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(54) Title: METHIONINE AMINOPEPTIDASE AND METHODS OF USE

(57) Abstract: MetAP crystalline structures are disclosed. Also disclosed are inhibitors of bacterial methionine aminopeptidases, useful in treating bacterial infections and methods of identifying inhibitors of this aminopepticlase and methods of inhibiting MetAP using inhibitors with certain structural and spatial characteristics.

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METHIONINE AMINOPEPTIDASE AND METHODS OF USE

FIELD OF THE INVENTION

The present invention relates to the identification of novel bacterial methionine aminopeptidase (herein "MetAP") crystalline structures. In particular, it provides novel methionine aminopeptidase active sites of crystalline structures and active sites of crystalline structures in complex with inhibitors and methods to use these crystalline forms and their active sites to identify and improve methionine aminopeptidase inhibitor compounds, among other uses. These compounds are characterized by the ability to competitively inhibit binding of substrates or other like-molecules to the active site of MetAP, a member of the aminopeptidase family.

BACKGROUND OF THE INVENTION

Methionine aminopeptidases are ubiquitously distributed in all living organisms. They catalyze the removal of the initiator methionine from newly translated polypeptides using divalent metal ions as cofactors. Two distantly related MetAP enzymes, type 1 and type 2, are found in eukaryotes, which at least in yeast, are both required for normal growth; whereas one MetAP is currently known in eubacteria (type 1) and archaebacteria (type 2). The N-terminal extension region distinguishes the MetAPs in eukaryotes from those in procaryotes. A 64-amino acid sequence insertion (from residues 381 to 444 in hMetAP2) in a catalytic C-terminal domain distinguishes the MetAP-2 family from the MetAP-1 family. Despite the difference in the gene structure, MetAP enzymes appear to share a highly conserved catalytic scaffold termed "pita-bread" fold (Bazan, et al. (1994) *Proc. Natl. Acad. Sci. U.S.A. 91*, 2473) containing six strictly conserved residues implicated in the coordination of the metal cofactors.

N-terminal methionine removal in bacteria is a two-step process requiring first the removal on the N-formyl group by polypeptide deformylase followed by cleavage of the N-terminal methionine when the adjacent amino acid is small (e.g., Ala, Pro, Ser, Thr, Gly, Cys, and Val). Both of these steps appear to be essential for cell viability. Failure to remove the N-terminal methionine can lead to inactive enzymes (e.g., glutamine phosphoribosylpyrophosphate amidotransferase and N-terminal nucleophile hydrolases). Therefore, inhibition or other modulation of MetAP may have a wide-ranging effect inhibiting or otherwise modulating the action of essential enzymes involved in varied cellular processes.

MetAP is an attractive antibacterial target as this enzyme has been demonstrated to be essential for bacterial growth *in vitro* (Chang, et al. (1989) *J. Bacteriol. 171*, 4071, and Miller et al. (1989) *J. Bacteriol. 171*, 5215.); and appears to be universally conserved in prokaryotes. This indicates that inhibitors or other modulators directed against this target will be broad-spectrum agents and will kill bacteria. Further, this inventions provides that this gene may be transcribed in thigh lesion and pyelonephritis models of infection with *S. aureus* as well as both early and late in murine respiratory tract infection with *S. pneumoniae*. These models indicate the importance of this process in infection.

SUMMARY OF THE INVENTION

In one aspect, the present invention relates to methionine aminopeptidase (herein "MetAP") crystalline structures, for example, a MetAP in crystalline form derived from *S. aureus* or *S. pneumoniae.*

In another aspect, the present invention provides a crystalline form of a *S. aureus* methionine aminopeptidase in complex with a MetAP inhibitor or other modulator, for example a triazole, for example, a 1,2,3 triazole.

In another aspect, the present invention provides a crystalline form of a *S. aureus* methionine aminopeptidase in complex with an inhibitor or other modulator, 5-benzofuran-2-yl-1-H-[1,2,3]triazole or 5-(3-Iodo-phenyl)-1-H-[1,2,3]triazole.

In yet another aspect, the invention provides a role for residues in an active site responsible for binding of aminopeptidase inhibitors or other modulators by MetAP.

In yet another aspect, the invention provides a method of modulating an activity of a bacterial MetAP comprising administering to a mammal in need therof a compound that spatially fits into an active site of MetAP.

In yet another aspect, the invention provides a structural basis to identify positions of amino acid residues and metals bound to those residues with respect to an inhibitor or other modulator and a method for identifying inhibitors or other modulators of MetAP.

Another aspect of this invention comprises machine-readable media encoded with data representing coordinates of a three-dimensional structure of a MetAP crystal structure alone or in complex with an inhibitor or other modulator.

A further aspect of the invention provides for a *Staphylococcus aureus* MetAP defined by three dimensional protein coordinates of Table I in an essentially pure form or a homolog thereof.

Another aspect of this invention includes a *Staphylococcus aureus* MetAP wherein the MetAP crystal form comprises cubic crystals with a space group I23.

In yet another aspect, the invention provides a *Staphylococcus aureus* MetAP wherein cubic crystals comprise a lattice constant of about a=121.36 Ångstroms (Å).

Another aspect of this invention includes a *Staphylococcus aureus* MetAP wherein a MetAP crystal form comprises monoclinic crystals with a space group $P2_1$ and lattice constants of about a=41.19Å, about b=76.78Å, and about c=41.71Å, β=104.165°.

Another aspect of this invention includes a *Staphylococcus aureus* MetAP wherein a MetAP crystal form is in complex with a MetAP inhibitor or other modulator, for example, 5-(3-Iodo-phenyl)-1-H-[1,2,3] triazole and 5-benzofuran-2-yl-1-H-[1,2,3]triazole.

A further aspect of the invention provides a *Streptococcus pneumoniae* MetAP defined by three dimensional protein coordinates of Table VIII in an essentially pure form, partially pure form, pure form, or a homolog of any thereof.

Another aspect of this invention includes a *Streptococcus pneumoniae* MetAP wherein a crystal form comprises orthorhombic crystals with a space group $P2_12_12_1$, wherein said orthorhombic crystals comprise lattice constants of about a=56.77Å, about b=69.16Å, and about c=80.51Å.

In yet another aspect, the invention provides a *Streptococcus pneumoniae* MetAP in complex with a MetAP inhibitor or other modulator, such as a triazole, for example a 1,2,3 triazole.

Another aspect of this invention includes a process for determining a bacterial MetAP crystalline form of other bacteria or species by using structural coordinates of a *Staphylococcus aureus* MetAP crystal or portions thereof, to determine a crystal structure of a mutant, homologue, or co-complex of a binding pocket or active site by molecular replacement.

Another aspect of this invention includes a process for determining a bacterial MetAP crystalline form of other bacteria or species by using structural coordinates of a *Streptococcus pneumoniae* MetAP crystal or portions thereof, to determine a crystal structure of a mutant, homologue, or co-complex of a binding pocket or active site by molecular replacement.

A further aspect of the invention provides a process of identifying a bacterial MetAP inhibitor or other modulator capable of binding to and inhibiting or otherwise modulating an enzymatic activity of a bacterial MetAP said process comprising:

introducing into a suitable computer program information defining an active site conformation of a MetAP molecule comprising a conformation defined by crystal coordinates comprising those listed in Tables I to X wherein said program displays a three-dimensional structure;

creating a three dimensional structure of a test compound in said computer program;

displaying and superimposing a model of said test compound on a model of said active site;

incorporating said test compound in a biological methionine aminopeptidase activity assay for a methionine aminopeptidase characterized by said active site; and

determining whether said test compound inhibits or otherwise modulates an enzymatic activity in said assay.

Another aspect of this invention includes a process for designing inhibitors or other modulators of MetAP activity using atomic coordinates of a bacterial MetAP in crystalline form to computationally evaluate a chemical entity for associating with an active site of a MetAP enzyme.

In yet another aspect, the invention provides a method of modifying a test bacterial MetAP polypeptide comprising:

providing a test bacterial MetAP polypeptide sequence having a characteristic that is targeted for modification;

aligning the test bacterial MetAP polypeptide sequence with a reference bacterial MetAP polypeptide sequence for which an X-ray structure is available, wherein the reference bacterial MetAP polypeptide sequence has a characteristic that is desired for the test bacterial MetAP polypeptide;

building a three-dimensional model for the test bacterial MetAP polypeptide using the three-dimensional coordinates of the X-ray structure(s) of a reference bacterial MetAP polypeptide and its sequence alignment with the test bacterial MetAP polypeptide sequence;

examining the three-dimensional model of the test bacterial MetAP polypeptide for a difference in an amino acid residue as compared to a reference bacterial MetAP polypeptide, wherein the residues are associated with the desired characteristic; and

mutating an amino acid residue in the test bacterial MetAP polypeptide sequence located at a difference identified in step (d) to a residue associated

with the desired characteristic, whereby the test bacterial MetAP polypeptide is modified.

Another aspect of the invention provides a method for the treatment of an individual having need to inhibit or other wise modulate a bacterial methionine aminopeptidase comprising: administering to the individual an amount, for example, a therapeutically effective amount, of a compound that binds to, alters the structure of, or interacts with, an active site of a bacterial MetAP enzyme. In a further embodiment, a compound is selected from the group consisting of 5-(3-Iodo-phenyl)-1-H-[1,2,3] triazole and 5-benzofuran-2-yl-1-H-[1,2,3]triazole, or a pharmaceutically active salt or solvate thereof.

In yet another aspect, the invention provides a method of drug design comprising using the structural coordinates of a MetAP crystal to computationally evaluate a chemical entity for associating with the inhibitor or modulator binding site of MetAP.

A further aspect of the invention provides a method for modulating an activity of a bacterial methionine aminopeptidase comprising: contacting a methionine aminopeptidase with a compound that binds to, alters a structure of, or interacts with, an active site of a bacterial MetAP enzyme and modulates said activity of said methionine aminopeptidase. In a further embodiment, a compound is selected from the group consisting of 5-(3-Iodo-phenyl)-1-H-[1,2,3] triazole and 5-benzofuran-2-yl-1-H-[1,2,3]triazole, or a pharmaceutically active salt or solvate thereof. Another aspect of this invention provides a method for modulating an activity of a bacterial methionine aminopeptidase comprising: contacting a methionine aminopeptidase with a compound that comprises an activity selected from the group consisting of: bonding with, complexing with, coordinating with and/or cocrystalizing with an amino acid residue or residues defined by a protein coordinate or coordinates set forth in Table I; bonding with, complexing with, coordinating with and/or cocrystalizing with a *Staphylococcus aureus* MetAP crystal form comprising cubic crystals comprising a space group I23; bonding with, complexing with, coordinating with and/or cocrystalizing with a *Staphylococcus aureus* MetAP cubic crystal comprising a lattice constant of about a=121.36 Ångstroms (Å); bonding with, complexing with, coordinating with and/or cocrystalizing with a *Staphylococcus aureus* MetAP crystal form comprising a monoclinic crystal with a space group $P2_1$ and lattice constants of about a=41.19Å, about b=76.78Å, and about c=41.71Å, β=104.165°; bonding with, complexing with, coordinating with and/or cocrystalizing with an amino acid residue or residues defined by

a protein coordinate or coordinates set forth in Table VIII; bonding with, complexing with, coordinating with and/or cocrystalizing with a *Streptococcus pneumoniae* MetAP crystal form comprising orthorhombic crystals with a space group $P2_12_12_1$, wherein said orthorhombic crystals comprise lattice constants of about a=56.77Å, about b=69.16Å, and about c=80.51Å; bonding with, coordinating with and/or cocrystalizing with a *Streptococcus pneumoniae* MetAP in complex with a MetAP inhibitor or other modulator; and bonding with, complexing with, coordinating with and/or cocrystalizing with a bacterial MetAP enzyme.

A further embodiment of the inventions provides a compound or composition comprising a compound that modulates an activity of a bacterial methionine aminopeptidase, wherein said activity comprises binding to, altering a structure of, or interacting with, an active site of a bacterial MetAP enzyme, for example, a compound selected from the group consisting of 5-(3-Iodo-phenyl)-1-H-[1,2,3] triazole and 5-benzofuran-2-yl-1-H-[1,2,3]triazole, or a pharmaceutically active salt or solvate thereof.

Another aspect of this invention provides a compound or composition comprising a compound that modulates an activity of a bacterial methionine aminopeptidase, wherein said activity is selected from the group consisting of: bonding with, complexing with, coordinating with and/or cocrystalizing with an amino acid residue or residues defined by a protein coordinate or coordinates set forth in Table I; bonding with, complexing with, coordinating with and/or cocrystalizing with a *Staphylococcus aureus* MetAP crystal form comprising cubic crystals comprising a space group I23; bonding with, complexing with, coordinating with and/or cocrystalizing with a *Staphylococcus aureus* MetAP cubic crystal comprising a lattice constant of about a=121.36 Ångstroms (Å); bonding with, complexing with, coordinating with and/or cocrystalizing with a *Staphylococcus aureus* MetAP crystal form comprising a monoclinic crystal with a space group $P2_1$ and lattice constants of about a=41.19Å, about b=76.78Å, and about c=41.71Å, β=104.165°; bonding with, complexing with, coordinating with and/or cocrystalizing with an amino acid residue or residues defined by a protein coordinate or coordinates set forth in Table VIII; bonding with, complexing with, coordinating with and/or cocrystalizing with a *Streptococcus pneumoniae* MetAP crystal form comprising orthorhombic crystals with a space group $P2_12_12_1$, wherein said orthorhombic crystals comprise lattice constants of about a=56.77Å, about b=69.16Å, and about c=80.51Å; bonding with, coordinating with and/or cocrystalizing with a *Streptococcus pneumoniae* MetAP in complex with a MetAP inhibitor or other

modulator; and bonding with, complexing with, coordinating with and/or cocrystalizing with a bacterial MetAP enzyme.

DESCRIPTION OF THE FIGURES

Figure 1 is a ribbon diagram of *S. aureus* methionine aminopeptidase. Amino and carboxyl-termini are indicated by N and C. The drawing was produced using the program MOLSCRIPT [Kraulis, P., *J. Appl. Crystallogr.*, 24, 946-950 (1991)].

Figure 2 is an illustration of an active site of *S. aureus* methionine aminopeptidase.

Figure 3 is a stereoview of an active site of *S. aureus* methionine aminopeptidase. For clarity, no hydrogen atoms or water molecules are shown.

Figure 4 is an illustration of an active site of *S. aureus* methionine aminopeptidase in complex with an inhibitor, 5-(3-Iodo-phenyl)-1-H-[1,2,3]triazole, of *S. aureus* methionine aminopeptidase. The exemplary view depicts an interaction of this inhibitor with atoms of residues of an active site of *S. aureus* methionine aminopeptidase within 5Å of this inhibitor. For clarity, no hydrogen atoms or water molecules are shown. 2 active site metal atoms are represented as spheres.

Figure 5 is a stereoview of an active site of *S. aureus* methionine aminopeptidase in complex with an inhibitor, 5-(3-Iodo-phenyl)-1-H-[1,2,3]triazole, of *S. aureus* methionine aminopeptidase. This figure is a stereo drawing of an interaction of this inhibitor with atoms of residues of an active site of *S. aureus* methionine aminopeptidase within 5Å of this inhibitor. Water molecules and 2 active site metal atoms are shown as crosses in the figure.

Figure 6 is an illustration of an active site of *S. aureus* methionine aminopeptidase in complex with an inhibitor, 5-benzofuran-2-yl-1-H-[1,2,3]triazole, of *S. aureus* methionine aminopeptidase. This view depicts an interaction of an inhibitor with atoms of residues of an active site of *S. aureus* methionine aminopeptidase within 5Å of this inhibitor. For clarity, no hydrogen atoms or water molecules are shown. 2 active site metal atoms are represented as spheres.

Figure 7 is a stereoview of an active site of *S. aureus* methionine aminopeptidase in complex with an inhibitor, 5-benzofuran-2-yl-1-H-[1,2,3]triazole, of *S. aureus* methionine aminopeptidase. This figure is a stereo drawing of an interaction of this inhibitor with atoms of residues of an active site of *S. aureus* methionine aminopeptidase within 5Å of this inhibitor. Water molecules and 2 active site metal atoms are shown as crosses in the figure.

Figure 8 is a ribbon diagram of *S. pneumoniae* methionine aminopeptidase. Amino and carboxyl-termini are indicated by N and C respectively.

Figure 9 is an illustration of an active site of *S. pneumoniae* methionine aminopeptidase.

Figure 10 is a stereoview of an active site of *S. pneumoniae* methionine aminopeptidase. For clarity, no hydrogen atoms or water molecules other than a water molecule bridging metal atoms are shown.

DETAILED DESCRIPTION OF THE INVENTION

The present invention provides a method for inhibiting or otherwise modulating bacterial methionine aminopeptidase (MetAP) by administering compounds with certain structural, physical and/or spatial characteristics that allow for an interaction of said compounds with specific residues of an inhibitor or modulator binding site of a bacterial methionine aminopeptidase. This interaction inhibits or otherwise modulates an activity of bacterial MetAP and, thus, treats diseases where bacterial replication is a factor.

The present invention provides for bacterial MetAP crystalline structures, and methods for identifying inhibitors or modulators of MetAP that bind to or interacts with an active site of a bacterial MetAP enzyme. In addition, the invention provides for active sites of a crystalline structure of MetAP, in complex with inhibitor or other modulator compounds and methods to use these crystalline forms and their active sites to identify and improve MEtAP inhibitor or other modulator compounds, such as peptide, peptidomimetic or synthetic compositions. These compounds may be characterized by an ability to competitively inhibit binding of substrates or other like-molecules to an active site of MetAP.

Crystallization and structure solution of S. *pneumoniae* methionine aminopeptidase

Examplary crystals of *S. pneumoniae* methionine aminopeptidase grew to a size of approximately 0.2 mm^3 overnight. In this example, the concentration of *S. pneumoniae* methionine aminopeptidase used in crystallization was approximately 15 mg/ml. A method of vapor diffusion in sitting drops was used to grow crystals from ta solution of *S. pneumoniae* methionine aminopeptidase. Crystals grew at root temperature from drops containing protein in a solution of 10% glycerol in 20mM Hepes buffer at pH 7.4 containing 0.10M NaCl, 0.5mM $CoCl_2$. This solution was mixed in equal volumes with a reservoir solution of 10% isopropanol, 20% PEG 4000 and

100mM Hepes at pH 7.5. Crystals are orthorhombic, space group $P2_12_12_1$, with cell constants of a=56.77, b=69.16, c=80.51 Ångstroms. These exemplary crystals contained one molecule in the asymmetric unit and approximately 57% solvent with a V_m value of 2.93 A^3/Dalton. X-ray diffraction data were measured from a single crystal using synchrotron radiation provided by beamline 17-ID at the Advanced Photon Source, Argonne National Laboratory. A structure was determined by molecular replacement using CNX (Molecular Simulations Inc). A starting model consisted of all protein atoms of the structure of *S. aureus* methionine aminopeptidase determined as described below. This exemplary model was refined by rigid-body refinement, and resulting phases were used to calculate Fourier maps with coefficients $|F_o-F_c|$ and $|2F_o-F_c|$, into which an atomic model of *S. pneumoniae* methionine aminopeptidase was built using a molecular graphics system XtalView (Molecular Simulations Inc). Conventional positional refinement was carried out during protein model building using CNX to a final R_c-value of 0.22 at 1.0 Ångstroms resolution.

Crystallization and structure solution of S. *aureus* methionine aminopeptidase

Exemplary crystals of *S. aureus* methionine aminopeptidase grew under two different conditions. For example, Form I crystals grew to a size of approximately 0.2 mm^3 in about two days. The concentration of S. *aureus* methionine aminopeptidase used in this exemplary crystallization was approximately 12 mg./ml. Amethod of vapor diffusion in sitting drops was used to grow crystals from a solution of *S. aureus* methionine aminopeptidase. Crystals grew at room temperature from drops containing protein in a solution of 10% glycerol in 10mM Hepes buffer at pH 7.4 containing 0.20M NaCl, 1 mM $CoCl_2$. This solution was mixed in equal volumes with a reservoir solution of 30% peg 400, 0.2M NaCl and 0.1M Hepes at pH 7.5. Exemplary crystals of Form I comprise a cubic, space group I23, with cell constants of a=121.36 Ångstroms. Exemplary crystals contain one molecule in the asymmetric unit and approximately 53% solvent with a V_m value of 2.71 A^3/Dalton. X-ray diffraction data were measured from a single crystal using synchrotron radiation provided by beamline 17-ID at the Advance Photon Source, Argonne National Laboratory. A structure was determined by molecular replacement using CNX (Molecular Simulations Inc). A starting model consisted of all protein atoms of the published structure of *E. coli* methionine aminopeptidase published by Roderick and Matthews [S.L.Roderick, B.W.Matthews. Structure of the Cobalt-dependent Methionine Aminopeptidase from *Escherichia coli*:

a New Type of Proteolytic Enzyme, *Biochemistry* 32 ,3907 (1993)]. This model was refined by rigid-body refinement, and resulting phases were used to calculate Fourier maps with coefficients $|F_O-F_C|$ and $|2F_O-F_C|$, into which an atomic model of *S. aureus* methionine aminopeptidase was built using a molecular graphics system XtalView (Molecular Simulations Inc). Conventional positional refinement was carried out during protein model building using CNX to a final R_C-value of 0.25 at 2.5 Ångstroms resolution.

Exemplary Form II crystals grew to a size of approximately 0.2 mm^3 in about two days at room temperature. The concentration of *S. aureus* methionine aminopeptidase used in crystallization was approximately 12 mg/ml. A method of vapor diffusion in sitting drops was used to grow crystals from the solution of *S. aureus* methionine aminopeptidase. Exemplary crystals grew from drops containing protein in a solution of 10% glycerol in 10mM Hepes buffer at pH 7.4 containing 0.20M NaCl, 1mM $CoCl_2$. This solution was mixed in equal volumes with a solution of 18% PEG 8000, 0.12M Na-acetate, 0.06M Na-cacodylate-acetate, pH 6.5 and equilibrate with a reservoir containing 15% PEG 8000, 0.10M Na-acetate, 0.05M Na-cacodylate-acetate, pH 6.5. These crystals of Form II comprise a monoclinic space group $P2_1$, with cell constants of a=41.19, b=76.78, and c=41.71 Ångstroms β=104.165°. Crystals contain a molecule in an asymmetric unit and approximately 46% solvent with a V_m value of 2.33 A^3/Dalton. X-ray diffraction data were measured from a single crystal using synchrotron radiation provided by beamline 17-ID at the Advance Photon Source, Argonne National Laboratory. A structure was determined by molecular replacement as described above. Conventional positional refinement was carried out using CNX to a final R_C-value of 0.22 at 1.8 Ångstroms resolution.

Structure solution of S. *aureus* methionine aminopeptidase inhibitor complexes

Exemplary complexes were prepared by introducing solid inhibitor into a crystal mother liquor after crystal formation and allowed to incubate for 24 to 48 hours. Form II crystal were used to determine the structure of inhibitor complexes of *S. aureus* methionine aminopeptidase. Structures were refined as described above at 1.8 Ångstroms resolution.

Abbreviations

mM, milliMolar

$R_c = \Sigma|(F_o - F_c)| / F_o$

F_o = observed structure amplitude

F_c = calculated structure amplitude

The present invention also provides bacterial MetAP crystalline structures in complex with inhibitors and provides methods to use these crystalline forms to identify and improve bacterial MetAP inhibitor compounds. Such compounds are characterized by their ability to inhibit MetAP activity.

It has now been discovered that substituted triazoles, for example, substituted 1,2,3-triazoles of formula (I) and formula (IA) are inhibitors of bacterial MetAP. It has also now been discovered that selective inhibition of MetAP enzyme mechanisms by treatment with inhibitors of formula (I) and formula (IA), or a pharmaceutically acceptable salt thereof, represents a novel therapeutic and preventative approach to the treatment of a variety of disease states, including, but not limited to, diseases in which bacterial replication is a factor.

The term "Ph" represents a phenyl ring. The terms "Het" or "heterocyclic" as used herein interchangeably, mean a stable heterocyclic ring, that are either saturated or unsaturated, and consist of carbon atoms and from one to three heteroatoms selected from a group consisting of N, O and S, and wherein nitrogen may optionally be oxidized or quaternized, and including any bicyclic group in which any of the above-defined heterocyclic rings is fused to a benzene ring. Ph and Het may be substituted with up to five of C_{2-6}alkyl-, C_{1-6}alkoxy-, $R^4R^5N(CH_2)_{1-6}$-, $R^4R^5N(CH_2)_{2-6}O$-, -CO_2R^6, -CF_3 or, halogen.

The term "C_{1-6}alkyl" as used herein means a substituted and unsubstituted, straight or branched chain radical of 1 to 6 carbon atoms, unless the chain length is limited thereto, including, but not limited to methyl, ethyl, n-propyl, isopropyl, n-butyl, isobutyl and t-butyl, pentyl, n-pentyl, isopentyl, neopentyl and hexyl and the simple aliphatic isomers thereof. Any C_{1-6}alkyl group may be optionally substituted independently by one or more of OR^4, R^4, NR^4R^5.

The term "C_{3-7}cycloalkyl" as used herein means substituted or unsubstituted cyclic radicals having 3 to 7 carbons, including but not limited to cyclopropyl, cyclopentyl, cyclohexyl and cycloheptyl radicals.

The term "C_{2-6}alkenyl" as used herein means an alkyl group of 2 to 6 carbons wherein a carbon-carbon single bond is replaced by a carbon-carbon double bond. C_{2-6}alkenyl includes ethylene, 1-propene, 2-propene, 1-butene, 2-butene, isobutene and isomeric pentenes and hexenes. Both cis and trans isomers are included within the scope of this invention. Any C_{2-6}alkenyl group may be optionally substituted independently by one or more of Ph-C_{0-6}alkyl-, Het-C_{0-6} alkyl-, C_{1-6}alkyl-, C_{1-6}alkoxy-, C_{1-6}mercaptyl-, Ph-C_{0-6}alkoxy-, Het-C_{0-6}alkoxy-, HO-, R^4R^5N-, Het-S-C_{0-6}alkyl-, Ph-S-C_{0-6}alkyl-, $HO(CH_2)_{1-6}$-, $R^4R^5N(CH_2)_{2-6}$-, $R^4R^5N(CH_2)_{2-6}O$-, $R^6CO_2(CH_2)_{0-6}$-, $R^6CO_2(CH_2)_{1-6}O$-, $R^6SO_2(CH_2)_{1-6}$-, $-CF_3$, $-OCF_3$, or halogen.

The term " C_{2-6}alkynyl" as used herein means an alkyl group of 2 to 6 carbons wherein one carbon-carbon single bond is replaced by a carbon-carbon triple bond. C_{2-6}alkynyl includes acetylene, 1-propyne, 2-propyne, 1-butyne, 2-butyne, 3-butyne and the simple isomers of pentyne and hexyne.

The term "alkoxy" as used herein means a straight or branched chain radical of 1 to 6 carbon atoms, unless the chain length is limited thereto, bonded to an oxygen atom, including, but not limited to, methoxy, ethoxy, n- propoxy, isopropoxy, and the like.

The term "mercaptyl" as used herein means a straight or branched chain radical of 1 to 6 carbon atoms, unless the chain length is limited thereto, bonded to a sulfur atom, including, but not limited to, methylthio, ethylthio, n- propylthio, isopropylthio, and the like.

The terms "hetero" or "heteroatom" as used hereineach mean oxygen, nitrogen and sulfur.

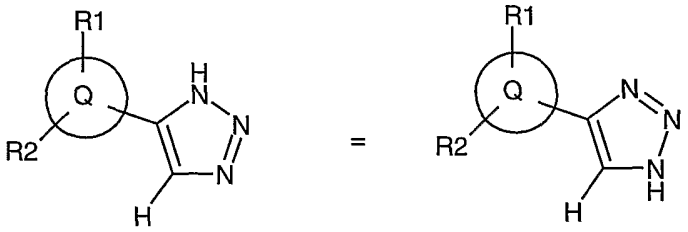
The terms "halo" or "halogen" as used hereineach mean F, Cl, Br, and I.

Herein the term C_0 means the absence of the substituent group immediately following; for instance, in the moiety PhC_{0-6}alkyl, when C is 0, the substituent is phenyl.

It will be understood that for compounds of formula (I) and formula (IA), the triazole ring can exist in either of two tautomeric forms as shown in Structure 1. Hydrogen on the triazole ring can exist on either N1 or N3, thus the name for a compound of Structure 1 can be any of the following: 4-(Q)-1*H*-1,2,3-triazole, 5-(Q)-1*H*-1,2,3-triazole, 4-(Q)-3*H*-1,2,3-triazole, 5-(Q)-3*H*-1,2,3-triazole. These compounds

are equivalent and represented herin as one structure and one name (4-(Q)-1*H*-1,2,3-triazole).

Structure 1



The term "Q" is used herein to represent a 5- or 6-membered monocyclic ring optionally containing up to two heteroatoms selected from N, O, or S, or an 8- to 11-membered fused bicyclic ring optionally containing up to four heteroatoms selected from N, O, or S. A bicyclic ring is defined as two rings that are fused together by two adjacent atoms. Suitably, the ring may be saturated or unsaturated, wherein the nitrogen may optionally be oxidized or quaternized. It will be understood that if Q is a heterocyclic ring, it may be attached to the triazole ring through any heteroatom or carbon atom of Q which results in the creation of a stable structure.

Examples of Q include, but are not limited to phenyl, napthyl, piperidinyl, piperazinyl, 2-oxopiperazinyl, 2-oxopiperidinyl, 2-oxopyrrolodinyl, 2-oxoazepinyl, azepinyl, pyrrolyl, 4-piperidonyl, pyrrolidinyl, pyrazolyl, pyrazolidinyl, imidazolyl, pyridinyl, pyrazinyl, oxazolidinyl, oxazolinyl, oxazolyl, isoxazolyl, morpholinyl, thiazolidinyl, thiazolinyl, thiazolyl, quinuclidinyl, indolyl, quinolinyl, isoquinolinyl, benzimidazolyl, benzopyranyl, benzoxazolyl, furyl, pyranyl, tetrahydrofuryl, tetrahydropyranyl, thienyl, benzoxazolyl, benzofuranyl, benzothiophenyl, thiamorpholinyl sulfoxide, thiamorpholinyl sulfone, oxadiazolyl, triazolyl, thiadiazolyl, oxadiazolyl, isoxazolyl, isothiazolyl, imidazolyl, pyridazinyl, pyrimidinyl and triazinyl which moieties are available commercially or can be made by routine chemical synthesis and are stable.

Suitably, Q is a 5- or 6-membered unsaturated ring or a 9-membered bicyclic ring. For example, Q is thiophene, phenyl, pyridine, benzofuran, or benzo[1,3]dioxole.

It will be understood that for compounds of formula (I), Q is substituted by up to eight of R^1 and if Q is Ph, Q is additionally substituted by one or more R^2.

It will be understood that for compounds of this invention, Q is substituted by up to eight substituents, selected independently from R^1 and R^2.

Suitably, R^1 is H-, Ph-C_{0-6}alkyl-, Het-C_{0-6} alkyl-, C_{1-6}alkyl-, C_{1-6}alkoxy-, C_{1-6}mercaptyl-, Ph-C_{0-6}alkoxy-, Het-C_{0-6}alkoxy-, HO-, R^4R^5N-, Het-S-C_{0-6}alkyl-, Ph-S-C_{0-6}alkyl-, $HO(CH_2)_{1-6}$-, $R^4R^5N(CH_2)_{2-6}$-, $R^4R^5N(CH_2)_{2-6}O$-, $R^6CO_2(CH_2)_{0-6}$-, $R^6CO_2(CH_2)_{1-6}O$-, $R^6SO_2(CH_2)_{1-6}$-, $-CF_3$, $-OCF_3$, or halogen, and Ph or Het are substituted with up to five of C_{2-6}alkyl-, C_{1-6}alkoxy-, $R^4R^5N(CH_2)_{1-6}$-, $R^4R^5N(CH_2)_{2-6}O$-, $-CO_2R^6$, $-CF_3$ or, halogen. For example, R^1 is halogen, C_{1-6}alkyl-, C_{1-6}alkoxy-, or -OH. For example, R^1 is bromine, chlorine, methyl, ethyl, methoxyl, or hydroxyl.

Suitably, R^2 is Ph-C_{0-6}alkyl-, Het-C_{0-6} alkyl-, C_{5-6}alkyl-, C_{2-6}alkoxy-, C_{1-6}mercaptyl-, Ph-C_{0-6}alkoxy-, Het-C_{0-6}alkoxy-, HO-, R^4R^5N-, Het-S-C_{0-6}alkyl-, Ph-S-C_{0-6}alkyl-, $HO(CH_2)_{1-6}$-, $R^4R^5N(CH_2)_{2-6}$-, $R^4R^5N(CH_2)_{2-6}O$-, $R^6CO_2(CH_2)_{0-6}$-, $R^6CO_2(CH_2)_{1-6}O$-, $R^6SO_2(CH_2)_{1-6}$-, $-CF_3$ or $-OCF_3$, and Ph or Het are substituted with up to five of C_{2-6}alkyl-, C_{1-6}alkoxy-, $R^4R^5N(CH_2)_{1-6}$-, $R^4R^5N(CH_2)_{2-6}O$-, $-CO_2R^6$, $-CF_3$ or, halogen; wherein R^4, R^5, and R^6 are independently selected from H, C_{2-6}alkyl, C_{3-6}alkenyl, C_{3-6}alkynyl, Ph-C_{0-6}alkyl, Het-C_{0-6}alkyl, or C_{3-7}cycloalkyl-C_{0-6}alkyl. For example, R^2 is $-NR^4R^5$, $-CF_3$, Ph-S-C_{0-6}alkyl-, Ph-C_{0-6}alkoxy-. For example, R^2 is benzylamine, propylamine, furan-3-ylmethylamine, furan-2-ylmethylamine, $-CF_3$, Ph-CH_2-O-, (4-Cl)Ph-S-.

For compounds of formula IA, R^3 is suitably H-, halogen, or R^3 and Q together form a fused bicyclic or tricyclic saturated or unsaturated ring system wherein R^3 is -C-, or -C=C-. For example, R^3 is hydrogen, bromine, or is fused to Q by -C- to form a dihydro-indenotriazole or by -C=C- to form a napthotriazole or an acetonapthotriazole.

Suitably, R^4, R^5, and R^6 are independently selected from H-, C_{2-6}alkyl-, C_{3-6}alkenyl-, C_{3-6}alkynyl-, Ph-C_{0-6}alkyl-, Het-C_{0-6}alkyl-, or C_{3-7}cycloalkyl-C_{0-6}alkyl-. For example R^4, R^5, and R^6 are independently selected hydrogen, benzyl, furanyl, and propyl.

Further, it will be understood that when a moiety is "optionally substituted" the moiety may have one or more optional substituents, each optional substituent being independently selected.

Suitably, pharmaceutically acceptable salts of formula (I) include, but are not limited to, salts with inorganic acids such as hydrochloride, sulfate, phosphate, diphosphate, hydrobromide, and nitrate, or salts with an organic acid such as malate, maleate, fumarate, tartrate, succinate, citrate, acetate, lactate, methanesulfonate, p-toluenesulfonate, palmitate, salicylate, and stearate.

The compounds of the present invention may contain one or more asymmetric carbon atoms and may exist in racemic and optically active forms. The stereocenters may be (R), (S) or any combination of R and S configuration, for example, (R,R), (R,S), (S,S) or (S,R). All of these compounds are within the scope of the present invention.

Novel intermediates useful in making compounds of this invention are as follows:

4-ethynyl-benzo[1,3]dioxole;

1-(4-chloro-phenylsulfanyl)-2-ethynylbenzene;

(3-phenyl-propyl)-(3-ethynylphenyl)amine;

phenethyl-(3-ethynylphenyl)-amine;

furan-2-ylmethyl-(3-ethynylphenyl)-amine;

furan-3-ylmethyl-(3-ethynylphenyl)-amine;

napthalene-1-ylmethyl-(3-ethynylphenyl)-amine; and

napthalene-2-ylmethyl-(3-ethynylphenyl)-amine.

The intermediates useful for this invention were made according to the Schemes herein.

Among the compounds of the formula (IA) are the following compounds:

3-(1*H*-1,2,3-triazol-4-yl)-phenol;

4-(3-iodophenyl)-1*H*-1,2,3-triazole;

4-(2-fluorophenyl)-1*H*-1,2,3-triazole;

4-(4-n-butylphenyl)-1*H*-1,2,3-triazole;

4-(2-chlorophenyl)-1*H*-1,2,3-triazole;

N-(3-[1*H*-1,2,3-triazol-4-yl]phenyl)benzamide;

3-(1*H*-1,2,3-triazol-4-yl)-phenylamine;

N-(3-[1*H*-1,2,3-triazol-4-yl]phenyl)acetamide;

4-(4-trifouoromethylphenyl)-1*H*-1,2,3-triazole;

4-(3-trifouoromethylphenyl)-1*H*-1,2,3-triazole;

4-(4-n-propylphenyl)-1*H*-1,2,3-triazole;

4-(4-methoxyphenyl)-1*H*-1,2,3-triazole;

4-(3-methylphenyl)-1*H*-1,2,3-triazole;
2-(1*H*-1,2,3-triazol-4-yl)-pyridine;
4-(4-chlorophenyl)-1*H*-1,2,3-triazole;
4-(4-ethylphenyl)-1*H*-1,2,3-triazole;
4-(1*H*-1,2,3-triazol-4-yl)-phenylamine;
4-(4-methylphenyl)-1*H*-1,2,3-triazole;
2-(1*H*-1,2,3-triazol-4-yl)-5-methylpyridine;
2-(1*H*-1,2,3-triazol-4-yl)-4-methyl-pyridine;
1-(1*H*-1,2,3-triazol-4-yl)cyclohexanol;
4-(thiophen-2-yl)-1*H*-1,2,3-triazole;
4-(thiophen-3-yl)-1*H*-1,2,3-triazole;
4-(2-methylphenyl)-1*H*-1,2,3-triazole;
4-(1,3-dimethylphenyl)-1*H*-1,2,3-triazole;
4-(4-bromophenyl)-1*H*-1,2,3-triazole;
4-(1,3-dichlorophenyl)-1*H*-1,2,3-triazole;
4-(1-biphenyl-2-yl)-1*H*-1,2,3-triazole;
4-(2-benzyloxy-phenyl)-1*H*-1,2,3-triazole;
2-(1*H*-1,2,3-triazol-4-yl)-6-methylpyridine;
3-(1*H*-1,2,3-triazol-4-yl)-pyridine;
4-(1*H*-1,2,3-triazol-4-yl)-pyridine;
4-(2-methoxyphenyl)-1*H*-1,2,3-triazole;
4-(2-bromophenyl)-1*H*-1,2,3-triazole;
4-benzo[1,3]dioxol-5-yl-1*H*-1,2,3-triazole;
2-(1*H*-1,2,3-triazol-4-yl)-benzofuran;
4-benzo[1,3]dioxol-4-yl-1*H*-1,2,3-triazole;
4-(2-[4-chloro-phenylsulfanyl]-phenyl)-1*H*-1,2,3-triazole;
(3-phenyl-propyl)-(3-[1*H*-1,2,3-triazol-4-yl]phenyl)amine;
phenethyl-(3-[1*H*-1,2,3-triazol-4-yl]phenyl)amine;
furan-2-ylmethyl-(3-[1*H*-1,2,3-triazol-4-yl]phenyl)amine;
furan-3-ylmethyl-(3-[1*H*-1,2,3-triazol-4-yl]phenyl)amine;
napthalene-1-ylmethyl-(3-[1*H*-1,2,3-triazol-4-yl]phenyl)amine;
napthalene-2-ylmethyl-(3-[1*H*-1,2,3-triazol-4-yl]phenyl)amine;
4-(1*H*-1,2,3-triazol-4-yl)-phenol;
benzyl-(3-[1*H*-1,2,3-triazol-4-yl]phenyl)amine;
4-(4-fluorophenyl)-1*H*-1,2,3-triazole;

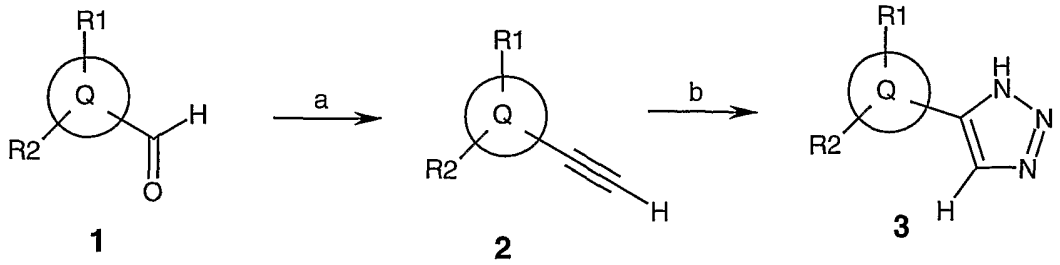
2-bromo-5-(1*H*-1,2,3-triazol-4-yl)-phenol;
2,6-dibromo-5-(1*H*-1,2,3-triazol-4-yl)-phenol;
2,4-dibromo-5-(*1H*-1,2,3-triazol-4-yl)-phenol;
2-(5-bromo-1H-1,2,3-triazol-4-yl)-4-methyl-pyridine;
1*H*-naptho[1,2-*d*]-1,2,3-triazole;
2,8-dihydro-indeno[1,2-*d*]-1,2,3-triazole;
4-phenyl-1*H*-1,2,3-triazole; and
5,5a,6,8-tetrahydro-4*H*-acenaphtho[4,5-*d*]-1,2,3-triazole.

Among the most compounds of the formula (IA) are the following compounds:
4-(3-iodophenyl)-1*H*-1,2,3-triazole;
4-(2-fluorophenyl)-1*H*-1,2,3-triazole;
4-(2-chlorophenyl)-1*H*-1,2,3-triazole;
4-(3-methylphenyl)-1*H*-1,2,3-triazole;
4-(4-chlorophenyl)-1*H*-1,2,3-triazole;
4-(4-ethylphenyl)-1*H*-1,2,3-triazole;
4-(4-methylphenyl)-1*H*-1,2,3-triazole;
2-(1*H*-1,2,3-triazol-4-yl)-5-methylpyridine;
2-(1*H*-1,2,3-triazol-4-yl)-4-methyl-pyridine;
4-(thiophen-3-yl)-1*H*-1,2,3-triazole;
4-(4-bromophenyl)-1*H*-1,2,3-triazole;
4-(1,3-dichlorophenyl)-1*H*-1,2,3-triazole;
2-(1*H*-1,2,3-triazol-4-yl)-benzofuran;
furan-2-ylmethyl-(3-[1*H*-1,2,3-triazol-4-yl]phenyl)amine;
furan-3-ylmethyl-(3-[1*H*-1,2,3-triazol-4-yl]phenyl)amine;
benzyl-(3-[1*H*-1,2,3-triazol-4-yl]phenyl)amine;
4-(4-fluorophenyl)-1*H*-1,2,3-triazole;
2-bromo-5-(1*H*-1,2,3-triazol-4-yl)-phenol;
2,4-dibromo-5-(*1H*-1,2,3-triazol-4-yl)-phenol; and
2-(5-bromo-1H-1,2,3-triazol-4-yl)-4-methyl-pyridine.

Methods of Preparation

Compounds of the formulae (I) or (IA), were prepared by methods analogous to those described in Scheme 1.

Scheme 1



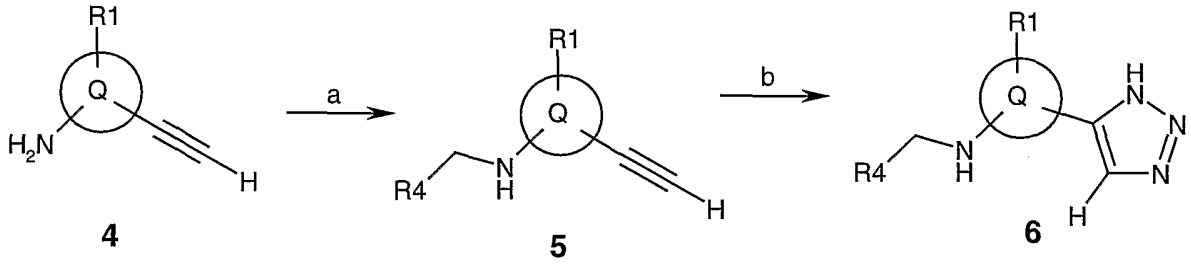
1 2 3

a) $P(O)(OMe)_2C(N_2)C(O)CH_3$, K_2CO_3, MeOH b) 1. Me_3SiN_3, $PhCH_3$, 110 °C; 2. H_2O.

An aldehyde (such as 2-thiophenecarboxaldehyde) (1-Scheme1) was treated with 1-diazo-2-oxopropylphosphonate and potassium carbonate in dry methanol to provide 2-Scheme1. Treatment of the acetylene (such as 2-ethynylthiophene) (2-Scheme1) with azidotrimethylsilane in refluxing toluene, followed by addition of water afforded 3-Scheme1.

Compounds of the formulae (I) or (IA), were R^2 is NHR^4 were prepared by methods analogous to those described in Scheme 2.

Scheme 2



4 5 6

a) R4-C(O)H, $Na(OAc)_3BH$, $ClCH_2CH_2Cl$, AcOH b) 1. Me_3SiN_3, $PhCH_3$, 110 °C; 2. H_2O.

An alkynyl aniline (such as 3-ethynylphenylamine) was substituted by a reductive amination reaction with an aldehyde to provide 5-Scheme2. Treatment of the acetylene (5-Scheme2) with azidotrimethylsilane in refluxing toluene, followed by addition of water afforded 6-Scheme2.

Formulation of Pharmaceutical Compositions

Pharmaceutically effective compounds of this invention (and pharmaceutically acceptable salts thereof) may be administered in conventional dosage forms prepared by, for example, combining a compound of this invention of formula (I) or (IA) ("active

ingredient") in an amount sufficient to treat diseases in which bacterial replication is a factor ("MetAP-mediated disease states") with standard pharmaceutical carriers or diluents according to conventional procedures well known in the art. These procedures may involve mixing, granulating and compressing or dissolving the ingredients as appropriate to the desired preparation.

The pharmaceutical carrier employed may be, for example, either a solid or liquid. Exemplary of solid carriers are lactose, terra alba, sucrose, talc, gelatin, agar, pectin, acacia, magnesium stearate, stearic acid and the like. Exemplary of liquid carriers are syrup, peanut oil, olive oil, water and the like. Similarly, the carrier or diluent may include time delay material well known to the art, such as glyceryl monostearate or glyceryl distearate alone or with a wax.

A wide variety of pharmaceutical forms can be employed. Thus, if a solid carrier is used, a preparation may be tableted, placed in a hard gelatin capsule in powder or pellet form or in the form of a troche or lozenge. An amount of solid carrier may vary widely but may be from about 25 mg to about 1000 mg. When a liquid carrier is used, a preparation may be in the form of a syrup, emulsion, soft gelatin capsule, sterile injectable liquid such as an ampule or nonaqueous liquid suspension.

An active ingredient may also be administered topically to a mammal in need of treatment or prophylaxis of MetAP-mediated disease states. An amount of active ingredient required for therapeutic effect on topical administration may vary with a compound chosen, nature and severity of a disease state being treated and the mammal undergoing treatment, and may ultimately be at the discretion of a physician. A suitable dose of an active ingredient may be 1.5 mg to 500 mg for topical administration, an examplarydosage being 1 mg to 100 mg, for example 5 to 25 mg administered two or three times daily.

By topical administration is meant non-systemic administration and may include an application of an active ingredient externally to epidermis, to the buccal cavity, instillation of such a compound into the ear, eye or nose, or where a compound does not significantly enter the blood stream. By systemic administration is meant oral, intravenous, intraperitoneal and intramuscular administration, among others.

While it is possible for an active ingredient to be administered alone as a raw chemical, it may also be present as a pharmaceutical formulation. An active ingredient may comprise, for topical administration, from 0.001% to 10% w/w, e.g. from 1% to 2% by weight of the formulation although it may comprise as much as 10% w/w but in certain

embodiments will not be excess of 5% w/w and in other embodiments will range from 0.1% to 1% w/w of the formulation.

Topical formulations of the present invention, both for veterinary and for human medical use, may comprise an active ingredient together with one or more acceptable carrier(s) therefor and optionally any other therapeutic ingredient(s). Exemplary carrier(s) are 'acceptable' in the sense of being compatible with the other ingredients of the formulation and not deleterious to the recipient thereof.

Formulations suitable for topical administration include, but are not limited to, liquid or semi-liquid preparations suitable for penetration through the skin to a site of inflammation, such as liniments, lotions, creams, ointments or pastes, and drops suitable for administration to the eye, ear or nose, among others.

Drops according to the present invention may comprise sterile aqueous or oily solutions or suspensions and may be prepared by dissolving the active ingredient in a suitable aqueous or alcoholic solution of a bactericidal and/or fungicidal agent and/or any other suitable preservative, and may, for example, include a surface active agent. A resulting solution may then be clarified by filtration, transferred to a suitable container which is then sealed and sterilized by autoclaving or maintaining at 98-100°C for half an hour, among other ways. Alternatively, a solution may be sterilized by filtration and transferred to a container by an aseptic technique. Examples of bactericidal and fungicidal agents suitable for inclusion in drops may comprise phenylmercuric nitrate or acetate (0.002%), benzalkonium chloride (0.01%) and chlorhexidine acetate (0.01%). Suitable solvents for preparation of an oily solution may include glycerol, diluted alcohol and propylene glycol.

Lotions according to the present invention include, but are not limited to, those suitable for application to the skin or eye. An eye lotion may comprise a sterile aqueous solution optionally containing a bactericide and may be prepared by methods similar to those for the preparation of drops. Lotions or liniments for application to the skin may also include an agent to hasten drying and to cool the skin, such as an alcohol or acetone, and/or a moisturizer such as glycerol or an oil such as castor oil or arachis oil, among others.

Creams, ointments or pastes according to the present invention may be semi-solid formulations of an active ingredient for external application. They may be made by mixing an active ingredient in finely divided or powdered form, alone or in solution or suspension in an aqueous or non-aqueous fluid, with the aid of suitable machinery, with a greasy or non-greasy basis. A basis may comprise hydrocarbons, such as hard, soft or

liquid paraffin, glycerol, beeswax, a metallic soap; a mucilage; an oil of natural origin such as almond, corn, arachis, castor or olive oil; wool fat or its derivatives, or a fatty acid such as stearic or oleic acid together with an alcohol such as propylene glycol. A formulation may incorporate any suitable surface-active agent such as an anionic, cationic or non-ionic surfactant such as esters or polyoxyethylene derivatives thereof. Suspending agents such as natural gums, cellulose derivatives or inorganic materials such as silicaceous silicas, and other ingredients such as lanolin, may also be included.

An active ingredient may also be administered by inhalation. By "inhalation" is meant intranasal or oral inhalation administration. Appropriate dosage forms for such administration, such as an aerosol formulation or a metered dose inhaler, may be prepared by conventional techniques. A daily dosage amount of an active ingredient administered by inhalation is from about 0.1 mg to about 100 mg per day, for example about 1 mg to about 10 mg per day.

By the term "treating" is meant either prophylactic or therapeutic therapy. Such compound may be administered to such mammal in a conventional dosage form prepared by combining the compound of this invention with a conventional pharmaceutically acceptable carrier or diluent according to known techniques. It will be recognized by one of skill in the art that the form and character of the pharmaceutically acceptable carrier or diluent may be dictated by the amount of active ingredient with which it is to be combined, the route of administration and other well-known variables. The compound is administered to a mammal in need of treatment for diseases in which bacterial replication is a factor, in an amount sufficient to decrease or eliminate symptoms associated with these disease states. The route of administration may be oral or parenteral, among others.

The term parenteral as used herein includes, but is not limited to, intravenous, intramuscular, subcutaneous, intra-rectal, intravaginal or intraperitoneal administration. A daily parenteral dosage regimen may for example be from about 30 mg to about 300 mg per day of active ingredient. The daily oral dosage regimen may, for example, be from about 100 mg to about 2000 mg per day of active ingredient.

It will be recognized by one of skill in the art that a quantity and spacing of individual dosages of a compound of this invention may be determined by the nature and extent of a condition being treated, a form, route and site of administration, and mammal being treated, and that such quantity and spacing may be determined by conventional techniques. It will also be appreciated by one of skill in the art that an exemplary course of treatment, i.e., the number of doses of a compound given per day

for a defined number of days, may be ascertained by those skilled in the art using conventional course of treatment determination tests.

Definitions

Herein, the terms "a" and "an" mean "one or more" when used in this application, including the claims.

The invention further provides for homologues, co-complexes, mutants and derivatives of a MetAP crystal structure of the invention.

The term "co-complex" and "cocrystal" each mean a MetAP or a mutant or homologue of a MetAP in covalent or non-covalent association with a chemical entity or compound.

As used herein, the terms "antagonist" and "inhibitor" as herein mean an agent that (i) decreases or inhibits an activity of a MetAP gene or protein or (ii) decreases or inhibits an activity of a gene or polypeptide encoded by a gene that is up- or down-regulated by a MetAP polypeptide.

As used herein, the term "active site" refers to a region of a MetAP binding pocket where a molecule binds and catalysis takes place. It may be comprised and bound by amino acid residues that are in contact with a substrate or that interact with a substrate(s) through water molecules or amino acids that, although not being in contact with a substarte(s), nonetheless allow certain positioning of amino acids that are in contact and that without certain positioning they would not be able to interact in a way conducent to catalysis with a substrate(s). These interactions between amino acids and substrate(s) may be responsible for binding of a substrate to MetAP, for certain positioning of a substrate for catalysis, and for stabilization of any reaction intermediates and for binding or release of a product from an active site. An active site may also be comprised of amino acids that are responsible for catalysis. These amino acids interact with a substrate(s) through hydrogen bonds or by close proximity to electron-donor or electron-acceptor centers in a substrate. These amino acids may act themselves as electron-donor or electron-acceptor centers for catalysis to take place.

As used herein, the term "biological activity" or "activity" means (i) any observable effect flowing from an interaction between anenzyme or polypeptide and a modulator, (ii) transcription regulation, modulator binding, and polypeptide binding, (iii) an interaction or association between (1) a compound and an enzyme, for example, a bacterial methionine aminopeptidase, or (2) a component of a complex comprising a compound and an enzyme, for example, a bacterial methionine aminopeptidase, or (3)

a compound and a subunit(s) or a cofactor(s) of an enzyme , for example, a bacterial methionine aminopeptidase, or (iv) active site catalysis of an enzyme, for example, a bacterial methionine aminopeptidase, or (vi) a chemical reaction carried out by or correlated with an enzyme, for example, a bacterial methionine aminopeptidase.

As used herein, the terms "candidate substance" and "candidate compound" are used interchangeably and refer to a substance that is believed to interact with another moiety, for example an modulator that is believed to interact with a complete, or a fragment of, an enzyme, such as a MetAP polypeptide, and which can be evaluated for such an interaction. Representative candidate substances or compounds include, but are not limited to, xenobiotics such as drugs and other therapeutic agents, carcinogens and environmental pollutants, natural products and extracts, as well as endobiotics such as glucocorticosteroids, steroids, fatty acids and prostaglandins. Other examples of candidate compounds that can be investigated using methods of the present invention include, but are not restricted to, agonists and antagonists of a MetAP polypeptide, toxins and venoms, viral epitopes, hormones (e.g., glucocorticosteroids, opioid peptides, steroids, etc.), hormone receptors, peptides, enzymes, enzyme substrates, co-factors, lectins, sugars, oligonucleotides or nucleic acids, oligosaccharides, proteins, small molecules and monoclonal antibodies.

As used herein, the terms "cells" or "host organism" are used interchangeably and mean not only to a particular subject cell, but also to any progeny or potential progeny of such a cell. Because certain modifications can occur in succeeding generations due to either mutation or environmental influences, such progeny might not, in fact, be identical to the parent cell, but are still included within the scope of the term as used herein.

"Bacteria(al)" means a (i) prokaryote, including but not limited to, a member of the genus *Streptococcus, Staphylococcus, Bordetella, Corynebacterium, Mycobacterium, Neisseria, Haemophilus, Actinomycetes, Streptomycetes, Nocardia, Enterobacter, Yersinia, Fancisella, Pasturella, Moraxella, Acinetobacter, Erysipelothrix, Branhamella, Actinobacillus, Streptobacillus, Listeria, Calymmatobacterium, Brucella, Bacillus, Clostridium, Treponema, Escherichia, Salmonella, Kleibsiella, Vibrio, Proteus, Erwinia, Borrelia, Leptospira, Spirillum, Campylobacter, Shigella, Legionella, Pseudomonas, Aeromonas, Rickettsia, Chlamydia, Borrelia* and *Mycoplasma*, and further including, but not limited to, a member of the species or group, Group A *Streptococcus,* Group B *Streptococcus,* Group C *Streptococcus,* Group D *Streptococcus,* Group G *Streptococcus, Streptococcus pneumoniae, Streptococcus pyogenes, Streptococcus*

agalactiae, Streptococcus faecalis, Streptococcus faecium, Streptococcus durans, Neisseria gonorrheae, Neisseria meningitidis, Staphylococcus aureus, Staphylococcus epidermidis, Corynebacterium diptheriae, Gardnerella vaginalis, Mycobacterium tuberculosis, Mycobacterium bovis, Mycobacterium ulcerans, Mycobacterium leprae, Actinomyctes israelii, Listeria monocytogenes, Bordetella pertusis, Bordatella parapertusis, Bordetella bronchiseptica, Escherichia coli, Shigella dysenteriae, Haemophilus influenzae, Haemophilus aegyptius, Haemophilus parainfluenzae, Haemophilus ducreyi, Bordetella, Salmonella typhi, Citrobacter freundii, Proteus mirabilis, Proteus vulgaris, Yersinia pestis, Kleibsiella pneumoniae, Serratia marcessens, Serratia liquefaciens, Vibrio cholera, Shigella dysenterii, Shigella flexneri, Pseudomonas aeruginosa, Franscisella tularensis, Brucella abortis, Bacillus anthracis, Bacillus cereus, Clostridium perfringens, Clostridium tetani, Clostridium botulinum, Treponema pallidum, Rickettsia rickettsii and *Chlamydia trachomitis,* and (ii) an archaeon, including but not limited to *Archaebacter.*

As used herein, the term "detecting" means confirming presence of a target entity by observing an occurrence of a detectable signal, such as a radiologic or spectroscopic signal that will appear exclusively in the presence of the target entity.

As used herein, the term "expression" generally refers to the cellular processes by which a biologically active polypeptide is produced.

As used herein, the term "gene" is used for simplicity to refer to a functional protein, polypeptide or peptide encoding unit. As will be understood by those in the art, this functional term includes both genomic sequences and cDNA sequences.

As used herein, the term "crystal lattice" means an array of points defined by vertices of packed unit cells.

As used herein, "hexagonal unit cell" means a unit cell wherein $a = b \neq c$; and $\alpha = \beta = 90$, $\gamma = 120^{\circ}$. The vectors a, b, and c describe unit cell edges and angles α, β, and γ describe unit cell angles. In an embodiment of the present invention, for example *S. pneumoniae,* a unit cell has lattice constants of, a=56.77, b=69.16, c=80.51 Ångstroms. While certain lattice constants are provided, a crystalline polypeptide of the present invention also comprises variations from certain lattice constants, wherein varations range from about one to about two percent.

As used herein, the term "hybridization" means binding of a probe molecule, a molecule to which a detectable moiety has been bound, to a target sample.

As used herein, the term "interact" means detectable interactions between molecules, such as can be detected using, for example, a yeast two hybrid assay. The

term "interact" is also meant to include "binding" interactions between molecules. Interactions can, for example, be protein-protein or protein-nucleic acid in nature.

As used herein, the term "isolated" means oligonucleotides substantially free of other nucleic acids, proteins, lipids, carbohydrates or other materials with which they may be associated, such association being either in cellular material or in a synthesis medium. The term can also be applied to polypeptides, in which case the polypeptide will be substantially free of nucleic acids, carbohydrates, lipids and other undesired polypeptides.

As used herein, the term "labeled" means attachment of a moiety, capable of detection by spectroscopic, radiologic or other methods, to a probe molecule.

As used herein, the term "modified" means an alteration from an entity's normally occurring state. An entity can be modified by removing discrete chemical units or by adding discrete chemical units. The term "modified" encompasses detectable labels as well as those entities added as aids in purification.

"Modulation," "modulating," to "modulate" means with reference to a mechanism of action, activty, enzyme activity, enzyme, polynucleotide, crystal or coordinate herein (i) altering, modulating, raising, enhancing, increasing, lowering, diminishing, preventing or stopping an activity or activities of an enzyme, for example, a bacterial methionine aminopeptidase, or (ii) enhancing, improving, or stabilizing an interaction or association between (1) a compound and an enzyme, for example, a bacterial methionine aminopeptidase, or (2) a component of a complex comprising a compound and an enzyme, for example, a bacterial methionine aminopeptidase, or (3) a compound and subunit(s) or cofactor(s) of an enzyme , for example, a bacterial methionine aminopeptidase, or (iii) altering, modulating, lowering, diminishing, preventing or stopping an active site activity of an enzyme, for example, a bacterial methionine aminopeptidase, or (iv) up-regulation (i.e., activation or stimulation) and down-regulation (i.e. inhibition or suppression) of an activity of an enzyme, for example, a bacterial methionine aminopeptidase.

"Modulator(s)" means a compound or composition that causes, affects, or correlates with, modulation, modulating, or may modulate through cause, affect or correlation.

As used herein, the term "molecular replacement" means a method that involves generating a preliminary model of a wild-type MetAP ligand binding domain, or a MetAP mutant crystal whose structure coordinates are unknown, by orienting and positioning a molecule or model whose structure coordinates are known within a unit

cell of the unknown crystal so as best to account for an observed diffraction pattern of the unknown crystal. Phases can then be calculated from this model and combined with observed amplitudes to give an approximate Fourier synthesis of a structure whose coordinates are unknown. This, in turn, may be subject to any of the several forms of refinement to provide a final, accurate structure of an unknown crystal. See, e.g., *Lattman*, (1985) *Method Enzymol.*, 115: 55-77; *Rossmann*, ed, (1972) *The Molecular Replacement Method*, Gordon & Breach, New York. Using the structure coordinates of an active site of MetAP provided by this invention, molecular replacement may be used to determine the structure coordinates of a crystalline mutant or homologue of an MetAP active site, or of a different crystal form of an MetAP active site.

As used herein, the term "polypeptide" means any polymer comprising any of the 20 protein amino acids, regardless of its size. Although "protein" is often used in reference to relatively large polypeptides, and "peptide" is often used in reference to small polypeptides, usage of these terms in the art overlaps and varies. The term "polypeptide" as used herein refers to peptides, polypeptides and proteins, unless otherwise noted. As used herein, the terms "protein", "polypeptide" and "peptide" are used interchangeably herein when referring to a gene product.

As used herein, the terms "structure coordinates" and "structural coordinates" mean mathematical or spatial coordinates derived from mathematical equations related to patterns obtained on diffraction of a monochromatic beam of X-rays by atoms (scattering centers) of a molecule in crystal form. The diffraction data may be used to calculate an electron density map of a repeating unit of a crystal. Electron density maps may be used to establish positions of individual atoms within a unit cell of a crystal.

Those of skill in the art understand that a set of coordinates determined by X-ray crystallography is not without standard error. An error in assigned coordinates may become reduced as resolution is increased, since more experimental diffraction data may available for model fitting and refinement. Thus, for example, more diffraction data may be collected from a crystal that diffracts to a resolution of 2.8 angstroms than from a crystal that diffracts to a lower resolution, such as 3.5 angstroms. Consequently, refined structural coordinates may be more accurate when fitted and refined using data from a crystal that diffracts to higher resolution. The design of agonists, antagonists, and modulators for MetAP depends on the accuracy of the structural coordinates. If the coordinates are not sufficiently accurate, then a design process may be ineffective. In certain cases, it may be difficult or impossible to

collect sufficient diffraction data to define atomic coordinates precisely when a crystal diffracts to a resolution of 3.5 angstroms or poorer. Thus, in certain cases, it may be difficult to use X-ray structures in structure-based agonist and antagonist design when X-ray structures are based on crystals that diffract to a resolution of 3.5 angstroms or poorer. However, crystals diffracting to 2.8 angstroms or better may yield X-ray structures with an accuracy enabling structure-based drug design. Further improvement in resolution may further facilitate structure-based design, but the coordinates obtained at 2.8 angstroms resolution may be adequate for certain purposes.

Also, those of skill in the art will understand that MetAP proteins may adopt different conformations when different agonists, antagonists, and modulators are bound. Subtle variations in a conformation may also occur when different agonists are bound, and when different antagonists are bound. Structure-based design of MetAP modulators may depend to some degree on a knowledge of differences in conformation that occur when agonists and antagonists are bound. Thus, structure-based modulator design may be facilitated by an availability of X-ray structures of complexes with agonists as well as antagonists.

As used herein, the term "substantially pure" means that a polynucleotide or polypeptide is substantially free of the sequences and molecules with which it is or may be associated in its natural state or synthetic state, and those molecules used in an isolation procedure. The term "substantially free" means that a sample is at least 50%, or may be at least 70%, or may also be at least 80% or at least 90% free of materials and compounds with which it is or may be associated in nature.

As used herein, the term "transcription" means a process involving an interaction of an RNA polymerase with a gene that directs expression of RNA. The process includes, but is not limited to the following steps: (a) transcription initiation, (b) transcript elongation, (c) transcript splicing, (d) transcript capping, (e) transcript termination, (f) transcript polyadenylation, (g) nuclear export of a transcript, (h) transcript editing, and (i) stabilizing a transcript.

As used herein, the term "unit cell" means a basic parallelipiped shaped block. A volume of a crystal may be constructed by regular assembly of such blocks. Each unit cell may comprise a complete representation of a unit of pattern, any repetition of which builds up a crystal. Thus, the term "unit cell" means a fundamental portion of a crystal structure that may be repeated infinitely by translation in three dimensions. A unit cell may be characterized by three vectors a, b, and c, not colocated in a plane,

which form the edges of a parallelepiped. Angles α, β, and γ define angles between the vectors: angle α is an angle between vectors b and c; angle β is an angle between vectors a and c; and angle γ is an angle between vectors a and b. The volume of a crystal may be constructed by regular assembly of unit cells; each unit cell comprises a complete representation of a unit of pattern, any repetition of which builds up a crystal.

As used herein, the term "mutant" or "mutation" carries its traditional connotation and means a change, inherited, naturally occurring or introduced, in a nucleic acid or polypeptide sequence, and is used in its sense as generally known to those of skill in the art. For example, a MetAP polypeptide, i.e., a polypeptide displaying a biological activity of wild-type MetAP activity, characterized by a replacement of an active-site amino acid from a wild-type prenyltransferase sequence.

MetAP mutants may also be generated by site-specific incorporation of unnatural amino acids into a MetAP protein using biosynthetic methods of C. J. Noren et al, *Science*, 244:182-188 (1989), among other methods. In this method, a codon encoding an amino acid of interest in wild-type MetAP is replaced by a "blank" nonsense codon, TAG, using oligonucleotide-directed mutagenesis. A suppressor directed against this codon is then chemically aminoacylated *in vitro* with a desired unnatural amino acid. The aminoacylated residue is then added to an *in vitro* translation system to yield a mutant MetAP with a site-specific incorporated unnatural amino acid.

Selenocysteine or selenomethionine may be incorporated into wild-type or mutant metallo MetAP by expression of MetAP-encoding cDNAs in auxotrophic *E. coli* strains (W. A. Hendrickson et al, *EMBO J.*, 9(5):1665-1672 (1990)) or a normal strain grown in a medium supplemented with appropriate nutrients that will prevent endogenous synthesis of methionine. In either of these methods, the wild-type or mutated MetAP cDNA may be expressed in a host organism on a growth medium depleted of either natural cysteine or methionine (or both) but enriched in selenocysteine or selenomethionine (or both).

The term "heavy atom derivative" refers to derivatives of MetAP produced by chemically modifying a crystal of MetAP. A native crystal may be treated by immersing it in a solution containing a desired metal salt, or organometallic compound, e.g., lead chloride, gold thiomalate, thimerosal or uranyl acetate, which upon diffusion into a protein crystal may bind to the protein. The location of the bound heavy metal atom site(s) may be determined by X-ray diffraction analysis of the treated crystal. This

information may be used to generate phase angle information needed to construct a three-dimensional electron density map from which a model of an atomic structure of an enzyme may be derived (T. L. Blundel and N. L. Johnson, *Protein Crystallography*, Academic Press (1976)).

The term "space group" refers to an arrangement of symmetry elements (i.e. molecules) throughout a crystal. There are 132 possible arrangements, each one identified by a symbol. The space group symbol is denoted by a letter (P, F, I, C) and numbers with or without subscripts, for example: $P2_1$, I222, $C2_12_12_1$, etc.

Methods of Identifying Inhibitors of MetAP from *Streptococcus pneumoniae* Crystalline Structure

An aspect of this invention involves a method for identifying inhibitors of a MetAP characterized by a crystal structure and an active site described herein, and crystal structures of complexes with its substrates. An exemplary crystalline structure of the invention permits identification of inhibitors of methionine aminopeptidase activity. Such inhibitors may be competitive, binding to all or a portion of an active site of MetAP; or non-competitive and bind to and inhibit methionine aminopeptidase whether or not it is bound to another chemical entity.

One design approach is to probe a MetAP crystal of the invention with molecules composed of a variety of different chemical entities to determine sites for interaction between candidate MetAP inhibitors and an enzyme. For example, high resolution X-ray diffraction data collected from crystals saturated with solvent allows the determination of where each type of solvent molecule binds. Small molecules that bind tightly to those sites may then be designed and synthesized and tested for a MetAP inhibitor activity (J. Travis, *Science*, 262:1374 (1993)).

This invention also enables the development of compounds that may isomerize to short-lived reaction intermediates in a chemical reaction of a substrate or other compound that binds to or with an exemplary MetAP. Thus, time-dependent analysis of structural changes in a MetAP during its interaction with other molecules may be permitted. Reaction intermediates of a MetAP can also be deduced from a reaction product in co-complex with a MetAP. Such information may be useful to design improved analogues of known MetAP inhibitors or to design novel classes of inhibitors based on reaction intermediates of a MetAP enzyme and MetAP inhibitor co-complex. This provides a route for designing MetAP inhibitors with both specificity and stability.

Another approach made possible by this invention, is to screen computationally small molecule data bases for elements or compounds that may bind in whole, or in part, to a MetAP enzyme. In this screening, the quality of fit of such entities or compounds to the binding site may be judged either by shape complementarity or by estimated interaction energy (E. C. Meng et al, *J. Comp. Chem.*, 13:505-524 (1992)).

Because MetAP may crystallize in more than one crystal form, the structure coordinates of MetAP, or portions thereof, as provided by this invention are particularly useful to solve a structure of those other crystal forms of MetAP. They may also be used to solve a structure of MetAP mutant co-complexes, or of a crystalline form of any other protein with significant amino acid sequence homology to any functional domain of MetAP.

One method that may be employed for this purpose is molecular replacement. In this method, an unknown crystal structure, whether it is another crystal form of MetAP, a MetAP mutant, a MetAP co-complex, a MetAP from a different bacterial species, or a crystal of some other protein with significant amino acid sequence homology to any domain of MetAP, may be determined using MetAP structure coordinates of this invention, such as those provided in Figures 1-10 and Tables I - X. This method may provide an accurate structural form for an unknown crystal.

Thus, MetAP structures provided herein permits screening of known molecules and/or the designing of new molecules that bind to a structure, particularly at a binding pocket or active site, via use of computerized evaluation systems. For example, computer modeling systems are available in which a sequence of a MetAP, and a MetAP structure (i.e., atomic coordinates, bond distances between atoms in the active site region, etc. as provided, for example, by Tables I - X herein) may be input. Thus, a machine readable medium may be encoded with data representing coordinates of Tables I - X. The computer may then generate structural details of a site into which a test compound may bind, thereby enabling determination of a complementary structural details of this test compound.

More particularly, design of compounds that bind to or inhibit MetAP according to this invention generally involves consideration of two factors. First, a compound must be capable of physically and structurally associating with MetAP. Non-covalent molecular interactions important in an association of MetAP with its substrate include hydrogen bonding, van der Waals, and hydrophobic interactions.

Second, a compound must be able to assume a conformation that allows it to associate with MetAP. Although certain portions of a compound may not directly

participate in this association with MetAP, those portions may still influence an overall conformation of a molecule. This, in turn, may have a significant impact on potency. Such conformational requirements include an overall three-dimensional structure and orientation of the chemical entity or compound in relation to all or a portion of a binding site, e.g., binding pocket, active site, or substrate binding sites of MetAP, or a spacing between functional groups of a compound comprising several chemical entities that directly interact with MetAP.

Another approach made possible by this invention is to screen computationally small molecule databases for chemical entities or compounds that can bind in whole, or in part, to a MetAP enzyme. Details on this process and the results it can provide are now documented in the art. For a description of this type of technology please refer to PCT application WO 97/16177 published 09 May 1997; the techniques described there for computer modeling are incorporated herein by reference.

Once identified by modeling techniques, a MetAP inhibitor may be tested for bio-activity using standard techniques. For example, a structure of the invention may be used in enzymatic activity assays to determine an inhibitory activity of compounds or binding assays using conventional formats to screen inhibitors. One particularly suitable assay format includes a enzyme-linked immunosorbent assay (herein "ELISA"). Other assay formats may be used; these assay formats are not a limitation on the present invention.

A potential inhibitory or binding effect of a chemical compound on MetAP may be analyzed prior to its actual synthesis and testing by the use of computer modelling techniques. If a theoretical structure of a given compound suggests insufficient interaction and association between it and MetAP, synthesis and testing of the compound is obviated. However, if computer modelling indicates a strong interaction, a molecule may then be synthesized and tested for its ability to bind to MetAP and inhibit using a suitable assay. In this manner, synthesis of inoperative compounds may be avoided.

An inhibitory or other binding compound of MetAP may be computationally evaluated and designed by means of a series of steps in that chemical entities or fragments are screened and selected for their ability to associate with an individual binding pockets or other areas of MetAP.

One skilled in the art may use one of several methods to screen chemical entities or fragments for their ability to associate with MetAP and more particularly with individual binding pockets of a MetAP active site or accessory binding site. This

process may begin by visual inspection of, for example, an active site on a computer screen based on MetAP coordinates in Tables I-X. Selected fragments or chemical entities may then be positioned in a variety of orientations, or docked, within an binding pocket or active site of MetAP. Docking may be accomplished using software such as Quanta and Sybyl, followed by energy minimization and molecular dynamics with standard molecular mechanics forcefields, such as CHARMM and AMBER.

Specialized computer programs may also assist in the process of selecting fragments or chemical entities. These include, but are not limited to:

1. GRID (P. J. Goodford, "A Computational Procedure for Determining Energetically Favorable Binding Sites on Biologically Important Macromolecules", *J. Med. Chem.*, 28:849-857 (1985)). GRID is available from Oxford University, Oxford, UK.

2. MCSS (A. Miranker and M. Karplus, "Functionality Maps of Binding Sites: A Multiple Copy Simultaneous Search Method", *Proteins: Structure, Function and Genetics*, 11:29-34 (1991)). MCSS is available from Molecular Simulations, Burlington, MA.

3. AUTODOCK (D. S. Goodsell and A. J. Olsen, "Automated Docking of Substrates to Proteins by Simulated Annealing", *Proteins: Structure, Function, and Genetics*, 8:195-202 (1990)). AUTODOCK is available from Scripps Research Institute, La Jolla, CA.

4. DOCK (I. D. Kuntz et al., "A Geometric Approach to Macromolecule-Ligand Interactions", J. Mol. Biol., 161:269-288 (1982)). DOCK is available from University of California, San Francisco, CA.

In addition, other commercially available computer databases for small molecular compounds includes Cambridge Structural Database, Fine Chemical Database, and CONCORD, for a review see Rusinko, A., Chem. Des. Auto. News 8, 44-47 (1993).

Once suitable chemical entities or fragments have been selected, they may be assembled into a single compound or inhibitor. Assembly may be proceed by visual inspection of a relationship of the fragments to each other on a three-dimensional image displayed on a computer screen in relation to structural coordinates of MetAP. This may be followed by manual model building using software such as Quanta or Sybyl.

Useful programs to aid one of skill in the art in connecting the individual chemical entities or fragments include, but are not limited to:

1. CAVEAT (P. A. Bartlett et al, "CAVEAT: A Program to Facilitate the Structure-Derived Design of Biologically Active Molecules", in Molecular Recognition in Chemical and Biological Problems", Speical Pub., Royal Chem. Soc. 78, pp. 182-196 (1989)]. CAVEAT is available from the University of California, Berkeley, CA.

2. 3D Database systems such as MACCS-3D (MDL Information Systems, San Leandro, CA). This area is reviewed in Y. C. Martin, "3D Database Searching in Drug Design," J. Med. Chem., 35:2145-2154 (1992).

3. HOOK (available from Molecular Simulations, Burlington, MA).

Instead of proceeding to build a MetAP modulator in a step-wise fashion a fragment or chemical entity at a time as described above, inhibitory, modulatory or other MetAP binding compounds may be designed as a whole or "*de novo*" using an empty active site or optionally including some portion(s) of a known ligand(s). These methods include, but are not limited to:

1. LUDI (H.J. Bohm, "The Computer Program LUDI: A New Method for the De Novo Design of Enzyme Inhibitors", *J. Comp. Aid. Molec. Design*, 6:61-78 (1992)). LUDI is available from Biosym Technologies, San Diego, CA.

2. LEGEND (Y. Nishibata and A. Itai, *Tetrahedron*, 47:8985 (1991)). LEGEND is available from Molecular Simulations, Burlington, MA.

3. LeapFrog (available from Tripos Associates, St. Louis, MO).

Other molecular modelling techniques may also be employed in accordance with this invention. See, e.g., N. C. Cohen et al, "Molecular Modeling Software and Methods for Medicinal Chemistry", *J. Med. Chem.*, 33:883-894 (1990). See also, M. A. Navia and M. A. Murcko, "The Use of Structural Information in Drug Design", *Current Opinions in Structural Biology*, 2:202-210 (1992). For example, where the structures of test compounds are known, a model of a test compound may be superimposed over a model of a structure of the invention. Numerous methods and techniques are known in the art for performing this step, any of which may be used. See, e.g., P.S. Farmer, Drug Design, Ariens, E.J., ed., Vol. 10, pp 119-143 (Academic Press, New York, 1980); U.S. Patent No. 5,331,573; U.S. Patent No. 5,500,807; C. Verlinde, *Structure*, 2:577-587 (1994); and I. D. Kuntz, *Science*, 257:1078-1082 (1992). Model building techniques and computer evaluation systems described herein are not a limitation on the present invention.

Thus, using these computer evaluation systems, a large number of compounds may be examined. Moreover, the need for synthesis of many compounds may be eliminated.

In another aspect, a bacterial methionine aminopeptidase structure of the invention may permit design and identification of synthetic compounds and/or other molecules that may be characterized by a conformation of a bacterial methionine aminopeptidase of the invention. Using known computer systems, coordinates of the bacterial methionine aminopeptidase structures of the invention may be provided in machine readable form, test compounds designed and/or screened and their conformations superimposed on a structure of the methionine aminopeptidases of the invention. Subsequently, suitable candidates identified as above may be screened for a desired methionine aminopeptidase inhibitory activity, stability, and the like.

Once identified and screened for activity, these inhibitors may be used therapeutically or prophylactically to block methionine aminopeptidase activity, and thus, overcome bacterial resistance to antibiotics, for example, of the beta-lactam class, *e.g.* imipenem, penicillins, cephalosporins, *etc.* by using a different mechanism of attacking bacteria in diseases produced by bacterial infection.

All publications, including, but not limited to, patents and patent applications cited in this specification, are herein incorporated by reference as if each individual publication were specifically and individually indicated to be incorporated by reference herein as though fully set forth.

Tables

Table I provides three dimensional protein coordinates of the *S. aureus* methionine aminopeptidase crystalline structure of the invention.

Table II provides three dimensional coordinates for a *S. aureus* methionine aminopeptidase complex with a specific inhibitor of the present invention, 5-(3-Iodo-phenyl)-1-H-[1,2,3]triazole.

Table III provides three dimensional coordinates for a *S. aureus* methionine aminopeptidase complex with a specific inhibitor of the present invention, 5-benzofuran-2-yl-1-H-[1,2,3]triazole.

Table IV provides distances between interresidue atoms that are within 5 Ångstroms apart in an active site of *S. aureus* methionine aminopeptidase for inhibitor complexes of a specific inhibitor of the present invention, 5-(3-Iodo-phenyl)-1-H-[1,2,3]triazole.

Table V provides distances between interresidue atoms that are within 5 Ångstroms apart in an active site of *S. aureus* methionine aminopeptidase for

inhibitor complexes of a specific inhibitor of the present invention, 5-benzofuran-2-yl-1-H-[1,2,3]triazole.

Table VI provides angles between interresidue atoms that are within 5 Ångstroms apart in an active site of *S. aureus* methionine aminopeptidase for inhibitor complexes of a specific inhibitor of the present invention, 5-(3-Iodo-phenyl)-1-H-[1,2,3]triazole.

TableVII provides angles between interresidue atoms that are within 5 Ångstroms apart in an active site of *S. aureus* methionine aminopeptidase for inhibitor complexes of a specific inhibitor of the present invention, 5-benzofuran-2-yl-1-H-[1,2,3]triazole.

Table VIII provides three dimensional protein coordinates of an *S. pneumoniae* methionine aminopeptidase crystalline structure of the invention.

Table IX provides distances between interresidue atoms that are within 5 Ångstroms apart in an active site of *S. pneumoniae* methionine aminopeptidase.

Table X provides angles between interresidue atoms that are within 5 Ångstroms apart in an active site of *S. pneumoniae.*

Table Legend:

1. Under the heading ATOM appears a "atom number" (e.g. 1,2,3,4...etc) and the "atom name" (e.g. CA, CB, N,... etc) such that to each "atom name" in a coordinate list corresponds an "atom number".

2. Under the heading RESIDUE appears a three-letter "residue name" (e.g. THR, ASP, etc), a "chain identifier" represented by a capital letter (e.g. A, B, C D, etc) and a "residue number", such that to each residue (or amino acid) in an amino acid sequence of a particular protein in a structure corresponds a name that identifies it, a number according to its position along an amino acid sequence, and a chain name. A chain name identifies a particular molecule in a crystal structure. For instance, if there is more than one molecule that forms a unit that is repeated throughout a crystal lattice, then each unit is identified as molecule A, or molecule B, or molecule C, *etc.*

3. Under the headings X, Y, or Z appear Cartesian coordinates of the atoms in a structure.

4. Under the heading B appears the "B-factor" or "temperature factor" that may adopt, in principle, any value. It is meant to represent an atomic displacement around that position.

EXAMPLES

The invention will now be described by reference to the following examples which are merely illustrative and are not to be construed as a limitation of the scope of the present invention. In the Examples, proton NMR spectra were performed upon a Bruker 400 MHz NMR spectrometer, unless otherwise indicated.

Example 1

Preparation of 3-(1*H*-1,2,3-triazol-4-yl)-phenol

To a stirring solution of 3-ethynylphenol (0.55 g, 4.0 mmol) in 4 ml of toluene under an inert atmosphere was added trimethylsilylazide (1 ml, 8 mmol). The resulting solution was heated to reflux for 3 days. To this mixture was added water (1 ml) and after evaporation, the resulting residue was purified by preparative HPLC to afford the title compound as a white solid (0.12 g, 18%). ^{1}H-NMR (400MHz, CD_3OD): δ 8.09 (s, 1H), 7.27 (m, 3H), 6.81 (m, 1H). MS (ESI) 162.2 $(M+H)^+$. (This procedure was adapted from Tanaka, Y.; Velen, S. R.; Miller, S. I. *Tetrahedron*, **1973**, *29*, 3271.)

Example 2

Preparation of 4-(3-iodophenyl)-1*H*-1,2,3-triazole

Following the procedure of Example 1, except substituting 1-ethynyl-3-iodobenzene for 3-ethynylphenol, the title compound was prepared as a white solid (20 %). ^{1}H-NMR (400MHz, $CDCl_3$): δ 8.21 (s, 1H), 7.98 (s, 1H), 7.81 (d, J=7.8 Hz, 1H), 7.73 (d, J=8.1 Hz, 1H), 7.21 (t, J=7.8 Hz, 1H). MS (ESI) 272.0 $(M+H)^+$.

Example 3

Preparation of 4-(2-fluorophenyl)-1*H*-1,2,3-triazole

Following the procedure of Example 1, except substituting 1-ethynyl-2-fluorobenzene for 3-ethynylphenol, the title compound was prepared as a white solid (21 %). ^{1}H-NMR (400MHz, $CDCl_3$): δ 11.54 (br s, 1H), 8.19 (s, 1H), 8.11 (t, J=7.5 Hz, 1H), 7.18-7.40 (m, 3H). MS (ESI) 164.2 $(M+H)^+$.

Example 4

Preparation of 4-(4-n-butylphenyl)-1*H*-1,2,3-triazole

Following the procedure of Example 1, except substituting 1-ethynyl-4-n-butylbenzene for 3-ethynylphenol, the title compound was prepared as a white solid (16 %). ^{1}H-NMR (400MHz, CD_3OD): δ 8.11 (s, 1H), 7.74 (d, J=7.8 Hz, 2H), 7.28 (d,

J=8.0 Hz, 2H), 2.67 (t, J=7.6 Hz, 2H), 1.61-1.69 (m, 2H), 1.37-1.43 (m, 2H), 0.97 (t, J=7.3 Hz, 3H). MS (ESI) 202.2 $(M+H)^+$.

Example 5

Preparation of 4-(2-chlorophenyl)-1*H*-1,2,3-triazole

Following the procedure of Example 1, except substituting 1-chloro-2-ethynylbenzene for 3-ethynylphenol, the title compound was prepared as a white solid (35 %). ^{1}H-NMR (400MHz, CD_3OD): δ 8.29 (s, 1H), 7.90 (d, J=7.0 Hz, 1H), 7.53-7.56 (m, 1H), 737-7.44 (m, 2H). MS (ESI) 180.0 $(M+H)^+$.

Example 6

Preparation of N-(3-[1*H*-1,2,3-triazol-4-yl]phenyl)benzamide

Following the procedure of Example 1, except substituting N-(3-ethynylphenyl)benzamide for 3-ethynylphenol, the title compound was prepared as a white solid (12 %). ^{1}H-NMR (400MHz, CD_3OD): δ 8.18-8.20 (m, 2H), 7.93-8.00 (m, 2H), 7.45-7.76 (m, 6H). MS (ESI) 265.2 $(M+H)^+$.

Example 7

Preparation of 3-(1*H*-1,2,3-triazol-4-yl)-phenylamine

Following the procedure of Example 1, except substituting 3-ethynyl-phenylamine for 3-ethynylphenol, the title compound was prepared as a tan solid (19 %). ^{1}H-NMR (400MHz, CD_3OD): δ 8.05 (s, 1H), 7.12-7.20 (m, 3H), 6.73-6.75 (m, 1H). MS (ESI) 161.2 $(M+H)^+$.

Example 8

Preparation of N-(3-[1*H*-1,2,3-triazol-4-yl]phenyl)acetamide

Following the procedure of Example 1, except substituting N-(3-ethynylphenyl)acetamide for 3-ethynylphenol, the title compound was prepared as a tan solid (49%). ^{1}H-NMR (400MHz, DMSO-d_6): δ 10.04 (s, 1H), 8.11-8.50 (m, 2H), 7.35-7.58 (m, 3H), 2.06 (s, 3H). MS (ESI) 203.2 $(M+H)^+$.

Example 9

Preparation of 4-(4-trifouoromethylphenyl)-1*H*-1,2,3-triazole

Following the procedure of Example 1, except substituting 1-ethynyl-4-trifouoromethylphenyl for 3-ethynylphenol, the title compound was prepared as a white solid (50 %). ^{1}H-NMR (400MHz, CD_3OD): δ 8.30 (s, 1H), 8.06 (d, J=8.2 Hz, 2H), 7.76 (d, J=8.2 Hz, 2H). MS (ESI) 214.2 $(M+H)^+$.

Example 10

Preparation of 4-(3-trifouoromethylphenyl)-1*H*-1,2,3-triazole

Following the procedure of Example 1, except substituting 1-ethynyl-3-trifouoromethylphenyl for 3-ethynylphenol, the title compound was prepared as a white solid (16 %). ^{1}H-NMR (400MHz, CD_3OD): δ 8.32, (s, 1H), 8.10-8.18 (m, 2H), 7.64-7.68 (m, 1H). MS (ESI) 214.2 $(M+H)^+$.

Example 11

Preparation of 4-(4-n-propylphenyl)-1*H*-1,2,3-triazole

Following the procedure of Example 1, except substituting 1-ethynyl-4-n-propylbenzene for 3-ethynylphenol, the title compound was prepared as a white solid (26 %). ^{1}H-NMR (400MHz, CD_3OD): δ 8.11 (s, 1H), 7.74 (d, J=7.5 Hz, 2H), 7.28 (d, J=8.0 Hz, 2H), 2.64 (t, J=7.6 Hz, 2H), 1.64-1.73 (m, 2H), 0.97 (t, J=7.3 Hz, 3H). MS (ESI) 188.2 $(M+H)^+$.

Example 12

Preparation of 4-(4-methoxyphenyl)-1*H*-1,2,3-triazole

Following the procedure of Example 1, except substituting 1-ethynyl-4-methoxybenzene for 3-ethynylphenol, the title compound was prepared as a white solid (34 %). ^{1}H-NMR (400MHz, $CDCl_3$): δ 7.92 (s, 1H), 7.76 (d, J=8.8 Hz, 2H), 7.01 (d, J=8.8 Hz, 2H), 3.88 (s, 3H). MS (ESI) 176.2 $(M+H)^+$.

Example 13

Preparation of 4-(3-methylphenyl)-1*H*-1,2,3-triazole

Following the procedure of Example 1, except substituting 3-ethynyltoluene for 3-ethynylphenol, the title compound was prepared as a white solid (23 %). ^{1}H-NMR (400MHz, CD_3OD): δ 8.14 (s, 1H), 7.67 (s, 1H), 7.62 (d, J=7.7 Hz, 1H), 7.34 (t, J=7.6 Hz, 1H), 7.20 (d, J=7.6 Hz, 1H), 2.41 (s, 3H). MS (ESI) 160.2 $(M+H)^+$.

Example 14

Preparation of 2-(1*H*-1,2,3-triazol-4-yl)-pyridine

Following the procedure of Example 1, except substituting 2-ethynylpyridine for 3-ethynylphenol, the title compound was prepared as a white solid (16 %). ^{1}H-NMR (400MHz, CD_3OD): δ 8.60-8.61 (m, 1H), 8.32 (s, 1H), 8.06 (d, J=8.0 Hz, 1H), 7.90-7.95 (m, 1H), 7.38-7.41 (m, 1H). MS (ESI) 147.2 $(M+H)^+$.

Example 15

Preparation of 4-(4-chlorophenyl)-1*H*-1,2,3-triazole

Following the procedure of Example 1, except substituting 1-chloro-4-ethynylbenzene for 3-ethynylphenol, the title compound was prepared as a white solid (35 %). ^{1}H-NMR (400MHz, CD_3OD): δ 8.18 (s, 1H), 7.85 (d, J=8.6 Hz, 2H), 7.47 (d, J = 8.7 Hz, 2H). MS (ESI) 180.0 $(M+H)^+$.

Example 16

Preparation of 4-(4-ethylphenyl)-1*H*-1,2,3-triazole

Following the procedure of Example 1, except substituting 1-ethyl-4-ethynylbenzene for 3-ethynylphenol, the title compound was prepared as a white solid (11 %). ^{1}H-NMR (400MHz, CD_3OD): δ 8.11 (s, 1H), 7.74 (d, J=8.2 Hz, 2H), 7.30 (d, J = 8.2 Hz, 2H), 2.69 (q, J = 7.6, 2H), 1.27 (t, J = 7.6 Hz, 3H). MS (ESI) 174.2 $(M+H)^+$.

Example 17

Preparation of 4-(1*H*-1,2,3-triazol-4-yl)-phenylamine

Following the procedure of Example 1, except substituting 4-ethynylphenylamine for 3-ethynylphenol, the title compound was prepared as an orange solid (9 %). ^{1}H-NMR (400MHz, CD_3OD): δ 7.94 (s, 1H), 7.54 (d, J=8.6 Hz, 2H), 6.78 (d, J=8.6 Hz, 2H). MS (ESI) 161.2 $(M+H)^+$.

Example 18

Preparation of 4-(4-methylphenyl)-1*H*-1,2,3-triazole

Following the procedure of Example 1, except substituting 4-ethynyltoluene for 3-ethynylphenol, the title compound was prepared as a white solid (14 %). ^{1}H-NMR (400MHz, $CDCl_3$): δ 7.96 (s, 1H), 7.73 (d, J = 8.0 Hz, 2H), 7.28-7.30 (m, 2H), 1.57 (s, 3H). MS (ESI) 160.2 $(M+H)^+$.

Example 19

Preparation of 2-(1*H*-1,2,3-triazol-4-yl)-5-methylpyridine

Following the procedure of Example 1, except substituting 2-ethynyl-5-methylpyridine (Sakamoto, T.; Nagata, H.; Kondo, Y.; Sato, K.; Yamanaka, H. *Chem. Pharm. Bull.* **1984**, *32*, 4866) for 3-ethynylphenol, the title compound was prepared as a white solid (28 %). ^{1}H-NMR (400MHz, CD_3OD): δ 8.45 (s, 1H), 8.27 (s, 1H), 7.95 (d, J = 8.1 Hz, 1H), 7.76 (d, J = 8.1 Hz, 1H), 2.41 (s, 3H). MS (ESI) 161.2 $(M+H)^+$.

Example 20

Preparation of 2-(1*H*-1,2,3-triazol-4-yl)-4-methyl-pyridine

Following the procedure of Example 1, except substituting 2-ethynyl-4-methylpyridine (Sakamoto, T.; Nagata, H.; Kondo, Y.; Sato, K.; Yamanaka, H. *Chem. Pharm. Bull.* **1984**, *32*, 4866) for 3-ethynylphenol, the title compound was prepared as a white solid (54 %). ^{1}H-NMR (400MHz, CD_3OD): δ 8.45 (d, J = 5.1 Hz, 1H), 8.29 (s, 1H), 7.91 (s, 1H), 7.23 (d, J = 5.1 Hz, 1H), 2.46 (s, 3H). MS (ESI) 161.2 $(M+H)^+$.

Example 21

Preparation of 1-(1*H*-1,2,3-triazol-4-yl)cyclohexanol

Following the procedure of Example 1, except substituting 1-ethynylcyclohexanol for 3-ethynylphenol, the title compound was prepared as a white solid (10%). ^{1}H-NMR (400MHz, CD_3OD): δ 7.70 (s, 1H), 1.39-1.99 (m, 10H). MS (ESI) 168.2 $(M+H)^+$.

Example 22

Preparation of 4-(thiophen-2-yl)-1*H*-1,2,3-triazole

a) 2-ethynylthiophene

To a stirring solution of 2-thiophenecarboxaldehyde (0.33 g, 3.0 mmol) in dry methanol (30 ml) was added potassium carbonate (0.87 g, 6.3 mmol) and 1-diazo-2-oxopropylphosphonate (0.78 g, 4.1 mmol, Calant, P.; D'Haenens, L.; Vandewalle, M. *Synth. Commun.* **1984**, *14*, 155). After 4 h of stirring at room temperature, aqueous sodium bicarbonate (5%, 50 ml) and hexanes (50 ml) were added. The organic layer was collected, dried ($MgSO_4$) and filtered through a short silica plug. Evaporation

yielded the title compound as a clear oil. (This procedure was adapted from Muller, S.; Liepold, B.; Roth, G. J.; Bestmann, H. J. *Synlett* **1996**, 521.)

b) 4-(thiophen-2-yl)-1*H*-1,2,3-triazole

Following the procedure of Example 1, except substituting 2-ethynylthiophene for 3-ethynylphenol, the title compound was prepared as a white solid (2 steps, 7%). ^{1}H-NMR (400MHz, CD_3OD): δ 8.05 (s, 1H), 7.43-7.47 (m, 2H), 7.10-7.13 (m, 1H). MS (ESI) 152.2 $(M+H)^+$.

Example 23

Preparation of 4-(thiophen-3-yl)-1*H*-1,2,3-triazole

Following the procedure of Example 22, except substituting 3-thiophenecarboxaldehyde for 2-thiophenecarboxaldehyde in step a, the title compound was prepared as a white solid (2 steps, 8 %). ^{1}H-NMR (400MHz, CD_3OD): δ 8.07 (s, 1H), 7.79 (s, 1H), 7.53 (s, 2H). MS (ESI) 152.2 $(M+H)^+$.

Example 24

Preparation of 4-(2-methylphenyl)-1*H*-1,2,3-triazole

Following the procedure of Example 22, except substituting o-tolualdehyde for 2-thiophenecarboxaldehyde in step a, the title compound was prepared as a white solid (2 steps, 3 %). ^{1}H-NMR (400MHz, CD_3OD): δ 7.97 (s, 1H), 7.55-7.58 (m, 1H), 7.26-7.33 (m, 3H), 2.44 (s, 3H). MS (ESI) 160.2 $(M+H)^+$.

Example 25

Preparation of 4-(1,3-dimethylphenyl)-1*H*-1,2,3-triazole

Following the procedure of Example 22, except substituting 2,4-dimethylbenzaldehyde for 2-thiophenecarboxaldehyde in step a, the title compound was prepared as a white solid (2 steps, 3 %). ^{1}H-NMR (400MHz, CD_3OD): δ 7.92 (s, 1H), 7.44 (d, J=7.8 Hz, 1H), 7.14 (s, 1H), 7.10 (d, J=7.3 Hz, 1H), 2.40 (s, 3H), 2.36 (s, 3H). MS (ESI) 174.2 $(M+H)^+$.

Example 26

Preparation of 4-(4-bromophenyl)-1*H*-1,2,3-triazole

Following the procedure of Example 22, except substituting 4-bromobenzaldehyde for 2-thiophenecarboxaldehyde in step a, the title compound was

prepared as a white solid (2 steps, 7 %). ^{1}H-NMR (400MHz, CD_3OD): δ 8.19 (s, 1H), 7.77 (d, J=8.6 Hz, 2H), 7.61 (d, J=8.6, 2H). MS (ESI) 224.0 $(M+H)^+$.

Example 27

Preparation of 4-(1,3-dichlorophenyl)-1*H*-1,2,3-triazole

Following the procedure of Example 22, except substituting 2,4-dichlorobenzaldehyde for 2-thiophenecarboxaldehyde in step a, the title compound was prepared as a white solid (2 steps, 6 %). ^{1}H-NMR (400MHz, CD_3OD): δ (s, 1H), 7.91-7.94 (m, 1H), 7.61-7.62 (m, 1H) 7.44-7.48 (m, 1H). MS (ESI) 214.0 $(M+H)^+$.

Example 28

Preparation of 4-(1-biphenyl-2-yl)-1*H*-1,2,3-triazole

Following the procedure of Example 22, except substituting 2-biphenylcarboxaldehyde for 2-thiophenecarboxaldehyde in step a, the title compound was prepared as a clear oil (2 steps, 27 %). ^{1}H-NMR (400MHz, CD_3OD): δ 7.80 (s, 1H), 7.47-7.49 (m, 2H), 7.36-7.40 (m, 4 H), 7.20-7.22 (m, 2H), 6.88 (s, 1H). MS (ESI) 222.2 $(M+H)^+$.

Example 29

Preparation of 4-(2-benzyloxy-phenyl)-1*H*-1,2,3-triazole

Following the procedure of Example 22, except substituting 2-benzyloxybenzaldehyde for 2-thiophenecarboxaldehyde in step a, the title compound was prepared as a white solid (2 steps, 25 %). ^{1}H-NMR (400MHz, CD_3OD): δ 8.09 (s, 1H), 8.00 (d, J = 7.7 Hz, 1H), 7.33-7.43 (m, 6H), 7.20 (d, J = 8.3 Hz, 1H), 7.07 (t, J = 7.5, 1H), 5.25 (s, 2H). MS (ESI) 252.2 $(M+H)^+$.

Example 30

Preparation of 2-(1*H*-1,2,3-triazol-4-yl)-6-methylpyridine

Following the procedure of Example 22, except substituting 6-methyl-2-pyridine carboxaldehyde for 2-thiophenecarboxaldehyde in step a, the title compound was prepared as a clear oil (2 steps, 39 %). ^{1}H-NMR (400MHz, CD_3OD): δ 8.33 (s, 1H), 7.77-7.85 (m, 2H), 7.26 (d, J = 7.4 Hz, 1H), 2.60 (s, 3H). MS (ESI) 161.2 $(M+H)^+$.

Example 31

Preparation of 3-(1*H*-1,2,3-triazol-4-yl)-pyridine

Following the procedure of Example 22, except substituting 3-pyridine carboxaldehyde for 2-thiophenecarboxaldehyde in step a, the title compound was prepared as a white solid (2 steps, 25 %). %). ^{1}H-NMR (400MHz, CD_3OD): δ 9.06 (s, 1H), 8.54 (d, J = 3.4 Hz, 1H), 8.31-8.33 (m, 2H), 7.54 (m, 1H). MS (ESI) 147.2 $(M+H)^+$.

Example 32

Preparation of 4-(1*H*-1,2,3-triazol-4-yl)-pyridine

Following the procedure of Example 22, except substituting 4-pyridine carboxaldehyde for 2-thiophenecarboxaldehyde in step a, the title compound was prepared as a white solid (2 steps, 15 %). ^{1}H-NMR (400MHz, CD_3OD): δ 8.61-8.62 (m, 2H), 8.42 (s, 1H), 7.91-7.93 (m, 2H). MS (ESI) 147.2 $(M+H)^+$.

Example 33

Preparation of 4-(2-methoxyphenyl)-1*H*-1,2,3-triazole

Following the procedure of Example 22, except substituting o-anisaldehyde for 2-thiophenecarboxaldehyde in step a, the title compound was prepared as a white solid (2 steps, 6 %). ^{1}H-NMR (400MHz, CD_3OD): δ 8.19 (s, 1H), 7.95 (d, J = 6.8 Hz, 1H), 7.35-7.40 (m, 1H), 7.14 (d, J = 8.3 z, 1H), 7.04-7.08 (m, 1H), 4.90 (s, 3H). MS (ESI) 176.2 $(M+H)^+$.

Example 34

Preparation of 4-(2-bromophenyl)-1*H*-1,2,3-triazole

Following the procedure of Example 22, except substituting 2-bromobenzaldehyde for 2-thiophenecarboxaldehyde in step a, the title compound was prepared as a white solid (2 steps, 15 %). ^{1}H-NMR (400MHz, CD_3OD): δ 8.27 (s, 1H), 7.73-7.79 (m, 2H), 7.45-7.79 (m, 1H), 7.30-7.34 (m, 1H).MS (ESI) 224.0 $(M+H)^+$.

Example 35

Preparation of 4-benzo[1,3]dioxol-5-yl-1*H*-1,2,3-triazole

Following the procedure of Example 22, except substituting piperonal for 2-thiophenecarboxaldehyde in step a, the title compound was prepared as a white solid

(2 steps, 10 %). ^{1}H-NMR (400MHz, CD_3OD): δ 8.05 (s, 1H), 7.32-7.34 (m, 2H), 6.89-6.91 (m, 1H), 6.00 (s, 2H). MS (ESI) 190.2 $(M+H)^+$.

Example 36

Preparation of 2-(1*H*-1,2,3-triazol-4-yl)-benzofuran

Following the procedure of Example 22, except substituting benzofuran-2-carboxaldehyde for 2-thiophenecarboxaldehyde in step a, the title compound was prepared as a white solid (2 steps, 25 %). ^{1}H-NMR (400MHz, CD_3OD): δ 8.25 (s, 1H), 7.65 (d, J = 7.6 Hz, 1H), 7.56 (d, J = 8.0 Hz, 1H), 7.23-7.36 (m, 3H). MS (ESI) 186.0 $(M+H)^+$.

Example 37

Preparation of 4-benzo[1,3]dioxol-4-yl-1*H*-1,2,3-triazole

a) 4-ethynyl-benzo[1,3]dioxole

Following the procedure of Example 22, except substituting benzo[1,3]dioxole-4-carbaldehyde for 2-thiophenecarboxaldehyde in step a, the title compound was obtained as an oil (98 %). ^{1}H-NMR (400MHz, $CDCl_3$): δ 6.94-6.96 (m, 1H), 6.80-6.85 (m, 2H), 6.05 (s, 2H), 3.30 (s, 1H).

b) 4-benzo[1,3]dioxol-4-yl-1*H*-1,2,3-triazole

Following the procedure of Example 1, except substituting 4-ethynyl-benzo[1,3]dioxole for 3-ethynylphenol, the title compound was prepared as a white solid (24 %). ^{1}H-NMR (400MHz, CD_3OD): δ 8.13 (s, 1H), 7.45 (d, J = 8.0 Hz, 1H), 6.94-6.97 (m, 1H), 6.81-6.83 (m, 1H), 6.08 (s, 2H). MS (ESI) 190.2 $(M+H)^+$.

Example 38

Preparation of 4-(2-[4-chloro-phenylsulfanyl]-phenyl)-1*H*-1,2,3-triazole

a) 1-(4-chloro-phenylsulfanyl)-2-ethynylbenzene

Following the procedure of Example 22, except substituting 2-(4-chlorophenylthio)benzaldehyde for 2-thiophenecarboxaldehyde in step a, the title compound was obtained as an oil (91 %). ^{1}H-NMR (400MHz, $CDCl_3$): δ 7.53-7.55 (m, 1H), 7.17-7.40 (m, 6H), 7.03-7.05 (m, 1H), 3.43 (s, 1H).

b) 4-(2-[4-chloro-phenylsulfanyl]-phenyl)-1*H*-1,2,3-triazole

Following the procedure of Example 1, except substituting 1-(4-chloro-phenylsulfanyl)-2-ethynylbenzene for 3-ethynylphenol, the title compound was

prepared as a white solid (21 %). ^{1}H-NMR (400MHz, CD_3OD): δ 8.10 (s, 1H), 7.77-7.79 (m, 1H), 7.39-7.46 (m, 3H), 7.28-7.30 (m, 2H), 7.15-7.17 (m, 2H).MS (ESI) 288.2 $(M+H)^+$.

Example 39

Preparation of (3-phenyl-propyl)-(3-[1*H*-1,2,3-triazol-4-yl]phenyl)amine

a) (3-phenyl-propyl)-(3-ethynylphenyl)amine

To a stirring solution of 3-ethynylphenylamine (0.59 g, 5.0 mmol) and 3-phenylpropionaldehyde (0.66 g, 5.0 mmol) in 1,2-dichloroethane (15 ml) was added acetic acid (0.29 ml, 5.0 mmol) and sodium triacetoxyborohydride (1.6 g, 7.5 mmol). After stirring at room temperature for 72 h, aqueous sodium bicarbonate (saturated) and diethyl ether were added. The organic layer was washed with additional sodium bicarbonate, dried ($MgSO_4$) and evaporated. Purification via silica gel chromatography gave the title compound as a clear oil (42 %). MS (ESI) 236.2 $(M+H)^+$.

b) (3-phenyl-propyl)-(3-[1*H*-1,2,3-triazol-4-yl]phenyl)amine

Following the procedure of Example 1, except substituting (3-phenyl-propyl)-(3-ethynylphenyl)amine for 3-ethynylphenol, the title compound was prepared as a clear oil (16 %). ^{1}H-NMR (400MHz, CD_3OD): δ 8.03 (s, 1H), 7.6.62-7.30 (m, 9H), 3.17 (t, J = 7.0 Hz, 2H), 2.77 (t, J = 7.4 Hz, 2H), 1.97 (t, J = 7.7 Hz, 2H). MS (ESI) 279.4 $(M+H)^+$.

Example 40

Preparation of phenethyl-(3-[1*H*-1,2,3-triazol-4-yl]phenyl)amine

a) phenethyl-(3-ethynylphenyl)-amine

Following the procedure of Example 39, except substituting phenylacetaldehyde for 3-phenylpropionaldehyde in step a, the title compound was prepared as a clear oil (47 %). MS (ESI) 222.2 $(M+H)^+$.

b) phenethyl-(3-[1*H*-1,2,3-triazol-4-yl]phenyl)amine

Following the procedure of Example 1, except substituting phenethyl-(3-ethynylphenyl)-amine for 3-ethynylphenol, the title compound was prepared as a clear oil (19 %). ^{1}H-NMR (400MHz, CD_3OD): δ 8.07 (s, 1H), 7.06-7.31 (m, 8H), 6.67 (d, J = 8.1 Hz, 1H), 3.41 (t, J = 7.2 Hz, 2H), 2.94 (t, J = 7.1 Hz, 2H). MS (ESI) 265.2 $(M+H)^+$.

Example 41

Preparation of furan-2-ylmethyl-(3-[1*H*-1,2,3-triazol-4-yl]phenyl)amine

a) furan-2-ylmethyl-(3-ethynylphenyl)-amine

Following the procedure of Example 39, except substituting furfural for 3-phenylpropionaldehyde in step a, the title compound was prepared as a clear oil (75 %). MS (ESI) 198.2 $(M+H)^+$.

b) furan-2-ylmethyl-(3-[1*H*-1,2,3-triazol-4-yl]phenyl)amine

Following the procedure of Example 1, except substituting furan-2-ylmethyl-(3-ethynylphenyl)-amine for 3-ethynylphenol, the title compound was prepared as a white solid (18 %). ^{1}H-NMR (400MHz, CD_3OD): δ 8.06 (s, 1H), 7.43 (d, J = 1.0 Hz, 1H), 7.09-7.22 (m, 3H), 6.72 (d, J = 8.1 Hz, 1H), 6.34-6.35 (m, 1H), 6.28 (d, J = 3.2 Hz, 1H), 4.36 (s, 2H). MS (ESI) 241.2 $(M+H)^+$.

Example 42

Preparation of furan-3-ylmethyl-(3-[1*H*-1,2,3-triazol-4-yl]phenyl)amine

a) furan-3-ylmethyl-(3-ethynylphenyl)-amine

Following the procedure of Example 39, except substituting 3-furaldehyde for 3-phenylpropionaldehyde in step a, the title compound was prepared as a clear oil (70 %). MS (ESI) 198.2 $(M+H)^+$.

b) furan-3-ylmethyl-(3-[1*H*-1,2,3-triazol-4-yl]phenyl)amine

Following the procedure of Example 1, except substituting furan-3-ylmethyl-(3-ethynylphenyl)-amine for 3-ethynylphenol, the title compound was prepared as a white solid (20 %). ^{1}H-NMR (400MHz, CD_3OD): δ 8.06 (s, 1H), 7.49 (s, 1H), 7.45-7.46 (m, 1H), 7.08-7.22 (m, 3H), 6.71 (dd, J = 6.5, 1.5 Hz, 1H), 6.47 (s, 1H) 4.22 (s, 2H). MS (ESI) 241.2 $(M+H)^+$.

Example 43

Preparation of napthalene-1-ylmethyl-(3-[1*H*-1,2,3-triazol-4-yl]phenyl)amine

a) napthalene-1-ylmethyl-(3-ethynylphenyl)-amine

Following the procedure of Example 39, except substituting 1-napthaldehyde for 3-phenylpropionaldehyde in step a, the title compound was prepared as a clear oil (80 %). MS (ESI) 258.2 $(M+H)^+$.

b) napthalene-1-ylmethyl-(3-[1*H*-1,2,3-triazol-4-yl]phenyl)amine

Following the procedure of Example 1, except substituting napthalene-1-ylmethyl-(3-ethynylphenyl)-amine for 3-ethynylphenol, the title compound was

prepared as a white solid (18 %). ^{1}H-NMR (400MHz, CD_3OD): δ 8.16 (d, J = 8.2 Hz, 1H), 7.99 (br s, 1H), 7.91 (d, J = 8.1 Hz, 1H), 7.81 (d, J = 8.4 Hz, 1H), 7.42-7.60 (m, 4H), 7.09-7.21 (m, 3H) 6.71 (d, J = 8.0 Hz, 1H), 4.83 (s, 2H). MS (ESI) 301.2 $(M+H)^+$.

Example 44

Preparation of napthalene-2-ylmethyl-(3-[1*H*-1,2,3-triazol-4-yl]phenyl)amine

a) napthalene-2-ylmethyl-(3-ethynylphenyl)-amine

Following the procedure of Example 39, except substituting 2-napthaldehyde for 3-phenylpropionaldehyde in step a, the title compound was prepared as a clear oil (90 %). MS (ESI) 258.2 $(M+H)^+$.

b) napthalene-2-ylmethyl-(3-[1*H*-1,2,3-triazol-4-yl]phenyl)amine

Following the procedure of Example 1, except substituting napthalene-2-ylmethyl-(3-ethynylphenyl)-amine for 3-ethynylphenol, the title compound was prepared as a white solid (15 %). ^{1}H-NMR (400MHz, CD_3OD): δ 8.01 (s, 1H), 7.80-7.87 (m, 4H), 7.41-7.56 (m, 3H), 7.05-7.19 (m, 3H), 6.70 (d, J = 1.6 Hz, 1H), 4.56 (s, 2H). MS (ESI) 301.2 $(M+H)^+$.

Example 45

Preparation of 4-(1*H*-1,2,3-triazol-4-yl)-phenol

To 4-(4-methoxyphenyl)-1*H*-1,2,3-triazole (83 mg, 0.5 mmol, from Example 12) was added hydrobromic acid (48% in water, 2 ml) and the solution was heated to 100 °C. After three hours, water (10 ml) and ethyl acetate (10 ml) were added. The water layer was washed with ethyl acetate three times and the collected organic layers were dried, filtered, and evaporated. The resulting residue was purified by preparative HPLC to afford the title compound as a white solid (40 %). ^{1}H-NMR (400MHz, CD_3OD): δ 8.01 (s, 1H), 7.65 (d, J=8.7 Hz, 2H), 6.87 (d, J=8.7 Hz, 2H). MS (ESI) 162.2 $(M+H)^+$.

Example 46

Preparation of benzyl-(3-[1*H*-1,2,3-triazol-4-yl]phenyl)amine

To a cooled (0 °C) solution of N-(3-[1*H*-1,2,3-triazol-4-yl]phenyl)benzamide (50 mg, 0.19 mmol, from Example 6) in THF (0.5 ml) and dioxane (0.5 ml) was added lithium aluminum hydride (1.0 M in THF, 0.2 ml) and the reaction was allowed to warm to room temperature overnight. Additional dioxane (1 ml) and lithium aluminum hydride (0.2 ml) were added with heating to 50 °C to force the reaction to completion.

Water and Na_2SO_4 were added and the residue was filtered. The filtrate was evaporated and purified by preparative HPLC to afford the title compound as a tan oil (60 %). ^{1}H-NMR (400MHz, CD_3OD): δ 7.96 (s, 1H), 7.40-7.43 (m, 2H) 7.30-7.35 (m, 2H), 7.04-7.25 (m, 4H), 6.63 (d, J = 8.0 Hz, 1H), 4.38 (s, 2H). MS (ESI) 251.2 $(M+H)^+$.

Example 47

Preparation of 4-(4-fluorophenyl)-1*H*-1,2,3-triazole

a) 1-chloroethynyl-4-fluorobenzene

To a stirring solution of 1-ethynyl-4-fluorobenzene (1.30 g, 10 mmol) in carbon tetrachloride (5 ml) was added potassium carbonate (1.56 g, 11 mmol) and TBAF (0.23 g, 1.0 mmol). After stirring the reaction at RT for 1 h, water (20 ml) was added and the organic material was collected by extraction into chloroform. The combined chloroform extracts were dried ($MgSO_4$) and evaporated. Purification by silica gel chromatography (100% hexanes) gave the title compound as a clear oil (60%). (This procedure was adapted from Sasson, Y.; Webster, O. W. *J. Chem. Soc., Chem. Commun.* **1992**, 1200.)

b) 4-fluorophenylethynyltriphenylphosphonium chloride

To triphenylphosphine (1.7 g, 6.3 mmol) in ether (50 ml) was added 1-chloroethynyl-4-fluorobenzene (1.0 g, 6.3 mmol). After sitting for 10 days at RT, the white phosphonium salt was collected by filtration (18%). (This procedure was adapted from Tanaka, Y.; Miller, S. I. J. Org. Chem. 1973, 38, 2708.)

c) 4-(4-fluorophenyl)-1*H*-1,2,3-triazole

To a warm (60 °C) solution of sodium azide (74 mg, 1.1 mmol) in DMF (4 ml) was added 4-fluorophenylethynyltriphenylphosphonium chloride (476 mg, 1.1 mmol) in DMF (4 ml) dropwise. After the mixture was stirred for 3 h at 60 °C, the DMF was removed by evaporation. The residue was dissolved in chloroform, filtered, and the filtrate was evaporated to give a yellow solid. This solid was dissolved in ethanol (5.5 ml) and a sodium hydroxide solution (0.25 M, 11 ml) was added. After stirring and heating to 90 °C for 2 h, water (20 ml) was added and the aqueous layer was extracted with chloroform (10 ml X 2). (The organic layers were discarded.) The aqueous layer was neutralized with HCl (6 N) and again extracted with chloroform (10 ml X 3). The organic layers were combined, dried ($MgSO_4$) and evaporated. Purification by preparative HPLC to afforded the title compound as a yellow solid (20%). ^{1}H-NMR

(400MHz, CD_3OD): δ 8.13 (s, 1H), 7.84-7.88 (m, 2H), 7.16-7.21 (m, 2H). MS (ESI) 164.2 $(M+H)^+$. (This procedure was adapted from Tanaka, Y.; Miller, S. I. *J. Org. Chem.* **1973**, *38*, 2708.)

Example 48

Preparation of 2-bromo-5-(1*H*-1,2,3-triazol-4-yl)-phenol, 2,6-dibromo-5-(1*H*-1,2,3-triazol-4-yl)-phenol, and 2,4-dibromo-5-(*1H*-1,2,3-triazol-4-yl)-phenol

To 3-(1*H*-1,2,3-triazol-4-yl)-phenol (54 mg, 0.33 mmol, from Example 1) in acetic acid (1 ml) was added bromine (18 uL, 0.33 mmol). After 1 h of stirring at RT, water (10 ml) and ethyl acetate (10 ml) were added. The aqueous layer was neutralized with saturated $NaHCO_3$. The water layer was washed with ethyl acetate three times and the collected organic layers were dried, filtered, and evaporated. The resulting residue was purified by preparative HPLC to afford the three compounds, each as a white solid. 2-bromo-5-(1*H*-1,2,3-triazol-4-yl)-phenol (14 %): ^{1}H-NMR (400MHz, CD_3OD): δ 8.12 (s, 1H), 7.53 (d, J = 8.2 Hz, 1H), 7.40 (d, J = 2.0 Hz, 1H), 7.22 (dd, J = 8.2, 2.0 Hz, 1H). MS (ESI) 240.0 $(M+H)^+$. 2,6-dibromo-5-(1*H*-1,2,3-triazol-4-yl)-phenol (7 %): ^{1}H-NMR (400MHz, CD_3OD): δ 8.24 (s, 1H), 7.56 (d, J=8.3 Hz, 1H), 7.16 (d, J = 8.3 Hz, 1H). MS (ESI) 319.9 $(M+H)^+$. 2,4-dibromo-5-(1*H*-1,2,3-triazol-4-yl)-phenol (8 %): ^{1}H-NMR (400MHz, CD_3OD): δ 8.29 (s, 1H), 7.80 (s, 1H), 7.36 (s, 1H). MS (ESI) 319.9 $(M+H)^+$.

Example 49

Preparation of 2-(5-bromo-1H-1,2,3-triazol-4-yl)-4-methyl-pyridine

Following the procedure of Example 48, except substituting 2-(1H-1,2,3-triazol-4-yl)-4-methyl-pyridine (Example 21) for 3-(1*H*-1,2,3-triazol-4-yl)-phenol, the title compound was prepared as an orange solid (16 %). ^{1}H-NMR (400MHz, CD_3OD): δ 8.53 (d, J = 5.0 Hz, 1H), 7.92 (s, 1H), 7.32 (d, J = 5.0 Hz, 1H), 2.48 (s, 3H). MS (ESI) 239.0 $(M+H)^+$.

Example 50

Preparation of 1*H*-naptho[1,2-*d*]-1,2,3-triazole

Morgan, G.; *J. Chem. Soc.* **1910**, *97*, 1719. MS (ESI) 170.0 $(M+H)^+$.

Example 51

Preparation of 2,8-dihydro-indeno[1,2-*d*]-1,2,3-triazole

Rapoport, H.; Chen, H. H. *J. Org. Chem.* **1960**, *25*; 313. MS (ESI) 158.0 $(M+H)^+$.

Example 52

Preparation of 4-phenyl-1*H*-1,2,3-triazole

Tanaka, Y.; Velen, S. R.; Miller, S. I. *Tetrahedron*, **1973**, *29*, 3271. MS (ESI) 146.0 $(M+H)^+$.

Example 53

Preparation of 5,5a,6,8-tetrahydro-4*H*-acenaphtho[4,5-*d*]-1,2,3-triazole

Rapoport, H.; Nilsson, W. *J .Am. Chem. Soc.* **1961**; *83*, 4262. MS (ESI) 198.0 $(M+H)^+$.

Table I

Provides a three dimensional protein coordinate set of a *S. aureus* methionine aminopeptidase crystalline structure.

Residue	Atom	X	Y	Z	B
1	MET CB	6.43	53.27	9.67	15.13
1	MET CG	6.59	52.03	10.54	15.35
1	MET SD	5.17	51.70	11.63	15.46
1	MET CE	5.42	52.97	12.89	15.71
1	MET C	8.88	53.65	9.80	15.04
1	MET O	9.76	52.80	9.72	14.99
1	MET N	7.90	52.64	7.77	14.99
1	MET CA	7.68	53.63	8.86	15.06
2	ILE N	8.91	54.64	10.69	15.08
2	ILE CA	9.98	54.75	11.68	15.12
2	ILE CB	10.58	56.18	11.74	15.11
2	ILE CG2	11.69	56.23	12.77	15.13
2	ILE CG1	11.12	56.60	10.37	15.10
2	ILE CD1	12.16	55.66	9.81	15.02
2	ILE C	9.34	54.43	13.02	15.15
2	ILE O	8.43	55.14	13.47	15.15
3	VAL N	9.79	53.36	13.66	15.21
3	VAL CA	9.26	52.96	14.96	15.31
3	VAL CB	9.75	51.54	15.37	15.33
3	VAL CG1	9.22	51.17	16.74	15.35
3	VAL CG2	9.31	50.51	14.33	15.31

3 VAL C	9.71	53.94	16.03	15.41
3 VAL O	10.90	54.19	16.20	15.43
4 LYS N	8.74	54.51	16.75	15.50
4 LYS CA	9.06	55.47	17.81	15.61
4 LYS CB	8.48	56.85	17.47	15.77
4 LYS CG	9.22	57.62	16.36	16.09
4 LYS CD	10.62	58.06	16.79	16.35
4 LYS CE	11.71	57.16	16.20	16.55
4 LYS NZ	13.09	57.58	16.59	16.80
4 LYS C	8.55	55.04	19.18	15.58
4 LYS O	9.00	55.57	20.20	15.62
5 THR N	7.61	54.11	19.21	15.49
5 THR CA	7.06	53.66	20.49	15.51
5 THR CB	5.63	54.18	20.71	15.51
5 THR OG1	4.74	53.52	19.80	15.56
5 THR CG2	5.56	55.68	20.48	15.54
5 THR C	7.02	52.14	20.63	15.55
5 THR O	7.05	51.40	19.64	15.50
6 GLU N	6.92	51.69	21.87	15.55
6 GLU CA	6.86	50.27	22.20	15.56
6 GLU CB	6.88	50.10	23.72	15.81
6 GLU CG	6.98	48.66	24.23	16.26
6 GLU CD	8.35	48.06	24.03	16.49
6 GLU OE1	9.36	48.76	24.27	16.76
6 GLU OE2	8.43	46.87	23.65	16.71
6 GLU C	5.58	49.68	21.61	15.27
6 GLU O	5.54	48.53	21.17	15.37
7 GLU N	4.51	50.48	21.62	15.00
7 GLU CA	3.22	50.03	21.09	14.67
7 GLU CB	2.14	51.09	21.34	14.95
7 GLU CG	1.69	51.24	22.80	15.30
7 GLU CD	2.77	51.79	23.74	15.51
7 GLU OE1	3.57	52.66	23.31	15.59
7 GLU OE2	2.81	51.36	24.91	15.76
7 GLU C	3.30	49.72	19.59	14.29
7 GLU O	2.76	48.72	19.12	14.21
8 GLU N	3.99	50.58	18.84	13.86
8 GLU CA	4.12	50.37	17.40	13.29
8 GLU CB	4.80	51.58	16.75	13.39
8 GLU CG	4.06	52.88	16.97	13.55
8 GLU CD	4.73	54.08	16.32	13.59
8 GLU OE1	5.97	54.11	16.27	13.66
8 GLU OE2	4.01	54.99	15.86	13.76

8 GLU C	4.96	49.12	17.16	12.88
8 GLU O	4.65	48.31	16.29	12.87
9 LEU N	6.02	48.96	17.95	12.40
9 LEU CA	6.88	47.80	17.82	12.00
9 LEU CB	8.04	47.86	18.81	12.11
9 LEU CG	8.95	46.63	18.86	12.20
9 LEU CD1	9.63	46.43	17.52	12.27
9 LEU CD2	9.99	46.81	19.96	12.19
9 LEU C	6.06	46.52	18.04	11.68
9 LEU O	6.15	45.57	17.27	11.59
10 GLN N	5.27	46.51	19.10	11.43
10 GLN CA	4.45	45.33	19.40	11.04
10 GLN CB	3.73	45.52	20.74	11.15
10 GLN CG	4.68	45.90	21.87	11.40
10 GLN CD	3.96	46.15	23.18	11.56
10 GLN OE1	2.77	46.45	23.19	11.74
10 GLN NE2	4.70	46.06	24.28	11.68
10 GLN C	3.44	45.08	18.29	10.68
10 GLN O	3.20	43.93	17.92	10.61
11 ALA N	2.86	46.14	17.75	10.23
11 ALA CA	1.89	45.99	16.67	9.81
11 ALA CB	1.28	47.34	16.32	9.92
11 ALA C	2.54	45.38	15.44	9.56
11 ALA O	1.95	44.54	14.76	9.43
12 LEU N	3.78	45.78	15.16	9.18
12 LEU CA	4.50	45.26	14.01	8.86
12 LEU CB	5.76	46.10	13.75	8.81
12 LEU CG	5.45	47.50	13.19	8.76
12 LEU CD1	6.69	48.40	13.25	8.74
12 LEU CD2	4.98	47.35	11.75	8.67
12 LEU C	4.88	43.80	14.22	8.73
12 LEU O	4.74	42.97	13.32	8.65
13 LYS N	5.35	43.47	15.42	8.53
13 LYS CA	5.71	42.10	15.72	8.41
13 LYS CB	6.34	42.02	17.11	8.63
13 LYS CG	7.72	42.62	17.18	8.98
13 LYS CD	8.24	42.59	18.61	9.38
13 LYS CE	9.70	42.96	18.66	9.70
13 LYS NZ	10.17	42.99	20.08	10.07
13 LYS C	4.48	41.21	15.66	8.24
13 LYS O	4.56	40.05	15.23	8.19
14 GLU N	3.34	41.74	16.07	8.06
14 GLU CA	2.10	40.96	16.04	7.92

14 GLU CB	0.94	41.75	16.67	8.16
14 GLU CG	-0.45	41.11	16.50	8.49
14 GLU CD	-0.64	39.84	17.32	8.63
14 GLU OE1	0.26	39.45	18.09	8.80
14 GLU OE2	-1.72	39.23	17.21	8.81
14 GLU C	1.74	40.54	14.62	7.74
14 GLU O	1.61	39.35	14.33	7.61
15 ILE N	1.60	41.51	13.72	7.57
15 ILE CA	1.23	41.20	12.34	7.36
15 ILE CB	0.85	42.48	11.54	7.27
15 ILE CG2	2.04	43.45	11.48	7.26
15 ILE CG1	0.35	42.10	10.15	7.18
15 ILE CD1	-0.96	41.35	10.15	7.09
15 ILE C	2.34	40.42	11.62	7.32
15 ILE O	2.07	39.62	10.73	7.18
16 GLY N	3.58	40.65	12.04	7.28
16 GLY CA	4.70	39.94	11.45	7.07
16 GLY C	4.58	38.46	11.77	6.91
16 GLY O	4.76	37.61	10.89	7.16
17 TYR N	4.25	38.13	13.02	6.79
17 TYR CA	4.10	36.74	13.43	6.80
17 TYR CB	3.75	36.62	14.91	7.14
17 TYR CG	3.40	35.19	15.31	7.09
17 TYR CD1	4.39	34.22	15.47	7.20
17 TYR CE1	4.05	32.87	15.71	7.37
17 TYR CD2	2.06	34.78	15.41	7.25
17 TYR CE2	1.72	33.45	15.64	7.33
17 TYR CZ	2.71	32.51	15.79	7.40
17 TYR OH	2.38	31.19	16.01	7.56
17 TYR C	2.98	36.08	12.63	6.75
17 TYR O	3.12	34.95	12.16	6.70
18 ILE N	1.86	36.77	12.52	6.69
18 ILE CA	0.71	36.24	11.81	6.68
18 ILE CB	-0.45	37.25	11.81	6.72
18 ILE CG2	-1.61	36.74	10.94	6.69
18 ILE CG1	-0.95	37.44	13.25	6.80
18 ILE CD1	-2.00	38.55	13.40	6.98
18 ILE C	1.05	35.88	10.37	6.67
18 ILE O	0.75	34.76	9.92	6.57
19 CYS N	1.70	36.79	9.66	6.72
19 CYS CA	2.06	36.50	8.27	6.84
19 CYS CB	2.62	37.75	7.58	7.20
19 CYS SG	1.39	39.09	7.40	7.57

19 CYS C	3.06	35.34	8.16	6.71
19 CYS O	2.97	34.52	7.25	6.49
20 ALA N	4.00	35.28	9.10	6.63
20 ALA CA	4.98	34.21	9.10	6.57
20 ALA CB	6.04	34.45	10.19	6.67
20 ALA C	4.28	32.87	9.35	6.54
20 ALA O	4.58	31.86	8.70	6.52
21 LYS N	3.34	32.88	10.28	6.45
21 LYS CA	2.58	31.67	10.61	6.56
21 LYS CB	1.61	31.94	11.76	6.69
21 LYS CG	0.93	30.69	12.33	7.10
21 LYS CD	1.97	29.70	12.86	7.42
21 LYS CE	1.34	28.55	13.62	7.70
21 LYS NZ	2.39	27.66	14.18	7.91
21 LYS C	1.81	31.19	9.39	6.45
21 LYS O	1.78	30.00	9.08	6.36
22 VAL N	1.17	32.13	8.71	6.45
22 VAL CA	0.39	31.80	7.52	6.41
22 VAL CB	-0.35	33.04	7.00	6.34
22 VAL CG1	-0.99	32.75	5.64	6.41
22 VAL CG2	-1.41	33.44	8.01	6.53
22 VAL C	1.31	31.23	6.44	6.40
22 VAL O	1.03	30.19	5.83	6.33
23 ARG N	2.41	31.94	6.20	6.40
23 ARG CA	3.40	31.53	5.21	6.30
23 ARG CB	4.58	32.51	5.24	6.19
23 ARG CG	5.63	32.31	4.16	6.30
23 ARG CD	6.93	32.94	4.62	6.30
23 ARG NE	7.45	32.23	5.79	6.30
23 ARG CZ	8.05	32.81	6.83	6.36
23 ARG NH1	8.21	34.12	6.86	6.29
23 ARG NH2	8.46	32.07	7.85	6.22
23 ARG C	3.89	30.10	5.49	6.27
23 ARG O	3.95	29.26	4.58	6.26
24 ASN N	4.24	29.81	6.75	6.41
24 ASN CA	4.70	28.46	7.09	6.60
24 ASN CB	5.18	28.39	8.54	6.95
24 ASN CG	6.48	29.13	8.77	7.09
24 ASN OD1	7.25	29.36	7.84	7.26
24 ASN ND2	6.74	29.50	10.02	7.37
24 ASN C	3.62	27.40	6.89	6.59
24 ASN O	3.90	26.32	6.36	6.64
25 THR N	2.39	27.71	7.31	6.71

25 THR CA	1.30	26.76	7.18	6.79
25 THR CB	0.03	27.28	7.91	6.77
25 THR OG1	0.36	27.63	9.26	6.87
25 THR CG2	-1.05	26.20	7.95	6.91
25 THR C	1.00	26.46	5.70	6.87
25 THR O	0.82	25.30	5.32	6.68
26 MET N	0.97	27.50	4.87	7.05
26 MET CA	0.73	27.32	3.44	7.14
26 MET CB	0.60	28.67	2.73	7.12
26 MET CG	-0.64	29.44	3.15	7.34
26 MET SD	-0.79	31.09	2.43	7.05
26 MET CE	-1.04	30.70	0.73	7.35
26 MET C	1.84	26.50	2.78	7.12
26 MET O	1.57	25.60	1.98	7.04
27 GLN N	3.08	26.81	3.12	7.19
27 GLN CA	4.20	26.09	2.54	7.31
27 GLN CB	5.54	26.65	3.04	7.31
27 GLN CG	6.75	25.87	2.52	7.37
27 GLN CD	8.06	26.55	2.83	7.41
27 GLN OE1	8.10	27.51	3.58	7.44
27 GLN NE2	9.15	26.04	2.26	7.41
27 GLN C	4.14	24.59	2.85	7.46
27 GLN O	4.31	23.75	1.95	7.45
28 ALA N	3.90	24.26	4.12	7.61
28 ALA CA	3.83	22.88	4.56	7.74
28 ALA CB	3.62	22.83	6.07	7.64
28 ALA C	2.71	22.12	3.87	7.82
28 ALA O	2.79	20.91	3.67	7.93
29 ALA N	1.66	22.84	3.49	8.04
29 ALA CA	0.52	22.25	2.82	8.20
29 ALA CB	-0.76	23.01	3.20	8.31
29 ALA C	0.65	22.18	1.30	8.39
29 ALA O	-0.20	21.59	0.62	8.33
30 THR N	1.71	22.79	0.76	8.61
30 THR CA	1.92	22.79	-0.68	8.69
30 THR CB	2.86	23.95	-1.13	8.69
30 THR OG1	2.30	25.20	-0.70	8.77
30 THR CG2	2.98	23.99	-2.66	8.72
30 THR C	2.50	21.45	-1.15	8.82
30 THR O	3.71	21.21	-1.05	8.85
31 LYS N	1.63	20.59	-1.65	8.92
31 LYS CA	2.02	19.28	-2.16	8.94
31 LYS CB	1.62	18.18	-1.16	9.33

31 LYS CG	0.13	18.13	-0.84	9.68
31 LYS CD	-0.21	16.89	-0.01	10.00
31 LYS CE	0.05	15.61	-0.82	10.30
31 LYS NZ	0.14	14.40	0.02	10.46
31 LYS C	1.31	19.02	-3.48	9.07
31 LYS O	0.33	19.70	-3.82	9.07
32 PRO N	1.79	18.05	-4.27	9.23
32 PRO CD	3.05	17.29	-4.12	9.24
32 PRO CA	1.14	17.75	-5.55	9.25
32 PRO CB	1.94	16.56	-6.07	9.39
32 PRO CG	3.32	16.83	-5.53	9.26
32 PRO C	-0.34	17.41	-5.32	9.45
32 PRO O	-0.68	16.70	-4.38	9.64
33 GLY N	-1.21	17.93	-6.17	9.66
33 GLY CA	-2.62	17.63	-6.03	9.78
33 GLY C	-3.44	18.72	-5.38	9.77
33 GLY O	-4.67	18.73	-5.49	9.99
34 ILE N	-2.80	19.65	-4.68	9.59
34 ILE CA	-3.55	20.73	-4.06	9.39
34 ILE CB	-2.89	21.19	-2.73	9.22
34 ILE CG2	-1.56	21.86	-3.00	9.10
34 ILE CG1	-3.83	22.14	-1.99	9.11
34 ILE CD1	-3.39	22.44	-0.59	9.02
34 ILE C	-3.62	21.89	-5.05	9.25
34 ILE O	-2.71	22.05	-5.87	9.40
35 THR N	-4.69	22.67	-5.03	9.25
35 THR CA	-4.78	23.80	-5.95	9.22
35 THR CB	-6.21	24.06	-6.46	9.19
35 THR OG1	-7.03	24.54	-5.38	9.18
35 THR CG2	-6.82	22.79	-7.05	9.18
35 THR C	-4.29	25.05	-5.23	9.07
35 THR O	-4.30	25.09	-4.00	9.07
36 THR N	-3.89	26.06	-5.98	9.13
36 THR CA	-3.42	27.27	-5.34	9.25
36 THR CB	-2.79	28.26	-6.36	9.29
36 THR OG1	-3.74	28.59	-7.38	9.20
36 THR CG2	-1.55	27.64	-7.00	9.23
36 THR C	-4.55	27.95	-4.59	9.23
36 THR O	-4.31	28.60	-3.58	9.32
37 LYS N	-5.79	27.78	-5.05	9.33
37 LYS CA	-6.91	28.40	-4.35	9.43
37 LYS CB	-8.20	28.30	-5.18	9.55
37 LYS CG	-9.33	29.19	-4.64	9.66

37 LYS CD	-8.88	30.64	-4.56	9.79
37 LYS CE	-9.81	31.50	-3.72	9.85
37 LYS NZ	-9.20	32.86	-3.54	9.91
37 LYS C	-7.10	27.72	-2.99	9.46
37 LYS O	-7.44	28.38	-2.01	9.43
38 GLU N	-6.88	26.41	-2.92	9.48
38 GLU CA	-7.01	25.70	-1.66	9.49
38 GLU CB	-6.88	24.19	-1.86	9.76
38 GLU CG	-8.02	23.62	-2.69	10.29
38 GLU CD	-7.93	22.11	-2.84	10.65
38 GLU OE1	-6.95	21.62	-3.43	10.83
38 GLU OE2	-8.86	21.43	-2.37	11.08
38 GLU C	-5.96	26.20	-0.67	9.31
38 GLU O	-6.22	26.27	0.54	9.17
39 LEU N	-4.78	26.52	-1.18	9.18
39 LEU CA	-3.71	27.04	-0.33	9.06
39 LEU CB	-2.39	27.15	-1.11	9.16
39 LEU CG	-1.68	25.85	-1.47	9.23
39 LEU CD1	-0.46	26.16	-2.33	9.29
39 LEU CD2	-1.25	25.12	-0.19	9.25
39 LEU C	-4.10	28.43	0.17	8.98
39 LEU O	-3.87	28.77	1.32	8.92
40 ASP N	-4.71	29.21	-0.71	8.97
40 ASP CA	-5.14	30.56	-0.36	8.93
40 ASP CB	-5.69	31.27	-1.61	8.89
40 ASP CG	-5.87	32.75	-1.40	8.96
40 ASP OD1	-4.86	33.45	-1.16	8.83
40 ASP OD2	-7.02	33.23	-1.46	9.04
40 ASP C	-6.21	30.49	0.72	8.94
40 ASP O	-6.27	31.36	1.59	8.90
41 ASN N	-7.04	29.45	0.69	9.03
41 ASN CA	-8.10	29.29	1.68	9.17
41 ASN CB	-9.00	28.12	1.31	9.22
41 ASN CG	-9.87	28.42	0.11	9.40
41 ASN OD1	-10.04	29.59	-0.25	9.51
41 ASN ND2	-10.42	27.38	-0.51	9.36
41 ASN C	-7.56	29.11	3.09	9.23
41 ASN O	-8.23	29.43	4.07	9.17
42 ILE N	-6.35	28.57	3.18	9.33
42 ILE CA	-5.71	28.38	4.46	9.41
42 ILE CB	-4.37	27.62	4.31	9.26
42 ILE CG2	-3.66	27.53	5.66	9.31
42 ILE CG1	-4.64	26.23	3.75	9.29

42 ILE CD1	-3.38	25.43	3.45	9.19
42 ILE C	-5.44	29.77	5.04	9.55
42 ILE O	-5.73	30.02	6.21	9.59
43 ALA N	-4.91	30.67	4.22	9.69
43 ALA CA	-4.63	32.03	4.68	9.85
43 ALA CB	-3.96	32.84	3.57	9.88
43 ALA C	-5.92	32.70	5.12	9.99
43 ALA O	-5.96	33.39	6.14	9.97
44 LYS N	-6.99	32.51	4.34	10.19
44 LYS CA	-8.28	33.11	4.69	10.53
44 LYS CB	-9.35	32.66	3.69	10.58
44 LYS CG	-10.77	33.15	4.01	10.83
44 LYS CD	-11.79	32.53	3.06	11.07
44 LYS CE	-13.20	33.03	3.33	11.32
44 LYS NZ	-13.30	34.51	3.20	11.65
44 LYS C	-8.70	32.73	6.12	10.64
44 LYS O	-9.05	33.59	6.92	10.64
45 GLU N	-8.64	31.44	6.44	10.98
45 GLU CA	-9.04	30.98	7.78	11.30
45 GLU CB	-9.12	29.45	7.83	11.78
45 GLU CG	-10.14	28.84	6.88	12.72
45 GLU CD	-11.54	29.44	7.04	13.19
45 GLU OE1	-12.03	29.55	8.18	13.63
45 GLU OE2	-12.15	29.79	6.00	13.66
45 GLU C	-8.11	31.46	8.89	11.24
45 GLU O	-8.58	31.79	9.99	11.18
46 LEU N	-6.81	31.49	8.63	11.18
46 LEU CA	-5.87	31.94	9.65	11.19
46 LEU CB	-4.43	31.57	9.26	11.17
46 LEU CG	-4.09	30.07	9.34	11.24
46 LEU CD1	-2.63	29.86	8.93	11.21
46 LEU CD2	-4.32	29.56	10.75	11.23
46 LEU C	-5.99	33.44	9.87	11.23
46 LEU O	-5.95	33.91	11.02	11.22
47 PHE N	-6.14	34.21	8.80	11.24
47 PHE CA	-6.28	35.66	8.97	11.27
47 PHE CB	-6.46	36.38	7.63	10.95
47 PHE CG	-5.20	36.51	6.81	10.75
47 PHE CD1	-3.95	36.55	7.42	10.60
47 PHE CD2	-5.28	36.62	5.43	10.58
47 PHE CE1	-2.78	36.71	6.64	10.51
47 PHE CE2	-4.13	36.77	4.65	10.51
47 PHE CZ	-2.88	36.82	5.25	10.46

47 PHE C	-7.48	35.94	9.87	11.40
47 PHE O	-7.41	36.79	10.76	11.37
48 GLU N	-8.57	35.22	9.65	11.75
48 GLU CA	-9.77	35.40	10.46	12.12
48 GLU CB	-10.91	34.56	9.89	12.54
48 GLU CG	-12.21	34.62	10.68	13.33
48 GLU CD	-12.76	36.03	10.79	13.70
48 GLU OE1	-12.83	36.73	9.75	14.19
48 GLU OE2	-13.15	36.43	11.91	14.10
48 GLU C	-9.52	35.02	11.92	12.12
48 GLU O	-9.94	35.72	12.84	12.16
49 GLU N	-8.81	33.91	12.11	12.32
49 GLU CA	-8.48	33.41	13.45	12.49
49 GLU CB	-7.77	32.06	13.32	12.89
49 GLU CG	-7.43	31.38	14.65	13.71
49 GLU CD	-6.86	29.98	14.46	14.11
49 GLU OE1	-7.56	29.12	13.88	14.52
49 GLU OE2	-5.71	29.74	14.88	14.52
49 GLU C	-7.61	34.38	14.25	12.42
49 GLU O	-7.82	34.57	15.45	12.25
50 TYR N	-6.62	34.99	13.59	12.35
50 TYR CA	-5.71	35.93	14.24	12.25
50 TYR CB	-4.32	35.83	13.62	12.28
50 TYR CG	-3.61	34.53	13.91	12.54
50 TYR CD1	-3.05	34.28	15.16	12.57
50 TYR CE1	-2.40	33.08	15.44	12.69
50 TYR CD2	-3.52	33.53	12.94	12.58
50 TYR CE2	-2.87	32.33	13.21	12.66
50 TYR CZ	-2.32	32.11	14.45	12.71
50 TYR OH	-1.68	30.92	14.70	12.87
50 TYR C	-6.17	37.39	14.20	12.14
50 TYR O	-5.47	38.27	14.70	12.18
51 GLY N	-7.32	37.64	13.59	11.95
51 GLY CA	-7.83	38.99	13.52	11.69
51 GLY C	-7.09	39.92	12.58	11.51
51 GLY O	-7.02	41.13	12.83	11.49
52 ALA N	-6.54	39.37	11.51	11.26
52 ALA CA	-5.82	40.16	10.52	10.96
52 ALA CB	-4.43	39.57	10.29	10.92
52 ALA C	-6.59	40.18	9.21	10.80
52 ALA O	-7.52	39.40	9.00	10.69
53 ILE N	-6.19	41.08	8.32	10.74
53 ILE CA	-6.83	41.22	7.03	10.76

53 ILE CB	-7.59	42.55	6.93	11.09
53 ILE CG2	-8.12	42.75	5.54	11.08
53 ILE CG1	-8.74	42.55	7.94	11.34
53 ILE CD1	-9.71	41.43	7.75	11.84
53 ILE C	-5.82	41.18	5.90	10.65
53 ILE O	-4.71	41.70	6.02	10.56
54 SER N	-6.21	40.55	4.80	10.57
54 SER CA	-5.36	40.43	3.61	10.72
54 SER CB	-6.10	39.63	2.54	10.72
54 SER OG	-5.47	39.78	1.27	10.63
54 SER C	-4.99	41.80	3.04	10.77
54 SER O	-5.88	42.60	2.74	10.76
55 ALA N	-3.70	42.08	2.87	10.90
55 ALA CA	-3.29	43.36	2.31	11.05
55 ALA CB	-1.80	43.61	2.54	10.96
55 ALA C	-3.61	43.45	0.81	11.16
55 ALA O	-4.05	44.48	0.34	11.10
56 PRO N	-3.39	42.36	0.05	11.37
56 PRO CD	-2.66	41.12	0.38	11.33
56 PRO CA	-3.69	42.41	-1.38	11.44
56 PRO CB	-3.42	40.98	-1.85	11.44
56 PRO CG	-2.25	40.60	-1.01	11.38
56 PRO C	-5.14	42.82	-1.62	11.71
56 PRO O	-5.44	43.65	-2.48	11.70
57 ILE N	-6.04	42.23	-0.84	11.87
57 ILE CA	-7.46	42.53	-0.97	12.01
57 ILE CB	-8.32	41.55	-0.16	12.02
57 ILE CG2	-9.77	42.06	-0.11	12.05
57 ILE CG1	-8.23	40.16	-0.79	11.93
57 ILE CD1	-8.96	39.08	0.01	11.78
57 ILE C	-7.82	43.94	-0.49	12.22
57 ILE O	-8.53	44.67	-1.17	12.22
58 HIS N	-7.32	44.30	0.69	12.37
58 HIS CA	-7.60	45.60	1.28	12.63
58 HIS CB	-7.13	45.60	2.74	12.73
58 HIS CG	-7.25	46.94	3.42	12.73
58 HIS CD2	-8.22	47.44	4.22	12.78
58 HIS ND1	-6.29	47.92	3.31	12.80
58 HIS CE1	-6.66	48.97	4.02	12.82
58 HIS NE2	-7.82	48.71	4.58	12.84
58 HIS C	-6.97	46.77	0.53	12.81
58 HIS O	-7.62	47.79	0.32	12.82
59 ASP N	-5.71	46.60	0.12	12.96

59 ASP CA	-4.94	47.63	-0.58	13.19
59 ASP CB	-3.44	47.41	-0.39	13.25
59 ASP CG	-2.98	47.57	1.05	13.42
59 ASP OD1	-3.78	47.95	1.92	13.43
59 ASP OD2	-1.77	47.33	1.29	13.51
59 ASP C	-5.16	47.77	-2.08	13.27
59 ASP O	-5.28	48.89	-2.59	13.39
60 GLU N	-5.16	46.65	-2.80	13.34
60 GLU CA	-5.29	46.67	-4.26	13.30
60 GLU CB	-4.10	45.94	-4.91	13.77
60 GLU CG	-2.73	46.19	-4.30	14.47
60 GLU CD	-2.37	47.65	-4.23	14.81
60 GLU OE1	-2.75	48.41	-5.16	15.14
60 GLU OE2	-1.69	48.04	-3.25	15.19
60 GLU C	-6.54	46.02	-4.82	13.01
60 GLU O	-6.73	45.99	-6.04	12.97
61 ASN N	-7.39	45.50	-3.95	12.60
61 ASN CA	-8.59	44.80	-4.39	12.28
61 ASN CB	-9.54	45.71	-5.17	12.26
61 ASN CG	-10.89	45.06	-5.43	12.34
61 ASN OD1	-11.35	44.22	-4.65	12.33
61 ASN ND2	-11.54	45.46	-6.53	12.36
61 ASN C	-8.14	43.64	-5.27	12.04
61 ASN O	-8.72	43.37	-6.32	11.90
62 PHE N	-7.08	42.97	-4.82	11.76
62 PHE CA	-6.51	41.81	-5.50	11.47
62 PHE CB	-5.15	41.46	-4.89	11.52
62 PHE CG	-4.47	40.29	-5.53	11.77
62 PHE CD1	-3.81	40.43	-6.75	11.88
62 PHE CD2	-4.47	39.04	-4.91	11.85
62 PHE CE1	-3.15	39.35	-7.33	11.91
62 PHE CE2	-3.82	37.95	-5.50	11.88
62 PHE CZ	-3.16	38.10	-6.71	11.91
62 PHE C	-7.48	40.66	-5.26	11.24
62 PHE O	-7.98	40.50	-4.14	11.11
63 PRO N	-7.76	39.86	-6.29	11.08
63 PRO CD	-7.35	40.06	-7.70	10.99
63 PRO CA	-8.68	38.72	-6.18	10.84
63 PRO CB	-9.06	38.46	-7.64	10.94
63 PRO CG	-7.77	38.76	-8.35	11.00
63 PRO C	-8.03	37.50	-5.53	10.71
63 PRO O	-7.88	36.45	-6.15	10.70
64 GLY N	-7.65	37.65	-4.26	10.53

64 GLY CA	-7.01	36.56	-3.55	10.28
64 GLY C	-6.47	37.03	-2.22	10.11
64 GLY O	-6.09	38.19	-2.08	10.11
65 GLN N	-6.43	36.14	-1.23	9.93
65 GLN CA	-5.92	36.49	0.09	9.84
65 GLN CB	-6.17	35.34	1.07	9.86
65 GLN CG	-7.64	35.04	1.34	10.07
65 GLN CD	-8.30	36.09	2.21	10.18
65 GLN OE1	-7.66	36.67	3.10	10.15
65 GLN NE2	-9.59	36.34	1.96	10.31
65 GLN C	-4.42	36.78	0.04	9.68
65 GLN O	-3.94	37.73	0.67	9.61
66 THR N	-3.71	35.94	-0.70	9.64
66 THR CA	-2.26	36.02	-0.86	9.57
66 THR CB	-1.57	34.85	-0.14	9.54
66 THR OG1	-1.96	33.61	-0.76	9.57
66 THR CG2	-1.97	34.80	1.33	9.59
66 THR C	-1.88	35.90	-2.33	9.54
66 THR O	-2.74	35.66	-3.18	9.47
67 CYS N	-0.59	36.06	-2.62	9.58
67 CYS CA	-0.09	35.93	-3.98	9.69
67 CYS CB	0.86	37.07	-4.33	10.27
67 CYS SG	0.04	38.68	-4.41	10.95
67 CYS C	0.66	34.60	-4.01	9.38
67 CYS O	1.51	34.34	-3.17	9.38
68 ILE N	0.31	33.76	-4.98	9.24
68 ILE CA	0.94	32.45	-5.12	9.20
68 ILE CB	-0.05	31.33	-4.78	9.22
68 ILE CG2	0.65	29.97	-4.90	9.09
68 ILE CG1	-0.59	31.54	-3.36	9.16
68 ILE CD1	-1.65	30.53	-2.94	9.32
68 ILE C	1.34	32.34	-6.58	9.23
68 ILE O	0.48	32.24	-7.46	9.15
69 SER N	2.64	32.35	-6.83	9.40
69 SER CA	3.17	32.30	-8.18	9.44
69 SER CB	4.12	33.48	-8.38	9.50
69 SER OG	3.54	34.67	-7.84	9.31
69 SER C	3.87	30.98	-8.47	9.48
69 SER O	4.70	30.54	-7.67	9.68
70 VAL N	3.54	30.35	-9.59	9.51
70 VAL CA	4.16	29.06	-9.90	9.65
70 VAL CB	3.10	27.93	-9.93	9.70
70 VAL CG1	3.79	26.59	-10.19	9.57

70 VAL CG2	2.35	27.89	-8.61	9.59
70 VAL C	4.93	29.04	-11.22	9.79
70 VAL O	4.47	29.56	-12.23	9.89
71 ASN N	6.12	28.45	-11.18	10.00
71 ASN CA	7.00	28.30	-12.35	10.15
71 ASN CB	6.50	27.14	-13.21	10.16
71 ASN CG	6.49	25.83	-12.46	10.32
71 ASN OD1	7.40	25.55	-11.67	10.33
71 ASN ND2	5.48	25.00	-12.71	10.38
71 ASN C	7.25	29.54	-13.21	10.18
71 ASN O	8.11	30.35	-12.89	10.13
72 GLU N	6.50	29.68	-14.31	10.29
72 GLU CA	6.70	30.83	-15.18	10.24
72 GLU CB	5.90	30.66	-16.49	10.29
72 GLU CG	4.40	30.90	-16.41	10.47
72 GLU CD	3.63	29.76	-15.78	10.52
72 GLU OE1	4.22	28.69	-15.52	10.61
72 GLU OE2	2.41	29.92	-15.55	10.59
72 GLU C	6.33	32.14	-14.48	10.16
72 GLU O	6.86	33.19	-14.83	10.23
73 GLU N	5.45	32.07	-13.48	10.17
73 GLU CA	5.07	33.27	-12.74	10.16
73 GLU CB	3.70	33.09	-12.10	10.39
73 GLU CG	2.64	32.63	-13.07	10.62
73 GLU CD	1.36	32.28	-12.37	10.77
73 GLU OE1	1.43	31.66	-11.28	10.88
73 GLU OE2	0.28	32.62	-12.91	10.93
73 GLU C	6.08	33.52	-11.63	10.13
73 GLU O	6.46	32.61	-10.90	10.04
74 VAL N	6.52	34.77	-11.52	10.35
74 VAL CA	7.50	35.19	-10.53	10.46
74 VAL CB	8.49	36.20	-11.14	10.53
74 VAL CG1	9.49	36.69	-10.08	10.53
74 VAL CG2	9.23	35.56	-12.31	10.54
74 VAL C	6.86	35.85	-9.31	10.56
74 VAL O	7.29	35.66	-8.17	10.57
75 ALA N	5.83	36.64	-9.57	10.70
75 ALA CA	5.14	37.34	-8.49	10.79
75 ALA CB	5.96	38.56	-8.08	10.84
75 ALA C	3.74	37.77	-8.90	10.84
75 ALA O	3.43	37.83	-10.08	10.81
76 HIS N	2.92	38.05	-7.90	10.94
76 HIS CA	1.54	38.48	-8.11	11.16

76 HIS CB	1.53	39.77	-8.95	11.62
76 HIS CG	2.11	40.97	-8.26	12.06
76 HIS CD2	1.62	42.22	-8.06	12.29
76 HIS ND1	3.36	40.96	-7.66	12.32
76 HIS CE1	3.60	42.14	-7.13	12.37
76 HIS NE2	2.57	42.93	-7.36	12.45
76 HIS C	0.64	37.42	-8.74	11.03
76 HIS O	-0.40	37.75	-9.33	11.11
77 GLY N	1.00	36.15	-8.62	10.90
77 GLY CA	0.16	35.09	-9.18	10.76
77 GLY C	-1.19	35.06	-8.46	10.74
77 GLY O	-1.25	35.25	-7.24	10.61
78 ILE N	-2.27	34.83	-9.21	10.69
78 ILE CA	-3.62	34.79	-8.63	10.77
78 ILE CB	-4.67	35.36	-9.63	10.80
78 ILE CG2	-6.06	35.29	-9.01	10.82
78 ILE CG1	-4.33	36.81	-10.00	10.90
78 ILE CD1	-5.20	37.39	-11.13	11.05
78 ILE C	-4.03	33.36	-8.26	10.69
78 ILE O	-4.05	32.49	-9.12	10.75
79 PRO N	-4.34	33.10	-6.97	10.64
79 PRO CD	-4.24	34.00	-5.81	10.79
79 PRO CA	-4.75	31.76	-6.55	10.78
79 PRO CB	-5.12	31.95	-5.08	10.74
79 PRO CG	-4.16	33.03	-4.65	10.72
79 PRO C	-5.94	31.32	-7.40	10.74
79 PRO O	-6.85	32.12	-7.66	10.77
80 SER N	-5.94	30.07	-7.82	10.76
80 SER CA	-6.99	29.57	-8.70	10.89
80 SER CB	-6.71	30.02	-10.12	10.91
80 SER OG	-5.49	29.44	-10.57	10.83
80 SER C	-7.09	28.05	-8.68	10.97
80 SER O	-6.63	27.39	-7.75	10.96
81 LYS N	-7.68	27.50	-9.74	11.05
81 LYS CA	-7.85	26.06	-9.87	11.11
81 LYS CB	-8.93	25.77	-10.91	11.30
81 LYS CG	-10.29	26.34	-10.54	11.69
81 LYS CD	-11.26	26.34	-11.71	12.04
81 LYS CE	-12.62	26.91	-11.30	12.20
81 LYS NZ	-13.55	27.00	-12.46	12.37
81 LYS C	-6.54	25.38	-10.26	10.98
81 LYS O	-6.47	24.15	-10.31	10.91
82 ARG N	-5.51	26.18	-10.55	10.88

82 ARG CA	-4.21	25.63	-10.93	10.79
82 ARG CB	-3.16	26.74	-11.07	10.81
82 ARG CG	-1.79	26.21	-11.43	10.88
82 ARG CD	-0.82	27.33	-11.77	11.00
82 ARG NE	0.41	26.79	-12.36	11.17
82 ARG CZ	1.25	27.50	-13.11	11.12
82 ARG NH1	1.00	28.77	-13.37	11.26
82 ARG NH2	2.35	26.93	-13.61	11.15
82 ARG C	-3.74	24.62	-9.89	10.73
82 ARG O	-3.60	24.94	-8.72	10.61
83 VAL N	-3.48	23.39	-10.34	10.71
83 VAL CA	-3.03	22.35	-9.43	10.66
83 VAL CB	-3.58	20.97	-9.86	10.88
83 VAL CG1	-3.00	20.58	-11.20	11.18
83 VAL CG2	-3.24	19.93	-8.81	11.07
83 VAL C	-1.50	22.28	-9.33	10.53
83 VAL O	-0.80	22.34	-10.34	10.33
84 ILE N	-1.01	22.16	-8.10	10.44
84 ILE CA	0.43	22.05	-7.86	10.41
84 ILE CB	0.78	22.17	-6.36	10.49
84 ILE CG2	2.24	21.79	-6.14	10.39
84 ILE CG1	0.48	23.59	-5.87	10.59
84 ILE CD1	1.13	24.69	-6.68	10.80
84 ILE C	0.89	20.67	-8.32	10.41
84 ILE O	0.20	19.68	-8.10	10.33
85 ARG N	2.05	20.62	-8.96	10.45
85 ARG CA	2.62	19.37	-9.46	10.65
85 ARG CB	2.66	19.39	-10.99	11.00
85 ARG CG	1.30	19.54	-11.64	11.42
85 ARG CD	0.48	18.29	-11.41	11.83
85 ARG NE	1.04	17.16	-12.15	12.31
85 ARG CZ	0.60	16.75	-13.34	12.40
85 ARG NH1	-0.43	17.36	-13.91	12.49
85 ARG NH2	1.19	15.73	-13.95	12.62
85 ARG C	4.03	19.16	-8.93	10.67
85 ARG O	4.71	20.11	-8.54	10.63
86 GLU N	4.46	17.91	-8.90	10.68
86 GLU CA	5.80	17.55	-8.43	10.76
86 GLU CB	5.99	16.03	-8.60	11.03
86 GLU CG	7.34	15.46	-8.16	11.44
86 GLU CD	7.51	15.40	-6.67	11.57
86 GLU OE1	6.50	15.46	-5.93	11.74
86 GLU OE2	8.68	15.28	-6.21	11.75

86	GLU	C	6.84	18.32	-9.25	10.57
86	GLU	O	6.76	18.36	-10.48	10.62
87	GLY	N	7.81	18.93	-8.57	10.32
87	GLY	CA	8.84	19.67	-9.27	9.84
87	GLY	C	8.54	21.15	-9.50	9.48
87	GLY	O	9.38	21.88	-10.04	9.46
88	ASP	N	7.35	21.59	-9.11	9.17
88	ASP	CA	6.97	23.00	-9.29	8.91
88	ASP	CB	5.49	23.23	-8.93	9.17
88	ASP	CG	4.53	22.89	-10.06	9.36
88	ASP	OD1	4.97	22.61	-11.19	9.56
88	ASP	OD2	3.30	22.92	-9.80	9.35
88	ASP	C	7.80	23.92	-8.39	8.57
88	ASP	O	8.13	23.57	-7.26	8.51
89	LEU	N	8.13	25.10	-8.91	8.39
89	LEU	CA	8.86	26.11	-8.14	8.03
89	LEU	CB	9.90	26.82	-9.02	8.06
89	LEU	CG	10.69	27.97	-8.37	8.15
89	LEU	CD1	11.29	27.55	-7.04	8.16
89	LEU	CD2	11.80	28.41	-9.34	8.15
89	LEU	C	7.75	27.08	-7.74	7.81
89	LEU	O	7.15	27.75	-8.58	7.78
90	VAL	N	7.48	27.14	-6.44	7.61
90	VAL	CA	6.40	27.97	-5.94	7.45
90	VAL	CB	5.36	27.10	-5.19	7.48
90	VAL	CG1	4.15	27.93	-4.80	7.64
90	VAL	CG2	4.95	25.92	-6.06	7.67
90	VAL	C	6.80	29.10	-5.00	7.23
90	VAL	O	7.65	28.93	-4.13	7.21
91	ASN	N	6.21	30.27	-5.22	7.18
91	ASN	CA	6.44	31.40	-4.33	7.02
91	ASN	CB	6.99	32.63	-5.05	7.35
91	ASN	CG	7.15	33.81	-4.10	7.73
91	ASN	OD1	6.29	34.70	-4.03	8.01
91	ASN	ND2	8.24	33.82	-3.34	7.95
91	ASN	C	5.12	31.77	-3.69	6.84
91	ASN	O	4.09	31.94	-4.36	6.56
92	ILE	N	5.16	31.88	-2.38	6.72
92	ILE	CA	3.99	32.26	-1.62	6.72
92	ILE	CB	3.65	31.19	-0.56	6.92
92	ILE	CG2	2.50	31.67	0.32	7.04
92	ILE	CG1	3.30	29.87	-1.26	7.31
92	ILE	CD1	3.10	28.69	-0.33	7.69

92	ILE	C	4.39	33.56	-0.95	6.57
92	ILE	O	5.38	33.61	-0.22	6.50
93	ASP	N	3.64	34.62	-1.23	6.66
93	ASP	CA	3.93	35.92	-0.67	6.75
93	ASP	CB	4.21	36.93	-1.78	7.16
93	ASP	CG	4.79	38.23	-1.25	7.51
93	ASP	OD1	4.32	38.70	-0.21	7.76
93	ASP	OD2	5.71	38.78	-1.89	7.87
93	ASP	C	2.72	36.35	0.15	6.68
93	ASP	O	1.63	36.56	-0.38	6.56
94	VAL	N	2.94	36.46	1.46	6.81
94	VAL	CA	1.89	36.81	2.40	6.91
94	VAL	CB	1.88	35.78	3.55	6.97
94	VAL	CG1	0.77	36.10	4.54	7.20
94	VAL	CG2	1.70	34.37	2.98	7.24
94	VAL	C	2.06	38.21	2.98	6.83
94	VAL	O	3.11	38.52	3.55	6.83
95	SER	N	1.04	39.05	2.81	6.97
95	SER	CA	1.05	40.41	3.34	7.04
95	SER	CB	1.39	41.44	2.26	7.24
95	SER	OG	0.46	41.42	1.20	7.21
95	SER	C	-0.32	40.67	3.94	7.05
95	SER	O	-1.35	40.29	3.38	7.08
96	ALA	N	-0.33	41.31	5.11	7.08
96	ALA	CA	-1.56	41.60	5.82	7.05
96	ALA	CB	-2.02	40.35	6.57	7.10
96	ALA	C	-1.37	42.75	6.80	7.11
96	ALA	O	-0.24	43.20	7.04	6.96
97	LEU	N	-2.47	43.19	7.38	7.18
97	LEU	CA	-2.46	44.27	8.36	7.37
97	LEU	CB	-2.91	45.59	7.71	7.46
97	LEU	CG	-4.33	45.69	7.14	7.59
97	LEU	CD1	-4.78	47.15	7.16	7.72
97	LEU	CD2	-4.38	45.14	5.71	7.62
97	LEU	C	-3.39	43.94	9.52	7.47
97	LEU	O	-4.37	43.21	9.34	7.49
98	LYS	N	-3.06	44.44	10.70	7.66
98	LYS	CA	-3.88	44.24	11.90	7.93
98	LYS	CB	-3.43	43.01	12.70	7.99
98	LYS	CG	-4.20	42.81	14.02	8.11
98	LYS	CD	-3.86	41.48	14.69	8.29
98	LYS	CE	-4.66	41.28	15.98	8.47
98	LYS	NZ	-4.37	39.97	16.64	8.69

98 LYS C	-3.69	45.50	12.73	8.15
98 LYS O	-2.56	45.92	12.98	8.19
99 ASN N	-4.80	46.11	13.12	8.43
99 ASN CA	-4.78	47.34	13.90	8.51
99 ASN CB	-4.24	47.09	15.32	8.67
99 ASN CG	-5.12	46.13	16.12	8.73
99 ASN OD1	-6.35	46.14	15.99	8.91
99 ASN ND2	-4.50	45.30	16.96	8.82
99 ASN C	-3.96	48.45	13.22	8.56
99 ASN O	-3.28	49.23	13.89	8.66
100 GLY N	-4.03	48.49	11.89	8.45
100 GLY CA	-3.33	49.51	11.12	8.36
100 GLY C	-1.87	49.27	10.75	8.21
100 GLY O	-1.29	50.05	10.00	8.19
101 TYR N	-1.28	48.19	11.27	8.04
101 TYR CA	0.12	47.86	11.01	7.75
101 TYR CB	0.86	47.62	12.32	7.87
101 TYR CG	0.96	48.88	13.15	8.16
101 TYR CD1	2.01	49.78	12.98	8.29
101 TYR CE1	2.05	50.99	13.68	8.58
101 TYR CD2	-0.05	49.22	14.05	8.29
101 TYR CE2	-0.02	50.43	14.75	8.54
101 TYR CZ	1.03	51.31	14.55	8.61
101 TYR OH	1.04	52.52	15.22	8.95
101 TYR C	0.28	46.67	10.07	7.52
101 TYR O	-0.46	45.69	10.16	7.45
102 TYR N	1.28	46.76	9.20	7.38
102 TYR CA	1.55	45.74	8.18	7.22
102 TYR CB	1.68	46.42	6.81	7.30
102 TYR CG	0.41	47.03	6.23	7.57
102 TYR CD1	-0.22	48.12	6.83	7.54
102 TYR CE1	-1.35	48.72	6.25	7.75
102 TYR CD2	-0.13	46.54	5.04	7.61
102 TYR CE2	-1.25	47.12	4.46	7.68
102 TYR CZ	-1.86	48.20	5.07	7.86
102 TYR OH	-2.97	48.77	4.48	7.96
102 TYR C	2.78	44.86	8.34	7.07
102 TYR O	3.73	45.21	9.04	6.95
103 ALA N	2.74	43.72	7.65	7.07
103 ALA CA	3.84	42.76	7.57	6.90
103 ALA CB	3.64	41.60	8.52	6.96
103 ALA C	3.79	42.29	6.12	6.75
103 ALA O	2.73	42.31	5.48	6.84

104 ASP N	4.94	41.87	5.60	6.61
104 ASP CA	5.06	41.42	4.22	6.57
104 ASP CB	5.46	42.62	3.36	6.79
104 ASP CG	5.39	42.35	1.87	6.84
104 ASP OD1	5.12	41.20	1.47	6.89
104 ASP OD2	5.61	43.31	1.10	6.72
104 ASP C	6.18	40.38	4.24	6.47
104 ASP O	7.30	40.66	4.67	6.38
105 THR N	5.88	39.16	3.80	6.50
105 THR CA	6.90	38.13	3.80	6.44
105 THR CB	6.94	37.40	5.17	6.46
105 THR OG1	8.02	36.46	5.19	6.45
105 THR CG2	5.62	36.69	5.43	6.53
105 THR C	6.62	37.14	2.67	6.46
105 THR O	5.49	37.05	2.19	6.55
106 GLY N	7.63	36.40	2.25	6.43
106 GLY CA	7.42	35.46	1.17	6.51
106 GLY C	8.54	34.46	1.06	6.59
106 GLY O	9.64	34.67	1.56	6.44
107 ILE N	8.25	33.36	0.38	6.68
107 ILE CA	9.25	32.32	0.23	6.71
107 ILE CB	9.26	31.42	1.49	6.73
107 ILE CG2	7.89	30.77	1.67	6.75
107 ILE CG1	10.36	30.37	1.37	7.04
107 ILE CD1	10.63	29.65	2.66	7.53
107 ILE C	9.02	31.45	-1.00	6.69
107 ILE O	7.89	31.09	-1.32	6.47
108 SER N	10.11	31.14	-1.69	6.84
108 SER CA	10.04	30.27	-2.86	7.04
108 SER CB	10.87	30.83	-4.02	7.01
108 SER OG	10.27	31.98	-4.58	7.00
108 SER C	10.64	28.94	-2.42	7.18
108 SER O	11.60	28.91	-1.65	7.03
109 PHE N	10.07	27.86	-2.93	7.45
109 PHE CA	10.54	26.52	-2.62	7.76
109 PHE CB	9.95	26.02	-1.29	7.72
109 PHE CG	8.45	26.09	-1.23	7.67
109 PHE CD1	7.81	27.29	-0.92	7.72
109 PHE CD2	7.67	24.97	-1.50	7.74
109 PHE CE1	6.41	27.38	-0.88	7.73
109 PHE CE2	6.27	25.04	-1.46	7.72
109 PHE CZ	5.64	26.25	-1.15	7.66
109 PHE C	10.15	25.59	-3.75	8.02

109 PHE O	9.33	25.94	-4.59	7.97
110 VAL N	10.77	24.41	-3.78	8.40
110 VAL CA	10.48	23.41	-4.79	8.73
110 VAL CB	11.78	22.72	-5.26	8.76
110 VAL CG1	11.46	21.58	-6.22	8.69
110 VAL CG2	12.69	23.74	-5.94	8.75
110 VAL C	9.56	22.37	-4.17	9.11
110 VAL O	9.80	21.93	-3.04	9.12
111 VAL N	8.51	22.00	-4.89	9.46
111 VAL CA	7.57	21.00	-4.42	9.96
111 VAL CB	6.20	21.16	-5.11	9.94
111 VAL CG1	5.24	20.07	-4.63	9.81
111 VAL CG2	5.63	22.53	-4.80	9.87
111 VAL C	8.16	19.64	-4.77	10.35
111 VAL O	8.31	19.31	-5.94	10.37
112 GLY N	8.52	18.88	-3.74	10.81
112 GLY CA	9.11	17.58	-3.98	11.24
112 GLY C	10.44	17.73	-4.69	11.57
112 GLY O	11.32	18.46	-4.24	11.67
113 GLU N	10.59	17.03	-5.82	11.85
113 GLU CA	11.82	17.09	-6.58	12.17
113 GLU CB	12.58	15.77	-6.45	12.54
113 GLU CG	12.85	15.33	-5.02	13.07
113 GLU CD	13.30	13.89	-4.97	13.36
113 GLU OE1	12.56	13.03	-5.50	13.72
113 GLU OE2	14.38	13.61	-4.42	13.60
113 GLU C	11.59	17.38	-8.06	12.22
113 GLU O	10.62	16.91	-8.66	12.19
114 SER N	12.51	18.14	-8.64	12.26
114 SER CA	12.49	18.50	-10.05	12.29
114 SER CB	12.64	20.02	-10.21	12.45
114 SER OG	12.82	20.38	-11.56	12.71
114 SER C	13.69	17.82	-10.72	12.19
114 SER O	14.65	17.47	-10.04	12.16
115 ASP N	13.62	17.60	-12.04	12.18
115 ASP CA	14.73	16.97	-12.76	12.17
115 ASP CB	14.28	16.48	-14.13	12.77
115 ASP CG	13.67	17.59	-14.97	13.26
115 ASP OD1	12.73	18.24	-14.47	13.73
115 ASP OD2	14.12	17.81	-16.11	13.79
115 ASP C	15.87	17.95	-12.95	11.89
115 ASP O	16.99	17.57	-13.31	11.74
116 ASP N	15.57	19.23	-12.72	11.63

116	ASP	CA	16.56	20.29	-12.88	11.41
116	ASP	CB	16.02	21.40	-13.78	11.67
116	ASP	CG	17.11	22.33	-14.27	11.80
116	ASP	OD1	18.14	22.47	-13.57	11.94
116	ASP	OD2	16.93	22.93	-15.35	11.91
116	ASP	C	16.91	20.87	-11.52	11.19
116	ASP	O	16.08	21.53	-10.89	11.12
117	PRO	N	18.14	20.65	-11.04	11.03
117	PRO	CD	19.23	19.91	-11.71	11.03
117	PRO	CA	18.57	21.16	-9.75	10.91
117	PRO	CB	19.92	20.46	-9.54	10.95
117	PRO	CG	20.44	20.34	-10.93	11.01
117	PRO	C	18.68	22.69	-9.68	10.85
117	PRO	O	18.85	23.26	-8.60	10.70
118	MET	N	18.56	23.36	-10.82	10.86
118	MET	CA	18.64	24.81	-10.85	10.83
118	MET	CB	18.60	25.33	-12.29	11.18
118	MET	CG	18.58	26.86	-12.42	11.64
118	MET	SD	20.07	27.66	-11.76	12.14
118	MET	CE	21.19	27.45	-13.13	12.08
118	MET	C	17.49	25.43	-10.05	10.57
118	MET	O	17.62	26.53	-9.52	10.48
119	LYS	N	16.35	24.74	-9.99	10.28
119	LYS	CA	15.23	25.28	-9.23	10.14
119	LYS	CB	13.99	24.38	-9.36	10.21
119	LYS	CG	13.34	24.45	-10.74	10.29
119	LYS	CD	11.99	23.73	-10.78	10.35
119	LYS	CE	11.26	24.00	-12.10	10.55
119	LYS	NZ	9.99	23.23	-12.22	10.63
119	LYS	C	15.63	25.44	-7.76	9.96
119	LYS	O	15.46	26.51	-7.19	9.99
120	GLN	N	16.19	24.39	-7.17	9.82
120	GLN	CA	16.63	24.47	-5.79	9.62
120	GLN	CB	17.09	23.09	-5.29	9.62
120	GLN	CG	17.45	23.06	-3.79	9.62
120	GLN	CD	16.29	23.50	-2.91	9.61
120	GLN	OE1	15.16	23.04	-3.08	9.62
120	GLN	NE2	16.56	24.40	-1.97	9.65
120	GLN	C	17.78	25.48	-5.65	9.52
120	GLN	O	17.87	26.18	-4.64	9.51
121	LYS	N	18.64	25.57	-6.67	9.41
121	LYS	CA	19.77	26.50	-6.61	9.37
121	LYS	CB	20.64	26.41	-7.89	9.37

121	LYS	CG	21.89	27.30	-7.82	9.37
121	LYS	CD	22.84	27.13	-9.02	9.39
121	LYS	CE	24.02	28.10	-8.92	9.51
121	LYS	NZ	25.07	27.90	-9.96	9.57
121	LYS	C	19.33	27.93	-6.41	9.29
121	LYS	O	19.83	28.62	-5.52	9.51
122	VAL	N	18.38	28.41	-7.22	9.33
122	VAL	CA	17.94	29.79	-7.07	9.34
122	VAL	CB	16.96	30.21	-8.19	9.47
122	VAL	CG1	17.68	30.20	-9.53	9.60
122	VAL	CG2	15.74	29.30	-8.23	9.54
122	VAL	C	17.31	30.00	-5.69	9.17
122	VAL	O	17.39	31.09	-5.14	9.09
123	CYS	N	16.70	28.95	-5.13	9.21
123	CYS	CA	16.13	29.07	-3.80	9.07
123	CYS	CB	15.26	27.86	-3.46	9.11
123	CYS	SG	13.69	27.80	-4.39	8.94
123	CYS	C	17.26	29.21	-2.78	9.04
123	CYS	O	17.18	30.04	-1.89	8.96
124	ASP	N	18.30	28.38	-2.91	9.10
124	ASP	CA	19.42	28.46	-1.98	9.25
124	ASP	CB	20.49	27.39	-2.29	9.57
124	ASP	CG	19.98	25.96	-2.12	9.96
124	ASP	OD1	19.07	25.72	-1.29	10.11
124	ASP	OD2	20.52	25.07	-2.81	10.21
124	ASP	C	20.10	29.82	-2.05	9.25
124	ASP	O	20.46	30.39	-1.01	9.16
125	VAL	N	20.28	30.36	-3.25	9.27
125	VAL	CA	20.95	31.65	-3.40	9.34
125	VAL	CB	21.45	31.82	-4.87	9.27
125	VAL	CG1	22.22	33.13	-5.03	9.38
125	VAL	CG2	22.37	30.65	-5.22	9.33
125	VAL	C	20.07	32.82	-2.96	9.33
125	VAL	O	20.57	33.84	-2.49	9.32
126	ALA	N	18.76	32.67	-3.11	9.40
126	ALA	CA	17.85	33.71	-2.67	9.55
126	ALA	CB	16.40	33.34	-3.02	9.53
126	ALA	C	18.01	33.85	-1.16	9.65
126	ALA	O	18.02	34.96	-0.62	9.60
127	THR	N	18.15	32.72	-0.47	9.87
127	THR	CA	18.32	32.72	0.98	10.18
127	THR	CB	18.20	31.30	1.56	10.35
127	THR	OG1	16.87	30.81	1.35	10.71

127	THR	CG2	18.49	31.29	3.06	10.60
127	THR	C	19.67	33.33	1.36	10.23
127	THR	O	19.74	34.15	2.28	10.12
128	MET	N	20.73	32.94	0.67	10.48
128	MET	CA	22.05	33.49	0.96	10.71
128	MET	CB	23.11	32.83	0.09	11.37
128	MET	CG	23.45	31.42	0.48	12.33
128	MET	SD	24.82	30.84	-0.52	13.45
128	MET	CE	24.03	30.57	-2.04	13.45
128	MET	C	22.05	34.99	0.70	10.48
128	MET	O	22.59	35.76	1.50	10.30
129	ALA	N	21.43	35.40	-0.40	10.37
129	ALA	CA	21.37	36.82	-0.74	10.39
129	ALA	CB	20.64	37.02	-2.05	10.48
129	ALA	C	20.69	37.60	0.38	10.35
129	ALA	O	21.14	38.68	0.76	10.42
130	PHE	N	19.60	37.05	0.91	10.29
130	PHE	CA	18.90	37.73	1.98	10.16
130	PHE	CB	17.62	36.98	2.36	10.04
130	PHE	CG	16.90	37.61	3.50	9.87
130	PHE	CD1	16.11	38.74	3.31	9.82
130	PHE	CD2	17.07	37.13	4.79	9.87
130	PHE	CE1	15.51	39.39	4.38	9.72
130	PHE	CE2	16.47	37.77	5.88	9.79
130	PHE	CZ	15.69	38.91	5.67	9.70
130	PHE	C	19.80	37.85	3.21	10.19
130	PHE	O	19.91	38.92	3.81	10.16
131	GLU	N	20.45	36.75	3.57	10.29
131	GLU	CA	21.35	36.72	4.73	10.39
131	GLU	CB	21.95	35.31	4.91	10.58
131	GLU	CG	20.92	34.20	5.14	11.12
131	GLU	CD	21.56	32.81	5.15	11.40
131	GLU	OE1	22.64	32.65	4.54	11.61
131	GLU	OE2	20.96	31.89	5.76	11.68
131	GLU	C	22.49	37.72	4.58	10.35
131	GLU	O	22.86	38.40	5.54	10.21
132	ASN	N	23.06	37.79	3.38	10.46
132	ASN	CA	24.16	38.71	3.15	10.68
132	ASN	CB	24.82	38.41	1.81	10.77
132	ASN	CG	25.50	37.07	1.79	10.94
132	ASN	OD1	25.77	36.49	2.85	11.09
132	ASN	ND2	25.80	36.56	0.60	11.00
132	ASN	C	23.70	40.16	3.23	10.90

132 ASN O	24.45	41.03	3.68	10.77
133 ALA N	22.47	40.41	2.80	11.27
133 ALA CA	21.92	41.77	2.83	11.71
133 ALA CB	20.65	41.84	2.00	11.66
133 ALA C	21.63	42.20	4.26	12.01
133 ALA O	22.00	43.30	4.67	12.17
134 ILE N	20.98	41.34	5.04	12.39
134 ILE CA	20.67	41.74	6.41	12.81
134 ILE CB	19.72	40.75	7.08	12.92
134 ILE CG2	18.41	40.70	6.30	13.10
134 ILE CG1	20.36	39.37	7.16	13.08
134 ILE CD1	19.61	38.41	8.05	13.19
134 ILE C	21.92	41.88	7.27	12.95
134 ILE O	21.90	42.57	8.29	12.97
135 ALA N	23.01	41.23	6.85	13.25
135 ALA CA	24.27	41.27	7.59	13.54
135 ALA CB	25.36	40.55	6.80	13.43
135 ALA C	24.76	42.66	7.97	13.78
135 ALA O	25.27	42.85	9.08	14.02
136 LYS N	24.64	43.64	7.09	14.12
136 LYS CA	25.10	44.98	7.46	14.38
136 LYS CB	26.24	45.44	6.55	14.80
136 LYS CG	27.59	44.79	6.83	15.14
136 LYS CD	28.67	45.41	5.95	15.50
136 LYS CE	29.92	44.56	5.89	15.73
136 LYS NZ	30.80	45.03	4.76	16.03
136 LYS C	24.00	46.03	7.52	14.44
136 LYS O	24.26	47.23	7.36	14.57
137 VAL N	22.77	45.59	7.75	14.41
137 VAL CA	21.66	46.53	7.89	14.37
137 VAL CB	20.30	45.82	7.73	14.47
137 VAL CG1	19.18	46.73	8.20	14.47
137 VAL CG2	20.09	45.43	6.27	14.42
137 VAL C	21.78	47.11	9.30	14.30
137 VAL O	21.57	46.40	10.29	14.32
138 LYS N	22.16	48.38	9.38	14.21
138 LYS CA	22.31	49.08	10.65	14.10
138 LYS CB	23.73	48.88	11.21	14.25
138 LYS CG	24.07	47.42	11.56	14.53
138 LYS CD	25.23	47.32	12.56	14.70
138 LYS CE	24.83	47.88	13.94	14.84
138 LYS NZ	23.62	47.17	14.50	15.00
138 LYS C	22.04	50.57	10.45	13.84

138 LYS O	22.07	51.06	9.32	13.78
139 PRO N	21.76	51.31	11.54	13.62
139 PRO CD	21.53	50.85	12.92	13.62
139 PRO CA	21.49	52.75	11.42	13.44
139 PRO CB	21.24	53.17	12.87	13.48
139 PRO CG	20.66	51.96	13.48	13.54
139 PRO C	22.69	53.48	10.82	13.30
139 PRO O	23.83	53.21	11.19	13.29
140 GLY N	22.42	54.40	9.89	13.05
140 GLY CA	23.49	55.17	9.28	12.85
140 GLY C	24.13	54.55	8.05	12.75
140 GLY O	24.90	55.22	7.36	12.72
141 THR N	23.83	53.28	7.77	12.65
141 THR CA	24.39	52.61	6.61	12.58
141 THR CB	24.45	51.07	6.81	12.80
141 THR OG1	23.11	50.54	6.86	13.18
141 THR CG2	25.16	50.74	8.11	13.07
141 THR C	23.58	52.92	5.36	12.27
141 THR O	22.39	53.24	5.44	12.24
142 LYS N	24.22	52.81	4.21	12.00
142 LYS CA	23.56	53.10	2.94	11.76
142 LYS CB	24.61	53.24	1.83	11.96
142 LYS CG	25.55	54.42	2.04	12.16
142 LYS CD	26.70	54.38	1.05	12.55
142 LYS CE	27.64	55.56	1.22	12.85
142 LYS NZ	28.77	55.47	0.26	13.24
142 LYS C	22.55	52.02	2.56	11.54
142 LYS O	22.79	50.83	2.73	11.48
143 LEU N	21.41	52.49	2.07	11.36
143 LEU CA	20.34	51.62	1.63	11.24
143 LEU CB	19.16	52.47	1.15	11.33
143 LEU CG	18.00	51.73	0.49	11.35
143 LEU CD1	17.25	50.94	1.56	11.40
143 LEU CD2	17.05	52.73	-0.18	11.36
143 LEU C	20.86	50.76	0.48	11.12
143 LEU O	20.55	49.57	0.39	11.16
144 SER N	21.68	51.38	-0.36	10.97
144 SER CA	22.25	50.70	-1.52	10.92
144 SER CB	23.07	51.70	-2.36	11.18
144 SER OG	24.21	52.16	-1.66	11.42
144 SER C	23.11	49.48	-1.18	10.76
144 SER O	23.39	48.67	-2.06	10.67
145 ASN N	23.54	49.36	0.08	10.61

145	ASN	CA	24.34	48.20	0.47	10.40
145	ASN	CB	24.82	48.29	1.92	10.65
145	ASN	CG	25.83	49.40	2.13	11.01
145	ASN	OD1	26.76	49.57	1.36	11.26
145	ASN	ND2	25.64	50.16	3.20	11.32
145	ASN	C	23.51	46.92	0.33	10.15
145	ASN	O	24.06	45.83	0.14	10.00
146	ILE	N	22.19	47.05	0.45	9.92
146	ILE	CA	21.31	45.90	0.33	9.80
146	ILE	CB	19.84	46.27	0.66	9.83
146	ILE	CG2	18.92	45.06	0.45	9.74
146	ILE	CG1	19.74	46.71	2.13	10.03
146	ILE	CD1	18.37	47.24	2.53	10.28
146	ILE	C	21.39	45.31	-1.08	9.68
146	ILE	O	21.77	44.15	-1.25	9.64
147	GLY	N	21.06	46.12	-2.08	9.67
147	GLY	CA	21.12	45.64	-3.45	9.62
147	GLY	C	22.52	45.23	-3.87	9.61
147	GLY	O	22.71	44.28	-4.63	9.62
148	LYS	N	23.52	45.94	-3.36	9.54
148	LYS	CA	24.90	45.62	-3.70	9.49
148	LYS	CB	25.84	46.62	-3.03	9.74
148	LYS	CG	27.29	46.45	-3.39	10.06
148	LYS	CD	28.11	47.60	-2.82	10.49
148	LYS	CE	29.48	47.63	-3.45	10.81
148	LYS	NZ	29.36	47.97	-4.90	11.31
148	LYS	C	25.21	44.20	-3.25	9.36
148	LYS	O	25.82	43.42	-3.98	9.26
149	ALA	N	24.78	43.86	-2.03	9.27
149	ALA	CA	25.02	42.53	-1.48	9.22
149	ALA	CB	24.63	42.50	0.00	9.08
149	ALA	C	24.22	41.46	-2.23	9.21
149	ALA	O	24.72	40.36	-2.47	9.09
150	VAL	N	22.98	41.79	-2.58	9.31
150	VAL	CA	22.13	40.86	-3.30	9.42
150	VAL	CB	20.71	41.44	-3.51	9.49
150	VAL	CG1	19.87	40.49	-4.35	9.56
150	VAL	CG2	20.04	41.67	-2.17	9.57
150	VAL	C	22.73	40.52	-4.66	9.48
150	VAL	O	22.86	39.34	-5.00	9.50
151	HIS	N	23.11	41.53	-5.42	9.61
151	HIS	CA	23.68	41.30	-6.75	9.73
151	HIS	CB	23.79	42.62	-7.51	10.01

151	HIS	CG	24.18	42.46	-8.95	10.40
151	HIS	CD2	23.43	42.40	-10.07	10.64
151	HIS	ND1	25.49	42.34	-9.36	10.64
151	HIS	CE1	25.53	42.20	-10.68	10.76
151	HIS	NE2	24.29	42.23	-11.13	10.75
151	HIS	C	25.04	40.60	-6.70	9.75
151	HIS	O	25.34	39.73	-7.53	9.51
152	ASN	N	25.86	40.96	-5.71	9.84
152	ASN	CA	27.17	40.34	-5.56	9.98
152	ASN	CB	27.96	41.04	-4.44	10.11
152	ASN	CG	29.35	40.46	-4.25	10.41
152	ASN	OD1	29.50	39.26	-4.02	10.73
152	ASN	ND2	30.37	41.30	-4.33	10.37
152	ASN	C	26.97	38.85	-5.25	10.07
152	ASN	O	27.68	37.99	-5.78	9.98
153	THR	N	25.99	38.54	-4.40	10.14
153	THR	CA	25.71	37.15	-4.05	10.32
153	THR	CB	24.60	37.04	-2.98	10.30
153	THR	OG1	24.99	37.75	-1.80	10.34
153	THR	CG2	24.34	35.58	-2.63	10.34
153	THR	C	25.27	36.38	-5.29	10.42
153	THR	O	25.69	35.24	-5.51	10.42
154	ALA	N	24.41	37.00	-6.11	10.56
154	ALA	CA	23.95	36.34	-7.32	10.81
154	ALA	CB	22.94	37.22	-8.05	10.76
154	ALA	C	25.15	36.06	-8.22	10.97
154	ALA	O	25.31	34.95	-8.74	11.05
155	ARG	N	26.00	37.06	-8.40	11.20
155	ARG	CA	27.18	36.94	-9.25	11.47
155	ARG	CB	27.92	38.28	-9.29	11.94
155	ARG	CG	28.66	38.53	-10.59	12.70
155	ARG	CD	29.76	37.52	-10.80	13.28
155	ARG	NE	30.14	37.43	-12.21	13.81
155	ARG	CZ	31.10	36.64	-12.68	13.99
155	ARG	NH1	31.78	35.85	-11.85	14.19
155	ARG	NH2	31.37	36.62	-13.97	14.23
155	ARG	C	28.13	35.83	-8.79	11.39
155	ARG	O	28.70	35.12	-9.62	11.28
156	GLN	N	28.29	35.69	-7.47	11.33
156	GLN	CA	29.17	34.66	-6.92	11.30
156	GLN	CB	29.26	34.75	-5.40	11.36
156	GLN	CG	29.81	36.04	-4.85	11.52
156	GLN	CD	30.00	35.96	-3.35	11.66

156	GLN	OE1	30.04	36.98	-2.65	11.84
156	GLN	NE2	30.11	34.73	-2.83	11.66
156	GLN	C	28.68	33.26	-7.26	11.26
156	GLN	O	29.43	32.29	-7.18	11.23
157	ASN	N	27.40	33.15	-7.61	11.30
157	ASN	CA	26.83	31.84	-7.94	11.37
157	ASN	CB	25.68	31.53	-6.99	11.56
157	ASN	CG	26.14	31.44	-5.56	11.71
157	ASN	OD1	26.12	32.43	-4.82	11.91
157	ASN	ND2	26.57	30.25	-5.16	11.81
157	ASN	C	26.37	31.72	-9.38	11.37
157	ASN	O	25.50	30.90	-9.69	11.28
158	ASP	N	26.94	32.54	-10.24	11.45
158	ASP	CA	26.61	32.53	-11.66	11.57
158	ASP	CB	27.14	31.24	-12.30	12.05
158	ASP	CG	28.65	31.09	-12.14	12.47
158	ASP	OD1	29.40	31.93	-12.68	12.83
158	ASP	OD2	29.09	30.14	-11.46	12.93
158	ASP	C	25.12	32.67	-11.92	11.41
158	ASP	O	24.55	31.97	-12.76	11.39
159	LEU	N	24.49	33.58	-11.19	11.20
159	LEU	CA	23.07	33.83	-11.34	11.00
159	LEU	CB	22.30	33.32	-10.12	11.02
159	LEU	CG	22.30	31.79	-9.97	11.06
159	LEU	CD1	21.67	31.41	-8.64	11.02
159	LEU	CD2	21.52	31.17	-11.13	11.05
159	LEU	C	22.81	35.32	-11.54	10.86
159	LEU	O	23.72	36.14	-11.46	10.85
160	LYS	N	21.55	35.65	-11.80	10.79
160	LYS	CA	21.14	37.03	-12.04	10.74
160	LYS	CB	20.56	37.16	-13.45	10.96
160	LYS	CG	21.55	36.92	-14.58	11.19
160	LYS	CD	22.74	37.86	-14.46	11.58
160	LYS	CE	23.63	37.83	-15.70	11.85
160	LYS	NZ	24.08	36.45	-16.06	12.14
160	LYS	C	20.09	37.44	-11.02	10.62
160	LYS	O	19.62	36.62	-10.23	10.47
161	VAL	N	19.73	38.72	-11.02	10.59
161	VAL	CA	18.69	39.20	-10.12	10.59
161	VAL	CB	19.23	40.29	-9.12	10.61
161	VAL	CG1	20.41	39.74	-8.34	10.70
161	VAL	CG2	19.64	41.54	-9.88	10.71
161	VAL	C	17.60	39.82	-11.00	10.50

161 VAL O	17.85	40.13	-12.17	10.56
162 ILE N	16.40	39.96	-10.46	10.41
162 ILE CA	15.30	40.59	-11.20	10.41
162 ILE CB	13.91	40.11	-10.72	10.51
162 ILE CG2	12.81	40.89	-11.43	10.39
162 ILE CG1	13.74	38.61	-10.98	10.47
162 ILE CD1	13.82	38.21	-12.44	10.55
162 ILE C	15.48	42.06	-10.86	10.36
162 ILE O	15.32	42.45	-9.71	10.42
163 LYS N	15.82	42.86	-11.86	10.37
163 LYS CA	16.07	44.28	-11.64	10.45
163 LYS CB	16.91	44.84	-12.79	10.71
163 LYS CG	18.29	44.21	-12.94	11.10
163 LYS CD	19.00	44.79	-14.15	11.53
163 LYS CE	20.34	44.12	-14.40	11.90
163 LYS NZ	21.36	44.45	-13.37	12.31
163 LYS C	14.84	45.16	-11.48	10.40
163 LYS O	14.88	46.16	-10.77	10.37
164 ASN N	13.74	44.79	-12.13	10.36
164 ASN CA	12.54	45.60	-12.04	10.28
164 ASN CB	11.87	45.72	-13.43	10.27
164 ASN CG	11.31	44.40	-13.92	10.25
164 ASN OD1	11.81	43.32	-13.60	10.09
164 ASN ND2	10.26	44.49	-14.74	10.29
164 ASN C	11.54	45.21	-10.97	10.20
164 ASN O	10.36	45.54	-11.05	10.32
165 LEU N	12.01	44.50	-9.95	10.08
165 LEU CA	11.19	44.12	-8.80	10.06
165 LEU CB	10.94	42.61	-8.76	9.99
165 LEU CG	9.85	42.09	-9.72	9.94
165 LEU CD1	9.70	40.59	-9.55	9.76
165 LEU CD2	8.53	42.79	-9.43	9.89
165 LEU C	12.03	44.56	-7.61	10.09
165 LEU O	13.23	44.30	-7.57	10.08
166 THR N	11.41	45.23	-6.64	10.06
166 THR CA	12.16	45.72	-5.48	10.01
166 THR CB	12.50	47.21	-5.65	9.95
166 THR OG1	11.35	47.99	-5.28	10.06
166 THR CG2	12.83	47.53	-7.10	9.95
166 THR C	11.46	45.62	-4.14	9.99
166 THR O	10.26	45.34	-4.06	9.93
167 GLY N	12.23	45.88	-3.08	9.94
167 GLY CA	11.72	45.87	-1.73	9.93

167 GLY C	11.11	47.24	-1.49	9.96
167 GLY O	11.08	48.06	-2.40	9.92
168 HIS N	10.68	47.53	-0.27	9.98
168 HIS CA	10.03	48.81	0.00	9.96
168 HIS CB	8.66	48.77	-0.67	9.94
168 HIS CG	7.88	47.54	-0.32	9.79
168 HIS CD2	7.77	46.35	-0.95	9.82
168 HIS ND1	7.19	47.41	0.87	9.83
168 HIS CE1	6.69	46.19	0.95	9.83
168 HIS NE2	7.03	45.53	-0.14	9.82
168 HIS C	9.83	49.02	1.48	9.97
168 HIS O	9.89	48.08	2.26	10.06
169 GLY N	9.58	50.27	1.88	10.07
169 GLY CA	9.33	50.53	3.28	10.11
169 GLY C	7.97	49.93	3.61	10.24
169 GLY O	7.13	49.78	2.72	10.27
170 VAL N	7.77	49.58	4.88	10.35
170 VAL CA	6.50	49.00	5.32	10.48
170 VAL CB	6.54	47.44	5.35	10.55
170 VAL CG1	7.60	46.96	6.30	10.71
170 VAL CG2	5.17	46.89	5.75	10.67
170 VAL C	6.19	49.52	6.71	10.48
170 VAL O	7.08	50.03	7.39	10.44
171 GLY N	4.93	49.44	7.11	10.58
171 GLY CA	4.55	49.91	8.44	10.66
171 GLY C	3.08	50.23	8.51	10.75
171 GLY O	2.29	49.44	9.04	10.69
172 LEU N	2.70	51.38	7.98	10.96
172 LEU CA	1.30	51.82	7.97	11.30
172 LEU CB	1.23	53.31	8.30	11.37
172 LEU CG	1.74	53.65	9.70	11.48
172 LEU CD1	1.91	55.16	9.85	11.51
172 LEU CD2	0.77	53.09	10.73	11.36
172 LEU C	0.67	51.55	6.60	11.55
172 LEU O	-0.51	51.80	6.37	11.53
173 SER N	1.50	51.02	5.71	11.91
173 SER CA	1.11	50.67	4.35	12.31
173 SER CB	1.08	51.91	3.45	12.24
173 SER OG	2.40	52.34	3.16	12.16
173 SER C	2.17	49.72	3.83	12.65
173 SER O	3.15	49.42	4.51	12.60
174 LEU N	1.98	49.27	2.59	13.10
174 LEU CA	2.89	48.35	1.94	13.58

174 LEU CB	2.09	47.32	1.14	13.60
174 LEU CG	2.78	46.11	0.52	13.54
174 LEU CD1	2.52	44.89	1.41	13.50
174 LEU CD2	2.20	45.85	-0.88	13.48
174 LEU C	3.81	49.13	0.99	13.87
174 LEU O	4.67	48.56	0.32	14.11
175 HIS N	3.61	50.44	0.93	14.09
175 HIS CA	4.44	51.26	0.07	14.23
175 HIS CB	3.80	51.40	-1.32	14.53
175 HIS CG	4.54	50.65	-2.40	14.68
175 HIS CD2	5.33	51.09	-3.40	14.77
175 HIS ND1	4.55	49.27	-2.48	14.83
175 HIS CE1	5.31	48.90	-3.50	14.77
175 HIS NE2	5.80	49.98	-4.08	14.82
175 HIS C	4.75	52.64	0.65	14.13
175 HIS O	4.05	53.62	0.40	14.31
176 GLU N	5.82	52.69	1.44	13.85
176 GLU CA	6.28	53.92	2.04	13.47
176 GLU CB	5.79	54.05	3.48	13.51
176 GLU CG	5.74	52.76	4.29	13.57
176 GLU CD	4.92	52.91	5.55	13.66
176 GLU OE1	5.50	53.01	6.66	13.70
176 GLU OE2	3.67	52.93	5.44	13.69
176 GLU C	7.79	54.01	1.97	13.23
176 GLU O	8.45	53.04	1.59	13.12
177 ALA N	8.35	55.17	2.30	13.05
177 ALA CA	9.79	55.36	2.24	12.97
177 ALA CB	10.14	56.76	2.71	12.80
177 ALA C	10.55	54.33	3.06	12.90
177 ALA O	10.17	54.02	4.19	12.93
178 PRO N	11.63	53.75	2.50	12.91
178 PRO CD	12.50	52.82	3.22	13.04
178 PRO CA	12.15	54.02	1.16	12.99
178 PRO CB	13.56	53.44	1.22	13.06
178 PRO CG	13.39	52.27	2.13	13.08
178 PRO C	11.29	53.36	0.09	12.94
178 PRO O	10.90	52.20	0.22	12.99
179 ALA N	10.98	54.11	-0.96	12.77
179 ALA CA	10.12	53.62	-2.04	12.74
179 ALA CB	9.97	54.70	-3.11	12.69
179 ALA C	10.60	52.32	-2.69	12.70
179 ALA O	9.80	51.40	-2.89	12.59
180 HIS N	11.88	52.26	-3.01	12.66

180	HIS	CA	12.42	51.07	-3.65	12.68
180	HIS	CB	12.62	51.33	-5.15	12.86
180	HIS	CG	11.37	51.72	-5.87	13.18
180	HIS	CD2	10.36	50.96	-6.36	13.25
180	HIS	ND1	11.05	53.02	-6.17	13.35
180	HIS	CE1	9.90	53.06	-6.81	13.39
180	HIS	NE2	9.46	51.82	-6.95	13.43
180	HIS	C	13.72	50.58	-3.07	12.56
180	HIS	O	14.68	51.33	-2.92	12.63
181	VAL	N	13.75	49.29	-2.76	12.47
181	VAL	CA	14.94	48.65	-2.23	12.42
181	VAL	CB	14.60	47.79	-1.01	12.51
181	VAL	CG1	15.86	47.15	-0.45	12.52
181	VAL	CG2	13.91	48.64	0.05	12.44
181	VAL	C	15.41	47.76	-3.38	12.44
181	VAL	O	14.93	46.64	-3.54	12.38
182	LEU	N	16.33	48.29	-4.18	12.48
182	LEU	CA	16.83	47.57	-5.35	12.51
182	LEU	CB	17.73	48.49	-6.19	12.46
182	LEU	CG	17.17	49.84	-6.65	12.52
182	LEU	CD1	18.29	50.64	-7.31	12.49
182	LEU	CD2	16.01	49.65	-7.62	12.49
182	LEU	C	17.61	46.31	-5.02	12.55
182	LEU	O	18.12	46.14	-3.92	12.51
183	ASN	N	17.67	45.43	-6.01	12.67
183	ASN	CA	18.39	44.17	-5.90	12.80
183	ASN	CB	17.60	43.05	-6.57	12.86
183	ASN	CG	16.34	42.71	-5.81	12.96
183	ASN	OD1	16.36	42.57	-4.59	12.95
183	ASN	ND2	15.23	42.56	-6.53	13.02
183	ASN	C	19.76	44.30	-6.53	12.88
183	ASN	O	20.44	43.30	-6.79	12.79
184	TYR	N	20.16	45.54	-6.79	13.07
184	TYR	CA	21.47	45.80	-7.36	13.25
184	TYR	CB	21.42	45.84	-8.90	13.19
184	TYR	CG	20.50	46.88	-9.46	13.24
184	TYR	CD1	19.12	46.65	-9.53	13.16
184	TYR	CE1	18.25	47.62	-10.01	13.27
184	TYR	CD2	20.99	48.13	-9.89	13.22
184	TYR	CE2	20.12	49.11	-10.37	13.29
184	TYR	CZ	18.75	48.85	-10.42	13.29
184	TYR	OH	17.88	49.80	-10.86	13.44
184	TYR	C	21.98	47.13	-6.82	13.46

184 TYR O	21.24	47.89	-6.20	13.50
185 PHE N	23.25	47.40	-7.08	13.73
185 PHE CA	23.91	48.60	-6.59	14.07
185 PHE CB	25.41	48.32	-6.43	14.10
185 PHE CG	26.21	49.51	-5.98	14.16
185 PHE CD1	25.87	50.20	-4.82	14.21
185 PHE CD2	27.32	49.94	-6.71	14.20
185 PHE CE1	26.61	51.30	-4.39	14.25
185 PHE CE2	28.07	51.04	-6.29	14.32
185 PHE CZ	27.71	51.72	-5.13	14.29
185 PHE C	23.71	49.85	-7.45	14.32
185 PHE O	23.91	49.83	-8.66	14.30
186 ASP N	23.30	50.94	-6.79	14.66
186 ASP CA	23.10	52.23	-7.45	15.02
186 ASP CB	21.66	52.73	-7.31	15.11
186 ASP CG	21.47	54.11	-7.93	15.34
186 ASP OD1	22.38	54.57	-8.66	15.50
186 ASP OD2	20.41	54.72	-7.71	15.44
186 ASP C	24.05	53.20	-6.75	15.16
186 ASP O	23.76	53.70	-5.66	15.11
187 PRO N	25.20	53.47	-7.38	15.32
187 PRO CD	25.54	52.99	-8.73	15.36
187 PRO CA	26.24	54.37	-6.88	15.49
187 PRO CB	27.32	54.28	-7.95	15.46
187 PRO CG	26.51	54.04	-9.20	15.44
187 PRO C	25.82	55.82	-6.62	15.62
187 PRO O	26.55	56.57	-5.97	15.69
188 LYS N	24.64	56.22	-7.10	15.72
188 LYS CA	24.18	57.59	-6.90	15.81
188 LYS CB	23.41	58.09	-8.12	16.04
188 LYS CG	22.03	57.48	-8.22	16.29
188 LYS CD	21.13	58.20	-9.21	16.52
188 LYS CE	19.68	57.78	-8.96	16.61
188 LYS NZ	19.32	58.05	-7.54	16.74
188 LYS C	23.29	57.77	-5.67	15.77
188 LYS O	23.10	58.89	-5.19	15.78
189 ASP N	22.72	56.67	-5.18	15.64
189 ASP CA	21.82	56.75	-4.03	15.56
189 ASP CB	21.01	55.45	-3.90	15.65
189 ASP CG	19.95	55.54	-2.83	15.79
189 ASP OD1	19.62	56.67	-2.40	15.80
189 ASP OD2	19.42	54.48	-2.44	15.85
189 ASP C	22.55	57.02	-2.72	15.40

189 ASP O	23.46	56.29	-2.34	15.37
190 LYS N	22.14	58.09	-2.04	15.25
190 LYS CA	22.77	58.45	-0.77	15.04
190 LYS CB	23.17	59.93	-0.80	15.21
190 LYS CG	24.21	60.27	-1.87	15.49
190 LYS CD	24.56	61.75	-1.85	15.72
190 LYS CE	25.54	62.12	-2.95	15.89
190 LYS NZ	25.76	63.59	-3.05	16.07
190 LYS C	21.82	58.19	0.40	14.76
190 LYS O	22.11	58.55	1.54	14.81
191 THR N	20.68	57.57	0.11	14.44
191 THR CA	19.70	57.27	1.15	14.10
191 THR CB	18.46	56.56	0.57	14.26
191 THR OG1	17.91	57.36	-0.48	14.42
191 THR CG2	17.41	56.38	1.66	14.37
191 THR C	20.30	56.37	2.21	13.73
191 THR O	20.98	55.39	1.89	13.66
192 LEU N	20.06	56.71	3.46	13.41
192 LEU CA	20.58	55.93	4.57	13.11
192 LEU CB	21.39	56.82	5.51	13.24
192 LEU CG	22.58	57.58	4.93	13.32
192 LEU CD1	23.24	58.38	6.05	13.46
192 LEU CD2	23.57	56.60	4.32	13.42
192 LEU C	19.48	55.28	5.38	12.86
192 LEU O	18.34	55.75	5.39	12.71
193 LEU N	19.82	54.19	6.06	12.74
193 LEU CA	18.87	53.49	6.91	12.69
193 LEU CB	19.25	52.02	7.06	12.81
193 LEU CG	19.42	51.23	5.76	12.91
193 LEU CD1	19.69	49.77	6.08	13.00
193 LEU CD2	18.16	51.36	4.92	13.04
193 LEU C	18.99	54.20	8.25	12.63
193 LEU O	20.07	54.66	8.62	12.63
194 THR N	17.88	54.30	8.97	12.54
194 THR CA	17.88	54.97	10.27	12.52
194 THR CB	17.06	56.28	10.20	12.60
194 THR OG1	15.71	55.98	9.85	12.63
194 THR CG2	17.65	57.23	9.16	12.67
194 THR C	17.30	54.09	11.37	12.44
194 THR O	16.62	53.10	11.10	12.36
195 GLU N	17.59	54.46	12.61	12.40
195 GLU CA	17.10	53.73	13.77	12.33
195 GLU CB	17.60	54.43	15.04	12.55

195 GLU CG	17.09	53.86	16.36	12.99
195 GLU CD	17.58	52.46	16.64	13.22
195 GLU OE1	18.76	52.16	16.33	13.44
195 GLU OE2	16.80	51.65	17.19	13.41
195 GLU C	15.57	53.70	13.74	12.13
195 GLU O	14.92	54.74	13.64	12.09
196 GLY N	15.00	52.50	13.80	11.89
196 GLY CA	13.55	52.36	13.78	11.57
196 GLY C	12.92	52.21	12.40	11.42
196 GLY O	11.72	51.97	12.29	11.33
197 MET N	13.72	52.34	11.35	11.29
197 MET CA	13.20	52.22	9.99	11.09
197 MET CB	14.27	52.62	8.97	11.33
197 MET CG	13.75	52.72	7.55	11.61
197 MET SD	15.05	53.09	6.35	11.77
197 MET CE	14.94	54.87	6.31	11.87
197 MET C	12.73	50.80	9.71	10.84
197 MET O	13.46	49.84	9.99	10.76
198 VAL N	11.53	50.66	9.18	10.65
198 VAL CA	10.98	49.34	8.87	10.51
198 VAL CB	9.55	49.16	9.44	10.52
198 VAL CG1	9.08	47.73	9.25	10.52
198 VAL CG2	9.55	49.52	10.91	10.49
198 VAL C	10.96	49.16	7.35	10.47
198 VAL O	10.38	49.98	6.62	10.40
199 LEU N	11.59	48.08	6.89	10.50
199 LEU CA	11.71	47.80	5.47	10.40
199 LEU CB	13.14	48.04	5.00	10.56
199 LEU CG	13.95	49.14	5.66	10.91
199 LEU CD1	15.36	49.16	5.08	11.00
199 LEU CD2	13.25	50.47	5.38	11.08
199 LEU C	11.37	46.36	5.13	10.16
199 LEU O	11.48	45.47	5.97	10.18
200 ALA N	10.96	46.15	3.89	9.98
200 ALA CA	10.68	44.81	3.41	9.74
200 ALA CB	9.36	44.77	2.66	9.83
200 ALA C	11.84	44.55	2.46	9.50
200 ALA O	12.05	45.30	1.50	9.58
201 ILE N	12.62	43.52	2.74	9.35
201 ILE CA	13.75	43.18	1.89	9.18
201 ILE CB	15.02	42.96	2.74	9.27
201 ILE CG2	16.17	42.47	1.86	9.08
201 ILE CG1	15.38	44.28	3.44	9.24

201 ILE CD1	16.71	44.27	4.19	9.46
201 ILE C	13.35	41.90	1.16	9.04
201 ILE O	13.04	40.89	1.79	8.99
202 GLU N	13.33	41.94	-0.17	9.05
202 GLU CA	12.92	40.77	-0.94	9.03
202 GLU CB	11.43	40.88	-1.33	9.20
202 GLU CG	10.97	42.26	-1.78	9.45
202 GLU CD	9.45	42.35	-1.99	9.60
202 GLU OE1	8.88	43.41	-1.67	9.74
202 GLU OE2	8.82	41.40	-2.48	9.74
202 GLU C	13.76	40.48	-2.17	8.86
202 GLU O	13.36	40.78	-3.30	8.91
203 PRO N	14.94	39.89	-1.98	8.68
203 PRO CD	15.60	39.46	-0.74	8.71
203 PRO CA	15.77	39.59	-3.15	8.67
203 PRO CB	17.07	39.06	-2.54	8.70
203 PRO CG	16.62	38.45	-1.24	8.72
203 PRO C	15.10	38.57	-4.07	8.49
203 PRO O	14.44	37.64	-3.60	8.45
204 PHE N	15.24	38.79	-5.38	8.36
204 PHE CA	14.71	37.89	-6.40	8.35
204 PHE CB	13.79	38.61	-7.39	8.34
204 PHE CG	12.43	38.91	-6.84	8.45
204 PHE CD1	12.22	40.00	-6.01	8.45
204 PHE CD2	11.34	38.09	-7.16	8.47
204 PHE CE1	10.96	40.28	-5.49	8.57
204 PHE CE2	10.08	38.36	-6.64	8.54
204 PHE CZ	9.89	39.45	-5.81	8.52
204 PHE C	15.94	37.41	-7.17	8.28
204 PHE O	16.62	38.22	-7.78	8.21
205 ILE N	16.21	36.11	-7.12	8.26
205 ILE CA	17.35	35.52	-7.82	8.22
205 ILE CB	18.14	34.59	-6.87	8.27
205 ILE CG2	19.27	33.90	-7.63	8.20
205 ILE CG1	18.69	35.39	-5.69	8.24
205 ILE CD1	19.61	36.53	-6.09	8.30
205 ILE C	16.83	34.74	-9.02	8.16
205 ILE O	15.92	33.92	-8.88	8.29
206 SER N	17.42	34.98	-10.20	8.11
206 SER CA	16.98	34.35	-11.45	8.25
206 SER CB	16.53	35.44	-12.41	8.34
206 SER OG	16.29	34.92	-13.71	8.32
206 SER C	18.02	33.46	-12.15	8.34

206	SER	O	19.21	33.75	-12.10	8.18
207	SER	N	17.57	32.40	-12.80	8.58
207	SER	CA	18.48	31.51	-13.52	8.76
207	SER	CB	17.82	30.16	-13.80	8.62
207	SER	OG	16.63	30.31	-14.57	8.68
207	SER	C	18.97	32.11	-14.84	8.92
207	SER	O	19.94	31.63	-15.42	8.87
208	ASN	N	18.29	33.15	-15.32	9.17
208	ASN	CA	18.70	33.79	-16.57	9.46
208	ASN	CB	18.30	32.93	-17.77	9.81
208	ASN	CG	18.84	33.47	-19.08	9.97
208	ASN	OD1	18.08	33.88	-19.96	10.29
208	ASN	ND2	20.15	33.47	-19.22	10.13
208	ASN	C	18.19	35.22	-16.79	9.54
208	ASN	O	18.98	36.15	-16.97	9.60
209	ALA	N	16.87	35.39	-16.79	9.59
209	ALA	CA	16.26	36.70	-17.00	9.69
209	ALA	CB	14.75	36.56	-17.09	9.68
209	ALA	C	16.62	37.72	-15.93	9.77
209	ALA	O	16.70	37.39	-14.75	9.75
210	SER	N	16.85	38.97	-16.34	9.91
210	SER	CA	17.20	40.03	-15.40	9.94
210	SER	CB	18.40	40.81	-15.91	10.24
210	SER	OG	18.09	41.53	-17.09	10.82
210	SER	C	16.03	40.98	-15.16	9.77
210	SER	O	16.20	42.05	-14.58	9.75
211	PHE	N	14.84	40.59	-15.61	9.72
211	PHE	CA	13.64	41.40	-15.44	9.80
211	PHE	CB	13.63	42.57	-16.42	9.74
211	PHE	CG	13.56	42.15	-17.87	9.86
211	PHE	CD1	14.70	41.73	-18.54	9.91
211	PHE	CD2	12.35	42.15	-18.55	9.95
211	PHE	CE1	14.63	41.31	-19.87	10.07
211	PHE	CE2	12.27	41.74	-19.88	10.05
211	PHE	CZ	13.42	41.33	-20.54	10.07
211	PHE	C	12.40	40.55	-15.69	9.95
211	PHE	O	12.49	39.45	-16.23	9.81
212	VAL	N	11.24	41.05	-15.27	10.40
212	VAL	CA	9.97	40.35	-15.48	10.92
212	VAL	CB	9.23	40.03	-14.15	10.99
212	VAL	CG1	10.06	39.07	-13.30	11.17
212	VAL	CG2	8.94	41.31	-13.39	11.16
212	VAL	C	9.05	41.21	-16.34	11.16

212 VAL O	9.24	42.42	-16.46	11.11
213 THR N	8.05	40.57	-16.93	11.54
213 THR CA	7.08	41.26	-17.77	12.05
213 THR CB	7.33	40.99	-19.27	12.08
213 THR OG1	7.41	39.57	-19.49	11.95
213 THR CG2	8.62	41.65	-19.72	12.14
213 THR C	5.65	40.84	-17.43	12.30
213 THR O	5.44	39.86	-16.71	12.36
214 GLU N	4.68	41.58	-17.94	12.79
214 GLU CA	3.26	41.29	-17.70	13.29
214 GLU CB	2.39	42.26	-18.50	13.67
214 GLU CG	0.91	42.16	-18.22	14.26
214 GLU CD	0.12	43.24	-18.95	14.60
214 GLU OE1	0.50	44.42	-18.82	14.94
214 GLU OE2	-0.86	42.90	-19.64	14.92
214 GLU C	2.98	39.85	-18.14	13.42
214 GLU O	3.42	39.43	-19.21	13.54
215 GLY N	2.25	39.11	-17.32	13.58
215 GLY CA	1.96	37.73	-17.63	13.89
215 GLY C	0.61	37.41	-18.24	14.12
215 GLY O	0.03	38.23	-18.96	14.08
216 LYS N	0.11	36.22	-17.93	14.31
216 LYS CA	-1.17	35.72	-18.45	14.45
216 LYS CB	-1.38	34.27	-18.01	14.41
216 LYS CG	-1.55	34.10	-16.50	14.33
216 LYS CD	-1.74	32.64	-16.10	14.31
216 LYS CE	-0.52	31.78	-16.42	14.35
216 LYS NZ	0.74	32.29	-15.79	14.28
216 LYS C	-2.40	36.54	-18.07	14.58
216 LYS O	-3.48	36.33	-18.62	14.64
217 ASN N	-2.24	37.47	-17.13	14.65
217 ASN CA	-3.35	38.32	-16.72	14.74
217 ASN CB	-4.14	37.69	-15.57	14.74
217 ASN CG	-3.26	37.34	-14.39	14.62
217 ASN OD1	-2.54	38.19	-13.85	14.62
217 ASN ND2	-3.31	36.07	-13.97	14.55
217 ASN C	-2.83	39.69	-16.31	14.77
217 ASN O	-1.64	39.95	-16.40	14.86
218 GLU N	-3.72	40.57	-15.86	14.85
218 GLU CA	-3.33	41.92	-15.48	14.88
218 GLU CB	-4.55	42.84	-15.48	15.23
218 GLU CG	-5.68	42.36	-14.58	15.82
218 GLU CD	-6.83	43.36	-14.50	16.20

218 GLU OE1	-7.30	43.83	-15.56	16.52
218 GLU OE2	-7.26	43.66	-13.36	16.42
218 GLU C	-2.63	42.01	-14.13	14.67
218 GLU O	-2.32	43.10	-13.67	14.70
219 TRP N	-2.37	40.87	-13.50	14.43
219 TRP CA	-1.71	40.88	-12.20	14.16
219 TRP CB	-2.59	40.22	-11.15	14.13
219 TRP CG	-3.76	41.05	-10.73	14.22
219 TRP CD2	-3.74	42.15	-9.82	14.15
219 TRP CE2	-5.07	42.60	-9.67	14.32
219 TRP CE3	-2.72	42.80	-9.10	14.31
219 TRP CD1	-5.07	40.88	-11.10	14.15
219 TRP NE1	-5.86	41.81	-10.47	14.24
219 TRP CZ2	-5.42	43.67	-8.85	14.38
219 TRP CZ3	-3.06	43.87	-8.28	14.41
219 TRP CH2	-4.40	44.29	-8.16	14.42
219 TRP C	-0.34	40.21	-12.18	13.99
219 TRP O	0.66	40.84	-11.83	13.90
220 ALA N	-0.29	38.94	-12.54	13.87
220 ALA CA	0.96	38.18	-12.51	13.64
220 ALA CB	0.68	36.72	-12.86	13.82
220 ALA C	2.09	38.71	-13.39	13.49
220 ALA O	1.86	39.23	-14.48	13.51
221 PHE N	3.30	38.59	-12.86	13.28
221 PHE CA	4.52	38.97	-13.57	13.05
221 PHE CB	5.42	39.86	-12.71	13.33
221 PHE CG	4.82	41.19	-12.39	13.52
221 PHE CD1	4.21	41.95	-13.38	13.64
221 PHE CD2	4.87	41.69	-11.09	13.60
221 PHE CE1	3.64	43.19	-13.09	13.72
221 PHE CE2	4.31	42.93	-10.79	13.67
221 PHE CZ	3.70	43.68	-11.79	13.73
221 PHE C	5.23	37.66	-13.87	12.74
221 PHE O	5.28	36.77	-13.02	12.83
222 GLU N	5.77	37.55	-15.07	12.46
222 GLU CA	6.45	36.34	-15.52	12.17
222 GLU CB	5.50	35.56	-16.44	12.26
222 GLU CG	4.18	35.10	-15.79	12.32
222 GLU CD	3.18	34.52	-16.78	12.49
222 GLU OE1	3.62	33.97	-17.82	12.51
222 GLU OE2	1.95	34.59	-16.52	12.55
222 GLU C	7.73	36.66	-16.29	11.98
222 GLU O	8.16	37.81	-16.36	11.86

223 THR N	8.36	35.62	-16.84	11.84
223 THR CA	9.54	35.78	-17.68	11.67
223 THR CB	10.85	35.20	-17.06	11.61
223 THR OG1	10.72	33.79	-16.86	11.66
223 THR CG2	11.19	35.89	-15.75	11.56
223 THR C	9.21	34.99	-18.93	11.60
223 THR O	8.74	33.85	-18.84	11.61
224 SER N	9.43	35.59	-20.10	11.51
224 SER CA	9.14	34.91	-21.35	11.46
224 SER CB	9.32	35.87	-22.53	11.65
224 SER OG	8.30	36.85	-22.53	11.85
224 SER C	10.05	33.69	-21.54	11.33
224 SER O	9.62	32.70	-22.12	11.25
225 ASP N	11.28	33.76	-21.04	11.20
225 ASP CA	12.18	32.63	-21.19	11.05
225 ASP CB	13.66	33.07	-21.21	11.01
225 ASP CG	14.11	33.72	-19.92	11.17
225 ASP OD1	13.38	33.67	-18.91	11.02
225 ASP OD2	15.23	34.28	-19.91	11.24
225 ASP C	11.95	31.58	-20.11	10.92
225 ASP O	12.68	30.59	-20.02	10.88
226 LYS N	10.92	31.79	-19.30	10.88
226 LYS CA	10.56	30.86	-18.24	10.78
226 LYS CB	9.94	29.60	-18.85	11.09
226 LYS CG	8.62	29.89	-19.56	11.51
226 LYS CD	8.09	28.68	-20.31	12.10
226 LYS CE	6.72	28.98	-20.89	12.39
226 LYS NZ	6.71	30.30	-21.59	12.93
226 LYS C	11.73	30.48	-17.33	10.60
226 LYS O	11.92	29.31	-17.00	10.56
227 SER N	12.49	31.49	-16.93	10.51
227 SER CA	13.63	31.27	-16.04	10.35
227 SER CB	14.41	32.57	-15.82	10.72
227 SER OG	15.10	32.98	-17.00	11.09
227 SER C	13.07	30.81	-14.70	10.05
227 SER O	11.88	30.98	-14.43	10.07
228 PHE N	13.93	30.23	-13.87	9.79
228 PHE CA	13.52	29.82	-12.54	9.55
228 PHE CB	14.26	28.54	-12.12	9.79
228 PHE CG	14.03	27.39	-13.06	9.98
228 PHE CD1	12.77	27.15	-13.58	10.13
228 PHE CD2	15.07	26.55	-13.42	10.18
228 PHE CE1	12.54	26.09	-14.46	10.28

228	PHE	CE2	14.86	25.48	-14.30	10.25
228	PHE	CZ	13.59	25.26	-14.82	10.31
228	PHE	C	13.93	30.96	-11.63	9.31
228	PHE	O	15.10	31.32	-11.56	9.16
229	VAL	N	12.96	31.55	-10.95	9.25
229	VAL	CA	13.23	32.68	-10.08	9.07
229	VAL	CB	12.51	33.95	-10.59	9.03
229	VAL	CG1	12.83	35.13	-9.68	9.02
229	VAL	CG2	12.95	34.24	-12.02	9.11
229	VAL	C	12.76	32.39	-8.66	8.93
229	VAL	O	11.67	31.86	-8.46	9.04
230	ALA	N	13.59	32.73	-7.68	8.78
230	ALA	CA	13.24	32.51	-6.29	8.62
230	ALA	CB	14.18	31.47	-5.65	8.70
230	ALA	C	13.30	33.81	-5.50	8.54
230	ALA	O	14.19	34.64	-5.72	8.52
231	GLN	N	12.35	33.98	-4.59	8.47
231	GLN	CA	12.27	35.15	-3.72	8.45
231	GLN	CB	10.95	35.90	-3.98	8.54
231	GLN	CG	10.79	37.23	-3.22	8.84
231	GLN	CD	9.45	37.36	-2.47	9.00
231	GLN	OE1	8.90	38.46	-2.34	9.22
231	GLN	NE2	8.94	36.24	-1.97	8.95
231	GLN	C	12.28	34.71	-2.26	8.39
231	GLN	O	11.85	33.60	-1.93	8.20
232	ILE	N	12.80	35.58	-1.40	8.41
232	ILE	CA	12.82	35.38	0.05	8.44
232	ILE	CB	14.21	34.94	0.61	8.55
232	ILE	CG2	14.21	35.04	2.14	8.79
232	ILE	CG1	14.53	33.50	0.20	8.88
232	ILE	CD1	13.52	32.47	0.70	9.18
232	ILE	C	12.54	36.80	0.55	8.25
232	ILE	O	13.28	37.72	0.23	8.25
233	GLU	N	11.46	36.98	1.30	8.17
233	GLU	CA	11.14	38.30	1.80	8.10
233	GLU	CB	9.95	38.88	1.03	8.32
233	GLU	CG	9.37	40.17	1.61	8.52
233	GLU	CD	8.23	40.73	0.77	8.67
233	GLU	OE1	7.42	39.92	0.27	8.77
233	GLU	OE2	8.14	41.97	0.61	8.88
233	GLU	C	10.82	38.29	3.29	8.00
233	GLU	O	10.18	37.37	3.81	7.98
234	HIS	N	11.30	39.33	3.98	8.06

234 HIS CA	11.06	39.48	5.40	8.07
234 HIS CB	12.26	38.97	6.21	8.29
234 HIS CG	12.23	37.49	6.47	8.34
234 HIS CD2	13.01	36.48	6.00	8.48
234 HIS ND1	11.31	36.90	7.31	8.45
234 HIS CE1	11.52	35.60	7.35	8.52
234 HIS NE2	12.55	35.32	6.56	8.49
234 HIS C	10.87	40.96	5.68	8.05
234 HIS O	11.41	41.82	4.98	7.87
235 THR N	10.07	41.24	6.70	8.21
235 THR CA	9.85	42.62	7.13	8.40
235 THR CB	8.43	42.84	7.64	8.25
235 THR OG1	7.51	42.74	6.54	8.13
235 THR CG2	8.29	44.23	8.27	8.27
235 THR C	10.89	42.79	8.23	8.49
235 THR O	10.95	42.00	9.17	8.42
236 VAL N	11.71	43.83	8.07	8.84
236 VAL CA	12.81	44.11	8.98	9.36
236 VAL CB	14.14	44.00	8.21	9.30
236 VAL CG1	15.31	44.22	9.15	9.41
236 VAL CG2	14.23	42.64	7.53	9.40
236 VAL C	12.76	45.48	9.63	9.38
236 VAL O	12.31	46.44	9.01	9.51
237 ILE N	13.20	45.56	10.88	9.82
237 ILE CA	13.26	46.83	11.58	10.45
237 ILE CB	12.45	46.80	12.89	10.41
237 ILE CG2	12.44	48.20	13.51	10.29
237 ILE CG1	11.01	46.36	12.60	10.51
237 ILE CD1	10.11	46.32	13.83	10.86
237 ILE C	14.73	47.06	11.89	10.59
237 ILE O	15.41	46.18	12.42	10.62
238 VAL N	15.23	48.24	11.52	11.06
238 VAL CA	16.62	48.62	11.75	11.85
238 VAL CB	17.07	49.73	10.77	11.74
238 VAL CG1	18.55	50.04	10.97	11.75
238 VAL CG2	16.80	49.32	9.34	11.79
238 VAL C	16.78	49.13	13.18	12.12
238 VAL O	16.14	50.11	13.56	12.18
239 THR N	17.62	48.47	13.96	12.65
239 THR CA	17.87	48.89	15.34	13.26
239 THR CB	17.19	47.95	16.37	13.14
239 THR OG1	18.07	46.87	16.69	13.43
239 THR CG2	15.89	47.40	15.81	13.31

239 THR C	19.37	48.89	15.62	13.46
239 THR O	20.14	48.22	14.94	13.46
240 LYS N	19.77	49.66	16.62	13.89
240 LYS CA	21.18	49.78	16.98	14.34
240 LYS CB	21.34	50.83	18.09	14.50
240 LYS CG	20.42	50.63	19.29	14.82
240 LYS CD	20.43	51.86	20.21	15.14
240 LYS CE	19.52	51.66	21.42	15.34
240 LYS NZ	18.12	51.27	21.03	15.57
240 LYS C	21.76	48.45	17.44	14.50
240 LYS O	22.98	48.24	17.38	14.60
241 ASP N	20.89	47.55	17.89	14.69
241 ASP CA	21.33	46.25	18.38	14.83
241 ASP CB	20.56	45.89	19.65	15.16
241 ASP CG	20.86	46.83	20.80	15.41
241 ASP OD1	22.05	47.14	21.00	15.60
241 ASP OD2	19.91	47.26	21.48	15.65
241 ASP C	21.18	45.14	17.35	14.72
241 ASP O	21.29	43.95	17.68	14.88
242 GLY N	20.95	45.52	16.10	14.47
242 GLY CA	20.79	44.53	15.06	14.18
242 GLY C	19.38	44.53	14.49	13.89
242 GLY O	18.43	44.94	15.17	13.91
243 PRO N	19.21	44.07	13.24	13.59
243 PRO CD	20.24	43.60	12.31	13.53
243 PRO CA	17.89	44.03	12.62	13.37
243 PRO CB	18.20	43.65	11.18	13.32
243 PRO CG	19.43	42.81	11.31	13.44
243 PRO C	16.91	43.07	13.28	13.02
243 PRO O	17.28	41.98	13.73	13.03
244 ILE N	15.65	43.48	13.34	12.67
244 ILE CA	14.60	42.67	13.91	12.43
244 ILE CB	13.73	43.48	14.89	12.43
244 ILE CG2	12.57	42.64	15.38	12.42
244 ILE CG1	14.58	43.98	16.05	12.52
244 ILE CD1	13.78	44.68	17.14	12.70
244 ILE C	13.71	42.20	12.77	12.09
244 ILE O	13.16	43.02	12.04	12.05
245 LEU N	13.60	40.89	12.60	11.88
245 LEU CA	12.74	40.35	11.55	11.62
245 LEU CB	13.35	39.08	10.95	11.62
245 LEU CG	14.42	39.27	9.87	11.75
245 LEU CD1	15.54	40.16	10.39	11.78

245 LEU CD2	14.97	37.91	9.46	11.77
245 LEU C	11.39	40.02	12.18	11.39
245 LEU O	11.27	39.05	12.93	11.43
246 THR N	10.38	40.83	11.88	11.22
246 THR CA	9.06	40.59	12.45	11.08
246 THR CB	8.13	41.80	12.23	10.99
246 THR OG1	7.85	41.93	10.84	10.89
246 THR CG2	8.80	43.09	12.72	10.94
246 THR C	8.41	39.36	11.85	10.92
246 THR O	7.53	38.76	12.46	10.84
247 THR N	8.87	38.96	10.66	11.03
247 THR CA	8.30	37.81	9.96	11.10
247 THR CB	8.09	38.14	8.48	10.97
247 THR OG1	9.31	38.63	7.92	10.93
247 THR CG2	7.00	39.20	8.32	10.94
247 THR C	9.11	36.52	10.08	11.25
247 THR O	8.92	35.59	9.29	11.08
248 LYS N	10.00	36.48	11.06	11.62
248 LYS CA	10.81	35.29	11.30	12.10
248 LYS CB	12.30	35.65	11.38	12.27
248 LYS CG	13.18	34.46	11.71	12.62
248 LYS CD	14.62	34.87	11.96	13.00
248 LYS CE	15.45	33.67	12.36	13.30
248 LYS NZ	16.85	34.08	12.68	13.72
248 LYS C	10.36	34.70	12.62	12.35
248 LYS O	10.33	35.39	13.64	12.36
249 ILE N	9.98	33.42	12.60	12.68
249 ILE CA	9.54	32.72	13.80	13.06
249 ILE CB	8.29	31.85	13.52	12.88
249 ILE CG2	8.01	30.93	14.71	12.97
249 ILE CG1	7.08	32.73	13.25	12.80
249 ILE CD1	5.84	31.95	12.85	12.43
249 ILE C	10.67	31.81	14.27	13.35
249 ILE O	11.13	30.99	13.45	13.62
249 ILE OT	11.07	31.93	15.45	13.77
301 HOH O	10.52	34.41	4.34	9.04
302 HOH O	5.68	43.84	10.75	7.39
303 HOH O	-1.54	38.06	1.99	12.17
304 HOH O	9.58	31.37	-7.05	11.42
305 HOH O	3.84	35.16	-5.21	13.13
306 HOH O	15.54	21.70	-8.21	11.28
307 HOH O	1.27	24.06	-11.29	10.96
308 HOH O	2.83	15.97	-9.91	13.21

309	HOH	O	7.75	29.41	5.29	11.48
310	HOH	O	0.00	23.10	6.79	13.97
311	HOH	O	15.64	45.67	-8.01	12.06
312	HOH	O	9.80	28.82	-15.22	13.56
313	HOH	O	17.62	39.52	-19.14	15.74
314	HOH	O	-0.83	44.37	14.52	11.62
315	HOH	O	-0.42	38.31	20.32	14.43
316	HOH	O	-1.83	34.36	-12.10	11.01
317	HOH	O	19.18	48.28	-2.44	14.08
318	HOH	O	-0.15	30.63	-9.41	14.58
319	HOH	O	1.31	39.36	-0.48	15.80
320	HOH	O	17.43	50.70	-3.01	11.91
321	HOH	O	16.96	43.75	-2.50	15.47
322	HOH	O	27.70	32.63	-2.22	17.18
323	HOH	O	7.13	38.87	15.05	13.04
324	HOH	O	6.69	25.10	6.71	15.96
325	HOH	O	12.13	26.59	2.42	16.87
326	HOH	O	9.11	23.19	1.27	16.15
327	HOH	O	12.01	32.52	8.22	15.82
328	HOH	O	-10.14	24.71	0.78	18.07
329	HOH	O	10.19	30.74	-11.11	12.76
330	HOH	O	27.52	34.99	-0.31	22.73
331	HOH	O	25.00	45.61	-8.38	15.19
332	HOH	O	-1.54	30.46	-12.60	15.24
333	HOH	O	19.47	56.55	13.08	16.06
334	HOH	O	-8.38	38.74	4.73	12.15
335	HOH	O	-6.73	18.96	-3.18	15.71
336	HOH	O	-10.97	34.30	0.08	13.27
337	HOH	O	21.12	50.41	-4.73	16.42
338	HOH	O	21.28	28.77	1.36	19.93
339	HOH	O	21.90	54.50	-0.49	15.36
340	HOH	O	6.31	38.98	-4.46	15.11
341	HOH	O	0.28	47.87	20.07	17.85
342	HOH	O	10.30	52.79	6.53	13.97
343	HOH	O	21.05	22.71	-6.43	18.60
344	HOH	O	24.76	54.33	-3.46	17.89
345	HOH	O	8.27	55.29	6.13	17.47
346	HOH	O	14.63	39.13	14.67	17.13
347	HOH	O	26.93	45.54	0.58	16.06
348	HOH	O	22.00	40.33	-12.38	18.56
349	HOH	O	22.94	37.71	8.22	17.56
350	HOH	O	-9.57	25.12	-6.14	17.84
351	HOH	O	14.01	37.19	-21.87	21.98

352	HOH	O	4.97	28.02	11.97	18.66
353	HOH	O	-5.14	33.79	-15.46	19.79
354	HOH	O	0.89	27.80	-16.88	20.55
355	HOH	O	0.04	44.37	19.31	19.74
356	HOH	O	-3.82	23.00	-13.39	19.63
357	HOH	O	-5.33	28.61	-13.52	20.29
358	HOH	O	-1.83	19.71	1.80	18.07
359	HOH	O	6.32	20.97	-0.93	18.32
360	HOH	O	27.95	42.43	-8.15	16.27
361	HOH	O	-12.42	27.09	-2.81	19.70
362	HOH	O	6.92	56.74	10.12	19.28
363	HOH	O	4.38	48.07	26.38	17.88
364	HOH	O	19.09	59.51	4.00	22.51
365	HOH	O	0.29	20.44	5.95	21.11
366	HOH	O	22.32	49.11	4.73	22.73
367	HOH	O	-7.96	33.86	-5.80	15.94
368	HOH	O	10.38	12.96	-7.37	19.87
369	HOH	O	10.83	20.64	-13.14	20.14
370	HOH	O	14.02	19.19	-4.63	17.34
371	HOH	O	27.65	28.59	-6.88	22.89
372	HOH	O	-6.46	47.08	10.42	18.12
373	HOH	O	-10.07	39.53	10.48	21.30
374	HOH	O	26.55	63.94	0.02	19.49
375	HOH	O	3.08	24.90	9.68	23.60
376	HOH	O	-2.68	51.64	4.49	18.77
377	HOH	O	13.98	54.38	-2.78	20.57
378	HOH	O	6.01	26.98	-17.07	18.20
379	HOH	O	10.76	28.22	8.28	21.31
380	HOH	O	7.21	21.14	-12.51	22.12
381	HOH	O	-0.01	47.70	24.74	20.57
382	HOH	O	26.14	36.21	-13.19	18.02
383	HOH	O	8.71	24.35	-14.71	17.36
384	HOH	O	-1.02	26.70	-15.46	21.86
385	HOH	O	11.63	19.79	-2.08	20.87
386	HOH	O	24.46	45.23	4.56	21.68
387	HOH	O	-10.35	35.86	6.34	17.79
388	HOH	O	9.16	13.56	-4.09	24.33
389	HOH	O	14.88	29.32	2.52	23.60
390	HOH	O	7.93	59.35	12.82	21.92
391	HOH	O	-0.39	23.55	11.16	24.02
392	HOH	O	-12.19	39.32	7.34	20.29
393	HOH	O	4.62	40.47	-21.40	20.86
394	HOH	O	10.83	29.71	6.02	18.68

395	HOH	O	24.32	29.38	-12.36	22.37
396	HOH	O	28.11	43.37	-0.40	21.07
397	HOH	O	-6.47	51.51	11.11	21.48
398	HOH	O	-13.50	29.57	1.74	21.65
399	HOH	O	19.82	47.00	12.43	19.88
400	HOH	O	4.96	19.65	5.04	23.26
401	HOH	O	20.66	22.51	-14.45	21.14
402	HOH	O	23.27	50.91	-11.12	19.97
403	HOH	O	24.73	27.34	-2.60	22.99
404	HOH	O	10.48	25.34	-17.84	20.43
405	HOH	O	12.29	57.56	5.75	21.45
406	HOH	O	4.36	24.78	-15.46	23.33
407	HOH	O	27.81	38.95	4.53	25.57
408	HOH	O	16.80	29.38	-17.21	18.25
409	HOH	O	11.24	56.92	-1.08	23.15
410	HOH	O	27.14	41.96	3.63	19.44
411	HOH	O	8.80	44.92	-17.88	21.62
412	HOH	O	7.99	47.13	-4.60	21.32
413	HOH	O	4.03	21.88	-13.51	21.83
414	HOH	O	10.11	30.56	-23.57	19.04
415	HOH	O	2.49	20.92	9.21	23.07
416	HOH	O	-3.68	18.23	-0.95	23.22
417	HOH	O	2.21	18.16	2.62	24.12
418	HOH	O	-7.20	45.05	12.15	17.72
419	HOH	O	3.33	30.32	-20.15	23.20
420	HOH	O	-10.10	21.91	-7.96	24.45
421	HOH	O	6.20	32.93	-19.28	20.30
422	HOH	O	26.47	50.59	-1.04	20.30
423	HOH	O	4.73	12.67	-7.41	20.45
424	HOH	O	30.96	47.29	7.54	23.26
425	HOH	O	5.48	21.45	8.98	23.62
426	HOH	O	7.63	53.70	24.03	20.67
427	HOH	O	24.84	33.85	3.40	19.47
428	HOH	O	-6.35	22.25	2.44	21.89
429	HOH	O	14.70	22.58	-16.76	21.77
430	HOH	O	3.75	54.62	-2.08	23.59
431	HOH	O	22.02	24.22	-11.35	20.43
432	HOH	O	-3.17	29.64	-17.10	24.33
433	HOH	O	13.43	57.79	1.30	20.34
434	HOH	O	12.73	49.05	18.00	22.94
435	HOH	O	-1.86	47.35	18.38	20.80
436	HOH	O	-8.80	32.90	-9.68	22.48
437	HOH	O	7.68	56.75	-0.80	23.53

438	HOH	O	2.12	54.11	19.73	20.27
439	HOH	O	20.02	27.96	5.22	22.64
440	HOH	O	27.87	54.67	-2.71	21.05
441	HOH	O	5.68	17.32	-1.75	21.40
442	HOH	O	-2.40	21.46	9.46	25.37
443	HOH	O	14.70	33.35	6.08	20.03
444	HOH	O	9.71	29.38	10.63	15.52
445	HOH	O	24.87	51.89	13.40	19.22
446	HOH	O	26.44	38.92	-13.22	22.46
447	HOH	O	25.13	34.40	7.66	23.31
448	HOH	O	26.10	25.40	-8.41	22.30
449	HOH	O	25.14	25.44	-5.06	23.19
450	HOH	O	8.38	17.72	-15.21	23.09
451	HOH	O	22.19	29.97	-15.30	23.57
452	HOH	O	18.33	34.74	-23.33	24.25
453	HOH	O	10.42	50.74	19.99	23.68
454	HOH	O	3.82	37.92	-5.15	11.14
455	HOH	O	2.27	13.52	-8.36	12.29
456	HOH	O	-2.78	30.00	-9.48	13.74
457	HOH	O	-9.55	38.20	7.08	17.08
458	HOH	O	-3.75	32.18	-11.75	14.53
459	HOH	O	19.30	52.33	-4.24	16.15
460	HOH	O	13.16	27.86	0.31	14.90
461	HOH	O	8.48	26.74	-16.17	16.16
462	HOH	O	-9.40	32.09	-0.23	14.19
463	HOH	O	14.64	44.03	-1.79	12.77
464	HOH	O	26.82	44.37	-6.48	10.19
465	HOH	O	-1.79	44.63	17.17	17.83
466	HOH	O	9.95	34.41	-7.10	16.75
467	HOH	O	1.11	22.95	9.12	20.95
468	HOH	O	12.16	38.23	-18.69	15.18
469	HOH	O	7.37	23.04	5.01	18.28
470	HOH	O	-11.15	38.22	12.41	20.33
471	HOH	O	28.61	30.24	-0.81	17.78
472	HOH	O	-0.96	26.32	11.35	20.16
473	HOH	O	24.13	38.95	-11.62	18.68
474	HOH	O	4.45	14.71	-12.00	19.97
475	HOH	O	-0.69	18.90	4.10	19.92
476	HOH	O	6.05	24.26	8.94	23.08
477	HOH	O	-8.40	22.26	-10.37	18.50
478	HOH	O	-3.90	21.03	3.27	19.43
479	HOH	O	-9.00	28.94	-12.03	19.69
480	HOH	O	5.72	43.88	-19.58	21.53

481	HOH	O	-10.34	40.76	3.80	19.91
482	HOH	O	4.65	19.40	-14.69	21.72
483	HOH	O	14.18	31.10	4.58	21.73
484	HOH	O	30.32	41.65	-7.82	19.22
485	HOH	O	21.32	35.97	9.01	20.31
486	HOH	O	4.48	29.50	16.49	20.31
487	HOH	O	29.18	37.40	0.15	19.97
488	HOH	O	20.08	54.41	17.08	21.63
489	HOH	O	15.85	30.46	-19.41	20.67
490	HOH	O	20.53	60.95	2.00	16.09
491	HOH	O	23.10	22.71	-8.27	21.27
492	HOH	O	-4.11	51.39	-1.95	22.75
493	HOH	O	-11.18	28.95	3.76	20.88
494	HOH	O	7.02	22.64	-15.50	20.80
253	ZN2	ZN	7.01	43.39	-0.45	14.29
254	ZN2	ZN	5.57	40.37	-0.35	13.09

Table II

Provides a three dimensional protein coordinate set of a *S. aureus* methionine aminopeptidase crystalline structure of an inhibitor complex with 5-(3-Iodo-phenyl)-1-H-[1,2,3]triazole.

Residue	Atom	X	Y	Z	B
1	MET	CB	6.21	53.26	9.50	19.23
1	MET	CG	6.45	52.04	10.38	19.33
1	MET	SD	5.09	51.62	11.50	19.46
1	MET	CE	5.33	52.85	12.79	19.56
1	MET	C	8.65	53.68	9.58	19.14
1	MET	O	9.57	52.88	9.43	19.09
1	MET	N	7.67	52.67	7.58	19.08
1	MET	CA	7.43	53.66	8.67	19.14
2	ILE	N	8.64	54.61	10.53	19.17
2	ILE	CA	9.72	54.73	11.50	19.25
2	ILE	CB	10.30	56.16	11.56	19.26
2	ILE	CG2	11.43	56.21	12.59	19.29
2	ILE	CG1	10.81	56.58	10.18	19.29
2	ILE	CD1	11.96	55.74	9.67	19.29
2	ILE	C	9.14	54.40	12.87	19.27
2	ILE	O	8.24	55.10	13.34	19.28
3	VAL	N	9.63	53.34	13.49	19.35

3 VAL CA	9.14	52.94	14.81	19.44
3 VAL CB	9.62	51.52	15.18	19.43
3 VAL CG1	9.22	51.19	16.61	19.46
3 VAL CG2	9.04	50.51	14.21	19.46
3 VAL C	9.63	53.91	15.88	19.52
3 VAL O	10.82	54.15	16.01	19.54
4 LYS N	8.69	54.46	16.64	19.62
4 LYS CA	9.03	55.40	17.70	19.71
4 LYS CB	8.34	56.75	17.45	19.88
4 LYS CG	8.73	57.46	16.16	20.17
4 LYS CD	10.09	58.16	16.26	20.41
4 LYS CE	11.25	57.20	16.09	20.58
4 LYS NZ	12.56	57.91	16.16	20.77
4 LYS C	8.60	54.88	19.07	19.68
4 LYS O	9.24	55.18	20.08	19.72
5 THR N	7.53	54.09	19.11	19.59
5 THR CA	7.03	53.57	20.38	19.50
5 THR CB	5.61	54.09	20.67	19.53
5 THR OG1	4.67	53.41	19.82	19.54
5 THR CG2	5.52	55.59	20.39	19.53
5 THR C	6.98	52.05	20.52	19.43
5 THR O	6.99	51.32	19.53	19.44
6 GLU N	6.91	51.60	21.76	19.31
6 GLU CA	6.84	50.18	22.09	19.16
6 GLU CB	6.88	50.01	23.62	19.39
6 GLU CG	6.60	48.60	24.14	19.71
6 GLU CD	7.64	47.58	23.73	19.87
6 GLU OE1	8.83	47.95	23.63	20.04
6 GLU OE2	7.28	46.40	23.53	20.01
6 GLU C	5.55	49.59	21.53	18.92
6 GLU O	5.53	48.45	21.07	18.90
7 GLU N	4.47	50.37	21.57	18.58
7 GLU CA	3.18	49.92	21.06	18.24
7 GLU CB	2.10	50.97	21.36	18.47
7 GLU CG	1.70	51.09	22.83	18.77
7 GLU CD	2.82	51.62	23.71	18.95
7 GLU OE1	3.53	52.57	23.31	19.05
7 GLU OE2	2.98	51.09	24.84	19.23
7 GLU C	3.24	49.66	19.55	17.81
7 GLU O	2.63	48.72	19.05	17.76
8 GLU N	3.97	50.50	18.83	17.30
8 GLU CA	4.10	50.33	17.39	16.78
8 GLU CB	4.81	51.53	16.76	16.90

8 GLU CG	4.07	52.84	16.93	17.05
8 GLU CD	4.83	54.03	16.36	17.13
8 GLU OE1	6.07	54.05	16.49	17.26
8 GLU OE2	4.18	54.95	15.81	17.30
8 GLU C	4.90	49.06	17.12	16.32
8 GLU O	4.57	48.27	16.23	16.25
9 LEU N	5.95	48.86	17.91	15.83
9 LEU CA	6.80	47.68	17.78	15.30
9 LEU CB	7.94	47.73	18.80	15.39
9 LEU CG	8.87	46.51	18.84	15.42
9 LEU CD1	9.53	46.28	17.49	15.48
9 LEU CD2	9.92	46.71	19.92	15.51
9 LEU C	5.97	46.41	17.98	14.95
9 LEU O	6.10	45.46	17.22	14.78
10 GLN N	5.14	46.42	19.02	14.50
10 GLN CA	4.30	45.27	19.32	14.04
10 GLN CB	3.58	45.49	20.65	14.12
10 GLN CG	4.53	45.54	21.84	14.31
10 GLN CD	3.84	45.99	23.11	14.39
10 GLN OE1	2.64	46.24	23.13	14.55
10 GLN NE2	4.62	46.09	24.19	14.46
10 GLN C	3.29	45.01	18.20	13.72
10 GLN O	3.04	43.86	17.84	13.59
11 ALA N	2.71	46.07	17.66	13.26
11 ALA CA	1.75	45.92	16.59	12.85
11 ALA CB	1.16	47.27	16.22	12.91
11 ALA C	2.42	45.28	15.37	12.60
11 ALA O	1.85	44.41	14.72	12.49
12 LEU N	3.64	45.72	15.07	12.27
12 LEU CA	4.38	45.18	13.92	11.98
12 LEU CB	5.63	46.03	13.65	12.00
12 LEU CG	5.32	47.44	13.14	12.01
12 LEU CD1	6.56	48.31	13.23	12.05
12 LEU CD2	4.82	47.36	11.70	12.04
12 LEU C	4.77	43.72	14.15	11.78
12 LEU O	4.73	42.90	13.23	11.73
13 LYS N	5.14	43.40	15.38	11.61
13 LYS CA	5.52	42.03	15.71	11.46
13 LYS CB	6.13	41.96	17.11	11.73
13 LYS CG	7.51	42.58	17.20	12.09
13 LYS CD	8.05	42.46	18.61	12.47
13 LYS CE	9.50	42.88	18.69	12.78
13 LYS NZ	10.04	42.64	20.06	13.07

13 LYS C	4.31	41.11	15.62	11.20
13 LYS O	4.42	39.95	15.21	11.18
14 GLU N	3.15	41.63	16.01	10.92
14 GLU CA	1.91	40.85	15.97	10.59
14 GLU CB	0.75	41.67	16.56	10.78
14 GLU CG	-0.64	41.05	16.39	10.96
14 GLU CD	-0.84	39.79	17.21	11.11
14 GLU OE1	0.06	39.40	17.98	11.34
14 GLU OE2	-1.93	39.18	17.08	11.36
14 GLU C	1.56	40.45	14.54	10.33
14 GLU O	1.42	39.26	14.24	10.20
15 ILE N	1.44	41.43	13.65	10.01
15 ILE CA	1.09	41.13	12.26	9.77
15 ILE CB	0.70	42.44	11.50	9.70
15 ILE CG2	1.89	43.38	11.41	9.67
15 ILE CG1	0.17	42.10	10.10	9.57
15 ILE CD1	-1.07	41.23	10.11	9.36
15 ILE C	2.21	40.37	11.54	9.65
15 ILE O	1.95	39.58	10.63	9.68
16 GLY N	3.46	40.59	11.97	9.53
16 GLY CA	4.57	39.87	11.37	9.25
16 GLY C	4.47	38.39	11.71	9.14
16 GLY O	4.71	37.53	10.86	8.92
17 TYR N	4.13	38.09	12.96	9.12
17 TYR CA	3.99	36.70	13.38	9.13
17 TYR CB	3.66	36.61	14.88	9.34
17 TYR CG	3.26	35.22	15.29	9.68
17 TYR CD1	4.21	34.22	15.46	9.90
17 TYR CE1	3.83	32.91	15.74	10.16
17 TYR CD2	1.91	34.87	15.40	9.92
17 TYR CE2	1.51	33.56	15.68	10.14
17 TYR CZ	2.49	32.58	15.84	10.18
17 TYR OH	2.12	31.27	16.08	10.55
17 TYR C	2.87	36.03	12.60	8.95
17 TYR O	3.02	34.90	12.12	8.87
18 ILE N	1.74	36.73	12.47	8.81
18 ILE CA	0.60	36.20	11.74	8.65
18 ILE CB	-0.57	37.22	11.76	8.59
18 ILE CG2	-1.68	36.77	10.81	8.56
18 ILE CG1	-1.11	37.35	13.19	8.62
18 ILE CD1	-2.17	38.43	13.36	8.71
18 ILE C	0.97	35.87	10.30	8.59
18 ILE O	0.64	34.80	9.79	8.55

	19 CYS N	1.69	36.78	9.65	8.55
	19 CYS CA	2.07	36.52	8.27	8.47
	19 CYS CB	2.67	37.78	7.63	8.47
	19 CYS SG	1.39	39.01	7.25	8.50
5	19 CYS C	3.04	35.35	8.16	8.50
	19 CYS O	2.96	34.55	7.22	8.51
	20 ALA N	3.96	35.24	9.13	8.51
	20 ALA CA	4.92	34.14	9.13	8.54
	20 ALA CB	5.96	34.38	10.23	8.61
10	20 ALA C	4.20	32.81	9.36	8.66
	20 ALA O	4.50	31.81	8.71	8.52
	21 LYS N	3.25	32.82	10.28	8.77
	21 LYS CA	2.48	31.61	10.59	9.01
	21 LYS CB	1.50	31.90	11.73	9.34
15	21 LYS CG	0.59	30.73	12.11	10.01
	21 LYS CD	1.38	29.55	12.63	10.53
	21 LYS CE	0.44	28.50	13.22	10.90
	21 LYS NZ	1.13	27.23	13.58	11.29
	21 LYS C	1.73	31.15	9.35	8.95
20	21 LYS O	1.70	29.96	9.02	9.02
	22 VAL N	1.11	32.10	8.65	8.94
	22 VAL CA	0.36	31.78	7.44	8.95
	22 VAL CB	-0.40	33.03	6.93	8.97
	22 VAL CG1	-0.97	32.79	5.53	8.97
25	22 VAL CG2	-1.53	33.35	7.89	9.01
	22 VAL C	1.30	31.25	6.35	8.96
	22 VAL O	1.02	30.25	5.70	8.97
	23 ARG N	2.44	31.92	6.17	8.93
	23 ARG CA	3.42	31.50	5.18	8.94
30	23 ARG CB	4.62	32.45	5.23	8.90
	23 ARG CG	5.67	32.23	4.16	8.91
	23 ARG CD	6.96	32.89	4.60	8.94
	23 ARG NE	7.46	32.22	5.80	8.98
	23 ARG CZ	7.99	32.83	6.86	8.98
35	23 ARG NH1	8.12	34.16	6.88	8.99
	23 ARG NH2	8.38	32.11	7.90	8.95
	23 ARG C	3.88	30.07	5.45	9.00
	23 ARG O	3.91	29.23	4.54	9.00
	24 ASN N	4.23	29.78	6.70	9.15
40	24 ASN CA	4.69	28.44	7.05	9.21
	24 ASN CB	5.13	28.37	8.52	9.46
	24 ASN CG	6.39	29.16	8.79	9.66
	24 ASN OD1	7.17	29.45	7.89	9.82

24 ASN ND2	6.60	29.50	10.06	9.94
24 ASN C	3.62	27.38	6.82	9.27
24 ASN O	3.92	26.30	6.31	9.24
25 THR N	2.39	27.68	7.22	9.27
25 THR CA	1.29	26.74	7.08	9.30
25 THR CB	0.01	27.28	7.76	9.36
25 THR OG1	0.31	27.61	9.13	9.55
25 THR CG2	-1.09	26.22	7.76	9.41
25 THR C	1.03	26.44	5.60	9.35
25 THR O	0.87	25.28	5.21	9.34
26 MET N	1.01	27.48	4.78	9.38
26 MET CA	0.79	27.30	3.35	9.43
26 MET CB	0.66	28.66	2.66	9.32
26 MET CG	-0.65	29.37	2.96	9.07
26 MET SD	-0.73	31.04	2.29	8.85
26 MET CE	-1.03	30.69	0.55	8.82
26 MET C	1.93	26.49	2.72	9.62
26 MET O	1.68	25.58	1.92	9.69
27 GLN N	3.17	26.81	3.06	9.86
27 GLN CA	4.29	26.06	2.50	10.12
27 GLN CB	5.62	26.63	3.00	10.25
27 GLN CG	6.83	25.82	2.53	10.36
27 GLN CD	8.15	26.48	2.87	10.53
27 GLN OE1	8.20	27.44	3.63	10.60
27 GLN NE2	9.23	25.96	2.30	10.56
27 GLN C	4.20	24.58	2.87	10.33
27 GLN O	4.41	23.70	2.03	10.33
28 ALA N	3.89	24.30	4.13	10.50
28 ALA CA	3.79	22.93	4.61	10.78
28 ALA CB	3.52	22.91	6.10	10.75
28 ALA C	2.70	22.15	3.88	10.99
28 ALA O	2.80	20.93	3.73	11.11
29 ALA N	1.66	22.86	3.44	11.17
29 ALA CA	0.54	22.24	2.75	11.29
29 ALA CB	-0.74	23.02	3.05	11.35
29 ALA C	0.72	22.12	1.24	11.43
29 ALA O	-0.10	21.52	0.55	11.44
30 THR N	1.80	22.70	0.73	11.52
30 THR CA	2.06	22.65	-0.70	11.67
30 THR CB	2.98	23.80	-1.14	11.62
30 THR OG1	2.42	25.06	-0.74	11.60
30 THR CG2	3.12	23.81	-2.65	11.57
30 THR C	2.65	21.31	-1.11	11.87

30 THR O	3.82	21.02	-0.86	11.99
31 LYS N	1.82	20.48	-1.74	11.99
31 LYS CA	2.21	19.15	-2.18	12.15
31 LYS CB	1.71	18.12	-1.17	12.43
31 LYS CG	0.21	18.19	-0.96	12.97
31 LYS CD	-0.33	17.17	0.04	13.38
31 LYS CE	-0.41	15.78	-0.55	13.70
31 LYS NZ	-1.09	14.84	0.38	13.97
31 LYS C	1.54	18.89	-3.52	12.07
31 LYS O	0.58	19.57	-3.88	11.94
32 PRO N	2.05	17.91	-4.28	12.10
32 PRO CD	3.26	17.10	-4.08	12.06
32 PRO CA	1.42	17.61	-5.58	12.11
32 PRO CB	2.22	16.40	-6.07	12.12
32 PRO CG	3.58	16.63	-5.48	12.06
32 PRO C	-0.05	17.27	-5.34	12.22
32 PRO O	-0.38	16.55	-4.40	12.32
33 GLY N	-0.94	17.79	-6.18	12.33
33 GLY CA	-2.34	17.49	-6.01	12.37
33 GLY C	-3.20	18.57	-5.40	12.38
33 GLY O	-4.43	18.52	-5.51	12.55
34 ILE N	-2.59	19.55	-4.74	12.25
34 ILE CA	-3.37	20.63	-4.15	12.14
34 ILE CB	-2.77	21.09	-2.79	12.07
34 ILE CG2	-1.49	21.86	-3.02	12.01
34 ILE CG1	-3.77	21.97	-2.05	12.05
34 ILE CD1	-3.37	22.28	-0.62	12.08
34 ILE C	-3.37	21.79	-5.14	12.00
34 ILE O	-2.40	21.98	-5.88	12.04
35 THR N	-4.46	22.56	-5.19	11.92
35 THR CA	-4.53	23.70	-6.10	11.90
35 THR CB	-5.96	23.95	-6.59	11.88
35 THR OG1	-6.80	24.28	-5.47	11.85
35 THR CG2	-6.51	22.73	-7.31	11.94
35 THR C	-4.07	24.94	-5.35	11.78
35 THR O	-4.11	24.98	-4.12	11.74
36 THR N	-3.66	25.96	-6.09	11.80
36 THR CA	-3.22	27.18	-5.43	11.82
36 THR CB	-2.53	28.15	-6.42	11.77
36 THR OG1	-3.41	28.45	-7.51	11.73
36 THR CG2	-1.27	27.51	-6.97	11.66
36 THR C	-4.39	27.86	-4.71	11.88
36 THR O	-4.19	28.52	-3.70	11.80

37 LYS N	-5.60	27.66	-5.21	11.99
37 LYS CA	-6.78	28.24	-4.56	12.18
37 LYS CB	-8.04	27.96	-5.38	12.39
37 LYS CG	-9.34	28.44	-4.73	12.76
37 LYS CD	-9.36	29.95	-4.57	13.07
37 LYS CE	-10.66	30.44	-3.94	13.28
37 LYS NZ	-10.66	31.91	-3.75	13.53
37 LYS C	-6.93	27.62	-3.17	12.12
37 LYS O	-7.22	28.31	-2.19	12.14
38 GLU N	-6.75	26.30	-3.08	12.09
38 GLU CA	-6.85	25.61	-1.81	12.08
38 GLU CB	-6.67	24.11	-2.01	12.41
38 GLU CG	-7.87	23.43	-2.62	12.97
38 GLU CD	-7.56	22.00	-2.95	13.28
38 GLU OE1	-6.94	21.76	-4.01	13.62
38 GLU OE2	-7.92	21.11	-2.14	13.67
38 GLU C	-5.82	26.12	-0.81	11.91
38 GLU O	-6.10	26.21	0.38	11.83
39 LEU N	-4.63	26.45	-1.31	11.71
39 LEU CA	-3.59	26.98	-0.45	11.58
39 LEU CB	-2.27	27.06	-1.22	11.48
39 LEU CG	-1.60	25.72	-1.55	11.42
39 LEU CD1	-0.39	25.97	-2.44	11.41
39 LEU CD2	-1.18	25.02	-0.27	11.41
39 LEU C	-4.00	28.36	0.03	11.54
39 LEU O	-3.82	28.70	1.20	11.42
40 ASP N	-4.58	29.15	-0.87	11.58
40 ASP CA	-5.03	30.50	-0.55	11.69
40 ASP CB	-5.56	31.18	-1.81	11.71
40 ASP CG	-5.75	32.68	-1.64	11.73
40 ASP OD1	-4.75	33.37	-1.35	11.76
40 ASP OD2	-6.89	33.17	-1.79	11.87
40 ASP C	-6.12	30.45	0.52	11.76
40 ASP O	-6.22	31.36	1.34	11.76
41 ASN N	-6.92	29.39	0.51	11.94
41 ASN CA	-8.00	29.26	1.48	12.11
41 ASN CB	-8.88	28.04	1.16	12.08
41 ASN CG	-9.75	28.26	-0.06	12.15
41 ASN OD1	-9.97	29.38	-0.49	12.25
41 ASN ND2	-10.27	27.17	-0.61	12.08
41 ASN C	-7.44	29.12	2.89	12.21
41 ASN O	-8.10	29.48	3.87	12.29
42 ILE N	-6.23	28.59	2.99	12.31

42 ILE CA	-5.59	28.44	4.29	12.49
42 ILE CB	-4.25	27.68	4.16	12.45
42 ILE CG2	-3.48	27.75	5.47	12.47
42 ILE CG1	-4.52	26.23	3.77	12.45
42 ILE CD1	-3.26	25.40	3.55	12.39
42 ILE C	-5.35	29.83	4.85	12.64
42 ILE O	-5.60	30.08	6.03	12.59
43 ALA N	-4.89	30.75	4.01	12.86
43 ALA CA	-4.66	32.12	4.46	13.08
43 ALA CB	-3.99	32.94	3.36	13.03
43 ALA C	-5.99	32.76	4.86	13.31
43 ALA O	-6.06	33.47	5.86	13.27
44 LYS N	-7.04	32.51	4.08	13.59
44 LYS CA	-8.34	33.08	4.40	13.91
44 LYS CB	-9.41	32.57	3.42	14.05
44 LYS CG	-10.82	33.11	3.71	14.28
44 LYS CD	-11.85	32.54	2.73	14.54
44 LYS CE	-13.27	32.99	3.06	14.74
44 LYS NZ	-13.48	34.45	2.84	15.04
44 LYS C	-8.73	32.69	5.82	14.13
44 LYS O	-9.10	33.54	6.63	14.12
45 GLU N	-8.65	31.40	6.13	14.37
45 GLU CA	-9.02	30.91	7.45	14.69
45 GLU CB	-8.98	29.39	7.48	15.07
45 GLU CG	-10.02	28.74	6.57	15.74
45 GLU CD	-11.42	29.26	6.82	16.05
45 GLU OE1	-11.90	29.15	7.97	16.40
45 GLU OE2	-12.05	29.77	5.87	16.39
45 GLU C	-8.14	31.47	8.57	14.69
45 GLU O	-8.65	31.93	9.59	14.68
46 LEU N	-6.82	31.43	8.38	14.73
46 LEU CA	-5.92	31.94	9.41	14.79
46 LEU CB	-4.47	31.57	9.09	14.74
46 LEU CG	-4.14	30.07	9.20	14.80
46 LEU CD1	-2.67	29.85	8.87	14.78
46 LEU CD2	-4.45	29.57	10.61	14.81
46 LEU C	-6.04	33.44	9.62	14.78
46 LEU O	-6.02	33.91	10.76	14.79
47 PHE N	-6.18	34.21	8.54	14.85
47 PHE CA	-6.32	35.66	8.70	14.98
47 PHE CB	-6.50	36.37	7.35	14.71
47 PHE CG	-5.22	36.53	6.56	14.45
47 PHE CD1	-3.97	36.55	7.19	14.33

47 PHE CD2	-5.27	36.72	5.18	14.30
47 PHE CE1	-2.80	36.76	6.45	14.26
47 PHE CE2	-4.11	36.92	4.43	14.28
47 PHE CZ	-2.87	36.95	5.07	14.21
47 PHE C	-7.54	35.93	9.59	15.29
47 PHE O	-7.49	36.75	10.50	15.21
48 GLU N	-8.64	35.24	9.30	15.64
48 GLU CA	-9.87	35.39	10.08	16.08
48 GLU CB	-10.96	34.48	9.51	16.42
48 GLU CG	-12.23	34.42	10.33	17.03
48 GLU CD	-12.84	35.78	10.56	17.34
48 GLU OE1	-12.79	36.62	9.63	17.70
48 GLU OE2	-13.37	36.02	11.67	17.62
48 GLU C	-9.62	35.02	11.53	16.18
48 GLU O	-10.05	35.72	12.45	16.19
49 GLU N	-8.91	33.92	11.73	16.29
49 GLU CA	-8.59	33.41	13.06	16.47
49 GLU CB	-7.83	32.09	12.94	16.79
49 GLU CG	-7.60	31.39	14.26	17.31
49 GLU CD	-6.79	30.11	14.10	17.56
49 GLU OE1	-7.02	29.40	13.09	17.88
49 GLU OE2	-5.95	29.82	14.97	17.88
49 GLU C	-7.77	34.38	13.91	16.42
49 GLU O	-8.02	34.54	15.10	16.42
50 TYR N	-6.79	35.03	13.28	16.32
50 TYR CA	-5.90	35.96	13.98	16.20
50 TYR CB	-4.47	35.82	13.45	16.37
50 TYR CG	-3.83	34.48	13.77	16.61
50 TYR CD1	-3.47	34.15	15.08	16.73
50 TYR CE1	-2.89	32.92	15.37	16.88
50 TYR CD2	-3.60	33.55	12.77	16.74
50 TYR CE2	-3.02	32.31	13.05	16.84
50 TYR CZ	-2.67	32.00	14.36	16.89
50 TYR OH	-2.09	30.78	14.64	17.06
50 TYR C	-6.33	37.42	13.91	16.00
50 TYR O	-5.60	38.30	14.37	15.99
51 GLY N	-7.49	37.68	13.33	15.80
51 GLY CA	-7.99	39.04	13.23	15.52
51 GLY C	-7.25	39.95	12.28	15.36
51 GLY O	-7.20	41.16	12.49	15.33
52 ALA N	-6.67	39.38	11.23	15.16
52 ALA CA	-5.94	40.17	10.25	15.02
52 ALA CB	-4.55	39.57	10.01	14.95

52 ALA C	-6.70	40.23	8.93	14.92
52 ALA O	-7.66	39.49	8.72	14.84
53 ILE N	-6.25	41.12	8.04	14.89
53 ILE CA	-6.87	41.29	6.73	14.92
53 ILE CB	-7.61	42.66	6.64	15.05
53 ILE CG2	-8.02	42.93	5.20	15.17
53 ILE CG1	-8.82	42.65	7.56	15.21
53 ILE CD1	-9.85	41.59	7.21	15.39
53 ILE C	-5.80	41.24	5.64	14.88
53 ILE O	-4.70	41.77	5.81	14.72
54 SER N	-6.13	40.58	4.54	14.87
54 SER CA	-5.23	40.45	3.40	15.01
54 SER CB	-5.90	39.62	2.30	14.89
54 SER OG	-5.27	39.86	1.05	14.78
54 SER C	-4.86	41.81	2.83	15.15
54 SER O	-5.74	42.61	2.48	15.16
55 ALA N	-3.56	42.08	2.72	15.34
55 ALA CA	-3.09	43.34	2.17	15.57
55 ALA CB	-1.59	43.49	2.40	15.51
55 ALA C	-3.41	43.40	0.68	15.80
55 ALA O	-3.78	44.45	0.16	15.79
56 PRO N	-3.26	42.27	-0.03	16.00
56 PRO CD	-2.50	41.06	0.30	16.01
56 PRO CA	-3.58	42.30	-1.46	16.26
56 PRO CB	-3.23	40.89	-1.91	16.17
56 PRO CG	-2.04	40.57	-1.06	16.07
56 PRO C	-5.02	42.68	-1.76	16.53
56 PRO O	-5.30	43.45	-2.68	16.59
57 ILE N	-5.94	42.14	-0.98	16.85
57 ILE CA	-7.35	42.44	-1.18	17.17
57 ILE CB	-8.25	41.46	-0.40	17.13
57 ILE CG2	-9.70	41.91	-0.47	17.13
57 ILE CG1	-8.08	40.04	-0.95	17.10
57 ILE CD1	-8.77	38.97	-0.13	17.01
57 ILE C	-7.68	43.85	-0.73	17.50
57 ILE O	-8.34	44.61	-1.44	17.57
58 HIS N	-7.19	44.21	0.46	17.84
58 HIS CA	-7.44	45.52	1.04	18.18
58 HIS CB	-6.97	45.52	2.50	18.23
58 HIS CG	-7.19	46.82	3.22	18.32
58 HIS CD2	-8.15	47.20	4.09	18.38
58 HIS ND1	-6.34	47.89	3.09	18.37
58 HIS CE1	-6.77	48.88	3.85	18.38

58 HIS NE2	-7.87	48.49	4.47	18.39
58 HIS C	-6.82	46.70	0.29	18.38
58 HIS O	-7.51	47.67	0.00	18.43
59 ASP N	-5.53	46.60	-0.01	18.61
59 ASP CA	-4.80	47.67	-0.70	18.84
59 ASP CB	-3.30	47.59	-0.37	18.99
59 ASP CG	-2.96	48.10	1.03	19.14
59 ASP OD1	-3.67	47.75	1.99	19.19
59 ASP OD2	-1.97	48.86	1.18	19.27
59 ASP C	-4.96	47.69	-2.23	18.90
59 ASP O	-4.99	48.77	-2.83	19.03
60 GLU N	-5.06	46.52	-2.86	18.91
60 GLU CA	-5.16	46.45	-4.32	18.85
60 GLU CB	-3.95	45.70	-4.88	19.15
60 GLU CG	-2.62	46.06	-4.26	19.60
60 GLU CD	-2.31	47.53	-4.34	19.85
60 GLU OE1	-2.50	48.12	-5.44	20.14
60 GLU OE2	-1.88	48.11	-3.32	20.10
60 GLU C	-6.41	45.81	-4.91	18.59
60 GLU O	-6.59	45.82	-6.13	18.61
61 ASN N	-7.28	45.27	-4.07	18.31
61 ASN CA	-8.48	44.59	-4.54	17.99
61 ASN CB	-9.39	45.55	-5.33	18.12
61 ASN CG	-10.80	45.00	-5.51	18.17
61 ASN OD1	-11.22	44.11	-4.78	18.25
61 ASN ND2	-11.53	45.55	-6.48	18.20
61 ASN C	-8.02	43.43	-5.42	17.72
61 ASN O	-8.64	43.10	-6.43	17.76
62 PHE N	-6.91	42.82	-5.01	17.30
62 PHE CA	-6.31	41.68	-5.69	16.83
62 PHE CB	-4.96	41.34	-5.05	16.89
62 PHE CG	-4.23	40.18	-5.70	16.90
62 PHE CD1	-3.63	40.33	-6.94	16.96
62 PHE CD2	-4.14	38.95	-5.05	16.94
62 PHE CE1	-2.94	39.27	-7.53	16.96
62 PHE CE2	-3.45	37.89	-5.63	16.96
62 PHE CZ	-2.85	38.05	-6.87	16.97
62 PHE C	-7.28	40.52	-5.52	16.47
62 PHE O	-7.83	40.32	-4.43	16.39
63 PRO N	-7.50	39.73	-6.58	16.11
63 PRO CD	-7.04	39.90	-7.97	16.07
63 PRO CA	-8.42	38.60	-6.47	15.77
63 PRO CB	-8.77	38.31	-7.92	15.90

63 PRO CG	-7.49	38.60	-8.62	15.98
63 PRO C	-7.79	37.39	-5.77	15.37
63 PRO O	-7.65	36.32	-6.37	15.39
64 GLY N	-7.41	37.58	-4.51	14.88
64 GLY CA	-6.80	36.50	-3.75	14.26
64 GLY C	-6.27	36.97	-2.41	13.78
64 GLY O	-5.83	38.12	-2.28	13.74
65 GLN N	-6.30	36.10	-1.40	13.36
65 GLN CA	-5.80	36.46	-0.07	12.86
65 GLN CB	-6.04	35.31	0.91	12.86
65 GLN CG	-7.50	34.96	1.17	12.99
65 GLN CD	-8.24	36.03	1.93	13.11
65 GLN OE1	-7.68	36.70	2.80	13.08
65 GLN NE2	-9.53	36.18	1.63	13.16
65 GLN C	-4.30	36.73	-0.15	12.53
65 GLN O	-3.80	37.69	0.45	12.41
66 THR N	-3.61	35.88	-0.90	12.14
66 THR CA	-2.16	35.96	-1.06	11.77
66 THR CB	-1.48	34.80	-0.32	11.76
66 THR OG1	-1.84	33.56	-0.95	11.65
66 THR CG2	-1.93	34.77	1.13	11.69
66 THR C	-1.76	35.83	-2.53	11.62
66 THR O	-2.61	35.60	-3.39	11.52
67 CYS N	-0.47	35.96	-2.80	11.43
67 CYS CA	0.06	35.80	-4.15	11.27
67 CYS CB	1.01	36.94	-4.52	11.39
67 CYS SG	0.24	38.57	-4.63	11.80
67 CYS C	0.81	34.49	-4.19	11.08
67 CYS O	1.70	34.25	-3.38	10.93
68 ILE N	0.44	33.62	-5.12	10.86
68 ILE CA	1.10	32.33	-5.26	10.79
68 ILE CB	0.15	31.18	-4.91	10.71
68 ILE CG2	0.87	29.84	-5.09	10.62
68 ILE CG1	-0.33	31.31	-3.46	10.66
68 ILE CD1	-1.37	30.30	-3.05	10.71
68 ILE C	1.53	32.26	-6.71	10.80
68 ILE O	0.70	32.23	-7.62	10.86
69 SER N	2.84	32.23	-6.92	10.83
69 SER CA	3.41	32.22	-8.27	10.87
69 SER CB	4.36	33.42	-8.41	10.79
69 SER OG	3.73	34.61	-7.95	10.68
69 SER C	4.16	30.93	-8.53	10.96
69 SER O	5.03	30.54	-7.75	10.94

70 VAL N	3.83	30.26	-9.63	11.06
70 VAL CA	4.46	28.98	-9.94	11.23
70 VAL CB	3.41	27.84	-9.95	11.16
70 VAL CG1	4.08	26.50	-10.16	11.21
70 VAL CG2	2.64	27.84	-8.64	11.25
70 VAL C	5.23	28.93	-11.26	11.38
70 VAL O	4.77	29.43	-12.28	11.43
71 ASN N	6.42	28.32	-11.19	11.49
71 ASN CA	7.31	28.12	-12.33	11.78
71 ASN CB	6.79	26.96	-13.19	11.77
71 ASN CG	6.79	25.64	-12.43	11.74
71 ASN OD1	7.67	25.39	-11.60	11.67
71 ASN ND2	5.82	24.78	-12.72	11.76
71 ASN C	7.59	29.33	-13.21	11.95
71 ASN O	8.51	30.10	-12.94	12.06
72 GLU N	6.81	29.51	-14.28	12.13
72 GLU CA	7.04	30.64	-15.16	12.27
72 GLU CB	6.23	30.48	-16.46	12.36
72 GLU CG	4.74	30.78	-16.35	12.60
72 GLU CD	3.93	29.63	-15.77	12.64
72 GLU OE1	4.50	28.55	-15.49	12.77
72 GLU OE2	2.71	29.82	-15.58	12.82
72 GLU C	6.69	31.96	-14.48	12.29
72 GLU O	7.20	33.02	-14.86	12.30
73 GLU N	5.82	31.90	-13.47	12.35
73 GLU CA	5.42	33.09	-12.74	12.44
73 GLU CB	4.03	32.90	-12.13	12.54
73 GLU CG	2.96	32.56	-13.14	12.67
73 GLU CD	1.66	32.20	-12.48	12.81
73 GLU OE1	1.71	31.57	-11.40	12.80
73 GLU OE2	0.59	32.52	-13.05	12.97
73 GLU C	6.41	33.40	-11.64	12.46
73 GLU O	6.76	32.52	-10.84	12.46
74 VAL N	6.87	34.64	-11.60	12.51
74 VAL CA	7.84	35.09	-10.61	12.66
74 VAL CB	8.83	36.10	-11.24	12.58
74 VAL CG1	9.82	36.60	-10.21	12.64
74 VAL CG2	9.55	35.46	-12.42	12.65
74 VAL C	7.18	35.75	-9.40	12.77
74 VAL O	7.62	35.58	-8.26	12.66
75 ALA N	6.12	36.51	-9.66	12.86
75 ALA CA	5.43	37.23	-8.59	13.04
75 ALA CB	6.23	38.48	-8.23	13.11

75 ALA C	4.02	37.62	-8.98	13.24
75 ALA O	3.67	37.64	-10.16	13.20
76 HIS N	3.21	37.92	-7.97	13.43
76 HIS CA	1.83	38.35	-8.15	13.63
76 HIS CB	1.80	39.66	-8.94	14.05
76 HIS CG	2.43	40.81	-8.23	14.51
76 HIS CD2	2.20	42.15	-8.31	14.67
76 HIS ND1	3.47	40.66	-7.34	14.73
76 HIS CE1	3.86	41.85	-6.91	14.81
76 HIS NE2	3.10	42.77	-7.48	14.89
76 HIS C	0.92	37.32	-8.82	13.65
76 HIS O	-0.07	37.68	-9.45	13.62
77 GLY N	1.24	36.03	-8.68	13.56
77 GLY CA	0.40	35.01	-9.27	13.53
77 GLY C	-0.95	34.94	-8.57	13.57
77 GLY O	-1.03	35.10	-7.36	13.44
78 ILE N	-2.01	34.70	-9.34	13.65
78 ILE CA	-3.36	34.63	-8.79	13.67
78 ILE CB	-4.41	35.12	-9.81	13.74
78 ILE CG2	-5.77	35.22	-9.15	13.79
78 ILE CG1	-4.01	36.47	-10.40	13.79
78 ILE CD1	-4.88	36.91	-11.58	13.86
78 ILE C	-3.75	33.21	-8.38	13.80
78 ILE O	-3.73	32.31	-9.21	13.76
79 PRO N	-4.10	32.99	-7.10	13.88
79 PRO CD	-4.06	33.92	-5.96	13.83
79 PRO CA	-4.49	31.65	-6.68	13.82
79 PRO CB	-4.93	31.86	-5.23	13.87
79 PRO CG	-4.00	32.97	-4.77	13.87
79 PRO C	-5.64	31.20	-7.59	14.00
79 PRO O	-6.54	31.99	-7.89	14.07
80 SER N	-5.60	29.95	-8.04	14.07
80 SER CA	-6.61	29.45	-8.96	14.16
80 SER CB	-6.23	29.87	-10.38	14.16
80 SER OG	-5.05	29.19	-10.78	14.14
80 SER C	-6.72	27.93	-8.92	14.27
80 SER O	-6.23	27.28	-8.01	14.26
81 LYS N	-7.38	27.37	-9.94	14.37
81 LYS CA	-7.56	25.93	-10.03	14.49
81 LYS CB	-8.68	25.61	-11.03	14.81
81 LYS CG	-10.01	26.25	-10.65	15.25
81 LYS CD	-11.02	26.18	-11.79	15.64
81 LYS CE	-12.31	26.92	-11.44	15.87

81	LYS	NZ	-13.25	26.97	-12.59	16.08
81	LYS	C	-6.27	25.23	-10.44	14.34
81	LYS	O	-6.22	24.01	-10.57	14.37
82	ARG	N	-5.21	26.02	-10.62	14.20
82	ARG	CA	-3.92	25.46	-11.01	14.03
82	ARG	CB	-2.88	26.57	-11.14	14.03
82	ARG	CG	-1.50	26.06	-11.52	14.05
82	ARG	CD	-0.53	27.18	-11.80	14.04
82	ARG	NE	0.72	26.68	-12.37	14.08
82	ARG	CZ	1.54	27.41	-13.11	14.04
82	ARG	NH1	1.26	28.67	-13.37	14.07
82	ARG	NH2	2.65	26.87	-13.61	14.04
82	ARG	C	-3.47	24.44	-9.97	13.93
82	ARG	O	-3.39	24.75	-8.78	13.83
83	VAL	N	-3.16	23.23	-10.42	13.85
83	VAL	CA	-2.72	22.17	-9.53	13.77
83	VAL	CB	-3.25	20.79	-9.98	13.89
83	VAL	CG1	-2.60	20.39	-11.29	14.05
83	VAL	CG2	-2.99	19.75	-8.91	13.96
83	VAL	C	-1.20	22.10	-9.42	13.63
83	VAL	O	-0.49	22.17	-10.43	13.57
84	ILE	N	-0.71	21.99	-8.19	13.53
84	ILE	CA	0.72	21.88	-7.92	13.43
84	ILE	CB	1.01	22.04	-6.41	13.41
84	ILE	CG2	2.48	21.71	-6.13	13.36
84	ILE	CG1	0.66	23.46	-5.95	13.40
84	ILE	CD1	1.46	24.56	-6.63	13.43
84	ILE	C	1.19	20.51	-8.38	13.40
84	ILE	O	0.51	19.51	-8.17	13.33
85	ARG	N	2.37	20.47	-8.99	13.37
85	ARG	CA	2.95	19.23	-9.48	13.41
85	ARG	CB	3.03	19.25	-11.02	13.72
85	ARG	CG	1.69	19.35	-11.72	14.26
85	ARG	CD	0.82	18.14	-11.41	14.77
85	ARG	NE	1.38	16.91	-11.94	15.32
85	ARG	CZ	1.29	16.52	-13.21	15.49
85	ARG	NH1	0.65	17.28	-14.09	15.73
85	ARG	NH2	1.85	15.38	-13.61	15.78
85	ARG	C	4.35	19.02	-8.92	13.25
85	ARG	O	5.02	19.97	-8.51	13.18
86	GLU	N	4.79	17.77	-8.90	13.02
86	GLU	CA	6.12	17.41	-8.42	12.82
86	GLU	CB	6.36	15.92	-8.65	13.02

86	GLU	CG	7.71	15.40	-8.18	13.26
86	GLU	CD	7.82	15.28	-6.68	13.38
86	GLU	OE1	6.81	15.50	-5.97	13.63
86	GLU	OE2	8.93	14.95	-6.19	13.48
86	GLU	C	7.13	18.23	-9.21	12.57
86	GLU	O	7.04	18.32	-10.44	12.61
87	GLY	N	8.09	18.83	-8.51	12.27
87	GLY	CA	9.11	19.62	-9.17	11.85
87	GLY	C	8.81	21.10	-9.38	11.54
87	GLY	O	9.67	21.84	-9.83	11.56
88	ASP	N	7.59	21.53	-9.05	11.25
88	ASP	CA	7.24	22.94	-9.22	10.94
88	ASP	CB	5.76	23.18	-8.88	11.06
88	ASP	CG	4.80	22.75	-9.97	11.19
88	ASP	OD1	5.25	22.32	-11.06	11.42
88	ASP	OD2	3.58	22.86	-9.73	11.29
88	ASP	C	8.06	23.86	-8.33	10.60
88	ASP	O	8.41	23.50	-7.20	10.48
89	LEU	N	8.38	25.05	-8.84	10.34
89	LEU	CA	9.09	26.06	-8.07	10.13
89	LEU	CB	10.16	26.75	-8.91	10.01
89	LEU	CG	10.87	27.96	-8.29	9.88
89	LEU	CD1	11.40	27.62	-6.89	9.84
89	LEU	CD2	12.00	28.41	-9.20	9.94
89	LEU	C	7.98	27.04	-7.71	10.00
89	LEU	O	7.45	27.74	-8.57	10.05
90	VAL	N	7.64	27.08	-6.42	9.84
90	VAL	CA	6.55	27.91	-5.94	9.76
90	VAL	CB	5.55	27.04	-5.14	9.72
90	VAL	CG1	4.36	27.87	-4.68	9.84
90	VAL	CG2	5.10	25.86	-5.99	9.91
90	VAL	C	6.96	29.06	-5.03	9.74
90	VAL	O	7.82	28.90	-4.17	9.70
91	ASN	N	6.36	30.22	-5.24	9.72
91	ASN	CA	6.61	31.36	-4.37	9.77
91	ASN	CB	7.19	32.57	-5.09	10.13
91	ASN	CG	7.36	33.75	-4.15	10.36
91	ASN	OD1	6.42	34.52	-3.93	10.60
91	ASN	ND2	8.54	33.87	-3.55	10.68
91	ASN	C	5.28	31.76	-3.75	9.66
91	ASN	O	4.28	31.95	-4.45	9.62
92	ILE	N	5.28	31.86	-2.43	9.49
92	ILE	CA	4.09	32.26	-1.69	9.43

92	ILE	CB	3.70	31.20	-0.64	9.45
92	ILE	CG2	2.52	31.69	0.19	9.51
92	ILE	CG1	3.39	29.87	-1.34	9.57
92	ILE	CD1	3.01	28.75	-0.40	9.63
92	ILE	C	4.46	33.57	-1.01	9.40
92	ILE	O	5.45	33.62	-0.26	9.28
93	ASP	N	3.69	34.62	-1.29	9.42
93	ASP	CA	3.94	35.94	-0.72	9.50
93	ASP	CB	4.15	36.97	-1.83	9.83
93	ASP	CG	4.77	38.27	-1.31	10.11
93	ASP	OD1	4.26	38.80	-0.30	10.33
93	ASP	OD2	5.75	38.77	-1.91	10.66
93	ASP	C	2.73	36.30	0.12	9.36
93	ASP	O	1.62	36.46	-0.40	9.24
94	VAL	N	2.95	36.45	1.43	9.26
94	VAL	CA	1.89	36.75	2.39	9.38
94	VAL	CB	1.89	35.71	3.55	9.33
94	VAL	CG1	0.73	35.96	4.50	9.37
94	VAL	CG2	1.83	34.29	2.99	9.33
94	VAL	C	2.07	38.14	3.00	9.40
94	VAL	O	3.07	38.40	3.66	9.40
95	SER	N	1.10	39.02	2.78	9.48
95	SER	CA	1.15	40.36	3.36	9.63
95	SER	CB	1.57	41.40	2.31	9.71
95	SER	OG	0.65	41.48	1.24	9.65
95	SER	C	-0.23	40.66	3.92	9.78
95	SER	O	-1.24	40.26	3.34	9.80
96	ALA	N	-0.29	41.35	5.05	9.93
96	ALA	CA	-1.57	41.64	5.68	10.12
96	ALA	CB	-2.10	40.38	6.37	10.17
96	ALA	C	-1.44	42.76	6.68	10.29
96	ALA	O	-0.33	43.24	6.97	10.36
97	LEU	N	-2.57	43.18	7.22	10.52
97	LEU	CA	-2.59	44.24	8.21	10.71
97	LEU	CB	-3.04	45.57	7.58	10.77
97	LEU	CG	-4.43	45.63	6.92	10.80
97	LEU	CD1	-4.93	47.07	6.96	10.92
97	LEU	CD2	-4.35	45.12	5.48	10.83
97	LEU	C	-3.52	43.89	9.36	10.87
97	LEU	O	-4.51	43.17	9.18	10.82
98	LYS	N	-3.18	44.38	10.54	10.99
98	LYS	CA	-3.99	44.18	11.74	11.29
98	LYS	CB	-3.55	42.95	12.54	11.30

98 LYS CG	-4.33	42.76	13.84	11.32
98 LYS CD	-4.04	41.42	14.49	11.31
98 LYS CE	-4.74	41.28	15.84	11.41
98 LYS NZ	-4.57	39.91	16.40	11.40
98 LYS C	-3.82	45.44	12.58	11.52
98 LYS O	-2.70	45.87	12.84	11.52
99 ASN N	-4.94	46.03	13.00	11.80
99 ASN CA	-4.92	47.25	13.80	12.02
99 ASN CB	-4.39	46.96	15.21	12.33
99 ASN CG	-5.30	46.02	15.99	12.49
99 ASN OD1	-6.52	46.14	15.92	12.87
99 ASN ND2	-4.70	45.10	16.73	12.66
99 ASN C	-4.09	48.35	13.13	11.93
99 ASN O	-3.41	49.13	13.81	12.16
100 GLY N	-4.15	48.40	11.80	11.86
100 GLY CA	-3.44	49.43	11.07	11.71
100 GLY C	-1.99	49.20	10.73	11.55
100 GLY O	-1.39	50.02	10.03	11.62
101 TYR N	-1.40	48.11	11.21	11.34
101 TYR CA	0.00	47.84	10.94	11.09
101 TYR CB	0.76	47.64	12.25	11.18
101 TYR CG	0.81	48.91	13.06	11.36
101 TYR CD1	1.84	49.84	12.88	11.49
101 TYR CE1	1.85	51.05	13.56	11.75
101 TYR CD2	-0.22	49.24	13.94	11.52
101 TYR CE2	-0.22	50.45	14.63	11.70
101 TYR CZ	0.81	51.35	14.43	11.74
101 TYR OH	0.81	52.56	15.11	12.10
101 TYR C	0.17	46.65	10.00	10.85
101 TYR O	-0.61	45.69	10.04	10.76
102 TYR N	1.21	46.72	9.18	10.63
102 TYR CA	1.48	45.71	8.16	10.42
102 TYR CB	1.62	46.38	6.80	10.54
102 TYR CG	0.36	46.98	6.22	10.69
102 TYR CD1	-0.29	48.04	6.86	10.80
102 TYR CE1	-1.42	48.63	6.28	10.97
102 TYR CD2	-0.14	46.53	5.00	10.79
102 TYR CE2	-1.25	47.11	4.43	10.92
102 TYR CZ	-1.89	48.16	5.06	10.96
102 TYR OH	-2.97	48.75	4.46	11.17
102 TYR C	2.72	44.84	8.33	10.28
102 TYR O	3.67	45.20	9.02	10.13
103 ALA N	2.69	43.71	7.63	10.05

103 ALA CA	3.80	42.77	7.57	9.86
103 ALA CB	3.60	41.61	8.54	9.99
103 ALA C	3.81	42.27	6.13	9.73
103 ALA O	2.77	42.24	5.47	9.61
104 ASP N	4.97	41.86	5.65	9.45
104 ASP CA	5.12	41.39	4.28	9.35
104 ASP CB	5.49	42.59	3.40	9.41
104 ASP CG	5.56	42.27	1.93	9.50
104 ASP OD1	5.16	41.16	1.51	9.51
104 ASP OD2	6.03	43.15	1.18	9.58
104 ASP C	6.24	40.36	4.29	9.25
104 ASP O	7.37	40.65	4.69	9.20
105 THR N	5.93	39.14	3.87	9.15
105 THR CA	6.94	38.09	3.85	9.09
105 THR CB	7.01	37.38	5.22	8.97
105 THR OG1	8.08	36.43	5.22	8.87
105 THR CG2	5.69	36.69	5.54	9.03
105 THR C	6.61	37.10	2.74	9.14
105 THR O	5.47	37.01	2.29	9.17
106 GLY N	7.62	36.38	2.27	9.08
106 GLY CA	7.40	35.43	1.20	9.10
106 GLY C	8.54	34.44	1.09	8.98
106 GLY O	9.63	34.67	1.62	8.92
107 ILE N	8.29	33.35	0.39	8.93
107 ILE CA	9.31	32.33	0.23	8.93
107 ILE CB	9.35	31.43	1.50	9.03
107 ILE CG2	8.01	30.73	1.69	9.00
107 ILE CG1	10.47	30.40	1.41	9.11
107 ILE CD1	10.87	29.82	2.76	9.42
107 ILE C	9.10	31.47	-1.01	8.91
107 ILE O	7.97	31.12	-1.37	8.71
108 SER N	10.21	31.15	-1.67	8.97
108 SER CA	10.20	30.29	-2.85	9.06
108 SER CB	11.04	30.88	-3.99	9.02
108 SER OG	10.43	32.02	-4.56	8.97
108 SER C	10.80	28.97	-2.42	9.25
108 SER O	11.76	28.93	-1.65	9.17
109 PHE N	10.23	27.88	-2.92	9.39
109 PHE CA	10.70	26.55	-2.59	9.65
109 PHE CB	10.09	26.07	-1.26	9.56
109 PHE CG	8.59	26.12	-1.23	9.47
109 PHE CD1	7.92	27.31	-0.97	9.45
109 PHE CD2	7.84	24.98	-1.49	9.47

109 PHE CE1	6.53	27.36	-0.97	9.45
109 PHE CE2	6.45	25.02	-1.50	9.43
109 PHE CZ	5.79	26.22	-1.23	9.38
109 PHE C	10.32	25.58	-3.71	9.85
109 PHE O	9.48	25.89	-4.56	9.84
110 VAL N	10.95	24.41	-3.69	10.15
110 VAL CA	10.70	23.38	-4.68	10.42
110 VAL CB	12.01	22.70	-5.11	10.42
110 VAL CG1	11.73	21.56	-6.08	10.42
110 VAL CG2	12.93	23.73	-5.75	10.42
110 VAL C	9.78	22.33	-4.08	10.69
110 VAL O	9.97	21.91	-2.93	10.70
111 VAL N	8.77	21.91	-4.84	11.04
111 VAL CA	7.85	20.88	-4.37	11.45
111 VAL CB	6.47	21.00	-5.05	11.42
111 VAL CG1	5.55	19.88	-4.58	11.38
111 VAL CG2	5.85	22.35	-4.73	11.40
111 VAL C	8.48	19.54	-4.75	11.82
111 VAL O	8.64	19.24	-5.93	11.87
112 GLY N	8.84	18.75	-3.75	12.25
112 GLY CA	9.46	17.46	-4.03	12.82
112 GLY C	10.77	17.59	-4.76	13.15
112 GLY O	11.66	18.33	-4.34	13.32
113 GLU N	10.91	16.87	-5.87	13.57
113 GLU CA	12.14	16.92	-6.65	13.87
113 GLU CB	12.83	15.55	-6.66	14.12
113 GLU CG	13.10	14.97	-5.29	14.61
113 GLU CD	13.60	13.55	-5.38	14.82
113 GLU OE1	12.95	12.72	-6.05	15.15
113 GLU OE2	14.65	13.25	-4.77	15.06
113 GLU C	11.89	17.32	-8.09	13.94
113 GLU O	10.91	16.89	-8.70	13.95
114 SER N	12.79	18.14	-8.62	14.05
114 SER CA	12.74	18.58	-10.01	14.18
114 SER CB	12.99	20.08	-10.12	14.18
114 SER OG	13.23	20.45	-11.47	14.21
114 SER C	13.88	17.84	-10.68	14.29
114 SER O	14.81	17.39	-10.01	14.31
115 ASP N	13.82	17.71	-12.00	14.40
115 ASP CA	14.90	17.03	-12.71	14.52
115 ASP CB	14.40	16.53	-14.07	15.02
115 ASP CG	14.08	17.66	-15.03	15.42
115 ASP OD1	13.48	18.66	-14.59	15.80

115	ASP	OD2	14.43	17.54	-16.22	15.84
115	ASP	C	16.05	18.02	-12.91	14.33
115	ASP	O	17.16	17.63	-13.30	14.31
116	ASP	N	15.79	19.29	-12.62	14.08
116	ASP	CA	16.81	20.33	-12.77	13.88
116	ASP	CB	16.28	21.45	-13.68	13.95
116	ASP	CG	17.37	22.38	-14.15	14.02
116	ASP	OD1	18.42	22.47	-13.48	14.02
116	ASP	OD2	17.18	23.04	-15.20	14.16
116	ASP	C	17.18	20.92	-11.42	13.67
116	ASP	O	16.37	21.59	-10.78	13.62
117	PRO	N	18.42	20.68	-10.96	13.47
117	PRO	CD	19.47	19.84	-11.56	13.45
117	PRO	CA	18.84	21.21	-9.66	13.36
117	PRO	CB	20.20	20.54	-9.44	13.44
117	PRO	CG	20.70	20.30	-10.84	13.48
117	PRO	C	18.91	22.74	-9.59	13.19
117	PRO	O	19.11	23.30	-8.52	13.12
118	MET	N	18.75	23.40	-10.73	13.10
118	MET	CA	18.79	24.86	-10.76	12.99
118	MET	CB	18.75	25.37	-12.20	13.33
118	MET	CG	18.67	26.89	-12.33	13.66
118	MET	SD	20.13	27.78	-11.71	14.22
118	MET	CE	21.24	27.60	-13.09	14.15
118	MET	C	17.63	25.48	-9.97	12.75
118	MET	O	17.75	26.58	-9.44	12.67
119	LYS	N	16.50	24.78	-9.91	12.46
119	LYS	CA	15.37	25.31	-9.17	12.15
119	LYS	CB	14.14	24.40	-9.33	12.11
119	LYS	CG	13.47	24.55	-10.69	12.12
119	LYS	CD	12.18	23.73	-10.77	12.06
119	LYS	CE	11.36	24.11	-12.00	12.16
119	LYS	NZ	10.15	23.24	-12.16	12.16
119	LYS	C	15.72	25.46	-7.69	11.99
119	LYS	O	15.46	26.51	-7.09	11.92
120	GLN	N	16.33	24.44	-7.10	11.85
120	GLN	CA	16.72	24.53	-5.70	11.67
120	GLN	CB	17.13	23.15	-5.17	11.72
120	GLN	CG	17.50	23.13	-3.68	11.77
120	GLN	CD	16.38	23.64	-2.78	11.84
120	GLN	OE1	15.24	23.16	-2.85	12.03
120	GLN	NE2	16.70	24.60	-1.92	11.96
120	GLN	C	17.89	25.51	-5.55	11.53

120 GLN O	17.98	26.22	-4.55	11.45
121 LYS N	18.77	25.57	-6.54	11.39
121 LYS CA	19.91	26.48	-6.47	11.33
121 LYS CB	20.79	26.39	-7.72	11.49
121 LYS CG	22.00	27.32	-7.64	11.69
121 LYS CD	22.94	27.20	-8.82	11.96
121 LYS CE	24.11	28.16	-8.68	12.14
121 LYS NZ	25.10	28.03	-9.79	12.40
121 LYS C	19.48	27.92	-6.28	11.21
121 LYS O	20.03	28.61	-5.43	11.17
122 VAL N	18.53	28.39	-7.08	11.11
122 VAL CA	18.11	29.78	-6.92	10.87
122 VAL CB	17.15	30.25	-8.05	10.88
122 VAL CG1	17.89	30.28	-9.37	10.86
122 VAL CG2	15.93	29.34	-8.14	10.78
122 VAL C	17.48	30.01	-5.55	10.85
122 VAL O	17.56	31.12	-5.01	10.89
123 CYS N	16.85	28.98	-4.99	10.78
123 CYS CA	16.26	29.14	-3.66	10.79
123 CYS CB	15.38	27.93	-3.30	10.68
123 CYS SG	13.86	27.79	-4.26	10.46
123 CYS C	17.39	29.27	-2.65	10.96
123 CYS O	17.32	30.10	-1.75	10.92
124 ASP N	18.41	28.43	-2.79	11.15
124 ASP CA	19.55	28.46	-1.88	11.39
124 ASP CB	20.59	27.38	-2.23	11.57
124 ASP CG	20.09	25.97	-1.99	11.81
124 ASP OD1	19.15	25.78	-1.18	12.07
124 ASP OD2	20.65	25.04	-2.60	12.04
124 ASP C	20.25	29.82	-1.94	11.44
124 ASP O	20.59	30.40	-0.91	11.41
125 VAL N	20.45	30.34	-3.14	11.56
125 VAL CA	21.14	31.61	-3.27	11.72
125 VAL CB	21.66	31.79	-4.72	11.69
125 VAL CG1	22.36	33.14	-4.85	11.64
125 VAL CG2	22.65	30.67	-5.05	11.67
125 VAL C	20.29	32.80	-2.84	11.93
125 VAL O	20.83	33.80	-2.37	11.95
126 ALA N	18.97	32.70	-2.99	12.11
126 ALA CA	18.09	33.78	-2.56	12.30
126 ALA CB	16.64	33.50	-3.00	12.35
126 ALA C	18.17	33.90	-1.04	12.50
126 ALA O	18.11	34.99	-0.48	12.39

127	THR	N	18.28	32.75	-0.38	12.73
127	THR	CA	18.38	32.72	1.07	13.08
127	THR	CB	18.28	31.28	1.59	13.23
127	THR	OG1	17.09	30.68	1.07	13.57
127	THR	CG2	18.21	31.26	3.11	13.41
127	THR	C	19.71	33.35	1.49	13.18
127	THR	O	19.76	34.15	2.41	13.11
128	MET	N	20.78	32.98	0.80	13.36
128	MET	CA	22.09	33.55	1.10	13.56
128	MET	CB	23.19	32.87	0.28	14.16
128	MET	CG	23.58	31.48	0.77	14.95
128	MET	SD	25.11	30.89	0.01	15.92
128	MET	CE	24.54	30.60	-1.63	15.74
128	MET	C	22.09	35.04	0.82	13.36
128	MET	O	22.67	35.83	1.56	13.21
129	ALA	N	21.41	35.44	-0.26	13.16
129	ALA	CA	21.36	36.85	-0.61	13.03
129	ALA	CB	20.63	37.04	-1.94	12.96
129	ALA	C	20.66	37.65	0.49	12.99
129	ALA	O	21.09	38.76	0.82	12.90
130	PHE	N	19.59	37.10	1.06	13.04
130	PHE	CA	18.89	37.81	2.12	13.10
130	PHE	CB	17.60	37.08	2.52	12.86
130	PHE	CG	16.87	37.74	3.65	12.61
130	PHE	CD1	16.01	38.81	3.42	12.52
130	PHE	CD2	17.12	37.38	4.97	12.50
130	PHE	CE1	15.42	39.51	4.47	12.40
130	PHE	CE2	16.54	38.07	6.03	12.41
130	PHE	CZ	15.69	39.14	5.78	12.37
130	PHE	C	19.77	37.97	3.36	13.34
130	PHE	O	19.84	39.05	3.94	13.23
131	GLU	N	20.44	36.89	3.75	13.72
131	GLU	CA	21.33	36.91	4.91	14.11
131	GLU	CB	21.96	35.52	5.12	14.41
131	GLU	CG	20.96	34.39	5.28	15.11
131	GLU	CD	21.63	33.02	5.32	15.48
131	GLU	OE1	22.63	32.81	4.59	15.86
131	GLU	OE2	21.16	32.14	6.08	15.91
131	GLU	C	22.45	37.92	4.71	14.18
131	GLU	O	22.82	38.64	5.64	14.14
132	ASN	N	23.00	37.97	3.50	14.33
132	ASN	CA	24.08	38.90	3.23	14.54
132	ASN	CB	24.74	38.57	1.89	14.71

132 ASN CG	25.51	37.26	1.94	14.92
132 ASN OD1	25.94	36.82	3.01	15.13
132 ASN ND2	25.71	36.65	0.78	15.08
132 ASN C	23.56	40.33	3.23	14.63
132 ASN O	24.26	41.26	3.65	14.57
133 ALA N	22.33	40.51	2.77	14.73
133 ALA CA	21.73	41.84	2.71	14.96
133 ALA CB	20.41	41.77	1.95	14.88
133 ALA C	21.50	42.44	4.10	15.11
133 ALA O	21.75	43.63	4.30	15.14
134 ILE N	21.02	41.64	5.05	15.31
134 ILE CA	20.77	42.19	6.38	15.60
134 ILE CB	19.58	41.50	7.07	15.63
134 ILE CG2	18.31	41.74	6.28	15.66
134 ILE CG1	19.87	40.01	7.24	15.65
134 ILE CD1	18.95	39.34	8.24	15.69
134 ILE C	21.95	42.13	7.33	15.79
134 ILE O	21.90	42.69	8.42	15.78
135 ALA N	23.03	41.48	6.90	16.11
135 ALA CA	24.22	41.30	7.73	16.52
135 ALA CB	25.34	40.68	6.90	16.49
135 ALA C	24.74	42.55	8.44	16.81
135 ALA O	25.13	42.47	9.61	16.98
136 LYS N	24.75	43.68	7.75	17.13
136 LYS CA	25.26	44.91	8.36	17.41
136 LYS CB	26.53	45.36	7.62	17.59
136 LYS CG	27.72	44.41	7.79	17.84
136 LYS CD	28.93	44.85	6.97	18.06
136 LYS CE	28.67	44.74	5.47	18.20
136 LYS NZ	29.85	45.22	4.68	18.33
136 LYS C	24.26	46.06	8.43	17.49
136 LYS O	24.64	47.20	8.72	17.54
137 VAL N	22.99	45.77	8.16	17.52
137 VAL CA	21.94	46.79	8.22	17.53
137 VAL CB	20.55	46.18	7.90	17.59
137 VAL CG1	19.45	47.17	8.24	17.73
137 VAL CG2	20.47	45.80	6.43	17.66
137 VAL C	21.92	47.41	9.61	17.49
137 VAL O	21.78	46.71	10.61	17.50
138 LYS N	22.09	48.73	9.66	17.43
138 LYS CA	22.10	49.45	10.92	17.30
138 LYS CB	23.45	49.32	11.63	17.56
138 LYS CG	23.50	48.29	12.74	17.88

138 LYS CD	24.80	48.40	13.51	18.14
138 LYS CE	24.89	47.36	14.62	18.30
138 LYS NZ	24.99	45.98	14.07	18.42
138 LYS C	21.83	50.92	10.66	17.07
138 LYS O	21.90	51.38	9.51	17.06
139 PRO N	21.52	51.69	11.71	16.83
139 PRO CD	21.28	51.30	13.11	16.81
139 PRO CA	21.26	53.12	11.51	16.62
139 PRO CB	21.03	53.63	12.93	16.68
139 PRO CG	20.43	52.45	13.62	16.74
139 PRO C	22.47	53.79	10.85	16.40
139 PRO O	23.61	53.49	11.19	16.42
140 GLY N	22.20	54.67	9.89	16.12
140 GLY CA	23.27	55.38	9.20	15.77
140 GLY C	23.88	54.71	7.99	15.59
140 GLY O	24.61	55.35	7.22	15.54
141 THR N	23.60	53.42	7.79	15.41
141 THR CA	24.16	52.70	6.65	15.29
141 THR CB	24.15	51.17	6.87	15.35
141 THR OG1	22.80	50.72	7.05	15.48
141 THR CG2	24.96	50.81	8.10	15.45
141 THR C	23.40	53.03	5.38	15.09
141 THR O	22.23	53.44	5.43	15.12
142 LYS N	24.05	52.84	4.24	14.95
142 LYS CA	23.44	53.14	2.96	14.75
142 LYS CB	24.52	53.28	1.89	14.93
142 LYS CG	25.47	54.44	2.13	15.11
142 LYS CD	26.56	54.50	1.08	15.37
142 LYS CE	27.51	55.66	1.36	15.59
142 LYS NZ	28.61	55.74	0.37	15.89
142 LYS C	22.43	52.10	2.51	14.61
142 LYS O	22.69	50.90	2.57	14.49
143 LEU N	21.28	52.58	2.06	14.42
143 LEU CA	20.22	51.71	1.58	14.29
143 LEU CB	19.05	52.56	1.08	14.30
143 LEU CG	17.87	51.84	0.43	14.31
143 LEU CD1	17.18	50.96	1.45	14.40
143 LEU CD2	16.89	52.86	-0.15	14.36
143 LEU C	20.78	50.86	0.44	14.23
143 LEU O	20.48	49.67	0.34	14.11
144 SER N	21.60	51.48	-0.40	14.20
144 SER CA	22.19	50.79	-1.54	14.18
144 SER CB	23.02	51.75	-2.40	14.24

144	SER	OG	24.14	52.24	-1.68	14.40
144	SER	C	23.05	49.58	-1.16	14.11
144	SER	O	23.36	48.76	-2.02	14.11
145	ASN	N	23.43	49.47	0.12	14.07
145	ASN	CA	24.23	48.32	0.56	13.98
145	ASN	CB	24.61	48.41	2.04	14.22
145	ASN	CG	25.64	49.47	2.32	14.40
145	ASN	OD1	26.42	49.84	1.45	14.65
145	ASN	ND2	25.67	49.93	3.56	14.66
145	ASN	C	23.44	47.04	0.38	13.80
145	ASN	O	24.01	45.98	0.15	13.74
146	ILE	N	22.12	47.13	0.54	13.61
146	ILE	CA	21.26	45.97	0.40	13.44
146	ILE	CB	19.80	46.34	0.71	13.42
146	ILE	CG2	18.88	45.13	0.47	13.41
146	ILE	CG1	19.69	46.79	2.17	13.49
146	ILE	CD1	18.31	47.25	2.58	13.54
146	ILE	C	21.37	45.41	-1.01	13.38
146	ILE	O	21.73	44.25	-1.20	13.28
147	GLY	N	21.07	46.23	-2.01	13.31
147	GLY	CA	21.14	45.77	-3.39	13.29
147	GLY	C	22.56	45.36	-3.77	13.30
147	GLY	O	22.75	44.41	-4.53	13.26
148	LYS	N	23.55	46.08	-3.25	13.35
148	LYS	CA	24.93	45.75	-3.56	13.38
148	LYS	CB	25.87	46.71	-2.83	13.65
148	LYS	CG	27.32	46.63	-3.29	14.00
148	LYS	CD	28.20	47.59	-2.50	14.48
148	LYS	CE	29.53	47.79	-3.18	14.80
148	LYS	NZ	29.39	48.54	-4.46	15.27
148	LYS	C	25.22	44.31	-3.11	13.30
148	LYS	O	25.80	43.52	-3.85	13.22
149	ALA	N	24.80	43.99	-1.89	13.20
149	ALA	CA	25.01	42.66	-1.33	13.10
149	ALA	CB	24.61	42.65	0.14	13.05
149	ALA	C	24.23	41.58	-2.08	13.12
149	ALA	O	24.75	40.49	-2.33	13.03
150	VAL	N	22.98	41.88	-2.43	13.21
150	VAL	CA	22.14	40.93	-3.15	13.28
150	VAL	CB	20.71	41.49	-3.39	13.27
150	VAL	CG1	19.90	40.53	-4.25	13.27
150	VAL	CG2	20.02	41.70	-2.05	13.27
150	VAL	C	22.75	40.58	-4.50	13.38

150 VAL O	22.89	39.40	-4.84	13.30
151 HIS N	23.14	41.59	-5.27	13.61
151 HIS CA	23.72	41.35	-6.59	13.92
151 HIS CB	23.84	42.67	-7.36	14.15
151 HIS CG	24.29	42.51	-8.77	14.48
151 HIS CD2	23.59	42.40	-9.92	14.64
151 HIS ND1	25.62	42.41	-9.13	14.64
151 HIS CE1	25.71	42.25	-10.44	14.72
151 HIS NE2	24.49	42.24	-10.95	14.75
151 HIS C	25.08	40.67	-6.49	14.00
151 HIS O	25.42	39.85	-7.34	13.95
152 ASN N	25.86	40.99	-5.46	14.13
152 ASN CA	27.17	40.37	-5.31	14.31
152 ASN CB	27.95	41.04	-4.16	14.54
152 ASN CG	29.35	40.48	-4.02	14.84
152 ASN OD1	29.54	39.32	-3.65	15.13
152 ASN ND2	30.36	41.30	-4.31	15.00
152 ASN C	27.00	38.88	-5.04	14.24
152 ASN O	27.73	38.05	-5.59	14.22
153 THR N	26.03	38.55	-4.20	14.24
153 THR CA	25.75	37.15	-3.87	14.24
153 THR CB	24.63	37.03	-2.83	14.18
153 THR OG1	25.01	37.73	-1.64	14.13
153 THR CG2	24.36	35.58	-2.48	14.07
153 THR C	25.34	36.39	-5.13	14.38
153 THR O	25.74	35.24	-5.34	14.32
154 ALA N	24.54	37.04	-5.97	14.50
154 ALA CA	24.10	36.40	-7.21	14.67
154 ALA CB	23.10	37.30	-7.93	14.62
154 ALA C	25.30	36.13	-8.12	14.86
154 ALA O	25.47	35.02	-8.62	14.82
155 ARG N	26.14	37.14	-8.30	15.16
155 ARG CA	27.32	37.01	-9.14	15.47
155 ARG CB	28.05	38.36	-9.19	15.89
155 ARG CG	28.79	38.62	-10.48	16.59
155 ARG CD	29.90	37.62	-10.73	17.12
155 ARG NE	30.41	37.74	-12.09	17.64
155 ARG CZ	31.42	37.03	-12.58	17.80
155 ARG NH1	32.06	36.15	-11.82	18.01
155 ARG NH2	31.79	37.20	-13.85	17.97
155 ARG C	28.27	35.92	-8.65	15.43
155 ARG O	28.85	35.17	-9.45	15.42
156 GLN N	28.45	35.83	-7.33	15.42

156	GLN	CA	29.34	34.81	-6.76	15.43
156	GLN	CB	29.45	34.98	-5.25	15.62
156	GLN	CG	30.08	36.26	-4.76	16.01
156	GLN	CD	30.31	36.20	-3.27	16.19
156	GLN	OE1	30.34	37.23	-2.59	16.43
156	GLN	NE2	30.48	34.99	-2.74	16.35
156	GLN	C	28.85	33.40	-7.02	15.30
156	GLN	O	29.57	32.43	-6.80	15.29
157	ASN	N	27.61	33.28	-7.47	15.18
157	ASN	CA	27.03	31.97	-7.75	15.08
157	ASN	CB	25.88	31.69	-6.78	15.09
157	ASN	CG	26.36	31.60	-5.33	15.05
157	ASN	OD1	26.33	32.58	-4.58	15.18
157	ASN	ND2	26.82	30.41	-4.95	15.11
157	ASN	C	26.54	31.85	-9.19	15.04
157	ASN	O	25.65	31.05	-9.49	14.98
158	ASP	N	27.14	32.64	-10.07	15.03
158	ASP	CA	26.80	32.63	-11.49	15.04
158	ASP	CB	27.33	31.34	-12.12	15.35
158	ASP	CG	28.81	31.16	-11.89	15.66
158	ASP	OD1	29.57	32.12	-12.18	15.93
158	ASP	OD2	29.23	30.08	-11.42	15.97
158	ASP	C	25.32	32.79	-11.78	14.89
158	ASP	O	24.78	32.17	-12.70	14.88
159	LEU	N	24.66	33.65	-11.01	14.64
159	LEU	CA	23.24	33.90	-11.19	14.41
159	LEU	CB	22.45	33.36	-9.99	14.31
159	LEU	CG	22.49	31.84	-9.83	14.25
159	LEU	CD1	21.85	31.43	-8.52	14.17
159	LEU	CD2	21.78	31.18	-11.01	14.20
159	LEU	C	22.98	35.39	-11.37	14.32
159	LEU	O	23.90	36.20	-11.28	14.24
160	LYS	N	21.73	35.74	-11.62	14.27
160	LYS	CA	21.33	37.13	-11.84	14.17
160	LYS	CB	20.77	37.30	-13.25	14.41
160	LYS	CG	21.71	36.92	-14.38	14.73
160	LYS	CD	22.97	37.78	-14.37	15.07
160	LYS	CE	23.86	37.50	-15.58	15.31
160	LYS	NZ	24.21	36.06	-15.70	15.60
160	LYS	C	20.26	37.54	-10.84	14.04
160	LYS	O	19.80	36.74	-10.04	13.91
161	VAL	N	19.88	38.81	-10.90	13.89
161	VAL	CA	18.83	39.33	-10.03	13.79

161	VAL	CB	19.37	40.43	-9.08	13.77
161	VAL	CG1	20.53	39.90	-8.25	13.77
161	VAL	CG2	19.81	41.65	-9.88	13.85
161	VAL	C	17.74	39.93	-10.91	13.70
161	VAL	O	17.98	40.27	-12.07	13.75
162	ILE	N	16.53	40.05	-10.37	13.61
162	ILE	CA	15.45	40.66	-11.14	13.49
162	ILE	CB	14.06	40.12	-10.74	13.43
162	ILE	CG2	12.96	40.92	-11.44	13.46
162	ILE	CG1	13.94	38.64	-11.12	13.40
162	ILE	CD1	14.10	38.38	-12.62	13.34
162	ILE	C	15.57	42.14	-10.78	13.48
162	ILE	O	15.30	42.53	-9.64	13.45
163	LYS	N	15.98	42.94	-11.75	13.51
163	LYS	CA	16.20	44.36	-11.53	13.57
163	LYS	CB	17.13	44.91	-12.62	13.78
163	LYS	CG	18.49	44.24	-12.65	14.09
163	LYS	CD	19.31	44.69	-13.84	14.46
163	LYS	CE	20.74	44.22	-13.72	14.73
163	LYS	NZ	21.43	44.89	-12.59	15.10
163	LYS	C	14.96	45.23	-11.44	13.51
163	LYS	O	14.97	46.25	-10.75	13.48
164	ASN	N	13.88	44.83	-12.11	13.44
164	ASN	CA	12.68	45.65	-12.08	13.43
164	ASN	CB	12.08	45.79	-13.49	13.23
164	ASN	CG	11.58	44.48	-14.06	13.18
164	ASN	OD1	12.05	43.41	-13.69	12.97
164	ASN	ND2	10.63	44.57	-14.98	13.15
164	ASN	C	11.60	45.27	-11.07	13.47
164	ASN	O	10.43	45.59	-11.24	13.60
165	LEU	N	12.02	44.59	-10.01	13.52
165	LEU	CA	11.14	44.24	-8.90	13.53
165	LEU	CB	10.84	42.74	-8.84	13.67
165	LEU	CG	9.85	42.24	-9.91	13.75
165	LEU	CD1	9.53	40.78	-9.65	13.80
165	LEU	CD2	8.58	43.09	-9.88	13.79
165	LEU	C	11.96	44.68	-7.69	13.48
165	LEU	O	13.15	44.40	-7.61	13.55
166	THR	N	11.32	45.40	-6.76	13.38
166	THR	CA	12.05	45.92	-5.62	13.24
166	THR	CB	12.30	47.43	-5.77	13.22
166	THR	OG1	11.06	48.12	-5.55	13.29
166	THR	CG2	12.79	47.75	-7.17	13.22

166 THR C	11.37	45.74	-4.28	13.12
166 THR O	10.19	45.45	-4.20	13.14
167 GLY N	12.17	45.93	-3.23	12.98
167 GLY CA	11.68	45.87	-1.87	12.90
167 GLY C	11.07	47.23	-1.61	12.88
167 GLY O	11.03	48.08	-2.51	12.88
168 HIS N	10.63	47.49	-0.38	12.79
168 HIS CA	9.98	48.76	-0.10	12.78
168 HIS CB	8.62	48.76	-0.78	12.76
168 HIS CG	7.82	47.52	-0.49	12.74
168 HIS CD2	7.74	46.35	-1.16	12.76
168 HIS ND1	7.05	47.37	0.65	12.76
168 HIS CE1	6.53	46.16	0.67	12.73
168 HIS NE2	6.93	45.52	-0.42	12.73
168 HIS C	9.78	48.98	1.38	12.79
168 HIS O	9.79	48.03	2.16	12.76
169 GLY N	9.56	50.23	1.76	12.83
169 GLY CA	9.29	50.51	3.15	12.88
169 GLY C	7.92	49.94	3.40	12.99
169 GLY O	7.12	49.80	2.47	12.89
170 VAL N	7.63	49.59	4.65	13.09
170 VAL CA	6.34	49.01	5.00	13.26
170 VAL CB	6.38	47.46	4.78	13.30
170 VAL CG1	7.36	46.83	5.74	13.34
170 VAL CG2	4.99	46.86	4.93	13.40
170 VAL C	6.02	49.35	6.45	13.38
170 VAL O	6.91	49.70	7.23	13.41
171 GLY N	4.74	49.30	6.83	13.51
171 GLY CA	4.39	49.61	8.20	13.74
171 GLY C	2.95	50.07	8.37	13.93
171 GLY O	2.14	49.36	8.96	13.79
172 LEU N	2.64	51.26	7.88	14.20
172 LEU CA	1.29	51.78	7.98	14.54
172 LEU CB	1.31	53.26	8.36	14.60
172 LEU CG	1.73	53.49	9.81	14.67
172 LEU CD1	1.92	54.98	10.08	14.80
172 LEU CD2	0.67	52.91	10.74	14.68
172 LEU C	0.59	51.57	6.64	14.81
172 LEU O	-0.56	51.95	6.45	14.71
173 SER N	1.32	50.95	5.73	15.15
173 SER CA	0.81	50.64	4.40	15.55
173 SER CB	0.78	51.89	3.52	15.53
173 SER OG	2.09	52.28	3.15	15.47

173 SER C	1.77	49.62	3.81	15.91
173 SER O	2.86	49.38	4.33	15.91
174 LEU N	1.35	49.02	2.71	16.34
174 LEU CA	2.17	48.03	2.06	16.77
174 LEU CB	1.40	47.40	0.92	16.91
174 LEU CG	2.30	46.51	0.10	17.13
174 LEU CD1	2.45	45.16	0.79	17.23
174 LEU CD2	1.71	46.41	-1.30	17.19
174 LEU C	3.44	48.68	1.50	16.89
174 LEU O	4.54	48.16	1.69	17.05
175 HIS N	3.25	49.80	0.82	17.03
175 HIS CA	4.35	50.54	0.20	17.11
175 HIS CB	4.18	50.55	-1.32	17.48
175 HIS CG	4.58	49.26	-1.98	17.81
175 HIS CD2	5.52	49.00	-2.92	17.96
175 HIS ND1	3.98	48.06	-1.70	17.98
175 HIS CE1	4.53	47.10	-2.43	18.00
175 HIS NE2	5.47	47.65	-3.18	18.08
175 HIS C	4.51	51.99	0.68	16.94
175 HIS O	3.62	52.82	0.47	17.03
176 GLU N	5.64	52.27	1.32	16.72
176 GLU CA	5.96	53.61	1.80	16.44
176 GLU CB	5.40	53.83	3.21	16.38
176 GLU CG	5.67	52.73	4.22	16.29
176 GLU CD	4.74	52.82	5.42	16.30
176 GLU OE1	5.19	52.57	6.55	16.26
176 GLU OE2	3.54	53.12	5.22	16.29
176 GLU C	7.49	53.80	1.76	16.34
176 GLU O	8.21	52.87	1.43	16.26
177 ALA N	7.97	55.00	2.07	16.21
177 ALA CA	9.41	55.27	2.01	16.18
177 ALA CB	9.68	56.71	2.42	16.15
177 ALA C	10.24	54.32	2.87	16.14
177 ALA O	9.87	54.00	4.00	16.17
178 PRO N	11.38	53.84	2.33	16.11
178 PRO CD	12.31	53.00	3.11	16.17
178 PRO CA	11.93	54.12	1.00	16.09
178 PRO CB	13.36	53.61	1.11	16.14
178 PRO CG	13.23	52.46	2.04	16.16
178 PRO C	11.13	53.43	-0.10	16.08
178 PRO O	10.83	52.24	-0.01	16.01
179 ALA N	10.82	54.19	-1.14	16.08
179 ALA CA	10.04	53.68	-2.27	16.05

179 ALA CB	9.97	54.74	-3.36	16.06
179 ALA C	10.55	52.38	-2.85	16.00
179 ALA O	9.78	51.45	-3.09	16.04
180 HIS N	11.86	52.30	-3.08	15.96
180 HIS CA	12.44	51.10	-3.67	15.97
180 HIS CB	12.69	51.33	-5.16	16.11
180 HIS CG	11.46	51.65	-5.95	16.34
180 HIS CD2	10.52	50.84	-6.49	16.39
180 HIS ND1	11.06	52.94	-6.23	16.46
180 HIS CE1	9.93	52.91	-6.91	16.48
180 HIS NE2	9.58	51.65	-7.08	16.54
180 HIS C	13.72	50.61	-3.04	15.84
180 HIS O	14.66	51.37	-2.81	15.88
181 VAL N	13.74	49.31	-2.76	15.72
181 VAL CA	14.91	48.65	-2.20	15.63
181 VAL CB	14.54	47.77	-0.99	15.64
181 VAL CG1	15.76	47.01	-0.51	15.65
181 VAL CG2	13.96	48.65	0.12	15.67
181 VAL C	15.38	47.78	-3.36	15.60
181 VAL O	14.86	46.69	-3.59	15.51
182 LEU N	16.36	48.29	-4.11	15.61
182 LEU CA	16.88	47.59	-5.28	15.63
182 LEU CB	17.80	48.51	-6.08	15.62
182 LEU CG	17.21	49.83	-6.58	15.59
182 LEU CD1	18.31	50.62	-7.28	15.61
182 LEU CD2	16.05	49.58	-7.51	15.64
182 LEU C	17.63	46.31	-4.98	15.72
182 LEU O	18.15	46.11	-3.88	15.65
183 ASN N	17.70	45.45	-5.99	15.83
183 ASN CA	18.42	44.19	-5.89	16.02
183 ASN CB	17.66	43.09	-6.62	15.84
183 ASN CG	16.39	42.69	-5.90	15.78
183 ASN OD1	16.41	42.45	-4.70	15.67
183 ASN ND2	15.28	42.62	-6.62	15.66
183 ASN C	19.82	44.33	-6.47	16.28
183 ASN O	20.50	43.34	-6.70	16.22
184 TYR N	20.22	45.57	-6.72	16.64
184 TYR CA	21.55	45.84	-7.26	17.08
184 TYR CB	21.54	45.83	-8.79	17.02
184 TYR CG	20.61	46.85	-9.41	17.03
184 TYR CD1	19.25	46.61	-9.50	17.03
184 TYR CE1	18.38	47.56	-10.03	17.05
184 TYR CD2	21.10	48.07	-9.87	17.04

184	TYR	CE2	20.25	49.03	-10.39	17.08
184	TYR	CZ	18.89	48.77	-10.47	17.09
184	TYR	OH	18.04	49.73	-10.97	17.18
184	TYR	C	22.02	47.20	-6.75	17.46
184	TYR	O	21.25	47.95	-6.14	17.41
185	PHE	N	23.29	47.51	-7.00	17.98
185	PHE	CA	23.89	48.74	-6.53	18.57
185	PHE	CB	25.38	48.50	-6.25	18.65
185	PHE	CG	26.13	49.74	-5.85	18.85
185	PHE	CD1	25.81	50.42	-4.68	18.86
185	PHE	CD2	27.14	50.23	-6.66	18.90
185	PHE	CE1	26.50	51.58	-4.32	18.96
185	PHE	CE2	27.84	51.39	-6.31	18.99
185	PHE	CZ	27.51	52.06	-5.14	19.00
185	PHE	C	23.75	49.96	-7.44	18.93
185	PHE	O	24.11	49.92	-8.61	19.00
186	ASP	N	23.21	51.04	-6.87	19.37
186	ASP	CA	23.02	52.31	-7.57	19.83
186	ASP	CB	21.56	52.75	-7.48	20.05
186	ASP	CG	21.32	54.12	-8.09	20.24
186	ASP	OD1	21.76	54.35	-9.24	20.42
186	ASP	OD2	20.69	54.97	-7.42	20.37
186	ASP	C	23.92	53.30	-6.84	20.04
186	ASP	O	23.59	53.79	-5.76	20.07
187	PRO	N	25.09	53.61	-7.42	20.26
187	PRO	CD	25.49	53.22	-8.78	20.31
187	PRO	CA	26.07	54.54	-6.85	20.42
187	PRO	CB	27.20	54.52	-7.88	20.41
187	PRO	CG	26.47	54.31	-9.16	20.39
187	PRO	C	25.61	55.95	-6.53	20.55
187	PRO	O	26.26	56.65	-5.75	20.68
188	LYS	N	24.51	56.40	-7.13	20.68
188	LYS	CA	24.04	57.75	-6.87	20.77
188	LYS	CB	23.39	58.33	-8.14	20.95
188	LYS	CG	22.13	57.62	-8.62	21.18
188	LYS	CD	20.93	57.96	-7.76	21.39
188	LYS	CE	19.63	57.46	-8.38	21.48
188	LYS	NZ	18.47	57.71	-7.48	21.69
188	LYS	C	23.08	57.89	-5.69	20.73
188	LYS	O	22.75	59.00	-5.29	20.77
189	ASP	N	22.65	56.77	-5.12	20.62
189	ASP	CA	21.72	56.82	-4.00	20.45
189	ASP	CB	20.95	55.51	-3.88	20.52

189 ASP CG 19.82 55.58 -2.86 20.63
189 ASP OD1 19.43 56.70 -2.49 20.65
189 ASP OD2 19.32 54.51 -2.45 20.64
189 ASP C 22.43 57.13 -2.69 20.29
189 ASP O 23.32 56.40 -2.27 20.29
190 LYS N 22.02 58.22 -2.05 20.07
190 LYS CA 22.61 58.63 -0.78 19.81
190 LYS CB 22.92 60.13 -0.81 20.02
190 LYS CG 24.00 60.53 -1.79 20.26
190 LYS CD 24.14 62.04 -1.87 20.45
190 LYS CE 25.28 62.44 -2.78 20.59
190 LYS NZ 25.39 63.92 -2.92 20.71
190 LYS C 21.67 58.33 0.38 19.48
190 LYS O 21.96 58.67 1.53 19.52
191 THR N 20.53 57.71 0.07 19.05
191 THR CA 19.53 57.37 1.08 18.60
191 THR CB 18.33 56.62 0.46 18.67
191 THR OG1 17.72 57.46 -0.53 18.84
191 THR CG2 17.30 56.29 1.53 18.74
191 THR C 20.12 56.49 2.17 18.18
191 THR O 20.81 55.50 1.88 18.05
192 LEU N 19.85 56.84 3.42 17.72
192 LEU CA 20.37 56.06 4.55 17.28
192 LEU CB 21.17 56.96 5.49 17.26
192 LEU CG 22.36 57.75 4.97 17.26
192 LEU CD1 22.89 58.60 6.11 17.25
192 LEU CD2 23.44 56.81 4.45 17.29
192 LEU C 19.25 55.42 5.35 17.02
192 LEU O 18.11 55.88 5.34 16.98
193 LEU N 19.60 54.34 6.05 16.75
193 LEU CA 18.64 53.65 6.90 16.48
193 LEU CB 19.05 52.19 7.09 16.50
193 LEU CG 19.21 51.36 5.81 16.48
193 LEU CD1 19.55 49.93 6.19 16.50
193 LEU CD2 17.94 51.40 4.99 16.53
193 LEU C 18.72 54.39 8.24 16.39
193 LEU O 19.79 54.89 8.61 16.29
194 THR N 17.60 54.47 8.95 16.20
194 THR CA 17.59 55.15 10.23 16.13
194 THR CB 16.78 56.47 10.15 16.19
194 THR OG1 15.40 56.17 9.89 16.28
194 THR CG2 17.31 57.36 9.04 16.20
194 THR C 17.00 54.26 11.31 16.00

194 THR O	16.30	53.29	11.03	16.03
195 GLU N	17.30	54.59	12.56	15.89
195 GLU CA	16.79	53.84	13.70	15.75
195 GLU CB	17.24	54.51	14.99	15.91
195 GLU CG	16.64	53.94	16.26	16.23
195 GLU CD	17.11	52.54	16.57	16.35
195 GLU OE1	18.33	52.30	16.56	16.53
195 GLU OE2	16.25	51.67	16.83	16.55
195 GLU C	15.26	53.77	13.65	15.50
195 GLU O	14.59	54.80	13.60	15.53
196 GLY N	14.72	52.55	13.65	15.25
196 GLY CA	13.28	52.37	13.63	14.82
196 GLY C	12.66	52.20	12.25	14.52
196 GLY O	11.47	51.93	12.13	14.53
197 MET N	13.47	52.35	11.21	14.19
197 MET CA	12.97	52.21	9.85	13.86
197 MET CB	14.06	52.61	8.84	13.93
197 MET CG	13.62	52.54	7.39	13.98
197 MET SD	14.90	53.13	6.27	14.10
197 MET CE	14.70	54.89	6.42	14.09
197 MET C	12.52	50.77	9.58	13.58
197 MET O	13.22	49.82	9.91	13.58
198 VAL N	11.34	50.63	8.98	13.28
198 VAL CA	10.80	49.31	8.66	13.03
198 VAL CB	9.36	49.16	9.18	13.03
198 VAL CG1	8.90	47.72	9.02	13.02
198 VAL CG2	9.28	49.58	10.64	12.97
198 VAL C	10.84	49.09	7.15	12.91
198 VAL O	10.28	49.88	6.38	12.89
199 LEU N	11.49	48.00	6.75	12.68
199 LEU CA	11.65	47.68	5.34	12.51
199 LEU CB	13.13	47.81	4.94	12.76
199 LEU CG	13.91	49.09	5.19	12.92
199 LEU CD1	15.37	48.87	4.86	13.03
199 LEU CD2	13.34	50.20	4.33	13.01
199 LEU C	11.26	46.26	4.99	12.34
199 LEU O	11.44	45.34	5.79	12.29
200 ALA N	10.72	46.08	3.79	12.03
200 ALA CA	10.42	44.75	3.29	11.86
200 ALA CB	9.11	44.74	2.51	11.79
200 ALA C	11.61	44.52	2.35	11.70
200 ALA O	11.76	45.22	1.34	11.61
201 ILE N	12.48	43.59	2.72	11.57

201	ILE	CA	13.65	43.27	1.93	11.53
201	ILE	CB	14.90	43.16	2.83	11.42
201	ILE	CG2	16.10	42.68	2.03	11.40
201	ILE	CG1	15.18	44.53	3.45	11.39
201	ILE	CD1	16.30	44.55	4.47	11.42
201	ILE	C	13.32	41.95	1.24	11.54
201	ILE	O	13.04	40.95	1.90	11.45
202	GLU	N	13.32	41.97	-0.09	11.67
202	GLU	CA	12.93	40.80	-0.86	11.84
202	GLU	CB	11.46	40.93	-1.26	12.25
202	GLU	CG	11.07	42.33	-1.67	12.76
202	GLU	CD	9.64	42.43	-2.17	13.10
202	GLU	OE1	9.07	43.53	-2.10	13.26
202	GLU	OE2	9.09	41.42	-2.64	13.49
202	GLU	C	13.75	40.49	-2.10	11.74
202	GLU	O	13.29	40.68	-3.23	11.72
203	PRO	N	14.96	39.98	-1.91	11.62
203	PRO	CD	15.62	39.64	-0.64	11.63
203	PRO	CA	15.81	39.65	-3.06	11.55
203	PRO	CB	17.08	39.12	-2.40	11.58
203	PRO	CG	16.59	38.59	-1.08	11.61
203	PRO	C	15.19	38.61	-4.00	11.53
203	PRO	O	14.55	37.66	-3.55	11.34
204	PHE	N	15.38	38.83	-5.29	11.55
204	PHE	CA	14.92	37.91	-6.33	11.65
204	PHE	CB	14.06	38.60	-7.39	11.88
204	PHE	CG	12.64	38.85	-6.98	12.13
204	PHE	CD1	12.28	40.03	-6.35	12.29
204	PHE	CD2	11.65	37.92	-7.30	12.27
204	PHE	CE1	10.95	40.30	-6.04	12.49
204	PHE	CE2	10.31	38.18	-6.99	12.40
204	PHE	CZ	9.96	39.37	-6.36	12.45
204	PHE	C	16.18	37.41	-7.04	11.61
204	PHE	O	16.94	38.22	-7.58	11.69
205	ILE	N	16.39	36.10	-7.03	11.58
205	ILE	CA	17.55	35.49	-7.67	11.56
205	ILE	CB	18.29	34.57	-6.70	11.54
205	ILE	CG2	19.44	33.88	-7.41	11.49
205	ILE	CG1	18.81	35.39	-5.51	11.60
205	ILE	CD1	19.79	36.48	-5.89	11.64
205	ILE	C	17.05	34.70	-8.88	11.60
205	ILE	O	16.19	33.83	-8.74	11.55
206	SER	N	17.61	35.00	-10.05	11.69

206	SER	CA	17.21	34.38	-11.31	11.82
206	SER	CB	16.74	35.49	-12.26	11.75
206	SER	OG	16.54	35.01	-13.58	11.77
206	SER	C	18.26	33.53	-12.01	12.02
206	SER	O	19.45	33.86	-11.99	11.93
207	SER	N	17.82	32.45	-12.65	12.27
207	SER	CA	18.73	31.58	-13.37	12.62
207	SER	CB	18.05	30.24	-13.70	12.63
207	SER	OG	16.95	30.42	-14.57	12.72
207	SER	C	19.27	32.22	-14.65	12.88
207	SER	O	20.28	31.77	-15.20	12.90
208	ASN	N	18.61	33.26	-15.14	13.16
208	ASN	CA	19.06	33.94	-16.35	13.48
208	ASN	CB	18.75	33.09	-17.59	13.79
208	ASN	CG	19.21	33.76	-18.88	14.04
208	ASN	OD1	18.40	34.13	-19.72	14.35
208	ASN	ND2	20.52	33.93	-19.02	14.21
208	ASN	C	18.50	35.34	-16.58	13.53
208	ASN	O	19.26	36.31	-16.66	13.61
209	ALA	N	17.18	35.46	-16.69	13.56
209	ALA	CA	16.54	36.76	-16.93	13.59
209	ALA	CB	15.04	36.58	-17.07	13.63
209	ALA	C	16.85	37.76	-15.83	13.62
209	ALA	O	16.88	37.42	-14.65	13.56
210	SER	N	17.07	39.01	-16.23	13.67
210	SER	CA	17.38	40.07	-15.29	13.77
210	SER	CB	18.59	40.88	-15.77	13.87
210	SER	OG	18.33	41.50	-17.02	14.18
210	SER	C	16.19	41.00	-15.09	13.75
210	SER	O	16.32	42.06	-14.49	13.70
211	PHE	N	15.04	40.60	-15.62	13.77
211	PHE	CA	13.82	41.39	-15.50	13.88
211	PHE	CB	13.84	42.56	-16.49	13.84
211	PHE	CG	13.85	42.13	-17.94	13.85
211	PHE	CD1	15.04	41.77	-18.56	13.92
211	PHE	CD2	12.67	42.08	-18.67	13.91
211	PHE	CE1	15.05	41.36	-19.90	13.98
211	PHE	CE2	12.67	41.68	-20.00	13.97
211	PHE	CZ	13.87	41.32	-20.62	13.99
211	PHE	C	12.59	40.53	-15.75	14.04
211	PHE	O	12.70	39.42	-16.27	13.89
212	VAL	N	11.42	41.04	-15.37	14.30
212	VAL	CA	10.16	40.35	-15.58	14.69

212 VAL CB	9.39	40.10	-14.26	14.70
212 VAL CG1	10.09	39.02	-13.45	14.73
212 VAL CG2	9.28	41.39	-13.46	14.75
212 VAL C	9.27	41.20	-16.49	15.00
212 VAL O	9.49	42.40	-16.65	15.00
213 THR N	8.26	40.56	-17.08	15.40
213 THR CA	7.32	41.25	-17.95	15.81
213 THR CB	7.59	40.93	-19.44	15.82
213 THR OG1	7.63	39.51	-19.63	15.83
213 THR CG2	8.90	41.56	-19.89	15.90
213 THR C	5.90	40.80	-17.61	16.16
213 THR O	5.71	39.86	-16.85	16.09
214 GLU N	4.90	41.48	-18.18	16.59
214 GLU CA	3.50	41.14	-17.93	17.08
214 GLU CB	2.57	42.06	-18.73	17.38
214 GLU CG	1.09	41.77	-18.50	17.97
214 GLU CD	0.18	42.67	-19.31	18.22
214 GLU OE1	0.28	43.91	-19.17	18.57
214 GLU OE2	-0.63	42.15	-20.11	18.57
214 GLU C	3.26	39.69	-18.33	17.19
214 GLU O	3.65	39.26	-19.42	17.28
215 GLY N	2.60	38.95	-17.45	17.39
215 GLY CA	2.32	37.55	-17.71	17.63
215 GLY C	0.99	37.21	-18.36	17.79
215 GLY O	0.43	38.01	-19.11	17.84
216 LYS N	0.50	36.01	-18.06	17.91
216 LYS CA	-0.75	35.49	-18.61	18.05
216 LYS CB	-0.95	34.04	-18.15	18.04
216 LYS CG	-1.17	33.89	-16.65	17.98
216 LYS CD	-1.44	32.44	-16.25	18.01
216 LYS CE	-0.26	31.52	-16.57	18.00
216 LYS NZ	1.01	31.98	-15.93	17.99
216 LYS C	-2.00	36.30	-18.25	18.16
216 LYS O	-3.07	36.05	-18.80	18.23
217 ASN N	-1.85	37.24	-17.33	18.22
217 ASN CA	-2.97	38.09	-16.94	18.32
217 ASN CB	-3.80	37.42	-15.84	18.26
217 ASN CG	-2.97	37.00	-14.64	18.22
217 ASN OD1	-2.30	37.83	-14.03	18.20
217 ASN ND2	-3.00	35.72	-14.31	18.16
217 ASN C	-2.46	39.46	-16.48	18.40
217 ASN O	-1.27	39.73	-16.54	18.44
218 GLU N	-3.37	40.32	-16.04	18.51

218 GLU CA	-3.00	41.67	-15.62	18.54
218 GLU CB	-4.24	42.56	-15.61	18.88
218 GLU CG	-5.35	42.05	-14.71	19.43
218 GLU CD	-6.64	42.80	-14.90	19.72
218 GLU OE1	-7.17	42.78	-16.04	20.03
218 GLU OE2	-7.14	43.40	-13.93	20.04
218 GLU C	-2.30	41.76	-14.28	18.33
218 GLU O	-1.99	42.86	-13.82	18.37
219 TRP N	-2.03	40.62	-13.65	18.06
219 TRP CA	-1.37	40.63	-12.35	17.79
219 TRP CB	-2.25	39.95	-11.30	17.92
219 TRP CG	-3.48	40.73	-10.95	18.07
219 TRP CD2	-3.54	41.88	-10.11	18.14
219 TRP CE2	-4.90	42.28	-10.04	18.17
219 TRP CE3	-2.59	42.63	-9.41	18.17
219 TRP CD1	-4.76	40.47	-11.34	18.12
219 TRP NE1	-5.62	41.40	-10.80	18.15
219 TRP CZ2	-5.32	43.38	-9.30	18.20
219 TRP CZ3	-3.01	43.73	-8.67	18.21
219 TRP CH2	-4.36	44.10	-8.62	18.25
219 TRP C	0.01	39.98	-12.32	17.54
219 TRP O	1.00	40.61	-11.94	17.48
220 ALA N	0.07	38.72	-12.72	17.25
220 ALA CA	1.31	37.95	-12.69	16.94
220 ALA CB	1.02	36.52	-13.11	16.99
220 ALA C	2.48	38.50	-13.50	16.73
220 ALA O	2.31	39.01	-14.60	16.71
221 PHE N	3.68	38.39	-12.91	16.46
221 PHE CA	4.92	38.80	-13.56	16.21
221 PHE CB	5.82	39.59	-12.60	16.43
221 PHE CG	5.40	41.02	-12.41	16.64
221 PHE CD1	5.53	41.94	-13.44	16.77
221 PHE CD2	4.88	41.44	-11.19	16.77
221 PHE CE1	5.14	43.27	-13.26	16.86
221 PHE CE2	4.48	42.77	-11.00	16.87
221 PHE CZ	4.62	43.68	-12.04	16.88
221 PHE C	5.62	37.50	-13.95	15.93
221 PHE O	5.68	36.56	-13.15	15.85
222 GLU N	6.13	37.44	-15.17	15.59
222 GLU CA	6.81	36.23	-15.64	15.32
222 GLU CB	5.86	35.44	-16.56	15.34
222 GLU CG	4.56	34.98	-15.89	15.50
222 GLU CD	3.58	34.32	-16.85	15.61

222 GLU OE1	4.04	33.76	-17.87	15.75
222 GLU OE2	2.36	34.36	-16.58	15.60
222 GLU C	8.05	36.62	-16.44	15.10
222 GLU O	8.35	37.80	-16.58	15.04
223 THR N	8.77	35.62	-16.92	14.92
223 THR CA	9.94	35.85	-17.77	14.75
223 THR CB	11.27	35.33	-17.16	14.67
223 THR OG1	11.20	33.91	-16.98	14.50
223 THR CG2	11.55	36.00	-15.82	14.56
223 THR C	9.63	35.04	-19.01	14.77
223 THR O	9.18	33.89	-18.92	14.75
224 SER N	9.83	35.63	-20.18	14.79
224 SER CA	9.54	34.93	-21.42	14.79
224 SER CB	9.66	35.88	-22.62	14.80
224 SER OG	8.56	36.78	-22.64	14.94
224 SER C	10.43	33.71	-21.63	14.72
224 SER O	9.99	32.73	-22.24	14.72
225 ASP N	11.66	33.75	-21.12	14.67
225 ASP CA	12.57	32.61	-21.27	14.62
225 ASP CB	14.04	33.07	-21.25	14.77
225 ASP CG	14.44	33.75	-19.95	14.93
225 ASP OD1	13.78	33.52	-18.92	14.86
225 ASP OD2	15.45	34.50	-19.96	15.13
225 ASP C	12.34	31.56	-20.18	14.54
225 ASP O	13.07	30.57	-20.10	14.58
226 LYS N	11.32	31.78	-19.36	14.43
226 LYS CA	10.95	30.88	-18.28	14.28
226 LYS CB	10.33	29.60	-18.86	14.53
226 LYS CG	9.05	29.87	-19.63	14.91
226 LYS CD	8.36	28.57	-20.06	15.34
226 LYS CE	7.06	28.86	-20.78	15.60
226 LYS NZ	7.32	29.65	-22.01	15.93
226 LYS C	12.09	30.54	-17.33	14.02
226 LYS O	12.31	29.38	-16.97	13.99
227 SER N	12.82	31.58	-16.93	13.72
227 SER CA	13.92	31.42	-15.99	13.45
227 SER CB	14.62	32.75	-15.75	13.59
227 SER OG	15.35	33.19	-16.88	13.71
227 SER C	13.35	30.94	-14.67	13.24
227 SER O	12.17	31.13	-14.38	13.17
228 PHE N	14.21	30.33	-13.86	12.95
228 PHE CA	13.79	29.89	-12.54	12.69
228 PHE CB	14.46	28.58	-12.16	12.83

228	PHE	CG	14.13	27.46	-13.09	12.93
228	PHE	CD1	12.82	27.27	-13.53	13.03
228	PHE	CD2	15.11	26.59	-13.54	13.06
228	PHE	CE1	12.49	26.23	-14.39	13.02
228	PHE	CE2	14.80	25.55	-14.40	13.09
228	PHE	CZ	13.48	25.37	-14.84	13.05
228	PHE	C	14.20	31.03	-11.62	12.44
228	PHE	O	15.37	31.42	-11.56	12.33
229	VAL	N	13.22	31.58	-10.92	12.20
229	VAL	CA	13.47	32.71	-10.05	12.03
229	VAL	CB	12.77	33.97	-10.59	12.00
229	VAL	CG1	13.14	35.18	-9.75	12.02
229	VAL	CG2	13.16	34.18	-12.05	12.03
229	VAL	C	12.98	32.43	-8.64	11.94
229	VAL	O	11.86	31.95	-8.44	11.99
230	ALA	N	13.83	32.72	-7.66	11.78
230	ALA	CA	13.47	32.50	-6.27	11.78
230	ALA	CB	14.41	31.47	-5.64	11.74
230	ALA	C	13.53	33.80	-5.48	11.78
230	ALA	O	14.36	34.68	-5.74	11.68
231	GLN	N	12.64	33.91	-4.51	11.78
231	GLN	CA	12.59	35.08	-3.67	11.88
231	GLN	CB	11.39	35.94	-4.05	12.21
231	GLN	CG	11.13	37.07	-3.10	12.71
231	GLN	CD	10.00	37.95	-3.56	12.96
231	GLN	OE1	8.94	37.46	-3.96	13.24
231	GLN	NE2	10.21	39.26	-3.50	13.22
231	GLN	C	12.48	34.69	-2.20	11.78
231	GLN	O	11.93	33.65	-1.86	11.81
232	ILE	N	13.06	35.53	-1.34	11.66
232	ILE	CA	12.97	35.36	0.11	11.66
232	ILE	CB	14.30	34.91	0.75	11.80
232	ILE	CG2	14.22	35.07	2.27	11.90
232	ILE	CG1	14.60	33.46	0.38	11.98
232	ILE	CD1	13.56	32.47	0.88	12.15
232	ILE	C	12.64	36.77	0.56	11.58
232	ILE	O	13.34	37.71	0.20	11.65
233	GLU	N	11.58	36.91	1.35	11.43
233	GLU	CA	11.16	38.22	1.80	11.27
233	GLU	CB	9.94	38.67	0.99	11.59
233	GLU	CG	9.28	39.94	1.49	12.15
233	GLU	CD	8.13	40.38	0.60	12.42
233	GLU	OE1	7.29	39.53	0.23	12.46

233 GLU OE2	8.08	41.58	0.27	12.86
233 GLU C	10.83	38.27	3.28	11.00
233 GLU O	10.21	37.36	3.82	10.79
234 HIS N	11.27	39.34	3.93	10.79
234 HIS CA	11.02	39.56	5.34	10.60
234 HIS CB	12.19	39.10	6.20	10.47
234 HIS CG	12.21	37.63	6.47	10.27
234 HIS CD2	13.09	36.67	6.09	10.23
234 HIS ND1	11.25	37.00	7.22	10.25
234 HIS CE1	11.52	35.71	7.30	10.24
234 HIS NE2	12.64	35.48	6.62	10.27
234 HIS C	10.80	41.03	5.63	10.60
234 HIS O	11.30	41.91	4.92	10.46
235 THR N	10.03	41.29	6.68	10.71
235 THR CA	9.80	42.66	7.12	10.90
235 THR CB	8.38	42.86	7.67	10.73
235 THR OG1	7.45	42.74	6.59	10.47
235 THR CG2	8.24	44.25	8.29	10.59
235 THR C	10.85	42.84	8.22	11.17
235 THR O	10.90	42.07	9.18	11.15
236 VAL N	11.68	43.86	8.04	11.56
236 VAL CA	12.79	44.13	8.93	12.10
236 VAL CB	14.12	44.02	8.14	12.05
236 VAL CG1	15.32	44.20	9.06	12.16
236 VAL CG2	14.18	42.68	7.40	12.05
236 VAL C	12.74	45.52	9.56	12.41
236 VAL O	12.44	46.50	8.89	12.45
237 ILE N	13.06	45.59	10.85	12.88
237 ILE CA	13.10	46.87	11.55	13.46
237 ILE CB	12.38	46.80	12.90	13.41
237 ILE CG2	12.40	48.18	13.56	13.48
237 ILE CG1	10.93	46.34	12.70	13.51
237 ILE CD1	10.12	46.29	13.99	13.61
237 ILE C	14.57	47.13	11.82	13.83
237 ILE O	15.26	46.27	12.38	13.85
238 VAL N	15.05	48.30	11.41	14.39
238 VAL CA	16.44	48.68	11.61	15.04
238 VAL CB	16.86	49.74	10.57	14.98
238 VAL CG1	18.32	50.12	10.77	15.06
238 VAL CG2	16.62	49.21	9.16	15.10
238 VAL C	16.61	49.26	13.02	15.42
238 VAL O	15.94	50.23	13.38	15.55
239 THR N	17.47	48.65	13.83	15.99

239 THR CA	17.72	49.14	15.19	16.57
239 THR CB	17.02	48.27	16.26	16.57
239 THR OG1	17.81	47.11	16.53	16.68
239 THR CG2	15.62	47.85	15.80	16.66
239 THR C	19.21	49.13	15.48	16.93
239 THR O	19.98	48.42	14.82	16.98
240 LYS N	19.63	49.91	16.47	17.40
240 LYS CA	21.04	50.00	16.83	17.87
240 LYS CB	21.24	51.07	17.91	18.07
240 LYS CG	20.39	50.88	19.14	18.31
240 LYS CD	20.61	52.00	20.15	18.57
240 LYS CE	19.68	51.88	21.34	18.74
240 LYS NZ	18.25	51.89	20.92	18.95
240 LYS C	21.62	48.68	17.30	18.09
240 LYS O	22.83	48.46	17.20	18.22
241 ASP N	20.77	47.80	17.80	18.33
241 ASP CA	21.22	46.50	18.29	18.48
241 ASP CB	20.50	46.14	19.59	18.81
241 ASP CG	20.80	47.12	20.70	19.03
241 ASP OD1	22.00	47.31	21.02	19.26
241 ASP OD2	19.84	47.70	21.25	19.26
241 ASP C	21.01	45.39	17.27	18.42
241 ASP O	21.00	44.21	17.64	18.49
242 GLY N	20.84	45.76	16.01	18.26
242 GLY CA	20.65	44.75	14.98	18.01
242 GLY C	19.26	44.75	14.39	17.79
242 GLY O	18.32	45.29	14.98	17.91
243 PRO N	19.09	44.16	13.20	17.56
243 PRO CD	20.11	43.57	12.31	17.53
243 PRO CA	17.77	44.12	12.57	17.29
243 PRO CB	18.08	43.72	11.13	17.35
243 PRO CG	19.27	42.83	11.30	17.44
243 PRO C	16.80	43.15	13.24	17.01
243 PRO O	17.18	42.05	13.63	17.04
244 ILE N	15.55	43.58	13.36	16.67
244 ILE CA	14.50	42.76	13.95	16.32
244 ILE CB	13.61	43.56	14.92	16.40
244 ILE CG2	12.45	42.69	15.41	16.43
244 ILE CG1	14.43	44.07	16.10	16.49
244 ILE CD1	13.62	44.89	17.10	16.63
244 ILE C	13.60	42.30	12.81	15.98
244 ILE O	13.01	43.12	12.12	15.97
245 LEU N	13.51	40.99	12.60	15.63

245 LEU CA	12.65	40.45	11.55	15.26
245 LEU CB	13.27	39.20	10.92	15.29
245 LEU CG	14.36	39.36	9.87	15.41
245 LEU CD1	15.57	40.07	10.46	15.45
245 LEU CD2	14.74	37.98	9.35	15.44
245 LEU C	11.31	40.09	12.16	15.01
245 LEU O	11.20	39.09	12.87	15.02
246 THR N	10.29	40.90	11.90	14.65
246 THR CA	8.97	40.65	12.46	14.33
246 THR CB	8.02	41.83	12.23	14.19
246 THR OG1	7.74	41.95	10.83	13.98
246 THR CG2	8.64	43.13	12.73	14.07
246 THR C	8.33	39.41	11.84	14.27
246 THR O	7.44	38.81	12.43	14.09
247 THR N	8.81	39.02	10.66	14.28
247 THR CA	8.24	37.88	9.96	14.41
247 THR CB	8.06	38.17	8.47	14.24
247 THR OG1	9.28	38.68	7.94	14.02
247 THR CG2	6.95	39.19	8.27	14.06
247 THR C	9.02	36.58	10.11	14.72
247 THR O	8.84	35.63	9.35	14.58
248 LYS N	9.91	36.54	11.10	15.14
248 LYS CA	10.68	35.34	11.35	15.67
248 LYS CB	12.18	35.62	11.38	15.82
248 LYS CG	13.01	34.36	11.62	16.14
248 LYS CD	14.49	34.66	11.63	16.43
248 LYS CE	15.29	33.43	12.02	16.61
248 LYS NZ	16.75	33.73	12.07	16.87
248 LYS C	10.26	34.77	12.70	15.94
248 LYS O	10.18	35.49	13.70	16.02
249 ILE N	9.95	33.48	12.70	16.30
249 ILE CA	9.55	32.77	13.90	16.70
249 ILE CB	8.39	31.80	13.62	16.72
249 ILE CG2	8.12	30.92	14.84	16.75
249 ILE CG1	7.13	32.59	13.24	16.71
249 ILE CD1	5.91	31.73	12.96	16.67
249 ILE C	10.78	31.99	14.34	16.95
249 ILE O	10.93	30.84	13.88	17.20
249 ILE OT	11.59	32.55	15.11	17.26
301 HOH O	10.50	34.31	4.32	9.06
302 HOH O	5.57	43.83	10.68	9.81
303 HOH O	-1.47	37.94	1.86	12.48
304 HOH O	9.79	31.23	-7.03	11.64

305	HOH	O	3.89	34.95	-5.27	11.03
306	HOH	O	15.78	21.59	-8.09	10.36
307	HOH	O	1.48	24.02	-11.09	12.98
308	HOH	O	2.97	15.64	-9.85	13.15
309	HOH	O	7.92	29.43	5.32	13.72
310	HOH	O	0.01	23.07	6.64	14.54
311	HOH	O	15.63	45.72	-8.03	12.44
312	HOH	O	10.09	28.99	-15.19	11.95
313	HOH	O	18.01	39.43	-18.99	16.32
314	HOH	O	-0.95	44.41	14.47	13.37
315	HOH	O	-0.66	38.44	20.34	14.96
316	HOH	O	-1.55	34.10	-12.27	12.53
317	HOH	O	19.17	48.37	-2.30	15.29
318	HOH	O	0.12	30.41	-9.59	13.28
319	HOH	O	1.38	39.43	-0.52	14.20
320	HOH	O	17.49	50.72	-2.91	16.84
321	HOH	O	17.02	43.84	-2.49	13.68
322	HOH	O	28.15	32.65	-2.10	15.80
323	HOH	O	6.84	38.82	15.12	12.81
324	HOH	O	6.59	25.34	6.77	15.48
325	HOH	O	12.11	26.54	2.56	15.55
326	HOH	O	9.17	23.20	1.33	16.34
327	HOH	O	12.02	32.56	8.27	16.56
328	HOH	O	-9.74	24.52	0.67	20.03
329	HOH	O	10.45	30.81	-11.10	14.20
330	HOH	O	27.52	35.27	-0.58	18.28
331	HOH	O	25.11	45.75	-8.22	17.53
332	HOH	O	-1.30	30.42	-12.80	15.06
333	HOH	O	19.02	56.83	12.96	16.84
334	HOH	O	-8.50	38.80	4.37	16.78
335	HOH	O	-6.38	18.76	-3.02	19.40
336	HOH	O	-10.59	34.20	-0.11	17.10
337	HOH	O	21.30	50.53	-4.76	18.10
338	HOH	O	21.45	28.88	1.32	19.23
339	HOH	O	21.88	54.48	-0.26	16.58
340	HOH	O	6.49	38.98	-4.48	17.69
341	HOH	O	0.11	48.00	19.88	17.22
342	HOH	O	10.10	52.62	6.29	15.23
343	HOH	O	21.00	22.73	-6.38	16.72
344	HOH	O	24.86	54.24	-3.40	22.28
345	HOH	O	7.92	55.12	5.89	19.85
346	HOH	O	14.71	39.07	14.56	19.07
347	HOH	O	26.86	45.72	0.92	19.88

348	HOH	O	22.02	40.61	-12.44	18.41
349	HOH	O	22.74	38.00	8.33	19.02
350	HOH	O	-9.45	24.82	-6.24	21.83
351	HOH	O	13.78	37.27	-21.84	19.18
352	HOH	O	4.99	28.20	12.08	20.77
353	HOH	O	-5.01	33.74	-15.69	20.64
354	HOH	O	1.17	27.89	-16.92	20.59
355	HOH	O	0.17	44.15	19.11	19.87
356	HOH	O	-3.41	22.84	-13.56	21.42
357	HOH	O	-5.14	28.62	-13.47	20.90
358	HOH	O	-1.85	19.72	1.80	20.71
359	HOH	O	6.48	21.09	-1.06	20.45
360	HOH	O	28.11	42.45	-8.13	18.62
361	HOH	O	-12.26	26.83	-2.91	22.09
362	HOH	O	6.67	56.62	9.97	19.68
363	HOH	O	4.01	47.86	26.45	17.27
364	HOH	O	18.69	59.47	3.77	23.06
365	HOH	O	0.16	20.37	6.01	23.36
366	HOH	O	22.30	49.21	4.75	18.77
367	HOH	O	-7.86	33.69	-6.02	19.95
368	HOH	O	10.46	12.87	-7.36	18.01
369	HOH	O	11.00	20.66	-13.11	21.77
370	HOH	O	14.21	19.07	-4.63	19.48
371	HOH	O	27.85	28.82	-6.89	22.74
372	HOH	O	-6.38	47.34	10.32	18.97
373	HOH	O	-10.01	39.83	10.28	20.93
374	HOH	O	26.70	64.11	0.15	20.24
375	HOH	O	3.20	24.97	9.63	25.45
376	HOH	O	-2.60	51.70	4.38	20.78
377	HOH	O	13.88	54.45	-2.97	20.82
378	HOH	O	6.18	26.81	-16.96	18.19
379	HOH	O	10.58	28.33	8.39	23.90
380	HOH	O	7.39	21.08	-12.28	23.32
381	HOH	O	0.13	47.78	24.35	22.62
382	HOH	O	26.15	36.21	-12.96	20.40
383	HOH	O	8.96	24.34	-14.66	17.57
384	HOH	O	-1.01	26.64	-15.30	20.12
385	HOH	O	11.88	19.84	-2.20	20.50
386	HOH	O	24.49	44.87	4.87	22.28
387	HOH	O	-10.21	35.98	5.99	18.66
388	HOH	O	9.21	13.44	-4.01	25.85
389	HOH	O	14.98	29.54	2.33	24.61
390	HOH	O	7.93	59.43	12.87	24.17

391	HOH	O	-0.26	23.55	11.19	23.78
392	HOH	O	-12.06	39.39	7.08	24.15
393	HOH	O	4.98	40.38	-21.60	22.64
394	HOH	O	10.69	29.72	6.01	18.43
395	HOH	O	24.36	29.29	-12.38	22.73
396	HOH	O	28.22	43.44	-0.25	25.25
397	HOH	O	-6.56	51.42	11.24	21.57
398	HOH	O	-13.34	29.31	1.75	23.21
399	HOH	O	19.63	47.05	12.32	20.88
400	HOH	O	4.95	19.45	5.14	23.22
401	HOH	O	20.89	22.41	-14.55	24.54
402	HOH	O	23.32	50.74	-11.13	22.14
403	HOH	O	24.62	27.54	-2.49	22.10
404	HOH	O	10.41	25.28	-17.89	22.27
405	HOH	O	12.30	57.28	5.52	24.16
406	HOH	O	4.64	24.76	-15.47	24.23
407	HOH	O	27.73	38.82	4.59	24.95
408	HOH	O	17.31	29.62	-17.22	21.80
409	HOH	O	11.27	56.97	-1.16	23.68
410	HOH	O	26.93	42.10	3.67	21.90
411	HOH	O	8.72	44.98	-17.85	21.75
412	HOH	O	8.03	47.25	-4.59	21.41
413	HOH	O	4.14	21.80	-13.55	24.99
414	HOH	O	10.17	30.45	-23.51	22.48
415	HOH	O	2.62	20.87	9.35	24.58
416	HOH	O	-3.74	18.10	-1.15	25.06
417	HOH	O	2.04	18.34	2.49	25.70
418	HOH	O	-7.43	45.03	12.12	22.88
419	HOH	O	3.58	30.30	-20.07	26.38
420	HOH	O	-10.04	21.86	-8.06	26.34
421	HOH	O	6.53	32.82	-19.37	22.03
422	HOH	O	26.25	50.66	-1.04	22.34
423	HOH	O	4.96	12.79	-7.27	21.96
424	HOH	O	30.77	47.25	7.48	24.89
425	HOH	O	5.92	21.44	8.83	26.99
426	HOH	O	7.46	53.62	23.92	23.43
427	HOH	O	24.97	34.17	3.43	22.85
428	HOH	O	-6.37	22.14	2.31	24.19
429	HOH	O	14.77	22.58	-16.65	23.42
430	HOH	O	3.57	54.77	-1.91	25.37
431	HOH	O	22.09	24.38	-11.40	21.89
432	HOH	O	-3.17	29.64	-17.16	24.28
433	HOH	O	13.39	57.89	1.13	23.28

434	HOH	O	12.52	49.15	17.84	24.31
435	HOH	O	-2.08	47.31	18.20	24.25
436	HOH	O	-8.48	32.84	-9.78	23.74
437	HOH	O	7.89	56.57	-0.91	25.49
438	HOH	O	2.24	54.17	19.67	21.14
439	HOH	O	20.06	27.95	5.10	26.39
440	HOH	O	27.74	54.69	-2.52	22.59
441	HOH	O	5.78	17.42	-1.67	24.72
442	HOH	O	-2.46	21.51	9.49	26.75
443	HOH	O	14.66	33.57	6.02	25.13
444	HOH	O	9.66	29.46	10.67	17.72
445	HOH	O	24.67	52.28	13.32	23.17
446	HOH	O	26.52	38.92	-13.27	24.93
447	HOH	O	25.12	34.05	7.68	26.03
448	HOH	O	26.01	25.28	-8.92	24.50
449	HOH	O	25.09	25.29	-5.13	25.06
450	HOH	O	8.27	17.86	-15.20	26.25
451	HOH	O	22.34	30.07	-15.27	24.43
452	HOH	O	18.62	34.74	-23.36	24.16
453	HOH	O	10.20	50.69	19.86	25.64
454	HOH	O	4.22	37.79	-5.22	11.06
455	HOH	O	2.45	13.45	-8.33	15.64
456	HOH	O	-2.56	29.86	-9.55	15.16
457	HOH	O	-9.51	38.40	6.83	15.69
458	HOH	O	-3.38	31.98	-11.92	14.11
459	HOH	O	19.26	52.40	-4.23	17.67
460	HOH	O	13.22	27.93	0.45	17.00
461	HOH	O	8.82	26.70	-16.12	17.14
462	HOH	O	-9.17	31.97	-0.82	16.61
463	HOH	O	14.39	43.99	-1.92	14.00
464	HOH	O	26.84	44.47	-6.39	16.06
465	HOH	O	-1.84	44.64	17.02	19.03
466	HOH	O	10.06	34.39	-7.29	15.99
467	HOH	O	1.18	23.04	9.02	18.90
468	HOH	O	12.44	38.17	-18.77	15.25
469	HOH	O	7.30	23.12	5.05	19.32
470	HOH	O	-11.23	38.31	12.21	20.31
471	HOH	O	28.60	30.16	-0.68	18.62
472	HOH	O	-0.73	26.20	11.41	21.74
473	HOH	O	24.27	39.15	-11.42	19.76
474	HOH	O	4.55	14.77	-12.02	19.53
475	HOH	O	-0.59	18.81	4.03	21.27
476	HOH	O	5.93	24.23	9.11	22.95

477	HOH	O	-8.21	22.36	-10.67	21.87
478	HOH	O	-3.98	21.05	3.15	22.46
479	HOH	O	-8.85	28.81	-12.01	22.91
480	HOH	O	5.97	44.02	-19.72	23.69
481	HOH	O	-10.40	40.78	3.46	22.30
482	HOH	O	4.50	19.36	-14.69	22.88
483	HOH	O	14.04	31.14	4.55	21.83
484	HOH	O	30.51	41.31	-7.64	23.60
485	HOH	O	21.07	36.06	8.80	23.18
486	HOH	O	4.08	29.47	16.54	23.69
487	HOH	O	29.17	37.84	-0.16	21.62
488	HOH	O	20.00	54.35	17.19	23.32
489	HOH	O	15.94	30.37	-19.31	24.71
490	HOH	O	20.46	60.80	2.12	23.18
491	HOH	O	23.44	22.82	-8.19	24.08
492	HOH	O	-4.17	51.23	-1.97	24.09
493	HOH	O	-11.19	28.95	3.59	22.64
494	HOH	O	6.98	22.69	-15.48	23.33
495	HOH	O	8.12	30.80	-9.06	13.51
496	HOH	O	13.70	31.03	-1.77	16.61
497	HOH	O	-13.99	28.89	-2.79	22.29
498	HOH	O	-5.62	32.23	-13.46	19.99
499	HOH	O	8.76	17.86	8.23	23.45
500	HOH	O	19.03	37.00	-21.38	22.06
300	737	C1	1.79	42.89	-2.36	31.43
300	737	C2	3.20	42.72	-2.05	31.13
300	737	C3	1.29	42.49	-3.63	31.62
300	737	C4	0.88	43.44	-1.42	31.83
300	737	C5	4.24	43.62	-1.92	31.00
300	737	N6	3.81	41.53	-1.80	30.99
300	737	C7	-0.08	42.66	-3.93	31.70
300	737	C8	-0.49	43.61	-1.73	31.96
300	737	N9	5.39	42.96	-1.62	30.83
300	737	N10	5.12	41.67	-1.54	30.83
300	737	C11	-0.97	43.22	-2.99	31.79
300	737	I12	-0.82	42.07	-5.76	31.66
253	ZN2	ZN	6.76	43.46	-0.66	18.13
254	ZN2	ZN	5.51	40.30	-0.30	13.79

Table III

Provides a three dimensional protein coordinate set of an *S. aureus* methionine aminopeptidase crystalline structure of an inhibitor complex with 5-benzofuran-2-yl-1-H-[1,2,3]triazole.

Residue	Atom	X	Y	Z	B
1	MET CB	6.23	53.31	9.47	20.78
1	MET CG	6.51	52.11	10.37	20.85
1	MET SD	5.13	51.60	11.41	21.11
1	MET CE	5.27	52.76	12.79	21.00
1	MET C	8.66	53.80	9.55	20.75
1	MET O	9.60	53.03	9.40	20.70
1	MET N	7.67	52.75	7.54	20.67
1	MET CA	7.44	53.73	8.64	20.72
2	ILE N	8.62	54.73	10.50	20.85
2	ILE CA	9.70	54.87	11.47	20.87
2	ILE CB	10.29	56.30	11.47	20.94
2	ILE CG2	11.44	56.37	12.46	21.01
2	ILE CG1	10.75	56.69	10.06	21.03
2	ILE CD1	11.83	55.79	9.48	21.06
2	ILE C	9.12	54.61	12.85	20.86
2	ILE O	8.28	55.37	13.32	20.90
3	VAL N	9.55	53.52	13.49	20.88
3	VAL CA	9.07	53.16	14.82	20.92
3	VAL CB	9.53	51.74	15.22	20.97
3	VAL CG1	9.06	51.41	16.63	20.98
3	VAL CG2	8.96	50.72	14.23	21.00
3	VAL C	9.60	54.13	15.87	21.00
3	VAL O	10.78	54.47	15.88	20.98
4	LYS N	8.71	54.57	16.76	21.11
4	LYS CA	9.07	55.49	17.83	21.18
4	LYS CB	8.49	56.88	17.57	21.34
4	LYS CG	9.12	57.66	16.42	21.64
4	LYS CD	10.60	57.93	16.66	21.83
4	LYS CE	11.19	58.79	15.55	22.01
4	LYS NZ	12.66	58.96	15.69	22.18
4	LYS C	8.60	55.01	19.20	21.13
4	LYS O	9.21	55.33	20.22	21.15
5	THR N	7.50	54.25	19.24	21.00
5	THR CA	6.97	53.76	20.52	20.92
5	THR CB	5.52	54.26	20.76	20.92
5	THR OG1	4.63	53.63	19.83	20.79
5	THR CG2	5.44	55.77	20.61	20.97
5	THR C	6.95	52.24	20.65	20.90
5	THR O	6.92	51.51	19.65	20.87

6 GLU N	6.94	51.77	21.89	20.82
6 GLU CA	6.90	50.35	22.19	20.66
6 GLU CB	6.96	50.14	23.71	21.01
6 GLU CG	6.69	48.72	24.21	21.47
6 GLU CD	7.79	47.74	23.85	21.71
6 GLU OE1	8.97	48.04	24.12	22.01
6 GLU OE2	7.47	46.65	23.30	21.88
6 GLU C	5.61	49.75	21.62	20.36
6 GLU O	5.59	48.61	21.17	20.34
7 GLU N	4.53	50.54	21.62	19.97
7 GLU CA	3.25	50.07	21.11	19.65
7 GLU CB	2.14	51.09	21.39	19.99
7 GLU CG	1.90	51.35	22.87	20.37
7 GLU CD	3.12	51.88	23.58	20.60
7 GLU OE1	3.70	52.89	23.12	20.78
7 GLU OE2	3.52	51.29	24.60	20.94
7 GLU C	3.31	49.78	19.61	19.22
7 GLU O	2.76	48.77	19.14	19.19
8 GLU N	3.96	50.66	18.85	18.76
8 GLU CA	4.07	50.45	17.41	18.24
8 GLU CB	4.80	51.62	16.75	18.37
8 GLU CG	4.10	52.95	16.93	18.47
8 GLU CD	4.88	54.13	16.34	18.61
8 GLU OE1	6.12	54.15	16.47	18.62
8 GLU OE2	4.24	55.04	15.77	18.60
8 GLU C	4.84	49.16	17.16	17.83
8 GLU O	4.47	48.36	16.30	17.74
9 LEU N	5.92	48.97	17.92	17.39
9 LEU CA	6.74	47.77	17.78	16.96
9 LEU CB	7.94	47.83	18.73	17.07
9 LEU CG	8.84	46.59	18.79	17.08
9 LEU CD1	9.61	46.42	17.49	17.25
9 LEU CD2	9.82	46.74	19.95	17.22
9 LEU C	5.93	46.51	18.05	16.71
9 LEU O	6.06	45.52	17.34	16.62
10 GLN N	5.10	46.55	19.09	16.29
10 GLN CA	4.29	45.38	19.42	15.87
10 GLN CB	3.57	45.61	20.75	15.94
10 GLN CG	4.47	46.02	21.89	16.18
10 GLN CD	3.70	46.16	23.18	16.27
10 GLN OE1	2.49	46.40	23.16	16.32
10 GLN NE2	4.39	46.03	24.31	16.41
10 GLN C	3.27	45.10	18.32	15.52

10 GLN O	3.00	43.95	17.99	15.45
11 ALA N	2.71	46.16	17.75	15.03
11 ALA CA	1.73	45.98	16.69	14.60
11 ALA CB	1.09	47.31	16.35	14.54
11 ALA C	2.39	45.37	15.45	14.31
11 ALA O	1.81	44.50	14.81	14.30
12 LEU N	3.60	45.81	15.13	13.92
12 LEU CA	4.33	45.31	13.96	13.64
12 LEU CB	5.56	46.19	13.69	13.67
12 LEU CG	5.21	47.59	13.15	13.74
12 LEU CD1	6.39	48.55	13.25	13.76
12 LEU CD2	4.77	47.43	11.71	13.80
12 LEU C	4.76	43.86	14.18	13.43
12 LEU O	4.74	43.05	13.25	13.36
13 LYS N	5.14	43.52	15.41	13.19
13 LYS CA	5.54	42.16	15.72	13.00
13 LYS CB	6.16	42.09	17.10	13.18
13 LYS CG	7.50	42.76	17.19	13.41
13 LYS CD	8.02	42.67	18.60	13.64
13 LYS CE	9.47	43.09	18.69	13.93
13 LYS NZ	9.92	43.01	20.10	14.02
13 LYS C	4.32	41.24	15.64	12.76
13 LYS O	4.43	40.09	15.21	12.72
14 GLU N	3.17	41.76	16.05	12.46
14 GLU CA	1.93	40.99	16.02	12.11
14 GLU CB	0.77	41.80	16.62	12.31
14 GLU CG	-0.62	41.17	16.42	12.52
14 GLU CD	-0.81	39.88	17.21	12.69
14 GLU OE1	0.13	39.43	17.88	12.87
14 GLU OE2	-1.93	39.32	17.15	12.91
14 GLU C	1.58	40.58	14.59	11.74
14 GLU O	1.42	39.39	14.30	11.61
15 ILE N	1.46	41.56	13.69	11.42
15 ILE CA	1.12	41.28	12.29	11.11
15 ILE CB	0.78	42.60	11.50	11.27
15 ILE CG2	2.03	43.48	11.35	11.24
15 ILE CG1	0.24	42.25	10.11	11.31
15 ILE CD1	-0.99	41.37	10.13	11.43
15 ILE C	2.25	40.52	11.60	10.90
15 ILE O	2.02	39.76	10.65	10.72
16 GLY N	3.48	40.72	12.09	10.67
16 GLY CA	4.62	40.03	11.52	10.38
16 GLY C	4.49	38.55	11.79	10.35

16 GLY O	4.72	37.72	10.91	10.24
17 TYR N	4.11	38.21	13.02	10.35
17 TYR CA	3.94	36.81	13.42	10.40
17 TYR CB	3.61	36.70	14.91	10.66
17 TYR CG	3.27	35.28	15.31	11.00
17 TYR CD1	4.27	34.31	15.39	11.22
17 TYR CE1	3.95	32.97	15.62	11.39
17 TYR CD2	1.94	34.88	15.49	11.15
17 TYR CE2	1.61	33.53	15.72	11.36
17 TYR CZ	2.62	32.59	15.78	11.45
17 TYR OH	2.32	31.26	15.97	11.77
17 TYR C	2.84	36.12	12.63	10.23
17 TYR O	2.99	34.96	12.22	10.16
18 ILE N	1.73	36.83	12.46	10.03
18 ILE CA	0.59	36.30	11.73	9.79
18 ILE CB	-0.58	37.31	11.72	9.69
18 ILE CG2	-1.73	36.80	10.87	9.62
18 ILE CG1	-1.09	37.53	13.15	9.55
18 ILE CD1	-2.16	38.61	13.25	9.44
18 ILE C	0.97	35.95	10.29	9.75
18 ILE O	0.61	34.87	9.80	9.71
19 CYS N	1.70	36.84	9.62	9.73
19 CYS CA	2.11	36.60	8.24	9.68
19 CYS CB	2.73	37.86	7.65	9.70
19 CYS SG	1.44	39.11	7.32	10.06
19 CYS C	3.07	35.42	8.14	9.66
19 CYS O	2.97	34.60	7.22	9.70
20 ALA N	3.99	35.34	9.09	9.68
20 ALA CA	4.95	34.25	9.11	9.59
20 ALA CB	5.97	34.48	10.22	9.56
20 ALA C	4.20	32.95	9.35	9.67
20 ALA O	4.44	31.95	8.67	9.54
21 LYS N	3.30	32.95	10.33	9.79
21 LYS CA	2.50	31.78	10.66	10.05
21 LYS CB	1.51	32.15	11.78	10.30
21 LYS CG	0.58	31.04	12.20	10.86
21 LYS CD	1.31	29.84	12.79	11.34
21 LYS CE	0.26	28.87	13.32	11.72
21 LYS NZ	0.83	27.67	13.98	12.13
21 LYS C	1.75	31.27	9.43	9.97
21 LYS O	1.74	30.06	9.12	9.98
22 VAL N	1.12	32.20	8.72	9.93
22 VAL CA	0.38	31.88	7.50	9.95

22 VAL CB	-0.36	33.13	6.98	10.03
22 VAL CG1	-0.96	32.87	5.60	10.07
22 VAL CG2	-1.42	33.53	7.96	10.08
22 VAL C	1.31	31.35	6.42	9.85
22 VAL O	1.04	30.32	5.80	9.82
23 ARG N	2.42	32.06	6.20	9.83
23 ARG CA	3.39	31.65	5.19	9.75
23 ARG CB	4.59	32.59	5.21	9.74
23 ARG CG	5.64	32.34	4.13	9.71
23 ARG CD	6.95	32.96	4.58	9.70
23 ARG NE	7.41	32.29	5.79	9.57
23 ARG CZ	7.94	32.88	6.86	9.58
23 ARG NH1	8.11	34.20	6.88	9.29
23 ARG NH2	8.27	32.15	7.91	9.55
23 ARG C	3.86	30.23	5.48	9.81
23 ARG O	3.94	29.39	4.57	9.75
24 ASN N	4.18	29.96	6.74	9.88
24 ASN CA	4.64	28.62	7.09	10.04
24 ASN CB	5.06	28.56	8.57	9.93
24 ASN CG	6.37	29.29	8.85	9.88
24 ASN OD1	7.20	29.50	7.95	9.56
24 ASN ND2	6.58	29.65	10.11	9.88
24 ASN C	3.59	27.55	6.81	10.17
24 ASN O	3.89	26.51	6.21	10.24
25 THR N	2.35	27.79	7.24	10.41
25 THR CA	1.26	26.83	7.05	10.44
25 THR CB	-0.04	27.34	7.73	10.52
25 THR OG1	0.23	27.61	9.11	10.64
25 THR CG2	-1.14	26.28	7.67	10.62
25 THR C	1.00	26.52	5.57	10.50
25 THR O	0.81	25.36	5.18	10.34
26 MET N	1.00	27.56	4.74	10.47
26 MET CA	0.79	27.37	3.31	10.49
26 MET CB	0.64	28.73	2.61	10.26
26 MET CG	-0.64	29.45	3.00	10.07
26 MET SD	-0.73	31.14	2.39	9.79
26 MET CE	-0.94	30.86	0.63	9.76
26 MET C	1.92	26.57	2.68	10.63
26 MET O	1.68	25.70	1.83	10.61
27 GLN N	3.15	26.84	3.10	10.93
27 GLN CA	4.30	26.11	2.57	11.23
27 GLN CB	5.62	26.70	3.10	11.29
27 GLN CG	6.85	25.91	2.64	11.57

27 GLN CD	8.17	26.61	2.95	11.74
27 GLN OE1	8.25	27.45	3.85	11.92
27 GLN NE2	9.21	26.27	2.20	11.86
27 GLN C	4.20	24.62	2.93	11.35
27 GLN O	4.36	23.76	2.07	11.29
28 ALA N	3.90	24.32	4.20	11.48
28 ALA CA	3.79	22.93	4.62	11.66
28 ALA CB	3.62	22.85	6.15	11.56
28 ALA C	2.66	22.17	3.93	11.83
28 ALA O	2.69	20.94	3.84	11.78
29 ALA N	1.66	22.90	3.45	11.99
29 ALA CA	0.51	22.28	2.79	12.13
29 ALA CB	-0.76	23.07	3.09	12.00
29 ALA C	0.70	22.19	1.28	12.31
29 ALA O	-0.13	21.61	0.57	12.29
30 THR N	1.77	22.79	0.79	12.52
30 THR CA	2.05	22.76	-0.64	12.72
30 THR CB	3.00	23.90	-1.03	12.75
30 THR OG1	2.40	25.16	-0.70	12.88
30 THR CG2	3.27	23.87	-2.52	12.81
30 THR C	2.65	21.42	-1.05	12.80
30 THR O	3.78	21.10	-0.69	12.93
31 LYS N	1.86	20.64	-1.78	12.96
31 LYS CA	2.28	19.33	-2.26	13.21
31 LYS CB	1.95	18.25	-1.23	13.42
31 LYS CG	0.47	18.02	-1.01	13.76
31 LYS CD	0.22	16.85	-0.06	14.09
31 LYS CE	-1.17	16.30	-0.25	14.29
31 LYS NZ	-1.46	15.12	0.63	14.48
31 LYS C	1.57	19.02	-3.57	13.26
31 LYS O	0.56	19.65	-3.90	13.22
32 PRO N	2.10	18.07	-4.35	13.40
32 PRO CD	3.33	17.28	-4.14	13.45
32 PRO CA	1.46	17.71	-5.62	13.55
32 PRO CB	2.25	16.49	-6.08	13.54
32 PRO CG	3.62	16.77	-5.53	13.44
32 PRO C	-0.01	17.38	-5.34	13.68
32 PRO O	-0.32	16.74	-4.33	13.73
33 GLY N	-0.92	17.84	-6.20	13.78
33 GLY CA	-2.33	17.55	-6.00	13.83
33 GLY C	-3.19	18.67	-5.44	13.87
33 GLY O	-4.41	18.67	-5.63	13.98
34 ILE N	-2.59	19.64	-4.76	13.80

34 ILE CA	-3.36	20.74	-4.20	13.72
34 ILE CB	-2.76	21.18	-2.84	13.65
34 ILE CG2	-1.49	21.98	-3.06	13.55
34 ILE CG1	-3.76	22.06	-2.09	13.66
34 ILE CD1	-3.31	22.35	-0.67	13.71
34 ILE C	-3.39	21.93	-5.16	13.68
34 ILE O	-2.43	22.15	-5.90	13.69
35 THR N	-4.47	22.70	-5.18	13.68
35 THR CA	-4.53	23.86	-6.06	13.67
35 THR CB	-5.95	24.13	-6.60	13.59
35 THR OG1	-6.77	24.64	-5.54	13.57
35 THR CG2	-6.56	22.86	-7.17	13.64
35 THR C	-4.10	25.10	-5.28	13.73
35 THR O	-4.19	25.14	-4.05	13.65
36 THR N	-3.64	26.12	-6.00	13.87
36 THR CA	-3.21	27.36	-5.39	14.04
36 THR CB	-2.60	28.34	-6.44	14.10
36 THR OG1	-3.55	28.61	-7.48	14.22
36 THR CG2	-1.34	27.74	-7.05	14.07
36 THR C	-4.38	28.01	-4.67	14.06
36 THR O	-4.21	28.67	-3.65	14.06
37 LYS N	-5.58	27.80	-5.20	14.22
37 LYS CA	-6.77	28.35	-4.56	14.33
37 LYS CB	-8.02	28.10	-5.40	14.58
37 LYS CG	-9.30	28.61	-4.76	14.86
37 LYS CD	-9.25	30.12	-4.54	15.26
37 LYS CE	-10.58	30.65	-4.05	15.48
37 LYS NZ	-10.49	32.09	-3.71	15.79
37 LYS C	-6.94	27.70	-3.18	14.31
37 LYS O	-7.29	28.37	-2.22	14.34
38 GLU N	-6.70	26.39	-3.10	14.28
38 GLU CA	-6.81	25.69	-1.82	14.31
38 GLU CB	-6.57	24.19	-1.98	14.63
38 GLU CG	-7.73	23.43	-2.62	15.20
38 GLU CD	-7.35	22.01	-2.95	15.58
38 GLU OE1	-6.74	21.79	-4.01	15.73
38 GLU OE2	-7.64	21.11	-2.12	15.93
38 GLU C	-5.79	26.25	-0.83	14.17
38 GLU O	-6.07	26.38	0.36	14.01
39 LEU N	-4.60	26.57	-1.34	13.96
39 LEU CA	-3.55	27.14	-0.51	13.89
39 LEU CB	-2.24	27.23	-1.29	13.76
39 LEU CG	-1.60	25.88	-1.61	13.65

39 LEU CD1	-0.39	26.12	-2.51	13.52
39 LEU CD2	-1.19	25.19	-0.31	13.61
39 LEU C	-3.94	28.53	-0.01	13.98
39 LEU O	-3.63	28.91	1.11	13.90
40 ASP N	-4.65	29.27	-0.86	14.04
40 ASP CA	-5.09	30.61	-0.51	14.16
40 ASP CB	-5.63	31.31	-1.76	14.31
40 ASP CG	-5.79	32.81	-1.57	14.39
40 ASP OD1	-4.78	33.51	-1.34	14.45
40 ASP OD2	-6.95	33.29	-1.64	14.56
40 ASP C	-6.16	30.56	0.59	14.22
40 ASP O	-6.24	31.46	1.42	14.16
41 ASN N	-6.97	29.51	0.60	14.28
41 ASN CA	-8.02	29.39	1.61	14.49
41 ASN CB	-8.93	28.19	1.32	14.41
41 ASN CG	-9.72	28.35	0.05	14.38
41 ASN OD1	-9.99	29.46	-0.38	14.50
41 ASN ND2	-10.10	27.23	-0.56	14.33
41 ASN C	-7.46	29.25	3.02	14.61
41 ASN O	-8.13	29.61	3.99	14.66
42 ILE N	-6.25	28.73	3.12	14.83
42 ILE CA	-5.61	28.58	4.42	14.92
42 ILE CB	-4.29	27.81	4.32	14.87
42 ILE CG2	-3.60	27.75	5.67	14.92
42 ILE CG1	-4.55	26.40	3.79	14.81
42 ILE CD1	-3.29	25.63	3.48	14.72
42 ILE C	-5.35	29.98	4.97	15.07
42 ILE O	-5.57	30.23	6.16	15.08
43 ALA N	-4.91	30.89	4.11	15.25
43 ALA CA	-4.64	32.25	4.54	15.48
43 ALA CB	-3.99	33.05	3.40	15.40
43 ALA C	-5.95	32.91	4.97	15.67
43 ALA O	-6.00	33.59	5.99	15.74
44 LYS N	-7.01	32.70	4.19	15.93
44 LYS CA	-8.32	33.28	4.51	16.17
44 LYS CB	-9.36	32.84	3.49	16.28
44 LYS CG	-10.78	33.29	3.82	16.45
44 LYS CD	-11.77	32.81	2.77	16.76
44 LYS CE	-13.18	33.30	3.07	16.99
44 LYS NZ	-13.29	34.79	3.02	17.35
44 LYS C	-8.77	32.87	5.92	16.35
44 LYS O	-9.24	33.69	6.70	16.37
45 GLU N	-8.61	31.59	6.23	16.65

45 GLU CA	-9.00	31.06	7.54	16.98
45 GLU CB	-9.00	29.53	7.52	17.25
45 GLU CG	-10.07	28.91	6.62	17.69
45 GLU CD	-11.46	29.50	6.85	17.93
45 GLU OE1	-11.97	29.42	7.99	18.09
45 GLU OE2	-12.05	30.04	5.88	18.15
45 GLU C	-8.09	31.55	8.66	17.07
45 GLU O	-8.57	31.95	9.72	17.12
46 LEU N	-6.78	31.52	8.44	17.15
46 LEU CA	-5.86	31.99	9.47	17.23
46 LEU CB	-4.41	31.65	9.11	17.24
46 LEU CG	-4.04	30.16	9.22	17.35
46 LEU CD1	-2.65	29.94	8.68	17.41
46 LEU CD2	-4.14	29.71	10.67	17.46
46 LEU C	-6.00	33.49	9.71	17.26
46 LEU O	-5.94	33.94	10.86	17.31
47 PHE N	-6.19	34.27	8.65	17.24
47 PHE CA	-6.35	35.71	8.82	17.29
47 PHE CB	-6.52	36.44	7.47	17.23
47 PHE CG	-5.25	36.59	6.67	17.23
47 PHE CD1	-4.00	36.58	7.29	17.13
47 PHE CD2	-5.31	36.78	5.29	17.08
47 PHE CE1	-2.83	36.75	6.54	17.14
47 PHE CE2	-4.15	36.95	4.53	17.19
47 PHE CZ	-2.90	36.93	5.16	17.09
47 PHE C	-7.58	35.98	9.70	17.45
47 PHE O	-7.53	36.78	10.63	17.32
48 GLU N	-8.69	35.31	9.40	17.65
48 GLU CA	-9.91	35.49	10.18	17.88
48 GLU CB	-11.06	34.68	9.56	18.04
48 GLU CG	-12.38	34.74	10.33	18.44
48 GLU CD	-12.91	36.14	10.55	18.66
48 GLU OE1	-12.67	37.02	9.69	18.90
48 GLU OE2	-13.58	36.37	11.60	18.86
48 GLU C	-9.68	35.06	11.62	17.94
48 GLU O	-10.20	35.67	12.56	17.98
49 GLU N	-8.87	34.03	11.81	17.99
49 GLU CA	-8.57	33.53	13.15	18.12
49 GLU CB	-7.87	32.18	13.06	18.41
49 GLU CG	-7.23	31.73	14.36	18.92
49 GLU CD	-6.67	30.32	14.28	19.22
49 GLU OE1	-6.08	29.96	13.23	19.52
49 GLU OE2	-6.82	29.58	15.27	19.44

49 GLU C	-7.71	34.50	13.96	18.04
49 GLU O	-7.88	34.63	15.18	17.91
50 TYR N	-6.79	35.17	13.29	17.86
50 TYR CA	-5.90	36.10	13.97	17.83
50 TYR CB	-4.49	35.95	13.43	17.91
50 TYR CG	-3.87	34.63	13.78	18.11
50 TYR CD1	-3.57	34.32	15.11	18.16
50 TYR CE1	-2.96	33.11	15.44	18.23
50 TYR CD2	-3.55	33.70	12.80	18.11
50 TYR CE2	-2.94	32.49	13.12	18.19
50 TYR CZ	-2.64	32.20	14.44	18.23
50 TYR OH	-2.00	31.03	14.76	18.38
50 TYR C	-6.32	37.55	13.90	17.67
50 TYR O	-5.56	38.44	14.28	17.65
51 GLY N	-7.53	37.79	13.40	17.53
51 GLY CA	-8.03	39.15	13.30	17.33
51 GLY C	-7.27	40.02	12.32	17.21
51 GLY O	-7.21	41.24	12.50	17.19
52 ALA N	-6.70	39.41	11.29	17.02
52 ALA CA	-5.96	40.17	10.30	16.91
52 ALA CB	-4.57	39.57	10.09	16.88
52 ALA C	-6.71	40.21	8.98	16.86
52 ALA O	-7.67	39.46	8.76	16.70
53 ILE N	-6.26	41.08	8.10	16.87
53 ILE CA	-6.88	41.23	6.80	17.02
53 ILE CB	-7.69	42.54	6.74	17.18
53 ILE CG2	-8.16	42.79	5.33	17.31
53 ILE CG1	-8.87	42.45	7.71	17.44
53 ILE CD1	-9.86	41.35	7.36	17.57
53 ILE C	-5.84	41.24	5.71	16.94
53 ILE O	-4.76	41.82	5.86	16.82
54 SER N	-6.17	40.58	4.60	16.99
54 SER CA	-5.28	40.50	3.45	17.08
54 SER CB	-5.94	39.69	2.33	16.90
54 SER OG	-5.23	39.85	1.12	16.41
54 SER C	-4.91	41.88	2.93	17.32
54 SER O	-5.78	42.71	2.68	17.26
55 ALA N	-3.61	42.12	2.75	17.63
55 ALA CA	-3.14	43.41	2.24	18.01
55 ALA CB	-1.66	43.59	2.53	17.90
55 ALA C	-3.41	43.53	0.74	18.28
55 ALA O	-3.81	44.59	0.27	18.31
56 PRO N	-3.18	42.45	-0.02	18.54

56 PRO CD	-2.46	41.19	0.28	18.58
56 PRO CA	-3.44	42.57	-1.46	18.80
56 PRO CB	-3.06	41.20	-2.00	18.79
56 PRO CG	-1.96	40.77	-1.08	18.68
56 PRO C	-4.91	42.91	-1.75	19.07
56 PRO O	-5.20	43.70	-2.64	19.17
57 ILE N	-5.83	42.33	-0.98	19.37
57 ILE CA	-7.25	42.60	-1.20	19.70
57 ILE CB	-8.14	41.57	-0.47	19.69
57 ILE CG2	-9.62	41.98	-0.59	19.71
57 ILE CG1	-7.92	40.18	-1.08	19.71
57 ILE CD1	-8.63	39.07	-0.34	19.71
57 ILE C	-7.64	43.99	-0.73	19.92
57 ILE O	-8.40	44.70	-1.40	19.97
58 HIS N	-7.09	44.39	0.41	20.16
58 HIS CA	-7.38	45.69	1.01	20.33
58 HIS CB	-6.96	45.67	2.48	20.34
58 HIS CG	-7.20	46.96	3.20	20.45
58 HIS CD2	-8.11	47.30	4.13	20.46
58 HIS ND1	-6.43	48.09	2.99	20.42
58 HIS CE1	-6.86	49.06	3.76	20.39
58 HIS NE2	-7.89	48.62	4.46	20.41
58 HIS C	-6.75	46.88	0.29	20.43
58 HIS O	-7.42	47.88	0.02	20.40
59 ASP N	-5.46	46.77	-0.05	20.51
59 ASP CA	-4.74	47.85	-0.73	20.62
59 ASP CB	-3.24	47.77	-0.41	20.68
59 ASP CG	-2.91	48.16	1.03	20.73
59 ASP OD1	-3.56	47.64	1.96	20.81
59 ASP OD2	-1.98	48.97	1.24	20.80
59 ASP C	-4.90	47.87	-2.25	20.68
59 ASP O	-5.13	48.93	-2.84	20.80
60 GLU N	-4.77	46.71	-2.89	20.72
60 GLU CA	-4.85	46.63	-4.36	20.69
60 GLU CB	-3.64	45.86	-4.89	20.92
60 GLU CG	-2.32	46.09	-4.15	21.32
60 GLU CD	-1.73	47.48	-4.33	21.60
60 GLU OE1	-1.55	47.93	-5.49	21.88
60 GLU OE2	-1.42	48.13	-3.30	21.74
60 GLU C	-6.12	45.98	-4.91	20.50
60 GLU O	-6.30	45.89	-6.13	20.56
61 ASN N	-7.00	45.54	-4.03	20.25
61 ASN CA	-8.22	44.86	-4.46	19.98

61 ASN CB	-9.14	45.81	-5.24	20.16
61 ASN CG	-10.53	45.24	-5.43	20.17
61 ASN OD1	-10.95	44.36	-4.68	20.33
61 ASN ND2	-11.25	45.74	-6.42	20.31
61 ASN C	-7.83	43.67	-5.32	19.73
61 ASN O	-8.51	43.32	-6.28	19.74
62 PHE N	-6.71	43.05	-4.94	19.36
62 PHE CA	-6.18	41.88	-5.62	18.95
62 PHE CB	-4.80	41.52	-5.03	18.93
62 PHE CG	-4.10	40.39	-5.75	18.92
62 PHE CD1	-3.39	40.63	-6.92	18.93
62 PHE CD2	-4.13	39.09	-5.23	18.93
62 PHE CE1	-2.71	39.59	-7.57	18.90
62 PHE CE2	-3.46	38.05	-5.88	18.89
62 PHE CZ	-2.75	38.30	-7.05	18.88
62 PHE C	-7.14	40.73	-5.41	18.61
62 PHE O	-7.66	40.52	-4.31	18.51
63 PRO N	-7.42	39.97	-6.47	18.30
63 PRO CD	-6.99	40.22	-7.86	18.33
63 PRO CA	-8.33	38.83	-6.40	18.07
63 PRO CB	-8.63	38.54	-7.87	18.18
63 PRO CG	-7.34	38.93	-8.55	18.26
63 PRO C	-7.65	37.65	-5.70	17.71
63 PRO O	-7.32	36.65	-6.34	17.70
64 GLY N	-7.45	37.77	-4.39	17.34
64 GLY CA	-6.82	36.69	-3.65	16.84
64 GLY C	-6.29	37.13	-2.29	16.44
64 GLY O	-5.88	38.27	-2.12	16.41
65 GLN N	-6.31	36.22	-1.32	16.13
65 GLN CA	-5.83	36.54	0.01	15.75
65 GLN CB	-6.07	35.37	0.96	15.78
65 GLN CG	-7.53	35.01	1.20	16.03
65 GLN CD	-8.30	36.09	1.94	16.19
65 GLN OE1	-7.73	36.82	2.77	16.25
65 GLN NE2	-9.59	36.20	1.65	16.19
65 GLN C	-4.33	36.83	-0.05	15.43
65 GLN O	-3.84	37.75	0.60	15.38
66 THR N	-3.63	36.04	-0.85	15.13
66 THR CA	-2.18	36.16	-1.01	14.82
66 THR CB	-1.47	35.04	-0.25	14.86
66 THR OG1	-1.82	33.79	-0.84	14.85
66 THR CG2	-1.87	35.04	1.22	14.77
66 THR C	-1.77	36.01	-2.48	14.65

66 THR O	-2.62	35.77	-3.34	14.73
67 CYS N	-0.47	36.12	-2.74	14.43
67 CYS CA	0.08	35.97	-4.08	14.14
67 CYS CB	1.04	37.12	-4.40	14.24
67 CYS SG	0.24	38.73	-4.58	14.54
67 CYS C	0.84	34.65	-4.15	13.93
67 CYS O	1.75	34.41	-3.36	13.81
68 ILE N	0.46	33.79	-5.09	13.74
68 ILE CA	1.11	32.49	-5.27	13.59
68 ILE CB	0.14	31.33	-4.95	13.56
68 ILE CG2	0.86	29.99	-5.11	13.63
68 ILE CG1	-0.36	31.46	-3.51	13.59
68 ILE CD1	-1.49	30.51	-3.19	13.73
68 ILE C	1.52	32.40	-6.73	13.51
68 ILE O	0.67	32.35	-7.62	13.59
69 SER N	2.82	32.37	-6.96	13.39
69 SER CA	3.40	32.34	-8.30	13.25
69 SER CB	4.37	33.51	-8.43	13.19
69 SER OG	3.75	34.72	-7.98	13.10
69 SER C	4.13	31.02	-8.54	13.23
69 SER O	4.99	30.63	-7.75	13.18
70 VAL N	3.81	30.33	-9.64	13.19
70 VAL CA	4.43	29.04	-9.93	13.24
70 VAL CB	3.38	27.90	-9.94	13.33
70 VAL CG1	4.01	26.57	-10.34	13.39
70 VAL CG2	2.73	27.80	-8.57	13.35
70 VAL C	5.22	28.99	-11.23	13.32
70 VAL O	4.75	29.45	-12.26	13.25
71 ASN N	6.43	28.43	-11.17	13.35
71 ASN CA	7.30	28.27	-12.33	13.56
71 ASN CB	6.81	27.10	-13.19	13.48
71 ASN CG	6.78	25.78	-12.42	13.47
71 ASN OD1	7.59	25.55	-11.54	13.42
71 ASN ND2	5.84	24.92	-12.78	13.51
71 ASN C	7.54	29.50	-13.21	13.75
71 ASN O	8.45	30.29	-12.95	13.68
72 GLU N	6.75	29.66	-14.28	13.97
72 GLU CA	6.96	30.79	-15.16	14.22
72 GLU CB	6.20	30.61	-16.49	14.17
72 GLU CG	4.69	30.83	-16.46	14.32
72 GLU CD	3.93	29.72	-15.76	14.34
72 GLU OE1	4.44	28.58	-15.69	14.40
72 GLU OE2	2.81	29.99	-15.30	14.51

72 GLU C	6.57	32.11	-14.50	14.31
72 GLU O	7.02	33.18	-14.89	14.39
73 GLU N	5.72	32.03	-13.48	14.45
73 GLU CA	5.30	33.23	-12.76	14.57
73 GLU CB	3.94	33.02	-12.13	14.70
73 GLU CG	2.92	32.54	-13.10	14.77
73 GLU CD	1.60	32.27	-12.42	14.88
73 GLU OE1	1.62	31.63	-11.34	14.80
73 GLU OE2	0.57	32.70	-12.97	14.97
73 GLU C	6.31	33.53	-11.66	14.65
73 GLU O	6.66	32.66	-10.88	14.65
74 VAL N	6.76	34.78	-11.62	14.82
74 VAL CA	7.75	35.23	-10.65	14.95
74 VAL CB	8.74	36.24	-11.29	14.94
74 VAL CG1	9.76	36.71	-10.26	14.91
74 VAL CG2	9.44	35.59	-12.48	14.96
74 VAL C	7.11	35.90	-9.45	15.05
74 VAL O	7.60	35.80	-8.33	15.04
75 ALA N	6.00	36.59	-9.68	15.21
75 ALA CA	5.36	37.28	-8.57	15.38
75 ALA CB	6.21	38.49	-8.17	15.28
75 ALA C	3.95	37.73	-8.94	15.47
75 ALA O	3.60	37.79	-10.11	15.49
76 HIS N	3.16	38.02	-7.91	15.64
76 HIS CA	1.78	38.47	-8.08	15.89
76 HIS CB	1.74	39.77	-8.88	16.35
76 HIS CG	2.41	40.92	-8.21	16.73
76 HIS CD2	2.27	42.26	-8.40	16.99
76 HIS ND1	3.41	40.77	-7.28	16.99
76 HIS CE1	3.87	41.96	-6.92	17.05
76 HIS NE2	3.19	42.88	-7.58	17.22
76 HIS C	0.88	37.43	-8.75	15.89
76 HIS O	-0.10	37.79	-9.39	15.82
77 GLY N	1.23	36.15	-8.60	15.84
77 GLY CA	0.43	35.09	-9.19	15.84
77 GLY C	-0.93	35.04	-8.52	15.82
77 GLY O	-1.05	35.26	-7.31	15.72
78 ILE N	-1.97	34.74	-9.30	15.85
78 ILE CA	-3.33	34.69	-8.79	15.94
78 ILE CB	-4.33	35.20	-9.87	16.19
78 ILE CG2	-5.73	35.27	-9.31	16.15
78 ILE CG1	-3.91	36.60	-10.34	16.30
78 ILE CD1	-4.73	37.11	-11.51	16.42

78 ILE C -3.75 33.27 -8.39 15.98
78 ILE O -3.65 32.35 -9.19 15.92
79 PRO N -4.19 33.09 -7.13 16.02
79 PRO CD -4.17 34.04 -6.00 16.03
79 PRO CA -4.62 31.76 -6.67 15.97
79 PRO CB -5.06 32.02 -5.24 16.04
79 PRO CG -4.12 33.12 -4.80 16.00
79 PRO C -5.76 31.30 -7.57 16.02
79 PRO O -6.66 32.09 -7.89 16.05
80 SER N -5.75 30.04 -7.96 16.04
80 SER CA -6.78 29.54 -8.86 16.13
80 SER CB -6.48 30.07 -10.26 16.17
80 SER OG -5.24 29.55 -10.72 16.26
80 SER C -6.81 28.02 -8.90 16.20
80 SER O -6.23 27.36 -8.04 16.22
81 LYS N -7.47 27.48 -9.91 16.18
81 LYS CA -7.58 26.03 -10.06 16.14
81 LYS CB -8.66 25.70 -11.09 16.29
81 LYS CG -10.01 26.35 -10.79 16.59
81 LYS CD -10.85 26.52 -12.05 16.89
81 LYS CE -12.16 27.25 -11.74 17.00
81 LYS NZ -12.99 27.54 -12.94 17.15
81 LYS C -6.26 25.37 -10.45 15.94
81 LYS O -6.19 24.15 -10.59 15.98
82 ARG N -5.22 26.18 -10.65 15.73
82 ARG CA -3.92 25.63 -11.02 15.55
82 ARG CB -2.87 26.75 -11.10 15.55
82 ARG CG -1.47 26.24 -11.35 15.43
82 ARG CD -0.56 27.33 -11.85 15.54
82 ARG NE 0.66 26.78 -12.43 15.55
82 ARG CZ 1.54 27.50 -13.13 15.62
82 ARG NH1 1.33 28.79 -13.33 15.58
82 ARG NH2 2.62 26.92 -13.63 15.58
82 ARG C -3.47 24.59 -9.98 15.46
82 ARG O -3.42 24.89 -8.79 15.34
83 VAL N -3.16 23.38 -10.43 15.34
83 VAL CA -2.74 22.33 -9.50 15.21
83 VAL CB -3.25 20.93 -9.93 15.31
83 VAL CG1 -2.54 20.45 -11.18 15.43
83 VAL CG2 -3.05 19.94 -8.80 15.39
83 VAL C -1.22 22.25 -9.36 15.04
83 VAL O -0.49 22.32 -10.35 14.99
84 ILE N -0.75 22.10 -8.13 14.81

84	ILE	CA	0.69	21.99	-7.87	14.67
84	ILE	CB	1.01	22.15	-6.36	14.60
84	ILE	CG2	2.47	21.84	-6.11	14.51
84	ILE	CG1	0.67	23.58	-5.90	14.63
84	ILE	CD1	1.49	24.66	-6.57	14.70
84	ILE	C	1.18	20.62	-8.33	14.58
84	ILE	O	0.54	19.60	-8.08	14.55
85	ARG	N	2.33	20.61	-8.99	14.53
85	ARG	CA	2.92	19.37	-9.50	14.51
85	ARG	CB	2.99	19.43	-11.03	14.88
85	ARG	CG	1.64	19.53	-11.70	15.43
85	ARG	CD	0.82	18.27	-11.47	15.80
85	ARG	NE	1.46	17.12	-12.10	16.29
85	ARG	CZ	1.21	16.72	-13.35	16.50
85	ARG	NH1	0.33	17.37	-14.10	16.70
85	ARG	NH2	1.87	15.68	-13.85	16.75
85	ARG	C	4.33	19.13	-8.96	14.35
85	ARG	O	5.02	20.06	-8.56	14.10
86	GLU	N	4.75	17.87	-8.95	14.10
86	GLU	CA	6.08	17.52	-8.49	14.00
86	GLU	CB	6.33	16.04	-8.77	14.17
86	GLU	CG	7.68	15.51	-8.32	14.45
86	GLU	CD	7.80	15.34	-6.83	14.55
86	GLU	OE1	6.78	15.44	-6.11	14.66
86	GLU	OE2	8.93	15.09	-6.36	14.63
86	GLU	C	7.09	18.38	-9.25	13.76
86	GLU	O	6.95	18.60	-10.45	13.74
87	GLY	N	8.11	18.88	-8.54	13.49
87	GLY	CA	9.13	19.71	-9.17	13.16
87	GLY	C	8.80	21.19	-9.34	12.97
87	GLY	O	9.65	21.97	-9.78	12.91
88	ASP	N	7.59	21.59	-8.98	12.75
88	ASP	CA	7.21	23.01	-9.14	12.65
88	ASP	CB	5.73	23.24	-8.79	12.74
88	ASP	CG	4.80	22.89	-9.94	12.76
88	ASP	OD1	5.29	22.49	-11.00	12.87
88	ASP	OD2	3.56	23.03	-9.76	12.81
88	ASP	C	8.06	23.94	-8.28	12.41
88	ASP	O	8.47	23.59	-7.17	12.45
89	LEU	N	8.32	25.13	-8.81	12.24
89	LEU	CA	9.06	26.15	-8.08	11.94
89	LEU	CB	10.11	26.80	-8.97	11.90
89	LEU	CG	10.82	28.02	-8.37	11.89

89 LEU CD1 11.40 27.69 -6.98 11.89
89 LEU CD2 11.91 28.47 -9.32 11.91
89 LEU C 7.98 27.15 -7.69 11.92
89 LEU O 7.46 27.88 -8.54 11.86
90 VAL N 7.64 27.17 -6.41 11.81
90 VAL CA 6.58 28.02 -5.88 11.74
90 VAL CB 5.58 27.16 -5.07 11.66
90 VAL CG1 4.41 28.01 -4.57 11.68
90 VAL CG2 5.08 26.01 -5.93 11.69
90 VAL C 7.03 29.18 -4.98 11.69
90 VAL O 7.86 29.01 -4.10 11.49
91 ASN N 6.45 30.35 -5.23 11.78
91 ASN CA 6.71 31.56 -4.45 11.80
91 ASN CB 7.19 32.70 -5.34 12.23
91 ASN CG 7.51 33.97 -4.54 12.73
91 ASN OD1 6.70 34.42 -3.72 12.94
91 ASN ND2 8.69 34.55 -4.79 13.23
91 ASN C 5.37 31.94 -3.82 11.68
91 ASN O 4.38 32.18 -4.52 11.62
92 ILE N 5.35 31.98 -2.49 11.43
92 ILE CA 4.15 32.34 -1.74 11.31
92 ILE CB 3.79 31.26 -0.70 11.29
92 ILE CG2 2.67 31.75 0.22 11.25
92 ILE CG1 3.40 29.96 -1.42 11.35
92 ILE CD1 3.06 28.79 -0.47 11.33
92 ILE C 4.48 33.64 -1.04 11.36
92 ILE O 5.44 33.72 -0.28 11.14
93 ASP N 3.68 34.67 -1.31 11.37
93 ASP CA 3.91 35.98 -0.71 11.37
93 ASP CB 4.19 37.01 -1.81 11.47
93 ASP CG 4.78 38.30 -1.27 11.61
93 ASP OD1 4.29 38.78 -0.23 11.73
93 ASP OD2 5.72 38.82 -1.90 11.96
93 ASP C 2.70 36.37 0.11 11.35
93 ASP O 1.59 36.50 -0.41 11.29
94 VAL N 2.92 36.55 1.41 11.32
94 VAL CA 1.86 36.88 2.34 11.43
94 VAL CB 1.82 35.84 3.50 11.42
94 VAL CG1 0.57 36.03 4.34 11.32
94 VAL CG2 1.88 34.42 2.93 11.50
94 VAL C 2.06 38.27 2.96 11.50
94 VAL O 3.12 38.56 3.51 11.50
95 SER N 1.05 39.12 2.85 11.58

95 SER CA	1.11	40.45	3.46	11.61
95 SER CB	1.59	41.53	2.46	11.67
95 SER OG	0.74	41.66	1.34	11.64
95 SER C	-0.29	40.76	3.97	11.72
95 SER O	-1.29	40.39	3.35	11.60
96 ALA N	-0.37	41.41	5.12	11.79
96 ALA CA	-1.66	41.71	5.73	11.94
96 ALA CB	-2.16	40.48	6.49	11.82
96 ALA C	-1.52	42.88	6.69	12.08
96 ALA O	-0.44	43.41	6.87	12.16
97 LEU N	-2.64	43.26	7.29	12.30
97 LEU CA	-2.64	44.35	8.25	12.48
97 LEU CB	-3.13	45.66	7.60	12.53
97 LEU CG	-4.51	45.66	6.94	12.61
97 LEU CD1	-5.03	47.10	6.83	12.64
97 LEU CD2	-4.44	45.03	5.57	12.64
97 LEU C	-3.54	44.01	9.43	12.56
97 LEU O	-4.50	43.25	9.29	12.54
98 LYS N	-3.21	44.54	10.59	12.67
98 LYS CA	-4.01	44.33	11.79	12.86
98 LYS CB	-3.54	43.10	12.58	12.93
98 LYS CG	-4.31	42.88	13.90	12.99
98 LYS CD	-3.88	41.59	14.59	13.13
98 LYS CE	-4.65	41.36	15.88	13.25
98 LYS NZ	-4.30	40.03	16.49	13.32
98 LYS C	-3.85	45.59	12.62	13.01
98 LYS O	-2.74	46.08	12.82	12.96
99 ASN N	-4.98	46.16	13.05	13.13
99 ASN CA	-4.97	47.38	13.83	13.29
99 ASN CB	-4.42	47.10	15.23	13.37
99 ASN CG	-5.32	46.17	16.02	13.41
99 ASN OD1	-6.54	46.33	16.01	13.54
99 ASN ND2	-4.74	45.19	16.69	13.45
99 ASN C	-4.18	48.52	13.18	13.26
99 ASN O	-3.60	49.36	13.87	13.41
100 GLY N	-4.15	48.53	11.85	13.22
100 GLY CA	-3.46	49.58	11.12	13.11
100 GLY C	-1.99	49.36	10.82	12.97
100 GLY O	-1.34	50.23	10.25	13.07
101 TYR N	-1.45	48.20	11.20	12.75
101 TYR CA	-0.04	47.92	10.95	12.45
101 TYR CB	0.69	47.75	12.27	12.65
101 TYR CG	0.70	49.02	13.10	12.97

101	TYR	CD1	1.71	49.96	12.95	13.10
101	TYR	CE1	1.72	51.14	13.71	13.37
101	TYR	CD2	-0.32	49.27	14.01	13.14
101	TYR	CE2	-0.34	50.45	14.78	13.41
101	TYR	CZ	0.69	51.37	14.62	13.48
101	TYR	OH	0.69	52.51	15.40	13.70
101	TYR	C	0.14	46.71	10.05	12.16
101	TYR	O	-0.58	45.71	10.17	11.97
102	TYR	N	1.10	46.81	9.14	11.96
102	TYR	CA	1.36	45.77	8.15	11.76
102	TYR	CB	1.47	46.41	6.76	11.76
102	TYR	CG	0.22	47.05	6.22	12.03
102	TYR	CD1	-0.39	48.13	6.86	12.07
102	TYR	CE1	-1.54	48.74	6.31	12.26
102	TYR	CD2	-0.34	46.60	5.03	12.00
102	TYR	CE2	-1.46	47.19	4.49	12.25
102	TYR	CZ	-2.06	48.26	5.12	12.29
102	TYR	OH	-3.17	48.80	4.53	12.39
102	TYR	C	2.62	44.94	8.34	11.60
102	TYR	O	3.54	45.33	9.05	11.50
103	ALA	N	2.64	43.79	7.67	11.49
103	ALA	CA	3.79	42.89	7.64	11.39
103	ALA	CB	3.61	41.72	8.60	11.42
103	ALA	C	3.84	42.39	6.19	11.35
103	ALA	O	2.82	42.37	5.49	11.34
104	ASP	N	5.02	41.99	5.73	11.30
104	ASP	CA	5.17	41.52	4.37	11.25
104	ASP	CB	5.50	42.72	3.46	11.41
104	ASP	CG	5.57	42.37	1.99	11.55
104	ASP	OD1	5.20	41.23	1.62	11.59
104	ASP	OD2	5.97	43.25	1.21	11.51
104	ASP	C	6.29	40.49	4.35	11.15
104	ASP	O	7.43	40.79	4.73	11.03
105	THR	N	5.98	39.28	3.91	11.09
105	THR	CA	6.99	38.24	3.87	10.99
105	THR	CB	7.07	37.53	5.26	11.07
105	THR	OG1	8.08	36.52	5.24	11.02
105	THR	CG2	5.74	36.93	5.64	11.10
105	THR	C	6.65	37.27	2.76	10.95
105	THR	O	5.50	37.18	2.33	10.96
106	GLY	N	7.66	36.55	2.27	10.87
106	GLY	CA	7.42	35.61	1.20	10.72
106	GLY	C	8.54	34.60	1.11	10.71

106 GLY O	9.61	34.78	1.68	10.51
107 ILE N	8.29	33.52	0.39	10.68
107 ILE CA	9.31	32.49	0.25	10.67
107 ILE CB	9.39	31.61	1.55	10.54
107 ILE CG2	8.08	30.88	1.79	10.60
107 ILE CG1	10.54	30.61	1.44	10.66
107 ILE CD1	10.89	29.95	2.78	10.77
107 ILE C	9.09	31.62	-0.98	10.69
107 ILE O	7.95	31.35	-1.38	10.50
108 SER N	10.20	31.25	-1.61	10.70
108 SER CA	10.18	30.38	-2.78	10.85
108 SER CB	11.02	30.96	-3.93	10.76
108 SER OG	10.46	32.15	-4.45	10.72
108 SER C	10.81	29.08	-2.33	11.03
108 SER O	11.79	29.07	-1.59	10.89
109 PHE N	10.22	27.98	-2.78	11.24
109 PHE CA	10.71	26.65	-2.45	11.61
109 PHE CB	10.07	26.15	-1.15	11.60
109 PHE CG	8.56	26.15	-1.17	11.68
109 PHE CD1	7.86	27.33	-0.94	11.76
109 PHE CD2	7.85	24.99	-1.45	11.78
109 PHE CE1	6.46	27.36	-0.99	11.74
109 PHE CE2	6.45	25.01	-1.51	11.88
109 PHE CZ	5.76	26.20	-1.28	11.77
109 PHE C	10.36	25.71	-3.60	11.82
109 PHE O	9.56	26.07	-4.48	11.67
110 VAL N	10.97	24.54	-3.60	12.16
110 VAL CA	10.72	23.53	-4.63	12.47
110 VAL CB	12.04	22.85	-5.08	12.54
110 VAL CG1	11.74	21.69	-6.04	12.54
110 VAL CG2	12.94	23.87	-5.76	12.54
110 VAL C	9.79	22.48	-4.04	12.73
110 VAL O	9.94	22.08	-2.88	12.74
111 VAL N	8.82	22.04	-4.83	12.96
111 VAL CA	7.88	21.02	-4.38	13.20
111 VAL CB	6.52	21.17	-5.05	13.26
111 VAL CG1	5.54	20.12	-4.52	13.35
111 VAL CG2	5.99	22.57	-4.81	13.30
111 VAL C	8.48	19.68	-4.76	13.44
111 VAL O	8.67	19.39	-5.95	13.34
112 GLY N	8.78	18.86	-3.76	13.65
112 GLY CA	9.36	17.57	-4.04	14.12
112 GLY C	10.69	17.71	-4.75	14.37

112 GLY O	11.56	18.47	-4.31	14.43
113 GLU N	10.85	17.00	-5.86	14.73
113 GLU CA	12.09	17.05	-6.62	15.11
113 GLU CB	12.79	15.71	-6.57	15.34
113 GLU CG	13.02	15.19	-5.17	15.81
113 GLU CD	13.53	13.77	-5.17	16.07
113 GLU OE1	12.82	12.88	-5.71	16.38
113 GLU OE2	14.63	13.54	-4.63	16.29
113 GLU C	11.86	17.43	-8.08	15.24
113 GLU O	10.88	17.02	-8.69	15.23
114 SER N	12.80	18.20	-8.62	15.34
114 SER CA	12.79	18.64	-10.01	15.49
114 SER CB	12.95	20.17	-10.08	15.62
114 SER OG	13.28	20.60	-11.39	15.85
114 SER C	13.99	17.98	-10.68	15.56
114 SER O	15.00	17.73	-10.03	15.53
115 ASP N	13.88	17.70	-11.98	15.71
115 ASP CA	15.00	17.09	-12.70	15.84
115 ASP CB	14.53	16.54	-14.05	16.37
115 ASP CG	14.12	17.63	-15.00	16.79
115 ASP OD1	13.53	18.61	-14.52	17.18
115 ASP OD2	14.37	17.50	-16.22	17.31
115 ASP C	16.09	18.13	-12.94	15.69
115 ASP O	17.19	17.79	-13.38	15.64
116 ASP N	15.78	19.40	-12.68	15.48
116 ASP CA	16.76	20.46	-12.86	15.38
116 ASP CB	16.19	21.61	-13.70	15.50
116 ASP CG	17.28	22.57	-14.19	15.55
116 ASP OD1	18.36	22.61	-13.57	15.62
116 ASP OD2	17.04	23.29	-15.19	15.61
116 ASP C	17.14	20.98	-11.48	15.27
116 ASP O	16.32	21.59	-10.80	15.21
117 PRO N	18.39	20.76	-11.07	15.13
117 PRO CD	19.47	20.03	-11.77	15.16
117 PRO CA	18.83	21.23	-9.75	15.04
117 PRO CB	20.20	20.55	-9.59	15.12
117 PRO CG	20.70	20.43	-10.99	15.09
117 PRO C	18.89	22.76	-9.60	14.97
117 PRO O	18.98	23.28	-8.49	14.92
118 MET N	18.80	23.48	-10.72	14.94
118 MET CA	18.84	24.95	-10.73	14.94
118 MET CB	18.83	25.47	-12.17	15.14
118 MET CG	18.72	26.99	-12.30	15.53

118	MET	SD	20.20	27.88	-11.68	15.88
118	MET	CE	21.33	27.62	-13.04	15.90
118	MET	C	17.68	25.57	-9.96	14.83
118	MET	O	17.79	26.68	-9.44	14.73
119	LYS	N	16.56	24.85	-9.89	14.75
119	LYS	CA	15.42	25.36	-9.16	14.63
119	LYS	CB	14.23	24.40	-9.32	14.60
119	LYS	CG	13.52	24.52	-10.67	14.64
119	LYS	CD	12.19	23.76	-10.70	14.70
119	LYS	CE	11.37	24.10	-11.94	14.76
119	LYS	NZ	10.13	23.25	-12.05	14.66
119	LYS	C	15.80	25.56	-7.70	14.53
119	LYS	O	15.60	26.65	-7.15	14.56
120	GLN	N	16.39	24.54	-7.07	14.42
120	GLN	CA	16.80	24.64	-5.67	14.29
120	GLN	CB	17.28	23.28	-5.15	14.35
120	GLN	CG	17.56	23.23	-3.64	14.30
120	GLN	CD	16.40	23.76	-2.81	14.26
120	GLN	OE1	15.28	23.28	-2.90	14.27
120	GLN	NE2	16.68	24.77	-1.97	14.18
120	GLN	C	17.91	25.68	-5.52	14.22
120	GLN	O	17.91	26.46	-4.57	14.28
121	LYS	N	18.85	25.69	-6.47	14.09
121	LYS	CA	19.96	26.63	-6.42	13.95
121	LYS	CB	20.83	26.52	-7.68	14.09
121	LYS	CG	22.05	27.42	-7.62	14.24
121	LYS	CD	22.99	27.19	-8.80	14.46
121	LYS	CE	24.24	28.06	-8.67	14.56
121	LYS	NZ	25.11	27.96	-9.86	14.64
121	LYS	C	19.51	28.08	-6.26	13.76
121	LYS	O	20.03	28.79	-5.40	13.77
122	VAL	N	18.55	28.52	-7.07	13.55
122	VAL	CA	18.11	29.90	-6.94	13.26
122	VAL	CB	17.14	30.32	-8.09	13.29
122	VAL	CG1	17.87	30.24	-9.42	13.16
122	VAL	CG2	15.89	29.45	-8.10	13.06
122	VAL	C	17.49	30.15	-5.57	13.24
122	VAL	O	17.58	31.26	-5.04	13.24
123	CYS	N	16.88	29.12	-4.98	13.15
123	CYS	CA	16.30	29.26	-3.65	13.17
123	CYS	CB	15.42	28.05	-3.29	12.84
123	CYS	SG	13.89	27.93	-4.26	12.42
123	CYS	C	17.40	29.39	-2.60	13.46

123 CYS O	17.29	30.18	-1.68	13.59
124 ASP N	18.45	28.57	-2.72	13.81
124 ASP CA	19.54	28.64	-1.75	14.08
124 ASP CB	20.56	27.51	-1.98	14.29
124 ASP CG	19.99	26.13	-1.72	14.48
124 ASP OD1	18.95	26.02	-1.03	14.63
124 ASP OD2	20.60	25.15	-2.19	14.51
124 ASP C	20.28	29.96	-1.82	14.14
124 ASP O	20.70	30.50	-0.80	14.20
125 VAL N	20.45	30.48	-3.03	14.25
125 VAL CA	21.14	31.75	-3.23	14.33
125 VAL CB	21.57	31.92	-4.72	14.42
125 VAL CG1	22.31	33.25	-4.89	14.41
125 VAL CG2	22.49	30.78	-5.13	14.41
125 VAL C	20.27	32.92	-2.81	14.40
125 VAL O	20.77	33.95	-2.38	14.41
126 ALA N	18.95	32.75	-2.93	14.49
126 ALA CA	18.03	33.80	-2.53	14.56
126 ALA CB	16.60	33.44	-2.94	14.57
126 ALA C	18.11	33.95	-1.01	14.66
126 ALA O	17.96	35.04	-0.48	14.56
127 THR N	18.32	32.83	-0.34	14.79
127 THR CA	18.42	32.83	1.11	14.94
127 THR CB	18.34	31.41	1.67	15.05
127 THR OG1	17.03	30.89	1.44	15.29
127 THR CG2	18.62	31.42	3.17	15.24
127 THR C	19.73	33.45	1.54	14.94
127 THR O	19.80	34.16	2.54	14.90
128 MET N	20.79	33.18	0.79	15.08
128 MET CA	22.07	33.77	1.12	15.15
128 MET CB	23.20	33.11	0.33	15.52
128 MET CG	23.52	31.68	0.75	16.12
128 MET SD	25.13	31.17	0.09	17.15
128 MET CE	24.73	30.96	-1.62	16.79
128 MET C	22.02	35.26	0.81	14.99
128 MET O	22.57	36.07	1.56	14.95
129 ALA N	21.36	35.63	-0.28	14.84
129 ALA CA	21.26	37.04	-0.64	14.81
129 ALA CB	20.46	37.22	-1.93	14.74
129 ALA C	20.60	37.82	0.51	14.82
129 ALA O	21.07	38.90	0.87	14.77
130 PHE N	19.53	37.27	1.08	14.87
130 PHE CA	18.84	37.94	2.17	14.99

130 PHE CB	17.57	37.18	2.58	14.90
130 PHE CG	16.86	37.80	3.75	14.91
130 PHE CD1	16.01	38.89	3.57	14.92
130 PHE CD2	17.12	37.35	5.03	14.99
130 PHE CE1	15.43	39.53	4.67	14.84
130 PHE CE2	16.55	37.98	6.13	14.95
130 PHE CZ	15.70	39.07	5.95	14.96
130 PHE C	19.72	38.12	3.41	15.17
130 PHE O	19.74	39.20	4.02	15.07
131 GLU N	20.45	37.06	3.78	15.45
131 GLU CA	21.34	37.07	4.93	15.81
131 GLU CB	21.95	35.68	5.16	16.12
131 GLU CG	20.94	34.57	5.21	16.71
131 GLU CD	21.57	33.20	5.39	16.99
131 GLU OE1	22.53	32.87	4.65	17.20
131 GLU OE2	21.11	32.46	6.28	17.36
131 GLU C	22.48	38.07	4.75	15.87
131 GLU O	22.87	38.75	5.69	15.81
132 ASN N	23.03	38.14	3.54	16.02
132 ASN CA	24.12	39.07	3.30	16.23
132 ASN CB	24.77	38.81	1.95	16.57
132 ASN CG	25.57	37.53	1.92	16.96
132 ASN OD1	26.25	37.18	2.89	17.40
132 ASN ND2	25.52	36.84	0.79	17.21
132 ASN C	23.60	40.50	3.33	16.25
132 ASN O	24.29	41.41	3.80	16.09
133 ALA N	22.38	40.68	2.85	16.35
133 ALA CA	21.74	41.99	2.81	16.64
133 ALA CB	20.41	41.90	2.06	16.49
133 ALA C	21.51	42.59	4.19	16.87
133 ALA O	21.80	43.76	4.42	16.89
134 ILE N	20.97	41.80	5.11	17.20
134 ILE CA	20.72	42.32	6.45	17.59
134 ILE CB	19.57	41.57	7.14	17.68
134 ILE CG2	18.28	41.77	6.36	17.80
134 ILE CG1	19.91	40.09	7.27	17.76
134 ILE CD1	19.02	39.32	8.24	17.84
134 ILE C	21.95	42.23	7.34	17.79
134 ILE O	21.91	42.68	8.49	17.73
135 ALA N	23.03	41.67	6.81	18.09
135 ALA CA	24.28	41.49	7.56	18.49
135 ALA CB	25.40	41.08	6.60	18.54
135 ALA C	24.74	42.68	8.40	18.75

135 ALA O	25.02	42.52	9.59	18.80
136 LYS N	24.84	43.85	7.79	19.02
136 LYS CA	25.29	45.03	8.52	19.28
136 LYS CB	26.62	45.52	7.93	19.50
136 LYS CG	27.82	44.63	8.29	19.80
136 LYS CD	29.05	44.98	7.47	20.05
136 LYS CE	28.89	44.50	6.03	20.13
136 LYS NZ	30.02	44.93	5.15	20.24
136 LYS C	24.26	46.17	8.55	19.27
136 LYS O	24.61	47.31	8.88	19.41
137 VAL N	23.01	45.86	8.21	19.23
137 VAL CA	21.95	46.86	8.22	19.12
137 VAL CB	20.57	46.24	7.86	19.15
137 VAL CG1	19.45	47.23	8.14	19.26
137 VAL CG2	20.55	45.85	6.38	19.22
137 VAL C	21.87	47.52	9.59	19.03
137 VAL O	21.66	46.85	10.61	18.99
138 LYS N	22.04	48.84	9.61	18.90
138 LYS CA	22.00	49.63	10.83	18.76
138 LYS CB	23.31	49.52	11.61	18.99
138 LYS CG	23.27	48.53	12.76	19.38
138 LYS CD	24.55	48.60	13.59	19.66
138 LYS CE	24.80	47.28	14.30	19.83
138 LYS NZ	25.05	46.18	13.32	20.04
138 LYS C	21.77	51.10	10.53	18.47
138 LYS O	21.96	51.55	9.41	18.35
139 PRO N	21.36	51.87	11.55	18.25
139 PRO CD	21.02	51.45	12.92	18.24
139 PRO CA	21.12	53.29	11.37	18.17
139 PRO CB	20.82	53.77	12.78	18.12
139 PRO CG	20.15	52.58	13.39	18.20
139 PRO C	22.36	53.94	10.77	18.07
139 PRO O	23.48	53.64	11.20	18.00
140 GLY N	22.15	54.78	9.77	17.92
140 GLY CA	23.26	55.47	9.12	17.84
140 GLY C	23.84	54.78	7.90	17.72
140 GLY O	24.52	55.42	7.10	17.81
141 THR N	23.57	53.48	7.73	17.60
141 THR CA	24.11	52.75	6.59	17.39
141 THR CB	24.09	51.19	6.83	17.45
141 THR OG1	22.74	50.70	6.87	17.43
141 THR CG2	24.78	50.85	8.15	17.41
141 THR C	23.36	53.08	5.31	17.26

141 THR O	22.19	53.44	5.32	17.27
142 LYS N	24.06	52.96	4.18	17.06
142 LYS CA	23.46	53.28	2.90	16.93
142 LYS CB	24.54	53.40	1.83	17.04
142 LYS CG	25.56	54.47	2.12	17.30
142 LYS CD	26.63	54.50	1.04	17.61
142 LYS CE	27.57	55.69	1.22	17.83
142 LYS NZ	28.54	55.82	0.09	18.18
142 LYS C	22.43	52.24	2.48	16.75
142 LYS O	22.69	51.04	2.56	16.71
143 LEU N	21.27	52.71	2.04	16.65
143 LEU CA	20.19	51.83	1.59	16.50
143 LEU CB	19.02	52.67	1.07	16.57
143 LEU CG	17.82	51.95	0.44	16.61
143 LEU CD1	17.13	51.10	1.48	16.78
143 LEU CD2	16.85	52.99	-0.13	16.73
143 LEU C	20.73	50.95	0.47	16.39
143 LEU O	20.47	49.75	0.41	16.43
144 SER N	21.50	51.58	-0.42	16.25
144 SER CA	22.09	50.91	-1.56	16.10
144 SER CB	22.88	51.91	-2.42	16.04
144 SER OG	24.03	52.35	-1.74	15.94
144 SER C	22.98	49.71	-1.22	16.08
144 SER O	23.31	48.92	-2.10	16.02
145 ASN N	23.37	49.58	0.05	16.10
145 ASN CA	24.21	48.44	0.45	16.14
145 ASN CB	24.72	48.56	1.89	16.20
145 ASN CG	25.76	49.64	2.06	16.36
145 ASN OD1	26.50	49.97	1.14	16.46
145 ASN ND2	25.84	50.18	3.28	16.59
145 ASN C	23.45	47.12	0.34	16.07
145 ASN O	24.05	46.05	0.15	15.98
146 ILE N	22.13	47.19	0.48	16.03
146 ILE CA	21.26	46.01	0.39	16.02
146 ILE CB	19.78	46.39	0.72	16.04
146 ILE CG2	18.84	45.21	0.43	15.93
146 ILE CG1	19.67	46.80	2.19	16.10
146 ILE CD1	18.30	47.32	2.60	16.04
146 ILE C	21.36	45.41	-1.01	16.02
146 ILE O	21.73	44.23	-1.18	15.99
147 GLY N	21.05	46.22	-2.01	16.08
147 GLY CA	21.11	45.76	-3.39	16.04
147 GLY C	22.53	45.39	-3.77	16.06

147	GLY	O	22.76	44.43	-4.50	16.01
148	LYS	N	23.50	46.15	-3.26	16.09
148	LYS	CA	24.89	45.86	-3.57	16.05
148	LYS	CB	25.80	46.88	-2.89	16.28
148	LYS	CG	27.25	46.77	-3.31	16.49
148	LYS	CD	28.10	47.77	-2.53	16.80
148	LYS	CE	29.47	47.91	-3.13	16.94
148	LYS	NZ	29.40	48.53	-4.48	17.28
148	LYS	C	25.21	44.44	-3.09	15.98
148	LYS	O	25.84	43.67	-3.81	15.86
149	ALA	N	24.75	44.09	-1.90	15.88
149	ALA	CA	24.99	42.76	-1.34	15.88
149	ALA	CB	24.62	42.74	0.14	15.68
149	ALA	C	24.20	41.69	-2.09	15.87
149	ALA	O	24.71	40.60	-2.35	15.81
150	VAL	N	22.95	42.00	-2.42	15.99
150	VAL	CA	22.11	41.06	-3.14	16.15
150	VAL	CB	20.68	41.62	-3.34	16.17
150	VAL	CG1	19.85	40.67	-4.20	16.18
150	VAL	CG2	20.01	41.79	-1.99	16.12
150	VAL	C	22.73	40.73	-4.50	16.24
150	VAL	O	22.94	39.56	-4.83	16.34
151	HIS	N	23.06	41.76	-5.28	16.44
151	HIS	CA	23.66	41.54	-6.59	16.71
151	HIS	CB	23.77	42.88	-7.34	16.89
151	HIS	CG	24.27	42.73	-8.75	17.05
151	HIS	CD2	23.60	42.65	-9.92	17.15
151	HIS	ND1	25.60	42.60	-9.06	17.14
151	HIS	CE1	25.74	42.45	-10.37	17.19
151	HIS	NE2	24.53	42.47	-10.91	17.13
151	HIS	C	25.02	40.84	-6.53	16.80
151	HIS	O	25.38	40.09	-7.43	16.68
152	ASN	N	25.77	41.09	-5.46	16.97
152	ASN	CA	27.08	40.47	-5.30	17.14
152	ASN	CB	27.84	41.13	-4.14	17.36
152	ASN	CG	29.24	40.55	-3.96	17.63
152	ASN	OD1	29.40	39.46	-3.40	17.87
152	ASN	ND2	30.25	41.28	-4.44	17.74
152	ASN	C	26.94	38.98	-5.03	17.09
152	ASN	O	27.70	38.16	-5.55	17.21
153	THR	N	25.95	38.63	-4.21	17.05
153	THR	CA	25.71	37.23	-3.89	16.99
153	THR	CB	24.62	37.08	-2.82	16.99

153	THR	OG1	25.03	37.76	-1.63	16.88
153	THR	CG2	24.40	35.61	-2.49	16.90
153	THR	C	25.28	36.47	-5.13	17.05
153	THR	O	25.60	35.30	-5.31	17.02
154	ALA	N	24.54	37.16	-6.00	17.09
154	ALA	CA	24.07	36.53	-7.23	17.20
154	ALA	CB	23.04	37.40	-7.91	17.17
154	ALA	C	25.25	36.28	-8.16	17.25
154	ALA	O	25.36	35.22	-8.77	17.27
155	ARG	N	26.14	37.26	-8.25	17.39
155	ARG	CA	27.29	37.13	-9.13	17.62
155	ARG	CB	28.00	38.47	-9.27	17.94
155	ARG	CG	28.41	38.78	-10.70	18.55
155	ARG	CD	29.51	37.84	-11.16	19.01
155	ARG	NE	29.81	37.98	-12.58	19.37
155	ARG	CZ	30.82	37.38	-13.21	19.55
155	ARG	NH1	31.64	36.58	-12.53	19.64
155	ARG	NH2	30.99	37.56	-14.52	19.55
155	ARG	C	28.25	36.06	-8.61	17.54
155	ARG	O	28.82	35.30	-9.39	17.54
156	GLN	N	28.40	35.98	-7.29	17.56
156	GLN	CA	29.29	34.98	-6.71	17.53
156	GLN	CB	29.39	35.15	-5.21	17.66
156	GLN	CG	30.15	36.36	-4.72	18.00
156	GLN	CD	30.29	36.33	-3.22	18.19
156	GLN	OE1	30.55	37.35	-2.58	18.31
156	GLN	NE2	30.09	35.15	-2.63	18.30
156	GLN	C	28.79	33.57	-7.00	17.45
156	GLN	O	29.53	32.60	-6.86	17.36
157	ASN	N	27.53	33.44	-7.40	17.36
157	ASN	CA	26.98	32.11	-7.70	17.32
157	ASN	CB	25.82	31.79	-6.75	17.27
157	ASN	CG	26.27	31.65	-5.30	17.29
157	ASN	OD1	26.23	32.61	-4.53	17.33
157	ASN	ND2	26.73	30.46	-4.93	17.12
157	ASN	C	26.54	31.95	-9.14	17.31
157	ASN	O	25.69	31.12	-9.46	17.33
158	ASP	N	27.14	32.75	-10.03	17.31
158	ASP	CA	26.83	32.67	-11.45	17.32
158	ASP	CB	27.33	31.33	-12.00	17.60
158	ASP	CG	28.82	31.14	-11.76	17.85
158	ASP	OD1	29.61	31.93	-12.31	18.05
158	ASP	OD2	29.20	30.21	-11.00	18.11

158	ASP	C	25.34	32.83	-11.74	17.17
158	ASP	O	24.78	32.15	-12.60	17.21
159	LEU	N	24.70	33.74	-11.02	17.01
159	LEU	CA	23.28	33.99	-11.20	16.85
159	LEU	CB	22.50	33.45	-10.00	16.85
159	LEU	CG	22.57	31.93	-9.80	16.82
159	LEU	CD1	21.84	31.53	-8.53	16.77
159	LEU	CD2	21.95	31.24	-11.01	16.80
159	LEU	C	23.00	35.47	-11.39	16.84
159	LEU	O	23.91	36.30	-11.32	16.75
160	LYS	N	21.74	35.80	-11.64	16.81
160	LYS	CA	21.33	37.18	-11.86	16.76
160	LYS	CB	20.80	37.33	-13.29	16.93
160	LYS	CG	21.85	37.21	-14.39	17.27
160	LYS	CD	22.92	38.28	-14.24	17.53
160	LYS	CE	23.76	38.43	-15.52	17.74
160	LYS	NZ	24.38	37.14	-15.94	17.92
160	LYS	C	20.24	37.60	-10.88	16.64
160	LYS	O	19.78	36.81	-10.07	16.58
161	VAL	N	19.85	38.87	-10.94	16.56
161	VAL	CA	18.80	39.39	-10.07	16.48
161	VAL	CB	19.36	40.47	-9.11	16.50
161	VAL	CG1	20.54	39.90	-8.30	16.47
161	VAL	CG2	19.82	41.69	-9.91	16.49
161	VAL	C	17.71	40.02	-10.93	16.42
161	VAL	O	17.95	40.34	-12.09	16.44
162	ILE	N	16.50	40.18	-10.38	16.31
162	ILE	CA	15.43	40.82	-11.14	16.20
162	ILE	CB	14.03	40.33	-10.70	16.18
162	ILE	CG2	12.94	41.12	-11.43	16.13
162	ILE	CG1	13.89	38.83	-10.97	16.16
162	ILE	CD1	14.17	38.42	-12.40	16.13
162	ILE	C	15.57	42.30	-10.81	16.12
162	ILE	O	15.30	42.72	-9.69	16.22
163	LYS	N	16.00	43.09	-11.79	16.08
163	LYS	CA	16.22	44.52	-11.58	16.01
163	LYS	CB	17.15	45.06	-12.68	16.13
163	LYS	CG	18.55	44.49	-12.61	16.32
163	LYS	CD	19.43	45.05	-13.72	16.46
163	LYS	CE	20.87	44.61	-13.57	16.66
163	LYS	NZ	21.43	45.01	-12.23	16.68
163	LYS	C	14.97	45.38	-11.49	15.89
163	LYS	O	14.96	46.40	-10.80	15.78

164 ASN N	13.91	44.98	-12.19	15.71
164 ASN CA	12.69	45.77	-12.18	15.65
164 ASN CB	12.06	45.76	-13.58	15.73
164 ASN CG	11.60	44.39	-13.99	15.84
164 ASN OD1	12.15	43.38	-13.56	15.98
164 ASN ND2	10.59	44.34	-14.86	16.02
164 ASN C	11.66	45.34	-11.12	15.55
164 ASN O	10.47	45.56	-11.28	15.53
165 LEU N	12.14	44.71	-10.05	15.46
165 LEU CA	11.28	44.32	-8.93	15.40
165 LEU CB	10.99	42.81	-8.92	15.50
165 LEU CG	9.91	42.36	-9.92	15.52
165 LEU CD1	9.65	40.86	-9.79	15.40
165 LEU CD2	8.64	43.13	-9.66	15.58
165 LEU C	12.07	44.74	-7.69	15.32
165 LEU O	13.24	44.40	-7.56	15.29
166 THR N	11.44	45.48	-6.79	15.23
166 THR CA	12.15	45.97	-5.62	15.22
166 THR CB	12.45	47.46	-5.76	15.24
166 THR OG1	11.27	48.20	-5.42	15.38
166 THR CG2	12.83	47.80	-7.19	15.22
166 THR C	11.42	45.84	-4.30	15.16
166 THR O	10.21	45.60	-4.26	15.11
167 GLY N	12.19	46.03	-3.23	15.10
167 GLY CA	11.65	46.00	-1.89	14.99
167 GLY C	11.04	47.36	-1.64	15.01
167 GLY O	10.97	48.19	-2.56	14.96
168 HIS N	10.61	47.62	-0.41	14.93
168 HIS CA	9.95	48.88	-0.11	14.90
168 HIS CB	8.60	48.90	-0.82	14.90
168 HIS CG	7.79	47.65	-0.62	14.94
168 HIS CD2	7.63	46.56	-1.40	14.92
168 HIS ND1	7.07	47.41	0.53	15.02
168 HIS CE1	6.50	46.22	0.45	14.97
168 HIS NE2	6.82	45.69	-0.71	15.02
168 HIS C	9.72	49.06	1.38	14.86
168 HIS O	9.73	48.09	2.14	14.84
169 GLY N	9.51	50.30	1.79	14.86
169 GLY CA	9.23	50.56	3.19	14.88
169 GLY C	7.86	49.98	3.43	14.92
169 GLY O	7.09	49.80	2.48	14.96
170 VAL N	7.54	49.69	4.68	14.98
170 VAL CA	6.24	49.12	5.03	15.11

170 VAL CB	6.23	47.57	4.83	15.20
170 VAL CG1	7.23	46.92	5.76	15.19
170 VAL CG2	4.82	47.01	5.05	15.26
170 VAL C	5.94	49.49	6.48	15.15
170 VAL O	6.85	49.88	7.22	15.12
171 GLY N	4.68	49.42	6.88	15.28
171 GLY CA	4.33	49.77	8.24	15.58
171 GLY C	2.88	50.18	8.39	15.74
171 GLY O	2.09	49.44	8.96	15.67
172 LEU N	2.54	51.36	7.88	16.08
172 LEU CA	1.17	51.87	7.94	16.42
172 LEU CB	1.19	53.37	8.29	16.64
172 LEU CG	1.71	53.71	9.69	16.88
172 LEU CD1	1.96	55.21	9.82	17.03
172 LEU CD2	0.70	53.23	10.72	16.95
172 LEU C	0.47	51.66	6.60	16.59
172 LEU O	-0.69	52.03	6.41	16.58
173 SER N	1.19	51.04	5.67	16.80
173 SER CA	0.69	50.75	4.33	17.10
173 SER CB	0.71	52.01	3.46	17.01
173 SER OG	2.04	52.31	3.06	17.12
173 SER C	1.64	49.71	3.74	17.32
173 SER O	2.72	49.48	4.28	17.43
174 LEU N	1.26	49.11	2.62	17.59
174 LEU CA	2.10	48.09	2.00	17.97
174 LEU CB	1.30	47.30	0.96	18.07
174 LEU CG	1.97	46.09	0.32	18.14
174 LEU CD1	2.47	45.13	1.39	18.13
174 LEU CD2	0.95	45.39	-0.59	18.21
174 LEU C	3.34	48.71	1.34	18.15
174 LEU O	4.42	48.12	1.36	18.23
175 HIS N	3.18	49.90	0.76	18.25
175 HIS CA	4.28	50.58	0.08	18.42
175 HIS CB	4.04	50.59	-1.44	18.61
175 HIS CG	4.17	49.23	-2.08	18.85
175 HIS CD2	4.94	48.81	-3.11	18.95
175 HIS ND1	3.45	48.13	-1.67	18.99
175 HIS CE1	3.77	47.09	-2.41	18.96
175 HIS NE2	4.68	47.47	-3.30	19.08
175 HIS C	4.49	52.03	0.56	18.34
175 HIS O	3.65	52.90	0.33	18.40
176 GLU N	5.61	52.28	1.24	18.24
176 GLU CA	5.93	53.63	1.70	18.03

176	GLU	CB	5.33	53.88	3.10	18.11
176	GLU	CG	5.67	52.86	4.18	18.06
176	GLU	CD	4.71	52.91	5.37	18.15
176	GLU	OE1	5.17	52.70	6.51	18.07
176	GLU	OE2	3.50	53.15	5.16	18.21
176	GLU	C	7.45	53.86	1.68	17.99
176	GLU	O	8.22	52.96	1.34	17.91
177	ALA	N	7.88	55.08	2.01	17.92
177	ALA	CA	9.31	55.41	1.99	17.96
177	ALA	CB	9.53	56.84	2.48	17.88
177	ALA	C	10.12	54.44	2.83	17.98
177	ALA	O	9.72	54.08	3.94	17.95
178	PRO	N	11.28	53.97	2.31	18.09
178	PRO	CD	12.20	53.09	3.05	18.06
178	PRO	CA	11.82	54.30	0.99	18.05
178	PRO	CB	13.26	53.80	1.08	18.09
178	PRO	CG	13.13	52.60	1.96	18.15
178	PRO	C	11.02	53.62	-0.12	18.12
178	PRO	O	10.65	52.45	0.00	18.11
179	ALA	N	10.75	54.36	-1.18	18.08
179	ALA	CA	9.97	53.86	-2.31	18.04
179	ALA	CB	9.95	54.91	-3.43	18.07
179	ALA	C	10.45	52.53	-2.86	18.02
179	ALA	O	9.67	51.59	-3.01	17.95
180	HIS	N	11.74	52.45	-3.16	18.03
180	HIS	CA	12.31	51.23	-3.72	18.10
180	HIS	CB	12.59	51.42	-5.21	18.27
180	HIS	CG	11.38	51.76	-6.02	18.41
180	HIS	CD2	10.39	50.97	-6.50	18.41
180	HIS	ND1	11.04	53.05	-6.36	18.52
180	HIS	CE1	9.90	53.04	-7.03	18.46
180	HIS	NE2	9.48	51.79	-7.12	18.51
180	HIS	C	13.59	50.74	-3.05	18.07
180	HIS	O	14.48	51.51	-2.70	18.04
181	VAL	N	13.66	49.43	-2.87	17.99
181	VAL	CA	14.82	48.78	-2.29	17.99
181	VAL	CB	14.43	47.92	-1.09	17.93
181	VAL	CG1	15.68	47.23	-0.54	17.99
181	VAL	CG2	13.75	48.77	-0.02	17.87
181	VAL	C	15.32	47.89	-3.41	18.04
181	VAL	O	14.89	46.74	-3.54	17.87
182	LEU	N	16.23	48.42	-4.23	18.15
182	LEU	CA	16.76	47.70	-5.38	18.28

182	LEU	CB	17.66	48.63	-6.22	18.30
182	LEU	CG	17.08	49.95	-6.73	18.37
182	LEU	CD1	18.18	50.75	-7.44	18.37
182	LEU	CD2	15.92	49.68	-7.67	18.45
182	LEU	C	17.55	46.45	-5.04	18.41
182	LEU	O	18.11	46.32	-3.95	18.36
183	ASN	N	17.61	45.54	-6.00	18.53
183	ASN	CA	18.35	44.30	-5.83	18.76
183	ASN	CB	17.60	43.14	-6.46	18.76
183	ASN	CG	16.38	42.75	-5.66	18.80
183	ASN	OD1	16.46	42.59	-4.44	18.80
183	ASN	ND2	15.24	42.60	-6.33	18.88
183	ASN	C	19.75	44.42	-6.43	18.90
183	ASN	O	20.41	43.42	-6.69	18.79
184	TYR	N	20.18	45.66	-6.66	19.15
184	TYR	CA	21.51	45.92	-7.20	19.45
184	TYR	CB	21.52	45.90	-8.73	19.31
184	TYR	CG	20.61	46.93	-9.37	19.35
184	TYR	CD1	19.23	46.74	-9.41	19.28
184	TYR	CE1	18.39	47.70	-9.96	19.27
184	TYR	CD2	21.14	48.11	-9.91	19.32
184	TYR	CE2	20.30	49.08	-10.46	19.31
184	TYR	CZ	18.93	48.87	-10.48	19.30
184	TYR	OH	18.10	49.84	-10.99	19.38
184	TYR	C	21.99	47.27	-6.69	19.73
184	TYR	O	21.22	48.03	-6.11	19.62
185	PHE	N	23.27	47.55	-6.91	20.14
185	PHE	CA	23.89	48.78	-6.45	20.57
185	PHE	CB	25.41	48.57	-6.30	20.66
185	PHE	CG	26.15	49.81	-5.86	20.88
185	PHE	CD1	25.84	50.43	-4.66	20.87
185	PHE	CD2	27.15	50.36	-6.66	20.96
185	PHE	CE1	26.50	51.59	-4.25	20.95
185	PHE	CE2	27.83	51.52	-6.26	21.07
185	PHE	CZ	27.50	52.13	-5.05	20.97
185	PHE	C	23.64	50.01	-7.33	20.87
185	PHE	O	23.79	49.97	-8.55	20.82
186	ASP	N	23.26	51.11	-6.68	21.25
186	ASP	CA	23.00	52.37	-7.37	21.64
186	ASP	CB	21.52	52.73	-7.28	21.78
186	ASP	CG	21.21	54.09	-7.89	22.06
186	ASP	OD1	21.88	54.47	-8.88	22.17
186	ASP	OD2	20.30	54.77	-7.38	22.18

186	ASP	C	23.86	53.44	-6.72	21.81
186	ASP	O	23.54	53.97	-5.66	21.77
187	PRO	N	24.99	53.78	-7.36	22.04
187	PRO	CD	25.36	53.33	-8.71	22.02
187	PRO	CA	25.94	54.79	-6.88	22.12
187	PRO	CB	27.03	54.78	-7.95	22.13
187	PRO	CG	26.26	54.46	-9.19	22.06
187	PRO	C	25.39	56.19	-6.63	22.29
187	PRO	O	25.97	56.96	-5.87	22.43
188	LYS	N	24.28	56.53	-7.27	22.39
188	LYS	CA	23.74	57.88	-7.08	22.50
188	LYS	CB	22.83	58.25	-8.25	22.67
188	LYS	CG	21.56	57.43	-8.31	22.90
188	LYS	CD	20.43	58.19	-9.00	23.09
188	LYS	CE	19.08	57.62	-8.59	23.18
188	LYS	NZ	18.87	57.74	-7.11	23.28
188	LYS	C	22.95	58.02	-5.78	22.48
188	LYS	O	22.93	59.09	-5.18	22.53
189	ASP	N	22.31	56.94	-5.36	22.45
189	ASP	CA	21.50	56.96	-4.15	22.28
189	ASP	CB	20.72	55.65	-4.05	22.42
189	ASP	CG	19.71	55.65	-2.92	22.58
189	ASP	OD1	19.08	56.71	-2.69	22.65
189	ASP	OD2	19.54	54.59	-2.29	22.55
189	ASP	C	22.28	57.22	-2.87	22.11
189	ASP	O	23.25	56.52	-2.56	22.13
190	LYS	N	21.85	58.23	-2.12	21.87
190	LYS	CA	22.48	58.60	-0.86	21.58
190	LYS	CB	22.88	60.08	-0.89	21.79
190	LYS	CG	24.05	60.40	-1.83	22.07
190	LYS	CD	24.19	61.89	-2.06	22.28
190	LYS	CE	25.42	62.21	-2.90	22.41
190	LYS	NZ	25.46	63.65	-3.30	22.59
190	LYS	C	21.54	58.33	0.30	21.22
190	LYS	O	21.83	58.69	1.45	21.28
191	THR	N	20.40	57.72	0.01	20.83
191	THR	CA	19.42	57.40	1.04	20.38
191	THR	CB	18.25	56.60	0.47	20.44
191	THR	OG1	17.64	57.35	-0.60	20.58
191	THR	CG2	17.21	56.33	1.56	20.48
191	THR	C	20.04	56.56	2.14	19.97
191	THR	O	20.74	55.59	1.87	19.84
192	LEU	N	19.78	56.95	3.38	19.60

192 LEU CA	20.33	56.21	4.51	19.23
192 LEU CB	21.14	57.15	5.41	19.30
192 LEU CG	22.37	57.83	4.79	19.35
192 LEU CD1	23.02	58.72	5.84	19.39
192 LEU CD2	23.34	56.78	4.30	19.38
192 LEU C	19.23	55.57	5.33	18.95
192 LEU O	18.07	56.00	5.29	18.85
193 LEU N	19.59	54.52	6.06	18.63
193 LEU CA	18.65	53.83	6.92	18.35
193 LEU CB	19.08	52.37	7.13	18.28
193 LEU CG	19.36	51.55	5.87	18.21
193 LEU CD1	19.73	50.12	6.27	18.19
193 LEU CD2	18.14	51.53	4.97	18.19
193 LEU C	18.66	54.56	8.26	18.22
193 LEU O	19.71	55.01	8.72	18.20
194 THR N	17.50	54.67	8.90	18.00
194 THR CA	17.44	55.35	10.18	17.86
194 THR CB	16.54	56.60	10.09	17.92
194 THR OG1	15.17	56.20	9.93	18.08
194 THR CG2	16.94	57.46	8.89	17.92
194 THR C	16.92	54.43	11.27	17.66
194 THR O	16.32	53.39	10.99	17.58
195 GLU N	17.18	54.80	12.52	17.44
195 GLU CA	16.71	54.01	13.66	17.18
195 GLU CB	17.17	54.66	14.97	17.32
195 GLU CG	16.60	54.04	16.25	17.58
195 GLU CD	17.12	52.64	16.54	17.71
195 GLU OE1	18.36	52.43	16.54	17.75
195 GLU OE2	16.28	51.74	16.79	17.91
195 GLU C	15.19	53.92	13.60	16.93
195 GLU O	14.50	54.93	13.48	16.84
196 GLY N	14.67	52.70	13.67	16.63
196 GLY CA	13.23	52.50	13.65	16.30
196 GLY C	12.63	52.33	12.26	16.10
196 GLY O	11.43	52.07	12.13	16.02
197 MET N	13.45	52.47	11.23	15.88
197 MET CA	12.96	52.33	9.86	15.62
197 MET CB	14.06	52.72	8.86	15.66
197 MET CG	13.61	52.66	7.42	15.69
197 MET SD	14.88	53.15	6.23	15.97
197 MET CE	14.71	54.91	6.26	15.86
197 MET C	12.52	50.89	9.60	15.51
197 MET O	13.24	49.94	9.93	15.43

198 VAL N	11.33	50.74	9.03	15.40
198 VAL CA	10.80	49.42	8.72	15.29
198 VAL CB	9.36	49.23	9.23	15.28
198 VAL CG1	8.92	47.78	8.99	15.33
198 VAL CG2	9.29	49.57	10.70	15.26
198 VAL C	10.82	49.22	7.22	15.23
198 VAL O	10.24	50.00	6.46	15.07
199 LEU N	11.48	48.15	6.81	15.15
199 LEU CA	11.64	47.83	5.41	15.10
199 LEU CB	13.12	47.97	5.03	15.18
199 LEU CG	13.85	49.25	5.42	15.43
199 LEU CD1	15.34	49.08	5.18	15.50
199 LEU CD2	13.30	50.40	4.59	15.42
199 LEU C	11.22	46.41	5.06	15.00
199 LEU O	11.28	45.51	5.90	14.97
200 ALA N	10.80	46.23	3.81	14.88
200 ALA CA	10.44	44.92	3.29	14.79
200 ALA CB	9.13	44.99	2.49	14.85
200 ALA C	11.62	44.63	2.36	14.74
200 ALA O	11.75	45.27	1.32	14.57
201 ILE N	12.49	43.70	2.76	14.69
201 ILE CA	13.65	43.34	1.95	14.73
201 ILE CB	14.91	43.17	2.84	14.73
201 ILE CG2	16.14	42.87	1.98	14.64
201 ILE CG1	15.14	44.47	3.63	14.74
201 ILE CD1	16.27	44.40	4.64	14.87
201 ILE C	13.31	42.03	1.26	14.86
201 ILE O	13.02	41.03	1.91	14.72
202 GLU N	13.31	42.05	-0.07	15.03
202 GLU CA	12.93	40.89	-0.86	15.23
202 GLU CB	11.44	40.97	-1.21	15.70
202 GLU CG	10.96	42.35	-1.62	16.37
202 GLU CD	9.49	42.36	-2.03	16.74
202 GLU OE1	8.92	43.45	-2.23	17.06
202 GLU OE2	8.90	41.26	-2.16	17.24
202 GLU C	13.75	40.64	-2.12	15.14
202 GLU O	13.30	40.92	-3.24	15.18
203 PRO N	14.95	40.08	-1.97	15.00
203 PRO CD	15.57	39.65	-0.70	14.95
203 PRO CA	15.83	39.79	-3.10	14.80
203 PRO CB	17.13	39.37	-2.43	14.93
203 PRO CG	16.67	38.72	-1.17	14.97
203 PRO C	15.26	38.72	-4.02	14.86

203 PRO O	14.69	37.73	-3.56	14.73
204 PHE N	15.39	38.95	-5.32	14.81
204 PHE CA	14.94	38.03	-6.35	14.77
204 PHE CB	14.10	38.73	-7.42	14.87
204 PHE CG	12.70	39.01	-7.00	15.14
204 PHE CD1	12.37	40.22	-6.40	15.15
204 PHE CD2	11.70	38.08	-7.25	15.18
204 PHE CE1	11.05	40.50	-6.06	15.35
204 PHE CE2	10.39	38.34	-6.92	15.30
204 PHE CZ	10.06	39.56	-6.32	15.32
204 PHE C	16.19	37.51	-7.04	14.65
204 PHE O	17.00	38.30	-7.50	14.68
205 ILE N	16.34	36.19	-7.10	14.51
205 ILE CA	17.49	35.59	-7.75	14.35
205 ILE CB	18.22	34.62	-6.82	14.37
205 ILE CG2	19.36	33.92	-7.57	14.34
205 ILE CG1	18.77	35.38	-5.61	14.42
205 ILE CD1	19.82	36.43	-5.97	14.39
205 ILE C	16.97	34.84	-8.98	14.25
205 ILE O	16.04	34.04	-8.87	14.18
206 SER N	17.59	35.11	-10.12	14.20
206 SER CA	17.19	34.52	-11.39	14.18
206 SER CB	16.78	35.62	-12.36	14.18
206 SER OG	16.50	35.09	-13.65	13.98
206 SER C	18.25	33.65	-12.07	14.23
206 SER O	19.44	33.97	-12.04	14.08
207 SER N	17.80	32.58	-12.71	14.35
207 SER CA	18.71	31.69	-13.42	14.55
207 SER CB	18.02	30.36	-13.74	14.39
207 SER OG	16.86	30.58	-14.52	14.75
207 SER C	19.25	32.33	-14.70	14.70
207 SER O	20.26	31.89	-15.24	14.74
208 ASN N	18.57	33.36	-15.20	14.97
208 ASN CA	19.03	34.02	-16.42	15.29
208 ASN CB	18.68	33.17	-17.64	15.62
208 ASN CG	19.16	33.80	-18.95	15.88
208 ASN OD1	18.43	34.58	-19.58	16.25
208 ASN ND2	20.38	33.47	-19.36	16.23
208 ASN C	18.48	35.42	-16.61	15.36
208 ASN O	19.24	36.40	-16.61	15.34
209 ALA N	17.16	35.52	-16.78	15.46
209 ALA CA	16.51	36.81	-16.99	15.60
209 ALA CB	15.01	36.62	-17.11	15.50

209 ALA C	16.83	37.80	-15.87	15.74
209 ALA O	16.81	37.44	-14.69	15.71
210 SER N	17.09	39.04	-16.25	15.95
210 SER CA	17.41	40.08	-15.27	16.16
210 SER CB	18.63	40.88	-15.73	16.25
210 SER OG	18.37	41.56	-16.95	16.30
210 SER C	16.23	41.02	-15.05	16.31
210 SER O	16.36	42.06	-14.40	16.36
211 PHE N	15.08	40.66	-15.60	16.42
211 PHE CA	13.86	41.45	-15.45	16.55
211 PHE CB	13.84	42.61	-16.44	16.50
211 PHE CG	13.81	42.17	-17.87	16.55
211 PHE CD1	14.98	41.86	-18.54	16.55
211 PHE CD2	12.60	42.04	-18.54	16.55
211 PHE CE1	14.96	41.42	-19.85	16.56
211 PHE CE2	12.57	41.59	-19.86	16.56
211 PHE CZ	13.75	41.28	-20.52	16.52
211 PHE C	12.62	40.59	-15.70	16.67
211 PHE O	12.73	39.45	-16.16	16.65
212 VAL N	11.46	41.15	-15.38	16.75
212 VAL CA	10.19	40.46	-15.59	16.95
212 VAL CB	9.43	40.21	-14.25	17.00
212 VAL CG1	10.28	39.38	-13.31	17.04
212 VAL CG2	9.05	41.52	-13.60	17.07
212 VAL C	9.28	41.28	-16.50	17.20
212 VAL O	9.52	42.47	-16.73	17.16
213 THR N	8.24	40.64	-17.02	17.39
213 THR CA	7.28	41.31	-17.89	17.65
213 THR CB	7.56	41.01	-19.38	17.64
213 THR OG1	7.64	39.59	-19.58	17.57
213 THR CG2	8.85	41.66	-19.83	17.66
213 THR C	5.87	40.88	-17.54	18.01
213 THR O	5.66	39.94	-16.77	17.88
214 GLU N	4.89	41.57	-18.11	18.45
214 GLU CA	3.49	41.25	-17.86	18.82
214 GLU CB	2.59	42.16	-18.69	19.08
214 GLU CG	1.10	41.98	-18.43	19.59
214 GLU CD	0.27	43.06	-19.09	19.87
214 GLU OE1	0.40	44.24	-18.68	20.15
214 GLU OE2	-0.50	42.73	-20.02	19.93
214 GLU C	3.26	39.80	-18.23	18.94
214 GLU O	3.73	39.33	-19.27	18.97
215 GLY N	2.56	39.08	-17.37	19.16

215	GLY	CA	2.29	37.67	-17.61	19.41
215	GLY	C	0.97	37.35	-18.30	19.60
215	GLY	O	0.42	38.19	-19.01	19.60
216	LYS	N	0.48	36.14	-18.06	19.72
216	LYS	CA	-0.77	35.64	-18.64	19.90
216	LYS	CB	-0.99	34.18	-18.24	19.92
216	LYS	CG	-1.17	33.95	-16.73	19.88
216	LYS	CD	-1.38	32.46	-16.39	19.88
216	LYS	CE	-0.16	31.60	-16.71	19.86
216	LYS	NZ	1.05	31.94	-15.91	19.72
216	LYS	C	-2.00	36.46	-18.26	20.01
216	LYS	O	-3.10	36.18	-18.74	20.08
217	ASN	N	-1.82	37.45	-17.39	20.11
217	ASN	CA	-2.92	38.31	-16.97	20.17
217	ASN	CB	-3.73	37.64	-15.85	20.15
217	ASN	CG	-2.87	37.27	-14.64	20.08
217	ASN	OD1	-2.25	38.12	-14.02	20.11
217	ASN	ND2	-2.84	35.98	-14.32	19.98
217	ASN	C	-2.42	39.67	-16.52	20.25
217	ASN	O	-1.23	39.96	-16.55	20.34
218	GLU	N	-3.35	40.53	-16.11	20.42
218	GLU	CA	-3.00	41.88	-15.68	20.46
218	GLU	CB	-4.26	42.73	-15.68	20.71
218	GLU	CG	-5.29	42.24	-14.67	21.21
218	GLU	CD	-6.70	42.34	-15.17	21.50
218	GLU	OE1	-7.06	41.59	-16.11	21.77
218	GLU	OE2	-7.46	43.17	-14.63	21.76
218	GLU	C	-2.36	41.94	-14.29	20.26
218	GLU	O	-2.17	43.02	-13.75	20.26
219	TRP	N	-2.03	40.79	-13.71	20.11
219	TRP	CA	-1.41	40.80	-12.39	19.87
219	TRP	CB	-2.32	40.13	-11.36	20.05
219	TRP	CG	-3.62	40.85	-11.11	20.27
219	TRP	CD2	-3.81	42.02	-10.31	20.38
219	TRP	CE2	-5.20	42.32	-10.34	20.46
219	TRP	CE3	-2.96	42.85	-9.57	20.47
219	TRP	CD1	-4.85	40.50	-11.58	20.32
219	TRP	NE1	-5.80	41.37	-11.12	20.35
219	TRP	CZ2	-5.75	43.41	-9.66	20.48
219	TRP	CZ3	-3.51	43.93	-8.89	20.51
219	TRP	CH2	-4.89	44.20	-8.94	20.54
219	TRP	C	-0.04	40.15	-12.35	19.69
219	TRP	O	0.96	40.81	-12.12	19.59

220	ALA	N	0.00	38.84	-12.59	19.51
220	ALA	CA	1.24	38.08	-12.54	19.25
220	ALA	CB	0.97	36.63	-12.92	19.25
220	ALA	C	2.40	38.61	-13.37	19.12
220	ALA	O	2.22	39.17	-14.45	19.08
221	PHE	N	3.60	38.42	-12.84	18.89
221	PHE	CA	4.83	38.82	-13.51	18.74
221	PHE	CB	5.70	39.63	-12.55	18.94
221	PHE	CG	5.31	41.08	-12.46	19.00
221	PHE	CD1	5.68	41.98	-13.46	19.09
221	PHE	CD2	4.58	41.56	-11.38	19.11
221	PHE	CE1	5.34	43.33	-13.38	19.14
221	PHE	CE2	4.23	42.92	-11.29	19.18
221	PHE	CZ	4.62	43.80	-12.29	19.15
221	PHE	C	5.53	37.55	-13.94	18.55
221	PHE	O	5.52	36.55	-13.23	18.59
222	GLU	N	6.15	37.59	-15.11	18.27
222	GLU	CA	6.83	36.41	-15.62	18.12
222	GLU	CB	5.86	35.62	-16.51	18.26
222	GLU	CG	4.63	35.09	-15.80	18.52
222	GLU	CD	3.64	34.48	-16.77	18.69
222	GLU	OE1	4.10	33.85	-17.75	18.85
222	GLU	OE2	2.41	34.62	-16.56	18.82
222	GLU	C	8.07	36.75	-16.43	17.90
222	GLU	O	8.44	37.91	-16.57	17.79
223	THR	N	8.72	35.71	-16.94	17.70
223	THR	CA	9.89	35.90	-17.80	17.51
223	THR	CB	11.22	35.43	-17.14	17.48
223	THR	OG1	11.19	34.02	-16.91	17.44
223	THR	CG2	11.45	36.15	-15.82	17.47
223	THR	C	9.60	35.08	-19.04	17.44
223	THR	O	9.18	33.92	-18.96	17.45
224	SER	N	9.79	35.69	-20.21	17.33
224	SER	CA	9.53	34.99	-21.46	17.23
224	SER	CB	9.71	35.95	-22.64	17.38
224	SER	OG	8.62	36.86	-22.70	17.48
224	SER	C	10.41	33.76	-21.63	17.10
224	SER	O	9.97	32.75	-22.17	17.02
225	ASP	N	11.65	33.83	-21.15	16.90
225	ASP	CA	12.55	32.68	-21.28	16.73
225	ASP	CB	14.02	33.14	-21.29	16.73
225	ASP	CG	14.46	33.75	-19.96	16.81
225	ASP	OD1	13.65	33.85	-19.02	16.77

225	ASP	OD2	15.66	34.11	-19.87	16.89
225	ASP	C	12.33	31.64	-20.18	16.56
225	ASP	O	13.05	30.64	-20.10	16.51
226	LYS	N	11.31	31.87	-19.36	16.40
226	LYS	CA	10.94	30.98	-18.26	16.33
226	LYS	CB	10.36	29.67	-18.79	16.51
226	LYS	CG	9.05	29.85	-19.56	16.77
226	LYS	CD	8.47	28.50	-19.99	17.17
226	LYS	CE	7.14	28.68	-20.71	17.26
226	LYS	NZ	7.27	29.60	-21.87	17.54
226	LYS	C	12.09	30.68	-17.30	16.20
226	LYS	O	12.28	29.54	-16.87	16.10
227	SER	N	12.87	31.71	-16.96	16.08
227	SER	CA	13.97	31.57	-16.02	15.95
227	SER	CB	14.70	32.91	-15.81	16.03
227	SER	OG	15.51	33.29	-16.91	16.31
227	SER	C	13.41	31.12	-14.68	15.82
227	SER	O	12.24	31.38	-14.37	15.82
228	PHE	N	14.22	30.45	-13.88	15.63
228	PHE	CA	13.79	30.03	-12.55	15.45
228	PHE	CB	14.47	28.70	-12.16	15.62
228	PHE	CG	14.11	27.55	-13.07	15.67
228	PHE	CD1	12.79	27.34	-13.44	15.84
228	PHE	CD2	15.10	26.71	-13.57	15.80
228	PHE	CE1	12.44	26.30	-14.31	15.82
228	PHE	CE2	14.77	25.66	-14.44	15.84
228	PHE	CZ	13.43	25.46	-14.81	15.83
228	PHE	C	14.18	31.15	-11.60	15.24
228	PHE	O	15.36	31.46	-11.44	15.22
229	VAL	N	13.19	31.79	-10.99	15.08
229	VAL	CA	13.44	32.90	-10.08	14.85
229	VAL	CB	12.71	34.18	-10.56	14.85
229	VAL	CG1	13.06	35.34	-9.65	14.82
229	VAL	CG2	13.10	34.49	-12.00	14.91
229	VAL	C	12.95	32.56	-8.68	14.68
229	VAL	O	11.87	32.00	-8.51	14.62
230	ALA	N	13.75	32.88	-7.67	14.53
230	ALA	CA	13.36	32.60	-6.30	14.46
230	ALA	CB	14.28	31.55	-5.67	14.43
230	ALA	C	13.43	33.89	-5.49	14.45
230	ALA	O	14.26	34.76	-5.74	14.30
231	GLN	N	12.54	34.00	-4.51	14.42
231	GLN	CA	12.52	35.18	-3.68	14.46

231	GLN	CB	11.35	36.08	-4.09	14.81
231	GLN	CG	11.08	37.22	-3.12	15.42
231	GLN	CD	9.93	38.12	-3.57	15.89
231	GLN	OE1	8.88	37.65	-4.01	16.22
231	GLN	NE2	10.14	39.44	-3.45	16.19
231	GLN	C	12.40	34.81	-2.21	14.32
231	GLN	O	11.82	33.77	-1.85	14.22
232	ILE	N	12.98	35.64	-1.35	14.25
232	ILE	CA	12.89	35.45	0.09	14.16
232	ILE	CB	14.23	35.00	0.72	14.31
232	ILE	CG2	14.13	35.10	2.24	14.35
232	ILE	CG1	14.54	33.56	0.32	14.40
232	ILE	CD1	13.45	32.55	0.68	14.48
232	ILE	C	12.53	36.85	0.54	14.10
232	ILE	O	13.18	37.81	0.14	14.07
233	GLU	N	11.48	36.99	1.34	14.08
233	GLU	CA	11.07	38.32	1.81	14.04
233	GLU	CB	9.84	38.79	1.01	14.33
233	GLU	CG	9.27	40.14	1.47	14.79
233	GLU	CD	8.21	40.71	0.51	15.04
233	GLU	OE1	7.36	39.94	0.02	15.11
233	GLU	OE2	8.24	41.95	0.26	15.46
233	GLU	C	10.77	38.36	3.31	13.88
233	GLU	O	10.19	37.44	3.87	13.77
234	HIS	N	11.20	39.45	3.95	13.74
234	HIS	CA	10.97	39.65	5.38	13.62
234	HIS	CB	12.17	39.17	6.22	13.64
234	HIS	CG	12.16	37.70	6.52	13.64
234	HIS	CD2	12.97	36.70	6.10	13.71
234	HIS	ND1	11.23	37.12	7.35	13.58
234	HIS	CE1	11.47	35.82	7.43	13.70
234	HIS	NE2	12.52	35.54	6.68	13.68
234	HIS	C	10.77	41.13	5.66	13.69
234	HIS	O	11.28	41.99	4.94	13.41
235	THR	N	10.00	41.41	6.70	13.74
235	THR	CA	9.77	42.77	7.12	14.10
235	THR	CB	8.34	42.95	7.67	13.95
235	THR	OG1	7.41	42.77	6.59	14.05
235	THR	CG2	8.14	44.34	8.25	14.01
235	THR	C	10.80	42.95	8.23	14.34
235	THR	O	10.81	42.19	9.21	14.21
236	VAL	N	11.67	43.94	8.06	14.72
236	VAL	CA	12.75	44.20	9.00	15.16

236 VAL CB	14.13	44.04	8.30	15.24
236 VAL CG1	15.25	44.23	9.30	15.36
236 VAL CG2	14.23	42.68	7.63	15.41
236 VAL C	12.72	45.61	9.58	15.38
236 VAL O	12.45	46.57	8.87	15.38
237 ILE N	13.01	45.73	10.87	15.72
237 ILE CA	13.06	47.02	11.53	16.09
237 ILE CB	12.30	47.01	12.86	16.19
237 ILE CG2	12.44	48.38	13.54	16.19
237 ILE CG1	10.83	46.67	12.64	16.14
237 ILE CD1	10.00	46.61	13.92	16.23
237 ILE C	14.54	47.28	11.81	16.43
237 ILE O	15.22	46.44	12.40	16.46
238 VAL N	15.03	48.44	11.38	16.76
238 VAL CA	16.42	48.81	11.59	17.25
238 VAL CB	16.86	49.87	10.54	17.25
238 VAL CG1	18.34	50.19	10.69	17.33
238 VAL CG2	16.55	49.35	9.14	17.35
238 VAL C	16.58	49.38	13.00	17.55
238 VAL O	15.87	50.32	13.37	17.65
239 THR N	17.47	48.80	13.80	17.94
239 THR CA	17.70	49.28	15.16	18.35
239 THR CB	17.01	48.40	16.23	18.40
239 THR OG1	17.94	47.42	16.70	18.56
239 THR CG2	15.79	47.70	15.64	18.48
239 THR C	19.19	49.29	15.46	18.59
239 THR O	19.97	48.59	14.82	18.59
240 LYS N	19.58	50.09	16.46	18.88
240 LYS CA	20.98	50.19	16.84	19.14
240 LYS CB	21.13	51.17	18.01	19.18
240 LYS CG	20.26	50.84	19.20	19.31
240 LYS CD	20.32	51.95	20.24	19.42
240 LYS CE	19.32	51.70	21.35	19.54
240 LYS NZ	17.94	51.52	20.78	19.63
240 LYS C	21.58	48.85	17.23	19.31
240 LYS O	22.76	48.59	16.99	19.41
241 ASP N	20.76	47.99	17.82	19.56
241 ASP CA	21.23	46.68	18.26	19.74
241 ASP CB	20.45	46.25	19.50	19.96
241 ASP CG	20.56	47.25	20.62	20.19
241 ASP OD1	21.70	47.51	21.06	20.32
241 ASP OD2	19.51	47.77	21.06	20.24
241 ASP C	21.13	45.61	17.20	19.71

241 ASP O	21.30	44.42	17.49	19.76
242 GLY N	20.85	46.01	15.96	19.64
242 GLY CA	20.72	45.05	14.89	19.44
242 GLY C	19.32	44.98	14.31	19.27
242 GLY O	18.37	45.49	14.91	19.42
243 PRO N	19.15	44.36	13.13	19.10
243 PRO CD	20.19	43.72	12.30	19.09
243 PRO CA	17.84	44.25	12.49	18.93
243 PRO CB	18.19	43.76	11.08	18.96
243 PRO CG	19.37	42.91	11.32	18.97
243 PRO C	16.86	43.32	13.20	18.84
243 PRO O	17.24	42.26	13.71	18.83
244 ILE N	15.60	43.72	13.22	18.63
244 ILE CA	14.56	42.94	13.85	18.44
244 ILE CB	13.77	43.77	14.87	18.58
244 ILE CG2	12.60	42.95	15.40	18.60
244 ILE CG1	14.69	44.22	16.00	18.60
244 ILE CD1	14.01	45.12	17.01	18.87
244 ILE C	13.61	42.46	12.77	18.24
244 ILE O	12.97	43.27	12.10	18.19
245 LEU N	13.53	41.15	12.60	18.04
245 LEU CA	12.64	40.57	11.60	17.82
245 LEU CB	13.26	39.30	11.01	17.85
245 LEU CG	14.34	39.49	9.95	17.94
245 LEU CD1	15.49	40.33	10.50	17.98
245 LEU CD2	14.82	38.13	9.50	17.98
245 LEU C	11.30	40.23	12.25	17.67
245 LEU O	11.21	39.28	13.02	17.72
246 THR N	10.27	40.99	11.93	17.42
246 THR CA	8.96	40.73	12.50	17.16
246 THR CB	8.01	41.92	12.28	17.11
246 THR OG1	7.78	42.08	10.88	16.92
246 THR CG2	8.61	43.21	12.84	17.02
246 THR C	8.31	39.49	11.87	17.16
246 THR O	7.41	38.90	12.46	17.01
247 THR N	8.79	39.10	10.69	17.17
247 THR CA	8.23	37.97	9.96	17.28
247 THR CB	8.10	38.30	8.47	17.17
247 THR OG1	9.38	38.69	7.96	17.06
247 THR CG2	7.10	39.43	8.27	17.15
247 THR C	9.02	36.67	10.07	17.60
247 THR O	8.81	35.72	9.31	17.40
248 LYS N	9.95	36.63	11.02	18.00

248	LYS	CA	10.76	35.45	11.26	18.41
248	LYS	CB	12.25	35.81	11.21	18.46
248	LYS	CG	13.18	34.62	11.42	18.68
248	LYS	CD	14.29	34.98	12.41	18.86
248	LYS	CE	15.29	33.85	12.59	18.87
248	LYS	NZ	16.27	33.83	11.46	18.92
248	LYS	C	10.41	34.95	12.65	18.63
248	LYS	O	10.35	35.72	13.61	18.70
249	ILE	N	10.15	33.65	12.73	18.88
249	ILE	CA	9.82	32.99	13.98	19.17
249	ILE	CB	8.69	31.97	13.79	19.27
249	ILE	CG2	8.35	31.30	15.12	19.37
249	ILE	CG1	7.47	32.68	13.20	19.19
249	ILE	CD1	6.26	31.78	13.00	19.11
249	ILE	C	11.07	32.24	14.44	19.30
249	ILE	O	11.17	31.05	14.12	19.48
249	ILE	OT	11.94	32.88	15.08	19.56
301	HOH	O	15.58	45.78	-8.07	13.29
302	HOH	O	8.20	30.81	-9.11	9.94
303	HOH	O	27.39	35.54	-0.53	14.83
304	HOH	O	5.50	43.91	10.59	9.76
305	HOH	O	10.59	34.42	4.24	7.93
306	HOH	O	19.45	47.41	12.36	15.72
307	HOH	O	-1.29	38.04	1.88	14.01
308	HOH	O	13.24	24.25	-1.59	14.18
309	HOH	O	-13.22	32.82	-2.07	15.50
310	HOH	O	18.12	39.61	-19.01	14.85
311	HOH	O	0.03	23.25	6.53	17.05
312	HOH	O	1.50	24.00	-11.29	15.56
313	HOH	O	-9.35	32.09	-0.58	13.40
314	HOH	O	10.19	52.79	6.21	17.63
315	HOH	O	-8.01	22.26	-10.70	14.85
316	HOH	O	-2.36	51.98	8.35	14.01
317	HOH	O	6.27	15.67	-3.49	17.58
318	HOH	O	10.53	30.89	-11.09	17.26
319	HOH	O	10.13	38.60	-20.14	12.45
320	HOH	O	30.28	34.23	-0.09	17.92
321	HOH	O	-0.84	44.52	14.44	16.58
322	HOH	O	26.21	57.81	7.05	13.30
323	HOH	O	19.17	48.50	-2.42	17.17
324	HOH	O	13.11	36.66	-20.68	15.09
325	HOH	O	6.96	38.85	14.99	15.43
326	HOH	O	9.75	31.91	10.28	14.40

327	HOH	O	4.86	28.36	12.29	19.91
328	HOH	O	21.80	54.71	-0.54	16.23
329	HOH	O	6.66	25.26	6.89	14.98
330	HOH	O	24.86	54.37	-3.29	21.95
331	HOH	O	7.98	55.20	5.75	15.42
332	HOH	O	-3.38	22.91	-13.66	19.49
333	HOH	O	10.11	34.59	-7.28	17.80
334	HOH	O	9.10	26.82	-16.09	17.48
335	HOH	O	3.05	15.74	-9.90	15.64
336	HOH	O	6.54	57.38	3.22	19.58
337	HOH	O	4.19	48.03	26.45	17.54
338	HOH	O	6.37	21.07	-0.89	16.77
339	HOH	O	2.25	19.30	6.94	19.90
340	HOH	O	10.04	28.93	-15.26	15.12
341	HOH	O	0.00	48.16	19.92	16.41
342	HOH	O	26.78	44.53	-6.33	17.16
343	HOH	O	-5.06	33.66	-15.77	16.23
344	HOH	O	13.65	54.53	-3.06	19.30
345	HOH	O	-17.57	28.43	10.03	18.58
346	HOH	O	3.93	35.26	-5.28	17.46
347	HOH	O	-8.81	29.06	-11.84	17.53
348	HOH	O	-1.49	34.38	-12.13	16.89
349	HOH	O	-12.43	26.89	-3.00	15.32
350	HOH	O	10.54	30.05	6.06	16.74
351	HOH	O	1.05	28.19	-16.99	18.50
352	HOH	O	21.27	28.86	1.27	19.15
353	HOH	O	11.88	20.15	-2.30	18.43
354	HOH	O	10.52	47.72	-15.77	19.17
355	HOH	O	22.27	40.37	-12.00	16.97
356	HOH	O	10.42	12.95	-7.41	19.92
357	HOH	O	9.19	23.21	1.40	13.30
358	HOH	O	6.64	26.05	16.30	22.39
359	HOH	O	-9.67	25.19	-6.10	21.60
360	HOH	O	14.70	25.83	-0.04	19.19
361	HOH	O	-5.83	29.97	-21.37	21.00
362	HOH	O	17.48	51.03	-2.79	18.87
363	HOH	O	17.34	25.55	-18.63	19.45
364	HOH	O	21.00	22.98	-6.51	16.39
365	HOH	O	19.18	57.03	12.95	17.28
366	HOH	O	24.93	34.77	7.98	20.06
367	HOH	O	29.01	42.16	-7.78	21.98
368	HOH	O	7.30	21.19	-12.40	20.66
369	HOH	O	1.85	39.52	-1.07	21.23

370	HOH	O	-11.25	37.95	12.27	18.94
371	HOH	O	5.68	17.09	-12.51	14.63
372	HOH	O	18.83	59.66	4.15	19.42
373	HOH	O	-2.45	39.18	-20.31	20.20
374	HOH	O	-2.89	51.67	4.45	18.29
375	HOH	O	-3.65	18.15	-1.24	20.93
376	HOH	O	-7.38	24.80	2.09	20.51
377	HOH	O	-1.20	30.35	-12.83	16.70
378	HOH	O	-11.24	29.00	3.59	17.09
379	HOH	O	11.02	20.77	-13.07	20.24
380	HOH	O	20.19	60.08	-2.96	22.38
381	HOH	O	-5.47	56.35	23.01	20.13
382	HOH	O	14.16	56.73	-10.30	23.05
383	HOH	O	5.84	30.08	17.45	23.80
384	HOH	O	-1.10	26.40	11.23	18.74
385	HOH	O	13.21	53.06	17.30	20.35
386	HOH	O	26.15	36.60	-12.84	18.40
387	HOH	O	26.31	44.66	4.11	22.33
388	HOH	O	7.42	53.55	24.05	20.26
389	HOH	O	-15.40	25.50	-5.02	21.75
390	HOH	O	-9.94	49.33	0.99	21.69
391	HOH	O	-9.82	30.09	-18.49	22.08
392	HOH	O	8.73	17.60	-15.37	22.36
393	HOH	O	14.56	39.48	14.70	18.48
394	HOH	O	33.14	35.08	-14.69	21.34
395	HOH	O	-11.29	30.98	10.83	21.35
396	HOH	O	6.51	57.12	9.90	21.88
397	HOH	O	4.94	40.34	-21.52	21.03
398	HOH	O	18.05	58.88	-4.38	22.13
399	HOH	O	22.46	37.96	8.51	16.98
400	HOH	O	-6.56	43.63	18.04	20.38
401	HOH	O	6.20	21.84	9.02	22.53
402	HOH	O	11.54	60.10	2.44	19.72
403	HOH	O	10.16	58.97	-13.02	20.98
404	HOH	O	20.30	28.25	5.09	22.10
405	HOH	O	-8.58	38.95	4.27	15.56
406	HOH	O	15.79	36.64	-21.40	24.14
407	HOH	O	-3.69	16.22	2.31	20.43
408	HOH	O	11.80	57.04	5.08	17.94
409	HOH	O	20.26	54.34	17.28	22.77
410	HOH	O	28.85	64.98	-2.73	20.92
411	HOH	O	24.31	29.52	-12.44	19.06
412	HOH	O	9.29	13.36	-4.52	19.92

413	HOH	O	-6.69	47.05	9.87	22.55
414	HOH	O	27.01	45.74	0.80	12.75
415	HOH	O	-1.12	19.80	8.30	19.44
416	HOH	O	30.00	56.11	-14.13	25.81
417	HOH	O	12.09	32.76	8.32	18.82
418	HOH	O	-14.13	30.16	-15.63	23.51
419	HOH	O	8.46	45.06	-17.68	20.53
420	HOH	O	-8.04	37.23	17.14	22.73
421	HOH	O	0.05	58.45	19.88	22.71
422	HOH	O	10.70	49.46	-10.16	23.04
423	HOH	O	4.89	19.70	5.08	21.10
424	HOH	O	14.98	28.19	13.97	24.08
425	HOH	O	9.93	49.36	26.74	23.28
426	HOH	O	20.91	22.21	-14.82	23.68
427	HOH	O	9.41	61.42	20.20	22.72
428	HOH	O	3.22	25.20	9.62	21.33
429	HOH	O	12.87	22.23	-15.08	23.34
430	HOH	O	25.93	58.76	-9.31	22.03
431	HOH	O	16.69	63.09	-4.55	21.66
432	HOH	O	17.10	20.16	-17.44	23.82
300	458	C1	2.38	43.13	-3.65	24.20
300	458	C2	3.30	42.69	-2.65	24.07
300	458	C3	1.28	42.47	-4.17	24.18
300	458	O4	2.50	44.37	-4.25	24.25
300	458	C5	3.34	41.56	-1.89	24.16
300	458	N6	4.41	43.38	-2.25	24.12
300	458	C7	0.68	43.32	-5.14	24.19
300	458	C8	1.48	44.49	-5.15	24.18
300	458	N9	4.43	41.60	-1.07	24.13
300	458	N10	5.08	42.72	-1.30	24.14
300	458	C11	-0.45	43.24	-6.02	24.24
300	458	C12	1.23	45.61	-5.99	24.24
300	458	C13	-0.73	44.36	-6.88	24.21
300	458	C14	0.10	45.52	-6.86	24.22
253	ZN2	ZN	6.77	43.47	-0.65	25.04
254	ZN2	ZN	5.53	40.31	-0.32	19.29

Table IV

Provides distances between interresidue atoms that are within 5 Ångstroms apart in an active site of a *S. aureus* methionine aminopeptidase for an inhibitor complex with 5-(3-Iodo-phenyl)-1-H-[1,2,3]triazole.

Atom 1	Atom 2	Distance
300C1	174CD2	3.679
300C1	174CD1	3.938
300C1	95OG	4.030
300C1	174CG	4.403
300C1	56CG	4.667
300C1	95CB	4.911
174CD2	300C1	38.87
174CD2	300C1	93.98
174CD2	300C1	19.13
174CD2	300C1	112.04
174CD2	300C1	90.77
174CD1	300C1	62.23
174CD1	300C1	20.05
174CD1	300C1	101.60
174CD1	300C1	54.57
95OG	300C1	79.66
95OG	300C1	49.06
95OG	300C1	14.32
174CG	300C1	110.30
174CG	300C1	73.86
56CG	300C1	63.06
300C2	174CD1	3.810
300C2	174CD2	4.047
300C2	104OD2	4.313
300C2	95OG	4.340
300C2	104OD1	4.348
300C2	93OD1	4.424
300C2	174CG	4.440
300C2	175CE1	4.592
300C2	104CG	4.643
300C2	93OD2	4.711
300C2	93CG	4.779
300C2	95CB	4.839
300C2	168NE2	4.936
300C2	76CE1	4.981
174CD1	300C2	37.67
174CD1	300C2	60.60
174CD1	300C2	60.29
174CD1	300C2	73.12
174CD1	300C2	108.68
174CD1	300C2	19.40
174CD1	300C2	60.61
174CD1	300C2	61.72
174CD1	300C2	128.46
174CD1	300C2	123.04
174CD1	300C2	55.80
174CD1	300C2	62.72
174CD1	300C2	149.72
174CD2	300C2	90.84
174CD2	300C2	84.48
174CD2	300C2	110.04
174CD2	300C2	145.44
174CD2	300C2	19.96
174CD2	300C2	41.70
174CD2	300C2	96.88
174CD2	300C2	163.77
174CD2	300C2	160.31
174CD2	300C2	87.57
174CD2	300C2	72.77
174CD2	300C2	112.84
104OD2	300C2	81.21
104OD2	300C2	29.39
104OD2	300C2	68.62
104OD2	300C2	71.81
104OD2	300C2	77.23
104OD2	300C2	15.46
104OD2	300C2	72.94
104OD2	300C2	76.26
104OD2	300C2	64.77
104OD2	300C2	36.99
104OD2	300C2	131.39
95OG	300C2	62.76
95OG	300C2	65.66
95OG	300C2	76.06
95OG	300C2	120.36

95OG 300C2 67.82
95OG 300C2 93.20
95OG 300C2 78.95
95OG 300C2 16.63
95OG 300C2 110.85
95OG 300C2 139.96
104OD1 300C2 41.49
104OD1 300C2 90.16
104OD1 300C2 106.34
104OD1 300C2 15.52
104OD1 300C2 55.34
104OD1 300C2 52.55
104OD1 300C2 46.89
104OD1 300C2 66.01
104OD1 300C2 132.51
93OD1 300C2 127.87
93OD1 300C2 144.11
93OD1 300C2 56.86
93OD1 300C2 27.59
93OD1 300C2 14.94
93OD1 300C2 58.87
93OD1 300C2 100.98
93OD1 300C2 101.42
174CG 300C2 44.45
174CG 300C2 76.95
174CG 300C2 144.30
174CG 300C2 141.84
174CG 300C2 74.28
174CG 300C2 60.83
174CG 300C2 130.32
175CE1 300C2 91.08
175CE1 300C2 130.38
175CE1 300C2 143.91
175CE1 300C2 115.63
175CE1 300C2 43.13
175CE1 300C2 92.75
104CG 300C2 67.53
104CG 300C2 67.06
104CG 300C2 51.19
104CG 300C2 52.35
104CG 300C2 138.66
93OD2 300C2 15.23
93OD2 300C2 85.84
93OD2 300C2 93.24
93OD2 300C2 79.01
93CG 300C2 73.55
93CG 300C2 103.25
93CG 300C2 86.79
95CB 300C2 96.40
95CB 300C2 151.12
168NE2 300C2 108.77
300C3 67SG 4.179
300C3 76CE1 4.211
300C3 76NE2 4.261
300C3 174CD2 4.578
300C3 56CG 4.626
300C3 76ND1 4.673
300C3 76CD2 4.774
67SG 300C3 79.93
67SG 300C3 87.30
67SG 300C3 161.25
67SG 300C3 64.01
67SG 300C3 63.97
67SG 300C3 75.35
76CE1 300C3 17.93
76CE1 300C3 118.10
76CE1 300C3 143.92
76CE1 300C3 16.05
76CE1 300C3 27.36
76NE2 300C3 111.44
76NE2 300C3 146.59
76NE2 300C3 27.26
76NE2 300C3 16.26
174CD2 300C3 97.93
174CD2 300C3 134.15
174CD2 300C3 122.89
56CG 300C3 127.90
56CG 300C3 130.60
76ND1 300C3 26.71
300C4 174CD2 3.079
300C4 174CD1 3.203
300C4 95OG 3.309
300C4 174CG 3.697
300C4 56CG 4.117
300C4 95CB 4.307
300C4 56CD 4.483

300C4 56N 4.525
300C4 55CB 4.551
300C4 56CA 4.603
300C4 174CB 4.621
300C4 55C 4.782
300C4 56CB 4.870
174CD2 300C4 47.78
174CD2 300C4 124.03
174CD2 300C4 23.77
174CD2 300C4 149.20
174CD2 300C4 112.41
174CD2 300C4 134.39
174CD2 300C4 118.79
174CD2 300C4 95.90
174CD2 300C4 119.82
174CD2 300C4 29.29
174CD2 300C4 103.37
174CD2 300C4 137.29
174CD1 300C4 78.45
174CD1 300C4 24.16
174CD1 300C4 131.51
174CD1 300C4 65.13
174CD1 300C4 112.99
174CD1 300C4 112.13
174CD1 300C4 71.48
174CD1 300C4 127.87
174CD1 300C4 30.61
174CD1 300C4 98.20
174CD1 300C4 139.91
95OG 300C4 100.94
95OG 300C4 57.79
95OG 300C4 15.30
95OG 300C4 47.45
95OG 300C4 62.45
95OG 300C4 45.17
95OG 300C4 78.07
95OG 300C4 96.24
95OG 300C4 65.17
95OG 300C4 73.22
174CG 300C4 144.62
174CG 300C4 88.68
174CG 300C4 124.94
174CG 300C4 116.07
174CG 300C4 81.68
174CG 300C4 125.45
174CG 300C4 16.66
174CG 300C4 99.87
174CG 300C4 143.13
56CG 300C4 73.01
56CG 300C4 19.80
56CG 300C4 30.94
56CG 300C4 63.24
56CG 300C4 30.65
56CG 300C4 129.25
56CG 300C4 47.01
56CG 300C4 16.62
95CB 300C4 62.34
95CB 300C4 76.04
95CB 300C4 50.54
95CB 300C4 92.61
95CB 300C4 87.06
95CB 300C4 76.06
95CB 300C4 88.52
56CD 300C4 18.86
56CD 300C4 43.44
56CD 300C4 30.79
56CD 300C4 110.17
56CD 300C4 31.69
56CD 300C4 28.60
56N 300C4 41.27
56N 300C4 18.42
56N 300C4 99.66
56N 300C4 16.30
56N 300C4 28.51
55CB 300C4 59.00
55CB 300C4 68.02
55CB 300C4 31.10
55CB 300C4 68.44
56CA 300C4 108.93
56CA 300C4 29.74
56CA 300C4 18.26
174CB 300C4 83.39
174CB 300C4 126.48
55C 300C4 44.03
300C5 175CE1 3.532
300C5 174CD1 3.593

300C5 104OD2 3.613
300C5 168NE2 3.619
300C5 174CD2 3.821
300C5 174CG 4.022
300C5 168CE1 4.288
300C5 104CG 4.289
300C5 104OD1 4.320
300C5 175NE2 4.393
300C5 175ND1 4.453
300C5 168CD2 4.498
300C5 202OE1 4.829
300C5 233OE2 4.868
175CE1 300C5 74.10
175CE1 300C5 102.23
175CE1 300C5 58.91
175CE1 300C5 49.97
175CE1 300C5 53.35
175CE1 300C5 57.33
175CE1 300C5 114.55
175CE1 300C5 131.18
175CE1 300C5 14.62
175CE1 300C5 13.75
175CE1 300C5 50.49
175CE1 300C5 86.19
175CE1 300C5 114.50
174CD1 300C5 69.77
174CD1 300C5 80.34
174CD1 300C5 40.03
174CD1 300C5 22.15
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174CD1 300C5 67.11
174CD1 300C5 75.50
174CD1 300C5 87.86
174CD1 300C5 60.36
174CD1 300C5 89.95
174CD1 300C5 122.27
174CD1 300C5 103.38
104OD2 300C5 48.89
104OD2 300C5 106.49
104OD2 300C5 84.33
104OD2 300C5 45.07
104OD2 300C5 15.33
104OD2 300C5 30.53
104OD2 300C5 103.16
104OD2 300C5 96.64
104OD2 300C5 63.15
104OD2 300C5 62.28
104OD2 300C5 33.68
168NE2 300C5 92.51
168NE2 300C5 76.98
168NE2 300C5 16.60
168NE2 300C5 64.09
168NE2 300C5 79.05
168NE2 300C5 55.42
168NE2 300C5 60.08
168NE2 300C5 15.06
168NE2 300C5 44.18
168NE2 300C5 56.34
174CD2 300C5 22.17
174CD2 300C5 79.92
174CD2 300C5 106.76
174CD2 300C5 115.25
174CD2 300C5 64.07
174CD2 300C5 39.17
174CD2 300C5 92.61
174CD2 300C5 133.13
174CD2 300C5 139.07
174CG 300C5 62.02
174CG 300C5 85.66
174CG 300C5 96.42
174CG 300C5 67.72
174CG 300C5 39.70
174CG 300C5 81.66
174CG 300C5 121.02
174CG 300C5 117.05
168CE1 300C5 58.70
168CE1 300C5 75.16
168CE1 300C5 58.81
168CE1 300C5 53.96
168CE1 300C5 28.78
168CE1 300C5 59.99
168CE1 300C5 63.52
104CG 300C5 16.67
104CG 300C5 117.46
104CG 300C5 106.71
104CG 300C5 78.47

104CG 300C5 73.75
104CG 300C5 38.78
104OD1 300C5 133.68
104OD1 300C5 122.67
104OD1 300C5 92.63
104OD1 300C5 78.88
104OD1 300C5 40.21
175NE2 300C5 28.03
175NE2 300C5 43.66
175NE2 300C5 74.27
175NE2 300C5 107.09
175ND1 300C5 55.46
175ND1 300C5 94.63
175ND1 300C5 116.21
168CD2 300C5 40.71
168CD2 300C5 64.23
202OE1 300C5 38.87
300N6 93OD1 3.143
300N6 93OD2 3.381
300N6 93CG 3.432
300N6 104OD1 3.591
300N6 104OD2 4.058
300N6 104CG 4.184
300N6 95OG 4.376
300N6 233OE1 4.497
300N6 93CB 4.567
300N6 174CD1 4.658
300N6 95CB 4.680
300N6 233OE2 4.750
93OD1 300N6 39.13
93OD1 300N6 21.29
93OD1 300N6 54.47
93OD1 300N6 85.29
93OD1 300N6 70.65
93OD1 300N6 76.44
93OD1 300N6 44.59
93OD1 300N6 29.20
93OD1 300N6 117.00
93OD1 300N6 68.18
93OD1 300N6 70.83
93OD2 300N6 21.29
93OD2 300N6 74.41
93OD2 300N6 92.03
93OD2 300N6 86.14
93OD2 300N6 115.48
93OD2 300N6 37.50
93OD2 300N6 30.89
93OD2 300N6 145.34
93OD2 300N6 106.46
93OD2 300N6 60.37
93CG 300N6 70.57
93CG 300N6 97.02
93CG 300N6 85.64
93CG 300N6 95.35
93CG 300N6 45.40
93CG 300N6 14.73
93CG 300N6 137.95
93CG 300N6 89.07
93CG 300N6 72.37
104OD1 300N6 32.66
104OD1 300N6 16.29
104OD1 300N6 68.37
104OD1 300N6 41.24
104OD1 300N6 82.86
104OD1 300N6 71.17
104OD1 300N6 50.82
104OD1 300N6 42.33
104OD2 300N6 17.34
104OD2 300N6 83.69
104OD2 300N6 54.67
104OD2 300N6 111.21
104OD2 300N6 55.92
104OD2 300N6 68.14
104OD2 300N6 35.07
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104CG 300N6 49.60
104CG 300N6 98.62
104CG 300N6 59.32
104CG 300N6 54.76
104CG 300N6 39.82
95OG 300N6 103.90
95OG 300N6 92.79
95OG 300N6 54.13
95OG 300N6 17.58
95OG 300N6 110.22
233OE1 300N6 60.09

233OE1 300N6 108.68
233OE1 300N6 87.80
233OE1 300N6 27.34
93CB 300N6 143.39
93CB 300N6 90.88
93CB 300N6 86.89
174CD1 300N6 52.74
174CD1 300N6 90.57
95CB 300N6 92.67
300C7 56CG 4.051
300C7 56CB 4.136
300C7 67SG 4.162
300C7 60CG 4.251
300C7 56CA 4.290
300C7 76NE2 4.772
300C7 174CD2 4.915
300C7 76CD2 4.964
56CG 300C7 21.05
56CG 300C7 69.49
56CG 300C7 100.39
56CG 300C7 32.59
56CG 300C7 149.40
56CG 300C7 101.04
56CG 300C7 142.44
56CB 300C7 73.79
56CB 300C7 85.83
56CB 300C7 20.77
56CB 300C7 151.69
56CB 300C7 110.08
56CB 300C7 137.33
67SG 300C7 144.99
67SG 300C7 94.55
67SG 300C7 81.09
67SG 300C7 144.17
67SG 300C7 73.41
60CG 300C7 68.06
60CG 300C7 108.70
60CG 300C7 69.46
60CG 300C7 106.64
56CA 300C7 166.68
56CA 300C7 92.98
56CA 300C7 150.76
76NE2 300C7 97.90
76NE2 300C7 16.08
174CD2 300C7 112.52
300C8 56CA 3.364
300C8 56CG 3.482
300C8 56N 3.515
300C8 174CD2 3.578
300C8 55C 3.794
300C8 95OG 3.823
300C8 56CD 3.833
300C8 56CB 3.872
300C8 55O 3.889
300C8 60CG 4.116
300C8 174CD1 4.164
300C8 55CB 4.276
300C8 174CG 4.410
300C8 56C 4.628
300C8 55CA 4.695
300C8 56O 4.906
300C8 60OE2 4.967
300C8 174CB 4.987
56CA 300C8 40.13
56CA 300C8 24.43
56CA 300C8 148.99
56CA 300C8 38.85
56CA 300C8 89.78
56CA 300C8 38.52
56CA 300C8 23.00
56CA 300C8 42.98
56CA 300C8 78.72
56CA 300C8 138.18
56CA 300C8 71.18
56CA 300C8 143.40
56CA 300C8 12.37
56CA 300C8 53.45
56CA 300C8 26.21
56CA 300C8 96.90
56CA 300C8 126.90
56CG 300C8 39.05
56CG 300C8 159.09
56CG 300C8 59.14
56CG 300C8 59.87
56CG 300C8 23.38
56CG 300C8 22.71

56CG	300C8	73.69
56CG	300C8	113.93
56CG	300C8	121.65
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56CG	300C8	140.99
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56CG	300C8	62.94
56CG	300C8	64.61
56CG	300C8	136.67
56CG	300C8	136.95
56N	300C8	136.40
56N	300C8	20.74
56N	300C8	69.52
56N	300C8	22.66
56N	300C8	36.48
56N	300C8	34.91
56N	300C8	96.57
56N	300C8	114.10
56N	300C8	47.25
56N	300C8	123.35
56N	300C8	32.19
56N	300C8	30.81
56N	300C8	46.18
56N	300C8	106.13
56N	300C8	109.35
174CD2	300C8	116.13
174CD2	300C8	99.28
174CD2	300C8	141.25
174CD2	300C8	171.87
174CD2	300C8	107.01
174CD2	300C8	85.76
174CD2	300C8	37.45
174CD2	300C8	93.73
174CD2	300C8	18.45
174CD2	300C8	139.30
174CD2	300C8	106.59
174CD2	300C8	130.49
174CD2	300C8	60.17
174CD2	300C8	27.49
55C	300C8	72.99
55C	300C8	39.00
55C	300C8	56.33
55C	300C8	18.39
55C	300C8	91.45
55C	300C8	100.49
55C	300C8	35.64
55C	300C8	105.15
55C	300C8	40.40
55C	300C8	16.83
55C	300C8	50.68
55C	300C8	92.17
55C	300C8	89.79
95OG	300C8	51.29
95OG	300C8	81.74
95OG	300C8	89.88
95OG	300C8	164.34
95OG	300C8	61.90
95OG	300C8	46.59
95OG	300C8	81.81
95OG	300C8	100.70
95OG	300C8	59.32
95OG	300C8	115.17
95OG	300C8	146.80
95OG	300C8	84.18
56CD	300C8	35.36
56CD	300C8	56.17
56CD	300C8	116.79
56CD	300C8	107.38
56CD	300C8	48.33
56CD	300C8	123.40
56CD	300C8	49.90
56CD	300C8	39.81
56CD	300C8	64.35
56CD	300C8	128.78
56CD	300C8	115.02
56CB	300C8	64.88
56CB	300C8	91.22
56CB	300C8	142.25
56CB	300C8	81.07
56CB	300C8	158.36
56CB	300C8	33.27
56CB	300C8	66.90
56CB	300C8	43.35
56CB	300C8	115.01
56CB	300C8	145.83
55O	300C8	74.46

55O 300C8 103.04
55O 300C8 47.15
55O 300C8 101.14
55O 300C8 38.47
55O 300C8 30.73
55O 300C8 43.20
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55O 300C8 84.19
60CG 300C8 121.13
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60CG 300C8 101.07
60CG 300C8 66.93
60CG 300C8 105.05
60CG 300C8 52.56
60CG 300C8 28.38
60CG 300C8 94.18
174CD1 300C8 67.01
174CD1 300C8 20.20
174CD1 300C8 140.42
174CD1 300C8 84.90
174CD1 300C8 145.29
174CD1 300C8 93.20
174CD1 300C8 29.70
55CB 300C8 77.41
55CB 300C8 75.50
55CB 300C8 18.83
55CB 300C8 86.30
55CB 300C8 105.28
55CB 300C8 66.76
174CG 300C8 138.93
174CG 300C8 92.54
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174CG 300C8 73.50
174CG 300C8 17.14
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56C 300C8 14.49
56C 300C8 84.57
56C 300C8 121.79
55CA 300C8 67.51
55CA 300C8 99.40
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56O 300C8 72.09
56O 300C8 119.94
60OE2 300C8 65.82
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300N9 168NE2 3.218
300N9 233OE2 3.558
300N9 104OD1 3.610
300N9 104CG 3.612
300N9 202OE1 3.749
300N9 168CE1 4.092
300N9 202OE2 4.127
300N9 168CD2 4.147
300N9 93OD2 4.216
300N9 202CD 4.312
300N9 175CE1 4.316
300N9 233OE1 4.326
300N9 233CD 4.362
300N9 174CD1 4.390
300N9 93OD1 4.504
300N9 93CG 4.740
300N9 175NE2 4.947
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104OD2 300N9 37.49
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168NE2 300N9 57.24
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168NE2 300N9 15.93

168NE2 300N9 140.91
168NE2 300N9 71.02
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168NE2 300N9 105.18
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233OE2 300N9 51.03
233OE2 300N9 52.33
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233OE2 300N9 65.76
233OE2 300N9 43.83
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104OD1 300N9 96.62
104OD1 300N9 128.87
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104OD1 300N9 138.27
104CG 300N9 96.40
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104CG 300N9 75.78
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202OE1 300N9 15.80
202OE1 300N9 91.49
202OE1 300N9 75.39
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202OE1 300N9 130.62
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168CE1 300N9 142.46
168CE1 300N9 83.87
168CE1 300N9 53.79
168CE1 300N9 105.05
168CE1 300N9 90.25
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168CE1 300N9 128.99
168CE1 300N9 140.78
168CE1 300N9 55.30
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202OE2 300N9 49.09
202OE2 300N9 157.23
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202OE2 300N9 76.49
202OE2 300N9 105.16
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168CD2 300N9 94.18
168CD2 300N9 84.70
168CD2 300N9 149.86
168CD2 300N9 151.28
168CD2 300N9 41.49
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93OD2 300N9 163.57
93OD2 300N9 37.44
93OD2 300N9 52.80
93OD2 300N9 126.45
93OD2 300N9 28.93
93OD2 300N9 14.72
93OD2 300N9 156.79
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202CD 300N9 61.82
202CD 300N9 51.34
202CD 300N9 142.29
202CD 300N9 99.92
202CD 300N9 91.03
202CD 300N9 93.50
175CE1 300N9 158.35
175CE1 300N9 142.15
175CE1 300N9 59.08
175CE1 300N9 153.05
175CE1 300N9 159.41
175CE1 300N9 14.43
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233OE1 300N9 117.17
233OE1 300N9 41.84
233OE1 300N9 41.20
233OE1 300N9 151.60
233CD 300N9 116.05
233CD 300N9 57.65
233CD 300N9 57.76
233CD 300N9 135.37
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174CD1 300N9 111.84
174CD1 300N9 72.98
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93OD1 300N9 166.22
93CG 300N9 163.81
300N10 93OD2 2.996
300N10 104OD1 3.091
300N10 104OD2 3.230
300N10 93OD1 3.241
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300N10 104CG 3.546
300N10 233CD 3.916
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93OD1 300N10 117.06
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93CG 300N10 96.56
93CG 300N10 73.46
93CG 300N10 93.21
93CG 300N10 153.23
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93CG 300N10 105.78
93CG 300N10 9.22
93CG 300N10 127.63
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233OE2 300N10 52.20
233OE2 300N10 18.18
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233OE2 300N10 62.41
233OE2 300N10 46.54
233OE2 300N10 40.73
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233OE1 300N10 62.21
233OE1 300N10 18.45
233OE1 300N10 60.34
233OE1 300N10 98.51
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233OE1 300N10 121.40
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104CG 300N10 63.34
104CG 300N10 86.64
104CG 300N10 89.02
104CG 300N10 104.35
104CG 300N10 59.40
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233CD 300N10 80.24
233CD 300N10 61.15
233CD 300N10 51.37
233CD 300N10 82.23
233CD 300N10 112.87
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202OE2 300N10 29.35
202OE2 300N10 14.98
202OE2 300N10 96.76
202OE2 300N10 133.12
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168NE2 300N10 59.20
168NE2 300N10 162.34
168NE2 300N10 59.19
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202OE1 300N10 125.82
202OE1 300N10 104.17
202CD 300N10 110.39
202CD 300N10 118.20
93CB 300N10 127.36
300C11 56CA 3.156
300C11 56CB 3.421
300C11 56CG 3.445
300C11 60CG 3.523
300C11 56N 3.858
300C11 56CD 4.223
300C11 56C 4.268
300C11 60CB 4.320
300C11 56O 4.346

300C11 55O 4.402
300C11 55C 4.414
300C11 174CD2 4.492
300C11 60CD 4.721
300C11 95OG 4.846
300C11 62CB 4.869
300C11 60OE2 4.986
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56CA 300C11 41.44
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56CA 300C11 21.20
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56CA 300C11 32.73
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56CB 300C11 25.19
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60CD 300C11 14.49
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95OG 300C11 118.05
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300I12 67SG 3.828
300I12 62CG 3.904
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300I12 219CE3 4.092
300I12 76CG 4.264
300I12 62CB 4.265
300I12 76NE2 4.337
300I12 62CD2 4.610
300I12 60CG 4.623
300I12 62CZ 4.643
300I12 56CB 4.692
300I12 76CB 4.770
300I12 76ND1 4.782
300I12 76CE1 4.820
300I12 60CB 4.875
300I12 62CE2 4.945
300I12 219CH2 4.988
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62CD1 300I12 20.77
62CD1 300I12 20.60
62CD1 300I12 113.76
62CD1 300I12 61.51
62CD1 300I12 54.62
62CD1 300I12 105.54
62CD1 300I12 36.28
62CD1 300I12 132.00
62CD1 300I12 30.68
62CD1 300I12 103.00
62CD1 300I12 30.61
62CD1 300I12 74.90
62CD1 300I12 87.89
62CD1 300I12 117.42
62CD1 300I12 132.34
62CD1 300I12 85.12
62CD1 300I12 33.19
62CD1 300I12 55.86
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67SG 300I12 68.36
67SG 300I12 89.86
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67SG 300I12 93.65
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76CD2 300I12 18.49
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76CD2 300I12 131.52
76CD2 300I12 119.26
76CD2 300I12 101.38
76CD2 300I12 158.00
76CD2 300I12 32.99
76CD2 300I12 26.87
76CD2 300I12 26.69
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76CD2 300I12 116.15
76CD2 300I12 99.45
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62CB 300I12 151.11
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62CB 300I12 48.19
62CB 300I12 58.26
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76NE2 300I12 15.46
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62CD2 300I12 16.30
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60CG 300I12 63.77
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56CB 300I12 59.40
56CB 300I12 101.91
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76CB 300I12 44.50
76CB 300I12 147.98
76CB 300I12 83.25
76CB 300I12 102.26
76ND1 300I12 15.82
76ND1 300I12 148.74
76ND1 300I12 103.77
76ND1 300I12 124.59
76CE1 300I12 134.45
76CE1 300I12 119.02
76CE1 300I12 124.87
60CB 300I12 106.40
60CB 300I12 48.92
62CE2 300I12 88.84
253ZN 104OD2 2.002
253ZN 168NE2 2.077
253ZN 233OE2 2.478
253ZN 202OE1 2.724
253ZN 168CE1 3.012
253ZN 104CG 3.089
253ZN 168CD2 3.090

253ZN 202CD 3.412
253ZN 104OD1 3.542
253ZN 233CD 3.600
253ZN 202OE2 3.676
253ZN 233OE1 4.064
253ZN 168ND1 4.134
253ZN 168CG 4.202
253ZN 104CB 4.344
253ZN 202CG 4.573
253ZN 175CE1 4.626
253ZN 233CG 4.836
253ZN 174CD1 4.849
253ZN 93OD2 4.962
104OD2 253ZN 94.40
104OD2 253ZN 74.39
104OD2 253ZN 143.03
104OD2 253ZN 73.00
104OD2 253ZN 14.18
104OD2 253ZN 114.10
104OD2 253ZN 131.83
104OD2 253ZN 34.22
104OD2 253ZN 71.69
104OD2 253ZN 129.77
104OD2 253ZN 72.33
104OD2 253ZN 83.25
104OD2 253ZN 101.83
104OD2 253ZN 4.87
104OD2 253ZN 120.51
104OD2 253ZN 107.34
104OD2 253ZN 70.68
104OD2 253ZN 57.15
104OD2 253ZN 90.69
168NE2 253ZN 131.44
168NE2 253ZN 88.08
168NE2 253ZN 21.44
168NE2 253ZN 108.51
168NE2 253ZN 21.13
168NE2 253ZN 106.27
168NE2 253ZN 127.51
168NE2 253ZN 140.75
168NE2 253ZN 124.02
168NE2 253ZN 157.03
168NE2 253ZN 11.72
168NE2 253ZN 10.72
168NE2 253ZN 96.50
168NE2 253ZN 101.04
168NE2 253ZN 46.01
168NE2 253ZN 128.77
168NE2 253ZN 72.14
168NE2 253ZN 169.34
233OE2 253ZN 76.50
233OE2 253ZN 123.58
233OE2 253ZN 66.35
233OE2 253ZN 126.95
233OE2 253ZN 59.18
233OE2 253ZN 61.23
233OE2 253ZN 10.43
233OE2 253ZN 56.28
233OE2 253ZN 27.78
233OE2 253ZN 124.11
233OE2 253ZN 125.70
233OE2 253ZN 69.71
233OE2 253ZN 52.63
233OE2 253ZN 176.65
233OE2 253ZN 4.26
233OE2 253ZN 128.78
233OE2 253ZN 59.04
202OE1 253ZN 105.92
202OE1 253ZN 141.42
202OE1 253ZN 67.86
202OE1 253ZN 19.49
202OE1 253ZN 136.35
202OE1 253ZN 83.25
202OE1 253ZN 36.04
202OE1 253ZN 91.70
202OE1 253ZN 94.81
202OE1 253ZN 77.48
202OE1 253ZN 138.51
202OE1 253ZN 24.41
202OE1 253ZN 100.77
202OE1 253ZN 79.13
202OE1 253ZN 154.44
202OE1 253ZN 93.50
168CE1 253ZN 87.09
168CE1 253ZN 42.10
168CE1 253ZN 121.90

168CE1 253ZN 106.15
168CE1 253ZN 129.88
168CE1 253ZN 141.41
168CE1 253ZN 141.19
168CE1 253ZN 11.37
168CE1 253ZN 30.24
168CE1 253ZN 75.27
168CE1 253ZN 112.89
168CE1 253ZN 55.05
168CE1 253ZN 119.78
168CE1 253ZN 59.29
168CE1 253ZN 160.53
104CG 253ZN 128.27
104CG 253ZN 125.52
104CG 253ZN 20.26
104CG 253ZN 61.66
104CG 253ZN 118.83
104CG 253ZN 59.57
104CG 253ZN 97.42
104CG 253ZN 116.00
104CG 253ZN 13.28
104CG 253ZN 117.07
104CG 253ZN 115.95
104CG 253ZN 63.20
104CG 253ZN 62.71
104CG 253ZN 76.54
168CD2 253ZN 86.80
168CD2 253ZN 148.07
168CD2 253ZN 137.38
168CD2 253ZN 103.40
168CD2 253ZN 153.94
168CD2 253ZN 31.14
168CD2 253ZN 12.27
168CD2 253ZN 115.51
168CD2 253ZN 84.09
168CD2 253ZN 49.79
168CD2 253ZN 126.06
168CD2 253ZN 90.11
168CD2 253ZN 155.17
202CD 253ZN 117.15
202CD 253ZN 64.75
202CD 253ZN 19.78
202CD 253ZN 72.22
202CD 253ZN 111.47
202CD 253ZN 95.56
202CD 253ZN 126.96
202CD 253ZN 14.32
202CD 253ZN 118.43
202CD 253ZN 62.36
202CD 253ZN 170.90
202CD 253ZN 76.87
104OD1 253ZN 53.39
104OD1 253ZN 104.82
104OD1 253ZN 45.35
104OD1 253ZN 116.95
104OD1 253ZN 135.84
104OD1 253ZN 33.47
104OD1 253ZN 113.66
104OD1 253ZN 121.81
104OD1 253ZN 59.41
104OD1 253ZN 69.10
104OD1 253ZN 56.56
233CD 253ZN 58.09
233CD 253ZN 17.51
233CD 253ZN 132.27
233CD 253ZN 135.82
233CD 253ZN 67.35
233CD 253ZN 60.35
233CD 253ZN 172.75
233CD 253ZN 12.10
233CD 253ZN 122.31
233CD 253ZN 49.89
202OE2 253ZN 59.91
202OE2 253ZN 130.61
202OE2 253ZN 113.49
202OE2 253ZN 125.40
202OE2 253ZN 31.41
202OE2 253ZN 122.43
202OE2 253ZN 60.31
202OE2 253ZN 156.50
202OE2 253ZN 57.74
233OE1 253ZN 146.80
233OE1 253ZN 153.31
233OE1 253ZN 68.93
233OE1 253ZN 71.73
233OE1 253ZN 155.26

233OE1 253ZN 29.55
233OE1 253ZN 112.87
233OE1 253ZN 33.55
168ND1 253ZN 19.04
168ND1 253ZN 85.10
168ND1 253ZN 103.69
168ND1 253ZN 53.83
168ND1 253ZN 120.85
168ND1 253ZN 68.77
168ND1 253ZN 171.64
168CG 253ZN 103.29
168CG 253ZN 90.55
168CG 253ZN 51.36
168CG 253ZN 123.76
168CG 253ZN 82.76
168CG 253ZN 167.39
104CB 253ZN 115.71
104CB 253ZN 111.94
104CB 253ZN 65.96
104CB 253ZN 62.01
104CB 253ZN 89.31
202CG 253ZN 124.45
202CG 253ZN 54.97
202CG 253ZN 171.98
202CG 253ZN 84.33
175CE1 253ZN 174.69
175CE1 253ZN 53.82
175CE1 253ZN 123.42
233CG 253ZN 125.86
233CG 253ZN 61.82
174CD1 253ZN 103.10
254ZN 93OD1 1.948
254ZN 233OE1 2.009
254ZN 104OD1 2.039
254ZN 93OD2 2.234
254ZN 93CG 2.383
254ZN 233CD 2.777
254ZN 233OE2 2.932
254ZN 104CG 2.977
254ZN 104OD2 3.259
254ZN 93CB 3.899
254ZN 233CG 4.190
254ZN 104CB 4.361
254ZN 202OE2 4.418
254ZN 93CA 4.651
254ZN 104C 4.653
254ZN 104CA 4.729
254ZN 95CB 4.855
254ZN 93C 4.886
254ZN 233CB 4.893
93OD1 254ZN 105.84
93OD1 254ZN 102.39
93OD1 254ZN 62.92
93OD1 254ZN 31.47
93OD1 254ZN 128.84
93OD1 254ZN 153.84
93OD1 254ZN 121.26
93OD1 254ZN 140.80
93OD1 254ZN 28.71
93OD1 254ZN 120.57
93OD1 254ZN 113.59
93OD1 254ZN 135.56
93OD1 254ZN 20.63
93OD1 254ZN 96.27
93OD1 254ZN 97.12
93OD1 254ZN 69.85
93OD1 254ZN 6.97
93OD1 254ZN 108.86
233OE1 254ZN 94.44
233OE1 254ZN 80.38
233OE1 254ZN 93.64
233OE1 254ZN 24.22
233OE1 254ZN 48.56
233OE1 254ZN 92.12
233OE1 254ZN 94.04
233OE1 254ZN 94.96
233OE1 254ZN 19.36
233OE1 254ZN 88.80
233OE1 254ZN 61.38
233OE1 254ZN 87.96
233OE1 254ZN 66.56
233OE1 254ZN 84.36
233OE1 254ZN 131.39
233OE1 254ZN 99.74
233OE1 254ZN 3.02
104OD1 254ZN 161.74

104OD1 254ZN 133.07
104OD1 254ZN 82.02
104OD1 254ZN 77.86
104OD1 254ZN 19.27
104OD1 254ZN 41.51
104OD1 254ZN 130.44
104OD1 254ZN 79.14
104OD1 254ZN 11.46
104OD1 254ZN 120.14
104OD1 254ZN 114.72
104OD1 254ZN 31.12
104OD1 254ZN 13.12
104OD1 254ZN 44.32
104OD1 254ZN 99.81
104OD1 254ZN 93.51
93OD2 254ZN 31.45
93OD2 254ZN 98.64
93OD2 254ZN 110.23
93OD2 254ZN 172.35
93OD2 254ZN 155.56
93OD2 254ZN 34.22
93OD2 254ZN 98.59
93OD2 254ZN 166.77
93OD2 254ZN 72.78
93OD2 254ZN 48.01
93OD2 254ZN 134.59
93OD2 254ZN 149.89
93OD2 254ZN 129.30
93OD2 254ZN 64.27
93OD2 254ZN 82.14
93CG 254ZN 117.19
93CG 254ZN 136.84
93CG 254ZN 152.30
93CG 254ZN 171.03
93CG 254ZN 2.77
93CG 254ZN 112.77
93CG 254ZN 143.67
93CG 254ZN 104.18
93CG 254ZN 19.90
93CG 254ZN 118.47
93CG 254ZN 125.48
93CG 254ZN 99.73
93CG 254ZN 33.28
93CG 254ZN 96.36
233CD 254ZN 25.03
233CD 254ZN 73.74
233CD 254ZN 70.98
233CD 254ZN 118.73
233CD 254ZN 9.27
233CD 254ZN 73.33
233CD 254ZN 53.06
233CD 254ZN 112.04
233CD 254ZN 61.95
233CD 254ZN 75.81
233CD 254ZN 125.78
233CD 254ZN 122.28
233CD 254ZN 21.28
233OE2 254ZN 63.04
233OE2 254ZN 52.10
233OE2 254ZN 139.06
233OE2 254ZN 33.32
233OE2 254ZN 66.81
233OE2 254ZN 44.20
233OE2 254ZN 136.36
233OE2 254ZN 70.21
233OE2 254ZN 77.23
233OE2 254ZN 120.33
233OE2 254ZN 147.17
233OE2 254ZN 45.54
104CG 254ZN 22.51
104CG 254ZN 149.64
104CG 254ZN 73.79
104CG 254ZN 9.75
104CG 254ZN 102.36
104CG 254ZN 133.83
104CG 254ZN 41.30
104CG 254ZN 28.60
104CG 254ZN 57.30
104CG 254ZN 119.02
104CG 254ZN 90.30
104OD2 254ZN 168.55
104OD2 254ZN 74.72
104OD2 254ZN 32.05
104OD2 254ZN 83.62
104OD2 254ZN 156.22
104OD2 254ZN 60.90

104OD2 254ZN 50.89
104OD2 254ZN 71.64
104OD2 254ZN 140.08
104OD2 254ZN 91.44
93CB 254ZN 113.94
93CB 254ZN 141.16
93CB 254ZN 106.95
93CB 254ZN 18.04
93CB 254ZN 116.79
93CB 254ZN 123.14
93CB 254ZN 97.05
93CB 254ZN 30.63
93CB 254ZN 97.73
233CG 254ZN 71.76
233CG 254ZN 61.28
233CG 254ZN 105.07
233CG 254ZN 55.74
233CG 254ZN 71.25
233CG 254ZN 121.27
233CG 254ZN 113.84
233CG 254ZN 16.95
104CB 254ZN 108.68
104CB 254ZN 124.55
104CB 254ZN 32.31
104CB 254ZN 18.89
104CB 254ZN 54.38
104CB 254ZN 110.65
104CB 254ZN 87.40
202OE2 254ZN 117.65
202OE2 254ZN 113.05
202OE2 254ZN 121.35
202OE2 254ZN 152.12
202OE2 254ZN 135.66
202OE2 254ZN 59.45
93CA 254ZN 98.76
93CA 254ZN 105.94
93CA 254ZN 89.31
93CA 254ZN 18.16
93CA 254ZN 90.97
104C 254ZN 18.64
104C 254ZN 65.97
104C 254ZN 90.76
104C 254ZN 66.41
104CA 254ZN 50.13
104CA 254ZN 93.27
104CA 254ZN 83.88
95CB 254ZN 71.15
95CB 254ZN 131.83
93C 254ZN 102.74

Table V

Provides distances between interresidue atoms that are within 5 Ångstroms apart in an active site of a *S. aureus* methionine aminopeptidase for an inhibitor complex with 5-benzofuran-2-yl-1-H-[1,2,3]triazole.

Atom 1	Atom 2	Distance
300C1	76CE1	3.780
300C1	76NE2	4.027
300C1	174CD2	4.064
300C1	175CE1	4.370
300C1	76ND1	4.454
300C1	76CD2	4.830
300C1	175NE2	4.920
300C1	174CG	4.960
300C1	67SG	4.988
76CE1	300C1	19.14
76CE1	300C1	164.38
76CE1	300C1	113.69
76CE1	300C1	15.95
76CE1	300C1	26.06
76CE1	300C1	98.82
76CE1	300C1	155.51
76CE1	300C1	74.42
76NE2	300C1	147.39
76NE2	300C1	105.69
76NE2	300C1	28.72
76NE2	300C1	14.53
76NE2	300C1	91.86

76NE2 300C1 146.70
76NE2 300C1 81.18
174CD2 300C1 52.87
174CD2 300C1 172.05
174CD2 300C1 146.40
174CD2 300C1 67.72
174CD2 300C1 15.79
174CD2 300C1 118.71
175CE1 300C1 129.65
175CE1 300C1 116.73
175CE1 300C1 14.91
175CE1 300C1 42.43
175CE1 300C1 171.48
76ND1 300C1 26.83
76ND1 300C1 114.78
76ND1 300C1 170.79
76ND1 300C1 58.47
76CD2 300C1 103.95
76CD2 300C1 153.05
76CD2 300C1 69.24
175NE2 300C1 57.13
175NE2 300C1 173.03
174CG 300C1 129.75
300C2 174CD2 4.134
300C2 76CE1 4.368
300C2 175CE1 4.430
300C2 93OD2 4.624
300C2 93OD1 4.702
300C2 174CG 4.705
300C2 104OD2 4.723
300C2 174CD1 4.797
300C2 93CG 4.837
300C2 95OG 4.856
300C2 104OD1 4.899
300C2 76NE2 4.938
174CD2 300C2 132.15
174CD2 300C2 52.02
174CD2 300C2 139.66
174CD2 300C2 113.90
174CD2 300C2 18.44
174CD2 300C2 80.51
174CD2 300C2 31.45
174CD2 300C2 128.63
174CD2 300C2 55.04
174CD2 300C2 88.85
174CD2 300C2 117.47
76CE1 300C2 101.87
76CE1 300C2 87.27
76CE1 300C2 109.71
76CE1 300C2 140.71
76CE1 300C2 138.19
76CE1 300C2 158.66
76CE1 300C2 95.03
76CE1 300C2 146.77
76CE1 300C2 138.79
76CE1 300C2 14.74
175CE1 300C2 140.03
175CE1 300C2 140.77
175CE1 300C2 43.86
175CE1 300C2 77.13
175CE1 300C2 57.79
175CE1 300C2 148.67
175CE1 300C2 102.80
175CE1 300C2 102.01
175CE1 300C2 91.07
93OD2 300C2 27.20
93OD2 300C2 130.52
93OD2 300C2 70.80
93OD2 300C2 112.31
93OD2 300C2 14.93
93OD2 300C2 87.95
93OD2 300C2 53.47
93OD2 300C2 101.97
93OD1 300C2 109.58
93OD1 300C2 63.87
93OD1 300C2 91.49
93OD1 300C2 14.94
93OD1 300C2 60.76
93OD1 300C2 38.83
93OD1 300C2 123.45
174CG 300C2 63.86
174CG 300C2 18.41
174CG 300C2 124.25
174CG 300C2 58.94
174CG 300C2 77.06
174CG 300C2 126.57

104OD2 300C2 49.42
104OD2 300C2 72.72
104OD2 300C2 69.61
104OD2 300C2 26.43
104OD2 300C2 145.50
174CD1 300C2 105.98
174CD1 300C2 47.37
174CD1 300C2 59.00
174CD1 300C2 144.92
93CG 300C2 74.56
93CG 300C2 50.31
93CG 300C2 109.09
95OG 300C2 54.84
95OG 300C2 144.86
104OD1 300C2 153.06
300C3 76CE1 3.808
300C3 67SG 3.904
300C3 76NE2 3.933
300C3 76ND1 4.133
300C3 76CD2 4.345
300C3 76CG 4.470
300C3 174CD2 4.637
300C3 56CG 4.786
76CE1 300C3 88.64
76CE1 300C3 19.56
76CE1 300C3 18.60
76CE1 300C3 30.32
76CE1 300C3 29.53
76CE1 300C3 133.72
76CE1 300C3 151.39
67SG 300C3 97.91
67SG 300C3 70.36
67SG 300C3 84.94
67SG 300C3 68.93
67SG 300C3 131.79
67SG 300C3 63.16
76NE2 300C3 30.70
76NE2 300C3 18.26
76NE2 300C3 29.44
76NE2 300C3 129.79
76NE2 300C3 157.76
76ND1 300C3 29.74
76ND1 300C3 17.88
76ND1 300C3 151.31
76ND1 300C3 133.50
76CD2 300C3 17.62
76CD2 300C3 142.99
76CD2 300C3 139.86
76CG 300C3 159.17
76CG 300C3 129.15
174CD2 300C3 71.10
300O4 175CE1 3.522
300O4 76NE2 3.714
300O4 76CE1 3.846
300O4 175NE2 3.910
300O4 174CD2 4.110
300O4 76CD2 4.656
300O4 175ND1 4.663
300O4 76ND1 4.790
300O4 174CG 4.910
175CE1 300O4 135.39
175CE1 300O4 135.94
175CE1 300O4 19.62
175CE1 300O4 58.51
175CE1 300O4 146.44
175CE1 300O4 9.44
175CE1 300O4 147.36
175CE1 300O4 44.17
76NE2 300O4 20.02
76NE2 300O4 115.77
76NE2 300O4 165.92
76NE2 300O4 13.84
76NE2 300O4 141.55
76NE2 300O4 25.39
76NE2 300O4 174.40
76CE1 300O4 118.02
76CE1 300O4 155.30
76CE1 300O4 27.89
76CE1 300O4 144.90
76CE1 300O4 12.39
76CE1 300O4 154.63
175NE2 300O4 78.13
175NE2 300O4 127.25
175NE2 300O4 27.17
175NE2 300O4 130.20
175NE2 300O4 63.60

174CD2 300O4 152.62
174CD2 300O4 51.81
174CD2 300O4 145.29
174CD2 300O4 16.61
76CD2 300O4 150.34
76CD2 300O4 26.70
76CD2 300O4 168.88
175ND1 300O4 156.65
175ND1 300O4 39.13
76ND1 300O4 150.63
300C5 93OD1 3.375
300C5 93CG 3.623
300C5 93OD2 3.631
300C5 104OD1 3.988
300C5 95OG 4.148
300C5 104OD2 4.399
300C5 104CG 4.545
300C5 93CB 4.628
300C5 95CB 4.691
300C5 174CD2 4.695
300C5 233OE1 4.735
300C5 174CD1 4.925
300C5 67SG 4.989
93OD1 300C5 20.13
93OD1 300C5 36.26
93OD1 300C5 50.64
93OD1 300C5 79.27
93OD1 300C5 78.56
93OD1 300C5 65.61
93OD1 300C5 29.58
93OD1 300C5 69.09
93OD1 300C5 132.75
93OD1 300C5 43.84
93OD1 300C5 108.66
93OD1 300C5 88.44
93CG 300C5 19.79
93CG 300C5 65.68
93CG 300C5 97.90
93CG 300C5 89.37
93CG 300C5 79.56
93CG 300C5 15.86
93CG 300C5 89.03
93CG 300C5 152.83
93CG 300C5 44.29
93CG 300C5 127.62
93CG 300C5 79.99
93OD2 300C5 68.37
93OD2 300C5 115.49
93OD2 300C5 84.21
93OD2 300C5 79.26
93OD2 300C5 30.45
93OD2 300C5 103.93
93OD2 300C5 161.69
93OD2 300C5 35.41
93OD2 300C5 131.66
93OD2 300C5 88.68
104OD1 300C5 67.01
104OD1 300C5 30.00
104OD1 300C5 15.11
104OD1 300C5 79.44
104OD1 300C5 50.02
104OD1 300C5 93.57
104OD1 300C5 38.72
104OD1 300C5 63.77
104OD1 300C5 135.84
95OG 300C5 79.50
95OG 300C5 68.75
95OG 300C5 97.18
95OG 300C5 16.99
95OG 300C5 56.35
95OG 300C5 103.03
95OG 300C5 49.70
95OG 300C5 92.59
104OD2 300C5 16.02
104OD2 300C5 104.86
104OD2 300C5 64.77
104OD2 300C5 78.21
104OD2 300C5 48.81
104OD2 300C5 50.15
104OD2 300C5 165.81
104CG 300C5 93.97
104CG 300C5 52.56
104CG 300C5 82.43
104CG 300C5 45.66
104CG 300C5 52.45
104CG 300C5 149.92

93CB 300C5 92.58
93CB 300C5 152.83
93CB 300C5 59.99
93CB 300C5 137.20
93CB 300C5 64.15
95CB 300C5 63.84
95CB 300C5 86.55
95CB 300C5 47.31
95CB 300C5 105.36
174CD2 300C5 126.85
174CD2 300C5 30.04
174CD2 300C5 107.31
233OE1 300C5 97.53
233OE1 300C5 123.27
174CD1 300C5 131.42
300N6 168NE2 3.672
300N6 175CE1 3.765
300N6 104OD2 3.797
300N6 175NE2 4.231
300N6 174CD2 4.332
300N6 168CE1 4.440
300N6 174CG 4.460
300N6 174CD1 4.485
300N6 104OD1 4.502
300N6 202OE1 4.508
300N6 104CG 4.516
300N6 168CD2 4.605
300N6 93OD2 4.758
300N6 233OE2 4.801
300N6 175ND1 4.884
300N6 76CE1 4.910
300N6 202OE2 4.964
168NE2 300N6 60.66
168NE2 300N6 50.92
168NE2 300N6 56.93
168NE2 300N6 94.08
168NE2 300N6 15.28
168NE2 300N6 74.77
168NE2 300N6 72.46
168NE2 300N6 79.88
168NE2 300N6 48.07
168NE2 300N6 65.13
168NE2 300N6 14.11
168NE2 300N6 112.91
168NE2 300N6 56.29
168NE2 300N6 57.85
168NE2 300N6 130.73
168NE2 300N6 70.53
175CE1 300N6 98.09
175CE1 300N6 17.84
175CE1 300N6 54.88
175CE1 300N6 58.33
175CE1 300N6 48.25
175CE1 300N6 64.93
175CE1 300N6 122.48
175CE1 300N6 98.82
175CE1 300N6 107.72
175CE1 300N6 56.36
175CE1 300N6 173.40
175CE1 300N6 116.81
175CE1 300N6 9.41
175CE1 300N6 103.10
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300C13 219CZ3 3.458
300C13 60CG 3.606
300C13 219CE3 3.806
300C13 60CB 3.831
300C13 60OE1 3.919
300C13 76CD2 3.963
300C13 60CD 4.154
300C13 76NE2 4.248
300C13 62CD1 4.582
300C13 219CH2 4.648
300C13 76CG 4.839
219CZ3 300C13 98.24
219CZ3 300C13 21.41
219CZ3 300C13 74.89
219CZ3 300C13 98.52
219CZ3 300C13 108.71
219CZ3 300C13 104.78
219CZ3 300C13 127.05
219CZ3 300C13 55.11
219CZ3 300C13 10.78
219CZ3 300C13 105.93
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60CG 300C13 23.43
60CG 300C13 36.93
60CG 300C13 151.60
60CG 300C13 21.17
60CG 300C13 134.55
60CG 300C13 98.17
60CG 300C13 87.47
60CG 300C13 146.80
219CE3 300C13 94.41
219CE3 300C13 119.19
219CE3 300C13 87.88
219CE3 300C13 126.17
219CE3 300C13 106.58
219CE3 300C13 47.95

219CE3 300C13 31.58
219CE3 300C13 84.51
60CB 300C13 45.48
60CB 300C13 168.93
60CB 300C13 37.22
60CB 300C13 157.45
60CB 300C13 83.32
60CB 300C13 64.11
60CB 300C13 156.05
60OE1 300C13 141.03
60OE1 300C13 17.57
60OE1 300C13 124.77
60OE1 300C13 128.54
60OE1 300C13 89.96
60OE1 300C13 151.73
76CD2 300C13 144.65
76CD2 300C13 18.87
76CD2 300C13 90.26
76CD2 300C13 119.33
76CD2 300C13 13.57
60CD 300C13 125.88
60CD 300C13 118.60
60CD 300C13 94.69
60CD 300C13 149.20
76NE2 300C13 104.52
76NE2 300C13 137.79
76NE2 300C13 26.99
62CD1 300C13 56.52
62CD1 300C13 78.23
219CH2 300C13 115.76
300C14 60OE1 3.226
300C14 60CG 3.682
300C14 60CD 3.687
300C14 76NE2 4.132
300C14 76CD2 4.209
300C14 60CB 4.238
300C14 219CZ3 4.431
300C14 60OE2 4.666
300C14 219CE3 4.879
60OE1 300C14 40.01
60OE1 300C14 19.48
60OE1 300C14 159.20
60OE1 300C14 176.13
60OE1 300C14 44.84
60OE1 300C14 92.59
60OE1 300C14 24.76
60OE1 300C14 108.89
60CG 300C14 23.87
60CG 300C14 136.08
60CG 300C14 136.74
60CG 300C14 20.73
60CG 300C14 81.80
60CG 300C14 30.39
60CG 300C14 94.66
60CD 300C14 146.21
60CD 300C14 156.68
60CD 300C14 36.97
60CD 300C14 95.82
60CD 300C14 10.83
60CD 300C14 111.20
76NE2 300C14 18.94
76NE2 300C14 142.41
76NE2 300C14 107.48
76NE2 300C14 137.23
76NE2 300C14 91.26
76CD2 300C14 133.38
76CD2 300C14 88.62
76CD2 300C14 151.52
76CD2 300C14 72.36
60CB 300C14 61.59
60CB 300C14 46.67
60CB 300C14 75.50
219CZ3 300C14 106.54
219CZ3 300C14 16.30
60OE2 300C14 121.70
253ZN 104OD2 2.030
253ZN 168NE2 2.220
253ZN 233OE2 2.301
253ZN 202OE1 2.663
253ZN 168CE1 2.976
253ZN 104CG 3.105
253ZN 202CD 3.239
253ZN 168CD2 3.295
253ZN 233CD 3.319
253ZN 202OE2 3.413
253ZN 104OD1 3.554

253ZN 233OE1 3.643
253ZN 168ND1 4.123
253ZN 168CG 4.306
253ZN 104CB 4.368
253ZN 202CG 4.439
253ZN 233CG 4.666
253ZN 93OD2 4.924
104OD2 253ZN 98.10
104OD2 253ZN 79.80
104OD2 253ZN 149.19
104OD2 253ZN 74.01
104OD2 253ZN 14.80
104OD2 253ZN 133.12
104OD2 253ZN 114.19
104OD2 253ZN 76.43
104OD2 253ZN 125.52
104OD2 253ZN 34.58
104OD2 253ZN 78.09
104OD2 253ZN 82.40
104OD2 253ZN 100.92
104OD2 253ZN 7.30
104OD2 253ZN 123.08
104OD2 253ZN 73.89
104OD2 253ZN 92.73
168NE2 253ZN 131.31
168NE2 253ZN 88.36
168NE2 253ZN 24.30
168NE2 253ZN 112.86
168NE2 253ZN 108.18
168NE2 253ZN 18.22
168NE2 253ZN 146.31
168NE2 253ZN 128.30
168NE2 253ZN 131.18
168NE2 253ZN 166.31
168NE2 253ZN 18.64
168NE2 253ZN 12.73
168NE2 253ZN 101.89
168NE2 253ZN 103.01
168NE2 253ZN 135.74
168NE2 253ZN 159.98
233OE2 253ZN 73.52
233OE2 253ZN 121.77
233OE2 253ZN 71.23
233OE2 253ZN 53.63
233OE2 253ZN 123.02
233OE2 253ZN 15.48
233OE2 253ZN 49.42
233OE2 253ZN 67.24
233OE2 253ZN 35.31
233OE2 253ZN 118.24
233OE2 253ZN 119.25
233OE2 253ZN 72.59
233OE2 253ZN 47.04
233OE2 253ZN 7.48
233OE2 253ZN 67.16
202OE1 253ZN 107.39
202OE1 253ZN 144.62
202OE1 253ZN 21.74
202OE1 253ZN 70.17
202OE1 253ZN 81.57
202OE1 253ZN 39.94
202OE1 253ZN 136.93
202OE1 253ZN 88.54
202OE1 253ZN 96.73
202OE1 253ZN 79.57
202OE1 253ZN 142.31
202OE1 253ZN 27.09
202OE1 253ZN 80.48
202OE1 253ZN 90.92
168CE1 253ZN 88.81
168CE1 253ZN 123.47
168CE1 253ZN 40.57
168CE1 253ZN 132.89
168CE1 253ZN 144.93
168CE1 253ZN 107.88
168CE1 253ZN 147.63
168CE1 253ZN 10.75
168CE1 253ZN 28.46
168CE1 253ZN 77.60
168CE1 253ZN 113.63
168CE1 253ZN 122.92
168CE1 253ZN 161.11
104CG 253ZN 124.49
104CG 253ZN 128.92
104CG 253ZN 64.96
104CG 253ZN 112.83

104CG 253ZN 20.25
104CG 253ZN 64.01
104CG 253ZN 97.12
104CG 253ZN 115.54
104CG 253ZN 13.04
104CG 253ZN 117.61
104CG 253ZN 64.48
104CG 253ZN 78.31
202CD 253ZN 90.35
202CD 253ZN 60.09
202CD 253ZN 21.49
202CD 253ZN 115.21
202CD 253ZN 67.19
202CD 253ZN 112.85
202CD 253ZN 97.86
202CD 253ZN 125.83
202CD 253ZN 14.34
202CD 253ZN 60.08
202CD 253ZN 75.41
168CD2 253ZN 138.30
168CD2 253ZN 110.10
168CD2 253ZN 148.44
168CD2 253ZN 155.56
168CD2 253ZN 31.80
168CD2 253ZN 13.72
168CD2 253ZN 116.84
168CD2 253ZN 86.59
168CD2 253ZN 129.37
168CD2 253ZN 152.00
233CD 253ZN 49.27
233CD 253ZN 56.27
233CD 253ZN 20.07
233CD 253ZN 131.49
233CD 253ZN 134.58
233CD 253ZN 69.79
233CD 253ZN 57.26
233CD 253ZN 10.68
233CD 253ZN 52.92
202OE2 253ZN 98.59
202OE2 253ZN 49.82
202OE2 253ZN 134.33
202OE2 253ZN 118.90
202OE2 253ZN 119.05
202OE2 253ZN 32.25
202OE2 253ZN 53.59
202OE2 253ZN 53.93
104OD1 253ZN 48.85
104OD1 253ZN 116.85
104OD1 253ZN 135.46
104OD1 253ZN 33.13
104OD1 253ZN 113.44
104OD1 253ZN 59.78
104OD1 253ZN 58.16
233OE1 253ZN 149.60
233OE1 253ZN 154.55
233OE1 253ZN 72.97
233OE1 253ZN 69.26
233OE1 253ZN 30.58
233OE1 253ZN 33.44
168ND1 253ZN 18.68
168ND1 253ZN 85.16
168ND1 253ZN 103.55
168ND1 253ZN 120.91
168ND1 253ZN 171.66
168CG 253ZN 103.24
168CG 253ZN 91.25
168CG 253ZN 124.30
168CG 253ZN 165.70
104CB 253ZN 115.89
104CB 253ZN 66.80
104CB 253ZN 90.83
202CG 253ZN 54.29
202CG 253ZN 84.78
233CG 253ZN 63.60
254ZN 233OE1 1.901
254ZN 93OD1 1.967
254ZN 104OD1 2.171
254ZN 93OD2 2.177
254ZN 93CG 2.351
254ZN 233CD 2.841
254ZN 104CG 3.093
254ZN 233OE2 3.221
254ZN 104OD2 3.343
254ZN 93CB 3.859
254ZN 202OE2 3.953
254ZN 233CG 4.151

254ZN 104CB 4.485
254ZN 93CA 4.641
254ZN 104C 4.736
254ZN 233CB 4.765
254ZN 202CD 4.772
254ZN 104CA 4.854
254ZN 93C 4.873
254ZN 95CB 4.973
254ZN 202OE1 4.997
233OE1 254ZN 115.97
233OE1 254ZN 93.69
233OE1 254ZN 84.63
233OE1 254ZN 101.91
233OE1 254ZN 20.60
233OE1 254ZN 89.10
233OE1 254ZN 41.97
233OE1 254ZN 87.96
233OE1 254ZN 103.44
233OE1 254ZN 46.39
233OE1 254ZN 17.35
233OE1 254ZN 87.62
233OE1 254ZN 99.36
233OE1 254ZN 70.88
233OE1 254ZN 9.58
233OE1 254ZN 49.53
233OE1 254ZN 86.84
233OE1 254ZN 112.39
233OE1 254ZN 135.20
233OE1 254ZN 62.68
93OD1 254ZN 101.07
93OD1 254ZN 63.70
93OD1 254ZN 32.03
93OD1 254ZN 133.29
93OD1 254ZN 119.26
93OD1 254ZN 155.93
93OD1 254ZN 138.28
93OD1 254ZN 30.19
93OD1 254ZN 137.94
93OD1 254ZN 120.64
93OD1 254ZN 111.96
93OD1 254ZN 19.84
93OD1 254ZN 94.80
93OD1 254ZN 107.63
93OD1 254ZN 150.44
93OD1 254ZN 95.80
93OD1 254ZN 3.92
93OD1 254ZN 70.60
93OD1 254ZN 158.70
104OD1 254ZN 161.45
104OD1 254ZN 132.41
104OD1 254ZN 79.55
104OD1 254ZN 18.77
104OD1 254ZN 75.53
104OD1 254ZN 40.61
104OD1 254ZN 130.77
104OD1 254ZN 116.13
104OD1 254ZN 76.43
104OD1 254ZN 10.96
104OD1 254ZN 114.56
104OD1 254ZN 29.02
104OD1 254ZN 90.96
104OD1 254ZN 105.21
104OD1 254ZN 11.53
104OD1 254ZN 100.04
104OD1 254ZN 43.85
104OD1 254ZN 100.24
93OD2 254ZN 31.67
93OD2 254ZN 102.81
93OD2 254ZN 173.72
93OD2 254ZN 113.67
93OD2 254ZN 157.10
93OD2 254ZN 33.54
93OD2 254ZN 75.68
93OD2 254ZN 101.55
93OD2 254ZN 167.83
93OD2 254ZN 47.98
93OD2 254ZN 136.30
93OD2 254ZN 84.34
93OD2 254ZN 87.76
93OD2 254ZN 150.94
93OD2 254ZN 64.01
93OD2 254ZN 130.04
93OD2 254ZN 95.40
93CG 254ZN 122.50
93CG 254ZN 151.03
93CG 254ZN 140.78

93CG 254ZN 168.95
93CG 254ZN 1.98
93CG 254ZN 106.83
93CG 254ZN 114.98
93CG 254ZN 142.99
93CG 254ZN 18.97
93CG 254ZN 118.73
93CG 254ZN 97.17
93CG 254ZN 119.15
93CG 254ZN 125.36
93CG 254ZN 32.54
93CG 254ZN 100.61
93CG 254ZN 126.93
233CD 254ZN 71.07
233CD 254ZN 22.94
233CD 254ZN 67.50
233CD 254ZN 124.03
233CD 254ZN 45.24
233CD 254ZN 13.34
233CD 254ZN 71.45
233CD 254ZN 118.86
233CD 254ZN 63.36
233CD 254ZN 26.67
233CD 254ZN 42.29
233CD 254ZN 75.58
233CD 254ZN 129.43
233CD 254ZN 123.38
233CD 254ZN 51.88
104CG 254ZN 61.18
104CG 254ZN 22.04
104CG 254ZN 149.31
104CG 254ZN 100.18
104CG 254ZN 72.17
104CG 254ZN 9.19
104CG 254ZN 133.32
104CG 254ZN 40.08
104CG 254ZN 89.42
104CG 254ZN 88.42
104CG 254ZN 27.56
104CG 254ZN 118.51
104CG 254ZN 55.21
104CG 254ZN 81.96
233OE2 254ZN 50.18
233OE2 254ZN 142.64
233OE2 254ZN 40.80
233OE2 254ZN 35.30
233OE2 254ZN 65.17
233OE2 254ZN 141.33
233OE2 254ZN 70.48
233OE2 254ZN 49.35
233OE2 254ZN 31.54
233OE2 254ZN 76.20
233OE2 254ZN 152.01
233OE2 254ZN 116.29
233OE2 254ZN 34.78
104OD2 254ZN 167.02
104OD2 254ZN 83.53
104OD2 254ZN 73.76
104OD2 254ZN 31.07
104OD2 254ZN 154.92
104OD2 254ZN 59.63
104OD2 254ZN 91.85
104OD2 254ZN 71.08
104OD2 254ZN 49.47
104OD2 254ZN 138.44
104OD2 254ZN 68.60
104OD2 254ZN 62.07
93CB 254ZN 108.79
93CB 254ZN 116.21
93CB 254ZN 141.43
93CB 254ZN 17.95
93CB 254ZN 117.92
93CB 254ZN 98.50
93CB 254ZN 121.10
93CB 254ZN 123.97
93CB 254ZN 30.80
93CB 254ZN 98.63
93CB 254ZN 128.71
202OE2 254ZN 56.03
202OE2 254ZN 105.47
202OE2 254ZN 118.78
202OE2 254ZN 108.02
202OE2 254ZN 55.62
202OE2 254ZN 12.51
202OE2 254ZN 116.78
202OE2 254ZN 136.93

202OE2	254ZN	151.23
202OE2	254ZN	25.03
233CG	254ZN	70.30
233CG	254ZN	107.98
233CG	254ZN	55.26
233CG	254ZN	18.14
233CG	254ZN	54.84
233CG	254ZN	70.12
233CG	254ZN	116.73
233CG	254ZN	118.84
233CG	254ZN	65.14
104CB	254ZN	124.69
104CB	254ZN	31.57
104CB	254ZN	86.46
104CB	254ZN	94.35
104CB	254ZN	18.41
104CB	254ZN	110.83
104CB	254ZN	52.61
104CB	254ZN	89.34
93CA	254ZN	100.00
93CA	254ZN	92.20
93CA	254ZN	131.19
93CA	254ZN	106.65
93CA	254ZN	18.17
93CA	254ZN	89.97
93CA	254ZN	142.22
104C	254ZN	65.66
104C	254ZN	101.60
104C	254ZN	18.20
104C	254ZN	92.10
104C	254ZN	64.34
104C	254ZN	104.00
233CB	254ZN	59.11
233CB	254ZN	82.75
233CB	254ZN	103.93
233CB	254ZN	129.54
233CB	254ZN	72.20
202CD	254ZN	107.42
202CD	254ZN	149.36
202CD	254ZN	138.83
202CD	254ZN	14.45
104CA	254ZN	94.12
104CA	254ZN	48.74
104CA	254ZN	105.19
93C	254ZN	71.81
93C	254ZN	159.41
95CB	254ZN	126.71

Table VI

Provides bond angles between interresidue atoms that are within 5 Ångstroms apart in an active site of *S. aureus* methionine aminopeptidase for an inhibitor complex with 5-(3-Iodo-phenyl)-1-H-[1,2,3]triazole.

Atom 1	Atom 2	Atom 3	Angle
174CD2	300C1	174CD1	38.87
174CD2	300C1	95OG	93.98
174CD2	300C1	174CG	19.13
174CD2	300C1	95CB	90.77
174CD1	300C1	95OG	62.23
174CD1	300C1	174CG	20.05
174CD1	300C1	95CB	54.57
95OG	300C1	174CG	79.66
95OG	300C1	56CG	49.06
95OG	300C1	95CB	14.32
174CG	300C1	95CB	73.86
56CG	300C1	95CB	63.06
174CD1	300C2	174CD2	37.67
174CD1	300C2	104OD2	60.60
174CD1	300C2	95OG	60.29
174CD1	300C2	104OD1	73.12
174CD1	300C2	174CG	19.40
174CD1	300C2	175CE1	60.61
174CD1	300C2	104CG	61.72
174CD1	300C2	95CB	55.80
174CD1	300C2	168NE2	62.72
174CD2	300C2	104OD2	90.84

174CD2 300C2 95OG 84.48
174CD2 300C2 174CG 19.96
174CD2 300C2 175CE1 41.70
174CD2 300C2 104CG 96.88
174CD2 300C2 95CB 87.57
174CD2 300C2 168NE2 72.77
104OD2 300C2 95OG 81.21
104OD2 300C2 104OD1 29.39
104OD2 300C2 93OD1 68.62
104OD2 300C2 174CG 71.81
104OD2 300C2 175CE1 77.23
104OD2 300C2 104CG 15.46
104OD2 300C2 93OD2 72.94
104OD2 300C2 93CG 76.26
104OD2 300C2 95CB 64.77
104OD2 300C2 168NE2 36.99
95OG 300C2 104OD1 62.76
95OG 300C2 93OD1 65.66
95OG 300C2 174CG 76.06
95OG 300C2 104CG 67.82
95OG 300C2 93OD2 93.20
95OG 300C2 93CG 78.95
95OG 300C2 95CB 16.63
104OD1 300C2 93OD1 41.49
104OD1 300C2 174CG 90.16
104OD1 300C2 104CG 15.52
104OD1 300C2 93OD2 55.34
104OD1 300C2 93CG 52.55
104OD1 300C2 95CB 46.89
104OD1 300C2 168NE2 66.01
93OD1 300C2 104CG 56.86
93OD1 300C2 93OD2 27.59
93OD1 300C2 93CG 14.94
93OD1 300C2 95CB 58.87
174CG 300C2 175CE1 44.45
174CG 300C2 104CG 76.95
174CG 300C2 95CB 74.28
174CG 300C2 168NE2 60.83
175CE1 300C2 104CG 91.08
175CE1 300C2 168NE2 43.13
175CE1 300C2 76CE1 92.75
104CG 300C2 93OD2 67.53
104CG 300C2 93CG 67.06
104CG 300C2 95CB 51.19
104CG 300C2 168NE2 52.35
93OD2 300C2 93CG 15.23
93OD2 300C2 95CB 85.84
93OD2 300C2 168NE2 93.24
93OD2 300C2 76CE1 79.01
93CG 300C2 95CB 73.55
93CG 300C2 76CE1 86.79
95CB 300C2 168NE2 96.40
67SG 300C3 76CE1 79.93
67SG 300C3 76NE2 87.30
67SG 300C3 56CG 64.01
67SG 300C3 76ND1 63.97
67SG 300C3 76CD2 75.35
76CE1 300C3 76NE2 17.93
76CE1 300C3 76ND1 16.05
76CE1 300C3 76CD2 27.36
76NE2 300C3 76ND1 27.26
76NE2 300C3 76CD2 16.26
174CD2 300C3 56CG 97.93
76ND1 300C3 76CD2 26.71
174CD2 300C4 174CD1 47.78
174CD2 300C4 174CG 23.77
174CD2 300C4 55CB 95.90
174CD2 300C4 174CB 29.29
174CD1 300C4 95OG 78.45
174CD1 300C4 174CG 24.16
174CD1 300C4 95CB 65.13
174CD1 300C4 55CB 71.48
174CD1 300C4 174CB 30.61
174CD1 300C4 55C 98.20
95OG 300C4 56CG 57.79
95OG 300C4 95CB 15.30
95OG 300C4 56CD 47.45
95OG 300C4 56N 62.45
95OG 300C4 55CB 45.17
95OG 300C4 56CA 78.07
95OG 300C4 174CB 96.24
95OG 300C4 55C 65.17
95OG 300C4 56CB 73.22
174CG 300C4 95CB 88.68
174CG 300C4 55CB 81.68
174CG 300C4 174CB 16.66

174CG 300C4 55C 99.87
56CG 300C4 95CB 73.01
56CG 300C4 56CD 19.80
56CG 300C4 56N 30.94
56CG 300C4 55CB 63.24
56CG 300C4 56CA 30.65
56CG 300C4 55C 47.01
56CG 300C4 56CB 16.62
95CB 300C4 56CD 62.34
95CB 300C4 56N 76.04
95CB 300C4 55CB 50.54
95CB 300C4 56CA 92.61
95CB 300C4 174CB 87.06
95CB 300C4 55C 76.06
95CB 300C4 56CB 88.52
56CD 300C4 56N 18.86
56CD 300C4 55CB 43.44
56CD 300C4 56CA 30.79
56CD 300C4 55C 31.69
56CD 300C4 56CB 28.60
56N 300C4 55CB 41.27
56N 300C4 56CA 18.42
56N 300C4 174CB 99.66
56N 300C4 55C 16.30
56N 300C4 56CB 28.51
55CB 300C4 56CA 59.00
55CB 300C4 174CB 68.02
55CB 300C4 55C 31.10
55CB 300C4 56CB 68.44
56CA 300C4 55C 29.74
56CA 300C4 56CB 18.26
174CB 300C4 55C 83.39
55C 300C4 56CB 44.03
175CE1 300C5 174CD1 74.10
175CE1 300C5 168NE2 58.91
175CE1 300C5 174CD2 49.97
175CE1 300C5 174CG 53.35
175CE1 300C5 168CE1 57.33
175CE1 300C5 175NE2 14.62
175CE1 300C5 175ND1 13.75
175CE1 300C5 168CD2 50.49
175CE1 300C5 202OE1 86.19
174CD1 300C5 104OD2 69.77
174CD1 300C5 168NE2 80.34
174CD1 300C5 174CD2 40.03
174CD1 300C5 174CG 22.15
174CD1 300C5 168CE1 63.75
174CD1 300C5 104CG 67.11
174CD1 300C5 104OD1 75.50
174CD1 300C5 175NE2 87.86
174CD1 300C5 175ND1 60.36
174CD1 300C5 168CD2 89.95
104OD2 300C5 168NE2 48.89
104OD2 300C5 174CG 84.33
104OD2 300C5 168CE1 45.07
104OD2 300C5 104CG 15.33
104OD2 300C5 104OD1 30.53
104OD2 300C5 175ND1 96.64
104OD2 300C5 168CD2 63.15
104OD2 300C5 202OE1 62.28
104OD2 300C5 233OE2 33.68
168NE2 300C5 174CD2 92.51
168NE2 300C5 174CG 76.98
168NE2 300C5 168CE1 16.60
168NE2 300C5 104CG 64.09
168NE2 300C5 104OD1 79.05
168NE2 300C5 175NE2 55.42
168NE2 300C5 175ND1 60.08
168NE2 300C5 168CD2 15.06
168NE2 300C5 202OE1 44.18
168NE2 300C5 233OE2 56.34
174CD2 300C5 174CG 22.17
174CD2 300C5 168CE1 79.92
174CD2 300C5 175NE2 64.07
174CD2 300C5 175ND1 39.17
174CD2 300C5 168CD2 92.61
174CG 300C5 168CE1 62.02
174CG 300C5 104CG 85.66
174CG 300C5 104OD1 96.42
174CG 300C5 175NE2 67.72
174CG 300C5 175ND1 39.70
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202OE1 300C5 233OE2 38.87
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93OD2 300N6 104CG 86.14
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93OD2 300N6 233OE2 60.37
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93CG 300N6 104OD2 97.02
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93CG 300N6 95OG 95.35
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93CG 300N6 93CB 14.73
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67SG 300C7 56CA 94.55
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60CG 300C7 56CA 68.06
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55CB 300C8 56O 86.30
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174CG 300C8 174CB 17.14
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56O 300C8 60OE2 72.09
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93CG 300N10 233CD 73.46
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76CD2 300I12 219CE3 75.63

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76CD2 300I12 76CE1 26.69
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104OD2 253ZN 233CD 71.69
104OD2 253ZN 233OE1 72.33
104OD2 253ZN 168ND1 83.25
104OD2 253ZN 104CB 4.87
104OD2 253ZN 233CG 70.68
104OD2 253ZN 174CD1 57.15
104OD2 253ZN 93OD2 90.69
168NE2 253ZN 202OE1 88.08
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168NE2 253ZN 174CD1 72.14

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233OE2 253ZN 104OD1 61.23
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233OE2 253ZN 233OE1 27.78
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233OE2 253ZN 233CG 4.26
233OE2 253ZN 93OD2 59.04
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202OE1 253ZN 168CG 77.48
202OE1 253ZN 202CG 24.41
202OE1 253ZN 233CG 79.13
202OE1 253ZN 93OD2 93.50
168CE1 253ZN 104CG 87.09
168CE1 253ZN 168CD2 42.10
168CE1 253ZN 168ND1 11.37
168CE1 253ZN 168CG 30.24
168CE1 253ZN 104CB 75.27
168CE1 253ZN 175CE1 55.05
168CE1 253ZN 174CD1 59.29
104CG 253ZN 104OD1 20.26
104CG 253ZN 233CD 61.66
104CG 253ZN 233OE1 59.57
104CG 253ZN 168ND1 97.42
104CG 253ZN 104CB 13.28
104CG 253ZN 233CG 63.20
104CG 253ZN 174CD1 62.71
104CG 253ZN 93OD2 76.54
168CD2 253ZN 202CD 86.80
168CD2 253ZN 168ND1 31.14
168CD2 253ZN 168CG 12.27
168CD2 253ZN 202CG 84.09
168CD2 253ZN 175CE1 49.79
168CD2 253ZN 174CD1 90.11
202CD 253ZN 233CD 64.75
202CD 253ZN 202OE2 19.78
202CD 253ZN 233OE1 72.22
202CD 253ZN 168CG 95.56
202CD 253ZN 202CG 14.32
202CD 253ZN 233CG 62.36
202CD 253ZN 93OD2 76.87
104OD1 253ZN 233CD 53.39
104OD1 253ZN 233OE1 45.35
104OD1 253ZN 104CB 33.47
104OD1 253ZN 233CG 59.41
104OD1 253ZN 174CD1 69.10
104OD1 253ZN 93OD2 56.56
233CD 253ZN 202OE2 58.09
233CD 253ZN 233OE1 17.51
233CD 253ZN 104CB 67.35
233CD 253ZN 202CG 60.35
233CD 253ZN 233CG 12.10
233CD 253ZN 93OD2 49.89
202OE2 253ZN 233OE1 59.91
202OE2 253ZN 202CG 31.41
202OE2 253ZN 233CG 60.31
202OE2 253ZN 93OD2 57.74
233OE1 253ZN 104CB 68.93
233OE1 253ZN 202CG 71.73
233OE1 253ZN 233CG 29.55
233OE1 253ZN 93OD2 33.55
168ND1 253ZN 168CG 19.04
168ND1 253ZN 104CB 85.10
168ND1 253ZN 175CE1 53.83
168ND1 253ZN 174CD1 68.77
168CG 253ZN 202CG 90.55
168CG 253ZN 175CE1 51.36
168CG 253ZN 174CD1 82.76
104CB 253ZN 233CG 65.96
104CB 253ZN 174CD1 62.01
104CB 253ZN 93OD2 89.31
202CG 253ZN 233CG 54.97
202CG 253ZN 93OD2 84.33
175CE1 253ZN 174CD1 53.82
233CG 253ZN 93OD2 61.82
93OD1 254ZN 93OD2 62.92
93OD1 254ZN 93CG 31.47
93OD1 254ZN 93CB 28.71

93OD1 254ZN 93CA 20.63
93OD1 254ZN 104C 96.27
93OD1 254ZN 104CA 97.12
93OD1 254ZN 95CB 69.85
93OD1 254ZN 93C 6.97
233OE1 254ZN 104OD1 94.44
233OE1 254ZN 93OD2 80.38
233OE1 254ZN 93CG 93.64
233OE1 254ZN 233CD 24.22
233OE1 254ZN 233OE2 48.56
233OE1 254ZN 104CG 92.12
233OE1 254ZN 104OD2 94.04
233OE1 254ZN 93CB 94.96
233OE1 254ZN 233CG 19.36
233OE1 254ZN 104CB 88.80
233OE1 254ZN 202OE2 61.38
233OE1 254ZN 93CA 87.96
233OE1 254ZN 104C 66.56
233OE1 254ZN 104CA 84.36
233OE1 254ZN 93C 99.74
233OE1 254ZN 233CB 3.02
104OD1 254ZN 233CD 82.02
104OD1 254ZN 233OE2 77.86
104OD1 254ZN 104CG 19.27
104OD1 254ZN 104OD2 41.51
104OD1 254ZN 233CG 79.14
104OD1 254ZN 104CB 11.46
104OD1 254ZN 104C 31.12
104OD1 254ZN 104CA 13.12
104OD1 254ZN 95CB 44.32
104OD1 254ZN 93C 99.81
104OD1 254ZN 233CB 93.51
93OD2 254ZN 93CG 31.45
93OD2 254ZN 233CD 98.64
93OD2 254ZN 93CB 34.22
93OD2 254ZN 233CG 98.59
93OD2 254ZN 202OE2 72.78
93OD2 254ZN 93CA 48.01
93OD2 254ZN 93C 64.27
93OD2 254ZN 233CB 82.14
93CG 254ZN 93CB 2.77
93CG 254ZN 93CA 19.90
93CG 254ZN 95CB 99.73
93CG 254ZN 93C 33.28
93CG 254ZN 233CB 96.36
233CD 254ZN 233OE2 25.03
233CD 254ZN 104CG 73.74
233CD 254ZN 104OD2 70.98
233CD 254ZN 233CG 9.27
233CD 254ZN 104CB 73.33
233CD 254ZN 202OE2 53.06
233CD 254ZN 104C 61.95
233CD 254ZN 104CA 75.81
233CD 254ZN 233CB 21.28
233OE2 254ZN 104CG 63.04
233OE2 254ZN 104OD2 52.10
233OE2 254ZN 233CG 33.32
233OE2 254ZN 104CB 66.81
233OE2 254ZN 202OE2 44.20
233OE2 254ZN 104C 70.21
233OE2 254ZN 104CA 77.23
233OE2 254ZN 233CB 45.54
104CG 254ZN 104OD2 22.51
104CG 254ZN 233CG 73.79
104CG 254ZN 104CB 9.75
104CG 254ZN 104C 41.30
104CG 254ZN 104CA 28.60
104CG 254ZN 95CB 57.30
104CG 254ZN 233CB 90.30
104OD2 254ZN 233CG 74.72
104OD2 254ZN 104CB 32.05
104OD2 254ZN 202OE2 83.62
104OD2 254ZN 104C 60.90
104OD2 254ZN 104CA 50.89
104OD2 254ZN 95CB 71.64
104OD2 254ZN 233CB 91.44
93CB 254ZN 93CA 18.04
93CB 254ZN 95CB 97.05
93CB 254ZN 93C 30.63
93CB 254ZN 233CB 97.73
233CG 254ZN 104CB 71.76
233CG 254ZN 202OE2 61.28
233CG 254ZN 104C 55.74
233CG 254ZN 104CA 71.25
233CG 254ZN 233CB 16.95
104CB 254ZN 104C 32.31

104CB	254ZN	104CA	18.89
104CB	254ZN	95CB	54.38
104CB	254ZN	233CB	87.40
202OE2	254ZN	233CB	59.45
93CA	254ZN	104C	98.76
93CA	254ZN	95CB	89.31
93CA	254ZN	93C	18.16
93CA	254ZN	233CB	90.97
104C	254ZN	104CA	18.64
104C	254ZN	95CB	65.97
104C	254ZN	93C	90.76
104C	254ZN	233CB	66.41
104CA	254ZN	95CB	50.13
104CA	254ZN	93C	93.27
104CA	254ZN	233CB	83.88
95CB	254ZN	93C	71.15

Table VII

Provides bond angles between interresidue atoms that are within 5 Ångstroms apart in an active site of an *S. aureus* methionine aminopeptidase for an inhibitor complex with 5-benzofuran-2-yl-1-H-[1,2,3]triazole.

Atom 1	Atom 2	Atom 3	Angle
76CE1	300C1	76NE2	19.14
76CE1	300C1	76ND1	15.95
76CE1	300C1	76CD2	26.06
76CE1	300C1	175NE2	98.82
76CE1	300C1	67SG	74.42
76NE2	300C1	76ND1	28.72
76NE2	300C1	76CD2	14.53
76NE2	300C1	175NE2	91.86
76NE2	300C1	67SG	81.18
174CD2	300C1	175CE1	52.87
174CD2	300C1	175NE2	67.72
174CD2	300C1	174CG	15.79
175CE1	300C1	175NE2	14.91
175CE1	300C1	174CG	42.43
76ND1	300C1	76CD2	26.83
76ND1	300C1	67SG	58.47
76CD2	300C1	67SG	69.24
175NE2	300C1	174CG	57.13
174CD2	300C2	175CE1	52.02
174CD2	300C2	174CG	18.44
174CD2	300C2	104OD2	80.51
174CD2	300C2	174CD1	31.45
174CD2	300C2	95OG	55.04
174CD2	300C2	104OD1	88.85
76CE1	300C2	93OD2	87.27
76CE1	300C2	93CG	95.03
76CE1	300C2	76NE2	14.74
175CE1	300C2	174CG	43.86
175CE1	300C2	104OD2	77.13
175CE1	300C2	174CD1	57.79
175CE1	300C2	76NE2	91.07
93OD2	300C2	93OD1	27.20
93OD2	300C2	104OD2	70.80
93OD2	300C2	93CG	14.93
93OD2	300C2	95OG	87.95
93OD2	300C2	104OD1	53.47
93OD1	300C2	104OD2	63.87
93OD1	300C2	174CD1	91.49
93OD1	300C2	93CG	14.94
93OD1	300C2	95OG	60.76
93OD1	300C2	104OD1	38.83
174CG	300C2	104OD2	63.86
174CG	300C2	174CD1	18.41
174CG	300C2	95OG	58.94
174CG	300C2	104OD1	77.06
104OD2	300C2	174CD1	49.42
104OD2	300C2	93CG	72.72
104OD2	300C2	95OG	69.61
104OD2	300C2	104OD1	26.43
174CD1	300C2	95OG	47.37
174CD1	300C2	104OD1	59.00
93CG	300C2	95OG	74.56
93CG	300C2	104OD1	50.31
95OG	300C2	104OD1	54.84
76CE1	300C3	67SG	88.64

76CE1 300C3 76NE2 19.56
76CE1 300C3 76ND1 18.60
76CE1 300C3 76CD2 30.32
76CE1 300C3 76CG 29.53
67SG 300C3 76NE2 97.91
67SG 300C3 76ND1 70.36
67SG 300C3 76CD2 84.94
67SG 300C3 76CG 68.93
67SG 300C3 56CG 63.16
76NE2 300C3 76ND1 30.70
76NE2 300C3 76CD2 18.26
76NE2 300C3 76CG 29.44
76ND1 300C3 76CD2 29.74
76ND1 300C3 76CG 17.88
76CD2 300C3 76CG 17.62
174CD2 300C3 56CG 71.10
175CE1 300O4 175NE2 19.62
175CE1 300O4 174CD2 58.51
175CE1 300O4 175ND1 9.44
175CE1 300O4 174CG 44.17
76NE2 300O4 76CE1 20.02
76NE2 300O4 76CD2 13.84
76NE2 300O4 76ND1 25.39
76CE1 300O4 76CD2 27.89
76CE1 300O4 76ND1 12.39
175NE2 300O4 174CD2 78.13
175NE2 300O4 175ND1 27.17
175NE2 300O4 174CG 63.60
174CD2 300O4 175ND1 51.81
174CD2 300O4 174CG 16.61
76CD2 300O4 76ND1 26.70
175ND1 300O4 174CG 39.13
93OD1 300C5 93CG 20.13
93OD1 300C5 93OD2 36.26
93OD1 300C5 104OD1 50.64
93OD1 300C5 95OG 79.27
93OD1 300C5 104OD2 78.56
93OD1 300C5 104CG 65.61
93OD1 300C5 93CB 29.58
93OD1 300C5 95CB 69.09
93OD1 300C5 233OE1 43.84
93OD1 300C5 67SG 88.44
93CG 300C5 93OD2 19.79
93CG 300C5 104OD1 65.68
93CG 300C5 95OG 97.90
93CG 300C5 104OD2 89.37
93CG 300C5 104CG 79.56
93CG 300C5 93CB 15.86
93CG 300C5 95CB 89.03
93CG 300C5 233OE1 44.29
93CG 300C5 67SG 79.99
93OD2 300C5 104OD1 68.37
93OD2 300C5 104OD2 84.21
93OD2 300C5 104CG 79.26
93OD2 300C5 93CB 30.45
93OD2 300C5 233OE1 35.41
93OD2 300C5 67SG 88.68
104OD1 300C5 95OG 67.01
104OD1 300C5 104OD2 30.00
104OD1 300C5 104CG 15.11
104OD1 300C5 93CB 79.44
104OD1 300C5 95CB 50.02
104OD1 300C5 174CD2 93.57
104OD1 300C5 233OE1 38.72
104OD1 300C5 174CD1 63.77
95OG 300C5 104OD2 79.50
95OG 300C5 104CG 68.75
95OG 300C5 93CB 97.18
95OG 300C5 95CB 16.99
95OG 300C5 174CD2 56.35
95OG 300C5 174CD1 49.70
95OG 300C5 67SG 92.59
104OD2 300C5 104CG 16.02
104OD2 300C5 95CB 64.77
104OD2 300C5 174CD2 78.21
104OD2 300C5 233OE1 48.81
104OD2 300C5 174CD1 50.15
104CG 300C5 93CB 93.97
104CG 300C5 95CB 52.56
104CG 300C5 174CD2 82.43
104CG 300C5 233OE1 45.66
104CG 300C5 174CD1 52.45
93CB 300C5 95CB 92.58
93CB 300C5 233OE1 59.99
93CB 300C5 67SG 64.15
95CB 300C5 174CD2 63.84

95CB 300C5 233OE1 86.55
95CB 300C5 174CD1 47.31
174CD2 300C5 174CD1 30.04
233OE1 300C5 174CD1 97.53
168NE2 300N6 175CE1 60.66
168NE2 300N6 104OD2 50.92
168NE2 300N6 175NE2 56.93
168NE2 300N6 174CD2 94.08
168NE2 300N6 168CE1 15.28
168NE2 300N6 174CG 74.77
168NE2 300N6 174CD1 72.46
168NE2 300N6 104OD1 79.88
168NE2 300N6 202OE1 48.07
168NE2 300N6 104CG 65.13
168NE2 300N6 168CD2 14.11
168NE2 300N6 233OE2 56.29
168NE2 300N6 175ND1 57.85
168NE2 300N6 202OE2 70.53
175CE1 300N6 104OD2 98.09
175CE1 300N6 175NE2 17.84
175CE1 300N6 174CD2 54.88
175CE1 300N6 168CE1 58.33
175CE1 300N6 174CG 48.25
175CE1 300N6 174CD1 64.93
175CE1 300N6 202OE1 98.82
175CE1 300N6 168CD2 56.36
175CE1 300N6 175ND1 9.41
104OD2 300N6 174CD2 89.62
104OD2 300N6 168CE1 43.45
104OD2 300N6 174CG 73.82
104OD2 300N6 174CD1 56.73
104OD2 300N6 104OD1 29.29
104OD2 300N6 202OE1 65.42
104OD2 300N6 104CG 14.26
104OD2 300N6 168CD2 64.32
104OD2 300N6 93OD2 77.65
104OD2 300N6 233OE2 35.43
104OD2 300N6 175ND1 90.27
104OD2 300N6 202OE2 66.17
175NE2 300N6 174CD2 72.37
175NE2 300N6 168CE1 60.10
175NE2 300N6 174CG 65.80
175NE2 300N6 174CD1 81.37
175NE2 300N6 202OE1 85.55
175NE2 300N6 168CD2 48.21
175NE2 300N6 175ND1 25.94
175NE2 300N6 76CE1 93.02
174CD2 300N6 168CE1 81.04
174CD2 300N6 174CG 19.90
174CD2 300N6 174CD1 32.93
174CD2 300N6 104OD1 91.82
174CD2 300N6 104CG 86.97
174CD2 300N6 168CD2 99.59
174CD2 300N6 175ND1 49.15
168CE1 300N6 174CG 61.25
168CE1 300N6 174CD1 57.27
168CE1 300N6 104OD1 72.53
168CE1 300N6 202OE1 61.10
168CE1 300N6 104CG 56.75
168CE1 300N6 168CD2 28.01
168CE1 300N6 233OE2 59.87
168CE1 300N6 175ND1 52.93
168CE1 300N6 202OE2 80.57
174CG 300N6 174CD1 19.60
174CG 300N6 104OD1 83.78
174CG 300N6 104CG 74.67
174CG 300N6 168CD2 81.82
174CG 300N6 175ND1 39.92
174CD1 300N6 104OD1 64.19
174CD1 300N6 104CG 55.61
174CD1 300N6 168CD2 83.26
174CD1 300N6 233OE2 92.15
174CD1 300N6 175ND1 55.79
104OD1 300N6 202OE1 80.00
104OD1 300N6 104CG 15.94
104OD1 300N6 168CD2 92.72
104OD1 300N6 93OD2 55.13
104OD1 300N6 233OE2 42.79
104OD1 300N6 202OE2 67.63
202OE1 300N6 104CG 75.06
202OE1 300N6 168CD2 44.66
202OE1 300N6 93OD2 74.87
202OE1 300N6 233OE2 37.23
202OE1 300N6 76CE1 96.91
202OE1 300N6 202OE2 26.19
104CG 300N6 168CD2 78.58

104CG 300N6 93OD2 69.09
104CG 300N6 233OE2 40.23
104CG 300N6 175ND1 99.04
104CG 300N6 202OE2 69.75
168CD2 300N6 233OE2 63.34
168CD2 300N6 175ND1 56.18
168CD2 300N6 202OE2 70.04
93OD2 300N6 233OE2 56.91
93OD2 300N6 76CE1 79.88
93OD2 300N6 202OE2 48.71
233OE2 300N6 202OE2 30.74
76CE1 300N6 202OE2 89.70
76NE2 300C7 76CD2 21.35
76NE2 300C7 76CE1 19.73
76NE2 300C7 76CG 30.99
76NE2 300C7 76ND1 29.72
76NE2 300C7 67SG 91.58
76CD2 300C7 76CE1 33.21
76CD2 300C7 76CG 18.17
76CD2 300C7 76ND1 30.49
76CD2 300C7 67SG 82.30
76CE1 300C7 76CG 30.96
76CE1 300C7 76ND1 17.67
76CE1 300C7 67SG 77.73
60CG 300C7 60CD 17.36
76CG 300C7 76ND1 18.51
76CG 300C7 67SG 64.49
76ND1 300C7 67SG 62.25
76NE2 300C8 76CE1 19.24
76NE2 300C8 76CD2 19.05
76NE2 300C8 76ND1 24.47
76NE2 300C8 76CG 24.20
76CE1 300C8 76CD2 32.14
76CE1 300C8 76ND1 14.15
76CE1 300C8 175NE2 99.96
76CE1 300C8 76CG 27.00
76CD2 300C8 76ND1 27.63
76CD2 300C8 76CG 14.59
60CG 300C8 175CE1 95.50
60CG 300C8 60CD 19.94
60CG 300C8 60OE1 31.19
60CG 300C8 174CD2 66.15
175CE1 300C8 60CD 82.18
175CE1 300C8 60OE1 87.00
175CE1 300C8 174CD2 48.76
175CE1 300C8 175NE2 16.06
60CD 300C8 60OE1 15.83
60CD 300C8 174CD2 67.06
60CD 300C8 175NE2 89.46
60OE1 300C8 174CD2 81.55
60OE1 300C8 175NE2 90.17
174CD2 300C8 175NE2 64.81
76ND1 300C8 76CG 16.66
104OD1 300N9 93OD1 67.33
104OD1 300N9 93OD2 91.27
104OD1 300N9 104OD2 42.33
104OD1 300N9 93CG 84.17
104OD1 300N9 104CG 21.21
104OD1 300N9 233OE1 54.45
104OD1 300N9 233OE2 56.07
104OD1 300N9 233CD 50.71
104OD1 300N9 95OG 73.08
104OD1 300N9 95CB 55.01
104OD1 300N9 202OE2 87.17
104OD1 300N9 93CB 92.10
104OD1 300N9 174CD1 73.50
104OD1 300N9 168NE2 84.53
104OD1 300N9 104CB 21.22
104OD1 300N9 202OE1 91.43
93OD1 300N9 93OD2 41.87
93OD1 300N9 93CG 21.87
93OD1 300N9 104CG 88.49
93OD1 300N9 233OE1 60.03
93OD1 300N9 233OE2 91.88
93OD1 300N9 233CD 74.45
93OD1 300N9 95OG 79.50
93OD1 300N9 95CB 74.48
93OD1 300N9 202OE2 92.50
93OD1 300N9 93CB 25.77
93OD1 300N9 104CB 87.91
93OD2 300N9 93CG 21.96
93OD2 300N9 233OE1 48.11
93OD2 300N9 233OE2 77.20
93OD2 300N9 233CD 63.02
93OD2 300N9 202OE2 58.74
93OD2 300N9 93CB 27.95

93OD2 300N9 202OE1 84.27
104OD2 300N9 104CG 21.90
104OD2 300N9 233OE1 68.14
104OD2 300N9 233OE2 43.26
104OD2 300N9 233CD 53.81
104OD2 300N9 95OG 90.32
104OD2 300N9 95CB 75.87
104OD2 300N9 202OE2 74.95
104OD2 300N9 174CD1 56.27
104OD2 300N9 168NE2 42.37
104OD2 300N9 104CB 25.94
104OD2 300N9 202OE1 62.73
93CG 300N9 233OE1 57.69
93CG 300N9 233OE2 90.42
93CG 300N9 233CD 73.65
93CG 300N9 95OG 97.71
93CG 300N9 95CB 95.53
93CG 300N9 202OE2 79.21
93CG 300N9 93CB 10.65
104CG 300N9 233OE1 63.05
104CG 300N9 233OE2 50.44
104CG 300N9 233CD 53.11
104CG 300N9 95OG 77.28
104CG 300N9 95CB 60.27
104CG 300N9 202OE2 84.53
104CG 300N9 174CD1 59.66
104CG 300N9 168NE2 64.22
104CG 300N9 104CB 6.81
104CG 300N9 202OE1 79.83
233OE1 300N9 233OE2 33.02
233OE1 300N9 233CD 15.97
233OE1 300N9 202OE2 40.30
233OE1 300N9 93CB 68.23
233OE1 300N9 168NE2 88.11
233OE1 300N9 104CB 68.47
233OE1 300N9 202OE1 60.24
233OE2 300N9 233CD 17.51
233OE2 300N9 202OE2 34.11
233OE2 300N9 174CD1 98.97
233OE2 300N9 168NE2 55.17
233OE2 300N9 104CB 57.25
233OE2 300N9 202OE1 36.75
233CD 300N9 202OE2 36.85
233CD 300N9 93CB 84.19
233CD 300N9 168NE2 72.63
233CD 300N9 104CB 59.40
233CD 300N9 202OE1 49.92
95OG 300N9 95CB 18.09
95OG 300N9 93CB 93.26
95OG 300N9 174CD1 50.01
95OG 300N9 104CB 70.50
95CB 300N9 93CB 94.31
95CB 300N9 174CD1 49.20
95CB 300N9 104CB 53.61
202OE2 300N9 93CB 86.68
202OE2 300N9 168NE2 66.02
202OE2 300N9 104CB 91.34
202OE2 300N9 202OE1 26.02
174CD1 300N9 168NE2 61.74
174CD1 300N9 104CB 55.02
168NE2 300N9 104CB 67.39
168NE2 300N9 202OE1 41.02
104CB 300N9 202OE1 86.09
104OD2 300N10 104OD1 41.92
104OD2 300N10 104CG 20.72
104OD2 300N10 168NE2 60.90
104OD2 300N10 233OE2 49.96
104OD2 300N10 233OE1 68.40
104OD2 300N10 202OE1 82.23
104OD2 300N10 233CD 56.26
104OD2 300N10 93OD1 90.74
104OD2 300N10 168CE1 48.25
104OD2 300N10 202OE2 87.71
104OD2 300N10 174CD1 61.83
104OD2 300N10 202CD 81.05
104OD2 300N10 168CD2 70.97
104OD2 300N10 175CE1 97.18
104OD2 300N10 104CB 18.37
104OD2 300N10 174CG 76.46
104OD2 300N10 174CD2 91.88
104OD1 300N10 104CG 21.75
104OD1 300N10 233OE2 59.10
104OD1 300N10 233OE1 48.81
104OD1 300N10 93OD2 71.62
104OD1 300N10 233CD 50.39
104OD1 300N10 93OD1 49.29

104OD1 300N10 168CE1 89.80
104OD1 300N10 202OE2 89.52
104OD1 300N10 93CG 62.88
104OD1 300N10 174CD1 74.41
104OD1 300N10 202CD 94.20
104OD1 300N10 104CB 27.15
104OD1 300N10 174CG 92.46
104OD1 300N10 174CD2 98.46
104CG 300N10 168NE2 81.55
104CG 300N10 233OE2 54.99
104CG 300N10 233OE1 59.95
104CG 300N10 93OD2 91.28
104CG 300N10 202OE1 96.30
104CG 300N10 233CD 53.81
104CG 300N10 93OD1 71.03
104CG 300N10 168CE1 68.08
104CG 300N10 202OE2 91.96
104CG 300N10 93CG 84.23
104CG 300N10 174CD1 63.17
104CG 300N10 202CD 90.60
104CG 300N10 168CD2 91.69
104CG 300N10 104CB 6.87
104CG 300N10 174CG 80.73
104CG 300N10 174CD2 92.02
168NE2 300N10 233OE2 70.99
168NE2 300N10 202OE1 53.66
168NE2 300N10 233CD 87.94
168NE2 300N10 168CE1 17.13
168NE2 300N10 202OE2 82.91
168NE2 300N10 174CD1 74.30
168NE2 300N10 202CD 66.81
168NE2 300N10 168CD2 11.35
168NE2 300N10 175CE1 52.09
168NE2 300N10 104CB 77.85
168NE2 300N10 174CG 70.92
168NE2 300N10 174CD2 86.03
233OE2 300N10 233OE1 34.46
233OE2 300N10 93OD2 73.52
233OE2 300N10 202OE1 45.76
233OE2 300N10 233CD 17.07
233OE2 300N10 93OD1 81.56
233OE2 300N10 168CE1 72.64
233OE2 300N10 202OE2 38.11
233OE2 300N10 93CG 81.06
233OE2 300N10 202CD 36.07
233OE2 300N10 168CD2 72.78
233OE2 300N10 104CB 59.52
233OE1 300N10 93OD2 41.19
233OE1 300N10 202OE1 69.28
233OE1 300N10 233CD 17.60
233OE1 300N10 93OD1 48.36
233OE1 300N10 202OE2 43.49
233OE1 300N10 93CG 46.65
233OE1 300N10 202CD 54.15
233OE1 300N10 104CB 66.72
93OD2 300N10 202OE1 89.54
93OD2 300N10 233CD 58.07
93OD2 300N10 93OD1 31.19
93OD2 300N10 202OE2 58.88
93OD2 300N10 93CG 15.95
93OD2 300N10 202CD 74.99
93OD2 300N10 104CB 97.79
202OE1 300N10 233CD 57.83
202OE1 300N10 168CE1 67.58
202OE1 300N10 202OE2 31.00
202OE1 300N10 202CD 15.72
202OE1 300N10 168CD2 46.72
202OE1 300N10 175CE1 92.31
202OE1 300N10 104CB 98.44
233CD 300N10 93OD1 64.63
233CD 300N10 168CE1 88.20
233CD 300N10 202OE2 39.53
233CD 300N10 93CG 64.23
233CD 300N10 202CD 44.64
233CD 300N10 168CD2 89.80
233CD 300N10 104CB 59.85
93OD1 300N10 202OE2 84.08
93OD1 300N10 93CG 16.30
93OD1 300N10 202CD 98.85
93OD1 300N10 104CB 76.16
168CE1 300N10 202OE2 93.99
168CE1 300N10 174CD1 59.33
168CE1 300N10 202CD 78.57
168CE1 300N10 168CD2 28.38
168CE1 300N10 175CE1 53.85
168CE1 300N10 104CB 63.39

168CE1 300N10 174CG 59.66
168CE1 300N10 174CD2 76.62
202OE2 300N10 93CG 73.54
202OE2 300N10 202CD 16.15
202OE2 300N10 168CD2 77.36
202OE2 300N10 104CB 97.16
93CG 300N10 202CD 89.39
93CG 300N10 104CB 90.02
174CD1 300N10 168CD2 83.41
174CD1 300N10 175CE1 58.32
174CD1 300N10 104CB 56.74
174CD1 300N10 174CG 18.11
174CD1 300N10 174CD2 30.15
202CD 300N10 168CD2 61.30
202CD 300N10 104CB 94.35
168CD2 300N10 175CE1 51.16
168CD2 300N10 104CB 88.46
168CD2 300N10 174CG 77.49
168CD2 300N10 174CD2 90.76
175CE1 300N10 174CG 41.85
175CE1 300N10 174CD2 45.70
104CB 300N10 174CG 74.10
104CB 300N10 174CD2 86.01
174CG 300N10 174CD2 17.78
76CD2 300C11 76NE2 20.21
76CD2 300C11 219CZ3 97.90
76CD2 300C11 76CG 17.87
76CD2 300C11 219CE3 83.02
76CD2 300C11 62CE1 86.24
76CD2 300C11 76CE1 28.25
76CD2 300C11 76ND1 26.53
76CD2 300C11 67SG 80.67
60CG 300C11 219CZ3 81.89
60CG 300C11 60CB 20.85
60CG 300C11 62CG 92.45
60CG 300C11 60CD 16.94
60CG 300C11 62CB 74.10
60CG 300C11 60OE1 29.42
76NE2 300C11 76CG 30.56
76NE2 300C11 76CE1 15.73
76NE2 300C11 76ND1 26.55
76NE2 300C11 67SG 84.24
62CD1 300C11 219CZ3 55.30
62CD1 300C11 60CB 85.01
62CD1 300C11 76CG 91.20
62CD1 300C11 219CE3 48.79
62CD1 300C11 62CE1 17.31
62CD1 300C11 62CG 16.67
62CD1 300C11 67SG 63.98
62CD1 300C11 62CB 31.83
219CZ3 300C11 60CB 62.77
219CZ3 300C11 219CE3 18.54
219CZ3 300C11 62CE1 62.87
219CZ3 300C11 62CG 64.74
219CZ3 300C11 60CD 84.31
219CZ3 300C11 62CB 62.83
219CZ3 300C11 60OE1 75.66
60CB 300C11 219CE3 80.87
60CB 300C11 62CG 76.95
60CB 300C11 60CD 32.56
60CB 300C11 62CB 59.19
60CB 300C11 60OE1 37.72
76CG 300C11 219CE3 85.39
76CG 300C11 62CE1 73.99
76CG 300C11 76CE1 28.49
76CG 300C11 76ND1 16.49
76CG 300C11 67SG 63.03
219CE3 300C11 62CE1 50.69
219CE3 300C11 62CG 62.59
219CE3 300C11 62CB 67.18
219CE3 300C11 60OE1 92.58
62CE1 300C11 62CG 30.57
62CE1 300C11 76ND1 84.08
62CE1 300C11 67SG 54.56
62CE1 300C11 62CB 48.06
76CE1 300C11 76ND1 16.15
76CE1 300C11 67SG 70.09
62CG 300C11 67SG 61.11
62CG 300C11 62CB 18.35
60CD 300C11 62CB 90.17
60CD 300C11 60OE1 15.00
76ND1 300C11 67SG 58.10
67SG 300C11 62CB 74.33
62CB 300C11 60OE1 96.80
60OE1 300C12 60CD 18.90
60OE1 300C12 60CG 35.99

60OE1 300C12 60OE2 28.67
60OE1 300C12 175CE1 96.27
60OE1 300C12 60CB 36.55
76NE2 300C12 76CD2 18.32
76NE2 300C12 76CE1 13.70
76NE2 300C12 175NE2 98.52
60CD 300C12 60CG 22.11
60CD 300C12 60OE2 14.58
60CD 300C12 175CE1 86.18
60CD 300C12 175NE2 96.96
60CD 300C12 60CB 30.42
60CG 300C12 60OE2 31.63
60CG 300C12 175CE1 95.29
60CG 300C12 60CB 15.14
76CD2 300C12 76CE1 28.36
60OE2 300C12 175CE1 71.64
60OE2 300C12 175NE2 82.51
60OE2 300C12 60CB 43.37
76CE1 300C12 175CE1 95.45
76CE1 300C12 175NE2 90.57
175CE1 300C12 175NE2 16.13
219CZ3 300C13 60CG 98.24
219CZ3 300C13 219CE3 21.41
219CZ3 300C13 60CB 74.89
219CZ3 300C13 60OE1 98.52
219CZ3 300C13 62CD1 55.11
219CZ3 300C13 219CH2 10.78
60CG 300C13 60CB 23.43
60CG 300C13 60OE1 36.93
60CG 300C13 60CD 21.17
60CG 300C13 62CD1 98.17
60CG 300C13 219CH2 87.47
219CE3 300C13 60CB 94.41
219CE3 300C13 76CD2 87.88
219CE3 300C13 62CD1 47.95
219CE3 300C13 219CH2 31.58
219CE3 300C13 76CG 84.51
60CB 300C13 60OE1 45.48
60CB 300C13 60CD 37.22
60CB 300C13 62CD1 83.32
60CB 300C13 219CH2 64.11
60OE1 300C13 60CD 17.57
60OE1 300C13 219CH2 89.96
76CD2 300C13 76NE2 18.87
76CD2 300C13 62CD1 90.26
76CD2 300C13 76CG 13.57
60CD 300C13 219CH2 94.69
76NE2 300C13 76CG 26.99
62CD1 300C13 219CH2 56.52
62CD1 300C13 76CG 78.23
60OE1 300C14 60CG 40.01
60OE1 300C14 60CD 19.48
60OE1 300C14 60CB 44.84
60OE1 300C14 219CZ3 92.59
60OE1 300C14 60OE2 24.76
60CG 300C14 60CD 23.87
60CG 300C14 60CB 20.73
60CG 300C14 219CZ3 81.80
60CG 300C14 60OE2 30.39
60CG 300C14 219CE3 94.66
60CD 300C14 60CB 36.97
60CD 300C14 219CZ3 95.82
60CD 300C14 60OE2 10.83
76NE2 300C14 76CD2 18.94
76NE2 300C14 219CE3 91.26
76CD2 300C14 219CZ3 88.62
76CD2 300C14 219CE3 72.36
60CB 300C14 219CZ3 61.59
60CB 300C14 60OE2 46.67
60CB 300C14 219CE3 75.50
219CZ3 300C14 219CE3 16.30
104OD2 253ZN 168NE2 98.10
104OD2 253ZN 233OE2 79.80
104OD2 253ZN 168CE1 74.01
104OD2 253ZN 104CG 14.80
104OD2 253ZN 233CD 76.43
104OD2 253ZN 104OD1 34.58
104OD2 253ZN 233OE1 78.09
104OD2 253ZN 168ND1 82.40
104OD2 253ZN 104CB 7.30
104OD2 253ZN 233CG 73.89
104OD2 253ZN 93OD2 92.73
168NE2 253ZN 202OE1 88.36
168NE2 253ZN 168CE1 24.30
168NE2 253ZN 168CD2 18.22
168NE2 253ZN 168ND1 18.64

168NE2 253ZN 168CG 12.73
233OE2 253ZN 202OE1 73.52
233OE2 253ZN 104CG 71.23
233OE2 253ZN 202CD 53.63
233OE2 253ZN 233CD 15.48
233OE2 253ZN 202OE2 49.42
233OE2 253ZN 104OD1 67.24
233OE2 253ZN 233OE1 35.31
233OE2 253ZN 104CB 72.59
233OE2 253ZN 202CG 47.04
233OE2 253ZN 233CG 7.48
233OE2 253ZN 93OD2 67.16
202OE1 253ZN 202CD 21.74
202OE1 253ZN 168CD2 70.17
202OE1 253ZN 233CD 81.57
202OE1 253ZN 202OE2 39.94
202OE1 253ZN 233OE1 88.54
202OE1 253ZN 168ND1 96.73
202OE1 253ZN 168CG 79.57
202OE1 253ZN 202CG 27.09
202OE1 253ZN 233CG 80.48
202OE1 253ZN 93OD2 90.92
168CE1 253ZN 104CG 88.81
168CE1 253ZN 168CD2 40.57
168CE1 253ZN 168ND1 10.75
168CE1 253ZN 168CG 28.46
168CE1 253ZN 104CB 77.60
104CG 253ZN 233CD 64.96
104CG 253ZN 104OD1 20.25
104CG 253ZN 233OE1 64.01
104CG 253ZN 168ND1 97.12
104CG 253ZN 104CB 13.04
104CG 253ZN 233CG 64.48
104CG 253ZN 93OD2 78.31
202CD 253ZN 168CD2 90.35
202CD 253ZN 233CD 60.09
202CD 253ZN 202OE2 21.49
202CD 253ZN 233OE1 67.19
202CD 253ZN 168CG 97.86
202CD 253ZN 202CG 14.34
202CD 253ZN 233CG 60.08
202CD 253ZN 93OD2 75.41
168CD2 253ZN 168ND1 31.80
168CD2 253ZN 168CG 13.72
168CD2 253ZN 202CG 86.59
233CD 253ZN 202OE2 49.27
233CD 253ZN 104OD1 56.27
233CD 253ZN 233OE1 20.07
233CD 253ZN 104CB 69.79
233CD 253ZN 202CG 57.26
233CD 253ZN 233CG 10.68
233CD 253ZN 93OD2 52.92
202OE2 253ZN 104OD1 98.59
202OE2 253ZN 233OE1 49.82
202OE2 253ZN 202CG 32.25
202OE2 253ZN 233CG 53.59
202OE2 253ZN 93OD2 53.93
104OD1 253ZN 233OE1 48.85
104OD1 253ZN 104CB 33.13
104OD1 253ZN 233CG 59.78
104OD1 253ZN 93OD2 58.16
233OE1 253ZN 104CB 72.97
233OE1 253ZN 202CG 69.26
233OE1 253ZN 233CG 30.58
233OE1 253ZN 93OD2 33.44
168ND1 253ZN 168CG 18.68
168ND1 253ZN 104CB 85.16
168CG 253ZN 202CG 91.25
104CB 253ZN 233CG 66.80
104CB 253ZN 93OD2 90.83
202CG 253ZN 233CG 54.29
202CG 253ZN 93OD2 84.78
233CG 253ZN 93OD2 63.60
233OE1 254ZN 104OD1 93.69
233OE1 254ZN 93OD2 84.63
233OE1 254ZN 233CD 20.60
233OE1 254ZN 104CG 89.10
233OE1 254ZN 233OE2 41.97
233OE1 254ZN 104OD2 87.96
233OE1 254ZN 202OE2 46.39
233OE1 254ZN 233CG 17.35
233OE1 254ZN 104CB 87.62
233OE1 254ZN 93CA 99.36
233OE1 254ZN 104C 70.88
233OE1 254ZN 233CB 9.58
233OE1 254ZN 202CD 49.53

233OE1 254ZN 104CA 86.84
233OE1 254ZN 202OE1 62.68
93OD1 254ZN 93OD2 63.70
93OD1 254ZN 93CG 32.03
93OD1 254ZN 93CB 30.19
93OD1 254ZN 93CA 19.84
93OD1 254ZN 104C 94.80
93OD1 254ZN 104CA 95.80
93OD1 254ZN 93C 3.92
93OD1 254ZN 95CB 70.60
104OD1 254ZN 233CD 79.55
104OD1 254ZN 104CG 18.77
104OD1 254ZN 233OE2 75.53
104OD1 254ZN 104OD2 40.61
104OD1 254ZN 233CG 76.43
104OD1 254ZN 104CB 10.96
104OD1 254ZN 104C 29.02
104OD1 254ZN 233CB 90.96
104OD1 254ZN 104CA 11.53
104OD1 254ZN 95CB 43.85
93OD2 254ZN 93CG 31.67
93OD2 254ZN 93CB 33.54
93OD2 254ZN 202OE2 75.68
93OD2 254ZN 93CA 47.98
93OD2 254ZN 233CB 84.34
93OD2 254ZN 202CD 87.76
93OD2 254ZN 93C 64.01
93OD2 254ZN 202OE1 95.40
93CG 254ZN 93CB 1.98
93CG 254ZN 93CA 18.97
93CG 254ZN 233CB 97.17
93CG 254ZN 93C 32.54
233CD 254ZN 104CG 71.07
233CD 254ZN 233OE2 22.94
233CD 254ZN 104OD2 67.50
233CD 254ZN 202OE2 45.24
233CD 254ZN 233CG 13.34
233CD 254ZN 104CB 71.45
233CD 254ZN 104C 63.36
233CD 254ZN 233CB 26.67
233CD 254ZN 202CD 42.29
233CD 254ZN 104CA 75.58
233CD 254ZN 202OE1 51.88
104CG 254ZN 233OE2 61.18
104CG 254ZN 104OD2 22.04
104CG 254ZN 233CG 72.17
104CG 254ZN 104CB 9.19
104CG 254ZN 104C 40.08
104CG 254ZN 233CB 89.42
104CG 254ZN 202CD 88.42
104CG 254ZN 104CA 27.56
104CG 254ZN 95CB 55.21
104CG 254ZN 202OE1 81.96
233OE2 254ZN 104OD2 50.18
233OE2 254ZN 202OE2 40.80
233OE2 254ZN 233CG 35.30
233OE2 254ZN 104CB 65.17
233OE2 254ZN 104C 70.48
233OE2 254ZN 233CB 49.35
233OE2 254ZN 202CD 31.54
233OE2 254ZN 104CA 76.20
233OE2 254ZN 202OE1 34.78
104OD2 254ZN 202OE2 83.53
104OD2 254ZN 233CG 73.76
104OD2 254ZN 104CB 31.07
104OD2 254ZN 104C 59.63
104OD2 254ZN 233CB 91.85
104OD2 254ZN 202CD 71.08
104OD2 254ZN 104CA 49.47
104OD2 254ZN 95CB 68.60
104OD2 254ZN 202OE1 62.07
93CB 254ZN 93CA 17.95
93CB 254ZN 233CB 98.50
93CB 254ZN 93C 30.80
93CB 254ZN 95CB 98.63
202OE2 254ZN 233CG 56.03
202OE2 254ZN 233CB 55.62
202OE2 254ZN 202CD 12.51
202OE2 254ZN 202OE1 25.03
233CG 254ZN 104CB 70.30
233CG 254ZN 104C 55.26
233CG 254ZN 233CB 18.14
233CG 254ZN 202CD 54.84
233CG 254ZN 104CA 70.12
233CG 254ZN 202OE1 65.14
104CB 254ZN 104C 31.57

104CB	254ZN	233CB	86.46
104CB	254ZN	202CD	94.35
104CB	254ZN	104CA	18.41
104CB	254ZN	95CB	52.61
104CB	254ZN	202OE1	89.34
93CA	254ZN	233CB	92.20
93CA	254ZN	93C	18.17
93CA	254ZN	95CB	89.97
104C	254ZN	233CB	65.66
104C	254ZN	104CA	18.20
104C	254ZN	93C	92.10
104C	254ZN	95CB	64.34
233CB	254ZN	202CD	59.11
233CB	254ZN	104CA	82.75
233CB	254ZN	202OE1	72.20
202CD	254ZN	202OE1	14.45
104CA	254ZN	93C	94.12
104CA	254ZN	95CB	48.74
93C	254ZN	95CB	71.81

Table VIII

Provides a three dimensional protein coordinate set of an *S. pneumoniae* methionine aminopeptidase crystalline structure.

Residue	Atom	X	Y	Z	B
2 ILE	CB	10.87	40.59	15.61	18.51
2 ILE	CG2	11.88	41.49	16.31	18.53
2 ILE	CG1	9.48	41.23	15.62	18.55
2 ILE	CD1	8.91	41.42	17.02	18.56
2 ILE	C	12.69	39.66	14.19	18.35
2 ILE	O	12.84	38.57	14.74	18.43
2 ILE	N	10.34	39.47	13.43	18.53
2 ILE	CA	11.32	40.33	14.16	18.45
3 THR	N	13.68	40.32	13.60	18.20
3 THR	CA	15.03	39.77	13.60	17.99
3 THR	CB	15.75	40.02	12.25	18.05
3 THR	OG1	15.92	41.43	12.05	18.08
3 THR	CG2	14.95	39.44	11.10	18.08
3 THR	C	15.86	40.40	14.70	17.77
3 THR	O	15.71	41.58	15.01	17.79
4 LEU	N	16.73	39.59	15.31	17.46
4 LEU	CA	17.62	40.07	16.35	17.13
4 LEU	CB	17.71	39.05	17.48	17.20
4 LEU	CG	16.37	38.76	18.18	17.22
4 LEU	CD1	16.59	37.74	19.29	17.29
4 LEU	CD2	15.79	40.04	18.74	17.25
4 LEU	C	18.95	40.22	15.62	16.87
4 LEU	O	19.55	39.24	15.18	16.89
5 LYS	N	19.39	41.46	15.47	16.51
5 LYS	CA	20.60	41.79	14.74	16.14

5 LYS CB	20.71	43.30	14.58	16.07
5 LYS CG	19.79	43.89	13.52	15.97
5 LYS CD	18.32	43.63	13.82	15.88
5 LYS CE	17.43	44.27	12.77	15.83
5 LYS NZ	15.98	43.99	12.99	15.72
5 LYS C	21.94	41.25	15.23	15.94
5 LYS O	22.20	41.12	16.43	15.92
6 SER N	22.80	40.95	14.25	15.67
6 SER CA	24.14	40.46	14.49	15.40
6 SER CB	24.62	39.65	13.28	15.40
6 SER OG	24.72	40.50	12.15	15.33
6 SER C	25.04	41.67	14.66	15.19
6 SER O	24.62	42.80	14.38	15.07
7 ALA N	26.27	41.45	15.09	14.97
7 ALA CA	27.21	42.55	15.27	14.71
7 ALA CB	28.53	42.03	15.81	14.86
7 ALA C	27.42	43.24	13.92	14.48
7 ALA O	27.52	44.47	13.85	14.38
8 ARG N	27.49	42.45	12.86	14.19
8 ARG CA	27.69	42.98	11.51	13.88
8 ARG CB	27.81	41.83	10.50	14.13
8 ARG CG	27.96	42.28	9.05	14.47
8 ARG CD	28.14	41.09	8.12	14.85
8 ARG NE	29.39	40.37	8.39	15.19
8 ARG CZ	29.74	39.23	7.79	15.38
8 ARG NH1	28.94	38.68	6.89	15.52
8 ARG NH2	30.89	38.65	8.11	15.58
8 ARG C	26.56	43.92	11.10	13.54
8 ARG O	26.79	45.01	10.58	13.34
9 GLU N	25.32	43.49	11.33	13.23
9 GLU CA	24.16	44.29	10.97	13.00
9 GLU CB	22.88	43.46	11.13	13.22
9 GLU CG	22.86	42.25	10.20	13.63
9 GLU CD	21.73	41.28	10.47	13.85
9 GLU OE1	21.37	41.10	11.66	13.95
9 GLU OE2	21.20	40.68	9.51	14.15
9 GLU C	24.08	45.58	11.80	12.70
9 GLU O	23.72	46.63	11.29	12.42
10 ILE N	24.43	45.48	13.08	12.55
10 ILE CA	24.41	46.64	13.96	12.52
10 ILE CB	24.64	46.23	15.44	12.69
10 ILE CG2	24.78	47.47	16.31	12.79
10 ILE CG1	23.47	45.36	15.92	12.88

10 ILE CD1	23.68	44.76	17.30	13.16
10 ILE C	25.47	47.66	13.53	12.30
10 ILE O	25.22	48.86	13.55	12.22
11 GLU N	26.65	47.17	13.15	12.14
11 GLU CA	27.71	48.06	12.71	11.97
11 GLU CB	28.99	47.28	12.39	12.31
11 GLU CG	30.10	48.16	11.81	12.85
11 GLU CD	31.37	47.40	11.48	13.15
11 GLU OE1	31.38	46.16	11.60	13.44
11 GLU OE2	32.36	48.05	11.08	13.40
11 GLU C	27.28	48.85	11.47	11.62
11 GLU O	27.51	50.05	11.38	11.50
12 ALA N	26.65	48.16	10.53	11.28
12 ALA CA	26.18	48.82	9.31	10.93
12 ALA CB	25.57	47.79	8.36	10.97
12 ALA C	25.16	49.90	9.66	10.68
12 ALA O	25.21	51.00	9.11	10.51
13 MET N	24.25	49.61	10.58	10.59
13 MET CA	23.25	50.59	10.98	10.55
13 MET CB	22.20	49.97	11.89	10.71
13 MET CG	21.29	48.99	11.21	11.13
13 MET SD	20.14	48.33	12.41	11.37
13 MET CE	18.89	47.63	11.34	11.74
13 MET C	23.89	51.77	11.71	10.43
13 MET O	23.49	52.92	11.52	10.31
14 ASP N	24.87	51.48	12.55	10.50
14 ASP CA	25.54	52.52	13.31	10.60
14 ASP CB	26.56	51.90	14.27	11.07
14 ASP CG	27.13	52.90	15.25	11.47
14 ASP OD1	26.38	53.78	15.71	11.60
14 ASP OD2	28.33	52.79	15.57	12.16
14 ASP C	26.21	53.52	12.36	10.37
14 ASP O	26.18	54.73	12.59	10.27
15 LYS N	26.80	53.00	11.28	10.20
15 LYS CA	27.46	53.86	10.30	10.14
15 LYS CB	28.25	53.01	9.31	10.33
15 LYS CG	29.49	52.35	9.89	10.62
15 LYS CD	30.08	51.38	8.89	10.95
15 LYS CE	31.35	50.74	9.40	11.14
15 LYS NZ	31.88	49.77	8.40	11.26
15 LYS C	26.44	54.71	9.55	9.97
15 LYS O	26.64	55.91	9.36	9.78
16 ALA N	25.35	54.09	9.12	9.82

16	ALA	CA	24.31	54.83	8.41	9.73
16	ALA	CB	23.20	53.88	7.95	9.77
16	ALA	C	23.75	55.90	9.33	9.62
16	ALA	O	23.46	57.02	8.90	9.49
17	GLY	N	23.61	55.56	10.61	9.52
17	GLY	CA	23.09	56.50	11.59	9.61
17	GLY	C	24.04	57.66	11.86	9.59
17	GLY	O	23.60	58.77	12.14	9.47
18	ASP	N	25.34	57.39	11.79	9.70
18	ASP	CA	26.34	58.44	11.99	9.83
18	ASP	CB	27.75	57.86	12.03	10.29
18	ASP	CG	28.09	57.21	13.36	10.61
18	ASP	OD1	27.28	57.28	14.31	10.72
18	ASP	OD2	29.19	56.62	13.46	11.34
18	ASP	C	26.24	59.44	10.84	9.77
18	ASP	O	26.36	60.65	11.03	9.70
19	PHE	N	26.04	58.92	9.63	9.74
19	PHE	CA	25.92	59.78	8.45	9.74
19	PHE	CB	25.88	58.94	7.17	10.16
19	PHE	CG	25.61	59.73	5.93	10.66
19	PHE	CD1	26.47	60.75	5.51	10.96
19	PHE	CD2	24.48	59.47	5.17	10.87
19	PHE	CE1	26.20	61.48	4.36	11.24
19	PHE	CE2	24.20	60.20	4.01	11.18
19	PHE	CZ	25.07	61.21	3.61	11.28
19	PHE	C	24.65	60.63	8.57	9.51
19	PHE	O	24.68	61.84	8.35	9.38
20	LEU	N	23.54	59.99	8.93	9.33
20	LEU	CA	22.28	60.70	9.09	9.22
20	LEU	CB	21.16	59.72	9.47	9.35
20	LEU	CG	19.72	60.15	9.21	9.46
20	LEU	CD1	18.80	58.95	9.31	9.54
20	LEU	CD2	19.30	61.24	10.19	9.65
20	LEU	C	22.45	61.79	10.16	9.13
20	LEU	O	22.04	62.93	9.97	8.91
21	ALA	N	23.09	61.43	11.27	9.20
21	ALA	CA	23.32	62.40	12.34	9.31
21	ALA	CB	24.02	61.73	13.52	9.48
21	ALA	C	24.16	63.58	11.84	9.43
21	ALA	O	23.91	64.73	12.22	9.41
22	SER	N	25.14	63.31	10.98	9.59
22	SER	CA	25.98	64.38	10.45	9.86
22	SER	CB	27.17	63.81	9.65	10.10

22 SER OG	26.79	63.37	8.36	10.99
22 SER C	25.16	65.32	9.59	9.78
22 SER O	25.44	66.52	9.51	9.83
23 ILE N	24.13	64.79	8.93	9.73
23 ILE CA	23.26	65.63	8.11	9.74
23 ILE CB	22.34	64.76	7.21	9.95
23 ILE CG2	21.18	65.58	6.67	10.00
23 ILE CG1	23.18	64.17	6.07	10.15
23 ILE CD1	22.41	63.25	5.16	10.47
23 ILE C	22.45	66.54	9.03	9.62
23 ILE O	22.31	67.73	8.75	9.53
24 HIS N	21.93	66.00	10.13	9.61
24 HIS CA	21.19	66.84	11.07	9.63
24 HIS CB	20.61	66.01	12.21	9.44
24 HIS CG	19.29	65.39	11.89	9.18
24 HIS CD2	18.85	64.12	11.97	9.16
24 HIS ND1	18.23	66.13	11.40	9.17
24 HIS CE1	17.19	65.33	11.21	9.08
24 HIS NE2	17.55	64.11	11.54	9.09
24 HIS C	22.10	67.94	11.62	9.77
24 HIS O	21.68	69.09	11.76	9.77
25 ILE N	23.35	67.61	11.91	10.02
25 ILE CA	24.28	68.61	12.42	10.39
25 ILE CB	25.65	67.97	12.78	10.65
25 ILE CG2	26.67	69.06	13.07	10.81
25 ILE CG1	25.47	67.06	13.99	10.87
25 ILE CD1	26.66	66.16	14.27	11.21
25 ILE C	24.45	69.71	11.37	10.48
25 ILE O	24.47	70.90	11.70	10.46
26 GLY N	24.55	69.32	10.10	10.67
26 GLY CA	24.70	70.31	9.04	10.94
26 GLY C	23.46	71.17	8.87	11.09
26 GLY O	23.55	72.35	8.55	11.09
27 LEU N	22.28	70.57	9.07	11.28
27 LEU CA	21.03	71.31	8.93	11.54
27 LEU CB	19.83	70.36	9.04	11.49
27 LEU CG	19.60	69.42	7.85	11.48
27 LEU CD1	18.44	68.48	8.16	11.52
27 LEU CD2	19.30	70.24	6.60	11.61
27 LEU C	20.89	72.43	9.95	11.79
27 LEU O	20.14	73.38	9.74	11.70
28 ARG N	21.62	72.33	11.06	12.16
28 ARG CA	21.57	73.36	12.09	12.67

28 ARG CB	22.50	73.02	13.24	12.54
28 ARG CG	22.14	71.74	13.97	12.43
28 ARG CD	23.18	71.39	15.01	12.25
28 ARG NE	22.93	70.08	15.60	12.21
28 ARG CZ	23.71	69.50	16.49	12.20
28 ARG NH1	24.82	70.10	16.91	12.41
28 ARG NH2	23.40	68.31	16.97	12.28
28 ARG C	21.97	74.72	11.52	13.09
28 ARG O	21.43	75.75	11.92	13.24
29 ASP N	22.92	74.72	10.59	13.59
29 ASP CA	23.39	75.96	9.99	14.06
29 ASP CB	24.84	75.81	9.53	14.57
29 ASP CG	25.78	75.47	10.67	14.98
29 ASP OD1	25.68	76.11	11.74	15.40
29 ASP OD2	26.62	74.57	10.49	15.40
29 ASP C	22.55	76.41	8.80	14.11
29 ASP O	22.53	77.59	8.46	14.23
30 LEU N	21.85	75.47	8.18	14.13
30 LEU CA	21.04	75.77	7.00	14.14
30 LEU CB	20.92	74.52	6.13	14.27
30 LEU CG	20.13	74.65	4.83	14.41
30 LEU CD1	20.75	75.72	3.95	14.63
30 LEU CD2	20.13	73.31	4.11	14.60
30 LEU C	19.64	76.30	7.31	14.07
30 LEU O	19.16	77.21	6.65	14.15
31 ILE N	19.00	75.73	8.32	13.96
31 ILE CA	17.66	76.12	8.70	13.86
31 ILE CB	16.98	74.99	9.51	13.73
31 ILE CG2	15.59	75.40	9.96	13.75
31 ILE CG1	16.92	73.73	8.63	13.62
31 ILE CD1	16.45	72.48	9.34	13.56
31 ILE C	17.64	77.44	9.47	13.88
31 ILE O	17.81	77.47	10.69	13.97
32 LYS N	17.41	78.52	8.74	13.87
32 LYS CA	17.38	79.87	9.30	13.83
32 LYS CB	18.73	80.56	9.06	14.41
32 LYS CG	19.93	79.78	9.52	15.02
32 LYS CD	21.22	80.48	9.12	15.69
32 LYS CE	21.33	81.85	9.77	16.03
32 LYS NZ	22.55	82.58	9.32	16.41
32 LYS C	16.30	80.69	8.61	13.54
32 LYS O	15.83	80.34	7.53	13.31
33 PRO N	15.88	81.81	9.23	13.34

33 PRO CD	16.25	82.31	10.57	13.34
33 PRO CA	14.85	82.65	8.62	13.22
33 PRO CB	14.71	83.81	9.61	13.26
33 PRO CG	15.05	83.17	10.93	13.31
33 PRO C	15.30	83.13	7.24	13.11
33 PRO O	16.47	83.48	7.06	13.07
34 GLY N	14.39	83.12	6.28	12.96
34 GLY CA	14.73	83.57	4.94	12.87
34 GLY C	15.18	82.49	3.98	12.72
34 GLY O	15.23	82.71	2.77	12.83
35 VAL N	15.51	81.32	4.51	12.53
35 VAL CA	15.95	80.20	3.69	12.31
35 VAL CB	16.86	79.25	4.49	12.38
35 VAL CG1	17.22	78.02	3.66	12.44
35 VAL CG2	18.12	79.98	4.93	12.47
35 VAL C	14.75	79.43	3.15	12.10
35 VAL O	13.76	79.25	3.86	11.96
36 ASP N	14.85	78.98	1.91	11.90
36 ASP CA	13.78	78.20	1.28	11.69
36 ASP CB	14.02	78.15	-0.24	11.89
36 ASP CG	12.90	77.44	-0.99	11.93
36 ASP OD1	12.04	76.80	-0.35	11.90
36 ASP OD2	12.90	77.53	-2.24	12.34
36 ASP C	13.83	76.79	1.86	11.50
36 ASP O	14.87	76.14	1.82	11.39
37 MET N	12.71	76.33	2.41	11.32
37 MET CA	12.62	75.00	3.01	11.22
37 MET CB	11.17	74.70	3.42	11.61
37 MET CG	10.98	73.37	4.17	12.20
37 MET SD	9.32	72.62	3.96	13.13
37 MET CE	8.27	73.79	4.82	13.09
37 MET C	13.09	73.92	2.03	10.99
37 MET O	13.63	72.89	2.44	10.74
38 TRP N	12.89	74.17	0.74	10.87
38 TRP CA	13.29	73.20	-0.27	10.86
38 TRP CB	12.93	73.72	-1.67	11.05
38 TRP CG	13.34	72.77	-2.75	11.24
38 TRP CD2	12.78	71.48	-3.03	11.40
38 TRP CE2	13.54	70.91	-4.07	11.49
38 TRP CE3	11.71	70.75	-2.50	11.46
38 TRP CD1	14.38	72.93	-3.62	11.35
38 TRP NE1	14.52	71.81	-4.41	11.42
38 TRP CZ2	13.28	69.64	-4.59	11.61

38	TRP	CZ3	11.44	69.48	-3.02	11.61
38	TRP	CH2	12.22	68.94	-4.05	11.64
38	TRP	C	14.77	72.88	-0.19	10.73
38	TRP	O	15.20	71.78	-0.55	10.63
39	GLU	N	15.57	73.83	0.28	10.68
39	GLU	CA	17.00	73.60	0.39	10.72
39	GLU	CB	17.74	74.91	0.72	11.23
39	GLU	CG	17.73	75.91	-0.43	12.24
39	GLU	CD	18.18	75.30	-1.75	12.79
39	GLU	OE1	19.20	74.58	-1.76	13.14
39	GLU	OE2	17.51	75.53	-2.78	13.50
39	GLU	C	17.35	72.50	1.39	10.34
39	GLU	O	18.45	71.96	1.35	10.22
40	VAL	N	16.42	72.17	2.28	10.07
40	VAL	CA	16.65	71.09	3.24	9.83
40	VAL	CB	15.50	70.98	4.27	9.88
40	VAL	CG1	15.60	69.68	5.05	9.96
40	VAL	CG2	15.55	72.17	5.22	9.99
40	VAL	C	16.74	69.80	2.42	9.71
40	VAL	O	17.65	68.98	2.60	9.57
41	GLU	N	15.80	69.62	1.50	9.62
41	GLU	CA	15.77	68.45	0.63	9.69
41	GLU	CB	14.51	68.47	-0.23	9.62
41	GLU	CG	14.42	67.40	-1.32	9.47
41	GLU	CD	14.21	65.98	-0.79	9.33
41	GLU	OE1	13.94	65.81	0.42	9.36
41	GLU	OE2	14.31	65.04	-1.60	9.25
41	GLU	C	17.02	68.44	-0.25	9.78
41	GLU	O	17.65	67.39	-0.43	9.69
42	GLU	N	17.39	69.59	-0.80	9.95
42	GLU	CA	18.57	69.67	-1.65	10.21
42	GLU	CB	18.72	71.08	-2.24	10.72
42	GLU	CG	17.59	71.45	-3.19	11.61
42	GLU	CD	17.75	70.84	-4.58	12.08
42	GLU	OE1	18.43	69.81	-4.73	12.51
42	GLU	OE2	17.17	71.42	-5.52	12.70
42	GLU	C	19.84	69.29	-0.89	10.07
42	GLU	O	20.70	68.60	-1.43	9.90
43	TYR	N	19.95	69.74	0.35	9.99
43	TYR	CA	21.12	69.43	1.16	9.95
43	TYR	CB	21.04	70.15	2.51	10.35
43	TYR	CG	22.19	69.83	3.44	10.77
43	TYR	CD1	23.49	70.24	3.13	11.10

43	TYR	CE1	24.56	69.94	3.98	11.45
43	TYR	CD2	21.98	69.11	4.61	11.00
43	TYR	CE2	23.04	68.80	5.46	11.28
43	TYR	CZ	24.32	69.21	5.14	11.41
43	TYR	OH	25.36	68.90	5.99	11.81
43	TYR	C	21.24	67.92	1.39	9.72
43	TYR	O	22.32	67.34	1.24	9.56
44	VAL	N	20.14	67.28	1.76	9.59
44	VAL	CA	20.16	65.85	1.99	9.63
44	VAL	CB	18.82	65.36	2.58	9.59
44	VAL	CG1	18.82	63.84	2.71	9.75
44	VAL	CG2	18.59	66.00	3.95	9.71
44	VAL	C	20.49	65.11	0.70	9.61
44	VAL	O	21.28	64.16	0.71	9.46
45	ARG	N	19.91	65.53	-0.42	9.76
45	ARG	CA	20.20	64.88	-1.69	10.00
45	ARG	CB	19.36	65.49	-2.83	10.27
45	ARG	CG	17.88	65.19	-2.73	10.61
45	ARG	CD	17.15	65.58	-4.00	11.03
45	ARG	NE	15.74	65.19	-3.95	11.30
45	ARG	CZ	14.95	65.09	-5.01	11.53
45	ARG	NH1	15.41	65.34	-6.23	11.82
45	ARG	NH2	13.68	64.72	-4.85	11.71
45	ARG	C	21.68	65.03	-2.03	10.07
45	ARG	O	22.32	64.07	-2.48	9.97
46	ARG	N	22.23	66.22	-1.83	10.29
46	ARG	CA	23.63	66.46	-2.12	10.60
46	ARG	CB	23.99	67.93	-1.90	10.96
46	ARG	CG	25.48	68.22	-2.04	11.57
46	ARG	CD	25.76	69.71	-2.17	12.15
46	ARG	NE	25.54	70.46	-0.93	12.71
46	ARG	CZ	26.38	70.48	0.10	12.98
46	ARG	NH1	27.50	69.79	0.07	13.26
46	ARG	NH2	26.09	71.22	1.16	13.28
46	ARG	C	24.55	65.58	-1.27	10.61
46	ARG	O	25.47	64.96	-1.80	10.50
47	ARG	N	24.30	65.53	0.03	10.66
47	ARG	CA	25.13	64.72	0.91	10.86
47	ARG	CB	24.72	64.91	2.38	11.39
47	ARG	CG	25.00	66.30	2.97	12.17
47	ARG	CD	26.50	66.61	3.08	12.90
47	ARG	NE	27.24	65.66	3.91	13.49
47	ARG	CZ	27.12	65.54	5.23	13.94

47	ARG	NH1	26.29	66.32	5.92	14.29
47	ARG	NH2	27.85	64.64	5.87	14.19
47	ARG	C	25.04	63.24	0.53	10.71
47	ARG	O	26.05	62.53	0.54	10.57
48	CYS	N	23.84	62.77	0.17	10.69
48	CYS	CA	23.67	61.38	-0.23	10.74
48	CYS	CB	22.20	61.08	-0.52	10.75
48	CYS	SG	21.20	60.81	0.96	10.77
48	CYS	C	24.50	61.08	-1.47	10.86
48	CYS	O	25.15	60.04	-1.56	10.67
49	LYS	N	24.49	61.99	-2.43	11.07
49	LYS	CA	25.27	61.79	-3.65	11.50
49	LYS	CB	24.86	62.81	-4.72	11.73
49	LYS	CG	23.48	62.54	-5.30	12.10
49	LYS	CD	23.12	63.53	-6.40	12.58
49	LYS	CE	21.78	63.20	-7.04	13.00
49	LYS	NZ	21.83	61.95	-7.85	13.41
49	LYS	C	26.77	61.87	-3.37	11.63
49	LYS	O	27.56	61.15	-3.99	11.76
50	GLU	N	27.18	62.73	-2.44	11.82
50	GLU	CA	28.59	62.87	-2.12	12.09
50	GLU	CB	28.83	64.11	-1.25	12.47
50	GLU	CG	28.48	65.42	-1.94	13.13
50	GLU	CD	28.69	66.63	-1.05	13.46
50	GLU	OE1	28.64	66.48	0.19	13.90
50	GLU	OE2	28.89	67.74	-1.59	13.80
50	GLU	C	29.16	61.64	-1.40	12.04
50	GLU	O	30.32	61.27	-1.63	12.06
51	GLU	N	28.36	61.00	-0.55	11.99
51	GLU	CA	28.83	59.85	0.21	11.97
51	GLU	CB	28.47	60.03	1.69	12.48
51	GLU	CG	28.96	61.34	2.29	13.24
51	GLU	CD	30.45	61.57	2.07	13.67
51	GLU	OE1	31.21	60.59	2.13	14.03
51	GLU	OE2	30.85	62.73	1.84	14.15
51	GLU	C	28.32	58.49	-0.27	11.64
51	GLU	O	28.65	57.45	0.30	11.54
52	ASN	N	27.51	58.51	-1.32	11.27
52	ASN	CA	26.94	57.30	-1.92	10.99
52	ASN	CB	28.05	56.36	-2.40	11.09
52	ASN	CG	27.73	55.74	-3.76	11.19
52	ASN	OD1	27.39	56.46	-4.70	11.28
52	ASN	ND2	27.84	54.42	-3.86	11.27

52	ASN	C	25.94	56.54	-1.04	10.74
52	ASN	O	26.06	55.33	-0.82	10.77
53	PHE	N	24.94	57.28	-0.56	10.56
53	PHE	CA	23.86	56.74	0.25	10.50
53	PHE	CB	23.70	57.51	1.56	10.73
53	PHE	CG	24.59	57.05	2.66	11.04
53	PHE	CD1	25.95	57.34	2.65	11.25
53	PHE	CD2	24.06	56.34	3.73	11.30
53	PHE	CE1	26.77	56.93	3.69	11.50
53	PHE	CE2	24.88	55.93	4.78	11.58
53	PHE	CZ	26.23	56.22	4.76	11.60
53	PHE	C	22.56	56.91	-0.53	10.37
53	PHE	O	22.39	57.90	-1.24	10.34
54	LEU	N	21.65	55.96	-0.37	10.33
54	LEU	CA	20.36	56.06	-1.03	10.31
54	LEU	CB	19.82	54.68	-1.42	10.60
54	LEU	CG	20.31	54.01	-2.70	10.82
54	LEU	CD1	19.74	52.60	-2.77	11.07
54	LEU	CD2	19.89	54.82	-3.91	11.04
54	LEU	C	19.34	56.70	-0.10	10.18
54	LEU	O	19.30	56.40	1.09	9.97
55	PRO	N	18.52	57.61	-0.64	10.13
55	PRO	CD	18.69	58.27	-1.95	10.28
55	PRO	CA	17.47	58.27	0.14	10.05
55	PRO	CB	17.23	59.56	-0.63	10.24
55	PRO	CG	17.47	59.14	-2.05	10.41
55	PRO	C	16.32	57.26	0.03	9.92
55	PRO	O	15.52	57.32	-0.91	9.80
56	LEU	N	16.27	56.33	0.97	9.87
56	LEU	CA	15.30	55.25	0.95	9.88
56	LEU	CB	15.59	54.28	2.10	9.94
56	LEU	CG	16.97	53.62	2.07	9.97
56	LEU	CD1	17.14	52.71	3.27	10.21
56	LEU	CD2	17.16	52.82	0.78	10.09
56	LEU	C	13.82	55.60	0.92	9.85
56	LEU	O	13.00	54.76	0.55	9.79
57	GLN	N	13.46	56.83	1.29	9.87
57	GLN	CA	12.05	57.21	1.26	10.08
57	GLN	CB	11.81	58.48	2.06	10.49
57	GLN	CG	12.02	58.31	3.55	11.18
57	GLN	CD	11.77	59.58	4.33	11.73
57	GLN	OE1	12.10	59.65	5.51	12.28
57	GLN	NE2	11.19	60.58	3.67	12.12

57	GLN	C	11.54	57.41	-0.16	10.00
57	GLN	O	10.33	57.31	-0.39	9.89
58	ILE	N	12.42	57.71	-1.10	9.98
58	ILE	CA	11.97	57.92	-2.47	10.12
58	ILE	CB	13.07	58.56	-3.36	10.15
58	ILE	CG2	12.52	58.81	-4.76	10.27
58	ILE	CG1	13.54	59.87	-2.73	10.20
58	ILE	CD1	14.57	60.64	-3.55	10.31
58	ILE	C	11.52	56.60	-3.08	10.17
58	ILE	O	12.32	55.70	-3.33	10.24
59	GLY	N	10.21	56.49	-3.29	10.21
59	GLY	CA	9.65	55.27	-3.85	10.33
59	GLY	C	8.79	54.49	-2.88	10.34
59	GLY	O	8.21	53.47	-3.24	10.41
60	VAL	N	8.70	54.95	-1.63	10.31
60	VAL	CA	7.87	54.24	-0.65	10.38
60	VAL	CB	8.01	54.88	0.76	10.53
60	VAL	CG1	6.93	54.35	1.70	10.74
60	VAL	CG2	9.40	54.58	1.34	10.63
60	VAL	C	6.40	54.24	-1.08	10.30
60	VAL	O	5.88	55.28	-1.50	10.21
61	ASP	N	5.75	53.08	-1.00	10.34
61	ASP	CA	4.34	52.93	-1.38	10.43
61	ASP	CB	3.76	51.59	-0.87	10.62
61	ASP	CG	4.19	50.39	-1.69	10.82
61	ASP	OD1	4.86	50.52	-2.74	11.09
61	ASP	OD2	3.83	49.27	-1.25	11.02
61	ASP	C	3.43	54.01	-0.80	10.45
61	ASP	O	3.47	54.30	0.40	10.44
62	GLY	N	2.57	54.56	-1.66	10.46
62	GLY	CA	1.60	55.57	-1.26	10.51
62	GLY	C	0.38	55.36	-2.15	10.42
62	GLY	O	0.54	55.10	-3.34	10.43
63	ALA	N	-0.83	55.48	-1.60	10.45
63	ALA	CA	-2.05	55.25	-2.37	10.51
63	ALA	CB	-3.25	55.23	-1.43	10.64
63	ALA	C	-2.31	56.22	-3.52	10.54
63	ALA	O	-2.81	55.81	-4.57	10.52
64	MET	N	-2.00	57.49	-3.32	10.56
64	MET	CA	-2.21	58.48	-4.37	10.71
64	MET	CB	-2.64	59.82	-3.76	11.02
64	MET	CG	-3.92	59.74	-2.96	11.50
64	MET	SD	-4.57	61.33	-2.41	11.77

64 MET CE	-5.40	61.88	-3.91	12.10
64 MET C	-0.95	58.68	-5.20	10.59
64 MET O	-1.02	59.03	-6.38	10.57
65 MET N	0.19	58.44	-4.57	10.53
65 MET CA	1.49	58.59	-5.23	10.52
65 MET CB	1.76	60.08	-5.47	10.87
65 MET CG	1.84	60.90	-4.19	11.38
65 MET SD	1.72	62.69	-4.41	12.03
65 MET CE	3.35	63.06	-5.08	12.18
65 MET C	2.54	58.03	-4.29	10.27
65 MET O	2.36	58.03	-3.07	10.10
66 ASP N	3.64	57.52	-4.83	10.07
66 ASP CA	4.69	57.01	-3.97	9.94
66 ASP CB	5.67	56.13	-4.75	10.17
66 ASP CG	5.09	54.76	-5.06	10.26
66 ASP OD1	4.12	54.35	-4.37	10.27
66 ASP OD2	5.61	54.09	-5.97	10.50
66 ASP C	5.40	58.23	-3.38	9.79
66 ASP O	5.31	59.33	-3.94	9.84
67 TYR N	6.09	58.06	-2.26	9.61
67 TYR CA	6.76	59.21	-1.65	9.55
67 TYR CB	7.32	58.85	-0.28	9.34
67 TYR CG	7.58	60.10	0.52	9.11
67 TYR CD1	6.53	60.85	1.05	9.14
67 TYR CE1	6.75	62.08	1.66	8.99
67 TYR CD2	8.87	60.61	0.64	8.95
67 TYR CE2	9.10	61.84	1.25	8.82
67 TYR CZ	8.03	62.57	1.75	8.88
67 TYR OH	8.23	63.82	2.29	8.74
67 TYR C	7.88	59.68	-2.58	9.66
67 TYR O	8.75	58.90	-2.96	9.69
68 PRO N	7.90	60.97	-2.94	9.80
68 PRO CD	6.88	62.01	-2.73	9.99
68 PRO CA	8.94	61.46	-3.85	9.89
68 PRO CB	8.22	62.54	-4.67	10.14
68 PRO CG	6.80	62.63	-4.09	10.22
68 PRO C	10.23	62.03	-3.31	9.76
68 PRO O	11.17	62.24	-4.08	9.83
69 TYR N	10.31	62.25	-2.00	9.61
69 TYR CA	11.47	62.92	-1.45	9.48
69 TYR CB	11.00	64.23	-0.82	9.82
69 TYR CG	10.10	65.03	-1.75	10.26
69 TYR CD1	10.61	65.65	-2.88	10.51

69	TYR	CE1	9.79	66.38	-3.74	10.85
69	TYR	CD2	8.72	65.14	-1.50	10.51
69	TYR	CE2	7.89	65.86	-2.36	10.87
69	TYR	CZ	8.43	66.47	-3.48	10.98
69	TYR	OH	7.62	67.19	-4.33	11.40
69	TYR	C	12.35	62.17	-0.46	9.26
69	TYR	O	11.93	61.20	0.17	9.06
70	ALA	N	13.58	62.65	-0.32	9.11
70	ALA	CA	14.54	62.07	0.60	9.08
70	ALA	CB	15.92	62.65	0.35	9.09
70	ALA	C	14.10	62.38	2.04	9.03
70	ALA	O	14.30	61.57	2.95	9.03
71	THR	N	13.50	63.55	2.21	8.94
71	THR	CA	13.06	64.00	3.52	9.03
71	THR	CB	13.70	65.37	3.90	9.02
71	THR	OG1	13.14	66.40	3.06	9.06
71	THR	CG2	15.20	65.34	3.74	9.16
71	THR	C	11.57	64.23	3.65	8.95
71	THR	O	10.84	64.28	2.66	8.86
72	CYS	N	11.16	64.37	4.90	9.13
72	CYS	CA	9.80	64.74	5.26	9.21
72	CYS	CB	9.12	63.72	6.16	9.42
72	CYS	SG	8.58	62.24	5.31	9.76
72	CYS	C	10.08	66.02	6.05	9.17
72	CYS	O	10.90	66.02	6.97	9.29
73	CYS	N	9.43	67.10	5.65	9.11
73	CYS	CA	9.58	68.39	6.31	9.17
73	CYS	CB	10.12	69.44	5.33	9.40
73	CYS	SG	11.86	69.23	4.89	9.88
73	CYS	C	8.19	68.78	6.79	9.09
73	CYS	O	7.33	69.15	5.99	9.24
74	SER	N	7.98	68.68	8.10	9.04
74	SER	CA	6.69	68.98	8.70	9.04
74	SER	CB	6.25	67.79	9.54	8.93
74	SER	OG	6.17	66.62	8.72	8.79
74	SER	C	6.75	70.25	9.52	9.17
74	SER	O	7.42	70.33	10.56	9.04
75	LEU	N	6.03	71.25	9.03	9.46
75	LEU	CA	5.98	72.58	9.61	9.82
75	LEU	CB	5.91	73.58	8.46	10.54
75	LEU	CG	5.84	75.10	8.64	11.18
75	LEU	CD1	7.15	75.60	9.21	11.54
75	LEU	CD2	5.56	75.75	7.29	11.53

75 LEU C	4.83	72.84	10.57	9.75
75 LEU O	3.68	72.54	10.26	9.68
76 ASN N	5.15	73.39	11.73	9.69
76 ASN CA	4.17	73.78	12.73	9.64
76 ASN CB	3.58	75.13	12.30	9.71
76 ASN CG	4.67	76.19	12.15	9.72
76 ASN OD1	5.59	76.24	12.96	9.81
76 ASN ND2	4.57	77.03	11.12	9.97
76 ASN C	3.08	72.77	13.09	9.58
76 ASN O	3.35	71.84	13.85	9.51
77 ASP N	1.86	72.94	12.57	9.59
77 ASP CA	0.77	72.01	12.88	9.66
77 ASP CB	-0.60	72.68	12.70	10.11
77 ASP CG	-0.85	73.18	11.29	10.40
77 ASP OD1	0.12	73.56	10.61	11.01
77 ASP OD2	-2.03	73.21	10.87	10.73
77 ASP C	0.85	70.70	12.09	9.48
77 ASP O	0.04	69.80	12.30	9.48
78 GLU N	1.81	70.60	11.18	9.36
78 GLU CA	2.01	69.37	10.43	9.23
78 GLU CB	2.86	69.62	9.18	9.34
78 GLU CG	2.16	70.54	8.19	9.61
78 GLU CD	2.98	70.88	6.96	9.71
78 GLU OE1	4.22	70.71	6.99	9.73
78 GLU OE2	2.38	71.34	5.97	10.16
78 GLU C	2.71	68.42	11.39	9.16
78 GLU O	3.72	68.77	12.01	9.06
79 VAL N	2.16	67.22	11.52	9.06
79 VAL CA	2.67	66.22	12.44	9.09
79 VAL CB	1.51	65.28	12.86	9.20
79 VAL CG1	2.02	64.16	13.74	9.36
79 VAL CG2	0.44	66.08	13.57	9.32
79 VAL C	3.81	65.39	11.88	9.04
79 VAL O	4.84	65.20	12.54	8.97
80 ALA N	3.63	64.89	10.67	9.09
80 ALA CA	4.63	64.05	10.03	9.22
80 ALA CB	4.72	62.71	10.77	9.33
80 ALA C	4.26	63.80	8.58	9.33
80 ALA O	3.14	64.09	8.15	9.16
81 HIS N	5.23	63.28	7.83	9.58
81 HIS CA	5.06	62.91	6.43	9.91
81 HIS CB	3.99	61.81	6.34	10.63
81 HIS CG	4.28	60.61	7.18	11.50

81	HIS	CD2	5.40	60.21	7.83	11.88
81	HIS	ND1	3.33	59.65	7.44	12.00
81	HIS	CE1	3.85	58.70	8.20	12.05
81	HIS	NE2	5.11	59.02	8.45	12.09
81	HIS	C	4.74	64.01	5.42	9.68
81	HIS	O	4.28	63.72	4.32	9.75
82	ALA	N	4.98	65.26	5.79	9.53
82	ALA	CA	4.74	66.37	4.88	9.49
82	ALA	CB	4.46	67.65	5.66	9.49
82	ALA	C	5.97	66.55	3.98	9.47
82	ALA	O	7.09	66.16	4.34	9.34
83	PHE	N	5.76	67.15	2.81	9.71
83	PHE	CA	6.83	67.33	1.83	9.93
83	PHE	CB	6.29	67.46	0.40	10.21
83	PHE	CG	5.37	66.38	-0.08	10.50
83	PHE	CD1	5.48	65.06	0.35	10.63
83	PHE	CD2	4.46	66.68	-1.09	10.79
83	PHE	CE1	4.70	64.06	-0.23	10.81
83	PHE	CE2	3.67	65.70	-1.67	10.97
83	PHE	CZ	3.79	64.39	-1.25	10.99
83	PHE	C	7.71	68.56	1.94	9.98
83	PHE	O	7.28	69.62	2.39	9.86
84	PRO	N	8.97	68.42	1.50	10.05
84	PRO	CD	9.76	67.21	1.25	10.06
84	PRO	CA	9.82	69.61	1.53	10.16
84	PRO	CB	11.20	69.06	1.16	10.08
84	PRO	CG	10.90	67.75	0.45	10.04
84	PRO	C	9.16	70.36	0.36	10.30
84	PRO	O	8.64	69.72	-0.57	10.33
85	ARG	N	9.14	71.69	0.39	10.52
85	ARG	CA	8.48	72.45	-0.66	10.92
85	ARG	CB	6.98	72.54	-0.36	11.19
85	ARG	CG	6.66	73.55	0.75	11.49
85	ARG	CD	5.45	73.17	1.59	11.58
85	ARG	NE	5.74	72.06	2.50	11.59
85	ARG	CZ	5.09	71.82	3.63	11.44
85	ARG	NH1	4.09	72.61	4.00	11.59
85	ARG	NH2	5.43	70.79	4.39	11.31
85	ARG	C	9.07	73.85	-0.69	11.03
85	ARG	O	9.80	74.24	0.21	10.93
86	HIS	N	8.75	74.61	-1.74	11.28
86	HIS	CA	9.23	75.98	-1.82	11.59
86	HIS	CB	9.08	76.52	-3.24	12.02

86	HIS	CG	10.07	75.94	-4.20	12.51
86	HIS	CD2	9.90	75.19	-5.31	12.80
86	HIS	ND1	11.43	76.08	-4.03	12.66
86	HIS	CE1	12.06	75.43	-5.00	12.95
86	HIS	NE2	11.15	74.88	-5.79	13.10
86	HIS	C	8.41	76.80	-0.84	11.56
86	HIS	O	7.21	76.98	-1.00	11.75
87	TYR	N	9.10	77.27	0.19	11.47
87	TYR	CA	8.48	78.06	1.25	11.44
87	TYR	CB	7.75	77.13	2.23	11.38
87	TYR	CG	7.40	77.79	3.54	11.30
87	TYR	CD1	6.40	78.76	3.62	11.36
87	TYR	CE1	6.11	79.40	4.82	11.32
87	TYR	CD2	8.10	77.48	4.71	11.20
87	TYR	CE2	7.82	78.11	5.91	11.20
87	TYR	CZ	6.83	79.08	5.96	11.21
87	TYR	OH	6.55	79.72	7.14	11.19
87	TYR	C	9.61	78.77	1.99	11.41
87	TYR	O	10.57	78.13	2.41	11.37
88	ILE	N	9.51	80.08	2.12	11.50
88	ILE	CA	10.54	80.83	2.81	11.59
88	ILE	CB	10.53	82.31	2.38	11.84
88	ILE	CG2	11.59	83.09	3.14	11.91
88	ILE	CG1	10.77	82.40	0.86	12.04
88	ILE	CD1	12.04	81.72	0.38	12.32
88	ILE	C	10.31	80.71	4.32	11.50
88	ILE	O	9.31	81.20	4.85	11.40
89	LEU	N	11.24	80.05	4.99	11.42
89	LEU	CA	11.14	79.84	6.43	11.43
89	LEU	CB	12.36	79.06	6.93	11.43
89	LEU	CG	12.48	77.63	6.37	11.41
89	LEU	CD1	13.85	77.07	6.70	11.54
89	LEU	CD2	11.38	76.75	6.95	11.43
89	LEU	C	11.01	81.16	7.19	11.50
89	LEU	O	11.72	82.13	6.90	11.51
90	LYS	N	10.10	81.19	8.15	11.67
90	LYS	CA	9.85	82.38	8.95	11.94
90	LYS	CB	8.35	82.62	9.09	12.29
90	LYS	CG	7.59	82.83	7.79	12.79
90	LYS	CD	6.10	83.01	8.08	13.24
90	LYS	CE	5.28	83.11	6.81	13.63
90	LYS	NZ	5.69	84.26	5.97	13.91
90	LYS	C	10.43	82.25	10.35	11.89

90 LYS O	10.47	81.16	10.93	11.78
91 ASP N	10.87	83.38	10.90	11.98
91 ASP CA	11.40	83.41	12.25	12.05
91 ASP CB	11.85	84.83	12.60	12.62
91 ASP CG	12.77	84.87	13.80	13.09
91 ASP OD1	12.41	84.28	14.84	13.56
91 ASP OD2	13.84	85.49	13.70	13.74
91 ASP C	10.21	83.00	13.13	11.83
91 ASP O	9.16	83.64	13.10	12.01
92 GLY N	10.38	81.93	13.90	11.49
92 GLY CA	9.30	81.47	14.75	11.11
92 GLY C	8.72	80.13	14.33	10.82
92 GLY O	8.02	79.49	15.11	10.82
93 ASP N	9.02	79.71	13.10	10.51
93 ASP CA	8.53	78.43	12.59	10.25
93 ASP CB	8.86	78.25	11.10	10.19
93 ASP CG	7.87	78.94	10.18	10.10
93 ASP OD1	6.71	79.20	10.59	10.16
93 ASP OD2	8.25	79.19	9.01	10.09
93 ASP C	9.18	77.27	13.34	10.11
93 ASP O	10.29	77.39	13.88	10.12
94 LEU N	8.48	76.14	13.34	9.97
94 LEU CA	8.96	74.90	13.95	9.92
94 LEU CB	8.00	74.43	15.04	10.10
94 LEU CG	8.23	73.02	15.58	10.27
94 LEU CD1	9.63	72.90	16.18	10.53
94 LEU CD2	7.17	72.68	16.61	10.60
94 LEU C	8.97	73.89	12.80	9.74
94 LEU O	7.94	73.61	12.20	9.74
95 LEU N	10.15	73.35	12.51	9.64
95 LEU CA	10.29	72.41	11.40	9.52
95 LEU CB	11.20	73.01	10.33	10.05
95 LEU CG	11.42	72.18	9.06	10.56
95 LEU CD1	10.11	72.06	8.30	11.11
95 LEU CD2	12.47	72.84	8.18	10.82
95 LEU C	10.85	71.06	11.85	9.20
95 LEU O	11.94	71.00	12.42	9.16
96 LYS N	10.11	69.99	11.58	8.91
96 LYS CA	10.55	68.64	11.92	8.77
96 LYS CB	9.40	67.81	12.51	8.82
96 LYS CG	8.94	68.25	13.91	9.02
96 LYS CD	7.97	69.42	13.88	9.17
96 LYS CE	6.61	69.01	13.35	9.28

96	LYS	NZ	5.68	70.18	13.26	9.36
96	LYS	C	11.05	67.99	10.63	8.67
96	LYS	O	10.30	67.86	9.66	8.74
97	VAL	N	12.32	67.59	10.61	8.56
97	VAL	CA	12.91	66.97	9.43	8.53
97	VAL	CB	14.20	67.70	8.99	8.64
97	VAL	CG1	14.76	67.07	7.72	8.87
97	VAL	CG2	13.92	69.17	8.77	8.84
97	VAL	C	13.24	65.51	9.71	8.36
97	VAL	O	14.03	65.20	10.61	8.30
98	ASP	N	12.61	64.61	8.96	8.34
98	ASP	CA	12.82	63.17	9.11	8.38
98	ASP	CB	11.49	62.50	9.48	8.42
98	ASP	CG	11.66	61.12	10.13	8.44
98	ASP	OD1	12.77	60.54	10.09	8.33
98	ASP	OD2	10.67	60.61	10.68	8.63
98	ASP	C	13.35	62.64	7.78	8.39
98	ASP	O	13.07	63.20	6.71	8.48
99	MET	N	14.12	61.56	7.85	8.34
99	MET	CA	14.70	60.94	6.67	8.48
99	MET	CB	15.90	61.76	6.16	8.66
99	MET	CG	17.11	61.71	7.08	8.98
99	MET	SD	18.35	62.96	6.71	9.33
99	MET	CE	17.62	64.39	7.51	9.50
99	MET	C	15.16	59.53	7.01	8.49
99	MET	O	15.39	59.21	8.17	8.45
100	VAL	N	15.27	58.69	5.98	8.46
100	VAL	CA	15.73	57.32	6.14	8.61
100	VAL	CB	14.60	56.29	5.93	8.70
100	VAL	CG1	15.13	54.89	6.17	8.87
100	VAL	CG2	13.44	56.59	6.88	8.82
100	VAL	C	16.80	57.15	5.06	8.73
100	VAL	O	16.54	57.35	3.87	8.71
101	LEU	N	18.01	56.79	5.49	8.92
101	LEU	CA	19.14	56.65	4.58	9.17
101	LEU	CB	20.20	57.71	4.92	9.45
101	LEU	CG	19.70	59.14	5.14	9.76
101	LEU	CD1	20.85	60.01	5.59	10.04
101	LEU	CD2	19.08	59.69	3.86	10.01
101	LEU	C	19.78	55.27	4.63	9.24
101	LEU	O	19.88	54.67	5.70	9.19
102	GLY	N	20.21	54.79	3.47	9.31
102	GLY	CA	20.85	53.49	3.39	9.54

102	GLY	C	22.20	53.57	2.70	9.75
102	GLY	O	22.31	54.08	1.59	9.71
103	GLY	N	23.23	53.06	3.37	9.94
103	GLY	CA	24.56	53.09	2.80	10.39
103	GLY	C	25.63	52.91	3.86	10.70
103	GLY	O	25.30	52.59	5.00	10.73
104	PRO	N	26.91	53.12	3.52	10.98
104	PRO	CD	28.04	53.01	4.45	11.14
104	PRO	CA	27.37	53.51	2.18	11.32
104	PRO	CB	28.77	54.02	2.45	11.31
104	PRO	CG	29.24	53.09	3.52	11.26
104	PRO	C	27.35	52.35	1.20	11.55
104	PRO	O	27.67	51.22	1.56	11.68
105	ILE	N	26.97	52.64	-0.04	11.82
105	ILE	CA	26.92	51.62	-1.07	12.14
105	ILE	CB	25.73	51.89	-2.02	12.29
105	ILE	CG2	25.76	50.94	-3.21	12.38
105	ILE	CG1	24.42	51.74	-1.23	12.45
105	ILE	CD1	23.23	52.38	-1.90	12.56
105	ILE	C	28.23	51.62	-1.86	12.23
105	ILE	O	28.84	52.67	-2.05	12.08
106	ALA	N	28.65	50.44	-2.30	12.53
106	ALA	CA	29.89	50.32	-3.08	12.97
106	ALA	CB	30.15	48.86	-3.42	13.00
106	ALA	C	29.76	51.15	-4.35	13.34
106	ALA	O	28.85	50.94	-5.15	13.16
107	LYS	N	30.69	52.08	-4.52	13.94
107	LYS	CA	30.71	52.98	-5.67	14.61
107	LYS	CB	31.97	53.85	-5.62	15.02
107	LYS	CG	31.97	55.06	-6.54	15.57
107	LYS	CD	31.02	56.14	-6.04	16.00
107	LYS	CE	31.16	57.41	-6.87	16.19
107	LYS	NZ	30.30	58.51	-6.37	16.45
107	LYS	C	30.66	52.23	-7.00	14.81
107	LYS	O	29.99	52.67	-7.94	14.99
108	SER	N	31.36	51.11	-7.08	14.96
108	SER	CA	31.40	50.32	-8.31	15.12
108	SER	CB	32.61	49.40	-8.30	15.29
108	SER	OG	32.67	48.64	-7.11	15.62
108	SER	C	30.13	49.51	-8.58	15.11
108	SER	O	29.97	48.95	-9.66	15.15
109	ASP	N	29.23	49.45	-7.60	15.11
109	ASP	CA	27.98	48.72	-7.77	15.20

109	ASP	CB	27.60	47.96	-6.50	15.13
109	ASP	CG	28.53	46.80	-6.21	15.05
109	ASP	OD1	29.28	46.39	-7.13	14.76
109	ASP	OD2	28.50	46.27	-5.08	15.20
109	ASP	C	26.86	49.68	-8.14	15.28
109	ASP	O	26.01	49.37	-8.98	15.36
110	LEU	N	26.85	50.85	-7.51	15.38
110	LEU	CA	25.83	51.85	-7.77	15.44
110	LEU	CB	24.59	51.56	-6.91	15.65
110	LEU	CG	23.30	52.32	-7.23	15.83
110	LEU	CD1	22.78	51.88	-8.59	15.95
110	LEU	CD2	22.26	52.05	-6.16	15.98
110	LEU	C	26.36	53.24	-7.45	15.37
110	LEU	O	26.68	53.53	-6.30	15.41
111	ASN	N	26.47	54.09	-8.47	15.23
111	ASN	CA	26.95	55.45	-8.28	15.11
111	ASN	CB	27.72	55.94	-9.51	15.42
111	ASN	CG	28.43	57.25	-9.26	15.67
111	ASN	OD1	27.93	58.11	-8.54	15.83
111	ASN	ND2	29.61	57.42	-9.86	15.96
111	ASN	C	25.73	56.34	-8.06	14.84
111	ASN	O	25.08	56.77	-9.01	14.71
112	VAL	N	25.44	56.62	-6.80	14.60
112	VAL	CA	24.29	57.44	-6.44	14.38
112	VAL	CB	24.20	57.58	-4.90	14.32
112	VAL	CG1	23.01	58.44	-4.52	14.25
112	VAL	CG2	24.08	56.19	-4.26	14.29
112	VAL	C	24.26	58.82	-7.09	14.34
112	VAL	O	23.19	59.33	-7.42	14.15
113	SER	N	25.43	59.42	-7.31	14.39
113	SER	CA	25.47	60.74	-7.93	14.57
113	SER	CB	26.90	61.30	-7.91	14.67
113	SER	OG	27.75	60.59	-8.78	14.92
113	SER	C	24.95	60.71	-9.37	14.60
113	SER	O	24.57	61.74	-9.92	14.74
114	LYS	N	24.94	59.53	-9.98	14.56
114	LYS	CA	24.47	59.38	-11.35	14.56
114	LYS	CB	25.45	58.55	-12.17	14.85
114	LYS	CG	26.77	59.26	-12.42	15.26
114	LYS	CD	27.71	58.38	-13.22	15.56
114	LYS	CE	29.04	59.07	-13.44	15.75
114	LYS	NZ	29.98	58.16	-14.14	15.96
114	LYS	C	23.08	58.77	-11.44	14.37

114	LYS	O	22.64	58.36	-12.52	14.47
115	LEU	N	22.39	58.70	-10.31	14.06
115	LEU	CA	21.03	58.17	-10.28	13.80
115	LEU	CB	20.76	57.41	-8.98	13.93
115	LEU	CG	21.61	56.17	-8.70	14.04
115	LEU	CD1	21.13	55.52	-7.41	14.10
115	LEU	CD2	21.51	55.20	-9.86	14.12
115	LEU	C	20.10	59.37	-10.38	13.57
115	LEU	O	20.43	60.46	-9.93	13.48
116	ASN	N	18.93	59.16	-10.98	13.35
116	ASN	CA	17.97	60.24	-11.12	13.20
116	ASN	CB	17.26	60.13	-12.47	13.27
116	ASN	CG	16.22	61.21	-12.66	13.33
116	ASN	OD1	16.14	62.15	-11.88	13.34
116	ASN	ND2	15.42	61.08	-13.72	13.44
116	ASN	C	16.95	60.21	-9.99	13.07
116	ASN	O	15.97	59.47	-10.04	12.97
117	PHE	N	17.19	61.02	-8.96	12.93
117	PHE	CA	16.31	61.08	-7.80	12.85
117	PHE	CB	16.88	62.04	-6.75	12.73
117	PHE	CG	18.07	61.50	-5.98	12.57
117	PHE	CD1	18.70	60.31	-6.34	12.61
117	PHE	CD2	18.55	62.20	-4.88	12.63
117	PHE	CE1	19.80	59.84	-5.61	12.60
117	PHE	CE2	19.64	61.74	-4.15	12.63
117	PHE	CZ	20.27	60.56	-4.51	12.51
117	PHE	C	14.89	61.53	-8.15	12.94
117	PHE	O	13.96	61.27	-7.39	12.85
118	ASN	N	14.74	62.20	-9.29	13.08
118	ASN	CA	13.42	62.69	-9.70	13.25
118	ASN	CB	13.56	63.90	-10.63	13.52
118	ASN	CG	14.01	65.14	-9.89	13.76
118	ASN	OD1	13.76	65.30	-8.70	13.95
118	ASN	ND2	14.67	66.05	-10.61	14.10
118	ASN	C	12.55	61.63	-10.37	13.26
118	ASN	O	11.37	61.87	-10.60	13.29
119	ASN	N	13.14	60.49	-10.70	13.28
119	ASN	CA	12.38	59.41	-11.32	13.31
119	ASN	CB	13.23	58.65	-12.33	13.60
119	ASN	CG	12.45	57.59	-13.09	13.77
119	ASN	OD1	11.46	57.05	-12.58	13.93
119	ASN	ND2	12.89	57.27	-14.30	13.98
119	ASN	C	11.99	58.48	-10.18	13.19

119 ASN O	12.73	57.56	-9.83	13.04
120 VAL N	10.83	58.73	-9.58	13.16
120 VAL CA	10.37	57.93	-8.45	13.16
120 VAL CB	9.05	58.49	-7.88	13.13
120 VAL CG1	8.61	57.68	-6.68	13.13
120 VAL CG2	9.25	59.95	-7.49	13.18
120 VAL C	10.21	56.45	-8.80	13.24
120 VAL O	10.56	55.58	-8.01	13.11
121 GLU N	9.70	56.17	-10.00	13.43
121 GLU CA	9.50	54.79	-10.45	13.74
121 GLU CB	8.87	54.80	-11.84	14.20
121 GLU CG	8.75	53.44	-12.50	14.95
121 GLU CD	8.17	53.53	-13.90	15.35
121 GLU OE1	6.98	53.89	-14.02	15.68
121 GLU OE2	8.90	53.25	-14.87	15.83
121 GLU C	10.81	54.01	-10.47	13.63
121 GLU O	10.87	52.86	-10.03	13.65
122 GLN N	11.87	54.63	-10.98	13.58
122 GLN CA	13.17	53.96	-11.03	13.52
122 GLN CB	14.10	54.68	-12.01	13.95
122 GLN CG	15.49	54.07	-12.12	14.62
122 GLN CD	15.46	52.60	-12.51	14.97
122 GLN OE1	14.90	52.23	-13.53	15.38
122 GLN NE2	16.08	51.76	-11.68	15.26
122 GLN C	13.81	53.91	-9.65	13.21
122 GLN O	14.38	52.89	-9.26	13.21
123 MET N	13.72	55.01	-8.90	12.90
123 MET CA	14.29	55.03	-7.56	12.67
123 MET CB	14.09	56.40	-6.90	12.51
123 MET CG	14.97	57.51	-7.47	12.35
123 MET SD	16.75	57.16	-7.33	12.05
123 MET CE	16.98	57.34	-5.54	12.42
123 MET C	13.68	53.94	-6.69	12.60
123 MET O	14.37	53.33	-5.87	12.50
124 LYS N	12.39	53.68	-6.87	12.60
124 LYS CA	11.68	52.65	-6.11	12.69
124 LYS CB	10.24	52.54	-6.59	12.52
124 LYS CG	9.36	51.61	-5.76	12.32
124 LYS CD	8.01	51.42	-6.43	12.17
124 LYS CE	6.98	50.79	-5.49	11.98
124 LYS NZ	6.48	51.77	-4.49	11.91
124 LYS C	12.38	51.30	-6.27	12.87
124 LYS O	12.47	50.53	-5.32	12.79

	125 LYS N	12.87	51.03	-7.47	13.18
	125 LYS CA	13.55	49.77	-7.74	13.55
	125 LYS CB	13.91	49.66	-9.23	13.97
	125 LYS CG	12.71	49.63	-10.16	14.55
5	125 LYS CD	13.15	49.48	-11.61	15.02
	125 LYS CE	11.97	49.52	-12.56	15.38
	125 LYS NZ	11.03	48.39	-12.34	15.77
	125 LYS C	14.81	49.63	-6.89	13.51
	125 LYS O	15.15	48.53	-6.45	13.71
10	126 TYR N	15.50	50.74	-6.66	13.39
	126 TYR CA	16.71	50.74	-5.86	13.37
	126 TYR CB	17.57	51.97	-6.16	13.49
	126 TYR CG	18.07	52.10	-7.58	13.69
	126 TYR CD1	18.82	51.08	-8.17	13.83
15	126 TYR CE1	19.33	51.22	-9.45	14.02
	126 TYR CD2	17.84	53.26	-8.31	13.79
	126 TYR CE2	18.35	53.41	-9.59	13.97
	126 TYR CZ	19.10	52.39	-10.16	14.00
	126 TYR OH	19.62	52.54	-11.42	14.25
20	126 TYR C	16.44	50.75	-4.35	13.31
	126 TYR O	17.02	49.96	-3.60	13.26
	127 THR N	15.57	51.66	-3.92	13.31
	127 THR CA	15.28	51.82	-2.51	13.40
	127 THR CB	14.58	53.17	-2.25	13.17
25	127 THR OG1	13.30	53.17	-2.89	12.85
	127 THR CG2	15.42	54.31	-2.80	13.12
	127 THR C	14.45	50.73	-1.84	13.70
	127 THR O	14.74	50.33	-0.71	13.71
	128 GLN N	13.43	50.24	-2.53	14.09
30	128 GLN CA	12.57	49.23	-1.95	14.59
	128 GLN CB	11.14	49.41	-2.48	14.66
	128 GLN CG	10.66	50.88	-2.43	14.80
	128 GLN CD	10.73	51.49	-1.04	14.81
	128 GLN OE1	10.02	51.07	-0.12	14.89
35	128 GLN NE2	11.59	52.50	-0.88	14.86
	128 GLN C	13.08	47.80	-2.18	14.81
	128 GLN O	12.32	46.84	-2.06	15.04
	129 SER N	14.36	47.69	-2.50	14.94
	129 SER CA	15.02	46.40	-2.73	14.97
40	129 SER CB	15.19	46.12	-4.23	15.26
	129 SER OG	16.18	46.96	-4.80	15.90
	129 SER C	16.41	46.46	-2.07	14.69
	129 SER O	17.19	45.52	-2.16	14.85

130	TYR	N	16.68	47.59	-1.41	14.25
130	TYR	CA	17.95	47.81	-0.74	13.73
130	TYR	CB	18.00	49.25	-0.19	13.33
130	TYR	CG	19.21	49.53	0.66	12.81
130	TYR	CD1	20.46	49.72	0.07	12.65
130	TYR	CE1	21.59	49.95	0.85	12.38
130	TYR	CD2	19.12	49.58	2.05	12.58
130	TYR	CE2	20.24	49.80	2.84	12.30
130	TYR	CZ	21.48	49.98	2.23	12.22
130	TYR	OH	22.60	50.19	3.00	11.91
130	TYR	C	18.24	46.84	0.40	13.56
130	TYR	O	17.35	46.50	1.18	13.58
131	SER	N	19.49	46.40	0.50	13.36
131	SER	CA	19.91	45.49	1.55	13.18
131	SER	CB	20.16	44.09	1.00	13.41
131	SER	OG	20.52	43.19	2.04	13.96
131	SER	C	21.20	46.05	2.15	12.83
131	SER	O	22.20	46.22	1.45	12.97
132	GLY	N	21.18	46.33	3.45	12.41
132	GLY	CA	22.36	46.86	4.10	11.86
132	GLY	C	21.99	47.77	5.25	11.44
132	GLY	O	20.83	47.85	5.65	11.38
133	GLY	N	23.00	48.46	5.78	11.05
133	GLY	CA	22.75	49.35	6.89	10.65
133	GLY	C	21.84	50.51	6.53	10.35
133	GLY	O	21.95	51.09	5.45	10.18
134	LEU	N	20.92	50.84	7.43	10.20
134	LEU	CA	20.02	51.95	7.22	10.11
134	LEU	CB	18.74	51.52	6.49	10.59
134	LEU	CG	17.67	50.71	7.23	11.09
134	LEU	CD1	16.41	50.65	6.39	11.43
134	LEU	CD2	18.18	49.31	7.52	11.43
134	LEU	C	19.68	52.58	8.56	9.79
134	LEU	O	19.74	51.92	9.61	9.82
135	ALA	N	19.33	53.86	8.52	9.46
135	ALA	CA	18.98	54.61	9.72	9.24
135	ALA	CB	20.18	55.40	10.20	9.59
135	ALA	C	17.80	55.53	9.45	8.99
135	ALA	O	17.60	56.01	8.33	8.78
136	ASP	N	17.05	55.79	10.52	8.80
136	ASP	CA	15.84	56.59	10.49	8.77
136	ASP	CB	14.66	55.61	10.59	9.03
136	ASP	CG	13.31	56.29	10.75	9.23

136	ASP	OD1	12.31	55.55	10.93	9.96
136	ASP	OD2	13.24	57.53	10.69	9.15
136	ASP	C	15.85	57.54	11.70	8.70
136	ASP	O	15.96	57.09	12.83	8.63
137	SER	N	15.77	58.85	11.45	8.61
137	SER	CA	15.73	59.81	12.56	8.68
137	SER	CB	17.12	59.99	13.19	8.66
137	SER	OG	17.10	61.03	14.17	8.77
137	SER	C	15.17	61.18	12.23	8.73
137	SER	O	15.69	61.90	11.37	8.86
138	CYS	N	14.10	61.53	12.94	8.95
138	CYS	CA	13.46	62.83	12.80	8.88
138	CYS	CB	11.96	62.71	13.04	9.06
138	CYS	SG	11.06	64.28	12.96	8.93
138	CYS	C	14.04	63.74	13.89	8.88
138	CYS	O	14.20	63.31	15.03	8.82
139	TRP	N	14.40	64.97	13.53	8.87
139	TRP	CA	14.88	65.92	14.53	8.96
139	TRP	CB	16.40	66.13	14.46	9.16
139	TRP	CG	16.97	66.42	15.84	9.27
139	TRP	CD2	17.03	65.50	16.94	9.35
139	TRP	CE2	17.51	66.22	18.06	9.39
139	TRP	CE3	16.72	64.14	17.09	9.43
139	TRP	CD1	17.41	67.62	16.32	9.45
139	TRP	NE1	17.74	67.51	17.65	9.45
139	TRP	CZ2	17.68	65.62	19.31	9.52
139	TRP	CZ3	16.89	63.55	18.33	9.48
139	TRP	CH2	17.37	64.29	19.42	9.52
139	TRP	C	14.13	67.23	14.28	8.94
139	TRP	O	13.82	67.57	13.13	8.90
140	ALA	N	13.82	67.95	15.35	9.04
140	ALA	CA	13.07	69.20	15.26	9.25
140	ALA	CB	12.02	69.26	16.36	9.27
140	ALA	C	13.97	70.42	15.33	9.44
140	ALA	O	14.96	70.43	16.07	9.50
141	TYR	N	13.59	71.45	14.58	9.66
141	TYR	CA	14.34	72.70	14.51	10.07
141	TYR	CB	15.02	72.83	13.14	10.02
141	TYR	CG	16.00	71.73	12.85	9.93
141	TYR	CD1	15.57	70.49	12.37	9.82
141	TYR	CE1	16.47	69.45	12.17	9.75
141	TYR	CD2	17.35	71.91	13.12	9.96
141	TYR	CE2	18.26	70.89	12.93	9.90

141 TYR CZ	17.82	69.66	12.46	9.81
141 TYR OH	18.72	68.64	12.31	9.93
141 TYR C	13.49	73.93	14.72	10.38
141 TYR O	12.40	74.05	14.15	10.33
142 ALA N	13.99	74.85	15.53	10.80
142 ALA CA	13.31	76.11	15.76	11.26
142 ALA CB	13.54	76.59	17.19	11.40
142 ALA C	13.95	77.08	14.77	11.58
142 ALA O	15.17	77.25	14.77	11.70
143 VAL N	13.14	77.68	13.90	11.93
143 VAL CA	13.66	78.63	12.93	12.34
143 VAL CB	12.73	78.75	11.71	12.36
143 VAL CG1	13.32	79.72	10.69	12.51
143 VAL CG2	12.54	77.37	11.08	12.44
143 VAL C	13.77	79.99	13.61	12.59
143 VAL O	12.77	80.52	14.10	12.55
144 GLY N	14.97	80.54	13.65	12.98
144 GLY CA	15.16	81.82	14.30	13.52
144 GLY C	14.93	81.69	15.80	13.88
144 GLY O	15.43	80.76	16.43	14.06
145 THR N	14.15	82.61	16.36	14.21
145 THR CA	13.85	82.58	17.78	14.53
145 THR CB	13.96	83.99	18.39	14.71
145 THR OG1	15.27	84.52	18.15	15.01
145 THR CG2	13.70	83.95	19.89	14.89
145 THR C	12.44	82.04	18.01	14.55
145 THR O	11.46	82.67	17.63	14.71
146 PRO N	12.33	80.86	18.63	14.52
146 PRO CD	13.39	79.95	19.09	14.57
146 PRO CA	11.01	80.28	18.88	14.42
146 PRO CB	11.33	78.82	19.16	14.52
146 PRO CG	12.62	78.92	19.91	14.55
146 PRO C	10.33	80.95	20.07	14.25
146 PRO O	10.99	81.51	20.93	14.25
147 SER N	9.00	80.90	20.11	14.07
147 SER CA	8.28	81.46	21.24	13.80
147 SER CB	6.78	81.49	20.97	14.00
147 SER OG	6.26	80.17	20.91	14.19
147 SER C	8.59	80.48	22.37	13.53
147 SER O	9.00	79.35	22.11	13.29
148 GLU N	8.41	80.90	23.62	13.32
148 GLU CA	8.70	80.00	24.73	13.24
148 GLU CB	8.60	80.75	26.05	13.36

148	GLU	CG	9.68	81.81	26.20	13.61
148	GLU	CD	9.57	82.59	27.49	13.71
148	GLU	OE1	9.71	81.98	28.57	13.78
148	GLU	OE2	9.33	83.81	27.42	13.92
148	GLU	C	7.76	78.80	24.70	13.12
148	GLU	O	8.15	77.70	25.10	12.97
149	GLU	N	6.54	79.00	24.21	13.11
149	GLU	CA	5.58	77.90	24.14	13.19
149	GLU	CB	4.21	78.42	23.72	13.76
149	GLU	CG	3.07	77.48	24.09	14.60
149	GLU	CD	1.71	77.99	23.65	15.03
149	GLU	OE1	1.52	79.22	23.57	15.47
149	GLU	OE2	0.82	77.14	23.39	15.52
149	GLU	C	6.08	76.87	23.12	12.86
149	GLU	O	5.97	75.67	23.34	12.69
150	VAL	N	6.63	77.35	22.01	12.58
150	VAL	CA	7.16	76.45	21.00	12.30
150	VAL	CB	7.58	77.22	19.72	12.37
150	VAL	CG1	8.42	76.32	18.82	12.52
150	VAL	CG2	6.34	77.69	18.97	12.53
150	VAL	C	8.36	75.68	21.54	12.02
150	VAL	O	8.47	74.47	21.34	11.87
151	LYS	N	9.26	76.37	22.24	11.83
151	LYS	CA	10.43	75.69	22.78	11.72
151	LYS	CB	11.46	76.69	23.32	12.26
151	LYS	CG	12.82	76.06	23.63	12.99
151	LYS	CD	13.45	75.41	22.40	13.68
151	LYS	CE	14.77	74.73	22.75	14.14
151	LYS	NZ	15.36	74.02	21.59	14.71
151	LYS	C	10.03	74.69	23.86	11.35
151	LYS	O	10.66	73.65	24.00	11.14
152	ASN	N	8.99	75.00	24.63	11.06
152	ASN	CA	8.52	74.08	25.66	10.82
152	ASN	CB	7.36	74.67	26.47	11.13
152	ASN	CG	7.82	75.47	27.67	11.31
152	ASN	OD1	8.96	75.34	28.12	11.60
152	ASN	ND2	6.92	76.28	28.21	11.53
152	ASN	C	8.05	72.79	24.99	10.55
152	ASN	O	8.35	71.69	25.46	10.40
153	LEU	N	7.31	72.93	23.90	10.32
153	LEU	CA	6.81	71.77	23.16	10.12
153	LEU	CB	5.97	72.22	21.97	10.23
153	LEU	CG	5.61	71.14	20.95	10.34

153 LEU CD1	4.71	70.09	21.57	10.49
153 LEU CD2	4.93	71.78	19.75	10.48
153 LEU C	7.99	70.93	22.68	9.96
153 LEU O	7.97	69.70	22.80	9.73
154 MET N	9.01	71.59	22.13	9.91
154 MET CA	10.18	70.88	21.64	9.97
154 MET CB	11.18	71.86	21.02	10.08
154 MET CG	10.70	72.52	19.73	10.30
154 MET SD	11.82	73.80	19.12	10.24
154 MET CE	13.20	72.80	18.54	10.71
154 MET C	10.87	70.11	22.76	9.93
154 MET O	11.15	68.92	22.63	9.72
155 ASP N	11.12	70.79	23.88	10.03
155 ASP CA	11.79	70.14	25.00	10.21
155 ASP CB	12.08	71.16	26.11	10.64
155 ASP CG	13.20	72.12	25.74	10.98
155 ASP OD1	13.82	71.95	24.67	11.30
155 ASP OD2	13.46	73.05	26.54	11.42
155 ASP C	10.99	68.98	25.57	10.13
155 ASP O	11.56	67.94	25.90	10.06
156 VAL N	9.68	69.15	25.70	10.11
156 VAL CA	8.84	68.08	26.23	10.17
156 VAL CB	7.38	68.56	26.44	10.38
156 VAL CG1	6.47	67.37	26.73	10.79
156 VAL CG2	7.32	69.55	27.59	10.71
156 VAL C	8.86	66.87	25.31	9.96
156 VAL O	8.95	65.73	25.77	9.93
157 THR N	8.79	67.11	24.00	9.79
157 THR CA	8.81	66.02	23.04	9.63
157 THR CB	8.59	66.55	21.61	9.54
157 THR OG1	7.35	67.27	21.56	9.58
157 THR CG2	8.55	65.41	20.61	9.60
157 THR C	10.14	65.27	23.09	9.60
157 THR O	10.17	64.03	23.11	9.51
158 LYS N	11.23	66.01	23.13	9.74
158 LYS CA	12.55	65.40	23.17	9.93
158 LYS CB	13.63	66.48	23.03	10.23
158 LYS CG	15.04	65.90	22.88	10.73
158 LYS CD	16.06	66.98	22.58	11.25
158 LYS CE	16.24	67.93	23.75	11.60
158 LYS NZ	17.11	69.09	23.37	11.97
158 LYS C	12.77	64.60	24.46	9.94
158 LYS O	13.29	63.49	24.42	9.78

159 GLU N	12.38	65.17	25.59	10.09
159 GLU CA	12.56	64.46	26.86	10.37
159 GLU CB	12.29	65.39	28.04	10.95
159 GLU CG	12.54	64.76	29.41	12.07
159 GLU CD	13.92	64.13	29.56	12.62
159 GLU OE1	14.87	64.60	28.91	13.15
159 GLU OE2	14.04	63.16	30.34	13.36
159 GLU C	11.65	63.24	26.91	10.14
159 GLU O	12.04	62.20	27.46	10.08
160 ALA N	10.45	63.34	26.35	10.00
160 ALA CA	9.54	62.20	26.33	9.82
160 ALA CB	8.22	62.59	25.68	9.95
160 ALA C	10.21	61.07	25.56	9.68
160 ALA O	10.13	59.90	25.95	9.59
161 MET N	10.87	61.41	24.45	9.62
161 MET CA	11.56	60.41	23.65	9.58
161 MET CB	12.22	61.06	22.43	9.65
161 MET CG	13.08	60.09	21.62	9.78
161 MET SD	14.20	60.91	20.46	9.87
161 MET CE	15.26	61.81	21.61	10.09
161 MET C	12.63	59.72	24.49	9.52
161 MET O	12.71	58.49	24.52	9.37
162 TYR N	13.46	60.51	25.18	9.65
162 TYR CA	14.52	59.92	26.00	9.90
162 TYR CB	15.47	61.01	26.50	10.02
162 TYR CG	16.46	61.47	25.44	10.22
162 TYR CD1	17.38	60.58	24.88	10.36
162 TYR CE1	18.29	61.00	23.91	10.49
162 TYR CD2	16.48	62.79	25.00	10.35
162 TYR CE2	17.39	63.22	24.03	10.60
162 TYR CZ	18.29	62.32	23.49	10.53
162 TYR OH	19.19	62.74	22.54	10.72
162 TYR C	13.96	59.10	27.16	9.97
162 TYR O	14.57	58.11	27.56	9.95
163 LYS N	12.80	59.50	27.69	10.15
163 LYS CA	12.17	58.74	28.77	10.33
163 LYS CB	10.93	59.47	29.29	10.83
163 LYS CG	11.22	60.67	30.17	11.56
163 LYS CD	11.79	60.26	31.52	12.21
163 LYS CE	11.99	61.46	32.42	12.68
163 LYS NZ	12.50	61.05	33.76	13.19
163 LYS C	11.77	57.37	28.22	10.16
163 LYS O	11.86	56.35	28.91	10.24

164 GLY N	11.31	57.36	26.97	10.06
164 GLY CA	10.92	56.11	26.34	10.01
164 GLY C	12.13	55.22	26.11	9.95
164 GLY O	12.10	54.02	26.40	9.88
165 ILE N	13.20	55.80	25.58	10.06
165 ILE CA	14.41	55.04	25.30	10.27
165 ILE CB	15.48	55.94	24.62	10.27
165 ILE CG2	16.79	55.18	24.47	10.42
165 ILE CG1	14.96	56.41	23.26	10.26
165 ILE CD1	15.86	57.41	22.55	10.34
165 ILE C	14.98	54.41	26.57	10.46
165 ILE O	15.46	53.28	26.55	10.39
166 GLU N	14.89	55.14	27.68	10.85
166 GLU CA	15.39	54.65	28.96	11.33
166 GLU CB	15.18	55.72	30.03	12.06
166 GLU CG	15.56	55.31	31.44	13.23
166 GLU CD	15.44	56.47	32.41	13.85
166 GLU OE1	14.34	57.06	32.49	14.29
166 GLU OE2	16.44	56.78	33.08	14.48
166 GLU C	14.71	53.34	29.39	11.21
166 GLU O	15.30	52.52	30.09	11.16
167 GLN N	13.47	53.16	28.95	11.18
167 GLN CA	12.70	51.96	29.28	11.30
167 GLN CB	11.20	52.26	29.22	11.48
167 GLN CG	10.70	53.24	30.25	11.91
167 GLN CD	10.87	52.72	31.66	12.19
167 GLN OE1	10.61	51.54	31.93	12.44
167 GLN NE2	11.30	53.58	32.57	12.53
167 GLN C	12.99	50.78	28.36	11.29
167 GLN O	12.55	49.66	28.63	11.23
168 ALA N	13.72	51.03	27.28	11.32
168 ALA CA	14.03	49.98	26.31	11.53
168 ALA CB	14.30	50.61	24.94	11.49
168 ALA C	15.21	49.11	26.73	11.71
168 ALA O	16.27	49.13	26.10	11.72
169 VAL N	15.00	48.34	27.79	11.97
169 VAL CA	16.03	47.45	28.31	12.38
169 VAL CB	16.37	47.78	29.78	12.47
169 VAL CG1	16.94	49.19	29.88	12.59
169 VAL CG2	15.13	47.64	30.66	12.56
169 VAL C	15.56	46.00	28.23	12.64
169 VAL O	14.36	45.72	28.23	12.60
170 VAL N	16.51	45.07	28.15	12.98

170 VAL CA	16.19	43.65	28.07	13.37
170 VAL CB	17.47	42.78	28.14	13.53
170 VAL CG1	17.09	41.30	28.18	13.74
170 VAL CG2	18.36	43.07	26.95	13.67
170 VAL C	15.28	43.28	29.22	13.50
170 VAL O	15.53	43.65	30.37	13.53
171 GLY N	14.22	42.55	28.93	13.57
171 GLY CA	13.31	42.15	29.98	13.52
171 GLY C	12.11	43.06	30.14	13.33
171 GLY O	11.06	42.61	30.61	13.59
172 ASN N	12.25	44.33	29.79	12.99
172 ASN CA	11.12	45.25	29.87	12.51
172 ASN CB	11.57	46.71	29.79	12.65
172 ASN CG	11.60	47.40	31.14	12.73
172 ASN OD1	11.69	48.62	31.23	12.92
172 ASN ND2	11.54	46.61	32.21	12.87
172 ASN C	10.21	44.91	28.71	12.15
172 ASN O	10.48	43.98	27.95	12.08
173 ARG N	9.12	45.66	28.56	11.79
173 ARG CA	8.17	45.38	27.50	11.45
173 ARG CB	6.94	44.72	28.13	11.89
173 ARG CG	7.34	43.52	28.98	12.50
173 ARG CD	6.19	42.91	29.74	12.99
173 ARG NE	5.21	42.31	28.85	13.46
173 ARG CZ	4.36	41.35	29.21	13.68
173 ARG NH1	4.37	40.88	30.45	13.99
173 ARG NH2	3.49	40.88	28.33	13.84
173 ARG C	7.79	46.64	26.73	10.99
173 ARG O	8.03	47.75	27.19	10.70
174 ILE N	7.23	46.45	25.54	10.61
174 ILE CA	6.84	47.58	24.69	10.33
174 ILE CB	6.09	47.08	23.42	10.36
174 ILE CG2	5.40	48.23	22.72	10.42
174 ILE CG1	7.08	46.38	22.47	10.51
174 ILE CD1	8.04	47.31	21.74	10.67
174 ILE C	5.97	48.59	25.45	10.11
174 ILE O	6.12	49.80	25.27	9.86
175 GLY N	5.08	48.09	26.31	10.06
175 GLY CA	4.21	48.97	27.08	10.15
175 GLY C	4.95	49.89	28.05	10.16
175 GLY O	4.45	50.97	28.38	10.15
176 ASP N	6.12	49.47	28.52	10.20
176 ASP CA	6.88	50.30	29.44	10.27

176 ASP CB	8.10	49.55	29.98	10.52
176 ASP CG	7.71	48.37	30.84	10.72
176 ASP OD1	6.85	48.55	31.73	11.08
176 ASP OD2	8.25	47.26	30.63	10.93
176 ASP C	7.33	51.57	28.73	10.15
176 ASP O	7.37	52.65	29.31	10.05
177 ILE N	7.68	51.42	27.45	10.09
177 ILE CA	8.12	52.55	26.64	10.04
177 ILE CB	8.61	52.08	25.26	10.09
177 ILE CG2	8.83	53.27	24.34	10.11
177 ILE CG1	9.90	51.26	25.43	10.15
177 ILE CD1	10.30	50.48	24.19	10.22
177 ILE C	6.96	53.53	26.46	10.02
177 ILE O	7.09	54.72	26.72	9.90
178 GLY N	5.81	53.01	26.03	10.04
178 GLY CA	4.65	53.85	25.81	10.16
178 GLY C	4.14	54.53	27.06	10.17
178 GLY O	3.77	55.70	27.02	10.19
179 ALA N	4.12	53.80	28.17	10.24
179 ALA CA	3.64	54.37	29.43	10.29
179 ALA CB	3.62	53.30	30.51	10.41
179 ALA C	4.50	55.55	29.87	10.30
179 ALA O	3.98	56.55	30.37	10.27
180 ALA N	5.81	55.43	29.68	10.36
180 ALA CA	6.74	56.49	30.08	10.44
180 ALA CB	8.18	56.00	29.97	10.60
180 ALA C	6.55	57.75	29.23	10.50
180 ALA O	6.51	58.86	29.76	10.43
181 ILE N	6.45	57.57	27.92	10.61
181 ILE CA	6.26	58.69	27.01	10.84
181 ILE CB	6.26	58.20	25.54	10.83
181 ILE CG2	5.90	59.35	24.61	10.88
181 ILE CG1	7.63	57.62	25.20	10.88
181 ILE CD1	7.67	56.89	23.87	11.00
181 ILE C	4.93	59.38	27.30	10.99
181 ILE O	4.87	60.61	27.44	10.92
182 GLN N	3.88	58.59	27.42	11.27
182 GLN CA	2.54	59.09	27.69	11.66
182 GLN CB	1.55	57.93	27.74	11.91
182 GLN CG	0.10	58.35	27.81	12.34
182 GLN CD	-0.82	57.18	28.06	12.56
182 GLN OE1	-0.53	56.05	27.66	12.64
182 GLN NE2	-1.95	57.44	28.70	12.76

182 GLN C	2.44	59.89	28.98	11.77
182 GLN O	1.90	61.00	28.99	11.74
183 GLU N	2.96	59.34	30.07	11.97
183 GLU CA	2.90	60.03	31.36	12.17
183 GLU CB	3.46	59.15	32.47	12.70
183 GLU CG	3.54	59.80	33.85	13.57
183 GLU CD	2.21	60.36	34.35	14.04
183 GLU OE1	1.15	59.81	33.97	14.62
183 GLU OE2	2.22	61.34	35.13	14.55
183 GLU C	3.65	61.35	31.31	11.98
183 GLU O	3.16	62.37	31.80	11.88
184 TYR N	4.84	61.34	30.72	11.80
184 TYR CA	5.63	62.55	30.66	11.69
184 TYR CB	7.00	62.27	30.01	11.94
184 TYR CG	7.93	63.45	30.10	12.23
184 TYR CD1	7.91	64.45	29.13	12.39
184 TYR CE1	8.70	65.59	29.25	12.67
184 TYR CD2	8.77	63.62	31.20	12.50
184 TYR CE2	9.57	64.75	31.33	12.71
184 TYR CZ	9.52	65.73	30.35	12.77
184 TYR OH	10.28	66.87	30.46	13.14
184 TYR C	4.92	63.68	29.91	11.51
184 TYR O	4.86	64.81	30.40	11.41
185 ALA N	4.37	63.36	28.75	11.36
185 ALA CA	3.68	64.36	27.94	11.36
185 ALA CB	3.58	63.88	26.50	11.35
185 ALA C	2.29	64.75	28.45	11.43
185 ALA O	1.98	65.94	28.57	11.38
186 GLU N	1.46	63.76	28.75	11.61
186 GLU CA	0.10	64.06	29.22	11.84
186 GLU CB	-0.74	62.78	29.30	12.05
186 GLU CG	-0.91	62.08	27.95	12.39
186 GLU CD	-2.00	61.02	27.96	12.55
186 GLU OE1	-2.29	60.46	29.05	12.75
186 GLU OE2	-2.54	60.72	26.88	12.72
186 GLU C	0.05	64.78	30.56	11.88
186 GLU O	-0.79	65.66	30.75	11.89
187 SER N	0.95	64.44	31.48	11.93
187 SER CA	0.94	65.09	32.79	12.05
187 SER CB	1.95	64.43	33.73	12.11
187 SER OG	3.28	64.66	33.30	12.15
187 SER C	1.27	66.58	32.66	12.06
187 SER O	0.96	67.37	33.55	12.13

188	ARG	N	1.88	66.95	31.54	12.04
188	ARG	CA	2.25	68.34	31.29	12.06
188	ARG	CB	3.65	68.41	30.69	12.05
188	ARG	CG	4.73	68.04	31.70	12.08
188	ARG	CD	6.10	67.88	31.06	12.07
188	ARG	NE	7.13	67.68	32.08	12.15
188	ARG	CZ	7.24	66.60	32.86	12.21
188	ARG	NH1	6.37	65.61	32.73	12.25
188	ARG	NH2	8.19	66.53	33.78	12.37
188	ARG	C	1.23	69.07	30.41	12.03
188	ARG	O	1.45	70.22	30.01	12.10
189	GLY	N	0.13	68.39	30.10	11.98
189	GLY	CA	-0.93	69.00	29.30	11.94
189	GLY	C	-0.90	68.81	27.80	11.84
189	GLY	O	-1.67	69.45	27.08	12.10
190	TYR	N	-0.02	67.94	27.31	11.60
190	TYR	CA	0.08	67.70	25.88	11.39
190	TYR	CB	1.55	67.57	25.46	11.40
190	TYR	CG	2.37	68.81	25.71	11.48
190	TYR	CD1	2.89	69.09	26.98	11.57
190	TYR	CE1	3.63	70.24	27.20	11.61
190	TYR	CD2	2.62	69.71	24.68	11.52
190	TYR	CE2	3.36	70.87	24.90	11.60
190	TYR	CZ	3.87	71.12	26.16	11.59
190	TYR	OH	4.60	72.27	26.38	11.85
190	TYR	C	-0.68	66.46	25.42	11.25
190	TYR	O	-1.01	65.58	26.22	11.23
191	GLY	N	-0.94	66.40	24.12	11.10
191	GLY	CA	-1.64	65.27	23.54	10.98
191	GLY	C	-0.63	64.36	22.85	10.89
191	GLY	O	0.33	64.83	22.23	10.97
192	VAL	N	-0.85	63.05	22.95	10.86
192	VAL	CA	0.04	62.08	22.34	10.88
192	VAL	CB	0.41	60.97	23.35	11.03
192	VAL	CG1	1.33	59.95	22.71	11.18
192	VAL	CG2	1.07	61.59	24.58	11.17
192	VAL	C	-0.62	61.44	21.12	10.85
192	VAL	O	-1.64	60.75	21.24	10.85
193	VAL	N	-0.05	61.69	19.94	10.83
193	VAL	CA	-0.59	61.12	18.71	10.98
193	VAL	CB	0.30	61.52	17.50	10.87
193	VAL	CG1	-0.08	60.72	16.27	10.97
193	VAL	CG2	0.14	63.01	17.22	10.89

193 VAL C	-0.66	59.60	18.85	11.19
193 VAL O	0.31	58.97	19.29	11.00
194 ARG N	-1.80	59.02	18.49	11.61
194 ARG CA	-2.00	57.58	18.61	12.18
194 ARG CB	-3.36	57.29	19.27	12.58
194 ARG CG	-3.58	57.92	20.63	13.24
194 ARG CD	-4.97	57.58	21.15	13.86
194 ARG NE	-5.26	58.22	22.43	14.45
194 ARG CZ	-6.41	58.08	23.08	14.72
194 ARG NH1	-7.37	57.32	22.58	15.00
194 ARG NH2	-6.60	58.70	24.24	15.03
194 ARG C	-1.96	56.82	17.29	12.31
194 ARG O	-1.62	55.63	17.27	12.39
195 ASP N	-2.31	57.49	16.20	12.48
195 ASP CA	-2.35	56.85	14.89	12.67
195 ASP CB	-3.08	57.74	13.90	13.13
195 ASP CG	-4.57	57.84	14.18	13.52
195 ASP OD1	-5.04	57.21	15.15	13.95
195 ASP OD2	-5.26	58.55	13.43	13.90
195 ASP C	-1.01	56.44	14.30	12.53
195 ASP O	-0.93	55.47	13.54	12.74
196 LEU N	0.04	57.18	14.63	12.18
196 LEU CA	1.38	56.89	14.11	11.86
196 LEU CB	1.96	58.14	13.45	12.14
196 LEU CG	1.06	58.70	12.34	12.45
196 LEU CD1	1.64	60.01	11.84	12.51
196 LEU CD2	0.95	57.69	11.20	12.67
196 LEU C	2.25	56.40	15.26	11.50
196 LEU O	2.16	56.90	16.38	11.39
197 VAL N	3.11	55.42	14.97	11.17
197 VAL CA	3.95	54.82	15.99	10.88
197 VAL CB	3.34	53.46	16.43	10.96
197 VAL CG1	1.94	53.67	17.00	11.05
197 VAL CG2	3.29	52.51	15.24	11.10
197 VAL C	5.40	54.56	15.60	10.64
197 VAL O	5.78	54.68	14.43	10.65
198 GLY N	6.20	54.21	16.61	10.42
198 GLY CA	7.60	53.86	16.40	10.15
198 GLY C	7.58	52.47	15.79	9.97
198 GLY O	6.52	51.85	15.71	9.86
199 HIS N	8.75	51.95	15.43	9.89
199 HIS CA	8.78	50.66	14.75	9.85
199 HIS CB	8.38	50.91	13.30	9.78

199 HIS CG	9.20	52.00	12.66	9.67
199 HIS CD2	9.02	53.34	12.62	9.67
199 HIS ND1	10.43	51.77	12.09	9.61
199 HIS CE1	10.98	52.92	11.73	9.65
199 HIS NE2	10.14	53.89	12.04	9.74
199 HIS C	10.15	50.02	14.75	9.88
199 HIS O	11.15	50.65	15.10	9.80
200 GLY N	10.19	48.75	14.34	10.04
200 GLY CA	11.45	48.06	14.24	10.28
200 GLY C	12.08	48.47	12.92	10.51
200 GLY O	11.41	49.01	12.03	10.37
201 VAL N	13.38	48.23	12.79	10.91
201 VAL CA	14.12	48.55	11.57	11.46
201 VAL CB	14.95	49.85	11.75	11.50
201 VAL CG1	15.76	50.14	10.49	11.57
201 VAL CG2	14.02	51.02	12.05	11.75
201 VAL C	15.06	47.40	11.23	11.82
201 VAL O	15.64	46.79	12.13	11.71
202 GLY N	15.19	47.09	9.95	12.33
202 GLY CA	16.06	46.02	9.51	13.15
202 GLY C	15.29	44.72	9.31	13.77
202 GLY O	14.71	44.20	10.26	13.73
203 PRO N	15.29	44.16	8.09	14.29
203 PRO CD	14.67	42.84	7.85	14.52
203 PRO CA	15.96	44.64	6.87	14.74
203 PRO CB	15.99	43.39	5.99	14.77
203 PRO CG	14.70	42.73	6.33	14.70
203 PRO C	15.33	45.84	6.15	15.06
203 PRO O	15.97	46.45	5.30	15.24
204 THR N	14.09	46.17	6.50	15.40
204 THR CA	13.40	47.30	5.87	15.69
204 THR CB	11.99	46.87	5.38	15.94
204 THR OG1	12.13	45.82	4.41	16.34
204 THR CG2	11.25	48.03	4.74	16.21
204 THR C	13.27	48.46	6.85	15.61
204 THR O	13.53	48.30	8.04	15.50
205 MET N	12.86	49.63	6.36	15.62
205 MET CA	12.70	50.80	7.22	15.65
205 MET CB	12.57	52.09	6.39	15.70
205 MET CG	11.24	52.28	5.66	15.78
205 MET SD	11.08	53.93	4.89	15.74
205 MET CE	12.21	53.78	3.53	15.97
205 MET C	11.50	50.67	8.15	15.65

205 MET O	11.34	51.45	9.08	15.67
206 HIS N	10.65	49.67	7.89	15.66
206 HIS CA	9.47	49.46	8.71	15.67
206 HIS CB	8.22	49.98	7.99	16.09
206 HIS CG	7.01	50.07	8.87	16.54
206 HIS CD2	5.96	49.23	9.03	16.71
206 HIS ND1	6.81	51.12	9.74	16.77
206 HIS CE1	5.68	50.92	10.40	16.83
206 HIS NE2	5.15	49.78	9.99	16.88
206 HIS C	9.30	47.97	9.02	15.42
206 HIS O	8.95	47.18	8.14	15.45
207 GLU N	9.55	47.60	10.27	15.11
207 GLU CA	9.45	46.21	10.69	14.87
207 GLU CB	10.84	45.59	10.85	14.98
207 GLU CG	11.71	45.64	9.61	15.25
207 GLU CD	11.35	44.58	8.59	15.45
207 GLU OE1	11.94	44.59	7.50	15.60
207 GLU OE2	10.47	43.73	8.89	15.62
207 GLU C	8.74	46.11	12.03	14.69
207 GLU O	8.59	47.11	12.74	14.53
208 GLU N	8.31	44.90	12.37	14.51
208 GLU CA	7.69	44.66	13.65	14.38
208 GLU CB	7.06	43.26	13.68	14.79
208 GLU CG	5.73	43.19	12.98	15.50
208 GLU CD	4.63	43.85	13.78	15.84
208 GLU OE1	3.69	44.41	13.17	16.25
208 GLU OE2	4.70	43.80	15.03	16.23
208 GLU C	8.87	44.72	14.62	14.00
208 GLU O	10.02	44.53	14.21	13.96
209 PRO N	8.62	45.02	15.90	13.63
209 PRO CD	9.69	44.96	16.92	13.61
209 PRO CA	7.33	45.30	16.52	13.28
209 PRO CB	7.57	44.87	17.96	13.44
209 PRO CG	8.96	45.38	18.19	13.51
209 PRO C	7.00	46.78	16.44	12.90
209 PRO O	7.89	47.61	16.22	12.79
210 MET N	5.73	47.11	16.60	12.51
210 MET CA	5.34	48.51	16.59	12.16
210 MET CB	3.84	48.66	16.32	12.69
210 MET CG	3.44	48.27	14.91	13.41
210 MET SD	4.33	49.20	13.63	14.20
210 MET CE	5.65	48.05	13.21	14.10
210 MET C	5.68	49.03	17.99	11.58

210 MET O	5.68	48.27	18.96	11.41
211 VAL N	5.99	50.31	18.07	11.04
211 VAL CA	6.35	50.93	19.34	10.66
211 VAL CB	7.85	51.33	19.35	10.64
211 VAL CG1	8.25	51.81	20.73	10.67
211 VAL CG2	8.72	50.15	18.93	10.72
211 VAL C	5.49	52.16	19.56	10.41
211 VAL O	5.90	53.29	19.29	10.18
212 PRO N	4.25	51.96	20.05	10.26
212 PRO CD	3.59	50.67	20.32	10.27
212 PRO CA	3.34	53.07	20.31	10.27
212 PRO CB	2.08	52.38	20.82	10.32
212 PRO CG	2.14	51.03	20.18	10.34
212 PRO C	3.90	54.05	21.34	10.23
212 PRO O	4.66	53.66	22.22	10.11
213 ASN N	3.49	55.31	21.23	10.26
213 ASN CA	3.95	56.34	22.15	10.49
213 ASN CB	4.09	57.66	21.40	10.45
213 ASN CG	5.20	57.61	20.39	10.49
213 ASN OD1	6.36	57.44	20.74	10.48
213 ASN ND2	4.85	57.74	19.11	10.65
213 ASN C	3.05	56.48	23.36	10.74
213 ASN O	3.17	57.42	24.14	10.71
214 TYR N	2.14	55.52	23.51	11.14
214 TYR CA	1.23	55.46	24.64	11.58
214 TYR CB	-0.14	56.05	24.30	12.28
214 TYR CG	-0.90	55.29	23.24	13.02
214 TYR CD1	-0.58	55.43	21.89	13.29
214 TYR CE1	-1.26	54.72	20.91	13.72
214 TYR CD2	-1.92	54.41	23.59	13.44
214 TYR CE2	-2.60	53.68	22.62	13.82
214 TYR CZ	-2.27	53.84	21.29	13.87
214 TYR OH	-2.95	53.12	20.33	14.36
214 TYR C	1.11	53.97	24.95	11.57
214 TYR O	1.24	53.13	24.05	11.41
215 GLY N	0.87	53.64	26.21	11.67
215 GLY CA	0.75	52.24	26.57	11.86
215 GLY C	0.66	52.03	28.06	11.99
215 GLY O	0.59	52.98	28.83	11.95
216 ILE N	0.67	50.76	28.45	12.15
216 ILE CA	0.56	50.38	29.86	12.36
216 ILE CB	-0.67	49.48	30.08	12.57
216 ILE CG2	-0.76	49.06	31.54	12.64

	216 ILE CG1	-1.93	50.23	29.65	12.79
	216 ILE CD1	-3.20	49.42	29.78	13.03
	216 ILE C	1.81	49.63	30.31	12.35
	216 ILE O	2.25	48.69	29.65	12.22
	217 ALA N	2.37	50.06	31.43	12.42
	217 ALA CA	3.56	49.44	31.97	12.50
	217 ALA CB	3.98	50.14	33.26	12.63
	217 ALA C	3.35	47.95	32.22	12.51
	217 ALA O	2.27	47.52	32.63	12.53
	218 GLY N	4.39	47.17	31.95	12.51
	218 GLY CA	4.33	45.74	32.17	12.54
	218 GLY C	3.56	44.94	31.13	12.48
	218 GLY O	3.37	43.74	31.31	12.62
	219 ARG N	3.14	45.58	30.05	12.42
	219 ARG CA	2.39	44.89	29.01	12.26
	219 ARG CB	0.95	45.42	28.95	12.39
	219 ARG CG	0.21	45.30	30.27	12.41
	219 ARG CD	-1.27	45.56	30.10	12.45
	219 ARG NE	-1.98	45.47	31.37	12.47
	219 ARG CZ	-3.30	45.45	31.49	12.44
	219 ARG NH1	-4.07	45.52	30.41	12.39
	219 ARG NH2	-3.85	45.36	32.69	12.61
	219 ARG C	3.05	45.02	27.64	12.14
	219 ARG O	3.92	45.86	27.44	12.00
	220 GLY N	2.62	44.18	26.71	12.05
	220 GLY CA	3.18	44.22	25.37	12.06
	220 GLY C	4.33	43.26	25.18	12.00
	220 GLY O	4.73	42.56	26.12	11.91
	221 LEU N	4.88	43.23	23.97	12.07
	221 LEU CA	5.98	42.33	23.67	12.15
	221 LEU CB	6.37	42.46	22.19	12.49
	221 LEU CG	5.43	41.82	21.16	12.88
	221 LEU CD1	5.87	42.20	19.77	13.17
	221 LEU CD2	5.43	40.31	21.33	13.05
	221 LEU C	7.21	42.56	24.53	12.12
	221 LEU O	7.57	43.70	24.84	11.86
	222 ARG N	7.85	41.47	24.93	12.26
	222 ARG CA	9.05	41.54	25.75	12.53
	222 ARG CB	9.31	40.19	26.43	13.02
	222 ARG CG	8.26	39.83	27.48	13.83
	222 ARG CD	8.41	38.40	27.98	14.49
	222 ARG NE	7.33	38.01	28.89	15.10
	222 ARG CZ	7.22	38.41	30.15	15.38

222 ARG NH1	8.13	39.22	30.67	15.69
222 ARG NH2	6.20	38.01	30.90	15.64
222 ARG C	10.24	41.95	24.88	12.43
222 ARG O	10.43	41.42	23.77	12.33
223 LEU N	11.03	42.89	25.37	12.39
223 LEU CA	12.19	43.38	24.64	12.53
223 LEU CB	12.60	44.76	25.17	12.43
223 LEU CG	11.46	45.79	25.14	12.45
223 LEU CD1	11.95	47.10	25.74	12.44
223 LEU CD2	10.99	46.00	23.71	12.52
223 LEU C	13.35	42.41	24.75	12.71
223 LEU O	13.63	41.88	25.83	12.78
224 ARG N	14.02	42.17	23.63	12.93
224 ARG CA	15.14	41.24	23.58	13.26
224 ARG CB	14.79	40.03	22.71	13.61
224 ARG CG	13.56	39.26	23.15	14.08
224 ARG CD	13.73	38.66	24.53	14.61
224 ARG NE	12.57	37.86	24.91	15.11
224 ARG CZ	12.34	37.40	26.13	15.29
224 ARG NH1	13.19	37.65	27.11	15.55
224 ARG NH2	11.25	36.69	26.38	15.53
224 ARG C	16.40	41.88	23.02	13.30
224 ARG O	16.34	42.80	22.20	13.18
225 GLU N	17.54	41.37	23.47	13.45
225 GLU CA	18.84	41.85	23.02	13.56
225 GLU CB	19.95	41.04	23.70	14.11
225 GLU CG	21.36	41.49	23.38	14.98
225 GLU CD	22.40	40.56	23.98	15.45
225 GLU OE1	22.25	40.19	25.16	15.92
225 GLU OE2	23.37	40.22	23.28	15.91
225 GLU C	18.90	41.63	21.51	13.28
225 GLU O	18.56	40.56	21.02	13.32
226 GLY N	19.32	42.66	20.77	13.02
226 GLY CA	19.41	42.52	19.33	12.69
226 GLY C	18.29	43.22	18.59	12.41
226 GLY O	18.36	43.40	17.38	12.37
227 MET N	17.23	43.60	19.30	12.13
227 MET CA	16.14	44.31	18.66	11.89
227 MET CB	14.92	44.43	19.59	12.17
227 MET CG	14.12	43.16	19.78	12.51
227 MET SD	12.67	43.49	20.79	12.81
227 MET CE	11.39	43.52	19.53	13.34
227 MET C	16.60	45.72	18.30	11.57

227 MET O	17.30	46.36	19.09	11.51
228 VAL N	16.22	46.18	17.12	11.26
228 VAL CA	16.55	47.53	16.68	11.01
228 VAL CB	17.35	47.53	15.36	11.02
228 VAL CG1	17.53	48.96	14.87	11.04
228 VAL CG2	18.70	46.88	15.57	11.13
228 VAL C	15.21	48.22	16.48	10.80
228 VAL O	14.39	47.79	15.67	10.74
229 LEU N	15.00	49.29	17.24	10.64
229 LEU CA	13.74	50.01	17.20	10.52
229 LEU CB	12.96	49.78	18.49	10.82
229 LEU CG	12.81	48.36	19.04	11.04
229 LEU CD1	12.18	48.41	20.43	11.28
229 LEU CD2	11.96	47.55	18.09	11.24
229 LEU C	13.94	51.51	17.09	10.44
229 LEU O	15.05	52.02	17.22	10.24
230 THR N	12.83	52.19	16.84	10.41
230 THR CA	12.84	53.64	16.84	10.45
230 THR CB	12.41	54.28	15.51	10.69
230 THR OG1	11.03	53.98	15.26	10.96
230 THR CG2	13.28	53.80	14.37	10.91
230 THR C	11.79	54.02	17.86	10.25
230 THR O	10.81	53.30	18.10	10.48
231 ILE N	12.03	55.14	18.52	9.90
231 ILE CA	11.09	55.72	19.45	9.60
231 ILE CB	11.62	55.68	20.90	9.54
231 ILE CG2	10.89	56.70	21.76	9.63
231 ILE CG1	11.40	54.26	21.45	9.58
231 ILE CD1	11.97	54.02	22.82	9.58
231 ILE C	11.00	57.12	18.87	9.51
231 ILE O	11.99	57.84	18.77	9.27
232 GLU N	9.79	57.47	18.44	9.51
232 GLU CA	9.56	58.74	17.77	9.66
232 GLU CB	9.59	58.50	16.26	9.80
232 GLU CG	8.67	57.39	15.76	10.16
232 GLU CD	8.88	57.11	14.29	10.20
232 GLU OE1	8.56	58.00	13.47	10.68
232 GLU OE2	9.39	56.02	13.96	10.38
232 GLU C	8.26	59.42	18.15	9.62
232 GLU O	7.36	59.57	17.33	9.71
233 PRO N	8.16	59.87	19.40	9.67
233 PRO CD	9.17	59.88	20.47	9.83
233 PRO CA	6.93	60.53	19.83	9.65

233 PRO CB	7.20	60.83	21.31	9.86
233 PRO CG	8.69	61.00	21.35	10.03
233 PRO C	6.54	61.78	19.06	9.57
233 PRO O	7.37	62.64	18.76	9.47
234 MET N	5.25	61.85	18.73	9.64
234 MET CA	4.64	62.99	18.06	9.70
234 MET CB	3.87	62.55	16.82	9.97
234 MET CG	4.79	62.21	15.66	10.20
234 MET SD	4.12	60.97	14.56	10.39
234 MET CE	4.43	59.49	15.54	10.56
234 MET C	3.72	63.54	19.14	9.71
234 MET O	2.75	62.88	19.55	9.63
235 ILE N	4.05	64.73	19.61	9.74
235 ILE CA	3.33	65.39	20.68	9.89
235 ILE CB	4.33	65.72	21.82	9.97
235 ILE CG2	3.62	66.40	22.98	10.11
235 ILE CG1	5.06	64.45	22.27	10.04
235 ILE CD1	4.15	63.34	22.80	10.07
235 ILE C	2.66	66.66	20.19	9.98
235 ILE O	3.28	67.47	19.49	9.80
236 ASN N	1.38	66.82	20.54	10.22
236 ASN CA	0.62	67.99	20.12	10.56
236 ASN CB	-0.72	67.58	19.49	10.58
236 ASN CG	-0.56	66.66	18.30	10.55
236 ASN OD1	0.52	66.57	17.70	10.58
236 ASN ND2	-1.64	65.97	17.93	10.68
236 ASN C	0.32	68.89	21.32	10.83
236 ASN O	0.22	68.42	22.45	10.84
237 THR N	0.16	70.19	21.07	11.21
237 THR CA	-0.14	71.10	22.17	11.70
237 THR CB	0.03	72.58	21.74	11.76
237 THR OG1	-0.79	72.84	20.60	11.80
237 THR CG2	1.48	72.87	21.41	11.88
237 THR C	-1.56	70.89	22.68	12.00
237 THR O	-1.85	71.16	23.84	12.10
238 GLY N	-2.44	70.41	21.81	12.30
238 GLY CA	-3.83	70.19	22.20	12.73
238 GLY C	-4.31	68.76	22.02	13.01
238 GLY O	-3.78	67.83	22.63	13.10
239 ASP N	-5.31	68.58	21.16	13.30
239 ASP CA	-5.88	67.27	20.90	13.66
239 ASP CB	-7.15	67.40	20.05	14.30
239 ASP CG	-8.24	68.19	20.75	14.85

239 ASP OD1	-8.61	67.84	21.88	15.33
239 ASP OD2	-8.74	69.18	20.15	15.40
239 ASP C	-4.89	66.33	20.21	13.63
239 ASP O	-4.03	66.77	19.45	13.47
240 TRP N	-5.04	65.03	20.46	13.71
240 TRP CA	-4.15	64.03	19.88	13.91
240 TRP CB	-4.08	62.79	20.78	14.27
240 TRP CG	-5.40	62.14	21.06	14.70
240 TRP CD2	-6.05	61.14	20.27	14.90
240 TRP CE2	-7.27	60.82	20.91	15.03
240 TRP CE3	-5.72	60.47	19.08	15.02
240 TRP CD1	-6.23	62.38	22.12	14.87
240 TRP NE1	-7.35	61.59	22.04	15.05
240 TRP CZ2	-8.15	59.86	20.40	15.13
240 TRP CZ3	-6.60	59.52	18.57	15.10
240 TRP CH2	-7.80	59.23	19.24	15.15
240 TRP C	-4.53	63.58	18.46	13.89
240 TRP O	-3.71	62.99	17.76	13.71
241 GLU N	-5.76	63.86	18.05	13.96
241 GLU CA	-6.23	63.45	16.73	14.15
241 GLU CB	-7.75	63.61	16.63	14.47
241 GLU CG	-8.52	62.71	17.59	15.07
241 GLU CD	-8.92	63.42	18.88	15.43
241 GLU OE1	-8.17	64.31	19.34	15.74
241 GLU OE2	-9.98	63.08	19.43	15.80
241 GLU C	-5.55	64.17	15.56	14.10
241 GLU O	-5.24	65.36	15.65	13.92
242 ILE N	-5.35	63.44	14.47	14.19
242 ILE CA	-4.71	63.98	13.27	14.42
242 ILE CB	-3.26	63.45	13.11	14.27
242 ILE CG2	-2.45	63.78	14.35	14.21
242 ILE CG1	-3.27	61.94	12.87	14.26
242 ILE CD1	-1.90	61.36	12.52	14.25
242 ILE C	-5.50	63.61	12.01	14.72
242 ILE O	-6.37	62.74	12.04	14.69
243 ASP N	-5.18	64.29	10.91	15.15
243 ASP CA	-5.84	64.04	9.63	15.68
243 ASP CB	-6.64	65.27	9.18	16.05
243 ASP CG	-5.76	66.43	8.75	16.27
243 ASP OD1	-4.52	66.31	8.81	16.61
243 ASP OD2	-6.32	67.47	8.34	16.60
243 ASP C	-4.78	63.72	8.57	15.86
243 ASP O	-3.59	63.68	8.88	15.92

244 THR N	-5.21	63.50	7.34	16.13
244 THR CA	-4.29	63.20	6.25	16.47
244 THR CB	-4.34	61.72	5.84	16.53
244 THR OG1	-4.02	60.90	6.97	16.58
244 THR CG2	-3.33	61.43	4.73	16.61
244 THR C	-4.62	64.05	5.03	16.68
244 THR O	-5.79	64.24	4.69	16.72
245 ASP N	-3.58	64.55	4.37	16.94
245 ASP CA	-3.73	65.38	3.18	17.25
245 ASP CB	-2.35	65.66	2.59	17.38
245 ASP CG	-2.37	66.72	1.51	17.53
245 ASP OD1	-3.20	66.61	0.58	17.71
245 ASP OD2	-1.55	67.66	1.58	17.64
245 ASP C	-4.59	64.64	2.15	17.40
245 ASP O	-4.24	63.55	1.70	17.39
246 MET N	-5.71	65.25	1.77	17.61
246 MET CA	-6.61	64.64	0.80	17.79
246 MET CB	-8.01	65.23	0.92	18.44
246 MET CG	-8.69	64.91	2.24	19.24
246 MET SD	-8.81	63.13	2.51	20.36
246 MET CE	-10.32	62.76	1.63	20.14
246 MET C	-6.12	64.79	-0.64	17.51
246 MET O	-6.62	64.12	-1.55	17.50
247 LYS N	-5.14	65.66	-0.84	17.14
247 LYS CA	-4.60	65.91	-2.17	16.71
247 LYS CB	-4.14	67.36	-2.27	17.09
247 LYS CG	-3.71	67.79	-3.66	17.54
247 LYS CD	-3.26	69.25	-3.68	17.91
247 LYS CE	-4.34	70.17	-3.13	18.12
247 LYS NZ	-5.62	70.06	-3.88	18.39
247 LYS C	-3.44	64.98	-2.52	16.15
247 LYS O	-3.30	64.56	-3.67	16.21
248 THR N	-2.63	64.64	-1.53	15.42
248 THR CA	-1.46	63.79	-1.75	14.68
248 THR CB	-0.17	64.50	-1.34	14.73
248 THR OG1	-0.15	64.66	0.08	14.63
248 THR CG2	-0.09	65.88	-1.99	14.74
248 THR C	-1.47	62.47	-0.98	14.10
248 THR O	-0.79	61.52	-1.36	13.96
249 GLY N	-2.23	62.43	0.11	13.50
249 GLY CA	-2.29	61.23	0.93	12.80
249 GLY C	-1.07	61.08	1.83	12.29
249 GLY O	-0.89	60.04	2.46	12.16

	250 TRP N	-0.24	62.12	1.90	11.88
	250 TRP CA	0.96	62.04	2.72	11.58
	250 TRP CB	2.19	62.37	1.86	11.46
	250 TRP CG	2.56	61.23	0.96	11.24
5	250 TRP CD2	3.09	59.97	1.38	11.18
	250 TRP CE2	3.24	59.17	0.23	11.15
	250 TRP CE3	3.46	59.43	2.62	11.24
	250 TRP CD1	2.42	61.15	-0.39	11.22
	250 TRP NE1	2.82	59.92	-0.84	11.15
10	250 TRP CZ2	3.73	57.86	0.28	11.17
	250 TRP CZ3	3.95	58.14	2.68	11.35
	250 TRP CH2	4.08	57.36	1.51	11.34
	250 TRP C	0.97	62.86	4.01	11.48
	250 TRP O	0.93	62.29	5.10	11.40
15	251 ALA N	1.01	64.18	3.91	11.46
	251 ALA CA	1.07	65.02	5.10	11.51
	251 ALA CB	1.13	66.49	4.70	11.53
	251 ALA C	-0.06	64.83	6.12	11.55
	251 ALA O	-1.23	64.72	5.75	11.58
20	252 HIS N	0.32	64.79	7.39	11.67
	252 HIS CA	-0.64	64.66	8.48	11.85
	252 HIS CB	-0.27	63.51	9.41	12.33
	252 HIS CG	-0.25	62.18	8.73	12.69
	252 HIS CD2	0.76	61.32	8.48	12.88
25	252 HIS ND1	-1.39	61.62	8.18	12.96
	252 HIS CE1	-1.07	60.47	7.62	13.03
	252 HIS NE2	0.23	60.26	7.78	12.92
	252 HIS C	-0.58	65.96	9.27	11.75
	252 HIS O	0.50	66.50	9.51	11.53
30	253 LYS N	-1.75	66.45	9.68	11.73
	253 LYS CA	-1.84	67.68	10.46	11.76
	253 LYS CB	-2.44	68.82	9.63	12.32
	253 LYS CG	-1.59	69.30	8.47	12.96
	253 LYS CD	-2.21	70.54	7.85	13.57
35	253 LYS CE	-1.34	71.13	6.75	13.96
	253 LYS NZ	-1.93	72.39	6.22	14.33
	253 LYS C	-2.72	67.44	11.68	11.48
	253 LYS O	-3.53	66.51	11.70	11.36
	254 THR N	-2.57	68.29	12.69	11.21
40	254 THR CA	-3.40	68.18	13.88	11.08
	254 THR CB	-2.93	69.14	14.98	10.94
	254 THR OG1	-2.95	70.48	14.48	10.63
	254 THR CG2	-1.53	68.79	15.44	10.82

254 THR C	-4.82	68.56	13.48	11.20
254 THR O	-5.03	69.45	12.66	11.19
255 ILE N	-5.80	67.88	14.06	11.42
255 ILE CA	-7.19	68.19	13.77	11.75
255 ILE CB	-8.14	67.12	14.36	12.05
255 ILE CG2	-9.57	67.65	14.42	12.34
255 ILE CG1	-8.06	65.83	13.53	12.30
255 ILE CD1	-8.59	65.98	12.12	12.62
255 ILE C	-7.55	69.55	14.36	11.75
255 ILE O	-8.30	70.31	13.75	11.86
256 ASP N	-7.01	69.87	15.53	11.73
256 ASP CA	-7.34	71.14	16.17	11.78
256 ASP CB	-7.27	71.00	17.71	12.21
256 ASP CG	-5.85	70.90	18.24	12.55
256 ASP OD1	-4.89	70.87	17.45	12.69
256 ASP OD2	-5.70	70.85	19.48	13.00
256 ASP C	-6.57	72.37	15.71	11.58
256 ASP O	-6.89	73.49	16.11	11.42
257 GLY N	-5.55	72.17	14.87	11.40
257 GLY CA	-4.79	73.30	14.38	11.48
257 GLY C	-3.62	73.70	15.26	11.42
257 GLY O	-2.86	74.61	14.92	11.64
258 GLY N	-3.47	73.02	16.39	11.23
258 GLY CA	-2.37	73.32	17.29	11.01
258 GLY C	-1.06	72.77	16.75	10.72
258 GLY O	-1.04	72.01	15.79	10.58
259 LEU N	0.04	73.16	17.39	10.52
259 LEU CA	1.35	72.71	16.97	10.29
259 LEU CB	2.43	73.57	17.62	10.68
259 LEU CG	2.43	75.06	17.28	11.00
259 LEU CD1	3.45	75.77	18.13	11.39
259 LEU CD2	2.72	75.25	15.80	11.28
259 LEU C	1.61	71.25	17.33	9.92
259 LEU O	0.99	70.70	18.24	9.95
260 SER N	2.54	70.65	16.60	9.52
260 SER CA	2.96	69.27	16.83	9.19
260 SER CB	2.35	68.33	15.80	9.10
260 SER OG	2.69	66.98	16.08	8.89
260 SER C	4.48	69.23	16.71	8.96
260 SER O	5.07	70.01	15.97	8.89
261 CYS N	5.11	68.32	17.45	8.81
261 CYS CA	6.55	68.18	17.38	8.69
261 CYS CB	7.24	68.96	18.51	8.87

261	CYS	SG	9.02	69.20	18.27	9.13
261	CYS	C	6.92	66.70	17.48	8.59
261	CYS	O	6.18	65.91	18.08	8.57
262	GLN	N	8.05	66.34	16.90	8.55
262	GLN	CA	8.53	64.97	16.91	8.61
262	GLN	CB	8.03	64.22	15.66	8.59
262	GLN	CG	8.54	62.79	15.56	8.64
262	GLN	CD	8.01	62.03	14.37	8.74
262	GLN	OE1	7.89	62.58	13.27	8.83
262	GLN	NE2	7.71	60.76	14.57	8.97
262	GLN	C	10.05	64.91	16.94	8.68
262	GLN	O	10.72	65.70	16.28	8.76
263	TYR	N	10.56	63.97	17.73	8.79
263	TYR	CA	11.99	63.69	17.82	8.94
263	TYR	CB	12.62	64.16	19.13	9.14
263	TYR	CG	12.92	65.63	19.22	9.24
263	TYR	CD1	11.96	66.53	19.68	9.36
263	TYR	CE1	12.25	67.88	19.83	9.56
263	TYR	CD2	14.18	66.12	18.89	9.43
263	TYR	CE2	14.48	67.48	19.02	9.54
263	TYR	CZ	13.51	68.35	19.50	9.60
263	TYR	OH	13.80	69.68	19.69	9.93
263	TYR	C	12.07	62.18	17.74	8.97
263	TYR	O	11.19	61.48	18.25	8.99
264	GLU	N	13.13	61.67	17.12	9.04
264	GLU	CA	13.29	60.24	16.95	9.15
264	GLU	CB	12.64	59.82	15.63	9.25
264	GLU	CG	13.00	58.43	15.13	9.25
264	GLU	CD	12.35	58.11	13.80	9.20
264	GLU	OE1	12.21	59.04	12.97	9.12
264	GLU	OE2	11.98	56.93	13.59	9.27
264	GLU	C	14.73	59.77	16.95	9.16
264	GLU	O	15.63	60.46	16.45	9.36
265	HIS	N	14.95	58.59	17.51	9.11
265	HIS	CA	16.25	57.95	17.50	9.08
265	HIS	CB	16.99	58.07	18.83	9.19
265	HIS	CG	17.87	59.27	18.94	9.18
265	HIS	CD2	18.01	60.18	19.93	9.33
265	HIS	ND1	18.77	59.64	17.96	9.29
265	HIS	CE1	19.41	60.72	18.34	9.31
265	HIS	NE2	18.97	61.07	19.54	9.39
265	HIS	C	16.04	56.48	17.22	9.09
265	HIS	O	15.03	55.90	17.63	8.96

266 GLN N	16.99	55.90	16.50	9.21
266 GLN CA	16.99	54.48	16.20	9.46
266 GLN CB	17.42	54.24	14.76	9.57
266 GLN CG	17.52	52.77	14.37	9.74
266 GLN CD	17.82	52.59	12.89	9.79
266 GLN OE1	18.63	51.74	12.50	10.19
266 GLN NE2	17.16	53.39	12.06	9.62
266 GLN C	18.05	53.94	17.17	9.57
266 GLN O	19.09	54.57	17.35	9.60
267 PHE N	17.77	52.81	17.79	9.85
267 PHE CA	18.71	52.25	18.75	10.21
267 PHE CB	18.40	52.80	20.15	10.24
267 PHE CG	17.00	52.49	20.63	10.27
267 PHE CD1	16.71	51.30	21.28	10.40
267 PHE CD2	15.96	53.38	20.37	10.31
267 PHE CE1	15.41	50.99	21.67	10.49
267 PHE CE2	14.66	53.09	20.76	10.40
267 PHE CZ	14.38	51.89	21.41	10.47
267 PHE C	18.62	50.73	18.78	10.47
267 PHE O	17.66	50.15	18.29	10.36
268 VAL N	19.64	50.11	19.35	10.90
268 VAL CA	19.65	48.66	19.47	11.46
268 VAL CB	20.91	48.04	18.81	11.56
268 VAL CG1	22.18	48.62	19.42	11.74
268 VAL CG2	20.88	46.52	18.98	11.70
268 VAL C	19.63	48.34	20.96	11.85
268 VAL O	20.28	49.01	21.77	11.76
269 ILE N	18.86	47.33	21.33	12.39
269 ILE CA	18.79	46.93	22.72	13.05
269 ILE CB	17.43	46.27	23.03	13.14
269 ILE CG2	17.43	45.72	24.45	13.25
269 ILE CG1	16.32	47.30	22.83	13.27
269 ILE CD1	14.93	46.78	23.10	13.40
269 ILE C	19.94	45.96	22.99	13.45
269 ILE O	20.05	44.92	22.35	13.46
270 THR N	20.81	46.33	23.93	14.04
270 THR CA	21.95	45.49	24.29	14.61
270 THR CB	23.29	46.23	24.12	14.61
270 THR OG1	23.49	47.12	25.23	14.59
270 THR CG2	23.32	47.02	22.82	14.69
270 THR C	21.80	45.06	25.74	15.00
270 THR O	20.98	45.61	26.47	15.04
271 LYS N	22.62	44.10	26.16	15.49

271 LYS CA	22.56	43.62	27.54	15.96
271 LYS CB	23.54	42.46	27.74	16.30
271 LYS CG	25.03	42.83	27.81	16.76
271 LYS CD	25.63	43.16	26.45	17.18
271 LYS CE	25.45	44.62	26.09	17.40
271 LYS NZ	26.07	44.95	24.77	17.64
271 LYS C	22.85	44.73	28.54	16.05
271 LYS O	22.38	44.67	29.68	16.26
272 ASP N	23.60	45.73	28.12	16.07
272 ASP CA	23.95	46.84	29.00	16.03
272 ASP CB	25.42	47.22	28.80	16.49
272 ASP CG	26.36	46.11	29.23	16.83
272 ASP OD1	26.33	45.75	30.43	17.17
272 ASP OD2	27.12	45.60	28.39	17.21
272 ASP C	23.08	48.08	28.82	15.68
272 ASP O	23.34	49.12	29.41	15.83
273 GLY N	22.03	47.95	28.01	15.16
273 GLY CA	21.14	49.08	27.80	14.48
273 GLY C	21.00	49.48	26.34	13.97
273 GLY O	21.74	48.99	25.49	13.95
274 PRO N	20.06	50.37	26.03	13.54
274 PRO CD	19.08	51.02	26.92	13.49
274 PRO CA	19.88	50.80	24.64	13.12
274 PRO CB	18.56	51.58	24.70	13.24
274 PRO CG	18.59	52.17	26.07	13.39
274 PRO C	21.04	51.65	24.14	12.74
274 PRO O	21.54	52.53	24.84	12.77
275 VAL N	21.48	51.37	22.92	12.25
275 VAL CA	22.57	52.12	22.31	11.83
275 VAL CB	23.74	51.20	21.89	11.99
275 VAL CG1	24.82	52.01	21.19	12.20
275 VAL CG2	24.32	50.51	23.12	12.24
275 VAL C	22.03	52.85	21.09	11.34
275 VAL O	21.59	52.22	20.12	11.15
276 ILE N	22.04	54.17	21.15	10.91
276 ILE CA	21.52	55.00	20.07	10.57
276 ILE CB	21.31	56.45	20.57	10.56
276 ILE CG2	20.93	57.36	19.41	10.51
276 ILE CG1	20.21	56.45	21.63	10.65
276 ILE CD1	20.09	57.75	22.40	10.79
276 ILE C	22.45	54.96	18.86	10.36
276 ILE O	23.65	55.22	18.96	10.46
277 LEU N	21.86	54.65	17.70	10.11

277	LEU	CA	22.58	54.52	16.44	9.96
277	LEU	CB	21.98	53.35	15.65	10.19
277	LEU	CG	22.04	52.00	16.36	10.38
277	LEU	CD1	21.06	51.02	15.74	10.55
277	LEU	CD2	23.46	51.47	16.30	10.71
277	LEU	C	22.57	55.77	15.58	9.76
277	LEU	O	23.31	55.87	14.60	9.72
278	THR	N	21.73	56.74	15.95	9.57
278	THR	CA	21.59	57.99	15.22	9.54
278	THR	CB	20.13	58.17	14.78	9.44
278	THR	OG1	19.26	57.89	15.88	9.20
278	THR	CG2	19.80	57.21	13.63	9.37
278	THR	C	21.99	59.19	16.09	9.65
278	THR	O	21.44	60.28	15.95	9.56
279	SER	N	22.96	58.98	16.98	9.91
279	SER	CA	23.39	60.04	17.88	10.19
279	SER	CB	24.26	59.45	19.00	10.29
279	SER	OG	24.76	60.48	19.84	10.44
279	SER	C	24.16	61.18	17.22	10.39
279	SER	O	25.05	60.95	16.41	10.38
280	GLN	N	23.80	62.40	17.60	10.64
280	GLN	CA	24.47	63.59	17.07	11.05
280	GLN	CB	23.44	64.69	16.79	10.71
280	GLN	CG	22.45	64.37	15.69	10.38
280	GLN	CD	21.30	65.34	15.64	10.14
280	GLN	OE1	21.48	66.56	15.75	10.09
280	GLN	NE2	20.09	64.82	15.46	9.95
280	GLN	C	25.50	64.12	18.07	11.50
280	GLN	O	26.16	65.12	17.82	11.62
281	GLY	N	25.63	63.44	19.21	12.05
281	GLY	CA	26.57	63.85	20.23	12.81
281	GLY	C	26.07	63.49	21.62	13.31
281	GLY	O	25.24	62.58	21.76	13.32
282	GLU	N	26.56	64.17	22.65	13.84
282	GLU	CA	26.14	63.90	24.02	14.38
282	GLU	CB	26.78	64.90	24.99	14.80
282	GLU	CG	26.66	64.51	26.45	15.53
282	GLU	CD	27.20	65.58	27.38	15.90
282	GLU	OE1	28.22	66.22	27.03	16.30
282	GLU	OE2	26.62	65.77	28.47	16.31
282	GLU	C	24.62	64.03	24.07	14.45
282	GLU	O	24.08	65.09	23.77	14.46
283	GLU	N	23.94	62.96	24.46	14.56

283 GLU CA	22.48	62.98	24.50	14.61
283 GLU CB	21.93	61.61	24.92	14.32
283 GLU CG	22.40	60.44	24.07	13.88
283 GLU CD	22.30	60.68	22.57	13.57
283 GLU OE1	21.47	61.51	22.14	13.27
283 GLU OE2	23.05	60.03	21.82	13.29
283 GLU C	21.91	64.06	25.42	14.85
283 GLU O	22.37	64.25	26.54	14.99
284 GLY N	20.88	64.74	24.91	15.03
284 GLY CA	20.22	65.78	25.67	15.24
284 GLY C	20.78	67.17	25.43	15.30
284 GLY O	20.16	68.16	25.82	15.48
285 THR N	21.93	67.26	24.78	15.29
285 THR CA	22.57	68.55	24.51	15.19
285 THR CB	24.10	68.45	24.66	15.41
285 THR OG1	24.63	67.63	23.62	15.63
285 THR CG2	24.46	67.85	26.02	15.53
285 THR C	22.28	69.15	23.14	14.89
285 THR O	22.80	70.22	22.81	15.02
286 TYR N	21.46	68.47	22.34	14.43
286 TYR CA	21.14	68.97	21.00	13.94
286 TYR CB	22.06	68.31	19.97	13.50
286 TYR CG	21.93	66.80	19.91	12.93
286 TYR CD1	20.99	66.20	19.08	12.69
286 TYR CE1	20.86	64.81	19.02	12.33
286 TYR CD2	22.75	65.97	20.68	12.75
286 TYR CE2	22.63	64.59	20.63	12.40
286 TYR CZ	21.68	64.02	19.79	12.25
286 TYR OH	21.56	62.65	19.71	11.82
286 TYR C	19.68	68.73	20.66	13.86
286 TYR O	18.99	68.07	21.46	13.85
286 TYR OT1	19.23	69.21	19.59	13.77
314 HOH O	25.62	55.76	14.77	6.45
315 HOH O	19.71	62.07	14.66	10.04
316 HOH O	7.77	55.56	19.39	10.43
317 HOH O	3.09	68.32	2.12	11.83
318 HOH O	8.58	65.39	9.46	10.26
319 HOH O	1.83	56.58	19.07	10.84
321 HOH O	25.04	56.74	17.00	10.83
322 HOH O	5.29	66.33	15.09	10.00
323 HOH O	-4.26	71.72	11.39	13.32
324 HOH O	2.94	60.11	19.41	11.38
325 HOH O	4.26	51.36	23.80	11.70

326	HOH	O	11.05	74.47	-8.06	12.27
327	HOH	O	7.63	65.04	11.99	8.99
328	HOH	O	8.02	61.07	11.02	9.06
329	HOH	O	3.55	45.00	22.11	12.90
330	HOH	O	15.14	59.07	2.21	9.87
332	HOH	O	0.50	57.96	1.35	10.07
333	HOH	O	31.03	44.64	9.37	13.64
334	HOH	O	5.86	77.62	15.40	12.45
335	HOH	O	29.15	56.87	8.75	12.35
336	HOH	O	-0.47	58.78	-1.28	11.81
337	HOH	O	7.03	69.60	-2.88	15.16
338	HOH	O	-3.31	60.11	-7.59	13.69
339	HOH	O	0.20	58.17	-8.65	10.69
340	HOH	O	30.78	56.80	1.88	13.04
341	HOH	O	0.23	54.29	-5.91	10.84
342	HOH	O	0.00	54.02	31.24	15.18
343	HOH	O	27.34	48.05	-1.33	11.07
344	HOH	O	17.05	71.62	17.19	11.59
345	HOH	O	30.92	54.46	-1.29	13.42
346	HOH	O	16.45	74.31	17.01	13.33
347	HOH	O	-3.50	60.43	16.50	12.93
348	HOH	O	2.60	52.75	-5.83	12.71
349	HOH	O	24.41	57.86	22.69	16.07
350	HOH	O	20.93	68.90	-4.11	12.68
351	HOH	O	4.43	57.87	-7.65	12.98
352	HOH	O	-3.55	68.44	25.36	16.96
353	HOH	O	-3.51	46.12	27.66	15.41
354	HOH	O	22.20	46.46	8.94	13.79
355	HOH	O	22.93	71.60	-1.05	15.48
356	HOH	O	-3.01	62.19	24.73	13.30
357	HOH	O	22.88	45.00	6.72	13.28
358	HOH	O	6.45	54.38	-8.47	14.25
359	HOH	O	26.36	50.78	6.62	14.16
360	HOH	O	14.66	70.38	22.56	17.51
361	HOH	O	5.96	56.76	-9.70	14.63
362	HOH	O	7.80	62.74	8.86	10.67
363	HOH	O	7.09	53.05	32.05	13.64
364	HOH	O	25.66	67.75	18.62	14.72
365	HOH	O	19.61	65.67	22.69	14.17
366	HOH	O	5.61	60.10	-6.56	13.66
367	HOH	O	19.50	44.33	9.43	12.20
368	HOH	O	2.04	49.75	23.74	14.45
369	HOH	O	30.02	57.15	4.45	16.93

370	HOH	O	4.07	74.27	24.72	12.60
371	HOH	O	1.60	69.84	3.83	16.22
372	HOH	O	27.75	58.99	-5.61	14.15
373	HOH	O	20.41	73.61	-4.06	18.67
374	HOH	O	29.68	48.03	8.00	13.57
375	HOH	O	11.84	62.90	-6.57	14.25
376	HOH	O	-5.98	60.61	15.01	16.51
377	HOH	O	6.53	51.96	-9.71	13.76
378	HOH	O	29.59	55.43	6.52	14.50
379	HOH	O	-3.29	59.92	23.22	12.68
380	HOH	O	7.44	80.80	17.52	14.85
381	HOH	O	-0.32	50.95	23.16	16.14
382	HOH	O	9.02	50.85	-10.01	14.59
383	HOH	O	18.27	65.67	-7.56	17.17
384	HOH	O	2.49	76.71	9.26	17.89
385	HOH	O	-0.27	72.64	25.56	17.47
386	HOH	O	19.13	46.16	28.38	16.29
387	HOH	O	15.73	65.96	26.72	15.71
388	HOH	O	16.49	70.41	19.60	14.12
389	HOH	O	3.09	69.12	34.79	17.17
390	HOH	O	10.94	85.73	9.20	17.07
391	HOH	O	12.67	44.52	13.98	16.08
392	HOH	O	31.71	53.61	6.43	13.68
393	HOH	O	1.47	56.29	31.56	17.83
394	HOH	O	13.03	42.61	11.83	18.02
395	HOH	O	0.91	49.01	26.18	15.79
396	HOH	O	14.28	68.25	26.50	13.86
397	HOH	O	1.07	52.18	33.02	15.45
398	HOH	O	11.78	56.39	31.65	14.05
399	HOH	O	9.24	39.28	22.61	14.96
400	HOH	O	4.52	52.40	2.46	13.42
401	HOH	O	24.78	40.94	7.52	15.67
402	HOH	O	9.80	60.21	7.67	17.48
403	HOH	O	19.53	70.60	16.80	19.96
404	HOH	O	4.51	48.49	-4.55	13.61
405	HOH	O	8.88	60.40	-11.11	18.67
406	HOH	O	18.12	52.54	30.33	19.37
407	HOH	O	-1.43	47.64	26.58	20.92
408	HOH	O	7.35	50.68	33.44	17.13
409	HOH	O	28.20	66.59	22.26	22.52
410	HOH	O	24.98	39.30	9.73	17.60
411	HOH	O	17.19	79.62	0.27	17.92
412	HOH	O	28.11	39.55	13.03	19.37

413	HOH	O	3.97	66.56	35.23	15.09
414	HOH	O	14.78	44.15	15.58	15.13
415	HOH	O	17.33	57.88	27.34	17.14
416	HOH	O	12.90	79.65	24.70	16.70
417	HOH	O	-2.63	67.22	6.11	20.55
418	HOH	O	27.79	69.95	5.47	21.96
419	HOH	O	19.14	63.10	-9.29	13.90
420	HOH	O	23.68	45.09	-0.56	21.61
421	HOH	O	22.14	71.39	-3.61	15.32
422	HOH	O	-4.23	58.88	10.66	23.46
423	HOH	O	1.90	47.27	22.61	21.15
424	HOH	O	17.49	39.11	25.29	17.82
425	HOH	O	-5.48	67.75	17.10	15.68
426	HOH	O	7.39	50.64	-0.53	15.87
427	HOH	O	11.13	54.18	8.65	17.67
428	HOH	O	23.17	55.55	23.46	15.47
429	HOH	O	-2.21	58.01	3.82	18.25
430	HOH	O	11.33	73.53	28.12	15.62
431	HOH	O	0.62	72.27	28.21	21.53
432	HOH	O	7.70	45.27	32.27	19.69
433	HOH	O	6.87	73.81	-3.87	17.81
434	HOH	O	4.17	62.70	36.21	18.21
435	HOH	O	11.27	79.11	16.02	15.79
436	HOH	O	-6.39	69.33	10.15	22.08
437	HOH	O	31.26	49.21	-12.14	20.40
438	HOH	O	4.27	46.02	19.65	15.49
439	HOH	O	31.55	41.96	9.49	19.34
440	HOH	O	11.22	84.88	6.53	18.07
441	HOH	O	22.02	40.78	7.03	18.67
442	HOH	O	3.08	72.05	31.31	21.08
443	HOH	O	25.49	56.12	20.89	20.37
444	HOH	O	7.18	81.53	1.11	18.85
445	HOH	O	1.47	74.61	24.45	19.91
446	HOH	O	0.70	73.42	5.81	22.03
447	HOH	O	26.78	38.90	16.38	22.73
448	HOH	O	3.61	45.02	17.14	18.57
449	HOH	O	9.55	57.27	32.97	15.50
450	HOH	O	33.45	53.77	8.57	14.93
451	HOH	O	9.70	38.74	19.96	20.16
452	HOH	O	4.42	70.35	-2.38	20.63
453	HOH	O	14.95	75.11	25.96	17.69
454	HOH	O	25.38	53.64	-11.16	22.80
455	HOH	O	28.54	45.80	16.18	20.64

456	HOH	O	2.03	65.80	1.47	20.62
457	HOH	O	18.75	75.70	12.69	22.34
458	HOH	O	17.48	79.35	12.91	19.93
459	HOH	O	20.64	43.53	6.59	19.01
460	HOH	O	-2.49	58.34	25.35	19.38
461	HOH	O	-7.22	72.24	21.40	19.81
462	HOH	O	14.62	85.03	1.42	23.03
463	HOH	O	-2.15	50.13	25.20	20.07
464	HOH	O	5.24	53.40	-12.01	20.22
465	HOH	O	24.19	62.36	-13.11	15.83
466	HOH	O	21.09	46.56	-1.93	22.13
467	HOH	O	-0.31	75.21	19.44	17.33
468	HOH	O	29.36	59.62	8.81	20.27
469	HOH	O	27.90	67.78	9.73	19.54
470	HOH	O	13.31	67.69	-7.50	22.51
471	HOH	O	-2.52	54.24	27.56	18.21
472	HOH	O	19.59	54.60	29.40	21.25
473	HOH	O	-5.70	60.97	1.77	24.93
474	HOH	O	1.52	42.24	32.47	20.62
475	HOH	O	31.78	56.83	-2.20	19.80
476	HOH	O	7.47	83.72	23.89	21.43
477	HOH	O	6.28	63.24	34.52	16.16
478	HOH	O	3.04	64.99	37.33	20.01
479	HOH	O	5.99	59.55	12.06	19.34
480	HOH	O	20.93	72.99	0.15	18.98
481	HOH	O	7.72	55.28	33.48	22.07
482	HOH	O	16.95	74.17	-5.66	20.90
483	HOH	O	33.43	49.96	-4.87	21.06
484	HOH	O	5.67	62.29	-8.07	20.76
485	HOH	O	-3.50	56.43	2.19	17.54
486	HOH	O	18.75	47.78	25.97	19.25
487	HOH	O	25.48	60.77	25.80	21.32
488	HOH	O	7.80	58.03	-11.36	20.49
489	HOH	O	7.54	83.13	4.21	18.81
490	HOH	O	22.16	66.88	-5.27	23.37
491	HOH	O	9.97	50.45	34.16	20.41
492	HOH	O	6.26	50.35	1.93	21.49
493	HOH	O	-2.25	70.37	18.92	16.53
494	HOH	O	17.82	41.67	9.84	22.92
495	HOH	O	16.95	78.58	16.18	22.58
496	HOH	O	-0.45	67.19	35.90	21.51
497	HOH	O	26.13	68.33	21.37	20.98
498	HOH	O	-0.73	50.81	34.63	24.81

499	HOH	O	30.75	56.45	11.00	21.52
500	HOH	O	8.59	42.77	10.47	16.92
501	HOH	O	7.62	60.95	34.08	20.29
502	HOH	O	-0.72	69.16	-0.51	21.80
503	HOH	O	-4.11	56.13	25.96	20.12
504	HOH	O	3.83	71.47	34.02	22.03
505	HOH	O	25.36	73.24	6.50	24.79
506	HOH	O	31.78	46.62	-5.92	21.25
507	HOH	O	0.03	42.48	27.49	22.25
508	HOH	O	3.44	70.15	-0.02	22.38
509	HOH	O	4.60	81.12	17.60	22.00
510	HOH	O	4.26	45.69	-4.29	21.06
511	HOH	O	14.73	50.32	2.07	21.60
512	HOH	O	20.15	50.62	30.68	21.15
513	HOH	O	12.05	67.07	32.27	22.10
514	HOH	O	-0.64	75.97	15.09	23.07
515	HOH	O	20.00	47.71	30.91	21.88
516	HOH	O	26.56	72.54	12.35	22.54
517	HOH	O	13.52	69.16	29.05	19.15
518	HOH	O	27.45	60.31	20.30	21.45
519	HOH	O	8.00	59.40	32.00	19.52
520	HOH	O	15.39	85.53	15.74	23.07
521	HOH	O	5.83	56.55	12.59	24.73
522	HOH	O	19.04	44.91	4.74	21.60
523	HOH	O	28.06	61.53	13.01	22.18
524	HOH	O	19.98	39.23	26.66	22.96
525	HOH	O	6.73	83.88	11.98	19.98
526	HOH	O	-0.09	58.45	32.08	20.31
527	HOH	O	3.61	78.95	16.26	19.95
528	HOH	O	-4.79	64.05	25.65	22.66
529	HOH	O	23.72	64.14	-9.62	20.87
530	HOH	O	-2.56	74.11	8.29	22.03
531	HOH	O	30.90	44.14	13.46	23.73
532	HOH	O	5.51	65.89	-5.22	21.87
533	HOH	O	6.81	47.79	-7.93	22.41
534	HOH	O	23.37	56.01	-13.72	23.15
535	HOH	O	-10.60	71.39	16.90	21.76
536	HOH	O	17.32	72.28	21.42	23.04
537	HOH	O	15.02	51.36	32.82	23.81
538	HOH	O	5.40	53.27	12.14	21.09
540	HOH	O	18.96	55.80	27.01	23.49
541	HOH	O	34.56	60.04	2.17	23.60
542	HOH	O	15.22	76.50	-3.73	21.84

543	HOH	O	28.57	48.62	16.32	23.52
545	HOH	O	0.12	76.37	10.30	21.07
547	HOH	O	32.52	58.58	1.80	16.49
549	HOH	O	16.82	36.91	14.38	22.51
550	HOH	O	26.17	48.07	25.22	21.54
551	HOH	O	9.79	64.32	-7.51	25.56
552	HOH	O	9.13	85.46	4.86	24.49
554	HOH	O	15.79	47.89	2.91	22.12
556	HOH	O	8.92	43.02	32.25	21.25
557	HOH	O	9.33	48.39	-8.70	23.77
559	HOH	O	12.66	50.32	3.58	22.02
560	HOH	O	5.50	47.13	-1.19	19.70
561	HOH	O	4.21	57.58	11.07	20.67
562	HOH	O	-2.10	64.46	-6.00	21.42
565	HOH	O	-3.58	72.97	20.53	20.33
566	HOH	O	5.15	81.64	23.84	21.73
567	HOH	O	2.86	74.92	2.91	23.52
568	HOH	O	-0.26	45.98	33.72	22.01
569	HOH	O	36.81	49.98	-8.54	22.28
570	HOH	O	-3.48	51.99	26.44	21.30
571	HOH	O	10.85	58.69	35.02	21.96
574	HOH	O	9.58	58.70	5.62	28.90
575	HOH	O	14.88	87.03	11.84	23.94
576	HOH	O	8.51	56.74	4.55	24.46
577	HOH	O	19.14	48.40	-4.28	22.63
578	HOH	O	2.29	78.38	13.61	21.50
579	HOH	O	0.95	45.84	16.79	20.93
580	HOH	O	-5.15	73.68	22.71	23.34
581	HOH	O	8.86	68.48	-6.29	23.28
582	HOH	O	15.97	38.02	27.28	23.18
585	HOH	O	29.59	55.27	15.87	22.11
587	HOH	O	28.98	56.33	18.23	20.66
588	HOH	O	34.65	46.54	-5.61	21.69
590	HOH	O	18.54	84.32	8.80	23.61
593	HOH	O	27.01	54.68	18.19	24.38
601	HOH	O	10.69	69.18	28.99	23.32
602	HOH	O	22.51	48.74	-2.80	24.21
603	HOH	O	-2.73	66.02	28.47	21.85
604	HOH	O	-6.55	67.81	3.05	24.57
605	HOH	O	33.48	59.82	6.28	24.71
606	HOH	O	7.93	83.52	17.49	23.44
610	HOH	O	17.19	78.89	-2.32	22.39
611	HOH	O	11.32	54.82	-15.30	23.51

614	HOH	O	-1.82	60.34	31.64	23.08
615	HOH	O	17.79	44.50	31.66	23.97
616	HOH	O	5.95	81.58	12.22	26.87
617	HOH	O	13.30	78.15	-6.87	26.85
618	HOH	O	11.07	42.45	6.02	24.18
619	HOH	O	0.40	65.16	37.45	24.44
620	HOH	O	15.44	78.74	23.41	25.05
621	HOH	O	10.15	47.78	34.39	24.19
622	HOH	O	3.65	80.72	20.28	22.24
623	HOH	O	26.64	63.48	-12.01	25.94
625	HOH	O	8.66	49.94	-12.65	23.77
626	HOH	O	12.07	52.23	-13.98	25.56
627	HOH	O	30.91	59.44	5.61	30.73
628	HOH	O	4.72	80.56	0.69	23.63
629	HOH	O	9.84	71.51	-6.15	31.12
633	HOH	O	32.67	54.55	11.08	23.40
634	HOH	O	27.25	44.92	18.37	24.08
635	HOH	O	29.55	68.33	2.13	22.95
636	HOH	O	18.86	46.30	7.18	26.04
638	HOH	O	30.69	58.96	-3.48	22.96
640	HOH	O	16.51	75.33	19.53	23.27
642	HOH	O	28.96	67.43	24.75	24.99
643	HOH	O	20.47	71.46	18.92	23.03
644	HOH	O	28.36	70.87	3.05	25.69
645	HOH	O	25.19	45.77	20.02	23.64
649	HOH	O	-7.68	57.11	15.91	26.16
650	HOH	O	29.29	61.88	7.51	22.66
651	HOH	O	30.34	53.30	-10.77	25.90
652	HOH	O	27.63	38.11	10.37	23.80
653	HOH	O	10.15	84.70	16.36	24.69
654	HOH	O	13.06	49.74	33.82	25.88
655	HOH	O	-10.35	69.12	18.18	23.77
656	HOH	O	-2.08	53.04	17.47	24.18
657	HOH	O	15.41	60.75	30.17	26.79
658	HOH	O	8.21	50.70	4.12	24.45
659	HOH	O	0.64	70.35	35.28	25.78
660	HOH	O	7.70	48.53	-2.38	22.91
661	HOH	O	35.00	48.28	-10.01	25.41
662	HOH	O	21.69	78.93	11.71	27.63
663	HOH	O	7.60	62.42	-9.91	24.53
664	HOH	O	2.98	53.47	34.59	24.15
665	HOH	O	6.18	86.10	10.47	24.56
666	HOH	O	3.06	67.19	-5.27	29.34

667	HOH	O	-0.03	46.12	24.07	24.93
668	HOH	O	13.02	87.37	9.86	23.55
669	HOH	O	30.13	62.84	5.13	24.61
670	HOH	O	6.73	47.03	-5.41	22.73
671	HOH	O	18.24	63.72	28.40	25.21
672	HOH	O	16.13	56.69	-10.76	22.10
673	HOH	O	6.04	71.82	30.96	25.26
674	HOH	O	-1.28	49.98	20.87	24.08
675	HOH	O	1.59	47.59	19.12	25.26
676	HOH	O	0.62	78.05	16.15	24.35
677	HOH	O	24.64	58.08	25.78	23.95
678	HOH	O	4.19	83.63	16.78	24.64
679	HOH	O	-2.76	54.35	11.79	24.22
680	HOH	O	24.94	54.22	25.04	23.55
681	HOH	O	-0.92	62.44	33.08	24.41
683	HOH	O	25.95	72.80	16.14	25.24
684	HOH	O	17.82	67.65	27.64	25.87
685	HOH	O	29.21	65.94	11.73	27.58
686	HOH	O	-5.11	59.90	26.63	22.58
687	HOH	O	9.53	85.35	25.14	24.70
688	HOH	O	16.93	48.52	-11.69	26.84
689	HOH	O	-3.73	51.75	33.39	28.01
690	HOH	O	25.99	48.39	20.23	27.48
691	HOH	O	4.93	77.99	0.20	25.82
692	HOH	O	-0.98	69.53	3.23	24.46
693	HOH	O	13.06	86.70	5.50	25.80
694	HOH	O	-4.12	72.37	25.16	25.50
695	HOH	O	32.03	52.55	12.83	23.94
696	HOH	O	14.62	81.94	-2.30	28.15
697	HOH	O	19.13	73.67	19.87	28.03
698	HOH	O	24.41	43.07	23.62	22.94
699	HOH	O	-11.38	60.83	18.91	28.63
700	HOH	O	13.81	64.17	33.23	24.40
701	HOH	O	-9.26	66.77	17.67	27.19
702	HOH	O	28.65	61.97	-11.14	24.05
703	HOH	O	-2.19	74.92	26.01	26.63
704	HOH	O	-5.43	65.69	23.69	23.47
705	HOH	O	30.72	39.51	13.13	25.31
706	HOH	O	-8.68	59.80	15.17	25.88
707	HOH	O	23.82	62.58	28.39	25.61
708	HOH	O	27.55	57.95	16.86	23.71
709	HOH	O	8.98	69.48	32.94	22.81
710	HOH	O	19.95	58.71	26.08	24.64

711	HOH	O	5.40	41.87	33.09	25.37
712	HOH	O	23.80	48.54	-5.14	24.53
713	HOH	O	10.60	39.95	31.40	23.19
714	HOH	O	23.01	51.94	27.26	24.37
715	HOH	O	1.74	76.11	6.68	24.61
716	HOH	O	6.08	82.67	14.55	22.35
717	HOH	O	17.99	47.36	33.21	25.38
718	HOH	O	12.29	81.85	23.22	25.39
719	HOH	O	1.58	42.75	22.30	25.49
720	HOH	O	22.80	43.93	21.05	24.55
721	HOH	O	18.57	83.82	4.79	24.51
722	HOH	O	0.85	48.37	34.99	26.02
723	HOH	O	12.21	47.49	-5.30	23.82
724	HOH	O	20.23	74.06	16.07	25.19
725	HOH	O	-0.67	50.96	18.33	25.39
726	HOH	O	16.94	68.40	-6.42	25.90
727	HOH	O	28.39	70.52	9.63	24.39
728	HOH	O	17.39	85.88	11.12	25.86
729	HOH	O	13.81	39.41	7.60	26.16
730	HOH	O	22.58	53.60	-12.80	27.37
731	HOH	O	7.50	71.39	-4.97	25.83
732	HOH	O	21.27	39.86	18.56	23.57
733	HOH	O	35.67	49.44	-6.15	25.91
734	HOH	O	0.08	74.63	8.21	25.05
735	HOH	O	19.20	70.45	24.90	24.94
736	HOH	O	23.39	71.70	20.20	26.92
738	HOH	O	20.65	40.15	29.15	25.47
739	HOH	O	-9.06	62.29	13.08	25.76
740	HOH	O	9.75	63.89	-10.10	25.02
741	HOH	O	23.32	72.22	24.80	24.88
742	HOH	O	19.61	71.77	22.62	25.68
743	HOH	O	-3.41	61.18	9.75	25.55
744	HOH	O	14.06	79.57	-3.48	25.35
745	HOH	O	3.63	81.35	3.06	26.94
746	HOH	O	-3.66	71.16	28.13	25.25
747	HOH	O	7.29	47.30	34.13	25.37
748	HOH	O	1.82	71.84	1.20	25.66
749	HOH	O	24.45	73.71	-0.14	23.90
750	HOH	O	31.78	41.85	12.32	27.58
751	HOH	O	-5.89	60.50	9.29	24.52
752	HOH	O	20.34	47.90	8.55	28.66
753	HOH	O	28.19	69.18	17.09	26.56
754	HOH	O	16.62	67.85	-8.93	26.55

755	HOH	O	9.22	47.99	-4.54	25.91
756	HOH	O	21.68	56.70	25.60	27.54
757	HOH	O	12.55	86.43	1.99	27.42
758	HOH	O	9.95	86.42	2.30	24.86
759	HOH	O	18.95	39.77	11.68	24.89
760	HOH	O	21.34	75.46	-0.39	27.65
761	HOH	O	-1.90	56.40	34.01	27.94
762	HOH	O	-7.87	64.96	21.91	25.75
763	HOH	O	10.29	50.48	2.35	25.43
764	HOH	O	-0.94	69.76	33.06	26.40
765	HOH	O	-8.20	56.03	20.28	26.25
766	HOH	O	14.68	54.76	34.57	28.83
767	HOH	O	-5.50	69.51	0.99	27.56
768	HOH	O	-5.77	70.12	25.30	26.53
769	HOH	O	32.18	59.01	-0.64	25.31
770	HOH	O	14.91	49.39	-14.49	28.33
771	HOH	O	8.47	74.57	-8.39	27.05
772	HOH	O	27.30	70.51	24.96	26.24
773	HOH	O	14.18	46.00	-7.72	27.27
774	HOH	O	8.16	85.03	19.99	26.88
775	HOH	O	27.31	46.33	22.79	28.48
776	HOH	O	27.10	50.17	18.22	27.70
777	HOH	O	12.86	45.30	0.54	28.03
778	HOH	O	29.05	65.07	17.18	26.29
779	HOH	O	16.18	70.09	25.83	27.45
780	HOH	O	5.77	72.80	28.61	26.22
781	HOH	O	12.57	41.90	3.75	27.47
782	HOH	O	23.72	38.29	26.52	27.15
783	HOH	O	2.62	78.60	5.08	27.48
784	HOH	O	27.24	60.99	28.04	27.30
785	HOH	O	3.09	83.56	21.96	28.25
786	HOH	O	9.54	62.42	34.93	28.70
787	HOH	O	-0.21	62.57	36.04	28.47
788	HOH	O	8.47	86.82	9.12	27.38
789	HOH	O	0.57	68.11	-5.92	28.59
790	HOH	O	26.45	65.68	-4.66	27.55
791	HOH	O	24.48	79.51	8.63	27.10
792	HOH	O	17.35	75.25	14.78	28.54
793	HOH	O	5.48	41.85	16.75	27.99
794	HOH	O	12.58	37.82	19.90	27.74
795	HOH	O	25.21	78.73	11.98	27.98
796	HOH	O	11.04	80.21	-2.38	28.78
299	HOH	O	20.33	68.86	14.90	10.41

290	HOH	O	10.01	57.54	11.33	10.75
291	HOH	O	21.46	79.00	5.63	24.93
292	HOH	O	-10.74	57.08	19.29	25.97
293	HOH	O	17.81	59.62	29.37	25.06
294	HOH	O	-9.38	68.28	1.29	25.84
295	HOH	O	-6.46	55.28	18.30	25.89
296	HOH	O	22.37	47.06	32.44	26.10
297	HOH	O	15.31	43.97	2.12	25.16
298	HOH	O	11.20	58.31	8.87	10.62
287	ZN2	ZN	11.66	58.72	10.96	9.72
288	ZN2	ZN	10.75	55.89	12.28	13.36

Table IX

Provides distances between interresidue atoms that are within 5 Ångstroms apart in an active site of an *S. pneumoniae* methionine aminopeptidase.

Atom 1	Atom 2	Distance
287ZN	136OD2	1.992
287ZN	264OE1	2.112
287ZN	98OD2	2.154
287ZN	98OD1	2.299
287ZN	98CG	2.539
287ZN	136CG	2.943
287ZN	264CD	2.989
287ZN	264OE2	3.196
287ZN	136OD1	3.229
287ZN	232OE1	4.056
287ZN	98CB	4.059
287ZN	137N	4.137
287ZN	138N	4.218
287ZN	136CB	4.331
287ZN	264CG	4.393
287ZN	136C	4.411
287ZN	137C	4.471
287ZN	137CA	4.505
287ZN	138CB	4.510
287ZN	232CD	4.632
287ZN	232OE2	4.641
287ZN	99O	4.672
287ZN	136CA	4.710
287ZN	138CA	4.856
287ZN	99N	4.877
287ZN	264CB	4.902
287ZN	100CG2	4.928
287ZN	98CA	4.957
287ZN	136O	4.962
136OD2	287ZN	90.61
136OD2	287ZN	150.95
136OD2	287ZN	92.52
136OD2	287ZN	121.53
136OD2	287ZN	19.04
136OD2	287ZN	79.83
136OD2	287ZN	72.33
136OD2	287ZN	41.87
136OD2	287ZN	125.43
136OD2	287ZN	122.88
136OD2	287ZN	41.43
136OD2	287ZN	90.24
136OD2	287ZN	9.33
136OD2	287ZN	81.14
136OD2	287ZN	27.39
136OD2	287ZN	75.32
136OD2	287ZN	58.50
136OD2	287ZN	122.59
136OD2	287ZN	111.26
136OD2	287ZN	97.20
136OD2	287ZN	49.76
136OD2	287ZN	10.22
136OD2	287ZN	105.29

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136OD2 287ZN 95.97
136OD2 287ZN 49.30
136OD2 287ZN 107.66
136OD2 287ZN 33.80
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136OD1 288ZN 87.62
199NE2 288ZN 87.65
199NE2 288ZN 106.25
199NE2 288ZN 108.47
199NE2 288ZN 21.48
199NE2 288ZN 21.37
199NE2 288ZN 151.20
199NE2 288ZN 117.38
199NE2 288ZN 128.57
199NE2 288ZN 170.75
199NE2 288ZN 66.77
199NE2 288ZN 74.80
199NE2 288ZN 80.02
199NE2 288ZN 13.14
199NE2 288ZN 12.54
199NE2 288ZN 99.19
199NE2 288ZN 106.24
199NE2 288ZN 139.81
199NE2 288ZN 121.87
199NE2 288ZN 149.29
232OE2 288ZN 20.97
232OE2 288ZN 157.04
232OE2 288ZN 104.05
232OE2 288ZN 67.12
232OE2 288ZN 84.34
232OE2 288ZN 42.10
232OE2 288ZN 143.05
232OE2 288ZN 93.22
232OE2 288ZN 55.14
232OE2 288ZN 91.22
232OE2 288ZN 69.74
232OE2 288ZN 92.54
232OE2 288ZN 75.60
232OE2 288ZN 152.41
232OE2 288ZN 18.73
232OE2 288ZN 77.64
232OE2 288ZN 35.89
232OE2 288ZN 100.54
232CD 288ZN 144.63
232CD 288ZN 124.38
232CD 288ZN 84.98
232CD 288ZN 72.72
232CD 288ZN 22.53
232CD 288ZN 125.15
232CD 288ZN 76.40
232CD 288ZN 72.79
232CD 288ZN 105.15
232CD 288ZN 83.02
232CD 288ZN 112.75
232CD 288ZN 94.89
232CD 288ZN 149.46
232CD 288ZN 11.65
232CD 288ZN 69.60
232CD 288ZN 24.79
232CD 288ZN 79.59
136CG 288ZN 88.59
136CG 288ZN 129.84
136CG 288ZN 73.67
136CG 288ZN 132.11
136CG 288ZN 21.49
136CG 288ZN 68.25
136CG 288ZN 115.51
136CG 288ZN 77.94
136CG 288ZN 96.39
136CG 288ZN 100.04
136CG 288ZN 118.86
136CG 288ZN 13.55
136CG 288ZN 140.57
136CG 288ZN 79.55
136CG 288ZN 122.91
136CG 288ZN 74.13

199CE1 288ZN 41.86
199CE1 288ZN 138.14
199CE1 288ZN 138.52
199CE1 288ZN 109.70
199CE1 288ZN 151.22
199CE1 288ZN 67.52
199CE1 288ZN 61.35
199CE1 288ZN 73.57
199CE1 288ZN 11.65
199CE1 288ZN 30.28
199CE1 288ZN 78.25
199CE1 288ZN 121.38
199CE1 288ZN 129.78
199CE1 288ZN 133.31
199CE1 288ZN 150.83
199CD2 288ZN 144.52
199CD2 288ZN 96.67
199CD2 288ZN 149.65
199CD2 288ZN 160.11
199CD2 288ZN 60.64
199CD2 288ZN 82.07
199CD2 288ZN 79.08
199CD2 288ZN 31.07
199CD2 288ZN 12.47
199CD2 288ZN 120.11
199CD2 288ZN 85.85
199CD2 288ZN 133.15
199CD2 288ZN 102.48
199CD2 288ZN 143.55
264CD 288ZN 72.89
264CD 288ZN 60.52
264CD 288ZN 20.48
264CD 288ZN 86.11
264CD 288ZN 77.76
264CD 288ZN 71.24
264CD 288ZN 140.08
264CD 288ZN 143.10
264CD 288ZN 76.83
264CD 288ZN 66.90
264CD 288ZN 11.89
264CD 288ZN 49.27
264CD 288ZN 59.51
232OE1 288ZN 110.63
232OE1 288ZN 68.35
232OE1 288ZN 95.30
232OE1 288ZN 125.85
232OE1 288ZN 104.10
232OE1 288ZN 127.48
232OE1 288ZN 108.49
232OE1 288ZN 143.21
232OE1 288ZN 32.73
232OE1 288ZN 74.59
232OE1 288ZN 36.87
232OE1 288ZN 59.59
136OD2 288ZN 49.85
136OD2 288ZN 126.65
136OD2 288ZN 91.95
136OD2 288ZN 105.70
136OD2 288ZN 121.27
136OD2 288ZN 139.80
136OD2 288ZN 33.93
136OD2 288ZN 124.35
136OD2 288ZN 69.46
136OD2 288ZN 107.29
136OD2 288ZN 53.31
264OE1 288ZN 106.31
264OE1 288ZN 95.97
264OE1 288ZN 91.63
264OE1 288ZN 157.82
264OE1 288ZN 163.17
264OE1 288ZN 75.94
264OE1 288ZN 74.50
264OE1 288ZN 32.27
264OE1 288ZN 57.66
264OE1 288ZN 39.41
230OG1 288ZN 37.69
230OG1 288ZN 21.01
230OG1 288ZN 60.54
230OG1 288ZN 57.00
230OG1 288ZN 103.06
230OG1 288ZN 63.16
230OG1 288ZN 74.22
230OG1 288ZN 67.83
230OG1 288ZN 141.17
230CG2 288ZN 22.15
230CG2 288ZN 62.50

230CG2	288ZN	72.14
230CG2	288ZN	65.36
230CG2	288ZN	93.81
230CG2	288ZN	68.45
230CG2	288ZN	90.19
230CG2	288ZN	133.81
230CB	288ZN	70.40
230CB	288ZN	72.83
230CB	288ZN	85.06
230CB	288ZN	71.75
230CB	288ZN	59.82
230CB	288ZN	69.74
230CB	288ZN	130.63
199ND1	288ZN	18.99
199ND1	288ZN	89.26
199ND1	288ZN	110.17
199ND1	288ZN	129.68
199ND1	288ZN	123.28
199ND1	288ZN	158.13
199CG	288ZN	108.25
199CG	288ZN	94.03
199CG	288ZN	131.21
199CG	288ZN	109.36
199CG	288ZN	154.06
136CB	288ZN	141.50
136CB	288ZN	80.09
136CB	288ZN	125.01
136CB	288ZN	87.17
232CG	288ZN	61.80
232CG	288ZN	17.67
232CG	288ZN	85.44
264CG	288ZN	44.93
264CG	288ZN	70.81
232CB	288ZN	75.59

Table X

Provides angles between interresidue atoms that are within 5 Ångstroms apart in an active site of an *S. pneumoniae* methionine aminopeptidase.

Atom 1	Atom 2	Atom 3	Angle
136OD2	287ZN	264OE1	90.61
136OD2	287ZN	98OD1	92.52
136OD2	287ZN	136CG	19.04
136OD2	287ZN	264CD	79.83
136OD2	287ZN	264OE2	72.33
136OD2	287ZN	136OD1	41.87
136OD2	287ZN	137N	41.43
136OD2	287ZN	138N	90.24
136OD2	287ZN	136CB	9.33
136OD2	287ZN	264CG	81.14
136OD2	287ZN	136C	27.39
136OD2	287ZN	137C	75.32
136OD2	287ZN	137CA	58.50
136OD2	287ZN	232OE2	97.20
136OD2	287ZN	99O	49.76
136OD2	287ZN	136CA	10.22
136OD2	287ZN	99N	82.28
136OD2	287ZN	264CB	95.97
136OD2	287ZN	100CG2	49.30
136OD2	287ZN	136O	33.80
264OE1	287ZN	98OD2	96.24
264OE1	287ZN	98OD1	96.44
264OE1	287ZN	98CG	99.57
264OE1	287ZN	136CG	92.65
264OE1	287ZN	264CD	20.50
264OE1	287ZN	264OE2	43.43
264OE1	287ZN	136OD1	95.93
264OE1	287ZN	232OE1	68.59
264OE1	287ZN	137N	67.80
264OE1	287ZN	138N	45.65
264OE1	287ZN	136CB	90.60
264OE1	287ZN	264CG	12.68
264OE1	287ZN	136C	68.51
264OE1	287ZN	137C	55.97
264OE1	287ZN	137CA	52.32
264OE1	287ZN	138CB	53.79
264OE1	287ZN	232CD	61.47
264OE1	287ZN	232OE2	66.31
264OE1	287ZN	136CA	86.04
264OE1	287ZN	138CA	54.03

264OE1 287ZN 264CB 5.53
264OE1 287ZN 98CA 99.05
264OE1 287ZN 136O 57.60
98OD2 287ZN 98OD1 58.71
98OD2 287ZN 98CG 29.46
98OD2 287ZN 232OE1 83.12
98OD2 287ZN 98CB 28.08
98OD2 287ZN 138N 75.05
98OD2 287ZN 137C 85.25
98OD2 287ZN 138CB 46.58
98OD2 287ZN 232CD 96.72
98OD2 287ZN 138CA 58.47
98OD2 287ZN 99N 69.02
98OD2 287ZN 264CB 90.87
98OD2 287ZN 98CA 43.39
98OD1 287ZN 98CG 29.42
98OD1 287ZN 98CB 31.47
98OD1 287ZN 137N 62.80
98OD1 287ZN 138N 50.86
98OD1 287ZN 136C 79.51
98OD1 287ZN 137C 45.02
98OD1 287ZN 137CA 60.54
98OD1 287ZN 138CB 55.97
98OD1 287ZN 99O 46.43
98OD1 287ZN 136CA 83.96
98OD1 287ZN 138CA 44.98
98OD1 287ZN 99N 19.36
98OD1 287ZN 264CB 94.81
98OD1 287ZN 100CG2 81.89
98OD1 287ZN 98CA 15.47
98OD1 287ZN 136O 89.20
98CG 287ZN 98CB 3.38
98CG 287ZN 137N 90.56
98CG 287ZN 138N 61.38
98CG 287ZN 137C 64.66
98CG 287ZN 137CA 83.55
98CG 287ZN 138CB 46.58
98CG 287ZN 99O 73.04
98CG 287ZN 138CA 47.31
98CG 287ZN 99N 40.72
98CG 287ZN 264CB 95.54
98CG 287ZN 100CG2 98.06
98CG 287ZN 98CA 13.98
136CG 287ZN 264CD 76.76
136CG 287ZN 264OE2 62.66
136CG 287ZN 136OD1 22.84
136CG 287ZN 137N 58.63
136CG 287ZN 136CB 9.82
136CG 287ZN 264CG 80.95
136CG 287ZN 136C 42.30
136CG 287ZN 137C 92.06
136CG 287ZN 137CA 73.70
136CG 287ZN 232CD 95.72
136CG 287ZN 232OE2 80.72
136CG 287ZN 99O 66.37
136CG 287ZN 136CA 28.84
136CG 287ZN 99N 98.91
136CG 287ZN 264CB 98.16
136CG 287ZN 100CG2 51.97
136CG 287ZN 136O 43.17
264CD 287ZN 264OE2 23.07
264CD 287ZN 136OD1 76.24
264CD 287ZN 232OE1 63.17
264CD 287ZN 137N 70.41
264CD 287ZN 138N 63.68
264CD 287ZN 136CB 77.16
264CD 287ZN 264CG 9.03
264CD 287ZN 136C 64.48
264CD 287ZN 137C 70.17
264CD 287ZN 137CA 60.22
264CD 287ZN 138CB 74.08
264CD 287ZN 232CD 51.78
264CD 287ZN 232OE2 51.48
264CD 287ZN 136CA 78.38
264CD 287ZN 138CA 74.06
264CD 287ZN 264CB 24.80
264CD 287ZN 136O 51.35
264OE2 287ZN 136OD1 55.85
264OE2 287ZN 232OE1 57.71
264OE2 287ZN 137N 79.65
264OE2 287ZN 138N 85.96
264OE2 287ZN 136CB 66.49
264OE2 287ZN 264CG 31.91
264OE2 287ZN 136C 67.60
264OE2 287ZN 137C 89.73
264OE2 287ZN 137CA 75.65

264OE2 287ZN 138CB 96.22
264OE2 287ZN 232CD 43.32
264OE2 287ZN 232OE2 35.86
264OE2 287ZN 136CA 74.96
264OE2 287ZN 138CA 97.11
264OE2 287ZN 264CB 47.22
264OE2 287ZN 136O 54.51
136OD1 287ZN 232OE1 89.01
136OD1 287ZN 137N 80.41
136OD1 287ZN 136CB 32.66
136OD1 287ZN 264CG 83.25
136OD1 287ZN 136C 63.25
136OD1 287ZN 137CA 93.36
136OD1 287ZN 232CD 77.59
136OD1 287ZN 232OE2 62.09
136OD1 287ZN 99O 86.50
136OD1 287ZN 136CA 51.64
136OD1 287ZN 100CG2 59.94
136OD1 287ZN 136O 60.50
232OE1 287ZN 264CG 68.41
232OE1 287ZN 138CB 85.49
232OE1 287ZN 232CD 14.69
232OE1 287ZN 232OE2 28.30
232OE1 287ZN 264CB 66.44
98CB 287ZN 137N 93.28
98CB 287ZN 138N 64.75
98CB 287ZN 137C 67.95
98CB 287ZN 137CA 86.76
98CB 287ZN 138CB 49.16
98CB 287ZN 99O 73.82
98CB 287ZN 138CA 50.57
98CB 287ZN 99N 41.25
98CB 287ZN 264CB 98.31
98CB 287ZN 100CG2 96.77
98CB 287ZN 98CA 16.02
137N 287ZN 138N 49.38
137N 287ZN 136CB 49.25
137N 287ZN 264CG 65.52
137N 287ZN 136C 17.56
137N 287ZN 137C 33.89
137N 287ZN 137CA 18.89
137N 287ZN 138CB 81.50
137N 287ZN 99O 43.79
137N 287ZN 136CA 31.37
137N 287ZN 138CA 63.88
137N 287ZN 99N 63.76
137N 287ZN 264CB 71.43
137N 287ZN 100CG2 75.86
137N 287ZN 98CA 77.57
137N 287ZN 136O 26.64
138N 287ZN 136CB 96.89
138N 287ZN 264CG 54.65
138N 287ZN 136C 63.33
138N 287ZN 137C 17.28
138N 287ZN 137CA 31.79
138N 287ZN 138CB 32.35
138N 287ZN 99O 75.48
138N 287ZN 136CA 80.51
138N 287ZN 138CA 16.59
138N 287ZN 99N 67.54
138N 287ZN 264CB 44.56
138N 287ZN 98CA 55.90
138N 287ZN 136O 62.74
136CB 287ZN 264CG 79.89
136CB 287ZN 136C 33.58
136CB 287ZN 137C 82.96
136CB 287ZN 137CA 65.16
136CB 287ZN 232OE2 88.66
136CB 287ZN 99O 58.24
136CB 287ZN 136CA 19.02
136CB 287ZN 99N 90.88
136CB 287ZN 264CB 96.11
136CB 287ZN 100CG2 50.97
136CB 287ZN 136O 36.70
264CG 287ZN 136C 62.27
264CG 287ZN 137C 61.70
264CG 287ZN 137CA 53.30
264CG 287ZN 138CB 66.38
264CG 287ZN 232CD 58.39
264CG 287ZN 232OE2 59.72
264CG 287ZN 136CA 78.10
264CG 287ZN 138CA 65.22
264CG 287ZN 264CB 17.77
264CG 287ZN 136O 49.92
136C 287ZN 137C 49.81
136C 287ZN 137CA 31.58

136C 287ZN 138CB 95.59
136C 287ZN 99O 51.08
136C 287ZN 136CA 18.96
136C 287ZN 138CA 79.10
136C 287ZN 99N 77.51
136C 287ZN 264CB 73.28
136C 287ZN 100CG2 71.42
136C 287ZN 98CA 94.62
136C 287ZN 136O 13.48
137C 287ZN 137CA 19.50
137C 287ZN 138CB 47.95
137C 287ZN 99O 59.16
137C 287ZN 136CA 65.23
137C 287ZN 138CA 30.03
137C 287ZN 99N 57.65
137C 287ZN 264CB 56.53
137C 287ZN 98CA 55.11
137C 287ZN 136O 52.73
137CA 287ZN 138CB 64.12
137CA 287ZN 99O 57.85
137CA 287ZN 136CA 48.96
137CA 287ZN 138CA 47.59
137CA 287ZN 99N 68.34
137CA 287ZN 264CB 55.04
137CA 287ZN 100CG2 94.22
137CA 287ZN 98CA 72.83
137CA 287ZN 136O 33.23
138CB 287ZN 232CD 90.81
138CB 287ZN 99O 97.50
138CB 287ZN 138CA 18.33
138CB 287ZN 99N 75.23
138CB 287ZN 264CB 49.30
138CB 287ZN 98CA 50.29
138CB 287ZN 136O 93.47
232CD 287ZN 232OE2 15.49
232CD 287ZN 264CB 60.67
232CD 287ZN 136O 97.68
232OE2 287ZN 264CB 67.06
232OE2 287ZN 136O 89.33
99O 287ZN 136CA 44.16
99O 287ZN 138CA 80.94
99O 287ZN 99N 32.65
99O 287ZN 100CG2 42.76
99O 287ZN 98CA 59.92
99O 287ZN 136O 64.54
136CA 287ZN 138CA 95.25
136CA 287ZN 99N 75.75
136CA 287ZN 264CB 91.12
136CA 287ZN 100CG2 53.46
136CA 287ZN 98CA 99.35
136CA 287ZN 136O 28.47
138CA 287ZN 99N 63.97
138CA 287ZN 264CB 51.18
138CA 287ZN 98CA 45.03
138CA 287ZN 136O 79.30
99N 287ZN 100CG2 62.83
99N 287ZN 98CA 28.56
99N 287ZN 136O 89.76
264CB 287ZN 98CA 96.08
264CB 287ZN 136O 62.75
100CG2 287ZN 98CA 89.80
100CG2 287ZN 136O 81.88
264OE2 288ZN 136OD1 92.52
264OE2 288ZN 232OE2 81.54
264OE2 288ZN 232CD 75.02
264OE2 288ZN 136CG 75.50
264OE2 288ZN 264CD 15.25
264OE2 288ZN 232OE1 80.90
264OE2 288ZN 136OD2 67.40
264OE2 288ZN 264OE1 35.47
264OE2 288ZN 230OG1 72.15
264OE2 288ZN 230CG2 63.00
264OE2 288ZN 230CB 56.16
264OE2 288ZN 136CB 74.97
264OE2 288ZN 232CG 66.62
264OE2 288ZN 264CG 6.40
264OE2 288ZN 232CB 50.24
264OE2 288ZN 98OD2 74.73
136OD1 288ZN 199NE2 89.61
136OD1 288ZN 136CG 19.54
136OD1 288ZN 199CE1 70.81
136OD1 288ZN 264CD 92.63
136OD1 288ZN 136OD2 39.10
136OD1 288ZN 264OE1 87.68
136OD1 288ZN 230CG2 76.96
136OD1 288ZN 230CB 98.46

136OD1 288ZN 199ND1 82.45
136OD1 288ZN 136CB 18.07
136OD1 288ZN 264CG 97.29
136OD1 288ZN 98OD2 87.62
199NE2 288ZN 232OE2 87.65
199NE2 288ZN 199CE1 21.48
199NE2 288ZN 199CD2 21.37
199NE2 288ZN 230OG1 66.77
199NE2 288ZN 230CG2 74.80
199NE2 288ZN 230CB 80.02
199NE2 288ZN 199ND1 13.14
199NE2 288ZN 199CG 12.54
199NE2 288ZN 136CB 99.19
232OE2 288ZN 232CD 20.97
232OE2 288ZN 199CD2 67.12
232OE2 288ZN 264CD 84.34
232OE2 288ZN 232OE1 42.10
232OE2 288ZN 264OE1 93.22
232OE2 288ZN 230OG1 55.14
232OE2 288ZN 230CG2 91.22
232OE2 288ZN 230CB 69.74
232OE2 288ZN 199ND1 92.54
232OE2 288ZN 199CG 75.60
232OE2 288ZN 232CG 18.73
232OE2 288ZN 264CG 77.64
232OE2 288ZN 232CB 35.89
232CD 288ZN 199CD2 84.98
232CD 288ZN 264CD 72.72
232CD 288ZN 232OE1 22.53
232CD 288ZN 264OE1 76.40
232CD 288ZN 230OG1 72.79
232CD 288ZN 230CB 83.02
232CD 288ZN 199CG 94.89
232CD 288ZN 232CG 11.65
232CD 288ZN 264CG 69.60
232CD 288ZN 232CB 24.79
232CD 288ZN 98OD2 79.59
136CG 288ZN 199CE1 88.59
136CG 288ZN 264CD 73.67
136CG 288ZN 136OD2 21.49
136CG 288ZN 264OE1 68.25
136CG 288ZN 230CG2 77.94
136CG 288ZN 230CB 96.39
136CG 288ZN 136CB 13.55
136CG 288ZN 264CG 79.55
136CG 288ZN 98OD2 74.13
199CE1 288ZN 199CD2 41.86
199CE1 288ZN 230OG1 67.52
199CE1 288ZN 230CG2 61.35
199CE1 288ZN 230CB 73.57
199CE1 288ZN 199ND1 11.65
199CE1 288ZN 199CG 30.28
199CE1 288ZN 136CB 78.25
199CD2 288ZN 232OE1 96.67
199CD2 288ZN 230OG1 60.64
199CD2 288ZN 230CG2 82.07
199CD2 288ZN 230CB 79.08
199CD2 288ZN 199ND1 31.07
199CD2 288ZN 199CG 12.47
199CD2 288ZN 232CG 85.85
264CD 288ZN 232OE1 72.89
264CD 288ZN 136OD2 60.52
264CD 288ZN 264OE1 20.48
264CD 288ZN 230OG1 86.11
264CD 288ZN 230CG2 77.76
264CD 288ZN 230CB 71.24
264CD 288ZN 136CB 76.83
264CD 288ZN 232CG 66.90
264CD 288ZN 264CG 11.89
264CD 288ZN 232CB 49.27
264CD 288ZN 98OD2 59.51
232OE1 288ZN 264OE1 68.35
232OE1 288ZN 230OG1 95.30
232OE1 288ZN 232CG 32.73
232OE1 288ZN 264CG 74.59
232OE1 288ZN 232CB 36.87
232OE1 288ZN 98OD2 59.59
136OD2 288ZN 264OE1 49.85
136OD2 288ZN 230CG2 91.95
136OD2 288ZN 136CB 33.93
136OD2 288ZN 264CG 69.46
136OD2 288ZN 98OD2 53.31
264OE1 288ZN 230CG2 95.97
264OE1 288ZN 230CB 91.63
264OE1 288ZN 136CB 75.94
264OE1 288ZN 232CG 74.50

264OE1 288ZN 264CG 32.27
264OE1 288ZN 232CB 57.66
264OE1 288ZN 98OD2 39.41
230OG1 288ZN 230CG2 37.69
230OG1 288ZN 230CB 21.01
230OG1 288ZN 199ND1 60.54
230OG1 288ZN 199CG 57.00
230OG1 288ZN 232CG 63.16
230OG1 288ZN 264CG 74.22
230OG1 288ZN 232CB 67.83
230CG2 288ZN 230CB 22.15
230CG2 288ZN 199ND1 62.50
230CG2 288ZN 199CG 72.14
230CG2 288ZN 136CB 65.36
230CG2 288ZN 232CG 93.81
230CG2 288ZN 264CG 68.45
230CG2 288ZN 232CB 90.19
230CB 288ZN 199ND1 70.40
230CB 288ZN 199CG 72.83
230CB 288ZN 136CB 85.06
230CB 288ZN 232CG 71.75
230CB 288ZN 264CG 59.82
230CB 288ZN 232CB 69.74
199ND1 288ZN 199CG 18.99
199ND1 288ZN 136CB 89.26
199CG 288ZN 232CG 94.03
136CB 288ZN 264CG 80.09
136CB 288ZN 98OD2 87.17
232CG 288ZN 264CG 61.80
232CG 288ZN 232CB 17.67
232CG 288ZN 98OD2 85.44
264CG 288ZN 232CB 44.93
264CG 288ZN 98OD2 70.81
232CB 288ZN 98OD2 75.59

The above description fully discloses the invention including certain embodiments thereof. Modifications and improvements of the embodiments specifically disclosed herein are within the scope of the following claims. Without further elaboration it is believed that one skilled in the art can, given the preceding description, utilize the present invention to its fullest extent. Therefore any examples are to be construed as merely illustrative and not a limitation on the scope of the present invention in any way. The embodiments of the invention in which an exclusive property or privilege is claimed are defined as follows.

What is claimed is:

1. A composition comprising a bacterial MetAP in crystalline form.
2. The composition according to claim 1 wherein said MetAP is a *Staphylococcus aureus* MetAP.
3. The composition according to claim 2, wherein the crystalline form is defined by three dimensional protein coordinates of Table I in an essentially pure form or a homolog thereof.
4. The composition according to claim 2, wherein said crystalline form comprises cubic crystals with a space group I23.
5. The composition according to claim 4, wherein said cubic crystals comprise a lattice constant of a=121.36 Ångstroms (Å).
6. The composition according to claim 2, wherein said crystalline form comprises monoclinic crystals with a space group $P2_1$.
7. The composition according to claim 6, wherein said monoclinic crystals comprise lattice constants of a=41.19Å, b=76.78Å, and c=41.71Å, β=104.165°.
8. A composition comprising a *Staphylococcus aureus* MetAP in complex with a MetAP inhibitor.
9. The composition according to claim 8, wherein said MetAP inhibitor is a 1,2,3 triazole.
10. The composition according to claim 8 wherein the MetAP inhibitor is selected from the group consisting of 5-(3-Iodo-phenyl)-1-H-[1,2,3] triazole and 5-benzofuran-2-yl-1-H-[1,2,3]triazole.
11. The composition according to claim 1 wherein said MetAP is a *Streptococcus pneumoniae* MetAP.
12. The composition according to claim 11, wherein the crystalline form is defined by three dimensional protein coordinates of Table VIII in an essentially pure form or a homolog thereof.
13. The composition according to claim 11, wherein said crystalline form comprises orthorhombic crystals with a space group $P2_12_12_1$.
14. The composition according to claim 11, wherein said orthorhombic crystals comprise lattice constants of a=56.77Å, b=69.16Å, c=80.51Å.
15. A composition comprising a *Streptococcus pneumoniae* MetAP in complex with a MetAP inhibitor.

16. The composition according to claim 15, wherein said MetAP inhibitor is a 1,2,3 triazole.

17. A process for determining a bacterial MetAP crystalline form by using structural coordinates of a *Staphylococcus aureus* MetAP crystal or portions thereof, to determine a crystal structure of a mutant, homologue, or co-complex of a binding pocket or active site by molecular replacement.

18. A process for determining a bacterial MetAP crystalline form by using structural coordinates of a *Streptococcus pneumoniae* MetAP crystal or portions thereof, to determine a crystal structure of a mutant, homologue, or co-complex of a binding pocket or active site by molecular replacement.

19. A process of identifying a bacterial MetAP inhibitor capable of binding to and inhibiting the enzymatic activity of a bacterial MetAP said process comprising:

(a) introducing into a suitable computer program information defining an active site conformation of a MetAP molecule comprising a conformation defined by MetAP crystal coordinates and listed in Tables I to X wherein said program displays a three-dimensional structure;

(b) creating a three dimensional structure of a test compound in said computer program;

(c) displaying and superimposing a model of said test compound on a model of said active site;

(d) incorporating said test compound in a biological methionine aminopeptidase activity assay for a methionine aminopeptidase characterized by said active site; and

(e) determining whether said test compound inhibits enzymatic activity in said assay.

20. A process for designing inhibitors of bacterial MetAP activity using the atomic coordinates of a MetAP in crystalline form to computationally evaluate a chemical entity for associating with an active site of a MetAP enzyme.

21. A method of modifying a test bacterial MetAP polypeptide comprising:

providing a test bacterial MetAP polypeptide sequence having a characteristic that is targeted for modification;

aligning the test bacterial MetAP polypeptide sequence with a reference bacterial MetAP polypeptide sequence for which an X-ray structure is available, wherein a reference bacterial MetAP polypeptide sequence has a characteristic that is desired for the test bacterial MetAP polypeptide;

building a three-dimensional model for the test bacterial MetAP polypeptide using the three-dimensional coordinates of the X-ray structure(s) of a reference bacterial MetAP

polypeptide and its sequence alignment with the test bacterial MetAP polypeptide sequence;

examining the three-dimensional model of the test bacterial MetAP polypeptide for a difference in an amino acid residue as compared to a reference bacterial MetAP polypeptide, wherein the residues are associated with the desired characteristic; and

mutating an amino acid residue in the test bacterial MetAP polypeptide sequence located at a difference identified in step (d) to a residue associated with the desired characteristic, whereby the test bacterial MetAP polypeptide is modified.

22. A method for the treatment of an individual having need to inhibit a bacterial methionine aminopeptidase comprising: administering to the individual a therapeutically effective amount of a compound that binds to or interacts with an active site of a bacterial MetAP enzyme.

23. A method of drug design comprising using the structural coordinates of a MetAP crystal to computationally evaluate a chemical entity for associating with the inhibitor binding site of MetAP.

Figure 1

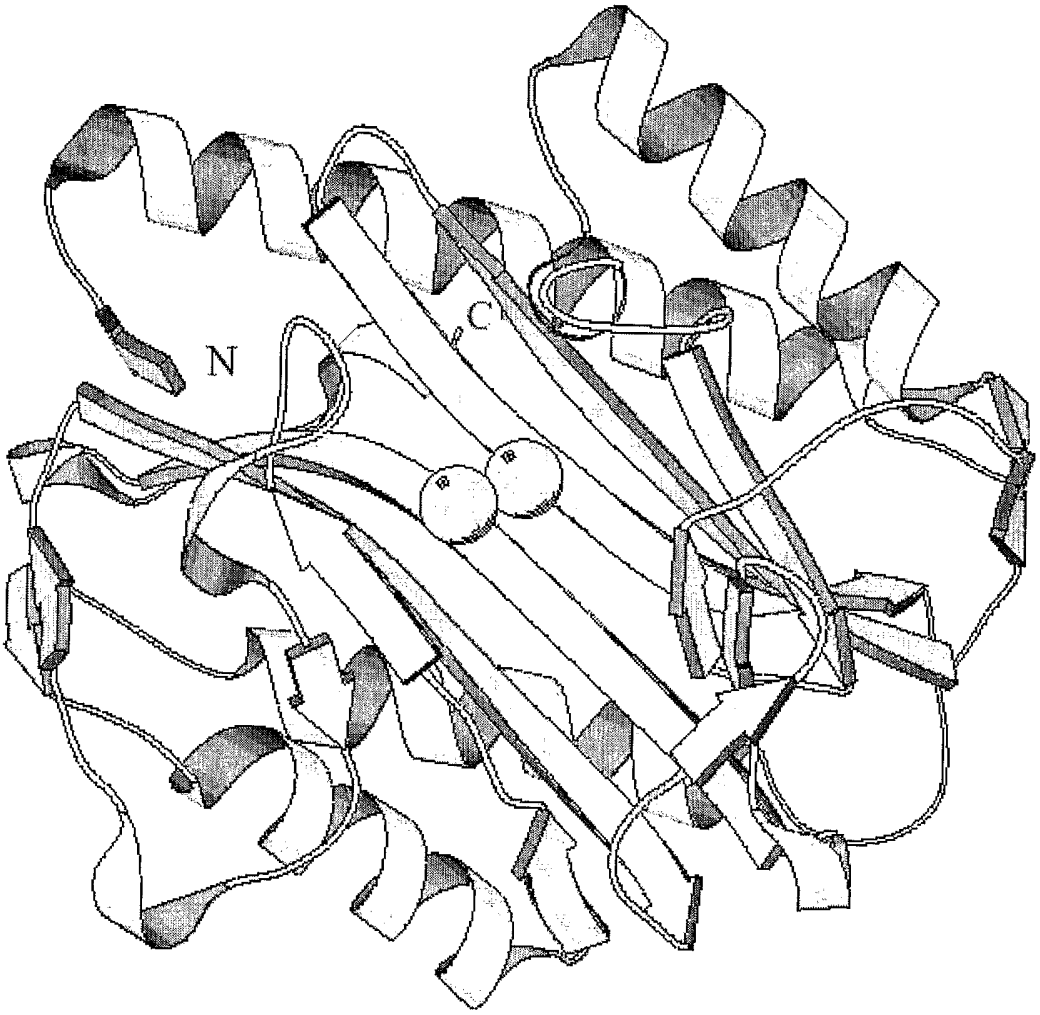


Figure 2

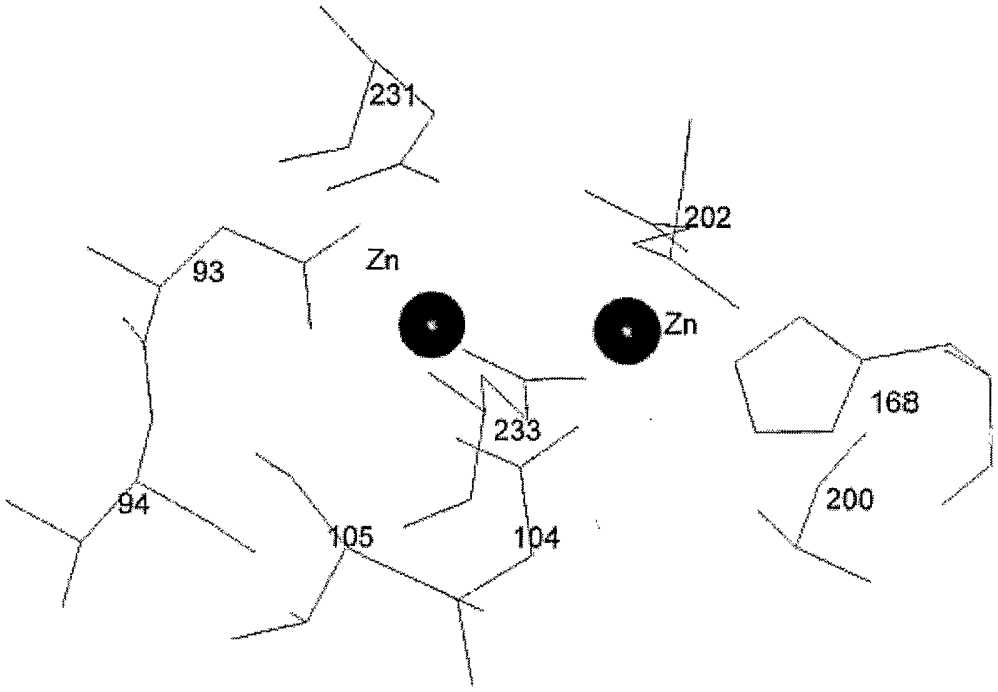


Figure 3

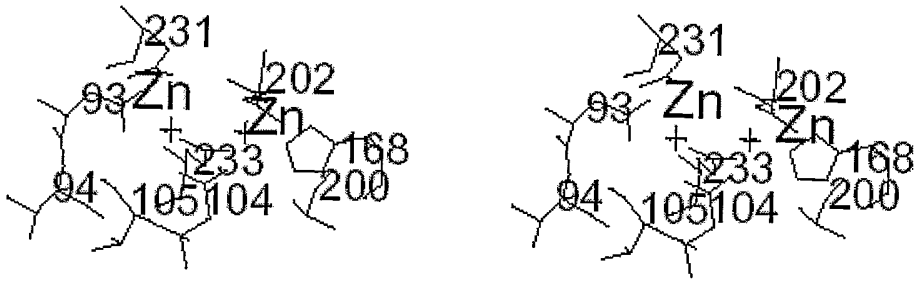

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Figure 4

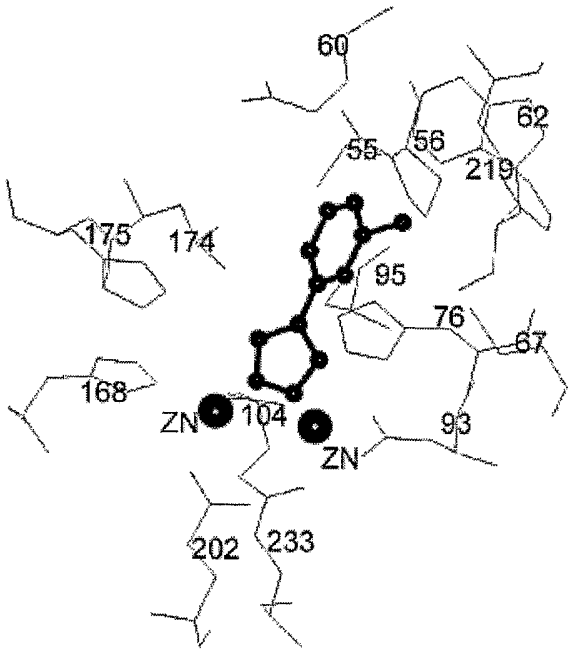


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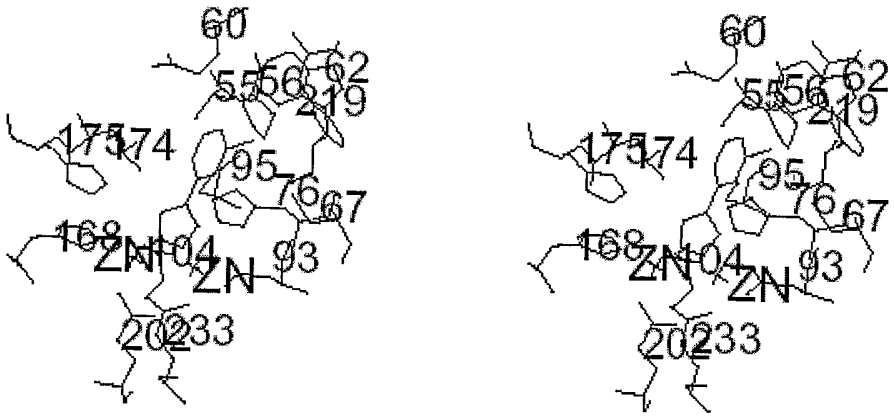

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Figure 6

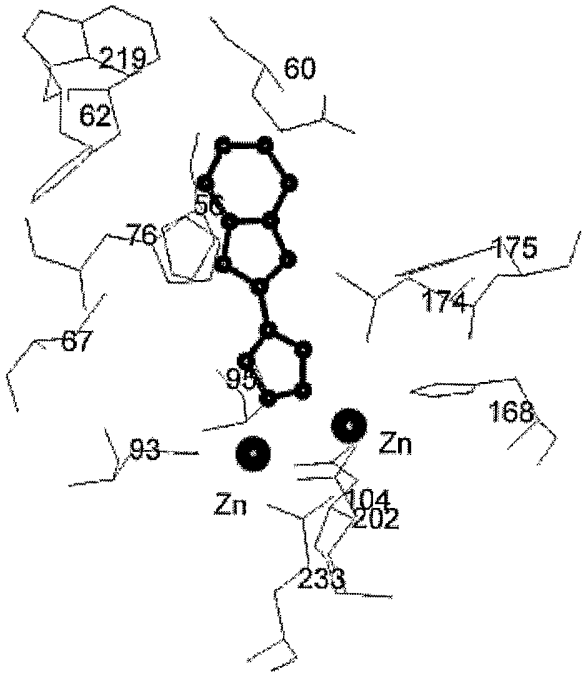


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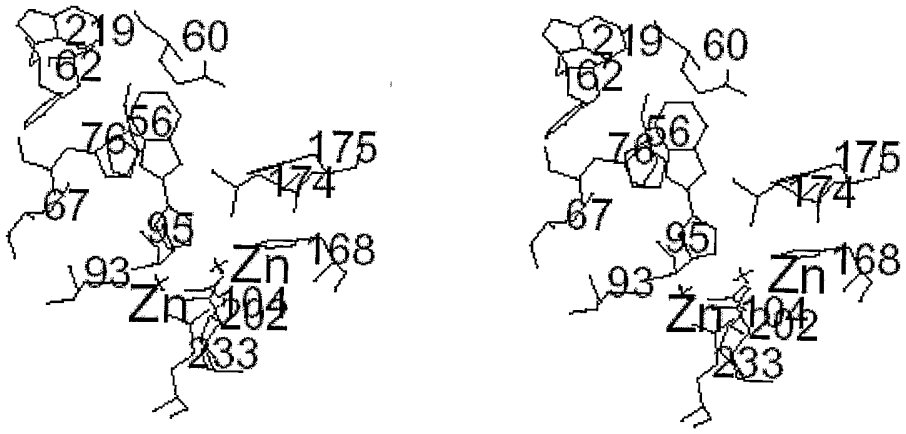

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Figure 8

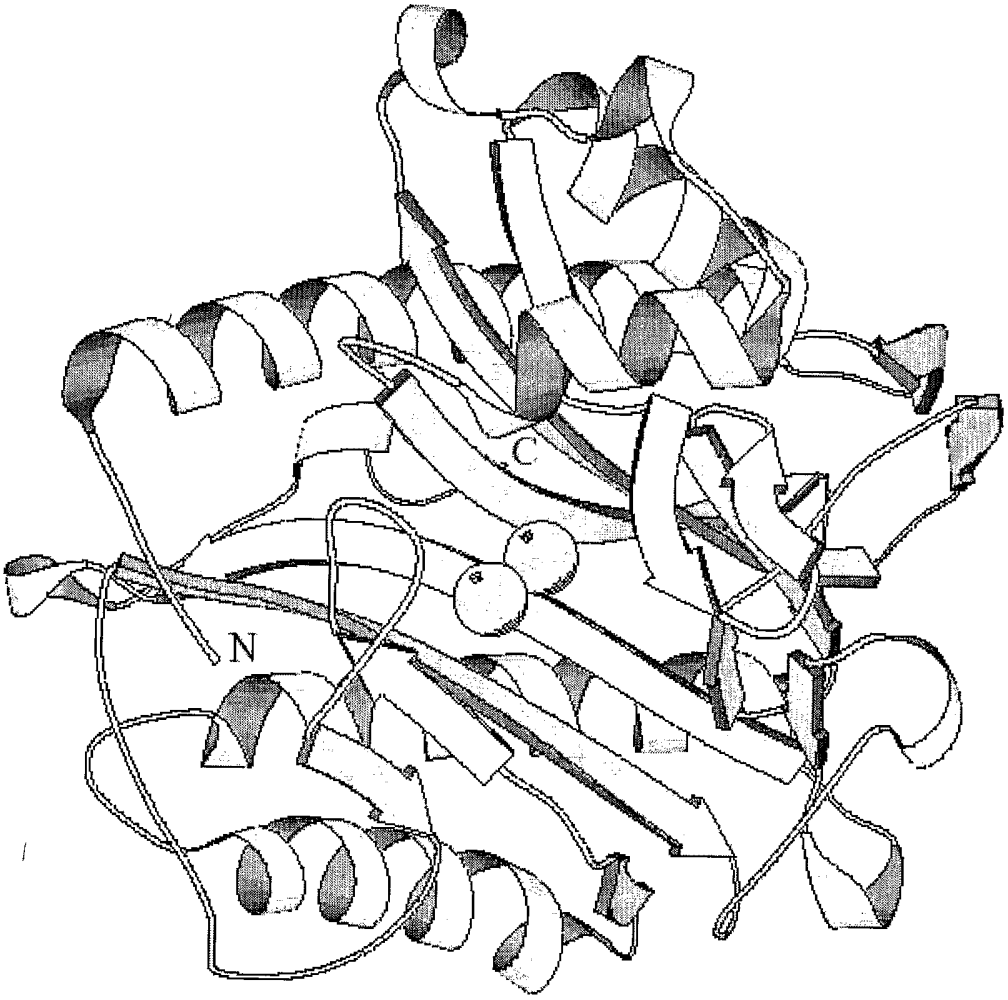


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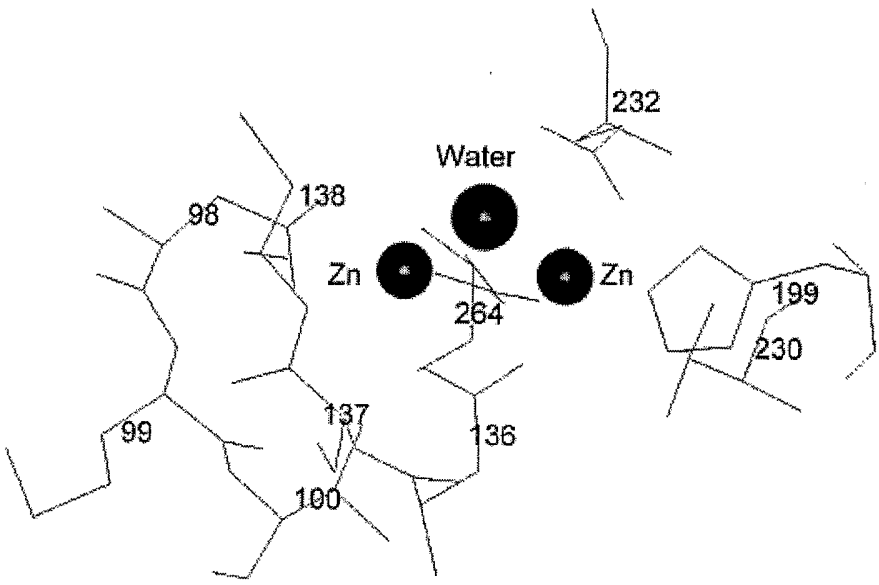
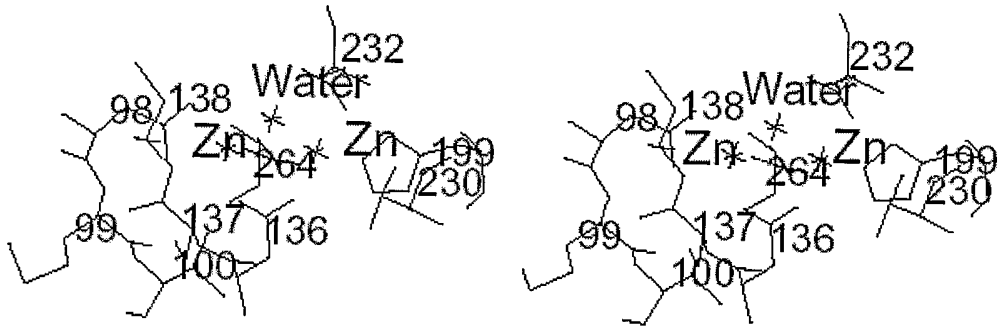


Figure 10


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