447    430   -554    C
ATOM   4517  CB  GLU E 396      41.104 -33.664 -10.542  1.00 29.27        C
ANISOU 4517  CB  GLU E 396     4134   2013   4973    547    344   -494    C
ATOM   4518  CG  GLU E 396      42.271 -34.530 -10.972  1.00 32.63        C
ANISOU 4518  CG  GLU E 396     4474   2363   5563    729    311   -631    C
ATOM   4519  CD  GLU E 396      42.372 -35.851 -10.218  1.00 36.07        C
ANISOU 4519  CD  GLU E 396     5002   2534   6168    858    191   -529    C
ATOM   4520  OE1 GLU E 396      41.525 -36.109  -9.323  1.00 38.71        O
ANISOU 4520  OE1 GLU E 396     5482   2756   6470    779    143   -330    O
ATOM   4521  OE2 GLU E 396      43.304 -36.647 -10.530  1.00 42.02        O
ANISOU 4521  OE2 GLU E 396     5684   3188   7095   1039    148   -649    O
ATOM   4522  C   GLU E 396      39.785 -31.557 -11.059  1.00 25.08        C
ANISOU 4522  C   GLU E 396     3601   1751   4176    284    471   -475    C
ATOM   4523  O   GLU E 396      39.134 -31.458 -12.082  1.00 25.02        O
ANISOU 4523  O   GLU E 396     3608   1763   4135    209    531   -560    O
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Figure 18 (continued)

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ATOM   4524  N   ALA E 397      39.382 -31.055  -9.898  1.00 24.77           N
ANISOU 4524  N   ALA E 397    3603   1741   4069    238    435   -329       N
ATOM   4525  CA  ALA E 397      38.105 -30.350  -9.702  1.00 22.83           C
ANISOU 4525  CA  ALA E 397    3407   1538   3729    104    473   -267       C
ATOM   4526  CB  ALA E 397      37.845 -30.182  -8.227  1.00 22.80           C
ANISOU 4526  CB  ALA E 397    3447   1548   3667     81    431   -123       C
ATOM   4527  C   ALA E 397      38.054 -29.011 -10.421  1.00 21.75           C
ANISOU 4527  C   ALA E 397    3209   1549   3504     43    529   -331       C
ATOM   4528  O   ALA E 397      37.043 -28.663 -11.030  1.00 22.91           O
ANISOU 4528  O   ALA E 397    3380   1710   3614    -37    562   -349       O
ATOM   4529  N   ILE E 398      39.136 -28.247 -10.344  1.00 20.67           N
ANISOU 4529  N   ILE E 398    2993   1518   3341     75    531   -358       N
ATOM   4530  CA  ILE E 398      39.245 -27.004 -11.079  1.00 19.58           C
ANISOU 4530  CA  ILE E 398    2812   1492   3134      8    585   -403       C
ATOM   4531  CB  ILE E 398      40.575 -26.213 -10.741  1.00 19.57           C
ANISOU 4531  CB  ILE E 398    2713   1599   3124     24    586   -429       C
ATOM   4532  CG1 ILE E 398      40.619 -25.880  -9.246  1.00 18.51           C
ANISOU 4532  CG1 ILE E 398    2582   1481   2970     32    523   -352       C
ATOM   4533  CD1 ILE E 398      41.963 -25.363  -8.757  1.00 20.95           C
ANISOU 4533  CD1 ILE E 398    2779   1896   3284     56    495   -393       C
ATOM   4534  CG2 ILE E 398      40.655 -24.936 -11.565  1.00 17.52           C
ANISOU 4534  CG2 ILE E 398    2432   1422   2802    -73    651   -453       C
ATOM   4535  C   ILE E 398      39.063 -27.223 -12.597  1.00 19.20           C
ANISOU 4535  C   ILE E 398    2768   1457   3070    -19    639   -494       C
ATOM   4536  O   ILE E 398      38.259 -26.545 -13.226  1.00 17.87           O
ANISOU 4536  O   ILE E 398    2634   1320   2835    -95    659   -479       O
ATOM   4537  N   ILE E 399      39.791 -28.190 -13.148  1.00 20.46           N
ANISOU 4537  N   ILE E 399    2890   1594   3288     52    653   -593       N
ATOM   4538  CA  ILE E 399      39.703 -28.555 -14.570  1.00 20.68           C
ANISOU 4538  CA  ILE E 399    2920   1655   3284     28    710   -714       C
ATOM   4539  CB  ILE E 399      40.619 -29.774 -14.904  1.00 22.08           C
ANISOU 4539  CB  ILE E 399    3039   1784   3565    141    723   -855       C
ATOM   4540  CG1 ILE E 399      42.093 -29.371 -14.774  1.00 21.85           C
ANISOU 4540  CG1 ILE E 399    2876   1872   3554    198    754   -907       C
ATOM   4541  CD1 ILE E 399      43.088 -30.515 -14.781  1.00 23.92           C
ANISOU 4541  CD1 ILE E 399    3050   2078   3961    353    742  -1039       C
ATOM   4542  CG2 ILE E 399      40.306 -30.345 -16.312  1.00 21.12           C
ANISOU 4542  CG2 ILE E 399    2936   1684   3405    110    780  -1011       C
ATOM   4543  C   ILE E 399      38.254 -28.856 -14.984  1.00 21.30           C
ANISOU 4543  C   ILE E 399    3087   1671   3335    -37    690   -699       C
ATOM   4544  O   ILE E 399      37.753 -28.319 -15.969  1.00 21.55           O
ANISOU 4544  O   ILE E 399    3137   1788   3263   -112    713   -722       O
ATOM   4545  N   VAL E 400      37.593 -29.728 -14.229  1.00 21.79           N
ANISOU 4545  N   VAL E 400    3203   1590   3488    -18    641   -655       N
ATOM   4546  CA  VAL E 400      36.210 -30.104 -14.507  1.00 21.47           C
ANISOU 4546  CA  VAL E 400    3221   1492   3445    -94    623   -654       C
ATOM   4547  CB  VAL E 400      35.728 -31.255 -13.542  1.00 21.73           C
ANISOU 4547  CB  VAL E 400    3313   1344   3600    -85    586   -598       C
ATOM   4548  CG1 VAL E 400      34.263 -31.478 -13.660  1.00 19.99           C
ANISOU 4548  CG1 VAL E 400    3126   1090   3380   -194    578   -590       C
ATOM   4549  CG2 VAL E 400      36.493 -32.517 -13.815  1.00 21.84           C
ANISOU 4549  CG2 VAL E 400    3339   1224   3736      3    579   -696       C
ATOM   4550  C   VAL E 400      35.249 -28.902 -14.461  1.00 20.50           C
ANISOU 4550  C   VAL E 400    3099   1460   3229    -173    613   -571       C
ATOM   4551  O   VAL E 400      34.363 -28.774 -15.302  1.00 20.28           O
ANISOU 4551  O   VAL E 400    3080   1476   3150    -232    600   -610       O
ATOM   4552  N   ALA E 401      35.406 -28.048 -13.458  1.00 19.91           N
ANISOU 4552  N   ALA E 401    3010   1412   3141    -166    607   -470       N
ATOM   4553  CA  ALA E 401      34.606 -26.819 -13.352  1.00 19.36           C
ANISOU 4553  CA  ALA E 401    2933   1408   3014    -214    597   -410       C
ATOM   4554  CB  ALA E 401      34.872 -26.101 -12.008  1.00 17.52           C
ANISOU 4554  CB  ALA E 401    2687   1183   2788    -199    596   -333       C
ATOM   4555  C   ALA E 401      34.832 -25.862 -14.533  1.00 19.87           C
ANISOU 4555  C   ALA E 401    2992   1566   2990    -237    605   -427       C
ATOM   4556  O   ALA E 401      33.877 -25.259 -15.044  1.00 19.29           O
ANISOU 4556  O   ALA E 401    2928   1525   2877    -270    570   -403       O
ATOM   4557  N   MSE E 402      36.089 -25.714 -14.954  1.00 20.42           N
ANISOU 4557  N   MSE E 402    3042   1687   3029    -222    647   -461       N
ATOM   4558  CA  MSE E 402      36.416 -24.804 -16.059  1.00 21.29           C
ANISOU 4558  CA  MSE E 402    3161   1895   3034    -271    672   -454       C
ATOM   4559  CB  MSE E 402      37.926 -24.599 -16.154  1.00 21.70           C
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Figure 18 (continued)

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ANISOU 4559  CB  MSE E 402     3161   2012   3074   -271    741   -491       C
ATOM   4560  CG  MSE E 402       38.500 -23.683 -15.106  1.00 22.22         C
ANISOU 4560  CG  MSE E 402     3194   2063   3185   -274    741   -428       C
ATOM   4561 SE   MSE E 402       40.412 -23.696 -15.293  0.90 27.13        SE
ANISOU 4561 SE   MSE E 402     3703   2793   3811   -278    825   -514      SE
ATOM   4562  CE  MSE E 402       40.877 -22.320 -13.992  1.00 24.57         C
ANISOU 4562  CE  MSE E 402     3347   2452   3536   -321    801   -441       C
ATOM   4563  C   MSE E 402       35.859 -25.299 -17.400  1.00 20.61         C
ANISOU 4563  C   MSE E 402     3105   1865   2859   -305    663   -518       C
ATOM   4564  O   MSE E 402       35.362 -24.495 -18.187  1.00 19.44         O
ANISOU 4564  O   MSE E 402     2995   1781   2610   -352    634   -461       O
ATOM   4565  N   VAL E 403       35.951 -26.621 -17.650  1.00 20.69         N
ANISOU 4565  N   VAL E 403     3106   1848   2909   -277    678   -639       N
ATOM   4566  CA  VAL E 403       35.357 -27.238 -18.838  1.00 21.22         C
ANISOU 4566  CA  VAL E 403     3197   1968   2897   -315    663   -740       C
ATOM   4567  CB  VAL E 403       35.749 -28.745 -19.039  1.00 22.85         C
ANISOU 4567  CB  VAL E 403     3389   2108   3184   -275    696   -911       C
ATOM   4568  CG1 VAL E 403       34.962 -29.365 -20.219  1.00 22.24         C
ANISOU 4568  CG1 VAL E 403     3339   2087   3026   -332    670  -1042       C
ATOM   4569  CG2 VAL E 403       37.257 -28.917 -19.283  1.00 22.02         C
ANISOU 4569  CG2 VAL E 403     3230   2058   3078   -225    785  -1003       C
ATOM   4570  C   VAL E 403       33.831 -27.076 -18.810  1.00 21.70         C
ANISOU 4570  C   VAL E 403     3278   2007   2959   -349    573   -688       C
ATOM   4571  O   VAL E 403       33.223 -26.611 -19.775  1.00 22.35         O
ANISOU 4571  O   VAL E 403     3382   2190   2919   -393    524   -677       O
ATOM   4572  N   PHE E 404       33.229 -27.437 -17.677  1.00 21.32         N
ANISOU 4572  N   PHE E 404     3216   1843   3042   -331    550   -651       N
ATOM   4573  CA  PHE E 404       31.791 -27.400 -17.481  1.00 21.21         C
ANISOU 4573  CA  PHE E 404     3184   1815   3059   -366    483   -626       C
ATOM   4574  CB  PHE E 404       31.482 -27.898 -16.078  1.00 20.30         C
ANISOU 4574  CB  PHE E 404     3054   1582   3076   -361    502   -585       C
ATOM   4575  CG  PHE E 404       30.035 -27.900 -15.746  1.00 19.75         C
ANISOU 4575  CG  PHE E 404     2939   1514   3051   -412    461   -575       C
ATOM   4576  CD1 PHE E 404       29.247 -29.023 -16.055  1.00 19.38         C
ANISOU 4576  CD1 PHE E 404     2879   1427   3057   -483    446   -667       C
ATOM   4577  CE1 PHE E 404       27.907 -29.040 -15.754  1.00 19.00         C
ANISOU 4577  CE1 PHE E 404     2759   1402   3058   -547    417   -672       C
ATOM   4578  CZ  PHE E 404       27.319 -27.946 -15.109  1.00 19.40         C
ANISOU 4578  CZ  PHE E 404     2745   1515   3110   -518    407   -596       C
ATOM   4579  CE2 PHE E 404       28.097 -26.822 -14.789  1.00 17.30         C
ANISOU 4579  CE2 PHE E 404     2507   1267   2799   -435    418   -512       C
ATOM   4580  CD2 PHE E 404       29.458 -26.815 -15.107  1.00 15.18         C
ANISOU 4580  CD2 PHE E 404     2315    974   2477   -394    445   -496       C
ATOM   4581  C   PHE E 404       31.176 -26.003 -17.703  1.00 21.45         C
ANISOU 4581  C   PHE E 404     3204   1924   3023   -364    423   -525       C
ATOM   4582  O   PHE E 404       30.026 -25.880 -18.163  1.00 22.44         O
ANISOU 4582  O   PHE E 404     3300   2097   3129   -384    344   -535       O
ATOM   4583  N   SER E 405       31.953 -24.969 -17.400  1.00 21.06         N
ANISOU 4583  N   SER E 405     3173   1878   2951   -336    451   -437       N
ATOM   4584  CA  SER E 405       31.531 -23.571 -17.521  1.00 21.22         C
ANISOU 4584  CA  SER E 405     3201   1919   2941   -322    396   -331       C
ATOM   4585  CB  SER E 405       32.564 -22.651 -16.867  1.00 20.19         C
ANISOU 4585  CB  SER E 405     3090   1748   2835   -309    450   -261       C
ATOM   4586  OG  SER E 405       33.724 -22.537 -17.685  1.00 22.95         O
ANISOU 4586  OG  SER E 405     3477   2159   3084   -349    505   -260       O
ATOM   4587  C   SER E 405       31.306 -23.154 -18.975  1.00 22.42         C
ANISOU 4587  C   SER E 405     3398   2173   2949   -348    331   -301       C
ATOM   4588  O   SER E 405       30.560 -22.202 -19.254  1.00 23.42         O
ANISOU 4588  O   SER E 405     3532   2307   3060   -324    239   -211       O
ATOM   4589  N   GLN E 406       31.952 -23.865 -19.900  1.00 23.01         N
ANISOU 4589  N   GLN E 406     3502   2329   2912   -392    374   -379       N
ATOM   4590  CA  GLN E 406       31.820 -23.613 -21.329  1.00 23.93         C
ANISOU 4590  CA  GLN E 406     3671   2581   2840   -437    323   -363       C
ATOM   4591  CB  GLN E 406       30.363 -23.731 -21.769  1.00 23.93         C
ANISOU 4591  CB  GLN E 406     3642   2627   2824   -428    184   -375       C
ATOM   4592  CG  GLN E 406       29.800 -25.108 -21.530  1.00 25.61         C
ANISOU 4592  CG  GLN E 406     3790   2817   3125   -445    190   -542       C
ATOM   4593  CD  GLN E 406       28.374 -25.265 -22.015  1.00 26.20         C
ANISOU 4593  CD  GLN E 406     3807   2964   3185   -456     52   -581       C
ATOM   4594  OE1 GLN E 406       27.534 -24.417 -21.751  1.00 27.21         O
ANISOU 4594  OE1 GLN E 406     3891   3085   3361   -406    -42   -484       O
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Figure 18 (continued)

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ATOM   4595  NE2 GLN E 406      28.100 -26.358 -22.741  1.00 26.20           N
ANISOU 4595  NE2 GLN E 406    3793   3035   3128   -519     35   -744        N
ATOM   4596  C   GLN E 406      32.420 -22.265 -21.765  1.00 24.66           C
ANISOU 4596  C   GLN E 406    3837   2702   2830   -463    327   -203        C
ATOM   4597  O   GLN E 406      32.100 -21.780 -22.848  1.00 26.26           O
ANISOU 4597  O   GLN E 406    4104   3005   2869   -497    254   -125        O
ATOM   4598  N   GLU E 407      33.294 -21.675 -20.941  1.00 23.80           N
ANISOU 4598  N   GLU E 407    3726   2506   2810   -459    407   -149        N
ATOM   4599  CA  GLU E 407      33.961 -20.391 -21.287  1.00 25.17           C
ANISOU 4599  CA  GLU E 407    3974   2678   2913   -513    429      1        C
ATOM   4600  CB  GLU E 407      34.926 -19.945 -20.188  1.00 24.30           C
ANISOU 4600  CB  GLU E 407    3829   2469   2934   -515    519      5        C
ATOM   4601  CG  GLU E 407      34.281 -19.528 -18.878  1.00 24.55           C
ANISOU 4601  CG  GLU E 407    3821   2356   3150   -436    467     19        C
ATOM   4602  CD  GLU E 407      34.947 -18.299 -18.237  1.00 25.54           C
ANISOU 4602  CD  GLU E 407    3969   2380   3355   -464    499     96        C
ATOM   4603  OE1 GLU E 407      35.873 -17.724 -18.827  1.00 30.35           O
ANISOU 4603  OE1 GLU E 407    4626   3019   3887   -559    558    160        O
ATOM   4604  OE2 GLU E 407      34.530 -17.876 -17.153  1.00 23.13           O
ANISOU 4604  OE2 GLU E 407    3631   1969   3188   -407    470     83        O
ATOM   4605  C   GLU E 407      34.732 -20.428 -22.598  1.00 27.34           C
ANISOU 4605  C   GLU E 407    4309   3114   2966   -616    494     10        C
ATOM   4606  O   GLU E 407      35.326 -21.447 -22.949  1.00 27.53           O
ANISOU 4606  O   GLU E 407    4289   3241   2928   -640    584   -143        O
ATOM   4607  N   ASP E 408      34.720 -19.296 -23.313  1.00 30.09           N
ANISOU 4607  N   ASP E 408    4761   3478   3194   -677    453    192        N
ATOM   4608  CA  ASP E 408      35.466 -19.149 -24.567  1.00 32.41           C
ANISOU 4608  CA  ASP E 408    5129   3945   3239   -807    529    238        C
ATOM   4609  CB  ASP E 408      35.129 -17.845 -25.296  1.00 34.46           C
ANISOU 4609  CB  ASP E 408    5534   4184   3374   -865    434    495        C
ATOM   4610  CG  ASP E 408      35.833 -17.727 -26.652  1.00 38.94           C
ANISOU 4610  CG  ASP E 408    6196   4964   3636  -1025    519    562        C
ATOM   4611  OD1 ASP E 408      35.458 -18.436 -27.618  1.00 39.82           O
ANISOU 4611  OD1 ASP E 408    6324   5271   3536  -1043    486    487        O
ATOM   4612  OD2 ASP E 408      36.777 -16.908 -26.746  1.00 42.86           O
ANISOU 4612  OD2 ASP E 408    6747   5443   4095  -1150    628    682        O
ATOM   4613  C   ASP E 408      36.971 -19.282 -24.378  1.00 32.45           C
ANISOU 4613  C   ASP E 408    5078   4004   3248   -892    721    155        C
ATOM   4614  O   ASP E 408      37.656 -19.768 -25.273  1.00 34.09           O
ANISOU 4614  O   ASP E 408    5278   4400   3273   -979    829     69        O
ATOM   4615  N  ACYS E 409      37.497 -18.881 -23.224  0.50 31.13           N
ANISOU 4615  N  ACYS E 409    4853   3694   3283   -867    764    157        N
ATOM   4616  N  BCYS E 409      37.455 -18.823 -23.224  0.50 31.33           N
ANISOU 4616  N  BCYS E 409    4884   3713   3309   -867    757    167        N
ATOM   4617  CA ACYS E 409      38.945 -18.986 -22.993  0.50 31.70           C
ANISOU 4617  CA ACYS E 409    4839   3830   3375   -943    929     67        C
ATOM   4618  CA BCYS E 409      38.853 -18.961 -22.819  0.50 31.92           C
ANISOU 4618  CA BCYS E 409    4865   3831   3435   -926    915     70        C
ATOM   4619  CB ACYS E 409      39.418 -17.964 -21.963  0.50 31.37           C
ANISOU 4619  CB ACYS E 409    4782   3631   3504   -966    941    149        C
ATOM   4620  CB BCYS E 409      39.050 -18.424 -21.402  0.50 30.51           C
ANISOU 4620  CB BCYS E 409    4633   3474   3486   -876    897     85        C
ATOM   4621  SG ACYS E 409      39.457 -18.589 -20.296  0.50 30.93           S
ANISOU 4621  SG ACYS E 409    4597   3457   3698   -823    915      5        S
ATOM   4622  SG BCYS E 409      39.461 -16.682 -21.315  0.50 36.34           S
ANISOU 4622  SG BCYS E 409    5462   4091   4256  -1005    908    284        S
ATOM   4623  C   ACYS E 409      39.403 -20.401 -22.601  0.50 30.56           C
ANISOU 4623  C   ACYS E 409    4560   3745   3307   -857    994   -170        C
ATOM   4624  C   BCYS E 409      39.290 -20.414 -22.846  0.50 31.07           C
ANISOU 4624  C   BCYS E 409    4642   3832   3331   -867    989   -162        C
ATOM   4625  O   ACYS E 409      40.607 -20.690 -22.587  0.50 31.33           O
ANISOU 4625  O   ACYS E 409    4558   3935   3409   -897   1126   -280        O
ATOM   4626  O   BCYS E 409      40.354 -20.744 -23.379  0.50 32.50           O
ANISOU 4626  O   BCYS E 409    4760   4166   3424   -938   1128   -266        O
ATOM   4627  N    MSE E 410      38.447 -21.267 -22.266  1.00 28.89           N
ANISOU 4627  N    MSE E 410    4337   3470   3171   -740    899   -246        N
ATOM   4628  CA   MSE E 410      38.702 -22.687 -22.159  1.00 27.78           C
ANISOU 4628  CA   MSE E 410    4109   3364   3084   -665    940   -452        C
ATOM   4629  CB   MSE E 410      37.602 -23.336 -21.317  1.00 25.84           C
ANISOU 4629  CB   MSE E 410    3858   2970   2988   -556    826   -475        C
ATOM   4630  CG   MSE E 410      37.745 -24.812 -21.107  1.00 24.62           C
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Figure 18 (continued)

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ANISOU 4630  CG  MSE E 410     3640   2790   2925   -480    849   -661      C
ATOM   4631 SE   MSE E 410      36.814 -25.805 -22.457  0.90 25.74          SE
ANISOU 4631 SE   MSE E 410     3827   3028   2924   -506    808   -801      SE
ATOM   4632  CE  MSE E 410      35.017 -25.128 -22.097  1.00 23.87           C
ANISOU 4632  CE  MSE E 410     3650   2703   2716   -500    633   -631      C
ATOM   4633  C   MSE E 410      38.792 -23.291 -23.566  1.00 29.33           C
ANISOU 4633  C   MSE E 410     4324   3746   3072   -725    995   -564      C
ATOM   4634  O   MSE E 410      39.716 -24.018 -23.894  1.00 29.96           O
ANISOU 4634  O   MSE E 410     4323   3928   3131   -726   1112   -737      O
ATOM   4635  N   ILE E 411      37.828 -22.957 -24.405  1.00 30.56           N
ANISOU 4635  N   ILE E 411     4583   3960   3069   -769    906   -474      N
ATOM   4636  CA  ILE E 411      37.776 -23.470 -25.766  1.00 32.47           C
ANISOU 4636  CA  ILE E 411     4859   4406   3073   -837    938   -578      C
ATOM   4637  CB  ILE E 411      36.401 -23.150 -26.397  1.00 32.92           C
ANISOU 4637  CB  ILE E 411     5019   4490   3001   -847    769   -462      C
ATOM   4638  CG1 ILE E 411      35.373 -24.172 -25.895  1.00 33.37           C
ANISOU 4638  CG1 ILE E 411     5025   4439   3216   -745    664   -594      C
ATOM   4639  CD1 ILE E 411      33.977 -23.673 -25.783  1.00 34.15           C
ANISOU 4639  CD1 ILE E 411     5163   4473   3339   -708    481   -458      C
ATOM   4640  CG2 ILE E 411      36.431 -23.283 -27.907  1.00 35.77           C
ANISOU 4640  CG2 ILE E 411     5446   5105   3040   -954    792   -507      C
ATOM   4641  C   ILE E 411      38.973 -22.985 -26.599  1.00 34.59           C
ANISOU 4641  C   ILE E 411     5130   4868   3144   -972   1100   -571      C
ATOM   4642  O   ILE E 411      39.547 -23.735 -27.392  1.00 36.40           O
ANISOU 4642  O   ILE E 411     5312   5278   3240  -1009   1214   -766      O
ATOM   4643  N   LYS E 412      39.383 -21.744 -26.380  1.00 34.85           N
ANISOU 4643  N   LYS E 412     5209   4862   3172  -1052   1123   -363      N
ATOM   4644  CA  LYS E 412      40.525 -21.193 -27.085  1.00 36.94           C
ANISOU 4644  CA  LYS E 412     5471   5303   3261  -1213   1291   -333      C
ATOM   4645  CB  LYS E 412      40.472 -19.660 -27.055  1.00 37.70           C
ANISOU 4645  CB  LYS E 412     5690   5312   3323  -1323   1253    -33      C
ATOM   4646  CG  LYS E 412      39.344 -19.044 -27.912  1.00 38.14           C
ANISOU 4646  CG  LYS E 412     5929   5383   3179  -1358   1097    184      C
ATOM   4647  CD  LYS E 412      39.476 -19.441 -29.388  1.00 42.37           C
ANISOU 4647  CD  LYS E 412     6522   6218   3360  -1478   1167    132      C
ATOM   4648  CE  LYS E 412      38.440 -18.757 -30.263  1.00 43.95           C
ANISOU 4648  CE  LYS E 412     6909   6454   3335  -1517    992    376      C
ATOM   4649  NZ  LYS E 412      37.050 -19.198 -29.938  1.00 43.30           N
ANISOU 4649  NZ  LYS E 412     6823   6258   3371  -1341    770    345      N
ATOM   4650  C   LYS E 412      41.870 -21.724 -26.575  1.00 37.07           C
ANISOU 4650  C   LYS E 412     5308   5363   3414  -1197   1460   -534      C
ATOM   4651  O   LYS E 412      42.886 -21.588 -27.252  1.00 39.36           O
ANISOU 4651  O   LYS E 412     5545   5853   3557  -1327   1633   -594      O
ATOM   4652  N   ALA E 413      41.872 -22.336 -25.390  1.00 35.02           N
ANISOU 4652  N   ALA E 413     4949   4932   3426  -1041   1408   -635      N
ATOM   4653  CA  ALA E 413      43.087 -22.942 -24.833  1.00 34.68           C
ANISOU 4653  CA  ALA E 413     4723   4918   3536   -985   1526   -827      C
ATOM   4654  CB  ALA E 413      43.016 -22.990 -23.309  1.00 31.70           C
ANISOU 4654  CB  ALA E 413     4291   4318   3437   -852   1426   -795      C
ATOM   4655  C   ALA E 413      43.387 -24.329 -25.422  1.00 35.53           C
ANISOU 4655  C   ALA E 413     4738   5144   3617   -907   1600  -1111      C
ATOM   4656  O   ALA E 413      44.438 -24.908 -25.156  1.00 36.10           O
ANISOU 4656  O   ALA E 413     4646   5265   3807   -844   1701  -1297      O
ATOM   4657  N   VAL E 414      42.471 -24.854 -26.229  1.00 36.17           N
ANISOU 4657  N   VAL E 414     4917   5270   3556   -905   1543  -1161      N
ATOM   4658  CA  VAL E 414      42.703 -26.137 -26.896  1.00 37.60           C
ANISOU 4658  CA  VAL E 414     5026   5559   3703   -846   1616  -1457      C
ATOM   4659  CB  VAL E 414      41.425 -26.689 -27.557  1.00 37.84           C
ANISOU 4659  CB  VAL E 414     5176   5586   3615   -840   1499  -1498      C
ATOM   4660  CG1 VAL E 414      41.758 -27.878 -28.499  1.00 39.24           C
ANISOU 4660  CG1 VAL E 414     5290   5919   3703   -822   1602  -1834      C
ATOM   4661  CG2 VAL E 414      40.407 -27.088 -26.498  1.00 33.57           C
ANISOU 4661  CG2 VAL E 414     4671   4769   3316   -713   1324  -1430      C
ATOM   4662  C   VAL E 414      43.829 -26.037 -27.933  1.00 41.28           C
ANISOU 4662  C   VAL E 414     5406   6318   3960   -969   1828  -1600      C
ATOM   4663  O   VAL E 414      43.854 -25.126 -28.772  1.00 41.91           O
ANISOU 4663  O   VAL E 414     5575   6580   3769  -1151   1889  -1455      O
ATOM   4664  N   ARG E 415      44.752 -26.995 -27.862  1.00 43.28           N
ANISOU 4664  N   ARG E 415     5485   6615   4345   -866   1940  -1885      N
ATOM   4665  CA  ARG E 415      45.838 -27.092 -28.822  1.00 47.04           C
ANISOU 4665  CA  ARG E 415     5837   7389   4648   -962   2163  -2091      C
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Figure 18 (continued)

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ATOM   4666  CB  ARG E 415      47.205 -27.002 -28.123  1.00 47.50           C
ANISOU 4666  CB  ARG E 415    5672   7467   4909   -912   2278  -2175           C
ATOM   4667  CG  ARG E 415      47.450 -25.686 -27.389  1.00 46.34           C
ANISOU 4667  CG  ARG E 415    5545   7256   4804  -1020   2250  -1881           C
ATOM   4668  CD  ARG E 415      47.536 -24.502 -28.344  1.00 49.52           C
ANISOU 4668  CD  ARG E 415    6053   7875   4887  -1292   2366  -1695           C
ATOM   4669  NE  ARG E 415      47.747 -23.254 -27.607  1.00 48.95           N
ANISOU 4669  NE  ARG E 415    6011   7694   4895  -1396   2332  -1427           N
ATOM   4670  CZ  ARG E 415      46.795 -22.365 -27.330  1.00 46.89           C
ANISOU 4670  CZ  ARG E 415    5952   7256   4608  -1446   2181  -1130           C
ATOM   4671  NH1 ARG E 415      45.553 -22.573 -27.751  1.00 46.50           N
ANISOU 4671  NH1 ARG E 415    6082   7142   4444  -1404   2044  -1050           N
ATOM   4672  NH2 ARG E 415      47.094 -21.257 -26.644  1.00 44.45           N
ANISOU 4672  NH2 ARG E 415    5654   6838   4397  -1538   2164   -932           N
ATOM   4673  C   ARG E 415      45.722 -28.376 -29.633  1.00 49.40           C
ANISOU 4673  C   ARG E 415    6100   7778   4892   -885   2213  -2430           C
ATOM   4674  O   ARG E 415      45.571 -29.466 -29.075  1.00 49.22           O
ANISOU 4674  O   ARG E 415    6023   7550   5130   -691   2135  -2605           O
ATOM   4675  N   GLY E 416      45.791 -28.237 -30.952  1.00 52.08           N
ANISOU 4675  N   GLY E 416    6480   8422   4887  -1048   2344  -2521           N
ATOM   4676  CA  GLY E 416      45.624 -29.371 -31.844  1.00 54.89           C
ANISOU 4676  CA  GLY E 416    6816   8897   5143  -1004   2397  -2865           C
ATOM   4677  C   GLY E 416      44.169 -29.796 -31.969  1.00 53.94           C
ANISOU 4677  C   GLY E 416    6874   8627   4993   -972   2190  -2820           C
ATOM   4678  O   GLY E 416      43.287 -29.229 -31.316  1.00 51.70           O
ANISOU 4678  O   GLY E 416    6715   8147   4783   -967   2007  -2522           O
ATOM   4679  N   ASP E 417      43.932 -30.798 -32.812  1.00 56.14           N
ANISOU 4679  N   ASP E 417    7149   9009   5171   -954   2224  -3142           N
ATOM   4680  CA  ASP E 417      42.594 -31.308 -33.083  1.00 55.99           C
ANISOU 4680  CA  ASP E 417    7273   8893   5107   -947   2041  -3164           C
ATOM   4681  CB  ASP E 417      42.535 -31.971 -34.471  1.00 59.31           C
ANISOU 4681  CB  ASP E 417    7703   9606   5227  -1034   2138  -3503           C
ATOM   4682  CG  ASP E 417      42.443 -30.958 -35.618  1.00 61.53           C
ANISOU 4682  CG  ASP E 417    8097  10274   5009  -1270   2196  -3338           C
ATOM   4683  OD1 ASP E 417      42.191 -29.761 -35.352  1.00 58.40           O
ANISOU 4683  OD1 ASP E 417    7803   9867   4522  -1359   2119  -2936           O
ATOM   4684  OD2 ASP E 417      42.607 -31.366 -36.801  1.00 64.87           O
ANISOU 4684  OD2 ASP E 417    8516  11011   5120  -1369   2315  -3613           O
ATOM   4685  C   ASP E 417      42.153 -32.295 -32.013  1.00 54.22           C
ANISOU 4685  C   ASP E 417    7020   8277   5303   -748   1903  -3244           C
ATOM   4686  O   ASP E 417      42.985 -32.986 -31.415  1.00 54.68           O
ANISOU 4686  O   ASP E 417    6940   8187   5651   -592   1974  -3422           O
ATOM   4687  N   LEU E 418      40.845 -32.359 -31.782  1.00 52.57           N
ANISOU 4687  N   LEU E 418    6940   7908   5127   -756   1703  -3107           N
ATOM   4688  CA  LEU E 418      40.294 -33.303 -30.826  1.00 51.40           C
ANISOU 4688  CA  LEU E 418    6787   7397   5344   -610   1576  -3164           C
ATOM   4689  CB  LEU E 418      39.353 -32.585 -29.850  1.00 48.14           C
ANISOU 4689  CB  LEU E 418    6464   6792   5037   -613   1398  -2795           C
ATOM   4690  CG  LEU E 418      39.926 -31.400 -29.056  1.00 45.99           C
ANISOU 4690  CG  LEU E 418    6170   6504   4798   -611   1421  -2486           C
ATOM   4691  CD1 LEU E 418      38.849 -30.744 -28.220  1.00 44.92           C
ANISOU 4691  CD1 LEU E 418    6125   6198   4746   -616   1247  -2179           C
ATOM   4692  CD2 LEU E 418      41.082 -31.819 -28.178  1.00 46.73           C
ANISOU 4692  CD2 LEU E 418    6131   6455   5169   -468   1509  -2568           C
ATOM   4693  C   LEU E 418      39.612 -34.486 -31.533  1.00 53.69           C
ANISOU 4693  C   LEU E 418    7109   7665   5627   -615   1533  -3488           C
ATOM   4694  O   LEU E 418      38.647 -34.299 -32.289  1.00 54.45           O
ANISOU 4694  O   LEU E 418    7301   7912   5477   -742   1440  -3471           O
ATOM   4695  N   ASN E 419      40.129 -35.693 -31.277  1.00 55.13           N
ANISOU 4695  N   ASN E 419    7208   7649   6090   -474   1588  -3786           N
ATOM   4696  CA  ASN E 419      39.644 -36.931 -31.904  1.00 57.91           C
ANISOU 4696  CA  ASN E 419    7578   7933   6493   -469   1567  -4150           C
ATOM   4697  CB  ASN E 419      40.546 -37.300 -33.088  1.00 61.18           C
ANISOU 4697  CB  ASN E 419    7904   8639   6703   -488   1763  -4536           C
ATOM   4698  CG  ASN E 419      40.444 -36.311 -34.223  1.00 62.11           C
ANISOU 4698  CG  ASN E 419    8073   9206   6320   -687   1822  -4458           C
ATOM   4699  OD1 ASN E 419      39.366 -36.093 -34.773  1.00 61.35           O
ANISOU 4699  OD1 ASN E 419    8092   9224   5995   -820   1694  -4388           O
ATOM   4700  ND2 ASN E 419      41.572 -35.692 -34.576  1.00 64.20           N
ANISOU 4700  ND2 ASN E 419    8248   9736   6409   -717   2012  -4458           N
ATOM   4701  C   ASN E 419      39.519 -38.140 -30.958  1.00 58.48           C
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Figure 18 (continued)

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ANISOU 4701  C   ASN E 419     7640   7561   7019   -310   1493  -4262      C
ATOM   4702  O   ASN E 419      39.706 -39.289 -31.387  1.00 60.83          O
ANISOU 4702  O   ASN E 419     7906   7757   7451   -247   1539  -4636      O
ATOM   4703  N   PHE E 420      39.191 -37.883 -29.687  1.00 56.70          N
ANISOU 4703  N   PHE E 420     7451   7072   7023   -252   1380  -3940      N
ATOM   4704  CA  PHE E 420      39.084 -38.931 -28.651  1.00 57.43          C
ANISOU 4704  CA  PHE E 420     7556   6734   7531   -114   1302  -3962      C
ATOM   4705  CB  PHE E 420      38.919 -38.322 -27.244  1.00 54.05          C
ANISOU 4705  CB  PHE E 420     7156   6122   7256    -69   1207  -3556      C
ATOM   4706  CG  PHE E 420      40.157 -37.660 -26.718  1.00 53.02          C
ANISOU 4706  CG  PHE E 420     6924   6072   7150     40   1288  -3429      C
ATOM   4707  CD1 PHE E 420      40.232 -36.271 -26.623  1.00 49.71          C
ANISOU 4707  CD1 PHE E 420     6500   5880   6506    -48   1302  -3156      C
ATOM   4708  CE1 PHE E 420      41.378 -35.643 -26.140  1.00 48.97          C
ANISOU 4708  CE1 PHE E 420     6301   5865   6440     27   1377  -3055      C
ATOM   4709  CZ  PHE E 420      42.477 -36.409 -25.744  1.00 51.30          C
ANISOU 4709  CZ  PHE E 420     6475   6032   6983    212   1429  -3226      C
ATOM   4710  CE2 PHE E 420      42.419 -37.803 -25.839  1.00 54.45          C
ANISOU 4710  CE2 PHE E 420     6879   6193   7615    329   1405  -3490      C
ATOM   4711  CD2 PHE E 420      41.259 -38.425 -26.323  1.00 54.30          C
ANISOU 4711  CD2 PHE E 420     6985   6074   7573    234   1341  -3591      C
ATOM   4712  C   PHE E 420      37.958 -39.927 -28.902  1.00 59.71          C
ANISOU 4712  C   PHE E 420     7933   6829   7924   -188   1203  -4135      C
ATOM   4713  O   PHE E 420      36.885 -39.562 -29.385  1.00 59.38          O
ANISOU 4713  O   PHE E 420     7955   6933   7674   -352   1122  -4078      O
ATOM   4714  N   VAL E 421      38.221 -41.179 -28.526  1.00 62.76          N
ANISOU 4714  N   VAL E 421     8318   6873   8656    -62   1198  -4339      N
ATOM   4715  CA  VAL E 421      37.341 -42.318 -28.779  1.00 66.10          C
ANISOU 4715  CA  VAL E 421     8817   7058   9241   -128   1126  -4568      C
ATOM   4716  CB  VAL E 421      37.809 -43.068 -30.056  1.00 69.65          C
ANISOU 4716  CB  VAL E 421     9215   7633   9617   -116   1235  -5067      C
ATOM   4717  CG1 VAL E 421      37.690 -44.582 -29.918  1.00 73.52          C
ANISOU 4717  CG1 VAL E 421     9747   7695  10491    -41   1203  -5363      C
ATOM   4718  CG2 VAL E 421      37.063 -42.546 -31.282  1.00 70.73          C
ANISOU 4718  CG2 VAL E 421     9372   8169   9332   -327   1231  -5178      C
ATOM   4719  C   VAL E 421      37.312 -43.237 -27.547  1.00 66.76          C
ANISOU 4719  C   VAL E 421     8958   6647   9763    -10   1048  -4463      C
ATOM   4720  O   VAL E 421      38.339 -43.406 -26.881  1.00 67.09          O
ANISOU 4720  O   VAL E 421     8949   6536  10006    185   1081  -4409      O
ATOM   4721  N   ASN E 422      36.145 -43.820 -27.243  1.00 67.53          N
ANISOU 4721  N   ASN E 422     9155   6503   9999   -136    942  -4424      N
ATOM   4722  CA  ASN E 422      35.987 -44.671 -26.041  1.00 68.08          C
ANISOU 4722  CA  ASN E 422     9309   6098  10459    -68    865  -4271      C
ATOM   4723  CB  ASN E 422      34.522 -44.727 -25.572  1.00 67.27          C
ANISOU 4723  CB  ASN E 422     9296   5877  10386   -278    760  -4080      C
ATOM   4724  CG  ASN E 422      33.535 -44.977 -26.713  1.00 69.70          C
ANISOU 4724  CG  ASN E 422     9604   6341  10538   -481    739  -4363      C
ATOM   4725  OD1 ASN E 422      32.448 -44.388 -26.738  1.00 68.72          O
ANISOU 4725  OD1 ASN E 422     9477   6388  10245   -657    670  -4214      O
ATOM   4726  ND2 ASN E 422      33.905 -45.848 -27.657  1.00 72.67          N
ANISOU 4726  ND2 ASN E 422     9970   6669  10973   -451    789  -4791      N
ATOM   4727  C   ASN E 422      36.580 -46.085 -26.139  1.00 71.50          C
ANISOU 4727  C   ASN E 422     9766   6157  11244     78    884  -4587      C
ATOM   4728  O   ASN E 422      36.751 -46.632 -27.227  1.00 74.15          O
ANISOU 4728  O   ASN E 422    10065   6559  11547     73    946  -5000      O
ATOM   4729  N   ARG E 427      33.161 -42.328 -30.481  1.00 65.32          N
ANISOU 4729  N   ARG E 427     8875   7278   8664   -761    800  -4699      N
ATOM   4730  CA  ARG E 427      33.763 -40.998 -30.490  1.00 62.98          C
ANISOU 4730  CA  ARG E 427     8546   7283   8101   -712    849  -4431      C
ATOM   4731  CB  ARG E 427      33.673 -40.369 -31.883  1.00 65.03          C
ANISOU 4731  CB  ARG E 427     8792   8005   7911   -823    864  -4564      C
ATOM   4732  CG  ARG E 427      34.458 -39.089 -31.984  1.00 64.47          C
ANISOU 4732  CG  ARG E 427     8699   8216   7579   -784    943  -4317      C
ATOM   4733  CD  ARG E 427      33.754 -38.015 -32.796  1.00 67.22          C
ANISOU 4733  CD  ARG E 427     9082   8944   7515   -926    854  -4158      C
ATOM   4734  NE  ARG E 427      34.445 -36.739 -32.601  1.00 67.49          N
ANISOU 4734  NE  ARG E 427     9116   9147   7382   -892    917  -3843      N
ATOM   4735  CZ  ARG E 427      35.598 -36.405 -33.186  1.00 69.71          C
ANISOU 4735  CZ  ARG E 427     9366   9652   7467   -875   1082  -3922      C
ATOM   4736  NH1 ARG E 427      36.196 -37.243 -34.034  1.00 71.76          N
ANISOU 4736  NH1 ARG E 427     9587  10022   7658   -875   1208  -4324      N
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Figure 18 (continued)

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ATOM   4737  NH2 ARG E 427      36.152 -35.226 -32.920  1.00 67.88           N
ANISOU 4737  NH2 ARG E 427     9137   9538   7117   -868   1131  -3614        N
ATOM   4738  C   ARG E 427      33.075 -40.091 -29.485  1.00 58.80           C
ANISOU 4738  C   ARG E 427     8035   6711   7596   -740    749  -3994        C
ATOM   4739  O   ARG E 427      31.865 -39.867 -29.575  1.00 58.91           O
ANISOU 4739  O   ARG E 427     8061   6791   7533   -873    626  -3912        O
ATOM   4740  N   LEU E 428      33.848 -39.555 -28.545  1.00 55.36           N
ANISOU 4740  N   LEU E 428     7586   6185   7263   -612    800  -3735        N
ATOM   4741  CA  LEU E 428      33.293 -38.797 -27.419  1.00 50.88           C
ANISOU 4741  CA  LEU E 428     7034   5531   6765   -619    721  -3349        C
ATOM   4742  CB  LEU E 428      34.399 -38.397 -26.432  1.00 48.72           C
ANISOU 4742  CB  LEU E 428     6740   5151   6618   -464    792  -3144        C
ATOM   4743  CG  LEU E 428      35.420 -39.432 -25.919  1.00 49.33           C
ANISOU 4743  CG  LEU E 428     6806   4945   6991   -304    858  -3284        C
ATOM   4744  CD1 LEU E 428      36.268 -38.834 -24.795  1.00 44.63           C
ANISOU 4744  CD1 LEU E 428     6182   4285   6491   -173    879  -3013        C
ATOM   4745  CD2 LEU E 428      34.776 -40.760 -25.451  1.00 49.60           C
ANISOU 4745  CD2 LEU E 428     6906   4603   7335   -323    795  -3387        C
ATOM   4746  C   LEU E 428      32.532 -37.565 -27.894  1.00 49.08           C
ANISOU 4746  C   LEU E 428     6802   5617   6229   -725    643  -3163        C
ATOM   4747  O   LEU E 428      32.874 -36.983 -28.932  1.00 49.55           O
ANISOU 4747  O   LEU E 428     6855   5985   5989   -757    677  -3230        O
ATOM   4748  N   ASN E 429      31.494 -37.179 -27.148  1.00 46.94           N
ANISOU 4748  N   ASN E 429     6534   5270   6032   -780    538  -2933        N
ATOM   4749  CA  ASN E 429      30.814 -35.909 -27.424  1.00 45.15           C
ANISOU 4749  CA  ASN E 429     6294   5299   5563   -837    448  -2718        C
ATOM   4750  CB  ASN E 429      29.427 -35.795 -26.731  1.00 44.53           C
ANISOU 4750  CB  ASN E 429     6183   5130   5604   -909    324  -2571        C
ATOM   4751  CG  ASN E 429      29.505 -35.650 -25.216  1.00 43.04           C
ANISOU 4751  CG  ASN E 429     5995   4702   5656   -844    356  -2335        C
ATOM   4752  OD1 ASN E 429      30.552 -35.375 -24.647  1.00 44.36           O
ANISOU 4752  OD1 ASN E 429     6185   4799   5871   -736    441  -2227        O
ATOM   4753  ND2 ASN E 429      28.369 -35.826 -24.559  1.00 44.32           N
ANISOU 4753  ND2 ASN E 429     6122   4763   5956   -921    286  -2262        N
ATOM   4754  C   ASN E 429      31.770 -34.724 -27.176  1.00 42.35           C
ANISOU 4754  C   ASN E 429     5946   5058   5088   -750    517  -2486        C
ATOM   4755  O   ASN E 429      32.811 -34.903 -26.528  1.00 41.08           O
ANISOU 4755  O   ASN E 429     5779   4756   5072   -648    619  -2464        O
ATOM   4756  N   PRO E 430      31.476 -33.549 -27.774  1.00 41.73           N
ANISOU 4756  N   PRO E 430     5879   5236   4742   -793    458  -2330        N
ATOM   4757  CA  PRO E 430      32.316 -32.355 -27.629  1.00 39.46           C
ANISOU 4757  CA  PRO E 430     5608   5050   4333   -744    520  -2107        C
ATOM   4758  CB  PRO E 430      31.423 -31.252 -28.194  1.00 40.25           C
ANISOU 4758  CB  PRO E 430     5736   5353   4205   -805    385  -1924        C
ATOM   4759  CG  PRO E 430      30.653 -31.948 -29.274  1.00 42.76           C
ANISOU 4759  CG  PRO E 430     6052   5820   4376   -896    299  -2151        C
ATOM   4760  CD  PRO E 430      30.346 -33.303 -28.705  1.00 43.03           C
ANISOU 4760  CD  PRO E 430     6044   5611   4695   -894    315  -2363        C
ATOM   4761  C   PRO E 430      32.774 -32.033 -26.201  1.00 36.38           C
ANISOU 4761  C   PRO E 430     5201   4442   4180   -650    563  -1910        C
ATOM   4762  O   PRO E 430      33.960 -31.739 -25.993  1.00 35.32           O
ANISOU 4762  O   PRO E 430     5056   4315   4049   -592    673  -1876        O
ATOM   4763  N   MSE E 431      31.873 -32.122 -25.223  1.00 34.13           N
ANISOU 4763  N   MSE E 431     4901   3985   4083   -644    482  -1799        N
ATOM   4764  CA  MSE E 431      32.236 -31.766 -23.826  1.00 31.35           C
ANISOU 4764  CA  MSE E 431     4538   3456   3919   -566    515  -1608        C
ATOM   4765  CB  MSE E 431      30.985 -31.620 -22.945  1.00 30.30           C
ANISOU 4765  CB  MSE E 431     4383   3219   3912   -594    423  -1477        C
ATOM   4766  CG  MSE E 431      30.087 -30.421 -23.323  1.00 29.63           C
ANISOU 4766  CG  MSE E 431     4282   3300   3676   -624    317  -1334        C
ATOM   4767  SE  MSE E 431      30.966 -28.722 -22.996  0.90 32.22          SE
ANISOU 4767  SE  MSE E 431     4642   3693   3906   -556    353  -1079        SE
ATOM   4768  CE  MSE E 431      31.056 -28.819 -21.067  1.00 26.36           C
ANISOU 4768  CE  MSE E 431     3867   2715   3434   -492    401   -968        C
ATOM   4769  C   MSE E 431      33.244 -32.741 -23.208  1.00 30.85           C
ANISOU 4769  C   MSE E 431     4469   3203   4050   -485    609  -1710        C
ATOM   4770  O   MSE E 431      34.119 -32.348 -22.445  1.00 29.27           O
ANISOU 4770  O   MSE E 431     4255   2950   3916   -408    662  -1595        O
ATOM   4771  N   HIS E 432      33.128 -34.014 -23.562  1.00 32.32           N
ANISOU 4771  N   HIS E 432     4662   3283   4336   -499    617  -1934        N
ATOM   4772  CA  HIS E 432      34.063 -35.044 -23.091  1.00 34.03           C
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Figure 18 (continued)

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ANISOU 4772  CA  HIS E 432     4877   3292   4760   -399    685  -2050      C
ATOM   4773  CB  HIS E 432      33.392 -36.424 -23.076  1.00 36.39          C
ANISOU 4773  CB  HIS E 432     5209   3369   5248   -441    649  -2222      C
ATOM   4774  CG  HIS E 432      32.433 -36.595 -21.940  1.00 38.68          C
ANISOU 4774  CG  HIS E 432     5527   3471   5699   -494    584  -2041      C
ATOM   4775  ND1 HIS E 432      31.189 -35.998 -21.920  1.00 39.39          N
ANISOU 4775  ND1 HIS E 432     5597   3668   5702   -607    513  -1936      N
ATOM   4776  CE1 HIS E 432      30.584 -36.288 -20.782  1.00 39.89          C
ANISOU 4776  CE1 HIS E 432     5675   3550   5932   -643    494  -1795      C
ATOM   4777  NE2 HIS E 432      31.391 -37.043 -20.058  1.00 41.36          N
ANISOU 4777  NE2 HIS E 432     5911   3505   6297   -559    536  -1776      N
ATOM   4778  CD2 HIS E 432      32.561 -37.241 -20.754  1.00 40.10          C
ANISOU 4778  CD2 HIS E 432     5748   3382   6107   -450    584  -1933      C
ATOM   4779  C   HIS E 432      35.358 -35.061 -23.901  1.00 35.10          C
ANISOU 4779  C   HIS E 432     4973   3565   4797   -332    791  -2220      C
ATOM   4780  O   HIS E 432      36.402 -35.469 -23.410  1.00 35.53          O
ANISOU 4780  O   HIS E 432     4993   3505   5002   -212    850  -2259      O
ATOM   4781  N   GLN E 433      35.258 -34.625 -25.152  1.00 35.90          N
ANISOU 4781  N   GLN E 433     5072   3931   4639   -414    811  -2323      N
ATOM   4782  CA  GLN E 433      36.394 -34.264 -25.999  1.00 36.69          C
ANISOU 4782  CA  GLN E 433     5128   4254   4558   -397    931  -2434      C
ATOM   4783  CB  GLN E 433      35.808 -33.686 -27.294  1.00 38.40          C
ANISOU 4783  CB  GLN E 433     5382   4764   4444   -531    907  -2469      C
ATOM   4784  CG  GLN E 433      36.487 -33.958 -28.567  1.00 42.26          C
ANISOU 4784  CG  GLN E 433     5849   5489   4720   -569   1019  -2729      C
ATOM   4785  CD  GLN E 433      36.743 -35.422 -28.835  1.00 46.49          C
ANISOU 4785  CD  GLN E 433     6351   5891   5423   -510   1069  -3088      C
ATOM   4786  OE1 GLN E 433      37.885 -35.864 -28.762  1.00 46.73          O
ANISOU 4786  OE1 GLN E 433     6307   5883   5565   -406   1191  -3246      O
ATOM   4787  NE2 GLN E 433      35.701 -36.170 -29.196  1.00 49.59          N
ANISOU 4787  NE2 GLN E 433     6786   6216   5839   -577    974  -3240      N
ATOM   4788  C   GLN E 433      37.266 -33.209 -25.278  1.00 33.83          C
ANISOU 4788  C   GLN E 433     4728   3932   4195   -345    981  -2204      C
ATOM   4789  O   GLN E 433      38.456 -33.403 -25.081  1.00 34.24          O
ANISOU 4789  O   GLN E 433     4705   3974   4330   -254   1077  -2284      O
ATOM   4790  N   LEU E 434      36.650 -32.110 -24.866  1.00 31.07          N
ANISOU 4790  N   LEU E 434     4418   3619   3768   -399    908  -1937      N
ATOM   4791  CA  LEU E 434      37.329 -31.034 -24.128  1.00 28.78          C
ANISOU 4791  CA  LEU E 434     4102   3346   3486   -372    939  -1719      C
ATOM   4792  CB  LEU E 434      36.367 -29.855 -23.924  1.00 26.01          C
ANISOU 4792  CB  LEU E 434     3811   3033   3038   -442    841  -1468      C
ATOM   4793  CG  LEU E 434      35.966 -29.145 -25.222  1.00 25.54          C
ANISOU 4793  CG  LEU E 434     3805   3209   2689   -551    822  -1442      C
ATOM   4794  CD1 LEU E 434      34.729 -28.299 -25.018  1.00 24.35          C
ANISOU 4794  CD1 LEU E 434     3706   3042   2504   -583    681  -1235      C
ATOM   4795  CD2 LEU E 434      37.121 -28.319 -25.799  1.00 22.38          C
ANISOU 4795  CD2 LEU E 434     3397   2995   2113   -602    943  -1400      C
ATOM   4796  C   LEU E 434      37.900 -31.483 -22.783  1.00 27.76          C
ANISOU 4796  C   LEU E 434     3927   2997   3622   -250    939  -1675      C
ATOM   4797  O   LEU E 434      39.014 -31.136 -22.430  1.00 27.07          O
ANISOU 4797  O   LEU E 434     3771   2946   3569   -196   1008  -1653      O
ATOM   4798  N   LEU E 435      37.110 -32.250 -22.042  1.00 27.99          N
ANISOU 4798  N   LEU E 435     3994   2811   3829   -220    856  -1657      N
ATOM   4799  CA  LEU E 435      37.487 -32.722 -20.719  1.00 27.82          C
ANISOU 4799  CA  LEU E 435     3960   2577   4035   -116    832  -1578      C
ATOM   4800  CB  LEU E 435      36.316 -33.464 -20.074  1.00 27.22          C
ANISOU 4800  CB  LEU E 435     3951   2294   4097   -145    746  -1530      C
ATOM   4801  CG  LEU E 435      36.445 -33.810 -18.591  1.00 28.04          C
ANISOU 4801  CG  LEU E 435     4075   2192   4388    -72    705  -1378      C
ATOM   4802  CD1 LEU E 435      36.646 -32.562 -17.667  1.00 24.26          C
ANISOU 4802  CD1 LEU E 435     3574   1799   3846    -69    694  -1159      C
ATOM   4803  CD2 LEU E 435      35.226 -34.633 -18.191  1.00 25.93          C
ANISOU 4803  CD2 LEU E 435     3877   1742   4232   -145    648  -1354      C
ATOM   4804  C   LEU E 435      38.771 -33.577 -20.768  1.00 29.75          C
ANISOU 4804  C   LEU E 435     4131   2762   4410     14    896  -1756      C
ATOM   4805  O   LEU E 435      39.778 -33.201 -20.144  1.00 28.71          O
ANISOU 4805  O   LEU E 435     3929   2650   4330     95    921  -1690      O
ATOM   4806  N   ARG E 436      38.741 -34.676 -21.534  1.00 32.34          N
ANISOU 4806  N   ARG E 436     4465   3030   4795     35    920  -1999      N
ATOM   4807  CA  ARG E 436      39.909 -35.546 -21.722  1.00 35.45          C
ANISOU 4807  CA  ARG E 436     4775   3363   5331    178    982  -2217      C
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Figure 18 (continued)

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ATOM   4808  CB  ARG E 436      39.663 -36.647 -22.752  1.00 39.05           C
ANISOU 4808  CB  ARG E 436    5249   3770   5817    172   1014  -2522           C
ATOM   4809  CG  ARG E 436      38.505 -37.569 -22.494  1.00 44.53           C
ANISOU 4809  CG  ARG E 436    6055   4209   6656    124    920  -2530           C
ATOM   4810  CD  ARG E 436      38.611 -38.440 -21.233  1.00 52.12           C
ANISOU 4810  CD  ARG E 436    7061   4819   7923    242    842  -2421           C
ATOM   4811  NE  ARG E 436      37.245 -38.756 -20.802  1.00 57.30           N
ANISOU 4811  NE  ARG E 436    7831   5312   8631    112    760  -2299           N
ATOM   4812  CZ  ARG E 436      36.618 -38.200 -19.764  1.00 57.95           C
ANISOU 4812  CZ  ARG E 436    7958   5361   8701     53    702  -2012           C
ATOM   4813  NH1 ARG E 436      37.239 -37.329 -18.967  1.00 55.93           N
ANISOU 4813  NH1 ARG E 436    7660   5194   8395    119    701  -1810           N
ATOM   4814  NH2 ARG E 436      35.361 -38.551 -19.498  1.00 60.15           N
ANISOU 4814  NH2 ARG E 436    8312   5518   9024    -81    651  -1946           N
ATOM   4815  C   ARG E 436      41.160 -34.801 -22.148  1.00 35.22           C
ANISOU 4815  C   ARG E 436    4619   3580   5182    206   1094  -2273           C
ATOM   4816  O   ARG E 436      42.231 -35.071 -21.622  1.00 35.85           O
ANISOU 4816  O   ARG E 436    4598   3608   5416    348   1111  -2313           O
ATOM   4817  N   HIS E 437      41.028 -33.904 -23.128  1.00 34.80           N
ANISOU 4817  N   HIS E 437    4568   3798   4857     67   1165  -2278           N
ATOM   4818  CA  HIS E 437      42.118 -33.014 -23.525  1.00 34.74           C
ANISOU 4818  CA  HIS E 437    4454   4042   4705     38   1285  -2284           C
ATOM   4819  CB  HIS E 437      41.679 -32.053 -24.633  1.00 34.55           C
ANISOU 4819  CB  HIS E 437    4489   4283   4357   -146   1338  -2235           C
ATOM   4820  CG  HIS E 437      42.748 -31.068 -25.013  1.00 35.10           C
ANISOU 4820  CG  HIS E 437    4468   4599   4270   -217   1471  -2204           C
ATOM   4821  ND1 HIS E 437      43.851 -31.420 -25.764  1.00 37.41           N
ANISOU 4821  ND1 HIS E 437    4626   5075   4513   -200   1631  -2455           N
ATOM   4822  CE1 HIS E 437      44.631 -30.366 -25.924  1.00 38.18           C
ANISOU 4822  CE1 HIS E 437    4658   5375   4475   -302   1736  -2358           C
ATOM   4823  NE2 HIS E 437      44.081 -29.345 -25.292  1.00 35.48           N
ANISOU 4823  NE2 HIS E 437    4413   4960   4108   -374   1640  -2054           N
ATOM   4824  CD2 HIS E 437      42.906 -29.759 -24.711  1.00 32.73           C
ANISOU 4824  CD2 HIS E 437    4181   4382   3872   -313   1477  -1962           C
ATOM   4825  C   HIS E 437      42.749 -32.194 -22.375  1.00 33.02           C
ANISOU 4825  C   HIS E 437    4176   3799   4570     79   1259  -2066           C
ATOM   4826  O   HIS E 437      43.972 -32.101 -22.278  1.00 33.79           O
ANISOU 4826  O   HIS E 437    4129   3988   4720    145   1337  -2148           O
ATOM   4827  N   PHE E 438      41.926 -31.574 -21.532  1.00 31.16           N
ANISOU 4827  N   PHE E 438    4035   3462   4342     33   1153  -1812           N
ATOM   4828  CA  PHE E 438      42.449 -30.736 -20.445  1.00 29.88           C
ANISOU 4828  CA  PHE E 438    3826   3289   4236     53   1124  -1624           C
ATOM   4829  CB  PHE E 438      41.489 -29.603 -20.094  1.00 26.95           C
ANISOU 4829  CB  PHE E 438    3561   2923   3757    -63   1061  -1384           C
ATOM   4830  CG  PHE E 438      41.464 -28.502 -21.121  1.00 27.09           C
ANISOU 4830  CG  PHE E 438    3604   3149   3541   -212   1134  -1338           C
ATOM   4831  CD1 PHE E 438      42.603 -27.741 -21.370  1.00 25.13           C
ANISOU 4831  CD1 PHE E 438    3262   3064   3221   -267   1241  -1344           C
ATOM   4832  CE1 PHE E 438      42.595 -26.732 -22.328  1.00 25.50           C
ANISOU 4832  CE1 PHE E 438    3355   3289   3044   -424   1312  -1272           C
ATOM   4833  CZ  PHE E 438      41.445 -26.464 -23.056  1.00 25.46           C
ANISOU 4833  CZ  PHE E 438    3487   3307   2880   -504   1254  -1191           C
ATOM   4834  CE2 PHE E 438      40.295 -27.218 -22.825  1.00 25.44           C
ANISOU 4834  CE2 PHE E 438    3552   3162   2953   -438   1138  -1209           C
ATOM   4835  CD2 PHE E 438      40.308 -28.232 -21.858  1.00 26.06           C
ANISOU 4835  CD2 PHE E 438    3586   3055   3260   -305   1090  -1283           C
ATOM   4836  C   PHE E 438      42.892 -31.546 -19.216  1.00 30.99           C
ANISOU 4836  C   PHE E 438    3923   3228   4624    221   1042  -1610           C
ATOM   4837  O   PHE E 438      43.758 -31.116 -18.459  1.00 30.57           O
ANISOU 4837  O   PHE E 438    3776   3208   4631    274   1032  -1547           O
ATOM   4838  N   GLN E 439      42.333 -32.746 -19.058  1.00 32.94           N
ANISOU 4838  N   GLN E 439    4237   3267   5012    299    977  -1674           N
ATOM   4839  CA  GLN E 439      42.793 -33.691 -18.041  1.00 34.33           C
ANISOU 4839  CA  GLN E 439    4390   3229   5424    468    892  -1664           C
ATOM   4840  CB  GLN E 439      41.809 -34.835 -17.889  1.00 34.98           C
ANISOU 4840  CB  GLN E 439    4604   3055   5634    485    819  -1673           C
ATOM   4841  CG  GLN E 439      40.528 -34.421 -17.151  1.00 33.80           C
ANISOU 4841  CG  GLN E 439    4583   2832   5428    365    747  -1440           C
ATOM   4842  CD  GLN E 439      39.593 -35.607 -16.908  1.00 35.82           C
ANISOU 4842  CD  GLN E 439    4957   2826   5828    357    684  -1441           C
ATOM   4843  OE1 GLN E 439      39.605 -36.585 -17.663  1.00 36.28           O
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Figure 18 (continued)

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ANISOU 4843  OE1 GLN E 439     5025   2780   5979    391    705  -1646      O
ATOM   4844  NE2 GLN E 439      38.782 -35.521 -15.849  1.00 34.67          N
ANISOU 4844  NE2 GLN E 439     4899   2575   5700    299    617  -1224      N
ATOM   4845  C   GLN E 439      44.181 -34.224 -18.355  1.00 36.88          C
ANISOU 4845  C   GLN E 439     4548   3601   5863    621    947  -1875      C
ATOM   4846  O   GLN E 439      44.947 -34.537 -17.454  1.00 38.31          O
ANISOU 4846  O   GLN E 439     4655   3695   6205    771    873  -1834      O
ATOM   4847  N   LYS E 440      44.506 -34.307 -19.639  1.00 38.67          N
ANISOU 4847  N   LYS E 440     4708   3989   5997    585   1074  -2109      N
ATOM   4848  CA  LYS E 440      45.830 -34.701 -20.085  1.00 41.00          C
ANISOU 4848  CA  LYS E 440     4811   4387   6378    713   1162  -2352      C
ATOM   4849  CB  LYS E 440      45.760 -35.237 -21.517  1.00 43.24          C
ANISOU 4849  CB  LYS E 440     5080   4772   6575    674   1289  -2647      C
ATOM   4850  CG  LYS E 440      44.974 -36.564 -21.628  1.00 44.39          C
ANISOU 4850  CG  LYS E 440     5348   4632   6884    748   1215  -2766      C
ATOM   4851  CD  LYS E 440      45.302 -37.362 -22.891  1.00 47.55          C
ANISOU 4851  CD  LYS E 440     5680   5105   7282    784   1335  -3147      C
ATOM   4852  CE  LYS E 440      44.512 -38.715 -22.929  1.00 50.57          C
ANISOU 4852  CE  LYS E 440     6192   5155   7866    848   1250  -3276      C
ATOM   4853  NZ  LYS E 440      45.145 -39.840 -23.728  1.00 54.88          N
ANISOU 4853  NZ  LYS E 440     6641   5641   8568    993   1329  -3685      N
ATOM   4854  C   LYS E 440      46.860 -33.566 -19.953  1.00 41.06          C
ANISOU 4854  C   LYS E 440     4658   4652   6290    666   1236  -2303      C
ATOM   4855  O   LYS E 440      48.025 -33.808 -19.611  1.00 42.57          O
ANISOU 4855  O   LYS E 440     4664   4881   6629    813   1240  -2407      O
ATOM   4856  N   ASP E 441      46.435 -32.336 -20.226  1.00 39.79          N
ANISOU 4856  N   ASP E 441     4560   4659   5898    463   1287  -2149      N
ATOM   4857  CA  ASP E 441      47.317 -31.180 -20.142  1.00 40.18          C
ANISOU 4857  CA  ASP E 441     4482   4932   5855    373   1365  -2091      C
ATOM   4858  CB  ASP E 441      48.154 -31.013 -21.419  1.00 43.33          C
ANISOU 4858  CB  ASP E 441     4737   5607   6118    295   1564  -2319      C
ATOM   4859  CG  ASP E 441      49.325 -30.041 -21.231  1.00 46.39          C
ANISOU 4859  CG  ASP E 441     4939   6211   6477    220   1653  -2302      C
ATOM   4860  OD1 ASP E 441      49.448 -29.440 -20.140  1.00 48.49          O
ANISOU 4860  OD1 ASP E 441     5197   6410   6818    225   1551  -2118      O
ATOM   4861  OD2 ASP E 441      50.129 -29.879 -22.174  1.00 51.62          O
ANISOU 4861  OD2 ASP E 441     5456   7122   7035    143   1834  -2486      O
ATOM   4862  C   ASP E 441      46.537 -29.904 -19.828  1.00 37.74          C
ANISOU 4862  C   ASP E 441     4310   4644   5386    194   1329  -1822      C
ATOM   4863  O   ASP E 441      45.864 -29.332 -20.693  1.00 37.25          O
ANISOU 4863  O   ASP E 441     4355   4675   5122     36   1387  -1775      O
ATOM   4864  N   ALA E 442      46.636 -29.476 -18.570  1.00 35.71          N
ANISOU 4864  N   ALA E 442     4047   4299   5223    231   1222  -1652      N
ATOM   4865  CA  ALA E 442      45.931 -28.299 -18.098  1.00 33.38          C
ANISOU 4865  CA  ALA E 442     3868   3993   4822     92   1177  -1423      C
ATOM   4866  CB  ALA E 442      45.419 -28.529 -16.675  1.00 31.22          C
ANISOU 4866  CB  ALA E 442     3665   3526   4672    185   1020  -1271      C
ATOM   4867  C   ALA E 442      46.776 -27.016 -18.181  1.00 33.32          C
ANISOU 4867  C   ALA E 442     3761   4170   4728    -46   1265  -1384      C
ATOM   4868  O   ALA E 442      46.260 -25.945 -17.903  1.00 32.99          O
ANISOU 4868  O   ALA E 442     3816   4112   4608   -168   1240  -1212      O
ATOM   4869  N   LYS E 443      48.043 -27.134 -18.584  1.00 34.87          N
ANISOU 4869  N   LYS E 443     3760   4535   4953    -31   1371  -1554      N
ATOM   4870  CA  LYS E 443      49.006 -26.014 -18.612  1.00 35.36          C
ANISOU 4870  CA  LYS E 443     3692   4779   4964   -175   1466  -1542      C
ATOM   4871  CB  LYS E 443      50.372 -26.455 -19.164  1.00 38.05          C
ANISOU 4871  CB  LYS E 443     3778   5324   5355   -134   1599  -1786      C
ATOM   4872  CG  LYS E 443      51.263 -27.243 -18.219  1.00 40.17          C
ANISOU 4872  CG  LYS E 443     3849   5559   5857     88   1500  -1903      C
ATOM   4873  CD  LYS E 443      52.487 -27.764 -18.987  1.00 43.53          C
ANISOU 4873  CD  LYS E 443     4010   6196   6334    144   1649  -2186      C
ATOM   4874  CE  LYS E 443      53.103 -28.956 -18.285  1.00 48.78          C
ANISOU 4874  CE  LYS E 443     4515   6765   7255    440   1522  -2328      C
ATOM   4875  NZ  LYS E 443      54.154 -29.631 -19.120  1.00 53.55          N
ANISOU 4875  NZ  LYS E 443     4860   7551   7935    536   1667  -2646      N
ATOM   4876  C   LYS E 443      48.554 -24.806 -19.413  1.00 33.77          C
ANISOU 4876  C   LYS E 443     3618   4659   4554   -414   1561  -1408      C
ATOM   4877  O   LYS E 443      48.684 -23.694 -18.948  1.00 33.32          O
ANISOU 4877  O   LYS E 443     3574   4600   4484   -537   1551  -1276      O
ATOM   4878  N   VAL E 444      48.057 -25.015 -20.627  1.00 33.39          N
ANISOU 4878  N   VAL E 444     3664   4680   4342   -482   1645  -1446      N
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Figure 18 (continued)

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ATOM   4879  CA  VAL E 444      47.578 -23.901 -21.443  1.00 32.51           C
ANISOU 4879  CA  VAL E 444    3697   4640   4016   -699   1710  -1287          C
ATOM   4880  CB  VAL E 444      47.325 -24.320 -22.913  1.00 33.98           C
ANISOU 4880  CB  VAL E 444    3940   4981   3988   -767   1820  -1385          C
ATOM   4881  CG1 VAL E 444      46.849 -23.117 -23.727  1.00 33.93           C
ANISOU 4881  CG1 VAL E 444    4100   5048   3745   -989   1863  -1177          C
ATOM   4882  CG2 VAL E 444      48.595 -24.935 -23.530  1.00 35.29           C
ANISOU 4882  CG2 VAL E 444    3886   5374   4147   -757   1997  -1653          C
ATOM   4883  C   VAL E 444      46.325 -23.248 -20.824  1.00 30.69           C
ANISOU 4883  C   VAL E 444    3666   4204   3792   -710   1557  -1054          C
ATOM   4884  O   VAL E 444      46.204 -22.012 -20.791  1.00 30.76           O
ANISOU 4884  O   VAL E 444    3753   4195   3741   -856   1561   -883          O
ATOM   4885  N   LEU E 445      45.419 -24.090 -20.332  1.00 28.79           N
ANISOU 4885  N   LEU E 445    3497   3803   3639   -557   1429  -1058          N
ATOM   4886  CA  LEU E 445      44.175 -23.667 -19.699  1.00 27.40           C
ANISOU 4886  CA  LEU E 445    3476   3448   3487   -543   1291   -880          C
ATOM   4887  CB  LEU E 445      43.334 -24.905 -19.324  1.00 26.06           C
ANISOU 4887  CB  LEU E 445    3348   3141   3410   -390   1191   -938          C
ATOM   4888  CG  LEU E 445      42.005 -24.714 -18.603  1.00 24.67           C
ANISOU 4888  CG  LEU E 445    3297   2800   3277   -363   1061   -794          C
ATOM   4889  CD1 LEU E 445      41.045 -23.943 -19.450  1.00 23.86           C
ANISOU 4889  CD1 LEU E 445    3319   2724   3024   -467   1044   -683          C
ATOM   4890  CD2 LEU E 445      41.388 -26.048 -18.167  1.00 23.79           C
ANISOU 4890  CD2 LEU E 445    3204   2560   3276   -238    987   -863          C
ATOM   4891  C   LEU E 445      44.416 -22.841 -18.438  1.00 26.46           C
ANISOU 4891  C   LEU E 445    3330   3240   3486   -548   1230   -777          C
ATOM   4892  O   LEU E 445      43.801 -21.786 -18.261  1.00 26.04           O
ANISOU 4892  O   LEU E 445    3381   3112   3400   -630   1188   -624          O
ATOM   4893  N   PHE E 446      45.272 -23.353 -17.551  1.00 26.46           N
ANISOU 4893  N   PHE E 446    3188   3241   3625   -447   1211   -870          N
ATOM   4894  CA  PHE E 446      45.576 -22.697 -16.274  1.00 25.67           C
ANISOU 4894  CA  PHE E 446    3046   3084   3625   -444   1141   -806          C
ATOM   4895  CB  PHE E 446      46.347 -23.663 -15.363  1.00 26.39           C
ANISOU 4895  CB  PHE E 446    2995   3178   3856   -282   1079   -912          C
ATOM   4896  CG  PHE E 446      45.490 -24.679 -14.652  1.00 24.94           C
ANISOU 4896  CG  PHE E 446    2898   2839   3740   -131    959   -875          C
ATOM   4897  CD1 PHE E 446      44.152 -24.830 -14.944  1.00 24.46           C
ANISOU 4897  CD1 PHE E 446    2999   2671   3625   -146    932   -796          C
ATOM   4898  CE1 PHE E 446      43.370 -25.769 -14.271  1.00 25.96           C
ANISOU 4898  CE1 PHE E 446    3262   2721   3881    -40    838   -760          C
ATOM   4899  CZ  PHE E 446      43.927 -26.577 -13.306  1.00 26.29           C
ANISOU 4899  CZ  PHE E 446    3242   2714   4034     92    761   -778          C
ATOM   4900  CE2 PHE E 446      45.274 -26.429 -12.996  1.00 28.95           C
ANISOU 4900  CE2 PHE E 446    3418   3158   4423    134    764   -850          C
ATOM   4901  CD2 PHE E 446      46.045 -25.494 -13.676  1.00 27.06           C
ANISOU 4901  CD2 PHE E 446    3080   3073   4128     20    868   -912          C
ATOM   4902  C   PHE E 446      46.389 -21.403 -16.496  1.00 26.52           C
ANISOU 4902  C   PHE E 446    3097   3289   3693   -623   1230   -777          C
ATOM   4903  O   PHE E 446      46.081 -20.387 -15.902  1.00 26.04           O
ANISOU 4903  O   PHE E 446    3101   3142   3650   -697   1185   -672          O
ATOM   4904  N   GLN E 447      47.407 -21.441 -17.364  1.00 28.42           N
ANISOU 4904  N   GLN E 447    3213   3703   3882   -703   1367   -882          N
ATOM   4905  CA  GLN E 447      48.255 -20.272 -17.631  1.00 30.21           C
ANISOU 4905  CA  GLN E 447    3374   4031   4073   -906   1474   -858          C
ATOM   4906  CB  GLN E 447      49.558 -20.665 -18.370  1.00 32.70           C
ANISOU 4906  CB  GLN E 447    3479   4581   4365   -956   1632  -1034          C
ATOM   4907  CG  GLN E 447      50.469 -21.664 -17.619  1.00 33.25           C
ANISOU 4907  CG  GLN E 447    3317   4717   4599   -768   1585  -1223          C
ATOM   4908  CD  GLN E 447      51.134 -21.082 -16.361  1.00 34.07           C
ANISOU 4908  CD  GLN E 447    3297   4813   4836   -777   1499  -1223          C
ATOM   4909  OE1 GLN E 447      50.681 -20.084 -15.801  1.00 33.58           O
ANISOU 4909  OE1 GLN E 447    3351   4637   4770   -881   1442  -1088          O
ATOM   4910  NE2 GLN E 447      52.215 -21.716 -15.914  1.00 33.89           N
ANISOU 4910  NE2 GLN E 447    3028   4913   4937   -660   1480  -1391          N
ATOM   4911  C   GLN E 447      47.535 -19.110 -18.348  1.00 30.32           C
ANISOU 4911  C   GLN E 447    3585   3978   3959  -1087   1508   -671          C
ATOM   4912  O   GLN E 447      47.924 -17.962 -18.215  1.00 31.49           O
ANISOU 4912  O   GLN E 447    3740   4105   4121  -1252   1546   -595          O
ATOM   4913  N   ASN E 448      46.468 -19.409 -19.073  1.00 30.31           N
ANISOU 4913  N   ASN E 448    3744   3928   3845  -1051   1477   -595          N
ATOM   4914  CA  ASN E 448      45.761 -18.409 -19.873  1.00 30.88           C
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Figure 18 (continued)

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ANISOU 4914  CA  ASN E 448     4004   3947   3783  -1195   1485   -407    C
ATOM   4915  CB  ASN E 448      45.584 -18.920 -21.309  1.00 32.53         C
ANISOU 4915  CB  ASN E 448     4268   4311   3782  -1240   1569   -424    C
ATOM   4916  CG  ASN E 448      46.858 -18.826 -22.104  1.00 35.40         C
ANISOU 4916  CG  ASN E 448     4506   4905   4040  -1401   1764   -514    C
ATOM   4917  OD1 ASN E 448      47.280 -17.741 -22.458  1.00 39.32         O
ANISOU 4917  OD1 ASN E 448     5044   5427   4468  -1605   1846   -389    O
ATOM   4918  ND2 ASN E 448      47.482 -19.960 -22.378  1.00 37.31         N
ANISOU 4918  ND2 ASN E 448     4588   5308   4280  -1312   1845   -737    N
ATOM   4919  C   ASN E 448      44.419 -17.982 -19.291  1.00 29.13         C
ANISOU 4919  C   ASN E 448     3941   3507   3618  -1115   1326   -267    C
ATOM   4920  O   ASN E 448      43.766 -17.081 -19.821  1.00 29.93         O
ANISOU 4920  O   ASN E 448     4198   3528   3646  -1201   1297    -98    O
ATOM   4921  N   TRP E 449      44.039 -18.593 -18.176  1.00 27.59         N
ANISOU 4921  N   TRP E 449     3703   3222   3558   -952   1225   -333    N
ATOM   4922  CA  TRP E 449      42.729 -18.370 -17.542  1.00 26.76         C
ANISOU 4922  CA  TRP E 449     3713   2942   3513   -861   1090   -243    C
ATOM   4923  CB  TRP E 449      42.475 -19.424 -16.454  1.00 24.28         C
ANISOU 4923  CB  TRP E 449     3331   2590   3304   -695   1016   -340    C
ATOM   4924  CG  TRP E 449      41.137 -19.316 -15.787  1.00 23.02         C
ANISOU 4924  CG  TRP E 449     3262   2290   3195   -614    905   -273    C
ATOM   4925  CD1 TRP E 449      40.863 -18.715 -14.596  1.00 21.45         C
ANISOU 4925  CD1 TRP E 449     3066   1994   3092   -591    847   -256    C
ATOM   4926  NE1 TRP E 449      39.515 -18.822 -14.298  1.00 20.39         N
ANISOU 4926  NE1 TRP E 449     3000   1770   2976   -516    770   -215    N
ATOM   4927  CE2 TRP E 449      38.885 -19.504 -15.306  1.00 21.49         C
ANISOU 4927  CE2 TRP E 449     3183   1943   3039   -494    763   -200    C
ATOM   4928  CD2 TRP E 449      39.876 -19.846 -16.270  1.00 24.86         C
ANISOU 4928  CD2 TRP E 449     3576   2486   3383   -553    846   -240    C
ATOM   4929  CE3 TRP E 449      39.491 -20.568 -17.422  1.00 23.76         C
ANISOU 4929  CE3 TRP E 449     3472   2418   3138   -550    858   -261    C
ATOM   4930  CZ3 TRP E 449      38.128 -20.936 -17.561  1.00 23.43         C
ANISOU 4930  CZ3 TRP E 449     3491   2323   3088   -492    771   -235    C
ATOM   4931  CH2 TRP E 449      37.172 -20.568 -16.574  1.00 21.37         C
ANISOU 4931  CH2 TRP E 449     3244   1947   2927   -437    692   -188    C
ATOM   4932  CZ2 TRP E 449      37.535 -19.864 -15.450  1.00 20.61         C
ANISOU 4932  CZ2 TRP E 449     3121   1786   2923   -435    694   -175    C
ATOM   4933  C   TRP E 449      42.490 -16.955 -16.983  1.00 27.51         C
ANISOU 4933  C   TRP E 449     3882   2888   3683   -936   1047   -131    C
ATOM   4934  O   TRP E 449      41.353 -16.459 -16.959  1.00 28.76         O
ANISOU 4934  O   TRP E 449     4157   2914   3855   -897    959    -29    O
ATOM   4935  N   GLY E 450      43.527 -16.296 -16.504  1.00 28.21         N
ANISOU 4935  N   GLY E 450     3890   2989   3838  -1037   1102   -166    N
ATOM   4936  CA  GLY E 450      43.293 -14.993 -15.886  1.00 27.79         C
ANISOU 4936  CA  GLY E 450     3907   2766   3884  -1103   1057    -93    C
ATOM   4937  C   GLY E 450      43.612 -15.062 -14.403  1.00 26.81         C
ANISOU 4937  C   GLY E 450     3678   2623   3885  -1038   1007   -216    C
ATOM   4938  O   GLY E 450      43.219 -16.005 -13.720  1.00 25.75         O
ANISOU 4938  O   GLY E 450     3501   2518   3763   -889    946   -282    O
ATOM   4939  N   ILE E 451      44.331 -14.049 -13.925  1.00 27.46         N
ANISOU 4939  N   ILE E 451     3725   2659   4049  -1166   1031   -243    N
ATOM   4940  CA  ILE E 451      44.805 -13.944 -12.563  1.00 26.27         C
ANISOU 4940  CA  ILE E 451     3467   2521   3994  -1141    984   -372    C
ATOM   4941  CB  ILE E 451      46.380 -13.916 -12.516  1.00 27.56         C
ANISOU 4941  CB  ILE E 451     3449   2845   4177  -1267   1061   -479    C
ATOM   4942  CG1 ILE E 451      46.919 -14.436 -11.178  1.00 27.57         C
ANISOU 4942  CG1 ILE E 451     3300   2949   4228  -1173    981   -627    C
ATOM   4943  CD1 ILE E 451      47.068 -15.951 -11.141  1.00 22.34         C
ANISOU 4943  CD1 ILE E 451     2547   2426   3515   -998    952   -669    C
ATOM   4944  CG2 ILE E 451      46.958 -12.547 -12.840  1.00 28.46         C
ANISOU 4944  CG2 ILE E 451     3590   2876   4349  -1500   1134   -445    C
ATOM   4945  C   ILE E 451      44.170 -12.690 -11.957  1.00 26.81         C
ANISOU 4945  C   ILE E 451     3641   2382   4162  -1182    931   -349    C
ATOM   4946  O   ILE E 451      43.942 -11.712 -12.669  1.00 27.27         O
ANISOU 4946  O   ILE E 451     3818   2296   4248  -1289    957   -238    O
ATOM   4947  N   GLU E 452      43.846 -12.740 -10.657  1.00 26.34         N
ANISOU 4947  N   GLU E 452     3548   2306   4155  -1090    853   -453    N
ATOM   4948  CA  GLU E 452      43.223 -11.616  -9.949  1.00 27.25         C
ANISOU 4948  CA  GLU E 452     3743   2237   4375  -1105    806   -486    C
ATOM   4949  CB  GLU E 452      41.711 -11.797  -9.805  1.00 26.07         C
ANISOU 4949  CB  GLU E 452     3691   1990   4224   -947    745   -441    C
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Figure 18 (continued)

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ATOM   4950  CG  GLU E 452      41.266 -12.939  -8.853  1.00 25.31           C
ANISOU 4950  CG  GLU E 452    3530   2030   4058   -801    701   -515          C
ATOM   4951  CD  GLU E 452      39.756 -13.124  -8.803  1.00 24.53           C
ANISOU 4951  CD  GLU E 452    3504   1856   3961   -674    661   -476          C
ATOM   4952  OE1 GLU E 452      39.068 -12.217  -9.314  1.00 25.81           O
ANISOU 4952  OE1 GLU E 452    3753   1850   4202   -676    647   -420          O
ATOM   4953  OE2 GLU E 452      39.251 -14.177  -8.283  1.00 23.51           O
ANISOU 4953  OE2 GLU E 452    3341   1829   3761   -574    642   -494          O
ATOM   4954  C   GLU E 452      43.848 -11.432  -8.580  1.00 28.43           C
ANISOU 4954  C   GLU E 452    3783   2458   4563  -1127    771   -662          C
ATOM   4955  O   GLU E 452      44.286 -12.399  -7.949  1.00 27.98           O
ANISOU 4955  O   GLU E 452    3614   2584   4434  -1053    740   -731          O
ATOM   4956  N   HIS E 453      43.923 -10.180  -8.146  1.00 30.69           N
ANISOU 4956  N   HIS E 453    4104   2592   4964  -1232    766   -734          N
ATOM   4957  CA  HIS E 453      44.200  -9.865  -6.747  1.00 32.45           C
ANISOU 4957  CA  HIS E 453    4251   2864   5216  -1241    715   -926          C
ATOM   4958  CB  HIS E 453      44.444  -8.372  -6.528  1.00 34.20           C
ANISOU 4958  CB  HIS E 453    4517   2885   5593  -1398    727  -1017          C
ATOM   4959  CG  HIS E 453      45.250  -8.092  -5.296  1.00 39.68           C
ANISOU 4959  CG  HIS E 453    5086   3695   6296  -1476    688  -1238          C
ATOM   4960  ND1 HIS E 453      44.724  -7.482  -4.169  1.00 43.34           N
ANISOU 4960  ND1 HIS E 453    5574   4092   6801  -1445    640  -1415          N
ATOM   4961  CE1 HIS E 453      45.664  -7.391  -3.246  1.00 44.55           C
ANISOU 4961  CE1 HIS E 453    5596   4407   6924  -1535    601  -1598          C
ATOM   4962  NE2 HIS E 453      46.769  -7.945  -3.718  1.00 42.51           N
ANISOU 4962  NE2 HIS E 453    5213   4316   6621  -1609    617  -1544          N
ATOM   4963  CD2 HIS E 453      46.540  -8.383  -4.997  1.00 40.32           C
ANISOU 4963  CD2 HIS E 453    5000   3982   6338  -1576    682  -1329          C
ATOM   4964  C   HIS E 453      43.055 -10.310  -5.860  1.00 31.39           C
ANISOU 4964  C   HIS E 453    4153   2749   5027  -1069    658   -973          C
ATOM   4965  O   HIS E 453      41.890 -10.357  -6.286  1.00 30.46           O
ANISOU 4965  O   HIS E 453    4134   2517   4921   -967    656   -882          O
ATOM   4966  N   ILE E 454      43.380 -10.638  -4.618  1.00 31.87           N
ANISOU 4966  N   ILE E 454    4122   2971   5015  -1043    609  -1116          N
ATOM   4967  CA  ILE E 454      42.346 -11.093  -3.700  1.00 31.42           C
ANISOU 4967  CA  ILE E 454    4094   2967   4875   -909    573  -1161          C
ATOM   4968  CB  ILE E 454      42.380 -12.627  -3.506  1.00 30.33           C
ANISOU 4968  CB  ILE E 454    3911   3030   4585   -798    542  -1074          C
ATOM   4969  CG1 ILE E 454      43.610 -13.057  -2.681  1.00 31.20           C
ANISOU 4969  CG1 ILE E 454    3893   3350   4610   -830    478  -1157          C
ATOM   4970  CD1 ILE E 454      43.581 -14.534  -2.282  1.00 29.25           C
ANISOU 4970  CD1 ILE E 454    3622   3268   4225   -703    423  -1067          C
ATOM   4971  CG2 ILE E 454      42.334 -13.309  -4.878  1.00 29.40           C
ANISOU 4971  CG2 ILE E 454    3820   2871   4478   -764    580   -902          C
ATOM   4972  C   ILE E 454      42.322 -10.396  -2.359  1.00 32.96           C
ANISOU 4972  C   ILE E 454    4262   3196   5064   -942    541  -1372          C
ATOM   4973  O   ILE E 454      43.289  -9.765  -1.929  1.00 34.56           O
ANISOU 4973  O   ILE E 454    4398   3432   5303  -1065    521  -1505          O
ATOM   4974  N   ASP E 455      41.171 -10.489  -1.720  1.00 33.18           N
ANISOU 4974  N   ASP E 455    4337   3225   5046   -841    545  -1419          N
ATOM   4975  CA  ASP E 455      41.040 -10.071  -0.349  1.00 34.92           C
ANISOU 4975  CA  ASP E 455    4527   3541   5200   -856    525  -1632          C
ATOM   4976  CB  ASP E 455      39.607  -9.614  -0.072  1.00 35.97           C
ANISOU 4976  CB  ASP E 455    4721   3562   5384   -767    570  -1709          C
ATOM   4977  CG  ASP E 455      39.150  -8.513  -1.016  1.00 38.40           C
ANISOU 4977  CG  ASP E 455    5103   3558   5931   -768    596  -1692          C
ATOM   4978  OD1 ASP E 455      39.930  -7.575  -1.295  1.00 43.88           O
ANISOU 4978  OD1 ASP E 455    5809   4103   6759   -885    588  -1746          O
ATOM   4979  OD2 ASP E 455      38.012  -8.581  -1.493  1.00 39.86           O
ANISOU 4979  OD2 ASP E 455    5332   3641   6173   -656    616  -1617          O
ATOM   4980  C   ASP E 455      41.428 -11.210   0.583  1.00 34.38           C
ANISOU 4980  C   ASP E 455    4395   3761   4905   -821    470  -1620          C
ATOM   4981  O   ASP E 455      41.239 -12.372   0.267  1.00 33.22           O
ANISOU 4981  O   ASP E 455    4259   3693   4672   -739    463  -1447          O
ATOM   4982  N   ASN E 456      42.001 -10.857   1.727  1.00 36.29           N
ANISOU 4982  N   ASN E 456    4579   4155   5054   -888    421  -1805          N
ATOM   4983  CA  ASN E 456      42.242 -11.804   2.805  1.00 36.41           C
ANISOU 4983  CA  ASN E 456    4556   4451   4827   -852    350  -1799          C
ATOM   4984  CB  ASN E 456      43.157 -11.172   3.870  1.00 38.96           C
ANISOU 4984  CB  ASN E 456    4797   4935   5071   -959    274  -2023          C
ATOM   4985  CG  ASN E 456      44.549 -10.827   3.334  1.00 40.45           C
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Figure 18 (continued)

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ANISOU 4985  CG  ASN E 456     4881   5107   5382  -1060    220  -2046      C
ATOM   4986  OD1 ASN E 456      45.178 -11.638   2.635  1.00 41.16          O
ANISOU 4986  OD1 ASN E 456     4920   5233   5486  -1020    191  -1874      O
ATOM   4987  ND2 ASN E 456      45.040  -9.624   3.669  1.00 39.97          N
ANISOU 4987  ND2 ASN E 456     4777   4994   5418  -1199    215  -2279      N
ATOM   4988  C   ASN E 456      40.922 -12.229   3.444  1.00 35.91          C
ANISOU 4988  C   ASN E 456     4561   4451   4631   -773    404  -1790      C
ATOM   4989  O   ASN E 456      40.246 -11.425   4.099  1.00 37.52          O
ANISOU 4989  O   ASN E 456     4782   4643   4833   -794    455  -1984      O
ATOM   4990  N   VAL E 457      40.543 -13.483   3.230  1.00 33.98          N
ANISOU 4990  N   VAL E 457     4351   4269   4291   -689    402  -1578      N
ATOM   4991  CA  VAL E 457      39.365 -14.080   3.867  1.00 33.82          C
ANISOU 4991  CA  VAL E 457     4385   4343   4122   -641    458  -1541      C
ATOM   4992  CB  VAL E 457      38.259 -14.476   2.836  1.00 32.61          C
ANISOU 4992  CB  VAL E 457     4279   4018   4093   -568    540  -1399      C
ATOM   4993  CG1 VAL E 457      37.029 -15.057   3.553  1.00 32.25          C
ANISOU 4993  CG1 VAL E 457     4264   4088   3900   -547    614  -1383      C
ATOM   4994  CG2 VAL E 457      37.839 -13.264   1.956  1.00 34.28          C
ANISOU 4994  CG2 VAL E 457     4492   3983   4548   -564    592  -1495      C
ATOM   4995  C   VAL E 457      39.833 -15.326   4.626  1.00 33.51          C
ANISOU 4995  C   VAL E 457     4356   4530   3847   -623    373  -1398      C
ATOM   4996  O   VAL E 457      40.368 -16.254   4.027  1.00 32.47          O
ANISOU 4996  O   VAL E 457     4224   4372   3741   -570    314  -1210      O
ATOM   4997  N   MSE E 458      39.663 -15.333   5.946  1.00 34.54          N
ANISOU 4997  N   MSE E 458     4498   4881   3746   -664    361  -1491      N
ATOM   4998  CA  MSE E 458      40.077 -16.485   6.758  1.00 34.73          C
ANISOU 4998  CA  MSE E 458     4554   5121   3522   -649    262  -1328      C
ATOM   4999  CB  MSE E 458      39.930 -16.198   8.270  1.00 36.83          C
ANISOU 4999  CB  MSE E 458     4834   5661   3500   -725    252  -1475      C
ATOM   5000  CG  MSE E 458      40.556 -17.267   9.149  1.00 36.65          C
ANISOU 5000  CG  MSE E 458     4852   5870   3203   -714    109  -1293      C
ATOM   5001  SE  MSE E 458      40.273 -16.954  11.015  0.90 41.76         SE
ANISOU 5001  SE  MSE E 458     5537   6903   3425   -827    106  -1458      SE
ATOM   5002  CE  MSE E 458      41.315 -18.332  11.797  1.00 45.02          C
ANISOU 5002  CE  MSE E 458     6009   7547   3550   -781   -137  -1152      C
ATOM   5003  C   MSE E 458      39.307 -17.753   6.367  1.00 33.55          C
ANISOU 5003  C   MSE E 458     4487   4909   3352   -591    305  -1072      C
ATOM   5004  O   MSE E 458      38.099 -17.701   6.110  1.00 32.64          O
ANISOU 5004  O   MSE E 458     4404   4712   3286   -596    437  -1080      O
ATOM   5005  N   GLY E 459      40.010 -18.883   6.316  1.00 33.52          N
ANISOU 5005  N   GLY E 459     4507   4934   3293   -532    189   -859      N
ATOM   5006  CA  GLY E 459      39.389 -20.156   5.923  1.00 33.09          C
ANISOU 5006  CA  GLY E 459     4540   4788   3245   -484    216   -617      C
ATOM   5007  C   GLY E 459      39.465 -20.494   4.445  1.00 31.02          C
ANISOU 5007  C   GLY E 459     4259   4286   3242   -413    236   -537      C
ATOM   5008  O   GLY E 459      38.878 -21.472   4.003  1.00 29.76          O
ANISOU 5008  O   GLY E 459     4166   4024   3119   -382    269   -374      O
ATOM   5009  N   MSE E 460      40.234 -19.707   3.697  1.00 31.09          N
ANISOU 5009  N   MSE E 460     4178   4216   3419   -401    216   -654      N
ATOM   5010  CA  MSE E 460      40.276 -19.773   2.235  1.00 31.27          C
ANISOU 5010  CA  MSE E 460     4178   4037   3665   -358    258   -615      C
ATOM   5011  CB  MSE E 460      39.161 -18.884   1.732  1.00 30.55          C
ANISOU 5011  CB  MSE E 460     4104   3830   3674   -400    385   -715      C
ATOM   5012  CG  MSE E 460      38.666 -19.120   0.368  1.00 31.73          C
ANISOU 5012  CG  MSE E 460     4270   3798   3987   -364    442   -641      C
ATOM   5013  SE  MSE E 460      37.264 -17.775   0.139  0.90 36.29         SE
ANISOU 5013  SE  MSE E 460     4850   4272   4665   -398    558   -792      SE
ATOM   5014  CE  MSE E 460      35.900 -18.531   1.319  1.00 33.17          C
ANISOU 5014  CE  MSE E 460     4495   4021   4089   -418    629   -764      C
ATOM   5015  C   MSE E 460      41.595 -19.181   1.740  1.00 29.41          C
ANISOU 5015  C   MSE E 460     3836   3797   3541   -360    197   -704      C
ATOM   5016  O   MSE E 460      42.123 -18.243   2.345  1.00 30.18          O
ANISOU 5016  O   MSE E 460     3874   3990   3604   -424    166   -859      O
ATOM   5017  N   VAL E 461      42.129 -19.739   0.654  1.00 27.19          N
ANISOU 5017  N   VAL E 461     3522   3418   3392   -302    187   -625      N
ATOM   5018  CA  VAL E 461      43.328 -19.186   0.002  1.00 26.63          C
ANISOU 5018  CA  VAL E 461     3332   3346   3439   -324    164   -711      C
ATOM   5019  CB  VAL E 461      44.678 -19.981   0.317  1.00 27.57          C
ANISOU 5019  CB  VAL E 461     3343   3596   3535   -245    -26   -678      C
ATOM   5020  CG1 VAL E 461      45.146 -19.726   1.712  1.00 30.38          C
ANISOU 5020  CG1 VAL E 461     3661   4147   3734   -267    -90   -741      C
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Figure 18 (continued)

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ATOM   5021  CG2 VAL E 461      44.544 -21.476   0.054  1.00 27.15           C
ANISOU 5021  CG2 VAL E 461    3343   3486   3488   -113    -15   -505       C
ATOM   5022  C   VAL E 461      43.155 -19.117  -1.507  1.00 24.12           C
ANISOU 5022  C   VAL E 461    3020   2866   3278   -326    258   -681       C
ATOM   5023  O   VAL E 461      42.324 -19.841  -2.080  1.00 22.67           O
ANISOU 5023  O   VAL E 461    2916   2584   3112   -275    303   -577       O
ATOM   5024  N   GLY E 462      43.947 -18.249  -2.140  1.00 23.16           N
ANISOU 5024  N   GLY E 462    2816   2728   3258   -401    288   -772       N
ATOM   5025  CA  GLY E 462      44.112 -18.282  -3.598  1.00 21.82           C
ANISOU 5025  CA  GLY E 462    2635   2456   3200   -412    367   -733       C
ATOM   5026  C   GLY E 462      44.981 -19.456  -4.067  1.00 21.42           C
ANISOU 5026  C   GLY E 462    2500   2467   3173   -317    329   -687       C
ATOM   5027  O   GLY E 462      45.717 -20.046  -3.299  1.00 20.90           O
ANISOU 5027  O   GLY E 462    2354   2517   3068   -248    226   -695       O
ATOM   5028  N   VAL E 463      44.888 -19.781  -5.350  1.00 21.09           N
ANISOU 5028  N   VAL E 463    2471   2348   3194   -308    408   -648       N
ATOM   5029  CA  VAL E 463      45.725 -20.807  -5.947  1.00 20.88           C
ANISOU 5029  CA  VAL E 463    2351   2370   3213   -218    396   -648       C
ATOM   5030  CB  VAL E 463      44.939 -22.151  -6.066  1.00 21.07           C
ANISOU 5030  CB  VAL E 463    2475   2306   3226    -91    372   -548       C
ATOM   5031  CG1 VAL E 463      43.726 -22.012  -7.015  1.00 18.51           C
ANISOU 5031  CG1 VAL E 463    2276   1857   2899   -139    466   -501       C
ATOM   5032  CG2 VAL E 463      45.863 -23.303  -6.490  1.00 19.87           C
ANISOU 5032  CG2 VAL E 463    2221   2184   3145     35    338   -572       C
ATOM   5033  C   VAL E 463      46.254 -20.270  -7.294  1.00 20.93           C
ANISOU 5033  C   VAL E 463    2297   2378   3279   -312    513   -699       C
ATOM   5034  O   VAL E 463      45.503 -19.667  -8.067  1.00 20.04           O
ANISOU 5034  O   VAL E 463    2287   2170   3159   -394    595   -659       O
ATOM   5035  N   LEU E 464      47.555 -20.432  -7.522  1.00 21.97           N
ANISOU 5035  N   LEU E 464    2253   2633   3461   -308    516   -787       N
ATOM   5036  CA  LEU E 464      48.217 -20.037  -8.768  1.00 22.38           C
ANISOU 5036  CA  LEU E 464    2222   2733   3549   -412    644   -844       C
ATOM   5037  CB  LEU E 464      49.692 -19.686  -8.481  1.00 23.67           C
ANISOU 5037  CB  LEU E 464    2157   3066   3770   -468    634   -973       C
ATOM   5038  CG  LEU E 464      50.020 -18.579  -7.451  1.00 24.00           C
ANISOU 5038  CG  LEU E 464    2156   3149   3816   -587    574  -1026       C
ATOM   5039  CD1 LEU E 464      51.527 -18.280  -7.395  1.00 23.87           C
ANISOU 5039  CD1 LEU E 464    1881   3320   3868   -665    578  -1172       C
ATOM   5040  CD2 LEU E 464      49.204 -17.298  -7.711  1.00 19.83           C
ANISOU 5040  CD2 LEU E 464    1791   2471   3272   -757    652   -975       C
ATOM   5041  C   LEU E 464      48.096 -21.191  -9.796  1.00 23.25           C
ANISOU 5041  C   LEU E 464    2340   2827   3666   -306    696   -838       C
ATOM   5042  O   LEU E 464      47.759 -22.317  -9.404  1.00 23.03           O
ANISOU 5042  O   LEU E 464    2348   2749   3651   -145    614   -807       O
ATOM   5043  N   PRO E 465      48.325 -20.915 -11.110  1.00 24.19           N
ANISOU 5043  N   PRO E 465    2442   2983   3768   -407    835   -868       N
ATOM   5044  CA  PRO E 465      48.340 -21.987 -12.127  1.00 25.02           C
ANISOU 5044  CA  PRO E 465    2532   3105   3868   -317    897   -912       C
ATOM   5045  CB  PRO E 465      48.816 -21.267 -13.393  1.00 25.21           C
ANISOU 5045  CB  PRO E 465    2515   3230   3834   -493   1061   -949       C
ATOM   5046  CG  PRO E 465      48.349 -19.856 -13.215  1.00 25.13           C
ANISOU 5046  CG  PRO E 465    2621   3143   3785   -666   1072   -842       C
ATOM   5047  CD  PRO E 465      48.511 -19.577 -11.724  1.00 25.08           C
ANISOU 5047  CD  PRO E 465    2570   3111   3849   -623    944   -853       C
ATOM   5048  C   PRO E 465      49.235 -23.225 -11.820  1.00 27.35           C
ANISOU 5048  C   PRO E 465    2659   3471   4261   -129    835  -1023       C
ATOM   5049  O   PRO E 465      48.830 -24.361 -12.130  1.00 26.54           O
ANISOU 5049  O   PRO E 465    2609   3290   4185      9    814  -1032       O
ATOM   5050  N   ASP E 466      50.418 -23.018 -11.230  1.00 29.43           N
ANISOU 5050  N   ASP E 466    2720   3869   4592   -119    795  -1113       N
ATOM   5051  CA  ASP E 466      51.243 -24.148 -10.769  1.00 32.32           C
ANISOU 5051  CA  ASP E 466    2921   4288   5071     93    692  -1202       C
ATOM   5052  CB  ASP E 466      52.739 -23.769 -10.621  1.00 34.50           C
ANISOU 5052  CB  ASP E 466    2906   4779   5422     65    702  -1353       C
ATOM   5053  CG  ASP E 466      53.011 -22.725  -9.515  1.00 36.86           C
ANISOU 5053  CG  ASP E 466    3166   5140   5698    -48    612  -1323       C
ATOM   5054  OD1 ASP E 466      52.104 -22.374  -8.726  1.00 36.45           O
ANISOU 5054  OD1 ASP E 466    3303   4971   5575    -73    529  -1195       O
ATOM   5055  OD2 ASP E 466      54.164 -22.236  -9.438  1.00 40.79           O
ANISOU 5055  OD2 ASP E 466    3426   5820   6251   -123    630  -1452       O
ATOM   5056  C   ASP E 466      50.683 -24.859  -9.498  1.00 32.48           C
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Figure 18 (continued)

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ANISOU 5056  C   ASP E 466     3053   4182   5108    257    499  -1082      C
ATOM   5057  O   ASP E 466      51.316 -25.787  -8.955  1.00 34.03          O
ANISOU 5057  O   ASP E 466     3140   4392   5398    449    373  -1114      O
ATOM   5058  N   MSE E 467      49.498 -24.434  -9.038  1.00 30.80          N
ANISOU 5058  N   MSE E 467     3052   3848   4801    183    475   -942      N
ATOM   5059  CA  MSE E 467      48.846 -25.020  -7.854  1.00 30.56          C
ANISOU 5059  CA  MSE E 467     3147   3717   4746    291    324   -814      C
ATOM   5060  CB  MSE E 467      48.762 -26.561  -7.943  1.00 31.92          C
ANISOU 5060  CB  MSE E 467     3352   3770   5007    491    255   -788      C
ATOM   5061  CG  MSE E 467      47.737 -27.121  -8.964  1.00 31.71          C
ANISOU 5061  CG  MSE E 467     3477   3592   4981    477    356   -771      C
ATOM   5062  SE  MSE E 467      45.883 -26.433  -8.795  0.90 34.47          SE
ANISOU 5062  SE  MSE E 467     4082   3825   5191    312    402   -618      SE
ATOM   5063  CE  MSE E 467      45.524 -26.906  -6.992  1.00 31.60          C
ANISOU 5063  CE  MSE E 467     3808   3411   4787    390    232   -460      C
ATOM   5064  C   MSE E 467      49.441 -24.599  -6.507  1.00 31.54          C
ANISOU 5064  C   MSE E 467     3189   3953   4840    301    184   -803      C
ATOM   5065  O   MSE E 467      49.044 -25.120  -5.466  1.00 31.93          O
ANISOU 5065  O   MSE E 467     3332   3957   4844    388     53   -692      O
ATOM   5066  N   THR E 468      50.376 -23.644  -6.523  1.00 32.10          N
ANISOU 5066  N   THR E 468     3090   4182   4925    193    214   -918      N
ATOM   5067  CA  THR E 468      50.923 -23.058  -5.298  1.00 32.25          C
ANISOU 5067  CA  THR E 468     3023   4330   4900    163     86   -940      C
ATOM   5068  CB  THR E 468      52.209 -22.245  -5.586  1.00 33.45          C
ANISOU 5068  CB  THR E 468     2925   4665   5118     52    132  -1109      C
ATOM   5069  OG1 THR E 468      53.248 -23.146  -5.974  1.00 36.74          O
ANISOU 5069  OG1 THR E 468     3131   5176   5652    209     99  -1199      O
ATOM   5070  CG2 THR E 468      52.708 -21.493  -4.365  1.00 35.62          C
ANISOU 5070  CG2 THR E 468     3114   5077   5342    -16      5  -1160      C
ATOM   5071  C   THR E 468      49.829 -22.192  -4.665  1.00 30.54          C
ANISOU 5071  C   THR E 468     2997   4041   4564     33     99   -864      C
ATOM   5072  O   THR E 468      49.160 -21.413  -5.371  1.00 28.58          O
ANISOU 5072  O   THR E 468     2848   3706   4305   -106    236   -861      O
ATOM   5073  N   PRO E 469      49.621 -22.346  -3.345  1.00 30.70          N
ANISOU 5073  N   PRO E 469     3072   4103   4490     85    -46   -802      N
ATOM   5074  CA  PRO E 469      48.656 -21.488  -2.669  1.00 30.08          C
ANISOU 5074  CA  PRO E 469     3144   3989   4298    -36    -24   -774      C
ATOM   5075  CB  PRO E 469      48.508 -22.138  -1.284  1.00 31.30          C
ANISOU 5075  CB  PRO E 469     3355   4213   4324     65   -191   -683      C
ATOM   5076  CG  PRO E 469      49.779 -22.851  -1.077  1.00 33.03          C
ANISOU 5076  CG  PRO E 469     3396   4554   4601    203   -334   -705      C
ATOM   5077  CD  PRO E 469      50.246 -23.308  -2.421  1.00 32.56          C
ANISOU 5077  CD  PRO E 469     3238   4425   4708    260   -238   -754      C
ATOM   5078  C   PRO E 469      49.205 -20.071  -2.547  1.00 30.36          C
ANISOU 5078  C   PRO E 469     3079   4112   4345   -212     15   -921      C
ATOM   5079  O   PRO E 469      50.414 -19.874  -2.451  1.00 32.17          O
ANISOU 5079  O   PRO E 469     3111   4488   4626   -230    -38  -1031      O
ATOM   5080  N   SER E 470      48.312 -19.099  -2.559  1.00 28.84          N
ANISOU 5080  N   SER E 470     3014   3820   4123   -340    103   -932      N
ATOM   5081  CA  SER E 470      48.702 -17.729  -2.427  1.00 29.49          C
ANISOU 5081  CA  SER E 470     3037   3929   4238   -515    142  -1067      C
ATOM   5082  CB  SER E 470      48.867 -17.093  -3.809  1.00 28.97          C
ANISOU 5082  CB  SER E 470     2956   3760   4289   -635    295  -1082      C
ATOM   5083  OG  SER E 470      49.175 -15.713  -3.679  1.00 29.55          O
ANISOU 5083  OG  SER E 470     3000   3813   4414   -824    336  -1197      O
ATOM   5084  C   SER E 470      47.631 -16.997  -1.653  1.00 28.74          C
ANISOU 5084  C   SER E 470     3092   3763   4065   -573    150  -1083      C
ATOM   5085  O   SER E 470      46.443 -17.255  -1.843  1.00 26.47          O
ANISOU 5085  O   SER E 470     2958   3353   3748   -526    203   -985      O
ATOM   5086  N   THR E 471      48.069 -16.067  -0.807  1.00 30.16          N
ANISOU 5086  N   THR E 471     3210   4030   4222   -681    102  -1231      N
ATOM   5087  CA  THR E 471      47.155 -15.195  -0.063  1.00 30.86          C
ANISOU 5087  CA  THR E 471     3415   4056   4254   -749    123  -1307      C
ATOM   5088  CB  THR E 471      47.566 -15.088   1.420  1.00 32.72          C
ANISOU 5088  CB  THR E 471     3592   4500   4342   -760    -10  -1427      C
ATOM   5089  OG1 THR E 471      48.951 -14.718   1.504  1.00 37.22          O
ANISOU 5089  OG1 THR E 471     3970   5205   4968   -843    -80  -1556      O
ATOM   5090  CG2 THR E 471      47.380 -16.453   2.138  1.00 32.82          C
ANISOU 5090  CG2 THR E 471     3640   4649   4181   -599   -122  -1281      C
ATOM   5091  C   THR E 471      47.026 -13.797  -0.691  1.00 30.99          C
ANISOU 5091  C   THR E 471     3462   3895   4418   -908    233  -1402      C
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Figure 18 (continued)

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ATOM   5092  O   THR E 471      46.403 -12.895  -0.095  1.00 32.41           O
ANISOU 5092  O   THR E 471    3716   4003   4595   -969    251  -1512          O
ATOM   5093  N   GLU E 472      47.585 -13.628  -1.893  1.00 30.24           N
ANISOU 5093  N   GLU E 472    3317   3723   4448   -974    310  -1358          N
ATOM   5094  CA  GLU E 472      47.662 -12.324  -2.573  1.00 30.68           C
ANISOU 5094  CA  GLU E 472    3405   3604   4648   -1148   408  -1413          C
ATOM   5095  CB  GLU E 472      49.108 -11.861  -2.654  1.00 32.44           C
ANISOU 5095  CB  GLU E 472    3444   3937   4945   -1303   403  -1532          C
ATOM   5096  CG  GLU E 472      49.779 -11.668  -1.290  1.00 37.76           C
ANISOU 5096  CG  GLU E 472    3990   4801   5555   -1337   276  -1720          C
ATOM   5097  CD  GLU E 472      51.175 -12.305  -1.215  1.00 43.37           C
ANISOU 5097  CD  GLU E 472    4460   5762   6256   -1331   199  -1771          C
ATOM   5098  OE1 GLU E 472      52.173 -11.548  -1.139  1.00 44.91           O
ANISOU 5098  OE1 GLU E 472    4502   6025   6538   -1509   199  -1925          O
ATOM   5099  OE2 GLU E 472      51.270 -13.569  -1.236  1.00 42.62           O
ANISOU 5099  OE2 GLU E 472    4322   5787   6083   -1147   136  -1663          O
ATOM   5100  C   GLU E 472      47.062 -12.382  -3.974  1.00 28.59           C
ANISOU 5100  C   GLU E 472    3251   3164   4447   -1137   517  -1248          C
ATOM   5101  O   GLU E 472      46.385 -11.449  -4.397  1.00 28.12           O
ANISOU 5101  O   GLU E 472    3316   2897   4471   -1205   576  -1225          O
ATOM   5102  N   MSE E 473      47.284 -13.494  -4.682  1.00 27.02           N
ANISOU 5102  N   MSE E 473    3012   3048   4206   -1042   532  -1137          N
ATOM   5103  CA  MSE E 473      46.791 -13.651  -6.073  1.00 25.54           C
ANISOU 5103  CA  MSE E 473    2919   2739   4045   -1038   629   -993          C
ATOM   5104  CB  MSE E 473      47.927 -13.574  -7.115  1.00 25.96           C
ANISOU 5104  CB  MSE E 473    2858   2862   4144   -1159   717   -991          C
ATOM   5105  CG  MSE E 473      48.808 -12.339  -7.049  1.00 27.29           C
ANISOU 5105  CG  MSE E 473    2952   3011   4406   -1379   758  -1091          C
ATOM   5106  SE  MSE E 473      47.910 -10.662  -7.515  0.90 31.81          SE
ANISOU 5106  SE  MSE E 473    3749   3250   5087   -1541   823  -1021          SE
ATOM   5107  CE  MSE E 473      47.552 -10.998  -9.390  1.00 22.17           C
ANISOU 5107  CE  MSE E 473    2643   1969   3812   -1555   942   -793          C
ATOM   5108  C   MSE E 473      46.107 -14.980  -6.236  1.00 23.39           C
ANISOU 5108  C   MSE E 473    2695   2501   3691   -856    603   -890          C
ATOM   5109  O   MSE E 473      46.393 -15.922  -5.503  1.00 22.98           O
ANISOU 5109  O   MSE E 473    2572   2580   3579   -744    522   -910          O
ATOM   5110  N   SER E 474      45.225 -15.055  -7.218  1.00 21.86           N
ANISOU 5110  N   SER E 474    2624   2183   3498   -833    662   -776          N
ATOM   5111  CA  SER E 474      44.566 -16.309  -7.532  1.00 21.14           C
ANISOU 5111  CA  SER E 474    2578   2108   3346   -687    648   -690          C
ATOM   5112  CB  SER E 474      43.337 -16.499  -6.641  1.00 19.96           C
ANISOU 5112  CB  SER E 474    2523   1903   3156   -597    594   -671          C
ATOM   5113  OG  SER E 474      42.904 -17.839  -6.691  1.00 17.66           O
ANISOU 5113  OG  SER E 474    2253   1645   2812   -475    569   -603          O
ATOM   5114  C   SER E 474      44.153 -16.398  -9.009  1.00 21.27           C
ANISOU 5114  C   SER E 474    2672   2053   3359   -708    727   -592          C
ATOM   5115  O   SER E 474      43.946 -15.384  -9.652  1.00 20.89           O
ANISOU 5115  O   SER E 474    2694   1900   3342   -814    775   -549          O
ATOM   5116  N   MSE E 475      44.041 -17.620  -9.536  1.00 22.35           N
ANISOU 5116  N   MSE E 475    2683   2123   3336   -608    732   -558          N
ATOM   5117  CA  MSE E 475      43.337 -17.808 -10.790  1.00 22.35           C
ANISOU 5117  CA  MSE E 475    2894   2181   3417   -609    783   -475          C
ATOM   5118  CB  MSE E 475      43.262 -19.297 -11.154  1.00 21.85           C
ANISOU 5118  CB  MSE E 475    2809   2173   3321   -490    776   -482          C
ATOM   5119  CG  MSE E 475      44.593 -19.830 -11.643  1.00 24.48           C
ANISOU 5119  CG  MSE E 475    3003   2637   3663   -493    828   -563          C
ATOM   5120  SE  MSE E 475      44.487 -21.578 -12.470  0.90 25.13          SE
ANISOU 5120  SE  MSE E 475    3073   2746   3730   -353    842   -603          SE
ATOM   5121  CE  MSE E 475      44.118 -22.622 -10.880  1.00 14.68           C
ANISOU 5121  CE  MSE E 475    1759   1354   2463   -188    701   -580          C
ATOM   5122  C   MSE E 475      41.951 -17.191 -10.626  1.00 21.56           C
ANISOU 5122  C   MSE E 475    2925   1942   3326   -596    747   -409          C
ATOM   5123  O   MSE E 475      41.300 -17.398  -9.596  1.00 20.22           O
ANISOU 5123  O   MSE E 475    2769   1750   3164   -523    691   -430          O
ATOM   5124  N   ARG E 476      41.543 -16.382 -11.605  1.00 22.84           N
ANISOU 5124  N   ARG E 476    3174   2018   3486   -669    779   -331          N
ATOM   5125  CA  ARG E 476      40.252 -15.645 -11.593  1.00 23.43           C
ANISOU 5125  CA  ARG E 476    3359   1948   3596   -642    734   -269          C
ATOM   5126  CB  ARG E 476      40.013 -14.999 -12.975  1.00 24.07           C
ANISOU 5126  CB  ARG E 476    3538   1961   3647   -714    755   -147          C
ATOM   5127  CG  ARG E 476      38.593 -14.426 -13.168  1.00 27.79           C
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Figure 18 (continued)

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ANISOU 5127  CG  ARG E 476     4110   2292   4159   -646    680    -70  C
ATOM   5128  CD  ARG E 476      38.209 -14.075 -14.619  1.00 28.50      C
ANISOU 5128  CD  ARG E 476     4305   2345   4177   -684    665     79  C
ATOM   5129  NE  ARG E 476      38.636 -14.995 -15.699  1.00 32.45      N
ANISOU 5129  NE  ARG E 476     4797   3003   4528   -722    716    104  N
ATOM   5130  CZ  ARG E 476      37.899 -15.993 -16.202  1.00 31.12      C
ANISOU 5130  CZ  ARG E 476     4629   2913   4282   -642    682     96  C
ATOM   5131  NH1 ARG E 476      36.693 -16.294 -15.685  1.00 30.33      N
ANISOU 5131  NH1 ARG E 476     4521   2762   4240   -526    601     71  N
ATOM   5132  NH2 ARG E 476      38.385 -16.718 -17.191  1.00 25.61      N
ANISOU 5132  NH2 ARG E 476     3925   2354   3452   -687    739     89  N
ATOM   5133  C   ARG E 476      39.015 -16.489 -11.142  1.00 21.83      C
ANISOU 5133  C   ARG E 476     3173   1741   3380   -513    681   -273  C
ATOM   5134  O   ARG E 476      38.679 -17.503 -11.745  1.00 21.04      O
ANISOU 5134  O   ARG E 476     3079   1693   3224   -465    681   -247  O
ATOM   5135  N   GLY E 477      38.372 -16.052 -10.058  1.00 21.70      N
ANISOU 5135  N   GLY E 477     3157   1672   3416   -473    646   -324  N
ATOM   5136  CA  GLY E 477      37.207 -16.716  -9.484  1.00 20.09      C
ANISOU 5136  CA  GLY E 477     2953   1479   3200   -382    617   -338  C
ATOM   5137  C   GLY E 477      37.443 -18.027  -8.755  1.00 19.41      C
ANISOU 5137  C   GLY E 477     2821   1499   3053   -341    617   -363  C
ATOM   5138  O   GLY E 477      36.471 -18.609  -8.296  1.00 19.64      O
ANISOU 5138  O   GLY E 477     2856   1537   3067   -294    607   -361  O
ATOM   5139  N   ILE E 478      38.696 -18.502  -8.647  1.00 18.91      N
ANISOU 5139  N   ILE E 478     2708   1514   2965   -357    623   -381  N
ATOM   5140  CA  ILE E 478      39.017 -19.810  -8.023  1.00 17.77      C
ANISOU 5140  CA  ILE E 478     2530   1443   2777   -297    599   -380  C
ATOM   5141  CB  ILE E 478      40.039 -20.648  -8.855  1.00 18.55      C
ANISOU 5141  CB  ILE E 478     2584   1586   2878   -277    612   -379  C
ATOM   5142  CG1 ILE E 478      39.751 -20.616 -10.374  1.00 17.27      C
ANISOU 5142  CG1 ILE E 478     2459   1391   2711   -306    659   -354  C
ATOM   5143  CD1 ILE E 478      38.418 -21.271 -10.824  1.00 13.13      C
ANISOU 5143  CD1 ILE E 478     2003    811   2174   -270    646   -315  C
ATOM   5144  CG2 ILE E 478      40.182 -22.098  -8.267  1.00 18.35      C
ANISOU 5144  CG2 ILE E 478     2547   1581   2843   -186    567   -361  C
ATOM   5145  C   ILE E 478      39.616 -19.651  -6.599  1.00 18.69      C
ANISOU 5145  C   ILE E 478     2602   1637   2863   -298    561   -430  C
ATOM   5146  O   ILE E 478      40.569 -18.901  -6.395  1.00 18.45      O
ANISOU 5146  O   ILE E 478     2515   1647   2850   -348    556   -490  O
ATOM   5147  N   ARG E 479      39.035 -20.351  -5.617  1.00 18.39      N
ANISOU 5147  N   ARG E 479     2589   1632   2767   -257    533   -405  N
ATOM   5148  CA  ARG E 479      39.554 -20.346  -4.253  1.00 19.06      C
ANISOU 5148  CA  ARG E 479     2644   1820   2777   -256    483   -435  C
ATOM   5149  CB  ARG E 479      38.638 -19.533  -3.312  1.00 19.09      C
ANISOU 5149  CB  ARG E 479     2674   1845   2733   -297    507   -498  C
ATOM   5150  CG  ARG E 479      38.471 -18.073  -3.712  1.00 20.34      C
ANISOU 5150  CG  ARG E 479     2824   1925   2979   -348    545   -592  C
ATOM   5151  CD  ARG E 479      39.752 -17.232  -3.507  1.00 22.85      C
ANISOU 5151  CD  ARG E 479     3081   2279   3322   -408    517   -680  C
ATOM   5152  NE  ARG E 479      39.500 -15.800  -3.765  1.00 25.19      N
ANISOU 5152  NE  ARG E 479     3393   2459   3718   -468    552   -765  N
ATOM   5153  CZ  ARG E 479      39.487 -15.222  -4.979  1.00 27.21      C
ANISOU 5153  CZ  ARG E 479     3679   2582   4078   -498    582   -718  C
ATOM   5154  NH1 ARG E 479      39.709 -15.928  -6.090  1.00 26.37      N
ANISOU 5154  NH1 ARG E 479     3581   2470   3970   -482    595   -610  N
ATOM   5155  NH2 ARG E 479      39.248 -13.924  -5.085  1.00 26.41      N
ANISOU 5155  NH2 ARG E 479     3609   2347   4078   -547    597   -780  N
ATOM   5156  C   ARG E 479      39.697 -21.757  -3.727  1.00 19.49      C
ANISOU 5156  C   ARG E 479     2720   1912   2775   -189    429   -345  C
ATOM   5157  O   ARG E 479      38.976 -22.661  -4.158  1.00 18.74      O
ANISOU 5157  O   ARG E 479     2681   1743   2697   -162    449   -271  O
ATOM   5158  N   VAL E 480      40.609 -21.940  -2.772  1.00 20.82      N
ANISOU 5158  N   VAL E 480     2847   2187   2876   -166    349   -348  N
ATOM   5159  CA  VAL E 480      40.767 -23.248  -2.116  1.00 21.96      C
ANISOU 5159  CA  VAL E 480     3031   2353   2960    -92    271   -232  C
ATOM   5160  CB  VAL E 480      42.207 -23.838  -2.322  1.00 22.03      C
ANISOU 5160  CB  VAL E 480     2948   2393   3028      3    178   -229  C
ATOM   5161  CG1 VAL E 480      42.429 -25.077  -1.472  1.00 22.81      C
ANISOU 5161  CG1 VAL E 480     3098   2500   3069     95     63    -94  C
ATOM   5162  CG2 VAL E 480      42.460 -24.160  -3.772  1.00 20.19      C
ANISOU 5162  CG2 VAL E 480     2677   2061   2932     38    234   -261  C
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Figure 18 (continued)

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ATOM   5163  C   VAL E 480      40.412 -23.122  -0.620  1.00 23.54           C
ANISOU 5163  C   VAL E 480    3277   2674   2994   -131    235   -206          C
ATOM   5164  O   VAL E 480      40.953 -22.280   0.097  1.00 24.05           O
ANISOU 5164  O   VAL E 480    3287   2864   2988   -167    198   -300          O
ATOM   5165  N   SER E 481      39.492 -23.966  -0.161  1.00 24.81           N
ANISOU 5165  N   SER E 481    3538   2808   3083   -141    253    -88          N
ATOM   5166  CA  SER E 481      39.093 -24.015   1.249  1.00 26.08           C
ANISOU 5166  CA  SER E 481    3757   3104   3048   -193    236    -40          C
ATOM   5167  CB  SER E 481      37.836 -24.872   1.399  1.00 25.78           C
ANISOU 5167  CB  SER E 481    3824   3003   2969   -243    310     83          C
ATOM   5168  OG  SER E 481      37.426 -24.964   2.750  1.00 25.77           O
ANISOU 5168  OG  SER E 481    3886   3155   2752   -316    315    141          O
ATOM   5169  C   SER E 481      40.194 -24.566   2.157  1.00 28.89           C
ANISOU 5169  C   SER E 481    4114   3570   3294   -131     82     47          C
ATOM   5170  O   SER E 481      40.829 -25.579   1.858  1.00 29.34           O
ANISOU 5170  O   SER E 481    4181   3543   3423    -30     -9    161          O
ATOM   5171  N   LYS E 482      40.406 -23.902   3.280  1.00 31.33           N
ANISOU 5171  N   LYS E 482    4407   4070   3426   -183     44    -16          N
ATOM   5172  CA  LYS E 482      41.264 -24.437   4.320  1.00 35.34           C
ANISOU 5172  CA  LYS E 482    4931   4720   3776   -135   -119     86          C
ATOM   5173  CB  LYS E 482      42.004 -23.295   5.021  1.00 36.93           C
ANISOU 5173  CB  LYS E 482    5031   5127   3875   -177   -179    -95          C
ATOM   5174  CG  LYS E 482      43.111 -22.672   4.207  1.00 38.22           C
ANISOU 5174  CG  LYS E 482    5038   5259   4224   -134   -219   -240          C
ATOM   5175  CD  LYS E 482      43.698 -21.521   4.982  1.00 44.98           C
ANISOU 5175  CD  LYS E 482    5803   6309   4977   -211   -267   -433          C
ATOM   5176  CE  LYS E 482      45.223 -21.561   4.968  1.00 47.96           C
ANISOU 5176  CE  LYS E 482    6028   6783   5410   -142   -430   -476          C
ATOM   5177  NZ  LYS E 482      45.777 -20.298   5.551  1.00 50.79           N
ANISOU 5177  NZ  LYS E 482    6280   7307   5710   -250   -458   -708          N
ATOM   5178  C   LYS E 482      40.480 -25.277   5.345  1.00 37.85           C
ANISOU 5178  C   LYS E 482    5402   5097   3882   -186   -120    278          C
ATOM   5179  O   LYS E 482      41.059 -25.722   6.324  1.00 40.42           O
ANISOU 5179  O   LYS E 482    5770   5557   4030   -157   -263    396          O
ATOM   5180  N   MSE E 483      39.178 -25.477   5.113  1.00 38.08           N
ANISOU 5180  N   MSE E 483    5507   5039   3923   -271     35    313          N
ATOM   5181  CA  MSE E 483      38.319 -26.309   5.975  1.00 41.13           C
ANISOU 5181  CA  MSE E 483    6038   5469   4121   -357     73    501          C
ATOM   5182  CB  MSE E 483      36.882 -25.754   6.064  1.00 40.37           C
ANISOU 5182  CB  MSE E 483    5941   5421   3976   -498    279    393          C
ATOM   5183  CG  MSE E 483      36.761 -24.265   6.345  1.00 40.01           C
ANISOU 5183  CG  MSE E 483    5787   5531   3882   -542    350    123          C
ATOM   5184  SE  MSE E 483      37.684 -23.720   7.991  0.90 48.53          SE
ANISOU 5184  SE  MSE E 483    6871   6944   4625   -576    224     65          SE
ATOM   5185  CE  MSE E 483      36.796 -24.873   9.310  1.00 39.30           C
ANISOU 5185  CE  MSE E 483    5885   5939   3108   -711    273    332          C
ATOM   5186  C   MSE E 483      38.246 -27.706   5.373  1.00 42.30           C
ANISOU 5186  C   MSE E 483    6281   5381   4412   -297     34    716          C
ATOM   5187  O   MSE E 483      37.810 -27.893   4.207  1.00 41.41           O
ANISOU 5187  O   MSE E 483    6140   5074   4520   -280    115    669          O
ATOM   5188  OXT MSE E 483      38.610 -28.668   6.048  1.00 45.09           O
ANISOU 5188  OXT MSE E 483    6745   5727   4660   -266    -87    937          O
ATOM   5189  N   SER F 322      34.011   6.452 -60.832  1.00 64.98           N
ANISOU 5189  N   SER F 322   10039  10556   4093  -1803    691   1251          N
ATOM   5190  CA  SER F 322      32.816   6.735 -59.979  1.00 62.59           C
ANISOU 5190  CA  SER F 322    9734  10002   4046  -1536    361   1309          C
ATOM   5191  CB  SER F 322      32.604   8.243 -59.821  1.00 64.65           C
ANISOU 5191  CB  SER F 322   10337   9931   4296  -1631    298   1564          C
ATOM   5192  OG  SER F 322      33.389   8.747 -58.754  1.00 65.13           O
ANISOU 5192  OG  SER F 322   10229   9915   4604  -1806    456   1515          O
ATOM   5193  C   SER F 322      31.562   6.093 -60.548  1.00 61.62           C
ANISOU 5193  C   SER F 322    9683   9900   3831  -1253     68   1295          C
ATOM   5194  O   SER F 322      31.304   6.186 -61.745  1.00 64.33           O
ANISOU 5194  O   SER F 322   10330  10282   3832  -1271     13   1407          O
ATOM   5195  N   PHE F 323      30.793   5.447 -59.672  1.00 57.78           N
ANISOU 5195  N   PHE F 323    8921   9391   3643  -1013   -115   1152          N
ATOM   5196  CA  PHE F 323      29.540   4.774 -60.034  1.00 56.60           C
ANISOU 5196  CA  PHE F 323    8754   9271   3481   -759   -400   1094          C
ATOM   5197  CB  PHE F 323      29.803   3.472 -60.817  1.00 56.49           C
ANISOU 5197  CB  PHE F 323    8646   9535   3285   -767   -321    906          C
ATOM   5198  CG  PHE F 323      30.640   2.458 -60.073  1.00 53.82           C
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Figure 18 (continued)

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ANISOU 5198  CG  PHE F 323     7956   9345   3148   -799   -105    669       C
ATOM   5199  CD1 PHE F 323      30.039   1.474 -59.298  1.00 49.66           C
ANISOU 5199  CD1 PHE F 323     7167   8820   2880   -621   -219    487       C
ATOM   5200  CE1 PHE F 323      30.800   0.533 -58.628  1.00 48.33           C
ANISOU 5200  CE1 PHE F 323     6732   8755   2877   -621    -52    290       C
ATOM   5201  CZ  PHE F 323      32.182   0.565 -58.719  1.00 49.24           C
ANISOU 5201  CZ  PHE F 323     6772   9006   2930   -778    220    248       C
ATOM   5202  CE2 PHE F 323      32.796   1.537 -59.491  1.00 52.46           C
ANISOU 5202  CE2 PHE F 323     7386   9446   3100   -985    365    404       C
ATOM   5203  CD2 PHE F 323      32.028   2.476 -60.167  1.00 54.43           C
ANISOU 5203  CD2 PHE F 323     7968   9559   3154  -1005    210    625       C
ATOM   5204  C   PHE F 323      28.693   4.508 -58.789  1.00 53.34           C
ANISOU 5204  C   PHE F 323     8069   8746   3453   -555   -559    984       C
ATOM   5205  O   PHE F 323      28.952   5.075 -57.735  1.00 52.04           O
ANISOU 5205  O   PHE F 323     7823   8434   3515   -588   -490   1003       O
ATOM   5206  N   SER F 324      27.717   3.610 -58.913  1.00 52.31           N
ANISOU 5206  N   SER F 324     7801   8693   3380   -371   -751    850       N
ATOM   5207  CA  SER F 324      26.659   3.430 -57.923  1.00 50.15           C
ANISOU 5207  CA  SER F 324     7311   8311   3432   -183   -917    760       C
ATOM   5208  CB  SER F 324      25.461   4.292 -58.342  1.00 52.27           C
ANISOU 5208  CB  SER F 324     7742   8435   3685     -5  -1217    905       C
ATOM   5209  OG  SER F 324      24.546   4.524 -57.289  1.00 51.91           O
ANISOU 5209  OG  SER F 324     7504   8244   3975    161  -1325    848       O
ATOM   5210  C   SER F 324      26.254   1.948 -57.864  1.00 48.44           C
ANISOU 5210  C   SER F 324     6852   8258   3293   -116   -945    520       C
ATOM   5211  O   SER F 324      26.075   1.322 -58.895  1.00 50.04           O
ANISOU 5211  O   SER F 324     7125   8610   3280   -114  -1019    464       O
ATOM   5212  N   PHE F 325      26.129   1.389 -56.660  1.00 45.78           N
ANISOU 5212  N   PHE F 325     6271   7878   3245    -79   -878    379       N
ATOM   5213  CA  PHE F 325      25.670  -0.004 -56.478  1.00 43.79           C
ANISOU 5213  CA  PHE F 325     5824   7722   3091    -32   -896    158       C
ATOM   5214  CB  PHE F 325      26.785  -1.009 -56.819  1.00 43.32           C
ANISOU 5214  CB  PHE F 325     5751   7815   2894   -128   -702     38       C
ATOM   5215  CG  PHE F 325      26.407  -2.453 -56.596  1.00 42.81           C
ANISOU 5215  CG  PHE F 325     5543   7795   2927    -86   -705   -186       C
ATOM   5216  CD1 PHE F 325      25.471  -3.087 -57.424  1.00 45.16           C
ANISOU 5216  CD1 PHE F 325     5857   8167   3136    -52   -875   -288       C
ATOM   5217  CE1 PHE F 325      25.112  -4.424 -57.209  1.00 44.54           C
ANISOU 5217  CE1 PHE F 325     5674   8097   3153    -49   -865   -503       C
ATOM   5218  CZ  PHE F 325      25.706  -5.150 -56.167  1.00 42.37           C
ANISOU 5218  CZ  PHE F 325     5311   7741   3047    -53   -689   -594       C
ATOM   5219  CE2 PHE F 325      26.651  -4.536 -55.348  1.00 40.54           C
ANISOU 5219  CE2 PHE F 325     5059   7456   2890    -58   -547   -487       C
ATOM   5220  CD2 PHE F 325      26.989  -3.188 -55.561  1.00 41.44           C
ANISOU 5220  CD2 PHE F 325     5244   7577   2924    -88   -552   -295       C
ATOM   5221  C   PHE F 325      25.132  -0.224 -55.053  1.00 41.64           C
ANISOU 5221  C   PHE F 325     5353   7325   3145     26   -873     66       C
ATOM   5222  O   PHE F 325      25.807   0.091 -54.067  1.00 39.51           O
ANISOU 5222  O   PHE F 325     5054   6968   2990    -20   -727     92       O
ATOM   5223  N   GLY F 326      23.906  -0.747 -54.969  1.00 41.53           N
ANISOU 5223  N   GLY F 326     5205   7311   3264    109  -1015    -51       N
ATOM   5224  CA  GLY F 326      23.229  -1.041 -53.700  1.00 39.72           C
ANISOU 5224  CA  GLY F 326     4794   6976   3322    140   -970   -158       C
ATOM   5225  C   GLY F 326      23.119   0.104 -52.706  1.00 39.23           C
ANISOU 5225  C   GLY F 326     4733   6746   3427    187   -931    -57       C
ATOM   5226  O   GLY F 326      23.248  -0.105 -51.503  1.00 37.01           O
ANISOU 5226  O   GLY F 326     4384   6376   3302    155   -790   -119       O
ATOM   5227  N   GLY F 327      22.887   1.309 -53.220  1.00 40.74           N
ANISOU 5227  N   GLY F 327     5040   6875   3563    264  -1061     99       N
ATOM   5228  CA  GLY F 327      22.741   2.501 -52.404  1.00 41.28           C
ANISOU 5228  CA  GLY F 327     5152   6754   3780    325  -1040    192       C
ATOM   5229  C   GLY F 327      24.066   3.126 -51.996  1.00 40.95           C
ANISOU 5229  C   GLY F 327     5272   6631   3655    195   -873    305       C
ATOM   5230  O   GLY F 327      24.101   4.024 -51.162  1.00 40.80           O
ANISOU 5230  O   GLY F 327     5305   6440   3756    207   -821    353       O
ATOM   5231  N   PHE F 328      25.160   2.646 -52.578  1.00 40.57           N
ANISOU 5231  N   PHE F 328     5289   6716   3411     64   -781    323       N
ATOM   5232  CA  PHE F 328      26.480   3.152 -52.254  1.00 40.14           C
ANISOU 5232  CA  PHE F 328     5327   6634   3289    -87   -619    398       C
ATOM   5233  CB  PHE F 328      27.337   2.054 -51.593  1.00 38.59           C
ANISOU 5233  CB  PHE F 328     4985   6548   3129   -161   -471    255       C
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Figure 18 (continued)

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ATOM   5234  CG  PHE F 328      26.937   1.747 -50.172  1.00 36.26           C
ANISOU 5234  CG  PHE F 328    4584   6146   3047   -114   -436    152       C
ATOM   5235  CD1 PHE F 328      27.509   2.439 -49.118  1.00 35.56           C
ANISOU 5235  CD1 PHE F 328    4532   5943   3037   -180   -359    178       C
ATOM   5236  CE1 PHE F 328      27.135   2.179 -47.794  1.00 35.95           C
ANISOU 5236  CE1 PHE F 328    4532   5891   3238   -147   -318     85       C
ATOM   5237  CZ  PHE F 328      26.175   1.205 -47.525  1.00 35.59           C
ANISOU 5237  CZ  PHE F 328    4392   5853   3279    -67   -328    -30       C
ATOM   5238  CE2 PHE F 328      25.579   0.501 -48.591  1.00 35.31           C
ANISOU 5238  CE2 PHE F 328    4292   5930   3195    -16   -406    -67       C
ATOM   5239  CD2 PHE F 328      25.972   0.772 -49.896  1.00 36.57           C
ANISOU 5239  CD2 PHE F 328    4509   6196   3191    -31   -472     21       C
ATOM   5240  C   PHE F 328      27.164   3.747 -53.487  1.00 42.14           C
ANISOU 5240  C   PHE F 328    5784   6945   3284   -188   -612    551       C
ATOM   5241  O   PHE F 328      27.123   3.162 -54.574  1.00 43.04           O
ANISOU 5241  O   PHE F 328    5930   7212   3211   -186   -657    538       O
ATOM   5242  N   THR F 329      27.753   4.931 -53.308  1.00 43.06           N
ANISOU 5242  N   THR F 329    6063   6922   3376   -296   -547    691       N
ATOM   5243  CA  THR F 329      28.590   5.562 -54.324  1.00 44.99           C
ANISOU 5243  CA  THR F 329    6526   7199   3369   -463   -471    842       C
ATOM   5244  CB  THR F 329      28.582   7.124 -54.212  1.00 47.13           C
ANISOU 5244  CB  THR F 329    7067   7201   3639   -520   -492   1036       C
ATOM   5245  OG1 THR F 329      27.239   7.622 -54.309  1.00 47.99           O
ANISOU 5245  OG1 THR F 329    7274   7135   3825   -281   -725   1105       O
ATOM   5246  CG2 THR F 329      29.435   7.782 -55.313  1.00 49.33           C
ANISOU 5246  CG2 THR F 329    7622   7494   3626   -739   -385   1209       C
ATOM   5247  C   THR F 329      30.011   5.037 -54.169  1.00 44.33           C
ANISOU 5247  C   THR F 329    6307   7296   3238   -659   -242    750       C
ATOM   5248  O   THR F 329      30.661   5.270 -53.164  1.00 43.50           O
ANISOU 5248  O   THR F 329    6103   7145   3278   -750   -146    702       O
ATOM   5249  N   PHE F 330      30.485   4.299 -55.160  1.00 45.43           N
ANISOU 5249  N   PHE F 330    6430   7653   3179   -712   -166    704       N
ATOM   5250  CA  PHE F 330      31.856   3.815 -55.144  1.00 45.51           C
ANISOU 5250  CA  PHE F 330    6284   7859   3150   -873     57    599       C
ATOM   5251  CB  PHE F 330      31.974   2.448 -55.811  1.00 44.24           C
ANISOU 5251  CB  PHE F 330    5998   7924   2886   -793     95    438       C
ATOM   5252  CG  PHE F 330      31.265   1.341 -55.083  1.00 41.56           C
ANISOU 5252  CG  PHE F 330    5484   7570   2737   -593    -24    281       C
ATOM   5253  CD1 PHE F 330      31.970   0.227 -54.643  1.00 39.01           C
ANISOU 5253  CD1 PHE F 330    4950   7373   2501   -551     72     97       C
ATOM   5254  CE1 PHE F 330      31.319  -0.811 -53.999  1.00 36.87           C
ANISOU 5254  CE1 PHE F 330    4580   7051   2379   -392    -23    -32       C
ATOM   5255  CZ  PHE F 330      29.941  -0.742 -53.767  1.00 36.29           C
ANISOU 5255  CZ  PHE F 330    4566   6835   2390   -298   -191      0       C
ATOM   5256  CE2 PHE F 330      29.229   0.364 -54.190  1.00 37.65           C
ANISOU 5256  CE2 PHE F 330    4887   6913   2505   -313   -297    159       C
ATOM   5257  CD2 PHE F 330      29.886   1.396 -54.852  1.00 39.87           C
ANISOU 5257  CD2 PHE F 330    5319   7211   2619   -446   -227    310       C
ATOM   5258  C   PHE F 330      32.713   4.818 -55.875  1.00 48.65           C
ANISOU 5258  C   PHE F 330    6873   8264   3348  -1124    219    745       C
ATOM   5259  O   PHE F 330      32.259   5.448 -56.807  1.00 50.59           O
ANISOU 5259  O   PHE F 330    7408   8428   3384  -1150    160    912       O
ATOM   5260  N   LYS F 331      33.946   4.979 -55.416  1.00 50.04           N
ANISOU 5260  N   LYS F 331    6892   8531   3590  -1318    414    680       N
ATOM   5261  CA  LYS F 331      34.964   5.753 -56.116  1.00 53.68           C
ANISOU 5261  CA  LYS F 331    7471   9055   3869  -1620    639    769       C
ATOM   5262  CB  LYS F 331      35.231   7.083 -55.410  1.00 55.11           C
ANISOU 5262  CB  LYS F 331    7777   9006   4157  -1811    660    889       C
ATOM   5263  CG  LYS F 331      34.021   7.996 -55.305  1.00 58.38           C
ANISOU 5263  CG  LYS F 331    8516   9084   4581  -1684    447   1080       C
ATOM   5264  CD  LYS F 331      34.421   9.467 -55.258  1.00 65.79           C
ANISOU 5264  CD  LYS F 331    9739   9778   5479  -1948    534   1252       C
ATOM   5265  CE  LYS F 331      33.390  10.311 -56.018  1.00 69.37           C
ANISOU 5265  CE  LYS F 331   10638   9954   5763  -1842    370   1498       C
ATOM   5266  NZ  LYS F 331      33.674  11.800 -55.808  1.00 74.95           N
ANISOU 5266  NZ  LYS F 331   11678  10334   6466  -2070    432   1671       N
ATOM   5267  C   LYS F 331      36.204   4.910 -56.034  1.00 53.61           C
ANISOU 5267  C   LYS F 331    7117   9344   3907  -1704    845    557       C
ATOM   5268  O   LYS F 331      36.661   4.624 -54.932  1.00 51.96           O
ANISOU 5268  O   LYS F 331    6638   9168   3938  -1666    824    424       O
ATOM   5269  N   ARG F 332      36.740   4.480 -57.175  1.00 55.82           N
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Figure 18 (continued)

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ANISOU 5269  N   ARG F 332     7406   9846   3958  -1795   1035    512       N
ATOM   5270  CA  ARG F 332      37.975   3.711 -57.141  1.00 56.45           C
ANISOU 5270  CA  ARG F 332     7126  10222   4102  -1854   1251    286       C
ATOM   5271  CB  ARG F 332      38.200   2.902 -58.417  1.00 58.54           C
ANISOU 5271  CB  ARG F 332     7413  10718   4111  -1836   1419    191       C
ATOM   5272  CG  ARG F 332      39.426   1.993 -58.330  1.00 58.83           C
ANISOU 5272  CG  ARG F 332     7035  11059   4257  -1823   1632    -82       C
ATOM   5273  CD  ARG F 332      39.626   1.183 -59.593  1.00 60.93           C
ANISOU 5273  CD  ARG F 332     7343  11542   4265  -1793   1821   -205       C
ATOM   5274  NE  ARG F 332      40.094   1.998 -60.711  1.00 63.73           N
ANISOU 5274  NE  ARG F 332     7925  11986   4305  -2121   2102    -93       N
ATOM   5275  CZ  ARG F 332      39.945   1.662 -61.989  1.00 67.27           C
ANISOU 5275  CZ  ARG F 332     8607  12545   4407  -2151   2238   -103       C
ATOM   5276  NH1 ARG F 332      39.334   0.528 -62.321  1.00 65.85           N
ANISOU 5276  NH1 ARG F 332     8448  12400   4171  -1873   2106   -235       N
ATOM   5277  NH2 ARG F 332      40.400   2.464 -62.946  1.00 71.36           N
ANISOU 5277  NH2 ARG F 332     9373  13127   4613  -2480   2512     18       N
ATOM   5278  C   ARG F 332      39.138   4.648 -56.879  1.00 58.97           C
ANISOU 5278  C   ARG F 332     7335  10596   4475  -2189   1464    297       C
ATOM   5279  O   ARG F 332      39.386   5.586 -57.629  1.00 61.80           O
ANISOU 5279  O   ARG F 332     7943  10911   4627  -2474   1635    449       O
ATOM   5280  N   THR F 333      39.841   4.386 -55.789  1.00 58.21           N
ANISOU 5280  N   THR F 333     6878  10586   4652  -2165   1442    134       N
ATOM   5281  CA  THR F 333      40.945   5.229 -55.366  1.00 60.07           C
ANISOU 5281  CA  THR F 333     6945  10888   4991  -2487   1602    103       C
ATOM   5282  CB  THR F 333      40.955   5.395 -53.809  1.00 57.87           C
ANISOU 5282  CB  THR F 333     6499  10485   5005  -2405   1378     45       C
ATOM   5283  OG1 THR F 333      40.820   4.116 -53.173  1.00 53.94           O
ANISOU 5283  OG1 THR F 333     5755  10082   4659  -2055   1210   -124       O
ATOM   5284  CG2 THR F 333      39.781   6.265 -53.360  1.00 55.42           C
ANISOU 5284  CG2 THR F 333     6572   9793   4692  -2367   1177    257       C
ATOM   5285  C   THR F 333      42.260   4.664 -55.913  1.00 63.49           C
ANISOU 5285  C   THR F 333     7009  11703   5413  -2612   1892   -115       C
ATOM   5286  O   THR F 333      43.229   5.410 -56.156  1.00 66.66           O
ANISOU 5286  O   THR F 333     7310  12223   5793  -2977   2143   -133       O
ATOM   5287  N   SER F 334      42.274   3.351 -56.144  1.00 62.58           N
ANISOU 5287  N   SER F 334     6695  11769   5312  -2317   1875   -291       N
ATOM   5288  CA  SER F 334      43.502   2.644 -56.507  1.00 65.70           C
ANISOU 5288  CA  SER F 334     6674  12530   5758  -2338   2121   -550       C
ATOM   5289  CB  SER F 334      44.291   2.301 -55.244  1.00 65.54           C
ANISOU 5289  CB  SER F 334     6199  12626   6076  -2225   1985   -745       C
ATOM   5290  OG  SER F 334      44.801   3.472 -54.626  1.00 68.04           O
ANISOU 5290  OG  SER F 334     6457  12896   6498  -2553   2002   -685       O
ATOM   5291  C   SER F 334      43.246   1.357 -57.283  1.00 65.13           C
ANISOU 5291  C   SER F 334     6595  12586   5565  -2050   2161   -684       C
ATOM   5292  O   SER F 334      42.223   0.701 -57.097  1.00 62.02           O
ANISOU 5292  O   SER F 334     6381  12018   5168  -1758   1918   -644       O
ATOM   5293  N   GLY F 335      44.195   0.999 -58.142  1.00 68.40           N
ANISOU 5293  N   GLY F 335     6793  13307   5888  -2150   2488   -866       N
ATOM   5294  CA  GLY F 335      44.157  -0.277 -58.850  1.00 68.50           C
ANISOU 5294  CA  GLY F 335     6754  13467   5808  -1876   2563  -1055       C
ATOM   5295  C   GLY F 335      43.389  -0.225 -60.154  1.00 68.74           C
ANISOU 5295  C   GLY F 335     7239  13435   5445  -1951   2668   -925       C
ATOM   5296  O   GLY F 335      43.026   0.858 -60.629  1.00 69.46           O
ANISOU 5296  O   GLY F 335     7680  13399   5314  -2236   2722   -681       O
ATOM   5297  N   SER F 336      43.149  -1.405 -60.731  1.00 68.37           N
ANISOU 5297  N   SER F 336     7212  13464   5303  -1688   2679  -1092       N
ATOM   5298  CA  SER F 336      42.397  -1.531 -61.986  1.00 69.05           C
ANISOU 5298  CA  SER F 336     7727  13513   4996  -1723   2739  -1010       C
ATOM   5299  CB  SER F 336      43.217  -1.023 -63.178  1.00 73.61           C
ANISOU 5299  CB  SER F 336     8375  14331   5263  -2063   3179  -1036       C
ATOM   5300  OG  SER F 336      44.204  -1.967 -63.529  1.00 76.75           O
ANISOU 5300  OG  SER F 336     8413  15033   5715  -1957   3464  -1374       O
ATOM   5301  C   SER F 336      41.939  -2.968 -62.240  1.00 67.73           C
ANISOU 5301  C   SER F 336     7568  13350   4817  -1369   2631  -1214       C
ATOM   5302  O   SER F 336      42.344  -3.898 -61.517  1.00 66.67           O
ANISOU 5302  O   SER F 336     7102  13257   4972  -1096   2562  -1428       O
ATOM   5303  N   SER F 337      41.095  -3.128 -63.279  1.00 68.08           N
ANISOU 5303  N   SER F 337     8018  13336   4512  -1379   2602  -1144       N
ATOM   5304  CA  SER F 337      40.508  -4.417 -63.644  1.00 67.00           C
ANISOU 5304  CA  SER F 337     7973  13170   4315  -1097   2486  -1327       C
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Figure 18 (continued)

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ATOM   5305  CB  SER F 337      39.336  -4.739 -62.720  1.00 62.53           C
ANISOU 5305  CB  SER F 337    7481  12315   3961   -875   2064  -1229         C
ATOM   5306  OG  SER F 337      38.333  -3.755 -62.848  1.00 60.99           O
ANISOU 5306  OG  SER F 337    7612  11944   3619  -1016   1861   -934         O
ATOM   5307  C   SER F 337      40.018  -4.501 -65.096  1.00 69.66           C
ANISOU 5307  C   SER F 337    8719  13566   4183  -1202   2583  -1314         C
ATOM   5308  O   SER F 337      39.755  -3.477 -65.752  1.00 70.99           O
ANISOU 5308  O   SER F 337    9208  13715   4051  -1462   2625  -1078         O
ATOM   5309  N   ILE F 338      39.898  -5.738 -65.580  1.00 70.19           N
ANISOU 5309  N   ILE F 338    8806  13686   4178   -994   2605  -1570         N
ATOM   5310  CA  ILE F 338      39.155  -6.038 -66.796  1.00 71.90           C
ANISOU 5310  CA  ILE F 338    9439  13908   3972  -1029   2574  -1583         C
ATOM   5311  CB  ILE F 338      40.002  -6.853 -67.853  1.00 76.35           C
ANISOU 5311  CB  ILE F 338    9987  14730   4290  -1023   2965  -1906         C
ATOM   5312  CG1 ILE F 338      40.263  -8.298 -67.393  1.00 75.23           C
ANISOU 5312  CG1 ILE F 338    9575  14570   4439   -678   2951  -2246         C
ATOM   5313  CD1 ILE F 338      40.863  -9.201 -68.486  1.00 80.18           C
ANISOU 5313  CD1 ILE F 338   10254  15401   4810   -623   3291  -2589         C
ATOM   5314  CG2 ILE F 338      41.320  -6.112 -68.205  1.00 78.90           C
ANISOU 5314  CG2 ILE F 338   10131  15320   4527  -1288   3428  -1925         C
ATOM   5315  C   ILE F 338      37.828  -6.734 -66.425  1.00 68.91           C
ANISOU 5315  C   ILE F 338    9200  13287   3697   -806   2150  -1576         C
ATOM   5316  O   ILE F 338      37.757  -7.445 -65.419  1.00 66.10           O
ANISOU 5316  O   ILE F 338    8600  12808   3708   -581   2005  -1683         O
ATOM   5317  N   LYS F 339      36.784  -6.500 -67.226  1.00 69.74           N
ANISOU 5317  N   LYS F 339    9700  13325   3473   -882   1949  -1445         N
ATOM   5318  CA  LYS F 339      35.463  -7.116 -67.021  1.00 67.74           C
ANISOU 5318  CA  LYS F 339    9570  12878   3290   -720   1556  -1458         C
ATOM   5319  CB  LYS F 339      34.333  -6.139 -67.371  1.00 67.59           C
ANISOU 5319  CB  LYS F 339    9864  12753   3064   -831   1250  -1160         C
ATOM   5320  CG  LYS F 339      34.393  -4.798 -66.699  1.00 66.44           C
ANISOU 5320  CG  LYS F 339    9674  12510   3061   -940   1203   -852         C
ATOM   5321  CD  LYS F 339      33.675  -3.720 -67.540  1.00 68.91           C
ANISOU 5321  CD  LYS F 339   10398  12778   3007  -1082   1029   -569         C
ATOM   5322  CE  LYS F 339      34.362  -2.348 -67.345  1.00 70.79           C
ANISOU 5322  CE  LYS F 339   10682  12989   3227  -1292   1208   -308         C
ATOM   5323  NZ  LYS F 339      34.350  -1.864 -65.889  1.00 67.41           N
ANISOU 5323  NZ  LYS F 339    9955  12387   3271  -1227   1105   -208         N
ATOM   5324  C   LYS F 339      35.324  -8.349 -67.910  1.00 70.21           C
ANISOU 5324  C   LYS F 339   10033  13263   3382   -630   1607  -1759         C
ATOM   5325  O   LYS F 339      35.364  -8.238 -69.132  1.00 73.21           O
ANISOU 5325  O   LYS F 339   10707  13787   3321   -763   1726  -1788         O
ATOM   5326  N   ARG F 340      35.143  -9.514 -67.302  1.00 68.86           N
ANISOU 5326  N   ARG F 340    9700  12972   3492   -415   1515  -1980         N
ATOM   5327  CA  ARG F 340      35.046 -10.755 -68.056  1.00 71.85           C
ANISOU 5327  CA  ARG F 340   10224  13375   3699   -321   1570  -2296         C
ATOM   5328  CB  ARG F 340      36.226 -11.677 -67.715  1.00 72.59           C
ANISOU 5328  CB  ARG F 340   10046  13519   4016   -132   1871  -2586         C
ATOM   5329  CG  ARG F 340      36.403 -12.842 -68.679  1.00 76.97           C
ANISOU 5329  CG  ARG F 340   10775  14131   4338    -46   2034  -2942         C
ATOM   5330  CD  ARG F 340      37.468 -13.841 -68.233  1.00 78.54           C
ANISOU 5330  CD  ARG F 340   10696  14325   4818    215   2278  -3243         C
ATOM   5331  NE  ARG F 340      37.621 -14.943 -69.196  1.00 86.31           N
ANISOU 5331  NE  ARG F 340   11880  15342   5571    307   2449  -3605         N
ATOM   5332  CZ  ARG F 340      36.819 -16.011 -69.279  1.00 87.14           C
ANISOU 5332  CZ  ARG F 340   12201  15224   5684    409   2247  -3787         C
ATOM   5333  NH1 ARG F 340      35.781 -16.154 -68.451  1.00 84.58           N
ANISOU 5333  NH1 ARG F 340   11903  14639   5593    422   1877  -3641         N
ATOM   5334  NH2 ARG F 340      37.058 -16.949 -70.188  1.00 89.57           N
ANISOU 5334  NH2 ARG F 340   12702  15565   5765    482   2435  -4134         N
ATOM   5335  C   ARG F 340      33.708 -11.429 -67.754  1.00 70.08           C
ANISOU 5335  C   ARG F 340   10105  12931   3592   -240   1188  -2333         C
ATOM   5336  O   ARG F 340      33.361 -11.615 -66.587  1.00 67.34           O
ANISOU 5336  O   ARG F 340    9563  12392   3630   -132   1021  -2278         O
ATOM   5337  N   GLU F 341      32.949 -11.763 -68.797  1.00 72.62           N
ANISOU 5337  N   GLU F 341   10737  13286   3568   -315   1050  -2429         N
ATOM   5338  CA  GLU F 341      31.665 -12.460 -68.643  1.00 72.00           C
ANISOU 5338  CA  GLU F 341   10745  13030   3582   -280    699  -2511         C
ATOM   5339  CB  GLU F 341      30.833 -12.346 -69.924  1.00 75.35           C
ANISOU 5339  CB  GLU F 341   11521  13561   3548   -419    499  -2531         C
ATOM   5340  CG  GLU F 341      29.378 -12.802 -69.795  1.00 75.43           C
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Figure 18 (continued)

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ANISOU 5340  CG  GLU F 341    11576  13430   3654   -432     82  -2580    C
ATOM   5341  CD  GLU F 341      28.386 -11.646 -69.818  1.00 75.78        C
ANISOU 5341  CD  GLU F 341    11656  13495   3643   -509   -266  -2273    C
ATOM   5342  OE1 GLU F 341      27.661 -11.539 -70.835  1.00 78.56        O
ANISOU 5342  OE1 GLU F 341    12266  13948   3635   -593   -508  -2290    O
ATOM   5343  OE2 GLU F 341      28.329 -10.858 -68.835  1.00 72.03        O
ANISOU 5343  OE2 GLU F 341    10963  12933   3474   -469   -311  -2029    O
ATOM   5344  C   GLU F 341      31.866 -13.933 -68.254  1.00 72.08        C
ANISOU 5344  C   GLU F 341    10682  12885   3819   -116    781  -2838    C
ATOM   5345  O   GLU F 341      32.667 -14.650 -68.854  1.00 74.94        O
ANISOU 5345  O   GLU F 341    11113  13324   4035    -49   1050  -3099    O
ATOM   5346  N   GLU F 342      31.125 -14.370 -67.245  1.00 69.62        N
ANISOU 5346  N   GLU F 342    10251  12340   3862    -54    560  -2823    N
ATOM   5347  CA  GLU F 342      31.293 -15.693 -66.653  1.00 69.64        C
ANISOU 5347  CA  GLU F 342    10208  12126   4127    103    619  -3074    C
ATOM   5348  CB  GLU F 342      32.322 -15.633 -65.514  1.00 67.97        C
ANISOU 5348  CB  GLU F 342     9720  11849   4259    282    797  -3004    C
ATOM   5349  CG  GLU F 342      33.695 -16.187 -65.890  1.00 72.52        C
ANISOU 5349  CG  GLU F 342    10240  12529   4785    450   1138  -3236    C
ATOM   5350  CD  GLU F 342      34.866 -15.386 -65.320  1.00 73.01        C
ANISOU 5350  CD  GLU F 342     9998  12742   5001    520   1337  -3091    C
ATOM   5351  OE1 GLU F 342      35.691 -14.915 -66.127  1.00 76.14        O
ANISOU 5351  OE1 GLU F 342    10366  13400   5165    460   1597  -3130    O
ATOM   5352  OE2 GLU F 342      34.977 -15.234 -64.084  1.00 71.41        O
ANISOU 5352  OE2 GLU F 342     9591  12405   5135    615   1243  -2952    O
ATOM   5353  C   GLU F 342      29.962 -16.216 -66.134  1.00 67.95        C
ANISOU 5353  C   GLU F 342    10035  11683   4100     41    312  -3093    C
ATOM   5354  O   GLU F 342      29.181 -15.466 -65.550  1.00 65.42        O
ANISOU 5354  O   GLU F 342     9603  11333   3922    -40    100  -2859    O
ATOM   5355  N   GLU F 343      29.706 -17.498 -66.380  1.00 69.90        N
ANISOU 5355  N   GLU F 343    10445  11769   4346     66    308  -3389    N
ATOM   5356  CA  GLU F 343      28.559 -18.194 -65.805  1.00 69.18        C
ANISOU 5356  CA  GLU F 343    10385  11429   4472    -16     79  -3457    C
ATOM   5357  CB  GLU F 343      28.115 -19.373 -66.685  1.00 72.48        C
ANISOU 5357  CB  GLU F 343    11077  11759   4703    -93     38  -3804    C
ATOM   5358  CG  GLU F 343      26.910 -19.055 -67.631  1.00 74.73        C
ANISOU 5358  CG  GLU F 343    11479  12200   4715   -329   -260  -3829    C
ATOM   5359  CD  GLU F 343      26.608 -20.312 -68.539  1.00 78.55        C
ANISOU 5359  CD  GLU F 343    12260  12593   4990   -414   -279  -4224    C
ATOM   5360  OE1 GLU F 343      26.210 -21.396 -67.996  1.00 78.42        O
ANISOU 5360  OE1 GLU F 343    12303  12280   5215   -445   -298  -4412    O
ATOM   5361  OE2 GLU F 343      26.759 -20.210 -69.802  1.00 81.28        O
ANISOU 5361  OE2 GLU F 343    12817  13155   4912   -468   -271  -4349    O
ATOM   5362  C   GLU F 343      28.962 -18.700 -64.434  1.00 66.86        C
ANISOU 5362  C   GLU F 343     9963  10869   4573    140    169  -3421    C
ATOM   5363  O   GLU F 343      30.023 -19.295 -64.287  1.00 68.01        O
ANISOU 5363  O   GLU F 343    10119  10944   4777    342    387  -3549    O
ATOM   5364  N   VAL F 344      28.126 -18.450 -63.434  1.00 64.55        N
ANISOU 5364  N   VAL F 344     9551  10437   4540     58      0  -3253    N
ATOM   5365  CA  VAL F 344      28.351 -18.977 -62.081  1.00 62.97        C
ANISOU 5365  CA  VAL F 344     9292   9954   4679    175     57  -3208    C
ATOM   5366  CB  VAL F 344      28.623 -17.848 -61.021  1.00 59.59        C
ANISOU 5366  CB  VAL F 344     8616   9585   4440    225     51  -2890    C
ATOM   5367  CG1 VAL F 344      29.883 -17.084 -61.375  1.00 59.63        C
ANISOU 5367  CG1 VAL F 344     8500   9834   4323    357    219  -2806    C
ATOM   5368  CG2 VAL F 344      27.435 -16.885 -60.878  1.00 57.61        C
ANISOU 5368  CG2 VAL F 344     8250   9422   4217     29   -159  -2700    C
ATOM   5369  C   VAL F 344      27.175 -19.874 -61.683  1.00 63.62        C
ANISOU 5369  C   VAL F 344     9499   9764   4910     11    -81  -3328    C
ATOM   5370  O   VAL F 344      26.167 -19.933 -62.404  1.00 65.05        O
ANISOU 5370  O   VAL F 344     9736  10016   4963   -196   -243  -3431    O
ATOM   5371  N   LEU F 345      27.309 -20.581 -60.561  1.00 62.81        N
ANISOU 5371  N   LEU F 345     9450   9352   5063     92    -20  -3322    N
ATOM   5372  CA  LEU F 345      26.254 -21.491 -60.114  1.00 64.00        C
ANISOU 5372  CA  LEU F 345     9749   9208   5359    -98    -99  -3437    C
ATOM   5373  CB  LEU F 345      26.623 -22.938 -60.433  1.00 66.98        C
ANISOU 5373  CB  LEU F 345    10440   9302   5705    -18      4  -3726    C
ATOM   5374  CG  LEU F 345      25.588 -24.015 -60.112  1.00 69.00        C
ANISOU 5374  CG  LEU F 345    10916   9216   6083   -256    -48  -3887    C
ATOM   5375  CD1 LEU F 345      25.216 -24.820 -61.343  1.00 72.57        C
ANISOU 5375  CD1 LEU F 345    11584   9653   6334   -394    -85  -4220    C
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Figure 18 (continued)

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ATOM   5376  CD2 LEU F 345      26.113 -24.915 -59.016  1.00 69.88           C
ANISOU 5376  CD2 LEU F 345   11247   8912   6394    -92     72  -3866       C
ATOM   5377  C   LEU F 345      25.911 -21.302 -58.632  1.00 61.95           C
ANISOU 5377  C   LEU F 345    9405   8757   5376   -129   -105  -3225       C
ATOM   5378  O   LEU F 345      26.775 -21.464 -57.754  1.00 61.11           O
ANISOU 5378  O   LEU F 345    9333   8496   5389     83     -3  -3125       O
ATOM   5379  N   THR F 346      24.649 -20.944 -58.369  1.00 61.45           N
ANISOU 5379  N   THR F 346    9224   8720   5404   -389   -230  -3169       N
ATOM   5380  CA  THR F 346      24.186 -20.634 -57.011  1.00 59.61           C
ANISOU 5380  CA  THR F 346    8895   8347   5406   -459   -215  -2976       C
ATOM   5381  CB  THR F 346      22.830 -19.857 -56.990  1.00 59.00           C
ANISOU 5381  CB  THR F 346    8570   8441   5406   -711   -358  -2918       C
ATOM   5382  OG1 THR F 346      21.739 -20.769 -57.159  1.00 61.25           O
ANISOU 5382  OG1 THR F 346    8940   8578   5755   -989   -400  -3137       O
ATOM   5383  CG2 THR F 346      22.775 -18.783 -58.068  1.00 58.59           C
ANISOU 5383  CG2 THR F 346    8329   8761   5170   -678   -507  -2868       C
ATOM   5384  C   THR F 346      24.058 -21.898 -56.162  1.00 61.14           C
ANISOU 5384  C   THR F 346    9368   8119   5743   -514   -112  -3065       C
ATOM   5385  O   THR F 346      24.144 -23.020 -56.681  1.00 64.20           O
ANISOU 5385  O   THR F 346   10015   8309   6069   -530    -77  -3293       O
ATOM   5386  N   GLY F 347      23.851 -21.703 -54.861  1.00 59.58           N
ANISOU 5386  N   GLY F 347    9155   7768   5717   -548    -58  -2884       N
ATOM   5387  CA  GLY F 347      23.695 -22.800 -53.910  1.00 61.10           C
ANISOU 5387  CA  GLY F 347    9656   7535   6025   -620     47  -2913       C
ATOM   5388  C   GLY F 347      22.384 -23.558 -54.037  1.00 63.56           C
ANISOU 5388  C   GLY F 347   10062   7682   6405  -1000     56  -3100       C
ATOM   5389  O   GLY F 347      22.088 -24.419 -53.209  1.00 65.10           O
ANISOU 5389  O   GLY F 347   10531   7510   6694  -1136    166  -3112       O
ATOM   5390  N   ASN F 348      21.594 -23.215 -55.055  1.00 64.06           N
ANISOU 5390  N   ASN F 348    9904   8019   6416  -1185    -68  -3241       N
ATOM   5391  CA  ASN F 348      20.382 -23.946 -55.409  1.00 66.83           C
ANISOU 5391  CA  ASN F 348   10293   8274   6823  -1558    -97  -3477       C
ATOM   5392  CB  ASN F 348      19.142 -23.043 -55.278  1.00 66.16           C
ANISOU 5392  CB  ASN F 348    9806   8464   6867  -1802   -190  -3437       C
ATOM   5393  CG  ASN F 348      17.840 -23.839 -55.092  1.00 69.65           C
ANISOU 5393  CG  ASN F 348   10255   8745   7462  -2237   -149  -3647       C
ATOM   5394  OD1 ASN F 348      17.773 -24.763 -54.278  1.00 72.02           O
ANISOU 5394  OD1 ASN F 348   10853   8662   7850  -2387     37  -3669       O
ATOM   5395  ND2 ASN F 348      16.799 -23.468 -55.839  1.00 69.91           N
ANISOU 5395  ND2 ASN F 348    9964   9072   7527  -2447   -330  -3802       N
ATOM   5396  C   ASN F 348      20.544 -24.474 -56.834  1.00 69.06           C
ANISOU 5396  C   ASN F 348   10684   8640   6915  -1547   -200  -3738       C
ATOM   5397  O   ASN F 348      19.582 -24.911 -57.473  1.00 71.54           O
ANISOU 5397  O   ASN F 348   10974   8984   7225  -1844   -293  -3970       O
ATOM   5398  N   LEU F 349      21.791 -24.430 -57.308  1.00 68.36           N
ANISOU 5398  N   LEU F 349   10708   8599   6666  -1207   -176  -3713       N
ATOM   5399  CA  LEU F 349      22.186 -24.875 -58.655  1.00 70.41           C
ANISOU 5399  CA  LEU F 349   11104   8949   6701  -1136   -228  -3954       C
ATOM   5400  CB  LEU F 349      22.034 -26.402 -58.833  1.00 74.30           C
ANISOU 5400  CB  LEU F 349   11995   9037   7197  -1269   -153  -4240       C
ATOM   5401  CG  LEU F 349      23.212 -27.314 -58.448  1.00 75.35           C
ANISOU 5401  CG  LEU F 349   12494   8800   7338   -960     11  -4265       C
ATOM   5402  CD1 LEU F 349      23.480 -27.324 -56.942  1.00 73.43           C
ANISOU 5402  CD1 LEU F 349   12321   8288   7290   -860    111  -4005       C
ATOM   5403  CD2 LEU F 349      22.971 -28.730 -58.948  1.00 79.27           C
ANISOU 5403  CD2 LEU F 349   13395   8930   7794  -1104     54  -4593       C
ATOM   5404  C   LEU F 349      21.494 -24.087 -59.774  1.00 70.46           C
ANISOU 5404  C   LEU F 349   10850   9370   6551  -1276   -435  -4021       C
ATOM   5405  O   LEU F 349      21.080 -24.656 -60.785  1.00 73.71           O
ANISOU 5405  O   LEU F 349   11378   9813   6815  -1431   -529  -4288       O
ATOM   5406  N   GLN F 350      21.378 -22.778 -59.579  1.00 67.14           N
ANISOU 5406  N   GLN F 350   10108   9250   6152  -1213   -519  -3778       N
ATOM   5407  CA  GLN F 350      20.865 -21.888 -60.610  1.00 67.20           C
ANISOU 5407  CA  GLN F 350    9898   9645   5989  -1271   -738  -3784       C
ATOM   5408  CB  GLN F 350      19.977 -20.807 -59.982  1.00 65.17           C
ANISOU 5408  CB  GLN F 350    9286   9560   5916  -1363   -855  -3582       C
ATOM   5409  CG  GLN F 350      19.282 -19.897 -60.986  1.00 66.25           C
ANISOU 5409  CG  GLN F 350    9203  10065   5904  -1411  -1134  -3582       C
ATOM   5410  CD  GLN F 350      18.266 -18.962 -60.350  1.00 65.23           C
ANISOU 5410  CD  GLN F 350    8713  10069   6003  -1493  -1259  -3436       C
ATOM   5411  OE1 GLN F 350      18.433 -18.500 -59.215  1.00 63.41           O
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Figure 18 (continued)

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ANISOU 5411  OE1 GLN F 350     8380   9742   5972  -1419  -1115  -3235      O
ATOM   5412  NE2 GLN F 350      17.205 -18.670 -61.091  1.00 67.82          N
ANISOU 5412  NE2 GLN F 350     8845  10626   6297  -1630  -1540  -3552      N
ATOM   5413  C   GLN F 350      22.031 -21.267 -61.393  1.00 66.19          C
ANISOU 5413  C   GLN F 350     9811   9742   5597   -994   -707  -3697      C
ATOM   5414  O   GLN F 350      23.053 -20.903 -60.811  1.00 63.73          O
ANISOU 5414  O   GLN F 350     9487   9398   5327   -760   -551  -3513      O
ATOM   5415  N   THR F 351      21.873 -21.162 -62.711  1.00 68.30          N
ANISOU 5415  N   THR F 351    10130  10239   5581  -1042   -850  -3841      N
ATOM   5416  CA  THR F 351      22.896 -20.578 -63.589  1.00 68.33          C
ANISOU 5416  CA  THR F 351    10199  10477   5286   -837   -796  -3781      C
ATOM   5417  CB  THR F 351      22.933 -21.313 -64.957  1.00 72.47          C
ANISOU 5417  CB  THR F 351    10986  11065   5483   -903   -838  -4090      C
ATOM   5418  OG1 THR F 351      23.426 -22.645 -64.764  1.00 74.33          O
ANISOU 5418  OG1 THR F 351    11477  10978   5788   -858   -645  -4327      O
ATOM   5419  CG2 THR F 351      23.822 -20.584 -65.965  1.00 72.87          C
ANISOU 5419  CG2 THR F 351    11102  11406   5178   -749   -781  -4024      C
ATOM   5420  C   THR F 351      22.726 -19.054 -63.781  1.00 66.46          C
ANISOU 5420  C   THR F 351     9733  10556   4964   -796   -942  -3503      C
ATOM   5421  O   THR F 351      21.670 -18.577 -64.223  1.00 67.46          O
ANISOU 5421  O   THR F 351     9740  10849   5042   -941  -1208  -3500      O
ATOM   5422  N   LEU F 352      23.774 -18.303 -63.438  1.00 63.82          N
ANISOU 5422  N   LEU F 352     9338  10288   4622   -594   -780  -3279      N
ATOM   5423  CA  LEU F 352      23.783 -16.849 -63.611  1.00 62.08          C
ANISOU 5423  CA  LEU F 352     8962  10317   4309   -548   -879  -3005      C
ATOM   5424  CB  LEU F 352      23.883 -16.122 -62.257  1.00 58.40          C
ANISOU 5424  CB  LEU F 352     8278   9763   4150   -474   -815  -2744      C
ATOM   5425  CG  LEU F 352      22.734 -16.210 -61.252  1.00 57.71          C
ANISOU 5425  CG  LEU F 352     8017   9528   4381   -599   -923  -2723      C
ATOM   5426  CD1 LEU F 352      23.172 -15.633 -59.924  1.00 54.58          C
ANISOU 5426  CD1 LEU F 352     7487   9024   4226   -496   -788  -2494      C
ATOM   5427  CD2 LEU F 352      21.468 -15.522 -61.746  1.00 59.33          C
ANISOU 5427  CD2 LEU F 352     8065   9916   4561   -720  -1217  -2699      C
ATOM   5428  C   LEU F 352      24.939 -16.408 -64.496  1.00 62.47          C
ANISOU 5428  C   LEU F 352     9140  10557   4038   -426   -732  -2963      C
ATOM   5429  O   LEU F 352      26.059 -16.914 -64.364  1.00 62.17          O
ANISOU 5429  O   LEU F 352     9174  10448   4001   -291   -475  -3039      O
ATOM   5430  N   LYS F 353      24.665 -15.457 -65.384  1.00 63.27          N
ANISOU 5430  N   LYS F 353     9272  10900   3869   -470   -892  -2843      N
ATOM   5431  CA  LYS F 353      25.722 -14.814 -66.150  1.00 64.14          C
ANISOU 5431  CA  LYS F 353     9502  11201   3667   -397   -727  -2748      C
ATOM   5432  CB  LYS F 353      25.257 -14.567 -67.589  1.00 67.60          C
ANISOU 5432  CB  LYS F 353    10164  11852   3670   -499   -919  -2806      C
ATOM   5433  CG  LYS F 353      26.308 -14.823 -68.681  1.00 70.46          C
ANISOU 5433  CG  LYS F 353    10783  12357   3632   -480   -672  -2941      C
ATOM   5434  CD  LYS F 353      25.734 -14.438 -70.067  1.00 74.26          C
ANISOU 5434  CD  LYS F 353    11530  13051   3636   -595   -907  -2954      C
ATOM   5435  CE  LYS F 353      26.582 -14.974 -71.227  1.00 78.07          C
ANISOU 5435  CE  LYS F 353    12316  13659   3685   -614   -662  -3177      C
ATOM   5436  NZ  LYS F 353      25.986 -14.635 -72.572  1.00 81.80          N
ANISOU 5436  NZ  LYS F 353    13103  14333   3646   -737   -916  -3190      N
ATOM   5437  C   LYS F 353      26.085 -13.500 -65.445  1.00 61.18          C
ANISOU 5437  C   LYS F 353     8950  10869   3425   -333   -686  -2411      C
ATOM   5438  O   LYS F 353      25.259 -12.592 -65.346  1.00 60.54          O
ANISOU 5438  O   LYS F 353     8789  10834   3380   -374   -920  -2221      O
ATOM   5439  N   ILE F 354      27.308 -13.410 -64.930  1.00 59.64          N
ANISOU 5439  N   ILE F 354     8685  10652   3322   -226   -399  -2355      N
ATOM   5440  CA  ILE F 354      27.766 -12.181 -64.259  1.00 57.21          C
ANISOU 5440  CA  ILE F 354     8224  10380   3133   -191   -340  -2061      C
ATOM   5441  CB  ILE F 354      27.922 -12.336 -62.706  1.00 53.63          C
ANISOU 5441  CB  ILE F 354     7553   9725   3099   -105   -280  -1999      C
ATOM   5442  CG1 ILE F 354      29.041 -13.330 -62.353  1.00 54.06          C
ANISOU 5442  CG1 ILE F 354     7590   9699   3250     27    -30  -2177      C
ATOM   5443  CD1 ILE F 354      29.514 -13.275 -60.917  1.00 51.17          C
ANISOU 5443  CD1 ILE F 354     7045   9181   3215    133     39  -2074      C
ATOM   5444  CG2 ILE F 354      26.599 -12.724 -62.050  1.00 51.74          C
ANISOU 5444  CG2 ILE F 354     7246   9318   3094   -161   -499  -2033      C
ATOM   5445  C   ILE F 354      29.064 -11.642 -64.869  1.00 58.84          C
ANISOU 5445  C   ILE F 354     8491  10766   3100   -178    -75  -2003      C
ATOM   5446  O   ILE F 354      29.891 -12.409 -65.373  1.00 60.22          O
ANISOU 5446  O   ILE F 354     8735  10998   3147   -131    148  -2215      O
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Figure 18 (continued)

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ATOM   5447  N   ARG F 355      29.226 -10.318 -64.815  1.00 58.63           N
ANISOU 5447  N   ARG F 355    8438  10819   3021   -229    -85  -1728          N
ATOM   5448  CA  ARG F 355      30.437  -9.658 -65.305  1.00 60.49           C
ANISOU 5448  CA  ARG F 355    8713  11221   3050   -274    189  -1647          C
ATOM   5449  CB  ARG F 355      30.117  -8.263 -65.852  1.00 61.44           C
ANISOU 5449  CB  ARG F 355    8992  11418   2933   -394     74  -1361          C
ATOM   5450  CG  ARG F 355      31.245  -7.634 -66.651  1.00 64.96           C
ANISOU 5450  CG  ARG F 355    9569  12047   3066   -511    373  -1292          C
ATOM   5451  CD  ARG F 355      30.886  -6.237 -67.160  1.00 66.33           C
ANISOU 5451  CD  ARG F 355    9972  12237   2992   -636    245   -979          C
ATOM   5452  NE  ARG F 355      30.037  -6.239 -68.360  1.00 71.70           N
ANISOU 5452  NE  ARG F 355   10987  12983   3272   -678     11   -971          N
ATOM   5453  CZ  ARG F 355      29.472  -5.154 -68.895  1.00 73.47           C
ANISOU 5453  CZ  ARG F 355   11472  13191   3252   -738   -203   -704          C
ATOM   5454  NH1 ARG F 355      29.634  -3.953 -68.346  1.00 73.36           N
ANISOU 5454  NH1 ARG F 355   11440  13073   3362   -773   -196   -423          N
ATOM   5455  NH2 ARG F 355      28.736  -5.268 -69.988  1.00 77.30           N
ANISOU 5455  NH2 ARG F 355   12262  13752   3359   -754   -445   -722          N
ATOM   5456  C   ARG F 355      31.472  -9.601 -64.187  1.00 57.93           C
ANISOU 5456  C   ARG F 355    8122  10848   3041   -191    403  -1623          C
ATOM   5457  O   ARG F 355      31.365  -8.802 -63.252  1.00 55.72           O
ANISOU 5457  O   ARG F 355    7705  10480   2987   -196    329  -1419          O
ATOM   5458  N   VAL F 356      32.454 -10.488 -64.286  1.00 59.00           N
ANISOU 5458  N   VAL F 356    8187  11038   3193    -99    649  -1853          N
ATOM   5459  CA  VAL F 356      33.472 -10.669 -63.254  1.00 57.54           C
ANISOU 5459  CA  VAL F 356    7731  10818   3314     26    815  -1887          C
ATOM   5460  CB  VAL F 356      34.034 -12.124 -63.294  1.00 59.07           C
ANISOU 5460  CB  VAL F 356    7892  10969   3584    215    953  -2208          C
ATOM   5461  CG1 VAL F 356      35.263 -12.285 -62.413  1.00 58.90           C
ANISOU 5461  CG1 VAL F 356    7583  10962   3833    377   1122  -2261          C
ATOM   5462  CG2 VAL F 356      32.959 -13.120 -62.889  1.00 58.12           C
ANISOU 5462  CG2 VAL F 356    7884  10597   3601    282    725  -2309          C
ATOM   5463  C   VAL F 356      34.594  -9.647 -63.446  1.00 58.53           C
ANISOU 5463  C   VAL F 356    7742  11144   3352    -77   1059  -1769          C
ATOM   5464  O   VAL F 356      35.136  -9.510 -64.553  1.00 61.27           O
ANISOU 5464  O   VAL F 356    8201  11690   3390   -175   1273  -1838          O
ATOM   5465  N   HIS F 357      34.942  -8.926 -62.380  1.00 56.02           N
ANISOU 5465  N   HIS F 357    7219  10776   3291    -82   1041  -1603          N
ATOM   5466  CA  HIS F 357      36.060  -7.989 -62.470  1.00 57.30           C
ANISOU 5466  CA  HIS F 357    7240  11120   3411   -212   1281  -1516          C
ATOM   5467  CB  HIS F 357      35.754  -6.682 -61.737  1.00 55.20           C
ANISOU 5467  CB  HIS F 357    6955  10760   3259   -343   1148  -1222          C
ATOM   5468  CG  HIS F 357      34.762  -5.810 -62.460  1.00 56.04           C
ANISOU 5468  CG  HIS F 357    7368  10819   3105   -492    995  -1005          C
ATOM   5469  ND1 HIS F 357      35.108  -4.564 -62.960  1.00 57.20           N
ANISOU 5469  ND1 HIS F 357    7641  11040   3052   -709   1109   -802          N
ATOM   5470  CE1 HIS F 357      34.034  -4.029 -63.539  1.00 57.73           C
ANISOU 5470  CE1 HIS F 357    8005  11020   2910   -757    890   -629          C
ATOM   5471  NE2 HIS F 357      33.002  -4.895 -63.453  1.00 56.73           N
ANISOU 5471  NE2 HIS F 357    7904  10798   2853   -597    644   -736          N
ATOM   5472  CD2 HIS F 357      33.429  -6.007 -62.764  1.00 55.77           C
ANISOU 5472  CD2 HIS F 357    7539  10666   2984   -449    720   -964          C
ATOM   5473  C   HIS F 357      37.379  -8.623 -62.026  1.00 57.96           C
ANISOU 5473  C   HIS F 357    7008  11315   3698    -68   1502  -1730          C
ATOM   5474  O   HIS F 357      37.441  -9.312 -61.010  1.00 56.64           O
ANISOU 5474  O   HIS F 357    6685  11010   3825    136   1387  -1810          O
ATOM   5475  N   GLU F 358      38.424  -8.396 -62.813  1.00 60.88           N
ANISOU 5475  N   GLU F 358    7293  11938   3900   -169   1821  -1829          N
ATOM   5476  CA  GLU F 358      39.720  -9.030 -62.584  1.00 62.68           C
ANISOU 5476  CA  GLU F 358    7182  12324   4310    -13   2054  -2080          C
ATOM   5477  CB  GLU F 358      40.114  -9.904 -63.775  1.00 66.22           C
ANISOU 5477  CB  GLU F 358    7711  12931   4519     53   2310  -2364          C
ATOM   5478  CG  GLU F 358      39.357 -11.213 -63.855  1.00 66.22           C
ANISOU 5478  CG  GLU F 358    7904  12729   4529    286   2137  -2540          C
ATOM   5479  CD  GLU F 358      39.723 -12.027 -65.081  1.00 70.08           C
ANISOU 5479  CD  GLU F 358    8515  13362   4752    337   2398  -2837          C
ATOM   5480  OE1 GLU F 358      40.884 -11.947 -65.532  1.00 73.92           O
ANISOU 5480  OE1 GLU F 358    8787  14108   5193    324   2746  -3000          O
ATOM   5481  OE2 GLU F 358      38.844 -12.747 -65.596  1.00 70.92           O
ANISOU 5481  OE2 GLU F 358    8924  13330   4693    377   2265  -2927          O
ATOM   5482  C   GLU F 358      40.822  -8.024 -62.297  1.00 63.33           C
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Figure 18 (continued)

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ANISOU 5482  C   GLU F 358     6971  12606   4485   -186   2258  -2010      C
ATOM   5483  O   GLU F 358      41.201  -7.245 -63.165  1.00 65.86         O
ANISOU 5483  O   GLU F 358     7365  13110   4550   -452   2506  -1950      O
ATOM   5484  N   GLY F 359      41.349  -8.079 -61.081  1.00 61.35         N
ANISOU 5484  N   GLY F 359     6404  12317   4590    -48   2153  -2027      N
ATOM   5485  CA  GLY F 359      42.408  -7.178 -60.650  1.00 62.41         C
ANISOU 5485  CA  GLY F 359     6211  12637   4866   -213   2303  -1990      C
ATOM   5486  C   GLY F 359      42.221  -6.774 -59.198  1.00 59.15         C
ANISOU 5486  C   GLY F 359     5681  12045   4748   -161   2011  -1834      C
ATOM   5487  O   GLY F 359      41.145  -6.954 -58.626  1.00 55.46         O
ANISOU 5487  O   GLY F 359     5438  11308   4326    -64   1725  -1700      O
ATOM   5488  N   TYR F 360      43.272  -6.231 -58.597  1.00 60.49         N
ANISOU 5488  N   TYR F 360     5491  12378   5116   -241   2091  -1868      N
ATOM   5489  CA  TYR F 360      43.140  -5.679 -57.274  1.00 58.50         C
ANISOU 5489  CA  TYR F 360     5160  11974   5092   -248   1830  -1716      C
ATOM   5490  CB  TYR F 360      44.441  -5.768 -56.483  1.00 61.17         C
ANISOU 5490  CB  TYR F 360     5016  12510   5718   -156   1845  -1890      C
ATOM   5491  CG  TYR F 360      44.405  -5.033 -55.139  1.00 60.37         C
ANISOU 5491  CG  TYR F 360     4845  12280   5811   -223   1588  -1737      C
ATOM   5492  CD1 TYR F 360      44.129  -5.711 -53.941  1.00 57.83         C
ANISOU 5492  CD1 TYR F 360     4525  11766   5682     75   1267  -1742      C
ATOM   5493  CE1 TYR F 360      44.117  -5.040 -52.728  1.00 55.89         C
ANISOU 5493  CE1 TYR F 360     4244  11416   5577      3   1045  -1619      C
ATOM   5494  CZ  TYR F 360      44.376  -3.669 -52.698  1.00 57.61         C
ANISOU 5494  CZ  TYR F 360     4417  11704   5768   -369   1137  -1499      C
ATOM   5495  OH  TYR F 360      44.375  -2.958 -51.515  1.00 56.33         O
ANISOU 5495  OH  TYR F 360     4240  11432   5729   -460    926  -1398      O
ATOM   5496  CE2 TYR F 360      44.640  -2.979 -53.864  1.00 60.25         C
ANISOU 5496  CE2 TYR F 360     4762  12201   5929   -672   1451  -1478      C
ATOM   5497  CD2 TYR F 360      44.645  -3.656 -55.072  1.00 61.36         C
ANISOU 5497  CD2 TYR F 360     4949  12461   5906   -601   1675  -1589      C
ATOM   5498  C   TYR F 360      42.675  -4.246 -57.382  1.00 57.20         C
ANISOU 5498  C   TYR F 360     5212  11733   4789   -608   1840  -1441      C
ATOM   5499  O   TYR F 360      43.193  -3.472 -58.181  1.00 59.56         O
ANISOU 5499  O   TYR F 360     5502  12205   4923   -901   2110  -1412      O
ATOM   5500  N   GLU F 361      41.695  -3.909 -56.553  1.00 53.97         N
ANISOU 5500  N   GLU F 361     5014  11047   4446   -581   1556  -1245      N
ATOM   5501  CA  GLU F 361      41.110  -2.579 -56.522  1.00 52.98         C
ANISOU 5501  CA  GLU F 361     5129  10781   4221   -857   1514   -981      C
ATOM   5502  CB  GLU F 361      39.809  -2.561 -57.329  1.00 51.91         C
ANISOU 5502  CB  GLU F 361     5403  10479   3840   -858   1435   -834      C
ATOM   5503  CG  GLU F 361      40.021  -2.601 -58.835  1.00 54.36         C
ANISOU 5503  CG  GLU F 361     5852  10968   3836   -989   1691   -875      C
ATOM   5504  CD  GLU F 361      38.780  -3.055 -59.586  1.00 54.79         C
ANISOU 5504  CD  GLU F 361     6252  10895   3671   -887   1552   -820      C
ATOM   5505  OE1 GLU F 361      38.124  -4.047 -59.150  1.00 52.19         O
ANISOU 5505  OE1 GLU F 361     5923  10445   3464   -635   1355   -913      O
ATOM   5506  OE2 GLU F 361      38.474  -2.410 -60.614  1.00 54.98         O
ANISOU 5506  OE2 GLU F 361     6559  10938   3391  -1074   1633   -684      O
ATOM   5507  C   GLU F 361      40.862  -2.085 -55.099  1.00 50.53         C
ANISOU 5507  C   GLU F 361     4782  10279   4137   -837   1267   -874      C
ATOM   5508  O   GLU F 361      40.743  -2.868 -54.158  1.00 48.99         O
ANISOU 5508  O   GLU F 361     4492   9997   4125   -585   1074   -955      O
ATOM   5509  N   GLU F 362      40.781  -0.769 -54.967  1.00 50.77         N
ANISOU 5509  N   GLU F 362     4930  10227   4132  -1111   1284   -690      N
ATOM   5510  CA  GLU F 362      40.569  -0.116 -53.696  1.00 49.49         C
ANISOU 5510  CA  GLU F 362     4773   9883   4149  -1141   1086   -593      C
ATOM   5511  CB  GLU F 362      41.853   0.602 -53.290  1.00 52.22         C
ANISOU 5511  CB  GLU F 362     4827  10402   4614  -1376   1204   -662      C
ATOM   5512  CG  GLU F 362      42.289   0.516 -51.833  1.00 53.76         C
ANISOU 5512  CG  GLU F 362     4795  10573   5058  -1278    995   -745      C
ATOM   5513  CD  GLU F 362      43.791   0.759 -51.700  1.00 59.82         C
ANISOU 5513  CD  GLU F 362     5136  11637   5954  -1447   1128   -920      C
ATOM   5514  OE1 GLU F 362      44.203   1.943 -51.674  1.00 63.47         O
ANISOU 5514  OE1 GLU F 362     5597  12108   6413  -1798   1232   -851      O
ATOM   5515  OE2 GLU F 362      44.566  -0.232 -51.658  1.00 61.55         O
ANISOU 5515  OE2 GLU F 362     5018  12080   6288  -1231   1134  -1137      O
ATOM   5516  C   GLU F 362      39.471   0.903 -53.950  1.00 47.93         C
ANISOU 5516  C   GLU F 362     4959   9439   3815   -345   1021   -345      C
ATOM   5517  O   GLU F 362      39.619   1.764 -54.816  1.00 50.08         O
ANISOU 5517  O   GLU F 362     5385   9735   3909  -1529   1187   -230      O
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Figure 18 (continued)

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ATOM   5518  N   PHE F 363      38.374   0.793 -53.206  1.00 44.53           N
ANISOU 5518  N   PHE F 363     4688   8767   3465  -1111    788   -267       NC
ATOM   5519  CA  PHE F 363      37.236   1.684 -53.350  1.00 43.24           C
ANISOU 5519  CA  PHE F 363     4850   8361   3218  -1169    690    -58       CC
ATOM   5520  CB  PHE F 363      35.981   0.878 -53.683  1.00 40.67           C
ANISOU 5520  CB  PHE F 363     4673   7941   2838   -939    548    -53       CC
ATOM   5521  CG  PHE F 363      36.051   0.171 -54.979  1.00 40.68           C
ANISOU 5521  CG  PHE F 363     4709   8111   2635   -910    655   -120       CC
ATOM   5522  CD1 PHE F 363      35.670   0.807 -56.150  1.00 41.53           C
ANISOU 5522  CD1 PHE F 363     5074   8214   2492  -1035    704     21       CC
ATOM   5523  CE1 PHE F 363      35.734   0.141 -57.373  1.00 42.89           C
ANISOU 5523  CE1 PHE F 363     5312   8550   2433  -1019    806    -55       CC
ATOM   5524  CZ  PHE F 363      36.189  -1.158 -57.422  1.00 42.89           C
ANISOU 5524  CZ  PHE F 363     5110   8707   2481   -871    874   -284       CC
ATOM   5525  CE2 PHE F 363      36.573  -1.800 -56.244  1.00 41.85           C
ANISOU 5525  CE2 PHE F 363     4721   8557   2623   -723    816   -416       CC
ATOM   5526  CD2 PHE F 363      36.503  -1.134 -55.038  1.00 39.67           C
ANISOU 5526  CD2 PHE F 363     4392   8132   2547   -749    702   -327       CC
ATOM   5527  C   PHE F 363      36.925   2.473 -52.094  1.00 42.77           C
ANISOU 5527  C   PHE F 363     4840   8086   3327  -1199    550     18       CO
ATOM   5528  O   PHE F 363      37.135   2.007 -50.973  1.00 41.83           O
ANISOU 5528  O   PHE F 363     4561   7954   3377  -1087    450    -85       ON
ATOM   5529  N   THR F 364      36.389   3.667 -52.305  1.00 43.89           N
ANISOU 5529  N   THR F 364     5240   8037   3400  -1337    537    201       NC
ATOM   5530  CA  THR F 364      35.644   4.393 -51.289  1.00 42.92           C
ANISOU 5530  CA  THR F 364     5254   7647   3406  -1303    388    282       CC
ATOM   5531  CB  THR F 364      35.989   5.912 -51.391  1.00 45.24           C
ANISOU 5531  CB  THR F 364     5738   7796   3655  -1580    468    427       CC
ATOM   5532  OG1 THR F 364      36.808   6.290 -50.279  1.00 45.24           O
ANISOU 5532  OG1 THR F 364     5587   7795   3810  -1716    475    338       OC
ATOM   5533  CG2 THR F 364      34.757   6.819 -51.449  1.00 46.04           C
ANISOU 5533  CG2 THR F 364     6170   7588   3736  -1510    345    604       CC
ATOM   5534  C   THR F 364      34.153   4.071 -51.527  1.00 41.58           C
ANISOU 5534  C   THR F 364     5252   7332   3215  -1076    236    345       CO
ATOM   5535  O   THR F 364      33.686   4.150 -52.663  1.00 43.15           O
ANISOU 5535  O   THR F 364     5607   7543   3244  -1066    239    436       ON
ATOM   5536  N   MSE F 365      33.435   3.668 -50.475  1.00 39.53           N
ANISOU 5536  N   MSE F 365     4952   6953   3115   -905    109    284       NC
ATOM   5537  CA  MSE F 365      31.970   3.467 -50.514  1.00 38.74           C
ANISOU 5537  CA  MSE F 365     4959   6713   3047   -717    -25    317       CC
ATOM   5538  CB  MSE F 365      31.558   2.102 -49.967  1.00 36.04           C
ANISOU 5538  CB  MSE F 365     4475   6423   2797   -544    -77    168       CC
ATOM   5539  CG  MSE F 365      32.040   0.907 -50.754  1.00 36.93           C
ANISOU 5539  CG  MSE F 365     4478   6743   2812   -498    -25     64       CC
ATOM   5540  SE  MSE F 365      31.519  -0.802 -49.939  0.90 39.05          SE
ANISOU 5540  SE  MSE F 365     4645   6991   3203   -298    -87   -113       SE
ATOM   5541  CE  MSE F 365      29.589  -0.577 -49.841  1.00 35.91           C
ANISOU 5541  CE  MSE F 365     4355   6406   2882   -215   -210    -68       CC
ATOM   5542  C   MSE F 365      31.317   4.540 -49.661  1.00 37.78           C
ANISOU 5542  C   MSE F 365     4972   6339   3046   -712    -92     392       CO
ATOM   5543  O   MSE F 365      31.692   4.733 -48.500  1.00 37.16           O
ANISOU 5543  O   MSE F 365     4845   6192   3080   -755    -78     332       ON
ATOM   5544  N   VAL F 366      30.362   5.267 -50.226  1.00 38.03           N
ANISOU 5544  N   VAL F 366     5182   6223   3045   -647   -175     514       NC
ATOM   5545  CA  VAL F 366      29.724   6.334 -49.460  1.00 38.03           C
ANISOU 5545  CA  VAL F 366     5316   5962   3171   -610   -229     570       CC
ATOM   5546  CB  VAL F 366      30.225   7.753 -49.873  1.00 40.41           C
ANISOU 5546  CB  VAL F 366     5862   6104   3387   -782   -188     733       CC
ATOM   5547  CG1 VAL F 366      29.484   8.835 -49.096  1.00 40.76           C
ANISOU 5547  CG1 VAL F 366     6072   5842   3573   -704   -250     771       CC
ATOM   5548  CG2 VAL F 366      31.728   7.887 -49.656  1.00 39.69           C
ANISOU 5548  CG2 VAL F 366     5703   6126   3250  -1053    -37     699       CC
ATOM   5549  C   VAL F 366      28.216   6.220 -49.565  1.00 37.81           C
ANISOU 5549  C   VAL F 366     5297   5841   3228   -377   -366     566       CO
ATOM   5550  O   VAL F 366      27.635   6.467 -50.626  1.00 39.06           O
ANISOU 5550  O   VAL F 366     5559   5991   3289   -297   -470     667       ON
ATOM   5551  N   GLY F 367      27.601   5.809 -48.458  1.00 36.34           N
ANISOU 5551  N   GLY F 367     4995   5600   3214   -276   -367     439       NC
ATOM   5552  CA  GLY F 367      26.149   5.662 -48.373  1.00 35.97           C
ANISOU 5552  CA  GLY F 367     4885   5486   3296    -73   -463     389       CC
ATOM   5553  C   GLY F 367      25.571   6.755 -47.502  1.00 37.01           C
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Figure 18 (continued)

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ANISOU 5553  C   GLY F 367     5111   5371   3580     -2   -460    393    C
ATOM   5554  O   GLY F 367      26.298   7.648 -47.027  1.00 37.55           O
ANISOU 5554  O   GLY F 367     5332   5300   3634   -122   -397    444    O
ATOM   5555  N   LYS F 368      24.263   6.678 -47.289  1.00 37.07           N
ANISOU 5555  N   LYS F 368     5015   5327   3743    187   -521    315    N
ATOM   5556  CA  LYS F 368      23.522   7.707 -46.596  1.00 39.14           C
ANISOU 5556  CA  LYS F 368     5344   5357   4169    313   -519    293    C
ATOM   5557  CB  LYS F 368      22.035   7.565 -46.942  1.00 40.86           C
ANISOU 5557  CB  LYS F 368     5388   5594   4542    553   -639    224    C
ATOM   5558  CG  LYS F 368      21.244   8.827 -46.755  1.00 45.35           C
ANISOU 5558  CG  LYS F 368     6044   5921   5265    758   -706    244    C
ATOM   5559  CD  LYS F 368      20.322   9.053 -47.934  1.00 52.09           C
ANISOU 5559  CD  LYS F 368     6847   6803   6142    988   -956    316    C
ATOM   5560  CE  LYS F 368      21.070   9.688 -49.121  1.00 54.74           C
ANISOU 5560  CE  LYS F 368     7484   7077   6236    936  -1094    561    C
ATOM   5561  NZ  LYS F 368      20.132  10.022 -50.240  1.00 57.30           N
ANISOU 5561  NZ  LYS F 368     7821   7398   6554   1192  -1381    650    N
ATOM   5562  C   LYS F 368      23.751   7.641 -45.067  1.00 37.84           C
ANISOU 5562  C   LYS F 368     5174   5115   4090    229   -347    158    C
ATOM   5563  O   LYS F 368      23.754   8.670 -44.375  1.00 38.54           O
ANISOU 5563  O   LYS F 368     5412   4988   4245    237   -298    153    O
ATOM   5564  N   ARG F 369      23.945   6.421 -44.577  1.00 35.65           N
ANISOU 5564  N   ARG F 369     4759   4999   3789    150   -265     51    N
ATOM   5565  CA  ARG F 369      24.089   6.136 -43.170  1.00 35.10           C
ANISOU 5565  CA  ARG F 369     4704   4880   3753     76   -120    -72    C
ATOM   5566  CB  ARG F 369      22.839   5.418 -42.628  1.00 35.16           C
ANISOU 5566  CB  ARG F 369     4548   4914   3898    172    -37   -226    C
ATOM   5567  CG  ARG F 369      21.534   6.240 -42.641  1.00 36.78           C
ANISOU 5567  CG  ARG F 369     4677   4998   4298    364    -46   -284    C
ATOM   5568  CD  ARG F 369      20.626   5.893 -41.434  1.00 39.03           C
ANISOU 5568  CD  ARG F 369     4867   5249   4714    379    152   -479    C
ATOM   5569  NE  ARG F 369      20.476   7.016 -40.493  1.00 39.37           N
ANISOU 5569  NE  ARG F 369     5053   5078   4826    428    260   -540    N
ATOM   5570  CZ  ARG F 369      20.294   6.888 -39.186  1.00 41.20           C
ANISOU 5570  CZ  ARG F 369     5349   5245   5059    356    470   -682    C
ATOM   5571  NH1 ARG F 369      20.260   5.688 -38.625  1.00 40.27           N
ANISOU 5571  NH1 ARG F 369     5187   5244   4870    225    594   -756    N
ATOM   5572  NH2 ARG F 369      20.172   7.967 -38.423  1.00 45.93           N
ANISOU 5572  NH2 ARG F 369     6100   5643   5708    408    562   -750    N
ATOM   5573  C   ARG F 369      25.349   5.297 -42.903  1.00 33.83           C
ANISOU 5573  C   ARG F 369     4557   4853   3444    -89    -92    -70    C
ATOM   5574  O   ARG F 369      25.582   4.876 -41.779  1.00 33.68           O
ANISOU 5574  O   ARG F 369     4575   4816   3407   -150     -7   -158    O
ATOM   5575  N   ALA F 370      26.165   5.072 -43.928  1.00 33.74           N
ANISOU 5575  N   ALA F 370     4525   4977   3319   -148   -165     25    N
ATOM   5576  CA  ALA F 370      27.433   4.376 -43.756  1.00 33.32           C
ANISOU 5576  CA  ALA F 370     4448   5061   3152   -271   -149     14    C
ATOM   5577  CB  ALA F 370      27.219   2.866 -43.786  1.00 32.53           C
ANISOU 5577  CB  ALA F 370     4229   5094   3036   -219   -139    -68    C
ATOM   5578  C   ALA F 370      28.480   4.805 -44.796  1.00 34.46           C
ANISOU 5578  C   ALA F 370     4607   5301   3186   -377   -183    124    C
ATOM   5579  O   ALA F 370      28.141   5.420 -45.821  1.00 35.44           O
ANISOU 5579  O   ALA F 370     4786   5396   3282   -351   -228    227    O
ATOM   5580  N   THR F 371      29.749   4.533 -44.485  1.00 34.41           N
ANISOU 5580  N   THR F 371     4557   5404   3113   -500   -162     97    N
ATOM   5581  CA  THR F 371      30.877   4.693 -45.401  1.00 35.72           C
ANISOU 5581  CA  THR F 371     4675   5719   3179   -628   -147    157    C
ATOM   5582  CB  THR F 371      31.658   6.063 -45.259  1.00 37.27           C
ANISOU 5582  CB  THR F 371     4983   5816   3361   -831   -115    222    C
ATOM   5583  OG1 THR F 371      32.299   6.139 -43.983  1.00 39.27           O
ANISOU 5583  OG1 THR F 371     5217   6048   3656   -912   -125    125    O
ATOM   5584  CG2 THR F 371      30.771   7.277 -45.436  1.00 38.77           C
ANISOU 5584  CG2 THR F 371     5387   5755   3590   -806   -128    324    C
ATOM   5585  C   THR F 371      31.864   3.567 -45.105  1.00 35.06           C
ANISOU 5585  C   THR F 371     4426   5831   3065   -633   -144     55    C
ATOM   5586  O   THR F 371      31.992   3.125 -43.961  1.00 34.68           O
ANISOU 5586  O   THR F 371     4370   5753   3055   -598   -175    -28    O
ATOM   5587  N   ALA F 372      32.582   3.125 -46.131  1.00 35.32           N
ANISOU 5587  N   ALA F 372     4346   6058   3017   -666   -110     60    N
ATOM   5588  CA  ALA F 372      33.520   2.019 -45.996  1.00 34.84           C
ANISOU 5588  CA  ALA F 372     4107   6186   2944   -621   -112    -50    C
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Figure 18 (continued)

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ATOM   5589  CB  ALA F 372      32.796   0.677 -46.224  1.00 33.58           C
ANISOU 5589  CB  ALA F 372    3933   6046   2781   -434   -136   -111       C
ATOM   5590  C   ALA F 372      34.709   2.162 -46.952  1.00 36.35           C
ANISOU 5590  C   ALA F 372    4157   6590   3064   -749    -25    -55       C
ATOM   5591  O   ALA F 372      34.637   2.846 -47.979  1.00 37.00           O
ANISOU 5591  O   ALA F 372    4314   6683   3060   -860     51     41       O
ATOM   5592  N   ILE F 373      35.809   1.530 -46.579  1.00 36.90           N
ANISOU 5592  N   ILE F 373    4028   6828   3166   -731    -35   -172       N
ATOM   5593  CA  ILE F 373      36.920   1.327 -47.482  1.00 38.46           C
ANISOU 5593  CA  ILE F 373    4023   7274   3317   -805     74   -232       C
ATOM   5594  CB  ILE F 373      38.271   1.774 -46.878  1.00 40.52           C
ANISOU 5594  CB  ILE F 373    4067   7677   3652   -954     71   -316       C
ATOM   5595  CG1 ILE F 373      38.285   3.292 -46.705  1.00 41.82           C
ANISOU 5595  CG1 ILE F 373    4365   7713   3813  -1228    112   -214       C
ATOM   5596  CD1 ILE F 373      38.951   3.744 -45.409  1.00 46.04           C
ANISOU 5596  CD1 ILE F 373    4819   8231   4445  -1323     -5   -292       C
ATOM   5597  CG2 ILE F 373      39.438   1.353 -47.777  1.00 42.20           C
ANISOU 5597  CG2 ILE F 373    3998   8188   3847   -998    208   -427       C
ATOM   5598  C   ILE F 373      36.917  -0.152 -47.827  1.00 37.80           C
ANISOU 5598  C   ILE F 373    3843   7296   3223   -576     62   -341       C
ATOM   5599  O   ILE F 373      37.018  -1.025 -46.943  1.00 36.27           O
ANISOU 5599  O   ILE F 373    3606   7073   3101   -402    -52   -425       O
ATOM   5600  N   LEU F 374      36.771  -0.409 -49.125  1.00 37.99           N
ANISOU 5600  N   LEU F 374    3882   7418   3136   -580    175   -333       N
ATOM   5601  CA  LEU F 374      36.835  -1.740 -49.675  1.00 37.72           C
ANISOU 5601  CA  LEU F 374    3776   7485   3070   -391    197   -455       C
ATOM   5602  CB  LEU F 374      35.600  -2.008 -50.541  1.00 36.81           C
ANISOU 5602  CB  LEU F 374    3865   7278   2844   -346    196   -396       C
ATOM   5603  CG  LEU F 374      35.410  -3.409 -51.127  1.00 35.70           C
ANISOU 5603  CG  LEU F 374    3719   7187   2659   -167    206   -529       C
ATOM   5604  CD1 LEU F 374      35.355  -4.482 -50.037  1.00 32.88           C
ANISOU 5604  CD1 LEU F 374    3345   6714   2434     29     94   -622       C
ATOM   5605  CD2 LEU F 374      34.154  -3.412 -51.980  1.00 36.04           C
ANISOU 5605  CD2 LEU F 374    3956   7151   2586   -180    174   -465       C
ATOM   5606  C   LEU F 374      38.114  -1.935 -50.495  1.00 40.40           C
ANISOU 5606  C   LEU F 374    3881   8101   3369   -441    359   -571       C
ATOM   5607  O   LEU F 374      38.330  -1.244 -51.491  1.00 41.59           O
ANISOU 5607  O   LEU F 374    4056   8354   3393   -631    516   -515       O
ATOM   5608  N   ARG F 375      38.958  -2.863 -50.040  1.00 41.39           N
ANISOU 5608  N   ARG F 375    3788   8340   3600   -264    322   -734       N
ATOM   5609  CA  ARG F 375      40.081  -3.367 -50.817  1.00 44.76           C
ANISOU 5609  CA  ARG F 375    3954   9037   4017   -227    480   -901       C
ATOM   5610  CB  ARG F 375      41.365  -3.461 -49.975  1.00 46.06           C
ANISOU 5610  CB  ARG F 375    3782   9363   4356   -167    416  -1037       C
ATOM   5611  CG  ARG F 375      41.765  -2.160 -49.277  1.00 47.35           C
ANISOU 5611  CG  ARG F 375    3874   9536   4580   -429    379   -955       C
ATOM   5612  CD  ARG F 375      43.214  -2.192 -48.753  1.00 51.18           C
ANISOU 5612  CD  ARG F 375    3943  10275   5227   -420    344  -1131       C
ATOM   5613  NE  ARG F 375      43.464  -1.175 -47.726  1.00 56.01           N
ANISOU 5613  NE  ARG F 375    4529  10837   5914   -618    213  -1075       N
ATOM   5614  CZ  ARG F 375      44.650  -0.608 -47.469  1.00 59.99           C
ANISOU 5614  CZ  ARG F 375    4690  11572   6531   -795    230  -1192       C
ATOM   5615  NH1 ARG F 375      45.730  -0.928 -48.175  1.00 63.23           N
ANISOU 5615  NH1 ARG F 375    4713  12304   7009   -801    399  -1375       N
ATOM   5616  NH2 ARG F 375      44.757   0.294 -46.496  1.00 61.29           N
ANISOU 5616  NH2 ARG F 375    4888  11655   6746   -981     88  -1145       N
ATOM   5617  C   ARG F 375      39.650  -4.740 -51.345  1.00 44.39           C
ANISOU 5617  C   ARG F 375    3991   8951   3922     26    478  -1009       C
ATOM   5618  O   ARG F 375      39.022  -5.515 -50.620  1.00 42.96           O
ANISOU 5618  O   ARG F 375    3945   8574   3804    217    312  -1010       O
ATOM   5619  N   LYS F 376      39.987  -5.036 -52.600  1.00 46.26           N
ANISOU 5619  N   LYS F 376    4176   9365   4035      5    679  -1106       N
ATOM   5620  CA  LYS F 376      39.348  -6.134 -53.320  1.00 46.24           C
ANISOU 5620  CA  LYS F 376    4340   9297   3933    173    694  -1190       C
ATOM   5621  CB  LYS F 376      38.040  -5.601 -53.905  1.00 45.02           C
ANISOU 5621  CB  LYS F 376    4494   9002   3608     21    666  -1020       C
ATOM   5622  CG  LYS F 376      37.218  -6.592 -54.639  1.00 45.84           C
ANISOU 5622  CG  LYS F 376    4788   9030   3597    138    648  -1099       C
ATOM   5623  CD  LYS F 376      36.312  -5.902 -55.630  1.00 45.93           C
ANISOU 5623  CD  LYS F 376    5028   9033   3391    -41    662   -965       C
ATOM   5624  CE  LYS F 376      35.659  -6.942 -56.497  1.00 47.28           C
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Figure 18 (continued)

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ANISOU 5624  CE  LYS F 376     5357   9181   3425     56    651  -1090    C
ATOM   5625  NZ  LYS F 376      36.674  -7.533 -57.410  1.00 49.17        N
ANISOU 5625  NZ  LYS F 376     5499   9636   3547    101    872  -1286    N
ATOM   5626  C   LYS F 376      40.212  -6.718 -54.445  1.00 49.04        C
ANISOU 5626  C   LYS F 376     4537   9897   4199    227    926  -1392    C
ATOM   5627  O   LYS F 376      40.914  -5.980 -55.142  1.00 51.37        O
ANISOU 5627  O   LYS F 376     4701  10414   4403     20   1140  -1400    O
ATOM   5628  N   ALA F 377      40.148  -8.041 -54.624  1.00 48.89        N
ANISOU 5628  N   ALA F 377     4554   9824   4200    490    905  -1564    N
ATOM   5629  CA  ALA F 377      40.819  -8.718 -55.746  1.00 50.86        C
ANISOU 5629  CA  ALA F 377     4702  10273   4349    573   1136  -1786    C
ATOM   5630  CB  ALA F 377      41.903  -9.649 -55.227  1.00 53.08        C
ANISOU 5630  CB  ALA F 377     4691  10631   4845    884   1125  -2013    C
ATOM   5631  C   ALA F 377      39.807  -9.480 -56.625  1.00 50.17        C
ANISOU 5631  C   ALA F 377     4938  10055   4069    617   1139  -1830    C
ATOM   5632  O   ALA F 377      38.594  -9.335 -56.445  1.00 47.07        O
ANISOU 5632  O   ALA F 377     4807   9454   3625    543    972  -1675    O
ATOM   5633  N   THR F 378      40.302 -10.282 -57.575  1.00 52.64        N
ANISOU 5633  N   THR F 378     5218  10501   4283    731   1331  -2062    N
ATOM   5634  CA  THR F 378      39.443 -11.109 -58.447  1.00 52.30        C
ANISOU 5634  CA  THR F 378     5480  10344   4050    774   1333  -2154    C
ATOM   5635  CB  THR F 378      40.261 -11.862 -59.508  1.00 56.31        C
ANISOU 5635  CB  THR F 378     5911  11045   4441    890   1603  -2444    C
ATOM   5636  OG1 THR F 378      41.023 -10.926 -60.282  1.00 58.56        O
ANISOU 5636  OG1 THR F 378     6043  11640   4566    661   1879  -2434    O
ATOM   5637  CG2 THR F 378      39.345 -12.685 -60.420  1.00 56.32        C
ANISOU 5637  CG2 THR F 378     6258  10920   4219    905   1590  -2552    C
ATOM   5638  C   THR F 378      38.624 -12.111 -57.623  1.00 50.10        C
ANISOU 5638  C   THR F 378     5380   9738   3920    974   1085  -2166    C
ATOM   5639  O   THR F 378      39.174 -13.029 -57.010  1.00 50.63        O
ANISOU 5639  O   THR F 378     5354   9711   4174   1249   1041  -2309    O
ATOM   5640  N   ARG F 379      37.307 -11.917 -57.630  1.00 47.53        N
ANISOU 5640  N   ARG F 379     5314   9237   3507    831    928  -2016    N
ATOM   5641  CA  ARG F 379      36.375 -12.691 -56.812  1.00 45.98        C
ANISOU 5641  CA  ARG F 379     5299   8730   3442    929    717  -1996    C
ATOM   5642  CB  ARG F 379      35.991 -13.986 -57.509  1.00 47.10        C
ANISOU 5642  CB  ARG F 379     5649   8750   3497   1039    741  -2218    C
ATOM   5643  CG  ARG F 379      35.553 -13.795 -58.975  1.00 49.36        C
ANISOU 5643  CG  ARG F 379     6077   9194   3483    864    839  -2280    C
ATOM   5644  CD  ARG F 379      34.872 -15.036 -59.519  1.00 49.19        C
ANISOU 5644  CD  ARG F 379     6310   8999   3381    920    800  -2486    C
ATOM   5645  NE  ARG F 379      33.688 -15.336 -58.716  1.00 48.20        N
ANISOU 5645  NE  ARG F 379     6327   8598   3390    864    582  -2392    N
ATOM   5646  CZ  ARG F 379      32.926 -16.417 -58.847  1.00 48.36        C
ANISOU 5646  CZ  ARG F 379     6569   8396   3409    870    509  -2542    C
ATOM   5647  NH1 ARG F 379      33.204 -17.326 -59.776  1.00 50.81        N
ANISOU 5647  NH1 ARG F 379     7015   8710   3582    951    618  -2802    N
ATOM   5648  NH2 ARG F 379      31.886 -16.587 -58.042  1.00 43.85        N
ANISOU 5648  NH2 ARG F 379     6090   7596   2976    779    346  -2448    N
ATOM   5649  C   ARG F 379      36.840 -12.931 -55.347  1.00 45.52        C
ANISOU 5649  C   ARG F 379     5126   8523   3646   1110    592  -1952    C
ATOM   5650  O   ARG F 379      36.679 -14.029 -54.799  1.00 46.28        O
ANISOU 5650  O   ARG F 379     5352   8383   3849   1302    501  -2041    O
ATOM   5651  N   ARG F 380      37.400 -11.897 -54.717  1.00 44.64        N
ANISOU 5651  N   ARG F 380     4807   8534   3618   1036    579  -1811    N
ATOM   5652  CA  ARG F 380      37.835 -11.998 -53.324  1.00 44.23        C
ANISOU 5652  CA  ARG F 380     4663   8367   3777   1184    430  -1758    C
ATOM   5653  CB  ARG F 380      39.209 -12.663 -53.248  1.00 47.80        C
ANISOU 5653  CB  ARG F 380     4876   8940   4345   1461    483  -1956    C
ATOM   5654  CG  ARG F 380      39.793 -12.813 -51.838  1.00 49.84        C
ANISOU 5654  CG  ARG F 380     5033   9103   4802   1655    286  -1915    C
ATOM   5655  CD  ARG F 380      41.062 -13.651 -51.917  1.00 56.80        C
ANISOU 5655  CD  ARG F 380     5680  10096   5807   1991    313  -2147    C
ATOM   5656  NE  ARG F 380      42.171 -13.087 -51.147  1.00 61.43        N
ANISOU 5656  NE  ARG F 380     5917  10875   6548   2062    223  -2147    N
ATOM   5657  CZ  ARG F 380      43.388 -12.828 -51.635  1.00 64.11        C
ANISOU 5657  CZ  ARG F 380     5845  11552   6964   2111    368  -2317    C
ATOM   5658  NH1 ARG F 380      43.677 -13.067 -52.908  1.00 65.91        N
ANISOU 5658  NH1 ARG F 380     5980  11960   7104   2099   -2496    N
ATOM   5659  NH2 ARG F 380      44.326 -12.326 -50.842  1.00 65.00        N
ANISOU 5659  NH2 ARG F 380     5629  11835   7234   2157    247  -2324    N
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Figure 18 (continued)

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ATOM   5660  C   ARG F 380      37.852 -10.660 -52.621  1.00 41.88           C
ANISOU 5660  C   ARG F 380    4256   8133   3523    993    370  -1553          C
ATOM   5661  O   ARG F 380      38.517  -9.734 -53.075  1.00 42.95           O
ANISOU 5661  O   ARG F 380    4196   8508   3614    848    494  -1530          O
ATOM   5662  N   LEU F 381      37.099 -10.574 -51.519  1.00 39.44           N
ANISOU 5662  N   LEU F 381    4100   7595   3292    975    200  -1415          N
ATOM   5663  CA  LEU F 381      37.138  -9.447 -50.574  1.00 37.48           C
ANISOU 5663  CA  LEU F 381    3781   7350   3109    840    116  -1247          C
ATOM   5664  CB  LEU F 381      35.919  -9.479 -49.643  1.00 35.32           C
ANISOU 5664  CB  LEU F 381    3754   6800   2866    791    -16  -1118          C
ATOM   5665  CG  LEU F 381      35.557  -8.300 -48.733  1.00 33.09           C
ANISOU 5665  CG  LEU F 381    3486   6465   2620    628    -85   -947          C
ATOM   5666  CD1 LEU F 381      34.028  -8.185 -48.630  1.00 28.32           C
ANISOU 5666  CD1 LEU F 381    3096   5671   1992    513   -108   -858          C
ATOM   5667  CD2 LEU F 381      36.185  -8.462 -47.322  1.00 32.20           C
ANISOU 5667  CD2 LEU F 381    3358   6270   2605    750   -225   -936          C
ATOM   5668  C   LEU F 381      38.412  -9.549 -49.763  1.00 38.85           C
ANISOU 5668  C   LEU F 381    3730   7616   3415   1002     44  -1313          C
ATOM   5669  O   LEU F 381      38.661 -10.569 -49.124  1.00 39.13           O
ANISOU 5669  O   LEU F 381    3822   7515   3530   1250    -72  -1389          O
ATOM   5670  N   VAL F 382      39.229  -8.500 -49.829  1.00 39.49           N
ANISOU 5670  N   VAL F 382    3562   7926   3518    858    106  -1289          N
ATOM   5671  CA  VAL F 382      40.512  -8.475 -49.144  1.00 41.58           C
ANISOU 5671  CA  VAL F 382    3538   8340   3920    980     28  -1378          C
ATOM   5672  CB  VAL F 382      41.603  -7.708 -49.966  1.00 43.41           C
ANISOU 5672  CB  VAL F 382    3420   8920   4155    821    228  -1467          C
ATOM   5673  CG1 VAL F 382      42.891  -7.551 -49.173  1.00 44.97           C
ANISOU 5673  CG1 VAL F 382    3263   9301   4525    909    121  -1569          C
ATOM   5674  CG2 VAL F 382      41.887  -8.422 -51.295  1.00 45.12           C
ANISOU 5674  CG2 VAL F 382    3569   9282   4293    909    448  -1638          C
ATOM   5675  C   VAL F 382      40.312  -7.883 -47.743  1.00 40.72           C
ANISOU 5675  C   VAL F 382    3510   8092   3870    921   -175  -1239          C
ATOM   5676  O   VAL F 382      40.756  -8.472 -46.752  1.00 41.67           O
ANISOU 5676  O   VAL F 382    3618   8139   4075   1138   -368  -1279          O
ATOM   5677  N   GLN F 383      39.620  -6.740 -47.677  1.00 39.32           N
ANISOU 5677  N   GLN F 383    3446   7862   3630    645   -138  -1080          N
ATOM   5678  CA  GLN F 383      39.373  -6.002 -46.438  1.00 38.54           C
ANISOU 5678  CA  GLN F 383    3444   7637   3564    546   -287   -961          C
ATOM   5679  CB  GLN F 383      40.628  -5.223 -46.012  1.00 40.51           C
ANISOU 5679  CB  GLN F 383    3390   8104   3898    455   -334  -1014          C
ATOM   5680  CG  GLN F 383      40.645  -4.744 -44.547  1.00 40.45           C
ANISOU 5680  CG  GLN F 383    3469   7978   3921    423   -545   -949          C
ATOM   5681  CD  GLN F 383      41.875  -3.885 -44.209  1.00 43.46           C
ANISOU 5681  CD  GLN F 383    3531   8595   4388    279   -598  -1023          C
ATOM   5682  OE1 GLN F 383      42.401  -3.158 -45.063  1.00 47.32           O
ANISOU 5682  OE1 GLN F 383    3803   9284   4893     65   -416  -1057          O
ATOM   5683  NE2 GLN F 383      42.331  -3.969 -42.958  1.00 43.22           N
ANISOU 5683  NE2 GLN F 383    3486   8538   4398    376   -848  -1052          N
ATOM   5684  C   GLN F 383      38.227  -5.022 -46.652  1.00 36.57           C
ANISOU 5684  C   GLN F 383    3400   7259   3236    306   -212   -801          C
ATOM   5685  O   GLN F 383      38.119  -4.405 -47.720  1.00 37.21           O
ANISOU 5685  O   GLN F 383    3447   7443   3248    144    -58   -768          O
ATOM   5686  N   LEU F 384      37.369  -4.907 -45.642  1.00 34.97           N
ANISOU 5686  N   LEU F 384    3425   6828   3036    299   -318   -709          N
ATOM   5687  CA  LEU F 384      36.306  -3.912 -45.594  1.00 33.66           C
ANISOU 5687  CA  LEU F 384    3428   6527   2834    111   -275   -576          C
ATOM   5688  CB  LEU F 384      34.924  -4.535 -45.873  1.00 31.81           C
ANISOU 5688  CB  LEU F 384    3403   6118   2566    163   -248   -546          C
ATOM   5689  CG  LEU F 384      33.659  -3.661 -45.748  1.00 30.14           C
ANISOU 5689  CG  LEU F 384    3344   5757   2352     32   -224   -435          C
ATOM   5690  CD1 LEU F 384      33.439  -2.719 -46.929  1.00 25.61           C
ANISOU 5690  CD1 LEU F 384    2737   5271   1724   -100   -144   -364          C
ATOM   5691  CD2 LEU F 384      32.413  -4.513 -45.509  1.00 29.87           C
ANISOU 5691  CD2 LEU F 384    3472   5546   2330    101   -229   -452          C
ATOM   5692  C   LEU F 384      36.364  -3.301 -44.207  1.00 33.92           C
ANISOU 5692  C   LEU F 384    3539   6450   2901     56   -390   -531          C
ATOM   5693  O   LEU F 384      36.411  -4.017 -43.192  1.00 34.45           O
ANISOU 5693  O   LEU F 384    3703   6414   2973    195   -514   -559          O
ATOM   5694  N   ILE F 385      36.419  -1.976 -44.173  1.00 34.62           N
ANISOU 5694  N   ILE F 385    3612   6550   2992   -150   -352   -464          N
ATOM   5695  CA  ILE F 385      36.450  -1.228 -42.930  1.00 35.04           C
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Figure 18 (continued)

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ANISOU 5695  CA  ILE F 385     3759   6494   3061   -238   -445   -436      C
ATOM   5696  CB  ILE F 385      37.718  -0.361 -42.822  1.00 36.95           C
ANISOU 5696  CB  ILE F 385     3794   6908   3338   -401   -473   -480      C
ATOM   5697  CG1 ILE F 385      38.985  -1.211 -43.001  1.00 38.55           C
ANISOU 5697  CG1 ILE F 385     3710   7352   3587   -268   -538   -611      C
ATOM   5698  CD1 ILE F 385      40.287  -0.384 -43.171  1.00 41.49           C
ANISOU 5698  CD1 ILE F 385     3783   7960   4019   -466   -520   -687      C
ATOM   5699  CG2 ILE F 385      37.746   0.385 -41.474  1.00 37.52           C
ANISOU 5699  CG2 ILE F 385     3994   6855   3407   -499   -592   -475      C
ATOM   5700  C   ILE F 385      35.213  -0.350 -42.996  1.00 34.38           C
ANISOU 5700  C   ILE F 385     3874   6223   2965   -350   -364   -332      C
ATOM   5701  O   ILE F 385      35.148   0.522 -43.864  1.00 35.97           O
ANISOU 5701  O   ILE F 385     4050   6456   3159   -485   -273   -270      O
ATOM   5702  N   VAL F 386      34.230  -0.603 -42.119  1.00 32.76           N
ANISOU 5702  N   VAL F 386     3871   5822   2755   -286   -389   -317      N
ATOM   5703  CA  VAL F 386      32.929   0.098 -42.139  1.00 31.18           C
ANISOU 5703  CA  VAL F 386     3822   5448   2576   -341   -310   -251      C
ATOM   5704  CB  VAL F 386      31.707  -0.895 -42.196  1.00 30.22           C
ANISOU 5704  CB  VAL F 386     3791   5226   2465   -223   -267   -266      C
ATOM   5705  CG1 VAL F 386      30.411  -0.170 -42.554  1.00 28.82           C
ANISOU 5705  CG1 VAL F 386     3669   4938   2344   -255   -195   -220      C
ATOM   5706  CG2 VAL F 386      31.928  -2.001 -43.194  1.00 31.56           C
ANISOU 5706  CG2 VAL F 386     3858   5519   2615   -125   -265   -303      C
ATOM   5707  C   VAL F 386      32.736   1.020 -40.921  1.00 31.34           C
ANISOU 5707  C   VAL F 386     3995   5314   2601   -430   -328   -248      C
ATOM   5708  O   VAL F 386      33.123   0.664 -39.792  1.00 31.29           O
ANISOU 5708  O   VAL F 386     4065   5275   2548   -406   -407   -298      O
ATOM   5709  N   SER F 387      32.167   2.205 -41.181  1.00 30.66           N
ANISOU 5709  N   SER F 387     3973   5122   2554   -523   -264   -192      N
ATOM   5710  CA  SER F 387      31.593   3.089 -40.168  1.00 30.93           C
ANISOU 5710  CA  SER F 387     4185   4961   2606   -577   -238   -204      C
ATOM   5711  CB  SER F 387      32.314   4.437 -40.147  1.00 32.15           C
ANISOU 5711  CB  SER F 387     4367   5081   2766   -752   -252   -182      C
ATOM   5712  OG  SER F 387      33.719   4.299 -40.027  1.00 33.45           O
ANISOU 5712  OG  SER F 387     4399   5419   2892   -849   -338   -224      O
ATOM   5713  C   SER F 387      30.123   3.319 -40.541  1.00 30.20           C
ANISOU 5713  C   SER F 387     4150   4737   2589   -496   -148   -176      C
ATOM   5714  O   SER F 387      29.797   3.411 -41.720  1.00 30.80           O
ANISOU 5714  O   SER F 387     4146   4862   2693   -463   -140   -113      O
ATOM   5715  N   GLY F 388      29.239   3.409 -39.556  1.00 29.35           N
ANISOU 5715  N   GLY F 388     4170   4476   2507   -463    -82   -233      N
ATOM   5716  CA  GLY F 388      27.829   3.707 -39.816  1.00 28.50           C
ANISOU 5716  CA  GLY F 388     4063   4258   2506   -376       4   -240      C
ATOM   5717  C   GLY F 388      27.081   4.361 -38.647  1.00 28.60           C
ANISOU 5717  C   GLY F 388     4224   4084   2558   -377     109   -322      C
ATOM   5718  O   GLY F 388      27.550   4.343 -37.526  1.00 27.72           O
ANISOU 5718  O   GLY F 388     4253   3926   2354   -450     122   -378      O
ATOM   5719  N   LYS F 389      25.894   4.911 -38.914  1.00 28.96           N
ANISOU 5719  N   LYS F 389     4235   4030   2737   -281     179   -343      N
ATOM   5720  CA  LYS F 389      25.150   5.640 -37.881  1.00 30.12           C
ANISOU 5720  CA  LYS F 389     4504   3998   2943   -260     308   -446      C
ATOM   5721  CB  LYS F 389      24.270   6.732 -38.500  1.00 31.54           C
ANISOU 5721  CB  LYS F 389     4640   4054   3289   -128     310   -434      C
ATOM   5722  CG  LYS F 389      25.065   7.735 -39.311  1.00 31.37           C
ANISOU 5722  CG  LYS F 389     4699   3977   3246   -167     180   -301      C
ATOM   5723  CD  LYS F 389      24.164   8.721 -39.993  1.00 32.90           C
ANISOU 5723  CD  LYS F 389     4890   4023   3587       1     146   -263      C
ATOM   5724  CE  LYS F 389      24.971   9.802 -40.644  1.00 33.28           C
ANISOU 5724  CE  LYS F 389     5107   3953   3584     -75      49   -123      C
ATOM   5725  NZ  LYS F 389      24.087  10.800 -41.284  1.00 36.05           N
ANISOU 5725  NZ  LYS F 389     5517   4114   4065     121     -12     -67      N
ATOM   5726  C   LYS F 389      24.345   4.720 -36.971  1.00 30.25           C
ANISOU 5726  C   LYS F 389     4529   4017   2950   -255     466   -565      C
ATOM   5727  O   LYS F 389      23.902   5.131 -35.891  1.00 31.37           O
ANISOU 5727  O   LYS F 389     4806   4031   3083   -274     611   -673      O
ATOM   5728  N   ASP F 390      24.204   3.466 -37.393  1.00 29.12           N
ANISOU 5728  N   ASP F 390     4269   4006   2789   -251     455   -550      N
ATOM   5729  CA  ASP F 390      23.576   2.440 -36.575  1.00 29.97           C
ANISOU 5729  CA  ASP F 390     4424   4105   2858   -296     612   -643      C
ATOM   5730  CB  ASP F 390      22.041   2.586 -36.553  1.00 30.71           C
ANISOU 5730  CB  ASP F 390     4366   4164   3137   -237    789   -763      C
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Figure 18 (continued)

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ATOM   5731  CG  ASP F 390      21.410   2.597 -37.954  1.00 30.11           C
ANISOU 5731  CG  ASP F 390    4012   4192   3236   -122    680   -736       C
ATOM   5732  OD1 ASP F 390      21.906   1.900 -38.876  1.00 31.34           O
ANISOU 5732  OD1 ASP F 390    4099   4466   3341   -128    537   -651       O
ATOM   5733  OD2 ASP F 390      20.396   3.303 -38.134  1.00 27.66           O
ANISOU 5733  OD2 ASP F 390    3554   3847   3110    -10    729   -811       O
ATOM   5734  C   ASP F 390      23.993   1.035 -37.017  1.00 29.58           C
ANISOU 5734  C   ASP F 390    4340   4171   2729   -323    541   -594       C
ATOM   5735  O   ASP F 390      24.751   0.863 -37.972  1.00 28.60           O
ANISOU 5735  O   ASP F 390    4127   4153   2588   -291    379   -507       O
ATOM   5736  N   GLU F 391      23.482   0.046 -36.293  1.00 30.84           N
ANISOU 5736  N   GLU F 391    4594   4290   2833   -389    685   -659       N
ATOM   5737  CA  GLU F 391      23.729  -1.385 -36.518  1.00 30.78           C
ANISOU 5737  CA  GLU F 391    4622   4325   2747   -417    652   -631       C
ATOM   5738  CB  GLU F 391      22.983  -2.177 -35.421  1.00 31.99           C
ANISOU 5738  CB  GLU F 391    4962   4364   2827   -533    875   -709       C
ATOM   5739  CG  GLU F 391      23.324  -3.638 -35.334  1.00 31.45           C
ANISOU 5739  CG  GLU F 391    5056   4259   2634   -576    853   -670       C
ATOM   5740  CD  GLU F 391      22.692  -4.319 -34.139  1.00 33.38           C
ANISOU 5740  CD  GLU F 391    5573   4355   2756   -724   1088   -721       C
ATOM   5741  OE1 GLU F 391      23.273  -5.342 -33.707  1.00 33.05           O
ANISOU 5741  OE1 GLU F 391    5804   4219   2535   -744   1036   -654       O
ATOM   5742  OE2 GLU F 391      21.639  -3.850 -33.633  1.00 30.81           O
ANISOU 5742  OE2 GLU F 391    5202   3997   2506   -814   1329   -829       O
ATOM   5743  C   GLU F 391      23.286  -1.857 -37.909  1.00 30.79           C
ANISOU 5743  C   GLU F 391    4372   4443   2884   -367    585   -630       C
ATOM   5744  O   GLU F 391      24.001  -2.594 -38.588  1.00 30.38           O
ANISOU 5744  O   GLU F 391    4307   4463   2773   -336    456   -576       O
ATOM   5745  N   GLN F 392      22.099  -1.421 -38.324  1.00 32.45           N
ANISOU 5745  N   GLN F 392    4380   4677   3273   -346    666   -706       N
ATOM   5746  CA  GLN F 392      21.515  -1.817 -39.610  1.00 32.48           C
ANISOU 5746  CA  GLN F 392    4144   4800   3398   -304    583   -727       C
ATOM   5747  CB  GLN F 392      20.092  -1.260 -39.718  1.00 34.09           C
ANISOU 5747  CB  GLN F 392    4120   5020   3814   -271    678   -843       C
ATOM   5748  CG  GLN F 392      19.442  -1.344 -41.095  1.00 35.80           C
ANISOU 5748  CG  GLN F 392    4067   5374   4160   -195    528   -866       C
ATOM   5749  CD  GLN F 392      19.152  -2.771 -41.513  1.00 38.28           C
ANISOU 5749  CD  GLN F 392    4332   5752   4461   -309    544   -935       C
ATOM   5750  OE1 GLN F 392      19.360  -3.713 -40.739  1.00 38.79           O
ANISOU 5750  OE1 GLN F 392    4575   5730   4433   -443    686   -960       O
ATOM   5751  NE2 GLN F 392      18.687  -2.945 -42.749  1.00 38.16           N
ANISOU 5751  NE2 GLN F 392    4110   5869   4519   -260    384   -963       N
ATOM   5752  C   GLN F 392      22.369  -1.346 -40.784  1.00 31.31           C
ANISOU 5752  C   GLN F 392    3932   4753   3213   -208    364   -613       C
ATOM   5753  O   GLN F 392      22.674  -2.123 -41.683  1.00 30.61           O
ANISOU 5753  O   GLN F 392    3793   4758   3081   -202    268   -594       O
ATOM   5754  N   SER F 393      22.754  -0.071 -40.752  1.00 31.83           N
ANISOU 5754  N   SER F 393    4026   4785   3285   -152    308   -546       N
ATOM   5755  CA  SER F 393      23.555   0.584 -41.804  1.00 31.84           C
ANISOU 5755  CA  SER F 393    4001   4859   3240    -99    140   -428       C
ATOM   5756  CB  SER F 393      23.778   2.031 -41.404  1.00 32.41           C
ANISOU 5756  CB  SER F 393    4160   4818   3334    -79    137   -379       C
ATOM   5757  OG  SER F 393      22.513   2.621 -41.159  1.00 36.78           O
ANISOU 5757  OG  SER F 393    4636   5288   4050       2    210   -458       O
ATOM   5758  C   SER F 393      24.904  -0.068 -42.095  1.00 31.09           C
ANISOU 5758  C   SER F 393    3969   4851   2992   -139     63   -365       C
ATOM   5759  O   SER F 393      25.370  -0.089 -43.238  1.00 31.67           O
ANISOU 5759  O   SER F 393    3975   5039   3019   -116    -36   -305       O
ATOM   5760  N   ILE F 394      25.531  -0.560 -41.031  1.00 30.78           N
ANISOU 5760  N   ILE F 394    4068   4760   2868   -190    110   -387       N
ATOM   5761  CA  ILE F 394      26.767  -1.307 -41.083  1.00 29.79           C
ANISOU 5761  CA  ILE F 394    3986   4710   2624   -191     33   -359       C
ATOM   5762  CB  ILE F 394      27.351  -1.480 -39.645  1.00 29.65           C
ANISOU 5762  CB  ILE F 394    4156   4598   2511   -226     48   -374       C
ATOM   5763  CG1 ILE F 394      27.823  -0.134 -39.098  1.00 29.52           C
ANISOU 5763  CG1 ILE F 394    4191   4541   2482   -279     24   -348       C
ATOM   5764  CD1 ILE F 394      27.916  -0.060 -37.553  1.00 31.10           C
ANISOU 5764  CD1 ILE F 394    4613   4618   2587   -330     64   -390       C
ATOM   5765  CG2 ILE F 394      28.466  -2.533 -39.621  1.00 29.07           C
ANISOU 5765  CG2 ILE F 394    4119   4590   2336   -174    -54   -367       C
ATOM   5766  C   ILE F 394      26.499  -2.669 -41.731  1.00 29.71           C
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Figure 18 (continued)

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ANISOU 5766  C   ILE F 394     3929   4753   2607   -158     31   -404      C
ATOM   5767  O   ILE F 394      27.278  -3.120 -42.577  1.00 29.55          O
ANISOU 5767  O   ILE F 394     3847   4847   2533   -116    -47   -388      O
ATOM   5768  N   ALA F 395      25.403  -3.316 -41.324  1.00 30.22          N
ANISOU 5768  N   ALA F 395     4027   4730   2726   -194    137   -478      N
ATOM   5769  CA  ALA F 395      25.009  -4.588 -41.908  1.00 30.57          C
ANISOU 5769  CA  ALA F 395     4048   4791   2775   -201    149   -541      C
ATOM   5770  CB  ALA F 395      23.837  -5.225 -41.145  1.00 31.36          C
ANISOU 5770  CB  ALA F 395     4215   4766   2934   -302    310   -630      C
ATOM   5771  C   ALA F 395      24.716  -4.452 -43.403  1.00 30.78          C
ANISOU 5771  C   ALA F 395     3889   4961   2846   -163     60   -548      C
ATOM   5772  O   ALA F 395      25.104  -5.325 -44.164  1.00 31.52          O
ANISOU 5772  O   ALA F 395     3978   5117   2882   -138     10   -576      O
ATOM   5773  N   GLU F 396      24.072  -3.354 -43.821  1.00 31.71          N
ANISOU 5773  N   GLU F 396     3881   5119   3047   -145     31   -523      N
ATOM   5774  CA  GLU F 396      23.861  -3.029 -45.257  1.00 31.94          C
ANISOU 5774  CA  GLU F 396     3780   5281   3073    -95    -93   -498      C
ATOM   5775  CB  GLU F 396      23.037  -1.743 -45.443  1.00 33.01          C
ANISOU 5775  CB  GLU F 396     3825   5402   3315    -41   -139   -461      C
ATOM   5776  CG  GLU F 396      21.538  -1.987 -45.467  1.00 35.48          C
ANISOU 5776  CG  GLU F 396     3973   5718   3789    -35   -123   -581      C
ATOM   5777  CD  GLU F 396      20.680  -0.802 -44.997  1.00 38.57          C
ANISOU 5777  CD  GLU F 396     4281   6037   4338     44   -103   -589      C
ATOM   5778  OE1 GLU F 396      21.223   0.325 -44.807  1.00 39.47          O
ANISOU 5778  OE1 GLU F 396     4500   6075   4423     99   -126   -482      O
ATOM   5779  OE2 GLU F 396      19.447  -1.008 -44.817  1.00 35.64          O
ANISOU 5779  OE2 GLU F 396     3729   5680   4133     47    -55   -721      O
ATOM   5780  C   GLU F 396      25.163  -2.938 -46.052  1.00 31.50          C
ANISOU 5780  C   GLU F 396     3762   5332   2874    -69   -168   -417      C
ATOM   5781  O   GLU F 396      25.290  -3.588 -47.089  1.00 32.61          O
ANISOU 5781  O   GLU F 396     3871   5579   2942    -56   -221   -449      O
ATOM   5782  N   ALA F 397      26.128  -2.156 -45.567  1.00 30.36          N
ANISOU 5782  N   ALA F 397     3680   5169   2688    -79   -159   -334      N
ATOM   5783  CA  ALA F 397      27.425  -2.017 -46.242  1.00 30.05          C
ANISOU 5783  CA  ALA F 397     3636   5250   2530    -86   -193   -277      C
ATOM   5784  CB  ALA F 397      28.335  -0.987 -45.512  1.00 29.70          C
ANISOU 5784  CB  ALA F 397     3637   5170   2479   -140   -180   -206      C
ATOM   5785  C   ALA F 397      28.164  -3.342 -46.421  1.00 29.77          C
ANISOU 5785  C   ALA F 397     3596   5288   2428    -49   -182   -356      C
ATOM   5786  O   ALA F 397      28.768  -3.583 -47.484  1.00 30.19          O
ANISOU 5786  O   ALA F 397     3600   5481   2390    -35   -195   -364      O
ATOM   5787  N   ILE F 398      28.116  -4.184 -45.387  1.00 29.18          N
ANISOU 5787  N   ILE F 398     3597   5103   2385    -28   -151   -416      N
ATOM   5788  CA  ILE F 398      28.785  -5.500 -45.391  1.00 29.82          C
ANISOU 5788  CA  ILE F 398     3721   5193   2418     45   -156   -491      C
ATOM   5789  CB  ILE F 398      28.763  -6.184 -43.978  1.00 30.01          C
ANISOU 5789  CB  ILE F 398     3908   5042   2453     64   -137   -511      C
ATOM   5790  CG1 ILE F 398      29.506  -5.325 -42.937  1.00 28.78          C
ANISOU 5790  CG1 ILE F 398     3784   4871   2279     53   -173   -446      C
ATOM   5791  CD1 ILE F 398      29.361  -5.799 -41.514  1.00 29.65          C
ANISOU 5791  CD1 ILE F 398     4105   4806   2357     54   -162   -447      C
ATOM   5792  CG2 ILE F 398      29.370  -7.571 -44.042  1.00 30.84          C
ANISOU 5792  CG2 ILE F 398     4096   5109   2512    173   -164   -580      C
ATOM   5793  C   ILE F 398      28.199  -6.428 -46.466  1.00 30.35          C
ANISOU 5793  C   ILE F 398     3770   5297   2466     59   -152   -577      C
ATOM   5794  O   ILE F 398      28.943  -7.040 -47.237  1.00 31.40          O
ANISOU 5794  O   ILE F 398     3877   5526   2528    124   -162   -630      O
ATOM   5795  N   ILE F 399      26.868  -6.485 -46.522  1.00 30.23          N
ANISOU 5795  N   ILE F 399     3752   5216   2518     -8   -136   -610      N
ATOM   5796  CA  ILE F 399      26.139  -7.273 -47.508  1.00 30.68          C
ANISOU 5796  CA  ILE F 399     3781   5309   2565    -31   -156   -710      C
ATOM   5797  CB  ILE F 399      24.585  -7.231 -47.249  1.00 31.14          C
ANISOU 5797  CB  ILE F 399     3785   5298   2749   -126   -136   -763      C
ATOM   5798  CG1 ILE F 399      24.226  -7.902 -45.914  1.00 29.45          C
ANISOU 5798  CG1 ILE F 399     3695   4892   2602   -193    -16   -803      C
ATOM   5799  CD1 ILE F 399      22.950  -7.376 -45.272  1.00 29.44          C
ANISOU 5799  CD1 ILE F 399     3606   4839   2739   -287     62   -831      C
ATOM   5800  CG2 ILE F 399      23.800  -7.896 -48.410  1.00 32.52          C
ANISOU 5800  CG2 ILE F 399     3891   5551   2914   -170   -202   -881      C
ATOM   5801  C   ILE F 399      26.479  -6.784 -48.919  1.00 31.25          C
ANISOU 5801  C   ILE F 399     3772   5569   2531    -226   -685      C
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Figure 18 (continued)

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ATOM   5802  O   ILE F 399      26.773  -7.594 -49.799  1.00 32.29           O
ANISOU 5802  O   ILE F 399    3926   5770   2572     20   -235   -772        O
ATOM   5803  N   VAL F 400      26.442  -5.468 -49.127  1.00 31.26           N
ANISOU 5803  N   VAL F 400    3717   5633   2527    -17   -266   -569        N
ATOM   5804  CA  VAL F 400      26.703  -4.862 -50.439  1.00 31.99           C
ANISOU 5804  CA  VAL F 400    3791   5879   2484    -16   -326   -512        C
ATOM   5805  CB  VAL F 400      26.552  -3.321 -50.424  1.00 32.28           C
ANISOU 5805  CB  VAL F 400    3826   5904   2535    -32   -369   -359        C
ATOM   5806  CG1 VAL F 400      27.154  -2.712 -51.702  1.00 31.55           C
ANISOU 5806  CG1 VAL F 400    3785   5949   2253    -57   -395   -270        C
ATOM   5807  CG2 VAL F 400      25.081  -2.906 -50.237  1.00 31.82           C
ANISOU 5807  CG2 VAL F 400    3714   5767   2609     -9   -454   -364        C
ATOM   5808  C   VAL F 400      28.110  -5.188 -50.913  1.00 32.53           C
ANISOU 5808  C   VAL F 400    3873   6063   2424      4   -258   -527        C
ATOM   5809  O   VAL F 400      28.320  -5.462 -52.094  1.00 33.48           O
ANISOU 5809  O   VAL F 400    4010   6312   2399      3   -262   -566        O
ATOM   5810  N   ALA F 401      29.054  -5.149 -49.973  1.00 31.73           N
ANISOU 5810  N   ALA F 401    3756   5926   2375     25   -198   -510        N
ATOM   5811  CA  ALA F 401      30.462  -5.417 -50.239  1.00 32.29           C
ANISOU 5811  CA  ALA F 401    3773   6123   2374     61   -131   -547        C
ATOM   5812  CB  ALA F 401      31.316  -4.940 -49.082  1.00 31.23           C
ANISOU 5812  CB  ALA F 401    3591   5955   2320     61   -122   -500        C
ATOM   5813  C   ALA F 401      30.738  -6.885 -50.529  1.00 32.85           C
ANISOU 5813  C   ALA F 401    3863   6199   2419    165   -106   -703        C
ATOM   5814  O   ALA F 401      31.652  -7.205 -51.280  1.00 34.52           O
ANISOU 5814  O   ALA F 401    4018   6556   2542    209    -41   -775        O
ATOM   5815  N   MSE F 402      29.963  -7.768 -49.913  1.00 32.87           N
ANISOU 5815  N   MSE F 402    3957   6031   2501    198   -138   -765        N
ATOM   5816  CA  MSE F 402      30.121  -9.221 -50.081  1.00 34.29           C
ANISOU 5816  CA  MSE F 402    4216   6142   2669    295   -120   -914        C
ATOM   5817  CB  MSE F 402      29.405 -10.001 -48.955  1.00 33.61           C
ANISOU 5817  CB  MSE F 402    4274   5812   2686    294   -135   -936        C
ATOM   5818  CG  MSE F 402      30.159 -10.004 -47.602  1.00 34.31           C
ANISOU 5818  CG  MSE F 402    4411   5796   2829    379   -152   -874        C
ATOM   5819  SE  MSE F 402      29.225 -10.945 -46.127  0.90 35.69          SE
ANISOU 5819  SE  MSE F 402    4858   5634   3068    337   -136   -872        SE
ATOM   5820  CE  MSE F 402      30.613 -10.934 -44.782  1.00 35.68           C
ANISOU 5820  CE  MSE F 402    4931   5574   3050    510   -223   -797        C
ATOM   5821  C   MSE F 402      29.589  -9.629 -51.439  1.00 34.50           C
ANISOU 5821  C   MSE F 402    4268   6255   2587    255   -119  -1011        C
ATOM   5822  O   MSE F 402      30.190 -10.441 -52.110  1.00 36.42           O
ANISOU 5822  O   MSE F 402    4535   6549   2753    337    -73  -1137        O
ATOM   5823  N   VAL F 403      28.465  -9.043 -51.840  1.00 34.25           N
ANISOU 5823  N   VAL F 403    4226   6243   2545    142   -183   -962        N
ATOM   5824  CA  VAL F 403      27.919  -9.227 -53.188  1.00 34.82           C
ANISOU 5824  CA  VAL F 403    4323   6427   2480     94   -232  -1038        C
ATOM   5825  CB  VAL F 403      26.495  -8.620 -53.318  1.00 34.53           C
ANISOU 5825  CB  VAL F 403    4248   6380   2494      0   -356   -989        C
ATOM   5826  CG1 VAL F 403      25.966  -8.754 -54.767  1.00 35.80           C
ANISOU 5826  CG1 VAL F 403    4442   6680   2479    -40   -460  -1064        C
ATOM   5827  CG2 VAL F 403      25.531  -9.291 -52.314  1.00 33.68           C
ANISOU 5827  CG2 VAL F 403    4139   6086   2573    -50   -354  -1061        C
ATOM   5828  C   VAL F 403      28.878  -8.653 -54.249  1.00 35.95           C
ANISOU 5828  C   VAL F 403    4446   6779   2433    106   -179  -1003        C
ATOM   5829  O   VAL F 403      29.190  -9.332 -55.244  1.00 37.21           O
ANISOU 5829  O   VAL F 403    4664   7031   2443    127   -138  -1133        O
ATOM   5830  N   PHE F 404      29.347  -7.420 -54.010  1.00 34.96           N
ANISOU 5830  N   PHE F 404    4259   6715   2308     72   -159   -839        N
ATOM   5831  CA  PHE F 404      30.282  -6.688 -54.895  1.00 36.53           C
ANISOU 5831  CA  PHE F 404    4449   7101   2332     28   -72   -777        C
ATOM   5832  CB  PHE F 404      30.606  -5.293 -54.309  1.00 35.90           C
ANISOU 5832  CB  PHE F 404    4324   7008   2310    -45    -63   -589        C
ATOM   5833  CG  PHE F 404      31.373  -4.375 -55.245  1.00 37.51           C
ANISOU 5833  CG  PHE F 404    4558   7371   2322   -153     35   -495        C
ATOM   5834  CD1 PHE F 404      30.713  -3.660 -56.254  1.00 38.35           C
ANISOU 5834  CD1 PHE F 404    4819   7508   2243   -225    -40   -382        C
ATOM   5835  CE1 PHE F 404      31.414  -2.801 -57.112  1.00 37.22           C
ANISOU 5835  CE1 PHE F 404    4768   7483   1890   -354     72   -274        C
ATOM   5836  CZ  PHE F 404      32.771  -2.645 -56.966  1.00 39.43           C
ANISOU 5836  CZ  PHE F 404    4931   7877   2174   -433    279   -303        C
ATOM   5837  CE2 PHE F 404      33.452  -3.342 -55.961  1.00 39.28           C
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Figure 18 (continued)

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ANISOU 5837  CE2 PHE F 404     4699   7858   2368   -343    332   -436      C
ATOM   5838  CD2 PHE F 404      32.747  -4.197 -55.097  1.00 38.17          C
ANISOU 5838  CD2 PHE F 404     4522   7571   2408   -192    198   -517      C
ATOM   5839  C   PHE F 404      31.571  -7.463 -55.140  1.00 37.46          C
ANISOU 5839  C   PHE F 404     4505   7327   2403    103     81   -918      C
ATOM   5840  O   PHE F 404      32.134  -7.391 -56.225  1.00 39.22          O
ANISOU 5840  O   PHE F 404     4747   7721   2433     66    186   -960      O
ATOM   5841  N   SER F 405      32.025  -8.203 -54.131  1.00 37.05          N
ANISOU 5841  N   SER F 405     4389   7171   2517    221     94   -995      N
ATOM   5842  CA  SER F 405      33.281  -8.958 -54.222  1.00 39.28          C
ANISOU 5842  CA  SER F 405     4576   7544   2804    352    212  -1143      C
ATOM   5843  CB  SER F 405      33.727  -9.455 -52.845  1.00 38.82          C
ANISOU 5843  CB  SER F 405     4463   7343   2945    492    158  -1160      C
ATOM   5844  OG  SER F 405      33.038 -10.651 -52.515  1.00 40.42          O
ANISOU 5844  OG  SER F 405     4824   7332   3201    585     93  -1254      O
ATOM   5845  C   SER F 405      33.166 -10.136 -55.180  1.00 40.69          C
ANISOU 5845  C   SER F 405     4856   7736   2869    429    260  -1340      C
ATOM   5846  O   SER F 405      34.178 -10.658 -55.653  1.00 42.13          O
ANISOU 5846  O   SER F 405     4962   8038   3005    534    391  -1487      O
ATOM   5847  N   GLN F 406      31.920 -10.534 -55.450  1.00 40.68          N
ANISOU 5847  N   GLN F 406     5011   7615   2832    371    155  -1361      N
ATOM   5848  CA  GLN F 406      31.572 -11.630 -56.381  1.00 42.61          C
ANISOU 5848  CA  GLN F 406     5392   7843   2954    399    169  -1558      C
ATOM   5849  CB  GLN F 406      31.955 -11.281 -57.824  1.00 44.04          C
ANISOU 5849  CB  GLN F 406     5602   8265   2868    332    270  -1606      C
ATOM   5850  CG  GLN F 406      31.191 -10.103 -58.371  1.00 43.15          C
ANISOU 5850  CG  GLN F 406     5540   8242   2614    163    170  -1425      C
ATOM   5851  CD  GLN F 406      31.738  -9.591 -59.677  1.00 44.42          C
ANISOU 5851  CD  GLN F 406     5768   8633   2476     81    291  -1422      C
ATOM   5852  OE1 GLN F 406      32.951  -9.500 -59.865  1.00 43.92          O
ANISOU 5852  OE1 GLN F 406     5611   8710   2369    105    499  -1468      O
ATOM   5853  NE2 GLN F 406      30.838  -9.241 -60.593  1.00 45.45          N
ANISOU 5853  NE2 GLN F 406     6064   8814   2393    -23    159  -1372      N
ATOM   5854  C   GLN F 406      32.173 -12.968 -55.971  1.00 43.95          C
ANISOU 5854  C   GLN F 406     5600   7871   3227    589    226  -1742      C
ATOM   5855  O   GLN F 406      32.433 -13.808 -56.819  1.00 46.15          O
ANISOU 5855  O   GLN F 406     5963   8178   3395    657    304  -1937      O
ATOM   5856  N   GLU F 407      32.373 -13.145 -54.666  1.00 43.66          N
ANISOU 5856  N   GLU F 407     5534   7667   3389    684    177  -1678      N
ATOM   5857  CA  GLU F 407      32.972 -14.356 -54.087  1.00 45.89          C
ANISOU 5857  CA  GLU F 407     5886   7768   3781    902    190  -1811      C
ATOM   5858  CB  GLU F 407      33.245 -14.162 -52.597  1.00 44.16          C
ANISOU 5858  CB  GLU F 407     5633   7413   3733    980    106  -1674      C
ATOM   5859  CG  GLU F 407      34.489 -13.382 -52.270  1.00 44.97          C
ANISOU 5859  CG  GLU F 407     5487   7716   3881   1066    133  -1614      C
ATOM   5860  CD  GLU F 407      35.177 -13.876 -51.008  1.00 45.76          C
ANISOU 5860  CD  GLU F 407     5591   7667   4127   1279     35  -1602      C
ATOM   5861  OE1 GLU F 407      34.788 -14.945 -50.485  1.00 46.21          O
ANISOU 5861  OE1 GLU F 407     5887   7443   4229   1387    -30  -1645      O
ATOM   5862  OE2 GLU F 407      36.126 -13.199 -50.553  1.00 46.06          O
ANISOU 5862  OE2 GLU F 407     5409   7866   4226   1332     14  -1552      O
ATOM   5863  C   GLU F 407      32.093 -15.581 -54.248  1.00 47.47          C
ANISOU 5863  C   GLU F 407     6337   7722   3977    890    155  -1951      C
ATOM   5864  O   GLU F 407      30.874 -15.486 -54.144  1.00 46.49          O
ANISOU 5864  O   GLU F 407     6303   7502   3860    703     80  -1898      O
ATOM   5865  N   ASP F 408      32.713 -16.737 -54.463  1.00 51.07          N
ANISOU 5865  N   ASP F 408     6898   8065   4441   1090    210  -2142      N
ATOM   5866  CA  ASP F 408      31.942 -17.949 -54.697  1.00 53.71          C
ANISOU 5866  CA  ASP F 408     7506   8138   4762   1059    193  -2300      C
ATOM   5867  CB  ASP F 408      32.753 -19.039 -55.396  1.00 56.74          C
ANISOU 5867  CB  ASP F 408     7989   8471   5099   1286    290  -2553      C
ATOM   5868  CG  ASP F 408      31.879 -19.947 -56.264  1.00 60.34          C
ANISOU 5868  CG  ASP F 408     8697   8784   5445   1155    300  -2755      C
ATOM   5869  OD1 ASP F 408      31.500 -19.542 -57.393  1.00 61.41          O
ANISOU 5869  OD1 ASP F 408     8794   9144   5396    993    324  -2821      O
ATOM   5870  OD2 ASP F 408      31.573 -21.074 -55.817  1.00 63.81          O
ANISOU 5870  OD2 ASP F 408     9399   8875   5969   1205    273  -2849      O
ATOM   5871  C   ASP F 408      31.241 -18.477 -53.441  1.00 53.40          C
ANISOU 5871  C   ASP F 408     7660   7761   4869   1016    107  -2210      C
ATOM   5872  O   ASP F 408      30.214 -19.139 -53.548  1.00 54.39          O
ANISOU 5872  O   ASP F 408     7984   7691   4992    852     89  -2287      O
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Figure 18 (continued)

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ATOM   5873  N   ACYS F 409      31.777 -18.185 -52.260  0.50 52.75           N
ANISOU 5873  N   ACYS F 409    7531   7613   4899   1137     60  -2057          N
ATOM   5874  N   BCYS F 409      31.777 -18.185 -52.260  0.50 52.75           N
ANISOU 5874  N   BCYS F 409    7531   7613   4899   1137     60  -2057          N
ATOM   5875  CA  ACYS F 409      31.089 -18.592 -51.034  0.50 52.65           C
ANISOU 5875  CA  ACYS F 409    7738   7288   4981   1065      2  -1951          C
ATOM   5876  CA  BCYS F 409      31.089 -18.592 -51.034  0.50 52.65           C
ANISOU 5876  CA  BCYS F 409    7738   7288   4981   1065      2  -1951          C
ATOM   5877  CB  ACYS F 409      32.047 -18.636 -49.835  0.50 52.96           C
ANISOU 5877  CB  ACYS F 409    7800   7221   5099   1305    -69  -1839          C
ATOM   5878  CB  BCYS F 409      32.047 -18.636 -49.835  0.50 52.96           C
ANISOU 5878  CB  BCYS F 409    7800   7221   5099   1305    -69  -1839          C
ATOM   5879  SG  ACYS F 409      32.091 -17.163 -48.811  0.50 52.55           S
ANISOU 5879  SG  ACYS F 409    7540   7342   5085   1205   -130  -1593          S
ATOM   5880  SG  BCYS F 409      32.091 -17.163 -48.811  0.50 52.55           S
ANISOU 5880  SG  BCYS F 409    7540   7342   5085   1205   -130  -1593          S
ATOM   5881  C   ACYS F 409      29.827 -17.739 -50.774  0.50 50.12           C
ANISOU 5881  C   ACYS F 409    7348   7022   4672    755    -13  -1821          C
ATOM   5882  C   BCYS F 409      29.827 -17.739 -50.774  0.50 50.12           C
ANISOU 5882  C   BCYS F 409    7348   7022   4672    755    -13  -1821          C
ATOM   5883  O   ACYS F 409      28.886 -18.205 -50.136  0.50 50.44           O
ANISOU 5883  O   ACYS F 409    7577   6823   4766    597     -7  -1802          O
ATOM   5884  O   BCYS F 409      28.886 -18.205 -50.136  0.50 50.44           O
ANISOU 5884  O   BCYS F 409    7577   6823   4766    597     -7  -1802          O
ATOM   5885  N    MSE F 410      29.811 -16.507 -51.289  1.00 48.14           N
ANISOU 5885  N    MSE F 410    6837   7079   4377    671    -19  -1743          N
ATOM   5886  CA   MSE F 410      28.586 -15.667 -51.329  1.00 46.32           C
ANISOU 5886  CA   MSE F 410    6511   6930   4158    419    -48  -1656          C
ATOM   5887  CB   MSE F 410      28.941 -14.221 -51.724  1.00 44.79           C
ANISOU 5887  CB   MSE F 410    6071   7035   3913    406    -68  -1529          C
ATOM   5888  CG   MSE F 410      27.762 -13.229 -51.931  1.00 42.99           C
ANISOU 5888  CG   MSE F 410    5730   6910   3694    209   -126  -1442          C
ATOM   5889 SE    MSE F 410      26.955 -13.098 -53.730  0.90 42.31          SE
ANISOU 5889 SE    MSE F 410    5600   7035   3439     86   -204  -1557          SE
ATOM   5890  CE   MSE F 410      28.542 -12.628 -54.751  1.00 41.76           C
ANISOU 5890  CE   MSE F 410    5476   7222   3170    230   -121  -1549          C
ATOM   5891  C    MSE F 410      27.565 -16.259 -52.323  1.00 47.69           C
ANISOU 5891  C    MSE F 410    6753   7090   4276    253    -60  -1820          C
ATOM   5892  O    MSE F 410      26.393 -16.467 -51.992  1.00 47.49           O
ANISOU 5892  O    MSE F 410    6775   6944   4327     57    -75  -1837          O
ATOM   5893  N   ILE F 411      28.020 -16.533 -53.544  1.00 48.99           N
ANISOU 5893  N   ILE F 411    6915   7393   4304    318    -48  -1959          N
ATOM   5894  CA  ILE F 411      27.176 -17.189 -54.556  1.00 50.31           C
ANISOU 5894  CA  ILE F 411    7177   7552   4386    171    -80  -2148          C
ATOM   5895  CB  ILE F 411      27.852 -17.190 -55.945  1.00 51.34           C
ANISOU 5895  CB  ILE F 411    7295   7903   4310    257    -53  -2275          C
ATOM   5896  CG1 ILE F 411      27.605 -15.837 -56.612  1.00 50.21           C
ANISOU 5896  CG1 ILE F 411    6965   8064   4047    166   -123  -2142          C
ATOM   5897  CD1 ILE F 411      28.722 -15.359 -57.495  1.00 52.42           C
ANISOU 5897  CD1 ILE F 411    7190   8586   4140    279    -32  -2145          C
ATOM   5898  CG2 ILE F 411      27.314 -18.312 -56.826  1.00 53.79           C
ANISOU 5898  CG2 ILE F 411    7799   8112   4525    167    -66  -2531          C
ATOM   5899  C   ILE F 411      26.671 -18.575 -54.108  1.00 51.93           C
ANISOU 5899  C   ILE F 411    7639   7413   4677    105    -50  -2292          C
ATOM   5900  O   ILE F 411      25.517 -18.904 -54.355  1.00 53.42           O
ANISOU 5900  O   ILE F 411    7863   7547   4889   -126    -93  -2390          O
ATOM   5901  N   LYS F 412      27.502 -19.356 -53.416  1.00 52.22           N
ANISOU 5901  N   LYS F 412    7857   7215   4771    298     14  -2301          N
ATOM   5902  CA  LYS F 412      27.074 -20.655 -52.866  1.00 53.75           C
ANISOU 5902  CA  LYS F 412    8365   7019   5038    237     51  -2401          C
ATOM   5903  CB  LYS F 412      28.288 -21.518 -52.480  1.00 55.14           C
ANISOU 5903  CB  LYS F 412    8752   6970   5227    556     88  -2438          C
ATOM   5904  CG  LYS F 412      29.038 -22.152 -53.648  1.00 57.75           C
ANISOU 5904  CG  LYS F 412    9134   7352   5454    744    126  -2667          C
ATOM   5905  CD  LYS F 412      28.231 -23.272 -54.325  1.00 61.07           C
ANISOU 5905  CD  LYS F 412    9825   7547   5831    564    149  -2906          C
ATOM   5906  CE  LYS F 412      28.940 -23.834 -55.572  1.00 63.36           C
ANISOU 5906  CE  LYS F 412   10174   7912   5988    740    204  -3162          C
ATOM   5907  NZ  LYS F 412      28.944 -22.908 -56.735  1.00 61.64           N
ANISOU 5907  NZ  LYS F 412    9691   8127   5602    663    198  -3197          N
ATOM   5908  C   LYS F 412      26.100 -20.546 -51.670  1.00 52.80           C
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Figure 18 (continued)

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ANISOU 5908  C   LYS F 412     8297   6719   5046     18     66  -2268   C
ATOM   5909  O   LYS F 412      25.481 -21.540 -51.279  1.00 54.85        O
ANISOU 5909  O   LYS F 412     8819   6665   5356   -135    119  -2349   O
ATOM   5910  N   ALA F 413      25.965 -19.345 -51.104  1.00 50.11        N
ANISOU 5910  N   ALA F 413     7723   6567   4749    -13     43  -2077   N
ATOM   5911  CA  ALA F 413      25.099 -19.097 -49.933  1.00 48.96        C
ANISOU 5911  CA  ALA F 413     7598   6290   4712   -206     90  -1956   C
ATOM   5912  CB  ALA F 413      25.724 -18.033 -49.014  1.00 46.53        C
ANISOU 5912  CB  ALA F 413     7166   6089   4424    -67     75  -1735   C
ATOM   5913  C   ALA F 413      23.642 -18.733 -50.269  1.00 48.81        C
ANISOU 5913  C   ALA F 413     7393   6390   4762   -515     84  -2024   C
ATOM   5914  O   ALA F 413      22.815 -18.557 -49.364  1.00 48.53        O
ANISOU 5914  O   ALA F 413     7342   6265   4831   -700    159  -1964   O
ATOM   5915  N   VAL F 414      23.341 -18.612 -51.562  1.00 49.08        N
ANISOU 5915  N   VAL F 414     7279   6637   4730   -561     -7  -2158   N
ATOM   5916  CA  VAL F 414      21.970 -18.436 -52.037  1.00 49.54        C
ANISOU 5916  CA  VAL F 414     7153   6817   4854   -830    -65  -2269   C
ATOM   5917  CB  VAL F 414      21.929 -18.102 -53.563  1.00 50.27        C
ANISOU 5917  CB  VAL F 414     7101   7196   4804   -801   -222  -2378   C
ATOM   5918  CG1 VAL F 414      20.491 -17.927 -54.072  1.00 49.09        C
ANISOU 5918  CG1 VAL F 414     6737   7190   4726  -1054   -341  -2505   C
ATOM   5919  CG2 VAL F 414      22.757 -16.861 -53.860  1.00 47.46        C
ANISOU 5919  CG2 VAL F 414     6588   7096   4350   -582   -280  -2198   C
ATOM   5920  C   VAL F 414      21.156 -19.706 -51.750  1.00 52.59        C
ANISOU 5920  C   VAL F 414     7748   6913   5322  -1091     27  -2442   C
ATOM   5921  O   VAL F 414      21.612 -20.824 -52.012  1.00 54.19        O
ANISOU 5921  O   VAL F 414     8243   6888   5458  -1056     66  -2564   O
ATOM   5922  N   ARG F 415      19.960 -19.513 -51.195  1.00 53.57        N
ANISOU 5922  N   ARG F 415     7719   7037   5597  -1355     78  -2459   N
ATOM   5923  CA  ARG F 415      19.009 -20.599 -50.933  1.00 56.86        C
ANISOU 5923  CA  ARG F 415     8279   7213   6113  -1686    189  -2636   C
ATOM   5924  CB  ARG F 415      18.679 -20.667 -49.434  1.00 56.75        C
ANISOU 5924  CB  ARG F 415     8382   6972   6208  -1824    400  -2512   C
ATOM   5925  CG  ARG F 415      19.868 -20.954 -48.513  1.00 56.55        C
ANISOU 5925  CG  ARG F 415     8721   6681   6086  -1584    482  -2321   C
ATOM   5926  CD  ARG F 415      20.259 -22.434 -48.501  1.00 61.81        C
ANISOU 5926  CD  ARG F 415     9852   6947   6685  -1607    548  -2415   C
ATOM   5927  NE  ARG F 415      21.475 -22.674 -47.715  1.00 62.49        N
ANISOU 5927  NE  ARG F 415    10262   6805   6676  -1304    561  -2235   N
ATOM   5928  CZ  ARG F 415      22.689 -22.855 -48.237  1.00 62.58        C
ANISOU 5928  CZ  ARG F 415    10363   6824   6592   -954    445  -2229   C
ATOM   5929  NH1 ARG F 415      22.868 -22.842 -49.557  1.00 61.25        N
ANISOU 5929  NH1 ARG F 415    10028   6864   6379   -878    340  -2390   N
ATOM   5930  NH2 ARG F 415      23.727 -23.063 -47.431  1.00 62.31        N
ANISOU 5930  NH2 ARG F 415    10583   6594   6498   -677    434  -2075   N
ATOM   5931  C   ARG F 415      17.730 -20.345 -51.734  1.00 58.42        C
ANISOU 5931  C   ARG F 415     8134   7663   6402  -1935     70  -2824   C
ATOM   5932  O   ARG F 415      17.145 -19.259 -51.654  1.00 58.20        O
ANISOU 5932  O   ARG F 415     7749   7898   6468  -1933      2  -2757   O
ATOM   5933  N   GLY F 416      17.295 -21.329 -52.509  1.00 61.08        N
ANISOU 5933  N   GLY F 416     8575   7920   6715  -2136     26  -3069   N
ATOM   5934  CA  GLY F 416      16.104 -21.163 -53.341  1.00 62.81        C
ANISOU 5934  CA  GLY F 416     8459   8396   7010  -2372   -136  -3277   C
ATOM   5935  C   GLY F 416      16.429 -20.481 -54.658  1.00 61.99        C
ANISOU 5935  C   GLY F 416     8200   8622   6732  -2155   -406  -3291   C
ATOM   5936  O   GLY F 416      17.592 -20.198 -54.941  1.00 59.93        O
ANISOU 5936  O   GLY F 416     8093   8382   6296  -1854   -424  -3155   O
ATOM   5937  N   ASP F 417      15.403 -20.224 -55.467  1.00 63.90        N
ANISOU 5937  N   ASP F 417     8138   9127   7013  -2314   -618  -3460   N
ATOM   5938  CA  ASP F 417      15.591 -19.601 -56.780  1.00 64.06        C
ANISOU 5938  CA  ASP F 417     8056   9458   6828  -2137   -900  -3476   C
ATOM   5939  CB  ASP F 417      14.602 -20.172 -57.801  1.00 67.95        C
ANISOU 5939  CB  ASP F 417     8438  10082   7298  -2398  -1118  -3786   C
ATOM   5940  CG  ASP F 417      15.090 -21.481 -58.420  1.00 70.01        C
ANISOU 5940  CG  ASP F 417     9098  10118   7385  -2495  -1067  -4000   C
ATOM   5941  OD1 ASP F 417      16.312 -21.756 -58.345  1.00 67.20        O
ANISOU 5941  OD1 ASP F 417     9070   9582   6879  -2269   -919  -3895   O
ATOM   5942  OD2 ASP F 417      14.257 -22.228 -58.994  1.00 73.52        O
ANISOU 5942  OD2 ASP F 417     9518  10568   7849  -2792  -1180  -4292   O
ATOM   5943  C   ASP F 417      15.497 -18.081 -56.723  1.00 62.18        C
ANISOU 5943  C   ASP F 417     7507   9500   6617  -1920  -1034  -3253   C
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Figure 18 (continued)

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ATOM   5944  O   ASP F 417      14.874 -17.529 -55.816  1.00 61.19           O
ANISOU 5944  O   ASP F 417    7135   9393   6721  -1970   -960  -3173         O
ATOM   5945  N   LEU F 418      16.133 -17.413 -57.685  1.00 61.75           N
ANISOU 5945  N   LEU F 418    7496   9647   6320  -1686  -1210  -3156         N
ATOM   5946  CA  LEU F 418      16.118 -15.948 -57.745  1.00 60.49           C
ANISOU 5946  CA  LEU F 418    7114   9719   6152  -1472  -1351  -2931         C
ATOM   5947  CB  LEU F 418      17.537 -15.398 -57.923  1.00 57.76           C
ANISOU 5947  CB  LEU F 418    6989   9374   5583  -1201  -1274  -2707         C
ATOM   5948  CG  LEU F 418      18.593 -15.816 -56.888  1.00 55.19           C
ANISOU 5948  CG  LEU F 418    6875   8788   5307  -1122   -976  -2599         C
ATOM   5949  CD1 LEU F 418      19.955 -15.240 -57.229  1.00 53.26           C
ANISOU 5949  CD1 LEU F 418    6775   8610   4852   -874   -930  -2422         C
ATOM   5950  CD2 LEU F 418      18.177 -15.419 -55.497  1.00 52.84           C
ANISOU 5950  CD2 LEU F 418    6426   8377   5273  -1162   -838  -2481         C
ATOM   5951  C   LEU F 418      15.138 -15.398 -58.802  1.00 63.79           C
ANISOU 5951  C   LEU F 418    7283  10437   6516  -1492  -1711  -3027         C
ATOM   5952  O   LEU F 418      15.392 -15.465 -60.017  1.00 65.29           O
ANISOU 5952  O   LEU F 418    7619  10766   6424  -1442  -1904  -3087         O
ATOM   5953  N   ASN F 419      14.019 -14.860 -58.308  1.00 65.15           N
ANISOU 5953  N   ASN F 419    7085  10711   6958  -1553  -1798  -3047         N
ATOM   5954  CA  ASN F 419      12.905 -14.410 -59.137  1.00 69.14           C
ANISOU 5954  CA  ASN F 419    7285  11496   7490  -1571  -2166  -3170         C
ATOM   5955  CB  ASN F 419      11.688 -15.328 -58.915  1.00 72.59           C
ANISOU 5955  CB  ASN F 419    7461  11934   8184  -1910  -2173  -3488         C
ATOM   5956  CG  ASN F 419      11.896 -16.734 -59.469  1.00 75.06           C
ANISOU 5956  CG  ASN F 419    8060  12114   8344  -2158  -2126  -3731         C
ATOM   5957  OD1 ASN F 419      12.169 -16.915 -60.657  1.00 76.13           O
ANISOU 5957  OD1 ASN F 419    8378  12363   8185  -2114  -2350  -3807         O
ATOM   5958  ND2 ASN F 419      11.741 -17.738 -58.608  1.00 76.18           N
ANISOU 5958  ND2 ASN F 419    8272  11998   8674  -2427  -1828  -3861         N
ATOM   5959  C   ASN F 419      12.492 -12.941 -58.929  1.00 68.82           C
ANISOU 5959  C   ASN F 419    6962  11617   7568  -1329  -2328  -2971         C
ATOM   5960  O   ASN F 419      11.329 -12.583 -59.159  1.00 71.70           O
ANISOU 5960  O   ASN F 419    6960  12179   8104  -1346  -2585  -3092         O
ATOM   5961  N   PHE F 420      13.438 -12.093 -58.525  1.00 65.87           N
ANISOU 5961  N   PHE F 420    6754  11162   7112  -1099  -2193  -2683         N
ATOM   5962  CA  PHE F 420      13.118 -10.705 -58.172  1.00 65.85           C
ANISOU 5962  CA  PHE F 420    6538  11242   7241   -872  -2295  -2489         C
ATOM   5963  CB  PHE F 420      14.226 -10.056 -57.331  1.00 61.88           C
ANISOU 5963  CB  PHE F 420    6236  10564   6710   -720  -2025  -2217         C
ATOM   5964  CG  PHE F 420      14.370 -10.644 -55.947  1.00 60.67           C
ANISOU 5964  CG  PHE F 420    6083  10193   6774   -865  -1658  -2251         C
ATOM   5965  CD1 PHE F 420      15.369 -11.592 -55.674  1.00 58.71           C
ANISOU 5965  CD1 PHE F 420    6148   9758   6401   -954  -1418  -2253         C
ATOM   5966  CE1 PHE F 420      15.511 -12.143 -54.394  1.00 56.02           C
ANISOU 5966  CE1 PHE F 420    5866   9196   6224  -1073  -1110  -2262         C
ATOM   5967  CZ  PHE F 420      14.657 -11.740 -53.367  1.00 56.93           C
ANISOU 5967  CZ  PHE F 420    5728   9288   6616  -1135   -998  -2278         C
ATOM   5968  CE2 PHE F 420      13.656 -10.794 -53.617  1.00 59.27           C
ANISOU 5968  CE2 PHE F 420    5671   9783   7065  -1048  -1201  -2302         C
ATOM   5969  CD2 PHE F 420      13.516 -10.248 -54.907  1.00 61.33           C
ANISOU 5969  CD2 PHE F 420    5874  10254   7176   -897  -1551  -2282         C
ATOM   5970  C   PHE F 420      12.752  -9.824 -59.370  1.00 68.72           C
ANISOU 5970  C   PHE F 420    6852  11834   7423   -675  -2718  -2421         C
ATOM   5971  O   PHE F 420      13.329  -9.934 -60.459  1.00 69.39           O
ANISOU 5971  O   PHE F 420    7220  11989   7156   -637  -2864  -2384         O
ATOM   5972  N   VAL F 421      11.776  -8.954 -59.131  1.00 70.81           N
ANISOU 5972  N   VAL F 421    6770  12208   7928   -541  -2906  -2410         N
ATOM   5973  CA  VAL F 421      11.229  -8.033 -60.118  1.00 74.14           C
ANISOU 5973  CA  VAL F 421    7105  12827   8236   -313  -3351  -2341         C
ATOM   5974  CB  VAL F 421       9.792  -8.485 -60.500  1.00 78.54           C
ANISOU 5974  CB  VAL F 421    7234  13606   9001   -421  -3660  -2651         C
ATOM   5975  CG1 VAL F 421       8.878  -7.313 -60.807  1.00 82.04           C
ANISOU 5975  CG1 VAL F 421    7378  14217   9575   -122  -4060  -2593         C
ATOM   5976  CG2 VAL F 421       9.832  -9.491 -61.650  1.00 80.93           C
ANISOU 5976  CG2 VAL F 421    7719  14022   9009   -611  -3856  -2839         C
ATOM   5977  C   VAL F 421      11.256  -6.621 -59.499  1.00 73.25           C
ANISOU 5977  C   VAL F 421    6923  12642   8268    -29  -3339  -2091         C
ATOM   5978  O   VAL F 421      11.324  -6.490 -58.270  1.00 71.13           O
ANISOU 5978  O   VAL F 421    6541  12226   8260    -56  -3019  -2067         O
ATOM   5979  N   ASN F 422      11.235  -5.578 -60.335  1.00 75.33           N
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Figure 18 (continued)

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ANISOU 5979  N   ASN F 422     7301  12982   8339    236  -3678  -1903     N
ATOM   5980  CA  ASN F 422      11.155  -4.182 -59.848  1.00 75.16          C
ANISOU 5980  CA  ASN F 422     7234  12867   8457    526  -3716  -1678     C
ATOM   5981  CB  ASN F 422      11.971  -3.211 -60.732  1.00 75.42          C
ANISOU 5981  CB  ASN F 422     7709  12848   8099    726  -3890  -1361     C
ATOM   5982  CG  ASN F 422      11.733  -3.403 -62.234  1.00 78.66          C
ANISOU 5982  CG  ASN F 422     8283  13451   8152    754  -4312  -1386     C
ATOM   5983  OD1 ASN F 422      12.644  -3.194 -63.032  1.00 78.39          O
ANISOU 5983  OD1 ASN F 422     8691  13389   7703    758  -4323  -1195     O
ATOM   5984  ND2 ASN F 422      10.515  -3.784 -62.621  1.00 82.48          N
ANISOU 5984  ND2 ASN F 422     8411  14140   8786    763  -4655  -1629     N
ATOM   5985  C   ASN F 422       9.730  -3.647 -59.623  1.00 78.75          C
ANISOU 5985  C   ASN F 422     7196  13446   9279    707  -3985  -1818     C
ATOM   5986  O   ASN F 422       8.770  -4.093 -60.259  1.00 82.55          O
ANISOU 5986  O   ASN F 422     7398  14147   9820    676  -4307  -2041     O
ATOM   5987  N   ASN F 425       7.024  -4.833 -63.856  1.00 98.86          N
ANISOU 5987  N   ASN F 425     9351  16900  11312    750  -5734  -2397     N
ATOM   5988  CA  ASN F 425       7.135  -6.277 -63.620  1.00 97.53          C
ANISOU 5988  CA  ASN F 425     9123  16747  11187    326  -5436  -2676     C
ATOM   5989  CB  ASN F 425       5.828  -6.981 -64.027  1.00102.75          C
ANISOU 5989  CB  ASN F 425     9296  17692  12053    177  -5785  -3064     C
ATOM   5990  CG  ASN F 425       5.624  -8.316 -63.314  1.00102.31          C
ANISOU 5990  CG  ASN F 425     9017  17603  12253   -265  -5400  -3381     C
ATOM   5991  OD1 ASN F 425       5.938  -8.463 -62.125  1.00 99.34          O
ANISOU 5991  OD1 ASN F 425     8595  17029  12122   -377  -4908  -3350     O
ATOM   5992  ND2 ASN F 425       5.084  -9.292 -64.040  1.00106.55          N
ANISOU 5992  ND2 ASN F 425     9446  18321  12716   -527  -5632  -3690     N
ATOM   5993  C   ASN F 425       8.361  -6.918 -64.312  1.00 94.87          C
ANISOU 5993  C   ASN F 425     9373  16317  10355    150  -5275  -2581     C
ATOM   5994  O   ASN F 425       8.342  -8.097 -64.685  1.00 95.60          O
ANISOU 5994  O   ASN F 425     9505  16474  10347   -145  -5240  -2830     O
ATOM   5995  N   GLN F 426       9.430  -6.136 -64.450  1.00 91.71          N
ANISOU 5995  N   GLN F 426     9420  15760   9667    322  -5153  -2238     N
ATOM   5996  CA  GLN F 426      10.599  -6.536 -65.229  1.00 89.89          C
ANISOU 5996  CA  GLN F 426     9732  15477   8946    211  -5027  -2133     C
ATOM   5997  CB  GLN F 426      11.215  -5.312 -65.891  1.00 90.44          C
ANISOU 5997  CB  GLN F 426    10206  15499   8656    478  -5188  -1769     C
ATOM   5998  CG  GLN F 426      10.299  -4.689 -66.940  1.00 97.68          C
ANISOU 5998  CG  GLN F 426    11101  16610   9404    704  -5808  -1744     C
ATOM   5999  CD  GLN F 426      10.355  -3.172 -66.960  1.00 99.86          C
ANISOU 5999  CD  GLN F 426    11537  16771   9635   1056  -5984  -1390     C
ATOM   6000  OE1 GLN F 426      10.705  -2.530 -65.963  1.00 97.48          O
ANISOU 6000  OE1 GLN F 426    11179  16268   9590   1145  -5681  -1230     O
ATOM   6001  NE2 GLN F 426       9.997  -2.588 -68.101  1.00105.16          N
ANISOU 6001  NE2 GLN F 426    12440  17552   9963   1259  -6492  -1268     N
ATOM   6002  C   GLN F 426      11.620  -7.231 -64.357  1.00 84.44          C
ANISOU 6002  C   GLN F 426     9182  14578   8323      4  -4459  -2135     C
ATOM   6003  O   GLN F 426      11.740  -6.912 -63.176  1.00 81.85          O
ANISOU 6003  O   GLN F 426     8691  14096   8313     37  -4164  -2056     O
ATOM   6004  N   ARG F 427      12.359  -8.169 -64.948  1.00 83.25          N
ANISOU 6004  N   ARG F 427     9349  14421   7862   -189  -4319  -2232     N
ATOM   6005  CA  ARG F 427      13.309  -9.025 -64.224  1.00 78.32          C
ANISOU 6005  CA  ARG F 427     8863  13606   7291   -373  -3826  -2279     C
ATOM   6006  CB  ARG F 427      13.485 -10.355 -64.972  1.00 80.10          C
ANISOU 6006  CB  ARG F 427     9276  13874   7285   -608  -3811  -2550     C
ATOM   6007  CG  ARG F 427      14.098 -11.462 -64.139  1.00 76.56          C
ANISOU 6007  CG  ARG F 427     8883  13214   6993   -803  -3370  -2682     C
ATOM   6008  CD  ARG F 427      14.519 -12.666 -64.971  1.00 77.87          C
ANISOU 6008  CD  ARG F 427     9339  13376   6870   -982  -3325  -2916     C
ATOM   6009  NE  ARG F 427      15.694 -13.289 -64.368  1.00 73.46          N
ANISOU 6009  NE  ARG F 427     9005  12591   6315  -1013  -2884  -2889     N
ATOM   6010  CZ  ARG F 427      15.669 -14.203 -63.397  1.00 71.27          C
ANISOU 6010  CZ  ARG F 427     8652  12105   6323  -1165  -2616  -3026     C
ATOM   6011  NH1 ARG F 427      14.518 -14.649 -62.913  1.00 72.31          N
ANISOU 6011  NH1 ARG F 427     8487  12227   6763  -1350  -2697  -3217     N
ATOM   6012  NH2 ARG F 427      16.809 -14.675 -62.908  1.00 67.90          N
ANISOU 6012  NH2 ARG F 427     8452  11478   5871  -1132  -2266  -2974     N
ATOM   6013  C   ARG F 427      14.672  -8.348 -64.009  1.00 74.70          C
ANISOU 6013  C   ARG F 427     8734  13001   6647   -251  -3533  -1973     C
ATOM   6014  O   ARG F 427      15.300  -7.904 -64.973  1.00 75.87          O
ANISOU 6014  O   ARG F 427     9220  13212   6395   -172  -3625  -1821     O
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Figure 18 (continued)

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ATOM   6015  N   LEU F 428      15.131  -8.282 -62.758  1.00 70.08           N
ANISOU 6015  N   LEU F 428    8058  12231   6337   -257  -3177  -1893          N
ATOM   6016  CA  LEU F 428      16.419  -7.647 -62.441  1.00 66.81           C
ANISOU 6016  CA  LEU F 428    7899  11689   5796   -165  -2899  -1630          C
ATOM   6017  CB  LEU F 428      16.562  -7.399 -60.921  1.00 63.57           C
ANISOU 6017  CB  LEU F 428    7303  11097   5755   -149  -2609  -1557          C
ATOM   6018  CG  LEU F 428      15.516  -6.574 -60.147  1.00 63.89           C
ANISOU 6018  CG  LEU F 428    7011  11121   6144    -34  -2730  -1518          C
ATOM   6019  CD1 LEU F 428      15.697  -6.733 -58.634  1.00 62.28           C
ANISOU 6019  CD1 LEU F 428    6672  10736   6257    -96  -2381  -1524          C
ATOM   6020  CD2 LEU F 428      15.535  -5.103 -60.527  1.00 64.62           C
ANISOU 6020  CD2 LEU F 428    7197  11227   6130    203  -2935  -1253          C
ATOM   6021  C   LEU F 428      17.636  -8.433 -62.980  1.00 65.60           C
ANISOU 6021  C   LEU F 428    8076  11517   5330   -268  -2664  -1675          C
ATOM   6022  O   LEU F 428      17.516  -9.608 -63.330  1.00 66.61           O
ANISOU 6022  O   LEU F 428    8239  11668   5402   -417  -2648  -1925          O
ATOM   6023  N   ASN F 429      18.796  -7.770 -63.056  1.00 63.59           N
ANISOU 6023  N   ASN F 429    8056  11222   4884   -191  -2477  -1450          N
ATOM   6024  CA  ASN F 429      20.054  -8.420 -63.463  1.00 62.44           C
ANISOU 6024  CA  ASN F 429    8171  11070   4485   -261  -2205  -1496          C
ATOM   6025  CB  ASN F 429      21.027  -7.413 -64.103  1.00 63.01           C
ANISOU 6025  CB  ASN F 429    8510  11197   4233   -193  -2135  -1245          C
ATOM   6026  CG  ASN F 429      21.529  -6.363 -63.128  1.00 60.93           C
ANISOU 6026  CG  ASN F 429    8175  10809   4167   -113  -1976   -998          C
ATOM   6027  OD1 ASN F 429      22.477  -6.593 -62.368  1.00 58.51           O
ANISOU 6027  OD1 ASN F 429    7839  10412   3980   -137  -1668   -990          O
ATOM   6028  ND2 ASN F 429      20.914  -5.187 -63.169  1.00 62.71           N
ANISOU 6028  ND2 ASN F 429    8387  11023   4418     -6  -2203   -799          N
ATOM   6029  C   ASN F 429      20.718  -9.203 -62.314  1.00 58.73           C
ANISOU 6029  C   ASN F 429    7615  10428   4271   -309  -1860  -1579          C
ATOM   6030  O   ASN F 429      20.508  -8.869 -61.159  1.00 56.33           O
ANISOU 6030  O   ASN F 429    7122  10004   4278   -277  -1781  -1501          O
ATOM   6031  N   PRO F 430      21.502 -10.253 -62.639  1.00 58.55           N
ANISOU 6031  N   PRO F 430    7752  10388   4107   -370  -1665  -1747          N
ATOM   6032  CA  PRO F 430      22.103 -11.214 -61.701  1.00 56.25           C
ANISOU 6032  CA  PRO F 430    7432   9919   4022   -392  -1387  -1860          C
ATOM   6033  CB  PRO F 430      23.143 -11.919 -62.569  1.00 57.92           C
ANISOU 6033  CB  PRO F 430    7882  10184   3943   -387  -1225  -1989          C
ATOM   6034  CG  PRO F 430      22.512 -11.934 -63.934  1.00 61.22           C
ANISOU 6034  CG  PRO F 430    8436  10778   4048   -454  -1472  -2086          C
ATOM   6035  CD  PRO F 430      21.832 -10.598 -64.041  1.00 61.60           C
ANISOU 6035  CD  PRO F 430    8395  10925   4087   -406  -1721  -1851          C
ATOM   6036  C   PRO F 430      22.770 -10.649 -60.433  1.00 53.25           C
ANISOU 6036  C   PRO F 430    6949   9412   3872   -310  -1184  -1672          C
ATOM   6037  O   PRO F 430      22.727 -11.279 -59.364  1.00 51.32           O
ANISOU 6037  O   PRO F 430    6623   8994   3881   -331  -1058  -1737          O
ATOM   6038  N   MSE F 431      23.393  -9.482 -60.550  1.00 52.56           N
ANISOU 6038  N   MSE F 431    6896   9398   3678   -235  -1153  -1444          N
ATOM   6039  CA  MSE F 431      24.056  -8.867 -59.414  1.00 49.48           C
ANISOU 6039  CA  MSE F 431    6418   8904   3479   -176   -983  -1278          C
ATOM   6040  CB  MSE F 431      25.096  -7.852 -59.885  1.00 49.34           C
ANISOU 6040  CB  MSE F 431    6508   8987   3253   -144   -888  -1088          C
ATOM   6041  CG  MSE F 431      26.338  -8.505 -60.487  1.00 49.79           C
ANISOU 6041  CG  MSE F 431    6683   9129   3106   -146   -670  -1196          C
ATOM   6042  SE  MSE F 431      27.421  -9.500 -59.208  0.90 48.52          SE
ANISOU 6042  SE  MSE F 431    6408   8820   3206    -65   -407  -1314          SE
ATOM   6043  CE  MSE F 431      28.095  -8.003 -58.164  1.00 42.60           C
ANISOU 6043  CE  MSE F 431    5533   8047   2607    -51   -331  -1034          C
ATOM   6044  C   MSE F 431      23.033  -8.245 -58.467  1.00 48.53           C
ANISOU 6044  C   MSE F 431    6111   8689   3637   -167  -1099  -1191          C
ATOM   6045  O   MSE F 431      23.151  -8.389 -57.249  1.00 46.67           O
ANISOU 6045  O   MSE F 431    5784   8310   3637   -162   -966  -1179          O
ATOM   6046  N   HIS F 432      22.022  -7.577 -59.025  1.00 50.21           N
ANISOU 6046  N   HIS F 432    6275   8987   3817   -152  -1351  -1142          N
ATOM   6047  CA  HIS F 432      20.939  -6.996 -58.216  1.00 50.13           C
ANISOU 6047  CA  HIS F 432    6049   8909   4088   -120  -1466  -1100          C
ATOM   6048  CB  HIS F 432      20.214  -5.876 -58.970  1.00 52.12           C
ANISOU 6048  CB  HIS F 432    6294   9261   4248    -24  -1753   -971          C
ATOM   6049  CG  HIS F 432      21.028  -4.628 -59.064  1.00 53.16           C
ANISOU 6049  CG  HIS F 432    6589   9363   4245     57  -1703   -709          C
ATOM   6050  ND1 HIS F 432      21.765  -4.303 -60.183  1.00 56.08           N
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Figure 18 (continued)

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ANISOU 6050  ND1 HIS F 432     7218   9830   4259     47  -1719   -603    N
ATOM   6051  CE1 HIS F 432      22.416  -3.175 -59.964  1.00 55.82         C
ANISOU 6051  CE1 HIS F 432     7296   9724   4188     81  -1633   -377    C
ATOM   6052  NE2 HIS F 432      22.146  -2.768 -58.736  1.00 53.78         N
ANISOU 6052  NE2 HIS F 432     6864   9325   4245    128  -1574   -342    N
ATOM   6053  CD2 HIS F 432      21.287  -3.664 -58.149  1.00 52.46         C
ANISOU 6053  CD2 HIS F 432     6466   9146   4318    116  -1604   -545    C
ATOM   6054  C   HIS F 432      19.976  -8.044 -57.680  1.00 50.25         C
ANISOU 6054  C   HIS F 432     5890   8868   4334   -223  -1472  -1325    C
ATOM   6055  O   HIS F 432      19.291  -7.825 -56.678  1.00 49.54         O
ANISOU 6055  O   HIS F 432     5610   8692   4520   -230  -1440  -1330    O
ATOM   6056  N   GLN F 433      19.961  -9.185 -58.363  1.00 51.26         N
ANISOU 6056  N   GLN F 433     6103   9036   4336   -321  -1489  -1523    N
ATOM   6057  CA  GLN F 433      19.267 -10.386 -57.940  1.00 51.44         C
ANISOU 6057  CA  GLN F 433     6036   8972   4537   -471  -1445  -1757    C
ATOM   6058  CB  GLN F 433      19.368 -11.415 -59.072  1.00 53.59         C
ANISOU 6058  CB  GLN F 433     6472   9312   4577   -558  -1515  -1959    C
ATOM   6059  CG  GLN F 433      18.243 -12.401 -59.174  1.00 56.54         C
ANISOU 6059  CG  GLN F 433     6733   9673   5078   -746  -1618  -2223    C
ATOM   6060  CD  GLN F 433      16.932 -11.816 -59.689  1.00 59.82         C
ANISOU 6060  CD  GLN F 433     6898  10278   5554   -765  -1945  -2270    C
ATOM   6061  OE1 GLN F 433      15.859 -12.218 -59.245  1.00 61.27         O
ANISOU 6061  OE1 GLN F 433     6840  10449   5990   -910  -1990  -2434    O
ATOM   6062  NE2 GLN F 433      17.012 -10.890 -60.639  1.00 62.13         N
ANISOU 6062  NE2 GLN F 433     7249  10744   5612   -622  -2176  -2135    N
ATOM   6063  C   GLN F 433      19.878 -10.921 -56.630  1.00 48.94         C
ANISOU 6063  C   GLN F 433     5764   8437   4393   -497  -1154  -1743    C
ATOM   6064  O   GLN F 433      19.161 -11.164 -55.657  1.00 48.75         O
ANISOU 6064  O   GLN F 433     5604   8301   4617   -588  -1080  -1799    O
ATOM   6065  N   LEU F 434      21.204 -11.080 -56.605  1.00 47.33         N
ANISOU 6065  N   LEU F 434     5750   8183   4051   -415   -991  -1671    N
ATOM   6066  CA  LEU F 434      21.915 -11.611 -55.435  1.00 45.33         C
ANISOU 6066  CA  LEU F 434     5572   7729   3923   -399   -763  -1651    C
ATOM   6067  CB  LEU F 434      23.375 -11.926 -55.764  1.00 44.35         C
ANISOU 6067  CB  LEU F 434     5621   7609   3622   -286   -638  -1633    C
ATOM   6068  CG  LEU F 434      23.737 -13.106 -56.671  1.00 46.26         C
ANISOU 6068  CG  LEU F 434     6031   7847   3701   -298   -613  -1839    C
ATOM   6069  CD1 LEU F 434      25.048 -12.834 -57.429  1.00 45.03         C
ANISOU 6069  CD1 LEU F 434     5961   7831   3320   -170   -529  -1797    C
ATOM   6070  CD2 LEU F 434      23.811 -14.406 -55.887  1.00 45.64         C
ANISOU 6070  CD2 LEU F 434     6075   7510   3756   -328   -486  -1973    C
ATOM   6071  C   LEU F 434      21.877 -10.621 -54.289  1.00 43.61         C
ANISOU 6071  C   LEU F 434     5240   7453   3875   -350   -703  -1470    C
ATOM   6072  O   LEU F 434      21.795 -11.014 -53.136  1.00 42.36         O
ANISOU 6072  O   LEU F 434     5094   7124   3877   -394   -569  -1478    O
ATOM   6073  N   LEU F 435      21.949  -9.337 -54.633  1.00 43.83         N
ANISOU 6073  N   LEU F 435     5202   7609   3845   -265   -801  -1307    N
ATOM   6074  CA  LEU F 435      21.877  -8.246 -53.682  1.00 42.80         C
ANISOU 6074  CA  LEU F 435     4980   7425   3858   -212   -765  -1145    C
ATOM   6075  CB  LEU F 435      22.151  -6.916 -54.393  1.00 43.44         C
ANISOU 6075  CB  LEU F 435     5072   7627   3806   -118   -883   -969    C
ATOM   6076  CG  LEU F 435      22.046  -5.590 -53.631  1.00 43.35         C
ANISOU 6076  CG  LEU F 435     4998   7552   3919    -51   -879   -798    C
ATOM   6077  CD1 LEU F 435      23.280  -5.323 -52.808  1.00 40.78         C
ANISOU 6077  CD1 LEU F 435     4764   7145   3587    -39   -699   -695    C
ATOM   6078  CD2 LEU F 435      21.811  -4.465 -54.623  1.00 46.94         C
ANISOU 6078  CD2 LEU F 435     5485   8107   4244     28  -1070   -665    C
ATOM   6079  C   LEU F 435      20.548  -8.204 -52.917  1.00 43.61         C
ANISOU 6079  C   LEU F 435     4899   7464   4207   -283   -781  -1217    C
ATOM   6080  O   LEU F 435      20.564  -8.107 -51.684  1.00 43.27         O
ANISOU 6080  O   LEU F 435     4845   7285   4311   -301   -630  -1181    O
ATOM   6081  N   ARG F 436      19.419  -8.281 -53.628  1.00 45.19         N
ANISOU 6081  N   ARG F 436     4950   7774   4447   -327   -958  -1331    N
ATOM   6082  CA  ARG F 436      18.092  -8.308 -52.997  1.00 46.39         C
ANISOU 6082  CA  ARG F 436     4861   7907   4858   -409   -963  -1447    C
ATOM   6083  CB  ARG F 436      16.958  -8.209 -54.025  1.00 49.83         C
ANISOU 6083  CB  ARG F 436     5092   8525   5315   -416  -1236  -1567    C
ATOM   6084  CG  ARG F 436      16.930  -6.953 -54.854  1.00 52.80         C
ANISOU 6084  CG  ARG F 436     5452   9031   5579   -222  -1482  -1411    C
ATOM   6085  CD  ARG F 436      16.008  -5.894 -54.293  1.00 58.94         C
ANISOU 6085  CD  ARG F 436     5980   9814   6599   -104  -1555  -1371    C
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Figure 18 (continued)

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ATOM   6086  NE  ARG F 436      15.996  -4.730 -55.183  1.00 65.22           N
ANISOU 6086  NE  ARG F 436    6825  10696   7261    100  -1823  -1207         N
ATOM   6087  CZ  ARG F 436      16.971  -3.816 -55.263  1.00 66.83           C
ANISOU 6087  CZ  ARG F 436    7266  10826   7300    211  -1789   -971         C
ATOM   6088  NH1 ARG F 436      18.065  -3.900 -54.498  1.00 64.44           N
ANISOU 6088  NH1 ARG F 436    7128  10393   6962    150  -1516   -886         N
ATOM   6089  NH2 ARG F 436      16.854  -2.803 -56.124  1.00 69.94           N
ANISOU 6089  NH2 ARG F 436    7744  11271   7558    377  -2041   -820         N
ATOM   6090  C   ARG F 436      17.859  -9.557 -52.166  1.00 45.64           C
ANISOU 6090  C   ARG F 436    4800   7659   4881   -598   -758  -1602         C
ATOM   6091  O   ARG F 436      17.216  -9.476 -51.121  1.00 45.62           O
ANISOU 6091  O   ARG F 436    4679   7574   5082   -674   -619  -1635         O
ATOM   6092  N   HIS F 437      18.342 -10.706 -52.646  1.00 45.31           N
ANISOU 6092  N   HIS F 437    4943   7568   4705   -678   -729  -1703         N
ATOM   6093  CA  HIS F 437      18.235 -11.973 -51.907  1.00 45.24           C
ANISOU 6093  CA  HIS F 437    5056   7358   4776   -856   -535  -1833         C
ATOM   6094  CB  HIS F 437      18.834 -13.126 -52.703  1.00 45.82           C
ANISOU 6094  CB  HIS F 437    5355   7378   4675   -890   -550  -1948         C
ATOM   6095  CG  HIS F 437      18.890 -14.416 -51.941  1.00 46.87           C
ANISOU 6095  CG  HIS F 437    5698   7245   4866  -1039   -355  -2050         C
ATOM   6096  ND1 HIS F 437      17.806 -15.262 -51.828  1.00 50.23           N
ANISOU 6096  ND1 HIS F 437    6073   7589   5423  -1302   -309  -2247         N
ATOM   6097  CE1 HIS F 437      18.145 -16.317 -51.107  1.00 49.92           C
ANISOU 6097  CE1 HIS F 437    6317   7264   5387  -1394   -120  -2277         C
ATOM   6098  NE2 HIS F 437      19.407 -16.186 -50.746  1.00 46.92           N
ANISOU 6098  NE2 HIS F 437    6143   6795   4890  -1170    -71  -2113         N
ATOM   6099  CD2 HIS F 437      19.897 -15.006 -51.253  1.00 45.46           C
ANISOU 6099  CD2 HIS F 437    5796   6848   4628   -964   -203  -1979         C
ATOM   6100  C   HIS F 437      18.888 -11.907 -50.513  1.00 43.18           C
ANISOU 6100  C   HIS F 437    4945   6899   4562   -822   -311  -1700         C
ATOM   6101  O   HIS F 437      18.278 -12.279 -49.506  1.00 43.17           O
ANISOU 6101  O   HIS F 437    4939   6759   4706   -972   -145  -1753         O
ATOM   6102  N   PHE F 438      20.125 -11.420 -50.468  1.00 41.26           N
ANISOU 6102  N   PHE F 438    4837   6655   4185   -641   -309  -1536         N
ATOM   6103  CA  PHE F 438      20.852 -11.273 -49.206  1.00 39.83           C
ANISOU 6103  CA  PHE F 438    4798   6315   4020   -587   -153  -1408         C
ATOM   6104  CB  PHE F 438      22.361 -11.316 -49.455  1.00 37.85           C
ANISOU 6104  CB  PHE F 438    4709   6069   3602   -417   -169  -1313         C
ATOM   6105  CG  PHE F 438      22.829 -12.660 -49.947  1.00 39.60           C
ANISOU 6105  CG  PHE F 438    5116   6198   3733   -418   -151  -1439         C
ATOM   6106  CD1 PHE F 438      22.572 -13.808 -49.195  1.00 40.19           C
ANISOU 6106  CD1 PHE F 438    5380   6026   3864   -522    -35  -1520         C
ATOM   6107  CE1 PHE F 438      22.977 -15.070 -49.651  1.00 41.92           C
ANISOU 6107  CE1 PHE F 438    5806   6113   4007   -509    -21  -1646         C
ATOM   6108  CZ  PHE F 438      23.645 -15.183 -50.862  1.00 41.42           C
ANISOU 6108  CZ  PHE F 438    5733   6193   3811   -388   -107  -1710         C
ATOM   6109  CE2 PHE F 438      23.898 -14.046 -51.625  1.00 40.68           C
ANISOU 6109  CE2 PHE F 438    5446   6370   3640   -307   -203  -1629         C
ATOM   6110  CD2 PHE F 438      23.490 -12.793 -51.171  1.00 37.92           C
ANISOU 6110  CD2 PHE F 438    4917   6123   3367   -324   -234  -1485         C
ATOM   6111  C   PHE F 438      20.402 -10.089 -48.336  1.00 39.24           C
ANISOU 6111  C   PHE F 438    4583   6259   4070   -568   -108  -1305         C
ATOM   6112  O   PHE F 438      20.540 -10.130 -47.106  1.00 39.25           O
ANISOU 6112  O   PHE F 438    4694   6107   4112   -601     45  -1255         O
ATOM   6113  N   GLN F 439      19.858  -9.049 -48.967  1.00 39.55           N
ANISOU 6113  N   GLN F 439    4408   6467   4154   -505   -247  -1277         N
ATOM   6114  CA  GLN F 439      19.215  -7.958 -48.236  1.00 40.07           C
ANISOU 6114  CA  GLN F 439    4319   6538   4370   -476   -210  -1224         C
ATOM   6115  CB  GLN F 439      18.927  -6.776 -49.172  1.00 40.77           C
ANISOU 6115  CB  GLN F 439    4244   6792   4456   -335   -421  -1156         C
ATOM   6116  CG  GLN F 439      20.154  -5.878 -49.485  1.00 38.76           C
ANISOU 6116  CG  GLN F 439    4134   6557   4035   -195   -480   -960         C
ATOM   6117  CD  GLN F 439      19.884  -4.831 -50.591  1.00 40.21           C
ANISOU 6117  CD  GLN F 439    4240   6875   4164    -74   -700   -876         C
ATOM   6118  OE1 GLN F 439      18.910  -4.924 -51.358  1.00 40.53           O
ANISOU 6118  OE1 GLN F 439    4129   7024   4247    -65   -866   -967         O
ATOM   6119  NE2 GLN F 439      20.765  -3.840 -50.676  1.00 38.72           N
ANISOU 6119  NE2 GLN F 439    4173   6671   3869     12   -714   -700         N
ATOM   6120  C   GLN F 439      17.937  -8.415 -47.506  1.00 41.99           C
ANISOU 6120  C   GLN F 439    4418   6725   4813   -648    -69  -1382         C
ATOM   6121  O   GLN F 439      17.606  -7.892 -46.434  1.00 42.49           O
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Figure 18 (continued)

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ANISOU 6121  O   GLN F 439     4446   6713   4984   -664     82  -1362      O
ATOM   6122  N   LYS F 440      17.235  -9.393 -48.079  1.00 43.71          N
ANISOU 6122  N   LYS F 440     4556   6978   5073   -798   -100  -1554      N
ATOM   6123  CA  LYS F 440      16.025  -9.948 -47.471  1.00 45.70          C
ANISOU 6123  CA  LYS F 440     4653   7190   5520  -1019     59  -1732      C
ATOM   6124  CB  LYS F 440      15.193 -10.701 -48.516  1.00 47.97          C
ANISOU 6124  CB  LYS F 440     4765   7600   5862  -1159    -81  -1933      C
ATOM   6125  CG  LYS F 440      13.730 -10.810 -48.165  1.00 52.65          C
ANISOU 6125  CG  LYS F 440     5024   8266   6716  -1355     10  -2138      C
ATOM   6126  CD  LYS F 440      13.005 -11.813 -49.037  1.00 57.78          C
ANISOU 6126  CD  LYS F 440     5548   8998   7410  -1567    -98  -2366      C
ATOM   6127  CE  LYS F 440      11.613 -12.094 -48.466  1.00 63.15          C
ANISOU 6127  CE  LYS F 440     5897   9727   8371  -1834     73  -2594      C
ATOM   6128  NZ  LYS F 440      10.726 -12.860 -49.401  1.00 67.40          N
ANISOU 6128  NZ  LYS F 440     6202  10408   8999  -2047    -88  -2852      N
ATOM   6129  C   LYS F 440      16.343 -10.851 -46.265  1.00 45.04          C
ANISOU 6129  C   LYS F 440     4857   6858   5399  -1184    337  -1726      C
ATOM   6130  O   LYS F 440      15.665 -10.779 -45.235  1.00 45.28          O
ANISOU 6130  O   LYS F 440     4834   6818   5553  -1319    556  -1776      O
ATOM   6131  N   ASP F 441      17.363 -11.702 -46.407  1.00 44.15          N
ANISOU 6131  N   ASP F 441     5059   6609   5107  -1164    329  -1670      N
ATOM   6132  CA  ASP F 441      17.851 -12.542 -45.301  1.00 44.37          C
ANISOU 6132  CA  ASP F 441     5434   6370   5057  -1258    537  -1623      C
ATOM   6133  CB  ASP F 441      17.083 -13.877 -45.220  1.00 47.39          C
ANISOU 6133  CB  ASP F 441     5912   6599   5494  -1550    681  -1796      C
ATOM   6134  CG  ASP F 441      17.580 -14.785 -44.081  1.00 49.62          C
ANISOU 6134  CG  ASP F 441     6630   6558   5663  -1643    885  -1723      C
ATOM   6135  OD1 ASP F 441      17.900 -14.261 -42.985  1.00 47.18          O
ANISOU 6135  OD1 ASP F 441     6449   6174   5305  -1586    997  -1590      O
ATOM   6136  OD2 ASP F 441      17.647 -16.033 -44.294  1.00 53.67          O
ANISOU 6136  OD2 ASP F 441     7391   6878   6124  -1769    920  -1801      O
ATOM   6137  C   ASP F 441      19.354 -12.779 -45.422  1.00 42.20          C
ANISOU 6137  C   ASP F 441     5438   6011   4585  -1054    445  -1484      C
ATOM   6138  O   ASP F 441      19.809 -13.476 -46.344  1.00 42.70          O
ANISOU 6138  O   ASP F 441     5580   6080   4565  -1008    336  -1539      O
ATOM   6139  N   ALA F 442      20.119 -12.200 -44.490  1.00 39.94          N
ANISOU 6139  N   ALA F 442     5287   5659   4228   -932    490  -1327      N
ATOM   6140  CA  ALA F 442      21.587 -12.254 -44.552  1.00 37.88          C
ANISOU 6140  CA  ALA F 442     5212   5367   3812   -718    385  -1206      C
ATOM   6141  CB  ALA F 442      22.194 -10.935 -44.070  1.00 35.76          C
ANISOU 6141  CB  ALA F 442     4870   5197   3522   -576    341  -1061      C
ATOM   6142  C   ALA F 442      22.206 -13.431 -43.786  1.00 38.27          C
ANISOU 6142  C   ALA F 442     5637   5147   3758   -720    460  -1181      C
ATOM   6143  O   ALA F 442      23.427 -13.627 -43.815  1.00 37.55          O
ANISOU 6143  O   ALA F 442     5683   5026   3559   -521    361  -1107      O
ATOM   6144  N   LYS F 443      21.364 -14.209 -43.117  1.00 39.15          N
ANISOU 6144  N   LYS F 443     5911   5060   3903   -941    634  -1246      N
ATOM   6145  CA  LYS F 443      21.830 -15.168 -42.119  1.00 40.19          C
ANISOU 6145  CA  LYS F 443     6467   4887   3916   -956    722  -1181      C
ATOM   6146  CB  LYS F 443      20.647 -15.777 -41.368  1.00 42.67          C
ANISOU 6146  CB  LYS F 443     6926   5010   4276  -1279    972  -1253      C
ATOM   6147  CG  LYS F 443      20.361 -15.115 -40.038  1.00 42.60          C
ANISOU 6147  CG  LYS F 443     7000   4958   4230  -1361   1138  -1163      C
ATOM   6148  CD  LYS F 443      19.175 -15.766 -39.380  1.00 45.79          C
ANISOU 6148  CD  LYS F 443     7535   5190   4676  -1716   1431  -1256      C
ATOM   6149  CE  LYS F 443      17.886 -15.276 -40.009  1.00 47.38          C
ANISOU 6149  CE  LYS F 443     7261   5629   5111  -1902   1514  -1439      C
ATOM   6150  NZ  LYS F 443      17.018 -16.416 -40.328  1.00 51.45          N
ANISOU 6150  NZ  LYS F 443     7824   6016   5707  -2211   1655  -1602      N
ATOM   6151  C   LYS F 443      22.727 -16.272 -42.669  1.00 40.29          C
ANISOU 6151  C   LYS F 443     6714   4754   3841   -804    609  -1201      C
ATOM   6152  O   LYS F 443      23.776 -16.559 -42.095  1.00 39.70          O
ANISOU 6152  O   LYS F 443     6892   4543   3650   -607    536  -1092      O
ATOM   6153  N   VAL F 444      22.306 -16.894 -43.771  1.00 40.93          N
ANISOU 6153  N   VAL F 444     6708   4865   3980   -884    583  -1356      N
ATOM   6154  CA  VAL F 444      23.106 -17.948 -44.424  1.00 41.02          C
ANISOU 6154  CA  VAL F 444     6929   4738   3917   -730    491  -1416      C
ATOM   6155  CB  VAL F 444      22.315 -18.633 -45.563  1.00 42.70          C
ANISOU 6155  CB  VAL F 444     7062   4969   4193   -911    498  -1626      C
ATOM   6156  CG1 VAL F 444      23.094 -19.832 -46.148  1.00 43.29          C
ANISOU 6156  CG1 VAL F 444     7417   4842   4187   -760    438  -1715      C
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Figure 18 (continued)

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ATOM   6157  CG2 VAL F 444      20.936 -19.073 -45.051  1.00 44.72           C
ANISOU 6157  CG2 VAL F 444    7368   5079   4545  -1289    687  -1713          C
ATOM   6158  C   VAL F 444      24.422 -17.346 -44.942  1.00 38.71           C
ANISOU 6158  C   VAL F 444    6494   4651   3563   -400    317  -1349          C
ATOM   6159  O   VAL F 444      25.494 -17.944 -44.813  1.00 39.03           O
ANISOU 6159  O   VAL F 444    6739   4560   3529   -169    245  -1320          O
ATOM   6160  N   LEU F 445      24.333 -16.142 -45.489  1.00 36.36           N
ANISOU 6160  N   LEU F 445    5845   4667   3303   -380    255  -1326          N
ATOM   6161  CA  LEU F 445      25.508 -15.420 -45.967  1.00 34.90           C
ANISOU 6161  CA  LEU F 445    5500   4697   3063   -133    131  -1260          C
ATOM   6162  CB  LEU F 445      25.098 -14.069 -46.554  1.00 32.55           C
ANISOU 6162  CB  LEU F 445    4867   4693   2805   -184     89  -1227          C
ATOM   6163  CG  LEU F 445      26.226 -13.137 -46.999  1.00 31.63           C
ANISOU 6163  CG  LEU F 445    4587   4801   2630      0     -2  -1143          C
ATOM   6164  CD1 LEU F 445      26.905 -13.645 -48.265  1.00 30.39           C
ANISOU 6164  CD1 LEU F 445    4401   4755   2391    115    -50  -1248          C
ATOM   6165  CD2 LEU F 445      25.692 -11.704 -47.173  1.00 30.43           C
ANISOU 6165  CD2 LEU F 445    4199   4843   2521    -73    -28  -1062          C
ATOM   6166  C   LEU F 445      26.542 -15.233 -44.853  1.00 35.09           C
ANISOU 6166  C   LEU F 445    5661   4635   3035     44     94  -1119          C
ATOM   6167  O   LEU F 445      27.710 -15.627 -44.999  1.00 35.50           O
ANISOU 6167  O   LEU F 445    5772   4680   3036    277      8  -1121          O
ATOM   6168  N   PHE F 446      26.090 -14.642 -43.743  1.00 35.06           N
ANISOU 6168  N   PHE F 446    5700   4578   3045    -65    157  -1016          N
ATOM   6169  CA  PHE F 446      26.937 -14.316 -42.610  1.00 35.44           C
ANISOU 6169  CA  PHE F 446    5879   4565   3023     66    102   -884          C
ATOM   6170  CB  PHE F 446      26.155 -13.442 -41.604  1.00 33.86           C
ANISOU 6170  CB  PHE F 446    5673   4356   2836   -109    206   -808          C
ATOM   6171  CG  PHE F 446      26.103 -11.980 -41.978  1.00 30.18           C
ANISOU 6171  CG  PHE F 446    4878   4157   2434   -115    174   -779          C
ATOM   6172  CD1 PHE F 446      26.572 -11.539 -43.229  1.00 28.69           C
ANISOU 6172  CD1 PHE F 446    4433   4194   2273    -20     77   -809          C
ATOM   6173  CE1 PHE F 446      26.527 -10.181 -43.583  1.00 26.71           C
ANISOU 6173  CE1 PHE F 446    3939   4146   2063    -34     47   -761          C
ATOM   6174  CZ  PHE F 446      25.987  -9.247 -42.674  1.00 27.01           C
ANISOU 6174  CZ  PHE F 446    3967   4156   2138   -123    111   -702          C
ATOM   6175  CE2 PHE F 446      25.498  -9.688 -41.439  1.00 24.47           C
ANISOU 6175  CE2 PHE F 446    3871   3634   1792   -215    223   -696          C
ATOM   6176  CD2 PHE F 446      25.556 -11.045 -41.101  1.00 28.12           C
ANISOU 6176  CD2 PHE F 446    4595   3899   2192   -223    257   -724          C
ATOM   6177  C   PHE F 446      27.501 -15.562 -41.943  1.00 38.56           C
ANISOU 6177  C   PHE F 446    6654   4667   3332    191     66   -864          C
ATOM   6178  O   PHE F 446      28.671 -15.593 -41.562  1.00 39.82           O
ANISOU 6178  O   PHE F 446    6870   4828   3433    430    -77   -804          O
ATOM   6179  N   GLN F 447      26.677 -16.596 -41.820  1.00 41.56           N
ANISOU 6179  N   GLN F 447    7294   4789   3708     31    185   -921          N
ATOM   6180  CA  GLN F 447      27.057 -17.775 -41.044  1.00 45.64           C
ANISOU 6180  CA  GLN F 447    8264   4954   4124    121    165   -873          C
ATOM   6181  CB  GLN F 447      25.815 -18.492 -40.478  1.00 47.48           C
ANISOU 6181  CB  GLN F 447    8800   4901   4339   -200    378   -890          C
ATOM   6182  CG  GLN F 447      25.073 -17.727 -39.352  1.00 48.48           C
ANISOU 6182  CG  GLN F 447    8957   5035   4427   -424    529   -798          C
ATOM   6183  CD  GLN F 447      23.680 -18.313 -39.041  1.00 50.68           C
ANISOU 6183  CD  GLN F 447    9403   5119   4735   -807    800   -867          C
ATOM   6184  OE1 GLN F 447      23.423 -19.504 -39.267  1.00 54.85           O
ANISOU 6184  OE1 GLN F 447   10205   5382   5253   -905    862   -931          O
ATOM   6185  NE2 GLN F 447      22.781 -17.469 -38.526  1.00 51.31           N
ANISOU 6185  NE2 GLN F 447    9309   5325   4860  -1031    975   -872          N
ATOM   6186  C   GLN F 447      27.949 -18.752 -41.824  1.00 47.16           C
ANISOU 6186  C   GLN F 447    8540   5061   4318    384     43   -961          C
ATOM   6187  O   GLN F 447      28.431 -19.731 -41.252  1.00 49.81           O
ANISOU 6187  O   GLN F 447    9258   5091   4576    537    -19   -919          O
ATOM   6188  N   ASN F 448      28.178 -18.487 -43.112  1.00 46.16           N
ANISOU 6188  N   ASN F 448    8083   5190   4265    451      9  -1083          N
ATOM   6189  CA  ASN F 448      29.028 -19.362 -43.933  1.00 47.96           C
ANISOU 6189  CA  ASN F 448    8359   5368   4497    707    -74  -1202          C
ATOM   6190  CB  ASN F 448      28.210 -20.041 -45.037  1.00 48.76           C
ANISOU 6190  CB  ASN F 448    8474   5419   4635    530     28  -1384          C
ATOM   6191  CG  ASN F 448      27.331 -21.142 -44.506  1.00 51.36           C
ANISOU 6191  CG  ASN F 448    9217   5346   4949    321    138  -1405          C
ATOM   6192  OD1 ASN F 448      27.684 -22.318 -44.583  1.00 56.22           O
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Figure 18 (continued)

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ANISOU 6192  OD1 ASN F 448    10163   5660   5540    452    119  -1474    O
ATOM   6193  ND2 ASN F 448      26.186 -20.775 -43.948  1.00 51.17        N
ANISOU 6193  ND2 ASN F 448     9191   5303   4948    -10    270  -1356    N
ATOM   6194  C   ASN F 448      30.261 -18.680 -44.526  1.00 47.16        C
ANISOU 6194  C   ASN F 448     7915   5590   4414    975   -193  -1223    C
ATOM   6195  O   ASN F 448      31.074 -19.318 -45.229  1.00 48.80        O
ANISOU 6195  O   ASN F 448     8107   5803   4633   1217   -243  -1344    O
ATOM   6196  N   TRP F 449      30.404 -17.396 -44.214  1.00 44.74        N
ANISOU 6196  N   TRP F 449     7344   5542   4115    923   -220  -1118    N
ATOM   6197  CA  TRP F 449      31.462 -16.558 -44.749  1.00 43.75        C
ANISOU 6197  CA  TRP F 449     6866   5746   4011   1087   -296  -1130    C
ATOM   6198  CB  TRP F 449      31.109 -15.093 -44.514  1.00 40.74        C
ANISOU 6198  CB  TRP F 449     6250   5589   3640    899   -272  -1021    C
ATOM   6199  CG  TRP F 449      32.099 -14.109 -45.064  1.00 39.18        C
ANISOU 6199  CG  TRP F 449     5708   5720   3459    989   -319  -1021    C
ATOM   6200  CD1 TRP F 449      33.122 -13.516 -44.388  1.00 38.41        C
ANISOU 6200  CD1 TRP F 449     5492   5733   3368   1111   -427   -956    C
ATOM   6201  NE1 TRP F 449      33.798 -12.649 -45.215  1.00 37.76        N
ANISOU 6201  NE1 TRP F 449     5082   5959   3306   1105   -405   -988    N
ATOM   6202  CE2 TRP F 449      33.212 -12.668 -46.456  1.00 38.35        C
ANISOU 6202  CE2 TRP F 449     5092   6121   3360    997   -290  -1060    C
ATOM   6203  CD2 TRP F 449      32.132 -13.577 -46.398  1.00 38.04        C
ANISOU 6203  CD2 TRP F 449     5310   5833   3311    927   -251  -1092    C
ATOM   6204  CE3 TRP F 449      31.347 -13.773 -47.545  1.00 37.88        C
ANISOU 6204  CE3 TRP F 449     5272   5859   3262    804   -169  -1181    C
ATOM   6205  CZ3 TRP F 449      31.668 -13.069 -48.703  1.00 37.87        C
ANISOU 6205  CZ3 TRP F 449     5043   6135   3213    771   -130  -1214    C
ATOM   6206  CH2 TRP F 449      32.756 -12.173 -48.731  1.00 37.69        C
ANISOU 6206  CH2 TRP F 449     4797   6336   3188    831   -137  -1165    C
ATOM   6207  CZ2 TRP F 449      33.536 -11.958 -47.622  1.00 37.45        C
ANISOU 6207  CZ2 TRP F 449     4735   6279   3216    935   -216  -1098    C
ATOM   6208  C   TRP F 449      32.844 -16.878 -44.167  1.00 45.96        C
ANISOU 6208  C   TRP F 449     7170   6002   4289   1417   -454  -1113    C
ATOM   6209  O   TRP F 449      33.846 -16.885 -44.895  1.00 46.57        O
ANISOU 6209  O   TRP F 449     7011   6277   4406   1622   -492  -1216    O
ATOM   6210  N   GLY F 450      32.904 -17.119 -42.858  1.00 47.36        N
ANISOU 6210  N   GLY F 450     7622   5957   4416   1470   -550   -991    N
ATOM   6211  CA  GLY F 450      34.169 -17.491 -42.226  1.00 50.09        C
ANISOU 6211  CA  GLY F 450     8014   6263   4756   1812   -756   -972    C
ATOM   6212  C   GLY F 450      34.684 -16.523 -41.180  1.00 49.91        C
ANISOU 6212  C   GLY F 450     7895   6373   4695   1820   -896   -845    C
ATOM   6213  O   GLY F 450      34.711 -15.310 -41.382  1.00 47.96        O
ANISOU 6213  O   GLY F 450     7334   6410   4479   1663   -853   -827    O
ATOM   6214  N   ILE F 451      35.112 -17.089 -40.061  1.00 52.64        N
ANISOU 6214  N   ILE F 451     8549   6492   4958   2009  -1079   -759    N
ATOM   6215  CA  ILE F 451      35.602 -16.346 -38.912  1.00 53.25        C
ANISOU 6215  CA  ILE F 451     8628   6646   4959   2031  -1254   -644    C
ATOM   6216  CB  ILE F 451      35.053 -16.971 -37.603  1.00 54.82        C
ANISOU 6216  CB  ILE F 451     9395   6461   4973   1996  -1306   -493    C
ATOM   6217  CG1 ILE F 451      33.541 -17.196 -37.695  1.00 53.93        C
ANISOU 6217  CG1 ILE F 451     9533   6138   4820   1646  -1016   -464    C
ATOM   6218  CD1 ILE F 451      32.730 -15.935 -37.885  1.00 50.90        C
ANISOU 6218  CD1 ILE F 451     8876   5986   4479   1312   -825   -462    C
ATOM   6219  CG2 ILE F 451      35.374 -16.122 -36.407  1.00 55.21        C
ANISOU 6219  CG2 ILE F 451     9489   6589   4899   1957  -1461   -380    C
ATOM   6220  C   ILE F 451      37.132 -16.370 -38.907  1.00 55.90        C
ANISOU 6220  C   ILE F 451     8691   7179   5368   2392  -1514   -716    C
ATOM   6221  O   ILE F 451      37.752 -17.379 -39.291  1.00 58.65        O
ANISOU 6221  O   ILE F 451     9074   7433   5779   2709  -1607   -809    O
ATOM   6222  N   GLU F 452      37.737 -15.263 -38.480  1.00 55.67        N
ANISOU 6222  N   GLU F 452     8380   7424   5347   2344  -1628   -694    N
ATOM   6223  CA  GLU F 452      39.200 -15.177 -38.353  1.00 58.58        C
ANISOU 6223  CA  GLU F 452     8434   8023   5801   2651  -1892   -778    C
ATOM   6224  CB  GLU F 452      39.802 -14.454 -39.564  1.00 57.37        C
ANISOU 6224  CB  GLU F 452     7708   8270   5820   2597  -1761   -932    C
ATOM   6225  CG  GLU F 452      39.359 -12.995 -39.696  1.00 53.46        C
ANISOU 6225  CG  GLU F 452     7007   7989   5316   2209  -1603   -881    C
ATOM   6226  CD  GLU F 452      40.063 -12.246 -40.809  1.00 54.15        C
ANISOU 6226  CD  GLU F 452     6579   8455   5541   2140  -1483  -1012    C
ATOM   6227  OE1 GLU F 452      40.983 -12.807 -41.443  1.00 57.04        O
ANISOU 6227  OE1 GLU F 452     6687   8967   6017   2391  -1514  -1163    O
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Figure 18 (continued)

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ATOM   6228  OE2 GLU F 452      39.690 -11.080 -41.056  1.00 52.63           O
ANISOU 6228  OE2 GLU F 452    6251   8404   5340   1830  -1342   -966         O
ATOM   6229  C   GLU F 452      39.607 -14.457 -37.070  1.00 59.73           C
ANISOU 6229  C   GLU F 452    8632   8226   5839   2623  -2130   -681         C
ATOM   6230  O   GLU F 452      38.882 -13.574 -36.594  1.00 57.59           O
ANISOU 6230  O   GLU F 452    8458   7952   5471   2304  -2021   -587         O
ATOM   6231  N  AHIS F 453      40.760 -14.833 -36.519  0.50 63.60           N
ANISOU 6231  N  AHIS F 453    9051   8768   6344   2968  -2465   -719         N
ATOM   6232  N  BHIS F 453      40.754 -14.846 -36.516  0.50 63.68           N
ANISOU 6232  N  BHIS F 453    9067   8774   6353   2970  -2465   -718         N
ATOM   6233  CA AHIS F 453      41.336 -14.158 -35.351  0.50 65.33           C
ANISOU 6233  CA AHIS F 453    9270   9092   6462   2971  -2752   -662         C
ATOM   6234  CA BHIS F 453      41.340 -14.156 -35.367  0.50 65.46           C
ANISOU 6234  CA BHIS F 453    9280   9111   6481   2971  -2750   -664         C
ATOM   6235  CB AHIS F 453      42.466 -15.006 -34.739  0.50 70.02           C
ANISOU 6235  CB AHIS F 453    9906   9644   7055   3446  -3172   -693         C
ATOM   6236  CB BHIS F 453      42.520 -14.952 -34.789  0.50 70.22           C
ANISOU 6236  CB BHIS F 453    9888   9698   7095   3444  -3170   -705         C
ATOM   6237  CG AHIS F 453      42.950 -14.519 -33.405  0.50 71.64           C
ANISOU 6237  CG AHIS F 453   10237   9889   7094   3472  -3522   -618         C
ATOM   6238  CG BHIS F 453      42.131 -16.251 -34.150  0.50 72.40           C
ANISOU 6238  CG BHIS F 453   10795   9514   7199   3687  -3298   -573         C
ATOM   6239  ND1AHIS F 453      44.132 -13.826 -33.248  0.50 73.20           N
ANISOU 6239  ND1AHIS F 453    9938  10466   7409   3561  -3786   -748         N
ATOM   6240  ND1BHIS F 453      41.800 -16.354 -32.815  0.50 73.75           N
ANISOU 6240  ND1BHIS F 453   11506   9424   7089   3657  -3486   -390         N
ATOM   6241  CE1AHIS F 453      44.303 -13.532 -31.971  0.50 74.77           C
ANISOU 6241  CE1AHIS F 453   10403  10611   7394   3557  -4093   -655         C
ATOM   6242  CE1BHIS F 453      41.511 -17.612 -32.531  0.50 76.18           C
ANISOU 6242  CE1BHIS F 453   12349   9316   7280   3883  -3551   -290         C
ATOM   6243  NE2AHIS F 453      43.277 -14.013 -31.292  0.50 73.86           N
ANISOU 6243  NE2AHIS F 453   10957  10092   7013   3469  -4011   -461         N
ATOM   6244  NE2BHIS F 453      41.648 -18.329 -33.632  0.50 76.34           N
ANISOU 6244  NE2BHIS F 453   12183   9314   7510   4069  -3421   -416         N
ATOM   6245  CD2AHIS F 453      42.418 -14.639 -32.164  0.50 71.98           C
ANISOU 6245  CD2AHIS F 453   10857   9646   6844   3407  -3652   -438         C
ATOM   6246  CD2BHIS F 453      42.038 -17.502 -34.658  0.50 73.83           C
ANISOU 6246  CD2BHIS F 453   11192   9429   7433   3954  -3259   -597         C
ATOM   6247  C  AHIS F 453      41.856 -12.786 -35.785  0.50 64.34           C
ANISOU 6247  C  AHIS F 453    8588   9388   6470   2743  -2688   -765         C
ATOM   6248  C  BHIS F 453      41.815 -12.774 -35.816  0.50 64.27           C
ANISOU 6248  C  BHIS F 453    8581   9378   6462   2731  -2673   -764         C
ATOM   6249  O  AHIS F 453      42.515 -12.669 -36.821  0.50 64.49           O
ANISOU 6249  O  AHIS F 453    8133   9680   6690   2808  -2604   -919         O
ATOM   6250  O  BHIS F 453      42.409 -12.638 -36.887  0.50 64.21           O
ANISOU 6250  O  BHIS F 453    8108   9637   6652   2778  -2569   -914         O
ATOM   6251  N   ILE F 454      41.544 -11.752 -35.009  1.00 63.53           N
ANISOU 6251  N   ILE F 454    8571   9322   6247   2459  -2702   -686         N
ATOM   6252  CA  ILE F 454      41.980 -10.396 -35.349  1.00 63.62           C
ANISOU 6252  CA  ILE F 454    8126   9678   6370   2202  -2634   -772         C
ATOM   6253  CB  ILE F 454      40.800  -9.375 -35.410  1.00 59.86           C
ANISOU 6253  CB  ILE F 454    7791   9130   5822   1781  -2331   -683         C
ATOM   6254  CG1 ILE F 454      40.225  -9.077 -34.026  1.00 59.78           C
ANISOU 6254  CG1 ILE F 454    8229   8907   5579   1656  -2428   -563         C
ATOM   6255  CD1 ILE F 454      38.978  -8.221 -34.069  1.00 56.89           C
ANISOU 6255  CD1 ILE F 454    8015   8437   5162   1302  -2116   -495         C
ATOM   6256  CG2 ILE F 454      39.713  -9.882 -36.346  1.00 57.55           C
ANISOU 6256  CG2 ILE F 454    7631   8673   5561   1711  -2013   -646         C
ATOM   6257  C   ILE F 454      43.171  -9.893 -34.513  1.00 67.95           C
ANISOU 6257  C   ILE F 454    8445  10453   6920   2290  -2997   -844         C
ATOM   6258  O   ILE F 454      43.466 -10.413 -33.431  1.00 70.35           O
ANISOU 6258  O   ILE F 454    9035  10620   7074   2507  -3324   -789         O
ATOM   6259  N   ASP F 455      43.850  -8.885 -35.059  1.00 69.56           N
ANISOU 6259  N   ASP F 455    8140  11002   7287   2108  -2939   -971         N
ATOM   6260  CA  ASP F 455      45.062  -8.311 -34.481  1.00 74.25           C
ANISOU 6260  CA  ASP F 455    8389  11882   7940   2136  -3255  -1090         C
ATOM   6261  CB  ASP F 455      45.985  -7.824 -35.605  1.00 75.13           C
ANISOU 6261  CB  ASP F 455    7842  12386   8318   2063  -3120  -1280         C
ATOM   6262  CG  ASP F 455      46.888  -8.925 -36.144  1.00 78.46           C
ANISOU 6262  CG  ASP F 455    7952  12945   8915   2492  -3242  -1425         C
ATOM   6263  OD1 ASP F 455      47.431  -9.720 -35.339  1.00 82.36           O
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Figure 18 (continued)

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ANISOU 6263  OD1 ASP F 455     8541  13377   9374   2866  -3625  -1440      O
ATOM   6264  OD2 ASP F 455      47.073  -8.983 -37.376  1.00 77.63          O
ANISOU 6264  OD2 ASP F 455     7515  13007   8974   2469  -2960  -1531      O
ATOM   6265  C   ASP F 455      44.811  -7.167 -33.493  1.00 74.78          C
ANISOU 6265  C   ASP F 455     8634  11930   7848   1812  -3331  -1036      C
ATOM   6266  O   ASP F 455      45.644  -6.915 -32.603  1.00 78.03          O
ANISOU 6266  O   ASP F 455     8955  12477   8215   1872  -3689  -1103      O
ATOM   6267  N   ASN F 456      43.670  -6.484 -33.647  1.00 72.42          N
ANISOU 6267  N   ASN F 456     8584  11465   7468   1486  -3010   -931      N
ATOM   6268  CA  ASN F 456      43.375  -5.246 -32.898  1.00 72.87          C
ANISOU 6268  CA  ASN F 456     8779  11502   7406   1147  -3004   -908      C
ATOM   6269  CB  ASN F 456      43.194  -5.502 -31.383  1.00 74.89          C
ANISOU 6269  CB  ASN F 456     9517  11553   7382   1230  -3287   -830      C
ATOM   6270  CG  ASN F 456      41.742  -5.352 -30.921  1.00 73.35          C
ANISOU 6270  CG  ASN F 456     9857  11028   6986   1044  -3027   -684      C
ATOM   6271  OD1 ASN F 456      40.804  -5.294 -31.734  1.00 71.27          O
ANISOU 6271  OD1 ASN F 456     9614  10661   6803    923  -2671   -632      O
ATOM   6272  ND2 ASN F 456      41.555  -5.287 -29.604  1.00 75.14          N
ANISOU 6272  ND2 ASN F 456    10508  11099   6942   1020  -3208   -632      N
ATOM   6273  C   ASN F 456      44.415  -4.143 -33.156  1.00 74.75          C
ANISOU 6273  C   ASN F 456     8515  12082   7807    933  -3067  -1065      C
ATOM   6274  O   ASN F 456      45.187  -3.760 -32.261  1.00 77.82          O
ANISOU 6274  O   ASN F 456     8830  12596   8142    912  -3384  -1148      O
ATOM   6275  N   VAL F 457      44.445  -3.683 -34.408  1.00 73.51          N
ANISOU 6275  N   VAL F 457     8021  12072   7836    767  -2766  -1110      N
ATOM   6276  CA  VAL F 457      45.134  -2.453 -34.786  1.00 74.40          C
ANISOU 6276  CA  VAL F 457     7745  12439   8083    443  -2695  -1225      C
ATOM   6277  CB  VAL F 457      45.522  -2.397 -36.298  1.00 73.96          C
ANISOU 6277  CB  VAL F 457     7258  12607   8237    380  -2410  -1296      C
ATOM   6278  CG1 VAL F 457      46.942  -2.910 -36.505  1.00 77.90          C
ANISOU 6278  CG1 VAL F 457     7228  13455   8917    586  -2608  -1493      C
ATOM   6279  CG2 VAL F 457      44.528  -3.164 -37.166  1.00 71.21          C
ANISOU 6279  CG2 VAL F 457     7123  12070   7862    520  -2146  -1181      C
ATOM   6280  C   VAL F 457      44.230  -1.295 -34.377  1.00 72.20          C
ANISOU 6280  C   VAL F 457     7797  11953   7683     96  -2535  -1135      C
ATOM   6281  O   VAL F 457      43.123  -1.523 -33.872  1.00 69.99          O
ANISOU 6281  O   VAL F 457     7977  11379   7238    134  -2467  -1004      O
ATOM   6282  N   MSE F 458      44.696  -0.064 -34.577  1.00 73.06          N
ANISOU 6282  N   MSE F 458     7679  12203   7878   -244  -2463  -1216      N
ATOM   6283  CA  MSE F 458      44.062   1.090 -33.940  1.00 72.35          C
ANISOU 6283  CA  MSE F 458     7904  11914   7672   -546  -2395  -1172      C
ATOM   6284  CB  MSE F 458      44.941   2.335 -34.025  1.00 74.88          C
ANISOU 6284  CB  MSE F 458     7928  12422   8101   -907  -2406  -1306      C
ATOM   6285  CG  MSE F 458      44.687   3.283 -32.866  1.00 77.18          C
ANISOU 6285  CG  MSE F 458     8543  12541   8241  -1133  -2523  -1331      C
ATOM   6286  SE  MSE F 458      44.951   5.167 -33.288  0.90 80.31         SE
ANISOU 6286  SE  MSE F 458     8839  12926   8747  -1693  -2306  -1407      SE
ATOM   6287  CE  MSE F 458      45.046   5.835 -31.442  1.00 81.22          C
ANISOU 6287  CE  MSE F 458     9312  12907   8640  -1838  -2642  -1526      C
ATOM   6288  C   MSE F 458      42.672   1.407 -34.465  1.00 66.67          C
ANISOU 6288  C   MSE F 458     7502  10919   6910   -636  -2053  -1019      C
ATOM   6289  O   MSE F 458      42.496   1.655 -35.655  1.00 65.37          O
ANISOU 6289  O   MSE F 458     7177  10798   6862   -727  -1796   -981      O
ATOM   6290  N   GLY F 459      41.699   1.395 -33.554  1.00 63.85          N
ANISOU 6290  N   GLY F 459     7594  10290   6378   -606  -2058   -941      N
ATOM   6291  CA  GLY F 459      40.324   1.802 -33.851  1.00 58.57          C
ANISOU 6291  CA  GLY F 459     7217   9360   5679   -691  -1761   -826      C
ATOM   6292  C   GLY F 459      39.477   0.783 -34.594  1.00 54.89          C
ANISOU 6292  C   GLY F 459     6812   8810   5236   -479  -1592   -722      C
ATOM   6293  O   GLY F 459      38.386   1.107 -35.066  1.00 52.95          O
ANISOU 6293  O   GLY F 459     6711   8400   5008   -543  -1352   -643      O
ATOM   6294  N   AMSE F 460      39.968  -0.449 -34.693  0.50 54.86          N
ANISOU 6294  N   AMSE F 460     6699   8908   5236   -220  -1732   -735      N
ATOM   6295  N   BMSE F 460      39.971  -0.452 -34.680  0.50 54.79          N
ANISOU 6295  N   BMSE F 460     6693   8900   5227   -219  -1735   -736      N
ATOM   6296  CA  AMSE F 460      39.261  -1.491 -35.431  0.50 51.87          C
ANISOU 6296  CA  AMSE F 460     6376   8449   4883    -31  -1585   -662      C
ATOM   6297  CA  BMSE F 460      39.302  -1.517 -35.430  0.50 51.83          C
ANISOU 6297  CA  BMSE F 460     6363   8450   4879    -25  -1593   -665      C
ATOM   6298  CB  AMSE F 460      40.169  -2.121 -36.484  0.50 52.65          C
ANISOU 6298  CB  AMSE F 460     6093   8789   5123    111  -1605   -728      C
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Figure 18 (continued)

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ATOM   6299  CB BMSE F 460     40.281  -2.170 -36.413  0.50 52.63           C
ANISOU 6299  CB BMSE F 460   6078   8800   5119    127  -1634   -737       C
ATOM   6300  CG AMSE F 460     40.769  -1.118 -37.435  0.50 52.90           C
ANISOU 6300  CG AMSE F 460   5781   9031   5286   -116  -1474   -781       C
ATOM   6301  CG BMSE F 460     40.942  -1.184 -37.354  0.50 52.67           C
ANISOU 6301  CG BMSE F 460   5723   9028   5261    -97  -1512   -797       C
ATOM   6302 SE  AMSE F 460     40.983  -1.865 -39.199  0.45 52.53          SE
ANISOU 6302 SE  AMSE F 460   5430   9166   5364      3  -1264   -808      SE
ATOM   6303 SE  BMSE F 460     39.627  -0.349 -38.511  0.45 48.23          SE
ANISOU 6303 SE  BMSE F 460   5294   8313   4718   -315  -1143   -673      SE
ATOM   6304  CE AMSE F 460     42.271  -0.575 -39.921  0.50 54.18           C
ANISOU 6304  CE AMSE F 460   5186   9698   5701   -319  -1174   -914       C
ATOM   6305  CE BMSE F 460     40.149   1.530 -38.358  0.50 49.90           C
ANISOU 6305  CE BMSE F 460   5422   8568   4968   -714  -1105   -700       C
ATOM   6306  C   AMSE F 460     38.707  -2.567 -34.517  0.50 51.44           C
ANISOU 6306  C   AMSE F 460   6684   8191   4671    169  -1681   -606       C
ATOM   6307  C   BMSE F 460     38.711  -2.576 -34.510  0.50 51.37           C
ANISOU 6307  C   BMSE F 460   6676   8181   4661    171  -1683   -606       C
ATOM   6308  O   AMSE F 460     39.431  -3.139 -33.701  0.50 54.01           O
ANISOU 6308  O   AMSE F 460   7068   8548   4908    330  -1952   -636       O
ATOM   6309  O   BMSE F 460     39.417  -3.146 -33.677  0.50 53.95           O
ANISOU 6309  O   BMSE F 460   7068   8534   4895    330  -1953   -635       O
ATOM   6310  N    VAL F 461     37.413  -2.830 -34.656  1.00 48.69           N
ANISOU 6310  N    VAL F 461   6584   7631   4285    151  -1461   -525       N
ATOM   6311  CA   VAL F 461     36.770  -3.939 -33.955  1.00 47.45           C
ANISOU 6311  CA   VAL F 461   6786   7259   3984    298  -1478   -464       C
ATOM   6312  CB   VAL F 461     35.734  -3.470 -32.897  1.00 47.00           C
ANISOU 6312  CB   VAL F 461   7111   6980   3768    144  -1360   -424       C
ATOM   6313  CG1  VAL F 461     36.434  -2.715 -31.786  1.00 49.19           C
ANISOU 6313  CG1  VAL F 461   7483   7296   3912     62  -1566   -471       C
ATOM   6314  CG2  VAL F 461     34.645  -2.627 -33.519  1.00 44.93           C
ANISOU 6314  CG2  VAL F 461   6793   6661   3616    -36  -1068   -416       C
ATOM   6315  C    VAL F 461     36.194  -4.970 -34.930  1.00 45.12           C
ANISOU 6315  C    VAL F 461   6467   6905   3770    421  -1327   -434       C
ATOM   6316  O    VAL F 461     35.935  -4.679 -36.100  1.00 43.35           O
ANISOU 6316  O    VAL F 461   6011   6774   3686    357  -1162   -447       O
ATOM   6317  N    GLY F 462     36.044  -6.197 -34.453  1.00 45.10           N
ANISOU 6317  N    GLY F 462   6732   6740   3664    596  -1399   -395       N
ATOM   6318  CA   GLY F 462     35.452  -7.240 -35.259  1.00 42.67           C
ANISOU 6318  CA   GLY F 462   6463   6335   3417    690  -1260   -382       C
ATOM   6319  C    GLY F 462     33.953  -7.209 -35.132  1.00 40.00           C
ANISOU 6319  C    GLY F 462   6361   5797   3042    512   -999   -335       C
ATOM   6320  O    GLY F 462     33.413  -6.646 -34.174  1.00 40.52           O
ANISOU 6320  O    GLY F 462   6646   5756   2995    370   -939   -306       O
ATOM   6321  N    VAL F 463     33.287  -7.800 -36.113  1.00 37.67           N
ANISOU 6321  N    VAL F 463   6002   5468   2845    514   -838   -350       N
ATOM   6322  CA   VAL F 463     31.848  -8.005 -36.073  1.00 35.82           C
ANISOU 6322  CA   VAL F 463   5947   5057   2604    360   -600   -333       C
ATOM   6323  CB   VAL F 463     31.095  -7.040 -37.020  1.00 33.67           C
ANISOU 6323  CB   VAL F 463   5405   4907   2481    210   -430   -364       C
ATOM   6324  CG1  VAL F 463     31.567  -7.173 -38.489  1.00 32.45           C
ANISOU 6324  CG1  VAL F 463   4944   4937   2447    292   -457   -406       C
ATOM   6325  CG2  VAL F 463     29.608  -7.232 -36.898  1.00 33.01           C
ANISOU 6325  CG2  VAL F 463   5453   4672   2418     63   -204   -375       C
ATOM   6326  C    VAL F 463     31.552  -9.483 -36.370  1.00 36.17           C
ANISOU 6326  C    VAL F 463   6172   4936   2636    457   -567   -337       C
ATOM   6327  O    VAL F 463     32.101 -10.045 -37.313  1.00 36.03           O
ANISOU 6327  O    VAL F 463   5987   5003   2702    603   -633   -384       O
ATOM   6328  N    LEU F 464     30.720 -10.110 -35.536  1.00 36.36           N
ANISOU 6328  N    LEU F 464   6560   4711   2543    365   -452   -297       N
ATOM   6329  CA   LEU F 464     30.401 -11.533 -35.679  1.00 37.09           C
ANISOU 6329  CA   LEU F 464   6903   4585   2604    418   -409   -295       C
ATOM   6330  CB   LEU F 464     30.195 -12.174 -34.286  1.00 39.07           C
ANISOU 6330  CB   LEU F 464   7666   4549   2628    385   -405   -204       C
ATOM   6331  CG   LEU F 464     31.419 -12.196 -33.354  1.00 40.94           C
ANISOU 6331  CG   LEU F 464   8086   4773   2696    599   -705   -130       C
ATOM   6332  CD1  LEU F 464     31.091 -12.743 -31.939  1.00 43.14           C
ANISOU 6332  CD1  LEU F 464   8942   4755   2695    535   -688    -20       C
ATOM   6333  CD2  LEU F 464     32.590 -12.974 -33.978  1.00 41.49           C
ANISOU 6333  CD2  LEU F 464   8040   4887   2837    924   -961   -154       C
ATOM   6334  C    LEU F 464     29.185 -11.752 -36.603  1.00 35.79           C
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Figure 18 (continued)

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ANISOU 6334  C   LEU F 464     6614   4407   2578    242   -171   -368       C
ATOM   6335  O   LEU F 464      28.472 -10.801 -36.896  1.00 33.02           O
ANISOU 6335  O   LEU F 464     6037   4188   2322     87    -41   -402       O
ATOM   6336  N   PRO F 465      28.971 -12.999 -37.096  1.00 37.43           N
ANISOU 6336  N   PRO F 465     6964   4455   2802    278   -137   -405       N
ATOM   6337  CA  PRO F 465      27.800 -13.306 -37.943  1.00 37.58           C
ANISOU 6337  CA  PRO F 465     6875   4460   2944     89     62   -496       C
ATOM   6338  CB  PRO F 465      27.950 -14.814 -38.211  1.00 39.80           C
ANISOU 6338  CB  PRO F 465     7426   4504   3193    175     38   -526       C
ATOM   6339  CG  PRO F 465      29.420 -15.040 -38.140  1.00 39.49           C
ANISOU 6339  CG  PRO F 465     7412   4494   3099    501   -217   -486       C
ATOM   6340  CD  PRO F 465      29.850 -14.180 -36.969  1.00 39.01           C
ANISOU 6340  CD  PRO F 465     7417   4482   2924    517   -307   -380       C
ATOM   6341  C   PRO F 465      26.410 -12.985 -37.360  1.00 38.58           C
ANISOU 6341  C   PRO F 465     7067   4510   3081   -204    314   -511       C
ATOM   6342  O   PRO F 465      25.432 -12.960 -38.117  1.00 38.80           O
ANISOU 6342  O   PRO F 465     6890   4606   3248   -359    449   -608       O
ATOM   6343  N   ASP F 466      26.316 -12.749 -36.047  1.00 39.71           N
ANISOU 6343  N   ASP F 466     7482   4529   3078   -278    375   -433       N
ATOM   6344  CA  ASP F 466      25.076 -12.246 -35.431  1.00 39.99           C
ANISOU 6344  CA  ASP F 466     7530   4535   3128   -543    642   -469       C
ATOM   6345  CB  ASP F 466      24.733 -13.040 -34.157  1.00 42.38           C
ANISOU 6345  CB  ASP F 466     8343   4540   3221   -688    795   -405       C
ATOM   6346  CG  ASP F 466      25.745 -12.838 -33.026  1.00 43.25           C
ANISOU 6346  CG  ASP F 466     8774   4573   3086   -539    618   -276       C
ATOM   6347  OD1 ASP F 466      26.686 -12.035 -33.161  1.00 40.47           O
ANISOU 6347  OD1 ASP F 466     8215   4411   2751   -348    390   -255       O
ATOM   6348  OD2 ASP F 466      25.589 -13.493 -31.976  1.00 46.27           O
ANISOU 6348  OD2 ASP F 466     9636   4699   3245   -632    706   -198       O
ATOM   6349  C   ASP F 466      25.070 -10.709 -35.183  1.00 38.76           C
ANISOU 6349  C   ASP F 466     7126   4585   3017   -543    641   -473       C
ATOM   6350  O   ASP F 466      24.221 -10.195 -34.450  1.00 39.42           O
ANISOU 6350  O   ASP F 466     7256   4637   3087   -715    852   -505       O
ATOM   6351  N   MSE F 467      26.016 -10.007 -35.819  1.00 37.33           N
ANISOU 6351  N   MSE F 467     6690   4601   2894   -358    423   -453       N
ATOM   6352  CA  MSE F 467      26.170  -8.534 -35.809  1.00 35.96           C
ANISOU 6352  CA  MSE F 467     6277   4607   2779   -345    387   -455       C
ATOM   6353  CB  MSE F 467      24.899  -7.811 -36.252  1.00 35.73           C
ANISOU 6353  CB  MSE F 467     5992   4658   2926   -482    577   -541       C
ATOM   6354  CG  MSE F 467      24.737  -7.701 -37.761  1.00 34.64           C
ANISOU 6354  CG  MSE F 467     5513   4688   2961   -427    503   -584       C
ATOM   6355  SE  MSE F 467      26.345  -7.142 -38.729  0.90 36.20          SE
ANISOU 6355  SE  MSE F 467     5518   5088   3149   -218    224   -515       SE
ATOM   6356  CE  MSE F 467      26.525  -5.301 -38.059  1.00 32.31           C
ANISOU 6356  CE  MSE F 467     4958   4657   2664   -246    217   -475       C
ATOM   6357  C   MSE F 467      26.703  -7.992 -34.476  1.00 37.22           C
ANISOU 6357  C   MSE F 467     6683   4702   2756   -343    341   -397       C
ATOM   6358  O   MSE F 467      26.687  -6.785 -34.186  1.00 35.87           O
ANISOU 6358  O   MSE F 467     6406   4617   2608   -377    355   -413       O
ATOM   6359  N   THR F 468      27.215  -8.919 -33.687  1.00 39.05           N
ANISOU 6359  N   THR F 468     7274   4768   2795   -291    262   -331       N
ATOM   6360  CA  THR F 468      27.716  -8.634 -32.358  1.00 40.94           C
ANISOU 6360  CA  THR F 468     7827   4923   2805   -287    187   -272       C
ATOM   6361  CB  THR F 468      27.372  -9.857 -31.476  1.00 43.19           C
ANISOU 6361  CB  THR F 468     8602   4931   2878   -353    280   -210       C
ATOM   6362  OG1 THR F 468      26.274  -9.513 -30.624  1.00 44.16           O
ANISOU 6362  OG1 THR F 468     8907   4957   2915   -594    586   -247       O
ATOM   6363  CG2 THR F 468      28.546 -10.408 -30.685  1.00 46.31           C
ANISOU 6363  CG2 THR F 468     9341   5221   3032   -165    -11   -103       C
ATOM   6364  C   THR F 468      29.201  -8.251 -32.487  1.00 40.62           C
ANISOU 6364  C   THR F 468     7654   5035   2745    -81   -147   -239       C
ATOM   6365  O   THR F 468      29.894  -8.776 -33.364  1.00 40.74           O
ANISOU 6365  O   THR F 468     7490   5133   2857     84   -302   -238       O
ATOM   6366  N   PRO F 469      29.679  -7.295 -31.671  1.00 41.09           N
ANISOU 6366  N   PRO F 469     7766   5150   2694   -102   -242   -236       N
ATOM   6367  CA  PRO F 469      31.083  -6.882 -31.768  1.00 41.16           C
ANISOU 6367  CA  PRO F 469     7605   5330   2704     54   -555   -230       C
ATOM   6368  CB  PRO F 469      31.077  -5.503 -31.123  1.00 40.81           C
ANISOU 6368  CB  PRO F 469     7543   5347   2614   -81   -534   -273       C
ATOM   6369  CG  PRO F 469      30.006  -5.598 -30.079  1.00 42.91           C
ANISOU 6369  CG  PRO F 469     8187   5411   2707   -237   -295   -271       C
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Figure 18 (continued)

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ATOM   6370  CD  PRO F 469      28.964  -6.555 -30.615  1.00 42.09           C
ANISOU 6370  CD  PRO F 469    8108   5193   2693   -283    -58   -262        C
ATOM   6371  C   PRO F 469      32.038  -7.820 -30.998  1.00 43.78           C
ANISOU 6371  C   PRO F 469    8232   5571   2832    239   -831   -163        C
ATOM   6372  O   PRO F 469      31.609  -8.515 -30.066  1.00 45.55           O
ANISOU 6372  O   PRO F 469    8901   5569   2839    206   -778    -99        O
ATOM   6373  N   SER F 470      33.313  -7.825 -31.394  1.00 43.90           N
ANISOU 6373  N   SER F 470    8000   5762   2916    433  -1119   -181        N
ATOM   6374  CA  SER F 470      34.346  -8.639 -30.751  1.00 46.64           C
ANISOU 6374  CA  SER F 470    8551   6062   3110    671  -1446   -135        C
ATOM   6375  CB  SER F 470      34.315 -10.073 -31.297  1.00 47.59           C
ANISOU 6375  CB  SER F 470    8779   6031   3271    863  -1454    -97        C
ATOM   6376  OG  SER F 470      35.473 -10.807 -30.918  1.00 49.69           O
ANISOU 6376  OG  SER F 470    9140   6283   3454   1168  -1812    -71        O
ATOM   6377  C   SER F 470      35.752  -8.045 -30.913  1.00 47.35           C
ANISOU 6377  C   SER F 470    8278   6429   3286    805  -1756   -203        C
ATOM   6378  O   SER F 470      36.105  -7.528 -31.963  1.00 45.73           O
ANISOU 6378  O   SER F 470    7626   6442   3306    790  -1714   -278        O
ATOM   6379  N   THR F 471      36.553  -8.143 -29.862  1.00 50.52           N
ANISOU 6379  N   THR F 471    8881   6821   3494    925  -2070   -182        N
ATOM   6380  CA  THR F 471      37.935  -7.704 -29.919  1.00 52.23           C
ANISOU 6380  CA  THR F 471    8738   7311   3795   1058  -2399   -268        C
ATOM   6381  CB  THR F 471      38.370  -7.063 -28.571  1.00 54.64           C
ANISOU 6381  CB  THR F 471    9275   7631   3857    989  -2649   -274        C
ATOM   6382  OG1 THR F 471      38.127  -7.985 -27.503  1.00 57.14           O
ANISOU 6382  OG1 THR F 471   10164   7680   3867   1111  -2776   -156        O
ATOM   6383  CG2 THR F 471      37.604  -5.758 -28.297  1.00 51.68           C
ANISOU 6383  CG2 THR F 471    8940   7250   3448    642  -2391   -311        C
ATOM   6384  C   THR F 471      38.872  -8.866 -30.315  1.00 54.76           C
ANISOU 6384  C   THR F 471    8937   7670   4198   1425  -2659   -278        C
ATOM   6385  O   THR F 471      40.081  -8.673 -30.459  1.00 56.74           O
ANISOU 6385  O   THR F 471    8822   8174   4560   1580  -2936   -374        O
ATOM   6386  N   GLU F 472      38.310 -10.061 -30.502  1.00 55.20           N
ANISOU 6386  N   GLU F 472    9286   7473   4215   1560  -2559   -198        N
ATOM   6387  CA  GLU F 472      39.103 -11.273 -30.764  1.00 58.61           C
ANISOU 6387  CA  GLU F 472    9708   7861   4701   1944  -2804   -203        C
ATOM   6388  CB  GLU F 472      38.944 -12.273 -29.615  1.00 61.64           C
ANISOU 6388  CB  GLU F 472   10735   7900   4787   2108  -2991    -57        C
ATOM   6389  CG  GLU F 472      39.602 -11.834 -28.294  1.00 66.05           C
ANISOU 6389  CG  GLU F 472   11497   8504   5096   2156  -3355    -23        C
ATOM   6390  CD  GLU F 472      39.044 -12.577 -27.088  1.00 68.99           C
ANISOU 6390  CD  GLU F 472   12632   8493   5089   2173  -3414    155        C
ATOM   6391  OE1 GLU F 472      39.536 -12.355 -25.958  1.00 74.88           O
ANISOU 6391  OE1 GLU F 472   13642   9238   5571   2229  -3734    199        O
ATOM   6392  OE2 GLU F 472      38.110 -13.393 -27.270  1.00 70.96           O
ANISOU 6392  OE2 GLU F 472   13234   8438   5289   2110  -3138    248        O
ATOM   6393  C   GLU F 472      38.814 -11.965 -32.106  1.00 56.75           C
ANISOU 6393  C   GLU F 472    9268   7606   4689   2022  -2575   -253        C
ATOM   6394  O   GLU F 472      39.740 -12.338 -32.826  0.50 57.96           O
ANISOU 6394  O   GLU F 472    9067   7930   5026   2279  -2713   -356        O
ATOM   6395  N   AMSE F 473      37.538 -12.106 -32.442  0.50 54.05           N
ANISOU 6395  N   AMSE F 473    9129   7077   4333   1792  -2225   -203        N
ATOM   6396  N   BMSE F 473      37.527 -12.152 -32.413  0.50 54.67           N
ANISOU 6396  N   BMSE F 473    9227   7140   4403   1798  -2228   -198        N
ATOM   6397  CA  AMSE F 473      37.154 -12.767 -33.686  0.50 52.38           C
ANISOU 6397  CA  AMSE F 473    8771   6831   4299   1830  -2013   -259        C
ATOM   6398  CA  BMSE F 473      37.061 -12.837 -33.638  0.50 53.57           C
ANISOU 6398  CA  BMSE F 473    8970   6950   4436   1823  -2000   -249        C
ATOM   6399  CB  AMSE F 473      36.349 -14.042 -33.398  0.50 53.56           C
ANISOU 6399  CB  AMSE F 473    9451   6579   4320   1866  -1917   -167        C
ATOM   6400  CB  BMSE F 473      36.126 -14.020 -33.278  0.50 54.56           C
ANISOU 6400  CB  BMSE F 473    9648   6665   4417   1812  -1876   -149        C
ATOM   6401  CG  AMSE F 473      37.019 -15.032 -32.430  0.50 57.16           C
ANISOU 6401  CG  AMSE F 473   10331   6794   4594   2182  -2241    -77        C
ATOM   6402  CG  BMSE F 473      36.799 -15.413 -33.076  0.50 59.08           C
ANISOU 6402  CG  BMSE F 473   10512   7000   4934   2193  -2125   -118        C
ATOM   6403  SE  AMSE F 473      38.682 -15.802 -33.103  0.45 58.91          SE
ANISOU 6403  SE  AMSE F 473   10192   7173   5018   2733  -2611   -206        SE
ATOM   6404  SE  BMSE F 473      35.701 -16.903 -32.302  0.45 62.74          SE
ANISOU 6404  SE  BMSE F 473   11838   6858   5142   2138  -1994     50        SE
ATOM   6405  CE  AMSE F 473      37.985 -17.029 -34.440  0.50 58.03           C
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Figure 18 (continued)

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ANISOU 6405  CE AMSE F 473    10158   6829   5063   2774  -2311   -279       C
ATOM   6406  CE BMSE F 473      34.039 -16.732 -33.323  0.50 58.44           C
ANISOU 6406  CE BMSE F 473    11168   6293   4743   1680  -1460    -22       C
ATOM   6407  C  AMSE F 473      36.353 -11.826 -34.583  0.50 48.62           C
ANISOU 6407  C  AMSE F 473     7996   6515   3962   1519  -1691   -310       C
ATOM   6408  C  BMSE F 473      36.326 -11.854 -34.571  0.50 49.21           C
ANISOU 6408  C  BMSE F 473     8085   6580   4033   1518  -1688   -307       C
ATOM   6409  O  AMSE F 473      35.756 -10.854 -34.118  0.50 46.99           O
ANISOU 6409  O  AMSE F 473     7827   6334   3694   1260  -1572   -275       O
ATOM   6410  O  BMSE F 473      35.750 -10.866 -34.112  0.50 47.60           O
ANISOU 6410  O  BMSE F 473     7908   6407   3769   1261  -1572   -274       O
ATOM   6411  N   SER F 474      36.355 -12.116 -35.876  1.00 47.59           N
ANISOU 6411  N   SER F 474     7586   6486   4008   1564  -1563   -398       N
ATOM   6412  CA  SER F 474      35.584 -11.319 -36.852  1.00 44.33           C
ANISOU 6412  CA  SER F 474     6917   6214   3712   1304  -1290   -437       C
ATOM   6413  CB  SER F 474      36.392 -10.097 -37.301  1.00 43.46           C
ANISOU 6413  CB  SER F 474     6360   6443   3709   1243  -1335   -499       C
ATOM   6414  OG  SER F 474      35.624  -9.222 -38.089  1.00 39.78           O
ANISOU 6414  OG  SER F 474     5726   6072   3317    997  -1104   -503       O
ATOM   6415  C   SER F 474      35.225 -12.160 -38.070  1.00 43.77           C
ANISOU 6415  C   SER F 474     6781   6105   3745   1359  -1143   -510       C
ATOM   6416  O   SER F 474      35.885 -13.164 -38.345  1.00 45.97           O
ANISOU 6416  O   SER F 474     7084   6329   4052   1623  -1256   -566       O
ATOM   6417  N   MSE F 475      34.196 -11.754 -38.806  1.00 41.25           N
ANISOU 6417  N   MSE F 475     6380   5813   3480   1127   -909   -523       N
ATOM   6418  CA  MSE F 475      34.003 -12.291 -40.149  1.00 40.97           C
ANISOU 6418  CA  MSE F 475     6197   5831   3539   1157   -792   -619       C
ATOM   6419  CB  MSE F 475      32.693 -11.806 -40.771  1.00 38.57           C
ANISOU 6419  CB  MSE F 475     5849   5536   3270    888   -576   -618       C
ATOM   6420  CG  MSE F 475      31.457 -12.502 -40.205  1.00 38.53           C
ANISOU 6420  CG  MSE F 475     6187   5241   3212    749   -456   -585       C
ATOM   6421 SE   MSE F 475      29.784 -11.880 -40.999  0.90 37.77          SE
ANISOU 6421 SE   MSE F 475     5943   5203   3204    437   -222   -623      SE
ATOM   6422  CE  MSE F 475      29.784 -10.021 -40.369  1.00 34.50           C
ANISOU 6422  CE  MSE F 475     5347   4962   2799    318   -223   -536       C
ATOM   6423  C   MSE F 475      35.210 -11.913 -41.018  1.00 41.26           C
ANISOU 6423  C   MSE F 475     5836   6174   3668   1296   -861   -711       C
ATOM   6424  O   MSE F 475      35.709 -10.786 -40.947  1.00 40.52           O
ANISOU 6424  O   MSE F 475     5499   6296   3600   1209   -892   -694       O
ATOM   6425  N   ARG F 476      35.662 -12.871 -41.825  1.00 42.54           N
ANISOU 6425  N   ARG F 476     5947   6338   3877   1494   -862   -821       N
ATOM   6426  CA  ARG F 476      36.908 -12.783 -42.592  1.00 43.25           C
ANISOU 6426  CA  ARG F 476     5676   6704   4054   1670   -906   -942       C
ATOM   6427  CB  ARG F 476      37.047 -14.035 -43.462  1.00 44.93           C
ANISOU 6427  CB  ARG F 476     5941   6831   4299   1877   -855  -1078       C
ATOM   6428  CG  ARG F 476      38.089 -13.966 -44.568  1.00 47.16           C
ANISOU 6428  CG  ARG F 476     5839   7416   4664   2010   -797  -1241       C
ATOM   6429  CD  ARG F 476      38.138 -15.267 -45.379  1.00 48.80           C
ANISOU 6429  CD  ARG F 476     6156   7498   4889   2224   -733  -1397       C
ATOM   6430  NE  ARG F 476      36.829 -15.772 -45.815  1.00 48.30           N
ANISOU 6430  NE  ARG F 476     6394   7206   4752   2046   -602  -1383       N
ATOM   6431  CZ  ARG F 476      36.126 -15.297 -46.843  1.00 47.93           C
ANISOU 6431  CZ  ARG F 476     6261   7289   4660   1803   -431  -1409       C
ATOM   6432  NH1 ARG F 476      36.574 -14.273 -47.565  1.00 48.79          N
ANISOU 6432  NH1 ARG F 476     6042   7730   4765   1693   -345  -1425       N
ATOM   6433  NH2 ARG F 476      34.962 -15.848 -47.154  1.00 46.79          N
ANISOU 6433  NH2 ARG F 476     6372   6939   4466   1657   -353  -1419       N
ATOM   6434  C   ARG F 476      37.030 -11.498 -43.416  1.00 41.10           C
ANISOU 6434  C   ARG F 476     5060   6740   3817   1453   -777   -953       C
ATOM   6435  O   ARG F 476      36.182 -11.199 -44.258  1.00 39.12           O
ANISOU 6435  O   ARG F 476     4810   6511   3545   1266   -612   -945       O
ATOM   6436  N   GLY F 477      38.082 -10.733 -43.140  1.00 41.43           N
ANISOU 6436  N   GLY F 477     4825   7009   3906   1471   -870   -969       N
ATOM   6437  CA  GLY F 477      38.354  -9.486 -43.850  1.00 40.53           C
ANISOU 6437  CA  GLY F 477     4413   7168   3820   1250   -748   -972       C
ATOM   6438  C   GLY F 477      37.457  -8.303 -43.526  1.00 37.97           C
ANISOU 6438  C   GLY F 477     4192   6789   3447    958   -686   -834       C
ATOM   6439  O   GLY F 477      37.588  -7.235 -44.118  1.00 37.40           O
ANISOU 6439  O   GLY F 477     3939   6888   3383    765   -584   -814       O
ATOM   6440  N   ILE F 478      36.549  -8.489 -42.574  1.00 37.64           N
ANISOU 6440  N   ILE F 478     4456   6494   3350    927   -734   -743       N
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Figure 18 (continued)

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ATOM   6441  CA  ILE F 478      35.552  -7.457 -42.189  1.00 35.63           C
ANISOU 6441  CA  ILE F 478    4320   6155   3064    685   -661   -635       C
ATOM   6442  CB  ILE F 478      34.126  -8.080 -42.125  1.00 34.02           C
ANISOU 6442  CB  ILE F 478    4389   5711   2826    640   -565   -600       C
ATOM   6443  CG1 ILE F 478      33.806  -8.827 -43.435  1.00 33.55           C
ANISOU 6443  CG1 ILE F 478    4276   5687   2784    683   -466   -676       C
ATOM   6444  CD1 ILE F 478      33.521  -7.945 -44.656  1.00 30.29           C
ANISOU 6444  CD1 ILE F 478    3677   5452   2378    537   -355   -670       C
ATOM   6445  CG2 ILE F 478      33.074  -7.027 -41.766  1.00 33.10           C
ANISOU 6445  CG2 ILE F 478    4345   5524   2706    427   -477   -518       C
ATOM   6446  C   ILE F 478      35.903  -6.782 -40.854  1.00 36.01           C
ANISOU 6446  C   ILE F 478    4438   6165   3079    636   -794   -583       C
ATOM   6447  O   ILE F 478      35.986  -7.446 -39.812  1.00 37.11           O
ANISOU 6447  O   ILE F 478    4791   6153   3155    758   -925   -568       O
ATOM   6448  N   ARG F 479      36.123  -5.467 -40.889  1.00 35.61           N
ANISOU 6448  N   ARG F 479    4243   6236   3052    452   -766   -558       N
ATOM   6449  CA  ARG F 479      36.358  -4.678 -39.648  1.00 35.25           C
ANISOU 6449  CA  ARG F 479    4285   6146   2962    361   -880   -526       C
ATOM   6450  CB  ARG F 479      37.771  -4.102 -39.604  1.00 37.00           C
ANISOU 6450  CB  ARG F 479    4220   6604   3234    340  -1006   -596       C
ATOM   6451  CG  ARG F 479      38.905  -5.105 -39.660  1.00 39.51           C
ANISOU 6451  CG  ARG F 479    4354   7064   3594    589  -1165   -694       C
ATOM   6452  CD  ARG F 479      38.890  -6.113 -38.506  1.00 39.37           C
ANISOU 6452  CD  ARG F 479    4610   6863   3485    811  -1371   -676       C
ATOM   6453  NE  ARG F 479      39.992  -7.062 -38.667  1.00 43.02           N
ANISOU 6453  NE  ARG F 479    4879   7454   4013   1100  -1539   -778       N
ATOM   6454  CZ  ARG F 479      39.943  -8.180 -39.394  1.00 42.54           C
ANISOU 6454  CZ  ARG F 479    4821   7349   3992   1310  -1482   -822       C
ATOM   6455  NH1 ARG F 479      38.836  -8.535 -40.045  1.00 39.17           N
ANISOU 6455  NH1 ARG F 479    4582   6764   3539   1240  -1271   -774       N
ATOM   6456  NH2 ARG F 479      41.014  -8.951 -39.460  1.00 44.32           N
ANISOU 6456  NH2 ARG F 479    4855   7691   4295   1600  -1648   -933       N
ATOM   6457  C   ARG F 479      35.379  -3.518 -39.523  1.00 33.52           C
ANISOU 6457  C   ARG F 479    4176   5824   2735    141   -749   -457       C
ATOM   6458  O   ARG F 479      34.960  -2.946 -40.533  1.00 33.11           O
ANISOU 6458  O   ARG F 479    4023   5824   2735     39   -613   -431       O
ATOM   6459  N   VAL F 480      35.010  -3.170 -38.293  1.00 33.05           N
ANISOU 6459  N   VAL F 480    4342   5614   2601     83   -794   -431       N
ATOM   6460  CA  VAL F 480      34.211  -1.973 -38.054  1.00 31.67           C
ANISOU 6460  CA  VAL F 480    4261   5340   2433   -100   -679   -394       C
ATOM   6461  CB  VAL F 480      32.975  -2.270 -37.150  1.00 31.19           C
ANISOU 6461  CB  VAL F 480    4503   5047   2302   -107   -586   -373       C
ATOM   6462  CG1 VAL F 480      32.299  -0.976 -36.650  1.00 29.99           C
ANISOU 6462  CG1 VAL F 480    4449   4788   2157   -263   -483   -369       C
ATOM   6463  CG2 VAL F 480      31.966  -3.168 -37.871  1.00 30.56           C
ANISOU 6463  CG2 VAL F 480    4439   4902   2268    -46   -452   -362       C
ATOM   6464  C   VAL F 480      35.128  -0.915 -37.429  1.00 32.95           C
ANISOU 6464  C   VAL F 480    4368   5575   2578   -225   -792   -424       C
ATOM   6465  O   VAL F 480      35.745  -1.151 -36.395  1.00 34.11           O
ANISOU 6465  O   VAL F 480    4604   5721   2637   -182   -961   -460       O
ATOM   6466  N   SER F 481      35.233   0.241 -38.068  1.00 33.25           N
ANISOU 6466  N   SER F 481    4278   5667   2688   -388   -713   -411       N
ATOM   6467  CA  SER F 481      36.017   1.336 -37.502  1.00 35.24           C
ANISOU 6467  CA  SER F 481    4499   5958   2933   -559   -797   -452       C
ATOM   6468  CB  SER F 481      36.437   2.355 -38.572  1.00 35.71           C
ANISOU 6468  CB  SER F 481    4370   6117   3082   -738   -702   -431       C
ATOM   6469  OG  SER F 481      37.145   3.457 -37.988  1.00 38.65           O
ANISOU 6469  OG  SER F 481    4738   6495   3454   -948   -769   -482       O
ATOM   6470  C   SER F 481      35.306   2.040 -36.341  1.00 35.43           C
ANISOU 6470  C   SER F 481    4816   5766   2882   -645   -777   -459       C
ATOM   6471  O   SER F 481      34.117   2.366 -36.409  1.00 34.16           O
ANISOU 6471  O   SER F 481    4805   5434   2740   -653   -618   -419       O
ATOM   6472  N   LYS F 482      36.073   2.261 -35.283  1.00 37.40           N
ANISOU 6472  N   LYS F 482    5126   6040   3045   -702   -948   -528       N
ATOM   6473  CA  LYS F 482      35.676   3.070 -34.149  1.00 38.68           C
ANISOU 6473  CA  LYS F 482    5562   6025   3110   -819   -945   -569       C
ATOM   6474  CB  LYS F 482      36.268   2.482 -32.863  1.00 40.92           C
ANISOU 6474  CB  LYS F 482    5998   6331   3219   -756  -1171   -627       C
ATOM   6475  CG  LYS F 482      35.631   1.192 -32.366  1.00 43.46           C
ANISOU 6475  CG  LYS F 482    6540   6556   3418   -560  -1164   -577       C
ATOM   6476  CD  LYS F 482      34.408   1.466 -31.467  1.00 47.95           C
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Figure 18 (continued)

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ANISOU 6476  CD  LYS F 482     7475   6881   3862   -619   -984   -579      C
ATOM   6477  CE  LYS F 482      33.121   1.568 -32.297  1.00 47.40          C
ANISOU 6477  CE  LYS F 482     7363   6708   3938   -612   -696   -534      C
ATOM   6478  NZ  LYS F 482      32.024   2.121 -31.458  1.00 48.36          N
ANISOU 6478  NZ  LYS F 482     7761   6627   3987   -690   -499   -580      N
ATOM   6479  C   LYS F 482      36.172   4.524 -34.290  1.00 39.57          C
ANISOU 6479  C   LYS F 482     5613   6135   3288  -1061   -935   -613      C
ATOM   6480  O   LYS F 482      35.963   5.337 -33.378  1.00 40.79          O
ANISOU 6480  O   LYS F 482     5995   6137   3367  -1181   -937   -673      O
ATOM   6481  N   MSE F 483      36.839   4.848 -35.404  1.00 38.62          N
ANISOU 6481  N   MSE F 483     5216   6167   3290  -1150   -910   -591      N
ATOM   6482  CA  MSE F 483      37.361   6.208 -35.607  1.00 39.11          C
ANISOU 6482  CA  MSE F 483     5242   6208   3412  -1419   -881   -623      C
ATOM   6483  CB  MSE F 483      38.321   6.273 -36.805  1.00 39.75          C
ANISOU 6483  CB  MSE F 483     4987   6519   3599  -1525   -853   -609      C
ATOM   6484  CG  MSE F 483      39.626   5.497 -36.598  1.00 41.96          C
ANISOU 6484  CG  MSE F 483     4958   7098   3887  -1482  -1052   -714      C
ATOM   6485 SE   MSE F 483      40.539   5.770 -34.876  0.90 50.05         SE
ANISOU 6485 SE   MSE F 483     6036   8169   4812  -1584  -1372   -884     SE
ATOM   6486  CE  MSE F 483      41.373   7.511 -35.168  1.00 48.50          C
ANISOU 6486  CE  MSE F 483     5726   7986   4714  -2058  -1303   -969      C
ATOM   6487  C   MSE F 483      36.227   7.226 -35.749  1.00 37.49          C
ANISOU 6487  C   MSE F 483     5289   5719   3238  -1481   -693   -566      C
ATOM   6488  O   MSE F 483      35.094   6.823 -36.053  1.00 35.28          O
ANISOU 6488  O   MSE F 483     5099   5332   2975  -1307   -572   -494      O
ATOM   6489  OXT MSE F 483      36.389   8.431 -35.532  1.00 37.47          O
ANISOU 6489  OXT MSE F 483     5406   5580   3252  -1689   -668   -602      O
ATOM   6490  O2G MGT A   1      48.431  21.314 -32.822  1.00 51.34          O
ANISOU 6490  O2G MGT A   1     5580   7344   6582   -151    662    268      O
ATOM   6491  PG  MGT A   1      47.642  21.644 -31.468  1.00 49.83          P
ANISOU 6491  PG  MGT A   1     5455   6960   6518   -139    518    275      P
ATOM   6492  O3G MGT A   1      46.906  20.295 -30.960  1.00 45.91          O
ANISOU 6492  O3G MGT A   1     5042   6412   5989     23    408    176      O
ATOM   6493  O1G MGT A   1      48.607  22.186 -30.469  1.00 50.23          O
ANISOU 6493  O1G MGT A   1     5363   7007   6715   -196    508    226      O
ATOM   6494  O3B MGT A   1      46.392  22.571 -31.946  1.00 49.90          O
ANISOU 6494  O3B MGT A   1     5618   6851   6491   -212    497    434      O
ATOM   6495  PB  MGT A   1      46.500  23.966 -32.785  1.00 50.34          P
ANISOU 6495  PB  MGT A   1     5693   6896   6537   -368    593    604      P
ATOM   6496  O2B MGT A   1      46.307  23.569 -34.337  1.00 50.62          O
ANISOU 6496  O2B MGT A   1     5793   7073   6368   -354    675    667      O
ATOM   6497  O1B MGT A   1      47.806  24.652 -32.528  1.00 51.47          O
ANISOU 6497  O1B MGT A   1     5686   7087   6785   -486    681    592      O
ATOM   6498  O3A MGT A   1      45.229  24.838 -32.232  1.00 49.00          O
ANISOU 6498  O3A MGT A   1     5651   6519   6447   -386    490    701      O
ATOM   6499  PA  MGT A   1      43.722  24.280 -31.756  1.00 44.78          P
ANISOU 6499  PA  MGT A   1     5239   5880   5896   -269    352    675      P
ATOM   6500  O2A MGT A   1      43.564  22.796 -32.345  1.00 45.17          O
ANISOU 6500  O2A MGT A   1     5307   6056   5798   -157    346    583      O
ATOM   6501  O1A MGT A   1      42.713  25.256 -32.229  1.00 46.58          O
ANISOU 6501  O1A MGT A   1     5577   6005   6118   -305    327    828      O
ATOM   6502  O5* MGT A   1      43.626  24.206 -30.136  1.00 42.80          O
ANISOU 6502  O5* MGT A   1     4955   5516   5792   -234    258    568      O
ATOM   6503  C5* MGT A   1      43.771  25.451 -29.389  1.00 38.57          C
ANISOU 6503  C5* MGT A   1     4398   4855   5403   -327    250    603      C
ATOM   6504  C4* MGT A   1      44.860  25.368 -28.297  1.00 34.92          C
ANISOU 6504  C4* MGT A   1     3808   4419   5042   -349    242    478      C
ATOM   6505  O4* MGT A   1      44.641  24.152 -27.533  1.00 33.27          O
ANISOU 6505  O4* MGT A   1     3599   4240   4800   -224    161    362      O
ATOM   6506  C3* MGT A   1      46.295  25.288 -28.821  1.00 34.19          C
ANISOU 6506  C3* MGT A   1     3578   4475   4937   -411    343    453      C
ATOM   6507  O3* MGT A   1      47.120  26.048 -27.945  1.00 35.75          O
ANISOU 6507  O3* MGT A   1     3669   4640   5274   -506    342    399      O
ATOM   6508  C2* MGT A   1      46.671  23.831 -28.682  1.00 33.94          C
ANISOU 6508  C2* MGT A   1     3496   4568   4833   -279    318    333      C
ATOM   6509  O2* MGT A   1      48.079  23.737 -28.438  1.00 37.14          O
ANISOU 6509  O2* MGT A   1     3729   5093   5289   -308    364    248      O
ATOM   6510  C1* MGT A   1      45.936  23.471 -27.403  1.00 30.89          C
ANISOU 6510  C1* MGT A   1     3166   4076   4495   -198    191    266      C
ATOM   6511  N9  MGT A   1      45.522  22.046 -27.080  1.00 29.66          N
ANISOU 6511  N9  MGT A   1     3059   3943   4269    -51    124    187      N
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Figure 18 (continued)

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ATOM   6512  C8  MGT A   1      44.505  21.434 -27.715  1.00 27.88           C
ANISOU 6512  C8  MGT A   1    2948   3695   3949      8    112    221       C
ATOM   6513  N7  MGT A   1      44.411  20.228 -27.155  1.00 27.01           N
ANISOU 6513  N7  MGT A   1    2858   3589   3815    120     53    134       N
ATOM   6514  CM7 MGT A   1      43.375  19.249 -27.561  1.00 25.30           C
ANISOU 6514  CM7 MGT A   1    2758   3341   3512    194     23    127       C
ATOM   6515  C5  MGT A   1      45.336  20.071 -26.191  1.00 27.24           C
ANISOU 6515  C5  MGT A   1    2792   3648   3910    147     21     59       C
ATOM   6516  C4  MGT A   1      46.053  21.249 -26.149  1.00 27.82           C
ANISOU 6516  C4  MGT A   1    2769   3743   4059     34     64     84       C
ATOM   6517  N3  MGT A   1      47.061  21.426 -25.271  1.00 27.51           N
ANISOU 6517  N3  MGT A   1    2607   3751   4096     24     36     11       N
ATOM   6518  C2  MGT A   1      47.423  20.471 -24.405  1.00 28.78           C
ANISOU 6518  C2  MGT A   1    2738   3945   4254    139    -41    -75       C
ATOM   6519  N2  MGT A   1      48.443  20.701 -23.575  1.00 29.71           N
ANISOU 6519  N2  MGT A   1    2722   4129   4439    129    -80   -146       N
ATOM   6520  N1  MGT A   1      46.712  19.246 -24.380  1.00 27.51           N
ANISOU 6520  N1  MGT A   1    2690   3743   4019    264    -84    -86       N
ATOM   6521  C6  MGT A   1      45.678  19.057 -25.295  1.00 26.68           C
ANISOU 6521  C6  MGT A   1    2705   3587   3846    258    -48    -26       C
ATOM   6522  O6  MGT A   1      45.070  17.997 -25.311  1.00 27.25           O
ANISOU 6522  O6  MGT A   1    2870   3620   3863    348    -80    -46       O
ATOM   6523  O2G MGT B   1       8.911   7.379 -30.815  1.00 52.96           O
ANISOU 6523  O2G MGT B   1    6523   7405   6194    480  -1101    341       O
ATOM   6524  PG  MGT B   1       8.686   7.207 -29.221  1.00 49.79           P
ANISOU 6524  PG  MGT B   1    5992   6928   5999    504  -1012    247       P
ATOM   6525  O3G MGT B   1      10.111   6.727 -28.566  1.00 47.34           O
ANISOU 6525  O3G MGT B   1    5764   6484   5738    339   -851    158       O
ATOM   6526  O1G MGT B   1       8.184   8.475 -28.631  1.00 50.87           O
ANISOU 6526  O1G MGT B   1    6159   6948   6223    702  -1015    339       O
ATOM   6527  O3B MGT B   1       7.735   5.911 -29.048  1.00 49.75           O
ANISOU 6527  O3B MGT B   1    5755   7120   6027    437  -1075    126       O
ATOM   6528  PB  MGT B   1       6.305   5.749 -29.792  1.00 51.97           P
ANISOU 6528  PB  MGT B   1    5864   7633   6251    512  -1261    156       P
ATOM   6529  O2B MGT B   1       6.621   5.123 -31.256  1.00 52.42           O
ANISOU 6529  O2B MGT B   1    6011   7805   6099    381  -1353    144       O
ATOM   6530  O1B MGT B   1       5.596   7.053 -29.893  1.00 53.94           O
ANISOU 6530  O1B MGT B   1    6111   7869   6514    750  -1339    301       O
ATOM   6531  O3A MGT B   1       5.465   4.683 -28.886  1.00 50.43           O
ANISOU 6531  O3A MGT B   1    5422   7553   6185    435  -1246     27       O
ATOM   6532  PA  MGT B   1       5.986   3.318 -28.093  1.00 45.51           P
ANISOU 6532  PA  MGT B   1    4771   6888   5634    227  -1122   -129       P
ATOM   6533  O2A MGT B   1       7.298   2.764 -28.782  1.00 43.17           O
ANISOU 6533  O2A MGT B   1    4672   6508   5222     84  -1068   -175       O
ATOM   6534  O1A MGT B   1       4.876   2.329 -28.139  1.00 43.87           O
ANISOU 6534  O1A MGT B   1    4348   6870   5450    131  -1206   -207       O
ATOM   6535  O5* MGT B   1       6.408   3.771 -26.568  1.00 42.04           O
ANISOU 6535  O5* MGT B   1    4356   6273   5345    294   -960   -138       O
ATOM   6536  C5* MGT B   1       5.376   4.024 -25.569  1.00 40.75           C
ANISOU 6536  C5* MGT B   1    4018   6158   5306    403   -935   -137       C
ATOM   6537  C4* MGT B   1       5.580   5.362 -24.810  1.00 38.17           C
ANISOU 6537  C4* MGT B   1    3791   5670   5043    591   -859    -67       C
ATOM   6538  O4* MGT B   1       6.866   5.317 -24.120  1.00 33.12           O
ANISOU 6538  O4* MGT B   1    3324   4841   4420    503   -736   -111       O
ATOM   6539  C3* MGT B   1       5.606   6.610 -25.719  1.00 38.56           C
ANISOU 6539  C3* MGT B   1    3962   5672   5018    750   -947     64       C
ATOM   6540  O3* MGT B   1       4.951   7.705 -25.060  1.00 39.09           O
ANISOU 6540  O3* MGT B   1    4007   5678   5169    978   -922    122       O
ATOM   6541  C2* MGT B   1       7.108   6.900 -25.892  1.00 36.08           C
ANISOU 6541  C2* MGT B   1    3897   5166   4648    655   -875     76       C
ATOM   6542  O2* MGT B   1       7.314   8.312 -26.089  1.00 40.76           O
ANISOU 6542  O2* MGT B   1    4655   5608   5223    807   -882    193       O
ATOM   6543  C1* MGT B   1       7.650   6.495 -24.540  1.00 30.98           C
ANISOU 6543  C1* MGT B   1    3257   4415   4100    578   -738    -22       C
ATOM   6544  N9  MGT B   1       9.078   6.082 -24.348  1.00 28.02           N
ANISOU 6544  N9  MGT B   1    3017   3924   3707    418   -654    -71       N
ATOM   6545  C8  MGT B   1       9.633   4.953 -24.839  1.00 26.32           C
ANISOU 6545  C8  MGT B   1    2789   3772   3439    259   -650   -132       C
ATOM   6546  N7  MGT B   1      10.913   4.962 -24.399  1.00 26.18           N
ANISOU 6546  N7  MGT B   1    2885   3627   3435    179   -562   -155       N
ATOM   6547  CM7 MGT B   1      11.908   3.911 -24.712  1.00 23.88           C
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Figure 18 (continued)

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ANISOU 6547  CM7 MGT B   1     2618   3350   3106     33   -517   -218       C
ATOM   6548  C5  MGT B   1      11.150   6.053 -23.649  1.00 26.92           C
ANISOU 6548  C5  MGT B   1     3066   3581   3583    257   -521   -117       C
ATOM   6549  C4  MGT B   1       9.951   6.759 -23.616  1.00 26.32           C
ANISOU 6549  C4  MGT B   1     2937   3533   3529    418   -573    -67       C
ATOM   6550  N3  MGT B   1       9.832   7.907 -22.934  1.00 26.49           N
ANISOU 6550  N3  MGT B   1     3046   3417   3601    542   -541    -32       N
ATOM   6551  C2  MGT B   1      10.866   8.432 -22.259  1.00 27.34           C
ANISOU 6551  C2  MGT B   1     3301   3354   3732    486   -471    -49       C
ATOM   6552  N2  MGT B   1      10.701   9.584 -21.612  1.00 27.16           N
ANISOU 6552  N2  MGT B   1     3394   3178   3749    604   -444    -27       N
ATOM   6553  N1  MGT B   1      12.111   7.743 -22.231  1.00 25.77           N
ANISOU 6553  N1  MGT B   1     3131   3144   3516    307   -431    -94       N
ATOM   6554  C6  MGT B   1      12.248   6.556 -22.934  1.00 25.10           C
ANISOU 6554  C6  MGT B   1     2952   3198   3385    209   -450   -125       C
ATOM   6555  O6  MGT B   1      13.319   5.964 -22.921  1.00 23.93           O
ANISOU 6555  O6  MGT B   1     2823   3040   3228     85   -407   -162       O
ATOM   6556  O2G MGT D   1      61.475 -17.770 -25.548  1.00 67.38           O
ANISOU 6556  O2G MGT D   1     9188   7995   8420    107    942  -1582       O
ATOM   6557  PG  MGT D   1      62.375 -16.755 -24.687  1.00 63.67           P
ANISOU 6557  PG  MGT D   1     8522   7594   8077    197    990  -1352       P
ATOM   6558  O3G MGT D   1      61.503 -15.362 -24.545  1.00 60.97           O
ANISOU 6558  O3G MGT D   1     8082   7476   7609     96    876  -1228       O
ATOM   6559  O1G MGT D   1      62.653 -17.429 -23.397  1.00 61.93           O
ANISOU 6559  O1G MGT D   1     8255   7184   8089    201    946  -1268       O
ATOM   6560  O3B MGT D   1      63.673 -16.536 -25.716  1.00 64.52           O
ANISOU 6560  O3B MGT D   1     8633   7752   8130    376   1208  -1392       O
ATOM   6561  PB  MGT D   1      64.918 -15.449 -25.741  1.00 62.58           P
ANISOU 6561  PB  MGT D   1     8215   7622   7940    497   1355  -1237       P
ATOM   6562  O2B MGT D   1      65.139 -15.212 -27.321  1.00 64.91           O
ANISOU 6562  O2B MGT D   1     8631   8045   7988    558   1524  -1348       O
ATOM   6563  O1B MGT D   1      66.180 -15.970 -25.139  1.00 63.51           O
ANISOU 6563  O1B MGT D   1     8220   7601   8311    635   1450  -1195       O
ATOM   6564  O3A MGT D   1      64.421 -13.964 -25.210  1.00 59.32           O
ANISOU 6564  O3A MGT D   1     7676   7379   7485    401   1242  -1049       O
ATOM   6565  PA  MGT D   1      65.432 -12.750 -24.675  1.00 56.96           P
ANISOU 6565  PA  MGT D   1     7170   7154   7317    450   1303   -853       P
ATOM   6566  O2A MGT D   1      64.807 -11.421 -25.326  1.00 57.92           O
ANISOU 6566  O2A MGT D   1     7315   7462   7229    384   1286   -780       O
ATOM   6567  O1A MGT D   1      66.884 -12.915 -25.008  1.00 57.06           O
ANISOU 6567  O1A MGT D   1     7089   7135   7457    589   1504   -851       O
ATOM   6568  O5* MGT D   1      65.125 -12.590 -23.090  1.00 52.24           O
ANISOU 6568  O5* MGT D   1     6467   6494   6888    382   1121   -735       O
ATOM   6569  C5* MGT D   1      66.139 -12.982 -22.146  1.00 47.19           C
ANISOU 6569  C5* MGT D   1     5707   5738   6485    461   1122   -671       C
ATOM   6570  C4* MGT D   1      65.571 -13.910 -21.075  1.00 41.42           C
ANISOU 6570  C4* MGT D   1     5036   4863   5837    416    977   -675       C
ATOM   6571  O4* MGT D   1      64.237 -13.425 -20.723  1.00 38.14           O
ANISOU 6571  O4* MGT D   1     4670   4525   5297    270    847   -650       O
ATOM   6572  C3* MGT D   1      65.400 -15.351 -21.574  1.00 41.82           C
ANISOU 6572  C3* MGT D   1     5242   4761   5887    450   1023   -828       C
ATOM   6573  O3* MGT D   1      66.052 -16.225 -20.646  1.00 42.77           O
ANISOU 6573  O3* MGT D   1     5339   4701   6212    533    987   -785       O
ATOM   6574  C2* MGT D   1      63.880 -15.578 -21.583  1.00 38.52           C
ANISOU 6574  C2* MGT D   1     4952   4355   5329    288    909   -890       C
ATOM   6575  O2* MGT D   1      63.571 -16.924 -21.181  1.00 41.39           O
ANISOU 6575  O2* MGT D   1     5434   4513   5779    262    869   -960       O
ATOM   6576  C1* MGT D   1      63.397 -14.606 -20.531  1.00 32.26           C
ANISOU 6576  C1* MGT D   1     4058   3655   4544    202    787   -739       C
ATOM   6577  N9  MGT D   1      61.985 -14.077 -20.575  1.00 30.62           N
ANISOU 6577  N9  MGT D   1     3877   3566   4190     57    691   -749       N
ATOM   6578  C8  MGT D   1      61.537 -13.152 -21.455  1.00 28.56           C
ANISOU 6578  C8  MGT D   1     3608   3474   3770     36    699   -767       C
ATOM   6579  N7  MGT D   1      60.245 -12.956 -21.135  1.00 28.87           N
ANISOU 6579  N7  MGT D   1     3649   3576   3745    -86    585   -769       N
ATOM   6580  CM7 MGT D   1      59.372 -12.016 -21.848  1.00 27.27           C
ANISOU 6580  CM7 MGT D   1     3432   3551   3377   -125    533   -779       C
ATOM   6581  C5  MGT D   1      59.872 -13.721 -20.082  1.00 29.90           C
ANISOU 6581  C5  MGT D   1     3792   3586   3983   -156    529   -750       C
ATOM   6582  C4  MGT D   1      61.017 -14.436 -19.739  1.00 29.44           C
ANISOU 6582  C4  MGT D   1     3754   3372   4059    -59    592   -730       C
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Figure 18 (continued)

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ATOM   6583  N3  MGT D   1      61.004 -15.292 -18.702  1.00 29.19           N
ANISOU 6583  N3  MGT D   1    3760   3183   4146    -86    553   -685          N
ATOM   6584  C2  MGT D   1      59.915 -15.502 -17.954  1.00 28.05           C
ANISOU 6584  C2  MGT D   1    3637   3026   3992   -223    481   -658          C
ATOM   6585  N2  MGT D   1      59.978 -16.375 -16.971  1.00 29.73           N
ANISOU 6585  N2  MGT D   1    3915   3072   4309   -246    463   -596          N
ATOM   6586  N1  MGT D   1      58.740 -14.829 -18.230  1.00 27.16           N
ANISOU 6586  N1  MGT D   1    3479   3073   3767   -332    434   -687          N
ATOM   6587  C6  MGT D   1      58.701 -13.917 -19.293  1.00 28.79           C
ANISOU 6587  C6  MGT D   1    3642   3444   3853   -290    443   -733          C
ATOM   6588  O6  MGT D   1      57.638 -13.327 -19.502  1.00 27.71           O
ANISOU 6588  O6  MGT D   1    3458   3444   3626   -368    381   -750          O
ATOM   6589  O2G MGT E   1      23.200 -31.391 -24.125  1.00 70.75           O
ANISOU 6589  O2G MGT E   1    9036   8796   9051   -973   -263  -1625          O
ATOM   6590  PG  MGT E   1      23.830 -31.142 -22.645  1.00 68.95           P
ANISOU 6590  PG  MGT E   1    8848   8360   8991   -906   -117  -1455          P
ATOM   6591  O3G MGT E   1      24.816 -29.813 -22.701  1.00 67.49           O
ANISOU 6591  O3G MGT E   1    8750   8226   8668   -768   -101  -1258          O
ATOM   6592  O1G MGT E   1      22.748 -30.981 -21.631  1.00 68.11           O
ANISOU 6592  O1G MGT E   1    8612   8217   9051   -935   -125  -1397          O
ATOM   6593  O3B MGT E   1      24.889 -32.361 -22.338  1.00 67.54           O
ANISOU 6593  O3B MGT E   1    8779   7972   8911   -938     27  -1554          O
ATOM   6594  PB  MGT E   1      24.785 -33.870 -22.938  1.00 68.18           P
ANISOU 6594  PB  MGT E   1    8880   7968   9058  -1057     39  -1813          P
ATOM   6595  O2B MGT E   1      25.148 -33.733 -24.532  1.00 69.37           O
ANISOU 6595  O2B MGT E   1    9066   8338   8953  -1050    -28  -1961          O
ATOM   6596  O1B MGT E   1      23.440 -34.487 -22.726  1.00 68.87           O
ANISOU 6596  O1B MGT E   1    8856   8032   9278  -1201    -15  -1906          O
ATOM   6597  O3A MGT E   1      25.997 -34.776 -22.240  1.00 65.43           O
ANISOU 6597  O3A MGT E   1    8646   7350   8863  -1017    183  -1825          O
ATOM   6598  PA  MGT E   1      27.307 -34.306 -21.288  1.00 59.20           P
ANISOU 6598  PA  MGT E   1    7934   6449   8110   -875    286  -1635          P
ATOM   6599  O2A MGT E   1      28.136 -33.197 -22.107  1.00 58.65           O
ANISOU 6599  O2A MGT E   1    7884   6588   7811   -779    280  -1588          O
ATOM   6600  O1A MGT E   1      28.129 -35.492 -20.942  1.00 59.66           O
ANISOU 6600  O1A MGT E   1    8071   6268   8331   -854    365  -1720          O
ATOM   6601  O5* MGT E   1      26.816 -33.620 -19.940  1.00 53.22           O
ANISOU 6601  O5* MGT E   1    7134   5651   7435   -863    299  -1411          O
ATOM   6602  C5* MGT E   1      26.613 -34.401 -18.761  1.00 47.71           C
ANISOU 6602  C5* MGT E   1    6458   4745   6925   -918    359  -1351          C
ATOM   6603  C4* MGT E   1      25.456 -33.830 -17.966  1.00 43.86           C
ANISOU 6603  C4* MGT E   1    5872   4324   6467   -983    346  -1240          C
ATOM   6604  O4* MGT E   1      25.786 -32.441 -17.660  1.00 39.94           O
ANISOU 6604  O4* MGT E   1    5354   3955   5866   -865    338  -1094          O
ATOM   6605  C3* MGT E   1      24.198 -33.807 -18.837  1.00 44.21           C
ANISOU 6605  C3* MGT E   1    5798   4523   6477  -1082    252  -1373          C
ATOM   6606  O3* MGT E   1      23.129 -34.318 -18.052  1.00 47.14           O
ANISOU 6606  O3* MGT E   1    6089   4833   6988  -1223    283  -1368          O
ATOM   6607  C2* MGT E   1      23.967 -32.325 -19.118  1.00 42.11           C
ANISOU 6607  C2* MGT E   1    5461   4470   6071   -979    178  -1280          C
ATOM   6608  O2* MGT E   1      22.556 -32.080 -19.141  1.00 44.49           O
ANISOU 6608  O2* MGT E   1    5604   4894   6405  -1051    104  -1318          O
ATOM   6609  C1* MGT E   1      24.614 -31.665 -17.889  1.00 36.11           C
ANISOU 6609  C1* MGT E   1    4744   3637   5341   -890    263  -1094          C
ATOM   6610  N9  MGT E   1      25.074 -30.253 -17.973  1.00 33.69           N
ANISOU 6610  N9  MGT E   1    4442   3438   4921   -758    232   -977          N
ATOM   6611  C8  MGT E   1      26.143 -29.848 -18.690  1.00 32.33           C
ANISOU 6611  C8  MGT E   1    4355   3300   4628   -678    226   -961          C
ATOM   6612  N7  MGT E   1      26.235 -28.515 -18.497  1.00 30.39           N
ANISOU 6612  N7  MGT E   1    4097   3125   4326   -592    200   -834          N
ATOM   6613  CM7 MGT E   1      27.291 -27.689 -19.147  1.00 30.36           C
ANISOU 6613  CM7 MGT E   1    4173   3175   4187   -519    196   -768          C
ATOM   6614  C5  MGT E   1      25.270 -28.075 -17.684  1.00 30.41           C
ANISOU 6614  C5  MGT E   1    4001   3137   4414   -594    187   -790          C
ATOM   6615  C4  MGT E   1      24.528 -29.207 -17.348  1.00 33.54           C
ANISOU 6615  C4  MGT E   1    4345   3484   4915   -708    216   -881          C
ATOM   6616  N3  MGT E   1      23.454 -29.116 -16.532  1.00 32.74           N
ANISOU 6616  N3  MGT E   1    4124   3405   4909   -756    232   -876          N
ATOM   6617  C2  MGT E   1      23.082 -27.949 -16.013  1.00 31.10           C
ANISOU 6617  C2  MGT E   1    3842   3265   4708   -674    218   -805          C
ATOM   6618  N2  MGT E   1      22.036 -27.912 -15.215  1.00 32.01           N
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Figure 18 (continued)

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ANISOU 6618  N2  MGT E   1     3821   3423   4917   -724    252   -831      N
ATOM   6619  N1  MGT E   1       23.783 -26.786 -16.310  1.00 30.29        N
ANISOU 6619  N1  MGT E   1     3801   3183   4526   -545    175   -716      N
ATOM   6620  C6  MGT E   1       24.887 -26.830 -17.148  1.00 31.43        C
ANISOU 6620  C6  MGT E   1     4072   3309   4562   -516    162   -696      C
ATOM   6621  O6  MGT E   1       25.482 -25.774 -17.398  1.00 30.00        O
ANISOU 6621  O6  MGT E   1     3944   3144   4312   -429    135   -607      O
ATOM   6622  O2G MGT F   1       30.350  -3.944 -65.480  1.00 99.58        O
ANISOU 6622  O2G MGT F   1    14031  16156   7647   -644      2   -439      O
ATOM   6623  PG  MGT F   1       28.875  -4.380 -64.937  1.00 97.98        P
ANISOU 6623  PG  MGT F   1    13719  15816   7693   -487   -380   -489      P
ATOM   6624  O3G MGT F   1       28.278  -5.473 -65.973  1.00100.06        O
ANISOU 6624  O3G MGT F   1    14125  16190   7703   -469   -516   -718      O
ATOM   6625  O1G MGT F   1       28.966  -4.930 -63.549  1.00 93.98        O
ANISOU 6625  O1G MGT F   1    12887  15191   7630   -397   -325   -595      O
ATOM   6626  O3B MGT F   1       27.926  -3.048 -65.157  1.00 97.20        O
ANISOU 6626  O3B MGT F   1    13810  15616   7506   -472   -688   -195      O
ATOM   6627  PB  MGT F   1       26.314  -3.046 -64.848  1.00 94.58        P
ANISOU 6627  PB  MGT F   1    13385  15180   7372   -321  -1114   -191      P
ATOM   6628  O2B MGT F   1       25.693  -3.980 -66.039  1.00 96.13        O
ANISOU 6628  O2B MGT F   1    13730  15529   7265   -323  -1304   -385      O
ATOM   6629  O1B MGT F   1       25.707  -1.684 -64.850  1.00 95.46        O
ANISOU 6629  O1B MGT F   1    13630  15170   7470   -262  -1343     89      O
ATOM   6630  O3A MGT F   1       26.194  -3.836 -63.403  1.00 86.47        O
ANISOU 6630  O3A MGT F   1    11980  14048   6828   -253  -1036   -362      O
ATOM   6631  PA  MGT F   1       25.747  -3.160 -61.969  1.00 79.76        P
ANISOU 6631  PA  MGT F   1    10904  13006   6395   -173  -1093   -247      P
ATOM   6632  O2A MGT F   1       25.428  -4.445 -61.045  1.00 77.01        O
ANISOU 6632  O2A MGT F   1    10293  12609   6357   -138  -1050   -494      O
ATOM   6633  O1A MGT F   1       24.575  -2.250 -62.103  1.00 81.05        O
ANISOU 6633  O1A MGT F   1    11113  13096   6587    -75  -1414    -96      O
ATOM   6634  O5* MGT F   1       27.022  -2.434 -61.277  1.00 74.56        O
ANISOU 6634  O5* MGT F   1    10228  12289   5813   -247   -803   -111      O
ATOM   6635  C5* MGT F   1       27.118  -0.995 -61.342  1.00 70.02        C
ANISOU 6635  C5* MGT F   1     9816  11623   5166   -279   -837    152      C
ATOM   6636  C4* MGT F   1       28.554  -0.539 -61.633  1.00 66.55        C
ANISOU 6636  C4* MGT F   1     9491  11251   4545   -450   -529    235      C
ATOM   6637  O4* MGT F   1       29.365  -1.421 -60.821  1.00 62.48        O
ANISOU 6637  O4* MGT F   1     8711  10787   4243   -457   -310     45      O
ATOM   6638  C3* MGT F   1       29.017  -0.716 -63.097  1.00 67.92        C
ANISOU 6638  C3* MGT F   1     9926  11602   4279   -559   -437    229      C
ATOM   6639  O3* MGT F   1       29.464   0.547 -63.638  1.00 71.23        O
ANISOU 6639  O3* MGT F   1    10633  11975   4455   -700   -363    483      O
ATOM   6640  C2* MGT F   1       30.204  -1.684 -63.020  1.00 65.40        C
ANISOU 6640  C2* MGT F   1     9433  11442   3975   -628   -112     11      C
ATOM   6641  O2* MGT F   1       31.280  -1.234 -63.872  1.00 65.11        O
ANISOU 6641  O2* MGT F   1     9573  11538   3626   -817    163     74      O
ATOM   6642  C1* MGT F   1       30.610  -1.563 -61.542  1.00 60.72        C
ANISOU 6642  C1* MGT F   1     8551  10736   3784   -595    -29      0      C
ATOM   6643  N9  MGT F   1       31.361  -2.695 -60.897  1.00 58.13        N
ANISOU 6643  N9  MGT F   1     7951  10481   3654   -540    147   -237      N
ATOM   6644  C8  MGT F   1       30.774  -3.809 -60.424  1.00 56.15        C
ANISOU 6644  C8  MGT F   1     7571  10180   3582   -396     36   -414      C
ATOM   6645  N7  MGT F   1       31.776  -4.546 -59.912  1.00 55.98        N
ANISOU 6645  N7  MGT F   1     7360  10216   3694   -359    232   -573      N
ATOM   6646  CM7 MGT F   1       31.556  -5.890 -59.278  1.00 54.61        C
ANISOU 6646  CM7 MGT F   1     7057   9970   3722   -208    191   -783      C
ATOM   6647  C5  MGT F   1       32.960  -3.927 -60.039  1.00 57.17        C
ANISOU 6647  C5  MGT F   1     7463  10481   3778   -476    459   -522      C
ATOM   6648  C4  MGT F   1       32.671  -2.722 -60.675  1.00 58.35        C
ANISOU 6648  C4  MGT F   1     7834  10615   3719   -617    418   -299      C
ATOM   6649  N3  MGT F   1       33.637  -1.831 -60.974  1.00 59.84        N
ANISOU 6649  N3  MGT F   1     8063  10888   3784   -804    632   -191      N
ATOM   6650  C2  MGT F   1       34.924  -2.053 -60.665  1.00 60.72        C
ANISOU 6650  C2  MGT F   1     7940  11139   3992   -862    890   -315      C
ATOM   6651  N2  MGT F   1       35.834  -1.129 -60.973  1.00 62.34        N
ANISOU 6651  N2  MGT F   1     8169  11434   4084  -1091   1115   -218      N
ATOM   6652  N1  MGT F   1       35.287  -3.254 -60.011  1.00 59.54        N
ANISOU 6652  N1  MGT F   1     7525  11029   4067   -680    912   -549      N
ATOM   6653  C6  MGT F   1       34.299  -4.207 -59.684  1.00 57.63        C
ANISOU 6653  C6  MGT F   1     7300  10661   3935   -485    696   -642      C
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Figure 18 (continued)

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ATOM   6654  O6  MGT F   1      34.635  -5.252 -59.114  1.00 55.72
ANISOU 6654  O6  MGT F   1    6882  10416   3874   -329    718   -828
ATOM   6655  OH2 WAT Z   1      22.010 -17.664  -4.923  1.00 24.01
ATOM   6656  OH2 WAT Z   2      35.587 -15.501 -13.579  1.00 25.92
ATOM   6657  OH2 WAT Z   3      24.874  18.972 -29.481  1.00 17.82
ATOM   6658  OH2 WAT Z   4      22.669  -1.536 -24.962  1.00 13.35
ATOM   6659  OH2 WAT Z   5      52.591 -14.211  -5.902  1.00 21.48
ATOM   6660  OH2 WAT Z   7      13.160   0.537   1.189  1.00 23.18
ATOM   6661  OH2 WAT Z   8      25.007  17.823 -32.038  1.00 17.76
ATOM   6662  OH2 WAT Z   9      57.764   0.177  -1.188  1.00 25.56
ATOM   6663  OH2 WAT Z  10      22.557  -2.907 -16.078  1.00 29.94
ATOM   6664  OH2 WAT Z  11       0.415  -4.929 -12.849  1.00 25.54
ATOM   6665  OH2 WAT Z  12      21.159   3.266  -9.320  1.00 33.91
ATOM   6666  OH2 WAT Z  13      29.894  16.381 -39.221  1.00 27.21
ATOM   6667  OH2 WAT Z  14      48.790  14.910 -10.474  1.00 28.71
ATOM   6668  OH2 WAT Z  15      51.978 -20.700 -11.448  1.00 26.98
ATOM   6669  OH2 WAT Z  16      52.522   8.682 -31.531  1.00 27.48
ATOM   6670  OH2 WAT Z  17      71.301  -1.768 -14.451  1.00 22.48
ATOM   6671  OH2 WAT Z  18      27.320 -22.307 -20.123  1.00 19.55
ATOM   6672  OH2 WAT Z  19      34.964  21.944  -4.871  1.00 23.06
ATOM   6673  OH2 WAT Z  21      23.902 -22.328 -16.923  1.00 23.97
ATOM   6674  OH2 WAT Z  22      48.357  -2.830 -15.780  1.00 34.81
ATOM   6675  OH2 WAT Z  23      58.588   5.961 -27.382  1.00 19.01
ATOM   6676  OH2 WAT Z  24      18.628  15.589 -17.793  1.00 30.46
ATOM   6677  OH2 WAT Z  25      19.270 -18.539 -13.641  1.00 21.85
ATOM   6678  OH2 WAT Z  26      43.558  13.915 -26.424  1.00 17.33
ATOM   6679  OH2 WAT Z  27      26.542 -12.581 -16.266  1.00 26.41
ATOM   6680  OH2 WAT Z  28      34.875  33.272 -20.697  1.00 21.41
ATOM   6681  OH2 WAT Z  29      13.457 -11.350 -34.721  1.00 35.91
ATOM   6682  OH2 WAT Z  30      25.564  10.236 -30.803  1.00 24.48
ATOM   6683  OH2 WAT Z  31      45.958 -26.847 -21.485  1.00 27.96
ATOM   6684  OH2 WAT Z  32      35.988 -22.594   2.913  1.00 21.42
ATOM   6685  OH2 WAT Z  33      54.562 -14.794 -17.888  1.00 22.27
ATOM   6686  OH2 WAT Z  34      22.529   2.193 -30.694  1.00 27.64
ATOM   6687  OH2 WAT Z  35      25.635  -4.794 -32.881  1.00 28.73
ATOM   6688  OH2 WAT Z  36      27.823  20.133  -0.039  1.00 36.81
ATOM   6689  OH2 WAT Z  37      20.246  12.658 -31.810  1.00 24.61
ATOM   6690  OH2 WAT Z  38      28.300 -37.005 -18.759  1.00 51.31
ATOM   6691  OH2 WAT Z  39      53.886 -12.268 -21.629  1.00 17.36
ATOM   6692  OH2 WAT Z  40      48.741  -7.083 -24.282  1.00 24.97
ATOM   6693  OH2 WAT Z  41      56.501 -23.941 -22.749  1.00 33.42
ATOM   6694  OH2 WAT Z  42      70.436   0.347 -12.882  1.00 19.32
ATOM   6695  OH2 WAT Z  43      25.679   6.098 -19.237  1.00 22.39
ATOM   6696  OH2 WAT Z  44      32.839  32.448 -18.714  1.00 35.80
ATOM   6697  OH2 WAT Z  45      13.259 -14.963 -26.829  1.00 23.85
ATOM   6698  OH2 WAT Z  46      45.572 -27.223 -24.539  1.00 26.82
ATOM   6699  OH2 WAT Z  47      18.892  12.226  -9.507  1.00 24.12
ATOM   6700  OH2 WAT Z  48      15.179  -6.957   4.889  1.00 33.18
ATOM   6701  OH2 WAT Z  49      28.351   4.517 -12.106  1.00 29.12
ATOM   6702  OH2 WAT Z  50      69.753  -7.784 -22.150  1.00 24.16
ATOM   6703  OH2 WAT Z  51      51.484 -18.920 -13.213  1.00 25.28
ATOM   6704  OH2 WAT Z  52      30.860  13.483  -5.891  1.00 23.31
ATOM   6705  OH2 WAT Z  53      30.542 -37.628 -17.641  1.00 34.32
ATOM   6706  OH2 WAT Z  54      17.077 -19.149 -12.084  1.00 24.17
ATOM   6707  OH2 WAT Z  55      31.540 -38.915 -14.093  1.00 29.25
ATOM   6708  OH2 WAT Z  56      32.031  10.317  -7.068  1.00 23.87
ATOM   6709  OH2 WAT Z  57      63.159 -12.048 -28.694  1.00 38.66
ATOM   6710  OH2 WAT Z  60      32.626 -17.204 -22.492  1.00 28.77
ATOM   6711  OH2 WAT Z  61      13.024 -14.857 -24.008  1.00 21.66
ATOM   6712  OH2 WAT Z  62      16.501   7.671 -21.877  1.00 22.39
ATOM   6713  OH2 WAT Z  63      26.459   8.287 -33.540  1.00 44.16
ATOM   6714  OH2 WAT Z  64      51.383 -16.236  -0.275  1.00 35.25
ATOM   6715  OH2 WAT Z  65      55.449   4.737 -37.070  1.00 38.33
ATOM   6716  OH2 WAT Z  66      18.627  -7.775 -42.508  1.00 43.11
ATOM   6717  OH2 WAT Z  67      25.172  -1.387 -16.895  1.00 32.89
ATOM   6718  OH2 WAT Z  68      63.541   6.400   3.498  1.00 39.85
ATOM   6719  OH2 WAT Z  69      58.234   5.010 -30.073  1.00 27.73
ATOM   6720  OH2 WAT Z  70      40.724  12.891 -10.774  1.00 30.83
ATOM   6721  OH2 WAT Z  71      24.900  12.576 -19.843  1.00 20.19
ATOM   6722  OH2 WAT Z  72      49.784  -6.304  -7.577  1.00 31.08
ATOM   6723  OH2 WAT Z  73      27.087  40.698 -13.760  1.00 41.38
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Figure 18 (continued)

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ATOM   6724  OH2 WAT Z  74      76.962   7.731  -7.980  1.00 33.08      O
ATOM   6725  OH2 WAT Z  75      23.651  14.328 -38.716  1.00 32.75      O
ATOM   6726  OH2 WAT Z  76      11.075   7.898  -8.738  1.00 37.62      O
ATOM   6727  OH2 WAT Z  77      17.338   4.404 -24.665  1.00 17.00      O
ATOM   6728  OH2 WAT Z  78      16.077 -25.529 -23.013  1.00 30.89      O
ATOM   6729  OH2 WAT Z  79      53.527  14.001 -17.979  1.00 27.27      O
ATOM   6730  OH2 WAT Z  80      34.264  14.194 -45.137  1.00 32.07      O
ATOM   6731  OH2 WAT Z  82      42.478  -8.305  -9.650  1.00 29.55      O
ATOM   6732  OH2 WAT Z  83      15.985  -6.541 -42.463  1.00 28.85      O
ATOM   6733  OH2 WAT Z  84      34.516   8.340 -25.756  1.00 25.94      O
ATOM   6734  OH2 WAT Z  85      58.379  -1.510 -36.376  1.00 38.41      O
ATOM   6735  OH2 WAT Z  86      37.811   8.922 -27.105  1.00 22.11      O
ATOM   6736  OH2 WAT Z  87      -0.391  -3.769 -14.739  1.00 35.30      O
ATOM   6737  OH2 WAT Z  88      43.490  14.702  -6.036  1.00 32.76      O
ATOM   6738  OH2 WAT Z  89      66.881   0.967 -35.813  1.00 29.64      O
ATOM   6739  OH2 WAT Z  90      50.228  23.440 -23.336  1.00 25.56      O
ATOM   6740  OH2 WAT Z  91      18.346 -19.140 -26.919  1.00 38.45      O
ATOM   6741  OH2 WAT Z  93      33.957  31.768 -27.497  1.00 34.70      O
ATOM   6742  OH2 WAT Z  94      15.782  16.563 -13.960  1.00 25.91      O
ATOM   6743  OH2 WAT Z  95      48.925   4.506   4.193  1.00 30.06      O
ATOM   6744  OH2 WAT Z  96      55.094   8.303   2.407  1.00 32.94      O
ATOM   6745  OH2 WAT Z  97      23.845  23.584 -12.034  1.00 27.82      O
ATOM   6746  OH2 WAT Z  98      19.282  13.117 -18.942  1.00 28.06      O
ATOM   6747  OH2 WAT Z  99      21.689 -13.748 -35.649  1.00 30.66      O
ATOM   6748  OH2 WAT Z 100      30.856  27.498 -24.106  1.00 31.84      O
ATOM   6749  OH2 WAT Z 101      46.475  15.139 -23.225  1.00 30.44      O
ATOM   6750  OH2 WAT Z 102      75.808   3.111  -8.446  1.00 33.80      O
ATOM   6751  OH2 WAT Z 103      22.117  -4.088 -48.032  1.00 47.28      O
ATOM   6752  OH2 WAT Z 104      19.417  -9.956 -43.103  1.00 37.00      O
ATOM   6753  OH2 WAT Z 105      50.959  14.958  -6.038  1.00 28.24      O
ATOM   6754  OH2 WAT Z 106      12.824 -14.262 -55.184  1.00 53.76      O
ATOM   6755  OH2 WAT Z 107      24.243 -15.291 -17.663  1.00 39.66      O
ATOM   6756  OH2 WAT Z 108      42.270  21.564 -34.734  1.00 24.55      O
ATOM   6757  OH2 WAT Z 109      16.713 -20.968  -7.090  1.00 27.98      O
ATOM   6758  OH2 WAT Z 110      36.477 -16.419 -21.410  1.00 48.83      O
ATOM   6759  OH2 WAT Z 111      35.351  16.445 -10.062  1.00 50.87      O
ATOM   6760  OH2 WAT Z 112      24.841  -4.261  -4.666  1.00 30.33      O
ATOM   6761  OH2 WAT Z 113       4.786  -8.000 -18.626  1.00 35.35      O
ATOM   6762  OH2 WAT Z 114      10.306  -1.689 -38.133  1.00 26.41      O
ATOM   6763  OH2 WAT Z 115      42.924 -19.244 -23.456  1.00 34.89      O
ATOM   6764  OH2 WAT Z 116      42.206  12.907  -6.861  1.00 25.28      O
ATOM   6765  OH2 WAT Z 117      51.605  13.100 -19.296  1.00 31.95      O
ATOM   6766  OH2 WAT Z 118      16.469  13.514  -8.427  1.00 45.86      O
ATOM   6767  OH2 WAT Z 119      50.036   4.161 -29.744  1.00 25.55      O
ATOM   6768  OH2 WAT Z 120      16.233  10.887 -35.555  1.00 41.62      O
ATOM   6769  OH2 WAT Z 121      22.532   0.490 -33.852  1.00 27.81      O
ATOM   6770  OH2 WAT Z 123      19.367 -19.611 -56.734  1.00 31.09      O
ATOM   6771  OH2 WAT Z 124      46.548 -25.852 -32.207  1.00 41.02      O
ATOM   6772  OH2 WAT Z 125      27.102 -32.879  -5.267  1.00 28.86      O
ATOM   6773  OH2 WAT Z 126      49.465   4.075  -4.211  1.00 29.62      O
ATOM   6774  OH2 WAT Z 127      68.660  -0.401 -18.608  1.00 38.81      O
ATOM   6775  OH2 WAT Z 128      28.488 -14.653  -2.031  1.00 33.34      O
ATOM   6776  OH2 WAT Z 129      38.691  29.556 -29.045  1.00 27.56      O
ATOM   6777  OH2 WAT Z 130      20.046  14.970  -5.630  1.00 35.59      O
ATOM   6778  OH2 WAT Z 131      21.161  -5.035  -2.609  1.00 24.94      O
ATOM   6779  OH2 WAT Z 132      39.421 -26.828   9.622  1.00 57.63      O
ATOM   6780  OH2 WAT Z 133      30.273 -15.692  -5.914  1.00 26.45      O
ATOM   6781  OH2 WAT Z 134      40.038 -33.801 -13.906  1.00 35.26      O
ATOM   6782  OH2 WAT Z 135      50.389   2.298 -27.656  1.00 26.52      O
ATOM   6783  OH2 WAT Z 136      42.086   7.582 -31.511  1.00 36.58      O
ATOM   6784  OH2 WAT Z 137      50.049 -21.915 -25.630  1.00 29.44      O
ATOM   6785  OH2 WAT Z 138      54.096  17.394 -14.365  1.00 26.83      O
ATOM   6786  OH2 WAT Z 139      53.457  22.759 -18.096  1.00 29.22      O
ATOM   6787  OH2 WAT Z 140      47.276 -14.555 -17.579  1.00 28.30      O
ATOM   6788  OH2 WAT Z 141      29.621  27.139  -8.722  1.00 19.74      O
ATOM   6789  OH2 WAT Z 142      21.551 -15.531 -46.177  1.00 37.12      O
ATOM   6790  OH2 WAT Z 143       0.081  -2.053  -6.723  1.00 35.12      O
ATOM   6791  OH2 WAT Z 145       2.708  -6.704 -12.288  1.00 29.20      O
ATOM   6792  OH2 WAT Z 146      48.187  -3.807 -23.913  1.00 39.45      O
ATOM   6793  OH2 WAT Z 147      35.518  -9.414 -58.946  1.00 49.19      O
ATOM   6794  OH2 WAT Z 149      50.661   6.651  -2.459  1.00 31.55      O
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Figure 18 (continued)

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ATOM   6795  OH2 WAT Z 150       6.977  -4.292   5.382  1.00 33.62      O
ATOM   6796  OH2 WAT Z 151      70.053  -2.697 -21.777  1.00 35.37      O
ATOM   6797  OH2 WAT Z 152      26.405 -25.745 -56.037  1.00 54.31      O
ATOM   6798  OH2 WAT Z 153      21.807 -11.348 -34.300  1.00 36.00      O
ATOM   6799  OH2 WAT Z 155      61.988  12.944  -9.997  1.00 37.17      O
ATOM   6800  OH2 WAT Z 156      48.957  -7.172  -3.666  1.00 35.39      O
ATOM   6801  OH2 WAT Z 157       9.240  15.496 -16.665  1.00 37.22      O
ATOM   6802  OH2 WAT Z 158      22.966  -4.323 -23.838  1.00 42.19      O
ATOM   6803  OH2 WAT Z 159       4.714 -15.721  -5.172  1.00 39.15      O
ATOM   6804  OH2 WAT Z 160      23.677  12.223 -38.115  1.00 37.72      O
ATOM   6805  OH2 WAT Z 161      40.873 -28.484 -31.719  1.00 49.84      O
ATOM   6806  OH2 WAT Z 162      20.764 -17.215 -48.256  1.00 30.64      O
ATOM   6807  OH2 WAT Z 163      46.257   2.134  -5.934  1.00 28.45      O
ATOM   6808  OH2 WAT Z 164       1.102  -0.339 -23.846  1.00 33.06      O
ATOM   6809  OH2 WAT Z 165      56.153 -23.889 -11.833  1.00 51.89      O
ATOM   6810  OH2 WAT Z 166      46.513 -37.594 -25.306  1.00 42.87      O
ATOM   6811  OH2 WAT Z 167      31.205 -31.346 -33.201  1.00 37.47      O
ATOM   6812  OH2 WAT Z 168      46.736 -32.410 -16.066  1.00 48.36      O
ATOM   6813  OH2 WAT Z 169      16.920 -25.816 -15.401  1.00 43.16      O
ATOM   6814  OH2 WAT Z 170      40.084  28.332 -35.998  1.00 31.80      O
ATOM   6815  OH2 WAT Z 171      43.734  19.350 -33.881  1.00 29.51      O
ATOM   6816  OH2 WAT Z 172      26.493  -8.330 -14.753  1.00 32.62      O
ATOM   6817  OH2 WAT Z 173      33.748   4.983 -37.285  1.00 33.47      O
ATOM   6818  OH2 WAT Z 175      56.484 -13.704  -3.695  1.00 32.87      O
ATOM   6819  OH2 WAT Z 176      27.269  -8.161 -63.691  1.00 43.49      O
ATOM   6820  OH2 WAT Z 177      50.087  -8.525  -2.162  1.00 26.01      O
ATOM   6821  OH2 WAT Z 179      36.074 -14.083  -7.400  1.00 33.95      O
ATOM   6822  OH2 WAT Z 180      21.712 -14.738 -31.372  1.00 41.69      O
ATOM   6823  OH2 WAT Z 181      66.636  -9.970  -8.729  1.00 30.38      O
ATOM   6824  OH2 WAT Z 182      65.403 -12.027  -5.047  1.00 39.48      O
ATOM   6825  OH2 WAT Z 183      25.708  11.169 -43.671  1.00 35.61      O
ATOM   6826  OH2 WAT Z 184      51.471 -10.298 -38.366  1.00 45.24      O
ATOM   6827  OH2 WAT Z 185      13.816  14.588 -29.069  1.00 30.39      O
ATOM   6828  OH2 WAT Z 186      25.401  24.637   0.808  1.00 42.63      O
ATOM   6829  OH2 WAT Z 187      24.141   3.660  -9.953  1.00 41.40      O
ATOM   6830  OH2 WAT Z 188      50.530  -7.054 -30.104  1.00 37.25      O
ATOM   6831  OH2 WAT Z 189      17.307 -28.578  -8.340  1.00 37.35      O
ATOM   6832  OH2 WAT Z 190      23.215  -2.485  -9.503  1.00 34.35      O
ATOM   6833  OH2 WAT Z 191      25.409 -36.972 -21.377  1.00 28.84      O
ATOM   6834  OH2 WAT Z 192      32.293   9.056 -52.850  1.00 53.81      O
ATOM   6835  OH2 WAT Z 194       9.854 -20.178  -8.716  1.00 47.33      O
ATOM   6836  OH2 WAT Z 195      45.448   7.502 -21.691  1.00 37.17      O
ATOM   6837  OH2 WAT Z 196      41.211 -41.959 -28.245  1.00 48.32      O
ATOM   6838  OH2 WAT Z 197      35.027 -38.234 -17.129  1.00 46.15      O
ATOM   6839  OH2 WAT Z 198      30.945   3.849 -33.630  1.00 38.01      O
ATOM   6840  OH2 WAT Z 199      10.582   3.216 -30.915  1.00 30.78      O
ATOM   6841  OH2 WAT Z 200      38.611 -12.140 -47.412  1.00 34.67      O
ATOM   6842  OH2 WAT Z 201      17.623  19.014 -29.499  1.00 56.25      O
ATOM   6843  OH2 WAT Z 202      48.293  17.619 -42.569  1.00 39.31      O
ATOM   6844  OH2 WAT Z 203      28.384  15.063  -3.883  1.00 41.61      O
ATOM   6845  OH2 WAT Z 204      35.579   3.773 -42.257  1.00 44.44      O
ATOM   6846  OH2 WAT Z 205      20.437 -13.266 -15.586  1.00 23.67      O
ATOM   6847  OH2 WAT Z 206      38.154   5.184 -40.233  1.00 49.51      O
ATOM   6848  OH2 WAT Z 207      45.198  22.725 -11.680  1.00 41.39      O
ATOM   6849  OH2 WAT Z 208      36.171 -18.123 -57.255  1.00 45.32      O
ATOM   6850  OH2 WAT Z 209      20.057   7.547  -4.988  1.00 40.68      O
ATOM   6851  OH2 WAT Z 210      40.148   3.860 -50.600  1.00 35.38      O
ATOM   6852  OH2 WAT Z 211      45.636  -6.474 -29.807  1.00 52.09      O
ATOM   6853  OH2 WAT Z 212      45.277  22.770  -9.176  1.00 24.03      O
ATOM   6854  OH2 WAT Z 213      33.172   4.773 -32.693  1.00 35.71      O
ATOM   6855  OH2 WAT Z 214      33.650 -19.496 -30.848  1.00 39.27      O
ATOM   6856  OH2 WAT Z 215      46.592  -5.388 -49.721  1.00 39.74      O
ATOM   6857  OH2 WAT Z 216      35.963 -38.228  -8.201  1.00 32.99      O
ATOM   6858  OH2 WAT Z 217      42.449 -15.437   1.419  1.00 33.54      O
ATOM   6859  OH2 WAT Z 218      17.500 -25.027  -8.417  1.00 31.46      O
ATOM   6860  OH2 WAT Z 219      24.656  -8.332 -63.244  1.00 41.72      O
ATOM   6861  OH2 WAT Z 220      30.837   2.476 -36.522  1.00 34.45      O
ATOM   6862  OH2 WAT Z 221      54.803 -22.398 -30.205  1.00 48.05      O
ATOM   6863  OH2 WAT Z 222      46.624  -6.685  -7.840  1.00 45.14      O
ATOM   6864  OH2 WAT Z 223      69.977   0.204  -6.062  1.00 29.12      O
ATOM   6865  OH2 WAT Z 224      27.484   9.235 -45.269  1.00 41.47      O
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Figure 18 (continued)

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ATOM   6866  OH2 WAT Z 225      39.053  12.272  -7.273  1.00 35.61           O
ATOM   6867  OH2 WAT Z 226      33.654 -11.620 -71.645  1.00 32.99           O
ATOM   6868  OH2 WAT Z 227      37.763 -36.609  -6.731  1.00 39.13           O
ATOM   6869  OH2 WAT Z 228      43.789  -6.817 -64.285  1.00 35.87           O
ATOM   6870  OH2 WAT Z 229      15.841   7.668 -39.846  1.00 42.57           O
ATOM   6871  OH2 WAT Z 230      49.470  -7.674 -32.876  1.00 39.94           O
ATOM   6872  OH2 WAT Z 231      73.132  -6.437 -11.485  1.00 43.64           O
ATOM   6873  OH2 WAT Z 232      69.189 -10.890  -8.124  1.00 43.10           O
ATOM   6874  OH2 WAT Z 233      68.220   1.931  -4.425  1.00 35.19           O
ATOM   6875  OH2 WAT Z 234      -0.117   0.428 -21.467  1.00 53.29           O
ATOM   6876  OH2 WAT Z 235      22.121  -3.444   6.017  1.00 34.04           O
ATOM   6877  OH2 WAT Z 236      12.296  14.675 -22.643  1.00 46.28           O
ATOM   6878  OH2 WAT Z 237      14.515  13.822  -6.990  1.00 44.07           O
ATOM   6879  OH2 WAT Z 238       8.264   1.618 -31.428  1.00 31.10           O
ATOM   6880  OH2 WAT Z 239      18.004  15.205  -9.508  1.00 43.87           O
ATOM   6881  OH2 WAT Z 240      26.138  -4.555  -6.867  1.00 38.79           O
ATOM   6882  OH2 WAT Z 241      44.614   6.587 -19.546  1.00 22.31           O
ATOM   6883  OH2 WAT Z 242      42.232  28.400 -29.247  1.00 39.83           O
ATOM   6884  OH2 WAT Z 243      35.090  10.219 -18.144  1.00 42.61           O
ATOM   6885  OH2 WAT Z 244      42.707   7.488 -22.667  1.00 26.48           O
ATOM   6886  OH2 WAT Z 245       5.481 -13.489 -33.682  1.00 42.88           O
ATOM   6887  OH2 WAT Z 246      24.380   4.187 -32.955  1.00 35.24           O
ATOM   6888  OH2 WAT Z 247      57.349  26.834 -15.600  1.00 57.46           O
ATOM   6889  OH2 WAT Z 248      36.055 -30.582   3.645  1.00 49.07           O
ATOM   6890  OH2 WAT Z 249      34.660 -36.210  -0.590  1.00 38.86           O
ATOM   6891  OH2 WAT Z 250      44.202   2.988 -16.631  1.00 34.41           O
ATOM   6892  OH2 WAT Z 251      28.312 -18.014 -27.408  1.00 47.07           O
ATOM   6893  OH2 WAT Z 252      43.871   7.890 -38.332  1.00 39.41           O
ATOM   6894  OH2 WAT Z 254      35.217 -18.557  -4.263  1.00 39.96           O
ATOM   6895  OH2 WAT Z 256      10.973  15.666 -13.469  1.00 51.73           O
ATOM   6896  OH2 WAT Z 257      63.806   8.757 -23.338  1.00 49.41           O
ATOM   6897  OH2 WAT Z 258      30.195  19.858 -45.928  1.00 40.05           O
ATOM   6898  OH2 WAT Z 259      45.473 -17.828 -14.547  1.00 34.13           O
ATOM   6899  OH2 WAT Z 261      32.026  -1.032 -32.780  1.00 55.96           O
ATOM   6900  OH2 WAT Z 263      11.334 -21.951 -13.454  1.00 54.94           O
ATOM   6901  OH2 WAT Z 264      34.852  11.262 -11.695  1.00 56.14           O
ATOM   6902  OH2 WAT Z 265      50.631 -23.856 -26.444  1.00 33.63           O
ATOM   6903  OH2 WAT Z 266      28.803  -8.481   0.380  1.00 46.99           O
ATOM   6904  OH2 WAT Z 268      60.910 -11.529 -36.250  1.00 42.92           O
ATOM   6905  OH2 WAT Z 269      29.242  24.796 -47.351  1.00 47.76           O
ATOM   6906  OH2 WAT Z 270      25.353 -10.071 -20.464  1.00 44.62           O
ATOM   6907  OH2 WAT Z 271      21.773 -15.534 -15.644  1.00 27.98           O
ATOM   6908  OH2 WAT Z 272      43.832  29.110 -16.193  1.00 29.32           O
ATOM   6909  OH2 WAT Z 274      24.253   7.923 -25.411  1.00 52.09           O
ATOM   6910  OH2 WAT Z 275      41.167  -6.372 -42.144  1.00 44.79           O
ATOM   6911  OH2 WAT Z 276      51.558 -15.128  -4.442  1.00 26.03           O
ATOM   6912  OH2 WAT Z 277      27.750 -30.861 -21.049  1.00 38.16           O
ATOM   6913  OH2 WAT Z 278      54.407   4.151   7.215  1.00 52.58           O
ATOM   6914  OH2 WAT Z 279      34.111  20.624  -3.191  1.00 50.26           O
ATOM   6915  OH2 WAT Z 280      47.178   7.039 -25.319  1.00 49.30           O
ATOM   6916  OH2 WAT Z 281      47.157 -37.019 -13.327  1.00 40.78           O
ATOM   6917  OH2 WAT Z 282      39.719 -34.762  -7.503  1.00 35.67           O
ATOM   6918  OH2 WAT Z 283      22.466 -13.541 -17.364  1.00 61.73           O
ATOM   6919  OH2 WAT Z 284      46.118  -4.589 -17.951  1.00 44.94           O
ATOM   6920  OH2 WAT Z 285      20.024 -16.482  -0.472  1.00 35.25           O
ATOM   6921  OH2 WAT Z 286      20.617  -3.221 -30.981  1.00 26.80           O
ATOM   6922  OH2 WAT Z 287      14.396  11.159  -7.209  1.00 48.86           O
ATOM   6923  OH2 WAT Z 288       1.963   6.454 -25.094  1.00 54.37           O
ATOM   6924  OH2 WAT Z 290      27.856  10.495 -28.946  1.00 31.74           O
ATOM   6925  OH2 WAT Z 291      20.937 -11.628 -24.894  1.00 33.25           O
ATOM   6926  OH2 WAT Z 293      29.682  29.704  -7.204  1.00 42.07           O
END
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