



166166

06 AUG 2002

THREE DIMENSIONAL STRUCTURES AND MODELS OF Fc RECEPTORS AND USES THEREOF

5

FIELD OF THE INVENTION

The present invention relates to three dimensional structures of Fc receptors (FcR), including crystalline FcγRIIa, crystalline FcεRI, three dimensional coordinates of FcγRIIa protein, a three dimensional structure of FcγRIIa, three dimensional structures of FcR, and particularly FcεRI and FcγRIIb, derived from the structure of FcγRIIa, models thereof, and uses of such structures and models.

15

BACKGROUND OF THE INVENTION

Fc receptors (FcR) are a family of highly related receptors that are specific for the Fc portion of immunoglobulin (Ig). These receptors have major roles in normal immunity and resistance to infection and provide the humoral immune system with a cellular effector arm. Receptors have been defined for each of the immunoglobulin classes and as such are defined by the class of Ig of which they bind (i.e. Fc gamma receptor (FcγR) bind gamma immunoglobulin (IgG), Fc epsilon receptor (FcεR) bind epsilon immunoglobulin (IgE), Fc alpha receptor (FcαR) bind alpha immunoglobulin (IgA)). Among the FcγR receptors, three subfamily members have been defined; FcγRI, which is a high affinity receptor for IgG; FcγRII, which are low affinity receptors for IgG that avidly bind to aggregates immune complexes; and FcγRIII, which are low affinity receptors that bind to immune complexes. These receptors are highly related structurally but perform different functions. The structure and function of FcγRII is of interest because of its interaction with immune complexes and its association with disease.

35

FcγR are expressed on most hematopoietic cells, and through the binding of IgG play a key role in homeostasis of the immune system and host protection against infection.

000000



000000

FcγRII is a low affinity receptor for IgG that essentially binds only to IgG immune complexes and is expressed on a variety of cell types including, for example monocytes, macrophages, neutrophils, eosinophils, platelets and B lymphocytes. FcγRII is involved in various immune and inflammatory responses including antibody-dependent cell-mediated cytotoxicity, clearance of immune complexes, release of inflammatory mediators and regulation of antibody production. The binding of IgG to an FcγR can lead to disease indications that involve regulation by FcγR. For example, the autoimmune disease thrombocytopenia purpura involves tissue (platelet) damage resulting from FcγR-dependent IgG immune complex activation of platelets or their destruction by FcγR+ phagocytes. In addition, various inflammatory disease are known to involve IgG immune complexes (e.g. rheumatoid arthritis, systemic lupus erythematosus), including type II and type III hypersensitivity reactions. Type II and type III hypersensitivity reactions are mediated by IgG, which can activate either complement-mediated or phagocytic effector mechanisms, leading to tissue damage.

The elucidation of the protein structure of FcγRIIa, FcεRI, or indeed any FcR is of importance in the formulation of therapeutic and diagnostic reagents for disease management. Until the discovery of the present invention, the structure and resulting mechanism by which FcγRIIa regulates immune responses was unknown. Thus, despite the general multifunctional role of FcγRIIa, development of useful reagents for treatment or diagnosis of disease was hindered by lack of structural information of the receptor. The linear nucleic acid and amino acid sequence of FcγRIIa have been previously reported (Hibbs et al. *Proc. Natl. Acad. Sci. USA*, vol. 85, pp. 2240-2244, 1988). Mutagenesis studies to identify regions of human FcγRIIa (Hulett et al., *Eur. J Immunol.*, vol. 23, pp.

40-645, 1993; Hulett et al., *J. Biol. Chem.*, vol. 69, pp. 15287-15293 1994; and Hulett et al., *J. Biol. Chem.*, vol. 270, pp. 21188-21194, 1995), human FcγRIIIb (Hibbs et al., *J. Immunol.*, vol. 152, p. 4466, 1994; and Tamm et al., *J. Biol. Chem.*, vol. 271, p. 3659, 1996) and mouse FcγRI (Hulett et al., *J. Immunol.*, vol. 148, pp. 1863-1868, 1991) have defined important regions of IgG binding to the FcγR. Information based on linear sequences, however, cannot accurately predict three dimensional structure of the protein and its functional domains. Huber et al. (*J. Mol. Biol.*, vol. 230, pp. 1077-1083, 1993) have described crystal formation of neonatal rat Fc receptor protein (FcRn). Burmeister et al. (*Nature*, vol. 372, pp. 336-343, 1994; and *Nature*, vol. 372, pp. 379-383, 1994) have described the structure of FcRn crystals. FcRn, however, is closely related to major histocompatibility protein complex and not related to the leukocyte FcγR family by function or structure. Thus, the protein structure of FcRn is not predictive of the FcR structure of the present invention.

FcεR are expressed on mast cells, and through the binding of IgE, trigger an inflammatory immune response which is primarily due to the release of inflammatory mediators upon degranulation of the mast cell (e.g., histamine and serotonin). Release of these mediators causes localized vascular permeability and increase in fluids in the local tissues, including an influx of polymorphonuclear cells into the site. Thus, binding of IgE to an FcεRI can lead to disease indications that involve discharge of fluids from the gut and increased mucus secretion and bronchial contraction, such indications typically being associated with diseases involving allergic inflammation. Therefore, the elucidation of protein structure of FcεRI is of importance in the formulation of therapeutic and diagnostic reagents for disease management,

and in particular, for the management of diseases related to allergic inflammation and other Th2-based immune responses. As for the FcγR described above, the linear nucleic acid and amino acid sequences of human FcεRI have
5 been previously reported (Kochan et al., 1998, *Nuc. Acid. Res.* 16:3584). Until the discovery of the present invention, however, the structure and resulting mechanism by which FcεR regulates immune responses was unknown. Thus, despite the knowledge of the general action of FcεRI,
10 the development of useful reagents for treatment or diagnosis of disease, such as diseases associated with allergic inflammation, was hindered by lack of structural information of the receptor.

Therefore, there is a need in the art to elucidate the
15 three dimensional structures and models of the Fc receptors, and to use such structures and models in therapeutic strategies, such as drug design.

SUMMARY OF THE INVENTION

20 The present invention relates to crystalline FcγRIIa and crystalline FcεRI, three dimensional coordinates of FcγRIIa protein, the three dimensional structure of FcγRIIa, three dimensional structures and models of Fc receptors (FcR) derived from the structure of FcγRIIa,
25 including FcεRI and FcγRIIb, and uses of such structures and models. Obtaining such crystals is an unexpected result. It is well known in the protein crystallographic art that obtaining crystals of quality sufficient for determining the structure of a protein is unpredictable.
30 In particular, obtaining crystals of quality sufficient for determining the three dimensional (3-D) structure of FcγRIIa has not been achievable until the crystallization of FcγRIIa as disclosed in the present application. As such, determination of the three dimensional structure of
35 FcγRIIa has not been possible until the discovery of the

present invention. Additionally, until the discovery of the present invention, derivation of the three dimensional structure and models of other Fc receptor (FcR) proteins has not been possible. The present inventors are also the first to define the three dimensional structure and provide three dimensional models for drug design for FcεRI and FcγRIIIb.

Accordingly, one object of the present invention is to provide crystals of sufficient quality to obtain a determination of the three dimensional structure of FcγRIIa to high resolution, preferably to the resolution of about 1.8 angstrom. The present invention also includes methods for producing crystalline FcγRIIa.

Yet another object of the present invention is to provide crystals of FcεRI protein, preferably of sufficient quality to obtain a determination of the three dimensional structure of FcεRI to high resolution. The present invention also includes methods for producing crystalline FcεRI.

The value of the crystals of FcγRIIa and FcεRI extends beyond merely being able to obtain such crystals. The knowledge obtained concerning the FcγRIIa crystal structure, for example, has been used by the present inventors to define the heretofore unknown tertiary structure of the FcγRIIa protein, to model and derive atomic coordinates for the heretofore unknown tertiary structure of the FcεRI protein and the heretofore unknown tertiary structure of the FcγRIIIb protein, and can be additionally used to model the heretofore unknown tertiary structure of other FcR proteins having substantially related linear amino acid sequence, such as for other members of the FcγR protein family and the FcαRI protein. There are three members of the FcγR family of proteins, FcγRI, FcγRII and FcγRIII, all of which act as immunoregulatory molecules and all of which bind to IgG.

Comparison of nucleic acid and amino acid sequences of the FcγR family of receptors indicates that the receptors are highly homologous. In addition, each member of the FcγR family of receptors belongs to the Ig super family of molecules, an assignment based on well established criteria (Hulett et al. 1994, *ibid.*). Moreover, FcγRII, FcγRIII, FcεRI and FcαRI each contain Ig-like domains, indicating the similarity between these receptors. FcγRI contains three Ig-like domains. The first and second domains, however, of FcγRI are substantially homologous to the Ig-like domains of FcγRII, FcγRIII, FcεRI and FcαRI. Current methods of tertiary structure determination that do not rely on x-ray diffraction techniques and thus do not require crystallization of the protein (e.g., computer modeling and nuclear magnetic resonance techniques) enable derivation and refinement of models of other FcγR proteins, FcεRI and FcαRI protein, extrapolated from a three dimensional structure of FcγRIIa protein. Thus, knowledge of the three dimensional structure of FcγRIIa protein has provided a starting point for investigation into the structure of all of these proteins.

Accordingly, a second object of the present invention is to provide information regarding the structure of FcγRIIa protein and models, atomic coordinates and derived three dimensional structures of other members of the FcγR family of proteins, FcεRI and FcαRI protein.

The knowledge of the three dimensional structure of FcγRIIa and models of other FcR provides a means for designing and producing compounds that regulate immune function and inflammation in an animal, including humans (i.e., structure based drug design). For example, chemical compounds can be designed to block binding of immunoglobulin to an Fc receptor protein using various computer programs and models.

Another embodiment of the present invention is to provide a three dimensional computer image of the three dimensional structure of an FcR.

5 Another embodiment of the present invention is to provide a computer-readable medium encoded with a set of three dimensional coordinates selected from the group of the three dimensional coordinates represented in Table 1, the three dimensional coordinates represented in Table 2, the three dimensional coordinates represented in Table 3,
10 the three dimensional coordinates represented in Table 4, and the three dimensional coordinates represented in Table 5, wherein, using a graphical display software program, the three dimensional coordinates create an electronic file that can be visualized on a computer capable of
15 representing said electronic file as a three dimensional image.

Accordingly, a third object of the present invention is to provide methods for using a three dimensional structure of FcR, such as FcγRIIa, and structures,
20 coordinates and models derived using such structure, for designing reagents for the treatment and diagnosis of disease, such as by binding to or mimicking the action of FcR protein, binding to or mimicking the action of an immunoglobulin (Ig), disrupting cellular signal
25 transduction through an FcR protein by, for example, preventing dimerization of two FcR proteins, or enhancing cellular signal transduction or binding to an FcR by, for example, enhancing dimerization of two FcR proteins.

The knowledge of the three dimensional structure of
30 FcR also provides a means for designing proteins that have altered beneficial functions by analyzing the structure and interactions between individual amino acids of the protein. For example, therapeutic proteins having improved binding to Ig or immune complexes of Ig can be designed to be used
35 as therapeutic compounds to prevent immune complex binding

to cells or enhance biological responses such as cellular signal transduction upon binding of FcR to Ig or complexes thereof. Thus recombinant soluble FcR engineered to contain improvements can be produced on the basis of the knowledge of the three dimensional structure.

Accordingly, a fourth object of the present invention is to provide for an extrapolation of the three dimensional structure of FcR to create recombinant protein having altered biological activity.

One embodiment of the present invention is a model of an FcR protein, wherein the model represents the three dimensional structure of FcR protein, in which the structure substantially conforms to the atomic coordinates represented by Table 1. Other embodiments of the present invention are the three dimensional structure of an FcγRIIa protein which substantially conforms to the atomic coordinates represented by Table 1; the three dimensional structure of a dimeric FcγRIIa protein which substantially conforms to the atomic coordinates represented by Table 2; the three dimensional structure of a monomeric FcεRI protein which substantially conforms to the atomic coordinates represented by Table 3; the three dimensional structure of a dimeric FcεRI protein which substantially conforms to the atomic coordinates represented by Table 4; the three dimensional structure of a dimeric FcγRIIIb protein which substantially conforms to the atomic coordinates represented by Table 5 and models representing such structures. Further embodiments of the present invention relate to a set of three dimensional coordinates of an FcγRIIa protein, wherein said coordinates are represented in Table 1; a set of three dimensional coordinates of a dimeric FcγRIIa protein, wherein said coordinates are represented in Table 2; a set of three dimensional coordinates of an FcεRI protein, wherein said coordinates are represented in Table 3; a set of three

dimensional coordinates of an FcεRI protein, wherein said coordinates are represented in Table 4; and a set of three dimensional coordinates of FcγRIIIb, wherein said coordinates are represented in Table 5. The present invention also includes methods to use such structures including structure based drug design and methods to derive models and images of target FcR structures.

Another embodiment of the present invention is a composition comprising FcγRIIa protein in a crystalline form. Yet another embodiment of the present invention is a composition comprising FcεRI protein in a crystalline form.

Yet another embodiment of the present invention is a method for producing crystals of FcγRIIa, comprising combining FcγRIIa protein with a mother liquor buffer selected from the group consisting of an acetate salt buffer and a sulphate buffer, and inducing crystal formation to produce said FcγRIIa crystals.

The present invention also includes a method for producing crystals of FcεRI, comprising combining FcεRI protein with a mother liquor buffer selected from the group consisting of an acetate salt buffer, a sodium cacodylate buffer and a sodium citrate buffer, and inducing crystal formation to produce said FcεRI crystals.

The present invention also includes a therapeutic composition that, when administered to an animal, reduces IgG-mediated tissue damage, said therapeutic composition comprising an inhibitory compound that inhibits the activity of an FcγRIIa protein, said inhibitory compound being identified by the method comprising: (a) providing a three dimensional structure of an FcγRIIa protein; (b) using said three dimensional structure to design a chemical compound selected from the group consisting of a compound that inhibits binding of FcγRIIa protein to IgG, a compound that substantially mimics the three dimensional structure

of FcγRIIa protein and a compound that inhibits binding of FcγRIIa protein with a molecule that stimulates cellular signal transduction through an FcγRIIa protein; (c) chemically synthesizing said chemical compound; and (d) evaluating the ability of said synthesized chemical compound to reduce IgG-mediated tissue damage.

Another embodiment of the present invention is a therapeutic composition that is capable of stimulating an IgG humoral immune response in an animal. Yet another embodiment of the present invention is a therapeutic composition that improves the therapeutic affects of an antibody that is administered to an animal to treat, by opsinization or FcγR-dependent effector functions (e.g. antibody-dependent FcγR-mediated cytotoxicity, phagocytosis or release of cellular mediators), a particular disease, including, but not limited to, cancer or infectious disease (e.g. oral infections such as HIV, herpes, bacterial infections, yeast infections or parasite infections). Such a therapeutic composition includes one or more stimulatory compounds that have increased binding to IgG, enhance binding of IgG to FcγR, enhance dimer formation of an FcγR and/or enhance signal transduction through the FcγR. Also included in the present invention is a method to stimulate a humoral immune response. The method includes the step of administering to an animal a therapeutic composition of the present invention.

The present invention also includes a therapeutic composition that, when administered to an animal, reduces IgG-mediated tissue damage, said therapeutic composition comprising an inhibitory compound that inhibits the activity of an FcγRIIb protein, said inhibitory compound being identified by the method comprising: (a) providing a three dimensional structure of an FcγRIIb protein; (b) using said three dimensional structure to design a chemical compound selected from the group consisting of a compound

that inhibits binding of FcγRIIIb protein to IgG, a compound that substantially mimics the three dimensional structure of FcγRIIIb protein and a compound that inhibits binding of FcγRIIIb protein with a molecule that stimulates cellular signal transduction through an FcγRIIIb protein; (c) chemically synthesizing said chemical compound; and (d) evaluating the ability of said synthesized chemical compound to reduce IgG-mediated tissue damage.

One embodiment of the present invention is a therapeutic composition that is capable of reducing IgE-mediated responses. Such therapeutic compositions are capable of reducing IgE-mediated responses resulting from IgE-mediated hypersensitivity, IgE-mediated release of inflammatory modulators or other biological mechanisms involved in IgE-mediated recruitment of inflammatory cells that involves FcεR protein. Such a therapeutic composition of the present invention can: (1) inhibit (i.e., prevent, block) binding of FcεR protein on a cell having an FcεR protein (e.g., mast cells) to an IgE immune complex by interfering with the IgE binding site of an FcεR protein; (2) inhibit precipitation of IgE or IgE immune complexes (i.e., prevent Fc:Fc interactions between two IgE); (3) inhibit immunoglobulin-mediated cellular signal transduction by interfering with the binding of an IgE to a cell surface receptor; and (4) inhibit FcεR-mediated cellular signal transduction by interfering with the binding of a cell signal inducing molecule (i.e., a molecule that induces cellular signal transduction through an FcεR protein) to an FcεR protein. Such therapeutic compositions include one or more inhibitory compounds that inhibit binding of IgE to FcεR protein, IgE to IgE, IgE to a cell surface receptor, or a cell signal inducing molecule to FcεR protein. Also included in the present invention are methods to reduce IgE-mediated responses, such as IgE-mediated inflammation.

Another embodiment of the present invention is a therapeutic composition that is capable of stimulating a IgE humoral immune response in an animal. Yet another embodiment of the present invention is a therapeutic composition that improves the therapeutic affects of an antibody that is administered to an animal to treat, by opsinization or FcεR-dependent effector functions (e.g. phagocytosis or release of cellular mediators), a particular disease. Such a therapeutic composition includes one or more stimulatory compounds that have increased binding to IgE, enhance binding of IgE to FcεRI, enhance dimer formation of FcεRI and/or otherwise enhance signal transduction through the FcεRI. Also included in the present invention is a method to stimulate a humoral immune response. The method includes the step of administering to an animal a therapeutic composition of the present invention.

BRIEF DESCRIPTION OF THE FIGURES

Fig. 1 is a scanned image of SDS-PAGE analysis of PsFcγRIIa protein during the purification process.

Fig. 2 is a scanned image of two-dimensional NEPHGE analysis of purified PsFcγRIIa protein.

Fig. 3 illustrates Langmuir plots of purified PsFcγRIIa protein binding to different isotypes of human immunoglobulin G.

Fig. 4 illustrates a graphical representation of the dimer of PFcγRIIa.

Fig. 5 illustrates the positions of the beta sheets in FcγRIIa Domains 1 and 2 and compares amino acid sequences of isomorphs of FcγRII.

Fig. 6 illustrates the stereo view of the FcγRIIa structure shown in Fig. 4.

Fig. 7 illustrates the location of amino acids involved in binding of FcγRIIa to IgG.

Fig. 8 illustrates an expanded view of an IgG binding region showing position and side chains of the involved amino acids.

5 Fig. 9 illustrates an expanded view of an IgG binding region showing amino acids which when mutated to alanine improves IgG binding to FcγRIIa.

Fig. 10 illustrates an expanded view of the region of one FcγRIIa monomer that contributes to the dimer interface.

10 Fig. 11 illustrates a comparison of the amino acid sequence of FcγRIIa protein with the amino acid sequences of FcγRI, FcγRIIb and FcεRI protein.

15 Fig. 12 illustrates a comparison of structural features shared by FcγRIIa, FcγRI, FcγRIIb and FcεRI proteins.

Fig. 13 illustrates a sequence alignment of the amino acid sequences of FcγRIIa and FcεRI.

Fig. 14 is a scanned image illustrating a worm representation of the structure of an FcεRI monomer.

20 Fig. 15 is a scanned image illustrating a worm representation of the structure of an FcεRI dimer.

Fig. 16 is a scanned image illustrating a molecular surface representation of an FcεRI dimer model.

25 Fig. 17 is a schematic representation of target sites in the FcR structure for drug design.

Fig. 18 illustrates a sequence alignment of the amino acid sequences of FcγRIIa and FcγRIIb.

DETAILED DESCRIPTION OF THE INVENTION

30 The present invention relates to the discovery of the three-dimensional structure of Fc receptor (FcR) proteins, models of such three-dimensional structures, a method of structure based drug design using such structures, the compounds identified by such methods and the use of such
35 compounds in therapeutic compositions. More particularly,

the present invention relates to novel crystals of Fc gamma receptor IIa (FcγRIIa), novel crystals of Fc epsilon receptor I (FcεRI), methods of production of such crystals, three dimensional coordinates of FcγRIIa protein, a three dimensional structure of FcγRIIa protein, FcR structures and models derived from the FcγRIIa structure, including FcεRI and FcγRIIb, and uses of such structure and models to derive other FcR structures and in drug design strategies. It is to be noted that the term "a" or "an" entity refers to one or more of that entity; for example, a compound refers to one or more compounds or at least one compound. As such, the terms "a" (or "an"), "one or more" and "at least one" can be used interchangeably herein. It is also to be noted that the terms "comprising", "including", and "having" can be used interchangeably. Furthermore, a compound "selected from the group consisting of" refers to one or more of the compounds in the list that follows, including mixtures (i.e., combinations) of two or more of the compounds. According to the present invention, an isolated, or pure, protein, is a protein that has been removed from its natural milieu. As such, "isolated" and "biologically pure" do not necessarily reflect the extent to which the protein has been purified. An isolated protein of the present invention can be obtained from its natural source, can be produced using recombinant DNA technology or can be produced by chemical synthesis. It is also to be noted that the terms "tertiary" and "three dimensional" can be used interchangeably. It is also to be noted that reference to an "FcR protein" can also be recited simply as "FcR" and such terms can be used to refer to a the complete FcR protein, a portion of the FcR protein, such as a polypeptide, and/or a monomer or a dimer of the FcR protein. When reference is specifically made to a monomer or dimer, for example, such term is typically used in conjunction with the FcR protein name.

The production of the crystal structure of FcγRIIa has been described in detail in U.S. Provisional Application Serial No. 60/073,972, filed February 6, 1998. The entire disclosure of U.S. Provisional Application Serial No. 60/073,972 is incorporated herein by reference in its entirety.

One embodiment of the present invention includes a model of an Fc receptor, in which the model represents a three dimensional structure of an Fc receptor (FcR) protein. Another embodiment of the present invention includes the three dimensional structure of an FcR protein. A three dimensional structure of an FcR protein encompassed by the present invention substantially conforms with the atomic coordinates represented in any one of Tables 1-5. According to the present invention, the use of the term "substantially conforms" refers to at least a portion of a three dimensional structure of an FcR protein which is sufficiently spatially similar to at least a portion of a specified three dimensional configuration of a particular set of atomic coordinates (e.g., those represented by Table 1) to allow the three dimensional structure of the FcR protein to be modeled or calculated (i.e., by molecular replacement) using the particular set of atomic coordinates as a basis for determining the atomic coordinates defining the three dimensional configuration of the FcR protein. According to the present invention, a three dimensional structure of a dimer of a first FcR can substantially conform to the atomic coordinates which represent a three dimensional structure of a monomer of a second FcR, and vice versa. In the first instance, at least a portion of the structure of the first FcR protein (i.e., a monomer of the first FcR protein dimer) substantially conforms to the atomic coordinates which represent the three dimensional configuration of the second FcR monomer. In the second reversed case, a first monomeric FcR protein substantially

conforms to at least a portion of the second FcR protein (i.e., a monomer of the second FcR protein dimer). Similarly, a three dimensional structure of a given portion or chain of a first FcR can substantially conform to at least a portion of the atomic coordinates which represent a three dimensional configuration of a second FcR.

More particularly, a structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 50% of such structure has an average root-mean-square deviation (RMSD) of less than about 1.5 Å for the backbone atoms in secondary structure elements in each domain, and more preferably, less than about 1.3 Å for the backbone atoms in secondary structure elements in each domain, and, in increasing preference, less than about 1.0 Å, less than about 0.7 Å, less than about 0.5 Å, and most preferably, less than about 0.3 Å for the backbone atoms in secondary structure elements in each domain. In a more preferred embodiment, a structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 75% of such structure has the recited average root-mean-square deviation (RMSD) value, and more preferably, at least about 90% of such structure has the recited average root-mean-square deviation (RMSD) value, and most preferably, about 100% of such structure has the recited average root-mean-square deviation (RMSD) value. In an even more preferred embodiment, the above definition of "substantially conforms" can be extended to include atoms of amino acid side chains. As used herein, the phrase "common amino acid side chains" refers to amino acid side chains that are common to both the structure which substantially conforms to a given set of atomic coordinates and the structure that is actually represented by such atomic coordinates. Preferably, a three dimensional structure that substantially conforms to a given set of atomic coordinates

is a structure wherein at least about 50% of the common amino acid side chains have an average root-mean-square deviation (RMSD) of less than about 1.5 Å, and more preferably, less than about 1.3 Å, and, in increasing preference, less than about 1.0 Å, less than about 0.7 Å, less than about 0.5 Å, and most preferably, less than about 0.3 Å. In a more preferred embodiment, a structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 75% of the common amino acid side chains have the recited average root-mean-square deviation (RMSD) value, and more preferably, at least about 90% of the common amino acid side chains have the recited average root-mean-square deviation (RMSD) value, and most preferably, about 100% of the common amino acid side chains have the recited average root-mean-square deviation (RMSD) value.

A three dimensional structure of an FcR protein which substantially conforms to a specified set of atomic coordinates can be modeled by a suitable modeling computer program such as MODELER (A. Sali and T.L. Blundell, *J. Mol. Biol.*, vol. 234:779-815, 1993 as implemented in the Insight II Homology software package (Insight II (97.0), MSI, San Diego)), using information, for example, derived from the following data: (1) the amino acid sequence of the FcR protein; (2) the amino acid sequence of the related portion(s) of the protein represented by the specified set of atomic coordinates having a three dimensional configuration; and, (3) the atomic coordinates of the specified three dimensional configuration. A three dimensional structure of an FcR protein which substantially conforms to a specified set of atomic coordinates can also be calculated by a method such as molecular replacement, which is described in detail below.

A suitable three dimensional structure of an FcR protein for use in modeling or calculating the three

dimensional structure of another FcR protein comprises the set of atomic coordinates represented in Table 1. The set of three dimensional coordinates set forth in Table 1 is represented in standard Protein Data Bank format.

5 According to the present invention, an FcR protein selected from the group of Fc γ RI, Fc γ RIIa, Fc γ RIIb, Fc γ RIIc, Fc γ RIIIb, Fc ϵ RI and Fc α RI have a three dimensional structure which substantially conforms to the set of atomic coordinates represented by Table 1. As used herein, a

10 three dimensional structure can also be a most probable, or significant, fit with a set of atomic coordinates. According to the present invention, a most probable or significant fit refers to the fit that a particular FcR protein has with a set of atomic coordinates derived from

15 that particular FcR protein. Such atomic coordinates can be derived, for example, from the crystal structure of the protein such as the coordinates determined for the Fc γ RIIa structure provided herein, or from a model of the structure of the protein as determined herein for Fc ϵ RI and Fc γ RIIIb.

20 For example, the three dimensional structure of a monomeric Fc γ RIIa protein, including a naturally occurring or recombinantly produced Fc γ RIIa protein, substantially conforms to and is a most probable fit, or significant fit, with the atomic coordinates of Table 1. The three

25 dimensional crystal structure of Fc γ RIIa that was determined by the present inventors comprises the atomic coordinates of Table 1. Also as an example, the three dimensional structure of an Fc ϵ RI protein substantially conforms to the atomic coordinates of Table 1 and both

30 substantially conforms to and is a most probable fit with the atomic coordinates of Table 3, and the three dimensional structure of the model of Fc ϵ RI monomer determined by the present inventors comprises the atomic coordinates of Table 3. This definition can be applied to

35 the other FcR proteins in a similar manner.

A preferred structure of an FcR protein according to the present invention substantially conforms to the atomic coordinates, and the B-values and/or the thermal parameters represented in Table 1. Such values as listed in Table 1
5 can be interpreted by one of skill in the art. A more preferred three dimensional structure of an FcR protein substantially conforms to the three dimensional coordinates represented in Table 1. An even more preferred three dimensional structure of an FcR protein is a most probable
10 fit with the three dimensional coordinates represented in Table 1. Methods to determine a substantially conforming and probable fit are within the expertise of skill in the art and are described herein in the Examples section.

A preferred FcR protein that has a three dimensional
15 structure which substantially conforms to the atomic coordinates represented by Table 1 includes an FcR protein having an amino acid sequence that is at least about 25%, preferably at least about 30%, more preferably at least about 40%, more preferably at least about 50%, more
20 preferably at least about 60%, more preferably at least about 70%, more preferably at least about 80% and more preferably at least about 90%, identical to an amino acid sequence of an FcγRIIa protein, preferably an amino acid sequence including SEQ ID NO:3, SEQ ID NO:10, SEQ ID NO:11
25 and/or SEQ ID NO:12, across the full-length of the FcR sequence when using, for example, a sequence alignment program such as the DNAsis™ program (available from Hitachi Software, San Bruno, CA) or the MacVector™ program (available from the Eastman Kodak Company, New Haven, CT)
30 or the GCY™ program (available from "GCY", University of Wisconsin, Madison, WI), such alignment being performed for example, using the standard default values accompanying such alignment programs.

One embodiment of the present invention includes a
35 three dimensional structure of FcγRIIa protein. A suitable

three dimensional structure of FcγRIIa protein substantially conforms with the atomic coordinates represented in Table 1. A suitable three dimensional structure of FcγRIIa also substantially conforms with the atomic coordinates represented by Tables 2-5. A suitable three dimensional structure of FcγRIIa protein also comprises the set of atomic coordinates represented in Table 1. The set of three dimensional coordinates of FcγRIIa protein is represented in standard Protein Data Bank format. A preferred structure of FcγRIIa protein substantially conforms to the atomic coordinates, and the B-values and/or the thermal parameters represented in Table 1 (monomeric FcγRIIa) or Table 2 (dimeric FcγRIIa). Such values as listed in Table 1 can be interpreted by one of skill in the art. A more preferred three dimensional structure of FcγRIIa protein has a most probable fit with the three dimensional coordinates represented in Table 1.

One embodiment of the present invention includes a three dimensional structure of FcεRI protein. A suitable three dimensional structure of FcεRI protein substantially conforms with the atomic coordinates represented in Table 1, Table 2, Table 3, Table 4 or Table 5. A more suitable three dimensional structure of FcεRI protein substantially conforms with the sets of atomic coordinates represented in Table 3 (monomeric FcεRI) or Table 4 (dimeric FcεRI). A suitable three dimensional structure of FcεRI protein also comprises the set of atomic coordinates represented in Tables 3 or 4. The sets of three dimensional coordinates of FcεRI protein are represented in standard Protein Data Bank format. Such coordinates as listed in Tables 1-5 can be interpreted by one of skill in the art. A more preferred three dimensional structure of FcεRI protein has a probable fit with the three dimensional coordinates represented in Table 3 or Table 4. One embodiment of the present invention includes a three dimensional structure of

FcγRIIIb protein. A suitable three dimensional structure of FcγRIIIb protein substantially conforms with the atomic coordinates represented in Table 1, Table 2, Table 3, Table 4 or Table 5. An even more suitable three dimensional structure of FcγRIIIb protein substantially conforms with the set of atomic coordinates represented in Table 5. A suitable three dimensional structure of FcγRIIIb protein also comprises the set of atomic coordinates represented in Table 5. The sets of three dimensional coordinates of FcγRIIIb protein are represented in standard Protein Data Bank format. A more preferred three dimensional structure of FcγRIIIb protein has a most probable fit with the three dimensional coordinates represented in Table 5. A three dimensional structure of any FcR protein can be modeled using methods generally known in the art based on information obtained from analysis of an FcγRIIa crystal, and from other FcR structures which are derived from an FcγRIIa crystal. The Examples section below discloses the production of an FcγRIIa crystal, the production of an FcεRI crystal, the three dimensional structure of an FcγRIIa protein monomer and dimer derived from the FcγRIIa crystal, and the model of the three dimensional structure of an FcεRI protein monomer and dimer using methods generally known in the art based on the information obtained from analysis of an FcγRIIa crystal. It is an embodiment of the present invention that the three dimensional structure of a crystalline FcR, such as the crystalline FcγRIIa, can be used to derive the three dimensional structure of any other FcR, such as the FcεRI disclosed herein. Subsequently, the derived three dimensional structure of such an FcR (e.g., FcεRI) derived from the crystalline structure of FcγRIIa can be used to derive the three dimensional structure of other FcR, such as FcγRIII. Therefore, the novel discovery herein of the crystalline FcγRIIa and the three dimensional structure of

FcyRIIa permits one of ordinary skill in the art to now derive the three dimensional structure, and models thereof, of any FcR. The derivation of the structure of any FcR can now be achieved even in the absence of having crystal structure data for such other FcR, and when the crystal structure of another FcR is available, the modeling of the three dimensional structure of the new FcR can be refined using the knowledge already gained from the FcyRIIa structure. It is an advantage of the present invention that, in the absence of crystal structure data for other FcR proteins, the three dimensional structures of other FcR proteins can be modeled, taking into account differences in the amino acid sequence of the other FcR. Indeed, the recent report of the crystallization of the monomeric FcεRI and publication of a model of the receptor (Garman et al., December 23, 1998, *Cell* 95:951-961) subsequent to the priority filing dates of the present application has confirmed that the monomeric FcεRI protein determined by the present inventors comprising the atomic coordinates represented in Table 3 has the overall gross structural features of the three dimensional structure of the crystalline FcεRI reported in Garman et al. Although the atomic coordinates of the crystalline FcεRI structure of Garman et al. are not currently publicly available, a review of the structural representations and discussion in Garman et al. indicates that the three dimensional structure of the crystalline FcεRI is expected to substantially conform to the atomic coordinates represented by Table 3. Moreover, the novel discoveries of the present invention allow for structure based drug design of compounds which affect the activity of virtually any FcR, and particularly, of FcyR and FcεRI.

Crystals are derivatized with heavy atom compounds such as complexes or salts of Pt, Hg, Au and Pb and X-ray diffraction data are measured for native and derivatized

crystals. Differences in diffraction intensities for native crystals and derivatized crystals can be used to determine phases for these data by the methods of MIR (multiple Isomorphous Replacement) or SIRAS (single isomorphous replacement with anomalous scattering). The Fourier transform of these data yield a low resolution electron density map for the protein. This electron density can be modified by image enhancement techniques. A molecular model for the protein is then placed in the electron density. This initial (partial) structure can be refined using a computer program (such as XPLOR) by modifying the parameters which describe the structure to minimize the difference between the measured and calculated diffraction patterns, while simultaneously restraining the model to conform to known geometric and chemical properties of proteins. New phases and a thus a new electron density map can be calculated for protein. Using this map as a guide the molecular model of the structure may be improved manually. This procedure is repeated to give the structure of the protein, represented herein for FcγRIIa as a set of atomic coordinates in Table 1.

One embodiment of the present invention includes a three dimensional structure of FcγRIIa protein, in which the atomic coordinates of the FcγRIIa protein are generated by the method comprising: (a) providing FcγRIIa protein in crystalline form; (b) generating an electron-density map of the crystalline FcγRIIa protein; and (c) analyzing the electron-density map to produce the atomic coordinates.

According to the present invention, a three dimensional structure of FcγRIIa protein of the present invention can be used to derive a model of the three dimensional structure of another FcR protein (i.e., a structure to be modeled). As used herein, a "structure" of a protein refers to the components and the manner of arrangement of the components to constitute the protein.

As used herein, the term "model" refers to a representation in a tangible medium of the three dimensional structure of a protein, polypeptide or peptide. For example, a model can be a representation of the three dimensional structure in an electronic file, on a computer screen, on a piece of paper (i.e., on a two dimensional medium), and/or as a ball-and-stick figure. Physical three-dimensional models are tangible and include, but are not limited to, stick models and space-filling models. The phrase "imaging the model on a computer screen" refers to the ability to express (or represent) and manipulate the model on a computer screen using appropriate computer hardware and software technology known to those skilled in the art. Such technology is available from a variety of sources including, for example, Evans and Sutherland, Salt Lake City, Utah, and Biosym Technologies, San Diego, CA. The phrase "providing a picture of the model" refers to the ability to generate a "hard copy" of the model. Hard copies include both motion and still pictures. Computer screen images and pictures of the model can be visualized in a number of formats including space-filling representations, α carbon traces, ribbon diagrams (see, for example, Fig. 14 which is a two dimensional ribbon diagram model of a three-dimensional structure of human Fc ϵ RI protein) and electron density maps.

Suitable target FcR structures to model using a method of the present invention include any FcR protein, polypeptide or peptide, including monomers, dimers and multimers of an FcR protein, that is substantially structurally related to an Fc γ RIIa protein. A preferred target FcR structure that is substantially structurally related to an Fc γ RIIa protein includes a target FcR structure having an amino acid sequence that is at least about 25%, preferably at least about 30%, more preferably at least about 36%, more preferably at least about 40%,

more preferably at least about 50%, more preferably at least about 60%, more preferably at least about 70%, more preferably at least about 80% and more preferably at least about 90%, identical to an amino acid sequence of an FcγRIIa protein, preferably an amino acid sequence including SEQ ID NO:3, SEQ ID NO:10, SEQ ID NO:11, SEQ ID NO:12, SEQ ID NO:14 and/or SEQ ID NO:15, across the full-length of the target FcR structure sequence when using, for example, a sequence alignment program such as the DNAsis™ program (available from Hitachi Software, San Bruno, CA) or the MacVector™ program (available from the Eastman Kodak Company, New Haven, CT) or the GCY™ program (available from "GCY", University of Wisconsin, Madison, WI), such alignment being performed for example, using the standard default values accompanying such alignment programs. More preferred target FcR structures to model include proteins comprising amino acid sequences that are at least about 50%, preferably at least about 60%, more preferably at least about 70%, more preferably at least about 80%, more preferably at least about 90%, and more preferably at least about 95%, identical to amino acid sequence SEQ ID NO:3, SEQ ID NO:5, SEQ ID NO:6, SEQ ID NO:7, SEQ ID NO:8, SEQ ID NO:9, SEQ ID NO:10, SEQ ID NO:11, SEQ ID NO:12, or SEQ ID NO:13 when comparing preferred regions of the sequence, such as the amino acid sequence for Domain 1 or Domain 2 of any one of the amino acid sequences, when using a DNA alignment program disclosed herein to align the amino acid sequences. A more preferred target FcR structure to model includes a structure comprising FcγRI, FcγRIIa, FcγRIIb, FcγRIIc, FcγRIIb, FcεRI or FcαRI protein, more preferably a structure comprising the amino acid sequence SEQ ID NO:3, SEQ ID NO:5, SEQ ID NO:6, SEQ ID NO:7, SEQ ID NO:8, SEQ ID NO:9, SEQ ID NO:10, SEQ ID NO:11, SEQ ID NO:12, or SEQ ID NO:13 and more preferably a structure consisting of the amino

acid sequence SEQ ID NO:3, SEQ ID NO:5, SEQ ID NO:6, SEQ ID NO:7, SEQ ID NO:8, SEQ ID NO:9, SEQ ID NO:10, SEQ ID NO:11, SEQ ID NO:12, or SEQ ID NO:13.

Preferred target FcR structures to model also include, but are not limited to, derivations of Fc receptor proteins, such as an Fc receptor having one or more amino acid residues substituted, deleted or added (referred to herein as Fc receptor mutants), or proteins encoded by natural allelic variants of a nucleic acid molecule encoding an Fc receptor. A preferred Fc receptor protein to model includes FcγRIIaTM (i.e., an FcγRIIa protein from which the transmembrane domain has been deleted), and mutants or natural allelic variants of a nucleic acid molecule encoding FcγRI, FcγRIIa, FcγRIIb, FcγRIIc, FcγRIIIb, FcεRI, FcαRI protein. More preferred Fc receptor proteins to model include Fc receptor proteins having an amino acid sequence including SEQ ID NO:5, SEQ ID NO:6, SEQ ID NO:7, SEQ ID NO:8, SEQ ID NO:9, SEQ ID NO:10, SEQ ID NO:11, SEQ ID NO:12, or SEQ ID NO:13 or mutants or natural allelic variants of SEQ ID NO:3, SEQ ID NO:5, SEQ ID NO:6, SEQ ID NO:7, SEQ ID NO:8, SEQ ID NO:9, SEQ ID NO:10, SEQ ID NO:11, SEQ ID NO:12, or SEQ ID NO:13. According to the present invention, an amino acid sequence for FcγRIIb is represented herein as SEQ ID NO:5, an amino acid sequence for FcγRIIc is represented herein as SEQ ID NO:6, an amino acid sequence for FcγRI is represented herein as SEQ ID NO:7, an amino acid sequence for FcγRIII is represented herein as SEQ ID NO:8, an amino acid sequence for FcεRI is represented herein as SEQ ID NO:9 and as set forth in Fig. 13, and an amino acid sequence for FcαRI is represented herein as SEQ ID NO:13. It is noted that the nucleotide and amino acid sequences for all of the above-known FcR are known and publicly available. Preferred allelic variants to model include, but are not limited to, FcγRIIa allelic variants having a glutamine at residue 27 of SEQ ID NO:3

and an arginine at residue 131 of SEQ ID NO:3, represented herein as SEQ ID NO:10; a tryptophan at residue 27 of SEQ ID NO:3 and a histidine at residue 131 of SEQ ID NO:3, represented herein as SEQ ID NO:11; or a tryptophan at residue 27 of SEQ ID NO:3 and an arginine at residue 131 of SEQ ID NO:3, represented herein as SEQ ID NO:12.

As used herein, a "natural allelic variant" refers to alternative forms of a gene that occupies corresponding loci on homologous chromosomes. Allelic variants typically encode proteins having similar activity to that of the protein encoded by the gene to which they are being compared. Allelic variants can also comprise alterations in the 5' or 3' untranslated regions of the gene (e.g., in regulatory control regions). Allelic variants are well known to those skilled in the art and would be expected to be found within a given group of genes encoding an Fc receptor in a given species of animal.

As used herein, "mutants of a nucleic acid molecule encoding an Fc receptor" refer to nucleic acid molecules modified by nucleotide insertions, deletions and/or substitutions. Preferably, a mutant of an Fc receptor nucleic acid molecule comprises modifications such that the protein encoded by the mutant of an Fc receptor nucleic acid molecule (i.e., an Fc receptor protein mutant) has one or more epitopes that can be targeted by a humoral or cellular immune response against a non-mutated Fc receptor protein. More preferably, the nucleic acid molecule encoding a mutant Fc receptor protein can form a stable hybrid with a nucleic acid sequence encoding a non-mutated Fc receptor nucleic acid molecule under stringent hybridization conditions. Even more preferably, the nucleic acid molecule encoding a mutant Fc receptor protein can form a stable hybrid, under stringent hybridization conditions, with a nucleic acid sequence encoding an amino acid sequence including SEQ ID NO:3, SEQ ID NO:5, SEQ ID

NO:6, SEQ ID NO:7, SEQ ID NO:8, SEQ ID NO:9, SEQ ID NO:10, SEQ ID NO:11, SEQ ID NO:12, or SEQ ID NO:13.

As used herein, stringent hybridization conditions refer to standard hybridization conditions under which nucleic acid molecules are used to identify similar nucleic acid molecules. Such standard conditions are disclosed, for example, in Sambrook et al., *Molecular Cloning: A Laboratory Manual*, Cold Spring Harbor Labs Press, 1989. Sambrook et al., *ibid.*, is incorporated by reference herein in its entirety (see specifically, pages 9.31-9.62, 11.7 and 11.45-11.61). In addition, formulae to calculate the appropriate hybridization and wash conditions to achieve hybridization permitting varying degrees of mismatch of nucleotides are disclosed, for example, in Meinkoth et al., 1984, *Anal. Biochem.* 138, 267-284; Meinkoth et al., *ibid.*, is incorporated by reference herein in its entirety.

More particularly, stringent hybridization conditions, as referred to herein, refer to conditions which permit isolation of nucleic acid molecules having at least about 70% nucleic acid sequence identity with the nucleic acid molecule being used to probe in the hybridization reaction, more particularly at least about 75%, and most particularly at least about 80%. Such conditions will vary, depending on whether DNA:RNA or DNA:DNA hybrids are being formed. Calculated melting temperatures for DNA:DNA hybrids are 10°C less than for DNA:RNA hybrids. In particular embodiments, stringent hybridization conditions for DNA:DNA hybrids include hybridization at an ionic strength of 0.1X SSC (0.157 M Na⁺) at a temperature of between about 20°C and about 35°C, more preferably, between about 28°C and about 40°C, and even more preferably, between about 35°C and about 45°C. In particular embodiments, stringent hybridization conditions for DNA:RNA hybrids include hybridization at an ionic strength of 0.1X SSC (0.157 M Na⁺) at a temperature of between about 30°C and about 45°C, more preferably, between

about 38°C and about 50°C, and even more preferably, between about 45°C and about 55°C. These values are based on calculations of a melting temperature for molecules larger than about 100 nucleotides, 0% formamide and a G + C content of about 50%. Alternatively, T_m can be calculated empirically as set forth in Sambrook et al., *supra*, pages 11.55 to 11.57.

A model of the present invention can be derived using conserved structural features between the known three dimensional structure of one FcR protein, such as FcγRIIa, and another target FcR structure. Such structural features include, but are not limited to, amino acid sequence, conserved di-sulphide bonds, and β-strands or β-sheets that are highly conserved in immunoglobulin superfamily members. For example, Figs. 5, 11 and 12 illustrate the relationship of β-strands with the linear amino acid sequence of various Fc receptor proteins. Preferably, a model of the present invention is derived by starting with the backbone of the three dimensional structure of FcγRIIa protein. Individual residues are then replaced according to the amino acid sequence of the target FcR structure at residues that differ from the amino acid sequence of an FcγRIIa protein. Care is taken that replacement of residues does not disturb the tertiary structure of the backbone. While procedures to model target FcR structures are generally known in the art, the present invention provides the first three dimensional structure of FcγRIIa protein and the first three dimensional structures of protein substantially related to a member of the family of FcγR receptors, an FcεRI and an FcγRIIIb. Thus, the present invention provides essential information to produce accurate, and therefore, useful models of a member of the family of FcγR receptors, of the FcεRI receptor and of the FcαRI receptor. As discussed above, once the three dimensional structure of a second FcR has been derived from a determined three

dimensional structure of a first FcR such as FcγRIIa disclosed herein, the second FcR three dimensional structure can be used to derive (i.e., model or calculate) the three dimensional structure of another FcR.

5 According to the present invention, a structure can be modeled using techniques generally described by, for example, Sali, *Current Opinions in Biotechnology*, vol. 6, pp. 437-451, 1995, and algorithms can be implemented in program packages such as Homology 95.0 (in the program
10 Insight II, available from Biosym/MSI, San Diego, CA). Use of Homology 95.0 requires an alignment of an amino acid sequence of a known structure having a known three dimensional structure with an amino acid sequence of a target structure to be modeled. The alignment can be a
15 pairwise alignment or a multiple sequence alignment including other related sequences (for example, using the method generally described by Rost, *Meth. Enzymol.*, vol. 266, pp. 525-539, 1996) to improve accuracy. Structurally conserved regions can be identified by comparing related
20 structural features, or by examining the degree of sequence homology between the known structure and the target structure. Certain coordinates for the target structure are assigned using known structures from the known structure. Coordinates for other regions of the target
25 structure can be generated from fragments obtained from known structures such as those found in the Protein Data Bank maintained by Brookhaven National Laboratory, Upton, NY. Conformation of side chains of the target structure can be assigned with reference to what is sterically allowable and using a library of rotamers and their
30 frequency of occurrence (as generally described in Ponder and Richards, *J. Mol. Biol.*, vol. 193, pp. 775-791, 1987).

The resulting model of the target structure, can be refined by molecular mechanics (such as embodied in the

program Discover, available from Biosym/MSI) to ensure that the model is chemically and conformationally reasonable.

Accordingly, one embodiment of the present invention is a method to derive a model of the three dimensional structure of a target FcR structure, the method comprising the steps of: (a) providing an amino acid sequence of an FcγRIIa protein and an amino acid sequence of a target FcR structure; (b) identifying structurally conserved regions shared between the FcγRIIa amino acid sequence and the target FcR structure amino acid sequence; (c) determining atomic coordinates for the target FcR structure by assigning said structurally conserved regions of the target FcR structure to a three dimensional structure using a three dimensional structure of an FcγRIIa protein based on atomic coordinates that substantially conform to the atomic coordinates represented in Table 1, to derive a model of the three dimensional structure of the target structure amino acid sequence. A model according to the present invention has been previously described herein. Preferably the model comprises a computer model. The method can further comprise the step of electronically simulating the structural assignments to derive a computer model of the three dimensional structure of the target structure amino acid sequence. Suitable target structures to model include proteins, polypeptides and peptides of Fc receptors disclosed herein, including monomers and dimers of such receptors. Preferred amino acid sequences to model are disclosed herein.

Another embodiment of the present invention is a method to derive a computer model of the three dimensional structure of a target FcR structure for which a crystal has been produced (referred to herein as a "crystallized target structure"). A suitable method to produce such a model includes the method comprising molecular replacement. Methods of molecular replacement are generally known by

those of skill in the art (generally described in Brunger, *Meth. Enzym.*, vol. 276, pp. 558-580, 1997; Navaza and Saludjian, *Meth. Enzym.*, vol. 276, pp. 581-594, 1997; Tong and Rossmann, *Meth. Enzym.*, vol. 276, pp. 594-611, 1997; 5 and Bentley, *Meth. Enzym.*, vol. 276, pp. 611-619, 1997, each of which are incorporated by this reference herein in their entirety) and are performed in a software program including, for example, XPLOR. According to the present invention, X-ray diffraction data is collected from the 10 crystal of a crystallized target structure. The X-ray diffraction data is transformed to calculate a Patterson function. The Patterson function of the crystallized target structure is compared with a Patterson function calculated from a known structure (referred to herein as a 15 search structure). The Patterson function of the crystallized target structure is rotated on the search structure Patterson function to determine the correct orientation of the crystallized target structure in the crystal. The translation function is then calculated to 20 determine the location of the target structure with respect to the crystal axes. Once the crystallized target structure has been correctly positioned in the unit cell, initial phases for the experimental data can be calculated. These phases are necessary for calculation of an electron 25 density map from which structural differences can be observed and for refinement of the structure. Preferably, the structural features (e.g., amino acid sequence, conserved di-sulphide bonds, and β -strands or β -sheets) of the search molecule are related to the crystallized target 30 structure. Preferably, a crystallized target FcR structure useful in a method of molecular replacement according to the present invention has an amino acid sequence that is at least about 25%, more preferably at least about 30%, more preferably at least about 40%, more preferably at least 35 about 50%, more preferably at least about 60%, more

preferably at least about 70%, more preferably at least about 80% and more preferably at least about 90% identical to the amino acid sequence of the search structure (e.g., FcγRIIa), when the two amino acid sequences are compared using a DNA alignment program disclosed herein. A preferred search structure of the present invention includes an FcγRIIa protein comprising an amino acid sequence including SEQ ID NO:3, SEQ ID NO:10, SEQ ID NO:11, SEQ ID NO:12, SEQ ID NO:14 or SEQ ID NO:15. A more preferred search structure of the present invention includes an FcγRIIa protein having a three dimensional structure that substantially conforms with the atomic coordinates listed in Table 1. Preferably, a Patterson function of a crystalline FcγRIIa protein is derived from X-ray diffraction of an FcγRIIa crystal of the present invention. A preferred target FcR structure for use in a molecular replacement strategy of the present invention includes FcγRI, FcγRIIb, FcγRIIc, FcγRIII, FcεRI and/or FcαRI, and most preferably, FcεRI and FcγRIIIb.

20 A preferred embodiment of the present invention includes a method to derive a three dimensional structure of a crystallized target FcR structure (i.e. a crystallized FcR protein), said method comprising the steps of: (a) comparing the Patterson function of a crystallized target FcR structure with the Patterson function of crystalline FcγRIIa protein to produce an electron-density map of said crystallized target FcR structure; and (b) analyzing the electron-density map to produce the three dimensional structure of the crystallized target FcR structure.

30 Another embodiment of the present invention is a method to determine a three dimensional structure of a target structure, in which the three dimensional structure of the target FcR structure is not known. Such a method is useful for identifying structures that are related to the three dimensional structure of an FcγRIIa protein based

only on the three dimensional structure of the target structure. Thus, the present method enables identification of structures that do not have high amino acid identity with an FcγRIIa protein but which do share three dimensional structure similarities. A preferred method to determine a three dimensional structure of a target FcR structure comprises: (a) providing an amino acid sequence of a target structure, wherein the three dimensional structure of the target structure is not known; (b) analyzing the pattern of folding of the amino acid sequence in a three dimensional conformation by fold recognition; and (c) comparing the pattern of folding of the target structure amino acid sequence with the three dimensional structure of FcγRIIa protein to determine the three dimensional structure of the target structure, wherein the three dimensional structure of the FcγRIIa protein substantially conforms to the atomic coordinates represented in Table 1. Preferred methods of fold recognition include the methods generally described in Jones, *Curr. Opin. Struc. Biol.*, vol. 7, pp. 377-387, 1997. Such folding can be analyzed based on hydrophobic and/or hydrophilic properties of a target structure.

One embodiment of the present invention includes a three dimensional computer image of the three dimensional structure of an FcR protein. Suitable structures of which to produce three dimensional computer images are disclosed herein. Preferably, a computer image is created to a structure substantially conforms with the three dimensional coordinates listed in Table 1. A computer image of the present invention can be produced using any suitable software program, including, but not limited to, MOLSCRIPT 2.0 (Avatar Software AB, Heleneborgsgatan 21C, SE-11731 Stockholm, Sweden), the graphical display program O (Jones et. al., *Acta Crystallography*, vol. A47, p. 110, 1991) or the graphical display program GRASP. Suitable computer

hardware useful for producing an image of the present invention are known to those of skill in the art. Preferred computer hardware includes a Silicon Graphics Workstation.

5 Another embodiment of the present invention relates to a computer-readable medium encoded with a set of three dimensional coordinates selected from the group of the three dimensional coordinates represented in Table 1, the three dimensional coordinates represented in Table 2, the
10 three dimensional coordinates represented in Table 3, the three dimensional coordinates represented in Table 4, and the three dimensional coordinates represented in Table 5, wherein, using a graphical display software program, the three dimensional coordinates create an electronic file
15 that can be visualized on a computer capable of representing said electronic file as a three dimensional image. Preferably, the three dimensional structure is of an FcR protein selected from the group of FcγRIIa, FcεRI, and FcγRIIIb.

20 Yet another embodiment of the present invention relates to a computer-readable medium encoded with a set of three dimensional coordinates of a three dimensional structure which substantially conforms to the three dimensional coordinates represented in Table 1, wherein,
25 using a graphical display software program, the set of three dimensional coordinates create an electronic file that can be visualized on a computer capable of representing said electronic file as a three dimensional image. Preferably, the three dimensional structure is of
30 an FcR protein selected from the group of FcγRI, FcγRIIa, FcγRIIb, FcγRIIc, FcγRIII, FcεRI and FcαRI.

 Another embodiment of the present invention relates to a two dimensional image of an FcR including those illustrated in Fig. 4, Fig. 6, Fig. 7, Fig. 8, Fig. 9, Fig.
35 10, Fig. 14, Fig. 15 or Fig. 16. Most of these figures

were drawn with MOLSCRIPT 2.0 (Avatar Software AB, Heleneborgsgatan 21C, SE-11731 Stockholm, Sweden).

One embodiment of the present invention includes an image of FcR protein that is generated when a set of three dimensional coordinates comprising the three dimensional coordinates represented in Table 1 are analyzed on a computer using a graphical display software program to create an electronic file of said image and visualizing said electronic file on a computer capable of representing electronic file as a three dimensional image. Suitable graphical software display programs include MOLSCRIPT 2.0, O and GRASP. A suitable computer to visualize such image includes a Silicon Graphics Workstation. Suitable structures and models to image are disclosed herein. Preferably, the three dimensional structures and/or models are of an FcR protein selected from the group of FcγRI, FcγRIIa, FcγRIIb, FcγRIIc, FcγRIII, FcεRI and FcαRI.

The present invention also includes a three dimensional model of the three dimensional structure of a target structure including FcγRI protein, FcγRIIa, FcγRIIb protein, FcγRIIc protein, FcγRIIIb protein, FcεRI protein, and FcαRI protein, such a three dimensional model being produced by the method comprising: (a) providing an amino acid sequences of an FcγRIIa protein and an amino acid sequence of a target FcR structure; (b) identifying structurally conserved regions shared between the FcγRIIa amino acid sequence and the target FcR structure amino acid sequence; (c) determining atomic coordinates for the FcR protein by assigning the structurally conserved regions of the target FcR structure to a three dimensional structure using a three dimensional structure of an FcγRIIa protein based on atomic coordinates that substantially conform to the atomic coordinates represented in Table 1 to derive a model of the three dimensional structure of the target FcR structure amino acid sequence. Preferably, the model

comprises a computer model. Preferably, the method further comprises the step of electronically simulating the structural assignments to derive a computer model of the three dimensional structure of the target FcR structure amino acid sequence. Preferred amino acid sequences of FcγRI protein, FcγRIIb protein, FcγRIIc protein, FcγRIIIb protein and FcεRI protein are disclosed herein.

One embodiment of the present invention includes a method for producing crystals of FcγRIIa, comprising combining FcγRIIa protein with a mother liquor and inducing crystal formation to produce the FcγRIIa crystals. Another embodiment of the present invention includes a method for producing crystals of FcεRI, comprising combining FcεRI protein with a mother liquor and inducing crystal formation to produce the FcεRI crystals. Although the production of crystals of FcγRIIa and FcεRI are specifically described herein, it is to be understood that such processes as are described herein can be adapted by those of skill in the art to produce crystals of other Fc receptors (FcR), particularly FcγRI, FcγRIIb, FcγRIIc, FcγRIIIb and FcαRI, the three dimensional structures of which are also encompassed by the present invention.

Preferably, crystals of FcγRIIa are formed using a solution containing a range of FcγRIIa protein from about 1 mg/ml to about 20 mg/ml, more preferably from about 2 mg/ml to about 15 mg/ml, and even more preferably from about 3 mg/ml to about 6 mg/ml of FcγRIIa protein in a mother liquor, with 3 mg/ml and 6 mg/ml of FcγRIIa protein in a mother liquor being more preferred. Preferably, crystals are formed using droplets containing from about 1 μg to about 30 μg, more preferably from about 5 μg to about 25 μg, and more preferably from about 4.5 μg to about 9 μg of FcγRIIa protein per 3 μl droplet.

A suitable mother liquor of the present invention comprises an acetate salt buffer. A preferred acetate salt

buffer of the present invention comprises ammonium acetate. The concentration of ammonium acetate in the buffer prior to crystallization can range from about 100 mM to about 500 mM ammonium acetate. Preferably, the concentration of ammonium acetate in the buffer ranges from about 150 mM to about 300 mM ammonium acetate. More preferably, the concentration of ammonium acetate in the buffer is 200 mM ammonium acetate. A suitable acetate salt buffer preferably includes a buffer having a pH of from about 5 to about 7, more preferably from about 5.5 to about 6.5, and more preferably a pH of about 5.6. Preferably, the pH of an acetate salt buffer or the present invention is controlled using sodium citrate. A suitable acetate salt buffer contains sodium citrate at a concentration of about 0.01 M sodium citrate, more preferably 0.05 M sodium citrate and more preferably 0.1 M sodium citrate. A suitable acetate salt buffer contains any polyethylene glycol (PEG), with PEG 4000 being more preferred. Suitable PEG 4000 concentrations in an acetate salt buffer of the present invention include a concentration of about 20%, preferably about 25%, and more preferably about 30% PEG 4000.

Another suitable mother liquor of the present invention comprises a sulphate buffer. A preferred sulphate buffer of the present invention comprises lithium sulfate. The concentration of lithium sulfate in the buffer prior to crystallization can range from about 100 mM to about 2.5 M lithium sulfate. Preferably, the concentration of lithium sulfate in the buffer ranges from about 500 mM to about 2 M lithium sulfate. More preferably, the concentration of lithium sulfate in the buffer is about 1.5 M lithium sulfate. A suitable sulphate buffer preferably includes a buffer having a pH of from about 5 to about 9, more preferably from about 6 to about 8, and more preferably a pH of about 7.5. Preferably, the

pH of a sulphate buffer or the present invention is controlled using HEPES. A suitable sulphate buffer contains HEPES at a concentration of about 0.01 M HEPES, more preferably 0.05 M HEPES and more preferably 0.1 M HEPES.

Supersaturated solutions of FcγRIIa protein can be induced to crystallize by several methods including, but not limited to, vapor diffusion, liquid diffusion, batch crystallization, constant temperature and temperature induction or a combination thereof. Preferably, supersaturated solutions of FcγRIIa protein are induced to crystallize by vapor diffusion (i.e., hanging drop method). In a vapor diffusion method, an FcγRIIa protein is combined with a mother liquor of the present invention that will cause the FcγRIIa protein solution to become supersaturated and form FcγRIIa crystals at a constant temperature. Vapor diffusion is preferably performed under a controlled temperature in the range of from about 15°C to about 30°C, more preferably from about 20°C to about 25°C, and more preferably at a constant temperature of about 22°C.

In a preferred embodiment, the present invention includes a method to produce crystals of FcγRIIa comprising the steps of: (a) preparing an about 3 mg/ml solution of FcγRIIa protein in an acetate salt buffer to form a supersaturated formulation, in which the buffer comprises about 200 mM ammonium acetate, about 100 mM sodium citrate and about 30% PEG 4000 and has a pH of about pH 5.8; (b) dropping about 3 μl droplets of the supersaturated formulation onto a coverslip and inverting this over a well containing about 1 ml of the acetate salt buffer; and (c) incubating until crystals of FcγRIIa form.

In another preferred embodiment, the present invention includes a method to produce crystals of FcγRIIa comprising the steps of: (a) preparing an about 3 mg/ml solution of FcγRIIa protein in a sulphate buffer to form a

supersaturated formulation, in which the buffer comprises about 0.15 M HEPES and about 1.5 M lithium sulphate and has a pH of about pH 7.5; (b) dropping about 3 μ l droplets of the supersaturated formulation onto a coverslip and
5 inverting this over a containing about 1 ml of the sulphate buffer; and (c) incubating until crystals of Fc γ RIIa form.

As discussed briefly above, another embodiment of the present invention is a method of producing Fc ϵ RI crystals and the Fc ϵ RI crystals produced thereby. Preferably,
10 crystals of Fc ϵ RI are formed using a solution containing a range of Fc ϵ RI protein from about 1 mg/ml to about 20 mg/ml, more preferably from about 2 mg/ml to about 15 mg/ml, and even more preferably from about 3 mg/ml to about 6 mg/ml of Fc ϵ RI protein in a mother liquor, with 3 mg/ml
15 and 6 mg/ml of Fc ϵ RI protein in a mother liquor being more preferred. Preferably, crystals are formed using droplets containing from about 1 μ g to about 30 μ g, more preferably from about 5 μ g to about 25 μ g, and more preferably from about 4.5 μ g to about 9 μ g of Fc ϵ RI protein per 3 μ l
20 droplet.

A suitable mother liquor of the present invention comprises an acetate salt buffer. A preferred acetate salt buffer of the present invention comprises calcium acetate. The concentration of calcium acetate in the buffer prior to
25 crystallization can range from about 100 mM to about 500 mM calcium acetate. Preferably, the concentration of calcium acetate in the buffer ranges from about 150 mM to about 300 mM calcium acetate. More preferably, the concentration of calcium acetate in the buffer is 200 mM calcium acetate.
30 A suitable acetate salt buffer preferably includes a buffer having a pH of from about 5.5 to about 7.5, more preferably from about 6.0 to about 7.0, and more preferably a pH of about 6.5. Preferably, the pH of an acetate salt buffer or the present invention is controlled using sodium
35 cacodylate. A suitable acetate salt buffer contains sodium

cacodylate at a concentration of about 0.01 M sodium cacodylate, more preferably 0.05 M sodium cacodylate and more preferably 0.1 M sodium cacodylate. A suitable acetate salt buffer contains any polyethylene glycol (PEG),
5 with PEG 8000 being more preferred. Suitable PEG 8000 concentrations in an acetate salt buffer of the present invention include a concentration of about 10% w/v, preferably about 15%, and more preferably about 20% w/v PEG 8000.

10 Another suitable mother liquor of the present invention comprises a buffer which includes sodium cacodylate together with 2-propanol and polyethylene glycol. A preferred sodium cacodylate buffer of the present invention comprises a concentration of sodium
15 cacodylate in the buffer prior to crystallization of about 0.01 M sodium cacodylate, more preferably 0.05 M sodium cacodylate and more preferably 0.1 M sodium cacodylate. A suitable sodium cacodylate buffer preferably includes a buffer having a pH of from about 5 to about 7, more
20 preferably from about 5.5 to about 6.5, and more preferably a pH of from about 5.5 to about 6.0. A suitable sodium cacodylate buffer contains 2-propanol at a concentration of about 5% v/v, more preferably 7% v/v and more preferably 10% v/v. A suitable sodium cacodylate buffer contains any
25 polyethylene glycol (PEG), with PEG 4000 being more preferred. Suitable PEG 4000 concentrations in an acetate salt buffer of the present invention include a concentration of about 10% w/v, preferably about 15%, and more preferably about 20% w/v PEG 4000.

30 Another suitable mother liquor of the present invention comprises a sodium citrate buffer which includes tri sodium citrate dihydrate together with sodium cacodylate and 2-propanol. A preferred sodium citrate buffer of the present invention comprises a concentration
35 of tri sodium citrate dihydrate in the buffer prior to

crystallization of about 0.05 M tri sodium citrate dihydrate, more preferably 0.1 M tri sodium citrate dihydrate and more preferably 0.2 M tri sodium citrate dihydrate. A suitable sodium citrate buffer preferably includes a buffer having a pH of from about 5.5 to about 7, more preferably from about 6.0 to about 7.0, and more preferably a pH of about 6.5. A preferred sodium citrate buffer of the present invention comprises a concentration of sodium cacodylate in the buffer prior to crystallization of about 0.01 M sodium cacodylate, more preferably 0.05 M sodium cacodylate and more preferably 0.1 M sodium cacodylate. A suitable sodium citrate buffer contains 2-propanol at a concentration of about 15% v/v, more preferably 20% v/v and more preferably 30% v/v.

Supersaturated solutions of FcεRI protein can be induced to crystallize by several methods including, but not limited to, vapor diffusion, liquid diffusion, batch crystallization, constant temperature and temperature induction or a combination thereof. Preferably, supersaturated solutions of FcεRI protein are induced to crystallize by vapor diffusion (i.e., hanging drop method). In a vapor diffusion method, an FcεRI protein is combined with a mother liquor of the present invention that will cause the FcεRI protein solution to become supersaturated and form FcεRI crystals at a constant temperature. Vapor diffusion is preferably performed under a controlled temperature in the range of from about 15°C to about 30°C, more preferably from about 20°C to about 25°C, and more preferably at a constant temperature of about 22°C.

In a preferred embodiment, the present invention includes a method to produce crystals of FcεRI comprising the steps of: (a) preparing an about 3 mg/ml solution of FcεRI protein in an acetate salt buffer to form a supersaturated formulation, in which the buffer comprises about 200 mM calcium acetate, about 100 mM sodium

cacodylate and about 18% w/v PEG 8000 and has a pH of about pH 6.5; (b) dropping about 3 μ l droplets of the supersaturated formulation onto a coverslip and inverting this over a well containing about 1 ml of the acetate salt buffer; and (c) incubating until crystals of Fc ϵ RI form.

In another preferred embodiment, the present invention includes a method to produce crystals of Fc ϵ RI comprising the steps of: (a) preparing an about 3 mg/ml solution of Fc ϵ RI protein in a sodium cacodylate buffer to form a supersaturated formulation, in which the buffer comprises about 100 mM sodium cacodylate, about 10% v/v 2-propanol and about 20% w/v PEG 4000 and has a pH of about pH 5.5-6.0; (b) dropping about 3 μ l droplets of the supersaturated formulation onto a coverslip and inverting this over a containing about 1 ml of the sulphate buffer; and (c) incubating until crystals of Fc ϵ RI form.

In another preferred embodiment, the present invention includes a method to produce crystals of Fc ϵ RI comprising the steps of: (a) preparing an about 3 mg/ml solution of Fc ϵ RI protein in a sodium citrate buffer to form a supersaturated formulation, in which the buffer comprises about 200 mM tri sodium citrate dihydrate, about 100 mM sodium cacodylate and about 30% v/v 2-propanol and has a pH of about pH 6.5; (b) dropping about 3 μ l droplets of the supersaturated formulation onto a coverslip and inverting this over a containing about 1 ml of the sulphate buffer; and (c) incubating until crystals of Fc ϵ RI form.

Any isolated FcR protein can be used with the present method. An isolated FcR protein can be isolated from its natural milieu or produced using recombinant DNA technology (e.g., polymerase chain reaction (PCR) amplification, cloning) or chemical synthesis. To produce recombinant FcR protein, a nucleic acid molecule encoding FcR protein can be inserted into any vector capable of delivering the nucleic acid molecule into a host cell. Suitable and

preferred nucleic acid molecules to include in recombinant vectors of the present invention are as disclosed herein. A preferred nucleic acid molecule of the present invention encodes a human FcR protein, and more preferably, a human FcγRIIa protein, a human FcεRI protein, or a human FcγRIIb protein. A nucleic acid molecule of the present invention can encode any portion of an FcR protein, preferably a full-length FcR protein, and more preferably a soluble form of FcR protein (i.e., a form of FcR protein capable of being secreted by a cell that produces such protein). A more preferred nucleic acid molecule to include in a recombinant vector, and particularly in a recombinant molecule, includes a nucleic acid molecule encoding a protein having the amino acid sequence represented by SEQ ID NO:3, SEQ ID NO:5, SEQ ID NO:6, SEQ ID NO:7, SEQ ID NO:8, SEQ ID NO:9, SEQ ID NO:10, SEQ ID NO:11, SEQ ID NO:12, or SEQ ID NO:13. A preferred nucleic acid molecule to include in a recombinant molecule includes sFcγRIIa and sFcεRI, the production of which are described in the Examples section.

A recombinant vector of the present invention can be either RNA or DNA, either prokaryotic or eukaryotic, and typically is a virus or a plasmid. Preferably, a nucleic acid molecule encoding an FcR protein is inserted into a vector comprising an expression vector to form a recombinant molecule. As used herein, an expression vector is a DNA or RNA vector that is capable of transforming a host cell and of affecting expression of a specified nucleic acid molecule. Expression vectors of the present invention include any vectors that function (i.e., direct gene expression) in recombinant cells of the present invention, including in bacterial, fungal, endoparasite, insect, other animal, and plant cells. Preferred expression vectors of the present invention direct expression in insect cells. A more preferred expression

vector of the present invention comprises pVL1392 baculovirus shuttle plasmid. A preferred recombinant molecule of the present invention comprises pVL-sFcγRIIa(a), pVL-sFcγRIIa(b), and pVL-sFcεRI.

5 An expression vector of the present invention can be transformed into any suitable host cell to form a recombinant cell. A suitable host cell includes any cell capable of expressing a nucleic acid molecule inserted into the expression vector. For example, a prokaryotic
10 expression vector can be transformed into a bacterial host cell. A preferred host cell of the present invention includes a cell capable of expressing a baculovirus, in particular an insect cell, with *Spodoptera frugiperda* or *Trichoplusia ni* cells being preferred. A preferred
15 recombinant cell of the present invention includes *S. frugiperda*:pVL-sFcγRIIa(a)/ pVL-sFcγRIIa(b) cells and *S. frugiperda*:pVL-sFcεRI the production of which is described herein.

One method to isolate FcR protein useful for producing
20 FcR crystals includes recovery of recombinant proteins from cell cultures of recombinant cells expressing such FcR protein. In one embodiment, an isolated recombinant FcR protein of the present invention is produced by culturing a cell capable of expressing the protein under conditions
25 effective to produce the protein, and recovering the protein. A preferred cell to culture is a recombinant cell of the present invention. Effective culture conditions include, but are not limited to, effective media, bioreactor, temperature, pH and oxygen conditions and
30 culture medium that permit protein production. Such culturing conditions are within the expertise of one of ordinary skill in the art. Examples of suitable conditions are included in the Examples section.

Preferably, a recombinant cell of the present
35 invention expresses a secreted form of FcR protein. FcR

proteins of the present invention can be purified using a variety of standard protein purification techniques, such as, but not limited to, affinity chromatography, ion exchange chromatography, filtration, electrophoresis, hydrophobic interaction chromatography, gel filtration chromatography, reverse phase chromatography, chromatofocusing and differential solubilization. Preferably, an FcR protein is purified in such a manner that the protein is purified sufficiently for formation of crystals useful for obtaining information related to the three dimensional structure of an FcR protein. Preferably, a composition of FcR protein is about 70%, more preferably 75%, more preferably 80%, more preferably 85% and more preferably 90% pure.

In one embodiment, a recombinant FcR protein is purified from a cell culture supernatant harvested between about 20 hours and about 60 hours post-infection, preferably between about 30 hours and about 50 hours post-infection, and more preferably about 40 hours post-infection. Preferably, an FcγRIIa protein is purified from a supernatant by a method comprising the steps: (a) applying supernatant from *S. frugiperda*:pVL-sFcγRIIa(a)/pVL-sFcγRIIa(b) cells to an ion exchange column; (b) collecting unbound protein from the ion exchange column and applying the unbound protein to an immuno-affinity chromatography column; (c) eluting proteins bound to the immuno-affinity chromatography column and applying the eluted proteins to a gel filtration column; and (d) collecting filtered proteins from the gel filtration column to obtain the FcγRIIa protein. Preferably, an FcεRI protein is purified from a supernatant by a method comprising the steps: (a) applying supernatant from *S. frugiperda*:pVL-sFcεRI cells to an ion exchange column; (b) collecting unbound protein from the ion exchange column and applying the unbound protein to an

immuno-affinity chromatography column; (c) eluting proteins bound to the immuno-affinity chromatography column and applying the eluted proteins to a gel filtration column; and (d) collecting filtered proteins from the gel
5 filtration column to obtain the FcεRI protein.

In view of the high degree of amino acid sequence homology between human FcγR proteins and other members of the FcγR family of proteins, the methods of purification of the present invention are applicable for each member of the
10 FcγR family. In addition, one of skill in the art will recognize that the purification methods of the present invention are generally useful for purifying any FcR protein, such as the FcεRI protein, except using IgE rather than IgG for the step of immuno-affinity chromatography purification, and such as the FcαRI protein, except using
15 IgA rather than IgG for the purification step. Isolated protein of the members of the FcγR family of proteins, FcεR protein and FcαR protein may be obtained through recombinant DNA technology or may be purified from natural sources, including but not limited to, monocytes,
20 macrophages, neutrophils, eosinophils, platelets and B lymphocytes (i.e., B cells). Descriptions of recombinant production of isolated FcγRIIa and FcεRI proteins are described in the Examples section.

Another embodiment of the present invention includes a composition comprising FcR protein in a crystalline form (i.e., FcR crystals). As used herein, the terms "crystalline FcR" and "FcR crystal" both refer to
25 crystallized FcR protein and are intended to be used interchangeably. Preferably, a crystalline FcR is produced using the crystal formation method described herein, in particular according to the method disclosed in Example 6 or Example 9. A FcR crystal of the present invention can comprise any crystal structure and preferably precipitates
30 as an orthorhombic crystal. A suitable crystalline FcR of
35

the present invention includes a monomer or a multimer of FcR protein. A preferred crystalline FcR comprises one FcR protein in an asymmetric unit. A more preferred crystalline FcR comprises a dimer of FcR proteins.

5 A particular embodiment of the present invention includes a composition comprising FcγRIIa protein in a crystalline form (i.e., FcγRIIa crystals). As used herein, the terms "crystalline FcγRIIa" and "FcγRIIa crystal" both refer to crystallized FcγRIIa protein and are intended to be used interchangeably. Preferably, a crystal FcγRIIa is produced using the crystal formation method described herein, in particular according to the method disclosed in Example 6. A FcγRIIa crystal of the present invention can comprise any crystal structure and preferably precipitates as an orthorhombic crystal. Preferably, a composition of the present invention includes FcγRIIa protein molecules arranged in a crystalline manner in a space group P2₁2₁2, so as to form a unit cell of dimensions $a = 78.80 \text{ \AA}$, $b = 100.55 \text{ \AA}$, $c = 27.85 \text{ \AA}$. A preferred crystal of the present invention provides X-ray diffraction data for determination of atomic coordinates of the FcγRIIa protein to a resolution of about 3.0 Å, preferably about 2.4 Å, and more preferably at about 1.8 Å.

25 A suitable crystalline FcγRIIa of the present invention includes a monomer or a multimer of FcγRIIa protein. A preferred crystalline FcγRIIa comprises one FcγRIIa proteins in an asymmetric unit. A more preferred crystalline FcγRIIa comprises a dimer of FcγRIIa proteins.

30 Another particular embodiment of the present invention includes a composition comprising FcεRI protein in a crystalline form (i.e., FcεRI crystals). As used herein, the terms "crystalline FcεRI" and "FcεRI crystal" both refer to crystallized FcεRI protein and are intended to be used interchangeably. Preferably, a crystal FcεRI is produced using the crystal formation method described

35

herein, in particular according to the method disclosed in Example 9. A FcεRI crystal of the present invention can comprise any crystal structure and preferably precipitates as an orthorhombic crystal. A suitable crystalline FcεRI of the present invention includes a monomer or a multimer of FcεRI protein. A preferred crystalline FcεRI comprises one FcεRI protein in an asymmetric unit. A more preferred crystalline FcεRI comprises a dimer of FcεRI proteins.

According to the present invention, crystalline FcR can be used to determine the ability of a chemical compound of the present invention to bind to FcγRIIa protein a manner predicted by a structure based drug design method of the present invention. Preferably, an FcγRIIa crystal is soaked in a solution containing a chemical compound of the present invention. Binding of the chemical compound to the crystal is then determined by methods standard in the art.

One embodiment of the present invention is a therapeutic composition. A therapeutic composition of the present invention comprises one or more therapeutic compounds. Preferred therapeutic compounds of the present invention include inhibitory compounds and stimulatory compounds.

One embodiment of the present invention is a therapeutic composition that is capable of reducing IgG-mediated tissue damage. Suitable therapeutic compositions are capable of reducing IgG-mediated tissue damage resulting from IgG-mediated hypersensitivity or other biological mechanisms involved in IgG-mediated recruitment of inflammatory cells that involves FcγR protein. For example, a therapeutic composition of the present invention can: (1) inhibit (i.e., prevent, block) binding of FcγR protein on a cell having an FcγR protein (e.g., B cells, macrophage, neutrophil, eosinophil or platelet cells) to an IgG immune complex by interfering with the IgG binding site of an FcγR protein; (2) binding

to the Fc portion of IgG to inhibit complement fixation by an IgG immune complex by interfering with the complement binding site of an IgG molecule; (3) inhibit precipitation of IgG or IgG immune complexes (i.e., prevent Fc:Fc interactions between two IgG); (4) inhibit immunoglobulin-mediated cellular signal transduction by interfering with the binding of an IgG to a cell surface receptor; (5) inhibit FcγR-mediated cellular signal transduction by interfering with the binding of a cell signal inducing molecule (i.e., a molecule that induces cellular signal transduction through an FcγR protein) to an FcγR protein; (6) inhibit opsinization of pathogens by inhibiting binding of IgG bound to a pathogen to FcγR protein on a phagocytic cell (e.g., to prevent antibody dependent enhancement (ADE) of viral infection, such as with flaviviruses and dengue virus); and (7) inhibit the binding of viral molecules to FcγR protein (e.g., measles virus nucleocapsid protein). As used herein, the term "immune complex" refers to a complex that is formed when an antibody binds to a soluble antigen. As used herein, the term "complement fixation" refers to complement activation by an antigen:antibody complex that results in recruitment of inflammatory cells, typically by assembly of a complex comprising C3a and C5a, or generation of cleaved C4. As used herein, the term "binding site" refers to the region of a molecule (e.g., a protein) to which another molecule specifically binds. Such therapeutic compositions include one or more inhibitory compounds that inhibit binding of IgG to FcγR protein, IgG to complement, IgG to IgG, IgG to a cell surface receptor, a cell signal inducing molecule to FcγR protein, FcγR protein to virus or inhibit opsinization. Also included in the present invention are methods to reduce IgG-mediated tissue damage. The method includes the step of administering to an animal a therapeutic composition of the present invention.

Another embodiment of the present invention is a therapeutic composition that is capable of stimulating an IgG humoral immune response in an animal. Yet another embodiment of the present invention is a therapeutic composition that improves the therapeutic affects of an antibody that is administered to an animal to treat, by opsinization or FcγR-dependent effector functions (e.g. antibody-dependent FcγR-mediated cytotoxicity, phagocytosis or release of cellular mediators), a particular disease, including, but not limited to, cancer or infectious disease (e.g. oral infections such as HIV, herpes, bacterial infections, yeast infections or parasite infections). Such a therapeutic composition includes one or more stimulatory compounds that have increased binding to IgG, enhance binding of IgG to FcγR, enhance dimer formation of an FcγR and/or enhance signal transduction through the FcγR. Also included in the present invention is a method to stimulate a humoral immune response. The method includes the step of administering to an animal a therapeutic composition of the present invention.

Suitable inhibitory compounds of the present invention are compounds that interact directly with an FcγR protein, preferably an FcγRIIa protein or an FcγRIIb protein, thereby inhibiting the binding of IgG to an FcγR protein, by either blocking the IgG binding site of an FcγR (referred to herein as substrate analogs) or by modifying other regions of the FcγR protein (such as in the upper groove of the IgG binding cleft between the monomers of an FcγR dimer, at the dimer interface, in the cleft or hinge region between D1 and D2 on each monomer, and/or underneath the IgG binding cleft in the lower groove formed by the monomers of an FcγR dimer) such that IgG cannot bind to the FcγR (e.g., by allosteric interaction). A FcγR substrate analog refers to a compound that interacts with (e.g., binds to, associates with, modifies) the IgG binding site

of an FcγR protein. A FcγR substrate analog can, for example, comprise a chemical compound that mimics the Fc portion of an IgG, or that binds specifically to the IgG binding site of an FcγR but does not mimic the Fc portion of an IgG. An inhibitory compound of the present invention can also include a compound that essentially mimics at least a portion of an FcγRIIa protein that binds to IgG (referred to herein as a peptidomimetic compound). Other suitable inhibitory compounds of the present invention include compounds that inhibit the binding of an FcγR protein to a cell signal inducing molecule other than IgG. Examples of such cell signal inducing molecules include another FcγR (i.e., to form a dimer of FcγR proteins), or a cell surface accessory molecule, an intracellular accessory molecule or virus (e.g., measles virus nucleocapsid protein).

One embodiment of the present invention is a therapeutic composition that is capable of reducing IgE-mediated responses. Suitable therapeutic compositions are capable of reducing IgE-mediated responses resulting from IgE-mediated hypersensitivity, IgE-mediated release of inflammatory modulators or other biological mechanisms involved in IgE-mediated recruitment of inflammatory cells that involves FcεR protein. For example, a therapeutic composition of the present invention can: (1) inhibit (i.e., prevent, block) binding of FcεR protein on a cell having an FcεR protein (e.g., mast cells) to an IgE immune complex by interfering with the IgE binding site of an FcεR protein; (2) inhibit precipitation of IgE or IgE immune complexes (i.e., prevent Fc:Fc interactions between two IgE); (3) inhibit immunoglobulin-mediated cellular signal transduction by interfering with the binding of an IgE to a cell surface receptor; and (4) inhibit FcεR-mediated cellular signal transduction by interfering with the binding of a cell signal inducing molecule (i.e., a

molecule that induces cellular signal transduction through an FcεR protein) to an FcεR protein. Such therapeutic compositions include one or more inhibitory compounds that inhibit binding of IgE to FcεR protein, IgE to IgE, IgE to a cell surface receptor, or a cell signal inducing molecule to FcεR protein. Also included in the present invention are methods to reduce IgE-mediated responses, such as IgE-mediated inflammation. The method includes the step of administering to an animal a therapeutic composition of the present invention.

Another embodiment of the present invention is a therapeutic composition that is capable of stimulating a IgE humoral immune response in an animal. Yet another embodiment of the present invention is a therapeutic composition that improves the therapeutic affects of an antibody that is administered to an animal to treat, by opsinization or FcεR-dependent effector functions (e.g. phagocytosis or release of cellular mediators), a particular disease. Such a therapeutic composition includes one or more stimulatory compounds that have increased binding to IgE, enhance binding of IgE to FcεRI, enhance dimer formation of FcεRI and/or otherwise enhance signal transduction through the FcεRI. Also included in the present invention is a method to stimulate a humoral immune response. The method includes the step of administering to an animal a therapeutic composition of the present invention.

Suitable inhibitory compounds of the present invention are compounds that interact directly with an FcεR protein, thereby inhibiting the binding of IgE to an FcεR protein, by either blocking the IgE binding site of an FcεR (referred to herein as substrate analogs) or by modifying other regions of the FcεR protein (such as in the upper groove of the IgE binding cleft between the monomers of an FcεRI dimer, at the dimer interface, in the cleft or hinge

region between D1 and D2 on each monomer, and/or underneath the IgE binding cleft in the lower groove formed by the monomers of an FcεRI dimer) such that IgE cannot bind to the FcεR (e.g., by allosteric interaction). A FcεR substrate analog refers to a compound that interacts with (e.g., binds to, associates with, modifies) the IgE binding site of an FcεR protein. A FcεR substrate analog can, for example, comprise a chemical compound that mimics the Fc portion of an IgE, or that binds specifically to the IgE binding site of an FcεR but does not mimic the Fc portion of an IgE. An inhibitory compound of the present invention can also include a compound that essentially mimics at least a portion of an FcεR protein that binds to IgE (referred to herein as a peptidomimetic compound). Other suitable inhibitory compounds of the present invention include compounds that inhibit the binding of an FcεR protein to a cell signal inducing molecule other than IgE. Examples of such cell signal inducing molecules include another FcεR (i.e., to form a dimer of FcεR proteins), or a cell surface accessory molecule, an intracellular accessory molecule or virus (e.g., measles virus nucleocapsid protein).

Inhibitory compounds of the present invention can be identified by various means known to those of skill in the art. For example, binding of an inhibitory compound to, or otherwise interaction with, an FcR protein, can be determined with FcR protein in solution or on cells using, for example, immunoassays such as enzyme linked immunoabsorbent assays (ELISA) and radioimmunoassays (RIA) or binding assays such as Biacore assays. Cell-based assays can include, for example, cytokine (e.g., IL-4, IL-6 or IL-12) secretion assays, or intracellular signal transduction assays that determine, for example, protein or lipid phosphorylation, mediator release or intracellular

Ca⁺⁺ mobilization upon FcR binding to a cell signal inducing molecule.

Suitable stimulatory therapeutic compounds of the present invention are compounds that exhibit improved
5 binding to Ig when compared with the ability of a natural FcR protein (e.g., an FcR protein isolated from its natural milieu) to bind to Ig, and also include compounds that enhance the binding of Ig to its FcR or enhance signal transduction through the FcR. Stimulatory compounds of the
10 present invention are identified by their ability to: (1) bind to, or otherwise interact with, Ig at a higher level than, for example, natural FcR protein; (2) enhance binding of Ig to its FcR; (3) enhance dimer formation of an FcR by binding either to the FcR, to an Ig that binds to the FcR
15 or to the combination of Ig bound to the FcR; and/or (4) enhance signal transduction through the FcR. Methods to determine improved binding of Ig to a stimulatory compound of the present invention compared with, for example, natural FcR protein, include binding assays that determine
20 the stability of binding, affinity or kinetics at which an Ig binds to a stimulatory compound and a natural FcR protein. Such methods are well known to those of skill in the art and are disclosed herein in the Examples section. A stimulatory compound of the present invention can also
25 include a compound that binds to an Ig or an FcR protein, thereby enhancing the binding of Ig to FcR protein or improving cellular signal transduction during or after the binding of Ig to FcR protein, by, for example, modifying other regions of the FcR or Ig by an allosteric interaction
30 that modifies the Ig-binding site of FcR or the Fc portion of Ig that binds to an FcR protein. Another stimulatory compound of the present invention can include a compound that binds to FcR protein in the absence of Ig, in such a manner that FcR-mediated cellular signal transduction is
35 stimulated.

One of skill in the art will understand that inhibitory or stimulatory compounds can also be developed based on the structure of any FcR and its Ig ligand, as described above for FcγR protein and IgG and FcεRI and IgE.

5 According to the present invention, suitable therapeutic compounds of the present invention include peptides or other organic molecules, and inorganic molecules. Suitable organic molecules include small organic molecules. Preferably, a therapeutic compound of
10 the present invention is not harmful (e.g., toxic) to an animal when such compound is administered to an animal. Peptides refer to a class of compounds that is small in molecular weight and yields two or more amino acids upon hydrolysis. A polypeptide is comprised of two or more
15 peptides. As used herein, a protein is comprised of one or more polypeptides. Preferred therapeutic compounds to design include peptides composed of "L" and/or "D" amino acids that are configured as normal or retroinverso peptides, peptidomimetic compounds, small organic
20 molecules, or homo- or hetero-polymers thereof, in linear or branched configurations.

Therapeutic compounds of the present invention can be designed using structure based drug design. Until the
25 discovery of the three dimensional structure of the present invention, no information was available for structure based development of therapeutic compounds based on the structure of FcR protein. Such rational development heretofore could not be executed *de novo* from available linear amino acid sequence information. Structure based drug design refers
30 to the use of computer simulation to predict a conformation of a peptide, polypeptide, protein, or conformational interaction between a peptide or polypeptide, and a therapeutic compound. For example, generally, for a protein to effectively interact with a therapeutic
35 compound, it is necessary that the three dimensional

structure of the therapeutic compound assume a compatible conformation that allows the compound to bind to the protein in such a manner that a desired result is obtained upon binding. Knowledge of the three dimensional structure of the protein enables a skilled artisan to design a therapeutic compound having such compatible conformation. For example, knowledge of the three dimensional structure of the IgG binding site of FcγRIIa protein enables one of skill in the art to design a therapeutic compound that binds to FcγRIIa, is stable and results in inhibition of a biological response such as IgG binding to cells having FcγR, or cellular signal transduction, upon such binding. In addition, for example, knowledge of the three dimensional structure of the IgG binding site of FcγRIIa protein enables a skilled artisan to design a substrate analog of FcγRIIa protein.

Suitable structures and models useful for structure based drug design are disclosed herein. Preferred structures to use in a method of structure based drug design include a structure of FcγRIIa protein, a structure of FcεRI protein, a structure of an FcγRIIb protein, and a model of a target FcR structure. Preferred models of target structures to use in a method of structure based drug design include models produced by any modeling method disclosed herein, including molecular replacement and fold recognition related methods.

One embodiment of the present invention is a computer-assisted method of structure based drug design of bioactive compounds, comprising: (a) providing a structure of a protein including a three dimensional structure of an FcR protein or a model of the present invention; (b) designing a chemical compound using the three dimensional structure or model; and (c) chemically synthesizing the chemical compound. Such a method can additionally include the step of (d) evaluating the bioactivity of the

synthesized chemical compound. Suitable three dimensional structures an FcR protein and models to use with the present method are disclosed herein. According to the present invention, the step of designing can include
5 creating a new chemical compound or searching databases of libraries of known compounds (e.g., a compound listed in a computational screening database containing three dimensional structures of known compounds). Designing can also be performed by simulating chemical compounds having
10 substitute moieties at certain structural features. The step of designing can include selecting a chemical compound based on a known function of the compound. A preferred step of designing comprises computational screening of one or more databases of compounds in which the three
15 dimensional structure of the compound is known and is interacted (e.g., docked, aligned, matched, interfaced) with the three dimensional structure of an FcR protein by computer (e.g. as described by Humblet and Dunbar, *Animal Reports in Medicinal Chemistry*, vol. 28, pp. 275-283, 1993, M Venuti, ed., Academic Press). Methods to synthesize
20 suitable chemical compounds are known to those of skill in the art and depend upon the structure of the chemical being synthesized. Methods to evaluate the bioactivity of the synthesized compound depend upon the bioactivity of the
25 compound (e.g., inhibitory or stimulatory) and are disclosed herein.

Various other methods of structure-based drug design are disclosed in Maulik et al., 1997, *Molecular Biotechnology: Therapeutic Applications and Strategies*,
30 Wiley-Liss, Inc., which is incorporated herein by reference in its entirety. Maulik et al. disclose, for example, methods of directed design, in which the user directs the process of creating novel molecules from a fragment library of appropriately selected fragments; random design, in
35 which the user uses a genetic or other algorithm to

randomly mutate fragments and their combinations while simultaneously applying a selection criterion to evaluate the fitness of candidate ligands; and a grid-based approach in which the user calculates the interaction energy between
5 three dimensional receptor structures and small fragment probes, followed by linking together of favorable probe sites.

Preferably, a chemical compound of the present invention that binds to the Ig binding site of an FcR
10 protein is known to originate from a chemical compound having chemical and/or stereochemical complementarity with FcR protein and/or Ig. Such complementarity is characteristic of a chemical compound that matches the surface of the receptor either in shape or in distribution
15 of chemical groups and binds to FcR protein to promote or inhibit Ig binding to the FcR protein, or to induce cellular signal transduction upon binding to FcR protein. More preferably, a chemical compound that binds to the Ig binding site of an FcR protein associates with an affinity
20 of at least about 10^{-6} M, and more preferably with an affinity of at least about 10^{-8} M.

Preferably, five sites of FcR protein are targets for structure based drug design. These sites include the Ig-binding site of FcR protein, the upper groove between
25 two FcR monomers, the dimerization interface between two FcR protein monomers, the lower groove between two FcR monomers, the interface, cleft or hinge region between Domains 1 and 2 of FcR protein, and combinations of any of these sites (e.g., interacting with the Ig-binding site and
30 the upper groove between monomers simultaneously). A schematic representation of these sites is shown in Fig. 17, with "a" representing the Ig-binding site of FcR protein, "b" representing the upper groove between two FcR monomers, "c" representing the dimerization interface
35 between two FcR protein monomers, "d" representing the

interface, cleft or hinge region between Domains 1 and 2 of FcR protein, and "e" representing the lower groove between two FcR monomers. The following discussion provides specific detail on drug-design using target sites of the FcR and as an example, references preferred target sites on the FcγRIIa structure. It is to be understood, however, that one of skill in the art, using the description of the FcεRI structure and the FcγRIIb structure provided herein, will be able to effectively select similar target sites on the FcεRI protein monomer and dimer for structure based drug design. Additionally, one of skill in the art, now being able to model the other FcR proteins based on the information provided herein, will also be able to effectively select similar target sites on the other FcR proteins for structure based drug design.

The Ig-binding site (Fig. 17; "a") is targeted to directly affect the binding of FcR to Ig (i.e., inhibition or enhancement). The IgG binding site of FcγRIIa protein, for example, includes, but is not limited to, residues 155, 156, 158-160, 113-116, 129, 131, 133 and 134 of SEQ ID NO:3, and can also include at least a portion of the second site described above (Fig. 17; "b"), the groove between the two IgG binding sites that form upon dimerization of FcγRIIa protein. Residues from site "b" that are included in IgG binding include, but are not limited to, residues 117-121, 125-129, 150-154 and 157-161 of SEQ ID NO:3. A suitable target site for structure based drug design comprising the IgG binding site of FcγRIIa protein is illustrated in Fig. 7. More specifically, mutagenesis studies have identified several residues which have an effect on the binding of IgG, and the three dimensional structure disclosed herein clearly identifies which residues are surface exposed (i.e., are likely to participate in binding of IgG and are not just having an allosteric effect). These residues can be classified in

three spatial groups: (1) Phe129, His131, Lys113, Pro114, Leu115, Val116; (2) Pro134 and Asp133; and (3) Leu159 and Ser161. Group (1) forms a continuous surface leading from the lip of the groove "b" (Fig. 17) across the binding surface "a" (Fig. 17), and represents the most preferred target of design work at the site of IgG binding. Group (2) is separated from Group (1) by Leu132, which is currently of unknown importance in the binding of IgG, and may well be part of the surface exposed residues. Group (3) contains residues which are remote from the other two groups and do not appear to be available to participate in binding of the IgG by the dimer structure.

The upper groove between the two monomers of the FcR (Fig. 17; "b") is also targeted to directly affect the binding of FcR to Ig (i.e., inhibition or enhancement). The upper groove provides an attractive site to build into in contrast to targeting a flat protein surface. The dimer structure of the FcγRIIa protein suggests targeting C2 or pseudo C2 symmetric inhibitors. Preferred residues to target in the FcγRIIa protein include Lys117, His131, Phe129, Asn154, Ser161, Leu159, Thr152 and Phe121, with Phe129, Lys117 and His131 being most preferred. In one embodiment, compounds can be designed which interact with both the upper groove "b" and the IgG binding surface "a" simultaneously. For example, improved Ig regulatory compounds may be obtained by designing regulatory compounds which flow out of the groove and bind to the binding surface of "a" as described above. Alternatively, a regulatory compound which binds to "b" may sterically hinder binding of IgG to "a" without actually interacting with the "a" binding surface.

The receptor dimer interface (Fig. 17; "c") is targeted to directly affect the ability of two FcR proteins to form a dimer, thereby affecting cellular signal transduction through one or both of the FcR proteins.

Without being bound by theory, the present inventors believe that dimer formation can affect cellular signal transduction or affect the conformation of the Ig binding of one or both of the FcR proteins involved in the dimer, thereby affecting cellular signal transduction. In addition, the dimer interface represents an excellent target site because one monomer provides ligand information for the other monomer and vice versa. A suitable target site for structure based drug design comprising the dimerization interface between two FcγRIIa proteins is illustrated in Fig. 10. More specifically, residues 117-131 and residues 150-164 make up the interfacial area of the FcγRIIa dimer, and peptides from these sequences or their mimics may be binding inhibitors. An examination of hydrogen bonding interactions from the crystal structure of FcγRIIa indicates relatively few interactions between the monomers in the interfacial area, but a notable cluster is spanned by the hexapeptide Phe121-Gln122-Asn123-Gly124-Lys125-Ser126. Additionally, there is a hydrogen bond between the monomers involving Gly124-Ser561 and Ser126-Leu559. There are also some hydrophobic contacts made by the Lys125 sidechain and by the Phe121 phenyl ring.

The interface between Domains 1 and 2 (Fig. 17; "d") is targeted to affect IgG binding to an FcγRIIa protein. The present inventors have discovered that in the three dimensional structure of FcγRIIa protein, Domain 1 makes close contact with Domain 2. In particular, a loop comprising residues 17-20 of SEQ ID NO:3 in Domain 1 lie close to the loops of Domain 2 to form at least a portion of the IgG-binding site. Interactions with IgG are believed to occur close to the D1D2 interface and so alterations at this site may effect Ig binding. Additionally, a cleft is defined by residues 12-14 (base), 6-10 and 77-80 (D1 face) and 93-96 and 101 (D2 face), and as such represents a potential site for inhibitor design.

A suitable target site for structure based drug design comprising the interface between Domain 1 and Domain 2 of an FcγRIIa protein is illustrated in Fig. 5.

5 The lower groove between the two monomers of the FcR (Fig. 17; "e") is also targeted to directly affect the binding of FcR to Ig (i.e., inhibition or enhancement). A similar design strategy can be used for this site as described above for the upper groove "b", although it is less clear whether compounds binding to this site would be
10 inhibitory, or more probably enhance IgG binding to the FcγR.

Drug design strategies as specifically described above with regard to residues and regions of the FcγRIIa monomer and dimer can be similarly applied to the other FcR
15 structures, including the FcγRIIIb and FcεRI structures disclosed herein. One of ordinary skill in the art, using the art recognized modeling programs and drug design methods, many of which are described herein, will be able to modify the FcγRIIa design strategy according to differences in amino acid sequence and more favored
20 structures, for example, in the other FcR, to similarly design compounds which regulate other FcR action. In addition, one of skill in the art could use lead compound structures derived from one FcR, such as the FcγRIIa protein, and taking into account differences in amino acid
25 residues in another FcR protein, such as FcεRI, modify the FcγRIIa lead compound to design lead compound structures for regulation of the FcεRI protein. For example, His131>Tyr131 in the upper groove pharmacophore could be
30 accommodated by changing an acidic moiety in an FcγRIIa lead compound structure to an electron deficient ketone moiety.

In the present method of structure based drug design, it is not necessary to align a candidate chemical compound
35 (i.e., a chemical compound being analyzed in, for example,

a computational screening method of the present invention) to each residue in a target site. Suitable candidate chemical compounds can align to a subset of residues described for a target site. Preferably, a candidate
5 chemical compound comprises a conformation that promotes the formation of covalent or noncovalent crosslinking between the target site and the candidate chemical compound. Preferably, a candidate chemical compound binds to a surface adjacent to a target site to provide an
10 additional site of interaction in a complex. When designing an antagonist (i.e., a chemical compound that inhibits the binding of a ligand to FCR protein by blocking a binding site or interface), the antagonist should bind with sufficient affinity to the binding site or to
15 substantially prohibit a ligand (i.e., a molecule that specifically binds to the target site) from binding to a target area. It will be appreciated by one of skill in the art that it is not necessary that the complementarity between a candidate chemical compound and a target site
20 extend over all residues specified here in order to inhibit or promote binding of a ligand.

In general, the design of a chemical compound possessing stereochemical complementarity can be accomplished by means of techniques that optimize,
25 chemically or geometrically, the "fit" between a chemical compound and a target site. Such techniques are disclosed by, for example, Sheridan and Venkataraghavan, *Acc. Chem Res.*, vol. 20, p. 322, 1987; Goodford, *J. Med. Chem.*, vol. 27, p. 557, 1984; Beddell, *Chem. Soc. Reviews*, vol. 279,
30 1985; Hol, *Angew. Chem.*, vol. 25, p. 767, 1986; and Verlinde and Hol, *Structure*, vol. 2, p. 577, 1994, each of which are incorporated by this reference herein in their entirety.

One embodiment of the present invention for structure
35 based drug design comprises identifying a chemical compound

that complements the shape of an FcR protein or a structure that is related to an FcR protein. Such method is referred to herein as a "geometric approach". In a geometric approach of the present invention, the number of internal degrees of freedom (and the corresponding local minima in the molecular conformation space) is reduced by considering only the geometric (hard-sphere) interactions of two rigid bodies, where one body (the active site) contains "pockets" or "grooves" that form binding sites for the second body (the complementing molecule, such as a ligand).

The geometric approach is described by Kuntz et al., *J. Mol. Biol.*, vol. 161, p. 269, 1982, which is incorporated by this reference herein in its entirety. The algorithm for chemical compound design can be implemented using the software program DOCK Package, Version 1.0 (available from the Regents of the University of California). Pursuant to the Kuntz algorithm, the shape of the cavity or groove on the surface of a structure (e.g., FcγRIIa protein) at a binding site or interface is defined as a series of overlapping spheres of different radii. One or more extant databases of crystallographic data (e.g., the Cambridge Structural Database System maintained by University Chemical Laboratory, Cambridge University, Lensfield Road, Cambridge CB2 1EW, U.K.) or the Protein Data Bank maintained by Brookhaven National Laboratory, is then searched for chemical compounds that approximate the shape thus defined.

Chemical compounds identified by the geometric approach can be modified to satisfy criteria associated with chemical complementarity, such as hydrogen bonding, ionic interactions or Van der Waals interactions.

Another embodiment of the present invention for structure based drug design comprises determining the interaction of chemical groups ("probes") with an active

site at sample positions within and around a binding site or interface, resulting in an array of energy values from which three dimensional contour surfaces at selected energy levels can be generated. This method is referred to herein as a "chemical-probe approach." The chemical-probe approach to the design of a chemical compound of the present invention is described by, for example, Goodford, *J. Med. Chem.*, vol. 28, p. 849, 1985, which is incorporated by this reference herein in its entirety, and is implemented using an appropriate software package, including for example, GRID (available from Molecular Discovery Ltd., Oxford OX2 9LL, U.K.). The chemical prerequisites for a site-complementing molecule can be identified at the outset, by probing the active site of an FcγRIIIa protein, for example, (as represented by the atomic coordinates shown in Table 1) with different chemical probes, e.g., water, a methyl group, an amine nitrogen, a carboxyl oxygen and/or a hydroxyl. Preferred sites for interaction between an active site and a probe are determined. Putative complementary chemical compounds can be generated using the resulting three dimensional pattern of such sites.

A therapeutic composition of the present invention can comprise one or more therapeutic compounds of the present invention. A therapeutic composition can further comprise other compounds capable of reducing Ig-mediated responses or increasing a humoral immune response. For example, a therapeutic composition of the present invention useful for reducing tissue damage can also include compounds that block recruitment of inflammatory cells, such as by, for example, blocking complement fixation, extravasation, block binding of viral proteins to FcR, block opsinization or enhance normal and passive antibody immunity. A therapeutic composition of the present invention useful for reducing Ig-mediated inflammation can include compounds

that block recruitment of inflammatory cells and/or block signal transduction pathway which leads to the release of inflammatory mediators.

5 A therapeutic composition of the present invention
useful for increasing a humoral response can also include
compounds that increase antibody production against an
antigen (i.e., adjuvants), including, but not limited to,
cytokines, chemokines, and compounds that induce the
production of cytokines and chemokines (e.g., granulocyte
10 macrophage colony stimulating factor (GM-CSF), granulocyte
colony stimulating factor (G-CSF), macrophage colony
stimulating factor (M-CSF), colony stimulating factor
(CSF), erythropoietin (EPO), interleukin 2 (IL-2),
interleukin-3 (IL-3), interleukin 4 (IL-4), interleukin 5
15 (IL-5), interleukin 6 (IL-6), interleukin 7 (IL-7),
interleukin 8 (IL-8), interleukin 10 (IL-10), interleukin
12 (IL-12), interferon gamma, interferon gamma inducing
factor I (IGIF), transforming growth factor beta, RANTES
(regulated upon activation, normal T cell expressed and
20 presumably secreted), macrophage inflammatory proteins
(e.g., MIP-1 alpha and MIP-1 beta), bacterial components
(e.g., endotoxins, in particular superantigens, exotoxins
and cell wall components); aluminum-based salts;
calcium-based salts; silica; polynucleotides; toxoids;
25 serum proteins, viral coat proteins; block copolymer
adjuvants (e.g., Hunter's Titermax™ adjuvant (Vaxcel™, Inc.
Norcross, GA), Ribi adjuvants (Ribi ImmunoChem Research,
Inc., Hamilton, MT); and saponins and their derivatives
(e.g., Quil A (Superfos Biosector A/S, Denmark)).

30 A therapeutic composition of the present invention can
be used to treat disease in an animal by administering such
composition to an animal in such a manner that desired
therapeutic results are obtained. Preferred animals to
treat include mammals, marsupials, reptiles and birds, with
35 humans, companion animals, food animals, zoo animals and

other economically relevant animals (e.g., race horses and animals valued for their coats, such as chinchillas and minks). More preferred animals to treat include humans, dogs, cats, horses, cattle, sheep, swine, chickens, ostriches, emus, turkeys, koalas and kangaroos. Particularly preferred animals to protect are humans, dogs and cats.

A preferred therapeutic composition of the present invention also includes an excipient, an adjuvant and/or carrier. Suitable excipients include compounds that the animal to be treated can tolerate. Examples of such excipients include water, saline, Ringer's solution, dextrose solution, Hank's solution, and other aqueous physiologically balanced salt solutions. Nonaqueous vehicles, such as fixed oils, sesame oil, ethyl oleate, or triglycerides may also be used. Other useful formulations include suspensions containing viscosity enhancing agents, such as sodium carboxymethylcellulose, sorbitol, or dextran. Excipients can also contain minor amounts of additives, such as substances that enhance isotonicity and chemical stability. Examples of buffers include phosphate buffer, bicarbonate buffer and Tris buffer, while examples of preservatives include thimerosal, o-cresol, formalin and benzyl alcohol. Standard formulations can either be liquid injectables or solids which can be taken up in a suitable liquid as a suspension or solution for injection. Thus, in a non-liquid formulation, the excipient can comprise dextrose, human serum albumin, preservatives, etc., to which sterile water or saline can be added prior to administration.

In one embodiment of the present invention, a therapeutic composition can include a carrier. Carriers include compounds that increase the half-life of a therapeutic composition in the treated animal. Suitable carriers include, but are not limited to, polymeric

controlled release vehicles, biodegradable implants, liposomes, bacteria, viruses, other cells, oils, esters, and glycols.

Acceptable protocols to administer therapeutic compositions of the present invention in an effective manner include individual dose size, number of doses, frequency of dose administration, and mode of administration. Determination of such protocols can be accomplished by those skilled in the art. Modes of administration can include, but are not limited to, subcutaneous, intradermal, intravenous, intranasal, oral, transdermal, intraocular and intramuscular routes.

Another embodiment of the present invention are diagnostic compounds capable of detecting altered FcR protein on or isolated from cells obtained from patients having abnormal immunity or inflammation. Using the methods of structure based drug design described herein, diagnostic reagents that bind to FcR protein can be developed using the three dimensional structure of FcR protein. Preferred diagnostic reagents of the present invention include molecules capable of binding to the Ig binding site of an FcR protein capable of binding to Ig and molecules capable of binding to circulating FcR protein obtained from patients with inflammation. Preferred diagnostic reagents include molecules that are immunogenic or can be chemically coupled to detectable compounds, such as radioisotopes, enzymes, dyes or biotin.

In a preferred embodiment, a therapeutic compound or diagnostic compound of the present invention comprises a protein engineered by recombinant DNA methods.

TABLE 1

REMARK Latest coordinates of the Fc Gamma Receptor IIa structure
 REMARK Written by O version 5.10.1
 REMARK Wed May 20 10:23:51 1998
 CRYST1 79.221 100.866 28.172 90.00 90.00 90.00
 ORIGX1 1.000000 0.000000 0.000000 0.000000
 ORIGX2 0.000000 1.000000 0.000000 0.000000
 ORIGX3 0.000000 0.000000 1.000000 0.000000
 SCALE1 0.012623 0.000000 0.000000 0.000000

70

	SCALE2	0.000000	0.009914	0.000000	0.000000				
	SCALE3	0.000000	0.000000	0.035496	0.000000				
	ATOM	1	CB	ALA	1	36.645	68.826	-4.702	1.00 51.37 6
	ATOM	2	C	ALA	1	36.199	68.294	-2.285	1.00 42.22 6
5	ATOM	3	O	ALA	1	36.801	67.492	-1.569	1.00 42.70 8
	ATOM	4	N	ALA	1	34.367	68.121	-3.997	1.00 45.74 7
	ATOM	5	CA	ALA	1	35.829	67.992	-3.724	1.00 43.68 6
	ATOM	6	N	PRO	2	35.903	69.499	-1.817	1.00 40.54 7
10	ATOM	7	CD	PRO	2	35.149	70.546	-2.533	1.00 38.91 6
	ATOM	8	CA	PRO	2	36.172	69.844	-0.425	1.00 38.61 6
	ATOM	9	CB	PRO	2	35.765	71.300	-0.322	1.00 39.86 6
	ATOM	10	CG	PRO	2	34.790	71.513	-1.426	1.00 41.36 6
	ATOM	11	C	PRO	2	35.294	68.931	0.434	1.00 36.70 6
	ATOM	12	O	PRO	2	34.188	68.654	-0.042	1.00 32.46 8
15	ATOM	13	N	PRO	3	35.789	68.496	1.579	1.00 33.82 7
	ATOM	14	CD	PRO	3	37.120	68.857	2.110	1.00 35.16 6
	ATOM	15	CA	PRO	3	35.069	67.637	2.491	1.00 38.25 6
	ATOM	16	CB	PRO	3	35.872	67.639	3.799	1.00 37.39 6
20	ATOM	17	CG	PRO	3	37.180	68.267	3.486	1.00 37.41 6
	ATOM	18	C	PRO	3	33.653	68.136	2.790	1.00 37.48 6
	ATOM	19	O	PRO	3	33.393	69.335	2.683	1.00 34.39 8
	ATOM	20	N	LYS	4	32.763	67.212	3.173	1.00 37.04 7
	ATOM	21	CA	LYS	4	31.399	67.678	3.424	1.00 34.97 6
	ATOM	22	CB	LYS	4	30.318	66.664	3.122	1.00 43.98 6
25	ATOM	23	CG	LYS	4	30.564	65.191	3.278	1.00 47.64 6
	ATOM	24	CD	LYS	4	29.775	64.349	2.292	1.00 52.03 6
	ATOM	25	CE	LYS	4	28.317	64.743	2.137	1.00 57.56 6
	ATOM	26	NZ	LYS	4	27.724	64.253	0.855	1.00 56.40 7
	ATOM	27	C	LYS	4	31.243	68.234	4.825	1.00 31.44 6
30	ATOM	28	O	LYS	4	31.846	67.769	5.784	1.00 29.91 8
	ATOM	29	N	ALA	5	30.416	69.280	4.908	1.00 28.75 7
	ATOM	30	CA	ALA	5	30.039	69.813	6.218	1.00 27.21 6
	ATOM	31	CB	ALA	5	29.155	71.032	6.110	1.00 21.94 6
35	ATOM	32	C	ALA	5	29.278	68.683	6.923	1.00 26.42 6
	ATOM	33	O	ALA	5	28.760	67.794	6.222	1.00 26.10 8
	ATOM	34	N	VAL	6	29.231	68.674	8.241	1.00 24.91 7
	ATOM	35	CA	VAL	6	28.515	67.632	8.985	1.00 26.95 6
	ATOM	36	CB	VAL	6	29.490	66.738	9.770	1.00 29.36 6
40	ATOM	37	CG1	VAL	6	28.779	65.726	10.676	1.00 29.86 6
	ATOM	38	CG2	VAL	6	30.434	66.024	8.801	1.00 26.74 6
	ATOM	39	C	VAL	6	27.503	68.253	9.942	1.00 28.93 6
	ATOM	40	O	VAL	6	27.846	68.994	10.866	1.00 31.46 8
	ATOM	41	N	LEU	7	26.233	67.929	9.758	1.00 30.08 7
	ATOM	42	CA	LEU	7	25.105	68.383	10.546	1.00 29.33 6
45	ATOM	43	CB	LEU	7	23.839	68.346	9.657	1.00 33.18 6
	ATOM	44	CG	LEU	7	22.828	69.458	9.960	1.00 34.94 6
	ATOM	45	CD1	LEU	7	22.082	69.876	8.721	1.00 27.55 6
	ATOM	46	CD2	LEU	7	21.887	69.002	11.069	1.00 32.30 6
	ATOM	47	C	LEU	7	24.816	67.565	11.794	1.00 29.57 6
50	ATOM	48	O	LEU	7	24.653	66.351	11.800	1.00 30.04 8
	ATOM	49	N	LYS	8	24.768	68.242	12.930	1.00 28.04 7
	ATOM	50	CA	LYS	8	24.568	67.692	14.257	1.00 25.12 6
	ATOM	51	CB	LYS	8	25.738	68.179	15.132	1.00 33.32 6
	ATOM	52	CG	LYS	8	25.777	67.611	16.532	1.00 39.37 6
55	ATOM	53	CD	LYS	8	25.967	68.598	17.652	1.00 43.84 6
	ATOM	54	CE	LYS	8	27.129	69.561	17.487	1.00 47.78 6
	ATOM	55	NZ	LYS	8	27.525	70.175	18.793	1.00 48.98 7
	ATOM	56	C	LYS	8	23.233	68.192	14.797	1.00 24.53 6
	ATOM	57	O	LYS	8	22.934	69.384	14.739	1.00 25.35 8
60	ATOM	58	N	LEU	9	22.423	67.310	15.333	1.00 24.78 7
	ATOM	59	CA	LEU	9	21.080	67.553	15.843	1.00 22.07 6
	ATOM	60	CB	LEU	9	20.189	66.483	15.190	1.00 20.04 6
	ATOM	61	CG	LEU	9	18.725	66.363	15.596	1.00 20.57 6
	ATOM	62	CD1	LEU	9	17.980	67.624	15.214	1.00 19.57 6
65	ATOM	63	CD2	LEU	9	18.084	65.137	14.903	1.00 23.44 6
	ATOM	64	C	LEU	9	21.019	67.415	17.346	1.00 21.01 6
	ATOM	65	O	LEU	9	21.424	66.393	17.869	1.00 22.38 8
	ATOM	66	N	GLU	10	20.583	68.410	18.118	1.00 22.53 7
	ATOM	67	CA	GLU	10	20.480	68.285	19.567	1.00 21.02 6
70	ATOM	68	CB	GLU	10	21.523	69.182	20.270	1.00 27.36 6
	ATOM	69	CGA	GLU	10	22.971	68.778	20.090	0.50 28.21 6

	ATOM	70	CGB	GLU	10	22.946	68.657	20.195	0.50	38.29	6
	ATOM	71	CDA	GLU	10	24.047	69.789	20.422	0.50	28.55	6
	ATOM	72	CDB	GLU	10	23.100	67.202	20.587	0.50	43.48	6
5	ATOM	73	OE1	GLU	10	25.131	69.365	20.907	0.50	26.56	8
	ATOM	74	OE1	GLU	10	22.443	66.771	21.565	0.50	47.24	8
	ATOM	75	OE2	GLU	10	23.888	71.008	20.186	0.50	22.10	8
	ATOM	76	OE2	GLU	10	23.871	66.486	19.908	0.50	46.42	8
	ATOM	77	C	GLU	10	19.096	68.728	20.008	1.00	19.76	6
10	ATOM	78	O	GLU	10	18.701	69.842	19.613	1.00	18.00	8
	ATOM	79	N	PRO	11	18.423	67.995	20.888	1.00	19.07	7
	ATOM	80	CD	PRO	11	17.058	68.340	21.390	1.00	18.71	6
	ATOM	81	CA	PRO	11	18.834	66.662	21.319	1.00	18.84	6
	ATOM	82	CB	PRO	11	17.807	66.272	22.365	1.00	17.38	6
15	ATOM	83	CG	PRO	11	16.560	67.000	21.944	1.00	18.86	6
	ATOM	84	C	PRO	11	18.787	65.758	20.090	1.00	20.01	6
	ATOM	85	O	PRO	11	18.310	66.212	19.051	1.00	16.22	8
	ATOM	86	N	PRO	12	19.232	64.517	20.155	1.00	19.94	7
	ATOM	87	CD	PRO	12	19.915	63.948	21.361	1.00	21.08	6
20	ATOM	88	CA	PRO	12	19.409	63.700	18.976	1.00	20.68	6
	ATOM	89	CB	PRO	12	20.455	62.656	19.397	1.00	19.82	6
	ATOM	90	CG	PRO	12	20.292	62.567	20.872	1.00	23.59	6
	ATOM	91	C	PRO	12	18.179	63.061	18.395	1.00	18.70	6
	ATOM	92	O	PRO	12	18.268	62.475	17.318	1.00	19.85	8
25	ATOM	93	N	TRP	13	17.039	63.169	19.059	1.00	15.64	7
	ATOM	94	CA	TRP	13	15.815	62.568	18.561	1.00	17.91	6
	ATOM	95	CB	TRP	13	14.688	62.840	19.562	1.00	14.32	6
	ATOM	96	CG	TRP	13	15.124	62.749	21.006	1.00	16.77	6
	ATOM	97	CD2	TRP	13	15.633	61.612	21.703	1.00	16.90	6
30	ATOM	98	CE2	TRP	13	15.899	62.005	23.032	1.00	16.87	6
	ATOM	99	CE3	TRP	13	15.867	60.279	21.350	1.00	18.03	6
	ATOM	100	CD1	TRP	13	15.106	63.769	21.916	1.00	18.97	6
	ATOM	101	NE1	TRP	13	15.589	63.343	23.137	1.00	11.16	7
	ATOM	102	CZ2	TRP	13	16.405	61.124	23.973	1.00	15.92	6
35	ATOM	103	CZ3	TRP	13	16.358	59.409	22.301	1.00	10.59	6
	ATOM	104	CH2	TRP	13	16.645	59.825	23.611	1.00	17.87	6
	ATOM	105	C	TRP	13	15.421	63.033	17.163	1.00	19.47	6
	ATOM	106	O	TRP	13	15.283	64.238	16.908	1.00	17.22	8
	ATOM	107	N	ILE	14	15.101	62.078	16.275	1.00	16.57	7
40	ATOM	108	CA	ILE	14	14.666	62.441	14.936	1.00	18.93	6
	ATOM	109	CB	ILE	14	15.185	61.523	13.816	1.00	16.07	6
	ATOM	110	CG2	ILE	14	16.720	61.521	13.840	1.00	16.61	6
	ATOM	111	CG1	ILE	14	14.582	60.119	13.972	1.00	21.35	6
	ATOM	112	CD1	ILE	14	15.045	59.150	12.896	1.00	26.28	6
45	ATOM	113	C	ILE	14	13.144	62.549	14.825	1.00	20.48	6
	ATOM	114	O	ILE	14	12.652	63.048	13.817	1.00	19.41	8
	ATOM	115	N	ASN	15	12.403	62.087	15.836	1.00	19.46	7
	ATOM	116	CA	ASN	15	10.935	62.270	15.778	1.00	18.11	6
	ATOM	117	CB	ASN	15	10.161	60.962	15.731	1.00	13.53	6
50	ATOM	118	CG	ASN	15	10.591	59.946	16.762	1.00	19.11	6
	ATOM	119	OD1	ASN	15	11.728	59.959	17.227	1.00	13.35	8
	ATOM	120	ND2	ASN	15	9.688	59.033	17.142	1.00	10.11	7
	ATOM	121	C	ASN	15	10.632	63.124	17.005	1.00	17.54	6
	ATOM	122	O	ASN	15	11.016	62.735	18.111	1.00	15.32	8
55	ATOM	123	N	VAL	16	10.122	64.331	16.805	1.00	16.86	7
	ATOM	124	CA	VAL	16	9.871	65.273	17.893	1.00	15.77	6
	ATOM	125	CB	VAL	16	10.761	66.534	17.748	1.00	16.54	6
	ATOM	126	CG1	VAL	16	12.251	66.141	17.733	1.00	13.42	6
	ATOM	127	CG2	VAL	16	10.490	67.345	16.491	1.00	18.04	6
60	ATOM	128	C	VAL	16	8.420	65.708	17.921	1.00	19.01	6
	ATOM	129	O	VAL	16	7.618	65.381	17.010	1.00	17.12	8
	ATOM	130	N	LEU	17	8.022	66.422	18.964	1.00	17.68	7
	ATOM	131	CA	LEU	17	6.664	66.962	19.068	1.00	15.11	6
	ATOM	132	CB	LEU	17	6.162	66.726	20.522	1.00	20.26	6
65	ATOM	133	CG	LEU	17	5.873	65.251	20.823	1.00	23.07	6
	ATOM	134	CD1	LEU	17	5.447	65.013	22.253	1.00	17.70	6
	ATOM	135	CD2	LEU	17	4.832	64.714	19.855	1.00	26.74	6
	ATOM	136	C	LEU	17	6.563	68.439	18.732	1.00	16.37	6
	ATOM	137	O	LEU	17	7.518	69.187	18.961	1.00	18.24	8
70	ATOM	138	N	GLN	18	5.424	68.931	18.227	1.00	18.55	7
	ATOM	139	CA	GLN	18	5.237	70.370	18.032	1.00	19.13	6
	ATOM	140	CB	GLN	18	3.790	70.721	17.696	1.00	31.65	6

	ATOM	141	CG	GLN	18	3.510	71.249	16.314	1.00	37.32	6
	ATOM	142	CD	GLN	18	2.120	70.902	15.800	1.00	36.92	6
	ATOM	143	OE1	GLN	18	1.953	70.032	14.943	1.00	30.97	8
	ATOM	144	NE2	GLN	18	1.135	71.618	16.333	1.00	31.73	7
5	ATOM	145	C	GLN	18	5.561	71.077	19.348	1.00	19.43	6
	ATOM	146	O	GLN	18	5.194	70.568	20.413	1.00	18.10	8
	ATOM	147	N	GLU	19	6.317	72.164	19.232	1.00	19.68	7
	ATOM	148	CA	GLU	19	6.727	73.045	20.293	1.00	18.88	6
	ATOM	149	CB	GLU	19	5.597	73.341	21.293	1.00	27.39	6
10	ATOM	150	CG	GLU	19	4.649	74.418	20.714	1.00	30.12	6
	ATOM	151	CD	GLU	19	3.558	74.699	21.720	1.00	41.87	6
	ATOM	152	OE1	GLU	19	3.857	75.330	22.758	1.00	48.83	8
	ATOM	153	OE2	GLU	19	2.421	74.272	21.464	1.00	46.61	8
	ATOM	154	C	GLU	19	8.004	72.622	20.998	1.00	21.46	6
15	ATOM	155	O	GLU	19	8.496	73.405	21.815	1.00	26.39	8
	ATOM	156	N	ASP	20	8.606	71.506	20.619	1.00	19.91	7
	ATOM	157	CA	ASP	20	9.898	71.094	21.114	1.00	20.76	6
	ATOM	158	CB	ASP	20	10.285	69.649	20.726	1.00	13.47	6
	ATOM	159	CG	ASP	20	9.587	68.578	21.526	1.00	13.93	6
20	ATOM	160	OD1	ASP	20	8.873	68.805	22.534	1.00	17.57	8
	ATOM	161	OD2	ASP	20	9.723	67.405	21.104	1.00	13.79	8
	ATOM	162	C	ASP	20	11.002	71.950	20.451	1.00	19.58	6
	ATOM	163	O	ASP	20	10.913	72.219	19.262	1.00	17.49	8
	ATOM	164	N	SER	21	12.071	72.198	21.174	1.00	17.22	7
25	ATOM	165	CA	SER	21	13.233	72.929	20.659	1.00	17.62	6
	ATOM	166	CBA	SER	21	14.011	73.525	21.844	0.50	17.49	6
	ATOM	167	CBB	SER	21	13.981	73.556	21.846	0.50	13.14	6
	ATOM	168	OGA	SER	21	14.900	74.516	21.355	0.50	22.95	8
	ATOM	169	OGB	SER	21	13.175	74.579	22.416	0.50	6.85	8
30	ATOM	170	C	SER	21	14.181	72.038	19.873	1.00	18.61	6
	ATOM	171	O	SER	21	14.424	70.884	20.265	1.00	21.41	8
	ATOM	172	N	VAL	22	14.638	72.512	18.721	1.00	15.80	7
	ATOM	173	CA	VAL	22	15.585	71.733	17.910	1.00	17.93	6
	ATOM	174	CB	VAL	22	15.052	71.234	16.560	1.00	20.37	6
35	ATOM	175	CG1	VAL	22	16.093	70.401	15.804	1.00	17.77	6
	ATOM	176	CG2	VAL	22	13.858	70.300	16.679	1.00	17.26	6
	ATOM	177	C	VAL	22	16.822	72.609	17.665	1.00	19.20	6
	ATOM	178	O	VAL	22	16.633	73.769	17.291	1.00	18.52	8
	ATOM	179	N	THR	23	18.021	72.107	17.917	1.00	16.32	7
40	ATOM	180	CA	THR	23	19.249	72.823	17.648	1.00	19.99	6
	ATOM	181	CB	THR	23	20.080	73.128	18.911	1.00	22.97	6
	ATOM	182	OG1	THR	23	19.192	73.749	19.850	1.00	18.42	8
	ATOM	183	CG2	THR	23	21.241	74.057	18.614	1.00	16.78	6
	ATOM	184	C	THR	23	20.098	72.016	16.658	1.00	24.68	6
45	ATOM	185	O	THR	23	20.509	70.880	16.897	1.00	22.59	8
	ATOM	186	N	LEU	24	20.257	72.618	15.467	1.00	23.73	7
	ATOM	187	CA	LEU	24	21.081	72.051	14.423	1.00	23.11	6
	ATOM	188	CB	LEU	24	20.427	72.206	13.046	1.00	20.25	6
	ATOM	189	CG	LEU	24	19.053	71.480	12.959	1.00	23.95	6
50	ATOM	190	CD1	LEU	24	18.324	71.856	11.681	1.00	20.78	6
	ATOM	191	CD2	LEU	24	19.251	69.985	13.049	1.00	22.74	6
	ATOM	192	C	LEU	24	22.444	72.763	14.450	1.00	25.87	6
	ATOM	193	O	LEU	24	22.470	74.008	14.537	1.00	24.57	8
	ATOM	194	N	THR	25	23.520	71.980	14.367	1.00	20.22	7
55	ATOM	195	CA	THR	25	24.847	72.600	14.336	1.00	23.21	6
	ATOM	196	CB	THR	25	25.656	72.265	15.597	1.00	27.69	6
	ATOM	197	OG1	THR	25	24.945	72.730	16.755	1.00	26.30	8
	ATOM	198	CG2	THR	25	27.041	72.925	15.590	1.00	28.49	6
	ATOM	199	C	THR	25	25.604	72.166	13.075	1.00	22.31	6
60	ATOM	200	O	THR	25	25.706	70.951	12.819	1.00	23.86	8
	ATOM	201	N	CYS	26	26.092	73.134	12.307	1.00	18.68	7
	ATOM	202	CA	CYS	26	26.832	72.888	11.075	1.00	23.20	6
	ATOM	203	C	CYS	26	28.345	72.910	11.346	1.00	23.06	6
	ATOM	204	O	CYS	26	28.957	73.980	11.556	1.00	23.76	8
65	ATOM	205	CB	CYS	26	26.509	73.881	9.958	1.00	17.92	6
	ATOM	206	SG	CYS	26	27.138	73.358	8.311	1.00	22.25	16
	ATOM	207	N	GLN	27	28.929	71.729	11.355	1.00	19.35	7
	ATOM	208	CA	GLN	27	30.332	71.521	11.658	1.00	23.30	6
	ATOM	209	CB	GLN	27	30.543	70.209	12.464	1.00	29.78	6
70	ATOM	210	CG	GLN	27	29.623	70.044	13.672	1.00	31.50	6
	ATOM	211	CD	GLN	27	29.927	68.828	14.518	1.00	33.01	6

	ATOM	212	OE1	GLN	27	30.322	67.774	14.032	1.00	38.67	8
	ATOM	213	NE2	GLN	27	29.792	68.895	15.834	1.00	36.36	7
	ATOM	214	C	GLN	27	31.169	71.417	10.377	1.00	26.33	6
5	ATOM	215	O	GLN	27	30.764	70.856	9.347	1.00	23.15	8
	ATOM	216	N	GLY	28	32.363	72.019	10.438	1.00	27.69	7
	ATOM	217	CA	GLY	28	33.289	72.019	9.313	1.00	28.02	6
	ATOM	218	C	GLY	28	34.022	73.360	9.215	1.00	29.41	6
	ATOM	219	O	GLY	28	33.639	74.335	9.862	1.00	28.46	8
10	ATOM	220	N	ALA	29	35.062	73.421	8.389	1.00	27.48	7
	ATOM	221	CA	ALA	29	35.824	74.640	8.210	1.00	27.39	6
	ATOM	222	CB	ALA	29	36.979	74.353	7.239	1.00	25.91	6
	ATOM	223	C	ALA	29	34.959	75.730	7.574	1.00	28.27	6
	ATOM	224	O	ALA	29	34.315	75.415	6.561	1.00	26.07	8
15	ATOM	225	N	ARG	30	35.060	76.951	8.064	1.00	23.97	7
	ATOM	226	CA	ARG	30	34.303	78.055	7.490	1.00	27.17	6
	ATOM	227	CB	ARG	30	33.571	78.823	8.601	1.00	30.34	6
	ATOM	228	CG	ARG	30	32.574	78.090	9.460	1.00	34.05	6
	ATOM	229	CD	ARG	30	32.365	78.880	10.761	1.00	33.86	6
20	ATOM	230	NE	ARG	30	32.407	77.902	11.836	1.00	38.60	7
	ATOM	231	CZ	ARG	30	32.487	78.082	13.126	1.00	38.08	6
	ATOM	232	NH1	ARG	30	32.567	79.298	13.635	1.00	36.51	7
	ATOM	233	NH2	ARG	30	32.467	76.990	13.879	1.00	46.13	7
	ATOM	234	C	ARG	30	35.194	79.148	6.880	1.00	26.70	6
25	ATOM	235	O	ARG	30	36.399	79.142	7.075	1.00	29.22	8
	ATOM	236	N	SER	31	34.573	80.129	6.246	1.00	26.85	7
	ATOM	237	CA	SER	31	35.315	81.284	5.738	1.00	26.56	6
	ATOM	238	CB	SER	31	34.682	81.846	4.476	1.00	25.03	6
	ATOM	239	OG	SER	31	34.562	80.875	3.477	1.00	27.59	8
30	ATOM	240	C	SER	31	35.273	82.321	6.861	1.00	26.58	6
	ATOM	241	O	SER	31	34.396	82.246	7.739	1.00	23.91	8
	ATOM	242	N	PRO	32	36.163	83.308	6.839	1.00	23.48	7
	ATOM	243	CD	PRO	32	37.224	83.483	5.842	1.00	22.70	6
	ATOM	244	CA	PRO	32	36.176	84.350	7.861	1.00	24.75	6
35	ATOM	245	CB	PRO	32	37.621	84.830	7.805	1.00	24.34	6
	ATOM	246	CG	PRO	32	38.095	84.571	6.414	1.00	23.77	6
	ATOM	247	C	PRO	32	35.172	85.449	7.549	1.00	29.23	6
	ATOM	248	O	PRO	32	35.472	86.609	7.223	1.00	28.28	8
	ATOM	249	N	GLU	33	33.913	85.121	7.709	1.00	29.77	7
40	ATOM	250	CA	GLU	33	32.725	85.896	7.417	1.00	33.37	6
	ATOM	251	CBA	GLU	33	32.177	85.426	6.073	0.50	35.18	6
	ATOM	252	CBB	GLU	33	32.123	85.457	6.084	0.50	31.98	6
	ATOM	253	CGA	GLU	33	30.795	84.829	5.952	0.50	39.40	6
	ATOM	254	CGB	GLU	33	31.776	83.990	5.954	0.50	34.05	6
45	ATOM	255	CDA	GLU	33	30.394	84.525	4.521	0.50	46.48	6
	ATOM	256	CDB	GLU	33	31.601	83.533	4.517	0.50	34.67	6
	ATOM	257	OE1	GLU	33	29.268	84.856	4.076	0.50	49.23	8
	ATOM	258	OE1	GLU	33	32.194	84.168	3.619	0.50	32.81	8
	ATOM	259	OE2	GLU	33	31.232	83.952	3.788	0.50	47.50	8
50	ATOM	260	OE2	GLU	33	30.877	82.542	4.275	0.50	24.64	8
	ATOM	261	C	GLU	33	31.683	85.689	8.519	1.00	32.61	6
	ATOM	262	O	GLU	33	31.612	84.600	9.085	1.00	28.72	8
	ATOM	263	N	SER	34	30.844	86.682	8.743	1.00	32.15	7
	ATOM	264	CA	SER	34	29.804	86.591	9.764	1.00	32.72	6
55	ATOM	265	CB	SER	34	29.277	88.013	10.037	1.00	34.26	6
	ATOM	266	OG	SER	34	28.320	87.931	11.093	1.00	45.88	8
	ATOM	267	C	SER	34	28.668	85.674	9.332	1.00	30.93	6
	ATOM	268	O	SER	34	28.156	84.883	10.124	1.00	28.87	8
	ATOM	269	N	ASP	35	28.222	85.773	8.082	1.00	28.02	7
60	ATOM	270	CA	ASP	35	27.167	84.858	7.599	1.00	28.62	6
	ATOM	271	CB	ASP	35	26.292	85.538	6.585	1.00	29.65	6
	ATOM	272	CG	ASP	35	25.357	86.639	7.057	1.00	37.43	6
	ATOM	273	OD1	ASP	35	25.027	86.769	8.258	1.00	33.53	8
	ATOM	274	OD2	ASP	35	24.902	87.396	6.154	1.00	36.01	8
65	ATOM	275	C	ASP	35	27.882	83.643	6.973	1.00	27.08	6
	ATOM	276	O	ASP	35	27.997	83.566	5.756	1.00	28.07	8
	ATOM	277	N	SER	36	28.461	82.748	7.774	1.00	25.55	7
	ATOM	278	CA	SER	36	29.282	81.680	7.225	1.00	27.45	6
	ATOM	279	CB	SER	36	30.440	81.431	8.213	1.00	34.87	6
70	ATOM	280	OG	SER	36	29.973	80.802	9.405	1.00	39.51	8
	ATOM	281	C	SER	36	28.558	80.382	6.890	1.00	27.14	6
	ATOM	282	O	SER	36	29.143	79.421	6.363	1.00	25.67	8

	ATOM	283	N	ILE	37	27.293	80.223	7.231	1.00	24.64	7
	ATOM	284	CA	ILE	37	26.580	78.973	6.977	1.00	24.33	6
	ATOM	285	CB	ILE	37	26.164	78.307	8.309	1.00	30.71	6
5	ATOM	286	CG2	ILE	37	25.561	76.931	8.032	1.00	26.94	6
	ATOM	287	CG1	ILE	37	27.333	78.221	9.308	1.00	21.66	6
	ATOM	288	CD1	ILE	37	28.443	77.278	8.867	1.00	27.66	6
	ATOM	289	C	ILE	37	25.336	79.159	6.128	1.00	24.08	6
	ATOM	290	O	ILE	37	24.515	80.033	6.390	1.00	23.50	8
10	ATOM	291	N	GLN	38	25.122	78.314	5.127	1.00	24.52	7
	ATOM	292	CA	GLN	38	23.862	78.296	4.399	1.00	23.13	6
	ATOM	293	CB	GLN	38	24.016	78.068	2.905	1.00	29.28	6
	ATOM	294	CG	GLN	38	24.458	79.296	2.123	1.00	29.86	6
	ATOM	295	CD	GLN	38	24.692	78.965	0.661	1.00	33.48	6
15	ATOM	296	OE1	GLN	38	25.540	78.122	0.323	1.00	28.34	8
	ATOM	297	NE2	GLN	38	23.922	79.668	-0.177	1.00	38.54	7
	ATOM	298	C	GLN	38	23.048	77.128	4.985	1.00	23.81	6
	ATOM	299	O	GLN	38	23.598	76.022	5.087	1.00	22.62	8
	ATOM	300	N	TRP	39	21.807	77.386	5.371	1.00	21.43	7
20	ATOM	301	CA	TRP	39	20.987	76.304	5.905	1.00	21.73	6
	ATOM	302	CB	TRP	39	20.345	76.633	7.257	1.00	21.01	6
	ATOM	303	CG	TRP	39	21.264	76.633	8.430	1.00	17.58	6
	ATOM	304	CD2	TRP	39	21.721	75.523	9.212	1.00	17.00	6
	ATOM	305	CE2	TRP	39	22.569	76.033	10.220	1.00	16.71	6
	ATOM	306	CE3	TRP	39	21.495	74.147	9.158	1.00	21.47	6
25	ATOM	307	CD1	TRP	39	21.844	77.750	8.974	1.00	19.92	6
	ATOM	308	NE1	TRP	39	22.626	77.400	10.061	1.00	22.18	7
	ATOM	309	CZ2	TRP	39	23.218	75.220	11.152	1.00	18.29	6
	ATOM	310	CZ3	TRP	39	22.109	73.329	10.091	1.00	21.62	6
30	ATOM	311	CH2	TRP	39	22.960	73.874	11.064	1.00	20.15	6
	ATOM	312	C	TRP	39	19.890	75.993	4.898	1.00	22.76	6
	ATOM	313	O	TRP	39	19.407	76.925	4.238	1.00	23.42	8
	ATOM	314	N	PHE	40	19.533	74.701	4.758	1.00	22.91	7
	ATOM	315	CA	PHE	40	18.512	74.389	3.754	1.00	26.86	6
35	ATOM	316	CB	PHE	40	19.121	73.722	2.513	1.00	24.16	6
	ATOM	317	CG	PHE	40	20.225	74.429	1.788	1.00	23.96	6
	ATOM	318	CD1	PHE	40	21.551	74.280	2.189	1.00	23.61	6
	ATOM	319	CD2	PHE	40	19.945	75.244	0.696	1.00	22.47	6
	ATOM	320	CE1	PHE	40	22.564	74.919	1.504	1.00	20.83	6
40	ATOM	321	CE2	PHE	40	20.967	75.880	0.020	1.00	21.69	6
	ATOM	322	CZ	PHE	40	22.267	75.740	0.432	1.00	21.86	6
	ATOM	323	C	PHE	40	17.466	73.435	4.349	1.00	23.51	6
	ATOM	324	O	PHE	40	17.838	72.588	5.151	1.00	21.94	8
	ATOM	325	N	HIS	41	16.232	73.575	3.905	1.00	21.59	7
45	ATOM	326	CA	HIS	41	15.107	72.771	4.366	1.00	24.07	6
	ATOM	327	CB	HIS	41	14.032	73.572	5.099	1.00	18.72	6
	ATOM	328	CG	HIS	41	12.864	72.727	5.548	1.00	23.41	6
	ATOM	329	CD2	HIS	41	12.794	71.415	5.899	1.00	21.85	6
	ATOM	330	ND1	HIS	41	11.588	73.218	5.709	1.00	21.97	7
50	ATOM	331	CE1	HIS	41	10.789	72.259	6.135	1.00	22.79	6
	ATOM	332	NE2	HIS	41	11.504	71.161	6.268	1.00	21.87	7
	ATOM	333	C	HIS	41	14.455	72.163	3.115	1.00	21.83	6
	ATOM	334	O	HIS	41	13.972	72.919	2.282	1.00	21.37	8
	ATOM	335	N	ASN	42	14.576	70.847	2.959	1.00	22.08	7
55	ATOM	336	CA	ASN	42	14.077	70.196	1.726	1.00	20.46	6
	ATOM	337	CB	ASN	42	12.562	70.322	1.722	1.00	18.21	6
	ATOM	338	CG	ASN	42	11.925	69.397	2.761	1.00	22.74	6
	ATOM	339	OD1	ASN	42	12.473	68.343	3.087	1.00	24.40	8
	ATOM	340	ND2	ASN	42	10.804	69.804	3.341	1.00	18.43	7
	ATOM	341	C	ASN	42	14.733	70.811	0.488	1.00	21.32	6
60	ATOM	342	O	ASN	42	14.085	71.047	-0.533	1.00	20.13	8
	ATOM	343	N	GLY	43	16.002	71.220	0.568	1.00	20.53	7
	ATOM	344	CA	GLY	43	16.767	71.861	-0.480	1.00	20.83	6
	ATOM	345	C	GLY	43	16.586	73.360	-0.661	1.00	24.51	6
65	ATOM	346	O	GLY	43	17.209	73.987	-1.550	1.00	25.30	8
	ATOM	347	N	ASN	44	15.633	73.970	0.051	1.00	21.27	7
	ATOM	348	CA	ASN	44	15.391	75.393	-0.112	1.00	20.46	6
	ATOM	349	CB	ASN	44	13.903	75.734	0.000	1.00	23.82	6
	ATOM	350	CG	ASN	44	13.049	74.834	-0.891	1.00	22.26	6
70	ATOM	351	OD1	ASN	44	12.148	74.144	-0.409	1.00	25.47	8
	ATOM	352	ND2	ASN	44	13.382	74.787	-2.171	1.00	21.59	7
	ATOM	353	C	ASN	44	16.208	76.143	0.937	1.00	19.78	6

	ATOM	354	O	ASN	44	16.180	75.778	2.107	1.00	22.07	8
	ATOM	355	N	LEU	45	16.907	77.188	0.523	1.00	22.22	7
	ATOM	356	CA	LEU	45	17.730	77.962	1.459	1.00	21.67	6
5	ATOM	357	CB	LEU	45	18.391	79.141	0.715	1.00	28.15	6
	ATOM	358	CG	LEU	45	19.159	80.171	1.538	1.00	29.14	6
	ATOM	359	CD1	LEU	45	20.479	79.571	2.002	1.00	25.07	6
	ATOM	360	CD2	LEU	45	19.452	81.466	0.775	1.00	28.51	6
	ATOM	361	C	LEU	45	16.825	78.559	2.525	1.00	22.27	6
10	ATOM	362	O	LEU	45	15.748	78.997	2.118	1.00	20.13	8
	ATOM	363	N	ILE	46	17.263	78.604	3.766	1.00	20.11	7
	ATOM	364	CA	ILE	46	16.539	79.322	4.835	1.00	24.64	6
	ATOM	365	CB	ILE	46	16.657	78.508	6.132	1.00	22.24	6
	ATOM	366	CG2	ILE	46	16.007	79.134	7.358	1.00	21.33	6
15	ATOM	367	CG1	ILE	46	16.111	77.072	5.945	1.00	20.74	6
	ATOM	368	CD1	ILE	46	16.664	76.147	7.024	1.00	20.48	6
	ATOM	369	C	ILE	46	17.351	80.625	5.006	1.00	25.53	6
	ATOM	370	O	ILE	46	18.419	80.600	5.624	1.00	22.91	8
	ATOM	371	N	PRO	47	16.937	81.747	4.444	1.00	30.56	7
20	ATOM	372	CD	PRO	47	15.704	81.884	3.620	1.00	32.61	6
	ATOM	373	CA	PRO	47	17.731	82.968	4.434	1.00	30.93	6
	ATOM	374	CB	PRO	47	17.030	83.836	3.363	1.00	31.28	6
	ATOM	375	CG	PRO	47	15.610	83.400	3.441	1.00	32.54	6
	ATOM	376	C	PRO	47	17.888	83.762	5.706	1.00	28.32	6
25	ATOM	377	O	PRO	47	18.733	84.670	5.747	1.00	29.24	8
	ATOM	378	N	THR	48	17.092	83.513	6.730	1.00	26.79	7
	ATOM	379	CA	THR	48	17.135	84.298	7.971	1.00	26.97	6
	ATOM	380	CB	THR	48	15.698	84.323	8.532	1.00	31.78	6
	ATOM	381	OG1	THR	48	15.241	82.958	8.520	1.00	31.45	8
30	ATOM	382	CG2	THR	48	14.798	85.150	7.605	1.00	27.40	6
	ATOM	383	C	THR	48	18.075	83.757	9.021	1.00	26.31	6
	ATOM	384	O	THR	48	18.206	84.334	10.113	1.00	28.00	8
	ATOM	385	N	HIS	49	18.698	82.602	8.772	1.00	24.44	7
	ATOM	386	CA	HIS	49	19.612	81.942	9.707	1.00	24.19	6
35	ATOM	387	CB	HIS	49	18.953	80.610	10.174	1.00	25.11	6
	ATOM	388	CG	HIS	49	17.722	80.939	10.961	1.00	22.20	6
	ATOM	389	CD2	HIS	49	16.430	81.109	10.624	1.00	27.86	6
	ATOM	390	ND1	HIS	49	17.809	81.225	12.306	1.00	29.80	7
	ATOM	391	CE1	HIS	49	16.595	81.526	12.762	1.00	28.91	6
40	ATOM	392	NE2	HIS	49	15.748	81.474	11.761	1.00	25.35	7
	ATOM	393	C	HIS	49	20.923	81.588	9.041	1.00	23.08	6
	ATOM	394	O	HIS	49	20.942	80.805	8.075	1.00	20.57	8
	ATOM	395	N	THR	50	22.038	82.162	9.497	1.00	25.11	7
	ATOM	396	CA	THR	50	23.321	81.974	8.807	1.00	22.98	6
45	ATOM	397	CB	THR	50	23.732	83.314	8.137	1.00	23.01	6
	ATOM	398	OG1	THR	50	23.843	84.252	9.231	1.00	18.66	8
	ATOM	399	CG2	THR	50	22.757	83.817	7.101	1.00	19.07	6
	ATOM	400	C	THR	50	24.460	81.645	9.766	1.00	24.61	6
	ATOM	401	O	THR	50	25.640	81.772	9.393	1.00	26.17	8
50	ATOM	402	N	GLN	51	24.126	81.274	10.985	1.00	24.52	7
	ATOM	403	CA	GLN	51	25.132	80.979	11.995	1.00	27.31	6
	ATOM	404	CB	GLN	51	24.708	81.505	13.378	1.00	28.63	6
	ATOM	405	CG	GLN	51	24.438	83.014	13.378	1.00	32.81	6
	ATOM	406	CD	GLN	51	25.677	83.810	12.995	1.00	38.53	6
55	ATOM	407	OE1	GLN	51	26.606	83.952	13.802	1.00	37.60	8
	ATOM	408	NE2	GLN	51	25.724	84.331	11.765	1.00	32.79	7
	ATOM	409	C	GLN	51	25.411	79.487	12.101	1.00	26.69	6
	ATOM	410	O	GLN	51	24.626	78.636	11.689	1.00	26.27	8
	ATOM	411	N	PRO	52	26.510	79.138	12.769	1.00	25.16	7
60	ATOM	412	CD	PRO	52	27.553	80.091	13.270	1.00	24.54	6
	ATOM	413	CA	PRO	52	26.917	77.763	12.974	1.00	25.24	6
	ATOM	414	CB	PRO	52	28.264	77.888	13.708	1.00	26.09	6
	ATOM	415	CG	PRO	52	28.804	79.217	13.257	1.00	23.35	6
	ATOM	416	C	PRO	52	25.900	76.915	13.722	1.00	25.71	6
	ATOM	417	O	PRO	52	25.877	75.687	13.542	1.00	21.61	8
65	ATOM	418	N	SER	53	25.044	77.497	14.556	1.00	24.05	7
	ATOM	419	CA	SER	53	23.991	76.773	15.239	1.00	25.63	6
	ATOM	420	CB	SER	53	24.105	76.711	16.758	1.00	31.86	6
	ATOM	421	OG	SER	53	24.778	75.495	17.094	1.00	42.46	8
70	ATOM	422	C	SER	53	22.681	77.460	14.854	1.00	24.85	6
	ATOM	423	O	SER	53	22.681	78.673	14.691	1.00	23.68	8
	ATOM	424	N	TYR	54	21.658	76.689	14.614	1.00	24.52	7

	ATOM	425	CA	TYR	54	20.333	77.167	14.212	1.00	26.29	6
	ATOM	426	CB	TYR	54	20.050	76.886	12.729	1.00	26.92	6
	ATOM	427	CG	TYR	54	18.612	76.998	12.274	1.00	30.15	6
5	ATOM	428	CD1	TYR	54	17.719	77.905	12.825	1.00	29.18	6
	ATOM	429	CE1	TYR	54	16.407	78.006	12.409	1.00	31.26	6
	ATOM	430	CD2	TYR	54	18.104	76.166	11.280	1.00	31.67	6
	ATOM	431	CE2	TYR	54	16.796	76.217	10.855	1.00	31.66	6
	ATOM	432	CZ	TYR	54	15.950	77.151	11.429	1.00	33.63	6
10	ATOM	433	OH	TYR	54	14.624	77.219	11.038	1.00	34.53	8
	ATOM	434	C	TYR	54	19.378	76.450	15.167	1.00	24.84	6
	ATOM	435	O	TYR	54	19.300	75.210	15.129	1.00	22.53	8
	ATOM	436	N	ARG	55	18.773	77.181	16.070	1.00	21.66	7
	ATOM	437	CA	ARG	55	17.864	76.650	17.070	1.00	23.60	6
	ATOM	438	CB	ARG	55	18.242	77.157	18.480	1.00	25.95	6
15	ATOM	439	CG	ARG	55	17.478	76.340	19.551	1.00	23.98	6
	ATOM	440	CD	ARG	55	17.651	76.982	20.918	1.00	35.38	6
	ATOM	441	NE	ARG	55	16.821	76.365	21.956	1.00	27.47	7
	ATOM	442	CZ	ARG	55	17.278	75.530	22.879	1.00	33.10	6
20	ATOM	443	NH1	ARG	55	18.570	75.209	22.904	1.00	30.00	7
	ATOM	444	NH2	ARG	55	16.418	75.049	23.778	1.00	32.66	7
	ATOM	445	C	ARG	55	16.434	77.103	16.802	1.00	27.49	6
	ATOM	446	O	ARG	55	16.275	78.312	16.569	1.00	22.62	8
	ATOM	447	N	PHE	56	15.455	76.174	16.781	1.00	23.78	7
25	ATOM	448	CA	PHE	56	14.092	76.636	16.510	1.00	21.92	6
	ATOM	449	CB	PHE	56	13.716	76.495	15.036	1.00	25.99	6
	ATOM	450	CG	PHE	56	13.819	75.131	14.386	1.00	20.84	6
	ATOM	451	CD1	PHE	56	15.019	74.653	13.897	1.00	21.33	6
	ATOM	452	CD2	PHE	56	12.705	74.319	14.264	1.00	20.31	6
30	ATOM	453	CE1	PHE	56	15.103	73.415	13.283	1.00	21.52	6
	ATOM	454	CE2	PHE	56	12.768	73.077	13.680	1.00	18.36	6
	ATOM	455	CZ	PHE	56	13.973	72.616	13.159	1.00	18.38	6
	ATOM	456	C	PHE	56	13.095	75.862	17.372	1.00	23.93	6
	ATOM	457	O	PHE	56	13.454	74.833	17.921	1.00	22.42	8
	ATOM	458	N	LYS	57	11.865	76.340	17.423	1.00	22.46	7
35	ATOM	459	CA	LYS	57	10.735	75.659	18.054	1.00	24.34	6
	ATOM	460	CBA	LYS	57	9.892	76.620	18.881	0.50	28.51	6
	ATOM	461	CBB	LYS	57	9.822	76.727	18.669	0.50	22.87	6
	ATOM	462	CGA	LYS	57	10.656	77.298	20.010	0.50	33.64	6
40	ATOM	463	CGB	LYS	57	8.769	76.208	19.632	0.50	24.29	6
	ATOM	464	CDA	LYS	57	11.436	76.342	20.892	0.50	40.75	6
	ATOM	465	CDB	LYS	57	8.631	77.186	20.798	0.50	26.90	6
	ATOM	466	CEA	LYS	57	12.612	76.990	21.603	0.50	43.07	6
	ATOM	467	CEB	LYS	57	9.138	76.604	22.092	0.50	29.79	6
45	ATOM	468	NZA	LYS	57	12.703	76.630	23.044	0.50	51.71	7
	ATOM	469	NZB	LYS	57	8.050	76.265	23.060	0.50	36.22	7
	ATOM	470	C	LYS	57	9.950	74.923	16.969	1.00	21.30	6
	ATOM	471	O	LYS	57	9.436	75.551	16.052	1.00	19.46	8
	ATOM	472	N	ALA	58	9.928	73.588	16.945	1.00	18.23	7
50	ATOM	473	CA	ALA	58	9.341	72.864	15.821	1.00	15.74	6
	ATOM	474	CB	ALA	58	9.612	71.361	16.094	1.00	9.09	6
	ATOM	475	C	ALA	58	7.841	73.034	15.614	1.00	20.26	6
	ATOM	476	O	ALA	58	7.067	73.064	16.574	1.00	18.04	8
	ATOM	477	N	ASN	59	7.392	73.126	14.367	1.00	18.31	7
55	ATOM	478	CA	ASN	59	5.986	73.071	14.019	1.00	23.04	6
	ATOM	479	CB	ASN	59	5.222	74.301	13.612	1.00	32.39	6
	ATOM	480	CG	ASN	59	5.880	75.643	13.665	1.00	38.26	6
	ATOM	481	OD1	ASN	59	5.855	76.279	14.716	1.00	42.50	8
	ATOM	482	ND2	ASN	59	6.426	76.066	12.529	1.00	43.39	7
60	ATOM	483	C	ASN	59	5.825	72.052	12.867	1.00	24.07	6
	ATOM	484	O	ASN	59	6.794	71.476	12.365	1.00	21.25	8
	ATOM	485	N	ASN	60	4.582	71.833	12.484	1.00	24.40	7
	ATOM	486	CA	ASN	60	4.192	70.823	11.519	1.00	31.47	6
	ATOM	487	CB	ASN	60	2.680	70.893	11.234	1.00	31.46	6
65	ATOM	488	CGA	ASN	60	2.272	69.776	10.274	0.50	31.26	6
	ATOM	489	CGB	ASN	60	2.221	72.272	10.814	0.50	35.72	6
	ATOM	490	OD1	ASN	60	2.337	68.582	10.597	0.50	22.52	8
	ATOM	491	OD1	ASN	60	2.985	73.240	10.768	0.50	33.04	8
	ATOM	492	ND2	ASN	60	1.863	70.175	9.070	0.50	26.04	7
70	ATOM	493	ND2	ASN	60	0.932	72.391	10.483	0.50	39.47	7
	ATOM	494	C	ASN	60	5.006	70.943	10.234	1.00	29.05	6
	ATOM	495	O	ASN	60	5.645	69.986	9.780	1.00	32.27	8

	ATOM	496	N	ASN	61	5.098	72.153	9.710	1.00	30.20	7
	ATOM	497	CAA	ASN	61	5.863	72.487	8.529	0.50	28.68	6
	ATOM	498	CAB	ASN	61	5.857	72.367	8.477	0.50	29.13	6
	ATOM	499	CBA	ASN	61	5.564	73.955	8.150	0.50	26.19	6
5	ATOM	500	CBB	ASN	61	5.403	73.671	7.806	0.50	30.25	6
	ATOM	501	CGA	ASN	61	4.101	74.127	7.792	0.50	27.01	6
	ATOM	502	CGB	ASN	61	5.608	74.882	8.678	0.50	32.36	6
	ATOM	503	OD1	ASN	61	3.502	75.125	8.184	0.50	28.58	8
10	ATOM	504	OD1	ASN	61	6.383	74.820	9.637	0.50	33.38	8
	ATOM	505	ND2	ASN	61	3.526	73.172	7.071	0.50	34.39	7
	ATOM	506	ND2	ASN	61	4.927	75.991	8.384	0.50	33.52	7
	ATOM	507	C	ASN	61	7.371	72.336	8.628	1.00	25.33	6
	ATOM	508	O	ASN	61	8.030	72.535	7.617	1.00	21.46	8
	ATOM	509	N	ASP	62	7.932	71.978	9.767	1.00	24.89	7
15	ATOM	510	CA	ASP	62	9.373	71.842	9.941	1.00	21.37	6
	ATOM	511	CB	ASP	62	9.749	72.284	11.372	1.00	16.89	6
	ATOM	512	CG	ASP	62	9.620	73.782	11.538	1.00	26.20	6
	ATOM	513	OD1	ASP	62	9.824	74.549	10.570	1.00	20.81	8
	ATOM	514	OD2	ASP	62	9.276	74.273	12.611	1.00	17.90	8
20	ATOM	515	C	ASP	62	9.887	70.439	9.645	1.00	18.69	6
	ATOM	516	O	ASP	62	11.104	70.209	9.654	1.00	20.50	8
	ATOM	517	N	SER	63	9.011	69.477	9.394	1.00	19.81	7
	ATOM	518	CA	SER	63	9.434	68.132	9.015	1.00	19.84	6
	ATOM	519	CB	SER	63	8.268	67.164	8.811	1.00	22.04	6
25	ATOM	520	OG	SER	63	7.506	67.018	10.009	1.00	20.02	8
	ATOM	521	C	SER	63	10.196	68.204	7.682	1.00	23.89	6
	ATOM	522	O	SER	63	10.015	69.160	6.911	1.00	17.92	8
	ATOM	523	N	GLY	64	11.056	67.195	7.467	1.00	19.50	7
30	ATOM	524	CA	GLY	64	11.769	67.191	6.190	1.00	22.23	6
	ATOM	525	C	GLY	64	13.272	66.965	6.340	1.00	19.81	6
	ATOM	526	O	GLY	64	13.744	66.564	7.399	1.00	18.93	8
	ATOM	527	N	GLU	65	13.980	67.226	5.238	1.00	17.01	7
	ATOM	528	CA	GLU	65	15.428	67.013	5.269	1.00	21.39	6
	ATOM	529	CBA	GLU	65	15.934	66.562	3.901	0.50	13.64	6
35	ATOM	530	CBB	GLU	65	15.933	66.446	3.947	0.50	23.81	6
	ATOM	531	CGA	GLU	65	16.507	65.158	3.813	0.50	15.71	6
	ATOM	532	CGB	GLU	65	15.409	65.059	3.602	0.50	32.15	6
	ATOM	533	CDA	GLU	65	16.656	64.679	2.381	0.50	22.33	6
	ATOM	534	CDB	GLU	65	15.898	63.965	4.520	0.50	40.56	6
40	ATOM	535	OE1	GLU	65	17.428	65.263	1.586	0.50	22.70	8
	ATOM	536	OE1	GLU	65	16.578	64.271	5.525	0.50	41.83	8
	ATOM	537	OE2	GLU	65	15.991	63.686	2.014	0.50	31.04	8
	ATOM	538	OE2	GLU	65	15.624	62.758	4.278	0.50	46.02	8
	ATOM	539	C	GLU	65	16.155	68.324	5.593	1.00	21.56	6
45	ATOM	540	O	GLU	65	15.756	69.325	5.007	1.00	21.41	8
	ATOM	541	N	TYR	66	17.172	68.268	6.458	1.00	21.38	7
	ATOM	542	CA	TYR	66	17.966	69.483	6.691	1.00	17.91	6
	ATOM	543	CB	TYR	66	17.954	69.984	8.129	1.00	17.39	6
	ATOM	544	CG	TYR	66	16.620	70.563	8.534	1.00	18.08	6
50	ATOM	545	CD1	TYR	66	15.605	69.686	8.957	1.00	18.56	6
	ATOM	546	CE1	TYR	66	14.369	70.147	9.323	1.00	16.48	6
	ATOM	547	CD2	TYR	66	16.348	71.921	8.485	1.00	18.23	6
	ATOM	548	CE2	TYR	66	15.102	72.382	8.867	1.00	18.37	6
	ATOM	549	CZ	TYR	66	14.124	71.516	9.279	1.00	18.98	6
55	ATOM	550	OH	TYR	66	12.872	71.939	9.624	1.00	14.14	8
	ATOM	551	C	TYR	66	19.379	69.231	6.212	1.00	13.96	6
	ATOM	552	O	TYR	66	19.923	68.135	6.353	1.00	18.14	8
	ATOM	553	N	THR	67	20.010	70.228	5.568	1.00	17.95	7
	ATOM	554	CA	THR	67	21.374	70.138	5.117	1.00	18.06	6
60	ATOM	555	CB	THR	67	21.514	69.844	3.599	1.00	22.52	6
	ATOM	556	OG1	THR	67	20.669	70.737	2.835	1.00	16.85	8
	ATOM	557	CG2	THR	67	21.215	68.371	3.309	1.00	17.46	6
	ATOM	558	C	THR	67	22.044	71.508	5.384	1.00	18.76	6
	ATOM	559	O	THR	67	21.354	72.515	5.567	1.00	17.47	8
65	ATOM	560	N	CYS	68	23.354	71.540	5.389	1.00	19.74	7
	ATOM	561	CA	CYS	68	24.099	72.792	5.597	1.00	23.50	6
	ATOM	562	C	CYS	68	25.382	72.759	4.758	1.00	23.12	6
	ATOM	563	O	CYS	68	25.791	71.712	4.279	1.00	25.07	8
	ATOM	564	CB	CYS	68	24.434	73.082	7.055	1.00	18.70	6
70	ATOM	565	SG	CYS	68	25.675	71.985	7.798	1.00	23.45	16
	ATOM	566	N	GLN	69	25.975	73.920	4.534	1.00	24.47	7

	ATOM	567	CA	GLN	69	27.174	74.121	3.770	1.00	24.99	6
	ATOM	568	CB	GLN	69	26.909	74.344	2.264	1.00	27.22	6
	ATOM	569	CG	GLN	69	28.155	74.057	1.419	1.00	25.14	6
5	ATOM	570	CD	GLN	69	27.857	74.022	-0.065	1.00	32.43	6
	ATOM	571	OE1	GLN	69	26.710	74.166	-0.487	1.00	31.34	8
	ATOM	572	NE2	GLN	69	28.896	73.814	-0.874	1.00	27.89	7
	ATOM	573	C	GLN	69	27.901	75.383	4.266	1.00	27.60	6
	ATOM	574	O	GLN	69	27.289	76.352	4.734	1.00	25.37	8
10	ATOM	575	N	THR	70	29.206	75.318	4.115	1.00	28.73	7
	ATOM	576	CA	THR	70	30.059	76.465	4.439	1.00	32.10	6
	ATOM	577	CB	THR	70	31.125	76.153	5.491	1.00	33.36	6
	ATOM	578	OG1	THR	70	30.619	75.311	6.553	1.00	45.26	8
	ATOM	579	CG2	THR	70	31.453	77.444	6.210	1.00	50.20	6
15	ATOM	580	C	THR	70	30.737	76.890	3.138	1.00	32.77	6
	ATOM	581	O	THR	70	30.680	76.170	2.130	1.00	30.75	8
	ATOM	582	N	GLY	71	31.472	78.007	3.175	1.00	31.83	7
	ATOM	583	CA	GLY	71	32.224	78.469	2.033	1.00	27.97	6
	ATOM	584	C	GLY	71	33.376	77.544	1.690	1.00	29.94	6
20	ATOM	585	O	GLY	71	33.938	77.668	0.596	1.00	32.37	8
	ATOM	586	N	GLN	72	33.842	76.707	2.594	1.00	24.86	7
	ATOM	587	CA	GLN	72	34.920	75.779	2.457	1.00	27.14	6
	ATOM	588	CB	GLN	72	35.868	75.974	3.667	1.00	27.31	6
	ATOM	589	CG	GLN	72	36.291	77.451	3.825	1.00	30.51	6
	ATOM	590	CD	GLN	72	36.961	77.995	2.567	1.00	30.53	6
25	ATOM	591	OE1	GLN	72	37.981	77.441	2.161	1.00	39.95	8
	ATOM	592	NE2	GLN	72	36.402	79.014	1.944	1.00	31.16	7
	ATOM	593	C	GLN	72	34.530	74.305	2.441	1.00	29.60	6
	ATOM	594	O	GLN	72	35.419	73.442	2.578	1.00	30.82	8
30	ATOM	595	N	THR	73	33.248	73.954	2.380	1.00	25.83	7
	ATOM	596	CA	THR	73	32.861	72.549	2.426	1.00	26.62	6
	ATOM	597	CB	THR	73	32.278	72.135	3.792	1.00	26.64	6
	ATOM	598	OG1	THR	73	31.226	73.051	4.138	1.00	27.54	8
	ATOM	599	CG2	THR	73	33.313	72.124	4.897	1.00	28.16	6
35	ATOM	600	C	THR	73	31.824	72.223	1.371	1.00	26.31	6
	ATOM	601	O	THR	73	31.210	73.110	0.776	1.00	28.00	8
	ATOM	602	N	SER	74	31.685	70.927	1.074	1.00	28.62	7
	ATOM	603	CA	SER	74	30.592	70.605	0.112	1.00	29.44	6
	ATOM	604	CB	SER	74	31.020	69.470	-0.803	1.00	30.45	6
40	ATOM	605	OG	SER	74	31.407	68.399	0.034	1.00	41.05	8
	ATOM	606	C	SER	74	29.366	70.395	0.992	1.00	26.65	6
	ATOM	607	O	SER	74	29.461	70.438	2.228	1.00	25.57	8
	ATOM	608	N	LEU	75	28.178	70.281	0.442	1.00	29.47	7
45	ATOM	609	CA	LEU	75	26.915	70.163	1.158	1.00	25.10	6
	ATOM	610	CB	LEU	75	25.749	70.141	0.159	1.00	27.83	6
	ATOM	611	CG	LEU	75	24.348	70.136	0.777	1.00	27.24	6
	ATOM	612	CD1	LEU	75	23.888	71.554	1.094	1.00	24.13	6
	ATOM	613	CD2	LEU	75	23.349	69.420	-0.133	1.00	24.42	6
	ATOM	614	C	LEU	75	26.884	68.973	2.087	1.00	25.84	6
50	ATOM	615	O	LEU	75	27.300	67.858	1.711	1.00	22.45	8
	ATOM	616	N	SER	76	26.376	69.158	3.315	1.00	23.31	7
	ATOM	617	CA	SER	76	26.357	68.009	4.219	1.00	25.20	6
	ATOM	618	CB	SER	76	25.916	68.402	5.644	1.00	26.64	6
	ATOM	619	OG	SER	76	24.514	68.663	5.624	1.00	29.43	8
55	ATOM	620	C	SER	76	25.346	66.955	3.738	1.00	23.00	6
	ATOM	621	O	SER	76	24.431	67.304	3.006	1.00	21.02	8
	ATOM	622	N	ASP	77	25.506	65.739	4.241	1.00	22.24	7
	ATOM	623	CA	ASP	77	24.493	64.712	4.094	1.00	26.03	6
	ATOM	624	CB	ASP	77	24.907	63.362	4.683	1.00	20.27	6
60	ATOM	625	CG	ASP	77	25.914	62.676	3.758	1.00	25.73	6
	ATOM	626	OD1	ASP	77	25.821	62.893	2.541	1.00	23.79	8
	ATOM	627	OD2	ASP	77	26.769	61.954	4.292	1.00	28.92	8
	ATOM	628	C	ASP	77	23.267	65.191	4.929	1.00	25.85	6
	ATOM	629	O	ASP	77	23.423	65.904	5.914	1.00	24.00	8
65	ATOM	630	N	PRO	78	22.098	64.758	4.492	1.00	27.37	7
	ATOM	631	CD	PRO	78	21.917	63.917	3.275	1.00	26.84	6
	ATOM	632	CA	PRO	78	20.849	65.130	5.098	1.00	25.42	6
	ATOM	633	CB	PRO	78	19.795	64.592	4.141	1.00	28.38	6
	ATOM	634	CG	PRO	78	20.453	63.586	3.272	1.00	27.24	6
70	ATOM	635	C	PRO	78	20.575	64.556	6.479	1.00	25.28	6
	ATOM	636	O	PRO	78	21.006	63.459	6.820	1.00	23.68	8
	ATOM	637	N	VAL	79	19.833	65.331	7.265	1.00	20.24	7

	ATOM	638	CA	VAL	79	19.287	64.861	8.535	1.00	18.86	6
	ATOM	639	CB	VAL	79	19.850	65.516	9.783	1.00	19.49	6
	ATOM	640	CG1	VAL	79	19.042	65.239	11.046	1.00	22.25	6
5	ATOM	641	CG2	VAL	79	21.275	64.959	10.036	1.00	21.95	6
	ATOM	642	C	VAL	79	17.777	65.046	8.399	1.00	19.76	6
	ATOM	643	O	VAL	79	17.283	66.130	8.076	1.00	22.34	8
	ATOM	644	N	HIS	80	17.024	63.955	8.566	1.00	19.43	7
	ATOM	645	CA	HIS	80	15.584	63.976	8.387	1.00	18.11	6
10	ATOM	646	CB	HIS	80	15.130	62.621	7.784	1.00	26.87	6
	ATOM	647	CG	HIS	80	13.712	62.754	7.293	1.00	31.93	6
	ATOM	648	CD2	HIS	80	13.194	62.983	6.069	1.00	27.05	6
	ATOM	649	ND1	HIS	80	12.637	62.697	8.176	1.00	34.35	7
	ATOM	650	CE1	HIS	80	11.525	62.847	7.480	1.00	34.80	6
15	ATOM	651	NE2	HIS	80	11.831	63.016	6.210	1.00	34.81	7
	ATOM	652	C	HIS	80	14.865	64.187	9.718	1.00	23.08	6
	ATOM	653	O	HIS	80	15.096	63.496	10.709	1.00	23.37	8
	ATOM	654	N	LEU	81	13.953	65.138	9.747	1.00	19.18	7
	ATOM	655	CA	LEU	81	13.244	65.478	10.957	1.00	21.58	6
20	ATOM	656	CB	LEU	81	13.567	66.937	11.331	1.00	18.20	6
	ATOM	657	CG	LEU	81	12.847	67.381	12.605	1.00	18.21	6
	ATOM	658	CD1	LEU	81	13.496	66.708	13.812	1.00	19.39	6
	ATOM	659	CD2	LEU	81	12.865	68.912	12.696	1.00	14.76	6
	ATOM	660	C	LEU	81	11.747	65.255	10.783	1.00	19.36	6
25	ATOM	661	O	LEU	81	11.225	65.543	9.720	1.00	20.96	8
	ATOM	662	N	THR	82	11.100	64.689	11.793	1.00	19.61	7
	ATOM	663	CA	THR	82	9.642	64.463	11.680	1.00	18.45	6
	ATOM	664	CB	THR	82	9.316	62.950	11.683	1.00	25.98	6
	ATOM	665	OG1	THR	82	9.907	62.351	10.527	1.00	18.89	8
30	ATOM	666	CG2	THR	82	7.795	62.775	11.666	1.00	24.98	6
	ATOM	667	C	THR	82	8.971	65.100	12.891	1.00	16.02	6
	ATOM	668	O	THR	82	9.248	64.735	14.035	1.00	14.79	8
	ATOM	669	N	VAL	83	8.075	66.045	12.647	1.00	16.23	7
	ATOM	670	CA	VAL	83	7.451	66.758	13.753	1.00	16.97	6
35	ATOM	671	CB	VAL	83	7.559	68.282	13.530	1.00	12.81	6
	ATOM	672	CG1	VAL	83	7.051	68.972	14.799	1.00	15.92	6
	ATOM	673	CG2	VAL	83	8.986	68.760	13.246	1.00	11.78	6
	ATOM	674	C	VAL	83	6.020	66.264	13.892	1.00	19.97	6
	ATOM	675	O	VAL	83	5.261	66.329	12.918	1.00	18.57	8
40	ATOM	676	N	LEU	84	5.686	65.756	15.075	1.00	16.89	7
	ATOM	677	CA	LEU	84	4.372	65.188	15.312	1.00	19.89	6
	ATOM	678	CB	LEU	84	4.621	63.786	15.890	1.00	18.15	6
	ATOM	679	CG	LEU	84	5.491	62.863	15.021	1.00	23.40	6
	ATOM	680	CD1	LEU	84	5.927	61.690	15.868	1.00	25.20	6
45	ATOM	681	CD2	LEU	84	4.752	62.396	13.758	1.00	20.46	6
	ATOM	682	C	LEU	84	3.487	66.016	16.228	1.00	22.29	6
	ATOM	683	O	LEU	84	3.928	66.891	16.975	1.00	23.90	8
	ATOM	684	N	PHE	85	2.189	65.750	16.218	1.00	21.03	7
	ATOM	685	CA	PHE	85	1.254	66.444	17.111	1.00	22.92	6
50	ATOM	686	CB	PHE	85	0.399	67.431	16.333	1.00	21.76	6
	ATOM	687	CG	PHE	85	-0.440	68.350	17.184	1.00	27.90	6
	ATOM	688	CD1	PHE	85	0.103	69.013	18.266	1.00	28.30	6
	ATOM	689	CD2	PHE	85	-1.787	68.533	16.899	1.00	26.61	6
	ATOM	690	CE1	PHE	85	-0.664	69.874	19.040	1.00	29.65	6
55	ATOM	691	CE2	PHE	85	-2.559	69.386	17.668	1.00	25.61	6
	ATOM	692	CZ	PHE	85	-1.996	70.047	18.733	1.00	28.75	6
	ATOM	693	C	PHE	85	0.455	65.399	17.852	1.00	21.99	6
	ATOM	694	O	PHE	85	-0.642	65.000	17.426	1.00	22.11	8
	ATOM	695	N	GLU	86	1.023	64.883	18.938	1.00	20.76	7
60	ATOM	696	CA	GLU	86	0.421	63.762	19.702	1.00	18.04	6
	ATOM	697	CB	GLU	86	1.142	62.463	19.210	1.00	20.84	6
	ATOM	698	CG	GLU	86	0.711	61.815	17.911	1.00	25.05	6
	ATOM	699	CD	GLU	86	1.647	61.048	17.019	1.00	41.96	6
	ATOM	700	OE1	GLU	86	2.719	60.507	17.416	1.00	46.14	8
65	ATOM	701	OE2	GLU	86	1.429	60.893	15.765	1.00	40.77	8
	ATOM	702	C	GLU	86	0.694	64.026	21.176	1.00	18.46	6
	ATOM	703	O	GLU	86	1.588	64.839	21.462	1.00	16.67	8
	ATOM	704	N	TRP	87	0.031	63.408	22.156	1.00	12.60	7
	ATOM	705	CA	TRP	87	0.328	63.631	23.553	1.00	13.01	6
70	ATOM	706	CB	TRP	87	-0.808	63.056	24.411	1.00	18.40	6
	ATOM	707	CG	TRP	87	-1.922	64.023	24.687	1.00	21.87	6
	ATOM	708	CD2	TRP	87	-1.812	65.176	25.521	1.00	21.14	6

	ATOM	709	CE2	TRP	87	-3.065	65.805	25.526	1.00	24.31	6
	ATOM	710	CE3	TRP	87	-0.767	65.738	26.255	1.00	24.84	6
	ATOM	711	CD1	TRP	87	-3.216	63.985	24.231	1.00	22.52	6
5	ATOM	712	NE1	TRP	87	-3.907	65.069	24.734	1.00	22.53	7
	ATOM	713	CZ2	TRP	87	-3.303	66.966	26.266	1.00	29.91	6
	ATOM	714	CZ3	TRP	87	-0.998	66.890	26.987	1.00	29.83	6
	ATOM	715	CH2	TRP	87	-2.254	67.499	26.970	1.00	29.09	6
	ATOM	716	C	TRP	87	1.599	62.967	24.068	1.00	15.44	6
10	ATOM	717	O	TRP	87	2.178	63.499	25.018	1.00	16.68	8
	ATOM	718	N	LEU	88	2.036	61.873	23.447	1.00	14.44	7
	ATOM	719	CA	LEU	88	3.153	61.051	23.861	1.00	20.07	6
	ATOM	720	CB	LEU	88	2.596	59.942	24.783	1.00	17.49	6
	ATOM	721	CG	LEU	88	3.608	59.303	25.769	1.00	16.97	6
	ATOM	722	CD1	LEU	88	4.062	60.299	26.830	1.00	17.38	6
15	ATOM	723	CD2	LEU	88	2.987	58.053	26.370	1.00	13.93	6
	ATOM	724	C	LEU	88	3.889	60.399	22.677	1.00	20.44	6
	ATOM	725	O	LEU	88	3.255	59.857	21.752	1.00	19.65	8
	ATOM	726	N	VAL	89	5.218	60.517	22.620	1.00	18.11	7
	ATOM	727	CA	VAL	89	5.998	59.926	21.542	1.00	14.66	6
20	ATOM	728	CBA	VAL	89	6.686	61.029	20.699	0.50	7.52	6
	ATOM	729	CBB	VAL	89	6.677	60.941	20.604	0.50	13.86	6
	ATOM	730	CG1	VAL	89	7.573	61.890	21.597	0.50	7.13	6
	ATOM	731	CG1	VAL	89	5.696	61.409	19.543	0.50	15.87	6
	ATOM	732	CG2	VAL	89	7.501	60.486	19.531	0.50	3.91	6
25	ATOM	733	CG2	VAL	89	7.264	62.090	21.402	0.50	18.65	6
	ATOM	734	C	VAL	89	7.109	59.032	22.107	1.00	15.71	6
	ATOM	735	O	VAL	89	7.689	59.262	23.179	1.00	14.52	8
	ATOM	736	N	LEU	90	7.379	57.958	21.386	1.00	15.13	7
30	ATOM	737	CA	LEU	90	8.520	57.133	21.703	1.00	13.72	6
	ATOM	738	CB	LEU	90	8.287	55.625	21.488	1.00	17.87	6
	ATOM	739	CG	LEU	90	9.650	54.978	21.873	1.00	26.07	6
	ATOM	740	CD1	LEU	90	9.479	54.066	23.036	1.00	30.57	6
	ATOM	741	CD2	LEU	90	10.373	54.463	20.662	1.00	25.07	6
35	ATOM	742	C	LEU	90	9.657	57.674	20.803	1.00	17.58	6
	ATOM	743	O	LEU	90	9.611	57.517	19.576	1.00	14.46	8
	ATOM	744	N	GLN	91	10.673	58.298	21.412	1.00	15.83	7
	ATOM	745	CA	GLN	91	11.745	58.908	20.623	1.00	17.70	6
	ATOM	746	CB	GLN	91	12.252	60.238	21.264	1.00	15.03	6
40	ATOM	747	CG	GLN	91	11.105	61.231	21.472	1.00	12.81	6
	ATOM	748	CD	GLN	91	11.564	62.636	21.868	1.00	15.79	6
	ATOM	749	OE1	GLN	91	12.023	62.823	22.988	1.00	14.61	8
	ATOM	750	NE2	GLN	91	11.409	63.610	20.984	1.00	16.27	7
	ATOM	751	C	GLN	91	12.971	58.042	20.375	1.00	17.71	6
45	ATOM	752	O	GLN	91	13.370	57.296	21.268	1.00	19.37	8
	ATOM	753	N	THR	92	13.607	58.207	19.218	1.00	14.05	7
	ATOM	754	CA	THR	92	14.853	57.488	18.934	1.00	19.01	6
	ATOM	755	CB	THR	92	14.562	56.225	18.089	1.00	16.40	6
	ATOM	756	OG1	THR	92	15.769	55.485	17.905	1.00	18.39	8
50	ATOM	757	CG2	THR	92	13.943	56.499	16.720	1.00	10.45	6
	ATOM	758	C	THR	92	15.803	58.416	18.173	1.00	18.96	6
	ATOM	759	O	THR	92	15.339	59.272	17.409	1.00	21.88	8
	ATOM	760	N	PRO	93	17.095	58.153	18.251	1.00	18.78	7
	ATOM	761	CD	PRO	93	17.747	57.169	19.135	1.00	22.16	6
55	ATOM	762	CA	PRO	93	18.090	58.929	17.530	1.00	24.37	6
	ATOM	763	CB	PRO	93	19.352	58.803	18.371	1.00	24.99	6
	ATOM	764	CG	PRO	93	19.162	57.609	19.235	1.00	26.05	6
	ATOM	765	C	PRO	93	18.285	58.362	16.138	1.00	27.02	6
	ATOM	766	O	PRO	93	18.852	59.019	15.248	1.00	27.04	8
60	ATOM	767	N	HIS	94	17.978	57.069	15.960	1.00	24.22	7
	ATOM	768	CA	HIS	94	18.114	56.421	14.651	1.00	25.72	6
	ATOM	769	CB	HIS	94	19.444	55.690	14.439	1.00	20.09	6
	ATOM	770	CG	HIS	94	20.639	56.587	14.595	1.00	21.67	6
	ATOM	771	CD2	HIS	94	21.161	57.530	13.798	1.00	23.30	6
65	ATOM	772	ND1	HIS	94	21.380	56.595	15.754	1.00	27.49	7
	ATOM	773	CE1	HIS	94	22.338	57.501	15.657	1.00	26.54	6
	ATOM	774	NE2	HIS	94	22.211	58.078	14.482	1.00	32.10	7
	ATOM	775	C	HIS	94	17.038	55.350	14.453	1.00	24.49	6
	ATOM	776	O	HIS	94	16.481	54.838	15.429	1.00	24.01	8
70	ATOM	777	N	LEU	95	16.847	54.929	13.214	1.00	21.96	7
	ATOM	778	CA	LEU	95	15.900	53.847	12.960	1.00	26.06	6
	ATOM	779	CB	LEU	95	15.014	54.118	11.741	1.00	26.66	6

	ATOM	780	CG	LEU	95	13.994	55.248	11.899	1.00	35.19	6
	ATOM	781	CD1	LEU	95	13.449	55.601	10.525	1.00	25.66	6
	ATOM	782	CD2	LEU	95	12.895	54.908	12.900	1.00	24.13	6
5	ATOM	783	C	LEU	95	16.626	52.525	12.720	1.00	26.30	6
	ATOM	784	O	LEU	95	15.999	51.464	12.790	1.00	26.83	8
	ATOM	785	N	GLU	96	17.884	52.601	12.326	1.00	25.44	7
	ATOM	786	CA	GLU	96	18.688	51.413	12.087	1.00	28.55	6
	ATOM	787	CB	GLU	96	19.062	51.144	10.634	1.00	28.97	6
10	ATOM	788	CG	GLU	96	17.977	51.334	9.605	1.00	34.46	6
	ATOM	789	CD	GLU	96	18.414	51.109	8.168	1.00	42.07	6
	ATOM	790	OE1	GLU	96	19.560	50.709	7.882	1.00	41.53	8
	ATOM	791	OE2	GLU	96	17.592	51.343	7.256	1.00	45.31	8
	ATOM	792	C	GLU	96	19.995	51.575	12.885	1.00	32.22	6
15	ATOM	793	O	GLU	96	20.525	52.686	13.015	1.00	31.68	8
	ATOM	794	N	PHE	97	20.396	50.487	13.538	1.00	29.38	7
	ATOM	795	CA	PHE	97	21.622	50.447	14.315	1.00	31.45	6
	ATOM	796	CB	PHE	97	21.388	50.351	15.832	1.00	29.88	6
	ATOM	797	CG	PHE	97	20.640	51.497	16.464	1.00	28.91	6
20	ATOM	798	CD1	PHE	97	19.256	51.580	16.386	1.00	19.88	6
	ATOM	799	CD2	PHE	97	21.311	52.503	17.131	1.00	27.06	6
	ATOM	800	CE1	PHE	97	18.557	52.624	16.971	1.00	23.29	6
	ATOM	801	CE2	PHE	97	20.622	53.545	17.719	1.00	23.27	6
	ATOM	802	CZ	PHE	97	19.244	53.626	17.636	1.00	25.87	6
25	ATOM	803	C	PHE	97	22.455	49.233	13.861	1.00	31.11	6
	ATOM	804	O	PHE	97	22.007	48.334	13.164	1.00	32.31	8
	ATOM	805	N	GLN	98	23.726	49.213	14.219	1.00	34.14	7
	ATOM	806	CA	GLN	98	24.636	48.131	13.939	1.00	33.31	6
	ATOM	807	CB	GLN	98	26.042	48.629	13.635	1.00	38.15	6
30	ATOM	808	CG	GLN	98	26.207	49.422	12.356	1.00	45.65	6
	ATOM	809	CD	GLN	98	25.763	48.712	11.097	1.00	49.99	6
	ATOM	810	OE1	GLN	98	26.455	47.828	10.589	1.00	52.58	8
	ATOM	811	NE2	GLN	98	24.603	49.088	10.563	1.00	53.06	7
	ATOM	812	C	GLN	98	24.662	47.218	15.172	1.00	31.48	6
35	ATOM	813	O	GLN	98	24.459	47.664	16.300	1.00	27.98	8
	ATOM	814	N	GLU	99	24.990	45.955	14.920	1.00	30.75	7
	ATOM	815	CA	GLU	99	25.112	44.978	16.009	1.00	32.56	6
	ATOM	816	CB	GLU	99	25.598	43.653	15.420	1.00	36.89	6
	ATOM	817	CG	GLU	99	25.204	42.392	16.141	1.00	44.86	6
40	ATOM	818	CD	GLU	99	24.771	41.288	15.184	1.00	48.45	6
	ATOM	819	OE1	GLU	99	23.802	40.573	15.521	1.00	53.90	8
	ATOM	820	OE2	GLU	99	25.400	41.148	14.118	1.00	50.56	8
	ATOM	821	C	GLU	99	26.130	45.551	16.980	1.00	31.14	6
	ATOM	822	O	GLU	99	27.136	46.048	16.475	1.00	31.94	8
45	ATOM	823	N	GLY	100	25.919	45.571	18.275	1.00	32.19	7
	ATOM	824	CA	GLY	100	26.874	46.123	19.217	1.00	31.10	6
	ATOM	825	C	GLY	100	26.643	47.541	19.696	1.00	31.51	6
	ATOM	826	O	GLY	100	27.082	47.931	20.789	1.00	30.30	8
	ATOM	827	N	GLU	101	25.948	48.369	18.921	1.00	34.41	7
50	ATOM	828	CA	GLU	101	25.675	49.746	19.297	1.00	34.07	6
	ATOM	829	CB	GLU	101	24.949	50.452	18.148	1.00	37.86	6
	ATOM	830	CG	GLU	101	25.777	50.676	16.889	1.00	48.38	6
	ATOM	831	CD	GLU	101	24.984	51.520	15.895	1.00	49.17	6
	ATOM	832	OE1	GLU	101	24.251	52.408	16.385	1.00	58.51	8
55	ATOM	833	OE2	GLU	101	25.046	51.333	14.669	1.00	48.56	8
	ATOM	834	C	GLU	101	24.783	49.848	20.537	1.00	33.06	6
	ATOM	835	O	GLU	101	24.086	48.888	20.886	1.00	27.70	8
	ATOM	836	N	THR	102	24.747	51.057	21.107	1.00	31.92	7
	ATOM	837	CA	THR	102	23.870	51.303	22.248	1.00	32.85	6
60	ATOM	838	CB	THR	102	24.508	52.161	23.341	1.00	35.75	6
	ATOM	839	OG1	THR	102	25.546	51.438	24.021	1.00	36.79	8
	ATOM	840	CG2	THR	102	23.532	52.577	24.441	1.00	35.82	6
	ATOM	841	C	THR	102	22.582	51.944	21.721	1.00	32.54	6
	ATOM	842	O	THR	102	22.650	52.932	20.991	1.00	30.03	8
65	ATOM	843	N	ILE	103	21.431	51.329	22.014	1.00	28.53	7
	ATOM	844	CA	ILE	103	20.162	51.939	21.590	1.00	25.40	6
	ATOM	845	CB	ILE	103	19.131	50.873	21.163	1.00	26.58	6
	ATOM	846	CG2	ILE	103	17.776	51.496	20.828	1.00	25.47	6
	ATOM	847	CG1	ILE	103	19.669	50.080	19.971	1.00	21.79	6
70	ATOM	848	CD1	ILE	103	18.739	49.003	19.438	1.00	19.73	6
	ATOM	849	C	ILE	103	19.624	52.753	22.767	1.00	25.27	6
	ATOM	850	O	ILE	103	19.439	52.181	23.853	1.00	23.06	8

	ATOM	851	N	MET	104	19.443	54.059	22.591	1.00	24.90	7
	ATOM	852	CA	MET	104	18.893	54.913	23.639	1.00	21.55	6
	ATOM	853	CB	MET	104	19.797	56.097	23.963	1.00	33.48	6
5	ATOM	854	CG	MET	104	20.810	55.826	25.101	1.00	29.68	6
	ATOM	855	SD	MET	104	21.940	57.256	25.242	1.00	46.02	16
	ATOM	856	CE	MET	104	22.667	57.216	23.589	1.00	31.10	6
	ATOM	857	C	MET	104	17.528	55.456	23.215	1.00	21.27	6
	ATOM	858	O	MET	104	17.374	55.991	22.106	1.00	22.96	8
10	ATOM	859	N	LEU	105	16.503	55.242	24.027	1.00	20.55	7
	ATOM	860	CA	LEU	105	15.134	55.668	23.728	1.00	22.33	6
	ATOM	861	CB	LEU	105	14.192	54.450	23.550	1.00	14.66	6
	ATOM	862	CG	LEU	105	14.713	53.389	22.561	1.00	18.89	6
	ATOM	863	CD1	LEU	105	13.796	52.178	22.489	1.00	19.44	6
	ATOM	864	CD2	LEU	105	14.882	54.056	21.186	1.00	18.70	6
15	ATOM	865	C	LEU	105	14.567	56.559	24.817	1.00	20.15	6
	ATOM	866	O	LEU	105	15.050	56.506	25.950	1.00	18.39	8
	ATOM	867	N	ARG	106	13.523	57.324	24.483	1.00	18.25	7
	ATOM	868	CA	ARG	106	12.912	58.174	25.516	1.00	17.87	6
	ATOM	869	CB	ARG	106	13.607	59.553	25.508	1.00	14.96	6
20	ATOM	870	CG	ARG	106	12.834	60.597	26.290	1.00	16.79	6
	ATOM	871	CD	ARG	106	13.699	61.788	26.757	1.00	19.51	6
	ATOM	872	NE	ARG	106	13.334	62.927	26.025	1.00	23.46	7
	ATOM	873	CZ	ARG	106	12.990	64.174	26.065	1.00	24.43	6
25	ATOM	874	NH1	ARG	106	12.923	64.892	27.176	1.00	25.93	7
	ATOM	875	NH2	ARG	106	12.697	64.795	24.936	1.00	18.72	7
	ATOM	876	C	ARG	106	11.422	58.321	25.304	1.00	18.56	6
	ATOM	877	O	ARG	106	10.998	58.479	24.142	1.00	20.43	8
	ATOM	878	N	CYS	107	10.642	58.246	26.378	1.00	15.23	7
30	ATOM	879	CA	CYS	107	9.189	58.419	26.292	1.00	14.89	6
	ATOM	880	C	CYS	107	8.934	59.891	26.583	1.00	15.28	6
	ATOM	881	O	CYS	107	9.296	60.294	27.690	1.00	15.96	8
	ATOM	882	CB	CYS	107	8.438	57.565	27.322	1.00	14.55	6
	ATOM	883	SG	CYS	107	6.691	57.368	27.013	1.00	13.91	16
35	ATOM	884	N	HIS	108	8.446	60.653	25.604	1.00	15.07	7
	ATOM	885	CA	HIS	108	8.334	62.103	25.811	1.00	11.91	6
	ATOM	886	CB	HIS	108	9.190	62.757	24.708	1.00	16.03	6
	ATOM	887	CG	HIS	108	9.119	64.240	24.572	1.00	16.94	6
	ATOM	888	CD2	HIS	108	9.068	65.023	23.462	1.00	17.64	6
40	ATOM	889	ND1	HIS	108	9.103	65.108	25.657	1.00	17.41	7
	ATOM	890	CE1	HIS	108	9.034	66.350	25.215	1.00	17.37	6
	ATOM	891	NE2	HIS	108	9.021	66.333	23.895	1.00	20.00	7
	ATOM	892	C	HIS	108	6.925	62.647	25.733	1.00	11.83	6
	ATOM	893	O	HIS	108	6.224	62.361	24.762	1.00	12.54	8
45	ATOM	894	N	SER	109	6.515	63.502	26.654	1.00	13.70	7
	ATOM	895	CA	SER	109	5.160	64.091	26.605	1.00	11.70	6
	ATOM	896	CB	SER	109	4.583	64.134	28.041	1.00	13.47	6
	ATOM	897	OG	SER	109	5.609	64.845	28.800	1.00	16.16	8
	ATOM	898	C	SER	109	5.190	65.459	25.970	1.00	14.21	6
50	ATOM	899	O	SER	109	6.180	66.232	25.903	1.00	14.63	8
	ATOM	900	N	TRP	110	4.047	65.804	25.381	1.00	16.58	7
	ATOM	901	CA	TRP	110	3.860	67.102	24.708	1.00	16.04	6
	ATOM	902	CB	TRP	110	2.480	67.158	24.072	1.00	18.73	6
	ATOM	903	CG	TRP	110	2.187	68.425	23.306	1.00	21.24	6
55	ATOM	904	CD2	TRP	110	1.135	69.339	23.589	1.00	20.70	6
	ATOM	905	CE2	TRP	110	1.193	70.361	22.616	1.00	25.92	6
	ATOM	906	CE3	TRP	110	0.112	69.372	24.549	1.00	24.16	6
	ATOM	907	CD1	TRP	110	2.827	68.908	22.214	1.00	22.22	6
	ATOM	908	NE1	TRP	110	2.233	70.069	21.765	1.00	22.81	7
60	ATOM	909	CZ2	TRP	110	0.276	71.404	22.568	1.00	24.18	6
	ATOM	910	CZ3	TRP	110	-0.781	70.434	24.509	1.00	30.15	6
	ATOM	911	CH2	TRP	110	-0.698	71.433	23.526	1.00	31.04	6
	ATOM	912	C	TRP	110	4.082	68.245	25.681	1.00	14.44	6
	ATOM	913	O	TRP	110	3.665	68.219	26.852	1.00	17.08	8
65	ATOM	914	N	LYS	111	4.928	69.199	25.294	1.00	19.42	7
	ATOM	915	CA	LYS	111	5.347	70.325	26.115	1.00	19.40	6
	ATOM	916	CB	LYS	111	4.131	71.241	26.418	1.00	21.00	6
	ATOM	917	CG	LYS	111	3.583	71.904	25.155	1.00	24.94	6
	ATOM	918	CD	LYS	111	2.124	72.287	25.337	1.00	34.17	6
70	ATOM	919	CE	LYS	111	1.952	73.719	25.781	1.00	37.49	6
	ATOM	920	NZ	LYS	111	2.783	74.668	24.987	1.00	52.66	7
	ATOM	921	C	LYS	111	5.940	69.921	27.450	1.00	20.33	6

	ATOM	922	O	LYS	111	5.905	70.694	28.419	1.00	16.80	8
	ATOM	923	N	ASP	112	6.444	68.695	27.602	1.00	18.28	7
	ATOM	924	CA	ASP	112	6.989	68.233	28.861	1.00	20.31	6
5	ATOM	925	CB	ASP	112	8.242	69.088	29.191	1.00	24.52	6
	ATOM	926	CG	ASP	112	9.306	68.737	28.155	1.00	31.39	6
	ATOM	927	OD1	ASP	112	9.700	67.545	28.119	1.00	39.68	8
	ATOM	928	OD2	ASP	112	9.719	69.588	27.360	1.00	35.00	8
	ATOM	929	C	ASP	112	6.015	68.203	30.018	1.00	23.40	6
10	ATOM	930	O	ASP	112	6.426	68.475	31.148	1.00	23.42	8
	ATOM	931	N	LYS	113	4.731	67.889	29.785	1.00	23.10	7
	ATOM	932	CA	LYS	113	3.792	67.721	30.891	1.00	22.35	6
	ATOM	933	CB	LYS	113	2.352	67.432	30.437	1.00	21.68	6
	ATOM	934	CG	LYS	113	1.758	68.611	29.659	1.00	27.09	6
	ATOM	935	CD	LYS	113	0.232	68.574	29.608	1.00	28.34	6
15	ATOM	936	CE	LYS	113	-0.269	69.780	28.816	1.00	32.92	6
	ATOM	937	NZ	LYS	113	-0.196	71.075	29.554	1.00	33.55	7
	ATOM	938	C	LYS	113	4.352	66.597	31.748	1.00	19.86	6
	ATOM	939	O	LYS	113	4.890	65.603	31.264	1.00	21.45	8
20	ATOM	940	N	PRO	114	4.288	66.761	33.066	1.00	20.08	7
	ATOM	941	CD	PRO	114	3.701	67.928	33.768	1.00	16.95	6
	ATOM	942	CA	PRO	114	4.923	65.801	33.957	1.00	17.00	6
	ATOM	943	CB	PRO	114	4.548	66.292	35.342	1.00	19.22	6
	ATOM	944	CG	PRO	114	4.169	67.733	35.176	1.00	21.34	6
	ATOM	945	C	PRO	114	4.451	64.405	33.636	1.00	16.83	6
25	ATOM	946	O	PRO	114	3.237	64.125	33.512	1.00	16.01	8
	ATOM	947	N	LEU	115	5.414	63.483	33.560	1.00	15.95	7
	ATOM	948	CA	LEU	115	5.081	62.104	33.215	1.00	17.10	6
	ATOM	949	CB	LEU	115	5.769	61.879	31.856	1.00	16.83	6
30	ATOM	950	CG	LEU	115	5.790	60.498	31.231	1.00	21.64	6
	ATOM	951	CD1	LEU	115	4.399	60.132	30.733	1.00	19.24	6
	ATOM	952	CD2	LEU	115	6.777	60.486	30.043	1.00	19.80	6
	ATOM	953	C	LEU	115	5.606	61.116	34.226	1.00	21.13	6
	ATOM	954	O	LEU	115	6.788	61.200	34.569	1.00	18.84	8
35	ATOM	955	N	VAL	116	4.839	60.105	34.630	1.00	20.51	7
	ATOM	956	CA	VAL	116	5.314	59.073	35.545	1.00	20.40	6
	ATOM	957	CB	VAL	116	4.787	59.277	36.971	1.00	18.72	6
	ATOM	958	CG1	VAL	116	5.313	60.547	37.644	1.00	22.67	6
	ATOM	959	CG2	VAL	116	3.257	59.328	36.998	1.00	22.12	6
40	ATOM	960	C	VAL	116	4.807	57.703	35.073	1.00	19.73	6
	ATOM	961	O	VAL	116	3.910	57.682	34.223	1.00	20.76	8
	ATOM	962	N	LYS	117	5.268	56.615	35.693	1.00	17.34	7
	ATOM	963	CA	LYS	117	4.760	55.290	35.381	1.00	20.33	6
	ATOM	964	CB	LYS	117	3.271	55.182	35.802	1.00	21.74	6
45	ATOM	965	CG	LYS	117	3.115	54.927	37.301	1.00	24.43	6
	ATOM	966	CD	LYS	117	1.793	55.445	37.832	1.00	32.69	6
	ATOM	967	CE	LYS	117	0.798	54.314	38.056	1.00	40.27	6
	ATOM	968	NZ	LYS	117	-0.568	54.865	38.266	1.00	44.06	7
	ATOM	969	C	LYS	117	4.956	54.936	33.914	1.00	18.58	6
50	ATOM	970	O	LYS	117	4.026	54.535	33.234	1.00	24.35	8
	ATOM	971	N	VAL	118	6.181	55.063	33.417	1.00	20.45	7
	ATOM	972	CA	VAL	118	6.542	54.798	32.039	1.00	19.15	6
	ATOM	973	CB	VAL	118	7.756	55.643	31.607	1.00	12.17	6
	ATOM	974	CG1	VAL	118	8.199	55.396	30.176	1.00	18.94	6
55	ATOM	975	CG2	VAL	118	7.408	57.129	31.794	1.00	16.75	6
	ATOM	976	C	VAL	118	6.868	53.330	31.797	1.00	18.58	6
	ATOM	977	O	VAL	118	7.606	52.717	32.564	1.00	17.16	8
	ATOM	978	N	THR	119	6.307	52.803	30.711	1.00	15.94	7
	ATOM	979	CA	THR	119	6.527	51.425	30.335	1.00	16.50	6
60	ATOM	980	CB	THR	119	5.291	50.523	30.367	1.00	19.59	6
	ATOM	981	OG1	THR	119	4.770	50.410	31.693	1.00	23.11	8
	ATOM	982	CG2	THR	119	5.695	49.123	29.872	1.00	24.83	6
	ATOM	983	C	THR	119	7.053	51.424	28.881	1.00	17.81	6
	ATOM	984	O	THR	119	6.436	52.130	28.095	1.00	14.36	8
65	ATOM	985	N	PHE	120	8.121	50.679	28.643	1.00	14.86	7
	ATOM	986	CA	PHE	120	8.616	50.608	27.259	1.00	13.85	6
	ATOM	987	CB	PHE	120	10.122	50.797	27.240	1.00	15.51	6
	ATOM	988	CG	PHE	120	10.553	52.230	27.463	1.00	13.38	6
	ATOM	989	CD1	PHE	120	10.748	52.701	28.750	1.00	20.15	6
70	ATOM	990	CD2	PHE	120	10.792	53.051	26.381	1.00	20.08	6
	ATOM	991	CE1	PHE	120	11.186	54.002	28.953	1.00	17.14	6
	ATOM	992	CE2	PHE	120	11.230	54.367	26.578	1.00	22.12	6

	ATOM	993	CZ	PHE	120	11.423	54.818	27.867	1.00	17.10	6
	ATOM	994	C	PHE	120	8.279	49.216	26.721	1.00	17.13	6
	ATOM	995	O	PHE	120	8.640	48.221	27.407	1.00	14.78	8
5	ATOM	996	N	PHE	121	7.626	49.166	25.575	1.00	16.20	7
	ATOM	997	CA	PHE	121	7.277	47.868	25.011	1.00	18.83	6
	ATOM	998	CB	PHE	121	5.799	47.821	24.616	1.00	13.50	6
	ATOM	999	CG	PHE	121	4.768	48.052	25.656	1.00	18.60	6
	ATOM	1000	CD1	PHE	121	4.368	49.339	26.017	1.00	17.37	6
10	ATOM	1001	CD2	PHE	121	4.208	46.961	26.334	1.00	18.44	6
	ATOM	1002	CE1	PHE	121	3.409	49.524	27.006	1.00	19.78	6
	ATOM	1003	CE2	PHE	121	3.260	47.173	27.313	1.00	22.69	6
	ATOM	1004	CZ	PHE	121	2.843	48.445	27.660	1.00	15.74	6
	ATOM	1005	C	PHE	121	8.074	47.539	23.749	1.00	18.44	6
15	ATOM	1006	O	PHE	121	8.351	48.454	22.987	1.00	15.63	8
	ATOM	1007	N	GLN	122	8.333	46.253	23.480	1.00	19.35	7
	ATOM	1008	CA	GLN	122	8.959	45.880	22.203	1.00	19.90	6
	ATOM	1009	CB	GLN	122	10.396	45.379	22.317	1.00	16.32	6
	ATOM	1010	CG	GLN	122	10.784	44.583	21.065	1.00	18.39	6
	ATOM	1011	CD	GLN	122	12.050	43.764	21.247	1.00	21.98	6
20	ATOM	1012	OE1	GLN	122	12.423	43.461	22.374	1.00	19.18	8
	ATOM	1013	NE2	GLN	122	12.700	43.396	20.153	1.00	24.51	7
	ATOM	1014	C	GLN	122	8.067	44.774	21.609	1.00	15.34	6
	ATOM	1015	O	GLN	122	7.789	43.832	22.321	1.00	17.30	8
25	ATOM	1016	N	ASN	123	7.474	44.931	20.439	1.00	18.98	7
	ATOM	1017	CA	ASN	123	6.542	43.975	19.859	1.00	22.95	6
	ATOM	1018	CB	ASN	123	7.241	42.708	19.332	1.00	19.57	6
	ATOM	1019	CG	ASN	123	8.228	43.130	18.244	1.00	26.31	6
	ATOM	1020	OD1	ASN	123	8.013	44.053	17.441	1.00	19.76	8
30	ATOM	1021	ND2	ASN	123	9.375	42.463	18.213	1.00	28.57	7
	ATOM	1022	C	ASN	123	5.397	43.643	20.803	1.00	21.02	6
	ATOM	1023	O	ASN	123	4.911	42.525	20.918	1.00	19.19	8
	ATOM	1024	N	GLY	124	4.951	44.632	21.579	1.00	19.77	7
	ATOM	1025	CA	GLY	124	3.852	44.516	22.495	1.00	16.41	6
35	ATOM	1026	C	GLY	124	4.159	43.885	23.844	1.00	14.85	6
	ATOM	1027	O	GLY	124	3.210	43.658	24.611	1.00	15.05	8
	ATOM	1028	N	LYS	125	5.405	43.610	24.133	1.00	13.81	7
	ATOM	1029	CA	LYS	125	5.830	42.997	25.379	1.00	21.18	6
	ATOM	1030	CB	LYS	125	6.700	41.738	25.247	1.00	14.85	6
40	ATOM	1031	CG	LYS	125	6.934	41.032	26.559	1.00	16.28	6
	ATOM	1032	CD	LYS	125	7.406	39.587	26.281	1.00	22.51	6
	ATOM	1033	CE	LYS	125	7.925	38.989	27.587	1.00	30.62	6
	ATOM	1034	NZ	LYS	125	8.822	37.818	27.330	1.00	36.72	7
	ATOM	1035	C	LYS	125	6.725	44.014	26.121	1.00	18.20	6
45	ATOM	1036	O	LYS	125	7.648	44.525	25.509	1.00	19.98	8
	ATOM	1037	N	SER	126	6.385	44.216	27.393	1.00	17.62	7
	ATOM	1038	CA	SER	126	7.107	45.241	28.155	1.00	20.03	6
	ATOM	1039	CB	SER	126	6.355	45.459	29.485	1.00	23.22	6
	ATOM	1040	OG	SER	126	7.317	45.773	30.466	1.00	38.12	8
50	ATOM	1041	C	SER	126	8.541	44.823	28.389	1.00	17.85	6
	ATOM	1042	O	SER	126	8.842	43.657	28.647	1.00	21.31	8
	ATOM	1043	N	GLN	127	9.490	45.718	28.254	1.00	17.16	7
	ATOM	1044	CA	GLN	127	10.898	45.515	28.408	1.00	17.45	6
	ATOM	1045	CB	GLN	127	11.723	46.073	27.225	1.00	20.82	6
55	ATOM	1046	CG	GLN	127	11.352	45.419	25.897	1.00	18.56	6
	ATOM	1047	CD	GLN	127	11.497	43.912	25.927	1.00	24.44	6
	ATOM	1048	OE1	GLN	127	12.606	43.416	26.116	1.00	31.62	8
	ATOM	1049	NE2	GLN	127	10.436	43.130	25.773	1.00	19.15	7
	ATOM	1050	C	GLN	127	11.386	46.251	29.661	1.00	20.94	6
60	ATOM	1051	O	GLN	127	12.439	45.929	30.179	1.00	18.25	8
	ATOM	1052	N	LYS	128	10.643	47.285	30.032	1.00	21.18	7
	ATOM	1053	CA	LYS	128	11.070	48.048	31.216	1.00	23.10	6
	ATOM	1054	CB	LYS	128	12.177	49.034	30.842	1.00	21.83	6
	ATOM	1055	CG	LYS	128	12.683	49.882	32.013	1.00	24.67	6
65	ATOM	1056	CD	LYS	128	13.739	50.905	31.589	1.00	18.23	6
	ATOM	1057	CE	LYS	128	14.048	51.746	32.870	1.00	27.02	6
	ATOM	1058	NZ	LYS	128	15.081	52.794	32.574	1.00	24.24	7
	ATOM	1059	C	LYS	128	9.884	48.844	31.754	1.00	24.93	6
	ATOM	1060	O	LYS	128	9.193	49.481	30.960	1.00	20.79	8
70	ATOM	1061	N	PHE	129	9.678	48.822	33.062	1.00	21.39	7
	ATOM	1062	CA	PHE	129	8.708	49.695	33.695	1.00	24.45	6
	ATOM	1063	CB	PHE	129	7.610	48.926	34.458	1.00	25.50	6

	ATOM	1064	CG	PHE	129	6.772	49.837	35.327	1.00	25.51	6
	ATOM	1065	CD1	PHE	129	5.799	50.630	34.762	1.00	19.40	6
	ATOM	1066	CD2	PHE	129	7.002	49.928	36.700	1.00	29.98	6
5	ATOM	1067	CE1	PHE	129	5.026	51.491	35.535	1.00	25.00	6
	ATOM	1068	CE2	PHE	129	6.249	50.788	37.491	1.00	28.84	6
	ATOM	1069	CZ	PHE	129	5.262	51.574	36.902	1.00	32.29	6
	ATOM	1070	C	PHE	129	9.480	50.577	34.687	1.00	27.88	6
	ATOM	1071	O	PHE	129	10.388	50.049	35.359	1.00	30.99	8
10	ATOM	1072	N	SER	130	9.134	51.846	34.853	1.00	26.67	7
	ATOM	1073	CA	SER	130	9.779	52.641	35.917	1.00	24.98	6
	ATOM	1074	CB	SER	130	11.025	53.344	35.422	1.00	21.29	6
	ATOM	1075	OG	SER	130	11.271	54.465	36.250	1.00	25.72	8
	ATOM	1076	C	SER	130	8.777	53.667	36.434	1.00	24.39	6
	ATOM	1077	O	SER	130	8.123	54.285	35.576	1.00	24.91	8
15	ATOM	1078	N	HIS	131	8.668	53.889	37.730	1.00	22.12	7
	ATOM	1079	CA	HIS	131	7.710	54.901	38.204	1.00	23.65	6
	ATOM	1080	CB	HIS	131	7.604	54.918	39.737	1.00	28.35	6
	ATOM	1081	CG	HIS	131	6.859	53.706	40.197	1.00	23.57	6
20	ATOM	1082	CD2	HIS	131	7.307	52.509	40.642	1.00	18.55	6
	ATOM	1083	ND1	HIS	131	5.478	53.666	40.170	1.00	26.69	7
	ATOM	1084	CE1	HIS	131	5.095	52.478	40.617	1.00	16.65	6
	ATOM	1085	NE2	HIS	131	6.173	51.764	40.890	1.00	23.94	7
	ATOM	1086	C	HIS	131	8.108	56.314	37.814	1.00	23.89	6
25	ATOM	1087	O	HIS	131	7.261	57.205	37.712	1.00	26.21	8
	ATOM	1088	N	LEU	132	9.426	56.548	37.689	1.00	21.77	7
	ATOM	1089	CA	LEU	132	9.886	57.900	37.480	1.00	20.70	6
	ATOM	1090	CB	LEU	132	10.630	58.361	38.760	1.00	30.28	6
	ATOM	1091	CG	LEU	132	10.022	58.084	40.148	1.00	26.56	6
30	ATOM	1092	CD1	LEU	132	11.073	58.316	41.229	1.00	29.07	6
	ATOM	1093	CD2	LEU	132	8.814	58.980	40.435	1.00	24.99	6
	ATOM	1094	C	LEU	132	10.762	58.144	36.279	1.00	22.94	6
	ATOM	1095	O	LEU	132	10.794	59.326	35.900	1.00	22.01	8
	ATOM	1096	N	ASP	133	11.541	57.181	35.778	1.00	21.75	7
35	ATOM	1097	CA	ASP	133	12.469	57.401	34.679	1.00	24.62	6
	ATOM	1098	CB	ASP	133	13.560	56.327	34.854	1.00	29.71	6
	ATOM	1099	CG	ASP	133	14.734	56.321	33.915	1.00	32.90	6
	ATOM	1100	OD1	ASP	133	14.837	57.254	33.083	1.00	32.91	8
	ATOM	1101	OD2	ASP	133	15.597	55.394	34.000	1.00	36.01	8
40	ATOM	1102	C	ASP	133	11.843	57.230	33.296	1.00	25.88	6
	ATOM	1103	O	ASP	133	11.419	56.136	32.940	1.00	24.36	8
	ATOM	1104	N	PRO	134	11.857	58.261	32.460	1.00	24.65	7
	ATOM	1105	CD	PRO	134	12.347	59.620	32.778	1.00	22.97	6
	ATOM	1106	CA	PRO	134	11.293	58.185	31.112	1.00	24.00	6
45	ATOM	1107	CB	PRO	134	10.889	59.662	30.870	1.00	24.02	6
	ATOM	1108	CG	PRO	134	11.987	60.433	31.544	1.00	23.04	6
	ATOM	1109	C	PRO	134	12.256	57.764	30.017	1.00	22.11	6
	ATOM	1110	O	PRO	134	11.970	57.930	28.824	1.00	19.00	8
50	ATOM	1111	N	THR	135	13.420	57.212	30.350	1.00	21.43	7
	ATOM	1112	CA	THR	135	14.424	56.805	29.401	1.00	24.98	6
	ATOM	1113	CB	THR	135	15.748	57.584	29.593	1.00	27.24	6
	ATOM	1114	OG1	THR	135	16.331	57.065	30.796	1.00	24.99	8
	ATOM	1115	CG2	THR	135	15.461	59.069	29.706	1.00	26.07	6
	ATOM	1116	C	THR	135	14.747	55.312	29.451	1.00	23.58	6
55	ATOM	1117	O	THR	135	14.445	54.629	30.423	1.00	26.14	8
	ATOM	1118	N	PHE	136	15.267	54.790	28.347	1.00	20.63	7
	ATOM	1119	CA	PHE	136	15.549	53.391	28.150	1.00	20.10	6
	ATOM	1120	CB	PHE	136	14.343	52.706	27.523	1.00	25.47	6
	ATOM	1121	CG	PHE	136	14.408	51.250	27.170	1.00	25.61	6
60	ATOM	1122	CD1	PHE	136	14.528	50.270	28.121	1.00	27.00	6
	ATOM	1123	CD2	PHE	136	14.332	50.847	25.841	1.00	27.45	6
	ATOM	1124	CE1	PHE	136	14.571	48.929	27.787	1.00	32.62	6
	ATOM	1125	CE2	PHE	136	14.385	49.516	25.490	1.00	28.46	6
	ATOM	1126	CZ	PHE	136	14.493	48.549	26.463	1.00	30.41	6
65	ATOM	1127	C	PHE	136	16.796	53.197	27.297	1.00	24.00	6
	ATOM	1128	O	PHE	136	16.952	53.801	26.230	1.00	24.50	8
	ATOM	1129	N	SER	137	17.665	52.294	27.730	1.00	21.97	7
	ATOM	1130	CA	SER	137	18.914	52.010	27.050	1.00	26.52	6
	ATOM	1131	CB	SER	137	20.120	52.418	27.908	1.00	30.03	6
70	ATOM	1132	OG	SER	137	20.769	53.559	27.412	1.00	44.19	8
	ATOM	1133	C	SER	137	19.128	50.507	26.840	1.00	27.38	6
	ATOM	1134	O	SER	137	18.911	49.694	27.721	1.00	27.33	8

	ATOM	1135	N	ILE	138	19.654	50.164	25.686	1.00	25.86	7
	ATOM	1136	CA	ILE	138	20.004	48.806	25.343	1.00	29.46	6
	ATOM	1137	CB	ILE	138	19.189	48.176	24.193	1.00	33.38	6
5	ATOM	1138	CG2	ILE	138	19.669	46.748	23.941	1.00	27.23	6
	ATOM	1139	CG1	ILE	138	17.679	48.197	24.472	1.00	30.55	6
	ATOM	1140	CD1	ILE	138	16.817	48.155	23.223	1.00	29.53	6
	ATOM	1141	C	ILE	138	21.477	48.875	24.926	1.00	29.88	6
	ATOM	1142	O	ILE	138	21.768	49.377	23.849	1.00	27.99	8
10	ATOM	1143	N	PRO	139	22.345	48.476	25.837	1.00	31.71	7
	ATOM	1144	CD	PRO	139	22.018	47.938	27.184	1.00	32.73	6
	ATOM	1145	CA	PRO	139	23.776	48.398	25.598	1.00	33.85	6
	ATOM	1146	CB	PRO	139	24.380	48.213	26.983	1.00	36.13	6
	ATOM	1147	CG	PRO	139	23.248	48.384	27.950	1.00	34.99	6
15	ATOM	1148	C	PRO	139	24.030	47.160	24.741	1.00	35.63	6
	ATOM	1149	O	PRO	139	23.324	46.160	24.888	1.00	38.22	8
	ATOM	1150	N	GLN	140	24.974	47.208	23.827	1.00	36.97	7
	ATOM	1151	CA	GLN	140	25.288	46.110	22.935	1.00	35.17	6
	ATOM	1152	CB	GLN	140	26.223	45.124	23.631	1.00	43.87	6
20	ATOM	1153	CG	GLN	140	27.518	45.802	24.088	1.00	49.77	6
	ATOM	1154	CD	GLN	140	27.883	45.282	25.468	1.00	56.21	6
	ATOM	1155	OE1	GLN	140	28.145	44.084	25.593	1.00	57.44	8
	ATOM	1156	NE2	GLN	140	27.883	46.161	26.468	1.00	57.25	7
	ATOM	1157	C	GLN	140	24.060	45.418	22.362	1.00	34.61	6
25	ATOM	1158	O	GLN	140	23.677	44.284	22.693	1.00	33.34	8
	ATOM	1159	N	ALA	141	23.473	46.111	21.391	1.00	29.80	7
	ATOM	1160	CA	ALA	141	22.287	45.634	20.694	1.00	30.02	6
	ATOM	1161	CB	ALA	141	21.778	46.745	19.774	1.00	27.89	6
	ATOM	1162	C	ALA	141	22.561	44.400	19.832	1.00	29.52	6
30	ATOM	1163	O	ALA	141	23.650	44.270	19.263	1.00	29.60	8
	ATOM	1164	N	ASN	142	21.528	43.582	19.665	1.00	30.60	7
	ATOM	1165	CA	ASN	142	21.642	42.435	18.738	1.00	31.55	6
	ATOM	1166	CB	ASN	142	21.985	41.139	19.453	1.00	30.39	6
	ATOM	1167	CG	ASN	142	21.012	40.749	20.534	1.00	31.63	6
35	ATOM	1168	OD1	ASN	142	19.838	40.423	20.268	1.00	27.57	8
	ATOM	1169	ND2	ASN	142	21.479	40.739	21.781	1.00	33.23	7
	ATOM	1170	C	ASN	142	20.357	42.321	17.936	1.00	32.33	6
	ATOM	1171	O	ASN	142	19.453	43.168	18.122	1.00	29.09	8
	ATOM	1172	N	HIS	143	20.223	41.257	17.134	1.00	29.40	7
40	ATOM	1173	CA	HIS	143	19.075	41.086	16.266	1.00	28.82	6
	ATOM	1174	CB	HIS	143	19.262	39.895	15.272	1.00	24.51	6
	ATOM	1175	CG	HIS	143	20.360	40.234	14.295	1.00	31.72	6
	ATOM	1176	CD2	HIS	143	20.704	41.420	13.740	1.00	33.88	6
	ATOM	1177	ND1	HIS	143	21.278	39.328	13.822	1.00	32.86	7
45	ATOM	1178	CE1	HIS	143	22.117	39.927	13.008	1.00	31.84	6
	ATOM	1179	NE2	HIS	143	21.794	41.202	12.941	1.00	31.48	7
	ATOM	1180	C	HIS	143	17.747	40.857	16.976	1.00	26.62	6
	ATOM	1181	O	HIS	143	16.696	41.098	16.366	1.00	25.96	8
	ATOM	1182	N	SER	144	17.812	40.412	18.221	1.00	20.85	7
50	ATOM	1183	CA	SER	144	16.557	40.128	18.941	1.00	24.82	6
	ATOM	1184	CB	SER	144	16.839	38.979	19.915	1.00	30.28	6
	ATOM	1185	OG	SER	144	17.739	39.389	20.930	1.00	39.11	8
	ATOM	1186	C	SER	144	15.976	41.423	19.474	1.00	24.89	6
	ATOM	1187	O	SER	144	14.775	41.518	19.755	1.00	25.22	8
55	ATOM	1188	N	HIS	145	16.746	42.522	19.463	1.00	20.33	7
	ATOM	1189	CA	HIS	145	16.306	43.861	19.811	1.00	19.38	6
	ATOM	1190	CB	HIS	145	17.474	44.762	20.302	1.00	19.40	6
	ATOM	1191	CG	HIS	145	18.145	44.212	21.534	1.00	18.37	6
	ATOM	1192	CD2	HIS	145	17.620	43.886	22.744	1.00	18.22	6
60	ATOM	1193	ND1	HIS	145	19.493	43.965	21.627	1.00	23.55	7
	ATOM	1194	CE1	HIS	145	19.768	43.492	22.829	1.00	26.33	6
	ATOM	1195	NE2	HIS	145	18.643	43.412	23.525	1.00	21.05	7
	ATOM	1196	C	HIS	145	15.589	44.553	18.657	1.00	22.05	6
	ATOM	1197	O	HIS	145	15.013	45.636	18.848	1.00	21.86	8
65	ATOM	1198	N	SER	146	15.569	43.997	17.440	1.00	20.66	7
	ATOM	1199	CA	SER	146	14.833	44.649	16.363	1.00	19.96	6
	ATOM	1200	CB	SER	146	15.075	44.009	14.986	1.00	20.48	6
	ATOM	1201	OG	SER	146	16.442	44.154	14.613	1.00	25.61	8
	ATOM	1202	C	SER	146	13.339	44.596	16.656	1.00	20.51	6
70	ATOM	1203	O	SER	146	12.915	43.614	17.287	1.00	22.06	8
	ATOM	1204	N	GLY	147	12.556	45.578	16.197	1.00	16.70	7
	ATOM	1205	CA	GLY	147	11.123	45.383	16.411	1.00	20.49	6

	ATOM	1206	C	GLY	147	10.385	46.714	16.555	1.00	22.63	6
	ATOM	1207	O	GLY	147	10.982	47.762	16.332	1.00	16.09	8
	ATOM	1208	N	ASP	148	9.111	46.560	16.951	1.00	20.62	7
5	ATOM	1209	CA	ASP	148	8.324	47.777	17.121	1.00	21.57	6
	ATOM	1210	CB	ASP	148	6.882	47.579	16.674	1.00	28.99	6
	ATOM	1211	CG	ASP	148	6.819	47.144	15.219	1.00	41.07	6
	ATOM	1212	OD1	ASP	148	7.849	47.338	14.540	1.00	39.21	8
	ATOM	1213	OD2	ASP	148	5.763	46.620	14.808	1.00	39.40	8
10	ATOM	1214	C	ASP	148	8.315	48.214	18.590	1.00	20.72	6
	ATOM	1215	O	ASP	148	7.817	47.469	19.447	1.00	20.27	8
	ATOM	1216	N	TYR	149	8.822	49.440	18.798	1.00	16.97	7
	ATOM	1217	CA	TYR	149	8.811	49.966	20.164	1.00	18.60	6
	ATOM	1218	CB	TYR	149	10.193	50.587	20.472	1.00	16.94	6
	ATOM	1219	CG	TYR	149	11.272	49.534	20.606	1.00	18.45	6
15	ATOM	1220	CD1	TYR	149	11.901	48.928	19.528	1.00	19.27	6
	ATOM	1221	CE1	TYR	149	12.877	47.948	19.737	1.00	20.18	6
	ATOM	1222	CD2	TYR	149	11.672	49.162	21.879	1.00	18.36	6
	ATOM	1223	CE2	TYR	149	12.636	48.216	22.116	1.00	15.60	6
	ATOM	1224	CZ	TYR	149	13.238	47.606	21.027	1.00	18.77	6
20	ATOM	1225	OH	TYR	149	14.211	46.660	21.253	1.00	18.41	8
	ATOM	1226	C	TYR	149	7.767	51.061	20.355	1.00	15.78	6
	ATOM	1227	O	TYR	149	7.539	51.859	19.450	1.00	15.86	8
	ATOM	1228	N	HIS	150	7.196	51.126	21.559	1.00	15.01	7
25	ATOM	1229	CA	HIS	150	6.247	52.171	21.925	1.00	12.99	6
	ATOM	1230	CB	HIS	150	4.849	51.980	21.372	1.00	11.96	6
	ATOM	1231	CG	HIS	150	3.942	51.032	22.117	1.00	17.71	6
	ATOM	1232	CD2	HIS	150	2.944	51.295	23.004	1.00	16.09	6
	ATOM	1233	ND1	HIS	150	3.988	49.660	21.971	1.00	11.60	7
	ATOM	1234	CE1	HIS	150	3.058	49.103	22.716	1.00	16.95	6
30	ATOM	1235	NE2	HIS	150	2.407	50.057	23.370	1.00	19.22	7
	ATOM	1236	C	HIS	150	6.263	52.270	23.462	1.00	13.37	6
	ATOM	1237	O	HIS	150	6.922	51.448	24.129	1.00	12.78	8
	ATOM	1238	N	CYS	151	5.680	53.355	23.957	1.00	14.21	7
35	ATOM	1239	CA	CYS	151	5.670	53.559	25.414	1.00	15.38	6
	ATOM	1240	C	CYS	151	4.301	53.982	25.880	1.00	16.27	6
	ATOM	1241	O	CYS	151	3.422	54.404	25.132	1.00	15.15	8
	ATOM	1242	CB	CYS	151	6.746	54.562	25.856	1.00	16.85	6
	ATOM	1243	SG	CYS	151	6.581	56.269	25.248	1.00	14.82	16
40	ATOM	1244	N	THR	152	4.080	53.805	27.186	1.00	17.41	7
	ATOM	1245	CA	THR	152	2.875	54.223	27.862	1.00	17.27	6
	ATOM	1246	CB	THR	152	1.899	53.131	28.305	1.00	21.80	6
	ATOM	1247	OG1	THR	152	2.527	52.212	29.205	1.00	17.53	8
	ATOM	1248	CG2	THR	152	1.356	52.388	27.075	1.00	17.12	6
45	ATOM	1249	C	THR	152	3.346	54.989	29.127	1.00	19.83	6
	ATOM	1250	O	THR	152	4.471	54.724	29.600	1.00	16.21	8
	ATOM	1251	N	GLY	153	2.496	55.913	29.534	1.00	17.84	7
	ATOM	1252	CA	GLY	153	2.815	56.706	30.731	1.00	20.33	6
	ATOM	1253	C	GLY	153	1.647	57.605	31.108	1.00	18.60	6
50	ATOM	1254	O	GLY	153	0.779	57.915	30.293	1.00	19.87	8
	ATOM	1255	N	ASN	154	1.603	58.000	32.373	1.00	20.99	7
	ATOM	1256	CA	ASN	154	0.560	58.815	32.959	1.00	20.36	6
	ATOM	1257	CB	ASN	154	0.512	58.556	34.478	1.00	26.77	6
	ATOM	1258	CG	ASN	154	-0.800	57.928	34.897	1.00	40.91	6
55	ATOM	1259	OD1	ASN	154	-1.700	58.580	35.441	1.00	46.67	8
	ATOM	1260	ND2	ASN	154	-0.927	56.639	34.633	1.00	40.24	7
	ATOM	1261	C	ASN	154	0.879	60.300	32.817	1.00	22.51	6
	ATOM	1262	O	ASN	154	1.973	60.685	33.272	1.00	22.15	8
	ATOM	1263	N	ILE	155	-0.018	61.067	32.202	1.00	19.40	7
60	ATOM	1264	CA	ILE	155	0.198	62.514	32.139	1.00	22.27	6
	ATOM	1265	CB	ILE	155	0.210	63.116	30.731	1.00	26.29	6
	ATOM	1266	CG2	ILE	155	0.327	64.640	30.831	1.00	23.31	6
	ATOM	1267	CG1	ILE	155	1.367	62.544	29.899	1.00	28.16	6
	ATOM	1268	CD1	ILE	155	1.371	62.874	28.434	1.00	29.42	6
65	ATOM	1269	C	ILE	155	-0.974	63.089	32.941	1.00	27.67	6
	ATOM	1270	O	ILE	155	-2.112	62.726	32.639	1.00	24.10	8
	ATOM	1271	N	GLY	156	-0.732	63.838	34.020	1.00	33.10	7
	ATOM	1272	CA	GLY	156	-1.942	64.285	34.780	1.00	37.62	6
	ATOM	1273	C	GLY	156	-2.447	63.053	35.527	1.00	38.80	6
	ATOM	1274	O	GLY	156	-1.659	62.512	36.299	1.00	43.91	8
70	ATOM	1275	N	TYR	157	-3.655	62.573	35.307	1.00	41.47	7
	ATOM	1276	CA	TYR	157	-4.182	61.357	35.894	1.00	43.65	6

	ATOM	1277	CB	TYR	157	-5.381	61.642	36.832	1.00	51.51	6
	ATOM	1278	CG	TYR	157	-5.020	62.592	37.961	1.00	57.42	6
	ATOM	1279	CD1	TYR	157	-5.523	63.885	37.982	1.00	60.45	6
5	ATOM	1280	CE1	TYR	157	-5.179	64.765	38.992	1.00	62.57	6
	ATOM	1281	CD2	TYR	157	-4.140	62.204	38.963	1.00	61.00	6
	ATOM	1282	CE2	TYR	157	-3.788	63.079	39.982	1.00	63.03	6
	ATOM	1283	CZ	TYR	157	-4.313	64.353	39.986	1.00	63.56	6
	ATOM	1284	OH	TYR	157	-3.979	65.237	40.984	1.00	66.68	8
10	ATOM	1285	C	TYR	157	-4.676	60.351	34.849	1.00	41.96	6
	ATOM	1286	O	TYR	157	-5.445	59.420	35.115	1.00	41.33	8
	ATOM	1287	N	THR	158	-4.298	60.547	33.594	1.00	36.77	7
	ATOM	1288	CA	THR	158	-4.722	59.693	32.496	1.00	30.71	6
	ATOM	1289	CB	THR	158	-5.260	60.597	31.364	1.00	30.82	6
15	ATOM	1290	OG1	THR	158	-6.237	61.471	31.942	1.00	30.47	8
	ATOM	1291	CG2	THR	158	-5.851	59.819	30.207	1.00	29.21	6
	ATOM	1292	C	THR	158	-3.532	58.944	31.912	1.00	25.66	6
	ATOM	1293	O	THR	158	-2.521	59.609	31.642	1.00	24.50	8
	ATOM	1294	N	LEU	159	-3.689	57.664	31.609	1.00	21.00	7
20	ATOM	1295	CA	LEU	159	-2.617	56.924	30.960	1.00	21.01	6
	ATOM	1296	CB	LEU	159	-2.737	55.435	31.284	1.00	26.53	6
	ATOM	1297	CG	LEU	159	-1.601	54.487	30.958	1.00	27.15	6
	ATOM	1298	CD1	LEU	159	-0.323	54.817	31.713	1.00	25.15	6
	ATOM	1299	CD2	LEU	159	-1.979	53.036	31.316	1.00	28.75	6
25	ATOM	1300	C	LEU	159	-2.654	57.179	29.461	1.00	22.04	6
	ATOM	1301	O	LEU	159	-3.711	57.248	28.844	1.00	22.64	8
	ATOM	1302	N	PHE	160	-1.484	57.396	28.855	1.00	20.79	7
	ATOM	1303	CA	PHE	160	-1.430	57.576	27.409	1.00	19.10	6
	ATOM	1304	CB	PHE	160	-0.821	58.946	27.060	1.00	20.91	6
30	ATOM	1305	CG	PHE	160	-1.848	60.034	27.216	1.00	19.50	6
	ATOM	1306	CD1	PHE	160	-1.971	60.676	28.442	1.00	24.86	6
	ATOM	1307	CD2	PHE	160	-2.645	60.409	26.156	1.00	21.03	6
	ATOM	1308	CE1	PHE	160	-2.903	61.709	28.588	1.00	29.44	6
	ATOM	1309	CE2	PHE	160	-3.582	61.421	26.296	1.00	19.89	6
35	ATOM	1310	CZ	PHE	160	-3.704	62.074	27.529	1.00	25.34	6
	ATOM	1311	C	PHE	160	-0.521	56.513	26.794	1.00	17.36	6
	ATOM	1312	O	PHE	160	0.346	55.982	27.504	1.00	18.36	8
	ATOM	1313	N	SER	161	-0.753	56.240	25.521	1.00	17.60	7
	ATOM	1314	CA	SER	161	0.087	55.302	24.785	1.00	14.63	6
40	ATOM	1315	CB	SER	161	-0.744	54.150	24.188	1.00	20.14	6
	ATOM	1316	OG	SER	161	0.115	53.054	23.901	1.00	21.55	8
	ATOM	1317	C	SER	161	0.662	56.037	23.561	1.00	18.96	6
	ATOM	1318	O	SER	161	-0.101	56.753	22.894	1.00	19.79	8
	ATOM	1319	N	SER	162	1.921	55.796	23.232	1.00	16.19	7
45	ATOM	1320	CA	SER	162	2.518	56.404	22.049	1.00	16.74	6
	ATOM	1321	CB	SER	162	4.029	56.678	22.233	1.00	16.78	6
	ATOM	1322	OG	SER	162	4.801	55.530	21.900	1.00	21.00	8
	ATOM	1323	C	SER	162	2.322	55.485	20.845	1.00	18.24	6
	ATOM	1324	O	SER	162	1.949	54.305	20.987	1.00	16.85	8
50	ATOM	1325	N	LYS	163	2.535	56.027	19.652	1.00	17.96	7
	ATOM	1326	CA	LYS	163	2.484	55.203	18.445	1.00	17.36	6
	ATOM	1327	CB	LYS	163	2.369	55.957	17.133	1.00	20.94	6
	ATOM	1328	CG	LYS	163	1.228	56.885	16.902	1.00	25.34	6
	ATOM	1329	CD	LYS	163	-0.128	56.271	16.685	1.00	29.02	6
55	ATOM	1330	CE	LYS	163	-0.954	57.131	15.721	1.00	42.35	6
	ATOM	1331	NZ	LYS	163	-0.495	58.558	15.692	1.00	38.14	7
	ATOM	1332	C	LYS	163	3.821	54.466	18.391	1.00	17.27	6
	ATOM	1333	O	LYS	163	4.817	54.906	18.978	1.00	16.54	8
	ATOM	1334	N	PRO	164	3.840	53.348	17.696	1.00	18.39	7
60	ATOM	1335	CD	PRO	164	2.702	52.743	16.952	1.00	20.79	6
	ATOM	1336	CA	PRO	164	5.060	52.572	17.546	1.00	19.84	6
	ATOM	1337	CB	PRO	164	4.545	51.177	17.142	1.00	17.33	6
	ATOM	1338	CG	PRO	164	3.254	51.416	16.475	1.00	21.76	6
	ATOM	1339	C	PRO	164	6.032	53.169	16.528	1.00	19.62	6
65	ATOM	1340	O	PRO	164	5.723	53.942	15.619	1.00	19.46	8
	ATOM	1341	N	VAL	165	7.295	52.833	16.674	1.00	17.22	7
	ATOM	1342	CA	VAL	165	8.427	53.162	15.841	1.00	20.36	6
	ATOM	1343	CB	VAL	165	9.405	54.190	16.450	1.00	20.84	6
	ATOM	1344	CG1	VAL	165	10.418	54.643	15.404	1.00	20.46	6
	ATOM	1345	CG2	VAL	165	8.699	55.475	16.899	1.00	23.72	6
70	ATOM	1346	C	VAL	165	9.173	51.833	15.590	1.00	22.05	6
	ATOM	1347	O	VAL	165	9.532	51.094	16.499	1.00	22.10	8

	ATOM	1348	N	THR	166	9.444	51.549	14.320	1.00	24.93	7
	ATOM	1349	CA	THR	166	10.111	50.317	13.939	1.00	26.07	6
	ATOM	1350	CB	THR	166	9.631	49.784	12.579	1.00	31.66	6
5	ATOM	1351	OG1	THR	166	9.737	50.811	11.569	1.00	38.39	8
	ATOM	1352	CG2	THR	166	8.180	49.353	12.694	1.00	23.71	6
	ATOM	1353	C	THR	166	11.611	50.597	13.909	1.00	25.06	6
	ATOM	1354	O	THR	166	11.985	51.536	13.244	1.00	21.88	8
	ATOM	1355	N	ILE	167	12.362	49.878	14.714	1.00	21.40	7
10	ATOM	1356	CA	ILE	167	13.784	49.907	14.909	1.00	25.06	6
	ATOM	1357	CB	ILE	167	14.088	50.164	16.424	1.00	26.21	6
	ATOM	1358	CG2	ILE	167	15.588	50.159	16.673	1.00	26.68	6
	ATOM	1359	CG1	ILE	167	13.415	51.472	16.825	1.00	26.56	6
	ATOM	1360	CD1	ILE	167	13.946	52.318	17.939	1.00	30.83	6
15	ATOM	1361	C	ILE	167	14.416	48.572	14.501	1.00	24.36	6
	ATOM	1362	O	ILE	167	14.013	47.482	14.920	1.00	23.36	8
	ATOM	1363	N	THR	168	15.412	48.591	13.630	1.00	22.83	7
	ATOM	1364	CA	THR	168	16.083	47.405	13.152	1.00	27.27	6
	ATOM	1365	CB	THR	168	15.945	47.266	11.622	1.00	31.88	6
20	ATOM	1366	OG1	THR	168	14.565	47.371	11.277	1.00	32.11	8
	ATOM	1367	CG2	THR	168	16.462	45.894	11.179	1.00	34.54	6
	ATOM	1368	C	THR	168	17.575	47.414	13.501	1.00	28.53	6
	ATOM	1369	O	THR	168	18.190	48.483	13.508	1.00	32.64	8
	ATOM	1370	N	VAL	169	18.090	46.260	13.863	1.00	23.55	7
25	ATOM	1371	CA	VAL	169	19.472	46.011	14.163	1.00	27.27	6
	ATOM	1372	CB	VAL	169	19.728	45.359	15.523	1.00	28.51	6
	ATOM	1373	CG1	VAL	169	21.227	45.133	15.757	1.00	26.42	6
	ATOM	1374	CG2	VAL	169	19.189	46.160	16.696	1.00	27.97	6
	ATOM	1375	C	VAL	169	20.011	45.022	13.098	1.00	32.65	6
30	ATOM	1376	O	VAL	169	19.332	44.056	12.710	1.00	33.21	8
	ATOM	1377	N	GLN	170	21.245	45.196	12.689	0.01	33.85	7
	ATOM	1378	CA	GLN	170	21.966	44.390	11.737	0.01	35.75	6
	ATOM	1379	CB	GLN	170	23.335	44.027	12.362	0.01	36.48	6
	ATOM	1380	CG	GLN	170	24.465	44.012	11.347	0.01	37.54	6
35	ATOM	1381	CD	GLN	170	25.478	45.110	11.599	0.01	37.91	6
	ATOM	1382	OE1	GLN	170	25.142	46.186	12.096	0.01	38.17	8
	ATOM	1383	NE2	GLN	170	26.735	44.846	11.257	0.01	38.21	7
	ATOM	1384	C	GLN	170	21.355	43.088	11.241	0.01	36.70	6
	ATOM	1385	O	GLN	170	21.049	42.167	11.995	0.01	36.81	8
40	ATOM	1386	N	VAL	171	21.273	42.959	9.919	0.01	37.51	7
	ATOM	1387	CA	VAL	171	20.781	41.772	9.240	0.01	38.20	6
	ATOM	1388	CB	VAL	171	19.483	41.208	9.842	0.01	38.61	6
	ATOM	1389	CG1	VAL	171	18.334	42.199	9.681	0.01	38.88	6
	ATOM	1390	CG2	VAL	171	19.115	39.881	9.180	0.01	38.83	6
45	ATOM	1391	C	VAL	171	20.587	42.048	7.750	0.01	38.42	6
	ATOM	1392	O	VAL	171	21.420	41.573	6.949	0.01	38.53	8
	ATOM	1393	OWO	WAT	201	13.958	68.106	19.930	1.00	18.36	8
	ATOM	1394	OWO	WAT	202	13.653	41.241	23.320	1.00	24.59	8
	ATOM	1395	OWO	WAT	203	5.895	57.410	18.965	1.00	14.14	8
50	ATOM	1396	OWO	WAT	204	9.519	72.688	30.514	1.00	42.11	8
	ATOM	1397	OWO	WAT	205	8.700	64.454	28.355	1.00	21.65	8
	ATOM	1398	OWO	WAT	206	25.548	65.664	7.898	1.00	24.88	8
	ATOM	1399	OWO	WAT	207	2.902	52.471	31.897	1.00	19.13	8
	ATOM	1400	OWO	WAT	208	14.303	45.256	23.676	1.00	24.28	8
55	ATOM	1401	OWO	WAT	209	10.371	62.552	29.076	1.00	27.73	8
	ATOM	1402	OWO	WAT	210	12.433	66.629	21.505	1.00	14.04	8
	ATOM	1403	OWO	WAT	211	5.417	47.499	21.002	1.00	16.89	8
	ATOM	1404	OWO	WAT	212	29.599	82.797	11.595	1.00	34.62	8
	ATOM	1405	OWO	WAT	213	17.813	70.187	2.648	1.00	16.34	8
60	ATOM	1406	OWO	WAT	214	6.656	58.315	16.413	1.00	24.31	8
	ATOM	1407	OWO	WAT	215	21.191	80.146	5.335	1.00	30.05	8
	ATOM	1408	OWO	WAT	216	15.621	66.766	18.319	1.00	18.82	8
	ATOM	1409	OWO	WAT	217	6.528	56.410	14.460	1.00	26.68	8
	ATOM	1410	OWO	WAT	218	6.213	69.723	22.792	1.00	19.89	8
65	ATOM	1411	OWO	WAT	219	12.935	67.874	24.109	1.00	29.95	8
	ATOM	1412	OWO	WAT	220	-2.277	62.236	20.953	1.00	28.34	8
	ATOM	1413	OWO	WAT	221	20.151	71.344	0.183	1.00	21.62	8
	ATOM	1414	OWO	WAT	222	27.773	65.203	6.295	1.00	20.74	8
	ATOM	1415	OWO	WAT	223	-0.481	58.864	19.811	1.00	24.67	8
	ATOM	1416	OWO	WAT	224	17.815	67.914	1.120	1.00	26.99	8
70	ATOM	1417	OWO	WAT	225	16.604	64.761	25.523	1.00	18.45	8
	ATOM	1418	OWO	WAT	226	-0.330	59.580	22.516	1.00	29.01	8

90

	ATOM	1419	OWO	WAT	227	13.324	40.955	17.129	1.00	40.98	8
	ATOM	1420	OWO	WAT	228	9.214	41.380	22.450	1.00	41.91	8
	ATOM	1421	OWO	WAT	229	20.146	82.270	13.850	1.00	50.03	8
5	ATOM	1422	OWO	WAT	230	21.707	80.353	12.325	1.00	18.46	8
	ATOM	1423	OWO	WAT	231	15.403	67.167	25.599	1.00	21.44	8
	ATOM	1424	OWO	WAT	232	12.703	63.258	30.174	1.00	37.28	8
	ATOM	1425	OWO	WAT	233	12.479	61.400	39.250	1.00	23.78	8
	ATOM	1426	OWO	WAT	234	13.921	59.460	9.106	1.00	40.49	8
10	ATOM	1427	OWO	WAT	235	7.230	72.381	24.432	1.00	41.81	8
	ATOM	1428	OWO	WAT	236	2.989	58.681	19.344	1.00	17.29	8
	ATOM	1429	OWO	WAT	237	12.865	75.036	10.180	1.00	47.19	8
	ATOM	1430	OWO	WAT	238	2.754	67.991	13.259	1.00	35.75	8
	ATOM	1431	OWO	WAT	239	17.416	57.608	26.641	1.00	32.09	8
	ATOM	1432	OWO	WAT	240	31.068	75.579	10.888	1.00	20.85	8
15	ATOM	1433	OWO	WAT	241	17.725	71.985	21.261	1.00	25.43	8
	ATOM	1434	OWO	WAT	242	32.760	65.251	6.079	1.00	38.04	8
	ATOM	1435	OWO	WAT	243	14.079	72.373	25.218	1.00	20.23	8
	ATOM	1436	OWO	WAT	244	16.644	77.936	-2.315	1.00	34.00	8
	ATOM	1437	OWO	WAT	245	1.790	62.643	35.518	1.00	30.63	8
20	ATOM	1438	OWO	WAT	246	10.026	76.840	13.639	1.00	31.10	8
	ATOM	1439	OWO	WAT	247	11.096	40.538	24.599	1.00	33.25	8
	ATOM	1440	OWO	WAT	248	19.457	73.016	-2.970	1.00	36.88	8
	ATOM	1441	OWO	WAT	249	18.578	60.108	26.756	1.00	30.86	8
	ATOM	1442	OWO	WAT	250	11.119	78.675	16.190	1.00	37.83	8
25	ATOM	1443	OWO	WAT	251	2.583	76.687	28.032	1.00	73.18	8
	ATOM	1444	OWO	WAT	252	0.243	75.153	22.803	1.00	34.15	8
	ATOM	1445	OWO	WAT	253	33.328	82.165	10.255	1.00	23.17	8
	ATOM	1446	OWO	WAT	254	22.212	87.081	5.080	1.00	51.41	8
	ATOM	1447	OWO	WAT	255	21.393	83.921	11.680	1.00	31.47	8
30	ATOM	1448	OWO	WAT	256	37.174	72.382	4.349	1.00	36.66	8
	ATOM	1449	OWO	WAT	257	23.291	53.950	13.981	1.00	45.02	8
	ATOM	1450	OWO	WAT	258	31.521	80.134	5.404	1.00	28.19	8
	ATOM	1451	OWO	WAT	259	11.904	78.169	8.209	1.00	61.39	8
35	ATOM	1452	OWO	WAT	260	7.393	36.160	24.668	1.00	45.96	8
	ATOM	1453	OWO	WAT	261	12.356	70.954	23.727	1.00	23.77	8
	ATOM	1454	OWO	WAT	262	33.898	69.078	7.353	1.00	32.96	8
	ATOM	1455	OWO	WAT	263	28.502	52.764	25.478	1.00	58.40	8
	ATOM	1456	OWO	WAT	264	23.414	37.810	18.427	1.00	35.16	8
40	ATOM	1457	OWO	WAT	265	4.792	74.631	16.778	1.00	44.49	8
	ATOM	1458	OWO	WAT	266	28.509	77.721	-1.620	1.00	50.51	8
	ATOM	1459	OWO	WAT	267	19.685	68.488	-0.712	1.00	45.74	8
	ATOM	1460	OWO	WAT	268	10.899	74.487	23.620	1.00	43.61	8
	ATOM	1461	OWO	WAT	269	-1.033	73.720	20.128	1.00	34.52	8
	ATOM	1462	OWO	WAT	270	15.215	67.397	0.077	1.00	27.35	8
45	ATOM	1463	OWO	WAT	271	8.748	79.989	16.508	1.00	51.59	8
	ATOM	1464	OWO	WAT	272	22.332	82.314	3.707	1.00	30.25	8
	ATOM	1465	OWO	WAT	273	23.373	70.771	17.610	1.00	22.44	8
	ATOM	1466	OWO	WAT	274	11.965	67.872	26.359	1.00	26.92	8
50	ATOM	1467	OWO	WAT	275	35.793	71.146	7.198	1.00	27.19	8
	ATOM	1468	OWO	WAT	276	10.333	72.530	25.867	1.00	46.78	8
	ATOM	1469	OWO	WAT	277	17.230	69.185	24.852	1.00	26.22	8
	ATOM	1470	OWO	WAT	278	17.594	51.432	30.830	1.00	32.58	8
	ATOM	1471	OWO	WAT	279	8.561	67.703	32.884	1.00	37.04	8
55	ATOM	1472	OWO	WAT	280	16.374	71.765	-4.195	1.00	31.45	8
	ATOM	1473	OWO	WAT	281	8.995	70.329	24.946	1.00	36.64	8
	ATOM	1474	OWO	WAT	282	19.019	47.051	28.676	1.00	48.06	8
	ATOM	1475	OWO	WAT	283	20.039	61.350	15.742	1.00	23.23	8
	ATOM	1476	OWO	WAT	284	21.308	55.309	20.658	1.00	28.24	8
60	ATOM	1477	OWO	WAT	285	7.405	70.019	5.261	1.00	41.47	8
	ATOM	1478	OWO	WAT	286	23.729	66.066	0.632	1.00	30.27	8
	ATOM	1479	OWO	WAT	287	15.826	40.095	23.946	1.00	41.94	8
	ATOM	1480	OWO	WAT	288	-0.119	50.371	24.812	0.50	25.93	8
	ATOM	1481	OWO	WAT	289	3.397	54.879	42.245	1.00	29.87	8
65	ATOM	1482	OWO	WAT	290	10.215	53.151	32.270	1.00	43.33	8
	ATOM	1483	OWO	WAT	291	8.440	65.109	33.883	1.00	34.09	8
	END										

TABLE 2

70

REMARK Written by O version 5.10.1

```

REMARK Wed May 20 10:23:51 1998
CRYST1 79.221 100.866 28.172 90.00 90.00 90.00
ORIGX1 1.000000 0.000000 0.000000 0.000000 0.000000
ORIGX2 0.000000 1.000000 0.000000 0.000000 0.000000
ORIGX3 0.000000 0.000000 1.000000 0.000000 0.000000
SCALE1 0.012623 0.000000 0.000000 0.000000 0.000000
SCALE2 0.000000 0.009914 0.000000 0.000000 0.000000
SCALE3 0.000000 0.000000 0.035496 0.000000 0.000000
  5  ATOM      1  CB  ALA      1  36.645  68.826 -4.702  1.00  51.37  6
    ATOM      2  C   ALA      1  36.199  68.294 -2.285  1.00  42.22  6
    ATOM      3  O   ALA      1  36.801  67.492 -1.569  1.00  42.70  8
    ATOM      4  N   ALA      1  34.367  68.121 -3.997  1.00  45.74  7
    ATOM      5  CA  ALA      1  35.829  67.992 -3.724  1.00  43.68  6
    ATOM      6  N   PRO      2  35.903  69.499 -1.817  1.00  40.54  7
  15  ATOM      7  CD  PRO      2  35.149  70.546 -2.533  1.00  38.91  6
    ATOM      8  CA  PRO      2  36.172  69.844 -0.425  1.00  38.61  6
    ATOM      9  CB  PRO      2  35.765  71.300 -0.322  1.00  39.86  6
    ATOM     10  CG  PRO      2  34.790  71.513 -1.426  1.00  41.36  6
    ATOM     11  C   PRO      2  35.294  68.931  0.434  1.00  36.70  6
  20  ATOM     12  O   PRO      2  34.188  68.654 -0.042  1.00  32.46  8
    ATOM     13  N   PRO      3  35.789  68.496  1.579  1.00  33.82  7
    ATOM     14  CD  PRO      3  37.120  68.857  2.110  1.00  35.16  6
    ATOM     15  CA  PRO      3  35.069  67.637  2.491  1.00  38.25  6
    ATOM     16  CB  PRO      3  35.872  67.639  3.799  1.00  37.39  6
  25  ATOM     17  CG  PRO      3  37.180  68.267  3.486  1.00  37.41  6
    ATOM     18  C   PRO      3  33.653  68.136  2.790  1.00  37.48  6
    ATOM     19  O   PRO      3  33.393  69.335  2.683  1.00  34.39  8
    ATOM     20  N   LYS      4  32.763  67.212  3.173  1.00  37.04  7
    ATOM     21  CA  LYS      4  31.399  67.678  3.424  1.00  34.97  6
  30  ATOM     22  CB  LYS      4  30.318  66.664  3.122  1.00  43.98  6
    ATOM     23  CG  LYS      4  30.564  65.191  3.278  1.00  47.64  6
    ATOM     24  CD  LYS      4  29.775  64.349  2.292  1.00  52.03  6
    ATOM     25  CE  LYS      4  28.317  64.743  2.137  1.00  57.56  6
    ATOM     26  NZ  LYS      4  27.724  64.253  0.855  1.00  56.40  7
  35  ATOM     27  C   LYS      4  31.243  68.234  4.825  1.00  31.44  6
    ATOM     28  O   LYS      4  31.846  67.769  5.784  1.00  29.91  8
    ATOM     29  N   ALA      5  30.416  69.280  4.908  1.00  28.75  7
    ATOM     30  CA  ALA      5  30.039  69.813  6.218  1.00  27.21  6
    ATOM     31  CB  ALA      5  29.155  71.032  6.110  1.00  21.94  6
  40  ATOM     32  C   ALA      5  29.278  68.683  6.923  1.00  26.42  6
    ATOM     33  O   ALA      5  28.760  67.794  6.222  1.00  26.10  8
    ATOM     34  N   VAL      6  29.231  68.674  8.241  1.00  24.91  7
    ATOM     35  CA  VAL      6  28.515  67.632  8.985  1.00  26.95  6
    ATOM     36  CB  VAL      6  29.490  66.738  9.770  1.00  29.36  6
  45  ATOM     37  CG1 VAL      6  28.779  65.726  10.676  1.00  29.86  6
    ATOM     38  CG2 VAL      6  30.434  66.024  8.801  1.00  26.74  6
    ATOM     39  C   VAL      6  27.503  68.253  9.942  1.00  28.93  6
    ATOM     40  O   VAL      6  27.846  68.994  10.866  1.00  31.46  8
  50  ATOM     41  N   LEU      7  26.233  67.929  9.758  1.00  30.08  7
    ATOM     42  CA  LEU      7  25.105  68.383  10.546  1.00  29.33  6
    ATOM     43  CB  LEU      7  23.839  68.346  9.657  1.00  33.18  6
    ATOM     44  CG  LEU      7  22.828  69.458  9.960  1.00  34.94  6
    ATOM     45  CD1 LEU      7  22.082  69.876  8.721  1.00  27.55  6
    ATOM     46  CD2 LEU      7  21.887  69.002  11.069  1.00  32.30  6
  55  ATOM     47  C   LEU      7  24.816  67.565  11.794  1.00  29.57  6
    ATOM     48  O   LEU      7  24.653  66.351  11.800  1.00  30.04  8
    ATOM     49  N   LYS      8  24.768  68.242  12.930  1.00  28.04  7
    ATOM     50  CA  LYS      8  24.568  67.692  14.257  1.00  25.12  6
    ATOM     51  CB  LYS      8  25.738  68.179  15.132  1.00  33.32  6
  60  ATOM     52  CG  LYS      8  25.777  67.611  16.532  1.00  39.37  6
    ATOM     53  CD  LYS      8  25.967  68.598  17.652  1.00  43.84  6
    ATOM     54  CE  LYS      8  27.129  69.561  17.487  1.00  47.78  6
    ATOM     55  NZ  LYS      8  27.525  70.175  18.793  1.00  48.98  7
    ATOM     56  C   LYS      8  23.233  68.192  14.797  1.00  24.53  6
  65  ATOM     57  O   LYS      8  22.934  69.384  14.739  1.00  25.35  8
    ATOM     58  N   LEU      9  22.423  67.310  15.333  1.00  24.78  7
    ATOM     59  CA  LEU      9  21.080  67.553  15.843  1.00  22.07  6
    ATOM     60  CB  LEU      9  20.189  66.483  15.190  1.00  20.04  6
    ATOM     61  CG  LEU      9  18.725  66.363  15.596  1.00  20.57  6
  70  ATOM     62  CD1 LEU      9  17.980  67.624  15.214  1.00  19.57  6
    ATOM     63  CD2 LEU      9  18.084  65.137  14.903  1.00  23.44  6

```

	ATOM	64	C	LEU	9	21.019	67.415	17.346	1.00	21.01	6
	ATOM	65	O	LEU	9	21.424	66.393	17.869	1.00	22.38	8
	ATOM	66	N	GLU	10	20.583	68.410	18.118	1.00	22.53	7
5	ATOM	67	CA	GLU	10	20.480	68.285	19.567	1.00	21.02	6
	ATOM	68	CB	GLU	10	21.523	69.182	20.270	1.00	27.36	6
	ATOM	69	CGA	GLU	10	22.971	68.778	20.090	0.50	28.21	6
	ATOM	70	CGB	GLU	10	22.946	68.657	20.195	0.50	38.29	6
	ATOM	71	CDA	GLU	10	24.047	69.789	20.422	0.50	28.55	6
10	ATOM	72	CDB	GLU	10	23.100	67.202	20.587	0.50	43.48	6
	ATOM	73	OE1	GLU	10	25.131	69.365	20.907	0.50	26.56	8
	ATOM	74	OE1	GLU	10	22.443	66.771	21.565	0.50	47.24	8
	ATOM	75	OE2	GLU	10	23.888	71.008	20.186	0.50	22.10	8
	ATOM	76	OE2	GLU	10	23.871	66.486	19.908	0.50	46.42	8
15	ATOM	77	C	GLU	10	19.096	68.728	20.008	1.00	19.76	6
	ATOM	78	O	GLU	10	18.701	69.842	19.613	1.00	18.00	8
	ATOM	79	N	PRO	11	18.423	67.995	20.888	1.00	19.07	7
	ATOM	80	CD	PRO	11	17.058	68.340	21.390	1.00	18.71	6
	ATOM	81	CA	PRO	11	18.834	66.662	21.319	1.00	18.84	6
20	ATOM	82	CB	PRO	11	17.807	66.272	22.365	1.00	17.38	6
	ATOM	83	CG	PRO	11	16.560	67.000	21.944	1.00	18.86	6
	ATOM	84	C	PRO	11	18.787	65.758	20.090	1.00	20.01	6
	ATOM	85	O	PRO	11	18.310	66.212	19.051	1.00	16.22	8
	ATOM	86	N	PRO	12	19.232	64.517	20.155	1.00	19.94	7
25	ATOM	87	CD	PRO	12	19.915	63.948	21.361	1.00	21.08	6
	ATOM	88	CA	PRO	12	19.409	63.700	18.976	1.00	20.68	6
	ATOM	89	CB	PRO	12	20.455	62.656	19.397	1.00	19.82	6
	ATOM	90	CG	PRO	12	20.292	62.567	20.872	1.00	23.59	6
	ATOM	91	C	PRO	12	18.179	63.061	18.395	1.00	18.70	6
30	ATOM	92	O	PRO	12	18.268	62.475	17.318	1.00	19.85	8
	ATOM	93	N	TRP	13	17.039	63.169	19.059	1.00	15.64	7
	ATOM	94	CA	TRP	13	15.815	62.568	18.561	1.00	17.91	6
	ATOM	95	CB	TRP	13	14.688	62.840	19.562	1.00	14.32	6
	ATOM	96	CG	TRP	13	15.124	62.749	21.006	1.00	16.77	6
35	ATOM	97	CD2	TRP	13	15.633	61.612	21.703	1.00	16.90	6
	ATOM	98	CE2	TRP	13	15.899	62.005	23.032	1.00	16.87	6
	ATOM	99	CE3	TRP	13	15.867	60.279	21.350	1.00	18.03	6
	ATOM	100	CD1	TRP	13	15.106	63.769	21.916	1.00	18.97	6
	ATOM	101	NE1	TRP	13	15.589	63.343	23.137	1.00	11.16	7
40	ATOM	102	CZ2	TRP	13	16.405	61.124	23.973	1.00	15.92	6
	ATOM	103	CZ3	TRP	13	16.358	59.409	22.301	1.00	10.59	6
	ATOM	104	CH2	TRP	13	16.645	59.825	23.611	1.00	17.87	6
	ATOM	105	C	TRP	13	15.421	63.033	17.163	1.00	19.47	6
	ATOM	106	O	TRP	13	15.283	64.238	16.908	1.00	17.22	8
45	ATOM	107	N	ILE	14	15.101	62.078	16.275	1.00	16.57	7
	ATOM	108	CA	ILE	14	14.666	62.441	14.936	1.00	18.93	6
	ATOM	109	CB	ILE	14	15.185	61.523	13.816	1.00	16.07	6
	ATOM	110	CG2	ILE	14	16.720	61.521	13.840	1.00	16.61	6
	ATOM	111	CG1	ILE	14	14.582	60.119	13.972	1.00	21.35	6
50	ATOM	112	CD1	ILE	14	15.045	59.150	12.896	1.00	26.28	6
	ATOM	113	C	ILE	14	13.144	62.549	14.825	1.00	20.48	6
	ATOM	114	O	ILE	14	12.652	63.048	13.817	1.00	19.41	8
	ATOM	115	N	ASN	15	12.403	62.087	15.836	1.00	19.46	7
	ATOM	116	CA	ASN	15	10.935	62.270	15.778	1.00	18.11	6
55	ATOM	117	CB	ASN	15	10.161	60.962	15.731	1.00	13.53	6
	ATOM	118	CG	ASN	15	10.591	59.946	16.762	1.00	19.11	6
	ATOM	119	OD1	ASN	15	11.728	59.959	17.227	1.00	13.35	8
	ATOM	120	ND2	ASN	15	9.688	59.033	17.142	1.00	10.11	7
	ATOM	121	C	ASN	15	10.632	63.124	17.005	1.00	17.54	6
60	ATOM	122	O	ASN	15	11.016	62.735	18.111	1.00	15.32	8
	ATOM	123	N	VAL	16	10.122	64.331	16.805	1.00	16.86	7
	ATOM	124	CA	VAL	16	9.871	65.273	17.893	1.00	15.77	6
	ATOM	125	CB	VAL	16	10.761	66.534	17.748	1.00	16.54	6
	ATOM	126	CG1	VAL	16	12.251	66.141	17.733	1.00	13.42	6
65	ATOM	127	CG2	VAL	16	10.490	67.345	16.491	1.00	18.04	6
	ATOM	128	C	VAL	16	8.420	65.708	17.921	1.00	19.01	6
	ATOM	129	O	VAL	16	7.618	65.381	17.010	1.00	17.12	8
	ATOM	130	N	LEU	17	8.022	66.422	18.964	1.00	17.68	7
	ATOM	131	CA	LEU	17	6.664	66.962	19.068	1.00	15.11	6
70	ATOM	132	CB	LEU	17	6.162	66.726	20.522	1.00	20.26	6
	ATOM	133	CG	LEU	17	5.873	65.251	20.823	1.00	23.07	6
	ATOM	134	CD1	LEU	17	5.447	65.013	22.253	1.00	17.70	6

	ATOM	135	CD2	LEU	17	4.832	64.714	19.855	1.00	26.74	6
	ATOM	136	C	LEU	17	6.563	68.439	18.732	1.00	16.37	6
	ATOM	137	O	LEU	17	7.518	69.187	18.961	1.00	18.24	8
5	ATOM	138	N	GLN	18	5.424	68.931	18.227	1.00	18.55	7
	ATOM	139	CA	GLN	18	5.237	70.370	18.032	1.00	19.13	6
	ATOM	140	CB	GLN	18	3.790	70.721	17.696	1.00	31.65	6
	ATOM	141	CG	GLN	18	3.510	71.249	16.314	1.00	37.32	6
	ATOM	142	CD	GLN	18	2.120	70.902	15.800	1.00	36.92	6
10	ATOM	143	OE1	GLN	18	1.953	70.032	14.943	1.00	30.97	8
	ATOM	144	NE2	GLN	18	1.135	71.618	16.333	1.00	31.73	7
	ATOM	145	C	GLN	18	5.561	71.077	19.348	1.00	19.43	6
	ATOM	146	O	GLN	18	5.194	70.568	20.413	1.00	18.10	8
	ATOM	147	N	GLU	19	6.317	72.164	19.232	1.00	19.68	7
	ATOM	148	CA	GLU	19	6.727	73.045	20.293	1.00	18.88	6
15	ATOM	149	CB	GLU	19	5.597	73.341	21.293	1.00	27.39	6
	ATOM	150	CG	GLU	19	4.649	74.418	20.714	1.00	30.12	6
	ATOM	151	CD	GLU	19	3.558	74.699	21.720	1.00	41.87	6
	ATOM	152	OE1	GLU	19	3.857	75.330	22.758	1.00	48.83	8
	ATOM	153	OE2	GLU	19	2.421	74.272	21.464	1.00	46.61	8
20	ATOM	154	C	GLU	19	8.004	72.622	20.998	1.00	21.46	6
	ATOM	155	O	GLU	19	8.496	73.405	21.815	1.00	26.39	8
	ATOM	156	N	ASP	20	8.606	71.506	20.619	1.00	19.91	7
	ATOM	157	CA	ASP	20	9.898	71.094	21.114	1.00	20.76	6
25	ATOM	158	CB	ASP	20	10.285	69.649	20.726	1.00	13.47	6
	ATOM	159	CG	ASP	20	9.587	68.578	21.526	1.00	13.93	6
	ATOM	160	OD1	ASP	20	8.873	68.805	22.534	1.00	17.57	8
	ATOM	161	OD2	ASP	20	9.723	67.405	21.104	1.00	13.79	8
	ATOM	162	C	ASP	20	11.002	71.950	20.451	1.00	19.58	6
30	ATOM	163	O	ASP	20	10.913	72.219	19.262	1.00	17.49	8
	ATOM	164	N	SER	21	12.071	72.198	21.174	1.00	17.22	7
	ATOM	165	CA	SER	21	13.233	72.929	20.659	1.00	17.62	6
	ATOM	166	CBA	SER	21	14.011	73.525	21.844	0.50	17.49	6
	ATOM	167	CBB	SER	21	13.981	73.556	21.846	0.50	13.14	6
35	ATOM	168	OGA	SER	21	14.900	74.516	21.355	0.50	22.95	8
	ATOM	169	OGB	SER	21	13.175	74.579	22.416	0.50	6.85	8
	ATOM	170	C	SER	21	14.181	72.038	19.873	1.00	18.61	6
	ATOM	171	O	SER	21	14.424	70.884	20.265	1.00	21.41	8
40	ATOM	172	N	VAL	22	14.638	72.512	18.721	1.00	15.80	7
	ATOM	173	CA	VAL	22	15.585	71.733	17.910	1.00	17.93	6
	ATOM	174	CB	VAL	22	15.052	71.234	16.560	1.00	20.37	6
	ATOM	175	CG1	VAL	22	16.093	70.401	15.804	1.00	17.77	6
	ATOM	176	CG2	VAL	22	13.858	70.300	16.679	1.00	17.26	6
	ATOM	177	C	VAL	22	16.822	72.609	17.665	1.00	19.20	6
45	ATOM	178	O	VAL	22	16.633	73.769	17.291	1.00	18.52	8
	ATOM	179	N	THR	23	18.021	72.107	17.917	1.00	16.32	7
	ATOM	180	CA	THR	23	19.249	72.823	17.648	1.00	19.99	6
	ATOM	181	CB	THR	23	20.080	73.128	18.911	1.00	22.97	6
	ATOM	182	OG1	THR	23	19.192	73.749	19.850	1.00	18.42	8
50	ATOM	183	CG2	THR	23	21.241	74.057	18.614	1.00	16.78	6
	ATOM	184	C	THR	23	20.098	72.016	16.658	1.00	24.68	6
	ATOM	185	O	THR	23	20.509	70.880	16.897	1.00	22.59	8
	ATOM	186	N	LEU	24	20.257	72.618	15.467	1.00	23.73	7
	ATOM	187	CA	LEU	24	21.081	72.051	14.423	1.00	23.11	6
55	ATOM	188	CB	LEU	24	20.427	72.206	13.046	1.00	20.25	6
	ATOM	189	CG	LEU	24	19.053	71.480	12.959	1.00	23.95	6
	ATOM	190	CD1	LEU	24	18.324	71.856	11.681	1.00	20.78	6
	ATOM	191	CD2	LEU	24	19.251	69.985	13.049	1.00	22.74	6
	ATOM	192	C	LEU	24	22.444	72.763	14.450	1.00	25.87	6
60	ATOM	193	O	LEU	24	22.470	74.008	14.537	1.00	24.57	8
	ATOM	194	N	THR	25	23.520	71.980	14.367	1.00	20.22	7
	ATOM	195	CA	THR	25	24.847	72.600	14.336	1.00	23.21	6
	ATOM	196	CB	THR	25	25.656	72.265	15.597	1.00	27.69	6
	ATOM	197	OG1	THR	25	24.945	72.730	16.755	1.00	26.30	8
65	ATOM	198	CG2	THR	25	27.041	72.925	15.590	1.00	28.49	6
	ATOM	199	C	THR	25	25.604	72.166	13.075	1.00	22.31	6
	ATOM	200	O	THR	25	25.706	70.951	12.819	1.00	23.86	8
	ATOM	201	N	CYS	26	26.092	73.134	12.307	1.00	18.68	7
	ATOM	202	CA	CYS	26	26.832	72.888	11.075	1.00	23.20	6
70	ATOM	203	C	CYS	26	28.345	72.910	11.346	1.00	23.06	6
	ATOM	204	O	CYS	26	28.957	73.980	11.556	1.00	23.76	8
	ATOM	205	CB	CYS	26	26.509	73.881	9.958	1.00	17.92	6

	ATOM	206	SG	CYS	26	27.138	73.358	8.311	1.00	22.25	16
	ATOM	207	N	GLN	27	28.929	71.729	11.355	1.00	19.35	7
	ATOM	208	CA	GLN	27	30.332	71.521	11.658	1.00	23.30	6
5	ATOM	209	CB	GLN	27	30.543	70.209	12.464	1.00	29.78	6
	ATOM	210	CG	GLN	27	29.623	70.044	13.672	1.00	31.50	6
	ATOM	211	CD	GLN	27	29.927	68.828	14.518	1.00	33.01	6
	ATOM	212	OE1	GLN	27	30.322	67.774	14.032	1.00	38.67	8
	ATOM	213	NE2	GLN	27	29.792	68.895	15.834	1.00	36.36	7
10	ATOM	214	C	GLN	27	31.169	71.417	10.377	1.00	26.33	6
	ATOM	215	O	GLN	27	30.764	70.856	9.347	1.00	23.15	8
	ATOM	216	N	GLY	28	32.363	72.019	10.438	1.00	27.69	7
	ATOM	217	CA	GLY	28	33.289	72.019	9.313	1.00	28.02	6
	ATOM	218	C	GLY	28	34.022	73.360	9.215	1.00	29.41	6
	ATOM	219	O	GLY	28	33.639	74.335	9.862	1.00	28.46	8
15	ATOM	220	N	ALA	29	35.062	73.421	8.389	1.00	27.48	7
	ATOM	221	CA	ALA	29	35.824	74.640	8.210	1.00	27.39	6
	ATOM	222	CB	ALA	29	36.979	74.353	7.239	1.00	25.91	6
	ATOM	223	C	ALA	29	34.959	75.730	7.574	1.00	28.27	6
	ATOM	224	O	ALA	29	34.315	75.415	6.561	1.00	26.07	8
20	ATOM	225	N	ARG	30	35.060	76.951	8.064	1.00	23.97	7
	ATOM	226	CA	ARG	30	34.303	78.055	7.490	1.00	27.17	6
	ATOM	227	CB	ARG	30	33.571	78.823	8.601	1.00	30.34	6
	ATOM	228	CG	ARG	30	32.574	78.090	9.460	1.00	34.05	6
	ATOM	229	CD	ARG	30	32.365	78.880	10.761	1.00	33.86	6
25	ATOM	230	NE	ARG	30	32.407	77.902	11.836	1.00	38.60	7
	ATOM	231	CZ	ARG	30	32.487	78.082	13.126	1.00	38.08	6
	ATOM	232	NH1	ARG	30	32.567	79.298	13.635	1.00	36.51	7
	ATOM	233	NH2	ARG	30	32.467	76.990	13.879	1.00	46.13	7
	ATOM	234	C	ARG	30	35.194	79.148	6.880	1.00	26.70	6
30	ATOM	235	O	ARG	30	36.399	79.142	7.075	1.00	29.22	8
	ATOM	236	N	SER	31	34.573	80.129	6.246	1.00	26.85	7
	ATOM	237	CA	SER	31	35.315	81.284	5.738	1.00	26.56	6
	ATOM	238	CB	SER	31	34.682	81.846	4.476	1.00	25.03	6
	ATOM	239	OG	SER	31	34.562	80.875	3.477	1.00	27.59	8
35	ATOM	240	C	SER	31	35.273	82.321	6.861	1.00	26.58	6
	ATOM	241	O	SER	31	34.396	82.246	7.739	1.00	23.91	8
	ATOM	242	N	PRO	32	36.163	83.308	6.839	1.00	23.48	7
	ATOM	243	CD	PRO	32	37.224	83.483	5.842	1.00	22.70	6
40	ATOM	244	CA	PRO	32	36.176	84.350	7.861	1.00	24.75	6
	ATOM	245	CB	PRO	32	37.621	84.830	7.805	1.00	24.34	6
	ATOM	246	CG	PRO	32	38.095	84.571	6.414	1.00	23.77	6
	ATOM	247	C	PRO	32	35.172	85.449	7.549	1.00	29.23	6
	ATOM	248	O	PRO	32	35.472	86.609	7.223	1.00	28.28	8
45	ATOM	249	N	GLU	33	33.913	85.121	7.709	1.00	29.77	7
	ATOM	250	CA	GLU	33	32.725	85.896	7.417	1.00	33.37	6
	ATOM	251	CBA	GLU	33	32.177	85.426	6.073	0.50	35.18	6
	ATOM	252	CBB	GLU	33	32.123	85.457	6.084	0.50	31.98	6
	ATOM	253	CGA	GLU	33	30.795	84.829	5.952	0.50	39.40	6
50	ATOM	254	CGB	GLU	33	31.776	83.990	5.954	0.50	34.05	6
	ATOM	255	CDA	GLU	33	30.394	84.525	4.521	0.50	46.48	6
	ATOM	256	CDB	GLU	33	31.601	83.533	4.517	0.50	34.67	6
	ATOM	257	OE1	GLU	33	29.268	84.856	4.076	0.50	49.23	8
	ATOM	258	OE1	GLU	33	32.194	84.168	3.619	0.50	32.81	8
55	ATOM	259	OE2	GLU	33	31.232	83.952	3.788	0.50	47.50	8
	ATOM	260	OE2	GLU	33	30.877	82.542	4.275	0.50	24.64	8
	ATOM	261	C	GLU	33	31.683	85.689	8.519	1.00	32.61	6
	ATOM	262	O	GLU	33	31.612	84.600	9.085	1.00	28.72	8
	ATOM	263	N	SER	34	30.844	86.682	8.743	1.00	32.15	7
60	ATOM	264	CA	SER	34	29.804	86.591	9.764	1.00	32.72	6
	ATOM	265	CB	SER	34	29.277	88.013	10.037	1.00	34.26	6
	ATOM	266	OG	SER	34	28.320	87.931	11.093	1.00	45.88	8
	ATOM	267	C	SER	34	28.668	85.674	9.332	1.00	30.93	6
	ATOM	268	O	SER	34	28.156	84.883	10.124	1.00	28.87	8
65	ATOM	269	N	ASP	35	28.222	85.773	8.082	1.00	28.02	7
	ATOM	270	CA	ASP	35	27.167	84.858	7.599	1.00	28.62	6
	ATOM	271	CB	ASP	35	26.292	85.538	6.585	1.00	29.65	6
	ATOM	272	CG	ASP	35	25.357	86.639	7.057	1.00	37.43	6
	ATOM	273	OD1	ASP	35	25.027	86.769	8.258	1.00	33.53	8
70	ATOM	274	OD2	ASP	35	24.902	87.396	6.154	1.00	36.01	8
	ATOM	275	C	ASP	35	27.882	83.643	6.973	1.00	27.08	6
	ATOM	276	O	ASP	35	27.997	83.566	5.756	1.00	28.07	8

	ATOM	277	N	SER	36	28.461	82.748	7.774	1.00	25.55	7
	ATOM	278	CA	SER	36	29.282	81.680	7.225	1.00	27.45	6
	ATOM	279	CB	SER	36	30.440	81.431	8.213	1.00	34.87	6
5	ATOM	280	OG	SER	36	29.973	80.802	9.405	1.00	39.51	8
	ATOM	281	C	SER	36	28.558	80.382	6.890	1.00	27.14	6
	ATOM	282	O	SER	36	29.143	79.421	6.363	1.00	25.67	8
	ATOM	283	N	ILE	37	27.293	80.223	7.231	1.00	24.64	7
	ATOM	284	CA	ILE	37	26.580	78.973	6.977	1.00	24.33	6
10	ATOM	285	CB	ILE	37	26.164	78.307	8.309	1.00	30.71	6
	ATOM	286	CG2	ILE	37	25.561	76.931	8.032	1.00	26.94	6
	ATOM	287	CG1	ILE	37	27.333	78.221	9.308	1.00	21.66	6
	ATOM	288	CD1	ILE	37	28.443	77.278	8.867	1.00	27.66	6
	ATOM	289	C	ILE	37	25.336	79.159	6.128	1.00	24.08	6
15	ATOM	290	O	ILE	37	24.515	80.033	6.390	1.00	23.50	8
	ATOM	291	N	GLN	38	25.122	78.314	5.127	1.00	24.52	7
	ATOM	292	CA	GLN	38	23.862	78.296	4.399	1.00	23.13	6
	ATOM	293	CB	GLN	38	24.016	78.068	2.905	1.00	29.28	6
	ATOM	294	CG	GLN	38	24.458	79.296	2.123	1.00	29.86	6
20	ATOM	295	CD	GLN	38	24.692	78.965	0.661	1.00	33.48	6
	ATOM	296	OE1	GLN	38	25.540	78.122	0.323	1.00	28.34	8
	ATOM	297	NE2	GLN	38	23.922	79.668	-0.177	1.00	38.54	7
	ATOM	298	C	GLN	38	23.048	77.128	4.985	1.00	23.81	6
	ATOM	299	O	GLN	38	23.598	76.022	5.087	1.00	22.62	8
25	ATOM	300	N	TRP	39	21.807	77.386	5.371	1.00	21.43	7
	ATOM	301	CA	TRP	39	20.987	76.304	5.905	1.00	21.73	6
	ATOM	302	CB	TRP	39	20.345	76.633	7.257	1.00	21.01	6
	ATOM	303	CG	TRP	39	21.264	76.633	8.430	1.00	17.58	6
	ATOM	304	CD2	TRP	39	21.721	75.523	9.212	1.00	17.00	6
30	ATOM	305	CE2	TRP	39	22.569	76.033	10.220	1.00	16.71	6
	ATOM	306	CE3	TRP	39	21.495	74.147	9.158	1.00	21.47	6
	ATOM	307	CD1	TRP	39	21.844	77.750	8.974	1.00	19.92	6
	ATOM	308	NE1	TRP	39	22.626	77.400	10.061	1.00	22.18	7
	ATOM	309	CZ2	TRP	39	23.218	75.220	11.152	1.00	18.29	6
35	ATOM	310	CZ3	TRP	39	22.109	73.329	10.091	1.00	21.62	6
	ATOM	311	CH2	TRP	39	22.960	73.874	11.064	1.00	20.15	6
	ATOM	312	C	TRP	39	19.890	75.993	4.898	1.00	22.76	6
	ATOM	313	O	TRP	39	19.407	76.925	4.238	1.00	23.42	8
	ATOM	314	N	PHE	40	19.533	74.701	4.758	1.00	22.91	7
40	ATOM	315	CA	PHE	40	18.512	74.389	3.754	1.00	26.86	6
	ATOM	316	CB	PHE	40	19.121	73.722	2.513	1.00	24.16	6
	ATOM	317	CG	PHE	40	20.225	74.429	1.788	1.00	23.96	6
	ATOM	318	CD1	PHE	40	21.551	74.280	2.189	1.00	23.61	6
	ATOM	319	CD2	PHE	40	19.945	75.244	0.696	1.00	22.47	6
45	ATOM	320	CE1	PHE	40	22.564	74.919	1.504	1.00	20.83	6
	ATOM	321	CE2	PHE	40	20.967	75.880	0.020	1.00	21.69	6
	ATOM	322	CZ	PHE	40	22.267	75.740	0.432	1.00	21.86	6
	ATOM	323	C	PHE	40	17.466	73.435	4.349	1.00	23.51	6
	ATOM	324	O	PHE	40	17.838	72.588	5.151	1.00	21.94	8
50	ATOM	325	N	HIS	41	16.232	73.575	3.905	1.00	21.59	7
	ATOM	326	CA	HIS	41	15.107	72.771	4.366	1.00	24.07	6
	ATOM	327	CB	HIS	41	14.032	73.572	5.099	1.00	18.72	6
	ATOM	328	CG	HIS	41	12.864	72.727	5.548	1.00	23.41	6
	ATOM	329	CD2	HIS	41	12.794	71.415	5.899	1.00	21.85	6
55	ATOM	330	ND1	HIS	41	11.588	73.218	5.709	1.00	21.97	7
	ATOM	331	CE1	HIS	41	10.789	72.259	6.135	1.00	22.79	6
	ATOM	332	NE2	HIS	41	11.504	71.161	6.268	1.00	21.87	7
	ATOM	333	C	HIS	41	14.455	72.163	3.115	1.00	21.83	6
	ATOM	334	O	HIS	41	13.972	72.919	2.282	1.00	21.37	8
60	ATOM	335	N	ASN	42	14.576	70.847	2.959	1.00	22.08	7
	ATOM	336	CA	ASN	42	14.077	70.196	1.726	1.00	20.46	6
	ATOM	337	CB	ASN	42	12.562	70.322	1.722	1.00	18.21	6
	ATOM	338	CG	ASN	42	11.925	69.397	2.761	1.00	22.74	6
	ATOM	339	OD1	ASN	42	12.473	68.343	3.087	1.00	24.40	8
65	ATOM	340	ND2	ASN	42	10.804	69.804	3.341	1.00	18.43	7
	ATOM	341	C	ASN	42	14.733	70.811	0.488	1.00	21.32	6
	ATOM	342	O	ASN	42	14.085	71.047	-0.533	1.00	20.13	8
	ATOM	343	N	GLY	43	16.002	71.220	0.568	1.00	20.53	7
	ATOM	344	CA	GLY	43	16.767	71.861	-0.480	1.00	20.83	6
70	ATOM	345	C	GLY	43	16.586	73.360	-0.661	1.00	24.51	6
	ATOM	346	O	GLY	43	17.209	73.987	-1.550	1.00	25.30	8
	ATOM	347	N	ASN	44	15.633	73.970	0.051	1.00	21.27	7

	ATOM	348	CA	ASN	44	15.391	75.393	-0.112	1.00	20.46	6
	ATOM	349	CB	ASN	44	13.903	75.734	0.000	1.00	23.82	6
	ATOM	350	CG	ASN	44	13.049	74.834	-0.891	1.00	22.26	6
5	ATOM	351	OD1	ASN	44	12.148	74.144	-0.409	1.00	25.47	8
	ATOM	352	ND2	ASN	44	13.382	74.787	-2.171	1.00	21.59	7
	ATOM	353	C	ASN	44	16.208	76.143	0.937	1.00	19.78	6
	ATOM	354	O	ASN	44	16.180	75.778	2.107	1.00	22.07	8
	ATOM	355	N	LEU	45	16.907	77.188	0.523	1.00	22.22	7
10	ATOM	356	CA	LEU	45	17.730	77.962	1.459	1.00	21.67	6
	ATOM	357	CB	LEU	45	18.391	79.141	0.715	1.00	28.15	6
	ATOM	358	CG	LEU	45	19.159	80.171	1.538	1.00	29.14	6
	ATOM	359	CD1	LEU	45	20.479	79.571	2.002	1.00	25.07	6
	ATOM	360	CD2	LEU	45	19.452	81.466	0.775	1.00	28.51	6
15	ATOM	361	C	LEU	45	16.825	78.559	2.525	1.00	22.27	6
	ATOM	362	O	LEU	45	15.748	78.997	2.118	1.00	20.13	8
	ATOM	363	N	ILE	46	17.263	78.604	3.766	1.00	20.11	7
	ATOM	364	CA	ILE	46	16.539	79.322	4.835	1.00	24.64	6
	ATOM	365	CB	ILE	46	16.657	78.508	6.132	1.00	22.24	6
20	ATOM	366	CG2	ILE	46	16.007	79.134	7.358	1.00	21.33	6
	ATOM	367	CG1	ILE	46	16.111	77.072	5.945	1.00	20.74	6
	ATOM	368	CD1	ILE	46	16.664	76.147	7.024	1.00	20.48	6
	ATOM	369	C	ILE	46	17.351	80.625	5.006	1.00	25.53	6
	ATOM	370	O	ILE	46	18.419	80.600	5.624	1.00	22.91	8
25	ATOM	371	N	PRO	47	16.937	81.747	4.444	1.00	30.56	7
	ATOM	372	CD	PRO	47	15.704	81.884	3.620	1.00	32.61	6
	ATOM	373	CA	PRO	47	17.731	82.968	4.434	1.00	30.93	6
	ATOM	374	CB	PRO	47	17.030	83.836	3.363	1.00	31.28	6
	ATOM	375	CG	PRO	47	15.610	83.400	3.441	1.00	32.54	6
30	ATOM	376	C	PRO	47	17.888	83.762	5.706	1.00	28.32	6
	ATOM	377	O	PRO	47	18.733	84.670	5.747	1.00	29.24	8
	ATOM	378	N	THR	48	17.092	83.513	6.730	1.00	26.79	7
	ATOM	379	CA	THR	48	17.135	84.298	7.971	1.00	26.97	6
	ATOM	380	CB	THR	48	15.698	84.323	8.532	1.00	31.78	6
35	ATOM	381	OG1	THR	48	15.241	82.958	8.520	1.00	31.45	8
	ATOM	382	CG2	THR	48	14.798	85.150	7.605	1.00	27.40	6
	ATOM	383	C	THR	48	18.075	83.757	9.021	1.00	26.31	6
	ATOM	384	O	THR	48	18.206	84.334	10.113	1.00	28.00	8
	ATOM	385	N	HIS	49	18.698	82.602	8.772	1.00	24.44	7
40	ATOM	386	CA	HIS	49	19.612	81.942	9.707	1.00	24.19	6
	ATOM	387	CB	HIS	49	18.953	80.610	10.174	1.00	25.11	6
	ATOM	388	CG	HIS	49	17.722	80.939	10.961	1.00	22.20	6
	ATOM	389	CD2	HIS	49	16.430	81.109	10.624	1.00	27.86	6
	ATOM	390	ND1	HIS	49	17.809	81.225	12.306	1.00	29.80	7
45	ATOM	391	CE1	HIS	49	16.595	81.526	12.762	1.00	28.91	6
	ATOM	392	NE2	HIS	49	15.748	81.474	11.761	1.00	25.35	7
	ATOM	393	C	HIS	49	20.923	81.588	9.041	1.00	23.08	6
	ATOM	394	O	HIS	49	20.942	80.805	8.075	1.00	20.57	8
	ATOM	395	N	THR	50	22.038	82.162	9.497	1.00	25.11	7
50	ATOM	396	CA	THR	50	23.321	81.974	8.807	1.00	22.98	6
	ATOM	397	CB	THR	50	23.732	83.314	8.137	1.00	23.01	6
	ATOM	398	OG1	THR	50	23.843	84.252	9.231	1.00	18.66	8
	ATOM	399	CG2	THR	50	22.757	83.817	7.101	1.00	19.07	6
	ATOM	400	C	THR	50	24.460	81.645	9.766	1.00	24.61	6
55	ATOM	401	O	THR	50	25.640	81.772	9.393	1.00	26.17	8
	ATOM	402	N	GLN	51	24.126	81.274	10.985	1.00	24.52	7
	ATOM	403	CA	GLN	51	25.132	80.979	11.995	1.00	27.31	6
	ATOM	404	CB	GLN	51	24.708	81.505	13.378	1.00	28.63	6
	ATOM	405	CG	GLN	51	24.438	83.014	13.378	1.00	32.81	6
60	ATOM	406	CD	GLN	51	25.677	83.810	12.995	1.00	38.53	6
	ATOM	407	OE1	GLN	51	26.606	83.952	13.802	1.00	37.60	8
	ATOM	408	NE2	GLN	51	25.724	84.331	11.765	1.00	32.79	7
	ATOM	409	C	GLN	51	25.411	79.487	12.101	1.00	26.69	6
	ATOM	410	O	GLN	51	24.626	78.636	11.689	1.00	26.27	8
65	ATOM	411	N	PRO	52	26.510	79.138	12.769	1.00	25.16	7
	ATOM	412	CD	PRO	52	27.553	80.091	13.270	1.00	24.54	6
	ATOM	413	CA	PRO	52	26.917	77.763	12.974	1.00	25.24	6
	ATOM	414	CB	PRO	52	28.264	77.888	13.708	1.00	26.09	6
	ATOM	415	CG	PRO	52	28.804	79.217	13.257	1.00	23.35	6
70	ATOM	416	C	PRO	52	25.900	76.915	13.722	1.00	25.71	6
	ATOM	417	O	PRO	52	25.877	75.687	13.542	1.00	21.61	8
	ATOM	418	N	SER	53	25.044	77.497	14.556	1.00	24.05	7

	ATOM	419	CA	SER	53	23.991	76.773	15.239	1.00	25.63	6
	ATOM	420	CB	SER	53	24.105	76.711	16.758	1.00	31.86	6
	ATOM	421	OG	SER	53	24.778	75.495	17.094	1.00	42.46	8
5	ATOM	422	C	SER	53	22.681	77.460	14.854	1.00	24.85	6
	ATOM	423	O	SER	53	22.681	78.673	14.691	1.00	23.68	8
	ATOM	424	N	TYR	54	21.658	76.689	14.614	1.00	24.52	7
	ATOM	425	CA	TYR	54	20.333	77.167	14.212	1.00	26.29	6
	ATOM	426	CB	TYR	54	20.050	76.886	12.729	1.00	26.92	6
10	ATOM	427	CG	TYR	54	18.612	76.998	12.274	1.00	30.15	6
	ATOM	428	CD1	TYR	54	17.719	77.905	12.825	1.00	29.18	6
	ATOM	429	CE1	TYR	54	16.407	78.006	12.409	1.00	31.26	6
	ATOM	430	CD2	TYR	54	18.104	76.166	11.280	1.00	31.67	6
	ATOM	431	CE2	TYR	54	16.796	76.217	10.855	1.00	31.66	6
15	ATOM	432	CZ	TYR	54	15.950	77.151	11.429	1.00	33.63	6
	ATOM	433	OH	TYR	54	14.624	77.219	11.038	1.00	34.53	8
	ATOM	434	C	TYR	54	19.378	76.450	15.167	1.00	24.84	6
	ATOM	435	O	TYR	54	19.300	75.210	15.129	1.00	22.53	8
	ATOM	436	N	ARG	55	18.773	77.181	16.070	1.00	21.66	7
20	ATOM	437	CA	ARG	55	17.864	76.650	17.070	1.00	23.60	6
	ATOM	438	CB	ARG	55	18.242	77.157	18.480	1.00	25.95	6
	ATOM	439	CG	ARG	55	17.478	76.340	19.551	1.00	23.98	6
	ATOM	440	CD	ARG	55	17.651	76.982	20.918	1.00	35.38	6
	ATOM	441	NE	ARG	55	16.821	76.365	21.956	1.00	27.47	7
25	ATOM	442	CZ	ARG	55	17.278	75.530	22.879	1.00	33.10	6
	ATOM	443	NH1	ARG	55	18.570	75.209	22.904	1.00	30.00	7
	ATOM	444	NH2	ARG	55	16.418	75.049	23.778	1.00	32.66	7
	ATOM	445	C	ARG	55	16.434	77.103	16.802	1.00	27.49	6
	ATOM	446	O	ARG	55	16.275	78.312	16.569	1.00	22.62	8
30	ATOM	447	N	PHE	56	15.455	76.174	16.781	1.00	23.78	7
	ATOM	448	CA	PHE	56	14.092	76.636	16.510	1.00	21.92	6
	ATOM	449	CB	PHE	56	13.716	76.495	15.036	1.00	25.99	6
	ATOM	450	CG	PHE	56	13.819	75.131	14.386	1.00	20.84	6
	ATOM	451	CD1	PHE	56	15.019	74.653	13.897	1.00	21.33	6
35	ATOM	452	CD2	PHE	56	12.705	74.319	14.264	1.00	20.31	6
	ATOM	453	CE1	PHE	56	15.103	73.415	13.283	1.00	21.52	6
	ATOM	454	CE2	PHE	56	12.768	73.077	13.680	1.00	18.36	6
	ATOM	455	CZ	PHE	56	13.973	72.616	13.159	1.00	18.38	6
	ATOM	456	C	PHE	56	13.095	75.862	17.372	1.00	23.93	6
40	ATOM	457	O	PHE	56	13.454	74.833	17.921	1.00	22.42	8
	ATOM	458	N	LYS	57	11.865	76.340	17.423	1.00	22.46	7
	ATOM	459	CA	LYS	57	10.735	75.659	18.054	1.00	24.34	6
	ATOM	460	CBA	LYS	57	9.892	76.620	18.881	0.50	28.51	6
	ATOM	461	CBB	LYS	57	9.822	76.727	18.669	0.50	22.87	6
45	ATOM	462	CGA	LYS	57	10.656	77.298	20.010	0.50	33.64	6
	ATOM	463	CGB	LYS	57	8.769	76.208	19.632	0.50	24.29	6
	ATOM	464	CDA	LYS	57	11.436	76.342	20.892	0.50	40.75	6
	ATOM	465	CDB	LYS	57	8.631	77.186	20.798	0.50	26.90	6
	ATOM	466	CEA	LYS	57	12.612	76.990	21.603	0.50	43.07	6
50	ATOM	467	CEB	LYS	57	9.138	76.604	22.092	0.50	29.79	6
	ATOM	468	NZA	LYS	57	12.703	76.630	23.044	0.50	51.71	7
	ATOM	469	NZB	LYS	57	8.050	76.265	23.060	0.50	36.22	7
	ATOM	470	C	LYS	57	9.950	74.923	16.969	1.00	21.30	6
55	ATOM	471	O	LYS	57	9.436	75.551	16.052	1.00	19.46	8
	ATOM	472	N	ALA	58	9.928	73.588	16.945	1.00	18.23	7
	ATOM	473	CA	ALA	58	9.341	72.864	15.821	1.00	15.74	6
	ATOM	474	CB	ALA	58	9.612	71.361	16.094	1.00	9.09	6
	ATOM	475	C	ALA	58	7.841	73.034	15.614	1.00	20.26	6
	ATOM	476	O	ALA	58	7.067	73.064	16.574	1.00	18.04	8
60	ATOM	477	N	ASN	59	7.392	73.126	14.367	1.00	18.31	7
	ATOM	478	CA	ASN	59	5.986	73.071	14.019	1.00	23.04	6
	ATOM	479	CB	ASN	59	5.222	74.301	13.612	1.00	32.39	6
	ATOM	480	CG	ASN	59	5.880	75.643	13.665	1.00	38.26	6
	ATOM	481	OD1	ASN	59	5.855	76.279	14.716	1.00	42.50	8
65	ATOM	482	ND2	ASN	59	6.426	76.066	12.529	1.00	43.39	7
	ATOM	483	C	ASN	59	5.825	72.052	12.867	1.00	24.07	6
	ATOM	484	O	ASN	59	6.794	71.476	12.365	1.00	21.25	8
	ATOM	485	N	ASN	60	4.582	71.833	12.484	1.00	24.40	7
	ATOM	486	CA	ASN	60	4.192	70.823	11.519	1.00	31.47	6
70	ATOM	487	CB	ASN	60	2.680	70.893	11.234	1.00	31.46	6
	ATOM	488	CGA	ASN	60	2.272	69.776	10.274	0.50	31.26	6
	ATOM	489	CGB	ASN	60	2.221	72.272	10.814	0.50	35.72	6

	ATOM	490	OD1 ASN	60	2.337	68.582	10.597	0.50	22.52	8
	ATOM	491	OD1 ASN	60	2.985	73.240	10.768	0.50	33.04	8
	ATOM	492	ND2 ASN	60	1.863	70.175	9.070	0.50	26.04	7
	ATOM	493	ND2 ASN	60	0.932	72.391	10.483	0.50	39.47	7
5	ATOM	494	C ASN	60	5.006	70.943	10.234	1.00	29.05	6
	ATOM	495	O ASN	60	5.645	69.986	9.780	1.00	32.27	8
	ATOM	496	N ASN	61	5.098	72.153	9.710	1.00	30.20	7
	ATOM	497	CAA ASN	61	5.863	72.487	8.529	0.50	28.68	6
	ATOM	498	CAB ASN	61	5.857	72.367	8.477	0.50	29.13	6
10	ATOM	499	CBA ASN	61	5.564	73.955	8.150	0.50	26.19	6
	ATOM	500	CBB ASN	61	5.403	73.671	7.806	0.50	30.25	6
	ATOM	501	CGA ASN	61	4.101	74.127	7.792	0.50	27.01	6
	ATOM	502	CGB ASN	61	5.608	74.882	8.678	0.50	32.36	6
	ATOM	503	OD1 ASN	61	3.502	75.125	8.184	0.50	28.58	8
15	ATOM	504	OD1 ASN	61	6.383	74.820	9.637	0.50	33.38	8
	ATOM	505	ND2 ASN	61	3.526	73.172	7.071	0.50	34.39	7
	ATOM	506	ND2 ASN	61	4.927	75.991	8.384	0.50	33.52	7
	ATOM	507	C ASN	61	7.371	72.336	8.628	1.00	25.33	6
20	ATOM	508	O ASN	61	8.030	72.535	7.617	1.00	21.46	8
	ATOM	509	N ASP	62	7.932	71.978	9.767	1.00	24.89	7
	ATOM	510	CA ASP	62	9.373	71.842	9.941	1.00	21.37	6
	ATOM	511	CB ASP	62	9.749	72.284	11.372	1.00	16.89	6
	ATOM	512	CG ASP	62	9.620	73.782	11.538	1.00	26.20	6
25	ATOM	513	OD1 ASP	62	9.824	74.549	10.570	1.00	20.81	8
	ATOM	514	OD2 ASP	62	9.276	74.273	12.611	1.00	17.90	8
	ATOM	515	C ASP	62	9.887	70.439	9.645	1.00	18.69	6
	ATOM	516	O ASP	62	11.104	70.209	9.654	1.00	20.50	8
	ATOM	517	N SER	63	9.011	69.477	9.394	1.00	19.81	7
30	ATOM	518	CA SER	63	9.434	68.132	9.015	1.00	19.84	6
	ATOM	519	CB SER	63	8.268	67.164	8.811	1.00	22.04	6
	ATOM	520	OG SER	63	7.506	67.018	10.009	1.00	20.02	8
	ATOM	521	C SER	63	10.196	68.204	7.682	1.00	23.89	6
	ATOM	522	O SER	63	10.015	69.160	6.911	1.00	17.92	8
35	ATOM	523	N GLY	64	11.056	67.195	7.467	1.00	19.50	7
	ATOM	524	CA GLY	64	11.769	67.191	6.190	1.00	22.23	6
	ATOM	525	C GLY	64	13.272	66.965	6.340	1.00	19.81	6
	ATOM	526	O GLY	64	13.744	66.564	7.399	1.00	18.93	8
	ATOM	527	N GLU	65	13.980	67.226	5.238	1.00	17.01	7
40	ATOM	528	CA GLU	65	15.428	67.013	5.269	1.00	21.39	6
	ATOM	529	CBA GLU	65	15.934	66.562	3.901	0.50	13.64	6
	ATOM	530	CBB GLU	65	15.933	66.446	3.947	0.50	23.81	6
	ATOM	531	CGA GLU	65	16.507	65.158	3.813	0.50	15.71	6
	ATOM	532	CGB GLU	65	15.409	65.059	3.602	0.50	32.15	6
45	ATOM	533	CDA GLU	65	16.656	64.679	2.381	0.50	22.33	6
	ATOM	534	CDB GLU	65	15.898	63.965	4.520	0.50	40.56	6
	ATOM	535	OE1 GLU	65	17.428	65.263	1.586	0.50	22.70	8
	ATOM	536	OE1 GLU	65	16.578	64.271	5.525	0.50	41.83	8
	ATOM	537	OE2 GLU	65	15.991	63.686	2.014	0.50	31.04	8
50	ATOM	538	OE2 GLU	65	15.624	62.758	4.278	0.50	46.02	8
	ATOM	539	C GLU	65	16.155	68.324	5.593	1.00	21.56	6
	ATOM	540	O GLU	65	15.756	69.325	5.007	1.00	21.41	8
	ATOM	541	N TYR	66	17.172	68.268	6.458	1.00	21.38	7
	ATOM	542	CA TYR	66	17.966	69.483	6.691	1.00	17.91	6
55	ATOM	543	CB TYR	66	17.954	69.984	8.129	1.00	17.39	6
	ATOM	544	CG TYR	66	16.620	70.563	8.534	1.00	18.08	6
	ATOM	545	CD1 TYR	66	15.605	69.686	8.957	1.00	18.56	6
	ATOM	546	CE1 TYR	66	14.369	70.147	9.323	1.00	16.48	6
	ATOM	547	CD2 TYR	66	16.348	71.921	8.485	1.00	18.23	6
60	ATOM	548	CE2 TYR	66	15.102	72.382	8.867	1.00	18.37	6
	ATOM	549	CZ TYR	66	14.124	71.516	9.279	1.00	18.98	6
	ATOM	550	OH TYR	66	12.872	71.939	9.624	1.00	14.14	8
	ATOM	551	C TYR	66	19.379	69.231	6.212	1.00	13.96	6
	ATOM	552	O TYR	66	19.923	68.135	6.353	1.00	18.14	8
65	ATOM	553	N THR	67	20.010	70.228	5.568	1.00	17.95	7
	ATOM	554	CA THR	67	21.374	70.138	5.117	1.00	18.06	6
	ATOM	555	CB THR	67	21.514	69.844	3.599	1.00	22.52	6
	ATOM	556	OG1 THR	67	20.669	70.737	2.835	1.00	16.85	8
	ATOM	557	CG2 THR	67	21.215	68.371	3.309	1.00	17.46	6
	ATOM	558	C THR	67	22.044	71.508	5.384	1.00	18.76	6
70	ATOM	559	O THR	67	21.354	72.515	5.567	1.00	17.47	8
	ATOM	560	N CYS	68	23.354	71.540	5.389	1.00	19.74	7

	ATOM	561	CA	CYS	68	24.099	72.792	5.597	1.00	23.50	6
	ATOM	562	C	CYS	68	25.382	72.759	4.758	1.00	23.12	6
	ATOM	563	O	CYS	68	25.791	71.712	4.279	1.00	25.07	8
	ATOM	564	CB	CYS	68	24.434	73.082	7.055	1.00	18.70	6
5	ATOM	565	SG	CYS	68	25.675	71.985	7.798	1.00	23.45	16
	ATOM	566	N	GLN	69	25.975	73.920	4.534	1.00	24.47	7
	ATOM	567	CA	GLN	69	27.174	74.121	3.770	1.00	24.99	6
	ATOM	568	CB	GLN	69	26.909	74.344	2.264	1.00	27.22	6
	ATOM	569	CG	GLN	69	28.155	74.057	1.419	1.00	25.14	6
10	ATOM	570	CD	GLN	69	27.857	74.022	-0.065	1.00	32.43	6
	ATOM	571	OE1	GLN	69	26.710	74.166	-0.487	1.00	31.34	8
	ATOM	572	NE2	GLN	69	28.896	73.814	-0.874	1.00	27.89	7
	ATOM	573	C	GLN	69	27.901	75.383	4.266	1.00	27.60	6
	ATOM	574	O	GLN	69	27.289	76.352	4.734	1.00	25.37	8
15	ATOM	575	N	THR	70	29.206	75.318	4.115	1.00	28.73	7
	ATOM	576	CA	THR	70	30.059	76.465	4.439	1.00	32.10	6
	ATOM	577	CB	THR	70	31.125	76.153	5.491	1.00	33.36	6
	ATOM	578	OG1	THR	70	30.619	75.311	6.553	1.00	45.26	8
	ATOM	579	CG2	THR	70	31.453	77.444	6.210	1.00	50.20	6
20	ATOM	580	C	THR	70	30.737	76.890	3.138	1.00	32.77	6
	ATOM	581	O	THR	70	30.680	76.170	2.130	1.00	30.75	8
	ATOM	582	N	GLY	71	31.472	78.007	3.175	1.00	31.83	7
	ATOM	583	CA	GLY	71	32.224	78.469	2.033	1.00	27.97	6
	ATOM	584	C	GLY	71	33.376	77.544	1.690	1.00	29.94	6
25	ATOM	585	O	GLY	71	33.938	77.668	0.596	1.00	32.37	8
	ATOM	586	N	GLN	72	33.842	76.707	2.594	1.00	24.86	7
	ATOM	587	CA	GLN	72	34.920	75.779	2.457	1.00	27.14	6
	ATOM	588	CB	GLN	72	35.868	75.974	3.667	1.00	27.31	6
	ATOM	589	CG	GLN	72	36.291	77.451	3.825	1.00	30.51	6
30	ATOM	590	CD	GLN	72	36.961	77.995	2.567	1.00	30.53	6
	ATOM	591	OE1	GLN	72	37.981	77.441	2.161	1.00	39.95	8
	ATOM	592	NE2	GLN	72	36.402	79.014	1.944	1.00	31.16	7
	ATOM	593	C	GLN	72	34.530	74.305	2.441	1.00	29.60	6
	ATOM	594	O	GLN	72	35.419	73.442	2.578	1.00	30.82	8
35	ATOM	595	N	THR	73	33.248	73.954	2.380	1.00	25.83	7
	ATOM	596	CA	THR	73	32.861	72.549	2.426	1.00	26.62	6
	ATOM	597	CB	THR	73	32.278	72.135	3.792	1.00	26.64	6
	ATOM	598	OG1	THR	73	31.226	73.051	4.138	1.00	27.54	8
	ATOM	599	CG2	THR	73	33.313	72.124	4.897	1.00	28.16	6
40	ATOM	600	C	THR	73	31.824	72.223	1.371	1.00	26.31	6
	ATOM	601	O	THR	73	31.210	73.110	0.776	1.00	28.00	8
	ATOM	602	N	SER	74	31.685	70.927	1.074	1.00	28.62	7
	ATOM	603	CA	SER	74	30.592	70.605	0.112	1.00	29.44	6
	ATOM	604	CB	SER	74	31.020	69.470	-0.803	1.00	30.45	6
45	ATOM	605	OG	SER	74	31.407	68.399	0.034	1.00	41.05	8
	ATOM	606	C	SER	74	29.366	70.395	0.992	1.00	26.65	6
	ATOM	607	O	SER	74	29.461	70.438	2.228	1.00	25.57	8
	ATOM	608	N	LEU	75	28.178	70.281	0.442	1.00	29.47	7
	ATOM	609	CA	LEU	75	26.915	70.163	1.158	1.00	25.10	6
50	ATOM	610	CB	LEU	75	25.749	70.141	0.159	1.00	27.83	6
	ATOM	611	CG	LEU	75	24.348	70.136	0.777	1.00	27.24	6
	ATOM	612	CD1	LEU	75	23.888	71.554	1.094	1.00	24.13	6
	ATOM	613	CD2	LEU	75	23.349	69.420	-0.133	1.00	24.42	6
	ATOM	614	C	LEU	75	26.884	68.973	2.087	1.00	25.84	6
55	ATOM	615	O	LEU	75	27.300	67.858	1.711	1.00	22.45	8
	ATOM	616	N	SER	76	26.376	69.158	3.315	1.00	23.31	7
	ATOM	617	CA	SER	76	26.357	68.009	4.219	1.00	25.20	6
	ATOM	618	CB	SER	76	25.916	68.402	5.644	1.00	26.64	6
	ATOM	619	OG	SER	76	24.514	68.663	5.624	1.00	29.43	8
60	ATOM	620	C	SER	76	25.346	66.955	3.738	1.00	23.00	6
	ATOM	621	O	SER	76	24.431	67.304	3.006	1.00	21.02	8
	ATOM	622	N	ASP	77	25.506	65.739	4.241	1.00	22.24	7
	ATOM	623	CA	ASP	77	24.493	64.712	4.094	1.00	26.03	6
	ATOM	624	CB	ASP	77	24.907	63.362	4.683	1.00	20.27	6
65	ATOM	625	CG	ASP	77	25.914	62.676	3.758	1.00	25.73	6
	ATOM	626	OD1	ASP	77	25.821	62.893	2.541	1.00	23.79	8
	ATOM	627	OD2	ASP	77	26.769	61.954	4.292	1.00	28.92	8
	ATOM	628	C	ASP	77	23.267	65.191	4.929	1.00	25.85	6
	ATOM	629	O	ASP	77	23.423	65.904	5.914	1.00	24.00	8
70	ATOM	630	N	PRO	78	22.098	64.758	4.492	1.00	27.37	7
	ATOM	631	CD	PRO	78	21.917	63.917	3.275	1.00	26.84	6

100

5	ATOM	632	CA	PRO	78	20.849	65.130	5.098	1.00	25.42	6
	ATOM	633	CB	PRO	78	19.795	64.592	4.141	1.00	28.38	6
	ATOM	634	CG	PRO	78	20.453	63.586	3.272	1.00	27.24	6
	ATOM	635	C	PRO	78	20.575	64.556	6.479	1.00	25.28	6
	ATOM	636	O	PRO	78	21.006	63.459	6.820	1.00	23.68	8
	ATOM	637	N	VAL	79	19.833	65.331	7.265	1.00	20.24	7
	ATOM	638	CA	VAL	79	19.287	64.861	8.535	1.00	18.86	6
	ATOM	639	CB	VAL	79	19.850	65.516	9.783	1.00	19.49	6
10	ATOM	640	CG1	VAL	79	19.042	65.239	11.046	1.00	22.25	6
	ATOM	641	CG2	VAL	79	21.275	64.959	10.036	1.00	21.95	6
	ATOM	642	C	VAL	79	17.777	65.046	8.399	1.00	19.76	6
	ATOM	643	O	VAL	79	17.283	66.130	8.076	1.00	22.34	8
	ATOM	644	N	HIS	80	17.024	63.955	8.566	1.00	19.43	7
15	ATOM	645	CA	HIS	80	15.584	63.976	8.387	1.00	18.11	6
	ATOM	646	CB	HIS	80	15.130	62.621	7.784	1.00	26.87	6
	ATOM	647	CG	HIS	80	13.712	62.754	7.293	1.00	31.93	6
	ATOM	648	CD2	HIS	80	13.194	62.983	6.069	1.00	27.05	6
	ATOM	649	ND1	HIS	80	12.637	62.697	8.176	1.00	34.35	7
20	ATOM	650	CE1	HIS	80	11.525	62.847	7.480	1.00	34.80	6
	ATOM	651	NE2	HIS	80	11.831	63.016	6.210	1.00	34.81	7
	ATOM	652	C	HIS	80	14.865	64.187	9.718	1.00	23.08	6
	ATOM	653	O	HIS	80	15.096	63.496	10.709	1.00	23.37	8
	ATOM	654	N	LEU	81	13.953	65.138	9.747	1.00	19.18	7
25	ATOM	655	CA	LEU	81	13.244	65.478	10.957	1.00	21.58	6
	ATOM	656	CB	LEU	81	13.567	66.937	11.331	1.00	18.20	6
	ATOM	657	CG	LEU	81	12.847	67.381	12.605	1.00	18.21	6
	ATOM	658	CD1	LEU	81	13.496	66.708	13.812	1.00	19.39	6
	ATOM	659	CD2	LEU	81	12.865	68.912	12.696	1.00	14.76	6
30	ATOM	660	C	LEU	81	11.747	65.255	10.783	1.00	19.36	6
	ATOM	661	O	LEU	81	11.225	65.543	9.720	1.00	20.96	8
	ATOM	662	N	THR	82	11.100	64.689	11.793	1.00	19.61	7
	ATOM	663	CA	THR	82	9.642	64.463	11.680	1.00	18.45	6
	ATOM	664	CB	THR	82	9.316	62.950	11.683	1.00	25.98	6
35	ATOM	665	OG1	THR	82	9.907	62.351	10.527	1.00	18.89	8
	ATOM	666	CG2	THR	82	7.795	62.775	11.666	1.00	24.98	6
	ATOM	667	C	THR	82	8.971	65.100	12.891	1.00	16.02	6
	ATOM	668	O	THR	82	9.248	64.735	14.035	1.00	14.79	8
	ATOM	669	N	VAL	83	8.075	66.045	12.647	1.00	16.23	7
40	ATOM	670	CA	VAL	83	7.451	66.758	13.753	1.00	16.97	6
	ATOM	671	CB	VAL	83	7.559	68.282	13.530	1.00	12.81	6
	ATOM	672	CG1	VAL	83	7.051	68.972	14.799	1.00	15.92	6
	ATOM	673	CG2	VAL	83	8.986	68.760	13.246	1.00	11.78	6
	ATOM	674	C	VAL	83	6.020	66.264	13.892	1.00	19.97	6
45	ATOM	675	O	VAL	83	5.261	66.329	12.918	1.00	18.57	8
	ATOM	676	N	LEU	84	5.686	65.756	15.075	1.00	16.89	7
	ATOM	677	CA	LEU	84	4.372	65.188	15.312	1.00	19.89	6
	ATOM	678	CB	LEU	84	4.621	63.786	15.890	1.00	18.15	6
	ATOM	679	CG	LEU	84	5.491	62.863	15.021	1.00	23.40	6
50	ATOM	680	CD1	LEU	84	5.927	61.690	15.868	1.00	25.20	6
	ATOM	681	CD2	LEU	84	4.752	62.396	13.758	1.00	20.46	6
	ATOM	682	C	LEU	84	3.487	66.016	16.228	1.00	22.29	6
	ATOM	683	O	LEU	84	3.928	66.891	16.975	1.00	23.90	8
	ATOM	684	N	PHE	85	2.189	65.750	16.218	1.00	21.03	7
55	ATOM	685	CA	PHE	85	1.254	66.444	17.111	1.00	22.92	6
	ATOM	686	CB	PHE	85	0.399	67.431	16.333	1.00	21.76	6
	ATOM	687	CG	PHE	85	-0.440	68.350	17.184	1.00	27.90	6
	ATOM	688	CD1	PHE	85	0.103	69.013	18.266	1.00	28.30	6
	ATOM	689	CD2	PHE	85	-1.787	68.533	16.899	1.00	26.61	6
60	ATOM	690	CE1	PHE	85	-0.664	69.874	19.040	1.00	29.65	6
	ATOM	691	CE2	PHE	85	-2.559	69.386	17.668	1.00	25.61	6
	ATOM	692	CZ	PHE	85	-1.996	70.047	18.733	1.00	28.75	6
	ATOM	693	C	PHE	85	0.455	65.399	17.852	1.00	21.99	6
	ATOM	694	O	PHE	85	-0.642	65.000	17.426	1.00	22.11	8
65	ATOM	695	N	GLU	86	1.023	64.883	18.938	1.00	20.76	7
	ATOM	696	CA	GLU	86	0.421	63.762	19.702	1.00	18.04	6
	ATOM	697	CB	GLU	86	1.142	62.463	19.210	1.00	20.84	6
	ATOM	698	CG	GLU	86	0.711	61.815	17.911	1.00	25.05	6
	ATOM	699	CD	GLU	86	1.647	61.048	17.019	1.00	41.96	6
70	ATOM	700	OE1	GLU	86	2.719	60.507	17.416	1.00	46.14	8
	ATOM	701	OE2	GLU	86	1.429	60.893	15.765	1.00	40.77	8
	ATOM	702	C	GLU	86	0.694	64.026	21.176	1.00	18.46	6

101

	ATOM	703	O	GLU	86	1.588	64.839	21.462	1.00	16.67	8
	ATOM	704	N	TRP	87	0.031	63.408	22.156	1.00	12.60	7
	ATOM	705	CA	TRP	87	0.328	63.631	23.553	1.00	13.01	6
	ATOM	706	CB	TRP	87	-0.808	63.056	24.411	1.00	18.40	6
5	ATOM	707	CG	TRP	87	-1.922	64.023	24.687	1.00	21.87	6
	ATOM	708	CD2	TRP	87	-1.812	65.176	25.521	1.00	21.14	6
	ATOM	709	CE2	TRP	87	-3.065	65.805	25.526	1.00	24.31	6
	ATOM	710	CE3	TRP	87	-0.767	65.738	26.255	1.00	24.84	6
	ATOM	711	CD1	TRP	87	-3.216	63.985	24.231	1.00	22.52	6
10	ATOM	712	NE1	TRP	87	-3.907	65.069	24.734	1.00	22.53	7
	ATOM	713	CZ2	TRP	87	-3.303	66.966	26.266	1.00	29.91	6
	ATOM	714	CZ3	TRP	87	-0.998	66.890	26.987	1.00	29.83	6
	ATOM	715	CH2	TRP	87	-2.254	67.499	26.970	1.00	29.09	6
	ATOM	716	C	TRP	87	1.599	62.967	24.068	1.00	15.44	6
15	ATOM	717	O	TRP	87	2.178	63.499	25.018	1.00	16.68	8
	ATOM	718	N	LEU	88	2.036	61.873	23.447	1.00	14.44	7
	ATOM	719	CA	LEU	88	3.153	61.051	23.861	1.00	20.07	6
	ATOM	720	CB	LEU	88	2.596	59.942	24.783	1.00	17.49	6
	ATOM	721	CG	LEU	88	3.608	59.303	25.769	1.00	16.97	6
20	ATOM	722	CD1	LEU	88	4.062	60.299	26.830	1.00	17.38	6
	ATOM	723	CD2	LEU	88	2.987	58.053	26.370	1.00	13.93	6
	ATOM	724	C	LEU	88	3.889	60.399	22.677	1.00	20.44	6
	ATOM	725	O	LEU	88	3.255	59.857	21.752	1.00	19.65	8
	ATOM	726	N	VAL	89	5.218	60.517	22.620	1.00	18.11	7
25	ATOM	727	CA	VAL	89	5.998	59.926	21.542	1.00	14.66	6
	ATOM	728	CBA	VAL	89	6.686	61.029	20.699	0.50	7.52	6
	ATOM	729	CBB	VAL	89	6.677	60.941	20.604	0.50	13.86	6
	ATOM	730	CG1	VAL	89	7.573	61.890	21.597	0.50	7.13	6
30	ATOM	731	CG1	VAL	89	5.696	61.409	19.543	0.50	15.87	6
	ATOM	732	CG2	VAL	89	7.501	60.486	19.531	0.50	3.91	6
	ATOM	733	CG2	VAL	89	7.264	62.090	21.402	0.50	18.65	6
	ATOM	734	C	VAL	89	7.109	59.032	22.107	1.00	15.71	6
	ATOM	735	O	VAL	89	7.689	59.262	23.179	1.00	14.52	8
	ATOM	736	N	LEU	90	7.379	57.958	21.386	1.00	15.13	7
35	ATOM	737	CA	LEU	90	8.520	57.133	21.703	1.00	13.72	6
	ATOM	738	CB	LEU	90	8.287	55.625	21.488	1.00	17.87	6
	ATOM	739	CG	LEU	90	9.650	54.978	21.873	1.00	26.07	6
	ATOM	740	CD1	LEU	90	9.479	54.066	23.036	1.00	30.57	6
40	ATOM	741	CD2	LEU	90	10.373	54.463	20.662	1.00	25.07	6
	ATOM	742	C	LEU	90	9.657	57.674	20.803	1.00	17.58	6
	ATOM	743	O	LEU	90	9.611	57.517	19.576	1.00	14.46	8
	ATOM	744	N	GLN	91	10.673	58.298	21.412	1.00	15.83	7
	ATOM	745	CA	GLN	91	11.745	58.908	20.623	1.00	17.70	6
	ATOM	746	CB	GLN	91	12.252	60.238	21.264	1.00	15.03	6
45	ATOM	747	CG	GLN	91	11.105	61.231	21.472	1.00	12.81	6
	ATOM	748	CD	GLN	91	11.564	62.636	21.868	1.00	15.79	6
	ATOM	749	OE1	GLN	91	12.023	62.823	22.988	1.00	14.61	8
	ATOM	750	NE2	GLN	91	11.409	63.610	20.984	1.00	16.27	7
50	ATOM	751	C	GLN	91	12.971	58.042	20.375	1.00	17.71	6
	ATOM	752	O	GLN	91	13.370	57.296	21.268	1.00	19.37	8
	ATOM	753	N	THR	92	13.607	58.207	19.218	1.00	14.05	7
	ATOM	754	CA	THR	92	14.853	57.488	18.934	1.00	19.01	6
	ATOM	755	CB	THR	92	14.562	56.225	18.089	1.00	16.40	6
55	ATOM	756	OG1	THR	92	15.769	55.485	17.905	1.00	18.39	8
	ATOM	757	CG2	THR	92	13.943	56.499	16.720	1.00	10.45	6
	ATOM	758	C	THR	92	15.803	58.416	18.173	1.00	18.96	6
	ATOM	759	O	THR	92	15.339	59.272	17.409	1.00	21.88	8
	ATOM	760	N	PRO	93	17.095	58.153	18.251	1.00	18.78	7
60	ATOM	761	CD	PRO	93	17.747	57.169	19.135	1.00	22.16	6
	ATOM	762	CA	PRO	93	18.090	58.929	17.530	1.00	24.37	6
	ATOM	763	CB	PRO	93	19.352	58.803	18.371	1.00	24.99	6
	ATOM	764	CG	PRO	93	19.162	57.609	19.235	1.00	26.05	6
	ATOM	765	C	PRO	93	18.285	58.362	16.138	1.00	27.02	6
65	ATOM	766	O	PRO	93	18.852	59.019	15.248	1.00	27.04	8
	ATOM	767	N	HIS	94	17.978	57.069	15.960	1.00	24.22	7
	ATOM	768	CA	HIS	94	18.114	56.421	14.651	1.00	25.72	6
	ATOM	769	CB	HIS	94	19.444	55.690	14.439	1.00	20.09	6
	ATOM	770	CG	HIS	94	20.639	56.587	14.595	1.00	21.67	6
	ATOM	771	CD2	HIS	94	21.161	57.530	13.798	1.00	23.30	6
70	ATOM	772	ND1	HIS	94	21.380	56.595	15.754	1.00	27.49	7
	ATOM	773	CE1	HIS	94	22.338	57.501	15.657	1.00	26.54	6

	ATOM	774	NE2	HIS	94	22.211	58.078	14.482	1.00	32.10	7
	ATOM	775	C	HIS	94	17.038	55.350	14.453	1.00	24.49	6
	ATOM	776	O	HIS	94	16.481	54.838	15.429	1.00	24.01	8
5	ATOM	777	N	LEU	95	16.847	54.929	13.214	1.00	21.96	7
	ATOM	778	CA	LEU	95	15.900	53.847	12.960	1.00	26.06	6
	ATOM	779	CB	LEU	95	15.014	54.118	11.741	1.00	26.66	6
	ATOM	780	CG	LEU	95	13.994	55.248	11.899	1.00	35.19	6
	ATOM	781	CD1	LEU	95	13.449	55.601	10.525	1.00	25.66	6
10	ATOM	782	CD2	LEU	95	12.895	54.908	12.900	1.00	24.13	6
	ATOM	783	C	LEU	95	16.626	52.525	12.720	1.00	26.30	6
	ATOM	784	O	LEU	95	15.999	51.464	12.790	1.00	26.83	8
	ATOM	785	N	GLU	96	17.884	52.601	12.326	1.00	25.44	7
	ATOM	786	CA	GLU	96	18.688	51.413	12.087	1.00	28.55	6
	ATOM	787	CB	GLU	96	19.062	51.144	10.634	1.00	28.97	6
15	ATOM	788	CG	GLU	96	17.977	51.334	9.605	1.00	34.46	6
	ATOM	789	CD	GLU	96	18.414	51.109	8.168	1.00	42.07	6
	ATOM	790	OE1	GLU	96	19.560	50.709	7.882	1.00	41.53	8
	ATOM	791	OE2	GLU	96	17.592	51.343	7.256	1.00	45.31	8
	ATOM	792	C	GLU	96	19.995	51.575	12.885	1.00	32.22	6
20	ATOM	793	O	GLU	96	20.525	52.686	13.015	1.00	31.68	8
	ATOM	794	N	PHE	97	20.396	50.487	13.538	1.00	29.38	7
	ATOM	795	CA	PHE	97	21.622	50.447	14.315	1.00	31.45	6
	ATOM	796	CB	PHE	97	21.388	50.351	15.832	1.00	29.88	6
	ATOM	797	CG	PHE	97	20.640	51.497	16.464	1.00	28.91	6
25	ATOM	798	CD1	PHE	97	19.256	51.580	16.386	1.00	19.88	6
	ATOM	799	CD2	PHE	97	21.311	52.503	17.131	1.00	27.06	6
	ATOM	800	CE1	PHE	97	18.557	52.624	16.971	1.00	23.29	6
	ATOM	801	CE2	PHE	97	20.622	53.545	17.719	1.00	23.27	6
30	ATOM	802	CZ	PHE	97	19.244	53.626	17.636	1.00	25.87	6
	ATOM	803	C	PHE	97	22.455	49.233	13.861	1.00	31.11	6
	ATOM	804	O	PHE	97	22.007	48.334	13.164	1.00	32.31	8
	ATOM	805	N	GLN	98	23.726	49.213	14.219	1.00	34.14	7
	ATOM	806	CA	GLN	98	24.636	48.131	13.939	1.00	33.31	6
35	ATOM	807	CB	GLN	98	26.042	48.629	13.635	1.00	38.15	6
	ATOM	808	CG	GLN	98	26.207	49.422	12.356	1.00	45.65	6
	ATOM	809	CD	GLN	98	25.763	48.712	11.097	1.00	49.99	6
	ATOM	810	OE1	GLN	98	26.455	47.828	10.589	1.00	52.58	8
	ATOM	811	NE2	GLN	98	24.603	49.088	10.563	1.00	53.06	7
40	ATOM	812	C	GLN	98	24.662	47.218	15.172	1.00	31.48	6
	ATOM	813	O	GLN	98	24.459	47.664	16.300	1.00	27.98	8
	ATOM	814	N	GLU	99	24.990	45.955	14.920	1.00	30.75	7
	ATOM	815	CA	GLU	99	25.112	44.978	16.009	1.00	32.56	6
	ATOM	816	CB	GLU	99	25.598	43.653	15.420	1.00	36.89	6
45	ATOM	817	CG	GLU	99	25.204	42.392	16.141	1.00	44.86	6
	ATOM	818	CD	GLU	99	24.771	41.288	15.184	1.00	48.45	6
	ATOM	819	OE1	GLU	99	23.802	40.573	15.521	1.00	53.90	8
	ATOM	820	OE2	GLU	99	25.400	41.148	14.118	1.00	50.56	8
	ATOM	821	C	GLU	99	26.130	45.551	16.980	1.00	31.14	6
50	ATOM	822	O	GLU	99	27.136	46.048	16.475	1.00	31.94	8
	ATOM	823	N	GLY	100	25.919	45.571	18.275	1.00	32.19	7
	ATOM	824	CA	GLY	100	26.874	46.123	19.217	1.00	31.10	6
	ATOM	825	C	GLY	100	26.643	47.541	19.696	1.00	31.51	6
	ATOM	826	O	GLY	100	27.082	47.931	20.789	1.00	30.30	8
55	ATOM	827	N	GLU	101	25.948	48.369	18.921	1.00	34.41	7
	ATOM	828	CA	GLU	101	25.675	49.746	19.297	1.00	34.07	6
	ATOM	829	CB	GLU	101	24.949	50.452	18.148	1.00	37.86	6
	ATOM	830	CG	GLU	101	25.777	50.676	16.889	1.00	48.38	6
	ATOM	831	CD	GLU	101	24.984	51.520	15.895	1.00	49.17	6
60	ATOM	832	OE1	GLU	101	24.251	52.408	16.385	1.00	58.51	8
	ATOM	833	OE2	GLU	101	25.046	51.333	14.669	1.00	48.56	8
	ATOM	834	C	GLU	101	24.783	49.848	20.537	1.00	33.06	6
	ATOM	835	O	GLU	101	24.086	48.888	20.886	1.00	27.70	8
	ATOM	836	N	THR	102	24.747	51.057	21.107	1.00	31.92	7
65	ATOM	837	CA	THR	102	23.870	51.303	22.248	1.00	32.85	6
	ATOM	838	CB	THR	102	24.508	52.161	23.341	1.00	35.75	6
	ATOM	839	OG1	THR	102	25.546	51.438	24.021	1.00	36.79	8
	ATOM	840	CG2	THR	102	23.532	52.577	24.441	1.00	35.82	6
	ATOM	841	C	THR	102	22.582	51.944	21.721	1.00	32.54	6
70	ATOM	842	O	THR	102	22.650	52.932	20.991	1.00	30.03	8
	ATOM	843	N	ILE	103	21.431	51.329	22.014	1.00	28.53	7
	ATOM	844	CA	ILE	103	20.162	51.939	21.590	1.00	25.40	6

103

5	ATOM	845	CB	ILE	103	19.131	50.873	21.163	1.00	26.58	6
	ATOM	846	CG2	ILE	103	17.776	51.496	20.828	1.00	25.47	6
	ATOM	847	CG1	ILE	103	19.669	50.080	19.971	1.00	21.79	6
	ATOM	848	CD1	ILE	103	18.739	49.003	19.438	1.00	19.73	6
	ATOM	849	C	ILE	103	19.624	52.753	22.767	1.00	25.27	6
	ATOM	850	O	ILE	103	19.439	52.181	23.853	1.00	23.06	8
	ATOM	851	N	MET	104	19.443	54.059	22.591	1.00	24.90	7
	ATOM	852	CA	MET	104	18.893	54.913	23.639	1.00	21.55	6
10	ATOM	853	CB	MET	104	19.797	56.097	23.963	1.00	33.48	6
	ATOM	854	CG	MET	104	20.810	55.826	25.101	1.00	29.68	6
	ATOM	855	SD	MET	104	21.940	57.256	25.242	1.00	46.02	16
	ATOM	856	CE	MET	104	22.667	57.216	23.589	1.00	31.10	6
	ATOM	857	C	MET	104	17.528	55.456	23.215	1.00	21.27	6
15	ATOM	858	O	MET	104	17.374	55.991	22.106	1.00	22.96	8
	ATOM	859	N	LEU	105	16.503	55.242	24.027	1.00	20.55	7
	ATOM	860	CA	LEU	105	15.134	55.668	23.728	1.00	22.33	6
	ATOM	861	CB	LEU	105	14.192	54.450	23.550	1.00	14.66	6
	ATOM	862	CG	LEU	105	14.713	53.389	22.561	1.00	18.89	6
20	ATOM	863	CD1	LEU	105	13.796	52.178	22.489	1.00	19.44	6
	ATOM	864	CD2	LEU	105	14.882	54.056	21.186	1.00	18.70	6
	ATOM	865	C	LEU	105	14.567	56.559	24.817	1.00	20.15	6
	ATOM	866	O	LEU	105	15.050	56.506	25.950	1.00	18.39	8
	ATOM	867	N	ARG	106	13.523	57.324	24.483	1.00	18.25	7
25	ATOM	868	CA	ARG	106	12.912	58.174	25.516	1.00	17.87	6
	ATOM	869	CB	ARG	106	13.607	59.553	25.508	1.00	14.96	6
	ATOM	870	CG	ARG	106	12.834	60.597	26.290	1.00	16.79	6
	ATOM	871	CD	ARG	106	13.699	61.788	26.757	1.00	19.51	6
	ATOM	872	NE	ARG	106	13.334	62.927	26.025	1.00	23.46	7
	ATOM	873	CZ	ARG	106	12.990	64.174	26.065	1.00	24.43	6
30	ATOM	874	NH1	ARG	106	12.923	64.892	27.176	1.00	25.93	7
	ATOM	875	NH2	ARG	106	12.697	64.795	24.936	1.00	18.72	7
	ATOM	876	C	ARG	106	11.422	58.321	25.304	1.00	18.56	6
	ATOM	877	O	ARG	106	10.998	58.479	24.142	1.00	20.43	8
	ATOM	878	N	CYS	107	10.642	58.246	26.378	1.00	15.23	7
35	ATOM	879	CA	CYS	107	9.189	58.419	26.292	1.00	14.89	6
	ATOM	880	C	CYS	107	8.934	59.891	26.583	1.00	15.28	6
	ATOM	881	O	CYS	107	9.296	60.294	27.690	1.00	15.96	8
	ATOM	882	CB	CYS	107	8.438	57.565	27.322	1.00	14.55	6
	ATOM	883	SG	CYS	107	6.691	57.368	27.013	1.00	13.91	16
40	ATOM	884	N	HIS	108	8.446	60.653	25.604	1.00	15.07	7
	ATOM	885	CA	HIS	108	8.334	62.103	25.811	1.00	11.91	6
	ATOM	886	CB	HIS	108	9.190	62.757	24.708	1.00	16.03	6
	ATOM	887	CG	HIS	108	9.119	64.240	24.572	1.00	16.94	6
	ATOM	888	CD2	HIS	108	9.068	65.023	23.462	1.00	17.64	6
45	ATOM	889	ND1	HIS	108	9.103	65.108	25.657	1.00	17.41	7
	ATOM	890	CE1	HIS	108	9.034	66.350	25.215	1.00	17.37	6
	ATOM	891	NE2	HIS	108	9.021	66.333	23.895	1.00	20.00	7
	ATOM	892	C	HIS	108	6.925	62.647	25.733	1.00	11.83	6
	ATOM	893	O	HIS	108	6.224	62.361	24.762	1.00	12.54	8
50	ATOM	894	N	SER	109	6.515	63.502	26.654	1.00	13.70	7
	ATOM	895	CA	SER	109	5.160	64.091	26.605	1.00	11.70	6
	ATOM	896	CB	SER	109	4.583	64.134	28.041	1.00	13.47	6
	ATOM	897	OG	SER	109	5.609	64.845	28.800	1.00	16.16	8
	ATOM	898	C	SER	109	5.190	65.459	25.970	1.00	14.21	6
55	ATOM	899	O	SER	109	6.180	66.232	25.903	1.00	14.63	8
	ATOM	900	N	TRP	110	4.047	65.804	25.381	1.00	16.58	7
	ATOM	901	CA	TRP	110	3.860	67.102	24.708	1.00	16.04	6
	ATOM	902	CB	TRP	110	2.480	67.158	24.072	1.00	18.73	6
	ATOM	903	CG	TRP	110	2.187	68.425	23.306	1.00	21.24	6
60	ATOM	904	CD2	TRP	110	1.135	69.339	23.589	1.00	20.70	6
	ATOM	905	CE2	TRP	110	1.193	70.361	22.616	1.00	25.92	6
	ATOM	906	CE3	TRP	110	0.112	69.372	24.549	1.00	24.16	6
	ATOM	907	CD1	TRP	110	2.827	68.908	22.214	1.00	22.22	6
	ATOM	908	NE1	TRP	110	2.233	70.069	21.765	1.00	22.81	7
65	ATOM	909	CZ2	TRP	110	0.276	71.404	22.568	1.00	24.18	6
	ATOM	910	CZ3	TRP	110	-0.781	70.434	24.509	1.00	30.15	6
	ATOM	911	CH2	TRP	110	-0.698	71.433	23.526	1.00	31.04	6
	ATOM	912	C	TRP	110	4.082	68.245	25.681	1.00	14.44	6
	ATOM	913	O	TRP	110	3.665	68.219	26.852	1.00	17.08	8
70	ATOM	914	N	LYS	111	4.928	69.199	25.294	1.00	19.42	7
	ATOM	915	CA	LYS	111	5.347	70.325	26.115	1.00	19.40	6

	ATOM	916	CB	LYS	111	4.131	71.241	26.418	1.00	21.00	6
	ATOM	917	CG	LYS	111	3.583	71.904	25.155	1.00	24.94	6
	ATOM	918	CD	LYS	111	2.124	72.287	25.337	1.00	34.17	6
5	ATOM	919	CE	LYS	111	1.952	73.719	25.781	1.00	37.49	6
	ATOM	920	NZ	LYS	111	2.783	74.668	24.987	1.00	52.66	7
	ATOM	921	C	LYS	111	5.940	69.921	27.450	1.00	20.33	6
	ATOM	922	O	LYS	111	5.905	70.694	28.419	1.00	16.80	8
	ATOM	923	N	ASP	112	6.444	68.695	27.602	1.00	18.28	7
10	ATOM	924	CA	ASP	112	6.989	68.233	28.861	1.00	20.31	6
	ATOM	925	CB	ASP	112	8.242	69.088	29.191	1.00	24.52	6
	ATOM	926	CG	ASP	112	9.306	68.737	28.155	1.00	31.39	6
	ATOM	927	OD1	ASP	112	9.700	67.545	28.119	1.00	39.68	8
	ATOM	928	OD2	ASP	112	9.719	69.588	27.360	1.00	35.00	8
15	ATOM	929	C	ASP	112	6.015	68.203	30.018	1.00	23.40	6
	ATOM	930	O	ASP	112	6.426	68.475	31.148	1.00	23.42	8
	ATOM	931	N	LYS	113	4.731	67.889	29.785	1.00	23.10	7
	ATOM	932	CA	LYS	113	3.792	67.721	30.891	1.00	22.35	6
	ATOM	933	CB	LYS	113	2.352	67.432	30.437	1.00	21.68	6
20	ATOM	934	CG	LYS	113	1.758	68.611	29.659	1.00	27.09	6
	ATOM	935	CD	LYS	113	0.232	68.574	29.608	1.00	28.34	6
	ATOM	936	CE	LYS	113	-0.269	69.780	28.816	1.00	32.92	6
	ATOM	937	NZ	LYS	113	-0.196	71.075	29.554	1.00	33.55	7
	ATOM	938	C	LYS	113	4.352	66.597	31.748	1.00	19.86	6
25	ATOM	939	O	LYS	113	4.890	65.603	31.264	1.00	21.45	8
	ATOM	940	N	PRO	114	4.288	66.761	33.066	1.00	20.08	7
	ATOM	941	CD	PRO	114	3.701	67.928	33.768	1.00	16.95	6
	ATOM	942	CA	PRO	114	4.923	65.801	33.957	1.00	17.00	6
	ATOM	943	CB	PRO	114	4.548	66.292	35.342	1.00	19.22	6
30	ATOM	944	CG	PRO	114	4.169	67.733	35.176	1.00	21.34	6
	ATOM	945	C	PRO	114	4.451	64.405	33.636	1.00	16.83	6
	ATOM	946	O	PRO	114	3.237	64.125	33.512	1.00	16.01	8
	ATOM	947	N	LEU	115	5.414	63.483	33.560	1.00	15.95	7
35	ATOM	948	CA	LEU	115	5.081	62.104	33.215	1.00	17.10	6
	ATOM	949	CB	LEU	115	5.769	61.879	31.856	1.00	16.83	6
	ATOM	950	CG	LEU	115	5.790	60.498	31.231	1.00	21.64	6
	ATOM	951	CD1	LEU	115	4.399	60.132	30.733	1.00	19.24	6
	ATOM	952	CD2	LEU	115	6.777	60.486	30.043	1.00	19.80	6
	ATOM	953	C	LEU	115	5.606	61.116	34.226	1.00	21.13	6
40	ATOM	954	O	LEU	115	6.788	61.200	34.569	1.00	18.84	8
	ATOM	955	N	VAL	116	4.839	60.105	34.630	1.00	20.51	7
	ATOM	956	CA	VAL	116	5.314	59.073	35.545	1.00	20.40	6
	ATOM	957	CB	VAL	116	4.787	59.277	36.971	1.00	18.72	6
	ATOM	958	CG1	VAL	116	5.313	60.547	37.644	1.00	22.67	6
45	ATOM	959	CG2	VAL	116	3.257	59.328	36.998	1.00	22.12	6
	ATOM	960	C	VAL	116	4.807	57.703	35.073	1.00	19.73	6
	ATOM	961	O	VAL	116	3.910	57.682	34.223	1.00	20.76	8
	ATOM	962	N	LYS	117	5.268	56.615	35.693	1.00	17.34	7
	ATOM	963	CA	LYS	117	4.760	55.290	35.381	1.00	20.33	6
50	ATOM	964	CB	LYS	117	3.271	55.182	35.802	1.00	21.74	6
	ATOM	965	CG	LYS	117	3.115	54.927	37.301	1.00	24.43	6
	ATOM	966	CD	LYS	117	1.793	55.445	37.832	1.00	32.69	6
	ATOM	967	CE	LYS	117	0.798	54.314	38.056	1.00	40.27	6
	ATOM	968	NZ	LYS	117	-0.568	54.865	38.266	1.00	44.06	7
55	ATOM	969	C	LYS	117	4.956	54.936	33.914	1.00	18.58	6
	ATOM	970	O	LYS	117	4.026	54.535	33.234	1.00	24.35	8
	ATOM	971	N	VAL	118	6.181	55.063	33.417	1.00	20.45	7
	ATOM	972	CA	VAL	118	6.542	54.798	32.039	1.00	19.15	6
	ATOM	973	CB	VAL	118	7.756	55.643	31.607	1.00	12.17	6
60	ATOM	974	CG1	VAL	118	8.199	55.396	30.176	1.00	18.94	6
	ATOM	975	CG2	VAL	118	7.408	57.129	31.794	1.00	16.75	6
	ATOM	976	C	VAL	118	6.868	53.330	31.797	1.00	18.58	6
	ATOM	977	O	VAL	118	7.606	52.717	32.564	1.00	17.16	8
	ATOM	978	N	THR	119	6.307	52.803	30.711	1.00	15.94	7
65	ATOM	979	CA	THR	119	6.527	51.425	30.335	1.00	16.50	6
	ATOM	980	CB	THR	119	5.291	50.523	30.367	1.00	19.59	6
	ATOM	981	OG1	THR	119	4.770	50.410	31.693	1.00	23.11	8
	ATOM	982	CG2	THR	119	5.695	49.123	29.872	1.00	24.83	6
	ATOM	983	C	THR	119	7.053	51.424	28.881	1.00	17.81	6
70	ATOM	984	O	THR	119	6.436	52.130	28.095	1.00	14.36	8
	ATOM	985	N	PHE	120	8.121	50.679	28.643	1.00	14.86	7
	ATOM	986	CA	PHE	120	8.616	50.608	27.259	1.00	13.85	6

	ATOM	987	CB	PHE	120	10.122	50.797	27.240	1.00	15.51	6
	ATOM	988	CG	PHE	120	10.553	52.230	27.463	1.00	13.38	6
	ATOM	989	CD1	PHE	120	10.748	52.701	28.750	1.00	20.15	6
5	ATOM	990	CD2	PHE	120	10.792	53.051	26.381	1.00	20.08	6
	ATOM	991	CE1	PHE	120	11.186	54.002	28.953	1.00	17.14	6
	ATOM	992	CE2	PHE	120	11.230	54.367	26.578	1.00	22.12	6
	ATOM	993	CZ	PHE	120	11.423	54.818	27.867	1.00	17.10	6
	ATOM	994	C	PHE	120	8.279	49.216	26.721	1.00	17.13	6
10	ATOM	995	O	PHE	120	8.640	48.221	27.407	1.00	14.78	8
	ATOM	996	N	PHE	121	7.626	49.166	25.575	1.00	16.20	7
	ATOM	997	CA	PHE	121	7.277	47.868	25.011	1.00	18.83	6
	ATOM	998	CB	PHE	121	5.799	47.821	24.616	1.00	13.50	6
	ATOM	999	CG	PHE	121	4.768	48.052	25.656	1.00	18.60	6
15	ATOM	1000	CD1	PHE	121	4.368	49.339	26.017	1.00	17.37	6
	ATOM	1001	CD2	PHE	121	4.208	46.961	26.334	1.00	18.44	6
	ATOM	1002	CE1	PHE	121	3.409	49.524	27.006	1.00	19.78	6
	ATOM	1003	CE2	PHE	121	3.260	47.173	27.313	1.00	22.69	6
	ATOM	1004	CZ	PHE	121	2.843	48.445	27.660	1.00	15.74	6
20	ATOM	1005	C	PHE	121	8.074	47.539	23.749	1.00	18.44	6
	ATOM	1006	O	PHE	121	8.351	48.454	22.987	1.00	15.63	8
	ATOM	1007	N	GLN	122	8.333	46.253	23.480	1.00	19.35	7
	ATOM	1008	CA	GLN	122	8.959	45.880	22.203	1.00	19.90	6
	ATOM	1009	CB	GLN	122	10.396	45.379	22.317	1.00	16.32	6
25	ATOM	1010	CG	GLN	122	10.784	44.583	21.065	1.00	18.39	6
	ATOM	1011	CD	GLN	122	12.050	43.764	21.247	1.00	21.98	6
	ATOM	1012	OE1	GLN	122	12.423	43.461	22.374	1.00	19.18	8
	ATOM	1013	NE2	GLN	122	12.700	43.396	20.153	1.00	24.51	7
	ATOM	1014	C	GLN	122	8.067	44.774	21.609	1.00	15.34	6
30	ATOM	1015	O	GLN	122	7.789	43.832	22.321	1.00	17.30	8
	ATOM	1016	N	ASN	123	7.474	44.931	20.439	1.00	18.98	7
	ATOM	1017	CA	ASN	123	6.542	43.975	19.859	1.00	22.95	6
	ATOM	1018	CB	ASN	123	7.241	42.708	19.332	1.00	19.57	6
	ATOM	1019	CG	ASN	123	8.228	43.130	18.244	1.00	26.31	6
35	ATOM	1020	OD1	ASN	123	8.013	44.053	17.441	1.00	19.76	8
	ATOM	1021	ND2	ASN	123	9.375	42.463	18.213	1.00	28.57	7
	ATOM	1022	C	ASN	123	5.397	43.643	20.803	1.00	21.02	6
	ATOM	1023	O	ASN	123	4.911	42.525	20.918	1.00	19.19	8
	ATOM	1024	N	GLY	124	4.951	44.632	21.579	1.00	19.77	7
40	ATOM	1025	CA	GLY	124	3.852	44.516	22.495	1.00	16.41	6
	ATOM	1026	C	GLY	124	4.159	43.885	23.844	1.00	14.85	6
	ATOM	1027	O	GLY	124	3.210	43.658	24.611	1.00	15.05	8
	ATOM	1028	N	LYS	125	5.405	43.610	24.133	1.00	13.81	7
	ATOM	1029	CA	LYS	125	5.830	42.997	25.379	1.00	21.18	6
45	ATOM	1030	CB	LYS	125	6.700	41.738	25.247	1.00	14.85	6
	ATOM	1031	CG	LYS	125	6.934	41.032	26.559	1.00	16.28	6
	ATOM	1032	CD	LYS	125	7.406	39.587	26.281	1.00	22.51	6
	ATOM	1033	CE	LYS	125	7.925	38.989	27.587	1.00	30.62	6
	ATOM	1034	NZ	LYS	125	8.822	37.818	27.330	1.00	36.72	7
50	ATOM	1035	C	LYS	125	6.725	44.014	26.121	1.00	18.20	6
	ATOM	1036	O	LYS	125	7.648	44.525	25.509	1.00	19.98	8
	ATOM	1037	N	SER	126	6.385	44.216	27.393	1.00	17.62	7
	ATOM	1038	CA	SER	126	7.107	45.241	28.155	1.00	20.03	6
	ATOM	1039	CB	SER	126	6.355	45.459	29.485	1.00	23.22	6
55	ATOM	1040	OG	SER	126	7.317	45.773	30.466	1.00	38.12	8
	ATOM	1041	C	SER	126	8.541	44.823	28.389	1.00	17.85	6
	ATOM	1042	O	SER	126	8.842	43.657	28.647	1.00	21.31	8
	ATOM	1043	N	GLN	127	9.490	45.718	28.254	1.00	17.16	7
	ATOM	1044	CA	GLN	127	10.898	45.515	28.408	1.00	17.45	6
60	ATOM	1045	CB	GLN	127	11.723	46.073	27.225	1.00	20.82	6
	ATOM	1046	CG	GLN	127	11.352	45.419	25.897	1.00	18.56	6
	ATOM	1047	CD	GLN	127	11.497	43.912	25.927	1.00	24.44	6
	ATOM	1048	OE1	GLN	127	12.606	43.416	26.116	1.00	31.62	8
	ATOM	1049	NE2	GLN	127	10.436	43.130	25.773	1.00	19.15	7
65	ATOM	1050	C	GLN	127	11.386	46.251	29.661	1.00	20.94	6
	ATOM	1051	O	GLN	127	12.439	45.929	30.179	1.00	18.25	8
	ATOM	1052	N	LYS	128	10.643	47.285	30.032	1.00	21.18	7
	ATOM	1053	CA	LYS	128	11.070	48.048	31.216	1.00	23.10	6
	ATOM	1054	CB	LYS	128	12.177	49.034	30.842	1.00	21.83	6
	ATOM	1055	CG	LYS	128	12.683	49.882	32.013	1.00	24.67	6
70	ATOM	1056	CD	LYS	128	13.739	50.905	31.589	1.00	18.23	6
	ATOM	1057	CE	LYS	128	14.048	51.746	32.870	1.00	27.02	6

106

	ATOM	1058	NZ	LYS	128	15.081	52.794	32.574	1.00	24.24	7
	ATOM	1059	C	LYS	128	9.884	48.844	31.754	1.00	24.93	6
	ATOM	1060	O	LYS	128	9.193	49.481	30.960	1.00	20.79	8
	ATOM	1061	N	PHE	129	9.678	48.822	33.062	1.00	21.39	7
5	ATOM	1062	CA	PHE	129	8.708	49.695	33.695	1.00	24.45	6
	ATOM	1063	CB	PHE	129	7.610	48.926	34.458	1.00	25.50	6
	ATOM	1064	CG	PHE	129	6.772	49.837	35.327	1.00	25.51	6
	ATOM	1065	CD1	PHE	129	5.799	50.630	34.762	1.00	19.40	6
	ATOM	1066	CD2	PHE	129	7.002	49.928	36.700	1.00	29.98	6
10	ATOM	1067	CE1	PHE	129	5.026	51.491	35.535	1.00	25.00	6
	ATOM	1068	CE2	PHE	129	6.249	50.788	37.491	1.00	28.84	6
	ATOM	1069	CZ	PHE	129	5.262	51.574	36.902	1.00	32.29	6
	ATOM	1070	C	PHE	129	9.480	50.577	34.687	1.00	27.88	6
	ATOM	1071	O	PHE	129	10.388	50.049	35.359	1.00	30.99	8
15	ATOM	1072	N	SER	130	9.134	51.846	34.853	1.00	26.67	7
	ATOM	1073	CA	SER	130	9.779	52.641	35.917	1.00	24.98	6
	ATOM	1074	CB	SER	130	11.025	53.344	35.422	1.00	21.29	6
	ATOM	1075	OG	SER	130	11.271	54.465	36.250	1.00	25.72	8
	ATOM	1076	C	SER	130	8.777	53.667	36.434	1.00	24.39	6
20	ATOM	1077	O	SER	130	8.123	54.285	35.576	1.00	24.91	8
	ATOM	1078	N	HIS	131	8.668	53.889	37.730	1.00	22.12	7
	ATOM	1079	CA	HIS	131	7.710	54.901	38.204	1.00	23.65	6
	ATOM	1080	CB	HIS	131	7.604	54.918	39.737	1.00	28.35	6
	ATOM	1081	CG	HIS	131	6.859	53.706	40.197	1.00	23.57	6
25	ATOM	1082	CD2	HIS	131	7.307	52.509	40.642	1.00	18.55	6
	ATOM	1083	ND1	HIS	131	5.478	53.666	40.170	1.00	26.69	7
	ATOM	1084	CE1	HIS	131	5.095	52.478	40.617	1.00	16.65	6
	ATOM	1085	NE2	HIS	131	6.173	51.764	40.890	1.00	23.94	7
	ATOM	1086	C	HIS	131	8.108	56.314	37.814	1.00	23.89	6
30	ATOM	1087	O	HIS	131	7.261	57.205	37.712	1.00	26.21	8
	ATOM	1088	N	LEU	132	9.426	56.548	37.689	1.00	21.77	7
	ATOM	1089	CA	LEU	132	9.886	57.900	37.480	1.00	20.70	6
	ATOM	1090	CB	LEU	132	10.630	58.361	38.760	1.00	30.28	6
	ATOM	1091	CG	LEU	132	10.022	58.084	40.148	1.00	26.56	6
35	ATOM	1092	CD1	LEU	132	11.073	58.316	41.229	1.00	29.07	6
	ATOM	1093	CD2	LEU	132	8.814	58.980	40.435	1.00	24.99	6
	ATOM	1094	C	LEU	132	10.762	58.144	36.279	1.00	22.94	6
	ATOM	1095	O	LEU	132	10.794	59.326	35.900	1.00	22.01	8
	ATOM	1096	N	ASP	133	11.541	57.181	35.778	1.00	21.75	7
40	ATOM	1097	CA	ASP	133	12.469	57.401	34.679	1.00	24.62	6
	ATOM	1098	CB	ASP	133	13.560	56.327	34.854	1.00	29.71	6
	ATOM	1099	CG	ASP	133	14.734	56.321	33.915	1.00	32.90	6
	ATOM	1100	OD1	ASP	133	14.837	57.254	33.083	1.00	32.91	8
	ATOM	1101	OD2	ASP	133	15.597	55.394	34.000	1.00	36.01	8
45	ATOM	1102	C	ASP	133	11.843	57.230	33.296	1.00	25.88	6
	ATOM	1103	O	ASP	133	11.419	56.136	32.940	1.00	24.36	8
	ATOM	1104	N	PRO	134	11.857	58.261	32.460	1.00	24.65	7
	ATOM	1105	CD	PRO	134	12.347	59.620	32.778	1.00	22.97	6
50	ATOM	1106	CA	PRO	134	11.293	58.185	31.112	1.00	24.00	6
	ATOM	1107	CB	PRO	134	10.889	59.662	30.870	1.00	24.02	6
	ATOM	1108	CG	PRO	134	11.987	60.433	31.544	1.00	23.04	6
	ATOM	1109	C	PRO	134	12.256	57.764	30.017	1.00	22.11	6
	ATOM	1110	O	PRO	134	11.970	57.930	28.824	1.00	19.00	8
	ATOM	1111	N	THR	135	13.420	57.212	30.350	1.00	21.43	7
55	ATOM	1112	CA	THR	135	14.424	56.805	29.401	1.00	24.98	6
	ATOM	1113	CB	THR	135	15.748	57.584	29.593	1.00	27.24	6
	ATOM	1114	OG1	THR	135	16.331	57.065	30.796	1.00	24.99	8
	ATOM	1115	CG2	THR	135	15.461	59.069	29.706	1.00	26.07	6
	ATOM	1116	C	THR	135	14.747	55.312	29.451	1.00	23.58	6
60	ATOM	1117	O	THR	135	14.445	54.629	30.423	1.00	26.14	8
	ATOM	1118	N	PHE	136	15.267	54.790	28.347	1.00	20.63	7
	ATOM	1119	CA	PHE	136	15.549	53.391	28.150	1.00	20.10	6
	ATOM	1120	CB	PHE	136	14.343	52.706	27.523	1.00	25.47	6
	ATOM	1121	CG	PHE	136	14.408	51.250	27.170	1.00	25.61	6
65	ATOM	1122	CD1	PHE	136	14.528	50.270	28.121	1.00	27.00	6
	ATOM	1123	CD2	PHE	136	14.332	50.847	25.841	1.00	27.45	6
	ATOM	1124	CE1	PHE	136	14.571	48.929	27.787	1.00	32.62	6
	ATOM	1125	CE2	PHE	136	14.385	49.516	25.490	1.00	28.46	6
	ATOM	1126	CZ	PHE	136	14.493	48.549	26.463	1.00	30.41	6
70	ATOM	1127	C	PHE	136	16.796	53.197	27.297	1.00	24.00	6
	ATOM	1128	O	PHE	136	16.952	53.801	26.230	1.00	24.50	8

	ATOM	1129	N	SER	137	17.665	52.294	27.730	1.00	21.97	7
	ATOM	1130	CA	SER	137	18.914	52.010	27.050	1.00	26.52	6
	ATOM	1131	CB	SER	137	20.120	52.418	27.908	1.00	30.03	6
5	ATOM	1132	OG	SER	137	20.769	53.559	27.412	1.00	44.19	8
	ATOM	1133	C	SER	137	19.128	50.507	26.840	1.00	27.38	6
	ATOM	1134	O	SER	137	18.911	49.694	27.721	1.00	27.33	8
	ATOM	1135	N	ILE	138	19.654	50.164	25.686	1.00	25.86	7
	ATOM	1136	CA	ILE	138	20.004	48.806	25.343	1.00	29.46	6
10	ATOM	1137	CB	ILE	138	19.189	48.176	24.193	1.00	33.38	6
	ATOM	1138	CG2	ILE	138	19.669	46.748	23.941	1.00	27.23	6
	ATOM	1139	CG1	ILE	138	17.679	48.197	24.472	1.00	30.55	6
	ATOM	1140	CD1	ILE	138	16.817	48.155	23.223	1.00	29.53	6
	ATOM	1141	C	ILE	138	21.477	48.875	24.926	1.00	29.88	6
	ATOM	1142	O	ILE	138	21.768	49.377	23.849	1.00	27.99	8
15	ATOM	1143	N	PRO	139	22.345	48.476	25.837	1.00	31.71	7
	ATOM	1144	CD	PRO	139	22.018	47.938	27.184	1.00	32.73	6
	ATOM	1145	CA	PRO	139	23.776	48.398	25.598	1.00	33.85	6
	ATOM	1146	CB	PRO	139	24.380	48.213	26.983	1.00	36.13	6
20	ATOM	1147	CG	PRO	139	23.248	48.384	27.950	1.00	34.99	6
	ATOM	1148	C	PRO	139	24.030	47.160	24.741	1.00	35.63	6
	ATOM	1149	O	PRO	139	23.324	46.160	24.888	1.00	38.22	8
	ATOM	1150	N	GLN	140	24.974	47.208	23.827	1.00	36.97	7
	ATOM	1151	CA	GLN	140	25.288	46.110	22.935	1.00	35.17	6
25	ATOM	1152	CB	GLN	140	26.223	45.124	23.631	1.00	43.87	6
	ATOM	1153	CG	GLN	140	27.518	45.802	24.088	1.00	49.77	6
	ATOM	1154	CD	GLN	140	27.883	45.282	25.468	1.00	56.21	6
	ATOM	1155	OE1	GLN	140	28.145	44.084	25.593	1.00	57.44	8
	ATOM	1156	NE2	GLN	140	27.883	46.161	26.468	1.00	57.25	7
30	ATOM	1157	C	GLN	140	24.060	45.418	22.362	1.00	34.61	6
	ATOM	1158	O	GLN	140	23.677	44.284	22.693	1.00	33.34	8
	ATOM	1159	N	ALA	141	23.473	46.111	21.391	1.00	29.80	7
	ATOM	1160	CA	ALA	141	22.287	45.634	20.694	1.00	30.02	6
	ATOM	1161	CB	ALA	141	21.778	46.745	19.774	1.00	27.89	6
35	ATOM	1162	C	ALA	141	22.561	44.400	19.832	1.00	29.52	6
	ATOM	1163	O	ALA	141	23.650	44.270	19.263	1.00	29.60	8
	ATOM	1164	N	ASN	142	21.528	43.582	19.665	1.00	30.60	7
	ATOM	1165	CA	ASN	142	21.642	42.435	18.738	1.00	31.55	6
	ATOM	1166	CB	ASN	142	21.985	41.139	19.453	1.00	30.39	6
40	ATOM	1167	CG	ASN	142	21.012	40.749	20.534	1.00	31.63	6
	ATOM	1168	OD1	ASN	142	19.838	40.423	20.268	1.00	27.57	8
	ATOM	1169	ND2	ASN	142	21.479	40.739	21.781	1.00	33.23	7
	ATOM	1170	C	ASN	142	20.357	42.321	17.936	1.00	32.33	6
	ATOM	1171	O	ASN	142	19.453	43.168	18.122	1.00	29.09	8
45	ATOM	1172	N	HIS	143	20.223	41.257	17.134	1.00	29.40	7
	ATOM	1173	CA	HIS	143	19.075	41.086	16.266	1.00	28.82	6
	ATOM	1174	CB	HIS	143	19.262	39.895	15.272	1.00	24.51	6
	ATOM	1175	CG	HIS	143	20.360	40.234	14.295	1.00	31.72	6
	ATOM	1176	CD2	HIS	143	20.704	41.420	13.740	1.00	33.88	6
50	ATOM	1177	ND1	HIS	143	21.278	39.328	13.822	1.00	32.86	7
	ATOM	1178	CE1	HIS	143	22.117	39.927	13.008	1.00	31.84	6
	ATOM	1179	NE2	HIS	143	21.794	41.202	12.941	1.00	31.48	7
	ATOM	1180	C	HIS	143	17.747	40.857	16.976	1.00	26.62	6
	ATOM	1181	O	HIS	143	16.696	41.098	16.366	1.00	25.96	8
55	ATOM	1182	N	SER	144	17.812	40.412	18.221	1.00	20.85	7
	ATOM	1183	CA	SER	144	16.557	40.128	18.941	1.00	24.82	6
	ATOM	1184	CB	SER	144	16.839	38.979	19.915	1.00	30.28	6
	ATOM	1185	OG	SER	144	17.739	39.389	20.930	1.00	39.11	8
	ATOM	1186	C	SER	144	15.976	41.423	19.474	1.00	24.89	6
	ATOM	1187	O	SER	144	14.775	41.518	19.755	1.00	25.22	8
60	ATOM	1188	N	HIS	145	16.746	42.522	19.463	1.00	20.33	7
	ATOM	1189	CA	HIS	145	16.306	43.861	19.811	1.00	19.38	6
	ATOM	1190	CB	HIS	145	17.474	44.762	20.302	1.00	19.40	6
	ATOM	1191	CG	HIS	145	18.145	44.212	21.534	1.00	18.37	6
65	ATOM	1192	CD2	HIS	145	17.620	43.886	22.744	1.00	18.22	6
	ATOM	1193	ND1	HIS	145	19.493	43.965	21.627	1.00	23.55	7
	ATOM	1194	CE1	HIS	145	19.768	43.492	22.829	1.00	26.33	6
	ATOM	1195	NE2	HIS	145	18.643	43.412	23.525	1.00	21.05	7
	ATOM	1196	C	HIS	145	15.589	44.553	18.657	1.00	22.05	6
	ATOM	1197	O	HIS	145	15.013	45.636	18.848	1.00	21.86	8
70	ATOM	1198	N	SER	146	15.569	43.997	17.440	1.00	20.66	7
	ATOM	1199	CA	SER	146	14.833	44.649	16.363	1.00	19.96	6

	ATOM	1200	CB	SER	146	15.075	44.009	14.986	1.00	20.48	6
	ATOM	1201	OG	SER	146	16.442	44.154	14.613	1.00	25.61	8
	ATOM	1202	C	SER	146	13.339	44.596	16.656	1.00	20.51	6
5	ATOM	1203	O	SER	146	12.915	43.614	17.287	1.00	22.06	8
	ATOM	1204	N	GLY	147	12.556	45.578	16.197	1.00	16.70	7
	ATOM	1205	CA	GLY	147	11.123	45.383	16.411	1.00	20.49	6
	ATOM	1206	C	GLY	147	10.385	46.714	16.555	1.00	22.63	6
	ATOM	1207	O	GLY	147	10.982	47.762	16.332	1.00	16.09	8
10	ATOM	1208	N	ASP	148	9.111	46.560	16.951	1.00	20.62	7
	ATOM	1209	CA	ASP	148	8.324	47.777	17.121	1.00	21.57	6
	ATOM	1210	CB	ASP	148	6.882	47.579	16.674	1.00	28.99	6
	ATOM	1211	CG	ASP	148	6.819	47.144	15.219	1.00	41.07	6
	ATOM	1212	OD1	ASP	148	7.849	47.338	14.540	1.00	39.21	8
15	ATOM	1213	OD2	ASP	148	5.763	46.620	14.808	1.00	39.40	8
	ATOM	1214	C	ASP	148	8.315	48.214	18.590	1.00	20.72	6
	ATOM	1215	O	ASP	148	7.817	47.469	19.447	1.00	20.27	8
	ATOM	1216	N	TYR	149	8.822	49.440	18.798	1.00	16.97	7
	ATOM	1217	CA	TYR	149	8.811	49.966	20.164	1.00	18.60	6
20	ATOM	1218	CB	TYR	149	10.193	50.587	20.472	1.00	16.94	6
	ATOM	1219	CG	TYR	149	11.272	49.534	20.606	1.00	18.45	6
	ATOM	1220	CD1	TYR	149	11.901	48.928	19.528	1.00	19.27	6
	ATOM	1221	CE1	TYR	149	12.877	47.948	19.737	1.00	20.18	6
	ATOM	1222	CD2	TYR	149	11.672	49.162	21.879	1.00	18.36	6
	ATOM	1223	CE2	TYR	149	12.636	48.216	22.116	1.00	15.60	6
25	ATOM	1224	CZ	TYR	149	13.238	47.606	21.027	1.00	18.77	6
	ATOM	1225	OH	TYR	149	14.211	46.660	21.253	1.00	18.41	8
	ATOM	1226	C	TYR	149	7.767	51.061	20.355	1.00	15.78	6
	ATOM	1227	O	TYR	149	7.539	51.859	19.450	1.00	15.86	8
30	ATOM	1228	N	HIS	150	7.196	51.126	21.559	1.00	15.01	7
	ATOM	1229	CA	HIS	150	6.247	52.171	21.925	1.00	12.99	6
	ATOM	1230	CB	HIS	150	4.849	51.980	21.372	1.00	11.96	6
	ATOM	1231	CG	HIS	150	3.942	51.032	22.117	1.00	17.71	6
	ATOM	1232	CD2	HIS	150	2.944	51.295	23.004	1.00	16.09	6
35	ATOM	1233	ND1	HIS	150	3.988	49.660	21.971	1.00	11.60	7
	ATOM	1234	CE1	HIS	150	3.058	49.103	22.716	1.00	16.95	6
	ATOM	1235	NE2	HIS	150	2.407	50.057	23.370	1.00	19.22	7
	ATOM	1236	C	HIS	150	6.263	52.270	23.462	1.00	13.37	6
	ATOM	1237	O	HIS	150	6.922	51.448	24.129	1.00	12.78	8
40	ATOM	1238	N	CYS	151	5.680	53.355	23.957	1.00	14.21	7
	ATOM	1239	CA	CYS	151	5.670	53.559	25.414	1.00	15.38	6
	ATOM	1240	C	CYS	151	4.301	53.982	25.880	1.00	16.27	6
	ATOM	1241	O	CYS	151	3.422	54.404	25.132	1.00	15.15	8
	ATOM	1242	CB	CYS	151	6.746	54.562	25.856	1.00	16.85	6
45	ATOM	1243	SG	CYS	151	6.581	56.269	25.248	1.00	14.82	16
	ATOM	1244	N	THR	152	4.080	53.805	27.186	1.00	17.41	7
	ATOM	1245	CA	THR	152	2.875	54.223	27.862	1.00	17.27	6
	ATOM	1246	CB	THR	152	1.899	53.131	28.305	1.00	21.80	6
	ATOM	1247	OG1	THR	152	2.527	52.212	29.205	1.00	17.53	8
50	ATOM	1248	CG2	THR	152	1.356	52.388	27.075	1.00	17.12	6
	ATOM	1249	C	THR	152	3.346	54.989	29.127	1.00	19.83	6
	ATOM	1250	O	THR	152	4.471	54.724	29.600	1.00	16.21	8
	ATOM	1251	N	GLY	153	2.496	55.913	29.534	1.00	17.84	7
	ATOM	1252	CA	GLY	153	2.815	56.706	30.731	1.00	20.33	6
55	ATOM	1253	C	GLY	153	1.647	57.605	31.108	1.00	18.60	6
	ATOM	1254	O	GLY	153	0.779	57.915	30.293	1.00	19.87	8
	ATOM	1255	N	ASN	154	1.603	58.000	32.373	1.00	20.99	7
	ATOM	1256	CA	ASN	154	0.560	58.815	32.959	1.00	20.36	6
	ATOM	1257	CB	ASN	154	0.512	58.556	34.478	1.00	26.77	6
	ATOM	1258	CG	ASN	154	-0.800	57.928	34.897	1.00	40.91	6
60	ATOM	1259	OD1	ASN	154	-1.700	58.580	35.441	1.00	46.67	8
	ATOM	1260	ND2	ASN	154	-0.927	56.639	34.633	1.00	40.24	7
	ATOM	1261	C	ASN	154	0.879	60.300	32.817	1.00	22.51	6
	ATOM	1262	O	ASN	154	1.973	60.685	33.272	1.00	22.15	8
65	ATOM	1263	N	ILE	155	-0.018	61.067	32.202	1.00	19.40	7
	ATOM	1264	CA	ILE	155	0.198	62.514	32.139	1.00	22.27	6
	ATOM	1265	CB	ILE	155	0.210	63.116	30.731	1.00	26.29	6
	ATOM	1266	CG2	ILE	155	0.327	64.640	30.831	1.00	23.31	6
	ATOM	1267	CG1	ILE	155	1.367	62.544	29.899	1.00	28.16	6
	ATOM	1268	CD1	ILE	155	1.371	62.874	28.434	1.00	29.42	6
70	ATOM	1269	C	ILE	155	-0.974	63.089	32.941	1.00	27.67	6
	ATOM	1270	O	ILE	155	-2.112	62.726	32.639	1.00	24.10	8

109

	ATOM	1271	N	GLY	156	-0.732	63.838	34.020	1.00	33.10	7
	ATOM	1272	CA	GLY	156	-1.942	64.285	34.780	1.00	37.62	6
	ATOM	1273	C	GLY	156	-2.447	63.053	35.527	1.00	38.80	6
5	ATOM	1274	O	GLY	156	-1.659	62.512	36.299	1.00	43.91	8
	ATOM	1275	N	TYR	157	-3.655	62.573	35.307	1.00	41.47	7
	ATOM	1276	CA	TYR	157	-4.182	61.357	35.894	1.00	43.65	6
	ATOM	1277	CB	TYR	157	-5.381	61.642	36.832	1.00	51.51	6
	ATOM	1278	CG	TYR	157	-5.020	62.592	37.961	1.00	57.42	6
10	ATOM	1279	CD1	TYR	157	-5.523	63.885	37.982	1.00	60.45	6
	ATOM	1280	CE1	TYR	157	-5.179	64.765	38.992	1.00	62.57	6
	ATOM	1281	CD2	TYR	157	-4.140	62.204	38.963	1.00	61.00	6
	ATOM	1282	CE2	TYR	157	-3.788	63.079	39.982	1.00	63.03	6
	ATOM	1283	CZ	TYR	157	-4.313	64.353	39.986	1.00	63.56	6
15	ATOM	1284	OH	TYR	157	-3.979	65.237	40.984	1.00	66.68	8
	ATOM	1285	C	TYR	157	-4.676	60.351	34.849	1.00	41.96	6
	ATOM	1286	O	TYR	157	-5.445	59.420	35.115	1.00	41.33	8
	ATOM	1287	N	THR	158	-4.298	60.547	33.594	1.00	36.77	7
	ATOM	1288	CA	THR	158	-4.722	59.693	32.496	1.00	30.71	6
20	ATOM	1289	CB	THR	158	-5.260	60.597	31.364	1.00	30.82	6
	ATOM	1290	OG1	THR	158	-6.237	61.471	31.942	1.00	30.47	8
	ATOM	1291	CG2	THR	158	-5.851	59.819	30.207	1.00	29.21	6
	ATOM	1292	C	THR	158	-3.532	58.944	31.912	1.00	25.66	6
	ATOM	1293	O	THR	158	-2.521	59.609	31.642	1.00	24.50	8
25	ATOM	1294	N	LEU	159	-3.689	57.664	31.609	1.00	21.00	7
	ATOM	1295	CA	LEU	159	-2.617	56.924	30.960	1.00	21.01	6
	ATOM	1296	CB	LEU	159	-2.737	55.435	31.284	1.00	26.53	6
	ATOM	1297	CG	LEU	159	-1.601	54.487	30.958	1.00	27.15	6
	ATOM	1298	CD1	LEU	159	-0.323	54.817	31.713	1.00	25.15	6
30	ATOM	1299	CD2	LEU	159	-1.979	53.036	31.316	1.00	28.75	6
	ATOM	1300	C	LEU	159	-2.654	57.179	29.461	1.00	22.04	6
	ATOM	1301	O	LEU	159	-3.711	57.248	28.844	1.00	22.64	8
	ATOM	1302	N	PHE	160	-1.484	57.396	28.855	1.00	20.79	7
	ATOM	1303	CA	PHE	160	-1.430	57.576	27.409	1.00	19.10	6
35	ATOM	1304	CB	PHE	160	-0.821	58.946	27.060	1.00	20.91	6
	ATOM	1305	CG	PHE	160	-1.848	60.034	27.216	1.00	19.50	6
	ATOM	1306	CD1	PHE	160	-1.971	60.676	28.442	1.00	24.86	6
	ATOM	1307	CD2	PHE	160	-2.645	60.409	26.156	1.00	21.03	6
	ATOM	1308	CE1	PHE	160	-2.903	61.709	28.588	1.00	29.44	6
40	ATOM	1309	CE2	PHE	160	-3.582	61.421	26.296	1.00	19.89	6
	ATOM	1310	CZ	PHE	160	-3.704	62.074	27.529	1.00	25.34	6
	ATOM	1311	C	PHE	160	-0.521	56.513	26.794	1.00	17.36	6
	ATOM	1312	O	PHE	160	0.346	55.982	27.504	1.00	18.36	8
	ATOM	1313	N	SER	161	-0.753	56.240	25.521	1.00	17.60	7
45	ATOM	1314	CA	SER	161	0.087	55.302	24.785	1.00	14.63	6
	ATOM	1315	CB	SER	161	-0.744	54.150	24.188	1.00	20.14	6
	ATOM	1316	OG	SER	161	0.115	53.054	23.901	1.00	21.55	8
	ATOM	1317	C	SER	161	0.662	56.037	23.561	1.00	18.96	6
	ATOM	1318	O	SER	161	-0.101	56.753	22.894	1.00	19.79	8
50	ATOM	1319	N	SER	162	1.921	55.796	23.232	1.00	16.19	7
	ATOM	1320	CA	SER	162	2.518	56.404	22.049	1.00	16.74	6
	ATOM	1321	CB	SER	162	4.029	56.678	22.233	1.00	16.78	6
	ATOM	1322	OG	SER	162	4.801	55.530	21.900	1.00	21.00	8
	ATOM	1323	C	SER	162	2.322	55.485	20.845	1.00	18.24	6
55	ATOM	1324	O	SER	162	1.949	54.305	20.987	1.00	16.85	8
	ATOM	1325	N	LYS	163	2.535	56.027	19.652	1.00	17.96	7
	ATOM	1326	CA	LYS	163	2.484	55.203	18.445	1.00	17.36	6
	ATOM	1327	CB	LYS	163	2.369	55.957	17.133	1.00	20.94	6
	ATOM	1328	CG	LYS	163	1.228	56.885	16.902	1.00	25.34	6
60	ATOM	1329	CD	LYS	163	-0.128	56.271	16.685	1.00	29.02	6
	ATOM	1330	CE	LYS	163	-0.954	57.131	15.721	1.00	42.35	6
	ATOM	1331	NZ	LYS	163	-0.495	58.558	15.692	1.00	38.14	7
	ATOM	1332	C	LYS	163	3.821	54.466	18.391	1.00	17.27	6
	ATOM	1333	O	LYS	163	4.817	54.906	18.978	1.00	16.54	8
65	ATOM	1334	N	PRO	164	3.840	53.348	17.696	1.00	18.39	7
	ATOM	1335	CD	PRO	164	2.702	52.743	16.952	1.00	20.79	6
	ATOM	1336	CA	PRO	164	5.060	52.572	17.546	1.00	19.84	6
	ATOM	1337	CB	PRO	164	4.545	51.177	17.142	1.00	17.33	6
	ATOM	1338	CG	PRO	164	3.254	51.416	16.475	1.00	21.76	6
	ATOM	1339	C	PRO	164	6.032	53.169	16.528	1.00	19.62	6
70	ATOM	1340	O	PRO	164	5.723	53.942	15.619	1.00	19.46	8
	ATOM	1341	N	VAL	165	7.295	52.833	16.674	1.00	17.22	7

	ATOM	1342	CA	VAL	165	8.427	53.162	15.841	1.00	20.36	6
	ATOM	1343	CB	VAL	165	9.405	54.190	16.450	1.00	20.84	6
	ATOM	1344	CG1	VAL	165	10.418	54.643	15.404	1.00	20.46	6
5	ATOM	1345	CG2	VAL	165	8.699	55.475	16.899	1.00	23.72	6
	ATOM	1346	C	VAL	165	9.173	51.833	15.590	1.00	22.05	6
	ATOM	1347	O	VAL	165	9.532	51.094	16.499	1.00	22.10	8
	ATOM	1348	N	THR	166	9.444	51.549	14.320	1.00	24.93	7
	ATOM	1349	CA	THR	166	10.111	50.317	13.939	1.00	26.07	6
10	ATOM	1350	CB	THR	166	9.631	49.784	12.579	1.00	31.66	6
	ATOM	1351	OG1	THR	166	9.737	50.811	11.569	1.00	38.39	8
	ATOM	1352	CG2	THR	166	8.180	49.353	12.694	1.00	23.71	6
	ATOM	1353	C	THR	166	11.611	50.597	13.909	1.00	25.06	6
	ATOM	1354	O	THR	166	11.985	51.536	13.244	1.00	21.88	8
	ATOM	1355	N	ILE	167	12.362	49.878	14.714	1.00	21.40	7
15	ATOM	1356	CA	ILE	167	13.784	49.907	14.909	1.00	25.06	6
	ATOM	1357	CB	ILE	167	14.088	50.164	16.424	1.00	26.21	6
	ATOM	1358	CG2	ILE	167	15.588	50.159	16.673	1.00	26.68	6
	ATOM	1359	CG1	ILE	167	13.415	51.472	16.825	1.00	26.56	6
	ATOM	1360	CD1	ILE	167	13.946	52.318	17.939	1.00	30.83	6
20	ATOM	1361	C	ILE	167	14.416	48.572	14.501	1.00	24.36	6
	ATOM	1362	O	ILE	167	14.013	47.482	14.920	1.00	23.36	8
	ATOM	1363	N	THR	168	15.412	48.591	13.630	1.00	22.83	7
	ATOM	1364	CA	THR	168	16.083	47.405	13.152	1.00	27.27	6
25	ATOM	1365	CB	THR	168	15.945	47.266	11.622	1.00	31.88	6
	ATOM	1366	OG1	THR	168	14.565	47.371	11.277	1.00	32.11	8
	ATOM	1367	CG2	THR	168	16.462	45.894	11.179	1.00	34.54	6
	ATOM	1368	C	THR	168	17.575	47.414	13.501	1.00	28.53	6
	ATOM	1369	O	THR	168	18.190	48.483	13.508	1.00	32.64	8
30	ATOM	1370	N	VAL	169	18.090	46.260	13.863	1.00	23.55	7
	ATOM	1371	CA	VAL	169	19.472	46.011	14.163	1.00	27.27	6
	ATOM	1372	CB	VAL	169	19.728	45.359	15.523	1.00	28.51	6
	ATOM	1373	CG1	VAL	169	21.227	45.133	15.757	1.00	26.42	6
	ATOM	1374	CG2	VAL	169	19.189	46.160	16.696	1.00	27.97	6
35	ATOM	1375	C	VAL	169	20.011	45.022	13.098	1.00	32.65	6
	ATOM	1376	O	VAL	169	19.332	44.056	12.710	1.00	33.21	8
	ATOM	1377	N	GLN	170	21.245	45.196	12.689	0.01	33.85	7
	ATOM	1378	CA	GLN	170	21.966	44.390	11.737	0.01	35.75	6
	ATOM	1379	CB	GLN	170	23.335	44.027	12.362	0.01	36.48	6
40	ATOM	1380	CG	GLN	170	24.465	44.012	11.347	0.01	37.54	6
	ATOM	1381	CD	GLN	170	25.478	45.110	11.599	0.01	37.91	6
	ATOM	1382	OE1	GLN	170	25.142	46.186	12.096	0.01	38.17	8
	ATOM	1383	NE2	GLN	170	26.735	44.846	11.257	0.01	38.21	7
	ATOM	1384	C	GLN	170	21.355	43.088	11.241	0.01	36.70	6
45	ATOM	1385	O	GLN	170	21.049	42.167	11.995	0.01	36.81	8
	ATOM	1386	N	VAL	171	21.273	42.959	9.919	0.01	37.51	7
	ATOM	1387	CA	VAL	171	20.781	41.772	9.240	0.01	38.20	6
	ATOM	1388	CB	VAL	171	19.483	41.208	9.842	0.01	38.61	6
	ATOM	1389	CG1	VAL	171	18.334	42.199	9.681	0.01	38.88	6
	ATOM	1390	CG2	VAL	171	19.115	39.881	9.180	0.01	38.83	6
50	ATOM	1391	C	VAL	171	20.587	42.048	7.750	0.01	38.42	6
	ATOM	1392	O	VAL	171	21.420	41.573	6.949	0.01	38.53	8
	ATOM	1393	OW0	WAT	201	13.958	68.106	19.930	1.00	18.36	8
	ATOM	1394	OW0	WAT	202	13.653	41.241	23.320	1.00	24.59	8
55	ATOM	1395	OW0	WAT	203	5.895	57.410	18.965	1.00	14.14	8
	ATOM	1396	OW0	WAT	204	9.519	72.688	30.514	1.00	42.11	8
	ATOM	1397	OW0	WAT	205	8.700	64.454	28.355	1.00	21.65	8
	ATOM	1398	OW0	WAT	206	25.548	65.664	7.898	1.00	24.88	8
	ATOM	1399	OW0	WAT	207	2.902	52.471	31.897	1.00	19.13	8
60	ATOM	1400	OW0	WAT	208	14.303	45.256	23.676	1.00	24.28	8
	ATOM	1401	OW0	WAT	209	10.371	62.552	29.076	1.00	27.73	8
	ATOM	1402	OW0	WAT	210	12.433	66.629	21.505	1.00	14.04	8
	ATOM	1403	OW0	WAT	211	5.417	47.499	21.002	1.00	16.89	8
	ATOM	1404	OW0	WAT	212	29.599	82.797	11.595	1.00	34.62	8
65	ATOM	1405	OW0	WAT	213	17.813	70.187	2.648	1.00	16.34	8
	ATOM	1406	OW0	WAT	214	6.656	58.315	16.413	1.00	24.31	8
	ATOM	1407	OW0	WAT	215	21.191	80.146	5.335	1.00	30.05	8
	ATOM	1408	OW0	WAT	216	15.621	66.766	18.319	1.00	18.82	8
	ATOM	1409	OW0	WAT	217	6.528	56.410	14.460	1.00	26.68	8
	ATOM	1410	OW0	WAT	218	6.213	69.723	22.792	1.00	19.89	8
70	ATOM	1411	OW0	WAT	219	12.935	67.874	24.109	1.00	29.95	8
	ATOM	1412	OW0	WAT	220	-2.277	62.236	20.953	1.00	28.34	8

111

	ATOM	1413	OWO	WAT	221	20.151	71.344	0.183	1.00	21.62	8
	ATOM	1414	OWO	WAT	222	27.773	65.203	6.295	1.00	20.74	8
	ATOM	1415	OWO	WAT	223	-0.481	58.864	19.811	1.00	24.67	8
5	ATOM	1416	OWO	WAT	224	17.815	67.914	1.120	1.00	26.99	8
	ATOM	1417	OWO	WAT	225	16.604	64.761	25.523	1.00	18.45	8
	ATOM	1418	OWO	WAT	226	-0.330	59.580	22.516	1.00	29.01	8
	ATOM	1419	OWO	WAT	227	13.324	40.955	17.129	1.00	40.98	8
	ATOM	1420	OWO	WAT	228	9.214	41.380	22.450	1.00	41.91	8
10	ATOM	1421	OWO	WAT	229	20.146	82.270	13.850	1.00	50.03	8
	ATOM	1422	OWO	WAT	230	21.707	80.353	12.325	1.00	18.46	8
	ATOM	1423	OWO	WAT	231	15.403	67.167	25.599	1.00	21.44	8
	ATOM	1424	OWO	WAT	232	12.703	63.258	30.174	1.00	37.28	8
	ATOM	1425	OWO	WAT	233	12.479	61.400	39.250	1.00	23.78	8
15	ATOM	1426	OWO	WAT	234	13.921	59.460	9.106	1.00	40.49	8
	ATOM	1427	OWO	WAT	235	7.230	72.381	24.432	1.00	41.81	8
	ATOM	1428	OWO	WAT	236	2.989	58.681	19.344	1.00	17.29	8
	ATOM	1429	OWO	WAT	237	12.865	75.036	10.180	1.00	47.19	8
	ATOM	1430	OWO	WAT	238	2.754	67.991	13.259	1.00	35.75	8
20	ATOM	1431	OWO	WAT	239	17.416	57.608	26.641	1.00	32.09	8
	ATOM	1432	OWO	WAT	240	31.068	75.579	10.888	1.00	20.85	8
	ATOM	1433	OWO	WAT	241	17.725	71.985	21.261	1.00	25.43	8
	ATOM	1434	OWO	WAT	242	32.760	65.251	6.079	1.00	38.04	8
	ATOM	1435	OWO	WAT	243	14.079	72.373	25.218	1.00	20.23	8
25	ATOM	1436	OWO	WAT	244	16.644	77.936	-2.315	1.00	34.00	8
	ATOM	1437	OWO	WAT	245	1.790	62.643	35.518	1.00	30.63	8
	ATOM	1438	OWO	WAT	246	10.026	76.840	13.639	1.00	31.10	8
	ATOM	1439	OWO	WAT	247	11.096	40.538	24.599	1.00	33.25	8
	ATOM	1440	OWO	WAT	248	19.457	73.016	-2.970	1.00	36.88	8
30	ATOM	1441	OWO	WAT	249	18.578	60.108	26.756	1.00	30.86	8
	ATOM	1442	OWO	WAT	250	11.119	78.675	16.190	1.00	37.83	8
	ATOM	1443	OWO	WAT	251	2.583	76.687	28.032	1.00	73.18	8
	ATOM	1444	OWO	WAT	252	0.243	75.153	22.803	1.00	34.15	8
	ATOM	1445	OWO	WAT	253	33.328	82.165	10.255	1.00	23.17	8
35	ATOM	1446	OWO	WAT	254	22.212	87.081	5.080	1.00	51.41	8
	ATOM	1447	OWO	WAT	255	21.393	83.921	11.680	1.00	31.47	8
	ATOM	1448	OWO	WAT	256	37.174	72.382	4.349	1.00	36.66	8
	ATOM	1449	OWO	WAT	257	23.291	53.950	13.981	1.00	45.02	8
	ATOM	1450	OWO	WAT	258	31.521	80.134	5.404	1.00	28.19	8
40	ATOM	1451	OWO	WAT	259	11.904	78.169	8.209	1.00	61.39	8
	ATOM	1452	OWO	WAT	260	7.393	36.160	24.668	1.00	45.96	8
	ATOM	1453	OWO	WAT	261	12.356	70.954	23.727	1.00	23.77	8
	ATOM	1454	OWO	WAT	262	33.898	69.078	7.353	1.00	32.96	8
	ATOM	1455	OWO	WAT	263	28.502	52.764	25.478	1.00	58.40	8
45	ATOM	1456	OWO	WAT	264	23.414	37.810	18.427	1.00	35.16	8
	ATOM	1457	OWO	WAT	265	4.792	74.631	16.778	1.00	44.49	8
	ATOM	1458	OWO	WAT	266	28.509	77.721	-1.620	1.00	50.51	8
	ATOM	1459	OWO	WAT	267	19.685	68.488	-0.712	1.00	45.74	8
	ATOM	1460	OWO	WAT	268	10.899	74.487	23.620	1.00	43.61	8
50	ATOM	1461	OWO	WAT	269	-1.033	73.720	20.128	1.00	34.52	8
	ATOM	1462	OWO	WAT	270	15.215	67.397	0.077	1.00	27.35	8
	ATOM	1463	OWO	WAT	271	8.748	79.989	16.508	1.00	51.59	8
	ATOM	1464	OWO	WAT	272	22.332	82.314	3.707	1.00	30.25	8
	ATOM	1465	OWO	WAT	273	23.373	70.771	17.610	1.00	22.44	8
55	ATOM	1466	OWO	WAT	274	11.965	67.872	26.359	1.00	26.92	8
	ATOM	1467	OWO	WAT	275	35.793	71.146	7.198	1.00	27.19	8
	ATOM	1468	OWO	WAT	276	10.333	72.530	25.867	1.00	46.78	8
	ATOM	1469	OWO	WAT	277	17.230	69.185	24.852	1.00	26.22	8
	ATOM	1470	OWO	WAT	278	17.594	51.432	30.830	1.00	32.58	8
60	ATOM	1471	OWO	WAT	279	8.561	67.703	32.884	1.00	37.04	8
	ATOM	1472	OWO	WAT	280	16.374	71.765	-4.195	1.00	31.45	8
	ATOM	1473	OWO	WAT	281	8.995	70.329	24.946	1.00	36.64	8
	ATOM	1474	OWO	WAT	282	19.019	47.051	28.676	1.00	48.06	8
	ATOM	1475	OWO	WAT	283	20.039	61.350	15.742	1.00	23.23	8
65	ATOM	1476	OWO	WAT	284	21.308	55.309	20.658	1.00	28.24	8
	ATOM	1477	OWO	WAT	285	7.405	70.019	5.261	1.00	41.47	8
	ATOM	1478	OWO	WAT	286	23.729	66.066	0.632	1.00	30.27	8
	ATOM	1479	OWO	WAT	287	15.826	40.095	23.946	1.00	41.94	8
	ATOM	1480	OWO	WAT	288	-0.119	50.371	24.812	0.50	25.93	8
70	ATOM	1481	OWO	WAT	289	3.397	54.879	42.245	1.00	29.87	8
	ATOM	1482	OWO	WAT	290	10.215	53.151	32.270	1.00	43.33	8
	ATOM	1483	OWO	WAT	291	8.440	65.109	33.883	1.00	34.09	8

112

	ATOM	1	CB	ALA	401	-36.645	32.040	-4.702	1.00	51.37	6
	ATOM	2	C	ALA	401	-36.199	32.572	-2.285	1.00	42.22	6
	ATOM	3	O	ALA	401	-36.801	33.374	-1.569	1.00	42.70	8
	ATOM	4	N	ALA	401	-34.367	32.745	-3.997	1.00	45.74	7
5	ATOM	5	CA	ALA	401	-35.829	32.874	-3.724	1.00	43.68	6
	ATOM	6	N	PRO	402	-35.903	31.367	-1.817	1.00	40.54	7
	ATOM	7	CD	PRO	402	-35.149	30.320	-2.533	1.00	38.91	6
	ATOM	8	CA	PRO	402	-36.172	31.022	-0.425	1.00	38.61	6
10	ATOM	9	CB	PRO	402	-35.765	29.566	-0.322	1.00	39.86	6
	ATOM	10	CG	PRO	402	-34.790	29.353	-1.426	1.00	41.36	6
	ATOM	11	C	PRO	402	-35.294	31.935	0.434	1.00	36.70	6
	ATOM	12	O	PRO	402	-34.188	32.212	-0.042	1.00	32.46	8
	ATOM	13	N	PRO	403	-35.789	32.370	1.579	1.00	33.82	7
15	ATOM	14	CD	PRO	403	-37.120	32.009	2.110	1.00	35.16	6
	ATOM	15	CA	PRO	403	-35.069	33.229	2.491	1.00	38.25	6
	ATOM	16	CB	PRO	403	-35.872	33.227	3.799	1.00	37.39	6
	ATOM	17	CG	PRO	403	-37.180	32.599	3.486	1.00	37.41	6
	ATOM	18	C	PRO	403	-33.653	32.730	2.790	1.00	37.48	6
20	ATOM	19	O	PRO	403	-33.393	31.531	2.683	1.00	34.39	8
	ATOM	20	N	LYS	404	-32.763	33.654	3.173	1.00	37.04	7
	ATOM	21	CA	LYS	404	-31.399	33.188	3.424	1.00	34.97	6
	ATOM	22	CB	LYS	404	-30.318	34.202	3.122	1.00	43.98	6
	ATOM	23	CG	LYS	404	-30.564	35.675	3.278	1.00	47.64	6
	ATOM	24	CD	LYS	404	-29.775	36.517	2.292	1.00	52.03	6
25	ATOM	25	CE	LYS	404	-28.317	36.123	2.137	1.00	57.56	6
	ATOM	26	NZ	LYS	404	-27.724	36.613	0.855	1.00	56.40	7
	ATOM	27	C	LYS	404	-31.243	32.632	4.825	1.00	31.44	6
	ATOM	28	O	LYS	404	-31.846	33.097	5.784	1.00	29.91	8
30	ATOM	29	N	ALA	405	-30.416	31.586	4.908	1.00	28.75	7
	ATOM	30	CA	ALA	405	-30.039	31.053	6.218	1.00	27.21	6
	ATOM	31	CB	ALA	405	-29.155	29.834	6.110	1.00	21.94	6
	ATOM	32	C	ALA	405	-29.278	32.183	6.923	1.00	26.42	6
	ATOM	33	O	ALA	405	-28.760	33.072	6.222	1.00	26.10	8
35	ATOM	34	N	VAL	406	-29.231	32.192	8.241	1.00	24.91	7
	ATOM	35	CA	VAL	406	-28.515	33.234	8.985	1.00	26.95	6
	ATOM	36	CB	VAL	406	-29.490	34.128	9.770	1.00	29.36	6
	ATOM	37	CG1	VAL	406	-28.779	35.140	10.676	1.00	29.86	6
	ATOM	38	CG2	VAL	406	-30.434	34.842	8.801	1.00	26.74	6
40	ATOM	39	C	VAL	406	-27.503	32.613	9.942	1.00	28.93	6
	ATOM	40	O	VAL	406	-27.846	31.872	10.866	1.00	31.46	8
	ATOM	41	N	LEU	407	-26.233	32.937	9.758	1.00	30.08	7
	ATOM	42	CA	LEU	407	-25.105	32.483	10.546	1.00	29.33	6
	ATOM	43	CB	LEU	407	-23.839	32.520	9.657	1.00	33.18	6
45	ATOM	44	CG	LEU	407	-22.828	31.408	9.960	1.00	34.94	6
	ATOM	45	CD1	LEU	407	-22.082	30.990	8.721	1.00	27.55	6
	ATOM	46	CD2	LEU	407	-21.887	31.864	11.069	1.00	32.30	6
	ATOM	47	C	LEU	407	-24.816	33.301	11.794	1.00	29.57	6
	ATOM	48	O	LEU	407	-24.653	34.515	11.800	1.00	30.04	8
50	ATOM	49	N	LYS	408	-24.768	32.624	12.930	1.00	28.04	7
	ATOM	50	CA	LYS	408	-24.568	33.174	14.257	1.00	25.12	6
	ATOM	51	CB	LYS	408	-25.738	32.687	15.132	1.00	33.32	6
	ATOM	52	CG	LYS	408	-25.777	33.255	16.532	1.00	39.37	6
	ATOM	53	CD	LYS	408	-25.967	32.268	17.652	1.00	43.84	6
55	ATOM	54	CE	LYS	408	-27.129	31.305	17.487	1.00	47.78	6
	ATOM	55	NZ	LYS	408	-27.525	30.691	18.793	1.00	48.98	7
	ATOM	56	C	LYS	408	-23.233	32.674	14.797	1.00	24.53	6
	ATOM	57	O	LYS	408	-22.934	31.482	14.739	1.00	25.35	8
	ATOM	58	N	LEU	409	-22.423	33.556	15.333	1.00	24.78	7
60	ATOM	59	CA	LEU	409	-21.080	33.313	15.843	1.00	22.07	6
	ATOM	60	CB	LEU	409	-20.189	34.383	15.190	1.00	20.04	6
	ATOM	61	CG	LEU	409	-18.725	34.503	15.596	1.00	20.57	6
	ATOM	62	CD1	LEU	409	-17.980	33.242	15.214	1.00	19.57	6
	ATOM	63	CD2	LEU	409	-18.084	35.729	14.903	1.00	23.44	6
65	ATOM	64	C	LEU	409	-21.019	33.451	17.346	1.00	21.01	6
	ATOM	65	O	LEU	409	-21.424	34.473	17.869	1.00	22.38	8
	ATOM	66	N	GLU	410	-20.583	32.456	18.118	1.00	22.53	7
	ATOM	67	CA	GLU	410	-20.480	32.581	19.567	1.00	21.02	6
	ATOM	68	CB	GLU	410	-21.523	31.684	20.270	1.00	27.36	6
70	ATOM	69	CGA	GLU	410	-22.971	32.088	20.090	0.50	28.21	6
	ATOM	70	CGB	GLU	410	-22.946	32.209	20.195	0.50	38.29	6
	ATOM	71	CDA	GLU	410	-24.047	31.077	20.422	0.50	28.55	6

113

	ATOM	72	CDB	GLU	410	-23.100	33.664	20.587	0.50	43.48	6
	ATOM	73	OE1	GLU	410	-25.131	31.501	20.907	0.50	26.56	8
	ATOM	74	OE1	GLU	410	-22.443	34.095	21.565	0.50	47.24	8
5	ATOM	75	OE2	GLU	410	-23.888	29.858	20.186	0.50	22.10	8
	ATOM	76	OE2	GLU	410	-23.871	34.380	19.908	0.50	46.42	8
	ATOM	77	C	GLU	410	-19.096	32.138	20.008	1.00	19.76	6
	ATOM	78	O	GLU	410	-18.701	31.024	19.613	1.00	18.00	8
	ATOM	79	N	PRO	411	-18.423	32.871	20.888	1.00	19.07	7
10	ATOM	80	CD	PRO	411	-17.058	32.526	21.390	1.00	18.71	6
	ATOM	81	CA	PRO	411	-18.834	34.204	21.319	1.00	18.84	6
	ATOM	82	CB	PRO	411	-17.807	34.594	22.365	1.00	17.38	6
	ATOM	83	CG	PRO	411	-16.560	33.866	21.944	1.00	18.86	6
	ATOM	84	C	PRO	411	-18.787	35.108	20.090	1.00	20.01	6
15	ATOM	85	O	PRO	411	-18.310	34.654	19.051	1.00	16.22	8
	ATOM	86	N	PRO	412	-19.232	36.349	20.155	1.00	19.94	7
	ATOM	87	CD	PRO	412	-19.915	36.918	21.361	1.00	21.08	6
	ATOM	88	CA	PRO	412	-19.409	37.166	18.976	1.00	20.68	6
	ATOM	89	CB	PRO	412	-20.455	38.210	19.397	1.00	19.82	6
20	ATOM	90	CG	PRO	412	-20.292	38.299	20.872	1.00	23.59	6
	ATOM	91	C	PRO	412	-18.179	37.805	18.395	1.00	18.70	6
	ATOM	92	O	PRO	412	-18.268	38.391	17.318	1.00	19.85	8
	ATOM	93	N	TRP	413	-17.039	37.697	19.059	1.00	15.64	7
	ATOM	94	CA	TRP	413	-15.815	38.298	18.561	1.00	17.91	6
25	ATOM	95	CB	TRP	413	-14.688	38.026	19.562	1.00	14.32	6
	ATOM	96	CG	TRP	413	-15.124	38.117	21.006	1.00	16.77	6
	ATOM	97	CD2	TRP	413	-15.633	39.254	21.703	1.00	16.90	6
	ATOM	98	CE2	TRP	413	-15.899	38.861	23.032	1.00	16.87	6
	ATOM	99	CE3	TRP	413	-15.867	40.587	21.350	1.00	18.03	6
30	ATOM	100	CD1	TRP	413	-15.106	37.097	21.916	1.00	18.97	6
	ATOM	101	NE1	TRP	413	-15.589	37.523	23.137	1.00	11.16	7
	ATOM	102	CZ2	TRP	413	-16.405	39.742	23.973	1.00	15.92	6
	ATOM	103	CZ3	TRP	413	-16.358	41.457	22.301	1.00	10.59	6
	ATOM	104	CH2	TRP	413	-16.645	41.041	23.611	1.00	17.87	6
35	ATOM	105	C	TRP	413	-15.421	37.833	17.163	1.00	19.47	6
	ATOM	106	O	TRP	413	-15.283	36.628	16.908	1.00	17.22	8
	ATOM	107	N	ILE	414	-15.101	38.788	16.275	1.00	16.57	7
	ATOM	108	CA	ILE	414	-14.666	38.425	14.936	1.00	18.93	6
	ATOM	109	CB	ILE	414	-15.185	39.343	13.816	1.00	16.07	6
40	ATOM	110	CG2	ILE	414	-16.720	39.345	13.840	1.00	16.61	6
	ATOM	111	CG1	ILE	414	-14.582	40.747	13.972	1.00	21.35	6
	ATOM	112	CD1	ILE	414	-15.045	41.716	12.896	1.00	26.28	6
	ATOM	113	C	ILE	414	-13.144	38.317	14.825	1.00	20.48	6
	ATOM	114	O	ILE	414	-12.652	37.818	13.817	1.00	19.41	8
45	ATOM	115	N	ASN	415	-12.403	38.779	15.836	1.00	19.46	7
	ATOM	116	CA	ASN	415	-10.935	38.596	15.778	1.00	18.11	6
	ATOM	117	CB	ASN	415	-10.161	39.904	15.731	1.00	13.53	6
	ATOM	118	CG	ASN	415	-10.591	40.920	16.762	1.00	19.11	6
	ATOM	119	OD1	ASN	415	-11.728	40.907	17.227	1.00	13.35	8
50	ATOM	120	ND2	ASN	415	-9.688	41.833	17.142	1.00	10.11	7
	ATOM	121	C	ASN	415	-10.632	37.742	17.005	1.00	17.54	6
	ATOM	122	O	ASN	415	-11.016	38.131	18.111	1.00	15.32	8
	ATOM	123	N	VAL	416	-10.122	36.535	16.805	1.00	16.86	7
	ATOM	124	CA	VAL	416	-9.871	35.593	17.893	1.00	15.77	6
55	ATOM	125	CB	VAL	416	-10.761	34.332	17.748	1.00	16.54	6
	ATOM	126	CG1	VAL	416	-12.251	34.725	17.733	1.00	13.42	6
	ATOM	127	CG2	VAL	416	-10.490	33.521	16.491	1.00	18.04	6
	ATOM	128	C	VAL	416	-8.420	35.158	17.921	1.00	19.01	6
	ATOM	129	O	VAL	416	-7.618	35.485	17.010	1.00	17.12	8
60	ATOM	130	N	LEU	417	-8.022	34.444	18.964	1.00	17.68	7
	ATOM	131	CA	LEU	417	-6.664	33.904	19.068	1.00	15.11	6
	ATOM	132	CB	LEU	417	-6.162	34.140	20.522	1.00	20.26	6
	ATOM	133	CG	LEU	417	-5.873	35.615	20.823	1.00	23.07	6
	ATOM	134	CD1	LEU	417	-5.447	35.853	22.253	1.00	17.70	6
65	ATOM	135	CD2	LEU	417	-4.832	36.152	19.855	1.00	26.74	6
	ATOM	136	C	LEU	417	-6.563	32.427	18.732	1.00	16.37	6
	ATOM	137	O	LEU	417	-7.518	31.679	18.961	1.00	18.24	8
	ATOM	138	N	GLN	418	-5.424	31.935	18.227	1.00	18.55	7
	ATOM	139	CA	GLN	418	-5.237	30.496	18.032	1.00	19.13	6
70	ATOM	140	CB	GLN	418	-3.790	30.145	17.696	1.00	31.65	6
	ATOM	141	CG	GLN	418	-3.510	29.617	16.314	1.00	37.32	6
	ATOM	142	CD	GLN	418	-2.120	29.964	15.800	1.00	36.92	6

	ATOM	143	OE1	GLN	418	-1.953	30.834	14.943	1.00	30.97	8
	ATOM	144	NE2	GLN	418	-1.135	29.248	16.333	1.00	31.73	7
	ATOM	145	C	GLN	418	-5.561	29.789	19.348	1.00	19.43	6
5	ATOM	146	O	GLN	418	-5.194	30.298	20.413	1.00	18.10	8
	ATOM	147	N	GLU	419	-6.317	28.702	19.232	1.00	19.68	7
	ATOM	148	CA	GLU	419	-6.727	27.821	20.293	1.00	18.88	6
	ATOM	149	CB	GLU	419	-5.597	27.525	21.293	1.00	27.39	6
	ATOM	150	CG	GLU	419	-4.649	26.448	20.714	1.00	30.12	6
10	ATOM	151	CD	GLU	419	-3.558	26.167	21.720	1.00	41.87	6
	ATOM	152	OE1	GLU	419	-3.857	25.536	22.758	1.00	48.83	8
	ATOM	153	OE2	GLU	419	-2.421	26.594	21.464	1.00	46.61	8
	ATOM	154	C	GLU	419	-8.004	28.244	20.998	1.00	21.46	6
	ATOM	155	O	GLU	419	-8.496	27.461	21.815	1.00	26.39	8
	ATOM	156	N	ASP	420	-8.606	29.360	20.619	1.00	19.91	7
15	ATOM	157	CA	ASP	420	-9.898	29.772	21.114	1.00	20.76	6
	ATOM	158	CB	ASP	420	-10.285	31.217	20.726	1.00	13.47	6
	ATOM	159	CG	ASP	420	-9.587	32.288	21.526	1.00	13.93	6
	ATOM	160	OD1	ASP	420	-8.873	32.061	22.534	1.00	17.57	8
20	ATOM	161	OD2	ASP	420	-9.723	33.461	21.104	1.00	13.79	8
	ATOM	162	C	ASP	420	-11.002	28.916	20.451	1.00	19.58	6
	ATOM	163	O	ASP	420	-10.913	28.647	19.262	1.00	17.49	8
	ATOM	164	N	SER	421	-12.071	28.668	21.174	1.00	17.22	7
	ATOM	165	CA	SER	421	-13.233	27.937	20.659	1.00	17.62	6
25	ATOM	166	CBA	SER	421	-14.011	27.341	21.844	0.50	17.49	6
	ATOM	167	CBB	SER	421	-13.981	27.310	21.846	0.50	13.14	6
	ATOM	168	OGA	SER	421	-14.900	26.350	21.355	0.50	22.95	8
	ATOM	169	OGB	SER	421	-13.175	26.287	22.416	0.50	6.85	8
	ATOM	170	C	SER	421	-14.181	28.828	19.873	1.00	18.61	6
	ATOM	171	O	SER	421	-14.424	29.982	20.265	1.00	21.41	8
30	ATOM	172	N	VAL	422	-14.638	28.354	18.721	1.00	15.80	7
	ATOM	173	CA	VAL	422	-15.585	29.133	17.910	1.00	17.93	6
	ATOM	174	CB	VAL	422	-15.052	29.632	16.560	1.00	20.37	6
	ATOM	175	CG1	VAL	422	-16.093	30.465	15.804	1.00	17.77	6
35	ATOM	176	CG2	VAL	422	-13.858	30.566	16.679	1.00	17.26	6
	ATOM	177	C	VAL	422	-16.822	28.257	17.665	1.00	19.20	6
	ATOM	178	O	VAL	422	-16.633	27.097	17.291	1.00	18.52	8
	ATOM	179	N	THR	423	-18.021	28.759	17.917	1.00	16.32	7
	ATOM	180	CA	THR	423	-19.249	28.043	17.648	1.00	19.99	6
40	ATOM	181	CB	THR	423	-20.080	27.738	18.911	1.00	22.97	6
	ATOM	182	OG1	THR	423	-19.192	27.117	19.850	1.00	18.42	8
	ATOM	183	CG2	THR	423	-21.241	26.809	18.614	1.00	16.78	6
	ATOM	184	C	THR	423	-20.098	28.850	16.658	1.00	24.68	6
	ATOM	185	O	THR	423	-20.509	29.986	16.897	1.00	22.59	8
45	ATOM	186	N	LEU	424	-20.257	28.248	15.467	1.00	23.73	7
	ATOM	187	CA	LEU	424	-21.081	28.815	14.423	1.00	23.11	6
	ATOM	188	CB	LEU	424	-20.427	28.660	13.046	1.00	20.25	6
	ATOM	189	CG	LEU	424	-19.053	29.386	12.959	1.00	23.95	6
	ATOM	190	CD1	LEU	424	-18.324	29.010	11.681	1.00	20.78	6
50	ATOM	191	CD2	LEU	424	-19.251	30.881	13.049	1.00	22.74	6
	ATOM	192	C	LEU	424	-22.444	28.103	14.450	1.00	25.87	6
	ATOM	193	O	LEU	424	-22.470	26.858	14.537	1.00	24.57	8
	ATOM	194	N	THR	425	-23.520	28.886	14.367	1.00	20.22	7
	ATOM	195	CA	THR	425	-24.847	28.266	14.336	1.00	23.21	6
55	ATOM	196	CB	THR	425	-25.656	28.601	15.597	1.00	27.69	6
	ATOM	197	OG1	THR	425	-24.945	28.136	16.755	1.00	26.30	8
	ATOM	198	CG2	THR	425	-27.041	27.941	15.590	1.00	28.49	6
	ATOM	199	C	THR	425	-25.604	28.700	13.075	1.00	22.31	6
	ATOM	200	O	THR	425	-25.706	29.915	12.819	1.00	23.86	8
60	ATOM	201	N	CYS	426	-26.092	27.732	12.307	1.00	18.68	7
	ATOM	202	CA	CYS	426	-26.832	27.978	11.075	1.00	23.20	6
	ATOM	203	C	CYS	426	-28.345	27.956	11.346	1.00	23.06	6
	ATOM	204	O	CYS	426	-28.957	26.886	11.556	1.00	23.76	8
	ATOM	205	CB	CYS	426	-26.509	26.985	9.958	1.00	17.92	6
65	ATOM	206	SG	CYS	426	-27.138	27.508	8.311	1.00	22.25	16
	ATOM	207	N	GLN	427	-28.929	29.137	11.355	1.00	19.35	7
	ATOM	208	CA	GLN	427	-30.332	29.345	11.658	1.00	23.30	6
	ATOM	209	CB	GLN	427	-30.543	30.657	12.464	1.00	29.78	6
	ATOM	210	CG	GLN	427	-29.623	30.822	13.672	1.00	31.50	6
70	ATOM	211	CD	GLN	427	-29.927	32.038	14.518	1.00	33.01	6
	ATOM	212	OE1	GLN	427	-30.322	33.092	14.032	1.00	38.67	8
	ATOM	213	NE2	GLN	427	-29.792	31.971	15.834	1.00	36.36	7

115

	ATOM	214	C	GLN	427	-31.169	29.449	10.377	1.00	26.33	6
	ATOM	215	O	GLN	427	-30.764	30.010	9.347	1.00	23.15	8
	ATOM	216	N	GLY	428	-32.363	28.847	10.438	1.00	27.69	7
5	ATOM	217	CA	GLY	428	-33.289	28.847	9.313	1.00	28.02	6
	ATOM	218	C	GLY	428	-34.022	27.506	9.215	1.00	29.41	6
	ATOM	219	O	GLY	428	-33.639	26.531	9.862	1.00	28.46	8
	ATOM	220	N	ALA	429	-35.062	27.445	8.389	1.00	27.48	7
	ATOM	221	CA	ALA	429	-35.824	26.226	8.210	1.00	27.39	6
10	ATOM	222	CB	ALA	429	-36.979	26.513	7.239	1.00	25.91	6
	ATOM	223	C	ALA	429	-34.959	25.136	7.574	1.00	28.27	6
	ATOM	224	O	ALA	429	-34.315	25.451	6.561	1.00	26.07	8
	ATOM	225	N	ARG	430	-35.060	23.915	8.064	1.00	23.97	7
	ATOM	226	CA	ARG	430	-34.303	22.811	7.490	1.00	27.17	6
15	ATOM	227	CB	ARG	430	-33.571	22.043	8.601	1.00	30.34	6
	ATOM	228	CG	ARG	430	-32.574	22.776	9.460	1.00	34.05	6
	ATOM	229	CD	ARG	430	-32.365	21.986	10.761	1.00	33.86	6
	ATOM	230	NE	ARG	430	-32.407	22.964	11.836	1.00	38.60	7
	ATOM	231	CZ	ARG	430	-32.487	22.784	13.126	1.00	38.08	6
20	ATOM	232	NH1	ARG	430	-32.567	21.568	13.635	1.00	36.51	7
	ATOM	233	NH2	ARG	430	-32.467	23.876	13.879	1.00	46.13	7
	ATOM	234	C	ARG	430	-35.194	21.718	6.880	1.00	26.70	6
	ATOM	235	O	ARG	430	-36.399	21.724	7.075	1.00	29.22	8
	ATOM	236	N	SER	431	-34.573	20.737	6.246	1.00	26.85	7
25	ATOM	237	CA	SER	431	-35.315	19.582	5.738	1.00	26.56	6
	ATOM	238	CB	SER	431	-34.682	19.020	4.476	1.00	25.03	6
	ATOM	239	OG	SER	431	-34.562	19.991	3.477	1.00	27.59	8
	ATOM	240	C	SER	431	-35.273	18.545	6.861	1.00	26.58	6
	ATOM	241	O	SER	431	-34.396	18.620	7.739	1.00	23.91	8
30	ATOM	242	N	PRO	432	-36.163	17.558	6.839	1.00	23.48	7
	ATOM	243	CD	PRO	432	-37.224	17.383	5.842	1.00	22.70	6
	ATOM	244	CA	PRO	432	-36.176	16.516	7.861	1.00	24.75	6
	ATOM	245	CB	PRO	432	-37.621	16.036	7.805	1.00	24.34	6
	ATOM	246	CG	PRO	432	-38.095	16.295	6.414	1.00	23.77	6
35	ATOM	247	C	PRO	432	-35.172	15.417	7.549	1.00	29.23	6
	ATOM	248	O	PRO	432	-35.472	14.257	7.223	1.00	28.28	8
	ATOM	249	N	GLU	433	-33.913	15.745	7.709	1.00	29.77	7
	ATOM	250	CA	GLU	433	-32.725	14.970	7.417	1.00	33.37	6
	ATOM	251	CBA	GLU	433	-32.177	15.440	6.073	0.50	35.18	6
40	ATOM	252	CBB	GLU	433	-32.123	15.409	6.084	0.50	31.98	6
	ATOM	253	CGA	GLU	433	-30.795	16.037	5.952	0.50	39.40	6
	ATOM	254	CGB	GLU	433	-31.776	16.876	5.954	0.50	34.05	6
	ATOM	255	CDA	GLU	433	-30.394	16.341	4.521	0.50	46.48	6
	ATOM	256	CDB	GLU	433	-31.601	17.333	4.517	0.50	34.67	6
45	ATOM	257	OE1	GLU	433	-29.268	16.010	4.076	0.50	49.23	8
	ATOM	258	OE1	GLU	433	-32.194	16.698	3.619	0.50	32.81	8
	ATOM	259	OE2	GLU	433	-31.232	16.914	3.788	0.50	47.50	8
	ATOM	260	OE2	GLU	433	-30.877	18.324	4.275	0.50	24.64	8
	ATOM	261	C	GLU	433	-31.683	15.177	8.519	1.00	32.61	6
50	ATOM	262	O	GLU	433	-31.612	16.266	9.085	1.00	28.72	8
	ATOM	263	N	SER	434	-30.844	14.184	8.743	1.00	32.15	7
	ATOM	264	CA	SER	434	-29.804	14.275	9.764	1.00	32.72	6
	ATOM	265	CB	SER	434	-29.277	12.853	10.037	1.00	34.26	6
	ATOM	266	OG	SER	434	-28.320	12.935	11.093	1.00	45.88	8
55	ATOM	267	C	SER	434	-28.668	15.192	9.332	1.00	30.93	6
	ATOM	268	O	SER	434	-28.156	15.983	10.124	1.00	28.87	8
	ATOM	269	N	ASP	435	-28.222	15.093	8.082	1.00	28.02	7
	ATOM	270	CA	ASP	435	-27.167	16.008	7.599	1.00	28.62	6
	ATOM	271	CB	ASP	435	-26.292	15.328	6.585	1.00	29.65	6
60	ATOM	272	CG	ASP	435	-25.357	14.227	7.057	1.00	37.43	6
	ATOM	273	OD1	ASP	435	-25.027	14.097	8.258	1.00	33.53	8
	ATOM	274	OD2	ASP	435	-24.902	13.470	6.154	1.00	36.01	8
	ATOM	275	C	ASP	435	-27.882	17.223	6.973	1.00	27.08	6
	ATOM	276	O	ASP	435	-27.997	17.300	5.756	1.00	28.07	8
65	ATOM	277	N	SER	436	-28.461	18.118	7.774	1.00	25.55	7
	ATOM	278	CA	SER	436	-29.282	19.186	7.225	1.00	27.45	6
	ATOM	279	CB	SER	436	-30.440	19.435	8.213	1.00	34.87	6
	ATOM	280	OG	SER	436	-29.973	20.064	9.405	1.00	39.51	8
	ATOM	281	C	SER	436	-28.558	20.484	6.890	1.00	27.14	6
70	ATOM	282	O	SER	436	-29.143	21.445	6.363	1.00	25.67	8
	ATOM	283	N	ILE	437	-27.293	20.643	7.231	1.00	24.64	7
	ATOM	284	CA	ILE	437	-26.580	21.893	6.977	1.00	24.33	6

	ATOM	285	CB	ILE	437	-26.164	22.559	8.309	1.00	30.71	6
	ATOM	286	CG2	ILE	437	-25.561	23.935	8.032	1.00	26.94	6
	ATOM	287	CG1	ILE	437	-27.333	22.645	9.308	1.00	21.66	6
5	ATOM	288	CD1	ILE	437	-28.443	23.588	8.867	1.00	27.66	6
	ATOM	289	C	ILE	437	-25.336	21.707	6.128	1.00	24.08	6
	ATOM	290	O	ILE	437	-24.515	20.833	6.390	1.00	23.50	8
	ATOM	291	N	GLN	438	-25.122	22.552	5.127	1.00	24.52	7
	ATOM	292	CA	GLN	438	-23.862	22.570	4.399	1.00	23.13	6
10	ATOM	293	CB	GLN	438	-24.016	22.798	2.905	1.00	29.28	6
	ATOM	294	CG	GLN	438	-24.458	21.570	2.123	1.00	29.86	6
	ATOM	295	CD	GLN	438	-24.692	21.901	0.661	1.00	33.48	6
	ATOM	296	OE1	GLN	438	-25.540	22.744	0.323	1.00	28.34	8
	ATOM	297	NE2	GLN	438	-23.922	21.198	-0.177	1.00	38.54	7
	ATOM	298	C	GLN	438	-23.048	23.738	4.985	1.00	23.81	6
15	ATOM	299	O	GLN	438	-23.598	24.844	5.087	1.00	22.62	8
	ATOM	300	N	TRP	439	-21.807	23.480	5.371	1.00	21.43	7
	ATOM	301	CA	TRP	439	-20.987	24.562	5.905	1.00	21.73	6
	ATOM	302	CB	TRP	439	-20.345	24.233	7.257	1.00	21.01	6
20	ATOM	303	CG	TRP	439	-21.264	24.233	8.430	1.00	17.58	6
	ATOM	304	CD2	TRP	439	-21.721	25.343	9.212	1.00	17.00	6
	ATOM	305	CE2	TRP	439	-22.569	24.833	10.220	1.00	16.71	6
	ATOM	306	CE3	TRP	439	-21.495	26.719	9.158	1.00	21.47	6
	ATOM	307	CD1	TRP	439	-21.844	23.116	8.974	1.00	19.92	6
25	ATOM	308	NE1	TRP	439	-22.626	23.466	10.061	1.00	22.18	7
	ATOM	309	CZ2	TRP	439	-23.218	25.646	11.152	1.00	18.29	6
	ATOM	310	CZ3	TRP	439	-22.109	27.537	10.091	1.00	21.62	6
	ATOM	311	CH2	TRP	439	-22.960	26.992	11.064	1.00	20.15	6
	ATOM	312	C	TRP	439	-19.890	24.873	4.898	1.00	22.76	6
30	ATOM	313	O	TRP	439	-19.407	23.941	4.238	1.00	23.42	8
	ATOM	314	N	PHE	440	-19.533	26.165	4.758	1.00	22.91	7
	ATOM	315	CA	PHE	440	-18.512	26.477	3.754	1.00	26.86	6
	ATOM	316	CB	PHE	440	-19.121	27.144	2.513	1.00	24.16	6
	ATOM	317	CG	PHE	440	-20.225	26.437	1.788	1.00	23.96	6
35	ATOM	318	CD1	PHE	440	-21.551	26.586	2.189	1.00	23.61	6
	ATOM	319	CD2	PHE	440	-19.945	25.622	0.696	1.00	22.47	6
	ATOM	320	CE1	PHE	440	-22.564	25.947	1.504	1.00	20.83	6
	ATOM	321	CE2	PHE	440	-20.967	24.986	0.020	1.00	21.69	6
	ATOM	322	CZ	PHE	440	-22.267	25.126	0.432	1.00	21.86	6
40	ATOM	323	C	PHE	440	-17.466	27.431	4.349	1.00	23.51	6
	ATOM	324	O	PHE	440	-17.838	28.278	5.151	1.00	21.94	8
	ATOM	325	N	HIS	441	-16.232	27.291	3.905	1.00	21.59	7
	ATOM	326	CA	HIS	441	-15.107	28.095	4.366	1.00	24.07	6
	ATOM	327	CB	HIS	441	-14.032	27.294	5.099	1.00	18.72	6
45	ATOM	328	CG	HIS	441	-12.864	28.139	5.548	1.00	23.41	6
	ATOM	329	CD2	HIS	441	-12.794	29.451	5.899	1.00	21.85	6
	ATOM	330	ND1	HIS	441	-11.588	27.648	5.709	1.00	21.97	7
	ATOM	331	CE1	HIS	441	-10.789	28.607	6.135	1.00	22.79	6
	ATOM	332	NE2	HIS	441	-11.504	29.705	6.268	1.00	21.87	7
50	ATOM	333	C	HIS	441	-14.455	28.703	3.115	1.00	21.83	6
	ATOM	334	O	HIS	441	-13.972	27.947	2.282	1.00	21.37	8
	ATOM	335	N	ASN	442	-14.576	30.019	2.959	1.00	22.08	7
	ATOM	336	CA	ASN	442	-14.077	30.670	1.726	1.00	20.46	6
	ATOM	337	CB	ASN	442	-12.562	30.544	1.722	1.00	18.21	6
55	ATOM	338	CG	ASN	442	-11.925	31.469	2.761	1.00	22.74	6
	ATOM	339	OD1	ASN	442	-12.473	32.523	3.087	1.00	24.40	8
	ATOM	340	ND2	ASN	442	-10.804	31.062	3.341	1.00	18.43	7
	ATOM	341	C	ASN	442	-14.733	30.055	0.488	1.00	21.32	6
	ATOM	342	O	ASN	442	-14.085	29.819	-0.533	1.00	20.13	8
60	ATOM	343	N	GLY	443	-16.002	29.646	0.568	1.00	20.53	7
	ATOM	344	CA	GLY	443	-16.767	29.005	-0.480	1.00	20.83	6
	ATOM	345	C	GLY	443	-16.586	27.506	-0.661	1.00	24.51	6
	ATOM	346	O	GLY	443	-17.209	26.879	-1.550	1.00	25.30	8
	ATOM	347	N	ASN	444	-15.633	26.896	0.051	1.00	21.27	7
65	ATOM	348	CA	ASN	444	-15.391	25.473	-0.112	1.00	20.46	6
	ATOM	349	CB	ASN	444	-13.903	25.132	0.000	1.00	23.82	6
	ATOM	350	CG	ASN	444	-13.049	26.032	-0.891	1.00	22.26	6
	ATOM	351	OD1	ASN	444	-12.148	26.722	-0.409	1.00	25.47	8
	ATOM	352	ND2	ASN	444	-13.382	26.079	-2.171	1.00	21.59	7
70	ATOM	353	C	ASN	444	-16.208	24.723	0.937	1.00	19.78	6
	ATOM	354	O	ASN	444	-16.180	25.088	2.107	1.00	22.07	8
	ATOM	355	N	LEU	445	-16.907	23.678	0.523	1.00	22.22	7

	ATOM	356	CA	LEU	445	-17.730	22.904	1.459	1.00	21.67	6
	ATOM	357	CB	LEU	445	-18.391	21.725	0.715	1.00	28.15	6
	ATOM	358	CG	LEU	445	-19.159	20.695	1.538	1.00	29.14	6
5	ATOM	359	CD1	LEU	445	-20.479	21.295	2.002	1.00	25.07	6
	ATOM	360	CD2	LEU	445	-19.452	19.400	0.775	1.00	28.51	6
	ATOM	361	C	LEU	445	-16.825	22.307	2.525	1.00	22.27	6
	ATOM	362	O	LEU	445	-15.748	21.869	2.118	1.00	20.13	8
	ATOM	363	N	ILE	446	-17.263	22.262	3.766	1.00	20.11	7
10	ATOM	364	CA	ILE	446	-16.539	21.544	4.835	1.00	24.64	6
	ATOM	365	CB	ILE	446	-16.657	22.358	6.132	1.00	22.24	6
	ATOM	366	CG2	ILE	446	-16.007	21.732	7.358	1.00	21.33	6
	ATOM	367	CG1	ILE	446	-16.111	23.794	5.945	1.00	20.74	6
	ATOM	368	CD1	ILE	446	-16.664	24.719	7.024	1.00	20.48	6
	ATOM	369	C	ILE	446	-17.351	20.241	5.006	1.00	25.53	6
15	ATOM	370	O	ILE	446	-18.419	20.266	5.624	1.00	22.91	8
	ATOM	371	N	PRO	447	-16.937	19.119	4.444	1.00	30.56	7
	ATOM	372	CD	PRO	447	-15.704	18.982	3.620	1.00	32.61	6
	ATOM	373	CA	PRO	447	-17.731	17.898	4.434	1.00	30.93	6
20	ATOM	374	CB	PRO	447	-17.030	17.030	3.363	1.00	31.28	6
	ATOM	375	CG	PRO	447	-15.610	17.466	3.441	1.00	32.54	6
	ATOM	376	C	PRO	447	-17.888	17.104	5.706	1.00	28.32	6
	ATOM	377	O	PRO	447	-18.733	16.196	5.747	1.00	29.24	8
	ATOM	378	N	THR	448	-17.092	17.353	6.730	1.00	26.79	7
25	ATOM	379	CA	THR	448	-17.135	16.568	7.971	1.00	26.97	6
	ATOM	380	CB	THR	448	-15.698	16.543	8.532	1.00	31.78	6
	ATOM	381	OG1	THR	448	-15.241	17.908	8.520	1.00	31.45	8
	ATOM	382	CG2	THR	448	-14.798	15.716	7.605	1.00	27.40	6
	ATOM	383	C	THR	448	-18.075	17.109	9.021	1.00	26.31	6
	ATOM	384	O	THR	448	-18.206	16.532	10.113	1.00	28.00	8
30	ATOM	385	N	HIS	449	-18.698	18.264	8.772	1.00	24.44	7
	ATOM	386	CA	HIS	449	-19.612	18.924	9.707	1.00	24.19	6
	ATOM	387	CB	HIS	449	-18.953	20.256	10.174	1.00	25.11	6
	ATOM	388	CG	HIS	449	-17.722	19.927	10.961	1.00	22.20	6
	ATOM	389	CD2	HIS	449	-16.430	19.757	10.624	1.00	27.86	6
35	ATOM	390	ND1	HIS	449	-17.809	19.641	12.306	1.00	29.80	7
	ATOM	391	CE1	HIS	449	-16.595	19.340	12.762	1.00	28.91	6
	ATOM	392	NE2	HIS	449	-15.748	19.392	11.761	1.00	25.35	7
	ATOM	393	C	HIS	449	-20.923	19.278	9.041	1.00	23.08	6
	ATOM	394	O	HIS	449	-20.942	20.061	8.075	1.00	20.57	8
40	ATOM	395	N	THR	450	-22.038	18.704	9.497	1.00	25.11	7
	ATOM	396	CA	THR	450	-23.321	18.892	8.807	1.00	22.98	6
	ATOM	397	CB	THR	450	-23.732	17.552	8.137	1.00	23.01	6
	ATOM	398	OG1	THR	450	-23.843	16.614	9.231	1.00	18.66	8
45	ATOM	399	CG2	THR	450	-22.757	17.049	7.101	1.00	19.07	6
	ATOM	400	C	THR	450	-24.460	19.221	9.766	1.00	24.61	6
	ATOM	401	O	THR	450	-25.640	19.094	9.393	1.00	26.17	8
	ATOM	402	N	GLN	451	-24.126	19.592	10.985	1.00	24.52	7
	ATOM	403	CA	GLN	451	-25.132	19.887	11.995	1.00	27.31	6
50	ATOM	404	CB	GLN	451	-24.708	19.361	13.378	1.00	28.63	6
	ATOM	405	CG	GLN	451	-24.438	17.852	13.378	1.00	32.81	6
	ATOM	406	CD	GLN	451	-25.677	17.056	12.995	1.00	38.53	6
	ATOM	407	OE1	GLN	451	-26.606	16.914	13.802	1.00	37.60	8
	ATOM	408	NE2	GLN	451	-25.724	16.535	11.765	1.00	32.79	7
55	ATOM	409	C	GLN	451	-25.411	21.379	12.101	1.00	26.69	6
	ATOM	410	O	GLN	451	-24.626	22.230	11.689	1.00	26.27	8
	ATOM	411	N	PRO	452	-26.510	21.728	12.769	1.00	25.16	7
	ATOM	412	CD	PRO	452	-27.553	20.775	13.270	1.00	24.54	6
	ATOM	413	CA	PRO	452	-26.917	23.103	12.974	1.00	25.24	6
60	ATOM	414	CB	PRO	452	-28.264	22.978	13.708	1.00	26.09	6
	ATOM	415	CG	PRO	452	-28.804	21.649	13.257	1.00	23.35	6
	ATOM	416	C	PRO	452	-25.900	23.951	13.722	1.00	25.71	6
	ATOM	417	O	PRO	452	-25.877	25.179	13.542	1.00	21.61	8
	ATOM	418	N	SER	453	-25.044	23.369	14.556	1.00	24.05	7
	ATOM	419	CA	SER	453	-23.991	24.093	15.239	1.00	25.63	6
65	ATOM	420	CB	SER	453	-24.105	24.155	16.758	1.00	31.86	6
	ATOM	421	OG	SER	453	-24.778	25.371	17.094	1.00	42.46	8
	ATOM	422	C	SER	453	-22.681	23.406	14.854	1.00	24.85	6
	ATOM	423	O	SER	453	-22.681	22.193	14.691	1.00	23.68	8
70	ATOM	424	N	TYR	454	-21.658	24.177	14.614	1.00	24.52	7
	ATOM	425	CA	TYR	454	-20.333	23.699	14.212	1.00	26.29	6
	ATOM	426	CB	TYR	454	-20.050	23.980	12.729	1.00	26.92	6

118

	ATOM	427	CG	TYR	454	-18.612	23.868	12.274	1.00	30.15	6
	ATOM	428	CD1	TYR	454	-17.719	22.961	12.825	1.00	29.18	6
	ATOM	429	CE1	TYR	454	-16.407	22.860	12.409	1.00	31.26	6
5	ATOM	430	CD2	TYR	454	-18.104	24.700	11.280	1.00	31.67	6
	ATOM	431	CE2	TYR	454	-16.796	24.649	10.855	1.00	31.66	6
	ATOM	432	CZ	TYR	454	-15.950	23.715	11.429	1.00	33.63	6
	ATOM	433	OH	TYR	454	-14.624	23.647	11.038	1.00	34.53	8
	ATOM	434	C	TYR	454	-19.378	24.416	15.167	1.00	24.84	6
10	ATOM	435	O	TYR	454	-19.300	25.656	15.129	1.00	22.53	8
	ATOM	436	N	ARG	455	-18.773	23.685	16.070	1.00	21.66	7
	ATOM	437	CA	ARG	455	-17.864	24.216	17.070	1.00	23.60	6
	ATOM	438	CB	ARG	455	-18.242	23.709	18.480	1.00	25.95	6
	ATOM	439	CG	ARG	455	-17.478	24.526	19.551	1.00	23.98	6
15	ATOM	440	CD	ARG	455	-17.651	23.884	20.918	1.00	35.38	6
	ATOM	441	NE	ARG	455	-16.821	24.501	21.956	1.00	27.47	7
	ATOM	442	CZ	ARG	455	-17.278	25.336	22.879	1.00	33.10	6
	ATOM	443	NH1	ARG	455	-18.570	25.657	22.904	1.00	30.00	7
	ATOM	444	NH2	ARG	455	-16.418	25.817	23.778	1.00	32.66	7
20	ATOM	445	C	ARG	455	-16.434	23.763	16.802	1.00	27.49	6
	ATOM	446	O	ARG	455	-16.275	22.554	16.569	1.00	22.62	8
	ATOM	447	N	PHE	456	-15.455	24.692	16.781	1.00	23.78	7
	ATOM	448	CA	PHE	456	-14.092	24.230	16.510	1.00	21.92	6
	ATOM	449	CB	PHE	456	-13.716	24.371	15.036	1.00	25.99	6
25	ATOM	450	CG	PHE	456	-13.819	25.735	14.386	1.00	20.84	6
	ATOM	451	CD1	PHE	456	-15.019	26.213	13.897	1.00	21.33	6
	ATOM	452	CD2	PHE	456	-12.705	26.547	14.264	1.00	20.31	6
	ATOM	453	CE1	PHE	456	-15.103	27.451	13.283	1.00	21.52	6
	ATOM	454	CE2	PHE	456	-12.768	27.789	13.680	1.00	18.36	6
30	ATOM	455	CZ	PHE	456	-13.973	28.250	13.159	1.00	18.38	6
	ATOM	456	C	PHE	456	-13.095	25.004	17.372	1.00	23.93	6
	ATOM	457	O	PHE	456	-13.454	26.033	17.921	1.00	22.42	8
	ATOM	458	N	LYS	457	-11.865	24.526	17.423	1.00	22.46	7
	ATOM	459	CA	LYS	457	-10.735	25.207	18.054	1.00	24.34	6
35	ATOM	460	CBA	LYS	457	-9.892	24.246	18.881	0.50	28.51	6
	ATOM	461	CBB	LYS	457	-9.822	24.139	18.669	0.50	22.87	6
	ATOM	462	CGA	LYS	457	-10.656	23.568	20.010	0.50	33.64	6
	ATOM	463	CGB	LYS	457	-8.769	24.658	19.632	0.50	24.29	6
	ATOM	464	CDA	LYS	457	-11.436	24.524	20.892	0.50	40.75	6
40	ATOM	465	CDB	LYS	457	-8.631	23.680	20.798	0.50	26.90	6
	ATOM	466	CEA	LYS	457	-12.612	23.876	21.603	0.50	43.07	6
	ATOM	467	CEB	LYS	457	-9.138	24.262	22.092	0.50	29.79	6
	ATOM	468	NZA	LYS	457	-12.703	24.236	23.044	0.50	51.71	7
	ATOM	469	NZB	LYS	457	-8.050	24.601	23.060	0.50	36.22	7
45	ATOM	470	C	LYS	457	-9.950	25.943	16.969	1.00	21.30	6
	ATOM	471	O	LYS	457	-9.436	25.315	16.052	1.00	19.46	8
	ATOM	472	N	ALA	458	-9.928	27.278	16.945	1.00	18.23	7
	ATOM	473	CA	ALA	458	-9.341	28.002	15.821	1.00	15.74	6
	ATOM	474	CB	ALA	458	-9.612	29.505	16.094	1.00	9.09	6
50	ATOM	475	C	ALA	458	-7.841	27.832	15.614	1.00	20.26	6
	ATOM	476	O	ALA	458	-7.067	27.802	16.574	1.00	18.04	8
	ATOM	477	N	ASN	459	-7.392	27.740	14.367	1.00	18.31	7
	ATOM	478	CA	ASN	459	-5.986	27.795	14.019	1.00	23.04	6
	ATOM	479	CB	ASN	459	-5.222	26.565	13.612	1.00	32.39	6
55	ATOM	480	CG	ASN	459	-5.880	25.223	13.665	1.00	38.26	6
	ATOM	481	OD1	ASN	459	-5.855	24.587	14.716	1.00	42.50	8
	ATOM	482	ND2	ASN	459	-6.426	24.800	12.529	1.00	43.39	7
	ATOM	483	C	ASN	459	-5.825	28.814	12.867	1.00	24.07	6
	ATOM	484	O	ASN	459	-6.794	29.390	12.365	1.00	21.25	8
60	ATOM	485	N	ASN	460	-4.582	29.033	12.484	1.00	24.40	7
	ATOM	486	CA	ASN	460	-4.192	30.043	11.519	1.00	31.47	6
	ATOM	487	CB	ASN	460	-2.680	29.973	11.234	1.00	31.46	6
	ATOM	488	CGA	ASN	460	-2.272	31.090	10.274	0.50	31.26	6
	ATOM	489	CGB	ASN	460	-2.221	28.594	10.814	0.50	35.72	6
65	ATOM	490	OD1	ASN	460	-2.337	32.284	10.597	0.50	22.52	8
	ATOM	491	OD1	ASN	460	-2.985	27.626	10.768	0.50	33.04	8
	ATOM	492	ND2	ASN	460	-1.863	30.691	9.070	0.50	26.04	7
	ATOM	493	ND2	ASN	460	-0.932	28.475	10.483	0.50	39.47	7
	ATOM	494	C	ASN	460	-5.006	29.923	10.234	1.00	29.05	6
70	ATOM	495	O	ASN	460	-5.645	30.880	9.780	1.00	32.27	8
	ATOM	496	N	ASN	461	-5.098	28.713	9.710	1.00	30.20	7
	ATOM	497	CAA	ASN	461	-5.863	28.379	8.529	0.50	28.68	6

	ATOM	498	CAB	ASN	461	-5.857	28.499	8.477	0.50	29.13	6
	ATOM	499	CBA	ASN	461	-5.564	26.911	8.150	0.50	26.19	6
	ATOM	500	CBB	ASN	461	-5.403	27.195	7.806	0.50	30.25	6
5	ATOM	501	CGA	ASN	461	-4.101	26.739	7.792	0.50	27.01	6
	ATOM	502	CGB	ASN	461	-5.608	25.984	8.678	0.50	32.36	6
	ATOM	503	OD1	ASN	461	-3.502	25.741	8.184	0.50	28.58	8
	ATOM	504	OD1	ASN	461	-6.383	26.046	9.637	0.50	33.38	8
	ATOM	505	ND2	ASN	461	-3.526	27.694	7.071	0.50	34.39	7
10	ATOM	506	ND2	ASN	461	-4.927	24.875	8.384	0.50	33.52	7
	ATOM	507	C	ASN	461	-7.371	28.530	8.628	1.00	25.33	6
	ATOM	508	O	ASN	461	-8.030	28.331	7.617	1.00	21.46	8
	ATOM	509	N	ASP	462	-7.932	28.888	9.767	1.00	24.89	7
	ATOM	510	CA	ASP	462	-9.373	29.024	9.941	1.00	21.37	6
	ATOM	511	CB	ASP	462	-9.749	28.582	11.372	1.00	16.89	6
15	ATOM	512	CG	ASP	462	-9.620	27.084	11.538	1.00	26.20	6
	ATOM	513	OD1	ASP	462	-9.824	26.317	10.570	1.00	20.81	8
	ATOM	514	OD2	ASP	462	-9.276	26.593	12.611	1.00	17.90	8
	ATOM	515	C	ASP	462	-9.887	30.427	9.645	1.00	18.69	6
	ATOM	516	O	ASP	462	-11.104	30.657	9.654	1.00	20.50	8
20	ATOM	517	N	SER	463	-9.011	31.389	9.394	1.00	19.81	7
	ATOM	518	CA	SER	463	-9.434	32.734	9.015	1.00	19.84	6
	ATOM	519	CB	SER	463	-8.268	33.702	8.811	1.00	22.04	6
	ATOM	520	OG	SER	463	-7.506	33.848	10.009	1.00	20.02	8
	ATOM	521	C	SER	463	-10.196	32.662	7.682	1.00	23.89	6
25	ATOM	522	O	SER	463	-10.015	31.706	6.911	1.00	17.92	8
	ATOM	523	N	GLY	464	-11.056	33.671	7.467	1.00	19.50	7
	ATOM	524	CA	GLY	464	-11.769	33.675	6.190	1.00	22.23	6
	ATOM	525	C	GLY	464	-13.272	33.901	6.340	1.00	19.81	6
	ATOM	526	O	GLY	464	-13.744	34.302	7.399	1.00	18.93	8
30	ATOM	527	N	GLU	465	-13.980	33.640	5.238	1.00	17.01	7
	ATOM	528	CA	GLU	465	-15.428	33.853	5.269	1.00	21.39	6
	ATOM	529	CBA	GLU	465	-15.934	34.304	3.901	0.50	13.64	6
	ATOM	530	CBB	GLU	465	-15.933	34.420	3.947	0.50	23.81	6
	ATOM	531	CGA	GLU	465	-16.507	35.708	3.813	0.50	15.71	6
35	ATOM	532	CGB	GLU	465	-15.409	35.807	3.602	0.50	32.15	6
	ATOM	533	CDA	GLU	465	-16.656	36.187	2.381	0.50	22.33	6
	ATOM	534	CDB	GLU	465	-15.898	36.901	4.520	0.50	40.56	6
	ATOM	535	OE1	GLU	465	-17.428	35.603	1.586	0.50	22.70	8
	ATOM	536	OE1	GLU	465	-16.578	36.595	5.525	0.50	41.83	8
40	ATOM	537	OE2	GLU	465	-15.991	37.180	2.014	0.50	31.04	8
	ATOM	538	OE2	GLU	465	-15.624	38.108	4.278	0.50	46.02	8
	ATOM	539	C	GLU	465	-16.155	32.542	5.593	1.00	21.56	6
	ATOM	540	O	GLU	465	-15.756	31.541	5.007	1.00	21.41	8
45	ATOM	541	N	TYR	466	-17.172	32.598	6.458	1.00	21.38	7
	ATOM	542	CA	TYR	466	-17.966	31.383	6.691	1.00	17.91	6
	ATOM	543	CB	TYR	466	-17.954	30.882	8.129	1.00	17.39	6
	ATOM	544	CG	TYR	466	-16.620	30.303	8.534	1.00	18.08	6
	ATOM	545	CD1	TYR	466	-15.605	31.180	8.957	1.00	18.56	6
50	ATOM	546	CE1	TYR	466	-14.369	30.719	9.323	1.00	16.48	6
	ATOM	547	CD2	TYR	466	-16.348	28.945	8.485	1.00	18.23	6
	ATOM	548	CE2	TYR	466	-15.102	28.484	8.867	1.00	18.37	6
	ATOM	549	CZ	TYR	466	-14.124	29.350	9.279	1.00	18.98	6
	ATOM	550	OH	TYR	466	-12.872	28.927	9.624	1.00	14.14	8
55	ATOM	551	C	TYR	466	-19.379	31.635	6.212	1.00	13.96	6
	ATOM	552	O	TYR	466	-19.923	32.731	6.353	1.00	18.14	8
	ATOM	553	N	THR	467	-20.010	30.638	5.568	1.00	17.95	7
	ATOM	554	CA	THR	467	-21.374	30.728	5.117	1.00	18.06	6
	ATOM	555	CB	THR	467	-21.514	31.022	3.599	1.00	22.52	6
60	ATOM	556	OG1	THR	467	-20.669	30.129	2.835	1.00	16.85	8
	ATOM	557	CG2	THR	467	-21.215	32.495	3.309	1.00	17.46	6
	ATOM	558	C	THR	467	-22.044	29.358	5.384	1.00	18.76	6
	ATOM	559	O	THR	467	-21.354	28.351	5.567	1.00	17.47	8
	ATOM	560	N	CYS	468	-23.354	29.326	5.389	1.00	19.74	7
65	ATOM	561	CA	CYS	468	-24.099	28.074	5.597	1.00	23.50	6
	ATOM	562	C	CYS	468	-25.382	28.107	4.758	1.00	23.12	6
	ATOM	563	O	CYS	468	-25.791	29.154	4.279	1.00	25.07	8
	ATOM	564	CB	CYS	468	-24.434	27.784	7.055	1.00	18.70	6
	ATOM	565	SG	CYS	468	-25.675	28.881	7.798	1.00	23.45	16
70	ATOM	566	N	GLN	469	-25.975	26.946	4.534	1.00	24.47	7
	ATOM	567	CA	GLN	469	-27.174	26.745	3.770	1.00	24.99	6
	ATOM	568	CB	GLN	469	-26.909	26.522	2.264	1.00	27.22	6

	ATOM	569	CG	GLN	469	-28.155	26.809	1.419	1.00	25.14	6
	ATOM	570	CD	GLN	469	-27.857	26.844	-0.065	1.00	32.43	6
	ATOM	571	OE1	GLN	469	-26.710	26.700	-0.487	1.00	31.34	8
5	ATOM	572	NE2	GLN	469	-28.896	27.052	-0.874	1.00	27.89	7
	ATOM	573	C	GLN	469	-27.901	25.483	4.266	1.00	27.60	6
	ATOM	574	O	GLN	469	-27.289	24.514	4.734	1.00	25.37	8
	ATOM	575	N	THR	470	-29.206	25.548	4.115	1.00	28.73	7
	ATOM	576	CA	THR	470	-30.059	24.401	4.439	1.00	32.10	6
10	ATOM	577	CB	THR	470	-31.125	24.713	5.491	1.00	33.36	6
	ATOM	578	OG1	THR	470	-30.619	25.555	6.553	1.00	45.26	8
	ATOM	579	CG2	THR	470	-31.453	23.422	6.210	1.00	50.20	6
	ATOM	580	C	THR	470	-30.737	23.976	3.138	1.00	32.77	6
	ATOM	581	O	THR	470	-30.680	24.696	2.130	1.00	30.75	8
15	ATOM	582	N	GLY	471	-31.472	22.859	3.175	1.00	31.83	7
	ATOM	583	CA	GLY	471	-32.224	22.397	2.033	1.00	27.97	6
	ATOM	584	C	GLY	471	-33.376	23.322	1.690	1.00	29.94	6
	ATOM	585	O	GLY	471	-33.938	23.198	0.596	1.00	32.37	8
	ATOM	586	N	GLN	472	-33.842	24.159	2.594	1.00	24.86	7
20	ATOM	587	CA	GLN	472	-34.920	25.087	2.457	1.00	27.14	6
	ATOM	588	CB	GLN	472	-35.868	24.892	3.667	1.00	27.31	6
	ATOM	589	CG	GLN	472	-36.291	23.415	3.825	1.00	30.51	6
	ATOM	590	CD	GLN	472	-36.961	22.871	2.567	1.00	30.53	6
	ATOM	591	OE1	GLN	472	-37.981	23.425	2.161	1.00	39.95	8
25	ATOM	592	NE2	GLN	472	-36.402	21.852	1.944	1.00	31.16	7
	ATOM	593	C	GLN	472	-34.530	26.561	2.441	1.00	29.60	6
	ATOM	594	O	GLN	472	-35.419	27.424	2.578	1.00	30.82	8
	ATOM	595	N	THR	473	-33.248	26.912	2.380	1.00	25.83	7
	ATOM	596	CA	THR	473	-32.861	28.317	2.426	1.00	26.62	6
30	ATOM	597	CB	THR	473	-32.278	28.731	3.792	1.00	26.64	6
	ATOM	598	OG1	THR	473	-31.226	27.815	4.138	1.00	27.54	8
	ATOM	599	CG2	THR	473	-33.313	28.742	4.897	1.00	28.16	6
	ATOM	600	C	THR	473	-31.824	28.643	1.371	1.00	26.31	6
	ATOM	601	O	THR	473	-31.210	27.756	0.776	1.00	28.00	8
35	ATOM	602	N	SER	474	-31.685	29.939	1.074	1.00	28.62	7
	ATOM	603	CA	SER	474	-30.592	30.261	0.112	1.00	29.44	6
	ATOM	604	CB	SER	474	-31.020	31.396	-0.803	1.00	30.45	6
	ATOM	605	OG	SER	474	-31.407	32.467	0.034	1.00	41.05	8
	ATOM	606	C	SER	474	-29.366	30.471	0.992	1.00	26.65	6
40	ATOM	607	O	SER	474	-29.461	30.428	2.228	1.00	25.57	8
	ATOM	608	N	LEU	475	-28.178	30.585	0.442	1.00	29.47	7
	ATOM	609	CA	LEU	475	-26.915	30.703	1.158	1.00	25.10	6
	ATOM	610	CB	LEU	475	-25.749	30.725	0.159	1.00	27.83	6
45	ATOM	611	CG	LEU	475	-24.348	30.730	0.777	1.00	27.24	6
	ATOM	612	CD1	LEU	475	-23.888	29.312	1.094	1.00	24.13	6
	ATOM	613	CD2	LEU	475	-23.349	31.446	-0.133	1.00	24.42	6
	ATOM	614	C	LEU	475	-26.884	31.893	2.087	1.00	25.84	6
	ATOM	615	O	LEU	475	-27.300	33.008	1.711	1.00	22.45	8
	ATOM	616	N	SER	476	-26.376	31.708	3.315	1.00	23.31	7
50	ATOM	617	CA	SER	476	-26.357	32.857	4.219	1.00	25.20	6
	ATOM	618	CB	SER	476	-25.916	32.464	5.644	1.00	26.64	6
	ATOM	619	OG	SER	476	-24.514	32.203	5.624	1.00	29.43	8
	ATOM	620	C	SER	476	-25.346	33.911	3.738	1.00	23.00	6
	ATOM	621	O	SER	476	-24.431	33.562	3.006	1.00	21.02	8
55	ATOM	622	N	ASP	477	-25.506	35.127	4.241	1.00	22.24	7
	ATOM	623	CA	ASP	477	-24.493	36.154	4.094	1.00	26.03	6
	ATOM	624	CB	ASP	477	-24.907	37.504	4.683	1.00	20.27	6
	ATOM	625	CG	ASP	477	-25.914	38.190	3.758	1.00	25.73	6
	ATOM	626	OD1	ASP	477	-25.821	37.973	2.541	1.00	23.79	8
60	ATOM	627	OD2	ASP	477	-26.769	38.912	4.292	1.00	28.92	8
	ATOM	628	C	ASP	477	-23.267	35.675	4.929	1.00	25.85	6
	ATOM	629	O	ASP	477	-23.423	34.962	5.914	1.00	24.00	8
	ATOM	630	N	PRO	478	-22.098	36.108	4.492	1.00	27.37	7
	ATOM	631	CD	PRO	478	-21.917	36.949	3.275	1.00	26.84	6
65	ATOM	632	CA	PRO	478	-20.849	35.736	5.098	1.00	25.42	6
	ATOM	633	CB	PRO	478	-19.795	36.274	4.141	1.00	28.38	6
	ATOM	634	CG	PRO	478	-20.453	37.280	3.272	1.00	27.24	6
	ATOM	635	C	PRO	478	-20.575	36.310	6.479	1.00	25.28	6
	ATOM	636	O	PRO	478	-21.006	37.407	6.820	1.00	23.68	8
70	ATOM	637	N	VAL	479	-19.833	35.535	7.265	1.00	20.24	7
	ATOM	638	CA	VAL	479	-19.287	36.005	8.535	1.00	18.86	6
	ATOM	639	CB	VAL	479	-19.850	35.350	9.783	1.00	19.49	6

121

	ATOM	640	CG1	VAL	479	-19.042	35.627	11.046	1.00	22.25	6
	ATOM	641	CG2	VAL	479	-21.275	35.907	10.036	1.00	21.95	6
	ATOM	642	C	VAL	479	-17.777	35.820	8.399	1.00	19.76	6
5	ATOM	643	O	VAL	479	-17.283	34.736	8.076	1.00	22.34	8
	ATOM	644	N	HIS	480	-17.024	36.911	8.566	1.00	19.43	7
	ATOM	645	CA	HIS	480	-15.584	36.890	8.387	1.00	18.11	6
	ATOM	646	CB	HIS	480	-15.130	38.245	7.784	1.00	26.87	6
	ATOM	647	CG	HIS	480	-13.712	38.112	7.293	1.00	31.93	6
10	ATOM	648	CD2	HIS	480	-13.194	37.883	6.069	1.00	27.05	6
	ATOM	649	ND1	HIS	480	-12.637	38.169	8.176	1.00	34.35	7
	ATOM	650	CE1	HIS	480	-11.525	38.019	7.480	1.00	34.80	6
	ATOM	651	NE2	HIS	480	-11.831	37.850	6.210	1.00	34.81	7
	ATOM	652	C	HIS	480	-14.865	36.679	9.718	1.00	23.08	6
15	ATOM	653	O	HIS	480	-15.096	37.370	10.709	1.00	23.37	8
	ATOM	654	N	LEU	481	-13.953	35.728	9.747	1.00	19.18	7
	ATOM	655	CA	LEU	481	-13.244	35.388	10.957	1.00	21.58	6
	ATOM	656	CB	LEU	481	-13.567	33.929	11.331	1.00	18.20	6
	ATOM	657	CG	LEU	481	-12.847	33.485	12.605	1.00	18.21	6
20	ATOM	658	CD1	LEU	481	-13.496	34.158	13.812	1.00	19.39	6
	ATOM	659	CD2	LEU	481	-12.865	31.954	12.696	1.00	14.76	6
	ATOM	660	C	LEU	481	-11.747	35.611	10.783	1.00	19.36	6
	ATOM	661	O	LEU	481	-11.225	35.323	9.720	1.00	20.96	8
	ATOM	662	N	THR	482	-11.100	36.177	11.793	1.00	19.61	7
25	ATOM	663	CA	THR	482	-9.642	36.403	11.680	1.00	18.45	6
	ATOM	664	CB	THR	482	-9.316	37.916	11.683	1.00	25.98	6
	ATOM	665	OG1	THR	482	-9.907	38.515	10.527	1.00	18.89	8
	ATOM	666	CG2	THR	482	-7.795	38.091	11.666	1.00	24.98	6
	ATOM	667	C	THR	482	-8.971	35.766	12.891	1.00	16.02	6
30	ATOM	668	O	THR	482	-9.248	36.131	14.035	1.00	14.79	8
	ATOM	669	N	VAL	483	-8.075	34.821	12.647	1.00	16.23	7
	ATOM	670	CA	VAL	483	-7.451	34.108	13.753	1.00	16.97	6
	ATOM	671	CB	VAL	483	-7.559	32.584	13.530	1.00	12.81	6
	ATOM	672	CG1	VAL	483	-7.051	31.894	14.799	1.00	15.92	6
35	ATOM	673	CG2	VAL	483	-8.986	32.106	13.246	1.00	11.78	6
	ATOM	674	C	VAL	483	-6.020	34.602	13.892	1.00	19.97	6
	ATOM	675	O	VAL	483	-5.261	34.537	12.918	1.00	18.57	8
	ATOM	676	N	LEU	484	-5.686	35.110	15.075	1.00	16.89	7
	ATOM	677	CA	LEU	484	-4.372	35.678	15.312	1.00	19.89	6
40	ATOM	678	CB	LEU	484	-4.621	37.080	15.890	1.00	18.15	6
	ATOM	679	CG	LEU	484	-5.491	38.003	15.021	1.00	23.40	6
	ATOM	680	CD1	LEU	484	-5.927	39.176	15.868	1.00	25.20	6
	ATOM	681	CD2	LEU	484	-4.752	38.470	13.758	1.00	20.46	6
	ATOM	682	C	LEU	484	-3.487	34.850	16.228	1.00	22.29	6
45	ATOM	683	O	LEU	484	-3.928	33.975	16.975	1.00	23.90	8
	ATOM	684	N	PHE	485	-2.189	35.116	16.218	1.00	21.03	7
	ATOM	685	CA	PHE	485	-1.254	34.422	17.111	1.00	22.92	6
	ATOM	686	CB	PHE	485	-0.399	33.435	16.333	1.00	21.76	6
	ATOM	687	CG	PHE	485	0.440	32.516	17.184	1.00	27.90	6
50	ATOM	688	CD1	PHE	485	-0.103	31.853	18.266	1.00	28.30	6
	ATOM	689	CD2	PHE	485	1.787	32.333	16.899	1.00	26.61	6
	ATOM	690	CE1	PHE	485	0.664	30.992	19.040	1.00	29.65	6
	ATOM	691	CE2	PHE	485	2.559	31.480	17.668	1.00	25.61	6
	ATOM	692	CZ	PHE	485	1.996	30.819	18.733	1.00	28.75	6
55	ATOM	693	C	PHE	485	-0.455	35.467	17.852	1.00	21.99	6
	ATOM	694	O	PHE	485	0.642	35.866	17.426	1.00	22.11	8
	ATOM	695	N	GLU	486	-1.023	35.983	18.938	1.00	20.76	7
	ATOM	696	CA	GLU	486	-0.421	37.104	19.702	1.00	18.04	6
	ATOM	697	CB	GLU	486	-1.142	38.403	19.210	1.00	20.84	6
60	ATOM	698	CG	GLU	486	-0.711	39.051	17.911	1.00	25.05	6
	ATOM	699	CD	GLU	486	-1.647	39.818	17.019	1.00	41.96	6
	ATOM	700	OE1	GLU	486	-2.719	40.359	17.416	1.00	46.14	8
	ATOM	701	OE2	GLU	486	-1.429	39.973	15.765	1.00	40.77	8
	ATOM	702	C	GLU	486	-0.694	36.840	21.176	1.00	18.46	6
65	ATOM	703	O	GLU	486	-1.588	36.027	21.462	1.00	16.67	8
	ATOM	704	N	TRP	487	-0.031	37.458	22.156	1.00	12.60	7
	ATOM	705	CA	TRP	487	-0.328	37.235	23.553	1.00	13.01	6
	ATOM	706	CB	TRP	487	0.808	37.810	24.411	1.00	18.40	6
	ATOM	707	CG	TRP	487	1.922	36.843	24.687	1.00	21.87	6
70	ATOM	708	CD2	TRP	487	1.812	35.690	25.521	1.00	21.14	6
	ATOM	709	CE2	TRP	487	3.065	35.061	25.526	1.00	24.31	6
	ATOM	710	CE3	TRP	487	0.767	35.128	26.255	1.00	24.84	6

	ATOM	711	CD1	TRP	487	3.216	36.881	24.231	1.00	22.52	6
	ATOM	712	NE1	TRP	487	3.907	35.797	24.734	1.00	22.53	7
	ATOM	713	CZ2	TRP	487	3.303	33.900	26.266	1.00	29.91	6
5	ATOM	714	CZ3	TRP	487	0.998	33.976	26.987	1.00	29.83	6
	ATOM	715	CH2	TRP	487	2.254	33.367	26.970	1.00	29.09	6
	ATOM	716	C	TRP	487	-1.599	37.899	24.068	1.00	15.44	6
	ATOM	717	O	TRP	487	-2.178	37.367	25.018	1.00	16.68	8
	ATOM	718	N	LEU	488	-2.036	38.993	23.447	1.00	14.44	7
10	ATOM	719	CA	LEU	488	-3.153	39.815	23.861	1.00	20.07	6
	ATOM	720	CB	LEU	488	-2.596	40.924	24.783	1.00	17.49	6
	ATOM	721	CG	LEU	488	-3.608	41.563	25.769	1.00	16.97	6
	ATOM	722	CD1	LEU	488	-4.062	40.567	26.830	1.00	17.38	6
	ATOM	723	CD2	LEU	488	-2.987	42.813	26.370	1.00	13.93	6
15	ATOM	724	C	LEU	488	-3.889	40.467	22.677	1.00	20.44	6
	ATOM	725	O	LEU	488	-3.255	41.009	21.752	1.00	19.65	8
	ATOM	726	N	VAL	489	-5.218	40.349	22.620	1.00	18.11	7
	ATOM	727	CA	VAL	489	-5.998	40.940	21.542	1.00	14.66	6
	ATOM	728	CBA	VAL	489	-6.686	39.837	20.699	0.50	7.52	6
20	ATOM	729	CBB	VAL	489	-6.677	39.925	20.604	0.50	13.86	6
	ATOM	730	CG1	VAL	489	-7.573	38.976	21.597	0.50	7.13	6
	ATOM	731	CG1	VAL	489	-5.696	39.457	19.543	0.50	15.87	6
	ATOM	732	CG2	VAL	489	-7.501	40.380	19.531	0.50	3.91	6
	ATOM	733	CG2	VAL	489	-7.264	38.776	21.402	0.50	18.65	6
25	ATOM	734	C	VAL	489	-7.109	41.834	22.107	1.00	15.71	6
	ATOM	735	O	VAL	489	-7.689	41.604	23.179	1.00	14.52	8
	ATOM	736	N	LEU	490	-7.379	42.908	21.386	1.00	15.13	7
	ATOM	737	CA	LEU	490	-8.520	43.733	21.703	1.00	13.72	6
	ATOM	738	CB	LEU	490	-8.287	45.241	21.488	1.00	17.87	6
30	ATOM	739	CG	LEU	490	-9.650	45.888	21.873	1.00	26.07	6
	ATOM	740	CD1	LEU	490	-9.479	46.800	23.036	1.00	30.57	6
	ATOM	741	CD2	LEU	490	-10.373	46.403	20.662	1.00	25.07	6
	ATOM	742	C	LEU	490	-9.657	43.192	20.803	1.00	17.58	6
	ATOM	743	O	LEU	490	-9.611	43.349	19.576	1.00	14.46	8
35	ATOM	744	N	GLN	491	-10.673	42.568	21.412	1.00	15.83	7
	ATOM	745	CA	GLN	491	-11.745	41.958	20.623	1.00	17.70	6
	ATOM	746	CB	GLN	491	-12.252	40.628	21.264	1.00	15.03	6
	ATOM	747	CG	GLN	491	-11.105	39.635	21.472	1.00	12.81	6
	ATOM	748	CD	GLN	491	-11.564	38.230	21.868	1.00	15.79	6
40	ATOM	749	OE1	GLN	491	-12.023	38.043	22.988	1.00	14.61	8
	ATOM	750	NE2	GLN	491	-11.409	37.256	20.984	1.00	16.27	7
	ATOM	751	C	GLN	491	-12.971	42.824	20.375	1.00	17.71	6
	ATOM	752	O	GLN	491	-13.370	43.570	21.268	1.00	19.37	8
	ATOM	753	N	THR	492	-13.607	42.659	19.218	1.00	14.05	7
45	ATOM	754	CA	THR	492	-14.853	43.378	18.934	1.00	19.01	6
	ATOM	755	CB	THR	492	-14.562	44.641	18.089	1.00	16.40	6
	ATOM	756	OG1	THR	492	-15.769	45.381	17.905	1.00	18.39	8
	ATOM	757	CG2	THR	492	-13.943	44.367	16.720	1.00	10.45	6
	ATOM	758	C	THR	492	-15.803	42.450	18.173	1.00	18.96	6
50	ATOM	759	O	THR	492	-15.339	41.594	17.409	1.00	21.88	8
	ATOM	760	N	PRO	493	-17.095	42.713	18.251	1.00	18.78	7
	ATOM	761	CD	PRO	493	-17.747	43.697	19.135	1.00	22.16	6
	ATOM	762	CA	PRO	493	-18.090	41.937	17.530	1.00	24.37	6
	ATOM	763	CB	PRO	493	-19.352	42.063	18.371	1.00	24.99	6
55	ATOM	764	CG	PRO	493	-19.162	43.257	19.235	1.00	26.05	6
	ATOM	765	C	PRO	493	-18.285	42.504	16.138	1.00	27.02	6
	ATOM	766	O	PRO	493	-18.852	41.847	15.248	1.00	27.04	8
	ATOM	767	N	HIS	494	-17.978	43.797	15.960	1.00	24.22	7
	ATOM	768	CA	HIS	494	-18.114	44.445	14.651	1.00	25.72	6
60	ATOM	769	CB	HIS	494	-19.444	45.176	14.439	1.00	20.09	6
	ATOM	770	CG	HIS	494	-20.639	44.279	14.595	1.00	21.67	6
	ATOM	771	CD2	HIS	494	-21.161	43.336	13.798	1.00	23.30	6
	ATOM	772	ND1	HIS	494	-21.380	44.271	15.754	1.00	27.49	7
	ATOM	773	CE1	HIS	494	-22.338	43.365	15.657	1.00	26.54	6
65	ATOM	774	NE2	HIS	494	-22.211	42.788	14.482	1.00	32.10	7
	ATOM	775	C	HIS	494	-17.038	45.516	14.453	1.00	24.49	6
	ATOM	776	O	HIS	494	-16.481	46.028	15.429	1.00	24.01	8
	ATOM	777	N	LEU	495	-16.847	45.937	13.214	1.00	21.96	7
	ATOM	778	CA	LEU	495	-15.900	47.019	12.960	1.00	26.06	6
70	ATOM	779	CB	LEU	495	-15.014	46.748	11.741	1.00	26.66	6
	ATOM	780	CG	LEU	495	-13.994	45.618	11.899	1.00	35.19	6
	ATOM	781	CD1	LEU	495	-13.449	45.265	10.525	1.00	25.66	6

123

	ATOM	782	CD2	LEU	495	-12.895	45.958	12.900	1.00	24.13	6
	ATOM	783	C	LEU	495	-16.626	48.341	12.720	1.00	26.30	6
	ATOM	784	O	LEU	495	-15.999	49.402	12.790	1.00	26.83	8
5	ATOM	785	N	GLU	496	-17.884	48.265	12.326	1.00	25.44	7
	ATOM	786	CA	GLU	496	-18.688	49.453	12.087	1.00	28.55	6
	ATOM	787	CB	GLU	496	-19.062	49.722	10.634	1.00	28.97	6
	ATOM	788	CG	GLU	496	-17.977	49.532	9.605	1.00	34.46	6
	ATOM	789	CD	GLU	496	-18.414	49.757	8.168	1.00	42.07	6
10	ATOM	790	OE1	GLU	496	-19.560	50.157	7.882	1.00	41.53	8
	ATOM	791	OE2	GLU	496	-17.592	49.523	7.256	1.00	45.31	8
	ATOM	792	C	GLU	496	-19.995	49.291	12.885	1.00	32.22	6
	ATOM	793	O	GLU	496	-20.525	48.180	13.015	1.00	31.68	8
	ATOM	794	N	PHE	497	-20.396	50.379	13.538	1.00	29.38	7
15	ATOM	795	CA	PHE	497	-21.622	50.419	14.315	1.00	31.45	6
	ATOM	796	CB	PHE	497	-21.388	50.515	15.832	1.00	29.88	6
	ATOM	797	CG	PHE	497	-20.640	49.369	16.464	1.00	28.91	6
	ATOM	798	CD1	PHE	497	-19.256	49.286	16.386	1.00	19.88	6
	ATOM	799	CD2	PHE	497	-21.311	48.363	17.131	1.00	27.06	6
20	ATOM	800	CE1	PHE	497	-18.557	48.242	16.971	1.00	23.29	6
	ATOM	801	CE2	PHE	497	-20.622	47.321	17.719	1.00	23.27	6
	ATOM	802	CZ	PHE	497	-19.244	47.240	17.636	1.00	25.87	6
	ATOM	803	C	PHE	497	-22.455	51.633	13.861	1.00	31.11	6
	ATOM	804	O	PHE	497	-22.007	52.532	13.164	1.00	32.31	8
25	ATOM	805	N	GLN	498	-23.726	51.653	14.219	1.00	34.14	7
	ATOM	806	CA	GLN	498	-24.636	52.735	13.939	1.00	33.31	6
	ATOM	807	CB	GLN	498	-26.042	52.237	13.635	1.00	38.15	6
	ATOM	808	CG	GLN	498	-26.207	51.444	12.356	1.00	45.65	6
	ATOM	809	CD	GLN	498	-25.763	52.154	11.097	1.00	49.99	6
30	ATOM	810	OE1	GLN	498	-26.455	53.038	10.589	1.00	52.58	8
	ATOM	811	NE2	GLN	498	-24.603	51.778	10.563	1.00	53.06	7
	ATOM	812	C	GLN	498	-24.662	53.648	15.172	1.00	31.48	6
	ATOM	813	O	GLN	498	-24.459	53.202	16.300	1.00	27.98	8
	ATOM	814	N	GLU	499	-24.990	54.911	14.920	1.00	30.75	7
35	ATOM	815	CA	GLU	499	-25.112	55.888	16.009	1.00	32.56	6
	ATOM	816	CB	GLU	499	-25.598	57.213	15.420	1.00	36.89	6
	ATOM	817	CG	GLU	499	-25.204	58.474	16.141	1.00	44.86	6
	ATOM	818	CD	GLU	499	-24.771	59.578	15.184	1.00	48.45	6
	ATOM	819	OE1	GLU	499	-23.802	60.293	15.521	1.00	53.90	8
40	ATOM	820	OE2	GLU	499	-25.400	59.718	14.118	1.00	50.56	8
	ATOM	821	C	GLU	499	-26.130	55.315	16.980	1.00	31.14	6
	ATOM	822	O	GLU	499	-27.136	54.818	16.475	1.00	31.94	8
	ATOM	823	N	GLY	500	-25.919	55.295	18.275	1.00	32.19	7
45	ATOM	824	CA	GLY	500	-26.874	54.743	19.217	1.00	31.10	6
	ATOM	825	C	GLY	500	-26.643	53.325	19.696	1.00	31.51	6
	ATOM	826	O	GLY	500	-27.082	52.935	20.789	1.00	30.30	8
	ATOM	827	N	GLU	501	-25.948	52.497	18.921	1.00	34.41	7
	ATOM	828	CA	GLU	501	-25.675	51.120	19.297	1.00	34.07	6
	ATOM	829	CB	GLU	501	-24.949	50.414	18.148	1.00	37.86	6
50	ATOM	830	CG	GLU	501	-25.777	50.190	16.889	1.00	48.38	6
	ATOM	831	CD	GLU	501	-24.984	49.346	15.895	1.00	49.17	6
	ATOM	832	OE1	GLU	501	-24.251	48.458	16.385	1.00	58.51	8
	ATOM	833	OE2	GLU	501	-25.046	49.533	14.669	1.00	48.56	8
	ATOM	834	C	GLU	501	-24.783	51.018	20.537	1.00	33.06	6
55	ATOM	835	O	GLU	501	-24.086	51.978	20.886	1.00	27.70	8
	ATOM	836	N	THR	502	-24.747	49.809	21.107	1.00	31.92	7
	ATOM	837	CA	THR	502	-23.870	49.563	22.248	1.00	32.85	6
	ATOM	838	CB	THR	502	-24.508	48.705	23.341	1.00	35.75	6
	ATOM	839	OG1	THR	502	-25.546	49.428	24.021	1.00	36.79	8
60	ATOM	840	CG2	THR	502	-23.532	48.289	24.441	1.00	35.82	6
	ATOM	841	C	THR	502	-22.582	48.922	21.721	1.00	32.54	6
	ATOM	842	O	THR	502	-22.650	47.934	20.991	1.00	30.03	8
	ATOM	843	N	ILE	503	-21.431	49.537	22.014	1.00	28.53	7
	ATOM	844	CA	ILE	503	-20.162	48.927	21.590	1.00	25.40	6
65	ATOM	845	CB	ILE	503	-19.131	49.993	21.163	1.00	26.58	6
	ATOM	846	CG2	ILE	503	-17.776	49.370	20.828	1.00	25.47	6
	ATOM	847	CG1	ILE	503	-19.669	50.786	19.971	1.00	21.79	6
	ATOM	848	CD1	ILE	503	-18.739	51.863	19.438	1.00	19.73	6
	ATOM	849	C	ILE	503	-19.624	48.113	22.767	1.00	25.27	6
70	ATOM	850	O	ILE	503	-19.439	48.685	23.853	1.00	23.06	8
	ATOM	851	N	MET	504	-19.443	46.807	22.591	1.00	24.90	7
	ATOM	852	CA	MET	504	-18.893	45.953	23.639	1.00	21.55	6

124

	ATOM	853	CB	MET	504	-19.797	44.769	23.963	1.00	33.48	6
	ATOM	854	CG	MET	504	-20.810	45.040	25.101	1.00	29.68	6
	ATOM	855	SD	MET	504	-21.940	43.610	25.242	1.00	46.02	16
5	ATOM	856	CE	MET	504	-22.667	43.650	23.589	1.00	31.10	6
	ATOM	857	C	MET	504	-17.528	45.410	23.215	1.00	21.27	6
	ATOM	858	O	MET	504	-17.374	44.875	22.106	1.00	22.96	8
	ATOM	859	N	LEU	505	-16.503	45.624	24.027	1.00	20.55	7
	ATOM	860	CA	LEU	505	-15.134	45.198	23.728	1.00	22.33	6
10	ATOM	861	CB	LEU	505	-14.192	46.416	23.550	1.00	14.66	6
	ATOM	862	CG	LEU	505	-14.713	47.477	22.561	1.00	18.89	6
	ATOM	863	CD1	LEU	505	-13.796	48.688	22.489	1.00	19.44	6
	ATOM	864	CD2	LEU	505	-14.882	46.810	21.186	1.00	18.70	6
	ATOM	865	C	LEU	505	-14.567	44.307	24.817	1.00	20.15	6
	ATOM	866	O	LEU	505	-15.050	44.360	25.950	1.00	18.39	8
15	ATOM	867	N	ARG	506	-13.523	43.542	24.483	1.00	18.25	7
	ATOM	868	CA	ARG	506	-12.912	42.692	25.516	1.00	17.87	6
	ATOM	869	CB	ARG	506	-13.607	41.313	25.508	1.00	14.96	6
	ATOM	870	CG	ARG	506	-12.834	40.269	26.290	1.00	16.79	6
20	ATOM	871	CD	ARG	506	-13.699	39.078	26.757	1.00	19.51	6
	ATOM	872	NE	ARG	506	-13.334	37.939	26.025	1.00	23.46	7
	ATOM	873	CZ	ARG	506	-12.990	36.692	26.065	1.00	24.43	6
	ATOM	874	NH1	ARG	506	-12.923	35.974	27.176	1.00	25.93	7
	ATOM	875	NH2	ARG	506	-12.697	36.071	24.936	1.00	18.72	7
25	ATOM	876	C	ARG	506	-11.422	42.545	25.304	1.00	18.56	6
	ATOM	877	O	ARG	506	-10.998	42.387	24.142	1.00	20.43	8
	ATOM	878	N	CYS	507	-10.642	42.620	26.378	1.00	15.23	7
	ATOM	879	CA	CYS	507	-9.189	42.447	26.292	1.00	14.89	6
	ATOM	880	C	CYS	507	-8.934	40.975	26.583	1.00	15.28	6
30	ATOM	881	O	CYS	507	-9.296	40.572	27.690	1.00	15.96	8
	ATOM	882	CB	CYS	507	-8.438	43.301	27.322	1.00	14.55	6
	ATOM	883	SG	CYS	507	-6.691	43.498	27.013	1.00	13.91	16
	ATOM	884	N	HIS	508	-8.446	40.213	25.604	1.00	15.07	7
	ATOM	885	CA	HIS	508	-8.334	38.763	25.811	1.00	11.91	6
35	ATOM	886	CB	HIS	508	-9.190	38.109	24.708	1.00	16.03	6
	ATOM	887	CG	HIS	508	-9.119	36.626	24.572	1.00	16.94	6
	ATOM	888	CD2	HIS	508	-9.068	35.843	23.462	1.00	17.64	6
	ATOM	889	ND1	HIS	508	-9.103	35.758	25.657	1.00	17.41	7
	ATOM	890	CE1	HIS	508	-9.034	34.516	25.215	1.00	17.37	6
40	ATOM	891	NE2	HIS	508	-9.021	34.533	23.895	1.00	20.00	7
	ATOM	892	C	HIS	508	-6.925	38.219	25.733	1.00	11.83	6
	ATOM	893	O	HIS	508	-6.224	38.505	24.762	1.00	12.54	8
	ATOM	894	N	SER	509	-6.515	37.364	26.654	1.00	13.70	7
	ATOM	895	CA	SER	509	-5.160	36.775	26.605	1.00	11.70	6
45	ATOM	896	CB	SER	509	-4.583	36.732	28.041	1.00	13.47	6
	ATOM	897	OG	SER	509	-5.609	36.021	28.800	1.00	16.16	8
	ATOM	898	C	SER	509	-5.190	35.407	25.970	1.00	14.21	6
	ATOM	899	O	SER	509	-6.180	34.634	25.903	1.00	14.63	8
	ATOM	900	N	TRP	510	-4.047	35.062	25.381	1.00	16.58	7
50	ATOM	901	CA	TRP	510	-3.860	33.764	24.708	1.00	16.04	6
	ATOM	902	CB	TRP	510	-2.480	33.708	24.072	1.00	18.73	6
	ATOM	903	CG	TRP	510	-2.187	32.441	23.306	1.00	21.24	6
	ATOM	904	CD2	TRP	510	-1.135	31.527	23.589	1.00	20.70	6
	ATOM	905	CE2	TRP	510	-1.193	30.505	22.616	1.00	25.92	6
55	ATOM	906	CE3	TRP	510	-0.112	31.494	24.549	1.00	24.16	6
	ATOM	907	CD1	TRP	510	-2.827	31.958	22.214	1.00	22.22	6
	ATOM	908	NE1	TRP	510	-2.233	30.797	21.765	1.00	22.81	7
	ATOM	909	CZ2	TRP	510	-0.276	29.462	22.568	1.00	24.18	6
	ATOM	910	CZ3	TRP	510	0.781	30.432	24.509	1.00	30.15	6
60	ATOM	911	CH2	TRP	510	0.698	29.433	23.526	1.00	31.04	6
	ATOM	912	C	TRP	510	-4.082	32.621	25.681	1.00	14.44	6
	ATOM	913	O	TRP	510	-3.665	32.647	26.852	1.00	17.08	8
	ATOM	914	N	LYS	511	-4.928	31.667	25.294	1.00	19.42	7
	ATOM	915	CA	LYS	511	-5.347	30.541	26.115	1.00	19.40	6
65	ATOM	916	CB	LYS	511	-4.131	29.625	26.418	1.00	21.00	6
	ATOM	917	CG	LYS	511	-3.583	28.962	25.155	1.00	24.94	6
	ATOM	918	CD	LYS	511	-2.124	28.579	25.337	1.00	34.17	6
	ATOM	919	CE	LYS	511	-1.952	27.147	25.781	1.00	37.49	6
	ATOM	920	NZ	LYS	511	-2.783	26.198	24.987	1.00	52.66	7
70	ATOM	921	C	LYS	511	-5.940	30.945	27.450	1.00	20.33	6
	ATOM	922	O	LYS	511	-5.905	30.172	28.419	1.00	16.80	8
	ATOM	923	N	ASP	512	-6.444	32.171	27.602	1.00	18.28	7

125

	ATOM	924	CA	ASP	512	-6.989	32.633	28.861	1.00	20.31	6
	ATOM	925	CB	ASP	512	-8.242	31.778	29.191	1.00	24.52	6
	ATOM	926	CG	ASP	512	-9.306	32.129	28.155	1.00	31.39	6
5	ATOM	927	OD1	ASP	512	-9.700	33.321	28.119	1.00	39.68	8
	ATOM	928	OD2	ASP	512	-9.719	31.278	27.360	1.00	35.00	8
	ATOM	929	C	ASP	512	-6.015	32.663	30.018	1.00	23.40	6
	ATOM	930	O	ASP	512	-6.426	32.391	31.148	1.00	23.42	8
	ATOM	931	N	LYS	513	-4.731	32.977	29.785	1.00	23.10	7
10	ATOM	932	CA	LYS	513	-3.792	33.145	30.891	1.00	22.35	6
	ATOM	933	CB	LYS	513	-2.352	33.434	30.437	1.00	21.68	6
	ATOM	934	CG	LYS	513	-1.758	32.255	29.659	1.00	27.09	6
	ATOM	935	CD	LYS	513	-0.232	32.292	29.608	1.00	28.34	6
	ATOM	936	CE	LYS	513	0.269	31.086	28.816	1.00	32.92	6
15	ATOM	937	NZ	LYS	513	0.196	29.791	29.554	1.00	33.55	7
	ATOM	938	C	LYS	513	-4.352	34.269	31.748	1.00	19.86	6
	ATOM	939	O	LYS	513	-4.890	35.263	31.264	1.00	21.45	8
	ATOM	940	N	PRO	514	-4.288	34.105	33.066	1.00	20.08	7
	ATOM	941	CD	PRO	514	-3.701	32.938	33.768	1.00	16.95	6
20	ATOM	942	CA	PRO	514	-4.923	35.065	33.957	1.00	17.00	6
	ATOM	943	CB	PRO	514	-4.548	34.574	35.342	1.00	19.22	6
	ATOM	944	CG	PRO	514	-4.169	33.133	35.176	1.00	21.34	6
	ATOM	945	C	PRO	514	-4.451	36.461	33.636	1.00	16.83	6
	ATOM	946	O	PRO	514	-3.237	36.741	33.512	1.00	16.01	8
25	ATOM	947	N	LEU	515	-5.414	37.383	33.560	1.00	15.95	7
	ATOM	948	CA	LEU	515	-5.081	38.762	33.215	1.00	17.10	6
	ATOM	949	CB	LEU	515	-5.769	38.987	31.856	1.00	16.83	6
	ATOM	950	CG	LEU	515	-5.790	40.368	31.231	1.00	21.64	6
	ATOM	951	CD1	LEU	515	-4.399	40.734	30.733	1.00	19.24	6
30	ATOM	952	CD2	LEU	515	-6.777	40.380	30.043	1.00	19.80	6
	ATOM	953	C	LEU	515	-5.606	39.750	34.226	1.00	21.13	6
	ATOM	954	O	LEU	515	-6.788	39.666	34.569	1.00	18.84	8
	ATOM	955	N	VAL	516	-4.839	40.761	34.630	1.00	20.51	7
	ATOM	956	CA	VAL	516	-5.314	41.793	35.545	1.00	20.40	6
35	ATOM	957	CB	VAL	516	-4.787	41.589	36.971	1.00	18.72	6
	ATOM	958	CG1	VAL	516	-5.313	40.319	37.644	1.00	22.67	6
	ATOM	959	CG2	VAL	516	-3.257	41.538	36.998	1.00	22.12	6
	ATOM	960	C	VAL	516	-4.807	43.163	35.073	1.00	19.73	6
	ATOM	961	O	VAL	516	-3.910	43.184	34.223	1.00	20.76	8
40	ATOM	962	N	LYS	517	-5.268	44.251	35.693	1.00	17.34	7
	ATOM	963	CA	LYS	517	-4.760	45.576	35.381	1.00	20.33	6
	ATOM	964	CB	LYS	517	-3.271	45.684	35.802	1.00	21.74	6
	ATOM	965	CG	LYS	517	-3.115	45.939	37.301	1.00	24.43	6
	ATOM	966	CD	LYS	517	-1.793	45.421	37.832	1.00	32.69	6
45	ATOM	967	CE	LYS	517	-0.798	46.552	38.056	1.00	40.27	6
	ATOM	968	NZ	LYS	517	0.568	46.001	38.266	1.00	44.06	7
	ATOM	969	C	LYS	517	-4.956	45.930	33.914	1.00	18.58	6
	ATOM	970	O	LYS	517	-4.026	46.331	33.234	1.00	24.35	8
	ATOM	971	N	VAL	518	-6.181	45.803	33.417	1.00	20.45	7
50	ATOM	972	CA	VAL	518	-6.542	46.068	32.039	1.00	19.15	6
	ATOM	973	CB	VAL	518	-7.756	45.223	31.607	1.00	12.17	6
	ATOM	974	CG1	VAL	518	-8.199	45.470	30.176	1.00	18.94	6
	ATOM	975	CG2	VAL	518	-7.408	43.737	31.794	1.00	16.75	6
	ATOM	976	C	VAL	518	-6.868	47.536	31.797	1.00	18.58	6
	ATOM	977	O	VAL	518	-7.606	48.149	32.564	1.00	17.16	8
55	ATOM	978	N	THR	519	-6.307	48.063	30.711	1.00	15.94	7
	ATOM	979	CA	THR	519	-6.527	49.441	30.335	1.00	16.50	6
	ATOM	980	CB	THR	519	-5.291	50.343	30.367	1.00	19.59	6
	ATOM	981	OG1	THR	519	-4.770	50.456	31.693	1.00	23.11	8
60	ATOM	982	CG2	THR	519	-5.695	51.743	29.872	1.00	24.83	6
	ATOM	983	C	THR	519	-7.053	49.442	28.881	1.00	17.81	6
	ATOM	984	O	THR	519	-6.436	48.736	28.095	1.00	14.36	8
	ATOM	985	N	PHE	520	-8.121	50.187	28.643	1.00	14.86	7
	ATOM	986	CA	PHE	520	-8.616	50.258	27.259	1.00	13.85	6
65	ATOM	987	CB	PHE	520	-10.122	50.069	27.240	1.00	15.51	6
	ATOM	988	CG	PHE	520	-10.553	48.636	27.463	1.00	13.38	6
	ATOM	989	CD1	PHE	520	-10.748	48.165	28.750	1.00	20.15	6
	ATOM	990	CD2	PHE	520	-10.792	47.815	26.381	1.00	20.08	6
	ATOM	991	CE1	PHE	520	-11.186	46.864	28.953	1.00	17.14	6
70	ATOM	992	CE2	PHE	520	-11.230	46.499	26.578	1.00	22.12	6
	ATOM	993	CZ	PHE	520	-11.423	46.048	27.867	1.00	17.10	6
	ATOM	994	C	PHE	520	-8.279	51.650	26.721	1.00	17.13	6

126

	ATOM	995	O	PHE	520	-8.640	52.645	27.407	1.00	14.78	8
	ATOM	996	N	PHE	521	-7.626	51.700	25.575	1.00	16.20	7
	ATOM	997	CA	PHE	521	-7.277	52.998	25.011	1.00	18.83	6
	ATOM	998	CB	PHE	521	-5.799	53.045	24.616	1.00	13.50	6
5	ATOM	999	CG	PHE	521	-4.768	52.814	25.656	1.00	18.60	6
	ATOM	1000	CD1	PHE	521	-4.368	51.527	26.017	1.00	17.37	6
	ATOM	1001	CD2	PHE	521	-4.208	53.905	26.334	1.00	18.44	6
	ATOM	1002	CE1	PHE	521	-3.409	51.342	27.006	1.00	19.78	6
10	ATOM	1003	CE2	PHE	521	-3.260	53.693	27.313	1.00	22.69	6
	ATOM	1004	CZ	PHE	521	-2.843	52.421	27.660	1.00	15.74	6
	ATOM	1005	C	PHE	521	-8.074	53.327	23.749	1.00	18.44	6
	ATOM	1006	O	PHE	521	-8.351	52.412	22.987	1.00	15.63	8
	ATOM	1007	N	GLN	522	-8.333	54.613	23.480	1.00	19.35	7
	ATOM	1008	CA	GLN	522	-8.959	54.986	22.203	1.00	19.90	6
15	ATOM	1009	CB	GLN	522	-10.396	55.487	22.317	1.00	16.32	6
	ATOM	1010	CG	GLN	522	-10.784	56.283	21.065	1.00	18.39	6
	ATOM	1011	CD	GLN	522	-12.050	57.102	21.247	1.00	21.98	6
	ATOM	1012	OE1	GLN	522	-12.423	57.405	22.374	1.00	19.18	8
	ATOM	1013	NE2	GLN	522	-12.700	57.470	20.153	1.00	24.51	7
20	ATOM	1014	C	GLN	522	-8.067	56.092	21.609	1.00	15.34	6
	ATOM	1015	O	GLN	522	-7.789	57.034	22.321	1.00	17.30	8
	ATOM	1016	N	ASN	523	-7.474	55.935	20.439	1.00	18.98	7
	ATOM	1017	CA	ASN	523	-6.542	56.891	19.859	1.00	22.95	6
	ATOM	1018	CB	ASN	523	-7.241	58.158	19.332	1.00	19.57	6
25	ATOM	1019	CG	ASN	523	-8.228	57.736	18.244	1.00	26.31	6
	ATOM	1020	OD1	ASN	523	-8.013	56.813	17.441	1.00	19.76	8
	ATOM	1021	ND2	ASN	523	-9.375	58.403	18.213	1.00	28.57	7
	ATOM	1022	C	ASN	523	-5.397	57.223	20.803	1.00	21.02	6
	ATOM	1023	O	ASN	523	-4.911	58.341	20.918	1.00	19.19	8
30	ATOM	1024	N	GLY	524	-4.951	56.234	21.579	1.00	19.77	7
	ATOM	1025	CA	GLY	524	-3.852	56.350	22.495	1.00	16.41	6
	ATOM	1026	C	GLY	524	-4.159	56.981	23.844	1.00	14.85	6
	ATOM	1027	O	GLY	524	-3.210	57.208	24.611	1.00	15.05	8
	ATOM	1028	N	LYS	525	-5.405	57.256	24.133	1.00	13.81	7
35	ATOM	1029	CA	LYS	525	-5.830	57.869	25.379	1.00	21.18	6
	ATOM	1030	CB	LYS	525	-6.700	59.128	25.247	1.00	14.85	6
	ATOM	1031	CG	LYS	525	-6.934	59.834	26.559	1.00	16.28	6
	ATOM	1032	CD	LYS	525	-7.406	61.279	26.281	1.00	22.51	6
	ATOM	1033	CE	LYS	525	-7.925	61.877	27.587	1.00	30.62	6
40	ATOM	1034	NZ	LYS	525	-8.822	63.048	27.330	1.00	36.72	7
	ATOM	1035	C	LYS	525	-6.725	56.852	26.121	1.00	18.20	6
	ATOM	1036	O	LYS	525	-7.648	56.341	25.509	1.00	19.98	8
	ATOM	1037	N	SER	526	-6.385	56.650	27.393	1.00	17.62	7
	ATOM	1038	CA	SER	526	-7.107	55.625	28.155	1.00	20.03	6
45	ATOM	1039	CB	SER	526	-6.355	55.407	29.485	1.00	23.22	6
	ATOM	1040	OG	SER	526	-7.317	55.093	30.466	1.00	38.12	8
	ATOM	1041	C	SER	526	-8.541	56.043	28.389	1.00	17.85	6
	ATOM	1042	O	SER	526	-8.842	57.209	28.647	1.00	21.31	8
	ATOM	1043	N	GLN	527	-9.490	55.148	28.254	1.00	17.16	7
50	ATOM	1044	CA	GLN	527	-10.898	55.351	28.408	1.00	17.45	6
	ATOM	1045	CB	GLN	527	-11.723	54.793	27.225	1.00	20.82	6
	ATOM	1046	CG	GLN	527	-11.352	55.447	25.897	1.00	18.56	6
	ATOM	1047	CD	GLN	527	-11.497	56.954	25.927	1.00	24.44	6
	ATOM	1048	OE1	GLN	527	-12.606	57.450	26.116	1.00	31.62	8
55	ATOM	1049	NE2	GLN	527	-10.436	57.736	25.773	1.00	19.15	7
	ATOM	1050	C	GLN	527	-11.386	54.615	29.661	1.00	20.94	6
	ATOM	1051	O	GLN	527	-12.439	54.937	30.179	1.00	18.25	8
	ATOM	1052	N	LYS	528	-10.643	53.581	30.032	1.00	21.18	7
	ATOM	1053	CA	LYS	528	-11.070	52.818	31.216	1.00	23.10	6
60	ATOM	1054	CB	LYS	528	-12.177	51.832	30.842	1.00	21.83	6
	ATOM	1055	CG	LYS	528	-12.683	50.984	32.013	1.00	24.67	6
	ATOM	1056	CD	LYS	528	-13.739	49.961	31.589	1.00	18.23	6
	ATOM	1057	CE	LYS	528	-14.048	49.120	32.870	1.00	27.02	6
	ATOM	1058	NZ	LYS	528	-15.081	48.072	32.574	1.00	24.24	7
65	ATOM	1059	C	LYS	528	-9.884	52.022	31.754	1.00	24.93	6
	ATOM	1060	O	LYS	528	-9.193	51.385	30.960	1.00	20.79	8
	ATOM	1061	N	PHE	529	-9.678	52.044	33.062	1.00	21.39	7
	ATOM	1062	CA	PHE	529	-8.708	51.171	33.695	1.00	24.45	6
	ATOM	1063	CB	PHE	529	-7.610	51.940	34.458	1.00	25.50	6
70	ATOM	1064	CG	PHE	529	-6.772	51.029	35.327	1.00	25.51	6
	ATOM	1065	CD1	PHE	529	-5.799	50.236	34.762	1.00	19.40	6

	ATOM	1066	CD2	PHE	529	-7.002	50.938	36.700	1.00	29.98	6
	ATOM	1067	CE1	PHE	529	-5.026	49.375	35.535	1.00	25.00	6
	ATOM	1068	CE2	PHE	529	-6.249	50.078	37.491	1.00	28.84	6
5	ATOM	1069	CZ	PHE	529	-5.262	49.292	36.902	1.00	32.29	6
	ATOM	1070	C	PHE	529	-9.480	50.289	34.687	1.00	27.88	6
	ATOM	1071	O	PHE	529	-10.388	50.817	35.359	1.00	30.99	8
	ATOM	1072	N	SER	530	-9.134	49.020	34.853	1.00	26.67	7
	ATOM	1073	CA	SER	530	-9.779	48.225	35.917	1.00	24.98	6
10	ATOM	1074	CB	SER	530	-11.025	47.522	35.422	1.00	21.29	6
	ATOM	1075	OG	SER	530	-11.271	46.401	36.250	1.00	25.72	8
	ATOM	1076	C	SER	530	-8.777	47.199	36.434	1.00	24.39	6
	ATOM	1077	O	SER	530	-8.123	46.581	35.576	1.00	24.91	8
	ATOM	1078	N	HIS	531	-8.668	46.977	37.730	1.00	22.12	7
15	ATOM	1079	CA	HIS	531	-7.710	45.965	38.204	1.00	23.65	6
	ATOM	1080	CB	HIS	531	-7.604	45.948	39.737	1.00	28.35	6
	ATOM	1081	CG	HIS	531	-6.859	47.160	40.197	1.00	23.57	6
	ATOM	1082	CD2	HIS	531	-7.307	48.357	40.642	1.00	18.55	6
	ATOM	1083	ND1	HIS	531	-5.478	47.200	40.170	1.00	26.69	7
20	ATOM	1084	CE1	HIS	531	-5.095	48.388	40.617	1.00	16.65	6
	ATOM	1085	NE2	HIS	531	-6.173	49.102	40.890	1.00	23.94	7
	ATOM	1086	C	HIS	531	-8.108	44.552	37.814	1.00	23.89	6
	ATOM	1087	O	HIS	531	-7.261	43.661	37.712	1.00	26.21	8
	ATOM	1088	N	LEU	532	-9.426	44.318	37.689	1.00	21.77	7
25	ATOM	1089	CA	LEU	532	-9.886	42.966	37.480	1.00	20.70	6
	ATOM	1090	CB	LEU	532	-10.630	42.505	38.760	1.00	30.28	6
	ATOM	1091	CG	LEU	532	-10.022	42.782	40.148	1.00	26.56	6
	ATOM	1092	CD1	LEU	532	-11.073	42.550	41.229	1.00	29.07	6
	ATOM	1093	CD2	LEU	532	-8.814	41.886	40.435	1.00	24.99	6
30	ATOM	1094	C	LEU	532	-10.762	42.722	36.279	1.00	22.94	6
	ATOM	1095	O	LEU	532	-10.794	41.540	35.900	1.00	22.01	8
	ATOM	1096	N	ASP	533	-11.541	43.685	35.778	1.00	21.75	7
	ATOM	1097	CA	ASP	533	-12.469	43.465	34.679	1.00	24.62	6
	ATOM	1098	CB	ASP	533	-13.560	44.539	34.854	1.00	29.71	6
35	ATOM	1099	CG	ASP	533	-14.734	44.545	33.915	1.00	32.90	6
	ATOM	1100	OD1	ASP	533	-14.837	43.612	33.083	1.00	32.91	8
	ATOM	1101	OD2	ASP	533	-15.597	45.472	34.000	1.00	36.01	8
	ATOM	1102	C	ASP	533	-11.843	43.636	33.296	1.00	25.88	6
	ATOM	1103	O	ASP	533	-11.419	44.730	32.940	1.00	24.36	8
40	ATOM	1104	N	PRO	534	-11.857	42.605	32.460	1.00	24.65	7
	ATOM	1105	CD	PRO	534	-12.347	41.246	32.778	1.00	22.97	6
	ATOM	1106	CA	PRO	534	-11.293	42.681	31.112	1.00	24.00	6
	ATOM	1107	CB	PRO	534	-10.889	41.204	30.870	1.00	24.02	6
	ATOM	1108	CG	PRO	534	-11.987	40.433	31.544	1.00	23.04	6
45	ATOM	1109	C	PRO	534	-12.256	43.102	30.017	1.00	22.11	6
	ATOM	1110	O	PRO	534	-11.970	42.936	28.824	1.00	19.00	8
	ATOM	1111	N	THR	535	-13.420	43.654	30.350	1.00	21.43	7
	ATOM	1112	CA	THR	535	-14.424	44.061	29.401	1.00	24.98	6
	ATOM	1113	CB	THR	535	-15.748	43.282	29.593	1.00	27.24	6
50	ATOM	1114	OG1	THR	535	-16.331	43.801	30.796	1.00	24.99	8
	ATOM	1115	CG2	THR	535	-15.461	41.797	29.706	1.00	26.07	6
	ATOM	1116	C	THR	535	-14.747	45.554	29.451	1.00	23.58	6
	ATOM	1117	O	THR	535	-14.445	46.237	30.423	1.00	26.14	8
55	ATOM	1118	N	PHE	536	-15.267	46.076	28.347	1.00	20.63	7
	ATOM	1119	CA	PHE	536	-15.549	47.475	28.150	1.00	20.10	6
	ATOM	1120	CB	PHE	536	-14.343	48.160	27.523	1.00	25.47	6
	ATOM	1121	CG	PHE	536	-14.408	49.616	27.170	1.00	25.61	6
	ATOM	1122	CD1	PHE	536	-14.528	50.596	28.121	1.00	27.00	6
60	ATOM	1123	CD2	PHE	536	-14.332	50.019	25.841	1.00	27.45	6
	ATOM	1124	CE1	PHE	536	-14.571	51.937	27.787	1.00	32.62	6
	ATOM	1125	CE2	PHE	536	-14.385	51.350	25.490	1.00	28.46	6
	ATOM	1126	CZ	PHE	536	-14.493	52.317	26.463	1.00	30.41	6
	ATOM	1127	C	PHE	536	-16.796	47.669	27.297	1.00	24.00	6
	ATOM	1128	O	PHE	536	-16.952	47.065	26.230	1.00	24.50	8
65	ATOM	1129	N	SER	537	-17.665	48.572	27.730	1.00	21.97	7
	ATOM	1130	CA	SER	537	-18.914	48.856	27.050	1.00	26.52	6
	ATOM	1131	CB	SER	537	-20.120	48.448	27.908	1.00	30.03	6
	ATOM	1132	OG	SER	537	-20.769	47.307	27.412	1.00	44.19	8
	ATOM	1133	C	SER	537	-19.128	50.359	26.840	1.00	27.38	6
70	ATOM	1134	O	SER	537	-18.911	51.172	27.721	1.00	27.33	8
	ATOM	1135	N	ILE	538	-19.654	50.702	25.686	1.00	25.86	7
	ATOM	1136	CA	ILE	538	-20.004	52.060	25.343	1.00	29.46	6

	ATOM	1137	CB	ILE	538	-19.189	52.690	24.193	1.00	33.38	6
	ATOM	1138	CG2	ILE	538	-19.669	54.118	23.941	1.00	27.23	6
	ATOM	1139	CG1	ILE	538	-17.679	52.669	24.472	1.00	30.55	6
5	ATOM	1140	CD1	ILE	538	-16.817	52.711	23.223	1.00	29.53	6
	ATOM	1141	C	ILE	538	-21.477	51.991	24.926	1.00	29.88	6
	ATOM	1142	O	ILE	538	-21.768	51.489	23.849	1.00	27.99	8
	ATOM	1143	N	PRO	539	-22.345	52.390	25.837	1.00	31.71	7
	ATOM	1144	CD	PRO	539	-22.018	52.928	27.184	1.00	32.73	6
10	ATOM	1145	CA	PRO	539	-23.776	52.468	25.598	1.00	33.85	6
	ATOM	1146	CB	PRO	539	-24.380	52.653	26.983	1.00	36.13	6
	ATOM	1147	CG	PRO	539	-23.248	52.482	27.950	1.00	34.99	6
	ATOM	1148	C	PRO	539	-24.030	53.706	24.741	1.00	35.63	6
	ATOM	1149	O	PRO	539	-23.324	54.706	24.888	1.00	38.22	8
	ATOM	1150	N	GLN	540	-24.974	53.658	23.827	1.00	36.97	7
15	ATOM	1151	CA	GLN	540	-25.288	54.756	22.935	1.00	35.17	6
	ATOM	1152	CB	GLN	540	-26.223	55.742	23.631	1.00	43.87	6
	ATOM	1153	CG	GLN	540	-27.518	55.064	24.088	1.00	49.77	6
	ATOM	1154	CD	GLN	540	-27.883	55.584	25.468	1.00	56.21	6
20	ATOM	1155	OE1	GLN	540	-28.145	56.782	25.593	1.00	57.44	8
	ATOM	1156	NE2	GLN	540	-27.883	54.705	26.468	1.00	57.25	7
	ATOM	1157	C	GLN	540	-24.060	55.448	22.362	1.00	34.61	6
	ATOM	1158	O	GLN	540	-23.677	56.582	22.693	1.00	33.34	8
	ATOM	1159	N	ALA	541	-23.473	54.755	21.391	1.00	29.80	7
25	ATOM	1160	CA	ALA	541	-22.287	55.232	20.694	1.00	30.02	6
	ATOM	1161	CB	ALA	541	-21.778	54.121	19.774	1.00	27.89	6
	ATOM	1162	C	ALA	541	-22.561	56.466	19.832	1.00	29.52	6
	ATOM	1163	O	ALA	541	-23.650	56.596	19.263	1.00	29.60	8
	ATOM	1164	N	ASN	542	-21.528	57.284	19.665	1.00	30.60	7
30	ATOM	1165	CA	ASN	542	-21.642	58.431	18.738	1.00	31.55	6
	ATOM	1166	CB	ASN	542	-21.985	59.727	19.453	1.00	30.39	6
	ATOM	1167	CG	ASN	542	-21.012	60.117	20.534	1.00	31.63	6
	ATOM	1168	OD1	ASN	542	-19.838	60.443	20.268	1.00	27.57	8
	ATOM	1169	ND2	ASN	542	-21.479	60.127	21.781	1.00	33.23	7
35	ATOM	1170	C	ASN	542	-20.357	58.545	17.936	1.00	32.33	6
	ATOM	1171	O	ASN	542	-19.453	57.698	18.122	1.00	29.09	8
	ATOM	1172	N	HIS	543	-20.223	59.609	17.134	1.00	29.40	7
	ATOM	1173	CA	HIS	543	-19.075	59.780	16.266	1.00	28.82	6
	ATOM	1174	CB	HIS	543	-19.262	60.971	15.272	1.00	24.51	6
40	ATOM	1175	CG	HIS	543	-20.360	60.632	14.295	1.00	31.72	6
	ATOM	1176	CD2	HIS	543	-20.704	59.446	13.740	1.00	33.88	6
	ATOM	1177	ND1	HIS	543	-21.278	61.538	13.822	1.00	32.86	7
	ATOM	1178	CE1	HIS	543	-22.117	60.939	13.008	1.00	31.84	6
	ATOM	1179	NE2	HIS	543	-21.794	59.664	12.941	1.00	31.48	7
45	ATOM	1180	C	HIS	543	-17.747	60.009	16.976	1.00	26.62	6
	ATOM	1181	O	HIS	543	-16.696	59.768	16.366	1.00	25.96	8
	ATOM	1182	N	SER	544	-17.812	60.454	18.221	1.00	20.85	7
	ATOM	1183	CA	SER	544	-16.557	60.738	18.941	1.00	24.82	6
	ATOM	1184	CB	SER	544	-16.839	61.887	19.915	1.00	30.28	6
	ATOM	1185	OG	SER	544	-17.739	61.477	20.930	1.00	39.11	8
50	ATOM	1186	C	SER	544	-15.976	59.443	19.474	1.00	24.89	6
	ATOM	1187	O	SER	544	-14.775	59.348	19.755	1.00	25.22	8
	ATOM	1188	N	HIS	545	-16.746	58.344	19.463	1.00	20.33	7
	ATOM	1189	CA	HIS	545	-16.306	57.005	19.811	1.00	19.38	6
55	ATOM	1190	CB	HIS	545	-17.474	56.104	20.302	1.00	19.40	6
	ATOM	1191	CG	HIS	545	-18.145	56.654	21.534	1.00	18.37	6
	ATOM	1192	CD2	HIS	545	-17.620	56.980	22.744	1.00	18.22	6
	ATOM	1193	ND1	HIS	545	-19.493	56.901	21.627	1.00	23.55	7
	ATOM	1194	CE1	HIS	545	-19.768	57.374	22.829	1.00	26.33	6
60	ATOM	1195	NE2	HIS	545	-18.643	57.454	23.525	1.00	21.05	7
	ATOM	1196	C	HIS	545	-15.589	56.313	18.657	1.00	22.05	6
	ATOM	1197	O	HIS	545	-15.013	55.230	18.848	1.00	21.86	8
	ATOM	1198	N	SER	546	-15.569	56.869	17.440	1.00	20.66	7
	ATOM	1199	CA	SER	546	-14.833	56.217	16.363	1.00	19.96	6
65	ATOM	1200	CB	SER	546	-15.075	56.857	14.986	1.00	20.48	6
	ATOM	1201	OG	SER	546	-16.442	56.712	14.613	1.00	25.61	8
	ATOM	1202	C	SER	546	-13.339	56.270	16.656	1.00	20.51	6
	ATOM	1203	O	SER	546	-12.915	57.252	17.287	1.00	22.06	8
	ATOM	1204	N	GLY	547	-12.556	55.288	16.197	1.00	16.70	7
70	ATOM	1205	CA	GLY	547	-11.123	55.483	16.411	1.00	20.49	6
	ATOM	1206	C	GLY	547	-10.385	54.152	16.555	1.00	22.63	6
	ATOM	1207	O	GLY	547	-10.982	53.104	16.332	1.00	16.09	8

	ATOM	1208	N	ASP	548	-9.111	54.306	16.951	1.00	20.62	7
	ATOM	1209	CA	ASP	548	-8.324	53.089	17.121	1.00	21.57	6
	ATOM	1210	CB	ASP	548	-6.882	53.287	16.674	1.00	28.99	6
5	ATOM	1211	CG	ASP	548	-6.819	53.722	15.219	1.00	41.07	6
	ATOM	1212	OD1	ASP	548	-7.849	53.528	14.540	1.00	39.21	8
	ATOM	1213	OD2	ASP	548	-5.763	54.246	14.808	1.00	39.40	8
	ATOM	1214	C	ASP	548	-8.315	52.652	18.590	1.00	20.72	6
	ATOM	1215	O	ASP	548	-7.817	53.397	19.447	1.00	20.27	7
10	ATOM	1216	N	TYR	549	-8.822	51.426	18.798	1.00	16.97	8
	ATOM	1217	CA	TYR	549	-8.811	50.900	20.164	1.00	18.60	6
	ATOM	1218	CB	TYR	549	-10.193	50.279	20.472	1.00	16.94	6
	ATOM	1219	CG	TYR	549	-11.272	51.332	20.606	1.00	18.45	6
	ATOM	1220	CD1	TYR	549	-11.901	51.938	19.528	1.00	19.27	6
15	ATOM	1221	CE1	TYR	549	-12.877	52.918	19.737	1.00	20.18	6
	ATOM	1222	CD2	TYR	549	-11.672	51.704	21.879	1.00	18.36	6
	ATOM	1223	CE2	TYR	549	-12.636	52.650	22.116	1.00	15.60	6
	ATOM	1224	CZ	TYR	549	-13.238	53.260	21.027	1.00	18.77	6
	ATOM	1225	OH	TYR	549	-14.211	54.206	21.253	1.00	18.41	8
20	ATOM	1226	C	TYR	549	-7.767	49.805	20.355	1.00	15.78	6
	ATOM	1227	O	TYR	549	-7.539	49.007	19.450	1.00	15.86	8
	ATOM	1228	N	HIS	550	-7.196	49.740	21.559	1.00	15.01	7
	ATOM	1229	CA	HIS	550	-6.247	48.695	21.925	1.00	12.99	6
	ATOM	1230	CB	HIS	550	-4.849	48.886	21.372	1.00	11.96	6
25	ATOM	1231	CG	HIS	550	-3.942	49.834	22.117	1.00	17.71	6
	ATOM	1232	CD2	HIS	550	-2.944	49.571	23.004	1.00	16.09	6
	ATOM	1233	ND1	HIS	550	-3.988	51.206	21.971	1.00	11.60	7
	ATOM	1234	CE1	HIS	550	-3.058	51.763	22.716	1.00	16.95	6
	ATOM	1235	NE2	HIS	550	-2.407	50.809	23.370	1.00	19.22	7
30	ATOM	1236	C	HIS	550	-6.263	48.596	23.462	1.00	13.37	6
	ATOM	1237	O	HIS	550	-6.922	49.418	24.129	1.00	12.78	8
	ATOM	1238	N	CYS	551	-5.680	47.511	23.957	1.00	14.21	7
	ATOM	1239	CA	CYS	551	-5.670	47.307	25.414	1.00	15.38	6
35	ATOM	1240	C	CYS	551	-4.301	46.884	25.880	1.00	16.27	6
	ATOM	1241	O	CYS	551	-3.422	46.462	25.132	1.00	15.15	8
	ATOM	1242	CB	CYS	551	-6.746	46.304	25.856	1.00	16.85	6
	ATOM	1243	SG	CYS	551	-6.581	44.597	25.248	1.00	14.82	16
	ATOM	1244	N	THR	552	-4.080	47.061	27.186	1.00	17.41	7
	ATOM	1245	CA	THR	552	-2.875	46.643	27.862	1.00	17.27	6
40	ATOM	1246	CB	THR	552	-1.899	47.735	28.305	1.00	21.80	6
	ATOM	1247	OG1	THR	552	-2.527	48.654	29.205	1.00	17.53	8
	ATOM	1248	CG2	THR	552	-1.356	48.478	27.075	1.00	17.12	6
	ATOM	1249	C	THR	552	-3.346	45.877	29.127	1.00	19.83	6
	ATOM	1250	O	THR	552	-4.471	46.142	29.600	1.00	16.21	8
45	ATOM	1251	N	GLY	553	-2.496	44.953	29.534	1.00	17.84	7
	ATOM	1252	CA	GLY	553	-2.815	44.160	30.731	1.00	20.33	6
	ATOM	1253	C	GLY	553	-1.647	43.261	31.108	1.00	18.60	6
	ATOM	1254	O	GLY	553	-0.779	42.951	30.293	1.00	19.87	8
	ATOM	1255	N	ASN	554	-1.603	42.866	32.373	1.00	20.99	7
50	ATOM	1256	CA	ASN	554	-0.560	42.051	32.959	1.00	20.36	6
	ATOM	1257	CB	ASN	554	-0.512	42.310	34.478	1.00	26.77	6
	ATOM	1258	CG	ASN	554	0.800	42.938	34.897	1.00	40.91	6
	ATOM	1259	OD1	ASN	554	1.700	42.286	35.441	1.00	46.67	8
	ATOM	1260	ND2	ASN	554	0.927	44.227	34.633	1.00	40.24	7
55	ATOM	1261	C	ASN	554	-0.879	40.566	32.817	1.00	22.51	6
	ATOM	1262	O	ASN	554	-1.973	40.181	33.272	1.00	22.15	8
	ATOM	1263	N	ILE	555	0.018	39.799	32.202	1.00	19.40	7
	ATOM	1264	CA	ILE	555	-0.198	38.352	32.139	1.00	22.27	6
	ATOM	1265	CB	ILE	555	-0.210	37.750	30.731	1.00	26.29	6
60	ATOM	1266	CG2	ILE	555	-0.327	36.226	30.831	1.00	23.31	6
	ATOM	1267	CG1	ILE	555	-1.367	38.322	29.899	1.00	28.16	6
	ATOM	1268	CD1	ILE	555	-1.371	37.992	28.434	1.00	29.42	6
	ATOM	1269	C	ILE	555	0.974	37.777	32.941	1.00	27.67	6
	ATOM	1270	O	ILE	555	2.112	38.140	32.639	1.00	24.10	8
65	ATOM	1271	N	GLY	556	0.732	37.028	34.020	1.00	33.10	7
	ATOM	1272	CA	GLY	556	1.942	36.581	34.780	1.00	37.62	6
	ATOM	1273	C	GLY	556	2.447	37.813	35.527	1.00	38.80	6
	ATOM	1274	O	GLY	556	1.659	38.354	36.299	1.00	43.91	8
	ATOM	1275	N	TYR	557	3.655	38.293	35.307	1.00	41.47	7
	ATOM	1276	CA	TYR	557	4.182	39.509	35.894	1.00	43.65	6
70	ATOM	1277	CB	TYR	557	5.381	39.224	36.832	1.00	51.51	6
	ATOM	1278	CG	TYR	557	5.020	38.274	37.961	1.00	57.42	6

130

	ATOM	1279	CD1	TYR	557	5.523	36.981	37.982	1.00	60.45	6
	ATOM	1280	CE1	TYR	557	5.179	36.101	38.992	1.00	62.57	6
	ATOM	1281	CD2	TYR	557	4.140	38.662	38.963	1.00	61.00	6
5	ATOM	1282	CE2	TYR	557	3.788	37.787	39.982	1.00	63.03	6
	ATOM	1283	CZ	TYR	557	4.313	36.513	39.986	1.00	63.56	6
	ATOM	1284	OH	TYR	557	3.979	35.629	40.984	1.00	66.68	8
	ATOM	1285	C	TYR	557	4.676	40.515	34.849	1.00	41.96	6
	ATOM	1286	O	TYR	557	5.445	41.446	35.115	1.00	41.33	8
10	ATOM	1287	N	THR	558	4.298	40.319	33.594	1.00	36.77	7
	ATOM	1288	CA	THR	558	4.722	41.173	32.496	1.00	30.71	6
	ATOM	1289	CB	THR	558	5.260	40.269	31.364	1.00	30.82	6
	ATOM	1290	OG1	THR	558	6.237	39.395	31.942	1.00	30.47	8
	ATOM	1291	CG2	THR	558	5.851	41.047	30.207	1.00	29.21	6
15	ATOM	1292	C	THR	558	3.532	41.922	31.912	1.00	25.66	6
	ATOM	1293	O	THR	558	2.521	41.257	31.642	1.00	24.50	8
	ATOM	1294	N	LEU	559	3.689	43.202	31.609	1.00	21.00	7
	ATOM	1295	CA	LEU	559	2.617	43.942	30.960	1.00	21.01	6
	ATOM	1296	CB	LEU	559	2.737	45.431	31.284	1.00	26.53	6
20	ATOM	1297	CG	LEU	559	1.601	46.379	30.958	1.00	27.15	6
	ATOM	1298	CD1	LEU	559	0.323	46.049	31.713	1.00	25.15	6
	ATOM	1299	CD2	LEU	559	1.979	47.830	31.316	1.00	28.75	6
	ATOM	1300	C	LEU	559	2.654	43.687	29.461	1.00	22.04	6
	ATOM	1301	O	LEU	559	3.711	43.618	28.844	1.00	22.64	8
25	ATOM	1302	N	PHE	560	1.484	43.470	28.855	1.00	20.79	7
	ATOM	1303	CA	PHE	560	1.430	43.290	27.409	1.00	19.10	6
	ATOM	1304	CB	PHE	560	0.821	41.920	27.060	1.00	20.91	6
	ATOM	1305	CG	PHE	560	1.848	40.832	27.216	1.00	19.50	6
	ATOM	1306	CD1	PHE	560	1.971	40.190	28.442	1.00	24.86	6
30	ATOM	1307	CD2	PHE	560	2.645	40.457	26.156	1.00	21.03	6
	ATOM	1308	CE1	PHE	560	2.903	39.157	28.588	1.00	29.44	6
	ATOM	1309	CE2	PHE	560	3.582	39.445	26.296	1.00	19.89	6
	ATOM	1310	CZ	PHE	560	3.704	38.792	27.529	1.00	25.34	6
35	ATOM	1311	C	PHE	560	0.521	44.353	26.794	1.00	17.36	6
	ATOM	1312	O	PHE	560	-0.346	44.884	27.504	1.00	18.36	8
	ATOM	1313	N	SER	561	0.753	44.626	25.521	1.00	17.60	7
	ATOM	1314	CA	SER	561	-0.087	45.564	24.785	1.00	14.63	6
	ATOM	1315	CB	SER	561	0.744	46.716	24.188	1.00	20.14	6
	ATOM	1316	OG	SER	561	-0.115	47.812	23.901	1.00	21.55	8
40	ATOM	1317	C	SER	561	-0.662	44.829	23.561	1.00	18.96	6
	ATOM	1318	O	SER	561	0.101	44.113	22.894	1.00	19.79	8
	ATOM	1319	N	SER	562	-1.921	45.070	23.232	1.00	16.19	7
	ATOM	1320	CA	SER	562	-2.518	44.462	22.049	1.00	16.74	6
	ATOM	1321	CB	SER	562	-4.029	44.188	22.233	1.00	16.78	6
45	ATOM	1322	OG	SER	562	-4.801	45.336	21.900	1.00	21.00	8
	ATOM	1323	C	SER	562	-2.322	45.381	20.845	1.00	18.24	6
	ATOM	1324	O	SER	562	-1.949	46.561	20.987	1.00	16.85	8
	ATOM	1325	N	LYS	563	-2.535	44.839	19.652	1.00	17.96	7
	ATOM	1326	CA	LYS	563	-2.484	45.663	18.445	1.00	17.36	6
50	ATOM	1327	CB	LYS	563	-2.369	44.909	17.133	1.00	20.94	6
	ATOM	1328	CG	LYS	563	-1.228	43.981	16.902	1.00	25.34	6
	ATOM	1329	CD	LYS	563	0.128	44.595	16.685	1.00	29.02	6
	ATOM	1330	CE	LYS	563	0.954	43.735	15.721	1.00	42.35	6
	ATOM	1331	NZ	LYS	563	0.495	42.308	15.692	1.00	38.14	7
55	ATOM	1332	C	LYS	563	-3.821	46.400	18.391	1.00	17.27	6
	ATOM	1333	O	LYS	563	-4.817	45.960	18.978	1.00	16.54	8
	ATOM	1334	N	PRO	564	-3.840	47.518	17.696	1.00	18.39	7
	ATOM	1335	CD	PRO	564	-2.702	48.123	16.952	1.00	20.79	6
	ATOM	1336	CA	PRO	564	-5.060	48.294	17.546	1.00	19.84	6
60	ATOM	1337	CB	PRO	564	-4.545	49.689	17.142	1.00	17.33	6
	ATOM	1338	CG	PRO	564	-3.254	49.450	16.475	1.00	21.76	6
	ATOM	1339	C	PRO	564	-6.032	47.697	16.528	1.00	19.62	6
	ATOM	1340	O	PRO	564	-5.723	46.924	15.619	1.00	19.46	8
	ATOM	1341	N	VAL	565	-7.295	48.033	16.674	1.00	17.22	7
65	ATOM	1342	CA	VAL	565	-8.427	47.704	15.841	1.00	20.36	6
	ATOM	1343	CB	VAL	565	-9.405	46.676	16.450	1.00	20.84	6
	ATOM	1344	CG1	VAL	565	-10.418	46.223	15.404	1.00	20.46	6
	ATOM	1345	CG2	VAL	565	-8.699	45.391	16.899	1.00	23.72	6
	ATOM	1346	C	VAL	565	-9.173	49.033	15.590	1.00	22.05	6
	ATOM	1347	O	VAL	565	-9.532	49.772	16.499	1.00	22.10	8
70	ATOM	1348	N	THR	566	-9.444	49.317	14.320	1.00	24.93	7
	ATOM	1349	CA	THR	566	-10.111	50.549	13.939	1.00	26.07	6

131

	ATOM	1350	CB	THR	566	-9.631	51.082	12.579	1.00	31.66	6
	ATOM	1351	OG1	THR	566	-9.737	50.055	11.569	1.00	38.39	8
	ATOM	1352	CG2	THR	566	-8.180	51.513	12.694	1.00	23.71	6
5	ATOM	1353	C	THR	566	-11.611	50.269	13.909	1.00	25.06	6
	ATOM	1354	O	THR	566	-11.985	49.330	13.244	1.00	21.88	8
	ATOM	1355	N	ILE	567	-12.362	50.988	14.714	1.00	21.40	7
	ATOM	1356	CA	ILE	567	-13.784	50.959	14.909	1.00	25.06	6
	ATOM	1357	CB	ILE	567	-14.088	50.702	16.424	1.00	26.21	6
10	ATOM	1358	CG2	ILE	567	-15.588	50.707	16.673	1.00	26.68	6
	ATOM	1359	CG1	ILE	567	-13.415	49.394	16.825	1.00	26.56	6
	ATOM	1360	CD1	ILE	567	-13.946	48.548	17.939	1.00	30.83	6
	ATOM	1361	C	ILE	567	-14.416	52.294	14.501	1.00	24.36	6
	ATOM	1362	O	ILE	567	-14.013	53.384	14.920	1.00	23.36	8
	ATOM	1363	N	THR	568	-15.412	52.275	13.630	1.00	22.83	7
15	ATOM	1364	CA	THR	568	-16.083	53.461	13.152	1.00	27.27	6
	ATOM	1365	CB	THR	568	-15.945	53.600	11.622	1.00	31.88	6
	ATOM	1366	OG1	THR	568	-14.565	53.495	11.277	1.00	32.11	8
	ATOM	1367	CG2	THR	568	-16.462	54.972	11.179	1.00	34.54	6
	ATOM	1368	C	THR	568	-17.575	53.452	13.501	1.00	28.53	6
20	ATOM	1369	O	THR	568	-18.190	52.383	13.508	1.00	32.64	8
	ATOM	1370	N	VAL	569	-18.090	54.606	13.863	1.00	23.55	7
	ATOM	1371	CA	VAL	569	-19.472	54.855	14.163	1.00	27.27	6
	ATOM	1372	CB	VAL	569	-19.728	55.507	15.523	1.00	28.51	6
	ATOM	1373	CG1	VAL	569	-21.227	55.733	15.757	1.00	26.42	6
25	ATOM	1374	CG2	VAL	569	-19.189	54.706	16.696	1.00	27.97	6
	ATOM	1375	C	VAL	569	-20.011	55.844	13.098	1.00	32.65	6
	ATOM	1376	O	VAL	569	-19.332	56.810	12.710	1.00	33.21	8
	ATOM	1377	N	GLN	570	-21.245	55.670	12.689	0.01	33.85	7
	ATOM	1378	CA	GLN	570	-21.966	56.476	11.737	0.01	35.75	6
30	ATOM	1379	CB	GLN	570	-23.335	56.839	12.362	0.01	36.48	6
	ATOM	1380	CG	GLN	570	-24.465	56.854	11.347	0.01	37.54	6
	ATOM	1381	CD	GLN	570	-25.478	55.756	11.599	0.01	37.91	6
	ATOM	1382	OE1	GLN	570	-25.142	54.680	12.096	0.01	38.17	8
	ATOM	1383	NE2	GLN	570	-26.735	56.020	11.257	0.01	38.21	7
35	ATOM	1384	C	GLN	570	-21.355	57.778	11.241	0.01	36.70	6
	ATOM	1385	O	GLN	570	-21.049	58.699	11.995	0.01	36.81	8
	ATOM	1386	N	VAL	571	-21.273	57.907	9.919	0.01	37.51	7
	ATOM	1387	CA	VAL	571	-20.781	59.094	9.240	0.01	38.20	6
	ATOM	1388	CB	VAL	571	-19.483	59.658	9.842	0.01	38.61	6
40	ATOM	1389	CG1	VAL	571	-18.334	58.667	9.681	0.01	38.88	6
	ATOM	1390	CG2	VAL	571	-19.115	60.985	9.180	0.01	38.83	6
	ATOM	1391	C	VAL	571	-20.587	58.818	7.750	0.01	38.42	6
	ATOM	1392	O	VAL	571	-21.420	59.293	6.949	0.01	38.53	8
45	ATOM	1	OWO	WAT	601	-13.958	32.760	19.930	1.00	18.36	8
	ATOM	2	OWO	WAT	602	-13.653	59.625	23.320	1.00	24.59	8
	ATOM	3	OWO	WAT	603	-5.895	43.456	18.965	1.00	14.14	8
	ATOM	4	OWO	WAT	604	-9.519	28.178	30.514	1.00	42.11	8
	ATOM	5	OWO	WAT	605	-8.700	36.412	28.355	1.00	21.65	8
50	ATOM	6	OWO	WAT	606	-25.548	35.202	7.898	1.00	24.88	8
	ATOM	7	OWO	WAT	607	-2.902	48.395	31.897	1.00	19.13	8
	ATOM	8	OWO	WAT	608	-14.303	55.610	23.676	1.00	24.28	8
	ATOM	9	OWO	WAT	609	-10.371	38.314	29.076	1.00	27.73	8
	ATOM	10	OWO	WAT	610	-12.433	34.237	21.505	1.00	14.04	8
55	ATOM	11	OWO	WAT	611	-5.417	53.367	21.002	1.00	16.89	8
	ATOM	12	OWO	WAT	612	-29.599	18.069	11.595	1.00	34.62	8
	ATOM	13	OWO	WAT	613	-17.813	30.679	2.648	1.00	16.34	8
	ATOM	14	OWO	WAT	614	-6.656	42.551	16.413	1.00	24.31	8
	ATOM	15	OWO	WAT	615	-21.191	20.720	5.335	1.00	30.05	8
60	ATOM	16	OWO	WAT	616	-15.621	34.100	18.319	1.00	18.82	8
	ATOM	17	OWO	WAT	617	-6.528	44.456	14.460	1.00	26.68	8
	ATOM	18	OWO	WAT	618	-6.213	31.143	22.792	1.00	19.89	8
	ATOM	19	OWO	WAT	619	-12.935	32.992	24.109	1.00	29.95	8
	ATOM	20	OWO	WAT	620	2.277	38.630	20.953	1.00	28.34	8
65	ATOM	21	OWO	WAT	621	-20.151	29.522	0.183	1.00	21.62	8
	ATOM	22	OWO	WAT	622	-27.773	35.663	6.295	1.00	20.74	8
	ATOM	23	OWO	WAT	623	0.481	42.002	19.811	1.00	24.67	8
	ATOM	24	OWO	WAT	624	-17.815	32.952	1.120	1.00	26.99	8
	ATOM	25	OWO	WAT	625	-16.604	36.105	25.523	1.00	18.45	8
	ATOM	26	OWO	WAT	626	0.330	41.286	22.516	1.00	29.01	8
70	ATOM	27	OWO	WAT	627	-13.324	59.911	17.129	1.00	40.98	8
	ATOM	28	OWO	WAT	628	-9.214	59.486	22.450	1.00	41.91	8

132

	ATOM	29	OWO	WAT	629	-20.146	18.596	13.850	1.00	50.03	8
	ATOM	30	OWO	WAT	630	-21.707	20.513	12.325	1.00	18.46	8
	ATOM	31	OWO	WAT	631	-15.403	33.699	25.599	1.00	21.44	8
5	ATOM	32	OWO	WAT	632	-12.703	37.608	30.174	1.00	37.28	8
	ATOM	33	OWO	WAT	633	-12.479	39.466	39.250	1.00	23.78	8
	ATOM	34	OWO	WAT	634	-13.921	41.406	9.106	1.00	40.49	8
	ATOM	35	OWO	WAT	635	-7.230	28.485	24.432	1.00	41.81	8
	ATOM	36	OWO	WAT	636	-2.989	42.185	19.344	1.00	17.29	8
10	ATOM	37	OWO	WAT	637	-12.865	25.830	10.180	1.00	47.19	8
	ATOM	38	OWO	WAT	638	-2.754	32.875	13.259	1.00	35.75	8
	ATOM	39	OWO	WAT	639	-17.416	43.258	26.641	1.00	32.09	8
	ATOM	40	OWO	WAT	640	-31.068	25.287	10.888	1.00	20.85	8
	ATOM	41	OWO	WAT	641	-17.725	28.881	21.261	1.00	25.43	8
15	ATOM	42	OWO	WAT	642	-32.760	35.615	6.079	1.00	38.04	8
	ATOM	43	OWO	WAT	643	-14.079	28.493	25.218	1.00	20.23	8
	ATOM	44	OWO	WAT	644	-16.644	22.930	-2.315	1.00	34.00	8
	ATOM	45	OWO	WAT	645	-1.790	38.223	35.518	1.00	30.63	8
	ATOM	46	OWO	WAT	646	-10.026	24.026	13.639	1.00	31.10	8
20	ATOM	47	OWO	WAT	647	-11.096	60.328	24.599	1.00	33.25	8
	ATOM	48	OWO	WAT	648	-19.457	27.850	-2.970	1.00	36.88	8
	ATOM	49	OWO	WAT	649	-18.578	40.758	26.756	1.00	30.86	8
	ATOM	50	OWO	WAT	650	-11.119	22.191	16.190	1.00	37.83	8
	ATOM	51	OWO	WAT	651	-2.583	24.179	28.032	1.00	73.18	8
25	ATOM	52	OWO	WAT	652	-0.243	25.713	22.803	1.00	34.15	8
	ATOM	53	OWO	WAT	653	-33.328	18.701	10.255	1.00	23.17	8
	ATOM	54	OWO	WAT	654	-22.212	13.785	5.080	1.00	51.41	8
	ATOM	55	OWO	WAT	655	-21.393	16.945	11.680	1.00	31.47	8
	ATOM	56	OWO	WAT	656	-37.174	28.484	4.349	1.00	36.66	8
30	ATOM	57	OWO	WAT	657	-23.291	46.916	13.981	1.00	45.02	8
	ATOM	58	OWO	WAT	658	-31.521	20.732	5.404	1.00	28.19	8
	ATOM	59	OWO	WAT	659	-11.904	22.697	8.209	1.00	61.39	8
	ATOM	60	OWO	WAT	660	-7.393	64.706	24.668	1.00	45.96	8
	ATOM	61	OWO	WAT	661	-12.356	29.912	23.727	1.00	23.77	8
35	ATOM	62	OWO	WAT	662	-33.898	31.788	7.353	1.00	32.96	8
	ATOM	63	OWO	WAT	663	-28.502	48.102	25.478	1.00	58.40	8
	ATOM	64	OWO	WAT	664	-23.414	63.056	18.427	1.00	35.16	8
	ATOM	65	OWO	WAT	665	-4.792	26.235	16.778	1.00	44.49	8
	ATOM	66	OWO	WAT	666	-28.509	23.145	-1.620	1.00	50.51	8
40	ATOM	67	OWO	WAT	667	-19.685	32.378	-0.712	1.00	45.74	8
	ATOM	68	OWO	WAT	668	-10.899	26.379	23.620	1.00	43.61	8
	ATOM	69	OWO	WAT	669	1.033	27.146	20.128	1.00	34.52	8
	ATOM	70	OWO	WAT	670	-15.215	33.469	0.077	1.00	27.35	8
	ATOM	71	OWO	WAT	671	-8.748	20.877	16.508	1.00	51.59	8
45	ATOM	72	OWO	WAT	672	-22.332	18.552	3.707	1.00	30.25	8
	ATOM	73	OWO	WAT	673	-23.373	30.095	17.610	1.00	22.44	8
	ATOM	74	OWO	WAT	674	-11.965	32.994	26.359	1.00	26.92	8
	ATOM	75	OWO	WAT	675	-35.793	29.720	7.198	1.00	27.19	8
	ATOM	76	OWO	WAT	676	-10.333	28.336	25.867	1.00	46.78	8
50	ATOM	77	OWO	WAT	677	-17.230	31.681	24.852	1.00	26.22	8
	ATOM	78	OWO	WAT	678	-17.594	49.434	30.830	1.00	32.58	8
	ATOM	79	OWO	WAT	679	-8.561	33.163	32.884	1.00	37.04	8
	ATOM	80	OWO	WAT	680	-16.374	29.101	-4.195	1.00	31.45	8
	ATOM	81	OWO	WAT	681	-8.995	30.537	24.946	1.00	36.64	8
55	ATOM	82	OWO	WAT	682	-19.019	53.815	28.676	1.00	48.06	8
	ATOM	83	OWO	WAT	683	-20.039	39.516	15.742	1.00	23.23	8
	ATOM	84	OWO	WAT	684	-21.308	45.557	20.658	1.00	28.24	8
	ATOM	85	OWO	WAT	685	-7.405	30.847	5.261	1.00	41.47	8
	ATOM	86	OWO	WAT	686	-23.729	34.800	0.632	1.00	30.27	8
60	ATOM	87	OWO	WAT	687	-15.826	60.771	23.946	1.00	41.94	8
	ATOM	88	OWO	WAT	688	0.119	50.495	24.812	0.50	25.93	8
	ATOM	89	OWO	WAT	689	-3.397	45.987	42.245	1.00	29.87	8
	ATOM	90	OWO	WAT	690	-10.215	47.715	32.270	1.00	43.33	8
	ATOM	91	OWO	WAT	691	-8.440	35.757	33.883	1.00	34.09	8
65	END										

TABLE 3

REMARK Homology model of Fc epsilon Receptor I by V. C. Epa; based on structure of FcγRIIa by K. Maxwell.

70

133

REMARK Produced by MODELLER: 24-Aug-98 01:02:51

1

REMARK MODELLER OBJECTIVE FUNCTION: 643.1817

5	ATOM	1	N	VAL	1	36.442	43.253	22.184	1.00	0.14	1SG	2
	ATOM	2	CA	VAL	1	37.922	43.321	22.176	1.00	0.14	1SG	3
	ATOM	3	CB	VAL	1	38.483	42.986	23.538	1.00	0.14	1SG	4
	ATOM	4	CG1	VAL	1	38.026	44.080	24.516	1.00	0.14	1SG	5
	ATOM	5	CG2	VAL	1	38.051	41.576	23.970	1.00	0.14	1SG	6
10	ATOM	6	C	VAL	1	38.614	42.508	21.119	1.00	0.14	1SG	7
	ATOM	7	O	VAL	1	39.758	42.821	20.796	1.00	0.14	1SG	8
	ATOM	8	N	PRO	2	38.026	41.492	20.533	1.00	0.15	1SG	9
	ATOM	9	CA	PRO	2	38.761	40.840	19.488	1.00	0.15	1SG	10
	ATOM	10	CD	PRO	2	37.208	40.531	21.266	1.00	0.15	1SG	11
15	ATOM	11	CB	PRO	2	38.099	39.483	19.270	1.00	0.15	1SG	12
	ATOM	12	CG	PRO	2	37.502	39.155	20.647	1.00	0.15	1SG	13
	ATOM	13	C	PRO	2	38.754	41.707	18.276	1.00	0.15	1SG	14
	ATOM	14	O	PRO	2	37.885	42.569	18.163	1.00	0.15	1SG	15
20	ATOM	15	N	GLN	3	39.714	41.495	17.359	1.00	0.19	1SG	16
	ATOM	16	CA	GLN	3	39.782	42.301	16.180	1.00	0.19	1SG	17
	ATOM	17	CB	GLN	3	40.951	41.913	15.260	1.00	0.19	1SG	18
	ATOM	18	CG	GLN	3	41.177	42.871	14.092	1.00	0.19	1SG	19
	ATOM	19	CD	GLN	3	42.430	42.400	13.369	1.00	0.19	1SG	20
	ATOM	20	OE1	GLN	3	42.839	41.249	13.508	1.00	0.19	1SG	21
25	ATOM	21	NE2	GLN	3	43.063	43.312	12.584	1.00	0.19	1SG	22
	ATOM	22	C	GLN	3	38.497	42.103	15.448	1.00	0.19	1SG	23
	ATOM	23	O	GLN	3	37.821	41.091	15.627	1.00	0.19	1SG	24
	ATOM	24	N	LYS	4	38.112	43.088	14.614	1.00	0.23	1SG	25
	ATOM	25	CA	LYS	4	36.855	42.998	13.932	1.00	0.23	1SG	26
30	ATOM	26	CB	LYS	4	36.146	44.354	13.776	1.00	0.23	1SG	27
	ATOM	27	CG	LYS	4	35.714	44.972	15.107	1.00	0.23	1SG	28
	ATOM	28	CD	LYS	4	35.315	46.446	14.996	1.00	0.23	1SG	29
	ATOM	29	CE	LYS	4	36.506	47.386	14.804	1.00	0.23	1SG	30
	ATOM	30	NZ	LYS	4	36.033	48.778	14.631	1.00	0.23	1SG	31
35	ATOM	31	C	LYS	4	37.089	42.464	12.560	1.00	0.23	1SG	32
	ATOM	32	O	LYS	4	37.990	42.883	11.834	1.00	0.23	1SG	33
	ATOM	33	N	PRO	5	36.261	41.520	12.218	1.00	0.25	1SG	34
	ATOM	34	CA	PRO	5	36.316	40.878	10.938	1.00	0.25	1SG	35
	ATOM	35	CD	PRO	5	34.937	41.436	12.804	1.00	0.25	1SG	36
40	ATOM	36	CB	PRO	5	35.140	39.910	10.930	1.00	0.25	1SG	37
	ATOM	37	CG	PRO	5	34.094	40.656	11.780	1.00	0.25	1SG	38
	ATOM	38	C	PRO	5	36.086	41.953	9.932	1.00	0.25	1SG	39
	ATOM	39	O	PRO	5	35.464	42.958	10.275	1.00	0.25	1SG	40
	ATOM	40	N	LYS	6	36.592	41.786	8.699	1.00	0.35	1SG	41
45	ATOM	41	CA	LYS	6	36.336	42.790	7.714	1.00	0.35	1SG	42
	ATOM	42	CB	LYS	6	37.597	43.344	7.030	1.00	0.35	1SG	43
	ATOM	43	CG	LYS	6	38.418	44.275	7.924	1.00	0.35	1SG	44
	ATOM	44	CD	LYS	6	39.065	43.574	9.120	1.00	0.35	1SG	45
	ATOM	45	CE	LYS	6	39.884	44.516	10.004	1.00	0.35	1SG	46
50	ATOM	46	NZ	LYS	6	40.469	43.767	11.137	1.00	0.35	1SG	47
	ATOM	47	C	LYS	6	35.491	42.168	6.659	1.00	0.35	1SG	48
	ATOM	48	O	LYS	6	35.686	41.011	6.289	1.00	0.35	1SG	49
	ATOM	49	N	VAL	7	34.498	42.928	6.165	1.00	0.35	1SG	50
	ATOM	50	CA	VAL	7	33.668	42.408	5.124	1.00	0.35	1SG	51
55	ATOM	51	CB	VAL	7	32.207	42.721	5.299	1.00	0.35	1SG	52
	ATOM	52	CG1	VAL	7	32.014	44.247	5.280	1.00	0.35	1SG	53
	ATOM	53	CG2	VAL	7	31.423	41.985	4.200	1.00	0.35	1SG	54
	ATOM	54	C	VAL	7	34.132	43.039	3.857	1.00	0.35	1SG	55
	ATOM	55	O	VAL	7	34.313	44.254	3.783	1.00	0.35	1SG	56
60	ATOM	56	N	SER	8	34.363	42.211	2.825	1.00	0.17	1SG	57
	ATOM	57	CA	SER	8	34.831	42.734	1.580	1.00	0.17	1SG	58
	ATOM	58	CB	SER	8	36.059	41.994	1.024	1.00	0.17	1SG	59
	ATOM	59	OG	SER	8	36.458	42.571	-0.210	1.00	0.17	1SG	60
	ATOM	60	C	SER	8	33.733	42.575	0.586	1.00	0.17	1SG	61
65	ATOM	61	O	SER	8	33.030	41.566	0.575	1.00	0.17	1SG	62
	ATOM	62	N	LEU	9	33.552	43.593	-0.272	1.00	0.11	1SG	63
	ATOM	63	CA	LEU	9	32.519	43.525	-1.257	1.00	0.11	1SG	64
	ATOM	64	CB	LEU	9	31.563	44.731	-1.198	1.00	0.11	1SG	65
	ATOM	65	CG	LEU	9	30.442	44.709	-2.253	1.00	0.11	1SG	66
70	ATOM	66	CD2	LEU	9	29.725	46.068	-2.316	1.00	0.11	1SG	67
	ATOM	67	CD1	LEU	9	29.474	43.536	-2.025	1.00	0.11	1SG	68

134

	ATOM	68	C	LEU	9	33.175	43.554	-2.597	1.00	0.11	1SG	69
	ATOM	69	O	LEU	9	33.992	44.428	-2.883	1.00	0.11	1SG	70
	ATOM	70	N	ASN	10	32.851	42.565	-3.450	1.00	0.17	1SG	71
5	ATOM	71	CA	ASN	10	33.401	42.565	-4.771	1.00	0.17	1SG	72
	ATOM	72	CB	ASN	10	34.406	41.428	-5.011	1.00	0.17	1SG	73
	ATOM	73	CG	ASN	10	35.623	41.693	-4.139	1.00	0.17	1SG	74
	ATOM	74	OD1	ASN	10	35.830	41.018	-3.132	1.00	0.17	1SG	75
	ATOM	75	ND2	ASN	10	36.451	42.698	-4.532	1.00	0.17	1SG	76
	ATOM	76	C	ASN	10	32.257	42.340	-5.702	1.00	0.17	1SG	77
10	ATOM	77	O	ASN	10	31.543	41.346	-5.585	1.00	0.17	1SG	78
	ATOM	78	N	PRO	11	32.037	43.241	-6.615	1.00	0.35	1SG	79
	ATOM	79	CA	PRO	11	32.836	44.431	-6.695	1.00	0.35	1SG	80
	ATOM	80	CD	PRO	11	31.554	42.825	-7.923	1.00	0.35	1SG	81
	ATOM	81	CB	PRO	11	32.565	45.023	-8.076	1.00	0.35	1SG	82
15	ATOM	82	CG	PRO	11	32.180	43.803	-8.930	1.00	0.35	1SG	83
	ATOM	83	C	PRO	11	32.450	45.345	-5.579	1.00	0.35	1SG	84
	ATOM	84	O	PRO	11	31.441	45.098	-4.920	1.00	0.35	1SG	85
	ATOM	85	N	PRO	12	33.234	46.363	-5.359	1.00	0.52	1SG	86
	ATOM	86	CA	PRO	12	32.980	47.289	-4.289	1.00	0.52	1SG	87
20	ATOM	87	CD	PRO	12	34.649	46.281	-5.684	1.00	0.52	1SG	88
	ATOM	88	CB	PRO	12	34.259	48.107	-4.134	1.00	0.52	1SG	89
	ATOM	89	CG	PRO	12	35.360	47.165	-4.647	1.00	0.52	1SG	90
	ATOM	90	C	PRO	12	31.775	48.132	-4.544	1.00	0.52	1SG	91
	ATOM	91	O	PRO	12	31.347	48.837	-3.632	1.00	0.52	1SG	92
25	ATOM	92	N	TRP	13	31.217	48.087	-5.767	1.00	0.35	1SG	93
	ATOM	93	CA	TRP	13	30.116	48.944	-6.099	1.00	0.35	1SG	94
	ATOM	94	CB	TRP	13	29.535	48.655	-7.492	1.00	0.35	1SG	95
	ATOM	95	CG	TRP	13	30.569	48.725	-8.590	1.00	0.35	1SG	96
	ATOM	96	CD2	TRP	13	31.368	49.880	-8.883	1.00	0.35	1SG	97
30	ATOM	97	CD1	TRP	13	30.982	47.743	-9.442	1.00	0.35	1SG	98
	ATOM	98	NE1	TRP	13	31.981	48.216	-10.257	1.00	0.35	1SG	99
	ATOM	99	CE2	TRP	13	32.232	49.530	-9.921	1.00	0.35	1SG	100
	ATOM	100	CE3	TRP	13	31.389	51.127	-8.327	1.00	0.35	1SG	101
	ATOM	101	CZ2	TRP	13	33.131	50.426	-10.422	1.00	0.35	1SG	102
35	ATOM	102	CZ3	TRP	13	32.292	52.032	-8.839	1.00	0.35	1SG	103
	ATOM	103	CH2	TRP	13	33.145	51.687	-9.867	1.00	0.35	1SG	104
	ATOM	104	C	TRP	13	29.028	48.729	-5.094	1.00	0.35	1SG	105
	ATOM	105	O	TRP	13	28.536	47.615	-4.920	1.00	0.35	1SG	106
	ATOM	106	N	ASN	14	28.646	49.808	-4.379	1.00	0.15	1SG	107
40	ATOM	107	CA	ASN	14	27.615	49.722	-3.385	1.00	0.15	1SG	108
	ATOM	108	CB	ASN	14	27.490	50.980	-2.504	1.00	0.15	1SG	109
	ATOM	109	CG	ASN	14	26.978	52.146	-3.340	1.00	0.15	1SG	110
	ATOM	110	OD1	ASN	14	27.409	52.366	-4.471	1.00	0.15	1SG	111
	ATOM	111	ND2	ASN	14	26.008	52.913	-2.773	1.00	0.15	1SG	112
45	ATOM	112	C	ASN	14	26.300	49.521	-4.065	1.00	0.15	1SG	113
	ATOM	113	O	ASN	14	25.463	48.747	-3.602	1.00	0.15	1SG	114
	ATOM	114	N	ARG	15	26.087	50.221	-5.196	1.00	0.13	1SG	115
	ATOM	115	CA	ARG	15	24.834	50.135	-5.884	1.00	0.13	1SG	116
	ATOM	116	CB	ARG	15	24.365	51.472	-6.487	1.00	0.13	1SG	117
50	ATOM	117	CG	ARG	15	24.050	52.558	-5.458	1.00	0.13	1SG	118
	ATOM	118	CD	ARG	15	23.590	53.872	-6.094	1.00	0.13	1SG	119
	ATOM	119	NE	ARG	15	23.349	54.844	-4.990	1.00	0.13	1SG	120
	ATOM	120	CZ	ARG	15	22.138	55.461	-4.864	1.00	0.13	1SG	121
	ATOM	121	NH1	ARG	15	21.143	55.212	-5.764	1.00	0.13	1SG	122
55	ATOM	122	NH2	ARG	15	21.924	56.330	-3.833	1.00	0.13	1SG	123
	ATOM	123	C	ARG	15	25.033	49.218	-7.039	1.00	0.13	1SG	124
	ATOM	124	O	ARG	15	25.976	49.374	-7.813	1.00	0.13	1SG	125
	ATOM	125	N	ILE	16	24.144	48.220	-7.185	1.00	0.12	1SG	126
	ATOM	126	CA	ILE	16	24.295	47.330	-8.294	1.00	0.12	1SG	127
60	ATOM	127	CB	ILE	16	24.817	45.969	-7.928	1.00	0.12	1SG	128
	ATOM	128	CG2	ILE	16	26.224	46.139	-7.331	1.00	0.12	1SG	129
	ATOM	129	CG1	ILE	16	23.828	45.237	-7.005	1.00	0.12	1SG	130
	ATOM	130	CD1	ILE	16	24.141	43.749	-6.850	1.00	0.12	1SG	131
	ATOM	131	C	ILE	16	22.948	47.120	-8.892	1.00	0.12	1SG	132
65	ATOM	132	O	ILE	16	21.939	47.597	-8.374	1.00	0.12	1SG	133
	ATOM	133	N	PHE	17	22.919	46.404	-10.030	1.00	0.17	1SG	134
	ATOM	134	CA	PHE	17	21.684	46.108	-10.688	1.00	0.17	1SG	135
	ATOM	135	CB	PHE	17	21.755	46.075	-12.223	1.00	0.17	1SG	136
	ATOM	136	CG	PHE	17	21.919	47.447	-12.765	1.00	0.17	1SG	137
70	ATOM	137	CD1	PHE	17	20.844	48.303	-12.811	1.00	0.17	1SG	138
	ATOM	138	CD2	PHE	17	23.137	47.862	-13.248	1.00	0.17	1SG	139

	ATOM	139	CE1	PHE	17	20.984	49.568	-13.324	1.00	0.17	1SG	140
	ATOM	140	CE2	PHE	17	23.283	49.126	-13.764	1.00	0.17	1SG	141
	ATOM	141	CZ	PHE	17	22.205	49.976	-13.800	1.00	0.17	1SG	142
5	ATOM	142	C	PHE	17	21.314	44.719	-10.316	1.00	0.17	1SG	143
	ATOM	143	O	PHE	17	22.151	43.922	-9.896	1.00	0.17	1SG	144
	ATOM	144	N	LYS	18	20.018	44.402	-10.462	1.00	0.22	1SG	145
	ATOM	145	CA	LYS	18	19.571	43.082	-10.162	1.00	0.22	1SG	146
	ATOM	146	CB	LYS	18	18.040	42.943	-10.187	1.00	0.22	1SG	147
10	ATOM	147	CG	LYS	18	17.424	43.301	-11.539	1.00	0.22	1SG	148
	ATOM	148	CD	LYS	18	15.961	42.882	-11.672	1.00	0.22	1SG	149
	ATOM	149	CE	LYS	18	15.353	43.196	-13.039	1.00	0.22	1SG	150
	ATOM	150	NZ	LYS	18	14.014	42.574	-13.142	1.00	0.22	1SG	151
	ATOM	151	C	LYS	18	20.141	42.189	-11.210	1.00	0.22	1SG	152
15	ATOM	152	O	LYS	18	20.335	42.596	-12.355	1.00	0.22	1SG	153
	ATOM	153	N	GLY	19	20.455	40.940	-10.824	1.00	0.21	1SG	154
	ATOM	154	CA	GLY	19	20.986	40.005	-11.767	1.00	0.21	1SG	155
	ATOM	155	C	GLY	19	22.474	40.059	-11.692	1.00	0.21	1SG	156
	ATOM	156	O	GLY	19	23.160	39.196	-12.236	1.00	0.21	1SG	157
20	ATOM	157	N	GLU	20	23.017	41.079	-11.005	1.00	0.23	1SG	158
	ATOM	158	CA	GLU	20	24.442	41.177	-10.910	1.00	0.23	1SG	159
	ATOM	159	CB	GLU	20	24.940	42.579	-10.523	1.00	0.23	1SG	160
	ATOM	160	CG	GLU	20	24.680	43.613	-11.619	1.00	0.23	1SG	161
	ATOM	161	CD	GLU	20	25.391	43.115	-12.870	1.00	0.23	1SG	162
25	ATOM	162	OE1	GLU	20	26.556	42.653	-12.741	1.00	0.23	1SG	163
	ATOM	163	OE2	GLU	20	24.774	43.175	-13.967	1.00	0.23	1SG	164
	ATOM	164	C	GLU	20	24.897	40.218	-9.864	1.00	0.23	1SG	165
	ATOM	165	O	GLU	20	24.122	39.806	-9.001	1.00	0.23	1SG	166
	ATOM	166	N	ASN	21	26.181	39.822	-9.930	1.00	0.16	1SG	167
30	ATOM	167	CA	ASN	21	26.694	38.898	-8.965	1.00	0.16	1SG	168
	ATOM	168	CB	ASN	21	27.686	37.880	-9.553	1.00	0.16	1SG	169
	ATOM	169	CG	ASN	21	26.895	36.971	-10.481	1.00	0.16	1SG	170
	ATOM	170	OD1	ASN	21	25.671	36.909	-10.394	1.00	0.16	1SG	171
	ATOM	171	ND2	ASN	21	27.602	36.251	-11.392	1.00	0.16	1SG	172
35	ATOM	172	C	ASN	21	27.415	39.694	-7.933	1.00	0.16	1SG	173
	ATOM	173	O	ASN	21	28.121	40.652	-8.246	1.00	0.16	1SG	174
	ATOM	174	N	VAL	22	27.217	39.327	-6.654	1.00	0.07	1SG	175
	ATOM	175	CA	VAL	22	27.876	40.026	-5.596	1.00	0.07	1SG	176
	ATOM	176	CB	VAL	22	26.922	40.670	-4.632	1.00	0.07	1SG	177
40	ATOM	177	CG1	VAL	22	27.727	41.288	-3.478	1.00	0.07	1SG	178
	ATOM	178	CG2	VAL	22	26.056	41.681	-5.405	1.00	0.07	1SG	179
	ATOM	179	C	VAL	22	28.661	39.015	-4.836	1.00	0.07	1SG	180
	ATOM	180	O	VAL	22	28.186	37.907	-4.590	1.00	0.07	1SG	181
	ATOM	181	N	THR	23	29.908	39.362	-4.469	1.00	0.06	1SG	182
45	ATOM	182	CA	THR	23	30.692	38.440	-3.706	1.00	0.06	1SG	183
	ATOM	183	CB	THR	23	31.980	38.047	-4.368	1.00	0.06	1SG	184
	ATOM	184	OG1	THR	23	31.714	37.430	-5.619	1.00	0.06	1SG	185
	ATOM	185	CG2	THR	23	32.727	37.067	-3.446	1.00	0.06	1SG	186
	ATOM	186	C	THR	23	31.044	39.117	-2.425	1.00	0.06	1SG	187
50	ATOM	187	O	THR	23	31.577	40.225	-2.418	1.00	0.06	1SG	188
	ATOM	188	N	LEU	24	30.731	38.460	-1.295	1.00	0.06	1SG	189
	ATOM	189	CA	LEU	24	31.057	39.021	-0.020	1.00	0.06	1SG	190
	ATOM	190	CB	LEU	24	29.871	39.048	0.956	1.00	0.06	1SG	191
	ATOM	191	CG	LEU	24	28.702	39.930	0.479	1.00	0.06	1SG	192
55	ATOM	192	CD2	LEU	24	29.182	41.346	0.123	1.00	0.06	1SG	193
	ATOM	193	CD1	LEU	24	27.548	39.924	1.495	1.00	0.06	1SG	194
	ATOM	194	C	LEU	24	32.076	38.112	0.572	1.00	0.06	1SG	195
	ATOM	195	O	LEU	24	31.886	36.898	0.615	1.00	0.06	1SG	196
	ATOM	196	N	THR	25	33.206	38.678	1.030	1.00	0.28	1SG	197
60	ATOM	197	CA	THR	25	34.202	37.838	1.616	1.00	0.28	1SG	198
	ATOM	198	CB	THR	25	35.507	37.852	0.876	1.00	0.28	1SG	199
	ATOM	199	OG1	THR	25	35.319	37.412	-0.461	1.00	0.28	1SG	200
	ATOM	200	CG2	THR	25	36.496	36.927	1.605	1.00	0.28	1SG	201
	ATOM	201	C	THR	25	34.460	38.367	2.979	1.00	0.28	1SG	202
65	ATOM	202	O	THR	25	34.579	39.572	3.187	1.00	0.28	1SG	203
	ATOM	203	N	CYS	26	34.543	37.462	3.960	1.00	0.52	1SG	204
	ATOM	204	CA	CYS	26	34.770	37.922	5.286	1.00	0.52	1SG	205
	ATOM	205	CB	CYS	26	33.724	37.332	6.226	1.00	0.52	1SG	206
	ATOM	206	SG	CYS	26	33.905	37.844	7.940	1.00	0.52	1SG	207
70	ATOM	207	C	CYS	26	36.111	37.410	5.681	1.00	0.52	1SG	208
	ATOM	208	O	CYS	26	36.327	36.201	5.748	1.00	0.52	1SG	209
	ATOM	209	N	ASN	27	37.050	38.332	5.961	1.00	0.35	1SG	210

136

	ATOM	210	CA	ASN	27	38.377	37.918	6.298	1.00	0.35	1SG 211
	ATOM	211	CB	ASN	27	39.472	38.673	5.527	1.00	0.35	1SG 212
	ATOM	212	CG	ASN	27	39.389	40.140	5.927	1.00	0.35	1SG 213
	ATOM	213	OD1	ASN	27	38.320	40.747	5.897	1.00	0.35	1SG 214
5	ATOM	214	ND2	ASN	27	40.549	40.726	6.326	1.00	0.35	1SG 215
	ATOM	215	C	ASN	27	38.595	38.211	7.743	1.00	0.35	1SG 216
	ATOM	216	O	ASN	27	37.972	39.107	8.310	1.00	0.35	1SG 217
	ATOM	217	N	GLY	28	39.483	37.427	8.381	1.00	0.15	1SG 218
	ATOM	218	CA	GLY	28	39.779	37.636	9.765	1.00	0.15	1SG 219
10	ATOM	219	C	GLY	28	40.251	36.330	10.306	1.00	0.15	1SG 220
	ATOM	220	O	GLY	28	40.302	35.333	9.587	1.00	0.15	1SG 221
	ATOM	221	N	ASN	29	40.604	36.299	11.606	1.00	0.16	1SG 222
	ATOM	222	CA	ASN	29	41.053	35.065	12.173	1.00	0.16	1SG 223
	ATOM	223	CB	ASN	29	41.554	35.176	13.624	1.00	0.16	1SG 224
15	ATOM	224	CG	ASN	29	42.895	35.895	13.621	1.00	0.16	1SG 225
	ATOM	225	OD1	ASN	29	43.494	36.131	12.573	1.00	0.16	1SG 226
	ATOM	226	ND2	ASN	29	43.391	36.241	14.838	1.00	0.16	1SG 227
	ATOM	227	C	ASN	29	39.883	34.143	12.168	1.00	0.16	1SG 228
	ATOM	228	O	ASN	29	38.741	34.566	12.336	1.00	0.16	1SG 229
20	ATOM	229	N	ASN	30	40.148	32.843	11.949	1.00	0.16	1SG 230
	ATOM	230	CA	ASN	30	39.080	31.893	11.889	1.00	0.16	1SG 231
	ATOM	231	CB	ASN	30	38.855	31.359	10.468	1.00	0.16	1SG 232
	ATOM	232	CG	ASN	30	37.718	30.355	10.511	1.00	0.16	1SG 233
	ATOM	233	OD1	ASN	30	36.716	30.535	11.200	1.00	0.16	1SG 234
25	ATOM	234	ND2	ASN	30	37.899	29.239	9.758	1.00	0.16	1SG 235
	ATOM	235	C	ASN	30	39.436	30.721	12.744	1.00	0.16	1SG 236
	ATOM	236	O	ASN	30	40.609	30.390	12.909	1.00	0.16	1SG 237
	ATOM	237	N	PHE	31	38.409	30.073	13.332	1.00	0.12	1SG 238
	ATOM	238	CA	PHE	31	38.628	28.899	14.123	1.00	0.12	1SG 239
30	ATOM	239	CB	PHE	31	37.510	28.639	15.146	1.00	0.12	1SG 240
	ATOM	240	CG	PHE	31	37.857	27.404	15.902	1.00	0.12	1SG 241
	ATOM	241	CD1	PHE	31	38.774	27.447	16.927	1.00	0.12	1SG 242
	ATOM	242	CD2	PHE	31	37.260	26.205	15.592	1.00	0.12	1SG 243
	ATOM	243	CE1	PHE	31	39.092	26.310	17.631	1.00	0.12	1SG 244
35	ATOM	244	CE2	PHE	31	37.575	25.064	16.292	1.00	0.12	1SG 245
	ATOM	245	CZ	PHE	31	38.495	25.115	17.312	1.00	0.12	1SG 246
	ATOM	246	C	PHE	31	38.639	27.765	13.155	1.00	0.12	1SG 247
	ATOM	247	O	PHE	31	38.118	27.888	12.049	1.00	0.12	1SG 248
	ATOM	248	N	PHE	32	39.248	26.626	13.528	1.00	0.11	1SG 249
40	ATOM	249	CA	PHE	32	39.265	25.565	12.570	1.00	0.11	1SG 250
	ATOM	250	CB	PHE	32	40.426	24.579	12.773	1.00	0.11	1SG 251
	ATOM	251	CG	PHE	32	41.663	25.381	12.563	1.00	0.11	1SG 252
	ATOM	252	CD1	PHE	32	42.195	26.109	13.602	1.00	0.11	1SG 253
	ATOM	253	CD2	PHE	32	42.284	25.417	11.337	1.00	0.11	1SG 254
45	ATOM	254	CE1	PHE	32	43.335	26.857	13.428	1.00	0.11	1SG 255
	ATOM	255	CE2	PHE	32	43.424	26.164	11.157	1.00	0.11	1SG 256
	ATOM	256	CZ	PHE	32	43.952	26.885	12.201	1.00	0.11	1SG 257
	ATOM	257	C	PHE	32	37.980	24.827	12.710	1.00	0.11	1SG 258
	ATOM	258	O	PHE	32	37.879	23.858	13.460	1.00	0.11	1SG 259
50	ATOM	259	N	GLU	33	36.949	25.287	11.977	1.00	0.10	1SG 260
	ATOM	260	CA	GLU	33	35.673	24.643	12.038	1.00	0.10	1SG 261
	ATOM	261	CB	GLU	33	34.682	25.327	12.994	1.00	0.10	1SG 262
	ATOM	262	CG	GLU	33	34.364	26.773	12.610	1.00	0.10	1SG 263
	ATOM	263	CD	GLU	33	33.383	27.314	13.638	1.00	0.10	1SG 264
55	ATOM	264	OE1	GLU	33	32.437	26.565	13.999	1.00	0.10	1SG 265
	ATOM	265	OE2	GLU	33	33.567	28.481	14.077	1.00	0.10	1SG 266
	ATOM	266	C	GLU	33	35.076	24.698	10.672	1.00	0.10	1SG 267
	ATOM	267	O	GLU	33	35.453	25.532	9.849	1.00	0.10	1SG 268
	ATOM	268	N	VAL	34	34.130	23.784	10.391	1.00	0.09	1SG 269
60	ATOM	269	CA	VAL	34	33.509	23.763	9.103	1.00	0.09	1SG 270
	ATOM	270	CB	VAL	34	32.562	22.612	8.943	1.00	0.09	1SG 271
	ATOM	271	CG1	VAL	34	31.945	22.676	7.538	1.00	0.09	1SG 272
	ATOM	272	CG2	VAL	34	33.335	21.310	9.215	1.00	0.09	1SG 273
	ATOM	273	C	VAL	34	32.742	25.032	8.926	1.00	0.09	1SG 274
65	ATOM	274	O	VAL	34	32.854	25.693	7.895	1.00	0.09	1SG 275
	ATOM	275	N	SER	35	31.953	25.431	9.942	1.00	0.11	1SG 276
	ATOM	276	CA	SER	35	31.202	26.645	9.800	1.00	0.11	1SG 277
	ATOM	277	CB	SER	35	29.838	26.613	10.522	1.00	0.11	1SG 278
	ATOM	278	OG	SER	35	30.011	26.400	11.915	1.00	0.11	1SG 279
70	ATOM	279	C	SER	35	32.033	27.743	10.378	1.00	0.11	1SG 280
	ATOM	280	O	SER	35	31.856	28.153	11.524	1.00	0.11	1SG 281

	ATOM	281	N	SER	36	32.974	28.249	9.563	1.00	0.27	1SG 282
	ATOM	282	CA	SER	36	33.906	29.251	9.984	1.00	0.27	1SG 283
	ATOM	283	CB	SER	36	34.962	29.539	8.905	1.00	0.27	1SG 284
5	ATOM	284	OG	SER	36	35.648	28.343	8.571	1.00	0.27	1SG 285
	ATOM	285	C	SER	36	33.204	30.541	10.256	1.00	0.27	1SG 286
	ATOM	286	O	SER	36	33.439	31.186	11.277	1.00	0.27	1SG 287
	ATOM	287	N	THR	37	32.290	30.954	9.360	1.00	0.48	1SG 288
	ATOM	288	CA	THR	37	31.752	32.266	9.550	1.00	0.48	1SG 289
10	ATOM	289	CB	THR	37	32.132	33.216	8.462	1.00	0.48	1SG 290
	ATOM	290	OG1	THR	37	31.579	34.490	8.737	1.00	0.48	1SG 291
	ATOM	291	CG2	THR	37	31.591	32.685	7.124	1.00	0.48	1SG 292
	ATOM	292	C	THR	37	30.265	32.253	9.596	1.00	0.48	1SG 293
	ATOM	293	O	THR	37	29.607	31.337	9.105	1.00	0.48	1SG 294
15	ATOM	294	N	LYS	38	29.708	33.307	10.225	1.00	0.41	1SG 295
	ATOM	295	CA	LYS	38	28.291	33.482	10.294	1.00	0.41	1SG 296
	ATOM	296	CB	LYS	38	27.770	33.754	11.715	1.00	0.41	1SG 297
	ATOM	297	CG	LYS	38	28.245	32.739	12.757	1.00	0.41	1SG 298
	ATOM	298	CD	LYS	38	29.734	32.877	13.087	1.00	0.41	1SG 299
	ATOM	299	CE	LYS	38	30.193	32.030	14.276	1.00	0.41	1SG 300
20	ATOM	300	NZ	LYS	38	31.621	32.301	14.565	1.00	0.41	1SG 301
	ATOM	301	C	LYS	38	28.013	34.720	9.506	1.00	0.41	1SG 302
	ATOM	302	O	LYS	38	28.709	35.726	9.652	1.00	0.41	1SG 303
	ATOM	303	N	TRP	39	26.998	34.677	8.624	1.00	0.18	1SG 304
25	ATOM	304	CA	TRP	39	26.680	35.852	7.870	1.00	0.18	1SG 305
	ATOM	305	CB	TRP	39	26.599	35.645	6.344	1.00	0.18	1SG 306
	ATOM	306	CG	TRP	39	27.940	35.495	5.663	1.00	0.18	1SG 307
	ATOM	307	CD2	TRP	39	28.804	36.606	5.377	1.00	0.18	1SG 308
	ATOM	308	CD1	TRP	39	28.585	34.378	5.220	1.00	0.18	1SG 309
	ATOM	309	NE1	TRP	39	29.800	34.725	4.672	1.00	0.18	1SG 310
30	ATOM	310	CE2	TRP	39	29.947	36.094	4.764	1.00	0.18	1SG 311
	ATOM	311	CE3	TRP	39	28.656	37.943	5.611	1.00	0.18	1SG 312
	ATOM	312	CZ2	TRP	39	30.964	36.918	4.374	1.00	0.18	1SG 313
	ATOM	313	CZ3	TRP	39	29.681	38.772	5.214	1.00	0.18	1SG 314
	ATOM	314	CH2	TRP	39	30.813	38.269	4.607	1.00	0.18	1SG 315
35	ATOM	315	C	TRP	39	25.345	36.329	8.319	1.00	0.18	1SG 316
	ATOM	316	O	TRP	39	24.473	35.536	8.668	1.00	0.18	1SG 317
	ATOM	317	N	PHE	40	25.166	37.662	8.355	1.00	0.08	1SG 318
	ATOM	318	CA	PHE	40	23.898	38.177	8.759	1.00	0.08	1SG 319
40	ATOM	319	CB	PHE	40	23.942	38.924	10.102	1.00	0.08	1SG 320
	ATOM	320	CG	PHE	40	24.268	37.911	11.142	1.00	0.08	1SG 321
	ATOM	321	CD1	PHE	40	25.575	37.560	11.393	1.00	0.08	1SG 322
	ATOM	322	CD2	PHE	40	23.262	37.311	11.865	1.00	0.08	1SG 323
	ATOM	323	CE1	PHE	40	25.872	36.623	12.352	1.00	0.08	1SG 324
45	ATOM	324	CE2	PHE	40	23.555	36.372	12.826	1.00	0.08	1SG 325
	ATOM	325	CZ	PHE	40	24.863	36.028	13.071	1.00	0.08	1SG 326
	ATOM	326	C	PHE	40	23.449	39.146	7.721	1.00	0.08	1SG 327
	ATOM	327	O	PHE	40	24.243	39.920	7.189	1.00	0.08	1SG 328
	ATOM	328	N	HIS	41	22.150	39.090	7.382	1.00	0.10	1SG 329
50	ATOM	329	CA	HIS	41	21.589	40.033	6.468	1.00	0.10	1SG 330
	ATOM	330	ND1	HIS	41	19.882	40.132	3.044	1.00	0.10	1SG 331
	ATOM	331	CG	HIS	41	20.491	40.427	4.242	1.00	0.10	1SG 332
	ATOM	332	CB	HIS	41	20.942	39.397	5.232	1.00	0.10	1SG 333
	ATOM	333	NE2	HIS	41	20.036	42.349	3.153	1.00	0.10	1SG 334
55	ATOM	334	CD2	HIS	41	20.577	41.784	4.294	1.00	0.10	1SG 335
	ATOM	335	CE1	HIS	41	19.631	41.317	2.434	1.00	0.10	1SG 336
	ATOM	336	C	HIS	41	20.508	40.722	7.226	1.00	0.10	1SG 337
	ATOM	337	O	HIS	41	19.557	40.090	7.682	1.00	0.10	1SG 338
	ATOM	338	N	ASN	42	20.632	42.049	7.386	1.00	0.11	1SG 339
60	ATOM	339	CA	ASN	42	19.651	42.772	8.132	1.00	0.11	1SG 340
	ATOM	340	CB	ASN	42	18.252	42.764	7.489	1.00	0.11	1SG 341
	ATOM	341	CG	ASN	42	18.291	43.691	6.283	1.00	0.11	1SG 342
	ATOM	342	OD1	ASN	42	19.275	44.395	6.062	1.00	0.11	1SG 343
	ATOM	343	ND2	ASN	42	17.185	43.710	5.492	1.00	0.11	1SG 344
65	ATOM	344	C	ASN	42	19.566	42.155	9.490	1.00	0.11	1SG 345
	ATOM	345	O	ASN	42	18.525	42.200	10.144	1.00	0.11	1SG 346
	ATOM	346	N	GLY	43	20.683	41.567	9.955	1.00	0.08	1SG 347
	ATOM	347	CA	GLY	43	20.714	41.014	11.277	1.00	0.08	1SG 348
	ATOM	348	C	GLY	43	20.172	39.620	11.264	1.00	0.08	1SG 349
	ATOM	349	O	GLY	43	20.036	39.001	12.318	1.00	0.08	1SG 350
70	ATOM	350	N	SER	44	19.844	39.074	10.079	1.00	0.15	1SG 351
	ATOM	351	CA	SER	44	19.330	37.735	10.068	1.00	0.15	1SG 352

138

	ATOM	352	CB	SER	44	18.218	37.498	9.034	1.00	0.15	1SG 353
	ATOM	353	OG	SER	44	18.737	37.641	7.720	1.00	0.15	1SG 354
	ATOM	354	C	SER	44	20.464	36.832	9.717	1.00	0.15	1SG 355
5	ATOM	355	O	SER	44	21.203	37.085	8.769	1.00	0.15	1SG 356
	ATOM	356	N	LEU	45	20.638	35.747	10.491	1.00	0.35	1SG 357
	ATOM	357	CA	LEU	45	21.720	34.843	10.241	1.00	0.35	1SG 358
	ATOM	358	CB	LEU	45	21.939	33.852	11.413	1.00	0.35	1SG 359
	ATOM	359	CG	LEU	45	23.091	32.823	11.298	1.00	0.35	1SG 360
10	ATOM	360	CD2	LEU	45	22.938	31.865	10.100	1.00	0.35	1SG 361
	ATOM	361	CD1	LEU	45	23.226	32.022	12.602	1.00	0.35	1SG 362
	ATOM	362	C	LEU	45	21.398	34.097	8.988	1.00	0.35	1SG 363
	ATOM	363	O	LEU	45	20.249	33.736	8.740	1.00	0.35	1SG 364
	ATOM	364	N	SER	46	22.430	33.863	8.153	1.00	0.48	1SG 365
	ATOM	365	CA	SER	46	22.263	33.118	6.938	1.00	0.48	1SG 366
15	ATOM	366	CB	SER	46	22.957	33.730	5.707	1.00	0.48	1SG 367
	ATOM	367	OG	SER	46	22.355	34.958	5.334	1.00	0.48	1SG 368
	ATOM	368	C	SER	46	22.960	31.813	7.135	1.00	0.48	1SG 369
	ATOM	369	O	SER	46	24.137	31.770	7.487	1.00	0.48	1SG 370
20	ATOM	370	N	GLU	47	22.221	30.711	6.936	1.00	0.44	1SG 371
	ATOM	371	CA	GLU	47	22.724	29.371	7.017	1.00	0.44	1SG 372
	ATOM	372	CB	GLU	47	21.604	28.321	7.026	1.00	0.44	1SG 373
	ATOM	373	CG	GLU	47	20.768	28.350	5.745	1.00	0.44	1SG 374
	ATOM	374	CD	GLU	47	19.700	27.272	5.839	1.00	0.44	1SG 375
	ATOM	375	OE1	GLU	47	19.539	26.690	6.945	1.00	0.44	1SG 376
25	ATOM	376	OE2	GLU	47	19.030	27.016	4.803	1.00	0.44	1SG 377
	ATOM	377	C	GLU	47	23.552	29.092	5.800	1.00	0.44	1SG 378
	ATOM	378	O	GLU	47	24.413	28.215	5.800	1.00	0.44	1SG 379
	ATOM	379	N	GLU	48	23.288	29.858	4.730	1.00	0.45	1SG 380
30	ATOM	380	CA	GLU	48	23.741	29.635	3.387	1.00	0.45	1SG 381
	ATOM	381	CB	GLU	48	23.284	30.775	2.465	1.00	0.45	1SG 382
	ATOM	382	CG	GLU	48	23.798	32.140	2.929	1.00	0.45	1SG 383
	ATOM	383	CD	GLU	48	23.187	33.215	2.041	1.00	0.45	1SG 384
	ATOM	384	OE1	GLU	48	22.440	32.852	1.094	1.00	0.45	1SG 385
	ATOM	385	OE2	GLU	48	23.459	34.417	2.302	1.00	0.45	1SG 386
35	ATOM	386	C	GLU	48	25.226	29.496	3.195	1.00	0.45	1SG 387
	ATOM	387	O	GLU	48	25.647	28.553	2.528	1.00	0.45	1SG 388
	ATOM	388	N	THR	49	26.087	30.365	3.758	1.00	0.55	1SG 389
	ATOM	389	CA	THR	49	27.427	30.251	3.247	1.00	0.55	1SG 390
40	ATOM	390	CB	THR	49	27.684	31.331	2.235	1.00	0.55	1SG 391
	ATOM	391	OG1	THR	49	28.936	31.166	1.589	1.00	0.55	1SG 392
	ATOM	392	CG2	THR	49	27.629	32.679	2.968	1.00	0.55	1SG 393
	ATOM	393	C	THR	49	28.482	30.361	4.310	1.00	0.55	1SG 394
	ATOM	394	O	THR	49	28.213	30.658	5.473	1.00	0.55	1SG 395
45	ATOM	395	N	ASN	50	29.736	30.090	3.881	1.00	0.44	1SG 396
	ATOM	396	CA	ASN	50	30.937	30.109	4.665	1.00	0.44	1SG 397
	ATOM	397	CB	ASN	50	31.925	28.990	4.291	1.00	0.44	1SG 398
	ATOM	398	CG	ASN	50	31.335	27.665	4.747	1.00	0.44	1SG 399
	ATOM	399	OD1	ASN	50	31.044	27.481	5.927	1.00	0.44	1SG 400
50	ATOM	400	ND2	ASN	50	31.153	26.715	3.790	1.00	0.44	1SG 401
	ATOM	401	C	ASN	50	31.648	31.407	4.437	1.00	0.44	1SG 402
	ATOM	402	O	ASN	50	31.038	32.472	4.355	1.00	0.44	1SG 403
	ATOM	403	N	SER	51	32.990	31.325	4.329	1.00	0.25	1SG 404
	ATOM	404	CA	SER	51	33.843	32.473	4.237	1.00	0.25	1SG 405
55	ATOM	405	CB	SER	51	35.323	32.099	4.049	1.00	0.25	1SG 406
	ATOM	406	OG	SER	51	35.506	31.465	2.792	1.00	0.25	1SG 407
	ATOM	407	C	SER	51	33.455	33.328	3.073	1.00	0.25	1SG 408
	ATOM	408	O	SER	51	33.338	34.545	3.215	1.00	0.25	1SG 409
	ATOM	409	N	SER	52	33.234	32.733	1.887	1.00	0.14	1SG 410
60	ATOM	410	CA	SER	52	32.906	33.575	0.772	1.00	0.14	1SG 411
	ATOM	411	CB	SER	52	33.750	33.288	-0.481	1.00	0.14	1SG 412
	ATOM	412	OG	SER	52	35.116	33.578	-0.227	1.00	0.14	1SG 413
	ATOM	413	C	SER	52	31.480	33.343	0.406	1.00	0.14	1SG 414
	ATOM	414	O	SER	52	31.035	32.204	0.274	1.00	0.14	1SG 415
65	ATOM	415	N	LEU	53	30.709	34.437	0.251	1.00	0.09	1SG 416
	ATOM	416	CA	LEU	53	29.346	34.271	-0.150	1.00	0.09	1SG 417
	ATOM	417	CB	LEU	53	28.319	34.889	0.816	1.00	0.09	1SG 418
	ATOM	418	CG	LEU	53	26.856	34.696	0.368	1.00	0.09	1SG 419
	ATOM	419	CD2	LEU	53	25.893	35.495	1.259	1.00	0.09	1SG 420
70	ATOM	420	CD1	LEU	53	26.482	33.208	0.298	1.00	0.09	1SG 421
	ATOM	421	C	LEU	53	29.195	34.941	-1.473	1.00	0.09	1SG 422
	ATOM	422	O	LEU	53	29.476	36.130	-1.619	1.00	0.09	1SG 423

139

	ATOM	423	N	ASN	54	28.760	34.174	-2.488	1.00	0.09	1SG 424
	ATOM	424	CA	ASN	54	28.584	34.749	-3.786	1.00	0.09	1SG 425
	ATOM	425	CB	ASN	54	29.349	34.011	-4.897	1.00	0.09	1SG 426
	ATOM	426	CG	ASN	54	29.234	34.837	-6.169	1.00	0.09	1SG 427
5	ATOM	427	OD1	ASN	54	28.770	35.975	-6.145	1.00	0.09	1SG 428
	ATOM	428	ND2	ASN	54	29.658	34.244	-7.317	1.00	0.09	1SG 429
	ATOM	429	C	ASN	54	27.137	34.629	-4.118	1.00	0.09	1SG 430
	ATOM	430	O	ASN	54	26.544	33.562	-3.972	1.00	0.09	1SG 431
10	ATOM	431	N	ILE	55	26.522	35.736	-4.566	1.00	0.08	1SG 432
	ATOM	432	CA	ILE	55	25.141	35.665	-4.922	1.00	0.08	1SG 433
	ATOM	433	CB	ILE	55	24.258	36.575	-4.120	1.00	0.08	1SG 434
	ATOM	434	CG2	ILE	55	24.346	36.152	-2.644	1.00	0.08	1SG 435
	ATOM	435	CG1	ILE	55	24.636	38.044	-4.369	1.00	0.08	1SG 436
	ATOM	436	CD1	ILE	55	23.600	39.030	-3.832	1.00	0.08	1SG 437
15	ATOM	437	C	ILE	55	25.039	36.115	-6.337	1.00	0.08	1SG 438
	ATOM	438	O	ILE	55	25.773	36.998	-6.779	1.00	0.08	1SG 439
	ATOM	439	N	VAL	56	24.119	35.493	-7.090	1.00	0.10	1SG 440
	ATOM	440	CA	VAL	56	23.922	35.858	-8.456	1.00	0.10	1SG 441
	ATOM	441	CB	VAL	56	23.985	34.683	-9.389	1.00	0.10	1SG 442
20	ATOM	442	CG1	VAL	56	23.615	35.140	-10.810	1.00	0.10	1SG 443
	ATOM	443	CG2	VAL	56	25.383	34.050	-9.280	1.00	0.10	1SG 444
	ATOM	444	C	VAL	56	22.544	36.412	-8.532	1.00	0.10	1SG 445
	ATOM	445	O	VAL	56	21.686	36.071	-7.719	1.00	0.10	1SG 446
	ATOM	446	N	ASN	57	22.312	37.292	-9.523	1.00	0.11	1SG 447
25	ATOM	447	CA	ASN	57	21.035	37.906	-9.706	1.00	0.11	1SG 448
	ATOM	448	CB	ASN	57	19.953	36.958	-10.250	1.00	0.11	1SG 449
	ATOM	449	CG	ASN	57	18.801	37.822	-10.747	1.00	0.11	1SG 450
	ATOM	450	OD1	ASN	57	18.420	38.801	-10.107	1.00	0.11	1SG 451
	ATOM	451	ND2	ASN	57	18.239	37.461	-11.932	1.00	0.11	1SG 452
30	ATOM	452	C	ASN	57	20.576	38.473	-8.404	1.00	0.11	1SG 453
	ATOM	453	O	ASN	57	19.548	38.066	-7.865	1.00	0.11	1SG 454
	ATOM	454	N	ALA	58	21.353	39.425	-7.850	1.00	0.21	1SG 455
	ATOM	455	CA	ALA	58	20.945	40.022	-6.615	1.00	0.21	1SG 456
	ATOM	456	CB	ALA	58	21.884	41.136	-6.118	1.00	0.21	1SG 457
35	ATOM	457	C	ALA	58	19.608	40.631	-6.871	1.00	0.21	1SG 458
	ATOM	458	O	ALA	58	19.393	41.275	-7.897	1.00	0.21	1SG 459
	ATOM	459	N	LYS	59	18.660	40.414	-5.941	1.00	0.31	1SG 460
	ATOM	460	CA	LYS	59	17.329	40.910	-6.123	1.00	0.31	1SG 461
	ATOM	461	CB	LYS	59	16.237	39.929	-5.664	1.00	0.31	1SG 462
40	ATOM	462	CG	LYS	59	16.172	38.657	-6.511	1.00	0.31	1SG 463
	ATOM	463	CD	LYS	59	15.844	38.913	-7.985	1.00	0.31	1SG 464
	ATOM	464	CE	LYS	59	15.812	37.638	-8.834	1.00	0.31	1SG 465
	ATOM	465	NZ	LYS	59	15.485	37.972	-10.239	1.00	0.31	1SG 466
	ATOM	466	C	LYS	59	17.157	42.162	-5.331	1.00	0.31	1SG 467
45	ATOM	467	O	LYS	59	18.068	42.622	-4.645	1.00	0.31	1SG 468
	ATOM	468	N	PHE	60	15.948	42.746	-5.431	1.00	0.23	1SG 469
	ATOM	469	CA	PHE	60	15.595	43.928	-4.704	1.00	0.23	1SG 470
	ATOM	470	CB	PHE	60	14.165	44.410	-4.999	1.00	0.23	1SG 471
	ATOM	471	CG	PHE	60	13.854	45.482	-4.011	1.00	0.23	1SG 472
50	ATOM	472	CD1	PHE	60	14.289	46.773	-4.202	1.00	0.23	1SG 473
	ATOM	473	CD2	PHE	60	13.119	45.189	-2.885	1.00	0.23	1SG 474
	ATOM	474	CE1	PHE	60	13.998	47.753	-3.282	1.00	0.23	1SG 475
	ATOM	475	CE2	PHE	60	12.825	46.165	-1.962	1.00	0.23	1SG 476
	ATOM	476	CZ	PHE	60	13.264	47.451	-2.161	1.00	0.23	1SG 477
55	ATOM	477	C	PHE	60	15.656	43.581	-3.255	1.00	0.23	1SG 478
	ATOM	478	O	PHE	60	16.056	44.387	-2.417	1.00	0.23	1SG 479
	ATOM	479	N	GLU	61	15.265	42.337	-2.942	1.00	0.15	1SG 480
	ATOM	480	CA	GLU	61	15.215	41.816	-1.609	1.00	0.15	1SG 481
	ATOM	481	CB	GLU	61	14.699	40.370	-1.604	1.00	0.15	1SG 482
60	ATOM	482	CG	GLU	61	15.521	39.448	-2.507	1.00	0.15	1SG 483
	ATOM	483	CD	GLU	61	14.713	38.185	-2.765	1.00	0.15	1SG 484
	ATOM	484	OE1	GLU	61	14.026	37.714	-1.820	1.00	0.15	1SG 485
	ATOM	485	OE2	GLU	61	14.761	37.681	-3.919	1.00	0.15	1SG 486
	ATOM	486	C	GLU	61	16.595	41.837	-1.028	1.00	0.15	1SG 487
65	ATOM	487	O	GLU	61	16.769	42.050	0.170	1.00	0.15	1SG 488
	ATOM	488	N	ASP	62	17.618	41.636	-1.877	1.00	0.16	1SG 489
	ATOM	489	CA	ASP	62	18.983	41.538	-1.440	1.00	0.16	1SG 490
	ATOM	490	CB	ASP	62	19.962	41.211	-2.582	1.00	0.16	1SG 491
	ATOM	491	CG	ASP	62	19.751	39.749	-2.954	1.00	0.16	1SG 492
70	ATOM	492	OD1	ASP	62	18.944	39.075	-2.259	1.00	0.16	1SG 493
	ATOM	493	OD2	ASP	62	20.401	39.282	-3.927	1.00	0.16	1SG 494

140

	ATOM	494	C	ASP	62	19.437	42.801	-0.773	1.00	0.16	1SG	495
	ATOM	495	O	ASP	62	20.299	42.749	0.100	1.00	0.16	1SG	496
	ATOM	496	N	SER	63	18.904	43.974	-1.168	1.00	0.20	1SG	497
5	ATOM	497	CA	SER	63	19.352	45.201	-0.565	1.00	0.20	1SG	498
	ATOM	498	CB	SER	63	18.578	46.439	-1.050	1.00	0.20	1SG	499
	ATOM	499	OG	SER	63	17.217	46.346	-0.655	1.00	0.20	1SG	500
	ATOM	500	C	SER	63	19.192	45.109	0.923	1.00	0.20	1SG	501
	ATOM	501	O	SER	63	18.201	44.586	1.430	1.00	0.20	1SG	502
10	ATOM	502	N	GLY	64	20.203	45.609	1.665	1.00	0.22	1SG	503
	ATOM	503	CA	GLY	64	20.164	45.561	3.098	1.00	0.22	1SG	504
	ATOM	504	C	GLY	64	21.570	45.701	3.585	1.00	0.22	1SG	505
	ATOM	505	O	GLY	64	22.472	46.032	2.817	1.00	0.22	1SG	506
	ATOM	506	N	GLU	65	21.792	45.447	4.892	1.00	0.19	1SG	507
	ATOM	507	CA	GLU	65	23.115	45.557	5.436	1.00	0.19	1SG	508
15	ATOM	508	CB	GLU	65	23.191	46.214	6.825	1.00	0.19	1SG	509
	ATOM	509	CG	GLU	65	22.869	47.707	6.845	1.00	0.19	1SG	510
	ATOM	510	CD	GLU	65	23.123	48.205	8.262	1.00	0.19	1SG	511
	ATOM	511	OE1	GLU	65	22.725	47.496	9.225	1.00	0.19	1SG	512
20	ATOM	512	OE2	GLU	65	23.734	49.299	8.401	1.00	0.19	1SG	513
	ATOM	513	C	GLU	65	23.647	44.176	5.620	1.00	0.19	1SG	514
	ATOM	514	O	GLU	65	22.902	43.245	5.925	1.00	0.19	1SG	515
	ATOM	515	N	TYR	66	24.970	44.009	5.422	1.00	0.22	1SG	516
	ATOM	516	CA	TYR	66	25.570	42.720	5.594	1.00	0.22	1SG	517
25	ATOM	517	CB	TYR	66	26.312	42.202	4.348	1.00	0.22	1SG	518
	ATOM	518	CG	TYR	66	25.308	41.992	3.266	1.00	0.22	1SG	519
	ATOM	519	CD1	TYR	66	24.943	43.031	2.440	1.00	0.22	1SG	520
	ATOM	520	CD2	TYR	66	24.726	40.759	3.079	1.00	0.22	1SG	521
	ATOM	521	CE1	TYR	66	24.019	42.842	1.440	1.00	0.22	1SG	522
30	ATOM	522	CE2	TYR	66	23.800	40.563	2.081	1.00	0.22	1SG	523
	ATOM	523	CZ	TYR	66	23.446	41.606	1.260	1.00	0.22	1SG	524
	ATOM	524	OH	TYR	66	22.497	41.407	0.236	1.00	0.22	1SG	525
	ATOM	525	C	TYR	66	26.580	42.828	6.692	1.00	0.22	1SG	526
	ATOM	526	O	TYR	66	27.258	43.845	6.835	1.00	0.22	1SG	527
35	ATOM	527	N	LYS	67	26.683	41.768	7.516	1.00	0.45	1SG	528
	ATOM	528	CA	LYS	67	27.618	41.753	8.602	1.00	0.45	1SG	529
	ATOM	529	CB	LYS	67	26.953	42.023	9.958	1.00	0.45	1SG	530
	ATOM	530	CG	LYS	67	26.340	43.420	10.055	1.00	0.45	1SG	531
	ATOM	531	CD	LYS	67	25.324	43.562	11.188	1.00	0.45	1SG	532
40	ATOM	532	CE	LYS	67	23.974	42.913	10.871	1.00	0.45	1SG	533
	ATOM	533	NZ	LYS	67	23.325	43.628	9.750	1.00	0.45	1SG	534
	ATOM	534	C	LYS	67	28.183	40.371	8.662	1.00	0.45	1SG	535
	ATOM	535	O	LYS	67	27.569	39.421	8.180	1.00	0.45	1SG	536
	ATOM	536	N	CYS	68	29.390	40.228	9.244	1.00	0.52	1SG	537
45	ATOM	537	CA	CYS	68	30.003	38.935	9.333	1.00	0.52	1SG	538
	ATOM	538	CB	CYS	68	31.059	38.703	8.250	1.00	0.52	1SG	539
	ATOM	539	SG	CYS	68	32.113	37.291	8.666	1.00	0.52	1SG	540
	ATOM	540	C	CYS	68	30.754	38.840	10.621	1.00	0.52	1SG	541
	ATOM	541	O	CYS	68	31.295	39.830	11.110	1.00	0.52	1SG	542
50	ATOM	542	N	GLN	69	30.796	37.631	11.218	1.00	0.27	1SG	543
	ATOM	543	CA	GLN	69	31.610	37.462	12.382	1.00	0.27	1SG	544
	ATOM	544	CB	GLN	69	30.855	37.549	13.718	1.00	0.27	1SG	545
	ATOM	545	CG	GLN	69	29.833	36.434	13.927	1.00	0.27	1SG	546
	ATOM	546	CD	GLN	69	29.290	36.575	15.342	1.00	0.27	1SG	547
55	ATOM	547	OE1	GLN	69	29.847	37.306	16.160	1.00	0.27	1SG	548
	ATOM	548	NE2	GLN	69	28.177	35.853	15.642	1.00	0.27	1SG	549
	ATOM	549	C	GLN	69	32.221	36.103	12.322	1.00	0.27	1SG	550
	ATOM	550	O	GLN	69	31.741	35.214	11.620	1.00	0.27	1SG	551
	ATOM	551	N	HIS	70	33.333	35.928	13.056	1.00	0.11	1SG	552
60	ATOM	552	CA	HIS	70	33.988	34.660	13.145	1.00	0.11	1SG	553
	ATOM	553	ND1	HIS	70	35.166	33.594	10.252	1.00	0.11	1SG	554
	ATOM	554	CG	HIS	70	35.399	34.688	11.056	1.00	0.11	1SG	555
	ATOM	555	CB	HIS	70	35.405	34.631	12.551	1.00	0.11	1SG	556
	ATOM	556	NE2	HIS	70	35.486	35.325	8.894	1.00	0.11	1SG	557
65	ATOM	557	CD2	HIS	70	35.593	35.736	10.211	1.00	0.11	1SG	558
	ATOM	558	CE1	HIS	70	35.229	34.031	8.970	1.00	0.11	1SG	559
	ATOM	559	C	HIS	70	34.110	34.372	14.599	1.00	0.11	1SG	560
	ATOM	560	O	HIS	70	33.793	35.212	15.438	1.00	0.11	1SG	561
	ATOM	561	N	GLN	71	34.541	33.146	14.938	1.00	0.12	1SG	562
70	ATOM	562	CA	GLN	71	34.685	32.822	16.322	1.00	0.12	1SG	563
	ATOM	563	CB	GLN	71	35.169	31.379	16.553	1.00	0.12	1SG	564
	ATOM	564	CG	GLN	71	34.160	30.298	16.156	1.00	0.12	1SG	565

141

	ATOM	565	CD	GLN	71	33.100	30.213	17.246	1.00	0.12	1SG 566
	ATOM	566	OE1	GLN	71	33.038	31.052	18.143	1.00	0.12	1SG 567
	ATOM	567	NE2	GLN	71	32.237	29.166	17.171	1.00	0.12	1SG 568
5	ATOM	568	C	GLN	71	35.731	33.730	16.880	1.00	0.12	1SG 569
	ATOM	569	O	GLN	71	35.580	34.277	17.970	1.00	0.12	1SG 570
	ATOM	570	N	GLN	72	36.827	33.913	16.123	1.00	0.21	1SG 571
	ATOM	571	CA	GLN	72	37.952	34.675	16.575	1.00	0.21	1SG 572
	ATOM	572	CB	GLN	72	39.129	34.611	15.587	1.00	0.21	1SG 573
10	ATOM	573	CG	GLN	72	39.531	33.182	15.217	1.00	0.21	1SG 574
	ATOM	574	CD	GLN	72	39.805	32.408	16.498	1.00	0.21	1SG 575
	ATOM	575	OE1	GLN	72	40.001	32.986	17.566	1.00	0.21	1SG 576
	ATOM	576	NE2	GLN	72	39.809	31.053	16.390	1.00	0.21	1SG 577
	ATOM	577	C	GLN	72	37.612	36.126	16.723	1.00	0.21	1SG 578
	ATOM	578	O	GLN	72	37.927	36.739	17.741	1.00	0.21	1SG 579
15	ATOM	579	N	VAL	73	36.943	36.714	15.712	1.00	0.31	1SG 580
	ATOM	580	CA	VAL	73	36.757	38.137	15.714	1.00	0.31	1SG 581
	ATOM	581	CB	VAL	73	36.891	38.749	14.349	1.00	0.31	1SG 582
	ATOM	582	CG1	VAL	73	38.329	38.520	13.852	1.00	0.31	1SG 583
	ATOM	583	CG2	VAL	73	35.809	38.152	13.433	1.00	0.31	1SG 584
20	ATOM	584	C	VAL	73	35.419	38.532	16.245	1.00	0.31	1SG 585
	ATOM	585	O	VAL	73	34.556	37.707	16.541	1.00	0.31	1SG 586
	ATOM	586	N	ASN	74	35.258	39.864	16.381	1.00	0.41	1SG 587
	ATOM	587	CA	ASN	74	34.078	40.535	16.838	1.00	0.41	1SG 588
	ATOM	588	CB	ASN	74	34.389	41.966	17.323	1.00	0.41	1SG 589
25	ATOM	589	CG	ASN	74	33.215	42.515	18.119	1.00	0.41	1SG 590
	ATOM	590	OD1	ASN	74	32.226	41.823	18.353	1.00	0.41	1SG 591
	ATOM	591	ND2	ASN	74	33.322	43.804	18.540	1.00	0.41	1SG 592
	ATOM	592	C	ASN	74	33.177	40.636	15.647	1.00	0.41	1SG 593
	ATOM	593	O	ASN	74	33.389	39.959	14.644	1.00	0.41	1SG 594
30	ATOM	594	N	GLU	75	32.113	41.457	15.746	1.00	0.48	1SG 595
	ATOM	595	CA	GLU	75	31.220	41.642	14.641	1.00	0.48	1SG 596
	ATOM	596	CB	GLU	75	29.879	42.271	15.056	1.00	0.48	1SG 597
	ATOM	597	CG	GLU	75	29.072	41.393	16.014	1.00	0.48	1SG 598
	ATOM	598	CD	GLU	75	28.504	40.229	15.218	1.00	0.48	1SG 599
35	ATOM	599	OE1	GLU	75	28.423	40.354	13.967	1.00	0.48	1SG 600
	ATOM	600	OE2	GLU	75	28.141	39.200	15.848	1.00	0.48	1SG 601
	ATOM	601	C	GLU	75	31.884	42.588	13.693	1.00	0.48	1SG 602
	ATOM	602	O	GLU	75	32.611	43.491	14.107	1.00	0.48	1SG 603
	ATOM	603	N	SER	76	31.657	42.386	12.381	1.00	0.42	1SG 604
40	ATOM	604	CA	SER	76	32.239	43.230	11.379	1.00	0.42	1SG 605
	ATOM	605	CB	SER	76	32.350	42.539	10.010	1.00	0.42	1SG 606
	ATOM	606	OG	SER	76	32.918	43.427	9.061	1.00	0.42	1SG 607
	ATOM	607	C	SER	76	31.346	44.416	11.208	1.00	0.42	1SG 608
	ATOM	608	O	SER	76	30.182	44.388	11.604	1.00	0.42	1SG 609
45	ATOM	609	N	GLU	77	31.884	45.509	10.627	1.00	0.31	1SG 610
	ATOM	610	CA	GLU	77	31.059	46.657	10.396	1.00	0.31	1SG 611
	ATOM	611	CB	GLU	77	31.813	47.908	9.915	1.00	0.31	1SG 612
	ATOM	612	CG	GLU	77	32.856	48.431	10.898	1.00	0.31	1SG 613
	ATOM	613	CD	GLU	77	34.144	47.681	10.608	1.00	0.31	1SG 614
50	ATOM	614	OE1	GLU	77	34.416	47.430	9.403	1.00	0.31	1SG 615
	ATOM	615	OE2	GLU	77	34.871	47.348	11.581	1.00	0.31	1SG 616
	ATOM	616	C	GLU	77	30.149	46.280	9.278	1.00	0.31	1SG 617
	ATOM	617	O	GLU	77	30.493	45.470	8.419	1.00	0.31	1SG 618
	ATOM	618	N	PRO	78	28.978	46.839	9.296	1.00	0.29	1SG 619
55	ATOM	619	CA	PRO	78	28.046	46.505	8.257	1.00	0.29	1SG 620
	ATOM	620	CD	PRO	78	28.309	47.037	10.573	1.00	0.29	1SG 621
	ATOM	621	CB	PRO	78	26.663	46.846	8.806	1.00	0.29	1SG 622
	ATOM	622	CG	PRO	78	26.830	46.701	10.328	1.00	0.29	1SG 623
	ATOM	623	C	PRO	78	28.349	47.178	6.959	1.00	0.29	1SG 624
60	ATOM	624	O	PRO	78	28.956	48.248	6.958	1.00	0.29	1SG 625
	ATOM	625	N	VAL	79	27.945	46.539	5.845	1.00	0.31	1SG 626
	ATOM	626	CA	VAL	79	28.075	47.100	4.536	1.00	0.31	1SG 627
	ATOM	627	CB	VAL	79	28.861	46.242	3.590	1.00	0.31	1SG 628
	ATOM	628	CG1	VAL	79	28.171	44.872	3.480	1.00	0.31	1SG 629
65	ATOM	629	CG2	VAL	79	28.983	46.983	2.247	1.00	0.31	1SG 630
	ATOM	630	C	VAL	79	26.678	47.181	4.020	1.00	0.31	1SG 631
	ATOM	631	O	VAL	79	25.899	46.245	4.193	1.00	0.31	1SG 632
	ATOM	632	N	TYR	80	26.305	48.306	3.381	1.00	0.19	1SG 633
	ATOM	633	CA	TYR	80	24.946	48.385	2.937	1.00	0.19	1SG 634
70	ATOM	634	CB	TYR	80	24.256	49.729	3.235	1.00	0.19	1SG 635
	ATOM	635	CG	TYR	80	22.813	49.553	2.905	1.00	0.19	1SG 636

	ATOM	636	CD1	TYR	80	22.346	49.756	1.626	1.00	0.19	1SG	637
	ATOM	637	CD2	TYR	80	21.926	49.172	3.886	1.00	0.19	1SG	638
	ATOM	638	CE1	TYR	80	21.013	49.586	1.333	1.00	0.19	1SG	639
5	ATOM	639	CE2	TYR	80	20.593	49.000	3.600	1.00	0.19	1SG	640
	ATOM	640	CZ	TYR	80	20.135	49.209	2.322	1.00	0.19	1SG	641
	ATOM	641	OH	TYR	80	18.767	49.033	2.023	1.00	0.19	1SG	642
	ATOM	642	C	TYR	80	24.940	48.188	1.459	1.00	0.19	1SG	643
	ATOM	643	O	TYR	80	25.745	48.771	0.734	1.00	0.19	1SG	644
10	ATOM	644	N	LEU	81	24.021	47.332	0.979	1.00	0.08	1SG	645
	ATOM	645	CA	LEU	81	23.950	47.054	-0.424	1.00	0.08	1SG	646
	ATOM	646	CB	LEU	81	24.024	45.551	-0.740	1.00	0.08	1SG	647
	ATOM	647	CG	LEU	81	23.950	45.230	-2.243	1.00	0.08	1SG	648
	ATOM	648	CD2	LEU	81	23.763	43.724	-2.484	1.00	0.08	1SG	649
	ATOM	649	CD1	LEU	81	25.157	45.810	-2.996	1.00	0.08	1SG	650
15	ATOM	650	C	LEU	81	22.632	47.548	-0.923	1.00	0.08	1SG	651
	ATOM	651	O	LEU	81	21.611	47.411	-0.251	1.00	0.08	1SG	652
	ATOM	652	N	GLU	82	22.633	48.166	-2.119	1.00	0.09	1SG	653
	ATOM	653	CA	GLU	82	21.417	48.652	-2.696	1.00	0.09	1SG	654
	ATOM	654	CB	GLU	82	21.424	50.176	-2.909	1.00	0.09	1SG	655
20	ATOM	655	CG	GLU	82	21.484	50.982	-1.610	1.00	0.09	1SG	656
	ATOM	656	CD	GLU	82	21.724	52.442	-1.972	1.00	0.09	1SG	657
	ATOM	657	OE1	GLU	82	21.178	52.895	-3.014	1.00	0.09	1SG	658
	ATOM	658	OE2	GLU	82	22.467	53.122	-1.216	1.00	0.09	1SG	659
	ATOM	659	C	GLU	82	21.317	48.028	-4.048	1.00	0.09	1SG	660
25	ATOM	660	O	GLU	82	22.273	48.049	-4.822	1.00	0.09	1SG	661
	ATOM	661	N	VAL	83	20.151	47.442	-4.369	1.00	0.09	1SG	662
	ATOM	662	CA	VAL	83	19.999	46.839	-5.659	1.00	0.09	1SG	663
	ATOM	663	CB	VAL	83	19.493	45.431	-5.602	1.00	0.09	1SG	664
	ATOM	664	CG1	VAL	83	20.533	44.566	-4.871	1.00	0.09	1SG	665
30	ATOM	665	CG2	VAL	83	18.111	45.445	-4.931	1.00	0.09	1SG	666
	ATOM	666	C	VAL	83	18.974	47.642	-6.383	1.00	0.09	1SG	667
	ATOM	667	O	VAL	83	17.973	48.052	-5.797	1.00	0.09	1SG	668
	ATOM	668	N	PHE	84	19.207	47.907	-7.682	1.00	0.23	1SG	669
	ATOM	669	CA	PHE	84	18.257	48.698	-8.403	1.00	0.23	1SG	670
35	ATOM	670	CB	PHE	84	18.805	50.055	-8.873	1.00	0.23	1SG	671
	ATOM	671	CG	PHE	84	19.450	50.743	-7.723	1.00	0.23	1SG	672
	ATOM	672	CD1	PHE	84	18.715	51.444	-6.799	1.00	0.23	1SG	673
	ATOM	673	CD2	PHE	84	20.812	50.670	-7.567	1.00	0.23	1SG	674
	ATOM	674	CE1	PHE	84	19.328	52.069	-5.740	1.00	0.23	1SG	675
40	ATOM	675	CE2	PHE	84	21.428	51.294	-6.510	1.00	0.23	1SG	676
	ATOM	676	CZ	PHE	84	20.689	51.999	-5.594	1.00	0.23	1SG	677
	ATOM	677	C	PHE	84	17.966	47.967	-9.668	1.00	0.23	1SG	678
	ATOM	678	O	PHE	84	18.750	47.124	-10.101	1.00	0.23	1SG	679
	ATOM	679	N	SER	85	16.802	48.247	-10.283	1.00	0.34	1SG	680
45	ATOM	680	CA	SER	85	16.544	47.653	-11.558	1.00	0.34	1SG	681
	ATOM	681	CB	SER	85	15.248	46.824	-11.611	1.00	0.34	1SG	682
	ATOM	682	OG	SER	85	14.121	47.637	-11.326	1.00	0.34	1SG	683
	ATOM	683	C	SER	85	16.439	48.779	-12.538	1.00	0.34	1SG	684
	ATOM	684	O	SER	85	15.403	49.431	-12.656	1.00	0.34	1SG	685
50	ATOM	685	N	ASP	86	17.538	49.042	-13.267	1.00	0.23	1SG	686
	ATOM	686	CA	ASP	86	17.542	50.101	-14.232	1.00	0.23	1SG	687
	ATOM	687	CB	ASP	86	18.144	51.413	-13.702	1.00	0.23	1SG	688
	ATOM	688	CG	ASP	86	17.182	51.997	-12.678	1.00	0.23	1SG	689
	ATOM	689	OD1	ASP	86	15.949	51.949	-12.931	1.00	0.23	1SG	690
55	ATOM	690	OD2	ASP	86	17.667	52.492	-11.625	1.00	0.23	1SG	691
	ATOM	691	C	ASP	86	18.413	49.652	-15.356	1.00	0.23	1SG	692
	ATOM	692	O	ASP	86	19.189	48.709	-15.213	1.00	0.23	1SG	693
	ATOM	693	N	TRP	87	18.280	50.297	-16.529	1.00	0.14	1SG	694
	ATOM	694	CA	TRP	87	19.116	49.918	-17.626	1.00	0.14	1SG	695
60	ATOM	695	CB	TRP	87	18.696	50.502	-18.982	1.00	0.14	1SG	696
	ATOM	696	CG	TRP	87	17.552	49.733	-19.589	1.00	0.14	1SG	697
	ATOM	697	CD2	TRP	87	17.711	48.410	-20.124	1.00	0.14	1SG	698
	ATOM	698	CD1	TRP	87	16.234	50.051	-19.727	1.00	0.14	1SG	699
	ATOM	699	NE1	TRP	87	15.562	49.008	-20.322	1.00	0.14	1SG	700
65	ATOM	700	CE2	TRP	87	16.460	47.990	-20.570	1.00	0.14	1SG	701
	ATOM	701	CE3	TRP	87	18.813	47.610	-20.230	1.00	0.14	1SG	702
	ATOM	702	CZ2	TRP	87	16.289	46.756	-21.133	1.00	0.14	1SG	703
	ATOM	703	CZ3	TRP	87	18.640	46.369	-20.801	1.00	0.14	1SG	704
	ATOM	704	CH2	TRP	87	17.402	45.949	-21.244	1.00	0.14	1SG	705
70	ATOM	705	C	TRP	87	20.535	50.295	-17.364	1.00	0.14	1SG	706
	ATOM	706	O	TRP	87	21.443	49.504	-17.607	1.00	0.14	1SG	707

143

	ATOM	707	N	LEU	88	20.772	51.514	-16.847	1.00	0.12	1SG 708
	ATOM	708	CA	LEU	88	22.128	51.938	-16.649	1.00	0.12	1SG 709
	ATOM	709	CB	LEU	88	22.571	52.993	-17.679	1.00	0.12	1SG 710
5	ATOM	710	CG	LEU	88	24.024	53.484	-17.521	1.00	0.12	1SG 711
	ATOM	711	CD2	LEU	88	24.277	54.759	-18.343	1.00	0.12	1SG 712
	ATOM	712	CD1	LEU	88	25.038	52.377	-17.830	1.00	0.12	1SG 713
	ATOM	713	C	LEU	88	22.224	52.584	-15.307	1.00	0.12	1SG 714
	ATOM	714	O	LEU	88	21.278	53.228	-14.856	1.00	0.12	1SG 715
10	ATOM	715	N	LEU	89	23.374	52.412	-14.622	1.00	0.11	1SG 716
	ATOM	716	CA	LEU	89	23.535	53.058	-13.352	1.00	0.11	1SG 717
	ATOM	717	CB	LEU	89	23.298	52.139	-12.138	1.00	0.11	1SG 718
	ATOM	718	CG	LEU	89	23.481	52.831	-10.774	1.00	0.11	1SG 719
	ATOM	719	CD2	LEU	89	23.511	51.805	-9.629	1.00	0.11	1SG 720
	ATOM	720	CD1	LEU	89	22.428	53.934	-10.560	1.00	0.11	1SG 721
15	ATOM	721	C	LEU	89	24.951	53.524	-13.265	1.00	0.11	1SG 722
	ATOM	722	O	LEU	89	25.847	52.949	-13.882	1.00	0.11	1SG 723
	ATOM	723	N	LEU	90	25.182	54.611	-12.507	1.00	0.11	1SG 724
	ATOM	724	CA	LEU	90	26.528	55.046	-12.310	1.00	0.11	1SG 725
20	ATOM	725	CB	LEU	90	26.688	56.576	-12.242	1.00	0.11	1SG 726
	ATOM	726	CG	LEU	90	28.146	57.033	-12.047	1.00	0.11	1SG 727
	ATOM	727	CD2	LEU	90	28.228	58.537	-11.741	1.00	0.11	1SG 728
	ATOM	728	CD1	LEU	90	29.013	56.629	-13.250	1.00	0.11	1SG 729
	ATOM	729	C	LEU	90	26.875	54.478	-10.975	1.00	0.11	1SG 730
25	ATOM	730	O	LEU	90	26.167	54.707	-9.996	1.00	0.11	1SG 731
	ATOM	731	N	GLN	91	27.972	53.704	-10.903	1.00	0.11	1SG 732
	ATOM	732	CA	GLN	91	28.255	53.028	-9.674	1.00	0.11	1SG 733
	ATOM	733	CB	GLN	91	28.619	51.545	-9.880	1.00	0.11	1SG 734
	ATOM	734	CG	GLN	91	27.482	50.714	-10.484	1.00	0.11	1SG 735
30	ATOM	735	CD	GLN	91	27.980	49.285	-10.669	1.00	0.11	1SG 736
	ATOM	736	OE1	GLN	91	29.136	49.064	-11.026	1.00	0.11	1SG 737
	ATOM	737	NE2	GLN	91	27.089	48.288	-10.419	1.00	0.11	1SG 738
	ATOM	738	C	GLN	91	29.413	53.684	-9.004	1.00	0.11	1SG 739
	ATOM	739	O	GLN	91	30.329	54.186	-9.654	1.00	0.11	1SG 740
35	ATOM	740	N	ALA	92	29.370	53.720	-7.658	1.00	0.18	1SG 741
	ATOM	741	CA	ALA	92	30.446	54.291	-6.909	1.00	0.18	1SG 742
	ATOM	742	CB	ALA	92	30.134	55.687	-6.346	1.00	0.18	1SG 743
	ATOM	743	C	ALA	92	30.703	53.398	-5.743	1.00	0.18	1SG 744
	ATOM	744	O	ALA	92	29.797	52.745	-5.231	1.00	0.18	1SG 745
40	ATOM	745	N	SER	93	31.975	53.316	-5.319	1.00	0.25	1SG 746
	ATOM	746	CA	SER	93	32.314	52.505	-4.192	1.00	0.25	1SG 747
	ATOM	747	CB	SER	93	33.830	52.393	-3.991	1.00	0.25	1SG 748
	ATOM	748	OG	SER	93	34.110	51.577	-2.865	1.00	0.25	1SG 749
	ATOM	749	C	SER	93	31.729	53.125	-2.961	1.00	0.25	1SG 750
45	ATOM	750	O	SER	93	31.113	52.443	-2.144	1.00	0.25	1SG 751
	ATOM	751	N	ALA	94	31.898	54.454	-2.798	1.00	0.19	1SG 752
	ATOM	752	CA	ALA	94	31.393	55.085	-1.611	1.00	0.19	1SG 753
	ATOM	753	CB	ALA	94	32.469	55.303	-0.534	1.00	0.19	1SG 754
	ATOM	754	C	ALA	94	30.843	56.428	-1.971	1.00	0.19	1SG 755
50	ATOM	755	O	ALA	94	31.285	57.069	-2.923	1.00	0.19	1SG 756
	ATOM	756	N	GLU	95	29.814	56.855	-1.216	1.00	0.12	1SG 757
	ATOM	757	CA	GLU	95	29.169	58.121	-1.400	1.00	0.12	1SG 758
	ATOM	758	CB	GLU	95	27.888	58.222	-0.553	1.00	0.12	1SG 759
	ATOM	759	CG	GLU	95	26.823	57.198	-0.963	1.00	0.12	1SG 760
55	ATOM	760	CD	GLU	95	25.743	57.151	0.108	1.00	0.12	1SG 761
	ATOM	761	OE1	GLU	95	25.714	58.073	0.966	1.00	0.12	1SG 762
	ATOM	762	OE2	GLU	95	24.930	56.188	0.080	1.00	0.12	1SG 763
	ATOM	763	C	GLU	95	30.096	59.221	-0.983	1.00	0.12	1SG 764
	ATOM	764	O	GLU	95	30.230	60.228	-1.676	1.00	0.12	1SG 765
60	ATOM	765	N	VAL	96	30.780	59.047	0.164	1.00	0.11	1SG 766
	ATOM	766	CA	VAL	96	31.626	60.097	0.652	1.00	0.11	1SG 767
	ATOM	767	CB	VAL	96	31.355	60.462	2.080	1.00	0.11	1SG 768
	ATOM	768	CG1	VAL	96	32.367	61.537	2.516	1.00	0.11	1SG 769
	ATOM	769	CG2	VAL	96	29.886	60.903	2.191	1.00	0.11	1SG 770
65	ATOM	770	C	VAL	96	33.039	59.638	0.573	1.00	0.11	1SG 771
	ATOM	771	O	VAL	96	33.336	58.455	0.737	1.00	0.11	1SG 772
	ATOM	772	N	VAL	97	33.954	60.587	0.303	1.00	0.10	1SG 773
	ATOM	773	CA	VAL	97	35.339	60.254	0.175	1.00	0.10	1SG 774
	ATOM	774	CB	VAL	97	35.826	60.312	-1.243	1.00	0.10	1SG 775
70	ATOM	775	CG1	VAL	97	35.078	59.249	-2.062	1.00	0.10	1SG 776
	ATOM	776	CG2	VAL	97	35.642	61.745	-1.768	1.00	0.10	1SG 777
	ATOM	777	C	VAL	97	36.119	61.271	0.931	1.00	0.10	1SG 778

144

	ATOM	778	O	VAL	97	35.603	62.323	1.300	1.00	0.10	1SG 779
	ATOM	779	N	MET	98	37.402	60.962	1.185	1.00	0.12	1SG 780
	ATOM	780	CA	MET	98	38.263	61.868	1.879	1.00	0.12	1SG 781
5	ATOM	781	CB	MET	98	39.295	61.145	2.762	1.00	0.12	1SG 782
	ATOM	782	CG	MET	98	38.651	60.261	3.835	1.00	0.12	1SG 783
	ATOM	783	SD	MET	98	37.735	61.156	5.127	1.00	0.12	1SG 784
	ATOM	784	CE	MET	98	39.181	61.447	6.184	1.00	0.12	1SG 785
	ATOM	785	C	MET	98	39.008	62.583	0.802	1.00	0.12	1SG 786
	ATOM	786	O	MET	98	39.188	62.048	-0.290	1.00	0.12	1SG 787
10	ATOM	787	N	GLU	99	39.440	63.830	1.057	1.00	0.10	1SG 788
	ATOM	788	CA	GLU	99	40.130	64.507	0.002	1.00	0.10	1SG 789
	ATOM	789	CB	GLU	99	40.449	65.986	0.286	1.00	0.10	1SG 790
	ATOM	790	CG	GLU	99	41.112	66.684	-0.906	1.00	0.10	1SG 791
	ATOM	791	CD	GLU	99	41.405	68.130	-0.533	1.00	0.10	1SG 792
15	ATOM	792	OE1	GLU	99	40.500	68.797	0.034	1.00	0.10	1SG 793
	ATOM	793	OE2	GLU	99	42.546	68.586	-0.812	1.00	0.10	1SG 794
	ATOM	794	C	GLU	99	41.427	63.806	-0.211	1.00	0.10	1SG 795
	ATOM	795	O	GLU	99	42.056	63.330	0.733	1.00	0.10	1SG 796
	ATOM	796	N	GLY	100	41.846	63.711	-1.486	1.00	0.20	1SG 797
20	ATOM	797	CA	GLY	100	43.097	63.098	-1.803	1.00	0.20	1SG 798
	ATOM	798	C	GLY	100	42.858	61.680	-2.198	1.00	0.20	1SG 799
	ATOM	799	O	GLY	100	43.718	61.061	-2.822	1.00	0.20	1SG 800
	ATOM	800	N	GLN	101	41.686	61.111	-1.860	1.00	0.50	1SG 801
	ATOM	801	CA	GLN	101	41.519	59.748	-2.261	1.00	0.50	1SG 802
25	ATOM	802	CB	GLN	101	40.589	58.891	-1.379	1.00	0.50	1SG 803
	ATOM	803	CG	GLN	101	39.119	59.298	-1.332	1.00	0.50	1SG 804
	ATOM	804	CD	GLN	101	38.416	58.229	-0.499	1.00	0.50	1SG 805
	ATOM	805	OE1	GLN	101	37.204	58.040	-0.574	1.00	0.50	1SG 806
	ATOM	806	NE2	GLN	101	39.213	57.489	0.318	1.00	0.50	1SG 807
30	ATOM	807	C	GLN	101	41.046	59.724	-3.672	1.00	0.50	1SG 808
	ATOM	808	O	GLN	101	40.446	60.674	-4.176	1.00	0.50	1SG 809
	ATOM	809	N	PRO	102	41.375	58.654	-4.332	1.00	0.57	1SG 810
	ATOM	810	CA	PRO	102	40.964	58.525	-5.698	1.00	0.57	1SG 811
	ATOM	811	CD	PRO	102	42.668	58.028	-4.098	1.00	0.57	1SG 812
35	ATOM	812	CB	PRO	102	41.873	57.469	-6.321	1.00	0.57	1SG 813
	ATOM	813	CG	PRO	102	43.156	57.556	-5.478	1.00	0.57	1SG 814
	ATOM	814	C	PRO	102	39.518	58.180	-5.764	1.00	0.57	1SG 815
	ATOM	815	O	PRO	102	39.021	57.507	-4.864	1.00	0.57	1SG 816
	ATOM	816	N	LEU	103	38.823	58.637	-6.818	1.00	0.26	1SG 817
40	ATOM	817	CA	LEU	103	37.446	58.299	-6.967	1.00	0.26	1SG 818
	ATOM	818	CB	LEU	103	36.529	59.508	-7.225	1.00	0.26	1SG 819
	ATOM	819	CG	LEU	103	35.043	59.129	-7.383	1.00	0.26	1SG 820
	ATOM	820	CD2	LEU	103	34.221	60.312	-7.920	1.00	0.26	1SG 821
	ATOM	821	CD1	LEU	103	34.473	58.542	-6.082	1.00	0.26	1SG 822
45	ATOM	822	C	LEU	103	37.366	57.422	-8.164	1.00	0.26	1SG 823
	ATOM	823	O	LEU	103	37.940	57.728	-9.207	1.00	0.26	1SG 824
	ATOM	824	N	PHE	104	36.674	56.279	-8.032	1.00	0.08	1SG 825
	ATOM	825	CA	PHE	104	36.542	55.422	-9.168	1.00	0.08	1SG 826
	ATOM	826	CB	PHE	104	37.073	53.998	-8.931	1.00	0.08	1SG 827
50	ATOM	827	CG	PHE	104	37.001	53.256	-10.222	1.00	0.08	1SG 828
	ATOM	828	CD1	PHE	104	37.981	53.414	-11.176	1.00	0.08	1SG 829
	ATOM	829	CD2	PHE	104	35.961	52.393	-10.476	1.00	0.08	1SG 830
	ATOM	830	CE1	PHE	104	37.919	52.727	-12.365	1.00	0.08	1SG 831
	ATOM	831	CE2	PHE	104	35.892	51.703	-11.664	1.00	0.08	1SG 832
55	ATOM	832	CZ	PHE	104	36.873	51.871	-12.611	1.00	0.08	1SG 833
	ATOM	833	C	PHE	104	35.081	55.331	-9.441	1.00	0.08	1SG 834
	ATOM	834	O	PHE	104	34.282	55.127	-8.528	1.00	0.08	1SG 835
	ATOM	835	N	LEU	105	34.691	55.515	-10.715	1.00	0.10	1SG 836
	ATOM	836	CA	LEU	105	33.306	55.440	-11.062	1.00	0.10	1SG 837
60	ATOM	837	CB	LEU	105	32.705	56.779	-11.524	1.00	0.10	1SG 838
	ATOM	838	CG	LEU	105	32.678	57.865	-10.432	1.00	0.10	1SG 839
	ATOM	839	CD2	LEU	105	32.015	57.352	-9.144	1.00	0.10	1SG 840
	ATOM	840	CD1	LEU	105	32.045	59.163	-10.958	1.00	0.10	1SG 841
	ATOM	841	C	LEU	105	33.203	54.497	-12.208	1.00	0.10	1SG 842
65	ATOM	842	O	LEU	105	34.173	54.269	-12.929	1.00	0.10	1SG 843
	ATOM	843	N	ARG	106	32.014	53.900	-12.389	1.00	0.15	1SG 844
	ATOM	844	CA	ARG	106	31.866	52.960	-13.452	1.00	0.15	1SG 845
	ATOM	845	CB	ARG	106	32.026	51.519	-12.938	1.00	0.15	1SG 846
	ATOM	846	CG	ARG	106	31.891	50.409	-13.977	1.00	0.15	1SG 847
70	ATOM	847	CD	ARG	106	32.273	49.049	-13.387	1.00	0.15	1SG 848
	ATOM	848	NE	ARG	106	32.035	48.004	-14.420	1.00	0.15	1SG 849

	ATOM	849	CZ	ARG	106	31.108	47.032	-14.187	1.00	0.15	1SG 850
	ATOM	850	NH1	ARG	106	30.419	47.031	-13.009	1.00	0.15	1SG 851
	ATOM	851	NH2	ARG	106	30.895	46.057	-15.119	1.00	0.15	1SG 852
	ATOM	852	C	ARG	106	30.491	53.116	-14.005	1.00	0.15	1SG 853
5	ATOM	853	O	ARG	106	29.531	53.327	-13.265	1.00	0.15	1SG 854
	ATOM	854	N	CYS	107	30.363	53.038	-15.342	1.00	0.16	1SG 855
	ATOM	855	CA	CYS	107	29.059	53.096	-15.924	1.00	0.16	1SG 856
	ATOM	856	CB	CYS	107	29.005	53.868	-17.255	1.00	0.16	1SG 857
	ATOM	857	SG	CYS	107	29.607	55.572	-17.068	1.00	0.16	1SG 858
10	ATOM	858	C	CYS	107	28.730	51.668	-16.190	1.00	0.16	1SG 859
	ATOM	859	O	CYS	107	29.442	50.988	-16.927	1.00	0.16	1SG 860
	ATOM	860	N	HIS	108	27.648	51.164	-15.572	1.00	0.11	1SG 861
	ATOM	861	CA	HIS	108	27.365	49.768	-15.705	1.00	0.11	1SG 862
	ATOM	862	ND1	HIS	108	25.867	46.991	-14.343	1.00	0.11	1SG 863
15	ATOM	863	CG	HIS	108	27.113	47.571	-14.417	1.00	0.11	1SG 864
	ATOM	864	CB	HIS	108	27.349	49.051	-14.343	1.00	0.11	1SG 865
	ATOM	865	NE2	HIS	108	27.329	45.329	-14.542	1.00	0.11	1SG 866
	ATOM	866	CD2	HIS	108	27.995	46.542	-14.541	1.00	0.11	1SG 867
	ATOM	867	CE1	HIS	108	26.055	45.649	-14.420	1.00	0.11	1SG 868
20	ATOM	868	C	HIS	108	26.033	49.600	-16.350	1.00	0.11	1SG 869
	ATOM	869	O	HIS	108	25.078	50.307	-16.033	1.00	0.11	1SG 870
	ATOM	870	N	GLY	109	25.949	48.636	-17.287	1.00	0.09	1SG 871
	ATOM	871	CA	GLY	109	24.722	48.381	-17.976	1.00	0.09	1SG 872
	ATOM	872	C	GLY	109	24.148	47.131	-17.403	1.00	0.09	1SG 873
25	ATOM	873	O	GLY	109	24.870	46.270	-16.904	1.00	0.09	1SG 874
	ATOM	874	N	TRP	110	22.812	47.003	-17.469	1.00	0.32	1SG 875
	ATOM	875	CA	TRP	110	22.150	45.862	-16.919	1.00	0.32	1SG 876
	ATOM	876	CB	TRP	110	20.623	46.057	-16.844	1.00	0.32	1SG 877
	ATOM	877	CG	TRP	110	19.843	44.901	-16.269	1.00	0.32	1SG 878
30	ATOM	878	CD2	TRP	110	18.944	44.087	-17.034	1.00	0.32	1SG 879
	ATOM	879	CD1	TRP	110	19.782	44.442	-14.985	1.00	0.32	1SG 880
	ATOM	880	NE1	TRP	110	18.904	43.387	-14.905	1.00	0.32	1SG 881
	ATOM	881	CE2	TRP	110	18.377	43.161	-16.158	1.00	0.32	1SG 882
	ATOM	882	CE3	TRP	110	18.613	44.112	-18.358	1.00	0.32	1SG 883
35	ATOM	883	CZ2	TRP	110	17.467	42.241	-16.595	1.00	0.32	1SG 884
	ATOM	884	CZ3	TRP	110	17.696	43.185	-18.796	1.00	0.32	1SG 885
	ATOM	885	CH2	TRP	110	17.134	42.268	-17.932	1.00	0.32	1SG 886
	ATOM	886	C	TRP	110	22.469	44.684	-17.783	1.00	0.32	1SG 887
	ATOM	887	O	TRP	110	22.612	44.803	-18.999	1.00	0.32	1SG 888
40	ATOM	888	N	ARG	111	22.622	43.507	-17.146	1.00	0.53	1SG 889
	ATOM	889	CA	ARG	111	22.948	42.292	-17.835	1.00	0.53	1SG 890
	ATOM	890	CB	ARG	111	21.891	41.812	-18.846	1.00	0.53	1SG 891
	ATOM	891	CG	ARG	111	20.728	41.061	-18.202	1.00	0.53	1SG 892
	ATOM	892	CD	ARG	111	19.970	40.150	-19.176	1.00	0.53	1SG 893
45	ATOM	893	NE	ARG	111	19.081	40.997	-20.019	1.00	0.53	1SG 894
	ATOM	894	CZ	ARG	111	18.507	40.481	-21.145	1.00	0.53	1SG 895
	ATOM	895	NH1	ARG	111	18.813	39.213	-21.550	1.00	0.53	1SG 896
	ATOM	896	NH2	ARG	111	17.649	41.243	-21.885	1.00	0.53	1SG 897
	ATOM	897	C	ARG	111	24.232	42.460	-18.581	1.00	0.53	1SG 898
50	ATOM	898	O	ARG	111	24.532	41.678	-19.482	1.00	0.53	1SG 899
	ATOM	899	N	ASN	112	25.038	43.468	-18.204	1.00	0.33	1SG 900
	ATOM	900	CA	ASN	112	26.311	43.678	-18.830	1.00	0.33	1SG 901
	ATOM	901	CB	ASN	112	27.335	42.576	-18.504	1.00	0.33	1SG 902
	ATOM	902	CG	ASN	112	27.731	42.721	-17.046	1.00	0.33	1SG 903
55	ATOM	903	OD1	ASN	112	28.052	43.819	-16.594	1.00	0.33	1SG 904
	ATOM	904	ND2	ASN	112	27.702	41.592	-16.288	1.00	0.33	1SG 905
	ATOM	905	C	ASN	112	26.153	43.727	-20.315	1.00	0.33	1SG 906
	ATOM	906	O	ASN	112	26.933	43.116	-21.046	1.00	0.33	1SG 907
	ATOM	907	N	TRP	113	25.146	44.464	-20.817	1.00	0.13	1SG 908
60	ATOM	908	CA	TRP	113	25.015	44.533	-22.240	1.00	0.13	1SG 909
	ATOM	909	CB	TRP	113	23.669	45.100	-22.722	1.00	0.13	1SG 910
	ATOM	910	CG	TRP	113	22.493	44.191	-22.444	1.00	0.13	1SG 911
	ATOM	911	CD2	TRP	113	22.228	42.976	-23.165	1.00	0.13	1SG 912
	ATOM	912	CD1	TRP	113	21.509	44.306	-21.504	1.00	0.13	1SG 913
65	ATOM	913	NE1	TRP	113	20.640	43.244	-21.602	1.00	0.13	1SG 914
	ATOM	914	CE2	TRP	113	21.075	42.416	-22.619	1.00	0.13	1SG 915
	ATOM	915	CE3	TRP	113	22.895	42.373	-24.195	1.00	0.13	1SG 916
	ATOM	916	CZ2	TRP	113	20.571	41.241	-23.102	1.00	0.13	1SG 917
	ATOM	917	CZ3	TRP	113	22.379	41.191	-24.679	1.00	0.13	1SG 918
70	ATOM	918	CH2	TRP	113	21.238	40.635	-24.142	1.00	0.13	1SG 919
	ATOM	919	C	TRP	113	26.119	45.405	-22.742	1.00	0.13	1SG 920

	ATOM	920	O	TRP	113	26.654	46.236	-22.011	1.00	0.13	1SG 921
	ATOM	921	N	ASP	114	26.496	45.227	-24.022	1.00	0.12	1SG 922
	ATOM	922	CA	ASP	114	27.588	45.975	-24.571	1.00	0.12	1SG 923
5	ATOM	923	CB	ASP	114	27.841	45.683	-26.059	1.00	0.12	1SG 924
	ATOM	924	CG	ASP	114	28.304	44.241	-26.189	1.00	0.12	1SG 925
	ATOM	925	OD1	ASP	114	29.314	43.875	-25.531	1.00	0.12	1SG 926
	ATOM	926	OD2	ASP	114	27.652	43.486	-26.958	1.00	0.12	1SG 927
	ATOM	927	C	ASP	114	27.248	47.423	-24.474	1.00	0.12	1SG 928
10	ATOM	928	O	ASP	114	26.138	47.838	-24.803	1.00	0.12	1SG 929
	ATOM	929	N	VAL	115	28.212	48.232	-23.999	1.00	0.21	1SG 930
	ATOM	930	CA	VAL	115	27.972	49.637	-23.884	1.00	0.21	1SG 931
	ATOM	931	CB	VAL	115	27.896	50.121	-22.466	1.00	0.21	1SG 932
	ATOM	932	CG1	VAL	115	27.643	51.639	-22.481	1.00	0.21	1SG 933
	ATOM	933	CG2	VAL	115	26.813	49.317	-21.728	1.00	0.21	1SG 934
15	ATOM	934	C	VAL	115	29.128	50.336	-24.516	1.00	0.21	1SG 935
	ATOM	935	O	VAL	115	30.265	49.873	-24.449	1.00	0.21	1SG 936
	ATOM	936	N	TYR	116	28.848	51.473	-25.172	1.00	0.44	1SG 937
	ATOM	937	CA	TYR	116	29.880	52.234	-25.804	1.00	0.44	1SG 938
20	ATOM	938	CB	TYR	116	30.062	51.874	-27.283	1.00	0.44	1SG 939
	ATOM	939	CG	TYR	116	28.712	52.007	-27.883	1.00	0.44	1SG 940
	ATOM	940	CD1	TYR	116	28.279	53.200	-28.399	1.00	0.44	1SG 941
	ATOM	941	CD2	TYR	116	27.864	50.929	-27.902	1.00	0.44	1SG 942
	ATOM	942	CE1	TYR	116	27.023	53.311	-28.945	1.00	0.44	1SG 943
	ATOM	943	CE2	TYR	116	26.607	51.031	-28.445	1.00	0.44	1SG 944
25	ATOM	944	CZ	TYR	116	26.183	52.225	-28.971	1.00	0.44	1SG 945
	ATOM	945	OH	TYR	116	24.892	52.332	-29.530	1.00	0.44	1SG 946
	ATOM	946	C	TYR	116	29.464	53.663	-25.712	1.00	0.44	1SG 947
	ATOM	947	O	TYR	116	28.359	53.962	-25.263	1.00	0.44	1SG 948
	ATOM	948	N	LYS	117	30.353	54.580	-26.142	1.00	0.45	1SG 949
30	ATOM	949	CA	LYS	117	30.080	55.988	-26.073	1.00	0.45	1SG 950
	ATOM	950	CB	LYS	117	29.019	56.496	-27.064	1.00	0.45	1SG 951
	ATOM	951	CG	LYS	117	29.519	56.616	-28.501	1.00	0.45	1SG 952
	ATOM	952	CD	LYS	117	28.443	57.089	-29.479	1.00	0.45	1SG 953
	ATOM	953	CE	LYS	117	28.988	57.432	-30.865	1.00	0.45	1SG 954
35	ATOM	954	NZ	LYS	117	29.035	56.215	-31.705	1.00	0.45	1SG 955
	ATOM	955	C	LYS	117	29.606	56.330	-24.702	1.00	0.45	1SG 956
	ATOM	956	O	LYS	117	28.453	56.713	-24.513	1.00	0.45	1SG 957
	ATOM	957	N	VAL	118	30.497	56.195	-23.704	1.00	0.21	1SG 958
	ATOM	958	CA	VAL	118	30.122	56.475	-22.352	1.00	0.21	1SG 959
40	ATOM	959	CB	VAL	118	30.761	55.541	-21.370	1.00	0.21	1SG 960
	ATOM	960	CG1	VAL	118	30.419	56.016	-19.953	1.00	0.21	1SG 961
	ATOM	961	CG2	VAL	118	30.294	54.109	-21.678	1.00	0.21	1SG 962
	ATOM	962	C	VAL	118	30.579	57.856	-22.012	1.00	0.21	1SG 963
	ATOM	963	O	VAL	118	31.688	58.262	-22.354	1.00	0.21	1SG 964
45	ATOM	964	N	ILE	119	29.704	58.631	-21.340	1.00	0.09	1SG 965
	ATOM	965	CA	ILE	119	30.083	59.955	-20.951	1.00	0.09	1SG 966
	ATOM	966	CB	ILE	119	29.298	61.032	-21.637	1.00	0.09	1SG 967
	ATOM	967	CG2	ILE	119	29.724	62.381	-21.035	1.00	0.09	1SG 968
	ATOM	968	CG1	ILE	119	29.490	60.945	-23.159	1.00	0.09	1SG 969
50	ATOM	969	CD1	ILE	119	28.509	61.812	-23.947	1.00	0.09	1SG 970
	ATOM	970	C	ILE	119	29.821	60.088	-19.488	1.00	0.09	1SG 971
	ATOM	971	O	ILE	119	28.827	59.579	-18.972	1.00	0.09	1SG 972
	ATOM	972	N	TYR	120	30.737	60.771	-18.778	1.00	0.09	1SG 973
55	ATOM	973	CA	TYR	120	30.560	61.006	-17.378	1.00	0.09	1SG 974
	ATOM	974	CB	TYR	120	31.820	60.775	-16.525	1.00	0.09	1SG 975
	ATOM	975	CG	TYR	120	31.970	59.317	-16.261	1.00	0.09	1SG 976
	ATOM	976	CD1	TYR	120	32.530	58.457	-17.178	1.00	0.09	1SG 977
	ATOM	977	CD2	TYR	120	31.540	58.817	-15.054	1.00	0.09	1SG 978
	ATOM	978	CE1	TYR	120	32.652	57.117	-16.885	1.00	0.09	1SG 979
60	ATOM	979	CE2	TYR	120	31.659	57.483	-14.755	1.00	0.09	1SG 980
	ATOM	980	CZ	TYR	120	32.217	56.631	-15.673	1.00	0.09	1SG 981
	ATOM	981	OH	TYR	120	32.335	55.263	-15.355	1.00	0.09	1SG 982
	ATOM	982	C	TYR	120	30.176	62.434	-17.220	1.00	0.09	1SG 983
	ATOM	983	O	TYR	120	30.750	63.318	-17.855	1.00	0.09	1SG 984
65	ATOM	984	N	TYR	121	29.163	62.691	-16.372	1.00	0.18	1SG 985
	ATOM	985	CA	TYR	121	28.723	64.038	-16.193	1.00	0.18	1SG 986
	ATOM	986	CB	TYR	121	27.258	64.245	-16.599	1.00	0.18	1SG 987
	ATOM	987	CG	TYR	121	27.150	63.949	-18.056	1.00	0.18	1SG 988
	ATOM	988	CD1	TYR	121	27.377	64.931	-18.993	1.00	0.18	1SG 989
70	ATOM	989	CD2	TYR	121	26.824	62.683	-18.486	1.00	0.18	1SG 990
	ATOM	990	CE1	TYR	121	27.275	64.654	-20.337	1.00	0.18	1SG 991

	ATOM	991	CE2	TYR	121	26.720	62.402	-19.827	1.00	0.18	1SG 992
	ATOM	992	CZ	TYR	121	26.942	63.389	-20.756	1.00	0.18	1SG 993
	ATOM	993	OH	TYR	121	26.834	63.101	-22.133	1.00	0.18	1SG 994
	ATOM	994	C	TYR	121	28.829	64.371	-14.740	1.00	0.18	1SG 995
5	ATOM	995	O	TYR	121	28.541	63.547	-13.874	1.00	0.18	1SG 996
	ATOM	996	N	LYS	122	29.284	65.605	-14.456	1.00	0.28	1SG 997
	ATOM	997	CA	LYS	122	29.428	66.129	-13.134	1.00	0.28	1SG 998
	ATOM	998	CB	LYS	122	30.880	66.537	-12.818	1.00	0.28	1SG 999
	ATOM	999	CG	LYS	122	31.137	66.957	-11.369	1.00	0.28	1SG1000
10	ATOM	1000	CD	LYS	122	32.608	67.287	-11.095	1.00	0.28	1SG1001
	ATOM	1001	CE	LYS	122	33.591	66.393	-11.855	1.00	0.28	1SG1002
	ATOM	1002	NZ	LYS	122	34.985	66.786	-11.541	1.00	0.28	1SG1003
	ATOM	1003	C	LYS	122	28.641	67.394	-13.143	1.00	0.28	1SG1004
	ATOM	1004	O	LYS	122	29.023	68.358	-13.804	1.00	0.28	1SG1005
15	ATOM	1005	N	ASP	123	27.517	67.417	-12.408	1.00	0.20	1SG1006
	ATOM	1006	CA	ASP	123	26.698	68.590	-12.349	1.00	0.20	1SG1007
	ATOM	1007	CB	ASP	123	27.342	69.736	-11.555	1.00	0.20	1SG1008
	ATOM	1008	CG	ASP	123	27.300	69.305	-10.096	1.00	0.20	1SG1009
	ATOM	1009	OD1	ASP	123	26.407	68.486	-9.750	1.00	0.20	1SG1010
20	ATOM	1010	OD2	ASP	123	28.159	69.781	-9.310	1.00	0.20	1SG1011
	ATOM	1011	C	ASP	123	26.373	69.035	-13.739	1.00	0.20	1SG1012
	ATOM	1012	O	ASP	123	26.275	70.230	-14.018	1.00	0.20	1SG1013
	ATOM	1013	N	GLY	124	26.196	68.062	-14.652	1.00	0.17	1SG1014
	ATOM	1014	CA	GLY	124	25.784	68.369	-15.990	1.00	0.17	1SG1015
25	ATOM	1015	C	GLY	124	26.969	68.690	-16.840	1.00	0.17	1SG1016
	ATOM	1016	O	GLY	124	26.818	69.053	-18.006	1.00	0.17	1SG1017
	ATOM	1017	N	GLU	125	28.189	68.566	-16.293	1.00	0.24	1SG1018
	ATOM	1018	CA	GLU	125	29.322	68.878	-17.110	1.00	0.24	1SG1019
	ATOM	1019	CB	GLU	125	30.365	69.739	-16.386	1.00	0.24	1SG1020
30	ATOM	1020	CG	GLU	125	31.381	70.369	-17.331	1.00	0.24	1SG1021
	ATOM	1021	CD	GLU	125	32.334	71.210	-16.497	1.00	0.24	1SG1022
	ATOM	1022	OE1	GLU	125	32.596	70.818	-15.328	1.00	0.24	1SG1023
	ATOM	1023	OE2	GLU	125	32.807	72.256	-17.015	1.00	0.24	1SG1024
	ATOM	1024	C	GLU	125	29.961	67.582	-17.482	1.00	0.24	1SG1025
35	ATOM	1025	O	GLU	125	30.165	66.716	-16.637	1.00	0.24	1SG1026
	ATOM	1026	N	ALA	126	30.306	67.396	-18.766	1.00	0.26	1SG1027
	ATOM	1027	CA	ALA	126	30.860	66.125	-19.130	1.00	0.26	1SG1028
	ATOM	1028	CB	ALA	126	30.790	65.834	-20.639	1.00	0.26	1SG1029
	ATOM	1029	C	ALA	126	32.302	66.112	-18.741	1.00	0.26	1SG1030
40	ATOM	1030	O	ALA	126	33.114	66.845	-19.302	1.00	0.26	1SG1031
	ATOM	1031	N	LEU	127	32.645	65.289	-17.731	1.00	0.39	1SG1032
	ATOM	1032	CA	LEU	127	34.008	65.183	-17.302	1.00	0.39	1SG1033
	ATOM	1033	CB	LEU	127	34.179	64.277	-16.074	1.00	0.39	1SG1034
	ATOM	1034	CG	LEU	127	33.482	64.807	-14.812	1.00	0.39	1SG1035
45	ATOM	1035	CD2	LEU	127	33.881	63.986	-13.576	1.00	0.39	1SG1036
	ATOM	1036	CD1	LEU	127	31.960	64.884	-15.010	1.00	0.39	1SG1037
	ATOM	1037	C	LEU	127	34.796	64.549	-18.400	1.00	0.39	1SG1038
	ATOM	1038	O	LEU	127	35.840	65.061	-18.800	1.00	0.39	1SG1039
	ATOM	1039	N	LYS	128	34.304	63.411	-18.933	1.00	0.43	1SG1040
50	ATOM	1040	CA	LYS	128	35.062	62.772	-19.966	1.00	0.43	1SG1041
	ATOM	1041	CB	LYS	128	36.120	61.788	-19.443	1.00	0.43	1SG1042
	ATOM	1042	CG	LYS	128	35.512	60.519	-18.844	1.00	0.43	1SG1043
	ATOM	1043	CD	LYS	128	36.528	59.394	-18.642	1.00	0.43	1SG1044
	ATOM	1044	CE	LYS	128	35.890	58.054	-18.279	1.00	0.43	1SG1045
55	ATOM	1045	NZ	LYS	128	35.161	57.519	-19.451	1.00	0.43	1SG1046
	ATOM	1046	C	LYS	128	34.135	61.974	-20.820	1.00	0.43	1SG1047
	ATOM	1047	O	LYS	128	33.048	61.582	-20.398	1.00	0.43	1SG1048
	ATOM	1048	N	TYR	129	34.557	61.737	-22.075	1.00	0.26	1SG1049
	ATOM	1049	CA	TYR	129	33.811	60.931	-22.993	1.00	0.26	1SG1050
60	ATOM	1050	CB	TYR	129	33.135	61.748	-24.108	1.00	0.26	1SG1051
	ATOM	1051	CG	TYR	129	32.753	60.810	-25.201	1.00	0.26	1SG1052
	ATOM	1052	CD1	TYR	129	31.645	59.997	-25.109	1.00	0.26	1SG1053
	ATOM	1053	CD2	TYR	129	33.524	60.758	-26.339	1.00	0.26	1SG1054
	ATOM	1054	CE1	TYR	129	31.320	59.142	-26.139	1.00	0.26	1SG1055
65	ATOM	1055	CE2	TYR	129	33.205	59.908	-27.369	1.00	0.26	1SG1056
	ATOM	1056	CZ	TYR	129	32.101	59.099	-27.271	1.00	0.26	1SG1057
	ATOM	1057	OH	TYR	129	31.779	58.229	-28.332	1.00	0.26	1SG1058
	ATOM	1058	C	TYR	129	34.778	59.999	-23.647	1.00	0.26	1SG1059
	ATOM	1059	O	TYR	129	35.824	60.422	-24.135	1.00	0.26	1SG1060
70	ATOM	1060	N	TRP	130	34.462	58.689	-23.653	1.00	0.16	1SG1061
	ATOM	1061	CA	TRP	130	35.333	57.766	-24.319	1.00	0.16	1SG1062

	ATOM	1062	CB	TRP	130	36.317	57.060	-23.376	1.00	0.16	1SG1063
	ATOM	1063	CG	TRP	130	37.415	56.304	-24.085	1.00	0.16	1SG1064
	ATOM	1064	CD2	TRP	130	38.743	56.820	-24.263	1.00	0.16	1SG1065
5	ATOM	1065	CD1	TRP	130	37.411	55.054	-24.630	1.00	0.16	1SG1066
	ATOM	1066	NE1	TRP	130	38.651	54.765	-25.146	1.00	0.16	1SG1067
	ATOM	1067	CE2	TRP	130	39.481	55.840	-24.923	1.00	0.16	1SG1068
	ATOM	1068	CE3	TRP	130	39.304	58.011	-23.900	1.00	0.16	1SG1069
	ATOM	1069	CZ2	TRP	130	40.797	56.035	-25.232	1.00	0.16	1SG1070
10	ATOM	1070	CZ3	TRP	130	40.631	58.206	-24.218	1.00	0.16	1SG1071
	ATOM	1071	CH2	TRP	130	41.364	57.237	-24.872	1.00	0.16	1SG1072
	ATOM	1072	C	TRP	130	34.445	56.710	-24.894	1.00	0.16	1SG1073
	ATOM	1073	O	TRP	130	33.462	56.312	-24.270	1.00	0.16	1SG1074
	ATOM	1074	N	TYR	131	34.742	56.241	-26.120	1.00	0.17	1SG1075
15	ATOM	1075	CA	TYR	131	33.876	55.242	-26.671	1.00	0.17	1SG1076
	ATOM	1076	CB	TYR	131	34.256	54.830	-28.102	1.00	0.17	1SG1077
	ATOM	1077	CG	TYR	131	33.897	55.923	-29.045	1.00	0.17	1SG1078
	ATOM	1078	CD1	TYR	131	34.677	57.051	-29.158	1.00	0.17	1SG1079
	ATOM	1079	CD2	TYR	131	32.777	55.801	-29.833	1.00	0.17	1SG1080
20	ATOM	1080	CE1	TYR	131	34.335	58.049	-30.040	1.00	0.17	1SG1081
	ATOM	1081	CE2	TYR	131	32.430	56.794	-30.716	1.00	0.17	1SG1082
	ATOM	1082	CZ	TYR	131	33.211	57.920	-30.821	1.00	0.17	1SG1083
	ATOM	1083	OH	TYR	131	32.855	58.940	-31.729	1.00	0.17	1SG1084
	ATOM	1084	C	TYR	131	33.952	53.988	-25.858	1.00	0.17	1SG1085
25	ATOM	1085	O	TYR	131	32.949	53.520	-25.323	1.00	0.17	1SG1086
	ATOM	1086	N	GLU	132	35.164	53.409	-25.753	1.00	0.19	1SG1087
	ATOM	1087	CA	GLU	132	35.336	52.145	-25.095	1.00	0.19	1SG1088
	ATOM	1088	CB	GLU	132	36.595	51.383	-25.550	1.00	0.19	1SG1089
	ATOM	1089	CG	GLU	132	37.918	52.085	-25.259	1.00	0.19	1SG1090
30	ATOM	1090	CD	GLU	132	39.023	51.244	-25.885	1.00	0.19	1SG1091
	ATOM	1091	OE1	GLU	132	38.999	49.998	-25.702	1.00	0.19	1SG1092
	ATOM	1092	OE2	GLU	132	39.905	51.838	-26.561	1.00	0.19	1SG1093
	ATOM	1093	C	GLU	132	35.334	52.226	-23.595	1.00	0.19	1SG1094
	ATOM	1094	O	GLU	132	34.804	51.333	-22.938	1.00	0.19	1SG1095
35	ATOM	1095	N	ASN	133	35.901	53.300	-23.008	1.00	0.18	1SG1096
	ATOM	1096	CA	ASN	133	36.132	53.303	-21.586	1.00	0.18	1SG1097
	ATOM	1097	CB	ASN	133	37.146	54.366	-21.119	1.00	0.18	1SG1098
	ATOM	1098	CG	ASN	133	37.569	54.017	-19.697	1.00	0.18	1SG1099
	ATOM	1099	OD1	ASN	133	36.964	53.162	-19.050	1.00	0.18	1SG1100
40	ATOM	1100	ND2	ASN	133	38.631	54.700	-19.191	1.00	0.18	1SG1101
	ATOM	1101	C	ASN	133	34.876	53.504	-20.800	1.00	0.18	1SG1102
	ATOM	1102	O	ASN	133	34.256	54.566	-20.828	1.00	0.18	1SG1103
	ATOM	1103	N	HIS	134	34.477	52.431	-20.089	1.00	0.16	1SG1104
	ATOM	1104	CA	HIS	134	33.342	52.361	-19.214	1.00	0.16	1SG1105
45	ATOM	1105	ND1	HIS	134	31.445	50.137	-20.751	1.00	0.16	1SG1106
	ATOM	1106	CG	HIS	134	32.655	50.103	-20.093	1.00	0.16	1SG1107
	ATOM	1107	CB	HIS	134	32.970	50.911	-18.870	1.00	0.16	1SG1108
	ATOM	1108	NE2	HIS	134	32.738	48.717	-21.871	1.00	0.16	1SG1109
	ATOM	1109	CD2	HIS	134	33.432	49.231	-20.790	1.00	0.16	1SG1110
50	ATOM	1110	CE1	HIS	134	31.550	49.291	-21.805	1.00	0.16	1SG1111
	ATOM	1111	C	HIS	134	33.620	53.068	-17.920	1.00	0.16	1SG1112
	ATOM	1112	O	HIS	134	32.711	53.632	-17.314	1.00	0.16	1SG1113
	ATOM	1113	N	ASN	135	34.887	53.046	-17.453	1.00	0.14	1SG1114
	ATOM	1114	CA	ASN	135	35.191	53.542	-16.136	1.00	0.14	1SG1115
55	ATOM	1115	CB	ASN	135	36.182	52.646	-15.379	1.00	0.14	1SG1116
	ATOM	1116	CG	ASN	135	35.543	51.277	-15.216	1.00	0.14	1SG1117
	ATOM	1117	OD1	ASN	135	34.446	51.144	-14.676	1.00	0.14	1SG1118
	ATOM	1118	ND2	ASN	135	36.246	50.224	-15.714	1.00	0.14	1SG1119
	ATOM	1119	C	ASN	135	35.824	54.896	-16.197	1.00	0.14	1SG1120
60	ATOM	1120	O	ASN	135	36.357	55.313	-17.223	1.00	0.14	1SG1121
	ATOM	1121	N	ILE	136	35.735	55.630	-15.065	1.00	0.19	1SG1122
	ATOM	1122	CA	ILE	136	36.343	56.921	-14.918	1.00	0.19	1SG1123
	ATOM	1123	CB	ILE	136	35.366	58.059	-14.963	1.00	0.19	1SG1124
	ATOM	1124	CG2	ILE	136	34.435	57.932	-13.746	1.00	0.19	1SG1125
65	ATOM	1125	CG1	ILE	136	36.110	59.402	-15.040	1.00	0.19	1SG1126
	ATOM	1126	CD1	ILE	136	35.202	60.579	-15.391	1.00	0.19	1SG1127
	ATOM	1127	C	ILE	136	36.965	56.952	-13.559	1.00	0.19	1SG1128
	ATOM	1128	O	ILE	136	36.449	56.350	-12.619	1.00	0.19	1SG1129
	ATOM	1129	N	SER	137	38.112	57.642	-13.419	1.00	0.24	1SG1130
70	ATOM	1130	CA	SER	137	38.739	57.700	-12.133	1.00	0.24	1SG1131
	ATOM	1131	CB	SER	137	39.970	56.783	-12.034	1.00	0.24	1SG1132
	ATOM	1132	OG	SER	137	40.555	56.873	-10.745	1.00	0.24	1SG1133

	ATOM	1133	C	SER	137	39.198	59.104	-11.907	1.00	0.24	1SG1134
	ATOM	1134	O	SER	137	39.686	59.763	-12.823	1.00	0.24	1SG1135
	ATOM	1135	N	ILE	138	39.035	59.607	-10.670	1.00	0.31	1SG1136
5	ATOM	1136	CA	ILE	138	39.486	60.933	-10.378	1.00	0.31	1SG1137
	ATOM	1137	CB	ILE	138	38.419	61.805	-9.789	1.00	0.31	1SG1138
	ATOM	1138	CG2	ILE	138	39.058	63.162	-9.443	1.00	0.31	1SG1139
	ATOM	1139	CG1	ILE	138	37.227	61.911	-10.757	1.00	0.31	1SG1140
	ATOM	1140	CD1	ILE	138	35.963	62.479	-10.116	1.00	0.31	1SG1141
10	ATOM	1141	C	ILE	138	40.547	60.785	-9.343	1.00	0.31	1SG1142
	ATOM	1142	O	ILE	138	40.328	60.190	-8.290	1.00	0.31	1SG1143
	ATOM	1143	N	THR	139	41.743	61.328	-9.610	1.00	0.40	1SG1144
	ATOM	1144	CA	THR	139	42.788	61.172	-8.648	1.00	0.40	1SG1145
	ATOM	1145	CB	THR	139	44.128	60.908	-9.262	1.00	0.40	1SG1146
15	ATOM	1146	OG1	THR	139	44.467	61.963	-10.149	1.00	0.40	1SG1147
	ATOM	1147	CG2	THR	139	44.075	59.569	-10.013	1.00	0.40	1SG1148
	ATOM	1148	C	THR	139	42.873	62.438	-7.870	1.00	0.40	1SG1149
	ATOM	1149	O	THR	139	42.513	63.503	-8.369	1.00	0.40	1SG1150
20	ATOM	1150	N	ASN	140	43.351	62.333	-6.613	1.00	0.29	1SG1151
	ATOM	1151	CA	ASN	140	43.471	63.472	-5.750	1.00	0.29	1SG1152
	ATOM	1152	CB	ASN	140	44.596	64.437	-6.160	1.00	0.29	1SG1153
	ATOM	1153	CG	ASN	140	45.928	63.762	-5.868	1.00	0.29	1SG1154
	ATOM	1154	OD1	ASN	140	46.306	62.785	-6.513	1.00	0.29	1SG1155
	ATOM	1155	ND2	ASN	140	46.667	64.304	-4.864	1.00	0.29	1SG1156
25	ATOM	1156	C	ASN	140	42.181	64.224	-5.754	1.00	0.29	1SG1157
	ATOM	1157	O	ASN	140	42.115	65.358	-6.226	1.00	0.29	1SG1158
	ATOM	1158	N	ALA	141	41.113	63.595	-5.227	1.00	0.26	1SG1159
	ATOM	1159	CA	ALA	141	39.821	64.215	-5.216	1.00	0.26	1SG1160
	ATOM	1160	CB	ALA	141	38.719	63.333	-4.603	1.00	0.26	1SG1161
30	ATOM	1161	C	ALA	141	39.898	65.471	-4.413	1.00	0.26	1SG1162
	ATOM	1162	O	ALA	141	40.719	65.603	-3.507	1.00	0.26	1SG1163
	ATOM	1163	N	THR	142	39.031	66.442	-4.762	1.00	0.35	1SG1164
	ATOM	1164	CA	THR	142	38.998	67.708	-4.097	1.00	0.35	1SG1165
	ATOM	1165	CB	THR	142	39.528	68.833	-4.935	1.00	0.35	1SG1166
35	ATOM	1166	OG1	THR	142	39.621	70.022	-4.165	1.00	0.35	1SG1167
	ATOM	1167	CG2	THR	142	38.582	69.043	-6.130	1.00	0.35	1SG1168
	ATOM	1168	C	THR	142	37.569	68.019	-3.789	1.00	0.35	1SG1169
	ATOM	1169	O	THR	142	36.665	67.266	-4.145	1.00	0.35	1SG1170
	ATOM	1170	N	VAL	143	37.343	69.150	-3.095	1.00	0.29	1SG1171
40	ATOM	1171	CA	VAL	143	36.032	69.574	-2.700	1.00	0.29	1SG1172
	ATOM	1172	CB	VAL	143	36.059	70.811	-1.856	1.00	0.29	1SG1173
	ATOM	1173	CG1	VAL	143	34.611	71.189	-1.502	1.00	0.29	1SG1174
	ATOM	1174	CG2	VAL	143	36.953	70.542	-0.631	1.00	0.29	1SG1175
	ATOM	1175	C	VAL	143	35.226	69.861	-3.926	1.00	0.29	1SG1176
45	ATOM	1176	O	VAL	143	34.025	69.598	-3.970	1.00	0.29	1SG1177
	ATOM	1177	N	GLU	144	35.880	70.403	-4.967	1.00	0.25	1SG1178
	ATOM	1178	CA	GLU	144	35.205	70.752	-6.183	1.00	0.25	1SG1179
	ATOM	1179	CB	GLU	144	36.143	71.376	-7.228	1.00	0.25	1SG1180
	ATOM	1180	CG	GLU	144	36.668	72.746	-6.801	1.00	0.25	1SG1181
50	ATOM	1181	CD	GLU	144	37.666	72.520	-5.676	1.00	0.25	1SG1182
	ATOM	1182	OE1	GLU	144	38.780	72.013	-5.971	1.00	0.25	1SG1183
	ATOM	1183	OE2	GLU	144	37.326	72.845	-4.507	1.00	0.25	1SG1184
	ATOM	1184	C	GLU	144	34.635	69.501	-6.767	1.00	0.25	1SG1185
	ATOM	1185	O	GLU	144	33.591	69.521	-7.417	1.00	0.25	1SG1186
55	ATOM	1186	N	ASP	145	35.312	68.367	-6.525	1.00	0.22	1SG1187
	ATOM	1187	CA	ASP	145	34.927	67.107	-7.086	1.00	0.22	1SG1188
	ATOM	1188	CB	ASP	145	35.835	65.959	-6.608	1.00	0.22	1SG1189
	ATOM	1189	CG	ASP	145	35.542	64.709	-7.427	1.00	0.22	1SG1190
	ATOM	1190	OD1	ASP	145	34.357	64.287	-7.484	1.00	0.22	1SG1191
60	ATOM	1191	OD2	ASP	145	36.511	64.160	-8.016	1.00	0.22	1SG1192
	ATOM	1192	C	ASP	145	33.523	66.785	-6.680	1.00	0.22	1SG1193
	ATOM	1193	O	ASP	145	32.759	66.255	-7.486	1.00	0.22	1SG1194
	ATOM	1194	N	SER	146	33.134	67.103	-5.430	1.00	0.20	1SG1195
	ATOM	1195	CA	SER	146	31.813	66.766	-4.974	1.00	0.20	1SG1196
65	ATOM	1196	CB	SER	146	31.492	67.291	-3.563	1.00	0.20	1SG1197
	ATOM	1197	OG	SER	146	31.476	68.711	-3.564	1.00	0.20	1SG1198
	ATOM	1198	C	SER	146	30.806	67.344	-5.914	1.00	0.20	1SG1199
	ATOM	1199	O	SER	146	31.006	68.414	-6.488	1.00	0.20	1SG1200
	ATOM	1200	N	GLY	147	29.691	66.614	-6.114	1.00	0.21	1SG1201
70	ATOM	1201	CA	GLY	147	28.676	67.077	-7.012	1.00	0.21	1SG1202
	ATOM	1202	C	GLY	147	27.818	65.904	-7.348	1.00	0.21	1SG1203
	ATOM	1203	O	GLY	147	27.869	64.869	-6.686	1.00	0.21	1SG1204

150

	ATOM	1204	N	THR	148	26.991	66.048	-8.399	1.00	0.17	1SG1205
	ATOM	1205	CA	THR	148	26.137	64.966	-8.774	1.00	0.17	1SG1206
	ATOM	1206	CB	THR	148	24.735	65.398	-9.070	1.00	0.17	1SG1207
5	ATOM	1207	OG1	THR	148	24.174	66.037	-7.933	1.00	0.17	1SG1208
	ATOM	1208	CG2	THR	148	23.912	64.152	-9.424	1.00	0.17	1SG1209
	ATOM	1209	C	THR	148	26.701	64.381	-10.022	1.00	0.17	1SG1210
	ATOM	1210	O	THR	148	27.063	65.103	-10.949	1.00	0.17	1SG1211
	ATOM	1211	N	TYR	149	26.809	63.040	-10.068	1.00	0.12	1SG1212
10	ATOM	1212	CA	TYR	149	27.360	62.412	-11.231	1.00	0.12	1SG1213
	ATOM	1213	CB	TYR	149	28.585	61.526	-10.948	1.00	0.12	1SG1214
	ATOM	1214	CG	TYR	149	29.753	62.381	-10.600	1.00	0.12	1SG1215
	ATOM	1215	CD1	TYR	149	29.899	62.900	-9.335	1.00	0.12	1SG1216
	ATOM	1216	CD2	TYR	149	30.712	62.647	-11.548	1.00	0.12	1SG1217
15	ATOM	1217	CE1	TYR	149	30.988	63.680	-9.026	1.00	0.12	1SG1218
	ATOM	1218	CE2	TYR	149	31.803	63.425	-11.245	1.00	0.12	1SG1219
	ATOM	1219	CZ	TYR	149	31.940	63.945	-9.981	1.00	0.12	1SG1220
	ATOM	1220	OH	TYR	149	33.057	64.744	-9.663	1.00	0.12	1SG1221
	ATOM	1221	C	TYR	149	26.341	61.495	-11.819	1.00	0.12	1SG1222
20	ATOM	1222	O	TYR	149	25.587	60.836	-11.105	1.00	0.12	1SG1223
	ATOM	1223	N	TYR	150	26.286	61.458	-13.164	1.00	0.12	1SG1224
	ATOM	1224	CA	TYR	150	25.436	60.528	-13.842	1.00	0.12	1SG1225
	ATOM	1225	CB	TYR	150	24.026	61.056	-14.177	1.00	0.12	1SG1226
	ATOM	1226	CG	TYR	150	24.091	62.236	-15.083	1.00	0.12	1SG1227
25	ATOM	1227	CD1	TYR	150	24.135	62.078	-16.450	1.00	0.12	1SG1228
	ATOM	1228	CD2	TYR	150	24.090	63.507	-14.559	1.00	0.12	1SG1229
	ATOM	1229	CE1	TYR	150	24.184	63.175	-17.277	1.00	0.12	1SG1230
	ATOM	1230	CE2	TYR	150	24.140	64.607	-15.380	1.00	0.12	1SG1231
	ATOM	1231	CZ	TYR	150	24.186	64.441	-16.741	1.00	0.12	1SG1232
30	ATOM	1232	OH	TYR	150	24.236	65.569	-17.586	1.00	0.12	1SG1233
	ATOM	1233	C	TYR	150	26.154	60.142	-15.092	1.00	0.12	1SG1234
	ATOM	1234	O	TYR	150	27.127	60.786	-15.483	1.00	0.12	1SG1235
	ATOM	1235	N	CYS	151	25.714	59.054	-15.747	1.00	0.27	1SG1236
	ATOM	1236	CA	CYS	151	26.449	58.615	-16.891	1.00	0.27	1SG1237
35	ATOM	1237	CB	CYS	151	27.202	57.301	-16.613	1.00	0.27	1SG1238
	ATOM	1238	SG	CYS	151	28.205	56.708	-18.002	1.00	0.27	1SG1239
	ATOM	1239	C	CYS	151	25.494	58.381	-18.012	1.00	0.27	1SG1240
	ATOM	1240	O	CYS	151	24.314	58.113	-17.797	1.00	0.27	1SG1241
	ATOM	1241	N	THR	152	25.991	58.533	-19.254	1.00	0.37	1SG1242
40	ATOM	1242	CA	THR	152	25.213	58.239	-20.419	1.00	0.37	1SG1243
	ATOM	1243	CB	THR	152	24.881	59.420	-21.283	1.00	0.37	1SG1244
	ATOM	1244	OG1	THR	152	26.039	60.203	-21.521	1.00	0.37	1SG1245
	ATOM	1245	CG2	THR	152	23.764	60.239	-20.631	1.00	0.37	1SG1246
	ATOM	1246	C	THR	152	25.993	57.273	-21.235	1.00	0.37	1SG1247
45	ATOM	1247	O	THR	152	27.222	57.258	-21.206	1.00	0.37	1SG1248
	ATOM	1248	N	GLY	153	25.276	56.407	-21.972	1.00	0.21	1SG1249
	ATOM	1249	CA	GLY	153	25.949	55.443	-22.782	1.00	0.21	1SG1250
	ATOM	1250	C	GLY	153	24.927	54.865	-23.693	1.00	0.21	1SG1251
	ATOM	1251	O	GLY	153	23.727	54.978	-23.449	1.00	0.21	1SG1252
50	ATOM	1252	N	LYS	154	25.384	54.221	-24.781	1.00	0.12	1SG1253
	ATOM	1253	CA	LYS	154	24.429	53.670	-25.687	1.00	0.12	1SG1254
	ATOM	1254	CB	LYS	154	24.681	54.054	-27.152	1.00	0.12	1SG1255
	ATOM	1255	CG	LYS	154	24.557	55.554	-27.414	1.00	0.12	1SG1256
	ATOM	1256	CD	LYS	154	25.103	55.976	-28.778	1.00	0.12	1SG1257
55	ATOM	1257	CE	LYS	154	24.981	57.477	-29.048	1.00	0.12	1SG1258
	ATOM	1258	NZ	LYS	154	25.536	57.801	-30.382	1.00	0.12	1SG1259
	ATOM	1259	C	LYS	154	24.520	52.188	-25.611	1.00	0.12	1SG1260
	ATOM	1260	O	LYS	154	25.575	51.600	-25.848	1.00	0.12	1SG1261
	ATOM	1261	N	VAL	155	23.395	51.548	-25.250	1.00	0.20	1SG1262
60	ATOM	1262	CA	VAL	155	23.342	50.123	-25.248	1.00	0.20	1SG1263
	ATOM	1263	CB	VAL	155	22.778	49.535	-23.985	1.00	0.20	1SG1264
	ATOM	1264	CG1	VAL	155	23.730	49.874	-22.824	1.00	0.20	1SG1265
	ATOM	1265	CG2	VAL	155	21.347	50.064	-23.790	1.00	0.20	1SG1266
	ATOM	1266	C	VAL	155	22.424	49.793	-26.367	1.00	0.20	1SG1267
65	ATOM	1267	O	VAL	155	21.364	50.401	-26.514	1.00	0.20	1SG1268
	ATOM	1268	N	TRP	156	22.830	48.847	-27.226	1.00	0.33	1SG1269
	ATOM	1269	CA	TRP	156	21.988	48.552	-28.338	1.00	0.33	1SG1270
	ATOM	1270	CB	TRP	156	20.541	48.207	-27.940	1.00	0.33	1SG1271
	ATOM	1271	CG	TRP	156	20.416	46.980	-27.065	1.00	0.33	1SG1272
	ATOM	1272	CD2	TRP	156	20.349	45.628	-27.548	1.00	0.33	1SG1273
70	ATOM	1273	CD1	TRP	156	20.351	46.905	-25.705	1.00	0.33	1SG1274
	ATOM	1274	NE1	TRP	156	20.250	45.593	-25.308	1.00	0.33	1SG1275

151

	ATOM	1275	CE2	TRP	156	20.248	44.795	-26.433	1.00	0.33	1SG1276
	ATOM	1276	CE3	TRP	156	20.371	45.122	-28.816	1.00	0.33	1SG1277
	ATOM	1277	CZ2	TRP	156	20.169	43.438	-26.570	1.00	0.33	1SG1278
	ATOM	1278	CZ3	TRP	156	20.290	43.752	-28.949	1.00	0.33	1SG1279
5	ATOM	1279	CH2	TRP	156	20.191	42.926	-27.848	1.00	0.33	1SG1280
	ATOM	1280	C	TRP	156	21.971	49.807	-29.139	1.00	0.33	1SG1281
	ATOM	1281	O	TRP	156	22.916	50.595	-29.101	1.00	0.33	1SG1282
	ATOM	1282	N	GLN	157	20.880	50.014	-29.892	1.00	0.49	1SG1283
	ATOM	1283	CA	GLN	157	20.742	51.178	-30.711	1.00	0.49	1SG1284
10	ATOM	1284	CB	GLN	157	19.491	51.114	-31.599	1.00	0.49	1SG1285
	ATOM	1285	CG	GLN	157	19.421	49.846	-32.447	1.00	0.49	1SG1286
	ATOM	1286	CD	GLN	157	20.718	49.744	-33.227	1.00	0.49	1SG1287
	ATOM	1287	OE1	GLN	157	21.154	50.709	-33.851	1.00	0.49	1SG1288
	ATOM	1288	NE2	GLN	157	21.358	48.547	-33.180	1.00	0.49	1SG1289
15	ATOM	1289	C	GLN	157	20.571	52.382	-29.842	1.00	0.49	1SG1290
	ATOM	1290	O	GLN	157	21.157	53.433	-30.097	1.00	0.49	1SG1291
	ATOM	1291	N	LEU	158	19.769	52.242	-28.769	1.00	0.41	1SG1292
	ATOM	1292	CA	LEU	158	19.383	53.372	-27.974	1.00	0.41	1SG1293
	ATOM	1293	CB	LEU	158	18.139	53.117	-27.106	1.00	0.41	1SG1294
20	ATOM	1294	CG	LEU	158	16.869	52.845	-27.933	1.00	0.41	1SG1295
	ATOM	1295	CD2	LEU	158	17.020	51.571	-28.782	1.00	0.41	1SG1296
	ATOM	1296	CD1	LEU	158	16.466	54.076	-28.762	1.00	0.41	1SG1297
	ATOM	1297	C	LEU	158	20.476	53.827	-27.067	1.00	0.41	1SG1298
	ATOM	1298	O	LEU	158	21.433	53.107	-26.787	1.00	0.41	1SG1299
25	ATOM	1299	N	ASP	159	20.333	55.089	-26.610	1.00	0.19	1SG1300
	ATOM	1300	CA	ASP	159	21.230	55.721	-25.689	1.00	0.19	1SG1301
	ATOM	1301	CB	ASP	159	21.643	57.142	-26.138	1.00	0.19	1SG1302
	ATOM	1302	CG	ASP	159	22.711	57.750	-25.227	1.00	0.19	1SG1303
	ATOM	1303	OD1	ASP	159	22.869	57.289	-24.067	1.00	0.19	1SG1304
30	ATOM	1304	OD2	ASP	159	23.385	58.706	-25.697	1.00	0.19	1SG1305
	ATOM	1305	C	ASP	159	20.460	55.850	-24.413	1.00	0.19	1SG1306
	ATOM	1306	O	ASP	159	19.280	56.200	-24.424	1.00	0.19	1SG1307
	ATOM	1307	N	TYR	160	21.100	55.535	-23.272	1.00	0.11	1SG1308
	ATOM	1308	CA	TYR	160	20.407	55.630	-22.022	1.00	0.11	1SG1309
35	ATOM	1309	CB	TYR	160	20.273	54.289	-21.280	1.00	0.11	1SG1310
	ATOM	1310	CG	TYR	160	19.308	53.437	-22.031	1.00	0.11	1SG1311
	ATOM	1311	CD1	TYR	160	19.672	52.822	-23.207	1.00	0.11	1SG1312
	ATOM	1312	CD2	TYR	160	18.036	53.241	-21.545	1.00	0.11	1SG1313
	ATOM	1313	CE1	TYR	160	18.776	52.036	-23.892	1.00	0.11	1SG1314
40	ATOM	1314	CE2	TYR	160	17.135	52.456	-22.225	1.00	0.11	1SG1315
	ATOM	1315	CZ	TYR	160	17.506	51.852	-23.402	1.00	0.11	1SG1316
	ATOM	1316	OH	TYR	160	16.587	51.045	-24.106	1.00	0.11	1SG1317
	ATOM	1317	C	TYR	160	21.173	56.539	-21.122	1.00	0.11	1SG1318
	ATOM	1318	O	TYR	160	22.366	56.770	-21.316	1.00	0.11	1SG1319
45	ATOM	1319	N	GLU	161	20.472	57.112	-20.124	1.00	0.12	1SG1320
	ATOM	1320	CA	GLU	161	21.125	57.944	-19.159	1.00	0.12	1SG1321
	ATOM	1321	CB	GLU	161	20.623	59.399	-19.119	1.00	0.12	1SG1322
	ATOM	1322	CG	GLU	161	21.484	60.299	-18.228	1.00	0.12	1SG1323
	ATOM	1323	CD	GLU	161	21.015	61.741	-18.382	1.00	0.12	1SG1324
50	ATOM	1324	OE1	GLU	161	19.816	62.015	-18.112	1.00	0.12	1SG1325
	ATOM	1325	OE2	GLU	161	21.860	62.592	-18.773	1.00	0.12	1SG1326
	ATOM	1326	C	GLU	161	20.870	57.327	-17.824	1.00	0.12	1SG1327
	ATOM	1327	O	GLU	161	19.815	56.739	-17.589	1.00	0.12	1SG1328
	ATOM	1328	N	SER	162	21.860	57.419	-16.919	1.00	0.11	1SG1329
55	ATOM	1329	CA	SER	162	21.729	56.834	-15.619	1.00	0.11	1SG1330
	ATOM	1330	CB	SER	162	23.065	56.348	-15.030	1.00	0.11	1SG1331
	ATOM	1331	OG	SER	162	22.857	55.774	-13.748	1.00	0.11	1SG1332
	ATOM	1332	C	SER	162	21.172	57.852	-14.688	1.00	0.11	1SG1333
	ATOM	1333	O	SER	162	21.083	59.035	-15.012	1.00	0.11	1SG1334
60	ATOM	1334	N	GLU	163	20.754	57.391	-13.495	1.00	0.13	1SG1335
	ATOM	1335	CA	GLU	163	20.245	58.279	-12.496	1.00	0.13	1SG1336
	ATOM	1336	CB	GLU	163	19.399	57.559	-11.433	1.00	0.13	1SG1337
	ATOM	1337	CG	GLU	163	20.166	56.464	-10.691	1.00	0.13	1SG1338
	ATOM	1338	CD	GLU	163	19.148	55.604	-9.957	1.00	0.13	1SG1339
65	ATOM	1339	OE1	GLU	163	18.185	55.142	-10.626	1.00	0.13	1SG1340
	ATOM	1340	OE2	GLU	163	19.315	55.396	-8.726	1.00	0.13	1SG1341
	ATOM	1341	C	GLU	163	21.427	58.899	-11.832	1.00	0.13	1SG1342
	ATOM	1342	O	GLU	163	22.501	58.306	-11.741	1.00	0.13	1SG1343
	ATOM	1343	N	PRO	164	21.247	60.108	-11.395	1.00	0.13	1SG1344
70	ATOM	1344	CA	PRO	164	22.340	60.787	-10.760	1.00	0.13	1SG1345
	ATOM	1345	CD	PRO	164	20.412	61.023	-12.159	1.00	0.13	1SG1346

152

	ATOM	1346	CB	PRO	164	21.993	62.271	-10.814	1.00	0.13	1SG1347
	ATOM	1347	CG	PRO	164	21.098	62.393	-12.057	1.00	0.13	1SG1348
	ATOM	1348	C	PRO	164	22.582	60.282	-9.378	1.00	0.13	1SG1349
	ATOM	1349	O	PRO	164	21.649	59.793	-8.745	1.00	0.13	1SG1350
5	ATOM	1350	N	LEU	165	23.838	60.371	-8.902	1.00	0.11	1SG1351
	ATOM	1351	CA	LEU	165	24.145	59.970	-7.563	1.00	0.11	1SG1352
	ATOM	1352	CB	LEU	165	25.043	58.726	-7.474	1.00	0.11	1SG1353
	ATOM	1353	CG	LEU	165	24.393	57.464	-8.071	1.00	0.11	1SG1354
10	ATOM	1354	CD2	LEU	165	22.957	57.275	-7.560	1.00	0.11	1SG1355
	ATOM	1355	CD1	LEU	165	25.276	56.226	-7.849	1.00	0.11	1SG1356
	ATOM	1356	C	LEU	165	24.887	61.114	-6.959	1.00	0.11	1SG1357
	ATOM	1357	O	LEU	165	25.628	61.811	-7.650	1.00	0.11	1SG1358
	ATOM	1358	N	ASN	166	24.696	61.358	-5.650	1.00	0.10	1SG1359
	ATOM	1359	CA	ASN	166	25.384	62.468	-5.065	1.00	0.10	1SG1360
15	ATOM	1360	CB	ASN	166	24.587	63.214	-3.980	1.00	0.10	1SG1361
	ATOM	1361	CG	ASN	166	23.476	64.012	-4.647	1.00	0.10	1SG1362
	ATOM	1362	OD1	ASN	166	23.226	63.888	-5.845	1.00	0.10	1SG1363
	ATOM	1363	ND2	ASN	166	22.794	64.872	-3.846	1.00	0.10	1SG1364
20	ATOM	1364	C	ASN	166	26.621	61.954	-4.414	1.00	0.10	1SG1365
	ATOM	1365	O	ASN	166	26.569	61.093	-3.537	1.00	0.10	1SG1366
	ATOM	1366	N	ILE	167	27.780	62.472	-4.857	1.00	0.22	1SG1367
	ATOM	1367	CA	ILE	167	29.021	62.087	-4.261	1.00	0.22	1SG1368
	ATOM	1368	CB	ILE	167	30.024	61.566	-5.249	1.00	0.22	1SG1369
25	ATOM	1369	CG2	ILE	167	31.364	61.380	-4.515	1.00	0.22	1SG1370
	ATOM	1370	CG1	ILE	167	29.500	60.285	-5.918	1.00	0.22	1SG1371
	ATOM	1371	CD1	ILE	167	30.315	59.855	-7.138	1.00	0.22	1SG1372
	ATOM	1372	C	ILE	167	29.588	63.326	-3.662	1.00	0.22	1SG1373
	ATOM	1373	O	ILE	167	29.637	64.372	-4.306	1.00	0.22	1SG1374
30	ATOM	1374	N	THR	168	30.016	63.251	-2.391	1.00	0.48	1SG1375
	ATOM	1375	CA	THR	168	30.555	64.431	-1.790	1.00	0.48	1SG1376
	ATOM	1376	CB	THR	168	29.789	64.932	-0.603	1.00	0.48	1SG1377
	ATOM	1377	OG1	THR	168	29.672	63.906	0.372	1.00	0.48	1SG1378
	ATOM	1378	CG2	THR	168	28.411	65.422	-1.054	1.00	0.48	1SG1379
35	ATOM	1379	C	THR	168	31.917	64.138	-1.288	1.00	0.48	1SG1380
	ATOM	1380	O	THR	168	32.229	63.015	-0.894	1.00	0.48	1SG1381
	ATOM	1381	N	VAL	169	32.784	65.163	-1.315	1.00	0.55	1SG1382
	ATOM	1382	CA	VAL	169	34.061	64.960	-0.722	1.00	0.55	1SG1383
	ATOM	1383	CB	VAL	169	35.186	65.749	-1.338	1.00	0.55	1SG1384
40	ATOM	1384	CG1	VAL	169	35.366	65.272	-2.785	1.00	0.55	1SG1385
	ATOM	1385	CG2	VAL	169	34.903	67.254	-1.220	1.00	0.55	1SG1386
	ATOM	1386	C	VAL	169	33.871	65.395	0.689	1.00	0.55	1SG1387
	ATOM	1387	O	VAL	169	33.425	66.509	0.960	1.00	0.55	1SG1388
	ATOM	1388	N	ILE	170	34.178	64.492	1.631	1.00	0.56	1SG1389
45	ATOM	1389	CA	ILE	170	33.974	64.776	3.017	1.00	0.56	1SG1390
	ATOM	1390	CB	ILE	170	34.332	63.609	3.909	1.00	0.56	1SG1391
	ATOM	1391	CG2	ILE	170	35.849	63.375	3.822	1.00	0.56	1SG1392
	ATOM	1392	CG1	ILE	170	33.816	63.807	5.348	1.00	0.56	1SG1393
	ATOM	1393	CD1	ILE	170	34.469	64.961	6.108	1.00	0.56	1SG1394
50	ATOM	1394	C	ILE	170	34.831	65.949	3.356	1.00	0.56	1SG1395
	ATOM	1395	O	ILE	170	34.414	66.833	4.103	1.00	0.56	1SG1396
	ATOM	1396	N	LYS	171	36.052	65.993	2.792	1.00	0.52	1SG1397
	ATOM	1397	CA	LYS	171	36.958	67.069	3.063	1.00	0.52	1SG1398
	ATOM	1398	CB	LYS	171	38.241	66.953	2.216	1.00	0.52	1SG1399
55	ATOM	1399	CG	LYS	171	39.411	67.838	2.650	1.00	0.52	1SG1400
	ATOM	1400	CD	LYS	171	39.151	69.334	2.515	1.00	0.52	1SG1401
	ATOM	1401	CE	LYS	171	40.396	70.193	2.745	1.00	0.52	1SG1402
	ATOM	1402	NZ	LYS	171	40.985	69.879	4.064	1.00	0.52	1SG1403
	ATOM	1403	C	LYS	171	36.237	68.329	2.704	1.00	0.52	1SG1404
60	ATOM	1404	O	LYS	171	35.772	68.490	1.578	1.00	0.52	1SG1405
	ATOM	1405	N	ALA	172	36.106	69.253	3.677	1.00	0.31	1SG1406
	ATOM	1406	CA	ALA	172	35.369	70.457	3.427	1.00	0.31	1SG1407
	ATOM	1407	CB	ALA	172	34.326	70.764	4.515	1.00	0.31	1SG1408
	ATOM	1408	C	ALA	172	36.321	71.645	3.385	1.00	0.31	1SG1409
65	ATOM	1409	O	ALA	172	35.863	72.767	3.726	1.00	0.31	1SG1410
	ATOM	1410	OXT	ALA	172	37.507	71.460	3.008	1.00	0.31	1SG1411
	END										

TABLE 4

REMARK Model of the Fc Epsilon Receptor I 'dimer'; V.C. Epa, 28/08/98.

153

	ATOM	1	N	VAL	A	1	35.035	67.423	-3.312	1.00	0.14	N1+
	ATOM	2	CA	VAL	A	1	36.312	67.082	-2.644	1.00	0.14	C
	ATOM	3	C	VAL	A	1	36.557	67.737	-1.314	1.00	0.14	C
5	ATOM	4	O	VAL	A	1	37.357	67.213	-0.542	1.00	0.14	O
	ATOM	5	CB	VAL	A	1	37.484	67.327	-3.566	1.00	0.14	C
	ATOM	6	CG1	VAL	A	1	37.364	66.351	-4.747	1.00	0.14	C
	ATOM	7	CG2	VAL	A	1	37.528	68.799	-4.005	1.00	0.14	C
	ATOM	8	1H	VAL	A	1	34.869	66.862	-4.138	1.00	0.00	H
10	ATOM	9	2H	VAL	A	1	34.241	67.268	-2.703	1.00	0.00	H
	ATOM	10	3H	VAL	A	1	34.995	68.390	-3.602	1.00	0.00	H
	ATOM	11	HA	VAL	A	1	36.235	66.006	-2.400	1.00	0.00	H
	ATOM	12	HB	VAL	A	1	38.411	67.089	-3.011	1.00	0.00	H
	ATOM	13	1HG1	VAL	A	1	38.229	66.431	-5.429	1.00	0.00	H
15	ATOM	14	2HG1	VAL	A	1	37.326	65.302	-4.406	1.00	0.00	H
	ATOM	15	3HG1	VAL	A	1	36.463	66.547	-5.351	1.00	0.00	H
	ATOM	16	1HG2	VAL	A	1	38.228	68.883	-4.860	1.00	0.00	H
	ATOM	17	2HG2	VAL	A	1	36.576	69.170	-4.412	1.00	0.00	H
	ATOM	18	3HG2	VAL	A	1	38.001	69.445	-3.249	1.00	0.00	H
20	ATOM	19	N	PRO	A	2	35.933	68.836	-0.959	1.00	0.15	N
	ATOM	20	CA	PRO	A	2	36.195	69.325	0.363	1.00	0.15	C
	ATOM	21	C	PRO	A	2	35.493	68.456	1.350	1.00	0.15	C
	ATOM	22	O	PRO	A	2	34.546	67.769	0.973	1.00	0.15	O
	ATOM	23	CB	PRO	A	2	35.731	70.778	0.391	1.00	0.15	C
25	ATOM	24	CG	PRO	A	2	35.897	71.231	-1.067	1.00	0.15	C
	ATOM	25	CD	PRO	A	2	35.709	69.942	-1.884	1.00	0.15	C
	ATOM	26	HA	PRO	A	2	37.285	69.336	0.558	1.00	0.00	H
	ATOM	27	1HB	PRO	A	2	36.304	71.370	1.118	1.00	0.00	H
	ATOM	28	2HB	PRO	A	2	34.669	70.840	0.677	1.00	0.00	H
30	ATOM	29	1HG	PRO	A	2	36.917	71.626	-1.212	1.00	0.00	H
	ATOM	30	2HG	PRO	A	2	35.203	72.033	-1.366	1.00	0.00	H
	ATOM	31	1HD	PRO	A	2	34.667	69.886	-2.239	1.00	0.00	H
	ATOM	32	2HD	PRO	A	2	36.339	70.042	-2.732	1.00	0.00	H
	ATOM	33	N	GLN	A	3	35.941	68.473	2.617	1.00	0.19	N
35	ATOM	34	CA	GLN	A	3	35.329	67.651	3.614	1.00	0.19	C
	ATOM	35	C	GLN	A	3	33.901	68.073	3.703	1.00	0.19	C
	ATOM	36	O	GLN	A	3	33.553	69.196	3.339	1.00	0.19	O
	ATOM	37	CB	GLN	A	3	35.986	67.803	4.996	1.00	0.19	C
	ATOM	38	CG	GLN	A	3	35.493	66.802	6.040	1.00	0.19	C
40	ATOM	39	CD	GLN	A	3	36.327	67.022	7.293	1.00	0.19	C
	ATOM	40	OE1	GLN	A	3	36.930	68.079	7.467	1.00	0.19	O
	ATOM	41	NE2	GLN	A	3	36.374	65.997	8.185	1.00	0.19	N
	ATOM	42	H	GLN	A	3	36.686	69.083	2.909	1.00	0.00	H
	ATOM	43	HA	GLN	A	3	35.401	66.596	3.289	1.00	0.00	H
45	ATOM	44	1HB	GLN	A	3	35.828	68.836	5.351	1.00	0.00	H
	ATOM	45	2HB	GLN	A	3	37.076	67.663	4.874	1.00	0.00	H
	ATOM	46	1HG	GLN	A	3	35.596	65.769	5.669	1.00	0.00	H
	ATOM	47	2HG	GLN	A	3	34.444	66.987	6.303	1.00	0.00	H
	ATOM	48	1HE2	GLN	A	3	36.281	65.050	7.857	1.00	0.00	H
50	ATOM	49	2HE2	GLN	A	3	37.049	66.168	8.921	1.00	0.00	H
	ATOM	50	N	LYS	A	4	33.024	67.165	4.172	1.00	0.23	N
	ATOM	51	CA	LYS	A	4	31.626	67.476	4.219	1.00	0.23	C
	ATOM	52	C	LYS	A	4	31.282	67.937	5.594	1.00	0.23	C
	ATOM	53	O	LYS	A	4	31.667	67.348	6.603	1.00	0.23	O
55	ATOM	54	CB	LYS	A	4	30.722	66.273	3.904	1.00	0.23	C
	ATOM	55	CG	LYS	A	4	30.861	65.765	2.467	1.00	0.23	C
	ATOM	56	CD	LYS	A	4	30.229	64.389	2.241	1.00	0.23	C
	ATOM	57	CE	LYS	A	4	31.032	63.242	2.856	1.00	0.23	C
	ATOM	58	NZ	LYS	A	4	30.320	61.959	2.659	1.00	0.23	N1+
60	ATOM	59	H	LYS	A	4	33.282	66.218	4.377	1.00	0.00	H
	ATOM	60	HA	LYS	A	4	31.442	68.204	3.416	1.00	0.00	H
	ATOM	61	1HB	LYS	A	4	29.665	66.523	4.096	1.00	0.00	H
	ATOM	62	2HB	LYS	A	4	30.952	65.468	4.623	1.00	0.00	H
	ATOM	63	1HG	LYS	A	4	31.919	65.737	2.150	1.00	0.00	H
65	ATOM	64	2HG	LYS	A	4	30.360	66.486	1.801	1.00	0.00	H
	ATOM	65	1HD	LYS	A	4	30.132	64.216	1.154	1.00	0.00	H
	ATOM	66	2HD	LYS	A	4	29.200	64.402	2.645	1.00	0.00	H
	ATOM	67	1HE	LYS	A	4	31.168	63.364	3.942	1.00	0.00	H
	ATOM	68	2HE	LYS	A	4	32.027	63.149	2.391	1.00	0.00	H
70	ATOM	69	1HZ	LYS	A	4	30.819	61.167	3.042	1.00	0.00	H
	ATOM	70	2HZ	LYS	A	4	29.420	61.981	3.134	1.00	0.00	H
	ATOM	71	3HZ	LYS	A	4	30.140	61.756	1.685	1.00	0.00	H

154

	ATOM	72	N	PRO	A	5	30.550	69.013	5.616	1.00	0.25	N
	ATOM	73	CA	PRO	A	5	30.108	69.615	6.840	1.00	0.25	C
	ATOM	74	C	PRO	A	5	29.273	68.587	7.522	1.00	0.25	C
5	ATOM	75	O	PRO	A	5	28.730	67.719	6.839	1.00	0.25	O
	ATOM	76	CB	PRO	A	5	29.231	70.784	6.411	1.00	0.25	C
	ATOM	77	CG	PRO	A	5	28.592	70.257	5.112	1.00	0.25	C
	ATOM	78	CD	PRO	A	5	29.678	69.350	4.507	1.00	0.25	C
	ATOM	79	HA	PRO	A	5	30.972	69.906	7.456	1.00	0.00	H
10	ATOM	80	1HB	PRO	A	5	29.730	71.743	6.357	1.00	0.00	H
	ATOM	81	2HB	PRO	A	5	28.453	70.955	7.178	1.00	0.00	H
	ATOM	82	1HG	PRO	A	5	28.174	70.972	4.412	1.00	0.00	H
	ATOM	83	2HG	PRO	A	5	27.910	69.522	5.421	1.00	0.00	H
	ATOM	84	1HD	PRO	A	5	29.236	68.469	4.044	1.00	0.00	H
	ATOM	85	2HD	PRO	A	5	30.320	69.821	3.774	1.00	0.00	H
15	ATOM	86	N	LYS	A	6	29.172	68.639	8.861	1.00	0.35	N
	ATOM	87	CA	LYS	A	6	28.336	67.685	9.520	1.00	0.35	C
	ATOM	88	C	LYS	A	6	27.209	68.437	10.136	1.00	0.35	C
	ATOM	89	O	LYS	A	6	27.391	69.533	10.666	1.00	0.35	O
20	ATOM	90	CB	LYS	A	6	29.033	66.897	10.641	1.00	0.35	C
	ATOM	91	CG	LYS	A	6	30.016	65.843	10.127	1.00	0.35	C
	ATOM	92	CD	LYS	A	6	31.243	66.430	9.427	1.00	0.35	C
	ATOM	93	CE	LYS	A	6	32.218	65.365	8.920	1.00	0.35	C
	ATOM	94	NZ	LYS	A	6	33.370	66.010	8.253	1.00	0.35	N1+
25	ATOM	95	H	LYS	A	6	29.530	69.396	9.434	1.00	0.00	H
	ATOM	96	HA	LYS	A	6	27.947	66.943	8.805	1.00	0.00	H
	ATOM	97	1HB	LYS	A	6	28.241	66.394	11.226	1.00	0.00	H
	ATOM	98	2HB	LYS	A	6	29.641	67.443	11.336	1.00	0.00	H
	ATOM	99	1HG	LYS	A	6	29.498	65.154	9.434	1.00	0.00	H
30	ATOM	100	2HG	LYS	A	6	30.343	65.221	10.981	1.00	0.00	H
	ATOM	101	1HD	LYS	A	6	31.763	67.118	10.116	1.00	0.00	H
	ATOM	102	2HD	LYS	A	6	30.880	67.022	8.600	1.00	0.00	H
	ATOM	103	1HE	LYS	A	6	31.740	64.699	8.183	1.00	0.00	H
	ATOM	104	2HE	LYS	A	6	32.610	64.746	9.743	1.00	0.00	H
35	ATOM	105	1HZ	LYS	A	6	33.989	65.352	7.805	1.00	0.00	H
	ATOM	106	2HZ	LYS	A	6	33.032	66.644	7.532	1.00	0.00	H
	ATOM	107	3HZ	LYS	A	6	33.939	66.555	8.889	1.00	0.00	H
	ATOM	108	N	VAL	A	7	25.995	67.867	10.051	1.00	0.35	N
	ATOM	109	CA	VAL	A	7	24.871	68.517	10.651	1.00	0.35	C
40	ATOM	110	C	VAL	A	7	24.592	67.792	11.922	1.00	0.35	C
	ATOM	111	O	VAL	A	7	24.524	66.564	11.950	1.00	0.35	O
	ATOM	112	CB	VAL	A	7	23.627	68.483	9.806	1.00	0.35	C
	ATOM	113	CG1	VAL	A	7	23.210	67.019	9.585	1.00	0.35	C
	ATOM	114	CG2	VAL	A	7	22.552	69.335	10.499	1.00	0.35	C
45	ATOM	115	H	VAL	A	7	25.821	66.977	9.615	1.00	0.00	H
	ATOM	116	HA	VAL	A	7	25.120	69.575	10.831	1.00	0.00	H
	ATOM	117	HB	VAL	A	7	23.863	68.941	8.827	1.00	0.00	H
	ATOM	118	1HG1	VAL	A	7	22.471	66.965	8.765	1.00	0.00	H
	ATOM	119	2HG1	VAL	A	7	24.031	66.350	9.285	1.00	0.00	H
50	ATOM	120	3HG1	VAL	A	7	22.693	66.586	10.456	1.00	0.00	H
	ATOM	121	1HG2	VAL	A	7	21.678	69.500	9.847	1.00	0.00	H
	ATOM	122	2HG2	VAL	A	7	22.176	68.844	11.412	1.00	0.00	H
	ATOM	123	3HG2	VAL	A	7	22.944	70.315	10.791	1.00	0.00	H
	ATOM	124	N	SER	A	8	24.448	68.548	13.023	1.00	0.17	N
55	ATOM	125	CA	SER	A	8	24.199	67.929	14.287	1.00	0.17	C
	ATOM	126	C	SER	A	8	22.807	68.274	14.689	1.00	0.17	C
	ATOM	127	O	SER	A	8	22.347	69.396	14.481	1.00	0.17	O
	ATOM	128	CB	SER	A	8	25.131	68.420	15.407	1.00	0.17	C
	ATOM	129	OG	SER	A	8	24.819	67.761	16.625	1.00	0.17	O
60	ATOM	130	H	SER	A	8	24.612	69.550	13.018	1.00	0.00	H
	ATOM	131	HA	SER	A	8	24.337	66.838	14.216	1.00	0.00	H
	ATOM	132	1HB	SER	A	8	25.070	69.509	15.536	1.00	0.00	H
	ATOM	133	2HB	SER	A	8	26.175	68.173	15.162	1.00	0.00	H
	ATOM	134	HG	SER	A	8	24.240	68.346	17.142	1.00	0.00	H
65	ATOM	135	N	LEU	A	9	22.092	67.295	15.268	1.00	0.11	N
	ATOM	136	CA	LEU	A	9	20.747	67.539	15.682	1.00	0.11	C
	ATOM	137	C	LEU	A	9	20.696	67.369	17.164	1.00	0.11	C
	ATOM	138	O	LEU	A	9	21.139	66.354	17.700	1.00	0.11	O
	ATOM	139	CB	LEU	A	9	19.749	66.532	15.080	1.00	0.11	C
70	ATOM	140	CG	LEU	A	9	18.287	66.745	15.512	1.00	0.11	C
	ATOM	141	CD1	LEU	A	9	17.732	68.081	14.988	1.00	0.11	C
	ATOM	142	CD2	LEU	A	9	17.418	65.542	15.111	1.00	0.11	C

155

	ATOM	143	H	LEU	A	9	22.476	66.399	15.518	1.00	0.00	H
	ATOM	144	HA	LEU	A	9	20.438	68.549	15.382	1.00	0.00	H
	ATOM	145	1HB	LEU	A	9	20.066	65.510	15.354	1.00	0.00	H
5	ATOM	146	2HB	LEU	A	9	19.815	66.582	13.978	1.00	0.00	H
	ATOM	147	HG	LEU	A	9	18.324	66.981	16.546	1.00	0.00	H
	ATOM	148	1HD1	LEU	A	9	16.651	68.121	15.191	1.00	0.00	H
	ATOM	149	2HD1	LEU	A	9	18.211	68.929	15.488	1.00	0.00	H
	ATOM	150	3HD1	LEU	A	9	17.848	68.122	13.899	1.00	0.00	H
10	ATOM	151	1HD2	LEU	A	9	16.368	65.690	15.400	1.00	0.00	H
	ATOM	152	2HD2	LEU	A	9	17.440	65.417	14.015	1.00	0.00	H
	ATOM	153	3HD2	LEU	A	9	17.775	64.610	15.558	1.00	0.00	H
	ATOM	154	N	ASN	A	10	20.176	68.388	17.872	1.00	0.17	N
	ATOM	155	CA	ASN	A	10	20.046	68.267	19.291	1.00	0.17	C
	ATOM	156	C	ASN	A	10	18.653	68.686	19.623	1.00	0.17	C
15	ATOM	157	O	ASN	A	10	18.240	69.797	19.295	1.00	0.17	O
	ATOM	158	CB	ASN	A	10	20.992	69.194	20.070	1.00	0.17	C
	ATOM	159	CG	ASN	A	10	22.415	68.721	19.819	1.00	0.17	C
	ATOM	160	OD1	ASN	A	10	23.167	69.361	19.086	1.00	0.17	O
20	ATOM	161	ND2	ASN	A	10	22.798	67.574	20.443	1.00	0.17	N
	ATOM	162	H	ASN	A	10	19.900	69.270	17.449	1.00	0.00	H
	ATOM	163	HA	ASN	A	10	20.331	67.257	19.576	1.00	0.00	H
	ATOM	164	1HB	ASN	A	10	20.746	69.138	21.144	1.00	0.00	H
	ATOM	165	2HB	ASN	A	10	20.917	70.239	19.756	1.00	0.00	H
	ATOM	166	1HD2	ASN	A	10	22.193	67.061	21.052	1.00	0.00	H
25	ATOM	167	2HD2	ASN	A	10	23.732	67.251	20.255	1.00	0.00	H
	ATOM	168	N	PRO	A	11	17.897	67.828	20.245	1.00	0.35	N
	ATOM	169	CA	PRO	A	11	18.370	66.510	20.559	1.00	0.35	C
	ATOM	170	C	PRO	A	11	18.404	65.700	19.305	1.00	0.35	C
30	ATOM	171	O	PRO	A	11	17.867	66.139	18.290	1.00	0.35	O
	ATOM	172	CB	PRO	A	11	17.403	65.958	21.604	1.00	0.35	C
	ATOM	173	CG	PRO	A	11	16.865	67.215	22.308	1.00	0.35	C
	ATOM	174	CD	PRO	A	11	16.938	68.307	21.228	1.00	0.35	C
	ATOM	175	HA	PRO	A	11	19.324	66.603	21.103	1.00	0.00	H
35	ATOM	176	1HB	PRO	A	11	17.862	65.215	22.273	1.00	0.00	H
	ATOM	177	2HB	PRO	A	11	16.571	65.464	21.082	1.00	0.00	H
	ATOM	178	1HG	PRO	A	11	17.522	67.473	23.155	1.00	0.00	H
	ATOM	179	2HG	PRO	A	11	15.851	67.097	22.721	1.00	0.00	H
	ATOM	180	1HD	PRO	A	11	15.961	68.435	20.733	1.00	0.00	H
	ATOM	181	2HD	PRO	A	11	17.234	69.288	21.626	1.00	0.00	H
40	ATOM	182	N	PRO	A	12	19.030	64.557	19.364	1.00	0.52	N
	ATOM	183	CA	PRO	A	12	19.156	63.710	18.209	1.00	0.52	C
	ATOM	184	C	PRO	A	12	17.853	63.101	17.809	1.00	0.52	C
	ATOM	185	O	PRO	A	12	17.789	62.501	16.737	1.00	0.52	O
45	ATOM	186	CB	PRO	A	12	20.215	62.672	18.568	1.00	0.52	C
	ATOM	187	CG	PRO	A	12	21.088	63.386	19.613	1.00	0.52	C
	ATOM	188	CD	PRO	A	12	20.128	64.371	20.299	1.00	0.52	C
	ATOM	189	HA	PRO	A	12	19.493	64.305	17.344	1.00	0.00	H
	ATOM	190	1HB	PRO	A	12	20.766	62.306	17.688	1.00	0.00	H
	ATOM	191	2HB	PRO	A	12	19.733	61.793	19.029	1.00	0.00	H
50	ATOM	192	1HG	PRO	A	12	21.889	63.941	19.096	1.00	0.00	H
	ATOM	193	2HG	PRO	A	12	21.583	62.706	20.323	1.00	0.00	H
	ATOM	194	1HD	PRO	A	12	19.742	63.953	21.242	1.00	0.00	H
	ATOM	195	2HD	PRO	A	12	20.663	65.299	20.521	1.00	0.00	H
55	ATOM	196	N	TRP	A	13	16.809	63.231	18.646	1.00	0.35	N
	ATOM	197	CA	TRP	A	13	15.559	62.588	18.359	1.00	0.35	C
	ATOM	198	C	TRP	A	13	15.107	63.016	16.998	1.00	0.35	C
	ATOM	199	O	TRP	A	13	14.934	64.204	16.731	1.00	0.35	O
	ATOM	200	CB	TRP	A	13	14.454	62.959	19.361	1.00	0.35	C
60	ATOM	201	CG	TRP	A	13	14.839	62.683	20.795	1.00	0.35	C
	ATOM	202	CD1	TRP	A	13	14.961	63.559	21.833	1.00	0.35	C
	ATOM	203	CD2	TRP	A	13	15.219	61.396	21.302	1.00	0.35	C
	ATOM	204	NE1	TRP	A	13	15.382	62.897	22.961	1.00	0.35	N
	ATOM	205	CE2	TRP	A	13	15.549	61.564	22.647	1.00	0.35	C
	ATOM	206	CE3	TRP	A	13	15.297	60.175	20.695	1.00	0.35	C
65	ATOM	207	CZ2	TRP	A	13	15.962	60.510	23.408	1.00	0.35	C
	ATOM	208	CZ3	TRP	A	13	15.707	59.110	21.468	1.00	0.35	C
	ATOM	209	CH2	TRP	A	13	16.031	59.276	22.798	1.00	0.35	C
	ATOM	210	H	TRP	A	13	16.881	63.779	19.484	1.00	0.00	H
70	ATOM	211	HA	TRP	A	13	15.723	61.498	18.375	1.00	0.00	H
	ATOM	212	1HB	TRP	A	13	13.543	62.407	19.077	1.00	0.00	H
	ATOM	213	2HB	TRP	A	13	14.206	64.025	19.251	1.00	0.00	H

156

	ATOM	214	HD1	TRP	A	13	14.739	64.617	21.844	1.00	0.00	H
	ATOM	215	HE1	TRP	A	13	15.809	63.343	23.741	1.00	0.00	H
	ATOM	216	HE3	TRP	A	13	15.045	60.031	19.655	1.00	0.00	H
5	ATOM	217	HZ2	TRP	A	13	16.229	60.748	24.420	1.00	0.00	H
	ATOM	218	HZ3	TRP	A	13	15.795	58.114	21.062	1.00	0.00	H
	ATOM	219	HH2	TRP	A	13	16.099	58.366	23.378	1.00	0.00	H
	ATOM	220	N	ASN	A	14	14.933	62.037	16.085	1.00	0.15	N
	ATOM	221	CA	ASN	A	14	14.506	62.327	14.747	1.00	0.15	C
	ATOM	222	C	ASN	A	14	13.076	62.758	14.777	1.00	0.15	C
10	ATOM	223	O	ASN	A	14	12.681	63.681	14.064	1.00	0.15	O
	ATOM	224	CB	ASN	A	14	14.605	61.127	13.785	1.00	0.15	C
	ATOM	225	CG	ASN	A	14	13.588	60.064	14.181	1.00	0.15	C
	ATOM	226	OD1	ASN	A	14	13.408	59.751	15.357	1.00	0.15	O
	ATOM	227	ND2	ASN	A	14	12.882	59.499	13.165	1.00	0.15	N
15	ATOM	228	H	ASN	A	14	15.126	61.062	16.292	1.00	0.00	H
	ATOM	229	HA	ASN	A	14	15.111	63.154	14.342	1.00	0.00	H
	ATOM	230	1HB	ASN	A	14	15.612	60.678	13.806	1.00	0.00	H
	ATOM	231	2HB	ASN	A	14	14.421	61.501	12.763	1.00	0.00	H
	ATOM	232	1HD2	ASN	A	14	12.990	59.778	12.202	1.00	0.00	H
20	ATOM	233	2HD2	ASN	A	14	12.220	58.777	13.379	1.00	0.00	H
	ATOM	234	N	ARG	A	15	12.257	62.093	15.615	1.00	0.13	N
	ATOM	235	CA	ARG	A	15	10.859	62.400	15.668	1.00	0.13	C
	ATOM	236	C	ARG	A	15	10.645	63.247	16.872	1.00	0.13	C
	ATOM	237	O	ARG	A	15	11.086	62.908	17.969	1.00	0.13	O
25	ATOM	238	CB	ARG	A	15	9.961	61.164	15.860	1.00	0.13	C
	ATOM	239	CG	ARG	A	15	9.990	60.171	14.698	1.00	0.13	C
	ATOM	240	CD	ARG	A	15	9.087	58.956	14.925	1.00	0.13	C
	ATOM	241	NE	ARG	A	15	9.233	58.061	13.742	1.00	0.13	N1+
	ATOM	242	CZ	ARG	A	15	8.137	57.682	13.023	1.00	0.13	C
30	ATOM	243	NH1	ARG	A	15	6.892	58.097	13.396	1.00	0.13	N
	ATOM	244	NH2	ARG	A	15	8.289	56.882	11.926	1.00	0.13	N
	ATOM	245	H	ARG	A	15	12.592	61.259	16.078	1.00	0.00	H
	ATOM	246	HA	ARG	A	15	10.563	62.903	14.736	1.00	0.00	H
	ATOM	247	1HB	ARG	A	15	8.996	61.516	16.214	1.00	0.00	H
35	ATOM	248	2HB	ARG	A	15	10.355	60.612	16.738	1.00	0.00	H
	ATOM	249	1HG	ARG	A	15	11.007	59.776	14.648	1.00	0.00	H
	ATOM	250	2HG	ARG	A	15	9.785	60.645	13.726	1.00	0.00	H
	ATOM	251	1HD	ARG	A	15	8.048	59.228	15.153	1.00	0.00	H
	ATOM	252	2HD	ARG	A	15	9.459	58.433	15.807	1.00	0.00	H
40	ATOM	253	HE	ARG	A	15	9.923	57.342	13.749	1.00	0.00	H
	ATOM	254	1HH1	ARG	A	15	6.719	58.668	14.192	1.00	0.00	H
	ATOM	255	2HH1	ARG	A	15	6.069	57.748	12.956	1.00	0.00	H
	ATOM	256	1HH2	ARG	A	15	7.535	56.853	11.277	1.00	0.00	H
	ATOM	257	2HH2	ARG	A	15	9.189	56.912	11.491	1.00	0.00	H
45	ATOM	258	N	ILE	A	16	9.959	64.390	16.699	1.00	0.12	N
	ATOM	259	CA	ILE	A	16	9.719	65.221	17.838	1.00	0.12	C
	ATOM	260	C	ILE	A	16	8.300	65.668	17.781	1.00	0.12	C
	ATOM	261	O	ILE	A	16	7.583	65.394	16.820	1.00	0.12	O
	ATOM	262	CB	ILE	A	16	10.558	66.467	17.883	1.00	0.12	C
50	ATOM	263	CG1	ILE	A	16	10.236	67.383	16.690	1.00	0.12	C
	ATOM	264	CG2	ILE	A	16	12.035	66.048	17.972	1.00	0.12	C
	ATOM	265	CD1	ILE	A	16	10.816	68.789	16.840	1.00	0.12	C
	ATOM	266	H	ILE	A	16	9.590	64.694	15.804	1.00	0.00	H
	ATOM	267	HA	ILE	A	16	9.806	64.637	18.761	1.00	0.00	H
55	ATOM	268	HB	ILE	A	16	10.323	67.011	18.816	1.00	0.00	H
	ATOM	269	1HG1	ILE	A	16	9.151	67.494	16.527	1.00	0.00	H
	ATOM	270	2HG1	ILE	A	16	10.633	66.927	15.766	1.00	0.00	H
	ATOM	271	1HG2	ILE	A	16	12.707	66.907	18.128	1.00	0.00	H
	ATOM	272	2HG2	ILE	A	16	12.205	65.359	18.814	1.00	0.00	H
60	ATOM	273	3HG2	ILE	A	16	12.376	65.543	17.052	1.00	0.00	H
	ATOM	274	1HD1	ILE	A	16	10.934	69.273	15.860	1.00	0.00	H
	ATOM	275	2HD1	ILE	A	16	10.156	69.429	17.440	1.00	0.00	H
	ATOM	276	3HD1	ILE	A	16	11.792	68.758	17.336	1.00	0.00	H
	ATOM	277	N	PHE	A	17	7.862	66.360	18.848	1.00	0.17	N
65	ATOM	278	CA	PHE	A	17	6.527	66.870	18.904	1.00	0.17	C
	ATOM	279	C	PHE	A	17	6.595	68.309	18.543	1.00	0.17	C
	ATOM	280	O	PHE	A	17	7.645	68.943	18.627	1.00	0.17	O
	ATOM	281	CB	PHE	A	17	5.886	66.867	20.300	1.00	0.17	C
	ATOM	282	CG	PHE	A	17	5.562	65.480	20.720	1.00	0.17	C
70	ATOM	283	CD1	PHE	A	17	4.468	64.838	20.192	1.00	0.17	C
	ATOM	284	CD2	PHE	A	17	6.337	64.840	21.657	1.00	0.17	C

157

	ATOM	285	CE1	PHE	A	17	4.154	63.561	20.585	1.00	0.17	C
	ATOM	286	CE2	PHE	A	17	6.027	63.563	22.057	1.00	0.17	C
	ATOM	287	CZ	PHE	A	17	4.935	62.927	21.518	1.00	0.17	C
5	ATOM	288	H	PHE	A	17	8.468	66.690	19.582	1.00	0.00	H
	ATOM	289	HA	PHE	A	17	5.913	66.277	18.229	1.00	0.00	H
	ATOM	290	1HB	PHE	A	17	4.946	67.418	20.184	1.00	0.00	H
	ATOM	291	2HB	PHE	A	17	6.495	67.400	21.041	1.00	0.00	H
	ATOM	292	HD1	PHE	A	17	3.883	65.351	19.440	1.00	0.00	H
10	ATOM	293	HD2	PHE	A	17	7.205	65.348	22.059	1.00	0.00	H
	ATOM	294	HE1	PHE	A	17	3.235	63.140	20.300	1.00	0.00	H
	ATOM	295	HE2	PHE	A	17	6.677	63.097	22.778	1.00	0.00	H
	ATOM	296	HZ	PHE	A	17	4.352	62.236	22.047	1.00	0.00	H
	ATOM	297	N	LYS	A	18	5.446	68.858	18.119	1.00	0.22	N
15	ATOM	298	CA	LYS	A	18	5.403	70.243	17.781	1.00	0.22	C
	ATOM	299	C	LYS	A	18	5.558	70.999	19.056	1.00	0.22	C
	ATOM	300	O	LYS	A	18	5.134	70.546	20.119	1.00	0.22	O
	ATOM	301	CB	LYS	A	18	4.077	70.663	17.126	1.00	0.22	C
	ATOM	302	CG	LYS	A	18	2.859	70.405	18.012	1.00	0.22	C
20	ATOM	303	CD	LYS	A	18	1.586	71.086	17.511	1.00	0.22	C
	ATOM	304	CE	LYS	A	18	0.375	70.870	18.418	1.00	0.22	C
	ATOM	305	NZ	LYS	A	18	-0.743	71.728	17.967	1.00	0.22	N1+
	ATOM	306	H	LYS	A	18	4.641	68.278	17.925	1.00	0.00	H
	ATOM	307	HA	LYS	A	18	6.267	70.377	17.128	1.00	0.00	H
25	ATOM	308	1HB	LYS	A	18	3.964	70.148	16.156	1.00	0.00	H
	ATOM	309	2HB	LYS	A	18	4.150	71.742	16.902	1.00	0.00	H
	ATOM	310	1HG	LYS	A	18	3.038	70.808	19.019	1.00	0.00	H
	ATOM	311	2HG	LYS	A	18	2.689	69.320	18.128	1.00	0.00	H
	ATOM	312	1HD	LYS	A	18	1.354	70.729	16.492	1.00	0.00	H
30	ATOM	313	2HD	LYS	A	18	1.792	72.168	17.428	1.00	0.00	H
	ATOM	314	1HE	LYS	A	18	0.596	71.147	19.461	1.00	0.00	H
	ATOM	315	2HE	LYS	A	18	0.024	69.828	18.411	1.00	0.00	H
	ATOM	316	1HZ	LYS	A	18	-1.576	71.594	18.528	1.00	0.00	H
	ATOM	317	2HZ	LYS	A	18	-0.522	72.713	18.013	1.00	0.00	H
35	ATOM	318	3HZ	LYS	A	18	-1.016	71.517	17.014	1.00	0.00	H
	ATOM	319	N	GLY	A	19	6.207	72.174	18.978	1.00	0.21	N
	ATOM	320	CA	GLY	A	19	6.383	72.980	20.146	1.00	0.21	C
	ATOM	321	C	GLY	A	19	7.708	72.652	20.746	1.00	0.21	C
	ATOM	322	O	GLY	A	19	8.192	73.365	21.623	1.00	0.21	O
40	ATOM	323	H	GLY	A	19	6.494	72.539	18.071	1.00	0.00	H
	ATOM	324	1HA	GLY	A	19	5.676	72.621	20.917	1.00	0.00	H
	ATOM	325	2HA	GLY	A	19	6.080	74.028	20.096	1.00	0.00	H
	ATOM	326	N	GLU	A	20	8.338	71.560	20.281	1.00	0.23	N
	ATOM	327	CA	GLU	A	20	9.610	71.201	20.830	1.00	0.23	C
45	ATOM	328	C	GLU	A	20	10.642	72.074	20.202	1.00	0.23	C
	ATOM	329	O	GLU	A	20	10.428	72.635	19.128	1.00	0.23	O
	ATOM	330	CB	GLU	A	20	10.002	69.736	20.574	1.00	0.23	C
	ATOM	331	CG	GLU	A	20	9.106	68.753	21.327	1.00	0.23	C
	ATOM	332	CD	GLU	A	20	9.228	69.092	22.806	1.00	0.23	C
50	ATOM	333	OE1	GLU	A	20	10.378	69.332	23.263	1.00	0.23	O
	ATOM	334	OE2	GLU	A	20	8.174	69.131	23.495	1.00	0.23	O1-
	ATOM	335	H	GLU	A	20	7.903	70.908	19.641	1.00	0.00	H
	ATOM	336	HA	GLU	A	20	9.596	71.403	21.915	1.00	0.00	H
	ATOM	337	1HB	GLU	A	20	11.054	69.593	20.883	1.00	0.00	H
55	ATOM	338	2HB	GLU	A	20	9.998	69.547	19.493	1.00	0.00	H
	ATOM	339	1HG	GLU	A	20	9.443	67.718	21.165	1.00	0.00	H
	ATOM	340	2HG	GLU	A	20	8.053	68.826	21.031	1.00	0.00	H
	ATOM	341	N	ASN	A	21	11.794	72.224	20.879	1.00	0.16	N
	ATOM	342	CA	ASN	A	21	12.833	73.051	20.346	1.00	0.16	C
60	ATOM	343	C	ASN	A	21	13.814	72.151	19.677	1.00	0.16	C
	ATOM	344	O	ASN	A	21	14.134	71.074	20.179	1.00	0.16	O
	ATOM	345	CB	ASN	A	21	13.589	73.859	21.415	1.00	0.16	C
	ATOM	346	CG	ASN	A	21	12.613	74.885	21.970	1.00	0.16	C
	ATOM	347	OD1	ASN	A	21	11.595	75.174	21.347	1.00	0.16	O
65	ATOM	348	ND2	ASN	A	21	12.923	75.448	23.168	1.00	0.16	N
	ATOM	349	H	ASN	A	21	12.004	71.689	21.705	1.00	0.00	H
	ATOM	350	HA	ASN	A	21	12.376	73.724	19.624	1.00	0.00	H
	ATOM	351	1HB	ASN	A	21	14.424	74.395	20.932	1.00	0.00	H
	ATOM	352	2HB	ASN	A	21	13.999	73.200	22.196	1.00	0.00	H
70	ATOM	353	1HD2	ASN	A	21	13.738	75.183	23.688	1.00	0.00	H
	ATOM	354	2HD2	ASN	A	21	12.260	76.106	23.540	1.00	0.00	H
	ATOM	355	N	VAL	A	22	14.289	72.567	18.490	1.00	0.07	N

	ATOM	356	CA	VAL	A	22	15.243	71.773	17.780	1.00	0.07	C
	ATOM	357	C	VAL	A	22	16.438	72.632	17.559	1.00	0.07	C
	ATOM	358	O	VAL	A	22	16.312	73.813	17.236	1.00	0.07	O
5	ATOM	359	CB	VAL	A	22	14.753	71.331	16.431	1.00	0.07	C
	ATOM	360	CG1	VAL	A	22	15.891	70.592	15.710	1.00	0.07	C
	ATOM	361	CG2	VAL	A	22	13.481	70.487	16.626	1.00	0.07	C
	ATOM	362	H	VAL	A	22	14.067	73.488	18.125	1.00	0.00	H
	ATOM	363	HA	VAL	A	22	15.511	70.880	18.368	1.00	0.00	H
	ATOM	364	HB	VAL	A	22	14.492	72.177	15.798	1.00	0.00	H
10	ATOM	365	1HG1	VAL	A	22	15.529	70.095	14.795	1.00	0.00	H
	ATOM	366	2HG1	VAL	A	22	16.697	71.275	15.398	1.00	0.00	H
	ATOM	367	3HG1	VAL	A	22	16.314	69.825	16.375	1.00	0.00	H
	ATOM	368	1HG2	VAL	A	22	13.124	70.080	15.667	1.00	0.00	H
	ATOM	369	2HG2	VAL	A	22	13.699	69.636	17.292	1.00	0.00	H
15	ATOM	370	3HG2	VAL	A	22	12.657	71.073	17.064	1.00	0.00	H
	ATOM	371	N	THR	A	23	17.641	72.066	17.762	1.00	0.06	N
	ATOM	372	CA	THR	A	23	18.823	72.838	17.530	1.00	0.06	C
	ATOM	373	C	THR	A	23	19.615	72.126	16.486	1.00	0.06	C
	ATOM	374	O	THR	A	23	19.909	70.939	16.612	1.00	0.06	O
20	ATOM	375	CB	THR	A	23	19.704	72.975	18.737	1.00	0.06	C
	ATOM	376	OG1	THR	A	23	18.992	73.612	19.787	1.00	0.06	O
	ATOM	377	CG2	THR	A	23	20.936	73.813	18.353	1.00	0.06	C
	ATOM	378	H	THR	A	23	17.775	71.115	18.098	1.00	0.00	H
	ATOM	379	HA	THR	A	23	18.556	73.850	17.211	1.00	0.00	H
25	ATOM	380	HB	THR	A	23	20.031	71.986	19.091	1.00	0.00	H
	ATOM	381	HG1	THR	A	23	18.059	73.402	19.624	1.00	0.00	H
	ATOM	382	1HG2	THR	A	23	21.551	74.025	19.243	1.00	0.00	H
	ATOM	383	2HG2	THR	A	23	21.585	73.297	17.628	1.00	0.00	H
	ATOM	384	3HG2	THR	A	23	20.634	74.784	17.926	1.00	0.00	H
30	ATOM	385	N	LEU	A	24	19.967	72.846	15.407	1.00	0.06	N
	ATOM	386	CA	LEU	A	24	20.752	72.253	14.368	1.00	0.06	C
	ATOM	387	C	LEU	A	24	22.058	72.966	14.393	1.00	0.06	C
	ATOM	388	O	LEU	A	24	22.104	74.195	14.388	1.00	0.06	O
	ATOM	389	CB	LEU	A	24	20.163	72.461	12.965	1.00	0.06	C
35	ATOM	390	CG	LEU	A	24	18.783	71.804	12.774	1.00	0.06	C
	ATOM	391	CD1	LEU	A	24	18.246	72.039	11.352	1.00	0.06	C
	ATOM	392	CD2	LEU	A	24	18.814	70.318	13.167	1.00	0.06	C
	ATOM	393	H	LEU	A	24	19.688	73.815	15.281	1.00	0.00	H
	ATOM	394	HA	LEU	A	24	20.869	71.185	14.552	1.00	0.00	H
40	ATOM	395	1HB	LEU	A	24	20.876	72.019	12.246	1.00	0.00	H
	ATOM	396	2HB	LEU	A	24	20.105	73.537	12.729	1.00	0.00	H
	ATOM	397	HG	LEU	A	24	18.071	72.302	13.461	1.00	0.00	H
	ATOM	398	1HD1	LEU	A	24	17.231	71.624	11.245	1.00	0.00	H
	ATOM	399	2HD1	LEU	A	24	18.193	73.115	11.117	1.00	0.00	H
45	ATOM	400	3HD1	LEU	A	24	18.893	71.560	10.600	1.00	0.00	H
	ATOM	401	1HD2	LEU	A	24	17.820	69.888	12.973	1.00	0.00	H
	ATOM	402	2HD2	LEU	A	24	19.551	69.756	12.571	1.00	0.00	H
	ATOM	403	3HD2	LEU	A	24	19.059	70.199	14.225	1.00	0.00	H
	ATOM	404	N	THR	A	25	23.167	72.207	14.441	1.00	0.28	N
50	ATOM	405	CA	THR	A	25	24.439	72.857	14.453	1.00	0.28	C
	ATOM	406	C	THR	A	25	25.210	72.309	13.308	1.00	0.28	C
	ATOM	407	O	THR	A	25	25.220	71.106	13.059	1.00	0.28	O
	ATOM	408	CB	THR	A	25	25.235	72.590	15.697	1.00	0.28	C
	ATOM	409	OG1	THR	A	25	24.523	73.038	16.841	1.00	0.28	O
55	ATOM	410	CG2	THR	A	25	26.580	73.327	15.588	1.00	0.28	C
	ATOM	411	H	THR	A	25	23.130	71.194	14.477	1.00	0.00	H
	ATOM	412	HA	THR	A	25	24.322	73.946	14.351	1.00	0.00	H
	ATOM	413	HB	THR	A	25	25.413	71.521	15.855	1.00	0.00	H
	ATOM	414	HG1	THR	A	25	24.344	73.978	16.692	1.00	0.00	H
60	ATOM	415	1HG2	THR	A	25	27.114	73.289	16.552	1.00	0.00	H
	ATOM	416	2HG2	THR	A	25	27.249	72.875	14.839	1.00	0.00	H
	ATOM	417	3HG2	THR	A	25	26.439	74.392	15.338	1.00	0.00	H
	ATOM	418	N	CYS	A	26	25.878	73.197	12.565	1.00	0.52	N
	ATOM	419	CA	CYS	A	26	26.616	72.723	11.446	1.00	0.52	C
65	ATOM	420	C	CYS	A	26	28.050	72.983	11.751	1.00	0.52	C
	ATOM	421	O	CYS	A	26	28.460	74.132	11.908	1.00	0.52	O
	ATOM	422	CB	CYS	A	26	26.230	73.510	10.198	1.00	0.52	C
	ATOM	423	SG	CYS	A	26	27.098	72.999	8.709	1.00	0.52	S
	ATOM	424	H	CYS	A	26	25.870	74.196	12.727	1.00	0.00	H
70	ATOM	425	HA	CYS	A	26	26.399	71.671	11.235	1.00	0.00	H
	ATOM	426	1HB	CYS	A	26	26.355	74.595	10.346	1.00	0.00	H

159

	ATOM	427	2HB	CYS	A	26	25.173	73.319	10.007	1.00	0.00	H
	ATOM	428	N	ASN	A	27	28.853	71.907	11.836	1.00	0.35	N
	ATOM	429	CA	ASN	A	27	30.232	72.073	12.176	1.00	0.35	C
5	ATOM	430	C	ASN	A	27	31.043	71.766	10.964	1.00	0.35	C
	ATOM	431	O	ASN	A	27	30.620	71.010	10.092	1.00	0.35	O
	ATOM	432	CB	ASN	A	27	30.713	71.117	13.280	1.00	0.35	C
	ATOM	433	CG	ASN	A	27	30.594	69.697	12.743	1.00	0.35	C
	ATOM	434	OD1	ASN	A	27	29.551	69.298	12.228	1.00	0.35	O
10	ATOM	435	ND2	ASN	A	27	31.698	68.912	12.855	1.00	0.35	N
	ATOM	436	H	ASN	A	27	28.542	70.946	11.685	1.00	0.00	H
	ATOM	437	HA	ASN	A	27	30.415	73.099	12.532	1.00	0.00	H
	ATOM	438	1HB	ASN	A	27	30.081	71.201	14.180	1.00	0.00	H
	ATOM	439	2HB	ASN	A	27	31.746	71.384	13.557	1.00	0.00	H
15	ATOM	440	1HD2	ASN	A	27	32.530	69.230	13.317	1.00	0.00	H
	ATOM	441	2HD2	ASN	A	27	31.597	67.953	12.575	1.00	0.00	H
	ATOM	442	N	GLY	A	28	32.237	72.381	10.876	1.00	0.15	N
	ATOM	443	CA	GLY	A	28	33.101	72.141	9.762	1.00	0.15	C
	ATOM	444	C	GLY	A	28	33.969	73.345	9.623	1.00	0.15	C
20	ATOM	445	O	GLY	A	28	33.839	74.305	10.382	1.00	0.15	O
	ATOM	446	H	GLY	A	28	32.528	73.118	11.502	1.00	0.00	H
	ATOM	447	1HA	GLY	A	28	32.514	72.014	8.837	1.00	0.00	H
	ATOM	448	2HA	GLY	A	28	33.710	71.234	9.918	1.00	0.00	H
	ATOM	449	N	ASN	A	29	34.882	73.329	8.633	1.00	0.16	N
25	ATOM	450	CA	ASN	A	29	35.730	74.467	8.454	1.00	0.16	C
	ATOM	451	C	ASN	A	29	34.852	75.590	8.021	1.00	0.16	C
	ATOM	452	O	ASN	A	29	33.866	75.388	7.315	1.00	0.16	O
	ATOM	453	CB	ASN	A	29	36.820	74.286	7.382	1.00	0.16	C
	ATOM	454	CG	ASN	A	29	37.876	73.331	7.919	1.00	0.16	C
30	ATOM	455	OD1	ASN	A	29	37.878	72.973	9.096	1.00	0.16	O
	ATOM	456	ND2	ASN	A	29	38.816	72.917	7.029	1.00	0.16	N
	ATOM	457	H	ASN	A	29	35.005	72.548	8.013	1.00	0.00	H
	ATOM	458	HA	ASN	A	29	36.207	74.723	9.419	1.00	0.00	H
	ATOM	459	1HB	ASN	A	29	37.363	75.225	7.240	1.00	0.00	H
35	ATOM	460	2HB	ASN	A	29	36.417	73.884	6.449	1.00	0.00	H
	ATOM	461	1HD2	ASN	A	29	38.833	73.235	6.078	1.00	0.00	H
	ATOM	462	2HD2	ASN	A	29	39.532	72.304	7.380	1.00	0.00	H
	ATOM	463	N	ASN	A	30	35.187	76.815	8.463	1.00	0.16	N
	ATOM	464	CA	ASN	A	30	34.377	77.945	8.127	1.00	0.16	C
40	ATOM	465	C	ASN	A	30	35.268	79.043	7.645	1.00	0.16	C
	ATOM	466	O	ASN	A	30	36.420	79.153	8.060	1.00	0.16	O
	ATOM	467	CB	ASN	A	30	33.609	78.491	9.339	1.00	0.16	C
	ATOM	468	CG	ASN	A	30	32.795	79.688	8.886	1.00	0.16	C
	ATOM	469	OD1	ASN	A	30	32.210	79.707	7.805	1.00	0.16	O
45	ATOM	470	ND2	ASN	A	30	32.781	80.740	9.746	1.00	0.16	N
	ATOM	471	H	ASN	A	30	36.004	77.014	9.015	1.00	0.00	H
	ATOM	472	HA	ASN	A	30	33.660	77.670	7.338	1.00	0.00	H
	ATOM	473	1HB	ASN	A	30	34.308	78.750	10.151	1.00	0.00	H
	ATOM	474	2HB	ASN	A	30	32.904	77.733	9.720	1.00	0.00	H
50	ATOM	475	1HD2	ASN	A	30	33.250	80.708	10.630	1.00	0.00	H
	ATOM	476	2HD2	ASN	A	30	32.054	81.435	9.600	1.00	0.00	H
	ATOM	477	N	PHE	A	31	34.745	79.879	6.724	1.00	0.12	N
	ATOM	478	CA	PHE	A	31	35.486	81.003	6.236	1.00	0.12	C
	ATOM	479	C	PHE	A	31	35.228	82.101	7.212	1.00	0.12	C
55	ATOM	480	O	PHE	A	31	34.243	82.061	7.945	1.00	0.12	O
	ATOM	481	CB	PHE	A	31	35.024	81.481	4.850	1.00	0.12	C
	ATOM	482	CG	PHE	A	31	35.870	82.641	4.458	1.00	0.12	C
	ATOM	483	CD1	PHE	A	31	37.137	82.444	3.958	1.00	0.12	C
	ATOM	484	CD2	PHE	A	31	35.395	83.926	4.581	1.00	0.12	C
60	ATOM	485	CE1	PHE	A	31	37.919	83.513	3.589	1.00	0.12	C
	ATOM	486	CE2	PHE	A	31	36.173	84.999	4.215	1.00	0.12	C
	ATOM	487	CZ	PHE	A	31	37.439	84.793	3.720	1.00	0.12	C
	ATOM	488	H	PHE	A	31	33.732	79.978	6.684	1.00	0.00	H
	ATOM	489	HA	PHE	A	31	36.560	80.758	6.226	1.00	0.00	H
65	ATOM	490	1HB	PHE	A	31	33.955	81.746	4.883	1.00	0.00	H
	ATOM	491	2HB	PHE	A	31	35.127	80.664	4.121	1.00	0.00	H
	ATOM	492	HD1	PHE	A	31	37.521	81.438	3.830	1.00	0.00	H
	ATOM	493	HD2	PHE	A	31	34.399	84.066	4.975	1.00	0.00	H
	ATOM	494	HE1	PHE	A	31	38.916	83.346	3.188	1.00	0.00	H
70	ATOM	495	HE2	PHE	A	31	35.783	86.009	4.316	1.00	0.00	H
	ATOM	496	HZ	PHE	A	31	38.053	85.642	3.428	1.00	0.00	H
	ATOM	497	N	PHE	A	32	36.111	83.113	7.268	1.00	0.11	N

160

	ATOM	498	CA	PHE	A	32	35.851	84.138	8.229	1.00	0.11	C
	ATOM	499	C	PHE	A	32	34.911	85.104	7.598	1.00	0.11	C
	ATOM	500	O	PHE	A	32	35.322	86.086	6.982	1.00	0.11	O
5	ATOM	501	CB	PHE	A	32	37.114	84.895	8.670	1.00	0.11	C
	ATOM	502	CG	PHE	A	32	37.971	83.875	9.336	1.00	0.11	C
	ATOM	503	CD1	PHE	A	32	38.800	83.076	8.583	1.00	0.11	C
	ATOM	504	CD2	PHE	A	32	37.941	83.706	10.700	1.00	0.11	C
	ATOM	505	CE1	PHE	A	32	39.597	82.127	9.178	1.00	0.11	C
10	ATOM	506	CE2	PHE	A	32	38.735	82.758	11.300	1.00	0.11	C
	ATOM	507	CZ	PHE	A	32	39.564	81.967	10.542	1.00	0.11	C
	ATOM	508	H	PHE	A	32	36.835	83.274	6.588	1.00	0.00	H
	ATOM	509	HA	PHE	A	32	35.409	83.699	9.143	1.00	0.00	H
	ATOM	510	1HB	PHE	A	32	36.811	85.700	9.358	1.00	0.00	H
	ATOM	511	2HB	PHE	A	32	37.630	85.368	7.820	1.00	0.00	H
15	ATOM	512	HD1	PHE	A	32	38.864	83.214	7.507	1.00	0.00	H
	ATOM	513	HD2	PHE	A	32	37.287	84.326	11.307	1.00	0.00	H
	ATOM	514	HE1	PHE	A	32	40.252	81.506	8.572	1.00	0.00	H
	ATOM	515	HE2	PHE	A	32	38.705	82.632	12.380	1.00	0.00	H
	ATOM	516	HZ	PHE	A	32	40.190	81.217	11.019	1.00	0.00	H
20	ATOM	517	N	GLU	A	33	33.600	84.832	7.738	1.00	0.10	N
	ATOM	518	CA	GLU	A	33	32.616	85.702	7.171	1.00	0.10	C
	ATOM	519	C	GLU	A	33	31.455	85.739	8.108	1.00	0.10	C
	ATOM	520	O	GLU	A	33	31.273	84.837	8.926	1.00	0.10	O
25	ATOM	521	CB	GLU	A	33	32.084	85.228	5.809	1.00	0.10	C
	ATOM	522	CG	GLU	A	33	31.401	83.860	5.863	1.00	0.10	C
	ATOM	523	CD	GLU	A	33	30.934	83.526	4.456	1.00	0.10	C
	ATOM	524	OE1	GLU	A	33	30.393	84.442	3.782	1.00	0.10	O
	ATOM	525	OE2	GLU	A	33	31.113	82.351	4.035	1.00	0.10	O1-
	ATOM	526	H	GLU	A	33	33.268	83.963	8.132	1.00	0.00	H
30	ATOM	527	HA	GLU	A	33	33.037	86.717	7.082	1.00	0.00	H
	ATOM	528	1HB	GLU	A	33	32.872	85.275	5.047	1.00	0.00	H
	ATOM	529	2HB	GLU	A	33	31.344	85.987	5.494	1.00	0.00	H
	ATOM	530	1HG	GLU	A	33	30.550	83.937	6.545	1.00	0.00	H
35	ATOM	531	2HG	GLU	A	33	32.063	83.066	6.242	1.00	0.00	H
	ATOM	532	N	VAL	A	34	30.644	86.808	8.020	1.00	0.09	N
	ATOM	533	CA	VAL	A	34	29.511	86.925	8.884	1.00	0.09	C
	ATOM	534	C	VAL	A	34	28.559	85.818	8.570	1.00	0.09	C
	ATOM	535	O	VAL	A	34	28.077	85.132	9.470	1.00	0.09	O
40	ATOM	536	CB	VAL	A	34	28.792	88.229	8.712	1.00	0.09	C
	ATOM	537	CG1	VAL	A	34	27.594	88.260	9.674	1.00	0.09	C
	ATOM	538	CG2	VAL	A	34	29.797	89.369	8.948	1.00	0.09	C
	ATOM	539	H	VAL	A	34	30.817	87.554	7.369	1.00	0.00	H
	ATOM	540	HA	VAL	A	34	29.835	86.811	9.932	1.00	0.00	H
45	ATOM	541	HB	VAL	A	34	28.403	88.320	7.681	1.00	0.00	H
	ATOM	542	1HG1	VAL	A	34	27.078	89.234	9.646	1.00	0.00	H
	ATOM	543	2HG1	VAL	A	34	26.840	87.496	9.421	1.00	0.00	H
	ATOM	544	3HG1	VAL	A	34	27.913	88.090	10.716	1.00	0.00	H
	ATOM	545	1HG2	VAL	A	34	29.295	90.352	8.942	1.00	0.00	H
	ATOM	546	2HG2	VAL	A	34	30.288	89.266	9.931	1.00	0.00	H
50	ATOM	547	3HG2	VAL	A	34	30.583	89.418	8.177	1.00	0.00	H
	ATOM	548	N	SER	A	35	28.277	85.587	7.274	1.00	0.11	N
	ATOM	549	CA	SER	A	35	27.364	84.531	6.942	1.00	0.11	C
	ATOM	550	C	SER	A	35	28.183	83.307	6.696	1.00	0.11	C
55	ATOM	551	O	SER	A	35	28.493	82.953	5.559	1.00	0.11	O
	ATOM	552	CB	SER	A	35	26.512	84.826	5.689	1.00	0.11	C
	ATOM	553	OG	SER	A	35	27.339	85.023	4.552	1.00	0.11	O
	ATOM	554	H	SER	A	35	28.711	86.062	6.500	1.00	0.00	H
	ATOM	555	HA	SER	A	35	26.653	84.371	7.771	1.00	0.00	H
60	ATOM	556	1HB	SER	A	35	25.922	85.742	5.827	1.00	0.00	H
	ATOM	557	2HB	SER	A	35	25.812	83.985	5.528	1.00	0.00	H
	ATOM	558	HG	SER	A	35	27.975	84.275	4.528	1.00	0.00	H
	ATOM	559	N	SER	A	36	28.548	82.623	7.794	1.00	0.27	N
	ATOM	560	CA	SER	A	36	29.398	81.472	7.742	1.00	0.27	C
65	ATOM	561	C	SER	A	36	28.707	80.338	7.057	1.00	0.27	C
	ATOM	562	O	SER	A	36	29.282	79.676	6.194	1.00	0.27	O
	ATOM	563	CB	SER	A	36	29.776	80.977	9.147	1.00	0.27	C
	ATOM	564	OG	SER	A	36	30.410	82.020	9.871	1.00	0.27	O
	ATOM	565	H	SER	A	36	28.273	82.996	8.696	1.00	0.00	H
	ATOM	566	HA	SER	A	36	30.311	81.701	7.172	1.00	0.00	H
70	ATOM	567	1HB	SER	A	36	30.374	80.065	9.130	1.00	0.00	H
	ATOM	568	2HB	SER	A	36	28.855	80.708	9.694	1.00	0.00	H

161

	ATOM	569	HG	SER	A	36	30.299	82.846	9.362	1.00	0.00	H
	ATOM	570	N	THR	A	37	27.431	80.089	7.399	1.00	0.48	N
	ATOM	571	CA	THR	A	37	26.842	78.902	6.858	1.00	0.48	C
5	ATOM	572	C	THR	A	37	25.567	79.191	6.148	1.00	0.48	C
	ATOM	573	O	THR	A	37	24.911	80.206	6.377	1.00	0.48	O
	ATOM	574	CB	THR	A	37	26.522	77.882	7.901	1.00	0.48	C
	ATOM	575	OG1	THR	A	37	25.965	76.737	7.283	1.00	0.48	O
	ATOM	576	CG2	THR	A	37	25.515	78.485	8.896	1.00	0.48	C
10	ATOM	577	H	THR	A	37	26.845	80.714	7.922	1.00	0.00	H
	ATOM	578	HA	THR	A	37	27.513	78.421	6.132	1.00	0.00	H
	ATOM	579	HB	THR	A	37	27.418	77.638	8.460	1.00	0.00	H
	ATOM	580	HG1	THR	A	37	25.715	76.122	7.988	1.00	0.00	H
	ATOM	581	1HG2	THR	A	37	25.307	77.711	9.648	1.00	0.00	H
15	ATOM	582	2HG2	THR	A	37	25.923	79.370	9.399	1.00	0.00	H
	ATOM	583	3HG2	THR	A	37	24.557	78.741	8.418	1.00	0.00	H
	ATOM	584	N	LYS	A	38	25.205	78.268	5.235	1.00	0.41	N
	ATOM	585	CA	LYS	A	38	23.972	78.360	4.517	1.00	0.41	C
	ATOM	586	C	LYS	A	38	23.171	77.183	4.969	1.00	0.41	C
20	ATOM	587	O	LYS	A	38	23.687	76.068	5.054	1.00	0.41	O
	ATOM	588	CB	LYS	A	38	24.131	78.210	2.995	1.00	0.41	C
	ATOM	589	CG	LYS	A	38	25.186	79.135	2.385	1.00	0.41	C
	ATOM	590	CD	LYS	A	38	26.617	78.728	2.751	1.00	0.41	C
	ATOM	591	CE	LYS	A	38	27.700	79.493	1.986	1.00	0.41	C
25	ATOM	592	NZ	LYS	A	38	29.037	78.966	2.348	1.00	0.41	N1+
	ATOM	593	H	LYS	A	38	25.629	77.348	5.315	1.00	0.00	H
	ATOM	594	HA	LYS	A	38	23.477	79.318	4.738	1.00	0.00	H
	ATOM	595	1HB	LYS	A	38	23.141	78.390	2.541	1.00	0.00	H
	ATOM	596	2HB	LYS	A	38	24.408	77.173	2.761	1.00	0.00	H
30	ATOM	597	1HG	LYS	A	38	24.996	80.183	2.681	1.00	0.00	H
	ATOM	598	2HG	LYS	A	38	25.082	79.106	1.285	1.00	0.00	H
	ATOM	599	1HD	LYS	A	38	26.726	77.658	2.649	1.00	0.00	H
	ATOM	600	2HD	LYS	A	38	26.849	78.975	3.795	1.00	0.00	H
	ATOM	601	1HE	LYS	A	38	27.684	80.565	2.244	1.00	0.00	H
35	ATOM	602	2HE	LYS	A	38	27.598	79.398	0.893	1.00	0.00	H
	ATOM	603	1HZ	LYS	A	38	29.782	79.444	1.855	1.00	0.00	H
	ATOM	604	2HZ	LYS	A	38	29.227	79.092	3.336	1.00	0.00	H
	ATOM	605	3HZ	LYS	A	38	29.137	77.982	2.132	1.00	0.00	H
	ATOM	606	N	TRP	A	39	21.884	77.401	5.297	1.00	0.18	N
40	ATOM	607	CA	TRP	A	39	21.073	76.294	5.707	1.00	0.18	C
	ATOM	608	C	TRP	A	39	20.040	76.079	4.659	1.00	0.18	C
	ATOM	609	O	TRP	A	39	19.565	77.025	4.034	1.00	0.18	O
	ATOM	610	CB	TRP	A	39	20.331	76.490	7.044	1.00	0.18	C
	ATOM	611	CG	TRP	A	39	21.211	76.379	8.268	1.00	0.18	C
45	ATOM	612	CD1	TRP	A	39	21.745	77.350	9.062	1.00	0.18	C
	ATOM	613	CD2	TRP	A	39	21.658	75.123	8.802	1.00	0.18	C
	ATOM	614	NE1	TRP	A	39	22.498	76.776	10.062	1.00	0.18	N
	ATOM	615	CE2	TRP	A	39	22.453	75.405	9.912	1.00	0.18	C
	ATOM	616	CE3	TRP	A	39	21.425	73.840	8.397	1.00	0.18	C
50	ATOM	617	CZ2	TRP	A	39	23.031	74.401	10.636	1.00	0.18	C
	ATOM	618	CZ3	TRP	A	39	22.006	72.830	9.130	1.00	0.18	C
	ATOM	619	CH2	TRP	A	39	22.793	73.105	10.228	1.00	0.18	C
	ATOM	620	H	TRP	A	39	21.424	78.294	5.236	1.00	0.00	H
	ATOM	621	HA	TRP	A	39	21.686	75.386	5.806	1.00	0.00	H
55	ATOM	622	1HB	TRP	A	39	19.541	75.720	7.109	1.00	0.00	H
	ATOM	623	2HB	TRP	A	39	19.802	77.454	7.048	1.00	0.00	H
	ATOM	624	HD1	TRP	A	39	21.773	78.413	8.875	1.00	0.00	H
	ATOM	625	HE1	TRP	A	39	23.073	77.294	10.699	1.00	0.00	H
	ATOM	626	HE3	TRP	A	39	20.762	73.621	7.571	1.00	0.00	H
60	ATOM	627	HZ2	TRP	A	39	23.619	74.619	11.521	1.00	0.00	H
	ATOM	628	HZ3	TRP	A	39	21.828	71.796	8.843	1.00	0.00	H
	ATOM	629	HH2	TRP	A	39	23.234	72.302	10.807	1.00	0.00	H
	ATOM	630	N	PHE	A	40	19.690	74.803	4.416	1.00	0.08	N
	ATOM	631	CA	PHE	A	40	18.688	74.538	3.434	1.00	0.08	C
65	ATOM	632	C	PHE	A	40	17.664	73.654	4.057	1.00	0.08	C
	ATOM	633	O	PHE	A	40	17.990	72.739	4.811	1.00	0.08	O
	ATOM	634	CB	PHE	A	40	19.229	73.816	2.190	1.00	0.08	C
	ATOM	635	CG	PHE	A	40	20.153	74.766	1.514	1.00	0.08	C
	ATOM	636	CD1	PHE	A	40	21.465	74.872	1.916	1.00	0.08	C
70	ATOM	637	CD2	PHE	A	40	19.703	75.553	0.478	1.00	0.08	C
	ATOM	638	CE1	PHE	A	40	22.315	75.752	1.291	1.00	0.08	C
	ATOM	639	CE2	PHE	A	40	20.551	76.435	-0.150	1.00	0.08	C

162

	ATOM	640	CZ	PHE	A	40	21.860	76.534	0.257	1.00	0.08	C
	ATOM	641	H	PHE	A	40	20.105	74.013	4.892	1.00	0.00	H
	ATOM	642	HA	PHE	A	40	18.309	75.494	3.136	1.00	0.00	H
5	ATOM	643	1HB	PHE	A	40	18.376	73.555	1.549	1.00	0.00	H
	ATOM	644	2HB	PHE	A	40	19.730	72.882	2.471	1.00	0.00	H
	ATOM	645	HD1	PHE	A	40	21.845	74.243	2.717	1.00	0.00	H
	ATOM	646	HD2	PHE	A	40	18.681	75.450	0.130	1.00	0.00	H
	ATOM	647	HE1	PHE	A	40	23.355	75.778	1.589	1.00	0.00	H
	ATOM	648	HE2	PHE	A	40	20.213	76.986	-1.023	1.00	0.00	H
10	ATOM	649	HZ	PHE	A	40	22.535	77.216	-0.253	1.00	0.00	H
	ATOM	650	N	HIS	A	41	16.383	73.945	3.777	1.00	0.10	N
	ATOM	651	CA	HIS	A	41	15.322	73.109	4.242	1.00	0.10	C
	ATOM	652	C	HIS	A	41	14.620	72.643	3.014	1.00	0.10	C
	ATOM	653	O	HIS	A	41	14.100	73.447	2.242	1.00	0.10	O
15	ATOM	654	CB	HIS	A	41	14.287	73.836	5.109	1.00	0.10	C
	ATOM	655	CG	HIS	A	41	13.274	72.893	5.682	1.00	0.10	C
	ATOM	656	ND1	HIS	A	41	12.236	73.278	6.499	1.00	0.10	N
	ATOM	657	CD2	HIS	A	41	13.159	71.544	5.541	1.00	0.10	C
	ATOM	658	CE1	HIS	A	41	11.548	72.151	6.810	1.00	0.10	C
20	ATOM	659	NE2	HIS	A	41	12.071	71.072	6.253	1.00	0.10	N
	ATOM	660	H	HIS	A	41	16.131	74.767	3.233	1.00	0.00	H
	ATOM	661	HA	HIS	A	41	15.740	72.280	4.830	1.00	0.00	H
	ATOM	662	1HB	HIS	A	41	13.796	74.642	4.539	1.00	0.00	H
	ATOM	663	2HB	HIS	A	41	14.822	74.338	5.936	1.00	0.00	H
25	ATOM	664	HD2	HIS	A	41	13.744	70.826	5.017	1.00	0.00	H
	ATOM	665	HE1	HIS	A	41	10.614	72.196	7.348	1.00	0.00	H
	ATOM	666	HE2	HIS	A	41	11.764	70.142	6.452	1.00	0.00	H
	ATOM	667	N	ASN	A	42	14.593	71.319	2.797	1.00	0.11	N
	ATOM	668	CA	ASN	A	42	13.967	70.801	1.622	1.00	0.11	C
30	ATOM	669	C	ASN	A	42	14.617	71.443	0.440	1.00	0.11	C
	ATOM	670	O	ASN	A	42	14.003	71.602	-0.614	1.00	0.11	O
	ATOM	671	CB	ASN	A	42	12.450	71.059	1.562	1.00	0.11	C
	ATOM	672	CG	ASN	A	42	11.781	70.123	2.558	1.00	0.11	C
	ATOM	673	OD1	ASN	A	42	12.427	69.246	3.129	1.00	0.11	O
35	ATOM	674	ND2	ASN	A	42	10.447	70.298	2.758	1.00	0.11	N
	ATOM	675	H	ASN	A	42	14.894	70.665	3.517	1.00	0.00	H
	ATOM	676	HA	ASN	A	42	14.186	69.722	1.529	1.00	0.00	H
	ATOM	677	1HB	ASN	A	42	12.064	70.773	0.568	1.00	0.00	H
	ATOM	678	2HB	ASN	A	42	12.165	72.105	1.744	1.00	0.00	H
40	ATOM	679	1HD2	ASN	A	42	9.946	71.057	2.334	1.00	0.00	H
	ATOM	680	2HD2	ASN	A	42	10.000	69.733	3.462	1.00	0.00	H
	ATOM	681	N	GLY	A	43	15.899	71.821	0.589	1.00	0.08	N
	ATOM	682	CA	GLY	A	43	16.624	72.378	-0.515	1.00	0.08	C
	ATOM	683	C	GLY	A	43	16.364	73.848	-0.611	1.00	0.08	C
45	ATOM	684	O	GLY	A	43	16.830	74.497	-1.546	1.00	0.08	O
	ATOM	685	H	GLY	A	43	16.250	71.979	1.521	1.00	0.00	H
	ATOM	686	1HA	GLY	A	43	16.323	71.897	-1.458	1.00	0.00	H
	ATOM	687	2HA	GLY	A	43	17.706	72.230	-0.374	1.00	0.00	H
	ATOM	688	N	SER	A	44	15.617	74.428	0.346	1.00	0.15	N
50	ATOM	689	CA	SER	A	44	15.375	75.838	0.255	1.00	0.15	C
	ATOM	690	C	SER	A	44	16.345	76.510	1.167	1.00	0.15	C
	ATOM	691	O	SER	A	44	16.513	76.111	2.317	1.00	0.15	O
	ATOM	692	CB	SER	A	44	13.964	76.262	0.694	1.00	0.15	C
	ATOM	693	OG	SER	A	44	13.788	76.006	2.080	1.00	0.15	O
55	ATOM	694	H	SER	A	44	15.032	73.916	0.998	1.00	0.00	H
	ATOM	695	HA	SER	A	44	15.484	76.176	-0.789	1.00	0.00	H
	ATOM	696	1HB	SER	A	44	13.195	75.690	0.158	1.00	0.00	H
	ATOM	697	2HB	SER	A	44	13.813	77.334	0.471	1.00	0.00	H
	ATOM	698	HG	SER	A	44	14.352	76.634	2.559	1.00	0.00	H
60	ATOM	699	N	LEU	A	45	17.025	77.556	0.666	1.00	0.35	N
	ATOM	700	CA	LEU	A	45	17.997	78.240	1.465	1.00	0.35	C
	ATOM	701	C	LEU	A	45	17.255	79.014	2.504	1.00	0.35	C
	ATOM	702	O	LEU	A	45	16.195	79.578	2.241	1.00	0.35	O
	ATOM	703	CB	LEU	A	45	18.886	79.190	0.622	1.00	0.35	C
65	ATOM	704	CG	LEU	A	45	20.000	79.986	1.345	1.00	0.35	C
	ATOM	705	CD1	LEU	A	45	20.847	80.767	0.328	1.00	0.35	C
	ATOM	706	CD2	LEU	A	45	19.465	80.938	2.433	1.00	0.35	C
	ATOM	707	H	LEU	A	45	16.859	77.916	-0.258	1.00	0.00	H
	ATOM	708	HA	LEU	A	45	18.652	77.484	1.916	1.00	0.00	H
70	ATOM	709	1HB	LEU	A	45	18.219	79.931	0.143	1.00	0.00	H
	ATOM	710	2HB	LEU	A	45	19.327	78.630	-0.212	1.00	0.00	H

163

	ATOM	711	HG	LEU	A	45	20.665	79.253	1.840	1.00	0.00	H
	ATOM	712	1HD1	LEU	A	45	21.676	81.302	0.821	1.00	0.00	H
	ATOM	713	2HD1	LEU	A	45	21.291	80.099	-0.428	1.00	0.00	H
5	ATOM	714	3HD1	LEU	A	45	20.234	81.514	-0.203	1.00	0.00	H
	ATOM	715	1HD2	LEU	A	45	19.719	81.980	2.158	1.00	0.00	H
	ATOM	716	2HD2	LEU	A	45	18.389	81.005	2.576	1.00	0.00	H
	ATOM	717	3HD2	LEU	A	45	20.074	80.759	3.311	1.00	0.00	H
	ATOM	718	N	SER	A	46	17.808	79.040	3.734	1.00	0.48	N
	ATOM	719	CA	SER	A	46	17.218	79.785	4.809	1.00	0.48	C
10	ATOM	720	C	SER	A	46	18.124	80.941	5.078	1.00	0.48	C
	ATOM	721	O	SER	A	46	19.320	80.771	5.301	1.00	0.48	O
	ATOM	722	CB	SER	A	46	17.159	79.037	6.154	1.00	0.48	C
	ATOM	723	OG	SER	A	46	16.268	77.937	6.093	1.00	0.48	O
15	ATOM	724	H	SER	A	46	18.589	78.436	3.972	1.00	0.00	H
	ATOM	725	HA	SER	A	46	16.185	80.070	4.554	1.00	0.00	H
	ATOM	726	1HB	SER	A	46	16.623	79.786	6.740	1.00	0.00	H
	ATOM	727	2HB	SER	A	46	18.133	78.779	6.591	1.00	0.00	H
	ATOM	728	HG	SER	A	46	16.014	77.771	7.023	1.00	0.00	H
20	ATOM	729	N	GLU	A	47	17.561	82.158	5.029	1.00	0.44	N
	ATOM	730	CA	GLU	A	47	18.248	83.383	5.316	1.00	0.44	C
	ATOM	731	C	GLU	A	47	18.453	83.486	6.797	1.00	0.44	C
	ATOM	732	O	GLU	A	47	19.343	84.188	7.271	1.00	0.44	O
	ATOM	733	CB	GLU	A	47	17.440	84.622	4.906	1.00	0.44	C
25	ATOM	734	CG	GLU	A	47	16.115	84.730	5.662	1.00	0.44	C
	ATOM	735	CD	GLU	A	47	15.396	85.988	5.203	1.00	0.44	C
	ATOM	736	OE1	GLU	A	47	15.858	86.606	4.206	1.00	0.44	O
	ATOM	737	OE2	GLU	A	47	14.373	86.349	5.844	1.00	0.44	O1-
	ATOM	738	H	GLU	A	47	16.607	82.284	4.724	1.00	0.00	H
30	ATOM	739	HA	GLU	A	47	19.239	83.381	4.833	1.00	0.00	H
	ATOM	740	1HB	GLU	A	47	17.273	84.585	3.815	1.00	0.00	H
	ATOM	741	2HB	GLU	A	47	18.068	85.508	5.110	1.00	0.00	H
	ATOM	742	1HG	GLU	A	47	16.248	84.814	6.752	1.00	0.00	H
	ATOM	743	2HG	GLU	A	47	15.450	83.868	5.495	1.00	0.00	H
35	ATOM	744	N	GLU	A	48	17.608	82.766	7.551	1.00	0.45	N
	ATOM	745	CA	GLU	A	48	17.419	82.881	8.969	1.00	0.45	C
	ATOM	746	C	GLU	A	48	18.648	82.740	9.823	1.00	0.45	C
	ATOM	747	O	GLU	A	48	18.857	83.579	10.697	1.00	0.45	O
	ATOM	748	CB	GLU	A	48	16.414	81.833	9.468	1.00	0.45	C
40	ATOM	749	CG	GLU	A	48	16.862	80.403	9.154	1.00	0.45	C
	ATOM	750	CD	GLU	A	48	15.749	79.447	9.560	1.00	0.45	C
	ATOM	751	OE1	GLU	A	48	14.717	79.928	10.099	1.00	0.45	O
	ATOM	752	OE2	GLU	A	48	15.917	78.219	9.333	1.00	0.45	O1-
	ATOM	753	H	GLU	A	48	16.949	82.175	7.075	1.00	0.00	H
45	ATOM	754	HA	GLU	A	48	17.016	83.885	9.188	1.00	0.00	H
	ATOM	755	1HB	GLU	A	48	15.437	82.052	8.999	1.00	0.00	H
	ATOM	756	2HB	GLU	A	48	16.290	81.972	10.557	1.00	0.00	H
	ATOM	757	1HG	GLU	A	48	17.655	80.150	9.869	1.00	0.00	H
	ATOM	758	2HG	GLU	A	48	17.413	80.258	8.238	1.00	0.00	H
50	ATOM	759	N	THR	A	49	19.523	81.735	9.626	1.00	0.55	N
	ATOM	760	CA	THR	A	49	20.475	81.591	10.695	1.00	0.55	C
	ATOM	761	C	THR	A	49	21.869	81.303	10.218	1.00	0.55	C
	ATOM	762	O	THR	A	49	22.124	81.078	9.036	1.00	0.55	O
	ATOM	763	CB	THR	A	49	20.062	80.467	11.603	1.00	0.55	C
55	ATOM	764	OG1	THR	A	49	20.882	80.388	12.757	1.00	0.55	O
	ATOM	765	CG2	THR	A	49	20.139	79.164	10.795	1.00	0.55	C
	ATOM	766	H	THR	A	49	19.450	81.037	8.909	1.00	0.00	H
	ATOM	767	HA	THR	A	49	20.596	82.511	11.285	1.00	0.00	H
	ATOM	768	HB	THR	A	49	19.051	80.768	11.920	1.00	0.00	H
60	ATOM	769	HG1	THR	A	49	20.723	79.538	13.198	1.00	0.00	H
	ATOM	770	1HG2	THR	A	49	19.326	78.450	10.800	1.00	0.00	H
	ATOM	771	2HG2	THR	A	49	20.226	79.357	9.715	1.00	0.00	H
	ATOM	772	3HG2	THR	A	49	21.061	78.660	11.101	1.00	0.00	H
	ATOM	773	N	ASN	A	50	22.808	81.331	11.191	1.00	0.44	N
65	ATOM	774	CA	ASN	A	50	24.216	81.101	11.036	1.00	0.44	C
	ATOM	775	C	ASN	A	50	24.526	79.690	11.431	1.00	0.44	C
	ATOM	776	O	ASN	A	50	23.788	78.756	11.124	1.00	0.44	O
	ATOM	777	CB	ASN	A	50	25.082	82.012	11.923	1.00	0.44	C
	ATOM	778	CG	ASN	A	50	24.987	83.430	11.383	1.00	0.44	C
	ATOM	779	OD1	ASN	A	50	25.306	83.682	10.223	1.00	0.44	O
70	ATOM	780	ND2	ASN	A	50	24.536	84.383	12.243	1.00	0.44	N
	ATOM	781	H	ASN	A	50	22.433	81.246	12.132	1.00	0.00	H

164

	ATOM	782	HA	ASN	A	50	24.490	81.217	9.974	1.00	0.00	H
	ATOM	783	1HB	ASN	A	50	26.160	81.813	11.801	1.00	0.00	H
	ATOM	784	2HB	ASN	A	50	24.811	81.939	12.988	1.00	0.00	H
5	ATOM	785	1HD2	ASN	A	50	24.226	84.171	13.172	1.00	0.00	H
	ATOM	786	2HD2	ASN	A	50	24.430	85.308	11.862	1.00	0.00	H
	ATOM	787	N	SER	A	51	25.661	79.521	12.140	1.00	0.25	N
	ATOM	788	CA	SER	A	51	26.182	78.233	12.494	1.00	0.25	C
	ATOM	789	C	SER	A	51	25.171	77.448	13.267	1.00	0.25	C
10	ATOM	790	O	SER	A	51	24.943	76.276	12.969	1.00	0.25	O
	ATOM	791	CB	SER	A	51	27.446	78.324	13.365	1.00	0.25	C
	ATOM	792	OG	SER	A	51	27.126	78.894	14.625	1.00	0.25	O
	ATOM	793	H	SER	A	51	26.206	80.301	12.462	1.00	0.00	H
	ATOM	794	HA	SER	A	51	26.417	77.665	11.581	1.00	0.00	H
15	ATOM	795	1HB	SER	A	51	28.230	78.908	12.849	1.00	0.00	H
	ATOM	796	2HB	SER	A	51	27.829	77.295	13.499	1.00	0.00	H
	ATOM	797	HG	SER	A	51	27.896	78.769	15.200	1.00	0.00	H
	ATOM	798	N	SER	A	52	24.525	78.056	14.278	1.00	0.14	N
	ATOM	799	CA	SER	A	52	23.591	77.273	15.036	1.00	0.14	C
20	ATOM	800	C	SER	A	52	22.214	77.760	14.740	1.00	0.14	C
	ATOM	801	O	SER	A	52	21.944	78.960	14.768	1.00	0.14	O
	ATOM	802	CB	SER	A	52	23.794	77.380	16.557	1.00	0.14	C
	ATOM	803	OG	SER	A	52	25.058	76.846	16.919	1.00	0.14	O
	ATOM	804	H	SER	A	52	24.837	78.941	14.640	1.00	0.00	H
25	ATOM	805	HA	SER	A	52	23.703	76.203	14.814	1.00	0.00	H
	ATOM	806	1HB	SER	A	52	22.983	76.804	17.042	1.00	0.00	H
	ATOM	807	2HB	SER	A	52	23.706	78.429	16.892	1.00	0.00	H
	ATOM	808	HG	SER	A	52	25.161	76.977	17.872	1.00	0.00	H
	ATOM	809	N	LEU	A	53	21.296	76.826	14.422	1.00	0.09	N
30	ATOM	810	CA	LEU	A	53	19.948	77.236	14.179	1.00	0.09	C
	ATOM	811	C	LEU	A	53	19.099	76.586	15.218	1.00	0.09	C
	ATOM	812	O	LEU	A	53	19.090	75.363	15.358	1.00	0.09	O
	ATOM	813	CB	LEU	A	53	19.400	76.833	12.798	1.00	0.09	C
	ATOM	814	CG	LEU	A	53	17.946	77.287	12.554	1.00	0.09	C
35	ATOM	815	CD1	LEU	A	53	17.822	78.817	12.594	1.00	0.09	C
	ATOM	816	CD2	LEU	A	53	17.391	76.694	11.251	1.00	0.09	C
	ATOM	817	H	LEU	A	53	21.500	75.830	14.376	1.00	0.00	H
	ATOM	818	HA	LEU	A	53	19.874	78.321	14.291	1.00	0.00	H
	ATOM	819	1HB	LEU	A	53	19.407	75.728	12.754	1.00	0.00	H
40	ATOM	820	2HB	LEU	A	53	20.106	77.112	12.014	1.00	0.00	H
	ATOM	821	HG	LEU	A	53	17.336	76.870	13.377	1.00	0.00	H
	ATOM	822	1HD1	LEU	A	53	16.830	79.056	13.024	1.00	0.00	H
	ATOM	823	2HD1	LEU	A	53	18.521	79.331	13.257	1.00	0.00	H
	ATOM	824	3HD1	LEU	A	53	17.754	79.272	11.609	1.00	0.00	H
45	ATOM	825	1HD2	LEU	A	53	16.302	76.848	11.201	1.00	0.00	H
	ATOM	826	2HD2	LEU	A	53	17.862	77.101	10.346	1.00	0.00	H
	ATOM	827	3HD2	LEU	A	53	17.544	75.602	11.226	1.00	0.00	H
	ATOM	828	N	ASN	A	54	18.372	77.405	15.998	1.00	0.09	N
	ATOM	829	CA	ASN	A	54	17.529	76.854	17.013	1.00	0.09	C
50	ATOM	830	C	ASN	A	54	16.131	77.235	16.666	1.00	0.09	C
	ATOM	831	O	ASN	A	54	15.849	78.395	16.374	1.00	0.09	O
	ATOM	832	CB	ASN	A	54	17.800	77.421	18.416	1.00	0.09	C
	ATOM	833	CG	ASN	A	54	16.982	76.612	19.411	1.00	0.09	C
	ATOM	834	OD1	ASN	A	54	16.409	75.580	19.069	1.00	0.09	O
55	ATOM	835	ND2	ASN	A	54	16.916	77.099	20.679	1.00	0.09	N
	ATOM	836	H	ASN	A	54	18.265	78.392	15.833	1.00	0.00	H
	ATOM	837	HA	ASN	A	54	17.682	75.775	17.052	1.00	0.00	H
	ATOM	838	1HB	ASN	A	54	17.555	78.493	18.473	1.00	0.00	H
	ATOM	839	2HB	ASN	A	54	18.867	77.298	18.670	1.00	0.00	H
60	ATOM	840	1HD2	ASN	A	54	17.381	77.945	20.949	1.00	0.00	H
	ATOM	841	2HD2	ASN	A	54	16.363	76.577	21.336	1.00	0.00	H
	ATOM	842	N	ILE	A	55	15.213	76.255	16.677	1.00	0.08	N
	ATOM	843	CA	ILE	A	55	13.854	76.575	16.377	1.00	0.08	C
	ATOM	844	C	ILE	A	55	13.041	76.131	17.542	1.00	0.08	C
65	ATOM	845	O	ILE	A	55	13.338	75.121	18.178	1.00	0.08	O
	ATOM	846	CB	ILE	A	55	13.310	75.856	15.178	1.00	0.08	C
	ATOM	847	CG1	ILE	A	55	13.293	74.339	15.424	1.00	0.08	C
	ATOM	848	CG2	ILE	A	55	14.135	76.277	13.950	1.00	0.08	C
	ATOM	849	CD1	ILE	A	55	12.481	73.570	14.384	1.00	0.08	C
70	ATOM	850	H	ILE	A	55	15.434	75.327	17.030	1.00	0.00	H
	ATOM	851	HA	ILE	A	55	13.731	77.661	16.238	1.00	0.00	H
	ATOM	852	HB	ILE	A	55	12.270	76.207	15.038	1.00	0.00	H

165

	ATOM	853	1HG1	ILE	A	55	12.813	74.025	16.355	1.00	0.00	H
	ATOM	854	2HG1	ILE	A	55	14.341	74.014	15.420	1.00	0.00	H
	ATOM	855	1HG2	ILE	A	55	13.703	75.895	13.010	1.00	0.00	H
5	ATOM	856	2HG2	ILE	A	55	14.181	77.375	13.855	1.00	0.00	H
	ATOM	857	3HG2	ILE	A	55	15.169	75.900	14.004	1.00	0.00	H
	ATOM	858	1HD1	ILE	A	55	12.528	72.482	14.547	1.00	0.00	H
	ATOM	859	2HD1	ILE	A	55	11.433	73.877	14.474	1.00	0.00	H
	ATOM	860	3HD1	ILE	A	55	12.805	73.762	13.349	1.00	0.00	H
10	ATOM	861	N	VAL	A	56	11.988	76.902	17.855	1.00	0.10	N
	ATOM	862	CA	VAL	A	56	11.128	76.559	18.942	1.00	0.10	C
	ATOM	863	C	VAL	A	56	9.803	76.269	18.333	1.00	0.10	C
	ATOM	864	O	VAL	A	56	9.483	76.775	17.259	1.00	0.10	O
	ATOM	865	CB	VAL	A	56	10.938	77.689	19.914	1.00	0.10	C
15	ATOM	866	CG1	VAL	A	56	9.887	77.287	20.962	1.00	0.10	C
	ATOM	867	CG2	VAL	A	56	12.308	78.053	20.510	1.00	0.10	C
	ATOM	868	H	VAL	A	56	11.643	77.623	17.244	1.00	0.00	H
	ATOM	869	HA	VAL	A	56	11.486	75.619	19.322	1.00	0.00	H
	ATOM	870	HB	VAL	A	56	10.550	78.573	19.374	1.00	0.00	H
20	ATOM	871	1HG1	VAL	A	56	10.078	77.797	21.922	1.00	0.00	H
	ATOM	872	2HG1	VAL	A	56	8.900	77.663	20.639	1.00	0.00	H
	ATOM	873	3HG1	VAL	A	56	9.712	76.240	21.212	1.00	0.00	H
	ATOM	874	1HG2	VAL	A	56	12.215	78.754	21.355	1.00	0.00	H
	ATOM	875	2HG2	VAL	A	56	12.874	77.183	20.866	1.00	0.00	H
	ATOM	876	3HG2	VAL	A	56	12.944	78.553	19.759	1.00	0.00	H
25	ATOM	877	N	ASN	A	57	9.004	75.433	19.021	1.00	0.11	N
	ATOM	878	CA	ASN	A	57	7.708	75.064	18.547	1.00	0.11	C
	ATOM	879	C	ASN	A	57	7.819	74.611	17.129	1.00	0.11	C
	ATOM	880	O	ASN	A	57	7.234	75.209	16.227	1.00	0.11	O
30	ATOM	881	CB	ASN	A	57	6.662	76.188	18.634	1.00	0.11	C
	ATOM	882	CG	ASN	A	57	5.291	75.545	18.470	1.00	0.11	C
	ATOM	883	OD1	ASN	A	57	5.099	74.663	17.634	1.00	0.11	O
	ATOM	884	ND2	ASN	A	57	4.310	75.986	19.303	1.00	0.11	N
	ATOM	885	H	ASN	A	57	9.360	74.950	19.839	1.00	0.00	H
35	ATOM	886	HA	ASN	A	57	7.598	74.194	19.108	1.00	0.00	H
	ATOM	887	1HB	ASN	A	57	6.807	76.960	17.861	1.00	0.00	H
	ATOM	888	2HB	ASN	A	57	6.743	76.690	19.613	1.00	0.00	H
	ATOM	889	1HD2	ASN	A	57	4.556	76.658	20.013	1.00	0.00	H
	ATOM	890	2HD2	ASN	A	57	3.546	75.358	19.482	1.00	0.00	H
40	ATOM	891	N	ALA	A	58	8.603	73.540	16.895	1.00	0.21	N
	ATOM	892	CA	ALA	A	58	8.722	73.047	15.556	1.00	0.21	C
	ATOM	893	C	ALA	A	58	7.341	72.692	15.120	1.00	0.21	C
	ATOM	894	O	ALA	A	58	6.578	72.084	15.870	1.00	0.21	O
45	ATOM	895	CB	ALA	A	58	9.596	71.785	15.430	1.00	0.21	C
	ATOM	896	H	ALA	A	58	9.197	73.133	17.613	1.00	0.00	H
	ATOM	897	HA	ALA	A	58	9.154	73.899	15.035	1.00	0.00	H
	ATOM	898	1HB	ALA	A	58	9.729	71.530	14.369	1.00	0.00	H
	ATOM	899	2HB	ALA	A	58	10.589	71.945	15.874	1.00	0.00	H
	ATOM	900	3HB	ALA	A	58	9.118	70.934	15.936	1.00	0.00	H
50	ATOM	901	N	LYS	A	59	6.977	73.095	13.889	1.00	0.31	N
	ATOM	902	CA	LYS	A	59	5.653	72.852	13.401	1.00	0.31	C
	ATOM	903	C	LYS	A	59	5.671	71.665	12.498	1.00	0.31	C
	ATOM	904	O	LYS	A	59	6.710	71.054	12.255	1.00	0.31	O
	ATOM	905	CB	LYS	A	59	5.066	74.025	12.597	1.00	0.31	C
55	ATOM	906	CG	LYS	A	59	4.819	75.274	13.445	1.00	0.31	C
	ATOM	907	CD	LYS	A	59	3.812	75.062	14.579	1.00	0.31	C
	ATOM	908	CE	LYS	A	59	3.593	76.308	15.443	1.00	0.31	C
	ATOM	909	NZ	LYS	A	59	2.607	76.020	16.509	1.00	0.31	N1+
	ATOM	910	H	LYS	A	59	7.667	73.546	13.283	1.00	0.00	H
60	ATOM	911	HA	LYS	A	59	4.994	72.593	14.243	1.00	0.00	H
	ATOM	912	1HB	LYS	A	59	4.188	73.779	11.986	1.00	0.00	H
	ATOM	913	2HB	LYS	A	59	5.917	74.358	11.995	1.00	0.00	H
	ATOM	914	1HG	LYS	A	59	4.449	76.103	12.824	1.00	0.00	H
	ATOM	915	2HG	LYS	A	59	5.784	75.617	13.863	1.00	0.00	H
65	ATOM	916	1HD	LYS	A	59	4.154	74.242	15.231	1.00	0.00	H
	ATOM	917	2HD	LYS	A	59	2.851	74.742	14.138	1.00	0.00	H
	ATOM	918	1HE	LYS	A	59	3.202	77.149	14.846	1.00	0.00	H
	ATOM	919	2HE	LYS	A	59	4.527	76.641	15.925	1.00	0.00	H
	ATOM	920	1HZ	LYS	A	59	2.435	76.829	17.091	1.00	0.00	H
70	ATOM	921	2HZ	LYS	A	59	1.719	75.717	16.136	1.00	0.00	H
	ATOM	922	3HZ	LYS	A	59	2.973	75.299	17.120	1.00	0.00	H
	ATOM	923	N	PHE	A	60	4.477	71.314	11.983	1.00	0.23	N

166

	ATOM	924	CA	PHE	A	60	4.318	70.228	11.063	1.00	0.23	C
	ATOM	925	C	PHE	A	60	5.095	70.579	9.839	1.00	0.23	C
	ATOM	926	O	PHE	A	60	5.704	69.726	9.197	1.00	0.23	O
5	ATOM	927	CB	PHE	A	60	2.858	70.016	10.632	1.00	0.23	C
	ATOM	928	CG	PHE	A	60	2.873	69.034	9.510	1.00	0.23	C
	ATOM	929	CD1	PHE	A	60	2.961	67.682	9.748	1.00	0.23	C
	ATOM	930	CD2	PHE	A	60	2.798	69.475	8.208	1.00	0.23	C
	ATOM	931	CE1	PHE	A	60	2.977	66.787	8.705	1.00	0.23	C
10	ATOM	932	CE2	PHE	A	60	2.813	68.584	7.161	1.00	0.23	C
	ATOM	933	CZ	PHE	A	60	2.902	67.236	7.409	1.00	0.23	C
	ATOM	934	H	PHE	A	60	3.633	71.764	12.295	1.00	0.00	H
	ATOM	935	HA	PHE	A	60	4.520	69.253	11.406	1.00	0.00	H
	ATOM	936	1HB	PHE	A	60	2.378	70.957	10.321	1.00	0.00	H
	ATOM	937	2HB	PHE	A	60	2.278	69.639	11.490	1.00	0.00	H
15	ATOM	938	HD1	PHE	A	60	3.027	67.313	10.769	1.00	0.00	H
	ATOM	939	HD2	PHE	A	60	2.735	70.540	7.999	1.00	0.00	H
	ATOM	940	HE1	PHE	A	60	3.056	65.721	8.908	1.00	0.00	H
	ATOM	941	HE2	PHE	A	60	2.763	68.947	6.138	1.00	0.00	H
20	ATOM	942	HZ	PHE	A	60	2.922	66.528	6.584	1.00	0.00	H
	ATOM	943	N	GLU	A	61	5.095	71.879	9.508	1.00	0.15	N
	ATOM	944	CA	GLU	A	61	5.748	72.420	8.354	1.00	0.15	C
	ATOM	945	C	GLU	A	61	7.218	72.152	8.459	1.00	0.15	C
	ATOM	946	O	GLU	A	61	7.889	71.928	7.454	1.00	0.15	O
25	ATOM	947	CB	GLU	A	61	5.528	73.936	8.259	1.00	0.15	C
	ATOM	948	CG	GLU	A	61	5.975	74.676	9.522	1.00	0.15	C
	ATOM	949	CD	GLU	A	61	5.349	76.063	9.510	1.00	0.15	C
	ATOM	950	OE1	GLU	A	61	5.260	76.667	8.408	1.00	0.15	O
	ATOM	951	OE2	GLU	A	61	4.938	76.533	10.605	1.00	0.15	O1-
30	ATOM	952	H	GLU	A	61	4.636	72.552	10.097	1.00	0.00	H
	ATOM	953	HA	GLU	A	61	5.382	71.916	7.445	1.00	0.00	H
	ATOM	954	1HB	GLU	A	61	4.456	74.129	8.074	1.00	0.00	H
	ATOM	955	2HB	GLU	A	61	6.074	74.289	7.366	1.00	0.00	H
	ATOM	956	1HG	GLU	A	61	7.066	74.750	9.599	1.00	0.00	H
35	ATOM	957	2HG	GLU	A	61	5.569	74.098	10.323	1.00	0.00	H
	ATOM	958	N	ASP	A	62	7.751	72.147	9.694	1.00	0.16	N
	ATOM	959	CA	ASP	A	62	9.160	71.997	9.932	1.00	0.16	C
	ATOM	960	C	ASP	A	62	9.664	70.682	9.421	1.00	0.16	C
	ATOM	961	O	ASP	A	62	10.828	70.586	9.041	1.00	0.16	O
40	ATOM	962	CB	ASP	A	62	9.539	72.120	11.419	1.00	0.16	C
	ATOM	963	CG	ASP	A	62	9.413	73.590	11.797	1.00	0.16	C
	ATOM	964	OD1	ASP	A	62	9.136	74.412	10.883	1.00	0.16	O
	ATOM	965	OD2	ASP	A	62	9.605	73.914	13.000	1.00	0.16	O1-
	ATOM	966	H	ASP	A	62	7.202	72.371	10.507	1.00	0.00	H
45	ATOM	967	HA	ASP	A	62	9.712	72.751	9.343	1.00	0.00	H
	ATOM	968	1HB	ASP	A	62	10.604	71.848	11.527	1.00	0.00	H
	ATOM	969	2HB	ASP	A	62	9.012	71.445	12.095	1.00	0.00	H
	ATOM	970	N	SER	A	63	8.832	69.622	9.415	1.00	0.20	N
	ATOM	971	CA	SER	A	63	9.308	68.342	8.962	1.00	0.20	C
50	ATOM	972	C	SER	A	63	9.869	68.484	7.579	1.00	0.20	C
	ATOM	973	O	SER	A	63	9.321	69.189	6.734	1.00	0.20	O
	ATOM	974	CB	SER	A	63	8.213	67.262	8.921	1.00	0.20	C
	ATOM	975	OG	SER	A	63	7.222	67.611	7.966	1.00	0.20	O
	ATOM	976	H	SER	A	63	7.856	69.781	9.622	1.00	0.00	H
55	ATOM	977	HA	SER	A	63	10.093	68.029	9.673	1.00	0.00	H
	ATOM	978	1HB	SER	A	63	7.772	67.106	9.916	1.00	0.00	H
	ATOM	979	2HB	SER	A	63	8.648	66.313	8.584	1.00	0.00	H
	ATOM	980	HG	SER	A	63	6.731	68.382	8.306	1.00	0.00	H
	ATOM	981	N	GLY	A	64	11.016	67.816	7.328	1.00	0.22	N
60	ATOM	982	CA	GLY	A	64	11.651	67.892	6.044	1.00	0.22	C
	ATOM	983	C	GLY	A	64	13.081	67.501	6.233	1.00	0.22	C
	ATOM	984	O	GLY	A	64	13.461	66.997	7.288	1.00	0.22	O
	ATOM	985	H	GLY	A	64	11.410	67.173	8.006	1.00	0.00	H
	ATOM	986	1HA	GLY	A	64	11.494	68.851	5.553	1.00	0.00	H
65	ATOM	987	2HA	GLY	A	64	11.200	67.149	5.359	1.00	0.00	H
	ATOM	988	N	GLU	A	65	13.918	67.728	5.199	1.00	0.19	N
	ATOM	989	CA	GLU	A	65	15.307	67.383	5.302	1.00	0.19	C
	ATOM	990	C	GLU	A	65	16.074	68.644	5.515	1.00	0.19	C
	ATOM	991	O	GLU	A	65	15.711	69.702	5.000	1.00	0.19	O
70	ATOM	992	CB	GLU	A	65	15.910	66.744	4.040	1.00	0.19	C
	ATOM	993	CG	GLU	A	65	15.403	65.337	3.730	1.00	0.19	C
	ATOM	994	CD	GLU	A	65	16.200	64.821	2.539	1.00	0.19	C

167

	ATOM	995	OE1	GLU	A	65	16.409	65.606	1.575	1.00	0.19	O
	ATOM	996	OE2	GLU	A	65	16.625	63.635	2.584	1.00	0.19	O1-
	ATOM	997	H	GLU	A	65	13.592	68.118	4.323	1.00	0.00	H
	ATOM	998	HA	GLU	A	65	15.418	66.667	6.112	1.00	0.00	H
5	ATOM	999	1HB	GLU	A	65	16.996	66.696	4.211	1.00	0.00	H
	ATOM	1000	2HB	GLU	A	65	15.743	67.417	3.182	1.00	0.00	H
	ATOM	1001	1HG	GLU	A	65	14.334	65.361	3.473	1.00	0.00	H
	ATOM	1002	2HG	GLU	A	65	15.576	64.670	4.587	1.00	0.00	H
10	ATOM	1003	N	TYR	A	66	17.164	68.560	6.304	1.00	0.22	N
	ATOM	1004	CA	TYR	A	66	17.970	69.718	6.549	1.00	0.22	C
	ATOM	1005	C	TYR	A	66	19.342	69.441	6.020	1.00	0.22	C
	ATOM	1006	O	TYR	A	66	19.839	68.318	6.099	1.00	0.22	O
	ATOM	1007	CB	TYR	A	66	18.124	70.071	8.040	1.00	0.22	C
15	ATOM	1008	CG	TYR	A	66	16.782	70.448	8.567	1.00	0.22	C
	ATOM	1009	CD1	TYR	A	66	15.918	69.482	9.033	1.00	0.22	C
	ATOM	1010	CD2	TYR	A	66	16.382	71.764	8.592	1.00	0.22	C
	ATOM	1011	CE1	TYR	A	66	14.679	69.825	9.522	1.00	0.22	C
	ATOM	1012	CE2	TYR	A	66	15.144	72.114	9.078	1.00	0.22	C
20	ATOM	1013	CZ	TYR	A	66	14.291	71.143	9.544	1.00	0.22	C
	ATOM	1014	OH	TYR	A	66	13.021	71.499	10.044	1.00	0.22	O
	ATOM	1015	H	TYR	A	66	17.342	67.720	6.847	1.00	0.00	H
	ATOM	1016	HA	TYR	A	66	17.532	70.591	6.047	1.00	0.00	H
	ATOM	1017	1HB	TYR	A	66	18.806	70.937	8.084	1.00	0.00	H
25	ATOM	1018	2HB	TYR	A	66	18.599	69.314	8.651	1.00	0.00	H
	ATOM	1019	HD1	TYR	A	66	16.191	68.433	9.006	1.00	0.00	H
	ATOM	1020	HD2	TYR	A	66	17.046	72.541	8.220	1.00	0.00	H
	ATOM	1021	HE1	TYR	A	66	13.997	69.066	9.847	1.00	0.00	H
	ATOM	1022	HE2	TYR	A	66	14.837	73.158	9.089	1.00	0.00	H
30	ATOM	1023	HH	TYR	A	66	12.339	71.120	9.464	1.00	0.00	H
	ATOM	1024	N	LYS	A	67	19.979	70.475	5.440	1.00	0.45	N
	ATOM	1025	CA	LYS	A	67	21.299	70.333	4.900	1.00	0.45	C
	ATOM	1026	C	LYS	A	67	22.038	71.587	5.238	1.00	0.45	C
	ATOM	1027	O	LYS	A	67	21.429	72.627	5.482	1.00	0.45	O
35	ATOM	1028	CB	LYS	A	67	21.302	70.211	3.371	1.00	0.45	C
	ATOM	1029	CG	LYS	A	67	20.591	68.953	2.871	1.00	0.45	C
	ATOM	1030	CD	LYS	A	67	20.205	69.019	1.394	1.00	0.45	C
	ATOM	1031	CE	LYS	A	67	18.982	69.902	1.129	1.00	0.45	C
	ATOM	1032	NZ	LYS	A	67	17.786	69.303	1.761	1.00	0.45	N1+
40	ATOM	1033	H	LYS	A	67	19.577	71.404	5.412	1.00	0.00	H
	ATOM	1034	HA	LYS	A	67	21.802	69.466	5.361	1.00	0.00	H
	ATOM	1035	1HB	LYS	A	67	22.349	70.191	3.016	1.00	0.00	H
	ATOM	1036	2HB	LYS	A	67	20.856	71.125	2.952	1.00	0.00	H
	ATOM	1037	1HG	LYS	A	67	19.696	68.714	3.468	1.00	0.00	H
45	ATOM	1038	2HG	LYS	A	67	21.325	68.161	3.088	1.00	0.00	H
	ATOM	1039	1HD	LYS	A	67	19.999	68.030	0.954	1.00	0.00	H
	ATOM	1040	2HD	LYS	A	67	21.053	69.426	0.812	1.00	0.00	H
	ATOM	1041	1HE	LYS	A	67	18.775	69.982	0.049	1.00	0.00	H
	ATOM	1042	2HE	LYS	A	67	19.096	70.919	1.529	1.00	0.00	H
50	ATOM	1043	1HZ	LYS	A	67	16.927	69.761	1.486	1.00	0.00	H
	ATOM	1044	2HZ	LYS	A	67	17.669	68.327	1.501	1.00	0.00	H
	ATOM	1045	3HZ	LYS	A	67	17.829	69.331	2.772	1.00	0.00	H
	ATOM	1046	N	CYS	A	68	23.383	71.512	5.281	1.00	0.52	N
	ATOM	1047	CA	CYS	A	68	24.163	72.670	5.606	1.00	0.52	C
55	ATOM	1048	C	CYS	A	68	25.428	72.644	4.811	1.00	0.52	C
	ATOM	1049	O	CYS	A	68	25.970	71.578	4.524	1.00	0.52	O
	ATOM	1050	CB	CYS	A	68	24.621	72.687	7.065	1.00	0.52	C
	ATOM	1051	SG	CYS	A	68	25.956	73.885	7.311	1.00	0.52	S
	ATOM	1052	H	CYS	A	68	23.896	70.694	5.003	1.00	0.00	H
60	ATOM	1053	HA	CYS	A	68	23.591	73.579	5.374	1.00	0.00	H
	ATOM	1054	1HB	CYS	A	68	24.992	71.688	7.349	1.00	0.00	H
	ATOM	1055	2HB	CYS	A	68	23.803	72.945	7.724	1.00	0.00	H
	ATOM	1056	N	GLN	A	69	25.931	73.832	4.420	1.00	0.27	N
	ATOM	1057	CA	GLN	A	69	27.206	73.865	3.771	1.00	0.27	C
65	ATOM	1058	C	GLN	A	69	27.926	75.086	4.234	1.00	0.27	C
	ATOM	1059	O	GLN	A	69	27.323	76.038	4.727	1.00	0.27	O
	ATOM	1060	CB	GLN	A	69	27.150	73.939	2.237	1.00	0.27	C
	ATOM	1061	CG	GLN	A	69	26.530	75.227	1.700	1.00	0.27	C
	ATOM	1062	CD	GLN	A	69	26.687	75.210	0.186	1.00	0.27	C
70	ATOM	1063	OE1	GLN	A	69	27.435	74.400	-0.360	1.00	0.27	O
	ATOM	1064	NE2	GLN	A	69	25.967	76.130	-0.511	1.00	0.27	N
	ATOM	1065	H	GLN	A	69	25.524	74.715	4.697	1.00	0.00	H

168

	ATOM	1066	HA	GLN	A	69	27.798	72.992	4.081	1.00	0.00	H
	ATOM	1067	1HB	GLN	A	69	26.598	73.064	1.859	1.00	0.00	H
	ATOM	1068	2HB	GLN	A	69	28.189	73.841	1.876	1.00	0.00	H
5	ATOM	1069	1HG	GLN	A	69	27.185	76.031	2.029	1.00	0.00	H
	ATOM	1070	2HG	GLN	A	69	25.497	75.374	2.036	1.00	0.00	H
	ATOM	1071	1HE2	GLN	A	69	25.234	76.647	-0.068	1.00	0.00	H
	ATOM	1072	2HE2	GLN	A	69	25.927	75.922	-1.496	1.00	0.00	H
	ATOM	1073	N	HIS	A	70	29.263	75.063	4.102	1.00	0.11	N
10	ATOM	1074	CA	HIS	A	70	30.076	76.188	4.443	1.00	0.11	C
	ATOM	1075	C	HIS	A	70	30.899	76.470	3.237	1.00	0.11	C
	ATOM	1076	O	HIS	A	70	30.877	75.716	2.267	1.00	0.11	O
	ATOM	1077	CB	HIS	A	70	31.043	75.946	5.612	1.00	0.11	C
	ATOM	1078	CG	HIS	A	70	30.339	75.869	6.930	1.00	0.11	C
15	ATOM	1079	ND1	HIS	A	70	29.937	76.975	7.646	1.00	0.11	N
	ATOM	1080	CD2	HIS	A	70	29.953	74.791	7.664	1.00	0.11	C
	ATOM	1081	CE1	HIS	A	70	29.331	76.515	8.768	1.00	0.11	C
	ATOM	1082	NE2	HIS	A	70	29.316	75.195	8.824	1.00	0.11	N
	ATOM	1083	H	HIS	A	70	29.699	74.376	3.501	1.00	0.00	H
20	ATOM	1084	HA	HIS	A	70	29.447	77.067	4.660	1.00	0.00	H
	ATOM	1085	1HB	HIS	A	70	31.767	76.777	5.657	1.00	0.00	H
	ATOM	1086	2HB	HIS	A	70	31.637	75.036	5.471	1.00	0.00	H
	ATOM	1087	HD2	HIS	A	70	30.099	73.743	7.447	1.00	0.00	H
	ATOM	1088	HE1	HIS	A	70	29.020	77.159	9.580	1.00	0.00	H
25	ATOM	1089	HE2	HIS	A	70	29.016	74.625	9.592	1.00	0.00	H
	ATOM	1090	N	GLN	A	71	31.625	77.600	3.251	1.00	0.12	N
	ATOM	1091	CA	GLN	A	71	32.441	77.912	2.121	1.00	0.12	C
	ATOM	1092	C	GLN	A	71	33.468	76.834	2.009	1.00	0.12	C
	ATOM	1093	O	GLN	A	71	33.753	76.341	0.920	1.00	0.12	O
30	ATOM	1094	CB	GLN	A	71	33.197	79.243	2.276	1.00	0.12	C
	ATOM	1095	CG	GLN	A	71	32.304	80.487	2.279	1.00	0.12	C
	ATOM	1096	CD	GLN	A	71	31.895	80.783	0.843	1.00	0.12	C
	ATOM	1097	OE1	GLN	A	71	32.123	79.983	-0.063	1.00	0.12	O
	ATOM	1098	NE2	GLN	A	71	31.272	81.970	0.623	1.00	0.12	N
35	ATOM	1099	H	GLN	A	71	31.670	78.217	4.051	1.00	0.00	H
	ATOM	1100	HA	GLN	A	71	31.834	77.889	1.204	1.00	0.00	H
	ATOM	1101	1HB	GLN	A	71	33.962	79.321	1.481	1.00	0.00	H
	ATOM	1102	2HB	GLN	A	71	33.758	79.212	3.225	1.00	0.00	H
	ATOM	1103	1HG	GLN	A	71	32.874	81.347	2.668	1.00	0.00	H
40	ATOM	1104	2HG	GLN	A	71	31.411	80.332	2.901	1.00	0.00	H
	ATOM	1105	1HE2	GLN	A	71	31.126	82.615	1.391	1.00	0.00	H
	ATOM	1106	2HE2	GLN	A	71	31.056	82.232	-0.322	1.00	0.00	H
	ATOM	1107	N	GLN	A	72	34.046	76.440	3.157	1.00	0.21	N
	ATOM	1108	CA	GLN	A	72	35.117	75.489	3.188	1.00	0.21	C
45	ATOM	1109	C	GLN	A	72	34.660	74.129	2.761	1.00	0.21	C
	ATOM	1110	O	GLN	A	72	35.308	73.483	1.940	1.00	0.21	O
	ATOM	1111	CB	GLN	A	72	35.698	75.320	4.602	1.00	0.21	C
	ATOM	1112	CG	GLN	A	72	36.104	76.644	5.252	1.00	0.21	C
	ATOM	1113	CD	GLN	A	72	37.057	77.372	4.316	1.00	0.21	C
50	ATOM	1114	OE1	GLN	A	72	37.630	76.784	3.400	1.00	0.21	O
	ATOM	1115	NE2	GLN	A	72	37.224	78.701	4.547	1.00	0.21	N
	ATOM	1116	H	GLN	A	72	33.776	76.855	4.029	1.00	0.00	H
	ATOM	1117	HA	GLN	A	72	35.857	75.781	2.433	1.00	0.00	H
	ATOM	1118	1HB	GLN	A	72	36.568	74.648	4.507	1.00	0.00	H
55	ATOM	1119	2HB	GLN	A	72	34.952	74.810	5.225	1.00	0.00	H
	ATOM	1120	1HG	GLN	A	72	36.614	76.581	6.211	1.00	0.00	H
	ATOM	1121	2HG	GLN	A	72	35.212	77.270	5.418	1.00	0.00	H
	ATOM	1122	1HE2	GLN	A	72	36.792	79.141	5.341	1.00	0.00	H
	ATOM	1123	2HE2	GLN	A	72	37.891	79.177	3.967	1.00	0.00	H
60	ATOM	1124	N	VAL	A	73	33.516	73.660	3.298	1.00	0.31	N
	ATOM	1125	CA	VAL	A	73	33.130	72.297	3.072	1.00	0.31	C
	ATOM	1126	C	VAL	A	73	32.145	72.164	1.959	1.00	0.31	C
	ATOM	1127	O	VAL	A	73	31.658	73.139	1.388	1.00	0.31	O
	ATOM	1128	CB	VAL	A	73	32.521	71.650	4.283	1.00	0.31	C
65	ATOM	1129	CG1	VAL	A	73	33.583	71.602	5.395	1.00	0.31	C
	ATOM	1130	CG2	VAL	A	73	31.247	72.424	4.666	1.00	0.31	C
	ATOM	1131	H	VAL	A	73	32.902	74.241	3.836	1.00	0.00	H
	ATOM	1132	HA	VAL	A	73	34.032	71.730	2.786	1.00	0.00	H
	ATOM	1133	HB	VAL	A	73	32.166	70.641	4.101	1.00	0.00	H
70	ATOM	1134	1HG1	VAL	A	73	33.219	71.046	6.275	1.00	0.00	H
	ATOM	1135	2HG1	VAL	A	73	34.505	71.104	5.053	1.00	0.00	H
	ATOM	1136	3HG1	VAL	A	73	33.855	72.612	5.740	1.00	0.00	H

	ATOM	1137	1HG2	VAL	A	73	31.260	72.697	5.729	1.00	0.00	H
	ATOM	1138	2HG2	VAL	A	73	31.174	73.376	4.129	1.00	0.00	H
	ATOM	1139	3HG2	VAL	A	73	30.331	71.901	4.407	1.00	0.00	H
5	ATOM	1140	N	ASN	A	74	31.857	70.887	1.634	1.00	0.41	N
	ATOM	1141	CA	ASN	A	74	30.932	70.453	0.630	1.00	0.41	C
	ATOM	1142	C	ASN	A	74	29.580	70.504	1.270	1.00	0.41	C
	ATOM	1143	O	ASN	A	74	29.409	71.115	2.322	1.00	0.41	O
	ATOM	1144	CB	ASN	A	74	31.202	68.997	0.200	1.00	0.41	C
	ATOM	1145	CG	ASN	A	74	30.458	68.687	-1.090	1.00	0.41	C
10	ATOM	1146	OD1	ASN	A	74	29.812	69.553	-1.676	1.00	0.41	O
	ATOM	1147	ND2	ASN	A	74	30.542	67.407	-1.542	1.00	0.41	N
	ATOM	1148	H	ASN	A	74	32.331	70.149	2.145	1.00	0.00	H
	ATOM	1149	HA	ASN	A	74	30.976	71.153	-0.222	1.00	0.00	H
	ATOM	1150	1HB	ASN	A	74	30.921	68.305	1.004	1.00	0.00	H
15	ATOM	1151	2HB	ASN	A	74	32.278	68.864	-0.003	1.00	0.00	H
	ATOM	1152	1HD2	ASN	A	74	30.976	66.687	-0.997	1.00	0.00	H
	ATOM	1153	2HD2	ASN	A	74	29.971	67.179	-2.339	1.00	0.00	H
	ATOM	1154	N	GLU	A	75	28.567	69.896	0.622	1.00	0.48	N
	ATOM	1155	CA	GLU	A	75	27.249	69.863	1.180	1.00	0.48	C
20	ATOM	1156	C	GLU	A	75	27.241	68.797	2.228	1.00	0.48	C
	ATOM	1157	O	GLU	A	75	27.925	67.781	2.100	1.00	0.48	O
	ATOM	1158	CB	GLU	A	75	26.170	69.500	0.145	1.00	0.48	C
	ATOM	1159	CG	GLU	A	75	26.047	70.526	-0.982	1.00	0.48	C
	ATOM	1160	CD	GLU	A	75	25.367	71.763	-0.418	1.00	0.48	C
25	ATOM	1161	OE1	GLU	A	75	24.699	71.637	0.643	1.00	0.48	O
	ATOM	1162	OE2	GLU	A	75	25.503	72.851	-1.039	1.00	0.48	O1-
	ATOM	1163	H	GLU	A	75	28.657	69.614	-0.346	1.00	0.00	H
	ATOM	1164	HA	GLU	A	75	27.017	70.847	1.621	1.00	0.00	H
	ATOM	1165	1HB	GLU	A	75	25.207	69.347	0.665	1.00	0.00	H
30	ATOM	1166	2HB	GLU	A	75	26.423	68.509	-0.272	1.00	0.00	H
	ATOM	1167	1HG	GLU	A	75	25.416	70.134	-1.797	1.00	0.00	H
	ATOM	1168	2HG	GLU	A	75	27.009	70.787	-1.450	1.00	0.00	H
	ATOM	1169	N	SER	A	76	26.469	69.018	3.309	1.00	0.42	N
	ATOM	1170	CA	SER	A	76	26.382	68.066	4.377	1.00	0.42	C
35	ATOM	1171	C	SER	A	76	25.336	67.064	4.009	1.00	0.42	C
	ATOM	1172	O	SER	A	76	24.507	67.313	3.136	1.00	0.42	O
	ATOM	1173	CB	SER	A	76	25.956	68.704	5.710	1.00	0.42	C
	ATOM	1174	OG	SER	A	76	25.873	67.713	6.720	1.00	0.42	O
	ATOM	1175	H	SER	A	76	26.027	69.921	3.444	1.00	0.00	H
40	ATOM	1176	HA	SER	A	76	27.347	67.548	4.497	1.00	0.00	H
	ATOM	1177	1HB	SER	A	76	24.918	69.048	5.529	1.00	0.00	H
	ATOM	1178	2HB	SER	A	76	26.368	69.600	6.179	1.00	0.00	H
	ATOM	1179	HG	SER	A	76	25.075	67.185	6.523	1.00	0.00	H
	ATOM	1180	N	GLU	A	77	25.365	65.881	4.660	1.00	0.31	N
45	ATOM	1181	CA	GLU	A	77	24.357	64.903	4.380	1.00	0.31	C
	ATOM	1182	C	GLU	A	77	23.106	65.426	4.998	1.00	0.31	C
	ATOM	1183	O	GLU	A	77	23.138	66.145	5.994	1.00	0.31	O
	ATOM	1184	CB	GLU	A	77	24.596	63.527	5.023	1.00	0.31	C
	ATOM	1185	CG	GLU	A	77	25.878	62.834	4.571	1.00	0.31	C
50	ATOM	1186	CD	GLU	A	77	26.987	63.328	5.483	1.00	0.31	C
	ATOM	1187	OE1	GLU	A	77	26.707	63.507	6.699	1.00	0.31	O
	ATOM	1188	OE2	GLU	A	77	28.123	63.535	4.981	1.00	0.31	O1-
	ATOM	1189	H	GLU	A	77	26.107	65.592	5.291	1.00	0.00	H
	ATOM	1190	HA	GLU	A	77	24.351	64.725	3.293	1.00	0.00	H
55	ATOM	1191	1HB	GLU	A	77	23.730	62.916	4.704	1.00	0.00	H
	ATOM	1192	2HB	GLU	A	77	24.496	63.579	6.121	1.00	0.00	H
	ATOM	1193	1HG	GLU	A	77	26.103	63.000	3.506	1.00	0.00	H
	ATOM	1194	2HG	GLU	A	77	25.778	61.745	4.715	1.00	0.00	H
	ATOM	1195	N	PRO	A	78	22.004	65.094	4.398	1.00	0.29	N
60	ATOM	1196	CA	PRO	A	78	20.764	65.579	4.932	1.00	0.29	C
	ATOM	1197	C	PRO	A	78	20.323	64.843	6.154	1.00	0.29	C
	ATOM	1198	O	PRO	A	78	20.684	63.679	6.323	1.00	0.29	O
	ATOM	1199	CB	PRO	A	78	19.756	65.509	3.788	1.00	0.29	C
	ATOM	1200	CG	PRO	A	78	20.627	65.643	2.527	1.00	0.29	C
65	ATOM	1201	CD	PRO	A	78	21.979	65.042	2.944	1.00	0.29	C
	ATOM	1202	HA	PRO	A	78	20.930	66.637	5.154	1.00	0.00	H
	ATOM	1203	1HB	PRO	A	78	18.975	66.271	3.881	1.00	0.00	H
	ATOM	1204	2HB	PRO	A	78	19.253	64.526	3.777	1.00	0.00	H
	ATOM	1205	1HG	PRO	A	78	20.743	66.647	2.155	1.00	0.00	H
70	ATOM	1206	2HG	PRO	A	78	20.192	65.085	1.679	1.00	0.00	H
	ATOM	1207	1HD	PRO	A	78	22.062	63.992	2.622	1.00	0.00	H

170

	ATOM	1208	2HD	PRO	A	78	22.791	65.613	2.482	1.00	0.00	H
	ATOM	1209	N	VAL	A	79	19.557	65.529	7.022	1.00	0.31	N
	ATOM	1210	CA	VAL	A	79	18.978	64.935	8.187	1.00	0.31	C
5	ATOM	1211	C	VAL	A	79	17.507	65.106	8.006	1.00	0.31	C
	ATOM	1212	O	VAL	A	79	17.055	66.173	7.593	1.00	0.31	O
	ATOM	1213	CB	VAL	A	79	19.362	65.618	9.465	1.00	0.31	C
	ATOM	1214	CG1	VAL	A	79	18.925	67.090	9.386	1.00	0.31	C
	ATOM	1215	CG2	VAL	A	79	18.732	64.848	10.638	1.00	0.31	C
10	ATOM	1216	H	VAL	A	79	19.361	66.506	6.860	1.00	0.00	H
	ATOM	1217	HA	VAL	A	79	19.257	63.869	8.216	1.00	0.00	H
	ATOM	1218	HB	VAL	A	79	20.462	65.577	9.567	1.00	0.00	H
	ATOM	1219	1HG1	VAL	A	79	19.391	67.661	10.210	1.00	0.00	H
	ATOM	1220	2HG1	VAL	A	79	19.283	67.547	8.460	1.00	0.00	H
	ATOM	1221	3HG1	VAL	A	79	17.846	67.223	9.523	1.00	0.00	H
15	ATOM	1222	1HG2	VAL	A	79	19.088	65.237	11.607	1.00	0.00	H
	ATOM	1223	2HG2	VAL	A	79	17.634	64.939	10.652	1.00	0.00	H
	ATOM	1224	3HG2	VAL	A	79	18.990	63.776	10.606	1.00	0.00	H
	ATOM	1225	N	TYR	A	80	16.709	64.061	8.294	1.00	0.19	N
20	ATOM	1226	CA	TYR	A	80	15.305	64.228	8.067	1.00	0.19	C
	ATOM	1227	C	TYR	A	80	14.649	64.401	9.394	1.00	0.19	C
	ATOM	1228	O	TYR	A	80	14.925	63.669	10.343	1.00	0.19	O
	ATOM	1229	CB	TYR	A	80	14.628	63.040	7.359	1.00	0.19	C
	ATOM	1230	CG	TYR	A	80	13.244	63.476	7.018	1.00	0.19	C
25	ATOM	1231	CD1	TYR	A	80	12.214	63.344	7.921	1.00	0.19	C
	ATOM	1232	CD2	TYR	A	80	12.983	64.029	5.785	1.00	0.19	C
	ATOM	1233	CE1	TYR	A	80	10.942	63.754	7.597	1.00	0.19	C
	ATOM	1234	CE2	TYR	A	80	11.714	64.441	5.454	1.00	0.19	C
	ATOM	1235	CZ	TYR	A	80	10.692	64.301	6.360	1.00	0.19	C
30	ATOM	1236	OH	TYR	A	80	9.387	64.723	6.025	1.00	0.19	O
	ATOM	1237	H	TYR	A	80	17.008	63.184	8.683	1.00	0.00	H
	ATOM	1238	HA	TYR	A	80	15.134	65.090	7.415	1.00	0.00	H
	ATOM	1239	1HB	TYR	A	80	14.633	62.141	7.994	1.00	0.00	H
	ATOM	1240	2HB	TYR	A	80	15.197	62.785	6.450	1.00	0.00	H
35	ATOM	1241	HD1	TYR	A	80	12.423	62.901	8.890	1.00	0.00	H
	ATOM	1242	HD2	TYR	A	80	13.756	64.049	5.036	1.00	0.00	H
	ATOM	1243	HE1	TYR	A	80	10.137	63.698	8.310	1.00	0.00	H
	ATOM	1244	HE2	TYR	A	80	11.519	64.850	4.465	1.00	0.00	H
	ATOM	1245	HH	TYR	A	80	8.972	65.029	6.840	1.00	0.00	H
40	ATOM	1246	N	LEU	A	81	13.760	65.406	9.490	1.00	0.08	N
	ATOM	1247	CA	LEU	A	81	13.094	65.671	10.729	1.00	0.08	C
	ATOM	1248	C	LEU	A	81	11.635	65.423	10.529	1.00	0.08	C
	ATOM	1249	O	LEU	A	81	11.076	65.757	9.485	1.00	0.08	O
	ATOM	1250	CB	LEU	A	81	13.250	67.130	11.191	1.00	0.08	C
45	ATOM	1251	CG	LEU	A	81	12.542	67.437	12.522	1.00	0.08	C
	ATOM	1252	CD1	LEU	A	81	13.157	66.632	13.678	1.00	0.08	C
	ATOM	1253	CD2	LEU	A	81	12.505	68.948	12.800	1.00	0.08	C
	ATOM	1254	H	LEU	A	81	13.531	65.997	8.697	1.00	0.00	H
	ATOM	1255	HA	LEU	A	81	13.489	64.991	11.494	1.00	0.00	H
50	ATOM	1256	1HB	LEU	A	81	12.768	67.742	10.414	1.00	0.00	H
	ATOM	1257	2HB	LEU	A	81	14.319	67.393	11.257	1.00	0.00	H
	ATOM	1258	HG	LEU	A	81	11.483	67.141	12.421	1.00	0.00	H
	ATOM	1259	1HD1	LEU	A	81	12.405	66.346	14.427	1.00	0.00	H
	ATOM	1260	2HD1	LEU	A	81	13.691	65.731	13.359	1.00	0.00	H
55	ATOM	1261	3HD1	LEU	A	81	13.915	67.235	14.207	1.00	0.00	H
	ATOM	1262	1HD2	LEU	A	81	11.952	69.171	13.726	1.00	0.00	H
	ATOM	1263	2HD2	LEU	A	81	13.519	69.368	12.903	1.00	0.00	H
	ATOM	1264	3HD2	LEU	A	81	12.001	69.489	11.981	1.00	0.00	H
	ATOM	1265	N	GLU	A	82	10.987	64.798	11.529	1.00	0.09	N
60	ATOM	1266	CA	GLU	A	82	9.582	64.537	11.444	1.00	0.09	C
	ATOM	1267	C	GLU	A	82	8.969	65.149	12.660	1.00	0.09	C
	ATOM	1268	O	GLU	A	82	9.443	64.940	13.776	1.00	0.09	O
	ATOM	1269	CB	GLU	A	82	9.250	63.035	11.486	1.00	0.09	C
	ATOM	1270	CG	GLU	A	82	9.774	62.251	10.282	1.00	0.09	C
65	ATOM	1271	CD	GLU	A	82	9.587	60.767	10.568	1.00	0.09	C
	ATOM	1272	OE1	GLU	A	82	8.557	60.408	11.201	1.00	0.09	O
	ATOM	1273	OE2	GLU	A	82	10.477	59.972	10.166	1.00	0.09	O1-
	ATOM	1274	H	GLU	A	82	11.437	64.495	12.385	1.00	0.00	H
	ATOM	1275	HA	GLU	A	82	9.165	64.964	10.521	1.00	0.00	H
	ATOM	1276	1HB	GLU	A	82	8.149	62.967	11.523	1.00	0.00	H
70	ATOM	1277	2HB	GLU	A	82	9.643	62.600	12.420	1.00	0.00	H
	ATOM	1278	1HG	GLU	A	82	10.829	62.451	10.073	1.00	0.00	H

171

	ATOM	1279	2HG	GLU	A	82	9.148	62.474	9.408	1.00	0.00	H
	ATOM	1280	N	VAL	A	83	7.896	65.936	12.476	1.00	0.09	N
	ATOM	1281	CA	VAL	A	83	7.263	66.538	13.611	1.00	0.09	C
5	ATOM	1282	C	VAL	A	83	5.907	65.928	13.711	1.00	0.09	C
	ATOM	1283	O	VAL	A	83	5.239	65.720	12.700	1.00	0.09	O
	ATOM	1284	CB	VAL	A	83	7.069	68.016	13.470	1.00	0.09	C
	ATOM	1285	CG1	VAL	A	83	8.451	68.684	13.377	1.00	0.09	C
	ATOM	1286	CG2	VAL	A	83	6.170	68.268	12.250	1.00	0.09	C
10	ATOM	1287	H	VAL	A	83	7.390	65.999	11.611	1.00	0.00	H
	ATOM	1288	HA	VAL	A	83	7.846	66.346	14.521	1.00	0.00	H
	ATOM	1289	HB	VAL	A	83	6.558	68.385	14.379	1.00	0.00	H
	ATOM	1290	1HG1	VAL	A	83	8.397	69.772	13.515	1.00	0.00	H
	ATOM	1291	2HG1	VAL	A	83	9.130	68.308	14.159	1.00	0.00	H
15	ATOM	1292	3HG1	VAL	A	83	8.933	68.497	12.403	1.00	0.00	H
	ATOM	1293	1HG2	VAL	A	83	6.508	69.061	11.601	1.00	0.00	H
	ATOM	1294	2HG2	VAL	A	83	6.129	67.447	11.520	1.00	0.00	H
	ATOM	1295	3HG2	VAL	A	83	5.180	68.342	12.716	1.00	0.00	H
	ATOM	1296	N	PHE	A	84	5.469	65.606	14.943	1.00	0.23	N
20	ATOM	1297	CA	PHE	A	84	4.182	64.994	15.076	1.00	0.23	C
	ATOM	1298	C	PHE	A	84	3.459	65.747	16.138	1.00	0.23	C
	ATOM	1299	O	PHE	A	84	4.077	66.424	16.959	1.00	0.23	O
	ATOM	1300	CB	PHE	A	84	4.229	63.552	15.606	1.00	0.23	C
	ATOM	1301	CG	PHE	A	84	5.215	62.773	14.810	1.00	0.23	C
25	ATOM	1302	CD1	PHE	A	84	4.889	62.234	13.590	1.00	0.23	C
	ATOM	1303	CD2	PHE	A	84	6.487	62.595	15.293	1.00	0.23	C
	ATOM	1304	CE1	PHE	A	84	5.814	61.522	12.865	1.00	0.23	C
	ATOM	1305	CE2	PHE	A	84	7.414	61.883	14.572	1.00	0.23	C
	ATOM	1306	CZ	PHE	A	84	7.081	61.341	13.357	1.00	0.23	C
30	ATOM	1307	H	PHE	A	84	6.045	65.661	15.777	1.00	0.00	H
	ATOM	1308	HA	PHE	A	84	3.619	65.035	14.132	1.00	0.00	H
	ATOM	1309	1HB	PHE	A	84	3.221	63.109	15.548	1.00	0.00	H
	ATOM	1310	2HB	PHE	A	84	4.503	63.548	16.673	1.00	0.00	H
	ATOM	1311	HD1	PHE	A	84	3.881	62.359	13.203	1.00	0.00	H
35	ATOM	1312	HD2	PHE	A	84	6.776	63.092	16.211	1.00	0.00	H
	ATOM	1313	HE1	PHE	A	84	5.532	61.066	11.919	1.00	0.00	H
	ATOM	1314	HE2	PHE	A	84	8.434	62.194	14.641	1.00	0.00	H
	ATOM	1315	HZ	PHE	A	84	7.738	60.588	13.011	1.00	0.00	H
	ATOM	1316	N	SER	A	85	2.115	65.679	16.131	1.00	0.34	N
40	ATOM	1317	CA	SER	A	85	1.395	66.292	17.204	1.00	0.34	C
	ATOM	1318	C	SER	A	85	0.673	65.190	17.915	1.00	0.34	C
	ATOM	1319	O	SER	A	85	-0.388	64.740	17.488	1.00	0.34	O
	ATOM	1320	CB	SER	A	85	0.370	67.346	16.748	1.00	0.34	C
	ATOM	1321	OG	SER	A	85	-0.610	66.760	15.906	1.00	0.34	O
45	ATOM	1322	H	SER	A	85	1.591	65.046	15.547	1.00	0.00	H
	ATOM	1323	HA	SER	A	85	2.077	66.796	17.905	1.00	0.00	H
	ATOM	1324	1HB	SER	A	85	0.858	68.148	16.180	1.00	0.00	H
	ATOM	1325	2HB	SER	A	85	-0.105	67.775	17.647	1.00	0.00	H
	ATOM	1326	HG	SER	A	85	-0.897	65.942	16.364	1.00	0.00	H
50	ATOM	1327	N	ASP	A	86	1.255	64.718	19.032	1.00	0.23	N
	ATOM	1328	CA	ASP	A	86	0.646	63.662	19.785	1.00	0.23	C
	ATOM	1329	C	ASP	A	86	0.958	63.925	21.219	1.00	0.23	C
	ATOM	1330	O	ASP	A	86	1.850	64.710	21.535	1.00	0.23	O
	ATOM	1331	CB	ASP	A	86	1.209	62.269	19.458	1.00	0.23	C
55	ATOM	1332	CG	ASP	A	86	0.750	61.889	18.058	1.00	0.23	C
	ATOM	1333	OD1	ASP	A	86	-0.436	62.161	17.730	1.00	0.23	O
	ATOM	1334	OD2	ASP	A	86	1.581	61.328	17.294	1.00	0.23	O1-
	ATOM	1335	H	ASP	A	86	2.097	65.076	19.438	1.00	0.00	H
	ATOM	1336	HA	ASP	A	86	-0.450	63.676	19.655	1.00	0.00	H
60	ATOM	1337	1HB	ASP	A	86	0.728	61.556	20.149	1.00	0.00	H
	ATOM	1338	2HB	ASP	A	86	2.265	62.020	19.445	1.00	0.00	H
	ATOM	1339	N	TRP	A	87	0.199	63.299	22.136	1.00	0.14	N
	ATOM	1340	CA	TRP	A	87	0.482	63.500	23.524	1.00	0.14	C
	ATOM	1341	C	TRP	A	87	1.782	62.871	23.895	1.00	0.14	C
65	ATOM	1342	O	TRP	A	87	2.587	63.476	24.598	1.00	0.14	O
	ATOM	1343	CB	TRP	A	87	-0.603	62.984	24.479	1.00	0.14	C
	ATOM	1344	CG	TRP	A	87	-1.760	63.943	24.577	1.00	0.14	C
	ATOM	1345	CD1	TRP	A	87	-3.025	63.873	24.074	1.00	0.14	C
	ATOM	1346	CD2	TRP	A	87	-1.660	65.206	25.254	1.00	0.14	C
70	ATOM	1347	NE1	TRP	A	87	-3.722	65.014	24.401	1.00	0.14	N
	ATOM	1348	CE2	TRP	A	87	-2.892	65.844	25.126	1.00	0.14	C
	ATOM	1349	CE3	TRP	A	87	-0.621	65.786	25.924	1.00	0.14	C

	ATOM	1350	CZ2	TRP	A	87	-3.106	67.080	25.670	1.00	0.14	C
	ATOM	1351	CZ3	TRP	A	87	-0.839	67.029	26.474	1.00	0.14	C
	ATOM	1352	CH2	TRP	A	87	-2.058	67.665	26.350	1.00	0.14	C
5	ATOM	1353	H	TRP	A	87	-0.549	62.677	21.872	1.00	0.00	H
	ATOM	1354	HA	TRP	A	87	0.614	64.581	23.692	1.00	0.00	H
	ATOM	1355	1HB	TRP	A	87	-0.152	62.874	25.482	1.00	0.00	H
	ATOM	1356	2HB	TRP	A	87	-0.938	61.974	24.197	1.00	0.00	H
	ATOM	1357	HD1	TRP	A	87	-3.478	63.070	23.505	1.00	0.00	H
10	ATOM	1358	HE1	TRP	A	87	-4.681	65.186	24.205	1.00	0.00	H
	ATOM	1359	HE3	TRP	A	87	0.335	65.286	26.045	1.00	0.00	H
	ATOM	1360	HZ2	TRP	A	87	-4.070	67.574	25.578	1.00	0.00	H
	ATOM	1361	HZ3	TRP	A	87	-0.071	67.493	27.066	1.00	0.00	H
	ATOM	1362	HH2	TRP	A	87	-2.209	68.629	26.826	1.00	0.00	H
15	ATOM	1363	N	LEU	A	88	2.035	61.637	23.423	1.00	0.12	N
	ATOM	1364	CA	LEU	A	88	3.244	60.972	23.818	1.00	0.12	C
	ATOM	1365	C	LEU	A	88	3.845	60.339	22.607	1.00	0.12	C
	ATOM	1366	O	LEU	A	88	3.126	59.888	21.717	1.00	0.12	O
	ATOM	1367	CB	LEU	A	88	2.988	59.838	24.827	1.00	0.12	C
20	ATOM	1368	CG	LEU	A	88	4.252	59.089	25.294	1.00	0.12	C
	ATOM	1369	CD1	LEU	A	88	5.169	59.984	26.135	1.00	0.12	C
	ATOM	1370	CD2	LEU	A	88	3.893	57.777	26.012	1.00	0.12	C
	ATOM	1371	H	LEU	A	88	1.475	61.180	22.722	1.00	0.00	H
	ATOM	1372	HA	LEU	A	88	3.945	61.699	24.244	1.00	0.00	H
25	ATOM	1373	1HB	LEU	A	88	2.285	59.119	24.367	1.00	0.00	H
	ATOM	1374	2HB	LEU	A	88	2.468	60.250	25.711	1.00	0.00	H
	ATOM	1375	HG	LEU	A	88	4.824	58.770	24.411	1.00	0.00	H
	ATOM	1376	1HD1	LEU	A	88	6.215	59.895	25.827	1.00	0.00	H
	ATOM	1377	2HD1	LEU	A	88	4.833	61.025	26.171	1.00	0.00	H
30	ATOM	1378	3HD1	LEU	A	88	5.148	59.665	27.192	1.00	0.00	H
	ATOM	1379	1HD2	LEU	A	88	4.792	57.191	26.258	1.00	0.00	H
	ATOM	1380	2HD2	LEU	A	88	3.353	57.971	26.954	1.00	0.00	H
	ATOM	1381	3HD2	LEU	A	88	3.238	57.148	25.391	1.00	0.00	H
	ATOM	1382	N	LEU	A	89	5.192	60.305	22.535	1.00	0.11	N
35	ATOM	1383	CA	LEU	A	89	5.817	59.659	21.418	1.00	0.11	C
	ATOM	1384	C	LEU	A	89	7.020	58.940	21.934	1.00	0.11	C
	ATOM	1385	O	LEU	A	89	7.608	59.330	22.942	1.00	0.11	O
	ATOM	1386	CB	LEU	A	89	6.316	60.624	20.325	1.00	0.11	C
	ATOM	1387	CG	LEU	A	89	6.996	59.930	19.129	1.00	0.11	C
40	ATOM	1388	CD1	LEU	A	89	6.001	59.044	18.356	1.00	0.11	C
	ATOM	1389	CD2	LEU	A	89	7.712	60.949	18.228	1.00	0.11	C
	ATOM	1390	H	LEU	A	89	5.789	60.680	23.262	1.00	0.00	H
	ATOM	1391	HA	LEU	A	89	5.072	59.108	20.865	1.00	0.00	H
	ATOM	1392	1HB	LEU	A	89	7.013	61.361	20.757	1.00	0.00	H
45	ATOM	1393	2HB	LEU	A	89	5.451	61.173	19.917	1.00	0.00	H
	ATOM	1394	HG	LEU	A	89	7.833	59.325	19.477	1.00	0.00	H
	ATOM	1395	1HD1	LEU	A	89	6.458	58.614	17.450	1.00	0.00	H
	ATOM	1396	2HD1	LEU	A	89	5.636	58.199	18.955	1.00	0.00	H
	ATOM	1397	3HD1	LEU	A	89	5.127	59.633	18.029	1.00	0.00	H
50	ATOM	1398	1HD2	LEU	A	89	8.143	60.354	17.418	1.00	0.00	H
	ATOM	1399	2HD2	LEU	A	89	7.008	61.683	17.815	1.00	0.00	H
	ATOM	1400	3HD2	LEU	A	89	8.510	61.485	18.761	1.00	0.00	H
	ATOM	1401	N	LEU	A	90	7.400	57.840	21.259	1.00	0.11	N
	ATOM	1402	CA	LEU	A	90	8.597	57.166	21.649	1.00	0.11	C
55	ATOM	1403	C	LEU	A	90	9.606	57.680	20.677	1.00	0.11	C
	ATOM	1404	O	LEU	A	90	9.404	57.600	19.467	1.00	0.11	O
	ATOM	1405	CB	LEU	A	90	8.527	55.634	21.510	1.00	0.11	C
	ATOM	1406	CG	LEU	A	90	9.818	54.918	21.950	1.00	0.11	C
	ATOM	1407	CD1	LEU	A	90	10.083	55.137	23.448	1.00	0.11	C
60	ATOM	1408	CD2	LEU	A	90	9.793	53.429	21.568	1.00	0.11	C
	ATOM	1409	H	LEU	A	90	7.168	57.724	20.279	1.00	0.00	H
	ATOM	1410	HA	LEU	A	90	8.845	57.420	22.688	1.00	0.00	H
	ATOM	1411	1HB	LEU	A	90	8.288	55.373	20.463	1.00	0.00	H
	ATOM	1412	2HB	LEU	A	90	7.684	55.257	22.117	1.00	0.00	H
65	ATOM	1413	HG	LEU	A	90	10.652	55.369	21.379	1.00	0.00	H
	ATOM	1414	1HD1	LEU	A	90	11.099	55.509	23.615	1.00	0.00	H
	ATOM	1415	2HD1	LEU	A	90	9.407	55.868	23.914	1.00	0.00	H
	ATOM	1416	3HD1	LEU	A	90	9.922	54.203	24.002	1.00	0.00	H
	ATOM	1417	1HD2	LEU	A	90	10.779	52.972	21.676	1.00	0.00	H
	ATOM	1418	2HD2	LEU	A	90	9.069	52.884	22.192	1.00	0.00	H
70	ATOM	1419	3HD2	LEU	A	90	9.493	53.311	20.514	1.00	0.00	H
	ATOM	1420	N	GLN	A	91	10.719	58.238	21.185	1.00	0.11	N

173

	ATOM	1421	CA	GLN	A	91	11.640	58.868	20.289	1.00	0.11	C
	ATOM	1422	C	GLN	A	91	12.857	58.018	20.152	1.00	0.11	C
	ATOM	1423	O	GLN	A	91	13.277	57.346	21.093	1.00	0.11	O
5	ATOM	1424	CB	GLN	A	91	12.096	60.254	20.782	1.00	0.11	C
	ATOM	1425	CG	GLN	A	91	10.956	61.273	20.886	1.00	0.11	C
	ATOM	1426	CD	GLN	A	91	11.531	62.582	21.415	1.00	0.11	C
	ATOM	1427	OE1	GLN	A	91	12.410	62.580	22.275	1.00	0.11	O
	ATOM	1428	NE2	GLN	A	91	11.026	63.730	20.890	1.00	0.11	N
10	ATOM	1429	H	GLN	A	91	10.880	58.341	22.182	1.00	0.00	H
	ATOM	1430	HA	GLN	A	91	11.164	59.029	19.308	1.00	0.00	H
	ATOM	1431	1HB	GLN	A	91	12.816	60.629	20.042	1.00	0.00	H
	ATOM	1432	2HB	GLN	A	91	12.614	60.147	21.748	1.00	0.00	H
	ATOM	1433	1HG	GLN	A	91	10.184	60.951	21.607	1.00	0.00	H
15	ATOM	1434	2HG	GLN	A	91	10.464	61.391	19.910	1.00	0.00	H
	ATOM	1435	1HE2	GLN	A	91	10.469	63.660	20.055	1.00	0.00	H
	ATOM	1436	2HE2	GLN	A	91	11.451	64.600	21.151	1.00	0.00	H
	ATOM	1437	N	ALA	A	92	13.435	58.011	18.936	1.00	0.18	N
	ATOM	1438	CA	ALA	A	92	14.630	57.261	18.701	1.00	0.18	C
20	ATOM	1439	C	ALA	A	92	15.533	58.108	17.870	1.00	0.18	C
	ATOM	1440	O	ALA	A	92	15.082	58.925	17.072	1.00	0.18	O
	ATOM	1441	CB	ALA	A	92	14.397	55.956	17.923	1.00	0.18	C
	ATOM	1442	H	ALA	A	92	13.116	58.559	18.152	1.00	0.00	H
	ATOM	1443	HA	ALA	A	92	15.098	56.977	19.650	1.00	0.00	H
25	ATOM	1444	1HB	ALA	A	92	15.351	55.416	17.814	1.00	0.00	H
	ATOM	1445	2HB	ALA	A	92	13.693	55.304	18.463	1.00	0.00	H
	ATOM	1446	3HB	ALA	A	92	13.990	56.146	16.918	1.00	0.00	H
	ATOM	1447	N	SER	A	93	16.852	57.959	18.076	1.00	0.25	N
	ATOM	1448	CA	SER	A	93	17.796	58.710	17.309	1.00	0.25	C
30	ATOM	1449	C	SER	A	93	17.756	58.227	15.893	1.00	0.25	C
	ATOM	1450	O	SER	A	93	17.703	59.024	14.957	1.00	0.25	O
	ATOM	1451	CB	SER	A	93	19.230	58.542	17.826	1.00	0.25	C
	ATOM	1452	OG	SER	A	93	20.123	59.308	17.034	1.00	0.25	O
	ATOM	1453	H	SER	A	93	17.208	57.332	18.779	1.00	0.00	H
35	ATOM	1454	HA	SER	A	93	17.535	59.779	17.322	1.00	0.00	H
	ATOM	1455	1HB	SER	A	93	19.526	57.478	17.807	1.00	0.00	H
	ATOM	1456	2HB	SER	A	93	19.278	58.881	18.878	1.00	0.00	H
	ATOM	1457	HG	SER	A	93	21.022	59.117	17.333	1.00	0.00	H
	ATOM	1458	N	ALA	A	94	17.769	56.893	15.694	1.00	0.19	N
40	ATOM	1459	CA	ALA	A	94	17.777	56.384	14.351	1.00	0.19	C
	ATOM	1460	C	ALA	A	94	16.919	55.161	14.290	1.00	0.19	C
	ATOM	1461	O	ALA	A	94	16.764	54.435	15.271	1.00	0.19	O
	ATOM	1462	CB	ALA	A	94	19.179	55.986	13.860	1.00	0.19	C
	ATOM	1463	H	ALA	A	94	17.675	56.216	16.429	1.00	0.00	H
45	ATOM	1464	HA	ALA	A	94	17.357	57.141	13.668	1.00	0.00	H
	ATOM	1465	1HB	ALA	A	94	19.119	55.626	12.821	1.00	0.00	H
	ATOM	1466	2HB	ALA	A	94	19.858	56.852	13.885	1.00	0.00	H
	ATOM	1467	3HB	ALA	A	94	19.610	55.186	14.481	1.00	0.00	H
	ATOM	1468	N	GLU	A	95	16.301	54.943	13.114	1.00	0.12	N
50	ATOM	1469	CA	GLU	A	95	15.454	53.816	12.861	1.00	0.12	C
	ATOM	1470	C	GLU	A	95	16.282	52.569	12.802	1.00	0.12	C
	ATOM	1471	O	GLU	A	95	15.920	51.545	13.378	1.00	0.12	O
	ATOM	1472	CB	GLU	A	95	14.711	53.966	11.522	1.00	0.12	C
	ATOM	1473	CG	GLU	A	95	13.753	55.164	11.506	1.00	0.12	C
55	ATOM	1474	CD	GLU	A	95	13.312	55.426	10.073	1.00	0.12	C
	ATOM	1475	OE1	GLU	A	95	13.538	54.538	9.208	1.00	0.12	O
	ATOM	1476	OE2	GLU	A	95	12.742	56.522	9.826	1.00	0.12	O1-
	ATOM	1477	H	GLU	A	95	16.317	55.628	12.375	1.00	0.00	H
	ATOM	1478	HA	GLU	A	95	14.723	53.702	13.677	1.00	0.00	H
60	ATOM	1479	1HB	GLU	A	95	14.147	53.030	11.359	1.00	0.00	H
	ATOM	1480	2HB	GLU	A	95	15.448	54.046	10.704	1.00	0.00	H
	ATOM	1481	1HG	GLU	A	95	14.200	56.089	11.906	1.00	0.00	H
	ATOM	1482	2HG	GLU	A	95	12.869	54.967	12.134	1.00	0.00	H
	ATOM	1483	N	VAL	A	96	17.436	52.630	12.110	1.00	0.11	N
65	ATOM	1484	CA	VAL	A	96	18.234	51.449	11.956	1.00	0.11	C
	ATOM	1485	C	VAL	A	96	19.504	51.637	12.709	1.00	0.11	C
	ATOM	1486	O	VAL	A	96	20.025	52.747	12.813	1.00	0.11	O
	ATOM	1487	CB	VAL	A	96	18.599	51.162	10.531	1.00	0.11	C
	ATOM	1488	CG1	VAL	A	96	19.514	49.924	10.495	1.00	0.11	C
	ATOM	1489	CG2	VAL	A	96	17.299	51.002	9.726	1.00	0.11	C
70	ATOM	1490	H	VAL	A	96	17.805	53.489	11.747	1.00	0.00	H
	ATOM	1491	HA	VAL	A	96	17.676	50.587	12.332	1.00	0.00	H

	ATOM	1492	HB	VAL	A	96	19.167	52.009	10.104	1.00	0.00	H
	ATOM	1493	1HG1	VAL	A	96	19.610	49.588	9.448	1.00	0.00	H
	ATOM	1494	2HG1	VAL	A	96	20.517	50.203	10.851	1.00	0.00	H
5	ATOM	1495	3HG1	VAL	A	96	19.099	49.089	11.077	1.00	0.00	H
	ATOM	1496	1HG2	VAL	A	96	17.491	50.648	8.699	1.00	0.00	H
	ATOM	1497	2HG2	VAL	A	96	16.617	50.282	10.198	1.00	0.00	H
	ATOM	1498	3HG2	VAL	A	96	16.754	51.957	9.632	1.00	0.00	H
	ATOM	1499	N	VAL	A	97	20.028	50.531	13.268	1.00	0.10	N
10	ATOM	1500	CA	VAL	A	97	21.230	50.600	14.039	1.00	0.10	C
	ATOM	1501	C	VAL	A	97	22.100	49.467	13.620	1.00	0.10	C
	ATOM	1502	O	VAL	A	97	21.654	48.534	12.957	1.00	0.10	O
	ATOM	1503	CB	VAL	A	97	20.992	50.432	15.511	1.00	0.10	C
	ATOM	1504	CG1	VAL	A	97	20.128	51.603	16.004	1.00	0.10	C
15	ATOM	1505	CG2	VAL	A	97	20.363	49.050	15.752	1.00	0.10	C
	ATOM	1506	H	VAL	A	97	19.530	49.654	13.277	1.00	0.00	H
	ATOM	1507	HA	VAL	A	97	21.758	51.533	13.789	1.00	0.00	H
	ATOM	1508	HB	VAL	A	97	21.926	50.382	16.060	1.00	0.00	H
	ATOM	1509	1HG1	VAL	A	97	20.116	51.663	17.104	1.00	0.00	H
20	ATOM	1510	2HG1	VAL	A	97	20.458	52.583	15.626	1.00	0.00	H
	ATOM	1511	3HG1	VAL	A	97	19.080	51.481	15.680	1.00	0.00	H
	ATOM	1512	1HG2	VAL	A	97	20.214	48.890	16.835	1.00	0.00	H
	ATOM	1513	2HG2	VAL	A	97	19.366	48.957	15.298	1.00	0.00	H
	ATOM	1514	3HG2	VAL	A	97	21.003	48.221	15.413	1.00	0.00	H
25	ATOM	1515	N	MET	A	98	23.386	49.536	14.004	1.00	0.12	N
	ATOM	1516	CA	MET	A	98	24.315	48.497	13.688	1.00	0.12	C
	ATOM	1517	C	MET	A	98	24.355	47.640	14.909	1.00	0.12	C
	ATOM	1518	O	MET	A	98	24.093	48.117	16.012	1.00	0.12	O
	ATOM	1519	CB	MET	A	98	25.737	49.029	13.442	1.00	0.12	C
30	ATOM	1520	CG	MET	A	98	25.810	50.033	12.286	1.00	0.12	C
	ATOM	1521	SD	MET	A	98	25.466	49.342	10.639	1.00	0.12	S
	ATOM	1522	CE	MET	A	98	27.170	48.804	10.325	1.00	0.12	C
	ATOM	1523	H	MET	A	98	23.734	50.300	14.559	1.00	0.00	H
	ATOM	1524	HA	MET	A	98	24.011	47.939	12.813	1.00	0.00	H
35	ATOM	1525	1HB	MET	A	98	26.406	48.172	13.257	1.00	0.00	H
	ATOM	1526	2HB	MET	A	98	26.107	49.527	14.356	1.00	0.00	H
	ATOM	1527	1HG	MET	A	98	26.805	50.510	12.241	1.00	0.00	H
	ATOM	1528	2HG	MET	A	98	25.093	50.856	12.444	1.00	0.00	H
	ATOM	1529	1HE	MET	A	98	27.192	48.311	9.342	1.00	0.00	H
40	ATOM	1530	2HE	MET	A	98	27.854	49.665	10.300	1.00	0.00	H
	ATOM	1531	3HE	MET	A	98	27.497	48.081	11.086	1.00	0.00	H
	ATOM	1532	N	GLU	A	99	24.653	46.339	14.755	1.00	0.10	N
	ATOM	1533	CA	GLU	A	99	24.662	45.530	15.936	1.00	0.10	C
	ATOM	1534	C	GLU	A	99	25.806	45.976	16.779	1.00	0.10	C
45	ATOM	1535	O	GLU	A	99	26.866	46.341	16.272	1.00	0.10	O
	ATOM	1536	CB	GLU	A	99	24.838	44.022	15.682	1.00	0.10	C
	ATOM	1537	CG	GLU	A	99	24.757	43.196	16.970	1.00	0.10	C
	ATOM	1538	CD	GLU	A	99	24.956	41.726	16.629	1.00	0.10	C
	ATOM	1539	OE1	GLU	A	99	24.323	41.247	15.652	1.00	0.10	O
50	ATOM	1540	OE2	GLU	A	99	25.752	41.063	17.347	1.00	0.10	O1-
	ATOM	1541	H	GLU	A	99	24.979	45.929	13.900	1.00	0.00	H
	ATOM	1542	HA	GLU	A	99	23.696	45.668	16.459	1.00	0.00	H
	ATOM	1543	1HB	GLU	A	99	25.788	43.861	15.155	1.00	0.00	H
	ATOM	1544	2HB	GLU	A	99	23.975	43.700	15.117	1.00	0.00	H
55	ATOM	1545	1HG	GLU	A	99	23.715	43.288	17.265	1.00	0.00	H
	ATOM	1546	2HG	GLU	A	99	25.443	43.481	17.776	1.00	0.00	H
	ATOM	1547	N	GLY	A	100	25.599	45.973	18.108	1.00	0.20	N
	ATOM	1548	CA	GLY	A	100	26.641	46.338	19.014	1.00	0.20	C
	ATOM	1549	C	GLY	A	100	26.474	47.770	19.396	1.00	0.20	C
60	ATOM	1550	O	GLY	A	100	27.034	48.210	20.399	1.00	0.20	O
	ATOM	1551	H	GLY	A	100	24.793	45.476	18.493	1.00	0.00	H
	ATOM	1552	1HA	GLY	A	100	27.635	46.198	18.562	1.00	0.00	H
	ATOM	1553	2HA	GLY	A	100	26.586	45.711	19.915	1.00	0.00	H
	ATOM	1554	N	GLN	A	101	25.696	48.551	18.624	1.00	0.50	N
65	ATOM	1555	CA	GLN	A	101	25.580	49.916	19.038	1.00	0.50	C
	ATOM	1556	C	GLN	A	101	24.520	50.006	20.078	1.00	0.50	C
	ATOM	1557	O	GLN	A	101	23.614	49.177	20.161	1.00	0.50	O
	ATOM	1558	CB	GLN	A	101	25.311	50.943	17.920	1.00	0.50	C
	ATOM	1559	CG	GLN	A	101	23.985	50.816	17.175	1.00	0.50	C
70	ATOM	1560	CD	GLN	A	101	23.925	52.009	16.224	1.00	0.50	C
	ATOM	1561	OE1	GLN	A	101	22.862	52.418	15.763	1.00	0.50	O
	ATOM	1562	NE2	GLN	A	101	25.114	52.601	15.932	1.00	0.50	N

175

	ATOM	1563	H	GLN	A	101	25.186	48.208	17.818	1.00	0.00	H
	ATOM	1564	HA	GLN	A	101	26.589	50.219	19.360	1.00	0.00	H
	ATOM	1565	1HB	GLN	A	101	26.170	50.832	17.236	1.00	0.00	H
5	ATOM	1566	2HB	GLN	A	101	25.362	51.936	18.402	1.00	0.00	H
	ATOM	1567	1HG	GLN	A	101	23.127	50.886	17.861	1.00	0.00	H
	ATOM	1568	2HG	GLN	A	101	23.855	50.016	16.515	1.00	0.00	H
	ATOM	1569	1HE2	GLN	A	101	25.979	52.314	16.347	1.00	0.00	H
	ATOM	1570	2HE2	GLN	A	101	25.070	53.427	15.358	1.00	0.00	H
10	ATOM	1571	N	PRO	A	102	24.671	50.987	20.918	1.00	0.57	N
	ATOM	1572	CA	PRO	A	102	23.702	51.170	21.956	1.00	0.57	C
	ATOM	1573	C	PRO	A	102	22.464	51.776	21.396	1.00	0.57	C
	ATOM	1574	O	PRO	A	102	22.552	52.542	20.440	1.00	0.57	O
	ATOM	1575	CB	PRO	A	102	24.375	52.030	23.023	1.00	0.57	C
15	ATOM	1576	CG	PRO	A	102	25.870	51.719	22.846	1.00	0.57	C
	ATOM	1577	CD	PRO	A	102	26.007	51.366	21.355	1.00	0.57	C
	ATOM	1578	HA	PRO	A	102	23.501	50.183	22.400	1.00	0.00	H
	ATOM	1579	1HB	PRO	A	102	23.985	51.835	24.034	1.00	0.00	H
	ATOM	1580	2HB	PRO	A	102	24.196	53.099	22.815	1.00	0.00	H
20	ATOM	1581	1HG	PRO	A	102	26.136	50.844	23.462	1.00	0.00	H
	ATOM	1582	2HG	PRO	A	102	26.539	52.537	23.155	1.00	0.00	H
	ATOM	1583	1HD	PRO	A	102	26.352	52.231	20.768	1.00	0.00	H
	ATOM	1584	2HD	PRO	A	102	26.737	50.556	21.257	1.00	0.00	H
	ATOM	1585	N	LEU	A	103	21.299	51.440	21.973	1.00	0.26	N
25	ATOM	1586	CA	LEU	A	103	20.081	52.025	21.517	1.00	0.26	C
	ATOM	1587	C	LEU	A	103	19.597	52.884	22.628	1.00	0.26	C
	ATOM	1588	O	LEU	A	103	19.568	52.462	23.782	1.00	0.26	O
	ATOM	1589	CB	LEU	A	103	18.971	51.003	21.213	1.00	0.26	C
	ATOM	1590	CG	LEU	A	103	17.661	51.649	20.720	1.00	0.26	C
30	ATOM	1591	CD1	LEU	A	103	17.856	52.350	19.366	1.00	0.26	C
	ATOM	1592	CD2	LEU	A	103	16.509	50.631	20.709	1.00	0.26	C
	ATOM	1593	H	LEU	A	103	21.252	50.742	22.706	1.00	0.00	H
	ATOM	1594	HA	LEU	A	103	20.277	52.609	20.607	1.00	0.00	H
	ATOM	1595	1HB	LEU	A	103	18.745	50.444	22.129	1.00	0.00	H
35	ATOM	1596	2HB	LEU	A	103	19.330	50.271	20.467	1.00	0.00	H
	ATOM	1597	HG	LEU	A	103	17.358	52.425	21.447	1.00	0.00	H
	ATOM	1598	1HD1	LEU	A	103	16.913	52.798	19.010	1.00	0.00	H
	ATOM	1599	2HD1	LEU	A	103	18.597	53.162	19.405	1.00	0.00	H
	ATOM	1600	3HD1	LEU	A	103	18.182	51.630	18.598	1.00	0.00	H
40	ATOM	1601	1HD2	LEU	A	103	15.604	51.038	20.237	1.00	0.00	H
	ATOM	1602	2HD2	LEU	A	103	16.779	49.714	20.160	1.00	0.00	H
	ATOM	1603	3HD2	LEU	A	103	16.227	50.355	21.735	1.00	0.00	H
	ATOM	1604	N	PHE	A	104	19.234	54.137	22.312	1.00	0.08	N
	ATOM	1605	CA	PHE	A	104	18.730	54.987	23.344	1.00	0.08	C
45	ATOM	1606	C	PHE	A	104	17.343	55.343	22.936	1.00	0.08	C
	ATOM	1607	O	PHE	A	104	17.099	55.705	21.785	1.00	0.08	O
	ATOM	1608	CB	PHE	A	104	19.527	56.291	23.513	1.00	0.08	C
	ATOM	1609	CG	PHE	A	104	18.986	57.015	24.699	1.00	0.08	C
	ATOM	1610	CD1	PHE	A	104	19.376	56.664	25.972	1.00	0.08	C
50	ATOM	1611	CD2	PHE	A	104	18.097	58.052	24.540	1.00	0.08	C
	ATOM	1612	CE1	PHE	A	104	18.881	57.333	27.066	1.00	0.08	C
	ATOM	1613	CE2	PHE	A	104	17.597	58.725	25.630	1.00	0.08	C
	ATOM	1614	CZ	PHE	A	104	17.990	58.364	26.896	1.00	0.08	C
	ATOM	1615	H	PHE	A	104	19.154	54.483	21.371	1.00	0.00	H
55	ATOM	1616	HA	PHE	A	104	18.727	54.463	24.309	1.00	0.00	H
	ATOM	1617	1HB	PHE	A	104	19.477	56.897	22.596	1.00	0.00	H
	ATOM	1618	2HB	PHE	A	104	20.592	56.046	23.663	1.00	0.00	H
	ATOM	1619	HD1	PHE	A	104	20.097	55.863	26.109	1.00	0.00	H
	ATOM	1620	HD2	PHE	A	104	18.020	58.419	23.527	1.00	0.00	H
60	ATOM	1621	HE1	PHE	A	104	19.224	57.065	28.062	1.00	0.00	H
	ATOM	1622	HE2	PHE	A	104	16.936	59.563	25.591	1.00	0.00	H
	ATOM	1623	HZ	PHE	A	104	17.766	59.003	27.735	1.00	0.00	H
	ATOM	1624	N	LEU	A	105	16.385	55.216	23.872	1.00	0.10	N
	ATOM	1625	CA	LEU	A	105	15.028	55.541	23.562	1.00	0.10	C
65	ATOM	1626	C	LEU	A	105	14.558	56.470	24.624	1.00	0.10	C
	ATOM	1627	O	LEU	A	105	15.108	56.504	25.724	1.00	0.10	O
	ATOM	1628	CB	LEU	A	105	14.079	54.330	23.569	1.00	0.10	C
	ATOM	1629	CG	LEU	A	105	14.388	53.284	22.481	1.00	0.10	C
	ATOM	1630	CD1	LEU	A	105	13.388	52.118	22.534	1.00	0.10	C
	ATOM	1631	CD2	LEU	A	105	14.485	53.930	21.090	1.00	0.10	C
70	ATOM	1632	H	LEU	A	105	16.573	54.928	24.828	1.00	0.00	H
	ATOM	1633	HA	LEU	A	105	14.968	56.061	22.597	1.00	0.00	H

	ATOM	1634	1HB	LEU	A	105	13.123	54.780	23.234	1.00	0.00	H
	ATOM	1635	2HB	LEU	A	105	13.791	53.897	24.481	1.00	0.00	H
	ATOM	1636	HG	LEU	A	105	15.382	52.848	22.697	1.00	0.00	H
5	ATOM	1637	1HD1	LEU	A	105	13.415	51.501	21.622	1.00	0.00	H
	ATOM	1638	2HD1	LEU	A	105	13.614	51.452	23.383	1.00	0.00	H
	ATOM	1639	3HD1	LEU	A	105	12.364	52.474	22.682	1.00	0.00	H
	ATOM	1640	1HD2	LEU	A	105	14.787	53.185	20.341	1.00	0.00	H
	ATOM	1641	2HD2	LEU	A	105	13.499	54.316	20.781	1.00	0.00	H
10	ATOM	1642	3HD2	LEU	A	105	15.189	54.755	20.996	1.00	0.00	H
	ATOM	1643	N	ARG	A	106	13.530	57.274	24.307	1.00	0.15	N
	ATOM	1644	CA	ARG	A	106	13.059	58.210	25.276	1.00	0.15	C
	ATOM	1645	C	ARG	A	106	11.579	58.303	25.130	1.00	0.15	C
	ATOM	1646	O	ARG	A	106	11.049	58.285	24.020	1.00	0.15	O
15	ATOM	1647	CB	ARG	A	106	13.663	59.604	25.034	1.00	0.15	C
	ATOM	1648	CG	ARG	A	106	13.241	60.704	26.004	1.00	0.15	C
	ATOM	1649	CD	ARG	A	106	14.061	61.978	25.787	1.00	0.15	C
	ATOM	1650	NE	ARG	A	106	13.541	63.034	26.698	1.00	0.15	N1+
	ATOM	1651	CZ	ARG	A	106	12.993	64.164	26.169	1.00	0.15	C
20	ATOM	1652	NH1	ARG	A	106	12.935	64.310	24.813	1.00	0.15	N
	ATOM	1653	NH2	ARG	A	106	12.531	65.148	26.995	1.00	0.15	N
	ATOM	1654	H	ARG	A	106	13.091	57.282	23.397	1.00	0.00	H
	ATOM	1655	HA	ARG	A	106	13.331	57.888	26.288	1.00	0.00	H
	ATOM	1656	1HB	ARG	A	106	13.453	59.931	24.002	1.00	0.00	H
25	ATOM	1657	2HB	ARG	A	106	14.740	59.440	25.151	1.00	0.00	H
	ATOM	1658	1HG	ARG	A	106	13.146	60.420	27.059	1.00	0.00	H
	ATOM	1659	2HG	ARG	A	106	12.200	60.978	25.736	1.00	0.00	H
	ATOM	1660	1HD	ARG	A	106	13.950	62.234	24.738	1.00	0.00	H
	ATOM	1661	2HD	ARG	A	106	15.136	61.855	25.994	1.00	0.00	H
30	ATOM	1662	HE	ARG	A	106	13.936	63.151	27.606	1.00	0.00	H
	ATOM	1663	1HH1	ARG	A	106	12.969	63.518	24.200	1.00	0.00	H
	ATOM	1664	2HH1	ARG	A	106	12.383	65.056	24.442	1.00	0.00	H
	ATOM	1665	1HH2	ARG	A	106	12.175	66.008	26.638	1.00	0.00	H
	ATOM	1666	2HH2	ARG	A	106	12.481	65.003	27.979	1.00	0.00	H
35	ATOM	1667	N	CYS	A	107	10.862	58.384	26.266	1.00	0.16	N
	ATOM	1668	CA	CYS	A	107	9.446	58.560	26.188	1.00	0.16	C
	ATOM	1669	C	CYS	A	107	9.261	60.020	26.416	1.00	0.16	C
	ATOM	1670	O	CYS	A	107	9.650	60.546	27.458	1.00	0.16	O
	ATOM	1671	CB	CYS	A	107	8.663	57.792	27.268	1.00	0.16	C
40	ATOM	1672	SG	CYS	A	107	9.006	56.009	27.207	1.00	0.16	S
	ATOM	1673	H	CYS	A	107	11.264	58.413	27.191	1.00	0.00	H
	ATOM	1674	HA	CYS	A	107	9.063	58.219	25.214	1.00	0.00	H
	ATOM	1675	1HB	CYS	A	107	7.591	57.974	27.085	1.00	0.00	H
	ATOM	1676	2HB	CYS	A	107	8.887	58.155	28.282	1.00	0.00	H
45	ATOM	1677	N	HIS	A	108	8.681	60.725	25.429	1.00	0.11	N
	ATOM	1678	CA	HIS	A	108	8.593	62.147	25.557	1.00	0.11	C
	ATOM	1679	C	HIS	A	108	7.159	62.550	25.545	1.00	0.11	C
	ATOM	1680	O	HIS	A	108	6.360	62.037	24.763	1.00	0.11	O
	ATOM	1681	CB	HIS	A	108	9.321	62.875	24.412	1.00	0.11	C
50	ATOM	1682	CG	HIS	A	108	9.314	64.372	24.517	1.00	0.11	C
	ATOM	1683	ND1	HIS	A	108	8.352	65.173	23.946	1.00	0.11	N
	ATOM	1684	CD2	HIS	A	108	10.189	65.217	25.126	1.00	0.11	C
	ATOM	1685	CE1	HIS	A	108	8.693	66.456	24.231	1.00	0.11	C
	ATOM	1686	NE2	HIS	A	108	9.799	66.533	24.946	1.00	0.11	N
55	ATOM	1687	H	HIS	A	108	8.344	60.317	24.563	1.00	0.00	H
	ATOM	1688	HA	HIS	A	108	9.067	62.476	26.494	1.00	0.00	H
	ATOM	1689	1HB	HIS	A	108	8.903	62.553	23.443	1.00	0.00	H
	ATOM	1690	2HB	HIS	A	108	10.372	62.547	24.407	1.00	0.00	H
	ATOM	1691	HD2	HIS	A	108	10.626	64.879	26.029	1.00	0.00	H
60	ATOM	1692	HE1	HIS	A	108	7.908	67.175	24.152	1.00	0.00	H
	ATOM	1693	HE2	HIS	A	108	9.908	67.286	25.608	1.00	0.00	H
	ATOM	1694	N	GLY	A	109	6.805	63.499	26.433	1.00	0.09	N
	ATOM	1695	CA	GLY	A	109	5.456	63.967	26.515	1.00	0.09	C
	ATOM	1696	C	GLY	A	109	5.417	65.310	25.871	1.00	0.09	C
65	ATOM	1697	O	GLY	A	109	6.414	66.029	25.839	1.00	0.09	O
	ATOM	1698	H	GLY	A	109	7.478	64.019	26.971	1.00	0.00	H
	ATOM	1699	1HA	GLY	A	109	5.161	64.080	27.574	1.00	0.00	H
	ATOM	1700	2HA	GLY	A	109	4.765	63.247	26.058	1.00	0.00	H
70	ATOM	1701	N	TRP	A	110	4.241	65.682	25.339	1.00	0.32	N
	ATOM	1702	CA	TRP	A	110	4.097	66.934	24.665	1.00	0.32	C
	ATOM	1703	C	TRP	A	110	4.162	68.019	25.691	1.00	0.32	C
	ATOM	1704	O	TRP	A	110	3.707	67.858	26.822	1.00	0.32	O

177

	ATOM	1705	CB	TRP	A	110	2.767	67.026	23.890	1.00	0.32	C
	ATOM	1706	CG	TRP	A	110	2.534	68.315	23.142	1.00	0.32	C
	ATOM	1707	CD1	TRP	A	110	3.146	68.796	22.021	1.00	0.32	C
5	ATOM	1708	CD2	TRP	A	110	1.525	69.270	23.495	1.00	0.32	C
	ATOM	1709	NE1	TRP	A	110	2.583	69.997	21.657	1.00	0.32	N
	ATOM	1710	CE2	TRP	A	110	1.580	70.298	22.553	1.00	0.32	C
	ATOM	1711	CE3	TRP	A	110	0.621	69.288	24.517	1.00	0.32	C
	ATOM	1712	CZ2	TRP	A	110	0.729	71.364	22.620	1.00	0.32	C
10	ATOM	1713	CZ3	TRP	A	110	-0.236	70.362	24.583	1.00	0.32	C
	ATOM	1714	CH2	TRP	A	110	-0.183	71.380	23.653	1.00	0.32	C
	ATOM	1715	H	TRP	A	110	3.501	64.994	25.214	1.00	0.00	H
	ATOM	1716	HA	TRP	A	110	4.922	67.038	23.933	1.00	0.00	H
	ATOM	1717	LHB	TRP	A	110	1.929	66.826	24.573	1.00	0.00	H
	ATOM	1718	2HB	TRP	A	110	2.766	66.199	23.167	1.00	0.00	H
15	ATOM	1719	HD1	TRP	A	110	4.013	68.408	21.524	1.00	0.00	H
	ATOM	1720	HE1	TRP	A	110	3.077	70.649	21.085	1.00	0.00	H
	ATOM	1721	HE3	TRP	A	110	0.604	68.488	25.237	1.00	0.00	H
	ATOM	1722	HZ2	TRP	A	110	0.771	72.167	21.889	1.00	0.00	H
20	ATOM	1723	HZ3	TRP	A	110	-1.037	70.345	25.317	1.00	0.00	H
	ATOM	1724	HH2	TRP	A	110	-0.902	72.196	23.710	1.00	0.00	H
	ATOM	1725	N	ARG	A	111	4.775	69.157	25.311	1.00	0.53	N
	ATOM	1726	CA	ARG	A	111	4.933	70.280	26.189	1.00	0.53	C
	ATOM	1727	C	ARG	A	111	5.683	69.866	27.413	1.00	0.53	C
25	ATOM	1728	O	ARG	A	111	5.653	70.566	28.425	1.00	0.53	O
	ATOM	1729	CB	ARG	A	111	3.620	70.933	26.655	1.00	0.53	C
	ATOM	1730	CG	ARG	A	111	3.020	71.896	25.633	1.00	0.53	C
	ATOM	1731	CD	ARG	A	111	2.053	72.917	26.245	1.00	0.53	C
	ATOM	1732	NE	ARG	A	111	0.754	72.237	26.508	1.00	0.53	N1+
30	ATOM	1733	CZ	ARG	A	111	-0.186	72.834	27.299	1.00	0.53	C
	ATOM	1734	NH1	ARG	A	111	0.095	74.017	27.921	1.00	0.53	N
	ATOM	1735	NH2	ARG	A	111	-1.396	72.233	27.493	1.00	0.53	N
	ATOM	1736	H	ARG	A	111	5.186	69.239	24.389	1.00	0.00	H
	ATOM	1737	HA	ARG	A	111	5.583	71.018	25.683	1.00	0.00	H
35	ATOM	1738	LHB	ARG	A	111	3.792	71.524	27.570	1.00	0.00	H
	ATOM	1739	2HB	ARG	A	111	2.899	70.159	26.910	1.00	0.00	H
	ATOM	1740	LHG	ARG	A	111	2.557	71.368	24.791	1.00	0.00	H
	ATOM	1741	2HG	ARG	A	111	3.855	72.472	25.192	1.00	0.00	H
	ATOM	1742	LHD	ARG	A	111	1.871	73.778	25.580	1.00	0.00	H
40	ATOM	1743	2HD	ARG	A	111	2.462	73.292	27.198	1.00	0.00	H
	ATOM	1744	HE	ARG	A	111	0.400	71.687	25.751	1.00	0.00	H
	ATOM	1745	LHH1	ARG	A	111	0.986	74.448	27.837	1.00	0.00	H
	ATOM	1746	2HH1	ARG	A	111	-0.584	74.483	28.480	1.00	0.00	H
	ATOM	1747	LHH2	ARG	A	111	-2.095	72.648	28.070	1.00	0.00	H
45	ATOM	1748	2HH2	ARG	A	111	-1.585	71.323	27.140	1.00	0.00	H
	ATOM	1749	N	ASN	A	112	6.402	68.732	27.343	1.00	0.33	N
	ATOM	1750	CA	ASN	A	112	7.191	68.280	28.452	1.00	0.33	C
	ATOM	1751	C	ASN	A	112	6.360	68.240	29.693	1.00	0.33	C
	ATOM	1752	O	ASN	A	112	6.800	68.685	30.754	1.00	0.33	O
50	ATOM	1753	CB	ASN	A	112	8.409	69.178	28.734	1.00	0.33	C
	ATOM	1754	CG	ASN	A	112	9.405	68.984	27.605	1.00	0.33	C
	ATOM	1755	OD1	ASN	A	112	9.721	67.852	27.241	1.00	0.33	O
	ATOM	1756	ND2	ASN	A	112	9.908	70.110	27.031	1.00	0.33	N
	ATOM	1757	H	ASN	A	112	6.362	68.142	26.519	1.00	0.00	H
55	ATOM	1758	HA	ASN	A	112	7.515	67.243	28.253	1.00	0.00	H
	ATOM	1759	LHB	ASN	A	112	8.936	68.822	29.637	1.00	0.00	H
	ATOM	1760	2HB	ASN	A	112	8.129	70.229	28.898	1.00	0.00	H
	ATOM	1761	LHD2	ASN	A	112	9.555	71.013	27.290	1.00	0.00	H
	ATOM	1762	2HD2	ASN	A	112	10.399	70.002	26.155	1.00	0.00	H
60	ATOM	1763	N	TRP	A	113	5.133	67.695	29.612	1.00	0.13	N
	ATOM	1764	CA	TRP	A	113	4.351	67.630	30.808	1.00	0.13	C
	ATOM	1765	C	TRP	A	113	4.945	66.562	31.665	1.00	0.13	C
	ATOM	1766	O	TRP	A	113	5.619	65.657	31.177	1.00	0.13	O
	ATOM	1767	CB	TRP	A	113	2.864	67.316	30.572	1.00	0.13	C
	ATOM	1768	CG	TRP	A	113	2.109	68.431	29.884	1.00	0.13	C
65	ATOM	1769	CD1	TRP	A	113	1.666	68.514	28.595	1.00	0.13	C
	ATOM	1770	CD2	TRP	A	113	1.737	69.663	30.524	1.00	0.13	C
	ATOM	1771	NE1	TRP	A	113	1.030	69.717	28.395	1.00	0.13	N
	ATOM	1772	CE2	TRP	A	113	1.071	70.435	29.574	1.00	0.13	C
	ATOM	1773	CE3	TRP	A	113	1.939	70.117	31.798	1.00	0.13	C
70	ATOM	1774	CZ2	TRP	A	113	0.593	71.676	29.891	1.00	0.13	C
	ATOM	1775	CZ3	TRP	A	113	1.451	71.367	32.110	1.00	0.13	C

178

	ATOM	1776	CH2	TRP	A	113	0.791	72.133	31.174	1.00	0.13	C
	ATOM	1777	H	TRP	A	113	4.706	67.474	28.722	1.00	0.00	H
	ATOM	1778	HA	TRP	A	113	4.416	68.602	31.331	1.00	0.00	H
5	ATOM	1779	1HB	TRP	A	113	2.398	67.120	31.554	1.00	0.00	H
	ATOM	1780	2HB	TRP	A	113	2.768	66.376	30.007	1.00	0.00	H
	ATOM	1781	HD1	TRP	A	113	1.720	67.746	27.844	1.00	0.00	H
	ATOM	1782	HE1	TRP	A	113	0.985	70.177	27.511	1.00	0.00	H
	ATOM	1783	HE3	TRP	A	113	2.453	69.524	32.547	1.00	0.00	H
10	ATOM	1784	HZ2	TRP	A	113	-0.140	72.215	29.363	1.00	0.00	H
	ATOM	1785	HZ3	TRP	A	113	1.587	71.753	33.118	1.00	0.00	H
	ATOM	1786	HH2	TRP	A	113	0.388	73.096	31.480	1.00	0.00	H
	ATOM	1787	N	ASP	A	114	4.712	66.648	32.988	1.00	0.12	N
	ATOM	1788	CA	ASP	A	114	5.293	65.702	33.895	1.00	0.12	C
15	ATOM	1789	C	ASP	A	114	4.813	64.344	33.513	1.00	0.12	C
	ATOM	1790	O	ASP	A	114	3.627	64.137	33.263	1.00	0.12	O
	ATOM	1791	CB	ASP	A	114	4.874	65.921	35.357	1.00	0.12	C
	ATOM	1792	CG	ASP	A	114	5.445	67.250	35.823	1.00	0.12	C
	ATOM	1793	OD1	ASP	A	114	6.688	67.432	35.731	1.00	0.12	O
20	ATOM	1794	OD2	ASP	A	114	4.640	68.101	36.285	1.00	0.12	O1-
	ATOM	1795	H	ASP	A	114	4.235	67.413	33.434	1.00	0.00	H
	ATOM	1796	HA	ASP	A	114	6.396	65.763	33.822	1.00	0.00	H
	ATOM	1797	1HB	ASP	A	114	5.326	65.104	35.943	1.00	0.00	H
	ATOM	1798	2HB	ASP	A	114	3.782	65.878	35.482	1.00	0.00	H
25	ATOM	1799	N	VAL	A	115	5.746	63.378	33.447	1.00	0.21	N
	ATOM	1800	CA	VAL	A	115	5.368	62.043	33.098	1.00	0.21	C
	ATOM	1801	C	VAL	A	115	5.975	61.133	34.112	1.00	0.21	C
	ATOM	1802	O	VAL	A	115	7.072	61.378	34.611	1.00	0.21	O
	ATOM	1803	CB	VAL	A	115	5.880	61.603	31.759	1.00	0.21	C
30	ATOM	1804	CG1	VAL	A	115	5.413	60.158	31.508	1.00	0.21	C
	ATOM	1805	CG2	VAL	A	115	5.402	62.604	30.694	1.00	0.21	C
	ATOM	1806	H	VAL	A	115	6.699	63.523	33.725	1.00	0.00	H
	ATOM	1807	HA	VAL	A	115	4.271	61.948	33.117	1.00	0.00	H
	ATOM	1808	HB	VAL	A	115	6.981	61.596	31.744	1.00	0.00	H
35	ATOM	1809	1HG1	VAL	A	115	5.622	59.852	30.468	1.00	0.00	H
	ATOM	1810	2HG1	VAL	A	115	5.940	59.432	32.142	1.00	0.00	H
	ATOM	1811	3HG1	VAL	A	115	4.326	60.047	31.656	1.00	0.00	H
	ATOM	1812	1HG2	VAL	A	115	6.242	63.234	30.360	1.00	0.00	H
	ATOM	1813	2HG2	VAL	A	115	5.022	62.106	29.788	1.00	0.00	H
40	ATOM	1814	3HG2	VAL	A	115	4.626	63.295	31.037	1.00	0.00	H
	ATOM	1815	N	TYR	A	116	5.249	60.058	34.455	1.00	0.44	N
	ATOM	1816	CA	TYR	A	116	5.738	59.110	35.407	1.00	0.44	C
	ATOM	1817	C	TYR	A	116	5.192	57.784	34.997	1.00	0.44	C
	ATOM	1818	O	TYR	A	116	4.387	57.702	34.070	1.00	0.44	O
45	ATOM	1819	CB	TYR	A	116	5.271	59.408	36.836	1.00	0.44	C
	ATOM	1820	CG	TYR	A	116	3.794	59.519	36.746	1.00	0.44	C
	ATOM	1821	CD1	TYR	A	116	2.990	58.419	36.891	1.00	0.44	C
	ATOM	1822	CD2	TYR	A	116	3.215	60.735	36.486	1.00	0.44	C
	ATOM	1823	CE1	TYR	A	116	1.624	58.535	36.797	1.00	0.44	C
50	ATOM	1824	CE2	TYR	A	116	1.851	60.859	36.391	1.00	0.44	C
	ATOM	1825	CZ	TYR	A	116	1.050	59.757	36.548	1.00	0.44	C
	ATOM	1826	OH	TYR	A	116	-0.352	59.883	36.451	1.00	0.44	O
	ATOM	1827	H	TYR	A	116	4.338	59.869	34.060	1.00	0.00	H
	ATOM	1828	HA	TYR	A	116	6.838	59.072	35.343	1.00	0.00	H
55	ATOM	1829	1HB	TYR	A	116	5.732	60.345	37.186	1.00	0.00	H
	ATOM	1830	2HB	TYR	A	116	5.607	58.618	37.523	1.00	0.00	H
	ATOM	1831	HD1	TYR	A	116	3.439	57.467	37.135	1.00	0.00	H
	ATOM	1832	HD2	TYR	A	116	3.838	61.619	36.358	1.00	0.00	H
	ATOM	1833	HE1	TYR	A	116	0.986	57.727	37.108	1.00	0.00	H
60	ATOM	1834	HE2	TYR	A	116	1.421	61.836	36.180	1.00	0.00	H
	ATOM	1835	HH	TYR	A	116	-0.572	60.683	35.940	1.00	0.00	H
	ATOM	1836	N	LYS	A	117	5.625	56.712	35.689	1.00	0.45	N
	ATOM	1837	CA	LYS	A	117	5.196	55.380	35.366	1.00	0.45	C
	ATOM	1838	C	LYS	A	117	5.361	55.152	33.903	1.00	0.45	C
65	ATOM	1839	O	LYS	A	117	4.381	54.992	33.177	1.00	0.45	O
	ATOM	1840	CB	LYS	A	117	3.732	55.063	35.716	1.00	0.45	C
	ATOM	1841	CG	LYS	A	117	3.486	54.831	37.205	1.00	0.45	C
	ATOM	1842	CD	LYS	A	117	2.021	54.552	37.540	1.00	0.45	C
	ATOM	1843	CE	LYS	A	117	1.803	54.093	38.982	1.00	0.45	C
70	ATOM	1844	NZ	LYS	A	117	1.648	55.268	39.868	1.00	0.45	N1+
	ATOM	1845	H	LYS	A	117	6.471	56.822	36.234	1.00	0.00	H
	ATOM	1846	HA	LYS	A	117	5.857	54.686	35.905	1.00	0.00	H

	ATOM	1847	1HB	LYS	A	117	3.423	54.134	35.202	1.00	0.00	H
	ATOM	1848	2HB	LYS	A	117	3.072	55.855	35.321	1.00	0.00	H
	ATOM	1849	1HG	LYS	A	117	4.032	55.470	37.906	1.00	0.00	H
5	ATOM	1850	2HG	LYS	A	117	3.730	53.803	37.280	1.00	0.00	H
	ATOM	1851	1HD	LYS	A	117	1.662	53.770	36.846	1.00	0.00	H
	ATOM	1852	2HD	LYS	A	117	1.404	55.440	37.399	1.00	0.00	H
	ATOM	1853	1HE	LYS	A	117	2.615	53.456	39.361	1.00	0.00	H
	ATOM	1854	2HE	LYS	A	117	0.875	53.505	39.082	1.00	0.00	H
10	ATOM	1855	1HZ	LYS	A	117	1.542	55.010	40.843	1.00	0.00	H
	ATOM	1856	2HZ	LYS	A	117	2.458	55.876	39.832	1.00	0.00	H
	ATOM	1857	3HZ	LYS	A	117	0.847	55.842	39.642	1.00	0.00	H
	ATOM	1858	N	VAL	A	118	6.621	55.134	33.433	1.00	0.21	N
	ATOM	1859	CA	VAL	A	118	6.873	54.949	32.037	1.00	0.21	C
15	ATOM	1860	C	VAL	A	118	7.212	53.512	31.806	1.00	0.21	C
	ATOM	1861	O	VAL	A	118	7.958	52.902	32.569	1.00	0.21	O
	ATOM	1862	CB	VAL	A	118	8.032	55.762	31.546	1.00	0.21	C
	ATOM	1863	CG1	VAL	A	118	8.313	55.380	30.088	1.00	0.21	C
	ATOM	1864	CG2	VAL	A	118	7.708	57.251	31.749	1.00	0.21	C
20	ATOM	1865	H	VAL	A	118	7.436	55.211	34.029	1.00	0.00	H
	ATOM	1866	HA	VAL	A	118	5.985	55.278	31.488	1.00	0.00	H
	ATOM	1867	HB	VAL	A	118	8.930	55.521	32.142	1.00	0.00	H
	ATOM	1868	1HG1	VAL	A	118	9.125	56.011	29.696	1.00	0.00	H
	ATOM	1869	2HG1	VAL	A	118	8.627	54.336	29.946	1.00	0.00	H
25	ATOM	1870	3HG1	VAL	A	118	7.399	55.589	29.526	1.00	0.00	H
	ATOM	1871	1HG2	VAL	A	118	8.495	57.906	31.341	1.00	0.00	H
	ATOM	1872	2HG2	VAL	A	118	6.771	57.514	31.231	1.00	0.00	H
	ATOM	1873	3HG2	VAL	A	118	7.597	57.515	32.814	1.00	0.00	H
	ATOM	1874	N	ILE	A	119	6.636	52.922	30.739	1.00	0.09	N
30	ATOM	1875	CA	ILE	A	119	6.937	51.557	30.434	1.00	0.09	C
	ATOM	1876	C	ILE	A	119	7.363	51.496	29.005	1.00	0.09	C
	ATOM	1877	O	ILE	A	119	6.814	52.188	28.149	1.00	0.09	O
	ATOM	1878	CB	ILE	A	119	5.765	50.634	30.583	1.00	0.09	C
	ATOM	1879	CG1	ILE	A	119	5.244	50.662	32.028	1.00	0.09	C
35	ATOM	1880	CG2	ILE	A	119	6.202	49.239	30.108	1.00	0.09	C
	ATOM	1881	CD1	ILE	A	119	3.887	49.980	32.199	1.00	0.09	C
	ATOM	1882	H	ILE	A	119	6.019	53.432	30.114	1.00	0.00	H
	ATOM	1883	HA	ILE	A	119	7.753	51.208	31.079	1.00	0.00	H
	ATOM	1884	HB	ILE	A	119	4.974	50.986	29.918	1.00	0.00	H
40	ATOM	1885	1HG1	ILE	A	119	5.127	51.696	32.388	1.00	0.00	H
	ATOM	1886	2HG1	ILE	A	119	5.962	50.087	32.618	1.00	0.00	H
	ATOM	1887	1HG2	ILE	A	119	5.476	48.458	30.381	1.00	0.00	H
	ATOM	1888	2HG2	ILE	A	119	6.342	49.174	29.021	1.00	0.00	H
	ATOM	1889	3HG2	ILE	A	119	7.135	48.928	30.599	1.00	0.00	H
45	ATOM	1890	1HD1	ILE	A	119	3.583	50.024	33.259	1.00	0.00	H
	ATOM	1891	2HD1	ILE	A	119	3.096	50.494	31.635	1.00	0.00	H
	ATOM	1892	3HD1	ILE	A	119	3.917	48.912	31.939	1.00	0.00	H
	ATOM	1893	N	TYR	A	120	8.383	50.666	28.722	1.00	0.09	N
	ATOM	1894	CA	TYR	A	120	8.837	50.488	27.377	1.00	0.09	C
50	ATOM	1895	C	TYR	A	120	8.350	49.159	26.923	1.00	0.09	C
	ATOM	1896	O	TYR	A	120	8.418	48.175	27.658	1.00	0.09	O
	ATOM	1897	CB	TYR	A	120	10.367	50.494	27.212	1.00	0.09	C
	ATOM	1898	CG	TYR	A	120	10.850	51.903	27.189	1.00	0.09	C
	ATOM	1899	CD1	TYR	A	120	11.051	52.631	28.339	1.00	0.09	C
55	ATOM	1900	CD2	TYR	A	120	11.111	52.492	25.973	1.00	0.09	C
	ATOM	1901	CE1	TYR	A	120	11.504	53.929	28.266	1.00	0.09	C
	ATOM	1902	CE2	TYR	A	120	11.563	53.785	25.893	1.00	0.09	C
	ATOM	1903	CZ	TYR	A	120	11.761	54.505	27.043	1.00	0.09	C
	ATOM	1904	OH	TYR	A	120	12.226	55.832	26.949	1.00	0.09	O
60	ATOM	1905	H	TYR	A	120	8.765	50.046	29.425	1.00	0.00	H
	ATOM	1906	HA	TYR	A	120	8.416	51.282	26.738	1.00	0.00	H
	ATOM	1907	1HB	TYR	A	120	10.609	49.990	26.261	1.00	0.00	H
	ATOM	1908	2HB	TYR	A	120	10.841	49.895	28.003	1.00	0.00	H
	ATOM	1909	HD1	TYR	A	120	10.804	52.180	29.294	1.00	0.00	H
65	ATOM	1910	HD2	TYR	A	120	10.959	51.928	25.055	1.00	0.00	H
	ATOM	1911	HE1	TYR	A	120	11.635	54.510	29.175	1.00	0.00	H
	ATOM	1912	HE2	TYR	A	120	11.814	54.215	24.941	1.00	0.00	H
	ATOM	1913	HH	TYR	A	120	11.980	56.270	27.778	1.00	0.00	H
	ATOM	1914	N	TYR	A	121	7.816	49.106	25.689	1.00	0.18	N
	ATOM	1915	CA	TYR	A	121	7.302	47.867	25.199	1.00	0.18	C
70	ATOM	1916	C	TYR	A	121	8.013	47.542	23.925	1.00	0.18	C
	ATOM	1917	O	TYR	A	121	8.291	48.417	23.108	1.00	0.18	O

180

	ATOM	1918	CB	TYR	A	121	5.803	47.929	24.877	1.00	0.18	C
	ATOM	1919	CG	TYR	A	121	5.083	48.219	26.150	1.00	0.18	C
	ATOM	1920	CD1	TYR	A	121	4.694	47.198	26.987	1.00	0.18	C
5	ATOM	1921	CD2	TYR	A	121	4.800	49.517	26.509	1.00	0.18	C
	ATOM	1922	CE1	TYR	A	121	4.028	47.469	28.160	1.00	0.18	C
	ATOM	1923	CE2	TYR	A	121	4.134	49.792	27.679	1.00	0.18	C
	ATOM	1924	CZ	TYR	A	121	3.744	48.768	28.506	1.00	0.18	C
	ATOM	1925	OH	TYR	A	121	3.059	49.051	29.707	1.00	0.18	O
10	ATOM	1926	H	TYR	A	121	7.631	49.920	25.112	1.00	0.00	H
	ATOM	1927	HA	TYR	A	121	7.436	47.107	25.959	1.00	0.00	H
	ATOM	1928	1HB	TYR	A	121	5.532	46.953	24.447	1.00	0.00	H
	ATOM	1929	2HB	TYR	A	121	5.646	48.703	24.116	1.00	0.00	H
	ATOM	1930	HD1	TYR	A	121	4.897	46.165	26.711	1.00	0.00	H
15	ATOM	1931	HD2	TYR	A	121	5.098	50.334	25.859	1.00	0.00	H
	ATOM	1932	HE1	TYR	A	121	3.695	46.652	28.797	1.00	0.00	H
	ATOM	1933	HE2	TYR	A	121	4.048	50.841	27.783	1.00	0.00	H
	ATOM	1934	HH	TYR	A	121	2.599	49.887	29.539	1.00	0.00	H
	ATOM	1935	N	LYS	A	122	8.347	46.249	23.757	1.00	0.28	N
20	ATOM	1936	CA	LYS	A	122	9.000	45.727	22.598	1.00	0.28	C
	ATOM	1937	C	LYS	A	122	8.109	44.630	22.126	1.00	0.28	C
	ATOM	1938	O	LYS	A	122	7.986	43.602	22.790	1.00	0.28	O
	ATOM	1939	CB	LYS	A	122	10.349	45.062	22.933	1.00	0.28	C
	ATOM	1940	CG	LYS	A	122	11.176	44.623	21.722	1.00	0.28	C
25	ATOM	1941	CD	LYS	A	122	12.535	44.030	22.111	1.00	0.28	C
	ATOM	1942	CE	LYS	A	122	13.183	44.715	23.316	1.00	0.28	C
	ATOM	1943	NZ	LYS	A	122	14.483	44.075	23.628	1.00	0.28	N1+
	ATOM	1944	H	LYS	A	122	8.145	45.567	24.483	1.00	0.00	H
	ATOM	1945	HA	LYS	A	122	9.164	46.528	21.864	1.00	0.00	H
30	ATOM	1946	1HB	LYS	A	122	10.242	44.240	23.659	1.00	0.00	H
	ATOM	1947	2HB	LYS	A	122	10.988	45.835	23.342	1.00	0.00	H
	ATOM	1948	1HG	LYS	A	122	11.311	45.492	21.057	1.00	0.00	H
	ATOM	1949	2HG	LYS	A	122	10.623	43.882	21.114	1.00	0.00	H
	ATOM	1950	1HD	LYS	A	122	13.201	44.012	21.232	1.00	0.00	H
35	ATOM	1951	2HD	LYS	A	122	12.369	42.972	22.385	1.00	0.00	H
	ATOM	1952	1HE	LYS	A	122	12.551	44.547	24.190	1.00	0.00	H
	ATOM	1953	2HE	LYS	A	122	13.425	45.746	23.185	1.00	0.00	H
	ATOM	1954	1HZ	LYS	A	122	14.925	44.473	24.445	1.00	0.00	H
	ATOM	1955	2HZ	LYS	A	122	14.393	43.081	23.789	1.00	0.00	H
	ATOM	1956	3HZ	LYS	A	122	15.133	44.201	22.860	1.00	0.00	H
40	ATOM	1957	N	ASP	A	123	7.464	44.826	20.965	1.00	0.20	N
	ATOM	1958	CA	ASP	A	123	6.591	43.826	20.428	1.00	0.20	C
	ATOM	1959	C	ASP	A	123	5.595	43.429	21.470	1.00	0.20	C
	ATOM	1960	O	ASP	A	123	5.193	42.269	21.556	1.00	0.20	O
45	ATOM	1961	CB	ASP	A	123	7.339	42.593	19.901	1.00	0.20	C
	ATOM	1962	CG	ASP	A	123	8.044	43.045	18.631	1.00	0.20	C
	ATOM	1963	OD1	ASP	A	123	7.553	44.021	18.001	1.00	0.20	O
	ATOM	1964	OD2	ASP	A	123	9.081	42.430	18.274	1.00	0.20	O1-
	ATOM	1965	H	ASP	A	123	7.666	45.628	20.369	1.00	0.00	H
50	ATOM	1966	HA	ASP	A	123	5.968	44.289	19.639	1.00	0.00	H
	ATOM	1967	1HB	ASP	A	123	6.613	41.815	19.612	1.00	0.00	H
	ATOM	1968	2HB	ASP	A	123	8.032	42.140	20.623	1.00	0.00	H
	ATOM	1969	N	GLY	A	124	5.173	44.404	22.296	1.00	0.17	N
	ATOM	1970	CA	GLY	A	124	4.147	44.159	23.266	1.00	0.17	C
55	ATOM	1971	C	GLY	A	124	4.739	43.612	24.523	1.00	0.17	C
	ATOM	1972	O	GLY	A	124	4.011	43.266	25.454	1.00	0.17	O
	ATOM	1973	H	GLY	A	124	5.538	45.337	22.192	1.00	0.00	H
	ATOM	1974	1HA	GLY	A	124	3.420	43.428	22.877	1.00	0.00	H
	ATOM	1975	2HA	GLY	A	124	3.606	45.080	23.485	1.00	0.00	H
60	ATOM	1976	N	GLU	A	125	6.076	43.516	24.601	1.00	0.24	N
	ATOM	1977	CA	GLU	A	125	6.638	42.987	25.806	1.00	0.24	C
	ATOM	1978	C	GLU	A	125	7.229	44.137	26.552	1.00	0.24	C
	ATOM	1979	O	GLU	A	125	7.934	44.962	25.980	1.00	0.24	O
	ATOM	1980	CB	GLU	A	125	7.747	41.958	25.550	1.00	0.24	C
65	ATOM	1981	CG	GLU	A	125	8.099	41.137	26.785	1.00	0.24	C
	ATOM	1982	CD	GLU	A	125	9.183	40.146	26.392	1.00	0.24	C
	ATOM	1983	OE1	GLU	A	125	10.013	40.500	25.512	1.00	0.24	O
	ATOM	1984	OE2	GLU	A	125	9.192	39.023	26.962	1.00	0.24	O1-
	ATOM	1985	H	GLU	A	125	6.662	43.562	23.773	1.00	0.00	H
	ATOM	1986	HA	GLU	A	125	5.870	42.467	26.400	1.00	0.00	H
70	ATOM	1987	1HB	GLU	A	125	8.638	42.476	25.156	1.00	0.00	H
	ATOM	1988	2HB	GLU	A	125	7.408	41.267	24.755	1.00	0.00	H

181

	ATOM	1989	1HG	GLU	A	125	7.225	40.613	27.203	1.00	0.00	H
	ATOM	1990	2HG	GLU	A	125	8.494	41.789	27.582	1.00	0.00	H
	ATOM	1991	N	ALA	A	126	6.967	44.237	27.865	1.00	0.26	N
5	ATOM	1992	CA	ALA	A	126	7.483	45.377	28.563	1.00	0.26	C
	ATOM	1993	C	ALA	A	126	8.923	45.129	28.870	1.00	0.26	C
	ATOM	1994	O	ALA	A	126	9.257	44.250	29.662	1.00	0.26	O
	ATOM	1995	CB	ALA	A	126	6.771	45.654	29.898	1.00	0.26	C
	ATOM	1996	H	ALA	A	126	6.357	43.601	28.352	1.00	0.00	H
10	ATOM	1997	HA	ALA	A	126	7.283	46.254	27.943	1.00	0.00	H
	ATOM	1998	1HB	ALA	A	126	7.244	46.526	30.375	1.00	0.00	H
	ATOM	1999	2HB	ALA	A	126	5.708	45.881	29.733	1.00	0.00	H
	ATOM	2000	3HB	ALA	A	126	6.836	44.803	30.593	1.00	0.00	H
	ATOM	2001	N	LEU	A	127	9.819	45.889	28.210	1.00	0.39	N
15	ATOM	2002	CA	LEU	A	127	11.223	45.746	28.455	1.00	0.39	C
	ATOM	2003	C	LEU	A	127	11.504	46.207	29.846	1.00	0.39	C
	ATOM	2004	O	LEU	A	127	12.150	45.505	30.622	1.00	0.39	O
	ATOM	2005	CB	LEU	A	127	12.082	46.623	27.532	1.00	0.39	C
	ATOM	2006	CG	LEU	A	127	11.973	46.250	26.046	1.00	0.39	C
20	ATOM	2007	CD1	LEU	A	127	10.541	46.453	25.527	1.00	0.39	C
	ATOM	2008	CD2	LEU	A	127	13.021	47.001	25.210	1.00	0.39	C
	ATOM	2009	H	LEU	A	127	9.483	46.608	27.583	1.00	0.00	H
	ATOM	2010	HA	LEU	A	127	11.516	44.689	28.359	1.00	0.00	H
	ATOM	2011	1HB	LEU	A	127	13.130	46.502	27.866	1.00	0.00	H
25	ATOM	2012	2HB	LEU	A	127	11.833	47.689	27.665	1.00	0.00	H
	ATOM	2013	HG	LEU	A	127	12.195	45.170	26.006	1.00	0.00	H
	ATOM	2014	1HD1	LEU	A	127	10.536	47.074	24.623	1.00	0.00	H
	ATOM	2015	2HD1	LEU	A	127	10.073	45.481	25.396	1.00	0.00	H
	ATOM	2016	3HD1	LEU	A	127	9.942	47.094	26.169	1.00	0.00	H
30	ATOM	2017	1HD2	LEU	A	127	12.582	46.866	24.252	1.00	0.00	H
	ATOM	2018	2HD2	LEU	A	127	13.035	48.076	25.442	1.00	0.00	H
	ATOM	2019	3HD2	LEU	A	127	14.037	46.592	25.281	1.00	0.00	H
	ATOM	2020	N	LYS	A	128	11.008	47.409	30.209	1.00	0.43	N
35	ATOM	2021	CA	LYS	A	128	11.294	47.881	31.530	1.00	0.43	C
	ATOM	2022	C	LYS	A	128	10.216	48.824	31.948	1.00	0.43	C
	ATOM	2023	O	LYS	A	128	9.524	49.417	31.122	1.00	0.43	O
	ATOM	2024	CB	LYS	A	128	12.614	48.659	31.641	1.00	0.43	C
	ATOM	2025	CG	LYS	A	128	12.560	50.028	30.960	1.00	0.43	C
	ATOM	2026	CD	LYS	A	128	13.718	50.948	31.350	1.00	0.43	C
40	ATOM	2027	CE	LYS	A	128	13.540	52.388	30.872	1.00	0.43	C
	ATOM	2028	NZ	LYS	A	128	12.447	53.031	31.635	1.00	0.43	N1+
	ATOM	2029	H	LYS	A	128	10.328	47.889	29.646	1.00	0.00	H
	ATOM	2030	HA	LYS	A	128	11.296	47.023	32.227	1.00	0.00	H
	ATOM	2031	1HB	LYS	A	128	13.445	48.056	31.235	1.00	0.00	H
45	ATOM	2032	2HB	LYS	A	128	12.825	48.793	32.717	1.00	0.00	H
	ATOM	2033	1HG	LYS	A	128	11.647	50.560	31.271	1.00	0.00	H
	ATOM	2034	2HG	LYS	A	128	12.473	49.888	29.880	1.00	0.00	H
	ATOM	2035	1HD	LYS	A	128	14.667	50.553	30.950	1.00	0.00	H
	ATOM	2036	2HD	LYS	A	128	13.841	50.944	32.449	1.00	0.00	H
50	ATOM	2037	1HE	LYS	A	128	13.239	52.423	29.841	1.00	0.00	H
	ATOM	2038	2HE	LYS	A	128	14.468	52.924	31.072	1.00	0.00	H
	ATOM	2039	1HZ	LYS	A	128	12.368	54.022	31.429	1.00	0.00	H
	ATOM	2040	2HZ	LYS	A	128	11.541	52.625	31.442	1.00	0.00	H
	ATOM	2041	3HZ	LYS	A	128	12.593	52.977	32.634	1.00	0.00	H
55	ATOM	2042	N	TYR	A	129	10.043	48.960	33.275	1.00	0.26	N
	ATOM	2043	CA	TYR	A	129	9.095	49.877	33.832	1.00	0.26	C
	ATOM	2044	C	TYR	A	129	9.784	50.604	34.940	1.00	0.26	C
	ATOM	2045	O	TYR	A	129	10.405	49.987	35.803	1.00	0.26	O
	ATOM	2046	CB	TYR	A	129	7.861	49.183	34.435	1.00	0.26	C
60	ATOM	2047	CG	TYR	A	129	7.171	50.160	35.325	1.00	0.26	C
	ATOM	2048	CD1	TYR	A	129	6.375	51.165	34.823	1.00	0.26	C
	ATOM	2049	CD2	TYR	A	129	7.327	50.051	36.687	1.00	0.26	C
	ATOM	2050	CE1	TYR	A	129	5.750	52.050	35.674	1.00	0.26	C
	ATOM	2051	CE2	TYR	A	129	6.707	50.930	37.540	1.00	0.26	C
65	ATOM	2052	CZ	TYR	A	129	5.916	51.931	37.035	1.00	0.26	C
	ATOM	2053	OH	TYR	A	129	5.283	52.830	37.916	1.00	0.26	O
	ATOM	2054	H	TYR	A	129	10.608	48.473	33.952	1.00	0.00	H
	ATOM	2055	HA	TYR	A	129	8.771	50.575	33.049	1.00	0.00	H
	ATOM	2056	1HB	TYR	A	129	8.174	48.298	35.013	1.00	0.00	H
70	ATOM	2057	2HB	TYR	A	129	7.213	48.793	33.637	1.00	0.00	H
	ATOM	2058	HD1	TYR	A	129	6.455	51.455	33.799	1.00	0.00	H
	ATOM	2059	HD2	TYR	A	129	7.952	49.261	37.097	1.00	0.00	H

182

	ATOM	2060	HE1	TYR	A	129	5.114	52.806	35.239	1.00	0.00	H
	ATOM	2061	HE2	TYR	A	129	6.841	50.791	38.607	1.00	0.00	H
	ATOM	2062	HH	TYR	A	129	5.829	52.879	38.713	1.00	0.00	H
5	ATOM	2063	N	TRP	A	130	9.712	51.950	34.931	1.00	0.16	N
	ATOM	2064	CA	TRP	A	130	10.311	52.685	36.006	1.00	0.16	C
	ATOM	2065	C	TRP	A	130	9.437	53.879	36.219	1.00	0.16	C
	ATOM	2066	O	TRP	A	130	8.929	54.461	35.261	1.00	0.16	O
	ATOM	2067	CB	TRP	A	130	11.716	53.211	35.683	1.00	0.16	C
10	ATOM	2068	CG	TRP	A	130	12.467	53.739	36.882	1.00	0.16	C
	ATOM	2069	CD1	TRP	A	130	12.409	54.960	37.486	1.00	0.16	C
	ATOM	2070	CD2	TRP	A	130	13.463	52.984	37.588	1.00	0.16	C
	ATOM	2071	NE1	TRP	A	130	13.299	55.007	38.532	1.00	0.16	N
	ATOM	2072	CE2	TRP	A	130	13.957	53.800	38.603	1.00	0.16	C
15	ATOM	2073	CE3	TRP	A	130	13.932	51.715	37.402	1.00	0.16	C
	ATOM	2074	CZ2	TRP	A	130	14.932	53.360	39.452	1.00	0.16	C
	ATOM	2075	CZ3	TRP	A	130	14.913	51.273	38.264	1.00	0.16	C
	ATOM	2076	CH2	TRP	A	130	15.404	52.079	39.270	1.00	0.16	C
	ATOM	2077	H	TRP	A	130	9.109	52.460	34.292	1.00	0.00	H
20	ATOM	2078	HA	TRP	A	130	10.329	52.061	36.916	1.00	0.00	H
	ATOM	2079	1HB	TRP	A	130	11.622	53.988	34.909	1.00	0.00	H
	ATOM	2080	2HB	TRP	A	130	12.306	52.403	35.220	1.00	0.00	H
	ATOM	2081	HD1	TRP	A	130	11.643	55.612	37.343	1.00	0.00	H
	ATOM	2082	HE1	TRP	A	130	13.577	55.818	39.058	1.00	0.00	H
25	ATOM	2083	HE3	TRP	A	130	13.550	51.063	36.623	1.00	0.00	H
	ATOM	2084	HZ2	TRP	A	130	15.318	54.001	40.242	1.00	0.00	H
	ATOM	2085	HZ3	TRP	A	130	15.309	50.266	38.152	1.00	0.00	H
	ATOM	2086	HH2	TRP	A	130	16.179	51.696	39.930	1.00	0.00	H
	ATOM	2087	N	TYR	A	131	9.204	54.267	37.487	1.00	0.17	N
30	ATOM	2088	CA	TYR	A	131	8.351	55.401	37.683	1.00	0.17	C
	ATOM	2089	C	TYR	A	131	8.991	56.631	37.120	1.00	0.17	C
	ATOM	2090	O	TYR	A	131	8.436	57.284	36.238	1.00	0.17	O
	ATOM	2091	CB	TYR	A	131	8.087	55.714	39.164	1.00	0.17	C
	ATOM	2092	CG	TYR	A	131	7.166	54.693	39.731	1.00	0.17	C
35	ATOM	2093	CD1	TYR	A	131	7.617	53.438	40.072	1.00	0.17	C
	ATOM	2094	CD2	TYR	A	131	5.844	55.009	39.937	1.00	0.17	C
	ATOM	2095	CE1	TYR	A	131	6.754	52.508	40.602	1.00	0.17	C
	ATOM	2096	CE2	TYR	A	131	4.977	54.084	40.465	1.00	0.17	C
	ATOM	2097	CZ	TYR	A	131	5.433	52.832	40.800	1.00	0.17	C
40	ATOM	2098	OH	TYR	A	131	4.542	51.882	41.345	1.00	0.17	O
	ATOM	2099	H	TYR	A	131	9.634	53.823	38.280	1.00	0.00	H
	ATOM	2100	HA	TYR	A	131	7.395	55.233	37.177	1.00	0.00	H
	ATOM	2101	1HB	TYR	A	131	7.635	56.719	39.216	1.00	0.00	H
	ATOM	2102	2HB	TYR	A	131	9.022	55.767	39.746	1.00	0.00	H
45	ATOM	2103	HD1	TYR	A	131	8.667	53.180	39.973	1.00	0.00	H
	ATOM	2104	HD2	TYR	A	131	5.494	56.012	39.704	1.00	0.00	H
	ATOM	2105	HE1	TYR	A	131	7.138	51.529	40.884	1.00	0.00	H
	ATOM	2106	HE2	TYR	A	131	3.963	54.370	40.710	1.00	0.00	H
	ATOM	2107	HH	TYR	A	131	5.048	51.342	41.965	1.00	0.00	H
50	ATOM	2108	N	GLU	A	132	10.189	56.977	37.630	1.00	0.19	N
	ATOM	2109	CA	GLU	A	132	10.842	58.196	37.249	1.00	0.19	C
	ATOM	2110	C	GLU	A	132	11.520	58.139	35.909	1.00	0.19	C
	ATOM	2111	O	GLU	A	132	11.501	59.125	35.175	1.00	0.19	O
	ATOM	2112	CB	GLU	A	132	11.851	58.705	38.295	1.00	0.19	C
55	ATOM	2113	CG	GLU	A	132	13.030	57.774	38.565	1.00	0.19	C
	ATOM	2114	CD	GLU	A	132	13.838	58.387	39.702	1.00	0.19	C
	ATOM	2115	OE1	GLU	A	132	14.098	59.618	39.651	1.00	0.19	O
	ATOM	2116	OE2	GLU	A	132	14.202	57.630	40.641	1.00	0.19	O1-
	ATOM	2117	H	GLU	A	132	10.574	56.510	38.434	1.00	0.00	H
60	ATOM	2118	HA	GLU	A	132	10.066	58.975	37.149	1.00	0.00	H
	ATOM	2119	1HB	GLU	A	132	11.321	58.901	39.245	1.00	0.00	H
	ATOM	2120	2HB	GLU	A	132	12.189	59.689	37.919	1.00	0.00	H
	ATOM	2121	1HG	GLU	A	132	13.639	57.522	37.692	1.00	0.00	H
	ATOM	2122	2HG	GLU	A	132	12.498	56.967	39.059	1.00	0.00	H
65	ATOM	2123	N	ASN	A	133	12.116	56.988	35.539	1.00	0.18	N
	ATOM	2124	CA	ASN	A	133	12.974	56.963	34.382	1.00	0.18	C
	ATOM	2125	C	ASN	A	133	12.209	57.009	33.098	1.00	0.18	C
	ATOM	2126	O	ASN	A	133	11.487	56.080	32.738	1.00	0.18	O
	ATOM	2127	CB	ASN	A	133	13.907	55.737	34.320	1.00	0.18	C
	ATOM	2128	CG	ASN	A	133	14.988	56.023	33.284	1.00	0.18	C
70	ATOM	2129	OD1	ASN	A	133	14.893	56.984	32.522	1.00	0.18	O
	ATOM	2130	ND2	ASN	A	133	16.041	55.162	33.248	1.00	0.18	N

183

	ATOM	2131	H	ASN A 133	12.152	56.184	36.126	1.00	0.00	H
	ATOM	2132	HA	ASN A 133	13.641	57.843	34.482	1.00	0.00	H
	ATOM	2133	1HB	ASN A 133	13.387	54.810	34.048	1.00	0.00	H
	ATOM	2134	2HB	ASN A 133	14.388	55.588	35.302	1.00	0.00	H
5	ATOM	2135	1HD2	ASN A 133	16.149	54.411	33.904	1.00	0.00	H
	ATOM	2136	2HD2	ASN A 133	16.735	55.326	32.538	1.00	0.00	H
	ATOM	2137	N	HIS A 134	12.358	58.148	32.393	1.00	0.16	N
	ATOM	2138	CA	HIS A 134	11.782	58.440	31.111	1.00	0.16	C
10	ATOM	2139	C	HIS A 134	12.510	57.713	30.020	1.00	0.16	C
	ATOM	2140	O	HIS A 134	11.908	57.336	29.016	1.00	0.16	O
	ATOM	2141	CB	HIS A 134	11.845	59.939	30.781	1.00	0.16	C
	ATOM	2142	CG	HIS A 134	11.133	60.773	31.803	1.00	0.16	C
	ATOM	2143	ND1	HIS A 134	9.767	60.954	31.837	1.00	0.16	N
15	ATOM	2144	CD2	HIS A 134	11.627	61.476	32.858	1.00	0.16	C
	ATOM	2145	CE1	HIS A 134	9.506	61.751	32.903	1.00	0.16	C
	ATOM	2146	NE2	HIS A 134	10.603	62.094	33.554	1.00	0.16	N
	ATOM	2147	H	HIS A 134	12.816	58.920	32.852	1.00	0.00	H
	ATOM	2148	HA	HIS A 134	10.736	58.098	31.094	1.00	0.00	H
20	ATOM	2149	1HB	HIS A 134	11.406	60.080	29.778	1.00	0.00	H
	ATOM	2150	2HB	HIS A 134	12.890	60.276	30.715	1.00	0.00	H
	ATOM	2151	HD2	HIS A 134	12.657	61.578	33.175	1.00	0.00	H
	ATOM	2152	HE1	HIS A 134	8.543	62.184	33.088	1.00	0.00	H
	ATOM	2153	HE2	HIS A 134	10.667	62.639	34.389	1.00	0.00	H
25	ATOM	2154	N	ASN A 135	13.835	57.507	30.179	1.00	0.14	N
	ATOM	2155	CA	ASN A 135	14.631	56.982	29.100	1.00	0.14	C
	ATOM	2156	C	ASN A 135	14.941	55.534	29.306	1.00	0.14	C
	ATOM	2157	O	ASN A 135	14.867	55.010	30.416	1.00	0.14	O
	ATOM	2158	CB	ASN A 135	15.986	57.690	28.963	1.00	0.14	C
	ATOM	2159	CG	ASN A 135	15.720	59.156	28.665	1.00	0.14	C
30	ATOM	2160	OD1	ASN A 135	15.032	59.498	27.704	1.00	0.14	O
	ATOM	2161	ND2	ASN A 135	16.270	60.053	29.528	1.00	0.14	N
	ATOM	2162	H	ASN A 135	14.277	57.581	31.090	1.00	0.00	H
	ATOM	2163	HA	ASN A 135	14.091	57.126	28.156	1.00	0.00	H
35	ATOM	2164	1HB	ASN A 135	16.465	57.199	28.112	1.00	0.00	H
	ATOM	2165	2HB	ASN A 135	16.609	57.530	29.857	1.00	0.00	H
	ATOM	2166	1HD2	ASN A 135	16.809	59.763	30.324	1.00	0.00	H
	ATOM	2167	2HD2	ASN A 135	16.088	61.027	29.364	1.00	0.00	H
	ATOM	2168	N	ILE A 136	15.270	54.846	28.190	1.00	0.19	N
40	ATOM	2169	CA	ILE A 136	15.665	53.467	28.207	1.00	0.19	C
	ATOM	2170	C	ILE A 136	16.831	53.341	27.279	1.00	0.19	C
	ATOM	2171	O	ILE A 136	16.909	54.042	26.272	1.00	0.19	O
	ATOM	2172	CB	ILE A 136	14.612	52.529	27.694	1.00	0.19	C
	ATOM	2173	CG1	ILE A 136	15.014	51.070	27.966	1.00	0.19	C
45	ATOM	2174	CG2	ILE A 136	14.381	52.844	26.207	1.00	0.19	C
	ATOM	2175	CD1	ILE A 136	13.874	50.077	27.751	1.00	0.19	C
	ATOM	2176	H	ILE A 136	15.312	55.307	27.283	1.00	0.00	H
	ATOM	2177	HA	ILE A 136	15.976	53.214	29.234	1.00	0.00	H
	ATOM	2178	HB	ILE A 136	13.653	52.762	28.141	1.00	0.00	H
50	ATOM	2179	1HG1	ILE A 136	15.391	50.970	28.996	1.00	0.00	H
	ATOM	2180	2HG1	ILE A 136	15.848	50.770	27.308	1.00	0.00	H
	ATOM	2181	1HG2	ILE A 136	13.544	52.256	25.812	1.00	0.00	H
	ATOM	2182	2HG2	ILE A 136	14.172	53.918	26.193	1.00	0.00	H
	ATOM	2183	3HG2	ILE A 136	15.231	52.583	25.560	1.00	0.00	H
55	ATOM	2184	1HD1	ILE A 136	14.060	49.114	28.250	1.00	0.00	H
	ATOM	2185	2HD1	ILE A 136	12.927	50.491	28.101	1.00	0.00	H
	ATOM	2186	3HD1	ILE A 136	13.745	49.876	26.675	1.00	0.00	H
	ATOM	2187	N	SER A 137	17.788	52.452	27.604	1.00	0.24	N
	ATOM	2188	CA	SER A 137	18.920	52.298	26.741	1.00	0.24	C
60	ATOM	2189	C	SER A 137	19.203	50.837	26.610	1.00	0.24	C
	ATOM	2190	O	SER A 137	19.102	50.085	27.577	1.00	0.24	O
	ATOM	2191	CB	SER A 137	20.185	52.972	27.299	1.00	0.24	C
	ATOM	2192	OG	SER A 137	21.276	52.795	26.411	1.00	0.24	O
	ATOM	2193	H	SER A 137	17.731	51.800	28.369	1.00	0.00	H
65	ATOM	2194	HA	SER A 137	18.669	52.741	25.782	1.00	0.00	H
	ATOM	2195	1HB	SER A 137	20.484	52.516	28.253	1.00	0.00	H
	ATOM	2196	2HB	SER A 137	20.000	54.044	27.484	1.00	0.00	H
	ATOM	2197	HG	SER A 137	20.990	53.121	25.543	1.00	0.00	H
	ATOM	2198	N	ILE A 138	19.553	50.391	25.389	1.00	0.31	N
70	ATOM	2199	CA	ILE A 138	19.872	49.009	25.203	1.00	0.31	C
	ATOM	2200	C	ILE A 138	21.299	48.973	24.779	1.00	0.31	C
	ATOM	2201	O	ILE A 138	21.688	49.613	23.804	1.00	0.31	O

184

	ATOM	2202	CB	ILE	A	138	19.075	48.358	24.114	1.00	0.31	C
	ATOM	2203	CG1	ILE	A	138	17.571	48.461	24.424	1.00	0.31	C
	ATOM	2204	CG2	ILE	A	138	19.578	46.912	23.962	1.00	0.31	C
5	ATOM	2205	CD1	ILE	A	138	16.674	48.147	23.229	1.00	0.31	C
	ATOM	2206	H	ILE	A	138	19.620	51.007	24.588	1.00	0.00	H
	ATOM	2207	HA	ILE	A	138	19.710	48.445	26.135	1.00	0.00	H
	ATOM	2208	HB	ILE	A	138	19.268	48.858	23.155	1.00	0.00	H
	ATOM	2209	1HG1	ILE	A	138	17.316	49.490	24.735	1.00	0.00	H
10	ATOM	2210	2HG1	ILE	A	138	17.309	47.817	25.281	1.00	0.00	H
	ATOM	2211	1HG2	ILE	A	138	18.854	46.237	23.492	1.00	0.00	H
	ATOM	2212	2HG2	ILE	A	138	20.505	46.865	23.369	1.00	0.00	H
	ATOM	2213	3HG2	ILE	A	138	19.788	46.455	24.944	1.00	0.00	H
	ATOM	2214	1HD1	ILE	A	138	15.696	48.643	23.340	1.00	0.00	H
15	ATOM	2215	2HD1	ILE	A	138	17.111	48.502	22.288	1.00	0.00	H
	ATOM	2216	3HD1	ILE	A	138	16.456	47.073	23.163	1.00	0.00	H
	ATOM	2217	N	THR	A	139	22.134	48.214	25.502	1.00	0.40	N
	ATOM	2218	CA	THR	A	139	23.515	48.187	25.136	1.00	0.40	C
	ATOM	2219	C	THR	A	139	23.749	46.939	24.359	1.00	0.40	C
20	ATOM	2220	O	THR	A	139	23.036	45.952	24.535	1.00	0.40	O
	ATOM	2221	CB	THR	A	139	24.443	48.189	26.311	1.00	0.40	C
	ATOM	2222	OG1	THR	A	139	24.163	47.077	27.147	1.00	0.40	O
	ATOM	2223	CG2	THR	A	139	24.261	49.504	27.085	1.00	0.40	C
	ATOM	2224	H	THR	A	139	21.880	47.655	26.299	1.00	0.00	H
25	ATOM	2225	HA	THR	A	139	23.767	49.068	24.524	1.00	0.00	H
	ATOM	2226	HB	THR	A	139	25.487	48.132	25.945	1.00	0.00	H
	ATOM	2227	HG1	THR	A	139	24.393	46.277	26.647	1.00	0.00	H
	ATOM	2228	1HG2	THR	A	139	24.974	49.573	27.923	1.00	0.00	H
	ATOM	2229	2HG2	THR	A	139	24.422	50.381	26.437	1.00	0.00	H
	ATOM	2230	3HG2	THR	A	139	23.249	49.577	27.515	1.00	0.00	H
30	ATOM	2231	N	ASN	A	140	24.763	46.972	23.470	1.00	0.29	N
	ATOM	2232	CA	ASN	A	140	25.086	45.844	22.647	1.00	0.29	C
	ATOM	2233	C	ASN	A	140	23.840	45.344	21.994	1.00	0.29	C
	ATOM	2234	O	ASN	A	140	23.385	44.235	22.272	1.00	0.29	O
35	ATOM	2235	CB	ASN	A	140	25.727	44.681	23.423	1.00	0.29	C
	ATOM	2236	CG	ASN	A	140	27.131	45.102	23.832	1.00	0.29	C
	ATOM	2237	OD1	ASN	A	140	27.317	45.982	24.671	1.00	0.29	O
	ATOM	2238	ND2	ASN	A	140	28.154	44.447	23.222	1.00	0.29	N
	ATOM	2239	H	ASN	A	140	25.351	47.783	23.365	1.00	0.00	H
40	ATOM	2240	HA	ASN	A	140	25.796	46.179	21.874	1.00	0.00	H
	ATOM	2241	1HB	ASN	A	140	25.766	43.791	22.770	1.00	0.00	H
	ATOM	2242	2HB	ASN	A	140	25.173	44.406	24.334	1.00	0.00	H
	ATOM	2243	1HD2	ASN	A	140	27.995	43.721	22.547	1.00	0.00	H
	ATOM	2244	2HD2	ASN	A	140	29.087	44.710	23.487	1.00	0.00	H
45	ATOM	2245	N	ALA	A	141	23.250	46.167	21.107	1.00	0.26	N
	ATOM	2246	CA	ALA	A	141	22.029	45.798	20.453	1.00	0.26	C
	ATOM	2247	C	ALA	A	141	22.269	44.561	19.652	1.00	0.26	C
	ATOM	2248	O	ALA	A	141	23.383	44.293	19.206	1.00	0.26	O
	ATOM	2249	CB	ALA	A	141	21.490	46.878	19.499	1.00	0.26	C
50	ATOM	2250	H	ALA	A	141	23.587	47.104	20.927	1.00	0.00	H
	ATOM	2251	HA	ALA	A	141	21.258	45.608	21.225	1.00	0.00	H
	ATOM	2252	1HB	ALA	A	141	20.549	46.526	19.046	1.00	0.00	H
	ATOM	2253	2HB	ALA	A	141	21.267	47.806	20.048	1.00	0.00	H
	ATOM	2254	3HB	ALA	A	141	22.201	47.104	18.690	1.00	0.00	H
55	ATOM	2255	N	THR	A	142	21.198	43.763	19.475	1.00	0.35	N
	ATOM	2256	CA	THR	A	142	21.277	42.535	18.746	1.00	0.35	C
	ATOM	2257	C	THR	A	142	20.122	42.498	17.797	1.00	0.35	C
	ATOM	2258	O	THR	A	142	19.288	43.401	17.779	1.00	0.35	O
	ATOM	2259	CB	THR	A	142	21.175	41.319	19.617	1.00	0.35	C
60	ATOM	2260	OG1	THR	A	142	21.424	40.145	18.859	1.00	0.35	O
	ATOM	2261	CG2	THR	A	142	19.764	41.270	20.230	1.00	0.35	C
	ATOM	2262	H	THR	A	142	20.268	44.072	19.709	1.00	0.00	H
	ATOM	2263	HA	THR	A	142	22.202	42.492	18.164	1.00	0.00	H
	ATOM	2264	HB	THR	A	142	21.924	41.382	20.430	1.00	0.00	H
	ATOM	2265	HG1	THR	A	142	20.924	39.425	19.314	1.00	0.00	H
65	ATOM	2266	1HG2	THR	A	142	19.677	40.455	20.966	1.00	0.00	H
	ATOM	2267	2HG2	THR	A	142	19.545	42.189	20.799	1.00	0.00	H
	ATOM	2268	3HG2	THR	A	142	19.002	41.155	19.495	1.00	0.00	H
	ATOM	2269	N	VAL	A	143	20.067	41.439	16.968	1.00	0.29	N
70	ATOM	2270	CA	VAL	A	143	19.038	41.271	15.985	1.00	0.29	C
	ATOM	2271	C	VAL	A	143	17.723	41.121	16.680	1.00	0.29	C
	ATOM	2272	O	VAL	A	143	16.696	41.601	16.203	1.00	0.29	O

185

	ATOM	2273	CB	VAL	A	143	19.256	40.063	15.127	1.00	0.29	C
	ATOM	2274	CG1	VAL	A	143	18.096	39.966	14.122	1.00	0.29	C
	ATOM	2275	CG2	VAL	A	143	20.644	40.180	14.470	1.00	0.29	C
5	ATOM	2276	H	VAL	A	143	20.761	40.704	17.079	1.00	0.00	H
	ATOM	2277	HA	VAL	A	143	18.850	42.036	15.329	1.00	0.00	H
	ATOM	2278	HB	VAL	A	143	19.249	39.139	15.730	1.00	0.00	H
	ATOM	2279	1HG1	VAL	A	143	18.282	39.173	13.377	1.00	0.00	H
	ATOM	2280	2HG1	VAL	A	143	17.142	39.710	14.609	1.00	0.00	H
10	ATOM	2281	3HG1	VAL	A	143	17.963	40.905	13.559	1.00	0.00	H
	ATOM	2282	1HG2	VAL	A	143	20.742	39.540	13.578	1.00	0.00	H
	ATOM	2283	2HG2	VAL	A	143	20.859	41.210	14.167	1.00	0.00	H
	ATOM	2284	3HG2	VAL	A	143	21.447	39.879	15.163	1.00	0.00	H
	ATOM	2285	N	GLU	A	144	17.728	40.452	17.845	1.00	0.25	N
15	ATOM	2286	CA	GLU	A	144	16.522	40.216	18.585	1.00	0.25	C
	ATOM	2287	C	GLU	A	144	15.953	41.542	18.969	1.00	0.25	C
	ATOM	2288	O	GLU	A	144	14.738	41.707	19.072	1.00	0.25	O
	ATOM	2289	CB	GLU	A	144	16.760	39.414	19.874	1.00	0.25	C
	ATOM	2290	CG	GLU	A	144	17.200	37.977	19.597	1.00	0.25	C
20	ATOM	2291	CD	GLU	A	144	18.626	38.030	19.072	1.00	0.25	C
	ATOM	2292	OE1	GLU	A	144	19.542	38.318	19.886	1.00	0.25	O
	ATOM	2293	OE2	GLU	A	144	18.817	37.791	17.849	1.00	0.25	O1-
	ATOM	2294	H	GLU	A	144	18.487	39.800	18.039	1.00	0.00	H
	ATOM	2295	HA	GLU	A	144	15.773	39.697	17.962	1.00	0.00	H
25	ATOM	2296	1HB	GLU	A	144	15.791	39.405	20.406	1.00	0.00	H
	ATOM	2297	2HB	GLU	A	144	17.460	39.925	20.552	1.00	0.00	H
	ATOM	2298	1HG	GLU	A	144	16.520	37.493	18.878	1.00	0.00	H
	ATOM	2299	2HG	GLU	A	144	17.181	37.402	20.537	1.00	0.00	H
	ATOM	2300	N	ASP	A	145	16.834	42.535	19.171	1.00	0.22	N
30	ATOM	2301	CA	ASP	A	145	16.438	43.836	19.619	1.00	0.22	C
	ATOM	2302	C	ASP	A	145	15.451	44.418	18.657	1.00	0.22	C
	ATOM	2303	O	ASP	A	145	14.495	45.069	19.079	1.00	0.22	O
	ATOM	2304	CB	ASP	A	145	17.632	44.802	19.718	1.00	0.22	C
	ATOM	2305	CG	ASP	A	145	17.196	46.073	20.435	1.00	0.22	C
35	ATOM	2306	OD1	ASP	A	145	16.201	46.706	19.992	1.00	0.22	O
	ATOM	2307	OD2	ASP	A	145	17.856	46.424	21.448	1.00	0.22	O1-
	ATOM	2308	H	ASP	A	145	17.800	42.416	18.901	1.00	0.00	H
	ATOM	2309	HA	ASP	A	145	15.940	43.745	20.598	1.00	0.00	H
	ATOM	2310	1HB	ASP	A	145	17.956	45.106	18.717	1.00	0.00	H
40	ATOM	2311	2HB	ASP	A	145	18.467	44.343	20.264	1.00	0.00	H
	ATOM	2312	N	SER	A	146	15.638	44.196	17.341	1.00	0.20	N
	ATOM	2313	CA	SER	A	146	14.748	44.779	16.374	1.00	0.20	C
	ATOM	2314	C	SER	A	146	13.344	44.384	16.696	1.00	0.20	C
	ATOM	2315	O	SER	A	146	13.085	43.287	17.191	1.00	0.20	O
45	ATOM	2316	CB	SER	A	146	15.037	44.343	14.926	1.00	0.20	C
	ATOM	2317	OG	SER	A	146	14.798	42.951	14.780	1.00	0.20	O
	ATOM	2318	H	SER	A	146	16.339	43.525	17.064	1.00	0.00	H
	ATOM	2319	HA	SER	A	146	14.867	45.875	16.450	1.00	0.00	H
	ATOM	2320	1HB	SER	A	146	16.065	44.568	14.651	1.00	0.00	H
50	ATOM	2321	2HB	SER	A	146	14.320	44.815	14.248	1.00	0.00	H
	ATOM	2322	HG	SER	A	146	15.341	42.471	15.433	1.00	0.00	H
	ATOM	2323	N	GLY	A	147	12.394	45.305	16.442	1.00	0.21	N
	ATOM	2324	CA	GLY	A	147	11.020	45.025	16.735	1.00	0.21	C
	ATOM	2325	C	GLY	A	147	10.301	46.331	16.762	1.00	0.21	C
55	ATOM	2326	O	GLY	A	147	10.814	47.349	16.299	1.00	0.21	O
	ATOM	2327	H	GLY	A	147	12.612	46.212	16.041	1.00	0.00	H
	ATOM	2328	1HA	GLY	A	147	10.941	44.526	17.716	1.00	0.00	H
	ATOM	2329	2HA	GLY	A	147	10.566	44.365	15.975	1.00	0.00	H
	ATOM	2330	N	THR	A	148	9.071	46.328	17.306	1.00	0.17	N
60	ATOM	2331	CA	THR	A	148	8.323	47.544	17.360	1.00	0.17	C
	ATOM	2332	C	THR	A	148	8.332	47.996	18.779	1.00	0.17	C
	ATOM	2333	O	THR	A	148	8.106	47.205	19.694	1.00	0.17	O
	ATOM	2334	CB	THR	A	148	6.895	47.375	16.948	1.00	0.17	C
	ATOM	2335	OG1	THR	A	148	6.829	46.867	15.623	1.00	0.17	O
65	ATOM	2336	CG2	THR	A	148	6.209	48.746	17.013	1.00	0.17	C
	ATOM	2337	H	THR	A	148	8.580	45.466	17.587	1.00	0.00	H
	ATOM	2338	HA	THR	A	148	8.769	48.280	16.678	1.00	0.00	H
	ATOM	2339	HB	THR	A	148	6.366	46.654	17.589	1.00	0.00	H
	ATOM	2340	HG1	THR	A	148	7.020	47.622	15.041	1.00	0.00	H
70	ATOM	2341	1HG2	THR	A	148	5.151	48.632	16.730	1.00	0.00	H
	ATOM	2342	2HG2	THR	A	148	6.285	49.123	18.038	1.00	0.00	H
	ATOM	2343	3HG2	THR	A	148	6.671	49.461	16.318	1.00	0.00	H

186

	ATOM	2344	N	TYR	A	149	8.616	49.292	19.001	1.00	0.12	N
	ATOM	2345	CA	TYR	A	149	8.660	49.790	20.343	1.00	0.12	C
	ATOM	2346	C	TYR	A	149	7.643	50.872	20.494	1.00	0.12	C
5	ATOM	2347	O	TYR	A	149	7.419	51.669	19.586	1.00	0.12	O
	ATOM	2348	CB	TYR	A	149	9.999	50.438	20.732	1.00	0.12	C
	ATOM	2349	CG	TYR	A	149	11.045	49.387	20.866	1.00	0.12	C
	ATOM	2350	CD1	TYR	A	149	11.674	48.868	19.759	1.00	0.12	C
	ATOM	2351	CD2	TYR	A	149	11.402	48.934	22.113	1.00	0.12	C
10	ATOM	2352	CE1	TYR	A	149	12.644	47.904	19.899	1.00	0.12	C
	ATOM	2353	CE2	TYR	A	149	12.372	47.971	22.260	1.00	0.12	C
	ATOM	2354	CZ	TYR	A	149	12.993	47.454	21.150	1.00	0.12	C
	ATOM	2355	OH	TYR	A	149	13.989	46.466	21.293	1.00	0.12	O
	ATOM	2356	H	TYR	A	149	8.800	49.943	18.247	1.00	0.00	H
15	ATOM	2357	HA	TYR	A	149	8.441	48.967	21.010	1.00	0.00	H
	ATOM	2358	1HB	TYR	A	149	9.845	50.916	21.708	1.00	0.00	H
	ATOM	2359	2HB	TYR	A	149	10.289	51.212	20.005	1.00	0.00	H
	ATOM	2360	HD1	TYR	A	149	11.401	49.211	18.764	1.00	0.00	H
	ATOM	2361	HD2	TYR	A	149	10.960	49.396	22.992	1.00	0.00	H
20	ATOM	2362	HE1	TYR	A	149	13.122	47.493	19.011	1.00	0.00	H
	ATOM	2363	HE2	TYR	A	149	13.003	48.093	23.120	1.00	0.00	H
	ATOM	2364	HH	TYR	A	149	14.639	46.549	20.554	1.00	0.00	H
	ATOM	2365	N	TYR	A	150	6.980	50.898	21.666	1.00	0.12	N
	ATOM	2366	CA	TYR	A	150	6.072	51.960	21.976	1.00	0.12	C
25	ATOM	2367	C	TYR	A	150	6.183	52.188	23.446	1.00	0.12	C
	ATOM	2368	O	TYR	A	150	6.750	51.369	24.169	1.00	0.12	O
	ATOM	2369	CB	TYR	A	150	4.570	51.774	21.565	1.00	0.12	C
	ATOM	2370	CG	TYR	A	150	3.990	50.559	22.220	1.00	0.12	C
	ATOM	2371	CD1	TYR	A	150	3.295	50.653	23.419	1.00	0.12	C
30	ATOM	2372	CD2	TYR	A	150	4.191	49.295	21.666	1.00	0.12	C
	ATOM	2373	CE1	TYR	A	150	2.907	49.520	24.112	1.00	0.12	C
	ATOM	2374	CE2	TYR	A	150	3.811	48.152	22.340	1.00	0.12	C
	ATOM	2375	CZ	TYR	A	150	3.225	48.255	23.614	1.00	0.12	C
	ATOM	2376	OH	TYR	A	150	3.066	47.123	24.350	1.00	0.12	O
35	ATOM	2377	H	TYR	A	150	7.166	50.227	22.400	1.00	0.00	H
	ATOM	2378	HA	TYR	A	150	6.447	52.877	21.485	1.00	0.00	H
	ATOM	2379	1HB	TYR	A	150	4.500	51.683	20.480	1.00	0.00	H
	ATOM	2380	2HB	TYR	A	150	4.025	52.689	21.836	1.00	0.00	H
	ATOM	2381	HD1	TYR	A	150	3.054	51.631	23.829	1.00	0.00	H
40	ATOM	2382	HD2	TYR	A	150	4.684	49.206	20.701	1.00	0.00	H
	ATOM	2383	HE1	TYR	A	150	2.366	49.635	25.050	1.00	0.00	H
	ATOM	2384	HE2	TYR	A	150	3.992	47.177	21.897	1.00	0.00	H
	ATOM	2385	HH	TYR	A	150	2.670	47.379	25.192	1.00	0.00	H
	ATOM	2386	N	CYS	A	151	5.668	53.328	23.936	1.00	0.27	N
	ATOM	2387	CA	CYS	A	151	5.851	53.607	25.325	1.00	0.27	C
45	ATOM	2388	C	CYS	A	151	4.536	53.997	25.912	1.00	0.27	C
	ATOM	2389	O	CYS	A	151	3.648	54.482	25.215	1.00	0.27	O
	ATOM	2390	CB	CYS	A	151	6.843	54.762	25.548	1.00	0.27	C
	ATOM	2391	SG	CYS	A	151	7.171	55.139	27.291	1.00	0.27	S
50	ATOM	2392	H	CYS	A	151	5.071	53.942	23.414	1.00	0.00	H
	ATOM	2393	HA	CYS	A	151	6.219	52.717	25.849	1.00	0.00	H
	ATOM	2394	1HB	CYS	A	151	6.499	55.675	25.037	1.00	0.00	H
	ATOM	2395	2HB	CYS	A	151	7.796	54.462	25.083	1.00	0.00	H
	ATOM	2396	N	THR	A	152	4.373	53.738	27.222	1.00	0.37	N
55	ATOM	2397	CA	THR	A	152	3.202	54.153	27.934	1.00	0.37	C
	ATOM	2398	C	THR	A	152	3.659	54.946	29.104	1.00	0.37	C
	ATOM	2399	O	THR	A	152	4.747	54.733	29.635	1.00	0.37	O
	ATOM	2400	CB	THR	A	152	2.327	53.042	28.434	1.00	0.37	C
	ATOM	2401	OG1	THR	A	152	3.105	52.054	29.091	1.00	0.37	O
60	ATOM	2402	CG2	THR	A	152	1.524	52.454	27.271	1.00	0.37	C
	ATOM	2403	H	THR	A	152	5.098	53.297	27.770	1.00	0.00	H
	ATOM	2404	HA	THR	A	152	2.623	54.822	27.283	1.00	0.00	H
	ATOM	2405	HB	THR	A	152	1.589	53.466	29.145	1.00	0.00	H
	ATOM	2406	HG1	THR	A	152	3.224	52.392	29.991	1.00	0.00	H
65	ATOM	2407	1HG2	THR	A	152	0.849	51.662	27.628	1.00	0.00	H
	ATOM	2408	2HG2	THR	A	152	0.960	53.241	26.770	1.00	0.00	H
	ATOM	2409	3HG2	THR	A	152	2.188	51.996	26.521	1.00	0.00	H
	ATOM	2410	N	GLY	A	153	2.829	55.919	29.520	1.00	0.21	N
	ATOM	2411	CA	GLY	A	153	3.195	56.730	30.637	1.00	0.21	C
	ATOM	2412	C	GLY	A	153	1.974	57.474	31.040	1.00	0.21	C
70	ATOM	2413	O	GLY	A	153	1.021	57.588	30.271	1.00	0.21	O
	ATOM	2414	H	GLY	A	153	1.886	56.034	29.142	1.00	0.00	H

187

	ATOM	2415	1HA	GLY	A	153	3.993	57.444	30.370	1.00	0.00	H
	ATOM	2416	2HA	GLY	A	153	3.543	56.101	31.450	1.00	0.00	H
	ATOM	2417	N	LYS	A	154	1.972	58.006	32.275	1.00	0.12	N
5	ATOM	2418	CA	LYS	A	154	0.807	58.711	32.702	1.00	0.12	C
	ATOM	2419	C	LYS	A	154	1.155	60.151	32.821	1.00	0.12	C
	ATOM	2420	O	LYS	A	154	2.059	60.530	33.565	1.00	0.12	O
	ATOM	2421	CB	LYS	A	154	0.290	58.265	34.077	1.00	0.12	C
	ATOM	2422	CG	LYS	A	154	-0.176	56.810	34.106	1.00	0.12	C
10	ATOM	2423	CD	LYS	A	154	-0.395	56.275	35.521	1.00	0.12	C
	ATOM	2424	CE	LYS	A	154	-0.863	54.818	35.557	1.00	0.12	C
	ATOM	2425	NZ	LYS	A	154	-1.046	54.378	36.959	1.00	0.12	N1+
	ATOM	2426	H	LYS	A	154	2.733	57.898	32.935	1.00	0.00	H
	ATOM	2427	HA	LYS	A	154	0.031	58.632	31.958	1.00	0.00	H
15	ATOM	2428	1HB	LYS	A	154	-0.526	58.939	34.362	1.00	0.00	H
	ATOM	2429	2HB	LYS	A	154	1.176	58.355	34.684	1.00	0.00	H
	ATOM	2430	1HG	LYS	A	154	0.548	56.156	33.586	1.00	0.00	H
	ATOM	2431	2HG	LYS	A	154	-1.115	56.752	33.543	1.00	0.00	H
	ATOM	2432	1HD	LYS	A	154	-1.072	56.939	36.083	1.00	0.00	H
20	ATOM	2433	2HD	LYS	A	154	0.602	56.301	35.950	1.00	0.00	H
	ATOM	2434	1HE	LYS	A	154	-0.129	54.147	35.080	1.00	0.00	H
	ATOM	2435	2HE	LYS	A	154	-1.829	54.686	35.041	1.00	0.00	H
	ATOM	2436	1HZ	LYS	A	154	-1.436	53.444	36.999	1.00	0.00	H
	ATOM	2437	2HZ	LYS	A	154	-0.179	54.358	37.466	1.00	0.00	H
25	ATOM	2438	3HZ	LYS	A	154	-1.701	54.977	37.445	1.00	0.00	H
	ATOM	2439	N	VAL	A	155	0.441	60.994	32.056	1.00	0.20	N
	ATOM	2440	CA	VAL	A	155	0.620	62.404	32.171	1.00	0.20	C
	ATOM	2441	C	VAL	A	155	-0.646	62.882	32.782	1.00	0.20	C
	ATOM	2442	O	VAL	A	155	-1.735	62.479	32.374	1.00	0.20	O
30	ATOM	2443	CB	VAL	A	155	0.804	63.105	30.854	1.00	0.20	C
	ATOM	2444	CG1	VAL	A	155	2.117	62.612	30.221	1.00	0.20	C
	ATOM	2445	CG2	VAL	A	155	-0.439	62.853	29.983	1.00	0.20	C
	ATOM	2446	H	VAL	A	155	-0.465	60.701	31.705	1.00	0.00	H
	ATOM	2447	HA	VAL	A	155	1.474	62.627	32.829	1.00	0.00	H
35	ATOM	2448	HB	VAL	A	155	0.898	64.185	31.070	1.00	0.00	H
	ATOM	2449	1HG1	VAL	A	155	2.526	63.319	29.484	1.00	0.00	H
	ATOM	2450	2HG1	VAL	A	155	2.861	62.443	31.007	1.00	0.00	H
	ATOM	2451	3HG1	VAL	A	155	1.975	61.644	29.711	1.00	0.00	H
	ATOM	2452	1HG2	VAL	A	155	-0.249	63.172	28.942	1.00	0.00	H
40	ATOM	2453	2HG2	VAL	A	155	-0.649	61.785	29.939	1.00	0.00	H
	ATOM	2454	3HG2	VAL	A	155	-1.343	63.391	30.285	1.00	0.00	H
	ATOM	2455	N	TRP	A	156	-0.539	63.723	33.820	1.00	0.33	N
	ATOM	2456	CA	TRP	A	156	-1.740	64.153	34.455	1.00	0.33	C
	ATOM	2457	C	TRP	A	156	-2.323	62.911	35.034	1.00	0.33	C
45	ATOM	2458	O	TRP	A	156	-1.605	61.962	35.350	1.00	0.33	O
	ATOM	2459	CB	TRP	A	156	-2.765	64.766	33.483	1.00	0.33	C
	ATOM	2460	CG	TRP	A	156	-2.277	66.008	32.771	1.00	0.33	C
	ATOM	2461	CD1	TRP	A	156	-1.694	66.113	31.543	1.00	0.33	C
	ATOM	2462	CD2	TRP	A	156	-2.345	67.341	33.303	1.00	0.33	C
50	ATOM	2463	NE1	TRP	A	156	-1.392	67.427	31.275	1.00	0.33	N
	ATOM	2464	CE2	TRP	A	156	-1.787	68.195	32.350	1.00	0.33	C
	ATOM	2465	CE3	TRP	A	156	-2.832	67.816	34.487	1.00	0.33	C
	ATOM	2466	CZ2	TRP	A	156	-1.705	69.541	32.569	1.00	0.33	C
	ATOM	2467	CZ3	TRP	A	156	-2.748	69.175	34.703	1.00	0.33	C
55	ATOM	2468	CH2	TRP	A	156	-2.195	70.021	33.763	1.00	0.33	C
	ATOM	2469	H	TRP	A	156	0.348	64.062	34.155	1.00	0.00	H
	ATOM	2470	HA	TRP	A	156	-1.505	64.859	35.270	1.00	0.00	H
	ATOM	2471	1HB	TRP	A	156	-3.617	65.114	34.092	1.00	0.00	H
	ATOM	2472	2HB	TRP	A	156	-3.230	64.080	32.765	1.00	0.00	H
60	ATOM	2473	HD1	TRP	A	156	-1.470	65.339	30.827	1.00	0.00	H
	ATOM	2474	HE1	TRP	A	156	-0.853	67.759	30.508	1.00	0.00	H
	ATOM	2475	HE3	TRP	A	156	-3.265	67.164	35.237	1.00	0.00	H
	ATOM	2476	HZ2	TRP	A	156	-1.272	70.204	31.826	1.00	0.00	H
	ATOM	2477	HZ3	TRP	A	156	-3.122	69.593	35.635	1.00	0.00	H
65	ATOM	2478	HH2	TRP	A	156	-2.143	71.087	33.972	1.00	0.00	H
	ATOM	2479	N	GLN	A	157	-3.656	62.899	35.190	1.00	0.49	N
	ATOM	2480	CA	GLN	A	157	-4.338	61.769	35.739	1.00	0.49	C
	ATOM	2481	C	GLN	A	157	-4.276	60.630	34.773	1.00	0.49	C
	ATOM	2482	O	GLN	A	157	-4.048	59.485	35.160	1.00	0.49	O
	ATOM	2483	CB	GLN	A	157	-5.830	62.050	35.969	1.00	0.49	C
70	ATOM	2484	CG	GLN	A	157	-6.082	63.297	36.814	1.00	0.49	C
	ATOM	2485	CD	GLN	A	157	-5.294	63.145	38.101	1.00	0.49	C

188

	ATOM	2486	OE1	GLN	A	157	-5.354	62.107	38.756	1.00	0.49	O
	ATOM	2487	NE2	GLN	A	157	-4.525	64.203	38.466	1.00	0.49	N
	ATOM	2488	H	GLN	A	157	-4.225	63.687	34.941	1.00	0.00	H
5	ATOM	2489	HA	GLN	A	157	-3.849	61.453	36.673	1.00	0.00	H
	ATOM	2490	1HB	GLN	A	157	-6.280	61.160	36.442	1.00	0.00	H
	ATOM	2491	2HB	GLN	A	157	-6.355	62.215	35.031	1.00	0.00	H
	ATOM	2492	1HG	GLN	A	157	-7.147	63.381	37.094	1.00	0.00	H
	ATOM	2493	2HG	GLN	A	157	-5.821	64.214	36.260	1.00	0.00	H
10	ATOM	2494	1HE2	GLN	A	157	-4.495	65.056	37.942	1.00	0.00	H
	ATOM	2495	2HE2	GLN	A	157	-3.997	64.103	39.316	1.00	0.00	H
	ATOM	2496	N	LEU	A	158	-4.459	60.932	33.473	1.00	0.41	N
	ATOM	2497	CA	LEU	A	158	-4.607	59.905	32.483	1.00	0.41	C
	ATOM	2498	C	LEU	A	158	-3.306	59.269	32.127	1.00	0.41	C
	ATOM	2499	O	LEU	A	158	-2.227	59.803	32.381	1.00	0.41	O
15	ATOM	2500	CB	LEU	A	158	-5.252	60.399	31.176	1.00	0.41	C
	ATOM	2501	CG	LEU	A	158	-6.699	60.889	31.364	1.00	0.41	C
	ATOM	2502	CD1	LEU	A	158	-7.628	59.742	31.796	1.00	0.41	C
	ATOM	2503	CD2	LEU	A	158	-6.758	62.101	32.310	1.00	0.41	C
	ATOM	2504	H	LEU	A	158	-4.372	61.876	33.144	1.00	0.00	H
20	ATOM	2505	HA	LEU	A	158	-5.247	59.120	32.926	1.00	0.00	H
	ATOM	2506	1HB	LEU	A	158	-5.231	59.590	30.425	1.00	0.00	H
	ATOM	2507	2HB	LEU	A	158	-4.656	61.226	30.773	1.00	0.00	H
	ATOM	2508	HG	LEU	A	158	-7.047	61.227	30.367	1.00	0.00	H
	ATOM	2509	1HD1	LEU	A	158	-8.682	60.066	31.788	1.00	0.00	H
25	ATOM	2510	2HD1	LEU	A	158	-7.548	58.883	31.108	1.00	0.00	H
	ATOM	2511	3HD1	LEU	A	158	-7.408	59.385	32.814	1.00	0.00	H
	ATOM	2512	1HD2	LEU	A	158	-7.652	62.708	32.086	1.00	0.00	H
	ATOM	2513	2HD2	LEU	A	158	-6.896	61.750	33.331	1.00	0.00	H
	ATOM	2514	3HD2	LEU	A	158	-5.894	62.776	32.222	1.00	0.00	H
30	ATOM	2515	N	ASP	A	159	-3.419	58.062	31.533	1.00	0.19	N
	ATOM	2516	CA	ASP	A	159	-2.310	57.288	31.058	1.00	0.19	C
	ATOM	2517	C	ASP	A	159	-2.414	57.323	29.566	1.00	0.19	C
	ATOM	2518	O	ASP	A	159	-3.504	57.198	29.009	1.00	0.19	O
	ATOM	2519	CB	ASP	A	159	-2.381	55.809	31.503	1.00	0.19	C
35	ATOM	2520	CG	ASP	A	159	-1.124	55.027	31.117	1.00	0.19	C
	ATOM	2521	OD1	ASP	A	159	-0.378	55.468	30.205	1.00	0.19	O
	ATOM	2522	OD2	ASP	A	159	-0.904	53.956	31.744	1.00	0.19	O1-
	ATOM	2523	H	ASP	A	159	-4.304	57.666	31.271	1.00	0.00	H
	ATOM	2524	HA	ASP	A	159	-1.394	57.724	31.412	1.00	0.00	H
40	ATOM	2525	1HB	ASP	A	159	-3.242	55.320	31.016	1.00	0.00	H
	ATOM	2526	2HB	ASP	A	159	-2.577	55.702	32.580	1.00	0.00	H
	ATOM	2527	N	TYR	A	160	-1.279	57.531	28.874	1.00	0.11	N
	ATOM	2528	CA	TYR	A	160	-1.321	57.584	27.443	1.00	0.11	C
	ATOM	2529	C	TYR	A	160	-0.381	56.562	26.901	1.00	0.11	C
45	ATOM	2530	O	TYR	A	160	0.535	56.111	27.589	1.00	0.11	O
	ATOM	2531	CB	TYR	A	160	-0.884	58.937	26.857	1.00	0.11	C
	ATOM	2532	CG	TYR	A	160	-1.939	59.942	27.171	1.00	0.11	C
	ATOM	2533	CD1	TYR	A	160	-2.067	60.462	28.439	1.00	0.11	C
	ATOM	2534	CD2	TYR	A	160	-2.794	60.378	26.185	1.00	0.11	C
50	ATOM	2535	CE1	TYR	A	160	-3.042	61.390	28.720	1.00	0.11	C
	ATOM	2536	CE2	TYR	A	160	-3.771	61.306	26.459	1.00	0.11	C
	ATOM	2537	CZ	TYR	A	160	-3.895	61.814	27.730	1.00	0.11	C
	ATOM	2538	OH	TYR	A	160	-4.895	62.767	28.019	1.00	0.11	O
	ATOM	2539	H	TYR	A	160	-0.429	57.158	29.312	1.00	0.00	H
55	ATOM	2540	HA	TYR	A	160	-2.323	57.325	27.087	1.00	0.00	H
	ATOM	2541	1HB	TYR	A	160	-0.756	58.828	25.769	1.00	0.00	H
	ATOM	2542	2HB	TYR	A	160	0.099	59.231	27.261	1.00	0.00	H
	ATOM	2543	HD1	TYR	A	160	-1.420	60.088	29.225	1.00	0.00	H
	ATOM	2544	HD2	TYR	A	160	-2.708	59.975	25.179	1.00	0.00	H
60	ATOM	2545	HE1	TYR	A	160	-3.087	61.827	29.711	1.00	0.00	H
	ATOM	2546	HE2	TYR	A	160	-4.440	61.623	25.662	1.00	0.00	H
	ATOM	2547	HH	TYR	A	160	-5.696	62.470	27.566	1.00	0.00	H
	ATOM	2548	N	GLU	A	161	-0.622	56.144	25.643	1.00	0.12	N
	ATOM	2549	CA	GLU	A	161	0.262	55.219	25.000	1.00	0.12	C
65	ATOM	2550	C	GLU	A	161	0.753	55.893	23.762	1.00	0.12	C
	ATOM	2551	O	GLU	A	161	0.033	56.669	23.135	1.00	0.12	O
	ATOM	2552	CB	GLU	A	161	-0.537	53.970	24.530	1.00	0.12	C
	ATOM	2553	CG	GLU	A	161	-1.765	53.494	25.343	1.00	0.12	C
	ATOM	2554	CD	GLU	A	161	-1.424	52.544	26.509	1.00	0.12	C
70	ATOM	2555	OE1	GLU	A	161	-1.294	51.360	26.186	1.00	0.12	O
	ATOM	2556	OE2	GLU	A	161	-1.270	53.072	27.616	1.00	0.12	O1-

189

	ATOM	2557	H	GLU	A	161	-1.390	56.468	25.083	1.00	0.00	H
	ATOM	2558	HA	GLU	A	161	1.082	54.949	25.668	1.00	0.00	H
	ATOM	2559	1HB	GLU	A	161	0.157	53.123	24.376	1.00	0.00	H
5	ATOM	2560	2HB	GLU	A	161	-0.927	54.220	23.531	1.00	0.00	H
	ATOM	2561	1HG	GLU	A	161	-2.415	52.932	24.651	1.00	0.00	H
	ATOM	2562	2HG	GLU	A	161	-2.358	54.344	25.709	1.00	0.00	H
	ATOM	2563	N	SER	A	162	2.020	55.632	23.397	1.00	0.11	N
	ATOM	2564	CA	SER	A	162	2.598	56.250	22.242	1.00	0.11	C
10	ATOM	2565	C	SER	A	162	2.381	55.367	21.065	1.00	0.11	C
	ATOM	2566	O	SER	A	162	1.967	54.216	21.196	1.00	0.11	O
	ATOM	2567	CB	SER	A	162	4.113	56.489	22.371	1.00	0.11	C
	ATOM	2568	OG	SER	A	162	4.614	57.110	21.196	1.00	0.11	O
	ATOM	2569	H	SER	A	162	2.604	55.025	23.964	1.00	0.00	H
	ATOM	2570	HA	SER	A	162	2.118	57.229	22.070	1.00	0.00	H
15	ATOM	2571	1HB	SER	A	162	4.627	55.527	22.518	1.00	0.00	H
	ATOM	2572	2HB	SER	A	162	4.316	57.117	23.249	1.00	0.00	H
	ATOM	2573	HG	SER	A	162	5.577	57.118	21.318	1.00	0.00	H
	ATOM	2574	N	GLU	A	163	2.640	55.915	19.864	1.00	0.13	N
	ATOM	2575	CA	GLU	A	163	2.517	55.151	18.661	1.00	0.13	C
20	ATOM	2576	C	GLU	A	163	3.757	54.333	18.544	1.00	0.13	C
	ATOM	2577	O	GLU	A	163	4.830	54.718	19.006	1.00	0.13	O
	ATOM	2578	CB	GLU	A	163	2.382	56.031	17.407	1.00	0.13	C
	ATOM	2579	CG	GLU	A	163	3.567	56.976	17.202	1.00	0.13	C
	ATOM	2580	CD	GLU	A	163	3.153	58.020	16.177	1.00	0.13	C
25	ATOM	2581	OE1	GLU	A	163	2.076	58.643	16.381	1.00	0.13	O
	ATOM	2582	OE2	GLU	A	163	3.900	58.212	15.181	1.00	0.13	O1-
	ATOM	2583	H	GLU	A	163	3.159	56.782	19.804	1.00	0.00	H
	ATOM	2584	HA	GLU	A	163	1.565	54.603	18.736	1.00	0.00	H
	ATOM	2585	1HB	GLU	A	163	1.438	56.596	17.501	1.00	0.00	H
30	ATOM	2586	2HB	GLU	A	163	2.265	55.357	16.540	1.00	0.00	H
	ATOM	2587	1HG	GLU	A	163	4.481	56.445	16.900	1.00	0.00	H
	ATOM	2588	2HG	GLU	A	163	3.766	57.518	18.137	1.00	0.00	H
	ATOM	2589	N	PRO	A	164	3.611	53.185	17.956	1.00	0.13	N
	ATOM	2590	CA	PRO	A	164	4.751	52.324	17.819	1.00	0.13	C
35	ATOM	2591	C	PRO	A	164	5.680	52.796	16.752	1.00	0.13	C
	ATOM	2592	O	PRO	A	164	5.235	53.459	15.818	1.00	0.13	O
	ATOM	2593	CB	PRO	A	164	4.189	50.930	17.565	1.00	0.13	C
	ATOM	2594	CG	PRO	A	164	2.815	50.957	18.251	1.00	0.13	C
	ATOM	2595	CD	PRO	A	164	2.385	52.429	18.167	1.00	0.13	C
40	ATOM	2596	HA	PRO	A	164	5.289	52.312	18.774	1.00	0.00	H
	ATOM	2597	1HB	PRO	A	164	4.769	50.185	18.092	1.00	0.00	H
	ATOM	2598	2HB	PRO	A	164	4.113	50.690	16.495	1.00	0.00	H
	ATOM	2599	1HG	PRO	A	164	2.920	50.648	19.303	1.00	0.00	H
	ATOM	2600	2HG	PRO	A	164	2.075	50.275	17.803	1.00	0.00	H
45	ATOM	2601	1HD	PRO	A	164	1.700	52.602	17.322	1.00	0.00	H
	ATOM	2602	2HD	PRO	A	164	1.875	52.702	19.099	1.00	0.00	H
	ATOM	2603	N	LEU	A	165	6.982	52.483	16.888	1.00	0.11	N
	ATOM	2604	CA	LEU	A	165	7.932	52.840	15.879	1.00	0.11	C
	ATOM	2605	C	LEU	A	165	8.678	51.587	15.565	1.00	0.11	C
50	ATOM	2606	O	LEU	A	165	8.896	50.754	16.444	1.00	0.11	O
	ATOM	2607	CB	LEU	A	165	8.953	53.897	16.327	1.00	0.11	C
	ATOM	2608	CG	LEU	A	165	8.309	55.248	16.688	1.00	0.11	C
	ATOM	2609	CD1	LEU	A	165	9.377	56.304	17.011	1.00	0.11	C
	ATOM	2610	CD2	LEU	A	165	7.321	55.708	15.605	1.00	0.11	C
55	ATOM	2611	H	LEU	A	165	7.333	52.020	17.718	1.00	0.00	H
	ATOM	2612	HA	LEU	A	165	7.399	53.174	14.975	1.00	0.00	H
	ATOM	2613	1HB	LEU	A	165	9.663	54.039	15.492	1.00	0.00	H
	ATOM	2614	2HB	LEU	A	165	9.540	53.512	17.180	1.00	0.00	H
	ATOM	2615	HG	LEU	A	165	7.725	55.110	17.619	1.00	0.00	H
60	ATOM	2616	1HD1	LEU	A	165	8.889	57.250	17.269	1.00	0.00	H
	ATOM	2617	2HD1	LEU	A	165	10.014	55.959	17.841	1.00	0.00	H
	ATOM	2618	3HD1	LEU	A	165	10.045	56.456	16.150	1.00	0.00	H
	ATOM	2619	1HD2	LEU	A	165	7.258	56.806	15.620	1.00	0.00	H
	ATOM	2620	2HD2	LEU	A	165	7.617	55.405	14.591	1.00	0.00	H
65	ATOM	2621	3HD2	LEU	A	165	6.293	55.405	15.796	1.00	0.00	H
	ATOM	2622	N	ASN	A	166	9.077	51.402	14.294	1.00	0.10	N
	ATOM	2623	CA	ASN	A	166	9.772	50.192	13.976	1.00	0.10	C
	ATOM	2624	C	ASN	A	166	11.234	50.478	14.008	1.00	0.10	C
	ATOM	2625	O	ASN	A	166	11.729	51.346	13.291	1.00	0.10	O
70	ATOM	2626	CB	ASN	A	166	9.460	49.623	12.581	1.00	0.10	C
	ATOM	2627	CG	ASN	A	166	8.056	49.035	12.593	1.00	0.10	C

	ATOM	2628	OD1	ASN	A	166	7.304	49.185	13.555	1.00	0.10	O
	ATOM	2629	ND2	ASN	A	166	7.695	48.328	11.490	1.00	0.10	N
	ATOM	2630	H	ASN	A	166	8.934	52.059	13.548	1.00	0.00	H
5	ATOM	2631	HA	ASN	A	166	9.513	49.396	14.694	1.00	0.00	H
	ATOM	2632	1HB	ASN	A	166	10.186	48.815	12.378	1.00	0.00	H
	ATOM	2633	2HB	ASN	A	166	9.555	50.379	11.786	1.00	0.00	H
	ATOM	2634	1HD2	ASN	A	166	8.315	48.199	10.712	1.00	0.00	H
	ATOM	2635	2HD2	ASN	A	166	6.774	47.924	11.489	1.00	0.00	H
10	ATOM	2636	N	ILE	A	167	11.959	49.747	14.873	1.00	0.22	N
	ATOM	2637	CA	ILE	A	167	13.378	49.904	14.942	1.00	0.22	C
	ATOM	2638	C	ILE	A	167	13.954	48.591	14.545	1.00	0.22	C
	ATOM	2639	O	ILE	A	167	13.535	47.544	15.035	1.00	0.22	O
	ATOM	2640	CB	ILE	A	167	13.880	50.216	16.322	1.00	0.22	C
15	ATOM	2641	CG1	ILE	A	167	13.316	51.562	16.805	1.00	0.22	C
	ATOM	2642	CG2	ILE	A	167	15.418	50.161	16.294	1.00	0.22	C
	ATOM	2643	CD1	ILE	A	167	13.532	51.815	18.297	1.00	0.22	C
	ATOM	2644	H	ILE	A	167	11.571	48.981	15.415	1.00	0.00	H
	ATOM	2645	HA	ILE	A	167	13.699	50.705	14.261	1.00	0.00	H
20	ATOM	2646	HB	ILE	A	167	13.530	49.426	17.014	1.00	0.00	H
	ATOM	2647	1HG1	ILE	A	167	12.227	51.610	16.623	1.00	0.00	H
	ATOM	2648	2HG1	ILE	A	167	13.758	52.388	16.219	1.00	0.00	H
	ATOM	2649	1HG2	ILE	A	167	15.829	50.322	17.306	1.00	0.00	H
	ATOM	2650	2HG2	ILE	A	167	15.817	49.186	15.976	1.00	0.00	H
25	ATOM	2651	3HG2	ILE	A	167	15.852	50.951	15.670	1.00	0.00	H
	ATOM	2652	1HD1	ILE	A	167	13.012	52.730	18.621	1.00	0.00	H
	ATOM	2653	2HD1	ILE	A	167	13.158	50.981	18.909	1.00	0.00	H
	ATOM	2654	3HD1	ILE	A	167	14.602	51.943	18.511	1.00	0.00	H
	ATOM	2655	N	THR	A	168	14.926	48.604	13.618	1.00	0.48	N
30	ATOM	2656	CA	THR	A	168	15.488	47.353	13.212	1.00	0.48	C
	ATOM	2657	C	THR	A	168	16.955	47.396	13.410	1.00	0.48	C
	ATOM	2658	O	THR	A	168	17.587	48.447	13.312	1.00	0.48	O
	ATOM	2659	CB	THR	A	168	15.289	47.020	11.764	1.00	0.48	C
	ATOM	2660	OG1	THR	A	168	15.798	48.064	10.948	1.00	0.48	O
35	ATOM	2661	CG2	THR	A	168	13.800	46.788	11.494	1.00	0.48	C
	ATOM	2662	H	THR	A	168	15.334	49.451	13.242	1.00	0.00	H
	ATOM	2663	HA	THR	A	168	15.086	46.551	13.823	1.00	0.00	H
	ATOM	2664	HB	THR	A	168	15.828	46.078	11.542	1.00	0.00	H
	ATOM	2665	HG1	THR	A	168	16.752	48.111	11.107	1.00	0.00	H
40	ATOM	2666	1HG2	THR	A	168	13.629	46.488	10.447	1.00	0.00	H
	ATOM	2667	2HG2	THR	A	168	13.392	45.995	12.141	1.00	0.00	H
	ATOM	2668	3HG2	THR	A	168	13.218	47.707	11.670	1.00	0.00	H
	ATOM	2669	N	VAL	A	169	17.538	46.228	13.724	1.00	0.55	N
	ATOM	2670	CA	VAL	A	169	18.958	46.199	13.795	1.00	0.55	C
45	ATOM	2671	C	VAL	A	169	19.375	45.828	12.415	1.00	0.55	C
	ATOM	2672	O	VAL	A	169	18.935	44.820	11.863	1.00	0.55	O
	ATOM	2673	CB	VAL	A	169	19.532	45.207	14.771	1.00	0.55	C
	ATOM	2674	CG1	VAL	A	169	19.096	45.621	16.183	1.00	0.55	C
	ATOM	2675	CG2	VAL	A	169	19.102	43.782	14.391	1.00	0.55	C
50	ATOM	2676	H	VAL	A	169	17.097	45.329	13.643	1.00	0.00	H
	ATOM	2677	HA	VAL	A	169	19.344	47.190	14.069	1.00	0.00	H
	ATOM	2678	HB	VAL	A	169	20.631	45.296	14.679	1.00	0.00	H
	ATOM	2679	1HG1	VAL	A	169	19.882	45.432	16.925	1.00	0.00	H
55	ATOM	2680	2HG1	VAL	A	169	18.919	46.708	16.250	1.00	0.00	H
	ATOM	2681	3HG1	VAL	A	169	18.150	45.151	16.482	1.00	0.00	H
	ATOM	2682	1HG2	VAL	A	169	19.961	43.256	14.838	1.00	0.00	H
	ATOM	2683	2HG2	VAL	A	169	18.107	43.608	14.822	1.00	0.00	H
	ATOM	2684	3HG2	VAL	A	169	19.091	43.378	13.385	1.00	0.00	H
	ATOM	2685	N	ILE	A	170	20.221	46.672	11.807	1.00	0.56	N
60	ATOM	2686	CA	ILE	A	170	20.637	46.451	10.457	1.00	0.56	C
	ATOM	2687	C	ILE	A	170	21.357	45.145	10.428	1.00	0.56	C
	ATOM	2688	O	ILE	A	170	21.198	44.364	9.490	1.00	0.56	O
	ATOM	2689	CB	ILE	A	170	21.546	47.545	9.942	1.00	0.56	C
	ATOM	2690	CG1	ILE	A	170	21.728	47.467	8.414	1.00	0.56	C
65	ATOM	2691	CG2	ILE	A	170	22.867	47.492	10.727	1.00	0.56	C
	ATOM	2692	CD1	ILE	A	170	22.467	46.223	7.921	1.00	0.56	C
	ATOM	2693	H	ILE	A	170	20.615	47.485	12.272	1.00	0.00	H
	ATOM	2694	HA	ILE	A	170	19.739	46.349	9.824	1.00	0.00	H
	ATOM	2695	HB	ILE	A	170	21.142	48.513	10.164	1.00	0.00	H
70	ATOM	2696	1HG1	ILE	A	170	22.296	48.360	8.094	1.00	0.00	H
	ATOM	2697	2HG1	ILE	A	170	20.748	47.543	7.909	1.00	0.00	H
	ATOM	2698	1HG2	ILE	A	170	23.219	48.524	10.855	1.00	0.00	H

	ATOM	2699	2HG2	ILE	A	170	22.796	47.047	11.714	1.00	0.00	H
	ATOM	2700	3HG2	ILE	A	170	23.675	46.954	10.210	1.00	0.00	H
	ATOM	2701	1HD1	ILE	A	170	23.115	46.497	7.070	1.00	0.00	H
5	ATOM	2702	2HD1	ILE	A	170	23.131	45.742	8.651	1.00	0.00	H
	ATOM	2703	3HD1	ILE	A	170	21.776	45.472	7.510	1.00	0.00	H
	ATOM	2704	N	LYS	A	171	22.156	44.867	11.475	1.00	0.52	N
	ATOM	2705	CA	LYS	A	171	22.902	43.646	11.537	1.00	0.52	C
	ATOM	2706	C	LYS	A	171	21.908	42.536	11.406	1.00	0.52	C
10	ATOM	2707	O	LYS	A	171	20.957	42.448	12.180	1.00	0.52	O
	ATOM	2708	CB	LYS	A	171	23.649	43.510	12.879	1.00	0.52	C
	ATOM	2709	CG	LYS	A	171	24.731	42.430	12.935	1.00	0.52	C
	ATOM	2710	CD	LYS	A	171	24.206	41.006	12.790	1.00	0.52	C
	ATOM	2711	CE	LYS	A	171	25.263	39.934	13.064	1.00	0.52	C
	ATOM	2712	NZ	LYS	A	171	26.436	40.153	12.190	1.00	0.52	N1+
15	ATOM	2713	H	LYS	A	171	22.064	45.419	12.309	1.00	0.00	H
	ATOM	2714	HA	LYS	A	171	23.632	43.648	10.707	1.00	0.00	H
	ATOM	2715	1HB	LYS	A	171	22.872	43.341	13.643	1.00	0.00	H
	ATOM	2716	2HB	LYS	A	171	24.129	44.479	13.070	1.00	0.00	H
20	ATOM	2717	1HG	LYS	A	171	25.345	42.498	13.836	1.00	0.00	H
	ATOM	2718	2HG	LYS	A	171	25.440	42.623	12.108	1.00	0.00	H
	ATOM	2719	1HD	LYS	A	171	23.964	40.933	11.730	1.00	0.00	H
	ATOM	2720	2HD	LYS	A	171	23.302	40.816	13.390	1.00	0.00	H
	ATOM	2721	1HE	LYS	A	171	24.877	38.923	12.853	1.00	0.00	H
25	ATOM	2722	2HE	LYS	A	171	25.630	39.937	14.101	1.00	0.00	H
	ATOM	2723	1HZ	LYS	A	171	27.152	39.454	12.333	1.00	0.00	H
	ATOM	2724	2HZ	LYS	A	171	26.174	40.112	11.214	1.00	0.00	H
	ATOM	2725	3HZ	LYS	A	171	26.861	41.053	12.366	1.00	0.00	H
	ATOM	2726	N	ALA	A	172	22.097	41.667	10.393	1.00	0.31	N
30	ATOM	2727	CA	ALA	A	172	21.148	40.617	10.164	1.00	0.31	C
	ATOM	2728	C	ALA	A	172	21.773	39.272	10.514	1.00	0.31	C
	ATOM	2729	O	ALA	A	172	21.353	38.260	9.895	1.00	0.31	O
	ATOM	2730	CB	ALA	A	172	20.692	40.524	8.698	1.00	0.31	C
	ATOM	2731	OXT	ALA	A	172	22.663	39.229	11.402	1.00	0.31	O1-
35	ATOM	2732	H	ALA	A	172	22.807	41.776	9.698	1.00	0.00	H
	ATOM	2733	HA	ALA	A	172	20.252	40.765	10.785	1.00	0.00	H
	ATOM	2734	1HB	ALA	A	172	19.857	39.810	8.602	1.00	0.00	H
	ATOM	2735	2HB	ALA	A	172	20.320	41.491	8.321	1.00	0.00	H
	ATOM	2736	3HB	ALA	A	172	21.505	40.199	8.030	1.00	0.00	H
40	ATOM	2737	N	VAL	B	1	-35.035	33.443	-3.312	1.00	0.14	N1+
	ATOM	2738	CA	VAL	B	1	-36.312	33.784	-2.644	1.00	0.14	C
	ATOM	2739	C	VAL	B	1	-36.557	33.129	-1.314	1.00	0.14	C
	ATOM	2740	O	VAL	B	1	-37.357	33.653	-0.542	1.00	0.14	O
	ATOM	2741	CB	VAL	B	1	-37.484	33.539	-3.566	1.00	0.14	C
45	ATOM	2742	CG1	VAL	B	1	-37.364	34.515	-4.747	1.00	0.14	C
	ATOM	2743	CG2	VAL	B	1	-37.528	32.067	-4.005	1.00	0.14	C
	ATOM	2744	1H	VAL	B	1	-34.869	34.004	-4.138	1.00	0.00	H
	ATOM	2745	2H	VAL	B	1	-34.241	33.598	-2.703	1.00	0.00	H
	ATOM	2746	3H	VAL	B	1	-34.995	32.476	-3.602	1.00	0.00	H
50	ATOM	2747	HA	VAL	B	1	-36.235	34.860	-2.400	1.00	0.00	H
	ATOM	2748	HB	VAL	B	1	-38.411	33.777	-3.011	1.00	0.00	H
	ATOM	2749	1HG1	VAL	B	1	-38.229	34.435	-5.429	1.00	0.00	H
	ATOM	2750	2HG1	VAL	B	1	-37.326	35.564	-4.406	1.00	0.00	H
	ATOM	2751	3HG1	VAL	B	1	-36.463	34.319	-5.351	1.00	0.00	H
55	ATOM	2752	1HG2	VAL	B	1	-38.228	31.983	-4.860	1.00	0.00	H
	ATOM	2753	2HG2	VAL	B	1	-36.576	31.696	-4.412	1.00	0.00	H
	ATOM	2754	3HG2	VAL	B	1	-38.001	31.421	-3.249	1.00	0.00	H
	ATOM	2755	N	PRO	B	2	-35.933	32.030	-0.959	1.00	0.15	N
	ATOM	2756	CA	PRO	B	2	-36.195	31.541	0.363	1.00	0.15	C
60	ATOM	2757	C	PRO	B	2	-35.493	32.410	1.350	1.00	0.15	C
	ATOM	2758	O	PRO	B	2	-34.546	33.097	0.973	1.00	0.15	O
	ATOM	2759	CB	PRO	B	2	-35.731	30.088	0.391	1.00	0.15	C
	ATOM	2760	CG	PRO	B	2	-35.897	29.635	-1.067	1.00	0.15	C
	ATOM	2761	CD	PRO	B	2	-35.709	30.924	-1.884	1.00	0.15	C
65	ATOM	2762	HA	PRO	B	2	-37.285	31.530	0.558	1.00	0.00	H
	ATOM	2763	1HB	PRO	B	2	-36.304	29.496	1.118	1.00	0.00	H
	ATOM	2764	2HB	PRO	B	2	-34.669	30.026	0.677	1.00	0.00	H
	ATOM	2765	1HG	PRO	B	2	-36.917	29.240	-1.212	1.00	0.00	H
	ATOM	2766	2HG	PRO	B	2	-35.203	28.833	-1.366	1.00	0.00	H
70	ATOM	2767	1HD	PRO	B	2	-34.667	30.980	-2.239	1.00	0.00	H
	ATOM	2768	2HD	PRO	B	2	-36.339	30.824	-2.732	1.00	0.00	H
	ATOM	2769	N	GLN	B	3	-35.941	32.393	2.617	1.00	0.19	N

	ATOM	2770	CA	GLN	B	3	-35.329	33.215	3.614	1.00	0.19	C
	ATOM	2771	C	GLN	B	3	-33.901	32.793	3.703	1.00	0.19	C
	ATOM	2772	O	GLN	B	3	-33.553	31.670	3.339	1.00	0.19	O
5	ATOM	2773	CB	GLN	B	3	-35.986	33.063	4.996	1.00	0.19	C
	ATOM	2774	CG	GLN	B	3	-35.493	34.064	6.040	1.00	0.19	C
	ATOM	2775	CD	GLN	B	3	-36.327	33.844	7.293	1.00	0.19	C
	ATOM	2776	OE1	GLN	B	3	-36.930	32.787	7.467	1.00	0.19	O
	ATOM	2777	NE2	GLN	B	3	-36.374	34.869	8.185	1.00	0.19	N
10	ATOM	2778	H	GLN	B	3	-36.686	31.783	2.909	1.00	0.00	H
	ATOM	2779	HA	GLN	B	3	-35.401	34.270	3.289	1.00	0.00	H
	ATOM	2780	1HB	GLN	B	3	-35.828	32.030	5.351	1.00	0.00	H
	ATOM	2781	2HB	GLN	B	3	-37.076	33.203	4.874	1.00	0.00	H
	ATOM	2782	1HG	GLN	B	3	-35.596	35.097	5.669	1.00	0.00	H
	ATOM	2783	2HG	GLN	B	3	-34.444	33.879	6.303	1.00	0.00	H
15	ATOM	2784	1HE2	GLN	B	3	-36.282	35.816	7.857	1.00	0.00	H
	ATOM	2785	2HE2	GLN	B	3	-37.049	34.698	8.921	1.00	0.00	H
	ATOM	2786	N	LYS	B	4	-33.024	33.701	4.172	1.00	0.23	N
	ATOM	2787	CA	LYS	B	4	-31.626	33.390	4.219	1.00	0.23	C
20	ATOM	2788	C	LYS	B	4	-31.282	32.929	5.594	1.00	0.23	C
	ATOM	2789	O	LYS	B	4	-31.667	33.518	6.603	1.00	0.23	O
	ATOM	2790	CB	LYS	B	4	-30.722	34.593	3.904	1.00	0.23	C
	ATOM	2791	CG	LYS	B	4	-30.861	35.101	2.467	1.00	0.23	C
	ATOM	2792	CD	LYS	B	4	-30.229	36.477	2.241	1.00	0.23	C
	ATOM	2793	CE	LYS	B	4	-31.032	37.624	2.856	1.00	0.23	C
25	ATOM	2794	NZ	LYS	B	4	-30.320	38.907	2.659	1.00	0.23	N1+
	ATOM	2795	H	LYS	B	4	-33.282	34.648	4.377	1.00	0.00	H
	ATOM	2796	HA	LYS	B	4	-31.442	32.662	3.416	1.00	0.00	H
	ATOM	2797	1HB	LYS	B	4	-29.665	34.343	4.096	1.00	0.00	H
	ATOM	2798	2HB	LYS	B	4	-30.952	35.398	4.623	1.00	0.00	H
30	ATOM	2799	1HG	LYS	B	4	-31.919	35.129	2.150	1.00	0.00	H
	ATOM	2800	2HG	LYS	B	4	-30.360	34.380	1.801	1.00	0.00	H
	ATOM	2801	1HD	LYS	B	4	-30.132	36.650	1.154	1.00	0.00	H
	ATOM	2802	2HD	LYS	B	4	-29.200	36.464	2.645	1.00	0.00	H
	ATOM	2803	1HE	LYS	B	4	-31.168	37.502	3.942	1.00	0.00	H
35	ATOM	2804	2HE	LYS	B	4	-32.027	37.717	2.391	1.00	0.00	H
	ATOM	2805	1HZ	LYS	B	4	-30.819	39.699	3.042	1.00	0.00	H
	ATOM	2806	2HZ	LYS	B	4	-29.420	38.885	3.134	1.00	0.00	H
	ATOM	2807	3HZ	LYS	B	4	-30.141	39.110	1.685	1.00	0.00	H
	ATOM	2808	N	PRO	B	5	-30.550	31.853	5.616	1.00	0.25	N
40	ATOM	2809	CA	PRO	B	5	-30.108	31.251	6.840	1.00	0.25	C
	ATOM	2810	C	PRO	B	5	-29.273	32.279	7.522	1.00	0.25	C
	ATOM	2811	O	PRO	B	5	-28.730	33.147	6.839	1.00	0.25	O
	ATOM	2812	CB	PRO	B	5	-29.231	30.082	6.411	1.00	0.25	C
45	ATOM	2813	CG	PRO	B	5	-28.592	30.609	5.112	1.00	0.25	C
	ATOM	2814	CD	PRO	B	5	-29.678	31.516	4.507	1.00	0.25	C
	ATOM	2815	HA	PRO	B	5	-30.972	30.960	7.456	1.00	0.00	H
	ATOM	2816	1HB	PRO	B	5	-29.730	29.123	6.357	1.00	0.00	H
	ATOM	2817	2HB	PRO	B	5	-28.453	29.911	7.178	1.00	0.00	H
	ATOM	2818	1HG	PRO	B	5	-28.174	29.894	4.412	1.00	0.00	H
50	ATOM	2819	2HG	PRO	B	5	-27.910	31.344	5.421	1.00	0.00	H
	ATOM	2820	1HD	PRO	B	5	-29.236	32.397	4.044	1.00	0.00	H
	ATOM	2821	2HD	PRO	B	5	-30.320	31.045	3.774	1.00	0.00	H
	ATOM	2822	N	LYS	B	6	-29.172	32.227	8.861	1.00	0.35	N
	ATOM	2823	CA	LYS	B	6	-28.336	33.181	9.520	1.00	0.35	C
55	ATOM	2824	C	LYS	B	6	-27.209	32.429	10.136	1.00	0.35	C
	ATOM	2825	O	LYS	B	6	-27.391	31.333	10.666	1.00	0.35	O
	ATOM	2826	CB	LYS	B	6	-29.033	33.969	10.641	1.00	0.35	C
	ATOM	2827	CG	LYS	B	6	-30.016	35.023	10.127	1.00	0.35	C
	ATOM	2828	CD	LYS	B	6	-31.243	34.436	9.427	1.00	0.35	C
60	ATOM	2829	CE	LYS	B	6	-32.218	35.501	8.920	1.00	0.35	C
	ATOM	2830	NZ	LYS	B	6	-33.370	34.856	8.253	1.00	0.35	N1+
	ATOM	2831	H	LYS	B	6	-29.531	31.470	9.434	1.00	0.00	H
	ATOM	2832	HA	LYS	B	6	-27.947	33.923	8.805	1.00	0.00	H
	ATOM	2833	1HB	LYS	B	6	-28.241	34.472	11.226	1.00	0.00	H
65	ATOM	2834	2HB	LYS	B	6	-29.641	33.423	11.336	1.00	0.00	H
	ATOM	2835	1HG	LYS	B	6	-29.498	35.712	9.434	1.00	0.00	H
	ATOM	2836	2HG	LYS	B	6	-30.343	35.645	10.981	1.00	0.00	H
	ATOM	2837	1HD	LYS	B	6	-31.763	33.748	10.116	1.00	0.00	H
	ATOM	2838	2HD	LYS	B	6	-30.880	33.844	8.600	1.00	0.00	H
70	ATOM	2839	1HE	LYS	B	6	-31.740	36.167	8.183	1.00	0.00	H
	ATOM	2840	2HE	LYS	B	6	-32.610	36.120	9.743	1.00	0.00	H

193

	ATOM	2841	1HZ	LYS	B	6	-33.989	35.514	7.805	1.00	0.00	H
	ATOM	2842	2HZ	LYS	B	6	-33.032	34.222	7.532	1.00	0.00	H
	ATOM	2843	3HZ	LYS	B	6	-33.939	34.311	8.889	1.00	0.00	H
5	ATOM	2844	N	VAL	B	7	-25.995	32.999	10.051	1.00	0.35	N
	ATOM	2845	CA	VAL	B	7	-24.871	32.349	10.651	1.00	0.35	C
	ATOM	2846	C	VAL	B	7	-24.592	33.074	11.922	1.00	0.35	C
	ATOM	2847	O	VAL	B	7	-24.524	34.302	11.950	1.00	0.35	O
	ATOM	2848	CB	VAL	B	7	-23.627	32.383	9.806	1.00	0.35	C
10	ATOM	2849	CG1	VAL	B	7	-23.210	33.847	9.585	1.00	0.35	C
	ATOM	2850	CG2	VAL	B	7	-22.552	31.531	10.499	1.00	0.35	C
	ATOM	2851	H	VAL	B	7	-25.821	33.888	9.614	1.00	0.00	H
	ATOM	2852	HA	VAL	B	7	-25.120	31.291	10.831	1.00	0.00	H
	ATOM	2853	HB	VAL	B	7	-23.863	31.925	8.827	1.00	0.00	H
15	ATOM	2854	1HG1	VAL	B	7	-22.471	33.901	8.765	1.00	0.00	H
	ATOM	2855	2HG1	VAL	B	7	-24.031	34.516	9.285	1.00	0.00	H
	ATOM	2856	3HG1	VAL	B	7	-22.693	34.280	10.456	1.00	0.00	H
	ATOM	2857	1HG2	VAL	B	7	-21.678	31.367	9.847	1.00	0.00	H
	ATOM	2858	2HG2	VAL	B	7	-22.176	32.022	11.412	1.00	0.00	H
	ATOM	2859	3HG2	VAL	B	7	-22.944	30.551	10.791	1.00	0.00	H
20	ATOM	2860	N	SER	B	8	-24.448	32.318	13.023	1.00	0.17	N
	ATOM	2861	CA	SER	B	8	-24.199	32.937	14.287	1.00	0.17	C
	ATOM	2862	C	SER	B	8	-22.807	32.592	14.689	1.00	0.17	C
	ATOM	2863	O	SER	B	8	-22.347	31.470	14.481	1.00	0.17	O
25	ATOM	2864	CB	SER	B	8	-25.131	32.446	15.407	1.00	0.17	C
	ATOM	2865	OG	SER	B	8	-24.819	33.105	16.625	1.00	0.17	O
	ATOM	2866	H	SER	B	8	-24.625	31.319	13.016	1.00	0.00	H
	ATOM	2867	HA	SER	B	8	-24.337	34.028	14.216	1.00	0.00	H
	ATOM	2868	1HB	SER	B	8	-25.073	31.358	15.536	1.00	0.00	H
30	ATOM	2869	2HB	SER	B	8	-26.174	32.697	15.163	1.00	0.00	H
	ATOM	2870	HG	SER	B	8	-24.204	32.543	17.125	1.00	0.00	H
	ATOM	2871	N	LEU	B	9	-22.092	33.571	15.268	1.00	0.11	N
	ATOM	2872	CA	LEU	B	9	-20.747	33.327	15.682	1.00	0.11	C
	ATOM	2873	C	LEU	B	9	-20.696	33.497	17.164	1.00	0.11	C
35	ATOM	2874	O	LEU	B	9	-21.139	34.512	17.700	1.00	0.11	O
	ATOM	2875	CB	LEU	B	9	-19.749	34.334	15.080	1.00	0.11	C
	ATOM	2876	CG	LEU	B	9	-18.287	34.121	15.512	1.00	0.11	C
	ATOM	2877	CD1	LEU	B	9	-17.732	32.785	14.988	1.00	0.11	C
	ATOM	2878	CD2	LEU	B	9	-17.418	35.324	15.111	1.00	0.11	C
40	ATOM	2879	H	LEU	B	9	-22.472	34.471	15.510	1.00	0.00	H
	ATOM	2880	HA	LEU	B	9	-20.438	32.317	15.382	1.00	0.00	H
	ATOM	2881	1HB	LEU	B	9	-20.066	35.356	15.354	1.00	0.00	H
	ATOM	2882	2HB	LEU	B	9	-19.814	34.285	13.978	1.00	0.00	H
	ATOM	2883	HG	LEU	B	9	-18.324	33.885	16.546	1.00	0.00	H
45	ATOM	2884	1HD1	LEU	B	9	-16.651	32.745	15.192	1.00	0.00	H
	ATOM	2885	2HD1	LEU	B	9	-18.211	31.936	15.488	1.00	0.00	H
	ATOM	2886	3HD1	LEU	B	9	-17.848	32.744	13.899	1.00	0.00	H
	ATOM	2887	1HD2	LEU	B	9	-16.368	35.176	15.400	1.00	0.00	H
	ATOM	2888	2HD2	LEU	B	9	-17.440	35.449	14.015	1.00	0.00	H
	ATOM	2889	3HD2	LEU	B	9	-17.775	36.256	15.559	1.00	0.00	H
50	ATOM	2890	N	ASN	B	10	-20.176	32.478	17.872	1.00	0.17	N
	ATOM	2891	CA	ASN	B	10	-20.046	32.599	19.291	1.00	0.17	C
	ATOM	2892	C	ASN	B	10	-18.653	32.180	19.623	1.00	0.17	C
	ATOM	2893	O	ASN	B	10	-18.240	31.069	19.295	1.00	0.17	O
55	ATOM	2894	CB	ASN	B	10	-20.992	31.672	20.070	1.00	0.17	C
	ATOM	2895	CG	ASN	B	10	-22.415	32.145	19.819	1.00	0.17	C
	ATOM	2896	OD1	ASN	B	10	-23.167	31.505	19.086	1.00	0.17	O
	ATOM	2897	ND2	ASN	B	10	-22.798	33.292	20.443	1.00	0.17	N
	ATOM	2898	H	ASN	B	10	-19.879	31.604	17.447	1.00	0.00	H
60	ATOM	2899	HA	ASN	B	10	-20.331	33.609	19.576	1.00	0.00	H
	ATOM	2900	1HB	ASN	B	10	-20.745	31.729	21.143	1.00	0.00	H
	ATOM	2901	2HB	ASN	B	10	-20.916	30.627	19.757	1.00	0.00	H
	ATOM	2902	1HD2	ASN	B	10	-22.191	33.807	21.049	1.00	0.00	H
	ATOM	2903	2HD2	ASN	B	10	-23.731	33.618	20.254	1.00	0.00	H
65	ATOM	2904	N	PRO	B	11	-17.897	33.038	20.245	1.00	0.35	N
	ATOM	2905	CA	PRO	B	11	-18.370	34.356	20.559	1.00	0.35	C
	ATOM	2906	C	PRO	B	11	-18.404	35.166	19.305	1.00	0.35	C
	ATOM	2907	O	PRO	B	11	-17.867	34.727	18.290	1.00	0.35	O
	ATOM	2908	CB	PRO	B	11	-17.403	34.908	21.604	1.00	0.35	C
70	ATOM	2909	CG	PRO	B	11	-16.865	33.651	22.308	1.00	0.35	C
	ATOM	2910	CD	PRO	B	11	-16.938	32.559	21.228	1.00	0.35	C
	ATOM	2911	HA	PRO	B	11	-19.324	34.263	21.103	1.00	0.00	H

	ATOM	2912	1HB	PRO	B	11	-17.861	35.651	22.273	1.00	0.00	H
	ATOM	2913	2HB	PRO	B	11	-16.571	35.402	21.082	1.00	0.00	H
	ATOM	2914	1HG	PRO	B	11	-17.522	33.393	23.155	1.00	0.00	H
	ATOM	2915	2HG	PRO	B	11	-15.851	33.769	22.721	1.00	0.00	H
5	ATOM	2916	1HD	PRO	B	11	-15.961	32.431	20.733	1.00	0.00	H
	ATOM	2917	2HD	PRO	B	11	-17.234	31.578	21.626	1.00	0.00	H
	ATOM	2918	N	PRO	B	12	-19.030	36.309	19.364	1.00	0.52	N
	ATOM	2919	CA	PRO	B	12	-19.156	37.156	18.209	1.00	0.52	C
10	ATOM	2920	C	PRO	B	12	-17.853	37.765	17.809	1.00	0.52	C
	ATOM	2921	O	PRO	B	12	-17.789	38.365	16.737	1.00	0.52	O
	ATOM	2922	CB	PRO	B	12	-20.215	38.194	18.568	1.00	0.52	C
	ATOM	2923	CG	PRO	B	12	-21.088	37.480	19.613	1.00	0.52	C
	ATOM	2924	CD	PRO	B	12	-20.128	36.495	20.299	1.00	0.52	C
15	ATOM	2925	HA	PRO	B	12	-19.493	36.561	17.344	1.00	0.00	H
	ATOM	2926	1HB	PRO	B	12	-20.767	38.562	17.689	1.00	0.00	H
	ATOM	2927	2HB	PRO	B	12	-19.734	39.074	19.029	1.00	0.00	H
	ATOM	2928	1HG	PRO	B	12	-21.889	36.926	19.096	1.00	0.00	H
	ATOM	2929	2HG	PRO	B	12	-21.583	38.161	20.323	1.00	0.00	H
20	ATOM	2930	1HD	PRO	B	12	-19.742	36.914	21.242	1.00	0.00	H
	ATOM	2931	2HD	PRO	B	12	-20.663	35.567	20.521	1.00	0.00	H
	ATOM	2932	N	TRP	B	13	-16.809	37.635	18.646	1.00	0.35	N
	ATOM	2933	CA	TRP	B	13	-15.559	38.278	18.359	1.00	0.35	C
	ATOM	2934	C	TRP	B	13	-15.107	37.850	16.998	1.00	0.35	C
25	ATOM	2935	O	TRP	B	13	-14.934	36.662	16.731	1.00	0.35	O
	ATOM	2936	CB	TRP	B	13	-14.454	37.907	19.361	1.00	0.35	C
	ATOM	2937	CG	TRP	B	13	-14.839	38.183	20.795	1.00	0.35	C
	ATOM	2938	CD1	TRP	B	13	-14.961	37.307	21.833	1.00	0.35	C
	ATOM	2939	CD2	TRP	B	13	-15.219	39.470	21.302	1.00	0.35	C
30	ATOM	2940	NE1	TRP	B	13	-15.382	37.969	22.961	1.00	0.35	N
	ATOM	2941	CE2	TRP	B	13	-15.549	39.302	22.647	1.00	0.35	C
	ATOM	2942	CE3	TRP	B	13	-15.297	40.691	20.695	1.00	0.35	C
	ATOM	2943	CZ2	TRP	B	13	-15.962	40.356	23.408	1.00	0.35	C
	ATOM	2944	CZ3	TRP	B	13	-15.707	41.756	21.468	1.00	0.35	C
35	ATOM	2945	CH2	TRP	B	13	-16.031	41.590	22.798	1.00	0.35	C
	ATOM	2946	H	TRP	B	13	-16.882	37.089	19.485	1.00	0.00	H
	ATOM	2947	HA	TRP	B	13	-15.723	39.368	18.375	1.00	0.00	H
	ATOM	2948	1HB	TRP	B	13	-13.543	38.459	19.077	1.00	0.00	H
	ATOM	2949	2HB	TRP	B	13	-14.206	36.841	19.251	1.00	0.00	H
40	ATOM	2950	HD1	TRP	B	13	-14.738	36.249	21.844	1.00	0.00	H
	ATOM	2951	HE1	TRP	B	13	-15.808	37.524	23.741	1.00	0.00	H
	ATOM	2952	HE3	TRP	B	13	-15.044	40.835	19.655	1.00	0.00	H
	ATOM	2953	HZ2	TRP	B	13	-16.229	40.119	24.420	1.00	0.00	H
	ATOM	2954	HZ3	TRP	B	13	-15.795	42.752	21.062	1.00	0.00	H
45	ATOM	2955	HZ2	TRP	B	13	-16.099	42.501	23.378	1.00	0.00	H
	ATOM	2956	N	ASN	B	14	-14.933	38.829	16.085	1.00	0.15	N
	ATOM	2957	CA	ASN	B	14	-14.506	38.539	14.747	1.00	0.15	C
	ATOM	2958	C	ASN	B	14	-13.076	38.108	14.777	1.00	0.15	C
	ATOM	2959	O	ASN	B	14	-12.681	37.185	14.064	1.00	0.15	O
50	ATOM	2960	CB	ASN	B	14	-14.605	39.739	13.785	1.00	0.15	C
	ATOM	2961	CG	ASN	B	14	-13.588	40.802	14.181	1.00	0.15	C
	ATOM	2962	OD1	ASN	B	14	-13.408	41.115	15.357	1.00	0.15	O
	ATOM	2963	ND2	ASN	B	14	-12.882	41.367	13.165	1.00	0.15	N
	ATOM	2964	H	ASN	B	14	-15.118	39.805	16.295	1.00	0.00	H
55	ATOM	2965	HA	ASN	B	14	-15.111	37.712	14.342	1.00	0.00	H
	ATOM	2966	1HB	ASN	B	14	-15.612	40.188	13.806	1.00	0.00	H
	ATOM	2967	2HB	ASN	B	14	-14.421	39.365	12.763	1.00	0.00	H
	ATOM	2968	1HD2	ASN	B	14	-12.987	41.087	12.202	1.00	0.00	H
	ATOM	2969	2HD2	ASN	B	14	-12.217	42.087	13.380	1.00	0.00	H
60	ATOM	2970	N	ARG	B	15	-12.257	38.773	15.615	1.00	0.13	N
	ATOM	2971	CA	ARG	B	15	-10.859	38.466	15.668	1.00	0.13	C
	ATOM	2972	C	ARG	B	15	-10.645	37.619	16.872	1.00	0.13	C
	ATOM	2973	O	ARG	B	15	-11.086	37.958	17.969	1.00	0.13	O
	ATOM	2974	CB	ARG	B	15	-9.961	39.702	15.860	1.00	0.13	C
65	ATOM	2975	CG	ARG	B	15	-9.990	40.695	14.698	1.00	0.13	C
	ATOM	2976	CD	ARG	B	15	-9.087	41.910	14.925	1.00	0.13	C
	ATOM	2977	NE	ARG	B	15	-9.233	42.805	13.742	1.00	0.13	N1+
	ATOM	2978	CZ	ARG	B	15	-8.137	43.184	13.023	1.00	0.13	C
	ATOM	2979	NH1	ARG	B	15	-6.892	42.769	13.396	1.00	0.13	N
	ATOM	2980	NH2	ARG	B	15	-8.289	43.984	11.926	1.00	0.13	N
70	ATOM	2981	H	ARG	B	15	-12.591	39.606	16.079	1.00	0.00	H
	ATOM	2982	HA	ARG	B	15	-10.563	37.963	14.736	1.00	0.00	H

	ATOM	2983	1HB	ARG	B	15	-8.996	39.350	16.214	1.00	0.00	H
	ATOM	2984	2HB	ARG	B	15	-10.354	40.254	16.738	1.00	0.00	H
	ATOM	2985	1HG	ARG	B	15	-11.007	41.090	14.649	1.00	0.00	H
5	ATOM	2986	2HG	ARG	B	15	-9.785	40.221	13.726	1.00	0.00	H
	ATOM	2987	1HD	ARG	B	15	-8.048	41.638	15.153	1.00	0.00	H
	ATOM	2988	2HD	ARG	B	15	-9.458	42.433	15.807	1.00	0.00	H
	ATOM	2989	HE	ARG	B	15	-9.921	43.526	13.751	1.00	0.00	H
	ATOM	2990	1HH1	ARG	B	15	-6.719	42.203	14.196	1.00	0.00	H
10	ATOM	2991	2HH1	ARG	B	15	-6.069	43.121	12.958	1.00	0.00	H
	ATOM	2992	1HH2	ARG	B	15	-7.535	44.013	11.277	1.00	0.00	H
	ATOM	2993	2HH2	ARG	B	15	-9.189	43.955	11.491	1.00	0.00	H
	ATOM	2994	N	ILE	B	16	-9.959	36.476	16.699	1.00	0.12	N
	ATOM	2995	CA	ILE	B	16	-9.719	35.645	17.838	1.00	0.12	C
	ATOM	2996	C	ILE	B	16	-8.300	35.198	17.781	1.00	0.12	C
15	ATOM	2997	O	ILE	B	16	-7.583	35.472	16.820	1.00	0.12	O
	ATOM	2998	CB	ILE	B	16	-10.558	34.399	17.883	1.00	0.12	C
	ATOM	2999	CG1	ILE	B	16	-10.236	33.483	16.690	1.00	0.12	C
	ATOM	3000	CG2	ILE	B	16	-12.035	34.818	17.972	1.00	0.12	C
20	ATOM	3001	CD1	ILE	B	16	-10.816	32.077	16.840	1.00	0.12	C
	ATOM	3002	H	ILE	B	16	-9.589	36.173	15.804	1.00	0.00	H
	ATOM	3003	HA	ILE	B	16	-9.806	36.229	18.761	1.00	0.00	H
	ATOM	3004	HB	ILE	B	16	-10.323	33.855	18.816	1.00	0.00	H
	ATOM	3005	1HG1	ILE	B	16	-9.151	33.372	16.527	1.00	0.00	H
25	ATOM	3006	2HG1	ILE	B	16	-10.632	33.939	15.766	1.00	0.00	H
	ATOM	3007	1HG2	ILE	B	16	-12.707	33.959	18.128	1.00	0.00	H
	ATOM	3008	2HG2	ILE	B	16	-12.205	35.507	18.814	1.00	0.00	H
	ATOM	3009	3HG2	ILE	B	16	-12.376	35.323	17.052	1.00	0.00	H
	ATOM	3010	1HD1	ILE	B	16	-10.934	31.593	15.860	1.00	0.00	H
30	ATOM	3011	2HD1	ILE	B	16	-10.156	31.437	17.441	1.00	0.00	H
	ATOM	3012	3HD1	ILE	B	16	-11.792	32.108	17.336	1.00	0.00	H
	ATOM	3013	N	PHE	B	17	-7.862	34.506	18.848	1.00	0.17	N
	ATOM	3014	CA	PHE	B	17	-6.527	33.996	18.904	1.00	0.17	C
	ATOM	3015	C	PHE	B	17	-6.595	32.557	18.543	1.00	0.17	C
35	ATOM	3016	O	PHE	B	17	-7.645	31.923	18.627	1.00	0.17	O
	ATOM	3017	CB	PHE	B	17	-5.886	33.999	20.300	1.00	0.17	C
	ATOM	3018	CG	PHE	B	17	-5.562	35.386	20.720	1.00	0.17	C
	ATOM	3019	CD1	PHE	B	17	-4.468	36.028	20.192	1.00	0.17	C
	ATOM	3020	CD2	PHE	B	17	-6.337	36.026	21.657	1.00	0.17	C
40	ATOM	3021	CE1	PHE	B	17	-4.154	37.305	20.585	1.00	0.17	C
	ATOM	3022	CE2	PHE	B	17	-6.027	37.303	22.057	1.00	0.17	C
	ATOM	3023	CZ	PHE	B	17	-4.935	37.939	21.518	1.00	0.17	C
	ATOM	3024	H	PHE	B	17	-8.467	34.178	19.583	1.00	0.00	H
45	ATOM	3025	HA	PHE	B	17	-5.913	34.589	18.229	1.00	0.00	H
	ATOM	3026	1HB	PHE	B	17	-4.946	33.448	20.184	1.00	0.00	H
	ATOM	3027	2HB	PHE	B	17	-6.495	33.466	21.041	1.00	0.00	H
	ATOM	3028	HD1	PHE	B	17	-3.883	35.515	19.440	1.00	0.00	H
	ATOM	3029	HD2	PHE	B	17	-7.205	35.518	22.059	1.00	0.00	H
	ATOM	3030	HE1	PHE	B	17	-3.236	37.726	20.300	1.00	0.00	H
50	ATOM	3031	HE2	PHE	B	17	-6.677	37.770	22.777	1.00	0.00	H
	ATOM	3032	HZ	PHE	B	17	-4.353	38.631	22.047	1.00	0.00	H
	ATOM	3033	N	LYS	B	18	-5.446	32.008	18.119	1.00	0.22	N
	ATOM	3034	CA	LYS	B	18	-5.403	30.623	17.781	1.00	0.22	C
	ATOM	3035	C	LYS	B	18	-5.558	29.867	19.056	1.00	0.22	C
55	ATOM	3036	O	LYS	B	18	-5.134	30.320	20.119	1.00	0.22	O
	ATOM	3037	CB	LYS	B	18	-4.077	30.203	17.126	1.00	0.22	C
	ATOM	3038	CG	LYS	B	18	-2.859	30.461	18.012	1.00	0.22	C
	ATOM	3039	CD	LYS	B	18	-1.586	29.780	17.511	1.00	0.22	C
	ATOM	3040	CE	LYS	B	18	-0.375	29.996	18.418	1.00	0.22	C
60	ATOM	3041	NZ	LYS	B	18	0.743	29.138	17.967	1.00	0.22	N1+
	ATOM	3042	H	LYS	B	18	-4.641	32.589	17.925	1.00	0.00	H
	ATOM	3043	HA	LYS	B	18	-6.267	30.489	17.128	1.00	0.00	H
	ATOM	3044	1HB	LYS	B	18	-3.964	30.718	16.156	1.00	0.00	H
	ATOM	3045	2HB	LYS	B	18	-4.150	29.124	16.902	1.00	0.00	H
65	ATOM	3046	1HG	LYS	B	18	-3.038	30.058	19.019	1.00	0.00	H
	ATOM	3047	2HG	LYS	B	18	-2.689	31.546	18.128	1.00	0.00	H
	ATOM	3048	1HD	LYS	B	18	-1.354	30.137	16.492	1.00	0.00	H
	ATOM	3049	2HD	LYS	B	18	-1.792	28.698	17.428	1.00	0.00	H
	ATOM	3050	1HE	LYS	B	18	-0.596	29.719	19.461	1.00	0.00	H
70	ATOM	3051	2HE	LYS	B	18	-0.024	31.038	18.411	1.00	0.00	H
	ATOM	3052	1HZ	LYS	B	18	1.576	29.272	18.528	1.00	0.00	H
	ATOM	3053	2HZ	LYS	B	18	0.522	28.153	18.013	1.00	0.00	H

	ATOM	3054	3HZ	LYS	B	18	1.016	29.349	17.015	1.00	0.00	H
	ATOM	3055	N	GLY	B	19	-6.207	28.692	18.978	1.00	0.21	N
	ATOM	3056	CA	GLY	B	19	-6.383	27.886	20.146	1.00	0.21	C
5	ATOM	3057	C	GLY	B	19	-7.708	28.214	20.746	1.00	0.21	C
	ATOM	3058	O	GLY	B	19	-8.192	27.501	21.623	1.00	0.21	O
	ATOM	3059	H	GLY	B	19	-6.495	28.327	18.071	1.00	0.00	H
	ATOM	3060	1HA	GLY	B	19	-5.676	28.245	20.917	1.00	0.00	H
	ATOM	3061	2HA	GLY	B	19	-6.080	26.838	20.096	1.00	0.00	H
10	ATOM	3062	N	GLU	B	20	-8.338	29.306	20.281	1.00	0.23	N
	ATOM	3063	CA	GLU	B	20	-9.610	29.665	20.830	1.00	0.23	C
	ATOM	3064	C	GLU	B	20	-10.642	28.792	20.202	1.00	0.23	C
	ATOM	3065	O	GLU	B	20	-10.428	28.231	19.128	1.00	0.23	O
	ATOM	3066	CB	GLU	B	20	-10.002	31.130	20.574	1.00	0.23	C
15	ATOM	3067	CG	GLU	B	20	-9.106	32.113	21.327	1.00	0.23	C
	ATOM	3068	CD	GLU	B	20	-9.228	31.774	22.806	1.00	0.23	C
	ATOM	3069	OE1	GLU	B	20	-10.378	31.534	23.263	1.00	0.23	O
	ATOM	3070	OE2	GLU	B	20	-8.174	31.735	23.495	1.00	0.23	O1-
	ATOM	3071	H	GLU	B	20	-7.903	29.958	19.641	1.00	0.00	H
20	ATOM	3072	HA	GLU	B	20	-9.596	29.463	21.915	1.00	0.00	H
	ATOM	3073	1HB	GLU	B	20	-11.054	31.273	20.883	1.00	0.00	H
	ATOM	3074	2HB	GLU	B	20	-9.998	31.319	19.493	1.00	0.00	H
	ATOM	3075	1HG	GLU	B	20	-9.443	33.148	21.165	1.00	0.00	H
	ATOM	3076	2HG	GLU	B	20	-8.053	32.040	21.031	1.00	0.00	H
25	ATOM	3077	N	ASN	B	21	-11.794	28.642	20.879	1.00	0.16	N
	ATOM	3078	CA	ASN	B	21	-12.833	27.815	20.346	1.00	0.16	C
	ATOM	3079	C	ASN	B	21	-13.814	28.715	19.677	1.00	0.16	C
	ATOM	3080	O	ASN	B	21	-14.134	29.792	20.179	1.00	0.16	O
	ATOM	3081	CB	ASN	B	21	-13.589	27.007	21.415	1.00	0.16	C
30	ATOM	3082	CG	ASN	B	21	-12.613	25.981	21.970	1.00	0.16	C
	ATOM	3083	OD1	ASN	B	21	-11.595	25.692	21.347	1.00	0.16	O
	ATOM	3084	ND2	ASN	B	21	-12.923	25.418	23.168	1.00	0.16	N
	ATOM	3085	H	ASN	B	21	-12.005	29.178	21.704	1.00	0.00	H
	ATOM	3086	HA	ASN	B	21	-12.376	27.142	19.624	1.00	0.00	H
35	ATOM	3087	1HB	ASN	B	21	-14.424	26.471	20.932	1.00	0.00	H
	ATOM	3088	2HB	ASN	B	21	-13.999	27.666	22.196	1.00	0.00	H
	ATOM	3089	1HD2	ASN	B	21	-13.739	25.683	23.687	1.00	0.00	H
	ATOM	3090	2HD2	ASN	B	21	-12.261	24.760	23.540	1.00	0.00	H
	ATOM	3091	N	VAL	B	22	-14.289	28.299	18.490	1.00	0.07	N
40	ATOM	3092	CA	VAL	B	22	-15.243	29.093	17.780	1.00	0.07	C
	ATOM	3093	C	VAL	B	22	-16.438	28.234	17.559	1.00	0.07	C
	ATOM	3094	O	VAL	B	22	-16.312	27.053	17.236	1.00	0.07	O
	ATOM	3095	CB	VAL	B	22	-14.753	29.535	16.431	1.00	0.07	C
	ATOM	3096	CG1	VAL	B	22	-15.891	30.274	15.710	1.00	0.07	C
45	ATOM	3097	CG2	VAL	B	22	-13.481	30.379	16.626	1.00	0.07	C
	ATOM	3098	H	VAL	B	22	-14.083	27.370	18.135	1.00	0.00	H
	ATOM	3099	HA	VAL	B	22	-15.511	29.985	18.368	1.00	0.00	H
	ATOM	3100	HB	VAL	B	22	-14.492	28.689	15.799	1.00	0.00	H
	ATOM	3101	1HG1	VAL	B	22	-15.529	30.772	14.795	1.00	0.00	H
50	ATOM	3102	2HG1	VAL	B	22	-16.697	29.591	15.399	1.00	0.00	H
	ATOM	3103	3HG1	VAL	B	22	-16.314	31.040	16.376	1.00	0.00	H
	ATOM	3104	1HG2	VAL	B	22	-13.124	30.786	15.667	1.00	0.00	H
	ATOM	3105	2HG2	VAL	B	22	-13.699	31.230	17.292	1.00	0.00	H
	ATOM	3106	3HG2	VAL	B	22	-12.657	29.793	17.064	1.00	0.00	H
55	ATOM	3107	N	THR	B	23	-17.641	28.800	17.762	1.00	0.06	N
	ATOM	3108	CA	THR	B	23	-18.823	28.028	17.530	1.00	0.06	C
	ATOM	3109	C	THR	B	23	-19.615	28.740	16.486	1.00	0.06	C
	ATOM	3110	O	THR	B	23	-19.909	29.927	16.612	1.00	0.06	O
	ATOM	3111	CB	THR	B	23	-19.704	27.891	18.737	1.00	0.06	C
60	ATOM	3112	OG1	THR	B	23	-18.992	27.254	19.787	1.00	0.06	O
	ATOM	3113	CG2	THR	B	23	-20.936	27.053	18.353	1.00	0.06	C
	ATOM	3114	H	THR	B	23	-17.770	29.719	18.174	1.00	0.00	H
	ATOM	3115	HA	THR	B	23	-18.554	27.016	17.215	1.00	0.00	H
	ATOM	3116	HB	THR	B	23	-20.030	28.886	19.078	1.00	0.00	H
	ATOM	3117	HG1	THR	B	23	-19.557	27.282	20.569	1.00	0.00	H
65	ATOM	3118	1HG2	THR	B	23	-21.569	26.856	19.233	1.00	0.00	H
	ATOM	3119	2HG2	THR	B	23	-21.569	27.557	17.607	1.00	0.00	H
	ATOM	3120	3HG2	THR	B	23	-20.629	26.075	17.945	1.00	0.00	H
	ATOM	3121	N	LEU	B	24	-19.967	28.020	15.407	1.00	0.06	N
70	ATOM	3122	CA	LEU	B	24	-20.752	28.613	14.368	1.00	0.06	C
	ATOM	3123	C	LEU	B	24	-22.058	27.900	14.393	1.00	0.06	C
	ATOM	3124	O	LEU	B	24	-22.104	26.671	14.388	1.00	0.06	O

197

	ATOM	3125	CB	LEU	B	24	-20.163	28.405	12.965	1.00	0.06	C
	ATOM	3126	CG	LEU	B	24	-18.783	29.062	12.774	1.00	0.06	C
	ATOM	3127	CD1	LEU	B	24	-18.246	28.827	11.352	1.00	0.06	C
5	ATOM	3128	CD2	LEU	B	24	-18.814	30.548	13.167	1.00	0.06	C
	ATOM	3129	H	LEU	B	24	-19.673	27.055	15.277	1.00	0.00	H
	ATOM	3130	HA	LEU	B	24	-20.868	29.681	14.551	1.00	0.00	H
	ATOM	3131	1HB	LEU	B	24	-20.876	28.847	12.246	1.00	0.00	H
	ATOM	3132	2HB	LEU	B	24	-20.105	27.329	12.729	1.00	0.00	H
10	ATOM	3133	HG	LEU	B	24	-18.071	28.564	13.461	1.00	0.00	H
	ATOM	3134	1HD1	LEU	B	24	-17.231	29.242	11.246	1.00	0.00	H
	ATOM	3135	2HD1	LEU	B	24	-18.193	27.751	11.117	1.00	0.00	H
	ATOM	3136	3HD1	LEU	B	24	-18.893	29.306	10.600	1.00	0.00	H
	ATOM	3137	1HD2	LEU	B	24	-17.820	30.978	12.972	1.00	0.00	H
15	ATOM	3138	2HD2	LEU	B	24	-19.551	31.110	12.571	1.00	0.00	H
	ATOM	3139	3HD2	LEU	B	24	-19.058	30.667	14.225	1.00	0.00	H
	ATOM	3140	N	THR	B	25	-23.167	28.659	14.441	1.00	0.28	N
	ATOM	3141	CA	THR	B	25	-24.439	28.009	14.453	1.00	0.28	C
	ATOM	3142	C	THR	B	25	-25.210	28.557	13.308	1.00	0.28	C
20	ATOM	3143	O	THR	B	25	-25.220	29.760	13.059	1.00	0.28	O
	ATOM	3144	CB	THR	B	25	-25.235	28.276	15.697	1.00	0.28	C
	ATOM	3145	OG1	THR	B	25	-24.523	27.828	16.841	1.00	0.28	O
	ATOM	3146	CG2	THR	B	25	-26.580	27.539	15.588	1.00	0.28	C
	ATOM	3147	H	THR	B	25	-23.128	29.672	14.385	1.00	0.00	H
25	ATOM	3148	HA	THR	B	25	-24.321	26.920	14.354	1.00	0.00	H
	ATOM	3149	HB	THR	B	25	-25.448	29.352	15.810	1.00	0.00	H
	ATOM	3150	HG1	THR	B	25	-23.678	28.304	16.823	1.00	0.00	H
	ATOM	3151	1HG2	THR	B	25	-27.114	27.581	16.552	1.00	0.00	H
	ATOM	3152	2HG2	THR	B	25	-27.247	27.990	14.837	1.00	0.00	H
30	ATOM	3153	3HG2	THR	B	25	-26.441	26.473	15.342	1.00	0.00	H
	ATOM	3154	N	CYS	B	26	-25.878	27.669	12.565	1.00	0.52	N
	ATOM	3155	CA	CYS	B	26	-26.616	28.143	11.446	1.00	0.52	C
	ATOM	3156	C	CYS	B	26	-28.050	27.883	11.751	1.00	0.52	C
	ATOM	3157	O	CYS	B	26	-28.460	26.734	11.908	1.00	0.52	O
35	ATOM	3158	CB	CYS	B	26	-26.230	27.356	10.198	1.00	0.52	C
	ATOM	3159	SG	CYS	B	26	-27.098	27.867	8.709	1.00	0.52	S
	ATOM	3160	H	CYS	B	26	-25.872	26.670	12.726	1.00	0.00	H
	ATOM	3161	HA	CYS	B	26	-26.399	29.195	11.235	1.00	0.00	H
	ATOM	3162	1HB	CYS	B	26	-26.355	26.271	10.346	1.00	0.00	H
40	ATOM	3163	2HB	CYS	B	26	-25.174	27.547	10.007	1.00	0.00	H
	ATOM	3164	N	ASN	B	27	-28.853	28.959	11.836	1.00	0.35	N
	ATOM	3165	CA	ASN	B	27	-30.232	28.793	12.176	1.00	0.35	C
	ATOM	3166	C	ASN	B	27	-31.043	29.100	10.964	1.00	0.35	C
	ATOM	3167	O	ASN	B	27	-30.620	29.856	10.092	1.00	0.35	O
45	ATOM	3168	CB	ASN	B	27	-30.713	29.749	13.280	1.00	0.35	C
	ATOM	3169	CG	ASN	B	27	-30.594	31.169	12.743	1.00	0.35	C
	ATOM	3170	OD1	ASN	B	27	-29.551	31.568	12.228	1.00	0.35	O
	ATOM	3171	ND2	ASN	B	27	-31.698	31.954	12.855	1.00	0.35	N
	ATOM	3172	H	ASN	B	27	-28.543	29.920	11.683	1.00	0.00	H
50	ATOM	3173	HA	ASN	B	27	-30.415	27.767	12.532	1.00	0.00	H
	ATOM	3174	1HB	ASN	B	27	-30.081	29.665	14.180	1.00	0.00	H
	ATOM	3175	2HB	ASN	B	27	-31.746	29.482	13.557	1.00	0.00	H
	ATOM	3176	1HD2	ASN	B	27	-32.530	31.636	13.316	1.00	0.00	H
	ATOM	3177	2HD2	ASN	B	27	-31.598	32.913	12.574	1.00	0.00	H
55	ATOM	3178	N	GLY	B	28	-32.237	28.485	10.876	1.00	0.15	N
	ATOM	3179	CA	GLY	B	28	-33.101	28.725	9.762	1.00	0.15	C
	ATOM	3180	C	GLY	B	28	-33.969	27.521	9.623	1.00	0.15	C
	ATOM	3181	O	GLY	B	28	-33.839	26.561	10.382	1.00	0.15	O
	ATOM	3182	H	GLY	B	28	-32.528	27.749	11.502	1.00	0.00	H
60	ATOM	3183	1HA	GLY	B	28	-32.514	28.852	8.837	1.00	0.00	H
	ATOM	3184	2HA	GLY	B	28	-33.710	29.632	9.918	1.00	0.00	H
	ATOM	3185	N	ASN	B	29	-34.882	27.537	8.633	1.00	0.16	N
	ATOM	3186	CA	ASN	B	29	-35.730	26.399	8.454	1.00	0.16	C
	ATOM	3187	C	ASN	B	29	-34.852	25.276	8.021	1.00	0.16	C
65	ATOM	3188	O	ASN	B	29	-33.866	25.478	7.315	1.00	0.16	O
	ATOM	3189	CB	ASN	B	29	-36.820	26.580	7.382	1.00	0.16	C
	ATOM	3190	CG	ASN	B	29	-37.876	27.535	7.919	1.00	0.16	C
	ATOM	3191	OD1	ASN	B	29	-37.878	27.893	9.096	1.00	0.16	O
	ATOM	3192	ND2	ASN	B	29	-38.816	27.949	7.029	1.00	0.16	N
70	ATOM	3193	H	ASN	B	29	-35.006	28.318	8.013	1.00	0.00	H
	ATOM	3194	HA	ASN	B	29	-36.207	26.143	9.419	1.00	0.00	H
	ATOM	3195	1HB	ASN	B	29	-37.363	25.641	7.240	1.00	0.00	H

	ATOM	3196	2HB	ASN	B	29	-36.417	26.982	6.449	1.00	0.00	H
	ATOM	3197	1HD2	ASN	B	29	-38.833	27.631	6.078	1.00	0.00	H
	ATOM	3198	2HD2	ASN	B	29	-39.532	28.562	7.380	1.00	0.00	H
5	ATOM	3199	N	ASN	B	30	-35.187	24.051	8.463	1.00	0.16	N
	ATOM	3200	CA	ASN	B	30	-34.377	22.921	8.127	1.00	0.16	C
	ATOM	3201	C	ASN	B	30	-35.268	21.823	7.645	1.00	0.16	C
	ATOM	3202	O	ASN	B	30	-36.420	21.713	8.060	1.00	0.16	O
	ATOM	3203	CB	ASN	B	30	-33.609	22.375	9.339	1.00	0.16	C
10	ATOM	3204	CG	ASN	B	30	-32.795	21.178	8.886	1.00	0.16	C
	ATOM	3205	OD1	ASN	B	30	-32.210	21.159	7.805	1.00	0.16	O
	ATOM	3206	ND2	ASN	B	30	-32.781	20.126	9.746	1.00	0.16	N
	ATOM	3207	H	ASN	B	30	-36.004	23.852	9.015	1.00	0.00	H
	ATOM	3208	HA	ASN	B	30	-33.660	23.196	7.338	1.00	0.00	H
	ATOM	3209	1HB	ASN	B	30	-34.307	22.117	10.152	1.00	0.00	H
15	ATOM	3210	2HB	ASN	B	30	-32.904	23.133	9.720	1.00	0.00	H
	ATOM	3211	1HD2	ASN	B	30	-33.323	20.099	10.587	1.00	0.00	H
	ATOM	3212	2HD2	ASN	B	30	-32.195	19.340	9.478	1.00	0.00	H
	ATOM	3213	N	PHE	B	31	-34.745	20.987	6.724	1.00	0.12	N
	ATOM	3214	CA	PHE	B	31	-35.486	19.863	6.236	1.00	0.12	C
20	ATOM	3215	C	PHE	B	31	-35.228	18.765	7.212	1.00	0.12	C
	ATOM	3216	O	PHE	B	31	-34.243	18.805	7.945	1.00	0.12	O
	ATOM	3217	CB	PHE	B	31	-35.024	19.385	4.850	1.00	0.12	C
	ATOM	3218	CG	PHE	B	31	-35.870	18.225	4.458	1.00	0.12	C
	ATOM	3219	CD1	PHE	B	31	-37.137	18.422	3.958	1.00	0.12	C
25	ATOM	3220	CD2	PHE	B	31	-35.395	16.940	4.581	1.00	0.12	C
	ATOM	3221	CE1	PHE	B	31	-37.919	17.353	3.589	1.00	0.12	C
	ATOM	3222	CE2	PHE	B	31	-36.173	15.867	4.215	1.00	0.12	C
	ATOM	3223	CZ	PHE	B	31	-37.439	16.073	3.720	1.00	0.12	C
	ATOM	3224	H	PHE	B	31	-33.732	20.891	6.678	1.00	0.00	H
30	ATOM	3225	HA	PHE	B	31	-36.560	20.108	6.225	1.00	0.00	H
	ATOM	3226	1HB	PHE	B	31	-33.955	19.120	4.883	1.00	0.00	H
	ATOM	3227	2HB	PHE	B	31	-35.127	20.202	4.121	1.00	0.00	H
	ATOM	3228	HD1	PHE	B	31	-37.521	19.428	3.830	1.00	0.00	H
	ATOM	3229	HD2	PHE	B	31	-34.399	16.800	4.975	1.00	0.00	H
35	ATOM	3230	HE1	PHE	B	31	-38.916	17.520	3.188	1.00	0.00	H
	ATOM	3231	HE2	PHE	B	31	-35.783	14.857	4.316	1.00	0.00	H
	ATOM	3232	HZ	PHE	B	31	-38.053	15.224	3.428	1.00	0.00	H
	ATOM	3233	N	PHE	B	32	-36.111	17.753	7.268	1.00	0.11	N
	ATOM	3234	CA	PHE	B	32	-35.851	16.728	8.229	1.00	0.11	C
40	ATOM	3235	C	PHE	B	32	-34.911	15.762	7.598	1.00	0.11	C
	ATOM	3236	O	PHE	B	32	-35.322	14.780	6.982	1.00	0.11	O
	ATOM	3237	CB	PHE	B	32	-37.114	15.971	8.670	1.00	0.11	C
	ATOM	3238	CG	PHE	B	32	-37.971	16.991	9.336	1.00	0.11	C
	ATOM	3239	CD1	PHE	B	32	-38.800	17.790	8.583	1.00	0.11	C
45	ATOM	3240	CD2	PHE	B	32	-37.941	17.160	10.700	1.00	0.11	C
	ATOM	3241	CE1	PHE	B	32	-39.597	18.739	9.178	1.00	0.11	C
	ATOM	3242	CE2	PHE	B	32	-38.735	18.108	11.300	1.00	0.11	C
	ATOM	3243	CZ	PHE	B	32	-39.564	18.899	10.542	1.00	0.11	C
	ATOM	3244	H	PHE	B	32	-36.832	17.591	6.586	1.00	0.00	H
50	ATOM	3245	HA	PHE	B	32	-35.409	17.166	9.143	1.00	0.00	H
	ATOM	3246	1HB	PHE	B	32	-36.811	15.166	9.358	1.00	0.00	H
	ATOM	3247	2HB	PHE	B	32	-37.630	15.498	7.820	1.00	0.00	H
	ATOM	3248	HD1	PHE	B	32	-38.864	17.652	7.507	1.00	0.00	H
	ATOM	3249	HD2	PHE	B	32	-37.287	16.539	11.307	1.00	0.00	H
55	ATOM	3250	HE1	PHE	B	32	-40.252	19.360	8.572	1.00	0.00	H
	ATOM	3251	HE2	PHE	B	32	-38.706	18.233	12.380	1.00	0.00	H
	ATOM	3252	HZ	PHE	B	32	-40.190	19.649	11.019	1.00	0.00	H
	ATOM	3253	N	GLU	B	33	-33.600	16.034	7.738	1.00	0.10	N
	ATOM	3254	CA	GLU	B	33	-32.616	15.164	7.171	1.00	0.10	C
60	ATOM	3255	C	GLU	B	33	-31.455	15.127	8.108	1.00	0.10	C
	ATOM	3256	O	GLU	B	33	-31.273	16.029	8.926	1.00	0.10	O
	ATOM	3257	CB	GLU	B	33	-32.084	15.638	5.809	1.00	0.10	C
	ATOM	3258	CG	GLU	B	33	-31.401	17.006	5.863	1.00	0.10	C
	ATOM	3259	CD	GLU	B	33	-30.934	17.340	4.456	1.00	0.10	C
65	ATOM	3260	OE1	GLU	B	33	-30.393	16.424	3.782	1.00	0.10	O
	ATOM	3261	OE2	GLU	B	33	-31.113	18.515	4.035	1.00	0.10	O1-
	ATOM	3262	H	GLU	B	33	-33.258	16.896	8.139	1.00	0.00	H
	ATOM	3263	HA	GLU	B	33	-33.037	14.148	7.082	1.00	0.00	H
	ATOM	3264	1HB	GLU	B	33	-32.872	15.591	5.047	1.00	0.00	H
70	ATOM	3265	2HB	GLU	B	33	-31.344	14.879	5.494	1.00	0.00	H
	ATOM	3266	1HG	GLU	B	33	-30.551	16.931	6.547	1.00	0.00	H

199

	ATOM	3267	2HG	GLU	B	33	-32.064	17.799	6.243	1.00	0.00	H
	ATOM	3268	N	VAL	B	34	-30.644	14.058	8.020	1.00	0.09	N
	ATOM	3269	CA	VAL	B	34	-29.511	13.941	8.884	1.00	0.09	C
	ATOM	3270	C	VAL	B	34	-28.559	15.048	8.570	1.00	0.09	C
5	ATOM	3271	O	VAL	B	34	-28.077	15.734	9.470	1.00	0.09	O
	ATOM	3272	CB	VAL	B	34	-28.792	12.637	8.712	1.00	0.09	C
	ATOM	3273	CG1	VAL	B	34	-27.594	12.606	9.674	1.00	0.09	C
	ATOM	3274	CG2	VAL	B	34	-29.797	11.497	8.948	1.00	0.09	C
10	ATOM	3275	H	VAL	B	34	-30.815	13.314	7.366	1.00	0.00	H
	ATOM	3276	HA	VAL	B	34	-29.835	14.056	9.932	1.00	0.00	H
	ATOM	3277	HB	VAL	B	34	-28.403	12.546	7.681	1.00	0.00	H
	ATOM	3278	1HG1	VAL	B	34	-27.078	11.632	9.646	1.00	0.00	H
	ATOM	3279	2HG1	VAL	B	34	-26.840	13.370	9.421	1.00	0.00	H
	ATOM	3280	3HG1	VAL	B	34	-27.914	12.776	10.716	1.00	0.00	H
15	ATOM	3281	1HG2	VAL	B	34	-29.295	10.514	8.942	1.00	0.00	H
	ATOM	3282	2HG2	VAL	B	34	-30.288	11.600	9.931	1.00	0.00	H
	ATOM	3283	3HG2	VAL	B	34	-30.583	11.448	8.178	1.00	0.00	H
	ATOM	3284	N	SER	B	35	-28.277	15.279	7.274	1.00	0.11	N
20	ATOM	3285	CA	SER	B	35	-27.364	16.335	6.942	1.00	0.11	C
	ATOM	3286	C	SER	B	35	-28.183	17.559	6.696	1.00	0.11	C
	ATOM	3287	O	SER	B	35	-28.493	17.913	5.559	1.00	0.11	O
	ATOM	3288	CB	SER	B	35	-26.512	16.040	5.689	1.00	0.11	C
	ATOM	3289	OG	SER	B	35	-27.339	15.843	4.552	1.00	0.11	O
25	ATOM	3290	H	SER	B	35	-28.722	14.814	6.501	1.00	0.00	H
	ATOM	3291	HA	SER	B	35	-26.655	16.496	7.772	1.00	0.00	H
	ATOM	3292	1HB	SER	B	35	-25.922	15.124	5.827	1.00	0.00	H
	ATOM	3293	2HB	SER	B	35	-25.813	16.882	5.528	1.00	0.00	H
	ATOM	3294	HG	SER	B	35	-27.978	16.589	4.533	1.00	0.00	H
30	ATOM	3295	N	SER	B	36	-28.548	18.243	7.794	1.00	0.27	N
	ATOM	3296	CA	SER	B	36	-29.398	19.394	7.742	1.00	0.27	C
	ATOM	3297	C	SER	B	36	-28.707	20.528	7.057	1.00	0.27	C
	ATOM	3298	O	SER	B	36	-29.282	21.190	6.194	1.00	0.27	O
	ATOM	3299	CB	SER	B	36	-29.776	19.889	9.147	1.00	0.27	C
	ATOM	3300	OG	SER	B	36	-30.410	18.846	9.871	1.00	0.27	O
35	ATOM	3301	H	SER	B	36	-28.475	17.775	8.692	1.00	0.00	H
	ATOM	3302	HA	SER	B	36	-30.315	19.170	7.176	1.00	0.00	H
	ATOM	3303	1HB	SER	B	36	-30.346	20.826	9.116	1.00	0.00	H
	ATOM	3304	2HB	SER	B	36	-28.841	20.156	9.675	1.00	0.00	H
40	ATOM	3305	HG	SER	B	36	-30.330	19.061	10.811	1.00	0.00	H
	ATOM	3306	N	THR	B	37	-27.431	20.777	7.399	1.00	0.48	N
	ATOM	3307	CA	THR	B	37	-26.842	21.964	6.858	1.00	0.48	C
	ATOM	3308	C	THR	B	37	-25.567	21.675	6.148	1.00	0.48	C
	ATOM	3309	O	THR	B	37	-24.911	20.660	6.377	1.00	0.48	O
	ATOM	3310	CB	THR	B	37	-26.522	22.984	7.901	1.00	0.48	C
45	ATOM	3311	OG1	THR	B	37	-25.965	24.129	7.283	1.00	0.48	O
	ATOM	3312	CG2	THR	B	37	-25.515	22.381	8.896	1.00	0.48	C
	ATOM	3313	H	THR	B	37	-26.848	20.135	7.907	1.00	0.00	H
	ATOM	3314	HA	THR	B	37	-27.514	22.445	6.132	1.00	0.00	H
50	ATOM	3315	HB	THR	B	37	-27.418	23.228	8.460	1.00	0.00	H
	ATOM	3316	HG1	THR	B	37	-25.716	24.744	7.987	1.00	0.00	H
	ATOM	3317	1HG2	THR	B	37	-25.307	23.154	9.649	1.00	0.00	H
	ATOM	3318	2HG2	THR	B	37	-25.923	21.495	9.398	1.00	0.00	H
	ATOM	3319	3HG2	THR	B	37	-24.557	22.126	8.418	1.00	0.00	H
55	ATOM	3320	N	LYS	B	38	-25.205	22.598	5.235	1.00	0.41	N
	ATOM	3321	CA	LYS	B	38	-23.972	22.506	4.517	1.00	0.41	C
	ATOM	3322	C	LYS	B	38	-23.171	23.683	4.969	1.00	0.41	C
	ATOM	3323	O	LYS	B	38	-23.687	24.798	5.054	1.00	0.41	O
	ATOM	3324	CB	LYS	B	38	-24.131	22.656	2.995	1.00	0.41	C
60	ATOM	3325	CG	LYS	B	38	-25.186	21.731	2.385	1.00	0.41	C
	ATOM	3326	CD	LYS	B	38	-26.617	22.138	2.751	1.00	0.41	C
	ATOM	3327	CE	LYS	B	38	-27.700	21.373	1.986	1.00	0.41	C
	ATOM	3328	NZ	LYS	B	38	-29.037	21.900	2.348	1.00	0.41	N1+
	ATOM	3329	H	LYS	B	38	-25.630	23.518	5.314	1.00	0.00	H
65	ATOM	3330	HA	LYS	B	38	-23.477	21.547	4.738	1.00	0.00	H
	ATOM	3331	1HB	LYS	B	38	-23.141	22.476	2.541	1.00	0.00	H
	ATOM	3332	2HB	LYS	B	38	-24.408	23.693	2.761	1.00	0.00	H
	ATOM	3333	1HG	LYS	B	38	-24.996	20.683	2.681	1.00	0.00	H
	ATOM	3334	2HG	LYS	B	38	-25.082	21.760	1.285	1.00	0.00	H
	ATOM	3335	1HD	LYS	B	38	-26.726	23.208	2.649	1.00	0.00	H
70	ATOM	3336	2HD	LYS	B	38	-26.849	21.891	3.795	1.00	0.00	H
	ATOM	3337	1HE	LYS	B	38	-27.684	20.301	2.244	1.00	0.00	H

200

	ATOM	3338	2HE	LYS	B	38	-27.598	21.468	0.893	1.00	0.00	H
	ATOM	3339	1HZ	LYS	B	38	-29.782	21.422	1.855	1.00	0.00	H
	ATOM	3340	2HZ	LYS	B	38	-29.227	21.774	3.336	1.00	0.00	H
	ATOM	3341	3HZ	LYS	B	38	-29.137	22.884	2.132	1.00	0.00	H
5	ATOM	3342	N	TRP	B	39	-21.884	23.465	5.297	1.00	0.18	N
	ATOM	3343	CA	TRP	B	39	-21.073	24.572	5.707	1.00	0.18	C
	ATOM	3344	C	TRP	B	39	-20.040	24.787	4.659	1.00	0.18	C
	ATOM	3345	O	TRP	B	39	-19.565	23.841	4.034	1.00	0.18	O
	ATOM	3346	CB	TRP	B	39	-20.331	24.376	7.044	1.00	0.18	C
10	ATOM	3347	CG	TRP	B	39	-21.211	24.487	8.268	1.00	0.18	C
	ATOM	3348	CD1	TRP	B	39	-21.745	23.516	9.062	1.00	0.18	C
	ATOM	3349	CD2	TRP	B	39	-21.658	25.743	8.802	1.00	0.18	C
	ATOM	3350	NE1	TRP	B	39	-22.498	24.090	10.062	1.00	0.18	N
	ATOM	3351	CE2	TRP	B	39	-22.453	25.461	9.912	1.00	0.18	C
15	ATOM	3352	CE3	TRP	B	39	-21.425	27.026	8.397	1.00	0.18	C
	ATOM	3353	CZ2	TRP	B	39	-23.031	26.465	10.636	1.00	0.18	C
	ATOM	3354	CZ3	TRP	B	39	-22.006	28.036	9.130	1.00	0.18	C
	ATOM	3355	CH2	TRP	B	39	-22.793	27.761	10.228	1.00	0.18	C
	ATOM	3356	H	TRP	B	39	-21.423	22.572	5.234	1.00	0.00	H
20	ATOM	3357	HA	TRP	B	39	-21.686	25.480	5.806	1.00	0.00	H
	ATOM	3358	1HB	TRP	B	39	-19.541	25.146	7.108	1.00	0.00	H
	ATOM	3359	2HB	TRP	B	39	-19.802	23.412	7.047	1.00	0.00	H
	ATOM	3360	HD1	TRP	B	39	-21.773	22.453	8.874	1.00	0.00	H
	ATOM	3361	HE1	TRP	B	39	-23.076	23.572	10.695	1.00	0.00	H
25	ATOM	3362	HE3	TRP	B	39	-20.762	27.244	7.571	1.00	0.00	H
	ATOM	3363	HZ2	TRP	B	39	-23.620	26.247	11.520	1.00	0.00	H
	ATOM	3364	HZ3	TRP	B	39	-21.828	29.070	8.842	1.00	0.00	H
	ATOM	3365	HH2	TRP	B	39	-23.235	28.564	10.806	1.00	0.00	H
	ATOM	3366	N	PHE	B	40	-19.690	26.063	4.416	1.00	0.08	N
30	ATOM	3367	CA	PHE	B	40	-18.688	26.328	3.434	1.00	0.08	C
	ATOM	3368	C	PHE	B	40	-17.664	27.212	4.057	1.00	0.08	C
	ATOM	3369	O	PHE	B	40	-17.990	28.127	4.811	1.00	0.08	O
	ATOM	3370	CB	PHE	B	40	-19.229	27.050	2.190	1.00	0.08	C
	ATOM	3371	CG	PHE	B	40	-20.153	26.100	1.514	1.00	0.08	C
35	ATOM	3372	CD1	PHE	B	40	-21.465	25.994	1.916	1.00	0.08	C
	ATOM	3373	CD2	PHE	B	40	-19.703	25.313	0.478	1.00	0.08	C
	ATOM	3374	CE1	PHE	B	40	-22.315	25.114	1.291	1.00	0.08	C
	ATOM	3375	CE2	PHE	B	40	-20.551	24.431	-0.150	1.00	0.08	C
	ATOM	3376	CZ	PHE	B	40	-21.860	24.332	0.257	1.00	0.08	C
40	ATOM	3377	H	PHE	B	40	-20.105	26.853	4.892	1.00	0.00	H
	ATOM	3378	HA	PHE	B	40	-18.309	25.372	3.136	1.00	0.00	H
	ATOM	3379	1HB	PHE	B	40	-18.376	27.311	1.549	1.00	0.00	H
	ATOM	3380	2HB	PHE	B	40	-19.730	27.984	2.471	1.00	0.00	H
	ATOM	3381	HD1	PHE	B	40	-21.845	26.623	2.717	1.00	0.00	H
45	ATOM	3382	HD2	PHE	B	40	-18.680	25.415	0.131	1.00	0.00	H
	ATOM	3383	HE1	PHE	B	40	-23.355	25.087	1.589	1.00	0.00	H
	ATOM	3384	HE2	PHE	B	40	-20.212	23.880	-1.022	1.00	0.00	H
	ATOM	3385	HZ	PHE	B	40	-22.535	23.650	-0.252	1.00	0.00	H
	ATOM	3386	N	HIS	B	41	-16.383	26.921	3.777	1.00	0.10	N
50	ATOM	3387	CA	HIS	B	41	-15.322	27.757	4.242	1.00	0.10	C
	ATOM	3388	C	HIS	B	41	-14.620	28.223	3.014	1.00	0.10	C
	ATOM	3389	O	HIS	B	41	-14.100	27.419	2.242	1.00	0.10	O
	ATOM	3390	CB	HIS	B	41	-14.287	27.030	5.109	1.00	0.10	C
	ATOM	3391	CG	HIS	B	41	-13.274	27.973	5.682	1.00	0.10	C
55	ATOM	3392	ND1	HIS	B	41	-12.236	27.588	6.499	1.00	0.10	N
	ATOM	3393	CD2	HIS	B	41	-13.159	29.322	5.541	1.00	0.10	C
	ATOM	3394	CE1	HIS	B	41	-11.548	28.715	6.810	1.00	0.10	C
	ATOM	3395	NE2	HIS	B	41	-12.071	29.794	6.253	1.00	0.10	N
	ATOM	3396	H	HIS	B	41	-16.137	26.064	3.279	1.00	0.00	H
60	ATOM	3397	HA	HIS	B	41	-15.740	28.586	4.831	1.00	0.00	H
	ATOM	3398	1HB	HIS	B	41	-13.799	26.218	4.545	1.00	0.00	H
	ATOM	3399	2HB	HIS	B	41	-14.824	26.533	5.938	1.00	0.00	H
	ATOM	3400	HD2	HIS	B	41	-13.745	30.040	5.019	1.00	0.00	H
	ATOM	3401	HE1	HIS	B	41	-10.615	28.670	7.349	1.00	0.00	H
65	ATOM	3402	HE2	HIS	B	41	-11.766	30.724	6.456	1.00	0.00	H
	ATOM	3403	N	ASN	B	42	-14.593	29.547	2.797	1.00	0.11	N
	ATOM	3404	CA	ASN	B	42	-13.967	30.065	1.622	1.00	0.11	C
	ATOM	3405	C	ASN	B	42	-14.617	29.423	0.440	1.00	0.11	C
	ATOM	3406	O	ASN	B	42	-14.003	29.264	-0.614	1.00	0.11	O
70	ATOM	3407	CB	ASN	B	42	-12.450	29.807	1.562	1.00	0.11	C
	ATOM	3408	CG	ASN	B	42	-11.781	30.743	2.558	1.00	0.11	C

201

	ATOM	3409	OD1	ASN	B	42	-12.427	31.620	3.129	1.00	0.11	O
	ATOM	3410	ND2	ASN	B	42	-10.447	30.568	2.758	1.00	0.11	N
	ATOM	3411	H	ASN	B	42	-14.895	30.202	3.517	1.00	0.00	H
	ATOM	3412	HA	ASN	B	42	-14.186	31.144	1.529	1.00	0.00	H
5	ATOM	3413	1HB	ASN	B	42	-12.064	30.095	0.568	1.00	0.00	H
	ATOM	3414	2HB	ASN	B	42	-12.163	28.762	1.744	1.00	0.00	H
	ATOM	3415	1HD2	ASN	B	42	-9.941	29.816	2.328	1.00	0.00	H
	ATOM	3416	2HD2	ASN	B	42	-9.999	31.137	3.458	1.00	0.00	H
10	ATOM	3417	N	GLY	B	43	-15.899	29.045	0.589	1.00	0.08	N
	ATOM	3418	CA	GLY	B	43	-16.624	28.488	-0.515	1.00	0.08	C
	ATOM	3419	C	GLY	B	43	-16.364	27.018	-0.611	1.00	0.08	C
	ATOM	3420	O	GLY	B	43	-16.830	26.369	-1.546	1.00	0.08	O
	ATOM	3421	H	GLY	B	43	-16.266	28.914	1.519	1.00	0.00	H
15	ATOM	3422	1HA	GLY	B	43	-16.323	28.969	-1.458	1.00	0.00	H
	ATOM	3423	2HA	GLY	B	43	-17.706	28.635	-0.374	1.00	0.00	H
	ATOM	3424	N	SER	B	44	-15.617	26.438	0.346	1.00	0.15	N
	ATOM	3425	CA	SER	B	44	-15.375	25.028	0.255	1.00	0.15	C
	ATOM	3426	C	SER	B	44	-16.345	24.356	1.167	1.00	0.15	C
20	ATOM	3427	O	SER	B	44	-16.513	24.755	2.317	1.00	0.15	O
	ATOM	3428	CB	SER	B	44	-13.964	24.604	0.694	1.00	0.15	C
	ATOM	3429	OG	SER	B	44	-13.788	24.860	2.080	1.00	0.15	O
	ATOM	3430	H	SER	B	44	-15.082	26.974	1.012	1.00	0.00	H
	ATOM	3431	HA	SER	B	44	-15.486	24.690	-0.788	1.00	0.00	H
25	ATOM	3432	1HB	SER	B	44	-13.183	25.094	0.087	1.00	0.00	H
	ATOM	3433	2HB	SER	B	44	-13.867	23.517	0.561	1.00	0.00	H
	ATOM	3434	HG	SER	B	44	-13.580	25.804	2.177	1.00	0.00	H
	ATOM	3435	N	LEU	B	45	-17.025	23.310	0.666	1.00	0.35	N
	ATOM	3436	CA	LEU	B	45	-17.997	22.626	1.465	1.00	0.35	C
30	ATOM	3437	C	LEU	B	45	-17.255	21.852	2.504	1.00	0.35	C
	ATOM	3438	O	LEU	B	45	-16.195	21.288	2.241	1.00	0.35	O
	ATOM	3439	CB	LEU	B	45	-18.886	21.676	0.622	1.00	0.35	C
	ATOM	3440	CG	LEU	B	45	-20.000	20.880	1.345	1.00	0.35	C
	ATOM	3441	CD1	LEU	B	45	-20.847	20.099	0.328	1.00	0.35	C
35	ATOM	3442	CD2	LEU	B	45	-19.465	19.928	2.433	1.00	0.35	C
	ATOM	3443	H	LEU	B	45	-16.840	22.935	-0.247	1.00	0.00	H
	ATOM	3444	HA	LEU	B	45	-18.651	23.382	1.916	1.00	0.00	H
	ATOM	3445	1HB	LEU	B	45	-18.218	20.935	0.143	1.00	0.00	H
	ATOM	3446	2HB	LEU	B	45	-19.327	22.235	-0.212	1.00	0.00	H
40	ATOM	3447	HG	LEU	B	45	-20.665	21.614	1.840	1.00	0.00	H
	ATOM	3448	1HD1	LEU	B	45	-21.676	19.564	0.821	1.00	0.00	H
	ATOM	3449	2HD1	LEU	B	45	-21.291	20.767	-0.428	1.00	0.00	H
	ATOM	3450	3HD1	LEU	B	45	-20.234	19.352	-0.203	1.00	0.00	H
	ATOM	3451	1HD2	LEU	B	45	-19.720	18.886	2.158	1.00	0.00	H
45	ATOM	3452	2HD2	LEU	B	45	-18.389	19.861	2.575	1.00	0.00	H
	ATOM	3453	3HD2	LEU	B	45	-20.074	20.108	3.311	1.00	0.00	H
	ATOM	3454	N	SER	B	46	-17.808	21.826	3.734	1.00	0.48	N
	ATOM	3455	CA	SER	B	46	-17.218	21.081	4.809	1.00	0.48	C
	ATOM	3456	C	SER	B	46	-18.124	19.925	5.078	1.00	0.48	C
50	ATOM	3457	O	SER	B	46	-19.320	20.095	5.301	1.00	0.48	O
	ATOM	3458	CB	SER	B	46	-17.159	21.829	6.154	1.00	0.48	C
	ATOM	3459	OG	SER	B	46	-16.268	22.929	6.093	1.00	0.48	O
	ATOM	3460	H	SER	B	46	-18.582	22.438	3.972	1.00	0.00	H
	ATOM	3461	HA	SER	B	46	-16.185	20.797	4.554	1.00	0.00	H
55	ATOM	3462	1HB	SER	B	46	-16.623	21.080	6.739	1.00	0.00	H
	ATOM	3463	2HB	SER	B	46	-18.133	22.087	6.591	1.00	0.00	H
	ATOM	3464	HG	SER	B	46	-16.007	23.091	7.021	1.00	0.00	H
	ATOM	3465	N	GLU	B	47	-17.561	18.708	5.029	1.00	0.44	N
	ATOM	3466	CA	GLU	B	47	-18.248	17.483	5.316	1.00	0.44	C
60	ATOM	3467	C	GLU	B	47	-18.453	17.380	6.797	1.00	0.44	C
	ATOM	3468	O	GLU	B	47	-19.343	16.678	7.271	1.00	0.44	O
	ATOM	3469	CB	GLU	B	47	-17.440	16.244	4.906	1.00	0.44	C
	ATOM	3470	CG	GLU	B	47	-16.115	16.136	5.662	1.00	0.44	C
	ATOM	3471	CD	GLU	B	47	-15.396	14.878	5.203	1.00	0.44	C
65	ATOM	3472	OE1	GLU	B	47	-15.858	14.260	4.206	1.00	0.44	O
	ATOM	3473	OE2	GLU	B	47	-14.373	14.517	5.844	1.00	0.44	O1-
	ATOM	3474	H	GLU	B	47	-16.607	18.583	4.722	1.00	0.00	H
	ATOM	3475	HA	GLU	B	47	-19.239	17.485	4.833	1.00	0.00	H
	ATOM	3476	1HB	GLU	B	47	-17.273	16.281	3.815	1.00	0.00	H
70	ATOM	3477	2HB	GLU	B	47	-18.068	15.358	5.110	1.00	0.00	H
	ATOM	3478	1HG	GLU	B	47	-16.248	16.052	6.752	1.00	0.00	H
	ATOM	3479	2HG	GLU	B	47	-15.450	16.998	5.494	1.00	0.00	H

202

	ATOM	3480	N	GLU	B	48	-17.608	18.100	7.551	1.00	0.45	N
	ATOM	3481	CA	GLU	B	48	-17.419	17.985	8.969	1.00	0.45	C
	ATOM	3482	C	GLU	B	48	-18.648	18.126	9.823	1.00	0.45	C
5	ATOM	3483	O	GLU	B	48	-18.857	17.287	10.697	1.00	0.45	O
	ATOM	3484	CB	GLU	B	48	-16.414	19.033	9.468	1.00	0.45	C
	ATOM	3485	CG	GLU	B	48	-16.862	20.463	9.154	1.00	0.45	C
	ATOM	3486	CD	GLU	B	48	-15.749	21.419	9.560	1.00	0.45	C
	ATOM	3487	OE1	GLU	B	48	-14.717	20.938	10.099	1.00	0.45	O
10	ATOM	3488	OE2	GLU	B	48	-15.917	22.647	9.333	1.00	0.45	Ol-
	ATOM	3489	H	GLU	B	48	-16.949	18.691	7.075	1.00	0.00	H
	ATOM	3490	HA	GLU	B	48	-17.016	16.981	9.188	1.00	0.00	H
	ATOM	3491	1HB	GLU	B	48	-15.437	18.814	8.999	1.00	0.00	H
	ATOM	3492	2HB	GLU	B	48	-16.290	18.894	10.557	1.00	0.00	H
15	ATOM	3493	1HG	GLU	B	48	-17.656	20.717	9.869	1.00	0.00	H
	ATOM	3494	2HG	GLU	B	48	-17.412	20.608	8.238	1.00	0.00	H
	ATOM	3495	N	THR	B	49	-19.523	19.131	9.626	1.00	0.55	N
	ATOM	3496	CA	THR	B	49	-20.475	19.275	10.695	1.00	0.55	C
	ATOM	3497	C	THR	B	49	-21.869	19.563	10.218	1.00	0.55	C
20	ATOM	3498	O	THR	B	49	-22.124	19.788	9.036	1.00	0.55	O
	ATOM	3499	CB	THR	B	49	-20.062	20.399	11.603	1.00	0.55	C
	ATOM	3500	OG1	THR	B	49	-20.882	20.478	12.757	1.00	0.55	O
	ATOM	3501	CG2	THR	B	49	-20.139	21.702	10.795	1.00	0.55	C
	ATOM	3502	H	THR	B	49	-19.450	19.828	8.907	1.00	0.00	H
25	ATOM	3503	HA	THR	B	49	-20.596	18.355	11.285	1.00	0.00	H
	ATOM	3504	HB	THR	B	49	-19.051	20.098	11.919	1.00	0.00	H
	ATOM	3505	HG1	THR	B	49	-20.702	21.317	13.210	1.00	0.00	H
	ATOM	3506	1HG2	THR	B	49	-19.326	22.416	10.800	1.00	0.00	H
	ATOM	3507	2HG2	THR	B	49	-20.226	21.509	9.715	1.00	0.00	H
30	ATOM	3508	3HG2	THR	B	49	-21.061	22.206	11.101	1.00	0.00	H
	ATOM	3509	N	ASN	B	50	-22.808	19.535	11.191	1.00	0.44	N
	ATOM	3510	CA	ASN	B	50	-24.216	19.765	11.036	1.00	0.44	C
	ATOM	3511	C	ASN	B	50	-24.526	21.176	11.431	1.00	0.44	C
	ATOM	3512	O	ASN	B	50	-23.788	22.110	11.124	1.00	0.44	O
35	ATOM	3513	CB	ASN	B	50	-25.082	18.854	11.923	1.00	0.44	C
	ATOM	3514	CG	ASN	B	50	-24.987	17.436	11.383	1.00	0.44	C
	ATOM	3515	OD1	ASN	B	50	-25.306	17.184	10.223	1.00	0.44	O
	ATOM	3516	ND2	ASN	B	50	-24.536	16.483	12.243	1.00	0.44	N
	ATOM	3517	H	ASN	B	50	-22.432	19.612	12.132	1.00	0.00	H
40	ATOM	3518	HA	ASN	B	50	-24.490	19.648	9.974	1.00	0.00	H
	ATOM	3519	1HB	ASN	B	50	-26.160	19.052	11.801	1.00	0.00	H
	ATOM	3520	2HB	ASN	B	50	-24.811	18.926	12.988	1.00	0.00	H
	ATOM	3521	1HD2	ASN	B	50	-24.229	16.692	13.173	1.00	0.00	H
	ATOM	3522	2HD2	ASN	B	50	-24.434	15.557	11.862	1.00	0.00	H
45	ATOM	3523	N	SER	B	51	-25.661	21.345	12.140	1.00	0.25	N
	ATOM	3524	CA	SER	B	51	-26.182	22.633	12.494	1.00	0.25	C
	ATOM	3525	C	SER	B	51	-25.171	23.418	13.267	1.00	0.25	C
	ATOM	3526	O	SER	B	51	-24.943	24.590	12.969	1.00	0.25	O
	ATOM	3527	CB	SER	B	51	-27.446	22.542	13.365	1.00	0.25	C
50	ATOM	3528	OG	SER	B	51	-27.126	21.972	14.625	1.00	0.25	O
	ATOM	3529	H	SER	B	51	-26.217	20.565	12.448	1.00	0.00	H
	ATOM	3530	HA	SER	B	51	-26.415	23.201	11.580	1.00	0.00	H
	ATOM	3531	1HB	SER	B	51	-28.208	21.903	12.897	1.00	0.00	H
	ATOM	3532	2HB	SER	B	51	-27.883	23.550	13.489	1.00	0.00	H
55	ATOM	3533	HG	SER	B	51	-26.652	22.654	15.134	1.00	0.00	H
	ATOM	3534	N	SER	B	52	-24.525	22.810	14.278	1.00	0.14	N
	ATOM	3535	CA	SER	B	52	-23.591	23.593	15.036	1.00	0.14	C
	ATOM	3536	C	SER	B	52	-22.214	23.106	14.740	1.00	0.14	C
	ATOM	3537	O	SER	B	52	-21.944	21.906	14.768	1.00	0.14	O
60	ATOM	3538	CB	SER	B	52	-23.794	23.486	16.557	1.00	0.14	C
	ATOM	3539	OG	SER	B	52	-25.058	24.020	16.919	1.00	0.14	O
	ATOM	3540	H	SER	B	52	-24.570	21.822	14.458	1.00	0.00	H
	ATOM	3541	HA	SER	B	52	-23.702	24.662	14.810	1.00	0.00	H
	ATOM	3542	1HB	SER	B	52	-22.979	24.029	17.070	1.00	0.00	H
65	ATOM	3543	2HB	SER	B	52	-23.770	22.444	16.905	1.00	0.00	H
	ATOM	3544	HG	SER	B	52	-24.950	24.982	16.985	1.00	0.00	H
	ATOM	3545	N	LEU	B	53	-21.296	24.040	14.422	1.00	0.09	N
	ATOM	3546	CA	LEU	B	53	-19.948	23.630	14.179	1.00	0.09	C
	ATOM	3547	C	LEU	B	53	-19.099	24.280	15.218	1.00	0.09	C
70	ATOM	3548	O	LEU	B	53	-19.090	25.503	15.358	1.00	0.09	O
	ATOM	3549	CB	LEU	B	53	-19.400	24.033	12.798	1.00	0.09	C
	ATOM	3550	CG	LEU	B	53	-17.946	23.579	12.554	1.00	0.09	C

203

	ATOM	3551	CD1	LEU	B	53	-17.822	22.049	12.594	1.00	0.09	C
	ATOM	3552	CD2	LEU	B	53	-17.391	24.172	11.251	1.00	0.09	C
	ATOM	3553	H	LEU	B	53	-21.497	25.037	14.378	1.00	0.00	H
5	ATOM	3554	HA	LEU	B	53	-19.873	22.545	14.292	1.00	0.00	H
	ATOM	3555	1HB	LEU	B	53	-19.407	25.138	12.754	1.00	0.00	H
	ATOM	3556	2HB	LEU	B	53	-20.106	23.754	12.014	1.00	0.00	H
	ATOM	3557	HG	LEU	B	53	-17.335	23.996	13.377	1.00	0.00	H
	ATOM	3558	1HD1	LEU	B	53	-16.829	21.811	13.024	1.00	0.00	H
10	ATOM	3559	2HD1	LEU	B	53	-18.521	21.535	13.257	1.00	0.00	H
	ATOM	3560	3HD1	LEU	B	53	-17.754	21.594	11.609	1.00	0.00	H
	ATOM	3561	1HD2	LEU	B	53	-16.302	24.018	11.201	1.00	0.00	H
	ATOM	3562	2HD2	LEU	B	53	-17.862	23.765	10.346	1.00	0.00	H
	ATOM	3563	3HD2	LEU	B	53	-17.544	25.264	11.226	1.00	0.00	H
15	ATOM	3564	N	ASN	B	54	-18.372	23.461	15.998	1.00	0.09	N
	ATOM	3565	CA	ASN	B	54	-17.529	24.012	17.013	1.00	0.09	C
	ATOM	3566	C	ASN	B	54	-16.131	23.631	16.666	1.00	0.09	C
	ATOM	3567	O	ASN	B	54	-15.849	22.471	16.374	1.00	0.09	O
	ATOM	3568	CB	ASN	B	54	-17.800	23.445	18.416	1.00	0.09	C
20	ATOM	3569	CG	ASN	B	54	-16.982	24.254	19.411	1.00	0.09	C
	ATOM	3570	OD1	ASN	B	54	-16.409	25.286	19.069	1.00	0.09	O
	ATOM	3571	ND2	ASN	B	54	-16.916	23.767	20.679	1.00	0.09	N
	ATOM	3572	H	ASN	B	54	-18.263	22.475	15.832	1.00	0.00	H
	ATOM	3573	HA	ASN	B	54	-17.682	25.091	17.053	1.00	0.00	H
	ATOM	3574	1HB	ASN	B	54	-17.555	22.373	18.473	1.00	0.00	H
25	ATOM	3575	2HB	ASN	B	54	-18.867	23.568	18.670	1.00	0.00	H
	ATOM	3576	1HD2	ASN	B	54	-17.372	22.916	20.949	1.00	0.00	H
	ATOM	3577	2HD2	ASN	B	54	-16.360	24.293	21.330	1.00	0.00	H
	ATOM	3578	N	ILE	B	55	-15.213	24.611	16.677	1.00	0.08	N
30	ATOM	3579	CA	ILE	B	55	-13.854	24.291	16.377	1.00	0.08	C
	ATOM	3580	C	ILE	B	55	-13.041	24.735	17.542	1.00	0.08	C
	ATOM	3581	O	ILE	B	55	-13.338	25.745	18.178	1.00	0.08	O
	ATOM	3582	CB	ILE	B	55	-13.310	25.010	15.178	1.00	0.08	C
	ATOM	3583	CG1	ILE	B	55	-13.293	26.527	15.424	1.00	0.08	C
35	ATOM	3584	CG2	ILE	B	55	-14.135	24.589	13.950	1.00	0.08	C
	ATOM	3585	CD1	ILE	B	55	-12.481	27.296	14.384	1.00	0.08	C
	ATOM	3586	H	ILE	B	55	-15.436	25.536	17.039	1.00	0.00	H
	ATOM	3587	HA	ILE	B	55	-13.731	23.205	16.238	1.00	0.00	H
	ATOM	3588	HB	ILE	B	55	-12.270	24.659	15.038	1.00	0.00	H
40	ATOM	3589	1HG1	ILE	B	55	-12.814	26.841	16.356	1.00	0.00	H
	ATOM	3590	2HG1	ILE	B	55	-14.341	26.851	15.420	1.00	0.00	H
	ATOM	3591	1HG2	ILE	B	55	-13.703	24.971	13.010	1.00	0.00	H
	ATOM	3592	2HG2	ILE	B	55	-14.181	23.491	13.855	1.00	0.00	H
	ATOM	3593	3HG2	ILE	B	55	-15.169	24.966	14.004	1.00	0.00	H
45	ATOM	3594	1HD1	ILE	B	55	-12.528	28.384	14.547	1.00	0.00	H
	ATOM	3595	2HD1	ILE	B	55	-11.433	26.989	14.474	1.00	0.00	H
	ATOM	3596	3HD1	ILE	B	55	-12.805	27.104	13.349	1.00	0.00	H
	ATOM	3597	N	VAL	B	56	-11.988	23.964	17.855	1.00	0.10	N
	ATOM	3598	CA	VAL	B	56	-11.128	24.307	18.942	1.00	0.10	C
50	ATOM	3599	C	VAL	B	56	-9.803	24.597	18.333	1.00	0.10	C
	ATOM	3600	O	VAL	B	56	-9.483	24.091	17.259	1.00	0.10	O
	ATOM	3601	CB	VAL	B	56	-10.938	23.177	19.914	1.00	0.10	C
	ATOM	3602	CG1	VAL	B	56	-9.887	23.579	20.962	1.00	0.10	C
	ATOM	3603	CG2	VAL	B	56	-12.308	22.813	20.510	1.00	0.10	C
55	ATOM	3604	H	VAL	B	56	-11.643	23.243	17.244	1.00	0.00	H
	ATOM	3605	HA	VAL	B	56	-11.486	25.247	19.322	1.00	0.00	H
	ATOM	3606	HB	VAL	B	56	-10.550	22.293	19.374	1.00	0.00	H
	ATOM	3607	1HG1	VAL	B	56	-10.078	23.069	21.922	1.00	0.00	H
	ATOM	3608	2HG1	VAL	B	56	-8.900	23.203	20.639	1.00	0.00	H
60	ATOM	3609	3HG1	VAL	B	56	-9.712	24.626	21.212	1.00	0.00	H
	ATOM	3610	1HG2	VAL	B	56	-12.215	22.112	21.356	1.00	0.00	H
	ATOM	3611	2HG2	VAL	B	56	-12.874	23.684	20.866	1.00	0.00	H
	ATOM	3612	3HG2	VAL	B	56	-12.944	22.313	19.759	1.00	0.00	H
	ATOM	3613	N	ASN	B	57	-9.004	25.433	19.021	1.00	0.11	N
65	ATOM	3614	CA	ASN	B	57	-7.708	25.802	18.547	1.00	0.11	C
	ATOM	3615	C	ASN	B	57	-7.819	26.255	17.129	1.00	0.11	C
	ATOM	3616	O	ASN	B	57	-7.234	25.657	16.227	1.00	0.11	O
	ATOM	3617	CB	ASN	B	57	-6.662	24.678	18.634	1.00	0.11	C
	ATOM	3618	CG	ASN	B	57	-5.291	25.321	18.470	1.00	0.11	C
70	ATOM	3619	OD1	ASN	B	57	-5.099	26.203	17.634	1.00	0.11	O
	ATOM	3620	ND2	ASN	B	57	-4.310	24.880	19.303	1.00	0.11	N
	ATOM	3621	H	ASN	B	57	-9.361	25.917	19.839	1.00	0.00	H

204

	ATOM	3622	HA	ASN	B	57	-7.598	26.672	19.108	1.00	0.00	H
	ATOM	3623	1HB	ASN	B	57	-6.807	23.906	17.861	1.00	0.00	H
	ATOM	3624	2HB	ASN	B	57	-6.743	24.176	19.613	1.00	0.00	H
5	ATOM	3625	1HD2	ASN	B	57	-4.557	24.208	20.013	1.00	0.00	H
	ATOM	3626	2HD2	ASN	B	57	-3.547	25.508	19.482	1.00	0.00	H
	ATOM	3627	N	ALA	B	58	-8.603	27.326	16.895	1.00	0.21	N
	ATOM	3628	CA	ALA	B	58	-8.722	27.819	15.556	1.00	0.21	C
	ATOM	3629	C	ALA	B	58	-7.341	28.174	15.120	1.00	0.21	C
10	ATOM	3630	O	ALA	B	58	-6.578	28.782	15.870	1.00	0.21	O
	ATOM	3631	CB	ALA	B	58	-9.596	29.081	15.430	1.00	0.21	C
	ATOM	3632	H	ALA	B	58	-9.197	27.733	17.613	1.00	0.00	H
	ATOM	3633	HA	ALA	B	58	-9.154	26.967	15.035	1.00	0.00	H
	ATOM	3634	1HB	ALA	B	58	-9.729	29.336	14.369	1.00	0.00	H
	ATOM	3635	2HB	ALA	B	58	-10.589	28.921	15.874	1.00	0.00	H
15	ATOM	3636	3HB	ALA	B	58	-9.118	29.932	15.936	1.00	0.00	H
	ATOM	3637	N	LYS	B	59	-6.977	27.771	13.889	1.00	0.31	N
	ATOM	3638	CA	LYS	B	59	-5.653	28.014	13.401	1.00	0.31	C
	ATOM	3639	C	LYS	B	59	-5.671	29.201	12.498	1.00	0.31	C
	ATOM	3640	O	LYS	B	59	-6.710	29.812	12.255	1.00	0.31	O
20	ATOM	3641	CB	LYS	B	59	-5.066	26.841	12.597	1.00	0.31	C
	ATOM	3642	CG	LYS	B	59	-4.819	25.592	13.445	1.00	0.31	C
	ATOM	3643	CD	LYS	B	59	-3.812	25.804	14.579	1.00	0.31	C
	ATOM	3644	CE	LYS	B	59	-3.593	24.558	15.443	1.00	0.31	C
	ATOM	3645	NZ	LYS	B	59	-2.607	24.846	16.509	1.00	0.31	N1+
25	ATOM	3646	H	LYS	B	59	-7.667	27.320	13.284	1.00	0.00	H
	ATOM	3647	HA	LYS	B	59	-4.994	28.273	14.243	1.00	0.00	H
	ATOM	3648	1HB	LYS	B	59	-4.188	27.087	11.986	1.00	0.00	H
	ATOM	3649	2HB	LYS	B	59	-5.917	26.508	11.995	1.00	0.00	H
	ATOM	3650	1HG	LYS	B	59	-4.449	24.763	12.824	1.00	0.00	H
30	ATOM	3651	2HG	LYS	B	59	-5.784	25.249	13.863	1.00	0.00	H
	ATOM	3652	1HD	LYS	B	59	-4.154	26.623	15.231	1.00	0.00	H
	ATOM	3653	2HD	LYS	B	59	-2.851	26.124	14.138	1.00	0.00	H
	ATOM	3654	1HE	LYS	B	59	-3.202	23.717	14.846	1.00	0.00	H
	ATOM	3655	2HE	LYS	B	59	-4.527	24.225	15.925	1.00	0.00	H
35	ATOM	3656	1HZ	LYS	B	59	-2.435	24.037	17.091	1.00	0.00	H
	ATOM	3657	2HZ	LYS	B	59	-1.719	25.149	16.136	1.00	0.00	H
	ATOM	3658	3HZ	LYS	B	59	-2.973	25.567	17.120	1.00	0.00	H
	ATOM	3659	N	PHE	B	60	-4.477	29.552	11.983	1.00	0.23	N
	ATOM	3660	CA	PHE	B	60	-4.318	30.638	11.063	1.00	0.23	C
40	ATOM	3661	C	PHE	B	60	-5.095	30.287	9.839	1.00	0.23	C
	ATOM	3662	O	PHE	B	60	-5.704	31.140	9.197	1.00	0.23	O
	ATOM	3663	CB	PHE	B	60	-2.858	30.850	10.632	1.00	0.23	C
	ATOM	3664	CG	PHE	B	60	-2.873	31.832	9.510	1.00	0.23	C
	ATOM	3665	CD1	PHE	B	60	-2.961	33.184	9.748	1.00	0.23	C
45	ATOM	3666	CD2	PHE	B	60	-2.798	31.391	8.208	1.00	0.23	C
	ATOM	3667	CE1	PHE	B	60	-2.977	34.079	8.705	1.00	0.23	C
	ATOM	3668	CE2	PHE	B	60	-2.813	32.282	7.161	1.00	0.23	C
	ATOM	3669	CZ	PHE	B	60	-2.902	33.630	7.409	1.00	0.23	C
	ATOM	3670	H	PHE	B	60	-3.633	29.102	12.295	1.00	0.00	H
50	ATOM	3671	HA	PHE	B	60	-4.520	31.613	11.406	1.00	0.00	H
	ATOM	3672	1HB	PHE	B	60	-2.378	29.909	10.321	1.00	0.00	H
	ATOM	3673	2HB	PHE	B	60	-2.278	31.227	11.490	1.00	0.00	H
	ATOM	3674	HD1	PHE	B	60	-3.027	33.553	10.769	1.00	0.00	H
	ATOM	3675	HD2	PHE	B	60	-2.735	30.326	7.999	1.00	0.00	H
55	ATOM	3676	HE1	PHE	B	60	-3.056	35.145	8.908	1.00	0.00	H
	ATOM	3677	HE2	PHE	B	60	-2.763	31.919	6.138	1.00	0.00	H
	ATOM	3678	HZ	PHE	B	60	-2.922	34.338	6.584	1.00	0.00	H
	ATOM	3679	N	GLU	B	61	-5.095	28.987	9.508	1.00	0.15	N
	ATOM	3680	CA	GLU	B	61	-5.748	28.446	8.354	1.00	0.15	C
60	ATOM	3681	C	GLU	B	61	-7.218	28.714	8.459	1.00	0.15	C
	ATOM	3682	O	GLU	B	61	-7.889	28.938	7.454	1.00	0.15	O
	ATOM	3683	CB	GLU	B	61	-5.528	26.930	8.259	1.00	0.15	C
	ATOM	3684	CG	GLU	B	61	-5.975	26.190	9.522	1.00	0.15	C
	ATOM	3685	CD	GLU	B	61	-5.349	24.803	9.510	1.00	0.15	C
65	ATOM	3686	OE1	GLU	B	61	-5.260	24.199	8.408	1.00	0.15	O
	ATOM	3687	OE2	GLU	B	61	-4.938	24.333	10.605	1.00	0.15	O1-
	ATOM	3688	H	GLU	B	61	-4.636	28.314	10.097	1.00	0.00	H
	ATOM	3689	HA	GLU	B	61	-5.382	28.950	7.445	1.00	0.00	H
	ATOM	3690	1HB	GLU	B	61	-4.456	26.737	8.074	1.00	0.00	H
70	ATOM	3691	2HB	GLU	B	61	-6.074	26.577	7.366	1.00	0.00	H
	ATOM	3692	1HG	GLU	B	61	-7.066	26.116	9.599	1.00	0.00	H

205

	ATOM	3693	2HG	GLU	B	61	-5.569	26.768	10.323	1.00	0.00	H
	ATOM	3694	N	ASP	B	62	-7.751	28.719	9.694	1.00	0.16	N
	ATOM	3695	CA	ASP	B	62	-9.160	28.869	9.932	1.00	0.16	C
5	ATOM	3696	C	ASP	B	62	-9.664	30.184	9.421	1.00	0.16	C
	ATOM	3697	O	ASP	B	62	-10.828	30.280	9.041	1.00	0.16	O
	ATOM	3698	CB	ASP	B	62	-9.539	28.746	11.419	1.00	0.16	C
	ATOM	3699	CG	ASP	B	62	-9.413	27.276	11.797	1.00	0.16	C
	ATOM	3700	OD1	ASP	B	62	-9.136	26.454	10.883	1.00	0.16	O
10	ATOM	3701	OD2	ASP	B	62	-9.605	26.952	13.000	1.00	0.16	O1-
	ATOM	3702	H	ASP	B	62	-7.202	28.495	10.507	1.00	0.00	H
	ATOM	3703	HA	ASP	B	62	-9.712	28.115	9.343	1.00	0.00	H
	ATOM	3704	1HB	ASP	B	62	-10.604	29.018	11.527	1.00	0.00	H
	ATOM	3705	2HB	ASP	B	62	-9.012	29.421	12.095	1.00	0.00	H
15	ATOM	3706	N	SER	B	63	-8.832	31.244	9.415	1.00	0.20	N
	ATOM	3707	CA	SER	B	63	-9.308	32.524	8.962	1.00	0.20	C
	ATOM	3708	C	SER	B	63	-9.869	32.382	7.579	1.00	0.20	C
	ATOM	3709	O	SER	B	63	-9.321	31.677	6.734	1.00	0.20	O
	ATOM	3710	CB	SER	B	63	-8.213	33.604	8.921	1.00	0.20	C
20	ATOM	3711	OG	SER	B	63	-7.222	33.255	7.966	1.00	0.20	O
	ATOM	3712	H	SER	B	63	-7.856	31.085	9.622	1.00	0.00	H
	ATOM	3713	HA	SER	B	63	-10.093	32.837	9.673	1.00	0.00	H
	ATOM	3714	1HB	SER	B	63	-7.772	33.760	9.916	1.00	0.00	H
	ATOM	3715	2HB	SER	B	63	-8.648	34.553	8.584	1.00	0.00	H
	ATOM	3716	HG	SER	B	63	-6.730	32.485	8.307	1.00	0.00	H
25	ATOM	3717	N	GLY	B	64	-11.016	33.050	7.328	1.00	0.22	N
	ATOM	3718	CA	GLY	B	64	-11.651	32.974	6.044	1.00	0.22	C
	ATOM	3719	C	GLY	B	64	-13.081	33.365	6.233	1.00	0.22	C
	ATOM	3720	O	GLY	B	64	-13.461	33.869	7.288	1.00	0.22	O
	ATOM	3721	H	GLY	B	64	-11.410	33.693	8.006	1.00	0.00	H
30	ATOM	3722	1HA	GLY	B	64	-11.495	32.015	5.554	1.00	0.00	H
	ATOM	3723	2HA	GLY	B	64	-11.200	33.716	5.359	1.00	0.00	H
	ATOM	3724	N	GLU	B	65	-13.918	33.138	5.199	1.00	0.19	N
	ATOM	3725	CA	GLU	B	65	-15.307	33.483	5.302	1.00	0.19	C
	ATOM	3726	C	GLU	B	65	-16.074	32.222	5.515	1.00	0.19	C
35	ATOM	3727	O	GLU	B	65	-15.711	31.164	5.000	1.00	0.19	O
	ATOM	3728	CB	GLU	B	65	-15.910	34.122	4.040	1.00	0.19	C
	ATOM	3729	CG	GLU	B	65	-15.403	35.529	3.730	1.00	0.19	C
	ATOM	3730	CD	GLU	B	65	-16.200	36.045	2.539	1.00	0.19	C
40	ATOM	3731	OE1	GLU	B	65	-16.409	35.260	1.575	1.00	0.19	O
	ATOM	3732	OE2	GLU	B	65	-16.625	37.231	2.584	1.00	0.19	O1-
	ATOM	3733	H	GLU	B	65	-13.592	32.750	4.322	1.00	0.00	H
	ATOM	3734	HA	GLU	B	65	-15.418	34.200	6.112	1.00	0.00	H
	ATOM	3735	1HB	GLU	B	65	-16.996	34.170	4.211	1.00	0.00	H
45	ATOM	3736	2HB	GLU	B	65	-15.743	33.449	3.182	1.00	0.00	H
	ATOM	3737	1HG	GLU	B	65	-14.334	35.505	3.473	1.00	0.00	H
	ATOM	3738	2HG	GLU	B	65	-15.576	36.196	4.587	1.00	0.00	H
	ATOM	3739	N	TYR	B	66	-17.164	32.306	6.304	1.00	0.22	N
	ATOM	3740	CA	TYR	B	66	-17.970	31.148	6.549	1.00	0.22	C
	ATOM	3741	C	TYR	B	66	-19.342	31.425	6.020	1.00	0.22	C
50	ATOM	3742	O	TYR	B	66	-19.839	32.548	6.099	1.00	0.22	O
	ATOM	3743	CB	TYR	B	66	-18.124	30.795	8.040	1.00	0.22	C
	ATOM	3744	CG	TYR	B	66	-16.782	30.418	8.567	1.00	0.22	C
	ATOM	3745	CD1	TYR	B	66	-15.918	31.384	9.033	1.00	0.22	C
55	ATOM	3746	CD2	TYR	B	66	-16.382	29.102	8.592	1.00	0.22	C
	ATOM	3747	CE1	TYR	B	66	-14.679	31.041	9.522	1.00	0.22	C
	ATOM	3748	CE2	TYR	B	66	-15.144	28.752	9.078	1.00	0.22	C
	ATOM	3749	CZ	TYR	B	66	-14.291	29.723	9.544	1.00	0.22	C
	ATOM	3750	OH	TYR	B	66	-13.021	29.367	10.044	1.00	0.22	O
60	ATOM	3751	H	TYR	B	66	-17.342	33.146	6.847	1.00	0.00	H
	ATOM	3752	HA	TYR	B	66	-17.532	30.275	6.047	1.00	0.00	H
	ATOM	3753	1HB	TYR	B	66	-18.806	29.929	8.084	1.00	0.00	H
	ATOM	3754	2HB	TYR	B	66	-18.599	31.552	8.651	1.00	0.00	H
	ATOM	3755	HD1	TYR	B	66	-16.191	32.433	9.006	1.00	0.00	H
	ATOM	3756	HD2	TYR	B	66	-17.046	28.325	8.221	1.00	0.00	H
65	ATOM	3757	HE1	TYR	B	66	-13.997	31.799	9.847	1.00	0.00	H
	ATOM	3758	HE2	TYR	B	66	-14.837	27.708	9.090	1.00	0.00	H
	ATOM	3759	HH	TYR	B	66	-12.338	29.749	9.466	1.00	0.00	H
	ATOM	3760	N	LYS	B	67	-19.979	30.391	5.440	1.00	0.45	N
70	ATOM	3761	CA	LYS	B	67	-21.299	30.533	4.900	1.00	0.45	C
	ATOM	3762	C	LYS	B	67	-22.038	29.279	5.238	1.00	0.45	C
	ATOM	3763	O	LYS	B	67	-21.429	28.239	5.482	1.00	0.45	O

206

	ATOM	3764	CB	LYS	B	67	-21.302	30.655	3.371	1.00	0.45	C
	ATOM	3765	CG	LYS	B	67	-20.591	31.913	2.871	1.00	0.45	C
	ATOM	3766	CD	LYS	B	67	-20.205	31.847	1.394	1.00	0.45	C
5	ATOM	3767	CE	LYS	B	67	-18.982	30.964	1.129	1.00	0.45	C
	ATOM	3768	NZ	LYS	B	67	-17.786	31.563	1.761	1.00	0.45	N1+
	ATOM	3769	H	LYS	B	67	-19.578	29.462	5.412	1.00	0.00	H
	ATOM	3770	HA	LYS	B	67	-21.802	31.400	5.361	1.00	0.00	H
	ATOM	3771	1HB	LYS	B	67	-22.349	30.675	3.016	1.00	0.00	H
10	ATOM	3772	2HB	LYS	B	67	-20.856	29.741	2.952	1.00	0.00	H
	ATOM	3773	1HG	LYS	B	67	-19.696	32.152	3.468	1.00	0.00	H
	ATOM	3774	2HG	LYS	B	67	-21.325	32.705	3.088	1.00	0.00	H
	ATOM	3775	1HD	LYS	B	67	-19.999	32.836	0.954	1.00	0.00	H
	ATOM	3776	2HD	LYS	B	67	-21.053	31.439	0.812	1.00	0.00	H
	ATOM	3777	1HE	LYS	B	67	-18.775	30.885	0.049	1.00	0.00	H
15	ATOM	3778	2HE	LYS	B	67	-19.097	29.947	1.529	1.00	0.00	H
	ATOM	3779	1HZ	LYS	B	67	-16.926	31.112	1.480	1.00	0.00	H
	ATOM	3780	2HZ	LYS	B	67	-17.675	32.541	1.507	1.00	0.00	H
	ATOM	3781	3HZ	LYS	B	67	-17.826	31.529	2.772	1.00	0.00	H
20	ATOM	3782	N	CYS	B	68	-23.383	29.354	5.281	1.00	0.52	N
	ATOM	3783	CA	CYS	B	68	-24.163	28.196	5.606	1.00	0.52	C
	ATOM	3784	C	CYS	B	68	-25.428	28.222	4.811	1.00	0.52	C
	ATOM	3785	O	CYS	B	68	-25.970	29.288	4.524	1.00	0.52	O
	ATOM	3786	CB	CYS	B	68	-24.621	28.179	7.065	1.00	0.52	C
	ATOM	3787	SG	CYS	B	68	-25.956	26.981	7.311	1.00	0.52	S
25	ATOM	3788	H	CYS	B	68	-23.896	30.171	5.002	1.00	0.00	H
	ATOM	3789	HA	CYS	B	68	-23.591	27.287	5.374	1.00	0.00	H
	ATOM	3790	1HB	CYS	B	68	-24.992	29.178	7.349	1.00	0.00	H
	ATOM	3791	2HB	CYS	B	68	-23.803	27.921	7.723	1.00	0.00	H
30	ATOM	3792	N	GLN	B	69	-25.931	27.034	4.420	1.00	0.27	N
	ATOM	3793	CA	GLN	B	69	-27.206	27.001	3.771	1.00	0.27	C
	ATOM	3794	C	GLN	B	69	-27.926	25.780	4.234	1.00	0.27	C
	ATOM	3795	O	GLN	B	69	-27.323	24.828	4.727	1.00	0.27	O
	ATOM	3796	CB	GLN	B	69	-27.150	26.927	2.237	1.00	0.27	C
	ATOM	3797	CG	GLN	B	69	-26.530	25.639	1.700	1.00	0.27	C
35	ATOM	3798	CD	GLN	B	69	-26.687	25.656	0.186	1.00	0.27	C
	ATOM	3799	OE1	GLN	B	69	-27.435	26.466	-0.360	1.00	0.27	O
	ATOM	3800	NE2	GLN	B	69	-25.967	24.736	-0.511	1.00	0.27	N
	ATOM	3801	H	GLN	B	69	-25.524	26.151	4.696	1.00	0.00	H
40	ATOM	3802	HA	GLN	B	69	-27.798	27.874	4.081	1.00	0.00	H
	ATOM	3803	1HB	GLN	B	69	-26.598	27.802	1.859	1.00	0.00	H
	ATOM	3804	2HB	GLN	B	69	-28.189	27.025	1.876	1.00	0.00	H
	ATOM	3805	1HG	GLN	B	69	-27.185	24.835	2.029	1.00	0.00	H
	ATOM	3806	2HG	GLN	B	69	-25.497	25.492	2.036	1.00	0.00	H
	ATOM	3807	1HE2	GLN	B	69	-25.235	24.219	-0.068	1.00	0.00	H
45	ATOM	3808	2HE2	GLN	B	69	-25.927	24.943	-1.496	1.00	0.00	H
	ATOM	3809	N	HIS	B	70	-29.263	25.803	4.102	1.00	0.11	N
	ATOM	3810	CA	HIS	B	70	-30.076	24.678	4.443	1.00	0.11	C
	ATOM	3811	C	HIS	B	70	-30.899	24.396	3.237	1.00	0.11	C
	ATOM	3812	O	HIS	B	70	-30.877	25.150	2.267	1.00	0.11	O
50	ATOM	3813	CB	HIS	B	70	-31.043	24.920	5.612	1.00	0.11	C
	ATOM	3814	CG	HIS	B	70	-30.339	24.997	6.930	1.00	0.11	C
	ATOM	3815	ND1	HIS	B	70	-29.937	23.891	7.646	1.00	0.11	N
	ATOM	3816	CD2	HIS	B	70	-29.953	26.075	7.664	1.00	0.11	C
	ATOM	3817	CE1	HIS	B	70	-29.331	24.351	8.768	1.00	0.11	C
55	ATOM	3818	NE2	HIS	B	70	-29.316	25.671	8.824	1.00	0.11	N
	ATOM	3819	H	HIS	B	70	-29.699	26.490	3.501	1.00	0.00	H
	ATOM	3820	HA	HIS	B	70	-29.447	23.799	4.660	1.00	0.00	H
	ATOM	3821	1HB	HIS	B	70	-31.766	24.089	5.657	1.00	0.00	H
	ATOM	3822	2HB	HIS	B	70	-31.637	25.829	5.471	1.00	0.00	H
60	ATOM	3823	HD2	HIS	B	70	-30.099	27.123	7.447	1.00	0.00	H
	ATOM	3824	HE1	HIS	B	70	-29.020	23.707	9.580	1.00	0.00	H
	ATOM	3825	HE2	HIS	B	70	-29.018	26.241	9.593	1.00	0.00	H
	ATOM	3826	N	GLN	B	71	-31.625	23.266	3.251	1.00	0.12	N
	ATOM	3827	CA	GLN	B	71	-32.441	22.954	2.121	1.00	0.12	C
65	ATOM	3828	C	GLN	B	71	-33.468	24.032	2.009	1.00	0.12	C
	ATOM	3829	O	GLN	B	71	-33.753	24.525	0.920	1.00	0.12	O
	ATOM	3830	CB	GLN	B	71	-33.197	21.623	2.276	1.00	0.12	C
	ATOM	3831	CG	GLN	B	71	-32.304	20.379	2.279	1.00	0.12	C
	ATOM	3832	CD	GLN	B	71	-31.895	20.083	0.843	1.00	0.12	C
70	ATOM	3833	OE1	GLN	B	71	-32.123	20.883	-0.063	1.00	0.12	O
	ATOM	3834	NE2	GLN	B	71	-31.272	18.896	0.623	1.00	0.12	N

207

	ATOM	3835	H	GLN	B	71	-31.669	22.648	4.050	1.00	0.00	H
	ATOM	3836	HA	GLN	B	71	-31.834	22.977	1.204	1.00	0.00	H
	ATOM	3837	1HB	GLN	B	71	-33.962	21.545	1.481	1.00	0.00	H
5	ATOM	3838	2HB	GLN	B	71	-33.758	21.654	3.225	1.00	0.00	H
	ATOM	3839	1HG	GLN	B	71	-32.874	19.519	2.668	1.00	0.00	H
	ATOM	3840	2HG	GLN	B	71	-31.411	20.534	2.901	1.00	0.00	H
	ATOM	3841	1HE2	GLN	B	71	-31.125	18.252	1.392	1.00	0.00	H
	ATOM	3842	2HE2	GLN	B	71	-31.056	18.634	-0.322	1.00	0.00	H
10	ATOM	3843	N	GLN	B	72	-34.046	24.426	3.157	1.00	0.21	N
	ATOM	3844	CA	GLN	B	72	-35.117	25.377	3.188	1.00	0.21	C
	ATOM	3845	C	GLN	B	72	-34.660	26.737	2.761	1.00	0.21	C
	ATOM	3846	O	GLN	B	72	-35.308	27.383	1.940	1.00	0.21	O
	ATOM	3847	CB	GLN	B	72	-35.698	25.546	4.602	1.00	0.21	C
15	ATOM	3848	CG	GLN	B	72	-36.104	24.222	5.252	1.00	0.21	C
	ATOM	3849	CD	GLN	B	72	-37.057	23.494	4.316	1.00	0.21	C
	ATOM	3850	OE1	GLN	B	72	-37.630	24.082	3.400	1.00	0.21	O
	ATOM	3851	NE2	GLN	B	72	-37.224	22.165	4.547	1.00	0.21	N
20	ATOM	3852	H	GLN	B	72	-33.776	24.011	4.029	1.00	0.00	H
	ATOM	3853	HA	GLN	B	72	-35.857	25.085	2.433	1.00	0.00	H
	ATOM	3854	1HB	GLN	B	72	-36.568	26.218	4.507	1.00	0.00	H
	ATOM	3855	2HB	GLN	B	72	-34.952	26.056	5.225	1.00	0.00	H
	ATOM	3856	1HG	GLN	B	72	-36.614	24.285	6.211	1.00	0.00	H
	ATOM	3857	2HG	GLN	B	72	-35.212	23.596	5.418	1.00	0.00	H
25	ATOM	3858	1HE2	GLN	B	72	-36.791	21.725	5.340	1.00	0.00	H
	ATOM	3859	2HE2	GLN	B	72	-37.890	21.689	3.966	1.00	0.00	H
	ATOM	3860	N	VAL	B	73	-33.516	27.206	3.298	1.00	0.31	N
	ATOM	3861	CA	VAL	B	73	-33.130	28.569	3.072	1.00	0.31	C
	ATOM	3862	C	VAL	B	73	-32.145	28.702	1.959	1.00	0.31	C
30	ATOM	3863	O	VAL	B	73	-31.658	27.727	1.388	1.00	0.31	O
	ATOM	3864	CB	VAL	B	73	-32.521	29.216	4.283	1.00	0.31	C
	ATOM	3865	CG1	VAL	B	73	-33.583	29.264	5.395	1.00	0.31	C
	ATOM	3866	CG2	VAL	B	73	-31.247	28.442	4.666	1.00	0.31	C
	ATOM	3867	H	VAL	B	73	-32.902	26.625	3.835	1.00	0.00	H
35	ATOM	3868	HA	VAL	B	73	-34.032	29.136	2.786	1.00	0.00	H
	ATOM	3869	HB	VAL	B	73	-32.166	30.225	4.101	1.00	0.00	H
	ATOM	3870	1HG1	VAL	B	73	-33.219	29.820	6.275	1.00	0.00	H
	ATOM	3871	2HG1	VAL	B	73	-34.505	29.762	5.053	1.00	0.00	H
	ATOM	3872	3HG1	VAL	B	73	-33.855	28.254	5.740	1.00	0.00	H
40	ATOM	3873	1HG2	VAL	B	73	-31.260	28.169	5.729	1.00	0.00	H
	ATOM	3874	2HG2	VAL	B	73	-31.174	27.490	4.129	1.00	0.00	H
	ATOM	3875	3HG2	VAL	B	73	-30.331	28.965	4.407	1.00	0.00	H
	ATOM	3876	N	ASN	B	74	-31.857	29.979	1.634	1.00	0.41	N
	ATOM	3877	CA	ASN	B	74	-30.932	30.413	0.630	1.00	0.41	C
45	ATOM	3878	C	ASN	B	74	-29.580	30.362	1.270	1.00	0.41	C
	ATOM	3879	O	ASN	B	74	-29.409	29.751	2.322	1.00	0.41	O
	ATOM	3880	CB	ASN	B	74	-31.202	31.869	0.200	1.00	0.41	C
	ATOM	3881	CG	ASN	B	74	-30.458	32.179	-1.090	1.00	0.41	C
	ATOM	3882	OD1	ASN	B	74	-29.812	31.313	-1.676	1.00	0.41	O
50	ATOM	3883	ND2	ASN	B	74	-30.542	33.459	-1.542	1.00	0.41	N
	ATOM	3884	H	ASN	B	74	-32.331	30.717	2.145	1.00	0.00	H
	ATOM	3885	HA	ASN	B	74	-30.976	29.713	-0.222	1.00	0.00	H
	ATOM	3886	1HB	ASN	B	74	-30.921	32.561	1.004	1.00	0.00	H
	ATOM	3887	2HB	ASN	B	74	-32.278	32.002	-0.003	1.00	0.00	H
55	ATOM	3888	1HD2	ASN	B	74	-30.976	34.179	-0.997	1.00	0.00	H
	ATOM	3889	2HD2	ASN	B	74	-29.971	33.687	-2.339	1.00	0.00	H
	ATOM	3890	N	GLU	B	75	-28.567	30.970	0.622	1.00	0.48	N
	ATOM	3891	CA	GLU	B	75	-27.249	31.003	1.180	1.00	0.48	C
	ATOM	3892	C	GLU	B	75	-27.241	32.069	2.228	1.00	0.48	C
60	ATOM	3893	O	GLU	B	75	-27.925	33.085	2.100	1.00	0.48	O
	ATOM	3894	CB	GLU	B	75	-26.170	31.366	0.145	1.00	0.48	C
	ATOM	3895	CG	GLU	B	75	-26.047	30.340	-0.982	1.00	0.48	C
	ATOM	3896	CD	GLU	B	75	-25.367	29.103	-0.418	1.00	0.48	C
	ATOM	3897	OE1	GLU	B	75	-24.699	29.229	0.643	1.00	0.48	O
65	ATOM	3898	OE2	GLU	B	75	-25.503	28.015	-1.039	1.00	0.48	O1-
	ATOM	3899	H	GLU	B	75	-28.657	31.252	-0.347	1.00	0.00	H
	ATOM	3900	HA	GLU	B	75	-27.017	30.019	1.621	1.00	0.00	H
	ATOM	3901	1HB	GLU	B	75	-25.207	31.519	0.665	1.00	0.00	H
	ATOM	3902	2HB	GLU	B	75	-26.423	32.357	-0.272	1.00	0.00	H
70	ATOM	3903	1HG	GLU	B	75	-25.416	30.732	-1.797	1.00	0.00	H
	ATOM	3904	2HG	GLU	B	75	-27.009	30.079	-1.450	1.00	0.00	H
	ATOM	3905	N	SER	B	76	-26.469	31.848	3.309	1.00	0.42	N

208

	ATOM	3906	CA	SER	B	76	-26.382	32.800	4.377	1.00	0.42	C
	ATOM	3907	C	SER	B	76	-25.336	33.802	4.009	1.00	0.42	C
	ATOM	3908	O	SER	B	76	-24.507	33.553	3.136	1.00	0.42	O
5	ATOM	3909	CB	SER	B	76	-25.956	32.162	5.710	1.00	0.42	C
	ATOM	3910	OG	SER	B	76	-25.873	33.153	6.720	1.00	0.42	O
	ATOM	3911	H	SER	B	76	-26.027	30.945	3.444	1.00	0.00	H
	ATOM	3912	HA	SER	B	76	-27.347	33.318	4.497	1.00	0.00	H
	ATOM	3913	1HB	SER	B	76	-24.918	31.818	5.529	1.00	0.00	H
10	ATOM	3914	2HB	SER	B	76	-26.368	31.266	6.179	1.00	0.00	H
	ATOM	3915	HG	SER	B	76	-25.076	33.682	6.522	1.00	0.00	H
	ATOM	3916	N	GLU	B	77	-25.365	34.985	4.660	1.00	0.31	N
	ATOM	3917	CA	GLU	B	77	-24.357	35.963	4.380	1.00	0.31	C
	ATOM	3918	C	GLU	B	77	-23.106	35.440	4.998	1.00	0.31	C
15	ATOM	3919	O	GLU	B	77	-23.138	34.721	5.994	1.00	0.31	O
	ATOM	3920	CB	GLU	B	77	-24.596	37.339	5.023	1.00	0.31	C
	ATOM	3921	CG	GLU	B	77	-25.878	38.032	4.571	1.00	0.31	C
	ATOM	3922	CD	GLU	B	77	-26.987	37.538	5.483	1.00	0.31	C
	ATOM	3923	OE1	GLU	B	77	-26.707	37.359	6.699	1.00	0.31	O
20	ATOM	3924	OE2	GLU	B	77	-28.123	37.331	4.981	1.00	0.31	O1-
	ATOM	3925	H	GLU	B	77	-26.107	35.274	5.290	1.00	0.00	H
	ATOM	3926	HA	GLU	B	77	-24.351	36.141	3.293	1.00	0.00	H
	ATOM	3927	1HB	GLU	B	77	-23.730	37.950	4.704	1.00	0.00	H
	ATOM	3928	2HB	GLU	B	77	-24.496	37.287	6.121	1.00	0.00	H
	ATOM	3929	1HG	GLU	B	77	-26.103	37.866	3.506	1.00	0.00	H
25	ATOM	3930	2HG	GLU	B	77	-25.778	39.121	4.715	1.00	0.00	H
	ATOM	3931	N	PRO	B	78	-22.004	35.772	4.398	1.00	0.29	N
	ATOM	3932	CA	PRO	B	78	-20.764	35.287	4.932	1.00	0.29	C
	ATOM	3933	C	PRO	B	78	-20.323	36.023	6.154	1.00	0.29	C
30	ATOM	3934	O	PRO	B	78	-20.684	37.187	6.323	1.00	0.29	O
	ATOM	3935	CB	PRO	B	78	-19.756	35.357	3.788	1.00	0.29	C
	ATOM	3936	CG	PRO	B	78	-20.627	35.223	2.527	1.00	0.29	C
	ATOM	3937	CD	PRO	B	78	-21.979	35.824	2.944	1.00	0.29	C
	ATOM	3938	HA	PRO	B	78	-20.930	34.229	5.154	1.00	0.00	H
35	ATOM	3939	1HB	PRO	B	78	-18.975	34.595	3.881	1.00	0.00	H
	ATOM	3940	2HB	PRO	B	78	-19.253	36.340	3.777	1.00	0.00	H
	ATOM	3941	1HG	PRO	B	78	-20.743	34.219	2.155	1.00	0.00	H
	ATOM	3942	2HG	PRO	B	78	-20.192	35.781	1.679	1.00	0.00	H
	ATOM	3943	1HD	PRO	B	78	-22.062	36.874	2.622	1.00	0.00	H
40	ATOM	3944	2HD	PRO	B	78	-22.791	35.253	2.482	1.00	0.00	H
	ATOM	3945	N	VAL	B	79	-19.557	35.337	7.022	1.00	0.31	N
	ATOM	3946	CA	VAL	B	79	-18.978	35.931	8.187	1.00	0.31	C
	ATOM	3947	C	VAL	B	79	-17.507	35.760	8.006	1.00	0.31	C
	ATOM	3948	O	VAL	B	79	-17.055	34.693	7.593	1.00	0.31	O
45	ATOM	3949	CB	VAL	B	79	-19.362	35.248	9.465	1.00	0.31	C
	ATOM	3950	CG1	VAL	B	79	-18.925	33.776	9.386	1.00	0.31	C
	ATOM	3951	CG2	VAL	B	79	-18.732	36.018	10.638	1.00	0.31	C
	ATOM	3952	H	VAL	B	79	-19.361	34.360	6.860	1.00	0.00	H
	ATOM	3953	HA	VAL	B	79	-19.257	36.997	8.216	1.00	0.00	H
50	ATOM	3954	HB	VAL	B	79	-20.462	35.289	9.567	1.00	0.00	H
	ATOM	3955	1HG1	VAL	B	79	-19.391	33.205	10.210	1.00	0.00	H
	ATOM	3956	2HG1	VAL	B	79	-19.283	33.319	8.460	1.00	0.00	H
	ATOM	3957	3HG1	VAL	B	79	-17.846	33.643	9.523	1.00	0.00	H
	ATOM	3958	1HG2	VAL	B	79	-19.088	35.629	11.607	1.00	0.00	H
55	ATOM	3959	2HG2	VAL	B	79	-17.634	35.926	10.652	1.00	0.00	H
	ATOM	3960	3HG2	VAL	B	79	-18.990	37.090	10.606	1.00	0.00	H
	ATOM	3961	N	TYR	B	80	-16.709	36.805	8.294	1.00	0.19	N
	ATOM	3962	CA	TYR	B	80	-15.305	36.638	8.067	1.00	0.19	C
	ATOM	3963	C	TYR	B	80	-14.649	36.465	9.394	1.00	0.19	C
60	ATOM	3964	O	TYR	B	80	-14.925	37.197	10.343	1.00	0.19	O
	ATOM	3965	CB	TYR	B	80	-14.628	37.826	7.359	1.00	0.19	C
	ATOM	3966	CG	TYR	B	80	-13.244	37.390	7.018	1.00	0.19	C
	ATOM	3967	CD1	TYR	B	80	-12.214	37.522	7.921	1.00	0.19	C
	ATOM	3968	CD2	TYR	B	80	-12.983	36.837	5.785	1.00	0.19	C
65	ATOM	3969	CE1	TYR	B	80	-10.942	37.112	7.597	1.00	0.19	C
	ATOM	3970	CE2	TYR	B	80	-11.714	36.425	5.454	1.00	0.19	C
	ATOM	3971	CZ	TYR	B	80	-10.692	36.565	6.360	1.00	0.19	C
	ATOM	3972	OH	TYR	B	80	-9.387	36.143	6.025	1.00	0.19	O
	ATOM	3973	H	TYR	B	80	-17.008	37.682	8.682	1.00	0.00	H
70	ATOM	3974	HA	TYR	B	80	-15.133	35.776	7.415	1.00	0.00	H
	ATOM	3975	1HB	TYR	B	80	-14.633	38.725	7.994	1.00	0.00	H
	ATOM	3976	2HB	TYR	B	80	-15.197	38.081	6.450	1.00	0.00	H

209

	ATOM	3977	HD1	TYR	B	80	-12.423	37.965	8.890	1.00	0.00	H
	ATOM	3978	HD2	TYR	B	80	-13.756	36.817	5.036	1.00	0.00	H
	ATOM	3979	HE1	TYR	B	80	-10.137	37.169	8.309	1.00	0.00	H
	ATOM	3980	HE2	TYR	B	80	-11.519	36.016	4.465	1.00	0.00	H
5	ATOM	3981	HH	TYR	B	80	-8.978	35.822	6.837	1.00	0.00	H
	ATOM	3982	N	LEU	B	81	-13.760	35.460	9.490	1.00	0.08	N
	ATOM	3983	CA	LEU	B	81	-13.094	35.195	10.729	1.00	0.08	C
	ATOM	3984	C	LEU	B	81	-11.635	35.443	10.529	1.00	0.08	C
	ATOM	3985	O	LEU	B	81	-11.076	35.109	9.485	1.00	0.08	O
10	ATOM	3986	CB	LEU	B	81	-13.250	33.736	11.191	1.00	0.08	C
	ATOM	3987	CG	LEU	B	81	-12.542	33.429	12.522	1.00	0.08	C
	ATOM	3988	CD1	LEU	B	81	-13.157	34.234	13.678	1.00	0.08	C
	ATOM	3989	CD2	LEU	B	81	-12.505	31.918	12.800	1.00	0.08	C
	ATOM	3990	H	LEU	B	81	-13.530	34.870	8.697	1.00	0.00	H
15	ATOM	3991	HA	LEU	B	81	-13.489	35.875	11.494	1.00	0.00	H
	ATOM	3992	1HB	LEU	B	81	-12.768	33.124	10.414	1.00	0.00	H
	ATOM	3993	2HB	LEU	B	81	-14.319	33.473	11.257	1.00	0.00	H
	ATOM	3994	HG	LEU	B	81	-11.483	33.725	12.421	1.00	0.00	H
	ATOM	3995	1HD1	LEU	B	81	-12.405	34.520	14.427	1.00	0.00	H
20	ATOM	3996	2HD1	LEU	B	81	-13.691	35.135	13.359	1.00	0.00	H
	ATOM	3997	3HD1	LEU	B	81	-13.915	33.631	14.207	1.00	0.00	H
	ATOM	3998	1HD2	LEU	B	81	-11.952	31.695	13.726	1.00	0.00	H
	ATOM	3999	2HD2	LEU	B	81	-13.519	31.498	12.903	1.00	0.00	H
	ATOM	4000	3HD2	LEU	B	81	-12.001	31.377	11.982	1.00	0.00	H
25	ATOM	4001	N	GLU	B	82	-10.987	36.068	11.529	1.00	0.09	N
	ATOM	4002	CA	GLU	B	82	-9.582	36.329	11.444	1.00	0.09	C
	ATOM	4003	C	GLU	B	82	-8.969	35.717	12.660	1.00	0.09	C
	ATOM	4004	O	GLU	B	82	-9.443	35.926	13.776	1.00	0.09	O
	ATOM	4005	CB	GLU	B	82	-9.250	37.831	11.486	1.00	0.09	C
30	ATOM	4006	CG	GLU	B	82	-9.774	38.615	10.282	1.00	0.09	C
	ATOM	4007	CD	GLU	B	82	-9.587	40.099	10.568	1.00	0.09	C
	ATOM	4008	OE1	GLU	B	82	-8.557	40.458	11.201	1.00	0.09	O
	ATOM	4009	OE2	GLU	B	82	-10.477	40.894	10.166	1.00	0.09	O1-
	ATOM	4010	H	GLU	B	82	-11.437	36.370	12.385	1.00	0.00	H
35	ATOM	4011	HA	GLU	B	82	-9.165	35.902	10.521	1.00	0.00	H
	ATOM	4012	1HB	GLU	B	82	-8.149	37.899	11.523	1.00	0.00	H
	ATOM	4013	2HB	GLU	B	82	-9.643	38.266	12.420	1.00	0.00	H
	ATOM	4014	1HG	GLU	B	82	-10.829	38.415	10.073	1.00	0.00	H
	ATOM	4015	2HG	GLU	B	82	-9.148	38.392	9.408	1.00	0.00	H
40	ATOM	4016	N	VAL	B	83	-7.896	34.930	12.476	1.00	0.09	N
	ATOM	4017	CA	VAL	B	83	-7.263	34.328	13.611	1.00	0.09	C
	ATOM	4018	C	VAL	B	83	-5.907	34.938	13.711	1.00	0.09	C
	ATOM	4019	O	VAL	B	83	-5.239	35.146	12.700	1.00	0.09	O
	ATOM	4020	CB	VAL	B	83	-7.069	32.850	13.470	1.00	0.09	C
45	ATOM	4021	CG1	VAL	B	83	-8.451	32.182	13.377	1.00	0.09	C
	ATOM	4022	CG2	VAL	B	83	-6.170	32.598	12.250	1.00	0.09	C
	ATOM	4023	H	VAL	B	83	-7.390	34.867	11.611	1.00	0.00	H
	ATOM	4024	HA	VAL	B	83	-7.846	34.520	14.521	1.00	0.00	H
	ATOM	4025	HB	VAL	B	83	-6.558	32.481	14.379	1.00	0.00	H
50	ATOM	4026	1HG1	VAL	B	83	-8.397	31.094	13.515	1.00	0.00	H
	ATOM	4027	2HG1	VAL	B	83	-9.129	32.558	14.160	1.00	0.00	H
	ATOM	4028	3HG1	VAL	B	83	-8.933	32.369	12.403	1.00	0.00	H
	ATOM	4029	1HG2	VAL	B	83	-6.508	31.805	11.601	1.00	0.00	H
	ATOM	4030	2HG2	VAL	B	83	-6.129	33.419	11.520	1.00	0.00	H
55	ATOM	4031	3HG2	VAL	B	83	-5.180	32.524	12.716	1.00	0.00	H
	ATOM	4032	N	PHE	B	84	-5.469	35.260	14.943	1.00	0.23	N
	ATOM	4033	CA	PHE	B	84	-4.182	35.872	15.076	1.00	0.23	C
	ATOM	4034	C	PHE	B	84	-3.459	35.119	16.138	1.00	0.23	C
	ATOM	4035	O	PHE	B	84	-4.077	34.442	16.959	1.00	0.23	O
60	ATOM	4036	CB	PHE	B	84	-4.229	37.314	15.606	1.00	0.23	C
	ATOM	4037	CG	PHE	B	84	-5.215	38.093	14.810	1.00	0.23	C
	ATOM	4038	CD1	PHE	B	84	-4.889	38.632	13.590	1.00	0.23	C
	ATOM	4039	CD2	PHE	B	84	-6.487	38.271	15.293	1.00	0.23	C
	ATOM	4040	CE1	PHE	B	84	-5.814	39.344	12.865	1.00	0.23	C
65	ATOM	4041	CE2	PHE	B	84	-7.414	38.983	14.572	1.00	0.23	C
	ATOM	4042	CZ	PHE	B	84	-7.081	39.525	13.357	1.00	0.23	C
	ATOM	4043	H	PHE	B	84	-6.045	35.205	15.777	1.00	0.00	H
	ATOM	4044	HA	PHE	B	84	-3.619	35.831	14.132	1.00	0.00	H
	ATOM	4045	1HB	PHE	B	84	-3.221	37.757	15.548	1.00	0.00	H
70	ATOM	4046	2HB	PHE	B	84	-4.503	37.318	16.673	1.00	0.00	H
	ATOM	4047	HD1	PHE	B	84	-3.881	38.507	13.203	1.00	0.00	H

210

	ATOM	4048	HD2	PHE	B	84	-6.776	37.774	16.212	1.00	0.00	H
	ATOM	4049	HE1	PHE	B	84	-5.532	39.800	11.919	1.00	0.00	H
	ATOM	4050	HE2	PHE	B	84	-8.434	38.672	14.642	1.00	0.00	H
5	ATOM	4051	HZ	PHE	B	84	-7.738	40.278	13.011	1.00	0.00	H
	ATOM	4052	N	SER	B	85	-2.115	35.187	16.131	1.00	0.34	N
	ATOM	4053	CA	SER	B	85	-1.395	34.574	17.204	1.00	0.34	C
	ATOM	4054	C	SER	B	85	-0.673	35.676	17.915	1.00	0.34	C
	ATOM	4055	O	SER	B	85	0.388	36.126	17.488	1.00	0.34	O
10	ATOM	4056	CB	SER	B	85	-0.370	33.520	16.748	1.00	0.34	C
	ATOM	4057	OG	SER	B	85	0.610	34.106	15.906	1.00	0.34	O
	ATOM	4058	H	SER	B	85	-1.592	35.821	15.547	1.00	0.00	H
	ATOM	4059	HA	SER	B	85	-2.077	34.071	17.905	1.00	0.00	H
	ATOM	4060	1HB	SER	B	85	-0.858	32.718	16.180	1.00	0.00	H
	ATOM	4061	2HB	SER	B	85	0.105	33.091	17.647	1.00	0.00	H
15	ATOM	4062	HG	SER	B	85	0.896	34.924	16.364	1.00	0.00	H
	ATOM	4063	N	ASP	B	86	-1.255	36.148	19.032	1.00	0.23	N
	ATOM	4064	CA	ASP	B	86	-0.646	37.204	19.785	1.00	0.23	C
	ATOM	4065	C	ASP	B	86	-0.958	36.941	21.219	1.00	0.23	C
	ATOM	4066	O	ASP	B	86	-1.850	36.156	21.535	1.00	0.23	O
20	ATOM	4067	CB	ASP	B	86	-1.209	38.597	19.458	1.00	0.23	C
	ATOM	4068	CG	ASP	B	86	-0.750	38.977	18.058	1.00	0.23	C
	ATOM	4069	OD1	ASP	B	86	0.436	38.705	17.730	1.00	0.23	O
	ATOM	4070	OD2	ASP	B	86	-1.581	39.538	17.294	1.00	0.23	O1-
	ATOM	4071	H	ASP	B	86	-2.098	35.791	19.438	1.00	0.00	H
25	ATOM	4072	HA	ASP	B	86	0.450	37.190	19.655	1.00	0.00	H
	ATOM	4073	1HB	ASP	B	86	-0.728	39.310	20.149	1.00	0.00	H
	ATOM	4074	2HB	ASP	B	86	-2.265	38.846	19.445	1.00	0.00	H
	ATOM	4075	N	TRP	B	87	-0.199	37.567	22.136	1.00	0.14	N
	ATOM	4076	CA	TRP	B	87	-0.482	37.366	23.524	1.00	0.14	C
30	ATOM	4077	C	TRP	B	87	-1.782	37.995	23.895	1.00	0.14	C
	ATOM	4078	O	TRP	B	87	-2.587	37.390	24.598	1.00	0.14	O
	ATOM	4079	CB	TRP	B	87	0.603	37.882	24.479	1.00	0.14	C
	ATOM	4080	CG	TRP	B	87	1.760	36.923	24.577	1.00	0.14	C
35	ATOM	4081	CD1	TRP	B	87	3.025	36.993	24.074	1.00	0.14	C
	ATOM	4082	CD2	TRP	B	87	1.660	35.660	25.254	1.00	0.14	C
	ATOM	4083	NE1	TRP	B	87	3.722	35.852	24.401	1.00	0.14	N
	ATOM	4084	CE2	TRP	B	87	2.892	35.022	25.126	1.00	0.14	C
	ATOM	4085	CE3	TRP	B	87	0.621	35.080	25.924	1.00	0.14	C
	ATOM	4086	CZ2	TRP	B	87	3.106	33.786	25.670	1.00	0.14	C
40	ATOM	4087	CZ3	TRP	B	87	0.839	33.837	26.474	1.00	0.14	C
	ATOM	4088	CH2	TRP	B	87	2.058	33.201	26.350	1.00	0.14	C
	ATOM	4089	H	TRP	B	87	0.548	38.189	21.872	1.00	0.00	H
	ATOM	4090	HA	TRP	B	87	-0.614	36.285	23.692	1.00	0.00	H
45	ATOM	4091	1HB	TRP	B	87	0.152	37.992	25.482	1.00	0.00	H
	ATOM	4092	2HB	TRP	B	87	0.938	38.892	24.197	1.00	0.00	H
	ATOM	4093	HD1	TRP	B	87	3.478	37.795	23.504	1.00	0.00	H
	ATOM	4094	HE1	TRP	B	87	4.680	35.678	24.202	1.00	0.00	H
	ATOM	4095	HE3	TRP	B	87	-0.335	35.580	26.045	1.00	0.00	H
	ATOM	4096	HZ2	TRP	B	87	4.070	33.292	25.578	1.00	0.00	H
50	ATOM	4097	HZ3	TRP	B	87	0.071	33.373	27.066	1.00	0.00	H
	ATOM	4098	HH2	TRP	B	87	2.209	32.237	26.826	1.00	0.00	H
	ATOM	4099	N	LEU	B	88	-2.035	39.229	23.423	1.00	0.12	N
	ATOM	4100	CA	LEU	B	88	-3.244	39.894	23.818	1.00	0.12	C
	ATOM	4101	C	LEU	B	88	-3.845	40.527	22.607	1.00	0.12	C
55	ATOM	4102	O	LEU	B	88	-3.126	40.978	21.717	1.00	0.12	O
	ATOM	4103	CB	LEU	B	88	-2.988	41.028	24.827	1.00	0.12	C
	ATOM	4104	CG	LEU	B	88	-4.252	41.777	25.294	1.00	0.12	C
	ATOM	4105	CD1	LEU	B	88	-5.169	40.882	26.135	1.00	0.12	C
	ATOM	4106	CD2	LEU	B	88	-3.893	43.089	26.012	1.00	0.12	C
60	ATOM	4107	H	LEU	B	88	-1.477	39.686	22.720	1.00	0.00	H
	ATOM	4108	HA	LEU	B	88	-3.946	39.167	24.244	1.00	0.00	H
	ATOM	4109	1HB	LEU	B	88	-2.285	41.747	24.367	1.00	0.00	H
	ATOM	4110	2HB	LEU	B	88	-2.468	40.616	25.711	1.00	0.00	H
	ATOM	4111	HG	LEU	B	88	-4.825	42.096	24.412	1.00	0.00	H
65	ATOM	4112	1HD1	LEU	B	88	-6.215	40.971	25.827	1.00	0.00	H
	ATOM	4113	2HD1	LEU	B	88	-4.833	39.841	26.171	1.00	0.00	H
	ATOM	4114	3HD1	LEU	B	88	-5.149	41.201	27.192	1.00	0.00	H
	ATOM	4115	1HD2	LEU	B	88	-4.793	43.673	26.263	1.00	0.00	H
	ATOM	4116	2HD2	LEU	B	88	-3.348	42.897	26.951	1.00	0.00	H
70	ATOM	4117	3HD2	LEU	B	88	-3.245	43.720	25.387	1.00	0.00	H
	ATOM	4118	N	LEU	B	89	-5.192	40.561	22.535	1.00	0.11	N

211

	ATOM	4119	CA	LEU	B	89	-5.817	41.207	21.418	1.00	0.11	C
	ATOM	4120	C	LEU	B	89	-7.020	41.926	21.934	1.00	0.11	C
	ATOM	4121	O	LEU	B	89	-7.608	41.536	22.942	1.00	0.11	O
5	ATOM	4122	CB	LEU	B	89	-6.316	40.242	20.325	1.00	0.11	C
	ATOM	4123	CG	LEU	B	89	-6.996	40.936	19.129	1.00	0.11	C
	ATOM	4124	CD1	LEU	B	89	-6.001	41.822	18.356	1.00	0.11	C
	ATOM	4125	CD2	LEU	B	89	-7.712	39.917	18.228	1.00	0.11	C
	ATOM	4126	H	LEU	B	89	-5.791	40.201	23.266	1.00	0.00	H
10	ATOM	4127	HA	LEU	B	89	-5.075	41.763	20.868	1.00	0.00	H
	ATOM	4128	1HB	LEU	B	89	-7.014	39.506	20.758	1.00	0.00	H
	ATOM	4129	2HB	LEU	B	89	-5.451	39.693	19.917	1.00	0.00	H
	ATOM	4130	HG	LEU	B	89	-7.828	41.548	19.479	1.00	0.00	H
	ATOM	4131	1HD1	LEU	B	89	-6.459	42.253	17.451	1.00	0.00	H
	ATOM	4132	2HD1	LEU	B	89	-5.641	42.666	18.958	1.00	0.00	H
15	ATOM	4133	3HD1	LEU	B	89	-5.126	41.235	18.030	1.00	0.00	H
	ATOM	4134	1HD2	LEU	B	89	-8.142	40.512	17.418	1.00	0.00	H
	ATOM	4135	2HD2	LEU	B	89	-7.007	39.183	17.817	1.00	0.00	H
	ATOM	4136	3HD2	LEU	B	89	-8.511	39.382	18.761	1.00	0.00	H
20	ATOM	4137	N	LEU	B	90	-7.400	43.026	21.259	1.00	0.11	N
	ATOM	4138	CA	LEU	B	90	-8.597	43.700	21.649	1.00	0.11	C
	ATOM	4139	C	LEU	B	90	-9.606	43.186	20.677	1.00	0.11	C
	ATOM	4140	O	LEU	B	90	-9.404	43.266	19.467	1.00	0.11	O
	ATOM	4141	CB	LEU	B	90	-8.527	45.232	21.510	1.00	0.11	C
25	ATOM	4142	CG	LEU	B	90	-9.818	45.948	21.950	1.00	0.11	C
	ATOM	4143	CD1	LEU	B	90	-10.083	45.729	23.448	1.00	0.11	C
	ATOM	4144	CD2	LEU	B	90	-9.793	47.437	21.568	1.00	0.11	C
	ATOM	4145	H	LEU	B	90	-6.910	43.370	20.450	1.00	0.00	H
	ATOM	4146	HA	LEU	B	90	-8.843	43.446	22.688	1.00	0.00	H
30	ATOM	4147	1HB	LEU	B	90	-8.289	45.492	20.463	1.00	0.00	H
	ATOM	4148	2HB	LEU	B	90	-7.683	45.608	22.117	1.00	0.00	H
	ATOM	4149	HG	LEU	B	90	-10.652	45.497	21.379	1.00	0.00	H
	ATOM	4150	1HD1	LEU	B	90	-11.099	45.356	23.615	1.00	0.00	H
	ATOM	4151	2HD1	LEU	B	90	-9.407	44.997	23.914	1.00	0.00	H
35	ATOM	4152	3HD1	LEU	B	90	-9.921	46.663	24.002	1.00	0.00	H
	ATOM	4153	1HD2	LEU	B	90	-10.779	47.894	21.677	1.00	0.00	H
	ATOM	4154	2HD2	LEU	B	90	-9.068	47.981	22.192	1.00	0.00	H
	ATOM	4155	3HD2	LEU	B	90	-9.494	47.554	20.513	1.00	0.00	H
	ATOM	4156	N	GLN	B	91	-10.719	42.628	21.185	1.00	0.11	N
40	ATOM	4157	CA	GLN	B	91	-11.640	41.998	20.289	1.00	0.11	C
	ATOM	4158	C	GLN	B	91	-12.857	42.848	20.152	1.00	0.11	C
	ATOM	4159	O	GLN	B	91	-13.277	43.520	21.093	1.00	0.11	O
	ATOM	4160	CB	GLN	B	91	-12.096	40.612	20.782	1.00	0.11	C
	ATOM	4161	CG	GLN	B	91	-10.956	39.593	20.886	1.00	0.11	C
45	ATOM	4162	CD	GLN	B	91	-11.531	38.284	21.415	1.00	0.11	C
	ATOM	4163	OE1	GLN	B	91	-12.410	38.286	22.275	1.00	0.11	O
	ATOM	4164	NE2	GLN	B	91	-11.026	37.136	20.890	1.00	0.11	N
	ATOM	4165	H	GLN	B	91	-10.874	42.521	22.183	1.00	0.00	H
	ATOM	4166	HA	GLN	B	91	-11.163	41.837	19.308	1.00	0.00	H
50	ATOM	4167	1HB	GLN	B	91	-12.816	40.237	20.042	1.00	0.00	H
	ATOM	4168	2HB	GLN	B	91	-12.614	40.719	21.748	1.00	0.00	H
	ATOM	4169	1HG	GLN	B	91	-10.184	39.916	21.606	1.00	0.00	H
	ATOM	4170	2HG	GLN	B	91	-10.464	39.476	19.910	1.00	0.00	H
	ATOM	4171	1HE2	GLN	B	91	-10.465	37.207	20.058	1.00	0.00	H
55	ATOM	4172	2HE2	GLN	B	91	-11.449	36.265	21.152	1.00	0.00	H
	ATOM	4173	N	ALA	B	92	-13.435	42.855	18.936	1.00	0.18	N
	ATOM	4174	CA	ALA	B	92	-14.630	43.605	18.701	1.00	0.18	C
	ATOM	4175	C	ALA	B	92	-15.533	42.758	17.870	1.00	0.18	C
	ATOM	4176	O	ALA	B	92	-15.082	41.941	17.072	1.00	0.18	O
60	ATOM	4177	CB	ALA	B	92	-14.397	44.910	17.923	1.00	0.18	C
	ATOM	4178	H	ALA	B	92	-13.113	42.309	18.152	1.00	0.00	H
	ATOM	4179	HA	ALA	B	92	-15.098	43.889	19.650	1.00	0.00	H
	ATOM	4180	1HB	ALA	B	92	-15.350	45.450	17.815	1.00	0.00	H
	ATOM	4181	2HB	ALA	B	92	-13.693	45.562	18.463	1.00	0.00	H
65	ATOM	4182	3HB	ALA	B	92	-13.990	44.720	16.918	1.00	0.00	H
	ATOM	4183	N	SER	B	93	-16.852	42.907	18.076	1.00	0.25	N
	ATOM	4184	CA	SER	B	93	-17.796	42.156	17.309	1.00	0.25	C
	ATOM	4185	C	SER	B	93	-17.756	42.639	15.893	1.00	0.25	C
	ATOM	4186	O	SER	B	93	-17.703	41.842	14.957	1.00	0.25	O
70	ATOM	4187	CB	SER	B	93	-19.230	42.324	17.826	1.00	0.25	C
	ATOM	4188	OG	SER	B	93	-20.123	41.558	17.034	1.00	0.25	O
	ATOM	4189	H	SER	B	93	-17.207	43.526	18.787	1.00	0.00	H

212

	ATOM	4190	HA	SER	B	93	-17.536	41.086	17.324	1.00	0.00	H
	ATOM	4191	1HB	SER	B	93	-19.542	43.384	17.844	1.00	0.00	H
	ATOM	4192	2HB	SER	B	93	-19.314	41.932	18.849	1.00	0.00	H
5	ATOM	4193	HG	SER	B	93	-20.011	41.846	16.114	1.00	0.00	H
	ATOM	4194	N	ALA	B	94	-17.769	43.973	15.694	1.00	0.19	N
	ATOM	4195	CA	ALA	B	94	-17.777	44.482	14.351	1.00	0.19	C
	ATOM	4196	C	ALA	B	94	-16.919	45.705	14.290	1.00	0.19	C
	ATOM	4197	O	ALA	B	94	-16.764	46.431	15.271	1.00	0.19	O
10	ATOM	4198	CB	ALA	B	94	-19.179	44.880	13.860	1.00	0.19	C
	ATOM	4199	H	ALA	B	94	-17.658	44.650	16.428	1.00	0.00	H
	ATOM	4200	HA	ALA	B	94	-17.356	43.726	13.667	1.00	0.00	H
	ATOM	4201	1HB	ALA	B	94	-19.117	45.246	12.823	1.00	0.00	H
	ATOM	4202	2HB	ALA	B	94	-19.858	44.014	13.878	1.00	0.00	H
15	ATOM	4203	3HB	ALA	B	94	-19.612	45.677	14.484	1.00	0.00	H
	ATOM	4204	N	GLU	B	95	-16.301	45.923	13.114	1.00	0.12	N
	ATOM	4205	CA	GLU	B	95	-15.454	47.050	12.861	1.00	0.12	C
	ATOM	4206	C	GLU	B	95	-16.282	48.297	12.802	1.00	0.12	C
	ATOM	4207	O	GLU	B	95	-15.920	49.321	13.378	1.00	0.12	O
20	ATOM	4208	CB	GLU	B	95	-14.711	46.900	11.522	1.00	0.12	C
	ATOM	4209	CG	GLU	B	95	-13.753	45.702	11.506	1.00	0.12	C
	ATOM	4210	CD	GLU	B	95	-13.312	45.440	10.073	1.00	0.12	C
	ATOM	4211	OE1	GLU	B	95	-13.538	46.328	9.208	1.00	0.12	O
	ATOM	4212	OE2	GLU	B	95	-12.742	44.344	9.826	1.00	0.12	O1-
25	ATOM	4213	H	GLU	B	95	-16.316	45.238	12.374	1.00	0.00	H
	ATOM	4214	HA	GLU	B	95	-14.722	47.164	13.677	1.00	0.00	H
	ATOM	4215	1HB	GLU	B	95	-14.146	47.836	11.359	1.00	0.00	H
	ATOM	4216	2HB	GLU	B	95	-15.448	46.820	10.703	1.00	0.00	H
	ATOM	4217	1HG	GLU	B	95	-14.200	44.777	11.906	1.00	0.00	H
30	ATOM	4218	2HG	GLU	B	95	-12.869	45.899	12.134	1.00	0.00	H
	ATOM	4219	N	VAL	B	96	-17.436	48.236	12.110	1.00	0.11	N
	ATOM	4220	CA	VAL	B	96	-18.234	49.417	11.956	1.00	0.11	C
	ATOM	4221	C	VAL	B	96	-19.504	49.229	12.709	1.00	0.11	C
	ATOM	4222	O	VAL	B	96	-20.025	48.119	12.813	1.00	0.11	O
35	ATOM	4223	CB	VAL	B	96	-18.599	49.704	10.531	1.00	0.11	C
	ATOM	4224	CG1	VAL	B	96	-19.514	50.942	10.495	1.00	0.11	C
	ATOM	4225	CG2	VAL	B	96	-17.299	49.864	9.726	1.00	0.11	C
	ATOM	4226	H	VAL	B	96	-17.804	47.378	11.744	1.00	0.00	H
	ATOM	4227	HA	VAL	B	96	-17.676	50.279	12.332	1.00	0.00	H
40	ATOM	4228	HB	VAL	B	96	-19.167	48.857	10.104	1.00	0.00	H
	ATOM	4229	1HG1	VAL	B	96	-19.610	51.278	9.448	1.00	0.00	H
	ATOM	4230	2HG1	VAL	B	96	-20.517	50.663	10.851	1.00	0.00	H
	ATOM	4231	3HG1	VAL	B	96	-19.099	51.777	11.077	1.00	0.00	H
	ATOM	4232	1HG2	VAL	B	96	-17.491	50.218	8.699	1.00	0.00	H
45	ATOM	4233	2HG2	VAL	B	96	-16.616	50.584	10.198	1.00	0.00	H
	ATOM	4234	3HG2	VAL	B	96	-16.754	48.909	9.632	1.00	0.00	H
	ATOM	4235	N	VAL	B	97	-20.028	50.335	13.268	1.00	0.10	N
	ATOM	4236	CA	VAL	B	97	-21.230	50.266	14.039	1.00	0.10	C
	ATOM	4237	C	VAL	B	97	-22.100	51.399	13.620	1.00	0.10	C
50	ATOM	4238	O	VAL	B	97	-21.654	52.332	12.957	1.00	0.10	O
	ATOM	4239	CB	VAL	B	97	-20.992	50.434	15.511	1.00	0.10	C
	ATOM	4240	CG1	VAL	B	97	-20.128	49.263	16.004	1.00	0.10	C
	ATOM	4241	CG2	VAL	B	97	-20.363	51.816	15.752	1.00	0.10	C
55	ATOM	4242	H	VAL	B	97	-19.530	51.212	13.277	1.00	0.00	H
	ATOM	4243	HA	VAL	B	97	-21.758	49.333	13.789	1.00	0.00	H
	ATOM	4244	HB	VAL	B	97	-21.926	50.484	16.060	1.00	0.00	H
	ATOM	4245	1HG1	VAL	B	97	-20.116	49.203	17.104	1.00	0.00	H
	ATOM	4246	2HG1	VAL	B	97	-20.458	48.283	15.626	1.00	0.00	H
	ATOM	4247	3HG1	VAL	B	97	-19.079	49.385	15.681	1.00	0.00	H
60	ATOM	4248	1HG2	VAL	B	97	-20.214	51.976	16.835	1.00	0.00	H
	ATOM	4249	2HG2	VAL	B	97	-19.366	51.909	15.298	1.00	0.00	H
	ATOM	4250	3HG2	VAL	B	97	-21.003	52.645	15.413	1.00	0.00	H
	ATOM	4251	N	MET	B	98	-23.386	51.330	14.004	1.00	0.12	N
	ATOM	4252	CA	MET	B	98	-24.315	52.369	13.688	1.00	0.12	C
65	ATOM	4253	C	MET	B	98	-24.355	53.226	14.909	1.00	0.12	C
	ATOM	4254	O	MET	B	98	-24.093	52.749	16.012	1.00	0.12	O
	ATOM	4255	CB	MET	B	98	-25.737	51.837	13.442	1.00	0.12	C
	ATOM	4256	CG	MET	B	98	-25.810	50.833	12.286	1.00	0.12	C
	ATOM	4257	SD	MET	B	98	-25.466	51.524	10.639	1.00	0.12	S
70	ATOM	4258	CE	MET	B	98	-27.170	52.062	10.325	1.00	0.12	C
	ATOM	4259	H	MET	B	98	-23.734	50.567	14.559	1.00	0.00	H
	ATOM	4260	HA	MET	B	98	-24.011	52.927	12.813	1.00	0.00	H

213

	ATOM	4261	1HB	MET	B	98	-26.406	52.694	13.257	1.00	0.00	H
	ATOM	4262	2HB	MET	B	98	-26.107	51.339	14.356	1.00	0.00	H
	ATOM	4263	1HG	MET	B	98	-26.805	50.356	12.241	1.00	0.00	H
5	ATOM	4264	2HG	MET	B	98	-25.093	50.010	12.444	1.00	0.00	H
	ATOM	4265	1HE	MET	B	98	-27.192	52.555	9.342	1.00	0.00	H
	ATOM	4266	2HE	MET	B	98	-27.854	51.201	10.300	1.00	0.00	H
	ATOM	4267	3HE	MET	B	98	-27.497	52.785	11.086	1.00	0.00	H
	ATOM	4268	N	GLU	B	99	-24.653	54.527	14.755	1.00	0.10	N
10	ATOM	4269	CA	GLU	B	99	-24.662	55.336	15.936	1.00	0.10	C
	ATOM	4270	C	GLU	B	99	-25.806	54.890	16.779	1.00	0.10	C
	ATOM	4271	O	GLU	B	99	-26.866	54.525	16.272	1.00	0.10	O
	ATOM	4272	CB	GLU	B	99	-24.838	56.844	15.682	1.00	0.10	C
	ATOM	4273	CG	GLU	B	99	-24.757	57.670	16.970	1.00	0.10	C
	ATOM	4274	CD	GLU	B	99	-24.956	59.140	16.629	1.00	0.10	C
15	ATOM	4275	OE1	GLU	B	99	-24.323	59.619	15.652	1.00	0.10	O
	ATOM	4276	OE2	GLU	B	99	-25.752	59.803	17.347	1.00	0.10	O1-
	ATOM	4277	H	GLU	B	99	-24.979	54.937	13.900	1.00	0.00	H
	ATOM	4278	HA	GLU	B	99	-23.696	55.198	16.459	1.00	0.00	H
	ATOM	4279	1HB	GLU	B	99	-25.788	57.005	15.155	1.00	0.00	H
20	ATOM	4280	2HB	GLU	B	99	-23.975	57.166	15.117	1.00	0.00	H
	ATOM	4281	1HG	GLU	B	99	-23.715	57.578	17.265	1.00	0.00	H
	ATOM	4282	2HG	GLU	B	99	-25.443	57.385	17.776	1.00	0.00	H
	ATOM	4283	N	GLY	B	100	-25.599	54.893	18.108	1.00	0.20	N
	ATOM	4284	CA	GLY	B	100	-26.641	54.528	19.014	1.00	0.20	C
25	ATOM	4285	C	GLY	B	100	-26.474	53.096	19.396	1.00	0.20	C
	ATOM	4286	O	GLY	B	100	-27.034	52.656	20.399	1.00	0.20	O
	ATOM	4287	H	GLY	B	100	-24.793	55.390	18.492	1.00	0.00	H
	ATOM	4288	1HA	GLY	B	100	-27.635	54.668	18.562	1.00	0.00	H
	ATOM	4289	2HA	GLY	B	100	-26.586	55.155	19.915	1.00	0.00	H
30	ATOM	4290	N	GLN	B	101	-25.696	52.315	18.624	1.00	0.50	N
	ATOM	4291	CA	GLN	B	101	-25.580	50.950	19.038	1.00	0.50	C
	ATOM	4292	C	GLN	B	101	-24.520	50.860	20.078	1.00	0.50	C
	ATOM	4293	O	GLN	B	101	-23.614	51.689	20.161	1.00	0.50	O
	ATOM	4294	CB	GLN	B	101	-25.311	49.923	17.920	1.00	0.50	C
35	ATOM	4295	CG	GLN	B	101	-23.985	50.050	17.175	1.00	0.50	C
	ATOM	4296	CD	GLN	B	101	-23.925	48.857	16.224	1.00	0.50	C
	ATOM	4297	OE1	GLN	B	101	-22.862	48.448	15.763	1.00	0.50	O
	ATOM	4298	NE2	GLN	B	101	-25.114	48.265	15.932	1.00	0.50	N
	ATOM	4299	H	GLN	B	101	-25.185	52.658	17.818	1.00	0.00	H
40	ATOM	4300	HA	GLN	B	101	-26.589	50.647	19.360	1.00	0.00	H
	ATOM	4301	1HB	GLN	B	101	-26.170	50.034	17.236	1.00	0.00	H
	ATOM	4302	2HB	GLN	B	101	-25.362	48.930	18.402	1.00	0.00	H
	ATOM	4303	1HG	GLN	B	101	-23.127	49.980	17.861	1.00	0.00	H
45	ATOM	4304	2HG	GLN	B	101	-23.855	50.850	16.515	1.00	0.00	H
	ATOM	4305	1HE2	GLN	B	101	-25.978	48.551	16.350	1.00	0.00	H
	ATOM	4306	2HE2	GLN	B	101	-25.070	47.437	15.362	1.00	0.00	H
	ATOM	4307	N	PRO	B	102	-24.671	49.879	20.918	1.00	0.57	N
	ATOM	4308	CA	PRO	B	102	-23.702	49.696	21.956	1.00	0.57	C
	ATOM	4309	C	PRO	B	102	-22.464	49.090	21.396	1.00	0.57	C
50	ATOM	4310	O	PRO	B	102	-22.552	48.324	20.440	1.00	0.57	O
	ATOM	4311	CB	PRO	B	102	-24.375	48.836	23.023	1.00	0.57	C
	ATOM	4312	CG	PRO	B	102	-25.870	49.147	22.846	1.00	0.57	C
	ATOM	4313	CD	PRO	B	102	-26.007	49.500	21.355	1.00	0.57	C
	ATOM	4314	HA	PRO	B	102	-23.501	50.683	22.400	1.00	0.00	H
55	ATOM	4315	1HB	PRO	B	102	-23.985	49.030	24.034	1.00	0.00	H
	ATOM	4316	2HB	PRO	B	102	-24.196	47.767	22.814	1.00	0.00	H
	ATOM	4317	1HG	PRO	B	102	-26.136	50.022	23.462	1.00	0.00	H
	ATOM	4318	2HG	PRO	B	102	-26.538	48.328	23.154	1.00	0.00	H
	ATOM	4319	1HD	PRO	B	102	-26.352	48.634	20.768	1.00	0.00	H
60	ATOM	4320	2HD	PRO	B	102	-26.737	50.310	21.257	1.00	0.00	H
	ATOM	4321	N	LEU	B	103	-21.299	49.426	21.973	1.00	0.26	N
	ATOM	4322	CA	LEU	B	103	-20.081	48.841	21.517	1.00	0.26	C
	ATOM	4323	C	LEU	B	103	-19.597	47.982	22.628	1.00	0.26	C
	ATOM	4324	O	LEU	B	103	-19.568	48.404	23.782	1.00	0.26	O
65	ATOM	4325	CB	LEU	B	103	-18.971	49.863	21.213	1.00	0.26	C
	ATOM	4326	CG	LEU	B	103	-17.661	49.217	20.720	1.00	0.26	C
	ATOM	4327	CD1	LEU	B	103	-17.856	48.516	19.366	1.00	0.26	C
	ATOM	4328	CD2	LEU	B	103	-16.509	50.235	20.709	1.00	0.26	C
	ATOM	4329	H	LEU	B	103	-21.251	50.111	22.718	1.00	0.00	H
70	ATOM	4330	HA	LEU	B	103	-20.277	48.257	20.607	1.00	0.00	H
	ATOM	4331	1HB	LEU	B	103	-18.745	50.421	22.129	1.00	0.00	H

214

	ATOM	4332	2HB	LEU	B	103	-19.330	50.595	20.468	1.00	0.00	H
	ATOM	4333	HG	LEU	B	103	-17.359	48.441	21.447	1.00	0.00	H
	ATOM	4334	1HD1	LEU	B	103	-16.913	48.068	19.010	1.00	0.00	H
5	ATOM	4335	2HD1	LEU	B	103	-18.596	47.704	19.406	1.00	0.00	H
	ATOM	4336	3HD1	LEU	B	103	-18.182	49.236	18.598	1.00	0.00	H
	ATOM	4337	1HD2	LEU	B	103	-15.604	49.827	20.237	1.00	0.00	H
	ATOM	4338	2HD2	LEU	B	103	-16.779	51.152	20.160	1.00	0.00	H
	ATOM	4339	3HD2	LEU	B	103	-16.227	50.511	21.735	1.00	0.00	H
10	ATOM	4340	N	PHE	B	104	-19.234	46.729	22.312	1.00	0.08	N
	ATOM	4341	CA	PHE	B	104	-18.730	45.879	23.344	1.00	0.08	C
	ATOM	4342	C	PHE	B	104	-17.343	45.523	22.936	1.00	0.08	C
	ATOM	4343	O	PHE	B	104	-17.099	45.161	21.785	1.00	0.08	O
	ATOM	4344	CB	PHE	B	104	-19.527	44.575	23.513	1.00	0.08	C
15	ATOM	4345	CG	PHE	B	104	-18.986	43.851	24.699	1.00	0.08	C
	ATOM	4346	CD1	PHE	B	104	-19.376	44.202	25.972	1.00	0.08	C
	ATOM	4347	CD2	PHE	B	104	-18.097	42.814	24.540	1.00	0.08	C
	ATOM	4348	CE1	PHE	B	104	-18.881	43.533	27.066	1.00	0.08	C
	ATOM	4349	CE2	PHE	B	104	-17.597	42.141	25.630	1.00	0.08	C
20	ATOM	4350	CZ	PHE	B	104	-17.990	42.502	26.896	1.00	0.08	C
	ATOM	4351	H	PHE	B	104	-19.164	46.378	21.373	1.00	0.00	H
	ATOM	4352	HA	PHE	B	104	-18.730	46.402	24.309	1.00	0.00	H
	ATOM	4353	1HB	PHE	B	104	-19.479	43.969	22.596	1.00	0.00	H
	ATOM	4354	2HB	PHE	B	104	-20.591	44.822	23.665	1.00	0.00	H
25	ATOM	4355	HD1	PHE	B	104	-20.096	45.005	26.104	1.00	0.00	H
	ATOM	4356	HD2	PHE	B	104	-18.020	42.448	23.527	1.00	0.00	H
	ATOM	4357	HE1	PHE	B	104	-19.224	43.802	28.062	1.00	0.00	H
	ATOM	4358	HE2	PHE	B	104	-16.936	41.303	25.591	1.00	0.00	H
	ATOM	4359	HZ	PHE	B	104	-17.766	41.863	27.735	1.00	0.00	H
30	ATOM	4360	N	LEU	B	105	-16.385	45.650	23.872	1.00	0.10	N
	ATOM	4361	CA	LEU	B	105	-15.028	45.325	23.562	1.00	0.10	C
	ATOM	4362	C	LEU	B	105	-14.558	44.396	24.624	1.00	0.10	C
	ATOM	4363	O	LEU	B	105	-15.108	44.362	25.724	1.00	0.10	O
	ATOM	4364	CB	LEU	B	105	-14.079	46.536	23.569	1.00	0.10	C
	ATOM	4365	CG	LEU	B	105	-14.388	47.582	22.481	1.00	0.10	C
35	ATOM	4366	CD1	LEU	B	105	-13.388	48.748	22.534	1.00	0.10	C
	ATOM	4367	CD2	LEU	B	105	-14.485	46.936	21.090	1.00	0.10	C
	ATOM	4368	H	LEU	B	105	-16.576	45.939	24.827	1.00	0.00	H
	ATOM	4369	HA	LEU	B	105	-14.968	44.805	22.597	1.00	0.00	H
40	ATOM	4370	1HB	LEU	B	105	-13.123	46.086	23.234	1.00	0.00	H
	ATOM	4371	2HB	LEU	B	105	-13.791	46.969	24.481	1.00	0.00	H
	ATOM	4372	HG	LEU	B	105	-15.382	48.018	22.698	1.00	0.00	H
	ATOM	4373	1HD1	LEU	B	105	-13.415	49.365	21.621	1.00	0.00	H
	ATOM	4374	2HD1	LEU	B	105	-13.615	49.414	23.383	1.00	0.00	H
45	ATOM	4375	3HD1	LEU	B	105	-12.365	48.392	22.683	1.00	0.00	H
	ATOM	4376	1HD2	LEU	B	105	-14.787	47.681	20.341	1.00	0.00	H
	ATOM	4377	2HD2	LEU	B	105	-13.499	46.550	20.781	1.00	0.00	H
	ATOM	4378	3HD2	LEU	B	105	-15.189	46.111	20.996	1.00	0.00	H
	ATOM	4379	N	ARG	B	106	-13.530	43.592	24.307	1.00	0.15	N
50	ATOM	4380	CA	ARG	B	106	-13.059	42.656	25.276	1.00	0.15	C
	ATOM	4381	C	ARG	B	106	-11.579	42.563	25.130	1.00	0.15	C
	ATOM	4382	O	ARG	B	106	-11.049	42.581	24.020	1.00	0.15	O
	ATOM	4383	CB	ARG	B	106	-13.663	41.262	25.034	1.00	0.15	C
	ATOM	4384	CG	ARG	B	106	-13.241	40.162	26.004	1.00	0.15	C
55	ATOM	4385	CD	ARG	B	106	-14.061	38.888	25.787	1.00	0.15	C
	ATOM	4386	NE	ARG	B	106	-13.541	37.832	26.698	1.00	0.15	N1+
	ATOM	4387	CZ	ARG	B	106	-12.993	36.702	26.169	1.00	0.15	C
	ATOM	4388	NH1	ARG	B	106	-12.935	36.556	24.813	1.00	0.15	N
	ATOM	4389	NH2	ARG	B	106	-12.531	35.718	26.995	1.00	0.15	N
60	ATOM	4390	H	ARG	B	106	-13.089	43.585	23.398	1.00	0.00	H
	ATOM	4391	HA	ARG	B	106	-13.331	42.978	26.288	1.00	0.00	H
	ATOM	4392	1HB	ARG	B	106	-13.453	40.935	24.002	1.00	0.00	H
	ATOM	4393	2HB	ARG	B	106	-14.740	41.426	25.150	1.00	0.00	H
	ATOM	4394	1HG	ARG	B	106	-13.146	40.446	27.059	1.00	0.00	H
65	ATOM	4395	2HG	ARG	B	106	-12.200	39.888	25.736	1.00	0.00	H
	ATOM	4396	1HD	ARG	B	106	-13.950	38.632	24.738	1.00	0.00	H
	ATOM	4397	2HD	ARG	B	106	-15.136	39.011	25.994	1.00	0.00	H
	ATOM	4398	HE	ARG	B	106	-13.935	37.715	27.606	1.00	0.00	H
	ATOM	4399	1HH1	ARG	B	106	-12.968	37.348	24.200	1.00	0.00	H
70	ATOM	4400	2HH1	ARG	B	106	-12.382	35.811	24.442	1.00	0.00	H
	ATOM	4401	1HH2	ARG	B	106	-12.173	34.859	26.638	1.00	0.00	H
	ATOM	4402	2HH2	ARG	B	106	-12.478	35.864	27.979	1.00	0.00	H

215

	ATOM	4403	N	CYS	B	107	-10.862	42.482	26.266	1.00	0.16	N
	ATOM	4404	CA	CYS	B	107	-9.446	42.306	26.188	1.00	0.16	C
	ATOM	4405	C	CYS	B	107	-9.261	40.846	26.416	1.00	0.16	C
5	ATOM	4406	O	CYS	B	107	-9.650	40.320	27.458	1.00	0.16	O
	ATOM	4407	CB	CYS	B	107	-8.663	43.074	27.268	1.00	0.16	C
	ATOM	4408	SG	CYS	B	107	-9.006	44.857	27.207	1.00	0.16	S
	ATOM	4409	H	CYS	B	107	-11.264	42.454	27.191	1.00	0.00	H
	ATOM	4410	HA	CYS	B	107	-9.062	42.647	25.214	1.00	0.00	H
10	ATOM	4411	1HB	CYS	B	107	-7.591	42.892	27.084	1.00	0.00	H
	ATOM	4412	2HB	CYS	B	107	-8.887	42.711	28.282	1.00	0.00	H
	ATOM	4413	N	HIS	B	108	-8.681	40.141	25.429	1.00	0.11	N
	ATOM	4414	CA	HIS	B	108	-8.593	38.719	25.557	1.00	0.11	C
	ATOM	4415	C	HIS	B	108	-7.159	38.316	25.545	1.00	0.11	C
15	ATOM	4416	O	HIS	B	108	-6.360	38.829	24.763	1.00	0.11	O
	ATOM	4417	CB	HIS	B	108	-9.321	37.991	24.412	1.00	0.11	C
	ATOM	4418	CG	HIS	B	108	-9.314	36.494	24.517	1.00	0.11	C
	ATOM	4419	ND1	HIS	B	108	-8.352	35.693	23.946	1.00	0.11	N
	ATOM	4420	CD2	HIS	B	108	-10.189	35.649	25.126	1.00	0.11	C
20	ATOM	4421	CE1	HIS	B	108	-8.693	34.410	24.231	1.00	0.11	C
	ATOM	4422	NE2	HIS	B	108	-9.799	34.333	24.946	1.00	0.11	N
	ATOM	4423	H	HIS	B	108	-8.343	40.550	24.563	1.00	0.00	H
	ATOM	4424	HA	HIS	B	108	-9.067	38.390	26.494	1.00	0.00	H
	ATOM	4425	1HB	HIS	B	108	-8.903	38.313	23.443	1.00	0.00	H
25	ATOM	4426	2HB	HIS	B	108	-10.372	38.319	24.407	1.00	0.00	H
	ATOM	4427	HD2	HIS	B	108	-10.626	35.988	26.029	1.00	0.00	H
	ATOM	4428	HE1	HIS	B	108	-7.908	33.691	24.152	1.00	0.00	H
	ATOM	4429	HE2	HIS	B	108	-9.908	33.580	25.609	1.00	0.00	H
	ATOM	4430	N	GLY	B	109	-6.805	37.367	26.433	1.00	0.09	N
30	ATOM	4431	CA	GLY	B	109	-5.456	36.899	26.515	1.00	0.09	C
	ATOM	4432	C	GLY	B	109	-5.417	35.556	25.871	1.00	0.09	C
	ATOM	4433	O	GLY	B	109	-6.414	34.837	25.839	1.00	0.09	O
	ATOM	4434	H	GLY	B	109	-7.478	36.848	26.971	1.00	0.00	H
	ATOM	4435	1HA	GLY	B	109	-5.161	36.786	27.574	1.00	0.00	H
35	ATOM	4436	2HA	GLY	B	109	-4.766	37.619	26.058	1.00	0.00	H
	ATOM	4437	N	TRP	B	110	-4.241	35.184	25.339	1.00	0.32	N
	ATOM	4438	CA	TRP	B	110	-4.097	33.932	24.665	1.00	0.32	C
	ATOM	4439	C	TRP	B	110	-4.162	32.847	25.691	1.00	0.32	C
	ATOM	4440	O	TRP	B	110	-3.707	33.008	26.822	1.00	0.32	O
40	ATOM	4441	CB	TRP	B	110	-2.767	33.840	23.890	1.00	0.32	C
	ATOM	4442	CG	TRP	B	110	-2.534	32.551	23.142	1.00	0.32	C
	ATOM	4443	CD1	TRP	B	110	-3.146	32.070	22.021	1.00	0.32	C
	ATOM	4444	CD2	TRP	B	110	-1.525	31.596	23.495	1.00	0.32	C
	ATOM	4445	NE1	TRP	B	110	-2.583	30.869	21.657	1.00	0.32	N
45	ATOM	4446	CE2	TRP	B	110	-1.580	30.568	22.553	1.00	0.32	C
	ATOM	4447	CE3	TRP	B	110	-0.621	31.578	24.517	1.00	0.32	C
	ATOM	4448	CZ2	TRP	B	110	-0.729	29.502	22.620	1.00	0.32	C
	ATOM	4449	CZ3	TRP	B	110	0.236	30.504	24.583	1.00	0.32	C
	ATOM	4450	CH2	TRP	B	110	0.183	29.486	23.653	1.00	0.32	C
50	ATOM	4451	H	TRP	B	110	-3.501	35.873	25.213	1.00	0.00	H
	ATOM	4452	HA	TRP	B	110	-4.922	33.828	23.933	1.00	0.00	H
	ATOM	4453	1HB	TRP	B	110	-1.929	34.040	24.572	1.00	0.00	H
	ATOM	4454	2HB	TRP	B	110	-2.766	34.667	23.167	1.00	0.00	H
	ATOM	4455	HD1	TRP	B	110	-4.013	32.458	21.524	1.00	0.00	H
55	ATOM	4456	HE1	TRP	B	110	-3.077	30.217	21.085	1.00	0.00	H
	ATOM	4457	HE3	TRP	B	110	-0.604	32.378	25.237	1.00	0.00	H
	ATOM	4458	HZ2	TRP	B	110	-0.771	28.699	21.889	1.00	0.00	H
	ATOM	4459	HZ3	TRP	B	110	1.037	30.521	25.317	1.00	0.00	H
	ATOM	4460	HH2	TRP	B	110	0.902	28.670	23.710	1.00	0.00	H
60	ATOM	4461	N	ARG	B	111	-4.775	31.709	25.311	1.00	0.53	N
	ATOM	4462	CA	ARG	B	111	-4.933	30.586	26.189	1.00	0.53	C
	ATOM	4463	C	ARG	B	111	-5.683	31.000	27.413	1.00	0.53	C
	ATOM	4464	O	ARG	B	111	-5.653	30.300	28.425	1.00	0.53	O
	ATOM	4465	CB	ARG	B	111	-3.620	29.933	26.655	1.00	0.53	C
65	ATOM	4466	CG	ARG	B	111	-3.020	28.970	25.633	1.00	0.53	C
	ATOM	4467	CD	ARG	B	111	-2.053	27.949	26.245	1.00	0.53	C
	ATOM	4468	NE	ARG	B	111	-0.754	28.629	26.508	1.00	0.53	N1+
	ATOM	4469	CZ	ARG	B	111	0.186	28.032	27.299	1.00	0.53	C
	ATOM	4470	NH1	ARG	B	111	-0.095	26.849	27.921	1.00	0.53	N
70	ATOM	4471	NH2	ARG	B	111	1.396	28.633	27.493	1.00	0.53	N
	ATOM	4472	H	ARG	B	111	-5.186	31.627	24.389	1.00	0.00	H
	ATOM	4473	HA	ARG	B	111	-5.583	29.848	25.683	1.00	0.00	H

216

	ATOM	4474	1HB	ARG	B	111	-3.792	29.342	27.570	1.00	0.00	H
	ATOM	4475	2HB	ARG	B	111	-2.899	30.707	26.910	1.00	0.00	H
	ATOM	4476	1HG	ARG	B	111	-2.557	29.498	24.791	1.00	0.00	H
5	ATOM	4477	2HG	ARG	B	111	-3.855	28.394	25.192	1.00	0.00	H
	ATOM	4478	1HD	ARG	B	111	-1.871	27.088	25.580	1.00	0.00	H
	ATOM	4479	2HD	ARG	B	111	-2.462	27.574	27.198	1.00	0.00	H
	ATOM	4480	HE	ARG	B	111	-0.400	29.179	25.751	1.00	0.00	H
	ATOM	4481	1HH1	ARG	B	111	-0.987	26.418	27.837	1.00	0.00	H
10	ATOM	4482	2HH1	ARG	B	111	0.584	26.383	28.480	1.00	0.00	H
	ATOM	4483	1HH2	ARG	B	111	2.095	28.219	28.070	1.00	0.00	H
	ATOM	4484	2HH2	ARG	B	111	1.585	29.543	27.140	1.00	0.00	H
	ATOM	4485	N	ASN	B	112	-6.402	32.134	27.343	1.00	0.33	N
	ATOM	4486	CA	ASN	B	112	-7.191	32.586	28.452	1.00	0.33	C
15	ATOM	4487	C	ASN	B	112	-6.360	32.626	29.693	1.00	0.33	C
	ATOM	4488	O	ASN	B	112	-6.800	32.181	30.754	1.00	0.33	O
	ATOM	4489	CB	ASN	B	112	-8.409	31.688	28.734	1.00	0.33	C
	ATOM	4490	CG	ASN	B	112	-9.405	31.882	27.605	1.00	0.33	C
	ATOM	4491	OD1	ASN	B	112	-9.721	33.014	27.241	1.00	0.33	O
20	ATOM	4492	ND2	ASN	B	112	-9.908	30.756	27.031	1.00	0.33	N
	ATOM	4493	H	ASN	B	112	-6.362	32.724	26.520	1.00	0.00	H
	ATOM	4494	HA	ASN	B	112	-7.515	33.623	28.253	1.00	0.00	H
	ATOM	4495	1HB	ASN	B	112	-8.936	32.044	29.637	1.00	0.00	H
	ATOM	4496	2HB	ASN	B	112	-8.129	30.637	28.898	1.00	0.00	H
	ATOM	4497	1HD2	ASN	B	112	-9.555	29.853	27.290	1.00	0.00	H
25	ATOM	4498	2HD2	ASN	B	112	-10.398	30.864	26.155	1.00	0.00	H
	ATOM	4499	N	TRP	B	113	-5.133	33.171	29.612	1.00	0.13	N
	ATOM	4500	CA	TRP	B	113	-4.351	33.236	30.808	1.00	0.13	C
	ATOM	4501	C	TRP	B	113	-4.945	34.304	31.665	1.00	0.13	C
30	ATOM	4502	O	TRP	B	113	-5.619	35.209	31.177	1.00	0.13	O
	ATOM	4503	CB	TRP	B	113	-2.864	33.550	30.572	1.00	0.13	C
	ATOM	4504	CG	TRP	B	113	-2.109	32.435	29.884	1.00	0.13	C
	ATOM	4505	CD1	TRP	B	113	-1.666	32.352	28.595	1.00	0.13	C
	ATOM	4506	CD2	TRP	B	113	-1.737	31.203	30.524	1.00	0.13	C
35	ATOM	4507	NE1	TRP	B	113	-1.030	31.149	28.395	1.00	0.13	N
	ATOM	4508	CE2	TRP	B	113	-1.071	30.431	29.574	1.00	0.13	C
	ATOM	4509	CE3	TRP	B	113	-1.939	30.749	31.798	1.00	0.13	C
	ATOM	4510	CZ2	TRP	B	113	-0.593	29.190	29.891	1.00	0.13	C
	ATOM	4511	CZ3	TRP	B	113	-1.451	29.499	32.110	1.00	0.13	C
40	ATOM	4512	CH2	TRP	B	113	-0.791	28.733	31.174	1.00	0.13	C
	ATOM	4513	H	TRP	B	113	-4.706	33.392	28.722	1.00	0.00	H
	ATOM	4514	HA	TRP	B	113	-4.416	32.264	31.331	1.00	0.00	H
	ATOM	4515	1HB	TRP	B	113	-2.398	33.746	31.554	1.00	0.00	H
	ATOM	4516	2HB	TRP	B	113	-2.768	34.490	30.007	1.00	0.00	H
45	ATOM	4517	HD1	TRP	B	113	-1.720	33.120	27.844	1.00	0.00	H
	ATOM	4518	HE1	TRP	B	113	-0.986	30.689	27.511	1.00	0.00	H
	ATOM	4519	HE3	TRP	B	113	-2.453	31.342	32.547	1.00	0.00	H
	ATOM	4520	HZ2	TRP	B	113	0.140	28.651	29.363	1.00	0.00	H
	ATOM	4521	HZ3	TRP	B	113	-1.587	29.113	33.118	1.00	0.00	H
50	ATOM	4522	HH2	TRP	B	113	-0.388	27.770	31.480	1.00	0.00	H
	ATOM	4523	N	ASP	B	114	-4.712	34.218	32.988	1.00	0.12	N
	ATOM	4524	CA	ASP	B	114	-5.293	35.164	33.895	1.00	0.12	C
	ATOM	4525	C	ASP	B	114	-4.813	36.522	33.513	1.00	0.12	C
	ATOM	4526	O	ASP	B	114	-3.627	36.729	33.263	1.00	0.12	O
55	ATOM	4527	CB	ASP	B	114	-4.874	34.945	35.357	1.00	0.12	C
	ATOM	4528	CG	ASP	B	114	-5.445	33.616	35.823	1.00	0.12	C
	ATOM	4529	OD1	ASP	B	114	-6.688	33.434	35.731	1.00	0.12	O
	ATOM	4530	OD2	ASP	B	114	-4.640	32.765	36.285	1.00	0.12	O1-
	ATOM	4531	H	ASP	B	114	-4.235	33.453	33.434	1.00	0.00	H
60	ATOM	4532	HA	ASP	B	114	-6.396	35.103	33.822	1.00	0.00	H
	ATOM	4533	1HB	ASP	B	114	-5.326	35.762	35.943	1.00	0.00	H
	ATOM	4534	2HB	ASP	B	114	-3.782	34.988	35.482	1.00	0.00	H
	ATOM	4535	N	VAL	B	115	-5.746	37.488	33.447	1.00	0.21	N
	ATOM	4536	CA	VAL	B	115	-5.368	38.823	33.098	1.00	0.21	C
65	ATOM	4537	C	VAL	B	115	-5.975	39.733	34.112	1.00	0.21	C
	ATOM	4538	O	VAL	B	115	-7.072	39.488	34.611	1.00	0.21	O
	ATOM	4539	CB	VAL	B	115	-5.880	39.263	31.759	1.00	0.21	C
	ATOM	4540	CG1	VAL	B	115	-5.413	40.708	31.508	1.00	0.21	C
	ATOM	4541	CG2	VAL	B	115	-5.402	38.262	30.694	1.00	0.21	C
70	ATOM	4542	H	VAL	B	115	-6.699	37.343	33.725	1.00	0.00	H
	ATOM	4543	HA	VAL	B	115	-4.271	38.918	33.117	1.00	0.00	H
	ATOM	4544	HB	VAL	B	115	-6.981	39.270	31.744	1.00	0.00	H

217

	ATOM	4545	1HG1	VAL	B	115	-5.622	41.014	30.468	1.00	0.00	H
	ATOM	4546	2HG1	VAL	B	115	-5.940	41.434	32.142	1.00	0.00	H
	ATOM	4547	3HG1	VAL	B	115	-4.326	40.819	31.656	1.00	0.00	H
5	ATOM	4548	1HG2	VAL	B	115	-6.242	37.632	30.360	1.00	0.00	H
	ATOM	4549	2HG2	VAL	B	115	-5.022	38.760	29.788	1.00	0.00	H
	ATOM	4550	3HG2	VAL	B	115	-4.626	37.571	31.037	1.00	0.00	H
	ATOM	4551	N	TYR	B	116	-5.249	40.808	34.455	1.00	0.44	N
	ATOM	4552	CA	TYR	B	116	-5.738	41.756	35.407	1.00	0.44	C
10	ATOM	4553	C	TYR	B	116	-5.192	43.082	34.997	1.00	0.44	C
	ATOM	4554	O	TYR	B	116	-4.387	43.164	34.070	1.00	0.44	O
	ATOM	4555	CB	TYR	B	116	-5.271	41.458	36.836	1.00	0.44	C
	ATOM	4556	CG	TYR	B	116	-3.794	41.347	36.746	1.00	0.44	C
	ATOM	4557	CD1	TYR	B	116	-2.990	42.447	36.891	1.00	0.44	C
	ATOM	4558	CD2	TYR	B	116	-3.215	40.131	36.486	1.00	0.44	C
15	ATOM	4559	CE1	TYR	B	116	-1.624	42.331	36.797	1.00	0.44	C
	ATOM	4560	CE2	TYR	B	116	-1.851	40.007	36.391	1.00	0.44	C
	ATOM	4561	CZ	TYR	B	116	-1.050	41.109	36.548	1.00	0.44	C
	ATOM	4562	OH	TYR	B	116	0.352	40.983	36.451	1.00	0.44	O
20	ATOM	4563	H	TYR	B	116	-4.340	40.999	34.057	1.00	0.00	H
	ATOM	4564	HA	TYR	B	116	-6.838	41.795	35.343	1.00	0.00	H
	ATOM	4565	1HB	TYR	B	116	-5.732	40.521	37.186	1.00	0.00	H
	ATOM	4566	2HB	TYR	B	116	-5.607	42.248	37.523	1.00	0.00	H
	ATOM	4567	HD1	TYR	B	116	-3.439	43.399	37.135	1.00	0.00	H
	ATOM	4568	HD2	TYR	B	116	-3.838	39.248	36.357	1.00	0.00	H
25	ATOM	4569	HE1	TYR	B	116	-0.986	43.139	37.108	1.00	0.00	H
	ATOM	4570	HE2	TYR	B	116	-1.421	39.030	36.180	1.00	0.00	H
	ATOM	4571	HH	TYR	B	116	0.572	40.183	35.940	1.00	0.00	H
	ATOM	4572	N	LYS	B	117	-5.625	44.154	35.689	1.00	0.45	N
	ATOM	4573	CA	LYS	B	117	-5.196	45.486	35.366	1.00	0.45	C
30	ATOM	4574	C	LYS	B	117	-5.361	45.714	33.903	1.00	0.45	C
	ATOM	4575	O	LYS	B	117	-4.381	45.874	33.177	1.00	0.45	O
	ATOM	4576	CB	LYS	B	117	-3.732	45.803	35.716	1.00	0.45	C
	ATOM	4577	CG	LYS	B	117	-3.486	46.035	37.205	1.00	0.45	C
	ATOM	4578	CD	LYS	B	117	-2.021	46.314	37.540	1.00	0.45	C
35	ATOM	4579	CE	LYS	B	117	-1.803	46.773	38.982	1.00	0.45	C
	ATOM	4580	NZ	LYS	B	117	-1.648	45.598	39.868	1.00	0.45	N1+
	ATOM	4581	H	LYS	B	117	-6.473	44.044	36.231	1.00	0.00	H
	ATOM	4582	HA	LYS	B	117	-5.857	46.181	35.904	1.00	0.00	H
40	ATOM	4583	1HB	LYS	B	117	-3.423	46.732	35.202	1.00	0.00	H
	ATOM	4584	2HB	LYS	B	117	-3.072	45.012	35.321	1.00	0.00	H
	ATOM	4585	1HG	LYS	B	117	-4.032	45.396	37.906	1.00	0.00	H
	ATOM	4586	2HG	LYS	B	117	-3.730	47.063	37.280	1.00	0.00	H
	ATOM	4587	1HD	LYS	B	117	-1.662	47.096	36.845	1.00	0.00	H
	ATOM	4588	2HD	LYS	B	117	-1.404	45.426	37.399	1.00	0.00	H
45	ATOM	4589	1HE	LYS	B	117	-2.615	47.410	39.361	1.00	0.00	H
	ATOM	4590	2HE	LYS	B	117	-0.875	47.361	39.082	1.00	0.00	H
	ATOM	4591	1HZ	LYS	B	117	-1.543	45.856	40.843	1.00	0.00	H
	ATOM	4592	2HZ	LYS	B	117	-2.458	44.990	39.832	1.00	0.00	H
50	ATOM	4593	3HZ	LYS	B	117	-0.847	45.024	39.642	1.00	0.00	H
	ATOM	4594	N	VAL	B	118	-6.621	45.732	33.433	1.00	0.21	N
	ATOM	4595	CA	VAL	B	118	-6.873	45.917	32.037	1.00	0.21	C
	ATOM	4596	C	VAL	B	118	-7.212	47.354	31.806	1.00	0.21	C
	ATOM	4597	O	VAL	B	118	-7.958	47.964	32.569	1.00	0.21	O
	ATOM	4598	CB	VAL	B	118	-8.032	45.104	31.546	1.00	0.21	C
55	ATOM	4599	CG1	VAL	B	118	-8.313	45.486	30.088	1.00	0.21	C
	ATOM	4600	CG2	VAL	B	118	-7.708	43.615	31.749	1.00	0.21	C
	ATOM	4601	H	VAL	B	118	-7.436	45.659	34.029	1.00	0.00	H
	ATOM	4602	HA	VAL	B	118	-5.985	45.589	31.488	1.00	0.00	H
	ATOM	4603	HB	VAL	B	118	-8.930	45.345	32.142	1.00	0.00	H
60	ATOM	4604	1HG1	VAL	B	118	-9.124	44.854	29.695	1.00	0.00	H
	ATOM	4605	2HG1	VAL	B	118	-8.627	46.530	29.946	1.00	0.00	H
	ATOM	4606	3HG1	VAL	B	118	-7.398	45.279	29.526	1.00	0.00	H
	ATOM	4607	1HG2	VAL	B	118	-8.494	42.960	31.340	1.00	0.00	H
	ATOM	4608	2HG2	VAL	B	118	-6.771	43.353	31.231	1.00	0.00	H
65	ATOM	4609	3HG2	VAL	B	118	-7.597	43.351	32.813	1.00	0.00	H
	ATOM	4610	N	ILE	B	119	-6.636	47.944	30.739	1.00	0.09	N
	ATOM	4611	CA	ILE	B	119	-6.937	49.309	30.434	1.00	0.09	C
	ATOM	4612	C	ILE	B	119	-7.363	49.370	29.005	1.00	0.09	C
	ATOM	4613	O	ILE	B	119	-6.814	48.678	28.149	1.00	0.09	O
70	ATOM	4614	CB	ILE	B	119	-5.765	50.232	30.583	1.00	0.09	C
	ATOM	4615	CG1	ILE	B	119	-5.244	50.204	32.028	1.00	0.09	C

218

	ATOM	4616	CG2	ILE	B	119	-6.202	51.627	30.108	1.00	0.09	C
	ATOM	4617	CD1	ILE	B	119	-3.887	50.886	32.199	1.00	0.09	C
	ATOM	4618	H	ILE	B	119	-5.959	47.463	30.152	1.00	0.00	H
5	ATOM	4619	HA	ILE	B	119	-7.753	49.658	31.079	1.00	0.00	H
	ATOM	4620	HB	ILE	B	119	-4.971	49.878	29.921	1.00	0.00	H
	ATOM	4621	1HG1	ILE	B	119	-5.125	49.169	32.385	1.00	0.00	H
	ATOM	4622	2HG1	ILE	B	119	-5.963	50.777	32.619	1.00	0.00	H
	ATOM	4623	1HG2	ILE	B	119	-5.476	52.407	30.381	1.00	0.00	H
10	ATOM	4624	2HG2	ILE	B	119	-6.341	51.692	29.021	1.00	0.00	H
	ATOM	4625	3HG2	ILE	B	119	-7.135	51.938	30.599	1.00	0.00	H
	ATOM	4626	1HD1	ILE	B	119	-3.575	50.833	33.256	1.00	0.00	H
	ATOM	4627	2HD1	ILE	B	119	-3.103	50.373	31.623	1.00	0.00	H
	ATOM	4628	3HD1	ILE	B	119	-3.918	51.955	31.943	1.00	0.00	H
15	ATOM	4629	N	TYR	B	120	-8.383	50.200	28.722	1.00	0.09	N
	ATOM	4630	CA	TYR	B	120	-8.837	50.378	27.377	1.00	0.09	C
	ATOM	4631	C	TYR	B	120	-8.350	51.707	26.923	1.00	0.09	C
	ATOM	4632	O	TYR	B	120	-8.418	52.691	27.658	1.00	0.09	O
	ATOM	4633	CB	TYR	B	120	-10.367	50.372	27.212	1.00	0.09	C
20	ATOM	4634	CG	TYR	B	120	-10.850	48.963	27.189	1.00	0.09	C
	ATOM	4635	CD1	TYR	B	120	-11.051	48.235	28.339	1.00	0.09	C
	ATOM	4636	CD2	TYR	B	120	-11.111	48.374	25.973	1.00	0.09	C
	ATOM	4637	CE1	TYR	B	120	-11.504	46.937	28.266	1.00	0.09	C
	ATOM	4638	CE2	TYR	B	120	-11.563	47.081	25.893	1.00	0.09	C
25	ATOM	4639	CZ	TYR	B	120	-11.761	46.361	27.043	1.00	0.09	C
	ATOM	4640	OH	TYR	B	120	-12.226	45.034	26.949	1.00	0.09	O
	ATOM	4641	H	TYR	B	120	-8.759	50.823	29.425	1.00	0.00	H
	ATOM	4642	HA	TYR	B	120	-8.416	49.584	26.738	1.00	0.00	H
	ATOM	4643	1HB	TYR	B	120	-10.609	50.876	26.261	1.00	0.00	H
30	ATOM	4644	2HB	TYR	B	120	-10.841	50.971	28.003	1.00	0.00	H
	ATOM	4645	HD1	TYR	B	120	-10.803	48.686	29.294	1.00	0.00	H
	ATOM	4646	HD2	TYR	B	120	-10.958	48.938	25.055	1.00	0.00	H
	ATOM	4647	HE1	TYR	B	120	-11.634	46.356	29.175	1.00	0.00	H
	ATOM	4648	HE2	TYR	B	120	-11.814	46.651	24.941	1.00	0.00	H
35	ATOM	4649	HH	TYR	B	120	-11.973	44.595	27.775	1.00	0.00	H
	ATOM	4650	N	TYR	B	121	-7.816	51.760	25.689	1.00	0.18	N
	ATOM	4651	CA	TYR	B	121	-7.302	52.999	25.199	1.00	0.18	C
	ATOM	4652	C	TYR	B	121	-8.013	53.324	23.925	1.00	0.18	C
	ATOM	4653	O	TYR	B	121	-8.291	52.449	23.108	1.00	0.18	O
40	ATOM	4654	CB	TYR	B	121	-5.803	52.937	24.877	1.00	0.18	C
	ATOM	4655	CG	TYR	B	121	-5.083	52.647	26.150	1.00	0.18	C
	ATOM	4656	CD1	TYR	B	121	-4.694	53.668	26.987	1.00	0.18	C
	ATOM	4657	CD2	TYR	B	121	-4.800	51.349	26.509	1.00	0.18	C
	ATOM	4658	CE1	TYR	B	121	-4.028	53.397	28.160	1.00	0.18	C
45	ATOM	4659	CE2	TYR	B	121	-4.134	51.074	27.679	1.00	0.18	C
	ATOM	4660	CZ	TYR	B	121	-3.744	52.098	28.506	1.00	0.18	C
	ATOM	4661	OH	TYR	B	121	-3.059	51.815	29.707	1.00	0.18	O
	ATOM	4662	H	TYR	B	121	-7.619	50.943	25.120	1.00	0.00	H
	ATOM	4663	HA	TYR	B	121	-7.431	53.759	25.960	1.00	0.00	H
50	ATOM	4664	1HB	TYR	B	121	-5.500	53.911	24.460	1.00	0.00	H
	ATOM	4665	2HB	TYR	B	121	-5.589	52.184	24.103	1.00	0.00	H
	ATOM	4666	HD1	TYR	B	121	-4.883	54.701	26.707	1.00	0.00	H
	ATOM	4667	HD2	TYR	B	121	-5.074	50.534	25.848	1.00	0.00	H
	ATOM	4668	HE1	TYR	B	121	-3.684	54.220	28.783	1.00	0.00	H
	ATOM	4669	HE2	TYR	B	121	-4.040	50.026	27.774	1.00	0.00	H
55	ATOM	4670	HH	TYR	B	121	-2.245	52.351	29.616	1.00	0.00	H
	ATOM	4671	N	LYS	B	122	-8.347	54.617	23.757	1.00	0.28	N
	ATOM	4672	CA	LYS	B	122	-9.000	55.139	22.598	1.00	0.28	C
	ATOM	4673	C	LYS	B	122	-8.109	56.236	22.126	1.00	0.28	C
60	ATOM	4674	O	LYS	B	122	-7.986	57.264	22.790	1.00	0.28	O
	ATOM	4675	CB	LYS	B	122	-10.349	55.804	22.933	1.00	0.28	C
	ATOM	4676	CG	LYS	B	122	-11.176	56.243	21.722	1.00	0.28	C
	ATOM	4677	CD	LYS	B	122	-12.535	56.836	22.111	1.00	0.28	C
	ATOM	4678	CE	LYS	B	122	-13.183	56.151	23.316	1.00	0.28	C
	ATOM	4679	NZ	LYS	B	122	-14.483	56.791	23.628	1.00	0.28	N1+
65	ATOM	4680	H	LYS	B	122	-8.144	55.299	24.484	1.00	0.00	H
	ATOM	4681	HA	LYS	B	122	-9.164	54.338	21.865	1.00	0.00	H
	ATOM	4682	1HB	LYS	B	122	-10.242	56.625	23.659	1.00	0.00	H
	ATOM	4683	2HB	LYS	B	122	-10.988	55.031	23.342	1.00	0.00	H
	ATOM	4684	1HG	LYS	B	122	-11.311	55.374	21.057	1.00	0.00	H
70	ATOM	4685	2HG	LYS	B	122	-10.623	56.984	21.114	1.00	0.00	H
	ATOM	4686	1HD	LYS	B	122	-13.201	56.854	21.232	1.00	0.00	H

	ATOM	4687	2HD	LYS	B	122	-12.369	57.894	22.385	1.00	0.00	H
	ATOM	4688	1HE	LYS	B	122	-12.551	56.319	24.190	1.00	0.00	H
	ATOM	4689	2HE	LYS	B	122	-13.425	55.120	23.185	1.00	0.00	H
5	ATOM	4690	1HZ	LYS	B	122	-14.924	56.393	24.445	1.00	0.00	H
	ATOM	4691	2HZ	LYS	B	122	-14.393	57.785	23.789	1.00	0.00	H
	ATOM	4692	3HZ	LYS	B	122	-15.134	56.665	22.860	1.00	0.00	H
	ATOM	4693	N	ASP	B	123	-7.464	56.040	20.965	1.00	0.20	N
	ATOM	4694	CA	ASP	B	123	-6.591	57.040	20.428	1.00	0.20	C
10	ATOM	4695	C	ASP	B	123	-5.595	57.437	21.470	1.00	0.20	C
	ATOM	4696	O	ASP	B	123	-5.193	58.597	21.556	1.00	0.20	O
	ATOM	4697	CB	ASP	B	123	-7.339	58.273	19.901	1.00	0.20	C
	ATOM	4698	CG	ASP	B	123	-8.044	57.821	18.631	1.00	0.20	C
	ATOM	4699	OD1	ASP	B	123	-7.553	56.845	18.001	1.00	0.20	O
	ATOM	4700	OD2	ASP	B	123	-9.081	58.436	18.274	1.00	0.20	O1-
15	ATOM	4701	H	ASP	B	123	-7.659	55.230	20.379	1.00	0.00	H
	ATOM	4702	HA	ASP	B	123	-5.967	56.577	19.640	1.00	0.00	H
	ATOM	4703	1HB	ASP	B	123	-6.613	59.051	19.613	1.00	0.00	H
	ATOM	4704	2HB	ASP	B	123	-8.032	58.726	20.624	1.00	0.00	H
20	ATOM	4705	N	GLY	B	124	-5.173	56.462	22.296	1.00	0.17	N
	ATOM	4706	CA	GLY	B	124	-4.147	56.707	23.266	1.00	0.17	C
	ATOM	4707	C	GLY	B	124	-4.739	57.254	24.523	1.00	0.17	C
	ATOM	4708	O	GLY	B	124	-4.011	57.600	25.454	1.00	0.17	O
	ATOM	4709	H	GLY	B	124	-5.500	55.518	22.162	1.00	0.00	H
25	ATOM	4710	1HA	GLY	B	124	-3.397	57.414	22.878	1.00	0.00	H
	ATOM	4711	2HA	GLY	B	124	-3.641	55.758	23.511	1.00	0.00	H
	ATOM	4712	N	GLU	B	125	-6.076	57.350	24.601	1.00	0.24	N
	ATOM	4713	CA	GLU	B	125	-6.638	57.879	25.806	1.00	0.24	C
	ATOM	4714	C	GLU	B	125	-7.229	56.729	26.552	1.00	0.24	C
30	ATOM	4715	O	GLU	B	125	-7.934	55.904	25.980	1.00	0.24	O
	ATOM	4716	CB	GLU	B	125	-7.747	58.908	25.550	1.00	0.24	C
	ATOM	4717	CG	GLU	B	125	-8.099	59.729	26.785	1.00	0.24	C
	ATOM	4718	CD	GLU	B	125	-9.183	60.720	26.392	1.00	0.24	C
	ATOM	4719	OE1	GLU	B	125	-10.013	60.366	25.512	1.00	0.24	O
35	ATOM	4720	OE2	GLU	B	125	-9.192	61.843	26.962	1.00	0.24	O1-
	ATOM	4721	H	GLU	B	125	-6.663	57.298	23.773	1.00	0.00	H
	ATOM	4722	HA	GLU	B	125	-5.870	58.399	26.400	1.00	0.00	H
	ATOM	4723	1HB	GLU	B	125	-8.638	58.390	25.156	1.00	0.00	H
	ATOM	4724	2HB	GLU	B	125	-7.408	59.599	24.755	1.00	0.00	H
40	ATOM	4725	1HG	GLU	B	125	-7.225	60.253	27.203	1.00	0.00	H
	ATOM	4726	2HG	GLU	B	125	-8.494	59.077	27.582	1.00	0.00	H
	ATOM	4727	N	ALA	B	126	-6.967	56.629	27.865	1.00	0.26	N
	ATOM	4728	CA	ALA	B	126	-7.483	55.489	28.563	1.00	0.26	C
	ATOM	4729	C	ALA	B	126	-8.923	55.737	28.870	1.00	0.26	C
45	ATOM	4730	O	ALA	B	126	-9.257	56.616	29.662	1.00	0.26	O
	ATOM	4731	CB	ALA	B	126	-6.771	55.212	29.898	1.00	0.26	C
	ATOM	4732	H	ALA	B	126	-6.347	57.258	28.348	1.00	0.00	H
	ATOM	4733	HA	ALA	B	126	-7.283	54.612	27.943	1.00	0.00	H
	ATOM	4734	1HB	ALA	B	126	-7.245	54.340	30.375	1.00	0.00	H
50	ATOM	4735	2HB	ALA	B	126	-5.708	54.984	29.733	1.00	0.00	H
	ATOM	4736	3HB	ALA	B	126	-6.835	56.063	30.593	1.00	0.00	H
	ATOM	4737	N	LEU	B	127	-9.819	54.977	28.210	1.00	0.39	N
	ATOM	4738	CA	LEU	B	127	-11.223	55.120	28.455	1.00	0.39	C
	ATOM	4739	C	LEU	B	127	-11.504	54.659	29.846	1.00	0.39	C
55	ATOM	4740	O	LEU	B	127	-12.150	55.361	30.622	1.00	0.39	O
	ATOM	4741	CB	LEU	B	127	-12.082	54.243	27.532	1.00	0.39	C
	ATOM	4742	CG	LEU	B	127	-11.973	54.616	26.046	1.00	0.39	C
	ATOM	4743	CD1	LEU	B	127	-10.541	54.413	25.527	1.00	0.39	C
	ATOM	4744	CD2	LEU	B	127	-13.021	53.865	25.210	1.00	0.39	C
60	ATOM	4745	H	LEU	B	127	-9.482	54.256	27.585	1.00	0.00	H
	ATOM	4746	HA	LEU	B	127	-11.515	56.177	28.359	1.00	0.00	H
	ATOM	4747	1HB	LEU	B	127	-13.130	54.364	27.866	1.00	0.00	H
	ATOM	4748	2HB	LEU	B	127	-11.833	53.177	27.665	1.00	0.00	H
	ATOM	4749	HG	LEU	B	127	-12.194	55.696	26.007	1.00	0.00	H
65	ATOM	4750	1HD1	LEU	B	127	-10.536	53.792	24.623	1.00	0.00	H
	ATOM	4751	2HD1	LEU	B	127	-10.073	55.385	25.396	1.00	0.00	H
	ATOM	4752	3HD1	LEU	B	127	-9.942	53.772	26.170	1.00	0.00	H
	ATOM	4753	1HD2	LEU	B	127	-12.582	54.000	24.252	1.00	0.00	H
	ATOM	4754	2HD2	LEU	B	127	-13.035	52.790	25.442	1.00	0.00	H
70	ATOM	4755	3HD2	LEU	B	127	-14.037	54.274	25.281	1.00	0.00	H
	ATOM	4756	N	LYS	B	128	-11.008	53.457	30.209	1.00	0.43	N
	ATOM	4757	CA	LYS	B	128	-11.294	52.985	31.530	1.00	0.43	C

220

	ATOM	4758	C	LYS	B	128	-10.216	52.042	31.948	1.00	0.43	C
	ATOM	4759	O	LYS	B	128	-9.524	51.449	31.122	1.00	0.43	O
	ATOM	4760	CB	LYS	B	128	-12.614	52.207	31.641	1.00	0.43	C
5	ATOM	4761	CG	LYS	B	128	-12.560	50.838	30.960	1.00	0.43	C
	ATOM	4762	CD	LYS	B	128	-13.718	49.918	31.350	1.00	0.43	C
	ATOM	4763	CE	LYS	B	128	-13.540	48.478	30.872	1.00	0.43	C
	ATOM	4764	NZ	LYS	B	128	-12.447	47.835	31.635	1.00	0.43	N1+
	ATOM	4765	H	LYS	B	128	-10.327	52.978	29.647	1.00	0.00	H
10	ATOM	4766	HA	LYS	B	128	-11.296	53.843	32.227	1.00	0.00	H
	ATOM	4767	1HB	LYS	B	128	-13.445	52.810	31.235	1.00	0.00	H
	ATOM	4768	2HB	LYS	B	128	-12.825	52.073	32.717	1.00	0.00	H
	ATOM	4769	1HG	LYS	B	128	-11.647	50.306	31.271	1.00	0.00	H
	ATOM	4770	2HG	LYS	B	128	-12.473	50.978	29.880	1.00	0.00	H
15	ATOM	4771	1HD	LYS	B	128	-14.667	50.313	30.950	1.00	0.00	H
	ATOM	4772	2HD	LYS	B	128	-13.841	49.922	32.449	1.00	0.00	H
	ATOM	4773	1HE	LYS	B	128	-13.239	48.443	29.841	1.00	0.00	H
	ATOM	4774	2HE	LYS	B	128	-14.468	47.942	31.072	1.00	0.00	H
	ATOM	4775	1HZ	LYS	B	128	-12.368	46.844	31.429	1.00	0.00	H
20	ATOM	4776	2HZ	LYS	B	128	-11.541	48.241	31.441	1.00	0.00	H
	ATOM	4777	3HZ	LYS	B	128	-12.592	47.889	32.634	1.00	0.00	H
	ATOM	4778	N	TYR	B	129	-10.043	51.906	33.275	1.00	0.26	N
	ATOM	4779	CA	TYR	B	129	-9.095	50.989	33.832	1.00	0.26	C
	ATOM	4780	C	TYR	B	129	-9.784	50.262	34.940	1.00	0.26	C
25	ATOM	4781	O	TYR	B	129	-10.405	50.879	35.803	1.00	0.26	O
	ATOM	4782	CB	TYR	B	129	-7.861	51.683	34.435	1.00	0.26	C
	ATOM	4783	CG	TYR	B	129	-7.171	50.706	35.325	1.00	0.26	C
	ATOM	4784	CD1	TYR	B	129	-6.375	49.701	34.823	1.00	0.26	C
	ATOM	4785	CD2	TYR	B	129	-7.327	50.815	36.687	1.00	0.26	C
30	ATOM	4786	CE1	TYR	B	129	-5.750	48.816	35.674	1.00	0.26	C
	ATOM	4787	CE2	TYR	B	129	-6.707	49.936	37.540	1.00	0.26	C
	ATOM	4788	CZ	TYR	B	129	-5.916	48.935	37.035	1.00	0.26	C
	ATOM	4789	OH	TYR	B	129	-5.283	48.036	37.916	1.00	0.26	O
	ATOM	4790	H	TYR	B	129	-10.607	52.393	33.952	1.00	0.00	H
35	ATOM	4791	HA	TYR	B	129	-8.771	50.291	33.049	1.00	0.00	H
	ATOM	4792	1HB	TYR	B	129	-8.174	52.568	35.013	1.00	0.00	H
	ATOM	4793	2HB	TYR	B	129	-7.213	52.072	33.637	1.00	0.00	H
	ATOM	4794	HD1	TYR	B	129	-6.453	49.410	33.799	1.00	0.00	H
	ATOM	4795	HD2	TYR	B	129	-7.952	51.605	37.097	1.00	0.00	H
40	ATOM	4796	HE1	TYR	B	129	-5.114	48.061	35.238	1.00	0.00	H
	ATOM	4797	HE2	TYR	B	129	-6.841	50.075	38.607	1.00	0.00	H
	ATOM	4798	HH	TYR	B	129	-5.832	47.984	38.711	1.00	0.00	H
	ATOM	4799	N	TRP	B	130	-9.712	48.916	34.931	1.00	0.16	N
	ATOM	4800	CA	TRP	B	130	-10.311	48.181	36.006	1.00	0.16	C
45	ATOM	4801	C	TRP	B	130	-9.437	46.987	36.219	1.00	0.16	C
	ATOM	4802	O	TRP	B	130	-8.929	46.405	35.261	1.00	0.16	O
	ATOM	4803	CB	TRP	B	130	-11.716	47.655	35.683	1.00	0.16	C
	ATOM	4804	CG	TRP	B	130	-12.467	47.127	36.882	1.00	0.16	C
	ATOM	4805	CD1	TRP	B	130	-12.409	45.906	37.486	1.00	0.16	C
50	ATOM	4806	CD2	TRP	B	130	-13.463	47.882	37.588	1.00	0.16	C
	ATOM	4807	NE1	TRP	B	130	-13.299	45.859	38.532	1.00	0.16	N
	ATOM	4808	CE2	TRP	B	130	-13.957	47.066	38.603	1.00	0.16	C
	ATOM	4809	CE3	TRP	B	130	-13.932	49.151	37.402	1.00	0.16	C
	ATOM	4810	CZ2	TRP	B	130	-14.932	47.506	39.452	1.00	0.16	C
55	ATOM	4811	CZ3	TRP	B	130	-14.913	49.593	38.264	1.00	0.16	C
	ATOM	4812	CH2	TRP	B	130	-15.404	48.787	39.270	1.00	0.16	C
	ATOM	4813	H	TRP	B	130	-9.108	48.407	34.292	1.00	0.00	H
	ATOM	4814	HA	TRP	B	130	-10.329	48.805	36.916	1.00	0.00	H
	ATOM	4815	1HB	TRP	B	130	-11.622	46.878	34.909	1.00	0.00	H
60	ATOM	4816	2HB	TRP	B	130	-12.306	48.463	35.220	1.00	0.00	H
	ATOM	4817	HD1	TRP	B	130	-11.644	45.253	37.343	1.00	0.00	H
	ATOM	4818	HE1	TRP	B	130	-13.577	45.048	39.057	1.00	0.00	H
	ATOM	4819	HE3	TRP	B	130	-13.550	49.803	36.623	1.00	0.00	H
	ATOM	4820	HZ2	TRP	B	130	-15.318	46.865	40.242	1.00	0.00	H
65	ATOM	4821	HZ3	TRP	B	130	-15.309	50.600	38.152	1.00	0.00	H
	ATOM	4822	HH2	TRP	B	130	-16.179	49.170	39.930	1.00	0.00	H
	ATOM	4823	N	TYR	B	131	-9.204	46.599	37.487	1.00	0.17	N
	ATOM	4824	CA	TYR	B	131	-8.351	45.465	37.683	1.00	0.17	C
	ATOM	4825	C	TYR	B	131	-8.991	44.235	37.120	1.00	0.17	C
70	ATOM	4826	O	TYR	B	131	-8.436	43.582	36.238	1.00	0.17	O
	ATOM	4827	CB	TYR	B	131	-8.087	45.152	39.164	1.00	0.17	C
	ATOM	4828	CG	TYR	B	131	-7.166	46.173	39.731	1.00	0.17	C

221

	ATOM	4829	CD1	TYR	B	131	-7.617	47.428	40.072	1.00	0.17	C
	ATOM	4830	CD2	TYR	B	131	-5.844	45.857	39.937	1.00	0.17	C
	ATOM	4831	CE1	TYR	B	131	-6.754	48.358	40.602	1.00	0.17	C
5	ATOM	4832	CE2	TYR	B	131	-4.977	46.782	40.465	1.00	0.17	C
	ATOM	4833	CZ	TYR	B	131	-5.433	48.034	40.800	1.00	0.17	C
	ATOM	4834	OH	TYR	B	131	-4.542	48.984	41.345	1.00	0.17	O
	ATOM	4835	H	TYR	B	131	-9.633	47.043	38.280	1.00	0.00	H
	ATOM	4836	HA	TYR	B	131	-7.395	45.633	37.177	1.00	0.00	H
10	ATOM	4837	1HB	TYR	B	131	-7.635	44.147	39.216	1.00	0.00	H
	ATOM	4838	2HB	TYR	B	131	-9.022	45.099	39.746	1.00	0.00	H
	ATOM	4839	HD1	TYR	B	131	-8.667	47.686	39.973	1.00	0.00	H
	ATOM	4840	HD2	TYR	B	131	-5.494	44.854	39.704	1.00	0.00	H
	ATOM	4841	HE1	TYR	B	131	-7.138	49.337	40.884	1.00	0.00	H
15	ATOM	4842	HE2	TYR	B	131	-3.963	46.496	40.710	1.00	0.00	H
	ATOM	4843	HH	TYR	B	131	-5.050	49.530	41.957	1.00	0.00	H
	ATOM	4844	N	GLU	B	132	-10.189	43.889	37.630	1.00	0.19	N
	ATOM	4845	CA	GLU	B	132	-10.842	42.670	37.249	1.00	0.19	C
	ATOM	4846	C	GLU	B	132	-11.520	42.727	35.909	1.00	0.19	C
20	ATOM	4847	O	GLU	B	132	-11.501	41.741	35.175	1.00	0.19	O
	ATOM	4848	CB	GLU	B	132	-11.851	42.161	38.295	1.00	0.19	C
	ATOM	4849	CG	GLU	B	132	-13.030	43.092	38.565	1.00	0.19	C
	ATOM	4850	CD	GLU	B	132	-13.838	42.479	39.702	1.00	0.19	C
	ATOM	4851	OE1	GLU	B	132	-14.098	41.248	39.651	1.00	0.19	O
	ATOM	4852	OE2	GLU	B	132	-14.202	43.236	40.641	1.00	0.19	O1-
25	ATOM	4853	H	GLU	B	132	-10.574	44.356	38.433	1.00	0.00	H
	ATOM	4854	HA	GLU	B	132	-10.066	41.891	37.149	1.00	0.00	H
	ATOM	4855	1HB	GLU	B	132	-11.321	41.965	39.245	1.00	0.00	H
	ATOM	4856	2HB	GLU	B	132	-12.189	41.177	37.919	1.00	0.00	H
30	ATOM	4857	1HG	GLU	B	132	-13.639	43.344	37.692	1.00	0.00	H
	ATOM	4858	2HG	GLU	B	132	-12.498	43.899	39.059	1.00	0.00	H
	ATOM	4859	N	ASN	B	133	-12.116	43.878	35.539	1.00	0.18	N
	ATOM	4860	CA	ASN	B	133	-12.974	43.903	34.382	1.00	0.18	C
	ATOM	4861	C	ASN	B	133	-12.209	43.857	33.098	1.00	0.18	C
35	ATOM	4862	O	ASN	B	133	-11.487	44.786	32.738	1.00	0.18	O
	ATOM	4863	CB	ASN	B	133	-13.907	45.129	34.320	1.00	0.18	C
	ATOM	4864	CG	ASN	B	133	-14.988	44.843	33.284	1.00	0.18	C
	ATOM	4865	OD1	ASN	B	133	-14.893	43.882	32.522	1.00	0.18	O
	ATOM	4866	ND2	ASN	B	133	-16.041	45.704	33.248	1.00	0.18	N
40	ATOM	4867	H	ASN	B	133	-12.148	44.684	36.122	1.00	0.00	H
	ATOM	4868	HA	ASN	B	133	-13.641	43.023	34.482	1.00	0.00	H
	ATOM	4869	1HB	ASN	B	133	-13.387	46.056	34.048	1.00	0.00	H
	ATOM	4870	2HB	ASN	B	133	-14.388	45.278	35.302	1.00	0.00	H
	ATOM	4871	1HD2	ASN	B	133	-16.148	46.456	33.904	1.00	0.00	H
45	ATOM	4872	2HD2	ASN	B	133	-16.734	45.541	32.536	1.00	0.00	H
	ATOM	4873	N	HIS	B	134	-12.358	42.718	32.393	1.00	0.16	N
	ATOM	4874	CA	HIS	B	134	-11.782	42.426	31.111	1.00	0.16	C
	ATOM	4875	C	HIS	B	134	-12.510	43.153	30.020	1.00	0.16	C
	ATOM	4876	O	HIS	B	134	-11.908	43.530	29.016	1.00	0.16	O
50	ATOM	4877	CB	HIS	B	134	-11.845	40.927	30.781	1.00	0.16	C
	ATOM	4878	CG	HIS	B	134	-11.133	40.093	31.803	1.00	0.16	C
	ATOM	4879	ND1	HIS	B	134	-9.767	39.912	31.837	1.00	0.16	N
	ATOM	4880	CD2	HIS	B	134	-11.627	39.390	32.858	1.00	0.16	C
	ATOM	4881	CE1	HIS	B	134	-9.506	39.115	32.903	1.00	0.16	C
55	ATOM	4882	NE2	HIS	B	134	-10.603	38.772	33.554	1.00	0.16	N
	ATOM	4883	H	HIS	B	134	-12.816	41.946	32.852	1.00	0.00	H
	ATOM	4884	HA	HIS	B	134	-10.736	42.768	31.094	1.00	0.00	H
	ATOM	4885	1HB	HIS	B	134	-11.406	40.786	29.778	1.00	0.00	H
	ATOM	4886	2HB	HIS	B	134	-12.890	40.590	30.715	1.00	0.00	H
60	ATOM	4887	HD2	HIS	B	134	-12.657	39.288	33.175	1.00	0.00	H
	ATOM	4888	HE1	HIS	B	134	-8.543	38.682	33.088	1.00	0.00	H
	ATOM	4889	HE2	HIS	B	134	-10.667	38.227	34.389	1.00	0.00	H
	ATOM	4890	N	ASN	B	135	-13.835	43.359	30.179	1.00	0.14	N
	ATOM	4891	CA	ASN	B	135	-14.631	43.884	29.100	1.00	0.14	C
65	ATOM	4892	C	ASN	B	135	-14.941	45.332	29.306	1.00	0.14	C
	ATOM	4893	O	ASN	B	135	-14.867	45.856	30.416	1.00	0.14	O
	ATOM	4894	CB	ASN	B	135	-15.986	43.176	28.963	1.00	0.14	C
	ATOM	4895	CG	ASN	B	135	-15.720	41.710	28.665	1.00	0.14	C
	ATOM	4896	OD1	ASN	B	135	-15.032	41.368	27.704	1.00	0.14	O
70	ATOM	4897	ND2	ASN	B	135	-16.270	40.813	29.528	1.00	0.14	N
	ATOM	4898	H	ASN	B	135	-14.277	43.286	31.091	1.00	0.00	H
	ATOM	4899	HA	ASN	B	135	-14.091	43.740	28.156	1.00	0.00	H

222

	ATOM	4900	1HB	ASN	B	135	-16.465	43.667	28.112	1.00	0.00	H
	ATOM	4901	2HB	ASN	B	135	-16.609	43.336	29.857	1.00	0.00	H
	ATOM	4902	1HD2	ASN	B	135	-16.809	41.103	30.323	1.00	0.00	H
5	ATOM	4903	2HD2	ASN	B	135	-16.088	39.839	29.364	1.00	0.00	H
	ATOM	4904	N	ILE	B	136	-15.270	46.020	28.190	1.00	0.19	N
	ATOM	4905	CA	ILE	B	136	-15.665	47.399	28.207	1.00	0.19	C
	ATOM	4906	C	ILE	B	136	-16.831	47.525	27.279	1.00	0.19	C
	ATOM	4907	O	ILE	B	136	-16.909	46.824	26.272	1.00	0.19	O
10	ATOM	4908	CB	ILE	B	136	-14.612	48.337	27.694	1.00	0.19	C
	ATOM	4909	CG1	ILE	B	136	-15.014	49.796	27.966	1.00	0.19	C
	ATOM	4910	CG2	ILE	B	136	-14.381	48.022	26.207	1.00	0.19	C
	ATOM	4911	CD1	ILE	B	136	-13.874	50.789	27.751	1.00	0.19	C
	ATOM	4912	H	ILE	B	136	-15.313	45.559	27.283	1.00	0.00	H
15	ATOM	4913	HA	ILE	B	136	-15.976	47.652	29.234	1.00	0.00	H
	ATOM	4914	HB	ILE	B	136	-13.653	48.104	28.141	1.00	0.00	H
	ATOM	4915	1HG1	ILE	B	136	-15.391	49.896	28.996	1.00	0.00	H
	ATOM	4916	2HG1	ILE	B	136	-15.848	50.096	27.307	1.00	0.00	H
	ATOM	4917	1HG2	ILE	B	136	-13.544	48.610	25.812	1.00	0.00	H
20	ATOM	4918	2HG2	ILE	B	136	-14.172	46.948	26.193	1.00	0.00	H
	ATOM	4919	3HG2	ILE	B	136	-15.231	48.283	25.560	1.00	0.00	H
	ATOM	4920	1HD1	ILE	B	136	-14.060	51.752	28.250	1.00	0.00	H
	ATOM	4921	2HD1	ILE	B	136	-12.927	50.375	28.101	1.00	0.00	H
	ATOM	4922	3HD1	ILE	B	136	-13.745	50.990	26.675	1.00	0.00	H
25	ATOM	4923	N	SER	B	137	-17.788	48.414	27.604	1.00	0.24	N
	ATOM	4924	CA	SER	B	137	-18.920	48.568	26.741	1.00	0.24	C
	ATOM	4925	C	SER	B	137	-19.203	50.029	26.610	1.00	0.24	C
	ATOM	4926	O	SER	B	137	-19.102	50.781	27.577	1.00	0.24	O
	ATOM	4927	CB	SER	B	137	-20.185	47.894	27.299	1.00	0.24	C
30	ATOM	4928	OG	SER	B	137	-21.276	48.071	26.411	1.00	0.24	O
	ATOM	4929	H	SER	B	137	-17.726	49.066	28.368	1.00	0.00	H
	ATOM	4930	HA	SER	B	137	-18.674	48.121	25.782	1.00	0.00	H
	ATOM	4931	1HB	SER	B	137	-20.436	48.283	28.302	1.00	0.00	H
	ATOM	4932	2HB	SER	B	137	-20.027	46.813	27.395	1.00	0.00	H
35	ATOM	4933	HG	SER	B	137	-21.483	49.017	26.401	1.00	0.00	H
	ATOM	4934	N	ILE	B	138	-19.553	50.475	25.389	1.00	0.31	N
	ATOM	4935	CA	ILE	B	138	-19.872	51.857	25.203	1.00	0.31	C
	ATOM	4936	C	ILE	B	138	-21.299	51.893	24.779	1.00	0.31	C
	ATOM	4937	O	ILE	B	138	-21.688	51.253	23.804	1.00	0.31	O
40	ATOM	4938	CB	ILE	B	138	-19.075	52.508	24.114	1.00	0.31	C
	ATOM	4939	CG1	ILE	B	138	-17.571	52.405	24.424	1.00	0.31	C
	ATOM	4940	CG2	ILE	B	138	-19.578	53.954	23.962	1.00	0.31	C
	ATOM	4941	CD1	ILE	B	138	-16.674	52.719	23.229	1.00	0.31	C
	ATOM	4942	H	ILE	B	138	-19.600	49.853	24.587	1.00	0.00	H
45	ATOM	4943	HA	ILE	B	138	-19.710	52.421	26.135	1.00	0.00	H
	ATOM	4944	HB	ILE	B	138	-19.268	52.008	23.155	1.00	0.00	H
	ATOM	4945	1HG1	ILE	B	138	-17.316	51.376	24.735	1.00	0.00	H
	ATOM	4946	2HG1	ILE	B	138	-17.308	53.049	25.281	1.00	0.00	H
	ATOM	4947	1HG2	ILE	B	138	-18.854	54.629	23.492	1.00	0.00	H
50	ATOM	4948	2HG2	ILE	B	138	-20.505	54.001	23.368	1.00	0.00	H
	ATOM	4949	3HG2	ILE	B	138	-19.788	54.411	24.944	1.00	0.00	H
	ATOM	4950	1HD1	ILE	B	138	-15.696	52.223	23.340	1.00	0.00	H
	ATOM	4951	2HD1	ILE	B	138	-17.111	52.364	22.288	1.00	0.00	H
	ATOM	4952	3HD1	ILE	B	138	-16.455	53.793	23.163	1.00	0.00	H
55	ATOM	4953	N	THR	B	139	-22.134	52.652	25.502	1.00	0.40	N
	ATOM	4954	CA	THR	B	139	-23.515	52.679	25.136	1.00	0.40	C
	ATOM	4955	C	THR	B	139	-23.749	53.927	24.359	1.00	0.40	C
	ATOM	4956	O	THR	B	139	-23.036	54.914	24.535	1.00	0.40	O
	ATOM	4957	CB	THR	B	139	-24.443	52.677	26.311	1.00	0.40	C
60	ATOM	4958	OG1	THR	B	139	-24.163	53.789	27.147	1.00	0.40	O
	ATOM	4959	CG2	THR	B	139	-24.261	51.362	27.085	1.00	0.40	C
	ATOM	4960	H	THR	B	139	-21.877	53.234	26.282	1.00	0.00	H
	ATOM	4961	HA	THR	B	139	-23.767	51.798	24.523	1.00	0.00	H
	ATOM	4962	HB	THR	B	139	-25.487	52.734	25.945	1.00	0.00	H
65	ATOM	4963	HG1	THR	B	139	-24.403	54.588	26.652	1.00	0.00	H
	ATOM	4964	1HG2	THR	B	139	-24.978	51.292	27.920	1.00	0.00	H
	ATOM	4965	2HG2	THR	B	139	-24.420	50.485	26.436	1.00	0.00	H
	ATOM	4966	3HG2	THR	B	139	-23.251	51.293	27.520	1.00	0.00	H
	ATOM	4967	N	ASN	B	140	-24.763	53.894	23.470	1.00	0.29	N
70	ATOM	4968	CA	ASN	B	140	-25.086	55.022	22.647	1.00	0.29	C
	ATOM	4969	C	ASN	B	140	-23.840	55.522	21.994	1.00	0.29	C
	ATOM	4970	O	ASN	B	140	-23.385	56.631	22.272	1.00	0.29	O

223

	ATOM	4971	CB	ASN	B	140	-25.727	56.185	23.423	1.00	0.29	C
	ATOM	4972	CG	ASN	B	140	-27.131	55.764	23.832	1.00	0.29	C
	ATOM	4973	OD1	ASN	B	140	-27.317	54.884	24.671	1.00	0.29	O
5	ATOM	4974	ND2	ASN	B	140	-28.154	56.419	23.222	1.00	0.29	N
	ATOM	4975	H	ASN	B	140	-25.351	53.083	23.363	1.00	0.00	H
	ATOM	4976	HA	ASN	B	140	-25.796	54.687	21.874	1.00	0.00	H
	ATOM	4977	1HB	ASN	B	140	-25.766	57.075	22.770	1.00	0.00	H
	ATOM	4978	2HB	ASN	B	140	-25.173	56.460	24.334	1.00	0.00	H
10	ATOM	4979	1HD2	ASN	B	140	-27.995	57.144	22.547	1.00	0.00	H
	ATOM	4980	2HD2	ASN	B	140	-29.087	56.156	23.487	1.00	0.00	H
	ATOM	4981	N	ALA	B	141	-23.250	54.699	21.107	1.00	0.26	N
	ATOM	4982	CA	ALA	B	141	-22.029	55.068	20.453	1.00	0.26	C
	ATOM	4983	C	ALA	B	141	-22.269	56.305	19.652	1.00	0.26	C
15	ATOM	4984	O	ALA	B	141	-23.383	56.573	19.206	1.00	0.26	O
	ATOM	4985	CB	ALA	B	141	-21.490	53.988	19.499	1.00	0.26	C
	ATOM	4986	H	ALA	B	141	-23.587	53.762	20.926	1.00	0.00	H
	ATOM	4987	HA	ALA	B	141	-21.258	55.258	21.225	1.00	0.00	H
	ATOM	4988	1HB	ALA	B	141	-20.549	54.340	19.046	1.00	0.00	H
20	ATOM	4989	2HB	ALA	B	141	-21.267	53.060	20.048	1.00	0.00	H
	ATOM	4990	3HB	ALA	B	141	-22.201	53.762	18.690	1.00	0.00	H
	ATOM	4991	N	THR	B	142	-21.198	57.103	19.475	1.00	0.35	N
	ATOM	4992	CA	THR	B	142	-21.277	58.331	18.746	1.00	0.35	C
	ATOM	4993	C	THR	B	142	-20.122	58.368	17.797	1.00	0.35	C
	ATOM	4994	O	THR	B	142	-19.288	57.465	17.779	1.00	0.35	O
25	ATOM	4995	CB	THR	B	142	-21.175	59.547	19.617	1.00	0.35	C
	ATOM	4996	OG1	THR	B	142	-21.424	60.721	18.859	1.00	0.35	O
	ATOM	4997	CG2	THR	B	142	-19.764	59.596	20.230	1.00	0.35	C
	ATOM	4998	H	THR	B	142	-20.268	56.794	19.709	1.00	0.00	H
	ATOM	4999	HA	THR	B	142	-22.202	58.374	18.164	1.00	0.00	H
30	ATOM	5000	HB	THR	B	142	-21.924	59.484	20.430	1.00	0.00	H
	ATOM	5001	HG1	THR	B	142	-20.924	61.441	19.314	1.00	0.00	H
	ATOM	5002	1HG2	THR	B	142	-19.677	60.411	20.966	1.00	0.00	H
	ATOM	5003	2HG2	THR	B	142	-19.545	58.677	20.799	1.00	0.00	H
	ATOM	5004	3HG2	THR	B	142	-19.002	59.711	19.495	1.00	0.00	H
35	ATOM	5005	N	VAL	B	143	-20.067	59.427	16.968	1.00	0.29	N
	ATOM	5006	CA	VAL	B	143	-19.038	59.595	15.985	1.00	0.29	C
	ATOM	5007	C	VAL	B	143	-17.723	59.745	16.680	1.00	0.29	C
	ATOM	5008	O	VAL	B	143	-16.696	59.265	16.203	1.00	0.29	O
40	ATOM	5009	CB	VAL	B	143	-19.256	60.803	15.127	1.00	0.29	C
	ATOM	5010	CG1	VAL	B	143	-18.096	60.900	14.122	1.00	0.29	C
	ATOM	5011	CG2	VAL	B	143	-20.644	60.686	14.470	1.00	0.29	C
	ATOM	5012	H	VAL	B	143	-20.761	60.162	17.079	1.00	0.00	H
	ATOM	5013	HA	VAL	B	143	-18.850	58.830	15.329	1.00	0.00	H
45	ATOM	5014	HB	VAL	B	143	-19.249	61.727	15.730	1.00	0.00	H
	ATOM	5015	1HG1	VAL	B	143	-18.282	61.693	13.377	1.00	0.00	H
	ATOM	5016	2HG1	VAL	B	143	-17.142	61.156	14.609	1.00	0.00	H
	ATOM	5017	3HG1	VAL	B	143	-17.963	59.961	13.559	1.00	0.00	H
	ATOM	5018	1HG2	VAL	B	143	-20.742	61.326	13.578	1.00	0.00	H
50	ATOM	5019	2HG2	VAL	B	143	-20.859	59.656	14.167	1.00	0.00	H
	ATOM	5020	3HG2	VAL	B	143	-21.447	60.987	15.163	1.00	0.00	H
	ATOM	5021	N	GLU	B	144	-17.728	60.414	17.845	1.00	0.25	N
	ATOM	5022	CA	GLU	B	144	-16.522	60.650	18.585	1.00	0.25	C
	ATOM	5023	C	GLU	B	144	-15.953	59.324	18.969	1.00	0.25	C
55	ATOM	5024	O	GLU	B	144	-14.738	59.159	19.072	1.00	0.25	O
	ATOM	5025	CB	GLU	B	144	-16.760	61.452	19.874	1.00	0.25	C
	ATOM	5026	CG	GLU	B	144	-17.200	62.889	19.597	1.00	0.25	C
	ATOM	5027	CD	GLU	B	144	-18.626	62.836	19.072	1.00	0.25	C
	ATOM	5028	OE1	GLU	B	144	-19.542	62.548	19.886	1.00	0.25	O
60	ATOM	5029	OE2	GLU	B	144	-18.817	63.075	17.849	1.00	0.25	O1-
	ATOM	5030	H	GLU	B	144	-18.487	61.065	18.039	1.00	0.00	H
	ATOM	5031	HA	GLU	B	144	-15.773	61.169	17.962	1.00	0.00	H
	ATOM	5032	1HB	GLU	B	144	-15.791	61.461	20.406	1.00	0.00	H
	ATOM	5033	2HB	GLU	B	144	-17.460	60.941	20.552	1.00	0.00	H
65	ATOM	5034	1HG	GLU	B	144	-16.520	63.373	18.878	1.00	0.00	H
	ATOM	5035	2HG	GLU	B	144	-17.181	63.464	20.537	1.00	0.00	H
	ATOM	5036	N	ASP	B	145	-16.834	58.331	19.171	1.00	0.22	N
	ATOM	5037	CA	ASP	B	145	-16.438	57.030	19.619	1.00	0.22	C
	ATOM	5038	C	ASP	B	145	-15.451	56.448	18.657	1.00	0.22	C
	ATOM	5039	O	ASP	B	145	-14.495	55.797	19.079	1.00	0.22	O
70	ATOM	5040	CB	ASP	B	145	-17.632	56.064	19.718	1.00	0.22	C
	ATOM	5041	CG	ASP	B	145	-17.196	54.793	20.435	1.00	0.22	C

224

	ATOM	5042	OD1	ASP	B	145	-16.201	54.160	19.992	1.00	0.22	O
	ATOM	5043	OD2	ASP	B	145	-17.856	54.442	21.448	1.00	0.22	O1-
	ATOM	5044	H	ASP	B	145	-17.800	58.450	18.901	1.00	0.00	H
5	ATOM	5045	HA	ASP	B	145	-15.940	57.121	20.598	1.00	0.00	H
	ATOM	5046	1HB	ASP	B	145	-17.956	55.760	18.717	1.00	0.00	H
	ATOM	5047	2HB	ASP	B	145	-18.467	56.523	20.264	1.00	0.00	H
	ATOM	5048	N	SER	B	146	-15.638	56.670	17.341	1.00	0.20	N
	ATOM	5049	CA	SER	B	146	-14.748	56.087	16.374	1.00	0.20	C
10	ATOM	5050	C	SER	B	146	-13.344	56.482	16.696	1.00	0.20	C
	ATOM	5051	O	SER	B	146	-13.085	57.579	17.191	1.00	0.20	O
	ATOM	5052	CB	SER	B	146	-15.037	56.523	14.926	1.00	0.20	C
	ATOM	5053	OG	SER	B	146	-14.798	57.915	14.780	1.00	0.20	O
	ATOM	5054	H	SER	B	146	-16.339	57.340	17.064	1.00	0.00	H
15	ATOM	5055	HA	SER	B	146	-14.867	54.991	16.450	1.00	0.00	H
	ATOM	5056	1HB	SER	B	146	-16.065	56.298	14.651	1.00	0.00	H
	ATOM	5057	2HB	SER	B	146	-14.320	56.051	14.248	1.00	0.00	H
	ATOM	5058	HG	SER	B	146	-15.343	58.395	15.432	1.00	0.00	H
	ATOM	5059	N	GLY	B	147	-12.394	55.561	16.442	1.00	0.21	N
20	ATOM	5060	CA	GLY	B	147	-11.020	55.841	16.735	1.00	0.21	C
	ATOM	5061	C	GLY	B	147	-10.301	54.535	16.762	1.00	0.21	C
	ATOM	5062	O	GLY	B	147	-10.814	53.517	16.299	1.00	0.21	O
	ATOM	5063	H	GLY	B	147	-12.613	54.654	16.041	1.00	0.00	H
	ATOM	5064	1HA	GLY	B	147	-10.942	56.340	17.716	1.00	0.00	H
25	ATOM	5065	2HA	GLY	B	147	-10.567	56.502	15.975	1.00	0.00	H
	ATOM	5066	N	THR	B	148	-9.071	54.538	17.306	1.00	0.17	N
	ATOM	5067	CA	THR	B	148	-8.323	53.322	17.360	1.00	0.17	C
	ATOM	5068	C	THR	B	148	-8.332	52.870	18.779	1.00	0.17	C
	ATOM	5069	O	THR	B	148	-8.106	53.661	19.694	1.00	0.17	O
30	ATOM	5070	CB	THR	B	148	-6.895	53.491	16.948	1.00	0.17	C
	ATOM	5071	OG1	THR	B	148	-6.829	53.999	15.623	1.00	0.17	O
	ATOM	5072	CG2	THR	B	148	-6.209	52.120	17.013	1.00	0.17	C
	ATOM	5073	H	THR	B	148	-8.624	55.388	17.678	1.00	0.00	H
	ATOM	5074	HA	THR	B	148	-8.767	52.588	16.674	1.00	0.00	H
35	ATOM	5075	HB	THR	B	148	-6.364	54.181	17.632	1.00	0.00	H
	ATOM	5076	HG1	THR	B	148	-7.244	54.874	15.660	1.00	0.00	H
	ATOM	5077	1HG2	THR	B	148	-5.147	52.241	16.751	1.00	0.00	H
	ATOM	5078	2HG2	THR	B	148	-6.308	51.719	18.025	1.00	0.00	H
	ATOM	5079	3HG2	THR	B	148	-6.655	51.422	16.289	1.00	0.00	H
40	ATOM	5080	N	TYR	B	149	-8.616	51.574	19.001	1.00	0.12	N
	ATOM	5081	CA	TYR	B	149	-8.660	51.076	20.343	1.00	0.12	C
	ATOM	5082	C	TYR	B	149	-7.643	49.994	20.494	1.00	0.12	C
	ATOM	5083	O	TYR	B	149	-7.419	49.197	19.586	1.00	0.12	O
	ATOM	5084	CB	TYR	B	149	-9.999	50.428	20.732	1.00	0.12	C
45	ATOM	5085	CG	TYR	B	149	-11.045	51.479	20.866	1.00	0.12	C
	ATOM	5086	CD1	TYR	B	149	-11.674	51.998	19.759	1.00	0.12	C
	ATOM	5087	CD2	TYR	B	149	-11.402	51.932	22.113	1.00	0.12	C
	ATOM	5088	CE1	TYR	B	149	-12.644	52.962	19.899	1.00	0.12	C
	ATOM	5089	CE2	TYR	B	149	-12.372	52.895	22.260	1.00	0.12	C
50	ATOM	5090	CZ	TYR	B	149	-12.993	53.412	21.150	1.00	0.12	C
	ATOM	5091	OH	TYR	B	149	-13.989	54.400	21.293	1.00	0.12	O
	ATOM	5092	H	TYR	B	149	-8.796	50.923	18.245	1.00	0.00	H
	ATOM	5093	HA	TYR	B	149	-8.441	51.899	21.010	1.00	0.00	H
	ATOM	5094	1HB	TYR	B	149	-9.845	49.950	21.708	1.00	0.00	H
55	ATOM	5095	2HB	TYR	B	149	-10.289	49.654	20.005	1.00	0.00	H
	ATOM	5096	HD1	TYR	B	149	-11.402	51.655	18.764	1.00	0.00	H
	ATOM	5097	HD2	TYR	B	149	-10.961	51.469	22.992	1.00	0.00	H
	ATOM	5098	HE1	TYR	B	149	-13.123	53.373	19.011	1.00	0.00	H
	ATOM	5099	HE2	TYR	B	149	-13.003	52.773	23.120	1.00	0.00	H
60	ATOM	5100	HH	TYR	B	149	-14.641	54.316	20.555	1.00	0.00	H
	ATOM	5101	N	TYR	B	150	-6.980	49.968	21.666	1.00	0.12	N
	ATOM	5102	CA	TYR	B	150	-6.072	48.906	21.976	1.00	0.12	C
	ATOM	5103	C	TYR	B	150	-6.183	48.678	23.446	1.00	0.12	C
	ATOM	5104	O	TYR	B	150	-6.750	49.497	24.169	1.00	0.12	O
65	ATOM	5105	CB	TYR	B	150	-4.574	49.181	21.581	1.00	0.12	C
	ATOM	5106	CG	TYR	B	150	-4.087	50.632	21.583	1.00	0.12	C
	ATOM	5107	CD1	TYR	B	150	-2.898	50.942	22.234	1.00	0.12	C
	ATOM	5108	CD2	TYR	B	150	-4.656	51.650	20.809	1.00	0.12	C
	ATOM	5109	CE1	TYR	B	150	-2.277	52.174	22.099	1.00	0.12	C
70	ATOM	5110	CE2	TYR	B	150	-4.087	52.909	20.709	1.00	0.12	C
	ATOM	5111	CZ	TYR	B	150	-2.865	53.188	21.343	1.00	0.12	C
	ATOM	5112	OH	TYR	B	150	-2.303	54.417	21.177	1.00	0.12	O

225

	ATOM	5113	H	TYR	B	150	-7.179	50.628	22.407	1.00	0.00	H
	ATOM	5114	HA	TYR	B	150	-6.417	47.983	21.478	1.00	0.00	H
	ATOM	5115	1HB	TYR	B	150	-4.376	48.771	20.583	1.00	0.00	H
5	ATOM	5116	2HB	TYR	B	150	-3.930	48.575	22.238	1.00	0.00	H
	ATOM	5117	HD1	TYR	B	150	-2.411	50.183	22.843	1.00	0.00	H
	ATOM	5118	HD2	TYR	B	150	-5.552	51.456	20.231	1.00	0.00	H
	ATOM	5119	HE1	TYR	B	150	-1.312	52.306	22.582	1.00	0.00	H
	ATOM	5120	HE2	TYR	B	150	-4.566	53.669	20.094	1.00	0.00	H
10	ATOM	5121	HH	TYR	B	150	-1.388	54.382	21.485	1.00	0.00	H
	ATOM	5122	N	CYS	B	151	-5.668	47.538	23.936	1.00	0.27	N
	ATOM	5123	CA	CYS	B	151	-5.851	47.259	25.325	1.00	0.27	C
	ATOM	5124	C	CYS	B	151	-4.536	46.869	25.912	1.00	0.27	C
	ATOM	5125	O	CYS	B	151	-3.648	46.384	25.215	1.00	0.27	O
15	ATOM	5126	CB	CYS	B	151	-6.843	46.104	25.548	1.00	0.27	C
	ATOM	5127	SG	CYS	B	151	-7.171	45.727	27.291	1.00	0.27	S
	ATOM	5128	H	CYS	B	151	-5.059	46.930	23.420	1.00	0.00	H
	ATOM	5129	HA	CYS	B	151	-6.218	48.148	25.849	1.00	0.00	H
	ATOM	5130	1HB	CYS	B	151	-6.499	45.191	25.037	1.00	0.00	H
20	ATOM	5131	2HB	CYS	B	151	-7.796	46.404	25.083	1.00	0.00	H
	ATOM	5132	N	THR	B	152	-4.373	47.128	27.222	1.00	0.37	N
	ATOM	5133	CA	THR	B	152	-3.202	46.713	27.934	1.00	0.37	C
	ATOM	5134	C	THR	B	152	-3.659	45.920	29.104	1.00	0.37	C
	ATOM	5135	O	THR	B	152	-4.747	46.133	29.635	1.00	0.37	O
25	ATOM	5136	CB	THR	B	152	-2.327	47.824	28.434	1.00	0.37	C
	ATOM	5137	OG1	THR	B	152	-3.105	48.812	29.091	1.00	0.37	O
	ATOM	5138	CG2	THR	B	152	-1.524	48.412	27.271	1.00	0.37	C
	ATOM	5139	H	THR	B	152	-5.082	47.588	27.778	1.00	0.00	H
	ATOM	5140	HA	THR	B	152	-2.623	46.045	27.283	1.00	0.00	H
30	ATOM	5141	HB	THR	B	152	-1.602	47.395	29.156	1.00	0.00	H
	ATOM	5142	HG1	THR	B	152	-2.553	49.611	29.152	1.00	0.00	H
	ATOM	5143	1HG2	THR	B	152	-0.892	49.248	27.611	1.00	0.00	H
	ATOM	5144	2HG2	THR	B	152	-0.852	47.655	26.850	1.00	0.00	H
	ATOM	5145	3HG2	THR	B	152	-2.185	48.790	26.476	1.00	0.00	H
35	ATOM	5146	N	GLY	B	153	-2.829	44.947	29.520	1.00	0.21	N
	ATOM	5147	CA	GLY	B	153	-3.195	44.136	30.637	1.00	0.21	C
	ATOM	5148	C	GLY	B	153	-1.974	43.392	31.040	1.00	0.21	C
	ATOM	5149	O	GLY	B	153	-1.021	43.278	30.271	1.00	0.21	O
	ATOM	5150	H	GLY	B	153	-1.886	44.837	29.146	1.00	0.00	H
40	ATOM	5151	1HA	GLY	B	153	-3.993	43.422	30.370	1.00	0.00	H
	ATOM	5152	2HA	GLY	B	153	-3.543	44.766	31.450	1.00	0.00	H
	ATOM	5153	N	LYS	B	154	-1.972	42.860	32.275	1.00	0.12	N
	ATOM	5154	CA	LYS	B	154	-0.807	42.155	32.702	1.00	0.12	C
	ATOM	5155	C	LYS	B	154	-1.155	40.715	32.821	1.00	0.12	C
45	ATOM	5156	O	LYS	B	154	-2.059	40.336	33.565	1.00	0.12	O
	ATOM	5157	CB	LYS	B	154	-0.290	42.601	34.077	1.00	0.12	C
	ATOM	5158	CG	LYS	B	154	0.176	44.056	34.106	1.00	0.12	C
	ATOM	5159	CD	LYS	B	154	0.395	44.591	35.521	1.00	0.12	C
	ATOM	5160	CE	LYS	B	154	0.863	46.048	35.557	1.00	0.12	C
50	ATOM	5161	NZ	LYS	B	154	1.046	46.488	36.959	1.00	0.12	N1+
	ATOM	5162	H	LYS	B	154	-2.733	42.972	32.935	1.00	0.00	H
	ATOM	5163	HA	LYS	B	154	-0.031	42.235	31.958	1.00	0.00	H
	ATOM	5164	1HB	LYS	B	154	0.526	41.927	34.362	1.00	0.00	H
	ATOM	5165	2HB	LYS	B	154	-1.176	42.511	34.684	1.00	0.00	H
55	ATOM	5166	1HG	LYS	B	154	-0.548	44.710	33.586	1.00	0.00	H
	ATOM	5167	2HG	LYS	B	154	1.115	44.114	33.543	1.00	0.00	H
	ATOM	5168	1HD	LYS	B	154	1.072	43.927	36.083	1.00	0.00	H
	ATOM	5169	2HD	LYS	B	154	-0.602	44.565	35.950	1.00	0.00	H
	ATOM	5170	1HE	LYS	B	154	0.129	46.719	35.080	1.00	0.00	H
60	ATOM	5171	2HE	LYS	B	154	1.829	46.180	35.041	1.00	0.00	H
	ATOM	5172	1HZ	LYS	B	154	1.435	47.422	36.999	1.00	0.00	H
	ATOM	5173	2HZ	LYS	B	154	0.179	46.508	37.465	1.00	0.00	H
	ATOM	5174	3HZ	LYS	B	154	1.701	45.889	37.446	1.00	0.00	H
	ATOM	5175	N	VAL	B	155	-0.441	39.872	32.056	1.00	0.20	N
65	ATOM	5176	CA	VAL	B	155	-0.620	38.462	32.171	1.00	0.20	C
	ATOM	5177	C	VAL	B	155	0.646	37.984	32.782	1.00	0.20	C
	ATOM	5178	O	VAL	B	155	1.735	38.387	32.374	1.00	0.20	O
	ATOM	5179	CB	VAL	B	155	-0.804	37.761	30.854	1.00	0.20	C
	ATOM	5180	CG1	VAL	B	155	-2.117	38.254	30.221	1.00	0.20	C
70	ATOM	5181	CG2	VAL	B	155	0.439	38.013	29.983	1.00	0.20	C
	ATOM	5182	H	VAL	B	155	0.465	40.165	31.706	1.00	0.00	H
	ATOM	5183	HA	VAL	B	155	-1.474	38.239	32.829	1.00	0.00	H

	ATOM	5184	HB	VAL	B	155	-0.898	36.681	31.070	1.00	0.00	H
	ATOM	5185	1HG1	VAL	B	155	-2.526	37.547	29.484	1.00	0.00	H
	ATOM	5186	2HG1	VAL	B	155	-2.861	38.423	31.007	1.00	0.00	H
5	ATOM	5187	3HG1	VAL	B	155	-1.975	39.222	29.711	1.00	0.00	H
	ATOM	5188	1HG2	VAL	B	155	0.249	37.694	28.942	1.00	0.00	H
	ATOM	5189	2HG2	VAL	B	155	0.649	39.081	29.939	1.00	0.00	H
	ATOM	5190	3HG2	VAL	B	155	1.343	37.475	30.285	1.00	0.00	H
	ATOM	5191	N	TRP	B	156	0.539	37.143	33.820	1.00	0.33	N
10	ATOM	5192	CA	TRP	B	156	1.740	36.713	34.455	1.00	0.33	C
	ATOM	5193	C	TRP	B	156	2.323	37.955	35.034	1.00	0.33	C
	ATOM	5194	O	TRP	B	156	1.605	38.904	35.350	1.00	0.33	O
	ATOM	5195	CB	TRP	B	156	2.765	36.100	33.483	1.00	0.33	C
	ATOM	5196	CG	TRP	B	156	2.277	34.858	32.771	1.00	0.33	C
15	ATOM	5197	CD1	TRP	B	156	1.694	34.753	31.543	1.00	0.33	C
	ATOM	5198	CD2	TRP	B	156	2.345	33.525	33.303	1.00	0.33	C
	ATOM	5199	NE1	TRP	B	156	1.392	33.439	31.275	1.00	0.33	N
	ATOM	5200	CE2	TRP	B	156	1.787	32.671	32.350	1.00	0.33	C
	ATOM	5201	CE3	TRP	B	156	2.832	33.050	34.487	1.00	0.33	C
20	ATOM	5202	CZ2	TRP	B	156	1.705	31.325	32.569	1.00	0.33	C
	ATOM	5203	CZ3	TRP	B	156	2.748	31.691	34.703	1.00	0.33	C
	ATOM	5204	CH2	TRP	B	156	2.195	30.845	33.763	1.00	0.33	C
	ATOM	5205	H	TRP	B	156	-0.349	36.804	34.155	1.00	0.00	H
	ATOM	5206	HA	TRP	B	156	1.505	36.007	35.270	1.00	0.00	H
25	ATOM	5207	1HB	TRP	B	156	3.617	35.752	34.092	1.00	0.00	H
	ATOM	5208	2HB	TRP	B	156	3.230	36.786	32.765	1.00	0.00	H
	ATOM	5209	HD1	TRP	B	156	1.470	35.527	30.827	1.00	0.00	H
	ATOM	5210	HE1	TRP	B	156	0.852	33.107	30.508	1.00	0.00	H
	ATOM	5211	HE3	TRP	B	156	3.265	33.702	35.237	1.00	0.00	H
30	ATOM	5212	HZ2	TRP	B	156	1.272	30.662	31.826	1.00	0.00	H
	ATOM	5213	HZ3	TRP	B	156	3.122	31.273	35.635	1.00	0.00	H
	ATOM	5214	HH2	TRP	B	156	2.143	29.779	33.972	1.00	0.00	H
	ATOM	5215	N	GLN	B	157	3.656	37.967	35.190	1.00	0.49	N
	ATOM	5216	CA	GLN	B	157	4.338	39.097	35.739	1.00	0.49	C
35	ATOM	5217	C	GLN	B	157	4.276	40.236	34.773	1.00	0.49	C
	ATOM	5218	O	GLN	B	157	4.048	41.381	35.160	1.00	0.49	O
	ATOM	5219	CB	GLN	B	157	5.830	38.816	35.969	1.00	0.49	C
	ATOM	5220	CG	GLN	B	157	6.082	37.569	36.814	1.00	0.49	C
	ATOM	5221	CD	GLN	B	157	5.294	37.721	38.101	1.00	0.49	C
40	ATOM	5222	OE1	GLN	B	157	5.354	38.759	38.756	1.00	0.49	O
	ATOM	5223	NE2	GLN	B	157	4.525	36.663	38.466	1.00	0.49	N
	ATOM	5224	H	GLN	B	157	4.224	37.178	34.941	1.00	0.00	H
	ATOM	5225	HA	GLN	B	157	3.849	39.413	36.673	1.00	0.00	H
	ATOM	5226	1HB	GLN	B	157	6.280	39.706	36.442	1.00	0.00	H
45	ATOM	5227	2HB	GLN	B	157	6.355	38.651	35.031	1.00	0.00	H
	ATOM	5228	1HG	GLN	B	157	7.147	37.485	37.094	1.00	0.00	H
	ATOM	5229	2HG	GLN	B	157	5.821	36.652	36.260	1.00	0.00	H
	ATOM	5230	1HE2	GLN	B	157	4.495	35.810	37.942	1.00	0.00	H
	ATOM	5231	2HE2	GLN	B	157	3.997	36.763	39.316	1.00	0.00	H
50	ATOM	5232	N	LEU	B	158	4.459	39.934	33.473	1.00	0.41	N
	ATOM	5233	CA	LEU	B	158	4.607	40.961	32.483	1.00	0.41	C
	ATOM	5234	C	LEU	B	158	3.306	41.597	32.127	1.00	0.41	C
	ATOM	5235	O	LEU	B	158	2.227	41.063	32.381	1.00	0.41	O
55	ATOM	5236	CB	LEU	B	158	5.252	40.467	31.176	1.00	0.41	C
	ATOM	5237	CG	LEU	B	158	6.699	39.977	31.364	1.00	0.41	C
	ATOM	5238	CD1	LEU	B	158	7.628	41.124	31.796	1.00	0.41	C
	ATOM	5239	CD2	LEU	B	158	6.758	38.765	32.310	1.00	0.41	C
	ATOM	5240	H	LEU	B	158	4.371	38.990	33.144	1.00	0.00	H
	ATOM	5241	HA	LEU	B	158	5.247	41.746	32.926	1.00	0.00	H
60	ATOM	5242	1HB	LEU	B	158	5.231	41.276	30.425	1.00	0.00	H
	ATOM	5243	2HB	LEU	B	158	4.656	39.640	30.773	1.00	0.00	H
	ATOM	5244	HG	LEU	B	158	7.047	39.639	30.367	1.00	0.00	H
	ATOM	5245	1HD1	LEU	B	158	8.682	40.800	31.788	1.00	0.00	H
	ATOM	5246	2HD1	LEU	B	158	7.548	41.983	31.109	1.00	0.00	H
65	ATOM	5247	3HD1	LEU	B	158	7.408	41.481	32.814	1.00	0.00	H
	ATOM	5248	1HD2	LEU	B	158	7.652	38.158	32.086	1.00	0.00	H
	ATOM	5249	2HD2	LEU	B	158	6.896	39.116	33.331	1.00	0.00	H
	ATOM	5250	3HD2	LEU	B	158	5.894	38.090	32.222	1.00	0.00	H
	ATOM	5251	N	ASP	B	159	3.419	42.804	31.533	1.00	0.19	N
70	ATOM	5252	CA	ASP	B	159	2.310	43.578	31.058	1.00	0.19	C
	ATOM	5253	C	ASP	B	159	2.414	43.543	29.566	1.00	0.19	C
	ATOM	5254	O	ASP	B	159	3.504	43.668	29.009	1.00	0.19	O

227

	ATOM	5255	CB	ASP	B	159	2.381	45.057	31.503	1.00	0.19	C
	ATOM	5256	CG	ASP	B	159	1.124	45.839	31.117	1.00	0.19	C
	ATOM	5257	OD1	ASP	B	159	0.378	45.398	30.205	1.00	0.19	O
	ATOM	5258	OD2	ASP	B	159	0.904	46.910	31.744	1.00	0.19	O1-
5	ATOM	5259	H	ASP	B	159	4.304	43.201	31.275	1.00	0.00	H
	ATOM	5260	HA	ASP	B	159	1.394	43.142	31.412	1.00	0.00	H
	ATOM	5261	1HB	ASP	B	159	3.242	45.547	31.017	1.00	0.00	H
	ATOM	5262	2HB	ASP	B	159	2.576	45.164	32.581	1.00	0.00	H
10	ATOM	5263	N	TYR	B	160	1.279	43.335	28.874	1.00	0.11	N
	ATOM	5264	CA	TYR	B	160	1.321	43.282	27.443	1.00	0.11	C
	ATOM	5265	C	TYR	B	160	0.381	44.304	26.901	1.00	0.11	C
	ATOM	5266	O	TYR	B	160	-0.535	44.755	27.589	1.00	0.11	O
	ATOM	5267	CB	TYR	B	160	0.884	41.929	26.857	1.00	0.11	C
15	ATOM	5268	CG	TYR	B	160	1.939	40.924	27.171	1.00	0.11	C
	ATOM	5269	CD1	TYR	B	160	2.067	40.404	28.439	1.00	0.11	C
	ATOM	5270	CD2	TYR	B	160	2.794	40.488	26.185	1.00	0.11	C
	ATOM	5271	CE1	TYR	B	160	3.042	39.476	28.720	1.00	0.11	C
	ATOM	5272	CE2	TYR	B	160	3.771	39.560	26.459	1.00	0.11	C
20	ATOM	5273	CZ	TYR	B	160	3.895	39.052	27.730	1.00	0.11	C
	ATOM	5274	OH	TYR	B	160	4.895	38.099	28.019	1.00	0.11	O
	ATOM	5275	H	TYR	B	160	0.420	43.679	29.317	1.00	0.00	H
	ATOM	5276	HA	TYR	B	160	2.324	43.539	27.087	1.00	0.00	H
	ATOM	5277	1HB	TYR	B	160	0.755	42.037	25.769	1.00	0.00	H
	ATOM	5278	2HB	TYR	B	160	-0.098	41.635	27.262	1.00	0.00	H
25	ATOM	5279	HD1	TYR	B	160	1.419	40.777	29.225	1.00	0.00	H
	ATOM	5280	HD2	TYR	B	160	2.708	40.890	25.178	1.00	0.00	H
	ATOM	5281	HE1	TYR	B	160	3.087	39.038	29.711	1.00	0.00	H
	ATOM	5282	HE2	TYR	B	160	4.440	39.242	25.662	1.00	0.00	H
	ATOM	5283	HH	TYR	B	160	5.695	38.392	27.561	1.00	0.00	H
30	ATOM	5284	N	GLU	B	161	0.622	44.722	25.643	1.00	0.12	N
	ATOM	5285	CA	GLU	B	161	-0.262	45.647	25.000	1.00	0.12	C
	ATOM	5286	C	GLU	B	161	-0.753	44.973	23.762	1.00	0.12	C
	ATOM	5287	O	GLU	B	161	-0.033	44.197	23.135	1.00	0.12	O
	ATOM	5288	CB	GLU	B	161	0.273	47.006	24.485	1.00	0.12	C
35	ATOM	5289	CG	GLU	B	161	-0.616	48.163	23.930	1.00	0.12	C
	ATOM	5290	CD	GLU	B	161	0.100	48.894	22.732	1.00	0.12	C
	ATOM	5291	OE1	GLU	B	161	0.523	48.163	21.832	1.00	0.12	O
	ATOM	5292	OE2	GLU	B	161	0.153	50.124	22.811	1.00	0.12	O1-
	ATOM	5293	H	GLU	B	161	1.327	44.317	25.048	1.00	0.00	H
40	ATOM	5294	HA	GLU	B	161	-1.119	45.827	25.660	1.00	0.00	H
	ATOM	5295	1HB	GLU	B	161	0.959	46.729	23.673	1.00	0.00	H
	ATOM	5296	2HB	GLU	B	161	0.855	47.435	25.316	1.00	0.00	H
	ATOM	5297	1HG	GLU	B	161	-0.844	48.899	24.714	1.00	0.00	H
	ATOM	5298	2HG	GLU	B	161	-1.583	47.807	23.551	1.00	0.00	H
45	ATOM	5299	N	SER	B	162	-2.020	45.234	23.397	1.00	0.11	N
	ATOM	5300	CA	SER	B	162	-2.598	44.616	22.242	1.00	0.11	C
	ATOM	5301	C	SER	B	162	-2.381	45.499	21.065	1.00	0.11	C
	ATOM	5302	O	SER	B	162	-1.967	46.650	21.196	1.00	0.11	O
	ATOM	5303	CB	SER	B	162	-4.113	44.377	22.371	1.00	0.11	C
50	ATOM	5304	OG	SER	B	162	-4.614	43.756	21.196	1.00	0.11	O
	ATOM	5305	H	SER	B	162	-2.583	45.884	23.935	1.00	0.00	H
	ATOM	5306	HA	SER	B	162	-2.119	43.636	22.074	1.00	0.00	H
	ATOM	5307	1HB	SER	B	162	-4.658	45.313	22.560	1.00	0.00	H
	ATOM	5308	2HB	SER	B	162	-4.320	43.696	23.199	1.00	0.00	H
55	ATOM	5309	HG	SER	B	162	-4.572	44.455	20.511	1.00	0.00	H
	ATOM	5310	N	GLU	B	163	-2.640	44.951	19.864	1.00	0.13	N
	ATOM	5311	CA	GLU	B	163	-2.517	45.715	18.661	1.00	0.13	C
	ATOM	5312	C	GLU	B	163	-3.757	46.533	18.544	1.00	0.13	C
	ATOM	5313	O	GLU	B	163	-4.830	46.148	19.006	1.00	0.13	O
60	ATOM	5314	CB	GLU	B	163	-2.382	44.835	17.407	1.00	0.13	C
	ATOM	5315	CG	GLU	B	163	-3.567	43.890	17.202	1.00	0.13	C
	ATOM	5316	CD	GLU	B	163	-3.153	42.846	16.177	1.00	0.13	C
	ATOM	5317	OE1	GLU	B	163	-2.076	42.223	16.381	1.00	0.13	O
	ATOM	5318	OE2	GLU	B	163	-3.900	42.654	15.181	1.00	0.13	O1-
65	ATOM	5319	H	GLU	B	163	-2.775	43.955	19.742	1.00	0.00	H
	ATOM	5320	HA	GLU	B	163	-1.567	46.269	18.725	1.00	0.00	H
	ATOM	5321	1HB	GLU	B	163	-1.436	44.272	17.498	1.00	0.00	H
	ATOM	5322	2HB	GLU	B	163	-2.268	45.510	16.541	1.00	0.00	H
	ATOM	5323	1HG	GLU	B	163	-4.480	44.422	16.897	1.00	0.00	H
70	ATOM	5324	2HG	GLU	B	163	-3.770	43.349	18.136	1.00	0.00	H
	ATOM	5325	N	PRO	B	164	-3.611	47.681	17.956	1.00	0.13	N

228

	ATOM	5326	CA	PRO	B	164	-4.751	48.542	17.819	1.00	0.13	C
	ATOM	5327	C	PRO	B	164	-5.680	48.070	16.752	1.00	0.13	C
	ATOM	5328	O	PRO	B	164	-5.235	47.407	15.818	1.00	0.13	O
5	ATOM	5329	CB	PRO	B	164	-4.189	49.936	17.565	1.00	0.13	C
	ATOM	5330	CG	PRO	B	164	-2.815	49.909	18.251	1.00	0.13	C
	ATOM	5331	CD	PRO	B	164	-2.385	48.437	18.167	1.00	0.13	C
	ATOM	5332	HA	PRO	B	164	-5.283	48.566	18.778	1.00	0.00	H
	ATOM	5333	1HB	PRO	B	164	-4.771	50.682	18.086	1.00	0.00	H
10	ATOM	5334	2HB	PRO	B	164	-4.110	50.174	16.494	1.00	0.00	H
	ATOM	5335	1HG	PRO	B	164	-2.913	50.209	19.302	1.00	0.00	H
	ATOM	5336	2HG	PRO	B	164	-2.076	50.592	17.804	1.00	0.00	H
	ATOM	5337	1HD	PRO	B	164	-1.699	48.263	17.323	1.00	0.00	H
	ATOM	5338	2HD	PRO	B	164	-1.875	48.165	19.100	1.00	0.00	H
15	ATOM	5339	N	LEU	B	165	-6.982	48.383	16.888	1.00	0.11	N
	ATOM	5340	CA	LEU	B	165	-7.932	48.026	15.879	1.00	0.11	C
	ATOM	5341	C	LEU	B	165	-8.678	49.279	15.565	1.00	0.11	C
	ATOM	5342	O	LEU	B	165	-8.896	50.112	16.444	1.00	0.11	O
	ATOM	5343	CB	LEU	B	165	-8.953	46.969	16.327	1.00	0.11	C
20	ATOM	5344	CG	LEU	B	165	-8.309	45.618	16.688	1.00	0.11	C
	ATOM	5345	CD1	LEU	B	165	-9.377	44.562	17.011	1.00	0.11	C
	ATOM	5346	CD2	LEU	B	165	-7.321	45.158	15.605	1.00	0.11	C
	ATOM	5347	H	LEU	B	165	-7.332	48.855	17.713	1.00	0.00	H
	ATOM	5348	HA	LEU	B	165	-7.399	47.693	14.975	1.00	0.00	H
	ATOM	5349	1HB	LEU	B	165	-9.663	46.827	15.492	1.00	0.00	H
25	ATOM	5350	2HB	LEU	B	165	-9.540	47.354	17.180	1.00	0.00	H
	ATOM	5351	HG	LEU	B	165	-7.725	45.756	17.619	1.00	0.00	H
	ATOM	5352	1HD1	LEU	B	165	-8.889	43.616	17.270	1.00	0.00	H
	ATOM	5353	2HD1	LEU	B	165	-10.014	44.907	17.841	1.00	0.00	H
	ATOM	5354	3HD1	LEU	B	165	-10.046	44.410	16.150	1.00	0.00	H
30	ATOM	5355	1HD2	LEU	B	165	-7.258	44.060	15.620	1.00	0.00	H
	ATOM	5356	2HD2	LEU	B	165	-7.617	45.460	14.591	1.00	0.00	H
	ATOM	5357	3HD2	LEU	B	165	-6.293	45.461	15.796	1.00	0.00	H
	ATOM	5358	N	ASN	B	166	-9.077	49.464	14.294	1.00	0.10	N
35	ATOM	5359	CA	ASN	B	166	-9.772	50.674	13.976	1.00	0.10	C
	ATOM	5360	C	ASN	B	166	-11.234	50.388	14.008	1.00	0.10	C
	ATOM	5361	O	ASN	B	166	-11.729	49.520	13.291	1.00	0.10	O
	ATOM	5362	CB	ASN	B	166	-9.460	51.243	12.581	1.00	0.10	C
	ATOM	5363	CG	ASN	B	166	-8.056	51.831	12.593	1.00	0.10	C
40	ATOM	5364	OD1	ASN	B	166	-7.304	51.681	13.555	1.00	0.10	O
	ATOM	5365	ND2	ASN	B	166	-7.695	52.538	11.490	1.00	0.10	N
	ATOM	5366	H	ASN	B	166	-8.920	48.814	13.545	1.00	0.00	H
	ATOM	5367	HA	ASN	B	166	-9.511	51.470	14.693	1.00	0.00	H
	ATOM	5368	1HB	ASN	B	166	-10.185	52.051	12.379	1.00	0.00	H
45	ATOM	5369	2HB	ASN	B	166	-9.555	50.487	11.785	1.00	0.00	H
	ATOM	5370	1HD2	ASN	B	166	-8.314	52.676	10.714	1.00	0.00	H
	ATOM	5371	2HD2	ASN	B	166	-6.780	52.955	11.511	1.00	0.00	H
	ATOM	5372	N	ILE	B	167	-11.959	51.119	14.873	1.00	0.22	N
	ATOM	5373	CA	ILE	B	167	-13.378	50.962	14.942	1.00	0.22	C
50	ATOM	5374	C	ILE	B	167	-13.954	52.275	14.545	1.00	0.22	C
	ATOM	5375	O	ILE	B	167	-13.535	53.322	15.035	1.00	0.22	O
	ATOM	5376	CB	ILE	B	167	-13.880	50.650	16.322	1.00	0.22	C
	ATOM	5377	CG1	ILE	B	167	-13.316	49.304	16.805	1.00	0.22	C
	ATOM	5378	CG2	ILE	B	167	-15.418	50.705	16.294	1.00	0.22	C
55	ATOM	5379	CD1	ILE	B	167	-13.532	49.051	18.297	1.00	0.22	C
	ATOM	5380	H	ILE	B	167	-11.568	51.884	15.416	1.00	0.00	H
	ATOM	5381	HA	ILE	B	167	-13.699	50.161	14.261	1.00	0.00	H
	ATOM	5382	HB	ILE	B	167	-13.530	51.440	17.014	1.00	0.00	H
	ATOM	5383	1HG1	ILE	B	167	-12.227	49.256	16.623	1.00	0.00	H
	ATOM	5384	2HG1	ILE	B	167	-13.758	48.478	16.219	1.00	0.00	H
60	ATOM	5385	1HG2	ILE	B	167	-15.829	50.544	17.306	1.00	0.00	H
	ATOM	5386	2HG2	ILE	B	167	-15.817	51.680	15.976	1.00	0.00	H
	ATOM	5387	3HG2	ILE	B	167	-15.851	49.914	15.670	1.00	0.00	H
	ATOM	5388	1HD1	ILE	B	167	-13.011	48.136	18.621	1.00	0.00	H
	ATOM	5389	2HD1	ILE	B	167	-13.158	49.884	18.909	1.00	0.00	H
65	ATOM	5390	3HD1	ILE	B	167	-14.602	48.923	18.511	1.00	0.00	H
	ATOM	5391	N	THR	B	168	-14.926	52.262	13.618	1.00	0.48	N
	ATOM	5392	CA	THR	B	168	-15.488	53.513	13.212	1.00	0.48	C
	ATOM	5393	C	THR	B	168	-16.955	53.470	13.410	1.00	0.48	C
	ATOM	5394	O	THR	B	168	-17.587	52.419	13.312	1.00	0.48	O
70	ATOM	5395	CB	THR	B	168	-15.289	53.846	11.764	1.00	0.48	C
	ATOM	5396	OG1	THR	B	168	-15.798	52.802	10.948	1.00	0.48	O

229

	ATOM	5397	CG2	THR	B	168	-13.800	54.078	11.494	1.00	0.48	C
	ATOM	5398	H	THR	B	168	-15.333	51.415	13.242	1.00	0.00	H
	ATOM	5399	HA	THR	B	168	-15.086	54.315	13.823	1.00	0.00	H
5	ATOM	5400	HB	THR	B	168	-15.828	54.788	11.542	1.00	0.00	H
	ATOM	5401	HG1	THR	B	168	-16.752	52.753	11.109	1.00	0.00	H
	ATOM	5402	1HG2	THR	B	168	-13.629	54.378	10.447	1.00	0.00	H
	ATOM	5403	2HG2	THR	B	168	-13.392	54.871	12.141	1.00	0.00	H
	ATOM	5404	3HG2	THR	B	168	-13.218	53.159	11.670	1.00	0.00	H
	ATOM	5405	N	VAL	B	169	-17.538	54.638	13.724	1.00	0.55	N
10	ATOM	5406	CA	VAL	B	169	-18.958	54.667	13.795	1.00	0.55	C
	ATOM	5407	C	VAL	B	169	-19.375	55.038	12.415	1.00	0.55	C
	ATOM	5408	O	VAL	B	169	-18.935	56.046	11.863	1.00	0.55	O
	ATOM	5409	CB	VAL	B	169	-19.532	55.659	14.771	1.00	0.55	C
	ATOM	5410	CG1	VAL	B	169	-19.096	55.245	16.183	1.00	0.55	C
15	ATOM	5411	CG2	VAL	B	169	-19.102	57.084	14.391	1.00	0.55	C
	ATOM	5412	H	VAL	B	169	-17.097	55.537	13.643	1.00	0.00	H
	ATOM	5413	HA	VAL	B	169	-19.344	53.676	14.069	1.00	0.00	H
	ATOM	5414	HB	VAL	B	169	-20.631	55.570	14.679	1.00	0.00	H
	ATOM	5415	1HG1	VAL	B	169	-19.882	55.434	16.925	1.00	0.00	H
20	ATOM	5416	2HG1	VAL	B	169	-18.919	54.158	16.250	1.00	0.00	H
	ATOM	5417	3HG1	VAL	B	169	-18.150	55.715	16.482	1.00	0.00	H
	ATOM	5418	1HG2	VAL	B	169	-19.962	57.610	14.838	1.00	0.00	H
	ATOM	5419	2HG2	VAL	B	169	-18.107	57.258	14.822	1.00	0.00	H
	ATOM	5420	3HG2	VAL	B	169	-19.091	57.488	13.385	1.00	0.00	H
25	ATOM	5421	N	ILE	B	170	-20.221	54.194	11.807	1.00	0.56	N
	ATOM	5422	CA	ILE	B	170	-20.637	54.415	10.457	1.00	0.56	C
	ATOM	5423	C	ILE	B	170	-21.357	55.721	10.428	1.00	0.56	C
	ATOM	5424	O	ILE	B	170	-21.198	56.502	9.490	1.00	0.56	O
	ATOM	5425	CB	ILE	B	170	-21.546	53.321	9.942	1.00	0.56	C
30	ATOM	5426	CG1	ILE	B	170	-21.728	53.399	8.414	1.00	0.56	C
	ATOM	5427	CG2	ILE	B	170	-22.867	53.374	10.727	1.00	0.56	C
	ATOM	5428	CD1	ILE	B	170	-22.467	54.643	7.921	1.00	0.56	C
	ATOM	5429	H	ILE	B	170	-20.615	53.381	12.272	1.00	0.00	H
	ATOM	5430	HA	ILE	B	170	-19.739	54.517	9.824	1.00	0.00	H
35	ATOM	5431	HB	ILE	B	170	-21.142	52.353	10.164	1.00	0.00	H
	ATOM	5432	1HG1	ILE	B	170	-22.296	52.506	8.094	1.00	0.00	H
	ATOM	5433	2HG1	ILE	B	170	-20.748	53.323	7.909	1.00	0.00	H
	ATOM	5434	1HG2	ILE	B	170	-23.219	52.342	10.855	1.00	0.00	H
	ATOM	5435	2HG2	ILE	B	170	-22.796	53.819	11.714	1.00	0.00	H
40	ATOM	5436	3HG2	ILE	B	170	-23.675	53.912	10.210	1.00	0.00	H
	ATOM	5437	1HD1	ILE	B	170	-23.115	54.369	7.070	1.00	0.00	H
	ATOM	5438	2HD1	ILE	B	170	-23.131	55.124	8.651	1.00	0.00	H
	ATOM	5439	3HD1	ILE	B	170	-21.776	55.394	7.510	1.00	0.00	H
	ATOM	5440	N	LYS	B	171	-22.156	55.999	11.475	1.00	0.52	N
45	ATOM	5441	CA	LYS	B	171	-22.902	57.220	11.537	1.00	0.52	C
	ATOM	5442	C	LYS	B	171	-21.908	58.330	11.406	1.00	0.52	C
	ATOM	5443	O	LYS	B	171	-20.957	58.418	12.180	1.00	0.52	O
	ATOM	5444	CB	LYS	B	171	-23.649	57.356	12.879	1.00	0.52	C
	ATOM	5445	CG	LYS	B	171	-24.731	58.436	12.935	1.00	0.52	C
50	ATOM	5446	CD	LYS	B	171	-24.206	59.860	12.790	1.00	0.52	C
	ATOM	5447	CE	LYS	B	171	-25.263	60.932	13.064	1.00	0.52	C
	ATOM	5448	NZ	LYS	B	171	-26.436	60.713	12.190	1.00	0.52	N1+
	ATOM	5449	H	LYS	B	171	-22.064	55.447	12.309	1.00	0.00	H
	ATOM	5450	HA	LYS	B	171	-23.632	57.218	10.707	1.00	0.00	H
55	ATOM	5451	1HB	LYS	B	171	-22.872	57.525	13.643	1.00	0.00	H
	ATOM	5452	2HB	LYS	B	171	-24.129	56.387	13.070	1.00	0.00	H
	ATOM	5453	1HG	LYS	B	171	-25.345	58.368	13.836	1.00	0.00	H
	ATOM	5454	2HG	LYS	B	171	-25.440	58.243	12.108	1.00	0.00	H
	ATOM	5455	1HD	LYS	B	171	-23.965	59.931	11.730	1.00	0.00	H
60	ATOM	5456	2HD	LYS	B	171	-23.301	60.050	13.389	1.00	0.00	H
	ATOM	5457	1HE	LYS	B	171	-24.878	61.943	12.854	1.00	0.00	H
	ATOM	5458	2HE	LYS	B	171	-25.630	60.929	14.101	1.00	0.00	H
	ATOM	5459	1HZ	LYS	B	171	-27.152	61.412	12.333	1.00	0.00	H
	ATOM	5460	2HZ	LYS	B	171	-26.174	60.754	11.214	1.00	0.00	H
65	ATOM	5461	3HZ	LYS	B	171	-26.861	59.813	12.366	1.00	0.00	H
	ATOM	5462	N	ALA	B	172	-22.097	59.199	10.393	1.00	0.31	N
	ATOM	5463	CA	ALA	B	172	-21.148	60.249	10.164	1.00	0.31	C
	ATOM	5464	C	ALA	B	172	-21.773	61.594	10.514	1.00	0.31	C
	ATOM	5465	O	ALA	B	172	-21.349	62.615	9.889	1.00	0.31	O
70	ATOM	5466	CB	ALA	B	172	-20.692	60.342	8.698	1.00	0.31	C
	ATOM	5467	OXT	ALA	B	172	-22.672	61.637	11.410	1.00	0.31	O1-

231

TABLE 5

REMARK Model of Fc Gamma Receptor type IIIb; V.C. Epa, Feb 02, 1999.

REMARK r3b_mod8.B99990013.pdb

REMARK Produced by MODELLER: 02-Feb-99 01:55:11

REMARK MODELLER OBJECTIVE FUNCTION:

933.2556

1

ATOM	1	N	ARG	1	36.333	78.544	5.582	1.00	0.75	1SG	2
ATOM	2	CA	ARG	1	36.665	78.748	7.009	1.00	0.75	1SG	3
ATOM	3	CB	ARG	1	37.362	80.102	7.211	1.00	0.75	1SG	4
ATOM	4	CG	ARG	1	38.684	80.236	6.455	1.00	0.75	1SG	5
ATOM	5	CD	ARG	1	39.381	81.577	6.691	1.00	0.75	1SG	6
ATOM	6	NE	ARG	1	38.454	82.648	6.231	1.00	0.75	1SG	7
ATOM	7	CZ	ARG	1	38.575	83.911	6.733	1.00	0.75	1SG	8
ATOM	8	NH1	ARG	1	39.561	84.195	7.632	1.00	0.75	1SG	9
ATOM	9	NH2	ARG	1	37.706	84.888	6.342	1.00	0.75	1SG	10
ATOM	10	C	ARG	1	35.413	78.755	7.815	1.00	0.75	1SG	11
ATOM	11	O	ARG	1	34.422	78.125	7.448	1.00	0.75	1SG	12
ATOM	12	N	THR	2	35.435	79.465	8.957	1.00	0.84	1SG	13
ATOM	13	CA	THR	2	34.253	79.541	9.758	1.00	0.84	1SG	14
ATOM	14	CB	THR	2	34.507	79.998	11.165	1.00	0.84	1SG	15
ATOM	15	OG1	THR	2	35.036	81.316	11.166	1.00	0.84	1SG	16
ATOM	16	CG2	THR	2	35.505	79.029	11.821	1.00	0.84	1SG	17
ATOM	17	C	THR	2	33.378	80.548	9.098	1.00	0.84	1SG	18
ATOM	18	O	THR	2	33.857	81.407	8.359	1.00	0.84	1SG	19
ATOM	19	N	GLU	3	32.057	80.458	9.329	1.00	0.71	1SG	20
ATOM	20	CA	GLU	3	31.181	81.396	8.699	1.00	0.71	1SG	21
ATOM	21	CB	GLU	3	29.830	80.782	8.299	1.00	0.71	1SG	22
ATOM	22	CG	GLU	3	29.965	79.711	7.214	1.00	0.71	1SG	23
ATOM	23	CD	GLU	3	30.554	80.365	5.972	1.00	0.71	1SG	24
ATOM	24	OE1	GLU	3	30.739	81.612	5.991	1.00	0.71	1SG	25
ATOM	25	OE2	GLU	3	30.827	79.627	4.988	1.00	0.71	1SG	26
ATOM	26	C	GLU	3	30.937	82.497	9.675	1.00	0.71	1SG	27
ATOM	27	O	GLU	3	30.388	82.277	10.753	1.00	0.71	1SG	28
ATOM	28	N	ASP	4	31.367	83.722	9.318	1.00	0.37	1SG	29
ATOM	29	CA	ASP	4	31.218	84.828	10.215	1.00	0.37	1SG	30
ATOM	30	CB	ASP	4	31.857	86.122	9.684	1.00	0.37	1SG	31
ATOM	31	CG	ASP	4	33.370	85.958	9.723	1.00	0.37	1SG	32
ATOM	32	OD1	ASP	4	33.845	85.029	10.428	1.00	0.37	1SG	33
ATOM	33	OD2	ASP	4	34.070	86.765	9.055	1.00	0.37	1SG	34
ATOM	34	C	ASP	4	29.767	85.099	10.401	1.00	0.37	1SG	35
ATOM	35	O	ASP	4	29.251	85.050	11.516	1.00	0.37	1SG	36
ATOM	36	N	LEU	5	29.059	85.370	9.294	1.00	0.17	1SG	37
ATOM	37	CA	LEU	5	27.667	85.668	9.399	1.00	0.17	1SG	38
ATOM	38	CB	LEU	5	27.075	86.177	8.075	1.00	0.17	1SG	39
ATOM	39	CG	LEU	5	27.732	87.486	7.592	1.00	0.17	1SG	40
ATOM	40	CD2	LEU	5	27.709	88.560	8.693	1.00	0.17	1SG	41
ATOM	41	CD1	LEU	5	27.115	87.974	6.271	1.00	0.17	1SG	42
ATOM	42	C	LEU	5	26.999	84.375	9.734	1.00	0.17	1SG	43
ATOM	43	O	LEU	5	27.436	83.315	9.290	1.00	0.17	1SG	44
ATOM	44	N	PRO	6	25.939	84.428	10.491	1.00	0.32	1SG	45
ATOM	45	CA	PRO	6	25.286	83.214	10.886	1.00	0.32	1SG	46
ATOM	46	CD	PRO	6	25.749	85.492	11.462	1.00	0.32	1SG	47
ATOM	47	CB	PRO	6	24.243	83.628	11.919	1.00	0.32	1SG	48
ATOM	48	CG	PRO	6	24.865	84.882	12.566	1.00	0.32	1SG	49
ATOM	49	C	PRO	6	24.755	82.520	9.679	1.00	0.32	1SG	50
ATOM	50	O	PRO	6	24.506	83.182	8.672	1.00	0.32	1SG	51
ATOM	51	N	LYS	7	24.603	81.184	9.741	1.00	0.49	1SG	52
ATOM	52	CA	LYS	7	24.184	80.476	8.572	1.00	0.49	1SG	53
ATOM	53	CB	LYS	7	24.543	78.979	8.570	1.00	0.49	1SG	54
ATOM	54	CG	LYS	7	26.045	78.697	8.611	1.00	0.49	1SG	55
ATOM	55	CD	LYS	7	26.398	77.211	8.617	1.00	0.49	1SG	56
ATOM	56	CE	LYS	7	25.652	76.398	9.673	1.00	0.49	1SG	57
ATOM	57	NZ	LYS	7	26.238	76.623	11.012	1.00	0.49	1SG	58

ATOM	58	C	LYS	7	22.703	80.560	8.420	1.00	0.49	1SG	59
ATOM	59	O	LYS	7	21.958	80.622	9.397	1.00	0.49	1SG	60
ATOM	60	N	ALA	8	22.243	80.568	7.155	1.00	0.29	1SG	61
ATOM	61	CA	ALA	8	20.838	80.543	6.890	1.00	0.29	1SG	62
ATOM	62	CB	ALA	8	20.483	80.789	5.413	1.00	0.29	1SG	63
ATOM	63	C	ALA	8	20.394	79.162	7.254	1.00	0.29	1SG	64
ATOM	64	O	ALA	8	21.215	78.248	7.328	1.00	0.29	1SG	65
ATOM	65	N	VAL	9	19.086	78.978	7.532	1.00	0.10	1SG	66
ATOM	66	CA	VAL	9	18.614	77.679	7.929	1.00	0.10	1SG	67
ATOM	67	CB	VAL	9	18.031	77.676	9.312	1.00	0.10	1SG	68
ATOM	68	CG1	VAL	9	17.521	76.263	9.638	1.00	0.10	1SG	69
ATOM	69	CG2	VAL	9	19.104	78.190	10.287	1.00	0.10	1SG	70
ATOM	70	C	VAL	9	17.537	77.242	6.979	1.00	0.10	1SG	71
ATOM	71	O	VAL	9	16.568	77.964	6.746	1.00	0.10	1SG	72
ATOM	72	N	VAL	10	17.674	76.015	6.431	1.00	0.19	1SG	73
ATOM	73	CA	VAL	10	16.740	75.508	5.463	1.00	0.19	1SG	74
ATOM	74	CB	VAL	10	17.398	74.689	4.392	1.00	0.19	1SG	75
ATOM	75	CG1	VAL	10	16.311	74.126	3.461	1.00	0.19	1SG	76
ATOM	76	CG2	VAL	10	18.435	75.572	3.678	1.00	0.19	1SG	77
ATOM	77	C	VAL	10	15.729	74.638	6.147	1.00	0.19	1SG	78
ATOM	78	O	VAL	10	16.071	73.734	6.909	1.00	0.19	1SG	79
ATOM	79	N	PHE	11	14.436	74.903	5.866	1.00	0.29	1SG	80
ATOM	80	CA	PHE	11	13.341	74.203	6.478	1.00	0.29	1SG	81
ATOM	81	CB	PHE	11	12.390	75.198	7.171	1.00	0.29	1SG	82
ATOM	82	CG	PHE	11	11.324	74.489	7.929	1.00	0.29	1SG	83
ATOM	83	CD1	PHE	11	11.626	73.789	9.074	1.00	0.29	1SG	84
ATOM	84	CD2	PHE	11	10.016	74.560	7.515	1.00	0.29	1SG	85
ATOM	85	CE1	PHE	11	10.640	73.144	9.783	1.00	0.29	1SG	86
ATOM	86	CE2	PHE	11	9.030	73.918	8.223	1.00	0.29	1SG	87
ATOM	87	CZ	PHE	11	9.337	73.205	9.357	1.00	0.29	1SG	88
ATOM	88	C	PHE	11	12.610	73.473	5.386	1.00	0.29	1SG	89
ATOM	89	O	PHE	11	12.366	74.029	4.317	1.00	0.29	1SG	90
ATOM	90	N	LEU	12	12.252	72.194	5.639	1.00	0.22	1SG	91
ATOM	91	CA	LEU	12	11.623	71.357	4.649	1.00	0.22	1SG	92
ATOM	92	CB	LEU	12	12.417	70.050	4.443	1.00	0.22	1SG	93
ATOM	93	CG	LEU	12	11.841	69.069	3.405	1.00	0.22	1SG	94
ATOM	94	CD2	LEU	12	12.543	67.702	3.485	1.00	0.22	1SG	95
ATOM	95	CD1	LEU	12	11.878	69.665	1.988	1.00	0.22	1SG	96
ATOM	96	C	LEU	12	10.245	70.996	5.122	1.00	0.22	1SG	97
ATOM	97	O	LEU	12	10.069	70.535	6.248	1.00	0.22	1SG	98
ATOM	98	N	GLU	13	9.214	71.217	4.272	1.00	0.16	1SG	99
ATOM	99	CA	GLU	13	7.873	70.835	4.636	1.00	0.16	1SG	100
ATOM	100	CB	GLU	13	6.922	72.012	4.907	1.00	0.16	1SG	101
ATOM	101	CG	GLU	13	7.239	72.794	6.177	1.00	0.16	1SG	102
ATOM	102	CD	GLU	13	6.214	73.912	6.297	1.00	0.16	1SG	103
ATOM	103	OE1	GLU	13	4.999	73.592	6.393	1.00	0.16	1SG	104
ATOM	104	OE2	GLU	13	6.630	75.102	6.291	1.00	0.16	1SG	105
ATOM	105	C	GLU	13	7.271	70.102	3.478	1.00	0.16	1SG	106
ATOM	106	O	GLU	13	7.330	70.573	2.342	1.00	0.16	1SG	107
ATOM	107	N	PRO	14	6.706	68.948	3.714	1.00	0.21	1SG	108
ATOM	108	CA	PRO	14	6.667	68.302	4.996	1.00	0.21	1SG	109
ATOM	109	CD	PRO	14	5.925	68.248	2.709	1.00	0.21	1SG	110
ATOM	110	CB	PRO	14	5.700	67.126	4.839	1.00	0.21	1SG	111
ATOM	111	CG	PRO	14	5.667	66.862	3.323	1.00	0.21	1SG	112
ATOM	112	C	PRO	14	8.071	67.870	5.287	1.00	0.21	1SG	113
ATOM	113	O	PRO	14	8.917	67.964	4.402	1.00	0.21	1SG	114
ATOM	114	N	GLN	15	8.326	67.394	6.518	1.00	0.25	1SG	115
ATOM	115	CA	GLN	15	9.620	67.052	7.049	1.00	0.25	1SG	116
ATOM	116	CB	GLN	15	9.550	66.690	8.541	1.00	0.25	1SG	117
ATOM	117	CG	GLN	15	9.071	67.839	9.430	1.00	0.25	1SG	118
ATOM	118	CD	GLN	15	9.049	67.340	10.867	1.00	0.25	1SG	119

ATOM	119	OE1	GLN	15	9.139	68.123	11.812	1.00	0.25	1SG	120
ATOM	120	NE2	GLN	15	8.927	65.996	11.040	1.00	0.25	1SG	121
ATOM	121	C	GLN	15	10.263	65.875	6.364	1.00	0.25	1SG	122
ATOM	122	O	GLN	15	11.479	65.714	6.432	1.00	0.25	1SG	123
ATOM	123	N	TRP	16	9.473	64.991	5.735	1.00	0.44	1SG	124
ATOM	124	CA	TRP	16	9.960	63.744	5.199	1.00	0.44	1SG	125
ATOM	125	CB	TRP	16	8.870	63.023	4.396	1.00	0.44	1SG	126
ATOM	126	CG	TRP	16	7.568	62.935	5.152	1.00	0.44	1SG	127
ATOM	127	CD2	TRP	16	7.393	62.263	6.408	1.00	0.44	1SG	128
ATOM	128	CD1	TRP	16	6.368	63.510	4.849	1.00	0.44	1SG	129
ATOM	129	NE1	TRP	16	5.454	63.236	5.837	1.00	0.44	1SG	130
ATOM	130	CE2	TRP	16	6.072	62.471	6.804	1.00	0.44	1SG	131
ATOM	131	CE3	TRP	16	8.263	61.541	7.173	1.00	0.44	1SG	132
ATOM	132	CZ2	TRP	16	5.599	61.956	7.976	1.00	0.44	1SG	133
ATOM	133	CZ3	TRP	16	7.780	61.016	8.351	1.00	0.44	1SG	134
ATOM	134	CH2	TRP	16	6.473	61.220	8.745	1.00	0.44	1SG	135
ATOM	135	C	TRP	16	11.131	63.929	4.267	1.00	0.44	1SG	136
ATOM	136	O	TRP	16	11.062	64.684	3.297	1.00	0.44	1SG	137
ATOM	137	N	TYR	17	12.261	63.242	4.567	1.00	0.57	1SG	138
ATOM	138	CA	TYR	17	13.440	63.252	3.737	1.00	0.57	1SG	139
ATOM	139	CB	TYR	17	14.749	62.870	4.463	1.00	0.57	1SG	140
ATOM	140	CG	TYR	17	14.639	61.516	5.071	1.00	0.57	1SG	141
ATOM	141	CD1	TYR	17	14.599	60.383	4.291	1.00	0.57	1SG	142
ATOM	142	CD2	TYR	17	14.616	61.383	6.440	1.00	0.57	1SG	143
ATOM	143	CE1	TYR	17	14.507	59.139	4.869	1.00	0.57	1SG	144
ATOM	144	CE2	TYR	17	14.524	60.142	7.024	1.00	0.57	1SG	145
ATOM	145	CZ	TYR	17	14.465	59.017	6.237	1.00	0.57	1SG	146
ATOM	146	OH	TYR	17	14.370	57.742	6.833	1.00	0.57	1SG	147
ATOM	147	C	TYR	17	13.280	62.371	2.530	1.00	0.57	1SG	148
ATOM	148	O	TYR	17	13.902	62.621	1.498	1.00	0.57	1SG	149
ATOM	149	N	SER	18	12.494	61.278	2.632	1.00	0.33	1SG	150
ATOM	150	CA	SER	18	12.317	60.414	1.493	1.00	0.33	1SG	151
ATOM	151	CB	SER	18	12.454	58.918	1.826	1.00	0.33	1SG	152
ATOM	152	OG	SER	18	11.412	58.518	2.704	1.00	0.33	1SG	153
ATOM	153	C	SER	18	10.925	60.641	0.986	1.00	0.33	1SG	154
ATOM	154	O	SER	18	9.960	60.479	1.730	1.00	0.33	1SG	155
ATOM	155	N	VAL	19	10.783	61.019	-0.304	1.00	0.11	1SG	156
ATOM	156	CA	VAL	19	9.477	61.311	-0.838	1.00	0.11	1SG	157
ATOM	157	CB	VAL	19	9.269	62.761	-1.167	1.00	0.11	1SG	158
ATOM	158	CG1	VAL	19	9.380	63.581	0.130	1.00	0.11	1SG	159
ATOM	159	CG2	VAL	19	10.274	63.169	-2.257	1.00	0.11	1SG	160
ATOM	160	C	VAL	19	9.271	60.547	-2.114	1.00	0.11	1SG	161
ATOM	161	O	VAL	19	10.165	59.855	-2.599	1.00	0.11	1SG	162
ATOM	162	N	LEU	20	8.048	60.648	-2.680	1.00	0.12	1SG	163
ATOM	163	CA	LEU	20	7.707	59.953	-3.890	1.00	0.12	1SG	164
ATOM	164	CB	LEU	20	6.371	59.199	-3.799	1.00	0.12	1SG	165
ATOM	165	CG	LEU	20	6.393	58.029	-2.795	1.00	0.12	1SG	166
ATOM	166	CD2	LEU	20	7.551	57.064	-3.096	1.00	0.12	1SG	167
ATOM	167	CD1	LEU	20	5.036	57.311	-2.743	1.00	0.12	1SG	168
ATOM	168	C	LEU	20	7.584	60.945	-5.006	1.00	0.12	1SG	169
ATOM	169	O	LEU	20	7.318	62.129	-4.797	1.00	0.12	1SG	170
ATOM	170	N	GLU	21	7.793	60.471	-6.250	1.00	0.27	1SG	171
ATOM	171	CA	GLU	21	7.682	61.341	-7.379	1.00	0.27	1SG	172
ATOM	172	CB	GLU	21	7.866	60.617	-8.725	1.00	0.27	1SG	173
ATOM	173	CG	GLU	21	9.271	60.049	-8.935	1.00	0.27	1SG	174
ATOM	174	CD	GLU	21	9.297	59.370	-10.297	1.00	0.27	1SG	175
ATOM	175	OE1	GLU	21	8.246	59.409	-10.992	1.00	0.27	1SG	176
ATOM	176	OE2	GLU	21	10.363	58.805	-10.660	1.00	0.27	1SG	177
ATOM	177	C	GLU	21	6.305	61.919	-7.359	1.00	0.27	1SG	178
ATOM	178	O	GLU	21	5.336	61.251	-7.002	1.00	0.27	1SG	179
ATOM	179	N	LYS	22	6.206	63.202	-7.752	1.00	0.41	1SG	180

ATOM	180	CA	LYS	22	4.977	63.941	-7.839	1.00	0.41	1SG 181
ATOM	181	CB	LYS	22	3.802	63.104	-8.379	1.00	0.41	1SG 182
ATOM	182	CG	LYS	22	2.521	63.919	-8.568	1.00	0.41	1SG 183
ATOM	183	CD	LYS	22	1.471	63.227	-9.442	1.00	0.41	1SG 184
ATOM	184	CE	LYS	22	1.782	63.301	-10.939	1.00	0.41	1SG 185
ATOM	185	NZ	LYS	22	0.726	62.610	-11.713	1.00	0.41	1SG 186
ATOM	186	C	LYS	22	4.576	64.522	-6.511	1.00	0.41	1SG 187
ATOM	187	O	LYS	22	3.617	65.290	-6.454	1.00	0.41	1SG 188
ATOM	188	N	ASP	23	5.298	64.220	-5.413	1.00	0.26	1SG 189
ATOM	189	CA	ASP	23	4.948	64.822	-4.152	1.00	0.26	1SG 190
ATOM	190	CB	ASP	23	5.586	64.148	-2.921	1.00	0.26	1SG 191
ATOM	191	CG	ASP	23	4.923	62.800	-2.666	1.00	0.26	1SG 192
ATOM	192	OD1	ASP	23	3.763	62.602	-3.117	1.00	0.26	1SG 193
ATOM	193	OD2	ASP	23	5.574	61.949	-2.004	1.00	0.26	1SG 194
ATOM	194	C	ASP	23	5.437	66.242	-4.163	1.00	0.26	1SG 195
ATOM	195	O	ASP	23	6.388	66.584	-4.872	1.00	0.26	1SG 196
ATOM	196	N	SER	24	4.784	67.104	-3.350	1.00	0.11	1SG 197
ATOM	197	CA	SER	24	5.124	68.497	-3.284	1.00	0.11	1SG 198
ATOM	198	CB	SER	24	3.932	69.399	-2.918	1.00	0.11	1SG 199
ATOM	199	OG	SER	24	4.336	70.760	-2.873	1.00	0.11	1SG 200
ATOM	200	C	SER	24	6.159	68.680	-2.222	1.00	0.11	1SG 201
ATOM	201	O	SER	24	6.104	68.045	-1.171	1.00	0.11	1SG 202
ATOM	202	N	VAL	25	7.164	69.537	-2.487	1.00	0.10	1SG 203
ATOM	203	CA	VAL	25	8.167	69.792	-1.492	1.00	0.10	1SG 204
ATOM	204	CB	VAL	25	9.530	69.287	-1.877	1.00	0.10	1SG 205
ATOM	205	CG1	VAL	25	10.534	69.704	-0.789	1.00	0.10	1SG 206
ATOM	206	CG2	VAL	25	9.453	67.767	-2.104	1.00	0.10	1SG 207
ATOM	207	C	VAL	25	8.278	71.276	-1.344	1.00	0.10	1SG 208
ATOM	208	O	VAL	25	8.336	71.999	-2.338	1.00	0.10	1SG 209
ATOM	209	N	THR	26	8.295	71.766	-0.084	1.00	0.09	1SG 210
ATOM	210	CA	THR	26	8.408	73.177	0.164	1.00	0.09	1SG 211
ATOM	211	CB	THR	26	7.254	73.732	0.946	1.00	0.09	1SG 212
ATOM	212	OG1	THR	26	6.040	73.502	0.247	1.00	0.09	1SG 213
ATOM	213	CG2	THR	26	7.467	75.243	1.142	1.00	0.09	1SG 214
ATOM	214	C	THR	26	9.640	73.398	0.982	1.00	0.09	1SG 215
ATOM	215	O	THR	26	9.791	72.831	2.073	1.00	0.09	1SG 216
ATOM	216	N	LEU	27	10.568	74.219	0.461	1.00	0.16	1SG 217
ATOM	217	CA	LEU	27	11.777	74.529	1.162	1.00	0.16	1SG 218
ATOM	218	CB	LEU	27	13.031	74.380	0.286	1.00	0.16	1SG 219
ATOM	219	CG	LEU	27	13.325	72.930	-0.140	1.00	0.16	1SG 220
ATOM	220	CD2	LEU	27	13.423	72.008	1.081	1.00	0.16	1SG 221
ATOM	221	CD1	LEU	27	14.585	72.854	-1.013	1.00	0.16	1SG 222
ATOM	222	C	LEU	27	11.683	75.974	1.550	1.00	0.16	1SG 223
ATOM	223	O	LEU	27	11.267	76.812	0.752	1.00	0.16	1SG 224
ATOM	224	N	LYS	28	12.051	76.300	2.806	1.00	0.26	1SG 225
ATOM	225	CA	LYS	28	11.982	77.664	3.253	1.00	0.26	1SG 226
ATOM	226	CB	LYS	28	11.025	77.848	4.443	1.00	0.26	1SG 227
ATOM	227	CG	LYS	28	9.559	77.562	4.112	1.00	0.26	1SG 228
ATOM	228	CD	LYS	28	8.696	77.332	5.355	1.00	0.26	1SG 229
ATOM	229	CE	LYS	28	8.759	78.477	6.369	1.00	0.26	1SG 230
ATOM	230	NZ	LYS	28	7.898	78.171	7.534	1.00	0.26	1SG 231
ATOM	231	C	LYS	28	13.350	78.065	3.716	1.00	0.26	1SG 232
ATOM	232	O	LYS	28	13.972	77.361	4.510	1.00	0.26	1SG 233
ATOM	233	N	CYS	29	13.855	79.221	3.231	1.00	0.25	1SG 234
ATOM	234	CA	CYS	29	15.166	79.665	3.623	1.00	0.25	1SG 235
ATOM	235	CB	CYS	29	15.989	80.261	2.466	1.00	0.25	1SG 236
ATOM	236	SG	CYS	29	17.746	80.487	2.876	1.00	0.25	1SG 237
ATOM	237	C	CYS	29	14.976	80.743	4.635	1.00	0.25	1SG 238
ATOM	238	O	CYS	29	14.520	81.842	4.318	1.00	0.25	1SG 239
ATOM	239	N	GLN	30	15.362	80.444	5.888	1.00	0.20	1SG 240
ATOM	240	CA	GLN	30	15.150	81.352	6.974	1.00	0.20	1SG 241

ATOM	241	CB	GLN	30	14.662	80.641	8.250	1.00	0.20	1SG	242
ATOM	242	CG	GLN	30	13.328	79.910	8.073	1.00	0.20	1SG	243
ATOM	243	CD	GLN	30	12.990	79.231	9.393	1.00	0.20	1SG	244
ATOM	244	OE1	GLN	30	13.436	79.665	10.434	1.00	0.20	1SG	245
ATOM	245	NE2	GLN	30	12.190	78.133	9.331	1.00	0.20	1SG	246
ATOM	246	C	GLN	30	16.447	82.021	7.307	1.00	0.20	1SG	247
ATOM	247	O	GLN	30	17.516	81.416	7.227	1.00	0.20	1SG	248
ATOM	248	N	GLY	31	16.370	83.318	7.670	1.00	0.17	1SG	249
ATOM	249	CA	GLY	31	17.534	84.063	8.057	1.00	0.17	1SG	250
ATOM	250	C	GLY	31	17.314	85.486	7.647	1.00	0.17	1SG	251
ATOM	251	O	GLY	31	16.372	85.790	6.917	1.00	0.17	1SG	252
ATOM	252	N	ALA	32	18.204	86.394	8.100	1.00	0.26	1SG	253
ATOM	253	CA	ALA	32	18.069	87.786	7.779	1.00	0.26	1SG	254
ATOM	254	CB	ALA	32	19.036	88.698	8.555	1.00	0.26	1SG	255
ATOM	255	C	ALA	32	18.361	87.941	6.323	1.00	0.26	1SG	256
ATOM	256	O	ALA	32	19.239	87.270	5.783	1.00	0.26	1SG	257
ATOM	257	N	TYR	33	17.622	88.851	5.656	1.00	0.37	1SG	258
ATOM	258	CA	TYR	33	17.742	89.029	4.237	1.00	0.37	1SG	259
ATOM	259	CB	TYR	33	16.403	88.888	3.494	1.00	0.37	1SG	260
ATOM	260	CG	TYR	33	15.701	87.652	3.939	1.00	0.37	1SG	261
ATOM	261	CD1	TYR	33	16.014	86.413	3.431	1.00	0.37	1SG	262
ATOM	262	CD2	TYR	33	14.701	87.754	4.878	1.00	0.37	1SG	263
ATOM	263	CE1	TYR	33	15.336	85.295	3.863	1.00	0.37	1SG	264
ATOM	264	CE2	TYR	33	14.020	86.642	5.313	1.00	0.37	1SG	265
ATOM	265	CZ	TYR	33	14.340	85.408	4.804	1.00	0.37	1SG	266
ATOM	266	OH	TYR	33	13.646	84.261	5.243	1.00	0.37	1SG	267
ATOM	267	C	TYR	33	18.105	90.462	3.998	1.00	0.37	1SG	268
ATOM	268	O	TYR	33	18.011	91.297	4.896	1.00	0.37	1SG	269
ATOM	269	N	SER	34	18.565	90.773	2.768	1.00	0.30	1SG	270
ATOM	270	CA	SER	34	18.837	92.136	2.411	1.00	0.30	1SG	271
ATOM	271	CB	SER	34	19.977	92.293	1.390	1.00	0.30	1SG	272
ATOM	272	OG	SER	34	21.202	91.842	1.949	1.00	0.30	1SG	273
ATOM	273	C	SER	34	17.592	92.664	1.776	1.00	0.30	1SG	274
ATOM	274	O	SER	34	16.777	91.896	1.264	1.00	0.30	1SG	275
ATOM	275	N	PRO	35	17.383	93.950	1.821	1.00	0.24	1SG	276
ATOM	276	CA	PRO	35	16.224	94.476	1.167	1.00	0.24	1SG	277
ATOM	277	CD	PRO	35	17.816	94.788	2.923	1.00	0.24	1SG	278
ATOM	278	CB	PRO	35	16.024	95.891	1.717	1.00	0.24	1SG	279
ATOM	279	CG	PRO	35	17.306	96.182	2.527	1.00	0.24	1SG	280
ATOM	280	C	PRO	35	16.414	94.377	-0.309	1.00	0.24	1SG	281
ATOM	281	O	PRO	35	17.086	95.235	-0.882	1.00	0.24	1SG	282
ATOM	282	N	GLU	36	15.796	93.358	-0.938	1.00	0.28	1SG	283
ATOM	283	CA	GLU	36	15.884	93.180	-2.356	1.00	0.28	1SG	284
ATOM	284	CB	GLU	36	17.245	92.670	-2.865	1.00	0.28	1SG	285
ATOM	285	CG	GLU	36	17.579	91.245	-2.422	1.00	0.28	1SG	286
ATOM	286	CD	GLU	36	18.911	90.862	-3.049	1.00	0.28	1SG	287
ATOM	287	OE1	GLU	36	18.954	90.706	-4.299	1.00	0.28	1SG	288
ATOM	288	OE2	GLU	36	19.906	90.723	-2.288	1.00	0.28	1SG	289
ATOM	289	C	GLU	36	14.878	92.137	-2.725	1.00	0.28	1SG	290
ATOM	290	O	GLU	36	14.517	91.286	-1.912	1.00	0.28	1SG	291
ATOM	291	N	ASP	37	14.393	92.191	-3.978	1.00	0.30	1SG	292
ATOM	292	CA	ASP	37	13.415	91.251	-4.436	1.00	0.30	1SG	293
ATOM	293	CB	ASP	37	12.885	91.582	-5.842	1.00	0.30	1SG	294
ATOM	294	CG	ASP	37	11.706	90.667	-6.145	1.00	0.30	1SG	295
ATOM	295	OD1	ASP	37	11.405	89.773	-5.310	1.00	0.30	1SG	296
ATOM	296	OD2	ASP	37	11.086	90.853	-7.226	1.00	0.30	1SG	297
ATOM	297	C	ASP	37	14.020	89.882	-4.499	1.00	0.30	1SG	298
ATOM	298	O	ASP	37	13.423	88.916	-4.026	1.00	0.30	1SG	299
ATOM	299	N	ASN	38	15.227	89.754	-5.088	1.00	0.32	1SG	300
ATOM	300	CA	ASN	38	15.808	88.444	-5.198	1.00	0.32	1SG	301
ATOM	301	CB	ASN	38	16.651	88.257	-6.472	1.00	0.32	1SG	302

ATOM	302	CG	ASN	38	15.715	88.249	-7.675	1.00	0.32	1SG 303
ATOM	303	OD1	ASN	38	14.501	88.106	-7.540	1.00	0.32	1SG 304
ATOM	304	ND2	ASN	38	16.300	88.393	-8.894	1.00	0.32	1SG 305
ATOM	305	C	ASN	38	16.722	88.253	-4.028	1.00	0.32	1SG 306
ATOM	306	O	ASN	38	17.941	88.343	-4.157	1.00	0.32	1SG 307
ATOM	307	N	SER	39	16.129	87.978	-2.851	1.00	0.48	1SG 308
ATOM	308	CA	SER	39	16.810	87.823	-1.597	1.00	0.48	1SG 309
ATOM	309	CB	SER	39	15.861	87.925	-0.392	1.00	0.48	1SG 310
ATOM	310	OG	SER	39	15.314	89.231	-0.308	1.00	0.48	1SG 311
ATOM	311	C	SER	39	17.535	86.510	-1.448	1.00	0.48	1SG 312
ATOM	312	O	SER	39	18.534	86.442	-0.737	1.00	0.48	1SG 313
ATOM	313	N	THR	40	17.061	85.405	-2.055	1.00	0.54	1SG 314
ATOM	314	CA	THR	40	17.721	84.170	-1.709	1.00	0.54	1SG 315
ATOM	315	CB	THR	40	16.821	83.202	-0.997	1.00	0.54	1SG 316
ATOM	316	OG1	THR	40	15.745	82.821	-1.841	1.00	0.54	1SG 317
ATOM	317	CG2	THR	40	16.283	83.878	0.276	1.00	0.54	1SG 318
ATOM	318	C	THR	40	18.276	83.447	-2.899	1.00	0.54	1SG 319
ATOM	319	O	THR	40	17.733	83.482	-4.001	1.00	0.54	1SG 320
ATOM	320	N	GLN	41	19.415	82.757	-2.678	1.00	0.31	1SG 321
ATOM	321	CA	GLN	41	20.021	81.948	-3.694	1.00	0.31	1SG 322
ATOM	322	CB	GLN	41	21.552	82.067	-3.738	1.00	0.31	1SG 323
ATOM	323	CG	GLN	41	22.071	83.453	-4.118	1.00	0.31	1SG 324
ATOM	324	CD	GLN	41	23.581	83.418	-3.944	1.00	0.31	1SG 325
ATOM	325	OE1	GLN	41	24.283	84.384	-4.235	1.00	0.31	1SG 326
ATOM	326	NE2	GLN	41	24.101	82.266	-3.443	1.00	0.31	1SG 327
ATOM	327	C	GLN	41	19.738	80.532	-3.297	1.00	0.31	1SG 328
ATOM	328	O	GLN	41	19.972	80.153	-2.150	1.00	0.31	1SG 329
ATOM	329	N	TRP	42	19.207	79.715	-4.229	1.00	0.13	1SG 330
ATOM	330	CA	TRP	42	18.948	78.336	-3.910	1.00	0.13	1SG 331
ATOM	331	CB	TRP	42	17.531	77.840	-4.248	1.00	0.13	1SG 332
ATOM	332	CG	TRP	42	16.469	78.313	-3.291	1.00	0.13	1SG 333
ATOM	333	CD2	TRP	42	16.139	77.634	-2.069	1.00	0.13	1SG 334
ATOM	334	CD1	TRP	42	15.660	79.406	-3.359	1.00	0.13	1SG 335
ATOM	335	NE1	TRP	42	14.849	79.450	-2.253	1.00	0.13	1SG 336
ATOM	336	CE2	TRP	42	15.130	78.368	-1.451	1.00	0.13	1SG 337
ATOM	337	CE3	TRP	42	16.638	76.495	-1.506	1.00	0.13	1SG 338
ATOM	338	CZ2	TRP	42	14.601	77.977	-0.255	1.00	0.13	1SG 339
ATOM	339	CZ3	TRP	42	16.101	76.100	-0.301	1.00	0.13	1SG 340
ATOM	340	CH2	TRP	42	15.101	76.827	0.312	1.00	0.13	1SG 341
ATOM	341	C	TRP	42	19.895	77.498	-4.701	1.00	0.13	1SG 342
ATOM	342	O	TRP	42	20.228	77.832	-5.836	1.00	0.13	1SG 343
ATOM	343	N	PHE	43	20.367	76.385	-4.099	1.00	0.11	1SG 344
ATOM	344	CA	PHE	43	21.302	75.544	-4.787	1.00	0.11	1SG 345
ATOM	345	CB	PHE	43	22.711	75.557	-4.166	1.00	0.11	1SG 346
ATOM	346	CG	PHE	43	23.295	76.925	-4.278	1.00	0.11	1SG 347
ATOM	347	CD1	PHE	43	23.030	77.879	-3.322	1.00	0.11	1SG 348
ATOM	348	CD2	PHE	43	24.113	77.251	-5.335	1.00	0.11	1SG 349
ATOM	349	CE1	PHE	43	23.572	79.139	-3.421	1.00	0.11	1SG 350
ATOM	350	CE2	PHE	43	24.658	78.510	-5.440	1.00	0.11	1SG 351
ATOM	351	CZ	PHE	43	24.386	79.457	-4.482	1.00	0.11	1SG 352
ATOM	352	C	PHE	43	20.843	74.120	-4.693	1.00	0.11	1SG 353
ATOM	353	O	PHE	43	20.285	73.695	-3.682	1.00	0.11	1SG 354
ATOM	354	N	HIS	44	21.065	73.353	-5.782	1.00	0.13	1SG 355
ATOM	355	CA	HIS	44	20.777	71.948	-5.815	1.00	0.13	1SG 356
ATOM	356	ND1	HIS	44	18.580	69.494	-7.813	1.00	0.13	1SG 357
ATOM	357	CG	HIS	44	19.360	70.111	-6.859	1.00	0.13	1SG 358
ATOM	358	CB	HIS	44	19.757	71.560	-6.902	1.00	0.13	1SG 359
ATOM	359	NE2	HIS	44	19.059	67.948	-6.288	1.00	0.13	1SG 360
ATOM	360	CD2	HIS	44	19.643	69.152	-5.935	1.00	0.13	1SG 361
ATOM	361	CE1	HIS	44	18.432	68.203	-7.422	1.00	0.13	1SG 362
ATOM	362	C	HIS	44	22.070	71.286	-6.166	1.00	0.13	1SG 363

ATOM	363	O	HIS	44	22.582	71.465	-7.270	1.00	0.13	1SG 364
ATOM	364	N	ASN	45	22.633	70.494	-5.234	1.00	0.21	1SG 365
ATOM	365	CA	ASN	45	23.888	69.850	-5.489	1.00	0.21	1SG 366
ATOM	366	CB	ASN	45	23.811	68.784	-6.595	1.00	0.21	1SG 367
ATOM	367	CG	ASN	45	23.006	67.606	-6.063	1.00	0.21	1SG 368
ATOM	368	OD1	ASN	45	22.804	67.465	-4.857	1.00	0.21	1SG 369
ATOM	369	ND2	ASN	45	22.542	66.723	-6.987	1.00	0.21	1SG 370
ATOM	370	C	ASN	45	24.885	70.895	-5.896	1.00	0.21	1SG 371
ATOM	371	O	ASN	45	25.698	70.672	-6.792	1.00	0.21	1SG 372
ATOM	372	N	GLU	46	24.851	72.063	-5.223	1.00	0.25	1SG 373
ATOM	373	CA	GLU	46	25.781	73.134	-5.465	1.00	0.25	1SG 374
ATOM	374	CB	GLU	46	27.239	72.652	-5.580	1.00	0.25	1SG 375
ATOM	375	CG	GLU	46	27.885	72.278	-4.245	1.00	0.25	1SG 376
ATOM	376	CD	GLU	46	28.429	73.558	-3.621	1.00	0.25	1SG 377
ATOM	377	OE1	GLU	46	28.277	74.634	-4.260	1.00	0.25	1SG 378
ATOM	378	OE2	GLU	46	29.006	73.479	-2.503	1.00	0.25	1SG 379
ATOM	379	C	GLU	46	25.473	73.880	-6.731	1.00	0.25	1SG 380
ATOM	380	O	GLU	46	26.222	74.785	-7.095	1.00	0.25	1SG 381
ATOM	381	N	SER	47	24.364	73.575	-7.430	1.00	0.17	1SG 382
ATOM	382	CA	SER	47	24.095	74.317	-8.633	1.00	0.17	1SG 383
ATOM	383	CB	SER	47	23.621	73.440	-9.806	1.00	0.17	1SG 384
ATOM	384	OG	SER	47	24.655	72.553	-10.206	1.00	0.17	1SG 385
ATOM	385	C	SER	47	22.995	75.284	-8.328	1.00	0.17	1SG 386
ATOM	386	O	SER	47	21.985	74.922	-7.728	1.00	0.17	1SG 387
ATOM	387	N	LEU	48	23.167	76.556	-8.743	1.00	0.23	1SG 388
ATOM	388	CA	LEU	48	22.186	77.559	-8.441	1.00	0.23	1SG 389
ATOM	389	CB	LEU	48	22.626	78.993	-8.790	1.00	0.23	1SG 390
ATOM	390	CG	LEU	48	21.562	80.060	-8.465	1.00	0.23	1SG 391
ATOM	391	CD2	LEU	48	21.917	81.419	-9.089	1.00	0.23	1SG 392
ATOM	392	CD1	LEU	48	21.311	80.151	-6.951	1.00	0.23	1SG 393
ATOM	393	C	LEU	48	20.947	77.283	-9.227	1.00	0.23	1SG 394
ATOM	394	O	LEU	48	21.009	76.888	-10.369	1.00	0.23	1SG 395
ATOM	395	N	ILE	49	19.775	77.464	-8.584	1.00	0.46	1SG 396
ATOM	396	CA	ILE	49	18.531	77.323	-9.283	1.00	0.46	1SG 397
ATOM	397	CB	ILE	49	17.549	76.400	-8.612	1.00	0.46	1SG 398
ATOM	398	CG2	ILE	49	18.080	74.962	-8.702	1.00	0.46	1SG 399
ATOM	399	CG1	ILE	49	17.241	76.864	-7.186	1.00	0.46	1SG 400
ATOM	400	CD1	ILE	49	16.161	76.019	-6.512	1.00	0.46	1SG 401
ATOM	401	C	ILE	49	17.942	78.697	-9.391	1.00	0.46	1SG 402
ATOM	402	O	ILE	49	17.639	79.357	-8.403	1.00	0.46	1SG 403
ATOM	403	N	SER	50	17.764	79.156	-10.636	1.00	0.56	1SG 404
ATOM	404	CA	SER	50	17.325	80.482	-10.966	1.00	0.56	1SG 405
ATOM	405	CB	SER	50	17.505	80.793	-12.460	1.00	0.56	1SG 406
ATOM	406	OG	SER	50	18.882	80.738	-12.803	1.00	0.56	1SG 407
ATOM	407	C	SER	50	15.878	80.719	-10.618	1.00	0.56	1SG 408
ATOM	408	O	SER	50	15.446	81.866	-10.519	1.00	0.56	1SG 409
ATOM	409	N	SER	51	15.082	79.649	-10.449	1.00	0.61	1SG 410
ATOM	410	CA	SER	51	13.649	79.730	-10.325	1.00	0.61	1SG 411
ATOM	411	CB	SER	51	13.004	78.340	-10.202	1.00	0.61	1SG 412
ATOM	412	OG	SER	51	13.266	77.580	-11.372	1.00	0.61	1SG 413
ATOM	413	C	SER	51	13.097	80.566	-9.184	1.00	0.61	1SG 414
ATOM	414	O	SER	51	12.185	81.348	-9.451	1.00	0.61	1SG 415
ATOM	415	N	GLN	52	13.569	80.481	-7.907	1.00	0.62	1SG 416
ATOM	416	CA	GLN	52	12.750	81.193	-6.937	1.00	0.62	1SG 417
ATOM	417	CB	GLN	52	11.586	80.313	-6.439	1.00	0.62	1SG 418
ATOM	418	CG	GLN	52	10.443	81.071	-5.758	1.00	0.62	1SG 419
ATOM	419	CD	GLN	52	9.317	80.075	-5.510	1.00	0.62	1SG 420
ATOM	420	OE1	GLN	52	9.529	78.864	-5.547	1.00	0.62	1SG 421
ATOM	421	NE2	GLN	52	8.086	80.594	-5.258	1.00	0.62	1SG 422
ATOM	422	C	GLN	52	13.480	81.759	-5.707	1.00	0.62	1SG 423
ATOM	423	O	GLN	52	14.681	81.533	-5.549	1.00	0.62	1SG 424

ATOM	424	N	ALA	53	12.693	82.502	-4.835	1.00	0.57	1SG	425
ATOM	425	CA	ALA	53	12.863	83.308	-3.621	1.00	0.57	1SG	426
ATOM	426	CB	ALA	53	11.846	84.457	-3.520	1.00	0.57	1SG	427
ATOM	427	C	ALA	53	12.782	82.536	-2.306	1.00	0.57	1SG	428
ATOM	428	O	ALA	53	13.156	81.373	-2.235	1.00	0.57	1SG	429
ATOM	429	N	SER	54	12.284	83.191	-1.212	1.00	0.58	1SG	430
ATOM	430	CA	SER	54	12.293	82.741	0.175	1.00	0.58	1SG	431
ATOM	431	CB	SER	54	11.521	83.693	1.105	1.00	0.58	1SG	432
ATOM	432	OG	SER	54	12.131	84.975	1.114	1.00	0.58	1SG	433
ATOM	433	C	SER	54	11.680	81.388	0.356	1.00	0.58	1SG	434
ATOM	434	O	SER	54	12.214	80.553	1.090	1.00	0.58	1SG	435
ATOM	435	N	SER	55	10.517	81.132	-0.255	1.00	0.46	1SG	436
ATOM	436	CA	SER	55	9.984	79.811	-0.133	1.00	0.46	1SG	437
ATOM	437	CB	SER	55	8.524	79.757	0.347	1.00	0.46	1SG	438
ATOM	438	OG	SER	55	7.666	80.343	-0.618	1.00	0.46	1SG	439
ATOM	439	C	SER	55	10.047	79.255	-1.508	1.00	0.46	1SG	440
ATOM	440	O	SER	55	9.761	79.953	-2.479	1.00	0.46	1SG	441
ATOM	441	N	TYR	56	10.485	77.992	-1.622	1.00	0.43	1SG	442
ATOM	442	CA	TYR	56	10.595	77.372	-2.903	1.00	0.43	1SG	443
ATOM	443	CB	TYR	56	12.067	77.058	-3.232	1.00	0.43	1SG	444
ATOM	444	CG	TYR	56	12.177	76.276	-4.492	1.00	0.43	1SG	445
ATOM	445	CD1	TYR	56	11.797	76.812	-5.701	1.00	0.43	1SG	446
ATOM	446	CD2	TYR	56	12.710	75.010	-4.460	1.00	0.43	1SG	447
ATOM	447	CE1	TYR	56	11.919	76.076	-6.857	1.00	0.43	1SG	448
ATOM	448	CE2	TYR	56	12.836	74.270	-5.612	1.00	0.43	1SG	449
ATOM	449	CZ	TYR	56	12.436	74.803	-6.814	1.00	0.43	1SG	450
ATOM	450	OH	TYR	56	12.563	74.048	-8.000	1.00	0.43	1SG	451
ATOM	451	C	TYR	56	9.801	76.113	-2.812	1.00	0.43	1SG	452
ATOM	452	O	TYR	56	10.155	75.196	-2.074	1.00	0.43	1SG	453
ATOM	453	N	PHE	57	8.684	76.046	-3.561	1.00	0.62	1SG	454
ATOM	454	CA	PHE	57	7.847	74.888	-3.487	1.00	0.62	1SG	455
ATOM	455	CB	PHE	57	6.421	75.206	-2.996	1.00	0.62	1SG	456
ATOM	456	CG	PHE	57	5.802	76.189	-3.932	1.00	0.62	1SG	457
ATOM	457	CD1	PHE	57	5.086	75.764	-5.028	1.00	0.62	1SG	458
ATOM	458	CD2	PHE	57	5.937	77.540	-3.710	1.00	0.62	1SG	459
ATOM	459	CE1	PHE	57	4.514	76.671	-5.889	1.00	0.62	1SG	460
ATOM	460	CE2	PHE	57	5.368	78.452	-4.567	1.00	0.62	1SG	461
ATOM	461	CZ	PHE	57	4.655	78.018	-5.659	1.00	0.62	1SG	462
ATOM	462	C	PHE	57	7.760	74.286	-4.844	1.00	0.62	1SG	463
ATOM	463	O	PHE	57	7.588	74.986	-5.840	1.00	0.62	1SG	464
ATOM	464	N	ILE	58	7.914	72.952	-4.921	1.00	0.54	1SG	465
ATOM	465	CA	ILE	58	7.807	72.349	-6.209	1.00	0.54	1SG	466
ATOM	466	CB	ILE	58	9.127	72.238	-6.929	1.00	0.54	1SG	467
ATOM	467	CG2	ILE	58	9.613	73.672	-7.192	1.00	0.54	1SG	468
ATOM	468	CG1	ILE	58	10.148	71.373	-6.163	1.00	0.54	1SG	469
ATOM	469	CD1	ILE	58	9.908	69.865	-6.239	1.00	0.54	1SG	470
ATOM	470	C	ILE	58	7.196	70.999	-6.075	1.00	0.54	1SG	471
ATOM	471	O	ILE	58	7.445	70.281	-5.109	1.00	0.54	1SG	472
ATOM	472	N	ASP	59	6.318	70.643	-7.038	1.00	0.34	1SG	473
ATOM	473	CA	ASP	59	5.869	69.286	-7.121	1.00	0.34	1SG	474
ATOM	474	CB	ASP	59	4.410	69.150	-7.587	1.00	0.34	1SG	475
ATOM	475	CG	ASP	59	3.516	69.675	-6.473	1.00	0.34	1SG	476
ATOM	476	OD1	ASP	59	4.061	70.282	-5.514	1.00	0.34	1SG	477
ATOM	477	OD2	ASP	59	2.277	69.465	-6.562	1.00	0.34	1SG	478
ATOM	478	C	ASP	59	6.741	68.771	-8.189	1.00	0.34	1SG	479
ATOM	479	O	ASP	59	6.411	67.882	-8.972	1.00	0.34	1SG	480
ATOM	480	N	ALA	60	7.950	69.337	-8.208	1.00	0.27	1SG	481
ATOM	481	CA	ALA	60	8.903	68.892	-9.141	1.00	0.27	1SG	482
ATOM	482	CB	ALA	60	9.978	69.945	-9.459	1.00	0.27	1SG	483
ATOM	483	C	ALA	60	9.569	67.769	-8.452	1.00	0.27	1SG	484
ATOM	484	O	ALA	60	10.713	67.472	-8.784	1.00	0.27	1SG	485

ATOM	485	N	ALA	61	8.892	67.133	-7.457	1.00	0.37	1SG	486
ATOM	486	CA	ALA	61	9.565	66.004	-6.941	1.00	0.37	1SG	487
ATOM	487	CB	ALA	61	8.825	65.293	-5.796	1.00	0.37	1SG	488
ATOM	488	C	ALA	61	9.623	65.065	-8.099	1.00	0.37	1SG	489
ATOM	489	O	ALA	61	8.603	64.547	-8.550	1.00	0.37	1SG	490
ATOM	490	N	THR	62	10.842	64.876	-8.632	1.00	0.56	1SG	491
ATOM	491	CA	THR	62	11.083	64.025	-9.750	1.00	0.56	1SG	492
ATOM	492	CB	THR	62	11.287	64.754	-11.044	1.00	0.56	1SG	493
ATOM	493	OG1	THR	62	12.411	65.617	-10.953	1.00	0.56	1SG	494
ATOM	494	CG2	THR	62	10.016	65.559	-11.364	1.00	0.56	1SG	495
ATOM	495	C	THR	62	12.357	63.334	-9.425	1.00	0.56	1SG	496
ATOM	496	O	THR	62	13.021	63.674	-8.449	1.00	0.56	1SG	497
ATOM	497	N	VAL	63	12.743	62.358	-10.258	1.00	0.52	1SG	498
ATOM	498	CA	VAL	63	13.904	61.569	-9.983	1.00	0.52	1SG	499
ATOM	499	CB	VAL	63	14.189	60.580	-11.080	1.00	0.52	1SG	500
ATOM	500	CG1	VAL	63	13.009	59.597	-11.163	1.00	0.52	1SG	501
ATOM	501	CG2	VAL	63	14.445	61.338	-12.394	1.00	0.52	1SG	502
ATOM	502	C	VAL	63	15.086	62.480	-9.863	1.00	0.52	1SG	503
ATOM	503	O	VAL	63	15.924	62.309	-8.980	1.00	0.52	1SG	504
ATOM	504	N	ASN	64	15.146	63.505	-10.731	1.00	0.32	1SG	505
ATOM	505	CA	ASN	64	16.248	64.419	-10.842	1.00	0.32	1SG	506
ATOM	506	CB	ASN	64	16.078	65.400	-12.013	1.00	0.32	1SG	507
ATOM	507	CG	ASN	64	16.191	64.599	-13.303	1.00	0.32	1SG	508
ATOM	508	OD1	ASN	64	15.323	63.792	-13.630	1.00	0.32	1SG	509
ATOM	509	ND2	ASN	64	17.296	64.827	-14.062	1.00	0.32	1SG	510
ATOM	510	C	ASN	64	16.425	65.225	-9.588	1.00	0.32	1SG	511
ATOM	511	O	ASN	64	17.531	65.680	-9.305	1.00	0.32	1SG	512
ATOM	512	N	ASP	65	15.338	65.442	-8.825	1.00	0.25	1SG	513
ATOM	513	CA	ASP	65	15.318	66.284	-7.655	1.00	0.25	1SG	514
ATOM	514	CB	ASP	65	13.909	66.571	-7.117	1.00	0.25	1SG	515
ATOM	515	CG	ASP	65	13.324	67.671	-7.985	1.00	0.25	1SG	516
ATOM	516	OD1	ASP	65	13.629	67.694	-9.207	1.00	0.25	1SG	517
ATOM	517	OD2	ASP	65	12.581	68.522	-7.428	1.00	0.25	1SG	518
ATOM	518	C	ASP	65	16.143	65.782	-6.505	1.00	0.25	1SG	519
ATOM	519	O	ASP	65	16.459	66.561	-5.609	1.00	0.25	1SG	520
ATOM	520	N	SER	66	16.465	64.481	-6.423	1.00	0.26	1SG	521
ATOM	521	CA	SER	66	17.211	64.032	-5.275	1.00	0.26	1SG	522
ATOM	522	CB	SER	66	17.558	62.533	-5.309	1.00	0.26	1SG	523
ATOM	523	OG	SER	66	16.372	61.755	-5.255	1.00	0.26	1SG	524
ATOM	524	C	SER	66	18.509	64.781	-5.185	1.00	0.26	1SG	525
ATOM	525	O	SER	66	19.017	65.300	-6.177	1.00	0.26	1SG	526
ATOM	526	N	GLY	67	19.071	64.884	-3.958	1.00	0.35	1SG	527
ATOM	527	CA	GLY	67	20.340	65.543	-3.821	1.00	0.35	1SG	528
ATOM	528	C	GLY	67	20.318	66.412	-2.603	1.00	0.35	1SG	529
ATOM	529	O	GLY	67	19.423	66.318	-1.765	1.00	0.35	1SG	530
ATOM	530	N	GLU	68	21.326	67.300	-2.473	1.00	0.40	1SG	531
ATOM	531	CA	GLU	68	21.354	68.137	-1.311	1.00	0.40	1SG	532
ATOM	532	CB	GLU	68	22.726	68.230	-0.620	1.00	0.40	1SG	533
ATOM	533	CG	GLU	68	23.845	68.792	-1.495	1.00	0.40	1SG	534
ATOM	534	CD	GLU	68	25.108	68.817	-0.647	1.00	0.40	1SG	535
ATOM	535	OE1	GLU	68	25.663	67.720	-0.373	1.00	0.40	1SG	536
ATOM	536	OE2	GLU	68	25.528	69.937	-0.250	1.00	0.40	1SG	537
ATOM	537	C	GLU	68	20.920	69.512	-1.698	1.00	0.40	1SG	538
ATOM	538	O	GLU	68	21.211	69.986	-2.795	1.00	0.40	1SG	539
ATOM	539	N	TYR	69	20.167	70.173	-0.796	1.00	0.34	1SG	540
ATOM	540	CA	TYR	69	19.709	71.508	-1.056	1.00	0.34	1SG	541
ATOM	541	CB	TYR	69	18.186	71.697	-0.940	1.00	0.34	1SG	542
ATOM	542	CG	TYR	69	17.520	71.002	-2.077	1.00	0.34	1SG	543
ATOM	543	CD1	TYR	69	17.280	69.648	-2.029	1.00	0.34	1SG	544
ATOM	544	CD2	TYR	69	17.127	71.715	-3.187	1.00	0.34	1SG	545
ATOM	545	CE1	TYR	69	16.661	69.014	-3.080	1.00	0.34	1SG	546

ATOM	546	CE2	TYR	69	16.507	71.087	-4.240	1.00	0.34	1SG	547
ATOM	547	CZ	TYR	69	16.275	69.733	-4.186	1.00	0.34	1SG	548
ATOM	548	OH	TYR	69	15.639	69.084	-5.265	1.00	0.34	1SG	549
ATOM	549	C	TYR	69	20.315	72.420	-0.037	1.00	0.34	1SG	550
ATOM	550	O	TYR	69	20.468	72.053	1.127	1.00	0.34	1SG	551
ATOM	551	N	ARG	70	20.700	73.640	-0.468	1.00	0.33	1SG	552
ATOM	552	CA	ARG	70	21.233	74.613	0.442	1.00	0.33	1SG	553
ATOM	553	CB	ARG	70	22.767	74.627	0.507	1.00	0.33	1SG	554
ATOM	554	CG	ARG	70	23.309	73.406	1.253	1.00	0.33	1SG	555
ATOM	555	CD	ARG	70	24.830	73.388	1.424	1.00	0.33	1SG	556
ATOM	556	NE	ARG	70	25.431	72.997	0.119	1.00	0.33	1SG	557
ATOM	557	CZ	ARG	70	26.690	72.472	0.081	1.00	0.33	1SG	558
ATOM	558	NH1	ARG	70	27.408	72.344	1.235	1.00	0.33	1SG	559
ATOM	559	NH2	ARG	70	27.226	72.071	-1.108	1.00	0.33	1SG	560
ATOM	560	C	ARG	70	20.752	75.964	0.004	1.00	0.33	1SG	561
ATOM	561	O	ARG	70	20.274	76.125	-1.117	1.00	0.33	1SG	562
ATOM	562	N	CYS	71	20.825	76.972	0.900	1.00	0.26	1SG	563
ATOM	563	CA	CYS	71	20.377	78.289	0.535	1.00	0.26	1SG	564
ATOM	564	CB	CYS	71	18.893	78.555	0.864	1.00	0.26	1SG	565
ATOM	565	SG	CYS	71	18.496	78.615	2.636	1.00	0.26	1SG	566
ATOM	566	C	CYS	71	21.235	79.307	1.221	1.00	0.26	1SG	567
ATOM	567	O	CYS	71	21.949	78.991	2.172	1.00	0.26	1SG	568
ATOM	568	N	GLN	72	21.215	80.559	0.711	1.00	0.14	1SG	569
ATOM	569	CA	GLN	72	22.005	81.615	1.278	1.00	0.14	1SG	570
ATOM	570	CB	GLN	72	23.405	81.712	0.643	1.00	0.14	1SG	571
ATOM	571	CG	GLN	72	24.303	82.785	1.260	1.00	0.14	1SG	572
ATOM	572	CD	GLN	72	25.638	82.750	0.528	1.00	0.14	1SG	573
ATOM	573	OE1	GLN	72	25.792	82.069	-0.485	1.00	0.14	1SG	574
ATOM	574	NE2	GLN	72	26.634	83.512	1.054	1.00	0.14	1SG	575
ATOM	575	C	GLN	72	21.301	82.918	1.026	1.00	0.14	1SG	576
ATOM	576	O	GLN	72	20.515	83.054	0.087	1.00	0.14	1SG	577
ATOM	577	N	THR	73	21.576	83.916	1.892	1.00	0.16	1SG	578
ATOM	578	CA	THR	73	21.012	85.228	1.773	1.00	0.16	1SG	579
ATOM	579	CB	THR	73	20.152	85.599	2.951	1.00	0.16	1SG	580
ATOM	580	OG1	THR	73	19.141	84.620	3.135	1.00	0.16	1SG	581
ATOM	581	CG2	THR	73	19.486	86.959	2.679	1.00	0.16	1SG	582
ATOM	582	C	THR	73	22.191	86.155	1.737	1.00	0.16	1SG	583
ATOM	583	O	THR	73	23.325	85.730	1.942	1.00	0.16	1SG	584
ATOM	584	N	ASN	74	21.971	87.447	1.435	1.00	0.21	1SG	585
ATOM	585	CA	ASN	74	23.072	88.368	1.377	1.00	0.21	1SG	586
ATOM	586	CB	ASN	74	22.697	89.763	0.849	1.00	0.21	1SG	587
ATOM	587	CG	ASN	74	22.617	89.670	-0.669	1.00	0.21	1SG	588
ATOM	588	OD1	ASN	74	22.270	90.635	-1.348	1.00	0.21	1SG	589
ATOM	589	ND2	ASN	74	22.961	88.475	-1.220	1.00	0.21	1SG	590
ATOM	590	C	ASN	74	23.669	88.525	2.743	1.00	0.21	1SG	591
ATOM	591	O	ASN	74	24.859	88.807	2.867	1.00	0.21	1SG	592
ATOM	592	N	LEU	75	22.825	88.433	3.790	1.00	0.22	1SG	593
ATOM	593	CA	LEU	75	23.180	88.556	5.181	1.00	0.22	1SG	594
ATOM	594	CB	LEU	75	21.987	88.944	6.070	1.00	0.22	1SG	595
ATOM	595	CG	LEU	75	21.434	90.348	5.763	1.00	0.22	1SG	596
ATOM	596	CD2	LEU	75	22.562	91.388	5.672	1.00	0.22	1SG	597
ATOM	597	CD1	LEU	75	20.333	90.745	6.759	1.00	0.22	1SG	598
ATOM	598	C	LEU	75	23.804	87.324	5.785	1.00	0.22	1SG	599
ATOM	599	O	LEU	75	24.481	87.437	6.802	1.00	0.22	1SG	600
ATOM	600	N	SER	76	23.574	86.107	5.251	1.00	0.32	1SG	601
ATOM	601	CA	SER	76	24.037	84.956	5.989	1.00	0.32	1SG	602
ATOM	602	CB	SER	76	22.883	84.027	6.399	1.00	0.32	1SG	603
ATOM	603	OG	SER	76	22.213	83.551	5.240	1.00	0.32	1SG	604
ATOM	604	C	SER	76	25.017	84.125	5.215	1.00	0.32	1SG	605
ATOM	605	O	SER	76	25.282	84.360	4.038	1.00	0.32	1SG	606
ATOM	606	N	THR	77	25.634	83.142	5.909	1.00	0.43	1SG	607

ATOM	607	CA	THR	77	26.525	82.222	5.261	1.00	0.43	1SG 608
ATOM	608	CB	THR	77	27.567	81.655	6.174	1.00	0.43	1SG 609
ATOM	609	OG1	THR	77	26.955	80.928	7.228	1.00	0.43	1SG 610
ATOM	610	CG2	THR	77	28.385	82.825	6.745	1.00	0.43	1SG 611
ATOM	611	C	THR	77	25.663	81.111	4.734	1.00	0.43	1SG 612
ATOM	612	O	THR	77	24.471	81.058	5.032	1.00	0.43	1SG 613
ATOM	613	N	LEU	78	26.241	80.196	3.928	1.00	0.27	1SG 614
ATOM	614	CA	LEU	78	25.474	79.156	3.293	1.00	0.27	1SG 615
ATOM	615	CB	LEU	78	26.307	78.312	2.309	1.00	0.27	1SG 616
ATOM	616	CG	LEU	78	25.499	77.245	1.545	1.00	0.27	1SG 617
ATOM	617	CD2	LEU	78	26.425	76.234	0.850	1.00	0.27	1SG 618
ATOM	618	CD1	LEU	78	24.498	77.891	0.572	1.00	0.27	1SG 619
ATOM	619	C	LEU	78	24.920	78.243	4.345	1.00	0.27	1SG 620
ATOM	620	O	LEU	78	25.581	77.931	5.333	1.00	0.27	1SG 621
ATOM	621	N	SER	79	23.667	77.783	4.149	1.00	0.11	1SG 622
ATOM	622	CA	SER	79	23.037	76.937	5.124	1.00	0.11	1SG 623
ATOM	623	CB	SER	79	21.513	76.815	4.955	1.00	0.11	1SG 624
ATOM	624	OG	SER	79	21.213	76.083	3.776	1.00	0.11	1SG 625
ATOM	625	C	SER	79	23.595	75.557	5.010	1.00	0.11	1SG 626
ATOM	626	O	SER	79	24.203	75.200	4.001	1.00	0.11	1SG 627
ATOM	627	N	ASP	80	23.417	74.752	6.079	1.00	0.14	1SG 628
ATOM	628	CA	ASP	80	23.841	73.383	6.047	1.00	0.14	1SG 629
ATOM	629	CB	ASP	80	23.747	72.664	7.406	1.00	0.14	1SG 630
ATOM	630	CG	ASP	80	24.820	73.215	8.338	1.00	0.14	1SG 631
ATOM	631	OD1	ASP	80	25.741	73.920	7.845	1.00	0.14	1SG 632
ATOM	632	OD2	ASP	80	24.733	72.931	9.562	1.00	0.14	1SG 633
ATOM	633	C	ASP	80	22.908	72.703	5.097	1.00	0.14	1SG 634
ATOM	634	O	ASP	80	21.786	73.158	4.880	1.00	0.14	1SG 635
ATOM	635	N	PRO	81	23.361	71.635	4.504	1.00	0.17	1SG 636
ATOM	636	CA	PRO	81	22.566	70.959	3.515	1.00	0.17	1SG 637
ATOM	637	CD	PRO	81	24.783	71.457	4.267	1.00	0.17	1SG 638
ATOM	638	CB	PRO	81	23.545	70.174	2.637	1.00	0.17	1SG 639
ATOM	639	CG	PRO	81	24.867	70.176	3.423	1.00	0.17	1SG 640
ATOM	640	C	PRO	81	21.445	70.127	4.045	1.00	0.17	1SG 641
ATOM	641	O	PRO	81	21.508	69.669	5.185	1.00	0.17	1SG 642
ATOM	642	N	VAL	82	20.396	69.960	3.216	1.00	0.16	1SG 643
ATOM	643	CA	VAL	82	19.285	69.101	3.498	1.00	0.16	1SG 644
ATOM	644	CB	VAL	82	17.966	69.817	3.475	1.00	0.16	1SG 645
ATOM	645	CG1	VAL	82	16.840	68.794	3.699	1.00	0.16	1SG 646
ATOM	646	CG2	VAL	82	18.008	70.940	4.524	1.00	0.16	1SG 647
ATOM	647	C	VAL	82	19.286	68.130	2.359	1.00	0.16	1SG 648
ATOM	648	O	VAL	82	19.289	68.539	1.198	1.00	0.16	1SG 649
ATOM	649	N	GLN	83	19.288	66.815	2.656	1.00	0.14	1SG 650
ATOM	650	CA	GLN	83	19.369	65.853	1.595	1.00	0.14	1SG 651
ATOM	651	CB	GLN	83	20.289	64.661	1.909	1.00	0.14	1SG 652
ATOM	652	CG	GLN	83	20.361	63.653	0.761	1.00	0.14	1SG 653
ATOM	653	CD	GLN	83	21.289	62.516	1.166	1.00	0.14	1SG 654
ATOM	654	OE1	GLN	83	21.088	61.372	0.761	1.00	0.14	1SG 655
ATOM	655	NE2	GLN	83	22.329	62.832	1.983	1.00	0.14	1SG 656
ATOM	656	C	GLN	83	18.000	65.310	1.325	1.00	0.14	1SG 657
ATOM	657	O	GLN	83	17.266	64.946	2.241	1.00	0.14	1SG 658
ATOM	658	N	LEU	84	17.623	65.249	0.031	1.00	0.13	1SG 659
ATOM	659	CA	LEU	84	16.313	64.773	-0.309	1.00	0.13	1SG 660
ATOM	660	CB	LEU	84	15.463	65.842	-1.024	1.00	0.13	1SG 661
ATOM	661	CG	LEU	84	14.045	65.379	-1.404	1.00	0.13	1SG 662
ATOM	662	CD2	LEU	84	13.376	66.379	-2.362	1.00	0.13	1SG 663
ATOM	663	CD1	LEU	84	13.193	65.093	-0.157	1.00	0.13	1SG 664
ATOM	664	C	LEU	84	16.463	63.601	-1.234	1.00	0.13	1SG 665
ATOM	665	O	LEU	84	17.358	63.578	-2.077	1.00	0.13	1SG 666
ATOM	666	N	GLU	85	15.609	62.565	-1.067	1.00	0.13	1SG 667
ATOM	667	CA	GLU	85	15.659	61.442	-1.962	1.00	0.13	1SG 668

ATOM	668	CB	GLU	85	16.128	60.122	-1.323	1.00	0.13	1SG 669
ATOM	669	CG	GLU	85	17.623	60.111	-0.993	1.00	0.13	1SG 670
ATOM	670	CD	GLU	85	18.029	58.680	-0.673	1.00	0.13	1SG 671
ATOM	671	OE1	GLU	85	17.391	58.068	0.224	1.00	0.13	1SG 672
ATOM	672	OE2	GLU	85	18.980	58.178	-1.330	1.00	0.13	1SG 673
ATOM	673	C	GLU	85	14.284	61.216	-2.512	1.00	0.13	1SG 674
ATOM	674	O	GLU	85	13.323	61.034	-1.765	1.00	0.13	1SG 675
ATOM	675	N	VAL	86	14.161	61.211	-3.855	1.00	0.18	1SG 676
ATOM	676	CA	VAL	86	12.880	61.025	-4.470	1.00	0.18	1SG 677
ATOM	677	CB	VAL	86	12.628	61.986	-5.593	1.00	0.18	1SG 678
ATOM	678	CG1	VAL	86	11.244	61.699	-6.195	1.00	0.18	1SG 679
ATOM	679	CG2	VAL	86	12.774	63.413	-5.038	1.00	0.18	1SG 680
ATOM	680	C	VAL	86	12.831	59.631	-5.014	1.00	0.18	1SG 681
ATOM	681	O	VAL	86	13.746	59.188	-5.708	1.00	0.18	1SG 682
ATOM	682	N	HIS	87	11.743	58.893	-4.710	1.00	0.34	1SG 683
ATOM	683	CA	HIS	87	11.681	57.522	-5.133	1.00	0.34	1SG 684
ATOM	684	ND1	HIS	87	13.107	57.437	-2.117	1.00	0.34	1SG 685
ATOM	685	CG	HIS	87	12.856	56.525	-3.119	1.00	0.34	1SG 686
ATOM	686	CB	HIS	87	11.614	56.524	-3.963	1.00	0.34	1SG 687
ATOM	687	NE2	HIS	87	14.860	56.069	-2.186	1.00	0.34	1SG 688
ATOM	688	CD2	HIS	87	13.936	55.697	-3.147	1.00	0.34	1SG 689
ATOM	689	CE1	HIS	87	14.318	57.118	-1.593	1.00	0.34	1SG 690
ATOM	690	C	HIS	87	10.467	57.302	-5.978	1.00	0.34	1SG 691
ATOM	691	O	HIS	87	9.539	58.109	-5.995	1.00	0.34	1SG 692
ATOM	692	N	ILE	88	10.485	56.205	-6.762	1.00	0.38	1SG 693
ATOM	693	CA	ILE	88	9.339	55.850	-7.542	1.00	0.38	1SG 694
ATOM	694	CB	ILE	88	9.605	55.807	-9.024	1.00	0.38	1SG 695
ATOM	695	CG2	ILE	88	10.824	54.912	-9.310	1.00	0.38	1SG 696
ATOM	696	CG1	ILE	88	8.323	55.418	-9.776	1.00	0.38	1SG 697
ATOM	697	CD1	ILE	88	8.409	55.623	-11.288	1.00	0.38	1SG 698
ATOM	698	C	ILE	88	8.899	54.495	-7.072	1.00	0.38	1SG 699
ATOM	699	O	ILE	88	9.501	53.472	-7.396	1.00	0.38	1SG 700
ATOM	700	N	GLY	89	7.809	54.464	-6.281	1.00	0.20	1SG 701
ATOM	701	CA	GLY	89	7.304	53.227	-5.757	1.00	0.20	1SG 702
ATOM	702	C	GLY	89	5.901	53.499	-5.315	1.00	0.20	1SG 703
ATOM	703	O	GLY	89	5.512	54.651	-5.141	1.00	0.20	1SG 704
ATOM	704	N	TRP	90	5.094	52.434	-5.147	1.00	0.12	1SG 705
ATOM	705	CA	TRP	90	3.723	52.586	-4.750	1.00	0.12	1SG 706
ATOM	706	CB	TRP	90	2.880	51.313	-4.922	1.00	0.12	1SG 707
ATOM	707	CG	TRP	90	2.518	51.031	-6.358	1.00	0.12	1SG 708
ATOM	708	CD2	TRP	90	1.448	51.700	-7.042	1.00	0.12	1SG 709
ATOM	709	CD1	TRP	90	3.076	50.170	-7.258	1.00	0.12	1SG 710
ATOM	710	NE1	TRP	90	2.414	50.255	-8.460	1.00	0.12	1SG 711
ATOM	711	CE2	TRP	90	1.410	51.195	-8.341	1.00	0.12	1SG 712
ATOM	712	CE3	TRP	90	0.569	52.657	-6.619	1.00	0.12	1SG 713
ATOM	713	CZ2	TRP	90	0.486	51.642	-9.241	1.00	0.12	1SG 714
ATOM	714	CZ3	TRP	90	-0.361	53.107	-7.529	1.00	0.12	1SG 715
ATOM	715	CH2	TRP	90	-0.400	52.608	-8.815	1.00	0.12	1SG 716
ATOM	716	C	TRP	90	3.580	53.037	-3.324	1.00	0.12	1SG 717
ATOM	717	O	TRP	90	2.663	53.800	-3.022	1.00	0.12	1SG 718
ATOM	718	N	LEU	91	4.446	52.560	-2.403	1.00	0.26	1SG 719
ATOM	719	CA	LEU	91	4.266	52.905	-1.015	1.00	0.26	1SG 720
ATOM	720	CB	LEU	91	3.562	51.776	-0.239	1.00	0.26	1SG 721
ATOM	721	CG	LEU	91	3.157	52.126	1.203	1.00	0.26	1SG 722
ATOM	722	CD2	LEU	91	2.734	50.869	1.981	1.00	0.26	1SG 723
ATOM	723	CD1	LEU	91	2.079	53.222	1.222	1.00	0.26	1SG 724
ATOM	724	C	LEU	91	5.614	53.138	-0.385	1.00	0.26	1SG 725
ATOM	725	O	LEU	91	6.577	52.431	-0.677	1.00	0.26	1SG 726
ATOM	726	N	LEU	92	5.719	54.138	0.522	1.00	0.38	1SG 727
ATOM	727	CA	LEU	92	6.998	54.439	1.103	1.00	0.38	1SG 728
ATOM	728	CB	LEU	92	7.560	55.735	0.473	1.00	0.38	1SG 729

ATOM	729	CG	LEU	92	9.071	56.015	0.609	1.00	0.38	1SG	730
ATOM	730	CD2	LEU	92	9.558	55.970	2.057	1.00	0.38	1SG	731
ATOM	731	CD1	LEU	92	9.434	57.344	-0.076	1.00	0.38	1SG	732
ATOM	732	C	LEU	92	6.810	54.634	2.588	1.00	0.38	1SG	733
ATOM	733	O	LEU	92	5.768	55.108	3.043	1.00	0.38	1SG	734
ATOM	734	N	LEU	93	7.804	54.221	3.402	1.00	0.28	1SG	735
ATOM	735	CA	LEU	93	7.741	54.488	4.812	1.00	0.28	1SG	736
ATOM	736	CB	LEU	93	8.385	53.414	5.695	1.00	0.28	1SG	737
ATOM	737	CG	LEU	93	8.272	53.774	7.184	1.00	0.28	1SG	738
ATOM	738	CD2	LEU	93	9.357	53.085	8.018	1.00	0.28	1SG	739
ATOM	739	CD1	LEU	93	6.842	53.566	7.705	1.00	0.28	1SG	740
ATOM	740	C	LEU	93	8.566	55.725	5.002	1.00	0.28	1SG	741
ATOM	741	O	LEU	93	9.775	55.710	4.770	1.00	0.28	1SG	742
ATOM	742	N	GLN	94	7.949	56.830	5.464	1.00	0.17	1SG	743
ATOM	743	CA	GLN	94	8.665	58.079	5.487	1.00	0.17	1SG	744
ATOM	744	CB	GLN	94	7.823	59.244	4.936	1.00	0.17	1SG	745
ATOM	745	CG	GLN	94	7.457	59.079	3.456	1.00	0.17	1SG	746
ATOM	746	CD	GLN	94	6.482	60.183	3.068	1.00	0.17	1SG	747
ATOM	747	OE1	GLN	94	5.403	60.300	3.646	1.00	0.17	1SG	748
ATOM	748	NE2	GLN	94	6.867	61.016	2.063	1.00	0.17	1SG	749
ATOM	749	C	GLN	94	9.119	58.445	6.869	1.00	0.17	1SG	750
ATOM	750	O	GLN	94	8.489	58.092	7.864	1.00	0.17	1SG	751
ATOM	751	N	ALA	95	10.270	59.157	6.949	1.00	0.22	1SG	752
ATOM	752	CA	ALA	95	10.807	59.602	8.209	1.00	0.22	1SG	753
ATOM	753	CB	ALA	95	11.868	58.652	8.789	1.00	0.22	1SG	754
ATOM	754	C	ALA	95	11.466	60.944	8.020	1.00	0.22	1SG	755
ATOM	755	O	ALA	95	11.923	61.281	6.929	1.00	0.22	1SG	756
ATOM	756	N	PRO	96	11.450	61.752	9.055	1.00	0.32	1SG	757
ATOM	757	CA	PRO	96	12.110	63.037	9.060	1.00	0.32	1SG	758
ATOM	758	CD	PRO	96	10.425	61.656	10.079	1.00	0.32	1SG	759
ATOM	759	CB	PRO	96	11.422	63.855	10.153	1.00	0.32	1SG	760
ATOM	760	CG	PRO	96	10.741	62.805	11.048	1.00	0.32	1SG	761
ATOM	761	C	PRO	96	13.591	62.923	9.280	1.00	0.32	1SG	762
ATOM	762	O	PRO	96	14.314	63.852	8.921	1.00	0.32	1SG	763
ATOM	763	N	ARG	97	14.065	61.820	9.898	1.00	0.53	1SG	764
ATOM	764	CA	ARG	97	15.473	61.698	10.174	1.00	0.53	1SG	765
ATOM	765	CB	ARG	97	15.898	62.263	11.541	1.00	0.53	1SG	766
ATOM	766	CG	ARG	97	15.826	63.783	11.675	1.00	0.53	1SG	767
ATOM	767	CD	ARG	97	16.303	64.269	13.047	1.00	0.53	1SG	768
ATOM	768	NE	ARG	97	16.192	65.754	13.073	1.00	0.53	1SG	769
ATOM	769	CZ	ARG	97	16.441	66.436	14.229	1.00	0.53	1SG	770
ATOM	770	NH1	ARG	97	16.772	65.759	15.367	1.00	0.53	1SG	771
ATOM	771	NH2	ARG	97	16.358	67.798	14.244	1.00	0.53	1SG	772
ATOM	772	C	ARG	97	15.838	60.245	10.235	1.00	0.53	1SG	773
ATOM	773	O	ARG	97	14.998	59.389	10.508	1.00	0.53	1SG	774
ATOM	774	N	TRP	98	17.112	59.947	9.899	1.00	0.63	1SG	775
ATOM	775	CA	TRP	98	17.708	58.639	9.981	1.00	0.63	1SG	776
ATOM	776	CB	TRP	98	19.044	58.563	9.225	1.00	0.63	1SG	777
ATOM	777	CG	TRP	98	18.963	58.722	7.727	1.00	0.63	1SG	778
ATOM	778	CD2	TRP	98	19.073	57.635	6.796	1.00	0.63	1SG	779
ATOM	779	CD1	TRP	98	18.829	59.858	6.982	1.00	0.63	1SG	780
ATOM	780	NE1	TRP	98	18.849	59.546	5.644	1.00	0.63	1SG	781
ATOM	781	CE2	TRP	98	19.000	58.181	5.515	1.00	0.63	1SG	782
ATOM	782	CE3	TRP	98	19.231	56.293	6.993	1.00	0.63	1SG	783
ATOM	783	CZ2	TRP	98	19.083	57.388	4.406	1.00	0.63	1SG	784
ATOM	784	CZ3	TRP	98	19.308	55.495	5.873	1.00	0.63	1SG	785
ATOM	785	CH2	TRP	98	19.235	56.033	4.604	1.00	0.63	1SG	786
ATOM	786	C	TRP	98	18.054	58.309	11.401	1.00	0.63	1SG	787
ATOM	787	O	TRP	98	17.880	57.176	11.851	1.00	0.63	1SG	788
ATOM	788	N	VAL	99	18.595	59.298	12.142	1.00	0.34	1SG	789
ATOM	789	CA	VAL	99	19.048	59.025	13.477	1.00	0.34	1SG	790

ATOM	790	CB	VAL	99	20.524	59.219	13.662	1.00	0.34	1SG 791
ATOM	791	CG1	VAL	99	20.863	58.957	15.139	1.00	0.34	1SG 792
ATOM	792	CG2	VAL	99	21.271	58.304	12.676	1.00	0.34	1SG 793
ATOM	793	C	VAL	99	18.367	59.959	14.419	1.00	0.34	1SG 794
ATOM	794	O	VAL	99	18.049	61.095	14.072	1.00	0.34	1SG 795
ATOM	795	N	PHE	100	18.120	59.475	15.651	1.00	0.22	1SG 796
ATOM	796	CA	PHE	100	17.482	60.261	16.666	1.00	0.22	1SG 797
ATOM	797	CB	PHE	100	16.050	59.805	17.011	1.00	0.22	1SG 798
ATOM	798	CG	PHE	100	15.147	60.050	15.850	1.00	0.22	1SG 799
ATOM	799	CD1	PHE	100	15.045	59.126	14.835	1.00	0.22	1SG 800
ATOM	800	CD2	PHE	100	14.393	61.200	15.781	1.00	0.22	1SG 801
ATOM	801	CE1	PHE	100	14.210	59.348	13.765	1.00	0.22	1SG 802
ATOM	802	CE2	PHE	100	13.557	61.428	14.714	1.00	0.22	1SG 803
ATOM	803	CZ	PHE	100	13.464	60.501	13.704	1.00	0.22	1SG 804
ATOM	804	C	PHE	100	18.269	60.096	17.929	1.00	0.22	1SG 805
ATOM	805	O	PHE	100	19.106	59.202	18.044	1.00	0.22	1SG 806
ATOM	806	N	LYS	101	18.022	60.982	18.914	1.00	0.37	1SG 807
ATOM	807	CA	LYS	101	18.685	60.871	20.179	1.00	0.37	1SG 808
ATOM	808	CB	LYS	101	19.121	62.219	20.781	1.00	0.37	1SG 809
ATOM	809	CG	LYS	101	20.001	62.084	22.025	1.00	0.37	1SG 810
ATOM	810	CD	LYS	101	20.705	63.381	22.431	1.00	0.37	1SG 811
ATOM	811	CE	LYS	101	21.583	63.228	23.674	1.00	0.37	1SG 812
ATOM	812	NZ	LYS	101	20.740	62.951	24.858	1.00	0.37	1SG 813
ATOM	813	C	LYS	101	17.693	60.252	21.105	1.00	0.37	1SG 814
ATOM	814	O	LYS	101	16.495	60.245	20.827	1.00	0.37	1SG 815
ATOM	815	N	GLU	102	18.163	59.687	22.231	1.00	0.39	1SG 816
ATOM	816	CA	GLU	102	17.220	59.044	23.095	1.00	0.39	1SG 817
ATOM	817	CB	GLU	102	17.844	58.321	24.301	1.00	0.39	1SG 818
ATOM	818	CG	GLU	102	16.843	57.503	25.120	1.00	0.39	1SG 819
ATOM	819	CD	GLU	102	17.615	56.757	26.198	1.00	0.39	1SG 820
ATOM	820	OE1	GLU	102	18.311	57.431	27.003	1.00	0.39	1SG 821
ATOM	821	OE2	GLU	102	17.521	55.500	26.228	1.00	0.39	1SG 822
ATOM	822	C	GLU	102	16.283	60.078	23.620	1.00	0.39	1SG 823
ATOM	823	O	GLU	102	16.670	61.220	23.867	1.00	0.39	1SG 824
ATOM	824	N	GLU	103	15.011	59.670	23.799	1.00	0.36	1SG 825
ATOM	825	CA	GLU	103	13.964	60.488	24.342	1.00	0.36	1SG 826
ATOM	826	CB	GLU	103	14.455	61.396	25.484	1.00	0.36	1SG 827
ATOM	827	CG	GLU	103	13.329	62.144	26.202	1.00	0.36	1SG 828
ATOM	828	CD	GLU	103	13.884	62.673	27.516	1.00	0.36	1SG 829
ATOM	829	OE1	GLU	103	14.575	63.727	27.492	1.00	0.36	1SG 830
ATOM	830	OE2	GLU	103	13.629	62.021	28.564	1.00	0.36	1SG 831
ATOM	831	C	GLU	103	13.304	61.337	23.292	1.00	0.36	1SG 832
ATOM	832	O	GLU	103	12.292	61.973	23.577	1.00	0.36	1SG 833
ATOM	833	N	ASP	104	13.805	61.348	22.040	1.00	0.43	1SG 834
ATOM	834	CA	ASP	104	13.164	62.158	21.035	1.00	0.43	1SG 835
ATOM	835	CB	ASP	104	14.062	62.472	19.824	1.00	0.43	1SG 836
ATOM	836	CG	ASP	104	15.128	63.467	20.261	1.00	0.43	1SG 837
ATOM	837	OD1	ASP	104	14.791	64.371	21.072	1.00	0.43	1SG 838
ATOM	838	OD2	ASP	104	16.289	63.343	19.786	1.00	0.43	1SG 839
ATOM	839	C	ASP	104	11.960	61.429	20.519	1.00	0.43	1SG 840
ATOM	840	O	ASP	104	11.861	60.207	20.619	1.00	0.43	1SG 841
ATOM	841	N	PRO	105	11.000	62.175	20.031	1.00	0.49	1SG 842
ATOM	842	CA	PRO	105	9.848	61.540	19.444	1.00	0.49	1SG 843
ATOM	843	CD	PRO	105	10.635	63.393	20.738	1.00	0.49	1SG 844
ATOM	844	CB	PRO	105	8.700	62.541	19.551	1.00	0.49	1SG 845
ATOM	845	CG	PRO	105	9.098	63.424	20.745	1.00	0.49	1SG 846
ATOM	846	C	PRO	105	10.124	61.111	18.035	1.00	0.49	1SG 847
ATOM	847	O	PRO	105	10.660	61.908	17.264	1.00	0.49	1SG 848
ATOM	848	N	ILE	106	9.727	59.883	17.652	1.00	0.36	1SG 849
ATOM	849	CA	ILE	106	9.943	59.473	16.295	1.00	0.36	1SG 850
ATOM	850	CB	ILE	106	10.523	58.093	16.165	1.00	0.36	1SG 851

ATOM	851	CG2	ILE	106	10.559	57.725	14.672	1.00	0.36	1SG	852
ATOM	852	CG1	ILE	106	11.905	58.028	16.839	1.00	0.36	1SG	853
ATOM	853	CD1	ILE	106	12.457	56.609	16.964	1.00	0.36	1SG	854
ATOM	854	C	ILE	106	8.601	59.479	15.637	1.00	0.36	1SG	855
ATOM	855	O	ILE	106	7.648	58.886	16.143	1.00	0.36	1SG	856
ATOM	856	N	HIS	107	8.487	60.185	14.495	1.00	0.24	1SG	857
ATOM	857	CA	HIS	107	7.250	60.266	13.772	1.00	0.24	1SG	858
ATOM	858	ND1	HIS	107	5.419	61.664	11.375	1.00	0.24	1SG	859
ATOM	859	CG	HIS	107	5.521	61.800	12.741	1.00	0.24	1SG	860
ATOM	860	CB	HIS	107	6.811	61.712	13.496	1.00	0.24	1SG	861
ATOM	861	NE2	HIS	107	3.359	62.008	12.134	1.00	0.24	1SG	862
ATOM	862	CD2	HIS	107	4.254	62.011	13.189	1.00	0.24	1SG	863
ATOM	863	CE1	HIS	107	4.105	61.797	11.065	1.00	0.24	1SG	864
ATOM	864	C	HIS	107	7.455	59.623	12.437	1.00	0.24	1SG	865
ATOM	865	O	HIS	107	8.426	59.919	11.743	1.00	0.24	1SG	866
ATOM	866	N	LEU	108	6.532	58.728	12.034	1.00	0.32	1SG	867
ATOM	867	CA	LEU	108	6.678	58.051	10.776	1.00	0.32	1SG	868
ATOM	868	CB	LEU	108	7.053	56.568	10.922	1.00	0.32	1SG	869
ATOM	869	CG	LEU	108	8.401	56.337	11.629	1.00	0.32	1SG	870
ATOM	870	CD2	LEU	108	9.528	57.138	10.963	1.00	0.32	1SG	871
ATOM	871	CD1	LEU	108	8.722	54.838	11.741	1.00	0.32	1SG	872
ATOM	872	C	LEU	108	5.365	58.089	10.057	1.00	0.32	1SG	873
ATOM	873	O	LEU	108	4.317	58.287	10.669	1.00	0.32	1SG	874
ATOM	874	N	ARG	109	5.391	57.926	8.715	1.00	0.56	1SG	875
ATOM	875	CA	ARG	109	4.152	57.926	7.992	1.00	0.56	1SG	876
ATOM	876	CB	ARG	109	3.759	59.308	7.445	1.00	0.56	1SG	877
ATOM	877	CG	ARG	109	2.437	59.292	6.678	1.00	0.56	1SG	878
ATOM	878	CD	ARG	109	1.919	60.679	6.297	1.00	0.56	1SG	879
ATOM	879	NE	ARG	109	2.988	61.367	5.522	1.00	0.56	1SG	880
ATOM	880	CZ	ARG	109	2.734	61.825	4.262	1.00	0.56	1SG	881
ATOM	881	NH1	ARG	109	1.540	61.534	3.664	1.00	0.56	1SG	882
ATOM	882	NH2	ARG	109	3.674	62.558	3.597	1.00	0.56	1SG	883
ATOM	883	C	ARG	109	4.246	56.981	6.835	1.00	0.56	1SG	884
ATOM	884	O	ARG	109	5.286	56.856	6.190	1.00	0.56	1SG	885
ATOM	885	N	CYS	110	3.129	56.286	6.547	1.00	0.57	1SG	886
ATOM	886	CA	CYS	110	3.049	55.357	5.458	1.00	0.57	1SG	887
ATOM	887	CB	CYS	110	2.169	54.160	5.827	1.00	0.57	1SG	888
ATOM	888	SG	CYS	110	2.263	52.785	4.659	1.00	0.57	1SG	889
ATOM	889	C	CYS	110	2.373	56.124	4.366	1.00	0.57	1SG	890
ATOM	890	O	CYS	110	1.224	56.532	4.524	1.00	0.57	1SG	891
ATOM	891	N	HIS	111	3.069	56.339	3.228	1.00	0.38	1SG	892
ATOM	892	CA	HIS	111	2.538	57.210	2.212	1.00	0.38	1SG	893
ATOM	893	ND1	HIS	111	3.845	59.725	-0.098	1.00	0.38	1SG	894
ATOM	894	CG	HIS	111	3.026	59.397	0.958	1.00	0.38	1SG	895
ATOM	895	CB	HIS	111	3.431	58.454	2.048	1.00	0.38	1SG	896
ATOM	896	NE2	HIS	111	1.950	60.848	-0.391	1.00	0.38	1SG	897
ATOM	897	CD2	HIS	111	1.872	60.091	0.765	1.00	0.38	1SG	898
ATOM	898	CE1	HIS	111	3.153	60.597	-0.874	1.00	0.38	1SG	899
ATOM	899	C	HIS	111	2.419	56.523	0.884	1.00	0.38	1SG	900
ATOM	900	O	HIS	111	3.335	55.837	0.435	1.00	0.38	1SG	901
ATOM	901	N	SER	112	1.273	56.736	0.198	1.00	0.32	1SG	902
ATOM	902	CA	SER	112	1.044	56.101	-1.070	1.00	0.32	1SG	903
ATOM	903	CB	SER	112	-0.389	55.569	-1.218	1.00	0.32	1SG	904
ATOM	904	OG	SER	112	-0.492	54.787	-2.396	1.00	0.32	1SG	905
ATOM	905	C	SER	112	1.307	57.088	-2.172	1.00	0.32	1SG	906
ATOM	906	O	SER	112	1.242	58.302	-1.980	1.00	0.32	1SG	907
ATOM	907	N	TRP	113	1.638	56.569	-3.372	1.00	0.30	1SG	908
ATOM	908	CA	TRP	113	1.963	57.399	-4.497	1.00	0.30	1SG	909
ATOM	909	CB	TRP	113	2.495	56.585	-5.697	1.00	0.30	1SG	910
ATOM	910	CG	TRP	113	2.901	57.379	-6.919	1.00	0.30	1SG	911
ATOM	911	CD2	TRP	113	2.390	57.139	-8.240	1.00	0.30	1SG	912

246

ATOM	912	CD1	TRP	113	3.833	58.368	-7.040	1.00	0.30	1SG 913
ATOM	913	NE1	TRP	113	3.923	58.771	-8.351	1.00	0.30	1SG 914
ATOM	914	CE2	TRP	113	3.046	58.019	-9.102	1.00	0.30	1SG 915
ATOM	915	CE3	TRP	113	1.459	56.252	-8.700	1.00	0.30	1SG 916
ATOM	916	CZ2	TRP	113	2.778	58.026	-10.441	1.00	0.30	1SG 917
ATOM	917	CZ3	TRP	113	1.187	56.267	-10.050	1.00	0.30	1SG 918
ATOM	918	CH2	TRP	113	1.834	57.139	-10.903	1.00	0.30	1SG 919
ATOM	919	C	TRP	113	0.745	58.163	-4.905	1.00	0.30	1SG 920
ATOM	920	O	TRP	113	-0.351	57.617	-5.020	1.00	0.30	1SG 921
ATOM	921	N	LYS	114	0.922	59.482	-5.109	1.00	0.27	1SG 922
ATOM	922	CA	LYS	114	-0.135	60.350	-5.539	1.00	0.27	1SG 923
ATOM	923	CB	LYS	114	-0.677	59.986	-6.931	1.00	0.27	1SG 924
ATOM	924	CG	LYS	114	0.364	60.164	-8.037	1.00	0.27	1SG 925
ATOM	925	CD	LYS	114	-0.039	59.543	-9.375	1.00	0.27	1SG 926
ATOM	926	CE	LYS	114	-0.974	60.429	-10.198	1.00	0.27	1SG 927
ATOM	927	NZ	LYS	114	-1.297	59.768	-11.480	1.00	0.27	1SG 928
ATOM	928	C	LYS	114	-1.266	60.310	-4.557	1.00	0.27	1SG 929
ATOM	929	O	LYS	114	-2.398	60.652	-4.895	1.00	0.27	1SG 930
ATOM	930	N	ASN	115	-0.981	59.925	-3.300	1.00	0.32	1SG 931
ATOM	931	CA	ASN	115	-1.970	59.921	-2.258	1.00	0.32	1SG 932
ATOM	932	CB	ASN	115	-2.435	61.333	-1.858	1.00	0.32	1SG 933
ATOM	933	CG	ASN	115	-1.305	61.990	-1.078	1.00	0.32	1SG 934
ATOM	934	OD1	ASN	115	-0.700	61.364	-0.209	1.00	0.32	1SG 935
ATOM	935	ND2	ASN	115	-1.011	63.280	-1.391	1.00	0.32	1SG 936
ATOM	936	C	ASN	115	-3.177	59.118	-2.626	1.00	0.32	1SG 937
ATOM	937	O	ASN	115	-4.302	59.534	-2.353	1.00	0.32	1SG 938
ATOM	938	N	THR	116	-2.997	57.932	-3.236	1.00	0.37	1SG 939
ATOM	939	CA	THR	116	-4.165	57.141	-3.495	1.00	0.37	1SG 940
ATOM	940	CB	THR	116	-3.909	55.918	-4.321	1.00	0.37	1SG 941
ATOM	941	OG1	THR	116	-5.135	55.293	-4.672	1.00	0.37	1SG 942
ATOM	942	CG2	THR	116	-3.039	54.961	-3.497	1.00	0.37	1SG 943
ATOM	943	C	THR	116	-4.668	56.703	-2.156	1.00	0.37	1SG 944
ATOM	944	O	THR	116	-3.888	56.517	-1.222	1.00	0.37	1SG 945
ATOM	945	N	ALA	117	-5.996	56.517	-2.030	1.00	0.24	1SG 946
ATOM	946	CA	ALA	117	-6.570	56.202	-0.752	1.00	0.24	1SG 947
ATOM	947	CB	ALA	117	-8.090	55.960	-0.804	1.00	0.24	1SG 948
ATOM	948	C	ALA	117	-5.923	54.971	-0.212	1.00	0.24	1SG 949
ATOM	949	O	ALA	117	-5.750	53.980	-0.917	1.00	0.24	1SG 950
ATOM	950	N	LEU	118	-5.541	55.021	1.081	1.00	0.13	1SG 951
ATOM	951	CA	LEU	118	-4.872	53.905	1.683	1.00	0.13	1SG 952
ATOM	952	CB	LEU	118	-3.382	54.199	1.945	1.00	0.13	1SG 953
ATOM	953	CG	LEU	118	-2.589	53.047	2.592	1.00	0.13	1SG 954
ATOM	954	CD2	LEU	118	-1.222	53.539	3.100	1.00	0.13	1SG 955
ATOM	955	CD1	LEU	118	-2.468	51.846	1.644	1.00	0.13	1SG 956
ATOM	956	C	LEU	118	-5.514	53.602	3.006	1.00	0.13	1SG 957
ATOM	957	O	LEU	118	-5.848	54.502	3.774	1.00	0.13	1SG 958
ATOM	958	N	HIS	119	-5.714	52.300	3.301	1.00	0.15	1SG 959
ATOM	959	CA	HIS	119	-6.265	51.906	4.567	1.00	0.15	1SG 960
ATOM	960	ND1	HIS	119	-8.820	53.706	5.627	1.00	0.15	1SG 961
ATOM	961	CG	HIS	119	-8.548	52.949	4.510	1.00	0.15	1SG 962
ATOM	962	CB	HIS	119	-7.782	51.660	4.549	1.00	0.15	1SG 963
ATOM	963	NE2	HIS	119	-9.697	54.792	3.897	1.00	0.15	1SG 964
ATOM	964	CD2	HIS	119	-9.091	53.626	3.461	1.00	0.15	1SG 965
ATOM	965	CE1	HIS	119	-9.508	54.796	5.205	1.00	0.15	1SG 966
ATOM	966	C	HIS	119	-5.579	50.648	5.009	1.00	0.15	1SG 967
ATOM	967	O	HIS	119	-4.757	50.091	4.284	1.00	0.15	1SG 968
ATOM	968	N	LYS	120	-5.895	50.183	6.236	1.00	0.15	1SG 969
ATOM	969	CA	LYS	120	-5.323	48.981	6.778	1.00	0.15	1SG 970
ATOM	970	CB	LYS	120	-5.711	47.726	5.981	1.00	0.15	1SG 971
ATOM	971	CG	LYS	120	-7.211	47.438	6.003	1.00	0.15	1SG 972
ATOM	972	CD	LYS	120	-7.654	46.446	4.927	1.00	0.15	1SG 973

ATOM	973	CE	LYS	120	-9.159	46.178	4.933	1.00	0.15	1SG 974
ATOM	974	NZ	LYS	120	-9.537	45.384	3.742	1.00	0.15	1SG 975
ATOM	975	C	LYS	120	-3.828	49.079	6.773	1.00	0.15	1SG 976
ATOM	976	O	LYS	120	-3.147	48.236	6.191	1.00	0.15	1SG 977
ATOM	977	N	VAL	121	-3.270	50.096	7.459	1.00	0.12	1SG 978
ATOM	978	CA	VAL	121	-1.847	50.293	7.458	1.00	0.12	1SG 979
ATOM	979	CB	VAL	121	-1.443	51.742	7.478	1.00	0.12	1SG 980
ATOM	980	CG1	VAL	121	0.090	51.832	7.576	1.00	0.12	1SG 981
ATOM	981	CG2	VAL	121	-2.025	52.431	6.232	1.00	0.12	1SG 982
ATOM	982	C	VAL	121	-1.240	49.648	8.662	1.00	0.12	1SG 983
ATOM	983	O	VAL	121	-1.756	49.748	9.775	1.00	0.12	1SG 984
ATOM	984	N	THR	122	-0.115	48.932	8.447	1.00	0.20	1SG 985
ATOM	985	CA	THR	122	0.569	48.321	9.545	1.00	0.20	1SG 986
ATOM	986	CB	THR	122	0.565	46.820	9.506	1.00	0.20	1SG 987
ATOM	987	OG1	THR	122	-0.770	46.335	9.535	1.00	0.20	1SG 988
ATOM	988	CG2	THR	122	1.344	46.294	10.725	1.00	0.20	1SG 989
ATOM	989	C	THR	122	1.993	48.778	9.503	1.00	0.20	1SG 990
ATOM	990	O	THR	122	2.590	48.895	8.433	1.00	0.20	1SG 991
ATOM	991	N	TYR	123	2.562	49.073	10.688	1.00	0.31	1SG 992
ATOM	992	CA	TYR	123	3.935	49.480	10.795	1.00	0.31	1SG 993
ATOM	993	CB	TYR	123	4.175	50.652	11.755	1.00	0.31	1SG 994
ATOM	994	CG	TYR	123	3.858	51.920	11.056	1.00	0.31	1SG 995
ATOM	995	CD1	TYR	123	2.569	52.379	10.913	1.00	0.31	1SG 996
ATOM	996	CD2	TYR	123	4.901	52.652	10.544	1.00	0.31	1SG 997
ATOM	997	CE1	TYR	123	2.334	53.568	10.261	1.00	0.31	1SG 998
ATOM	998	CE2	TYR	123	4.673	53.835	9.896	1.00	0.31	1SG 999
ATOM	999	CZ	TYR	123	3.391	54.291	9.756	1.00	0.31	1SG1000
ATOM	1000	OH	TYR	123	3.181	55.511	9.089	1.00	0.31	1SG1001
ATOM	1001	C	TYR	123	4.690	48.339	11.381	1.00	0.31	1SG1002
ATOM	1002	O	TYR	123	4.273	47.764	12.386	1.00	0.31	1SG1003
ATOM	1003	N	LEU	124	5.843	47.994	10.770	1.00	0.32	1SG1004
ATOM	1004	CA	LEU	124	6.599	46.877	11.259	1.00	0.32	1SG1005
ATOM	1005	CB	LEU	124	6.814	45.787	10.192	1.00	0.32	1SG1006
ATOM	1006	CG	LEU	124	5.515	45.183	9.624	1.00	0.32	1SG1007
ATOM	1007	CD2	LEU	124	4.590	44.673	10.739	1.00	0.32	1SG1008
ATOM	1008	CD1	LEU	124	5.817	44.105	8.571	1.00	0.32	1SG1009
ATOM	1009	C	LEU	124	7.971	47.343	11.640	1.00	0.32	1SG1010
ATOM	1010	O	LEU	124	8.523	48.248	11.017	1.00	0.32	1SG1011
ATOM	1011	N	GLN	125	8.543	46.757	12.714	1.00	0.33	1SG1012
ATOM	1012	CA	GLN	125	9.913	47.045	13.032	1.00	0.33	1SG1013
ATOM	1013	CB	GLN	125	10.152	47.788	14.359	1.00	0.33	1SG1014
ATOM	1014	CG	GLN	125	9.779	47.001	15.612	1.00	0.33	1SG1015
ATOM	1015	CD	GLN	125	10.320	47.768	16.812	1.00	0.33	1SG1016
ATOM	1016	OE1	GLN	125	11.527	47.814	17.044	1.00	0.33	1SG1017
ATOM	1017	NE2	GLN	125	9.403	48.390	17.600	1.00	0.33	1SG1018
ATOM	1018	C	GLN	125	10.597	45.721	13.137	1.00	0.33	1SG1019
ATOM	1019	O	GLN	125	10.185	44.856	13.907	1.00	0.33	1SG1020
ATOM	1020	N	ASN	126	11.665	45.529	12.346	1.00	0.22	1SG1021
ATOM	1021	CA	ASN	126	12.397	44.297	12.359	1.00	0.22	1SG1022
ATOM	1022	CB	ASN	126	13.085	44.005	13.704	1.00	0.22	1SG1023
ATOM	1023	CG	ASN	126	14.202	45.024	13.875	1.00	0.22	1SG1024
ATOM	1024	OD1	ASN	126	14.904	45.347	12.919	1.00	0.22	1SG1025
ATOM	1025	ND2	ASN	126	14.369	45.551	15.118	1.00	0.22	1SG1026
ATOM	1026	C	ASN	126	11.473	43.162	12.041	1.00	0.22	1SG1027
ATOM	1027	O	ASN	126	11.685	42.036	12.491	1.00	0.22	1SG1028
ATOM	1028	N	GLY	127	10.420	43.428	11.245	1.00	0.15	1SG1029
ATOM	1029	CA	GLY	127	9.558	42.371	10.800	1.00	0.15	1SG1030
ATOM	1030	C	GLY	127	8.459	42.097	11.784	1.00	0.15	1SG1031
ATOM	1031	O	GLY	127	7.651	41.197	11.556	1.00	0.15	1SG1032
ATOM	1032	N	LYS	128	8.386	42.841	12.907	1.00	0.28	1SG1033
ATOM	1033	CA	LYS	128	7.305	42.595	13.827	1.00	0.28	1SG1034

ATOM	1034	CB	LYS	128	7.746	42.359	15.281	1.00	0.28	1SG1035
ATOM	1035	CG	LYS	128	6.576	41.990	16.198	1.00	0.28	1SG1036
ATOM	1036	CD	LYS	128	6.996	41.432	17.558	1.00	0.28	1SG1037
ATOM	1037	CE	LYS	128	7.294	42.514	18.598	1.00	0.28	1SG1038
ATOM	1038	NZ	LYS	128	7.675	41.886	19.883	1.00	0.28	1SG1039
ATOM	1039	C	LYS	128	6.427	43.808	13.822	1.00	0.28	1SG1040
ATOM	1040	O	LYS	128	6.920	44.933	13.880	1.00	0.28	1SG1041
ATOM	1041	N	ASP	129	5.092	43.604	13.758	1.00	0.47	1SG1042
ATOM	1042	CA	ASP	129	4.182	44.713	13.654	1.00	0.47	1SG1043
ATOM	1043	CB	ASP	129	2.781	44.323	13.141	1.00	0.47	1SG1044
ATOM	1044	CG	ASP	129	2.148	43.334	14.108	1.00	0.47	1SG1045
ATOM	1045	OD1	ASP	129	2.903	42.693	14.887	1.00	0.47	1SG1046
ATOM	1046	OD2	ASP	129	0.896	43.199	14.070	1.00	0.47	1SG1047
ATOM	1047	C	ASP	129	4.040	45.423	14.964	1.00	0.47	1SG1048
ATOM	1048	O	ASP	129	3.732	44.821	15.991	1.00	0.47	1SG1049
ATOM	1049	N	ARG	130	4.370	46.733	14.954	1.00	0.54	1SG1050
ATOM	1050	CA	ARG	130	4.239	47.624	16.073	1.00	0.54	1SG1051
ATOM	1051	CB	ARG	130	5.171	48.845	15.964	1.00	0.54	1SG1052
ATOM	1052	CG	ARG	130	5.312	49.632	17.271	1.00	0.54	1SG1053
ATOM	1053	CD	ARG	130	4.047	50.382	17.689	1.00	0.54	1SG1054
ATOM	1054	NE	ARG	130	4.325	51.062	18.984	1.00	0.54	1SG1055
ATOM	1055	CZ	ARG	130	3.388	51.032	19.976	1.00	0.54	1SG1056
ATOM	1056	NH1	ARG	130	2.230	50.330	19.800	1.00	0.54	1SG1057
ATOM	1057	NH2	ARG	130	3.612	51.697	21.147	1.00	0.54	1SG1058
ATOM	1058	C	ARG	130	2.835	48.152	16.192	1.00	0.54	1SG1059
ATOM	1059	O	ARG	130	2.308	48.302	17.293	1.00	0.54	1SG1060
ATOM	1060	N	LYS	131	2.196	48.478	15.048	1.00	0.34	1SG1061
ATOM	1061	CA	LYS	131	0.921	49.141	15.109	1.00	0.34	1SG1062
ATOM	1062	CB	LYS	131	1.106	50.668	15.097	1.00	0.34	1SG1063
ATOM	1063	CG	LYS	131	-0.168	51.511	15.150	1.00	0.34	1SG1064
ATOM	1064	CD	LYS	131	0.143	53.009	15.235	1.00	0.34	1SG1065
ATOM	1065	CE	LYS	131	-1.058	53.916	14.962	1.00	0.34	1SG1066
ATOM	1066	NZ	LYS	131	-0.665	55.338	15.068	1.00	0.34	1SG1067
ATOM	1067	C	LYS	131	0.121	48.809	13.888	1.00	0.34	1SG1068
ATOM	1068	O	LYS	131	0.657	48.725	12.784	1.00	0.34	1SG1069
ATOM	1069	N	TYR	132	-1.202	48.610	14.067	1.00	0.18	1SG1070
ATOM	1070	CA	TYR	132	-2.078	48.392	12.952	1.00	0.18	1SG1071
ATOM	1071	CB	TYR	132	-2.580	46.941	12.832	1.00	0.18	1SG1072
ATOM	1072	CG	TYR	132	-3.692	46.919	11.840	1.00	0.18	1SG1073
ATOM	1073	CD1	TYR	132	-3.441	46.903	10.488	1.00	0.18	1SG1074
ATOM	1074	CD2	TYR	132	-4.999	46.936	12.267	1.00	0.18	1SG1075
ATOM	1075	CE1	TYR	132	-4.474	46.888	9.581	1.00	0.18	1SG1076
ATOM	1076	CE2	TYR	132	-6.037	46.920	11.364	1.00	0.18	1SG1077
ATOM	1077	CZ	TYR	132	-5.774	46.893	10.016	1.00	0.18	1SG1078
ATOM	1078	OH	TYR	132	-6.827	46.877	9.078	1.00	0.18	1SG1079
ATOM	1079	C	TYR	132	-3.270	49.277	13.136	1.00	0.18	1SG1080
ATOM	1080	O	TYR	132	-3.826	49.344	14.229	1.00	0.18	1SG1081
ATOM	1081	N	PHE	133	-3.674	50.009	12.073	1.00	0.16	1SG1082
ATOM	1082	CA	PHE	133	-4.842	50.847	12.146	1.00	0.16	1SG1083
ATOM	1083	CB	PHE	133	-4.561	52.324	12.491	1.00	0.16	1SG1084
ATOM	1084	CG	PHE	133	-4.409	52.420	13.969	1.00	0.16	1SG1085
ATOM	1085	CD1	PHE	133	-3.262	51.996	14.596	1.00	0.16	1SG1086
ATOM	1086	CD2	PHE	133	-5.424	52.951	14.731	1.00	0.16	1SG1087
ATOM	1087	CE1	PHE	133	-3.140	52.090	15.962	1.00	0.16	1SG1088
ATOM	1088	CE2	PHE	133	-5.307	53.049	16.097	1.00	0.16	1SG1089
ATOM	1089	CZ	PHE	133	-4.161	52.615	16.716	1.00	0.16	1SG1090
ATOM	1090	C	PHE	133	-5.527	50.820	10.821	1.00	0.16	1SG1091
ATOM	1091	O	PHE	133	-4.886	50.846	9.774	1.00	0.16	1SG1092
ATOM	1092	N	HIS	134	-6.869	50.736	10.828	1.00	0.26	1SG1093
ATOM	1093	CA	HIS	134	-7.547	50.719	9.569	1.00	0.26	1SG1094
ATOM	1094	ND1	HIS	134	-9.410	47.923	9.166	1.00	0.26	1SG1095

ATOM	1095	CG	HIS	134	-9.255	48.944	10.077	1.00	0.26	1SG1096
ATOM	1096	CB	HIS	134	-9.039	50.378	9.697	1.00	0.26	1SG1097
ATOM	1097	NE2	HIS	134	-9.537	46.998	11.184	1.00	0.26	1SG1098
ATOM	1098	CD2	HIS	134	-9.334	48.361	11.304	1.00	0.26	1SG1099
ATOM	1099	CE1	HIS	134	-9.576	46.782	9.881	1.00	0.26	1SG1100
ATOM	1100	C	HIS	134	-7.425	52.058	8.902	1.00	0.26	1SG1101
ATOM	1101	O	HIS	134	-7.150	52.143	7.709	1.00	0.26	1SG1102
ATOM	1102	N	HIS	135	-7.712	53.138	9.650	1.00	0.40	1SG1103
ATOM	1103	CA	HIS	135	-7.716	54.478	9.124	1.00	0.40	1SG1104
ATOM	1104	ND1	HIS	135	-8.378	55.032	12.360	1.00	0.40	1SG1105
ATOM	1105	CG	HIS	135	-8.228	55.796	11.224	1.00	0.40	1SG1106
ATOM	1106	CB	HIS	135	-8.708	55.391	9.862	1.00	0.40	1SG1107
ATOM	1107	NE2	HIS	135	-7.321	56.889	12.977	1.00	0.40	1SG1108
ATOM	1108	CD2	HIS	135	-7.581	56.926	11.619	1.00	0.40	1SG1109
ATOM	1109	CE1	HIS	135	-7.818	55.733	13.379	1.00	0.40	1SG1110
ATOM	1110	C	HIS	135	-6.411	55.226	9.122	1.00	0.40	1SG1111
ATOM	1111	O	HIS	135	-6.136	55.962	8.176	1.00	0.40	1SG1112
ATOM	1112	N	ASN	136	-5.579	55.078	10.177	1.00	0.34	1SG1113
ATOM	1113	CA	ASN	136	-4.497	56.015	10.365	1.00	0.34	1SG1114
ATOM	1114	CB	ASN	136	-4.255	56.339	11.847	1.00	0.34	1SG1115
ATOM	1115	CG	ASN	136	-3.317	57.529	11.904	1.00	0.34	1SG1116
ATOM	1116	OD1	ASN	136	-2.170	57.400	12.325	1.00	0.34	1SG1117
ATOM	1117	ND2	ASN	136	-3.806	58.715	11.451	1.00	0.34	1SG1118
ATOM	1118	C	ASN	136	-3.187	55.580	9.769	1.00	0.34	1SG1119
ATOM	1119	O	ASN	136	-2.653	54.518	10.075	1.00	0.34	1SG1120
ATOM	1120	N	SER	137	-2.651	56.454	8.892	1.00	0.23	1SG1121
ATOM	1121	CA	SER	137	-1.429	56.362	8.136	1.00	0.23	1SG1122
ATOM	1122	CB	SER	137	-1.431	57.298	6.916	1.00	0.23	1SG1123
ATOM	1123	OG	SER	137	-2.479	56.939	6.028	1.00	0.23	1SG1124
ATOM	1124	C	SER	137	-0.202	56.706	8.943	1.00	0.23	1SG1125
ATOM	1125	O	SER	137	0.906	56.514	8.445	1.00	0.23	1SG1126
ATOM	1126	N	ASP	138	-0.334	57.310	10.147	1.00	0.21	1SG1127
ATOM	1127	CA	ASP	138	0.853	57.763	10.837	1.00	0.21	1SG1128
ATOM	1128	CB	ASP	138	0.793	59.245	11.273	1.00	0.21	1SG1129
ATOM	1129	CG	ASP	138	-0.332	59.471	12.281	1.00	0.21	1SG1130
ATOM	1130	OD1	ASP	138	-0.325	58.810	13.354	1.00	0.21	1SG1131
ATOM	1131	OD2	ASP	138	-1.221	60.313	11.986	1.00	0.21	1SG1132
ATOM	1132	C	ASP	138	1.179	56.931	12.047	1.00	0.21	1SG1133
ATOM	1133	O	ASP	138	0.353	56.172	12.550	1.00	0.21	1SG1134
ATOM	1134	N	PHE	139	2.442	57.061	12.525	1.00	0.22	1SG1135
ATOM	1135	CA	PHE	139	2.972	56.316	13.635	1.00	0.22	1SG1136
ATOM	1136	CB	PHE	139	3.793	55.124	13.104	1.00	0.22	1SG1137
ATOM	1137	CG	PHE	139	4.421	54.316	14.186	1.00	0.22	1SG1138
ATOM	1138	CD1	PHE	139	3.664	53.563	15.055	1.00	0.22	1SG1139
ATOM	1139	CD2	PHE	139	5.792	54.273	14.287	1.00	0.22	1SG1140
ATOM	1140	CE1	PHE	139	4.270	52.812	16.034	1.00	0.22	1SG1141
ATOM	1141	CE2	PHE	139	6.404	53.523	15.263	1.00	0.22	1SG1142
ATOM	1142	CZ	PHE	139	5.640	52.793	16.141	1.00	0.22	1SG1143
ATOM	1143	C	PHE	139	3.858	57.225	14.441	1.00	0.22	1SG1144
ATOM	1144	O	PHE	139	4.645	57.992	13.885	1.00	0.22	1SG1145
ATOM	1145	N	HIS	140	3.748	57.165	15.789	1.00	0.24	1SG1146
ATOM	1146	CA	HIS	140	4.541	58.034	16.620	1.00	0.24	1SG1147
ATOM	1147	ND1	HIS	140	1.861	59.659	15.668	1.00	0.24	1SG1148
ATOM	1148	CG	HIS	140	2.970	60.039	16.391	1.00	0.24	1SG1149
ATOM	1149	CB	HIS	140	3.716	59.128	17.321	1.00	0.24	1SG1150
ATOM	1150	NE2	HIS	140	2.223	61.801	15.196	1.00	0.24	1SG1151
ATOM	1151	CD2	HIS	140	3.178	61.350	16.090	1.00	0.24	1SG1152
ATOM	1152	CE1	HIS	140	1.455	60.750	14.970	1.00	0.24	1SG1153
ATOM	1153	C	HIS	140	5.125	57.228	17.739	1.00	0.24	1SG1154
ATOM	1154	O	HIS	140	4.444	56.404	18.347	1.00	0.24	1SG1155
ATOM	1155	N	ILE	141	6.419	57.455	18.041	1.00	0.25	1SG1156

ATOM	1156	CA	ILE	141	7.045	56.791	19.144	1.00	0.25	1SG1157
ATOM	1157	CB	ILE	141	8.257	56.002	18.742	1.00	0.25	1SG1158
ATOM	1158	CG2	ILE	141	8.889	55.427	20.020	1.00	0.25	1SG1159
ATOM	1159	CG1	ILE	141	7.895	54.928	17.704	1.00	0.25	1SG1160
ATOM	1160	CD1	ILE	141	9.116	54.309	17.023	1.00	0.25	1SG1161
ATOM	1161	C	ILE	141	7.531	57.873	20.052	1.00	0.25	1SG1162
ATOM	1162	O	ILE	141	8.477	58.587	19.723	1.00	0.25	1SG1163
ATOM	1163	N	PRO	142	6.892	58.036	21.175	1.00	0.43	1SG1164
ATOM	1164	CA	PRO	142	7.352	59.024	22.107	1.00	0.43	1SG1165
ATOM	1165	CD	PRO	142	5.453	57.854	21.248	1.00	0.43	1SG1166
ATOM	1166	CB	PRO	142	6.139	59.430	22.947	1.00	0.43	1SG1167
ATOM	1167	CG	PRO	142	5.083	58.350	22.652	1.00	0.43	1SG1168
ATOM	1168	C	PRO	142	8.466	58.424	22.902	1.00	0.43	1SG1169
ATOM	1169	O	PRO	142	8.482	57.204	23.054	1.00	0.43	1SG1170
ATOM	1170	N	LYS	143	9.387	59.260	23.422	1.00	0.52	1SG1171
ATOM	1171	CA	LYS	143	10.473	58.801	24.241	1.00	0.52	1SG1172
ATOM	1172	CB	LYS	143	10.025	58.371	25.651	1.00	0.52	1SG1173
ATOM	1173	CG	LYS	143	9.356	59.483	26.461	1.00	0.52	1SG1174
ATOM	1174	CD	LYS	143	10.243	60.707	26.696	1.00	0.52	1SG1175
ATOM	1175	CE	LYS	143	9.553	61.806	27.508	1.00	0.52	1SG1176
ATOM	1176	NZ	LYS	143	8.346	62.283	26.794	1.00	0.52	1SG1177
ATOM	1177	C	LYS	143	11.135	57.616	23.605	1.00	0.52	1SG1178
ATOM	1178	O	LYS	143	10.991	56.492	24.083	1.00	0.52	1SG1179
ATOM	1179	N	ALA	144	11.886	57.840	22.508	1.00	0.40	1SG1180
ATOM	1180	CA	ALA	144	12.533	56.758	21.817	1.00	0.40	1SG1181
ATOM	1181	CB	ALA	144	13.097	57.155	20.441	1.00	0.40	1SG1182
ATOM	1182	C	ALA	144	13.672	56.228	22.636	1.00	0.40	1SG1183
ATOM	1183	O	ALA	144	14.282	56.947	23.427	1.00	0.40	1SG1184
ATOM	1184	N	THR	145	13.981	54.926	22.444	1.00	0.44	1SG1185
ATOM	1185	CA	THR	145	15.003	54.249	23.191	1.00	0.44	1SG1186
ATOM	1186	CB	THR	145	14.400	53.346	24.239	1.00	0.44	1SG1187
ATOM	1187	OG1	THR	145	13.520	54.104	25.056	1.00	0.44	1SG1188
ATOM	1188	CG2	THR	145	15.497	52.747	25.138	1.00	0.44	1SG1189
ATOM	1189	C	THR	145	15.788	53.422	22.200	1.00	0.44	1SG1190
ATOM	1190	O	THR	145	15.482	53.410	21.010	1.00	0.44	1SG1191
ATOM	1191	N	LEU	146	16.840	52.724	22.675	1.00	0.63	1SG1192
ATOM	1192	CA	LEU	146	17.739	51.323	21.890	1.00	0.63	1SG1193
ATOM	1193	CB	LEU	146	18.871	51.319	22.739	1.00	0.63	1SG1194
ATOM	1194	CG	LEU	146	19.780	52.375	23.396	1.00	0.63	1SG1195
ATOM	1195	CD2	LEU	146	21.044	51.733	23.988	1.00	0.63	1SG1196
ATOM	1196	CD1	LEU	146	19.008	53.219	24.424	1.00	0.63	1SG1197
ATOM	1197	C	LEU	146	17.007	50.780	21.252	1.00	0.63	1SG1198
ATOM	1198	O	LEU	146	17.373	50.337	20.165	1.00	0.63	1SG1199
ATOM	1199	N	LYS	147	15.970	50.250	21.924	1.00	0.64	1SG1200
ATOM	1200	CA	LYS	147	15.234	49.124	21.415	1.00	0.64	1SG1201
ATOM	1201	CB	LYS	147	14.155	48.611	22.381	1.00	0.64	1SG1202
ATOM	1202	CG	LYS	147	14.737	47.990	23.651	1.00	0.64	1SG1203
ATOM	1203	CD	LYS	147	15.708	46.838	23.378	1.00	0.64	1SG1204
ATOM	1204	CE	LYS	147	15.081	45.661	22.626	1.00	0.64	1SG1205
ATOM	1205	NZ	LYS	147	15.060	45.938	21.172	1.00	0.64	1SG1206
ATOM	1206	C	LYS	147	14.553	49.511	20.138	1.00	0.64	1SG1207
ATOM	1207	O	LYS	147	14.327	48.669	19.271	1.00	0.64	1SG1208
ATOM	1208	N	ASP	148	14.198	50.802	20.011	1.00	0.39	1SG1209
ATOM	1209	CA	ASP	148	13.491	51.371	18.897	1.00	0.39	1SG1210
ATOM	1210	CB	ASP	148	13.077	52.834	19.134	1.00	0.39	1SG1211
ATOM	1211	CG	ASP	148	11.977	52.847	20.187	1.00	0.39	1SG1212
ATOM	1212	OD1	ASP	148	11.064	51.984	20.096	1.00	0.39	1SG1213
ATOM	1213	OD2	ASP	148	12.030	53.724	21.090	1.00	0.39	1SG1214
ATOM	1214	C	ASP	148	14.314	51.324	17.639	1.00	0.39	1SG1215
ATOM	1215	O	ASP	148	13.763	51.464	16.551	1.00	0.39	1SG1216
ATOM	1216	N	SER	149	15.653	51.209	17.725	1.00	0.24	1SG1217

ATOM	1217	CA	SER	149	16.434	51.189	16.513	1.00	0.24	1SG1218
ATOM	1218	CB	SER	149	17.948	51.047	16.748	1.00	0.24	1SG1219
ATOM	1219	OG	SER	149	18.448	52.150	17.471	1.00	0.24	1SG1220
ATOM	1220	C	SER	149	16.031	49.996	15.702	1.00	0.24	1SG1221
ATOM	1221	O	SER	149	15.620	48.977	16.252	1.00	0.24	1SG1222
ATOM	1222	N	GLY	150	16.118	50.089	14.354	1.00	0.24	1SG1223
ATOM	1223	CA	GLY	150	15.795	48.914	13.596	1.00	0.24	1SG1224
ATOM	1224	C	GLY	150	15.308	49.283	12.229	1.00	0.24	1SG1225
ATOM	1225	O	GLY	150	15.351	50.442	11.818	1.00	0.24	1SG1226
ATOM	1226	N	SER	151	14.819	48.268	11.485	1.00	0.20	1SG1227
ATOM	1227	CA	SER	151	14.351	48.492	10.149	1.00	0.20	1SG1228
ATOM	1228	CB	SER	151	14.691	47.344	9.185	1.00	0.20	1SG1229
ATOM	1229	OG	SER	151	16.099	47.212	9.061	1.00	0.20	1SG1230
ATOM	1230	C	SER	151	12.862	48.605	10.193	1.00	0.20	1SG1231
ATOM	1231	O	SER	151	12.174	47.715	10.692	1.00	0.20	1SG1232
ATOM	1232	N	TYR	152	12.327	49.722	9.661	1.00	0.35	1SG1233
ATOM	1233	CA	TYR	152	10.906	49.925	9.663	1.00	0.35	1SG1234
ATOM	1234	CB	TYR	152	10.463	51.277	10.254	1.00	0.35	1SG1235
ATOM	1235	CG	TYR	152	10.639	51.246	11.735	1.00	0.35	1SG1236
ATOM	1236	CD1	TYR	152	11.873	51.440	12.314	1.00	0.35	1SG1237
ATOM	1237	CD2	TYR	152	9.549	51.036	12.550	1.00	0.35	1SG1238
ATOM	1238	CE1	TYR	152	12.015	51.412	13.682	1.00	0.35	1SG1239
ATOM	1239	CE2	TYR	152	9.685	51.007	13.917	1.00	0.35	1SG1240
ATOM	1240	CZ	TYR	152	10.921	51.195	14.485	1.00	0.35	1SG1241
ATOM	1241	OH	TYR	152	11.068	51.168	15.887	1.00	0.35	1SG1242
ATOM	1242	C	TYR	152	10.384	49.868	9.258	1.00	0.35	1SG1243
ATOM	1243	O	TYR	152	11.039	50.319	7.319	1.00	0.35	1SG1244
ATOM	1244	N	PHE	153	9.174	49.282	8.100	1.00	0.75	1SG1245
ATOM	1245	CA	PHE	153	8.500	49.142	6.835	1.00	0.75	1SG1246
ATOM	1246	CB	PHE	153	8.423	47.706	6.276	1.00	0.75	1SG1247
ATOM	1247	CG	PHE	153	9.717	46.992	6.083	1.00	0.75	1SG1248
ATOM	1248	CD1	PHE	153	10.350	46.400	7.151	1.00	0.75	1SG1249
ATOM	1249	CD2	PHE	153	10.267	46.861	4.828	1.00	0.75	1SG1250
ATOM	1250	CE1	PHE	153	11.531	45.716	6.977	1.00	0.75	1SG1251
ATOM	1251	CE2	PHE	153	11.445	46.177	4.647	1.00	0.75	1SG1252
ATOM	1252	CZ	PHE	153	12.083	45.607	5.724	1.00	0.75	1SG1253
ATOM	1253	C	PHE	153	7.044	49.335	7.134	1.00	0.75	1SG1254
ATOM	1254	O	PHE	153	6.626	49.319	8.292	1.00	0.75	1SG1255
ATOM	1255	N	CYS	154	6.226	49.481	6.071	1.00	0.86	1SG1256
ATOM	1256	CA	CYS	154	4.807	49.626	6.230	1.00	0.86	1SG1257
ATOM	1257	CB	CYS	154	4.356	51.084	6.045	1.00	0.86	1SG1258
ATOM	1258	SG	CYS	154	2.557	51.224	5.915	1.00	0.86	1SG1259
ATOM	1259	C	CYS	154	4.117	48.817	5.167	1.00	0.86	1SG1260
ATOM	1260	O	CYS	154	4.680	48.544	4.108	1.00	0.86	1SG1261
ATOM	1261	N	ARG	155	2.870	48.380	5.451	1.00	0.56	1SG1262
ATOM	1262	CA	ARG	155	2.050	47.690	4.499	1.00	0.56	1SG1263
ATOM	1263	CB	ARG	155	1.825	46.206	4.836	1.00	0.56	1SG1264
ATOM	1264	CG	ARG	155	3.105	45.370	4.777	1.00	0.56	1SG1265
ATOM	1265	CD	ARG	155	2.895	43.891	5.109	1.00	0.56	1SG1266
ATOM	1266	NE	ARG	155	2.510	43.797	6.545	1.00	0.56	1SG1267
ATOM	1267	CZ	ARG	155	1.952	42.646	7.022	1.00	0.56	1SG1268
ATOM	1268	NH1	ARG	155	1.743	41.593	6.180	1.00	0.56	1SG1269
ATOM	1269	NH2	ARG	155	1.603	42.548	8.338	1.00	0.56	1SG1270
ATOM	1270	C	ARG	155	0.716	48.370	4.543	1.00	0.56	1SG1271
ATOM	1271	O	ARG	155	0.343	48.942	5.569	1.00	0.56	1SG1272
ATOM	1272	N	GLY	156	-0.028	48.351	3.416	1.00	0.35	1SG1273
ATOM	1273	CA	GLY	156	-1.322	48.985	3.400	1.00	0.35	1SG1274
ATOM	1274	C	GLY	156	-2.002	48.644	2.110	1.00	0.35	1SG1275
ATOM	1275	O	GLY	156	-1.354	48.263	1.135	1.00	0.35	1SG1276
ATOM	1276	N	LEU	157	-3.344	48.794	2.057	1.00	0.37	1SG1277
ATOM	1277	CA	LEU	157	-4.007	48.431	0.841	1.00	0.37	1SG1278

ATOM	1278	CB	LEU	157	-5.300	47.603	1.002	1.00	0.37	1SG1279
ATOM	1279	CG	LEU	157	-6.616	48.389	1.183	1.00	0.37	1SG1280
ATOM	1280	CD2	LEU	157	-6.549	49.386	2.345	1.00	0.37	1SG1281
ATOM	1281	CD1	LEU	157	-7.805	47.425	1.325	1.00	0.37	1SG1282
ATOM	1282	C	LEU	157	-4.334	49.668	0.075	1.00	0.37	1SG1283
ATOM	1283	O	LEU	157	-4.844	50.650	0.612	1.00	0.37	1SG1284
ATOM	1284	N	VAL	158	-3.984	49.648	-1.223	1.00	0.25	1SG1285
ATOM	1285	CA	VAL	158	-4.299	50.717	-2.117	1.00	0.25	1SG1286
ATOM	1286	CB	VAL	158	-3.125	51.171	-2.929	1.00	0.25	1SG1287
ATOM	1287	CG1	VAL	158	-3.625	52.124	-4.027	1.00	0.25	1SG1288
ATOM	1288	CG2	VAL	158	-2.088	51.796	-1.981	1.00	0.25	1SG1289
ATOM	1289	C	VAL	158	-5.279	50.130	-3.065	1.00	0.25	1SG1290
ATOM	1290	O	VAL	158	-4.985	49.143	-3.738	1.00	0.25	1SG1291
ATOM	1291	N	GLY	159	-6.481	50.718	-3.149	1.00	0.14	1SG1292
ATOM	1292	CA	GLY	159	-7.440	50.118	-4.018	1.00	0.14	1SG1293
ATOM	1293	C	GLY	159	-7.690	48.744	-3.486	1.00	0.14	1SG1294
ATOM	1294	O	GLY	159	-8.016	48.562	-2.315	1.00	0.14	1SG1295
ATOM	1295	N	SER	160	-7.597	47.751	-4.385	1.00	0.21	1SG1296
ATOM	1296	CA	SER	160	-7.836	46.363	-4.117	1.00	0.21	1SG1297
ATOM	1297	CB	SER	160	-8.189	45.585	-5.397	1.00	0.21	1SG1298
ATOM	1298	OG	SER	160	-9.399	46.082	-5.951	1.00	0.21	1SG1299
ATOM	1299	C	SER	160	-6.697	45.631	-3.469	1.00	0.21	1SG1300
ATOM	1300	O	SER	160	-6.940	44.695	-2.707	1.00	0.21	1SG1301
ATOM	1301	N	LYS	161	-5.428	45.995	-3.753	1.00	0.33	1SG1302
ATOM	1302	CA	LYS	161	-4.384	45.112	-3.306	1.00	0.33	1SG1303
ATOM	1303	CB	LYS	161	-3.423	44.675	-4.426	1.00	0.33	1SG1304
ATOM	1304	CG	LYS	161	-4.077	43.773	-5.475	1.00	0.33	1SG1305
ATOM	1305	CD	LYS	161	-3.228	43.568	-6.732	1.00	0.33	1SG1306
ATOM	1306	CE	LYS	161	-2.135	42.511	-6.567	1.00	0.33	1SG1307
ATOM	1307	NZ	LYS	161	-1.386	42.355	-7.833	1.00	0.33	1SG1308
ATOM	1308	C	LYS	161	-3.550	45.700	-2.217	1.00	0.33	1SG1309
ATOM	1309	O	LYS	161	-3.514	46.909	-1.998	1.00	0.33	1SG1310
ATOM	1310	N	ASN	162	-2.847	44.800	-1.499	1.00	0.32	1SG1311
ATOM	1311	CA	ASN	162	-1.996	45.168	-0.406	1.00	0.32	1SG1312
ATOM	1312	CB	ASN	162	-1.860	44.057	0.653	1.00	0.32	1SG1313
ATOM	1313	CG	ASN	162	-0.975	44.545	1.794	1.00	0.32	1SG1314
ATOM	1314	OD1	ASN	162	0.206	44.834	1.613	1.00	0.32	1SG1315
ATOM	1315	ND2	ASN	162	-1.568	44.637	3.015	1.00	0.32	1SG1316
ATOM	1316	C	ASN	162	-0.634	45.444	-0.958	1.00	0.32	1SG1317
ATOM	1317	O	ASN	162	-0.169	44.764	-1.872	1.00	0.32	1SG1318
ATOM	1318	N	VAL	163	0.037	46.480	-0.419	1.00	0.27	1SG1319
ATOM	1319	CA	VAL	163	1.352	46.811	-0.881	1.00	0.27	1SG1320
ATOM	1320	CB	VAL	163	1.412	48.149	-1.564	1.00	0.27	1SG1321
ATOM	1321	CG1	VAL	163	2.865	48.442	-1.971	1.00	0.27	1SG1322
ATOM	1322	CG2	VAL	163	0.427	48.136	-2.746	1.00	0.27	1SG1323
ATOM	1323	C	VAL	163	2.256	46.869	0.311	1.00	0.27	1SG1324
ATOM	1324	O	VAL	163	1.803	47.074	1.437	1.00	0.27	1SG1325
ATOM	1325	N	SER	164	3.568	46.644	0.088	1.00	0.29	1SG1326
ATOM	1326	CA	SER	164	4.521	46.731	1.157	1.00	0.29	1SG1327
ATOM	1327	CB	SER	164	5.214	45.401	1.489	1.00	0.29	1SG1328
ATOM	1328	OG	SER	164	6.044	45.006	0.409	1.00	0.29	1SG1329
ATOM	1329	C	SER	164	5.591	47.688	0.728	1.00	0.29	1SG1330
ATOM	1330	O	SER	164	5.981	47.717	-0.438	1.00	0.29	1SG1331
ATOM	1331	N	SER	165	6.086	48.513	1.672	1.00	0.20	1SG1332
ATOM	1332	CA	SER	165	7.106	49.478	1.365	1.00	0.20	1SG1333
ATOM	1333	CB	SER	165	7.030	50.750	2.228	1.00	0.20	1SG1334
ATOM	1334	OG	SER	165	7.351	50.442	3.577	1.00	0.20	1SG1335
ATOM	1335	C	SER	165	8.449	48.865	1.616	1.00	0.20	1SG1336
ATOM	1336	O	SER	165	8.562	47.791	2.206	1.00	0.20	1SG1337
ATOM	1337	N	GLU	166	9.514	49.538	1.134	1.00	0.24	1SG1338
ATOM	1338	CA	GLU	166	10.849	49.081	1.386	1.00	0.24	1SG1339

ATOM	1339	CB	GLU	166	11.899	49.631	0.405	1.00	0.24	1SG1340
ATOM	1340	CG	GLU	166	11.737	49.101	-1.022	1.00	0.24	1SG1341
ATOM	1341	CD	GLU	166	12.830	49.716	-1.884	1.00	0.24	1SG1342
ATOM	1342	OE1	GLU	166	14.005	49.735	-1.432	1.00	0.24	1SG1343
ATOM	1343	OE2	GLU	166	12.500	50.180	-3.009	1.00	0.24	1SG1344
ATOM	1344	C	GLU	166	11.199	49.563	2.758	1.00	0.24	1SG1345
ATOM	1345	O	GLU	166	10.560	50.471	3.286	1.00	0.24	1SG1346
ATOM	1346	N	THR	167	12.223	48.948	3.382	1.00	0.37	1SG1347
ATOM	1347	CA	THR	167	12.579	49.311	4.726	1.00	0.37	1SG1348
ATOM	1348	CB	THR	167	13.348	48.260	5.469	1.00	0.37	1SG1349
ATOM	1349	OG1	THR	167	13.474	48.621	6.836	1.00	0.37	1SG1350
ATOM	1350	CG2	THR	167	14.741	48.133	4.831	1.00	0.37	1SG1351
ATOM	1351	C	THR	167	13.464	50.514	4.734	1.00	0.37	1SG1352
ATOM	1352	O	THR	167	14.103	50.863	3.742	1.00	0.37	1SG1353
ATOM	1353	N	VAL	168	13.478	51.191	5.899	1.00	0.32	1SG1354
ATOM	1354	CA	VAL	168	14.342	52.301	6.161	1.00	0.32	1SG1355
ATOM	1355	CB	VAL	168	13.619	53.606	6.332	1.00	0.32	1SG1356
ATOM	1356	CG1	VAL	168	14.652	54.707	6.628	1.00	0.32	1SG1357
ATOM	1357	CG2	VAL	168	12.777	53.870	5.071	1.00	0.32	1SG1358
ATOM	1358	C	VAL	168	14.985	51.983	7.477	1.00	0.32	1SG1359
ATOM	1359	O	VAL	168	14.311	51.562	8.417	1.00	0.32	1SG1360
ATOM	1360	N	ASN	169	16.315	52.167	7.582	1.00	0.27	1SG1361
ATOM	1361	CA	ASN	169	16.961	51.845	8.820	1.00	0.27	1SG1362
ATOM	1362	CB	ASN	169	18.405	51.332	8.659	1.00	0.27	1SG1363
ATOM	1363	CG	ASN	169	19.251	52.419	8.010	1.00	0.27	1SG1364
ATOM	1364	OD1	ASN	169	18.923	52.927	6.939	1.00	0.27	1SG1365
ATOM	1365	ND2	ASN	169	20.374	52.794	8.680	1.00	0.27	1SG1366
ATOM	1366	C	ASN	169	16.998	53.089	9.640	1.00	0.27	1SG1367
ATOM	1367	O	ASN	169	17.465	54.135	9.191	1.00	0.27	1SG1368
ATOM	1368	N	ILE	170	16.466	52.999	10.872	1.00	0.18	1SG1369
ATOM	1369	CA	ILE	170	16.432	54.120	11.759	1.00	0.18	1SG1370
ATOM	1370	CB	ILE	170	15.039	54.499	12.169	1.00	0.18	1SG1371
ATOM	1371	CG2	ILE	170	15.125	55.597	13.239	1.00	0.18	1SG1372
ATOM	1372	CG1	ILE	170	14.219	54.903	10.933	1.00	0.18	1SG1373
ATOM	1373	CD1	ILE	170	12.736	55.115	11.224	1.00	0.18	1SG1374
ATOM	1374	C	ILE	170	17.174	53.727	12.987	1.00	0.18	1SG1375
ATOM	1375	O	ILE	170	16.957	52.654	13.549	1.00	0.18	1SG1376
ATOM	1376	N	THR	171	18.089	54.595	13.443	1.00	0.23	1SG1377
ATOM	1377	CA	THR	171	18.828	54.212	14.600	1.00	0.23	1SG1378
ATOM	1378	CB	THR	171	20.303	54.095	14.351	1.00	0.23	1SG1379
ATOM	1379	OG1	THR	171	20.555	53.121	13.348	1.00	0.23	1SG1380
ATOM	1380	CG2	THR	171	20.992	53.691	15.665	1.00	0.23	1SG1381
ATOM	1381	C	THR	171	18.633	55.238	15.658	1.00	0.23	1SG1382
ATOM	1382	O	THR	171	18.599	56.440	15.396	1.00	0.23	1SG1383
ATOM	1383	N	ILE	172	18.448	54.760	16.899	1.00	0.52	1SG1384
ATOM	1384	CA	ILE	172	18.446	55.666	17.987	1.00	0.52	1SG1385
ATOM	1385	CB	ILE	172	17.615	55.233	19.175	1.00	0.52	1SG1386
ATOM	1386	CG2	ILE	172	18.032	53.833	19.655	1.00	0.52	1SG1387
ATOM	1387	CG1	ILE	172	17.636	56.325	20.257	1.00	0.52	1SG1388
ATOM	1388	CD1	ILE	172	16.588	56.119	21.349	1.00	0.52	1SG1389
ATOM	1389	C	ILE	172	19.882	55.716	18.301	1.00	0.52	1SG1390
ATOM	1390	O	ILE	172	20.463	54.767	18.833	1.00	0.52	1SG1391
ATOM	1391	N	THR	173	20.493	56.859	17.933	1.00	0.62	1SG1392
ATOM	1392	CA	THR	173	21.892	57.061	18.114	1.00	0.62	1SG1393
ATOM	1393	CB	THR	173	22.335	58.461	17.796	1.00	0.62	1SG1394
ATOM	1394	OG1	THR	173	23.752	58.546	17.821	1.00	0.62	1SG1395
ATOM	1395	CG2	THR	173	21.728	59.430	18.825	1.00	0.62	1SG1396
ATOM	1396	C	THR	173	22.118	56.823	19.551	1.00	0.62	1SG1397
ATOM	1397	O	THR	173	23.170	56.335	19.960	1.00	0.62	1SG1398
ATOM	1398	N	GLN	174	21.099	57.144	20.363	1.00	0.51	1SG1399
ATOM	1399	CA	GLN	174	21.327	56.893	21.735	1.00	0.51	1SG1400

ATOM	1400	CB	GLN	174	20.192	57.355	22.657	1.00	0.51	1SG1401
ATOM	1401	CG	GLN	174	20.594	57.287	24.130	1.00	0.51	1SG1402
ATOM	1402	CD	GLN	174	21.508	58.471	24.408	1.00	0.51	1SG1403
ATOM	1403	OE1	GLN	174	21.278	59.575	23.917	1.00	0.51	1SG1404
ATOM	1404	NE2	GLN	174	22.579	58.237	25.212	1.00	0.51	1SG1405
ATOM	1405	C	GLN	174	21.464	55.387	21.896	1.00	0.51	1SG1406
ATOM	1406	O	GLN	174	20.520	54.662	21.485	1.00	0.51	1SG1407
ATOM	1407	OXT	GLN	174	22.513	54.940	22.435	1.00	0.51	1SG1408
END										

2540.

The following examples are provided for the purposes of illustration and are not intended to limit the scope of the present invention.

5

EXAMPLES

Example 1

This example describes the construction of a recombinant baculovirus expressing soluble FcγRIIa protein and the production of such protein.

10

Recombinant molecule pFcγRIIa, containing a nucleic acid molecule encoding a soluble form of human FcγRII (sFcγRIIa) operatively linked to baculovirus polyhedron transcription control sequences was produced as follows. The nucleic acid molecule sFcγRIIa was polymerase chain reaction (PCR) amplified from about 10 nanogram (ng) of FcγRIIa^{LR} cDNA (described in detail in Ierino, et al., *J. Exp. Med.*, vol. 178, pp. 1617-1628, 1993) using about 100 ng of primer NR1 having the nucleic acid sequence 5'-TAC GAA TTC CTA TGG AGA CCC AAA TGT CTC-3' (denoted SEQ ID NO:1) and primer FI2 having the nucleic acid sequence 5'-CAT TCT AGA CTA TTG GAC AGT GAT GGT CAC-3' (denoted SEQ ID NO:2), using standard PCR methods. The resulting PCR product is 510 base pairs (referred to herein as sFcγRIIa(a)) and encodes the amino acid sequence represented herein by SEQ ID NO:3. Based on the results obtained in the Mass Spectroscopy experiment described in Example 7, a second protein product is present upon expression of a recombinant molecule comprising a PCR product of this Example. This data suggests that two PCR products were produced from the present method. The second PCR product is predicted to be 513 base pairs (referred to herein as sFcγRIIa(b)) and encodes the amino acid sequence represented herein by SEQ ID NO:12. The PCR products were digested with restriction endonucleases *EcoRI* and *XbaI* and ligated into unique *EcoRI* and *XbaI* sites of pVL1392

25

30

35

baculovirus shuttle plasmid (available from Pharmingen, San Diego, CA) to produce recombinant molecules referred to herein as pVL-sFcγRIIa(a) and pVL-sFcγRIIa(b).

5 The recombinant molecules pVL-sFcγRIIa(a) and pVL-sFcγRIIa(b) were co-transfected with baculovirus strain AcMNPV (available from Pharmingen) into *Spodoptera frugiperda* 21 (Sf-21) cells (available from Invitrogen Corp., San Diego, CA) to produce *S. frugiperda*:pVL-sFcγRIIa(a)/sFcγRIIa(b) cells. Putative
10 recombinant virus isolates were selected by screening on X-galactosidase plates for occlusion of β-galactosidase. Selected isolates were grown on monolayers of Sf-21 cells for infection using serum-free Sf900-II media (available from Gibco, New York) and the supernatant harvested about
15 40 hours post-infection. The presence of recombinant protein, referred to herein as PsFcγRIIa, in the supernatants was determined by ELISA using anti-FcγRII monoclonal antibodies 8.26 and 8.7 (described in detail in Ierino, et al., *ibid.*) using standard methods. Based on
20 the results described in Example 7, recombinant protein PsFcγRIIa includes the two species of protein having SEQ ID NO:3 and SEQ ID NO:12.

Example 2

25 This example describes the purification of PsFcγRIIa for crystallization of the protein.

 Supernatant from *S. frugiperda*: pVL-sFcγRIIa(a)/sFcγRIIa(b) cells described above in Example 1 was harvested and then centrifuged at about x2000 rpm to remove cellular debris. Supernatant from the centrifugation was
30 concentrated about five-fold using a Minitan[®] ultrafiltration system (available from Millipore, Bedford, MA) and then extensively dialyzed against a buffer containing 10 mM Tris-HCl pH 8.5, and 50 mM NaCl. The dialyzed solution was applied to a Q-Sepharose[®] fast-flow
35 ion exchange column (available from Pharmacia, Uppsala,

Sweden). The column was washed with 10 mM Tris-HCl, pH 8.5, and then protein was eluted from the column using a salt gradient from about 0 to about 500 mM NaCl, passed over the column over 4 hours. PsFcγRIIa was eluted from the column at approximately 150 mM NaCl. The partially purified product was dialyzed against a buffer containing 20 mM Tris-HCl pH 7.4, and 30 mM NaCl. The dialysate was applied to a HAGG immuno-affinity chromatography column (described in detail in Ierino, et al., *ibid.*). The column was washed with a buffer containing 20 mM Tris-HCl pH 7.4, and 30 mM NaCl. PsFcγRIIa was eluted from the column using a buffer containing 0.1 M sodium acetate pH 4.0, and 0.5 M NaCl. The eluant was neutralized using 3M Tris pH8.0 and the dialysed against PBS (3.5 mM NaH₂PO₄·2H₂O, 16 mM Na₂HPO₄, 150 mM NaCl). The dialysate was then concentrated approximately fifty-fold using macro and nanosep-10 ultra-filtration concentration devices (available from Filtron, Northborough, MA) and the applied to a G75 Superdex™ gel filtration column equilibrated in PBS (available from Pharmacia, Uppsala, Sweden). Filtered PsFcγRIIa was dialyzed against 1 mM Tris-HCl pH 7.4 and concentrated to about 6 milligram per milliliter (mg/ml) of protein using macro and nanosep-10 ultra-filtration concentration devices. The purity of PsFcγRIIa was assessed by resolving the concentrated protein by SDS-PAGE and staining the protein with crocein scarlet. An electronic scan of the resulting gel is shown in Fig. 1, in which lane A contains supernatant harvested from a *S. frugiperda*:pVL-sFcγRIIa(a)/sFcγRIIa(b) cell culture prior to the ion-exchange step, lane B contains protein eluted from the affinity column, lane C contains protein isolated from the gel filtration chromatography step and lane D contains a sample of the PsFcγRIIa concentrated to 6 mg/ml and that was used for further crystallization studies. The molecular weight markers are shown on the left side of the

figure. The results indicate that the purified PsFcγRIIa was about 90% pure with apparent molecular weights of 25,000 daltons.

Example 3

5 This example describes two-dimensional non-equilibrium pH gel electrophoresis analysis of purified PsFcγRIIa.

 Supernatant from *S. frugiperda*:pVL-sFcγRIIa(a)/sFcγRIIa(b) was incubated with about 20 microliter (ml) of packed Sepharose 4B beads conjugated with F(ab') fragments of anti-FcγRII monoclonal antibody 8.26 (IgG2b) (the
10 production of which is described in *J. Immunol.*, vol. 150, pp. 1-10, 1993) for about 1 hour at 4°C. The beads were then washed with buffer containing 10 mM Tris-HCl pH 7.4, 2% wt/vol bovine serum albumin (available from Commonwealth
15 Serum Laboratories, Melbourne, Australia), 1 mM PMSF (available from Sigma Chemical Co., St. Louis, MO), 0.1% vol/vol Aprotinin (available from Sigma Chemical Co.), and then with 10 mM Tris-HCl, pH 7.4. The beads were resuspended in about 50 ml isoelectric focusing
20 denaturation buffer (9.5 M urea, 4% acrylamide, 2% wt/vol NP-40, 2% total ampholines and 50 mM dithiothreitol), spun at about x13,000 rpm for about 2 minutes, loaded onto 4% tube gels and overlaid with about 10 ml of overlay buffer (9 M urea, 1% total ampholines) and anode buffer (0.01 M
25 phosphoric acid), and electrophoresed for about 5 hours at about 550 Volts. The gels were then removed from the glass tubes, equilibrated in SDS-PAGE sample buffer (62.5 mM Tris-HCl, pH 6.8, 50 mM dithiothreitol and 10% glycerol) for about 2 hours at room temperature and attached to the
30 top of a 13% slab gel for SDS-PAGE.

 The electrophoresed proteins were transferred to Immobilon-P PVDF membrane (available from Millipore) using a semi-dry transfer cell (Biorad, Australia) under a 20 mA current for about 30 minutes. The membrane was blocked in
35 PBS buffer containing 5% wt/vol skim milk for about 1 hour.

The membrane was then incubated overnight with a rabbit anti-FcγRII polyclonal antisera (diluted 1:10,000 in PBS containing 5% wt/vol skim milk) and then washed extensively with buffer (10 mM Tris-HCl, pH 8.0, 150 mM NaCl, 0.05% Tween-20). The polyclonal antisera was raised in rabbits by immunization with recombinant FcγRII protein. The animals were immunized with about 1 mg of FcγRII protein. For the first immunization, FcγRII protein was emulsified in complete Freund's adjuvant. Subsequent immunizations were performed using FcγRII protein emulsified in incomplete Freund's adjuvant. The membrane was then incubated with peroxidase-linked swine anti-rabbit antisera (available from Dako Corp., Denmark) (diluted 1:5000 in 10 mM Tris-HCl, pH 8.0, 150 mM NaCl and 0.05% Tween-20) for about 1 hour at room temperature. The membrane was washed before detection of the transferred protein using the enhanced chemiluminescence system (available from Amersham International, Australia).

An electronic scan of the resulting gels are shown in Figs. 2A and 2B. Fig. 2A illustrates the migration of protein isolated from supernatant harvested from *S. frugiperda*:pVL-sFcγRIIa(a)/sFcγRIIa(b) cell cultures after 34 hours. Fig. 2B illustrates the migration of protein isolated from supernatant harvested from *S. frugiperda*:pVL-sFcγRIIa(a)/sFcγRIIa(b) cell cultures after 73 hours. The molecular weight markers are shown on the left side of the figure. The results indicate that the purified PsFcγRIIa has an apparent molecular weight of 25,000 daltons and a pI at about pH 6.

Example 4

This example describes N-terminal peptide sequence of PsFcγRIIa.

Amino acid sequencing of purified PsFcγRIIa described in Example 2 using standard sequential Edman degradation method using an Applied Biosystem 470A gas phase sequencer

coupled to an Applied Biosystem 130 separation system for automatic on-line analysis of the first eight amino acids (available from Applied Biosystems, CA). The n-terminal sequence was determined to be Ala-Pro-Pro-Lys-Ala-Val-Leu-Lys (denoted as SEQ ID NO:4).

Example 5

This example describes the binding of PsFcγRIIa to monomeric immunoglobulin.

Analysis of the interaction between PsFcγRIIa and monomeric immunoglobulin was performed using a BIAcore[®] 2000 biosensor (available from Pharmacia Biotech, Uppsala, Sweden) at about 22°C in Hepes buffered saline (HBS; 10 mM Hepes [N-2-hydroxyethylpiperazine-N'-2-ethanesulfonic acid, available from Commonwealth Serum Laboratories, Parkville, Australia], pH 7.4, 150 mM NaCl, 3.4 mM EDTA and 0.005% Surfactant, available from Pharmacia). About 4000 to about 6000 response units (RU) of monomeric human immunoglobulin subclasses IgG1, IgG2, IgG3, and IgE (50 μg/ml of each) were covalently coupled to separate carboxymethylated dextran surface of each CM5 sensor-chips (available from BIAcore, Uppsala, Sweden) using a amine coupling kit (available from BIAcore), according to manufacturer's methods. A series of PsFcγRIIa concentrations (about 0.001 to about 1 mg/ml protein) was injected over each sensor-chip surface for about 1 minute at about 20 μl/min followed by about 3 minute dissociation phase. Following administration of the protein, the immunoglobulin surface was regenerated on each chip using a buffer containing 50 mM diethylamine pH 11.5, and 1 M NaCl. The equilibrium dissociation constants (K_D) for the interaction between PsFcγRIIa and immunoglobulin were obtained by non-linear curve fitting of a single site binding equation $[\text{Bound RU} = (B1_{\text{max}} \cdot C) / (K_{D1} + C)]$; or a two site binding equation $[\text{Bound RU} = ((B1_{\text{max}} \cdot C) / (K_{D1} + C)) + ((B2_{\text{max}} \cdot C) / (K_{D2} + C))]$, where ($B1_{\text{max}}$ refers to the maximum binding capacity of the surface at site 1; $B2_{\text{max}}$ refers to

the maximum binding capacity of the surface at site 2; C refers to the concentration of PsFcγRIIa) and by linear curve fitting to Scatchard plots. Data points obtained from the IgE channels were subtracted to correct for refractive index differences. Data points between 50 and 60 seconds were averaged to obtain the amount of PsFcγRIIa bound at equilibrium for each PsFcγRIIa concentration.

To determine the specificity of the interaction between PsFcγRIIa and immobilized immunoglobulin, the interaction between PsFcγRIIa with monomeric immunoglobulin was inhibited by the presence of excess monomeric IgG (Sandaglobulin, available from Sandoz, Basel, Switzerland). Using a fixed, half maximal dose of PsFcγRIIa (50 μg/ml), increasing concentrations of monomeric IgG (0 to 2 mg/ml IgG) were mixed with the PsFcγRIIa, at about 22°C for about 1 hour before passing the PsFcγRIIa over a sensor-chip surface coated with IgG1.

The results indicated that the binding of PsFcγRIIa to IgG3 and IgG1 was saturable over a broad range of protein concentrations. The maximum response units per protein concentration were plotted against the molar concentration of protein and curve fitting analyses undertaken. The curve of best fit suggests that there are two regions of PsFcγRIIa that interact with IgG3. At 50% of the sites, the affinity for IgG3 was about $2.7 \times 10^6 \text{ M}^{-1}$ and at the remaining 50% of the sites the affinity was about $1.2 \times 10^4 \text{ M}^{-1}$ (Fig. 3A). The interaction between PsFcγRIIa and IgG1 also occurred in two regions but the interaction was different from IgG3. Moreover, at about 90% of the ligand binding sites, the affinity of PsFcγRIIa for IgG1 was about $2.1 \times 10^6 \text{ M}^{-1}$ and at the remaining 10% of sites the affinity was about $2.3 \times 10^4 \text{ M}^{-1}$ (Fig. 3B). The interaction was specific for PsFcγRIIa since a six-fold molar excess of IgG completely inhibited binding of PsFcγRIIa to IgG. Analysis

of IgG2 binding was also performed and a K_d value of about $8 \times 10^{-5} M^{-1}$ was obtained (Fig. 3C).

Example 6

This example describes crystallization and X-ray diffraction of PsFcyRIIa.

A. Production of crystalline PsFcyRIIa

A series of alternative buffers were used to attempt to produce crystals of PsFcyRIIa by hanging drop vapor diffusion. Table 6 summarizes the different mother-liquor formulations used and the results obtained.

Table 6. Mother-liquor conditions and results of crystallization trial 3 mg/ml PsFcyRIIa.

No.	SALT	BUFFER	PRECIPITANT*	pH	RESULT
1	0.2M Calcium Chloride	0.1 M Acetate	30% MPD	4.6	clear drop
2	_____	_____	0.4M Na K Tartrate	_____	fine precipitation
3	_____	_____	0.4M Amm. Phosphate	_____	clear drop
4	_____	0.1M Tris	2.0M Amm. Sulphate	8.5	clear drop
5	0.2M Sodium Citrate	0.1M Hepes	40% MPD	7.5	phase separation
6	0.2M Mg Chloride	0.1M Tris	30% PEG 4000	8.5	dried up
7	_____	0.1M Cacodylate	1.4M Sodium Acetate	8.5	clear drop
8	0.2M Sodium Citrate	0.1M Cacodylate	30% Isopropanol	6.5	clear drop
9 ^b	0.2M Amm. Acetate	0.1M Sodium Citrate	30% PEG 4000	5.6	phase separation & crystal
10	0.2M Amm. Acetate	0.1M Acetate	30% PEG 4000	4.6	clear drop
11	_____	0.1M Citrate	1.0M Amm. Phosphate	5.6	clear drop
12	0.2M Mg Chloride	0.1M Hepes	30% Isopropanol	7.5	clear drop
13	0.2M Sodium Citrate	0.1M Tris	30% PEG 400	8.5	phase separation
14	0.2M Calcium Chloride	0.1M Hepes	28% PEG 400	7.5	precipitation
15	0.2M Amm. Sulphate	0.1M Cacodylate	30% PEG 8000	6.5	precipitation
16 ^c	_____	0.1M Hepes	1.5M Lithium Sulphate	7.5	splinters
17	0.2M Lithium Sulphate	0.1M Hepes	30% PEG 4000	7.5	phase separation
18	0.2M Mg Acetate	0.1M Cacodylate	20% PEG 8000	6.5	clear drop
19	0.2M Amm. Acetate	0.1M Tris	30% Isopropanol	8.5	clear drop
20	0.2M Amm. Sulphate	0.1M Acetate	25% PEG 4000	4.6	heavy precipitation
21	0.2M Mg Acetate	0.1M Cacodylate	30% MPD	6.5	fine precipitation
22	0.2M Sodium Acetate	0.1M Tris	30% PEG 4000	8.5	fine precipitation
23	0.2M Mg Chloride	0.1M Hepes	30% PEG 400	7.5	skin over drop
24	0.2M Calcium Chloride	0.1M Acetate	20% Isopropanol	4.6	clear drop
25 ^d	_____	0.1M Imidazole	1.0M Sodium Acetate	7.5	crystal
26	0.2M Amm. Acetate	0.1M Citrate	30% MPD	5.6	clear drop
27	0.2M Sodium Citrate	0.1M Hepes	20% Isopropanol	7.5	clear drop
28	0.2M Sodium Acetate	0.1M Cacodylate	30% PEG 8000	8.5	clear drop

262

No.	SALT	BUFFER	PRECIPITANT ^a	pH	RESULT
29	_____	0.1M Hepes	0.8M Na K Tartrate	7.5	clear drop
30	0.2M Amm. Sulphate	_____	30% PEG 8000	_____	precipitation
31	0.2M Amm. Sulphate	_____	30% PEG 4000	_____	precipitation
32	_____	_____	2.0M Amm. Sulphate	_____	clear drop
33	_____	_____	4.0M Sodium Formate	_____	precipitation
34	_____	0.1M Acetate	2.0M Sodium Formate	4.6	precipitation
35	_____	0.1M Hepes	2.0M Na K Phosphate	7.5	precipitation
36	_____	0.1M Tris	8% PEG 8000	8.5	precipitation
37	_____	0.1M Acetate	8% PEG 4000	4.6	aggregation
38	_____	0.1M Hepes	1.4M Na Citrate	7.5	heavy precipitation
39	_____	0.1M Hepes	2.0M Amm. Sulphate 2% PEG 400	7.5	fine precipitation
40	_____	0.1M Citrate	20% PEG 4000, 20% Isopropanol	5.6	fine aggregation
41	_____	0.1M Hepes	20% PEG 4000, 10% Isopropanol	7.5	clear drop
42	0.05M K Phosphate	_____	20% PEG 8000	_____	clear drop
43	_____	_____	30% PEG 1500	_____	clear drop
44	_____	_____	0.2M Mg Formate	_____	clear drop
45	0.2M Zn Acetate	0.1M Cacodylate	18% PEG 8000	6.5	heavy precipitation
46	0.2M Ca Acetate	0.1M Cacodylate	18% PEG 8000	6.5	fine precipitation
47	_____	0.1M Acetate	2.0M Amm. Sulphate	4.6	heavy precipitation
48	_____	0.1M Tris	2.0M Amm. Sulphate	8.5	fine precipitation
49	1.0M Li Sulphate	_____	2% PEG 8000	_____	med precipitation
50	1.0M Li Sulphate	_____	15% PEG 8000	_____	heavy precipitation

a. Final concentration of precipitant used to achieve the result listed.

b. Condition 9 produced two crystals in the single droplet.

c. Condition 16 produced a shower of splinters that have arisen from numerous nucleation points within the droplet.

d. Condition 25 produced an unusual crystal. Numerous crystalline plates appear to be joined together to form this crystal. X-ray diffraction analysis of this crystal was not successful.

A rapid screening method (generally described in McPherson, 1982, In: Preparation and Analysis of Protein Crystals, 1982, pp. 94-97, John Wiley and Sons, pub.; and *J. Crystal Growth*, vol. 122, pp. 161-167, 1992) was used. Briefly, hanging drop vapor diffusion experiments were performed using 24-well culture plates. Droplets (about 3 μ l) containing about 3 mg/ml of PsFcyRIIa in an equal volume of a mother-liquor were suspended from siliconized coverslips inverted into 24-well tissue culture plates well. The droplets were equilibrated at about 22°C against about 1 ml mother-liquor. Controlled temperature

incubation was performed in chambers (available from Linbro Inc, distributed by ICN Inc, Costa Mesa CA) at about 22°C. Successful PsFcyRIIa crystallization was performed using the mother-liquor 0.2 M ammonium acetate, 0.1 M citrate pH 5.6 and 30% PEG 4000, at 22°C for between about 3 to about 9 days, or up to 9 months depending upon the purity and concentration of the PsFcyRIIa, resulting in the production of orthorhombic crystals.

Successful PsFcyRIIa crystallization was also performed using the mother-liquor 0.1 M HEPES pH 7.5 with 1.5 M lithium sulphate, at 22°C for between about 3 to about 9 days, or up to 9 months depending upon the purity and concentration of the PsFcyRIIa, resulting in the production of a series of rod-like splinters of defined structure.

The rod-like splinters were analyzed by X-ray diffraction. B. X-ray Diffraction of Crystalline PsFcyRIIa and Determination of Electron Density Map

The PsFcyRIIa crystals produced as described above in section A were mounted in rayon loops and cryo-cooled to -165°C in mother liquor containing 20% glycerol. Twelve heavy atom compounds which sampled a broad range of activities were tested for binding to PsFcyRIIa. PIP (Di-p-iodo bis[ethylenediamine] di Platinum(II) nitrate) was found to be reactive. Crystals were derivatized by soaking overnight in mother liquor containing about 5 mM PIP. Diffraction measurements were made with a M18XHF rotating anode generator (Siemens, Germany) operating at about 40 KV and about 50 mA and using Ni filtered CuK α radiation. The generator was equipped with Franks mirrors (Molecular Structure Corporation, USA), a low-temperature system (Molecular Structure Corporation, USA) and RAXIS IIC and IV image plate detectors (Rigaku, Japan).

The crystals belong to the space group $P2_12_12$ ($a = 78.80 \text{ \AA}$, $b = 100.55 \text{ \AA}$, $c = 27.85 \text{ \AA}$) and diffracted to about 2.4 Å resolution with an $R(\text{merge})$ of 0.065. $R(\text{merge}) =$

$S(I_i - \langle IS \rangle) / I_i$ summed over all independent reflections where I = intensity. Native and derivative data were collected at 45 minute exposures with an oscillation range of about 1° . Diffraction intensities were integrated using DENZO (Otwinowski, et al., *Methods in Enzymology*, vol. 276, p. 307, 1996) and scaled with SCALEPACK (Otwinowski, et al., *ibid.*). A single heavy atom binding site was located by inspection of isomorphous and anomalous difference Patterson maps (Blundell, et al., In: Protein Crystallography, Horecker, B., Kaplan, N. O., Marmur, J., Scheraga, H. A., Eds., Academic Press, New York, 1976) calculated with the PROTEIN system (Steigeman, Ph.D. Thesis, Technical University, Munich, 1974). Heavy atom parameters were refined and phases were determined in a method of Single Isomorphous Replacement with Anomalous Scattering using the program SHARP (Statistical Heavy-Atom Refinement and Phasing (de La Fortelle, et al., *Methods in Enzymology*, vol. 276, p. 472, 1996). Merged data in the range of about 18 to about 2.7 Å resolution had an isomorphous R-factor of about 0.162, figure of merit for centric reflections 0.308 and acentric reflections 0.247 and phasing power of 1.127 for centric reflections and 1.081 for acentric reflections (Blundell, *ibid.*). Phases were modified in a protocol of solvent flattening (Wang, *Methods in Enzymology*, vol. 115, p. 90, 1985) and histogram mapping (Zhang, et al., *Acta Crystallography*, vol. A46, p. 377, 1990) in the density modification package DM (Cowtan, *Joint CCP4 and ESF-EACBM Newsletter on Protein Crystallography*, vol. 31, p. 34, 1994) in the CCP4 suite of programs (Cowtan, *ibid.*). 2Fo-Fc electron-density maps were displayed using the graphical display program O (Jones et. al., *Acta Crystallography*, vol. A47, p. 110, 1991). Secondary structural features could be identified at this stage, however the map was difficult to fully interpret and

trace of the polypeptide. To produce a simplified representation of the electron density, the map was skeletonised (Greer, *J. Mol. Biol.*, vol. 82, p. 279, 1974) using the program BONES (Jones, et al., *ibid.*).
5 Coordinates of Killer Inhibitory receptor (Fan, et. al., *Nature*, vol. 389, p. 96, 1997) and were used as a reference to trace the polypeptide and generate a partial model. To calculate subsequent maps density modified phases and phases calculated from the model were combined by the
10 Free-Sim method (Sim, *Acta Crystallography*, vol. 13, p. 511, 1960).

Additional data for structure refinement were collected at beam line X4A of the National Synchrotron Light Source at Brookhaven National Laboratory (Upton, New York).
15 Using radiation with a wavelength of about 1.058 Å, data were collected on Fuji image plates as exposures of about 100 seconds and oscillation ranges of about 1°. Diffraction images were digitized with a BAS 2000 scanner (Fuji, Japan) and processed as described above, giving an
20 *R*(merge) of 0.038 for data between about 10 Å and about 1.7 Å resolution. Structure refinement was performed with the XPLOR system (Brunger, et al., *Science*, vol. 235, p. 458, 1987) using protocols including individual temperature factor, energy minimization and slow-cool simulated
25 annealing refinement with bulk solvent correction.

The refined structure of PsFcyRIIa contains all amino acid residues from 1 to 170, together with 33 solvent molecules. The crystallographic residual *R*-factor and Free *R*-factor are about 0.253 and about 0.326 respectively for
30 data of from about 7 Å to about 2.0 Å resolution (Brunger, 1987, *ibid.*). Root mean squared deviations from ideality for bond lengths was about 0.01 Å and about 1.45° for angles (Brunger, et al., *Nature*, vol. 355, p. 472, 1992). The resulting data set of the atomic coordinates for
35 PsFcyRIIa is shown in Fig. 4.

C. PsFcγRIIa Structure

Using the atomic coordinates listed in Table 1, a structure of a dimer of PsFcγRIIa was derived. The structures were computer generated using MOLSCRIPT 2.0 program (available from Avatar Software AB, Heleneborgsgatan 21C, SE-11731 Stockholm, Sweden). The crystal structure reveals PsFcγRIIa in a dimeric form having two 170 amino acid monomers. The two monomers are structurally identical.

The structure of the PsFcγRIIa residues 1 to 170 consists of two immunoglobulin constant region 2 (C2) type immunoglobulin domains and each domain is comprised of two antiparallel β-sheets, pinned together by a disulfide bond. The first strand of each domain (A strand) is broken in the middle with part forming sheet I (ABE strands) and part forming sheet II (A'GFCC' strands). This structural feature occurs in immunoglobulin variable region (V) type domains and in the natural killer inhibitory receptor (KIR) but not in other C2 domains. The two immunoglobulin-like domains of PsFcγRIIa are quite similar to each other with the rms difference in Ca positions of 1.28 Å for 68 residues. Major differences are in the loops at the N-terminal end of the molecule (BC, C'E and FG loops) and in the position on the C' strand. Some of these loops have been implicated in binding Fc.

The region of association of the two domains in the PsFcγRIIa structure is quite bent, with the angle between the major axes of the domains being approximately 52°. This bend is more severe than other immunoglobulin super family members including 60° for KIR. The domain interface is composed of strands A' from Domain 1 and A & B from Domain 2, where sheet II from each domain forms the interface. Residues whose non-hydrogen atoms lie within 4 Å of the other domain. Water molecules 201, 211, 217-220, 227 and 232 also lie in the interface region.

Certain structural characteristics indicate that dimer formation between two PsFcγRIIa molecules in the crystal is a preferred interaction. Although the structure of only one PsFcγRIIa molecule (residues 1 to 170) of the crystal has been determined, each PsFcγRIIa molecule comprising the dimer in the crystal is related to the other PsFcγRIIa molecule in the crystal by a 2-fold crystallographic axis. By applying the transformation:

$$\begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \cdot \begin{pmatrix} x \\ y \\ z \end{pmatrix} + \begin{pmatrix} 0. \\ 100.55 \\ 0. \end{pmatrix}$$

to the coordinates given in Table 1 a dimer is formed (Fig. 4), with the interface composed of sheet II from each PsFcγRIIa molecule. The coordinates of the FcγRIIa dimer are represented in Table 2. The contact area is substantial (~400 Å²) and this interface has more hydrophobic character than the Domain 1-Domain 2 interface. Residues whose non-hydrogen atoms lie within 4 Å of the other molecule or water molecule 207 on the axis are 119, 121, 124-126, 150, 152 and 158-161, with residues 148, 163 and 164 also making a close approach. This type of domain interaction is not novel for immunoglobulins because V regions of antibodies pair in a similar manner. This type of interaction, however, has not been observed for C2 domains. Due to the size and character of this contact it suggests that this hitherto unforeseen interaction has physiological relevance.

Additional structural considerations support this conclusion. The crystal structure described above suggests that, if an FcγRIIa molecule is oriented with the C-terminus toward a cell membrane containing the receptor, then the putative Fc binding region of the receptor does not point away from the cell but to one side. Thus, forming a dimer between two FcγRIIa molecules in a cell membrane, the two potential Fc binding regions are brought

near each other and point away from the cell because the dimer axis points away from the cell. This orientation positions the potential Fc binding sites ideally for interaction with ligand (i.e., IgG), enabling the ligand binding site to be composed of regions from two receptor molecules. Involving two receptor molecules in a binding event has implications for cellular signal transduction because dimerization of the extracellular domains would bring the cytoplasmic domains of the two receptors together to initiate a cellular signal transduction response.

Fig. 4 shows a graphical representation of the dimer of PFcyRIIa. Two Ig-like domains (Domains 1 and 2) are shown in each monomer of each dimer. The first amino acid residue of the amino (NH₂) terminus of the protein is indicated by residue number 0. The last amino acid residue of the carboxyl (COOH) terminus of the protein is indicated by residue 170. Numbering of amino acid residues from the NH₂ terminus to the COOH terminus are shown where possible. Certain residues were omitted for clarity. Fig. 5 illustrates the amino acid residues that comprise each beta sheet of Domain 1 and Domain 2 of PFcyRIIa. In Domain 1, strand A includes residues 5-10, strand A' includes residues 14-17, strand B includes residues 20-28, strand C includes residues 37-41, strand C' includes residues 44-46, strand E includes residues 52-58, strand F includes residues 63-70 and strand G includes residues 78-84. In Domain 2, strand A includes residues 87-92, strand A' includes residues 95-97, strand B includes residues 102-110, strand C includes residues 117-122, strand C' includes residues 125-131, strand E includes residues 134-139, strand F includes residues 146-155, strand G includes residues 158-162 and strand G' includes residues 163-169. Fig. 6 shows the stereo view of the structure of the polypeptide shown in Fig. 4 in stereo.

A graphical representation of the three dimensional structure shown in Fig. 4 was used to determine the location of amino acid residues involved in the binding of FcγRIIa to IgG. Fig. 7 shows the location of the mutated alanine residues (indicated by the black balls) involved in the loss of binding of FcγRIIa to IgG. The residues shown in Fig. 7 were identified using recombinant mutants of FcγRIIa, in which residues were replaced with alanine and were found to disrupt or decrease IgG binding to FcγRIIa (described in Hulett, et al., 1994, *ibid.*; Hulett, et al., 1995, *ibid.*). Fig. 8 shows an expanded view of the IgG binding region showing position and side chains of amino acids involved in IgG binding to FcγRIIa, as shown by production of nucleic acid molecules having mutations in this region that encode an FcγRIIa protein having reduced binding to IgG.

Fig. 9 shows an expanded view of the IgG binding region and the amino acid residues, which when mutated to alanine, improve IgG binding.

The interface between the two dimers illustrated in the graphical representation of the three dimensional structure shown in Fig. 4 was further analyzed. Fig. 10 shows an expanded view of the region of one FcγRIIa monomer that contributes to the dimer interface. In Fig. 10, the region has been rotated about 90° in x, where x is horizontal to the page. The γ carbon of amino acid residues contributing to the interface are shown as black balls and are numbered according to the residue numbering of SEQ ID NO:3.

Example 7

This example describes analysis of N-terminal sequence of PsFcγRIIa protein by electrospray ionization mass spectrometry.

To determine the N-terminal amino acid sequence of PsFcγRIIa protein, the heterogeneity of the N-linked

glycosylation mass spectrometry was carried out as follows. Various samples were prepared by combining about 1 to about 100 picomolar (pmol) of PsFcγRIIa protein in about 2 μl to about 4 μl of 50% CH₃CN containing 0.1% acetic acid. The samples were infused at a flow rate of about 0.2 μl/min into a Perkin Elmer Sciex API-300 triple quadrupole mass spectrometer fitted with a micro-ionspray ion source and operated in the Q1 scan mode. The mass scale was calibrated at eight points over the 3000 u mass range, to an accuracy equivalent to ± 0.01%, using singly charged poly(propylene glycol) ions. Mass spectra (typically 30-100 scans) were recorded over the mass range m/z 200 u to 3000 u with a constant peak width of 0.6 u (peak width at half-height), and were processed by signal-averaging, manual mass determination and transformation using PE-Sciex Biomultiview software. The results indicated that two major species of protein having different N-terminal sequence were present in the solution of purified PsFcγRIIa protein. One species had a N-terminal sequence comprising SEQ ID NO:4 and the other species had a N-terminal sequence with an additional Ala at the 5' end of the protein (e.g., Ala-Ala-Pro-).

Example 8

This example describes the modeling of the three dimensional structure of the Fcε receptor I (FcεRI) in both monomeric and dimeric forms.

The extracellular regions of the human Fc epsilon receptor type I (FcεRI) and the human Fc gamma Receptor type II a (FcγRIIa) show a sequence identity of about 38% (for 172 residues). The final sequence alignment used in this modeling work is shown in Fig. 13. The X-ray crystallographic structure of the human FcγRIIa was determined by the present inventors (Table 1). The 3-dimensional coordinates of FcγRIIa in Table 1 differ from those used as the template to build a 3-dimensional model

of the human FcεRI by orientation of the imidazole ring of His 108 and one round of refinement.

5 Secondary structure prediction performed on FcεRI confirmed the validity of the alignment given in Fig. 13 and showed the pattern of β strands is the same in both FcεRI and FcγRIIa. The secondary structure prediction methods used were PHD (B. Rost et al., CABIOS, vol. 10, 266-275(1994)) and PREDATOR (D. Frishman and P. Argos, Proteins, vol. 27, 329-335(1997)).

10 MODELER (A. Sali and T.L. Blundell, J. Mol. Biol., vol. 234, 779-815(1993)) as implemented in the InsightII_Homology software package (Insight II (97.0), MSI, San Diego) was used to generate 3-dimensional models of FcεRI using a number of different initial sequence
15 alignments and two structural templates of FcγRIIa. One of the structural templates was the 3-dimensional coordinates of FcγRIIa where, for the residues that had alternative side-chain conformations (residue numbers 10, 21, 33, 57, 60, 61, 65, and 89), the conformations labeled 'A' were
20 selected while in the other template the conformations labeled 'B' were selected. In each Modeler run 5 structural models of FcεRI were generated. The following parameter values or options were used: 'library_schedule' of 1, 'max_var_iterations' of 300, 'md_level' of 'refine1',
25 'repeat_optimization' of 3, and 'max_molpdf' of 1e6. The best model from these runs had the sequence alignment given in Fig. 13, and used the structural template of FcγRIIa, where residues 10, 21, 33, 57, 60, 61, 65, and 89 had side-chains in the 'A' conformation. The criteria for
30 judging the 'best' model included the lowest value of the Modeler objective function (or $-1.0 \times \ln(\text{Molecular probability density function} = \text{Mpdf})$), 'well-behaved' PROSAIL (M. Sippl, Proteins, vol. 17, 355-362(1993)) residue energy plot for the model (for example, negative residue energy
35 scores throughout the sequence), and 'well-behaved'

PROFILES-3D (J.U. Bowie et al., Science, vol. 253, 164-170(1991)) local 3D-1D compatibility score plot (for example, positive plot scores throughout the sequence).

5 Next, Modeler was used to generate 20 different structural models of FcεRI using the sequence alignment and template selected above, and using the parameter values and options listed above. The model with the lowest $-\ln(\text{Mpdf})$ value (i.e. 957.2) was then selected as the template to generate structural models of the FcεRI sequence in the next cycle of Modeler runs. At the end of four such cycles, the 'best' 3-dimensional model of the FcεRI structure had a $-\ln(\text{Mpdf})$ value of 643.2. This was selected as the final structural model of the FcεRI monomer, and the corresponding heavy (non-hydrogen) atom cartesian coordinates are represented in Table 3. A 'worm' representation of the structure is shown in Fig. 14. This structure was validated with the programs PROSAIL, PROFILES-3D, and PROCHECK (R.M. Laskowski et al., J.Appl.Cryst. vol. 26, 283-291(1993)).

20 Finally, the same coordinate transformation that generates a dimer from the FcγRIIa monomer was applied to the above model of the FcεRI monomer. The interface of the resultant dimer was optimized by selecting alternative rotamers for the Glu 161 and Tyr 150 residues with the Auto_Rotamer option of the InsightII_Homology module (MSI, San Diego), and then adding hydrogen atoms to the dimer model and energy minimizing it keeping all heavy atoms fixed, except for Tyr 150 and Glu 161 where only the backbone atoms were kept fixed. The program Discover v. 2.98 (MSI, San Diego) was used for the energy minimization with the CFF91 force field and a distance-dependent dielectric constant of $1.0 \times r$, and the minimization was done with the conjugate gradients' method until the maximum energy gradient was less than 0.10 kcal/Å. The cartesian coordinates of the resultant model of the FcεRI dimer are

35

represented in Table 4 and a 'worm' representation of the dimer model is shown in Fig. 15. This model of the FcεRI dimer has a shape complementarity or Sc value (see M.C. Lawrence and P.M. Colman, *J. Mol. Biol.*, vol. 234, 946-950(1993)) at the monomer-monomer interface of 0.64 and an electrostatic complementarity value - for the fully solvated case, using the Spearman correlation coefficient - (see A. J. McCoy, V.C. Epa, and P.M. Colman, *J. Mol. Biol.*, vol. 268, 570-584(1997)) or ECSFS at the monomer-monomer interface of 0.08. These compare with 0.80 and 0.32, respectively, for the FcγRIIa dimer. These reduced complementarity values for the FcεRI dimer compared to the FcγRIIa dimer indicates that formation of the FcεRI dimer, as built herein, is energetically less favored than it is in the FcγRIIa case. However, we note that the interaction with the β or γ chains of the FcεRI has not been taken into consideration. Fig. 16 shows a molecular surface representation of the FcεRI dimer model.

The model of the 3-dimensional structure of FcεRI monomer represented by the coordinates in Table 3 or the FcεRI dimer represented by the coordinates in Table 4 may be used as a basis for drug design in the same manner as that described for the crystallographic coordinates of FcγRIIa herein.

25 Example 9

The following example demonstrates the crystallization of the Fcε receptor I (FcεRI).

Recombinant molecule pFcεRI, containing a nucleic acid molecule encoding a soluble form of human FcεRI (sFcεRI) operatively linked to baculovirus polyhedron transcription control sequences was produced as described for the pFcγRIIa molecule in Examples 1-3. Briefly, the recombinant soluble FcεRI was generated by placing a translation termination codon at the position 173 which normally encodes a Pro in the sequence Ile, Lys, Ala, Pro,

at the C-terminal end of the second domain as set forth in the sequence represented in Fig. 13. Soluble FcεRI was expressed in baculovirus expression system 'Bac to Bac' supplied by GIBCO. Infections of SF21 or Sf9 cells were performed as described by the manufacturer. Briefly, the recombinant FcγRIIa molecule was ligated into pVL1392 baculovirus shuttle plasmid (available from Pharmingen, San Diego, CA) to produce a recombinant molecule referred to herein as pVL-sFcεRI. The recombinant molecule pVL-sFcεRI was subsequently co-transfected with baculovirus strain AcMNPV (available from Pharmingen) into *Spodoptera frugiperda* 21 (Sf-21) cells (available from Invitrogen Corp., San Diego, CA) to produce *S. frugiperda*:pVL-sFcεRI cells. 65-70 hours following infection, supernatants were harvested and soluble receptor was purified by affinity chromatography on an anti-FcεRI antibody (3B4) monoclonal antibody-sepharose 4B affinity column, similar to the processes described for FcγRIIa in Example 5. The column was washed with 10 mM Tris pH 7.5 and eluted with 0.1 M sodium acetate, 0.5M sodium chloride, pH4.0. The purified protein was concentrated and used in crystallization trials as described above for FcγRIIa (Example 6). Crystals were produced under several conditions as follows:

(a) 0.2M calcium acetate; 0.1M sodium cacodylate, pH6.5; 18% w/v polyethylene glycol (PEG) 8000;

(b) 0.1M sodium cacodylate, pH6.0 or pH5.5; 10% v/v 2-propanol; 20% w/v PEG 4000;

(c) 0.2M tri sodium citrate dihydrate; 0.1M sodium cacodylate pH6.5; 30% v/v 2-propanol.

The structure of the FcεRI crystals obtained by these experiments can be used in X-ray diffraction analysis and/or in molecular replacement and modeling strategies as described herein.

Example 10

This example describes the modeling of the three dimensional structure of the Fcγ receptor III (FcγRIIIb) in monomeric form.

5 The extracellular regions of the human Fc gamma receptor type III (FcγRIIIb) and the human Fc gamma Receptor type II a (FcγRIIa) show a sequence identity of about 53% (for 174 residues). The final sequence alignment used in this modeling work is shown in Fig. 18. The X-ray
10 crystallographic structure of the human FcγRIIa was determined by the present inventors (Table 1) as described in Examples 1-7. The 3-dimensional coordinates of FcγRIIa in Table 1 differ from those used as the template to build a 3-dimensional model of the human FcγRIIIb by orientation
15 of the imidazole ring of His 108 and one round of refinement.

 MODELER (A. Sali and T.L. Blundell, J. Mol. Biol., vol. 234, 779-815(1993)) as implemented in the InsightII_Homology software package (Insight II (97.0),
20 MSI, San Diego) was used to generate 3-dimensional models of FcγRIIIb using a number of different initial sequence alignments and two structural templates of FcγRIIa. The structural template that was used was the 3-dimensional coordinates of FcγRIIa where, for the residues that had
25 alternative side-chain conformations (residue numbers 10, 21, 33, 57, 60, 61, 65, and 89), the conformations labeled 'A' were selected. In each Modeler run 5 structural models of FcγRIIIb were generated. The following parameter values or options were used: 'library_schedule' of 1,
30 'max_var_iterations' of 300, 'md_level' of 'refinel', 'repeat_optimization' of 3, and 'max_molpdf' of 1e6. The best model from these runs had the sequence alignment given in Fig. 18, and used the structural template of FcγRIIa, where residues 10, 21, 33, 57, 60, 61, 65, and 89 had
35 side-chains in the 'A' conformation. The criteria for

judging the 'best' model included the lowest value of the Modeler objective function (or $-1.0 \times \ln(\text{Molecular probability density function} = \text{Mpdf})$), 'well-behaved' PROSAIL (M. Sippl, Proteins, vol. 17, 355-362(1993)) residue energy plot for the model (for example, negative residue energy scores throughout the sequence), and 'well-behaved' PROFILES-3D (J.U. Bowie et al., Science, vol. 253, 164-170(1991)) local 3D-1D compatibility score plot (for example, positive plot scores throughout the sequence).

Next, Modeler was used to generate 20 different structural models of FcγRIIIb using the sequence alignment and template selected above, and using the parameter values and options listed above. The model with the lowest $-\ln(\text{Mpdf})$ value (i.e. 933.3) was then selected as the final structural model of the FcγRIIIb monomer, and the corresponding heavy (non-hydrogen) atom cartesian coordinates are represented in Table 5. This structure was validated with the programs PROSAIL, PROFILES-3D, and PROCHECK (R.M. Laskowski et al., J.Appl.Cryst. vol. 26, 283-291(1993)).

The model of the 3-dimensional structure of FcγRIIIb monomer represented by the coordinates in Table 5 may be used as a basis for drug design in the same manner as that described for the crystallographic coordinates of FcγRIIIa herein.

While various embodiments of the present invention have been described in detail, it is apparent that modifications and adaptations of those embodiments will occur to those skilled in the art. It is to be expressly understood, however, that such modifications and adaptations are within the scope of the present invention, as set forth in the following claims.

What is claimed is:

1. A model of an Fc receptor (FcR) protein, wherein said model represents a three dimensional structure that substantially conforms to the atomic coordinates of Table 1.
5
2. The model of Claim 1, wherein said structure substantially conforms to the atomic coordinates and B-values represented by Table 1.
3. The model of Claim 1, wherein said structure is monomeric.
10
4. The model of Claim 1, wherein said structure is dimeric.
5. The model of Claim 1, wherein said structure substantially conforms to the atomic coordinates of a table selected from the group consisting of Table 2, Table 3, Table 4 and Table 5.
15
6. The model of Claim 1, wherein at least about 50% of said structure has an average root-mean-square deviation (RMSD) of less than about 1.5Å for backbone atoms in secondary structure elements in each domain of said structure.
20
7. The model of Claim 1, wherein at least about 50% of common amino acid side chains between said structure and a structure comprising said atomic coordinates have an average root-mean-square deviation (RMSD) of less than about 1.5Å.
25
8. The model of Claim 1, wherein said FcR protein comprises an amino acid sequence that is at least about 25% identical to an amino acid sequence selected from the group consisting of SEQ ID NO:3, SEQ ID NO:10, SEQ ID NO:11 and SEQ ID NO:12.
30
9. The model of Claim 1, wherein said FcR protein comprises an amino acid sequence that is at least about 40% identical to an amino acid sequence selected from the group

consisting of SEQ ID NO:3, SEQ ID NO:10, SEQ ID NO:11 and SEQ ID NO:12.

10. The model of Claim 1, wherein said FcR protein comprises an amino acid sequence that is at least about 60% identical to an amino acid sequence selected from the group consisting of SEQ ID NO:3, SEQ ID NO:10, SEQ ID NO:11 and SEQ ID NO:12.

11. The model of Claim 1, wherein said FcR protein comprises an amino acid sequence selected from the group consisting of: SEQ ID NO:3, SEQ ID NO:5, SEQ ID NO:6, SEQ ID NO:7, SEQ ID NO:8, SEQ ID NO:9, SEQ ID NO:10, SEQ ID NO:11, SEQ ID NO:12, SEQ ID NO:13, a mutant of any of said amino acid sequences, and an allelic variant of any of said amino acid sequences.

12. The model of Claim 1, wherein said FcR protein comprises an amino acid sequence selected from the group consisting of: an amino acid sequence selected from the group consisting of SEQ ID NO:3, SEQ ID NO:5, SEQ ID NO:6, SEQ ID NO:7, SEQ ID NO:8, SEQ ID NO:9, SEQ ID NO:10, SEQ ID NO:11, SEQ ID NO:12, SEQ ID NO:13; a mutant of SEQ ID NO:3, SEQ ID NO:5, SEQ ID NO:6, SEQ ID NO:7, SEQ ID NO:8, SEQ ID NO:9, SEQ ID NO:10, SEQ ID NO:11, SEQ ID NO:12 or SEQ ID NO:13; and an allelic variant of SEQ ID NO:3, SEQ ID NO:5, SEQ ID NO:6, SEQ ID NO:7, SEQ ID NO:8, SEQ ID NO:9, SEQ ID NO:10, SEQ ID NO:11, SEQ ID NO:12 or SEQ ID NO:13.

13. The model of Claim 1, wherein said FcR protein is selected from the group consisting of FcγRI protein, FcγRIIa protein, FcγRIIb protein, FcγRIIc protein, FcγRIII protein, FcεRI protein, FcαRI protein and structural homologues of any of said FcR proteins.

14. The model of Claim 1, wherein said FcR protein is selected from the group consisting of FcγRI protein, FcγRIIa protein, FcγRIIb protein, FcγRIIc protein, FcγRIII protein, FcεRI protein and FcαRI protein.

15. The model of Claim 1, wherein said FcR protein is selected from the group consisting of an FcγRIIa protein monomer, an FcγRIIa protein dimer and structural homologues of said FcγRIIa proteins.

5 16. The model of Claim 1, wherein said FcR protein is selected from the group consisting of an FcεRI protein dimer, an FcεRI protein monomer and structural homologues of said FcεRI proteins.

10 17. The model of Claim 1, wherein said FcR protein is selected from the group consisting of an FcγRI protein dimer, an FcγRI protein monomer and structural homologues of said FcγRI protein.

15 18. The model of Claim 1, wherein said FcR protein is selected from the group consisting of an FcγRIIb protein dimer, an FcγRIIb protein monomer and structural homologues of said FcγRIIb protein.

20 19. The model of Claim 1, wherein said FcR protein is selected from the group consisting of an FcγRIIc protein dimer, an FcγRIIc protein monomer and structural homologues of said FcγRIIc protein.

25 20. The model of Claim 1, wherein said FcR protein is selected from the group consisting of an FcγRIIIb protein dimer, an FcγRIIIb protein monomer and structural homologues of said FcγRIIIb protein.

25 21. The model of Claim 1, wherein said FcR protein is selected from the group consisting of an FcαRI protein dimer, an FcαRI protein monomer and structural homologues of said FcαRI protein.

30 22. The model of Claim 1, wherein said atomic coordinates are generated by the method comprising:

 (a) providing an FcγRIIa protein in crystalline form;

 (b) generating an electron-density map of said crystalline FcγRIIa protein; and

(c) analyzing said electron-density map to produce said atomic coordinates.

23. The model of Claim 22, wherein said crystalline FcγRIIa protein is produced by a method comprising:
5 combining FcγRIIa protein with a mother liquor buffer selected from the group consisting of an acetate salt buffer and a sulphate buffer, and inducing crystal formation to produce said crystalline FcγRIIa protein.

24. The model of Claim 23, wherein said acetate
10 buffer comprises about 200 mM ammonium acetate, about 100 mM sodium citrate and about 30% PEG 4000, said buffer having a pH of about 5.6.

25. The model of Claim 23, wherein said sulphate
15 buffer comprises about 0.1 M HEPES and about 1.5 M lithium sulphate, said buffer having a pH of about 7.5.

26. The model of Claim 22, wherein said step of generating an electron-density map comprises analyzing said crystalline FcγRIIa protein by X-ray diffraction.

27. The model of Claim 22, wherein said crystalline
20 FcγRIIa protein is derivatized in Di-γ-iodo bis[ethylenediamine] di Platinum(II) nitrate prior to said X-ray diffraction.

28. The model of Claim 22, wherein said crystalline
25 FcγRIIa protein is derivatized in about 5 mM Di-γ-iodo bis[ethylenediamine] di Platinum(II) nitrate prior to said X-ray diffraction.

29. The model of Claim 1, wherein said model is a computer image generated by a computer-readable medium encoded with a set of three dimensional coordinates of said
30 three dimensional structure, wherein, using a graphical display software program, said three dimensional coordinates create an electronic file that can be visualized on a computer capable of representing said electronic file as a three dimensional image.

30. A computer-assisted method of structure based drug design of bioactive compounds, comprising:

a. providing a model of an Fc receptor (FcR) protein, wherein said model represents a three dimensional structure that substantially conforms to the atomic coordinates of Table 1;

b. designing a chemical compound using said model; and,

c. chemically synthesizing said chemical compound.

31. The method of Claim 30, wherein said method further comprises:

d. evaluating the bioactivity of said synthesized chemical compound.

32. The method of Claim 30, wherein said three dimensional structure comprises the atomic coordinates listed in Table 1.

33. The method of Claim 30, wherein said three dimensional structure is dimeric.

34. The method of Claim 30, wherein said three dimensional structure comprises the atomic coordinates listed in a table selected from the group consisting of Table 2, Table 3, Table 4, and Table 5.

35. The method of Claim 30, wherein said model comprises a computer image generated when the atomic coordinates listed in Table 1 are analyzed on a computer using a graphical display software program to create an electronic file of said image and visualizing said electronic file on a computer capable of representing said electronic file as a three dimensional image.

36. The method of Claim 30, wherein said step of designing comprises computational screening of one or more databases of chemical compounds in which the three dimensional structure of said compounds are known.

37. The method of Claim 36, further comprising interacting a compound identified by said screening step with said model by computer.

5 38. The method of Claim 30, wherein said step of designing comprises directed drug design.

39. The method of Claim 30, wherein said step of designing comprises random drug design.

40. The method of Claim 30, wherein said step of designing comprises grid-based drug design.

10 41. The method of Claim 30, wherein said step of designing comprises selecting compounds which are predicted to mimic said three dimensional structure of said FcR protein.

15 42. The method of Claim 30, wherein said step of designing comprises selecting compounds which are predicted to bind to said three dimensional structure of said FcR protein.

20 43. The method of Claim 30, wherein said bioactivity is selected from the group consisting of inhibiting binding of said FcR protein to an immunoglobulin protein, binding to said FcR protein, binding to an immunoglobulin which is capable of binding to said FcR protein, inhibiting phagocytosis of said immunoglobulin protein, inhibiting dimerization of said FcR protein, stimulating cellular
25 signal transduction through said FcR protein, and stimulating release of cytokines through said FcR protein.

30 44. The method of Claim 30, wherein said FcR protein is FcγRIIa and said bioactivity is selected from the group consisting of inhibiting binding of FcγRIIa protein to IgG, inhibiting phagocytosis of IgG, inhibiting dimerization of FcγRIIa protein, stimulating cellular signal transduction through an FcγRIIa protein, stimulating release of cytokines selected from the group consisting of IL-6 and IL-12.

35 45. The method of Claim 30, wherein said FcR protein is FcγRIIIb and said bioactivity is selected from the group

consisting of inhibiting binding of FcγRIIIb protein to IgG, inhibiting phagocytosis of IgG, inhibiting dimerization of FcγRIIIb protein, stimulating cellular signal transduction through an FcγRIIIb protein, stimulating
5 release of cytokines selected from the group consisting of IL-6 and IL-12.

46. The method of Claim 30, wherein said FcR protein is FcεRI and said bioactivity is selected from the group consisting of inhibiting binding of FcεRI protein to IgE,
10 inhibiting phagocytosis of IgE, inhibiting dimerization of FcεRI protein, stimulating cellular signal transduction through an FcεRI protein, stimulating release of histamine and serotonin by mast cells and inhibiting release of histamine and serotonin by mast cells.

15 47. A computer-assisted method of structure based drug design of bioactive compounds, comprising:

a. providing a model of an Fc receptor (FcR) protein, wherein said model represents a three dimensional structure that substantially conforms to the atomic
20 coordinates selected from the group consisting of atomic coordinates represented by Table 1; atomic coordinates represented by Table 2; atomic coordinates represented by Table 3; atomic coordinates represented by Table 4; and atomic coordinates represented by Table 5;

25 b. designing a chemical compound using said model; and,

c. chemically synthesizing said chemical compound.

48. A computer-assisted method of structure based drug design of bioactive compounds, comprising:

30 a. providing a model of a three dimensional structure of an Fc receptor (FcR) protein selected from the group consisting of FcγRIIa, FcγRIIIb and FcεRI;

b. designing a chemical compound using said model; and,

35 c. chemically synthesizing said chemical compound.

49. A three dimensional computer image of the three dimensional structure of an FcR protein.

50. The image of Claim 49, wherein said structure substantially conforms with the three dimensional coordinates selected from the group consisting of the three dimensional coordinates listed in Table 1; the three dimensional coordinates listed in Table 2; the three dimensional coordinates listed in Table 3; the three dimensional coordinates listed in Table 4; and the three dimensional coordinates listed in Table 5.

51. The image of Claim 49, wherein said computer image is generated when a set of three dimensional coordinates comprising said three dimensional coordinates are analyzed on a computer using a graphical display software program to create an electronic file of said image and visualizing said electronic file on a computer capable of representing electronic file as a three dimensional image.

52. The image of Claim 49, wherein said three dimensional computer image is represented by a two dimensional image selected from the group consisting of Fig. 4, Fig. 6, Fig. 7, Fig. 8, Fig. 9, Fig. 10, Fig. 14, Fig. 15 and Fig. 16.

53. The image of Claim 49, wherein said three dimensional computer image is used to design a therapeutic compound.

54. A computer-readable medium encoded with a set of three dimensional coordinates of an FcR protein having a three dimensional structure that substantially conforms to the atomic coordinates of Table 1, wherein, using a graphical display software program, said three dimensional coordinates create an electronic file that can be visualized on a computer capable of representing said electronic file as a three dimensional image.

55. A computer-readable medium encoded with a set of three dimensional coordinates selected from the group consisting of the three dimensional coordinates represented in Table 1, the three dimensional coordinates represented in Table 2, the three dimensional coordinates represented in Table 3, the three dimensional coordinates represented in Table 4, and the three dimensional coordinates represented in Table 5, wherein, using a graphical display software program, said three dimensional coordinates create an electronic file that can be visualized on a computer capable of representing said electronic file as a three dimensional image.

56. A model of the three dimensional structure of an FcR protein selected from the group consisting of FcγRI protein, FcγRIIb protein, FcγRIIc protein, FcγRIIb protein, FcεRI protein and FcαRI protein, said model being produced by the method comprising:

(a) providing an amino acid sequence of an FcγRIIa protein and an amino acid sequence of said FcR protein;

(b) identifying structurally conserved regions shared between said FcγRIIa amino acid sequence and said FcR protein amino acid sequence; and

(c) determining atomic coordinates for said FcR protein by assigning said structurally conserved regions of said FcR protein to a three dimensional structure using a three dimensional structure of said FcγRIIa protein which substantially conforms to the atomic coordinates represented in Table 1, to derive a model of said three dimensional structure of said FcR protein amino acid sequence.

57. The model of Claim 56, wherein said FcγRI protein amino acid sequence comprises SEQ ID NO:7; wherein said FcγRIIb protein amino acid sequence comprises SEQ ID NO:5; wherein said FcγRIIc protein amino acid sequence comprises

SEQ ID NO:6; wherein said FcγRIIIb protein amino acid sequence comprises SEQ ID NO:8; wherein said FcεRI protein amino acid sequence comprises SEQ ID NO:9; and wherein said FcαRI protein amino acid sequence comprises SEQ ID NO:13.

5 58. A therapeutic composition that, when administered to an animal, reduces IgG-mediated tissue damage, said therapeutic composition comprising an inhibitory compound that inhibits the activity of an Fcγ receptor (FcγR) protein, said inhibitory compound being identified by the
10 method comprising:

(a) providing a three dimensional structure of an FcγR protein selected from the group consisting of FcγRI, FcγRIIa, FcγRIIb, FcγRIIc and FcγRIIIb, wherein said three dimensional structure of said FcγR protein
15 substantially conforms to atomic coordinates represented by Table 1;

(b) using said three dimensional structure of said FcγR protein to design a chemical compound selected from the group consisting of a compound that inhibits
20 binding of FcγR protein to IgG, a compound that substantially mimics the three dimensional structure of FcγR protein and a compound that inhibits binding of FcγR protein with a molecule that stimulates cellular signal transduction through an FcγR protein;

25 (c) chemically synthesizing said chemical compound; and

(d) evaluating the ability of said synthesized chemical compound to reduce IgG-mediated tissue damage.

30 59. The composition of Claim 58, wherein said IgG-mediated tissue damage results from a biological response selected from the group consisting of IgG-mediated hypersensitivity, IgG-mediated recruitment of inflammatory cells, and IgG-mediated release of inflammatory modulators.

60. The composition of Claim 58, wherein said structure substantially conforms with the atomic coordinates represented in Table 1.

5 61. The composition of Claim 58, wherein said chemical compound is selected from the group consisting of an inorganic compound and an organic compound.

62. The composition of Claim 58, wherein said chemical compound is selected from the group consisting of oligonucleotides, peptides, peptidomimetic compounds and
10 small organic molecules.

63. The composition of Claim 58, wherein said chemical compound is selected from the group consisting of an analog of said FcγR protein, a substrate analog of said FcγR protein and a peptidomimetic compound of said FcγR
15 protein.

64. The composition of Claim 58, wherein said composition further comprises a component selected from the group consisting of an excipient, an adjuvant, and a carrier.

20 65. A therapeutic composition that, when administered to an animal, enhances IgG-mediated responses, said therapeutic composition comprising a stimulatory compound that stimulates the activity of an Fcγ receptor (FcγR) protein, said stimulatory compound being identified by the
25 method comprising:

(a) providing a three dimensional structure of an FcγR protein selected from the group consisting of FcγRI, FcγRIIa, FcγRIIb, FcγRIIc and FcγRIIIb, wherein said three dimensional structure of said FcγR protein
30 substantially conforms to atomic coordinates represented by Table 1;

(b) using said three dimensional structure of said FcγR protein to design a chemical compound selected from the group consisting of a compound that stimulates
35 binding of FcγR protein to IgG, a compound that

substantially mimics the three dimensional structure of FcγR protein and a compound that stimulates binding of FcγR protein with a molecule that stimulates cellular signal transduction through an FcγR protein;

5 (c) chemically synthesizing said chemical compound; and

 (d) evaluating the ability of said synthesized chemical compound to enhance IgG-mediated responses.

66. A therapeutic composition that, when administered
10 to an animal, reduces IgE-mediated responses, said therapeutic composition comprising an inhibitory compound that inhibits the activity of an Fcε receptor I (FcεRI) protein, said inhibitory compound being identified by the method comprising:

15 (a) providing a three dimensional structure of an FcεRI protein, wherein said three dimensional structure of said FcεRI protein substantially conforms to the atomic coordinates selected from the group consisting of the atomic coordinates represented by Table 1, the atomic
20 coordinates represented by Table 2, the atomic coordinates represented by Table 3, the atomic coordinates represented by Table 4 and the atomic coordinates represented by Table 5;

 (b) using said three dimensional structure of
25 said FcεRI protein to design a chemical compound selected from the group consisting of a compound that inhibits binding of FcεRI protein to IgE, a compound that substantially mimics the three dimensional structure of FcεRI protein and a compound that inhibits binding of FcεRI
30 protein with a molecule that stimulates cellular signal transduction through an FcεRI protein;

 (c) chemically synthesizing said chemical compound; and

 (d) evaluating the ability of said synthesized
35 chemical compound to reduce IgE-mediated responses.

67. The composition of Claim 66, wherein said IgE-mediated response results from a biological response selected from the group consisting of IgE-mediated hypersensitivity, IgE-mediated recruitment of inflammatory cells, and IgE-mediated release of inflammatory modulators.

68. The composition of Claim 66, wherein said structure comprises the atomic coordinates represented in Table 3.

69. The composition of Claim 66, wherein said structure comprises the atomic coordinates represented in Table 4.

70. The composition of Claim 66, wherein said chemical compound is selected from the group consisting of an inorganic compound and an organic compound.

71. The composition of Claim 66, wherein said chemical compound is selected from the group consisting of oligonucleotides, peptides, peptidomimetic compounds and small organic molecules.

72. The composition of Claim 66, wherein said chemical compound is selected from the group consisting of an analog of said FcεR protein, a substrate analog of said FcεRI protein and a peptidomimetic compound of said FcεRI protein.

73. The composition of Claim 66, wherein said composition further comprises a component selected from the group consisting of an excipient, an adjuvant, and a carrier.

74. A therapeutic composition that, when administered to an animal, enhances IgE-mediated responses, said therapeutic composition comprising a stimulatory compound that stimulates the activity of an Fcε receptor I (FcεRI) protein, said stimulatory compound being identified by the method comprising:

(a) providing a three dimensional structure of an FcεRI protein, wherein said three dimensional structure

of said FcεRI protein substantially conforms to the atomic coordinates selected from the group consisting of the atomic coordinates represented by Table 1, the atomic coordinates represented by Table 2, the atomic coordinates represented by Table 3, the atomic coordinates represented by Table 4 and the atomic coordinates represented by Table 5;

(b) using said three dimensional structure of said FcεRI protein to design a chemical compound selected from the group consisting of a compound that stimulates binding of FcεRI protein to IgE, a compound that substantially mimics the three dimensional structure of FcεRI protein and a compound that stimulates binding of FcεRI protein with a molecule that stimulates cellular signal transduction through an FcεRI protein;

(c) chemically synthesizing said chemical compound; and

(d) evaluating the ability of said synthesized chemical compound to enhance IgE-mediated responses.

75. A method to determine a three dimensional structure of an FcR protein, said method comprising

(a) providing an amino acid sequence of an FcR protein selected from the group consisting of FcγRI protein, FcγRIIb protein, FcγRIIc protein, FcγRIIIb protein, FcεRI protein and FcαRI protein, wherein the three dimensional structure of said FcR protein is not known;

(b) analyzing the pattern of folding of said amino acid sequence in a three dimensional conformation by fold recognition; and

(c) comparing said pattern of folding of said FcR protein amino acid sequence with the three dimensional structure of FcγRIIa protein to determine the three dimensional structure of said FcR protein, wherein said three dimensional structure of said FcγRIIa protein

substantially conforms to the atomic coordinates represented in Table 1.

76. A method to derive a model of the three dimensional structure of an FcR protein, said method comprising the steps of:

- (a) providing an amino acid sequence of an FcγRIIa protein and an amino acid sequence of an FcR protein;
- (b) identifying structurally conserved regions shared between said FcγRIIa amino acid sequence and said FcR protein amino acid sequence;
- (c) determining atomic coordinates for said target structure by assigning said structurally conserved regions of said FcR protein to a three dimensional structure using a three dimensional structure of an FcγRIIa protein based on atomic coordinates that substantially conform to the atomic coordinates represented in Table 1 to derive a model of the three dimensional structure of said FcR protein amino acid sequence.

77. The method of Claim 76, further comprising assigning atomic coordinates for side chains of said FcR protein by determining sterically allowable positions using a library of rotamers.

78. A method to derive a three dimensional structure of a crystallized FcR protein, said method comprising the steps of:

- (a) comparing the Patterson function of a crystallized FcR protein with the Patterson function of crystalline FcγRIIa protein to produce an electron-density map of said crystallized FcR protein; and
- (b) analyzing said electron-density map to produce said three dimensional structure of said crystallized FcR protein.

79. The method of Claim 78, further comprising the step of electronically simulating said three dimensional

structure of said crystallized FcR protein to derive a computer image of said three dimensional structure of said crystallized FcR protein.

80. The method of Claim 78, further comprising the step of rotating said Patterson function of said crystallized FcR protein on said Patterson function of said crystalline FcγRIIa protein to determine the correct orientation of said crystallized FcR protein in a crystal of said crystallized FcR protein to identify the initial phases of said crystallized FcR protein.

81. A composition comprising FcγRIIa protein in a crystalline form.

82. A computer for producing a three-dimensional model of a molecule or molecular structure, wherein said molecule or molecular structure comprises a three dimensional structure defined by atomic coordinates of an FcR protein, according to a table selected from the group consisting of Table 1, Table 2, Table 3, Table 4 and Table 5, or a three-dimensional model of a homologue of said molecule or molecular structure, wherein said homologue comprises a three dimensional structure that has an average root-mean-square deviation (RMSD) of less than about 1.5Å for the backbone atoms in secondary structure elements in each domain of said FcR protein, wherein said computer comprises:

(a) a computer-readable medium encoded with said atomic coordinates of an FcR protein, according to a table selected from the group consisting of Table 1, Table 2, Table 3, Table 4 and Table 5, to create an electronic file;

(b) a working memory for storing a graphical display software program for processing said electronic file;

(c) a processor coupled to said working memory and to said computer-readable medium which is capable of representing said electronic file as said three dimensional model; and,

AMENDED SHEET
IPEA/10

(12) (d) a display coupled to said processor for visualizing said three dimensional model.

83. The computer of Claim 82, wherein said molecule or molecular structure is dimeric.

5 84. The computer of Claim 82, wherein at least about 50% of said three dimensional structure of said homologue has an average root-mean-square deviation (RMSD) of less than about 1.5Å for the backbone atoms in secondary structure elements in each domain of said FcR protein.

10 85. The computer of Claim 82, wherein at least about 50% of common amino acid side chains between said three dimensional structure of said homologue and a said three dimensional structure defined by said atomic coordinates of an FcR protein have an average root-mean-square deviation (RMSD) of less than about 1.5Å.

15 86. The computer of Claim 82, wherein said FcR protein comprises an amino acid sequence selected from the group consisting of: an amino acid sequence selected from the group consisting of SEQ ID NO:3, SEQ ID NO:5, SEQ ID NO:6, SEQ ID NO:7, SEQ ID NO:8, SEQ ID NO:9, SEQ ID NO:10, SEQ ID NO:11, SEQ ID NO:12, SEQ ID NO:13.

20 87. The computer of Claim 82, wherein said FcR protein is selected from the group consisting of FcγRI protein, FcγRIIa protein, FcγRIIb protein, FcγRIIc protein, FcγRIII protein, FcεRI protein and FcαRI protein.