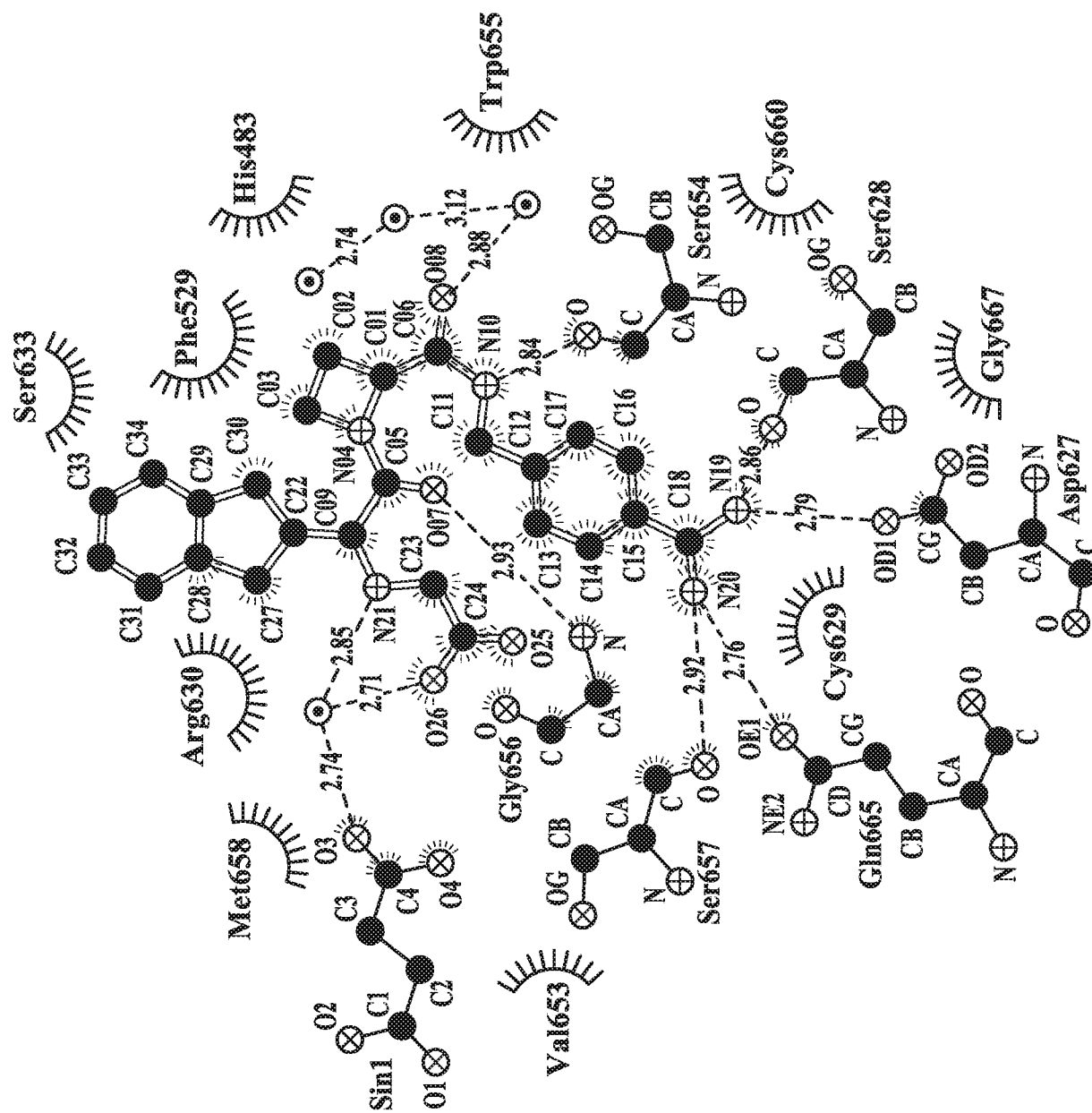




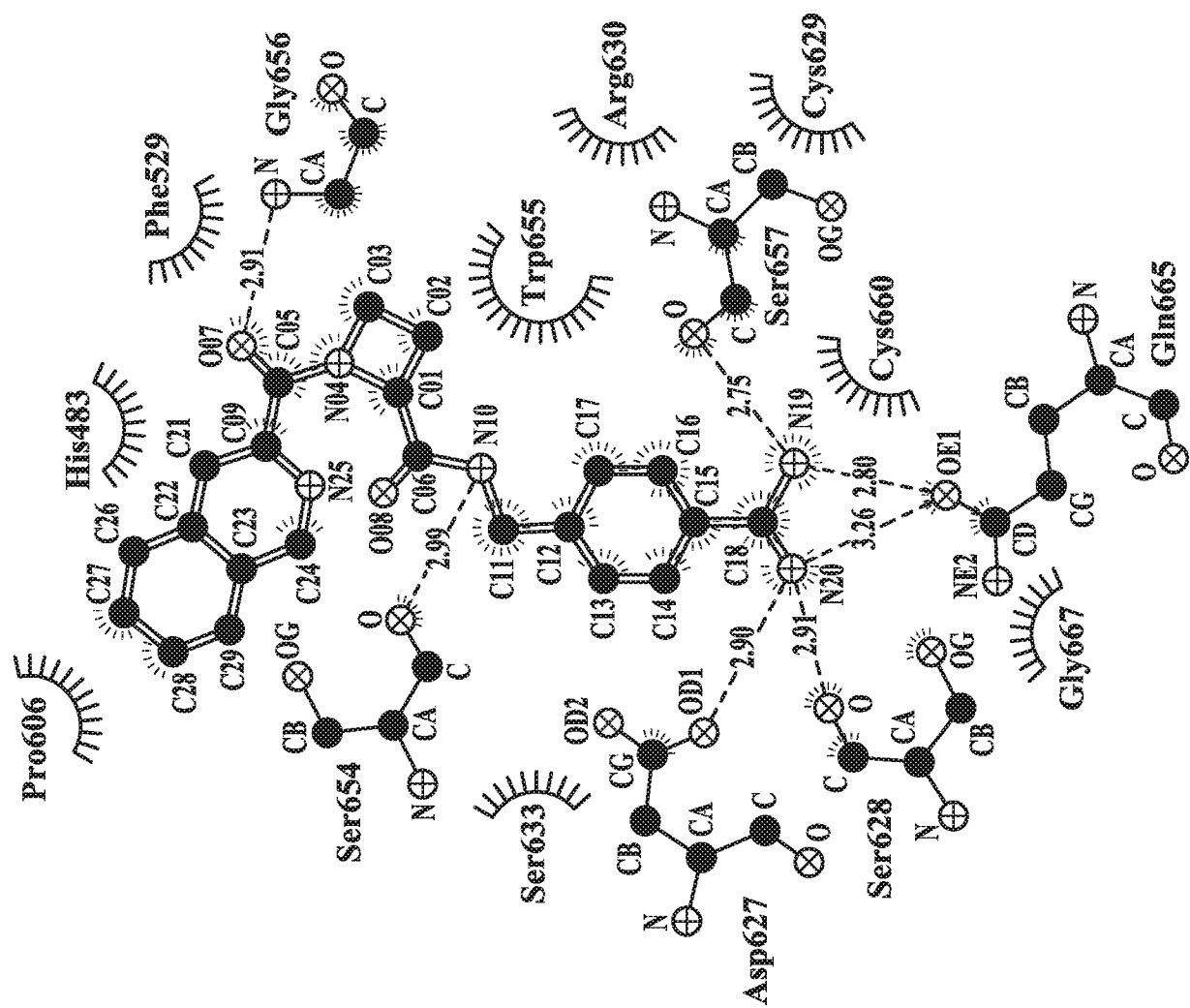


FIG.2

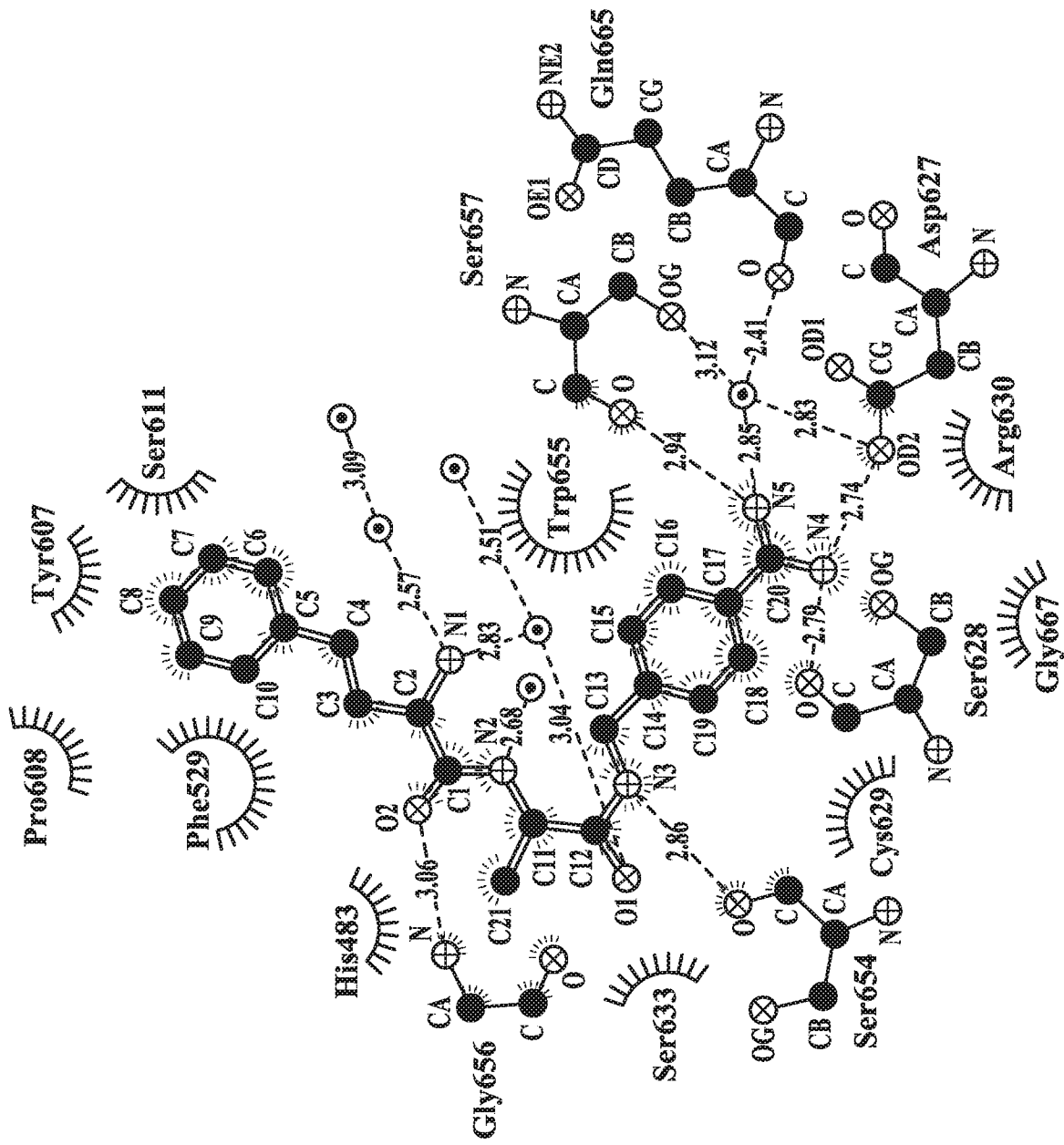


FIG.3

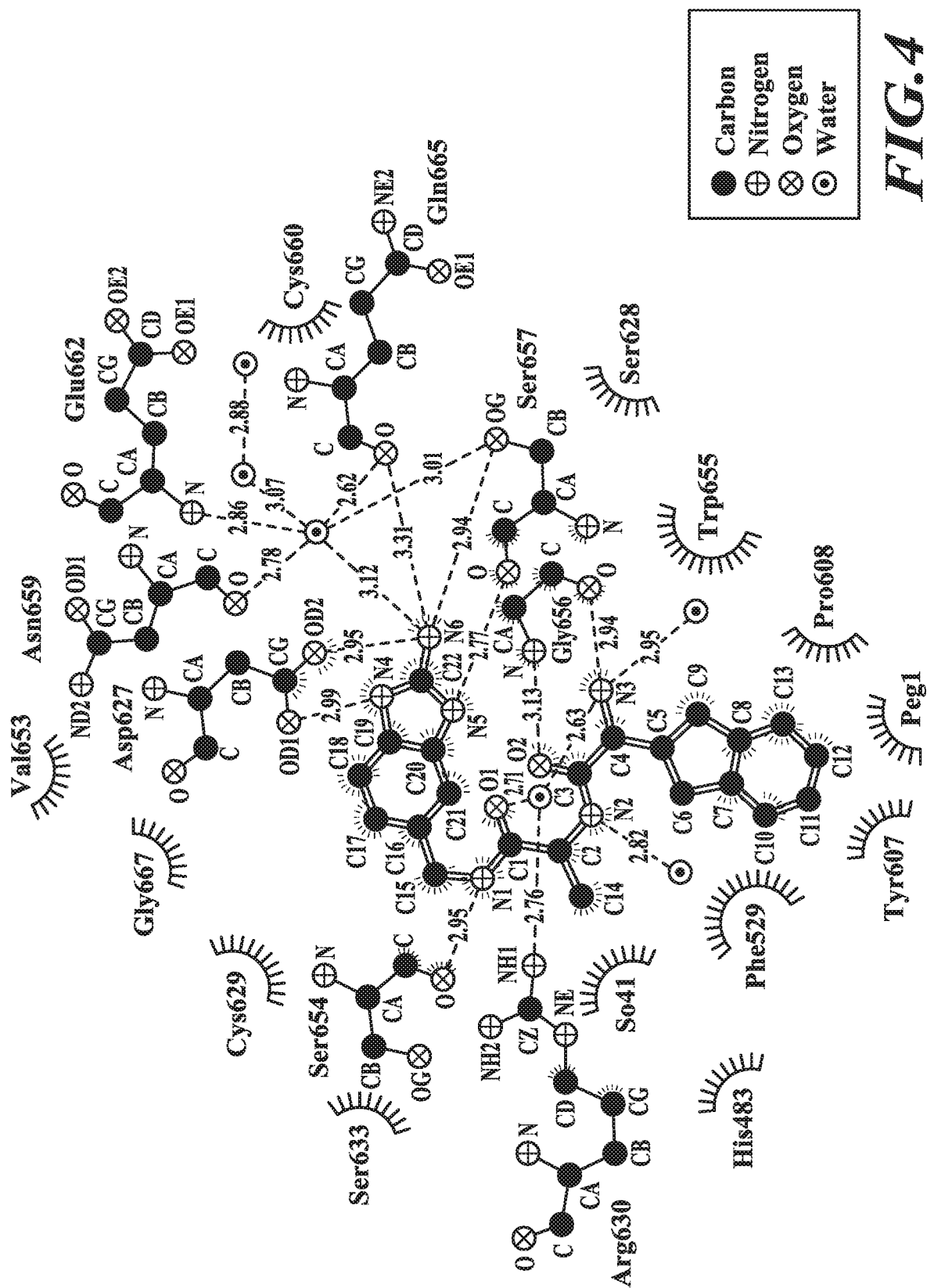
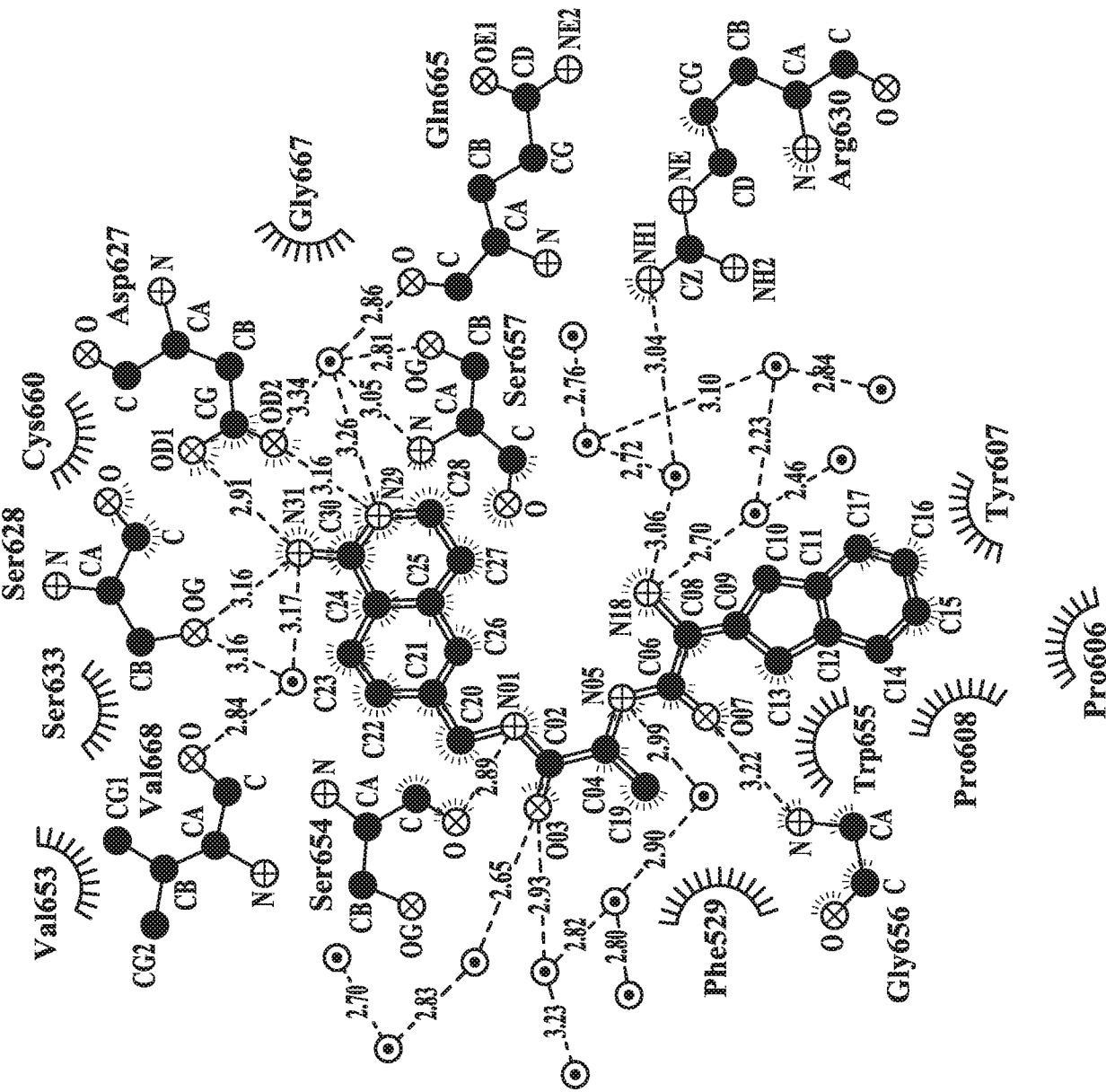


FIG. 4



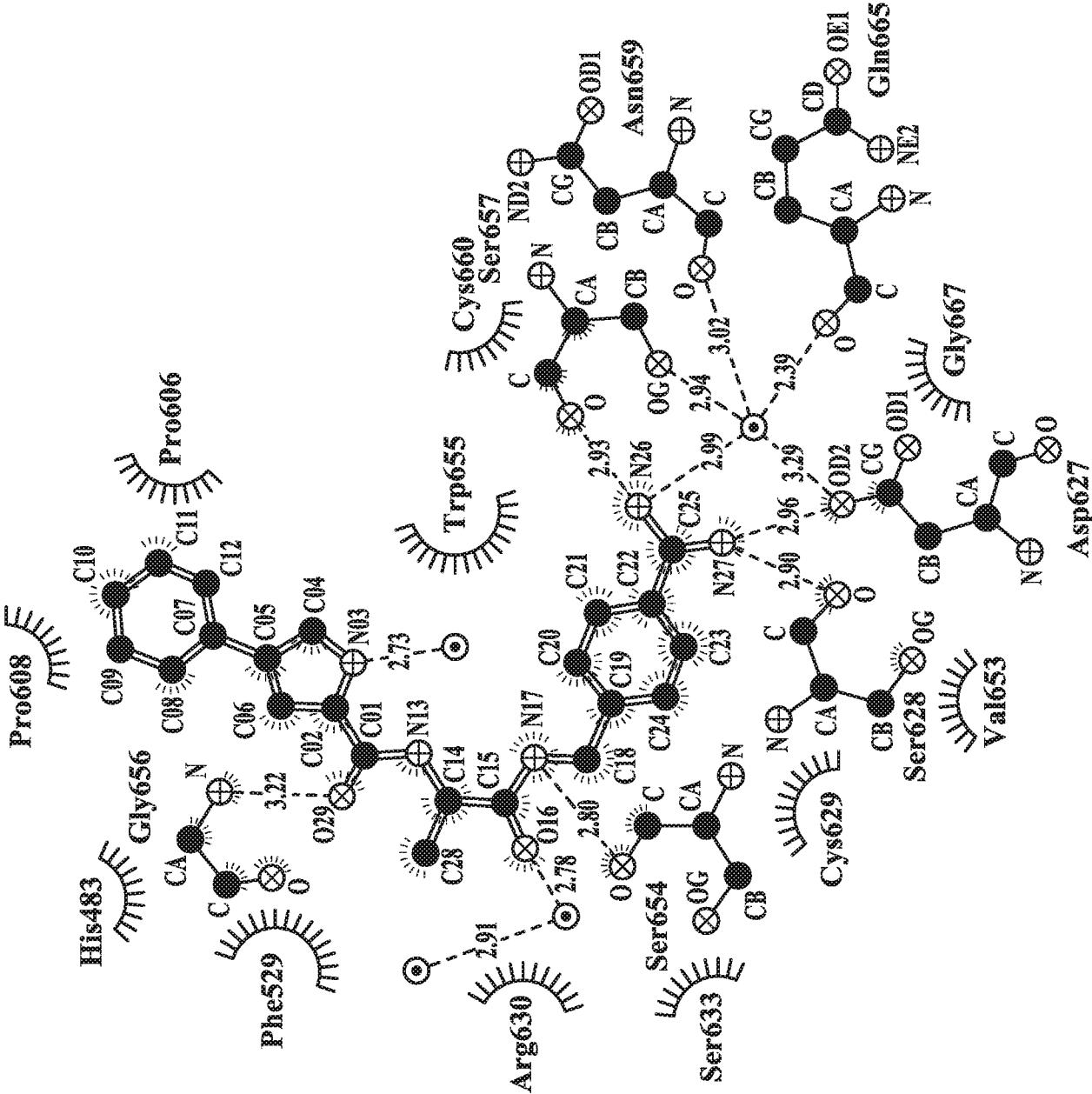
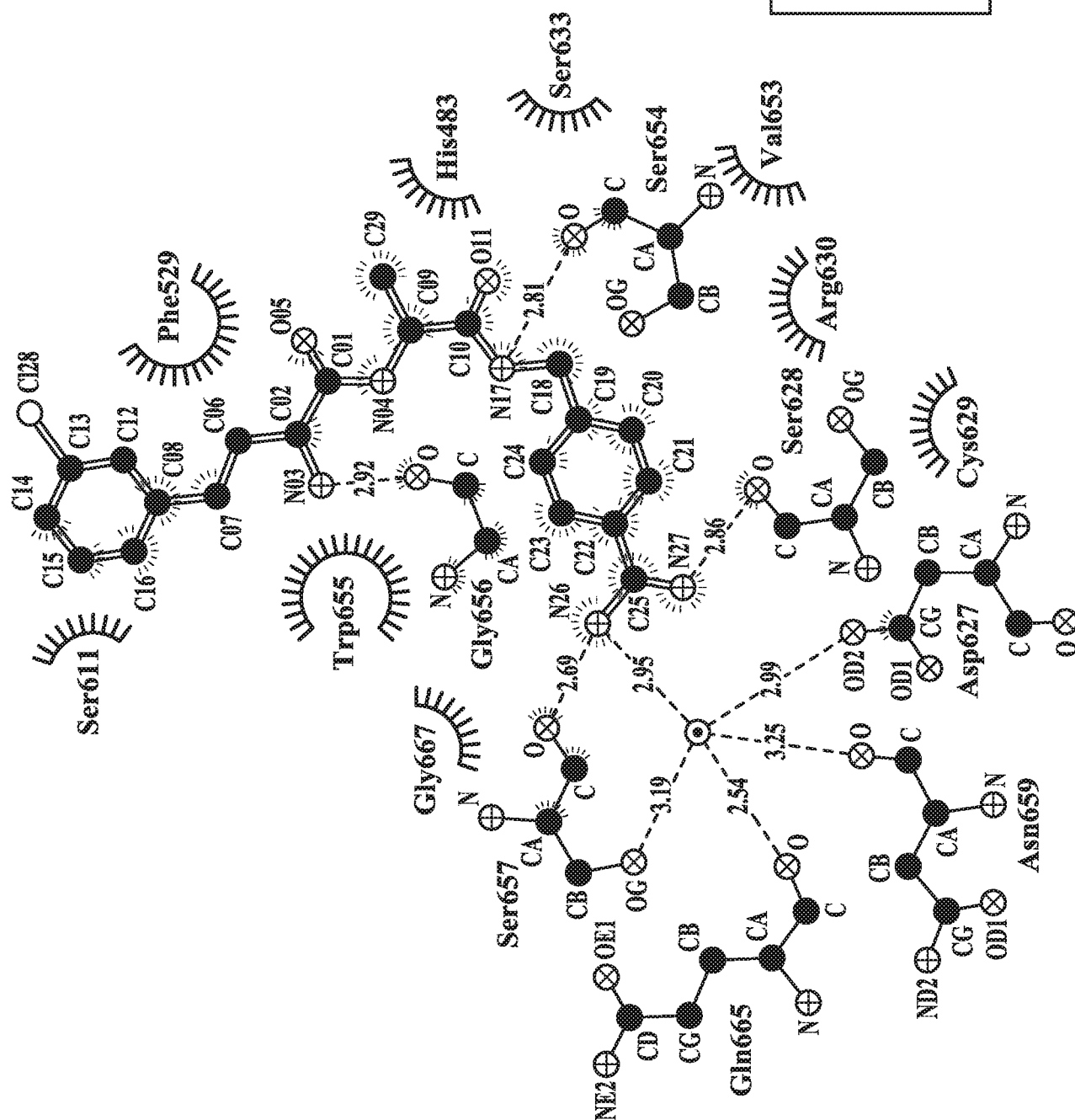


FIG. 6



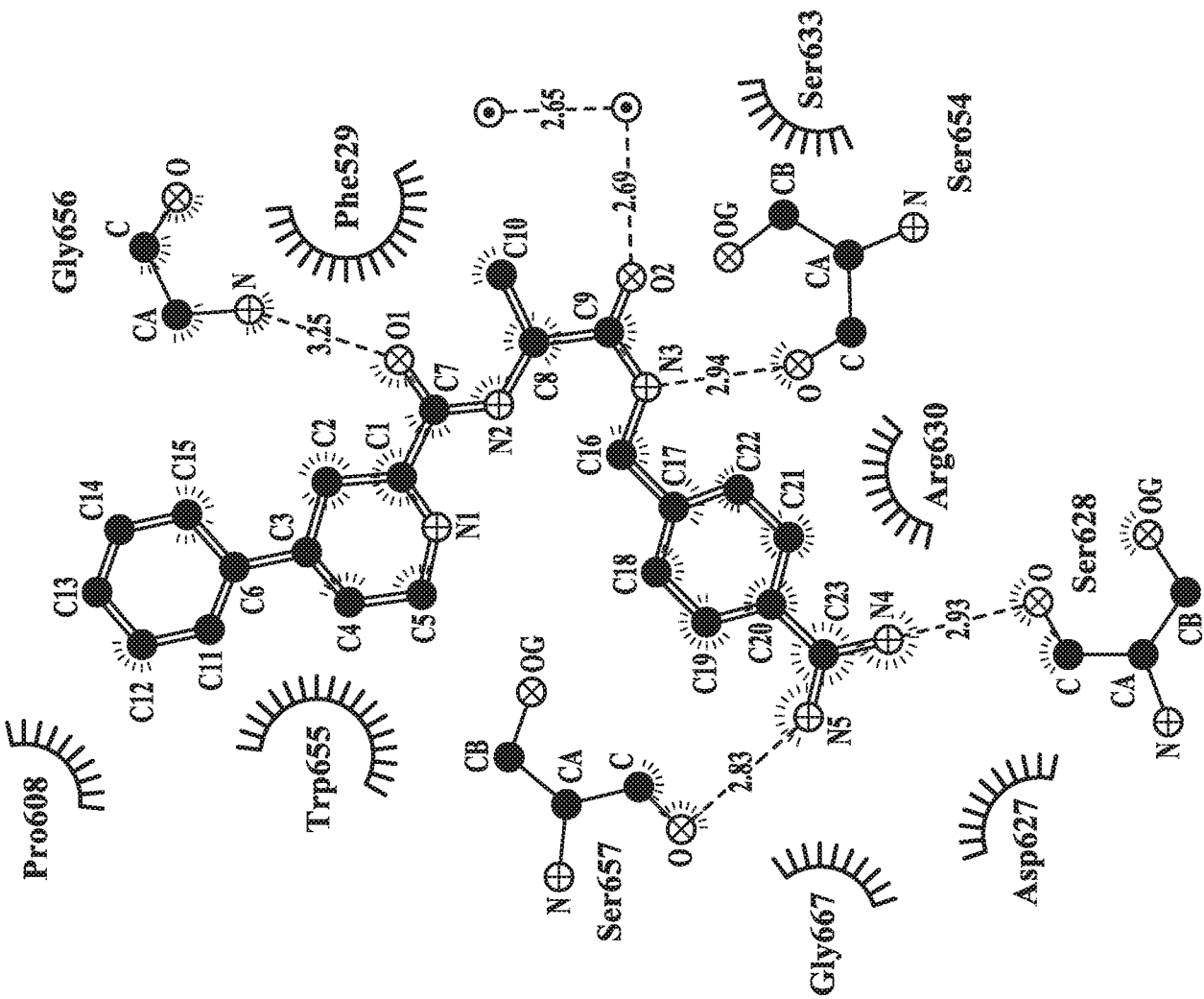


FIG.8

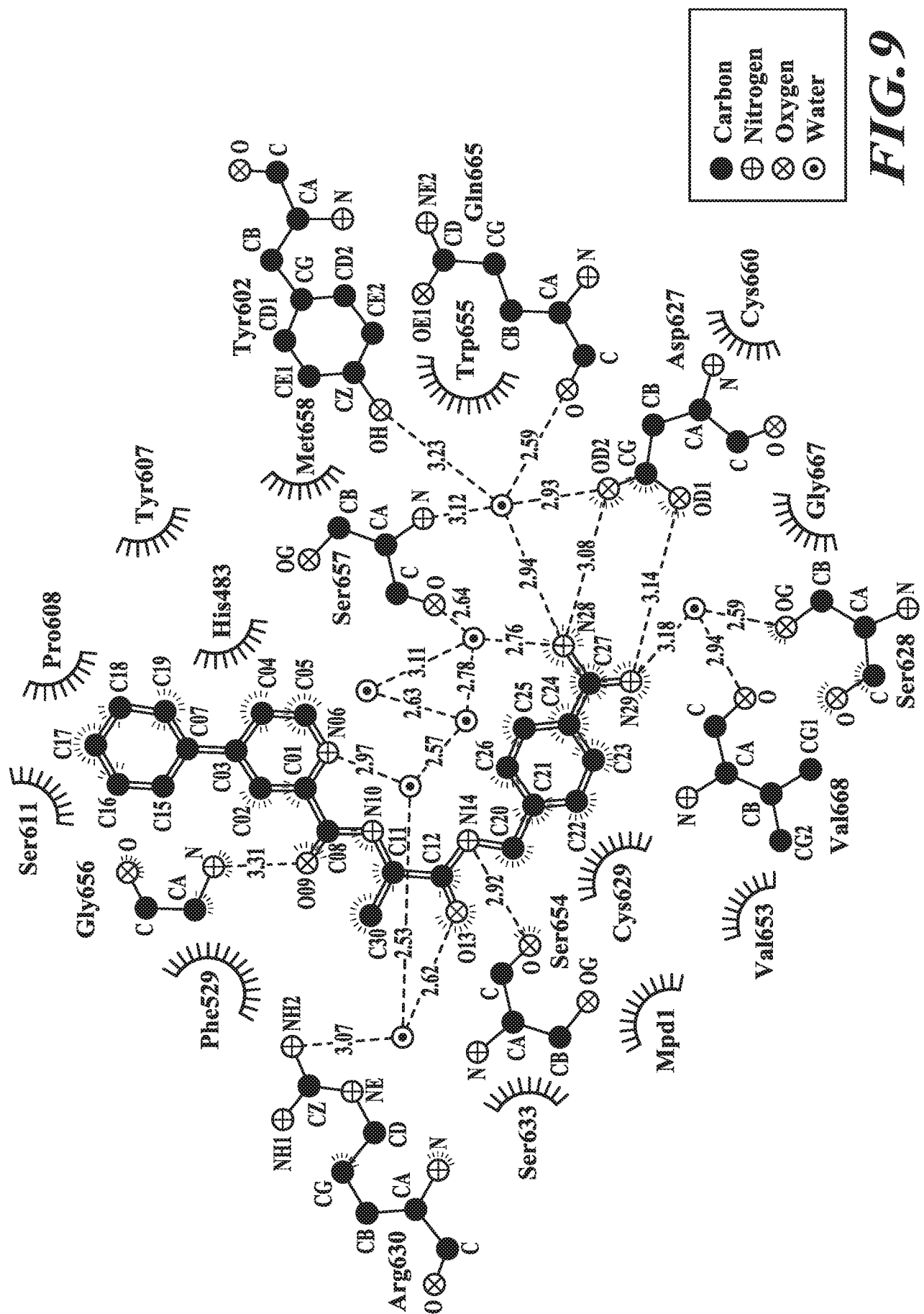


FIG. 9

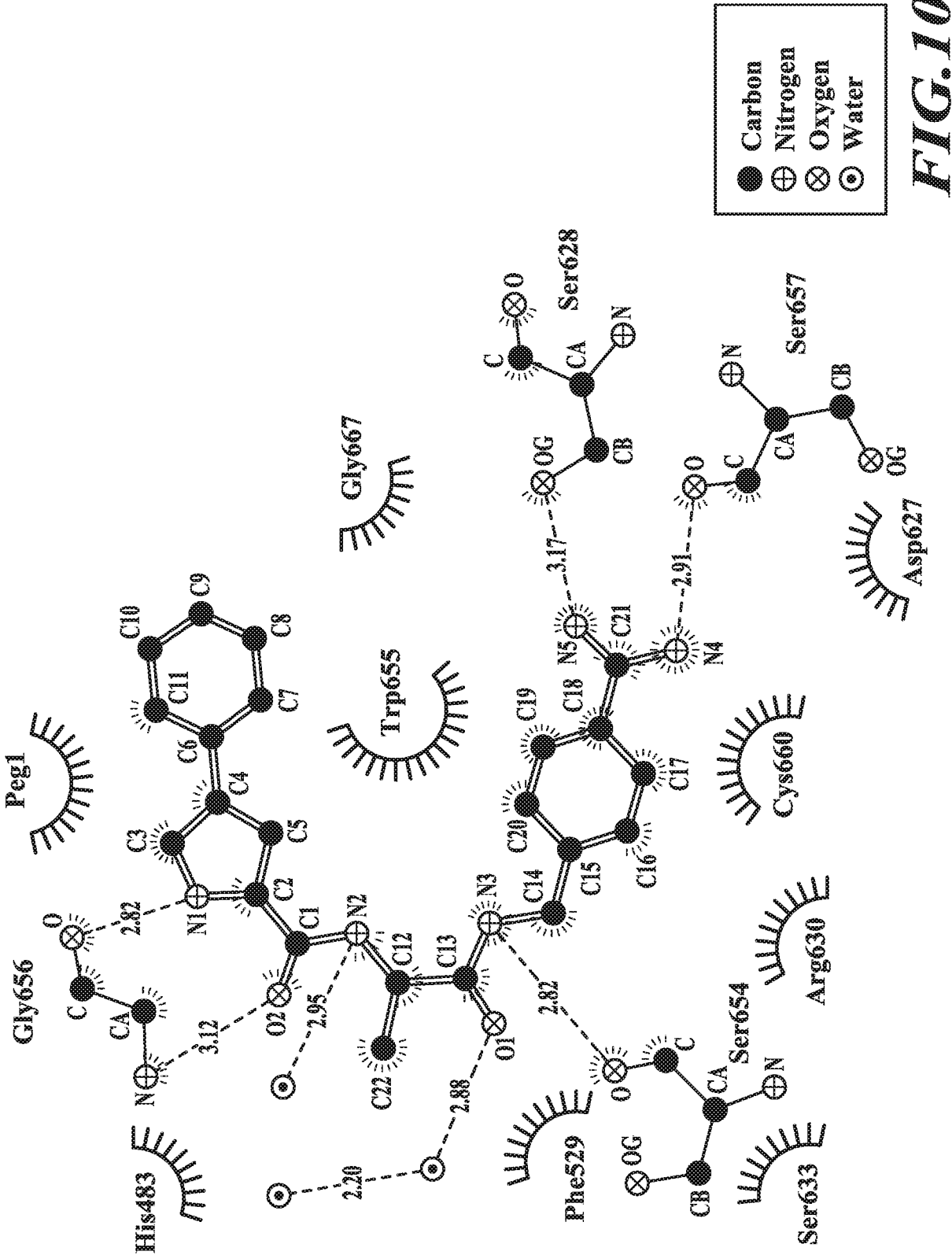
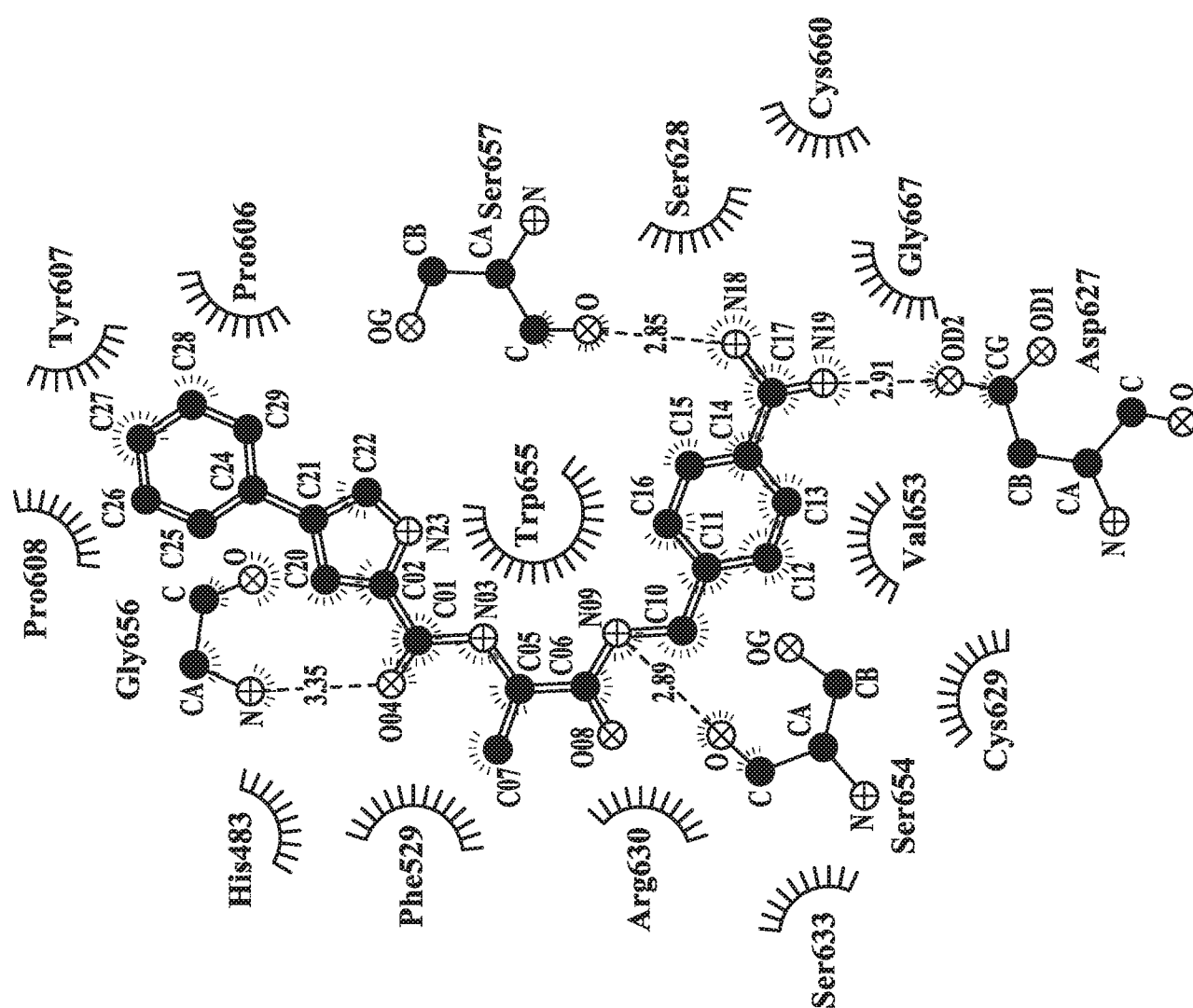


FIG.10



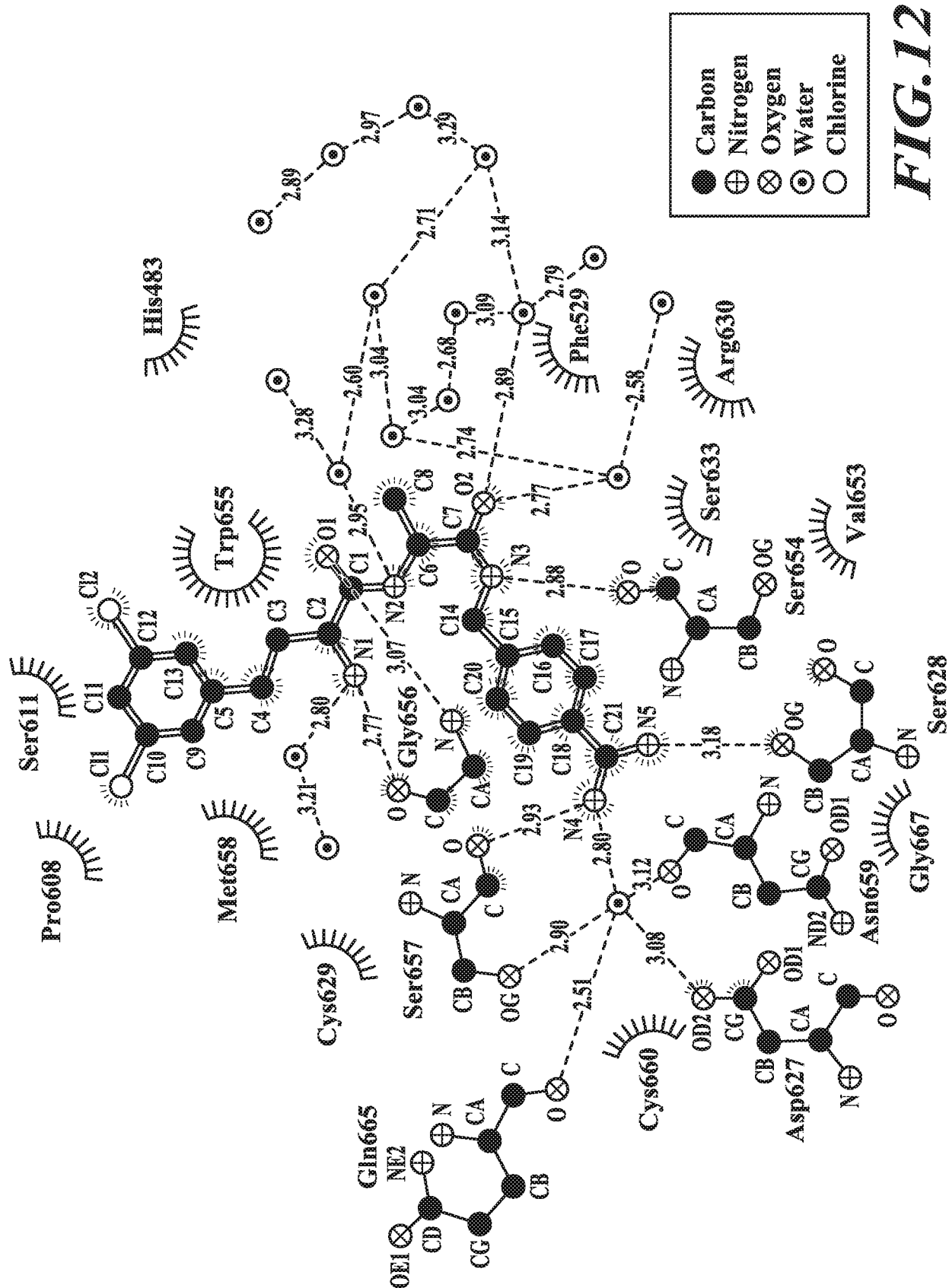


FIG. 12

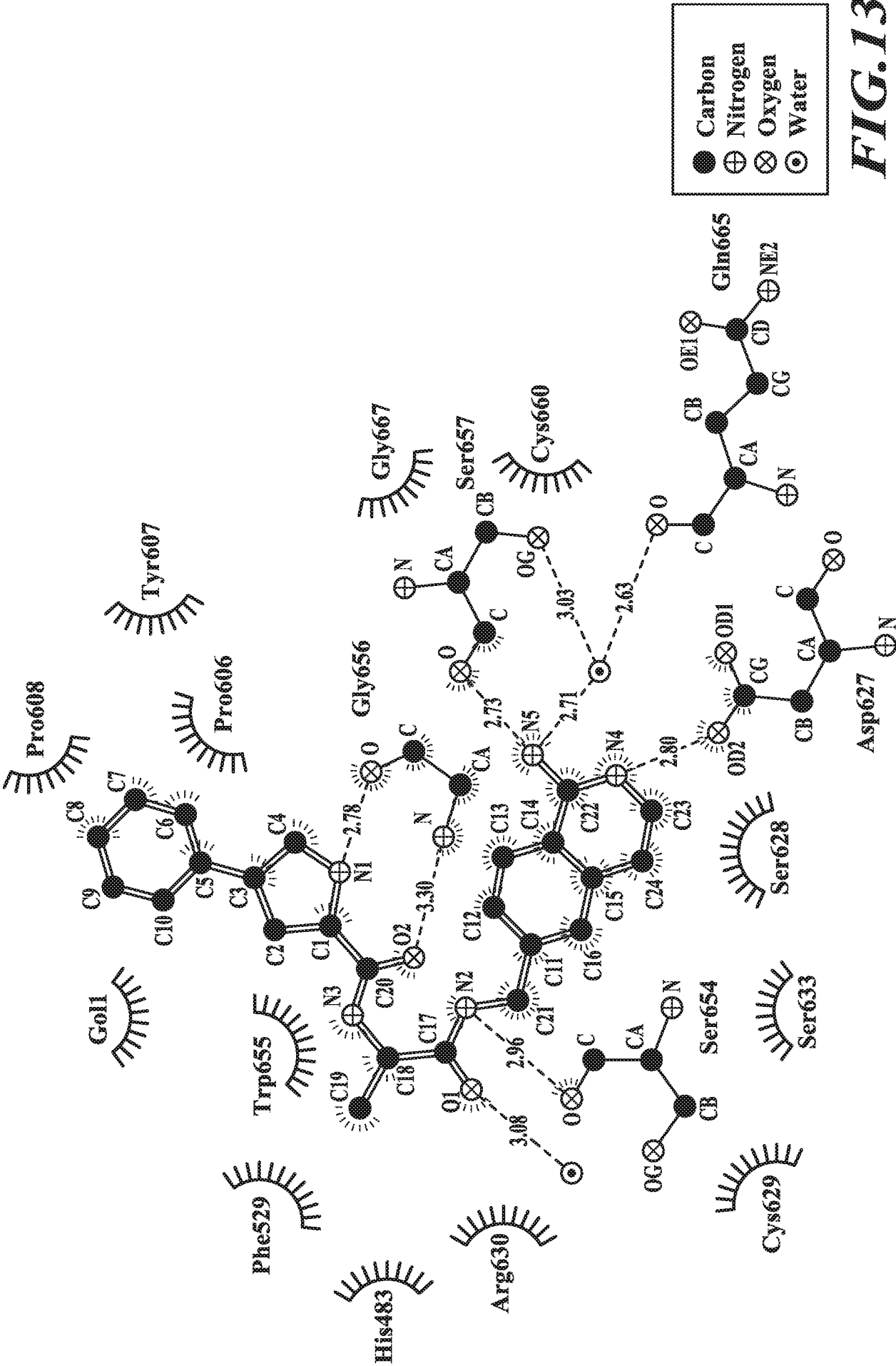
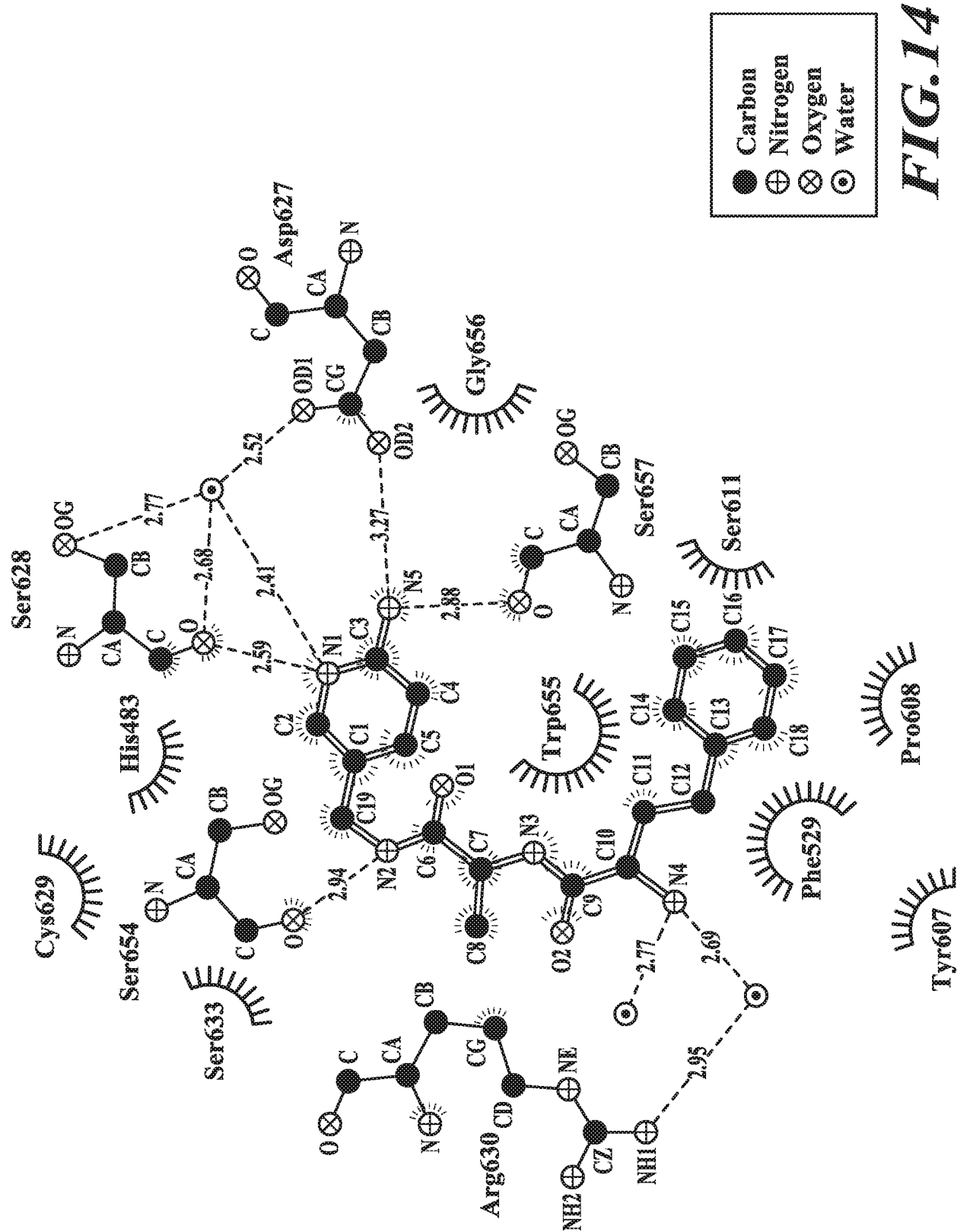


FIG.13



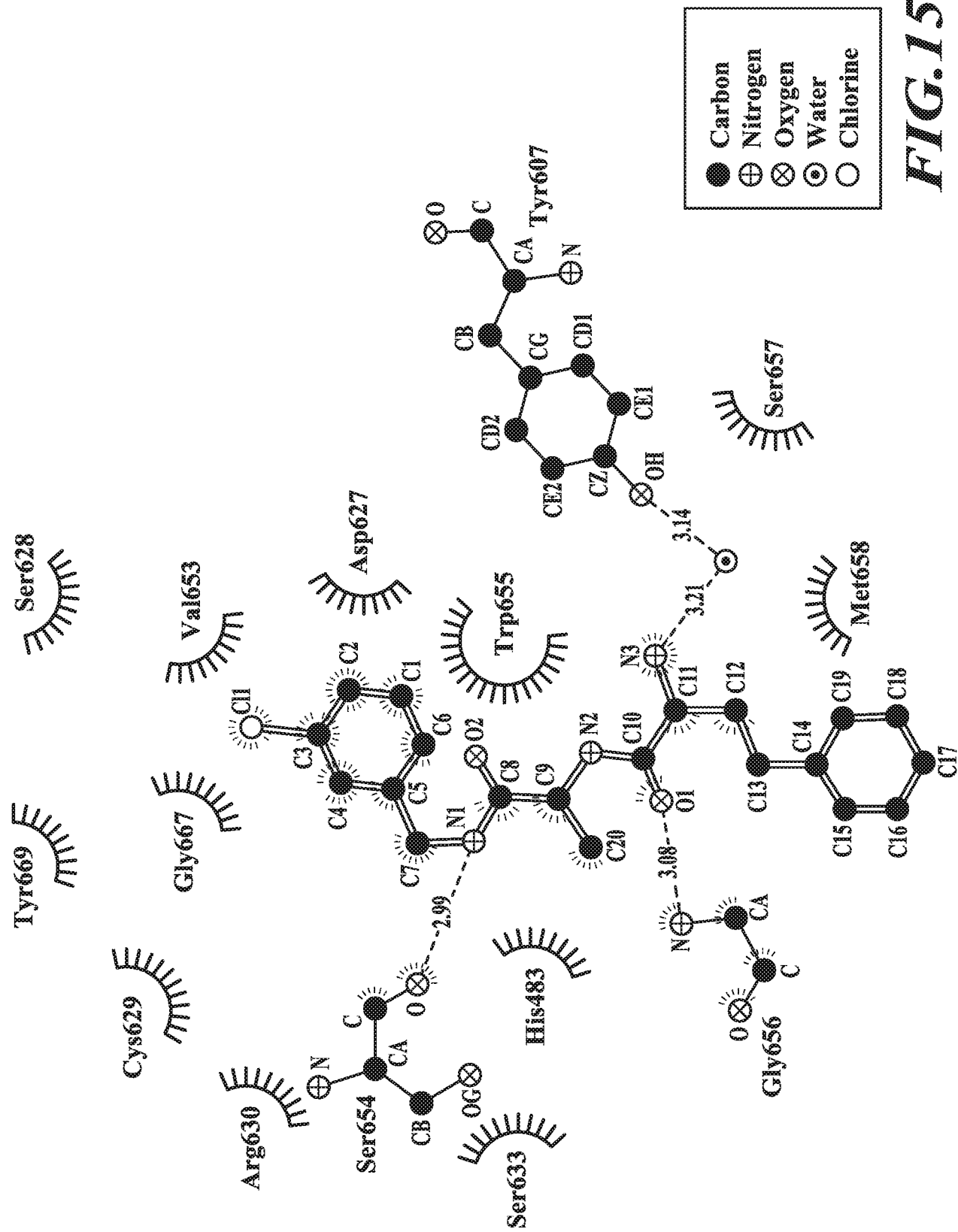
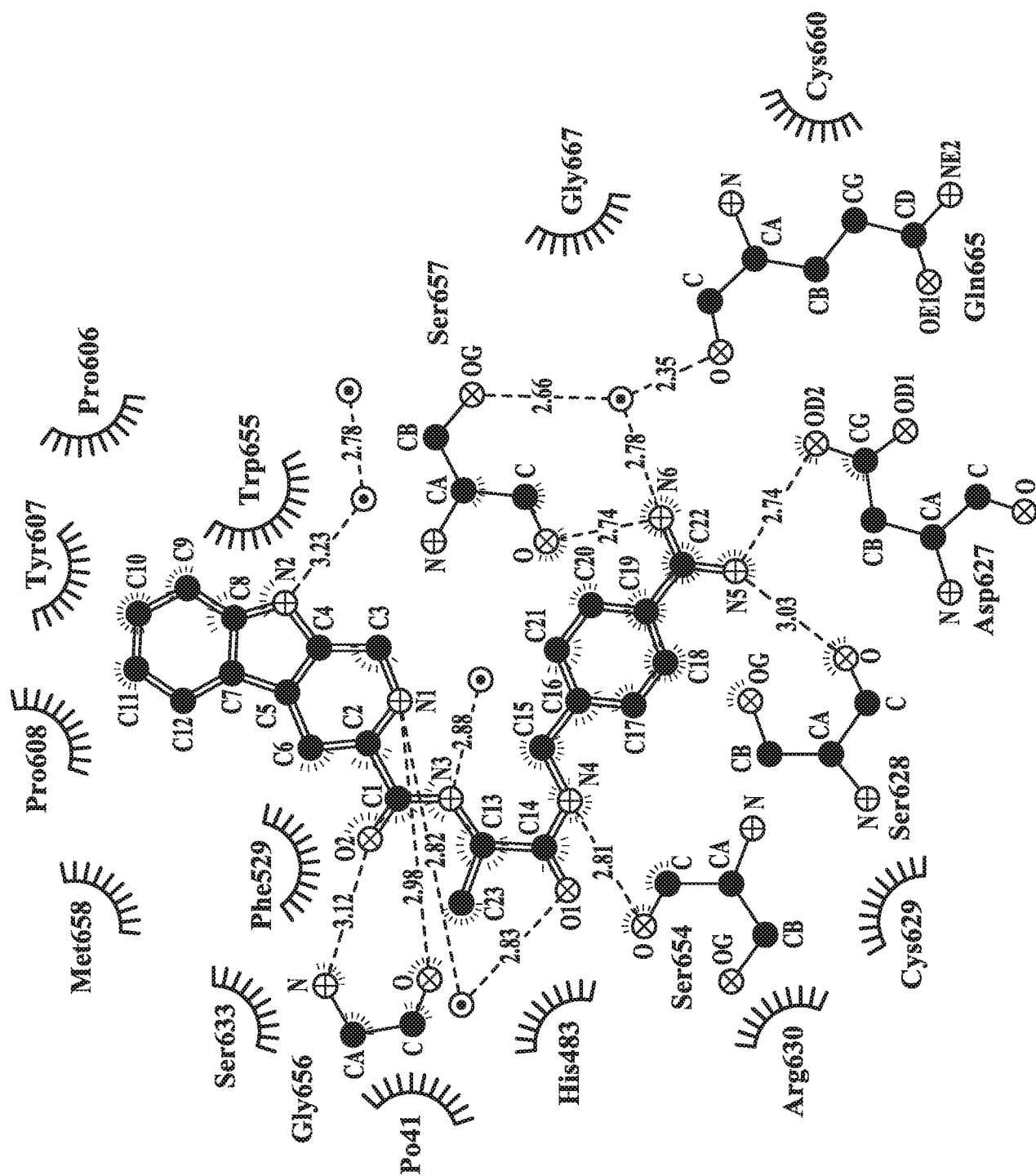


FIG.15



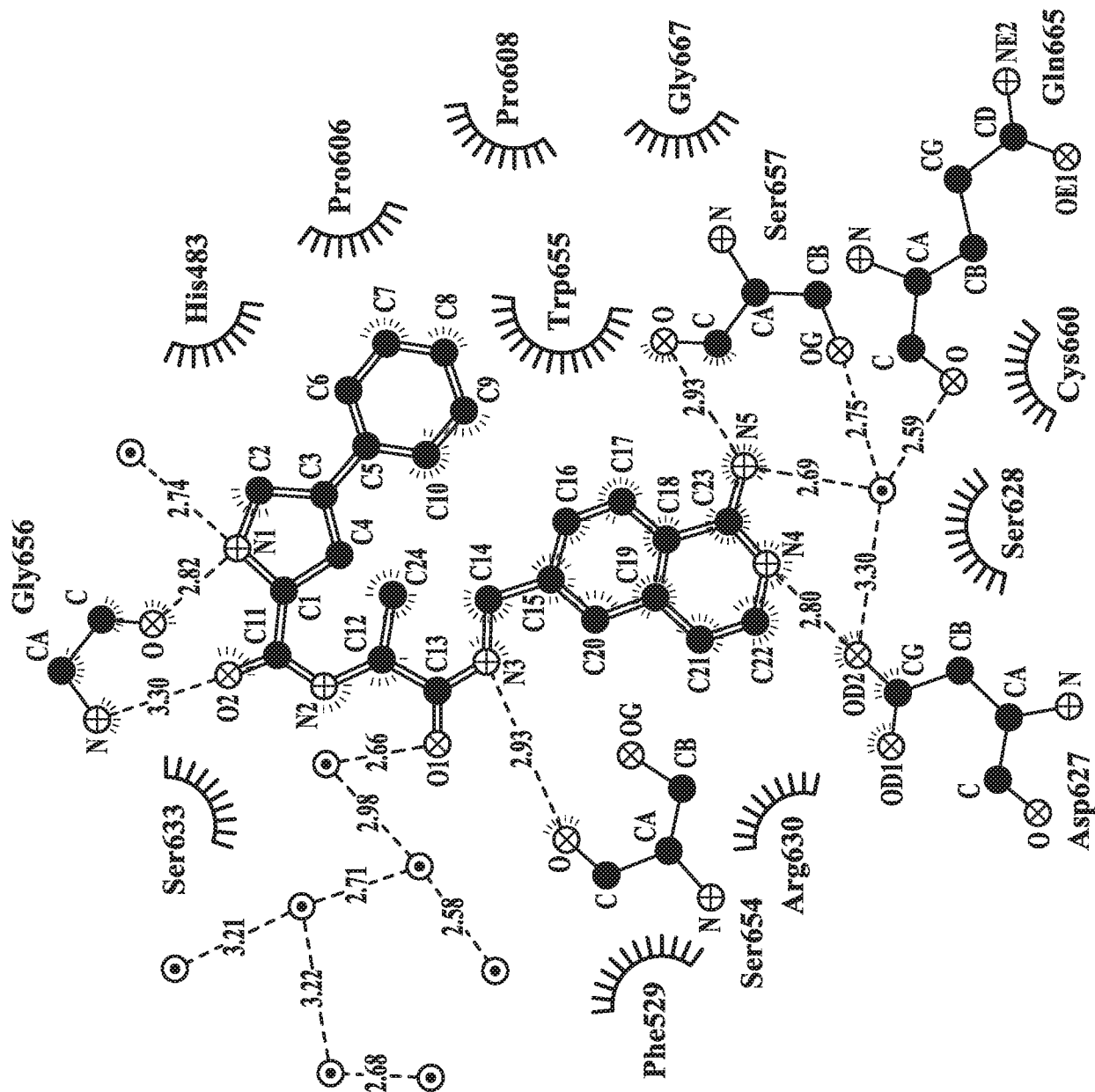
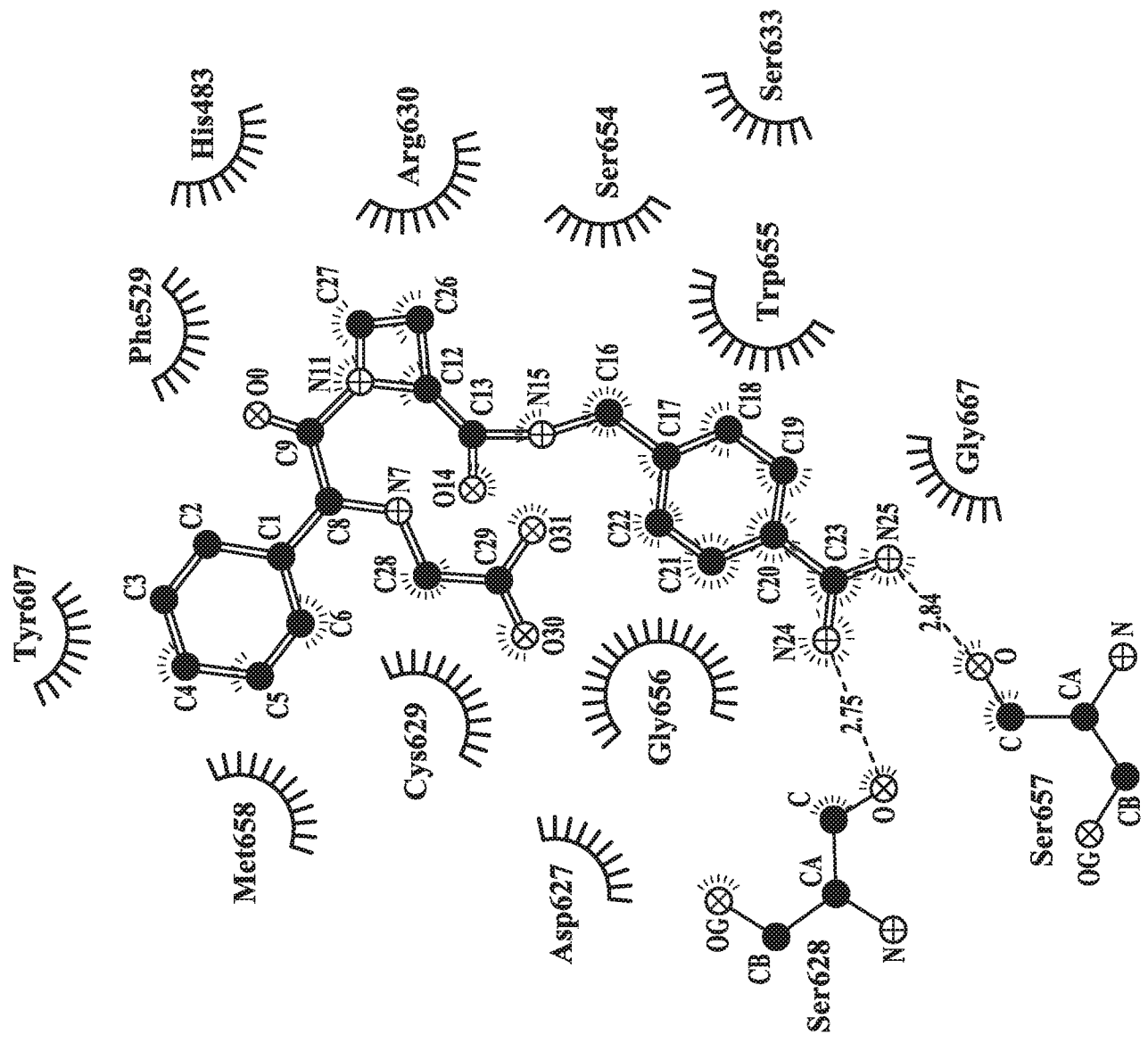
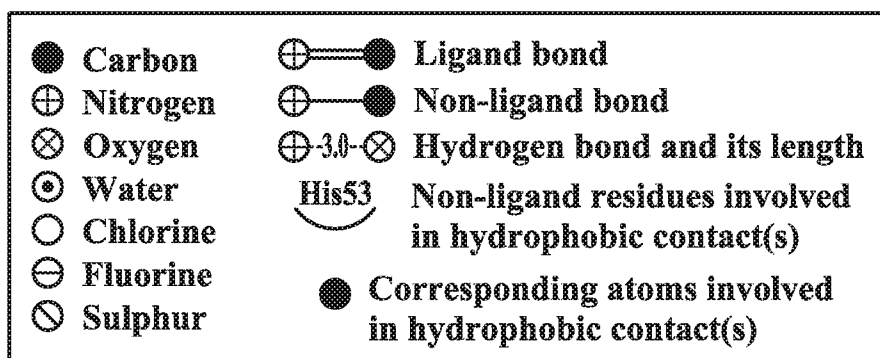
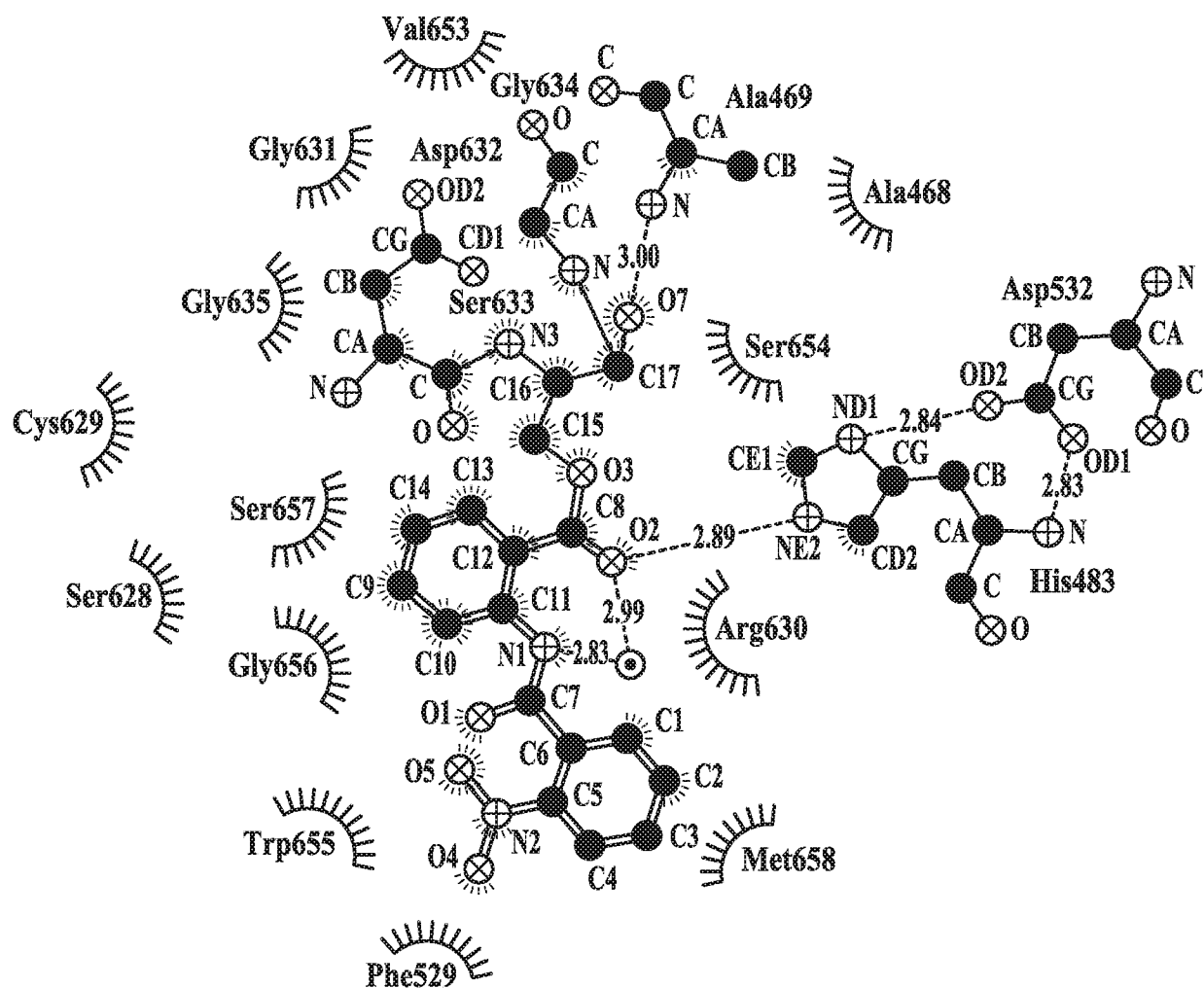


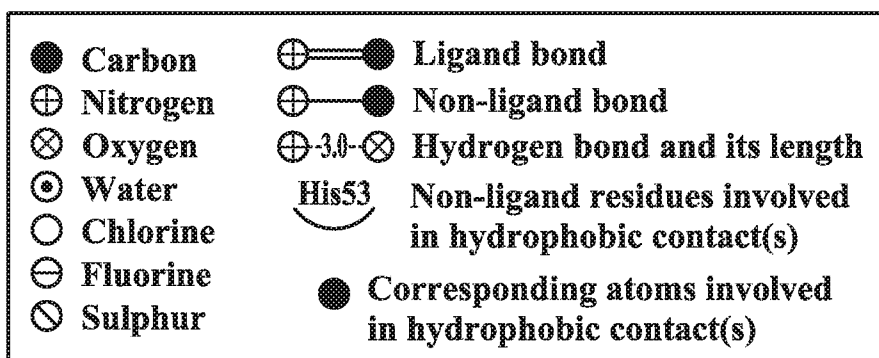
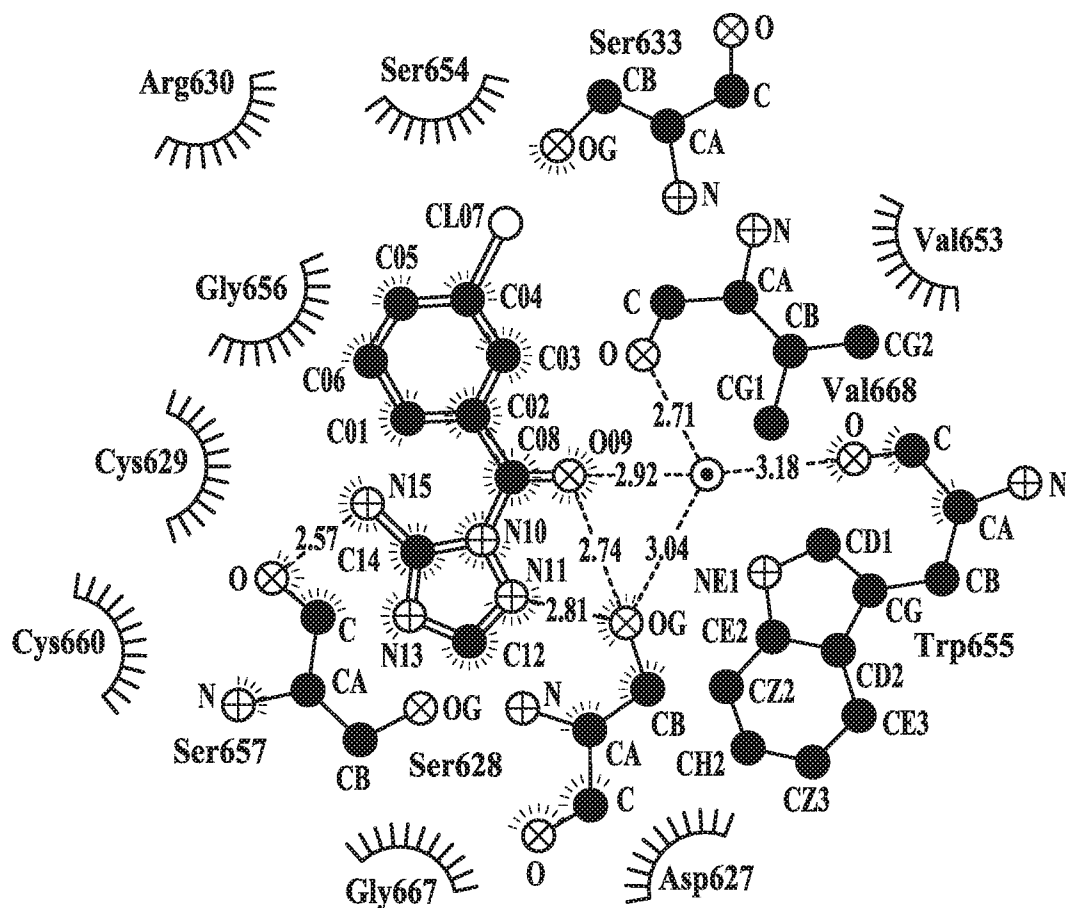
FIG. 17



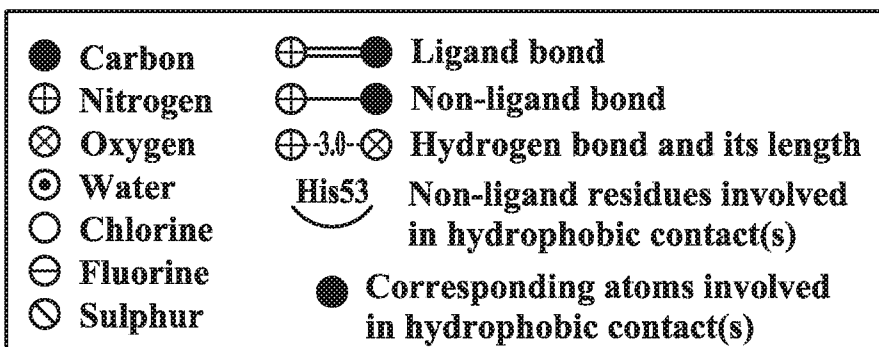
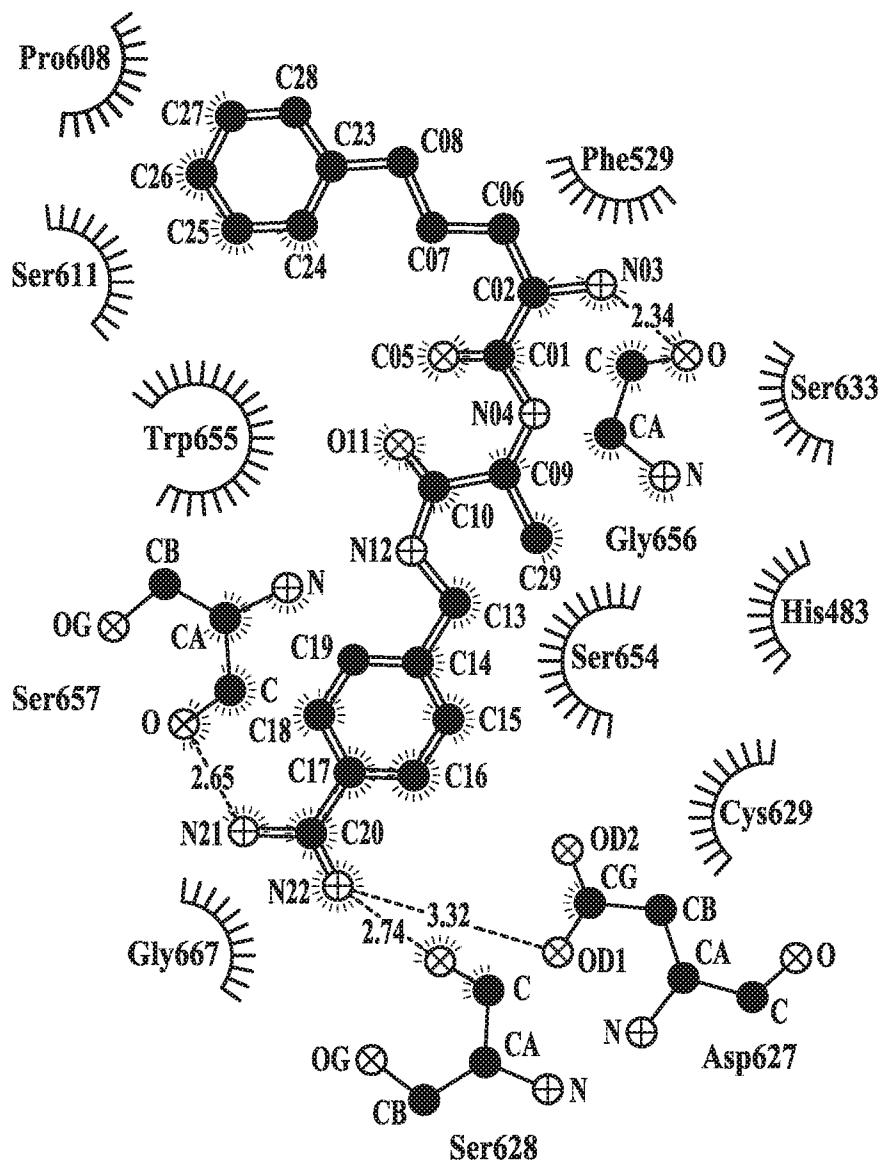
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**FIG.19**

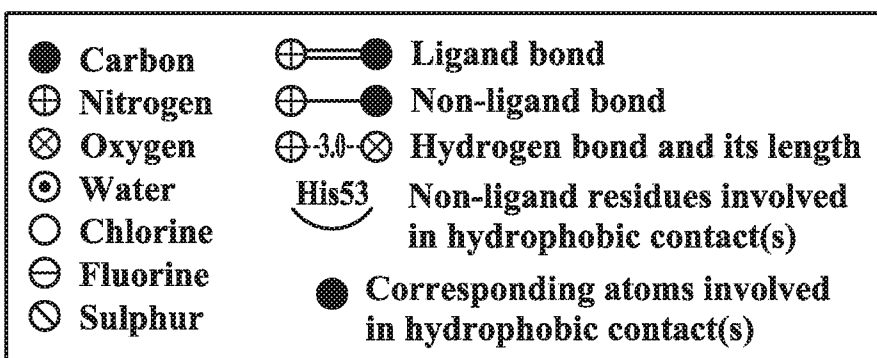
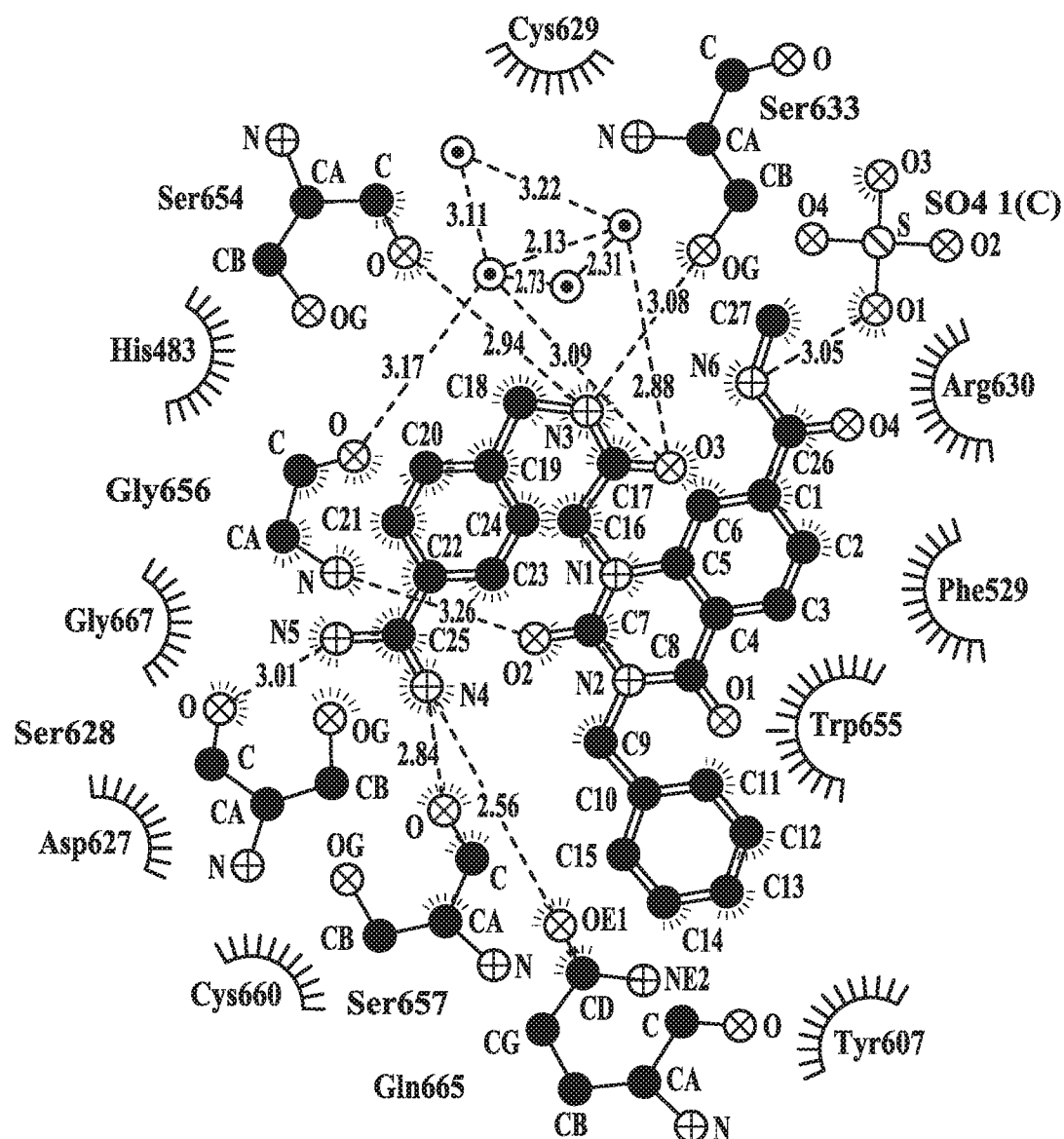
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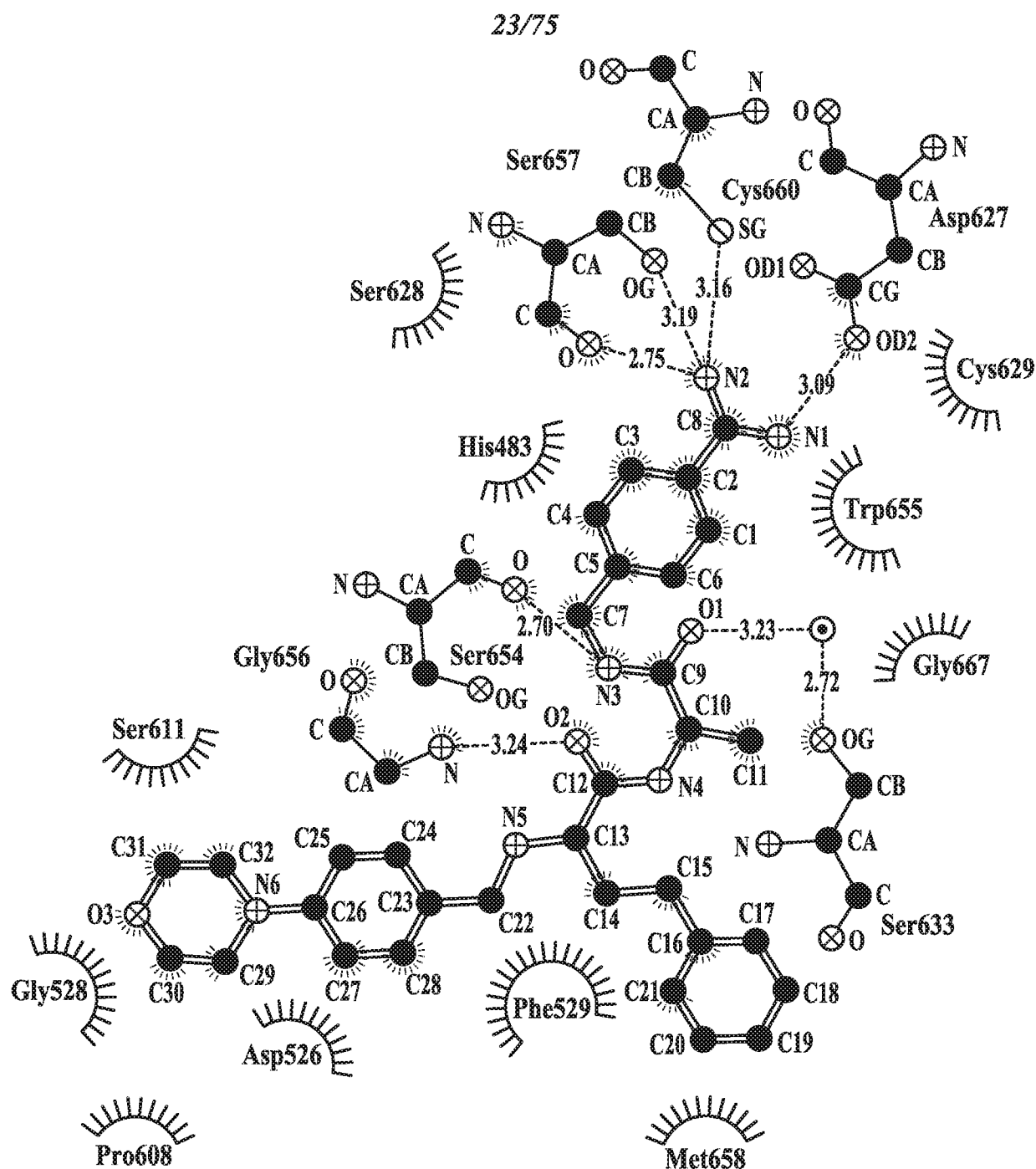
**FIG. 20**

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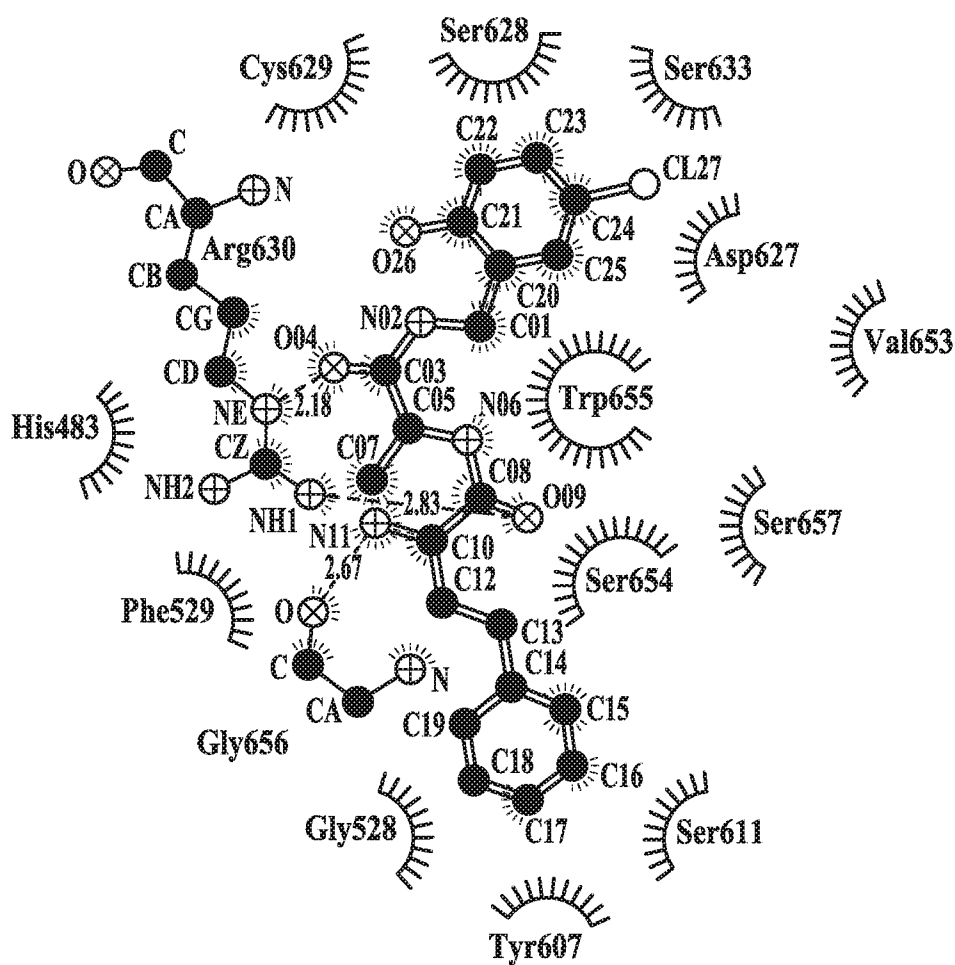
**FIG.21**

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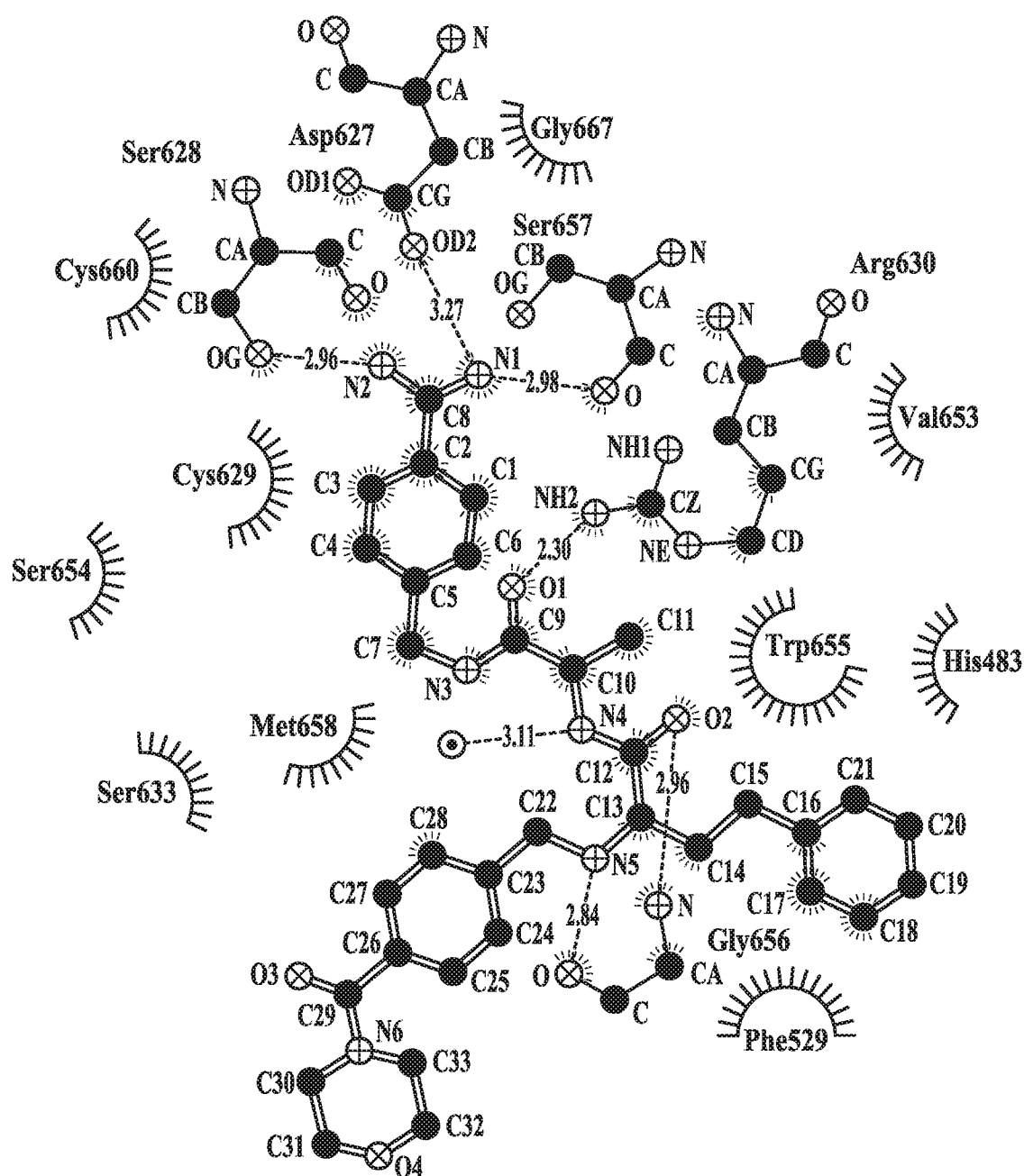
**FIG.22**

**FIG.23**

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**FIG. 24**

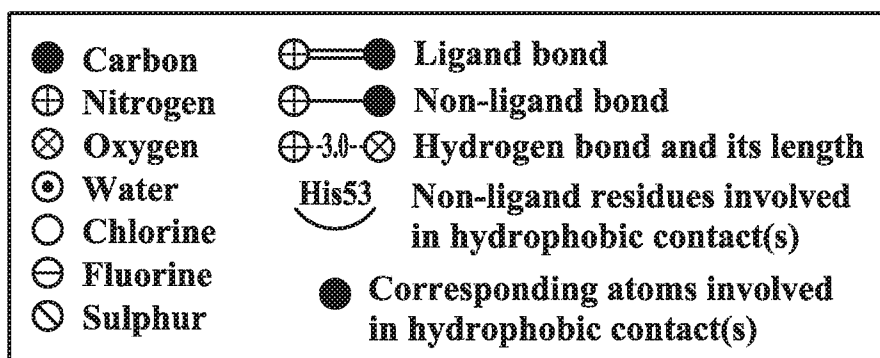
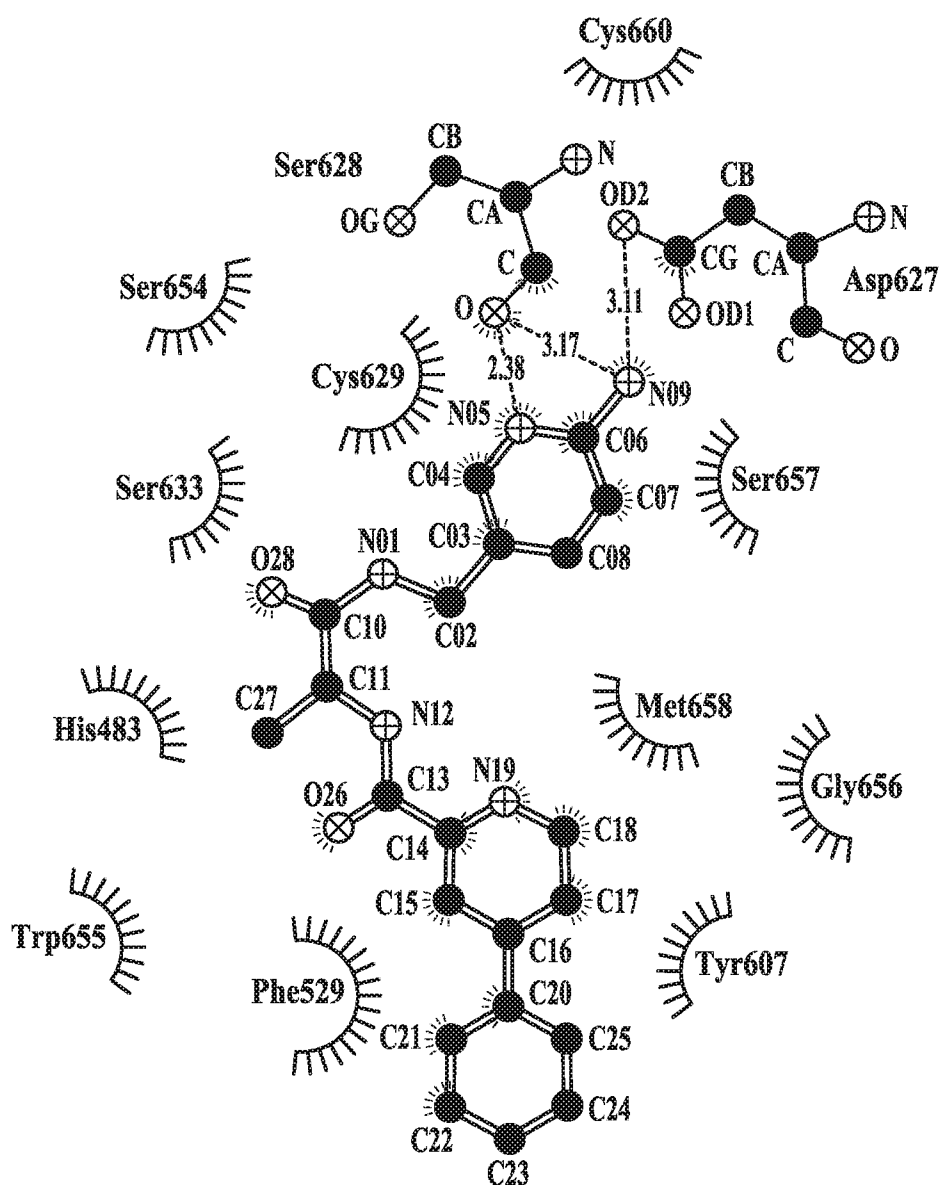
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- | | |
|------------|--|
| ● Carbon | ⊕—● Ligand bond |
| ⊕ Nitrogen | ⊕—● Non-ligand bond |
| ⊗ Oxygen | ⊕—3.0—⊗ Hydrogen bond and its length |
| ⊙ Water | His53 Non-ligand residues involved in hydrophobic contact(s) |
| ○ Chlorine | ● Corresponding atoms involved in hydrophobic contact(s) |
| ⊖ Fluorine | |
| ⊙ Sulphur | |

FIG.25

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**FIG. 26**

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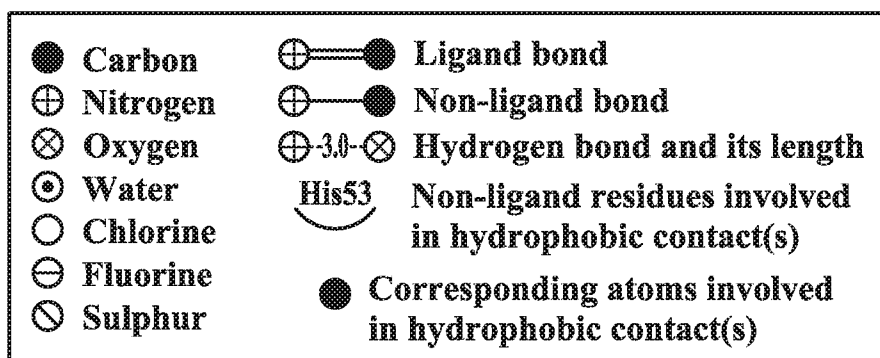
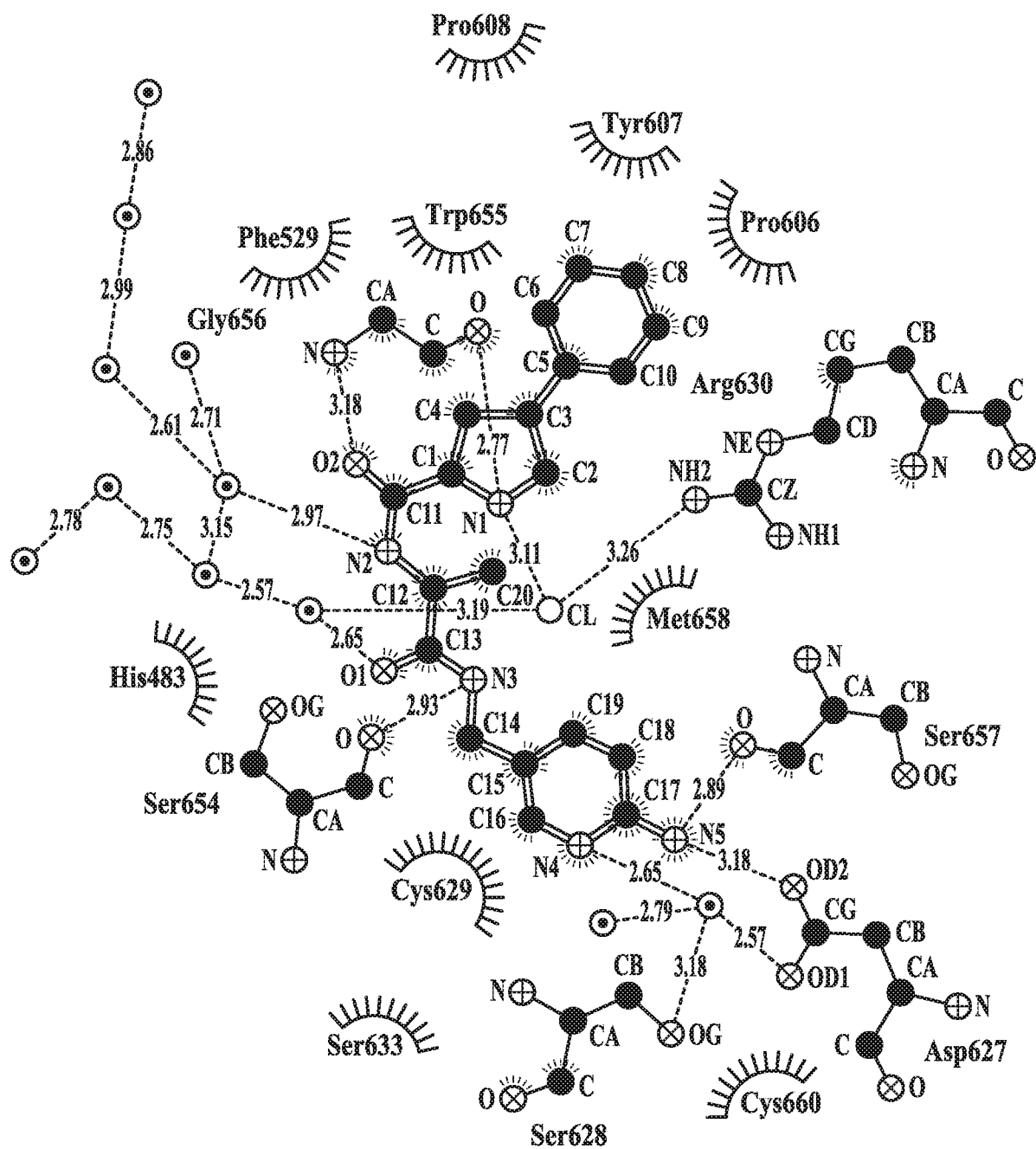
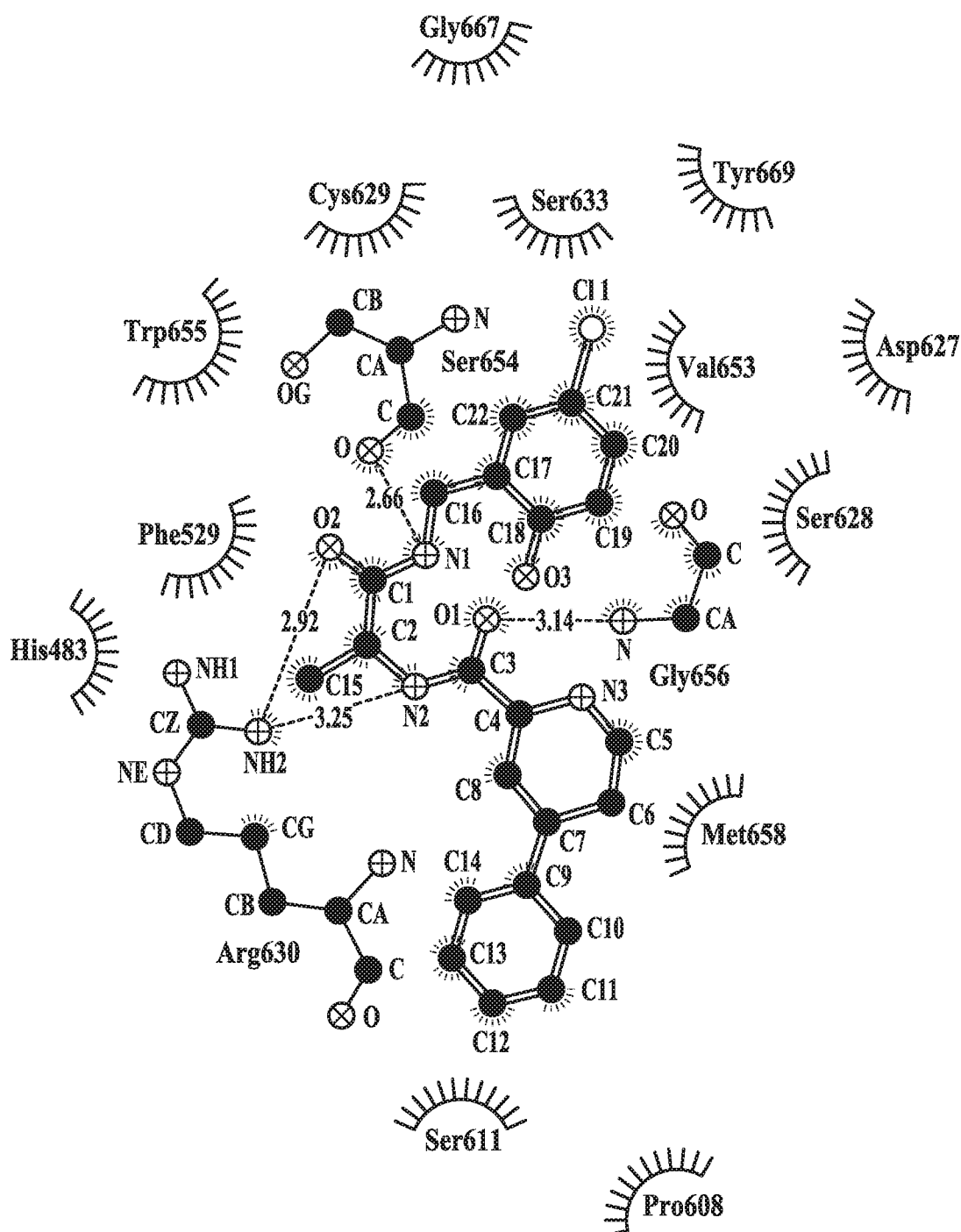
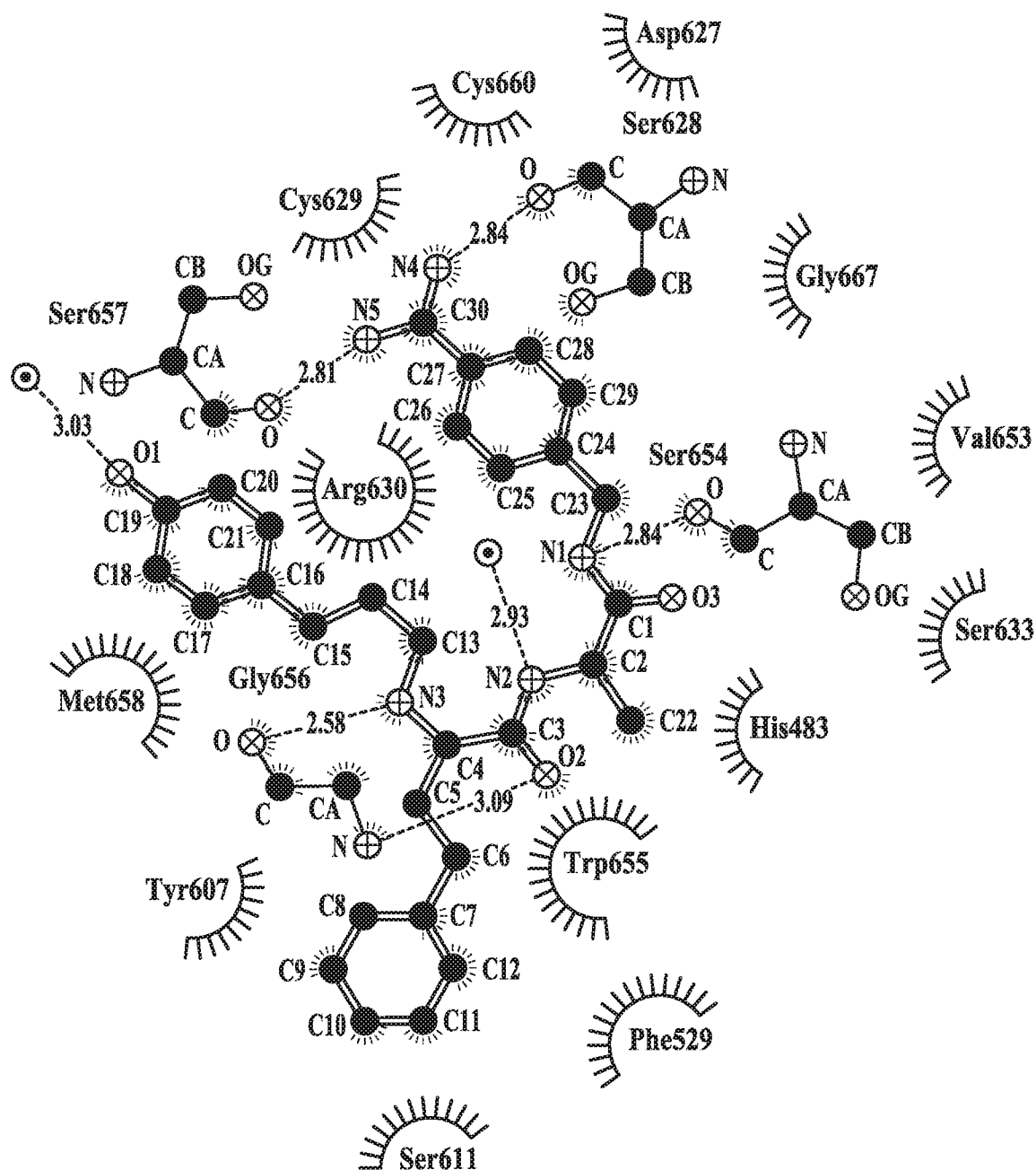


FIG. 27

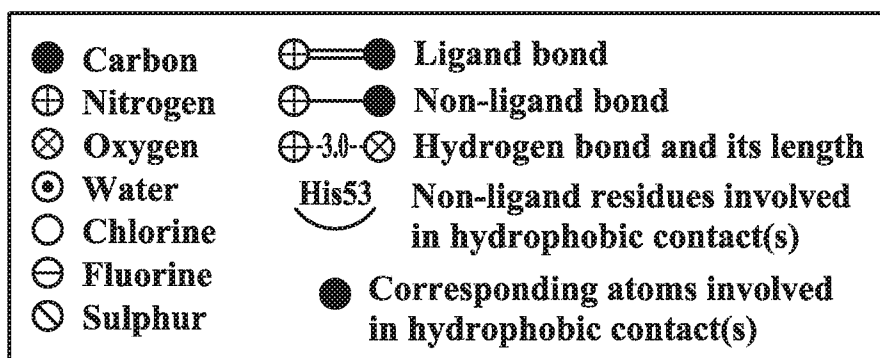
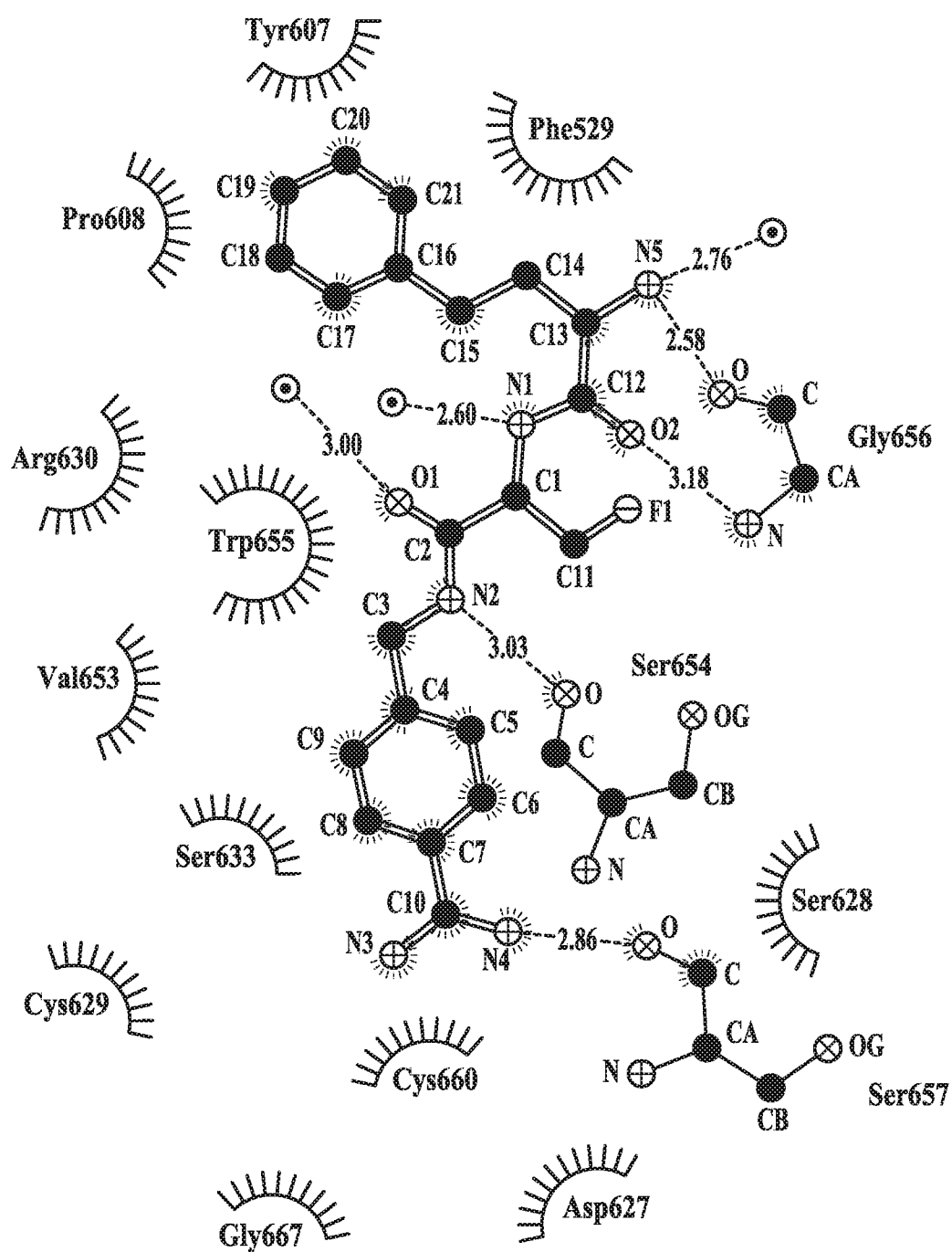
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**FIG. 28**

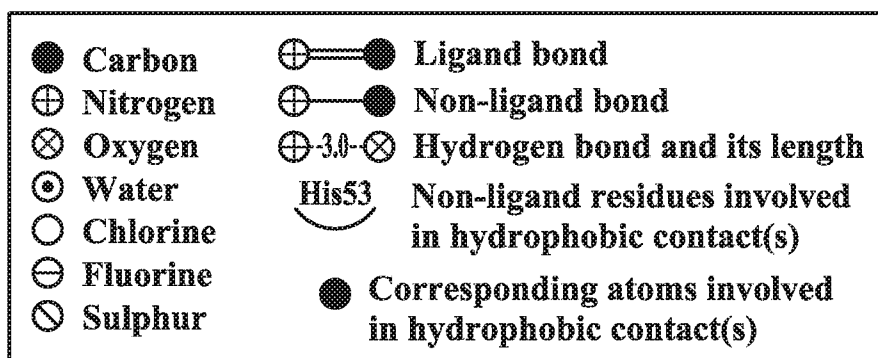
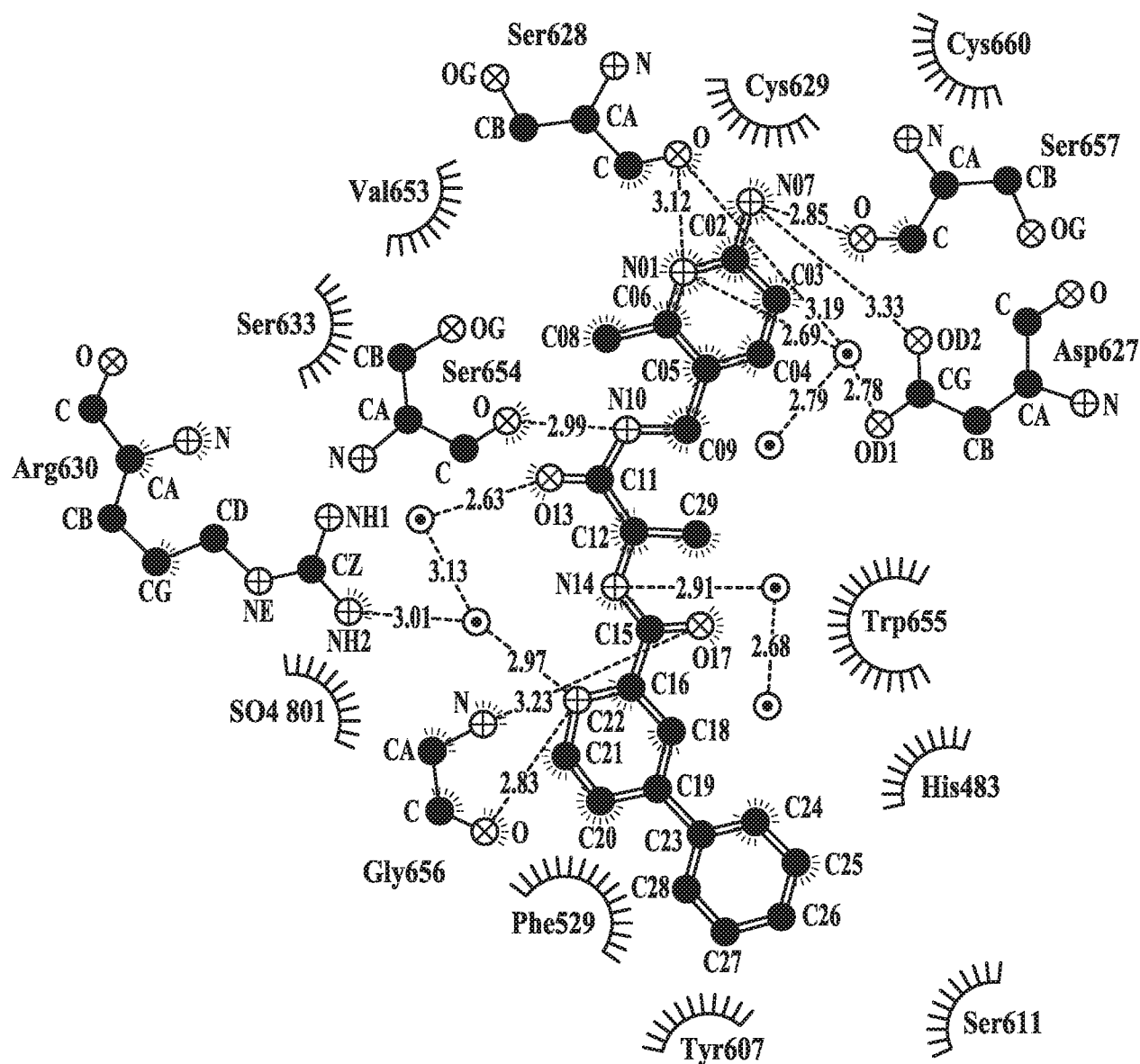
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**FIG. 29**

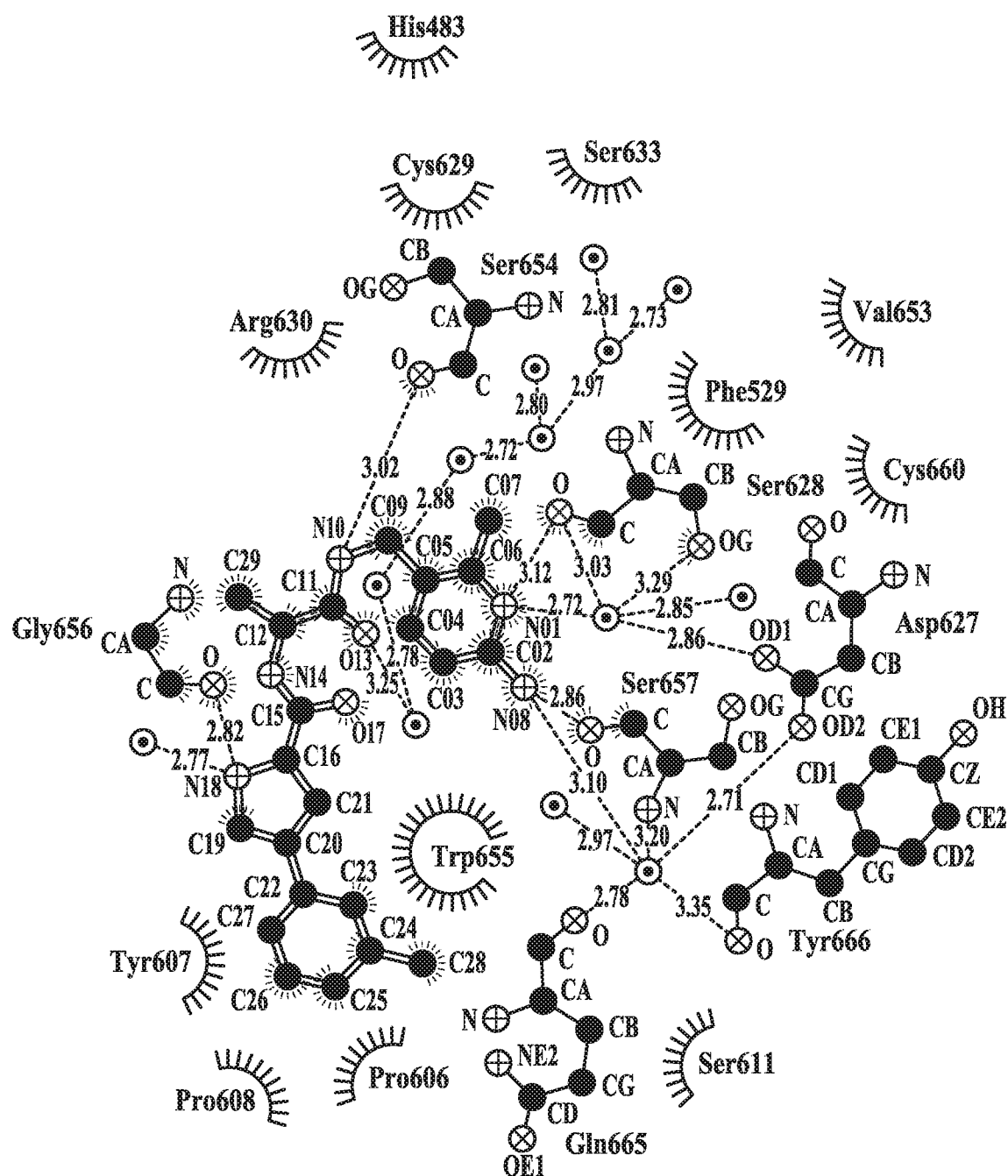
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**FIG.30**

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**FIG.31**

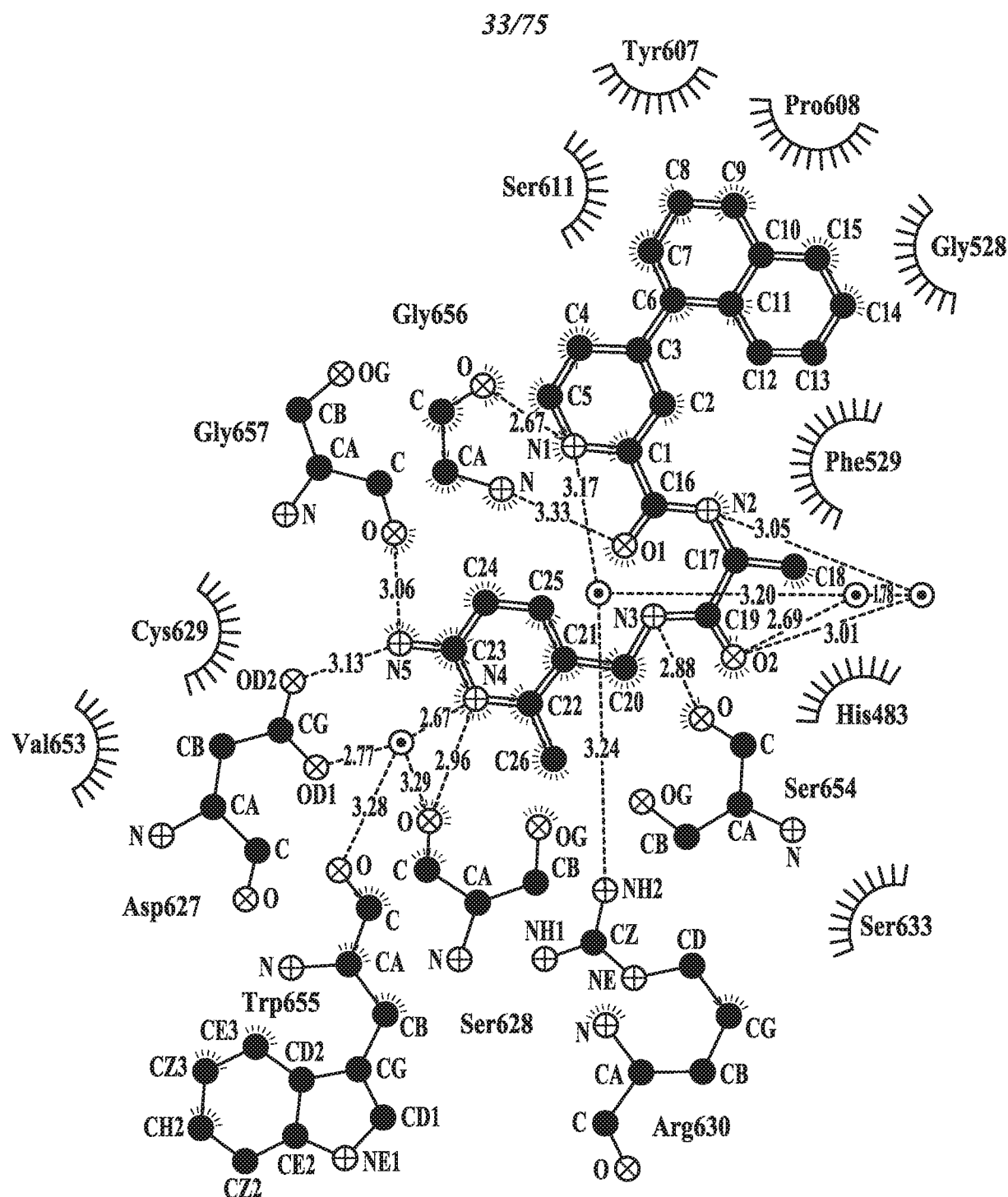
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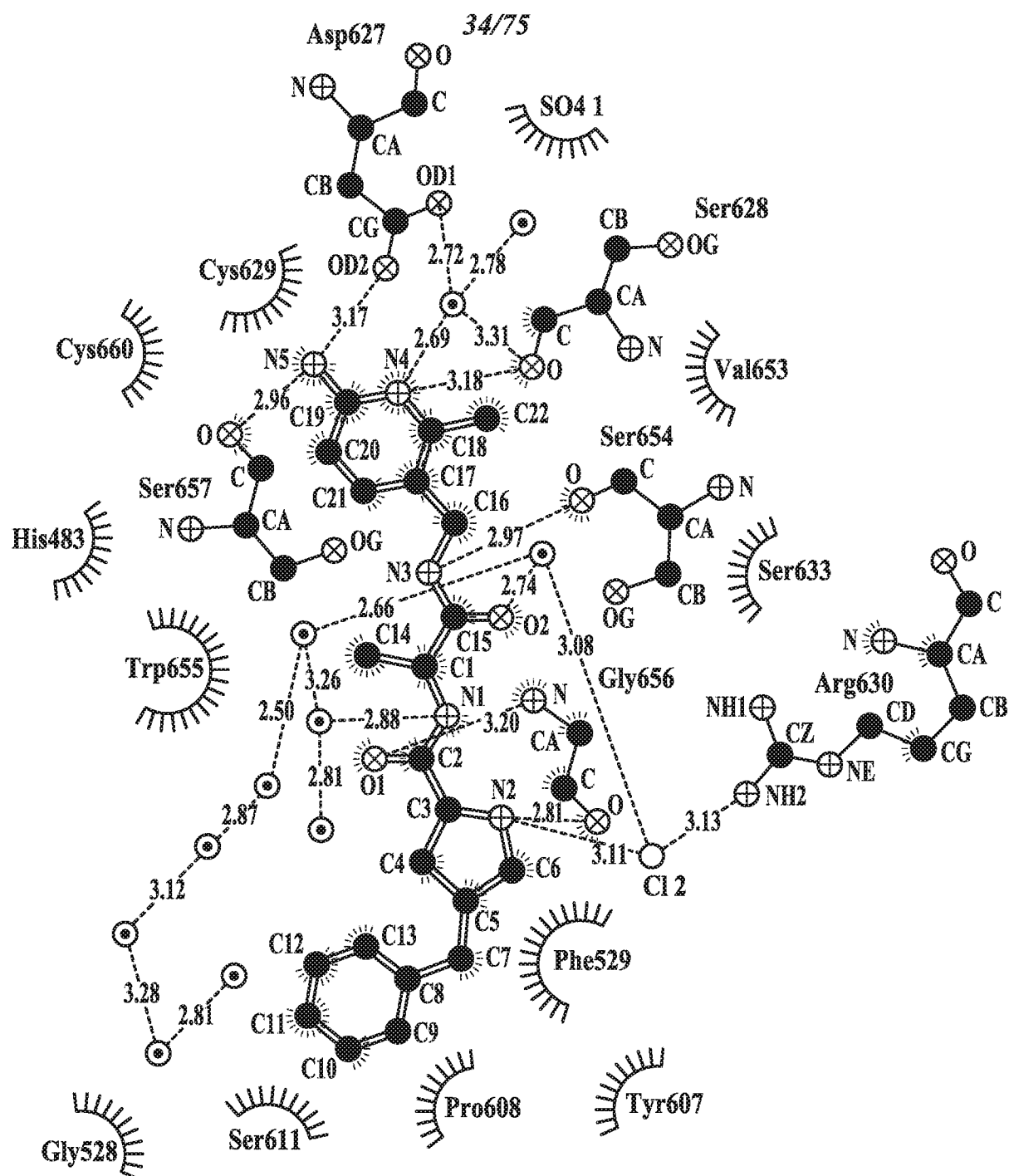


● Carbon
 ⊕ Nitrogen
 ⊗ Oxygen
 ⊙ Water
 ○ Chlorine
 ⊖ Fluorine
 ⊗ Sulphur

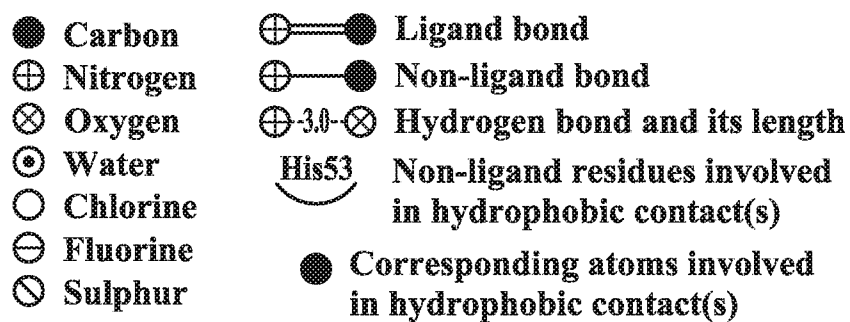
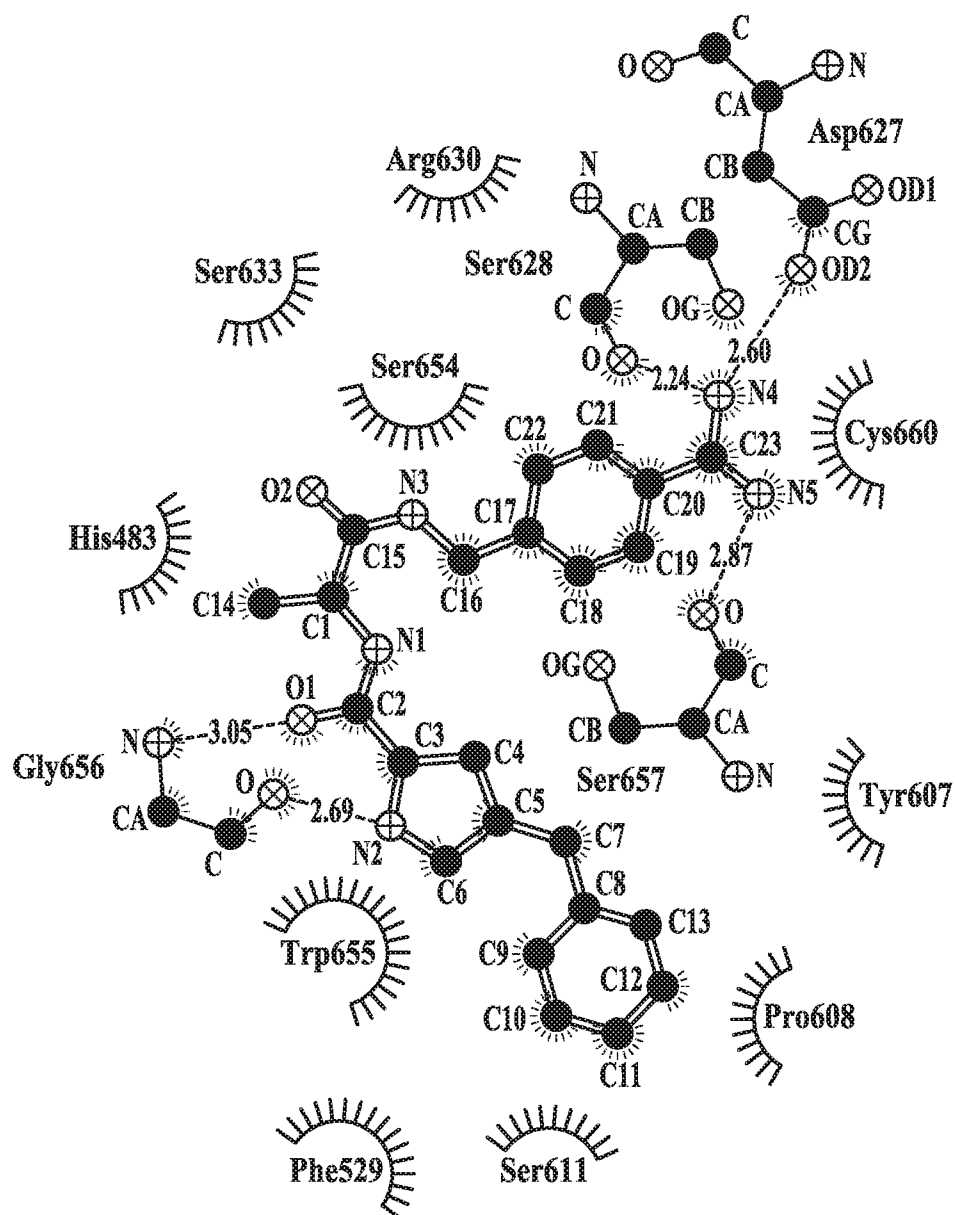
⊕=● Ligand bond
 ⊕—● Non-ligand bond
 ⊕-3.0-⊗ Hydrogen bond and its length
 His53 Non-ligand residues involved in hydrophobic contact(s)
 ● Corresponding atoms involved in hydrophobic contact(s)

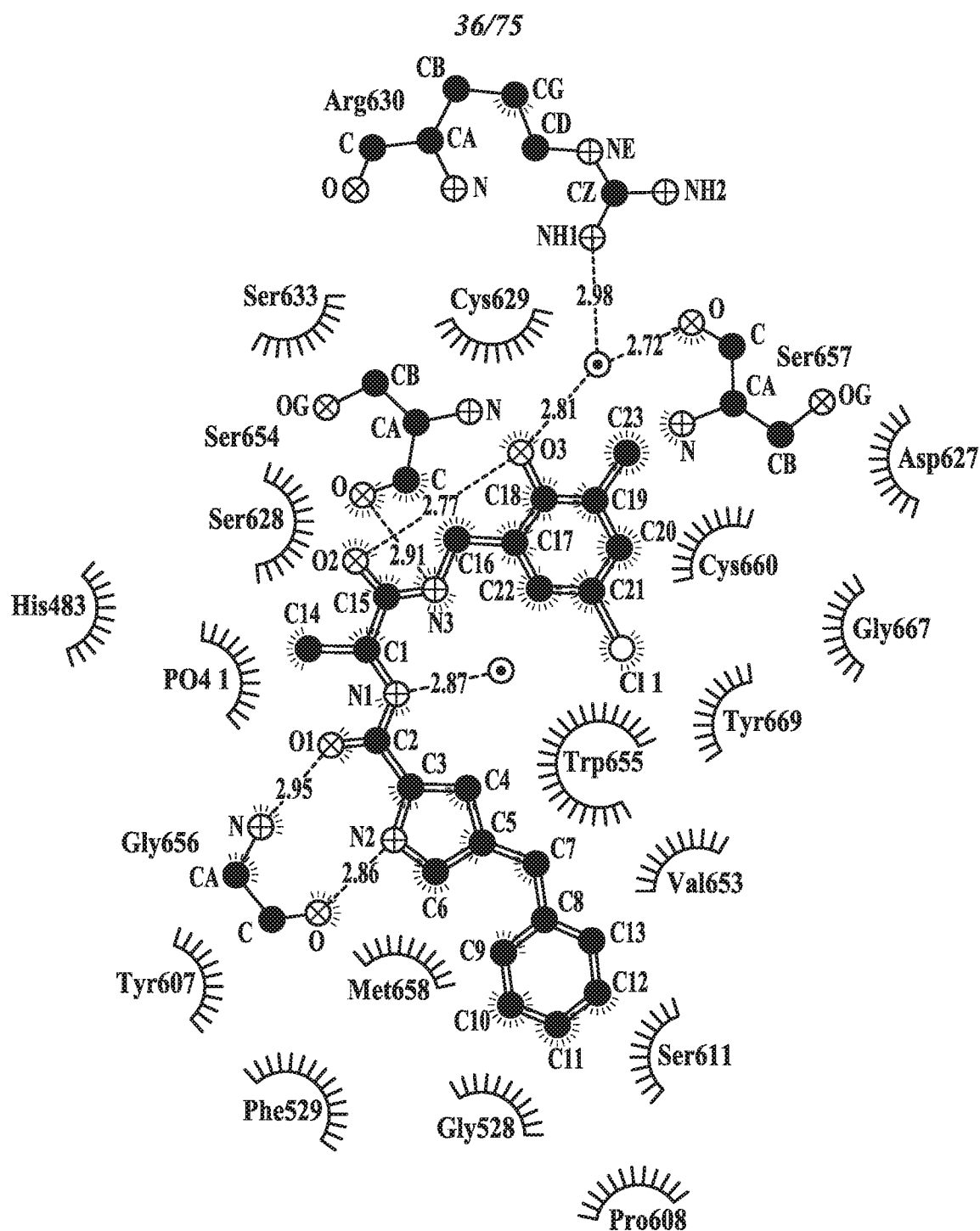
FIG. 32

**FIG.33**

**FIG.34**

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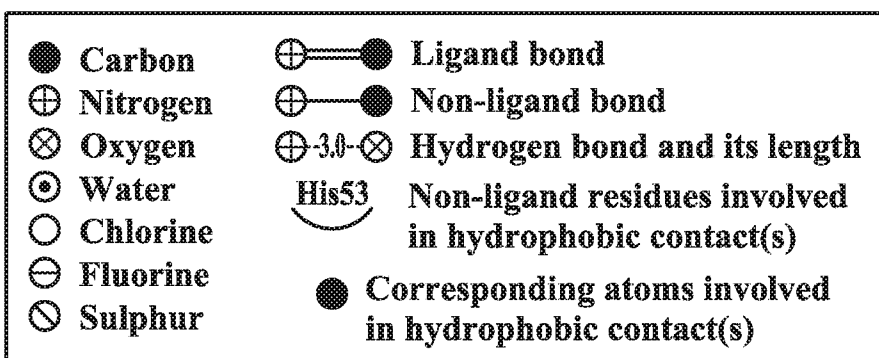
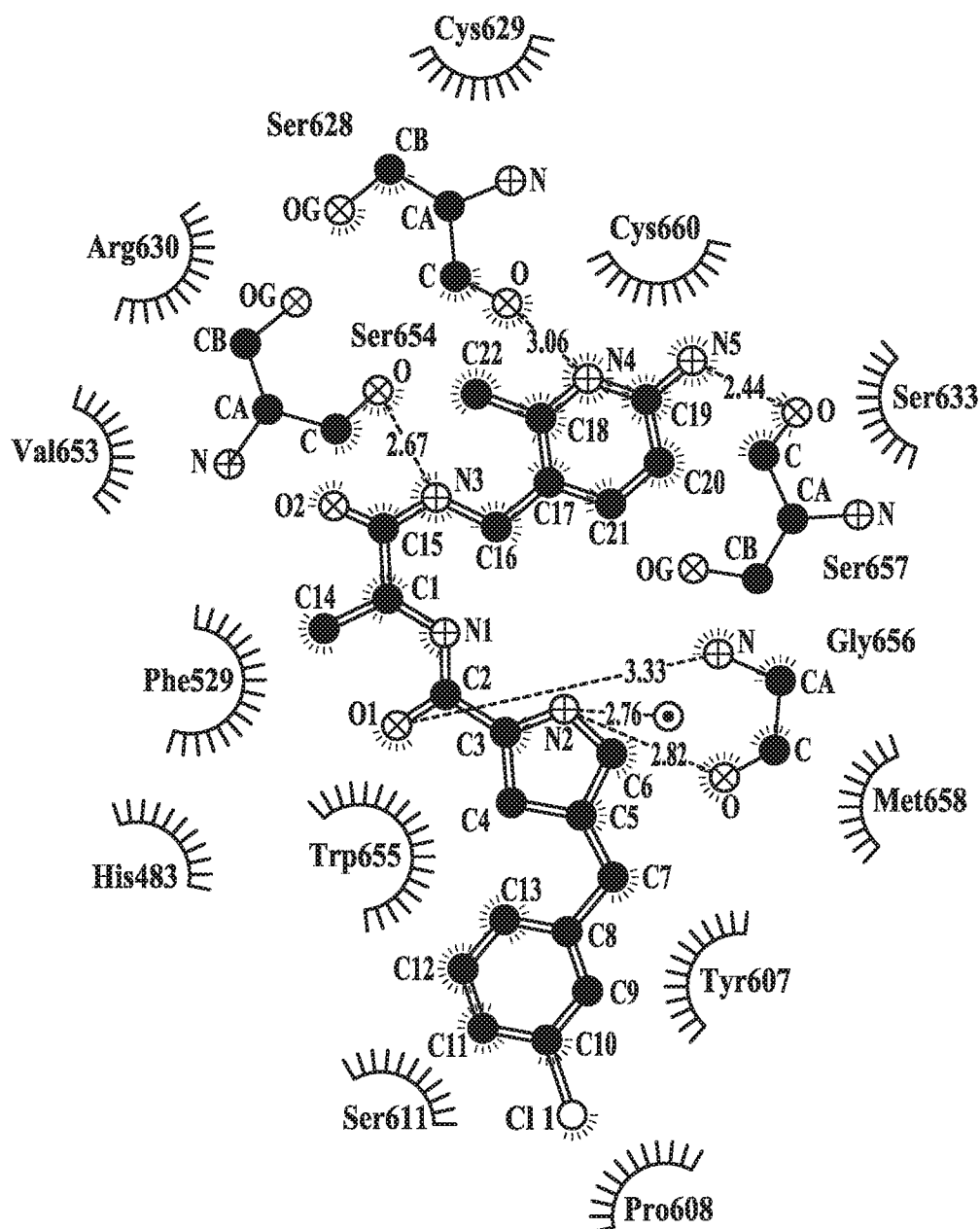
**FIG.35**

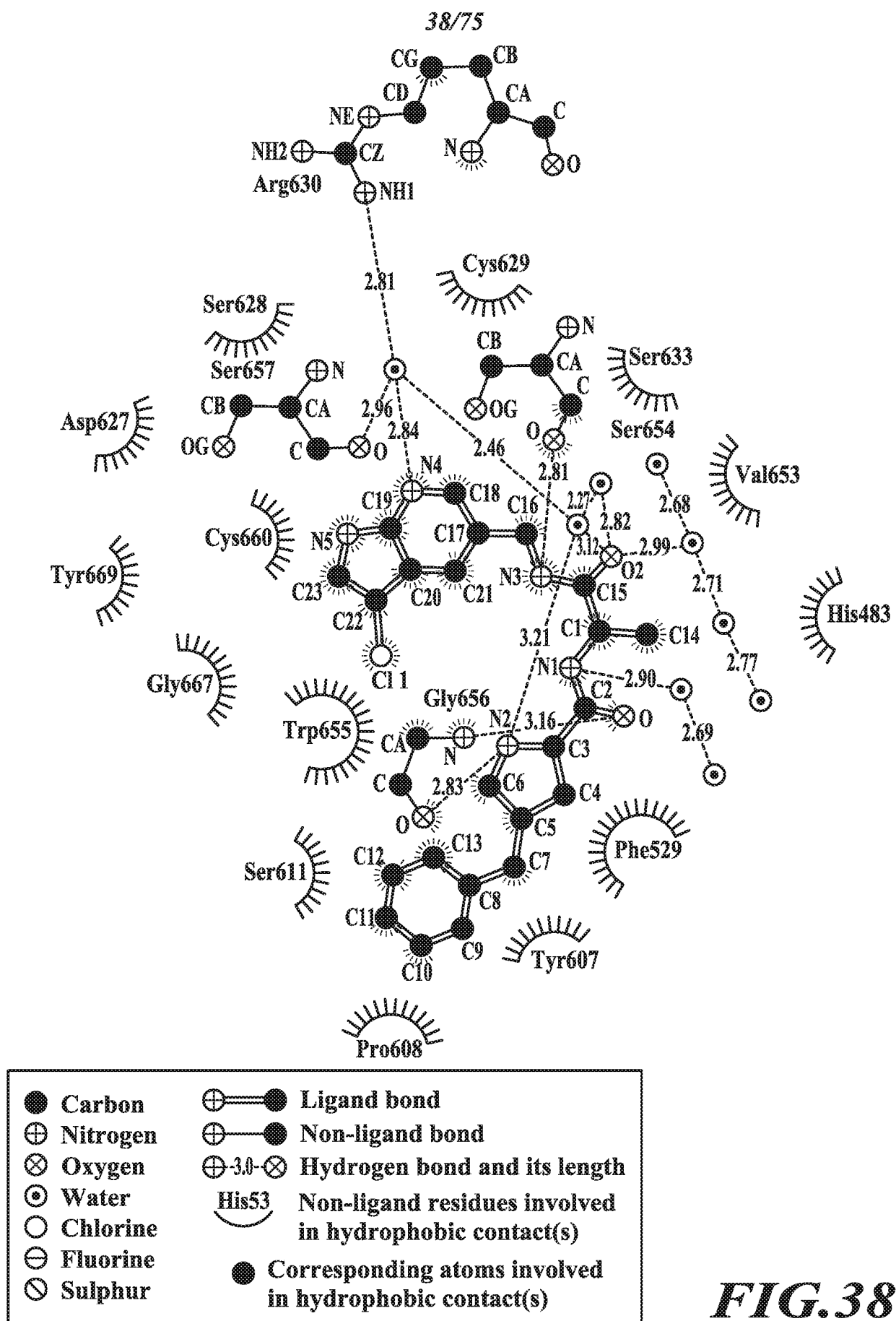


- | | |
|------------|--|
| ● Carbon | ⊕—● Ligand bond |
| ⊕ Nitrogen | ⊕—● Non-ligand bond |
| ⊗ Oxygen | ⊕—3.0—⊗ Hydrogen bond and its length |
| ⊙ Water | His53 Non-ligand residues involved in hydrophobic contact(s) |
| ○ Chlorine | ● Corresponding atoms involved in hydrophobic contact(s) |
| ⊖ Fluorine | |
| ⊙ Sulphur | |

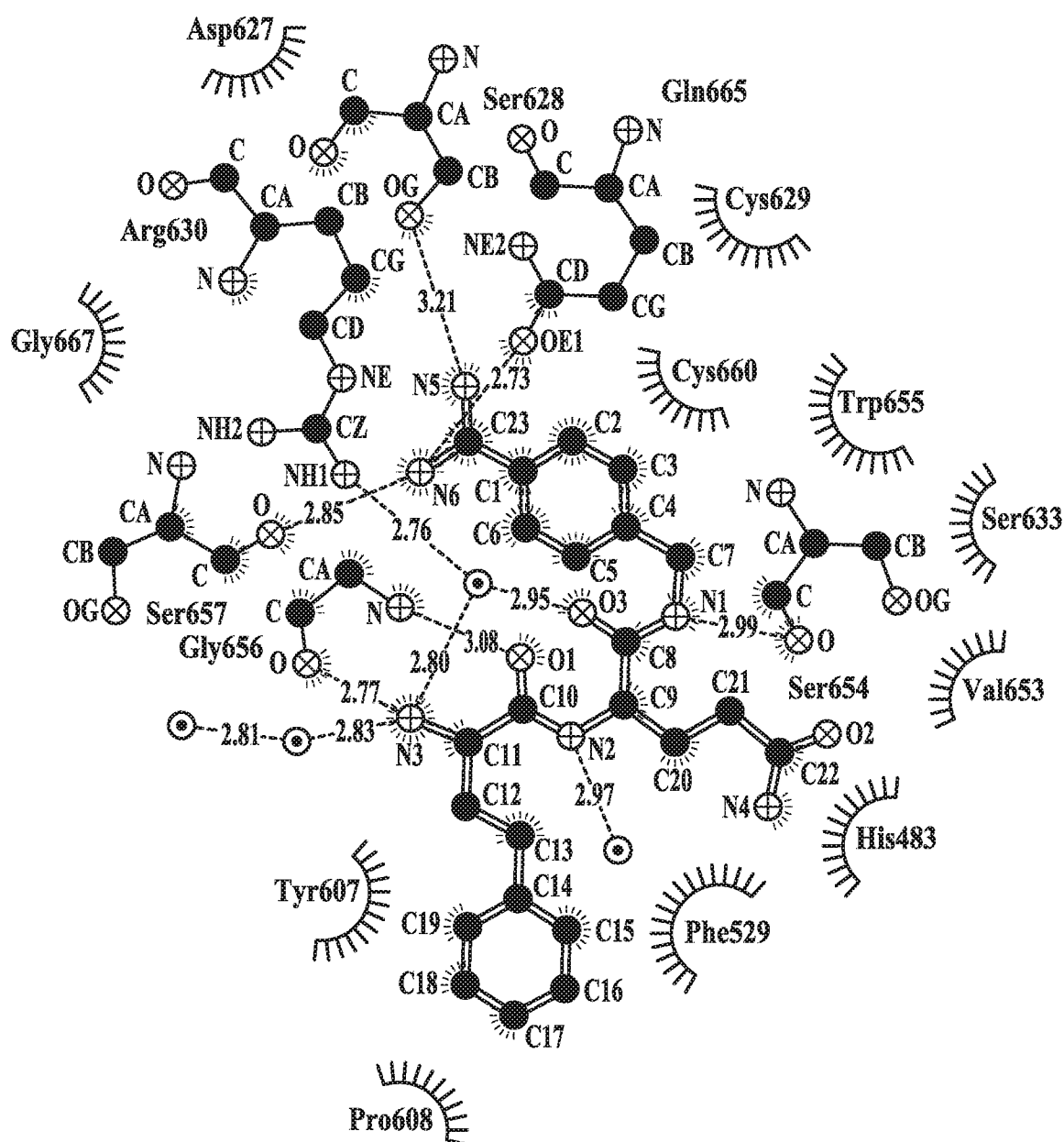
FIG.36

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**FIG.37**



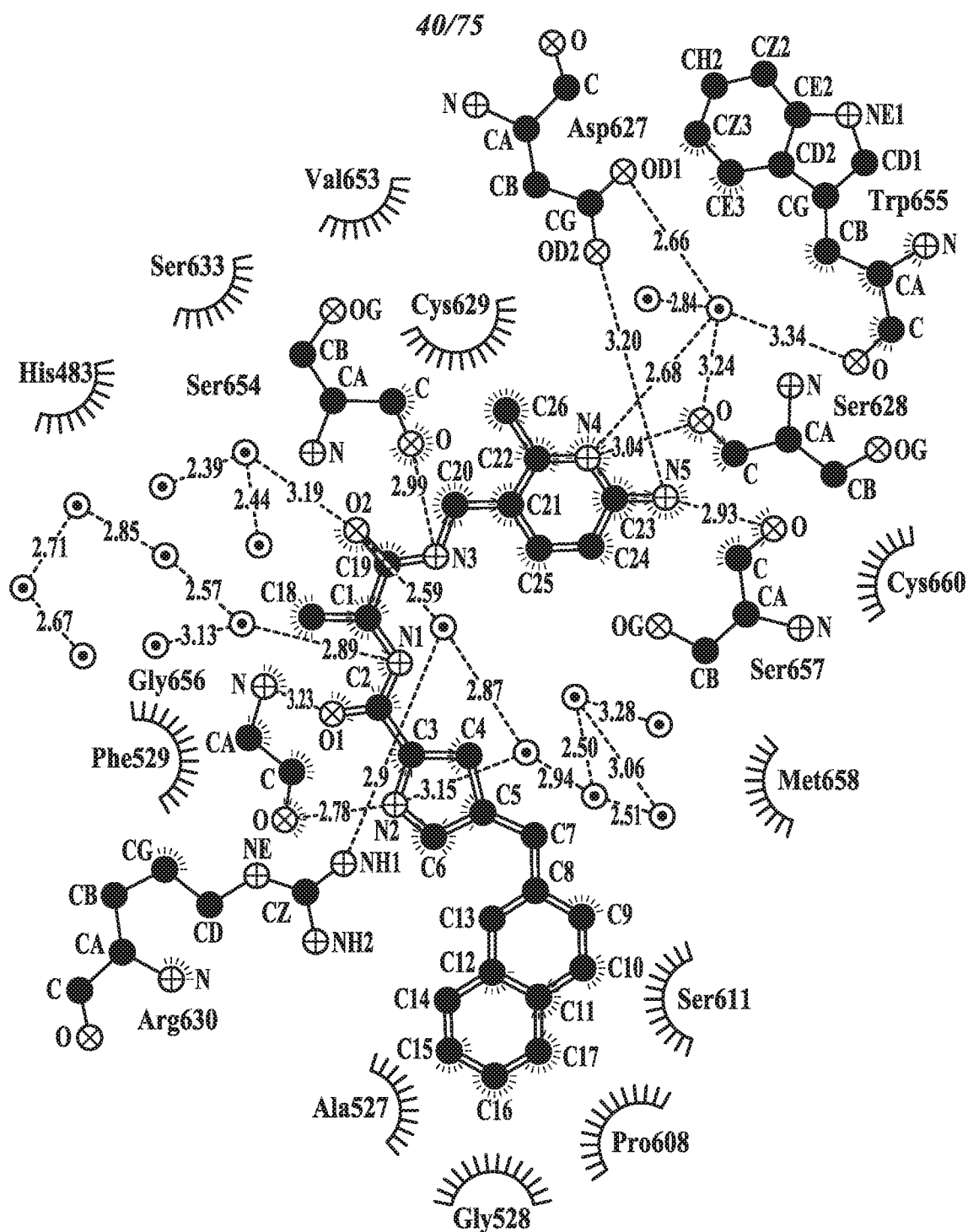
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● Carbon
 ⊕ Nitrogen
 ⊗ Oxygen
 ⊙ Water
 ○ Chlorine
 ⊖ Fluorine
 ⊙ Sulphur

⊕—● Ligand bond
 ⊕—● Non-ligand bond
 ⊕—3.0—⊗ Hydrogen bond and its length
 His53 Non-ligand residues involved in hydrophobic contact(s)
 ● Corresponding atoms involved in hydrophobic contact(s)

FIG.39

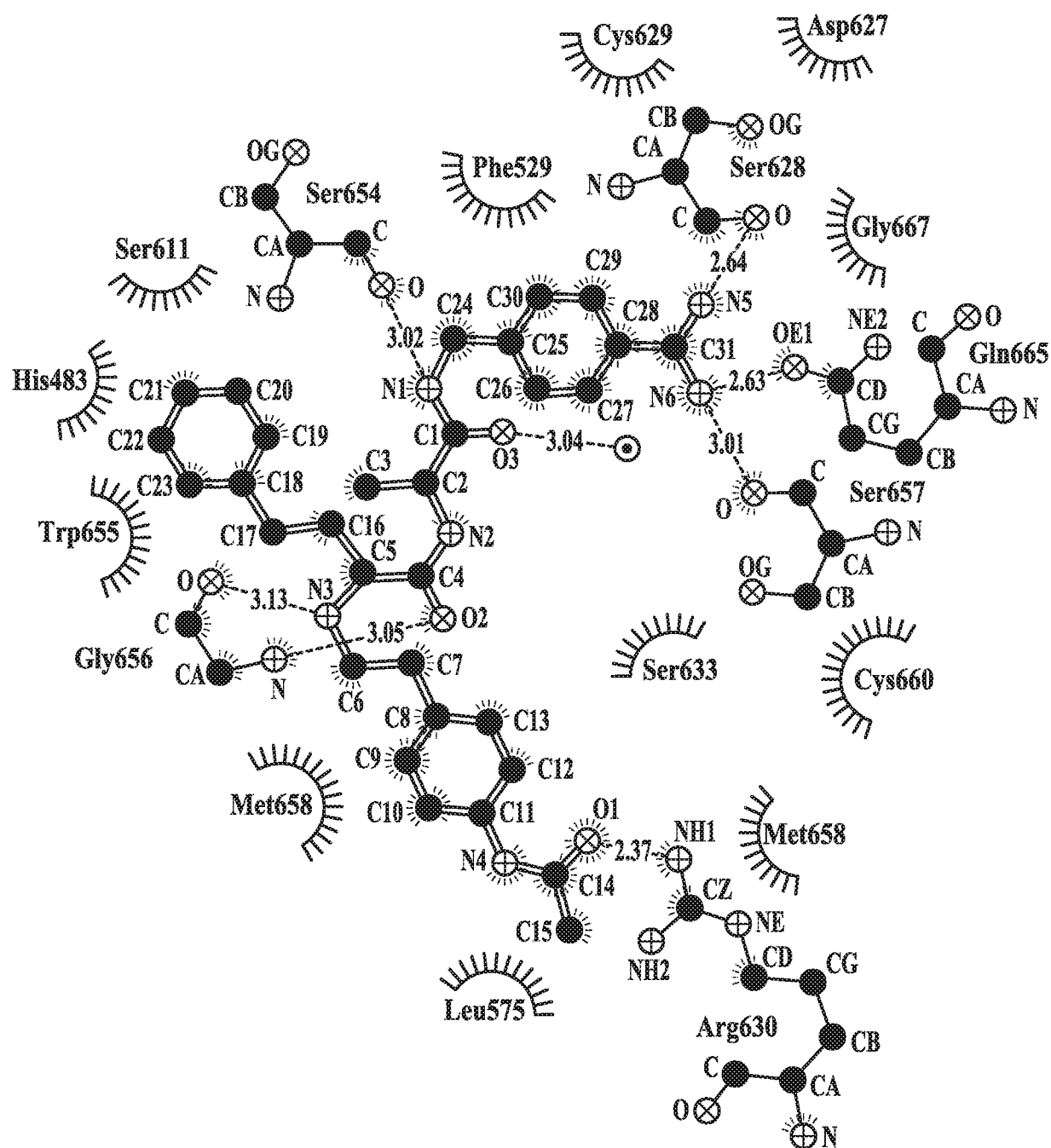


● Carbon
 ⊕ Nitrogen
 ⊗ Oxygen
 ⊙ Water
 ○ Chlorine
 ⊖ Fluorine
 ⊙ Sulphur

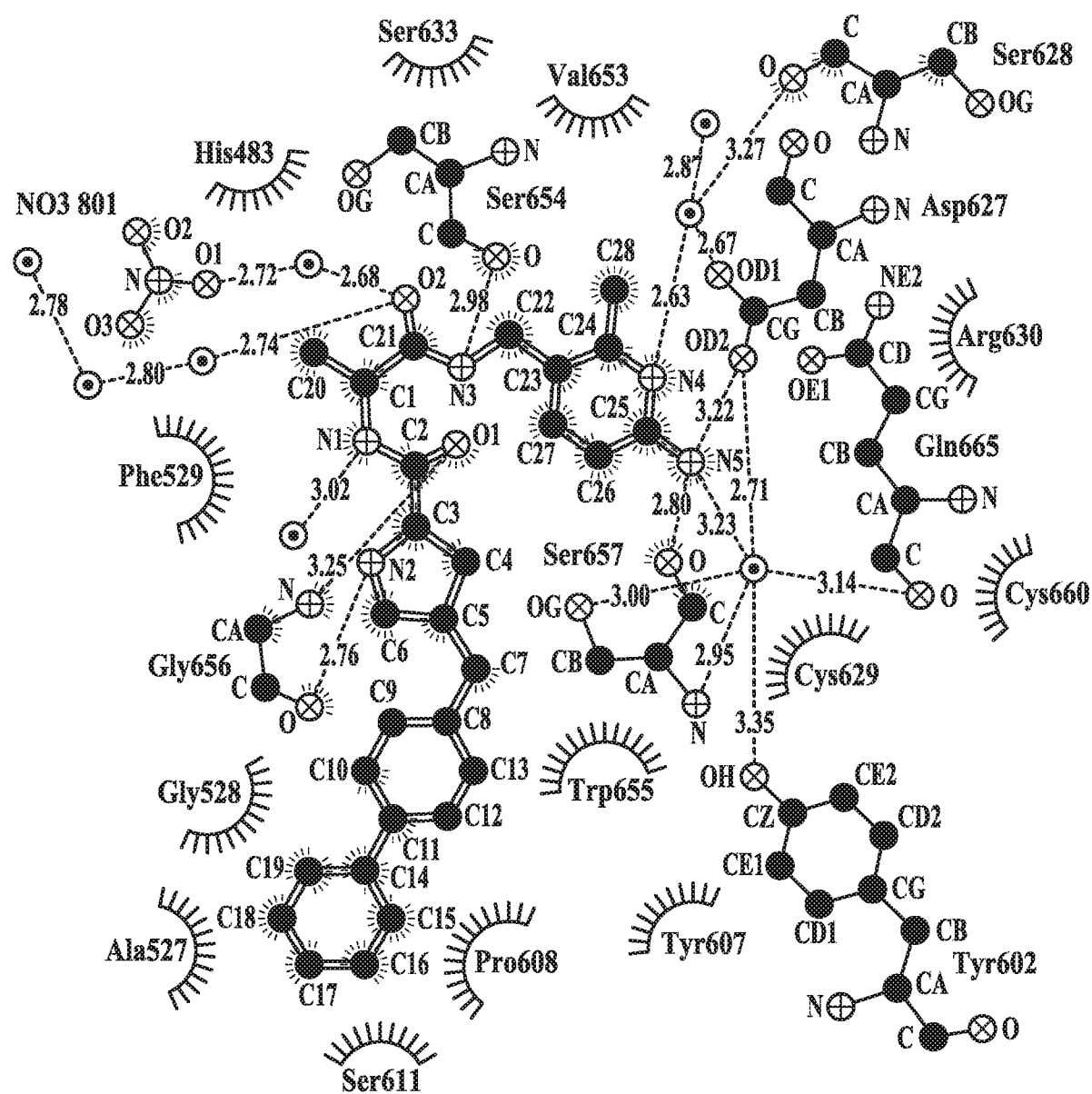
⊕—● Ligand bond
 ⊕—● Non-ligand bond
 ⊕—3.0—⊗ Hydrogen bond and its length
 His53 Non-ligand residues involved in hydrophobic contact(s)
 ● Corresponding atoms involved in hydrophobic contact(s)

FIG.40

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**FIG.41**

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● Carbon
 ⊕ Nitrogen
 ⊗ Oxygen
 ⊙ Water
 ○ Chlorine
 ⊖ Fluorine
 ⊙ Sulphur

⊕—● Ligand bond
 ⊕—● Non-ligand bond
 ⊕—3.0—⊗ Hydrogen bond and its length
 His53 Non-ligand residues involved in hydrophobic contact(s)
 ● Corresponding atoms involved in hydrophobic contact(s)

FIG.42

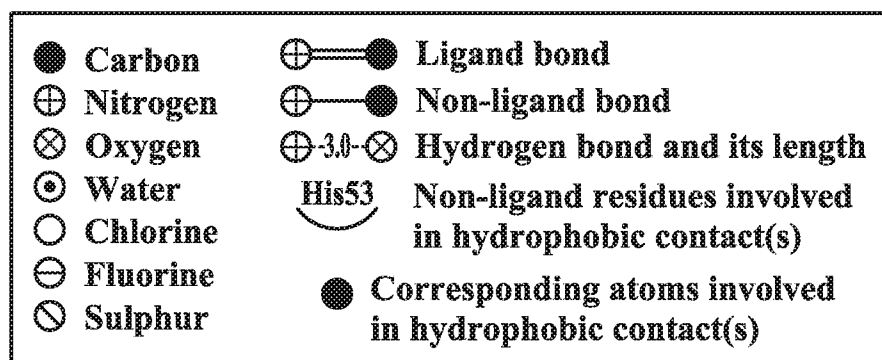
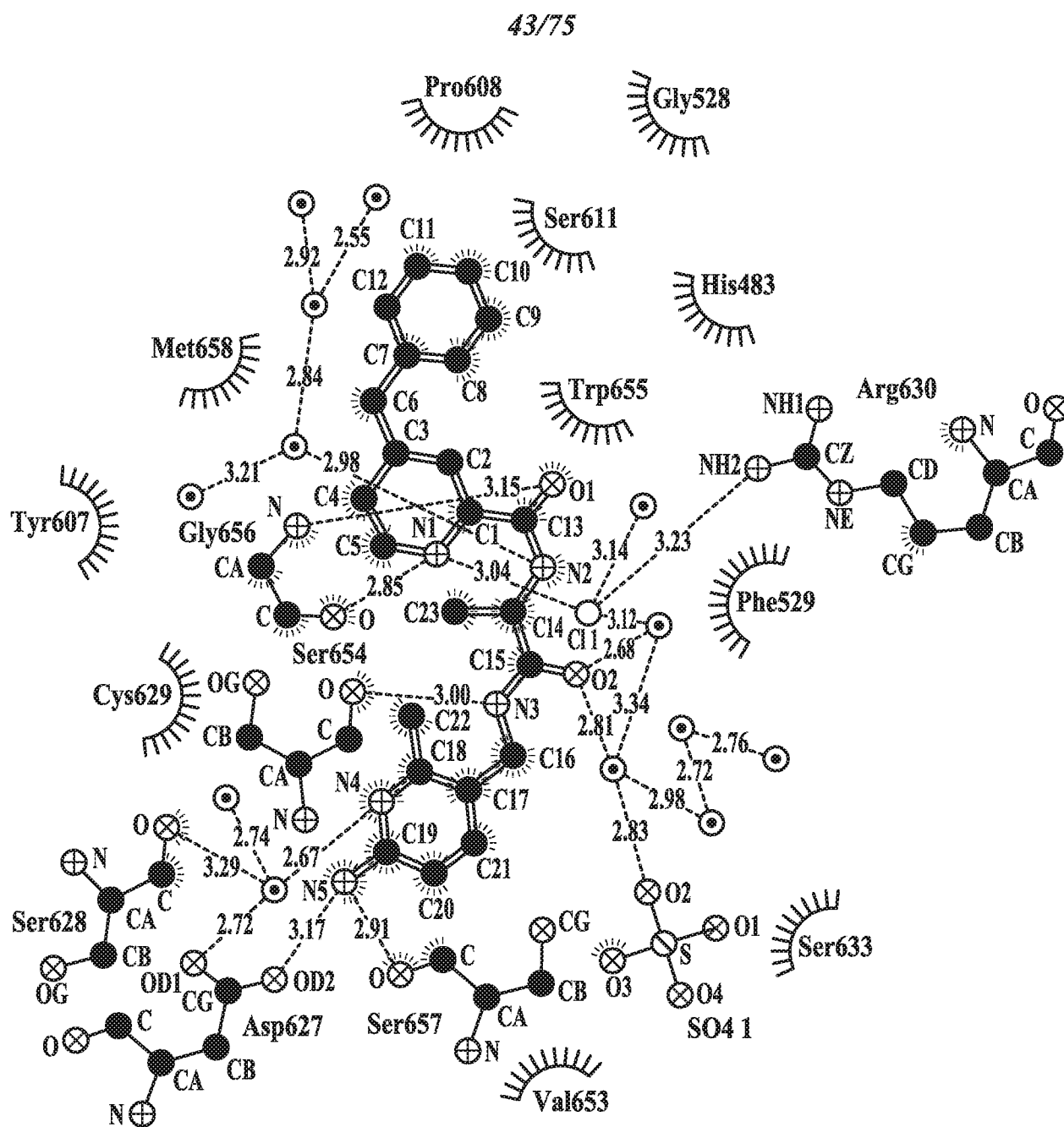
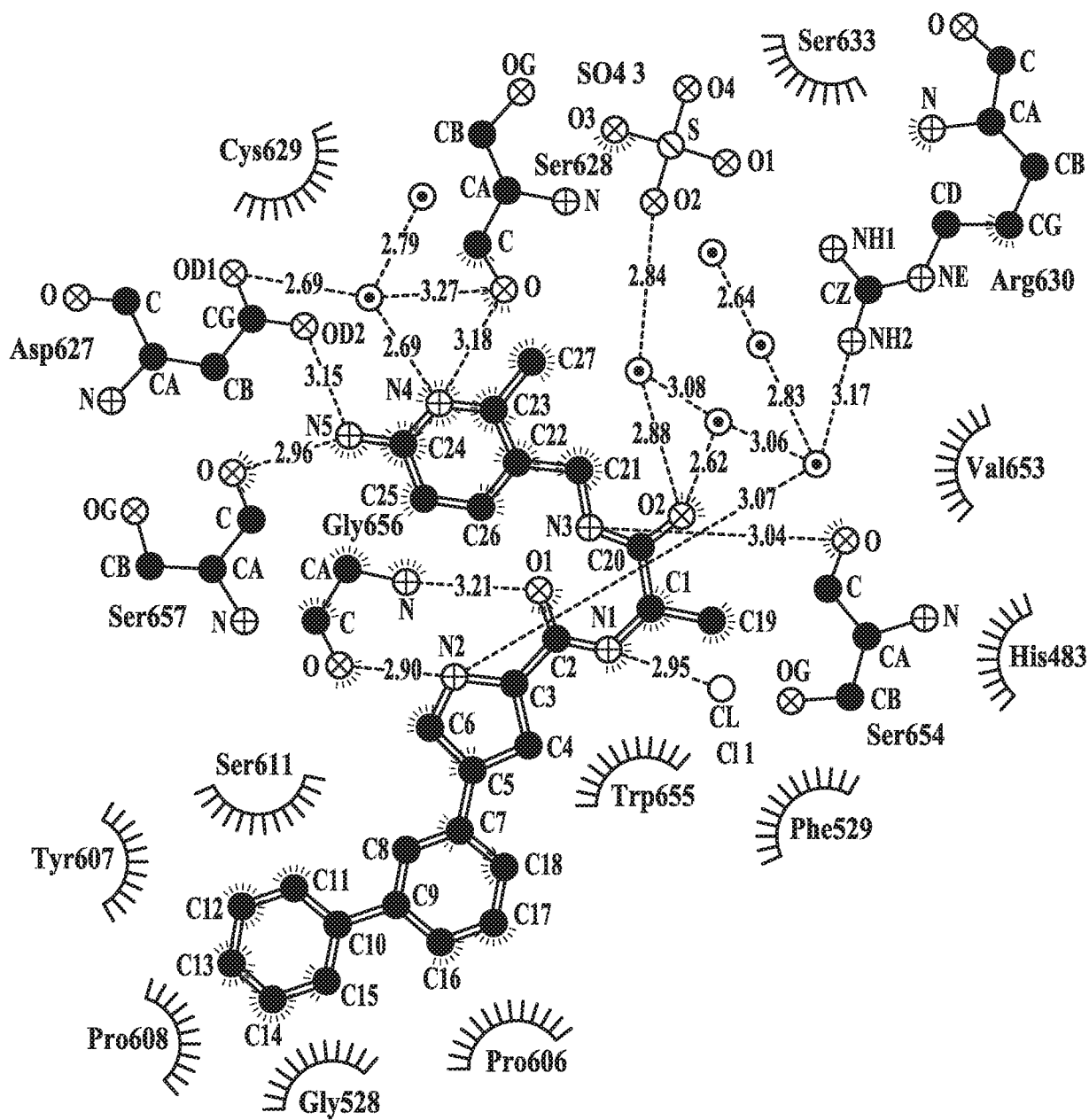
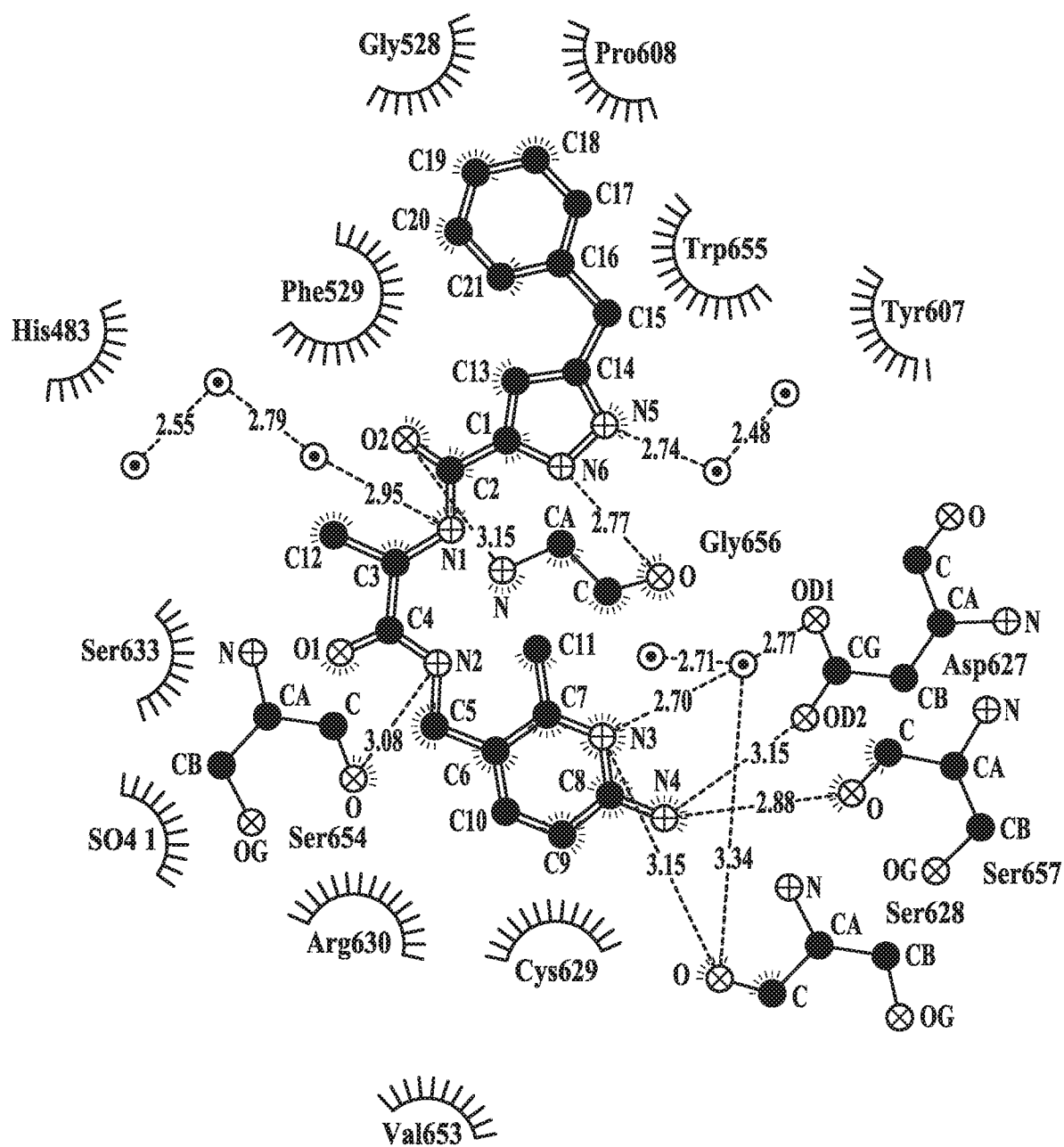


FIG. 43

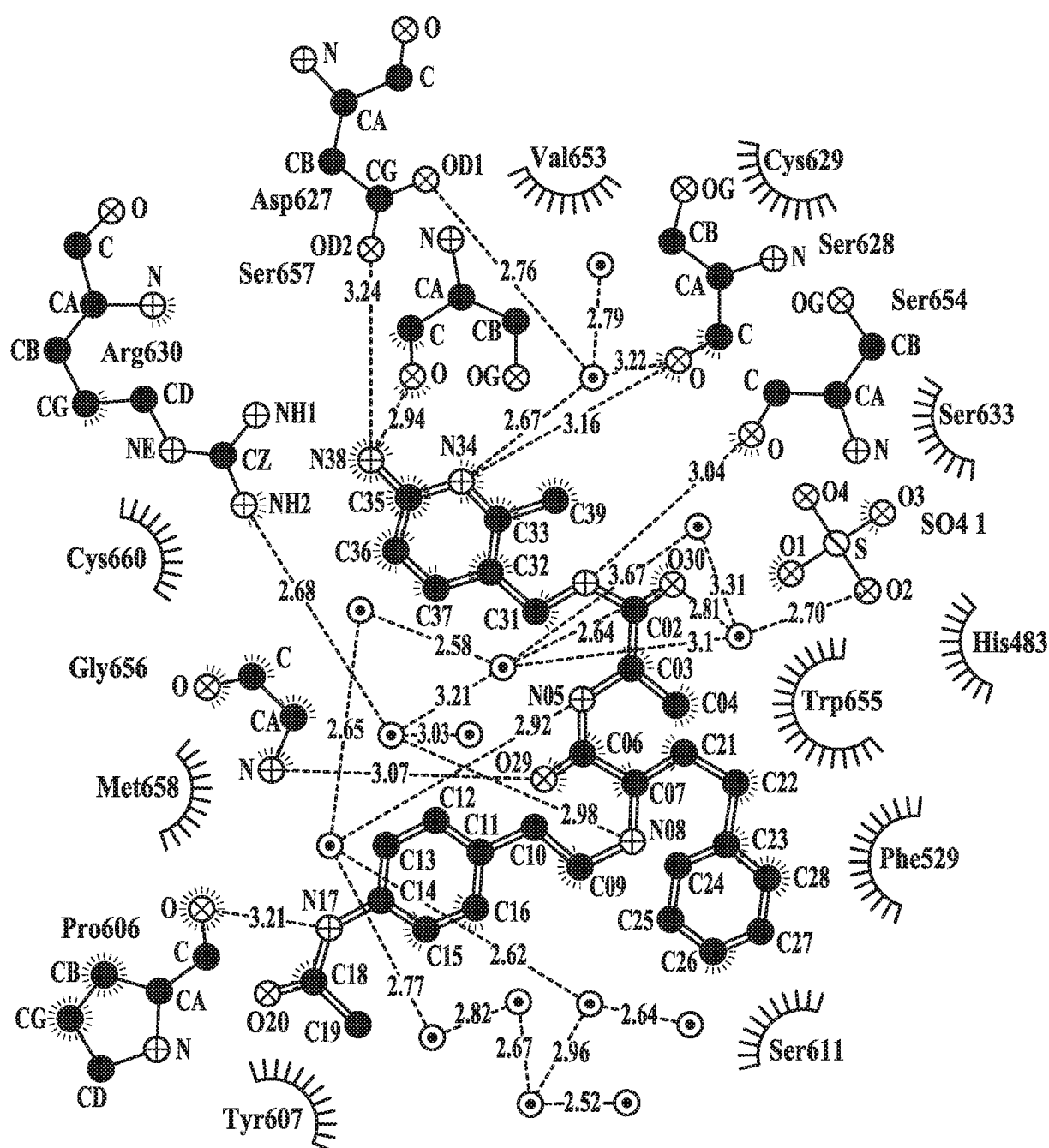
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**FIG.44**

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**FIG.45**

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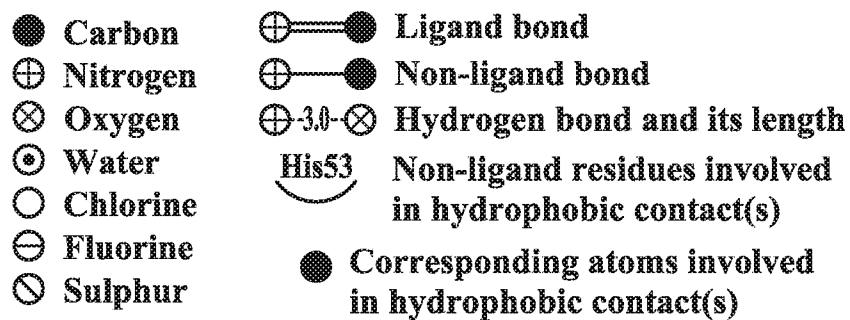
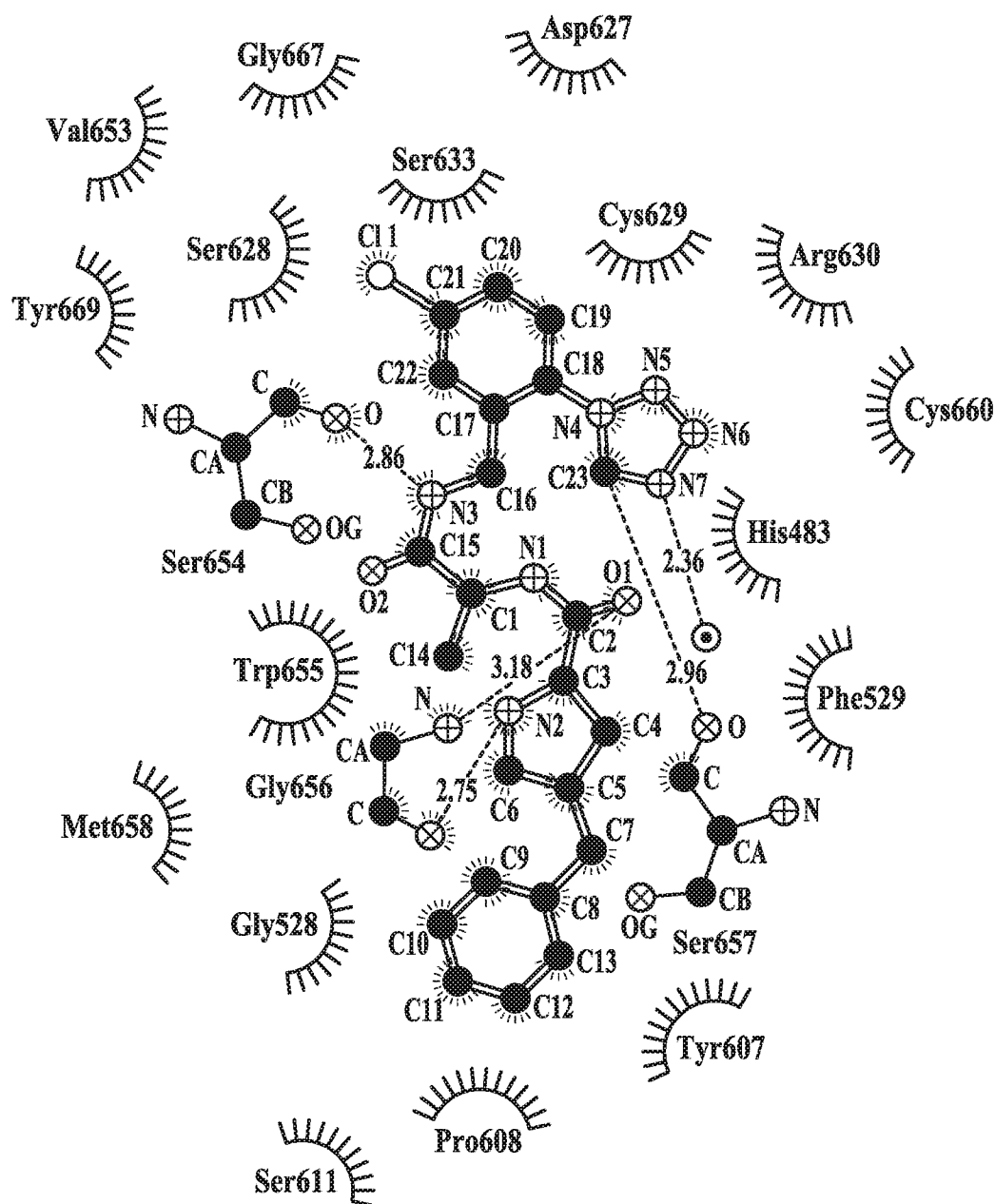


● Carbon
 ⊕ Nitrogen
 ⊗ Oxygen
 ⊙ Water
 ○ Chlorine
 ⊖ Fluorine
 ⊗ Sulphur

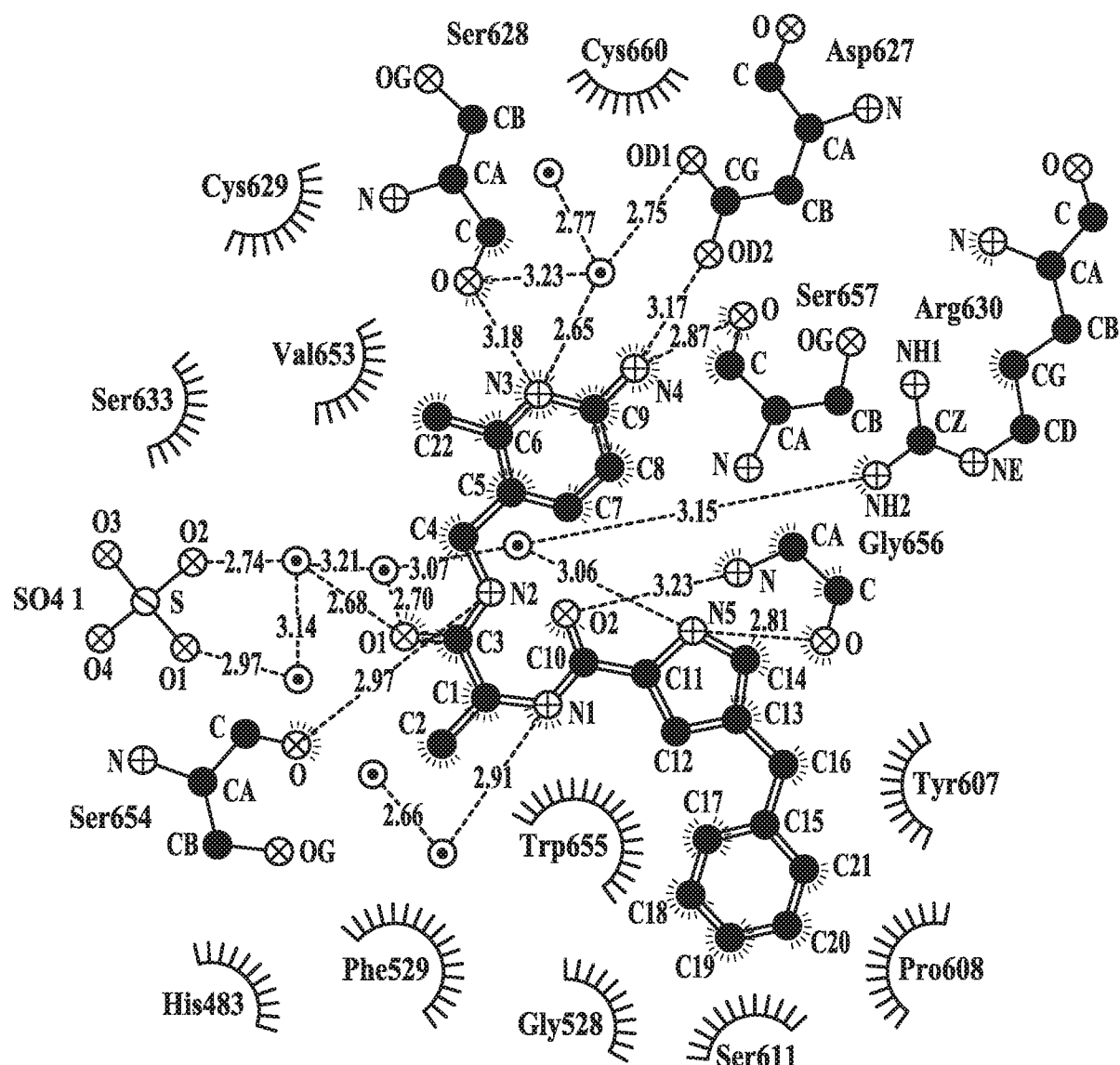
⊕—● Ligand bond
 ⊕—● Non-ligand bond
 ⊕-3.0-⊗ Hydrogen bond and its length
 His53 Non-ligand residues involved in hydrophobic contact(s)
 ● Corresponding atoms involved in hydrophobic contact(s)

FIG.46

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**FIG.47**

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● Carbon
 ⊕ Nitrogen
 ⊗ Oxygen
 ⊙ Water
 ○ Chlorine
 ⊖ Fluorine
 ⊙ Sulphur

⊕—● Ligand bond
 ⊕—● Non-ligand bond
 ⊕—3.0—⊗ Hydrogen bond and its length
 His53 Non-ligand residues involved in hydrophobic contact(s)
 ● Corresponding atoms involved in hydrophobic contact(s)

FIG.48

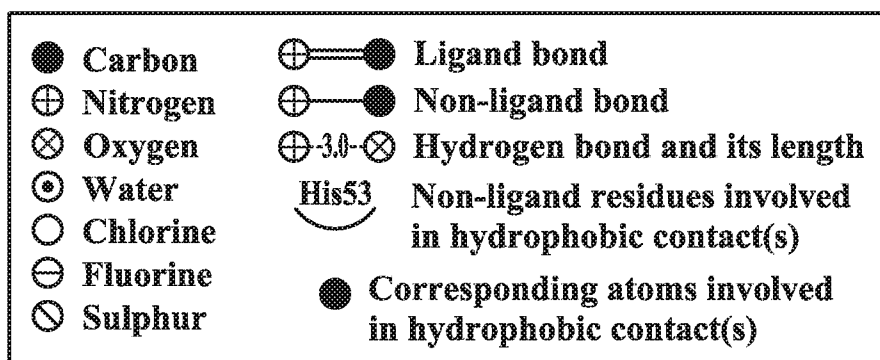
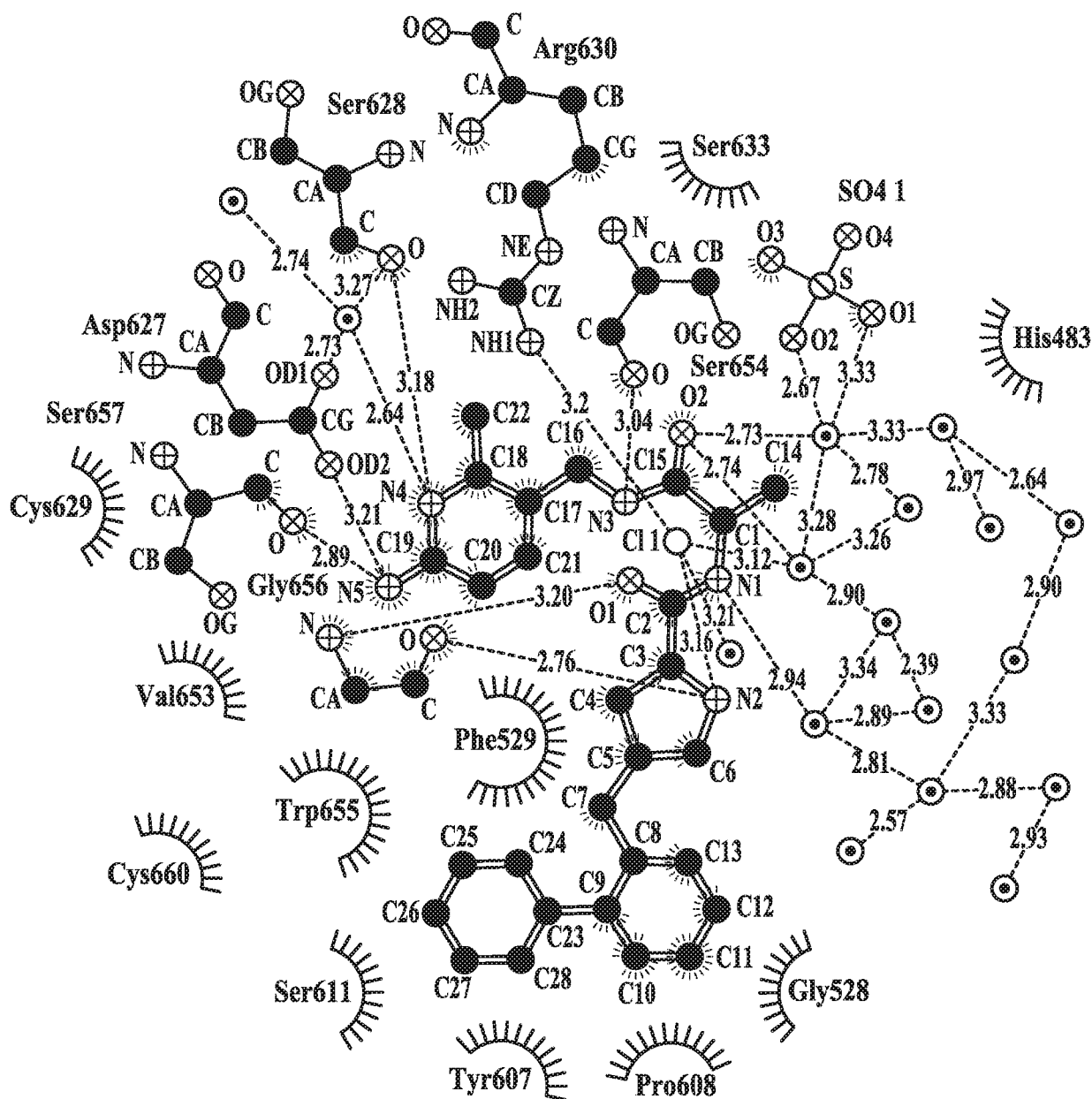
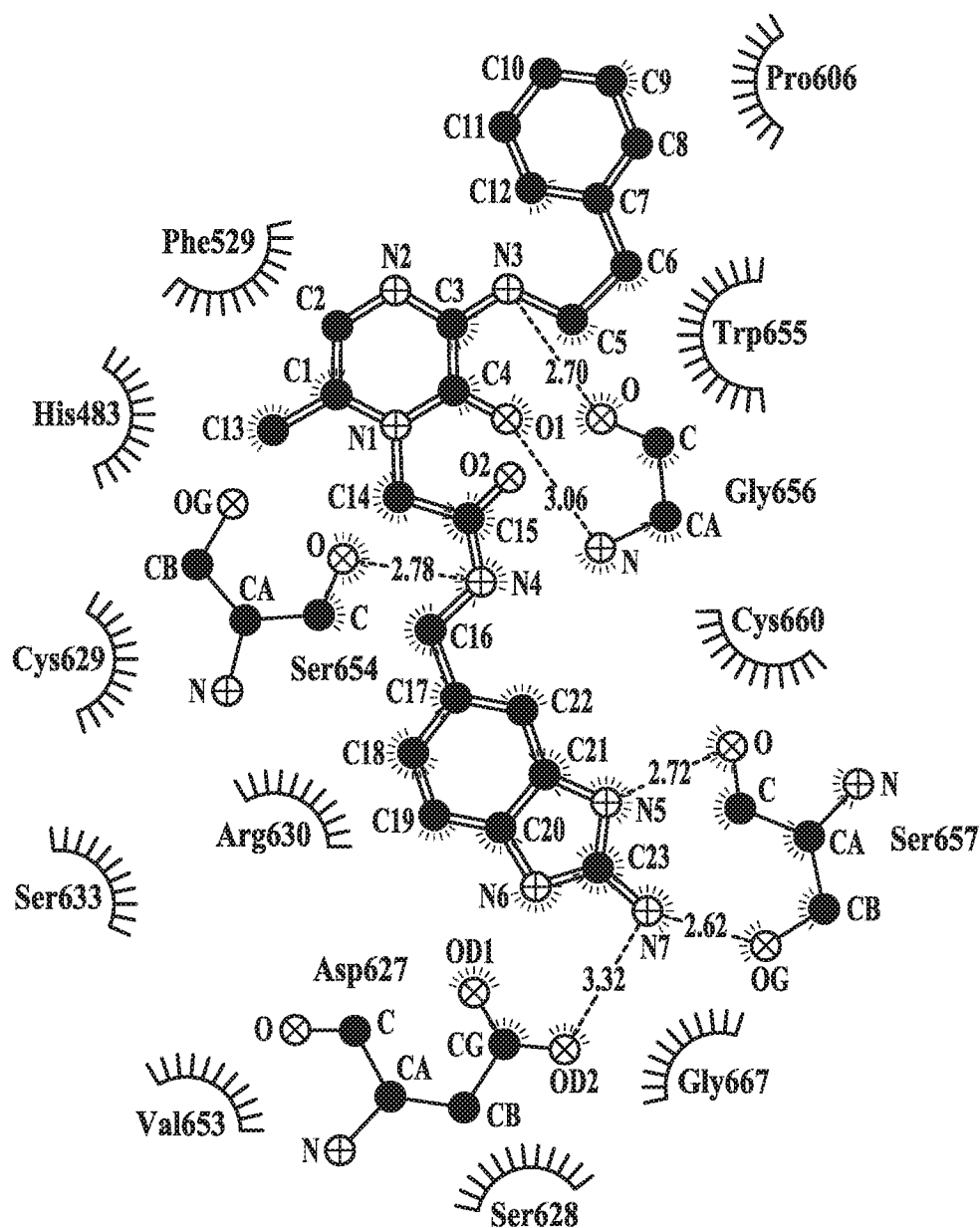
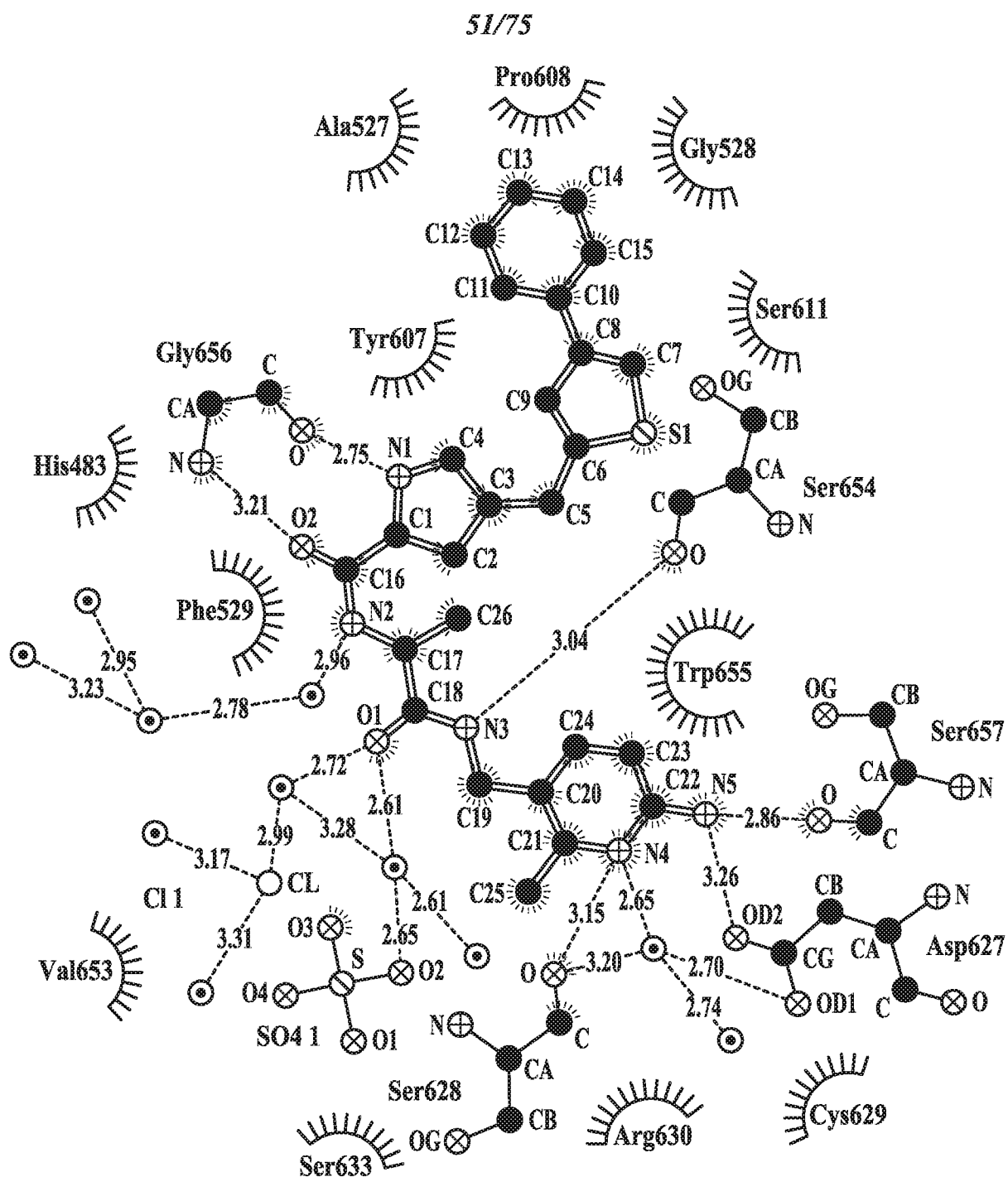


FIG. 49

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**FIG.50**

**FIG.51**

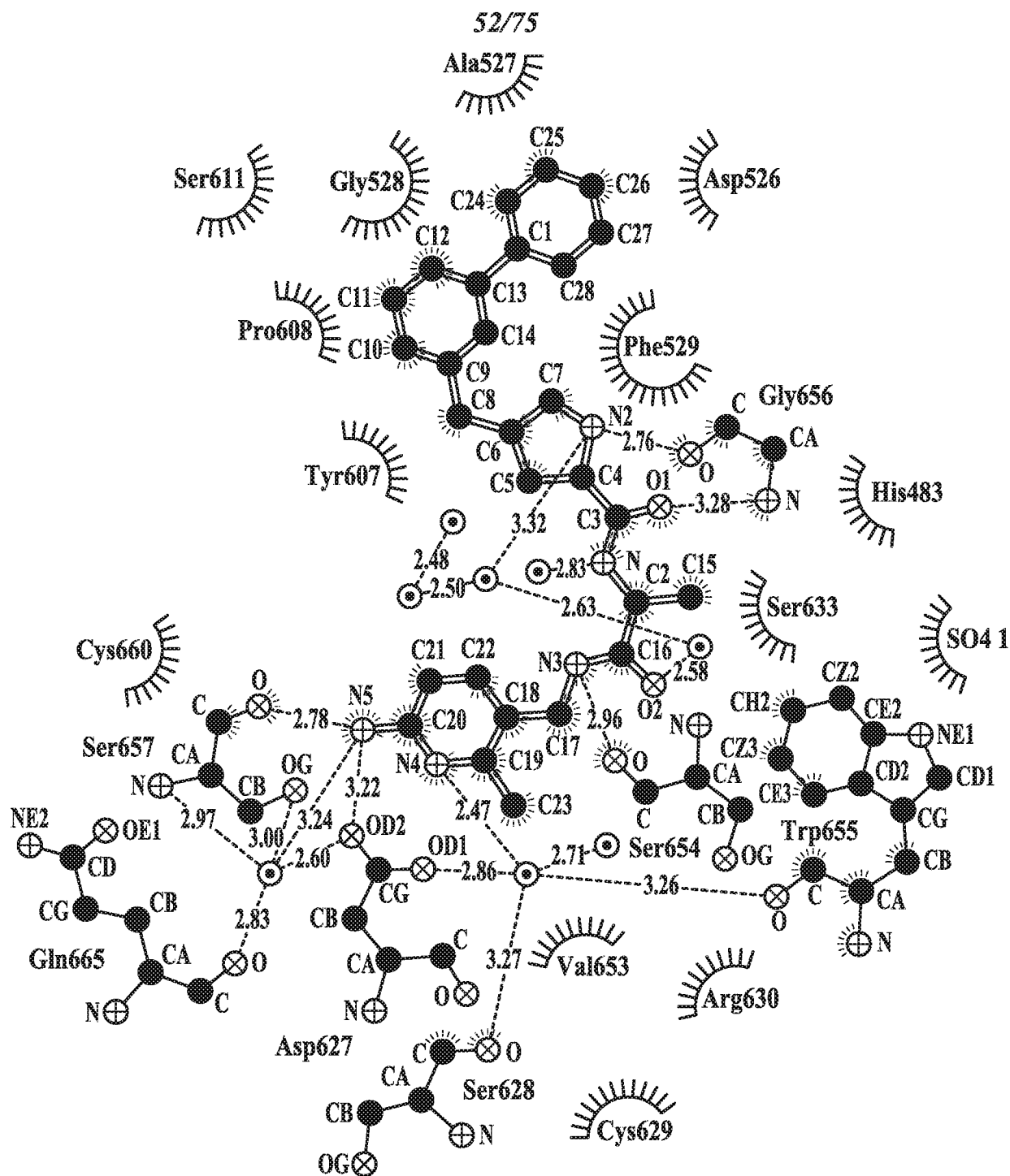
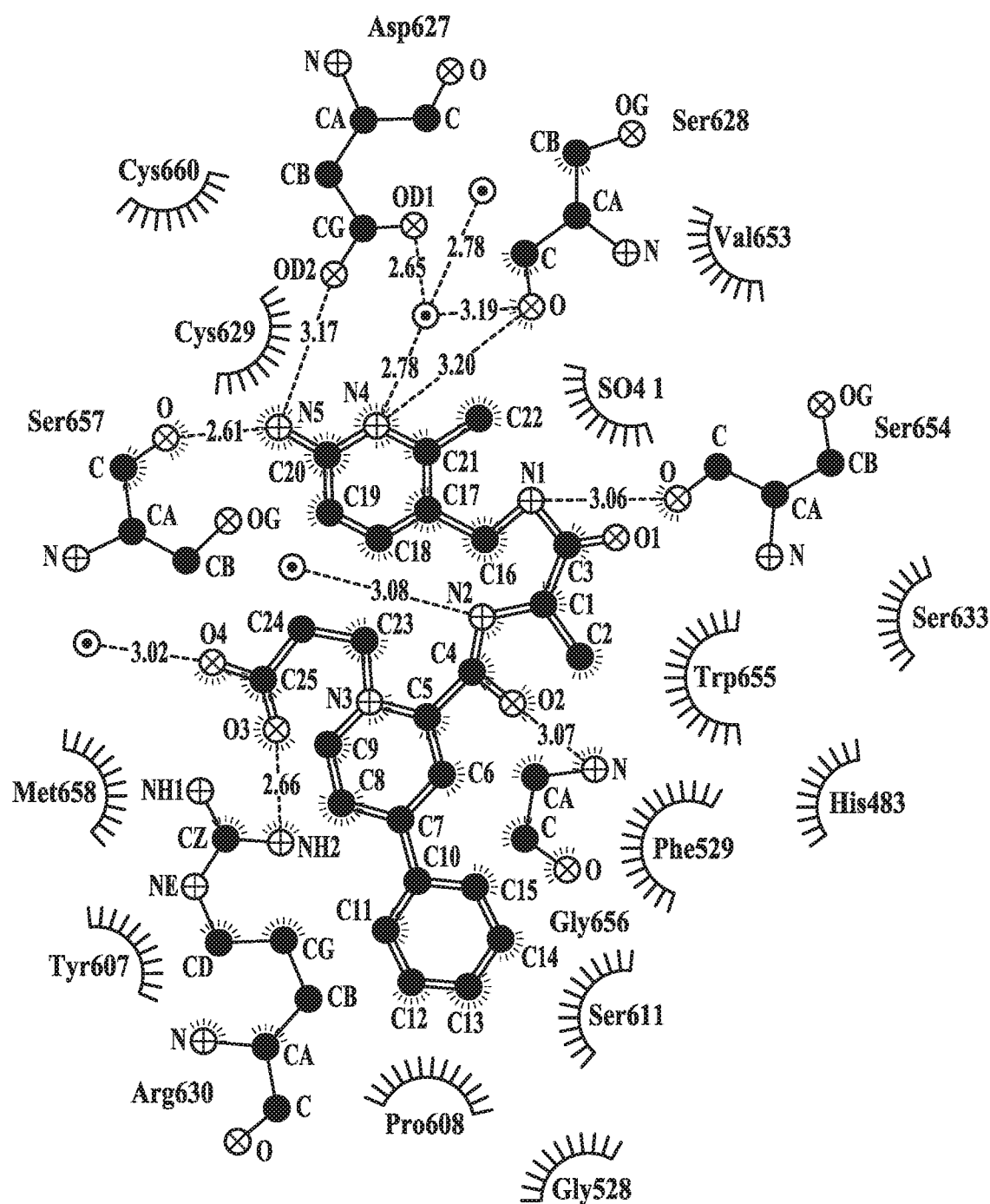


FIG. 52

● Carbon
 ⊕ Nitrogen
 ⊗ Oxygen
 ⊙ Water
 ○ Chlorine
 ⊖ Fluorine
 ⊘ Sulphur

⊕=● Ligand bond
 ⊕—● Non-ligand bond
 ⊕-3.0-⊗ Hydrogen bond and its length
 His53 Non-ligand residues involved in hydrophobic contact(s)
 ● Corresponding atoms involved in hydrophobic contact(s)

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**FIG.53**

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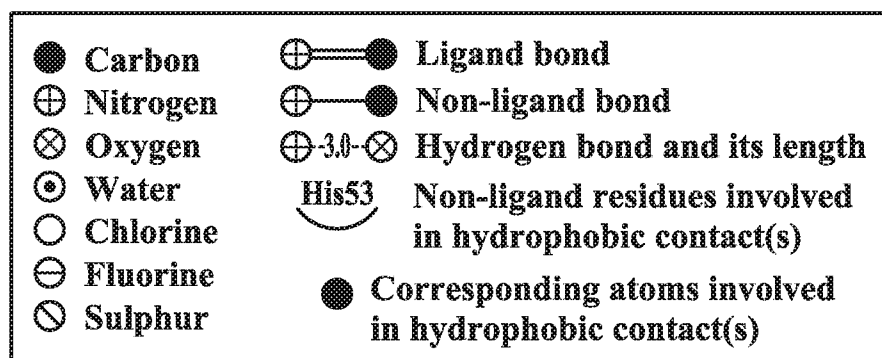
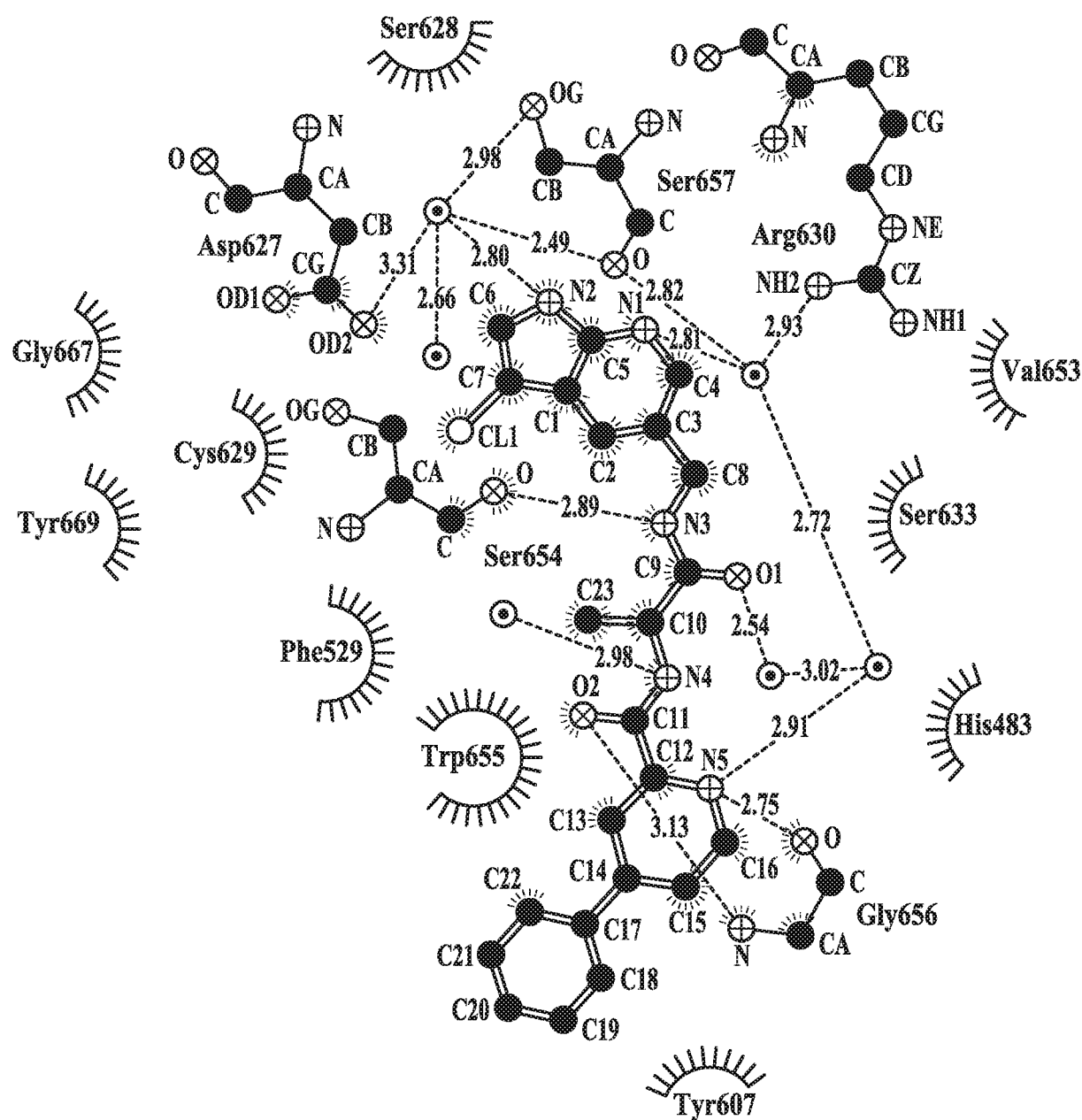
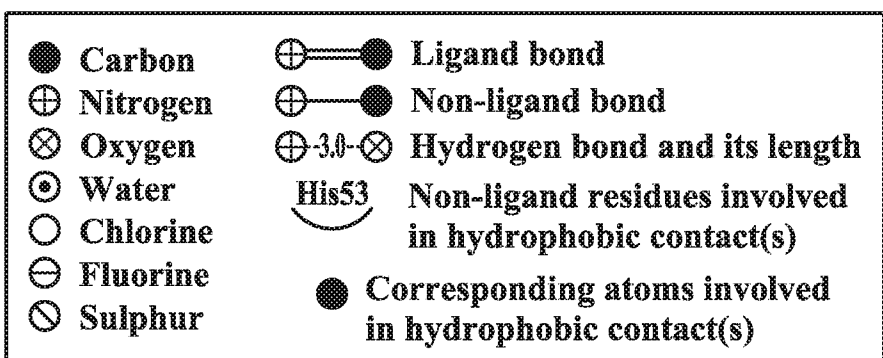
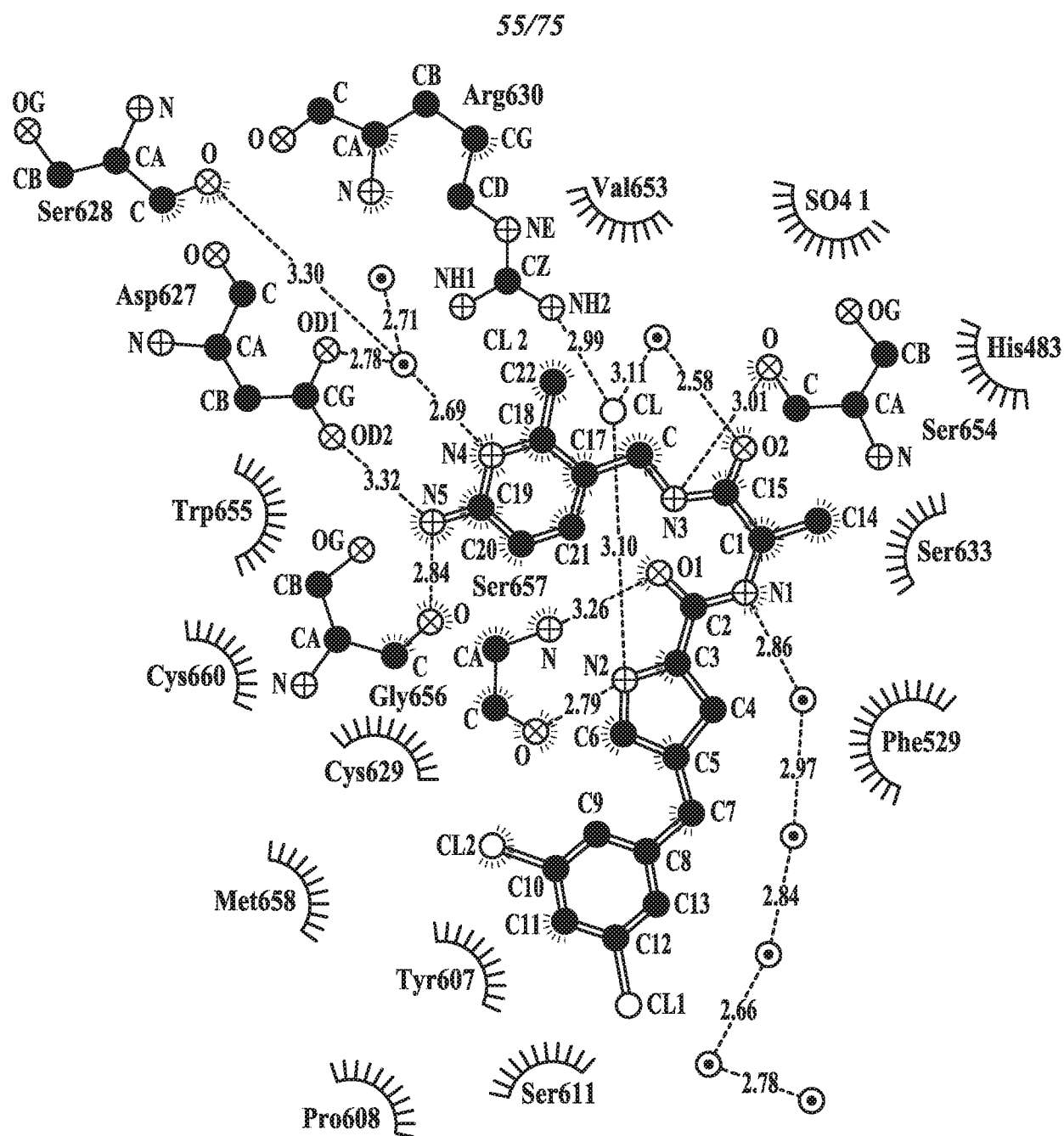


FIG. 54

**FIG.55**



- Carbon
 ⊕ Nitrogen
 ⊗ Oxygen
 ⊙ Water
 ○ Chlorine
 ⊖ Fluorine
 ⊘ Sulphur
- ⊕=● Ligand bond
 ⊕—● Non-ligand bond
 ⊕-3.0-⊗ Hydrogen bond and its length
 His53 Non-ligand residues involved in hydrophobic contact(s)
 ● Corresponding atoms involved in hydrophobic contact(s)

FIG. 56

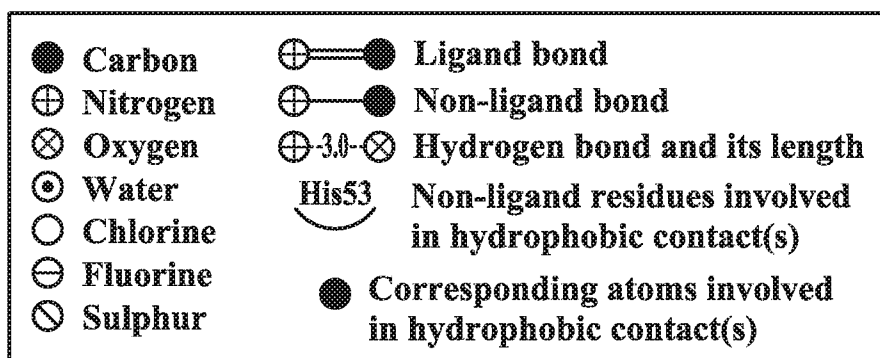
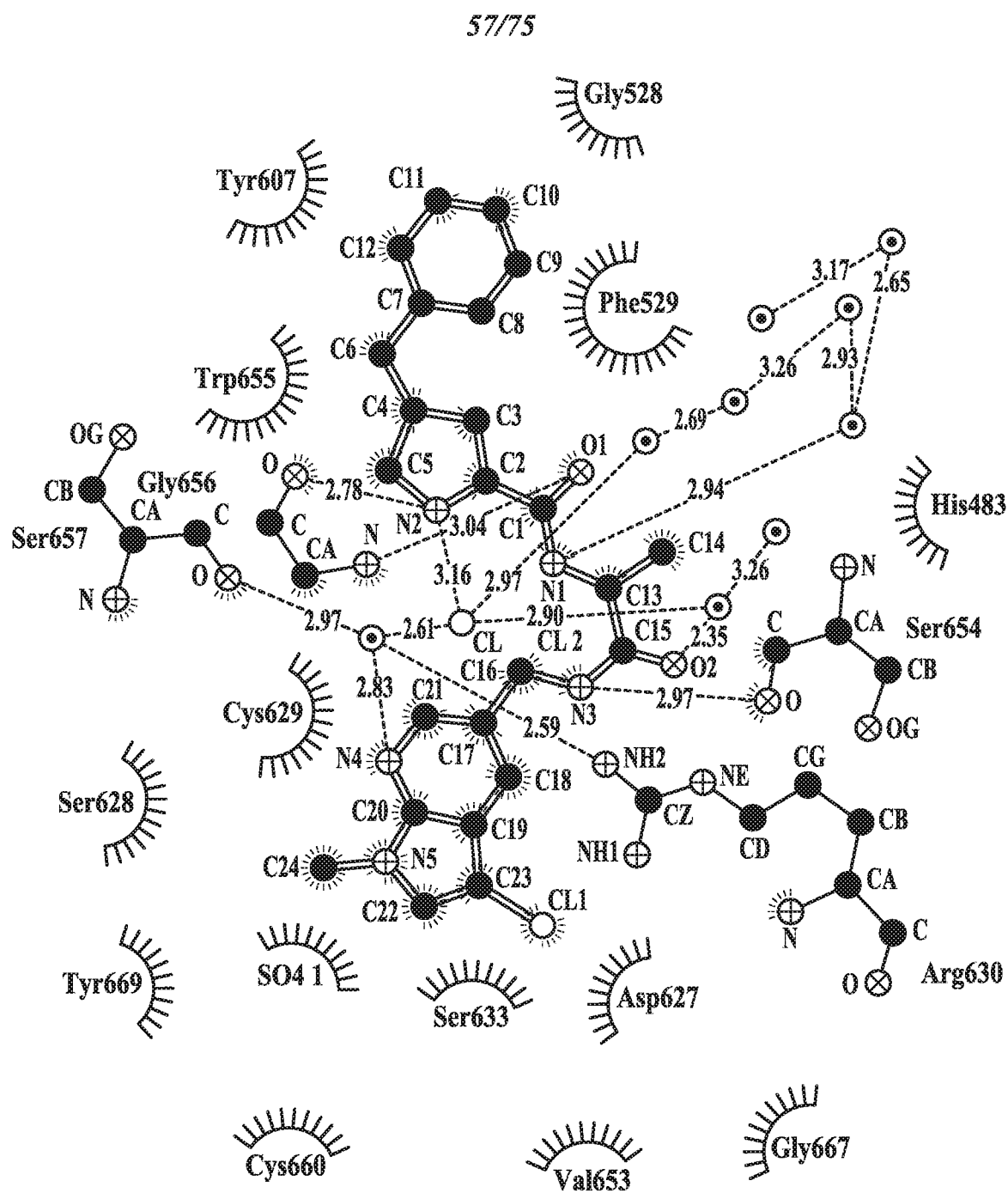


FIG. 57

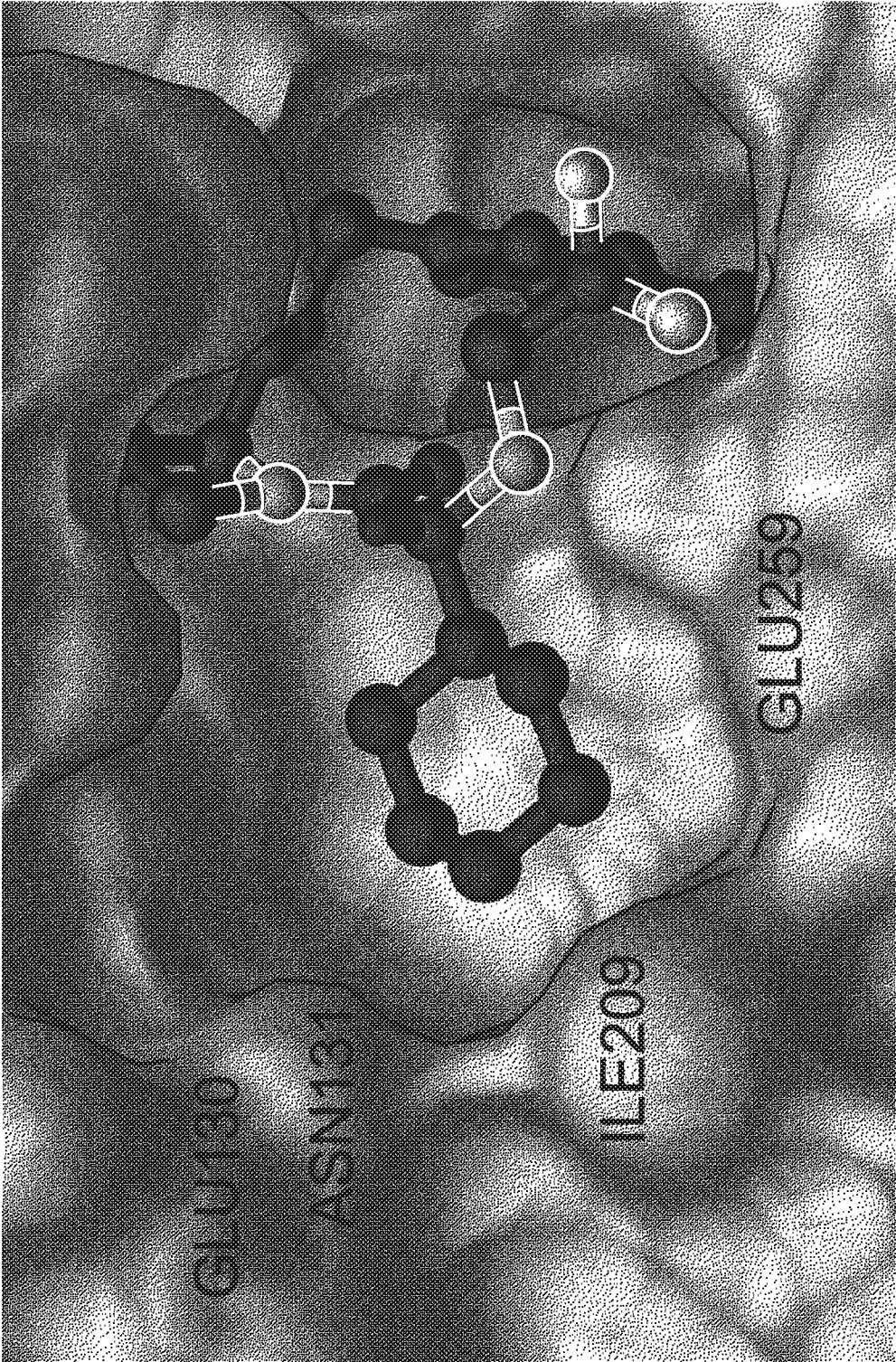


FIG. 58

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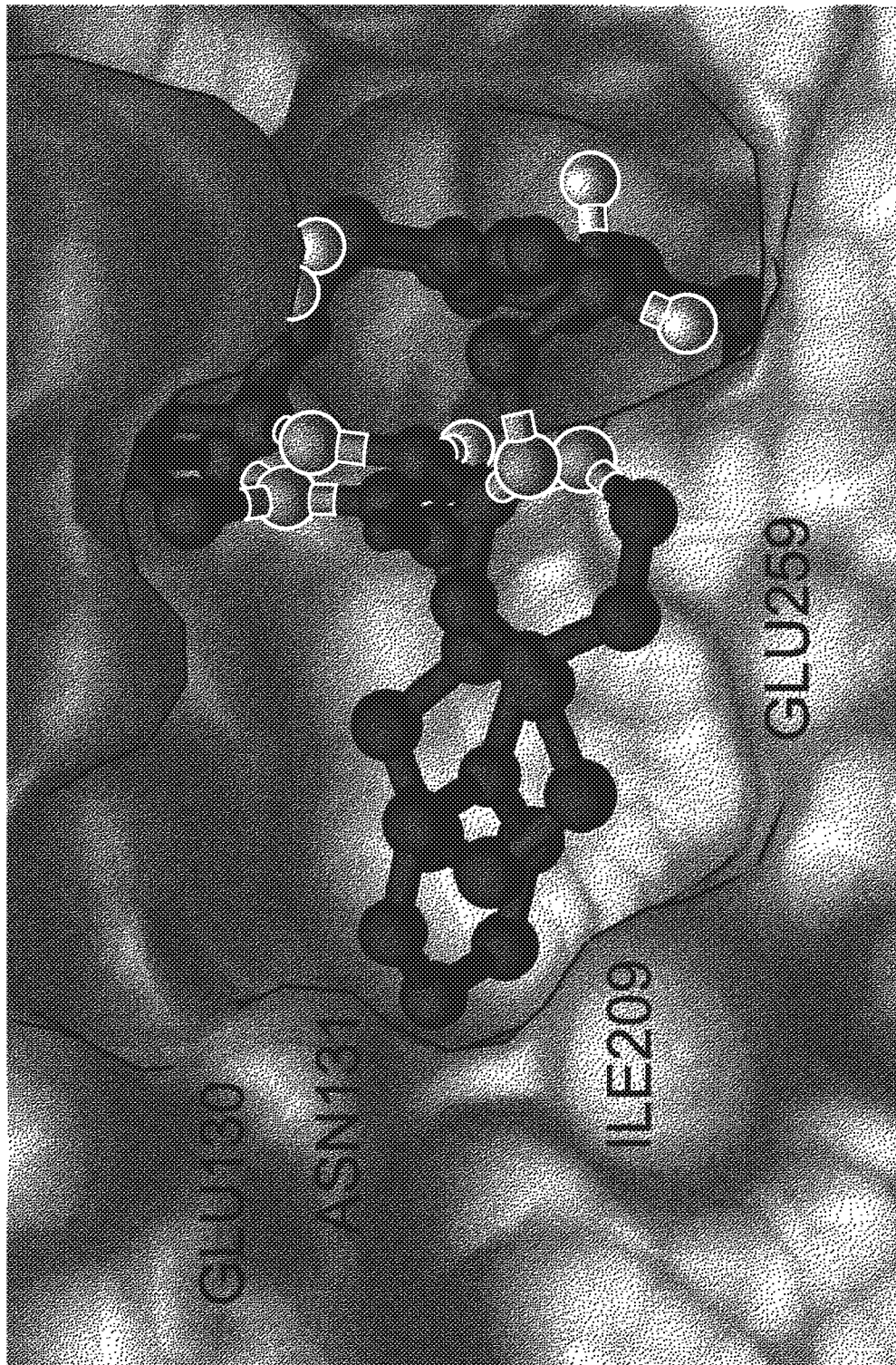


FIG.59

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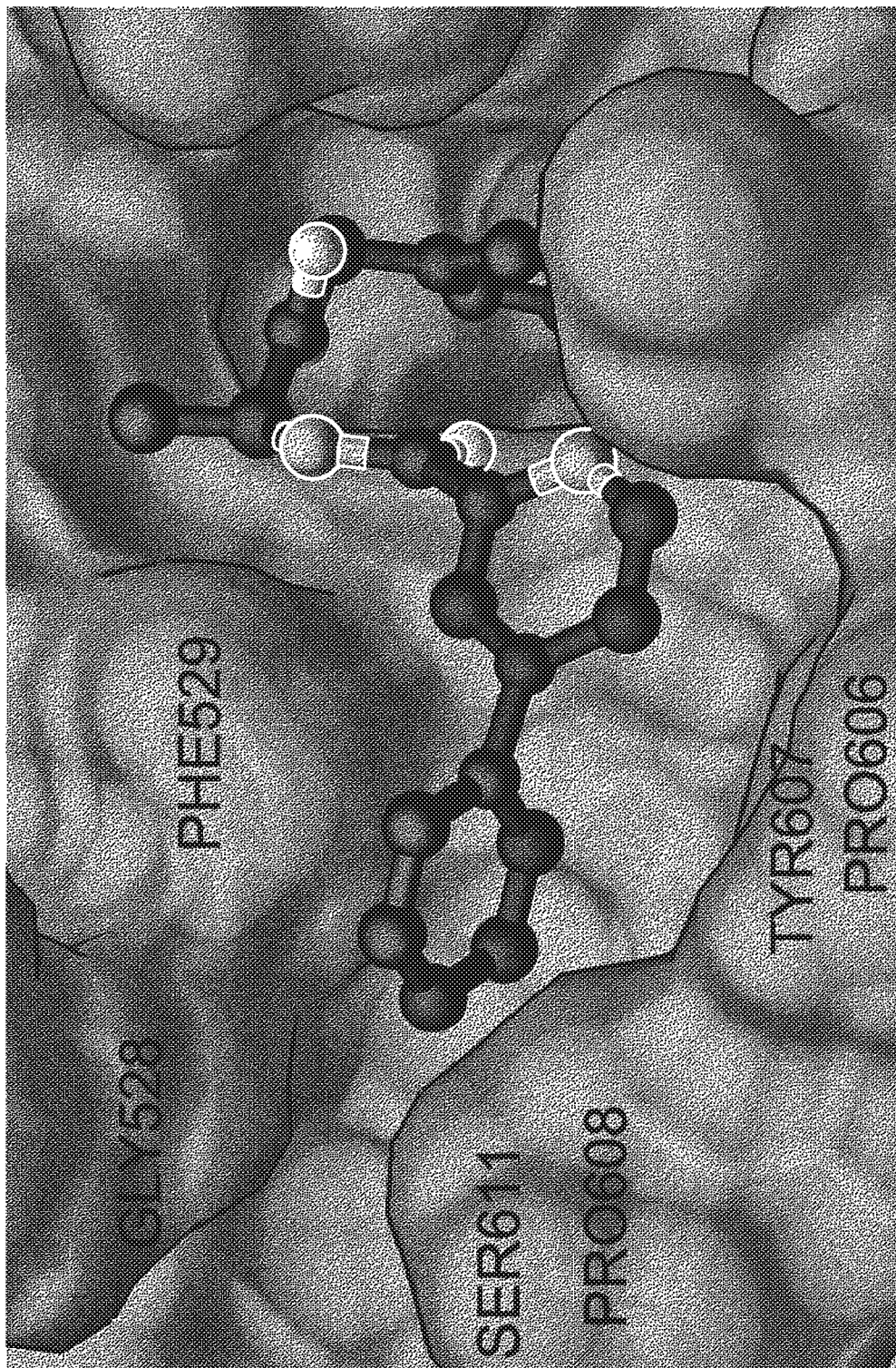


FIG. 60

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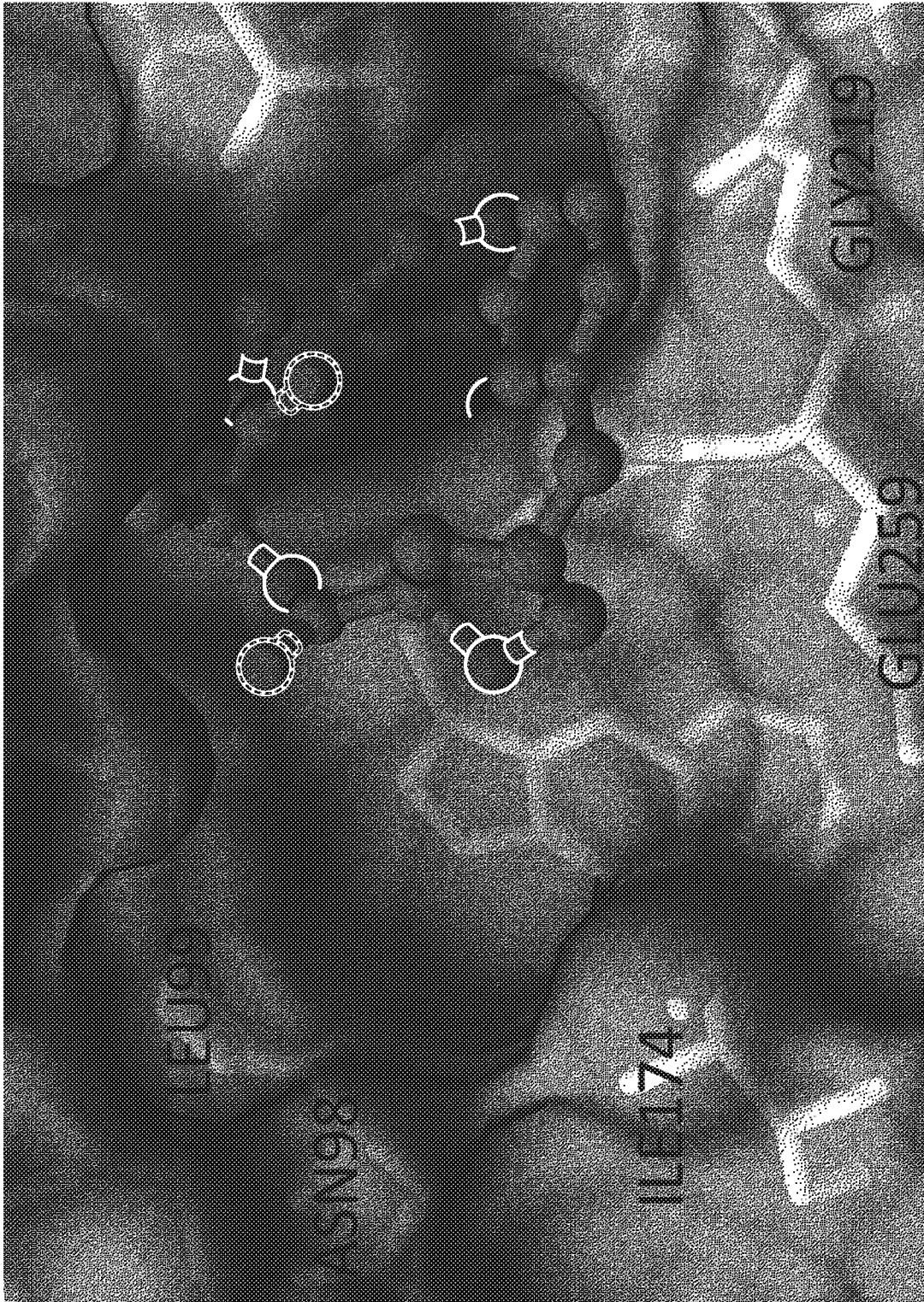


FIG.61

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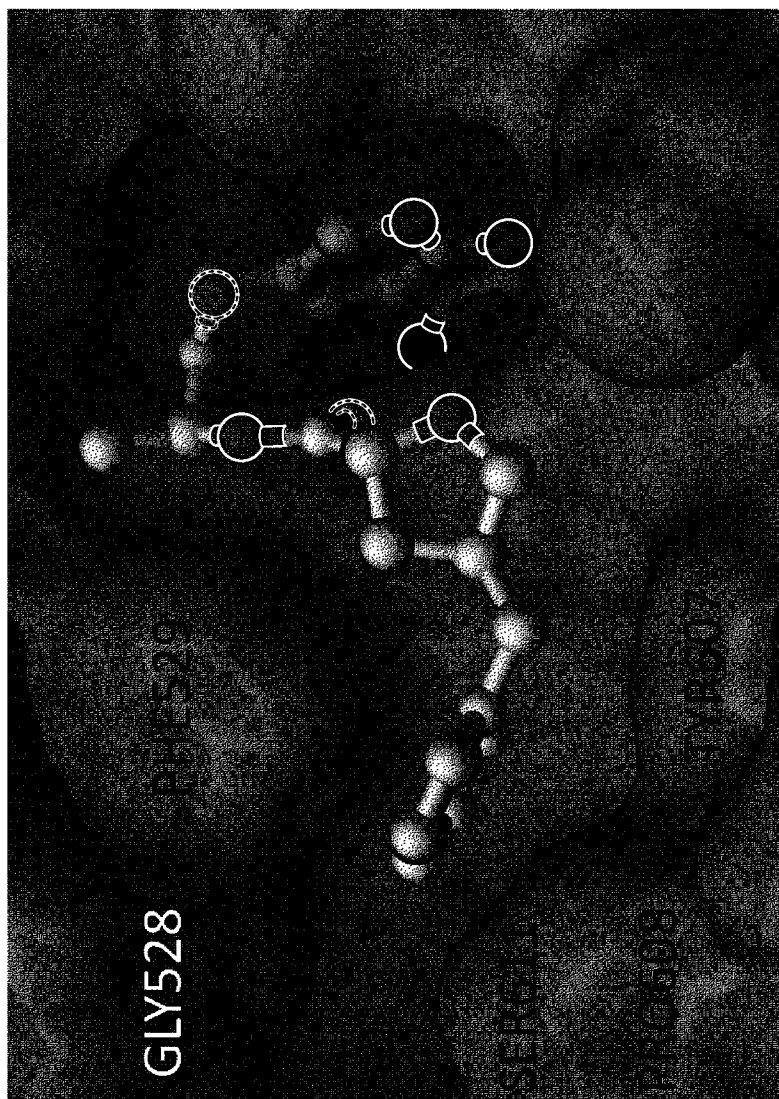


FIG. 62

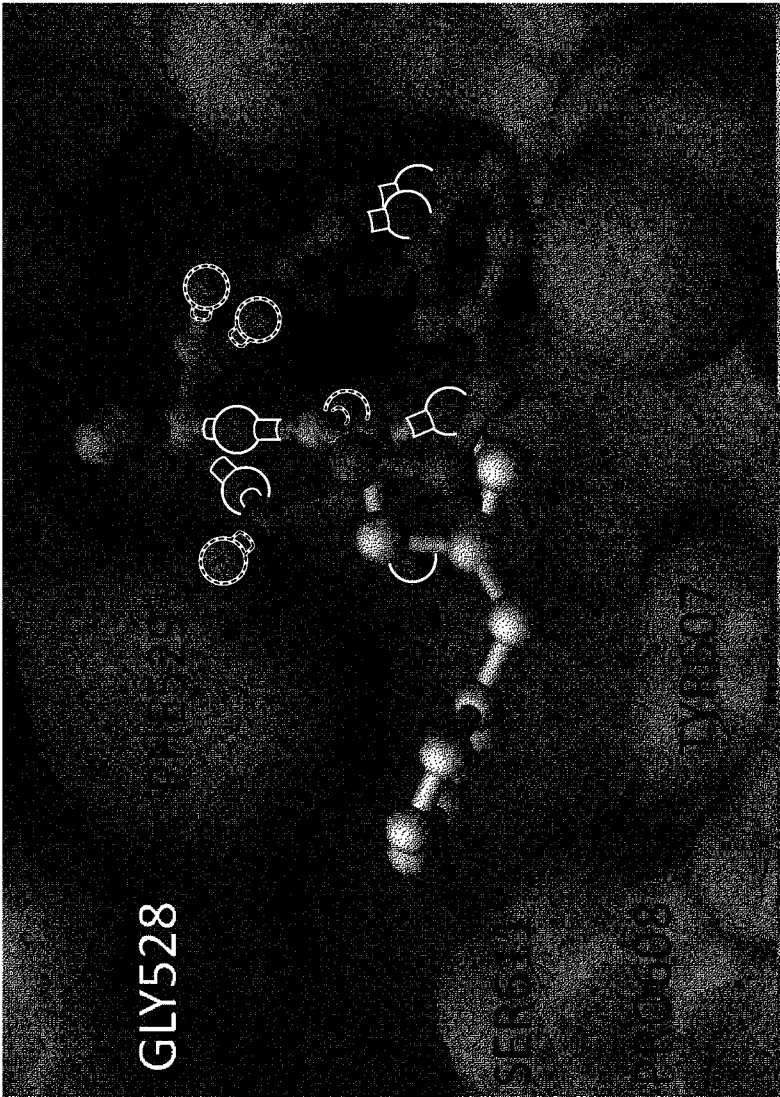


FIG.63

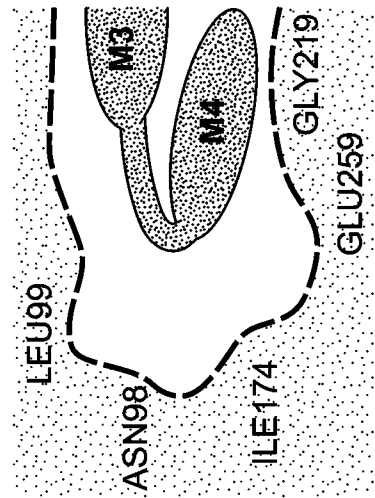


FIG.65

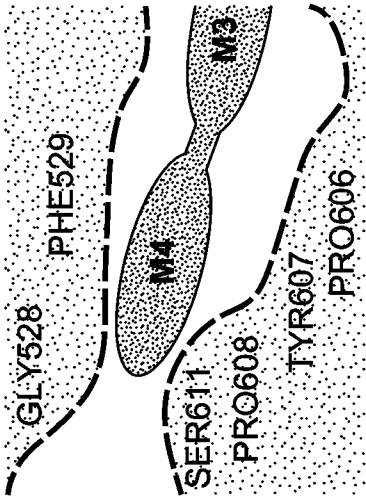


FIG.64

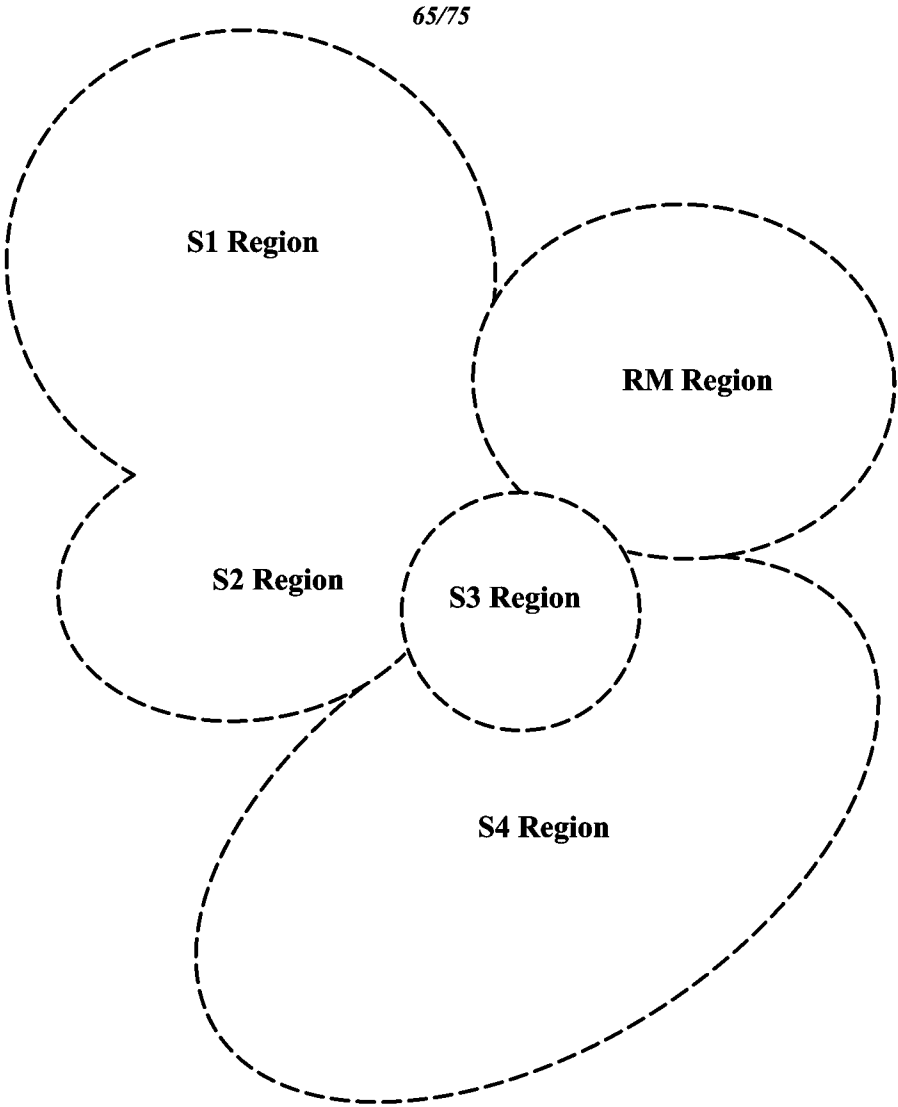
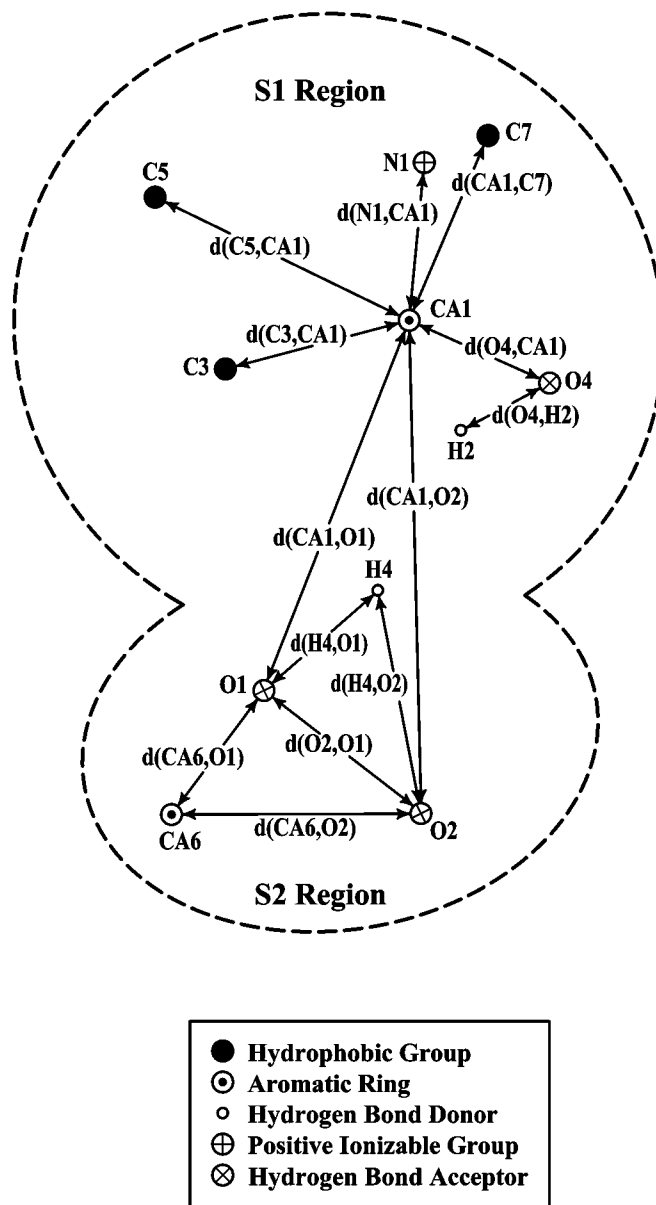
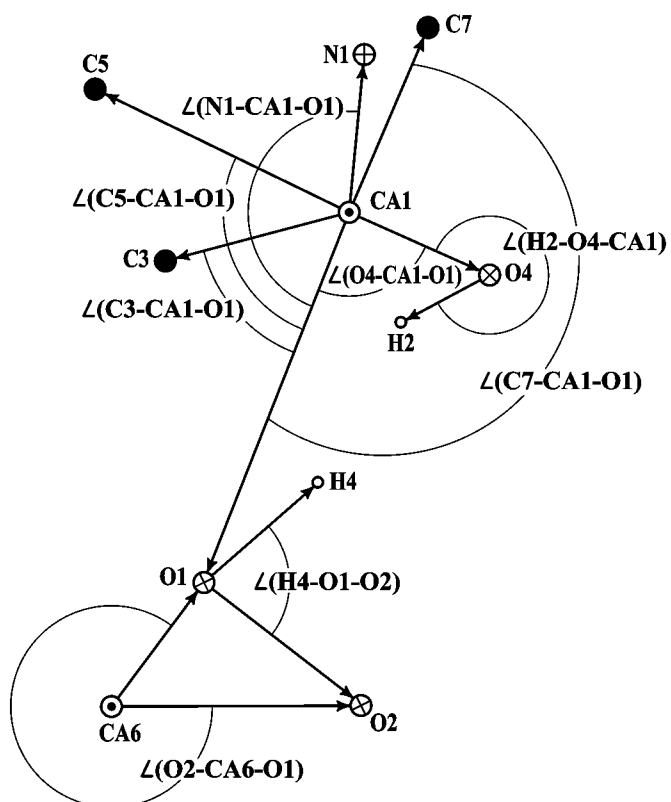


FIG.66

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**FIG.67**

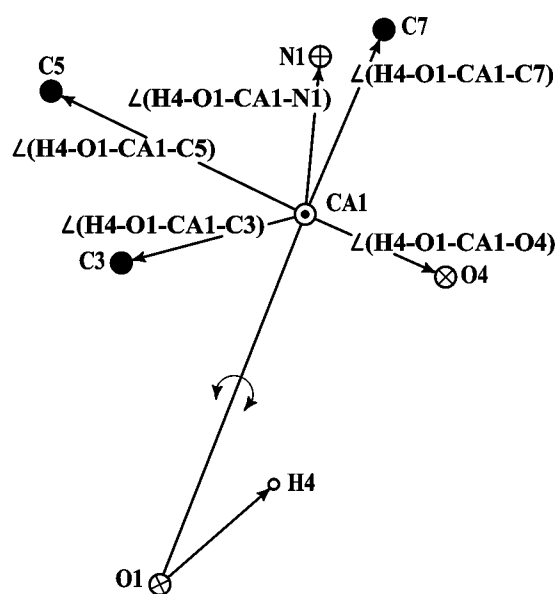
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- Hydrophobic Group
- ⊙ Aromatic Ring
- ∘ Hydrogen Bond Donor
- ⊕ Positive Ionizable Group
- ⊗ Hydrogen Bond Acceptor

FIG. 68

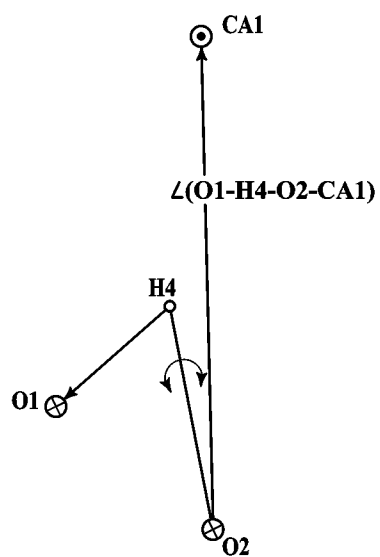
68/75



- Hydrophobic Group
- ⊙ Aromatic Ring
- Hydrogen Bond Donor
- ⊕ Positive Ionizable Group
- ⊗ Hydrogen Bond Acceptor

FIG. 69

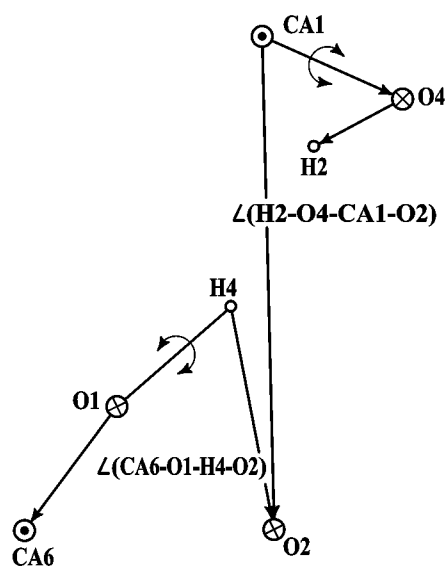
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- Hydrophobic Group
- ⊙ Aromatic Ring
- Hydrogen Bond Donor
- ⊕ Positive Ionizable Group
- ⊗ Hydrogen Bond Acceptor

FIG. 70

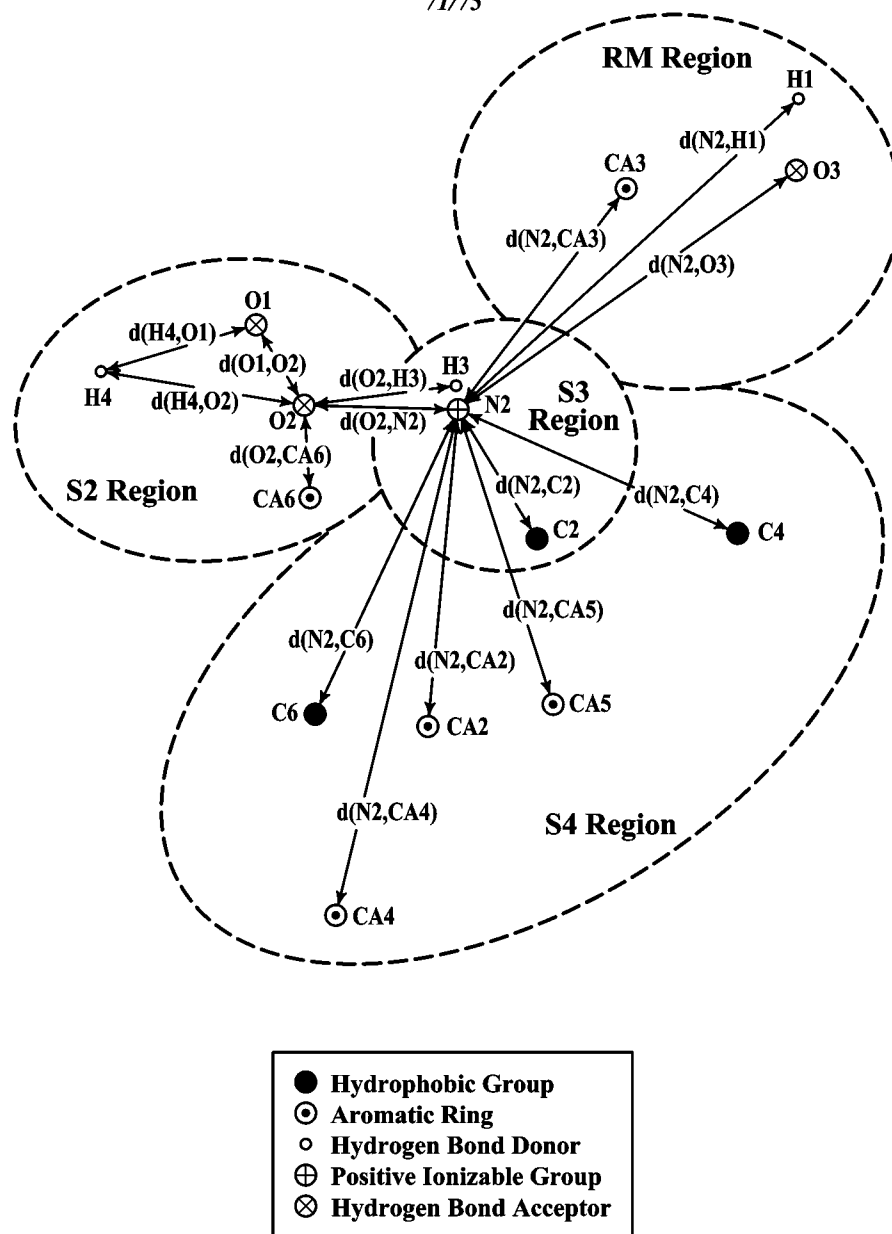
70/75



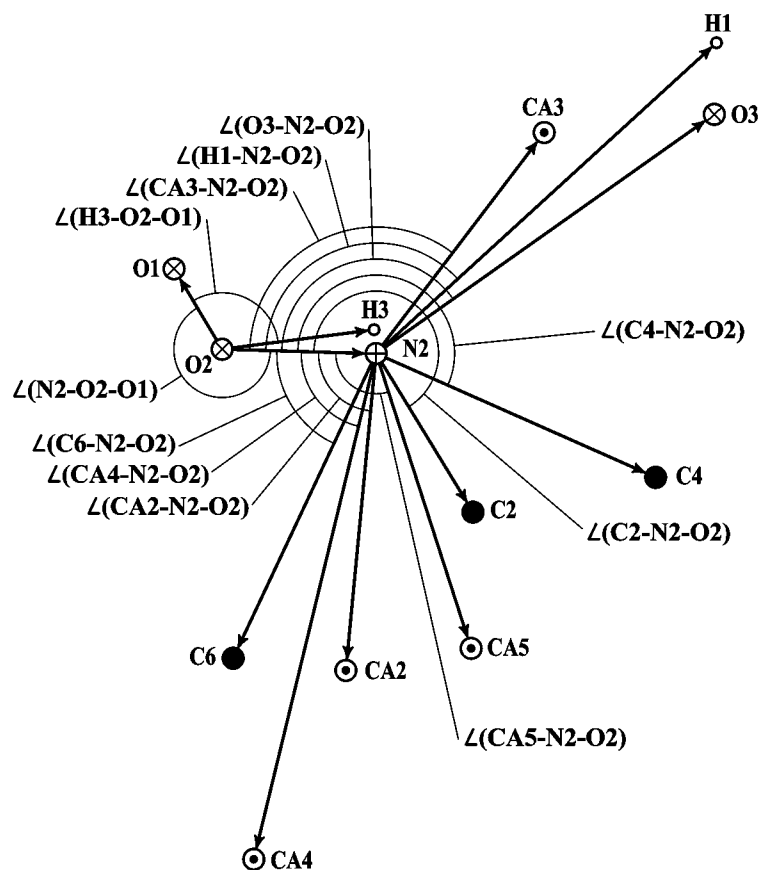
- Hydrophobic Group
- ⊙ Aromatic Ring
- Hydrogen Bond Donor
- ⊕ Positive Ionizable Group
- ⊗ Hydrogen Bond Acceptor

FIG. 71

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**FIG. 72**

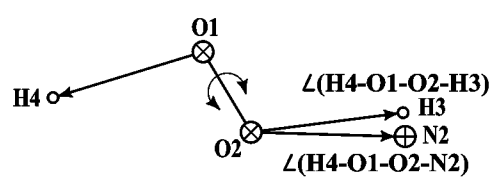
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- Hydrophobic Group
- ⊙ Aromatic Ring
- Hydrogen Bond Donor
- ⊕ Positive Ionizable Group
- ⊗ Hydrogen Bond Acceptor

FIG. 73

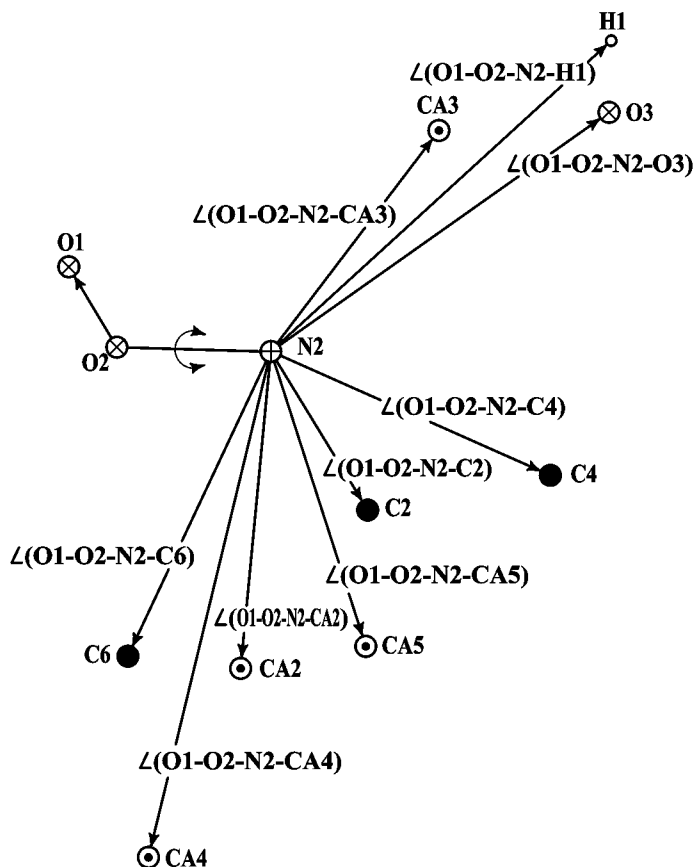
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- Hydrophobic Group
- ⊙ Aromatic Ring
- Hydrogen Bond Donor
- ⊕ Positive Ionizable Group
- ⊗ Hydrogen Bond Acceptor

FIG. 74

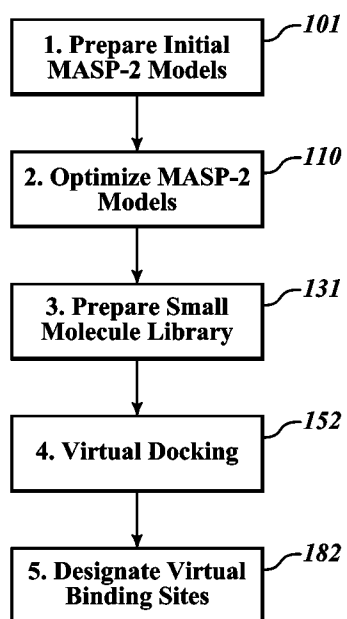
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- Hydrophobic Group
- ⊙ Aromatic Ring
- Hydrogen Bond Donor
- ⊕ Positive Ionizable Group
- ⊗ Hydrogen Bond Acceptor

FIG. 75

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**FIG. 76**