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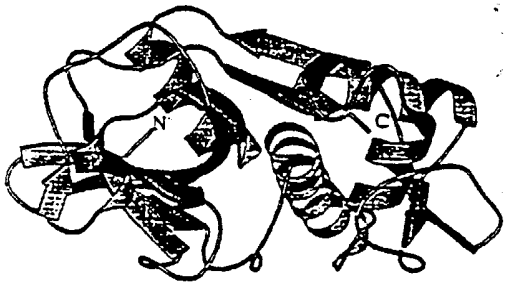
(54) Titre: Method of inhibiting cathepsin K.

(57) Abrégé: A novel cathepsin K crystalline structure is identified. Also disclosed are methods of identifying inhibitors of this protease and methods of inhibiting cathepsin K using inhibitors with certain structural, physical and spatial characteristics.



Human Cathepsin K

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METHOD OF INHIBITING CATHEPSIN K

Field of the Invention

This invention relates to a method of inhibiting cathepsin K by administering compounds with certain structural, physical and spatial characteristics that allow for the interaction of said compounds with specific residues of the active site of the enzyme. This interaction between the compounds of this invention and the active site inhibits the activity of cathepsin K and these compounds are useful for treating diseases in which said inhibition is indicated, such as osteoporosis and periodontal disease. This invention also relates to a novel crystalline structure of cathepsin K, the identification of a novel protease catalytic active site for this enzyme and methods enabling the design and selection of inhibitors of said active site.

Background of the Invention

Cathepsin K is a member of the family of enzymes which are part of the papain superfamily of cysteine proteases. Cathepsins B, H, L, N and S have been described in the literature. Recently, cathepsin K polypeptide and the cDNA encoding such polypeptide were disclosed in U.S. Patent No. 5,501,969 (called cathepsin O therein). Cathepsin K has been recently expressed, purified, and characterized. Bossard, M. J., et al., (1996) *J. Biol. Chem.* **271**, 12517-12524; Drake, F.H., et al., (1996) *J. Biol. Chem.* **271**, 12511-12516; Bromme, D., et al., (1996) *J. Biol. Chem.* **271**, 2126-2132.

Cathepsin K has been variously denoted as cathepsin O, cathepsin X or cathepsin O2 in the literature. The designation cathepsin K is considered to be the more appropriate one (name assigned by Nomenclature Committee of the International Union of Biochemistry and Molecular Biology).

Cathepsins of the papain superfamily of cysteine proteases function in the normal physiological process of protein degradation in animals, including humans, e.g., in the degradation of connective tissue. However, elevated levels of these enzymes in the body can result in pathological conditions leading to disease. Thus, cathepsins have been implicated in various disease states, including but not limited to, infections by pneumocystis carinii, trypsanoma cruzi, trypsanoma brucei brucei, and Crithidia fusiculata; as well as in schistosomiasis malaria, tumor metastasis, metachromatic leukodystrophy, muscular dystrophy, amytrophy, and the like. *See* International Publication Number WO 94/04172, published on March 3, 1994, and

references cited therein. *See also* European Patent Application EP 0 603 873 A1, and references cited therein. Two bacterial cysteine proteases from P. gingivallis, called gingipains, have been implicated in the pathogenesis of gingivitis. Potempa, J., et al. (1994) *Perspectives in Drug Discovery and Design*, **2**, 445-458.

Cathepsin K is believed to play a causative role in diseases of excessive bone or cartilage loss. Bone is composed of a protein matrix in which spindle- or plate-shaped crystals of hydroxyapatite are incorporated. Type I Collagen represents the major structural protein of bone comprising approximately 90% of the structural protein. The remaining 10% of matrix is composed of a number of non-collagenous proteins, including osteocalcin, proteoglycans, osteopontin, osteonectin, thrombospondin, fibronectin, and bone sialoprotein. Skeletal bone undergoes remodeling at discrete foci throughout life. These foci, or remodeling units, undergo a cycle consisting of a bone resorption phase followed by a phase of bone replacement.

Bone resorption is carried out by osteoclasts, which are multinuclear cells of hematopoietic lineage. The osteoclasts adhere to the bone surface and form a tight sealing zone, followed by extensive membrane ruffling on their apical (i.e., resorbing) surface. This creates an enclosed extracellular compartment on the bone surface that is acidified by proton pumps in the ruffled membrane, and into which the osteoclast secretes proteolytic enzymes. The low pH of the compartment dissolves hydroxyapatite crystals at the bone surface, while the proteolytic enzymes digest the protein matrix. In this way, a resorption lacuna, or pit, is formed. At the end of this phase of the cycle, osteoblasts lay down a new protein matrix that is subsequently mineralized. In several disease states, such as osteoporosis and Paget's disease, the normal balance between bone resorption and formation is disrupted, and there is a net loss of bone at each cycle. Ultimately, this leads to weakening of the bone and may result in increased fracture risk with minimal trauma.

The abundant selective expression of cathepsin K in osteoclasts strongly suggests that this enzyme is essential for bone resorption. Thus, selective inhibition of cathepsin K may provide an effective treatment for diseases of excessive bone loss, including, but not limited to, osteoporosis, gingival diseases such as gingivitis and periodontitis, Paget's disease, hypercalcemia of malignancy, and metabolic bone disease. Cathepsin K levels have also been demonstrated to be elevated in chondroclasts of osteoarthritic synovium. Thus, selective inhibition of cathepsin K may also be useful for treating diseases of excessive cartilage or matrix degradation, including, but not limited to, osteoarthritis and rheumatoid arthritis. Metastatic neoplastic cells also typically express high levels of proteolytic enzymes that

degrade the surrounding matrix. Thus, selective inhibition of cathepsin K may also be useful for treating certain neoplastic diseases.

Surprisingly, it has been found that a broad, structurally diverse series of compounds have common structural, physical and spatial characteristics that allow for the interaction of said compounds with specific residues of the active site of cathepsin K and are useful for treating diseases in which inhibition of bone resorption is indicated, such as osteoporosis and periodontal disease. Thus, this invention relates to the method of inhibiting cathepsin K using compounds having the characteristics hereinbelow defined.

Summary of the Invention

In one aspect, the present invention provides a method for inhibiting cathepsin K by administering compounds with certain structural, physical and spatial characteristics that allow for the interaction of said compounds with specific residues of the active site of the enzyme. This interaction inhibits the activity of cathepsin K and, thus, treats diseases in which bone resorption is a factor.

In another aspect, the present invention provides a novel cysteine protease in crystalline form.

In yet another aspect, the invention provides a novel protease composition characterized by a three dimensional catalytic site formed by the atoms of the amino acid residues listed in Table XXIX.

In still another aspect, the invention provides a method for identifying inhibitors of the compositions described above which methods involve the steps of: providing the coordinates of the protease structure of the invention to a computerized modeling system; identifying compounds which will bind to the structure; and screening the compounds or analogs derived therefrom identified for cathepsin K inhibitory bioactivity.

Other aspects and advantages of the present invention are described further in the following detailed description of the preferred embodiments thereof.

Brief Description of the Drawings

Figure 1 is the amino acid sequence of cathepsin K aligned with the amino acid sequences of other cysteine proteases.

Figure 2 is a ribbon diagram of cathepsin K. The 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 3 is a ribbon diagram of cathepsin K in complex with E-64, a known inhibitor of cysteine proteases. The drawing was produced using the program MOLSCRIPT.

Figure 4 is an illustration of the active site of cathepsin K. Figure 5 is a stereoview of the active site of cathepsin K. For clarity, no hydrogen atoms or water molecules are shown.

Figures 6, 8, 10, 12, 14, 16, 18, 20, and 22 are illustrations of the active site of cathepsin K in complex with novel inhibitors of cathepsin K. (Figure 6: Inhibitor = 3(S)-3-[(N-benzyloxycarbonyl)-L-leucinyl]amino-5-methyl-1-(1-propoxy)-2-hexane; Figure 8: Inhibitor = bis-(cbz-leucinyl)-1,3-diamino-propan-2-one; Figure 10: Inhibitor = 2,2'-N,N'-bis-benzyloxycarbonyl-L-leucinylcarbohydrazide; Figure 12: Inhibitor = (1S)-N-[2-[(1-benzyloxycarbonylamino)-3-methylbutyl]thiazol-4-ylcarbonyl]-N'-(N-benzyloxycarbonyl-L-leucinyl)hydrazide; Figure 14: Inhibitor = 2-[N-(3-benzyloxybenzoyl)]-2'-[N'-(N-benzyloxycarbonyl-L-leucinyl)]carbohydrazide; Figure 16: Inhibitor = 4-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-1-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-3-pyrrolidinone; Figure 18: Inhibitor = 4-[N-[(4-pyridylmethoxy)carbonyl]-L-leucyl]-1-[N-[(phenylmethoxy) carbonyl]-L-leucyl]-3-pyrrolidinone; Figure 20: Inhibitor = 4-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-1-N[N-(methyl)-L-leucyl)]-3-pyrrolidinone; Figure 22: Inhibitor = 1-N-(N-imidazole acetyl-leucinyl)-amino-3-N-(4-phenoxy-phenyl-sulfonyl)-amino-propan-2-one. Figures 7, 9, 11, 13, 15, 17, 19, 21 and 23 are stereoviews of the active site of cathepsin K in complex with novel inhibitors of cathepsin K. (Figure 7: Inhibitor = 3(S)-3-[(N-benzyloxycarbonyl)-L-leucinyl]amino-5-methyl-1-(1-propoxy)-2-hexane; Figure 9: Inhibitor = bis-(cbz-leucinyl)-1,3-diamino-propan-2-one; Figure 11: Inhibitor = 2,2'-N,N'-bis-benzyloxycarbonyl-L-leucinylcarbohydrazide; Figure 13: Inhibitor = (1S)-N-[2-[(1-benzyloxycarbonylamino)-3-methylbutyl]thiazol-4-ylcarbonyl]-N'-(N-benzyloxycarbonyl-L-leucinyl)hydrazide; Figure 15: Inhibitor = 2-[N-(3-benzyloxybenzoyl)]-2'-[N'-(N-benzyloxycarbonyl-L-leucinyl)]carbohydrazide; Figure 17: Inhibitor = 4-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-1-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-3-pyrrolidinone; Figure 19: Inhibitor = 4-[N-[(4-pyridylmethoxy)carbonyl]-L-leucyl]-1-[N-[(phenylmethoxy) carbonyl]-L-leucyl]-3-pyrrolidinone; Figure 21: Inhibitor = 4-[N-[(4-pyridylmethoxy)carbonyl]-L-leucyl]-1-[N-[(phenylmethoxy) carbonyl]-L-leucyl]-3-pyrrolidinone; Figure 23: Inhibitor = 1-N-(N-imidazole acetyl-leucinyl)-amino-3-N-(4-phenoxy-phenyl-sulfonyl)-amino-propan-2-one.

These views depict the interaction of each inhibitor with all atoms of residues of the active site of cathepsin K within 5Å of the inhibitors. For clarity, no hydrogen atoms or water molecules are shown.

Table I provides the three dimensional protein coordinates of the cathepsin K crystalline structure of the invention.

Tables II-X provide the three dimensional coordinates for the cathepsin K complex with specific inhibitors of the present invention.

Tables XI-XIX provide listings of the three atom angles between atoms of the inhibitors and the protein for all inhibitor atoms within 5 Ångstroms of the protein.

Tables XX-XXVIII provide listings of the distances between atoms of the inhibitors and the protein for all inhibitor atoms within 5 Ångstroms of the protein.

Table XXIX provides the atoms of the amino acid residues of the catalytic site.

Detailed Description of the Invention

The present invention provides a novel cysteine protease crystalline structure, a novel cysteine protease active site, and methods of use of the crystalline form and active site to identify protease inhibitor compounds.

In particular, the present invention provides a method for inhibiting cathepsin K by administering compounds with certain structural, physical and spatial characteristics that allow for the interaction of said compounds with specific residues of the active site of the enzyme. This interaction inhibits the activity of cathepsin K and, thus, treats diseases in which bone resorption is a factor.

Specifically, the inhibitors of cathepsin K used in the present invention interact with any two or more of the following:

1. Tyrosine 67 sidechain;
2. Hydrophobic pocket lined with atoms from methinoine 68, leucine 209, alanine 163, alanine 134 and portions of tyrosine 67;
3. Hydrogen bonds donated by glycine 66 amide nitrogen;
4. Cysteine 25 the active site nucleophile;
5. Mainchain interactions from residues glutamine 21, cysteine 22, and glycine 23;
6. Tryptophan 184 sidechain; and
7. Hydrophobic contacts with the sidechain atoms of glutamine 143 and asparagine 161 and the mainchain of alanine 137 and serine 138.

Preferably, the inhibitors of cathepsin K used in the present invention interact with any three or more of the above-identified regions of the active site.

The compounds used in the methods of the present invention possess an electrophilic carbon and either a hydrophobic group whose centroid is 5.44-6.94Å from the carbon or an aromatic group whose centroid is 9.24-11.24Å from the carbon, or both the hydrophobic and the aromatic groups in which case the centroids of these two groups should be 15.67-16.67Å apart. These features must be able to make the appropriate interactions with the cathepsin K active site. The electrophilic carbon atom should be 1.7-4.0Å from the side chain sulfur atom (SG) on the amino acid cysteine 25. The hydrophobic group should be near the following amino acids with appropriate distance ranges between the centroid of the side chain atoms and the centroid of the hydrophobic group given in parentheses: tyrosine 67 (4.91-5.91Å), methionine 68 (5.74-6.74Å), alanine 134 (4.15-5.15Å), leucine 160 (6.18-7.18Å), and leucine 209 (5.71-6.71Å). The aromatic group should be near the either tryptophan 184 (4.10-7.10Å) or tryptophan 188 (4.10-7.10Å) or both.

The key structural features of the inhibitors of the present invention include an electrophilic carbon, preferably the carbon of a carbonyl group, a hydrophobic group, preferably an isobutyl group, and an aromatic group, preferably a phenyl group. The electrophilic carbon of the inhibitor may be in the same compound with two hydrophobic groups, such as two isobutyl groups, or two aromatic groups, such as two phenyl groups, or one hydrophobic group and one aromatic group.

Suitably, the method of inhibiting cathepsin K of the present invention comprises administering to a mammal, preferably a human, in need thereof a compound that fits spatially into the active site of cathepsin K, said compound comprising any two or more of the following:

(i) an electrophilic carbon atom that binds to the side chain sulfur atom of cysteine 25 wherein said electrophilic carbon atom is 1.7-4.0Å from said sulfur atom;

(ii) a hydrophobic group that interacts with tryptophan 184 wherein the distance between the centroid of said hydrophobic group and the centroid of the side chain atoms of tryptophan 184 is 4.10-7.10Å;

(iii) a hydrophobic group that interacts with tyrosine 67, methionine 68, alanine 134, leucine 160, and leucine 209, creating a hydrophobic pocket, and has distance ranges between the centroid of said hydrophobic group and the centroids of the side chain atoms of the amino acid residues of said hydrophobic pocket which are tyrosine 67: 4.91- 5.91Å, methionine 68: 5.74-6.74Å, alanine 134: 4.15-5.15Å, leucine 160: 6.18-7.18Å, and leucine 209: 5.71-6.71Å;

(iv) a hydrophobic group that interacts with tyrosine 67 wherein the distance between the centroid of said hydrophobic group and the centroid of the side chain atoms of tyrosine 67 is 4.10-7.10Å;

(v) an amino group with a pKa of less than 7 or an oxygen atom, each of which interacts with a hydrogen atom donated by the amide nitrogen of glycine 66 wherein the distance between these two atoms is 2.7-3.5Å;

(vi) a hydrophobic group that interacts with the main chain atoms of glutamine 21, cysteine 22 and glycine 23 wherein the distance between the centroid of said hydrophobic group and the centroids of glutamine 21 , cysteine 22 and glycine 23 are 3.7-5.4, 4.9-5.7 and 5.4-6.7Å, respectively; or

(vii) a hydrophobic group that interacts with the side chain atoms of glutamine 143 and asparagine 161 and the main chain of alanine 137 and serine 138 wherein the distance between the centroid of the hydrophobic group and the centroids of glutamine 143, asparagine 161, alanine 137, and serine 138 are 7.9-9.6Å, 4.7-5.4Å, 4.2-5.5Å, and 4.6-6.4Å, respectively. Preferably, the inhibitors of cathepsin K used in the present invention comprise three or more of the above.

Suitably, the method of inhibiting cathepsin K of the present invention comprises administering to a mammal, preferably a human, in need thereof, a compound that fits spatially into the active site of cathepsin K, said compound comprising:

(i) an electrophilic carbon atom that binds to the side chain sulfur atom of cysteine 25 wherein said electrophilic carbon atom is 1.7-4.0Å from said sulfur atom; and

(ii) a hydrophobic group that interacts with tryptophan 184 wherein the distance between the centroid of said hydrophobic group and the centroid of the side chain atoms of tryptophan 184 is 4.10-7.10Å. Preferably, the hydrophobic group that interacts with tryptophan 184 is an aromatic group and the centroid of this aromatic group is 9.24-11.24Å from the centroid of the electrophilic carbon that binds to the side chain sulfur atom of cysteine 25.

Preferably, the electrophilic carbon that binds to the side chain sulfur atom of cysteine 25 is a carbonyl carbon.

Suitably, the method of the present invention further comprises a compound with a hydrophobic group that:

has a centroid which is 5.44-6.94Å from said electrophilic carbon;

interacts with tyrosine 67, methionine 68, alanine 134, leucine 160, and leucine 209, creating a hydrophobic pocket; and

has distance ranges between the centroid of said hydrophobic group and the centroids of the side chain atoms of the amino acid residues of said hydrophobic pocket which are tyrosine 67: 4.91- 5.91Å, methionine 68: 5.74-6.74Å, alanine 134: 4.15-5.15Å, leucine 160: 6.18-7.18Å, and leucine 209: 5.71-6.71Å. Preferably, this hydrophobic group is an isobutyl group.

Alternately, the method of the present invention further comprises a compound with a hydrophobic group that interacts with tyrosine 67 wherein the distance between the centroid of said hydrophobic group and the centroid of the side chain atoms of tyrosine 67 is 4.10-7.10Å. Preferably, this hydrophobic group is an aromatic group.

Alternately, the method of the present invention further comprises a compound with an amino group with a pKa of less than 7 or an oxygen atom, each of which interacts with a hydrogen atom donated by the amide nitrogen of glycine 66 wherein the distance between these two atoms is 2.7-3.5Å. Preferably, the compound comprises an oxygen atom, such as an oxygen atom of a carbonyl group or an oxygen atom of a hydroxyl group.

Alternately, the method of the present invention further comprises a compound with a hydrophobic group that interacts with the main chain atoms of glutamine 21, cysteine 22 and glycine 23 wherein the distance between the centroid of the hydrophobic group and the centroids of glutamine 21 , cysteine 22 and glycine 23 are 3.7-5.4, 4.9-5.7 and 5.4-6.7Å, respectively. Preferably, this hydrophobic group is an isobutyl group.

Alternately, the method of the present invention further comprises a compound with a hydrophobic group that interacts with the side chain atoms of glutamine 143 and asparagine 161 and the mainchain of alanine 137 and serine 138 wherein the distance between the centroid of the hydrophobic group and the centroids of glutamine 143, asparagine 161, alanine 137, and serine 138 are 7.9-9.6Å, 4.7-5.4Å, 4.2-5.5Å, and 4.6-6.4Å, respectively.

Compounds used in the method of the present invention include, but are not limited to, the following:

3(S)-3-[(N-benzyloxycarbonyl)-L-leucinyl]amino-5-methyl-1-(1-propoxy)-2-hexanone;

4-[N-[(4-pyridylmethoxy)carbonyl]-L-leucyl]-1-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-3-pyrrolidinone;

4-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-1-N-[N-(methyl)-L-leucyl)]-3-pyrrolidinone;

4-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-1-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-3-pyrrolidinone;

bis-(Cbz-leucinyl)-1,3-diamino-propan-2-one;

2-[N-(3-benzyloxybenzoyl)]-2'-[N'-(N-benzyloxycarbonyl-L-leucinyl)]carbohydrazide;

(1S)-N-[2-[(1-benzyloxycarbonylamino)-3-methylbutyl]thiazol-4-ylcarbonyl]-N'-(N-benzyloxycarbonyl-L-leucinyl)hydrazide;

1-N-(N-imidazole acetyl-leucinyl)-amino-3-N-(4-phenoxy-phenyl-sulfonyl)-amino-propan-2-one; and

2,2'-N,N'-bis-benzyloxycarbonyl-L-leucinylcarbohydrazide;

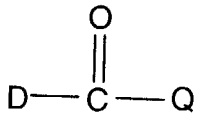
or a pharmaceutically acceptable salt thereof.

As stated herein, the interaction of the inhibitor at the side chain sulfur atom of cysteine 25 has as one of its requirements that the inhibitor contain an "electrophilic carbon" atom. By this term is meant an electron deficient carbon. This term includes, but is not limited to, a carbonyl carbon atom. This term also includes an epoxide, a thiocarbonyl, an imine, and a nitrile. Suitably, this term may also be represented by the formula -C=N-X, wherein X may be optionally tied back to C in a ring or wherein X is CH_2, H, O, S or NR^a in which R^a is H of C_{1-4}alkyl.

The hydrophobic groups that interact with tryptophan 184 or tyrosine 67 include, but are not limited to, aromatic groups. These hydrophobic groups include phenyl, C_{1-6}alkyl and heteroaryl, which is defined hereinbelow. The hydrophobic groups that interact with the hydrophobic pocket lined with atoms from tyrosine 67, methionine 68, alanine 134, leucine 160, and leucine 209 not only includes isobutyl, but also includes C_{1-6}alkyl, C_{3-6}cycloalkyl and adamantyl. The hydrophobic groups that interact with the main chain atoms of glutamine 21, cysteine 22 and glycine 23 or the side chain atoms of glutamine 143 and asparagine 161 and the mainchain of alanine 137 and serine 138 include C_{1-10}alkyl, C_bF_{2b+1}, in which b is 1-3, and aryl and heteroaryl, each of which are defined hereinbelow.

As used herein, the term "centroid" means the position for the stated atoms calculated by averaging the x coordinates of the atoms to obtain the x coordinate of the centroid, averaging the y coordinates of the atoms to obtain the y coordinate of the centroid, and averaging the z coordinates of the atoms to obtain the z coordinate of the centroid.

The compounds used in the method of the present invention include, but are not limited to, the compounds of formula (I):



I

wherein:

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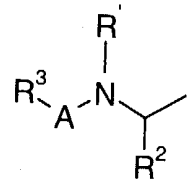
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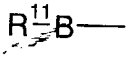
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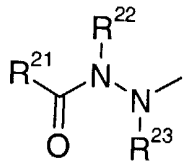
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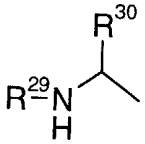
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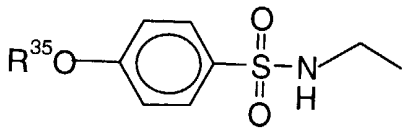
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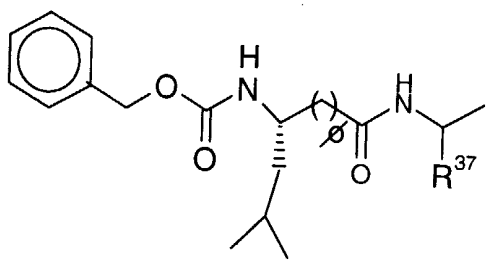
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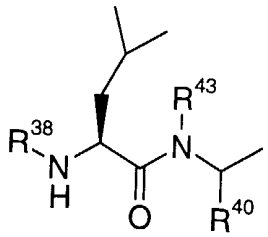
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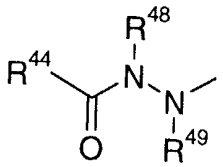
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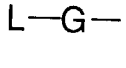
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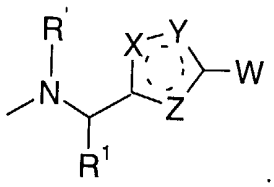
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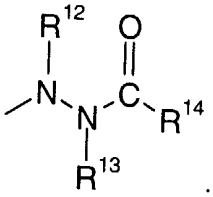
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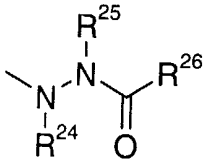
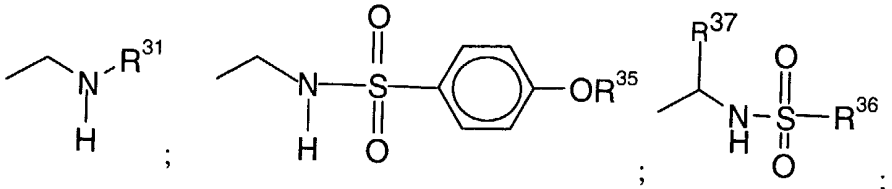
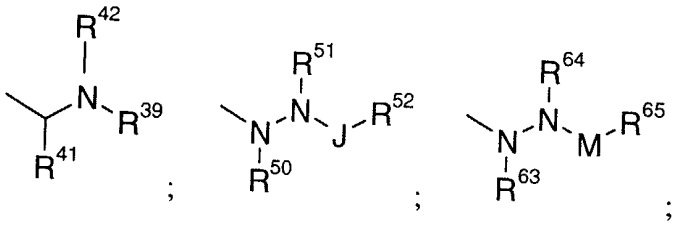
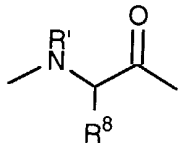
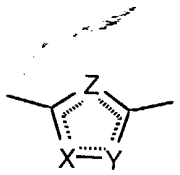
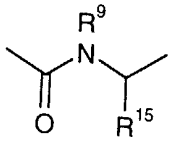



R31
N
H
O
S
O
OR35
R37
N
H
S
O
O
R36



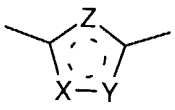
where:

A = absent,  ;

B =  ,  ;

L = C_{2-6}alkyl, Ar-C_{0-6}alkyl, Het-C_{0-6}alkyl, $CH(R^{66})NR^{60}R^{68}$, $CH(R^{66})Ar$, $CH(R^{66})OAr'$, $NR^{66}R^{67}$;

M = C(O), SO_2;

G = 

J = C(O), SO_2;

T = Ar, Het;

V = C_{3-7}cycloalkyl;

W = H, -CN, $-CF_3$, $-NO_2$, $-COR^7$, $-CO_2R^6$, $-CONHR^6$, $-SO_2NHR^6$, $-NHSO_2R^6$, $-NHCOR^7$, $-O-COR^6$, $-SR^6$, $NR'R^6$, $NR'(C=NH)NHR^5$, Cl, Br, I, F;

X = Y = Z = N, O, S or CR^4,

provided that at least two of X, Y and Z are heteroatoms and at least one of X, Y and Z is N, or one of X, Y and Z is C=N, C=C or N=N and the other two are CR^4 or N, provided that X, Y and Z together comprise at least two N;

$\doteq$ indicates a single or double bond in the five-membered heterocycle;

m = 0, 1, 2;

n = 1 to 6;

f = 0, 1, 2;

Ar = phenyl, naphthyl, optionally substituted by one or more of $Ph\text{-}C_{0\text{-}6}alkyl$, $Het\text{-}C_{0\text{-}6}alkyl$, $C_{1\text{-}6}alkoxy$, $Ph\text{-}C_{0\text{-}6}alkoxy$, $Het\text{-}C_{0\text{-}6}alkoxy$, OH, $(CH_2)_{1\text{-}6}NR^{58}R^{59}$, $O(CH_2)_{1\text{-}6}NR^{58}R^{59}$;

Ar' = phenyl or naphthyl, optionally substituted by one or more of $Ph\text{-}C_{0\text{-}6}alkyl$, $Het\text{-}C_{0\text{-}6}alkyl$, $C_{1\text{-}6}alkoxy$, $Ph\text{-}C_{0\text{-}6}alkoxy$, $Het\text{-}C_{0\text{-}6}alkoxy$, OH, $(CH_2)_{1\text{-}6}NR^{58}R^{59}$, $O(CH_2)_{1\text{-}6}NR^{58}R^{59}$, or halogen;

R' = H, $C_{1\text{-}6}alkyl$, $Ar\text{-}C_{0\text{-}6}alkyl$, $Het\text{-}C_{0\text{-}6}alkyl$;

R^1 = H, $C_{1\text{-}6}alkyl$;

R^2 = $C_{4\text{-}6}alkyl$, $C_{4\text{-}6}alkenyl$, benzyl;

R^3 = $C_{1\text{-}6}alkyl$, $Ar\text{-}C_{0\text{-}6}alkyl$, $Het\text{-}C_{0\text{-}6}alkyl$, R^5CO-, R^5SO_2-, $R^5OC(O)$-, R^5NHCO-;

R^4 = H, $C_{1\text{-}6}alkyl$, $Ar\text{-}C_{0\text{-}6}alkyl$, $Het\text{-}C_{0\text{-}6}alkyl$;

R^5 = $Ar\text{-}_{0\text{-}6}alkyl$, $Het\text{-}C_{0\text{-}6}alkyl$;

R^6 = H, $C_{1\text{-}6}alkyl$, CH_2CF_3, $Ar\text{-}C_{0\text{-}6}alkyl$, $Het\text{-}C_{0\text{-}6}alkyl$;

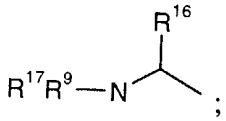
R^7 = $C_{1\text{-}6}alkyl$, $Ar\text{-}C_{0\text{-}6}alkyl$, $Het\text{-}C_{0\text{-}6}alkyl$;

R^8 = H; C_{2-6} alkenyl; C_{2-6}alkynyl; Het; Ar; C_{1-6}alkyl, optionally substituted by OR', SR', NR'_2, CO_2R', $CO_2NR'_2$, $N(C=NH)NH_2$, Het or Ar;

R^9 = H, C_{1-6}alkyl, Ar-C_{0-6}alkyl, Het-C_{0-6}alkyl;

R^{10} = C_{1-6}alkyl, Ar-C_{0-6}alkyl, Het-C_{0-6}alkyl;

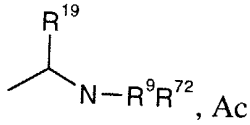
R^{11} = H, C_{1-6}alkyl, Ar-C_{1-6}alkyl, Het-C_{0-6}alkyl, or



;

R^{12} = H, C_{1-6}alkyl, Ar-C_{0-6}alkyl, Het-C_{0-6}alkyl;

R^{13} = H, C_{1-6}alkyl, Ar-C_{0-6}alkyl, Het-C_{0-6}alkyl;

R^{14} =  , Ac;

R^{15} = H, C_{1-6}alkyl, C_{2-6}alkenyl, C_{2-6}alkynyl, Ar, Het, or C_{1-6}alkyl optionally substituted by OR^9, NR^9_2, $CONR^9_2$, $N(C=NH)NH$-, Het or Ar;

R^{16} = C_{2-6}alkyl, C_{2-6}alkenyl, C_{2-6}alkynyl, Ar, Het, or C_{2-6}alkyl optionally substituted by OR^9, SR^9, NR^9_2, CO_2R^9, $CONR^9_2$, $N(C=NH)NH$-, Het or Ar;

R^{19} = H, C_{1-6}alkyl, C_{2-6}alkenyl, C_{2-6}alkynyl, Ar, Het, or C_{1-6}alkyl optionally substituted by OR^9, SR^9, NR^9_2, CO_2R^9, $CONR^9_2$, $N(C=NH)NH$-, Het or Ar;

R^{17} = R^{72} = H, C_{1-6}alkyl, R^{10}, $R^{10}C(O)$-, $R^{10}C(S)$-, $R^{10}OC(O)$-;

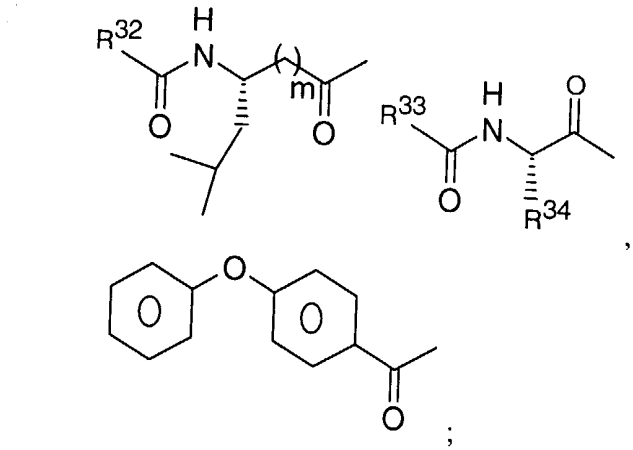
R^{21} = R^{26} = C_{5-6}alkyl; C_{2-6}alkenyl; C_{3-11}cycloalkyl; T-C_{3-6}alkyl; V-C_{1-6}alkyl; T-C_{2-6}alkenyl; T- $(CH_2)_nCH(T)(CH_2)_n$; optionally substituted by one or two halogens, SR^{20}, OR^{20},$NR^{20}R^{27}$ or C_{1-4}alkyl;

R^{27} = $R^{28}CO$, $R^{28}OCO$;

R^{28} = C_{1-6}alkyl; C_{3-11}cycloalkyl; Ar; Het; T-C_{1-6}alkyl; T-$(CH_2)_nCH(T)(CH_2)_n$; optionally substituted by one or two halogens, SR^{20}, OR^{20}, $NR^{20}R^{73}$, C_{1-6}alkyl;

R^{20} = R^{22} = R^{23} = R^{24} = R^{25} = R^{73} = H, C_{1-4}alkyl, Ar-C_{0-6}alkyl, Het-C_{0-6}alkyl;

R^{29} =



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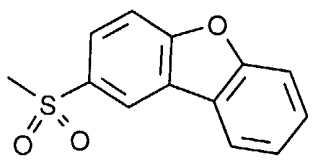
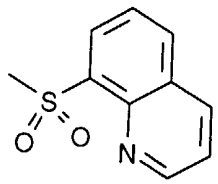
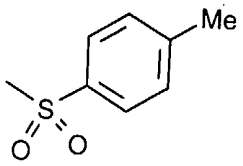
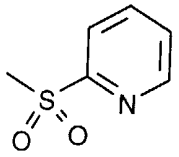
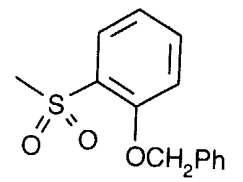
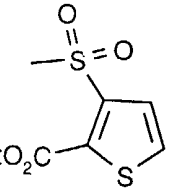








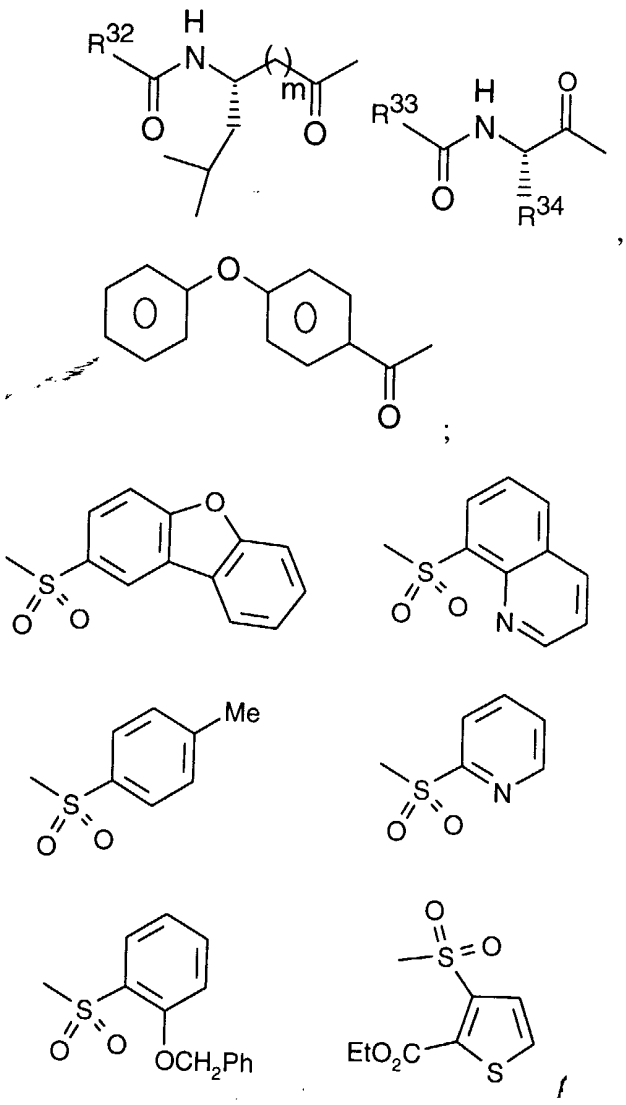




Cbz-leucinyl-; 2-, 3-, or 4-pyridyl methyloxycarbonyl-leucinyl-; 4-imidazole acetyl-leucinyl-, phenyl acetyl-leucinyl, N,N-dimethyl-glycinyl leucinyl, 4-pyridyl acetyl-leucinyl, 2-pyridyl sulfonyl-leucinyl, 4-pyridyl carbonyl-leucinyl, acetyl-leucinyl, benzoyl-leucinyl, 4-phenoxy-benzoyl-, 2- or 3-benzyloxybenzoyl-, biphenyl acetyl, lpha- isobutyl-biphenyl acetyl, Cbz-phenylalaninyl, Cbz-norleucinyl-, Cbz-norvalinyl-, Cbz-glutamyl-, Cbz-epsilon- (t-butyl ester)-glutamyl; acetyl-leucinyl-, 6- or 8- quinoline carbonyl, biphenyl acetyl, alpha- isobutyl-biphenyl acetyl, acetyl, benzoyl, 2- or 3- benzyloxy benzoyl, 4-phenoxy benzoyl-, Cbz-amino acid-; 2-,3-, or 4- pyridylmethyloxycarbonyl-aminoacid-; aryl C_0-C_6alkyloxy carbonyl-amino acid-, heteroaryl C_0-C_6alkyloxy carbonyl-amino acid-,aryl C_0-C_6alkyloxy carbonyl-amino acid-, heteroaryl C_0-C_6alkyloxy carbonyl-amino acid-, C_1-C_6alkyloxy carbonyl-amino acid-; C_1-C_6alkyl carbonyl, aryl C_0-C_6alkyl carbonyl, heteroaryl C_0-C_6alkyl carbonyl, aryl C_0-C_6alkyl carbonyl, heteroaryl C_0-C_6alkyl carbonyl, C_1-C_6alkyl sulfonyl, aryl C_0-C_6alkyl sulfonyl, heteroarylC_0-C_6alkyl sulfonyl, aryl C_0-C_6alkyl sulfonyl, heteroaryl C_0-C_6alkyl sulfonyl;

R^{30} = -H, C_1-6 alkyl;

R^{31} =



Cbz-leucinyl-; 2-, 3-, or 4-pyridyl methyloxycarbonyl-leucinyl-; 4-imidazole acetyl-leucinyl-, phenyl acetyl-leucinyl, N,N-dimethyl-glycinyl leucinyl, 4-pyridyl acetyl-leucinyl, 2-pyridyl sulfonyl-leucinyl, 4-pyridyl carbonyl-leucinyl, acetyl-leucinyl, benzoyl-leucinyl, 4-phenoxy-benzoyl-, 2- or 3-benzyloxybenzoyl-, biphenyl acetyl, alpha- isobutyl-biphenyl acetyl, Cbz-phenylalaninyl, Cbz-norleucinyl-, Cbz-norvalinyl-, Cbz-glutamyl-, Cbz-epsilon- (t-butyl ester)-glutamyl; acetyl-leucinyl-, 6- or 8- quinoline

carbonyl, biphenyl acetyl, alpha- isobutyl-biphenyl acetyl, acetyl, benzoyl, 2- or 3- benzyloxy benzoyl, 4-phenoxy benzoyl-, Cbz-amino acid-; 2-,3-, or 4- pyridylmethyloxycarbonyl-aminoacid-; aryl C_0-C_6alkyloxy carbonyl-amino acid-, heteroaryl C_0-C_6alkyloxy carbonyl-amino acid-,aryl C_0-C_6alkyloxy carbonyl-amino acid-, heteroaryl C_0-C_6alkyloxy carbonyl-amino acid-, C_1-C_6alkyloxy carbonyl-amino acid-; C_1-C_6alkyl carbonyl, aryl C_0-C_6alkyl carbonyl, heteroaryl C_0-C_6alkyl carbonyl, aryl C_0-C_6alkyl carbonyl, heteroaryl C_0-C_6alkyl carbonyl, C_1-C_6alkyl sulfonyl, aryl C_0-C_6alkyl sulfonyl, heteroaryl C_0-C_6alkyl sulfonyl, aryl C_0-C_6alkyl sulfonyl, heteroaryl C_0-C_6alkyl-sulfonyl;

R^{32} = OCH_2Ar, OCH2$C_{1\text{-}6}$alkyl, aryl substituted $C_{0\text{-}6}$alkyl, heteroaryl substituted $C_{0\text{-}6}$alkyl,4-imidazole methylene; 2-, 3-, or 4-pyridylmethylneneoxy; 4-pyridyl methylene, 2-pyridyl sulfonyl, 4-pyridyl, aryl substituted $C_{0\text{-}6}$alkyloxy, heteroaryl substituted $C_{0\text{-}6}$alkyloxy;

R^{33} = $C_{1\text{-}6}$alkyl, $-CH_2Ph$, $-CH_2CH_2CO_2R^{34}$;

R^{34} = -H, $C_{1\text{-}6}$alkyl;

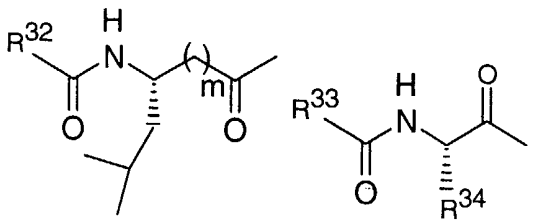
R^{35} = Ar, HetAr;

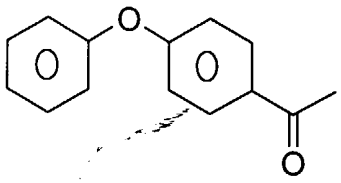
R^{36} = Aryl, heteroaryl, pyridyl, isoquinolinyl;

R^{37}= $C_{1\text{-}6}$alkyl, $-CH_2Ph$, $-CH_2CH_2CO_2R^{34}$;

R^{38} = Cbz; $C_{1\text{-}6}$alkyl or aryl substituted Cbz; $C_{1\text{-}6}$alkyl -CO; benzoyl; $C_{1\text{-}6}$alkyl or aryl substituted benzoyl;

R^{39} =





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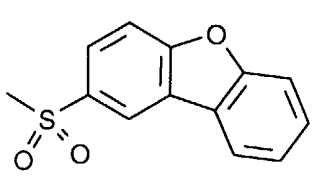
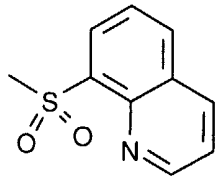
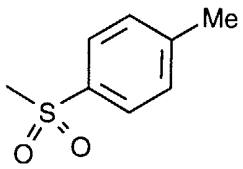
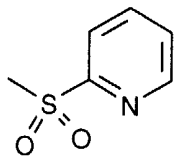
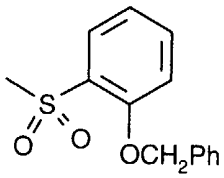
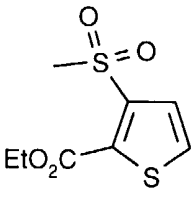












Cbz-leucinyl-; 2-, 3-, or 4-pyridyl methyloxycarbonyl-leucinyl-; 4-imidazole acetyl-leucinyl-, phenyl acetyl-leucinyl, N,N-dimethyl-glycinyl leucinyl, 4-pyridyl acetyl-leucinyl, 2-pyridyl sulfonyl-leucinyl, 4-pyridyl carbonyl-leucinyl, acetyl-leucinyl, benzoyl-leucinyl, 4-phenoxy-benzoyl-, 2- or 3-benzyloxybenzoyl-, biphenyl acetyl, alpha- isobutyl-biphenyl acetyl, Cbz-phenylalaninyl, Cbz-norleucinyl-, Cbz-norvalinyl-, Cbz-glutamyl-, Cbz-epsilon- (t-butyl ester)-glutamyl; acetyl-leucinyl-, 6- or 8- quinoline

carbonyl, biphenyl acetyl, alpha- isobutyl-biphenyl acetyl, acetyl, benzoyl, 2- or 3- benzyloxy benzoyl, 4-phenoxy benzoyl-, Cbz-amino acid-; 2-,3-, or 4- pyridylmethyloxycarbonyl-aminoacid-; aryl C_0-C_6alkyloxy carbonyl-amino acid-, heteroaryl C_0-C_6alkyloxy carbonyl-amino acid-,aryl C_0-C_6alkyloxy carbonyl-amino acid-,heteroaryl C_0-C_6alkyloxy carbonyl-amino acid-, C_1-C_6alkyloxy carbonyl-amino acid-; C_1-C_6alkyl carbonyl, aryl C_0-C_6alkyl carbonyl, heteroaryl C_0-C_6alkyl carbonyl, aryl C_0-C_6alkyl carbonyl, heteroaryl C_0-C_6alkyl carbonyl, C_1-C_6alkyl sulfonyl, aryl C_0-C_6alkyl sulfonyl, heteroaryl C_0-C_6alkyl sulfonyl, aryl C_0-C_6alkyl sulfonyl, heteroaryl C_0-C_6alkyl-sulfonyl;

R^{40} = H and C_{1-6}alkyl;

R^{41} = H and C_{1-6}alkyl;

R^{42} = C_{1-6}alkyl, aryl substituted C_{1-6}alkyl and hetero aryl substituted C_{1-6}alkyl,; H when R^{43} is C_{1-6}alkyl, aryl substituted C_{1-6}alkyl; and heteroaryl substituted C_{1-6}alkyl;

R^{43} = C_{1-6}alkyl, aryl substituted C_{1-6}alkyl and hetero aryl substituted C_{1-6}alkyl,; H when R^{42} is C_{1-6}alkyl, aryl substituted C_{1-6}alkyl; and heteroaryl substituted C_{1-6}alkyl;

R^{44} = $CH(R^{53})NR^{45}R^{54}$, $CH(R^{55})Ar$, C_{5-6}alkyl;

R^{45} = R^{46} = R^{47} = R^{48} = R^{49} = R^{50} = R^{51} = H, C_{1-6}alkyl, Ar-C_{0-6}alkyl, Het-C_{0-6}alkyl;

R^{52} = Ar, Het, $CH(R^{56})Ar$, $CH(R^{56})OAr$, $N(R^{56})Ar$, C_{1-6}alkyl, $CH(R^{56})NR^{46}R^{57}$;

R^{53} = C_{2-6}alkyl, Ar-C_{0-6}alkyl, Het-C_{0-6}alkyl, R^{53} and R^{45} may be connected to form a pyrrolidine or piperidine ring;

R^{54} = R^{57} = R^{47}, $R^{47}C(O)$, $R^{47}C(S)$, $R^{47}OC(O)$;

$R^{55} = R^{56} = R^{58} = R^{59} = H$, C_{1-6}alkyl, Ar-C_{0-6}alkyl, Het-C_{0-6}alkyl;

$R^{60} = R^{61} = R^{62} = R^{63} = R^{64} = H$, C_{1-6}alkyl, Ar-C_{0-6}alkyl, or Het-C_{0-6}alkyl;

R^{65} = C_{1-6}alkyl, Ar, Het, $CH(R^{69})Ar$, $CH(R^{69})OAr$, $N(R^{69})Ar$, $CH(R^{69})NR^{61}R^{70}$;

$R^{66} = R^{69} = R^{71} = H$, C_{1-6}alkyl, $(CH_2)_{0-6}$-C_{3-6}cycloalkyl, Ar-C_{0-6}alkyl, Het-C_{0-6}alkyl;

R^{67} = C_{1-6}alkyl, $(CH_2)_{0-6}$-C_{3-6}cycloalkyl, Ar-C_{0-6}alkyl, Het-C_{0-6}alkyl; R^{66} and R^{67} may be combined to form a 3-7 membered monocyclic or 7-10-membered bicyclic carbocyclic or heterocyclic ring, optionally substituted with 1-4 of C_{1-6}alkyl, Ph-C_{0-6}alkyl, Het-C_{0-6}alkyl, C_{1-6}alkoxy, Ph-C_{0-6}alkoxy, Het-C_{0-6}alkoxy, OH, $(CH_2)_{1-6}NR^{58}R^{59}$, $O(CH_2)_{1-6}NR^{58}R^{59}$;

$R^{68} = R^{70} = R^{62}$, $R^{62}C(O)$, $R^{62}C(S)$, $R^{62}OC(O)$, $R^{62}OC(O)NR^{59}CH(R^{71})(CO)$;

and pharmaceutically acceptable salts thereof.

The compounds of Formula I are hydrazidyl, bis-hydrazidyl and bis-aminomethyl carbonyl compounds having in common key structural features required of protease substrates, most particularly cathepsin K substrates. These structural features endow the present compounds with the appropriate molecular shape necessary to fit into the enzymatic active site, to bind to such active site, thereby blocking the site and inhibiting enzymatic biological activity. Referring to Formula I, such structural features include the central electrophilic carbonyl, a peptidyl or peptidomimetic molecular backbone on either side of the central carbonyl, a terminal carbobenzyloxy moiety (e.g., Cbz-leucinyl), or a mimic thereof, on the backbone on one or both sides of the carbonyl, and optionally, an isobutyl side chain extending from the backbone on one or both sides of the carbonyl.

Abbreviations and symbols commonly used in the peptide and chemical arts are used herein to describe the compounds of the present invention. In general, the amino acid abbreviations follow the IUPAC-IUB Joint Commission on Biochemical Nomenclature as described in *Eur. J. Biochem.*, 158, 9 (1984). The term "amino acid" as used herein refers to the D- or L- isomers of alanine, arginine, asparagine, aspartic acid, cysteine, glutamine, glutamic acid, glycine, histidine, isoleucine, leucine, lysine, methionine, phenylalanine, proline, serine, threonine, tryptophan, tyrosine and valine.

"C_{1-6}alkyl" as applied herein is meant to include substituted and unsubstituted 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 two halogens, SR', OR', $N(R')_2$, $C(O)N(R')_2$, carbamyl or C_{1-4}alkyl, where R' is C_{1-6}alkyl. C_0alkyl means that no alkyl group is present in the moiety. Thus, Ar-C_0alkyl is equivalent to Ar.

"C_{3-11}cycloalkyl" as applied herein is meant to include substituted and unsubstituted cyclopropane, cyclobutane, cyclopentane, cyclohexane, cycloheptane, cyclooctane, cyclononane, cyclodecane, cycloundecane.

"C_{2-6} alkenyl" as applied 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 the several isomeric pentenes and hexenes. Both cis and trans isomers are included.

"C_{2-6}alkynyl" 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.

"Halogen" means F, Cl, Br, and I.

"Ar" or "aryl" means phenyl or naphthyl, optionally substituted by one or more of Ph-C_{0-6}alkyl, Het-C_{0-6}alkyl, C_{1-6}alkoxy, Ph-C_{0-6}alkoxy, Het-C_{0-6}alkoxy, OH, $(CH_2)_{1-6}NR^{58}R^{59}$, $O(CH_2)_{1-6}NR^{58}R^{59}$; where R^{58}, R^{59} is H, C_{1-6}alkyl, Ar-C_{0-6}alkyl; Het-C_{0-6}alkyl, from C_{1-4}alkyl, OR', $N(R')_2$, SR', CF_3, NO_2, CN, CO_2R', CON(R'), F, Cl, Br and I.

As used herein "Het" or "heterocyclic" represents a stable 5- to 7-membered monocyclic or a stable 7- to 10-membered bicyclic heterocyclic ring, which is either saturated or unsaturated, and which consists of carbon atoms and from one to three heteroatoms selected from the group consisting of N, O and S, and wherein the

nitrogen and sulfur heteroatoms may optionally be oxidized, and the nitrogen heteroatom may optionally be quaternized, and including any bicyclic group in which any of the above-defined heterocyclic rings is fused to a benzene ring. The heterocyclic ring may be attached at any heteroatom or carbon atom which results in the creation of a stable structure, and may optionally be substituted with one or two moieties selected from C_{1-4}alkyl, OR', $N(R')_2$, SR', CF_3, NO_2, CN, CO_2R', CON(R'), F, Cl, Br and I, where R' is C_{1-6}alkyl. Examples of such heterocycles include piperidinyl, piperazinyl, 2-oxopiperazinyl, 2-oxopiperidinyl, 2-oxopyrrolodinyl, 2-oxoazepinyl, azepinyl, pyrrolyl, 4-piperidonyl, pyrrolidinyl, pyrazolyl, pyrazolidinyl, imidazolyl, pyridyl, pyrazinyl, oxazolidinyl, oxazolinyl, oxazolyl, isoxazolyl, morpholinyl, thiazolidinyl, thiazolinyl, thiazolyl, quinuclidinyl, indolyl, quinolinyl, isoquinolinyl, benzimidazolyl, benzopyranyl, benzoxazolyl, furyl, pyranyl, tetrahydrofuryl, tetrahydropyranyl, thienyl, benzoxazolyl, thiamorpholinyl sulfoxide, thiamorpholinyl sulfone, and oxadiazolyl.

"HetAr" or "heteroaryl" means any heterocyclic moiety encompassed by the above definition of Het which is aromatic in character, e.g., pyridine.

It will be appreciated that the heterocyclic ring,

, includes thiazoles, oxazoles, triazoles, thiadiazoles, oxadiazoles, isoxazoles, isothiazols, imidazoles, pyrazines, pyridazines, pyrimidines, triazines and tetrazines which are available by routine chemical synthesis and are stable. The single and double bonds (i.e., - -) in such heterocycles are arranged based upon the heteroatoms present so that the heterocycle is aromatic (e.g., it is a heteroaryl group). The term heteroatom as applied herein refers to oxygen, nitrogen and sulfur. When the heteroaryl group comprises a five membered ring, W is preferably an electron withdrawing group, such as halogen, -CN, $-CF_3$, $-NO_2$, $-COR^7$, $-CO_2R^6$, $-CONHR^6$, $-SO_2NHR^6$, $-NHSO_2R^6$, $-NHCOR^7$, $-O-COR^6$, $-SR^6$ or $NR'R^6$, or a similar electron withdrawing substituent as known in the art.

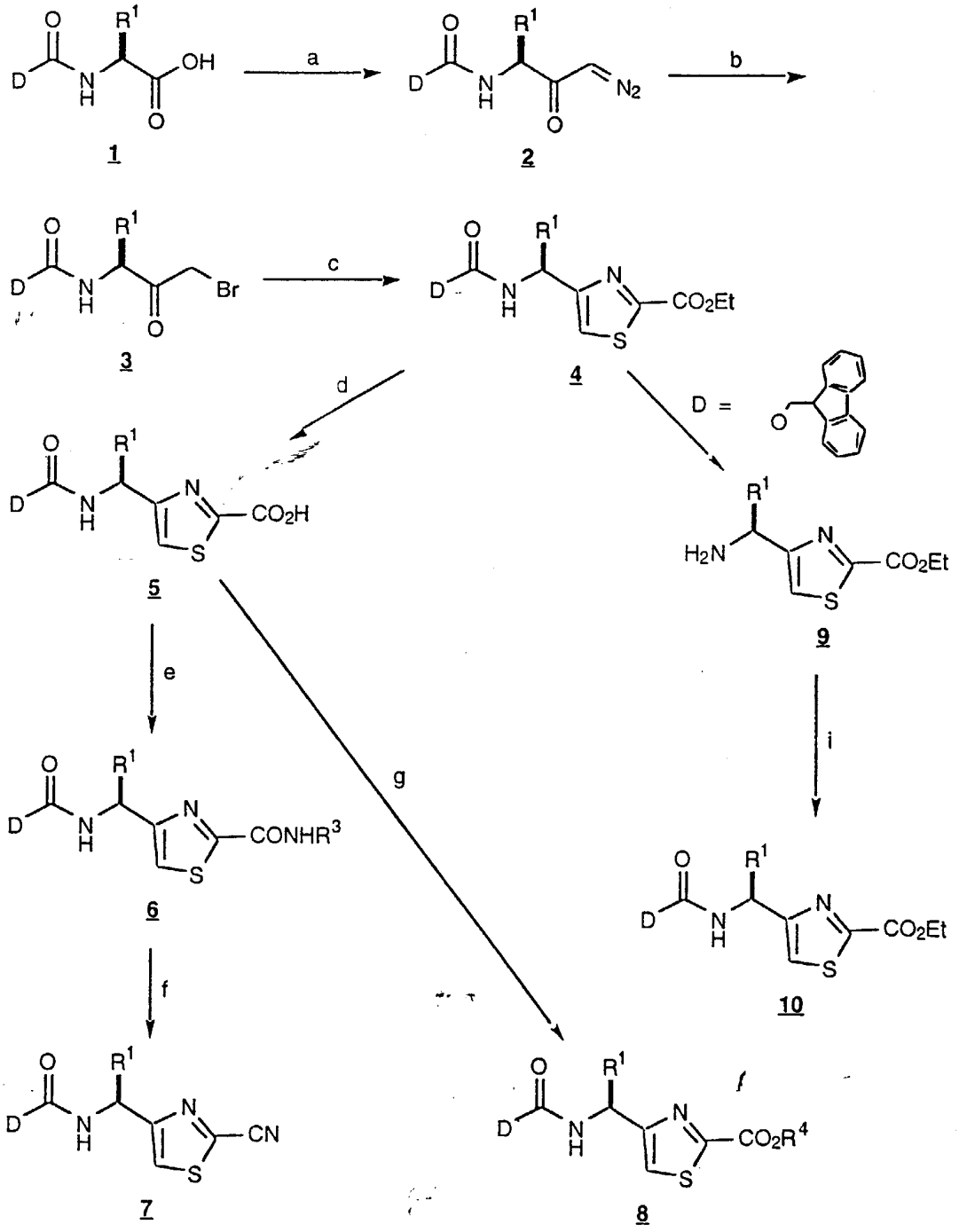
Certain radical groups are abbreviated herein. t-Bu refers to the tertiary butyl radical, Boc refers to the t-butyloxycarbonyl radical, Fmoc refers to the fluorenylmethoxycarbonyl radical, Ph refers to the phenyl radical, Cbz refers to the benzyloxycarbonyl radical.

Certain reagents are abbreviated herein. DCC refers to dicyclohexylcarbodiimide, DMAP is 2,6-dimethylaminopyridine, EDC refers to N-ethyl-N'(dimethylaminopropyl)-carbodiimide. HOBT refers to 1-hydroxybenzotriazole, DMF refers to dimethyl formamide, BOP refers to

benzotriazol-1-yloxy-tris(dimethylamino)phosphonium hexafluorophosphate, DMAP is dimethylaminopyridine, Lawesson's reagent is 2,4-bis(4-methoxyphenyl)-1,3-dithia-2,4-diphosphetane-2,4-disulfide, NMM is N-methylmorpholine, TFA refers to trifluoroacetic acid, TFAA refers to trifluoroacetic anhydride and THF refers to tetrahydrofuran. Jones reagent is a solution of chromium trioxide, water, and sulfuric acid well-known in the art.

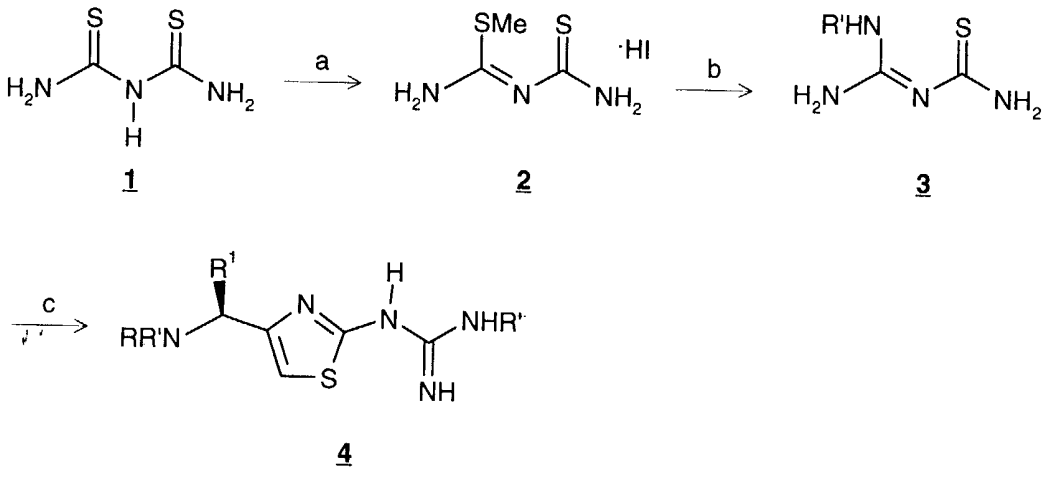
Compounds of formula (I) are prepared according to the methods detailed in Schemes 1-25.

Scheme 1



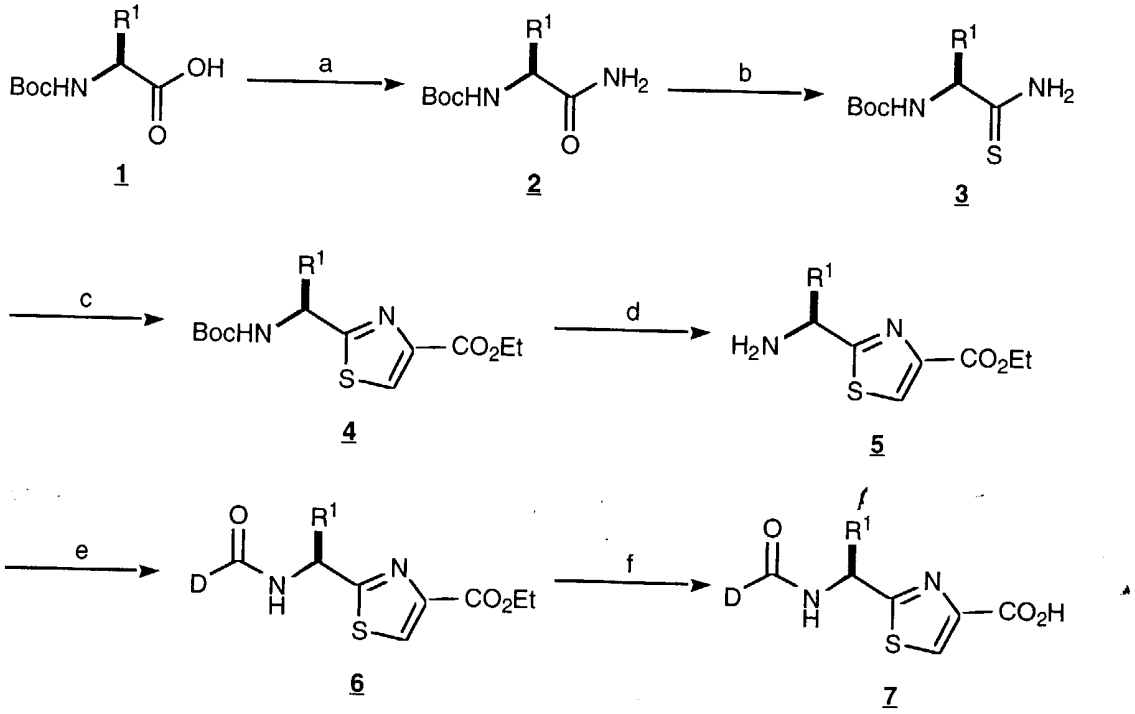
a) i-BuOCOCl, NMM, CH_2N_2, EtOAc, Et_2O; b) HBr, AcOH, EtOAc, Et_2O; c) H_2NCSCO_2Et, EtOH; d) NaOH, H_2O, THF; e) i-BuOCOCl, NMM, NH_2, THF or BOP, Et_3N, RNH_2, CH_2Cl_2; f) TFAA, pyridine, CH_2Cl_2; g) R^4OH, Boc_2O, Pyridine or R^4OH, EDCI, CH_2Cl_2; h) piperidine, DMF; i) BOP, Et_3N, D-CO_2H, CH_2Cl_2

Scheme 1A



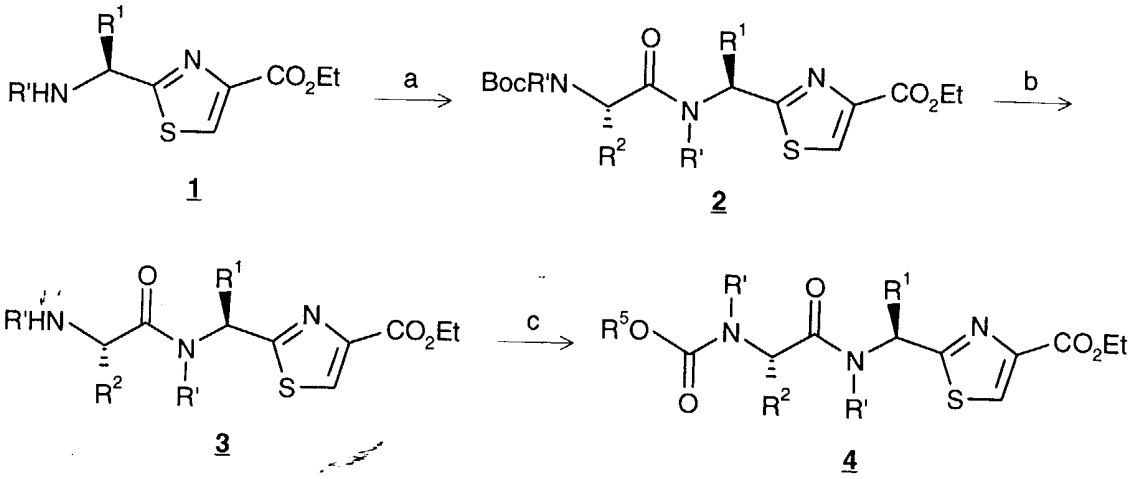
a) MeI, THF; b) $R'NH_2$, *i*-PrOH; c) Bromomethyl ketone, EtOH

Scheme 2



a) *i*-BuOCOCl, NMM, NH_3, THF; b) Lawesson's reagent, THF; c) $BrCH_2COCO_2Et$, TFAA, Pyridine, CH_2Cl_2; d) TFA; e) DCO_2H, EDC•HCl, HOBT, Et_3N, DMF; f) NaOH, H_2O, THF

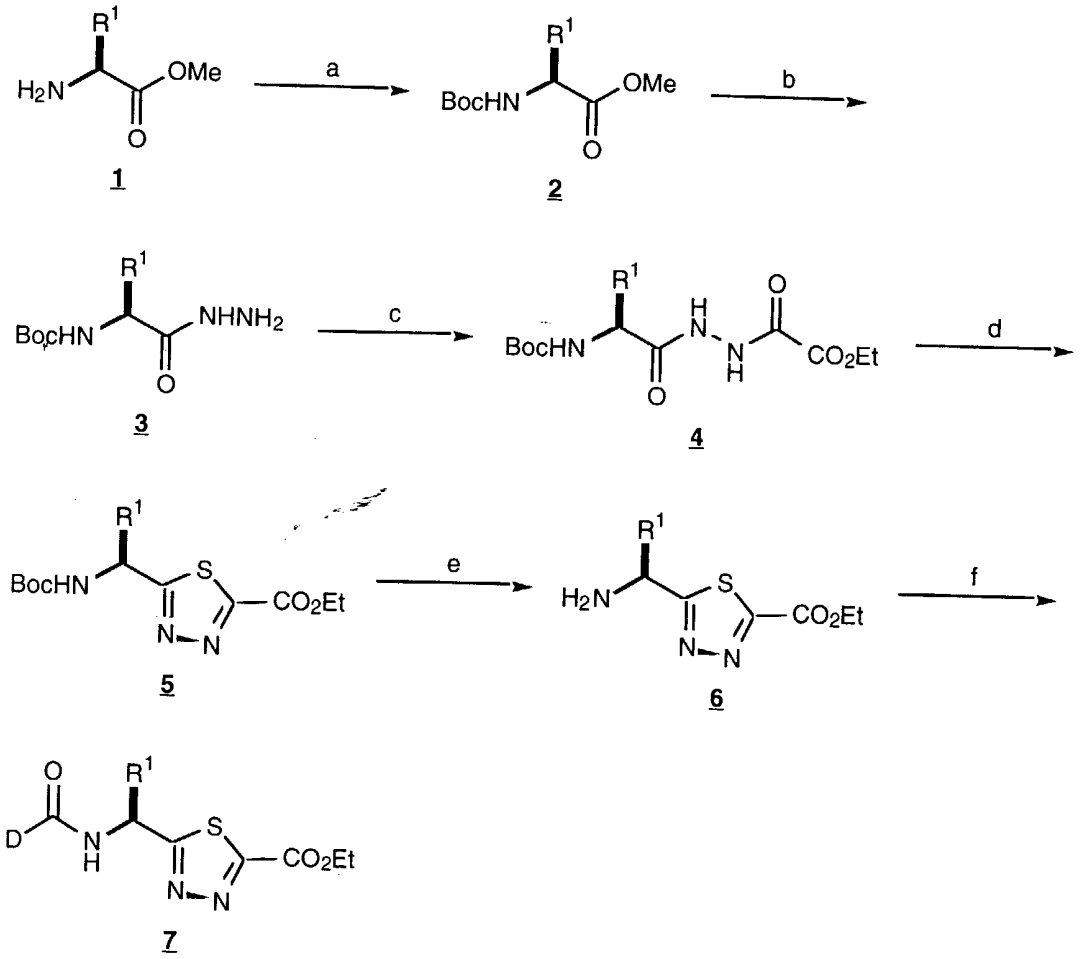
Scheme 2A



5

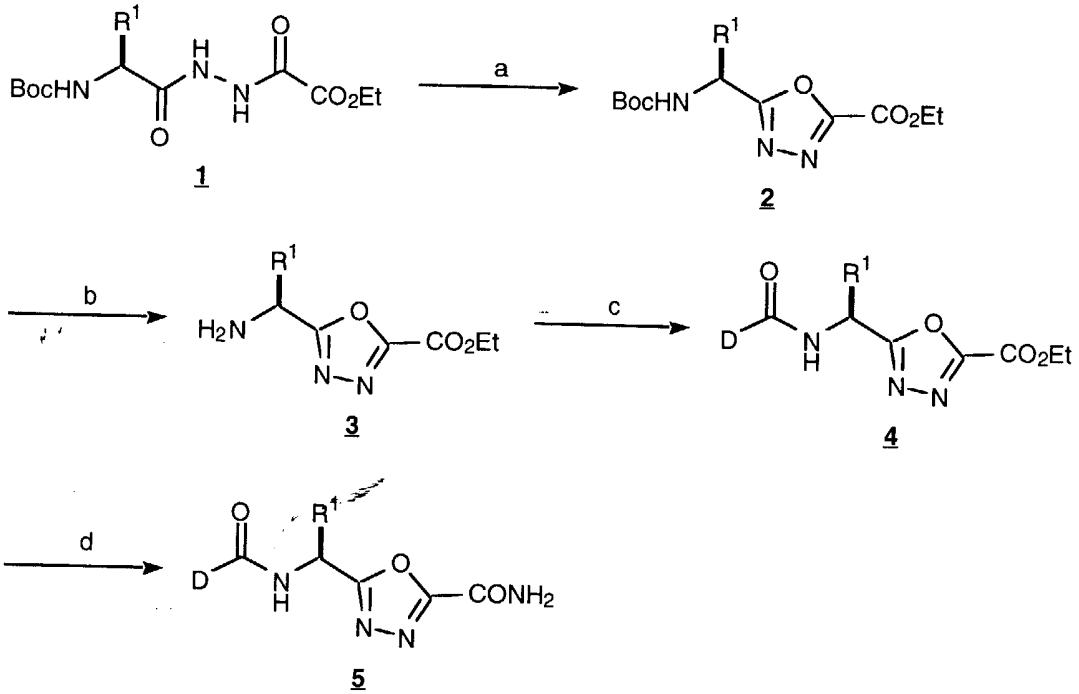
a) Boc-amino acid, EDC•HCl, 1-HOBT, DMF; b) TFA; c) R^5OCOCl, $i\text{-}Pr_2NEt$

Scheme 3



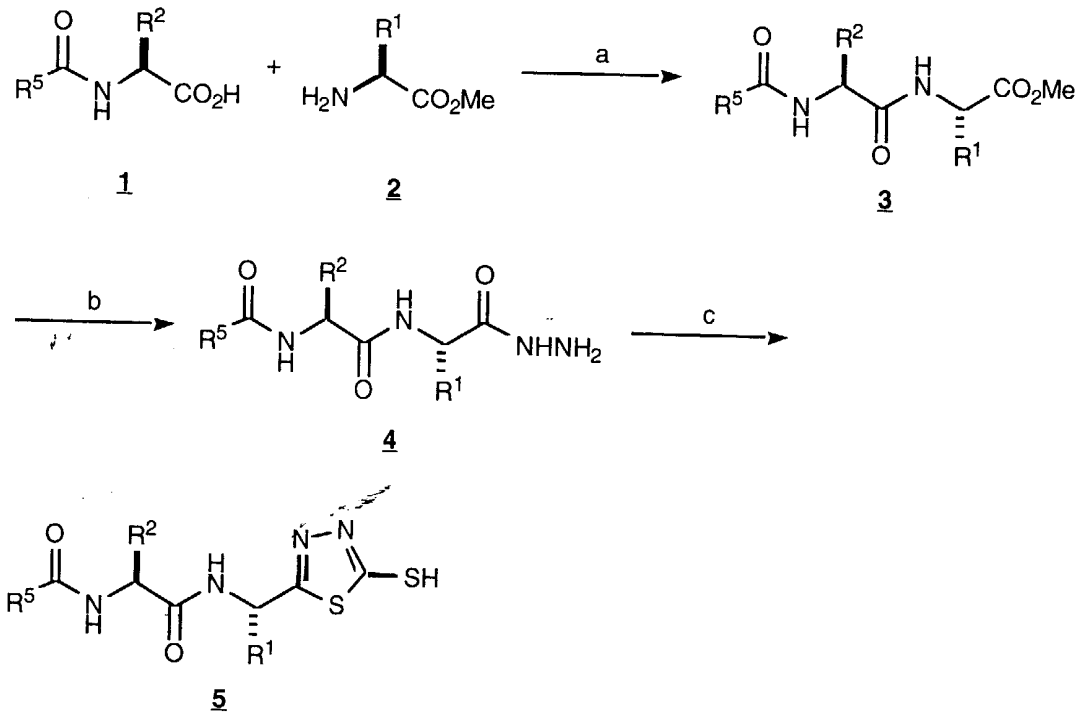
a) Boc_2O, Et_3N, THF; b) hydrazine hydrate, MeOH; c) EtO_2CCOCl, Pyridine, CH_2Cl_2; d) Lawesson's reagent, toluene; e) TFA, CH_2Cl_2; f) DCO_2H, EDC•HCl/HOBT, Et_3N, DMF

Scheme 4



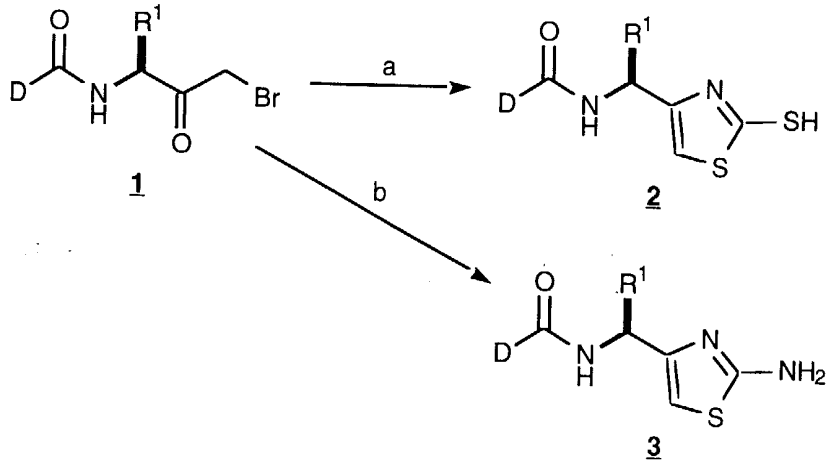
a) $SOCl_2$, pyridine, Et_2O, toluene; b) TFA, CH_2Cl_2; c) DCO_2H, EDC•HCl/HOBT, Et_3N, DMF; d) NH_3, EtOH

Scheme 5



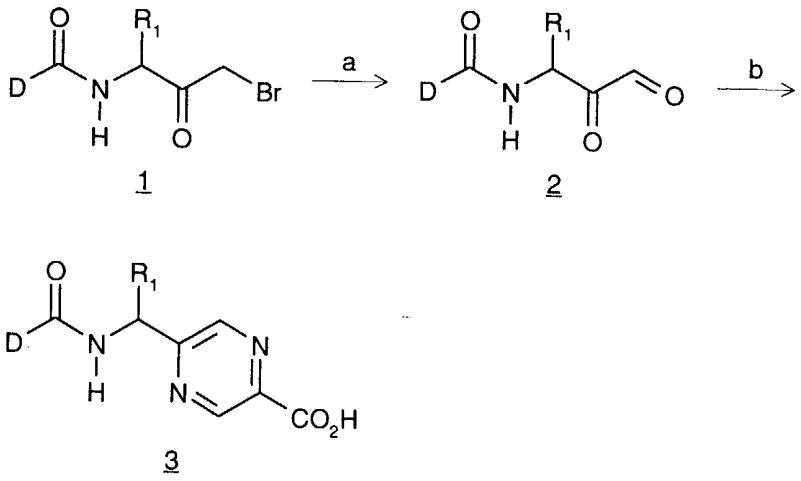
a) EDC•HCl/HOBT, Et_3N, DMF; b) $H_2NNH_2•H_2O$, MeOH; c) $CSCl_2$, Et_3N, $CHCl_3$

Scheme 6



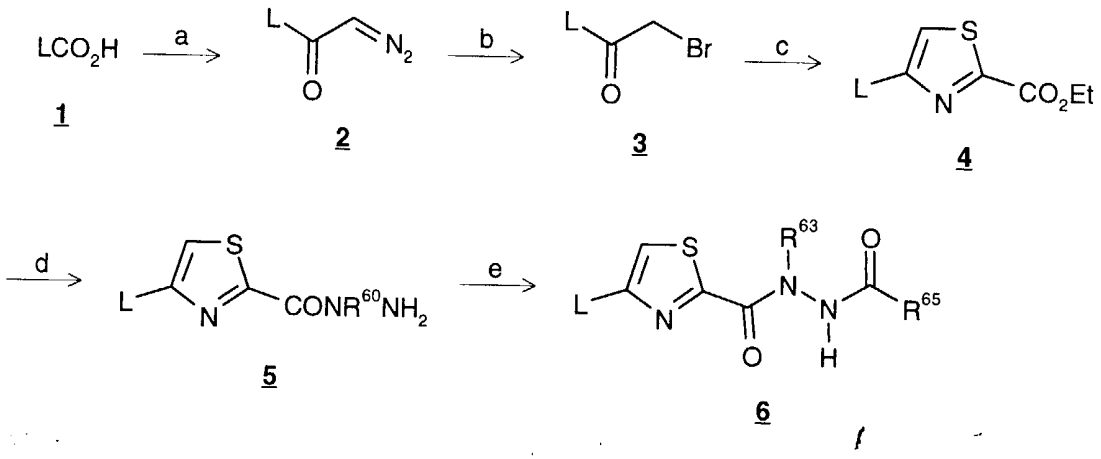
a) $H_2NCS_2\ NH_4^+$, EtOH; b) H_2NCSNH_2, EtOH

Scheme 7



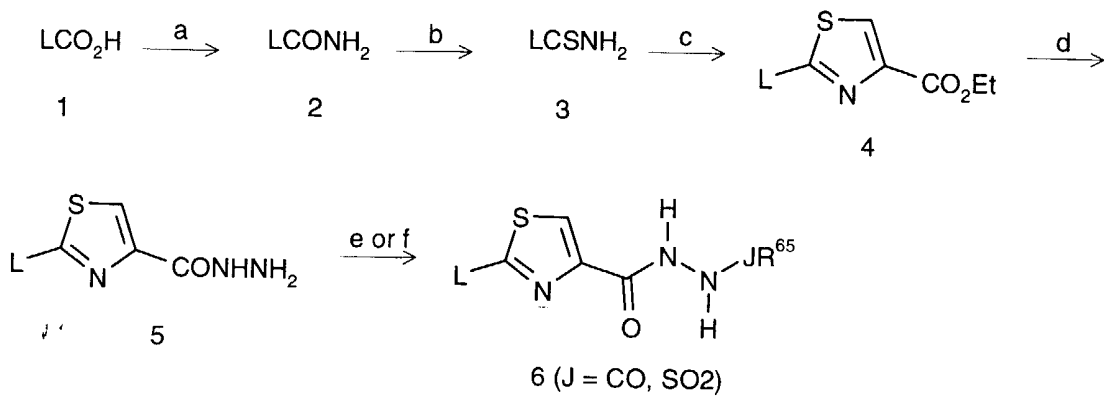
a) Et_2NO; b) $H_2NCH_2CH(NH_2)CO_2H$

Scheme 8



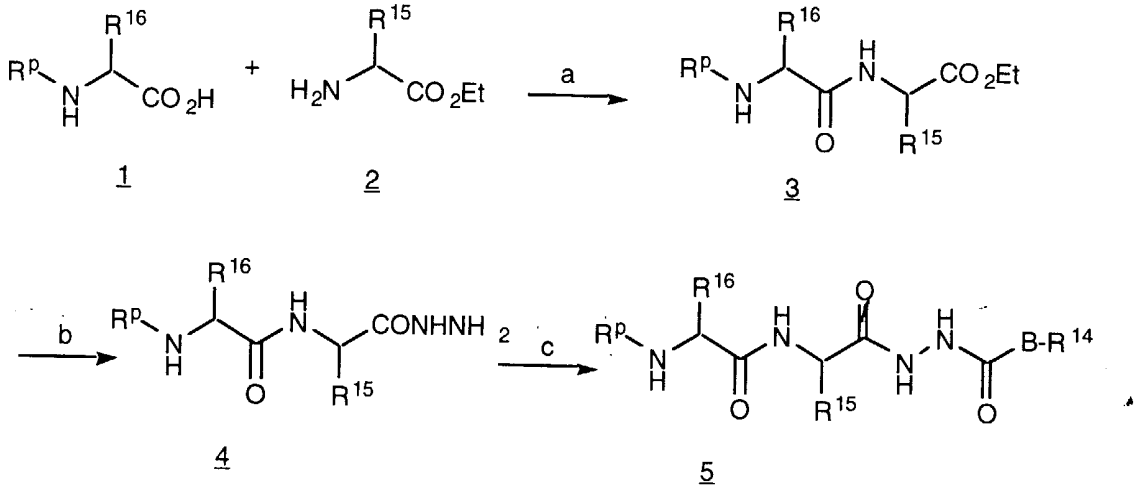
a) i. *i*-BuOCOCl, NMM, THF; ii. CH_2N_2, Et_2O; b) HBr, AcOH, Et_2O; c) H_2NCSCO_2Et, EtOH; d) $R^{63}NHNH_2$, EtOH; e) $R^{65}CO_2H$, EDC•HCl, 1-HOBT, DMF.

Scheme 9



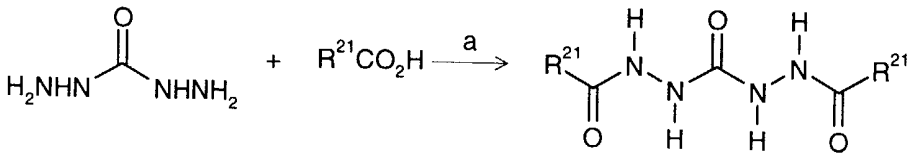
a) *i*-BuOCOCl, NMM, NH_3, THF; b) Lawesson's reagent, THF; c) i. EtO_2CCOCH_2Br; ii. TFAA, Py, CH_2Cl_2; d) $H_2NNH_2 \bullet H_2O$, EtOH; e) $R^{65}SO_2Cl$, Py, CH_2Cl_2; f) $R^{65}CO_2H$, EDC•HCl, 1-HOBT, DMF.

Scheme 10



a) EDC•HCl, HOBT, DMF; b) $H_2NNH_2 \bullet H_2O$, EtOH; c) R^{14}-B-CO_2H, EDC•HCL, HOBT, DMF

Scheme 11

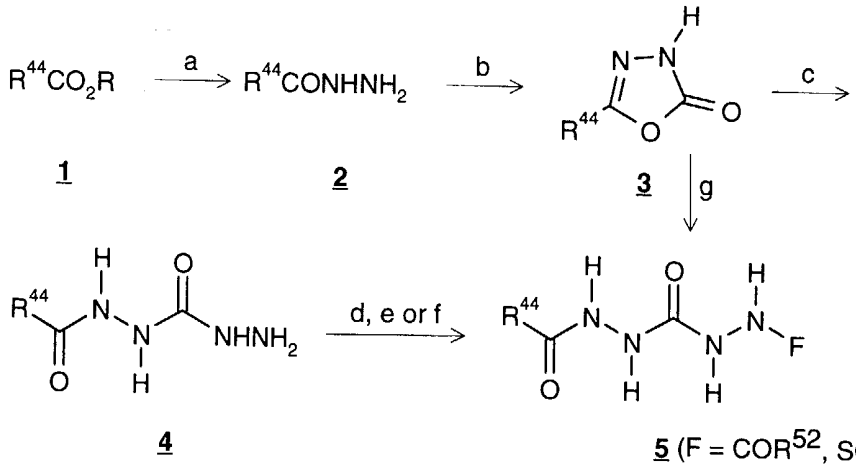


1

2

a) EDC.HCl, 1-HOBT, DMF

Scheme 12



1

2

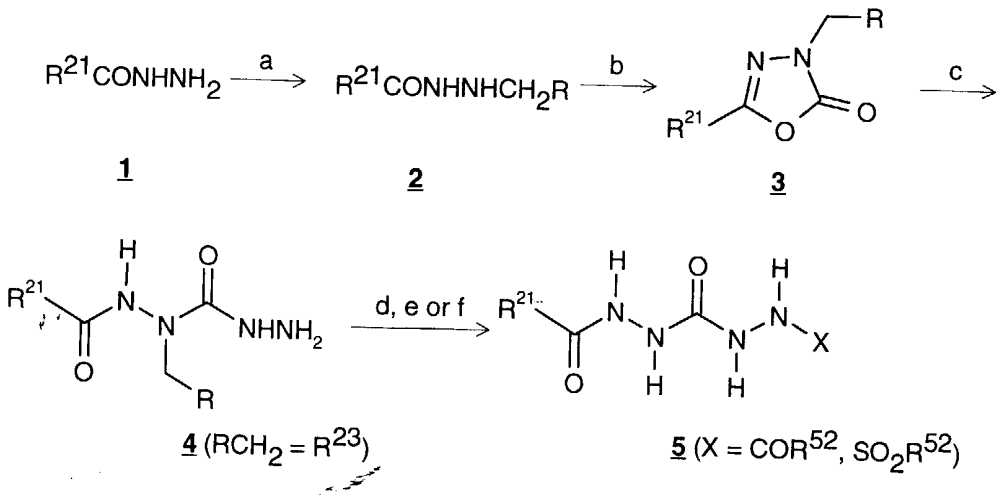
3

4

5 (F = COR^{52}, SO_2R^{52})

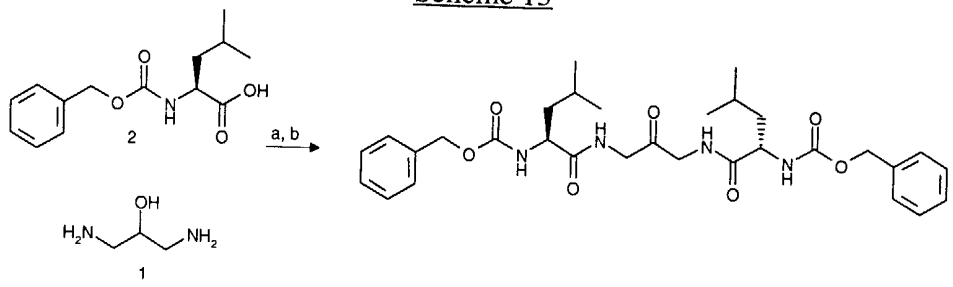
a) $H_2NNH_2 \cdot H_2O$, MeOH; b) Cl_2CO, PhMe; c) $H_2NNH_2 \cdot H_2O$, MeOH; d) $R^{49}CO_2H$,EDC·HCl, 1-HOBT, DMF; e) $R^{52}SO_2Cl$ or $R^{52}COCl$, pyridine, DMF; f) $R^{52}CO_2COR^{52}$; g) $R^{52}CONR^{51}NH_2$

Scheme 12A



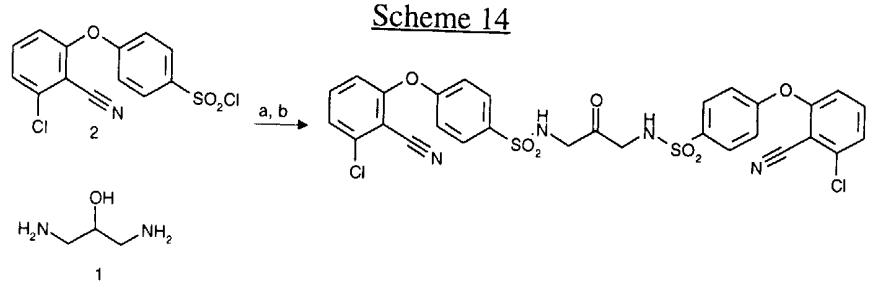
a) i. PhCHO, EtOH; ii. $BH_3 \cdot THF$; b) Cl_2CO, PhMe; c) $H_2NNH_2 \cdot H_2O$, MeOH; d) $R^{52}CO_2H$, EDC·HCl, 1-HOBT, DMF; e) $R^{52}SO_2Cl$ or $R^{52}COCl$, pyridine, DMF; f) $R^{52}CO_2COR^{52}$

Scheme 13



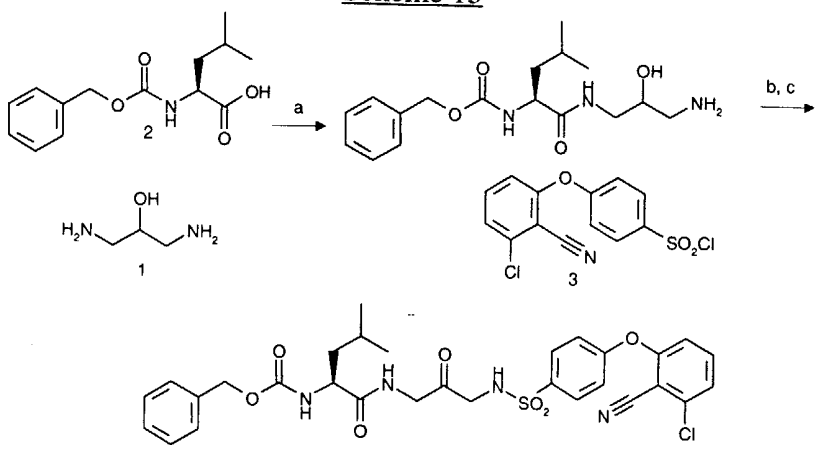
a) HBTU, NMM, DMF; b) Jones, acetone

Scheme 14



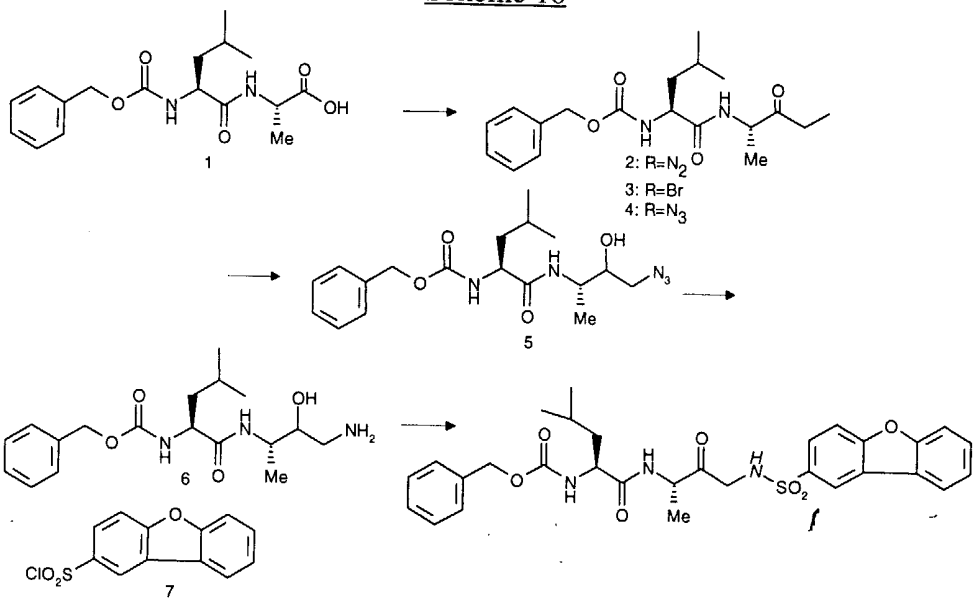
a) NMM, DMF; b) Jones, acetone

Scheme 15

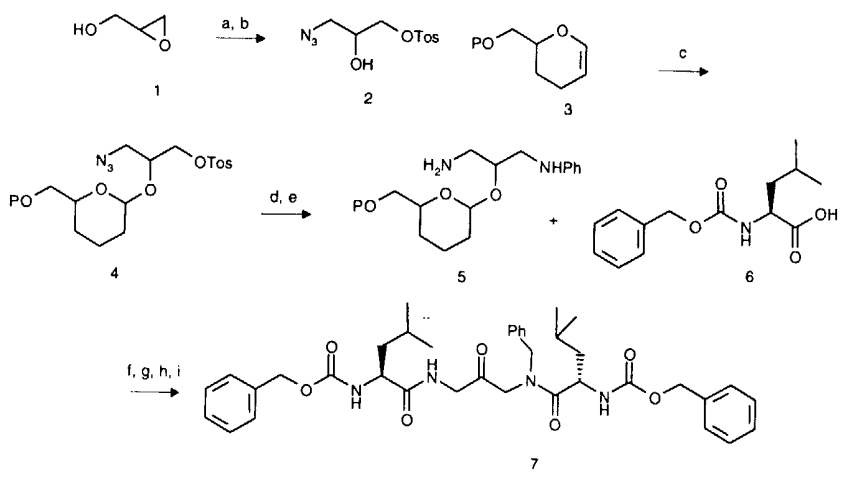


a) EDCI, HOBT, DMF; b) NMM, DMF, 3) Jones, acetone

Scheme 16

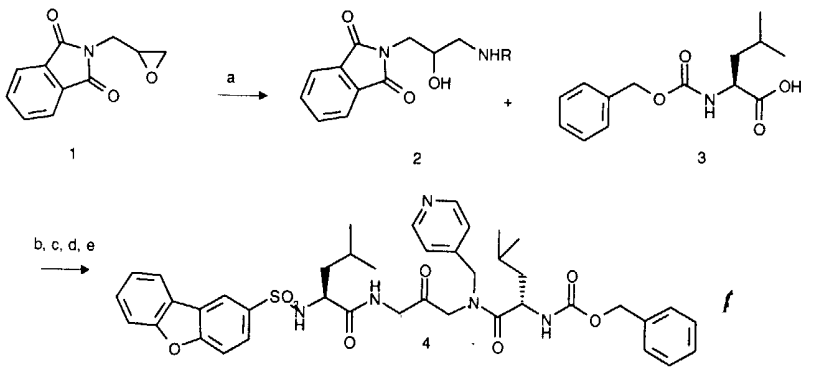


Scheme 17



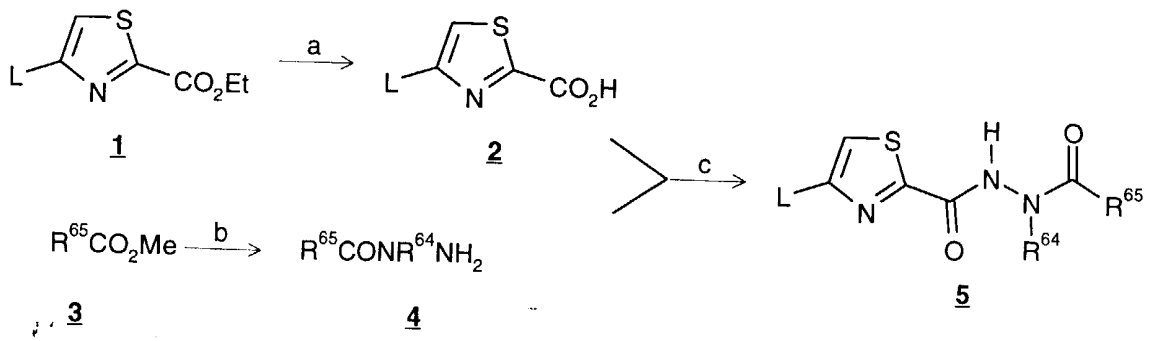
a) NaN_3, MeOH, H_2O; b) Tosyl chloride, triethylamine, CH_2Cl_2; c) Ellman dihydropyran resin (3), PPTS, $Cl(CH_2)_2Cl$; d) $PhCH_2NH_2$, toluene, 80 degrees C; e) HATU, N-methyl morpholine, NMP; f) $HS(CH_2)_3SH$, MeOH, Et_3N; g) Cbz-leucine (6), HBTU, N-methyl morpholine, NMP; h) TFA, CH_2Cl_2, Me_2S; i) Jones reagent, acetone

Scheme 18



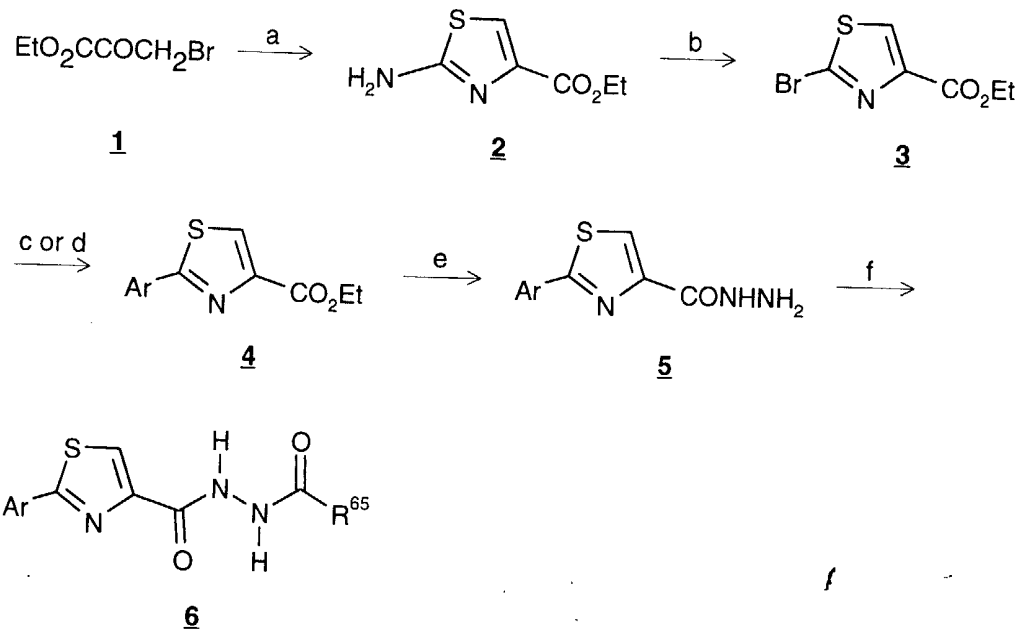
a) 4-pyridyl methyl amine, isopropanol, reflux; b) Cbz-leucine, HBTU, N-methyl morpholine, DMF; c) hydrazine, MeOH, reflux; d) 2-dibenzofuransulfonyl chloride, N-methyl morpholine, DMF; e) Jones reagent, acetone

Scheme 19



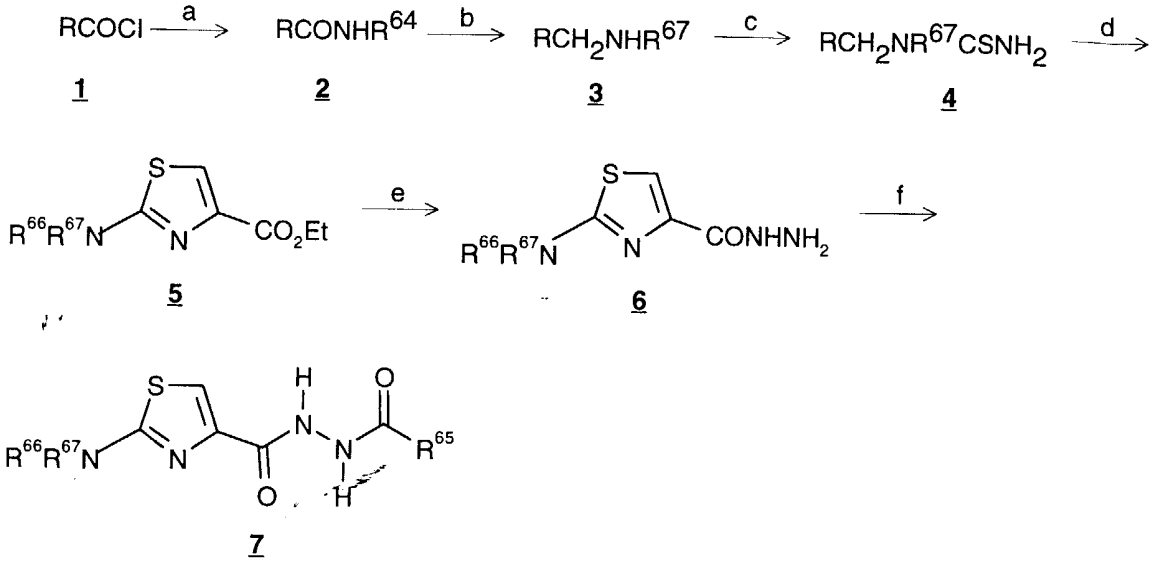
a) KOH, MeOH/H2O; b) $R^{66}NHNH_2$, EtOH; c) EDC•HCl, 1-HOBT, DMF

Scheme 20



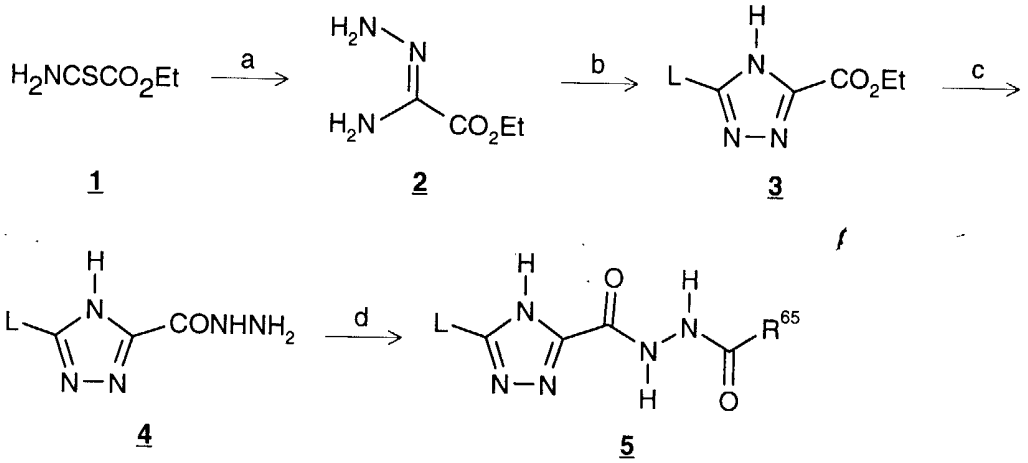
a) Thiourea, EtOH; b) i. $NaNO_2$, 16% aqueous HBr; ii. CuBr, 16% aqueous HBr; iii. HBr (cat.), EtOH; c) $ArB(OH)_2$, $Pd(PPh_3)_4$, CsF, DME; d) $ArSnMe_3$, $Pd(PPh_3)_4$, PhMe; e) $H_2NNH_2•H_2O$, EtOH; e) $R^{65}CO_2H$, EDC•HCl, 1-HOBT, DMF.

Scheme 21



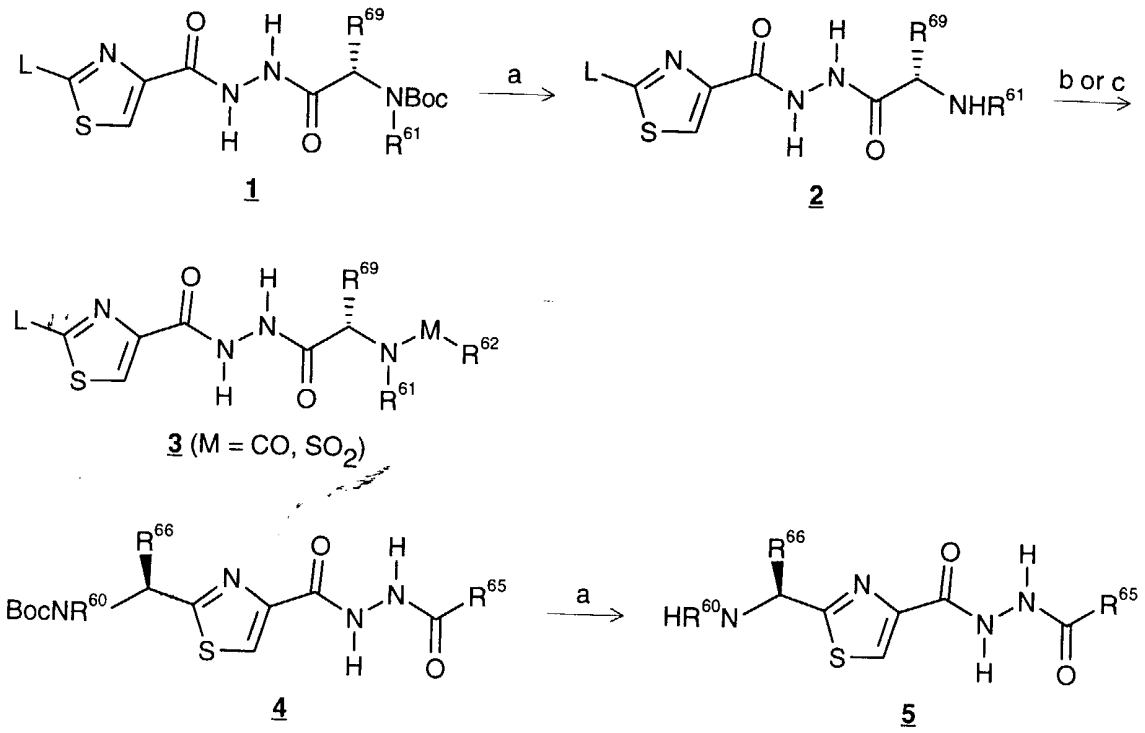
a) $R^{67}NH_2$, Py, CH_2Cl_2; b) $LiAlH_4$, THF; c) i. Cl_2CS, Py, CH_2Cl_2; ii. NH_3, MeOH or I. PhCONCS, $CHCl_3$; ii. K_2CO_3, MeOH, H_2O; d) EtO_2CCOCH_2Br, EtOH; e) $H_2NNH_2 \bullet H_2O$, EtOH; e) $R^{65}CO_2H$, EDC•HCl, 1-HOBT, DMF.

Scheme 22



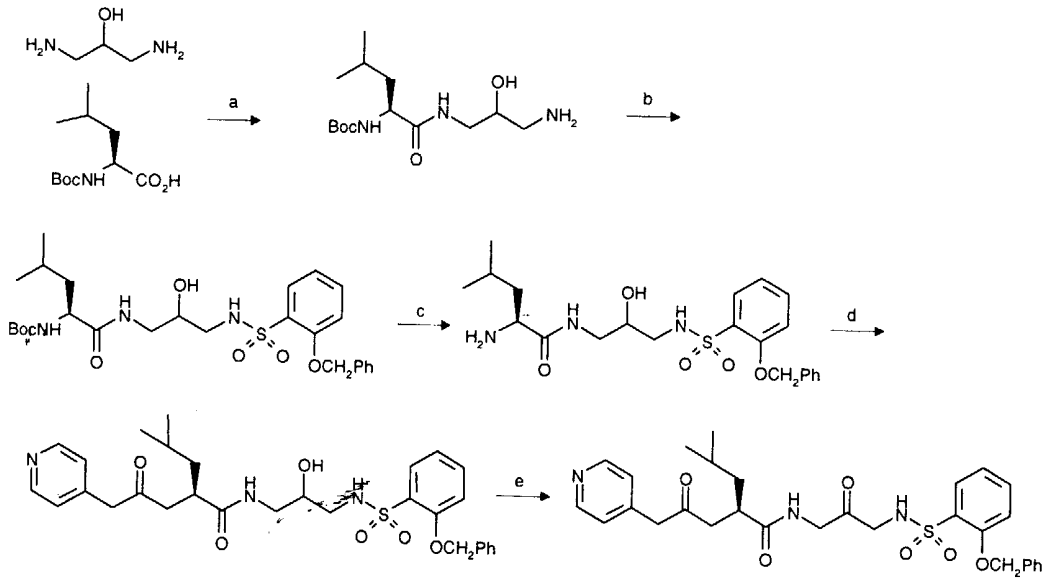
a) $H_2NNH_2 \bullet H_2O$, EtOH; b) LCO_2CO_2i-Bu, 200 °C; c) $H_2NNH_2 \bullet H_2O$, EtOH; d) $R^{65}CO_2H$, EDC•HCl, 1-HOBT, DMF

Scheme 23



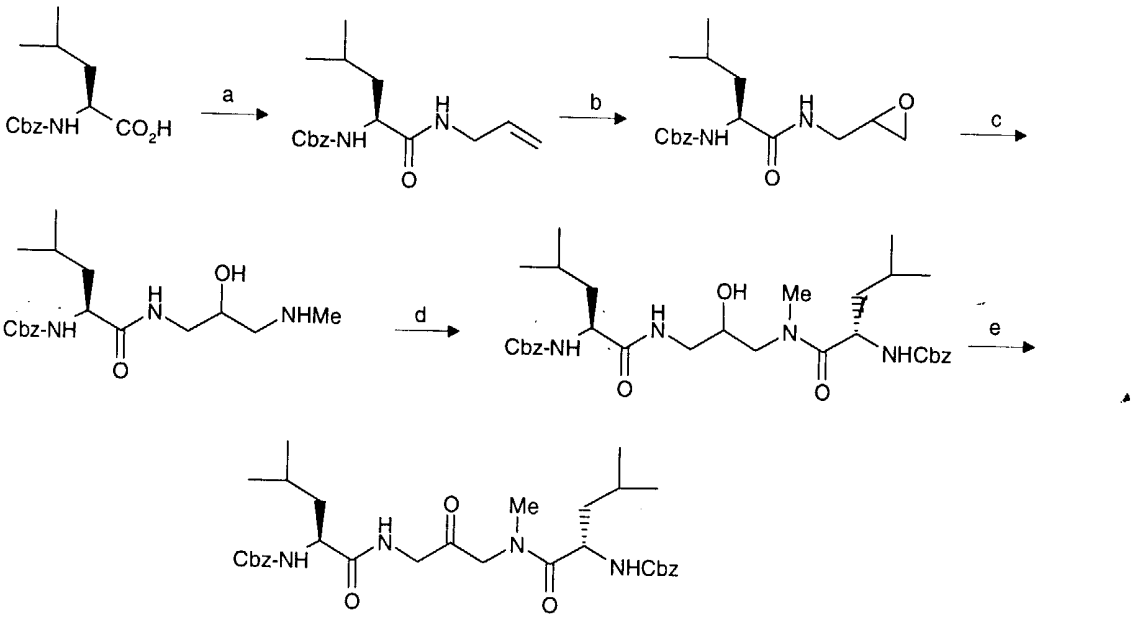
a) TFA; b) $R^{62}CO_2H$, EDC•HCl, 1-HOBT, DMF; c) $R^{62}SO_2Cl$, *i*-Pr_2NEt

Scheme 24



a) EDCI, DMF; b) 2-$PhCH_2OPhSO_2Cl$, NMM, DMF; c) TFA, DCM; d) 4-pyridyl acetic acid, HBTU, NMM, DMF; e) Jones

Scheme 25



a) HBTU, NMM, DMF, allyl amine; b) mCPBA, DCM; c) $MeNH_2$, isopropanol, 70 C; d) Cbz-leucine, EDCI, DMF; e) Jones, acetone

In another aspect, the present invention provides a novel cysteine protease in crystalline form, as defined by the positions in Table I herein.

In still another aspect, the present invention provides a novel protease composition characterized by a three dimensional catalytic site formed by the atoms of the amino acid residues listed in Table XXIX herein.

The three dimensional (3D) structure of the instant protease reveals that human cathepsin K is highly homologous to other known cysteine proteinases of the papain family. Cathepsin-K folds into two subdomains separated by the active site cleft, a characteristic of the papain family of cysteine proteases. The overall fold of cathepsin K is very similar to that of papain and actinidin. There is an insertion of one additional residue in cathepsin K at residue alanine 79 compared to papain. This insertion is easily accommodated in the turn at the carboxy terminal end of the helix formed by residues methionine 68-lysine 77 of cathepsin K. There is a different conformation for the backbone atoms of residues asparagine 99 to lysine 103 at the surface of cathepsin K compared to that in papain. Other differences in the backbone conformations between cathepsin K and papain are: a two residue insertion in loop residues 126-127, a two residue insertion at residue aspartate 152, the insertion of 4 residues at glutamine 172 and a difference in the conformation of the loop around residue lysine 200. There are many more differences in the structure of human cathepsin K and human cathepsin B, however, the secondary structure is preserved well between these two enzymes.

Listed in Figure 1 are the known amino acid sequences for the papain superfamily of cysteine proteases cathepsin K, cathepsin S, cathepsin L, papain, actinidin, cathepsin H and cathepsin B, aligned to illustrate the homologies there between.

According to the present invention the crystal structure of human cathepsin K has been determined in the absence of inhibitor and in complex with nine separate inhibitors at resolutions from 3.0 to 2.2 Ångstroms. The structures were determined using the method of molecular replacement and refined to R_c values ranging from 0.190-0.267 with the exception of the enzyme in the absence of inhibitor which was not refined.

Further refinement of the atomic coordinates will change the numbers in Table I. Refinement of the crystal structure from another crystal form will result in a new set of coordinates, determination of the crystal structure of another cysteine protease will also result in different set of numbers for coordinates in Table I which has an experimental error of approximately 0.4 Ångstroms. Also for example, the

amino acid sequence of the cysteine proteases can be varied by mutation derivatization or by use of a different source of the protein.

Human cathepsin K contains 215 amino acids and the model of the enzyme provided herein is represented by all 215 residues.

The cathepsin K crystal structure reveals an active site that is heretofor unknown and comprises a distinct three dimensional arrangement of atoms.

Table I discloses the protein coordinates of cathepsin K. These data are reported for the crystal structures described herein. The data are reported in Ångstroms with reference to an orthogonal coordinate system in standard format, illustrating the atom, i.e., nitrogen, oxygen, carbon, sulfur (at α, ß, γ, δ, or ε, positions in the amino acid residues); the amino acid residue in which the atom is located with amino acid number, and the coordinates X, Y and Z in Angstroms (Å) from the crystal structure. Note that each atom in the active site and the entire structure has an unique position in the crystal. The data also report the B or Temperature Factor values, which indicate the degree of thermal motion of the atom in root mean square displacement measurements ($Å^2$). Figure 2 illustrates the cathepsin K structure of the invention, including the active site.

The active site of cathepsin K bound to E-64 is shown in Figure 3. The conformation of E-64 bound to cathepsin K resembles that seen in the published structures of the papain-E-64 complex (Varughese, K.I., *Biochemistry* **28**, 1330-1332 (1989)) and actinidin-E-64 Varughese, K.I. , *Biochemistry* **31**, 5172-5176 (1992)). The covalent bond between the sulfur of cysteine 25 and the carbon C2 of the inhibitor is very clear in the electron density. Differences in the sidechain atoms lining the active site pockets on the enzyme of the various members of the papain family of cysteine proteases give rise to different interactions between the atoms of E-64 and the protein in these structures. In cathepsin K, the isobutyl atoms of the leucine lie well buried in the hydrophobic pocket formed by the side chain atoms of the cathepsin K residues leucine 160, alanine 134 and methionine 68 shielding these atoms of E-64 from solvent. In papain the leucyl side chain atoms of E-64 do not penetrate as deeply into this hydrophobic pocket. Another pocket of cathepsin K is occupied by the guanidinium atoms of E-64. A hydrogen bond forms between N4 of E-64 and the backbone carbonyl oxygen of glutamate 59 and the OD2 oxygen of aspartate 61. The carboxylate oxygen of aspartate 61 also makes a hydrogen bond with the N3 atom of E-64. The sidechain atoms of aspartate 61 lie at the entrance to this pocket in cathepsin K. These interactions are not possible in papain because the corresponding residue in papain is tyrosine 61 which blocks access. The carboxylate oxygens of E-64 make hydrogen bonding interactions with the ND1

atom of histidine 162 and the NE2 atom of glutamine 19. These interactions are also seen in papain and actinidin. The atoms of E-64 do not penetrate the complete region of the enzyme active site. As in papain, the backbone nitrogen atoms of residue glycine 66 in cathepsin K makes a hydrogen bond with the carbonyl oxygen atom O4 of the E-64. Also, the carbonyl oxygen of glycine 66 of cathepsin K forms a hydrogen bond with N2 of E-64. A portion of the regions of the active site are very similar in conformation in cathepsin K, papain and actinindin. A comparison of the active site of cathepsin K and cathepsin B reveals many more differences than observed in comparing papain or actinidin to cathepsin K. A portion of the active site of cathepsin B differs significantly from the corresponding portion of the active site in cathepsin K. The presence of the loop glutamate 107 - proline 116 in human cathepsin B is presumed responsible for the dipeptidyl carboxypeptidase activity of this enzyme and has no equivalent in cathepsin K, papain or actinidin. This loop makes this region of the active site of cathepsin B much smaller than in the other members of this papain family of cysteine proteases including cathepsin K. Despite the differences between the active sites of human cathepsin B and cathepsin K, the active site cysteine residues are almost exactly superimposed by an alignment of structurally homologous alpha carbon atoms in cathepsin B and cathepsin K. Differences in the hydrophobic pocket near leucine 160 in cathepsin K are also evident in cathepsin B. The residues forming this pocket are replaced by proline 78 in place of methionine 68 in cathepsin K and glutamate 243 in cathepsin B is structurally equivalent to leucine 160 in cathepsin K. Interestingly, the residues whose sidechain atoms form hydrogen bonds to the E-64 inhibitor in cathepsin K, namely histidine 162, glutamine 19 and aspartate 61, have structurally homologous residues in cathepsin B, namely histidine 197, glutamine 23 and aspartate 67 respectively.

Specific interactions of certain inhibitors of the present invention at the active site of cathepsin K are detailed hereinbelow.

3 (S)-3-[(N-benzyloxycarbonyl)-L-leucinyl]amino-5-methyl-1-(1-propoxy)-2-hexanone makes hydrophobic contacts with the enzyme residues indole ring of tryptophan 184 and the sidechain atom CG of glutamine 19. Oxygen O26 forms a bifurcated hydrogen bond with the amide nitrogen of cysteine 25 and the NE2 atom of glutamine 19. The active site nucleophilic sulfur of residue cysteine 25 is covalently linked to carbon C25 of the inhibitor, which adopts a tetrahedral conformation.

Bis-(Cbz-leucinyl)-1,3-diamino-propan-2-one exhibits the same interaction as 3 (S)-3-[(N-benzyloxycarbonyl)-L-leucinyl]amino-5-methyl-1-(1-propoxy)-2-

hexanone; carbon C21 of this inhibitor is covalently linked to SG of cysteine 25. The isopropyl atoms CC34,C35,C36 and C37 of the inhibitor form hydrophobic interactions with the sidechain atoms of residues on the enzyme surface, which form a hydrophobic pocket. This pocket is formed by atoms from methionine 68, leucine 209, alanine 163 and alanine 134 and portions of tyrosine 67.

2,2'-N,N'-bis-benzyloxycarbonyl-L-leucinylcarbohydrazide has interactions similar to bis-(Cbz-leucinyl)-1,3-diamino-propan-2-one and, in addition, the atoms C23-29 of the inhibitor CBZ group make an edge-face stacking interaction with the phenol ring of tyrosine 67. Inhibitor atom C21 is covalently bound the enzyme.

The sulfur atom of (1S)-N-[2-[(1-benzyloxycarbonylamino)-3-methylbutyl]thiazol-4-ylcarbonyl]-N'-(N-benzyloxycarbonyl-L-leucinyl)hydrazide contacts the ND1 atom of histidine 163 and the indole ring of tryptophan 184. Carbon C22 is covalently attached to SG of cysteine 25.

The CBZ atoms C20-26 of 2-[N-(3-benzyloxybenzoyl)]-2'-[N'-(N-benzyloxycarbonyl-L-leucinyl)]carbohydrazide interact with the sidechain atoms of leucine 160. Carbon C19 is covalently attached to SG of cysteine 25.

Cathepsin K binds selectively one stereoisomer of 4-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-1-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-3-pyrrolidinone. Carbon C22 is covalently attached to SG of cysteine 25. Atoms C14 and C15 of the inhibitor 4-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-1-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-3-pyrrolidinone form hydrophobic contacts with the sidechain atoms of glutamine 143 and asparagine 161 and the mainchain of alanine 137 and serine 138.

4-[N-[(4-pyridylmethoxy)carbonyl]-L-leucyl]-1-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-3-pyrrolidinone interacts in a similar manner to 4-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-1-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-3-pyrrolidinone. Again one stereoisomer is bound. Carbon C17 is covalently attached to SG of cysteine 25. The interaction of 4-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-1-N[N-(methyl)-L-leucyl)]-3-pyrrolidinone is the same as for 4-[N-[(4-pyridylmethoxy)carbonyl]-L-leucyl]-1-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-3-pyrrolidinone, except carbon C22 is covalently attached to SG of cysteine 25.

Atom O24 of 1-N-(N-imidazole acetyl-leucinyl)-amino-3-N-(4-phenoxy-phenyl-sulfonyl)-amino-propan-2-one forms a hydrogen bond interaction with the amide NH of glycine 66. Carbon C19 is covalently attached to SG of cysteine 25.

In summary, all inhibitors exhibit an aromatic interaction with atoms of the indole of Tryptophan 184. Isopropyl atoms C12-15 of 2,2'-N,N'-bis-

benzyloxycarbonyl-L-leucinylcarbohydrazide and (1S)-N-[2-[(1-benzyloxycarbonylamino)-3-methylbutyl]thiazol-4-ylcarbonyl]-N'-(N-benzyloxycarbonyl-L-leucinyl)hydrazide make hydrophobic contacts with main chain atoms of residues glutamine 21, cysteine 22 and glycine 23. The NE2 atom of glutamine 19 is able to donate a hydrogen bond to oxygen atom 2,2'-N,N'-bis-benzyloxycarbonyl-L-leucinylcarbohydrazide:O22, 1-N-(N-imidazole acetyl-leucinyl)-amino-3-N-(4-phenoxy-phenyl-sulfonyl)-amino-propan-2-one:O20, 2-[N-(3-benzyloxybenzoyl)]-2'-[N'-(N-benzyloxycarbonyl-L-leucinyl)]carbohydrazide:O20, 4-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-1-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-3-pyrrolidinone:O23, bis-(Cbz-leucinyl)-1,3-diamino-propan-2-one:O22, 3(S)-3-[(N-benzyloxycarbonyl)-L-leucinyl]amino-5-methyl-1-(1-propoxy)-2-hexanone:O26, 4-[N-[(4-pyridylmethoxy)carbonyl]-L-leucyl]-1-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-3-pyrrolidinone:O42, (1S, 2'R)-N-2-[[(1-benzyloxycarbonyl)amino]-3-methylbutyl]thiazol-4-ylcarbonyl-N'-2'-(benzyloxycarbonyl)amino-4'-methylpenanoylhydrazide:O23, 4-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-1-N[N-(methyl)-L-leucyl)]-3-pyrrolidinone:O23. The backbone amide nitrogen of glycine 66 donates a hydrogen bond to 2,2'-N,N'-bis-benzyloxycarbonyl-L-leucinylcarbohydrazide:O39, 1-N-(N-imidazole acetyl-leucinyl)-amino-3-N-(4-phenoxy-phenyl-sulfonyl)-amino-propan-2-one:O24, 2-[N-(3-benzyloxybenzoyl)]-2'-[N'-(N-benzyloxycarbonyl-L-leucinyl)]carbohydrazide:O37, 4-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-1-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-3-pyrrolidinone:O40, bis-(Cbz-leucinyl)-1,3-diamino-propan-2-one:O39, (1S, 2'R)-N-2-[[(1-benzyloxycarbonyl)amino]-3-methylbutyl]thiazol-4-ylcarbonyl-N'-2'-(benzyloxycarbonyl)amino-4'-methylpenanoylhydrazide:O40, 4-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-1-N[N-(methyl)-L-leucyl)]-3-pyrrolidinone:O31. The hydrophobic pocket lined with atoms from residues methionine 68, leucine 209, alanine 163 and alanine 134 and portions of tyrosine 67 interact with the isopropyl atoms; bis-(Cbz-leucinyl)-1,3-diamino-propan-2-one:C34-37, 2,2'-N,N'-bis-benzyloxycarbonyl-L-leucinylcarbohydrazide: C34-37, (1S)-N-[2-[(1-benzyloxycarbonylamino)-3-methylbutyl]thiazol-4-ylcarbonyl]-N'-(N-benzyloxycarbonyl-L-leucinyl)hydrazide; :C35-38, 2-[N-(3-benzyloxybenzoyl)]-2'-[N'-(N-benzyloxycarbonyl-L-leucinyl)]carbohydrazide:C32-35, 4-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-1-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-3-pyrrolidinone:C35-38, 4-[N-[(4-pyridylmethoxy)carbonyl]-L-leucyl]-1-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-3-pyrrolidinone:C19-22, 1 -N-(N-imidazole acetyl-leucinyl)-amino-3-N-(4-phenoxy-phenyl-sulfonyl)-amino-propan-2-one:C26-29. All inhibitors except 3(S)-3-[(N-

benzyloxycarbonyl)-L-leucinyl]amino-5-methyl-1-(1-propoxy)-2-hexanone and 4-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-1-N[N-(methyl)-L-leucyl)]-3-pyrrolidinone have aromatic groups that interact with tyrosine 67 on the protein. All inhibitors are covalently linked to the cysteine 25 SG atom through an inhibitor carbon atom.

The crystal structure of the protease of the present invention reveals the three dimensional structure of novel active site formed by the atoms of the amino acid residues listed in Table XXIX.

This structure is clearly useful in the structure-based design of protease inhibitors, which may be used as therapeutic agents against diseases in which inhibition of bone resorption is indicated. The discovery of the novel cathepsin K catalytic site permits the design of potent, highly selective protease inhibitors.

Another aspect of this invention involves a method for identifying inhibitors of cathepsin K characterized by the crystal structure and novel active site described herein, and the inhibitors themselves. The novel protease crystal structure of the invention permits the identification of inhibitors of protease activity. Such inhibitors may bind to all or a portion of the active site of cathepsin K; or even be competitive or non-competitive inhibitors. Once identified and screened for biological activity, these inhibitors may be used therapeutically or prophylactically to block protease activity.

One design approach is to probe the cathepsin K of the invention with molecules composed of a variety of different chemical entities to determine optimal sites for interaction between candidate cathepsin K inhibitors and the 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 sticks. Small molecules that bind tightly to those sites can then be designed and synthesized and tested for their cathepsin K inhibitor activity.

This invention also enables the development of compounds that can isomerize to short-lived reaction intermediates in the chemical reaction of a substrate or other compound that binds to or with cathepsin K. Thus, the time-dependent analysis of structural changes in cathepsin K during its interaction with other molecules is permitted. The reaction intermediates of cathepsin K can also be deduced from the reaction product in co-complex with cathepsin K. Such information is useful to design improved analogues of known cysteine protease inhibitors or to design novel classes of inhibitors based on the reaction intermediates of the cathepsin K enzyme and cathepsin K inhibitor co-complex. This provides a

novel route for designing cathepsin K inhibitors with both high specificity and stability.

Another approach made possible by this invention, is to screen computationally small molecule data bases for chemical entities or compounds that can bind in whole, or in part, to the cathepsin K enzyme. In this screening, the quality of fit of such entities or compounds to the binding site may be judged either by shape complementarity [R. L. DesJarlais et al., J. Med. Chem. 31:722-729 (1988)] or by estimated interaction energy [E. C. Meng et al, J. Comp. Chem., 13:505-524 (1992)].

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

One method that may be employed for this purpose is molecular replacement. In this method, the unknown crystal structure, whether it is another crystal form of cathepsin K, a cathepsin K mutant, or a cathepsin K co-complex, or the crystal of some other protein with significant amino acid sequence homology to any functional domain of cathepsin K, may be determined using the cathepsin K structure coordinates of this invention as provided in Table I. This method will provide an accurate structural form for the unknown crystal more quickly and efficiently than attempting to determine such information *ab initio*.

Thus, the cathepsin K structure provided herein permits the screening of known molecules and/or the designing of new molecules which bind to the protease structure, particularly at the active site, via the use of computerized evaluation systems. For example, computer modeling systems are available in which the sequence of the protease, and the protease structure (i.e., atomic coordinates of cathepsin K and/or the atomic coordinate of the active site cavity, bond angles, dihedral angles, distances between atoms in the active site region, etc. as provided by Table I may be input. Thus, a machine readable medium may be encoded with data representing the coordinates of Table I in this process. The computer then generates structural details of the site into which a test compound should bind, thereby enabling the determination of the complementary structural details of said test compound.

More particularly, the design of compounds that bind to or inhibit cathepsin K according to this invention generally involves consideration of two factors. First,

the compound must be capable of physically and structurally associating with cathepsin K. Non-covalent molecular interactions important in the association of cathepsin K with its substrate include hydrogen bonding, van der Waals and hydrophobic interactions.

Second, the compound must be able to assume a conformation that allows it to associate with cathepsin K. Although certain portions of the compound will not directly participate in this association with cathepsin K, those portions may still influence the overall conformation of the molecule. This, in turn, may have a significant impact on potency. Such conformational requirements include the overall three-dimensional structure and orientation of the chemical entity or compound in relation to all or a portion of the binding site, e.g., active site or accessory binding site of cathepsin K, or the spacing between functional groups of a compound comprising several chemical entities that directly interact with cathepsin K.

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

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

One skilled in the art may use one of several methods to screen chemical entities or fragments for their ability to associate with cathepsin K and more particularly with the individual binding pockets of the cathepsin K active site or accessory binding site. This process may begin by visual inspection of, for example, the active site on the computer screen based on the cathepsin K coordinates in Table I. Selected fragments or chemical entities may then be position cathepsin K. 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:

- 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.
- 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.
- 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.
- 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.

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

Once suitable chemical entities or fragments have been selected, they can be assembled into a single compound or inhibitor. Assembly may be proceeded by visual inspection of the relationship of the fragments to each other on the three-dimensional image displayed on a computer screen in relation to the structure coordinates of cathepsin K. This would 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:

- 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", Special Pub., Royal Chem. Soc. 78, pp. 182-196 (1989)]. CAVEAT is available from the University of California, Berkeley, CA.
- 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).
- HOOK (available from Molecular Simulations, Burlington, MA).

Instead of proceeding to build a cathepsin K inhibitor in a step-wise fashion one fragment or chemical entity at a time as described above, inhibitory or other

type of binding compounds may be designed as a whole or "*de novo*" using either an empty active site or optionally including some portion(s) of a known inhibitor(s). These methods include:

- 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.
- LEGEND [Y. Nishibata and A. Itai, Tetrahedron, 47:8985 (1991)]. LEGEND is available from Molecular Simulations, Burlington, MA.
- LeapFrog (available from Tripos Associates, St. Louis, MO).

Other molecular modeling 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 the test compound may be superimposed over the model of the 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). The 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 quickly and easily examined and expensive and lengthy biochemical testing avoided. Moreover, the need for actual synthesis of many compounds is effectively eliminated.

Once identified by the modeling techniques, the protease inhibitor may be tested for bioactivity using standard techniques. For example, structure of the invention may be used in binding assays using conventional formats to screen inhibitors. Suitable assays for use herein include, but are not limited to, the enzyme-linked immunosorbent assay (ELISA), or a fluoresence quench assay. See, for example, the cathepsin K activity assay of Example 2 below. Other assay formats may be used; these assay formats are not a limitation on the present invention.

In another aspect, the protease structure of the invention permit the design and identification of synthetic compounds and/or other molecules which have a shape complimentary to the conformation of the protease active site of the

invention. Using known computer systems, the coordinates of the protease structure of the invention may be provided in machine readable form, the test compounds designed and/or screened and their conformations superimposed on the structure of the protease of the invention. Subsequently, suitable candidates identified as above may be screened for the desired protease inhibitory bioactivity, stability, and the like.

Once identified and screened for biological activity, these inhibitors may be used therapeutically or prophylactically to block cathepsin K activity.

The following examples illustrate various aspects of this invention. These examples do not limit the scope of this invention which is defined by the appended claims.

EXAMPLE 1: Analysis of the Structure of Cathepsin K

A. ***Expression, Purification and Crystallization***

Cathepsin K (see Fig. 1) was expressed and purified as described in Bossard, M. J., et al., *J. Biol. Chem.* **271**, 12517-12524 (1996).

Crystals of cathepsin K were grown by vapor diffusion in hanging drops from a solution of 30% PEG 8000, 0.1 M Na^+/K^+ phosphate at pH 4.5 containing 0.2M Li_2SO_4. Crystals of the complex are tetragonal, space group $P4_32_12$, with cell constants of a=57.7 Ångstroms and c=131.1 Ångstroms. The crystals contain one molecule in the asymmetric unit and contain 36 % solvent with a V_m value of 2.3 $Å^3$/Dalton. The structure was determined by molecular replacement using X-PLOR [Brunger, A.T., et al., *Science*, **235**, 458-460 (1987)]. The starting model consisted of the protein atoms from the cathepsin K E-64 complex structure described herein.

B. ***Model Building and Refinement***

Using the three-dimensional electron density map obtained from above, the polypeptide chain of the cathepsin K can be traced without ambiguity. All 215 residues with side chains were built using the 3-D computer graphics program FRODO [Jones, T.A., *J. Appl. Crystallogr.*, **11**, 268-272 (1978)]. Each of these 215 amino acids residues was manually positioned in its electron density, allowing for a unique position for each atom in cathepsin K in which each position is defined by a unique set of atomic coordinates (X,Y,Z) as shown in Table I. Starting with these atomic coordinates, a diffraction pattern was calculated and compared to the experimental data. The difference between the calculated and experimentally determined diffraction patterns was monitored by the value of R_c. The refinement (using X-PLOR) of the structural model necessitates adjustments of

atomic positions to minimize the R-factor, where a value of below 20% is typical for a good quality protein structure and a value of higher than 25% usually indicates the need of further refinement.

EXAMPLE 2: Assays

Determination of cathepsin K proteolytic catalytic activity

All assays for cathepsin K were carried out with human recombinant enzyme. Standard assay conditions for the determination of kinetic constants used a fluorogenic peptide substrate, typically Cbz-Phe-Arg-AMC, and were determined in 100 mM Na acetate at pH 5.5 containing 20 mM cysteine and 5 mM EDTA. Stock substrate solutions were prepared at concentrations of 10 or 20 mM in DMSO with 20 uM final substrate concentration in the assays. All assays contained 10% DMSO. Independent experiments found that this level of DMSO had no effect on enzyme activity or kinetic constants. All assays were conducted at ambient temperature. Product fluorescence (excitation at 360 nM; emission at 460 nM) was monitored with a Perceptive Biosystems Cytofluor II fluorescent plate reader. Product progress curves were generated over 20 to 30 minutes following formation of AMC product.

Inhibition studies

Potential inhibitors were evaluated using the progress curve method. Assays were carried out in the presence of variable concentrations of test compound. Reactions were initiated by addition of enzyme to buffered solutions of inhibitor and substrate. Data analysis was conducted according to one of two procedures depending on the appearance of the progress curves in the presence of inhibitors. For those compounds whose progress curves were linear, apparent inhibition constants ($K_{i,app}$) were calculated according to equation 1 (Brandt *et al.*, *Biochemistry,* **1989**, *28*, 140):

$$v = V_m A / [K_a(1 + I/K_{i,\ app}) + A] \quad (1)$$

where v is the velocity of the reaction with maximal velocity V_m , A is the concentration of substrate with Michaelis constant of K_a, and I is the concentration of inhibitor.

For those compounds whose progress curves showed downward curvature characteristic of time-dependent inhibition, the data from individual sets was analyzed to give k_{obs} according to equation 2:

$$[AMC] = v_{ss}\, t + (v_0 - v_{ss})\,[1 - \exp(-k_{obs}t)] / k_{obs} \quad (2)$$

where [AMC] is the concentration of product formed over time t, v_0 is the initial reaction velocity and v_{ss} is the final steady state rate. Values for k_{obs} were then analyzed as a linear function of inhibitor concentration to generate an apparent second order rate constant (k_{obs} / inhibitor concentration or k_{obs} / [I]) describing the time-dependent inhibition. A complete discussion of this kinetic treatment has been fully described (Morrison *et al.*, *Adv. Enzymol. Relat. Areas Mol. Biol.*, **1988**, *61*, 201).

This assay measures the affinity of inhibitors to cathepsin K. One skilled in the art would consider any compound exhibiting a K_i value of less than 50 micromolar to be a potential lead compound for further research. Preferably, the compounds used in the method of the present invention have a K_i value of less than 1 micromolar. Most preferably, said compounds have a K_i value of less than 100 nanomolar.

Human Osteoclast Resorption Assay

Aliquots of osteoclastoma-derived cell suspensions were removed from liquid nitrogen storage, warmed rapidly at 37°C and washed x1 in RPMI-1640 medium by centrifugation (1000 rpm, 5 min at 4°C). The medium was aspirated and replaced with murine anti-HLA-DR antibody, diluted 1:3 in RPMI-1640 medium, and incubated for 30 min on ice The cell suspension was mixed frequently.

The cells were washed x2 with cold RPMI-1640 by centrifugation (1000 rpm, 5 min at 4°C) and then transferred to a sterile 15 mL centrifuge tube. The number of mononuclear cells were enumerated in an improved Neubauer counting chamber.

Sufficient magnetic beads (5 / mononuclear cell), coated with goat anti-mouse IgG, were removed from their stock bottle and placed into 5 mL of fresh medium (this washes away the toxic azide preservative). The medium was removed by immobilizing the beads on a magnet and is replaced with fresh medium.

The beads were mixed with the cells and the suspension was incubated for 30 min on ice. The suspension was mixed frequently. The bead-coated cells were immobilized on a magnet and the remaining cells (osteoclast-rich fraction) were

decanted into a sterile 50 mL centrifuge tube. Fresh medium was added to the bead-coated cells to dislodge any trapped osteoclasts. This wash process was repeated x10. The bead-coated cells were discarded.

The osteoclasts were enumerated in a counting chamber, using a large-bore disposable plastic Pasteur pipette to charge the chamber with the sample. The cells were pelleted by centrifugation and the density of osteoclasts adjusted to $1.5x10^4$/mL in EMEM medium, supplemented with 10% fetal calf serum and 1.7g/liter of sodium bicarbonate. 3 mL aliquots of the cell suspension (per treatment) were decanted into 15 mL centrifuge tubes. These cells were pelleted by centrifugation. To each tube 3 mL of the appropriate treatment was added (diluted to 50 uM in the EMEM medium). Also included were appropriate vehicle controls, a positive control (87MEM1 diluted to 100 ug/mL) and an isotype control (IgG2a diluted to 100 ug/mL). The tubes were incubate at 37°C for 30 min.

0.5 mL aliquots of the cells were seeded onto sterile dentine slices in a 48-well plate and incubated at 37°C for 2 h. Each treatment was screened in quadruplicate. The slices were washed in six changes of warm PBS (10 mL / well in a 6-well plate) and then placed into fresh treatment or control and incubated at 37°C for 48 h. The slices were then washed in phosphate buffered saline and fixed in 2% glutaraldehyde (in 0.2M sodium cacodylate) for 5 min., following which they were washed in water and incubated in buffer for 5 min at 37°C. The slices were then washed in cold water and incubated in cold acetate buffer / fast red garnet for 5 min at 4°C. Excess buffer was aspirated, and the slices were air dried following a wash in water.

The TRAP positive osteoclasts were enumerated by bright-field microscopy and were then removed from the surface of the dentine by sonication. Pit volumes were determined using the Nikon/Lasertec ILM21W confocal microscope.

EXAMPLE 3: Method of Detecting Inhibitors

The three dimensional atomic structure can be readily used as a template for selecting potent inhibitors. Various computer programs and databases are available for the purpose. A good inhibitor should at least have excellent steric and electrostatic complementarity to the target, a fair amount of hydrophobic surface buried and sufficient conformational rigidity to minimize entropy loss upon binding. The approach usually comprises several steps:

1) Define a region to target. the active site cavity of cathepsin K can be selected, but any place that is essential to the protease activity could become a

potential target. Since the crystal structure has been determined, the spatial and chemical properties of the target region is known.

2) Docking a small molecule onto the target. Many methods can be used to archive this. Computer databases of three-dimensional structures are available for screening millions of small molecular compounds. A negative image of these compounds can be calculated and used to match the shape of the target cavity. The profiles of hydrogen bond donor-acceptor and lipophilic points of these compounds can also be used to complement those of the target. Anyone skilled in the art would be able to identify many small molecules or fragments as hits.

3) Linking and extending recognition fragments. Using the hits identified by above procedure, one can incorporate different functional groups or small molecules into a single, larger molecule. The resulting molecule is likely to be more potent and have higher specificity. It is also possible to try to improve the "seed" inhibitor by adding more atoms or fragments that will interact with the target protein. The originally defined target region can be readily expanded to allow further necessary extension.

A limited number of promising compounds can be selected through the process. They can then be synthesized and assayed for their inhibitory properties. The success rate can sometimes be as high as 20%, and it may still be higher with the rapid progresses in computing methods.

EXAMPLE 4: Crystallization of Enzyme with Inhibitors

A. Preparation of Inhibitors

Compound 1. Preparation of 4-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-1-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-3-pyrrolidinone

a) 3-hydroxy-4-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-1-pyrrolidinecarboxylic acid 1,1dimethylethyl ester

To a solution of 3-hydroxy-4-amino-1-pyrrolidinecarboxylic acid, 1,1-dimethylethyl ester (202 mg, 1.14 mmol) in CH_2Cl_2 (5 mL) was added CBZ-leucine (302.9 mg, 1.14 mmol), HOBT (154 mg, 1.14 mmol) and EDC (262.2 mg, 1.37 mmol). The reaction was allowed to stir until complete by TLC analysis whereupon it was diluted with EtOAc and washed sequentially with pH 4 buffer, sat. K_2CO_3, water and brine. The organic layer was dried ($MgSO_4$), filtered and

concentrated. Column chromatography of the residue (3:1 EtOAc:hexanes) gave 325 mg of the title compound: MS (ES+) 450.3 (MH+), 472.2 (M+Na).

b) 3-hydroxy-4-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-1-pyrrolidine hydrochloride

To a solution of the carbamate (310 mg, 0.69 mmol) in dry EtOAc (5.0 mL) was bubbled HCl gas for approximately 5 minutes. The reaction was stirred until TLC analysis indicated the complete consumption of the starting material. The reaction was then concentrated *in vacuo* to give 249 mg of the title compound: MS (ES+) 350.3 (MH+)

c) 4-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-1-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-3-pyrrolidinol

To a solution of the amine hydrochloride from the previous step (249 mg, 0.64 mmol) in CH_2Cl_2 (10 mL) was added CBZ-leucine (170.4 mg, 0.64 mmol), HOBT (86.5 mg, 0.64 mmol), NMM (300 uL) and EDC (147.2 mg, 0.77 mmol). The reaction was allowed to stir at room temperature for 2 hours whereupon it was diluted with ethyl acetate and worked up as described previously. Column chromatography of the residue (3:1EtOAc:hexanes) gave 104 mg of the title compound: MS (ES+) 597.1 (MH+), 619.1 (M+Na).

d) 4-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-1-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-3-pyrrolidinone

To a 0°C solution of the alcohol (100 mg, 0.17 mmol) in acetone (5.0 mL) was added Jone's reagent dropwise until the brown color persisted. The reaction was allowed to warm to room temperature and stirred approximately 48 hours whereupon it was quenched with isopropanol, diluted with EtOAc and washed sequentially with sat. K_2CO_3, water and brine. The organic layer was dried ($MgSO_4$), filtered and concentrated. Column chromatography of the residue (3:1 EtOAc:hexanes) gave 31 mg of the title compound: MS (ES+) 595.1 (MH+), 617.0 (M+Na).

Compound 2. Preparation of 4-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-1-N[N-(methyl)-L-leucyl)]-3-pyrrolidinone

a) 4-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-1-[N-[(tert-butoxy)carbonyl]-N-(methyl)-L-leucyl]-3-pyrrolidinol

To a solution of 3-hydroxy-4-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-1-pyrrolidine (350 mg) was added N-BOC-N-methyl-leucine (222 mg, 0.0.91 mmol), HOBT(122.5 mg, 0.91 mmol), EDC (208.6 mg, 1.08 mmol) and N-methyl morpholine (0.3 mL, 2.72 mmol). The reaction was stirred at room temperature until complete by TLC analysis. Workup and column chromatography (1:1 Hex:EtOAc) gave 480 mg of the title compound which was used in the following reaction: MS (ES+) 477.4, 577.4 (MH+), 599.4 (M+Na).

b) 4-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-1-[N-[(tert-butoxy)carbonyl]-N-(methyl)-L-leucyl]-3-pyrrolidinone

To a -78°C solution of oxalyl chloride (0.11 mL, 1.23 mmol) in CH_2Cl_2 was added DMSO (0.17 mL, 2.46 mmol) dropwise. The reaction was allowed to stir at -78°C for 20 minutes whereupon a solution of the alcohol (474 mg, 0.82 mmol) in CH_2Cl_2 was added dropwise. The reaction was stirred at -78°C for 30 minutes whereupon triethylamine (0.57 mL) was added in a single portion and allowed to warm to room temperature. Workup and column chromatography (2:1 hexanes:ethyl acetate) gave 247 mg of the title compound: MS (ES+) 475, 575 (M+H), 597 (M+Na).

c) 4-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-1-N[N-(methyl)-L-leucyl)]-3-pyrrolidinone hydrochloride

To a room temperature solution EtOAc/HCl was added the carbamate. The reaction was stirred until complete by TLC analysis. Concentration gave the title compound: MS (ES+) 475 (M+H, 100%).

Compound 3. Preparation of 4-[N-[(4-pyridylmethoxy)carbonyl]-L-leucyl]-1-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-3-pyrrolidinone

a) 3-hydroxy-4-[N-[(4-pyridylmethoxy)carbonyl]-L-leucyl]-1-pyrrolidinecarboxylic acid 1,1dimethylethyl ester

3-hydroxy-4-amino-1-pyrrolidinecarboxylic acid, 1,1-dimethylethyl ester was coupled with iso-nicotinoyloxycarbonyl leucine in a similar manner as that described above to give 8.5 grams of the title compound: MS (ES+) 451 (MH+, 100%).

b) 3-hydroxy-4-[N-[(4-pyridylmethoxy)carbonyl]-L-leucyl]-1-pyrrolidine hydrochloride

The carbamate from the previous step was deprotected with EtOAc/HCl to give 8.4 grams of the title compound after concentration: MS (ES+)351 (MH+, 100%).

c) 4-[N-[(4-pyridylmethoxy)carbonyl]-L-leucyl]-1-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-3-pyrrolidinol

To a solution of CBZ leucinal (155 mg) in CH_2Cl_2 was added triethylamine (0.09 mL) and the amine hydrochloride (200 mg, 0.52 mmol) from the previous step. The reaction was stirred at room temperature for 2 hours whereupon the majority of the solvent was removed *in vacuo*. The mixture was redissolved in CH_2Cl_2 and sodium triacetoxyborohydride was added. The reaction was stirred at room temperature for 4 hours. Workup and column chromatography (5% methanol/chloroform) gave 200.5 mg of the title compound: MS(ES+) 583 (MH+, 100%).

d) 4-[N-[(4-pyridylmethoxy)carbonyl]-L-leucyl]-1-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-3-pyrrolidinone

To a DMSO (2 mL) solution of the alcohol (50 mg, 0.09 mmol) from the previous step was added triethylamine (0.07 mL, 0.52 mmol) and pyridine/sulfur trioxide complex (41 mg, 0.26 mmol). The reaction was maintained at room temperature until complete by TLC analysis. Workup and chromatography (5% methanol/chloroform) gave 37 mg of the title compound: MS (ES+) 582 (MH+, 100%).

Compound 4. Preparation of (3S)-3-[(N-benzyloxycarbonyl)-L-leucinyl]amino-1-(1-propoxy)-5-methyl-2-hexanone

(3S)-3-[(N-benzyloxycarbonyl)-L-leucinyl]amino-1-diazo-5-methyl-2-hexanone (150 mg, 0.37 mmol) was dissolved in 1-propanol (2.5 ml), then rhodium acetate (2 mg) was added and the reaction was stirred at RT for 2h. The reaction mixture was chromatographed (silica gel, 20% EtOAc/hexanes) to yield the title compound as a white solid (59 mg, 37%). MS(ES) $M+H^+ = 435$, $M+ NH_4^+ = 452$, $2M+H^+ = 869.6$.

Compound 5. Preparation of bis-(Cbz-leucinyl)-1,3-diamino-propan-2-one

Cbz-leucine (500 mg, 1.88 mmol), EDCI (558 mg, 1.88 mmol) was dissolved in DMF (4.0 ml) with 1,3-diamino-propan-2-ol (85 mg, 0.94 mmol) and Hunig's base (0.3 ml, 1.88 mmol) and was stirred at RT overnight. The reaction

was diluted with EtOAc (20 ml) and was extracted with water (2 x 20 ml). The combined organics were dried with magnesium sulfate, filtered, concentrated in vacuo. The intermediate was then dissolved in acetone (4.0 ml) and Jones reagent (2.0 ml, 1.5 M) was added dropwise and the reaction was stirred at RT overnight. The excess Jones reagent was then quenched with isopropanol (1.0 ml), then the reaction was diluted with EtOAc (20 ml) and was extracted with water (2x 20 ml) to remove the inorganic salts. The combined organics were dried with magnesium sulfate, filtered, concentrated, and chromatographed (silica gel, 2-5% MeOH/ methylene chloride) to give the title compound as a white solid (410 mg, 75%). MS(ES) $M+H^+$=583, $M+Na^+$=605.

Compound 6. Preparation of 2-[N-(3-benzyloxybenzoyl)]-2'-[N'-(N-benzyloxycarbonyl-L-leucinyl)]carbohydrazide

a) methyl 3-benzyloxybenzoate

To a suspension of NaH (0.395 g, 9.87 mmol, 60% in mineral oil) in DMF (20 mL) was added methyl 3-hydroxybenzoate (1.0 g, 6.58 mmol). After stirring for 15 min at room temperature, benzyl bromide (1.1 g, 6.58 mmol) was added. After stirring at room temperature for 3h, the solution was partitioned between ethyl acetate and water. The organic layer was washed with water (2 X 75 mL), saturated aqueous sodium bicarbonate, and brine, then dried ($MgSO_4$), filtered and concentrated to yield an off-white solid (1.013 g, 4.2 mmol). ^1H NMR (400 MHz, $CDCl_3$) d 7.67 (m, 2H), 7.48-7.34 (m. 6H), 7.19 (m, 1H), 5.12 (s, 2H), 3.95 (s, 3H).

b) 3-benzyloxybenzoic acid

To a solution of the compound of Example 6(a) (0.400 g, 1.65 mmol) in THF (2 mL) and water (2 mL) was added lithium hydroxide monohydrate (0.076 g, 1.82 mmol). After stirring at reflux for 5 h, the solution was partitioned between ethyl acetate and 3N HCl. The organic layer was washed with brine, dried ($MgSO_4$), filtered and concentrated to yield a white solid (0.355 g, 1.56 mmol). ^1H NMR (400 MHz, CD_3OD) d 7.58 (m, 2H), 7.36-7.24 (m. 6H), 7.10 (m, 1H), 5.04 (s, 2H).

c) 2-[N-(3-benzyloxybenzoyl)]-2'-[N'-(N-benzyloxycarbonyl-L-leucinyl)]carbohydrazide

Following the procedure of Example A, below, except substituting 3-benzyloxybenzoic acid for N-acetyl-L-leucine and 2-[N-(N-benzyloxycarbonyl-L-

leucinyl)]carbohydrazide for 2-[N-(N-benzyloxycarbonyl-L-alanyl)]carbohydrazide, the title compound was prepared as a white solid (0.062 g, 25%). MS(ESI): 548.1 $(M+H)^+$.

Example A

Preparation of 2-[N-(N-acetyl-L-leucinyl)]-2'-[N'-(N-benzyloxycarbonyl-L-alanyl)]carbohydrazide

To a stirring solution of 2-[N-(N-benzyloxycarbonyl-L-alanyl)]carbohydrazide (0.150g, 0.508mmol) in DMF (2mL) was added N-acetyl-L-leucine (0.092g, 0.534mmol), 1-hydroxybenzotriazole (0.014g, 0.102mmol), and 1-(3-dimethylaminopropyl)-3-ethylcarbodiimide hydrochloride (0.102g, 0.534mmol). After stirring at room temperature for 16h, the solution was diluted with ethyl acetate, washed successively with water, saturated aqueous sodium bicarbonate, and brine. The organic layer was dried (MgSO4), filtered and concentrated. The residue was purified by column chromatography (silica gel, methanol/dichloromethane) to yield the title compound as a white solid (0.028 g, 12%). MS(ESI): 451.1 (M+H)+.

Compound 7. Preparation of (1S)-N-[2-[(1-benzyloxycarbonylamino)-3-methylbutyl]thiazol-4-ylcarbonyl]-N'-(N-benzyloxycarbonyl-L-leucinyl)hydrazide

a) N-*tert*-butoxycarbonyl-(L)-leucinamide

To a solution of N-tert-butoxycarbonyl-(L)-leucine (7.0g, 28.1mmol) in dry THF (100mL) at -40°C was added isobutylchloroformate (3.8g, 28.1mmol) and N-methylmorphiline (6.0, 59mmol). After 15 minutes of stirring, ammonia was bubbled through the mixture for an additional 15 minutes, then warmed to room temperature and allowed to stir for 2 hours. Mixture filtered and filtrate concentrated in vacuo to yield title compound as a white solid (6.5, 28.0mmol). ^{1}HNMR (400MHz, $CDCl_3$) d 6.38 (br s, 1H), 5.79 (br s, 1H), 5.04 (br d, 1H), 4.13 (m, 1H), 1.71-1.49 (m, 3H), 1.39 (s, 9H), 0.92 (dd, 6H).

b) N-*tert*-butoxycarbonyl-(L)-leucinethioamide

To a stirring solution of the compound of Example 7(a) (6.5, 28.0 mmol) in dry THF was added Lawesson's reagent (6.8g, 16.9 mmol) and the mixture was stirred at room temperature under argon overnight. The solvent was evaporated and the residue chromatographed (silica gel, 12% ethyl acetate/hexane) to give the title compound as a white solid (5.4g, 77%). ^{1}HNMR (400MHz, $CDCl_3$) d 8.54 (br s,

1H), 7.97 (br s, 1H), 5.28 (br d, 1H), 4.52 (m, 1H), 1.72-1.58 (m, 3H), 1.40 (s, 9H), 0.92 (m, 6H).

c) (1S)-1-(tert-butoxycarbonyl)amino-1-(4-carboethoxythiazol-2-yl)-3-methylbutane

The compound of Example 7(b) (5.4g, 21.7 mmol) was stirred in dry acetone (100mL) under argon at -10°C. Ethylbromopyruvate (4.7g, 23.9mmol) was added and stirred for 1h at -10°C. The solution was poured into a well stirred mixture of chloroform and water and then into saturated sodium bicarbonate solution. The organic phase was separated and the aqueous layer extracted with chloroform. The combined organic extracts were dried over $MgSO_4$, filtered and concentrated to an oil. The oily residue was treated with TFAA (5.0g, 23.9mmol) and pyridine (3.8g, 47.8mmol) in dichloromethane for 1h at -20°C. Excess solvent was removed in vacuo and the residue was dissolved in dichloromethane. The solution was washed with saturated aqueous sodium bicarbonate and 1.0N $KHSO_4$ until pH 7. The solution was dried over magnesium sulfate, filtered and concentrated to an oil which was chromatographed (silica gel, 7.5% ethyl acetate/hexane) to give the title compound as a tan solid (4.5g, 61%). ^{1}HNMR (400MHz, $CDCl_3$) d 7.98 (s, 1H), 5.04 (br d, 1H), 4.95 (m, 1H), 4.31 (q, 2H), 1.88 (m, 1H), 1.63 (m, 2H), 1.40 (s, 9H),1.32 (t, 3H), 0.85 (dd, 6H).

d) (1S)-1-(Benzyloxycarbonyl)amino-1-(4-carboethoxythiazol-2-yl)-3-methylbutane

The compound of Example 7(c) (0.250g, 0.731mmol) was dissolved in TFA (2mL) and stirred at room temperature for 15 minutes when diluted with methanol and concentrated in vacuo. The residue was dissolved in methylene chloride and treated with triethylamine (0.739g, 7.31mmol) followed by benzyl chloroformate (1.2g, 7.31mmol). The solution stirred at room temperature for 2h when partition between ethyl acetate/water. The organic layer was washed with brine, collected, dried ($MgSO_4$) and concentrated to a residue that was chromatographed (silica gel, 15% ethyl acetate/hexane) to give the title compound as an oil (0.198g, 72%). ^{1}HNMR (400MHz, $CDCl_3$) d 8.01 (s, 1H), 7.32 (m, 5H), 5.51 (br d, 1H), 5.14 (m, 1H), 5.10 (s, 2H), 4.37 (q, 2H), 1.93 (m, 1H), 1.81-1.67 (m, 2H), 1.39 (t, 3H), 0.95 (m, 6H).

e) (1S)-N-[2-[(1-benzyloxycarbonylamino)-3-methylbutyl]thiazol-4-ylcarbonyl]-N'-(N-benzyloxycarbonyl-L-leucinyl)hydrazide

Following the procedure of Example B(a)-(d), below, except substituting (1S)-1-(Benzyloxycarbonyl)amino-1-(4-carboethoxythiazol-2-yl)-3-methylbutane for (1S)-1-benzyloxycarbonylamino-1-(2-carboethoxythiazol-4-yl)-3-methylbutane in step (c), the title compound was prepared. MS (MH^+): 610.0

Example B

Preparation of (1S,2'R)-N-4-[[(1-benzyloxycarbonyl)amino]-3-methylbutyl]thiazol-2-ylcarbonyl-N'-2'-(benzyloxycarbonyl)amino-4'-methylpentanoylhydrazide

a) N-benzyloxycarbonyl-L-leucinyl bromomethyl ketone

1-methyl-3-nitro-1-nitrosoguanidine (6.65 g, 45.2 mmol) in ether (225 mL) is cooled to 0°C. 40% sodium hydroxide is added slowly and the diazomethane is allowed to collect in the ether solution for 30 minutes at 0°C. The ether solution is then decanted and left at 0 °C.

N-Cbz-L-leucine (2.10 g, 7.6 mmol) was dissolved in THF (10 mL), cooled to -40 °C, and 4-methylmorpholine (0.77 g, 7.6 mmol, 0.83 mL) was added, followed by dropwise addition of isobutyl chloroformate (1.04 g, 7.6 mmol, 0.98 mL). After 15 min, the solution was filtered into the previously prepared 0 °C solution of ethereal diazomethane. The resulting solution was allowed to stand at 0 °C for 23 h. HBr (30% in acetic acid) (45.2 mmol, 9 mL) was added and the resulting solution was stirred at 0 °C for 5 min, then washed sequentially with 0.1 N HCl, saturated aqueous NaHCO3 and saturated brine, then dried (MgSO4), filtered and concentrated to give the title compound as a colorless oil (2.43 g, 94%).

b) (1S)-1-benzyloxycarbonylamino-1-(2-carboethoxythiazol-4-yl)-3-methylbutane

A solution of the compound of Example B(a) (1.57 g, 4.58 mmol) and ethyl thiooxamate (0.61 g, 4.58 mmol) in ethanol (10 mL) was heated at reflux for 4 h. The solution was then cooled , concentrated and the residue was purified by flash chromatography on 230-400 mesh silica gel, eluting with 1:4 ethyl acetate/hexanes, to give the title compound as a yellow oil (1.0 g, 58%). 1H NMR (400 MHz, CDCl3) d 7.41 (s, 1H), 7.34-7.31 (m, 5H), 5.40 (d, 1H), 5.10 (d, 1H), 5.05 (d, 1H), 4.98 (q, 1H), 4.48 (q, 2H), 1.80-1.76 (m, 2H), 1.57-1.53 (m, 1H), 1.44 (t, 3H), 0.95 (d, 3H), 0.93 (d, 3H).

c) (1S)-1-benzyloxycarbonylamino-1-(2-hydrazinocarbonylthiazol-4-yl)-3-methylbutane

A solution of the compound of Example B(b) (0.30 g, 0.8 mmol) and hydrazine hydrate (0.40 g, 8.0 mmol, 0.39 mL) in ethanol (8 mL) was allowed to stir at room temperature for 2 h. The solution was then concentrated to yield the title compound as a white foam (0.28 g, 98%). 1H NMR (400 MHz, CDCl3) d 8.29 (s, 1H), 7.37-7.35 (m, 5H), 5.18 (d, 1H), 5.09 (dd, 2H), 4.95 (q, 1H), 4.07 (d, 2H), 1.71 (t, 2H), 1.55 (m, 1H), 0.96 (d, 3H), 0.94 (d, 3H).

d) (1S,2'R)-N-4-[[(1-benzyloxycarbonyl)amino]-3-methylbutyl]thiazol-2-ylcarbonyl-N'-2'-(benzyloxycarbonyl)amino-4'-methylpentanoylhydrazide

A solution of the compound of Example B(c) (100 mg, 0.28 mmol), N-Cbz-L-leucine (80.5 mg, 0.30 mmol), 1-(3-dimethylaminopropyl)-3-ethylcarbodiimide hydrochloride (58.2 mg, 0.30 mmol) and 1-hydroxybenzotriazole (7.5 mg, 0.06 mmol) in DMF (0.6 mmol) was allowed to stir at room temperature for 18 h. The solution was diluted with ethyl acetate and washed successively with water, 0.1 N HCl, saturated aqueous NaHCO3 and saturated brine, then dried (MgSO4), filtered and concentrated. The residue was purified by flash chromatography on 230-400 mesh silica gel, eluting with 1:1 ethyl acetate/hexanes, to provide the title compound as a white solid (111.4 mg, 66%). mp 110-112 °C.

Compound 8. Preparation of 2,2'-N,N'-bis-benzyloxycarbonyl-L-leucinylcarbohydrazide

To a stirring solution of N-Cbz-L-leucine (Chemical Dynamics Corp.) (2.94 g, 11.1 mmol) in 22 mL of DMF was added carbohydrazide (0.5 g, 5.6 mmol), 1-(3-dimethylaminopropyl)-3-ethylcarbodiimide hydrochloride (2.13 g, 11.1 mmol) and 1-hydroxybenzotriazole (0.3 g, 2.2 mmol). After stirring at room temperature for 22 h, the solution was poured into 500 mL of water. The precipitate was collected by vacuum filtration and washed with water (4 X 150 mL) and dichloromethane (4 X 150 mL), then dried under vacuum to provide the title compound as a white solid (1.49 g, 46%). MS(ESI): 607.1 $(M+Na)^+$.

Compound 9. Preparation of 1-N-(N-imidazole acetyl-leucinyl)-amino-3-N-(4-phenoxy-phenyl-sulfonyl)-amino-propan-2-one

a) 1-N-(N-imidazole acetyl-leucinyl)-amino-3-N-(4-phenoxy phenyl sulfonyl)-amino-propan-2-one

Following the procedure of Example C(a)-(d), below, substituting "imidazole acetic acid" for "4-pyridyl acetic acid", the title compound was prepared: MS(ES) $M+H^+ = 542$.

Example C

Preparation of 1-N-(N-Cbz-leucinyl)-amino-3-N-(2-pyridyl-sulfonyl)-amino-propan-2-one

a) 1-N-(N-Cbz-leucinyl)-amino-3-N-(4-phenoxy-phenyl-sulfonyl)-amino-propan-2-ol

1,3-Diamino propan-2-ol (6.75 g, 75 mmol) was dissolved in DMF (100ml) and Cbz-leucine (20g, 75.5 mmol), HOBT-hydrate (11g, 81.5 mmol), and EDCI (15.5g, 81.2 mmol) were added. The reaction was stirred overnight at RT. A portion of the reaction mixture (30 ml) was concentrated in vacuo, then ether (50 ml) and MeOH (30 ml) were added. A 1N solution of hydrochloric acid in ether was added (1 M, 30 ml) and a white gum formed, which was washed several times with ether. MeOH-acetone were added and heated until the gum became a white solid. The white solid was dissolved in DMF (25 ml) and DIEA (5ml), then 4-phenoxy phenyl sulfonyl chloride was added. The reaction was stirred for 2h, concentrated in vacuo, then chromatographed (silica gel, 1:1 EtOAc: hexanes) to provide the desired product as a white solid.

b) Leucinyl-amino-3-N-(4-phenoxy phenyl sulfonyl)-amino-propan-2-ol

1-N-(Cbz-leucinyl)-amino-3-N-(4-phenoxy-phenyl-sulfonyl)-amino-propan-2-ol (1.0g, 1.8 mmol) was dissolved in EtOH (30 ml), then 10% Pd/C (0.22g) was added followed by 6N hydrochloric acid (2.5 ml), and the reaction was stirred under a balloon of hydrogen gas for 4h at RT. The reaction mixture was filtered, concentrated, and azeotroped with toluene to provide a white glass which was used in the next reaction without further purification.

c) 1-N-(N-4-pyridyl acetyl-leucinyl)-amino-3-N-(4-phenoxy-phenyl-sulfonyl)-amino-propan-2-ol

Leucinyl-amino-3-N-(4-phenoxy phenyl sulfonyl)-amino-propan-2-ol (0.36 g, 0.76 mmol) was dissolved in DMF (5 ml), then NMM (0.45 ml, 4 mmol) was added followed by 4-pyridyl acetic acid (0.13g, 0.75 mmol) and HBTU (0.29g, 0.76 mmol) and the reaction was stirred at RT overnight. The reaction mixture was concentrated in vacuo, then chromatographed (silica gel, 5%MeOH: methylene

chloride) to provide the desired product as a white solid (90 mg, MS(ES): $M+H^+$ = 555.

d) 1-N-(N-4-pyridyl acetyl-leucinyl)-amino-3-N-(4-phenoxy-phenyl-sulfonyl)-amino-propan-2-one

1-N-(N-4-pyridyl-acetyl-leucinyl)-amino-3-N-(4-phenoxy-phenyl-sulfonyl)-amino-propan-2-ol (45 mg, 0.08 mmol) was dissolved in acetone (5ml), then 1N hydrochloric acid (2 ml) was added. The reaction was concentrated in vacuo, then redissolved in acetone. Jones reagent (1.5 M, several drops) was added and the reaction mixture was stirred for 6h at RT. Isopropanol (0.5 ml) was added and the reaction mixture was concentrated in vacuo. The reaction was diluted with pH 7 buffer and then was extracted with EtOAc, dried with magnesium sulfate, filtered, concentrated in vacuo, then chromatographed (silica gel, 5% MeOH-methylene chloride) to give the desired product as a white solid (27 mg, 50%): MS(ES): $M+H^+$ = 553.

B. Crystallization of the protein and protein-inhibitor complexes

Human cathepsin K was expressed in *baculovirus* cells for the first eight of the nine inhibitors described below. Conditioned media containing expressed pro-cathepsin K was loaded directly onto an S-Sepharose column pre-equilibrated with 25 mM phosphate buffer at pH 8. The column was eluted with a NaCl gradient. Fractions containing pro-cathepsin K were pooled, concentrated to 2.5 mg/ml and activated to mature cathepsin K in 50 mM sodium acetate buffer pH 4.0 containing 20 mM L-cysteine and 1% mature cathepsin K as seed. The activation was monitored using CBZ-Phe-Arg-AMC,as fluorogenic substrate and by SDS-PAGE. When the increasing specific activity reached a plateau (*ca.* 15 µmol/min/mg), the reaction was stopped by the addition of inhibitor. The inhibited mature cathepsin K was concentrated and dialyzed against 20 mM MES, 50 mM NaCl, 2 mM L-cysteine, pH 6.

Protein preparation for cathepsin K complex with 4-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-1-N[N-(methyl)-L-leucyl)]-3-pyrrolidinone (only)

Human cathepsin K was expressed in *E. coli*. The cell pellet from 1 L of bacterial culture weighing 2.35 gm. was washed with 50 mL of 50 mM Tris/HCl, 5 mM EDTA, 150 mM NaCl, pH 8.0. After centrifugation at 13,000 x g for 15 mins,

the washed pellet was resuspended into 25 mL of the same buffer prepared at 4° C and lysed by passage twice through a cell disruptor (Avestin) at 10,000 psi. The lysate was centrifuged as above, the supernatant decanted and the pellet suspended in 25 mL 50 mM Tris/HCl, 10 mM DTT, 5 mM EDTA, 150 mM NaCl, pH 8.0 containing either 8 M urea or 6 M guanidine HCl. After stirring at 4° C for 30 mins, insoluble cellular debris was removed by centrifugation at 23,000 x g for 30 mins and the supernatant clarified by filtration (0.45 um, Millipore).

Varying amounts of the proenzyme form of cathepsin K were refolded by quick dilution into stirring, N_2 (g) sparged 50 mM Tris/HCl, 5 mM EDTA, 10 mM reduced and 1 mM oxidized glutathione, 0.7 M L-arginine pH 8.0 and stirred overnight at 4° C. After concentration to ca.1 mg/mL using a stirred cell fitted with a YM-10 membrane (Amicon), the sample was clarified by centrifugation and filtration then dialyzed against 25 mM Na_2PO_4, 1.0 M NaCl, pH 7.0. The dialysate was applied at a LFR= 23 cm/hr to a 2.6 x 90 cm column of Superdex 75 (Pharmacia) pre-equilibrated in 25 mM Na_2PO_4, 1.0 M NaCl, pH 7.0. The cathepsin K proenzyme was pooled based upon purity as observed on a reduced, SDS-PAGE gel.

Crystals of mature activated cathepsin K complexed with inhibitor grew to a size of approximately 0.2 mm^3 in about six days at 20°C. The concentration of inhibited cathepsin K used in the crystallization was approximately 8 mg./ml. The method of vapor diffusion in hanging drops was used to grow crystals from the solution of cathepsin K - inhibitor complex. The initial crystal structure to be determined was that of cathepsin K in complex with the cysteine protease inhibitor E64. Crystals of mature activated cathepsin K complexed with E-64 grew to a size of approximately 0.2 mm^3 in six days at 20°C. The concentration of E-64-inhibited cathepsin K used in the crystallization was 8 mg/ml. Vapor diffusion was used in hanging drops from a solution of 10% PEG 8000, 0.1 M Na^+/K^+ phosphate at pH 6.2 containing 0.2M NaCl. Crystals of the complex are orthorhombic, space group $P2_12_12_1$, with cell constants of a=38.4, b=50.7, and c=104.9 Ångstroms. This crystal form will be referred to as Form II. The crystals contain one molecule in the asymmetric unit and contain approximately 40% solvent with a Vm value of 2.1 A^3/Dalton. X-ray diffraction data were measured from a single crystal using a Siemens two-dimensional position-sensitive detector on a Siemens rotating anode generate operating a 5 KW. The structure was determined by molecular replacement using X-PLOR. The starting model consisted of all atoms of the main chain of papain and those side chain atoms predicted to be homologous between the two

proteins as determined from sequence alignment. The cross rotation function was calculated using x-ray diffraction data from 10 to 4 Å and a radius of integration of 32 Å. The highest peak was 6.0 σ. A translation search was carried out using data from 8 to 3.5 Ångstroms resulting in the highest peak of 12.5 σ.The resulting model gave an R_c factor of 0.488. This model was refined by rigid-body refinement, and the resulting phases were used to calculate Fourier maps with coefficients $|F_o-F_c|$ and $|2F_o-F_c|$, into which the atomic model of cathepsin K was built using the molecular graphics program FRODO. Conventional positional refinement was used to refine the structure during model building. The structure was refined using X-PLOR. The electron density for E-64 was clear in the maps. The inhibitor was built into density and several additional cycles of map fitting and refinement were carried out to a final R_c of 0.191.

Crystallization of the complex of cathepsin K with 3(S)-3-[(N-benzyloxycarbonyl)-L-leucinyl]amino-5-methyl-1-(1-propoxy)-2-hexanone

Crystals of mature activated cathepsin K complexed with the inhibitor grew from a solution of 10% isopropanol, 0.1 M $NaPO_4$ / citrate at pH 4.2. Crystals of the complex are tetragonal, space group $P4_32_12$, with cell constants of a=57.6 Å, and c=131.2 Å. This crystal form will be referred to as Form III. Diffraction data were collected as described above. The crystals contain one molecule in the asymmetric unit and contain 36% solvent with a V_m value of 2.3 $Å^3$/Dalton. The structure was determined by molecular replacement using X-PLOR at 2.5 Ångstroms resolution. The starting model consisted of all protein atoms of the orthorhombic form of cathepsin K-E64 structure. Molecular replacement was carried out as described above for the cathepsin K-E64 structure determination. The model was refined by rigid-body refinement using X-PLOR, and the resulting phases were used to calculate Fourier maps with coefficients $|F_o-F_c|$ and $|2F_o-F_c|$, into which the atomic model of the inhibitor was built using the molecular graphics program FRODO. Conventional positional refinement was used to refine the structure during model building. The structure was refined using X-PLOR. Several cycles of map fitting and refinement were carried out to a final R_c of 0.245.

Crystallization of the complex of cathepsin K with 2-[N-(3-benzyloxybenzoyl)]-2'-[N'-(N-benzyloxycarbonyl-L-leucinyl)]carbohydrazide

Crystals of mature activated cathepsin K complexed with the inhibitor grew from a solution of 22.5% PEG 8000, 0.075 M sodium acetate at pH 4.5 containing 0.15 M Li_2SO_4. Crystals of the complex grew as Form III. Diffraction data were collected as described above. The structure was determined by rigid body refinement with X-PLOR utilizing the previous Form III protein model at 2.4 Ångstroms resolution. Fourier maps with coefficients $|F_o-F_c|$ and $|2F_o-F_c|$ were used to fit the atomic model of the inhibitor using the molecular graphics program FRODO. Conventional positional refinement (X-PLOR) was used to refine the structure during model building. Several cycles of map fitting and refinement were carried out to a final R_c of 0.237.

Crystallization of the complex of cathepsin K with bis-(Cbz-leucinyl)-1,3-diamino-propan-2-one

Crystals of mature activated cathepsin K complexed with the inhibitor grew from a solution of 10% isopropanol, 0.1 M $NaPO_4$ / citrate at pH 4.2. Crystals of the complex grow as Form III. Diffraction data were collected as described above. The structure was determined by rigid body refinement of the previous Form III protein model at 2.6 Ångstroms resolution. Fourier maps with coefficients $|F_o-F_c|$ and $|2F_o-F_c|$ were used to fit the atomic model of the inhibitor using the molecular graphics program FRODO. Conventional positional refinement was used to refine the structure during model building. Several cycles of map fitting and refinement were carried out using X-PLOR to a final R_c of 0.210.

Crystallization of the complex of cathepsin K with 4-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-1-N[N-(methyl)-L-leucyl)]-3-pyrrolidinone

Crystals of mature activated cathepsin K complexed with the inhibitor grew from a solution 18% PEG 8000, 0.6 M sodium acetate at pH 4.5 containing 0.12 M Li_2SO_4. Crystals of the complex grow in Form III. Diffraction data were collected as described above. The structure was determined by rigid body refinement of the previous Form III protein model with X-PLOR at 2.4 Ångstroms resolution. Fourier maps with coefficients $|F_o-F_c|$ and $|2F_o-F_c|$, were used to the atomic model of the inhibitor using the molecular graphics program FRODO. Conventional positional refinement was used to refine the structure during model building using X-PLOR. Several cycles of map fitting and refinement were carried out to a final R_c of 0.218.

Crystallization of the complex of cathepsin K with (1S)-N-[2-[(1-benzyloxycarbonylamino)-3-methylbutyl]thiazol-4-ylcarbonyl]-N'-(N-benzyloxycarbonyl-L-leucinyl)hydrazide

Crystals of mature activated cathepsin K complexed with the inhibitor grew from a solution of 30% MPD, 0.1 M MES at pH 7.0 and 0.1 M tris buffer at pH 7.0. Crystals of the complex are Form II. Diffraction data were collected as described above. The structure was determined by rigid body refinement of the previous Form II protein model with X-PLOR at 2.3 Ångstroms resolution. Fourier maps with coefficients $|F_o-F_c|$ and $|2F_o-F_c|$, were used to the atomic model of the inhibitor using the molecular graphics program FRODO. Conventional positional refinement was used to refine the structure during model building using X-PLOR. Several cycles of map fitting and refinement were carried out to a final R_c of 0.211.

Crystallization of the complex of cathepsin K with 2,2'-N,N'-bis-benzyloxycarbonyl-L-leucinylcarbohydrazide

Crystals of mature activated cathepsin K complexed with the inhibitor grew from a solution of 33% MPD, 0.1 M MES at pH 7. Crystals of the complex grow as Form II. Diffraction data were collected as described above. The structure was determined by rigid body refinement of the previous Form II protein model with X-PLOR at 2.2 Ångstroms resolution.. Fourier maps with coefficients $|F_o-F_c|$ and $|2F_o-F_c|$, were used to the atomic model of the inhibitor using the molecular graphics program FRODO. Conventional positional refinement was used to refine the structure during model building using X-PLOR. Several cycles of map fitting and refinement were carried out to a final R_c of 0.208.

Crystallization of the complex of cathepsin K with 4-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-1-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-3-pyrrolidinone

Crystals of mature activated cathepsin K complexed with the inhibitor grew from a solution of 28% MPD, 0.1 M MES at pH 7.0 and 0.1 M tris buffer at pH 7.0. Crystals of the complex Form II. Diffraction data were collected as described above. The structure was determined by rigid body refinement of the previous Form II protein model with X-PLOR at 2.3 Ångstroms resolution. Fourier maps with coefficients $|F_o-F_c|$ and $|2F_o-F_c|$, were used to the atomic model of the inhibitor

using the molecular graphics program FRODO. Conventional positional refinement was used to refine the structure during model building using X-PLOR. Several cycles of map fitting and refinement were carried out to a final R_c of 0.193.

Crystallization of the complex of cathepsin K with 4-[N-[(4-pyridylmethoxy)carbonyl]-L-leucyl]-1-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-3-pyrrolidinone

Crystals of mature activated cathepsin K complexed with the inhibitor grew from a solution of 30% MPD, 0.1 M MES at pH 7.0 and 0.1 M tris buffer at pH 7.0. Crystals of the complex Form II. Diffraction data were collected as described above. The structure was determined by rigid body refinement of the previous Form II protein model with X-PLOR at 2.2 Ångstroms resolution.. Fourier maps with coefficients $|F_o-F_c|$ and $|2F_o-F_c|$, were used to the atomic model of the inhibitor using the molecular graphics program FRODO. Conventional positional refinement was used to refine the structure during model building using X-PLOR. Several cycles of map fitting and refinement were carried out to a final R_c of 0.267.

Crystallization of the complex of cathepsin K with 1-N-(N-imidazole acetyl-leucinyl)-amino-3-N-(4-phenoxy-phenyl-sulfonyl)-amino-propan-2-one

Crystals of mature activated cathepsin K complexed with the inhibitor grew from a solution of 18% PEG 8000, 0.6 M sodium acetate at pH 4.5 containing 0.12 M Li_2SO_4. Crystals of the complex are Form III. Diffraction data were collected as described above. The structure was determined by rigid body refinement of the previous Form II protein model at 2.5 Ångstroms resolution.. Fourier maps with coefficients $|F_o-F_c|$ and $|2F_o-F_c|$ were used to fit the atomic model of the inhibitor using the molecular graphics program FRODO. Conventional positional refinement was used to refine the structure during model building. Several cycles of map fitting and refinement were carried out using X-PLOR to a final R_c of 0.246.

Abbreviations

E-64, [1-[N-[(L-3-*trans*-carboxyoxirane-2carbonyl)-L-leucyl]amino]-4-guanidinobutane]
CBZ, benzyloxycarbonyl
AMC, aminomethylcoumarin
MPD, 2 methyl-2,4-pentanediol

PIPES, piperazone-N,N-bis(2-ethanesulfonic acid)
MES, 2-(N-morpholino)-ethanesulfonic acid
tris, tris(hydroxymethyl)-aminomethane
PEG, polyethyleneglycol
M, Molar
$R_C = \Sigma|(F_O - F_C)| / F_O$
F_O = observed structure amplitude
F_C = calculated structure amplitude
EDTA, ethylenediaminetetraacetic acid
DTT, 1,4-dithiothreitol
SDS-PAGE, sodium dodecylsulfate polyacrylamide gel electrophoresis

This invention is not to be limited in scope by the specific embodiments described herein. Indeed, various modifications of the invention in addition to those described herein will become apparent to those skilled in the art from the foregoing description. Such modifications are intended to fall within the scope of the appended claims.

The disclosures of the patents, patent applications and publications cited herein are incorporated by reference in their entireties.

TABLE I

Table of the orthogonal three dimensional coordinates in Ångstroms and B factors ($Å^2$) for cathepsin K.

Residue	Atom	X	Y	Z	B
1	ALA N	-3.94	11.01	90.45	15.00
1	ALA CA	-4.70	12.30	90.45	15.00
1	ALA C	-4.40	13.14	89.20	15.00
1	ALA O	-3.34	12.99	88.57	15.00
1	ALA CB	-4.36	13.12	91.73	15.00
2	PRO N	-5.36	14.01	88.80	15.00
2	PRO CA	-5.19	14.86	87.61	15.00
2	PRO C	-4.35	16.05	88.06	15.00
2	PRO O	-4.89	17.00	88.65	15.00
2	PRO CB	-6.62	15.33	87.31	15.00
2	PRO CG	-7.53	14.58	88.32	15.00
2	PRO CD	-6.63	14.31	89.47	15.00
3	ASP N	-3.04	16.00	87.87	15.00
3	ASP CA	-2.25	17.14	88.30	15.00
3	ASP C	-2.27	18.18	87.20	15.00
3	ASP O	-1.57	18.02	86.20	15.00
3	ASP CB	-0.82	16.75	88.67	15.00
3	ASP CG	-0.09	17.85	89.45	15.00
3	ASP OD1	-0.74	18.83	89.89	15.00
3	ASP OD2	1.14	17.73	89.63	15.00
4	SER N	-3.10	19.21	87.36	15.00
4	SER CA	-3.19	20.26	86.35	15.00
4	SER C	-3.97	21.51	86.77	15.00
4	SER O	-4.97	21.44	87.48	15.00
4	SER CB	-3.77	19.72	85.03	15.00
4	SER OG	-5.17	19.55	85.08	15.00
5	VAL N	-3.50	22.65	86.28	15.00
5	VAL CA	-4.10	23.94	86.54	15.00
5	VAL C	-4.27	24.65	85.17	15.00
5	VAL O	-3.43	24.48	84.28	15.00
5	VAL CB	-3.22	24.79	87.51	15.00
5	VAL CG1	-1.80	24.88	87.00	15.00
5	VAL CG2	-3.79	26.17	87.69	15.00
6	ASP N	-5.39	25.34	84.99	15.00
6	ASP CA	-5.67	26.08	83.76	15.00
6	ASP C	-6.40	27.34	84.22	15.00
6	ASP O	-7.63	27.33	84.43	15.00

TABLE I

6	ASP	CB	-6.55	25.25	82.82	15.00
6	ASP	CG	-6.81	25.95	81.48	15.00
6	ASP	OD1	-6.11	26.94	81.14	15.00
6	ASP	OD2	-7.72	25.49	80.75	15.00
7	TYR	N	-5.64	28.42	84.37	15.00
7	TYR	CA	-6.15	29.70	84.84	15.00
7	TYR	C	-7.18	30.35	83.96	15.00
7	TYR	O	-7.76	31.36	84.33	15.00
7	TYR	CB	-5.00	30.67	85.09	15.00
7	TYR	CG	-4.06	30.20	86.18	15.00
7	TYR	CD1	-4.41	30.29	87.52	15.00
7	TYR	CD2	-2.82	29.64	85.86	15.00
7	TYR	CE1	-3.55	29.86	88.52	15.00
7	TYR	CE2	-1.96	29.21	86.84	15.00
7	TYR	CZ	-2.33	29.31	88.17	15.00
7	TYR	OH	-1.48	28.86	89.14	15.00
8	ARG	N	-7.41	29.78	82.79	15.00
8	ARG	CA	-8.41	30.30	81.87	15.00
8	ARG	C	-9.77	30.07	82.53	15.00
8	ARG	O	-10.65	30.93	82.49	15.00
8	ARG	CB	-8.33	29.58	80.53	15.00
8	ARG	CG	-7.00	29.76	79.85	15.00
8	ARG	CD	-7.00	29.12	78.48	15.00
8	ARG	NE	-7.27	27.69	78.52	15.00
8	ARG	CZ	-6.85	26.83	77.58	15.00
8	ARG	NH1	-6.15	27.27	76.54	15.00
8	ARG	NH2	-7.15	25.54	77.69	15.00
9	LYS	N	-9.90	28.94	83.20	15.00
9	LYS	CA	-11.12	28.60	83.91	15.00
9	LYS	C	-11.16	29.33	85.28	15.00
9	LYS	O	-11.96	28.99	86.15	15.00
9	LYS	CB	-11.18	27.08	84.13	15.00
9	LYS	CG	-11.04	26.25	82.86	15.00
9	LYS	CD	-11.09	24.72	83.11	15.00
9	LYS	CE	-9.80	24.15	83.76	15.00
9	LYS	NZ	-9.78	22.65	83.99	15.00
10	LYS	N	-10.33	30.35	85.47	15.00
10	LYS	CA	-10.28	31.03	86.76	15.00
10	LYS	C	-10.23	32.55	86.69	15.00
10	LYS	O	-10.11	33.20	87.73	15.00
10	LYS	CB	-9.10	30.51	87.58	15.00
10	LYS	CG	-9.05	28.98	87.72	15.00

TABLE I

10	LYS	CD	-7.68	28.45	88.13	15.00
10	LYS	CE	-7.54	28.31	89.63	15.00
10	LYS	NZ	-7.61	29.62	90.36	15.00
11	GLY	N	-10.29	33.11	85.48	15.00
11	GLY	CA	-10.27	34.56	85.31	15.00
11	GLY	C	-8.96	35.28	85.53	15.00
11	GLY	O	-8.93	36.49	85.77	15.00
12	TYR	N	-7.86	34.54	85.44	15.00
12	TYR	CA	-6.54	35.11	85.64	15.00
12	TYR	C	-5.97	35.67	84.36	15.00
12	TYR	O	-5.13	36.58	84.39	15.00
12	TYR	CB	-5.57	34.04	86.13	15.00
12	TYR	CG	-5.76	33.63	87.56	15.00
12	TYR	CD1	-6.85	32.86	87.95	15.00
12	TYR	CD2	-4.82	33.98	88.52	15.00
12	TYR	CE1	-7.00	32.46	89.25	15.00
12	TYR	CE2	-4.96	33.58	89.83	15.00
12	TYR	CZ	-6.04	32.81	90.19	15.00
12	TYR	OH	-6.16	32.38	91.49	15.00
13	VAL	N	-6.40	35.09	83.24	15.00
13	VAL	CA	-5.92	35.47	81.92	15.00
13	VAL	C	-6.95	36.24	81.09	15.00
13	VAL	O	-8.15	36.03	81.21	15.00
13	VAL	CB	-5.41	34.21	81.15	15.00
13	VAL	CG1	-6.54	33.26	80.89	15.00
13	VAL	CG2	-4.73	34.61	79.86	15.00
14	THR	N	-6.45	37.19	80.31	15.00
14	THR	CA	-7.27	38.02	79.44	15.00
14	THR	C	-7.39	37.38	78.05	15.00
14	THR	O	-6.69	36.41	77.74	15.00
14	THR	CB	-6.63	39.42	79.32	15.00
14	THR	OG1	-5.21	39.28	79.27	15.00
14	THR	CG2	-7.00	40.28	80.52	15.00
15	PRO	N	-8.31	37.88	77.20	15.00
15	PRO	CA	-8.50	37.34	75.86	15.00
15	PRO	C	-7.23	37.45	75.01	15.00
15	PRO	O	-6.38	38.30	75.30	15.00
15	PRO	CB	-9.61	38.22	75.30	15.00
15	PRO	CG	-10.38	38.60	76.51	15.00
15	PRO	CD	-9.28	38.96	77.45	15.00
16	VAL	N	-7.14	36.65	73.95	15.00
16	VAL	CA	-5.97	36.64	73.08	15.00

TABLE I

16	VAL	C	-5.86	37.87	72.18	15.00
16	VAL	O	-6.80	38.23	71.47	15.00
16	VAL	CB	-5.94	35.38	72.22	15.00
16	VAL	CG1	-4.70	35.38	71.34	15.00
16	VAL	CG2	-5.97	34.18	73.10	15.00
17	LYS	N	-4.70	38.52	72.22	15.00
17	LYS	CA	-4.47	39.71	71.43	15.00
17	LYS	C	-3.49	39.39	70.31	15.00
17	LYS	O	-2.82	38.36	70.34	15.00
17	LYS	CB	-3.93	40.85	72.30	15.00
17	LYS	CG	-4.99	41.75	72.95	15.00
17	LYS	CD	-5.84	41.01	73.99	15.00
17	LYS	CE	-5.88	41.72	75.34	15.00
17	LYS	NZ	-4.53	41.86	75.97	15.00
18	ASN	N	-3.43	40.30	69.35	15.00
18	ASN	CA	-2.58	40.20	68.17	15.00
18	ASN	C	-1.54	41.29	68.24	15.00
18	ASN	O	-1.89	42.46	68.35	15.00
18	ASN	CB	-3.42	40.41	66.91	15.00
18	ASN	CG	-2.71	39.96	65.64	15.00
18	ASN	OD1	-1.74	40.58	65.19	15.00
18	ASN	ND2	-3.19	38.87	65.06	15.00
19	GLN	N	-0.27	40.92	68.15	15.00
19	GLN	CA	0.79	41.91	68.23	15.00
19	GLN	C	0.97	42.67	66.95	15.00
19	GLN	O	1.54	43.76	66.94	15.00
19	GLN	CB	2.10	41.26	68.59	15.00
19	GLN	CG	2.54	40.22	67.63	15.00
19	GLN	CD	3.88	39.71	67.99	15.00
19	GLN	OE1	4.04	38.93	68.92	15.00
19	GLN	NE2	4.89	40.20	67.31	15.00
20	GLY	N	0.51	42.07	65.86	15.00
20	GLY	CA	0.62	42.69	64.56	15.00
20	GLY	C	1.98	42.49	63.90	15.00
20	GLY	O	2.53	41.39	63.86	15.00
21	GLN	N	2.50	43.60	63.38	15.00
21	GLN	CA	3.77	43.62	62.67	15.00
21	GLN	C	4.94	43.82	63.62	15.00
21	GLN	O	6.05	43.35	63.36	15.00
21	GLN	CB	3.73	44.74	61.64	15.00
21	GLN	CG	2.68	44.55	60.56	15.00
21	GLN	CD	2.88	43.25	59.82	15.00

TABLE I

21	GLN	OE1	4.01	42.87	59.52	15.00
21	GLN	NE2	1.79	42.55	59.56	15.00
22	CYS	N	4.68	44.56	64.69	15.00
22	CYS	CA	5.65	44.87	65.73	15.00
22	CYS	C	6.15	43.60	66.46	15.00
22	CYS	O	5.37	42.68	66.72	15.00
22	CYS	CB	4.97	45.82	66.71	15.00
22	CYS	SG	5.96	46.40	68.11	15.00
23	GLY	N	7.45	43.53	66.73	15.00
23	GLY	CA	8.00	42.37	67.42	15.00
23	GLY	C	7.84	42.62	68.90	15.00
23	GLY	O	8.80	42.94	69.61	15.00
24	SER	N	6.60	42.54	69.37	15.00
24	SER	CA	6.33	42.80	70.77	15.00
24	SER	C	5.75	41.63	71.54	15.00
24	SER	O	4.72	41.77	72.20	15.00
24	SER	CB	5.44	44.05	70.90	15.00
24	SER	OG	4.14	43.81	70.40	15.00
25	CYC	N	6.39	40.47	71.48	15.00
25	CYC	CA	5.88	39.34	72.25	15.00
25	CYC	CB	6.32	38.03	71.63	15.00
25	CYC	SG	8.04	38.06	71.17	15.00
25	CYC	C	6.33	39.44	73.72	15.00
25	CYC	O	5.67	38.91	74.62	15.00
25	CYC	O1	7.96	38.09	69.44	15.00
26	TRP	N	7.45	40.14	73.95	15.00
26	TRP	CA	7.97	40.33	75.30	15.00
26	TRP	C	7.04	41.24	76.05	15.00
26	TRP	O	6.67	40.96	77.18	15.00
26	TRP	CB	9.37	40.92	75.27	15.00
26	TRP	CG	9.47	42.24	74.61	15.00
26	TRP	CD1	9.74	42.49	73.30	15.00
26	TRP	CD2	9.32	43.52	75.24	15.00
26	TRP	NE1	9.78	43.84	73.06	15.00
26	TRP	CE2	9.52	44.50	74.24	15.00
26	TRP	CE3	9.04	43.94	76.55	15.00
26	TRP	CZ2	9.45	45.88	74.51	15.00
26	TRP	CZ3	8.98	45.32	76.82	15.00
26	TRP	CH2	9.18	46.27	75.80	15.00
27	ALA	N	6.63	42.32	75.39	15.00
27	ALA	CA	5.70	43.30	75.95	15.00
27	ALA	C	4.40	42.61	76.34	15.00

TABLE I

27	ALA	O	3.92	42.75	77.47	15.00
27	ALA	CB	5.43	44.39	74.93	15.00
28	PHE	N	3.83	41.86	75.40	15.00
28	PHE	CA	2.60	41.13	75.63	15.00
28	PHE	C	2.79	40.08	76.73	15.00
28	PHE	O	2.00	40.02	77.66	15.00
28	PHE	CB	2.10	40.48	74.33	15.00
28	PHE	CG	1.41	41.44	73.39	15.00
28	PHE	CD1	2.14	42.29	72.57	15.00
28	PHE	CD2	0.02	41.51	73.33	15.00
28	PHE	CE1	1.51	43.18	71.73	15.00
28	PHE	CE2	-0.62	42.40	72.49	15.00
28	PHE	CZ	0.12	43.24	71.69	15.00
29	SER	N	3.85	39.28	76.64	15.00
29	SER	CA	4.15	38.25	77.64	15.00
29	SER	C	4.33	38.84	79.03	15.00
29	SER	O	3.95	38.23	80.03	15.00
29	SER	CB	5.43	37.50	77.25	15.00
29	SER	OG	5.78	36.51	78.20	15.00
30	SER	N	4.96	40.01	79.08	15.00
30	SER	CA	5.18	40.71	80.33	15.00
30	SER	C	3.84	41.16	80.89	15.00
30	SER	O	3.48	40.84	82.03	15.00
30	SER	CB	6.10	41.91	80.10	15.00
30	SER	OG	7.39	41.48	79.72	15.00
31	VAL	N	3.08	41.87	80.07	15.00
31	VAL	CA	1.75	42.34	80.48	15.00
31	VAL	C	0.85	41.18	80.88	15.00
31	VAL	O	0.03	41.31	81.77	15.00
31	VAL	CB	1.09	43.16	79.36	15.00
31	VAL	CG1	-0.41	43.10	79.47	15.00
31	VAL	CG2	1.57	44.60	79.43	15.00
32	GLY	N	1.05	40.04	80.24	15.00
32	GLY	CA	0.26	38.85	80.51	15.00
32	GLY	C	0.56	38.20	81.83	15.00
32	GLY	O	-0.24	37.41	82.32	15.00
33	ALA	N	1.74	38.46	82.39	15.00
33	ALA	CA	2.10	37.90	83.69	15.00
33	ALA	C	1.61	38.88	84.75	15.00
33	ALA	O	1.01	38.49	85.75	15.00
33	ALA	CB	3.59	37.68	83.80	15.00
34	LEU	N	1.79	40.17	84.49	15.00

TABLE I

34	LEU	CA	1.35	41.21	85.40	15.00
34	LEU	C	-0.15	41.08	85.64	15.00
34	LEU	O	-0.65	41.47	86.69	15.00
34	LEU	CB	1.64	42.59	84.83	15.00
34	LEU	CG	3.09	42.99	84.57	15.00
34	LEU	CD1	3.08	44.29	83.81	15.00
34	LEU	CD2	3.84	43.15	85.87	15.00
35	GLU	N	-0.88	40.56	84.67	15.00
35	GLU	CA	-2.32	40.39	84.82	15.00
35	GLU	C	-2.66	39.14	85.64	15.00
35	GLU	O	-3.66	39.11	86.37	15.00
35	GLU	CB	-2.98	40.28	83.45	15.00
35	GLU	CG	-2.84	41.50	82.57	15.00
35	GLU	CD	-3.34	41.23	81.17	15.00
35	GLU	OE1	-3.19	40.08	80.70	15.00
35	GLU	OE2	-3.87	42.16	80.54	15.00
36	GLY	N	-1.84	38.10	85.50	15.00
36	GLY	CA	-2.08	36.89	86.26	15.00
36	GLY	C	-1.99	37.16	87.76	15.00
36	GLY	O	-2.78	36.62	88.55	15.00
37	GLN	N	-1.03	37.99	88.17	15.00
37	GLN	CA	-0.86	38.31	89.57	15.00
37	GLN	C	-1.88	39.32	90.06	15.00
37	GLN	O	-2.40	39.18	91.17	15.00
37	GLN	CB	0.55	38.83	89.86	15.00
37	GLN	CG	1.61	37.74	90.00	15.00
37	GLN	CD	1.14	36.57	90.83	15.00
37	GLN	OE1	0.97	36.67	92.05	15.00
37	GLN	NE2	0.93	35.43	90.17	15.00
38	LEU	N	-2.17	40.32	89.23	15.00
38	LEU	CA	-3.14	41.34	89.61	15.00
38	LEU	C	-4.49	40.73	90.02	15.00
38	LEU	O	-5.12	41.20	90.95	15.00
38	LEU	CB	-3.34	42.35	88.48	15.00
38	LEU	CG	-4.22	43.54	88.86	15.00
38	LEU	CD1	-3.64	44.20	90.08	15.00
38	LEU	CD2	-4.33	44.53	87.71	15.00
39	LYS	N	-4.92	39.70	89.30	15.00
39	LYS	CA	-6.18	39.02	89.60	15.00
39	LYS	C	-6.00	38.22	90.90	15.00
39	LYS	O	-6.92	38.19	91.73	15.00
39	LYS	CB	-6.58	38.09	88.45	15.00

TABLE I

39	LYS	CG	-7.57	36.99	88.79	15.00
39	LYS	CD	-8.95	37.51	89.13	15.00
39	LYS	CE	-9.89	36.35	89.41	15.00
39	LYS	NZ	-11.25	36.77	89.82	15.00
40	LYS	N	-4.83	37.60	91.07	15.00
40	LYS	CA	-4.57	36.82	92.28	15.00
40	LYS	C	-4.64	37.74	93.49	15.00
40	LYS	O	-5.25	37.40	94.51	15.00
40	LYS	CB	-3.20	36.16	92.21	15.00
40	LYS	CG	-3.09	34.85	92.98	15.00
40	LYS	CD	-1.63	34.41	93.04	15.00
40	LYS	CE	-1.44	33.15	93.86	15.00
40	LYS	NZ	0.00	32.80	94.08	15.00
41	LYS	N	-4.06	38.93	93.36	15.00
41	LYS	CA	-4.06	39.93	94.43	15.00
41	LYS	C	-5.40	40.66	94.59	15.00
41	LYS	O	-6.17	40.38	95.49	15.00
41	LYS	CB	-2.93	40.95	94.23	15.00
41	LYS	CG	-1.55	40.33	94.11	15.00
41	LYS	CD	-1.34	39.26	95.18	15.00
41	LYS	CE	-0.06	38.46	94.95	15.00
41	LYS	NZ	-0.04	37.19	95.74	15.00
42	THR	N	-5.69	41.58	93.67	15.00
42	THR	CA	-6.91	42.36	93.75	15.00
42	THR	C	-8.23	41.65	93.40	15.00
42	THR	O	-9.28	42.28	93.37	15.00
42	THR	CB	-6.77	43.64	92.91	15.00
42	THR	OG1	-6.89	43.34	91.51	15.00
42	THR	CG2	-5.40	44.26	93.16	15.00
43	GLY	N	-8.17	40.35	93.10	15.00
43	GLY	CA	-9.38	39.62	92.78	15.00
43	GLY	C	-10.09	39.89	91.44	15.00
43	GLY	O	-10.94	39.09	91.03	15.00
44	LYS	N	-9.82	41.02	90.79	15.00
44	LYS	CA	-10.45	41.31	89.50	15.00
44	LYS	C	-9.41	41.72	88.45	15.00
44	LYS	O	-8.48	42.49	88.73	15.00
44	LYS	CB	-11.57	42.34	89.64	15.00
44	LYS	CG	-11.20	43.55	90.45	15.00
44	LYS	CD	-12.43	44.28	90.95	15.00
44	LYS	CE	-12.02	45.39	91.93	15.00
44	LYS	NZ	-11.26	44.88	93.11	15.00

TABLE I

45	LEU	N	-9.60	41.19	87.25	15.00
45	LEU	CA	-8.69	41.41	86.13	15.00
45	LEU	C	-8.92	42.66	85.26	15.00
45	LEU	O	-10.04	43.15	85.12	15.00
45	LEU	CB	-8.71	40.16	85.25	15.00
45	LEU	CG	-7.54	39.90	84.33	15.00
45	LEU	CD1	-6.25	39.87	85.12	15.00
45	LEU	CD2	-7.75	38.59	83.63	15.00
46	LEU	N	-7.83	43.15	84.69	15.00
46	LEU	CA	-7.84	44.31	83.80	15.00
46	LEU	C	-6.81	44.09	82.69	15.00
46	LEU	O	-5.76	43.51	82.93	15.00
46	LEU	CB	-7.44	45.58	84.55	15.00
46	LEU	CG	-8.49	46.47	85.20	15.00
46	LEU	CD1	-7.96	47.90	85.21	15.00
46	LEU	CD2	-9.77	46.43	84.42	15.00
47	ASN	N	-7.11	44.56	81.49	15.00
47	ASN	CA	-6.17	44.43	80.38	15.00
47	ASN	C	-5.12	45.50	80.56	15.00
47	ASN	O	-5.45	46.67	80.62	15.00
47	ASN	CB	-6.88	44.66	79.03	15.00
47	ASN	CG	-7.67	43.45	78.57	15.00
47	ASN	OD1	-7.13	42.37	78.38	15.00
47	ASN	ND2	-8.97	43.65	78.34	15.00
48	LEU	N	-3.86	45.10	80.70	15.00
48	LEU	CA	-2.77	46.07	80.88	15.00
48	LEU	C	-2.15	46.34	79.52	15.00
48	LEU	O	-2.28	45.53	78.61	15.00
48	LEU	CB	-1.74	45.56	81.90	15.00
48	LEU	CG	-2.26	45.06	83.27	15.00
48	LEU	CD1	-1.09	44.75	84.18	15.00
48	LEU	CD2	-3.18	46.08	83.91	15.00
49	SER	N	-1.46	47.47	79.36	15.00
49	SER	CA	-0.91	47.82	78.06	15.00
49	SER	C	0.51	47.42	77.67	15.00
49	SER	O	1.48	47.79	78.33	15.00
49	SER	CB	-1.10	49.32	77.77	15.00
49	SER	OG	-0.19	50.13	78.51	15.00
50	PRO	N	0.64	46.66	76.56	15.00
50	PRO	CA	1.94	46.22	76.04	15.00
50	PRO	C	2.59	47.44	75.41	15.00
50	PRO	O	3.80	47.52	75.25	15.00

TABLE I

50	PRO	CB	1.54	45.21	74.97	15.00
50	PRO	CG	0.21	44.71	75.44	15.00
50	PRO	CD	-0.45	45.98	75.85	15.00
51	GLN	N	1.74	48.40	75.03	15.00
51	GLN	CA	2.18	49.65	74.43	15.00
51	GLN	C	3.01	50.45	75.42	15.00
51	GLN	O	4.12	50.87	75.11	15.00
51	GLN	CB	0.97	50.49	74.00	15.00
51	GLN	CG	1.33	51.66	73.08	15.00
51	GLN	CD	1.77	51.20	71.71	15.00
51	GLN	OE1	0.96	50.74	70.92	15.00
51	GLN	NE2	3.06	51.26	71.44	15.00
52	ASN	N	2.47	50.66	76.62	15.00
52	ASN	CA	3.18	51.42	77.65	15.00
52	ASN	C	4.59	50.85	77.83	15.00
52	ASN	O	5.56	51.59	77.97	15.00
52	ASN	CB	2.42	51.35	78.97	15.00
52	ASN	CG	3.09	52.12	80.09	15.00
52	ASN	OD1	2.74	51.95	81.25	15.00
52	ASN	ND2	4.04	52.99	79.74	15.00
53	LEU	N	4.68	49.53	77.81	15.00
53	LEU	CA	5.95	48.86	77.94	15.00
53	LEU	C	6.82	49.21	76.72	15.00
53	LEU	O	7.87	49.84	76.88	15.00
53	LEU	CB	5.75	47.35	78.08	15.00
53	LEU	CG	5.11	46.95	79.41	15.00
53	LEU	CD1	4.91	45.45	79.49	15.00
53	LEU	CD2	6.00	47.41	80.54	15.00
54	VAL	N	6.33	48.87	75.52	15.00
54	VAL	CA	7.03	49.15	74.25	15.00
54	VAL	C	7.63	50.55	74.20	15.00
54	VAL	O	8.85	50.72	74.04	15.00
54	VAL	CB	6.06	49.01	73.03	15.00
54	VAL	CG1	6.70	49.55	71.75	15.00
54	VAL	CG2	5.67	47.56	72.83	15.00
55	ASP	N	6.76	51.55	74.37	15.00
55	ASP	CA	7.12	52.96	74.31	15.00
55	ASP	C	8.05	53.45	75.40	15.00
55	ASP	O	8.84	54.37	75.19	15.00
55	ASP	CB	5.85	53.84	74.36	15.00
55	ASP	CG	4.87	53.56	73.22	15.00
55	ASP	OD1	5.23	52.86	72.24	15.00

TABLE I

55	ASP	OD2	3.72	54.05	73.29	15.00
56	CYS	N	7.97	52.82	76.56	15.00
56	CYS	CA	8.76	53.27	77.70	15.00
56	CYS	C	9.97	52.47	78.16	15.00
56	CYS	O	10.98	53.06	78.54	15.00
56	CYS	CB	7.81	53.52	78.84	15.00
56	CYS	SG	6.36	54.45	78.28	15.00
57	VAL	N	9.87	51.15	78.17	15.00
57	VAL	CA	10.98	50.31	78.60	15.00
57	VAL	C	12.16	50.44	77.62	15.00
57	VAL	O	12.50	49.50	76.90	15.00
57	VAL	CB	10.54	48.83	78.71	15.00
57	VAL	CG1	11.66	47.98	79.32	15.00
57	VAL	CG2	9.26	48.72	79.52	15.00
58	SER	N	12.85	51.57	77.67	15.00
58	SER	CA	13.98	51.87	76.80	15.00
58	SER	C	15.15	50.91	76.84	15.00
58	SER	O	16.13	51.10	76.13	15.00
58	SER	CB	14.48	53.27	77.09	15.00
58	SER	OG	14.95	53.34	78.42	15.00
59	GLU	N	15.09	49.92	77.71	15.00
59	GLU	CA	16.15	48.93	77.82	15.00
59	GLU	C	15.93	47.86	76.73	15.00
59	GLU	O	16.77	46.99	76.50	15.00
59	GLU	CB	16.14	48.30	79.22	15.00
59	GLU	CG	16.39	49.27	80.39	15.00
59	GLU	CD	15.13	49.97	80.88	15.00
59	GLU	OE1	14.38	49.38	81.70	15.00
59	GLU	OE2	14.90	51.13	80.46	15.00
60	ASN	N	14.77	47.91	76.10	15.00
60	ASN	CA	14.43	46.98	75.04	15.00
60	ASN	C	14.26	47.73	73.71	15.00
60	ASN	O	13.99	48.94	73.69	15.00
60	ASN	CB	13.13	46.26	75.38	15.00
60	ASN	CG	13.27	45.35	76.57	15.00
60	ASN	OD1	12.35	45.22	77.38	15.00
60	ASN	ND2	14.41	44.68	76.68	15.00
61	ASP	N	14.39	47.02	72.61	15.00
61	ASP	CA	14.25	47.65	71.31	15.00
61	ASP	C	12.82	48.03	70.94	15.00
61	ASP	O	12.60	48.65	69.91	15.00
61	ASP	CB	14.84	46.75	70.23	15.00

TABLE I

61	ASP	CG	15.93	47.43	69.44	15.00
61	ASP	OD1	15.87	48.66	69.28	15.00
61	ASP	OD2	16.85	46.72	68.98	15.00
62	GLY	N	11.84	47.67	71.77	15.00
62	GLY	CA	10.46	47.99	71.45	15.00
62	GLY	C	9.91	47.03	70.41	15.00
62	GLY	O	9.71	45.85	70.70	15.00
63	CYS	N	9.68	47.50	69.20	15.00
63	CYS	CA	9.19	46.60	68.16	15.00
63	CYS	C	10.33	45.71	67.70	15.00
63	CYS	O	10.09	44.70	67.04	15.00
63	CYS	CB	8.59	47.36	66.99	15.00
63	CYS	SG	6.94	48.02	67.38	15.00
64	GLY	N	11.56	46.10	68.03	15.00
64	GLY	CA	12.72	45.32	67.68	15.00
64	GLY	C	12.90	44.16	68.64	15.00
64	GLY	O	13.65	43.21	68.37	15.00
65	GLY	N	12.20	44.23	69.78	15.00
65	GLY	CA	12.28	43.17	70.77	15.00
65	GLY	C	12.86	43.58	72.11	15.00
65	GLY	O	13.34	44.70	72.31	15.00
66	GLY	N	12.81	42.65	73.05	15.00
66	GLY	CA	13.34	42.92	74.37	15.00
66	GLY	C	13.08	41.77	75.32	15.00
66	GLY	O	12.42	40.80	74.94	15.00
67	TYR	N	13.57	41.90	76.55	15.00
67	TYR	CA	13.40	40.87	77.56	15.00
67	TYR	C	12.23	41.18	78.48	15.00
67	TYR	O	11.93	42.34	78.75	15.00
67	TYR	CB	14.68	40.76	78.39	15.00
67	TYR	CG	15.91	40.56	77.55	15.00
67	TYR	CD1	16.20	39.32	76.98	15.00
67	TYR	CD2	16.77	41.61	77.29	15.00
67	TYR	CE1	17.33	39.13	76.18	15.00
67	TYR	CE2	17.90	41.44	76.49	15.00
67	TYR	CZ	18.18	40.20	75.94	15.00
67	TYR	OH	19.27	40.05	75.12	15.00
68	MET	N	11.57	40.13	78.99	15.00
68	MET	CA	10.45	40.33	79.90	15.00
68	MET	C	10.90	40.92	81.23	15.00
68	MET	O	10.21	41.72	81.83	15.00
68	MET	CB	9.72	39.00	80.18	15.00

TABLE I

68	MET	CG	8.97	38.38	79.00	15.00
68	MET	SD	9.97	37.36	77.92	15.00
68	MET	CE	11.01	36.45	79.11	15.00
69	THR	N	12.09	40.53	81.68	15.00
69	THR	CA	12.62	41.03	82.94	15.00
69	THR	C	12.76	42.55	82.93	15.00
69	THR	O	12.33	43.21	83.87	15.00
69	THR	CB	13.98	40.37	83.29	15.00
69	THR	OG1	14.96	40.72	82.30	15.00
69	THR	CG2	13.84	38.85	83.35	15.00
70	ASN	N	13.33	43.09	81.85	15.00
70	ASN	CA	13.53	44.54	81.73	15.00
70	ASN	C	12.24	45.34	81.80	15.00
70	ASN	O	12.25	46.51	82.16	15.00
70	ASN	CB	14.28	44.87	80.45	15.00
70	ASN	CG	15.72	44.45	80.52	15.00
70	ASN	OD1	16.11	43.68	81.39	15.00
70	ASN	ND2	16.54	44.97	79.61	15.00
71	ALA	N	11.14	44.68	81.45	15.00
71	ALA	CA	9.81	45.28	81.50	15.00
71	ALA	C	9.27	45.18	82.93	15.00
71	ALA	O	8.72	46.14	83.46	15.00
71	ALA	CB	8.88	44.57	80.51	15.00
72	PHE	N	9.46	44.02	83.55	15.00
72	PHE	CA	9.02	43.79	84.93	15.00
72	PHE	C	9.63	44.86	85.81	15.00
72	PHE	O	8.94	45.51	86.59	15.00
72	PHE	CB	9.49	42.43	85.44	15.00
72	PHE	CG	8.73	41.28	84.88	15.00
72	PHE	CD1	7.40	41.42	84.52	15.00
72	PHE	CD2	9.34	40.04	84.73	15.00
72	PHE	CE1	6.67	40.35	84.03	15.00
72	PHE	CE2	8.62	38.96	84.24	15.00
72	PHE	CZ	7.29	39.12	83.89	15.00
73	GLN	N	10.93	45.05	85.64	15.00
73	GLN	CA	11.67	46.04	86.41	15.00
73	GLN	C	11.17	47.48	86.11	15.00
73	GLN	O	11.29	48.37	86.94	15.00
73	GLN	CB	13.16	45.86	86.13	15.00
73	GLN	CG	14.11	46.75	86.94	15.00
73	GLN	CD	14.52	46.20	88.32	15.00
73	GLN	OE1	15.45	46.73	88.93	15.00

TABLE I

73	GLN	NE2	13.85	45.16	88.80	15.00
74	TYR	N	10.54	47.68	84.96	15.00
74	TYR	CA	10.04	49.00	84.58	15.00
74	TYR	C	8.81	49.41	85.38	15.00
74	TYR	O	8.69	50.56	85.81	15.00
74	TYR	CB	9.72	49.05	83.08	15.00
74	TYR	CG	8.90	50.26	82.67	15.00
74	TYR	CD1	9.48	51.52	82.60	15.00
74	TYR	CD2	7.54	50.14	82.44	15.00
74	TYR	CE1	8.71	52.63	82.31	15.00
74	TYR	CE2	6.77	51.25	82.15	15.00
74	TYR	CZ	7.36	52.49	82.09	15.00
74	TYR	OH	6.58	53.59	81.84	15.00
75	VAL	N	7.87	48.48	85.54	15.00
75	VAL	CA	6.65	48.74	86.31	15.00
75	VAL	C	7.07	49.05	87.76	15.00
75	VAL	O	6.41	49.80	88.47	15.00
75	VAL	CB	5.73	47.48	86.38	15.00
75	VAL	CG1	4.32	47.87	86.73	15.00
75	VAL	CG2	5.77	46.72	85.07	15.00
76	GLN	N	8.18	48.44	88.18	15.00
76	GLN	CA	8.71	48.62	89.52	15.00
76	GLN	C	9.26	50.02	89.71	15.00
76	GLN	O	8.62	50.86	90.31	15.00
76	GLN	CB	9.78	47.57	89.79	15.00
76	GLN	CG	10.35	47.60	91.20	15.00
76	GLN	CD	11.53	46.64	91.36	15.00
76	GLN	OE1	12.17	46.25	90.38	15.00
76	GLN	NE2	11.80	46.25	92.59	15.00
77	LYS	N	10.43	50.30	89.15	15.00
77	LYS	CA	11.04	51.62	89.32	15.00
77	LYS	C	10.24	52.83	88.85	15.00
77	LYS	O	10.34	53.90	89.44	15.00
77	LYS	CB	12.44	51.64	88.71	15.00
77	LYS	CG	12.52	51.06	87.30	15.00
77	LYS	CD	13.96	50.69	86.97	15.00
77	LYS	CE	14.06	49.75	85.79	15.00
77	LYS	NZ	15.39	49.07	85.82	15.00
78	ASN	N	9.48	52.69	87.77	15.00
78	ASN	CA	8.67	53.81	87.31	15.00
78	ASN	C	7.51	53.96	88.28	15.00
78	ASN	O	6.94	55.03	88.41	15.00

TABLE I

78	ASN	CB	8.12	53.56	85.90	15.00
78	ASN	CG	7.17	54.66	85.44	15.00
78	ASN	OD1	7.61	55.76	85.09	15.00
78	ASN	ND2	5.88	54.37	85.44	15.00
79	ARG	N	7.19	52.86	88.95	15.00
79	ARG	CA	6.11	52.78	89.94	15.00
79	ARG	C	4.71	52.88	89.33	15.00
79	ARG	O	4.05	53.92	89.37	15.00
79	ARG	CB	6.31	53.81	91.08	15.00
79	ARG	CG	7.67	53.69	91.80	15.00
79	ARG	CD	7.80	54.56	93.06	15.00
79	ARG	NE	6.84	54.23	94.12	15.00
79	ARG	CZ	6.60	53.00	94.59	15.00
79	ARG	NH1	7.24	51.94	94.09	15.00
79	ARG	NH2	5.73	52.83	95.58	15.00
80	GLY	N	4.27	51.76	88.76	15.00
80	GLY	CA	2.95	51.68	88.15	15.00
80	GLY	C	2.98	51.54	86.64	15.00
80	GLY	O	3.87	52.07	85.97	15.00
81	ILE	N	1.98	50.85	86.10	15.00
81	ILE	CA	1.88	50.64	84.66	15.00
81	ILE	C	0.45	50.97	84.23	15.00
81	ILE	O	-0.49	50.68	84.96	15.00
81	ILE	CB	2.19	49.17	84.30	15.00
81	ILE	CG1	2.27	48.99	82.78	15.00
81	ILE	CG2	1.14	48.24	84.90	15.00
81	ILE	CD1	2.64	47.59	82.36	15.00
82	ASP	N	0.29	51.58	83.05	15.00
82	ASP	CA	-1.04	51.93	82.56	15.00
82	ASP	C	-1.89	50.76	82.07	15.00
82	ASP	O	-1.38	49.69	81.71	15.00
82	ASP	CB	-0.93	52.93	81.42	15.00
82	ASP	CG	-0.47	54.29	81.87	15.00
82	ASP	OD1	-0.66	54.63	83.06	15.00
82	ASP	OD2	0.08	55.02	81.02	15.00
83	SER	N	-3.20	50.96	82.05	15.00
83	SER	CA	-4.12	49.95	81.56	15.00
83	SER	C	-4.32	50.20	80.07	15.00
83	SER	O	-4.22	51.34	79.61	15.00
83	SER	CB	-5.46	50.02	82.32	15.00
83	SER	OG	-6.06	51.30	82.22	15.00
84	GLU	N	-4.61	49.14	79.32	15.00

TABLE I

84	GLU	CA	-4.81	49.22	77.86	15.00
84	GLU	C	-5.66	50.40	77.38	15.00
84	GLU	O	-5.20	51.19	76.57	15.00
84	GLU	CB	-5.39	47.91	77.33	15.00
84	GLU	CG	-5.73	47.89	75.85	15.00
84	GLU	CD	-4.51	47.97	74.94	15.00
84	GLU	OE1	-3.51	47.25	75.17	15.00
84	GLU	OE2	-4.57	48.74	73.96	15.00
85	ASP	N	-6.87	50.53	77.90	15.00
85	ASP	CA	-7.72	51.61	77.45	15.00
85	ASP	C	-7.12	52.99	77.70	15.00
85	ASP	O	-7.49	53.97	77.03	15.00
85	ASP	CB	-9.10	51.52	78.07	15.00
85	ASP	CG	-10.07	52.52	77.46	15.00
85	ASP	OD1	-9.97	52.79	76.24	15.00
85	ASP	OD2	-10.93	53.06	78.21	15.00
86	ALA	N	-6.18	53.08	78.64	15.00
86	ALA	CA	-5.54	54.36	78.93	15.00
86	ALA	C	-4.30	54.57	78.04	15.00
86	ALA	O	-3.90	55.70	77.78	15.00
86	ALA	CB	-5.16	54.45	80.40	15.00
87	TYR	N	-3.74	53.48	77.53	15.00
87	TYR	CA	-2.56	53.54	76.67	15.00
87	TYR	C	-2.69	52.41	75.64	15.00
87	TYR	O	-1.98	51.39	75.73	15.00
87	TYR	CB	-1.32	53.33	77.55	15.00
87	TYR	CG	-0.03	53.89	77.01	15.00
87	TYR	CD1	0.20	53.99	75.64	15.00
87	TYR	CD2	0.99	54.29	77.89	15.00
87	TYR	CE1	1.41	54.47	75.16	15.00
87	TYR	CE2	2.20	54.77	77.41	15.00
87	TYR	CZ	2.41	54.86	76.05	15.00
87	TYR	OH	3.61	55.32	75.57	15.00
88	PRO	N	-3.60	52.58	74.65	15.00
88	PRO	CA	-3.93	51.66	73.55	15.00
88	PRO	C	-2.80	51.22	72.61	15.00
88	PRO	O	-2.08	52.05	72.06	15.00
88	PRO	CB	-5.01	52.43	72.79	15.00
88	PRO	CG	-5.64	53.28	73.84	15.00
88	PRO	CD	-4.42	53.80	74.54	15.00
89	TYR	N	-2.74	49.92	72.34	15.00
89	TYR	CA	-1.71	49.35	71.48	15.00

TABLE I

89	TYR	C	-1.83	49.79	70.01	15.00
89	TYR	O	-2.46	49.11	69.21	15.00
89	TYR	CB	-1.74	47.82	71.56	15.00
89	TYR	CG	-0.54	47.18	70.92	15.00
89	TYR	CD1	0.75	47.59	71.30	15.00
89	TYR	CD2	-0.66	46.24	69.91	15.00
89	TYR	CE1	1.88	47.07	70.69	15.00
89	TYR	CE2	0.47	45.70	69.28	15.00
89	TYR	CZ	1.74	46.13	69.68	15.00
89	TYR	OH	2.87	45.65	69.09	15.00
90	VAL	N	-1.19	50.88	69.65	15.00
90	VAL	CA	-1.22	51.40	68.29	15.00
90	VAL	C	-0.55	50.51	67.23	15.00
90	VAL	O	-0.83	50.63	66.03	15.00
90	VAL	CB	-0.63	52.83	68.21	15.00
90	VAL	CG1	-1.26	53.71	69.28	15.00
90	VAL	CG2	0.88	52.80	68.33	15.00
91	GLY	N	0.37	49.65	67.64	15.00
91	GLY	CA	1.01	48.77	66.67	15.00
91	GLY	C	2.38	49.17	66.15	15.00
91	GLY	O	2.89	48.57	65.20	15.00
92	GLN	N	3.00	50.17	66.77	15.00
92	GLN	CA	4.32	50.61	66.35	15.00
92	GLN	C	4.96	51.34	67.52	15.00
92	GLN	O	4.33	51.51	68.57	15.00
92	GLN	CB	4.21	51.53	65.13	15.00
92	GLN	CG	3.46	52.85	65.38	15.00
92	GLN	CD	3.28	53.70	64.12	15.00
92	GLN	OE1	3.93	54.73	63.94	15.00
92	GLN	NE2	2.39	53.25	63.25	15.00
93	GLU	N	6.19	51.79	67.34	15.00
93	GLU	CA	6.90	52.49	68.39	15.00
93	GLU	C	6.60	53.99	68.38	15.00
93	GLU	O	6.84	54.67	67.38	15.00
93	GLU	CB	8.41	52.27	68.23	15.00
93	GLU	CG	8.80	50.81	68.17	15.00
93	GLU	CD	10.30	50.60	68.23	15.00
93	GLU	OE1	10.85	50.53	69.35	15.00
93	GLU	OE2	10.93	50.50	67.15	15.00
94	GLU	N	6.08	54.49	69.49	15.00
94	GLU	CA	5.76	55.90	69.63	15.00
94	GLU	C	6.54	56.47	70.80	15.00

TABLE I

94	GLU	O	7.40	55.80	71.37	15.00
94	GLU	CB	4.27	56.10	69.86	15.00
94	GLU	CG	3.45	56.13	68.58	15.00
94	GLU	CD	1.96	56.28	68.85	15.00
94	GLU	OE1	1.48	55.64	69.81	15.00
94	GLU	OE2	1.27	57.03	68.11	15.00
95	SER	N	6.22	57.71	71.14	15.00
95	SER	CA	6.84	58.41	72.26	15.00
95	SER	C	6.16	57.91	73.52	15.00
95	SER	O	4.92	57.82	73.58	15.00
95	SER	CB	6.63	59.93	72.12	15.00
95	SER	OG	5.25	60.23	71.89	15.00
96	CYS	N	6.96	57.55	74.51	15.00
96	CYS	CA	6.44	57.04	75.77	15.00
96	CYS	C	5.44	58.02	76.39	15.00
96	CYS	O	5.84	59.03	76.95	15.00
96	CYS	CB	7.59	56.77	76.74	15.00
96	CYS	SG	7.00	56.38	78.40	15.00
97	MET	N	4.15	57.73	76.21	15.00
97	MET	CA	3.06	58.55	76.74	15.00
97	MET	C	2.40	58.00	78.01	15.00
97	MET	O	1.16	57.90	78.06	15.00
97	MET	CB	1.97	58.73	75.69	15.00
97	MET	CG	2.36	59.52	74.45	15.00
97	MET	SD	1.29	58.98	73.09	15.00
97	MET	CE	-0.36	59.43	73.71	15.00
98	TYR	N	3.20	57.65	79.01	15.00
98	TYR	CA	2.67	57.13	80.26	15.00
98	TYR	C	1.93	58.21	81.06	15.00
98	TYR	O	2.48	59.26	81.38	15.00
98	TYR	CB	3.78	56.51	81.11	15.00
98	TYR	CG	3.32	56.04	82.48	15.00
98	TYR	CD1	3.24	56.92	83.56	15.00
98	TYR	CD2	2.95	54.72	82.69	15.00
98	TYR	CE1	2.81	56.49	84.80	15.00
98	TYR	CE2	2.52	54.29	83.95	15.00
98	TYR	CZ	2.45	55.18	84.99	15.00
98	TYR	OH	2.02	54.77	86.22	15.00
99	ASN	N	0.69	57.92	81.43	15.00
99	ASN	CA	-0.14	58.84	82.20	15.00
99	ASN	C	-0.54	58.20	83.54	15.00
99	ASN	O	-1.31	57.23	83.58	15.00

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TABLE I

99	ASN	CB	-1.37	59.22	81.36	15.00
99	ASN	CG	-2.38	60.08	82.13	15.00
99	ASN	OD1	-2.01	60.89	82.99	15.00
99	ASN	ND2	-3.66	59.90	81.80	15.00
100	PRO	N	-0.02	58.74	84.65	15.00
100	PRO	CA	-0.30	58.24	86.00	15.00
100	PRO	C	-1.77	58.23	86.33	15.00
100	PRO	O	-2.22	57.46	87.19	15.00
100	PRO	CB	0.45	59.22	86.90	15.00
100	PRO	CG	1.58	59.70	86.02	15.00
100	PRO	CD	0.86	59.92	84.71	15.00
101	THR	N	-2.53	59.08	85.65	15.00
101	THR	CA	-3.96	59.13	85.89	15.00
101	THR	C	-4.56	57.81	85.43	15.00
101	THR	O	-5.64	57.43	85.89	15.00
101	THR	CB	-4.63	60.25	85.10	15.00
101	THR	OG1	-3.86	61.45	85.21	15.00
101	THR	CG2	-6.03	60.52	85.66	15.00
102	GLY	N	-3.86	57.13	84.52	15.00
102	GLY	CA	-4.33	55.86	84.01	15.00
102	GLY	C	-3.55	54.62	84.42	15.00
102	GLY	O	-3.52	53.65	83.67	15.00
103	LYS	N	-2.90	54.62	85.59	15.00
103	LYS	CA	-2.15	53.44	86.02	15.00
103	LYS	C	-3.12	52.35	86.50	15.00
103	LYS	O	-4.26	52.65	86.86	15.00
103	LYS	CB	-1.13	53.83	87.11	15.00
103	LYS	CG	-1.51	53.50	88.56	15.00
103	LYS	CD	-0.97	52.13	88.98	15.00
103	LYS	CE	-1.39	51.77	90.40	15.00
103	LYS	NZ	-1.11	50.35	90.75	15.00
104	ALA	N	-2.68	51.10	86.52	15.00
104	ALA	CA	-3.55	50.01	86.96	15.00
104	ALA	C	-2.86	48.86	87.68	15.00
104	ALA	O	-3.52	47.92	88.12	15.00
104	ALA	CB	-4.37	49.49	85.79	15.00
105	ALA	N	-1.55	48.92	87.82	15.00
105	ALA	CA	-0.83	47.87	88.50	15.00
105	ALA	C	0.53	48.36	88.97	15.00
105	ALA	O	1.06	49.35	88.44	15.00
105	ALA	CB	-0.67	46.68	87.59	15.00
106	LYS	N	1.07	47.69	90.00	15.00

TABLE I

106	LYS	CA	2.39	48.03	90.56	15.00
106	LYS	C	3.24	46.76	90.62	15.00
106	LYS	O	2.73	45.65	90.44	15.00
106	LYS	CB	2.24	48.66	91.95	15.00
106	LYS	CG	1.78	50.12	91.94	15.00
106	LYS	CD	1.32	50.56	93.31	15.00
106	LYS	CE	2.44	50.52	94.34	15.00
106	LYS	NZ	3.48	51.56	94.06	15.00
107	CYS	N	4.54	46.92	90.90	15.00
107	CYS	CA	5.42	45.76	90.90	15.00
107	CYS	C	6.51	45.83	91.97	15.00
107	CYS	O	7.16	46.86	92.14	15.00
107	CYS	CB	6.07	45.65	89.52	15.00
107	CYS	SG	6.62	44.03	89.03	15.00
108	ARG	N	6.70	44.73	92.69	15.00
108	ARG	CA	7.71	44.62	93.74	15.00
108	ARG	C	8.93	43.86	93.19	15.00
108	ARG	O	9.61	43.14	93.93	15.00
108	ARG	CB	7.16	43.87	94.96	15.00
108	ARG	CG	6.08	44.58	95.79	15.00
108	ARG	CD	5.41	43.58	96.74	15.00
108	ARG	NE	6.38	42.60	97.25	15.00
108	ARG	CZ	6.16	41.29	97.39	15.00
108	ARG	NH1	4.99	40.74	97.08	15.00
108	ARG	NH2	7.16	40.52	97.80	15.00
109	GLY	N	9.21	44.02	91.90	15.00
109	GLY	CA	10.34	43.34	91.30	15.00
109	GLY	C	9.92	42.13	90.50	15.00
109	GLY	O	8.77	42.01	90.10	15.00
110	TYR	N	10.86	41.22	90.29	15.00
110	TYR	CA	10.59	39.99	89.54	15.00
110	TYR	C	11.44	38.82	90.02	15.00
110	TYR	O	12.41	38.99	90.75	15.00
110	TYR	CB	10.85	40.21	88.05	15.00
110	TYR	CG	12.30	40.42	87.70	15.00
110	TYR	CD1	13.13	39.33	87.46	15.00
110	TYR	CD2	12.82	41.70	87.58	15.00
110	TYR	CE1	14.46	39.52	87.10	15.00
110	TYR	CE2	14.14	41.89	87.22	15.00
110	TYR	CZ	14.95	40.80	86.98	15.00
110	TYR	OH	16.25	40.99	86.61	15.00
111	ARG	N	11.13	37.63	89.52	15.00

TABLE I

111	ARG	CA	11.87	36.45	89.91	15.00
111	ARG	C	11.88	35.46	88.75	15.00
111	ARG	O	10.90	35.34	88.03	15.00
111	ARG	CB	11.23	35.85	91.16	15.00
111	ARG	CG	12.14	34.90	91.88	15.00
111	ARG	CD	11.70	34.66	93.31	15.00
111	ARG	NE	12.85	34.20	94.09	15.00
111	ARG	CZ	13.87	34.98	94.44	15.00
111	ARG	NH1	13.87	36.28	94.12	15.00
111	ARG	NH2	14.89	34.48	95.13	15.00
112	GLU	N	13.00	34.76	88.58	15.00
112	GLU	CA	13.15	33.79	87.50	15.00
112	GLU	C	13.25	32.35	87.94	15.00
112	GLU	O	13.55	32.06	89.11	15.00
112	GLU	CB	14.38	34.11	86.66	15.00
112	GLU	CG	14.35	35.49	86.11	15.00
112	GLU	CD	15.46	35.72	85.14	15.00
112	GLU	OE1	15.30	35.30	83.97	15.00
112	GLU	OE2	16.49	36.31	85.56	15.00
113	ILE	N	12.98	31.46	86.99	15.00
113	ILE	CA	13.02	30.03	87.20	15.00
113	ILE	C	14.46	29.65	86.91	15.00
113	ILE	O	15.13	30.34	86.15	15.00
113	ILE	CB	12.04	29.30	86.23	15.00
113	ILE	CG1	10.60	29.50	86.70	15.00
113	ILE	CG2	12.36	27.81	86.13	15.00
113	ILE	CD1	10.10	30.93	86.65	15.00
114	PRO	N	15.01	28.64	87.60	15.00
114	PRO	CA	16.40	28.30	87.29	15.00
114	PRO	C	16.50	27.74	85.87	15.00
114	PRO	O	15.74	26.85	85.48	15.00
114	PRO	CB	16.77	27.29	88.39	15.00
114	PRO	CG	15.46	26.66	88.76	15.00
114	PRO	CD	14.52	27.85	88.75	15.00
115	GLU	N	17.41	28.32	85.09	15.00
115	GLU	CA	17.61	27.97	83.68	15.00
115	GLU	C	17.55	26.49	83.35	15.00
115	GLU	O	18.36	25.70	83.84	15.00
115	GLU	CB	18.93	28.56	83.15	15.00
115	GLU	CG	18.92	30.09	82.86	15.00
115	GLU	CD	20.11	30.56	81.97	15.00
115	GLU	OE1	20.75	29.70	81.31	15.00

TABLE I

115	GLU	OE2	20.39	31.79	81.92	15.00
116	GLY	N	16.55	26.11	82.56	15.00
116	GLY	CA	16.41	24.74	82.12	15.00
116	GLY	C	15.76	23.78	83.08	15.00
116	GLY	O	15.81	22.56	82.88	15.00
117	ASN	N	15.13	24.31	84.11	15.00
117	ASN	CA	14.47	23.47	85.10	15.00
117	ASN	C	12.97	23.47	84.87	15.00
117	ASN	O	12.28	24.43	85.22	15.00
117	ASN	CB	14.77	23.97	86.51	15.00
117	ASN	CG	14.21	23.05	87.58	15.00
117	ASN	OD1	13.32	22.23	87.32	15.00
117	ASN	ND2	14.72	23.19	88.80	15.00
118	GLU	N	12.47	22.38	84.29	15.00
118	GLU	CA	11.05	22.27	84.03	15.00
118	GLU	C	10.22	22.01	85.27	15.00
118	GLU	O	9.16	22.60	85.42	15.00
118	GLU	CB	10.75	21.20	82.99	15.00
118	GLU	CG	10.96	21.66	81.56	15.00
118	GLU	CD	10.34	20.72	80.56	15.00
118	GLU	OE1	9.11	20.82	80.33	15.00
118	GLU	OE2	11.08	19.88	80.01	15.00
119	LYS	N	10.73	21.18	86.18	15.00
119	LYS	CA	10.00	20.87	87.41	15.00
119	LYS	C	9.79	22.11	88.28	15.00
119	LYS	O	8.78	22.21	88.98	15.00
119	LYS	CB	10.68	19.76	88.21	15.00
119	LYS	CG	9.94	18.40	88.14	15.00
119	LYS	CD	10.13	17.64	86.81	15.00
119	LYS	CE	9.28	16.35	86.76	15.00
119	LYS	NZ	9.62	15.29	87.79	15.00
120	ALA	N	10.73	23.04	88.21	15.00
120	ALA	CA	10.61	24.30	88.94	15.00
120	ALA	C	9.57	25.15	88.23	15.00
120	ALA	O	8.72	25.75	88.88	15.00
120	ALA	CB	11.93	25.04	88.99	15.00
121	LEU	N	9.62	25.19	86.89	15.00
121	LEU	CA	8.66	25.96	86.09	15.00
121	LEU	C	7.23	25.51	86.39	15.00
121	LEU	O	6.34	26.34	86.52	15.00
121	LEU	CB	8.94	25.82	84.58	15.00
121	LEU	CG	7.91	26.43	83.60	15.00

TABLE I

121 LEU CD1	8.09	27.93	83.52	15.00
121 LEU CD2	8.08	25.84	82.22	15.00
122 LYS N	7.02	24.21	86.51	15.00
122 LYS CA	5.69	23.70	86.81	15.00
122 LYS C	5.24	24.18	88.19	15.00
122 LYS O	4.07	24.52	88.38	15.00
122 LYS CB	5.66	22.17	86.76	15.00
122 LYS CG	4.31	21.58	87.17	15.00
122 LYS CD	4.36	20.07	87.30	15.00
122 LYS CE	5.50	19.63	88.22	15.00
122 LYS NZ	5.63	18.14	88.27	15.00
123 ARG N	6.16	24.19	89.15	15.00
123 ARG CA	5.84	24.63	90.51	15.00
123 ARG C	5.51	26.11	90.47	15.00
123 ARG O	4.53	26.54	91.07	15.00
123 ARG CB	6.99	24.36	91.49	15.00
123 ARG CG	7.32	22.88	91.65	15.00
123 ARG CD	8.14	22.58	92.89	15.00
123 ARG NE	9.59	22.54	92.68	15.00
123 ARG CZ	10.40	23.60	92.76	15.00
123 ARG NH1	9.92	24.80	93.04	15.00
123 ARG NH2	11.71	23.43	92.63	15.00
124 ALA N	6.30	26.87	89.73	15.00
124 ALA CA	6.09	28.30	89.58	15.00
124 ALA C	4.72	28.57	88.98	15.00
124 ALA O	3.98	29.41	89.47	15.00
124 ALA CB	7.19	28.91	88.71	15.00
125 VAL N	4.37	27.84	87.92	15.00
125 VAL CA	3.07	28.02	87.28	15.00
125 VAL C	1.95	27.63	88.24	15.00
125 VAL O	0.88	28.23	88.22	15.00
125 VAL CB	2.96	27.17	85.98	15.00
125 VAL CG1	1.52	27.07	85.51	15.00
125 VAL CG2	3.78	27.79	84.88	15.00
126 ALA N	2.21	26.64	89.08	15.00
126 ALA CA	1.22	26.16	90.04	15.00
126 ALA C	1.10	26.92	91.36	15.00
126 ALA O	0.03	26.95	91.97	15.00
126 ALA CB	1.43	24.68	90.31	15.00
127 ARG N	2.20	27.51	91.82	15.00
127 ARG CA	2.21	28.25	93.07	15.00
127 ARG C	1.97	29.74	92.86	15.00

TABLE I

127 ARG O	1.45	30.43	93.75	15.00
127 ARG CB	3.55	28.07	93.81	15.00
127 ARG CG	3.44	27.25	95.07	15.00
127 ARG CD	3.83	25.82	94.84	15.00
127 ARG NE	5.24	25.57	95.18	15.00
127 ARG CZ	5.76	24.37	95.39	15.00
127 ARG NH1	5.03	23.27	95.29	15.00
127 ARG NH2	7.04	24.27	95.69	15.00
128 VAL N	2.38	30.23	91.69	15.00
128 VAL CA	2.22	31.64	91.36	15.00
128 VAL C	1.08	31.86	90.37	15.00
128 VAL O	0.06	32.47	90.67	15.00
128 VAL CB	3.53	32.20	90.78	15.00
128 VAL CG1	3.48	33.72	90.75	15.00
128 VAL CG2	4.72	31.71	91.58	15.00
129 GLY N	1.27	31.35	89.16	15.00
129 GLY CA	0.26	31.49	88.14	15.00
129 GLY C	0.98	31.73	86.84	15.00
129 GLY O	2.11	31.28	86.67	15.00
130 PRO N	0.36	32.47	85.91	15.00
130 PRO CA	0.96	32.76	84.62	15.00
130 PRO C	2.37	33.32	84.72	15.00
130 PRO O	2.60	34.37	85.32	15.00
130 PRO CB	-0.03	33.76	84.02	15.00
130 PRO CG	-1.33	33.27	84.53	15.00
130 PRO CD	-1.00	33.01	85.99	15.00
131 VAL N	3.32	32.57	84.15	15.00
131 VAL CA	4.72	32.96	84.13	15.00
131 VAL C	5.09	33.29	82.67	15.00
131 VAL O	4.48	32.77	81.73	15.00
131 VAL CB	5.63	31.83	84.73	15.00
131 VAL CG1	5.57	30.58	83.89	15.00
131 VAL CG2	7.07	32.28	84.86	15.00
132 SER N	6.03	34.23	82.49	15.00
132 SER CA	6.49	34.64	81.17	15.00
132 SER C	7.58	33.70	80.71	15.00
132 SER O	8.60	33.56	81.40	15.00
132 SER CB	7.08	36.05	81.25	15.00
132 SER OG	6.16	36.98	81.80	15.00
133 VAL N	7.39	33.03	79.58	15.00
133 VAL CA	8.39	32.10	79.03	15.00
133 VAL C	8.84	32.58	77.67	15.00

TABLE I

133 VAL O	8.20	33.43	77.06	15.00
133 VAL CB	7.86	30.66	78.87	15.00
133 VAL CG1	8.20	29.83	80.07	15.00
133 VAL CG2	6.37	30.65	78.66	15.00
134 ALA N	9.98	32.08	77.21	15.00
134 ALA CA	10.51	32.42	75.89	15.00
134 ALA C	10.71	31.08	75.20	15.00
134 ALA O	10.94	30.09	75.89	15.00
134 ALA CB	11.81	33.16	76.01	15.00
135 ILE N	10.58	31.02	73.88	15.00
135 ILE CA	10.74	29.75	73.17	15.00
135 ILE C	11.25	29.93	71.74	15.00
135 ILE O	11.54	31.04	71.29	15.00
135 ILE CB	9.39	29.00	73.05	15.00
135 ILE CG1	8.32	29.93	72.47	15.00
135 ILE CG2	8.98	28.39	74.37	15.00
135 ILE CD1	7.01	29.26	72.13	15.00
136 ASP N	11.37	28.80	71.04	15.00
136 ASP CA	11.80	28.77	69.65	15.00
136 ASP C	10.54	28.58	68.80	15.00
136 ASP O	10.02	27.47	68.67	15.00
136 ASP CB	12.79	27.62	69.36	15.00
136 ASP CG	13.23	27.57	67.89	15.00
136 ASP OD1	13.18	28.61	67.20	15.00
136 ASP OD2	13.64	26.49	67.41	15.00
137 ALA N	10.05	29.68	68.24	15.00
137 ALA CA	8.87	29.65	67.41	15.00
137 ALA C	9.23	29.70	65.91	15.00
137 ALA O	8.38	30.00	65.07	15.00
137 ALA CB	7.97	30.81	67.79	15.00
138 SER N	10.47	29.35	65.57	15.00
138 SER CA	10.91	29.38	64.18	15.00
138 SER C	10.40	28.27	63.28	15.00
138 SER O	10.47	28.39	62.06	15.00
138 SER CB	12.43	29.40	64.10	15.00
138 SER OG	12.93	30.59	64.68	15.00
139 LEU N	9.85	27.22	63.87	15.00
139 LEU CA	9.36	26.07	63.12	15.00
139 LEU C	8.06	26.32	62.36	15.00
139 LEU O	7.07	26.74	62.94	15.00
139 LEU CB	9.17	24.86	64.04	15.00
139 LEU CG	10.27	24.49	65.02	15.00

TABLE I

139 LEU CD1	11.61	24.35	64.30	15.00
139 LEU CD2	10.33	25.54	66.14	15.00
140 THR N	8.06	26.00	61.06	15.00
140 THR CA	6.87	26.19	60.24	15.00
140 THR C	5.73	25.38	60.86	15.00
140 THR O	4.56	25.75	60.77	15.00
140 THR CB	7.09	25.72	58.78	15.00
140 THR OG1	8.35	26.21	58.30	15.00
140 THR CG2	6.00	26.29	57.88	15.00
141 SER N	6.11	24.29	61.54	15.00
141 SER CA	5.14	23.42	62.20	15.00
141 SER C	4.49	24.13	63.38	15.00
141 SER O	3.32	23.91	63.69	15.00
141 SER CB	5.83	22.12	62.64	15.00
141 SER OG	7.14	22.36	63.15	15.00
142 PHE N	5.25	25.01	64.02	15.00
142 PHE CA	4.74	25.76	65.15	15.00
142 PHE C	3.80	26.83	64.66	15.00
142 PHE O	2.78	27.12	65.30	15.00
142 PHE CB	5.88	26.41	65.94	15.00
142 PHE CG	5.41	27.24	67.09	15.00
142 PHE CD1	5.07	28.58	66.91	15.00
142 PHE CD2	5.31	26.70	68.37	15.00
142 PHE CE1	4.64	29.36	67.97	15.00
142 PHE CE2	4.89	27.47	69.44	15.00
142 PHE CZ	4.55	28.81	69.24	15.00
143 GLN N	4.13	27.43	63.52	15.00
143 GLN CA	3.31	28.49	62.99	15.00
143 GLN C	1.93	28.03	62.57	15.00
143 GLN O	0.95	28.72	62.84	15.00
143 GLN CB	4.05	29.25	61.89	15.00
143 GLN CG	5.12	30.14	62.48	15.00
143 GLN CD	6.22	30.52	61.51	15.00
143 GLN OE1	5.97	31.14	60.47	15.00
143 GLN NE2	7.45	30.19	61.86	15.00
144 PHE N	1.84	26.82	62.00	15.00
144 PHE CA	0.54	26.30	61.57	15.00
144 PHE C	-0.14	25.30	62.52	15.00
144 PHE O	-1.02	24.53	62.12	15.00
144 PHE CB	0.56	25.79	60.11	15.00
144 PHE CG	1.57	24.68	59.84	15.00
144 PHE CD1	1.63	23.54	60.63	15.00

TABLE I

144	PHE	CD2	2.40	24.75	58.73	15.00
144	PHE	CE1	2.50	22.49	60.32	15.00
144	PHE	CE2	3.27	23.71	58.42	15.00
144	PHE	CZ	3.32	22.58	59.22	15.00
145	TYR	N	0.27	25.33	63.79	15.00
145	TYR	CA	-0.30	24.45	64.81	15.00
145	TYR	C	-1.80	24.73	64.93	15.00
145	TYR	O	-2.22	25.89	64.92	15.00
145	TYR	CB	0.36	24.72	66.17	15.00
145	TYR	CG	-0.43	24.13	67.33	15.00
145	TYR	CD1	-0.28	22.79	67.70	15.00
145	TYR	CD2	-1.38	24.90	68.01	15.00
145	TYR	CE1	-1.05	22.23	68.70	15.00
145	TYR	CE2	-2.15	24.35	69.01	15.00
145	TYR	CZ	-1.99	23.01	69.35	15.00
145	TYR	OH	-2.76	22.46	70.34	15.00
146	SER	N	-2.60	23.68	65.08	15.00
146	SER	CA	-4.04	23.84	65.20	15.00
146	SER	C	-4.65	22.98	66.30	15.00
146	SER	O	-5.72	23.29	66.81	15.00
146	SER	CB	-4.74	23.59	63.84	15.00
146	SER	OG	-4.46	22.30	63.31	15.00
147	LYS	N	-3.96	21.91	66.67	15.00
147	LYS	CA	-4.48	21.04	67.73	15.00
147	LYS	C	-3.46	20.00	68.23	15.00
147	LYS	O	-2.52	19.67	67.51	15.00
147	LYS	CB	-5.79	20.37	67.27	15.00
147	LYS	CG	-5.76	19.70	65.88	15.00
147	LYS	CD	-7.11	19.05	65.50	15.00
147	LYS	CE	-7.19	18.65	64.01	15.00
147	LYS	NZ	-7.28	19.82	63.07	15.00
148	GLY	N	-3.63	19.55	69.48	15.00
148	GLY	CA	-2.75	18.55	70.07	15.00
148	GLY	C	-1.56	19.09	70.85	15.00
148	GLY	O	-1.43	20.29	71.06	15.00
149	VAL	N	-0.71	18.18	71.31	15.00
149	VAL	CA	0.50	18.54	72.07	15.00
149	VAL	C	1.66	18.70	71.06	15.00
149	VAL	O	2.06	17.74	70.39	15.00
149	VAL	CB	0.83	17.46	73.14	15.00
149	VAL	CG1	2.06	17.86	73.93	15.00
149	VAL	CG2	-0.34	17.26	74.08	15.00

TABLE I

150 TYR N	2.21	19.90	70.99	15.00
150 TYR CA	3.25	20.21	70.03	15.00
150 TYR C	4.60	19.64	70.34	15.00
150 TYR O	5.26	20.08	71.28	15.00
150 TYR CB	3.39	21.72	69.86	15.00
150 TYR CG	4.42	22.11	68.81	15.00
150 TYR CD1	4.39	21.53	67.54	15.00
150 TYR CD2	5.44	23.02	69.11	15.00
150 TYR CE1	5.36	21.85	66.58	15.00
150 TYR CE2	6.41	23.33	68.15	15.00
150 TYR CZ	6.37	22.74	66.90	15.00
150 TYR OH	7.34	23.02	65.97	15.00
151 TYR N	5.03	18.69	69.53	15.00
151 TYR CA	6.35	18.11	69.70	15.00
151 TYR C	7.09	18.15	68.37	15.00
151 TYR O	6.65	17.56	67.39	15.00
151 TYR CB	6.30	16.68	70.20	15.00
151 TYR CG	7.67	16.22	70.63	15.00
151 TYR CD1	8.45	17.02	71.46	15.00
151 TYR CD2	8.20	15.02	70.17	15.00
151 TYR CE1	9.74	16.65	71.82	15.00
151 TYR CE2	9.50	14.63	70.52	15.00
151 TYR CZ	10.26	15.45	71.35	15.00
151 TYR OH	11.55	15.08	71.70	15.00
152 ASP N	8.21	18.85	68.35	15.00
152 ASP CA	8.98	18.96	67.12	15.00
152 ASP C	10.47	18.82	67.44	15.00
152 ASP O	11.08	19.72	68.03	15.00
152 ASP CB	8.70	20.31	66.45	15.00
152 ASP CG	9.22	20.37	65.03	15.00
152 ASP OD1	8.48	19.96	64.12	15.00
152 ASP OD2	10.37	20.82	64.82	15.00
153 GLU N	11.03	17.68	67.05	15.00
153 GLU CA	12.44	17.38	67.31	15.00
153 GLU C	13.40	18.37	66.69	15.00
153 GLU O	14.59	18.34	66.98	15.00
153 GLU CB	12.76	15.94	66.86	15.00
153 GLU CG	12.29	15.56	65.44	15.00
153 GLU CD	13.28	15.95	64.33	15.00
153 GLU OE1	14.38	15.36	64.28	15.00
153 GLU OE2	12.95	16.84	63.50	15.00
154 SER N	12.89	19.26	65.85	15.00

010786

TABLE I

154 SER CA	13.75	20.24	65.20	15.00
154 SER C	13.86	21.54	66.01	15.00
154 SER O	14.71	22.38	65.71	15.00
154 SER CB	13.20	20.54	63.80	15.00
154 SER OG	14.08	21.32	63.02	15.00
155 CYS N	13.02	21.69	67.03	15.00
155 CYS CA	13.01	22.90	67.86	15.00
155 CYS C	14.34	23.17	68.55	15.00
155 CYS O	14.74	22.42	69.45	15.00
155 CYS CB	11.86	22.85	68.87	15.00
155 CYS SG	11.05	24.47	69.10	15.00
156 ASN N	15.02	24.23	68.14	15.00
156 ASN CA	16.33	24.57	68.70	15.00
156 ASN C	16.29	25.23	70.07	15.00
156 ASN O	16.21	26.46	70.19	15.00
156 ASN CB	17.16	25.40	67.73	15.00
156 ASN CG	18.54	25.71	68.28	15.00
156 ASN OD1	18.89	26.86	68.48	15.00
156 ASN ND2	19.32	24.66	68.57	15.00
157 SER N	16.46	24.39	71.09	15.00
157 SER CA	16.46	24.79	72.50	15.00
157 SER C	17.39	25.95	72.87	15.00
157 SER O	17.24	26.54	73.94	15.00
157 SER CB	16.79	23.56	73.34	15.00
157 SER OG	16.11	22.42	72.84	15.00
158 ASP N	18.34	26.27	71.99	15.00
158 ASP CA	19.29	27.35	72.24	15.00
158 ASP C	18.88	28.70	71.64	15.00
158 ASP O	19.31	29.76	72.09	15.00
158 ASP CB	20.69	26.96	71.75	15.00
158 ASP CG	21.57	26.39	72.87	15.00
158 ASP OD1	21.02	25.82	73.85	15.00
158 ASP OD2	22.82	26.53	72.78	15.00
159 ASN N	18.07	28.66	70.59	15.00
159 ASN CA	17.63	29.89	69.97	15.00
159 ASN C	16.22	30.22	70.46	15.00
159 ASN O	15.25	29.58	70.04	15.00
159 ASN CB	17.69	29.76	68.45	15.00
159 ASN CG	16.80	30.75	67.73	15.00
159 ASN OD1	16.93	31.98	67.88	15.00
159 ASN ND2	15.86	30.22	66.96	15.00
160 LEU N	16.13	31.16	71.39	15.00

TABLE I

160 LEU CA	14.83	31.58	71.93	15.00
160 LEU C	14.48	32.83	71.16	15.00
160 LEU O	15.25	33.79	71.14	15.00
160 LEU CB	14.90	31.88	73.44	15.00
160 LEU CG	15.29	30.75	74.43	15.00
160 LEU CD1	15.63	31.34	75.78	15.00
160 LEU CD2	14.20	29.70	74.54	15.00
161 ASN N	13.32	32.82	70.51	15.00
161 ASN CA	12.91	33.94	69.69	15.00
161 ASN C	11.44	34.33	69.76	15.00
161 ASN O	10.94	34.97	68.85	15.00
161 ASN CB	13.25	33.62	68.24	15.00
161 ASN CG	12.59	32.35	67.78	15.00
161 ASN OD1	11.36	32.28	67.67	15.00
161 ASN ND2	13.38	31.31	67.58	15.00
162 HIS N	10.72	33.90	70.78	15.00
162 HIS CA	9.33	34.31	70.87	15.00
162 HIS C	8.84	34.19	72.29	15.00
162 HIS O	8.74	33.09	72.84	15.00
162 HIS CB	8.45	33.51	69.91	15.00
162 HIS CG	7.10	34.12	69.68	15.00
162 HIS ND1	6.93	35.47	69.42	15.00
162 HIS CD2	5.86	33.58	69.66	15.00
162 HIS CE1	5.64	35.72	69.24	15.00
162 HIS NE2	4.97	34.59	69.38	15.00
163 ALA N	8.58	35.35	72.90	15.00
163 ALA CA	8.09	35.40	74.26	15.00
163 ALA C	6.63	34.98	74.30	15.00
163 ALA O	5.78	35.55	73.61	15.00
163 ALA CB	8.27	36.79	74.81	15.00
164 VAL N	6.36	33.96	75.09	15.00
164 VAL CA	5.02	33.43	75.28	15.00
164 VAL C	4.69	33.44	76.78	15.00
164 VAL O	5.54	33.79	77.60	15.00
164 VAL CB	4.95	32.00	74.70	15.00
164 VAL CG1	5.97	31.10	75.37	15.00
164 VAL CG2	3.57	31.44	74.89	15.00
165 LEU N	3.45	33.09	77.15	15.00
165 LEU CA	3.04	33.03	78.55	15.00
165 LEU C	2.46	31.67	78.88	15.00
165 LEU O	1.65	31.15	78.12	15.00
165 LEU CB	1.96	34.09	78.85	15.00

TABLE I

165	LEU	CG	1.43	34.18	80.29	15.00
165	LEU	CD1	2.39	34.99	81.12	15.00
165	LEU	CD2	0.06	34.82	80.33	15.00
166	ALA	N	2.87	31.11	80.01	15.00
166	ALA	CA	2.35	29.81	80.46	15.00
166	ALA	C	1.08	30.09	81.24	15.00
166	ALA	O	1.06	30.96	82.11	15.00
166	ALA	CB	3.36	29.12	81.34	15.00
167	VAL	N	0.02	29.38	80.89	15.00
167	VAL	CA	-1.29	29.54	81.52	15.00
167	VAL	C	-1.67	28.28	82.34	15.00
167	VAL	O	-2.71	28.21	83.00	15.00
167	VAL	CB	-2.32	29.91	80.40	15.00
167	VAL	CG1	-3.67	29.28	80.59	15.00
167	VAL	CG2	-2.45	31.41	80.33	15.00
168	GLY	N	-0.76	27.32	82.38	15.00
168	GLY	CA	-0.99	26.12	83.13	15.00
168	GLY	C	-0.16	24.99	82.57	15.00
168	GLY	O	0.86	25.22	81.93	15.00
169	TYR	N	-0.61	23.78	82.81	15.00
169	TYR	CA	0.05	22.58	82.33	15.00
169	TYR	C	-1.02	21.51	82.42	15.00
169	TYR	O	-2.11	21.76	82.93	15.00
169	TYR	CB	1.27	22.22	83.20	15.00
169	TYR	CG	1.02	22.11	84.70	15.00
169	TYR	CD1	0.52	20.94	85.28	15.00
169	TYR	CD2	1.32	23.18	85.56	15.00
169	TYR	CE1	0.32	20.84	86.66	15.00
169	TYR	CE2	1.12	23.08	86.94	15.00
169	TYR	CZ	0.62	21.91	87.48	15.00
169	TYR	OH	0.44	21.83	88.85	15.00
170	GLY	N	-0.71	20.33	81.90	15.00
170	GLY	CA	-1.65	19.23	81.94	15.00
170	GLY	C	-1.16	18.11	81.05	15.00
170	GLY	O	-0.03	18.14	80.54	15.00
171	ILE	N	-2.04	17.15	80.81	15.00
171	ILE	CA	-1.78	15.98	79.97	15.00
171	ILE	C	-2.96	15.87	79.00	15.00
171	ILE	O	-3.95	16.60	79.14	15.00
171	ILE	CB	-1.62	14.73	80.86	15.00
171	ILE	CG1	-1.47	13.46	80.02	15.00
171	ILE	CG2	-2.76	14.65	81.87	15.00

TABLE I

171	ILE	CD1	-1.03	12.22	80.81	15.00
172	GLN	N	-2.86	15.03	77.96	15.00
172	GLN	CA	-3.97	14.90	77.01	15.00
172	GLN	C	-4.16	13.50	76.45	15.00
172	GLN	O	-5.04	12.76	76.88	15.00
172	GLN	CB	-3.79	15.89	75.87	15.00
172	GLN	CG	-4.95	15.94	74.92	15.00
172	GLN	CD	-4.83	17.08	73.95	15.00
172	GLN	OE1	-3.81	17.24	73.28	15.00
172	GLN	NE2	-5.86	17.91	73.88	15.00
173	LYS	N	-3.39	13.15	75.44	15.00
173	LYS	CA	-3.51	11.81	74.89	15.00
173	LYS	C	-2.36	11.09	75.55	15.00
173	LYS	O	-1.55	10.43	74.90	15.00
173	LYS	CB	-3.36	11.82	73.36	15.00
173	LYS	CG	-4.57	12.39	72.60	15.00
173	LYS	CD	-5.81	11.53	72.82	15.00
173	LYS	CE	-7.06	12.17	72.19	15.00
173	LYS	NZ	-8.35	11.45	72.50	15.00
174	GLY	N	-2.29	11.24	76.87	15.00
174	GLY	CA	-1.20	10.64	77.60	15.00
174	GLY	C	0.03	11.49	77.36	15.00
174	GLY	O	1.17	11.08	77.62	15.00
175	ASN	N	-0.19	12.72	76.92	15.00
175	ASN	CA	0.93	13.59	76.64	15.00
175	ASN	C	1.02	14.78	77.57	15.00
175	ASN	O	0.07	15.56	77.70	15.00
175	ASN	CB	0.88	14.04	75.18	15.00
175	ASN	CG	0.72	12.87	74.20	15.00
175	ASN	OD1	-0.28	12.77	73.49	15.00
175	ASN	ND2	1.71	11.97	74.19	15.00
176	LYS	N	2.15	14.88	78.27	15.00
176	LYS	CA	2.42	15.97	79.20	15.00
176	LYS	C	2.40	17.22	78.34	15.00
176	LYS	O	2.76	17.17	77.16	15.00
176	LYS	CB	3.83	15.84	79.78	15.00
176	LYS	CG	4.38	14.45	79.93	15.00
176	LYS	CD	4.27	13.97	81.36	15.00
176	LYS	CE	4.98	12.63	81.55	15.00
176	LYS	NZ	4.97	12.14	82.96	15.00
177	HIS	N	2.01	18.36	78.91	15.00
177	HIS	CA	1.99	19.58	78.13	15.00

TABLE I

177	HIS	C	1.88	20.86	78.95	15.00
177	HIS	O	1.47	20.84	80.12	15.00
177	HIS	CB	0.88	19.53	77.06	15.00
177	HIS	CG	-0.52	19.66	77.59	15.00
177	HIS	ND1	-1.43	18.63	77.56	15.00
177	HIS	CD2	-1.16	20.71	78.16	15.00
177	HIS	CE1	-2.57	19.03	78.08	15.00
177	HIS	NE2	-2.44	20.29	78.45	15.00
178	TRP	N	2.25	21.96	78.31	15.00
178	TRP	CA	2.17	23.29	78.89	15.00
178	TRP	C	1.16	24.04	78.03	15.00
178	TRP	O	1.20	23.95	76.79	15.00
178	TRP	CB	3.52	23.99	78.78	15.00
178	TRP	CG	4.66	23.32	79.46	15.00
178	TRP	CD1	5.71	22.70	78.87	15.00
178	TRP	CD2	4.94	23.34	80.86	15.00
178	TRP	NE1	6.65	22.35	79.80	15.00
178	TRP	CE2	6.21	22.73	81.03	15.00
178	TRP	CE3	4.26	23.83	81.99	15.00
178	TRP	CZ2	6.80	22.60	82.29	15.00
178	TRP	CZ3	4.85	23.70	83.23	15.00
178	TRP	CH2	6.12	23.09	83.38	15.00
179	ILE	N	0.22	24.75	78.66	15.00
179	ILE	CA	-0.79	25.51	77.92	15.00
179	ILE	C	-0.20	26.89	77.64	15.00
179	ILE	O	-0.07	27.71	78.54	15.00
179	ILE	CB	-2.08	25.66	78.74	15.00
179	ILE	CG1	-2.67	24.27	79.03	15.00
179	ILE	CG2	-3.07	26.56	78.02	15.00
179	ILE	CD1	-3.80	24.25	80.04	15.00
180	ILE	N	0.21	27.09	76.39	15.00
180	ILE	CA	0.83	28.33	75.96	15.00
180	ILE	C	-0.17	29.28	75.34	15.00
180	ILE	O	-1.09	28.85	74.65	15.00
180	ILE	CB	1.99	28.05	74.99	15.00
180	ILE	CG1	3.32	28.14	75.72	15.00
180	ILE	CG2	1.97	28.97	73.83	15.00
180	ILE	CD1	3.53	27.06	76.73	15.00
181	LYS	N	0.00	30.57	75.64	15.00
181	LYS	CA	-0.85	31.66	75.14	15.00
181	LYS	C	-0.01	32.55	74.22	15.00
181	LYS	O	0.91	33.23	74.68	15.00

TABLE I

181	LYS	CB	-1.38	32.51	76.30	15.00
181	LYS	CG	-2.27	33.66	75.84	15.00
181	LYS	CD	-2.51	34.72	76.91	15.00
181	LYS	CE	-3.38	35.84	76.37	15.00
181	LYS	NZ	-3.58	36.94	77.35	15.00
182	ASN	N	-0.32	32.56	72.93	15.00
182	ASN	CA	0.44	33.36	71.97	15.00
182	ASN	C	-0.18	34.74	71.73	15.00
182	ASN	O	-1.29	35.00	72.17	15.00
182	ASN	CB	0.55	32.59	70.66	15.00
182	ASN	CG	1.83	32.87	69.93	15.00
182	ASN	OD1	2.41	33.95	70.05	15.00
182	ASN	ND2	2.31	31.89	69.17	15.00
183	SER	N	0.55	35.64	71.08	15.00
183	SER	CA	0.03	36.98	70.82	15.00
183	SER	C	-0.32	37.19	69.34	15.00
183	SER	O	-0.25	38.31	68.82	15.00
183	SER	CB	1.03	38.04	71.25	15.00
183	SER	OG	2.31	37.80	70.69	15.00
184	TRP	N	-0.74	36.12	68.68	15.00
184	TRP	CA	-1.05	36.18	67.26	15.00
184	TRP	C	-2.53	36.23	66.88	15.00
184	TRP	O	-2.87	36.09	65.71	15.00
184	TRP	CB	-0.36	35.01	66.55	15.00
184	TRP	CG	1.12	35.12	66.54	15.00
184	TRP	CD1	1.85	36.23	66.82	15.00
184	TRP	CD2	2.05	34.09	66.23	15.00
184	TRP	NE1	3.18	35.97	66.69	15.00
184	TRP	CE2	3.34	34.66	66.33	15.00
184	TRP	CE3	1.94	32.75	65.87	15.00
184	TRP	CZ2	4.51	33.92	66.09	15.00
184	TRP	CZ3	3.10	32.01	65.63	15.00
184	TRP	CH2	4.37	32.60	65.74	15.00
185	GLY	N	-3.40	36.48	67.85	15.00
185	GLY	CA	-4.82	36.54	67.56	15.00
185	GLY	C	-5.46	35.18	67.75	15.00
185	GLY	O	-4.75	34.16	67.80	15.00
186	GLU	N	-6.78	35.15	67.86	15.00
186	GLU	CA	-7.54	33.91	68.07	15.00
186	GLU	C	-7.53	32.99	66.85	15.00
186	GLU	O	-7.65	31.78	67.00	15.00
186	GLU	CB	-8.98	34.24	68.44	15.00

TABLE I

186	GLU	CG	-9.10	35.32	69.49	15.00
186	GLU	CD	-10.45	36.03	69.45	15.00
186	GLU	OE1	-10.66	36.84	68.51	15.00
186	GLU	OE2	-11.29	35.77	70.34	15.00
187	ASN	N	-7.43	33.58	65.66	15.00
187	ASN	CA	-7.43	32.78	64.42	15.00
187	ASN	C	-6.14	31.97	64.30	15.00
187	ASN	O	-6.07	31.05	63.49	15.00
187	ASN	CB	-7.64	33.68	63.19	15.00
187	ASN	CG	-8.60	33.05	62.14	15.00
187	ASN	OD1	-8.17	32.52	61.10	15.00
187	ASN	ND2	-9.90	33.18	62.38	15.00
188	TRP	N	-5.12	32.31	65.10	15.00
188	TRP	CA	-3.87	31.57	65.07	15.00
188	TRP	C	-4.06	30.34	65.95	15.00
188	TRP	O	-4.78	30.41	66.95	15.00
188	TRP	CB	-2.71	32.38	65.64	15.00
188	TRP	CG	-1.45	31.59	65.56	15.00
188	TRP	CD1	-0.68	31.41	64.46	15.00
188	TRP	CD2	-0.89	30.74	66.58	15.00
188	TRP	NE1	0.30	30.49	64.71	15.00
188	TRP	CE2	0.20	30.06	66.00	15.00
188	TRP	CE3	-1.21	30.49	67.92	15.00
188	TRP	CZ2	0.97	29.14	66.71	15.00
188	TRP	CZ3	-0.44	29.57	68.62	15.00
188	TRP	CH2	0.64	28.92	68.02	15.00
189	GLY	N	-3.38	29.25	65.60	15.00
189	GLY	CA	-3.46	28.02	66.36	15.00
189	GLY	C	-4.84	27.67	66.87	15.00
189	GLY	O	-5.86	27.96	66.24	15.00
190	ASN	N	-4.87	27.07	68.04	15.00
190	ASN	CA	-6.10	26.65	68.68	15.00
190	ASN	C	-6.74	27.83	69.39	15.00
190	ASN	O	-6.67	27.92	70.61	15.00
190	ASN	CB	-5.76	25.58	69.71	15.00
190	ASN	CG	-6.97	24.84	70.19	15.00
190	ASN	OD1	-8.11	25.26	69.96	15.00
190	ASN	ND2	-6.73	23.72	70.87	15.00
191	LYS	N	-7.33	28.75	68.61	15.00
191	LYS	CA	-7.97	29.96	69.14	15.00
191	LYS	C	-7.01	30.82	69.95	15.00
191	LYS	O	-7.36	31.36	71.00	15.00

TABLE I

191	LYS	CB	-9.20	29.62	69.99	15.00
191	LYS	CG	-10.33	28.92	69.26	15.00
191	LYS	CD	-11.50	28.66	70.20	15.00
191	LYS	CE	-12.26	27.39	69.82	15.00
191	LYS	NZ	-11.42	26.16	70.01	15.00
192	GLY	N	-5.79	30.96	69.45	15.00
192	GLY	CA	-4.80	31.75	70.13	15.00
192	GLY	C	-3.88	30.93	70.99	15.00
192	GLY	O	-2.79	31.39	71.32	15.00
193	TYR	N	-4.28	29.72	71.35	15.00
193	TYR	CA	-3.43	28.86	72.18	15.00
193	TYR	C	-2.80	27.69	71.45	15.00
193	TYR	O	-3.25	27.27	70.39	15.00
193	TYR	CB	-4.21	28.31	73.39	15.00
193	TYR	CG	-4.63	29.36	74.36	15.00
193	TYR	CD1	-3.77	29.78	75.37	15.00
193	TYR	CD2	-5.85	30.00	74.22	15.00
193	TYR	CE1	-4.12	30.82	76.22	15.00
193	TYR	CE2	-6.21	31.05	75.06	15.00
193	TYR	CZ	-5.34	31.45	76.06	15.00
193	TYR	OH	-5.68	32.50	76.87	15.00
194	ILE	N	-1.73	27.17	72.05	15.00
194	ILE	CA	-1.01	26.02	71.53	15.00
194	ILE	C	-0.53	25.21	72.71	15.00
194	ILE	O	0.04	25.75	73.66	15.00
194	ILE	CB	0.20	26.40	70.62	15.00
194	ILE	CG1	1.05	25.15	70.32	15.00
194	ILE	CG2	1.04	27.49	71.24	15.00
194	ILE	CD1	2.33	25.42	69.60	15.00
195	LEU	N	-0.86	23.92	72.69	15.00
195	LEU	CA	-0.45	23.00	73.73	15.00
195	LEU	C	0.90	22.46	73.34	15.00
195	LEU	O	0.99	21.68	72.42	15.00
195	LEU	CB	-1.43	21.83	73.83	15.00
195	LEU	CG	-2.45	21.90	74.96	15.00
195	LEU	CD1	-3.38	23.07	74.76	15.00
195	LEU	CD2	-3.23	20.60	74.98	15.00
196	MET	N	1.95	22.94	74.01	15.00
196	MET	CA	3.31	22.50	73.75	15.00
196	MET	C	3.70	21.30	74.64	15.00
196	MET	O	2.97	20.96	75.57	15.00
196	MET	CB	4.27	23.66	73.96	15.00

TABLE I

196	MET	CG	4.16	24.69	72.88	15.00
196	MET	SD	5.11	26.17	73.23	15.00
196	MET	CE	6.79	25.64	72.90	15.00
197	ALA	N	4.85	20.69	74.38	15.00
197	ALA	CA	5.27	19.52	75.15	15.00
197	ALA	C	5.99	19.75	76.49	15.00
197	ALA	O	7.03	20.42	76.57	15.00
197	ALA	CB	6.07	18.58	74.28	15.00
198	ARG	N	5.43	19.14	77.54	15.00
198	ARG	CA	5.99	19.22	78.88	15.00
198	ARG	C	6.80	17.96	79.20	15.00
198	ARG	O	6.41	16.84	78.86	15.00
198	ARG	CB	4.89	19.44	79.92	15.00
198	ARG	CG	5.35	19.32	81.39	15.00
198	ARG	CD	4.48	20.12	82.35	15.00
198	ARG	NE	3.08	19.72	82.36	15.00
198	ARG	CZ	2.62	18.64	82.99	15.00
198	ARG	NH1	3.46	17.86	83.66	15.00
198	ARG	NH2	1.33	18.34	82.95	15.00
199	ASN	N	7.96	18.18	79.83	15.00
199	ASN	CA	8.87	17.11	80.24	15.00
199	ASN	C	9.57	16.30	79.13	15.00
199	ASN	O	10.36	15.40	79.43	15.00
199	ASN	CB	8.21	16.18	81.28	15.00
199	ASN	CG	8.15	16.81	82.68	15.00
199	ASN	OD1	7.06	17.06	83.21	15.00
199	ASN	ND2	9.31	17.07	83.27	15.00
200	LYS	N	9.31	16.63	77.88	15.00
200	LYS	CA	9.97	15.94	76.77	15.00
200	LYS	C	11.29	16.67	76.54	15.00
200	LYS	O	11.54	17.17	75.45	15.00
200	LYS	CB	9.11	15.96	75.49	15.00
200	LYS	CG	8.09	14.81	75.36	15.00
200	LYS	CD	8.32	14.01	74.06	15.00
200	LYS	CE	7.22	12.96	73.78	15.00
200	LYS	NZ	5.87	13.49	73.41	15.00
201	ASN	N	12.13	16.71	77.57	15.00
201	ASN	CA	13.42	17.39	77.56	15.00
201	ASN	C	13.27	18.81	77.00	15.00
201	ASN	O	13.24	18.99	75.80	15.00
201	ASN	CB	14.47	16.61	76.74	15.00
201	ASN	CG	15.92	17.21	76.86	15.00

TABLE I

201	ASN	OD1	16.88	16.46	77.06	15.00
201	ASN	ND2	16.06	18.52	76.67	15.00
202	ASN	N	13.15	19.80	77.89	15.00
202	ASN	CA	13.04	21.22	77.54	15.00
202	ASN	C	12.73	21.51	76.05	15.00
202	ASN	O	13.56	22.10	75.34	15.00
202	ASN	CB	14.35	21.92	77.95	15.00
202	ASN	CG	14.13	23.30	78.56	15.00
202	ASN	OD1	13.04	23.64	79.00	15.00
202	ASN	ND2	15.18	24.09	78.60	15.00
203	ALA	N	11.55	21.12	75.59	15.00
203	ALA	H	11.67	20.72	76.05	15.00
203	ALA	CA	11.15	21.27	74.19	15.00
203	ALA	CB	10.97	20.66	73.61	15.00
203	ALA	C	11.04	22.76	73.85	15.00
203	ALA	O	10.23	23.49	74.41	15.00
204	CYS	N	11.83	23.20	72.87	15.00
204	CYS	CA	11.81	24.59	72.40	15.00
204	CYS	C	12.38	25.57	73.42	15.00
204	CYS	O	12.06	26.76	73.36	15.00
204	CYS	CB	10.39	25.02	72.00	15.00
204	CYS	SG	9.66	24.16	70.56	15.00
205	GLY	N	13.21	25.07	74.33	15.00
205	GLY	CA	13.84	25.89	75.36	15.00
205	GLY	C	12.87	26.70	76.20	15.00
205	GLY	O	13.17	27.80	76.64	15.00
206	ILE	N	11.72	26.10	76.48	15.00
206	ILE	CA	10.67	26.74	77.23	15.00
206	ILE	C	11.05	27.11	78.67	15.00
206	ILE	O	10.90	28.27	79.08	15.00
206	ILE	CB	9.41	25.86	77.17	15.00
206	ILE	CG1	8.20	26.58	77.77	15.00
206	ILE	CG2	9.69	24.53	77.81	15.00
206	ILE	CD1	6.88	25.88	77.49	15.00
207	ALA	N	11.62	26.17	79.41	15.00
207	ALA	CA	12.03	26.40	80.79	15.00
207	ALA	C	13.38	27.11	80.93	15.00
207	ALA	O	13.98	27.10	82.01	15.00
207	ALA	CB	12.05	25.09	81.54	15.00
208	ASN	N	13.84	27.74	79.86	15.00
208	ASN	CA	15.12	28.43	79.86	15.00
208	ASN	C	15.08	29.92	80.08	15.00

TABLE I

208	ASN	O	16.13	30.53	80.28	15.00
208	ASN	CB	15.84	28.22	78.54	15.00
208	ASN	CG	16.81	27.09	78.60	15.00
208	ASN	OD1	16.50	26.04	79.14	15.00
208	ASN	ND2	17.99	27.30	78.04	15.00
209	LEU	N	13.91	30.54	79.98	15.00
209	LEU	CA	13.84	31.98	80.18	15.00
209	LEU	C	12.65	32.45	81.02	15.00
209	LEU	O	12.23	33.63	80.94	15.00
209	LEU	CB	13.89	32.69	78.83	15.00
209	LEU	CG	14.33	34.16	78.81	15.00
209	LEU	CD1	15.60	34.32	79.63	15.00
209	LEU	CD2	14.56	34.61	77.37	15.00
210	ALA	N	12.15	31.57	81.87	15.00
210	ALA	H	12.50	30.94	81.70	15.00
210	ALA	CA	10.99	31.87	82.71	15.00
210	ALA	CB	10.41	31.04	83.16	15.00
210	ALA	C	11.33	33.00	83.69	15.00
210	ALA	O	12.46	33.21	84.13	15.00
211	SER	N	10.26	33.74	84.06	15.00
211	SER	CA	10.37	34.83	85.02	15.00
211	SER	C	8.96	35.33	85.31	15.00
211	SER	O	8.09	35.24	84.45	15.00
211	SER	CB	11.22	35.98	84.46	15.00
211	SER	OG	10.50	36.76	83.53	15.00
212	PHE	N	8.72	35.78	86.53	15.00
212	PHE	CA	7.42	36.30	86.88	15.00
212	PHE	C	7.64	37.49	87.78	15.00
212	PHE	O	8.68	37.61	88.42	15.00
212	PHE	CB	6.57	35.23	87.56	15.00
212	PHE	CG	7.23	34.60	88.75	15.00
212	PHE	CD1	7.39	35.31	89.94	15.00
212	PHE	CD2	7.68	33.28	88.69	15.00
212	PHE	CE1	7.99	34.73	91.05	15.00
212	PHE	CE2	8.28	32.68	89.78	15.00
212	PHE	CZ	8.44	33.41	90.97	15.00
213	PRO	N	6.69	38.43	87.80	15.00
213	PRO	CA	6.84	39.62	88.65	15.00
213	PRO	C	6.38	39.34	90.09	15.00
213	PRO	O	5.56	38.44	90.33	15.00
213	PRO	CB	5.93	40.62	87.97	15.00
213	PRO	CG	4.79	39.75	87.52	15.00

TABLE I

213	PRO	CD	5.47	38.52	86.97	15.00
214	LYS	N	6.96	40.05	91.04	15.00
214	LYS	CA	6.57	39.89	92.42	15.00
214	LYS	C	5.65	41.06	92.68	15.00
214	LYS	O	6.12	42.17	92.91	15.00
214	LYS	CB	7.78	39.94	93.36	15.00
214	LYS	CG	8.68	38.72	93.27	15.00
214	LYS	CD	9.78	38.70	94.34	15.00
214	LYS	CE	10.67	39.94	94.26	15.00
214	LYS	NZ	11.94	39.80	95.03	15.00
215	MET	N	4.36	40.85	92.51	15.00
215	MET	CA	3.39	41.91	92.77	15.00
215	MET	C	2.86	41.71	94.19	15.00
215	MET	CB	2.25	41.86	91.76	15.00
215	MET	CG	1.06	42.74	92.12	15.00
215	MET	SD	-0.32	42.54	90.98	15.00
215	MET	CE	0.28	43.53	89.53	15.00

TABLE II

Table of the orthogonal three dimensional coordinates in Ångstroms and B factors ($Å^2$) for the cathepsin K complex with inhibitor 3(S)-3-[(N-benzyloxycarbonyl)-L-leucinyl]amino-5-methyl-1-(1-propoxy)-2-hexanone.

Residue	Atom	X	Y	Z	B
1 ALA	CB	-54.11	-32.66	67.34	15.00
1 ALA	C	-54.02	-32.71	64.82	15.00
1 ALA	O	-53.62	-33.85	64.58	15.00
1 ALA	N	-56.02	-33.44	65.99	15.00
1 ALA	CA	-54.90	-32.46	66.05	15.00
2 PRO	N	-53.80	-31.67	63.99	15.00
2 PRO	CD	-54.47	-30.37	64.11	15.00
2 PRO	CA	-52.98	-31.72	62.76	15.00
2 PRO	CB	-53.14	-30.31	62.20	15.00
2 PRO	CG	-54.52	-29.90	62.67	15.00
2 PRO	C	-51.51	-32.06	62.95	15.00
2 PRO	O	-50.99	-32.06	64.08	15.00
3 ASP	N	-50.81	-32.33	61.85	15.00
3 ASP	CA	-49.39	-32.67	61.91	15.00
3 ASP	CB	-49.04	-33.71	60.85	15.00
3 ASP	CG	-49.27	-35.14	61.32	15.00
3 ASP	OD1	-48.47	-35.61	62.17	15.00
3 ASP	OD2	-50.24	-35.79	60.85	15.00
3 ASP	C	-48.52	-31.44	61.73	15.00
3 ASP	O	-47.93	-31.24	60.68	15.00
4 SER	N	-48.41	-30.64	62.79	15.00
4 SER	CA	-47.62	-29.41	62.75	15.00
4 SER	CB	-48.55	-28.25	62.37	15.00
4 SER	OG	-47.82	-27.08	62.01	15.00
4 SER	C	-47.01	-29.13	64.12	15.00
4 SER	O	-47.59	-29.49	65.15	15.00
5 VAL	N	-45.83	-28.51	64.15	15.00
5 VAL	CA	-45.19	-28.15	65.41	15.00
5 VAL	CB	-44.36	-29.31	66.03	15.00
5 VAL	CG1	-43.06	-29.53	65.29	15.00
5 VAL	CG2	-44.08	-29.04	67.50	15.00
5 VAL	C	-44.34	-26.88	65.24	15.00
5 VAL	O	-43.64	-26.69	64.25	15.00

TABLE II

6	ASP	N	-44.48	-25.96	66.20	15.00
6	ASP	CA	-43.78	-24.69	66.19	15.00
6	ASP	CB	-44.75	-23.59	65.74	15.00
6	ASP	CG	-44.11	-22.19	65.67	15.00
6	ASP	OD1	-42.99	-21.99	66.18	15.00
6	ASP	OD2	-44.75	-21.27	65.13	15.00
6	ASP	C	-43.37	-24.47	67.64	15.00
6	ASP	O	-44.19	-24.09	68.48	15.00
7	TYR	N	-42.10	-24.68	67.95	15.00
7	TYR	CA	-41.65	-24.50	69.33	15.00
7	TYR	CB	-40.30	-25.18	69.53	15.00
7	TYR	CG	-40.41	-26.69	69.53	15.00
7	TYR	CD1	-40.91	-27.37	70.64	15.00
7	TYR	CE1	-41.02	-28.74	70.65	15.00
7	TYR	CD2	-40.02	-27.43	68.42	15.00
7	TYR	CE2	-40.13	-28.80	68.42	15.00
7	TYR	CZ	-40.63	-29.45	69.53	15.00
7	TYR	OH	-40.70	-30.82	69.53	15.00
7	TYR	C	-41.62	-23.07	69.82	15.00
7	TYR	O	-41.41	-22.81	71.00	15.00
8	ARG	N	-41.83	-22.12	68.92	15.00
8	ARG	CA	-41.84	-20.72	69.31	15.00
8	ARG	CB	-42.00	-19.80	68.09	15.00
8	ARG	CG	-40.82	-19.80	67.14	15.00
8	ARG	CD	-41.13	-18.98	65.91	15.00
8	ARG	NE	-42.05	-19.66	65.00	15.00
8	ARG	CZ	-42.68	-19.07	64.00	15.00
8	ARG	NH1	-42.49	-17.78	63.77	15.00
8	ARG	NH2	-43.50	-19.77	63.22	15.00
8	ARG	C	-43.00	-20.51	70.28	15.00
8	ARG	O	-42.87	-19.79	71.28	15.00
9	LYS	N	-44.10	-21.19	70.00	15.00
9	LYS	CA	-45.30	-21.10	70.82	15.00
9	LYS	CB	-46.49	-21.67	70.05	15.00
9	LYS	CG	-46.76	-21.07	68.69	15.00
9	LYS	CD	-48.04	-21.67	68.14	15.00
9	LYS	CE	-48.28	-21.36	66.69	15.00
9	LYS	NZ	-49.49	-22.07	66.19	15.00
9	LYS	C	-45.20	-21.83	72.16	15.00
9	LYS	O	-46.13	-21.78	72.97	15.00
10	LYS	N	-44.10	-22.53	72.40	15.00
10	LYS	CA	-43.92	-23.27	73.64	15.00

TABLE II

10	LYS	CB	-43.47	-24.71	73.36	15.00
10	LYS	CG	-43.75	-25.23	71.96	15.00
10	LYS	CD	-45.22	-25.49	71.73	15.00
10	LYS	CE	-45.52	-26.97	71.83	15.00
10	LYS	NZ	-45.21	-27.50	73.19	15.00
10	LYS	C	-42.88	-22.63	74.54	15.00
10	LYS	O	-42.67	-23.06	75.67	15.00
11	GLY	N	-42.16	-21.63	74.03	15.00
11	GLY	CA	-41.15	-20.98	74.83	15.00
11	GLY	C	-39.79	-21.63	74.68	15.00
11	GLY	O	-38.90	-21.42	75.50	15.00
12	TYR	N	-39.60	-22.38	73.60	15.00
12	TYR	CA	-38.34	-23.07	73.36	15.00
12	TYR	CB	-38.56	-24.39	72.61	15.00
12	TYR	CG	-39.12	-25.53	73.43	15.00
12	TYR	CD1	-40.27	-25.37	74.19	15.00
12	TYR	CE1	-40.82	-26.43	74.89	15.00
12	TYR	CD2	-38.53	-26.79	73.39	15.00
12	TYR	CE2	-39.08	-27.86	74.09	15.00
12	TYR	CZ	-40.23	-27.67	74.84	15.00
12	TYR	OH	-40.79	-28.71	75.55	15.00
12	TYR	C	-37.31	-22.26	72.60	15.00
12	TYR	O	-36.14	-22.61	72.57	15.00
13	VAL	N	-37.70	-21.18	71.93	15.00
13	VAL	CA	-36.72	-20.42	71.18	15.00
13	VAL	CB	-36.97	-20.48	69.67	15.00
13	VAL	CG1	-37.21	-21.91	69.23	15.00
13	VAL	CG2	-38.14	-19.62	69.30	15.00
13	VAL	C	-36.63	-18.98	71.64	15.00
13	VAL	O	-37.62	-18.38	72.02	15.00
14	THR	N	-35.41	-18.45	71.65	15.00
14	THR	CA	-35.16	-17.08	72.07	15.00
14	THR	CB	-33.75	-16.96	72.66	15.00
14	THR	OG1	-32.79	-17.40	71.71	15.00
14	THR	CG2	-33.63	-17.80	73.91	15.00
14	THR	C	-35.32	-16.08	70.91	15.00
14	THR	O	-35.57	-16.48	69.77	15.00
15	PRO	N	-35.24	-14.77	71.20	15.00
15	PRO	CD	-35.20	-14.14	72.53	15.00
15	PRO	CA	-35.37	-13.75	70.15	15.00
15	PRO	CB	-35.25	-12.44	70.93	15.00
15	PRO	CG	-35.83	-12.79	72.26	15.00

TABLE II

15 PRO C	-34.26	-13.87	69.11	15.00
15 PRO O	-33.13	-14.23	69.44	15.00
16 VAL N	-34.59	-13.55	67.85	15.00
16 VAL CA	-33.64	-13.61	66.75	15.00
16 VAL CB	-34.33	-13.31	65.40	15.00
16 VAL CG1	-33.34	-13.41	64.25	15.00
16 VAL CG2	-35.47	-14.26	65.19	15.00
16 VAL C	-32.48	-12.65	66.96	15.00
16 VAL O	-32.69	-11.49	67.32	15.00
17 LYS N	-31.28	-13.13	66.71	15.00
17 LYS CA	-30.07	-12.35	66.86	15.00
17 LYS CB	-29.12	-13.04	67.84	15.00
17 LYS CG	-29.68	-13.07	69.24	15.00
17 LYS CD	-28.91	-14.03	70.13	15.00
17 LYS CE	-29.54	-14.07	71.53	15.00
17 LYS NZ	-31.02	-14.22	71.43	15.00
17 LYS C	-29.39	-12.14	65.52	15.00
17 LYS O	-29.72	-12.79	64.54	15.00
18 ASN N	-28.42	-11.23	65.50	15.00
18 ASN CA	-27.68	-10.87	64.29	15.00
18 ASN CB	-27.77	-9.36	64.10	15.00
18 ASN CG	-27.26	-8.90	62.75	15.00
18 ASN OD1	-26.16	-9.25	62.32	15.00
18 ASN ND2	-28.07	-8.10	62.08	15.00
18 ASN C	-26.23	-11.28	64.45	15.00
18 ASN O	-25.55	-10.79	65.35	15.00
19 GLN N	-25.72	-12.16	63.60	15.00
19 GLN CA	-24.33	-12.56	63.73	15.00
19 GLN CB	-24.00	-13.81	62.90	15.00
19 GLN CG	-24.44	-13.80	61.45	15.00
19 GLN CD	-24.06	-15.09	60.72	15.00
19 GLN OE1	-24.91	-15.79	60.16	15.00
19 GLN NE2	-22.77	-15.41	60.71	15.00
19 GLN C	-23.40	-11.40	63.39	15.00
19 GLN O	-22.27	-11.33	63.88	15.00
20 GLY N	-23.91	-10.46	62.60	15.00
20 GLY CA	-23.14	-9.30	62.21	15.00
20 GLY C	-22.11	-9.67	61.16	15.00
20 GLY O	-22.39	-10.50	60.28	15.00
21 GLN N	-20.93	-9.08	61.26	15.00
21 GLN CA	-19.85	-9.33	60.32	15.00
21 GLN CB	-19.08	-8.03	60.01	15.00

TABLE II

21	GLN	CG	-19.94	-6.78	59.84	15.00
21	GLN	CD	-20.87	-6.85	58.64	15.00
21	GLN	OE1	-20.43	-6.78	57.49	15.00
21	GLN	NE2	-22.17	-6.95	58.90	15.00
21	GLN	C	-18.91	-10.35	60.98	15.00
21	GLN	O	-17.86	-10.01	61.52	15.00
22	CYS	N	-19.31	-11.61	60.97	15.00
22	CYS	CA	-18.53	-12.68	61.58	15.00
22	CYS	C	-19.27	-13.95	61.19	15.00
22	CYS	O	-20.48	-14.03	61.36	15.00
22	CYS	CB	-18.50	-12.50	63.11	15.00
22	CYS	SG	-17.85	-13.86	64.14	15.00
23	GLY	N	-18.56	-14.88	60.56	15.00
23	GLY	CA	-19.19	-16.12	60.13	15.00
23	GLY	C	-19.43	-17.05	61.30	15.00
23	GLY	O	-18.94	-18.17	61.31	15.00
24	SER	N	-20.24	-16.60	62.25	15.00
24	SER	CA	-20.56	-17.36	63.44	15.00
24	SER	CB	-20.46	-16.45	64.66	15.00
24	SER	OG	-21.23	-15.30	64.42	15.00
24	SER	C	-21.95	-17.97	63.37	15.00
24	SER	O	-22.54	-18.31	64.40	15.00
25	CYS	N	-22.49	-18.14	62.17	15.00
25	CYS	CA	-23.81	-18.74	62.02	15.00
25	CYS	CB	-24.21	-18.82	60.54	15.00
25	CYS	SG	-23.17	-19.85	59.47	15.00
25	CYS	C	-23.88	-20.12	62.68	15.00
25	CYS	O	-24.96	-20.59	63.04	15.00
25	INH	C1	-26.94	-9.70	58.69	15.00
25	INH	C2	-26.28	-10.48	59.65	15.00
25	INH	C3	-25.12	-11.19	59.30	15.00
25	INH	C4	-24.61	-11.12	58.00	15.00
25	INH	C5	-25.28	-10.33	57.05	15.00
25	INH	C6	-26.44	-9.62	57.39	15.00
25	INH	C7	-23.37	-11.90	57.62	15.00
25	INH	O8	-23.43	-13.32	57.82	15.00
25	INH	C9	-22.85	-14.36	57.02	15.00
25	INH	O10	-21.63	-14.58	56.99	15.00
25	INH	C11	-23.27	-16.14	55.41	15.00
25	INH	C12	-22.06	-15.67	54.58	15.00
25	INH	C13	-22.16	-15.18	53.14	15.00
25	INH	C14	-20.77	-15.22	52.56	15.00

TABLE II

25	INH	C15	-23.13	-16.04	52.32	15.00
25	INH	C16	-22.95	-17.51	56.01	15.00
25	INH	O17	-23.60	-18.50	55.66	15.00
25	INH	N18	-21.92	-17.60	56.86	15.00
25	INH	C19	-21.48	-18.89	57.42	15.00
25	INH	C20	-20.01	-19.11	57.02	15.00
25	INH	C21	-19.59	-19.34	55.56	15.00
25	INH	C22	-19.45	-20.84	55.30	15.00
25	INH	C23	-18.25	-18.64	55.30	15.00
25	INH	N24	-23.71	-15.07	56.30	15.00
25	INH	C25	-21.62	-19.06	58.94	15.00
25	INH	O26	-21.55	-17.95	59.50	15.00
25	INH	C27	-20.53	-20.00	59.45	15.00
25	INH	O28	-20.36	-21.26	58.72	15.00
25	INH	C29	-19.70	-22.40	59.29	15.00
25	INH	C30	-19.53	-23.60	58.35	15.00
25	INH	C31	-20.80	-24.42	58.08	15.00
26	TRP	N	-22.73	-20.75	62.90	15.00
26	TRP	CA	-22.65	-22.06	63.54	15.00
26	TRP	CB	-21.30	-22.75	63.25	15.00
26	TRP	CG	-20.09	-22.04	63.79	15.00
26	TRP	CD2	-19.48	-22.23	65.08	15.00
26	TRP	CE2	-18.36	-21.38	65.14	15.00
26	TRP	CE3	-19.77	-23.04	66.19	15.00
26	TRP	CD1	-19.33	-21.11	63.15	15.00
26	TRP	NE1	-18.29	-20.70	63.95	15.00
26	TRP	CZ2	-17.53	-21.31	66.27	15.00
26	TRP	CZ3	-18.94	-22.97	67.31	15.00
26	TRP	CH2	-17.83	-22.11	67.33	15.00
26	TRP	C	-22.89	-22.02	65.06	15.00
26	TRP	O	-23.59	-22.87	65.61	15.00
27	ALA	N	-22.34	-21.01	65.75	15.00
27	ALA	CA	-22.49	-20.86	67.19	15.00
27	ALA	CB	-21.58	-19.78	67.71	15.00
27	ALA	C	-23.93	-20.53	67.54	15.00
27	ALA	O	-24.46	-20.98	68.55	15.00
28	PHE	N	-24.55	-19.71	66.70	15.00
28	PHE	CA	-25.93	-19.33	66.91	15.00
28	PHE	CB	-26.33	-18.21	65.94	15.00
28	PHE	CG	-25.73	-16.88	66.28	15.00
28	PHE	CD1	-24.51	-16.49	65.73	15.00
28	PHE	CD2	-26.34	-16.04	67.19	15.00

TABLE II

28	PHE	CE1	-23.92	-15.30	66.11	15.00
28	PHE	CE2	-25.75	-14.85	67.57	15.00
28	PHE	CZ	-24.54	-14.48	67.02	15.00
28	PHE	C	-26.82	-20.55	66.75	15.00
28	PHE	O	-27.75	-20.75	67.51	15.00
29	SER	N	-26.49	-21.39	65.78	15.00
29	SER	CA	-27.25	-22.61	65.53	15.00
29	SER	CB	-26.69	-23.33	64.31	15.00
29	SER	OG	-27.48	-24.45	63.98	15.00
29	SER	C	-27.16	-23.52	66.74	15.00
29	SER	O	-28.17	-23.93	67.30	15.00
30	SER	N	-25.92	-23.82	67.14	15.00
30	SER	CA	-25.63	-24.69	68.27	15.00
30	SER	CB	-24.13	-24.77	68.46	15.00
30	SER	OG	-23.51	-24.96	67.22	15.00
30	SER	C	-26.27	-24.16	69.55	15.00
30	SER	O	-26.82	-24.92	70.35	15.00
31	VAL	N	-26.17	-22.85	69.75	15.00
31	VAL	CA	-26.75	-22.24	70.93	15.00
31	VAL	CB	-26.25	-20.78	71.09	15.00
31	VAL	CG1	-27.32	-19.87	71.63	15.00
31	VAL	CG2	-25.06	-20.75	72.01	15.00
31	VAL	C	-28.27	-22.35	70.84	15.00
31	VAL	O	-28.94	-22.62	71.82	15.00
32	GLY	N	-28.80	-22.28	69.63	15.00
32	GLY	CA	-30.23	-22.39	69.44	15.00
32	GLY	C	-30.80	-23.73	69.86	15.00
32	GLY	O	-31.91	-23.80	70.38	15.00
33	ALA	N	-30.05	-24.80	69.59	15.00
33	ALA	CA	-30.46	-26.15	69.95	15.00
33	ALA	CB	-29.65	-27.18	69.17	15.00
33	ALA	C	-30.28	-26.35	71.44	15.00
33	ALA	O	-31.16	-26.89	72.11	15.00
34	LEU	N	-29.14	-25.91	71.97	15.00
34	LEU	CA	-28.87	-26.01	73.40	15.00
34	LEU	CB	-27.54	-25.36	73.74	15.00
34	LEU	CG	-26.26	-26.09	73.37	15.00
34	LEU	CD1	-25.09	-25.16	73.59	15.00
34	LEU	CD2	-26.10	-27.34	74.21	15.00
34	LEU	C	-29.98	-25.32	74.18	15.00
34	LEU	O	-30.45	-25.85	75.18	15.00
35	GLU	N	-30.43	-24.16	73.69	15.00

TABLE II

35	GLU	CA	-31.51	-23.39	74.33	15.00
35	GLU	CB	-31.65	-22.03	73.66	15.00
35	GLU	CG	-30.44	-21.12	73.81	15.00
35	GLU	CD	-30.54	-19.82	73.03	15.00
35	GLU	OE1	-31.35	-19.71	72.09	15.00
35	GLU	OE2	-29.77	-18.91	73.35	15.00
35	GLU	C	-32.84	-24.12	74.28	15.00
35	GLU	O	-33.67	-24.00	75.19	15.00
36	GLY	N	-33.09	-24.86	73.21	15.00
36	GLY	CA	-34.33	-25.59	73.09	15.00
36	GLY	C	-34.37	-26.71	74.11	15.00
36	GLY	O	-35.37	-26.91	74.80	15.00
37	GLN	N	-33.26	-27.43	74.25	15.00
37	GLN	CA	-33.18	-28.52	75.20	15.00
37	GLN	CB	-31.92	-29.34	74.98	15.00
37	GLN	CG	-31.94	-30.12	73.69	15.00
37	GLN	CD	-33.17	-31.00	73.57	15.00
37	GLN	OE1	-33.42	-31.85	74.43	15.00
37	GLN	NE2	-33.95	-30.79	72.53	15.00
37	GLN	C	-33.24	-28.01	76.63	15.00
37	GLN	O	-33.97	-28.56	77.47	15.00
38	LEU	N	-32.52	-26.92	76.89	15.00
38	LEU	CA	-32.51	-26.31	78.21	15.00
38	LEU	CB	-31.79	-24.96	78.17	15.00
38	LEU	CG	-31.83	-24.13	79.46	15.00
38	LEU	CD1	-31.00	-24.83	80.53	15.00
38	LEU	CD2	-31.30	-22.73	79.20	15.00
38	LEU	C	-33.94	-26.11	78.69	15.00
38	LEU	O	-34.30	-26.51	79.79	15.00
39	LYS	N	-34.77	-25.51	77.85	15.00
39	LYS	CA	-36.16	-25.26	78.20	15.00
39	LYS	CB	-36.85	-24.43	77.11	15.00
39	LYS	CG	-38.06	-23.64	77.59	15.00
39	LYS	CD	-39.32	-24.48	77.65	15.00
39	LYS	CE	-40.53	-23.66	78.07	15.00
39	LYS	NZ	-40.50	-23.27	79.50	15.00
39	LYS	C	-36.89	-26.59	78.36	15.00
39	LYS	O	-37.71	-26.75	79.25	15.00
40	LYS	N	-36.57	-27.57	77.53	15.00
40	LYS	CA	-37.25	-28.86	77.63	15.00
40	LYS	CB	-36.85	-29.79	76.48	15.00
40	LYS	CG	-37.77	-31.00	76.39	15.00

TABLE II

40	LYS	CD	-37.48	-31.90	75.22	15.00
40	LYS	CE	-38.53	-32.99	75.17	15.00
40	LYS	NZ	-38.45	-33.78	73.92	15.00
40	LYS	C	-36.98	-29.55	78.95	15.00
40	LYS	O	-37.90	-30.11	79.56	15.00
41	LYS	N	-35.74	-29.45	79.42	15.00
41	LYS	CA	-35.35	-30.09	80.66	15.00
41	LYS	CB	-33.87	-30.48	80.61	15.00
41	LYS	CG	-33.50	-31.39	79.43	15.00
41	LYS	CD	-34.48	-32.55	79.32	15.00
41	LYS	CE	-34.33	-33.33	78.02	15.00
41	LYS	NZ	-35.59	-34.07	77.73	15.00
41	LYS	C	-35.67	-29.31	81.94	15.00
41	LYS	O	-36.36	-29.82	82.81	15.00
42	THR	N	-35.20	-28.08	82.07	15.00
42	THR	CA	-35.45	-27.32	83.29	15.00
42	THR	CB	-34.31	-26.34	83.57	15.00
42	THR	OG1	-34.40	-25.23	82.67	15.00
42	THR	CG2	-32.98	-27.04	83.36	15.00
42	THR	C	-36.77	-26.54	83.35	15.00
42	THR	O	-37.19	-26.11	84.43	15.00
43	GLY	N	-37.42	-26.34	82.21	15.00
43	GLY	CA	-38.67	-25.60	82.16	15.00
43	GLY	C	-38.49	-24.09	82.05	15.00
43	GLY	O	-39.45	-23.33	81.92	15.00
44	LYS	N	-37.25	-23.62	82.11	15.00
44	LYS	CA	-36.99	-22.20	82.03	15.00
44	LYS	CB	-36.47	-21.70	83.37	15.00
44	LYS	CG	-37.07	-22.42	84.57	15.00
44	LYS	CD	-36.69	-21.78	85.90	15.00
44	LYS	CE	-35.51	-22.46	86.59	15.00
44	LYS	NZ	-35.95	-23.54	87.52	15.00
44	LYS	C	-35.98	-21.94	80.92	15.00
44	LYS	O	-34.92	-22.58	80.87	15.00
45	LEU	N	-36.32	-21.02	80.04	15.00
45	LEU	CA	-35.47	-20.64	78.90	15.00
45	LEU	CB	-36.33	-20.13	77.75	15.00
45	LEU	CG	-35.67	-19.77	76.42	15.00
45	LEU	CD1	-35.27	-21.03	75.66	15.00
45	LEU	CD2	-36.67	-18.97	75.62	15.00
45	LEU	C	-34.47	-19.58	79.29	15.00
45	LEU	O	-34.68	-18.81	80.22	15.00

TABLE II

46	LEU	N	-33.38	-19.50	78.54	15.00
46	LEU	CA	-32.33	-18.54	78.81	15.00
46	LEU	CB	-31.43	-19.09	79.91	15.00
46	LEU	CG	-30.45	-18.17	80.63	15.00
46	LEU	CD1	-31.17	-16.89	81.03	15.00
46	LEU	CD2	-29.91	-18.88	81.84	15.00
46	LEU	C	-31.55	-18.33	77.51	15.00
46	LEU	O	-31.62	-19.14	76.60	15.00
47	ASN	N	-30.84	-17.22	77.39	15.00
47	ASN	CA	-30.04	-16.97	76.20	15.00
47	ASN	CB	-30.04	-15.48	75.85	15.00
47	ASN	CG	-31.37	-15.02	75.33	15.00
47	ASN	OD1	-32.19	-14.49	76.08	15.00
47	ASN	ND2	-31.59	-15.20	74.05	15.00
47	ASN	C	-28.62	-17.42	76.46	15.00
47	ASN	O	-27.96	-16.92	77.37	15.00
48	LEU	N	-28.15	-18.40	75.69	15.00
48	LEU	CA	-26.80	-18.91	75.86	15.00
48	LEU	CB	-26.74	-20.39	75.53	15.00
48	LEU	CG	-27.64	-21.29	76.40	15.00
48	LEU	CD1	-27.37	-22.73	76.07	15.00
48	LEU	CD2	-27.39	-21.05	77.86	15.00
48	LEU	C	-25.79	-18.10	75.06	15.00
48	LEU	O	-26.16	-17.33	74.17	15.00
49	SER	N	-24.51	-18.27	75.36	15.00
49	SER	CA	-23.45	-17.50	74.71	15.00
49	SER	CB	-22.34	-17.20	75.73	15.00
49	SER	OG	-21.21	-16.57	75.14	15.00
49	SER	C	-22.81	-18.05	73.44	15.00
49	SER	O	-22.00	-18.98	73.49	15.00
50	PRO	N	-23.17	-17.49	72.28	15.00
50	PRO	CD	-24.25	-16.53	71.99	15.00
50	PRO	CA	-22.56	-17.98	71.04	15.00
50	PRO	CB	-23.40	-17.29	69.95	15.00
50	PRO	CG	-23.89	-16.05	70.62	15.00
50	PRO	C	-21.10	-17.55	71.00	15.00
50	PRO	O	-20.25	-18.21	70.41	15.00
51	GLN	N	-20.79	-16.45	71.69	15.00
51	GLN	CA	-19.43	-15.93	71.75	15.00
51	GLN	CB	-19.40	-14.60	72.52	15.00
51	GLN	CG	-18.07	-13.86	72.44	15.00
51	GLN	CD	-17.86	-13.13	71.13	15.00

TABLE II

51	GLN	OE1	-18.70	-12.34	70.70	15.00
51	GLN	NE2	-16.72	-13.37	70.49	15.00
51	GLN	C	-18.52	-16.94	72.44	15.00
51	GLN	O	-17.43	-17.24	71.95	15.00
52	ASN	N	-18.97	-17.50	73.56	15.00
52	ASN	CA	-18.21	-18.49	74.31	15.00
52	ASN	CB	-19.13	-19.10	75.38	15.00
52	ASN	CG	-18.41	-20.00	76.37	15.00
52	ASN	OD1	-18.80	-20.05	77.53	15.00
52	ASN	ND2	-17.40	-20.73	75.93	15.00
52	ASN	C	-17.77	-19.57	73.34	15.00
52	ASN	O	-16.66	-20.11	73.43	15.00
53	LEU	N	-18.65	-19.89	72.39	15.00
53	LEU	CA	-18.37	-20.90	71.39	15.00
53	LEU	CB	-19.67	-21.37	70.73	15.00
53	LEU	CG	-20.66	-22.13	71.63	15.00
53	LEU	CD1	-21.88	-22.54	70.82	15.00
53	LEU	CD2	-20.00	-23.35	72.23	15.00
53	LEU	C	-17.40	-20.39	70.35	15.00
53	LEU	O	-16.45	-21.09	69.98	15.00
54	VAL	N	-17.59	-19.15	69.91	15.00
54	VAL	CA	-16.73	-18.54	68.89	15.00
54	VAL	CB	-17.24	-17.11	68.51	15.00
54	VAL	CG1	-16.31	-16.45	67.49	15.00
54	VAL	CG2	-18.63	-17.19	67.92	15.00
54	VAL	C	-15.27	-18.47	69.36	15.00
54	VAL	O	-14.36	-18.89	68.64	15.00
55	ASP	N	-15.06	-17.98	70.58	15.00
55	ASP	CA	-13.73	-17.83	71.15	15.00
55	ASP	CB	-13.78	-16.81	72.29	15.00
55	ASP	CG	-14.32	-15.46	71.87	15.00
55	ASP	OD1	-14.20	-15.10	70.68	15.00
55	ASP	OD2	-14.86	-14.76	72.75	15.00
55	ASP	C	-13.05	-19.09	71.70	15.00
55	ASP	O	-11.81	-19.13	71.78	15.00
56	CYS	N	-13.81	-20.12	72.07	15.00
56	CYS	CA	-13.22	-21.32	72.67	15.00
56	CYS	C	-13.29	-22.63	71.91	15.00
56	CYS	O	-12.56	-23.59	72.23	15.00
56	CYS	CB	-13.83	-21.53	74.05	15.00
56	CYS	SG	-14.01	-20.02	75.04	15.00
57	VAL	N	-14.19	-22.77	70.96	15.00

TABLE II

57	VAL	CA	-14.26	-24.02	70.22	15.00
57	VAL	CB	-15.60	-24.16	69.48	15.00
57	VAL	CG1	-15.62	-25.44	68.67	15.00
57	VAL	CG2	-16.73	-24.15	70.48	15.00
57	VAL	C	-13.09	-24.06	69.25	15.00
57	VAL	O	-13.23	-23.80	68.06	15.00
58	SER	N	-11.91	-24.40	69.77	15.00
58	SER	CA	-10.67	-24.46	69.00	15.00
58	SER	CB	-9.53	-24.83	69.93	15.00
58	SER	OG	-10.02	-25.66	70.98	15.00
58	SER	C	-10.66	-25.38	67.79	15.00
58	SER	O	-9.70	-25.38	67.02	15.00
59	GLU	N	-11.70	-26.18	67.64	15.00
59	GLU	CA	-11.82	-27.10	66.50	15.00
59	GLU	CB	-12.70	-28.31	66.86	15.00
59	GLU	CG	-12.16	-29.19	67.99	15.00
59	GLU	CD	-12.31	-28.56	69.36	15.00
59	GLU	OE1	-13.46	-28.38	69.83	15.00
59	GLU	OE2	-11.28	-28.23	69.97	15.00
59	GLU	C	-12.44	-26.34	65.33	15.00
59	GLU	O	-12.44	-26.81	64.19	15.00
60	ASN	N	-13.03	-25.19	65.61	15.00
60	ASN	CA	-13.64	-24.37	64.58	15.00
60	ASN	CB	-15.08	-23.98	64.97	15.00
60	ASN	CG	-16.03	-25.16	64.95	15.00
60	ASN	OD1	-17.08	-25.12	65.58	15.00
60	ASN	ND2	-15.68	-26.20	64.22	15.00
60	ASN	C	-12.79	-23.12	64.31	15.00
60	ASN	O	-11.88	-22.80	65.06	15.00
61	ASP	N	-13.13	-22.40	63.25	15.00
61	ASP	CA	-12.38	-21.21	62.87	15.00
61	ASP	CB	-12.30	-21.14	61.34	15.00
61	ASP	CG	-10.95	-20.64	60.84	15.00
61	ASP	OD1	-10.04	-20.40	61.65	15.00
61	ASP	OD2	-10.80	-20.50	59.60	15.00
61	ASP	C	-12.97	-19.91	63.44	15.00
61	ASP	O	-12.70	-18.83	62.93	15.00
62	GLY	N	-13.78	-19.99	64.49	15.00
62	GLY	CA	-14.37	-18.79	65.05	15.00
62	GLY	C	-15.25	-18.07	64.05	15.00
62	GLY	O	-16.26	-18.59	63.58	15.00
63	CYS	N	-14.89	-16.85	63.70	15.00

TABLE II

63	CYS	CA	-15.67	-16.11	62.72	15.00
63	CYS	C	-15.48	-16.70	61.33	15.00
63	CYS	O	-16.15	-16.28	60.39	15.00
63	CYS	CB	-15.30	-14.62	62.69	15.00
63	CYS	SG	-15.85	-13.63	64.12	15.00
64	GLY	N	-14.54	-17.62	61.19	15.00
64	GLY	CA	-14.29	-18.25	59.90	15.00
64	GLY	C	-15.24	-19.41	59.67	15.00
64	GLY	O	-15.32	-19.97	58.57	15.00
65	GLY	N	-15.97	-19.80	60.70	15.00
65	GLY	CA	-16.91	-20.91	60.56	15.00
65	GLY	C	-16.55	-22.16	61.33	15.00
65	GLY	O	-15.46	-22.30	61.90	15.00
66	GLY	N	-17.47	-23.10	61.38	15.00
66	GLY	CA	-17.25	-24.34	62.07	15.00
66	GLY	C	-18.51	-25.15	61.93	15.00
66	GLY	O	-19.46	-24.72	61.29	15.00
67	TYR	N	-18.50	-26.35	62.49	15.00
67	TYR	CA	-19.66	-27.22	62.44	15.00
67	TYR	CB	-19.25	-28.66	62.13	15.00
67	TYR	CG	-18.41	-28.83	60.89	15.00
67	TYR	CD1	-19.00	-29.00	59.64	15.00
67	TYR	CE1	-18.22	-29.18	58.51	15.00
67	TYR	CD2	-17.03	-28.83	60.98	15.00
67	TYR	CE2	-16.25	-29.01	59.86	15.00
67	TYR	CZ	-16.84	-29.18	58.63	15.00
67	TYR	OH	-16.03	-29.34	57.52	15.00
67	TYR	C	-20.27	-27.16	63.83	15.00
67	TYR	O	-19.59	-26.85	64.80	15.00
68	MET	N	-21.55	-27.48	63.93	15.00
68	MET	CA	-22.24	-27.45	65.20	15.00
68	MET	CB	-23.75	-27.51	65.00	15.00
68	MET	CG	-24.34	-26.31	64.22	15.00
68	MET	SD	-23.95	-26.25	62.46	15.00
68	MET	CE	-25.40	-26.96	61.77	15.00
68	MET	C	-21.76	-28.58	66.11	15.00
68	MET	O	-21.49	-28.37	67.29	15.00
69	THR	N	-21.57	-29.78	65.56	15.00
69	THR	CA	-21.13	-30.94	66.33	15.00
69	THR	CB	-20.92	-32.18	65.44	15.00
69	THR	OG1	-20.10	-31.83	64.31	15.00
69	THR	CG2	-22.26	-32.69	64.93	15.00

TABLE II

69	THR	C	-19.85	-30.65	67.12	15.00
69	THR	O	-19.69	-31.11	68.26	15.00
70	ASN	N	-18.95	-29.84	66.55	15.00
70	ASN	CA	-17.71	-29.46	67.22	15.00
70	ASN	CB	-16.73	-28.81	66.24	15.00
70	ASN	CG	-15.97	-29.81	65.39	15.00
70	ASN	OD1	-15.41	-29.45	64.37	15.00
70	ASN	ND2	-15.92	-31.06	65.83	15.00
70	ASN	C	-17.96	-28.52	68.39	15.00
70	ASN	O	-17.14	-28.42	69.30	15.00
71	ALA	N	-19.06	-27.78	68.35	15.00
71	ALA	CA	-19.42	-26.86	69.44	15.00
71	ALA	CB	-20.32	-25.76	68.92	15.00
71	ALA	C	-20.12	-27.66	70.53	15.00
71	ALA	O	-19.94	-27.42	71.73	15.00
72	PHE	N	-20.96	-28.60	70.13	15.00
72	PHE	CA	-21.67	-29.44	71.08	15.00
72	PHE	CB	-22.56	-30.44	70.34	15.00
72	PHE	CG	-23.74	-29.82	69.63	15.00
72	PHE	CD1	-24.33	-28.66	70.11	15.00
72	PHE	CD2	-24.27	-30.43	68.50	15.00
72	PHE	CE1	-25.45	-28.12	69.48	15.00
72	PHE	CE2	-25.39	-29.90	67.87	15.00
72	PHE	CZ	-25.98	-28.74	68.35	15.00
72	PHE	C	-20.60	-30.19	71.89	15.00
72	PHE	O	-20.60	-30.15	73.12	15.00
73	GLN	N	-19.64	-30.81	71.21	15.00
73	GLN	CA	-18.58	-31.56	71.87	15.00
73	GLN	CB	-17.64	-32.18	70.82	15.00
73	GLN	CG	-16.55	-33.13	71.36	15.00
73	GLN	CD	-17.07	-34.54	71.69	15.00
73	GLN	OE1	-17.16	-34.93	72.87	15.00
73	GLN	NE2	-17.37	-35.32	70.65	15.00
73	GLN	C	-17.81	-30.69	72.87	15.00
73	GLN	O	-17.46	-31.13	73.96	15.00
74	TYR	N	-17.55	-29.43	72.53	15.00
74	TYR	CA	-16.82	-28.56	73.44	15.00
74	TYR	CB	-16.43	-27.25	72.75	15.00
74	TYR	CG	-16.11	-26.12	73.70	15.00
74	TYR	CD1	-14.83	-25.93	74.20	15.00
74	TYR	CE1	-14.54	-24.93	75.11	15.00
74	TYR	CD2	-17.11	-25.25	74.14	15.00

TABLE II

74	TYR	CE2	-16.84	-24.23	75.06	15.00
74	TYR	CZ	-15.55	-24.08	75.53	15.00
74	TYR	OH	-15.28	-23.08	76.45	15.00
74	TYR	C	-17.62	-28.25	74.70	15.00
74	TYR	O	-17.05	-28.00	75.76	15.00
75	VAL	N	-18.94	-28.18	74.59	15.00
75	VAL	CA	-19.77	-27.89	75.75	15.00
75	VAL	CB	-21.21	-27.54	75.33	15.00
75	VAL	CG1	-22.04	-27.14	76.54	15.00
75	VAL	CG2	-21.20	-26.39	74.33	15.00
75	VAL	C	-19.74	-29.11	76.68	15.00
75	VAL	O	-19.87	-28.99	77.90	15.00
76	GLN	N	-19.50	-30.29	76.09	15.00
76	GLN	CA	-19.43	-31.54	76.84	15.00
76	GLN	CB	-19.51	-32.72	75.88	15.00
76	GLN	CG	-19.44	-34.10	76.53	15.00
76	GLN	CD	-19.41	-35.21	75.50	15.00
76	GLN	OE1	-20.45	-35.67	75.05	15.00
76	GLN	NE2	-18.23	-35.64	75.12	15.00
76	GLN	C	-18.15	-31.64	77.66	15.00
76	GLN	O	-18.20	-31.71	78.89	15.00
77	LYS	N	-17.00	-31.64	77.00	15.00
77	LYS	CA	-15.72	-31.75	77.70	15.00
77	LYS	CB	-14.60	-32.13	76.73	15.00
77	LYS	CG	-14.72	-31.53	75.36	15.00
77	LYS	CD	-13.52	-31.92	74.50	15.00
77	LYS	CE	-13.77	-31.61	73.03	15.00
77	LYS	NZ	-14.25	-30.21	72.83	15.00
77	LYS	C	-15.29	-30.55	78.56	15.00
77	LYS	O	-14.36	-30.63	79.36	15.00
78	ASN	N	-15.94	-29.41	78.38	15.00
78	ASN	CA	-15.62	-28.22	79.15	15.00
78	ASN	CB	-15.75	-26.98	78.27	15.00
78	ASN	CG	-15.54	-25.69	79.03	15.00
78	ASN	OD1	-14.43	-25.40	79.46	15.00
78	ASN	ND2	-16.60	-24.91	79.16	15.00
78	ASN	C	-16.60	-28.14	80.32	15.00
78	ASN	O	-16.47	-27.32	81.22	15.00
79	ARG	N	-17.60	-29.01	80.27	15.00
79	ARG	CA	-18.63	-29.08	81.29	15.00
79	ARG	CB	-18.06	-29.64	82.60	15.00
79	ARG	CG	-17.45	-31.04	82.42	15.00

TABLE II

79	ARG	CD	-17.13	-31.71	83.75	15.00
79	ARG	NE	-18.34	-32.20	84.40	15.00
79	ARG	CZ	-18.91	-33.37	84.15	15.00
79	ARG	NH1	-18.36	-34.20	83.26	15.00
79	ARG	NH2	-20.05	-33.70	84.75	15.00
79	ARG	C	-19.36	-27.77	81.50	15.00
79	ARG	O	-19.57	-27.33	82.64	15.00
80	GLY	N	-19.75	-27.14	80.39	15.00
80	GLY	CA	-20.48	-25.89	80.49	15.00
80	GLY	C	-20.34	-24.84	79.40	15.00
80	GLY	O	-19.34	-24.78	78.67	15.00
81	ILE	N	-21.39	-24.02	79.30	15.00
81	ILE	CA	-21.46	-22.91	78.36	15.00
81	ILE	CB	-22.22	-23.28	77.05	15.00
81	ILE	CG2	-23.65	-23.63	77.33	15.00
81	ILE	CG1	-22.16	-22.09	76.08	15.00
81	ILE	CD1	-22.80	-22.35	74.75	15.00
81	ILE	C	-22.15	-21.75	79.07	15.00
81	ILE	O	-23.20	-21.93	79.71	15.00
82	ASP	N	-21.51	-20.59	79.03	15.00
82	ASP	CA	-22.01	-19.37	79.65	15.00
82	ASP	CB	-20.99	-18.24	79.46	15.00
82	ASP	CG	-19.78	-18.37	80.35	15.00
82	ASP	OD1	-18.71	-17.88	79.95	15.00
82	ASP	OD2	-19.91	-18.93	81.47	15.00
82	ASP	C	-23.36	-18.86	79.13	15.00
82	ASP	O	-23.86	-19.29	78.09	15.00
83	SER	N	-23.91	-17.90	79.86	15.00
83	SER	CA	-25.16	-17.25	79.50	15.00
83	SER	CB	-25.99	-16.98	80.76	15.00
83	SER	OG	-25.21	-16.38	81.78	15.00
83	SER	C	-24.75	-15.93	78.85	15.00
83	SER	O	-23.63	-15.45	79.05	15.00
84	GLU	N	-25.64	-15.33	78.07	15.00
84	GLU	CA	-25.32	-14.09	77.39	15.00
84	GLU	CB	-26.48	-13.65	76.52	15.00
84	GLU	CG	-26.16	-12.52	75.57	15.00
84	GLU	CD	-25.34	-12.95	74.38	15.00
84	GLU	OE1	-24.85	-14.10	74.35	15.00
84	GLU	OE2	-25.19	-12.13	73.45	15.00
84	GLU	C	-24.88	-12.96	78.31	15.00
84	GLU	O	-24.03	-12.14	77.94	15.00

TABLE II

85	ASP	N	-25.44	-12.87	79.52	15.00
85	ASP	CA	-25.03	-11.81	80.45	15.00
85	ASP	CB	-25.92	-11.77	81.71	15.00
85	ASP	CG	-25.48	-10.69	82.73	15.00
85	ASP	OD1	-24.60	-9.85	82.41	15.00
85	ASP	OD2	-26.00	-10.66	83.87	15.00
85	ASP	C	-23.59	-12.02	80.86	15.00
85	ASP	O	-22.83	-11.07	81.00	15.00
86	ALA	N	-23.18	-13.27	81.05	15.00
86	ALA	CA	-21.82	-13.56	81.47	15.00
86	ALA	CB	-21.76	-14.91	82.14	15.00
86	ALA	C	-20.78	-13.48	80.36	15.00
86	ALA	O	-19.62	-13.15	80.59	15.00
87	TYR	N	-21.18	-13.74	79.12	15.00
87	TYR	CA	-20.23	-13.71	78.02	15.00
87	TYR	CB	-19.79	-15.15	77.74	15.00
87	TYR	CG	-18.44	-15.33	77.08	15.00
87	TYR	CD1	-17.91	-14.37	76.21	15.00
87	TYR	CE1	-16.69	-14.59	75.57	15.00
87	TYR	CD2	-17.72	-16.51	77.28	15.00
87	TYR	CE2	-16.50	-16.73	76.64	15.00
87	TYR	CZ	-16.00	-15.77	75.79	15.00
87	TYR	OH	-14.79	-16.02	75.16	15.00
87	TYR	C	-20.92	-13.13	76.79	15.00
87	TYR	O	-21.26	-13.88	75.86	15.00
88	PRO	N	-21.19	-11.80	76.79	15.00
88	PRO	CD	-21.02	-10.93	77.96	15.00
88	PRO	CA	-21.85	-11.07	75.70	15.00
88	PRO	CB	-21.91	-9.64	76.23	15.00
88	PRO	CG	-22.06	-9.86	77.72	15.00
88	PRO	C	-21.13	-11.13	74.36	15.00
88	PRO	O	-19.90	-11.11	74.31	15.00
89	TYR	N	-21.93	-11.18	73.31	15.00
89	TYR	CA	-21.47	-11.28	71.92	15.00
89	TYR	CB	-22.64	-11.80	71.09	15.00
89	TYR	CG	-22.28	-12.14	69.68	15.00
89	TYR	CD1	-21.43	-13.20	69.39	15.00
89	TYR	CE1	-21.07	-13.48	68.09	15.00
89	TYR	CD2	-22.75	-11.36	68.63	15.00
89	TYR	CE2	-22.39	-11.63	67.32	15.00
89	TYR	CZ	-21.55	-12.69	67.06	15.00
89	TYR	OH	-21.15	-12.93	65.77	15.00

TABLE II

89	TYR	C	-20.94	-9.96	71.34	15.00
89	TYR	O	-21.71	-9.04	71.08	15.00
90	VAL	N	-19.64	-9.86	71.12	15.00
90	VAL	CA	-19.06	-8.63	70.58	15.00
90	VAL	CB	-17.75	-8.27	71.27	15.00
90	VAL	CG1	-17.98	-8.12	72.76	15.00
90	VAL	CG2	-16.69	-9.32	70.99	15.00
90	VAL	C	-18.87	-8.65	69.07	15.00
90	VAL	O	-18.28	-7.74	68.50	15.00
91	GLY	N	-19.30	-9.73	68.44	15.00
91	GLY	CA	-19.20	-9.84	67.00	15.00
91	GLY	C	-17.86	-10.11	66.36	15.00
91	GLY	O	-17.67	-9.84	65.18	15.00
92	GLN	N	-16.91	-10.66	67.11	15.00
92	GLN	CA	-15.59	-10.97	66.57	15.00
92	GLN	CB	-14.80	-9.69	66.32	15.00
92	GLN	CG	-14.73	-8.76	67.51	15.00
92	GLN	CD	-13.95	-7.50	67.19	15.00
92	GLN	OE1	-12.73	-7.54	67.06	15.00
92	GLN	NE2	-14.65	-6.38	67.02	15.00
92	GLN	C	-14.83	-11.87	67.53	15.00
92	GLN	O	-15.17	-11.94	68.71	15.00
93	GLU	N	-13.80	-12.53	67.04	15.00
93	GLU	CA	-13.02	-13.45	67.85	15.00
93	GLU	CB	-12.36	-14.52	66.98	15.00
93	GLU	CG	-11.54	-13.97	65.80	15.00
93	GLU	CD	-11.57	-14.90	64.59	15.00
93	GLU	OE1	-10.51	-15.16	63.98	15.00
93	GLU	OE2	-12.67	-15.36	64.22	15.00
93	GLU	C	-11.99	-12.78	68.74	15.00
93	GLU	O	-11.29	-11.86	68.33	15.00
94	GLU	N	-11.89	-13.29	69.97	15.00
94	GLU	CA	-10.96	-12.78	70.96	15.00
94	GLU	CB	-11.65	-11.74	71.84	15.00
94	GLU	CG	-12.68	-12.34	72.79	15.00
94	GLU	CD	-13.96	-11.54	72.88	15.00
94	GLU	OE1	-13.96	-10.36	72.44	15.00
94	GLU	OE2	-14.97	-12.08	73.38	15.00
94	GLU	C	-10.54	-13.98	71.82	15.00
94	GLU	O	-10.95	-15.10	71.55	15.00
95	SER	N	-9.72	-13.74	72.84	15.00
95	SER	CA	-9.26	-14.80	73.73	15.00

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TABLE II

95	SER	CB	-8.26	-14.23	74.75	15.00
95	SER	OG	-7.14	-13.65	74.09	15.00
95	SER	C	-10.41	-15.51	74.46	15.00
95	SER	O	-11.34	-14.87	74.95	15.00
96	CYS	N	-10.37	-16.84	74.53	15.00
96	CYS	CA	-11.44	-17.57	75.21	15.00
96	CYS	C	-11.55	-17.03	76.62	15.00
96	CYS	O	-10.58	-17.04	77.37	15.00
96	CYS	CB	-11.13	-19.06	75.26	15.00
96	CYS	SG	-12.35	-20.02	76.20	15.00
97	MET	N	-12.72	-16.51	76.97	15.00
97	MET	CA	-12.95	-15.95	78.31	15.00
97	MET	CB	-13.50	-14.53	78.21	15.00
97	MET	CG	-12.65	-13.51	77.52	15.00
97	MET	SD	-13.49	-11.94	77.83	15.00
97	MET	CE	-14.95	-12.05	76.75	15.00
97	MET	C	-13.95	-16.74	79.15	15.00
97	MET	O	-14.60	-16.15	80.02	15.00
98	TYR	N	-14.08	-18.05	78.94	15.00
98	TYR	CA	-15.05	-18.82	79.70	15.00
98	TYR	CB	-14.89	-20.33	79.47	15.00
98	TYR	CG	-15.95	-21.14	80.19	15.00
98	TYR	CD1	-17.30	-21.01	79.88	15.00
98	TYR	CE1	-18.28	-21.71	80.58	15.00
98	TYR	CD2	-15.61	-22.00	81.23	15.00
98	TYR	CE2	-16.58	-22.70	81.94	15.00
98	TYR	CZ	-17.91	-22.55	81.62	15.00
98	TYR	OH	-18.86	-23.22	82.33	15.00
98	TYR	C	-14.99	-18.51	81.20	15.00
98	TYR	O	-13.92	-18.32	81.77	15.00
99	ASN	N	-16.16	-18.49	81.82	15.00
99	ASN	CA	-16.30	-18.18	83.23	15.00
99	ASN	CB	-16.73	-16.72	83.37	15.00
99	ASN	CG	-17.06	-16.32	84.81	15.00
99	ASN	OD1	-16.96	-17.13	85.74	15.00
99	ASN	ND2	-17.47	-15.06	84.98	15.00
99	ASN	C	-17.34	-19.10	83.86	15.00
99	ASN	O	-18.55	-18.87	83.72	15.00
100	PRO	N	-16.89	-20.13	84.60	15.00
100	PRO	CD	-15.46	-20.39	84.86	15.00
100	PRO	CA	-17.73	-21.12	85.29	15.00
100	PRO	CB	-16.74	-21.80	86.22	15.00

TABLE II

100	PRO	CG	-15.49	-21.81	85.41	15.00
100	PRO	C	-18.84	-20.46	86.07	15.00
100	PRO	O	-19.93	-21.02	86.20	15.00
101	THR	N	-18.58	-19.26	86.58	15.00
101	THR	CA	-19.58	-18.53	87.34	15.00
101	THR	CB	-18.99	-17.20	87.84	15.00
101	THR	OG1	-17.76	-17.48	88.53	15.00
101	THR	CG2	-19.95	-16.50	88.80	15.00
101	THR	C	-20.78	-18.25	86.46	15.00
101	THR	O	-21.93	-18.29	86.93	15.00
102	GLY	N	-20.52	-17.99	85.18	15.00
102	GLY	CA	-21.57	-17.69	84.23	15.00
102	GLY	C	-22.29	-18.89	83.62	15.00
102	GLY	O	-23.36	-18.73	83.04	15.00
103	LYS	N	-21.70	-20.07	83.72	15.00
103	LYS	CA	-22.30	-21.29	83.17	15.00
103	LYS	CB	-21.60	-22.52	83.76	15.00
103	LYS	CG	-22.34	-23.84	83.55	15.00
103	LYS	CD	-21.59	-24.99	84.23	15.00
103	LYS	CE	-22.56	-26.02	84.79	15.00
103	LYS	NZ	-23.48	-26.58	83.76	15.00
103	LYS	C	-23.81	-21.37	83.41	15.00
103	LYS	O	-24.27	-21.24	84.54	15.00
104	ALA	N	-24.58	-21.60	82.35	15.00
104	ALA	CA	-26.04	-21.70	82.45	15.00
104	ALA	CB	-26.69	-20.52	81.78	15.00
104	ALA	C	-26.60	-22.99	81.88	15.00
104	ALA	O	-27.76	-23.32	82.12	15.00
105	ALA	N	-25.81	-23.71	81.09	15.00
105	ALA	CA	-26.26	-24.97	80.50	15.00
105	ALA	CB	-26.99	-24.72	79.19	15.00
105	ALA	C	-25.10	-25.92	80.28	15.00
105	ALA	O	-23.93	-25.52	80.38	15.00
106	LYS	N	-25.41	-27.18	79.98	15.00
106	LYS	CA	-24.40	-28.19	79.72	15.00
106	LYS	CB	-23.77	-28.66	81.03	15.00
106	LYS	CG	-24.73	-29.25	82.04	15.00
106	LYS	CD	-24.01	-29.56	83.33	15.00
106	LYS	CE	-22.75	-30.37	83.07	15.00
106	LYS	NZ	-23.05	-31.63	82.31	15.00
106	LYS	C	-25.06	-29.34	78.99	15.00
106	LYS	O	-26.28	-29.39	78.94	15.00

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TABLE II

107	CYS	N	-24.27	-30.21	78.38	15.00
107	CYS	CA	-24.83	-31.36	77.65	15.00
107	CYS	CB	-25.14	-30.97	76.20	15.00
107	CYS	SG	-23.71	-31.01	75.11	15.00
107	CYS	C	-23.95	-32.61	77.67	15.00
107	CYS	O	-22.73	-32.53	77.81	15.00
108	ARG	N	-24.59	-33.76	77.53	15.00
108	ARG	CA	-23.92	-35.05	77.54	15.00
108	ARG	CB	-24.66	-36.03	78.46	15.00
108	ARG	CG	-26.18	-35.81	78.55	15.00
108	ARG	CD	-26.93	-37.01	79.17	15.00
108	ARG	NE	-27.06	-38.15	78.25	15.00
108	ARG	CZ	-28.19	-38.49	77.62	15.00
108	ARG	NH1	-29.31	-37.79	77.80	15.00
108	ARG	NH2	-28.22	-39.56	76.84	15.00
108	ARG	C	-23.70	-35.67	76.15	15.00
108	ARG	O	-23.77	-36.88	75.98	15.00
109	GLY	N	-23.44	-34.83	75.16	15.00
109	GLY	CA	-23.19	-35.32	73.82	15.00
109	GLY	C	-24.08	-34.73	72.75	15.00
109	GLY	O	-24.72	-33.69	72.94	15.00
110	TYR	N	-24.15	-35.41	71.61	15.00
110	TYR	CA	-24.97	-34.95	70.50	15.00
110	TYR	CB	-24.19	-33.91	69.71	15.00
110	TYR	CG	-22.97	-34.46	68.99	15.00
110	TYR	CD1	-21.71	-34.43	69.59	15.00
110	TYR	CE1	-20.59	-34.90	68.91	15.00
110	TYR	CD2	-23.07	-34.99	67.71	15.00
110	TYR	CE2	-21.97	-35.45	67.03	15.00
110	TYR	CZ	-20.73	-35.40	67.63	15.00
110	TYR	OH	-19.63	-35.82	66.93	15.00
110	TYR	C	-25.31	-36.11	69.57	15.00
110	TYR	O	-24.61	-37.12	69.54	15.00
111	ARG	N	-26.35	-35.94	68.76	15.00
111	ARG	CA	-26.74	-36.97	67.82	15.00
111	ARG	CB	-28.02	-37.68	68.29	15.00
111	ARG	CG	-27.87	-38.44	69.61	15.00
111	ARG	CD	-29.17	-39.16	70.00	15.00
111	ARG	NE	-29.49	-40.25	69.07	15.00
111	ARG	CZ	-28.84	-41.41	69.03	15.00
111	ARG	NH1	-29.20	-42.34	68.14	15.00
111	ARG	NH2	-27.85	-41.65	69.88	15.00

TABLE II

111	ARG	C	-27.00	-36.34	66.45	15.00
111	ARG	O	-27.71	-35.34	66.34	15.00
112	GLU	N	-26.39	-36.90	65.42	15.00
112	GLU	CA	-26.57	-36.42	64.06	15.00
112	GLU	CB	-25.27	-36.56	63.27	15.00
112	GLU	CG	-24.17	-35.62	63.74	15.00
112	GLU	CD	-22.80	-35.91	63.12	15.00
112	GLU	OE1	-22.22	-34.99	62.47	15.00
112	GLU	OE2	-22.29	-37.05	63.30	15.00
112	GLU	C	-27.68	-37.26	63.45	15.00
112	GLU	O	-27.84	-38.43	63.80	15.00
113	ILE	N	-28.50	-36.63	62.61	15.00
113	ILE	CA	-29.60	-37.28	61.90	15.00
113	ILE	CB	-30.69	-36.23	61.48	15.00
113	ILE	CG2	-31.45	-36.68	60.25	15.00
113	ILE	CG1	-31.68	-35.99	62.62	15.00
113	ILE	CD1	-31.14	-35.16	63.73	15.00
113	ILE	C	-29.00	-37.94	60.66	15.00
113	ILE	O	-28.03	-37.44	60.10	15.00
114	PRO	N	-29.54	-39.09	60.23	15.00
114	PRO	CD	-30.62	-39.89	60.83	15.00
114	PRO	CA	-29.00	-39.75	59.04	15.00
114	PRO	CB	-30.00	-40.89	58.81	15.00
114	PRO	CG	-30.41	-41.24	60.19	15.00
114	PRO	C	-28.97	-38.80	57.86	15.00
114	PRO	O	-29.98	-38.20	57.52	15.00
115	GLU	N	-27.80	-38.73	57.22	15.00
115	GLU	CA	-27.56	-37.86	56.07	15.00
115	GLU	CB	-26.14	-38.07	55.52	15.00
115	GLU	CG	-25.92	-37.52	54.10	15.00
115	GLU	CD	-24.48	-37.06	53.82	15.00
115	GLU	OE1	-23.52	-37.73	54.28	15.00
115	GLU	OE2	-24.30	-36.02	53.15	15.00
115	GLU	C	-28.55	-38.00	54.93	15.00
115	GLU	O	-28.57	-39.02	54.26	15.00
116	GLY	N	-29.31	-36.94	54.69	15.00
116	GLY	CA	-30.27	-36.94	53.60	15.00
116	GLY	C	-31.66	-37.41	53.97	15.00
116	GLY	O	-32.57	-37.40	53.14	15.00
117	ASN	N	-31.86	-37.78	55.24	15.00
117	ASN	CA	-33.15	-38.29	55.69	15.00
117	ASN	CB	-32.94	-39.38	56.73	15.00

TABLE II

117	ASN	CG	-34.19	-40.18	56.99	15.00
117	ASN	OD1	-35.32	-39.68	56.89	15.00
117	ASN	ND2	-34.00	-41.46	57.33	15.00
117	ASN	C	-34.07	-37.22	56.27	15.00
117	ASN	O	-33.93	-36.82	57.43	15.00
118	GLU	N	-35.06	-36.79	55.50	15.00
118	GLU	CA	-35.97	-35.78	55.99	15.00
118	GLU	CB	-36.70	-35.07	54.85	15.00
118	GLU	CG	-36.04	-33.77	54.42	15.00
118	GLU	CD	-36.91	-32.99	53.45	15.00
118	GLU	OE1	-36.81	-33.22	52.23	15.00
118	GLU	OE2	-37.72	-32.15	53.91	15.00
118	GLU	C	-36.97	-36.33	56.98	15.00
118	GLU	O	-37.46	-35.59	57.83	15.00
119	LYS	N	-37.32	-37.61	56.90	15.00
119	LYS	CA	-38.27	-38.14	57.87	15.00
119	LYS	CB	-38.85	-39.49	57.42	15.00
119	LYS	CG	-40.19	-39.34	56.68	15.00
119	LYS	CD	-40.08	-38.40	55.47	15.00
119	LYS	CE	-41.47	-38.06	54.90	15.00
119	LYS	NZ	-42.26	-37.19	55.83	15.00
119	LYS	C	-37.62	-38.24	59.24	15.00
119	LYS	O	-38.23	-37.90	60.26	15.00
120	ALA	N	-36.35	-38.62	59.28	15.00
120	ALA	CA	-35.63	-38.70	60.54	15.00
120	ALA	CB	-34.25	-39.25	60.33	15.00
120	ALA	C	-35.55	-37.30	61.16	15.00
120	ALA	O	-35.58	-37.15	62.38	15.00
121	LEU	N	-35.45	-36.27	60.32	15.00
121	LEU	CA	-35.38	-34.89	60.82	15.00
121	LEU	CB	-34.93	-33.91	59.73	15.00
121	LEU	CG	-34.80	-32.45	60.19	15.00
121	LEU	CD1	-33.77	-32.34	61.30	15.00
121	LEU	CD2	-34.42	-31.56	59.03	15.00
121	LEU	C	-36.74	-34.48	61.36	15.00
121	LEU	O	-36.83	-33.80	62.38	15.00
122	LYS	N	-37.79	-34.89	60.66	15.00
122	LYS	CA	-39.16	-34.58	61.05	15.00
122	LYS	CB	-40.14	-35.19	60.07	15.00
122	LYS	CG	-41.57	-34.80	60.31	15.00
122	LYS	CD	-42.49	-35.45	59.32	15.00
122	LYS	CE	-43.95	-35.16	59.67	15.00

TABLE II

122	LYS	NZ	-44.88	-35.66	58.60	15.00
122	LYS	C	-39.41	-35.15	62.44	15.00
122	LYS	O	-39.87	-34.44	63.33	15.00
123	ARG	N	-39.12	-36.44	62.62	15.00
123	ARG	CA	-39.29	-37.10	63.90	15.00
123	ARG	CB	-38.84	-38.58	63.84	15.00
123	ARG	CG	-39.74	-39.50	62.99	15.00
123	ARG	CD	-39.33	-40.97	63.13	15.00
123	ARG	NE	-37.95	-41.22	62.73	15.00
123	ARG	CZ	-37.42	-42.43	62.51	15.00
123	ARG	NH1	-38.15	-43.53	62.66	15.00
123	ARG	NH2	-36.17	-42.53	62.08	15.00
123	ARG	C	-38.46	-36.37	64.94	15.00
123	ARG	O	-39.01	-35.82	65.89	15.00
124	ALA	N	-37.15	-36.31	64.71	15.00
124	ALA	CA	-36.22	-35.65	65.62	15.00
124	ALA	CB	-34.86	-35.50	64.98	15.00
124	ALA	C	-36.70	-34.29	66.11	15.00
124	ALA	O	-36.67	-34.02	67.31	15.00
125	VAL	N	-37.16	-33.45	65.19	15.00
125	VAL	CA	-37.66	-32.13	65.55	15.00
125	VAL	CB	-38.00	-31.28	64.27	15.00
125	VAL	CG1	-38.50	-29.89	64.64	15.00
125	VAL	CG2	-36.77	-31.11	63.41	15.00
125	VAL	C	-38.87	-32.25	66.47	15.00
125	VAL	O	-39.03	-31.46	67.41	15.00
126	ALA	N	-39.71	-33.26	66.28	15.00
126	ALA	CA	-40.90	-33.44	67.11	15.00
126	ALA	CB	-42.00	-34.13	66.32	15.00
126	ALA	C	-40.64	-34.18	68.44	15.00
126	ALA	O	-41.32	-33.93	69.44	15.00
127	ARG	N	-39.67	-35.09	68.46	15.00
127	ARG	CA	-39.36	-35.83	69.68	15.00
127	ARG	CB	-38.79	-37.22	69.36	15.00
127	ARG	CG	-39.80	-38.34	69.36	15.00
127	ARG	CD	-40.24	-38.71	67.96	15.00
127	ARG	NE	-39.78	-40.04	67.58	15.00
127	ARG	CZ	-40.46	-40.88	66.80	15.00
127	ARG	NH1	-39.94	-42.06	66.52	15.00
127	ARG	NH2	-41.66	-40.57	66.33	15.00
127	ARG	C	-38.36	-35.09	70.56	15.00
127	ARG	O	-38.41	-35.20	71.78	15.00

TABLE II

128	VAL	N	-37.44	-34.37	69.94	15.00
128	VAL	CA	-36.42	-33.64	70.68	15.00
128	VAL	CB	-35.07	-33.78	69.99	15.00
128	VAL	CG1	-33.97	-33.24	70.88	15.00
128	VAL	CG2	-34.81	-35.23	69.64	15.00
128	VAL	C	-36.75	-32.17	70.84	15.00
128	VAL	O	-36.91	-31.68	71.94	15.00
129	GLY	N	-36.85	-31.47	69.72	15.00
129	GLY	CA	-37.13	-30.05	69.75	15.00
129	GLY	C	-36.29	-29.43	68.64	15.00
129	GLY	O	-35.92	-30.14	67.70	15.00
130	PRO	N	-35.92	-28.15	68.76	15.00
130	PRO	CD	-36.24	-27.22	69.86	15.00
130	PRO	CA	-35.11	-27.49	67.75	15.00
130	PRO	CB	-34.80	-26.14	68.39	15.00
130	PRO	CG	-36.01	-25.88	69.20	15.00
130	PRO	C	-33.83	-28.24	67.40	15.00
130	PRO	O	-33.02	-28.57	68.28	15.00
131	VAL	N	-33.63	-28.47	66.11	15.00
131	VAL	CA	-32.46	-29.17	65.62	15.00
131	VAL	CB	-32.89	-30.36	64.73	15.00
131	VAL	CG1	-31.68	-31.12	64.19	15.00
131	VAL	CG2	-33.78	-31.29	65.53	15.00
131	VAL	C	-31.59	-28.20	64.81	15.00
131	VAL	O	-32.10	-27.31	64.12	15.00
132	SER	N	-30.28	-28.33	64.94	15.00
132	SER	CA	-29.35	-27.48	64.21	15.00
132	SER	CB	-28.02	-27.41	64.95	15.00
132	SER	OG	-28.18	-26.80	66.21	15.00
132	SER	C	-29.16	-28.09	62.83	15.00
132	SER	O	-28.84	-29.27	62.71	15.00
133	VAL	N	-29.37	-27.32	61.78	15.00
133	VAL	CA	-29.21	-27.82	60.42	15.00
133	VAL	CB	-30.58	-28.02	59.71	15.00
133	VAL	CG1	-31.50	-28.91	60.54	15.00
133	VAL	CG2	-31.24	-26.68	59.44	15.00
133	VAL	C	-28.37	-26.84	59.60	15.00
133	VAL	O	-28.20	-25.68	59.99	15.00
134	ALA	N	-27.82	-27.30	58.48	15.00
134	ALA	CA	-27.00	-26.45	57.62	15.00
134	ALA	CB	-25.58	-26.95	57.57	15.00
134	ALA	C	-27.65	-26.50	56.26	15.00

TABLE II

134	ALA	O	-28.14	-27.55	55.86	15.00
135	ILE	N	-27.66	-25.38	55.55	15.00
135	ILE	CA	-28.30	-25.28	54.23	15.00
135	ILE	CB	-29.70	-24.57	54.29	15.00
135	ILE	CG2	-30.71	-25.39	55.10	15.00
135	ILE	CG1	-29.54	-23.15	54.87	15.00
135	ILE	CD1	-30.81	-22.34	54.88	15.00
135	ILE	C	-27.46	-24.44	53.29	15.00
135	ILE	O	-26.40	-23.92	53.66	15.00
136	ASP	N	-27.97	-24.32	52.07	15.00
136	ASP	CA	-27.34	-23.50	51.04	15.00
136	ASP	CB	-27.56	-24.11	49.65	15.00
136	ASP	CG	-27.02	-23.23	48.53	15.00
136	ASP	OD1	-27.80	-22.84	47.64	15.00
136	ASP	OD2	-25.83	-22.91	48.54	15.00
136	ASP	C	-28.06	-22.16	51.14	15.00
136	ASP	O	-29.21	-22.03	50.74	15.00
137	ALA	N	-27.43	-21.17	51.76	15.00
137	ALA	CA	-28.07	-19.87	51.86	15.00
137	ALA	CB	-27.97	-19.34	53.26	15.00
137	ALA	C	-27.47	-18.89	50.85	15.00
137	ALA	O	-27.92	-17.75	50.72	15.00
138	SER	N	-26.43	-19.33	50.15	15.00
138	SER	CA	-25.79	-18.51	49.14	15.00
138	SER	CB	-24.36	-19.00	48.90	15.00
138	SER	OG	-23.55	-18.75	50.04	15.00
138	SER	C	-26.61	-18.61	47.87	15.00
138	SER	O	-26.41	-19.53	47.07	15.00
139	LEU	N	-27.56	-17.70	47.74	15.00
139	LEU	CA	-28.46	-17.66	46.60	15.00
139	LEU	CB	-29.32	-18.92	46.55	15.00
139	LEU	CG	-30.03	-19.30	45.25	15.00
139	LEU	CD1	-29.04	-19.96	44.31	15.00
139	LEU	CD2	-31.14	-20.28	45.54	15.00
139	LEU	C	-29.35	-16.43	46.82	15.00
139	LEU	O	-29.99	-16.29	47.87	15.00
140	THR	N	-29.39	-15.54	45.83	15.00
140	THR	CA	-30.17	-14.30	45.90	15.00
140	THR	CB	-30.15	-13.57	44.52	15.00
140	THR	OG1	-29.95	-14.53	43.47	15.00
140	THR	CG2	-29.05	-12.52	44.48	15.00
140	THR	C	-31.60	-14.43	46.41	15.00

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TABLE II

140	THR	O	-32.02	-13.70	47.31	15.00
141	SER	N	-32.35	-15.38	45.88	15.00
141	SER	CA	-33.74	-15.58	46.27	15.00
141	SER	CB	-34.42	-16.62	45.36	15.00
141	SER	OG	-33.62	-17.78	45.21	15.00
141	SER	C	-33.92	-15.96	47.74	15.00
141	SER	O	-34.99	-15.74	48.33	15.00
142	PHE	N	-32.90	-16.52	48.37	15.00
142	PHE	CA	-33.01	-16.91	49.77	15.00
142	PHE	CB	-31.92	-17.91	50.15	15.00
142	PHE	CG	-31.91	-18.26	51.61	15.00
142	PHE	CD1	-32.74	-19.26	52.10	15.00
142	PHE	CD2	-31.09	-17.58	52.50	15.00
142	PHE	CE1	-32.74	-19.58	53.45	15.00
142	PHE	CE2	-31.09	-17.90	53.87	15.00
142	PHE	CZ	-31.92	-18.89	54.34	15.00
142	PHE	C	-32.87	-15.67	50.62	15.00
142	PHE	O	-33.64	-15.45	51.55	15.00
143	GLN	N	-31.90	-14.85	50.24	15.00
143	GLN	CA	-31.58	-13.63	50.96	15.00
143	GLN	CB	-30.25	-13.12	50.48	15.00
143	GLN	CG	-29.21	-14.20	50.55	15.00
143	GLN	CD	-27.89	-13.73	50.06	15.00
143	GLN	OE1	-27.33	-12.78	50.59	15.00
143	GLN	NE2	-27.36	-14.40	49.05	15.00
143	GLN	C	-32.63	-12.53	50.92	15.00
143	GLN	O	-32.79	-11.82	51.91	15.00
144	PHE	N	-33.31	-12.35	49.79	15.00
144	PHE	CA	-34.36	-11.32	49.70	15.00
144	PHE	CB	-34.28	-10.50	48.39	15.00
144	PHE	CG	-34.49	-11.30	47.11	15.00
144	PHE	CD1	-33.53	-11.26	46.11	15.00
144	PHE	CD2	-35.66	-12.02	46.88	15.00
144	PHE	CE1	-33.74	-11.93	44.90	15.00
144	PHE	CE2	-35.88	-12.69	45.67	15.00
144	PHE	CZ	-34.91	-12.64	44.68	15.00
144	PHE	C	-35.77	-11.88	49.96	15.00
144	PHE	O	-36.77	-11.36	49.45	15.00
145	TYR	N	-35.82	-12.95	50.76	15.00
145	TYR	CA	-37.05	-13.64	51.13	15.00
145	TYR	CB	-36.69	-14.96	51.83	15.00
145	TYR	CG	-37.83	-15.59	52.60	15.00

TABLE II

145	TYR	CD1	-38.64	-16.56	52.01	15.00
145	TYR	CE1	-39.71	-17.11	52.70	15.00
145	TYR	CD2	-38.11	-15.20	53.91	15.00
145	TYR	CE2	-39.18	-15.74	54.60	15.00
145	TYR	CZ	-39.98	-16.69	53.99	15.00
145	TYR	OH	-41.05	-17.22	54.66	15.00
145	TYR	C	-37.79	-12.74	52.10	15.00
145	TYR	O	-37.16	-12.04	52.89	15.00
146	SER	N	-39.12	-12.80	52.09	15.00
146	SER	CA	-39.93	-11.97	52.99	15.00
146	SER	CB	-40.22	-10.61	52.35	15.00
146	SER	OG	-40.75	-10.75	51.05	15.00
146	SER	C	-41.25	-12.62	53.43	15.00
146	SER	O	-41.83	-12.21	54.43	15.00
147	LYS	N	-41.74	-13.59	52.66	15.00
147	LYS	CA	-42.98	-14.28	52.99	15.00
147	LYS	CB	-44.19	-13.35	52.82	15.00
147	LYS	CG	-44.40	-12.86	51.40	15.00
147	LYS	CD	-45.58	-11.90	51.31	15.00
147	LYS	CE	-46.86	-12.63	50.95	15.00
147	LYS	NZ	-48.03	-11.69	50.96	15.00
147	LYS	C	-43.18	-15.52	52.13	15.00
147	LYS	O	-42.61	-15.62	51.04	15.00
148	GLY	N	-44.00	-16.45	52.62	15.00
148	GLY	CA	-44.27	-17.68	51.88	15.00
148	GLY	C	-43.30	-18.81	52.16	15.00
148	GLY	O	-42.38	-18.69	52.97	15.00
149	VAL	N	-43.52	-19.94	51.51	15.00
149	VAL	CA	-42.66	-21.10	51.68	15.00
149	VAL	CB	-43.47	-22.41	51.46	15.00
149	VAL	CG1	-42.59	-23.63	51.61	15.00
149	VAL	CG2	-44.62	-22.47	52.45	15.00
149	VAL	C	-41.57	-20.96	50.62	15.00
149	VAL	O	-41.84	-20.56	49.50	15.00
150	TYR	N	-40.34	-21.30	50.96	15.00
150	TYR	CA	-39.24	-21.14	50.02	15.00
150	TYR	CB	-38.02	-20.54	50.73	15.00
150	TYR	CG	-36.80	-20.39	49.85	15.00
150	TYR	CD1	-36.77	-19.48	48.80	15.00
150	TYR	CE1	-35.66	-19.36	47.97	15.00
150	TYR	CD2	-35.67	-21.18	50.05	15.00
150	TYR	CE2	-34.56	-21.07	49.24	15.00

TABLE II

150	TYR	CZ	-34.56	-20.16	48.20	15.00
150	TYR	OH	-33.45	-20.04	47.40	15.00
150	TYR	C	-38.83	-22.39	49.27	15.00
150	TYR	O	-38.66	-23.45	49.85	15.00
151	TYR	N	-38.62	-22.22	47.97	15.00
151	TYR	CA	-38.17	-23.31	47.12	15.00
151	TYR	CB	-39.33	-24.21	46.71	15.00
151	TYR	CG	-38.86	-25.44	45.98	15.00
151	TYR	CD1	-37.95	-26.30	46.56	15.00
151	TYR	CE1	-37.46	-27.40	45.87	15.00
151	TYR	CD2	-39.29	-25.71	44.68	15.00
151	TYR	CE2	-38.81	-26.81	43.98	15.00
151	TYR	CZ	-37.89	-27.65	44.58	15.00
151	TYR	OH	-37.37	-28.73	43.90	15.00
151	TYR	C	-37.49	-22.74	45.88	15.00
151	TYR	O	-37.97	-21.79	45.28	15.00
152	ASP	N	-36.36	-23.32	45.49	15.00
152	ASP	CA	-35.64	-22.85	44.31	15.00
152	ASP	CB	-34.72	-21.69	44.66	15.00
152	ASP	CG	-34.07	-21.09	43.44	15.00
152	ASP	OD1	-33.12	-21.69	42.92	15.00
152	ASP	OD2	-34.52	-20.01	43.01	15.00
152	ASP	C	-34.83	-23.96	43.66	15.00
152	ASP	O	-33.85	-24.45	44.23	15.00
153	GLU	N	-35.21	-24.32	42.44	15.00
153	GLU	CA	-34.53	-25.36	41.69	15.00
153	GLU	CB	-34.98	-25.36	40.21	15.00
153	GLU	CG	-35.22	-23.98	39.55	15.00
153	GLU	CD	-33.95	-23.34	38.93	15.00
153	GLU	OE1	-33.38	-22.41	39.56	15.00
153	GLU	OE2	-33.56	-23.73	37.80	15.00
153	GLU	C	-33.02	-25.27	41.80	15.00
153	GLU	O	-32.36	-26.29	42.00	15.00
154	SER	N	-32.48	-24.05	41.74	15.00
154	SER	CA	-31.02	-23.84	41.81	15.00
154	SER	CB	-30.65	-22.45	41.31	15.00
154	SER	OG	-30.66	-22.41	39.90	15.00
154	SER	C	-30.37	-24.06	43.16	15.00
154	SER	O	-29.14	-23.91	43.30	15.00
155	CYS	N	-31.15	-24.39	44.19	15.00
155	CYS	CA	-30.56	-24.61	45.49	15.00
155	CYS	C	-29.70	-25.86	45.37	15.00

TABLE II

155	CYS	O	-30.17	-26.88	44.86	15.00
155	CYS	CB	-31.63	-24.79	46.55	15.00
155	CYS	SG	-31.06	-24.07	48.11	15.00
156	ASN	N	-28.43	-25.75	45.74	15.00
156	ASN	CA	-27.50	-26.87	45.66	15.00
156	ASN	CB	-26.13	-26.39	45.18	15.00
156	ASN	CG	-25.14	-27.52	44.97	15.00
156	ASN	OD1	-25.51	-28.70	44.95	15.00
156	ASN	ND2	-23.88	-27.16	44.80	15.00
156	ASN	C	-27.34	-27.66	46.95	15.00
156	ASN	O	-26.57	-27.31	47.85	15.00
157	SER	N	-28.03	-28.79	46.98	15.00
157	SER	CA	-28.03	-29.71	48.10	15.00
157	SER	CB	-28.72	-31.00	47.65	15.00
157	SER	OG	-29.25	-30.85	46.33	15.00
157	SER	C	-26.63	-30.03	48.63	15.00
157	SER	O	-26.46	-30.47	49.77	15.00
158	ASP	N	-25.61	-29.83	47.80	15.00
158	ASP	CA	-24.23	-30.12	48.18	15.00
158	ASP	CB	-23.50	-30.73	47.00	15.00
158	ASP	CG	-23.99	-32.13	46.66	15.00
158	ASP	OD1	-24.82	-32.27	45.74	15.00
158	ASP	OD2	-23.57	-33.09	47.34	15.00
158	ASP	C	-23.44	-28.95	48.72	15.00
158	ASP	O	-22.48	-29.13	49.48	15.00
159	ASN	N	-23.80	-27.73	48.33	15.00
159	ASN	CA	-23.05	-26.56	48.81	15.00
159	ASN	CB	-23.07	-25.44	47.75	15.00
159	ASN	CG	-22.15	-24.26	48.11	15.00
159	ASN	OD1	-22.30	-23.64	49.16	15.00
159	ASN	ND2	-21.21	-23.95	47.22	15.00
159	ASN	C	-23.63	-26.08	50.13	15.00
159	ASN	O	-24.43	-25.14	50.17	15.00
160	LEU	N	-23.27	-26.74	51.23	15.00
160	LEU	CA	-23.78	-26.33	52.55	15.00
160	LEU	CB	-23.76	-27.50	53.53	15.00
160	LEU	CG	-24.57	-28.73	53.10	15.00
160	LEU	CD1	-24.08	-29.96	53.84	15.00
160	LEU	CD2	-26.06	-28.51	53.32	15.00
160	LEU	C	-22.87	-25.21	53.02	15.00
160	LEU	O	-21.70	-25.45	53.29	15.00
161	ASN	N	-23.41	-24.01	53.16	15.00

TABLE II

161	ASN	CA	-22.59	-22.86	53.54	15.00
161	ASN	CB	-22.43	-21.97	52.31	15.00
161	ASN	CG	-23.75	-21.64	51.67	15.00
161	ASN	OD1	-24.51	-20.79	52.17	15.00
161	ASN	ND2	-24.09	-22.36	50.62	15.00
161	ASN	C	-23.07	-22.00	54.70	15.00
161	ASN	O	-22.32	-21.20	55.27	15.00
162	HIS	N	-24.34	-22.10	55.06	15.00
162	HIS	CA	-24.87	-21.31	56.16	15.00
162	HIS	CB	-25.90	-20.34	55.60	15.00
162	HIS	CG	-26.42	-19.36	56.60	15.00
162	HIS	CD2	-27.67	-19.00	56.94	15.00
162	HIS	ND1	-25.58	-18.61	57.40	15.00
162	HIS	CE1	-26.30	-17.82	58.18	15.00
162	HIS	NE2	-27.57	-18.05	57.92	15.00
162	HIS	C	-25.52	-22.24	57.17	15.00
162	HIS	O	-26.26	-23.14	56.80	15.00
163	ALA	N	-25.22	-22.02	58.45	15.00
163	ALA	CA	-25.79	-22.84	59.53	15.00
163	ALA	CB	-24.77	-23.10	60.61	15.00
163	ALA	C	-27.00	-22.13	60.10	15.00
163	ALA	O	-26.93	-20.95	60.48	15.00
164	VAL	N	-28.10	-22.85	60.20	15.00
164	VAL	CA	-29.34	-22.30	60.70	15.00
164	VAL	CB	-30.25	-22.02	59.52	15.00
164	VAL	CG1	-31.04	-23.26	59.13	15.00
164	VAL	CG2	-31.11	-20.83	59.80	15.00
164	VAL	C	-29.96	-23.25	61.73	15.00
164	VAL	O	-29.32	-24.21	62.14	15.00
165	LEU	N	-31.20	-22.99	62.16	15.00
165	LEU	CA	-31.87	-23.83	63.17	15.00
165	LEU	CB	-31.87	-23.10	64.52	15.00
165	LEU	CG	-32.48	-23.78	65.74	15.00
165	LEU	CD1	-31.58	-24.90	66.23	15.00
165	LEU	CD2	-32.71	-22.77	66.84	15.00
165	LEU	C	-33.31	-24.16	62.81	15.00
165	LEU	O	-34.08	-23.27	62.49	15.00
166	ALA	N	-33.69	-25.43	62.90	15.00
166	ALA	CA	-35.06	-25.86	62.59	15.00
166	ALA	CB	-35.05	-27.27	62.00	15.00
166	ALA	C	-35.91	-25.81	63.86	15.00
166	ALA	O	-35.69	-26.57	64.80	15.00

TABLE II

167	VAL	N	-36.89	-24.92	63.85	15.00
167	VAL	CA	-37.78	-24.65	65.00	15.00
167	VAL	CB	-37.89	-23.09	65.18	15.00
167	VAL	CG1	-38.97	-22.71	66.15	15.00
167	VAL	CG2	-36.58	-22.55	65.68	15.00
167	VAL	C	-39.16	-25.32	64.93	15.00
167	VAL	O	-39.98	-25.21	65.84	15.00
168	GLY	N	-39.43	-26.06	63.87	15.00
168	GLY	CA	-40.71	-26.72	63.75	15.00
168	GLY	C	-40.98	-27.09	62.31	15.00
168	GLY	O	-40.05	-27.10	61.49	15.00
169	TYR	N	-42.23	-27.39	61.99	15.00
169	TYR	CA	-42.65	-27.76	60.65	15.00
169	TYR	CB	-42.15	-29.17	60.29	15.00
169	TYR	CG	-42.64	-30.27	61.22	15.00
169	TYR	CD1	-44.00	-30.58	61.31	15.00
169	TYR	CE1	-44.46	-31.57	62.15	15.00
169	TYR	CD2	-41.75	-30.99	62.01	15.00
169	TYR	CE2	-42.20	-31.99	62.85	15.00
169	TYR	CZ	-43.56	-32.28	62.91	15.00
169	TYR	OH	-44.04	-33.28	63.71	15.00
169	TYR	C	-44.16	-27.70	60.54	15.00
169	TYR	O	-44.85	-27.38	61.52	15.00
170	GLY	N	-44.70	-28.04	59.38	15.00
170	GLY	CA	-46.13	-28.00	59.18	15.00
170	GLY	C	-46.49	-27.76	57.73	15.00
170	GLY	O	-45.83	-28.26	56.83	15.00
171	ILE	N	-47.48	-26.92	57.48	15.00
171	ILE	CA	-47.95	-26.63	56.13	15.00
171	ILE	CB	-49.03	-27.66	55.72	15.00
171	ILE	CG2	-50.01	-27.09	54.71	15.00
171	ILE	CG1	-48.36	-28.95	55.21	15.00
171	ILE	CD1	-49.35	-30.05	54.82	15.00
171	ILE	C	-48.54	-25.23	56.14	15.00
171	ILE	O	-48.91	-24.71	57.20	15.00
172	GLN	N	-48.58	-24.55	55.00	15.00
172	GLN	CA	-49.16	-23.20	54.97	15.00
172	GLN	CB	-48.08	-22.18	54.62	15.00
172	GLN	CG	-48.58	-20.75	54.57	15.00
172	GLN	CD	-47.50	-19.79	54.12	15.00
172	GLN	OE1	-46.95	-19.93	53.02	15.00
172	GLN	NE2	-47.18	-18.82	54.96	15.00

TABLE II

172	GLN	C	-50.29	-23.15	53.96	15.00
172	GLN	O	-51.45	-22.89	54.32	15.00
173	LYS	N	-49.96	-23.36	52.68	15.00
173	LYS	CA	-50.96	-23.38	51.61	15.00
173	LYS	CB	-50.84	-22.14	50.69	15.00
173	LYS	CG	-51.09	-20.78	51.36	15.00
173	LYS	CD	-52.40	-20.72	52.16	15.00
173	LYS	CE	-53.63	-20.91	51.29	15.00
173	LYS	NZ	-54.88	-20.56	52.06	15.00
173	LYS	C	-50.66	-24.63	50.81	15.00
173	LYS	O	-50.20	-24.57	49.67	15.00
174	GLY	N	-50.86	-25.77	51.45	15.00
174	GLY	CA	-50.60	-27.04	50.79	15.00
174	GLY	C	-49.13	-27.39	50.91	15.00
174	GLY	O	-48.77	-28.52	51.28	15.00
175	ASN	N	-48.26	-26.42	50.63	15.00
175	ASN	CA	-46.83	-26.66	50.70	15.00
175	ASN	CB	-46.06	-25.48	50.10	15.00
175	ASN	CG	-46.31	-25.33	48.61	15.00
175	ASN	OD1	-47.34	-24.79	48.20	15.00
175	ASN	ND2	-45.38	-25.81	47.80	15.00
175	ASN	C	-46.33	-26.96	52.11	15.00
175	ASN	O	-46.55	-26.18	53.05	15.00
176	LYS	N	-45.69	-28.13	52.25	15.00
176	LYS	CA	-45.13	-28.55	53.53	15.00
176	LYS	CB	-44.68	-30.01	53.48	15.00
176	LYS	CG	-45.77	-31.03	53.17	15.00
176	LYS	CD	-45.27	-32.45	53.44	15.00
176	LYS	CE	-46.19	-33.50	52.85	15.00
176	LYS	NZ	-46.03	-33.64	51.36	15.00
176	LYS	C	-43.92	-27.66	53.74	15.00
176	LYS	O	-43.25	-27.27	52.77	15.00
177	HIS	N	-43.57	-27.37	54.99	15.00
177	HIS	CA	-42.44	-26.49	55.22	15.00
177	HIS	CB	-42.90	-25.04	55.10	15.00
177	HIS	CG	-43.81	-24.59	56.20	15.00
177	HIS	CD2	-43.59	-24.40	57.52	15.00
177	HIS	ND1	-45.13	-24.24	55.98	15.00
177	HIS	CE1	-45.67	-23.85	57.12	15.00
177	HIS	NE2	-44.76	-23.93	58.07	15.00
177	HIS	C	-41.73	-26.66	56.55	15.00
177	HIS	O	-42.31	-27.17	57.50	15.00

TABLE II

178	TRP	N	-40.48	-26.20	56.61	15.00
178	TRP	CA	-39.68	-26.25	57.82	15.00
178	TRP	CB	-38.26	-26.73	57.52	15.00
178	TRP	CG	-38.13	-28.11	57.02	15.00
178	TRP	CD2	-38.29	-29.32	57.78	15.00
178	TRP	CE2	-37.96	-30.39	56.93	15.00
178	TRP	CE3	-38.68	-29.59	59.10	15.00
178	TRP	CD1	-37.74	-28.49	55.78	15.00
178	TRP	NE1	-37.62	-29.86	55.72	15.00
178	TRP	CZ2	-38.00	-31.71	57.35	15.00
178	TRP	CZ3	-38.72	-30.91	59.52	15.00
178	TRP	CH2	-38.38	-31.96	58.64	15.00
178	TRP	C	-39.60	-24.81	58.34	15.00
178	TRP	O	-39.21	-23.90	57.60	15.00
179	ILE	N	-39.96	-24.57	59.59	15.00
179	ILE	CA	-39.89	-23.23	60.17	15.00
179	ILE	CB	-40.79	-23.11	61.41	15.00
179	ILE	CG2	-40.66	-21.74	62.03	15.00
179	ILE	CG1	-42.24	-23.42	61.02	15.00
179	ILE	CD1	-43.21	-23.40	62.15	15.00
179	ILE	C	-38.44	-23.00	60.58	15.00
179	ILE	O	-37.97	-23.57	61.56	15.00
180	ILE	N	-37.72	-22.17	59.81	15.00
180	ILE	CA	-36.31	-21.89	60.07	15.00
180	ILE	CB	-35.49	-21.93	58.76	15.00
180	ILE	CG2	-34.04	-21.77	59.05	15.00
180	ILE	CG1	-35.73	-23.25	58.02	15.00
180	ILE	CD1	-35.30	-24.46	58.78	15.00
180	ILE	C	-36.03	-20.55	60.77	15.00
180	ILE	O	-36.62	-19.52	60.42	15.00
181	LYS	N	-35.13	-20.57	61.74	15.00
181	LYS	CA	-34.73	-19.40	62.50	15.00
181	LYS	CB	-34.63	-19.75	63.99	15.00
181	LYS	CG	-34.15	-18.60	64.87	15.00
181	LYS	CD	-33.79	-19.04	66.29	15.00
181	LYS	CE	-33.65	-17.84	67.19	15.00
181	LYS	NZ	-33.21	-18.18	68.57	15.00
181	LYS	C	-33.36	-19.00	62.01	15.00
181	LYS	O	-32.43	-19.79	62.05	15.00
182	ASN	N	-33.20	-17.77	61.53	15.00
182	ASN	CA	-31.90	-17.34	61.04	15.00
182	ASN	CB	-32.07	-16.64	59.69	15.00

TABLE II

182	ASN	CG	-30.84	-16.74	58.82	15.00
182	ASN	OD1	-29.75	-17.06	59.30	15.00
182	ASN	ND2	-31.01	-16.50	57.53	15.00
182	ASN	C	-31.22	-16.43	62.06	15.00
182	ASN	O	-31.77	-16.14	63.11	15.00
183	SER	N	-30.00	-15.98	61.77	15.00
183	SER	CA	-29.29	-15.10	62.69	15.00
183	SER	CB	-28.07	-15.81	63.25	15.00
183	SER	OG	-27.40	-16.52	62.23	15.00
183	SER	C	-28.87	-13.82	61.98	15.00
183	SER	O	-27.82	-13.25	62.27	15.00
184	TRP	N	-29.70	-13.35	61.06	15.00
184	TRP	CA	-29.40	-12.13	60.34	15.00
184	TRP	CB	-29.58	-12.36	58.83	15.00
184	TRP	CG	-28.57	-13.29	58.22	15.00
184	TRP	CD2	-28.61	-13.87	56.90	15.00
184	TRP	CE2	-27.40	-14.58	56.72	15.00
184	TRP	CE3	-29.54	-13.84	55.86	15.00
184	TRP	CD1	-27.39	-13.69	58.76	15.00
184	TRP	NE1	-26.68	-14.46	57.87	15.00
184	TRP	CZ2	-27.11	-15.26	55.53	15.00
184	TRP	CZ3	-29.25	-14.52	54.67	15.00
184	TRP	CH2	-28.04	-15.22	54.52	15.00
184	TRP	C	-30.28	-10.98	60.82	15.00
184	TRP	O	-30.61	-10.09	60.04	15.00
185	GLY	N	-30.70	-11.02	62.09	15.00
185	GLY	CA	-31.53	-9.96	62.66	15.00
185	GLY	C	-33.03	-10.14	62.46	15.00
185	GLY	O	-33.46	-10.99	61.69	15.00
186	GLU	N	-33.84	-9.34	63.17	15.00
186	GLU	CA	-35.30	-9.44	63.04	15.00
186	GLU	CB	-36.00	-8.71	64.19	15.00
186	GLU	CG	-35.52	-9.13	65.56	15.00
186	GLU	CD	-36.52	-8.85	66.68	15.00
186	GLU	OE1	-36.30	-9.38	67.80	15.00
186	GLU	OE2	-37.51	-8.13	66.46	15.00
186	GLU	C	-35.74	-8.83	61.73	15.00
186	GLU	O	-36.83	-9.11	61.22	15.00
187	ASN	N	-34.89	-7.97	61.19	15.00
187	ASN	CA	-35.15	-7.28	59.95	15.00
187	ASN	CB	-34.04	-6.25	59.73	15.00
187	ASN	CG	-34.56	-4.94	59.17	15.00

TABLE II

187	ASN	OD1	-33.77	-4.07	58.80	15.00
187	ASN	ND2	-35.88	-4.76	59.16	15.00
187	ASN	C	-35.21	-8.22	58.75	15.00
187	ASN	O	-36.04	-8.04	57.86	15.00
188	TRP	N	-34.33	-9.22	58.73	15.00
188	TRP	CA	-34.26	-10.18	57.64	15.00
188	TRP	CB	-33.03	-11.07	57.79	15.00
188	TRP	CG	-32.85	-12.02	56.65	15.00
188	TRP	CD2	-33.28	-13.38	56.57	15.00
188	TRP	CE2	-32.98	-13.85	55.28	15.00
188	TRP	CE3	-33.90	-14.26	57.48	15.00
188	TRP	CD1	-32.31	-11.72	55.44	15.00
188	TRP	NE1	-32.39	-12.81	54.61	15.00
188	TRP	CZ2	-33.27	-15.15	54.86	15.00
188	TRP	CZ3	-34.20	-15.55	57.06	15.00
188	TRP	CH2	-33.88	-15.98	55.77	15.00
188	TRP	C	-35.50	-11.05	57.53	15.00
188	TRP	O	-36.10	-11.42	58.55	15.00
189	GLY	N	-35.85	-11.42	56.31	15.00
189	GLY	CA	-37.00	-12.26	56.07	15.00
189	GLY	C	-38.21	-11.92	56.90	15.00
189	GLY	O	-38.47	-10.76	57.23	15.00
190	ASN	N	-38.97	-12.94	57.27	15.00
190	ASN	CA	-40.16	-12.73	58.07	15.00
190	ASN	CB	-41.17	-13.86	57.83	15.00
190	ASN	CG	-42.55	-13.53	58.36	15.00
190	ASN	OD1	-42.70	-12.88	59.39	15.00
190	ASN	ND2	-43.57	-13.99	57.65	15.00
190	ASN	C	-39.79	-12.67	59.54	15.00
190	ASN	O	-39.85	-13.66	60.25	15.00
191	LYS	N	-39.32	-11.52	60.00	15.00
191	LYS	CA	-38.95	-11.34	61.39	15.00
191	LYS	CB	-40.19	-11.48	62.29	15.00
191	LYS	CG	-40.95	-10.18	62.44	15.00
191	LYS	CD	-42.19	-10.32	63.30	15.00
191	LYS	CE	-43.32	-10.98	62.52	15.00
191	LYS	NZ	-43.71	-10.21	61.31	15.00
191	LYS	C	-37.84	-12.24	61.88	15.00
191	LYS	O	-37.77	-12.55	63.06	15.00
192	GLY	N	-36.94	-12.61	60.98	15.00
192	GLY	CA	-35.83	-13.46	61.35	15.00
192	GLY	C	-36.05	-14.91	60.98	15.00

TABLE II

192	GLY	O	-35.12	-15.70	60.99	15.00
193	TYR	N	-37.29	-15.27	60.65	15.00
193	TYR	CA	-37.60	-16.64	60.28	15.00
193	TYR	CB	-38.84	-17.13	61.05	15.00
193	TYR	CG	-38.60	-17.31	62.52	15.00
193	TYR	CD1	-38.73	-16.25	63.41	15.00
193	TYR	CE1	-38.46	-16.41	64.76	15.00
193	TYR	CD2	-38.19	-18.55	63.03	15.00
193	TYR	CE2	-37.92	-18.71	64.38	15.00
193	TYR	CZ	-38.05	-17.64	65.23	15.00
193	TYR	OH	-37.77	-17.80	66.56	15.00
193	TYR	C	-37.83	-16.81	58.79	15.00
193	TYR	O	-38.02	-15.82	58.08	15.00
194	ILE	N	-37.82	-18.06	58.35	15.00
194	ILE	CA	-38.04	-18.41	56.95	15.00
194	ILE	CB	-36.75	-18.32	56.10	15.00
194	ILE	CG2	-35.64	-19.14	56.72	15.00
194	ILE	CG1	-37.03	-18.83	54.69	15.00
194	ILE	CD1	-35.86	-18.72	53.75	15.00
194	ILE	C	-38.61	-19.81	56.83	15.00
194	ILE	O	-38.11	-20.74	57.43	15.00
195	LEU	N	-39.72	-19.92	56.10	15.00
195	LEU	CA	-40.38	-21.19	55.85	15.00
195	LEU	CB	-41.88	-20.96	55.65	15.00
195	LEU	CG	-42.82	-20.84	56.86	15.00
195	LEU	CD1	-42.19	-20.08	58.01	15.00
195	LEU	CD2	-44.12	-20.18	56.42	15.00
195	LEU	C	-39.76	-21.78	54.59	15.00
195	LEU	O	-39.79	-21.16	53.53	15.00
196	MET	N	-39.11	-22.93	54.71	15.00
196	MET	CA	-38.46	-23.57	53.57	15.00
196	MET	CB	-37.03	-23.97	53.96	15.00
196	MET	CG	-36.09	-22.77	54.14	15.00
196	MET	SD	-34.43	-23.18	54.74	15.00
196	MET	CE	-33.67	-23.82	53.22	15.00
196	MET	C	-39.28	-24.78	53.11	15.00
196	MET	O	-40.09	-25.31	53.86	15.00
197	ALA	N	-39.08	-25.23	51.87	15.00
197	ALA	CA	-39.83	-26.37	51.32	15.00
197	ALA	CB	-39.62	-26.47	49.82	15.00
197	ALA	C	-39.52	-27.71	51.98	15.00
197	ALA	O	-38.37	-28.15	51.98	15.00

TABLE II

198	ARG	N	-40.56	-28.39	52.46	15.00
198	ARG	CA	-40.40	-29.68	53.11	15.00
198	ARG	CB	-41.17	-29.72	54.44	15.00
198	ARG	CG	-41.15	-31.07	55.15	15.00
198	ARG	CD	-41.43	-30.95	56.63	15.00
198	ARG	NE	-42.81	-30.59	56.92	15.00
198	ARG	CZ	-43.79	-31.47	57.10	15.00
198	ARG	NH1	-43.54	-32.78	57.01	15.00
198	ARG	NH2	-45.01	-31.05	57.42	15.00
198	ARG	C	-40.82	-30.85	52.23	15.00
198	ARG	O	-41.86	-30.80	51.57	15.00
199	ASN	N	-40.00	-31.89	52.23	15.00
199	ASN	CA	-40.25	-33.10	51.45	15.00
199	ASN	CB	-41.59	-33.75	51.83	15.00
199	ASN	CG	-41.57	-34.40	53.22	15.00
199	ASN	OD1	-42.60	-34.43	53.91	15.00
199	ASN	ND2	-40.42	-34.91	53.63	15.00
199	ASN	C	-40.15	-32.94	49.94	15.00
199	ASN	O	-40.49	-33.86	49.19	15.00
200	LYS	N	-39.67	-31.77	49.49	15.00
200	LYS	CA	-39.50	-31.55	48.05	15.00
200	LYS	CB	-39.77	-30.09	47.65	15.00
200	LYS	CG	-41.23	-29.79	47.39	15.00
200	LYS	CD	-41.42	-28.49	46.63	15.00
200	LYS	CE	-42.88	-28.03	46.65	15.00
200	LYS	NZ	-43.06	-26.68	46.03	15.00
200	LYS	C	-38.09	-31.95	47.69	15.00
200	LYS	O	-37.28	-31.12	47.26	15.00
201	ASN	N	-37.80	-33.22	47.95	15.00
201	ASN	CA	-36.50	-33.81	47.65	15.00
201	ASN	CB	-36.24	-33.83	46.13	15.00
201	ASN	CG	-37.32	-34.57	45.35	15.00
201	ASN	OD1	-37.09	-35.68	44.87	15.00
201	ASN	ND2	-38.46	-33.92	45.15	15.00
201	ASN	C	-35.31	-33.16	48.37	15.00
201	ASN	O	-34.31	-32.84	47.74	15.00
202	ASN	N	-35.43	-32.90	49.67	15.00
202	ASN	CA	-34.32	-32.33	50.44	15.00
202	ASN	CB	-33.19	-33.35	50.50	15.00
202	ASN	CG	-32.27	-33.14	51.68	15.00
202	ASN	OD1	-32.71	-32.70	52.75	15.00
202	ASN	ND2	-31.00	-33.48	51.51	15.00

TABLE II

202	ASN	C	-33.81	-30.99	49.89	15.00
202	ASN	O	-32.60	-30.77	49.75	15.00
203	ALA	N	-34.73	-30.09	49.59	15.00
203	ALA	H	-35.63	-30.29	49.94	15.00
203	ALA	CA	-34.40	-28.79	49.02	15.00
203	ALA	CB	-35.62	-27.88	48.98	15.00
203	ALA	C	-33.35	-28.09	49.90	15.00
203	ALA	O	-33.51	-27.93	51.10	15.00
204	CYS	N	-32.27	-27.66	49.25	15.00
204	CYS	CA	-31.18	-26.94	49.91	15.00
204	CYS	C	-30.38	-27.79	50.89	15.00
204	CYS	O	-29.60	-27.25	51.68	15.00
204	CYS	CB	-31.71	-25.68	50.59	15.00
204	CYS	SG	-32.51	-24.48	49.47	15.00
205	GLY	N	-30.56	-29.10	50.84	15.00
205	GLY	CA	-29.83	-30.00	51.71	15.00
205	GLY	C	-30.11	-29.81	53.19	15.00
205	GLY	O	-29.22	-29.98	54.02	15.00
206	ILE	N	-31.35	-29.51	53.52	15.00
206	ILE	CA	-31.77	-29.30	54.89	15.00
206	ILE	CB	-33.30	-29.10	54.96	15.00
206	ILE	CG2	-34.02	-30.31	54.38	15.00
206	ILE	CG1	-33.76	-28.86	56.41	15.00
206	ILE	CD1	-33.48	-27.47	56.92	15.00
206	ILE	C	-31.35	-30.45	55.82	15.00
206	ILE	O	-30.94	-30.23	56.97	15.00
207	ALA	N	-31.36	-31.68	55.31	15.00
207	ALA	CA	-31.00	-32.84	56.11	15.00
207	ALA	CB	-32.05	-33.93	55.95	15.00
207	ALA	C	-29.61	-33.42	55.88	15.00
207	ALA	O	-29.35	-34.57	56.24	15.00
208	ASN	N	-28.68	-32.65	55.31	15.00
208	ASN	CA	-27.33	-33.15	55.05	15.00
208	ASN	CB	-26.76	-32.53	53.77	15.00
208	ASN	CG	-27.34	-33.15	52.51	15.00
208	ASN	OD1	-28.21	-34.02	52.57	15.00
208	ASN	ND2	-26.89	-32.67	51.36	15.00
208	ASN	C	-26.32	-32.95	56.20	15.00
208	ASN	O	-25.17	-33.40	56.12	15.00
209	LEU	N	-26.72	-32.25	57.25	15.00
209	LEU	CA	-25.84	-32.03	58.40	15.00
209	LEU	CB	-24.76	-31.00	58.04	15.00

TABLE II

209	LEU	CG	-23.41	-30.99	58.78	15.00
209	LEU	CD1	-22.72	-32.35	58.64	15.00
209	LEU	CD2	-22.51	-29.86	58.24	15.00
209	LEU	C	-26.67	-31.60	59.63	15.00
209	LEU	O	-26.38	-30.59	60.28	15.00
210	ALA	N	-27.72	-32.37	59.95	15.00
210	ALA	H	-28.03	-32.90	59.19	15.00
210	ALA	CA	-28.61	-32.05	61.06	15.00
210	ALA	CB	-30.02	-32.57	60.81	15.00
210	ALA	C	-28.10	-32.73	62.34	15.00
210	ALA	O	-27.62	-33.86	62.34	15.00
211	SER	N	-28.18	-32.02	63.47	15.00
211	SER	CA	-27.75	-32.59	64.74	15.00
211	SER	CB	-26.24	-32.46	64.92	15.00
211	SER	OG	-25.84	-31.12	65.06	15.00
211	SER	C	-28.45	-31.88	65.88	15.00
211	SER	O	-29.03	-30.80	65.71	15.00
212	PHE	N	-28.50	-32.51	67.04	15.00
212	PHE	CA	-29.11	-31.91	68.21	15.00
212	PHE	CB	-30.59	-32.31	68.33	15.00
212	PHE	CG	-30.81	-33.79	68.43	15.00
212	PHE	CD1	-31.11	-34.54	67.30	15.00
212	PHE	CD2	-30.72	-34.44	69.66	15.00
212	PHE	CE1	-31.32	-35.91	67.39	15.00
212	PHE	CE2	-30.92	-35.81	69.77	15.00
212	PHE	CZ	-31.23	-36.55	68.63	15.00
212	PHE	C	-28.30	-32.39	69.40	15.00
212	PHE	O	-27.66	-33.43	69.32	15.00
213	PRO	N	-28.24	-31.58	70.46	15.00
213	PRO	CD	-28.77	-30.21	70.54	15.00
213	PRO	CA	-27.48	-31.92	71.67	15.00
213	PRO	CB	-27.21	-30.55	72.28	15.00
213	PRO	CG	-28.47	-29.82	71.97	15.00
213	PRO	C	-28.27	-32.81	72.64	15.00
213	PRO	O	-29.50	-32.76	72.69	15.00
214	LYS	N	-27.57	-33.62	73.42	15.00
214	LYS	CA	-28.23	-34.49	74.37	15.00
214	LYS	CB	-27.67	-35.90	74.28	15.00
214	LYS	CG	-28.06	-36.64	73.02	15.00
214	LYS	CD	-27.66	-38.11	73.07	15.00
214	LYS	CE	-26.16	-38.29	73.05	15.00
214	LYS	NZ	-25.79	-39.70	72.73	15.00

TABLE II

214	LYS	C	-28.03	-33.95	75.77	15.00
214	LYS	O	-26.90	-33.70	76.18	15.00
215	MET	N	-29.12	-33.69	76.47	15.00
215	MET	CA	-29.06	-33.18	77.83	15.00
215	MET	CB	-29.71	-31.80	77.93	15.00
215	MET	CG	-28.74	-30.64	77.75	15.00
215	MET	SD	-29.45	-29.00	78.06	15.00
215	MET	CE	-30.38	-29.32	79.56	15.00
215	MET	C	-29.72	-34.16	78.81	15.00
215	MET	OT1	-30.39	-35.12	78.35	15.00
215	MET	OT2	-29.55	-33.97	80.04	15.00
216	HOH	OH2	-28.46	-18.77	85.58	15.00
217	HOH	OH2	-24.63	-33.99	81.97	15.00
218	HOH	OH2	-31.11	-15.95	65.82	15.00
219	HOH	OH2	-30.23	-19.59	64.13	15.00
220	HOH	OH2	-8.58	-7.31	62.36	15.00
221	HOH	OH2	-6.71	-10.79	69.96	15.00
222	HOH	OH2	-34.27	-22.79	70.48	15.00
223	HOH	OH2	-16.88	-33.68	66.52	15.00
224	HOH	OH2	-15.68	-8.93	63.11	15.00
225	HOH	OH2	-24.93	-30.84	62.42	15.00
226	HOH	OH2	-7.02	-8.27	72.29	15.00
227	HOH	OH2	-13.39	-20.80	66.92	15.00
228	HOH	OH2	-44.55	-30.12	50.27	15.00
229	HOH	OH2	-44.14	-35.34	56.06	15.00
230	HOH	OH2	-37.95	-16.02	68.44	15.00
231	HOH	OH2	-36.41	-36.82	52.05	15.00
232	HOH	OH2	-20.00	-36.75	62.15	15.00
233	HOH	OH2	-30.13	-19.30	67.02	15.00
234	HOH	OH2	-28.16	-19.22	62.41	15.00
235	HOH	OH2	-22.03	-29.95	62.71	15.00
236	HOH	OH2	-25.92	-8.85	75.85	15.00
237	HOH	OH2	-41.00	-28.78	81.30	15.00
238	HOH	OH2	-32.73	-23.15	83.59	15.00
239	HOH	OH2	-40.55	-13.35	49.90	15.00
240	HOH	OH2	-35.40	-24.36	49.00	15.00
241	HOH	OH2	-48.40	-32.54	58.07	15.00
242	HOH	OH2	-27.39	-6.75	59.53	15.00
243	HOH	OH2	-41.50	-14.46	65.52	15.00
244	HOH	OH2	-22.40	-5.47	61.33	15.00
245	HOH	OH2	-33.17	-27.91	70.80	15.00
246	HOH	OH2	-45.87	-26.25	75.72	15.00

TABLE II

247	HOH	OH2	-12.64	-13.96	81.39	15.00
248	HOH	OH2	-3.78	-18.92	74.98	15.00
249	HOH	OH2	-8.03	-17.70	78.42	15.00
250	HOH	OH2	-27.41	-34.98	59.22	15.00
251	HOH	OH2	-34.88	-10.94	53.71	15.00
252	HOH	OH2	-32.92	-27.68	46.17	15.00
253	HOH	OH2	-39.35	-16.01	44.28	15.00
254	HOH	OH2	-41.38	-34.64	56.30	15.00
255	HOH	OH2	-44.42	-18.35	73.08	15.00
256	HOH	OH2	-32.35	-13.73	61.23	15.00
257	HOH	OH2	-39.40	-8.90	59.13	15.00
258	HOH	OH2	-28.41	-8.93	68.65	15.00
259	HOH	OH2	-31.58	-6.53	63.69	15.00
260	HOH	OH2	-19.27	-8.48	63.41	15.00
261	HOH	OH2	-33.33	-20.29	70.52	15.00
262	HOH	OH2	-13.49	-22.80	78.17	15.00
263	HOH	OH2	-8.72	-18.49	72.60	15.00
264	HOH	OH2	-10.39	-28.70	76.32	15.00
265	HOH	OH2	-20.24	-31.77	61.63	15.00
266	HOH	OH2	-24.78	-46.10	72.19	15.00
267	HOH	OH2	-13.26	-33.12	68.94	15.00
268	HOH	OH2	-12.60	-26.87	72.01	15.00
269	HOH	OH2	-17.76	-34.32	80.14	15.00
270	HOH	OH2	-22.51	-37.80	70.83	15.00
271	HOH	OH2	-7.33	-12.89	66.95	15.00
272	HOH	OH2	-9.75	-17.21	68.77	15.00
273	HOH	OH2	-30.86	-20.40	48.59	15.00
274	HOH	OH2	-25.79	-24.78	42.10	15.00
275	HOH	OH2	-33.50	-37.21	50.03	15.00
276	HOH	OH2	-23.21	-24.90	43.38	15.00
277	HOH	OH2	-37.83	-31.49	44.10	15.00
278	HOH	OH2	-37.02	-30.78	51.01	15.00

TABLE III

Table of the orthogonal three dimensional coordinates in Ångstroms and B factors (Å^2) for the cathepsin K complex with inhibitor bis-(cbz-leucinyl)-1,3-diamino-propan-2-one.

Residue	Atom	X	Y	Z	B
1	ALA CB	-54.29	-33.17	65.94	15.00
1	ALA C	-53.88	-32.69	63.50	15.00
1	ALA O	-53.42	-33.61	62.80	15.00
1	ALA N	-55.60	-34.28	64.17	15.00
1	ALA CA	-54.93	-33.01	64.57	15.00
2	PRO N	-53.52	-31.40	63.32	15.00
2	PRO CD	-53.99	-30.23	64.09	15.00
2	PRO CA	-52.52	-30.98	62.32	15.00
2	PRO CB	-52.49	-29.46	62.49	15.00
2	PRO CG	-52.83	-29.26	63.94	15.00
2	PRO C	-51.13	-31.59	62.52	15.00
2	PRO O	-50.62	-31.64	63.64	15.00
3	ASP N	-50.53	-32.08	61.44	15.00
3	ASP CA	-49.19	-32.65	61.51	15.00
3	ASP CB	-48.89	-33.49	60.27	15.00
3	ASP CG	-49.53	-34.88	60.32	15.00
3	ASP OD1	-49.43	-35.55	61.39	15.00
3	ASP OD2	-50.12	-35.29	59.28	15.00
3	ASP C	-48.24	-31.46	61.55	15.00
3	ASP O	-47.60	-31.14	60.54	15.00
4	SER N	-48.16	-30.78	62.68	15.00
4	SER CA	-47.29	-29.62	62.80	15.00
4	SER CB	-47.99	-28.35	62.27	15.00
4	SER OG	-48.14	-28.37	60.86	15.00
4	SER C	-46.84	-29.35	64.23	15.00
4	SER O	-47.54	-29.71	65.19	15.00
5	VAL N	-45.68	-28.72	64.36	15.00
5	VAL CA	-45.14	-28.35	65.65	15.00
5	VAL CB	-44.25	-29.47	66.25	15.00
5	VAL CG1	-43.09	-29.81	65.33	15.00
5	VAL CG2	-43.75	-29.04	67.62	15.00
5	VAL C	-44.36	-27.06	65.44	15.00
5	VAL O	-43.60	-26.93	64.48	15.00
6	ASP N	-44.59	-26.08	66.30	15.00

TABLE III

6	ASP	CA	-43.94	-24.79	66.20	15.00
6	ASP	CB	-44.95	-23.76	65.68	15.00
6	ASP	CG	-44.35	-22.38	65.47	15.00
6	ASP	OD1	-43.14	-22.26	65.21	15.00
6	ASP	OD2	-45.11	-21.39	65.56	15.00
6	ASP	C	-43.47	-24.45	67.60	15.00
6	ASP	O	-44.25	-24.02	68.45	15.00
7	TYR	N	-42.18	-24.61	67.86	15.00
7	TYR	CA	-41.62	-24.34	69.18	15.00
7	TYR	CB	-40.24	-24.98	69.29	15.00
7	TYR	CG	-40.34	-26.48	69.38	15.00
7	TYR	CD1	-40.73	-27.10	70.57	15.00
7	TYR	CE1	-40.88	-28.46	70.65	15.00
7	TYR	CD2	-40.08	-27.28	68.27	15.00
7	TYR	CE2	-40.23	-28.65	68.34	15.00
7	TYR	CZ	-40.63	-29.23	69.53	15.00
7	TYR	OH	-40.78	-30.58	69.62	15.00
7	TYR	C	-41.58	-22.91	69.65	15.00
7	TYR	O	-41.37	-22.64	70.84	15.00
8	ARG	N	-41.80	-21.97	68.74	15.00
8	ARG	CA	-41.78	-20.56	69.11	15.00
8	ARG	CB	-41.99	-19.67	67.87	15.00
8	ARG	CG	-40.88	-19.77	66.84	15.00
8	ARG	CD	-41.23	-19.01	65.57	15.00
8	ARG	NE	-42.50	-19.45	65.01	15.00
8	ARG	CZ	-42.96	-19.10	63.81	15.00
8	ARG	NH1	-42.24	-18.30	63.03	15.00
8	ARG	NH2	-44.15	-19.53	63.40	15.00
8	ARG	C	-42.85	-20.28	70.15	15.00
8	ARG	O	-42.57	-19.72	71.21	15.00
9	LYS	N	-44.06	-20.77	69.88	15.00
9	LYS	CA	-45.18	-20.55	70.78	15.00
9	LYS	CB	-46.50	-20.64	70.02	15.00
9	LYS	CG	-46.63	-21.81	69.10	15.00
9	LYS	CD	-47.93	-21.71	68.33	15.00
9	LYS	CE	-48.22	-22.99	67.54	15.00
9	LYS	NZ	-49.52	-22.90	66.80	15.00
9	LYS	C	-45.22	-21.43	72.02	15.00
9	LYS	O	-46.25	-21.56	72.67	15.00
10	LYS	N	-44.08	-22.02	72.38	15.00
10	LYS	CA	-43.97	-22.87	73.56	15.00
10	LYS	CB	-43.66	-24.32	73.16	15.00

TABLE III

10	LYS	CG	-44.79	-25.04	72.44	15.00
10	LYS	CD	-44.37	-26.46	72.08	15.00
10	LYS	CE	-45.44	-27.16	71.27	15.00
10	LYS	NZ	-45.80	-26.44	70.01	15.00
10	LYS	C	-42.90	-22.38	74.54	15.00
10	LYS	O	-42.69	-22.99	75.59	15.00
11	GLY	N	-42.19	-21.30	74.19	15.00
11	GLY	CA	-41.15	-20.78	75.05	15.00
11	GLY	C	-39.83	-21.52	74.90	15.00
11	GLY	O	-38.95	-21.41	75.74	15.00
12	TYR	N	-39.69	-22.25	73.79	15.00
12	TYR	CA	-38.48	-23.03	73.51	15.00
12	TYR	CB	-38.82	-24.26	72.67	15.00
12	TYR	CG	-39.21	-25.54	73.39	15.00
12	TYR	CD1	-40.43	-25.65	74.06	15.00
12	TYR	CE1	-40.85	-26.87	74.58	15.00
12	TYR	CD2	-38.41	-26.68	73.27	15.00
12	TYR	CE2	-38.83	-27.90	73.79	15.00
12	TYR	CZ	-40.05	-27.98	74.44	15.00
12	TYR	OH	-40.47	-29.19	74.93	15.00
12	TYR	C	-37.45	-22.25	72.72	15.00
12	TYR	O	-36.33	-22.72	72.54	15.00
13	VAL	N	-37.85	-21.09	72.19	15.00
13	VAL	CA	-36.94	-20.29	71.37	15.00
13	VAL	CB	-37.40	-20.32	69.88	15.00
13	VAL	CG1	-38.59	-19.43	69.67	15.00
13	VAL	CG2	-36.26	-19.93	68.97	15.00
13	VAL	C	-36.77	-18.86	71.87	15.00
13	VAL	O	-37.69	-18.26	72.43	15.00
14	THR	N	-35.55	-18.35	71.69	15.00
14	THR	CA	-35.15	-17.00	72.11	15.00
14	THR	CB	-33.72	-17.00	72.67	15.00
14	THR	OG1	-32.83	-17.53	71.69	15.00
14	THR	CG2	-33.64	-17.86	73.91	15.00
14	THR	C	-35.21	-15.98	70.97	15.00
14	THR	O	-35.26	-16.36	69.81	15.00
15	PRO	N	-35.22	-14.68	71.31	15.00
15	PRO	CD	-35.25	-14.08	72.65	15.00
15	PRO	CA	-35.27	-13.64	70.28	15.00
15	PRO	CB	-35.03	-12.35	71.08	15.00
15	PRO	CG	-34.46	-12.83	72.43	15.00
15	PRO	C	-34.23	-13.82	69.17	15.00

TABLE III

15	PRO	O	-33.14	-14.35	69.41	15.00
16	VAL	N	-34.60	-13.42	67.96	15.00
16	VAL	CA	-33.72	-13.53	66.81	15.00
16	VAL	CB	-34.45	-13.16	65.50	15.00
16	VAL	CG1	-33.63	-13.60	64.31	15.00
16	VAL	CG2	-35.81	-13.78	65.47	15.00
16	VAL	C	-32.52	-12.61	66.97	15.00
16	VAL	O	-32.67	-11.42	67.25	15.00
17	LYS	N	-31.32	-13.17	66.80	15.00
17	LYS	CA	-30.09	-12.42	66.91	15.00
17	LYS	CB	-29.08	-13.18	67.77	15.00
17	LYS	CG	-29.01	-12.72	69.22	15.00
17	LYS	CD	-30.27	-13.09	70.02	15.00
17	LYS	CE	-30.18	-14.48	70.64	15.00
17	LYS	NZ	-29.12	-14.54	71.68	15.00
17	LYS	C	-29.49	-12.15	65.54	15.00
17	LYS	O	-29.82	-12.81	64.56	15.00
18	ASN	N	-28.62	-11.15	65.49	15.00
18	ASN	CA	-27.91	-10.77	64.27	15.00
18	ASN	CB	-28.01	-9.26	64.05	15.00
18	ASN	CG	-27.09	-8.78	62.94	15.00
18	ASN	OD1	-26.98	-9.42	61.89	15.00
18	ASN	ND2	-26.38	-7.69	63.19	15.00
18	ASN	C	-26.45	-11.16	64.43	15.00
18	ASN	O	-25.79	-10.73	65.37	15.00
19	GLN	N	-25.94	-11.96	63.51	15.00
19	GLN	CA	-24.56	-12.40	63.60	15.00
19	GLN	CB	-24.34	-13.65	62.77	15.00
19	GLN	CG	-24.88	-13.58	61.37	15.00
19	GLN	CD	-24.42	-14.73	60.53	15.00
19	GLN	OE1	-25.17	-15.28	59.73	15.00
19	GLN	NE2	-23.15	-15.09	60.68	15.00
19	GLN	C	-23.52	-11.35	63.24	15.00
19	GLN	O	-22.35	-11.49	63.60	15.00
20	GLY	N	-23.94	-10.31	62.53	15.00
20	GLY	CA	-23.02	-9.26	62.14	15.00
20	GLY	C	-22.10	-9.67	61.00	15.00
20	GLY	O	-22.51	-10.40	60.11	15.00
21	GLN	N	-20.85	-9.20	61.04	15.00
21	GLN	CA	-19.86	-9.50	60.01	15.00
21	GLN	CB	-18.92	-8.30	59.78	15.00
21	GLN	CG	-19.60	-6.94	59.55	15.00

TABLE III

21	GLN	CD	-20.68	-6.99	58.49	15.00
21	GLN	OE1	-20.49	-7.53	57.41	15.00
21	GLN	NE2	-21.85	-6.43	58.81	15.00
21	GLN	C	-19.03	-10.74	60.38	15.00
21	GLN	O	-18.02	-11.06	59.74	15.00
22	CYS	N	-19.41	-11.42	61.44	15.00
22	CYS	CA	-18.69	-12.60	61.88	15.00
22	CYS	C	-19.37	-13.86	61.33	15.00
22	CYS	O	-20.59	-13.94	61.27	15.00
22	CYS	CB	-18.63	-12.61	63.41	15.00
22	CYS	SG	-17.84	-14.05	64.16	15.00
23	GLY	N	-18.58	-14.81	60.84	15.00
23	GLY	CA	-19.15	-16.03	60.30	15.00
23	GLY	C	-19.41	-17.03	61.41	15.00
23	GLY	O	-18.90	-18.15	61.38	15.00
24	SER	N	-20.22	-16.62	62.37	15.00
24	SER	CA	-20.56	-17.43	63.53	15.00
24	SER	CB	-20.36	-16.59	64.79	15.00
24	SER	OG	-21.14	-15.41	64.68	15.00
24	SER	C	-21.99	-17.95	63.49	15.00
24	SER	O	-22.60	-18.20	64.53	15.00
25	CYS	N	-22.55	-18.14	62.30	15.00
25	CYS	CA	-23.91	-18.65	62.20	15.00
25	CYS	CB	-24.41	-18.63	60.75	15.00
25	CYS	SG	-23.48	-19.60	59.54	15.00
25	CYS	C	-23.96	-20.05	62.82	15.00
25	CYS	O	-24.97	-20.45	63.40	15.00
25	INH	C1	-27.24	-9.28	57.72	15.00
25	INH	C2	-26.55	-9.60	58.90	15.00
25	INH	C3	-25.31	-10.22	58.84	15.00
25	INH	C4	-24.73	-10.54	57.61	15.00
25	INH	C5	-25.43	-10.21	56.44	15.00
25	INH	C6	-26.67	-9.59	56.49	15.00
25	INH	C7	-23.41	-11.26	57.54	15.00
25	INH	O8	-23.43	-12.63	57.98	15.00
25	INH	C9	-22.90	-13.56	57.08	15.00
25	INH	O10	-21.75	-13.43	56.65	15.00
25	INH	C11	-23.40	-15.62	55.77	15.00
25	INH	C12	-22.32	-15.20	54.77	15.00
25	INH	C13	-22.79	-14.65	53.42	15.00
25	INH	C14	-21.66	-14.80	52.41	15.00
25	INH	C15	-24.07	-15.33	52.91	15.00

TABLE III

25	INH	C16	-23.13	-17.06	56.23	15.00
25	INH	O17	-23.79	-17.98	55.74	15.00
25	INH	N18	-22.17	-17.29	57.12	15.00
25	INH	C19	-21.81	-18.63	57.60	15.00
25	INH	N20	-23.72	-14.55	56.73	15.00
25	INH	C21	-21.96	-18.81	59.10	15.00
25	INH	O22	-21.89	-17.72	59.66	15.00
25	INH	C23	-19.42	-29.07	54.27	15.00
25	INH	C24	-20.11	-28.05	54.90	15.00
25	INH	C25	-19.45	-26.88	55.23	15.00
25	INH	C26	-18.09	-26.70	54.93	15.00
25	INH	C27	-17.41	-27.74	54.30	15.00
25	INH	C28	-18.06	-28.92	53.96	15.00
25	INH	C29	-17.39	-25.41	55.26	15.00
25	INH	O30	-18.05	-24.15	55.06	15.00
25	INH	C31	-19.20	-23.80	55.81	15.00
25	INH	O32	-20.33	-23.84	55.32	15.00
25	INH	C33	-20.15	-23.05	57.92	15.00
25	INH	C34	-20.47	-24.13	58.95	15.00
25	INH	C35	-21.49	-25.18	58.56	15.00
25	INH	C36	-22.36	-24.69	57.40	15.00
25	INH	C37	-20.73	-26.42	58.16	15.00
25	INH	C38	-19.89	-21.74	58.63	15.00
25	INH	O39	-18.75	-21.39	58.90	15.00
25	INH	N40	-20.97	-21.01	58.95	15.00
25	INH	C41	-20.91	-19.72	59.64	15.00
25	INH	N42	-19.01	-23.44	57.08	15.00
26	TRP	N	-22.84	-20.77	62.76	15.00
26	TRP	CA	-22.76	-22.11	63.33	15.00
26	TRP	CB	-21.47	-22.81	62.88	15.00
26	TRP	CG	-20.24	-22.16	63.40	15.00
26	TRP	CD2	-19.56	-22.46	64.62	15.00
26	TRP	CE2	-18.51	-21.53	64.75	15.00
26	TRP	CE3	-19.74	-23.42	65.63	15.00
26	TRP	CD1	-19.59	-21.11	62.84	15.00
26	TRP	NE1	-18.55	-20.72	63.65	15.00
26	TRP	CZ2	-17.64	-21.52	65.85	15.00
26	TRP	CZ3	-18.88	-23.42	66.72	15.00
26	TRP	CH2	-17.84	-22.47	66.82	15.00
26	TRP	C	-22.82	-22.02	64.87	15.00
26	TRP	O	-23.31	-22.93	65.53	15.00
27	ALA	N	-22.34	-20.92	65.44	15.00

TABLE III

27	ALA	CA	-22.36	-20.73	66.89	15.00
27	ALA	CB	-21.43	-19.61	67.30	15.00
27	ALA	C	-23.79	-20.43	67.32	15.00
27	ALA	O	-24.29	-21.00	68.29	15.00
28	PHE	N	-24.48	-19.57	66.58	15.00
28	PHE	CA	-25.85	-19.25	66.92	15.00
28	PHE	CB	-26.38	-18.14	66.01	15.00
28	PHE	CG	-25.87	-16.78	66.39	15.00
28	PHE	CD1	-24.63	-16.33	65.94	15.00
28	PHE	CD2	-26.61	-15.96	67.22	15.00
28	PHE	CE1	-24.14	-15.10	66.33	15.00
28	PHE	CE2	-26.11	-14.72	67.62	15.00
28	PHE	CZ	-24.88	-14.29	67.17	15.00
28	PHE	C	-26.73	-20.49	66.83	15.00
28	PHE	O	-27.48	-20.80	67.75	15.00
29	SER	N	-26.60	-21.24	65.74	15.00
29	SER	CA	-27.36	-22.46	65.54	15.00
29	SER	CB	-26.91	-23.14	64.25	15.00
29	SER	OG	-27.55	-24.39	64.08	15.00
29	SER	C	-27.17	-23.43	66.70	15.00
29	SER	O	-28.14	-23.89	67.30	15.00
30	SER	N	-25.91	-23.75	67.01	15.00
30	SER	CA	-25.57	-24.67	68.09	15.00
30	SER	CB	-24.06	-24.68	68.33	15.00
30	SER	OG	-23.33	-25.06	67.19	15.00
30	SER	C	-26.28	-24.24	69.38	15.00
30	SER	O	-27.01	-25.02	70.01	15.00
31	VAL	N	-26.09	-22.97	69.73	15.00
31	VAL	CA	-26.67	-22.39	70.93	15.00
31	VAL	CB	-26.13	-20.95	71.14	15.00
31	VAL	CG1	-27.14	-20.07	71.79	15.00
31	VAL	CG2	-24.87	-20.99	71.99	15.00
31	VAL	C	-28.21	-22.46	70.89	15.00
31	VAL	O	-28.86	-22.68	71.92	15.00
32	GLY	N	-28.79	-22.36	69.70	15.00
32	GLY	CA	-30.23	-22.42	69.58	15.00
32	GLY	C	-30.77	-23.77	69.99	15.00
32	GLY	O	-31.84	-23.88	70.58	15.00
33	ALA	N	-30.04	-24.83	69.66	15.00
33	ALA	CA	-30.46	-26.18	70.01	15.00
33	ALA	CB	-29.67	-27.20	69.23	15.00
33	ALA	C	-30.27	-26.36	71.50	15.00

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TABLE III

33 ALA O	-31.10	-26.99	72.17	15.00
34 LEU N	-29.20	-25.80	72.04	15.00
34 LEU CA	-28.91	-25.88	73.47	15.00
34 LEU CB	-27.55	-25.25	73.77	15.00
34 LEU CG	-26.35	-26.14	73.47	15.00
34 LEU CD1	-25.07	-25.37	73.60	15.00
34 LEU CD2	-26.34	-27.30	74.42	15.00
34 LEU C	-30.00	-25.20	74.29	15.00
34 LEU O	-30.37	-25.66	75.38	15.00
35 GLU N	-30.56	-24.10	73.78	15.00
35 GLU CA	-31.61	-23.39	74.49	15.00
35 GLU CB	-31.82	-22.00	73.88	15.00
35 GLU CG	-30.62	-21.08	74.05	15.00
35 GLU CD	-30.60	-19.92	73.08	15.00
35 GLU OE1	-31.49	-19.83	72.21	15.00
35 GLU OE2	-29.66	-19.10	73.17	15.00
35 GLU C	-32.91	-24.18	74.47	15.00
35 GLU O	-33.62	-24.26	75.47	15.00
36 GLY N	-33.21	-24.80	73.33	15.00
36 GLY CA	-34.43	-25.58	73.22	15.00
36 GLY C	-34.49	-26.72	74.22	15.00
36 GLY O	-35.52	-26.94	74.86	15.00
37 GLN N	-33.38	-27.43	74.36	15.00
37 GLN CA	-33.27	-28.55	75.29	15.00
37 GLN CB	-31.99	-29.34	75.02	15.00
37 GLN CG	-32.04	-30.08	73.69	15.00
37 GLN CD	-33.27	-30.95	73.58	15.00
37 GLN OE1	-33.55	-31.77	74.45	15.00
37 GLN NE2	-34.04	-30.77	72.52	15.00
37 GLN C	-33.31	-28.07	76.74	15.00
37 GLN O	-33.94	-28.69	77.60	15.00
38 LEU N	-32.66	-26.94	77.00	15.00
38 LEU CA	-32.66	-26.34	78.34	15.00
38 LEU CB	-31.99	-24.97	78.30	15.00
38 LEU CG	-31.70	-24.28	79.63	15.00
38 LEU CD1	-30.58	-25.02	80.35	15.00
38 LEU CD2	-31.32	-22.84	79.40	15.00
38 LEU C	-34.11	-26.19	78.79	15.00
38 LEU O	-34.52	-26.71	79.82	15.00
39 LYS N	-34.91	-25.51	77.97	15.00
39 LYS CA	-36.31	-25.29	78.27	15.00
39 LYS CB	-36.98	-24.53	77.12	15.00

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TABLE III

39	LYS	CG	-38.48	-24.37	77.25	15.00
39	LYS	CD	-38.89	-23.62	78.49	15.00
39	LYS	CE	-40.38	-23.44	78.51	15.00
39	LYS	NZ	-40.84	-22.84	79.78	15.00
39	LYS	C	-37.01	-26.62	78.50	15.00
39	LYS	O	-37.78	-26.76	79.44	15.00
40	LYS	N	-36.70	-27.62	77.68	15.00
40	LYS	CA	-37.32	-28.93	77.83	15.00
40	LYS	CB	-36.78	-29.89	76.76	15.00
40	LYS	CG	-37.56	-31.18	76.57	15.00
40	LYS	CD	-36.89	-32.09	75.54	15.00
40	LYS	CE	-37.73	-33.32	75.24	15.00
40	LYS	NZ	-39.05	-32.97	74.63	15.00
40	LYS	C	-37.07	-29.52	79.22	15.00
40	LYS	O	-38.00	-29.92	79.93	15.00
41	LYS	N	-35.80	-29.51	79.64	15.00
41	LYS	CA	-35.41	-30.07	80.92	15.00
41	LYS	CB	-33.92	-30.40	80.91	15.00
41	LYS	CG	-33.48	-31.19	79.67	15.00
41	LYS	CD	-34.36	-32.41	79.42	15.00
41	LYS	CE	-34.05	-33.08	78.08	15.00
41	LYS	NZ	-34.99	-34.21	77.78	15.00
41	LYS	C	-35.76	-29.21	82.13	15.00
41	LYS	O	-36.58	-29.61	82.96	15.00
42	THR	N	-35.17	-28.02	82.25	15.00
42	THR	CA	-35.41	-27.14	83.39	15.00
42	THR	CB	-34.27	-26.12	83.52	15.00
42	THR	OG1	-34.29	-25.25	82.38	15.00
42	THR	CG2	-32.94	-26.82	83.57	15.00
42	THR	C	-36.72	-26.37	83.39	15.00
42	THR	O	-37.10	-25.79	84.41	15.00
43	GLY	N	-37.40	-26.33	82.25	15.00
43	GLY	CA	-38.65	-25.60	82.15	15.00
43	GLY	C	-38.47	-24.08	82.03	15.00
43	GLY	O	-39.43	-23.33	81.98	15.00
44	LYS	N	-37.24	-23.57	82.01	15.00
44	LYS	CA	-37.05	-22.13	81.89	15.00
44	LYS	CB	-36.55	-21.53	83.20	15.00
44	LYS	CG	-37.49	-21.67	84.38	15.00
44	LYS	CD	-36.91	-20.99	85.61	15.00
44	LYS	CE	-35.68	-21.70	86.11	15.00
44	LYS	NZ	-36.03	-23.03	86.65	15.00

TABLE III

44	LYS	C	-36.05	-21.83	80.80	15.00
44	LYS	O	-35.00	-22.48	80.70	15.00
45	LEU	N	-36.39	-20.84	79.97	15.00
45	LEU	CA	-35.55	-20.41	78.86	15.00
45	LEU	CB	-36.43	-19.88	77.73	15.00
45	LEU	CG	-35.82	-19.71	76.33	15.00
45	LEU	CD1	-35.62	-21.08	75.69	15.00
45	LEU	CD2	-36.74	-18.87	75.48	15.00
45	LEU	C	-34.58	-19.34	79.32	15.00
45	LEU	O	-34.92	-18.47	80.13	15.00
46	LEU	N	-33.36	-19.39	78.80	15.00
46	LEU	CA	-32.32	-18.44	79.15	15.00
46	LEU	CB	-31.47	-19.02	80.28	15.00
46	LEU	CG	-30.58	-18.14	81.17	15.00
46	LEU	CD1	-29.23	-17.96	80.55	15.00
46	LEU	CD2	-31.23	-16.81	81.44	15.00
46	LEU	C	-31.51	-18.26	77.86	15.00
46	LEU	O	-31.48	-19.15	77.01	15.00
47	ASN	N	-30.92	-17.08	77.67	15.00
47	ASN	CA	-30.14	-16.82	76.47	15.00
47	ASN	CB	-30.22	-15.35	76.06	15.00
47	ASN	CG	-31.33	-15.09	75.06	15.00
47	ASN	OD1	-32.44	-14.74	75.43	15.00
47	ASN	ND2	-31.04	-15.28	73.78	15.00
47	ASN	C	-28.69	-17.26	76.64	15.00
47	ASN	O	-27.98	-16.75	77.50	15.00
48	LEU	N	-28.27	-18.21	75.82	15.00
48	LEU	CA	-26.92	-18.73	75.89	15.00
48	LEU	CB	-26.89	-20.21	75.51	15.00
48	LEU	CG	-27.53	-21.15	76.55	15.00
48	LEU	CD1	-27.34	-22.60	76.17	15.00
48	LEU	CD2	-26.88	-20.92	77.88	15.00
48	LEU	C	-25.93	-17.89	75.07	15.00
48	LEU	O	-26.32	-17.11	74.20	15.00
49	SER	N	-24.64	-18.08	75.35	15.00
49	SER	CA	-23.56	-17.34	74.70	15.00
49	SER	CB	-22.47	-17.07	75.75	15.00
49	SER	OG	-21.31	-16.50	75.18	15.00
49	SER	C	-22.92	-17.91	73.43	15.00
49	SER	O	-22.16	-18.88	73.48	15.00
50	PRO	N	-23.22	-17.30	72.26	15.00
50	PRO	CD	-24.28	-16.31	72.02	15.00

TABLE III

50 PRO CA	-22.65	-17.75	70.98	15.00
50 PRO CB	-23.42	-16.92	69.95	15.00
50 PRO CG	-24.70	-16.64	70.62	15.00
50 PRO C	-21.16	-17.38	70.95	15.00
50 PRO O	-20.34	-18.08	70.35	15.00
51 GLN N	-20.81	-16.27	71.59	15.00
51 GLN CA	-19.43	-15.80	71.65	15.00
51 GLN CB	-19.35	-14.43	72.34	15.00
51 GLN CG	-17.95	-13.79	72.39	15.00
51 GLN CD	-17.46	-13.23	71.05	15.00
51 GLN OE1	-18.21	-12.62	70.30	15.00
51 GLN NE2	-16.19	-13.42	70.77	15.00
51 GLN C	-18.58	-16.83	72.38	15.00
51 GLN O	-17.46	-17.15	71.96	15.00
52 ASN N	-19.13	-17.42	73.44	15.00
52 ASN CA	-18.41	-18.42	74.24	15.00
52 ASN CB	-19.31	-18.96	75.35	15.00
52 ASN CG	-18.59	-19.90	76.31	15.00
52 ASN OD1	-19.23	-20.62	77.07	15.00
52 ASN ND2	-17.27	-19.89	76.28	15.00
52 ASN C	-17.91	-19.55	73.35	15.00
52 ASN O	-16.84	-20.12	73.59	15.00
53 LEU N	-18.67	-19.86	72.31	15.00
53 LEU CA	-18.33	-20.90	71.35	15.00
53 LEU CB	-19.58	-21.37	70.60	15.00
53 LEU CG	-20.63	-22.10	71.42	15.00
53 LEU CD1	-21.81	-22.44	70.55	15.00
53 LEU CD2	-20.01	-23.36	72.01	15.00
53 LEU C	-17.31	-20.42	70.34	15.00
53 LEU O	-16.37	-21.13	69.99	15.00
54 VAL N	-17.52	-19.19	69.87	15.00
54 VAL CA	-16.66	-18.57	68.87	15.00
54 VAL CB	-17.16	-17.14	68.56	15.00
54 VAL CG1	-16.22	-16.45	67.59	15.00
54 VAL CG2	-18.57	-17.20	68.00	15.00
54 VAL C	-15.20	-18.52	69.30	15.00
54 VAL O	-14.31	-18.88	68.53	15.00
55 ASP N	-14.96	-18.09	70.54	15.00
55 ASP CA	-13.61	-17.98	71.07	15.00
55 ASP CB	-13.58	-16.93	72.18	15.00
55 ASP CG	-14.14	-15.59	71.76	15.00
55 ASP OD1	-14.26	-15.33	70.55	15.00

TABLE III

55	ASP	OD2	-14.45	-14.78	72.67	15.00
55	ASP	C	-13.02	-19.26	71.65	15.00
55	ASP	O	-11.80	-19.39	71.72	15.00
56	CYS	N	-13.86	-20.19	72.09	15.00
56	CYS	CA	-13.36	-21.41	72.73	15.00
56	CYS	C	-13.29	-22.71	71.94	15.00
56	CYS	O	-12.43	-23.55	72.20	15.00
56	CYS	CB	-14.10	-21.61	74.04	15.00
56	CYS	SG	-14.21	-20.10	75.06	15.00
57	VAL	N	-14.17	-22.93	70.96	15.00
57	VAL	CA	-14.13	-24.17	70.18	15.00
57	VAL	CB	-15.44	-24.43	69.39	15.00
57	VAL	CG1	-15.38	-25.80	68.73	15.00
57	VAL	CG2	-16.63	-24.33	70.30	15.00
57	VAL	C	-12.97	-24.10	69.19	15.00
57	VAL	O	-13.17	-23.81	68.02	15.00
58	SER	N	-11.76	-24.40	69.66	15.00
58	SER	CA	-10.57	-24.35	68.82	15.00
58	SER	CB	-9.34	-24.73	69.63	15.00
58	SER	OG	-9.44	-26.08	70.07	15.00
58	SER	C	-10.65	-25.25	67.61	15.00
58	SER	O	-9.90	-25.09	66.65	15.00
59	GLU	N	-11.53	-26.25	67.65	15.00
59	GLU	CA	-11.69	-27.16	66.53	15.00
59	GLU	CB	-12.57	-28.35	66.92	15.00
59	GLU	CG	-12.00	-29.23	68.00	15.00
59	GLU	CD	-11.98	-28.56	69.36	15.00
59	GLU	OE1	-13.00	-27.95	69.73	15.00
59	GLU	OE2	-10.95	-28.66	70.06	15.00
59	GLU	C	-12.30	-26.41	65.35	15.00
59	GLU	O	-12.28	-26.89	64.22	15.00
60	ASN	N	-12.89	-25.26	65.63	15.00
60	ASN	CA	-13.53	-24.45	64.61	15.00
60	ASN	CB	-14.95	-24.06	65.03	15.00
60	ASN	CG	-15.92	-25.21	64.90	15.00
60	ASN	OD1	-17.09	-25.08	65.23	15.00
60	ASN	ND2	-15.45	-26.34	64.38	15.00
60	ASN	C	-12.71	-23.22	64.26	15.00
60	ASN	O	-11.73	-22.92	64.93	15.00
61	ASP	N	-13.13	-22.50	63.23	15.00
61	ASP	CA	-12.41	-21.34	62.75	15.00
61	ASP	CB	-12.53	-21.28	61.22	15.00

TABLE III

61 ASP CG	-11.20	-21.01	60.53	15.00
61 ASP OD1	-10.34	-20.32	61.12	15.00
61 ASP OD2	-11.03	-21.49	59.40	15.00
61 ASP C	-12.80	-19.99	63.35	15.00
61 ASP O	-12.23	-18.95	62.99	15.00
62 GLY N	-13.75	-19.97	64.28	15.00
62 GLY CA	-14.17	-18.71	64.87	15.00
62 GLY C	-15.12	-18.03	63.91	15.00
62 GLY O	-16.13	-18.61	63.51	15.00
63 CYS N	-14.80	-16.81	63.48	15.00
63 CYS CA	-15.65	-16.09	62.52	15.00
63 CYS C	-15.45	-16.63	61.12	15.00
63 CYS O	-16.10	-16.16	60.18	15.00
63 CYS CB	-15.34	-14.59	62.52	15.00
63 CYS SG	-15.84	-13.72	64.03	15.00
64 GLY N	-14.52	-17.56	60.95	15.00
64 GLY CA	-14.26	-18.14	59.65	15.00
64 GLY C	-15.17	-19.33	59.40	15.00
64 GLY O	-15.50	-19.67	58.26	15.00
65 GLY N	-15.60	-19.99	60.48	15.00
65 GLY CA	-16.47	-21.14	60.33	15.00
65 GLY C	-16.39	-22.20	61.41	15.00
65 GLY O	-15.56	-22.15	62.31	15.00
66 GLY N	-17.28	-23.18	61.30	15.00
66 GLY CA	-17.31	-24.25	62.27	15.00
66 GLY C	-18.50	-25.16	62.14	15.00
66 GLY O	-19.48	-24.83	61.48	15.00
67 TYR N	-18.43	-26.32	62.78	15.00
67 TYR CA	-19.51	-27.30	62.74	15.00
67 TYR CB	-18.97	-28.70	62.45	15.00
67 TYR CG	-18.28	-28.86	61.12	15.00
67 TYR CD1	-19.02	-29.00	59.94	15.00
67 TYR CE1	-18.40	-29.23	58.72	15.00
67 TYR CD2	-16.90	-28.94	61.04	15.00
67 TYR CE2	-16.26	-29.16	59.82	15.00
67 TYR CZ	-17.02	-29.31	58.67	15.00
67 TYR OH	-16.39	-29.51	57.46	15.00
67 TYR C	-20.17	-27.29	64.10	15.00
67 TYR O	-19.48	-27.14	65.12	15.00
68 MET N	-21.48	-27.47	64.12	15.00
68 MET CA	-22.26	-27.48	65.36	15.00
68 MET CB	-23.76	-27.60	65.07	15.00

TABLE III

68	MET	CG	-24.38	-26.42	64.29	15.00
68	MET	SD	-23.94	-26.32	62.55	15.00
68	MET	CE	-25.16	-27.35	61.83	15.00
68	MET	C	-21.81	-28.62	66.27	15.00
68	MET	O	-21.63	-28.43	67.47	15.00
69	THR	N	-21.58	-29.79	65.68	15.00
69	THR	CA	-21.15	-30.96	66.43	15.00
69	THR	CB	-20.90	-32.18	65.50	15.00
69	THR	OG1	-20.04	-31.81	64.42	15.00
69	THR	CG2	-22.21	-32.71	64.94	15.00
69	THR	C	-19.90	-30.65	67.25	15.00
69	THR	O	-19.80	-31.06	68.41	15.00
70	ASN	N	-18.98	-29.86	66.69	15.00
70	ASN	CA	-17.74	-29.49	67.37	15.00
70	ASN	CB	-16.79	-28.76	66.42	15.00
70	ASN	CG	-16.05	-29.71	65.50	15.00
70	ASN	OD1	-14.84	-29.64	65.39	15.00
70	ASN	ND2	-16.78	-30.58	64.83	15.00
70	ASN	C	-18.01	-28.62	68.59	15.00
70	ASN	O	-17.32	-28.74	69.60	15.00
71	ALA	N	-19.03	-27.77	68.48	15.00
71	ALA	CA	-19.43	-26.88	69.56	15.00
71	ALA	CB	-20.37	-25.81	69.04	15.00
71	ALA	C	-20.12	-27.68	70.67	15.00
71	ALA	O	-20.03	-27.32	71.84	15.00
72	PHE	N	-20.85	-28.72	70.28	15.00
72	PHE	CA	-21.54	-29.59	71.22	15.00
72	PHE	CB	-22.36	-30.65	70.47	15.00
72	PHE	CG	-23.54	-30.11	69.74	15.00
72	PHE	CD1	-24.28	-29.06	70.24	15.00
72	PHE	CD2	-23.91	-30.66	68.53	15.00
72	PHE	CE1	-25.36	-28.56	69.55	15.00
72	PHE	CE2	-25.00	-30.17	67.83	15.00
72	PHE	CZ	-25.72	-29.12	68.34	15.00
72	PHE	C	-20.46	-30.29	72.05	15.00
72	PHE	O	-20.43	-30.18	73.28	15.00
73	GLN	N	-19.58	-30.98	71.34	15.00
73	GLN	CA	-18.47	-31.71	71.92	15.00
73	GLN	CB	-17.53	-32.13	70.78	15.00
73	GLN	CG	-16.60	-33.30	71.06	15.00
73	GLN	CD	-17.31	-34.63	71.03	15.00
73	GLN	OE1	-17.80	-35.13	72.06	15.00

TABLE III

73	GLN	NE2	-17.35	-35.25	69.85	15.00
73	GLN	C	-17.74	-30.81	72.93	15.00
73	GLN	O	-17.27	-31.26	73.97	15.00
74	TYR	N	-17.66	-29.51	72.63	15.00
74	TYR	CA	-17.00	-28.57	73.51	15.00
74	TYR	CB	-16.75	-27.21	72.81	15.00
74	TYR	CG	-16.41	-26.08	73.77	15.00
74	TYR	CD1	-15.19	-26.05	74.43	15.00
74	TYR	CE1	-14.91	-25.06	75.37	15.00
74	TYR	CD2	-17.34	-25.09	74.06	15.00
74	TYR	CE2	-17.07	-24.10	75.00	15.00
74	TYR	CZ	-15.86	-24.09	75.66	15.00
74	TYR	OH	-15.60	-23.15	76.63	15.00
74	TYR	C	-17.75	-28.36	74.82	15.00
74	TYR	O	-17.14	-28.37	75.89	15.00
75	VAL	N	-19.07	-28.16	74.78	15.00
75	VAL	CA	-19.85	-27.94	76.02	15.00
75	VAL	CB	-21.30	-27.45	75.73	15.00
75	VAL	CG1	-22.06	-27.23	77.04	15.00
75	VAL	CG2	-21.27	-26.15	74.92	15.00
75	VAL	C	-19.87	-29.20	76.91	15.00
75	VAL	O	-20.07	-29.13	78.12	15.00
76	GLN	N	-19.65	-30.35	76.29	15.00
76	GLN	CA	-19.62	-31.60	77.01	15.00
76	GLN	CB	-19.93	-32.73	76.04	15.00
76	GLN	CG	-20.02	-34.11	76.67	15.00
76	GLN	CD	-19.74	-35.20	75.68	15.00
76	GLN	OE1	-20.14	-35.11	74.52	15.00
76	GLN	NE2	-19.01	-36.22	76.11	15.00
76	GLN	C	-18.25	-31.81	77.66	15.00
76	GLN	O	-18.14	-32.17	78.85	15.00
77	LYS	N	-17.18	-31.59	76.89	15.00
77	LYS	CA	-15.82	-31.78	77.39	15.00
77	LYS	CB	-14.83	-31.98	76.24	15.00
77	LYS	CG	-14.56	-30.75	75.41	15.00
77	LYS	CD	-13.69	-31.09	74.19	15.00
77	LYS	CE	-14.41	-32.05	73.24	15.00
77	LYS	NZ	-13.62	-32.45	72.02	15.00
77	LYS	C	-15.34	-30.65	78.29	15.00
77	LYS	O	-14.37	-30.81	79.01	15.00
78	ASN	N	-15.97	-29.49	78.22	15.00
78	ASN	CA	-15.60	-28.37	79.07	15.00

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TABLE III

78	ASN	CB	-15.58	-27.07	78.27	15.00
78	ASN	CG	-15.38	-25.85	79.16	15.00
78	ASN	OD1	-14.28	-25.58	79.64	15.00
78	ASN	ND2	-16.45	-25.11	79.37	15.00
78	ASN	C	-16.62	-28.28	80.20	15.00
78	ASN	O	-16.36	-27.67	81.23	15.00
79	ARG	N	-17.77	-28.91	79.97	15.00
79	ARG	CA	-18.89	-28.98	80.92	15.00
79	ARG	CB	-18.58	-29.92	82.11	15.00
79	ARG	CG	-17.47	-29.49	83.06	15.00
79	ARG	CD	-16.62	-30.66	83.51	15.00
79	ARG	NE	-17.44	-31.76	84.00	15.00
79	ARG	CZ	-17.90	-32.75	83.23	15.00
79	ARG	NH1	-17.60	-32.77	81.93	15.00
79	ARG	NH2	-18.73	-33.66	83.74	15.00
79	ARG	C	-19.45	-27.65	81.39	15.00
79	ARG	O	-19.42	-27.31	82.57	15.00
80	GLY	N	-20.00	-26.92	80.44	15.00
80	GLY	CA	-20.58	-25.63	80.75	15.00
80	GLY	C	-20.41	-24.62	79.63	15.00
80	GLY	O	-19.39	-24.61	78.93	15.00
81	ILE	N	-21.44	-23.82	79.44	15.00
81	ILE	CA	-21.45	-22.77	78.45	15.00
81	ILE	CB	-22.27	-23.14	77.21	15.00
81	ILE	CG2	-23.71	-23.46	77.59	15.00
81	ILE	CG1	-22.18	-22.01	76.17	15.00
81	ILE	CD1	-22.74	-22.34	74.79	15.00
81	ILE	C	-22.09	-21.59	79.18	15.00
81	ILE	O	-23.08	-21.77	79.89	15.00
82	ASP	N	-21.48	-20.42	79.06	15.00
82	ASP	CA	-21.99	-19.22	79.72	15.00
82	ASP	CB	-20.95	-18.10	79.68	15.00
82	ASP	CG	-19.75	-18.37	80.56	15.00
82	ASP	OD1	-18.66	-17.89	80.20	15.00
82	ASP	OD2	-19.89	-19.03	81.62	15.00
82	ASP	C	-23.27	-18.70	79.09	15.00
82	ASP	O	-23.67	-19.11	78.01	15.00
83	SER	N	-23.91	-17.78	79.79	15.00
83	SER	CA	-25.12	-17.15	79.30	15.00
83	SER	CB	-26.03	-16.79	80.46	15.00
83	SER	OG	-25.32	-16.05	81.44	15.00
83	SER	C	-24.66	-15.90	78.58	15.00

TABLE III

83	SER	O	-23.49	-15.51	78.67	15.00
84	GLU	N	-25.57	-15.24	77.87	15.00
84	GLU	CA	-25.22	-14.02	77.16	15.00
84	GLU	CB	-26.40	-13.50	76.35	15.00
84	GLU	CG	-26.09	-12.30	75.46	15.00
84	GLU	CD	-25.06	-12.58	74.36	15.00
84	GLU	OE1	-25.03	-13.69	73.78	15.00
84	GLU	OE2	-24.28	-11.66	74.06	15.00
84	GLU	C	-24.70	-12.95	78.14	15.00
84	GLU	O	-23.64	-12.37	77.92	15.00
85	ASP	N	-25.41	-12.69	79.23	15.00
85	ASP	CA	-24.95	-11.70	80.20	15.00
85	ASP	CB	-25.99	-11.46	81.31	15.00
85	ASP	CG	-25.59	-10.32	82.30	15.00
85	ASP	OD1	-26.24	-10.19	83.38	15.00
85	ASP	OD2	-24.66	-9.54	82.02	15.00
85	ASP	C	-23.63	-12.15	80.82	15.00
85	ASP	O	-22.86	-11.34	81.34	15.00
86	ALA	N	-23.31	-13.44	80.74	15.00
86	ALA	CA	-22.07	-13.91	81.32	15.00
86	ALA	CB	-22.24	-15.30	81.86	15.00
86	ALA	C	-20.90	-13.85	80.35	15.00
86	ALA	O	-19.74	-13.84	80.76	15.00
87	TYR	N	-21.19	-13.82	79.05	15.00
87	TYR	CA	-20.14	-13.77	78.03	15.00
87	TYR	CB	-19.67	-15.20	77.77	15.00
87	TYR	CG	-18.31	-15.36	77.13	15.00
87	TYR	CD1	-17.86	-14.49	76.13	15.00
87	TYR	CE1	-16.64	-14.70	75.51	15.00
87	TYR	CD2	-17.49	-16.43	77.48	15.00
87	TYR	CE2	-16.27	-16.64	76.86	15.00
87	TYR	CZ	-15.85	-15.78	75.88	15.00
87	TYR	OH	-14.65	-16.03	75.26	15.00
87	TYR	C	-20.73	-13.17	76.75	15.00
87	TYR	O	-20.92	-13.88	75.76	15.00
88	PRO	N	-20.99	-11.84	76.74	15.00
88	PRO	CD	-20.79	-10.92	77.87	15.00
88	PRO	CA	-21.57	-11.12	75.60	15.00
88	PRO	CB	-21.52	-9.66	76.07	15.00
88	PRO	CG	-21.75	-9.80	77.54	15.00
88	PRO	C	-20.91	-11.29	74.24	15.00
88	PRO	O	-19.71	-11.56	74.13	15.00

TABLE III

89	TYR	N	-21.72	-11.10	73.21	15.00
89	TYR	CA	-21.30	-11.23	71.83	15.00
89	TYR	CB	-22.51	-11.59	70.96	15.00
89	TYR	CG	-22.16	-12.03	69.56	15.00
89	TYR	CD1	-21.27	-13.09	69.35	15.00
89	TYR	CE1	-20.90	-13.46	68.07	15.00
89	TYR	CD2	-22.67	-11.37	68.45	15.00
89	TYR	CE2	-22.31	-11.74	67.17	15.00
89	TYR	CZ	-21.42	-12.78	66.98	15.00
89	TYR	OH	-21.02	-13.12	65.72	15.00
89	TYR	C	-20.67	-9.90	71.38	15.00
89	TYR	O	-21.33	-8.86	71.36	15.00
90	VAL	N	-19.38	-9.93	71.05	15.00
90	VAL	CA	-18.66	-8.73	70.61	15.00
90	VAL	CB	-17.25	-8.65	71.22	15.00
90	VAL	CG1	-17.32	-8.67	72.73	15.00
90	VAL	CG2	-16.37	-9.78	70.68	15.00
90	VAL	C	-18.54	-8.62	69.11	15.00
90	VAL	O	-17.85	-7.75	68.61	15.00
91	GLY	N	-19.14	-9.55	68.39	15.00
91	GLY	CA	-19.10	-9.49	66.94	15.00
91	GLY	C	-17.76	-9.77	66.31	15.00
91	GLY	O	-17.52	-9.39	65.15	15.00
92	GLN	N	-16.88	-10.44	67.03	15.00
92	GLN	CA	-15.56	-10.77	66.50	15.00
92	GLN	CB	-14.74	-9.51	66.31	15.00
92	GLN	CG	-14.49	-8.76	67.60	15.00
92	GLN	CD	-13.93	-7.40	67.35	15.00
92	GLN	OE1	-12.83	-7.06	67.80	15.00
92	GLN	NE2	-14.67	-6.59	66.60	15.00
92	GLN	C	-14.81	-11.73	67.41	15.00
92	GLN	O	-15.19	-11.95	68.57	15.00
93	GLU	N	-13.72	-12.26	66.89	15.00
93	GLU	CA	-12.90	-13.22	67.59	15.00
93	GLU	CB	-12.01	-13.95	66.59	15.00
93	GLU	CG	-12.77	-14.60	65.42	15.00
93	GLU	CD	-11.84	-15.07	64.31	15.00
93	GLU	OE1	-10.67	-15.37	64.62	15.00
93	GLU	OE2	-12.27	-15.13	63.13	15.00
93	GLU	C	-12.05	-12.56	68.66	15.00
93	GLU	O	-11.53	-11.46	68.49	15.00
94	GLU	N	-11.92	-13.25	69.78	15.00

TABLE III

94	GLU	CA	-11.13	-12.78	70.91	15.00
94	GLU	CB	-11.93	-11.79	71.76	15.00
94	GLU	CG	-13.39	-12.15	71.95	15.00
94	GLU	CD	-14.00	-11.50	73.18	15.00
94	GLU	OE1	-14.15	-10.26	73.18	15.00
94	GLU	OE2	-14.31	-12.24	74.14	15.00
94	GLU	C	-10.73	-13.98	71.74	15.00
94	GLU	O	-11.15	-15.10	71.47	15.00
95	SER	N	-9.88	-13.75	72.73	15.00
95	SER	CA	-9.40	-14.80	73.61	15.00
95	SER	CB	-8.39	-14.21	74.60	15.00
95	SER	OG	-7.22	-13.77	73.94	15.00
95	SER	C	-10.57	-15.44	74.35	15.00
95	SER	O	-11.48	-14.73	74.82	15.00
96	CYS	N	-10.55	-16.77	74.42	15.00
96	CYS	CA	-11.59	-17.52	75.13	15.00
96	CYS	C	-11.61	-17.01	76.56	15.00
96	CYS	O	-10.57	-16.90	77.21	15.00
96	CYS	CB	-11.31	-19.03	75.08	15.00
96	CYS	SG	-12.44	-20.07	76.07	15.00
97	MET	N	-12.80	-16.65	77.03	15.00
97	MET	CA	-12.96	-16.09	78.36	15.00
97	MET	CB	-13.24	-14.58	78.26	15.00
97	MET	CG	-12.05	-13.75	77.73	15.00
97	MET	SD	-12.56	-12.29	76.76	15.00
97	MET	CE	-13.48	-11.34	78.03	15.00
97	MET	C	-14.07	-16.78	79.14	15.00
97	MET	O	-14.87	-16.11	79.82	15.00
98	TYR	N	-14.13	-18.10	79.07	15.00
98	TYR	CA	-15.15	-18.84	79.78	15.00
98	TYR	CB	-15.00	-20.35	79.61	15.00
98	TYR	CG	-16.06	-21.14	80.35	15.00
98	TYR	CD1	-17.39	-21.10	79.94	15.00
98	TYR	CE1	-18.38	-21.80	80.65	15.00
98	TYR	CD2	-15.74	-21.90	81.48	15.00
98	TYR	CE2	-16.72	-22.60	82.18	15.00
98	TYR	CZ	-18.03	-22.54	81.76	15.00
98	TYR	OH	-19.00	-23.23	82.44	15.00
98	TYR	C	-15.08	-18.52	81.26	15.00
98	TYR	O	-14.04	-18.68	81.89	15.00
99	ASN	N	-16.19	-18.01	81.79	15.00
99	ASN	CA	-16.31	-17.67	83.19	15.00

TABLE III

99	ASN	CB	-16.96	-16.29	83.38	15.00
99	ASN	CG	-17.25	-15.98	84.84	15.00
99	ASN	OD1	-16.67	-16.58	85.75	15.00
99	ASN	ND2	-18.19	-15.06	85.07	15.00
99	ASN	C	-17.20	-18.74	83.81	15.00
99	ASN	O	-18.44	-18.61	83.82	15.00
100	PRO	N	-16.59	-19.79	84.39	15.00
100	PRO	CD	-15.15	-19.84	84.68	15.00
100	PRO	CA	-17.29	-20.92	85.02	15.00
100	PRO	CB	-16.19	-21.58	85.86	15.00
100	PRO	CG	-15.15	-20.47	86.03	15.00
100	PRO	C	-18.50	-20.55	85.87	15.00
100	PRO	O	-19.48	-21.29	85.92	15.00
101	THR	N	-18.46	-19.40	86.53	15.00
101	THR	CA	-19.58	-19.00	87.37	15.00
101	THR	CB	-19.22	-17.77	88.22	15.00
101	THR	OG1	-18.93	-16.65	87.36	15.00
101	THR	CG2	-17.99	-18.06	89.08	15.00
101	THR	C	-20.81	-18.70	86.52	15.00
101	THR	O	-21.94	-19.07	86.88	15.00
102	GLY	N	-20.59	-18.06	85.37	15.00
102	GLY	CA	-21.68	-17.73	84.47	15.00
102	GLY	C	-22.27	-18.92	83.72	15.00
102	GLY	O	-23.16	-18.73	82.87	15.00
103	LYS	N	-21.80	-20.14	84.00	15.00
103	LYS	CA	-22.32	-21.34	83.33	15.00
103	LYS	CB	-21.70	-22.60	83.93	15.00
103	LYS	CG	-22.23	-23.88	83.33	15.00
103	LYS	CD	-21.78	-25.11	84.11	15.00
103	LYS	CE	-22.56	-25.26	85.40	15.00
103	LYS	NZ	-24.02	-25.47	85.12	15.00
103	LYS	C	-23.83	-21.42	83.45	15.00
103	LYS	O	-24.39	-21.26	84.53	15.00
104	ALA	N	-24.50	-21.68	82.34	15.00
104	ALA	CA	-25.96	-21.77	82.34	15.00
104	ALA	CB	-26.56	-20.57	81.61	15.00
104	ALA	C	-26.48	-23.07	81.73	15.00
104	ALA	O	-27.69	-23.30	81.71	15.00
105	ALA	N	-25.59	-23.92	81.24	15.00
105	ALA	CA	-26.02	-25.18	80.65	15.00
105	ALA	CB	-26.71	-24.94	79.31	15.00
105	ALA	C	-24.89	-26.20	80.49	15.00

TABLE III

105	ALA	O	-23.72	-25.84	80.50	15.00
106	LYS	N	-25.28	-27.46	80.37	15.00
106	LYS	CA	-24.36	-28.59	80.21	15.00
106	LYS	CB	-24.28	-29.40	81.51	15.00
106	LYS	CG	-23.38	-28.89	82.62	15.00
106	LYS	CD	-23.65	-29.73	83.87	15.00
106	LYS	CE	-22.48	-29.72	84.85	15.00
106	LYS	NZ	-21.33	-30.54	84.36	15.00
106	LYS	C	-24.99	-29.49	79.16	15.00
106	LYS	O	-26.18	-29.32	78.83	15.00
107	CYS	N	-24.23	-30.42	78.61	15.00
107	CYS	CA	-24.77	-31.37	77.64	15.00
107	CYS	CB	-24.82	-30.77	76.22	15.00
107	CYS	SG	-23.38	-31.03	75.18	15.00
107	CYS	C	-23.93	-32.64	77.72	15.00
107	CYS	O	-22.76	-32.59	78.10	15.00
108	ARG	N	-24.54	-33.78	77.45	15.00
108	ARG	CA	-23.86	-35.07	77.52	15.00
108	ARG	CB	-24.60	-35.99	78.50	15.00
108	ARG	CG	-26.12	-35.73	78.59	15.00
108	ARG	CD	-26.86	-36.86	79.28	15.00
108	ARG	NE	-26.63	-38.14	78.60	15.00
108	ARG	CZ	-27.58	-38.89	78.03	15.00
108	ARG	NH1	-28.85	-38.51	78.05	15.00
108	ARG	NH2	-27.24	-40.03	77.45	15.00
108	ARG	C	-23.64	-35.78	76.18	15.00
108	ARG	O	-23.84	-36.99	76.06	15.00
109	GLY	N	-23.20	-35.03	75.17	15.00
109	GLY	CA	-22.97	-35.63	73.87	15.00
109	GLY	C	-23.82	-34.99	72.80	15.00
109	GLY	O	-24.27	-33.85	72.95	15.00
110	TYR	N	-24.09	-35.72	71.72	15.00
110	TYR	CA	-24.89	-35.19	70.63	15.00
110	TYR	CB	-24.12	-34.08	69.91	15.00
110	TYR	CG	-22.86	-34.56	69.20	15.00
110	TYR	CD1	-21.64	-34.62	69.87	15.00
110	TYR	CE1	-20.49	-35.03	69.22	15.00
110	TYR	CD2	-22.90	-34.93	67.85	15.00
110	TYR	CE2	-21.75	-35.34	67.19	15.00
110	TYR	CZ	-20.55	-35.39	67.88	15.00
110	TYR	OH	-19.39	-35.77	67.23	15.00
110	TYR	C	-25.22	-36.28	69.62	15.00

TABLE III

110	TYR	O	-24.44	-37.21	69.43	15.00
111	ARG	N	-26.34	-36.11	68.92	15.00
111	ARG	CA	-26.76	-37.08	67.92	15.00
111	ARG	CB	-28.02	-37.81	68.38	15.00
111	ARG	CG	-27.81	-38.84	69.48	15.00
111	ARG	CD	-28.75	-40.03	69.33	15.00
111	ARG	NE	-28.01	-41.28	69.36	15.00
111	ARG	CZ	-27.89	-42.06	70.44	15.00
111	ARG	NH1	-27.18	-43.18	70.36	15.00
111	ARG	NH2	-28.50	-41.73	71.58	15.00
111	ARG	C	-26.99	-36.46	66.54	15.00
111	ARG	O	-27.67	-35.45	66.41	15.00
112	GLU	N	-26.41	-37.06	65.50	15.00
112	GLU	CA	-26.56	-36.57	64.14	15.00
112	GLU	CB	-25.36	-37.00	63.29	15.00
112	GLU	CG	-24.03	-36.42	63.76	15.00
112	GLU	CD	-23.34	-35.56	62.70	15.00
112	GLU	OE1	-23.95	-34.57	62.22	15.00
112	GLU	OE2	-22.18	-35.88	62.33	15.00
112	GLU	C	-27.86	-37.13	63.56	15.00
112	GLU	O	-28.64	-37.75	64.27	15.00
113	ILE	N	-28.13	-36.87	62.29	15.00
113	ILE	CA	-29.35	-37.38	61.64	15.00
113	ILE	CB	-30.38	-36.25	61.34	15.00
113	ILE	CG2	-31.67	-36.83	60.78	15.00
113	ILE	CG1	-30.71	-35.45	62.60	15.00
113	ILE	CD1	-31.50	-36.20	63.65	15.00
113	ILE	C	-28.85	-37.98	60.33	15.00
113	ILE	O	-27.91	-37.46	59.73	15.00
114	PRO	N	-29.41	-39.13	59.92	15.00
114	PRO	CD	-30.48	-39.91	60.57	15.00
114	PRO	CA	-28.98	-39.77	58.68	15.00
114	PRO	CB	-30.10	-40.78	58.43	15.00
114	PRO	CG	-30.41	-41.23	59.83	15.00
114	PRO	C	-28.87	-38.79	57.54	15.00
114	PRO	O	-29.84	-38.12	57.20	15.00
115	GLU	N	-27.67	-38.66	56.99	15.00
115	GLU	CA	-27.46	-37.74	55.89	15.00
115	GLU	CB	-26.07	-37.92	55.28	15.00
115	GLU	CG	-24.92	-37.19	56.01	15.00
115	GLU	CD	-23.60	-37.16	55.20	15.00
115	GLU	OE1	-23.65	-37.20	53.94	15.00

TABLE III

115	GLU	OE2	-22.51	-37.08	55.82	15.00
115	GLU	C	-28.53	-37.91	54.82	15.00
115	GLU	O	-28.70	-39.00	54.27	15.00
116	GLY	N	-29.27	-36.83	54.59	15.00
116	GLY	CA	-30.30	-36.78	53.57	15.00
116	GLY	C	-31.63	-37.36	53.99	15.00
116	GLY	O	-32.46	-37.66	53.13	15.00
117	ASN	N	-31.88	-37.44	55.29	15.00
117	ASN	CA	-33.12	-38.03	55.77	15.00
117	ASN	CB	-32.80	-39.09	56.82	15.00
117	ASN	CG	-33.80	-40.21	56.84	15.00
117	ASN	OD1	-35.02	-39.99	56.90	15.00
117	ASN	ND2	-33.31	-41.44	56.76	15.00
117	ASN	C	-34.17	-37.06	56.31	15.00
117	ASN	O	-34.17	-36.72	57.50	15.00
118	GLU	N	-35.12	-36.66	55.48	15.00
118	GLU	CA	-36.15	-35.72	55.91	15.00
118	GLU	CB	-36.86	-35.08	54.72	15.00
118	GLU	CG	-36.09	-33.98	54.02	15.00
118	GLU	CD	-36.99	-33.14	53.15	15.00
118	GLU	OE1	-36.58	-32.75	52.04	15.00
118	GLU	OE2	-38.13	-32.87	53.57	15.00
118	GLU	C	-37.18	-36.33	56.83	15.00
118	GLU	O	-37.76	-35.64	57.66	15.00
119	LYS	N	-37.46	-37.61	56.66	15.00
119	LYS	CA	-38.43	-38.29	57.53	15.00
119	LYS	CB	-38.66	-39.71	57.03	15.00
119	LYS	CG	-39.20	-39.77	55.60	15.00
119	LYS	CD	-40.54	-39.04	55.49	15.00
119	LYS	CE	-41.04	-38.97	54.07	15.00
119	LYS	NZ	-40.26	-38.00	53.26	15.00
119	LYS	C	-37.89	-38.30	58.95	15.00
119	LYS	O	-38.55	-37.86	59.89	15.00
120	ALA	N	-36.64	-38.74	59.07	15.00
120	ALA	CA	-35.94	-38.81	60.34	15.00
120	ALA	CB	-34.58	-39.42	60.15	15.00
120	ALA	C	-35.81	-37.43	60.97	15.00
120	ALA	O	-35.88	-37.28	62.19	15.00
121	LEU	N	-35.56	-36.42	60.14	15.00
121	LEU	CA	-35.43	-35.06	60.66	15.00
121	LEU	CB	-34.96	-34.10	59.56	15.00
121	LEU	CG	-34.93	-32.61	59.96	15.00

TABLE III

121	LEU	CD1	-33.81	-32.34	60.93	15.00
121	LEU	CD2	-34.78	-31.76	58.72	15.00
121	LEU	C	-36.76	-34.60	61.25	15.00
121	LEU	O	-36.81	-33.98	62.31	15.00
122	LYS	N	-37.86	-34.91	60.57	15.00
122	LYS	CA	-39.17	-34.53	61.06	15.00
122	LYS	CB	-40.26	-35.04	60.11	15.00
122	LYS	CG	-41.65	-34.70	60.59	15.00
122	LYS	CD	-42.73	-35.28	59.72	15.00
122	LYS	CE	-44.10	-34.79	60.19	15.00
122	LYS	NZ	-45.21	-35.17	59.28	15.00
122	LYS	C	-39.36	-35.15	62.43	15.00
122	LYS	O	-39.79	-34.47	63.36	15.00
123	ARG	N	-39.02	-36.44	62.55	15.00
123	ARG	CA	-39.13	-37.17	63.81	15.00
123	ARG	CB	-38.72	-38.64	63.64	15.00
123	ARG	CG	-39.86	-39.56	63.26	15.00
123	ARG	CD	-39.43	-41.02	63.33	15.00
123	ARG	NE	-38.71	-41.48	62.14	15.00
123	ARG	CZ	-37.42	-41.79	62.12	15.00
123	ARG	NH1	-36.68	-41.70	63.21	15.00
123	ARG	NH2	-36.87	-42.22	60.99	15.00
123	ARG	C	-38.28	-36.55	64.90	15.00
123	ARG	O	-38.69	-36.51	66.05	15.00
124	ALA	N	-37.09	-36.07	64.55	15.00
124	ALA	CA	-36.20	-35.45	65.52	15.00
124	ALA	CB	-34.85	-35.18	64.89	15.00
124	ALA	C	-36.81	-34.15	66.03	15.00
124	ALA	O	-36.96	-33.96	67.23	15.00
125	VAL	N	-37.17	-33.25	65.12	15.00
125	VAL	CA	-37.77	-31.97	65.50	15.00
125	VAL	CB	-38.07	-31.11	64.25	15.00
125	VAL	CG1	-38.97	-29.94	64.59	15.00
125	VAL	CG2	-36.78	-30.59	63.67	15.00
125	VAL	C	-39.04	-32.20	66.30	15.00
125	VAL	O	-39.36	-31.43	67.20	15.00
126	ALA	N	-39.74	-33.29	66.00	15.00
126	ALA	CA	-40.97	-33.62	66.69	15.00
126	ALA	CB	-41.78	-34.61	65.88	15.00
126	ALA	C	-40.72	-34.17	68.09	15.00
126	ALA	O	-41.37	-33.76	69.06	15.00
127	ARG	N	-39.77	-35.10	68.19	15.00

TABLE III

127	ARG	CA	-39.41	-35.74	69.44	15.00
127	ARG	CB	-38.71	-37.07	69.18	15.00
127	ARG	CG	-39.58	-38.30	69.27	15.00
127	ARG	CD	-40.17	-38.70	67.94	15.00
127	ARG	NE	-39.87	-40.09	67.60	15.00
127	ARG	CZ	-40.52	-40.78	66.67	15.00
127	ARG	NH1	-40.18	-42.03	66.40	15.00
127	ARG	NH2	-41.55	-40.25	66.03	15.00
127	ARG	C	-38.52	-34.91	70.35	15.00
127	ARG	O	-38.86	-34.71	71.52	15.00
128	VAL	N	-37.37	-34.50	69.82	15.00
128	VAL	CA	-36.36	-33.72	70.56	15.00
128	VAL	CB	-34.95	-33.91	69.94	15.00
128	VAL	CG1	-33.88	-33.45	70.91	15.00
128	VAL	CG2	-34.73	-35.35	69.57	15.00
128	VAL	C	-36.62	-32.22	70.66	15.00
128	VAL	O	-36.44	-31.61	71.71	15.00
129	GLY	N	-36.99	-31.60	69.55	15.00
129	GLY	CA	-37.23	-30.17	69.54	15.00
129	GLY	C	-36.29	-29.54	68.53	15.00
129	GLY	O	-35.87	-30.22	67.58	15.00
130	PRO	N	-35.94	-28.25	68.71	15.00
130	PRO	CD	-36.46	-27.38	69.78	15.00
130	PRO	CA	-35.04	-27.50	67.83	15.00
130	PRO	CB	-34.80	-26.22	68.62	15.00
130	PRO	CG	-36.12	-26.00	69.26	15.00
130	PRO	C	-33.74	-28.21	67.50	15.00
130	PRO	O	-32.90	-28.46	68.37	15.00
131	VAL	N	-33.59	-28.51	66.21	15.00
131	VAL	CA	-32.42	-29.19	65.68	15.00
131	VAL	CB	-32.84	-30.34	64.73	15.00
131	VAL	CG1	-31.64	-31.06	64.18	15.00
131	VAL	CG2	-33.74	-31.33	65.48	15.00
131	VAL	C	-31.57	-28.19	64.90	15.00
131	VAL	O	-32.08	-27.25	64.28	15.00
132	SER	N	-30.25	-28.38	64.96	15.00
132	SER	CA	-29.32	-27.53	64.26	15.00
132	SER	CB	-28.00	-27.48	65.02	15.00
132	SER	OG	-28.18	-26.93	66.31	15.00
132	SER	C	-29.08	-28.14	62.88	15.00
132	SER	O	-28.67	-29.30	62.79	15.00
133	VAL	N	-29.38	-27.38	61.83	15.00

TABLE III

133 VAL CA	-29.21	-27.83	60.44	15.00
133 VAL CB	-30.57	-27.93	59.68	15.00
133 VAL CG1	-31.55	-28.81	60.43	15.00
133 VAL CG2	-31.16	-26.56	59.49	15.00
133 VAL C	-28.30	-26.86	59.68	15.00
133 VAL O	-28.06	-25.74	60.13	15.00
134 ALA N	-27.79	-27.28	58.52	15.00
134 ALA CA	-26.94	-26.44	57.69	15.00
134 ALA CB	-25.50	-26.93	57.73	15.00
134 ALA C	-27.49	-26.50	56.28	15.00
134 ALA O	-27.84	-27.57	55.79	15.00
135 ILE N	-27.58	-25.36	55.61	15.00
135 ILE CA	-28.14	-25.32	54.27	15.00
135 ILE CB	-29.58	-24.73	54.30	15.00
135 ILE CG2	-30.49	-25.57	55.19	15.00
135 ILE CG1	-29.53	-23.26	54.76	15.00
135 ILE CD1	-30.88	-22.58	54.88	15.00
135 ILE C	-27.33	-24.44	53.32	15.00
135 ILE O	-26.33	-23.82	53.72	15.00
136 ASP N	-27.75	-24.41	52.05	15.00
136 ASP CA	-27.12	-23.57	51.05	15.00
136 ASP CB	-27.25	-24.16	49.65	15.00
136 ASP CG	-26.77	-23.20	48.57	15.00
136 ASP OD1	-27.27	-23.28	47.43	15.00
136 ASP OD2	-25.90	-22.35	48.85	15.00
136 ASP C	-27.87	-22.24	51.10	15.00
136 ASP O	-29.05	-22.17	50.77	15.00
137 ALA N	-27.19	-21.21	51.59	15.00
137 ALA CA	-27.80	-19.89	51.68	15.00
137 ALA CB	-27.61	-19.32	53.08	15.00
137 ALA C	-27.23	-18.94	50.62	15.00
137 ALA O	-27.64	-17.78	50.53	15.00
138 SER N	-26.26	-19.43	49.84	15.00
138 SER CA	-25.66	-18.65	48.77	15.00
138 SER CB	-24.30	-19.22	48.37	15.00
138 SER OG	-23.28	-18.86	49.30	15.00
138 SER C	-26.61	-18.73	47.60	15.00
138 SER O	-26.51	-19.65	46.80	15.00
139 LEU N	-27.54	-17.77	47.57	15.00
139 LEU CA	-28.59	-17.66	46.55	15.00
139 LEU CB	-29.53	-18.86	46.65	15.00
139 LEU CG	-29.89	-19.63	45.38	15.00

TABLE III

139	LEU	CD1	-28.66	-20.27	44.80	15.00
139	LEU	CD2	-30.92	-20.68	45.71	15.00
139	LEU	C	-29.39	-16.39	46.85	15.00
139	LEU	O	-29.91	-16.22	47.96	15.00
140	THR	N	-29.52	-15.49	45.87	15.00
140	THR	CA	-30.23	-14.23	46.08	15.00
140	THR	CB	-30.06	-13.28	44.87	15.00
140	THR	OG1	-29.05	-13.81	43.99	15.00
140	THR	CG2	-29.62	-11.89	45.34	15.00
140	THR	C	-31.71	-14.37	46.42	15.00
140	THR	O	-32.23	-13.63	47.24	15.00
141	SER	N	-32.39	-15.35	45.83	15.00
141	SER	CA	-33.80	-15.59	46.10	15.00
141	SER	CB	-34.31	-16.76	45.27	15.00
141	SER	OG	-33.42	-17.86	45.34	15.00
141	SER	C	-34.00	-15.89	47.57	15.00
141	SER	O	-35.03	-15.57	48.16	15.00
142	PHE	N	-33.01	-16.51	48.18	15.00
142	PHE	CA	-33.07	-16.86	49.59	15.00
142	PHE	CB	-31.98	-17.88	49.93	15.00
142	PHE	CG	-31.93	-18.24	51.39	15.00
142	PHE	CD1	-32.72	-19.25	51.89	15.00
142	PHE	CD2	-31.10	-17.54	52.25	15.00
142	PHE	CE1	-32.68	-19.58	53.23	15.00
142	PHE	CE2	-31.05	-17.85	53.60	15.00
142	PHE	CZ	-31.85	-18.87	54.09	15.00
142	PHE	C	-32.88	-15.61	50.43	15.00
142	PHE	O	-33.66	-15.33	51.34	15.00
143	GLN	N	-31.86	-14.84	50.09	15.00
143	GLN	CA	-31.54	-13.64	50.83	15.00
143	GLN	CB	-30.25	-13.06	50.30	15.00
143	GLN	CG	-29.18	-14.11	50.24	15.00
143	GLN	CD	-27.84	-13.53	49.97	15.00
143	GLN	OE1	-27.41	-12.58	50.62	15.00
143	GLN	NE2	-27.15	-14.10	48.99	15.00
143	GLN	C	-32.63	-12.59	50.89	15.00
143	GLN	O	-32.90	-12.05	51.95	15.00
144	PHE	N	-33.29	-12.29	49.77	15.00
144	PHE	CA	-34.36	-11.28	49.80	15.00
144	PHE	CB	-34.33	-10.38	48.55	15.00
144	PHE	CG	-34.46	-11.12	47.24	15.00
144	PHE	CD1	-33.45	-11.04	46.30	15.00

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TABLE III

144	PHE	CD2	-35.59	-11.87	46.95	15.00
144	PHE	CE1	-33.56	-11.71	45.09	15.00
144	PHE	CE2	-35.71	-12.55	45.75	15.00
144	PHE	CZ	-34.70	-12.46	44.82	15.00
144	PHE	C	-35.76	-11.83	50.04	15.00
144	PHE	O	-36.76	-11.19	49.68	15.00
145	TYR	N	-35.83	-13.01	50.66	15.00
145	TYR	CA	-37.09	-13.68	50.97	15.00
145	TYR	CB	-36.80	-15.04	51.62	15.00
145	TYR	CG	-37.95	-15.65	52.36	15.00
145	TYR	CD1	-38.83	-16.52	51.73	15.00
145	TYR	CE1	-39.93	-17.05	52.41	15.00
145	TYR	CD2	-38.20	-15.31	53.69	15.00
145	TYR	CE2	-39.28	-15.83	54.38	15.00
145	TYR	CZ	-40.14	-16.69	53.73	15.00
145	TYR	OH	-41.24	-17.16	54.42	15.00
145	TYR	C	-37.87	-12.81	51.93	15.00
145	TYR	O	-37.27	-12.10	52.74	15.00
146	SER	N	-39.20	-12.88	51.89	15.00
146	SER	CA	-40.01	-12.07	52.78	15.00
146	SER	CB	-40.45	-10.78	52.10	15.00
146	SER	OG	-41.31	-11.05	51.01	15.00
146	SER	C	-41.23	-12.81	53.34	15.00
146	SER	O	-41.69	-12.52	54.45	15.00
147	LYS	N	-41.77	-13.75	52.58	15.00
147	LYS	CA	-42.93	-14.52	53.04	15.00
147	LYS	CB	-44.16	-13.62	53.21	15.00
147	LYS	CG	-44.84	-13.14	51.92	15.00
147	LYS	CD	-45.64	-11.86	52.19	15.00
147	LYS	CE	-44.71	-10.72	52.70	15.00
147	LYS	NZ	-45.41	-9.52	53.28	15.00
147	LYS	C	-43.27	-15.68	52.11	15.00
147	LYS	O	-43.03	-15.62	50.91	15.00
148	GLY	N	-43.83	-16.74	52.69	15.00
148	GLY	CA	-44.21	-17.90	51.90	15.00
148	GLY	C	-43.31	-19.08	52.16	15.00
148	GLY	O	-42.50	-19.07	53.08	15.00
149	VAL	N	-43.46	-20.12	51.35	15.00
149	VAL	CA	-42.65	-21.32	51.50	15.00
149	VAL	CB	-43.52	-22.60	51.39	15.00
149	VAL	CG1	-42.66	-23.84	51.53	15.00
149	VAL	CG2	-44.59	-22.59	52.45	15.00

TABLE III

149	VAL	C	-41.57	-21.27	50.42	15.00
149	VAL	O	-41.84	-21.44	49.24	15.00
150	TYR	N	-40.34	-21.01	50.84	15.00
150	TYR	CA	-39.21	-20.90	49.93	15.00
150	TYR	CB	-37.98	-20.37	50.67	15.00
150	TYR	CG	-36.75	-20.27	49.80	15.00
150	TYR	CD1	-36.73	-19.44	48.68	15.00
150	TYR	CE1	-35.61	-19.36	47.86	15.00
150	TYR	CD2	-35.61	-21.03	50.09	15.00
150	TYR	CE2	-34.48	-20.96	49.27	15.00
150	TYR	CZ	-34.49	-20.13	48.16	15.00
150	TYR	OH	-33.41	-20.06	47.32	15.00
150	TYR	C	-38.81	-22.16	49.19	15.00
150	TYR	O	-38.56	-23.19	49.80	15.00
151	TYR	N	-38.68	-22.03	47.88	15.00
151	TYR	CA	-38.24	-23.13	47.02	15.00
151	TYR	CB	-39.38	-24.11	46.72	15.00
151	TYR	CG	-38.89	-25.32	45.96	15.00
151	TYR	CD1	-37.74	-26.01	46.37	15.00
151	TYR	CE1	-37.23	-27.06	45.63	15.00
151	TYR	CD2	-39.52	-25.74	44.79	15.00
151	TYR	CE2	-39.01	-26.80	44.03	15.00
151	TYR	CZ	-37.87	-27.45	44.46	15.00
151	TYR	OH	-37.35	-28.50	43.72	15.00
151	TYR	C	-37.63	-22.58	45.73	15.00
151	TYR	O	-38.19	-21.69	45.08	15.00
152	ASP	N	-36.47	-23.12	45.37	15.00
152	ASP	CA	-35.74	-22.69	44.19	15.00
152	ASP	CB	-34.80	-21.56	44.59	15.00
152	ASP	CG	-34.09	-20.92	43.42	15.00
152	ASP	OD1	-33.27	-21.60	42.76	15.00
152	ASP	OD2	-34.35	-19.73	43.17	15.00
152	ASP	C	-34.93	-23.88	43.70	15.00
152	ASP	O	-33.98	-24.30	44.37	15.00
153	GLU	N	-35.23	-24.36	42.51	15.00
153	GLU	CA	-34.55	-25.53	41.95	15.00
153	GLU	CB	-35.15	-25.91	40.59	15.00
153	GLU	CG	-35.40	-24.74	39.62	15.00
153	GLU	CD	-34.12	-24.02	39.16	15.00
153	GLU	OE1	-33.16	-24.68	38.70	15.00
153	GLU	OE2	-34.09	-22.76	39.27	15.00
153	GLU	C	-33.03	-25.50	41.88	15.00

TABLE III

153 GLU O	-32.40	-26.49	41.49	15.00
154 SER N	-32.42	-24.37	42.22	15.00
154 SER CA	-30.96	-24.26	42.18	15.00
154 SER CB	-30.53	-23.00	41.43	15.00
154 SER OG	-30.93	-23.09	40.06	15.00
154 SER C	-30.27	-24.34	43.55	15.00
154 SER O	-29.04	-24.33	43.65	15.00
155 CYS N	-31.06	-24.43	44.61	15.00
155 CYS CA	-30.49	-24.54	45.95	15.00
155 CYS C	-29.66	-25.81	45.88	15.00
155 CYS O	-30.16	-26.88	45.54	15.00
155 CYS CB	-31.60	-24.69	46.96	15.00
155 CYS SG	-31.20	-23.89	48.53	15.00
156 ASN N	-28.36	-25.70	46.16	15.00
156 ASN CA	-27.50	-26.87	46.05	15.00
156 ASN CB	-26.20	-26.49	45.36	15.00
156 ASN CG	-25.34	-27.69	45.04	15.00
156 ASN OD1	-25.83	-28.82	44.97	15.00
156 ASN ND2	-24.05	-27.47	44.88	15.00
156 ASN C	-27.21	-27.66	47.33	15.00
156 ASN O	-26.37	-27.26	48.13	15.00
157 SER N	-27.82	-28.83	47.43	15.00
157 SER CA	-27.66	-29.72	48.57	15.00
157 SER CB	-28.41	-31.03	48.33	15.00
157 SER OG	-29.78	-30.78	48.03	15.00
157 SER C	-26.19	-30.04	48.87	15.00
157 SER O	-25.86	-30.54	49.96	15.00
158 ASP N	-25.31	-29.75	47.92	15.00
158 ASP CA	-23.89	-30.03	48.07	15.00
158 ASP CB	-23.30	-30.43	46.71	15.00
158 ASP CG	-24.01	-31.63	46.08	15.00
158 ASP OD1	-25.23	-31.53	45.79	15.00
158 ASP OD2	-23.34	-32.67	45.86	15.00
158 ASP C	-23.11	-28.86	48.64	15.00
158 ASP O	-22.00	-29.02	49.15	15.00
159 ASN N	-23.68	-27.66	48.60	15.00
159 ASN CA	-22.98	-26.49	49.11	15.00
159 ASN CB	-23.02	-25.36	48.07	15.00
159 ASN CG	-21.95	-24.29	48.31	15.00
159 ASN OD1	-21.61	-23.96	49.45	15.00
159 ASN ND2	-21.43	-23.72	47.22	15.00
159 ASN C	-23.59	-26.01	50.41	15.00

TABLE III

159	ASN	O	-24.34	-25.03	50.44	15.00
160	LEU	N	-23.31	-26.69	51.52	15.00
160	LEU	CA	-23.86	-26.27	52.80	15.00
160	LEU	CB	-23.99	-27.45	53.77	15.00
160	LEU	CG	-24.87	-28.62	53.30	15.00
160	LEU	CD1	-25.08	-29.56	54.47	15.00
160	LEU	CD2	-26.21	-28.16	52.76	15.00
160	LEU	C	-22.91	-25.21	53.33	15.00
160	LEU	O	-21.77	-25.51	53.65	15.00
161	ASN	N	-23.38	-23.97	53.35	15.00
161	ASN	CA	-22.55	-22.84	53.78	15.00
161	ASN	CB	-22.32	-21.90	52.60	15.00
161	ASN	CG	-23.61	-21.59	51.84	15.00
161	ASN	OD1	-24.49	-20.86	52.31	15.00
161	ASN	ND2	-23.75	-22.18	50.66	15.00
161	ASN	C	-23.10	-22.04	54.94	15.00
161	ASN	O	-22.37	-21.29	55.58	15.00
162	HIS	N	-24.38	-22.20	55.24	15.00
162	HIS	CA	-25.01	-21.44	56.31	15.00
162	HIS	CB	-26.00	-20.43	55.72	15.00
162	HIS	CG	-26.46	-19.38	56.68	15.00
162	HIS	CD2	-27.69	-18.91	56.97	15.00
162	HIS	ND1	-25.58	-18.66	57.46	15.00
162	HIS	CE1	-26.25	-17.79	58.19	15.00
162	HIS	NE2	-27.54	-17.92	57.90	15.00
162	HIS	C	-25.74	-22.34	57.31	15.00
162	HIS	O	-26.66	-23.07	56.94	15.00
163	ALA	N	-25.31	-22.30	58.57	15.00
163	ALA	CA	-25.93	-23.09	59.63	15.00
163	ALA	CB	-24.98	-23.25	60.81	15.00
163	ALA	C	-27.18	-22.33	60.08	15.00
163	ALA	O	-27.20	-21.09	60.08	15.00
164	VAL	N	-28.21	-23.05	60.48	15.00
164	VAL	CA	-29.44	-22.43	60.91	15.00
164	VAL	CB	-30.31	-22.10	59.66	15.00
164	VAL	CG1	-31.25	-23.23	59.31	15.00
164	VAL	CG2	-30.99	-20.79	59.85	15.00
164	VAL	C	-30.13	-23.35	61.91	15.00
164	VAL	O	-29.51	-24.32	62.35	15.00
165	LEU	N	-31.38	-23.10	62.28	15.00
165	LEU	CA	-32.05	-23.93	63.28	15.00
165	LEU	CB	-31.95	-23.25	64.64	15.00

TABLE III

165 LEU CG	-32.41	-23.97	65.90	15.00
165 LEU CD1	-31.39	-25.01	66.31	15.00
165 LEU CD2	-32.58	-22.96	67.00	15.00
165 LEU C	-33.51	-24.20	62.98	15.00
165 LEU O	-34.30	-23.27	62.86	15.00
166 ALA N	-33.88	-25.48	62.93	15.00
166 ALA CA	-35.27	-25.89	62.66	15.00
166 ALA CB	-35.30	-27.31	62.15	15.00
166 ALA C	-36.07	-25.78	63.95	15.00
166 ALA O	-35.74	-26.40	64.95	15.00
167 VAL N	-37.14	-24.99	63.93	15.00
167 VAL CA	-38.00	-24.75	65.09	15.00
167 VAL CB	-38.22	-23.21	65.30	15.00
167 VAL CG1	-39.07	-22.93	66.50	15.00
167 VAL CG2	-36.88	-22.50	65.47	15.00
167 VAL C	-39.35	-25.46	64.93	15.00
167 VAL O	-40.25	-25.34	65.77	15.00
168 GLY N	-39.51	-26.21	63.85	15.00
168 GLY CA	-40.75	-26.91	63.61	15.00
168 GLY C	-40.97	-27.18	62.14	15.00
168 GLY O	-40.03	-27.15	61.35	15.00
169 TYR N	-42.22	-27.45	61.78	15.00
169 TYR CA	-42.63	-27.75	60.41	15.00
169 TYR CB	-42.23	-29.18	60.00	15.00
169 TYR CG	-42.72	-30.27	60.93	15.00
169 TYR CD1	-44.07	-30.66	60.94	15.00
169 TYR CE1	-44.52	-31.66	61.81	15.00
169 TYR CD2	-41.85	-30.91	61.81	15.00
169 TYR CE2	-42.29	-31.91	62.68	15.00
169 TYR CZ	-43.63	-32.27	62.68	15.00
169 TYR OH	-44.07	-33.24	63.57	15.00
169 TYR C	-44.14	-27.59	60.31	15.00
169 TYR O	-44.81	-27.32	61.30	15.00
170 GLY N	-44.70	-27.76	59.12	15.00
170 GLY CA	-46.14	-27.63	58.97	15.00
170 GLY C	-46.56	-27.53	57.52	15.00
170 GLY O	-45.85	-27.94	56.61	15.00
171 ILE N	-47.74	-26.97	57.30	15.00
171 ILE CA	-48.28	-26.78	55.97	15.00
171 ILE CB	-49.43	-27.78	55.69	15.00
171 ILE CG2	-50.14	-27.44	54.38	15.00
171 ILE CG1	-48.91	-29.22	55.69	15.00

TABLE III

171	ILE	CD1	-48.38	-29.69	54.35	15.00
171	ILE	C	-48.89	-25.40	56.05	15.00
171	ILE	O	-49.85	-25.20	56.78	15.00
172	GLN	N	-48.29	-24.41	55.40	15.00
172	GLN	CA	-48.86	-23.07	55.47	15.00
172	GLN	CB	-47.96	-22.05	54.75	15.00
172	GLN	CG	-48.37	-20.59	54.97	15.00
172	GLN	CD	-47.48	-19.62	54.20	15.00
172	GLN	OE1	-46.94	-19.96	53.14	15.00
172	GLN	NE2	-47.33	-18.41	54.72	15.00
172	GLN	C	-50.22	-23.15	54.78	15.00
172	GLN	O	-51.26	-22.82	55.37	15.00
173	LYS	N	-50.21	-23.61	53.54	15.00
173	LYS	CA	-51.45	-23.77	52.79	15.00
173	LYS	CB	-52.00	-22.41	52.33	15.00
173	LYS	CG	-53.53	-22.35	52.25	15.00
173	LYS	CD	-54.00	-20.89	52.22	15.00
173	LYS	CE	-55.51	-20.75	52.34	15.00
173	LYS	NZ	-55.91	-19.31	52.33	15.00
173	LYS	C	-51.07	-24.63	51.61	15.00
173	LYS	O	-50.50	-24.16	50.63	15.00
174	GLY	N	-51.28	-25.93	51.80	15.00
174	GLY	CA	-50.97	-26.89	50.76	15.00
174	GLY	C	-49.51	-27.27	50.74	15.00
174	GLY	O	-49.17	-28.42	50.45	15.00
175	ASN	N	-48.63	-26.34	51.08	15.00
175	ASN	CA	-47.20	-26.64	51.05	15.00
175	ASN	CB	-46.44	-25.52	50.34	15.00
175	ASN	CG	-46.88	-25.35	48.88	15.00
175	ASN	OD1	-47.59	-24.39	48.54	15.00
175	ASN	ND2	-46.49	-26.29	48.03	15.00
175	ASN	C	-46.52	-26.98	52.38	15.00
175	ASN	O	-46.58	-26.21	53.35	15.00
176	LYS	N	-45.88	-28.15	52.40	15.00
176	LYS	CA	-45.15	-28.65	53.56	15.00
176	LYS	CB	-44.68	-30.09	53.34	15.00
176	LYS	CG	-45.74	-31.03	52.77	15.00
176	LYS	CD	-45.35	-32.49	52.97	15.00
176	LYS	CE	-46.23	-33.44	52.14	15.00
176	LYS	NZ	-45.80	-33.48	50.70	15.00
176	LYS	C	-43.94	-27.75	53.75	15.00
176	LYS	O	-43.26	-27.41	52.78	15.00

TABLE III

177 HIS N	-43.64	-27.39	55.00	15.00
177 HIS CA	-42.51	-26.50	55.25	15.00
177 HIS CB	-42.96	-25.05	55.09	15.00
177 HIS CG	-43.85	-24.56	56.20	15.00
177 HIS CD2	-43.59	-24.27	57.49	15.00
177 HIS ND1	-45.16	-24.20	55.99	15.00
177 HIS CE1	-45.67	-23.71	57.10	15.00
177 HIS NE2	-44.74	-23.75	58.03	15.00
177 HIS C	-41.82	-26.66	56.59	15.00
177 HIS O	-42.44	-27.05	57.57	15.00
178 TRP N	-40.52	-26.34	56.60	15.00
178 TRP CA	-39.67	-26.38	57.77	15.00
178 TRP CB	-38.26	-26.80	57.38	15.00
178 TRP CG	-38.11	-28.21	56.93	15.00
178 TRP CD2	-38.28	-29.38	57.73	15.00
178 TRP CE2	-38.02	-30.49	56.90	15.00
178 TRP CE3	-38.62	-29.60	59.08	15.00
178 TRP CD1	-37.77	-28.64	55.68	15.00
178 TRP NE1	-37.71	-30.01	55.65	15.00
178 TRP CZ2	-38.09	-31.80	57.37	15.00
178 TRP CZ3	-38.69	-30.89	59.54	15.00
178 TRP CH2	-38.43	-31.98	58.68	15.00
178 TRP C	-39.59	-24.94	58.28	15.00
178 TRP O	-39.26	-24.03	57.51	15.00
179 ILE N	-39.92	-24.71	59.55	15.00
179 ILE CA	-39.85	-23.36	60.09	15.00
179 ILE CB	-40.86	-23.17	61.23	15.00
179 ILE CG2	-40.80	-21.75	61.74	15.00
179 ILE CG1	-42.27	-23.50	60.72	15.00
179 ILE CD1	-43.38	-23.28	61.70	15.00
179 ILE C	-38.42	-23.13	60.55	15.00
179 ILE O	-37.94	-23.79	61.47	15.00
180 ILE N	-37.73	-22.22	59.88	15.00
180 ILE CA	-36.32	-21.94	60.17	15.00
180 ILE CB	-35.50	-22.02	58.86	15.00
180 ILE CG2	-34.06	-21.71	59.13	15.00
180 ILE CG1	-35.63	-23.40	58.22	15.00
180 ILE CD1	-34.94	-24.48	58.99	15.00
180 ILE C	-36.01	-20.62	60.88	15.00
180 ILE O	-36.59	-19.58	60.56	15.00
181 LYS N	-35.09	-20.68	61.84	15.00
181 LYS CA	-34.67	-19.51	62.60	15.00

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TABLE III

181 LYS CB	-34.58	-19.83	64.09	15.00
181 LYS CG	-34.19	-18.62	64.93	15.00
181 LYS CD	-33.86	-18.95	66.37	15.00
181 LYS CE	-33.68	-17.66	67.16	15.00
181 LYS NZ	-33.07	-17.85	68.50	15.00
181 LYS C	-33.30	-19.10	62.12	15.00
181 LYS O	-32.31	-19.74	62.48	15.00
182 ASN N	-33.22	-18.04	61.32	15.00
182 ASN CA	-31.93	-17.56	60.79	15.00
182 ASN CB	-32.17	-16.80	59.48	15.00
182 ASN CG	-30.98	-16.86	58.53	15.00
182 ASN OD1	-29.87	-17.20	58.92	15.00
182 ASN ND2	-31.21	-16.50	57.27	15.00
182 ASN C	-31.29	-16.65	61.84	15.00
182 ASN O	-31.86	-16.44	62.91	15.00
183 SER N	-30.11	-16.11	61.56	15.00
183 SER CA	-29.44	-15.21	62.52	15.00
183 SER CB	-28.26	-15.93	63.18	15.00
183 SER OG	-27.41	-16.54	62.21	15.00
183 SER C	-28.98	-13.90	61.87	15.00
183 SER O	-27.84	-13.44	62.08	15.00
184 TRP N	-29.85	-13.26	61.11	15.00
184 TRP CA	-29.52	-12.01	60.45	15.00
184 TRP CB	-29.70	-12.14	58.94	15.00
184 TRP CG	-28.74	-13.05	58.26	15.00
184 TRP CD2	-28.89	-13.61	56.96	15.00
184 TRP CE2	-27.72	-14.38	56.71	15.00
184 TRP CE3	-29.87	-13.53	55.98	15.00
184 TRP CD1	-27.54	-13.48	58.74	15.00
184 TRP NE1	-26.92	-14.29	57.81	15.00
184 TRP CZ2	-27.53	-15.07	55.51	15.00
184 TRP CZ3	-29.68	-14.22	54.78	15.00
184 TRP CH2	-28.52	-14.98	54.56	15.00
184 TRP C	-30.45	-10.91	60.98	15.00
184 TRP O	-31.16	-10.28	60.20	15.00
185 GLY N	-30.48	-10.71	62.29	15.00
185 GLY CA	-31.34	-9.69	62.86	15.00
185 GLY C	-32.79	-10.02	62.61	15.00
185 GLY O	-33.09	-11.01	61.96	15.00
186 GLU N	-33.73	-9.25	63.14	15.00
186 GLU CA	-35.13	-9.57	62.89	15.00
186 GLU CB	-36.01	-9.41	64.14	15.00

TABLE III

186 GLU CG	-36.02	-8.04	64.75	15.00
186 GLU CD	-37.04	-7.92	65.87	15.00
186 GLU OE1	-36.66	-7.55	67.00	15.00
186 GLU OE2	-38.23	-8.21	65.61	15.00
186 GLU C	-35.67	-8.78	61.72	15.00
186 GLU O	-36.84	-8.91	61.34	15.00
187 ASN N	-34.80	-7.96	61.13	15.00
187 ASN CA	-35.17	-7.15	59.99	15.00
187 ASN CB	-34.20	-5.97	59.84	15.00
187 ASN CG	-34.83	-4.76	59.13	15.00
187 ASN OD1	-34.15	-4.03	58.42	15.00
187 ASN ND2	-36.12	-4.54	59.36	15.00
187 ASN C	-35.15	-8.03	58.74	15.00
187 ASN O	-35.75	-7.72	57.72	15.00
188 TRP N	-34.45	-9.16	58.81	15.00
188 TRP CA	-34.37	-10.07	57.66	15.00
188 TRP CB	-33.13	-10.97	57.77	15.00
188 TRP CG	-33.03	-11.92	56.63	15.00
188 TRP CD2	-33.46	-13.29	56.62	15.00
188 TRP CE2	-33.26	-13.77	55.31	15.00
188 TRP CE3	-34.00	-14.15	57.58	15.00
188 TRP CD1	-32.60	-11.64	55.38	15.00
188 TRP NE1	-32.73	-12.74	54.58	15.00
188 TRP CZ2	-33.58	-15.08	54.93	15.00
188 TRP CZ3	-34.31	-15.45	57.20	15.00
188 TRP CH2	-34.10	-15.90	55.89	15.00
188 TRP C	-35.63	-10.94	57.55	15.00
188 TRP O	-36.34	-11.13	58.54	15.00
189 GLY N	-35.89	-11.44	56.34	15.00
189 GLY CA	-37.04	-12.29	56.09	15.00
189 GLY C	-38.26	-11.99	56.92	15.00
189 GLY O	-38.56	-10.84	57.23	15.00
190 ASN N	-38.99	-13.02	57.32	15.00
190 ASN CA	-40.18	-12.81	58.14	15.00
190 ASN CB	-41.17	-13.96	57.97	15.00
190 ASN CG	-42.58	-13.57	58.36	15.00
190 ASN OD1	-43.53	-13.95	57.69	15.00
190 ASN ND2	-42.72	-12.80	59.43	15.00
190 ASN C	-39.79	-12.68	59.61	15.00
190 ASN O	-39.86	-13.65	60.36	15.00
191 LYS N	-39.41	-11.47	60.02	15.00
191 LYS CA	-39.01	-11.18	61.41	15.00

TABLE III

191 LYS CB	-40.23	-11.26	62.34	15.00
191 LYS CG	-41.41	-10.38	61.96	15.00
191 LYS CD	-42.64	-10.75	62.79	15.00
191 LYS CE	-43.93	-10.18	62.20	15.00
191 LYS NZ	-45.15	-10.69	62.91	15.00
191 LYS C	-37.94	-12.14	61.90	15.00
191 LYS O	-38.00	-12.62	63.03	15.00
192 GLY N	-36.97	-12.45	61.05	15.00
192 GLY CA	-35.91	-13.35	61.43	15.00
192 GLY C	-36.06	-14.79	60.97	15.00
192 GLY O	-35.07	-15.51	60.83	15.00
193 TYR N	-37.30	-15.21	60.70	15.00
193 TYR CA	-37.56	-16.59	60.27	15.00
193 TYR CB	-38.79	-17.14	61.01	15.00
193 TYR CG	-38.57	-17.28	62.49	15.00
193 TYR CD1	-38.77	-16.20	63.35	15.00
193 TYR CE1	-38.49	-16.30	64.70	15.00
193 TYR CD2	-38.09	-18.47	63.04	15.00
193 TYR CE2	-37.81	-18.58	64.40	15.00
193 TYR CZ	-38.00	-17.48	65.22	15.00
193 TYR OH	-37.69	-17.57	66.55	15.00
193 TYR C	-37.77	-16.76	58.76	15.00
193 TYR O	-37.85	-15.80	57.99	15.00
194 ILE N	-37.83	-18.01	58.33	15.00
194 ILE CA	-38.06	-18.34	56.94	15.00
194 ILE CB	-36.77	-18.17	56.07	15.00
194 ILE CG2	-35.64	-19.02	56.60	15.00
194 ILE CG1	-37.07	-18.54	54.62	15.00
194 ILE CD1	-35.87	-18.54	53.71	15.00
194 ILE C	-38.59	-19.77	56.84	15.00
194 ILE O	-38.12	-20.68	57.53	15.00
195 LEU N	-39.65	-19.93	56.06	15.00
195 LEU CA	-40.27	-21.23	55.84	15.00
195 LEU CB	-41.76	-21.08	55.61	15.00
195 LEU CG	-42.62	-21.03	56.88	15.00
195 LEU CD1	-41.90	-20.32	58.01	15.00
195 LEU CD2	-43.94	-20.37	56.58	15.00
195 LEU C	-39.61	-21.79	54.60	15.00
195 LEU O	-39.53	-21.13	53.57	15.00
196 MET N	-39.08	-23.00	54.71	15.00
196 MET CA	-38.42	-23.63	53.58	15.00
196 MET CB	-36.96	-23.90	53.93	15.00

TABLE III

196 MET CG	-36.13	-22.63	54.11	15.00
196 MET SD	-34.43	-22.96	54.57	15.00
196 MET CE	-33.85	-23.77	53.09	15.00
196 MET C	-39.17	-24.90	53.20	15.00
196 MET O	-39.74	-25.58	54.05	15.00
197 ALA N	-39.23	-25.22	51.91	15.00
197 ALA CA	-39.93	-26.41	51.45	15.00
197 ALA CB	-39.79	-26.55	49.94	15.00
197 ALA C	-39.51	-27.70	52.15	15.00
197 ALA O	-38.32	-27.92	52.41	15.00
198 ARG N	-40.50	-28.53	52.47	15.00
198 ARG CA	-40.29	-29.81	53.12	15.00
198 ARG CB	-40.95	-29.84	54.50	15.00
198 ARG CG	-40.91	-31.22	55.15	15.00
198 ARG CD	-41.22	-31.19	56.63	15.00
198 ARG NE	-42.59	-30.84	56.98	15.00
198 ARG CZ	-43.60	-31.70	56.98	15.00
198 ARG NH1	-43.40	-32.96	56.63	15.00
198 ARG NH2	-44.79	-31.32	57.43	15.00
198 ARG C	-40.86	-30.94	52.27	15.00
198 ARG O	-42.03	-30.91	51.88	15.00
199 ASN N	-40.00	-31.90	51.96	15.00
199 ASN CA	-40.33	-33.08	51.17	15.00
199 ASN CB	-41.68	-33.69	51.58	15.00
199 ASN CG	-41.66	-34.26	53.00	15.00
199 ASN OD1	-42.63	-34.12	53.74	15.00
199 ASN ND2	-40.55	-34.91	53.38	15.00
199 ASN C	-40.22	-32.89	49.66	15.00
199 ASN O	-40.46	-33.83	48.89	15.00
200 LYS N	-39.80	-31.71	49.23	15.00
200 LYS CA	-39.60	-31.45	47.81	15.00
200 LYS CB	-39.83	-29.98	47.45	15.00
200 LYS CG	-41.27	-29.52	47.67	15.00
200 LYS CD	-41.61	-28.27	46.88	15.00
200 LYS CE	-43.08	-27.86	47.07	15.00
200 LYS NZ	-43.51	-26.73	46.16	15.00
200 LYS C	-38.15	-31.86	47.56	15.00
200 LYS O	-37.29	-31.02	47.31	15.00
201 ASN N	-37.90	-33.15	47.74	15.00
201 ASN CA	-36.58	-33.74	47.55	15.00
201 ASN CB	-36.23	-33.86	46.06	15.00
201 ASN CG	-37.27	-34.62	45.25	15.00

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TABLE III

201 ASN OD1	-37.46	-34.34	44.06	15.00
201 ASN ND2	-37.96	-35.58	45.88	15.00
201 ASN C	-35.48	-32.95	48.24	15.00
201 ASN O	-34.88	-32.07	47.64	15.00
202 ASN N	-35.27	-33.23	49.53	15.00
202 ASN CA	-34.21	-32.62	50.34	15.00
202 ASN CB	-33.01	-33.56	50.33	15.00
202 ASN CG	-31.96	-33.20	51.34	15.00
202 ASN OD1	-32.27	-32.76	52.45	15.00
202 ASN ND2	-30.71	-33.41	50.98	15.00
202 ASN C	-33.81	-31.18	49.94	15.00
202 ASN O	-32.63	-30.88	49.70	15.00
203 ALA N	-34.78	-30.29	49.91	15.00
203 ALA H	-35.58	-30.58	50.39	15.00
203 ALA CA	-34.60	-28.89	49.49	15.00
203 ALA CB	-35.83	-28.06	49.83	15.00
203 ALA C	-33.41	-28.27	50.25	15.00
203 ALA O	-33.31	-28.25	51.47	15.00
204 CYS N	-32.47	-27.71	49.46	15.00
204 CYS CA	-31.31	-27.02	50.02	15.00
204 CYS C	-30.43	-27.87	50.92	15.00
204 CYS O	-29.53	-27.34	51.59	15.00
204 CYS CB	-31.78	-25.79	50.79	15.00
204 CYS SG	-32.67	-24.58	49.75	15.00
205 GLY N	-30.64	-29.19	50.92	15.00
205 GLY CA	-29.86	-30.06	51.76	15.00
205 GLY C	-30.07	-29.75	53.23	15.00
205 GLY O	-29.14	-29.81	54.04	15.00
206 ILE N	-31.29	-29.37	53.59	15.00
206 ILE CA	-31.60	-29.06	54.98	15.00
206 ILE CB	-33.08	-28.64	55.16	15.00
206 ILE CG2	-34.01	-29.71	54.60	15.00
206 ILE CG1	-33.38	-28.40	56.63	15.00
206 ILE CD1	-34.65	-27.65	56.89	15.00
206 ILE C	-31.30	-30.24	55.91	15.00
206 ILE O	-30.92	-30.05	57.07	15.00
207 ALA N	-31.42	-31.46	55.39	15.00
207 ALA CA	-31.16	-32.64	56.19	15.00
207 ALA CB	-32.30	-33.64	56.03	15.00
207 ALA C	-29.82	-33.31	55.92	15.00
207 ALA O	-29.71	-34.52	55.99	15.00
208 ASN N	-28.75	-32.54	55.69	15.00

TABLE III

208 ASN CA	-27.44	-33.14	55.41	15.00
208 ASN CB	-26.91	-32.66	54.07	15.00
208 ASN CG	-27.50	-33.42	52.92	15.00
208 ASN OD1	-28.69	-33.32	52.66	15.00
208 ASN ND2	-26.68	-34.22	52.24	15.00
208 ASN C	-26.38	-32.91	56.46	15.00
208 ASN O	-25.30	-33.49	56.40	15.00
209 LEU N	-26.65	-32.01	57.40	15.00
209 LEU CA	-25.71	-31.72	58.47	15.00
209 LEU CB	-24.78	-30.58	58.07	15.00
209 LEU CG	-23.44	-30.57	58.80	15.00
209 LEU CD1	-22.65	-31.81	58.41	15.00
209 LEU CD2	-22.65	-29.33	58.46	15.00
209 LEU C	-26.52	-31.34	59.69	15.00
209 LEU O	-26.24	-30.34	60.34	15.00
210 ALA N	-27.55	-32.13	59.94	15.00
210 ALA H	-27.87	-32.61	59.15	15.00
210 ALA CA	-28.41	-31.91	61.10	15.00
210 ALA CB	-29.82	-32.45	60.85	15.00
210 ALA C	-27.84	-32.66	62.31	15.00
210 ALA O	-27.12	-33.64	62.12	15.00
211 SER N	-28.10	-32.14	63.49	15.00
211 SER CA	-27.62	-32.76	64.72	15.00
211 SER CB	-26.11	-32.53	64.90	15.00
211 SER OG	-25.80	-31.16	65.02	15.00
211 SER C	-28.35	-32.12	65.88	15.00
211 SER O	-28.97	-31.08	65.73	15.00
212 PHE N	-28.31	-32.77	67.03	15.00
212 PHE CA	-28.95	-32.21	68.21	15.00
212 PHE CB	-30.43	-32.63	68.32	15.00
212 PHE CG	-30.66	-34.13	68.43	15.00
212 PHE CD1	-31.05	-34.86	67.32	15.00
212 PHE CD2	-30.55	-34.79	69.67	15.00
212 PHE CE1	-31.34	-36.23	67.44	15.00
212 PHE CE2	-30.83	-36.15	69.79	15.00
212 PHE CZ	-31.23	-36.86	68.67	15.00
212 PHE C	-28.14	-32.62	69.42	15.00
212 PHE O	-27.50	-33.67	69.42	15.00
213 PRO N	-28.02	-31.73	70.40	15.00
213 PRO CD	-28.49	-30.34	70.46	15.00
213 PRO CA	-27.25	-32.08	71.59	15.00
213 PRO CB	-26.99	-30.73	72.23	15.00

TABLE III

213 PRO CG	-28.24	-29.98	71.91	15.00
213 PRO C	-28.08	-32.96	72.51	15.00
213 PRO O	-29.31	-32.92	72.48	15.00
214 LYS N	-27.43	-33.79	73.30	15.00
214 LYS CA	-28.14	-34.63	74.23	15.00
214 LYS CB	-27.49	-36.02	74.28	15.00
214 LYS CG	-28.32	-37.14	73.61	15.00
214 LYS CD	-27.43	-38.10	72.81	15.00
214 LYS CE	-26.30	-38.66	73.65	15.00
214 LYS NZ	-25.35	-39.45	72.81	15.00
214 LYS C	-28.02	-33.93	75.57	15.00
214 LYS O	-26.95	-33.45	75.91	15.00
215 MET N	-29.11	-33.79	76.30	15.00
215 MET CA	-29.01	-33.15	77.60	15.00
215 MET CB	-29.60	-31.73	77.56	15.00
215 MET CG	-28.77	-30.73	78.36	15.00
215 MET SD	-29.41	-29.06	78.37	15.00
215 MET CE	-30.41	-29.07	79.82	15.00
215 MET C	-29.66	-33.98	78.71	15.00
215 MET OT1	-30.59	-34.77	78.41	15.00
215 MET OT2	-29.20	-33.85	79.87	15.00
216 HOH OH2	-28.05	-18.06	84.86	15.00
217 HOH OH2	-23.19	-33.36	81.36	15.00
218 HOH OH2	-31.64	-15.80	65.41	15.00
219 HOH OH2	-30.17	-19.91	64.18	15.00
220 HOH OH2	-13.36	-11.60	62.86	15.00
221 HOH OH2	-9.95	-9.46	71.42	15.00
222 HOH OH2	-34.59	-22.68	70.30	15.00
223 HOH OH2	-17.52	-33.99	64.33	15.00
224 HOH OH2	-15.72	-11.02	61.35	15.00
225 HOH OH2	-24.41	-30.51	62.51	15.00
226 HOH OH2	-10.27	-5.38	68.19	15.00
227 HOH OH2	-11.06	-16.84	67.70	15.00
228 HOH OH2	-44.88	-30.73	49.92	15.00
229 HOH OH2	-44.59	-36.65	56.24	15.00
230 HOH OH2	-37.78	-15.40	68.33	15.00
231 HOH OH2	-38.40	-35.66	51.51	15.00
232 HOH OH2	-18.90	-36.86	61.93	15.00
233 HOH OH2	-41.75	-34.32	46.57	15.00
234 HOH OH2	-28.01	-19.38	62.11	15.00
235 HOH OH2	-21.94	-29.60	62.55	15.00
236 HOH OH2	-26.15	-8.89	74.53	15.00

TABLE III

237	HOH	OH2	-29.39	-20.71	79.14	15.00
238	HOH	OH2	-30.20	-22.42	84.30	15.00
239	HOH	OH2	-40.59	-13.37	49.72	15.00
240	HOH	OH2	-36.04	-24.57	49.50	15.00
241	HOH	OH2	-46.35	-34.82	56.72	15.00
242	HOH	OH2	-24.71	-3.06	61.99	15.00
243	HOH	OH2	-44.08	-16.56	65.62	15.00
244	HOH	OH2	-25.57	-5.90	65.10	15.00
245	HOH	OH2	-33.44	-27.60	71.31	15.00
246	HOH	OH2	-47.48	-27.33	77.05	15.00
247	HOH	OH2	-14.60	-14.01	81.32	15.00
248	HOH	OH2	-7.93	-18.05	73.48	15.00
249	HOH	OH2	-7.49	-16.70	75.98	15.00
250	HOH	OH2	-26.27	-35.42	59.26	15.00
251	HOH	OH2	-35.15	-10.72	53.73	15.00
252	HOH	OH2	-33.62	-27.20	46.10	15.00
253	HOH	OH2	-40.60	-16.73	45.07	15.00
254	HOH	OH2	-41.25	-34.55	55.94	15.00
255	HOH	OH2	-40.71	-18.20	72.64	15.00
256	HOH	OH2	-32.67	-13.41	60.76	15.00
257	HOH	OH2	-39.61	-9.04	58.76	15.00
258	HOH	OH2	-31.33	-8.54	65.90	15.00
259	HOH	OH2	-31.41	-5.90	63.60	15.00
260	HOH	OH2	-19.54	-8.02	63.36	15.00
261	HOH	OH2	-33.59	-19.88	70.38	15.00
262	HOH	OH2	-32.78	-42.12	66.81	15.00
263	HOH	OH2	-13.22	-22.75	77.99	15.00
264	HOH	OH2	-8.15	-22.46	73.27	15.00
265	HOH	OH2	-9.06	-29.93	75.92	15.00
266	HOH	OH2	-20.77	-33.56	62.36	15.00
267	HOH	OH2	-24.27	-45.12	64.98	15.00
268	HOH	OH2	-11.63	-32.82	70.13	15.00
269	HOH	OH2	-11.87	-26.78	72.10	15.00
270	HOH	OH2	-19.16	-34.47	79.41	15.00
271	HOH	OH2	-22.14	-37.69	70.75	15.00
272	HOH	OH2	-34.50	-24.81	88.02	15.00
273	HOH	OH2	-6.96	-12.16	66.61	15.00
274	HOH	OH2	-7.05	-22.45	69.94	15.00
275	HOH	OH2	-16.95	-20.23	55.91	15.00
276	HOH	OH2	-29.20	-20.58	48.90	15.00
277	HOH	OH2	-25.90	-22.48	45.16	15.00
278	HOH	OH2	-35.36	-37.73	52.91	15.00

TABLE III

279	HOH	OH2	-20.12	-27.71	43.74	15.00
280	HOH	OH2	-38.87	-31.38	41.99	15.00
281	HOH	OH2	-38.13	-30.43	51.07	15.00

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TABLE IV

Table of the orthogonal three dimensional coordinates in Ångstroms and B factors (Å2) for the cathepsin K complex with inhibitor 2,2'-N,N'-bis-benzyloxycarbonyl-L-leucinylcarbohydrazide.

Residue	Atom	X	Y	Z	B
1	ALA CB	-44.52	-37.54	64.26	15.00
1	ALA C	-46.72	-36.34	64.48	15.00
1	ALA O	-47.32	-36.96	63.59	15.00
1	ALA N	-46.03	-38.05	66.17	15.00
1	ALA CA	-45.55	-36.98	65.24	15.00
2	PRO N	-47.09	-35.10	64.86	15.00
2	PRO CD	-46.48	-34.27	65.92	15.00
2	PRO CA	-48.19	-34.39	64.20	15.00
2	PRO CB	-48.32	-33.13	65.04	15.00
2	PRO CG	-46.89	-32.89	65.50	15.00
2	PRO C	-47.85	-34.05	62.76	15.00
2	PRO O	-46.73	-34.29	62.29	15.00
3	ASP N	-48.84	-33.52	62.05	15.00
3	ASP CA	-48.64	-33.12	60.66	15.00
3	ASP CB	-49.97	-33.13	59.91	15.00
3	ASP CG	-50.31	-34.49	59.37	15.00
3	ASP OD1	-50.61	-34.58	58.16	15.00
3	ASP OD2	-50.25	-35.48	60.14	15.00
3	ASP C	-48.06	-31.73	60.63	15.00
3	ASP O	-47.45	-31.32	59.63	15.00
4	SER N	-48.18	-31.03	61.75	15.00
4	SER CA	-47.72	-29.67	61.87	15.00
4	SER CB	-48.86	-28.74	61.51	15.00
4	SER OG	-48.48	-27.37	61.57	15.00
4	SER C	-47.29	-29.41	63.29	15.00
4	SER O	-47.89	-29.91	64.23	15.00
5	VAL N	-46.20	-28.66	63.43	15.00
5	VAL CA	-45.71	-28.29	64.73	15.00
5	VAL CB	-44.98	-29.44	65.47	15.00
5	VAL CG1	-43.59	-29.68	64.89	15.00
5	VAL CG2	-44.88	-29.11	66.96	15.00
5	VAL C	-44.81	-27.08	64.62	15.00
5	VAL O	-44.04	-26.93	63.66	15.00
6	ASP N	-44.96	-26.20	65.59	15.00

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TABLE IV

6	ASP	CA	-44.19	-24.98	65.66	15.00
6	ASP	CB	-45.08	-23.81	65.22	15.00
6	ASP	CG	-44.31	-22.52	65.06	15.00
6	ASP	OD1	-43.13	-22.45	65.49	15.00
6	ASP	OD2	-44.88	-21.58	64.49	15.00
6	ASP	C	-43.72	-24.81	67.10	15.00
6	ASP	O	-44.50	-24.48	68.00	15.00
7	TYR	N	-42.42	-25.02	67.31	15.00
7	TYR	CA	-41.83	-24.90	68.64	15.00
7	TYR	CB	-40.43	-25.53	68.66	15.00
7	TYR	CG	-40.49	-27.05	68.76	15.00
7	TYR	CD1	-40.75	-27.66	69.98	15.00
7	TYR	CE1	-40.88	-29.04	70.08	15.00
7	TYR	CD2	-40.34	-27.85	67.63	15.00
7	TYR	CE2	-40.47	-29.24	67.72	15.00
7	TYR	CZ	-40.74	-29.83	68.95	15.00
7	TYR	OH	-40.89	-31.20	69.06	15.00
7	TYR	C	-41.80	-23.47	69.20	15.00
7	TYR	O	-41.66	-23.28	70.42	15.00
8	ARG	N	-41.93	-22.48	68.33	15.00
8	ARG	CA	-41.95	-21.08	68.77	15.00
8	ARG	CB	-42.06	-20.12	67.58	15.00
8	ARG	CG	-40.92	-20.21	66.57	15.00
8	ARG	CD	-41.19	-19.30	65.38	15.00
8	ARG	NE	-42.23	-19.84	64.51	15.00
8	ARG	CZ	-42.66	-19.26	63.38	15.00
8	ARG	NH1	-42.13	-18.11	62.97	15.00
8	ARG	NH2	-43.61	-19.84	62.66	15.00
8	ARG	C	-43.20	-20.93	69.64	15.00
8	ARG	O	-43.18	-20.25	70.68	15.00
9	LYS	N	-44.28	-21.58	69.21	15.00
9	LYS	CA	-45.54	-21.53	69.92	15.00
9	LYS	CB	-46.66	-22.14	69.08	15.00
9	LYS	CG	-47.11	-21.26	67.92	15.00
9	LYS	CD	-47.98	-22.07	66.95	15.00
9	LYS	CE	-48.74	-21.20	65.98	15.00
9	LYS	NZ	-49.84	-20.49	66.67	15.00
9	LYS	C	-45.45	-22.22	71.27	15.00
9	LYS	O	-46.19	-21.88	72.19	15.00
10	LYS	N	-44.53	-23.16	71.39	15.00
10	LYS	CA	-44.30	-23.91	72.63	15.00
10	LYS	CB	-43.82	-25.33	72.30	15.00

TABLE IV

10 LYS CG	-44.90	-26.25	71.75	15.00
10 LYS CD	-44.35	-27.64	71.47	15.00
10 LYS CE	-45.48	-28.63	71.20	15.00
10 LYS NZ	-44.99	-30.01	70.87	15.00
10 LYS C	-43.28	-23.22	73.53	15.00
10 LYS O	-42.94	-23.73	74.60	15.00
11 GLY N	-42.75	-22.09	73.09	15.00
11 GLY CA	-41.77	-21.37	73.88	15.00
11 GLY C	-40.41	-22.04	73.97	15.00
11 GLY O	-39.71	-21.91	74.97	15.00
12 TYR N	-40.02	-22.75	72.92	15.00
12 TYR CA	-38.73	-23.41	72.89	15.00
12 TYR CB	-38.86	-24.81	72.29	15.00
12 TYR CG	-39.47	-25.86	73.18	15.00
12 TYR CD1	-40.56	-25.59	73.99	15.00
12 TYR CE1	-41.12	-26.56	74.81	15.00
12 TYR CD2	-38.94	-27.15	73.21	15.00
12 TYR CE2	-39.49	-28.14	74.02	15.00
12 TYR CZ	-40.58	-27.84	74.82	15.00
12 TYR OH	-41.10	-28.81	75.64	15.00
12 TYR C	-37.73	-22.62	72.04	15.00
12 TYR O	-36.65	-23.14	71.72	15.00
13 VAL N	-38.08	-21.39	71.66	15.00
13 VAL CA	-37.21	-20.59	70.80	15.00
13 VAL CB	-37.82	-20.46	69.40	15.00
13 VAL CG1	-36.75	-20.07	68.38	15.00
13 VAL CG2	-38.52	-21.73	69.02	15.00
13 VAL C	-36.93	-19.17	71.30	15.00
13 VAL O	-37.86	-18.42	71.61	15.00
14 THR N	-35.66	-18.79	71.34	15.00
14 THR CA	-35.29	-17.45	71.78	15.00
14 THR CB	-33.84	-17.40	72.32	15.00
14 THR OG1	-32.91	-17.76	71.28	15.00
14 THR CG2	-33.67	-18.33	73.52	15.00
14 THR C	-35.46	-16.52	70.59	15.00
14 THR O	-35.55	-16.96	69.46	15.00
15 PRO N	-35.49	-15.20	70.84	15.00
15 PRO CD	-35.39	-14.48	72.12	15.00
15 PRO CA	-35.65	-14.27	69.72	15.00
15 PRO CB	-35.71	-12.90	70.42	15.00
15 PRO CG	-34.93	-13.12	71.67	15.00
15 PRO C	-34.54	-14.35	68.69	15.00

TABLE IV

15 PRO O	-33.45	-14.89	68.95	15.00
16 VAL N	-34.85	-13.85	67.50	15.00
16 VAL CA	-33.94	-13.84	66.37	15.00
16 VAL CB	-34.68	-13.41	65.08	15.00
16 VAL CG1	-33.72	-13.35	63.90	15.00
16 VAL CG2	-35.82	-14.39	64.78	15.00
16 VAL C	-32.71	-12.94	66.61	15.00
16 VAL O	-32.84	-11.79	67.04	15.00
17 LYS N	-31.54	-13.50	66.33	15.00
17 LYS CA	-30.27	-12.80	66.48	15.00
17 LYS CB	-29.26	-13.70	67.22	15.00
17 LYS CG	-29.85	-14.45	68.41	15.00
17 LYS CD	-30.15	-13.52	69.56	15.00
17 LYS CE	-31.10	-14.14	70.58	15.00
17 LYS NZ	-30.73	-15.52	70.94	15.00
17 LYS C	-29.70	-12.43	65.09	15.00
17 LYS O	-30.25	-12.81	64.05	15.00
18 ASN N	-28.59	-11.71	65.10	15.00
18 ASN CA	-27.93	-11.24	63.89	15.00
18 ASN CB	-28.25	-9.75	63.69	15.00
18 ASN CG	-27.74	-9.21	62.37	15.00
18 ASN OD1	-27.34	-9.95	61.49	15.00
18 ASN ND2	-27.75	-7.90	62.24	15.00
18 ASN C	-26.41	-11.47	63.99	15.00
18 ASN O	-25.70	-10.74	64.68	15.00
19 GLN N	-25.92	-12.47	63.27	15.00
19 GLN CA	-24.50	-12.81	63.27	15.00
19 GLN CB	-24.23	-14.05	62.39	15.00
19 GLN CG	-24.59	-13.91	60.91	15.00
19 GLN CD	-24.31	-15.17	60.10	15.00
19 GLN OE1	-25.15	-16.06	60.00	15.00
19 GLN NE2	-23.13	-15.23	59.50	15.00
19 GLN C	-23.59	-11.65	62.84	15.00
19 GLN O	-22.45	-11.56	63.30	15.00
20 GLY N	-24.09	-10.77	61.99	15.00
20 GLY CA	-23.28	-9.65	61.53	15.00
20 GLY C	-22.31	-10.07	60.45	15.00
20 GLY O	-22.59	-10.98	59.67	15.00
21 GLN N	-21.15	-9.43	60.41	15.00
21 GLN CA	-20.14	-9.75	59.41	15.00
21 GLN CB	-19.40	-8.48	58.96	15.00
21 GLN CG	-20.22	-7.59	58.06	15.00

TABLE IV

21 GLN CD	-20.48	-8.23	56.69	15.00
21 GLN OE1	-19.88	-9.26	56.33	15.00
21 GLN NE2	-21.37	-7.60	55.90	15.00
21 GLN C	-19.15	-10.78	59.98	15.00
21 GLN O	-17.95	-10.51	60.13	15.00
22 CYS N	-19.68	-11.95	60.30	15.00
22 CYS CA	-18.90	-13.04	60.86	15.00
22 CYS C	-19.59	-14.32	60.46	15.00
22 CYS O	-20.82	-14.40	60.50	15.00
22 CYS CB	-18.83	-12.90	62.40	15.00
22 CYS SG	-18.13	-14.32	63.33	15.00
23 GLY N	-18.81	-15.30	60.03	15.00
23 GLY CA	-19.36	-16.58	59.63	15.00
23 GLY C	-19.61	-17.48	60.83	15.00
23 GLY O	-19.23	-18.65	60.84	15.00
24 SER N	-20.32	-16.94	61.82	15.00
24 SER CA	-20.63	-17.67	63.03	15.00
24 SER CB	-20.58	-16.71	64.22	15.00
24 SER OG	-21.38	-15.58	64.00	15.00
24 SER C	-22.00	-18.34	62.98	15.00
24 SER O	-22.52	-18.78	64.01	15.00
25 CYS N	-22.59	-18.45	61.79	15.00
25 CYS CA	-23.90	-19.08	61.65	15.00
25 CYS CB	-24.31	-19.15	60.17	15.00
25 CYS SG	-23.12	-20.00	59.06	15.00
25 CYS C	-23.95	-20.47	62.29	15.00
25 CYS O	-24.95	-20.85	62.89	15.00
25 INH C1	-28.28	-9.31	55.94	15.00
25 INH C2	-28.07	-9.03	57.30	15.00
25 INH C3	-27.11	-9.78	58.03	15.00
25 INH C4	-26.37	-10.78	57.40	15.00
25 INH C5	-26.59	-11.05	56.05	15.00
25 INH C6	-27.54	-10.32	55.31	15.00
25 INH C7	-25.31	-11.54	58.16	15.00
25 INH O8	-24.19	-11.68	57.24	15.00
25 INH C9	-23.29	-12.79	57.20	15.00
25 INH O10	-22.50	-12.99	58.13	15.00
25 INH C11	-22.45	-14.71	55.88	15.00
25 INH C12	-21.05	-14.47	56.48	15.00
25 INH C13	-20.11	-13.38	55.92	15.00
25 INH C14	-19.15	-12.91	57.01	15.00
25 INH C15	-20.83	-12.17	55.23	15.00

TABLE IV

25	INH	C16	-23.00	-16.06	56.34	15.00
25	INH	O17	-24.16	-16.15	56.75	15.00
25	INH	N18	-22.19	-17.17	56.30	15.00
25	INH	N19	-22.62	-18.53	56.74	15.00
25	INH	N20	-23.34	-13.55	56.10	15.00
25	INH	C21	-22.09	-18.85	58.14	15.00
25	INH	O22	-22.10	-17.80	58.75	15.00
25	INH	C23	-12.78	-27.30	59.77	15.00
25	INH	C24	-13.75	-26.80	60.62	15.00
25	INH	C25	-14.61	-25.79	60.17	15.00
25	INH	C26	-14.52	-25.29	58.88	15.00
25	INH	C27	-13.54	-25.80	58.03	15.00
25	INH	C28	-12.67	-26.81	58.47	15.00
25	INH	C29	-15.45	-24.21	58.40	15.00
25	INH	O30	-16.52	-24.58	57.49	15.00
25	INH	C31	-17.56	-23.66	57.05	15.00
25	INH	O32	-17.32	-22.74	56.27	15.00
25	INH	C33	-19.95	-23.09	57.18	15.00
25	INH	C34	-21.23	-23.90	57.35	15.00
25	INH	C35	-21.11	-25.25	58.03	15.00
25	INH	C36	-22.32	-25.59	58.89	15.00
25	INH	C37	-20.84	-26.31	56.99	15.00
25	INH	C38	-20.07	-21.83	58.03	15.00
25	INH	O39	-19.74	-21.86	59.22	15.00
25	INH	N40	-20.56	-20.70	57.43	15.00
25	INH	N41	-20.70	-19.44	58.21	15.00
25	INH	N42	-18.78	-23.90	57.54	15.00
26	TRP	N	-22.83	-21.19	62.21	15.00
26	TRP	CA	-22.70	-22.53	62.79	15.00
26	TRP	CB	-21.33	-23.13	62.41	15.00
26	TRP	CG	-20.12	-22.32	62.88	15.00
26	TRP	CD2	-19.43	-22.44	64.14	15.00
26	TRP	CE2	-18.42	-21.46	64.16	15.00
26	TRP	CE3	-19.58	-23.27	65.26	15.00
26	TRP	CD1	-19.50	-21.31	62.20	15.00
26	TRP	NE1	-18.48	-20.79	62.96	15.00
26	TRP	CZ2	-17.56	-21.29	65.25	15.00
26	TRP	CZ3	-18.73	-23.10	66.34	15.00
26	TRP	CH2	-17.73	-22.11	66.33	15.00
26	TRP	C	-22.87	-22.47	64.31	15.00
26	TRP	O	-23.46	-23.36	64.91	15.00
27	ALA	N	-22.37	-21.39	64.90	15.00

TABLE IV

27 ALA CA	-22.43	-21.17	66.34	15.00
27 ALA CB	-21.53	-20.00	66.72	15.00
27 ALA C	-23.87	-20.90	66.77	15.00
27 ALA O	-24.34	-21.42	67.78	15.00
28 PHE N	-24.55	-20.06	65.99	15.00
28 PHE CA	-25.94	-19.71	66.23	15.00
28 PHE CB	-26.38	-18.58	65.29	15.00
28 PHE CG	-25.85	-17.23	65.70	15.00
28 PHE CD1	-24.59	-16.81	65.30	15.00
28 PHE CD2	-26.60	-16.39	66.52	15.00
28 PHE CE1	-24.08	-15.57	65.70	15.00
28 PHE CE2	-26.09	-15.15	66.93	15.00
28 PHE CZ	-24.83	-14.74	66.52	15.00
28 PHE C	-26.86	-20.93	66.07	15.00
28 PHE O	-27.82	-21.10	66.82	15.00
29 SER N	-26.54	-21.81	65.13	15.00
29 SER CA	-27.33	-23.01	64.93	15.00
29 SER CB	-26.85	-23.73	63.66	15.00
29 SER OG	-27.55	-24.93	63.47	15.00
29 SER C	-27.19	-23.93	66.16	15.00
29 SER O	-28.19	-24.39	66.71	15.00
30 SER N	-25.95	-24.16	66.59	15.00
30 SER CA	-25.63	-25.00	67.75	15.00
30 SER CB	-24.12	-24.97	68.04	15.00
30 SER OG	-23.34	-25.28	66.91	15.00
30 SER C	-26.36	-24.51	68.98	15.00
30 SER O	-27.02	-25.26	69.69	15.00
31 VAL N	-26.16	-23.23	69.26	15.00
31 VAL CA	-26.76	-22.55	70.39	15.00
31 VAL CB	-26.31	-21.07	70.38	15.00
31 VAL CG1	-27.42	-20.13	70.84	15.00
31 VAL CG2	-25.08	-20.92	71.26	15.00
31 VAL C	-28.28	-22.70	70.37	15.00
31 VAL O	-28.87	-23.11	71.37	15.00
32 GLY N	-28.89	-22.44	69.22	15.00
32 GLY CA	-30.32	-22.56	69.08	15.00
32 GLY C	-30.79	-23.96	69.45	15.00
32 GLY O	-31.80	-24.12	70.14	15.00
33 ALA N	-30.03	-24.96	69.01	15.00
33 ALA CA	-30.35	-26.35	69.30	15.00
33 ALA CB	-29.44	-27.29	68.48	15.00
33 ALA C	-30.24	-26.64	70.80	15.00

TABLE IV

33 ALA O	-31.11	-27.29	71.38	15.00
34 LEU N	-29.17	-26.15	71.42	15.00
34 LEU CA	-28.96	-26.37	72.84	15.00
34 LEU CB	-27.61	-25.82	73.28	15.00
34 LEU CG	-26.39	-26.66	72.87	15.00
34 LEU CD1	-25.12	-25.82	72.89	15.00
34 LEU CD2	-26.27	-27.87	73.78	15.00
34 LEU C	-30.09	-25.73	73.66	15.00
34 LEU O	-30.62	-26.34	74.59	15.00
35 GLU N	-30.48	-24.53	73.25	15.00
35 GLU CA	-31.55	-23.78	73.90	15.00
35 GLU CB	-31.70	-22.41	73.25	15.00
35 GLU CG	-30.49	-21.53	73.41	15.00
35 GLU CD	-30.59	-20.25	72.60	15.00
35 GLU OE1	-31.42	-20.17	71.67	15.00
35 GLU OE2	-29.81	-19.32	72.90	15.00
35 GLU C	-32.89	-24.52	73.87	15.00
35 GLU O	-33.66	-24.41	74.81	15.00
36 GLY N	-33.16	-25.25	72.79	15.00
36 GLY CA	-34.41	-25.97	72.72	15.00
36 GLY C	-34.42	-27.05	73.78	15.00
36 GLY O	-35.32	-27.13	74.61	15.00
37 GLN N	-33.35	-27.86	73.77	15.00
37 GLN CA	-33.18	-28.95	74.71	15.00
37 GLN CB	-31.95	-29.77	74.32	15.00
37 GLN CG	-32.01	-30.34	72.91	15.00
37 GLN CD	-33.22	-31.25	72.69	15.00
37 GLN OE1	-33.31	-32.35	73.26	15.00
37 GLN NE2	-34.16	-30.78	71.87	15.00
37 GLN C	-33.10	-28.48	76.17	15.00
37 GLN O	-33.70	-29.09	77.06	15.00
38 LEU N	-32.38	-27.39	76.40	15.00
38 LEU CA	-32.27	-26.87	77.75	15.00
38 LEU CB	-31.39	-25.63	77.79	15.00
38 LEU CG	-31.34	-25.01	79.18	15.00
38 LEU CD1	-30.49	-25.87	80.11	15.00
38 LEU CD2	-30.79	-23.61	79.08	15.00
38 LEU C	-33.65	-26.51	78.26	15.00
38 LEU O	-33.97	-26.73	79.43	15.00
39 LYS N	-34.45	-25.90	77.38	15.00
39 LYS CA	-35.81	-25.51	77.72	15.00
39 LYS CB	-36.42	-24.72	76.55	15.00

TABLE IV

39 LYS CG	-37.63	-23.88	76.91	15.00
39 LYS CD	-38.88	-24.71	77.08	15.00
39 LYS CE	-39.79	-24.14	78.15	15.00
39 LYS NZ	-39.99	-22.66	78.01	15.00
39 LYS C	-36.61	-26.78	78.00	15.00
39 LYS O	-37.28	-26.89	79.04	15.00
40 LYS N	-36.48	-27.75	77.11	15.00
40 LYS CA	-37.19	-29.01	77.23	15.00
40 LYS CB	-36.93	-29.90	76.01	15.00
40 LYS CG	-37.84	-31.13	75.91	15.00
40 LYS CD	-37.59	-31.87	74.60	15.00
40 LYS CE	-37.06	-33.28	74.85	15.00
40 LYS NZ	-36.36	-33.87	73.66	15.00
40 LYS C	-36.82	-29.76	78.51	15.00
40 LYS O	-37.69	-30.36	79.16	15.00
41 LYS N	-35.55	-29.66	78.92	15.00
41 LYS CA	-35.08	-30.37	80.10	15.00
41 LYS CB	-33.60	-30.71	79.95	15.00
41 LYS CG	-33.12	-31.74	80.95	15.00
41 LYS CD	-31.66	-32.10	80.76	15.00
41 LYS CE	-31.18	-33.02	81.87	15.00
41 LYS NZ	-31.86	-34.35	81.80	15.00
41 LYS C	-35.32	-29.68	81.45	15.00
41 LYS O	-35.76	-30.32	82.40	15.00
42 THR N	-35.04	-28.38	81.51	15.00
42 THR CA	-35.19	-27.62	82.75	15.00
42 THR CB	-34.00	-26.66	82.95	15.00
42 THR OG1	-34.10	-25.58	82.01	15.00
42 THR CG2	-32.68	-27.39	82.71	15.00
42 THR C	-36.46	-26.78	82.86	15.00
42 THR O	-36.86	-26.41	83.96	15.00
43 GLY N	-37.04	-26.42	81.73	15.00
43 GLY CA	-38.24	-25.60	81.75	15.00
43 GLY C	-37.95	-24.12	81.59	15.00
43 GLY O	-38.88	-23.31	81.62	15.00
44 LYS N	-36.67	-23.75	81.48	15.00
44 LYS CA	-36.28	-22.35	81.31	15.00
44 LYS CB	-35.14	-21.96	82.26	15.00
44 LYS CG	-35.58	-21.64	83.67	15.00
44 LYS CD	-35.80	-22.90	84.47	15.00
44 LYS CE	-34.48	-23.49	84.91	15.00
44 LYS NZ	-33.81	-22.59	85.90	15.00

TABLE IV

44	LYS	C	-35.82	-22.07	79.87	15.00
44	LYS	O	-35.33	-22.95	79.19	15.00
45	LEU	N	-35.97	-20.82	79.44	15.00
45	LEU	CA	-35.56	-20.40	78.11	15.00
45	LEU	CB	-36.79	-20.00	77.26	15.00
45	LEU	CG	-36.54	-19.61	75.80	15.00
45	LEU	CD1	-36.32	-20.88	74.98	15.00
45	LEU	CD2	-37.71	-18.81	75.22	15.00
45	LEU	C	-34.65	-19.18	78.26	15.00
45	LEU	O	-35.09	-18.11	78.69	15.00
46	LEU	N	-33.36	-19.38	78.00	15.00
46	LEU	CA	-32.41	-18.30	78.06	15.00
46	LEU	CB	-31.64	-18.25	79.40	15.00
46	LEU	CG	-30.80	-19.34	80.08	15.00
46	LEU	CD1	-31.61	-20.01	81.15	15.00
46	LEU	CD2	-30.27	-20.35	79.09	15.00
46	LEU	C	-31.46	-18.38	76.86	15.00
46	LEU	O	-31.39	-19.40	76.17	15.00
47	ASN	N	-30.79	-17.27	76.59	15.00
47	ASN	CA	-29.86	-17.18	75.47	15.00
47	ASN	CB	-29.74	-15.73	75.04	15.00
47	ASN	CG	-31.07	-15.14	74.66	15.00
47	ASN	OD1	-31.74	-15.64	73.75	15.00
47	ASN	ND2	-31.50	-14.13	75.39	15.00
47	ASN	C	-28.51	-17.75	75.81	15.00
47	ASN	O	-27.91	-17.37	76.81	15.00
48	LEU	N	-28.07	-18.74	75.05	15.00
48	LEU	CA	-26.77	-19.34	75.27	15.00
48	LEU	CB	-26.81	-20.84	74.95	15.00
48	LEU	CG	-27.74	-21.60	75.90	15.00
48	LEU	CD1	-27.67	-23.09	75.67	15.00
48	LEU	CD2	-27.37	-21.30	77.33	15.00
48	LEU	C	-25.77	-18.57	74.42	15.00
48	LEU	O	-26.17	-17.88	73.47	15.00
49	SER	N	-24.50	-18.67	74.76	15.00
49	SER	CA	-23.45	-17.92	74.09	15.00
49	SER	CB	-22.32	-17.62	75.08	15.00
49	SER	OG	-21.28	-16.87	74.48	15.00
49	SER	C	-22.83	-18.44	72.80	15.00
49	SER	O	-22.08	-19.40	72.82	15.00
50	PRO	N	-23.10	-17.78	71.67	15.00
50	PRO	CD	-24.13	-16.75	71.42	15.00

TABLE IV

50 PRO CA	-22.50	-18.23	70.41	15.00
50 PRO CB	-23.27	-17.43	69.35	15.00
50 PRO CG	-24.58	-17.10	70.04	15.00
50 PRO C	-21.01	-17.85	70.42	15.00
50 PRO O	-20.16	-18.58	69.92	15.00
51 GLN N	-20.70	-16.70	71.03	15.00
51 GLN CA	-19.34	-16.20	71.12	15.00
51 GLN CB	-19.32	-14.84	71.83	15.00
51 GLN CG	-18.00	-14.10	71.73	15.00
51 GLN CD	-17.72	-13.59	70.34	15.00
51 GLN OE1	-18.55	-12.90	69.73	15.00
51 GLN NE2	-16.55	-13.90	69.82	15.00
51 GLN C	-18.45	-17.21	71.86	15.00
51 GLN O	-17.28	-17.39	71.50	15.00
52 ASN N	-19.01	-17.87	72.87	15.00
52 ASN CA	-18.28	-18.88	73.62	15.00
52 ASN CB	-19.24	-19.57	74.60	15.00
52 ASN CG	-18.54	-20.47	75.63	15.00
52 ASN OD1	-19.19	-20.95	76.57	15.00
52 ASN ND2	-17.24	-20.70	75.48	15.00
52 ASN C	-17.74	-19.88	72.59	15.00
52 ASN O	-16.55	-20.22	72.60	15.00
53 LEU N	-18.60	-20.31	71.68	15.00
53 LEU CA	-18.22	-21.26	70.64	15.00
53 LEU CB	-19.47	-21.70	69.86	15.00
53 LEU CG	-20.37	-22.81	70.42	15.00
53 LEU CD1	-20.05	-23.13	71.87	15.00
53 LEU CD2	-21.83	-22.41	70.22	15.00
53 LEU C	-17.18	-20.69	69.68	15.00
53 LEU O	-16.17	-21.33	69.40	15.00
54 VAL N	-17.44	-19.48	69.18	15.00
54 VAL CA	-16.55	-18.82	68.23	15.00
54 VAL CB	-17.03	-17.36	67.92	15.00
54 VAL CG1	-15.96	-16.58	67.19	15.00
54 VAL CG2	-18.28	-17.40	67.05	15.00
54 VAL C	-15.10	-18.79	68.72	15.00
54 VAL O	-14.19	-19.17	67.98	15.00
55 ASP N	-14.90	-18.37	69.96	15.00
55 ASP CA	-13.56	-18.26	70.51	15.00
55 ASP CB	-13.56	-17.25	71.67	15.00
55 ASP CG	-14.04	-15.87	71.27	15.00
55 ASP OD1	-14.02	-15.54	70.06	15.00

TABLE IV

55 ASP OD2	-14.43	-15.10	72.18	15.00
55 ASP C	-12.93	-19.55	71.04	15.00
55 ASP O	-11.72	-19.70	71.00	15.00
56 CYS N	-13.76	-20.47	71.50	15.00
56 CYS CA	-13.26	-21.69	72.14	15.00
56 CYS C	-13.18	-23.02	71.37	15.00
56 CYS O	-12.34	-23.86	71.72	15.00
56 CYS CB	-14.03	-21.89	73.45	15.00
56 CYS SG	-14.05	-20.41	74.53	15.00
57 VAL N	-14.03	-23.22	70.37	15.00
57 VAL CA	-14.00	-24.47	69.62	15.00
57 VAL CB	-15.34	-24.76	68.86	15.00
57 VAL CG1	-15.38	-26.20	68.38	15.00
57 VAL CG2	-16.52	-24.51	69.77	15.00
57 VAL C	-12.80	-24.45	68.66	15.00
57 VAL O	-12.85	-23.83	67.60	15.00
58 SER N	-11.72	-25.10	69.08	15.00
58 SER CA	-10.48	-25.16	68.32	15.00
58 SER CB	-9.34	-25.68	69.21	15.00
58 SER OG	-9.70	-26.91	69.82	15.00
58 SER C	-10.53	-25.97	67.03	15.00
58 SER O	-9.67	-25.81	66.17	15.00
59 GLU N	-11.49	-26.88	66.92	15.00
59 GLU CA	-11.62	-27.68	65.70	15.00
59 GLU CB	-12.33	-29.00	65.99	15.00
59 GLU CG	-11.57	-29.96	66.92	15.00
59 GLU CD	-11.66	-29.59	68.40	15.00
59 GLU OE1	-10.69	-29.88	69.12	15.00
59 GLU OE2	-12.69	-29.03	68.85	15.00
59 GLU C	-12.37	-26.89	64.62	15.00
59 GLU O	-12.48	-27.34	63.49	15.00
60 ASN N	-12.91	-25.73	64.98	15.00
60 ASN CA	-13.65	-24.87	64.06	15.00
60 ASN CB	-14.99	-24.44	64.66	15.00
60 ASN CG	-16.08	-25.51	64.51	15.00
60 ASN OD1	-17.16	-25.38	65.08	15.00
60 ASN ND2	-15.79	-26.55	63.74	15.00
60 ASN C	-12.81	-23.65	63.73	15.00
60 ASN O	-11.76	-23.44	64.35	15.00
61 ASP N	-13.28	-22.85	62.78	15.00
61 ASP CA	-12.53	-21.67	62.38	15.00
61 ASP CB	-12.22	-21.74	60.88	15.00

TABLE IV

61 ASP CG	-11.54	-23.04	60.50	15.00
61 ASP OD1	-12.02	-23.72	59.56	15.00
61 ASP OD2	-10.54	-23.41	61.16	15.00
61 ASP C	-13.13	-20.31	62.74	15.00
61 ASP O	-12.89	-19.32	62.04	15.00
62 GLY N	-13.88	-20.27	63.83	15.00
62 GLY CA	-14.48	-19.03	64.30	15.00
62 GLY C	-15.34	-18.30	63.30	15.00
62 GLY O	-16.37	-18.81	62.87	15.00
63 CYS N	-14.96	-17.07	62.96	15.00
63 CYS CA	-15.71	-16.28	61.99	15.00
63 CYS C	-15.49	-16.79	60.56	15.00
63 CYS O	-16.19	-16.39	59.63	15.00
63 CYS CB	-15.37	-14.79	62.10	15.00
63 CYS SG	-16.14	-13.94	63.53	15.00
64 GLY N	-14.55	-17.71	60.41	15.00
64 GLY CA	-14.27	-18.27	59.10	15.00
64 GLY C	-15.11	-19.50	58.79	15.00
64 GLY O	-14.95	-20.10	57.73	15.00
65 GLY N	-15.94	-19.92	59.74	15.00
65 GLY CA	-16.78	-21.08	59.52	15.00
65 GLY C	-16.54	-22.20	60.51	15.00
65 GLY O	-15.54	-22.20	61.24	15.00
66 GLY N	-17.44	-23.18	60.52	15.00
66 GLY CA	-17.29	-24.31	61.41	15.00
66 GLY C	-18.41	-25.32	61.27	15.00
66 GLY O	-19.25	-25.19	60.37	15.00
67 TYR N	-18.41	-26.34	62.13	15.00
67 TYR CA	-19.42	-27.39	62.15	15.00
67 TYR CB	-18.78	-28.74	61.83	15.00
67 TYR CG	-18.30	-28.84	60.41	15.00
67 TYR CD1	-19.02	-29.55	59.47	15.00
67 TYR CE1	-18.62	-29.59	58.13	15.00
67 TYR CD2	-17.15	-28.16	60.00	15.00
67 TYR CE2	-16.74	-28.19	58.67	15.00
67 TYR CZ	-17.48	-28.90	57.74	15.00
67 TYR OH	-17.12	-28.88	56.42	15.00
67 TYR C	-20.12	-27.46	63.51	15.00
67 TYR O	-19.48	-27.31	64.54	15.00
68 MET N	-21.43	-27.73	63.50	15.00
68 MET CA	-22.22	-27.81	64.73	15.00
68 MET CB	-23.72	-27.83	64.41	15.00

TABLE IV

68 MET CG	-24.26	-26.60	63.63	15.00
68 MET SD	-24.05	-26.62	61.79	15.00
68 MET CE	-25.42	-27.66	61.31	15.00
68 MET C	-21.84	-29.02	65.61	15.00
68 MET O	-21.89	-28.95	66.84	15.00
69 THR N	-21.48	-30.12	64.98	15.00
69 THR CA	-21.08	-31.33	65.70	15.00
69 THR CB	-20.80	-32.51	64.73	15.00
69 THR OG1	-20.08	-32.02	63.58	15.00
69 THR CG2	-22.12	-33.15	64.27	15.00
69 THR C	-19.82	-31.05	66.53	15.00
69 THR O	-19.67	-31.55	67.66	15.00
70 ASN N	-18.94	-30.21	65.99	15.00
70 ASN CA	-17.72	-29.85	66.69	15.00
70 ASN CB	-16.76	-29.07	65.79	15.00
70 ASN CG	-15.89	-29.97	64.95	15.00
70 ASN OD1	-15.35	-29.56	63.93	15.00
70 ASN ND2	-15.72	-31.21	65.39	15.00
70 ASN C	-18.08	-29.02	67.91	15.00
70 ASN O	-17.57	-29.25	69.00	15.00
71 ALA N	-19.02	-28.09	67.71	15.00
71 ALA CA	-19.50	-27.22	68.77	15.00
71 ALA CB	-20.49	-26.20	68.21	15.00
71 ALA C	-20.14	-28.02	69.90	15.00
71 ALA O	-19.88	-27.76	71.07	15.00
72 PHE N	-20.90	-29.05	69.55	15.00
72 PHE CA	-21.56	-29.89	70.55	15.00
72 PHE CB	-22.55	-30.86	69.89	15.00
72 PHE CG	-23.72	-30.18	69.24	15.00
72 PHE CD1	-24.30	-29.05	69.82	15.00
72 PHE CD2	-24.23	-30.65	68.04	15.00
72 PHE CE1	-25.38	-28.41	69.21	15.00
72 PHE CE2	-25.31	-30.01	67.42	15.00
72 PHE CZ	-25.89	-28.89	68.01	15.00
72 PHE C	-20.53	-30.68	71.37	15.00
72 PHE O	-20.66	-30.76	72.60	15.00
73 GLN N	-19.55	-31.27	70.69	15.00
73 GLN CA	-18.50	-32.05	71.34	15.00
73 GLN CB	-17.52	-32.66	70.34	15.00
73 GLN CG	-18.09	-33.80	69.51	15.00
73 GLN CD	-17.03	-34.63	68.79	15.00
73 GLN OE1	-17.20	-35.01	67.62	15.00

TABLE IV

73	GLN	NE2	-15.95	-34.94	69.49	15.00
73	GLN	C	-17.75	-31.16	72.30	15.00
73	GLN	O	-17.35	-31.61	73.38	15.00
74	TYR	N	-17.55	-29.89	71.92	15.00
74	TYR	CA	-16.84	-28.94	72.75	15.00
74	TYR	CB	-16.75	-27.57	72.08	15.00
74	TYR	CG	-16.46	-26.43	73.03	15.00
74	TYR	CD1	-15.18	-26.26	73.58	15.00
74	TYR	CE1	-14.91	-25.23	74.50	15.00
74	TYR	CD2	-17.46	-25.54	73.42	15.00
74	TYR	CE2	-17.21	-24.51	74.34	15.00
74	TYR	CZ	-15.93	-24.36	74.88	15.00
74	TYR	OH	-15.69	-23.36	75.78	15.00
74	TYR	C	-17.58	-28.81	74.06	15.00
74	TYR	O	-17.02	-29.09	75.12	15.00
75	VAL	N	-18.84	-28.39	73.99	15.00
75	VAL	CA	-19.67	-28.21	75.17	15.00
75	VAL	CB	-21.14	-27.89	74.77	15.00
75	VAL	CG1	-22.00	-27.77	76.01	15.00
75	VAL	CG2	-21.20	-26.59	73.96	15.00
75	VAL	C	-19.61	-29.43	76.09	15.00
75	VAL	O	-19.55	-29.27	77.31	15.00
76	GLN	N	-19.56	-30.63	75.51	15.00
76	GLN	CA	-19.48	-31.85	76.29	15.00
76	GLN	CB	-19.68	-33.09	75.42	15.00
76	GLN	CG	-19.53	-34.39	76.19	15.00
76	GLN	CD	-19.73	-35.63	75.35	15.00
76	GLN	OE1	-19.39	-35.66	74.17	15.00
76	GLN	NE2	-20.27	-36.67	75.97	15.00
76	GLN	C	-18.15	-31.96	77.03	15.00
76	GLN	O	-18.14	-32.20	78.23	15.00
77	LYS	N	-17.05	-31.81	76.30	15.00
77	LYS	CA	-15.70	-31.90	76.87	15.00
77	LYS	CB	-14.63	-31.71	75.79	15.00
77	LYS	CG	-14.73	-32.63	74.61	15.00
77	LYS	CD	-14.44	-34.07	74.97	15.00
77	LYS	CE	-14.49	-34.96	73.73	15.00
77	LYS	NZ	-13.56	-34.52	72.63	15.00
77	LYS	C	-15.51	-30.80	77.93	15.00
77	LYS	O	-15.07	-31.05	79.04	15.00
78	ASN	N	-15.87	-29.58	77.55	15.00
78	ASN	CA	-15.78	-28.42	78.42	15.00

TABLE IV

78	ASN	CB	-16.11	-27.17	77.61	15.00
78	ASN	CG	-15.75	-25.90	78.33	15.00
78	ASN	OD1	-14.65	-25.77	78.86	15.00
78	ASN	ND2	-16.66	-24.93	78.33	15.00
78	ASN	C	-16.76	-28.55	79.61	15.00
78	ASN	O	-16.66	-27.82	80.59	15.00
79	ARG	N	-17.70	-29.48	79.47	15.00
79	ARG	CA	-18.73	-29.76	80.46	15.00
79	ARG	CB	-18.11	-30.22	81.77	15.00
79	ARG	CG	-17.42	-31.56	81.70	15.00
79	ARG	CD	-16.95	-31.93	83.08	15.00
79	ARG	NE	-16.17	-33.15	83.11	15.00
79	ARG	CZ	-14.86	-33.22	82.89	15.00
79	ARG	NH1	-14.17	-32.13	82.58	15.00
79	ARG	NH2	-14.21	-34.37	83.07	15.00
79	ARG	C	-19.66	-28.58	80.71	15.00
79	ARG	O	-20.27	-28.49	81.78	15.00
80	GLY	N	-19.79	-27.70	79.72	15.00
80	GLY	CA	-20.65	-26.55	79.87	15.00
80	GLY	C	-20.48	-25.48	78.81	15.00
80	GLY	O	-19.54	-25.52	78.01	15.00
81	ILE	N	-21.41	-24.53	78.80	15.00
81	ILE	CA	-21.40	-23.40	77.88	15.00
81	ILE	CB	-22.23	-23.68	76.58	15.00
81	ILE	CG2	-23.68	-24.05	76.93	15.00
81	ILE	CG1	-22.19	-22.46	75.64	15.00
81	ILE	CD1	-22.89	-22.66	74.31	15.00
81	ILE	C	-21.99	-22.20	78.62	15.00
81	ILE	O	-22.91	-22.35	79.43	15.00
82	ASP	N	-21.44	-21.02	78.37	15.00
82	ASP	CA	-21.91	-19.81	79.01	15.00
82	ASP	CB	-20.85	-18.71	78.94	15.00
82	ASP	CG	-19.73	-18.92	79.95	15.00
82	ASP	OD1	-18.66	-18.32	79.78	15.00
82	ASP	OD2	-19.93	-19.69	80.91	15.00
82	ASP	C	-23.21	-19.25	78.45	15.00
82	ASP	O	-23.63	-19.58	77.33	15.00
83	SER	N	-23.86	-18.43	79.26	15.00
83	SER	CA	-25.09	-17.78	78.85	15.00
83	SER	CB	-25.92	-17.36	80.08	15.00
83	SER	OG	-25.25	-16.38	80.86	15.00
83	SER	C	-24.65	-16.55	78.06	15.00

TABLE IV

83 SER O	-23.50	-16.10	78.17	15.00
84 GLU N	-25.56	-16.01	77.26	15.00
84 GLU CA	-25.27	-14.83	76.47	15.00
84 GLU CB	-26.53	-14.40	75.70	15.00
84 GLU CG	-26.39	-13.10	74.93	15.00
84 GLU CD	-25.30	-13.12	73.85	15.00
84 GLU OE1	-24.76	-12.04	73.52	15.00
84 GLU OE2	-24.98	-14.22	73.33	15.00
84 GLU C	-24.77	-13.70	77.38	15.00
84 GLU O	-23.77	-13.09	77.06	15.00
85 ASP N	-25.44	-13.47	78.51	15.00
85 ASP CA	-25.05	-12.41	79.46	15.00
85 ASP CB	-26.03	-12.35	80.65	15.00
85 ASP CG	-27.20	-11.39	80.42	15.00
85 ASP OD1	-27.86	-11.50	79.37	15.00
85 ASP OD2	-27.47	-10.53	81.29	15.00
85 ASP C	-23.62	-12.54	79.98	15.00
85 ASP O	-22.89	-11.55	80.07	15.00
86 ALA N	-23.23	-13.77	80.27	15.00
86 ALA CA	-21.91	-14.09	80.78	15.00
86 ALA CB	-21.95	-15.45	81.49	15.00
86 ALA C	-20.79	-14.09	79.71	15.00
86 ALA O	-19.61	-14.21	80.04	15.00
87 TYR N	-21.16	-13.98	78.44	15.00
87 TYR CA	-20.18	-13.99	77.36	15.00
87 TYR CB	-19.75	-15.44	77.09	15.00
87 TYR CG	-18.36	-15.67	76.52	15.00
87 TYR CD1	-17.82	-14.83	75.54	15.00
87 TYR CE1	-16.55	-15.09	74.99	15.00
87 TYR CD2	-17.60	-16.76	76.94	15.00
87 TYR CE2	-16.34	-17.03	76.40	15.00
87 TYR CZ	-15.82	-16.19	75.42	15.00
87 TYR OH	-14.59	-16.49	74.88	15.00
87 TYR C	-20.90	-13.42	76.14	15.00
87 TYR O	-21.25	-14.15	75.22	15.00
88 PRO N	-21.09	-12.09	76.11	15.00
88 PRO CD	-20.58	-11.10	77.08	15.00
88 PRO CA	-21.77	-11.42	75.00	15.00
88 PRO CB	-21.83	-9.97	75.47	15.00
88 PRO CG	-20.62	-9.82	76.28	15.00
88 PRO C	-21.13	-11.58	73.62	15.00
88 PRO O	-19.92	-11.77	73.47	15.00

TABLE IV

89 TYR N	-21.98	-11.45	72.61	15.00
89 TYR CA	-21.56	-11.59	71.22	15.00
89 TYR CB	-22.77	-11.93	70.35	15.00
89 TYR CG	-22.41	-12.26	68.92	15.00
89 TYR CD1	-21.67	-13.41	68.62	15.00
89 TYR CE1	-21.30	-13.71	67.32	15.00
89 TYR CD2	-22.78	-11.43	67.87	15.00
89 TYR CE2	-22.41	-11.72	66.56	15.00
89 TYR CZ	-21.68	-12.87	66.30	15.00
89 TYR OH	-21.29	-13.15	65.01	15.00
89 TYR C	-20.91	-10.31	70.72	15.00
89 TYR O	-21.45	-9.21	70.89	15.00
90 VAL N	-19.73	-10.45	70.13	15.00
90 VAL CA	-19.01	-9.31	69.58	15.00
90 VAL CB	-17.59	-9.14	70.23	15.00
90 VAL CG1	-17.71	-8.96	71.73	15.00
90 VAL CG2	-16.69	-10.31	69.89	15.00
90 VAL C	-18.88	-9.45	68.06	15.00
90 VAL O	-18.50	-8.50	67.38	15.00
91 GLY N	-19.17	-10.63	67.53	15.00
91 GLY CA	-19.08	-10.82	66.09	15.00
91 GLY C	-17.67	-10.74	65.55	15.00
91 GLY O	-17.44	-10.33	64.40	15.00
92 GLN N	-16.71	-11.14	66.37	15.00
92 GLN CA	-15.31	-11.12	66.00	15.00
92 GLN CB	-14.73	-9.72	66.26	15.00
92 GLN CG	-13.35	-9.49	65.65	15.00
92 GLN CD	-12.71	-8.19	66.08	15.00
92 GLN OE1	-12.20	-7.44	65.24	15.00
92 GLN NE2	-12.73	-7.92	67.39	15.00
92 GLN C	-14.60	-12.19	66.82	15.00
92 GLN O	-15.02	-12.50	67.94	15.00
93 GLU N	-13.54	-12.78	66.26	15.00
93 GLU CA	-12.77	-13.82	66.94	15.00
93 GLU CB	-11.86	-14.56	65.94	15.00
93 GLU CG	-12.59	-15.03	64.68	15.00
93 GLU CD	-11.65	-15.50	63.57	15.00
93 GLU OE1	-10.57	-14.88	63.36	15.00
93 GLU OE2	-12.02	-16.49	62.88	15.00
93 GLU C	-11.92	-13.20	68.04	15.00
93 GLU O	-11.31	-12.14	67.84	15.00
94 GLU N	-11.90	-13.84	69.20	15.00

TABLE IV

94 GLU CA	-11.15	-13.38	70.36	15.00
94 GLU CB	-12.03	-12.49	71.25	15.00
94 GLU CG	-12.71	-11.36	70.48	15.00
94 GLU CD	-13.30	-10.28	71.35	15.00
94 GLU OE1	-13.81	-10.60	72.43	15.00
94 GLU OE2	-13.27	-9.10	70.94	15.00
94 GLU C	-10.70	-14.63	71.11	15.00
94 GLU O	-11.13	-15.74	70.77	15.00
95 SER N	-9.82	-14.46	72.10	15.00
95 SER CA	-9.32	-15.60	72.86	15.00
95 SER CB	-8.13	-15.19	73.73	15.00
95 SER OG	-8.46	-14.11	74.58	15.00
95 SER C	-10.40	-16.21	73.74	15.00
95 SER O	-11.26	-15.51	74.26	15.00
96 CYS N	-10.31	-17.52	73.95	15.00
96 CYS CA	-11.30	-18.20	74.78	15.00
96 CYS C	-11.28	-17.68	76.21	15.00
96 CYS O	-10.25	-17.71	76.89	15.00
96 CYS CB	-11.10	-19.72	74.74	15.00
96 CYS SG	-12.37	-20.66	75.65	15.00
97 MET N	-12.43	-17.18	76.66	15.00
97 MET CA	-12.57	-16.63	77.99	15.00
97 MET CB	-12.71	-15.10	77.90	15.00
97 MET CG	-12.32	-14.33	79.15	15.00
97 MET SD	-10.53	-14.18	79.36	15.00
97 MET CE	-10.23	-15.44	80.61	15.00
97 MET C	-13.83	-17.23	78.62	15.00
97 MET O	-14.71	-16.50	79.08	15.00
98 TYR N	-13.95	-18.55	78.57	15.00
98 TYR CA	-15.11	-19.23	79.14	15.00
98 TYR CB	-15.04	-20.74	78.86	15.00
98 TYR CG	-16.04	-21.57	79.65	15.00
98 TYR CD1	-17.41	-21.44	79.44	15.00
98 TYR CE1	-18.32	-22.23	80.14	15.00
98 TYR CD2	-15.60	-22.52	80.59	15.00
98 TYR CE2	-16.51	-23.31	81.29	15.00
98 TYR CZ	-17.87	-23.16	81.06	15.00
98 TYR OH	-18.78	-23.95	81.71	15.00
98 TYR C	-15.16	-19.00	80.66	15.00
98 TYR O	-14.22	-19.33	81.36	15.00
99 ASN N	-16.23	-18.37	81.13	15.00
99 ASN CA	-16.39	-18.12	82.56	15.00

TABLE IV

99	ASN	CB	-17.13	-16.81	82.81	15.00
99	ASN	CG	-17.36	-16.54	84.30	15.00
99	ASN	OD1	-17.39	-17.46	85.12	15.00
99	ASN	ND2	-17.54	-15.27	84.65	15.00
99	ASN	C	-17.18	-19.27	83.16	15.00
99	ASN	O	-18.38	-19.39	82.93	15.00
100	PRO	N	-16.53	-20.09	83.98	15.00
100	PRO	CD	-15.13	-19.95	84.42	15.00
100	PRO	CA	-17.17	-21.24	84.63	15.00
100	PRO	CB	-16.08	-21.75	85.57	15.00
100	PRO	CG	-14.80	-21.33	84.89	15.00
100	PRO	C	-18.43	-20.86	85.40	15.00
100	PRO	O	-19.41	-21.59	85.40	15.00
101	THR	N	-18.41	-19.69	86.04	15.00
101	THR	CA	-19.54	-19.24	86.84	15.00
101	THR	CB	-19.09	-18.26	87.95	15.00
101	THR	OG1	-18.60	-17.04	87.37	15.00
101	THR	CG2	-17.99	-18.90	88.79	15.00
101	THR	C	-20.73	-18.68	86.08	15.00
101	THR	O	-21.79	-18.43	86.66	15.00
102	GLY	N	-20.57	-18.48	84.77	15.00
102	GLY	CA	-21.68	-17.98	83.97	15.00
102	GLY	C	-22.30	-19.14	83.21	15.00
102	GLY	O	-23.13	-18.94	82.32	15.00
103	LYS	N	-21.88	-20.35	83.54	15.00
103	LYS	CA	-22.36	-21.57	82.90	15.00
103	LYS	CB	-21.73	-22.79	83.58	15.00
103	LYS	CG	-22.11	-24.13	82.98	15.00
103	LYS	CD	-21.50	-25.25	83.81	15.00
103	LYS	CE	-21.82	-25.07	85.28	15.00
103	LYS	NZ	-21.22	-26.16	86.10	15.00
103	LYS	C	-23.89	-21.67	82.95	15.00
103	LYS	O	-24.50	-21.54	84.00	15.00
104	ALA	N	-24.50	-21.89	81.79	15.00
104	ALA	CA	-25.95	-21.97	81.72	15.00
104	ALA	CB	-26.48	-20.90	80.77	15.00
104	ALA	C	-26.45	-23.35	81.32	15.00
104	ALA	O	-27.63	-23.65	81.46	15.00
105	ALA	N	-25.55	-24.18	80.78	15.00
105	ALA	CA	-25.91	-25.53	80.36	15.00
105	ALA	CB	-26.98	-25.48	79.27	15.00
105	ALA	C	-24.70	-26.30	79.86	15.00

TABLE IV

105	ALA	O	-23.56	-25.84	80.00	15.00
106	LYS	N	-24.95	-27.48	79.33	15.00
106	LYS	CA	-23.93	-28.36	78.78	15.00
106	LYS	CB	-23.12	-29.05	79.90	15.00
106	LYS	CG	-23.87	-30.12	80.70	15.00
106	LYS	CD	-22.93	-30.93	81.56	15.00
106	LYS	CE	-23.66	-31.74	82.65	15.00
106	LYS	NZ	-24.38	-32.97	82.21	15.00
106	LYS	C	-24.70	-29.41	77.99	15.00
106	LYS	O	-25.89	-29.23	77.73	15.00
107	CYS	N	-24.03	-30.47	77.57	15.00
107	CYS	CA	-24.67	-31.55	76.85	15.00
107	CYS	CB	-24.96	-31.18	75.39	15.00
107	CYS	SG	-23.57	-31.18	74.26	15.00
107	CYS	C	-23.77	-32.77	76.95	15.00
107	CYS	O	-22.60	-32.67	77.31	15.00
108	ARG	N	-24.35	-33.94	76.70	15.00
108	ARG	CA	-23.62	-35.19	76.78	15.00
108	ARG	CB	-24.30	-36.10	77.80	15.00
108	ARG	CG	-24.56	-35.39	79.13	15.00
108	ARG	CD	-24.78	-36.37	80.25	15.00
108	ARG	NE	-26.08	-37.03	80.17	15.00
108	ARG	CZ	-26.31	-38.29	80.55	15.00
108	ARG	NH1	-25.34	-39.05	81.03	15.00
108	ARG	NH2	-27.55	-38.77	80.48	15.00
108	ARG	C	-23.52	-35.88	75.42	15.00
108	ARG	O	-23.75	-37.08	75.29	15.00
109	GLY	N	-23.15	-35.11	74.40	15.00
109	GLY	CA	-23.01	-35.66	73.07	15.00
109	GLY	C	-23.96	-35.04	72.06	15.00
109	GLY	O	-24.53	-33.97	72.30	15.00
110	TYR	N	-24.12	-35.71	70.92	15.00
110	TYR	CA	-24.99	-35.26	69.85	15.00
110	TYR	CB	-24.28	-34.21	68.99	15.00
110	TYR	CG	-23.06	-34.73	68.24	15.00
110	TYR	CD1	-21.77	-34.40	68.67	15.00
110	TYR	CE1	-20.65	-34.80	67.94	15.00
110	TYR	CD2	-23.19	-35.48	67.08	15.00
110	TYR	CE2	-22.08	-35.89	66.35	15.00
110	TYR	CZ	-20.81	-35.54	66.79	15.00
110	TYR	OH	-19.71	-35.91	66.03	15.00
110	TYR	C	-25.41	-36.44	68.98	15.00

TABLE IV

110	TYR	O	-24.81	-37.52	69.04	15.00
111	ARG	N	-26.39	-36.20	68.12	15.00
111	ARG	CA	-26.91	-37.23	67.23	15.00
111	ARG	CB	-28.22	-37.78	67.83	15.00
111	ARG	CG	-28.86	-38.97	67.11	15.00
111	ARG	CD	-29.48	-38.54	65.78	15.00
111	ARG	NE	-30.34	-39.56	65.17	15.00
111	ARG	CZ	-31.14	-39.34	64.13	15.00
111	ARG	NH1	-31.19	-38.13	63.58	15.00
111	ARG	NH2	-31.92	-40.30	63.68	15.00
111	ARG	C	-27.13	-36.60	65.85	15.00
111	ARG	O	-27.70	-35.51	65.74	15.00
112	GLU	N	-26.67	-37.29	64.81	15.00
112	GLU	CA	-26.82	-36.82	63.43	15.00
112	GLU	CB	-25.52	-37.09	62.65	15.00
112	GLU	CG	-24.30	-36.39	63.23	15.00
112	GLU	CD	-23.02	-36.62	62.42	15.00
112	GLU	OE1	-22.60	-35.70	61.69	15.00
112	GLU	OE2	-22.42	-37.70	62.55	15.00
112	GLU	C	-27.99	-37.52	62.76	15.00
112	GLU	O	-28.31	-38.67	63.08	15.00
113	ILE	N	-28.66	-36.80	61.85	15.00
113	ILE	CA	-29.79	-37.35	61.11	15.00
113	ILE	CB	-30.77	-36.21	60.69	15.00
113	ILE	CG2	-31.67	-36.67	59.56	15.00
113	ILE	CG1	-31.62	-35.77	61.89	15.00
113	ILE	CD1	-30.84	-35.23	63.06	15.00
113	ILE	C	-29.26	-38.07	59.87	15.00
113	ILE	O	-28.26	-37.65	59.27	15.00
114	PRO	N	-29.88	-39.21	59.49	15.00
114	PRO	CD	-31.02	-39.93	60.09	15.00
114	PRO	CA	-29.39	-39.90	58.30	15.00
114	PRO	CB	-30.43	-41.00	58.08	15.00
114	PRO	CG	-30.91	-41.30	59.46	15.00
114	PRO	C	-29.36	-38.89	57.15	15.00
114	PRO	O	-30.36	-38.22	56.87	15.00
115	GLU	N	-28.18	-38.70	56.57	15.00
115	GLU	CA	-27.97	-37.75	55.49	15.00
115	GLU	CB	-26.55	-37.89	54.96	15.00
115	GLU	CG	-26.25	-37.14	53.69	15.00
115	GLU	CD	-24.98	-37.66	53.04	15.00
115	GLU	OE1	-25.08	-38.38	52.01	15.00

TABLE IV

115	GLU	OE2	-23.89	-37.37	53.58	15.00
115	GLU	C	-28.99	-37.89	54.35	15.00
115	GLU	O	-29.14	-38.97	53.79	15.00
116	GLY	N	-29.66	-36.78	54.03	15.00
116	GLY	CA	-30.66	-36.76	52.98	15.00
116	GLY	C	-32.05	-37.27	53.37	15.00
116	GLY	O	-33.00	-37.16	52.59	15.00
117	ASN	N	-32.17	-37.77	54.60	15.00
117	ASN	CA	-33.43	-38.32	55.09	15.00
117	ASN	CB	-33.14	-39.42	56.11	15.00
117	ASN	CG	-34.25	-40.47	56.18	15.00
117	ASN	OD1	-35.40	-40.19	55.83	15.00
117	ASN	ND2	-33.91	-41.67	56.64	15.00
117	ASN	C	-34.36	-37.28	55.72	15.00
117	ASN	O	-34.34	-37.10	56.93	15.00
118	GLU	N	-35.19	-36.64	54.89	15.00
118	GLU	CA	-36.16	-35.64	55.36	15.00
118	GLU	CB	-36.86	-34.94	54.19	15.00
118	GLU	CG	-36.01	-33.88	53.50	15.00
118	GLU	CD	-36.83	-32.98	52.60	15.00
118	GLU	OE1	-36.94	-33.27	51.39	15.00
118	GLU	OE2	-37.37	-31.97	53.11	15.00
118	GLU	C	-37.21	-36.24	56.30	15.00
118	GLU	O	-37.72	-35.57	57.19	15.00
119	LYS	N	-37.53	-37.52	56.08	15.00
119	LYS	CA	-38.47	-38.23	56.93	15.00
119	LYS	CB	-38.64	-39.66	56.41	15.00
119	LYS	CG	-39.73	-39.83	55.38	15.00
119	LYS	CD	-39.53	-41.10	54.58	15.00
119	LYS	CE	-38.51	-40.88	53.46	15.00
119	LYS	NZ	-38.97	-39.83	52.48	15.00
119	LYS	C	-37.91	-38.29	58.36	15.00
119	LYS	O	-38.58	-37.89	59.32	15.00
120	ALA	N	-36.70	-38.81	58.51	15.00
120	ALA	CA	-36.06	-38.92	59.81	15.00
120	ALA	CB	-34.71	-39.60	59.68	15.00
120	ALA	C	-35.91	-37.54	60.41	15.00
120	ALA	O	-36.06	-37.38	61.61	15.00
121	LEU	N	-35.63	-36.55	59.56	15.00
121	LEU	CA	-35.48	-35.17	60.05	15.00
121	LEU	CB	-35.11	-34.21	58.90	15.00
121	LEU	CG	-34.87	-32.75	59.33	15.00

TABLE IV

121	LEU	CD1	-33.74	-32.69	60.38	15.00
121	LEU	CD2	-34.53	-31.88	58.12	15.00
121	LEU	C	-36.78	-34.71	60.72	15.00
121	LEU	O	-36.75	-34.17	61.83	15.00
122	LYS	N	-37.91	-34.94	60.05	15.00
122	LYS	CA	-39.23	-34.59	60.56	15.00
122	LYS	CB	-40.31	-35.02	59.58	15.00
122	LYS	CG	-41.74	-34.91	60.12	15.00
122	LYS	CD	-42.72	-35.57	59.17	15.00
122	LYS	CE	-44.11	-35.67	59.76	15.00
122	LYS	NZ	-45.10	-36.14	58.74	15.00
122	LYS	C	-39.44	-35.32	61.88	15.00
122	LYS	O	-39.88	-34.74	62.87	15.00
123	ARG	N	-39.14	-36.61	61.86	15.00
123	ARG	CA	-39.28	-37.46	63.03	15.00
123	ARG	CB	-38.80	-38.87	62.70	15.00
123	ARG	CG	-38.84	-39.87	63.86	15.00
123	ARG	CD	-37.70	-40.88	63.77	15.00
123	ARG	NE	-37.37	-41.20	62.38	15.00
123	ARG	CZ	-36.78	-42.32	61.98	15.00
123	ARG	NH1	-36.45	-43.25	62.87	15.00
123	ARG	NH2	-36.53	-42.51	60.69	15.00
123	ARG	C	-38.46	-36.88	64.19	15.00
123	ARG	O	-38.93	-36.84	65.32	15.00
124	ALA	N	-37.25	-36.42	63.89	15.00
124	ALA	CA	-36.37	-35.84	64.90	15.00
124	ALA	CB	-34.98	-35.61	64.35	15.00
124	ALA	C	-36.95	-34.53	65.45	15.00
124	ALA	O	-37.02	-34.33	66.66	15.00
125	VAL	N	-37.41	-33.66	64.57	15.00
125	VAL	CA	-37.99	-32.41	65.03	15.00
125	VAL	CB	-38.35	-31.48	63.87	15.00
125	VAL	CG1	-38.98	-30.19	64.39	15.00
125	VAL	CG2	-37.09	-31.17	63.06	15.00
125	VAL	C	-39.23	-32.65	65.89	15.00
125	VAL	O	-39.46	-31.94	66.87	15.00
126	ALA	N	-40.01	-33.67	65.53	15.00
126	ALA	CA	-41.22	-34.03	66.25	15.00
126	ALA	CB	-42.03	-35.02	65.44	15.00
126	ALA	C	-40.89	-34.61	67.62	15.00
126	ALA	O	-41.40	-34.14	68.64	15.00
127	ARG	N	-40.03	-35.62	67.64	15.00

TABLE IV

127	ARG	CA	-39.61	-36.29	68.86	15.00
127	ARG	CB	-38.83	-37.54	68.48	15.00
127	ARG	CG	-38.45	-38.44	69.64	15.00
127	ARG	CD	-39.63	-39.28	70.13	15.00
127	ARG	NE	-40.15	-40.18	69.10	15.00
127	ARG	CZ	-41.18	-39.90	68.31	15.00
127	ARG	NH1	-41.59	-40.78	67.41	15.00
127	ARG	NH2	-41.81	-38.73	68.42	15.00
127	ARG	C	-38.75	-35.47	69.83	15.00
127	ARG	O	-39.05	-35.36	71.01	15.00
128	VAL	N	-37.64	-34.94	69.31	15.00
128	VAL	CA	-36.66	-34.21	70.11	15.00
128	VAL	CB	-35.23	-34.54	69.59	15.00
128	VAL	CG1	-34.17	-33.72	70.32	15.00
128	VAL	CG2	-34.95	-36.02	69.74	15.00
128	VAL	C	-36.82	-32.70	70.26	15.00
128	VAL	O	-36.73	-32.17	71.36	15.00
129	GLY	N	-37.00	-32.01	69.14	15.00
129	GLY	CA	-37.16	-30.56	69.20	15.00
129	GLY	C	-36.36	-29.91	68.08	15.00
129	GLY	O	-35.89	-30.62	67.18	15.00
130	PRO	N	-36.19	-28.57	68.11	15.00
130	PRO	CD	-36.66	-27.66	69.17	15.00
130	PRO	CA	-35.45	-27.83	67.09	15.00
130	PRO	CB	-35.23	-26.47	67.74	15.00
130	PRO	CG	-36.51	-26.30	68.52	15.00
130	PRO	C	-34.13	-28.52	66.74	15.00
130	PRO	O	-33.37	-28.91	67.63	15.00
131	VAL	N	-33.90	-28.72	65.45	15.00
131	VAL	CA	-32.71	-29.40	64.97	15.00
131	VAL	CB	-33.13	-30.65	64.15	15.00
131	VAL	CG1	-31.93	-31.36	63.57	15.00
131	VAL	CG2	-33.92	-31.61	65.03	15.00
131	VAL	C	-31.82	-28.49	64.13	15.00
131	VAL	O	-32.32	-27.69	63.34	15.00
132	SER	N	-30.51	-28.59	64.32	15.00
132	SER	CA	-29.56	-27.79	63.55	15.00
132	SER	CB	-28.18	-27.83	64.22	15.00
132	SER	OG	-28.20	-27.34	65.55	15.00
132	SER	C	-29.44	-28.37	62.14	15.00
132	SER	O	-29.41	-29.59	61.96	15.00
133	VAL	N	-29.39	-27.50	61.13	15.00

TABLE IV

133	VAL	CA	-29.25	-27.94	59.75	15.00
133	VAL	CB	-30.63	-28.07	59.03	15.00
133	VAL	CG1	-31.40	-29.29	59.53	15.00
133	VAL	CG2	-31.45	-26.80	59.20	15.00
133	VAL	C	-28.37	-27.00	58.94	15.00
133	VAL	O	-28.12	-25.87	59.34	15.00
134	ALA	N	-27.86	-27.50	57.82	15.00
134	ALA	CA	-27.03	-26.73	56.91	15.00
134	ALA	CB	-25.65	-27.34	56.76	15.00
134	ALA	C	-27.75	-26.73	55.57	15.00
134	ALA	O	-28.29	-27.76	55.14	15.00
135	ILE	N	-27.80	-25.58	54.94	15.00
135	ILE	CA	-28.49	-25.45	53.66	15.00
135	ILE	CB	-29.82	-24.68	53.82	15.00
135	ILE	CG2	-30.80	-25.45	54.70	15.00
135	ILE	CG1	-29.52	-23.28	54.38	15.00
135	ILE	CD1	-30.72	-22.40	54.52	15.00
135	ILE	C	-27.64	-24.61	52.73	15.00
135	ILE	O	-26.59	-24.09	53.13	15.00
136	ASP	N	-28.09	-24.49	51.49	15.00
136	ASP	CA	-27.42	-23.66	50.51	15.00
136	ASP	CB	-27.50	-24.28	49.11	15.00
136	ASP	CG	-27.02	-23.32	48.02	15.00
136	ASP	OD1	-27.46	-23.49	46.88	15.00
136	ASP	OD2	-26.22	-22.40	48.29	15.00
136	ASP	C	-28.19	-22.36	50.54	15.00
136	ASP	O	-29.34	-22.29	50.10	15.00
137	ALA	N	-27.58	-21.33	51.11	15.00
137	ALA	CA	-28.19	-20.02	51.21	15.00
137	ALA	CB	-28.14	-19.54	52.65	15.00
137	ALA	C	-27.47	-19.04	50.30	15.00
137	ALA	O	-27.42	-17.85	50.60	15.00
138	SER	N	-26.94	-19.53	49.20	15.00
138	SER	CA	-26.20	-18.66	48.30	15.00
138	SER	CB	-25.12	-19.44	47.57	15.00
138	SER	OG	-25.71	-20.45	46.78	15.00
138	SER	C	-27.06	-17.91	47.29	15.00
138	SER	O	-26.76	-16.77	46.94	15.00
139	LEU	N	-28.12	-18.55	46.82	15.00
139	LEU	CA	-28.99	-17.95	45.82	15.00
139	LEU	CB	-30.12	-18.91	45.46	15.00
139	LEU	CG	-29.76	-20.02	44.48	15.00

TABLE IV

139	LEU	CD1	-29.30	-19.40	43.18	15.00
139	LEU	CD2	-28.67	-20.89	45.03	15.00
139	LEU	C	-29.56	-16.58	46.18	15.00
139	LEU	O	-29.93	-16.32	47.33	15.00
140	THR	N	-29.63	-15.71	45.19	15.00
140	THR	CA	-30.19	-14.37	45.38	15.00
140	THR	CB	-30.06	-13.54	44.09	15.00
140	THR	OG1	-28.67	-13.30	43.82	15.00
140	THR	CG2	-30.80	-12.20	44.20	15.00
140	THR	C	-31.65	-14.43	45.86	15.00
140	THR	O	-32.09	-13.62	46.69	15.00
141	SER	N	-32.38	-15.45	45.40	15.00
141	SER	CA	-33.77	-15.63	45.79	15.00
141	SER	CB	-34.39	-16.77	44.99	15.00
141	SER	OG	-33.78	-18.00	45.32	15.00
141	SER	C	-33.89	-15.89	47.29	15.00
141	SER	O	-34.94	-15.63	47.90	15.00
142	PHE	N	-32.82	-16.43	47.89	15.00
142	PHE	CA	-32.79	-16.70	49.33	15.00
142	PHE	CB	-31.71	-17.72	49.67	15.00
142	PHE	CG	-31.77	-18.20	51.08	15.00
142	PHE	CD1	-32.45	-19.38	51.39	15.00
142	PHE	CD2	-31.14	-17.49	52.10	15.00
142	PHE	CE1	-32.51	-19.85	52.70	15.00
142	PHE	CE2	-31.20	-17.95	53.41	15.00
142	PHE	CZ	-31.88	-19.14	53.72	15.00
142	PHE	C	-32.53	-15.40	50.08	15.00
142	PHE	O	-33.22	-15.09	51.06	15.00
143	GLN	N	-31.55	-14.64	49.60	15.00
143	GLN	CA	-31.19	-13.38	50.22	15.00
143	GLN	CB	-30.07	-12.72	49.44	15.00
143	GLN	CG	-29.68	-11.32	49.94	15.00
143	GLN	CD	-28.36	-10.81	49.37	15.00
143	GLN	OE1	-28.05	-9.62	49.47	15.00
143	GLN	NE2	-27.56	-11.71	48.80	15.00
143	GLN	C	-32.38	-12.43	50.33	15.00
143	GLN	O	-32.57	-11.75	51.35	15.00
144	PHE	N	-33.22	-12.40	49.30	15.00
144	PHE	CA	-34.36	-11.50	49.31	15.00
144	PHE	CB	-34.41	-10.73	47.98	15.00
144	PHE	CG	-33.22	-9.85	47.75	15.00
144	PHE	CD1	-33.13	-8.59	48.35	15.00

TABLE IV

144	PHE	CD2	-32.17	-10.27	46.94	15.00
144	PHE	CE1	-32.02	-7.77	48.15	15.00
144	PHE	CE2	-31.05	-9.46	46.73	15.00
144	PHE	CZ	-30.98	-8.21	47.34	15.00
144	PHE	C	-35.73	-12.13	49.64	15.00
144	PHE	O	-36.77	-11.52	49.38	15.00
145	TYR	N	-35.72	-13.30	50.26	15.00
145	TYR	CA	-36.97	-13.98	50.63	15.00
145	TYR	CB	-36.68	-15.35	51.26	15.00
145	TYR	CG	-37.89	-15.98	51.94	15.00
145	TYR	CD1	-38.72	-16.89	51.26	15.00
145	TYR	CE1	-39.83	-17.45	51.89	15.00
145	TYR	CD2	-38.21	-15.66	53.26	15.00
145	TYR	CE2	-39.33	-16.22	53.90	15.00
145	TYR	CZ	-40.13	-17.12	53.21	15.00
145	TYR	OH	-41.21	-17.68	53.85	15.00
145	TYR	C	-37.81	-13.16	51.62	15.00
145	TYR	O	-37.27	-12.49	52.50	15.00
146	SER	N	-39.13	-13.26	51.50	15.00
146	SER	CA	-40.03	-12.55	52.41	15.00
146	SER	CB	-40.33	-11.12	51.96	15.00
146	SER	OG	-40.50	-11.03	50.57	15.00
146	SER	C	-41.31	-13.30	52.73	15.00
146	SER	O	-41.74	-13.31	53.88	15.00
147	LYS	N	-41.89	-14.00	51.76	15.00
147	LYS	CA	-43.13	-14.74	51.99	15.00
147	LYS	CB	-44.34	-13.80	51.82	15.00
147	LYS	CG	-44.60	-12.90	53.05	15.00
147	LYS	CD	-45.56	-11.75	52.75	15.00
147	LYS	CE	-45.63	-10.76	53.91	15.00
147	LYS	NZ	-46.25	-11.32	55.15	15.00
147	LYS	C	-43.30	-15.99	51.13	15.00
147	LYS	O	-42.68	-16.13	50.07	15.00
148	GLY	N	-44.12	-16.92	51.60	15.00
148	GLY	CA	-44.36	-18.14	50.87	15.00
148	GLY	C	-43.35	-19.22	51.18	15.00
148	GLY	O	-42.39	-19.00	51.90	15.00
149	VAL	N	-43.60	-20.42	50.67	15.00
149	VAL	CA	-42.69	-21.53	50.90	15.00
149	VAL	CB	-43.43	-22.89	50.72	15.00
149	VAL	CG1	-42.46	-24.05	50.79	15.00
149	VAL	CG2	-44.49	-23.05	51.80	15.00

TABLE IV

149	VAL	C	-41.56	-21.34	49.88	15.00
149	VAL	O	-41.81	-21.30	48.67	15.00
150	TYR	N	-40.34	-21.13	50.37	15.00
150	TYR	CA	-39.19	-20.92	49.50	15.00
150	TYR	CB	-37.99	-20.42	50.30	15.00
150	TYR	CG	-36.72	-20.27	49.46	15.00
150	TYR	CD1	-36.48	-19.11	48.72	15.00
150	TYR	CE1	-35.31	-18.98	47.96	15.00
150	TYR	CD2	-35.77	-21.30	49.41	15.00
150	TYR	CE2	-34.59	-21.17	48.65	15.00
150	TYR	CZ	-34.37	-20.01	47.93	15.00
150	TYR	OH	-33.22	-19.88	47.19	15.00
150	TYR	C	-38.80	-22.18	48.76	15.00
150	TYR	O	-38.87	-23.29	49.30	15.00
151	TYR	N	-38.31	-21.98	47.54	15.00
151	TYR	CA	-37.87	-23.07	46.68	15.00
151	TYR	CB	-39.07	-23.95	46.31	15.00
151	TYR	CG	-38.80	-25.01	45.27	15.00
151	TYR	CD1	-38.36	-26.28	45.62	15.00
151	TYR	CE1	-38.19	-27.27	44.66	15.00
151	TYR	CD2	-39.05	-24.75	43.92	15.00
151	TYR	CE2	-38.88	-25.73	42.96	15.00
151	TYR	CZ	-38.46	-26.98	43.33	15.00
151	TYR	OH	-38.34	-27.95	42.36	15.00
151	TYR	C	-37.24	-22.44	45.44	15.00
151	TYR	O	-37.66	-21.37	45.00	15.00
152	ASP	N	-36.22	-23.11	44.89	15.00
152	ASP	CA	-35.52	-22.62	43.70	15.00
152	ASP	CB	-34.55	-21.50	44.08	15.00
152	ASP	CG	-33.97	-20.77	42.87	15.00
152	ASP	OD1	-33.75	-21.39	41.81	15.00
152	ASP	OD2	-33.72	-19.56	42.99	15.00
152	ASP	C	-34.75	-23.77	43.07	15.00
152	ASP	O	-33.90	-24.38	43.73	15.00
153	GLU	N	-35.01	-24.02	41.79	15.00
153	GLU	CA	-34.35	-25.09	41.04	15.00
153	GLU	CB	-34.78	-25.06	39.56	15.00
153	GLU	CG	-36.22	-25.45	39.26	15.00
153	GLU	CD	-36.59	-25.21	37.78	15.00
153	GLU	OE1	-37.05	-24.09	37.45	15.00
153	GLU	OE2	-36.40	-26.14	36.96	15.00
153	GLU	C	-32.84	-24.95	41.09	15.00

TABLE IV

153	GLU	O	-32.12	-25.93	40.99	15.00
154	SER	N	-32.38	-23.71	41.20	15.00
154	SER	CA	-30.95	-23.41	41.24	15.00
154	SER	CB	-30.73	-21.93	40.92	15.00
154	SER	OG	-31.33	-21.57	39.69	15.00
154	SER	C	-30.25	-23.78	42.55	15.00
154	SER	O	-29.02	-23.75	42.63	15.00
155	CYS	N	-31.02	-24.11	43.58	15.00
155	CYS	CA	-30.44	-24.46	44.87	15.00
155	CYS	C	-29.58	-25.72	44.76	15.00
155	CYS	O	-29.98	-26.72	44.17	15.00
155	CYS	CB	-31.53	-24.65	45.92	15.00
155	CYS	SG	-31.12	-23.81	47.48	15.00
156	ASN	N	-28.40	-25.67	45.35	15.00
156	ASN	CA	-27.48	-26.80	45.29	15.00
156	ASN	CB	-26.09	-26.28	44.91	15.00
156	ASN	CG	-25.15	-27.39	44.45	15.00
156	ASN	OD1	-25.21	-28.54	44.94	15.00
156	ASN	ND2	-24.26	-27.05	43.53	15.00
156	ASN	C	-27.42	-27.58	46.61	15.00
156	ASN	O	-26.99	-27.06	47.64	15.00
157	SER	N	-27.80	-28.85	46.54	15.00
157	SER	CA	-27.82	-29.72	47.71	15.00
157	SER	CB	-28.66	-30.98	47.45	15.00
157	SER	OG	-28.07	-31.81	46.47	15.00
157	SER	C	-26.43	-30.14	48.17	15.00
157	SER	O	-26.27	-30.76	49.23	15.00
158	ASP	N	-25.42	-29.82	47.37	15.00
158	ASP	CA	-24.06	-30.18	47.69	15.00
158	ASP	CB	-23.44	-30.99	46.55	15.00
158	ASP	CG	-23.70	-32.49	46.69	15.00
158	ASP	OD1	-24.30	-33.11	45.78	15.00
158	ASP	OD2	-23.32	-33.05	47.75	15.00
158	ASP	C	-23.21	-29.01	48.14	15.00
158	ASP	O	-22.19	-29.21	48.79	15.00
159	ASN	N	-23.67	-27.80	47.85	15.00
159	ASN	CA	-22.95	-26.60	48.28	15.00
159	ASN	CB	-23.04	-25.49	47.22	15.00
159	ASN	CG	-22.27	-24.23	47.61	15.00
159	ASN	OD1	-21.81	-24.09	48.74	15.00
159	ASN	ND2	-22.14	-23.31	46.67	15.00
159	ASN	C	-23.55	-26.10	49.61	15.00

TABLE IV

159	ASN	O	-24.20	-25.06	49.67	15.00
160	LEU	N	-23.38	-26.89	50.68	15.00
160	LEU	CA	-23.91	-26.47	51.98	15.00
160	LEU	CB	-23.83	-27.61	52.99	15.00
160	LEU	CG	-24.49	-28.94	52.62	15.00
160	LEU	CD1	-24.41	-29.89	53.81	15.00
160	LEU	CD2	-25.94	-28.71	52.23	15.00
160	LEU	C	-23.04	-25.30	52.41	15.00
160	LEU	O	-21.82	-25.42	52.46	15.00
161	ASN	N	-23.65	-24.15	52.70	15.00
161	ASN	CA	-22.86	-22.98	53.07	15.00
161	ASN	CB	-22.59	-22.13	51.83	15.00
161	ASN	CG	-23.82	-21.92	50.98	15.00
161	ASN	OD1	-24.77	-21.24	51.38	15.00
161	ASN	ND2	-23.83	-22.51	49.81	15.00
161	ASN	C	-23.40	-22.10	54.20	15.00
161	ASN	O	-22.80	-21.07	54.54	15.00
162	HIS	N	-24.47	-22.55	54.85	15.00
162	HIS	CA	-25.07	-21.78	55.92	15.00
162	HIS	CB	-26.12	-20.83	55.33	15.00
162	HIS	CG	-26.58	-19.75	56.27	15.00
162	HIS	CD2	-27.81	-19.22	56.48	15.00
162	HIS	ND1	-25.73	-19.08	57.12	15.00
162	HIS	CE1	-26.41	-18.20	57.83	15.00
162	HIS	NE2	-27.68	-18.27	57.46	15.00
162	HIS	C	-25.71	-22.76	56.91	15.00
162	HIS	O	-26.37	-23.71	56.50	15.00
163	ALA	N	-25.40	-22.58	58.19	15.00
163	ALA	CA	-25.96	-23.43	59.24	15.00
163	ALA	CB	-24.95	-23.66	60.35	15.00
163	ALA	C	-27.17	-22.65	59.74	15.00
163	ALA	O	-27.10	-21.42	59.92	15.00
164	VAL	N	-28.27	-23.34	59.96	15.00
164	VAL	CA	-29.51	-22.71	60.36	15.00
164	VAL	CB	-30.30	-22.38	59.08	15.00
164	VAL	CG1	-31.28	-23.48	58.75	15.00
164	VAL	CG2	-30.90	-20.99	59.15	15.00
164	VAL	C	-30.30	-23.60	61.34	15.00
164	VAL	O	-29.89	-24.73	61.62	15.00
165	LEU	N	-31.40	-23.09	61.89	15.00
165	LEU	CA	-32.18	-23.86	62.86	15.00
165	LEU	CB	-32.27	-23.11	64.20	15.00

TABLE IV

165	LEU	CG	-32.79	-23.87	65.44	15.00
165	LEU	CD1	-31.76	-24.89	65.90	15.00
165	LEU	CD2	-33.13	-22.90	66.57	15.00
165	LEU	C	-33.58	-24.27	62.40	15.00
165	LEU	O	-34.39	-23.42	62.03	15.00
166	ALA	N	-33.85	-25.57	62.43	15.00
166	ALA	CA	-35.15	-26.11	62.05	15.00
166	ALA	CB	-35.00	-27.51	61.50	15.00
166	ALA	C	-35.99	-26.11	63.33	15.00
166	ALA	O	-35.76	-26.91	64.25	15.00
167	VAL	N	-36.94	-25.19	63.39	15.00
167	VAL	CA	-37.80	-25.06	64.55	15.00
167	VAL	CB	-37.81	-23.60	65.03	15.00
167	VAL	CG1	-38.83	-22.75	64.24	15.00
167	VAL	CG2	-38.06	-23.55	66.50	15.00
167	VAL	C	-39.23	-25.58	64.33	15.00
167	VAL	O	-40.15	-25.31	65.14	15.00
168	GLY	N	-39.44	-26.31	63.24	15.00
168	GLY	CA	-40.76	-26.84	62.97	15.00
168	GLY	C	-40.97	-27.25	61.53	15.00
168	GLY	O	-40.02	-27.37	60.74	15.00
169	TYR	N	-42.23	-27.48	61.20	15.00
169	TYR	CA	-42.67	-27.89	59.87	15.00
169	TYR	CB	-42.21	-29.33	59.54	15.00
169	TYR	CG	-42.75	-30.41	60.46	15.00
169	TYR	CD1	-43.94	-31.09	60.16	15.00
169	TYR	CE1	-44.43	-32.10	60.99	15.00
169	TYR	CD2	-42.06	-30.79	61.61	15.00
169	TYR	CE2	-42.53	-31.80	62.45	15.00
169	TYR	CZ	-43.71	-32.45	62.13	15.00
169	TYR	OH	-44.15	-33.47	62.94	15.00
169	TYR	C	-44.18	-27.80	59.84	15.00
169	TYR	O	-44.84	-27.82	60.88	15.00
170	GLY	N	-44.73	-27.73	58.64	15.00
170	GLY	CA	-46.17	-27.63	58.48	15.00
170	GLY	C	-46.53	-27.64	57.01	15.00
170	GLY	O	-45.73	-28.04	56.18	15.00
171	ILE	N	-47.71	-27.14	56.69	15.00
171	ILE	CA	-48.16	-27.09	55.30	15.00
171	ILE	CB	-48.95	-28.37	54.91	15.00
171	ILE	CG2	-50.04	-28.69	55.91	15.00
171	ILE	CG1	-49.52	-28.25	53.51	15.00

TABLE IV

171	ILE	CD1	-50.20	-29.53	53.05	15.00
171	ILE	C	-48.97	-25.82	55.09	15.00
171	ILE	O	-49.84	-25.48	55.89	15.00
172	GLN	N	-48.59	-25.07	54.05	15.00
172	GLN	CA	-49.21	-23.80	53.72	15.00
172	GLN	CB	-48.19	-22.67	53.89	15.00
172	GLN	CG	-48.68	-21.32	53.45	15.00
172	GLN	CD	-47.73	-20.20	53.84	15.00
172	GLN	OE1	-47.84	-19.61	54.92	15.00
172	GLN	NE2	-46.78	-19.89	52.96	15.00
172	GLN	C	-49.73	-23.81	52.29	15.00
172	GLN	O	-48.96	-23.96	51.33	15.00
173	LYS	N	-51.04	-23.64	52.17	15.00
173	LYS	CA	-51.73	-23.62	50.88	15.00
173	LYS	CB	-51.37	-22.35	50.09	15.00
173	LYS	CG	-51.48	-21.01	50.88	15.00
173	LYS	CD	-52.85	-20.77	51.55	15.00
173	LYS	CE	-54.02	-20.84	50.56	15.00
173	LYS	NZ	-53.89	-19.90	49.41	15.00
173	LYS	C	-51.39	-24.87	50.08	15.00
173	LYS	O	-51.27	-24.82	48.87	15.00
174	GLY	N	-51.22	-25.99	50.77	15.00
174	GLY	CA	-50.91	-27.24	50.10	15.00
174	GLY	C	-49.43	-27.58	50.06	15.00
174	GLY	O	-49.07	-28.71	49.74	15.00
175	ASN	N	-48.59	-26.65	50.48	15.00
175	ASN	CA	-47.15	-26.87	50.44	15.00
175	ASN	CB	-46.44	-25.64	49.88	15.00
175	ASN	CG	-47.06	-25.14	48.59	15.00
175	ASN	OD1	-47.08	-25.86	47.58	15.00
175	ASN	ND2	-47.56	-23.91	48.62	15.00
175	ASN	C	-46.54	-27.23	51.79	15.00
175	ASN	O	-46.63	-26.46	52.74	15.00
176	LYS	N	-45.92	-28.40	51.87	15.00
176	LYS	CA	-45.28	-28.84	53.09	15.00
176	LYS	CB	-44.98	-30.33	53.02	15.00
176	LYS	CG	-46.23	-31.18	52.84	15.00
176	LYS	CD	-45.95	-32.63	53.09	15.00
176	LYS	CE	-47.17	-33.48	52.82	15.00
176	LYS	NZ	-46.84	-34.93	52.78	15.00
176	LYS	C	-44.00	-28.03	53.20	15.00
176	LYS	O	-43.37	-27.73	52.19	15.00

TABLE IV

177	HIS	N	-43.59	-27.69	54.42	15.00
177	HIS	CA	-42.39	-26.88	54.58	15.00
177	HIS	CB	-42.76	-25.39	54.51	15.00
177	HIS	CG	-43.62	-24.94	55.64	15.00
177	HIS	CD2	-43.32	-24.68	56.94	15.00
177	HIS	ND1	-44.96	-24.70	55.50	15.00
177	HIS	CE1	-45.46	-24.31	56.66	15.00
177	HIS	NE2	-44.48	-24.29	57.55	15.00
177	HIS	C	-41.68	-27.10	55.88	15.00
177	HIS	O	-42.20	-27.76	56.78	15.00
178	TRP	N	-40.52	-26.46	55.99	15.00
178	TRP	CA	-39.69	-26.51	57.18	15.00
178	TRP	CB	-38.24	-26.84	56.79	15.00
178	TRP	CG	-38.01	-28.23	56.31	15.00
178	TRP	CD2	-38.14	-29.45	57.06	15.00
178	TRP	CE2	-37.73	-30.50	56.22	15.00
178	TRP	CE3	-38.56	-29.74	58.37	15.00
178	TRP	CD1	-37.55	-28.59	55.07	15.00
178	TRP	NE1	-37.38	-29.95	55.01	15.00
178	TRP	CZ2	-37.73	-31.85	56.64	15.00
178	TRP	CZ3	-38.56	-31.08	58.79	15.00
178	TRP	CH2	-38.14	-32.12	57.92	15.00
178	TRP	C	-39.73	-25.11	57.74	15.00
178	TRP	O	-39.68	-24.14	56.97	15.00
179	ILE	N	-39.90	-24.97	59.05	15.00
179	ILE	CA	-39.91	-23.65	59.65	15.00
179	ILE	CB	-40.89	-23.55	60.84	15.00
179	ILE	CG2	-40.95	-22.10	61.34	15.00
179	ILE	CG1	-42.29	-24.02	60.43	15.00
179	ILE	CD1	-43.32	-23.95	61.55	15.00
179	ILE	C	-38.47	-23.41	60.08	15.00
179	ILE	O	-37.96	-24.05	61.00	15.00
180	ILE	N	-37.79	-22.52	59.36	15.00
180	ILE	CA	-36.40	-22.23	59.61	15.00
180	ILE	CB	-35.58	-22.34	58.29	15.00
180	ILE	CG2	-34.14	-21.97	58.52	15.00
180	ILE	CG1	-35.74	-23.74	57.68	15.00
180	ILE	CD1	-35.52	-24.88	58.66	15.00
180	ILE	C	-36.13	-20.88	60.25	15.00
180	ILE	O	-36.68	-19.85	59.84	15.00
181	LYS	N	-35.24	-20.90	61.25	15.00
181	LYS	CA	-34.84	-19.72	61.99	15.00

TABLE IV

181	LYS	CB	-34.77	-20.06	63.48	15.00
181	LYS	CG	-34.66	-18.84	64.35	15.00
181	LYS	CD	-34.34	-19.17	65.79	15.00
181	LYS	CE	-34.16	-17.89	66.56	15.00
181	LYS	NZ	-33.69	-18.09	67.94	15.00
181	LYS	C	-33.46	-19.27	61.49	15.00
181	LYS	O	-32.50	-20.03	61.56	15.00
182	ASN	N	-33.37	-18.05	60.98	15.00
182	ASN	CA	-32.11	-17.52	60.47	15.00
182	ASN	CB	-32.33	-16.76	59.15	15.00
182	ASN	CG	-31.05	-16.64	58.29	15.00
182	ASN	OD1	-30.00	-17.21	58.60	15.00
182	ASN	ND2	-31.15	-15.91	57.18	15.00
182	ASN	C	-31.43	-16.62	61.51	15.00
182	ASN	O	-32.00	-16.33	62.57	15.00
183	SER	N	-30.18	-16.25	61.24	15.00
183	SER	CA	-29.43	-15.38	62.14	15.00
183	SER	CB	-28.25	-16.13	62.75	15.00
183	SER	OG	-27.48	-16.78	61.76	15.00
183	SER	C	-28.96	-14.09	61.44	15.00
183	SER	O	-27.85	-13.63	61.66	15.00
184	TRP	N	-29.82	-13.52	60.59	15.00
184	TRP	CA	-29.50	-12.28	59.88	15.00
184	TRP	CB	-29.69	-12.45	58.37	15.00
184	TRP	CG	-28.71	-13.44	57.76	15.00
184	TRP	CD2	-28.74	-13.98	56.44	15.00
184	TRP	CE2	-27.62	-14.83	56.30	15.00
184	TRP	CE3	-29.60	-13.83	55.34	15.00
184	TRP	CD1	-27.60	-13.98	58.37	15.00
184	TRP	NE1	-26.95	-14.81	57.50	15.00
184	TRP	CZ2	-27.34	-15.53	55.13	15.00
184	TRP	CZ3	-29.33	-14.52	54.17	15.00
184	TRP	CH2	-28.21	-15.35	54.07	15.00
184	TRP	C	-30.35	-11.11	60.40	15.00
184	TRP	O	-30.51	-10.09	59.72	15.00
185	GLY	N	-30.84	-11.25	61.63	15.00
185	GLY	CA	-31.67	-10.22	62.24	15.00
185	GLY	C	-33.14	-10.43	61.94	15.00
185	GLY	O	-33.49	-11.18	61.03	15.00
186	GLU	N	-33.99	-9.73	62.68	15.00
186	GLU	CA	-35.45	-9.83	62.50	15.00
186	GLU	CB	-36.17	-9.31	63.74	15.00

TABLE IV

186	GLU	CG	-35.94	-10.14	64.97	15.00
186	GLU	CD	-37.15	-10.15	65.89	15.00
186	GLU	OE1	-38.26	-10.52	65.41	15.00
186	GLU	OE2	-37.01	-9.81	67.09	15.00
186	GLU	C	-36.05	-9.15	61.27	15.00
186	GLU	O	-37.10	-9.56	60.78	15.00
187	ASN	N	-35.38	-8.12	60.76	15.00
187	ASN	CA	-35.89	-7.42	59.59	15.00
187	ASN	CB	-35.32	-6.00	59.52	15.00
187	ASN	CG	-35.95	-5.04	60.53	15.00
187	ASN	OD1	-35.82	-3.83	60.39	15.00
187	ASN	ND2	-36.62	-5.58	61.56	15.00
187	ASN	C	-35.60	-8.14	58.29	15.00
187	ASN	O	-35.82	-7.57	57.22	15.00
188	TRP	N	-35.12	-9.38	58.37	15.00
188	TRP	CA	-34.81	-10.18	57.17	15.00
188	TRP	CB	-33.42	-10.84	57.28	15.00
188	TRP	CG	-33.16	-11.85	56.18	15.00
188	TRP	CD2	-33.54	-13.23	56.17	15.00
188	TRP	CE2	-33.19	-13.75	54.89	15.00
188	TRP	CE3	-34.14	-14.09	57.10	15.00
188	TRP	CD1	-32.60	-11.59	54.97	15.00
188	TRP	NE1	-32.63	-12.73	54.18	15.00
188	TRP	CZ2	-33.44	-15.08	54.52	15.00
188	TRP	CZ3	-34.39	-15.42	56.74	15.00
188	TRP	CH2	-34.03	-15.90	55.46	15.00
188	TRP	C	-35.88	-11.27	57.03	15.00
188	TRP	O	-36.45	-11.71	58.04	15.00
189	GLY	N	-36.14	-11.69	55.79	15.00
189	GLY	CA	-37.13	-12.72	55.53	15.00
189	GLY	C	-38.45	-12.40	56.21	15.00
189	GLY	O	-38.91	-11.26	56.15	15.00
190	ASN	N	-39.07	-13.38	56.85	15.00
190	ASN	CA	-40.33	-13.14	57.55	15.00
190	ASN	CB	-41.33	-14.27	57.29	15.00
190	ASN	CG	-42.74	-13.89	57.69	15.00
190	ASN	OD1	-42.98	-12.88	58.35	15.00
190	ASN	ND2	-43.69	-14.70	57.26	15.00
190	ASN	C	-40.03	-13.04	59.04	15.00
190	ASN	O	-40.09	-14.04	59.76	15.00
191	LYS	N	-39.68	-11.83	59.49	15.00
191	LYS	CA	-39.34	-11.59	60.90	15.00

TABLE IV

191	LYS	CB	-40.57	-11.79	61.81	15.00
191	LYS	CG	-41.66	-10.76	61.63	15.00
191	LYS	CD	-42.98	-11.23	62.27	15.00
191	LYS	CE	-43.69	-12.29	61.41	15.00
191	LYS	NZ	-42.88	-13.54	61.16	15.00
191	LYS	C	-38.18	-12.50	61.33	15.00
191	LYS	O	-38.18	-13.07	62.44	15.00
192	GLY	N	-37.22	-12.67	60.43	15.00
192	GLY	CA	-36.06	-13.51	60.71	15.00
192	GLY	C	-36.27	-14.99	60.45	15.00
192	GLY	O	-35.41	-15.81	60.78	15.00
193	TYR	N	-37.40	-15.34	59.87	15.00
193	TYR	CA	-37.69	-16.74	59.58	15.00
193	TYR	CB	-38.93	-17.20	60.33	15.00
193	TYR	CG	-38.68	-17.49	61.78	15.00
193	TYR	CD1	-38.81	-16.48	62.74	15.00
193	TYR	CE1	-38.56	-16.73	64.09	15.00
193	TYR	CD2	-38.31	-18.77	62.20	15.00
193	TYR	CE2	-38.06	-19.03	63.55	15.00
193	TYR	CZ	-38.18	-18.01	64.48	15.00
193	TYR	OH	-37.91	-18.26	65.81	15.00
193	TYR	C	-37.92	-16.95	58.10	15.00
193	TYR	O	-38.22	-16.01	57.36	15.00
194	ILE	N	-37.81	-18.21	57.68	15.00
194	ILE	CA	-38.04	-18.60	56.31	15.00
194	ILE	CB	-36.73	-18.55	55.43	15.00
194	ILE	CG2	-35.60	-19.33	56.09	15.00
194	ILE	CG1	-37.01	-19.10	54.03	15.00
194	ILE	CD1	-35.85	-18.96	53.07	15.00
194	ILE	C	-38.63	-20.00	56.30	15.00
194	ILE	O	-38.16	-20.88	57.01	15.00
195	LEU	N	-39.72	-20.18	55.55	15.00
195	LEU	CA	-40.34	-21.49	55.42	15.00
195	LEU	CB	-41.87	-21.37	55.28	15.00
195	LEU	CG	-42.73	-20.47	56.17	15.00
195	LEU	CD1	-44.18	-20.60	55.73	15.00
195	LEU	CD2	-42.58	-20.81	57.65	15.00
195	LEU	C	-39.76	-22.05	54.13	15.00
195	LEU	O	-39.93	-21.45	53.06	15.00
196	MET	N	-39.03	-23.15	54.22	15.00
196	MET	CA	-38.43	-23.75	53.02	15.00
196	MET	CB	-36.94	-24.02	53.26	15.00

TABLE IV

196	MET	CG	-36.14	-22.77	53.55	15.00
196	MET	SD	-34.44	-23.13	54.06	15.00
196	MET	CE	-33.70	-23.51	52.45	15.00
196	MET	C	-39.16	-25.05	52.64	15.00
196	MET	O	-39.62	-25.77	53.52	15.00
197	ALA	N	-39.26	-25.34	51.35	15.00
197	ALA	CA	-39.95	-26.53	50.86	15.00
197	ALA	CB	-39.82	-26.63	49.36	15.00
197	ALA	C	-39.52	-27.84	51.52	15.00
197	ALA	O	-38.32	-28.08	51.73	15.00
198	ARG	N	-40.50	-28.68	51.85	15.00
198	ARG	CA	-40.27	-29.98	52.48	15.00
198	ARG	CB	-41.04	-30.07	53.81	15.00
198	ARG	CG	-41.06	-31.45	54.43	15.00
198	ARG	CD	-41.33	-31.38	55.94	15.00
198	ARG	NE	-42.61	-30.75	56.26	15.00
198	ARG	CZ	-43.75	-31.42	56.44	15.00
198	ARG	NH1	-43.78	-32.74	56.32	15.00
198	ARG	NH2	-44.87	-30.76	56.70	15.00
198	ARG	C	-40.73	-31.09	51.56	15.00
198	ARG	O	-41.79	-31.00	50.96	15.00
199	ASN	N	-39.95	-32.17	51.52	15.00
199	ASN	CA	-40.22	-33.33	50.68	15.00
199	ASN	CB	-41.58	-33.97	50.99	15.00
199	ASN	CG	-41.67	-34.52	52.39	15.00
199	ASN	OD1	-40.69	-34.50	53.14	15.00
199	ASN	ND2	-42.85	-34.99	52.77	15.00
199	ASN	C	-40.16	-32.94	49.21	15.00
199	ASN	O	-40.84	-33.53	48.36	15.00
200	LYS	N	-39.35	-31.93	48.91	15.00
200	LYS	CA	-39.21	-31.49	47.55	15.00
200	LYS	CB	-39.47	-29.99	47.43	15.00
200	LYS	CG	-40.30	-29.64	46.22	15.00
200	LYS	CD	-41.12	-28.37	46.46	15.00
200	LYS	CE	-42.16	-28.18	45.36	15.00
200	LYS	NZ	-41.56	-28.02	43.99	15.00
200	LYS	C	-37.78	-31.85	47.17	15.00
200	LYS	O	-36.94	-30.98	46.93	15.00
201	ASN	N	-37.51	-33.15	47.20	15.00
201	ASN	CA	-36.21	-33.69	46.86	15.00
201	ASN	CB	-35.94	-33.51	45.37	15.00
201	ASN	CG	-36.89	-34.30	44.52	15.00

TABLE IV

201	ASN	OD1	-37.20	-35.46	44.81	15.00
201	ASN	ND2	-37.40	-33.66	43.47	15.00
201	ASN	C	-35.03	-33.16	47.67	15.00
201	ASN	O	-33.94	-32.96	47.11	15.00
202	ASN	N	-35.23	-33.00	48.98	15.00
202	ASN	CA	-34.18	-32.51	49.89	15.00
202	ASN	CB	-33.04	-33.54	49.99	15.00
202	ASN	CG	-32.05	-33.23	51.10	15.00
202	ASN	OD1	-32.41	-32.67	52.14	15.00
202	ASN	ND2	-30.79	-33.59	50.89	15.00
202	ASN	C	-33.66	-31.16	49.41	15.00
202	ASN	O	-32.46	-30.95	49.27	15.00
203	ALA	N	-34.57	-30.23	49.18	15.00
203	ALA	H	-35.42	-30.45	49.60	15.00
203	ALA	CA	-34.31	-28.90	48.63	15.00
203	ALA	CB	-35.55	-28.01	48.72	15.00
203	ALA	C	-33.20	-28.21	49.44	15.00
203	ALA	O	-33.27	-28.01	50.64	15.00
204	CYS	N	-32.19	-27.72	48.68	15.00
204	CYS	CA	-31.05	-26.98	49.22	15.00
204	CYS	C	-30.21	-27.75	50.22	15.00
204	CYS	O	-29.44	-27.14	50.97	15.00
204	CYS	CB	-31.51	-25.67	49.86	15.00
204	CYS	SG	-32.47	-24.53	48.82	15.00
205	GLY	N	-30.37	-29.07	50.27	15.00
205	GLY	CA	-29.60	-29.89	51.20	15.00
205	GLY	C	-30.01	-29.85	52.66	15.00
205	GLY	O	-29.23	-30.21	53.55	15.00
206	ILE	N	-31.27	-29.50	52.90	15.00
206	ILE	CA	-31.84	-29.38	54.25	15.00
206	ILE	CB	-33.38	-29.05	54.17	15.00
206	ILE	CG2	-34.13	-30.21	53.53	15.00
206	ILE	CG1	-33.94	-28.69	55.54	15.00
206	ILE	CD1	-33.54	-27.31	56.02	15.00
206	ILE	C	-31.59	-30.57	55.19	15.00
206	ILE	O	-31.42	-30.39	56.40	15.00
207	ALA	N	-31.52	-31.77	54.64	15.00
207	ALA	CA	-31.27	-32.95	55.49	15.00
207	ALA	CB	-32.38	-33.99	55.31	15.00
207	ALA	C	-29.89	-33.58	55.26	15.00
207	ALA	O	-29.62	-34.70	55.70	15.00
208	ASN	N	-28.99	-32.84	54.62	15.00

TABLE IV

208	ASN	CA	-27.66	-33.36	54.34	15.00
208	ASN	CB	-27.05	-32.65	53.13	15.00
208	ASN	CG	-27.49	-33.27	51.83	15.00
208	ASN	OD1	-27.92	-34.43	51.79	15.00
208	ASN	ND2	-27.39	-32.51	50.75	15.00
208	ASN	C	-26.67	-33.32	55.51	15.00
208	ASN	O	-25.80	-34.19	55.61	15.00
209	LEU	N	-26.82	-32.35	56.40	15.00
209	LEU	CA	-25.92	-32.20	57.53	15.00
209	LEU	CB	-24.79	-31.22	57.16	15.00
209	LEU	CG	-23.53	-31.18	58.02	15.00
209	LEU	CD1	-22.72	-32.44	57.77	15.00
209	LEU	CD2	-22.72	-29.93	57.68	15.00
209	LEU	C	-26.69	-31.68	58.75	15.00
209	LEU	O	-26.54	-30.52	59.15	15.00
210	ALA	N	-27.50	-32.55	59.34	15.00
210	ALA	H	-27.89	-32.98	58.56	15.00
210	ALA	CA	-28.32	-32.12	60.48	15.00
210	ALA	CB	-29.80	-32.37	60.21	15.00
210	ALA	C	-27.94	-32.94	61.72	15.00
210	ALA	O	-27.57	-34.09	61.63	15.00
211	SER	N	-28.10	-32.29	62.88	15.00
211	SER	CA	-27.80	-32.92	64.15	15.00
211	SER	CB	-26.28	-32.97	64.37	15.00
211	SER	OG	-25.71	-31.66	64.34	15.00
211	SER	C	-28.46	-32.19	65.33	15.00
211	SER	O	-29.01	-31.09	65.17	15.00
212	PHE	N	-28.43	-32.83	66.50	15.00
212	PHE	CA	-28.98	-32.24	67.71	15.00
212	PHE	CB	-30.46	-32.59	67.86	15.00
212	PHE	CG	-30.74	-34.06	67.93	15.00
212	PHE	CD1	-31.03	-34.79	66.77	15.00
212	PHE	CD2	-30.76	-34.72	69.16	15.00
212	PHE	CE1	-31.34	-36.13	66.83	15.00
212	PHE	CE2	-31.06	-36.08	69.22	15.00
212	PHE	CZ	-31.35	-36.79	68.05	15.00
212	PHE	C	-28.18	-32.66	68.96	15.00
212	PHE	O	-27.65	-33.77	69.03	15.00
213	PRO	N	-28.03	-31.76	69.92	15.00
213	PRO	CD	-28.51	-30.37	69.98	15.00
213	PRO	CA	-27.28	-32.11	71.13	15.00
213	PRO	CB	-27.07	-30.76	71.79	15.00

TABLE IV

213	PRO	CG	-28.33	-30.03	71.43	15.00
213	PRO	C	-28.10	-33.03	72.01	15.00
213	PRO	O	-29.33	-33.00	71.95	15.00
214	LYS	N	-27.42	-33.86	72.80	15.00
214	LYS	CA	-28.08	-34.78	73.73	15.00
214	LYS	CB	-27.64	-36.23	73.50	15.00
214	LYS	CG	-27.92	-36.75	72.10	15.00
214	LYS	CD	-27.72	-38.26	72.00	15.00
214	LYS	CE	-26.29	-38.66	72.30	15.00
214	LYS	NZ	-26.00	-39.99	71.69	15.00
214	LYS	C	-27.60	-34.34	75.10	15.00
214	LYS	O	-26.43	-34.00	75.26	15.00
215	MET	N	-28.50	-34.30	76.07	15.00
215	MET	CA	-28.12	-33.90	77.42	15.00
215	MET	CB	-28.97	-32.72	77.89	15.00
215	MET	CG	-28.96	-31.51	76.95	15.00
215	MET	SD	-29.63	-30.02	77.75	15.00
215	MET	CE	-28.68	-28.69	76.95	15.00
215	MET	C	-28.26	-35.09	78.36	15.00
215	MET	OT1	-27.93	-34.95	79.55	15.00
215	MET	OT2	-28.65	-36.17	77.89	15.00
216	HOH	OH2	-26.08	-16.55	83.97	15.00
217	HOH	OH2	-20.53	-32.33	79.43	15.00
218	HOH	OH2	-31.21	-16.22	65.49	15.00
219	HOH	OH2	-30.95	-18.19	68.23	15.00
220	HOH	OH2	-6.96	-10.59	69.84	15.00
221	HOH	OH2	-15.23	-12.63	73.08	15.00
222	HOH	OH2	-34.53	-23.51	69.96	15.00
223	HOH	OH2	-13.78	-33.08	69.63	15.00
224	HOH	OH2	-17.84	-17.71	57.57	15.00
225	HOH	OH2	-24.92	-31.02	61.65	15.00
226	HOH	OH2	-12.76	-8.21	61.82	15.00
227	HOH	OH2	-14.16	-21.69	66.48	15.00
228	HOH	OH2	-44.08	-26.87	48.48	15.00
229	HOH	OH2	-44.49	-35.40	55.40	15.00
230	HOH	OH2	-39.27	-16.80	68.54	15.00
231	HOH	OH2	-24.12	-35.40	48.13	15.00
232	HOH	OH2	-9.62	-25.46	63.42	15.00
233	HOH	OH2	-46.02	-25.14	44.36	15.00
234	HOH	OH2	-27.99	-19.44	61.96	15.00
235	HOH	OH2	-22.10	-30.02	61.67	15.00
236	HOH	OH2	-27.35	-15.73	71.93	15.00

TABLE IV

237	HOH	OH2	-29.19	-17.48	70.74	15.00
238	HOH	OH2	-29.55	-22.69	83.52	15.00
239	HOH	OH2	-35.73	-26.96	51.77	15.00
240	HOH	OH2	-36.27	-24.64	49.31	15.00
241	HOH	OH2	-46.67	-33.01	57.38	15.00
242	HOH	OH2	-27.40	-10.90	68.66	15.00
243	HOH	OH2	-42.01	-15.97	60.76	15.00
244	HOH	OH2	-18.00	-3.18	62.85	15.00
245	HOH	OH2	-33.49	-28.43	70.56	15.00
246	HOH	OH2	-44.87	-25.33	75.86	15.00
247	HOH	OH2	-17.32	-10.85	74.90	15.00
248	HOH	OH2	-11.45	-17.84	66.51	15.00
249	HOH	OH2	-11.56	-21.89	82.27	15.00
250	HOH	OH2	-28.01	-35.21	58.24	15.00
251	HOH	OH2	-35.05	-10.64	53.00	15.00
252	HOH	OH2	-31.64	-28.63	46.10	15.00
253	HOH	OH2	-35.04	-24.79	46.85	15.00
254	HOH	OH2	-41.38	-35.11	55.81	15.00
255	HOH	OH2	-40.44	-19.77	71.52	15.00
256	HOH	OH2	-43.66	-16.34	65.70	15.00
257	HOH	OH2	-39.00	-11.99	70.39	15.00
258	HOH	OH2	-30.92	-9.07	66.51	15.00
259	HOH	OH2	-32.51	-6.89	60.41	15.00
260	HOH	OH2	-19.20	-8.29	62.91	15.00
261	HOH	OH2	-33.67	-20.84	69.78	15.00
262	HOH	OH2	-32.87	-44.92	73.87	15.00
263	HOH	OH2	-13.20	-24.01	76.81	15.00
264	HOH	OH2	-8.83	-25.26	60.26	15.00
265	HOH	OH2	-17.23	-39.22	57.64	15.00
266	HOH	OH2	-21.10	-32.62	61.09	15.00
267	HOH	OH2	-24.50	-33.44	60.85	15.00
268	HOH	OH2	-6.37	-28.13	76.25	15.00
269	HOH	OH2	-10.20	-38.51	65.40	15.00
270	HOH	OH2	-21.41	-37.76	78.27	15.00
271	HOH	OH2	-22.56	-38.95	69.33	15.00
272	HOH	OH2	-30.18	-25.13	93.77	15.00
273	HOH	OH2	-12.08	-12.20	63.63	15.00
274	HOH	OH2	-1.36	-9.62	67.96	15.00
275	HOH	OH2	-28.39	-30.26	56.30	15.00
276	HOH	OH2	-29.74	-20.19	48.42	15.00
277	HOH	OH2	-26.12	-23.01	44.41	15.00
278	HOH	OH2	-29.92	-34.21	47.42	15.00

TABLE IV

279	HOH	OH2	-26.24	-33.39	47.92	15.00
280	HOH	OH2	-32.19	-28.29	42.42	15.00
281	HOH	OH2	-37.49	-30.33	50.55	15.00

TABLE V

Table of the orthogonal three dimensional coordinates in Ångstroms and B factors ($Å^2$) for the cathepsin K complex with inhibitor (1S)-N-[2-[(1-benzyloxycarbonylamino)-3-methylbutyl]thiazol-4-ylcarbonyl]-N'-(N-benzyloxycarbonyl-L-leucinyl)hydrazide.

Residue	Atom	X	Y	Z	B
1	ALA CB	-44.33	-37.20	63.83	15.00
1	ALA C	-46.76	-36.62	63.83	15.00
1	ALA O	-47.46	-36.94	62.86	15.00
1	ALA N	-46.07	-38.96	63.89	15.00
1	ALA CA	-45.70	-37.59	64.36	15.00
2	PRO N	-46.94	-35.47	64.51	15.00
2	PRO CD	-46.25	-35.02	65.74	15.00
2	PRO CA	-47.93	-34.49	64.07	15.00
2	PRO CB	-47.63	-33.28	64.97	15.00
2	PRO CG	-47.15	-33.90	66.23	15.00
2	PRO C	-47.63	-34.15	62.63	15.00
2	PRO O	-46.50	-34.30	62.16	15.00
3	ASP N	-48.65	-33.74	61.88	15.00
3	ASP CA	-48.39	-33.36	60.52	15.00
3	ASP CB	-49.60	-33.60	59.63	15.00
3	ASP CG	-49.78	-35.10	59.29	15.00
3	ASP OD1	-50.65	-35.42	58.45	15.00
3	ASP OD2	-49.05	-35.95	59.86	15.00
3	ASP C	-47.92	-31.92	60.51	15.00
3	ASP O	-47.44	-31.42	59.49	15.00
4	SER N	-47.94	-31.30	61.69	15.00
4	SER CA	-47.55	-29.91	61.87	15.00
4	SER CB	-48.70	-28.98	61.49	15.00
4	SER OG	-48.42	-27.64	61.85	15.00
4	SER C	-47.13	-29.61	63.29	15.00
4	SER O	-47.79	-30.03	64.24	15.00
5	VAL N	-46.04	-28.86	63.45	15.00
5	VAL CA	-45.60	-28.47	64.78	15.00
5	VAL CB	-44.86	-29.61	65.53	15.00
5	VAL CG1	-43.46	-29.81	64.97	15.00
5	VAL CG2	-44.83	-29.31	67.02	15.00
5	VAL C	-44.78	-27.20	64.70	15.00

TABLE V

5	VAL	O	-44.00	-26.98	63.77	15.00
6	ASP	N	-44.98	-26.34	65.69	15.00
6	ASP	CA	-44.29	-25.07	65.76	15.00
6	ASP	CB	-45.27	-23.94	65.39	15.00
6	ASP	CG	-44.57	-22.65	65.00	15.00
6	ASP	OD1	-43.38	-22.47	65.35	15.00
6	ASP	OD2	-45.21	-21.81	64.33	15.00
6	ASP	C	-43.72	-24.87	67.16	15.00
6	ASP	O	-44.44	-24.51	68.10	15.00
7	TYR	N	-42.41	-25.07	67.29	15.00
7	TYR	CA	-41.75	-24.90	68.58	15.00
7	TYR	CB	-40.35	-25.51	68.57	15.00
7	TYR	CG	-40.39	-27.00	68.75	15.00
7	TYR	CD1	-40.49	-27.57	70.02	15.00
7	TYR	CE1	-40.58	-28.94	70.20	15.00
7	TYR	CD2	-40.38	-27.87	67.65	15.00
7	TYR	CE2	-40.47	-29.25	67.81	15.00
7	TYR	CZ	-40.57	-29.77	69.09	15.00
7	TYR	OH	-40.68	-31.13	69.28	15.00
7	TYR	C	-41.75	-23.46	69.08	15.00
7	TYR	O	-41.62	-23.22	70.29	15.00
8	ARG	N	-41.91	-22.51	68.17	15.00
8	ARG	CA	-41.98	-21.10	68.55	15.00
8	ARG	CB	-42.05	-20.19	67.33	15.00
8	ARG	CG	-40.91	-20.36	66.38	15.00
8	ARG	CD	-41.09	-19.45	65.19	15.00
8	ARG	NE	-42.20	-19.81	64.32	15.00
8	ARG	CZ	-42.56	-19.12	63.24	15.00
8	ARG	NH1	-41.89	-18.03	62.89	15.00
8	ARG	NH2	-43.63	-19.48	62.56	15.00
8	ARG	C	-43.22	-20.92	69.42	15.00
8	ARG	O	-43.17	-20.22	70.43	15.00
9	LYS	N	-44.31	-21.59	69.04	15.00
9	LYS	CA	-45.55	-21.53	69.81	15.00
9	LYS	CB	-46.77	-21.98	68.99	15.00
9	LYS	CG	-47.20	-21.00	67.88	15.00
9	LYS	CD	-48.52	-21.46	67.22	15.00
9	LYS	CE	-48.99	-20.55	66.08	15.00
9	LYS	NZ	-49.38	-19.15	66.49	15.00
9	LYS	C	-45.44	-22.32	71.13	15.00
9	LYS	O	-46.27	-22.17	72.02	15.00
10	LYS	N	-44.41	-23.16	71.23	15.00

TABLE V

10	LYS	CA	-44.17	-23.94	72.43	15.00
10	LYS	CB	-43.58	-25.32	72.11	15.00
10	LYS	CG	-44.58	-26.34	71.57	15.00
10	LYS	CD	-43.93	-27.72	71.47	15.00
10	LYS	CE	-44.97	-28.81	71.25	15.00
10	LYS	NZ	-45.93	-28.85	72.39	15.00
10	LYS	C	-43.25	-23.20	73.40	15.00
10	LYS	O	-43.06	-23.65	74.53	15.00
11	GLY	N	-42.67	-22.09	72.95	15.00
11	GLY	CA	-41.78	-21.32	73.79	15.00
11	GLY	C	-40.38	-21.91	73.87	15.00
11	GLY	O	-39.64	-21.67	74.83	15.00
12	TYR	N	-40.01	-22.66	72.84	15.00
12	TYR	CA	-38.71	-23.31	72.77	15.00
12	TYR	CB	-38.80	-24.65	72.05	15.00
12	TYR	CG	-39.27	-25.80	72.87	15.00
12	TYR	CD1	-40.41	-25.71	73.66	15.00
12	TYR	CE1	-40.84	-26.79	74.42	15.00
12	TYR	CD2	-38.57	-27.00	72.85	15.00
12	TYR	CE2	-38.99	-28.09	73.59	15.00
12	TYR	CZ	-40.12	-27.98	74.38	15.00
12	TYR	OH	-40.50	-29.07	75.14	15.00
12	TYR	C	-37.64	-22.48	72.08	15.00
12	TYR	O	-36.46	-22.81	72.16	15.00
13	VAL	N	-38.06	-21.44	71.37	15.00
13	VAL	CA	-37.14	-20.62	70.58	15.00
13	VAL	CB	-37.66	-20.50	69.13	15.00
13	VAL	CG1	-36.66	-19.77	68.25	15.00
13	VAL	CG2	-37.95	-21.87	68.56	15.00
13	VAL	C	-36.89	-19.23	71.14	15.00
13	VAL	O	-37.84	-18.50	71.45	15.00
14	THR	N	-35.63	-18.84	71.23	15.00
14	THR	CA	-35.31	-17.51	71.72	15.00
14	THR	CB	-33.91	-17.47	72.36	15.00
14	THR	OG1	-32.93	-17.77	71.36	15.00
14	THR	CG2	-33.80	-18.49	73.47	15.00
14	THR	C	-35.44	-16.50	70.56	15.00
14	THR	O	-35.63	-16.89	69.40	15.00
15	PRO	N	-35.41	-15.19	70.86	15.00
15	PRO	CD	-35.34	-14.54	72.18	15.00
15	PRO	CA	-35.53	-14.18	69.79	15.00
15	PRO	CB	-35.29	-12.87	70.53	15.00

TABLE V

15	PRO	CG	-35.87	-13.15	71.89	15.00
15	PRO	C	-34.52	-14.37	68.66	15.00
15	PRO	O	-33.50	-15.04	68.82	15.00
16	VAL	N	-34.82	-13.76	67.52	15.00
16	VAL	CA	-33.93	-13.83	66.37	15.00
16	VAL	CB	-34.62	-13.31	65.09	15.00
16	VAL	CG1	-33.61	-13.11	63.98	15.00
16	VAL	CG2	-35.68	-14.31	64.65	15.00
16	VAL	C	-32.68	-13.01	66.64	15.00
16	VAL	O	-32.76	-11.88	67.11	15.00
17	LYS	N	-31.52	-13.61	66.39	15.00
17	LYS	CA	-30.24	-12.96	66.58	15.00
17	LYS	CB	-29.25	-13.89	67.30	15.00
17	LYS	CG	-29.81	-14.64	68.50	15.00
17	LYS	CD	-30.24	-13.71	69.61	15.00
17	LYS	CE	-30.58	-14.46	70.88	15.00
17	LYS	NZ	-31.75	-15.34	70.73	15.00
17	LYS	C	-29.67	-12.53	65.23	15.00
17	LYS	O	-30.20	-12.88	64.17	15.00
18	ASN	N	-28.57	-11.79	65.27	15.00
18	ASN	CA	-27.90	-11.32	64.06	15.00
18	ASN	CB	-28.17	-9.84	63.80	15.00
18	ASN	CG	-27.66	-9.39	62.45	15.00
18	ASN	OD1	-26.79	-10.02	61.85	15.00
18	ASN	ND2	-28.20	-8.29	61.95	15.00
18	ASN	C	-26.41	-11.58	64.19	15.00
18	ASN	O	-25.74	-11.03	65.08	15.00
19	GLN	N	-25.89	-12.42	63.30	15.00
19	GLN	CA	-24.48	-12.75	63.31	15.00
19	GLN	CB	-24.20	-14.02	62.48	15.00
19	GLN	CG	-24.56	-13.94	61.00	15.00
19	GLN	CD	-24.28	-15.24	60.27	15.00
19	GLN	OE1	-25.14	-15.79	59.60	15.00
19	GLN	NE2	-23.06	-15.74	60.40	15.00
19	GLN	C	-23.59	-11.60	62.86	15.00
19	GLN	O	-22.43	-11.51	63.27	15.00
20	GLY	N	-24.12	-10.71	62.03	15.00
20	GLY	CA	-23.32	-9.59	61.55	15.00
20	GLY	C	-22.33	-10.05	60.49	15.00
20	GLY	O	-22.59	-11.03	59.78	15.00
21	GLN	N	-21.19	-9.38	60.40	15.00
21	GLN	CA	-20.18	-9.73	59.39	15.00

TABLE V

21	GLN	CB	-19.51	-8.48	58.81	15.00
21	GLN	CG	-20.42	-7.63	57.93	15.00
21	GLN	CD	-20.79	-8.33	56.62	15.00
21	GLN	OE1	-20.02	-9.12	56.07	15.00
21	GLN	NE2	-21.97	-8.02	56.11	15.00
21	GLN	C	-19.15	-10.71	59.95	15.00
21	GLN	O	-17.96	-10.40	60.02	15.00
22	CYS	N	-19.63	-11.88	60.34	15.00
22	CYS	CA	-18.79	-12.94	60.89	15.00
22	CYS	C	-19.49	-14.24	60.53	15.00
22	CYS	O	-20.71	-14.34	60.62	15.00
22	CYS	CB	-18.61	-12.78	62.41	15.00
22	CYS	SG	-18.03	-14.24	63.33	15.00
23	GLY	N	-18.73	-15.19	60.00	15.00
23	GLY	CA	-19.29	-16.48	59.66	15.00
23	GLY	C	-19.53	-17.35	60.89	15.00
23	GLY	O	-19.04	-18.48	60.98	15.00
24	SER	N	-20.36	-16.86	61.81	15.00
24	SER	CA	-20.67	-17.60	63.03	15.00
24	SER	CB	-20.61	-16.66	64.22	15.00
24	SER	OG	-21.35	-15.49	63.95	15.00
24	SER	C	-22.01	-18.36	62.96	15.00
24	SER	O	-22.58	-18.73	63.99	15.00
25	CYS	N	-22.50	-18.58	61.74	15.00
25	CYS	CA	-23.76	-19.28	61.52	15.00
25	CYS	CB	-23.98	-19.51	60.01	15.00
25	CYS	SG	-22.57	-20.30	59.15	15.00
25	CYS	C	-23.86	-20.58	62.32	15.00
25	CYS	O	-24.84	-20.82	63.02	15.00
25	INH	C1	-28.50	-9.52	55.70	15.00
25	INH	C2	-28.63	-9.33	57.08	15.00
25	INH	C3	-27.56	-9.63	57.94	15.00
25	INH	C4	-26.35	-10.11	57.43	15.00
25	INH	C5	-26.23	-10.29	56.05	15.00
25	INH	C6	-27.29	-10.00	55.19	15.00
25	INH	C7	-25.20	-10.40	58.35	15.00
25	INH	O8	-24.73	-11.77	58.36	15.00
25	INH	C9	-24.03	-12.42	57.30	15.00
25	INH	O10	-24.33	-12.23	56.10	15.00
25	INH	C11	-22.27	-14.01	56.70	15.00
25	INH	C12	-20.77	-13.63	56.80	15.00
25	INH	C13	-20.18	-12.60	55.82	15.00

TABLE V

25	INH	C14	-19.01	-11.83	56.47	15.00
25	INH	C15	-21.22	-11.63	55.23	15.00
25	INH	C16	-22.50	-15.59	56.80	15.00
25	INH	S17	-23.78	-16.32	55.92	15.00
25	INH	N18	-21.80	-16.55	57.50	15.00
25	INH	C19	-22.21	-17.87	57.39	15.00
25	INH	N20	-23.05	-13.25	57.68	15.00
25	INH	C21	-23.27	-17.88	56.55	15.00
25	INH	C22	-21.58	-19.10	58.24	15.00
25	INH	O23	-21.37	-18.39	59.17	15.00
25	INH	C24	-13.79	-23.51	54.96	15.00
25	INH	C25	-14.23	-22.84	56.08	15.00
25	INH	C26	-14.83	-23.54	57.12	15.00
25	INH	C27	-15.00	-24.93	57.04	15.00
25	INH	C28	-14.54	-25.60	55.91	15.00
25	INH	C29	-13.94	-24.90	54.87	15.00
25	INH	C30	-15.72	-25.67	58.14	15.00
25	INH	O31	-17.10	-25.93	57.71	15.00
25	INH	C32	-17.91	-25.03	56.96	15.00
25	INH	O33	-17.69	-24.81	55.77	15.00
25	INH	C34	-19.82	-23.49	57.00	15.00
25	INH	C35	-21.22	-24.12	56.84	15.00
25	INH	C36	-21.92	-24.89	57.97	15.00
25	INH	C37	-21.43	-26.31	58.12	15.00
25	INH	C38	-21.86	-24.15	59.29	15.00
25	INH	C39	-19.87	-22.15	57.76	15.00
25	INH	O40	-19.60	-22.13	58.96	15.00
25	INH	N41	-20.18	-21.00	57.08	15.00
25	INH	N42	-20.20	-19.65	57.78	15.00
25	INH	N43	-18.90	-24.44	57.63	15.00
26	TRP	N	-22.80	-21.38	62.25	15.00
26	TRP	CA	-22.73	-22.65	62.97	15.00
26	TRP	CB	-21.39	-23.33	62.67	15.00
26	TRP	CG	-20.19	-22.46	62.98	15.00
26	TRP	CD2	-19.41	-22.45	64.19	15.00
26	TRP	CE2	-18.44	-21.44	64.05	15.00
26	TRP	CE3	-19.43	-23.21	65.37	15.00
26	TRP	CD1	-19.67	-21.48	62.19	15.00
26	TRP	NE1	-18.62	-20.86	62.82	15.00
26	TRP	CZ2	-17.50	-21.15	65.06	15.00
26	TRP	CZ3	-18.50	-22.92	66.37	15.00
26	TRP	CH2	-17.55	-21.91	66.21	15.00

TABLE V

26	TRP	C	-22.95	-22.50	64.49	15.00
26	TRP	O	-23.65	-23.30	65.10	15.00
27	ALA	N	-22.35	-21.46	65.08	15.00
27	ALA	CA	-22.45	-21.18	66.51	15.00
27	ALA	CB	-21.56	-20.02	66.89	15.00
27	ALA	C	-23.90	-20.90	66.88	15.00
27	ALA	O	-24.46	-21.56	67.74	15.00
28	PHE	N	-24.53	-19.94	66.19	15.00
28	PHE	CA	-25.93	-19.58	66.41	15.00
28	PHE	CB	-26.36	-18.44	65.48	15.00
28	PHE	CG	-25.83	-17.09	65.88	15.00
28	PHE	CD1	-24.66	-16.59	65.32	15.00
28	PHE	CD2	-26.48	-16.32	66.84	15.00
28	PHE	CE1	-24.14	-15.37	65.71	15.00
28	PHE	CE2	-25.97	-15.09	67.24	15.00
28	PHE	CZ	-24.80	-14.62	66.67	15.00
28	PHE	C	-26.87	-20.78	66.23	15.00
28	PHE	O	-27.85	-20.92	66.96	15.00
29	SER	N	-26.56	-21.64	65.26	15.00
29	SER	CA	-27.35	-22.83	64.99	15.00
29	SER	CB	-26.95	-23.45	63.64	15.00
29	SER	OG	-27.68	-24.63	63.36	15.00
29	SER	C	-27.21	-23.84	66.13	15.00
29	SER	O	-28.19	-24.49	66.50	15.00
30	SER	N	-26.01	-23.96	66.69	15.00
30	SER	CA	-25.73	-24.88	67.79	15.00
30	SER	CB	-24.23	-25.10	68.00	15.00
30	SER	OG	-23.60	-25.57	66.82	15.00
30	SER	C	-26.37	-24.39	69.09	15.00
30	SER	O	-26.95	-25.16	69.85	15.00
31	VAL	N	-26.23	-23.09	69.33	15.00
31	VAL	CA	-26.80	-22.45	70.51	15.00
31	VAL	CB	-26.39	-20.95	70.55	15.00
31	VAL	CG1	-27.42	-20.12	71.24	15.00
31	VAL	CG2	-25.07	-20.81	71.26	15.00
31	VAL	C	-28.31	-22.63	70.48	15.00
31	VAL	O	-28.91	-22.92	71.51	15.00
32	GLY	N	-28.89	-22.52	69.29	15.00
32	GLY	CA	-30.32	-22.68	69.11	15.00
32	GLY	C	-30.78	-24.09	69.45	15.00
32	GLY	O	-31.86	-24.28	69.99	15.00
33	ALA	N	-29.97	-25.08	69.09	15.00

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33	ALA	CA	-30.29	-26.47	69.38	15.00
33	ALA	CB	-29.33	-27.39	68.65	15.00
33	ALA	C	-30.19	-26.70	70.89	15.00
33	ALA	O	-31.08	-27.30	71.50	15.00
34	LEU	N	-29.13	-26.18	71.50	15.00
34	LEU	CA	-28.93	-26.32	72.93	15.00
34	LEU	CB	-27.58	-25.75	73.35	15.00
34	LEU	CG	-26.31	-26.50	72.95	15.00
34	LEU	CD1	-25.08	-25.64	73.21	15.00
34	LEU	CD2	-26.24	-27.79	73.73	15.00
34	LEU	C	-30.07	-25.65	73.69	15.00
34	LEU	O	-30.59	-26.21	74.64	15.00
35	GLU	N	-30.47	-24.47	73.22	15.00
35	GLU	CA	-31.55	-23.70	73.82	15.00
35	GLU	CB	-31.77	-22.39	73.08	15.00
35	GLU	CG	-30.84	-21.28	73.54	15.00
35	GLU	CD	-30.76	-20.13	72.55	15.00
35	GLU	OE1	-31.51	-20.14	71.54	15.00
35	GLU	OE2	-29.93	-19.22	72.76	15.00
35	GLU	C	-32.86	-24.47	73.95	15.00
35	GLU	O	-33.52	-24.39	75.00	15.00
36	GLY	N	-33.21	-25.21	72.90	15.00
36	GLY	CA	-34.42	-26.00	72.90	15.00
36	GLY	C	-34.35	-27.13	73.91	15.00
36	GLY	O	-35.29	-27.37	74.66	15.00
37	GLN	N	-33.22	-27.82	73.95	15.00
37	GLN	CA	-33.04	-28.92	74.90	15.00
37	GLN	CB	-31.77	-29.71	74.56	15.00
37	GLN	CG	-31.84	-30.38	73.19	15.00
37	GLN	CD	-33.17	-31.11	72.97	15.00
37	GLN	OE1	-33.60	-31.90	73.81	15.00
37	GLN	NE2	-33.82	-30.83	71.85	15.00
37	GLN	C	-33.05	-28.41	76.35	15.00
37	GLN	O	-33.63	-29.04	77.23	15.00
38	LEU	N	-32.45	-27.24	76.57	15.00
38	LEU	CA	-32.42	-26.63	77.90	15.00
38	LEU	CB	-31.61	-25.34	77.89	15.00
38	LEU	CG	-31.50	-24.54	79.20	15.00
38	LEU	CD1	-30.94	-25.41	80.34	15.00
38	LEU	CD2	-30.60	-23.34	78.95	15.00
38	LEU	C	-33.85	-26.35	78.35	15.00
38	LEU	O	-34.22	-26.60	79.50	15.00

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39	LYS	N	-34.66	-25.84	77.42	15.00
39	LYS	CA	-36.06	-25.56	77.68	15.00
39	LYS	CB	-36.71	-24.85	76.49	15.00
39	LYS	CG	-38.21	-24.62	76.62	15.00
39	LYS	CD	-38.52	-23.64	77.74	15.00
39	LYS	CE	-40.03	-23.47	77.92	15.00
39	LYS	NZ	-40.35	-22.39	78.91	15.00
39	LYS	C	-36.83	-26.83	78.04	15.00
39	LYS	O	-37.55	-26.89	79.04	15.00
40	LYS	N	-36.65	-27.87	77.23	15.00
40	LYS	CA	-37.33	-29.14	77.44	15.00
40	LYS	CB	-37.06	-30.09	76.28	15.00
40	LYS	CG	-37.54	-31.50	76.53	15.00
40	LYS	CD	-37.53	-32.32	75.26	15.00
40	LYS	CE	-38.47	-31.72	74.22	15.00
40	LYS	NZ	-38.75	-32.66	73.09	15.00
40	LYS	C	-37.01	-29.80	78.78	15.00
40	LYS	O	-37.92	-30.20	79.52	15.00
41	LYS	N	-35.73	-29.90	79.11	15.00
41	LYS	CA	-35.29	-30.52	80.36	15.00
41	LYS	CB	-33.84	-31.02	80.22	15.00
41	LYS	CG	-33.70	-32.50	79.87	15.00
41	LYS	CD	-34.49	-32.90	78.62	15.00
41	LYS	CE	-33.58	-33.12	77.41	15.00
41	LYS	NZ	-33.06	-31.85	76.83	15.00
41	LYS	C	-35.47	-29.73	81.68	15.00
41	LYS	O	-35.74	-30.32	82.73	15.00
42	THR	N	-35.28	-28.40	81.63	15.00
42	THR	CA	-35.41	-27.57	82.83	15.00
42	THR	CB	-34.17	-26.65	83.04	15.00
42	THR	OG1	-34.20	-25.57	82.10	15.00
42	THR	CG2	-32.87	-27.43	82.84	15.00
42	THR	C	-36.64	-26.66	82.82	15.00
42	THR	O	-37.07	-26.16	83.86	15.00
43	GLY	N	-37.17	-26.41	81.63	15.00
43	GLY	CA	-38.33	-25.55	81.52	15.00
43	GLY	C	-37.93	-24.10	81.41	15.00
43	GLY	O	-38.78	-23.23	81.26	15.00
44	LYS	N	-36.63	-23.82	81.53	15.00
44	LYS	CA	-36.11	-22.46	81.41	15.00
44	LYS	CB	-34.91	-22.24	82.33	15.00
44	LYS	CG	-35.25	-22.15	83.79	15.00

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44	LYS	CD	-34.06	-21.63	84.59	15.00
44	LYS	CE	-33.69	-20.18	84.17	15.00
44	LYS	NZ	-32.77	-19.50	85.16	15.00
44	LYS	C	-35.72	-22.17	79.96	15.00
44	LYS	O	-35.24	-23.05	79.25	15.00
45	LEU	N	-35.91	-20.93	79.54	15.00
45	LEU	CA	-35.56	-20.52	78.19	15.00
45	LEU	CB	-36.80	-20.28	77.31	15.00
45	LEU	CG	-36.49	-19.86	75.87	15.00
45	LEU	CD1	-36.01	-21.07	75.08	15.00
45	LEU	CD2	-37.69	-19.23	75.17	15.00
45	LEU	C	-34.71	-19.26	78.25	15.00
45	LEU	O	-35.22	-18.17	78.53	15.00
46	LEU	N	-33.41	-19.42	78.02	15.00
46	LEU	CA	-32.50	-18.29	78.00	15.00
46	LEU	CB	-31.75	-18.14	79.35	15.00
46	LEU	CG	-31.05	-19.27	80.11	15.00
46	LEU	CD1	-32.04	-20.12	80.86	15.00
46	LEU	CD2	-30.23	-20.09	79.17	15.00
46	LEU	C	-31.54	-18.34	76.80	15.00
46	LEU	O	-31.41	-19.37	76.14	15.00
47	ASN	N	-30.93	-17.20	76.48	15.00
47	ASN	CA	-30.00	-17.12	75.36	15.00
47	ASN	CB	-29.88	-15.69	74.84	15.00
47	ASN	CG	-31.21	-15.12	74.46	15.00
47	ASN	OD1	-31.91	-15.66	73.60	15.00
47	ASN	ND2	-31.59	-14.04	75.11	15.00
47	ASN	C	-28.64	-17.64	75.75	15.00
47	ASN	O	-28.10	-17.24	76.78	15.00
48	LEU	N	-28.12	-18.56	74.94	15.00
48	LEU	CA	-26.82	-19.15	75.18	15.00
48	LEU	CB	-26.80	-20.63	74.80	15.00
48	LEU	CG	-27.73	-21.45	75.71	15.00
48	LEU	CD1	-27.55	-22.93	75.44	15.00
48	LEU	CD2	-27.44	-21.15	77.17	15.00
48	LEU	C	-25.73	-18.36	74.47	15.00
48	LEU	O	-26.04	-17.44	73.71	15.00
49	SER	N	-24.48	-18.72	74.69	15.00
49	SER	CA	-23.36	-18.00	74.12	15.00
49	SER	CB	-22.27	-17.78	75.18	15.00
49	SER	OG	-21.19	-17.01	74.69	15.00
49	SER	C	-22.73	-18.50	72.83	15.00

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49	SER	O	-21.93	-19.43	72.84	15.00
50	PRO	N	-23.07	-17.87	71.68	15.00
50	PRO	CD	-24.14	-16.88	71.44	15.00
50	PRO	CA	-22.47	-18.30	70.42	15.00
50	PRO	CB	-23.33	-17.58	69.36	15.00
50	PRO	CG	-23.81	-16.35	70.07	15.00
50	PRO	C	-21.00	-17.83	70.39	15.00
50	PRO	O	-20.15	-18.48	69.77	15.00
51	GLN	N	-20.70	-16.73	71.10	15.00
51	GLN	CA	-19.34	-16.18	71.19	15.00
51	GLN	CB	-19.35	-14.78	71.82	15.00
51	GLN	CG	-18.06	-13.96	71.66	15.00
51	GLN	CD	-17.76	-13.49	70.22	15.00
51	GLN	OE1	-18.60	-12.89	69.54	15.00
51	GLN	NE2	-16.54	-13.74	69.77	15.00
51	GLN	C	-18.42	-17.16	71.95	15.00
51	GLN	O	-17.25	-17.33	71.59	15.00
52	ASN	N	-18.98	-17.86	72.94	15.00
52	ASN	CA	-18.23	-18.85	73.70	15.00
52	ASN	CB	-19.14	-19.54	74.73	15.00
52	ASN	CG	-18.40	-20.50	75.66	15.00
52	ASN	OD1	-18.99	-21.02	76.61	15.00
52	ASN	ND2	-17.11	-20.73	75.41	15.00
52	ASN	C	-17.68	-19.86	72.70	15.00
52	ASN	O	-16.50	-20.21	72.73	15.00
53	LEU	N	-18.55	-20.28	71.78	15.00
53	LEU	CA	-18.19	-21.24	70.74	15.00
53	LEU	CB	-19.44	-21.79	70.06	15.00
53	LEU	CG	-20.11	-23.02	70.67	15.00
53	LEU	CD1	-20.05	-22.96	72.19	15.00
53	LEU	CD2	-21.55	-23.11	70.17	15.00
53	LEU	C	-17.21	-20.66	69.72	15.00
53	LEU	O	-16.19	-21.29	69.42	15.00
54	VAL	N	-17.51	-19.46	69.21	15.00
54	VAL	CA	-16.65	-18.82	68.22	15.00
54	VAL	CB	-17.16	-17.39	67.85	15.00
54	VAL	CG1	-16.22	-16.73	66.85	15.00
54	VAL	CG2	-18.56	-17.47	67.25	15.00
54	VAL	C	-15.19	-18.75	68.68	15.00
54	VAL	O	-14.28	-19.13	67.94	15.00
55	ASP	N	-14.99	-18.33	69.93	15.00
55	ASP	CA	-13.65	-18.18	70.52	15.00

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55	ASP	CB	-13.64	-17.12	71.64	15.00
55	ASP	CG	-14.11	-15.73	71.18	15.00
55	ASP	OD1	-14.12	-15.43	69.96	15.00
55	ASP	OD2	-14.46	-14.93	72.06	15.00
55	ASP	C	-12.98	-19.44	71.08	15.00
55	ASP	O	-11.75	-19.53	71.15	15.00
56	CYS	N	-13.79	-20.43	71.47	15.00
56	CYS	CA	-13.26	-21.63	72.12	15.00
56	CYS	C	-13.13	-22.97	71.41	15.00
56	CYS	O	-12.36	-23.82	71.86	15.00
56	CYS	CB	-13.97	-21.81	73.45	15.00
56	CYS	SG	-13.91	-20.34	74.55	15.00
57	VAL	N	-13.92	-23.20	70.36	15.00
57	VAL	CA	-13.85	-24.48	69.64	15.00
57	VAL	CB	-15.13	-24.77	68.83	15.00
57	VAL	CG1	-15.08	-26.20	68.30	15.00
57	VAL	CG2	-16.37	-24.52	69.66	15.00
57	VAL	C	-12.67	-24.45	68.68	15.00
57	VAL	O	-12.73	-23.82	67.62	15.00
58	SER	N	-11.60	-25.15	69.04	15.00
58	SER	CA	-10.40	-25.18	68.22	15.00
58	SER	CB	-9.19	-25.66	69.02	15.00
58	SER	OG	-9.56	-26.66	69.95	15.00
58	SER	C	-10.54	-25.93	66.91	15.00
58	SER	O	-9.71	-25.75	66.02	15.00
59	GLU	N	-11.56	-26.78	66.79	15.00
59	GLU	CA	-11.79	-27.55	65.57	15.00
59	GLU	CB	-12.53	-28.86	65.84	15.00
59	GLU	CG	-11.72	-29.95	66.56	15.00
59	GLU	CD	-11.47	-29.63	68.03	15.00
59	GLU	OE1	-12.44	-29.48	68.79	15.00
59	GLU	OE2	-10.28	-29.54	68.42	15.00
59	GLU	C	-12.51	-26.74	64.50	15.00
59	GLU	O	-12.45	-27.06	63.32	15.00
60	ASN	N	-13.22	-25.69	64.92	15.00
60	ASN	CA	-13.91	-24.83	63.98	15.00
60	ASN	CB	-15.29	-24.45	64.49	15.00
60	ASN	CG	-16.25	-25.62	64.51	15.00
60	ASN	OD1	-17.17	-25.66	65.32	15.00
60	ASN	ND2	-16.04	-26.59	63.62	15.00
60	ASN	C	-13.03	-23.63	63.72	15.00
60	ASN	O	-12.01	-23.46	64.39	15.00

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61	ASP	N	-13.39	-22.81	62.74	15.00
61	ASP	CA	-12.56	-21.66	62.39	15.00
61	ASP	CB	-12.27	-21.64	60.88	15.00
61	ASP	CG	-11.96	-23.05	60.30	15.00
61	ASP	OD1	-12.89	-23.70	59.76	15.00
61	ASP	OD2	-10.78	-23.50	60.37	15.00
61	ASP	C	-13.12	-20.30	62.86	15.00
61	ASP	O	-12.75	-19.26	62.32	15.00
62	GLY	N	-13.97	-20.31	63.88	15.00
62	GLY	CA	-14.54	-19.06	64.36	15.00
62	GLY	C	-15.40	-18.39	63.30	15.00
62	GLY	O	-16.41	-18.95	62.84	15.00
63	CYS	N	-15.00	-17.18	62.90	15.00
63	CYS	CA	-15.71	-16.43	61.88	15.00
63	CYS	C	-15.44	-16.96	60.47	15.00
63	CYS	O	-16.00	-16.47	59.49	15.00
63	CYS	CB	-15.39	-14.94	61.97	15.00
63	CYS	SG	-16.00	-14.06	63.45	15.00
64	GLY	N	-14.57	-17.97	60.38	15.00
64	GLY	CA	-14.27	-18.57	59.09	15.00
64	GLY	C	-15.01	-19.88	58.84	15.00
64	GLY	O	-14.59	-20.68	58.01	15.00
65	GLY	N	-16.09	-20.12	59.59	15.00
65	GLY	CA	-16.86	-21.34	59.42	15.00
65	GLY	C	-16.66	-22.39	60.49	15.00
65	GLY	O	-15.77	-22.30	61.34	15.00
66	GLY	N	-17.52	-23.40	60.46	15.00
66	GLY	CA	-17.44	-24.49	61.42	15.00
66	GLY	C	-18.61	-25.44	61.32	15.00
66	GLY	O	-19.49	-25.27	60.48	15.00
67	TYR	N	-18.62	-26.44	62.18	15.00
67	TYR	CA	-19.68	-27.44	62.21	15.00
67	TYR	CB	-19.14	-28.83	61.87	15.00
67	TYR	CG	-18.68	-28.95	60.44	15.00
67	TYR	CD1	-19.58	-29.32	59.44	15.00
67	TYR	CE1	-19.18	-29.39	58.11	15.00
67	TYR	CD2	-17.37	-28.64	60.07	15.00
67	TYR	CE2	-16.96	-28.70	58.75	15.00
67	TYR	CZ	-17.88	-29.07	57.77	15.00
67	TYR	OH	-17.50	-29.10	56.45	15.00
67	TYR	C	-20.36	-27.48	63.56	15.00
67	TYR	O	-19.71	-27.30	64.59	15.00

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68	MET	N	-21.65	-27.77	63.56	15.00
68	MET	CA	-22.44	-27.85	64.78	15.00
68	MET	CB	-23.93	-28.03	64.44	15.00
68	MET	CG	-24.58	-26.86	63.66	15.00
68	MET	SD	-24.01	-26.58	61.93	15.00
68	MET	CE	-25.23	-27.50	61.01	15.00
68	MET	C	-21.91	-28.98	65.68	15.00
68	MET	O	-21.68	-28.77	66.87	15.00
69	THR	N	-21.68	-30.16	65.08	15.00
69	THR	CA	-21.17	-31.32	65.81	15.00
69	THR	CB	-20.89	-32.54	64.87	15.00
69	THR	OG1	-20.07	-32.14	63.76	15.00
69	THR	CG2	-22.20	-33.12	64.35	15.00
69	THR	C	-19.91	-31.01	66.64	15.00
69	THR	O	-19.80	-31.46	67.78	15.00
70	ASN	N	-18.97	-30.25	66.06	15.00
70	ASN	CA	-17.74	-29.87	66.77	15.00
70	ASN	CB	-16.76	-29.07	65.89	15.00
70	ASN	CG	-16.17	-29.89	64.75	15.00
70	ASN	OD1	-15.66	-29.34	63.79	15.00
70	ASN	ND2	-16.25	-31.20	64.86	15.00
70	ASN	C	-18.11	-29.01	67.98	15.00
70	ASN	O	-17.57	-29.19	69.08	15.00
71	ALA	N	-19.02	-28.07	67.74	15.00
71	ALA	CA	-19.50	-27.16	68.77	15.00
71	ALA	CB	-20.44	-26.11	68.16	15.00
71	ALA	C	-20.20	-27.92	69.91	15.00
71	ALA	O	-20.03	-27.59	71.08	15.00
72	PHE	N	-20.95	-28.97	69.56	15.00
72	PHE	CA	-21.63	-29.82	70.54	15.00
72	PHE	CB	-22.65	-30.75	69.86	15.00
72	PHE	CG	-23.80	-30.02	69.25	15.00
72	PHE	CD1	-24.32	-28.88	69.86	15.00
72	PHE	CD2	-24.37	-30.48	68.08	15.00
72	PHE	CE1	-25.40	-28.21	69.30	15.00
72	PHE	CE2	-25.46	-29.81	67.51	15.00
72	PHE	CZ	-25.97	-28.67	68.13	15.00
72	PHE	C	-20.64	-30.63	71.36	15.00
72	PHE	O	-20.69	-30.66	72.59	15.00
73	GLN	N	-19.71	-31.27	70.67	15.00
73	GLN	CA	-18.70	-32.08	71.33	15.00
73	GLN	CB	-17.83	-32.79	70.31	15.00

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73	GLN	CG	-16.90	-33.82	70.92	15.00
73	GLN	CD	-16.28	-34.73	69.87	15.00
73	GLN	OE1	-16.83	-34.92	68.78	15.00
73	GLN	NE2	-15.14	-35.30	70.20	15.00
73	GLN	C	-17.87	-31.21	72.25	15.00
73	GLN	O	-17.49	-31.64	73.33	15.00
74	TYR	N	-17.60	-29.98	71.82	15.00
74	TYR	CA	-16.83	-29.03	72.62	15.00
74	TYR	CB	-16.61	-27.69	71.89	15.00
74	TYR	CG	-16.39	-26.51	72.83	15.00
74	TYR	CD1	-15.18	-26.35	73.51	15.00
74	TYR	CE1	-15.02	-25.35	74.47	15.00
74	TYR	CD2	-17.43	-25.63	73.12	15.00
74	TYR	CE2	-17.28	-24.64	74.08	15.00
74	TYR	CZ	-16.08	-24.50	74.75	15.00
74	TYR	OH	-15.96	-23.57	75.75	15.00
74	TYR	C	-17.55	-28.79	73.94	15.00
74	TYR	O	-16.92	-28.75	75.00	15.00
75	VAL	N	-18.87	-28.62	73.86	15.00
75	VAL	CA	-19.70	-28.36	75.04	15.00
75	VAL	CB	-21.11	-27.88	74.63	15.00
75	VAL	CG1	-21.96	-27.66	75.85	15.00
75	VAL	CG2	-21.00	-26.57	73.83	15.00
75	VAL	C	-19.77	-29.55	75.98	15.00
75	VAL	O	-19.91	-29.38	77.19	15.00
76	GLN	N	-19.66	-30.74	75.42	15.00
76	GLN	CA	-19.66	-31.95	76.22	15.00
76	GLN	CB	-19.84	-33.21	75.36	15.00
76	GLN	CG	-19.80	-34.51	76.14	15.00
76	GLN	CD	-19.78	-35.75	75.25	15.00
76	GLN	OE1	-19.34	-35.70	74.09	15.00
76	GLN	NE2	-20.24	-36.86	75.79	15.00
76	GLN	C	-18.34	-32.00	77.00	15.00
76	GLN	O	-18.34	-32.09	78.22	15.00
77	LYS	N	-17.22	-31.90	76.29	15.00
77	LYS	CA	-15.89	-31.95	76.91	15.00
77	LYS	CB	-14.79	-32.01	75.85	15.00
77	LYS	CG	-14.77	-33.29	75.01	15.00
77	LYS	CD	-13.80	-33.14	73.84	15.00
77	LYS	CE	-13.62	-34.44	73.09	15.00
77	LYS	NZ	-12.55	-34.33	72.06	15.00
77	LYS	C	-15.63	-30.80	77.87	15.00

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77	LYS	O	-14.99	-30.98	78.91	15.00
78	ASN	N	-16.09	-29.61	77.50	15.00
78	ASN	CA	-15.91	-28.43	78.32	15.00
78	ASN	CB	-16.18	-27.16	77.51	15.00
78	ASN	CG	-15.95	-25.89	78.31	15.00
78	ASN	OD1	-14.90	-25.69	78.92	15.00
78	ASN	ND2	-16.93	-24.99	78.28	15.00
78	ASN	C	-16.83	-28.52	79.52	15.00
78	ASN	O	-16.64	-27.81	80.49	15.00
79	ARG	N	-17.81	-29.42	79.44	15.00
79	ARG	CA	-18.82	-29.64	80.47	15.00
79	ARG	CB	-18.19	-30.06	81.81	15.00
79	ARG	CG	-17.69	-31.48	81.85	15.00
79	ARG	CD	-16.75	-31.70	83.00	15.00
79	ARG	NE	-16.07	-32.98	82.88	15.00
79	ARG	CZ	-14.79	-33.13	82.56	15.00
79	ARG	NH1	-14.02	-32.08	82.33	15.00
79	ARG	NH2	-14.28	-34.36	82.41	15.00
79	ARG	C	-19.77	-28.45	80.65	15.00
79	ARG	O	-20.43	-28.32	81.69	15.00
80	GLY	N	-19.84	-27.58	79.66	15.00
80	GLY	CA	-20.72	-26.45	79.77	15.00
80	GLY	C	-20.50	-25.38	78.73	15.00
80	GLY	O	-19.60	-25.49	77.89	15.00
81	ILE	N	-21.38	-24.39	78.75	15.00
81	ILE	CA	-21.34	-23.24	77.85	15.00
81	ILE	CB	-22.12	-23.47	76.52	15.00
81	ILE	CG2	-23.54	-24.00	76.80	15.00
81	ILE	CG1	-22.15	-22.16	75.71	15.00
81	ILE	CD1	-22.81	-22.28	74.36	15.00
81	ILE	C	-21.98	-22.09	78.60	15.00
81	ILE	O	-23.00	-22.26	79.29	15.00
82	ASP	N	-21.37	-20.92	78.48	15.00
82	ASP	CA	-21.88	-19.75	79.15	15.00
82	ASP	CB	-20.83	-18.66	79.19	15.00
82	ASP	CG	-19.68	-19.00	80.10	15.00
82	ASP	OD1	-18.57	-18.52	79.85	15.00
82	ASP	OD2	-19.91	-19.76	81.07	15.00
82	ASP	C	-23.17	-19.21	78.57	15.00
82	ASP	O	-23.56	-19.54	77.45	15.00
83	SER	N	-23.85	-18.42	79.39	15.00
83	SER	CA	-25.09	-17.77	79.00	15.00

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83	SER	CB	-25.89	-17.34	80.22	15.00
83	SER	OG	-25.29	-16.22	80.86	15.00
83	SER	C	-24.70	-16.56	78.16	15.00
83	SER	O	-23.58	-16.04	78.30	15.00
84	GLU	N	-25.59	-16.10	77.30	15.00
84	GLU	CA	-25.30	-14.93	76.49	15.00
84	GLU	CB	-26.55	-14.46	75.73	15.00
84	GLU	CG	-26.40	-13.12	75.04	15.00
84	GLU	CD	-25.37	-13.12	73.92	15.00
84	GLU	OE1	-24.73	-12.07	73.72	15.00
84	GLU	OE2	-25.20	-14.15	73.23	15.00
84	GLU	C	-24.74	-13.81	77.37	15.00
84	GLU	O	-23.72	-13.20	77.06	15.00
85	ASP	N	-25.37	-13.60	78.53	15.00
85	ASP	CA	-24.94	-12.54	79.44	15.00
85	ASP	CB	-25.85	-12.44	80.66	15.00
85	ASP	CG	-27.22	-11.88	80.32	15.00
85	ASP	OD1	-28.19	-12.27	81.01	15.00
85	ASP	OD2	-27.33	-11.06	79.37	15.00
85	ASP	C	-23.49	-12.60	79.87	15.00
85	ASP	O	-22.78	-11.59	79.79	15.00
86	ALA	N	-23.05	-13.79	80.28	15.00
86	ALA	CA	-21.67	-14.00	80.73	15.00
86	ALA	CB	-21.59	-15.24	81.59	15.00
86	ALA	C	-20.61	-14.06	79.62	15.00
86	ALA	O	-19.42	-14.18	79.92	15.00
87	TYR	N	-21.04	-13.98	78.36	15.00
87	TYR	CA	-20.13	-14.04	77.22	15.00
87	TYR	CB	-19.69	-15.50	76.99	15.00
87	TYR	CG	-18.30	-15.71	76.41	15.00
87	TYR	CD1	-17.79	-14.89	75.41	15.00
87	TYR	CE1	-16.54	-15.12	74.86	15.00
87	TYR	CD2	-17.51	-16.78	76.84	15.00
87	TYR	CE2	-16.26	-17.02	76.29	15.00
87	TYR	CZ	-15.78	-16.18	75.30	15.00
87	TYR	OH	-14.54	-16.42	74.76	15.00
87	TYR	C	-20.88	-13.46	76.00	15.00
87	TYR	O	-21.14	-14.15	75.02	15.00
88	PRO	N	-21.17	-12.14	76.05	15.00
88	PRO	CD	-20.72	-11.16	77.06	15.00
88	PRO	CA	-21.90	-11.45	74.97	15.00
88	PRO	CB	-21.94	-9.99	75.46	15.00

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88	PRO	CG	-20.72	-9.87	76.27	15.00
88	PRO	C	-21.30	-11.57	73.58	15.00
88	PRO	O	-20.11	-11.80	73.42	15.00
89	TYR	N	-22.15	-11.39	72.58	15.00
89	TYR	CA	-21.74	-11.48	71.18	15.00
89	TYR	CB	-22.93	-11.78	70.27	15.00
89	TYR	CG	-22.53	-12.08	68.84	15.00
89	TYR	CD1	-21.82	-13.23	68.54	15.00
89	TYR	CE1	-21.40	-13.50	67.25	15.00
89	TYR	CD2	-22.83	-11.20	67.81	15.00
89	TYR	CE2	-22.40	-11.46	66.50	15.00
89	TYR	CZ	-21.69	-12.62	66.24	15.00
89	TYR	OH	-21.23	-12.90	64.98	15.00
89	TYR	C	-21.04	-10.21	70.71	15.00
89	TYR	O	-21.54	-9.11	70.94	15.00
90	VAL	N	-19.88	-10.36	70.08	15.00
90	VAL	CA	-19.15	-9.21	69.55	15.00
90	VAL	CB	-17.81	-8.94	70.27	15.00
90	VAL	CG1	-18.06	-8.15	71.55	15.00
90	VAL	CG2	-17.08	-10.23	70.56	15.00
90	VAL	C	-18.92	-9.31	68.05	15.00
90	VAL	O	-18.60	-8.32	67.40	15.00
91	GLY	N	-19.08	-10.51	67.50	15.00
91	GLY	CA	-18.90	-10.68	66.06	15.00
91	GLY	C	-17.46	-10.67	65.56	15.00
91	GLY	O	-17.19	-10.28	64.42	15.00
92	GLN	N	-16.54	-11.10	66.41	15.00
92	GLN	CA	-15.14	-11.17	66.04	15.00
92	GLN	CB	-14.46	-9.80	66.11	15.00
92	GLN	CG	-14.41	-9.16	67.49	15.00
92	GLN	CD	-14.16	-7.65	67.45	15.00
92	GLN	OE1	-14.60	-6.91	68.33	15.00
92	GLN	NE2	-13.46	-7.18	66.42	15.00
92	GLN	C	-14.45	-12.22	66.92	15.00
92	GLN	O	-14.82	-12.42	68.07	15.00
93	GLU	N	-13.51	-12.94	66.32	15.00
93	GLU	CA	-12.75	-13.98	66.99	15.00
93	GLU	CB	-11.92	-14.80	65.98	15.00
93	GLU	CG	-12.60	-15.10	64.64	15.00
93	GLU	CD	-11.66	-15.74	63.60	15.00
93	GLU	OE1	-10.42	-15.60	63.72	15.00
93	GLU	OE2	-12.17	-16.37	62.65	15.00

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93	GLU	C	-11.83	-13.34	68.03	15.00
93	GLU	O	-11.21	-12.30	67.75	15.00
94	GLU	N	-11.73	-13.97	69.20	15.00
94	GLU	CA	-10.88	-13.49	70.30	15.00
94	GLU	CB	-11.58	-12.42	71.15	15.00
94	GLU	CG	-11.71	-11.07	70.44	15.00
94	GLU	CD	-12.53	-10.04	71.21	15.00
94	GLU	OE1	-13.43	-10.42	71.98	15.00
94	GLU	OE2	-12.26	-8.84	71.02	15.00
94	GLU	C	-10.47	-14.70	71.15	15.00
94	GLU	O	-10.92	-15.82	70.89	15.00
95	SER	N	-9.61	-14.49	72.13	15.00
95	SER	CA	-9.17	-15.58	72.99	15.00
95	SER	CB	-7.98	-15.16	73.87	15.00
95	SER	OG	-8.29	-14.05	74.70	15.00
95	SER	C	-10.29	-16.20	73.83	15.00
95	SER	O	-11.16	-15.50	74.36	15.00
96	CYS	N	-10.27	-17.53	73.93	15.00
96	CYS	CA	-11.26	-18.23	74.72	15.00
96	CYS	C	-11.28	-17.62	76.13	15.00
96	CYS	O	-10.26	-17.58	76.83	15.00
96	CYS	CB	-10.97	-19.73	74.75	15.00
96	CYS	SG	-12.23	-20.69	75.64	15.00
97	MET	N	-12.44	-17.08	76.50	15.00
97	MET	CA	-12.64	-16.44	77.80	15.00
97	MET	CB	-12.80	-14.93	77.61	15.00
97	MET	CG	-12.60	-14.11	78.87	15.00
97	MET	SD	-10.92	-14.28	79.50	15.00
97	MET	CE	-10.06	-13.18	78.42	15.00
97	MET	C	-13.84	-17.05	78.53	15.00
97	MET	O	-14.64	-16.34	79.14	15.00
98	TYR	N	-13.96	-18.37	78.44	15.00
98	TYR	CA	-15.04	-19.09	79.10	15.00
98	TYR	CB	-15.03	-20.57	78.73	15.00
98	TYR	CG	-15.99	-21.40	79.55	15.00
98	TYR	CD1	-17.36	-21.36	79.31	15.00
98	TYR	CE1	-18.25	-22.09	80.09	15.00
98	TYR	CD2	-15.53	-22.21	80.59	15.00
98	TYR	CE2	-16.41	-22.95	81.38	15.00
98	TYR	CZ	-17.77	-22.88	81.13	15.00
98	TYR	OH	-18.64	-23.57	81.93	15.00
98	TYR	C	-15.01	-18.91	80.61	15.00

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98	TYR O	-14.00	-19.18	81.26	15.00
99	ASN N	-16.12	-18.44	81.16	15.00
99	ASN CA	-16.24	-18.23	82.58	15.00
99	ASN CB	-16.80	-16.84	82.89	15.00
99	ASN CG	-16.73	-16.50	84.38	15.00
99	ASN OD1	-16.91	-17.36	85.24	15.00
99	ASN ND2	-16.44	-15.25	84.68	15.00
99	ASN C	-17.14	-19.31	83.15	15.00
99	ASN O	-18.33	-19.37	82.85	15.00
100	PRO N	-16.59	-20.19	83.99	15.00
100	PRO CD	-15.16	-20.25	84.37	15.00
100	PRO CA	-17.34	-21.29	84.62	15.00
100	PRO CB	-16.27	-21.98	85.47	15.00
100	PRO CG	-15.00	-21.70	84.70	15.00
100	PRO C	-18.52	-20.82	85.48	15.00
100	PRO O	-19.53	-21.51	85.58	15.00
101	THR N	-18.37	-19.64	86.09	15.00
101	THR CA	-19.42	-19.05	86.93	15.00
101	THR CB	-18.92	-17.73	87.61	15.00
101	THR OG1	-17.73	-17.97	88.38	15.00
101	THR CG2	-19.99	-17.15	88.54	15.00
101	THR C	-20.68	-18.73	86.12	15.00
101	THR O	-21.77	-18.69	86.68	15.00
102	GLY N	-20.52	-18.51	84.81	15.00
102	GLY CA	-21.67	-18.18	83.97	15.00
102	GLY C	-22.36	-19.33	83.25	15.00
102	GLY O	-23.34	-19.12	82.53	15.00
103	LYS N	-21.87	-20.54	83.47	15.00
103	LYS CA	-22.41	-21.74	82.83	15.00
103	LYS CB	-21.73	-22.98	83.40	15.00
103	LYS CG	-21.93	-24.24	82.59	15.00
103	LYS CD	-21.93	-25.43	83.52	15.00
103	LYS CE	-20.80	-25.36	84.52	15.00
103	LYS NZ	-21.18	-26.01	85.80	15.00
103	LYS C	-23.91	-21.86	82.95	15.00
103	LYS O	-24.44	-21.97	84.05	15.00
104	ALA N	-24.60	-21.92	81.82	15.00
104	ALA CA	-26.05	-22.02	81.81	15.00
104	ALA CB	-26.65	-20.90	80.97	15.00
104	ALA C	-26.59	-23.38	81.35	15.00
104	ALA O	-27.77	-23.67	81.53	15.00
105	ALA N	-25.72	-24.20	80.77	15.00

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105	ALA	CA	-26.11	-25.53	80.29	15.00
105	ALA	CB	-27.03	-25.41	79.07	15.00
105	ALA	C	-24.88	-26.34	79.91	15.00
105	ALA	O	-23.75	-25.83	79.94	15.00
106	LYS	N	-25.12	-27.60	79.57	15.00
106	LYS	CA	-24.10	-28.54	79.11	15.00
106	LYS	CB	-23.33	-29.21	80.26	15.00
106	LYS	CG	-24.14	-30.16	81.14	15.00
106	LYS	CD	-23.57	-31.59	81.11	15.00
106	LYS	CE	-24.32	-32.54	82.06	15.00
106	LYS	NZ	-25.78	-32.68	81.70	15.00
106	LYS	C	-24.83	-29.57	78.27	15.00
106	LYS	O	-26.05	-29.54	78.19	15.00
107	CYS	N	-24.09	-30.44	77.60	15.00
107	CYS	CA	-24.70	-31.48	76.79	15.00
107	CYS	CB	-24.95	-31.05	75.34	15.00
107	CYS	SG	-23.54	-31.08	74.19	15.00
107	CYS	C	-23.84	-32.72	76.88	15.00
107	CYS	O	-22.66	-32.64	77.19	15.00
108	ARG	N	-24.45	-33.87	76.68	15.00
108	ARG	CA	-23.73	-35.13	76.74	15.00
108	ARG	CB	-24.36	-36.04	77.78	15.00
108	ARG	CG	-24.14	-35.57	79.21	15.00
108	ARG	CD	-24.54	-36.64	80.19	15.00
108	ARG	NE	-25.96	-36.93	80.10	15.00
108	ARG	CZ	-26.54	-38.01	80.61	15.00
108	ARG	NH1	-25.81	-38.91	81.24	15.00
108	ARG	NH2	-27.85	-38.18	80.50	15.00
108	ARG	C	-23.58	-35.82	75.39	15.00
108	ARG	O	-23.92	-36.99	75.24	15.00
109	GLY	N	-23.09	-35.08	74.41	15.00
109	GLY	CA	-22.90	-35.66	73.10	15.00
109	GLY	C	-23.96	-35.21	72.13	15.00
109	GLY	O	-24.80	-34.38	72.48	15.00
110	TYR	N	-23.95	-35.79	70.94	15.00
110	TYR	CA	-24.90	-35.45	69.88	15.00
110	TYR	CB	-24.35	-34.33	68.98	15.00
110	TYR	CG	-23.08	-34.72	68.26	15.00
110	TYR	CD1	-21.84	-34.52	68.86	15.00
110	TYR	CE1	-20.69	-34.96	68.26	15.00
110	TYR	CD2	-23.13	-35.37	67.04	15.00
110	TYR	CE2	-21.98	-35.82	66.43	15.00

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110	TYR	CZ	-20.76	-35.62	67.05	15.00
110	TYR	OH	-19.61	-36.09	66.45	15.00
110	TYR	C	-25.28	-36.66	69.02	15.00
110	TYR	O	-24.66	-37.72	69.09	15.00
111	ARG	N	-26.28	-36.45	68.18	15.00
111	ARG	CA	-26.77	-37.47	67.27	15.00
111	ARG	CB	-28.06	-38.10	67.78	15.00
111	ARG	CG	-29.00	-38.71	66.72	15.00
111	ARG	CD	-28.59	-40.10	66.19	15.00
111	ARG	NE	-29.56	-40.59	65.20	15.00
111	ARG	CZ	-29.24	-41.12	64.02	15.00
111	ARG	NH1	-27.97	-41.25	63.65	15.00
111	ARG	NH2	-30.20	-41.45	63.15	15.00
111	ARG	C	-26.95	-36.78	65.92	15.00
111	ARG	O	-27.32	-35.60	65.85	15.00
112	GLU	N	-26.60	-37.49	64.86	15.00
112	GLU	CA	-26.73	-36.98	63.50	15.00
112	GLU	CB	-25.44	-37.25	62.71	15.00
112	GLU	CG	-24.23	-36.54	63.29	15.00
112	GLU	CD	-22.94	-36.81	62.52	15.00
112	GLU	OE1	-22.55	-36.00	61.66	15.00
112	GLU	OE2	-22.30	-37.84	62.82	15.00
112	GLU	C	-27.95	-37.64	62.84	15.00
112	GLU	O	-28.32	-38.74	63.20	15.00
113	ILE	N	-28.60	-36.94	61.93	15.00
113	ILE	CA	-29.75	-37.51	61.24	15.00
113	ILE	CB	-30.79	-36.40	60.90	15.00
113	ILE	CG2	-31.82	-36.90	59.89	15.00
113	ILE	CG1	-31.47	-35.89	62.17	15.00
113	ILE	CD1	-32.11	-36.98	63.00	15.00
113	ILE	C	-29.23	-38.17	59.97	15.00
113	ILE	O	-28.24	-37.70	59.39	15.00
114	PRO	N	-29.81	-39.32	59.56	15.00
114	PRO	CD	-30.91	-40.08	60.16	15.00
114	PRO	CA	-29.34	-39.97	58.34	15.00
114	PRO	CB	-30.43	-41.01	58.08	15.00
114	PRO	CG	-30.84	-41.40	59.42	15.00
114	PRO	C	-29.30	-38.94	57.22	15.00
114	PRO	O	-30.29	-38.23	56.97	15.00
115	GLU	N	-28.14	-38.81	56.59	15.00
115	GLU	CA	-27.95	-37.85	55.52	15.00
115	GLU	CB	-26.52	-37.88	55.00	15.00

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115	GLU	CG	-26.24	-36.84	53.95	15.00
115	GLU	CD	-24.87	-36.97	53.34	15.00
115	GLU	OE1	-24.73	-37.74	52.35	15.00
115	GLU	OE2	-23.94	-36.29	53.84	15.00
115	GLU	C	-28.94	-38.05	54.38	15.00
115	GLU	O	-29.14	-39.17	53.91	15.00
116	GLY	N	-29.55	-36.96	53.95	15.00
116	GLY	CA	-30.51	-37.02	52.86	15.00
116	GLY	C	-31.93	-37.43	53.23	15.00
116	GLY	O	-32.85	-37.23	52.44	15.00
117	ASN	N	-32.12	-37.92	54.46	15.00
117	ASN	CA	-33.43	-38.37	54.93	15.00
117	ASN	CB	-33.27	-39.59	55.85	15.00
117	ASN	CG	-34.53	-40.48	55.92	15.00
117	ASN	OD1	-35.65	-40.02	55.70	15.00
117	ASN	ND2	-34.34	-41.74	56.27	15.00
117	ASN	C	-34.30	-37.30	55.60	15.00
117	ASN	O	-34.12	-37.00	56.79	15.00
118	GLU	N	-35.26	-36.75	54.86	15.00
118	GLU	CA	-36.18	-35.73	55.38	15.00
118	GLU	CB	-36.91	-34.98	54.26	15.00
118	GLU	CG	-36.01	-34.11	53.37	15.00
118	GLU	CD	-36.78	-33.09	52.55	15.00
118	GLU	OE1	-36.86	-33.26	51.32	15.00
118	GLU	OE2	-37.30	-32.11	53.13	15.00
118	GLU	C	-37.19	-36.37	56.35	15.00
118	GLU	O	-37.57	-35.76	57.35	15.00
119	LYS	N	-37.59	-37.60	56.06	15.00
119	LYS	CA	-38.53	-38.31	56.92	15.00
119	LYS	CB	-38.89	-39.68	56.33	15.00
119	LYS	CG	-40.10	-40.36	56.97	15.00
119	LYS	CD	-40.37	-41.75	56.35	15.00
119	LYS	CE	-39.71	-42.89	57.16	15.00
119	LYS	NZ	-39.80	-44.23	56.47	15.00
119	LYS	C	-37.89	-38.45	58.30	15.00
119	LYS	O	-38.53	-38.23	59.33	15.00
120	ALA	N	-36.59	-38.76	58.30	15.00
120	ALA	CA	-35.85	-38.91	59.54	15.00
120	ALA	CB	-34.44	-39.41	59.25	15.00
120	ALA	C	-35.78	-37.58	60.26	15.00
120	ALA	O	-35.89	-37.52	61.49	15.00
121	LEU	N	-35.61	-36.51	59.48	15.00

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121	LEU	CA	-35.52	-35.16	60.02	15.00
121	LEU	CB	-35.02	-34.18	58.94	15.00
121	LEU	CG	-34.84	-32.68	59.23	15.00
121	LEU	CD1	-33.98	-32.43	60.46	15.00
121	LEU	CD2	-34.25	-32.02	57.99	15.00
121	LEU	C	-36.83	-34.68	60.68	15.00
121	LEU	O	-36.79	-34.05	61.74	15.00
122	LYS	N	-37.97	-35.03	60.08	15.00
122	LYS	CA	-39.29	-34.65	60.60	15.00
122	LYS	CB	-40.42	-34.99	59.63	15.00
122	LYS	CG	-41.82	-34.90	60.26	15.00
122	LYS	CD	-42.89	-35.49	59.34	15.00
122	LYS	CE	-44.28	-35.44	59.97	15.00
122	LYS	NZ	-45.36	-35.91	59.03	15.00
122	LYS	C	-39.57	-35.33	61.92	15.00
122	LYS	O	-40.03	-34.70	62.88	15.00
123	ARG	N	-39.33	-36.63	61.96	15.00
123	ARG	CA	-39.55	-37.40	63.17	15.00
123	ARG	CB	-39.26	-38.88	62.91	15.00
123	ARG	CG	-40.26	-39.53	61.95	15.00
123	ARG	CD	-40.04	-41.04	61.79	15.00
123	ARG	NE	-38.71	-41.35	61.25	15.00
123	ARG	CZ	-37.76	-42.03	61.89	15.00
123	ARG	NH1	-37.99	-42.51	63.12	15.00
123	ARG	NH2	-36.57	-42.20	61.33	15.00
123	ARG	C	-38.72	-36.82	64.33	15.00
123	ARG	O	-39.21	-36.72	65.46	15.00
124	ALA	N	-37.50	-36.38	64.04	15.00
124	ALA	CA	-36.62	-35.79	65.05	15.00
124	ALA	CB	-35.21	-35.60	64.50	15.00
124	ALA	C	-37.17	-34.46	65.58	15.00
124	ALA	O	-37.17	-34.21	66.79	15.00
125	VAL	N	-37.64	-33.61	64.68	15.00
125	VAL	CA	-38.20	-32.33	65.09	15.00
125	VAL	CB	-38.57	-31.44	63.87	15.00
125	VAL	CG1	-39.39	-30.23	64.31	15.00
125	VAL	CG2	-37.30	-30.97	63.15	15.00
125	VAL	C	-39.41	-32.57	65.99	15.00
125	VAL	O	-39.53	-31.99	67.07	15.00
126	ALA	N	-40.27	-33.49	65.58	15.00
126	ALA	CA	-41.46	-33.83	66.34	15.00
126	ALA	CB	-42.27	-34.90	65.62	15.00

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126	ALA	C	-41.15	-34.29	67.77	15.00
126	ALA	O	-41.69	-33.74	68.73	15.00
127	ARG	N	-40.26	-35.26	67.93	15.00
127	ARG	CA	-39.95	-35.76	69.27	15.00
127	ARG	CB	-39.99	-37.28	69.30	15.00
127	ARG	CG	-38.95	-37.98	68.45	15.00
127	ARG	CD	-39.08	-39.48	68.63	15.00
127	ARG	NE	-40.43	-39.95	68.30	15.00
127	ARG	CZ	-41.25	-40.58	69.14	15.00
127	ARG	NH1	-42.47	-40.94	68.73	15.00
127	ARG	NH2	-40.88	-40.83	70.39	15.00
127	ARG	C	-38.72	-35.26	70.01	15.00
127	ARG	O	-38.50	-35.65	71.15	15.00
128	VAL	N	-37.91	-34.42	69.40	15.00
128	VAL	CA	-36.72	-33.94	70.07	15.00
128	VAL	CB	-35.46	-34.31	69.27	15.00
128	VAL	CG1	-34.25	-33.52	69.74	15.00
128	VAL	CG2	-35.18	-35.79	69.42	15.00
128	VAL	C	-36.78	-32.43	70.32	15.00
128	VAL	O	-36.54	-31.96	71.43	15.00
129	GLY	N	-37.12	-31.68	69.28	15.00
129	GLY	CA	-37.18	-30.24	69.39	15.00
129	GLY	C	-36.41	-29.69	68.22	15.00
129	GLY	O	-36.10	-30.46	67.30	15.00
130	PRO	N	-36.09	-28.39	68.19	15.00
130	PRO	CD	-36.46	-27.40	69.22	15.00
130	PRO	CA	-35.34	-27.75	67.11	15.00
130	PRO	CB	-35.01	-26.38	67.70	15.00
130	PRO	CG	-36.23	-26.08	68.51	15.00
130	PRO	C	-34.06	-28.52	66.73	15.00
130	PRO	O	-33.35	-29.05	67.61	15.00
131	VAL	N	-33.78	-28.58	65.44	15.00
131	VAL	CA	-32.61	-29.30	64.92	15.00
131	VAL	CB	-33.05	-30.57	64.15	15.00
131	VAL	CG1	-31.85	-31.31	63.57	15.00
131	VAL	CG2	-33.84	-31.50	65.07	15.00
131	VAL	C	-31.71	-28.42	64.02	15.00
131	VAL	O	-32.21	-27.71	63.14	15.00
132	SER	N	-30.41	-28.44	64.29	15.00
132	SER	CA	-29.40	-27.69	63.53	15.00
132	SER	CB	-28.07	-27.65	64.28	15.00
132	SER	OG	-28.22	-27.17	65.59	15.00

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132	SER	C	-29.19	-28.31	62.13	15.00
132	SER	O	-28.82	-29.48	62.02	15.00
133	VAL	N	-29.40	-27.52	61.08	15.00
133	VAL	CA	-29.23	-28.02	59.73	15.00
133	VAL	CB	-30.60	-28.18	58.99	15.00
133	VAL	CG1	-31.53	-29.06	59.80	15.00
133	VAL	CG2	-31.24	-26.84	58.70	15.00
133	VAL	C	-28.35	-27.10	58.89	15.00
133	VAL	O	-28.22	-25.92	59.20	15.00
134	ALA	N	-27.74	-27.66	57.85	15.00
134	ALA	CA	-26.88	-26.90	56.95	15.00
134	ALA	CB	-25.50	-27.56	56.83	15.00
134	ALA	C	-27.59	-26.86	55.59	15.00
134	ALA	O	-28.15	-27.87	55.15	15.00
135	ILE	N	-27.61	-25.69	54.96	15.00
135	ILE	CA	-28.28	-25.52	53.68	15.00
135	ILE	CB	-29.64	-24.75	53.86	15.00
135	ILE	CG2	-30.59	-25.51	54.77	15.00
135	ILE	CG1	-29.37	-23.34	54.39	15.00
135	ILE	CD1	-30.61	-22.47	54.50	15.00
135	ILE	C	-27.45	-24.69	52.71	15.00
135	ILE	O	-26.36	-24.22	53.04	15.00
136	ASP	N	-27.98	-24.56	51.49	15.00
136	ASP	CA	-27.37	-23.75	50.45	15.00
136	ASP	CB	-27.45	-24.42	49.07	15.00
136	ASP	CG	-26.86	-23.57	47.94	15.00
136	ASP	OD1	-26.91	-24.02	46.79	15.00
136	ASP	OD2	-26.35	-22.45	48.19	15.00
136	ASP	C	-28.21	-22.46	50.50	15.00
136	ASP	O	-29.41	-22.48	50.22	15.00
137	ALA	N	-27.58	-21.38	50.92	15.00
137	ALA	CA	-28.23	-20.08	51.04	15.00
137	ALA	CB	-28.30	-19.68	52.49	15.00
137	ALA	C	-27.45	-19.04	50.25	15.00
137	ALA	O	-27.31	-17.91	50.69	15.00
138	SER	N	-26.97	-19.44	49.08	15.00
138	SER	CA	-26.18	-18.56	48.22	15.00
138	SER	CB	-25.05	-19.36	47.56	15.00
138	SER	OG	-25.57	-20.33	46.67	15.00
138	SER	C	-26.99	-17.81	47.16	15.00
138	SER	O	-26.48	-16.88	46.52	15.00
139	LEU	N	-28.23	-18.24	46.97	15.00

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139	LEU	CA	-29.11	-17.68	45.97	15.00
139	LEU	CB	-30.17	-18.70	45.55	15.00
139	LEU	CG	-29.68	-19.89	44.71	15.00
139	LEU	CD1	-28.41	-20.51	45.27	15.00
139	LEU	CD2	-30.78	-20.93	44.65	15.00
139	LEU	C	-29.76	-16.35	46.31	15.00
139	LEU	O	-30.20	-16.13	47.44	15.00
140	THR	N	-29.82	-15.48	45.31	15.00
140	THR	CA	-30.41	-14.15	45.44	15.00
140	THR	CB	-30.31	-13.40	44.07	15.00
140	THR	OG1	-28.94	-13.06	43.81	15.00
140	THR	CG2	-31.17	-12.14	44.06	15.00
140	THR	C	-31.87	-14.27	45.91	15.00
140	THR	O	-32.36	-13.41	46.66	15.00
141	SER	N	-32.55	-15.34	45.50	15.00
141	SER	CA	-33.93	-15.58	45.89	15.00
141	SER	CB	-34.47	-16.84	45.23	15.00
141	SER	OG	-33.61	-17.94	45.44	15.00
141	SER	C	-34.00	-15.70	47.41	15.00
141	SER	O	-34.83	-15.07	48.07	15.00
142	PHE	N	-33.07	-16.47	47.97	15.00
142	PHE	CA	-32.99	-16.70	49.40	15.00
142	PHE	CB	-31.94	-17.76	49.73	15.00
142	PHE	CG	-31.90	-18.15	51.17	15.00
142	PHE	CD1	-32.77	-19.12	51.66	15.00
142	PHE	CD2	-31.02	-17.55	52.05	15.00
142	PHE	CE1	-32.75	-19.48	53.00	15.00
142	PHE	CE2	-31.00	-17.90	53.39	15.00
142	PHE	CZ	-31.86	-18.87	53.86	15.00
142	PHE	C	-32.73	-15.42	50.16	15.00
142	PHE	O	-33.46	-15.07	51.08	15.00
143	GLN	N	-31.67	-14.71	49.76	15.00
143	GLN	CA	-31.30	-13.45	50.40	15.00
143	GLN	CB	-30.10	-12.81	49.70	15.00
143	GLN	CG	-29.69	-11.45	50.28	15.00
143	GLN	CD	-28.34	-10.91	49.77	15.00
143	GLN	OE1	-27.73	-10.04	50.40	15.00
143	GLN	NE2	-27.85	-11.46	48.64	15.00
143	GLN	C	-32.50	-12.51	50.43	15.00
143	GLN	O	-32.76	-11.85	51.44	15.00
144	PHE	N	-33.28	-12.51	49.36	15.00
144	PHE	CA	-34.43	-11.62	49.26	15.00

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144	PHE	CB	-34.43	-10.90	47.89	15.00
144	PHE	CG	-33.21	-10.01	47.66	15.00
144	PHE	CD1	-32.96	-8.92	48.48	15.00
144	PHE	CD2	-32.31	-10.29	46.63	15.00
144	PHE	CE1	-31.83	-8.12	48.30	15.00
144	PHE	CE2	-31.17	-9.48	46.44	15.00
144	PHE	CZ	-30.94	-8.40	47.27	15.00
144	PHE	C	-35.79	-12.23	49.61	15.00
144	PHE	O	-36.83	-11.62	49.35	15.00
145	TYR	N	-35.78	-13.41	50.24	15.00
145	TYR	CA	-37.03	-14.08	50.64	15.00
145	TYR	CB	-36.76	-15.42	51.35	15.00
145	TYR	CG	-37.96	-16.00	52.08	15.00
145	TYR	CD1	-38.82	-16.92	51.46	15.00
145	TYR	CE1	-39.93	-17.45	52.13	15.00
145	TYR	CD2	-38.26	-15.62	53.38	15.00
145	TYR	CE2	-39.37	-16.13	54.05	15.00
145	TYR	CZ	-40.20	-17.04	53.43	15.00
145	TYR	OH	-41.29	-17.54	54.12	15.00
145	TYR	C	-37.90	-13.18	51.52	15.00
145	TYR	O	-37.38	-12.43	52.36	15.00
146	SER	N	-39.21	-13.31	51.38	15.00
146	SER	CA	-40.13	-12.49	52.15	15.00
146	SER	CB	-40.37	-11.15	51.45	15.00
146	SER	OG	-40.91	-11.35	50.15	15.00
146	SER	C	-41.46	-13.15	52.51	15.00
146	SER	O	-41.95	-12.96	53.62	15.00
147	LYS	N	-42.01	-13.92	51.58	15.00
147	LYS	CA	-43.30	-14.59	51.76	15.00
147	LYS	CB	-44.42	-13.76	51.10	15.00
147	LYS	CG	-44.60	-12.34	51.62	15.00
147	LYS	CD	-45.05	-12.34	53.08	15.00
147	LYS	CE	-45.37	-10.92	53.58	15.00
147	LYS	NZ	-46.00	-10.90	54.93	15.00
147	LYS	C	-43.37	-16.03	51.20	15.00
147	LYS	O	-42.63	-16.39	50.27	15.00
148	GLY	N	-44.29	-16.81	51.75	15.00
148	GLY	CA	-44.52	-18.16	51.28	15.00
148	GLY	C	-43.46	-19.22	51.49	15.00
148	GLY	O	-42.47	-18.99	52.18	15.00
149	VAL	N	-43.70	-20.41	50.95	15.00
149	VAL	CA	-42.78	-21.53	51.07	15.00

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149	VAL	CB	-43.53	-22.90	50.95	15.00
149	VAL	CG1	-42.55	-24.07	50.90	15.00
149	VAL	CG2	-44.47	-23.08	52.14	15.00
149	VAL	C	-41.69	-21.41	50.01	15.00
149	VAL	O	-41.94	-21.55	48.82	15.00
150	TYR	N	-40.49	-21.08	50.48	15.00
150	TYR	CA	-39.31	-20.92	49.63	15.00
150	TYR	CB	-38.12	-20.36	50.42	15.00
150	TYR	CG	-36.84	-20.29	49.60	15.00
150	TYR	CD1	-36.67	-19.30	48.63	15.00
150	TYR	CE1	-35.54	-19.29	47.81	15.00
150	TYR	CD2	-35.84	-21.25	49.74	15.00
150	TYR	CE2	-34.71	-21.24	48.92	15.00
150	TYR	CZ	-34.57	-20.26	47.96	15.00
150	TYR	OH	-33.48	-20.27	47.12	15.00
150	TYR	C	-38.89	-22.18	48.89	15.00
150	TYR	O	-38.88	-23.28	49.45	15.00
151	TYR	N	-38.47	-21.98	47.65	15.00
151	TYR	CA	-37.98	-23.03	46.77	15.00
151	TYR	CB	-39.09	-23.99	46.35	15.00
151	TYR	CG	-38.62	-25.09	45.42	15.00
151	TYR	CD1	-37.92	-26.20	45.91	15.00
151	TYR	CE1	-37.51	-27.23	45.06	15.00
151	TYR	CD2	-38.89	-25.04	44.05	15.00
151	TYR	CE2	-38.49	-26.07	43.19	15.00
151	TYR	CZ	-37.80	-27.16	43.70	15.00
151	TYR	OH	-37.46	-28.21	42.87	15.00
151	TYR	C	-37.35	-22.39	45.55	15.00
151	TYR	O	-37.80	-21.33	45.07	15.00
152	ASP	N	-36.30	-23.02	45.05	15.00
152	ASP	CA	-35.59	-22.54	43.86	15.00
152	ASP	CB	-34.66	-21.38	44.20	15.00
152	ASP	CG	-34.13	-20.68	42.97	15.00
152	ASP	OD1	-33.52	-19.60	43.12	15.00
152	ASP	OD2	-34.32	-21.20	41.84	15.00
152	ASP	C	-34.83	-23.70	43.25	15.00
152	ASP	O	-33.94	-24.27	43.89	15.00
153	GLU	N	-35.15	-24.04	42.01	15.00
153	GLU	CA	-34.50	-25.15	41.34	15.00
153	GLU	CB	-35.16	-25.45	40.00	15.00
153	GLU	CG	-34.95	-24.38	38.96	15.00
153	GLU	CD	-35.39	-24.81	37.56	15.00

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153	GLU	OE1	-35.72	-26.00	37.37	15.00
153	GLU	OE2	-35.40	-23.94	36.66	15.00
153	GLU	C	-32.98	-25.02	41.17	15.00
153	GLU	O	-32.30	-26.01	40.92	15.00
154	SER	N	-32.46	-23.80	41.32	15.00
154	SER	CA	-31.02	-23.56	41.18	15.00
154	SER	CB	-30.77	-22.15	40.66	15.00
154	SER	OG	-31.56	-21.91	39.50	15.00
154	SER	C	-30.23	-23.82	42.46	15.00
154	SER	O	-28.99	-23.76	42.45	15.00
155	CYS	N	-30.94	-24.13	43.53	15.00
155	CYS	CA	-30.35	-24.39	44.84	15.00
155	CYS	C	-29.60	-25.71	44.92	15.00
155	CYS	O	-30.20	-26.78	44.85	15.00
155	CYS	CB	-31.43	-24.32	45.91	15.00
155	CYS	SG	-30.84	-23.76	47.53	15.00
156	ASN	N	-28.29	-25.64	45.11	15.00
156	ASN	CA	-27.46	-26.84	45.20	15.00
156	ASN	CB	-26.08	-26.58	44.61	15.00
156	ASN	CG	-25.26	-27.85	44.48	15.00
156	ASN	OD1	-25.77	-28.97	44.56	15.00
156	ASN	ND2	-23.96	-27.69	44.26	15.00
156	ASN	C	-27.33	-27.51	46.58	15.00
156	ASN	O	-26.74	-26.95	47.51	15.00
157	SER	N	-27.78	-28.76	46.65	15.00
157	SER	CA	-27.73	-29.53	47.88	15.00
157	SER	CB	-28.66	-30.74	47.80	15.00
157	SER	OG	-28.22	-31.64	46.80	15.00
157	SER	C	-26.33	-29.97	48.29	15.00
157	SER	O	-26.16	-30.58	49.35	15.00
158	ASP	N	-25.34	-29.71	47.43	15.00
158	ASP	CA	-23.95	-30.07	47.71	15.00
158	ASP	CB	-23.35	-30.92	46.59	15.00
158	ASP	CG	-24.02	-32.27	46.47	15.00
158	ASP	OD1	-24.01	-33.04	47.47	15.00
158	ASP	OD2	-24.58	-32.55	45.38	15.00
158	ASP	C	-23.09	-28.84	47.97	15.00
158	ASP	O	-21.86	-28.90	47.96	15.00
159	ASN	N	-23.76	-27.70	48.14	15.00
159	ASN	CA	-23.08	-26.45	48.42	15.00
159	ASN	CB	-23.32	-25.45	47.30	15.00
159	ASN	CG	-22.57	-24.14	47.51	15.00

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159	ASN	OD1	-21.74	-24.00	48.41	15.00
159	ASN	ND2	-22.86	-23.16	46.67	15.00
159	ASN	C	-23.69	-25.99	49.73	15.00
159	ASN	O	-24.50	-25.06	49.75	15.00
160	LEU	N	-23.39	-26.71	50.81	15.00
160	LEU	CA	-23.89	-26.38	52.15	15.00
160	LEU	CB	-23.90	-27.62	53.06	15.00
160	LEU	CG	-24.57	-28.92	52.58	15.00
160	LEU	CD1	-24.38	-30.01	53.60	15.00
160	LEU	CD2	-26.04	-28.72	52.33	15.00
160	LEU	C	-23.01	-25.25	52.70	15.00
160	LEU	O	-21.92	-25.48	53.22	15.00
161	ASN	N	-23.52	-24.02	52.60	15.00
161	ASN	CA	-22.76	-22.83	53.00	15.00
161	ASN	CB	-22.57	-21.92	51.79	15.00
161	ASN	CG	-23.88	-21.63	51.05	15.00
161	ASN	OD1	-24.76	-20.95	51.55	15.00
161	ASN	ND2	-24.00	-22.18	49.86	15.00
161	ASN	C	-23.26	-22.01	54.20	15.00
161	ASN	O	-22.55	-21.12	54.69	15.00
162	HIS	N	-24.46	-22.32	54.68	15.00
162	HIS	CA	-25.05	-21.57	55.79	15.00
162	HIS	CB	-25.96	-20.49	55.23	15.00
162	HIS	CG	-26.59	-19.59	56.25	15.00
162	HIS	CD2	-27.87	-19.21	56.42	15.00
162	HIS	ND1	-25.86	-18.91	57.21	15.00
162	HIS	CE1	-26.66	-18.14	57.91	15.00
162	HIS	NE2	-27.89	-18.30	57.45	15.00
162	HIS	C	-25.78	-22.50	56.78	15.00
162	HIS	O	-26.69	-23.22	56.39	15.00
163	ALA	N	-25.32	-22.55	58.02	15.00
163	ALA	CA	-25.96	-23.37	59.05	15.00
163	ALA	CB	-24.98	-23.74	60.15	15.00
163	ALA	C	-27.13	-22.57	59.62	15.00
163	ALA	O	-26.96	-21.42	60.03	15.00
164	VAL	N	-28.29	-23.20	59.71	15.00
164	VAL	CA	-29.50	-22.54	60.16	15.00
164	VAL	CB	-30.35	-22.26	58.88	15.00
164	VAL	CG1	-31.36	-23.35	58.63	15.00
164	VAL	CG2	-30.92	-20.89	58.89	15.00
164	VAL	C	-30.20	-23.45	61.21	15.00
164	VAL	O	-29.65	-24.48	61.57	15.00

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165	LEU	N	-31.35	-23.06	61.74	15.00
165	LEU	CA	-32.05	-23.90	62.72	15.00
165	LEU	CB	-32.05	-23.25	64.11	15.00
165	LEU	CG	-32.78	-23.96	65.26	15.00
165	LEU	CD1	-32.01	-25.18	65.72	15.00
165	LEU	CD2	-32.97	-22.99	66.42	15.00
165	LEU	C	-33.48	-24.25	62.31	15.00
165	LEU	O	-34.26	-23.36	61.97	15.00
166	ALA	N	-33.83	-25.54	62.36	15.00
166	ALA	CA	-35.17	-26.00	62.00	15.00
166	ALA	CB	-35.08	-27.37	61.33	15.00
166	ALA	C	-36.09	-26.07	63.23	15.00
166	ALA	O	-36.08	-27.05	63.97	15.00
167	VAL	N	-36.92	-25.04	63.39	15.00
167	VAL	CA	-37.82	-24.95	64.54	15.00
167	VAL	CB	-37.90	-23.48	65.05	15.00
167	VAL	CG1	-36.52	-22.98	65.43	15.00
167	VAL	CG2	-38.52	-22.57	64.00	15.00
167	VAL	C	-39.23	-25.53	64.35	15.00
167	VAL	O	-40.12	-25.32	65.18	15.00
168	GLY	N	-39.43	-26.27	63.27	15.00
168	GLY	CA	-40.73	-26.86	63.04	15.00
168	GLY	C	-40.94	-27.30	61.61	15.00
168	GLY	O	-40.00	-27.42	60.82	15.00
169	TYR	N	-42.21	-27.55	61.29	15.00
169	TYR	CA	-42.63	-28.00	59.98	15.00
169	TYR	CB	-42.14	-29.44	59.67	15.00
169	TYR	CG	-42.65	-30.54	60.59	15.00
169	TYR	CD1	-43.92	-31.12	60.41	15.00
169	TYR	CE1	-44.37	-32.15	61.25	15.00
169	TYR	CD2	-41.86	-31.02	61.63	15.00
169	TYR	CE2	-42.31	-32.06	62.47	15.00
169	TYR	CZ	-43.57	-32.61	62.27	15.00
169	TYR	OH	-44.00	-33.61	63.11	15.00
169	TYR	C	-44.14	-27.91	59.91	15.00
169	TYR	O	-44.83	-27.98	60.92	15.00
170	GLY	N	-44.65	-27.78	58.70	15.00
170	GLY	CA	-46.08	-27.68	58.51	15.00
170	GLY	C	-46.38	-27.73	57.04	15.00
170	GLY	O	-45.57	-28.17	56.24	15.00
171	ILE	N	-47.52	-27.17	56.68	15.00
171	ILE	CA	-47.97	-27.14	55.30	15.00

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171	ILE	CB	-48.87	-28.38	55.01	15.00
171	ILE	CG2	-49.85	-28.63	56.15	15.00
171	ILE	CG1	-49.58	-28.25	53.67	15.00
171	ILE	CD1	-50.27	-29.51	53.26	15.00
171	ILE	C	-48.71	-25.83	55.06	15.00
171	ILE	O	-49.51	-25.40	55.88	15.00
172	GLN	N	-48.35	-25.13	53.99	15.00
172	GLN	CA	-48.99	-23.87	53.65	15.00
172	GLN	CB	-48.01	-22.70	53.72	15.00
172	GLN	CG	-48.67	-21.36	53.62	15.00
172	GLN	CD	-47.71	-20.23	53.89	15.00
172	GLN	OE1	-47.35	-19.97	55.05	15.00
172	GLN	NE2	-47.27	-19.55	52.84	15.00
172	GLN	C	-49.60	-24.00	52.25	15.00
172	GLN	O	-48.88	-24.13	51.26	15.00
173	LYS	N	-50.93	-23.99	52.20	15.00
173	LYS	CA	-51.68	-24.15	50.97	15.00
173	LYS	CB	-51.66	-22.89	50.10	15.00
173	LYS	CG	-52.38	-23.03	48.72	15.00
173	LYS	CD	-53.92	-23.15	48.79	15.00
173	LYS	CE	-54.45	-24.44	49.47	15.00
173	LYS	NZ	-54.10	-25.73	48.79	15.00
173	LYS	C	-51.15	-25.34	50.20	15.00
173	LYS	O	-50.54	-25.19	49.14	15.00
174	GLY	N	-51.31	-26.53	50.77	15.00
174	GLY	CA	-50.84	-27.73	50.10	15.00
174	GLY	C	-49.36	-27.74	49.76	15.00
174	GLY	O	-48.95	-28.42	48.82	15.00
175	ASN	N	-48.57	-26.97	50.50	15.00
175	ASN	CA	-47.12	-26.90	50.30	15.00
175	ASN	CB	-46.69	-25.54	49.74	15.00
175	ASN	CG	-46.88	-25.43	48.24	15.00
175	ASN	OD1	-45.91	-25.39	47.48	15.00
175	ASN	ND2	-48.13	-25.38	47.79	15.00
175	ASN	C	-46.40	-27.18	51.61	15.00
175	ASN	O	-46.33	-26.31	52.49	15.00
176	LYS	N	-45.91	-28.41	51.76	15.00
176	LYS	CA	-45.18	-28.82	52.97	15.00
176	LYS	CB	-44.88	-30.32	52.95	15.00
176	LYS	CG	-46.14	-31.18	52.92	15.00
176	LYS	CD	-45.83	-32.64	52.63	15.00
176	LYS	CE	-47.08	-33.51	52.74	15.00

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176	LYS	NZ	-47.62	-33.57	54.13	15.00
176	LYS	C	-43.90	-28.00	53.08	15.00
176	LYS	O	-43.34	-27.58	52.07	15.00
177	HIS	N	-43.42	-27.80	54.30	15.00
177	HIS	CA	-42.23	-26.99	54.52	15.00
177	HIS	CB	-42.58	-25.51	54.38	15.00
177	HIS	CG	-43.53	-25.04	55.43	15.00
177	HIS	CD2	-43.36	-24.83	56.76	15.00
177	HIS	ND1	-44.87	-24.83	55.18	15.00
177	HIS	CE1	-45.48	-24.50	56.31	15.00
177	HIS	NE2	-44.59	-24.50	57.28	15.00
177	HIS	C	-41.62	-27.24	55.88	15.00
177	HIS	O	-42.21	-27.92	56.71	15.00
178	TRP	N	-40.49	-26.58	56.12	15.00
178	TRP	CA	-39.74	-26.60	57.38	15.00
178	TRP	CB	-38.28	-27.02	57.18	15.00
178	TRP	CG	-38.08	-28.36	56.62	15.00
178	TRP	CD2	-38.10	-29.59	57.34	15.00
178	TRP	CE2	-37.84	-30.62	56.41	15.00
178	TRP	CE3	-38.30	-29.94	58.68	15.00
178	TRP	CD1	-37.82	-28.67	55.32	15.00
178	TRP	NE1	-37.68	-30.02	55.18	15.00
178	TRP	CZ2	-37.79	-31.98	56.77	15.00
178	TRP	CZ3	-38.25	-31.28	59.05	15.00
178	TRP	CH2	-37.99	-32.28	58.09	15.00
178	TRP	C	-39.76	-25.15	57.89	15.00
178	TRP	O	-39.63	-24.21	57.10	15.00
179	ILE	N	-39.96	-24.95	59.18	15.00
179	ILE	CA	-39.96	-23.60	59.72	15.00
179	ILE	CB	-40.92	-23.46	60.92	15.00
179	ILE	CG2	-41.00	-22.01	61.38	15.00
179	ILE	CG1	-42.33	-23.91	60.50	15.00
179	ILE	CD1	-43.31	-23.94	61.64	15.00
179	ILE	C	-38.50	-23.37	60.10	15.00
179	ILE	O	-37.97	-24.03	61.00	15.00
180	ILE	N	-37.84	-22.48	59.36	15.00
180	ILE	CA	-36.43	-22.18	59.55	15.00
180	ILE	CB	-35.67	-22.22	58.19	15.00
180	ILE	CG2	-34.25	-21.74	58.35	15.00
180	ILE	CG1	-35.73	-23.63	57.58	15.00
180	ILE	CD1	-35.19	-24.73	58.48	15.00
180	ILE	C	-36.14	-20.84	60.22	15.00

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180	ILE	O	-36.63	-19.80	59.79	15.00
181	LYS	N	-35.33	-20.88	61.27	15.00
181	LYS	CA	-34.93	-19.68	62.01	15.00
181	LYS	CB	-34.89	-19.94	63.51	15.00
181	LYS	CG	-34.35	-18.76	64.31	15.00
181	LYS	CD	-34.18	-19.11	65.77	15.00
181	LYS	CE	-33.68	-17.92	66.56	15.00
181	LYS	NZ	-33.51	-18.24	68.01	15.00
181	LYS	C	-33.55	-19.25	61.51	15.00
181	LYS	O	-32.61	-20.03	61.53	15.00
182	ASN	N	-33.43	-18.00	61.07	15.00
182	ASN	CA	-32.16	-17.49	60.56	15.00
182	ASN	CB	-32.35	-16.82	59.19	15.00
182	ASN	CG	-31.05	-16.69	58.41	15.00
182	ASN	OD1	-30.02	-17.26	58.78	15.00
182	ASN	ND2	-31.09	-15.95	57.31	15.00
182	ASN	C	-31.49	-16.53	61.56	15.00
182	ASN	O	-32.12	-16.09	62.52	15.00
183	SER	N	-30.20	-16.28	61.35	15.00
183	SER	CA	-29.44	-15.37	62.20	15.00
183	SER	CB	-28.30	-16.09	62.93	15.00
183	SER	OG	-27.53	-16.88	62.05	15.00
183	SER	C	-28.93	-14.14	61.42	15.00
183	SER	O	-27.77	-13.73	61.54	15.00
184	TRP	N	-29.81	-13.60	60.57	15.00
184	TRP	CA	-29.50	-12.41	59.78	15.00
184	TRP	CB	-29.71	-12.65	58.29	15.00
184	TRP	CG	-28.64	-13.47	57.67	15.00
184	TRP	CD2	-28.66	-14.06	56.37	15.00
184	TRP	CE2	-27.47	-14.81	56.23	15.00
184	TRP	CE3	-29.58	-14.04	55.31	15.00
184	TRP	CD1	-27.46	-13.86	58.25	15.00
184	TRP	NE1	-26.76	-14.67	57.39	15.00
184	TRP	CZ2	-27.18	-15.53	55.06	15.00
184	TRP	CZ3	-29.29	-14.76	54.16	15.00
184	TRP	CH2	-28.09	-15.49	54.04	15.00
184	TRP	C	-30.34	-11.22	60.27	15.00
184	TRP	O	-30.59	-10.27	59.53	15.00
185	GLY	N	-30.78	-11.31	61.52	15.00
185	GLY	CA	-31.57	-10.25	62.10	15.00
185	GLY	C	-33.05	-10.45	61.90	15.00
185	GLY	O	-33.50	-11.18	61.01	15.00

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186	GLU	N	-33.81	-9.76	62.75	15.00
186	GLU	CA	-35.27	-9.78	62.74	15.00
186	GLU	CB	-35.81	-9.15	64.05	15.00
186	GLU	CG	-37.34	-9.12	64.18	15.00
186	GLU	CD	-37.84	-9.82	65.44	15.00
186	GLU	OE1	-37.53	-9.33	66.55	15.00
186	GLU	OE2	-38.54	-10.87	65.33	15.00
186	GLU	C	-35.85	-9.11	61.50	15.00
186	GLU	O	-36.99	-9.36	61.12	15.00
187	ASN	N	-35.05	-8.27	60.84	15.00
187	ASN	CA	-35.52	-7.59	59.64	15.00
187	ASN	CB	-35.00	-6.16	59.56	15.00
187	ASN	CG	-36.02	-5.17	60.07	15.00
187	ASN	OD1	-35.91	-4.68	61.20	15.00
187	ASN	ND2	-37.05	-4.90	59.25	15.00
187	ASN	C	-35.23	-8.31	58.33	15.00
187	ASN	O	-35.26	-7.72	57.27	15.00
188	TRP	N	-34.94	-9.60	58.43	15.00
188	TRP	CA	-34.68	-10.39	57.25	15.00
188	TRP	CB	-33.32	-11.10	57.33	15.00
188	TRP	CG	-33.12	-12.00	56.19	15.00
188	TRP	CD2	-33.49	-13.38	56.12	15.00
188	TRP	CE2	-33.22	-13.81	54.80	15.00
188	TRP	CE3	-34.04	-14.29	57.03	15.00
188	TRP	CD1	-32.64	-11.66	54.96	15.00
188	TRP	NE1	-32.71	-12.74	54.12	15.00
188	TRP	CZ2	-33.48	-15.13	54.37	15.00
188	TRP	CZ3	-34.30	-15.60	56.60	15.00
188	TRP	CH2	-34.02	-16.00	55.28	15.00
188	TRP	C	-35.82	-11.39	57.10	15.00
188	TRP	O	-36.41	-11.81	58.09	15.00
189	GLY	N	-36.11	-11.76	55.85	15.00
189	GLY	CA	-37.16	-12.72	55.57	15.00
189	GLY	C	-38.43	-12.37	56.32	15.00
189	GLY	O	-38.82	-11.20	56.40	15.00
190	ASN	N	-39.08	-13.38	56.89	15.00
190	ASN	CA	-40.30	-13.15	57.64	15.00
190	ASN	CB	-41.37	-14.19	57.30	15.00
190	ASN	CG	-42.78	-13.73	57.68	15.00
190	ASN	OD1	-43.76	-14.38	57.34	15.00
190	ASN	ND2	-42.88	-12.59	58.37	15.00
190	ASN	C	-40.02	-13.14	59.13	15.00

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190 ASN O	-40.22	-14.15	59.80	15.00
191 LYS N	-39.56	-11.99	59.63	15.00
191 LYS CA	-39.23	-11.78	61.05	15.00
191 LYS CB	-40.40	-12.11	61.99	15.00
191 LYS CG	-41.62	-11.23	61.84	15.00
191 LYS CD	-42.63	-11.52	62.95	15.00
191 LYS CE	-43.99	-10.85	62.71	15.00
191 LYS NZ	-44.94	-11.70	61.92	15.00
191 LYS C	-37.98	-12.58	61.45	15.00
191 LYS O	-37.79	-12.95	62.61	15.00
192 GLY N	-37.13	-12.82	60.45	15.00
192 GLY CA	-35.90	-13.56	60.66	15.00
192 GLY C	-36.13	-15.04	60.40	15.00
192 GLY O	-35.29	-15.88	60.72	15.00
193 TYR N	-37.28	-15.34	59.80	15.00
193 TYR CA	-37.66	-16.70	59.49	15.00
193 TYR CB	-38.91	-17.11	60.25	15.00
193 TYR CG	-38.66	-17.45	61.68	15.00
193 TYR CD1	-38.59	-16.46	62.66	15.00
193 TYR CE1	-38.33	-16.78	63.98	15.00
193 TYR CD2	-38.48	-18.78	62.07	15.00
193 TYR CE2	-38.22	-19.11	63.38	15.00
193 TYR CZ	-38.15	-18.11	64.34	15.00
193 TYR OH	-37.89	-18.43	65.64	15.00
193 TYR C	-37.86	-16.93	58.01	15.00
193 TYR O	-37.92	-15.99	57.22	15.00
194 ILE N	-37.97	-18.20	57.65	15.00
194 ILE CA	-38.20	-18.60	56.28	15.00
194 ILE CB	-36.88	-18.58	55.44	15.00
194 ILE CG2	-35.81	-19.44	56.08	15.00
194 ILE CG1	-37.16	-19.03	54.00	15.00
194 ILE CD1	-36.05	-18.68	53.02	15.00
194 ILE C	-38.85	-20.00	56.28	15.00
194 ILE O	-38.54	-20.83	57.14	15.00
195 LEU N	-39.84	-20.20	55.42	15.00
195 LEU CA	-40.50	-21.49	55.30	15.00
195 LEU CB	-42.00	-21.36	55.08	15.00
195 LEU CG	-42.81	-20.66	56.16	15.00
195 LEU CD1	-44.27	-20.65	55.77	15.00
195 LEU CD2	-42.60	-21.36	57.49	15.00
195 LEU C	-39.83	-22.09	54.09	15.00
195 LEU O	-39.85	-21.47	53.04	15.00

TABLE V

196 MET N	-39.17	-23.23	54.23	15.00
196 MET CA	-38.49	-23.84	53.10	15.00
196 MET CB	-37.01	-24.08	53.39	15.00
196 MET CG	-36.15	-22.83	53.37	15.00
196 MET SD	-34.45	-23.19	53.93	15.00
196 MET CE	-33.63	-23.67	52.36	15.00
196 MET C	-39.17	-25.14	52.72	15.00
196 MET O	-39.59	-25.89	53.59	15.00
197 ALA N	-39.22	-25.41	51.41	15.00
197 ALA CA	-39.86	-26.62	50.87	15.00
197 ALA CB	-39.64	-26.70	49.36	15.00
197 ALA C	-39.42	-27.93	51.53	15.00
197 ALA O	-38.23	-28.21	51.67	15.00
198 ARG N	-40.41	-28.73	51.91	15.00
198 ARG CA	-40.18	-30.01	52.57	15.00
198 ARG CB	-40.77	-30.03	53.98	15.00
198 ARG CG	-40.78	-31.39	54.66	15.00
198 ARG CD	-41.18	-31.28	56.12	15.00
198 ARG NE	-42.52	-30.73	56.31	15.00
198 ARG CZ	-43.63	-31.47	56.40	15.00
198 ARG NH1	-43.55	-32.80	56.31	15.00
198 ARG NH2	-44.80	-30.89	56.62	15.00
198 ARG C	-40.74	-31.13	51.71	15.00
198 ARG O	-41.84	-31.00	51.16	15.00
199 ASN N	-39.98	-32.21	51.61	15.00
199 ASN CA	-40.35	-33.37	50.81	15.00
199 ASN CB	-41.72	-33.92	51.23	15.00
199 ASN CG	-41.71	-34.55	52.61	15.00
199 ASN OD1	-40.67	-34.60	53.26	15.00
199 ASN ND2	-42.87	-35.01	53.07	15.00
199 ASN C	-40.31	-33.04	49.32	15.00
199 ASN O	-41.18	-33.43	48.57	15.00
200 LYS N	-39.30	-32.27	48.92	15.00
200 LYS CA	-39.13	-31.88	47.54	15.00
200 LYS CB	-39.46	-30.41	47.32	15.00
200 LYS CG	-39.74	-30.07	45.87	15.00
200 LYS CD	-41.24	-30.05	45.59	15.00
200 LYS CE	-41.92	-28.93	46.40	15.00
200 LYS NZ	-43.41	-28.84	46.21	15.00
200 LYS C	-37.68	-32.17	47.16	15.00
200 LYS O	-36.89	-31.26	46.91	15.00
201 ASN N	-37.34	-33.46	47.14	15.00

TABLE V

201 ASN CA	-36.00	-33.95	46.83	15.00
201 ASN CB	-35.78	-34.02	45.31	15.00
201 ASN CG	-36.19	-32.75	44.59	15.00
201 ASN OD1	-37.20	-32.72	43.87	15.00
201 ASN ND2	-35.40	-31.70	44.76	15.00
201 ASN C	-34.84	-33.24	47.54	15.00
201 ASN O	-33.84	-32.88	46.92	15.00
202 ASN N	-34.98	-33.11	48.86	15.00
202 ASN CA	-33.97	-32.49	49.74	15.00
202 ASN CB	-32.74	-33.42	49.89	15.00
202 ASN CG	-31.91	-33.12	51.13	15.00
202 ASN OD1	-32.36	-32.48	52.07	15.00
202 ASN ND2	-30.67	-33.60	51.13	15.00
202 ASN C	-33.56	-31.08	49.33	15.00
202 ASN O	-32.39	-30.82	49.02	15.00
203 ALA N	-34.51	-30.16	49.36	15.00
203 ALA H	-35.31	-30.45	49.85	15.00
203 ALA CA	-34.34	-28.77	48.93	15.00
203 ALA CB	-35.57	-27.93	49.27	15.00
203 ALA C	-33.15	-28.14	49.67	15.00
203 ALA O	-33.11	-27.98	50.89	15.00
204 CYS N	-32.16	-27.74	48.86	15.00
204 CYS CA	-30.95	-27.06	49.31	15.00
204 CYS C	-30.08	-27.85	50.28	15.00
204 CYS O	-29.25	-27.26	50.98	15.00
204 CYS CB	-31.27	-25.68	49.90	15.00
204 CYS SG	-32.21	-24.52	48.84	15.00
205 GLY N	-30.24	-29.17	50.32	15.00
205 GLY CA	-29.45	-29.99	51.22	15.00
205 GLY C	-29.93	-29.89	52.66	15.00
205 GLY O	-29.14	-30.07	53.60	15.00
206 ILE N	-31.23	-29.68	52.83	15.00
206 ILE CA	-31.84	-29.52	54.15	15.00
206 ILE CB	-33.39	-29.24	54.01	15.00
206 ILE CG2	-34.12	-30.44	53.42	15.00
206 ILE CG1	-34.00	-28.84	55.35	15.00
206 ILE CD1	-33.66	-27.44	55.81	15.00
206 ILE C	-31.57	-30.69	55.11	15.00
206 ILE O	-31.39	-30.47	56.31	15.00
207 ALA N	-31.46	-31.91	54.59	15.00
207 ALA CA	-31.21	-33.09	55.42	15.00
207 ALA CB	-32.32	-34.12	55.21	15.00

TABLE V

207	ALA	C	-29.83	-33.73	55.24	15.00
207	ALA	O	-29.58	-34.86	55.66	15.00
208	ASN	N	-28.92	-32.98	54.65	15.00
208	ASN	CA	-27.58	-33.50	54.42	15.00
208	ASN	CB	-26.91	-32.79	53.25	15.00
208	ASN	CG	-27.23	-33.43	51.92	15.00
208	ASN	OD1	-27.61	-34.59	51.86	15.00
208	ASN	ND2	-27.06	-32.67	50.84	15.00
208	ASN	C	-26.68	-33.44	55.65	15.00
208	ASN	O	-25.80	-34.29	55.81	15.00
209	LEU	N	-26.91	-32.46	56.52	15.00
209	LEU	CA	-26.09	-32.29	57.72	15.00
209	LEU	CB	-24.96	-31.30	57.44	15.00
209	LEU	CG	-23.70	-31.44	58.30	15.00
209	LEU	CD1	-22.81	-32.53	57.75	15.00
209	LEU	CD2	-22.95	-30.12	58.33	15.00
209	LEU	C	-26.86	-31.91	58.99	15.00
209	LEU	O	-26.42	-31.04	59.74	15.00
210	ALA	N	-27.99	-32.56	59.23	15.00
210	ALA	H	-27.89	-32.43	58.64	15.00
210	ALA	CA	-28.78	-32.25	60.42	15.00
210	ALA	CB	-29.43	-31.67	60.51	15.00
210	ALA	C	-28.24	-33.03	61.63	15.00
210	ALA	O	-27.87	-34.20	61.51	15.00
211	SER	N	-28.17	-32.35	62.78	15.00
211	SER	CA	-27.71	-32.98	64.03	15.00
211	SER	CB	-26.19	-33.01	64.15	15.00
211	SER	OG	-25.65	-31.71	64.29	15.00
211	SER	C	-28.32	-32.28	65.24	15.00
211	SER	O	-28.93	-31.20	65.11	15.00
212	PHE	N	-28.18	-32.89	66.41	15.00
212	PHE	CA	-28.74	-32.30	67.61	15.00
212	PHE	CB	-30.25	-32.56	67.71	15.00
212	PHE	CG	-30.62	-34.00	67.79	15.00
212	PHE	CD1	-31.04	-34.69	66.66	15.00
212	PHE	CD2	-30.53	-34.69	69.00	15.00
212	PHE	CE1	-31.36	-36.03	66.73	15.00
212	PHE	CE2	-30.85	-36.04	69.07	15.00
212	PHE	CZ	-31.27	-36.71	67.94	15.00
212	PHE	C	-28.01	-32.78	68.87	15.00
212	PHE	O	-27.55	-33.94	68.95	15.00
213	PRO	N	-27.92	-31.91	69.88	15.00

TABLE V

213 PRO CD	-28.60	-30.60	69.99	15.00
213 PRO CA	-27.25	-32.25	71.13	15.00
213 PRO CB	-27.11	-30.89	71.80	15.00
213 PRO CG	-28.44	-30.26	71.47	15.00
213 PRO C	-28.13	-33.17	71.96	15.00
213 PRO O	-29.36	-33.23	71.79	15.00
214 LYS N	-27.48	-33.94	72.82	15.00
214 LYS CA	-28.19	-34.82	73.72	15.00
214 LYS CB	-27.71	-36.27	73.59	15.00
214 LYS CG	-27.91	-36.90	72.23	15.00
214 LYS CD	-27.28	-38.29	72.16	15.00
214 LYS CE	-25.79	-38.27	72.50	15.00
214 LYS NZ	-25.11	-39.56	72.18	15.00
214 LYS C	-27.84	-34.26	75.07	15.00
214 LYS O	-26.76	-33.71	75.24	15.00
215 MET N	-28.79	-34.27	75.99	15.00
215 MET CA	-28.55	-33.78	77.34	15.00
215 MET CB	-29.47	-32.60	77.70	15.00
215 MET CG	-29.12	-31.30	76.96	15.00
215 MET SD	-29.59	-29.73	77.80	15.00
215 MET CE	-28.68	-28.54	76.81	15.00
215 MET C	-28.66	-34.93	78.34	15.00
215 MET OT1	-27.81	-35.01	79.26	15.00
215 MET OT2	-29.54	-35.80	78.16	15.00
216 HOH OH2	-40.32	-20.86	90.40	15.00
217 HOH OH2	-20.71	-32.43	79.67	15.00
218 HOH OH2	-31.33	-16.38	65.47	15.00
219 HOH OH2	-29.76	-17.63	70.42	15.00
220 HOH OH2	-7.13	-18.39	66.48	15.00
221 HOH OH2	-15.45	-12.55	73.01	15.00
222 HOH OH2	-34.69	-23.23	69.94	15.00
223 HOH OH2	-11.03	-30.64	72.74	15.00
224 HOH OH2	-30.92	-18.33	68.20	15.00
225 HOH OH2	-24.49	-30.79	61.59	15.00
226 HOH OH2	-15.06	-10.95	61.61	15.00
227 HOH OH2	-14.14	-21.84	66.38	15.00
228 HOH OH2	-45.46	-29.94	49.49	15.00
229 HOH OH2	-45.53	-34.98	55.75	15.00
230 HOH OH2	-37.47	-12.36	67.54	15.00
231 HOH OH2	-32.59	-13.97	60.21	15.00
232 HOH OH2	-23.45	-33.51	51.76	15.00
233 HOH OH2	-9.95	-25.41	63.34	15.00

TABLE V

234	HOH	OH2	-57.83	-31.91	39.28	15.00
235	HOH	OH2	-30.05	-20.10	63.45	15.00
236	HOH	OH2	-22.11	-29.91	61.97	15.00
237	HOH	OH2	-26.54	-11.16	68.27	15.00
238	HOH	OH2	-28.19	-16.14	71.94	15.00
239	HOH	OH2	-26.07	-26.03	83.66	15.00
240	HOH	OH2	-35.84	-27.16	51.26	15.00
241	HOH	OH2	-35.66	-24.80	49.57	15.00
242	HOH	OH2	-46.96	-32.65	56.91	15.00
243	HOH	OH2	-25.39	-9.00	77.82	15.00
244	HOH	OH2	-41.61	-14.85	64.38	15.00
245	HOH	OH2	-18.39	-3.01	63.15	15.00
246	HOH	OH2	-33.49	-28.51	70.47	15.00
247	HOH	OH2	-48.24	-19.58	79.27	15.00
248	HOH	OH2	-17.16	-11.08	74.86	15.00
249	HOH	OH2	-7.77	-18.99	72.85	15.00
250	HOH	OH2	-12.50	-24.63	81.88	15.00
251	HOH	OH2	-28.11	-35.31	58.10	15.00
252	HOH	OH2	-35.24	-11.03	53.39	15.00
253	HOH	OH2	-31.85	-28.95	46.18	15.00
254	HOH	OH2	-35.11	-24.97	46.75	15.00
255	HOH	OH2	-42.46	-38.44	54.37	15.00
256	HOH	OH2	-37.82	-16.40	67.58	15.00
257	HOH	OH2	-43.11	-16.23	66.45	15.00
258	HOH	OH2	-36.79	-9.70	73.69	15.00
259	HOH	OH2	-34.92	-15.40	75.95	15.00
260	HOH	OH2	-32.03	-7.39	60.30	15.00
261	HOH	OH2	-19.94	-8.07	62.81	15.00
262	HOH	OH2	-33.79	-20.76	69.68	15.00
263	HOH	OH2	-33.86	-45.02	74.42	15.00
264	HOH	OH2	-11.97	-27.02	71.08	15.00
265	HOH	OH2	-8.26	-25.33	61.28	15.00
266	HOH	OH2	-19.53	-42.28	58.81	15.00
267	HOH	OH2	-20.68	-32.75	61.19	15.00
268	HOH	OH2	-24.87	-33.89	60.62	15.00
269	HOH	OH2	-2.83	-32.79	71.85	15.00
270	HOH	OH2	-14.43	-40.52	59.53	15.00
271	HOH	OH2	-21.46	-37.41	78.35	15.00
272	HOH	OH2	-19.79	-36.03	71.33	15.00
273	HOH	OH2	-28.57	-35.40	88.70	15.00
274	HOH	OH2	-13.04	-12.02	63.26	15.00
275	HOH	OH2	-8.63	-11.89	72.80	15.00

TABLE V

276	HOH	OH2	-28.58	-30.13	56.41	15.00
277	HOH	OH2	-29.86	-20.69	48.27	15.00
278	HOH	OH2	-26.77	-22.94	44.37	15.00
279	HOH	OH2	-25.17	-36.24	49.68	15.00
280	HOH	OH2	-19.40	-31.57	49.99	15.00
281	HOH	OH2	-34.95	-29.42	45.52	15.00
282	HOH	OH2	-37.69	-30.43	50.51	15.00

TABLE VI

Table of the orthogonal three dimensional coordinates in Ångstroms and B factors (Å^2) for the cathepsin K complex with inhibitor 2-[N-(3-benzyloxybenzoyl)]-2'-[N'-(N-benzyloxycarbonyl-L-leucinyl)]carbohydrazide.

Residue	Atom	X	Y	Z	B
1	ALA CB	-53.28	-28.69	64.46	15.00
1	ALA C	-53.74	-30.77	63.13	15.00
1	ALA O	-54.17	-31.71	63.79	15.00
1	ALA N	-55.61	-29.36	63.92	15.00
1	ALA CA	-54.20	-29.34	63.43	15.00
2	PRO N	-52.92	-30.93	62.07	15.00
2	PRO CD	-52.55	-29.87	61.11	15.00
2	PRO CA	-52.38	-32.23	61.65	15.00
2	PRO CB	-52.22	-32.03	60.15	15.00
2	PRO CG	-51.68	-30.61	60.09	15.00
2	PRO C	-51.02	-32.37	62.31	15.00
2	PRO O	-50.88	-32.09	63.50	15.00
3	ASP N	-50.02	-32.75	61.52	15.00
3	ASP CA	-48.67	-32.92	62.02	15.00
3	ASP CB	-47.96	-34.03	61.25	15.00
3	ASP CG	-48.48	-35.41	61.59	15.00
3	ASP OD1	-49.68	-35.69	61.38	15.00
3	ASP OD2	-47.66	-36.24	62.06	15.00
3	ASP C	-47.93	-31.60	61.84	15.00
3	ASP O	-47.35	-31.34	60.78	15.00
4	SER N	-48.02	-30.74	62.84	15.00
4	SER CA	-47.34	-29.45	62.82	15.00
4	SER CB	-48.32	-28.34	62.42	15.00
4	SER OG	-48.91	-28.65	61.17	15.00
4	SER C	-46.76	-29.17	64.20	15.00
4	SER O	-47.33	-29.58	65.22	15.00
5	VAL N	-45.60	-28.54	64.23	15.00
5	VAL CA	-45.00	-28.20	65.51	15.00
5	VAL CB	-44.16	-29.36	66.11	15.00
5	VAL CG1	-42.89	-29.57	65.35	15.00
5	VAL CG2	-43.87	-29.08	67.57	15.00
5	VAL C	-44.21	-26.91	65.37	15.00
5	VAL O	-43.46	-26.73	64.41	15.00

TABLE VI

6	ASP	N	-44.48	-25.98	66.27	15.00
6	ASP	CA	-43.81	-24.70	66.29	15.00
6	ASP	CB	-44.76	-23.60	65.80	15.00
6	ASP	CG	-44.06	-22.25	65.59	15.00
6	ASP	OD1	-42.88	-22.10	65.94	15.00
6	ASP	OD2	-44.73	-21.33	65.08	15.00
6	ASP	C	-43.41	-24.48	67.75	15.00
6	ASP	O	-44.26	-24.33	68.63	15.00
7	TYR	N	-42.12	-24.54	68.00	15.00
7	TYR	CA	-41.60	-24.37	69.34	15.00
7	TYR	CB	-40.20	-24.96	69.42	15.00
7	TYR	CG	-40.23	-26.49	69.41	15.00
7	TYR	CD1	-40.62	-27.20	70.55	15.00
7	TYR	CE1	-40.66	-28.57	70.55	15.00
7	TYR	CD2	-39.89	-27.21	68.27	15.00
7	TYR	CE2	-39.94	-28.60	68.26	15.00
7	TYR	CZ	-40.32	-29.27	69.41	15.00
7	TYR	OH	-40.40	-30.63	69.42	15.00
7	TYR	C	-41.64	-22.94	69.83	15.00
7	TYR	O	-41.52	-22.68	71.03	15.00
8	ARG	N	-41.85	-22.01	68.90	15.00
8	ARG	CA	-41.91	-20.58	69.22	15.00
8	ARG	CB	-42.07	-19.74	67.95	15.00
8	ARG	CG	-40.84	-19.78	67.04	15.00
8	ARG	CD	-41.01	-18.96	65.78	15.00
8	ARG	NE	-41.97	-19.57	64.86	15.00
8	ARG	CZ	-42.43	-18.97	63.77	15.00
8	ARG	NH1	-42.03	-17.75	63.46	15.00
8	ARG	NH2	-43.30	-19.60	62.98	15.00
8	ARG	C	-43.09	-20.36	70.15	15.00
8	ARG	O	-42.95	-19.71	71.18	15.00
9	LYS	N	-44.23	-20.95	69.82	15.00
9	LYS	CA	-45.41	-20.80	70.64	15.00
9	LYS	CB	-46.59	-21.48	69.96	15.00
9	LYS	CG	-46.93	-20.90	68.60	15.00
9	LYS	CD	-47.74	-21.89	67.79	15.00
9	LYS	CE	-48.07	-21.38	66.41	15.00
9	LYS	NZ	-48.46	-22.50	65.49	15.00
9	LYS	C	-45.16	-21.46	71.99	15.00
9	LYS	O	-45.70	-21.01	73.01	15.00
10	LYS	N	-44.29	-22.46	71.99	15.00
10	LYS	CA	-43.94	-23.25	73.18	15.00

TABLE VI

10	LYS	CB	-43.34	-24.60	72.77	15.00
10	LYS	CG	-44.19	-25.43	71.81	15.00
10	LYS	CD	-45.03	-26.48	72.52	15.00
10	LYS	CE	-46.23	-25.86	73.25	15.00
10	LYS	NZ	-47.28	-25.31	72.33	15.00
10	LYS	C	-42.97	-22.59	74.15	15.00
10	LYS	O	-42.91	-22.97	75.32	15.00
11	GLY	N	-42.15	-21.66	73.67	15.00
11	GLY	CA	-41.20	-21.02	74.57	15.00
11	GLY	C	-39.83	-21.68	74.55	15.00
11	GLY	O	-39.00	-21.42	75.42	15.00
12	TYR	N	-39.57	-22.49	73.53	15.00
12	TYR	CA	-38.29	-23.18	73.39	15.00
12	TYR	CB	-38.48	-24.53	72.68	15.00
12	TYR	CG	-39.09	-25.67	73.49	15.00
12	TYR	CD1	-40.24	-25.49	74.27	15.00
12	TYR	CE1	-40.82	-26.55	74.95	15.00
12	TYR	CD2	-38.55	-26.95	73.42	15.00
12	TYR	CE2	-39.13	-28.01	74.09	15.00
12	TYR	CZ	-40.26	-27.81	74.85	15.00
12	TYR	OH	-40.86	-28.88	75.47	15.00
12	TYR	C	-37.31	-22.37	72.55	15.00
12	TYR	O	-36.15	-22.73	72.44	15.00
13	VAL	N	-37.78	-21.29	71.94	15.00
13	VAL	CA	-36.94	-20.46	71.07	15.00
13	VAL	CB	-37.56	-20.37	69.65	15.00
13	VAL	CG1	-36.60	-19.70	68.68	15.00
13	VAL	CG2	-37.91	-21.76	69.16	15.00
13	VAL	C	-36.75	-19.06	71.62	15.00
13	VAL	O	-37.70	-18.41	72.02	15.00
14	THR	N	-35.51	-18.61	71.66	15.00
14	THR	CA	-35.21	-17.27	72.15	15.00
14	THR	CB	-33.80	-17.21	72.74	15.00
14	THR	OG1	-32.85	-17.58	71.74	15.00
14	THR	CG2	-33.69	-18.13	73.92	15.00
14	THR	C	-35.31	-16.23	71.02	15.00
14	THR	O	-35.46	-16.59	69.85	15.00
15	PRO	N	-35.25	-14.94	71.35	15.00
15	PRO	CD	-35.15	-14.35	72.71	15.00
15	PRO	CA	-35.34	-13.89	70.34	15.00
15	PRO	CB	-35.15	-12.62	71.16	15.00
15	PRO	CG	-35.72	-12.99	72.50	15.00

TABLE VI

15 PRO C	-34.26	-14.00	69.25	15.00
15 PRO O	-33.13	-14.41	69.53	15.00
16 VAL N	-34.61	-13.62	68.02	15.00
16 VAL CA	-33.69	-13.67	66.89	15.00
16 VAL CB	-34.39	-13.43	65.54	15.00
16 VAL CG1	-33.36	-13.27	64.43	15.00
16 VAL CG2	-35.29	-14.58	65.20	15.00
16 VAL C	-32.56	-12.66	67.05	15.00
16 VAL O	-32.79	-11.47	67.28	15.00
17 LYS N	-31.34	-13.17	66.92	15.00
17 LYS CA	-30.15	-12.36	67.04	15.00
17 LYS CB	-29.13	-13.09	67.91	15.00
17 LYS CG	-29.67	-13.49	69.27	15.00
17 LYS CD	-30.28	-12.30	69.96	15.00
17 LYS CE	-30.93	-12.65	71.28	15.00
17 LYS NZ	-31.68	-11.47	71.83	15.00
17 LYS C	-29.58	-12.08	65.65	15.00
17 LYS O	-30.13	-12.52	64.64	15.00
18 ASN N	-28.48	-11.33	65.60	15.00
18 ASN CA	-27.82	-10.98	64.34	15.00
18 ASN CB	-28.02	-9.49	64.05	15.00
18 ASN CG	-27.42	-9.05	62.72	15.00
18 ASN OD1	-26.35	-9.49	62.32	15.00
18 ASN ND2	-28.11	-8.15	62.03	15.00
18 ASN C	-26.32	-11.27	64.49	15.00
18 ASN O	-25.67	-10.71	65.37	15.00
19 GLN N	-25.79	-12.14	63.63	15.00
19 GLN CA	-24.38	-12.49	63.68	15.00
19 GLN CB	-24.08	-13.76	62.87	15.00
19 GLN CG	-24.55	-13.74	61.41	15.00
19 GLN CD	-24.19	-15.02	60.65	15.00
19 GLN OE1	-25.06	-15.85	60.37	15.00
19 GLN NE2	-22.92	-15.16	60.28	15.00
19 GLN C	-23.43	-11.34	63.29	15.00
19 GLN O	-22.26	-11.34	63.67	15.00
20 GLY N	-23.92	-10.39	62.50	15.00
20 GLY CA	-23.11	-9.25	62.11	15.00
20 GLY C	-22.23	-9.49	60.91	15.00
20 GLY O	-22.71	-9.92	59.87	15.00
21 GLN N	-20.96	-9.14	61.02	15.00
21 GLN CA	-20.02	-9.34	59.92	15.00
21 GLN CB	-19.11	-8.11	59.75	15.00

TABLE VI

21	GLN	CG	-19.78	-6.87	59.13	15.00
21	GLN	CD	-20.32	-7.11	57.72	15.00
21	GLN	OE1	-19.57	-7.44	56.79	15.00
21	GLN	NE2	-21.62	-6.95	57.55	15.00
21	GLN	C	-19.18	-10.59	60.17	15.00
21	GLN	O	-18.39	-11.01	59.33	15.00
22	CYS	N	-19.34	-11.17	61.36	15.00
22	CYS	CA	-18.63	-12.38	61.75	15.00
22	CYS	C	-19.40	-13.60	61.22	15.00
22	CYS	O	-20.64	-13.58	61.15	15.00
22	CYS	CB	-18.52	-12.41	63.27	15.00
22	CYS	SG	-17.94	-13.95	64.05	15.00
23	GLY	N	-18.68	-14.63	60.78	15.00
23	GLY	CA	-19.32	-15.82	60.25	15.00
23	GLY	C	-19.52	-16.87	61.32	15.00
23	GLY	O	-19.06	-18.00	61.18	15.00
24	SER	N	-20.24	-16.49	62.37	15.00
24	SER	CA	-20.52	-17.34	63.52	15.00
24	SER	CB	-20.42	-16.49	64.77	15.00
24	SER	OG	-21.27	-15.36	64.65	15.00
24	SER	C	-21.92	-17.95	63.44	15.00
24	SER	O	-22.54	-18.24	64.47	15.00
25	CYS	N	-22.40	-18.17	62.23	15.00
25	CYS	CA	-23.72	-18.75	62.04	15.00
25	CYS	CB	-24.08	-18.74	60.55	15.00
25	CYS	SG	-23.06	-19.79	59.52	15.00
25	CYS	C	-23.81	-20.15	62.66	15.00
25	CYS	O	-24.90	-20.59	63.05	15.00
25	INH	C1	-27.01	-9.79	58.47	15.00
25	INH	C2	-26.33	-10.46	59.49	15.00
25	INH	C3	-25.12	-11.10	59.22	15.00
25	INH	C4	-24.57	-11.08	57.94	15.00
25	INH	C5	-25.26	-10.40	56.92	15.00
25	INH	C6	-26.47	-9.76	57.18	15.00
25	INH	C7	-23.25	-11.75	57.65	15.00
25	INH	O8	-23.16	-13.18	57.51	15.00
25	INH	C9	-22.82	-13.83	56.29	15.00
25	INH	C10	-22.10	-13.30	55.22	15.00
25	INH	C11	-23.03	-15.93	55.08	15.00
25	INH	C12	-22.32	-15.39	54.01	15.00
25	INH	C13	-21.85	-14.07	54.07	15.00
25	INH	C14	-23.54	-17.29	55.29	15.00

TABLE VI

25	INH	O15	-24.49	-17.82	54.70	15.00
25	INH	N16	-22.71	-17.77	56.29	15.00
25	INH	N17	-22.76	-19.07	56.92	15.00
25	INH	C18	-23.27	-15.13	56.20	15.00
25	INH	C19	-22.05	-19.01	58.26	15.00
25	INH	O20	-21.78	-17.83	58.57	15.00
25	INH	C21	-21.27	-30.33	52.84	15.00
25	INH	C22	-20.95	-30.49	54.19	15.00
25	INH	C23	-20.34	-29.44	54.89	15.00
25	INH	C24	-20.03	-28.23	54.25	15.00
25	INH	C25	-20.35	-28.09	52.90	15.00
25	INH	C26	-20.96	-29.12	52.19	15.00
25	INH	C27	-19.35	-27.11	55.01	15.00
25	INH	O28	-20.01	-25.85	55.20	15.00
25	INH	C29	-20.09	-25.30	56.50	15.00
25	INH	O30	-19.34	-25.70	57.40	15.00
25	INH	C31	-21.28	-23.64	57.93	15.00
25	INH	C32	-21.14	-24.56	59.14	15.00
25	INH	C33	-22.16	-25.68	59.35	15.00
25	INH	C34	-23.25	-25.62	58.28	15.00
25	INH	C35	-21.45	-27.01	59.33	15.00
25	INH	C36	-20.52	-22.34	58.22	15.00
25	INH	O37	-19.37	-22.35	58.66	15.00
25	INH	N38	-21.23	-21.24	57.98	15.00
25	INH	N39	-20.81	-19.86	58.17	15.00
25	INH	N40	-21.01	-24.34	56.66	15.00
26	TRP	N	-22.67	-20.83	62.82	15.00
26	TRP	CA	-22.65	-22.16	63.44	15.00
26	TRP	CB	-21.35	-22.91	63.12	15.00
26	TRP	CG	-20.11	-22.22	63.59	15.00
26	TRP	CD2	-19.48	-22.37	64.87	15.00
26	TRP	CE2	-18.42	-21.44	64.92	15.00
26	TRP	CE3	-19.71	-23.18	65.98	15.00
26	TRP	CD1	-19.41	-21.27	62.93	15.00
26	TRP	NE1	-18.40	-20.78	63.72	15.00
26	TRP	CZ2	-17.59	-21.30	66.03	15.00
26	TRP	CZ3	-18.88	-23.05	67.10	15.00
26	TRP	CH2	-17.84	-22.11	67.11	15.00
26	TRP	C	-22.85	-22.06	64.96	15.00
26	TRP	O	-23.57	-22.86	65.55	15.00
27	ALA	N	-22.24	-21.04	65.57	15.00
27	ALA	CA	-22.33	-20.83	67.01	15.00

TABLE VI

27	ALA	CB	-21.35	-19.78	67.46	15.00
27	ALA	C	-23.74	-20.47	67.45	15.00
27	ALA	O	-24.21	-20.91	68.50	15.00
28	PHE	N	-24.42	-19.66	66.66	15.00
28	PHE	CA	-25.79	-19.27	66.96	15.00
28	PHE	CB	-26.23	-18.10	66.07	15.00
28	PHE	CG	-25.67	-16.77	66.49	15.00
28	PHE	CD1	-24.46	-16.32	65.99	15.00
28	PHE	CD2	-26.35	-15.98	67.42	15.00
28	PHE	CE1	-23.92	-15.11	66.41	15.00
28	PHE	CE2	-25.81	-14.78	67.84	15.00
28	PHE	CZ	-24.60	-14.35	67.34	15.00
28	PHE	C	-26.74	-20.47	66.82	15.00
28	PHE	O	-27.62	-20.68	67.66	15.00
29	SER	N	-26.56	-21.25	65.78	15.00
29	SER	CA	-27.40	-22.41	65.55	15.00
29	SER	CB	-27.05	-23.08	64.23	15.00
29	SER	OG	-27.68	-24.35	64.15	15.00
29	SER	C	-27.28	-23.44	66.66	15.00
29	SER	O	-28.27	-24.06	67.03	15.00
30	SER	N	-26.06	-23.65	67.16	15.00
30	SER	CA	-25.79	-24.61	68.22	15.00
30	SER	CB	-24.29	-24.72	68.44	15.00
30	SER	OG	-23.64	-25.04	67.22	15.00
30	SER	C	-26.44	-24.15	69.51	15.00
30	SER	O	-27.07	-24.93	70.25	15.00
31	VAL	N	-26.25	-22.87	69.80	15.00
31	VAL	CA	-26.81	-22.23	70.98	15.00
31	VAL	CB	-26.39	-20.75	71.00	15.00
31	VAL	CG1	-27.52	-19.85	71.44	15.00
31	VAL	CG2	-25.18	-20.58	71.92	15.00
31	VAL	C	-28.32	-22.41	70.92	15.00
31	VAL	O	-28.95	-22.72	71.94	15.00
32	GLY	N	-28.89	-22.27	69.73	15.00
32	GLY	CA	-30.32	-22.44	69.56	15.00
32	GLY	C	-30.76	-23.83	69.97	15.00
32	GLY	O	-31.77	-24.00	70.65	15.00
33	ALA	N	-30.00	-24.83	69.55	15.00
33	ALA	CA	-30.28	-26.21	69.89	15.00
33	ALA	CB	-29.29	-27.14	69.22	15.00
33	ALA	C	-30.20	-26.34	71.42	15.00
33	ALA	O	-31.19	-26.70	72.06	15.00

TABLE VI

34	LEU	N	-29.06	-25.98	71.99	15.00
34	LEU	CA	-28.87	-26.06	73.44	15.00
34	LEU	CB	-27.55	-25.42	73.85	15.00
34	LEU	CG	-26.25	-26.10	73.41	15.00
34	LEU	CD1	-25.07	-25.21	73.74	15.00
34	LEU	CD2	-26.11	-27.45	74.08	15.00
34	LEU	C	-30.02	-25.41	74.21	15.00
34	LEU	O	-30.59	-26.01	75.13	15.00
35	GLU	N	-30.39	-24.20	73.80	15.00
35	GLU	CA	-31.46	-23.44	74.44	15.00
35	GLU	CB	-31.63	-22.08	73.77	15.00
35	GLU	CG	-30.41	-21.18	73.87	15.00
35	GLU	CD	-30.58	-19.86	73.15	15.00
35	GLU	OE1	-31.46	-19.76	72.27	15.00
35	GLU	OE2	-29.83	-18.92	73.46	15.00
35	GLU	C	-32.79	-24.17	74.42	15.00
35	GLU	O	-33.51	-24.18	75.42	15.00
36	GLY	N	-33.11	-24.77	73.27	15.00
36	GLY	CA	-34.35	-25.52	73.13	15.00
36	GLY	C	-34.42	-26.67	74.11	15.00
36	GLY	O	-35.48	-26.98	74.65	15.00
37	GLN	N	-33.28	-27.30	74.37	15.00
37	GLN	CA	-33.21	-28.42	75.29	15.00
37	GLN	CB	-31.94	-29.22	75.05	15.00
37	GLN	CG	-32.00	-30.06	73.80	15.00
37	GLN	CD	-33.19	-31.00	73.80	15.00
37	GLN	OE1	-33.32	-31.84	74.69	15.00
37	GLN	NE2	-34.07	-30.83	72.84	15.00
37	GLN	C	-33.28	-27.96	76.74	15.00
37	GLN	O	-33.94	-28.58	77.58	15.00
38	LEU	N	-32.64	-26.83	77.01	15.00
38	LEU	CA	-32.62	-26.25	78.35	15.00
38	LEU	CB	-31.77	-24.98	78.37	15.00
38	LEU	CG	-31.54	-24.37	79.75	15.00
38	LEU	CD1	-30.73	-25.34	80.61	15.00
38	LEU	CD2	-30.82	-23.05	79.63	15.00
38	LEU	C	-34.04	-25.95	78.83	15.00
38	LEU	O	-34.31	-25.95	80.02	15.00
39	LYS	N	-34.94	-25.65	77.90	15.00
39	LYS	CA	-36.32	-25.38	78.26	15.00
39	LYS	CB	-37.04	-24.66	77.12	15.00
39	LYS	CG	-38.53	-24.45	77.32	15.00

TABLE VI

39	LYS	CD	-38.85	-23.47	78.43	15.00
39	LYS	CE	-40.35	-23.46	78.70	15.00
39	LYS	NZ	-40.71	-22.74	79.94	15.00
39	LYS	C	-36.98	-26.72	78.54	15.00
39	LYS	O	-37.63	-26.90	79.57	15.00
40	LYS	N	-36.73	-27.68	77.65	15.00
40	LYS	CA	-37.28	-29.03	77.72	15.00
40	LYS	CB	-36.61	-29.90	76.66	15.00
40	LYS	CG	-37.25	-31.25	76.41	15.00
40	LYS	CD	-38.51	-31.10	75.61	15.00
40	LYS	CE	-39.15	-32.44	75.34	15.00
40	LYS	NZ	-38.32	-33.29	74.44	15.00
40	LYS	C	-37.07	-29.66	79.08	15.00
40	LYS	O	-37.99	-30.28	79.63	15.00
41	LYS	N	-35.87	-29.50	79.64	15.00
41	LYS	CA	-35.54	-30.10	80.93	15.00
41	LYS	CB	-34.07	-30.55	80.94	15.00
41	LYS	CG	-33.59	-31.28	79.68	15.00
41	LYS	CD	-34.50	-32.44	79.28	15.00
41	LYS	CE	-34.05	-33.08	77.96	15.00
41	LYS	NZ	-35.06	-34.05	77.42	15.00
41	LYS	C	-35.79	-29.20	82.14	15.00
41	LYS	O	-36.48	-29.59	83.09	15.00
42	THR	N	-35.20	-28.01	82.11	15.00
42	THR	CA	-35.30	-27.03	83.19	15.00
42	THR	CB	-34.20	-25.98	82.99	15.00
42	THR	OG1	-32.95	-26.64	82.85	15.00
42	THR	CG2	-34.13	-25.03	84.17	15.00
42	THR	C	-36.64	-26.32	83.38	15.00
42	THR	O	-36.96	-25.86	84.48	15.00
43	GLY	N	-37.43	-26.23	82.31	15.00
43	GLY	CA	-38.70	-25.53	82.38	15.00
43	GLY	C	-38.52	-24.01	82.29	15.00
43	GLY	O	-39.48	-23.25	82.34	15.00
44	LYS	N	-37.27	-23.57	82.16	15.00
44	LYS	CA	-36.94	-22.15	82.05	15.00
44	LYS	CB	-36.25	-21.65	83.33	15.00
44	LYS	CG	-37.19	-21.45	84.50	15.00
44	LYS	CD	-36.45	-21.05	85.78	15.00
44	LYS	CE	-35.71	-22.21	86.39	15.00
44	LYS	NZ	-36.62	-23.38	86.62	15.00
44	LYS	C	-35.98	-21.98	80.87	15.00

TABLE VI

44	LYS	O	-35.10	-22.82	80.66	15.00
45	LEU	N	-36.17	-20.92	80.10	15.00
45	LEU	CA	-35.33	-20.65	78.93	15.00
45	LEU	CB	-36.23	-20.21	77.77	15.00
45	LEU	CG	-35.64	-20.07	76.38	15.00
45	LEU	CD1	-35.28	-21.42	75.82	15.00
45	LEU	CD2	-36.67	-19.42	75.52	15.00
45	LEU	C	-34.33	-19.56	79.25	15.00
45	LEU	O	-34.59	-18.70	80.09	15.00
46	LEU	N	-33.18	-19.57	78.58	15.00
46	LEU	CA	-32.16	-18.56	78.80	15.00
46	LEU	CB	-31.30	-18.93	80.01	15.00
46	LEU	CG	-30.51	-17.78	80.61	15.00
46	LEU	CD1	-31.46	-16.70	81.06	15.00
46	LEU	CD2	-29.69	-18.27	81.78	15.00
46	LEU	C	-31.27	-18.40	77.56	15.00
46	LEU	O	-31.02	-19.36	76.85	15.00
47	ASN	N	-30.83	-17.17	77.29	15.00
47	ASN	CA	-29.98	-16.89	76.13	15.00
47	ASN	CB	-29.92	-15.38	75.84	15.00
47	ASN	CG	-31.27	-14.80	75.53	15.00
47	ASN	OD1	-31.93	-14.22	76.41	15.00
47	ASN	ND2	-31.71	-14.94	74.29	15.00
47	ASN	C	-28.57	-17.36	76.39	15.00
47	ASN	O	-27.91	-16.86	77.30	15.00
48	LEU	N	-28.10	-18.32	75.61	15.00
48	LEU	CA	-26.75	-18.84	75.78	15.00
48	LEU	CB	-26.70	-20.31	75.39	15.00
48	LEU	CG	-27.60	-21.19	76.26	15.00
48	LEU	CD1	-27.18	-22.64	76.10	15.00
48	LEU	CD2	-27.50	-20.77	77.73	15.00
48	LEU	C	-25.77	-18.04	74.98	15.00
48	LEU	O	-26.14	-17.34	74.04	15.00
49	SER	N	-24.50	-18.13	75.34	15.00
49	SER	CA	-23.47	-17.36	74.67	15.00
49	SER	CB	-22.34	-17.06	75.64	15.00
49	SER	OG	-21.34	-16.25	75.03	15.00
49	SER	C	-22.89	-17.98	73.40	15.00
49	SER	O	-22.29	-19.06	73.45	15.00
50	PRO	N	-23.07	-17.31	72.24	15.00
50	PRO	CD	-24.05	-16.24	72.05	15.00
50	PRO	CA	-22.55	-17.77	70.95	15.00

TABLE VI

50	PRO	CB	-23.37	-16.96	69.95	15.00
50	PRO	CG	-24.61	-16.59	70.71	15.00
50	PRO	C	-21.09	-17.37	70.86	15.00
50	PRO	O	-20.29	-18.01	70.19	15.00
51	GLN	N	-20.74	-16.27	71.52	15.00
51	GLN	CA	-19.37	-15.78	71.56	15.00
51	GLN	CB	-19.30	-14.45	72.33	15.00
51	GLN	CG	-17.93	-13.77	72.34	15.00
51	GLN	CD	-17.55	-13.17	71.00	15.00
51	GLN	OE1	-18.39	-12.57	70.31	15.00
51	GLN	NE2	-16.29	-13.29	70.64	15.00
51	GLN	C	-18.53	-16.82	72.26	15.00
51	GLN	O	-17.45	-17.17	71.80	15.00
52	ASN	N	-19.03	-17.33	73.38	15.00
52	ASN	CA	-18.30	-18.34	74.14	15.00
52	ASN	CB	-19.20	-18.91	75.24	15.00
52	ASN	CG	-18.51	-19.98	76.10	15.00
52	ASN	OD1	-19.13	-20.54	76.99	15.00
52	ASN	ND2	-17.23	-20.22	75.86	15.00
52	ASN	C	-17.86	-19.45	73.19	15.00
52	ASN	O	-16.70	-19.87	73.22	15.00
53	LEU	N	-18.76	-19.88	72.32	15.00
53	LEU	CA	-18.42	-20.92	71.38	15.00
53	LEU	CB	-19.66	-21.39	70.63	15.00
53	LEU	CG	-20.68	-22.14	71.49	15.00
53	LEU	CD1	-21.63	-22.88	70.59	15.00
53	LEU	CD2	-19.98	-23.13	72.38	15.00
53	LEU	C	-17.35	-20.41	70.42	15.00
53	LEU	O	-16.28	-21.02	70.31	15.00
54	VAL	N	-17.61	-19.27	69.79	15.00
54	VAL	CA	-16.68	-18.63	68.86	15.00
54	VAL	CB	-17.16	-17.18	68.52	15.00
54	VAL	CG1	-16.02	-16.35	67.96	15.00
54	VAL	CG2	-18.31	-17.21	67.54	15.00
54	VAL	C	-15.24	-18.57	69.37	15.00
54	VAL	O	-14.31	-18.91	68.66	15.00
55	ASP	N	-15.07	-18.14	70.61	15.00
55	ASP	CA	-13.75	-18.00	71.21	15.00
55	ASP	CB	-13.78	-16.96	72.33	15.00
55	ASP	CG	-14.29	-15.61	71.87	15.00
55	ASP	OD1	-14.16	-15.30	70.67	15.00
55	ASP	OD2	-14.79	-14.85	72.72	15.00

TABLE VI

55	ASP	C	-13.10	-19.26	71.77	15.00
55	ASP	O	-11.88	-19.33	71.86	15.00
56	CYS	N	-13.89	-20.25	72.17	15.00
56	CYS	CA	-13.31	-21.45	72.77	15.00
56	CYS	C	-13.25	-22.75	71.96	15.00
56	CYS	O	-12.44	-23.62	72.27	15.00
56	CYS	CB	-13.98	-21.73	74.11	15.00
56	CYS	SG	-14.30	-20.24	75.11	15.00
57	VAL	N	-14.09	-22.89	70.94	15.00
57	VAL	CA	-14.08	-24.13	70.16	15.00
57	VAL	CB	-15.43	-24.34	69.42	15.00
57	VAL	CG1	-15.47	-25.73	68.80	15.00
57	VAL	CG2	-16.59	-24.17	70.38	15.00
57	VAL	C	-12.91	-24.19	69.18	15.00
57	VAL	O	-13.08	-24.04	67.98	15.00
58	SER	N	-11.71	-24.46	69.70	15.00
58	SER	CA	-10.50	-24.55	68.89	15.00
58	SER	CB	-9.34	-25.09	69.72	15.00
58	SER	OG	-9.08	-24.27	70.85	15.00
58	SER	C	-10.61	-25.37	67.62	15.00
58	SER	O	-9.84	-25.18	66.70	15.00
59	GLU	N	-11.57	-26.29	67.56	15.00
59	GLU	CA	-11.71	-27.13	66.38	15.00
59	GLU	CB	-12.49	-28.41	66.73	15.00
59	GLU	CG	-11.81	-29.30	67.75	15.00
59	GLU	CD	-11.90	-28.75	69.16	15.00
59	GLU	OE1	-12.96	-28.18	69.51	15.00
59	GLU	OE2	-10.92	-28.91	69.91	15.00
59	GLU	C	-12.39	-26.41	65.23	15.00
59	GLU	O	-12.46	-26.91	64.11	15.00
60	ASN	N	-12.93	-25.24	65.53	15.00
60	ASN	CA	-13.61	-24.41	64.53	15.00
60	ASN	CB	-14.99	-24.01	65.03	15.00
60	ASN	CG	-15.97	-25.16	65.02	15.00
60	ASN	OD1	-17.03	-25.09	65.63	15.00
60	ASN	ND2	-15.62	-26.23	64.31	15.00
60	ASN	C	-12.75	-23.19	64.27	15.00
60	ASN	O	-11.79	-22.94	64.98	15.00
61	ASP	N	-13.12	-22.41	63.25	15.00
61	ASP	CA	-12.36	-21.23	62.88	15.00
61	ASP	CB	-12.21	-21.20	61.35	15.00
61	ASP	CG	-10.99	-20.43	60.90	15.00

TABLE VI

61	ASP	OD1	-10.38	-19.70	61.71	15.00
61	ASP	OD2	-10.63	-20.55	59.71	15.00
61	ASP	C	-12.92	-19.89	63.39	15.00
61	ASP	O	-12.71	-18.86	62.76	15.00
62	GLY	N	-13.61	-19.89	64.52	15.00
62	GLY	CA	-14.16	-18.66	65.06	15.00
62	GLY	C	-15.11	-17.97	64.10	15.00
62	GLY	O	-16.17	-18.50	63.79	15.00
63	CYS	N	-14.73	-16.79	63.62	15.00
63	CYS	CA	-15.56	-16.06	62.67	15.00
63	CYS	C	-15.39	-16.55	61.24	15.00
63	CYS	O	-16.01	-16.03	60.31	15.00
63	CYS	CB	-15.28	-14.56	62.73	15.00
63	CYS	SG	-15.94	-13.72	64.20	15.00
64	GLY	N	-14.52	-17.54	61.06	15.00
64	GLY	CA	-14.28	-18.09	59.74	15.00
64	GLY	C	-15.24	-19.23	59.47	15.00
64	GLY	O	-15.42	-19.63	58.32	15.00
65	GLY	N	-15.85	-19.77	60.52	15.00
65	GLY	CA	-16.79	-20.86	60.33	15.00
65	GLY	C	-16.54	-22.03	61.25	15.00
65	GLY	O	-15.56	-22.04	62.00	15.00
66	GLY	N	-17.42	-23.02	61.19	15.00
66	GLY	CA	-17.29	-24.19	62.03	15.00
66	GLY	C	-18.50	-25.10	61.96	15.00
66	GLY	O	-19.48	-24.76	61.32	15.00
67	TYR	N	-18.43	-26.25	62.62	15.00
67	TYR	CA	-19.53	-27.20	62.62	15.00
67	TYR	CB	-19.02	-28.60	62.32	15.00
67	TYR	CG	-18.35	-28.77	60.99	15.00
67	TYR	CD1	-19.08	-29.16	59.86	15.00
67	TYR	CE1	-18.46	-29.38	58.65	15.00
67	TYR	CD2	-16.98	-28.59	60.86	15.00
67	TYR	CE2	-16.36	-28.81	59.65	15.00
67	TYR	CZ	-17.10	-29.20	58.55	15.00
67	TYR	OH	-16.46	-29.41	57.35	15.00
67	TYR	C	-20.23	-27.22	63.97	15.00
67	TYR	O	-19.59	-27.04	65.00	15.00
68	MET	N	-21.52	-27.51	63.96	15.00
68	MET	CA	-22.31	-27.57	65.19	15.00
68	MET	CB	-23.81	-27.69	64.91	15.00
68	MET	CG	-24.46	-26.48	64.23	15.00

TABLE VI

68	MET	SD	-24.10	-26.27	62.47	15.00
68	MET	CE	-25.07	-27.56	61.75	15.00
68	MET	C	-21.86	-28.72	66.09	15.00
68	MET	O	-21.76	-28.56	67.30	15.00
69	THR	N	-21.54	-29.86	65.49	15.00
69	THR	CA	-21.10	-31.02	66.26	15.00
69	THR	CB	-20.78	-32.22	65.35	15.00
69	THR	OG1	-20.01	-31.77	64.24	15.00
69	THR	CG2	-22.06	-32.86	64.85	15.00
69	THR	C	-19.88	-30.71	67.11	15.00
69	THR	O	-19.77	-31.19	68.25	15.00
70	ASN	N	-18.97	-29.89	66.59	15.00
70	ASN	CA	-17.77	-29.52	67.33	15.00
70	ASN	CB	-16.79	-28.76	66.46	15.00
70	ASN	CG	-15.98	-29.65	65.58	15.00
70	ASN	OD1	-15.42	-29.19	64.60	15.00
70	ASN	ND2	-15.89	-30.93	65.92	15.00
70	ASN	C	-18.11	-28.66	68.55	15.00
70	ASN	O	-17.46	-28.77	69.59	15.00
71	ALA	N	-19.12	-27.80	68.40	15.00
71	ALA	CA	-19.57	-26.91	69.47	15.00
71	ALA	CB	-20.58	-25.91	68.94	15.00
71	ALA	C	-20.15	-27.71	70.63	15.00
71	ALA	O	-19.80	-27.50	71.78	15.00
72	PHE	N	-21.03	-28.66	70.31	15.00
72	PHE	CA	-21.64	-29.51	71.33	15.00
72	PHE	CB	-22.57	-30.54	70.69	15.00
72	PHE	CG	-23.72	-29.93	69.96	15.00
72	PHE	CD1	-24.28	-28.73	70.39	15.00
72	PHE	CD2	-24.24	-30.55	68.84	15.00
72	PHE	CE1	-25.33	-28.16	69.70	15.00
72	PHE	CE2	-25.30	-29.98	68.15	15.00
72	PHE	CZ	-25.84	-28.78	68.58	15.00
72	PHE	C	-20.53	-30.25	72.07	15.00
72	PHE	O	-20.43	-30.18	73.31	15.00
73	GLN	N	-19.67	-30.90	71.31	15.00
73	GLN	CA	-18.56	-31.66	71.86	15.00
73	GLN	CB	-17.68	-32.20	70.72	15.00
73	GLN	CG	-16.78	-33.40	71.09	15.00
73	GLN	CD	-17.54	-34.73	71.21	15.00
73	GLN	OE1	-17.47	-35.58	70.31	15.00
73	GLN	NE2	-18.21	-34.94	72.35	15.00

TABLE VI

73	GLN	C	-17.76	-30.78	72.84	15.00
73	GLN	O	-17.33	-31.25	73.89	15.00
74	TYR	N	-17.62	-29.50	72.53	15.00
74	TYR	CA	-16.89	-28.59	73.40	15.00
74	TYR	CB	-16.70	-27.22	72.75	15.00
74	TYR	CG	-16.35	-26.13	73.74	15.00
74	TYR	CD1	-15.09	-26.05	74.30	15.00
74	TYR	CE1	-14.77	-25.07	75.22	15.00
74	TYR	CD2	-17.30	-25.18	74.12	15.00
74	TYR	CE2	-17.00	-24.19	75.04	15.00
74	TYR	CZ	-15.73	-24.14	75.59	15.00
74	TYR	OH	-15.42	-23.15	76.51	15.00
74	TYR	C	-17.58	-28.38	74.73	15.00
74	TYR	O	-16.93	-28.39	75.78	15.00
75	VAL	N	-18.88	-28.12	74.67	15.00
75	VAL	CA	-19.68	-27.89	75.88	15.00
75	VAL	CB	-21.15	-27.58	75.52	15.00
75	VAL	CG1	-21.95	-27.27	76.78	15.00
75	VAL	CG2	-21.22	-26.39	74.55	15.00
75	VAL	C	-19.62	-29.10	76.80	15.00
75	VAL	O	-19.60	-28.96	78.03	15.00
76	GLN	N	-19.59	-30.29	76.21	15.00
76	GLN	CA	-19.51	-31.51	76.98	15.00
76	GLN	CB	-19.75	-32.69	76.05	15.00
76	GLN	CG	-19.79	-34.05	76.69	15.00
76	GLN	CD	-19.56	-35.13	75.66	15.00
76	GLN	OE1	-20.03	-35.04	74.53	15.00
76	GLN	NE2	-18.78	-36.13	76.03	15.00
76	GLN	C	-18.14	-31.60	77.64	15.00
76	GLN	O	-18.03	-31.59	78.86	15.00
77	LYS	N	-17.08	-31.61	76.84	15.00
77	LYS	CA	-15.72	-31.70	77.36	15.00
77	LYS	CB	-14.70	-31.55	76.22	15.00
77	LYS	CG	-13.27	-31.34	76.69	15.00
77	LYS	CD	-12.32	-31.10	75.51	15.00
77	LYS	CE	-10.89	-30.81	75.97	15.00
77	LYS	NZ	-10.30	-31.95	76.76	15.00
77	LYS	C	-15.45	-30.64	78.42	15.00
77	LYS	O	-14.81	-30.91	79.45	15.00
78	ASN	N	-15.92	-29.42	78.17	15.00
78	ASN	CA	-15.74	-28.29	79.06	15.00
78	ASN	CB	-15.98	-27.00	78.28	15.00

TABLE VI

78	ASN	CG	-15.69	-25.76	79.10	15.00
78	ASN	OD1	-14.58	-25.59	79.62	15.00
78	ASN	ND2	-16.67	-24.87	79.19	15.00
78	ASN	C	-16.68	-28.34	80.25	15.00
78	ASN	O	-16.42	-27.72	81.28	15.00
79	ARG	N	-17.79	-29.06	80.11	15.00
79	ARG	CA	-18.78	-29.18	81.16	15.00
79	ARG	CB	-18.14	-29.76	82.43	15.00
79	ARG	CG	-17.67	-31.20	82.26	15.00
79	ARG	CD	-16.65	-31.59	83.33	15.00
79	ARG	NE	-17.15	-31.38	84.68	15.00
79	ARG	CZ	-18.16	-32.06	85.22	15.00
79	ARG	NH1	-18.78	-33.03	84.55	15.00
79	ARG	NH2	-18.62	-31.70	86.43	15.00
79	ARG	C	-19.45	-27.84	81.45	15.00
79	ARG	O	-19.31	-27.30	82.55	15.00
80	GLY	N	-20.13	-27.28	80.45	15.00
80	GLY	CA	-20.82	-26.02	80.66	15.00
80	GLY	C	-20.62	-24.91	79.64	15.00
80	GLY	O	-19.56	-24.82	79.00	15.00
81	ILE	N	-21.64	-24.08	79.48	15.00
81	ILE	CA	-21.59	-22.95	78.57	15.00
81	ILE	CB	-22.30	-23.23	77.22	15.00
81	ILE	CG2	-23.77	-23.52	77.45	15.00
81	ILE	CG1	-22.10	-22.05	76.27	15.00
81	ILE	CD1	-22.84	-22.16	74.96	15.00
81	ILE	C	-22.24	-21.75	79.25	15.00
81	ILE	O	-23.28	-21.89	79.90	15.00
82	ASP	N	-21.61	-20.59	79.11	15.00
82	ASP	CA	-22.11	-19.37	79.71	15.00
82	ASP	CB	-21.03	-18.29	79.64	15.00
82	ASP	CG	-19.90	-18.53	80.58	15.00
82	ASP	OD1	-18.82	-17.98	80.34	15.00
82	ASP	OD2	-20.09	-19.26	81.58	15.00
82	ASP	C	-23.36	-18.81	79.09	15.00
82	ASP	O	-23.69	-19.07	77.93	15.00
83	SER	N	-24.07	-18.02	79.89	15.00
83	SER	CA	-25.27	-17.36	79.44	15.00
83	SER	CB	-26.09	-16.90	80.64	15.00
83	SER	OG	-25.27	-16.23	81.59	15.00
83	SER	C	-24.75	-16.15	78.66	15.00
83	SER	O	-23.57	-15.79	78.79	15.00

TABLE VI

84	GLU	N	-25.61	-15.54	77.86	15.00
84	GLU	CA	-25.25	-14.36	77.07	15.00
84	GLU	CB	-26.46	-13.84	76.31	15.00
84	GLU	CG	-26.17	-12.64	75.43	15.00
84	GLU	CD	-25.31	-12.99	74.24	15.00
84	GLU	OE1	-24.08	-12.98	74.38	15.00
84	GLU	OE2	-25.87	-13.29	73.17	15.00
84	GLU	C	-24.70	-13.27	77.99	15.00
84	GLU	O	-23.53	-12.89	77.88	15.00
85	ASP	N	-25.51	-12.82	78.94	15.00
85	ASP	CA	-25.09	-11.79	79.87	15.00
85	ASP	CB	-26.13	-11.60	80.99	15.00
85	ASP	CG	-25.66	-10.63	82.08	15.00
85	ASP	OD1	-25.92	-10.88	83.29	15.00
85	ASP	OD2	-25.03	-9.60	81.73	15.00
85	ASP	C	-23.72	-12.09	80.49	15.00
85	ASP	O	-22.91	-11.18	80.65	15.00
86	ALA	N	-23.45	-13.34	80.81	15.00
86	ALA	CA	-22.18	-13.67	81.44	15.00
86	ALA	CB	-22.25	-15.05	82.03	15.00
86	ALA	C	-21.01	-13.56	80.47	15.00
86	ALA	O	-19.91	-13.17	80.86	15.00
87	TYR	N	-21.26	-13.89	79.21	15.00
87	TYR	CA	-20.23	-13.85	78.18	15.00
87	TYR	CB	-19.77	-15.27	77.87	15.00
87	TYR	CG	-18.42	-15.39	77.19	15.00
87	TYR	CD1	-17.96	-14.41	76.30	15.00
87	TYR	CE1	-16.74	-14.56	75.65	15.00
87	TYR	CD2	-17.62	-16.52	77.40	15.00
87	TYR	CE2	-16.40	-16.67	76.76	15.00
87	TYR	CZ	-15.96	-15.69	75.88	15.00
87	TYR	OH	-14.75	-15.83	75.25	15.00
87	TYR	C	-20.93	-13.23	76.97	15.00
87	TYR	O	-21.57	-13.94	76.19	15.00
88	PRO	N	-20.90	-11.90	76.86	15.00
88	PRO	CD	-20.42	-10.97	77.90	15.00
88	PRO	CA	-21.52	-11.15	75.78	15.00
88	PRO	CB	-21.33	-9.70	76.23	15.00
88	PRO	CG	-21.34	-9.81	77.71	15.00
88	PRO	C	-20.91	-11.38	74.39	15.00
88	PRO	O	-19.74	-11.74	74.25	15.00
89	TYR	N	-21.73	-11.12	73.38	15.00

TABLE VI

89	TYR	CA	-21.35	-11.29	71.99	15.00
89	TYR	CB	-22.56	-11.78	71.18	15.00
89	TYR	CG	-22.24	-12.15	69.76	15.00
89	TYR	CD1	-21.38	-13.20	69.47	15.00
89	TYR	CE1	-21.06	-13.53	68.17	15.00
89	TYR	CD2	-22.78	-11.44	68.70	15.00
89	TYR	CE2	-22.47	-11.76	67.39	15.00
89	TYR	CZ	-21.61	-12.79	67.13	15.00
89	TYR	OH	-21.27	-13.08	65.83	15.00
89	TYR	C	-20.85	-9.95	71.48	15.00
89	TYR	O	-21.52	-8.92	71.64	15.00
90	VAL	N	-19.65	-9.94	70.91	15.00
90	VAL	CA	-19.07	-8.71	70.39	15.00
90	VAL	CB	-17.75	-8.36	71.12	15.00
90	VAL	CG1	-17.97	-8.36	72.62	15.00
90	VAL	CG2	-16.65	-9.33	70.74	15.00
90	VAL	C	-18.88	-8.78	68.87	15.00
90	VAL	O	-18.54	-7.78	68.23	15.00
91	GLY	N	-19.08	-9.96	68.30	15.00
91	GLY	CA	-18.95	-10.12	66.86	15.00
91	GLY	C	-17.55	-10.23	66.27	15.00
91	GLY	O	-17.34	-9.87	65.12	15.00
92	GLN	N	-16.61	-10.80	67.01	15.00
92	GLN	CA	-15.24	-10.95	66.50	15.00
92	GLN	CB	-14.56	-9.58	66.41	15.00
92	GLN	CG	-14.68	-8.72	67.67	15.00
92	GLN	CD	-13.59	-7.67	67.79	15.00
92	GLN	OE1	-12.77	-7.72	68.72	15.00
92	GLN	NE2	-13.56	-6.72	66.85	15.00
92	GLN	C	-14.45	-11.86	67.43	15.00
92	GLN	O	-14.78	-11.97	68.62	15.00
93	GLU	N	-13.43	-12.52	66.89	15.00
93	GLU	CA	-12.64	-13.42	67.71	15.00
93	GLU	CB	-11.68	-14.28	66.89	15.00
93	GLU	CG	-12.31	-15.10	65.78	15.00
93	GLU	CD	-11.63	-14.87	64.44	15.00
93	GLU	OE1	-11.94	-15.61	63.48	15.00
93	GLU	OE2	-10.78	-13.94	64.33	15.00
93	GLU	C	-11.84	-12.62	68.71	15.00
93	GLU	O	-11.41	-11.49	68.44	15.00
94	GLU	N	-11.61	-13.26	69.85	15.00
94	GLU	CA	-10.88	-12.70	70.98	15.00

TABLE VI

94	GLU	CB	-11.81	-11.81	71.79	15.00
94	GLU	CG	-13.19	-12.42	71.93	15.00
94	GLU	CD	-14.06	-11.70	72.92	15.00
94	GLU	OE1	-13.99	-10.45	72.96	15.00
94	GLU	OE2	-14.83	-12.38	73.64	15.00
94	GLU	C	-10.52	-13.92	71.80	15.00
94	GLU	O	-10.89	-15.02	71.45	15.00
95	SER	N	-9.81	-13.73	72.91	15.00
95	SER	CA	-9.43	-14.85	73.75	15.00
95	SER	CB	-8.32	-14.42	74.71	15.00
95	SER	OG	-7.20	-13.94	73.98	15.00
95	SER	C	-10.62	-15.42	74.52	15.00
95	SER	O	-11.48	-14.67	75.02	15.00
96	CYS	N	-10.69	-16.75	74.57	15.00
96	CYS	CA	-11.76	-17.45	75.28	15.00
96	CYS	C	-11.74	-16.96	76.71	15.00
96	CYS	O	-10.73	-17.09	77.42	15.00
96	CYS	CB	-11.53	-18.97	75.20	15.00
96	CYS	SG	-12.62	-20.03	76.22	15.00
97	MET	N	-12.85	-16.38	77.14	15.00
97	MET	CA	-12.96	-15.85	78.49	15.00
97	MET	CB	-13.32	-14.36	78.39	15.00
97	MET	CG	-12.29	-13.51	77.69	15.00
97	MET	SD	-13.01	-11.98	77.03	15.00
97	MET	CE	-14.07	-11.44	78.40	15.00
97	MET	C	-14.03	-16.60	79.28	15.00
97	MET	O	-14.87	-15.99	79.96	15.00
98	TYR	N	-13.98	-17.93	79.21	15.00
98	TYR	CA	-14.96	-18.74	79.91	15.00
98	TYR	CB	-14.69	-20.23	79.71	15.00
98	TYR	CG	-15.74	-21.10	80.34	15.00
98	TYR	CD1	-17.08	-20.99	79.97	15.00
98	TYR	CE1	-18.07	-21.74	80.59	15.00
98	TYR	CD2	-15.41	-22.00	81.36	15.00
98	TYR	CE2	-16.40	-22.76	81.98	15.00
98	TYR	CZ	-17.72	-22.62	81.60	15.00
98	TYR	OH	-18.70	-23.34	82.23	15.00
98	TYR	C	-15.03	-18.43	81.39	15.00
98	TYR	O	-14.01	-18.38	82.08	15.00
99	ASN	N	-16.25	-18.27	81.88	15.00
99	ASN	CA	-16.49	-17.97	83.28	15.00
99	ASN	CB	-17.29	-16.66	83.38	15.00

TABLE VI

99	ASN	CG	-17.66	-16.33	84.80	15.00
99	ASN	OD1	-16.88	-16.57	85.74	15.00
99	ASN	ND2	-18.85	-15.79	84.99	15.00
99	ASN	C	-17.28	-19.10	83.92	15.00
99	ASN	O	-18.51	-19.16	83.78	15.00
100	PRO	N	-16.60	-19.99	84.67	15.00
100	PRO	CD	-15.22	-19.88	85.16	15.00
100	PRO	CA	-17.29	-21.11	85.32	15.00
100	PRO	CB	-16.20	-21.72	86.20	15.00
100	PRO	CG	-15.31	-20.55	86.51	15.00
100	PRO	C	-18.45	-20.63	86.16	15.00
100	PRO	O	-19.51	-21.24	86.15	15.00
101	THR	N	-18.28	-19.50	86.84	15.00
101	THR	CA	-19.33	-18.95	87.68	15.00
101	THR	CB	-18.86	-17.68	88.45	15.00
101	THR	OG1	-18.71	-16.57	87.55	15.00
101	THR	CG2	-17.51	-17.93	89.13	15.00
101	THR	C	-20.55	-18.59	86.82	15.00
101	THR	O	-21.68	-18.56	87.32	15.00
102	GLY	N	-20.32	-18.34	85.54	15.00
102	GLY	CA	-21.40	-17.98	84.64	15.00
102	GLY	C	-22.06	-19.12	83.88	15.00
102	GLY	O	-22.92	-18.86	83.03	15.00
103	LYS	N	-21.65	-20.36	84.12	15.00
103	LYS	CA	-22.24	-21.50	83.42	15.00
103	LYS	CB	-21.72	-22.83	83.98	15.00
103	LYS	CG	-22.32	-24.05	83.29	15.00
103	LYS	CD	-22.10	-25.33	84.06	15.00
103	LYS	CE	-22.96	-25.41	85.35	15.00
103	LYS	NZ	-24.41	-25.79	85.14	15.00
103	LYS	C	-23.75	-21.49	83.57	15.00
103	LYS	O	-24.26	-21.26	84.67	15.00
104	ALA	N	-24.47	-21.73	82.48	15.00
104	ALA	CA	-25.93	-21.75	82.53	15.00
104	ALA	CB	-26.51	-20.51	81.87	15.00
104	ALA	C	-26.52	-22.99	81.89	15.00
104	ALA	O	-27.73	-23.15	81.87	15.00
105	ALA	N	-25.66	-23.87	81.38	15.00
105	ALA	CA	-26.11	-25.10	80.75	15.00
105	ALA	CB	-26.84	-24.78	79.44	15.00
105	ALA	C	-24.95	-26.03	80.46	15.00
105	ALA	O	-23.79	-25.67	80.62	15.00

TABLE VI

106	LYS	N	-25.28	-27.26	80.07	15.00
106	LYS	CA	-24.29	-28.25	79.70	15.00
106	LYS	CB	-23.55	-28.80	80.92	15.00
106	LYS	CG	-24.41	-29.35	82.04	15.00
106	LYS	CD	-23.54	-29.64	83.27	15.00
106	LYS	CE	-22.40	-30.62	82.95	15.00
106	LYS	NZ	-21.34	-30.67	84.03	15.00
106	LYS	C	-24.99	-29.36	78.93	15.00
106	LYS	O	-26.21	-29.30	78.75	15.00
107	CYS	N	-24.23	-30.30	78.39	15.00
107	CYS	CA	-24.82	-31.40	77.64	15.00
107	CYS	CB	-25.06	-30.99	76.19	15.00
107	CYS	SG	-23.58	-30.95	75.18	15.00
107	CYS	C	-23.91	-32.61	77.68	15.00
107	CYS	O	-22.75	-32.49	78.06	15.00
108	ARG	N	-24.43	-33.77	77.32	15.00
108	ARG	CA	-23.64	-35.00	77.33	15.00
108	ARG	CB	-24.12	-35.97	78.42	15.00
108	ARG	CG	-25.63	-36.03	78.64	15.00
108	ARG	CD	-26.27	-37.28	78.04	15.00
108	ARG	NE	-27.73	-37.21	78.14	15.00
108	ARG	CZ	-28.57	-38.06	77.54	15.00
108	ARG	NH1	-28.09	-39.05	76.80	15.00
108	ARG	NH2	-29.88	-37.94	77.72	15.00
108	ARG	C	-23.55	-35.70	75.97	15.00
108	ARG	O	-23.77	-36.91	75.85	15.00
109	GLY	N	-23.19	-34.93	74.94	15.00
109	GLY	CA	-23.06	-35.50	73.61	15.00
109	GLY	C	-24.08	-34.95	72.65	15.00
109	GLY	O	-24.81	-34.01	72.97	15.00
110	TYR	N	-24.16	-35.57	71.48	15.00
110	TYR	CA	-25.07	-35.16	70.42	15.00
110	TYR	CB	-24.41	-34.09	69.55	15.00
110	TYR	CG	-23.10	-34.53	68.92	15.00
110	TYR	CD1	-21.91	-34.49	69.64	15.00
110	TYR	CE1	-20.71	-34.90	69.08	15.00
110	TYR	CD2	-23.06	-34.99	67.62	15.00
110	TYR	CE2	-21.87	-35.41	67.04	15.00
110	TYR	CZ	-20.70	-35.35	67.77	15.00
110	TYR	OH	-19.52	-35.75	67.18	15.00
110	TYR	C	-25.39	-36.37	69.57	15.00
110	TYR	O	-24.80	-37.44	69.77	15.00

TABLE VI

111	ARG	N	-26.29	-36.20	68.61	15.00
111	ARG	CA	-26.69	-37.28	67.73	15.00
111	ARG	CB	-27.96	-37.95	68.26	15.00
111	ARG	CG	-27.84	-38.48	69.67	15.00
111	ARG	CD	-29.18	-39.01	70.20	15.00
111	ARG	NE	-29.77	-40.08	69.39	15.00
111	ARG	CZ	-29.16	-41.20	69.02	15.00
111	ARG	NH1	-29.81	-42.09	68.27	15.00
111	ARG	NH2	-27.91	-41.45	69.40	15.00
111	ARG	C	-26.98	-36.73	66.35	15.00
111	ARG	O	-27.99	-36.05	66.17	15.00
112	GLU	N	-26.10	-36.96	65.39	15.00
112	GLU	CA	-26.32	-36.48	64.03	15.00
112	GLU	CB	-25.09	-36.71	63.15	15.00
112	GLU	CG	-23.91	-35.81	63.46	15.00
112	GLU	CD	-23.40	-35.09	62.22	15.00
112	GLU	OE1	-24.13	-34.21	61.69	15.00
112	GLU	OE2	-22.27	-35.41	61.77	15.00
112	GLU	C	-27.50	-37.23	63.45	15.00
112	GLU	O	-27.70	-38.41	63.76	15.00
113	ILE	N	-28.29	-36.55	62.64	15.00
113	ILE	CA	-29.46	-37.15	62.02	15.00
113	ILE	CB	-30.51	-36.04	61.71	15.00
113	ILE	CG2	-31.75	-36.60	61.05	15.00
113	ILE	CG1	-30.92	-35.38	63.02	15.00
113	ILE	CD1	-31.95	-34.32	62.87	15.00
113	ILE	C	-28.95	-37.84	60.75	15.00
113	ILE	O	-27.93	-37.44	60.20	15.00
114	PRO	N	-29.60	-38.95	60.34	15.00
114	PRO	CD	-30.69	-39.67	61.02	15.00
114	PRO	CA	-29.17	-39.68	59.14	15.00
114	PRO	CB	-30.28	-40.72	58.97	15.00
114	PRO	CG	-30.62	-41.05	60.38	15.00
114	PRO	C	-29.04	-38.79	57.93	15.00
114	PRO	O	-30.00	-38.17	57.47	15.00
115	GLU	N	-27.82	-38.75	57.41	15.00
115	GLU	CA	-27.50	-37.92	56.26	15.00
115	GLU	CB	-26.12	-38.30	55.74	15.00
115	GLU	CG	-25.58	-37.36	54.68	15.00
115	GLU	CD	-24.19	-37.76	54.22	15.00
115	GLU	OE1	-23.20	-37.34	54.86	15.00
115	GLU	OE2	-24.10	-38.51	53.22	15.00

TABLE VI

115	GLU	C	-28.52	-38.00	55.14	15.00
115	GLU	O	-28.72	-39.05	54.56	15.00
116	GLY	N	-29.21	-36.89	54.90	15.00
116	GLY	CA	-30.18	-36.81	53.83	15.00
116	GLY	C	-31.55	-37.41	54.07	15.00
116	GLY	O	-32.34	-37.53	53.14	15.00
117	ASN	N	-31.86	-37.73	55.32	15.00
117	ASN	CA	-33.15	-38.34	55.65	15.00
117	ASN	CB	-32.91	-39.54	56.56	15.00
117	ASN	CG	-34.17	-40.32	56.84	15.00
117	ASN	OD1	-35.26	-39.75	56.98	15.00
117	ASN	ND2	-34.04	-41.64	56.94	15.00
117	ASN	C	-34.11	-37.34	56.30	15.00
117	ASN	O	-34.16	-37.23	57.52	15.00
118	GLU	N	-34.90	-36.66	55.48	15.00
118	GLU	CA	-35.85	-35.67	55.98	15.00
118	GLU	CB	-36.67	-35.08	54.85	15.00
118	GLU	CG	-35.91	-34.08	54.01	15.00
118	GLU	CD	-36.80	-32.98	53.50	15.00
118	GLU	OE1	-37.51	-32.38	54.32	15.00
118	GLU	OE2	-36.79	-32.73	52.29	15.00
118	GLU	C	-36.80	-36.20	57.04	15.00
118	GLU	O	-37.05	-35.54	58.04	15.00
119	LYS	N	-37.34	-37.38	56.81	15.00
119	LYS	CA	-38.28	-37.95	57.77	15.00
119	LYS	CB	-38.87	-39.24	57.21	15.00
119	LYS	CG	-39.46	-39.06	55.80	15.00
119	LYS	CD	-40.57	-38.01	55.77	15.00
119	LYS	CE	-41.82	-38.49	56.49	15.00
119	LYS	NZ	-42.97	-37.55	56.32	15.00
119	LYS	C	-37.66	-38.15	59.15	15.00
119	LYS	O	-38.29	-37.87	60.16	15.00
120	ALA	N	-36.39	-38.56	59.19	15.00
120	ALA	CA	-35.73	-38.76	60.48	15.00
120	ALA	CB	-34.39	-39.43	60.30	15.00
120	ALA	C	-35.56	-37.41	61.15	15.00
120	ALA	O	-35.40	-37.34	62.37	15.00
121	LEU	N	-35.58	-36.35	60.34	15.00
121	LEU	CA	-35.45	-34.99	60.83	15.00
121	LEU	CB	-35.03	-34.03	59.71	15.00
121	LEU	CG	-34.92	-32.51	59.96	15.00
121	LEU	CD1	-33.98	-32.21	61.11	15.00

TABLE VI

121	LEU	CD2	-34.45	-31.82	58.71	15.00
121	LEU	C	-36.78	-34.54	61.43	15.00
121	LEU	O	-36.80	-33.96	62.51	15.00
122	LYS	N	-37.89	-34.84	60.76	15.00
122	LYS	CA	-39.20	-34.44	61.28	15.00
122	LYS	CB	-40.34	-34.86	60.35	15.00
122	LYS	CG	-41.71	-34.49	60.95	15.00
122	LYS	CD	-42.90	-34.72	60.02	15.00
122	LYS	CE	-43.21	-36.19	59.84	15.00
122	LYS	NZ	-42.13	-36.87	59.07	15.00
122	LYS	C	-39.43	-35.03	62.67	15.00
122	LYS	O	-40.00	-34.38	63.54	15.00
123	ARG	N	-39.02	-36.28	62.85	15.00
123	ARG	CA	-39.18	-36.96	64.12	15.00
123	ARG	CB	-38.90	-38.45	63.95	15.00
123	ARG	CG	-40.04	-39.22	63.30	15.00
123	ARG	CD	-39.53	-40.52	62.67	15.00
123	ARG	NE	-38.42	-41.08	63.44	15.00
123	ARG	CZ	-37.46	-41.85	62.92	15.00
123	ARG	NH1	-37.47	-42.16	61.62	15.00
123	ARG	NH2	-36.45	-42.23	63.68	15.00
123	ARG	C	-38.24	-36.34	65.14	15.00
123	ARG	O	-38.65	-36.04	66.25	15.00
124	ALA	N	-36.99	-36.12	64.76	15.00
124	ALA	CA	-36.05	-35.51	65.68	15.00
124	ALA	CB	-34.70	-35.31	65.02	15.00
124	ALA	C	-36.60	-34.17	66.19	15.00
124	ALA	O	-36.55	-33.91	67.39	15.00
125	VAL	N	-37.14	-33.34	65.30	15.00
125	VAL	CA	-37.68	-32.06	65.76	15.00
125	VAL	CB	-38.01	-31.03	64.60	15.00
125	VAL	CG1	-36.78	-30.27	64.19	15.00
125	VAL	CG2	-38.58	-31.72	63.39	15.00
125	VAL	C	-38.94	-32.28	66.58	15.00
125	VAL	O	-39.21	-31.52	67.50	15.00
126	ALA	N	-39.69	-33.32	66.27	15.00
126	ALA	CA	-40.93	-33.60	66.98	15.00
126	ALA	CB	-41.81	-34.52	66.16	15.00
126	ALA	C	-40.75	-34.16	68.38	15.00
126	ALA	O	-41.53	-33.84	69.28	15.00
127	ARG	N	-39.73	-35.00	68.55	15.00
127	ARG	CA	-39.42	-35.68	69.81	15.00

TABLE VI

127	ARG	CB	-39.04	-37.14	69.54	15.00
127	ARG	CG	-40.20	-37.95	69.00	15.00
127	ARG	CD	-39.78	-39.23	68.27	15.00
127	ARG	NE	-40.95	-39.80	67.60	15.00
127	ARG	CZ	-40.95	-40.88	66.83	15.00
127	ARG	NH1	-42.09	-41.30	66.28	15.00
127	ARG	NH2	-39.84	-41.56	66.63	15.00
127	ARG	C	-38.33	-35.04	70.66	15.00
127	ARG	O	-38.25	-35.30	71.86	15.00
128	VAL	N	-37.48	-34.22	70.04	15.00
128	VAL	CA	-36.40	-33.54	70.75	15.00
128	VAL	CB	-35.03	-33.81	70.10	15.00
128	VAL	CG1	-33.92	-33.34	71.02	15.00
128	VAL	CG2	-34.87	-35.29	69.78	15.00
128	VAL	C	-36.58	-32.02	70.88	15.00
128	VAL	O	-36.43	-31.46	71.95	15.00
129	GLY	N	-36.89	-31.35	69.77	15.00
129	GLY	CA	-37.08	-29.91	69.81	15.00
129	GLY	C	-36.26	-29.29	68.69	15.00
129	GLY	O	-36.02	-29.96	67.68	15.00
130	PRO	N	-35.83	-28.02	68.81	15.00
130	PRO	CD	-36.20	-27.06	69.86	15.00
130	PRO	CA	-35.04	-27.37	67.77	15.00
130	PRO	CB	-34.67	-26.05	68.43	15.00
130	PRO	CG	-35.92	-25.74	69.18	15.00
130	PRO	C	-33.81	-28.17	67.39	15.00
130	PRO	O	-33.07	-28.64	68.26	15.00
131	VAL	N	-33.60	-28.33	66.09	15.00
131	VAL	CA	-32.46	-29.08	65.58	15.00
131	VAL	CB	-32.94	-30.26	64.68	15.00
131	VAL	CG1	-31.76	-31.03	64.14	15.00
131	VAL	CG2	-33.82	-31.20	65.46	15.00
131	VAL	C	-31.50	-28.20	64.77	15.00
131	VAL	O	-31.93	-27.35	63.99	15.00
132	SER	N	-30.20	-28.39	64.96	15.00
132	SER	CA	-29.23	-27.61	64.22	15.00
132	SER	CB	-27.88	-27.61	64.94	15.00
132	SER	OG	-28.00	-26.96	66.20	15.00
132	SER	C	-29.08	-28.21	62.82	15.00
132	SER	O	-28.83	-29.41	62.68	15.00
133	VAL	N	-29.31	-27.39	61.80	15.00
133	VAL	CA	-29.22	-27.82	60.40	15.00

TABLE VI

133	VAL	CB	-30.60	-27.81	59.68	15.00
133	VAL	CG1	-31.51	-28.90	60.23	15.00
133	VAL	CG2	-31.27	-26.45	59.80	15.00
133	VAL	C	-28.26	-26.93	59.62	15.00
133	VAL	O	-27.88	-25.85	60.08	15.00
134	ALA	N	-27.93	-27.36	58.41	15.00
134	ALA	CA	-27.02	-26.64	57.54	15.00
134	ALA	CB	-25.69	-27.35	57.48	15.00
134	ALA	C	-27.64	-26.61	56.16	15.00
134	ALA	O	-27.92	-27.66	55.60	15.00
135	ILE	N	-27.84	-25.43	55.60	15.00
135	ILE	CA	-28.45	-25.31	54.28	15.00
135	ILE	CB	-29.84	-24.62	54.36	15.00
135	ILE	CG2	-30.82	-25.47	55.15	15.00
135	ILE	CG1	-29.70	-23.24	55.00	15.00
135	ILE	CD1	-30.95	-22.42	54.97	15.00
135	ILE	C	-27.59	-24.49	53.32	15.00
135	ILE	O	-26.49	-24.04	53.66	15.00
136	ASP	N	-28.09	-24.33	52.10	15.00
136	ASP	CA	-27.45	-23.52	51.07	15.00
136	ASP	CB	-27.50	-24.23	49.72	15.00
136	ASP	CG	-27.09	-23.32	48.57	15.00
136	ASP	OD1	-27.71	-23.40	47.49	15.00
136	ASP	OD2	-26.15	-22.50	48.73	15.00
136	ASP	C	-28.22	-22.21	50.99	15.00
136	ASP	O	-29.36	-22.17	50.52	15.00
137	ALA	N	-27.61	-21.13	51.46	15.00
137	ALA	CA	-28.26	-19.83	51.42	15.00
137	ALA	CB	-28.42	-19.30	52.83	15.00
137	ALA	C	-27.46	-18.84	50.56	15.00
137	ALA	O	-27.34	-17.66	50.89	15.00
138	SER	N	-26.92	-19.34	49.45	15.00
138	SER	CA	-26.12	-18.53	48.53	15.00
138	SER	CB	-25.09	-19.42	47.83	15.00
138	SER	OG	-25.71	-20.52	47.19	15.00
138	SER	C	-26.97	-17.80	47.49	15.00
138	SER	O	-26.60	-16.72	47.01	15.00
139	LEU	N	-28.12	-18.36	47.17	15.00
139	LEU	CA	-29.02	-17.79	46.19	15.00
139	LEU	CB	-30.07	-18.84	45.80	15.00
139	LEU	CG	-29.49	-20.25	45.62	15.00
139	LEU	CD1	-30.58	-21.21	45.21	15.00

TABLE VI

139	LEU	CD2	-28.37	-20.28	44.61	15.00
139	LEU	C	-29.70	-16.52	46.70	15.00
139	LEU	O	-30.06	-16.43	47.88	15.00
140	THR	N	-29.90	-15.54	45.81	15.00
140	THR	CA	-30.54	-14.29	46.18	15.00
140	THR	CB	-30.46	-13.21	45.07	15.00
140	THR	OG1	-30.85	-13.77	43.82	15.00
140	THR	CG2	-29.05	-12.66	44.96	15.00
140	THR	C	-32.00	-14.49	46.57	15.00
140	THR	O	-32.50	-13.79	47.45	15.00
141	SER	N	-32.68	-15.45	45.95	15.00
141	SER	CA	-34.08	-15.70	46.30	15.00
141	SER	CB	-34.66	-16.86	45.50	15.00
141	SER	OG	-33.72	-17.92	45.39	15.00
141	SER	C	-34.19	-15.94	47.79	15.00
141	SER	O	-35.04	-15.37	48.46	15.00
142	PHE	N	-33.27	-16.72	48.33	15.00
142	PHE	CA	-33.28	-17.01	49.76	15.00
142	PHE	CB	-32.21	-18.05	50.11	15.00
142	PHE	CG	-32.17	-18.41	51.57	15.00
142	PHE	CD1	-32.97	-19.43	52.08	15.00
142	PHE	CD2	-31.34	-17.72	52.45	15.00
142	PHE	CE1	-32.94	-19.75	53.43	15.00
142	PHE	CE2	-31.31	-18.04	53.80	15.00
142	PHE	CZ	-32.11	-19.05	54.29	15.00
142	PHE	C	-33.01	-15.75	50.54	15.00
142	PHE	O	-33.69	-15.45	51.52	15.00
143	GLN	N	-32.01	-15.00	50.09	15.00
143	GLN	CA	-31.61	-13.79	50.78	15.00
143	GLN	CB	-30.30	-13.26	50.21	15.00
143	GLN	CG	-29.18	-14.29	50.23	15.00
143	GLN	CD	-27.85	-13.72	49.81	15.00
143	GLN	OE1	-27.29	-12.84	50.48	15.00
143	GLN	NE2	-27.31	-14.22	48.70	15.00
143	GLN	C	-32.67	-12.70	50.84	15.00
143	GLN	O	-32.79	-12.04	51.86	15.00
144	PHE	N	-33.45	-12.51	49.78	15.00
144	PHE	CA	-34.50	-11.48	49.83	15.00
144	PHE	CB	-34.57	-10.60	48.55	15.00
144	PHE	CG	-34.78	-11.35	47.27	15.00
144	PHE	CD1	-33.92	-11.14	46.19	15.00
144	PHE	CD2	-35.84	-12.24	47.12	15.00

TABLE VI

144	PHE	CE1	-34.11	-11.81	44.99	15.00
144	PHE	CE2	-36.04	-12.92	45.91	15.00
144	PHE	CZ	-35.18	-12.71	44.85	15.00
144	PHE	C	-35.88	-12.04	50.20	15.00
144	PHE	O	-36.90	-11.36	50.02	15.00
145	TYR	N	-35.89	-13.28	50.71	15.00
145	TYR	CA	-37.12	-13.95	51.12	15.00
145	TYR	CB	-36.80	-15.21	51.94	15.00
145	TYR	CG	-37.98	-15.77	52.70	15.00
145	TYR	CD1	-38.84	-16.69	52.12	15.00
145	TYR	CE1	-39.96	-17.15	52.80	15.00
145	TYR	CD2	-38.27	-15.32	53.99	15.00
145	TYR	CE2	-39.40	-15.78	54.67	15.00
145	TYR	CZ	-40.24	-16.69	54.07	15.00
145	TYR	OH	-41.38	-17.11	54.73	15.00
145	TYR	C	-37.90	-12.98	51.97	15.00
145	TYR	O	-37.32	-12.24	52.74	15.00
146	SER	N	-39.21	-13.02	51.84	15.00
146	SER	CA	-40.07	-12.13	52.59	15.00
146	SER	CB	-40.63	-11.07	51.63	15.00
146	SER	OG	-41.38	-10.08	52.30	15.00
146	SER	C	-41.21	-12.89	53.24	15.00
146	SER	O	-41.48	-12.72	54.43	15.00
147	LYS	N	-41.86	-13.77	52.48	15.00
147	LYS	CA	-42.98	-14.54	53.01	15.00
147	LYS	CB	-44.25	-13.71	53.04	15.00
147	LYS	CG	-44.62	-13.11	51.70	15.00
147	LYS	CD	-46.07	-12.67	51.68	15.00
147	LYS	CE	-46.47	-12.13	50.31	15.00
147	LYS	NZ	-47.97	-12.11	50.14	15.00
147	LYS	C	-43.21	-15.79	52.19	15.00
147	LYS	O	-42.55	-16.01	51.17	15.00
148	GLY	N	-44.16	-16.61	52.64	15.00
148	GLY	CA	-44.49	-17.85	51.95	15.00
148	GLY	C	-43.47	-18.95	52.16	15.00
148	GLY	O	-42.52	-18.79	52.93	15.00
149	VAL	N	-43.64	-20.04	51.43	15.00
149	VAL	CA	-42.75	-21.19	51.52	15.00
149	VAL	CB	-43.57	-22.51	51.47	15.00
149	VAL	CG1	-42.66	-23.71	51.33	15.00
149	VAL	CG2	-44.41	-22.65	52.72	15.00
149	VAL	C	-41.67	-21.17	50.43	15.00

TABLE VI

149	VAL	O	-41.96	-21.34	49.24	15.00
150	TYR	N	-40.43	-20.96	50.84	15.00
150	TYR	CA	-39.30	-20.91	49.91	15.00
150	TYR	CB	-38.04	-20.41	50.64	15.00
150	TYR	CG	-36.82	-20.29	49.75	15.00
150	TYR	CD1	-36.78	-19.38	48.69	15.00
150	TYR	CE1	-35.67	-19.27	47.88	15.00
150	TYR	CD2	-35.69	-21.07	49.97	15.00
150	TYR	CE2	-34.56	-20.96	49.16	15.00
150	TYR	CZ	-34.56	-20.06	48.11	15.00
150	TYR	OH	-33.45	-19.93	47.32	15.00
150	TYR	C	-39.03	-22.26	49.27	15.00
150	TYR	O	-39.23	-23.31	49.88	15.00
151	TYR	N	-38.55	-22.22	48.03	15.00
151	TYR	CA	-38.21	-23.42	47.28	15.00
151	TYR	CB	-39.45	-24.26	46.99	15.00
151	TYR	CG	-39.15	-25.46	46.11	15.00
151	TYR	CD1	-38.22	-26.42	46.51	15.00
151	TYR	CE1	-37.94	-27.53	45.71	15.00
151	TYR	CD2	-39.79	-25.63	44.89	15.00
151	TYR	CE2	-39.52	-26.74	44.08	15.00
151	TYR	CZ	-38.59	-27.69	44.50	15.00
151	TYR	OH	-38.36	-28.83	43.75	15.00
151	TYR	C	-37.60	-23.00	45.97	15.00
151	TYR	O	-38.29	-22.44	45.11	15.00
152	ASP	N	-36.31	-23.25	45.80	15.00
152	ASP	CA	-35.66	-22.90	44.55	15.00
152	ASP	CB	-34.74	-21.69	44.71	15.00
152	ASP	CG	-34.02	-21.34	43.43	15.00
152	ASP	OD1	-34.60	-21.55	42.34	15.00
152	ASP	OD2	-32.87	-20.86	43.49	15.00
152	ASP	C	-34.87	-24.07	44.02	15.00
152	ASP	O	-33.84	-24.43	44.56	15.00
153	GLU	N	-35.33	-24.60	42.90	15.00
153	GLU	CA	-34.70	-25.74	42.26	15.00
153	GLU	CB	-35.49	-26.18	41.03	15.00
153	GLU	CG	-35.79	-25.08	40.01	15.00
153	GLU	CD	-37.17	-24.43	40.19	15.00
153	GLU	OE1	-38.12	-24.84	39.48	15.00
153	GLU	OE2	-37.29	-23.50	41.02	15.00
153	GLU	C	-33.22	-25.56	41.91	15.00
153	GLU	O	-32.59	-26.50	41.44	15.00

TABLE VI

154	SER	N	-32.66	-24.37	42.12	15.00
154	SER	CA	-31.24	-24.12	41.82	15.00
154	SER	CB	-31.02	-22.70	41.29	15.00
154	SER	OG	-32.05	-22.32	40.40	15.00
154	SER	C	-30.40	-24.30	43.08	15.00
154	SER	O	-29.17	-24.21	43.04	15.00
155	CYS	N	-31.08	-24.48	44.22	15.00
155	CYS	CA	-30.41	-24.66	45.49	15.00
155	CYS	C	-29.57	-25.91	45.40	15.00
155	CYS	O	-30.00	-26.91	44.82	15.00
155	CYS	CB	-31.44	-24.79	46.62	15.00
155	CYS	SG	-30.90	-24.05	48.19	15.00
156	ASN	N	-28.36	-25.87	45.94	15.00
156	ASN	CA	-27.47	-27.01	45.87	15.00
156	ASN	CB	-26.18	-26.59	45.19	15.00
156	ASN	CG	-25.28	-27.76	44.91	15.00
156	ASN	OD1	-25.73	-28.91	44.88	15.00
156	ASN	ND2	-23.99	-27.49	44.73	15.00
156	ASN	C	-27.20	-27.67	47.23	15.00
156	ASN	O	-26.43	-27.16	48.05	15.00
157	SER	N	-27.79	-28.85	47.41	15.00
157	SER	CA	-27.67	-29.64	48.62	15.00
157	SER	CB	-28.48	-30.92	48.45	15.00
157	SER	OG	-29.83	-30.63	48.13	15.00
157	SER	C	-26.24	-30.00	49.04	15.00
157	SER	O	-26.01	-30.36	50.19	15.00
158	ASP	N	-25.30	-29.93	48.10	15.00
158	ASP	CA	-23.89	-30.24	48.35	15.00
158	ASP	CB	-23.21	-30.69	47.07	15.00
158	ASP	CG	-23.72	-32.01	46.57	15.00
158	ASP	OD1	-24.95	-32.15	46.33	15.00
158	ASP	OD2	-22.86	-32.91	46.38	15.00
158	ASP	C	-23.14	-29.02	48.87	15.00
158	ASP	O	-22.11	-29.15	49.53	15.00
159	ASN	N	-23.62	-27.84	48.51	15.00
159	ASN	CA	-22.98	-26.62	48.94	15.00
159	ASN	CB	-23.10	-25.57	47.84	15.00
159	ASN	CG	-22.14	-24.40	48.03	15.00
159	ASN	OD1	-21.43	-24.30	49.04	15.00
159	ASN	ND2	-22.10	-23.51	47.04	15.00
159	ASN	C	-23.68	-26.14	50.20	15.00
159	ASN	O	-24.63	-25.37	50.12	15.00

TABLE VI

160	LEU	N	-23.25	-26.64	51.36	15.00
160	LEU	CA	-23.84	-26.23	52.63	15.00
160	LEU	CB	-23.88	-27.42	53.60	15.00
160	LEU	CG	-24.59	-28.72	53.22	15.00
160	LEU	CD1	-24.45	-29.70	54.37	15.00
160	LEU	CD2	-26.06	-28.49	52.89	15.00
160	LEU	C	-22.98	-25.11	53.22	15.00
160	LEU	O	-21.91	-25.35	53.78	15.00
161	ASN	N	-23.47	-23.89	53.16	15.00
161	ASN	CA	-22.70	-22.75	53.65	15.00
161	ASN	CB	-22.58	-21.73	52.53	15.00
161	ASN	CG	-23.89	-21.51	51.84	15.00
161	ASN	OD1	-24.74	-20.76	52.33	15.00
161	ASN	ND2	-24.10	-22.23	50.75	15.00
161	ASN	C	-23.23	-22.05	54.89	15.00
161	ASN	O	-22.45	-21.62	55.73	15.00
162	HIS	N	-24.54	-21.93	55.01	15.00
162	HIS	CA	-25.13	-21.27	56.16	15.00
162	HIS	CB	-26.18	-20.27	55.67	15.00
162	HIS	CG	-26.55	-19.22	56.67	15.00
162	HIS	CD2	-27.72	-18.61	56.93	15.00
162	HIS	ND1	-25.63	-18.66	57.53	15.00
162	HIS	CE1	-26.22	-17.74	58.27	15.00
162	HIS	NE2	-27.49	-17.69	57.93	15.00
162	HIS	C	-25.76	-22.27	57.12	15.00
162	HIS	O	-26.47	-23.19	56.69	15.00
163	ALA	N	-25.47	-22.12	58.41	15.00
163	ALA	CA	-26.01	-23.00	59.45	15.00
163	ALA	CB	-24.93	-23.33	60.47	15.00
163	ALA	C	-27.15	-22.28	60.13	15.00
163	ALA	O	-27.00	-21.13	60.54	15.00
164	VAL	N	-28.30	-22.94	60.24	15.00
164	VAL	CA	-29.48	-22.34	60.86	15.00
164	VAL	CB	-30.54	-21.99	59.79	15.00
164	VAL	CG1	-30.11	-20.79	58.99	15.00
164	VAL	CG2	-30.75	-23.16	58.86	15.00
164	VAL	C	-30.05	-23.28	61.91	15.00
164	VAL	O	-29.37	-24.21	62.33	15.00
165	LEU	N	-31.31	-23.07	62.30	15.00
165	LEU	CA	-31.97	-23.88	63.33	15.00
165	LEU	CB	-32.00	-23.11	64.64	15.00
165	LEU	CG	-32.59	-23.77	65.88	15.00

TABLE VI

165	LEU	CD1	-31.53	-24.65	66.49	15.00
165	LEU	CD2	-33.04	-22.71	66.87	15.00
165	LEU	C	-33.40	-24.17	62.94	15.00
165	LEU	O	-34.16	-23.24	62.72	15.00
166	ALA	N	-33.79	-25.44	62.92	15.00
166	ALA	CA	-35.15	-25.82	62.56	15.00
166	ALA	CB	-35.16	-27.19	61.92	15.00
166	ALA	C	-36.03	-25.80	63.80	15.00
166	ALA	O	-35.93	-26.66	64.66	15.00
167	VAL	N	-36.89	-24.80	63.88	15.00
167	VAL	CA	-37.79	-24.62	65.01	15.00
167	VAL	CB	-38.11	-23.11	65.18	15.00
167	VAL	CG1	-39.35	-22.88	66.00	15.00
167	VAL	CG2	-36.94	-22.42	65.84	15.00
167	VAL	C	-39.06	-25.46	64.92	15.00
167	VAL	O	-39.83	-25.56	65.87	15.00
168	GLY	N	-39.28	-26.10	63.78	15.00
168	GLY	CA	-40.48	-26.91	63.65	15.00
168	GLY	C	-40.77	-27.29	62.23	15.00
168	GLY	O	-39.85	-27.36	61.41	15.00
169	TYR	N	-42.04	-27.55	61.95	15.00
169	TYR	CA	-42.50	-27.93	60.62	15.00
169	TYR	CB	-42.09	-29.38	60.30	15.00
169	TYR	CG	-42.61	-30.41	61.28	15.00
169	TYR	CD1	-43.94	-30.82	61.25	15.00
169	TYR	CE1	-44.42	-31.76	62.13	15.00
169	TYR	CD2	-41.77	-30.98	62.23	15.00
169	TYR	CE2	-42.24	-31.93	63.13	15.00
169	TYR	CZ	-43.57	-32.31	63.07	15.00
169	TYR	OH	-44.04	-33.26	63.95	15.00
169	TYR	C	-44.02	-27.78	60.54	15.00
169	TYR	O	-44.70	-27.74	61.57	15.00
170	GLY	N	-44.55	-27.71	59.33	15.00
170	GLY	CA	-45.98	-27.55	59.16	15.00
170	GLY	C	-46.42	-27.49	57.72	15.00
170	GLY	O	-45.69	-27.89	56.82	15.00
171	ILE	N	-47.61	-26.95	57.49	15.00
171	ILE	CA	-48.20	-26.83	56.16	15.00
171	ILE	CB	-49.51	-27.69	56.06	15.00
171	ILE	CG2	-50.16	-27.55	54.70	15.00
171	ILE	CG1	-49.20	-29.18	56.27	15.00
171	ILE	CD1	-48.97	-29.59	57.73	15.00

TABLE VI

171	ILE	C	-48.55	-25.36	55.90	15.00
171	ILE	O	-48.58	-24.55	56.84	15.00
172	GLN	N	-48.73	-25.00	54.63	15.00
172	GLN	CA	-49.10	-23.64	54.25	15.00
172	GLN	CB	-47.90	-22.90	53.68	15.00
172	GLN	CG	-47.16	-22.04	54.69	15.00
172	GLN	CD	-47.81	-20.68	54.87	15.00
172	GLN	OE1	-47.24	-19.66	54.49	15.00
172	GLN	NE2	-49.00	-20.66	55.47	15.00
172	GLN	C	-50.24	-23.71	53.24	15.00
172	GLN	O	-51.31	-24.23	53.55	15.00
173	LYS	N	-50.05	-23.17	52.05	15.00
173	LYS	CA	-51.11	-23.24	51.05	15.00
173	LYS	CB	-51.04	-22.05	50.08	15.00
173	LYS	CG	-51.15	-20.70	50.77	15.00
173	LYS	CD	-50.94	-19.57	49.77	15.00
173	LYS	CE	-50.57	-18.27	50.50	15.00
173	LYS	NZ	-49.28	-18.39	51.26	15.00
173	LYS	C	-50.82	-24.55	50.34	15.00
173	LYS	O	-50.33	-24.58	49.21	15.00
174	GLY	N	-51.02	-25.63	51.08	15.00
174	GLY	CA	-50.77	-26.96	50.56	15.00
174	GLY	C	-49.30	-27.32	50.59	15.00
174	GLY	O	-48.95	-28.47	50.31	15.00
175	ASN	N	-48.44	-26.35	50.92	15.00
175	ASN	CA	-47.00	-26.60	50.98	15.00
175	ASN	CB	-46.20	-25.39	50.47	15.00
175	ASN	CG	-46.70	-24.86	49.14	15.00
175	ASN	OD1	-47.33	-23.79	49.08	15.00
175	ASN	ND2	-46.41	-25.58	48.06	15.00
175	ASN	C	-46.49	-26.95	52.38	15.00
175	ASN	O	-46.66	-26.16	53.33	15.00
176	LYS	N	-45.90	-28.13	52.53	15.00
176	LYS	CA	-45.33	-28.50	53.82	15.00
176	LYS	CB	-44.94	-29.98	53.84	15.00
176	LYS	CG	-46.10	-30.95	53.63	15.00
176	LYS	CD	-45.67	-32.36	53.98	15.00
176	LYS	CE	-46.71	-33.40	53.61	15.00
176	LYS	NZ	-46.36	-34.11	52.34	15.00
176	LYS	C	-44.08	-27.63	53.94	15.00
176	LYS	O	-43.52	-27.21	52.92	15.00
177	HIS	N	-43.62	-27.37	55.16	15.00

TABLE VI

177	HIS	CA	-42.44	-26.52	55.34	15.00
177	HIS	CB	-42.84	-25.05	55.23	15.00
177	HIS	CG	-43.71	-24.59	56.35	15.00
177	HIS	CD2	-43.41	-24.18	57.61	15.00
177	HIS	ND1	-45.09	-24.52	56.26	15.00
177	HIS	CE1	-45.59	-24.10	57.40	15.00
177	HIS	NE2	-44.59	-23.89	58.24	15.00
177	HIS	C	-41.74	-26.73	56.67	15.00
177	HIS	O	-42.32	-27.24	57.62	15.00
178	TRP	N	-40.49	-26.28	56.73	15.00
178	TRP	CA	-39.64	-26.34	57.91	15.00
178	TRP	CB	-38.24	-26.82	57.54	15.00
178	TRP	CG	-38.16	-28.22	57.08	15.00
178	TRP	CD2	-38.28	-29.41	57.88	15.00
178	TRP	CE2	-38.08	-30.51	57.03	15.00
178	TRP	CE3	-38.52	-29.64	59.24	15.00
178	TRP	CD1	-37.92	-28.65	55.81	15.00
178	TRP	NE1	-37.87	-30.02	55.77	15.00
178	TRP	CZ2	-38.13	-31.83	57.48	15.00
178	TRP	CZ3	-38.57	-30.95	59.70	15.00
178	TRP	CH2	-38.37	-32.03	58.83	15.00
178	TRP	C	-39.53	-24.91	58.39	15.00
178	TRP	O	-39.15	-24.04	57.61	15.00
179	ILE	N	-39.89	-24.63	59.63	15.00
179	ILE	CA	-39.79	-23.28	60.16	15.00
179	ILE	CB	-40.65	-23.09	61.42	15.00
179	ILE	CG2	-40.61	-21.64	61.85	15.00
179	ILE	CG1	-42.09	-23.52	61.15	15.00
179	ILE	CD1	-42.97	-23.45	62.38	15.00
179	ILE	C	-38.32	-23.04	60.52	15.00
179	ILE	O	-37.80	-23.66	61.45	15.00
180	ILE	N	-37.67	-22.16	59.78	15.00
180	ILE	CA	-36.27	-21.87	60.01	15.00
180	ILE	CB	-35.46	-22.00	58.70	15.00
180	ILE	CG2	-34.01	-21.64	58.91	15.00
180	ILE	CG1	-35.57	-23.42	58.16	15.00
180	ILE	CD1	-34.96	-24.46	59.08	15.00
180	ILE	C	-36.01	-20.52	60.69	15.00
180	ILE	O	-36.70	-19.53	60.44	15.00
181	LYS	N	-35.02	-20.53	61.58	15.00
181	LYS	CA	-34.60	-19.36	62.34	15.00
181	LYS	CB	-34.59	-19.69	63.84	15.00

TABLE VI

181	LYS	CG	-34.02	-18.59	64.70	15.00
181	LYS	CD	-33.87	-19.04	66.14	15.00
181	LYS	CE	-33.58	-17.85	67.01	15.00
181	LYS	NZ	-33.52	-18.17	68.45	15.00
181	LYS	C	-33.19	-19.02	61.91	15.00
181	LYS	O	-32.28	-19.85	62.04	15.00
182	ASN	N	-33.00	-17.82	61.37	15.00
182	ASN	CA	-31.68	-17.42	60.93	15.00
182	ASN	CB	-31.77	-16.80	59.54	15.00
182	ASN	CG	-30.45	-16.80	58.83	15.00
182	ASN	OD1	-29.40	-16.99	59.44	15.00
182	ASN	ND2	-30.48	-16.62	57.51	15.00
182	ASN	C	-31.10	-16.42	61.92	15.00
182	ASN	O	-31.81	-15.94	62.79	15.00
183	SER	N	-29.81	-16.14	61.82	15.00
183	SER	CA	-29.19	-15.20	62.74	15.00
183	SER	CB	-27.97	-15.85	63.38	15.00
183	SER	OG	-27.30	-16.66	62.44	15.00
183	SER	C	-28.79	-13.90	62.04	15.00
183	SER	O	-27.68	-13.40	62.23	15.00
184	TRP	N	-29.70	-13.34	61.25	15.00
184	TRP	CA	-29.44	-12.11	60.52	15.00
184	TRP	CB	-29.77	-12.29	59.03	15.00
184	TRP	CG	-28.79	-13.14	58.29	15.00
184	TRP	CD2	-28.97	-13.73	57.01	15.00
184	TRP	CE2	-27.80	-14.45	56.71	15.00
184	TRP	CE3	-30.01	-13.74	56.08	15.00
184	TRP	CD1	-27.55	-13.50	58.71	15.00
184	TRP	NE1	-26.94	-14.28	57.77	15.00
184	TRP	CZ2	-27.64	-15.17	55.52	15.00
184	TRP	CZ3	-29.85	-14.46	54.90	15.00
184	TRP	CH2	-28.67	-15.16	54.63	15.00
184	TRP	C	-30.23	-10.93	61.07	15.00
184	TRP	O	-30.32	-9.88	60.43	15.00
185	GLY	N	-30.78	-11.07	62.27	15.00
185	GLY	CA	-31.54	-9.98	62.83	15.00
185	GLY	C	-33.02	-10.16	62.62	15.00
185	GLY	O	-33.46	-11.00	61.84	15.00
186	GLU	N	-33.80	-9.35	63.33	15.00
186	GLU	CA	-35.26	-9.39	63.27	15.00
186	GLU	CB	-35.79	-8.71	64.53	15.00
186	GLU	CG	-37.29	-8.65	64.70	15.00

TABLE VI

186	GLU	CD	-37.71	-8.03	66.04	15.00
186	GLU	OE1	-36.83	-7.61	66.83	15.00
186	GLU	OE2	-38.93	-7.98	66.31	15.00
186	GLU	C	-35.73	-8.65	62.03	15.00
186	GLU	O	-36.89	-8.73	61.64	15.00
187	ASN	N	-34.78	-8.02	61.36	15.00
187	ASN	CA	-35.02	-7.21	60.18	15.00
187	ASN	CB	-34.03	-6.03	60.25	15.00
187	ASN	CG	-34.42	-4.86	59.37	15.00
187	ASN	OD1	-33.58	-4.33	58.64	15.00
187	ASN	ND2	-35.67	-4.40	59.48	15.00
187	ASN	C	-34.86	-7.97	58.86	15.00
187	ASN	O	-34.92	-7.36	57.80	15.00
188	TRP	N	-34.62	-9.28	58.92	15.00
188	TRP	CA	-34.47	-10.08	57.70	15.00
188	TRP	CB	-33.20	-10.94	57.77	15.00
188	TRP	CG	-33.05	-11.85	56.60	15.00
188	TRP	CD2	-33.41	-13.23	56.52	15.00
188	TRP	CE2	-33.18	-13.66	55.20	15.00
188	TRP	CE3	-33.92	-14.16	57.45	15.00
188	TRP	CD1	-32.61	-11.50	55.36	15.00
188	TRP	NE1	-32.69	-12.58	54.51	15.00
188	TRP	CZ2	-33.45	-14.96	54.76	15.00
188	TRP	CZ3	-34.18	-15.46	57.02	15.00
188	TRP	CH2	-33.94	-15.85	55.69	15.00
188	TRP	C	-35.66	-11.00	57.51	15.00
188	TRP	O	-36.23	-11.48	58.49	15.00
189	GLY	N	-36.02	-11.29	56.27	15.00
189	GLY	CA	-37.14	-12.17	56.00	15.00
189	GLY	C	-38.37	-11.86	56.84	15.00
189	GLY	O	-38.70	-10.69	57.08	15.00
190	ASN	N	-39.02	-12.91	57.32	15.00
190	ASN	CA	-40.22	-12.78	58.13	15.00
190	ASN	CB	-41.13	-14.00	57.93	15.00
190	ASN	CG	-42.58	-13.74	58.32	15.00
190	ASN	OD1	-42.87	-13.07	59.31	15.00
190	ASN	ND2	-43.50	-14.27	57.53	15.00
190	ASN	C	-39.86	-12.63	59.61	15.00
190	ASN	O	-39.81	-13.61	60.35	15.00
191	LYS	N	-39.55	-11.41	60.02	15.00
191	LYS	CA	-39.19	-11.14	61.41	15.00
191	LYS	CB	-40.43	-11.19	62.29	15.00

TABLE VI

191	LYS	CG	-41.44	-10.10	61.96	15.00
191	LYS	CD	-40.92	-8.71	62.35	15.00
191	LYS	CE	-41.18	-7.63	61.27	15.00
191	LYS	NZ	-40.19	-7.69	60.13	15.00
191	LYS	C	-38.10	-12.07	61.94	15.00
191	LYS	O	-38.11	-12.46	63.11	15.00
192	GLY	N	-37.15	-12.41	61.07	15.00
192	GLY	CA	-36.04	-13.26	61.47	15.00
192	GLY	C	-36.15	-14.73	61.13	15.00
192	GLY	O	-35.19	-15.48	61.32	15.00
193	TYR	N	-37.30	-15.16	60.63	15.00
193	TYR	CA	-37.50	-16.56	60.28	15.00
193	TYR	CB	-38.69	-17.14	61.04	15.00
193	TYR	CG	-38.47	-17.29	62.51	15.00
193	TYR	CD1	-38.57	-16.19	63.36	15.00
193	TYR	CE1	-38.34	-16.32	64.72	15.00
193	TYR	CD2	-38.13	-18.51	63.06	15.00
193	TYR	CE2	-37.91	-18.65	64.42	15.00
193	TYR	CZ	-38.01	-17.55	65.24	15.00
193	TYR	OH	-37.78	-17.71	66.59	15.00
193	TYR	C	-37.76	-16.73	58.80	15.00
193	TYR	O	-37.97	-15.76	58.08	15.00
194	ILE	N	-37.78	-17.99	58.37	15.00
194	ILE	CA	-38.03	-18.32	56.99	15.00
194	ILE	CB	-36.75	-18.27	56.13	15.00
194	ILE	CG2	-35.65	-19.10	56.76	15.00
194	ILE	CG1	-37.06	-18.74	54.72	15.00
194	ILE	CD1	-35.95	-18.54	53.75	15.00
194	ILE	C	-38.65	-19.70	56.88	15.00
194	ILE	O	-38.20	-20.64	57.51	15.00
195	LEU	N	-39.71	-19.79	56.09	15.00
195	LEU	CA	-40.40	-21.04	55.87	15.00
195	LEU	CB	-41.91	-20.78	55.71	15.00
195	LEU	CG	-42.77	-20.89	56.98	15.00
195	LEU	CD1	-42.08	-20.31	58.19	15.00
195	LEU	CD2	-44.09	-20.19	56.75	15.00
195	LEU	C	-39.83	-21.68	54.62	15.00
195	LEU	O	-40.04	-21.19	53.51	15.00
196	MET	N	-39.05	-22.73	54.81	15.00
196	MET	CA	-38.44	-23.44	53.70	15.00
196	MET	CB	-37.01	-23.80	54.04	15.00
196	MET	CG	-36.11	-22.58	54.16	15.00

TABLE VI

196	MET	SD	-34.46	-22.98	54.73	15.00
196	MET	CE	-33.78	-23.75	53.28	15.00
196	MET	C	-39.27	-24.68	53.38	15.00
196	MET	O	-40.03	-25.14	54.23	15.00
197	ALA	N	-39.15	-25.19	52.16	15.00
197	ALA	CA	-39.91	-26.36	51.72	15.00
197	ALA	CB	-39.86	-26.48	50.19	15.00
197	ALA	C	-39.51	-27.69	52.36	15.00
197	ALA	O	-38.33	-28.00	52.50	15.00
198	ARG	N	-40.52	-28.50	52.67	15.00
198	ARG	CA	-40.32	-29.81	53.28	15.00
198	ARG	CB	-41.08	-29.90	54.60	15.00
198	ARG	CG	-41.09	-31.28	55.23	15.00
198	ARG	CD	-41.40	-31.21	56.71	15.00
198	ARG	NE	-42.71	-30.64	57.00	15.00
198	ARG	CZ	-43.83	-31.35	57.04	15.00
198	ARG	NH1	-43.80	-32.66	56.80	15.00
198	ARG	NH2	-44.97	-30.76	57.34	15.00
198	ARG	C	-40.79	-30.90	52.34	15.00
198	ARG	O	-41.87	-30.81	51.76	15.00
199	ASN	N	-39.97	-31.93	52.20	15.00
199	ASN	CA	-40.28	-33.07	51.33	15.00
199	ASN	CB	-41.68	-33.62	51.60	15.00
199	ASN	CG	-41.76	-34.41	52.90	15.00
199	ASN	OD1	-42.80	-34.44	53.57	15.00
199	ASN	ND2	-40.65	-35.05	53.28	15.00
199	ASN	C	-40.08	-32.78	49.85	15.00
199	ASN	O	-40.45	-33.59	48.99	15.00
200	LYS	N	-39.47	-31.65	49.54	15.00
200	LYS	CA	-39.18	-31.30	48.16	15.00
200	LYS	CB	-39.18	-29.77	47.95	15.00
200	LYS	CG	-40.55	-29.15	47.76	15.00
200	LYS	CD	-41.24	-29.74	46.54	15.00
200	LYS	CE	-42.64	-29.19	46.34	15.00
200	LYS	NZ	-43.39	-29.98	45.32	15.00
200	LYS	C	-37.80	-31.87	47.84	15.00
200	LYS	O	-36.86	-31.13	47.56	15.00
201	ASN	N	-37.66	-33.19	48.01	15.00
201	ASN	CA	-36.40	-33.87	47.72	15.00
201	ASN	CB	-36.24	-33.99	46.19	15.00
201	ASN	CG	-35.16	-35.00	45.77	15.00
201	ASN	OD1	-35.27	-35.62	44.69	15.00

TABLE VI

201	ASN	ND2	-34.11	-35.15	46.58	15.00
201	ASN	C	-35.18	-33.16	48.34	15.00
201	ASN	O	-34.28	-32.70	47.62	15.00
202	ASN	N	-35.16	-33.09	49.67	15.00
202	ASN	CA	-34.05	-32.47	50.41	15.00
202	ASN	CB	-32.86	-33.43	50.47	15.00
202	ASN	CG	-31.99	-33.22	51.69	15.00
202	ASN	OD1	-32.43	-32.60	52.67	15.00
202	ASN	ND2	-30.77	-33.72	51.66	15.00
202	ASN	C	-33.61	-31.11	49.86	15.00
202	ASN	O	-32.42	-30.87	49.62	15.00
203	ALA	N	-34.58	-30.22	49.72	15.00
203	ALA	H	-35.43	-30.48	50.10	15.00
203	ALA	CA	-34.36	-28.88	49.17	15.00
203	ALA	CB	-35.62	-28.06	49.20	15.00
203	ALA	C	-33.31	-28.14	50.00	15.00
203	ALA	O	-33.47	-27.92	51.19	15.00
204	CYS	N	-32.23	-27.75	49.33	15.00
204	CYS	CA	-31.15	-27.01	49.98	15.00
204	CYS	C	-30.39	-27.80	51.03	15.00
204	CYS	O	-29.68	-27.21	51.83	15.00
204	CYS	CB	-31.68	-25.71	50.61	15.00
204	CYS	SG	-32.40	-24.49	49.47	15.00
205	GLY	N	-30.51	-29.13	51.01	15.00
205	GLY	CA	-29.80	-29.96	51.97	15.00
205	GLY	C	-30.19	-29.78	53.44	15.00
205	GLY	O	-29.39	-30.02	54.34	15.00
206	ILE	N	-31.43	-29.40	53.67	15.00
206	ILE	CA	-31.94	-29.18	55.01	15.00
206	ILE	CB	-33.46	-28.88	54.98	15.00
206	ILE	CG2	-34.18	-29.93	54.15	15.00
206	ILE	CG1	-34.03	-28.79	56.39	15.00
206	ILE	CD1	-33.55	-27.60	57.17	15.00
206	ILE	C	-31.63	-30.32	55.98	15.00
206	ILE	O	-31.31	-30.07	57.15	15.00
207	ALA	N	-31.68	-31.56	55.50	15.00
207	ALA	CA	-31.40	-32.72	56.36	15.00
207	ALA	CB	-32.50	-33.74	56.24	15.00
207	ALA	C	-30.07	-33.37	56.02	15.00
207	ALA	O	-29.89	-34.56	56.21	15.00
208	ASN	N	-29.11	-32.58	55.55	15.00
208	ASN	CA	-27.81	-33.10	55.16	15.00

TABLE VI

208	ASN	CB	-27.34	-32.39	53.88	15.00
208	ASN	CG	-27.15	-33.35	52.72	15.00
208	ASN	OD1	-28.12	-33.85	52.15	15.00
208	ASN	ND2	-25.90	-33.60	52.36	15.00
208	ASN	C	-26.72	-33.00	56.22	15.00
208	ASN	O	-25.66	-33.62	56.10	15.00
209	LEU	N	-26.96	-32.22	57.27	15.00
209	LEU	CA	-25.96	-32.06	58.31	15.00
209	LEU	CB	-24.98	-30.96	57.89	15.00
209	LEU	CG	-23.69	-30.69	58.67	15.00
209	LEU	CD1	-22.77	-31.90	58.61	15.00
209	LEU	CD2	-22.99	-29.49	58.09	15.00
209	LEU	C	-26.63	-31.70	59.63	15.00
209	LEU	O	-26.11	-30.91	60.41	15.00
210	ALA	N	-27.79	-32.31	59.90	15.00
210	ALA	H	-28.15	-32.83	59.17	15.00
210	ALA	CA	-28.56	-32.01	61.10	15.00
210	ALA	CB	-29.98	-32.52	60.98	15.00
210	ALA	C	-27.93	-32.71	62.32	15.00
210	ALA	O	-27.23	-33.70	62.23	15.00
211	SER	N	-28.20	-32.12	63.50	15.00
211	SER	CA	-27.73	-32.66	64.78	15.00
211	SER	CB	-26.21	-32.55	64.89	15.00
211	SER	OG	-25.79	-31.20	64.98	15.00
211	SER	C	-28.38	-31.89	65.92	15.00
211	SER	O	-28.93	-30.80	65.72	15.00
212	PHE	N	-28.35	-32.47	67.11	15.00
212	PHE	CA	-28.93	-31.84	68.28	15.00
212	PHE	CB	-30.43	-32.16	68.36	15.00
212	PHE	CG	-30.75	-33.63	68.34	15.00
212	PHE	CD1	-31.28	-34.23	67.20	15.00
212	PHE	CD2	-30.55	-34.43	69.48	15.00
212	PHE	CE1	-31.61	-35.57	67.19	15.00
212	PHE	CE2	-30.87	-35.79	69.48	15.00
212	PHE	CZ	-31.40	-36.35	68.33	15.00
212	PHE	C	-28.17	-32.36	69.50	15.00
212	PHE	O	-27.66	-33.48	69.48	15.00
213	PRO	N	-28.03	-31.54	70.55	15.00
213	PRO	CD	-28.53	-30.16	70.68	15.00
213	PRO	CA	-27.32	-31.95	71.76	15.00
213	PRO	CB	-26.95	-30.61	72.38	15.00
213	PRO	CG	-28.16	-29.81	72.11	15.00

TABLE VI

213	PRO	C	-28.20	-32.77	72.70	15.00
213	PRO	O	-29.42	-32.64	72.69	15.00
214	LYS	N	-27.58	-33.60	73.53	15.00
214	LYS	CA	-28.32	-34.41	74.49	15.00
214	LYS	CB	-27.85	-35.85	74.47	15.00
214	LYS	CG	-28.28	-36.60	73.23	15.00
214	LYS	CD	-27.98	-38.09	73.30	15.00
214	LYS	CE	-26.48	-38.39	73.31	15.00
214	LYS	NZ	-25.86	-38.24	74.66	15.00
214	LYS	C	-28.17	-33.84	75.89	15.00
214	LYS	O	-27.07	-33.47	76.29	15.00
215	MET	N	-29.28	-33.75	76.61	15.00
215	MET	CA	-29.29	-33.24	77.98	15.00
215	MET	CB	-30.27	-32.08	78.11	15.00
215	MET	CG	-29.79	-30.79	77.48	15.00
215	MET	SD	-28.97	-29.73	78.67	15.00
215	MET	CE	-30.38	-28.92	79.43	15.00
215	MET	C	-29.67	-34.33	78.99	15.00
215	MET	OT1	-30.25	-35.37	78.59	15.00
215	MET	OT2	-29.39	-34.13	80.20	15.00
216	HOH	OH2	-21.96	-40.63	81.12	15.00
217	HOH	OH2	-30.77	-17.16	67.86	15.00
218	HOH	OH2	-30.16	-20.07	64.02	15.00
219	HOH	OH2	-3.64	-10.82	59.75	15.00
220	HOH	OH2	-13.18	-7.77	71.57	15.00
221	HOH	OH2	-34.51	-22.61	70.17	15.00
222	HOH	OH2	-18.02	-34.44	65.29	15.00
223	HOH	OH2	-17.01	-5.28	69.42	15.00
224	HOH	OH2	-24.38	-30.77	62.26	15.00
225	HOH	OH2	0.36	-5.40	64.98	15.00
226	HOH	OH2	-13.68	-21.42	66.86	15.00
227	HOH	OH2	-46.72	-29.80	50.41	15.00
228	HOH	OH2	-45.10	-36.23	56.40	15.00
229	HOH	OH2	-39.09	-12.35	65.48	15.00
230	HOH	OH2	-35.85	-37.05	52.41	15.00
231	HOH	OH2	-19.20	-39.14	66.78	15.00
232	HOH	OH2	-30.09	-19.72	66.64	15.00
233	HOH	OH2	-27.95	-19.50	62.38	15.00
234	HOH	OH2	-21.75	-30.29	62.28	15.00
235	HOH	OH2	-30.30	-2.55	77.57	15.00
236	HOH	OH2	-33.08	-28.99	86.45	15.00
237	HOH	OH2	-30.07	-22.68	84.37	15.00

TABLE VI

238	HOH	OH2	-39.83	-16.82	48.34	15.00
239	HOH	OH2	-34.57	-24.95	47.01	15.00
240	HOH	OH2	-46.44	-34.07	57.12	15.00
241	HOH	OH2	-26.91	-7.02	56.22	15.00
242	HOH	OH2	-42.10	-15.05	61.98	15.00
243	HOH	OH2	-24.27	-7.11	65.05	15.00
244	HOH	OH2	-33.44	-27.69	70.80	15.00
245	HOH	OH2	-40.50	-27.38	80.61	15.00
246	HOH	OH2	-14.45	-17.44	86.64	15.00
247	HOH	OH2	-4.86	-12.23	73.56	15.00
248	HOH	OH2	-10.86	-20.50	79.87	15.00
249	HOH	OH2	-27.43	-35.04	59.25	15.00
250	HOH	OH2	-35.26	-10.90	53.73	15.00
251	HOH	OH2	-31.84	-29.20	46.92	15.00
252	HOH	OH2	-42.75	-9.71	40.49	15.00
253	HOH	OH2	-41.27	-34.56	56.25	15.00
254	HOH	OH2	-44.55	-15.65	65.22	15.00
255	HOH	OH2	-32.52	-13.49	60.73	15.00
256	HOH	OH2	-39.73	-4.62	63.34	15.00
257	HOH	OH2	-25.69	-11.84	70.98	15.00
258	HOH	OH2	-31.93	-6.64	63.98	15.00
259	HOH	OH2	-19.62	-7.72	62.94	15.00
260	HOH	OH2	-33.42	-20.20	70.53	15.00
261	HOH	OH2	-12.62	-24.00	79.04	15.00
262	HOH	OH2	-9.78	-21.46	77.40	15.00
263	HOH	OH2	-6.71	-27.36	80.84	15.00
264	HOH	OH2	-21.06	-35.71	57.19	15.00
265	HOH	OH2	-26.47	-48.97	59.68	15.00
266	HOH	OH2	-14.22	-32.57	69.97	15.00
267	HOH	OH2	-11.69	-25.57	76.63	15.00
268	HOH	OH2	-17.38	-27.79	86.86	15.00
269	HOH	OH2	-22.39	-37.94	70.91	15.00
270	HOH	OH2	-10.44	-11.32	63.69	15.00
271	HOH	OH2	-8.66	-22.33	72.95	15.00
272	HOH	OH2	-29.93	-20.17	48.73	15.00
273	HOH	OH2	-22.92	-30.27	39.30	15.00
274	HOH	OH2	-33.19	-37.20	49.46	15.00
275	HOH	OH2	-28.10	-25.82	41.06	15.00
276	HOH	OH2	-35.93	-29.91	44.54	15.00
277	HOH	OH2	-37.76	-30.41	51.24	15.00

TABLE VII

Table of the orthogonal three dimensional coordinates in Ångstroms and B factors ($Å^2$) for the cathepsin K complex with inhibitor 4-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-1-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-3-pyrrolidinone.

Residue	Atom	X	Y	Z	B
1 ALA	CB	-46.25	-39.17	62.96	30.60
1 ALA	C	-47.93	-37.51	63.80	29.74
1 ALA	O	-49.14	-37.57	63.58	32.13
1 ALA	N	-48.18	-39.83	64.36	28.23
1 ALA	CA	-47.15	-38.78	64.13	28.86
2 PRO	N	-47.26	-36.34	63.80	27.19
2 PRO	CD	-45.94	-36.10	64.40	26.45
2 PRO	CA	-47.92	-35.06	63.50	27.01
2 PRO	CB	-47.28	-34.10	64.52	26.65
2 PRO	CG	-46.25	-34.95	65.31	27.69
2 PRO	C	-47.73	-34.52	62.09	26.37
2 PRO	O	-46.67	-34.70	61.50	26.53
3 ASP	N	-48.76	-33.86	61.58	26.63
3 ASP	CA	-48.73	-33.23	60.26	24.49
3 ASP	CB	-50.14	-33.03	59.69	23.94
3 ASP	CG	-50.75	-34.32	59.17	24.73
3 ASP	OD1	-50.19	-34.88	58.21	31.10
3 ASP	OD2	-51.79	-34.76	59.71	23.79
3 ASP	C	-48.03	-31.88	60.39	24.62
3 ASP	O	-47.08	-31.59	59.67	23.92
4 SER	N	-48.55	-31.04	61.28	24.05
4 SER	CA	-47.98	-29.72	61.55	22.83
4 SER	CB	-49.04	-28.62	61.52	23.29
4 SER	OG	-49.84	-28.70	60.36	24.54
4 SER	C	-47.30	-29.75	62.91	23.31
4 SER	O	-47.71	-30.51	63.79	26.63
5 VAL	N	-46.27	-28.92	63.09	24.43
5 VAL	CA	-45.52	-28.80	64.34	22.41
5 VAL	CB	-44.44	-29.91	64.50	24.60
5 VAL	CG1	-43.39	-29.50	65.53	19.58
5 VAL	CG2	-45.09	-31.22	64.94	26.54
5 VAL	C	-44.80	-27.45	64.30	22.72

TABLE VII

5	VAL	O	-44.23	-27.09	63.27	24.78
6	ASP	N	-44.80	-26.74	65.41	22.25
6	ASP	CA	-44.17	-25.43	65.48	20.13
6	ASP	CB	-45.15	-24.34	65.04	20.94
6	ASP	CG	-44.49	-22.99	64.81	19.46
6	ASP	OD1	-43.28	-22.84	65.12	15.02
6	ASP	OD2	-45.20	-22.09	64.31	15.42
6	ASP	C	-43.67	-25.17	66.88	20.15
6	ASP	O	-44.45	-24.78	67.74	26.96
7	TYR	N	-42.37	-25.32	67.10	20.70
7	TYR	CA	-41.82	-25.08	68.42	19.50
7	TYR	CB	-40.44	-25.71	68.58	22.46
7	TYR	CG	-40.51	-27.21	68.76	22.69
7	TYR	CD1	-40.50	-27.78	70.03	24.39
7	TYR	CE1	-40.61	-29.16	70.20	23.01
7	TYR	CD2	-40.62	-28.05	67.66	17.84
7	TYR	CE2	-40.72	-29.42	67.82	17.55
7	TYR	CZ	-40.72	-29.97	69.08	16.70
7	TYR	OH	-40.84	-31.33	69.22	21.92
7	TYR	C	-41.77	-23.62	68.78	18.59
7	TYR	O	-41.12	-23.25	69.75	23.10
8	ARG	N	-42.39	-22.78	67.96	16.73
8	ARG	CA	-42.44	-21.36	68.25	17.40
8	ARG	CB	-42.56	-20.52	66.98	19.28
8	ARG	CG	-41.27	-20.40	66.17	22.66
8	ARG	CD	-41.41	-19.48	64.98	14.98
8	ARG	NE	-42.40	-19.99	64.04	17.92
8	ARG	CZ	-42.59	-19.53	62.81	22.05
8	ARG	NH1	-41.85	-18.52	62.36	24.53
8	ARG	NH2	-43.50	-20.10	62.03	26.01
8	ARG	C	-43.64	-21.14	69.17	15.35
8	ARG	O	-43.52	-20.55	70.24	14.09
9	LYS	N	-44.77	-21.73	68.79	13.90
9	LYS	CA	-46.01	-21.63	69.54	13.24
9	LYS	CB	-47.21	-21.84	68.62	10.93
9	LYS	CG	-47.27	-20.83	67.48	16.03
9	LYS	CD	-48.31	-21.19	66.44	13.55
9	LYS	CE	-49.69	-21.20	67.04	17.52
9	LYS	NZ	-50.71	-21.24	65.97	18.86
9	LYS	C	-46.01	-22.61	70.70	15.37
9	LYS	O	-47.06	-23.10	71.14	15.03
10	LYS	N	-44.81	-22.90	71.19	17.15

TABLE VII

10	LYS	CA	-44.58	-23.82	72.31	14.97
10	LYS	CB	-44.10	-25.19	71.81	13.68
10	LYS	CG	-45.15	-26.06	71.14	17.87
10	LYS	CD	-44.58	-27.44	70.87	17.96
10	LYS	CE	-45.67	-28.49	70.71	22.08
10	LYS	NZ	-45.07	-29.82	70.35	25.39
10	LYS	C	-43.52	-23.20	73.23	10.83
10	LYS	O	-43.08	-23.82	74.19	9.39
11	GLY	N	-43.07	-22.01	72.88	11.15
11	GLY	CA	-42.08	-21.35	73.70	14.48
11	GLY	C	-40.71	-21.99	73.69	15.75
11	GLY	O	-39.92	-21.75	74.60	16.24
12	TYR	N	-40.41	-22.80	72.67	16.05
12	TYR	CA	-39.09	-23.44	72.59	15.26
12	TYR	CB	-39.18	-24.83	71.96	16.85
12	TYR	CG	-39.84	-25.90	72.80	12.79
12	TYR	CD1	-41.22	-26.04	72.82	12.72
12	TYR	CE1	-41.82	-27.07	73.52	16.82
12	TYR	CD2	-39.08	-26.82	73.50	18.15
12	TYR	CE2	-39.67	-27.86	74.20	21.62
12	TYR	CZ	-41.04	-27.98	74.20	19.19
12	TYR	OH	-41.63	-29.03	74.89	22.22
12	TYR	C	-38.08	-22.61	71.81	16.45
12	TYR	O	-36.89	-22.92	71.82	18.97
13	VAL	N	-38.55	-21.55	71.16	16.26
13	VAL	CA	-37.67	-20.71	70.34	17.11
13	VAL	CB	-38.25	-20.58	68.90	17.86
13	VAL	CG1	-37.20	-20.07	67.96	18.97
13	VAL	CG2	-38.77	-21.92	68.41	19.17
13	VAL	C	-37.37	-19.31	70.89	16.02
13	VAL	O	-38.27	-18.51	71.14	16.61
14	THR	N	-36.08	-19.01	71.03	15.90
14	THR	CA	-35.65	-17.71	71.53	20.92
14	THR	CB	-34.21	-17.77	72.04	22.63
14	THR	OG1	-33.33	-18.11	70.97	28.59
14	THR	CG2	-34.09	-18.78	73.17	23.81
14	THR	C	-35.73	-16.67	70.41	25.69
14	THR	O	-36.01	-17.02	69.26	28.47
15	PRO	N	-35.50	-15.37	70.73	28.26
15	PRO	CD	-35.15	-14.82	72.05	27.19
15	PRO	CA	-35.56	-14.29	69.73	23.60
15	PRO	CB	-35.29	-13.04	70.58	24.84

TABLE VII

15	PRO	CG	-34.43	-13.55	71.68	26.75
15	PRO	C	-34.53	-14.44	68.62	19.41
15	PRO	O	-33.43	-14.94	68.84	15.67
16	VAL	N	-34.90	-13.96	67.43	16.42
16	VAL	CA	-34.03	-14.06	66.27	12.13
16	VAL	CB	-34.77	-13.71	64.95	9.20
16	VAL	CG1	-33.84	-13.89	63.77	7.84
16	VAL	CG2	-36.01	-14.56	64.78	6.59
16	VAL	C	-32.81	-13.16	66.39	11.22
16	VAL	O	-32.93	-11.94	66.44	11.47
17	LYS	N	-31.65	-13.79	66.45	10.35
17	LYS	CA	-30.39	-13.07	66.55	9.97
17	LYS	CB	-29.31	-13.93	67.22	14.75
17	LYS	CG	-29.17	-13.71	68.75	10.18
17	LYS	CD	-30.45	-14.02	69.52	5.48
17	LYS	CE	-30.69	-15.51	69.66	15.18
17	LYS	NZ	-29.75	-16.23	70.59	13.03
17	LYS	C	-29.98	-12.57	65.16	9.61
17	LYS	O	-30.72	-12.73	64.20	9.93
18	ASN	N	-28.76	-12.05	65.05	8.91
18	ASN	CA	-28.28	-11.47	63.80	8.23
18	ASN	CB	-28.78	-10.03	63.72	10.88
18	ASN	CG	-28.51	-9.36	62.39	13.91
18	ASN	OD1	-27.51	-9.63	61.72	9.48
18	ASN	ND2	-29.40	-8.44	62.03	13.48
18	ASN	C	-26.75	-11.54	63.75	8.02
18	ASN	O	-26.07	-10.64	64.22	13.56
19	GLN	N	-26.22	-12.59	63.14	7.59
19	GLN	CA	-24.78	-12.81	63.06	9.07
19	GLN	CB	-24.50	-14.08	62.26	11.76
19	GLN	CG	-24.91	-14.00	60.81	10.58
19	GLN	CD	-24.73	-15.33	60.11	10.05
19	GLN	OE1	-25.69	-16.07	59.88	8.08
19	GLN	NE2	-23.49	-15.66	59.80	3.31
19	GLN	C	-23.84	-11.70	62.60	12.84
19	GLN	O	-22.65	-11.71	62.95	14.67
20	GLY	N	-24.33	-10.75	61.81	9.97
20	GLY	CA	-23.45	-9.68	61.35	9.75
20	GLY	C	-22.40	-10.16	60.37	9.12
20	GLY	O	-22.56	-11.21	59.74	14.46
21	GLN	N	-21.32	-9.40	60.20	10.42
21	GLN	CA	-20.28	-9.80	59.25	13.95

TABLE VII

21	GLN	CB	-19.55	-8.58	58.66	13.14
21	GLN	CG	-20.40	-7.79	57.65	12.44
21	GLN	CD	-20.73	-8.61	56.41	13.48
21	GLN	OE1	-19.84	-9.15	55.76	14.90
21	GLN	NE2	-22.02	-8.71	56.08	9.41
21	GLN	C	-19.30	-10.83	59.81	15.26
21	GLN	O	-18.08	-10.64	59.79	16.33
22	CYS	N	-19.86	-11.93	60.29	17.72
22	CYS	CA	-19.10	-13.04	60.86	16.36
22	CYS	C	-19.82	-14.31	60.40	16.07
22	CYS	O	-21.05	-14.39	60.44	8.26
22	CYS	CB	-19.02	-12.91	62.40	16.53
22	CYS	SG	-18.36	-14.33	63.35	15.48
23	GLY	N	-19.04	-15.25	59.83	16.86
23	GLY	CA	-19.59	-16.52	59.35	14.89
23	GLY	C	-19.67	-17.49	60.52	13.50
23	GLY	O	-18.91	-18.45	60.61	11.64
24	SER	N	-20.61	-17.20	61.41	13.66
24	SER	CA	-20.82	-17.99	62.61	14.12
24	SER	CB	-20.65	-17.10	63.84	17.06
24	SER	OG	-21.37	-15.88	63.67	19.58
24	SER	C	-22.18	-18.67	62.64	14.42
24	SER	O	-22.63	-19.12	63.69	15.12
25	CYS	N	-22.83	-18.77	61.48	15.74
25	CYS	CA	-24.16	-19.38	61.40	12.45
25	CYS	CB	-24.61	-19.48	59.92	17.82
25	CYS	SG	-23.46	-20.34	58.77	15.84
25	CYS	C	-24.23	-20.73	62.12	12.21
25	CYS	O	-25.27	-21.09	62.66	8.88
25	INH	C1	-26.76	-10.18	57.23	37.63
25	INH	C2	-25.50	-10.64	57.58	37.16
25	INH	C3	-24.85	-11.61	56.79	34.05
25	INH	C4	-25.45	-12.12	55.64	32.87
25	INH	C5	-26.72	-11.65	55.30	36.05
25	INH	C6	-27.38	-10.68	56.09	37.28
25	INH	C7	-24.76	-13.16	54.79	31.70
25	INH	O8	-24.07	-14.24	55.46	33.18
25	INH	C9	-24.20	-15.65	55.36	32.90
25	INH	O10	-24.83	-16.33	56.19	27.65
25	INH	C11	-23.57	-17.64	54.11	33.43
25	INH	C12	-23.56	-17.98	52.63	29.93
25	INH	C13	-24.79	-17.58	51.82	30.09

TABLE VII

25	INH	C14	-24.84	-16.08	51.57	28.76
25	INH	C15	-24.70	-18.31	50.53	33.84
25	INH	C16	-22.36	-18.24	54.80	34.35
25	INH	O17	-21.26	-18.25	54.27	39.78
25	INH	N18	-22.58	-18.72	56.02	35.16
25	INH	C19	-21.64	-19.29	56.85	29.32
25	INH	N20	-23.57	-16.20	54.33	34.33
25	INH	C21	-21.16	-20.68	56.54	29.68
25	INH	C22	-22.10	-19.32	58.29	26.25
25	INH	O23	-22.30	-18.20	58.72	26.33
25	INH	C24	-13.39	-26.50	60.06	25.12
25	INH	C25	-13.12	-25.19	59.68	26.39
25	INH	C26	-14.04	-24.48	58.91	25.10
25	INH	C27	-15.23	-25.07	58.52	23.88
25	INH	C28	-15.49	-26.37	58.90	24.81
25	INH	C29	-14.58	-27.09	59.67	23.22
25	INH	C30	-16.20	-24.31	57.66	25.64
25	INH	O31	-16.99	-24.94	56.63	26.66
25	INH	C32	-18.41	-24.84	56.56	24.33
25	INH	O33	-19.08	-25.66	55.96	24.89
25	INH	C34	-20.39	-23.56	57.26	25.72
25	INH	C35	-21.15	-24.78	57.78	22.12
25	INH	C36	-21.80	-25.75	56.80	16.61
25	INH	C37	-23.15	-25.25	56.41	15.08
25	INH	C38	-21.91	-27.08	57.47	16.77
25	INH	C39	-20.56	-22.41	58.25	28.82
25	INH	O40	-20.39	-22.62	59.45	37.25
25	INH	N41	-20.88	-21.18	57.82	28.59
25	INH	C42	-21.00	-20.17	58.81	27.26
25	INH	N43	-18.95	-23.81	57.20	25.99
26	TRP	N	-23.11	-21.45	62.14	14.10
26	TRP	CA	-23.02	-22.74	62.82	15.29
26	TRP	CB	-21.66	-23.38	62.56	12.22
26	TRP	CG	-20.53	-22.49	62.90	15.74
26	TRP	CD2	-19.74	-22.52	64.10	17.65
26	TRP	CE2	-18.76	-21.51	63.98	15.49
26	TRP	CE3	-19.77	-23.30	65.27	18.53
26	TRP	CD1	-20.02	-21.49	62.14	16.57
26	TRP	NE1	-18.95	-20.90	62.77	17.92
26	TRP	CZ2	-17.82	-21.26	64.98	13.72
26	TRP	CZ3	-18.83	-23.05	66.26	16.53
26	TRP	CH2	-17.87	-22.04	66.11	15.09

TABLE VII

26	TRP	C	-23.24	-22.55	64.32	19.46
26	TRP	O	-24.09	-23.21	64.92	24.77
27	ALA	N	-22.52	-21.59	64.90	19.49
27	ALA	CA	-22.61	-21.25	66.31	12.94
27	ALA	CB	-21.77	-20.01	66.61	12.05
27	ALA	C	-24.07	-20.99	66.64	8.35
27	ALA	O	-24.61	-21.54	67.60	6.75
28	PHE	N	-24.72	-20.18	65.80	8.07
28	PHE	CA	-26.13	-19.83	65.95	9.51
28	PHE	CB	-26.51	-18.67	65.04	7.62
28	PHE	CG	-25.96	-17.35	65.48	4.72
28	PHE	CD1	-24.74	-16.91	65.01	4.11
28	PHE	CD2	-26.66	-16.56	66.38	2.92
28	PHE	CE1	-24.22	-15.69	65.41	4.53
28	PHE	CE2	-26.16	-15.33	66.79	2.38
28	PHE	CZ	-24.93	-14.89	66.31	2.00
28	PHE	C	-27.07	-21.01	65.72	10.66
28	PHE	O	-28.18	-21.04	66.26	14.07
29	SER	N	-26.64	-21.96	64.89	10.83
29	SER	CA	-27.44	-23.15	64.62	8.54
29	SER	CB	-26.92	-23.88	63.37	2.45
29	SER	OG	-27.80	-24.93	62.97	2.00
29	SER	C	-27.40	-24.05	65.86	7.86
29	SER	O	-28.44	-24.46	66.38	6.37
30	SER	N	-26.19	-24.29	66.36	5.14
30	SER	CA	-26.00	-25.14	67.52	7.65
30	SER	CB	-24.52	-25.27	67.84	10.56
30	SER	OG	-23.81	-25.61	66.67	14.28
30	SER	C	-26.76	-24.61	68.73	6.72
30	SER	O	-27.57	-25.32	69.34	8.64
31	VAL	N	-26.50	-23.35	69.06	6.44
31	VAL	CA	-27.15	-22.71	70.19	6.61
31	VAL	CB	-26.73	-21.23	70.25	6.76
31	VAL	CG1	-27.74	-20.40	71.03	9.71
31	VAL	CG2	-25.35	-21.14	70.90	2.00
31	VAL	C	-28.67	-22.86	70.18	9.86
31	VAL	O	-29.25	-23.30	71.17	13.64
32	GLY	N	-29.30	-22.56	69.05	12.98
32	GLY	CA	-30.75	-22.68	68.94	9.41
32	GLY	C	-31.27	-24.10	69.19	10.59
32	GLY	O	-32.42	-24.29	69.59	8.20
33	ALA	N	-30.44	-25.10	68.91	11.42

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33	ALA	CA	-30.82	-26.50	69.12	13.15
33	ALA	CB	-29.82	-27.42	68.47	10.51
33	ALA	C	-30.86	-26.73	70.64	14.58
33	ALA	O	-31.87	-27.19	71.19	12.75
34	LEU	N	-29.75	-26.39	71.29	12.77
34	LEU	CA	-29.62	-26.51	72.73	12.38
34	LEU	CB	-28.26	-26.01	73.20	4.32
34	LEU	CG	-27.04	-26.64	72.57	4.80
34	LEU	CD1	-25.82	-25.86	72.95	6.27
34	LEU	CD2	-26.92	-28.09	73.01	4.63
34	LEU	C	-30.73	-25.73	73.43	16.38
34	LEU	O	-31.32	-26.22	74.39	18.32
35	GLU	N	-31.00	-24.53	72.95	15.34
35	GLU	CA	-32.03	-23.71	73.54	15.20
35	GLU	CB	-32.17	-22.38	72.81	12.21
35	GLU	CG	-30.92	-21.55	72.88	18.17
35	GLU	CD	-31.07	-20.22	72.17	21.50
35	GLU	OE1	-31.87	-20.14	71.21	23.90
35	GLU	OE2	-30.40	-19.25	72.57	22.09
35	GLU	C	-33.37	-24.43	73.60	18.81
35	GLU	O	-34.06	-24.37	74.62	23.06
36	GLY	N	-33.73	-25.11	72.52	19.33
36	GLY	CA	-35.00	-25.83	72.48	19.77
36	GLY	C	-34.96	-27.02	73.42	21.74
36	GLY	O	-35.97	-27.38	74.05	18.02
37	GLN	N	-33.79	-27.63	73.53	23.70
37	GLN	CA	-33.61	-28.77	74.41	23.25
37	GLN	CB	-32.27	-29.48	74.15	22.37
37	GLN	CG	-32.08	-29.98	72.71	26.26
37	GLN	CD	-33.38	-30.28	71.94	30.06
37	GLN	OE1	-34.20	-31.11	72.36	29.64
37	GLN	NE2	-33.58	-29.57	70.83	31.26
37	GLN	C	-33.73	-28.32	75.86	24.67
37	GLN	O	-34.51	-28.89	76.62	25.08
38	LEU	N	-32.99	-27.27	76.22	22.29
38	LEU	CA	-33.04	-26.73	77.57	23.08
38	LEU	CB	-32.20	-25.46	77.70	21.38
38	LEU	CG	-32.11	-24.78	79.07	17.48
38	LEU	CD1	-31.77	-25.77	80.17	13.71
38	LEU	CD2	-31.07	-23.68	78.99	17.90
38	LEU	C	-34.47	-26.46	77.99	24.35
38	LEU	O	-34.92	-26.97	79.01	26.24

TABLE VII

39	LYS	N	-35.20	-25.71	77.17	26.25
39	LYS	CA	-36.59	-25.41	77.47	28.16
39	LYS	CB	-37.25	-24.61	76.34	28.65
39	LYS	CG	-38.35	-23.65	76.81	27.61
39	LYS	CD	-39.60	-24.37	77.25	27.20
39	LYS	CE	-40.68	-23.40	77.70	26.81
39	LYS	NZ	-41.94	-24.12	78.05	28.10
39	LYS	C	-37.37	-26.69	77.76	26.01
39	LYS	O	-38.28	-26.70	78.60	25.82
40	LYS	N	-37.00	-27.77	77.11	26.61
40	LYS	CA	-37.69	-29.03	77.34	27.03
40	LYS	CB	-37.64	-29.93	76.11	28.30
40	LYS	CG	-38.65	-31.06	76.16	29.91
40	LYS	CD	-38.79	-31.77	74.82	29.72
40	LYS	CE	-37.74	-32.83	74.61	26.31
40	LYS	NZ	-38.04	-33.61	73.37	31.45
40	LYS	C	-37.09	-29.72	78.56	25.36
40	LYS	O	-37.81	-30.32	79.35	23.91
41	LYS	N	-35.78	-29.57	78.73	25.39
41	LYS	CA	-35.06	-30.20	79.84	25.65
41	LYS	CB	-33.55	-30.06	79.66	24.57
41	LYS	CG	-32.72	-30.84	80.67	20.75
41	LYS	CD	-32.89	-32.34	80.50	26.88
41	LYS	CE	-31.76	-33.13	81.15	28.72
41	LYS	NZ	-31.63	-32.85	82.61	29.46
41	LYS	C	-35.50	-29.67	81.19	25.70
41	LYS	O	-35.92	-30.44	82.06	23.51
42	THR	N	-35.42	-28.35	81.34	26.91
42	THR	CA	-35.76	-27.67	82.58	25.94
42	THR	CB	-34.61	-26.77	83.03	26.05
42	THR	OG1	-34.60	-25.58	82.23	27.18
42	THR	CG2	-33.28	-27.49	82.85	28.99
42	THR	C	-37.00	-26.78	82.52	25.00
42	THR	O	-37.57	-26.43	83.55	28.90
43	GLY	N	-37.38	-26.35	81.32	24.41
43	GLY	CA	-38.54	-25.48	81.19	21.01
43	GLY	C	-38.09	-24.02	81.13	19.83
43	GLY	O	-38.92	-23.10	81.08	14.91
44	LYS	N	-36.78	-23.82	81.15	22.11
44	LYS	CA	-36.16	-22.50	81.10	24.14
44	LYS	CB	-35.06	-22.38	82.17	26.33
44	LYS	CG	-35.61	-22.19	83.60	25.46

TABLE VII

44	LYS	CD	-34.54	-22.37	84.69	26.23
44	LYS	CE	-33.36	-21.39	84.56	26.78
44	LYS	NZ	-32.26	-21.89	83.66	25.35
44	LYS	C	-35.63	-22.16	79.70	22.98
44	LYS	O	-34.86	-22.92	79.12	25.51
45	LEU	N	-36.06	-21.02	79.17	20.83
45	LEU	CA	-35.68	-20.55	77.84	14.37
45	LEU	CB	-36.93	-20.19	77.03	6.57
45	LEU	CG	-36.73	-19.98	75.54	7.56
45	LEU	CD1	-36.34	-21.28	74.88	7.35
45	LEU	CD2	-38.01	-19.44	74.92	7.68
45	LEU	C	-34.73	-19.36	77.92	12.93
45	LEU	O	-35.17	-18.22	78.02	12.18
46	LEU	N	-33.43	-19.62	77.91	12.78
46	LEU	CA	-32.45	-18.55	77.99	16.27
46	LEU	CB	-31.57	-18.68	79.23	17.06
46	LEU	CG	-32.20	-18.84	80.61	22.73
46	LEU	CD1	-33.29	-17.80	80.80	27.00
46	LEU	CD2	-32.76	-20.25	80.75	24.49
46	LEU	C	-31.59	-18.55	76.75	19.40
46	LEU	O	-31.38	-19.61	76.15	22.78
47	ASN	N	-31.05	-17.39	76.39	19.21
47	ASN	CA	-30.18	-17.27	75.21	16.88
47	ASN	CB	-30.12	-15.82	74.70	17.63
47	ASN	CG	-31.41	-15.38	74.02	19.44
47	ASN	OD1	-32.47	-15.31	74.64	24.63
47	ASN	ND2	-31.33	-15.04	72.74	18.95
47	ASN	C	-28.78	-17.79	75.50	14.05
47	ASN	O	-28.08	-17.23	76.36	11.81
48	LEU	N	-28.39	-18.87	74.83	12.40
48	LEU	CA	-27.05	-19.46	74.97	13.22
48	LEU	CB	-27.02	-20.94	74.58	14.23
48	LEU	CG	-27.64	-22.02	75.50	16.25
48	LEU	CD1	-26.96	-22.02	76.87	20.21
48	LEU	CD2	-29.13	-21.80	75.67	14.71
48	LEU	C	-26.08	-18.63	74.14	13.45
48	LEU	O	-26.51	-17.85	73.29	17.95
49	SER	N	-24.78	-18.80	74.36	15.33
49	SER	CA	-23.79	-17.98	73.65	13.70
49	SER	CB	-22.77	-17.41	74.65	14.72
49	SER	OG	-21.73	-16.68	74.02	13.12
49	SER	C	-23.05	-18.50	72.42	14.35

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49	SER	O	-22.14	-19.33	72.52	15.35
50	PRO	N	-23.38	-17.93	71.24	13.10
50	PRO	CD	-24.49	-16.99	71.00	13.10
50	PRO	CA	-22.73	-18.30	69.99	8.82
50	PRO	CB	-23.41	-17.39	68.98	10.23
50	PRO	CG	-24.79	-17.23	69.54	10.20
50	PRO	C	-21.25	-17.95	70.09	7.83
50	PRO	O	-20.40	-18.65	69.56	7.76
51	GLN	N	-20.96	-16.86	70.80	8.14
51	GLN	CA	-19.59	-16.38	70.97	8.89
51	GLN	CB	-19.58	-14.99	71.62	12.14
51	GLN	CG	-18.31	-14.16	71.33	13.72
51	GLN	CD	-18.18	-13.71	69.87	12.95
51	GLN	OE1	-19.12	-13.18	69.27	10.44
51	GLN	NE2	-16.99	-13.89	69.30	6.01
51	GLN	C	-18.70	-17.34	71.74	8.59
51	GLN	O	-17.49	-17.46	71.45	8.17
52	ASN	N	-19.27	-18.03	72.72	6.61
52	ASN	CA	-18.50	-19.01	73.49	6.19
52	ASN	CB	-19.36	-19.58	74.62	6.41
52	ASN	CG	-18.70	-20.74	75.34	7.63
52	ASN	OD1	-19.39	-21.64	75.81	9.07
52	ASN	ND2	-17.39	-20.70	75.48	4.94
52	ASN	C	-18.04	-20.09	72.50	9.66
52	ASN	O	-16.89	-20.56	72.54	9.03
53	LEU	N	-18.94	-20.43	71.58	10.50
53	LEU	CA	-18.69	-21.42	70.54	7.20
53	LEU	CB	-20.01	-21.83	69.89	6.76
53	LEU	CG	-20.74	-23.04	70.49	12.00
53	LEU	CD1	-20.47	-23.19	71.98	14.61
53	LEU	CD2	-22.22	-22.93	70.21	8.55
53	LEU	C	-17.69	-20.92	69.49	6.03
53	LEU	O	-16.75	-21.63	69.14	4.01
54	VAL	N	-17.87	-19.70	69.01	2.00
54	VAL	CA	-16.99	-19.14	68.00	6.81
54	VAL	CB	-17.34	-17.67	67.64	7.05
54	VAL	CG1	-16.27	-17.07	66.74	13.23
54	VAL	CG2	-18.66	-17.58	66.93	5.36
54	VAL	C	-15.55	-19.15	68.47	12.15
54	VAL	O	-14.66	-19.63	67.76	16.44
55	ASP	N	-15.32	-18.59	69.65	15.93
55	ASP	CA	-13.98	-18.48	70.22	17.26

TABLE VII

55	ASP	CB	-13.98	-17.47	71.37	19.77
55	ASP	CG	-14.33	-16.06	70.94	22.96
55	ASP	OD1	-14.48	-15.78	69.72	24.84
55	ASP	OD2	-14.44	-15.21	71.84	23.39
55	ASP	C	-13.37	-19.78	70.72	18.42
55	ASP	O	-12.18	-20.06	70.49	12.75
56	CYS	N	-14.18	-20.55	71.43	20.14
56	CYS	CA	-13.75	-21.79	72.06	19.35
56	CYS	C	-13.66	-23.12	71.30	16.79
56	CYS	O	-13.00	-24.05	71.77	19.07
56	CYS	CB	-14.52	-21.96	73.37	17.64
56	CYS	SG	-14.48	-20.45	74.39	15.52
57	VAL	N	-14.31	-23.23	70.14	14.99
57	VAL	CA	-14.24	-24.47	69.38	12.09
57	VAL	CB	-15.48	-24.72	68.51	9.25
57	VAL	CG1	-15.37	-26.09	67.85	2.60
57	VAL	CG2	-16.75	-24.62	69.34	5.09
57	VAL	C	-13.02	-24.48	68.47	12.69
57	VAL	O	-13.04	-23.91	67.39	15.30
58	SER	N	-11.96	-25.14	68.92	15.12
58	SER	CA	-10.72	-25.21	68.15	18.94
58	SER	CB	-9.59	-25.78	69.00	21.08
58	SER	OG	-9.92	-27.07	69.49	20.89
58	SER	C	-10.84	-25.98	66.83	19.38
58	SER	O	-10.00	-25.81	65.94	21.21
59	GLU	N	-11.83	-26.87	66.74	21.74
59	GLU	CA	-12.04	-27.68	65.53	20.63
59	GLU	CB	-12.88	-28.94	65.82	20.59
59	GLU	CG	-12.48	-29.76	67.06	21.89
59	GLU	CD	-13.08	-29.21	68.37	21.83
59	GLU	OE1	-14.32	-29.11	68.47	25.51
59	GLU	OE2	-12.31	-28.90	69.30	26.68
59	GLU	C	-12.69	-26.87	64.41	19.86
59	GLU	O	-12.56	-27.21	63.23	21.27
60	ASN	N	-13.43	-25.83	64.79	16.86
60	ASN	CA	-14.11	-24.97	63.83	10.64
60	ASN	CB	-15.49	-24.61	64.33	2.00
60	ASN	CG	-16.43	-25.78	64.27	6.50
60	ASN	OD1	-17.46	-25.83	64.96	3.71
60	ASN	ND2	-16.09	-26.75	63.42	3.21
60	ASN	C	-13.27	-23.76	63.49	13.09
60	ASN	O	-12.25	-23.51	64.13	14.35

TABLE VII

61	ASP	N	-13.67	-23.01	62.46	14.85
61	ASP	CA	-12.90	-21.86	62.02	15.28
61	ASP	CB	-12.74	-21.86	60.51	21.27
61	ASP	CG	-11.30	-22.08	60.07	23.24
61	ASP	OD1	-10.60	-21.08	59.84	26.41
61	ASP	OD2	-10.88	-23.25	59.97	20.64
61	ASP	C	-13.36	-20.50	62.51	15.18
61	ASP	O	-12.89	-19.47	62.01	13.47
62	GLY	N	-14.26	-20.50	63.48	15.64
62	GLY	CA	-14.75	-19.25	64.03	15.74
62	GLY	C	-15.68	-18.55	63.07	17.26
62	GLY	O	-16.72	-19.10	62.72	19.72
63	CYS	N	-15.30	-17.35	62.64	19.00
63	CYS	CA	-16.14	-16.62	61.70	18.17
63	CYS	C	-16.00	-17.19	60.29	19.74
63	CYS	O	-16.79	-16.86	59.41	22.59
63	CYS	CB	-15.85	-15.11	61.73	16.37
63	CYS	SG	-16.32	-14.21	63.25	14.06
64	GLY	N	-15.00	-18.05	60.09	17.99
64	GLY	CA	-14.81	-18.67	58.79	15.84
64	GLY	C	-15.66	-19.92	58.60	17.59
64	GLY	O	-15.50	-20.66	57.63	19.05
65	GLY	N	-16.59	-20.15	59.53	18.26
65	GLY	CA	-17.46	-21.31	59.44	12.24
65	GLY	C	-17.03	-22.45	60.34	10.78
65	GLY	O	-15.90	-22.47	60.83	9.37
66	GLY	N	-17.94	-23.40	60.53	8.77
66	GLY	CA	-17.68	-24.56	61.36	8.46
66	GLY	C	-18.83	-25.55	61.24	10.14
66	GLY	O	-19.79	-25.29	60.51	9.60
67	TYR	N	-18.69	-26.70	61.88	12.33
67	TYR	CA	-19.74	-27.73	61.84	14.13
67	TYR	CB	-19.18	-29.12	61.49	14.00
67	TYR	CG	-18.53	-29.22	60.13	16.82
67	TYR	CD1	-19.29	-29.29	58.96	19.29
67	TYR	CE1	-18.68	-29.37	57.70	19.34
67	TYR	CD2	-17.15	-29.24	60.02	17.85
67	TYR	CE2	-16.53	-29.32	58.77	21.15
67	TYR	CZ	-17.30	-29.39	57.61	22.41
67	TYR	OH	-16.66	-29.42	56.38	22.94
67	TYR	C	-20.44	-27.77	63.20	12.95
67	TYR	O	-19.80	-27.61	64.23	14.93

TABLE VII

68	MET	N	-21.75	-27.98	63.19	14.10
68	MET	CA	-22.51	-28.01	64.44	11.02
68	MET	CB	-24.02	-28.04	64.18	7.28
68	MET	CG	-24.57	-26.75	63.53	12.57
68	MET	SD	-24.82	-26.81	61.72	9.43
68	MET	CE	-23.29	-26.23	61.15	5.50
68	MET	C	-22.07	-29.15	65.34	10.25
68	MET	O	-21.98	-28.98	66.55	9.78
69	THR	N	-21.74	-30.30	64.76	11.11
69	THR	CA	-21.31	-31.45	65.54	9.38
69	THR	CB	-21.06	-32.69	64.65	7.39
69	THR	OG1	-20.19	-32.36	63.55	6.10
69	THR	CG2	-22.39	-33.24	64.11	6.49
69	THR	C	-20.08	-31.11	66.39	8.98
69	THR	O	-20.06	-31.41	67.57	15.86
70	ASN	N	-19.09	-30.44	65.81	5.69
70	ASN	CA	-17.89	-30.06	66.55	7.38
70	ASN	CB	-16.87	-29.34	65.67	9.34
70	ASN	CG	-16.43	-30.17	64.49	11.35
70	ASN	OD1	-16.13	-29.63	63.43	13.75
70	ASN	ND2	-16.38	-31.48	64.66	13.26
70	ASN	C	-18.26	-29.15	67.71	9.60
70	ASN	O	-17.68	-29.25	68.79	10.75
71	ALA	N	-19.24	-28.28	67.47	12.80
71	ALA	CA	-19.72	-27.33	68.48	15.69
71	ALA	CB	-20.62	-26.29	67.84	12.87
71	ALA	C	-20.48	-28.04	69.59	16.01
71	ALA	O	-20.50	-27.56	70.72	18.32
72	PHE	N	-21.14	-29.14	69.25	15.89
72	PHE	CA	-21.91	-29.90	70.23	15.72
72	PHE	CB	-22.88	-30.85	69.53	12.85
72	PHE	CG	-24.07	-30.17	68.91	10.89
72	PHE	CD1	-24.61	-29.03	69.48	13.23
72	PHE	CD2	-24.69	-30.70	67.78	13.69
72	PHE	CE1	-25.75	-28.43	68.93	14.17
72	PHE	CE2	-25.83	-30.10	67.23	11.57
72	PHE	CZ	-26.36	-28.96	67.80	8.27
72	PHE	C	-20.93	-30.66	71.11	17.93
72	PHE	O	-20.98	-30.59	72.34	16.27
73	GLN	N	-20.01	-31.36	70.44	19.40
73	GLN	CA	-18.97	-32.16	71.08	19.37
73	GLN	CB	-18.09	-32.78	70.00	17.22

TABLE VII

73	GLN	CG	-16.99	-33.70	70.46	19.79
73	GLN	CD	-16.30	-34.36	69.27	20.51
73	GLN	OE1	-16.73	-35.40	68.78	22.61
73	GLN	NE2	-15.24	-33.72	68.75	18.71
73	GLN	C	-18.15	-31.29	72.03	20.01
73	GLN	O	-17.74	-31.75	73.10	20.37
74	TYR	N	-17.92	-30.04	71.65	18.39
74	TYR	CA	-17.16	-29.12	72.48	15.45
74	TYR	CB	-16.90	-27.79	71.73	13.54
74	TYR	CG	-16.82	-26.58	72.63	12.20
74	TYR	CD1	-15.63	-26.22	73.26	10.63
74	TYR	CE1	-15.59	-25.18	74.18	11.99
74	TYR	CD2	-17.97	-25.84	72.93	9.97
74	TYR	CE2	-17.94	-24.79	73.84	7.22
74	TYR	CZ	-16.75	-24.47	74.47	11.24
74	TYR	OH	-16.74	-23.48	75.43	17.85
74	TYR	C	-17.93	-28.93	73.80	12.38
74	TYR	O	-17.38	-29.14	74.87	15.74
75	VAL	N	-19.21	-28.60	73.71	11.39
75	VAL	CA	-20.05	-28.38	74.88	11.24
75	VAL	CB	-21.50	-28.06	74.44	8.02
75	VAL	CG1	-22.42	-27.95	75.64	6.92
75	VAL	CG2	-21.54	-26.76	73.66	9.76
75	VAL	C	-20.05	-29.59	75.83	16.34
75	VAL	O	-20.35	-29.45	77.03	11.43
76	GLN	N	-19.74	-30.76	75.28	18.49
76	GLN	CA	-19.69	-32.02	76.03	17.15
76	GLN	CB	-19.98	-33.22	75.11	16.55
76	GLN	CG	-19.90	-34.60	75.78	17.80
76	GLN	CD	-20.05	-35.78	74.81	16.42
76	GLN	OE1	-19.33	-35.89	73.81	12.60
76	GLN	NE2	-20.98	-36.68	75.12	11.09
76	GLN	C	-18.33	-32.15	76.71	17.72
76	GLN	O	-18.25	-32.28	77.92	19.51
77	LYS	N	-17.25	-32.04	75.94	18.51
77	LYS	CA	-15.91	-32.16	76.50	18.56
77	LYS	CB	-14.84	-32.18	75.41	18.21
77	LYS	CG	-14.75	-33.47	74.62	18.16
77	LYS	CD	-13.48	-33.47	73.77	21.11
77	LYS	CE	-13.38	-34.69	72.84	22.51
77	LYS	NZ	-12.02	-34.81	72.23	21.73
77	LYS	C	-15.58	-31.08	77.52	20.04

TABLE VII

77	LYS	O	-14.76	-31.29	78.42	21.61
78	ASN	N	-16.20	-29.91	77.36	20.45
78	ASN	CA	-15.96	-28.79	78.27	19.68
78	ASN	CB	-15.88	-27.47	77.50	18.78
78	ASN	CG	-15.19	-26.36	78.30	19.30
78	ASN	OD1	-13.97	-26.34	78.44	16.41
78	ASN	ND2	-15.98	-25.40	78.79	20.55
78	ASN	C	-17.03	-28.73	79.35	18.44
78	ASN	O	-17.03	-27.83	80.18	20.10
79	ARG	N	-17.96	-29.68	79.32	16.26
79	ARG	CA	-19.04	-29.74	80.30	16.53
79	ARG	CB	-18.53	-30.31	81.63	16.34
79	ARG	CG	-17.65	-31.54	81.47	17.65
79	ARG	CD	-16.99	-31.93	82.78	19.26
79	ARG	NE	-16.03	-33.01	82.58	21.25
79	ARG	CZ	-14.74	-32.82	82.27	24.36
79	ARG	NH1	-14.27	-31.59	82.11	27.69
79	ARG	NH2	-13.93	-33.86	82.13	18.73
79	ARG	C	-19.74	-28.39	80.51	14.94
79	ARG	O	-19.91	-27.95	81.64	14.77
80	GLY	N	-20.12	-27.73	79.42	16.45
80	GLY	CA	-20.82	-26.46	79.56	14.39
80	GLY	C	-20.59	-25.34	78.56	13.10
80	GLY	O	-19.49	-25.18	78.00	10.43
81	ILE	N	-21.64	-24.54	78.38	9.15
81	ILE	CA	-21.62	-23.39	77.50	7.25
81	ILE	CB	-22.39	-23.68	76.19	6.85
81	ILE	CG2	-23.87	-23.89	76.48	4.07
81	ILE	CG1	-22.16	-22.55	75.18	8.21
81	ILE	CD1	-23.07	-22.63	73.97	11.83
81	ILE	C	-22.27	-22.21	78.25	8.64
81	ILE	O	-23.29	-22.38	78.94	9.51
82	ASP	N	-21.68	-21.03	78.13	11.32
82	ASP	CA	-22.20	-19.84	78.81	12.61
82	ASP	CB	-21.14	-18.75	78.92	10.86
82	ASP	CG	-19.95	-19.18	79.72	10.55
82	ASP	OD1	-18.81	-18.86	79.31	8.90
82	ASP	OD2	-20.14	-19.86	80.74	14.89
82	ASP	C	-23.46	-19.26	78.19	12.50
82	ASP	O	-23.92	-19.70	77.14	15.36
83	SER	N	-24.03	-18.28	78.87	11.91
83	SER	CA	-25.23	-17.61	78.39	12.55

TABLE VII

83	SER	CB	-26.14	-17.24	79.55	18.80
83	SER	OG	-25.48	-16.36	80.45	22.70
83	SER	C	-24.78	-16.35	77.64	9.20
83	SER	O	-23.59	-16.01	77.64	5.74
84	GLU	N	-25.71	-15.67	76.99	9.19
84	GLU	CA	-25.33	-14.43	76.31	14.72
84	GLU	CB	-26.47	-13.88	75.45	13.64
84	GLU	CG	-26.29	-14.13	73.96	13.53
84	GLU	CD	-25.09	-13.41	73.36	12.40
84	GLU	OE1	-24.88	-12.23	73.68	14.45
84	GLU	OE2	-24.38	-14.02	72.56	16.00
84	GLU	C	-24.86	-13.42	77.35	15.76
84	GLU	O	-23.85	-12.75	77.16	15.77
85	ASP	N	-25.57	-13.36	78.49	18.15
85	ASP	CA	-25.21	-12.45	79.58	18.14
85	ASP	CB	-26.05	-12.73	80.84	21.42
85	ASP	CG	-27.47	-12.20	80.72	27.07
85	ASP	OD1	-28.43	-12.97	80.98	25.69
85	ASP	OD2	-27.63	-11.01	80.38	28.79
85	ASP	C	-23.73	-12.56	79.90	20.03
85	ASP	O	-22.98	-11.59	79.78	24.76
86	ALA	N	-23.32	-13.77	80.28	17.91
86	ALA	CA	-21.93	-14.08	80.62	16.67
86	ALA	CB	-21.87	-15.44	81.30	15.93
86	ALA	C	-20.99	-14.07	79.41	19.50
86	ALA	O	-19.76	-14.03	79.57	22.48
87	TYR	N	-21.56	-14.13	78.21	16.64
87	TYR	CA	-20.72	-14.15	77.01	16.44
87	TYR	CB	-20.31	-15.59	76.69	12.21
87	TYR	CG	-18.90	-15.72	76.20	5.93
87	TYR	CD1	-18.37	-14.81	75.28	6.36
87	TYR	CE1	-17.08	-14.96	74.80	2.57
87	TYR	CD2	-18.10	-16.78	76.62	7.25
87	TYR	CE2	-16.81	-16.93	76.14	3.11
87	TYR	CZ	-16.31	-16.01	75.23	2.00
87	TYR	OH	-15.04	-16.18	74.72	8.83
87	TYR	C	-21.41	-13.49	75.82	16.77
87	TYR	O	-21.87	-14.18	74.91	22.23
88	PRO	N	-21.48	-12.15	75.80	15.42
88	PRO	CD	-20.91	-11.18	76.74	12.94
88	PRO	CA	-22.13	-11.44	74.70	13.08
88	PRO	CB	-21.96	-9.97	75.08	12.38

TABLE VII

88	PRO	CG	-21.82	-10.00	76.55	9.35
88	PRO	C	-21.49	-11.72	73.35	14.00
88	PRO	O	-20.33	-12.14	73.27	15.05
89	TYR	N	-22.25	-11.52	72.28	13.57
89	TYR	CA	-21.77	-11.73	70.93	14.96
89	TYR	CB	-22.90	-12.16	69.99	16.79
89	TYR	CG	-22.46	-12.46	68.56	19.46
89	TYR	CD1	-21.64	-13.54	68.28	17.96
89	TYR	CE1	-21.26	-13.85	66.98	20.62
89	TYR	CD2	-22.90	-11.67	67.49	17.49
89	TYR	CE2	-22.53	-11.96	66.17	17.03
89	TYR	CZ	-21.70	-13.06	65.92	17.44
89	TYR	OH	-21.28	-13.36	64.65	16.20
89	TYR	C	-21.11	-10.47	70.39	14.19
89	TYR	O	-21.79	-9.45	70.23	14.43
90	VAL	N	-19.80	-10.50	70.18	11.92
90	VAL	CA	-19.15	-9.33	69.61	12.81
90	VAL	CB	-17.69	-9.13	70.09	11.22
90	VAL	CG1	-17.68	-8.76	71.57	19.09
90	VAL	CG2	-16.84	-10.35	69.83	10.92
90	VAL	C	-19.21	-9.39	68.09	14.23
90	VAL	O	-19.09	-8.36	67.42	14.19
91	GLY	N	-19.44	-10.58	67.53	14.09
91	GLY	CA	-19.52	-10.72	66.09	15.26
91	GLY	C	-18.16	-10.68	65.44	18.32
91	GLY	O	-18.01	-10.38	64.24	16.36
92	GLN	N	-17.16	-11.06	66.23	20.31
92	GLN	CA	-15.78	-11.06	65.81	20.17
92	GLN	CB	-15.16	-9.69	66.09	23.65
92	GLN	CG	-13.83	-9.44	65.42	28.99
92	GLN	CD	-13.36	-8.00	65.62	34.47
92	GLN	OE1	-14.10	-7.15	66.15	34.75
92	GLN	NE2	-12.14	-7.72	65.19	37.63
92	GLN	C	-15.09	-12.17	66.60	20.89
92	GLN	O	-15.53	-12.53	67.70	18.43
93	GLU	N	-14.04	-12.73	66.03	22.82
93	GLU	CA	-13.31	-13.81	66.69	24.92
93	GLU	CB	-12.63	-14.74	65.66	27.98
93	GLU	CG	-12.23	-16.10	66.22	29.38
93	GLU	CD	-12.00	-17.17	65.15	34.25
93	GLU	OE1	-12.30	-16.93	63.95	35.80
93	GLU	OE2	-11.52	-18.26	65.52	34.14

TABLE VII

93	GLU	C	-12.31	-13.29	67.71	24.19
93	GLU	O	-11.61	-12.31	67.45	24.56
94	GLU	N	-12.28	-13.94	68.87	23.61
94	GLU	CA	-11.38	-13.58	69.96	24.32
94	GLU	CB	-12.02	-12.55	70.90	22.62
94	GLU	CG	-12.23	-11.20	70.27	23.90
94	GLU	CD	-12.86	-10.23	71.21	24.44
94	GLU	OE1	-12.18	-9.26	71.60	29.56
94	GLU	OE2	-14.04	-10.43	71.57	23.54
94	GLU	C	-10.99	-14.84	70.73	23.80
94	GLU	O	-11.64	-15.89	70.59	21.98
95	SER	N	-9.95	-14.73	71.55	20.75
95	SER	CA	-9.47	-15.86	72.36	19.71
95	SER	CB	-8.26	-15.46	73.19	20.00
95	SER	OG	-8.57	-14.41	74.09	24.28
95	SER	C	-10.60	-16.38	73.25	20.63
95	SER	O	-11.48	-15.60	73.65	22.33
96	CYS	N	-10.56	-17.66	73.58	17.74
96	CYS	CA	-11.60	-18.26	74.42	18.66
96	CYS	C	-11.59	-17.72	75.85	19.92
96	CYS	O	-10.58	-17.79	76.56	21.50
96	CYS	CB	-11.51	-19.78	74.41	16.39
96	CYS	SG	-12.75	-20.61	75.44	19.58
97	MET	N	-12.72	-17.14	76.26	17.89
97	MET	CA	-12.88	-16.59	77.60	18.67
97	MET	CB	-12.86	-15.07	77.57	17.60
97	MET	CG	-12.76	-14.43	78.94	18.29
97	MET	SD	-11.15	-13.66	79.17	26.40
97	MET	CE	-9.99	-15.01	78.76	19.16
97	MET	C	-14.18	-17.09	78.20	21.66
97	MET	O	-15.07	-16.31	78.52	25.61
98	TYR	N	-14.30	-18.41	78.29	23.47
98	TYR	CA	-15.49	-19.06	78.83	23.75
98	TYR	CB	-15.58	-20.50	78.30	21.70
98	TYR	CG	-16.39	-21.46	79.13	18.51
98	TYR	CD1	-17.74	-21.64	78.90	18.20
98	TYR	CE1	-18.49	-22.49	79.70	19.99
98	TYR	CD2	-15.80	-22.16	80.17	16.39
98	TYR	CE2	-16.53	-23.01	80.97	12.68
98	TYR	CZ	-17.87	-23.17	80.74	16.90
98	TYR	OH	-18.60	-23.99	81.57	22.57
98	TYR	C	-15.48	-19.01	80.37	26.07

TABLE VII

98	TYR	O	-14.44	-19.23	80.99	27.32
99	ASN	N	-16.63	-18.67	80.96	28.21
99	ASN	CA	-16.76	-18.59	82.42	27.40
99	ASN	CB	-17.24	-17.20	82.85	30.57
99	ASN	CG	-17.89	-17.21	84.22	33.86
99	ASN	OD1	-19.06	-16.84	84.36	33.41
99	ASN	ND2	-17.16	-17.66	85.24	34.39
99	ASN	C	-17.67	-19.66	83.03	25.48
99	ASN	O	-18.88	-19.64	82.82	25.31
100	PRO	N	-17.12	-20.53	83.87	22.21
100	PRO	CD	-15.70	-20.60	84.27	21.06
100	PRO	CA	-17.89	-21.60	84.50	19.72
100	PRO	CB	-16.89	-22.18	85.49	21.18
100	PRO	CG	-15.58	-22.01	84.75	22.13
100	PRO	C	-19.14	-21.08	85.22	19.80
100	PRO	O	-20.22	-21.65	85.09	15.82
101	THR	N	-18.98	-19.97	85.92	22.73
101	THR	CA	-20.07	-19.36	86.68	23.85
101	THR	CB	-19.53	-18.25	87.60	22.86
101	THR	OG1	-18.13	-18.47	87.87	20.58
101	THR	CG2	-20.28	-18.26	88.92	21.48
101	THR	C	-21.22	-18.80	85.82	24.75
101	THR	O	-22.30	-18.46	86.33	22.15
102	GLY	N	-20.96	-18.70	84.51	25.15
102	GLY	CA	-21.96	-18.20	83.59	21.81
102	GLY	C	-22.72	-19.34	82.94	19.11
102	GLY	O	-23.78	-19.12	82.36	19.57
103	LYS	N	-22.15	-20.55	83.03	18.20
103	LYS	CA	-22.73	-21.77	82.47	16.81
103	LYS	CB	-22.08	-23.02	83.07	16.94
103	LYS	CG	-22.90	-24.30	82.93	15.32
103	LYS	CD	-22.03	-25.53	83.10	18.87
103	LYS	CE	-21.32	-25.57	84.46	21.19
103	LYS	NZ	-20.02	-26.34	84.40	20.74
103	LYS	C	-24.24	-21.83	82.62	17.92
103	LYS	O	-24.78	-21.68	83.72	18.81
104	ALA	N	-24.92	-22.05	81.50	17.95
104	ALA	CA	-26.38	-22.11	81.49	17.78
104	ALA	CB	-26.93	-21.14	80.47	21.54
104	ALA	C	-26.84	-23.52	81.18	18.07
104	ALA	O	-27.99	-23.88	81.47	16.81
105	ALA	N	-25.95	-24.31	80.58	15.87

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105	ALA	CA	-26.27	-25.69	80.23	13.04
105	ALA	CB	-27.41	-25.72	79.22	10.01
105	ALA	C	-25.05	-26.40	79.66	11.95
105	ALA	O	-23.94	-25.86	79.68	8.46
106	LYS	N	-25.27	-27.63	79.20	12.25
106	LYS	CA	-24.24	-28.45	78.57	18.76
106	LYS	CB	-23.26	-29.07	79.58	23.73
106	LYS	CG	-23.89	-30.02	80.60	26.39
106	LYS	CD	-22.88	-31.05	81.09	29.44
106	LYS	CE	-23.54	-32.05	82.06	33.28
106	LYS	NZ	-24.76	-32.74	81.51	24.10
106	LYS	C	-24.95	-29.54	77.77	18.52
106	LYS	O	-26.18	-29.49	77.64	16.87
107	CYS	N	-24.21	-30.50	77.22	19.97
107	CYS	CA	-24.81	-31.59	76.45	21.83
107	CYS	CB	-25.13	-31.16	75.00	23.15
107	CYS	SG	-23.72	-30.88	73.87	21.75
107	CYS	C	-23.98	-32.87	76.48	22.08
107	CYS	O	-22.75	-32.84	76.60	21.41
108	ARG	N	-24.66	-34.00	76.40	22.61
108	ARG	CA	-23.96	-35.28	76.44	25.98
108	ARG	CB	-24.57	-36.18	77.53	25.00
108	ARG	CG	-24.76	-35.44	78.85	19.33
108	ARG	CD	-25.24	-36.32	79.99	17.89
108	ARG	NE	-26.61	-36.80	79.81	10.20
108	ARG	CZ	-27.00	-38.02	80.15	9.00
108	ARG	NH1	-26.12	-38.88	80.68	6.62
108	ARG	NH2	-28.26	-38.39	79.99	10.32
108	ARG	C	-23.91	-35.98	75.08	23.86
108	ARG	O	-24.38	-37.10	74.94	25.08
109	GLY	N	-23.34	-35.29	74.10	23.61
109	GLY	CA	-23.21	-35.84	72.76	20.68
109	GLY	C	-24.30	-35.35	71.82	18.95
109	GLY	O	-25.15	-34.56	72.22	19.25
110	TYR	N	-24.29	-35.85	70.58	18.18
110	TYR	CA	-25.27	-35.46	69.57	17.03
110	TYR	CB	-24.72	-34.38	68.64	14.76
110	TYR	CG	-23.48	-34.81	67.90	12.25
110	TYR	CD1	-22.21	-34.48	68.37	14.76
110	TYR	CE1	-21.06	-34.95	67.75	14.89
110	TYR	CD2	-23.56	-35.61	66.78	12.73
110	TYR	CE2	-22.41	-36.08	66.14	15.02

TABLE VII

110	TYR	CZ	-21.17	-35.75	66.64	17.33
110	TYR	OH	-20.03	-36.26	66.03	22.26
110	TYR	C	-25.70	-36.67	68.75	16.81
110	TYR	O	-25.01	-37.69	68.73	19.27
111	ARG	N	-26.83	-36.53	68.07	16.77
111	ARG	CA	-27.34	-37.57	67.19	18.25
111	ARG	CB	-28.73	-38.08	67.60	20.39
111	ARG	CG	-29.51	-38.81	66.48	21.92
111	ARG	CD	-28.94	-40.20	66.16	26.51
111	ARG	NE	-29.54	-40.85	64.98	25.17
111	ARG	CZ	-28.83	-41.49	64.03	26.40
111	ARG	NH1	-27.50	-41.55	64.12	21.95
111	ARG	NH2	-29.45	-42.10	63.02	18.73
111	ARG	C	-27.43	-36.92	65.81	20.54
111	ARG	O	-27.88	-35.77	65.69	23.20
112	GLU	N	-26.95	-37.62	64.79	17.24
112	GLU	CA	-27.01	-37.12	63.42	13.69
112	GLU	CB	-25.70	-37.34	62.69	12.60
112	GLU	CG	-24.59	-36.38	63.05	10.04
112	GLU	CD	-23.25	-36.92	62.62	11.35
112	GLU	OE1	-22.50	-36.23	61.89	10.65
112	GLU	OE2	-22.97	-38.06	63.01	14.44
112	GLU	C	-28.15	-37.85	62.72	15.47
112	GLU	O	-28.49	-38.97	63.09	17.83
113	ILE	N	-28.72	-37.25	61.70	17.43
113	ILE	CA	-29.82	-37.87	60.96	14.32
113	ILE	CB	-30.99	-36.87	60.90	13.01
113	ILE	CG2	-32.04	-37.32	59.87	11.54
113	ILE	CG1	-31.55	-36.70	62.33	10.24
113	ILE	CD1	-32.35	-35.44	62.57	7.36
113	ILE	C	-29.38	-38.34	59.57	12.75
113	ILE	O	-28.59	-37.68	58.91	11.81
114	PRO	N	-29.83	-39.53	59.13	15.44
114	PRO	CD	-30.82	-40.40	59.80	19.88
114	PRO	CA	-29.47	-40.08	57.81	15.21
114	PRO	CB	-30.54	-41.13	57.59	15.21
114	PRO	CG	-30.79	-41.66	58.96	16.85
114	PRO	C	-29.53	-39.00	56.73	18.58
114	PRO	O	-30.52	-38.27	56.64	21.69
115	GLU	N	-28.49	-38.91	55.91	17.93
115	GLU	CA	-28.45	-37.90	54.87	18.15
115	GLU	CB	-27.12	-37.95	54.11	21.41

TABLE VII

115	GLU	CG	-27.04	-39.05	53.06	28.55
115	GLU	CD	-25.73	-39.04	52.26	34.52
115	GLU	OE1	-25.24	-37.94	51.90	34.27
115	GLU	OE2	-25.21	-40.14	51.99	34.99
115	GLU	C	-29.63	-37.99	53.90	20.57
115	GLU	O	-30.10	-39.08	53.56	20.47
116	GLY	N	-30.13	-36.82	53.51	21.25
116	GLY	CA	-31.24	-36.73	52.58	19.05
116	GLY	C	-32.59	-37.14	53.12	19.97
116	GLY	O	-33.62	-36.74	52.56	24.15
117	ASN	N	-32.62	-37.87	54.23	17.37
117	ASN	CA	-33.90	-38.33	54.77	15.93
117	ASN	CB	-33.73	-39.57	55.64	10.26
117	ASN	CG	-35.03	-40.34	55.79	12.00
117	ASN	OD1	-36.12	-39.76	55.79	10.30
117	ASN	ND2	-34.92	-41.66	55.91	13.10
117	ASN	C	-34.73	-37.30	55.49	17.41
117	ASN	O	-34.57	-37.09	56.70	18.71
118	GLU	N	-35.66	-36.70	54.77	15.53
118	GLU	CA	-36.56	-35.71	55.34	15.33
118	GLU	CB	-37.27	-34.93	54.25	15.94
118	GLU	CG	-36.37	-34.00	53.46	22.20
118	GLU	CD	-37.14	-33.16	52.46	21.94
118	GLU	OE1	-37.27	-33.58	51.29	25.99
118	GLU	OE2	-37.64	-32.08	52.85	25.26
118	GLU	C	-37.57	-36.30	56.33	18.60
118	GLU	O	-38.02	-35.60	57.23	23.43
119	LYS	N	-37.93	-37.57	56.17	19.21
119	LYS	CA	-38.89	-38.21	57.08	17.16
119	LYS	CB	-39.39	-39.55	56.54	18.23
119	LYS	CG	-40.29	-39.44	55.34	23.03
119	LYS	CD	-41.48	-38.55	55.62	24.88
119	LYS	CE	-41.85	-37.77	54.36	33.17
119	LYS	NZ	-40.65	-37.07	53.78	35.51
119	LYS	C	-38.30	-38.39	58.44	13.83
119	LYS	O	-38.99	-38.27	59.45	14.48
120	ALA	N	-37.02	-38.74	58.47	11.43
120	ALA	CA	-36.30	-38.93	59.71	11.35
120	ALA	CB	-34.91	-39.44	59.43	12.94
120	ALA	C	-36.23	-37.57	60.34	14.11
120	ALA	O	-36.49	-37.41	61.53	20.36
121	LEU	N	-35.94	-36.57	59.52	14.09

TABLE VII

121	LEU	CA	-35.84	-35.19	59.98	14.37
121	LEU	CB	-35.35	-34.28	58.86	11.45
121	LEU	CG	-35.11	-32.82	59.20	13.53
121	LEU	CD1	-34.22	-32.69	60.44	17.91
121	LEU	CD2	-34.49	-32.13	57.98	13.43
121	LEU	C	-37.17	-34.71	60.57	14.14
121	LEU	O	-37.19	-34.08	61.63	17.50
122	LYS	N	-38.28	-35.01	59.90	14.51
122	LYS	CA	-39.61	-34.63	60.36	14.97
122	LYS	CB	-40.67	-34.97	59.32	15.25
122	LYS	CG	-42.09	-34.67	59.75	15.73
122	LYS	CD	-43.09	-35.54	59.00	15.63
122	LYS	CE	-44.48	-35.36	59.56	22.12
122	LYS	NZ	-45.45	-36.35	59.02	25.27
122	LYS	C	-39.93	-35.32	61.69	17.92
122	LYS	O	-40.58	-34.74	62.58	15.41
123	ARG	N	-39.51	-36.57	61.80	20.19
123	ARG	CA	-39.71	-37.36	63.00	24.53
123	ARG	CB	-39.36	-38.82	62.76	26.04
123	ARG	CG	-40.37	-39.57	61.92	29.94
123	ARG	CD	-39.79	-40.87	61.39	33.27
123	ARG	NE	-38.98	-41.56	62.39	38.93
123	ARG	CZ	-37.67	-41.79	62.26	38.64
123	ARG	NH1	-37.03	-41.37	61.18	39.92
123	ARG	NH2	-37.00	-42.45	63.20	34.71
123	ARG	C	-38.89	-36.77	64.14	25.64
123	ARG	O	-39.33	-36.76	65.30	25.72
124	ALA	N	-37.70	-36.26	63.80	23.74
124	ALA	CA	-36.80	-35.64	64.77	25.05
124	ALA	CB	-35.49	-35.23	64.09	22.46
124	ALA	C	-37.48	-34.41	65.37	24.90
124	ALA	O	-37.50	-34.23	66.59	25.58
125	VAL	N	-38.02	-33.57	64.50	25.44
125	VAL	CA	-38.69	-32.35	64.92	24.60
125	VAL	CB	-39.08	-31.46	63.72	20.30
125	VAL	CG1	-39.85	-30.23	64.19	13.27
125	VAL	CG2	-37.80	-31.05	62.95	19.58
125	VAL	C	-39.93	-32.66	65.73	24.17
125	VAL	O	-40.19	-32.01	66.73	26.08
126	ALA	N	-40.69	-33.66	65.32	25.26
126	ALA	CA	-41.90	-34.00	66.05	26.85
126	ALA	CB	-42.65	-35.08	65.34	27.49

TABLE VII

126	ALA	C	-41.59	-34.41	67.50	28.51
126	ALA	O	-42.22	-33.91	68.43	29.45
127	ARG	N	-40.60	-35.30	67.68	27.15
127	ARG	CA	-40.20	-35.80	69.01	26.50
127	ARG	CB	-39.52	-37.17	68.92	25.80
127	ARG	CG	-40.36	-38.31	68.39	29.17
127	ARG	CD	-41.39	-38.82	69.38	30.20
127	ARG	NE	-42.01	-40.06	68.90	31.67
127	ARG	CZ	-43.14	-40.57	69.38	31.87
127	ARG	NH1	-43.62	-41.70	68.87	32.34
127	ARG	NH2	-43.80	-39.97	70.36	33.34
127	ARG	C	-39.30	-34.88	69.83	26.63
127	ARG	O	-39.61	-34.54	70.98	29.49
128	VAL	N	-38.13	-34.58	69.27	24.07
128	VAL	CA	-37.14	-33.75	69.93	20.27
128	VAL	CB	-35.74	-33.96	69.29	17.18
128	VAL	CG1	-34.73	-33.00	69.87	16.62
128	VAL	CG2	-35.27	-35.40	69.51	16.17
128	VAL	C	-37.51	-32.28	69.92	19.91
128	VAL	O	-38.00	-31.75	70.91	21.31
129	GLY	N	-37.26	-31.63	68.79	21.40
129	GLY	CA	-37.56	-30.22	68.67	18.08
129	GLY	C	-36.62	-29.60	67.67	17.76
129	GLY	O	-36.22	-30.27	66.71	14.46
130	PRO	N	-36.25	-28.33	67.86	18.11
130	PRO	CD	-36.68	-27.44	68.96	20.59
130	PRO	CA	-35.35	-27.64	66.94	17.36
130	PRO	CB	-35.03	-26.36	67.70	17.67
130	PRO	CG	-36.33	-26.07	68.41	19.12
130	PRO	C	-34.10	-28.47	66.69	18.18
130	PRO	O	-33.43	-28.92	67.63	21.49
131	VAL	N	-33.81	-28.71	65.41	14.71
131	VAL	CA	-32.66	-29.47	64.99	10.15
131	VAL	CB	-33.09	-30.69	64.16	13.09
131	VAL	CG1	-31.88	-31.39	63.55	14.17
131	VAL	CG2	-33.88	-31.63	65.02	19.95
131	VAL	C	-31.80	-28.60	64.10	10.57
131	VAL	O	-32.33	-27.86	63.27	13.19
132	SER	N	-30.49	-28.71	64.25	7.45
132	SER	CA	-29.59	-27.93	63.42	7.72
132	SER	CB	-28.23	-27.81	64.07	9.68
132	SER	OG	-28.37	-27.45	65.44	20.96

TABLE VII

132	SER	C	-29.48	-28.55	62.02	6.88
132	SER	O	-29.18	-29.74	61.86	4.58
133	VAL	N	-29.75	-27.75	61.00	7.92
133	VAL	CA	-29.68	-28.20	59.62	6.47
133	VAL	CB	-31.09	-28.35	59.00	6.27
133	VAL	CG1	-31.92	-29.35	59.80	5.31
133	VAL	CG2	-31.80	-27.00	58.93	2.32
133	VAL	C	-28.88	-27.20	58.78	6.11
133	VAL	O	-28.93	-25.99	59.01	4.92
134	ALA	N	-28.09	-27.71	57.85	8.55
134	ALA	CA	-27.29	-26.90	56.94	10.56
134	ALA	CB	-25.90	-27.49	56.80	10.48
134	ALA	C	-28.01	-26.89	55.59	11.28
134	ALA	O	-28.61	-27.91	55.19	10.70
135	ILE	N	-28.00	-25.75	54.91	5.87
135	ILE	CA	-28.65	-25.64	53.61	9.02
135	ILE	CB	-30.05	-25.04	53.75	9.82
135	ILE	CG2	-30.96	-25.98	54.52	8.18
135	ILE	CG1	-29.97	-23.67	54.42	7.95
135	ILE	CD1	-31.24	-22.87	54.30	5.36
135	ILE	C	-27.84	-24.75	52.67	10.58
135	ILE	O	-26.82	-24.17	53.08	11.83
136	ASP	N	-28.27	-24.67	51.41	14.26
136	ASP	CA	-27.64	-23.83	50.39	12.77
136	ASP	CB	-27.59	-24.54	49.03	11.56
136	ASP	CG	-27.29	-23.58	47.87	11.70
136	ASP	OD1	-27.82	-23.80	46.77	16.82
136	ASP	OD2	-26.54	-22.61	48.06	6.89
136	ASP	C	-28.44	-22.53	50.29	11.76
136	ASP	O	-29.51	-22.50	49.69	12.86
137	ALA	N	-27.90	-21.45	50.83	12.10
137	ALA	CA	-28.63	-20.19	50.80	14.12
137	ALA	CB	-28.77	-19.64	52.22	16.96
137	ALA	C	-28.02	-19.14	49.87	15.39
137	ALA	O	-28.27	-17.94	50.04	11.83
138	SER	N	-27.20	-19.57	48.91	16.46
138	SER	CA	-26.56	-18.66	47.96	16.14
138	SER	CB	-25.45	-19.36	47.17	13.20
138	SER	OG	-25.91	-20.60	46.65	11.80
138	SER	C	-27.54	-17.97	47.02	17.22
138	SER	O	-27.42	-16.77	46.74	16.85
139	LEU	N	-28.50	-18.75	46.53	11.84

TABLE VII

139	LEU	CA	-29.51	-18.24	45.62	10.88
139	LEU	CB	-30.62	-19.27	45.41	10.28
139	LEU	CG	-30.39	-20.25	44.25	7.79
139	LEU	CD1	-28.98	-20.81	44.28	16.09
139	LEU	CD2	-31.39	-21.35	44.31	6.66
139	LEU	C	-30.07	-16.90	46.07	10.95
139	LEU	O	-30.56	-16.77	47.18	10.84
140	THR	N	-29.98	-15.89	45.20	12.65
140	THR	CA	-30.48	-14.56	45.55	10.04
140	THR	CB	-30.04	-13.47	44.54	8.74
140	THR	OG1	-30.71	-13.68	43.29	16.41
140	THR	CG2	-28.52	-13.50	44.33	5.90
140	THR	C	-31.98	-14.51	45.76	7.53
140	THR	O	-32.51	-13.48	46.16	7.86
141	SER	N	-32.69	-15.60	45.48	7.62
141	SER	CA	-34.13	-15.60	45.71	10.59
141	SER	CB	-34.81	-16.69	44.90	7.78
141	SER	OG	-34.14	-17.92	45.09	10.19
141	SER	C	-34.32	-15.81	47.21	14.46
141	SER	O	-35.31	-15.38	47.80	15.07
142	PHE	N	-33.33	-16.47	47.81	16.29
142	PHE	CA	-33.32	-16.75	49.24	18.29
142	PHE	CB	-32.26	-17.80	49.57	19.91
142	PHE	CG	-32.23	-18.22	51.01	19.34
142	PHE	CD1	-32.83	-19.42	51.40	19.10
142	PHE	CD2	-31.58	-17.44	51.96	17.86
142	PHE	CE1	-32.77	-19.84	52.72	18.29
142	PHE	CE2	-31.52	-17.86	53.29	16.09
142	PHE	CZ	-32.12	-19.06	53.67	17.03
142	PHE	C	-33.04	-15.46	49.98	18.87
142	PHE	O	-33.70	-15.13	50.96	20.82
143	GLN	N	-32.06	-14.71	49.48	17.89
143	GLN	CA	-31.69	-13.46	50.11	17.94
143	GLN	CB	-30.35	-12.98	49.56	20.86
143	GLN	CG	-29.29	-14.07	49.66	27.97
143	GLN	CD	-27.96	-13.66	49.06	35.25
143	GLN	OE1	-27.88	-12.65	48.36	42.66
143	GLN	NE2	-26.91	-14.44	49.35	32.14
143	GLN	C	-32.77	-12.40	49.97	16.38
143	GLN	O	-32.78	-11.43	50.72	21.06
144	PHE	N	-33.71	-12.62	49.07	16.70
144	PHE	CA	-34.81	-11.68	48.86	16.93

TABLE VII

144	PHE	CB	-34.83	-11.16	47.42	14.35
144	PHE	CG	-33.63	-10.34	47.06	9.94
144	PHE	CD1	-33.23	-9.28	47.87	7.40
144	PHE	CD2	-32.87	-10.63	45.94	11.47
144	PHE	CE1	-32.09	-8.54	47.58	2.23
144	PHE	CE2	-31.73	-9.89	45.63	11.16
144	PHE	CZ	-31.34	-8.85	46.45	5.01
144	PHE	C	-36.15	-12.29	49.26	19.07
144	PHE	O	-37.21	-11.75	48.94	23.82
145	TYR	N	-36.10	-13.42	49.95	21.54
145	TYR	CA	-37.31	-14.10	50.39	20.66
145	TYR	CB	-36.98	-15.43	51.09	19.50
145	TYR	CG	-38.13	-16.04	51.85	20.41
145	TYR	CD1	-38.96	-16.98	51.25	22.31
145	TYR	CE1	-40.05	-17.51	51.93	23.37
145	TYR	CD2	-38.43	-15.64	53.15	19.98
145	TYR	CE2	-39.52	-16.16	53.84	20.51
145	TYR	CZ	-40.33	-17.09	53.22	22.20
145	TYR	OH	-41.42	-17.60	53.89	24.45
145	TYR	C	-38.13	-13.18	51.31	19.31
145	TYR	O	-37.57	-12.41	52.09	16.29
146	SER	N	-39.44	-13.29	51.23	19.16
146	SER	CA	-40.31	-12.46	52.05	18.38
146	SER	CB	-40.69	-11.17	51.33	21.74
146	SER	OG	-41.24	-11.45	50.05	25.62
146	SER	C	-41.55	-13.21	52.52	17.33
146	SER	O	-41.87	-13.19	53.70	17.00
147	LYS	N	-42.21	-13.90	51.60	15.30
147	LYS	CA	-43.42	-14.63	51.94	16.47
147	LYS	CB	-44.65	-13.72	51.85	21.13
147	LYS	CG	-45.98	-14.43	52.13	26.90
147	LYS	CD	-47.15	-13.75	51.41	31.88
147	LYS	CE	-48.38	-14.69	51.35	38.13
147	LYS	NZ	-49.45	-14.23	50.41	36.35
147	LYS	C	-43.61	-15.88	51.09	16.19
147	LYS	O	-43.21	-15.91	49.92	18.85
148	GLY	N	-44.20	-16.91	51.69	14.07
148	GLY	CA	-44.47	-18.14	50.98	13.24
148	GLY	C	-43.46	-19.26	51.17	12.23
148	GLY	O	-42.39	-19.05	51.74	11.43
149	VAL	N	-43.82	-20.45	50.71	9.32
149	VAL	CA	-42.95	-21.61	50.81	8.20

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149	VAL	CB	-43.70	-22.96	50.60	5.83
149	VAL	CG1	-42.72	-24.11	50.73	2.00
149	VAL	CG2	-44.82	-23.12	51.61	4.34
149	VAL	C	-41.92	-21.43	49.70	11.54
149	VAL	O	-42.25	-21.45	48.50	12.48
150	TYR	N	-40.68	-21.21	50.13	12.91
150	TYR	CA	-39.55	-21.02	49.24	10.42
150	TYR	CB	-38.33	-20.58	50.03	4.78
150	TYR	CG	-37.10	-20.42	49.19	8.23
150	TYR	CD1	-36.83	-19.21	48.55	10.09
150	TYR	CE1	-35.68	-19.06	47.77	11.54
150	TYR	CD2	-36.21	-21.47	49.02	8.80
150	TYR	CE2	-35.07	-21.33	48.24	9.65
150	TYR	CZ	-34.81	-20.13	47.62	10.30
150	TYR	OH	-33.67	-19.97	46.88	18.73
150	TYR	C	-39.27	-22.30	48.46	14.00
150	TYR	O	-39.45	-23.40	48.96	16.63
151	TYR	N	-38.79	-22.13	47.24	15.66
151	TYR	CA	-38.48	-23.25	46.37	17.45
151	TYR	CB	-39.74	-24.04	46.01	21.54
151	TYR	CG	-39.53	-25.25	45.13	23.93
151	TYR	CD1	-38.93	-26.42	45.64	28.17
151	TYR	CE1	-38.74	-27.54	44.83	29.69
151	TYR	CD2	-39.94	-25.25	43.80	26.78
151	TYR	CE2	-39.76	-26.36	42.99	29.59
151	TYR	CZ	-39.16	-27.50	43.51	32.44
151	TYR	OH	-38.99	-28.60	42.70	37.61
151	TYR	C	-37.85	-22.60	45.15	18.03
151	TYR	O	-38.32	-21.56	44.68	16.75
152	ASP	N	-36.76	-23.17	44.68	19.75
152	ASP	CA	-36.05	-22.64	43.52	21.69
152	ASP	CB	-35.07	-21.53	43.91	21.35
152	ASP	CG	-34.48	-20.80	42.70	22.73
152	ASP	OD1	-34.58	-19.56	42.63	20.20
152	ASP	OD2	-33.90	-21.46	41.82	23.61
152	ASP	C	-35.33	-23.85	42.96	25.58
152	ASP	O	-34.67	-24.57	43.72	28.85
153	GLU	N	-35.50	-24.09	41.66	26.65
153	GLU	CA	-34.86	-25.25	41.03	26.63
153	GLU	CB	-35.52	-25.57	39.69	30.19
153	GLU	CG	-36.09	-24.38	38.92	34.99
153	GLU	CD	-35.04	-23.61	38.15	37.99

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153	GLU	OE1	-34.95	-22.38	38.34	40.14
153	GLU	OE2	-34.31	-24.24	37.34	40.23
153	GLU	C	-33.34	-25.20	40.91	24.39
153	GLU	O	-32.71	-26.22	40.70	23.54
154	SER	N	-32.75	-24.02	41.11	23.15
154	SER	CA	-31.30	-23.83	41.04	25.05
154	SER	CB	-30.95	-22.35	40.85	24.11
154	SER	OG	-31.81	-21.71	39.91	26.07
154	SER	C	-30.53	-24.38	42.26	25.62
154	SER	O	-29.37	-24.78	42.15	26.42
155	CYS	N	-31.19	-24.33	43.43	24.27
155	CYS	CA	-30.63	-24.77	44.71	19.73
155	CYS	C	-29.88	-26.08	44.59	17.05
155	CYS	O	-30.44	-27.08	44.16	14.86
155	CYS	CB	-31.72	-24.87	45.79	20.11
155	CYS	SG	-31.27	-24.12	47.40	19.94
156	ASN	N	-28.61	-26.07	44.99	19.11
156	ASN	CA	-27.76	-27.26	44.92	21.62
156	ASN	CB	-26.37	-26.87	44.41	19.84
156	ASN	CG	-25.47	-28.06	44.20	20.15
156	ASN	OD1	-25.86	-29.20	44.44	15.60
156	ASN	ND2	-24.23	-27.80	43.77	19.95
156	ASN	C	-27.67	-28.05	46.24	22.71
156	ASN	O	-27.08	-27.58	47.21	23.56
157	SER	N	-28.20	-29.28	46.23	22.09
157	SER	CA	-28.22	-30.17	47.40	16.83
157	SER	CB	-28.93	-31.49	47.06	14.81
157	SER	OG	-30.26	-31.26	46.66	19.44
157	SER	C	-26.86	-30.49	48.02	17.43
157	SER	O	-26.78	-31.10	49.10	16.02
158	ASP	N	-25.79	-30.19	47.30	17.73
158	ASP	CA	-24.46	-30.46	47.80	20.40
158	ASP	CB	-23.70	-31.42	46.88	24.69
158	ASP	CG	-24.27	-32.82	46.89	27.15
158	ASP	OD1	-24.93	-33.19	45.88	26.00
158	ASP	OD2	-24.08	-33.55	47.90	26.52
158	ASP	C	-23.68	-29.19	48.00	20.27
158	ASP	O	-22.46	-29.22	48.16	20.24
159	ASN	N	-24.39	-28.07	47.97	17.11
159	ASN	CA	-23.72	-26.81	48.19	16.88
159	ASN	CB	-24.01	-25.79	47.10	18.24
159	ASN	CG	-23.00	-24.66	47.10	21.17

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159	ASN	OD1	-21.83	-24.86	47.42	16.98
159	ASN	ND2	-23.46	-23.46	46.75	22.38
159	ASN	C	-24.12	-26.28	49.55	17.56
159	ASN	O	-24.64	-25.17	49.67	19.13
160	LEU	N	-23.93	-27.12	50.57	12.99
160	LEU	CA	-24.23	-26.73	51.94	8.24
160	LEU	CB	-24.00	-27.89	52.89	4.68
160	LEU	CG	-25.09	-28.95	53.11	5.66
160	LEU	CD1	-25.96	-29.16	51.89	3.96
160	LEU	CD2	-24.43	-30.24	53.54	6.24
160	LEU	C	-23.28	-25.58	52.23	8.29
160	LEU	O	-22.07	-25.75	52.11	8.75
161	ASN	N	-23.83	-24.41	52.54	9.39
161	ASN	CA	-23.02	-23.23	52.83	10.51
161	ASN	CB	-22.74	-22.43	51.56	14.18
161	ASN	CG	-24.01	-22.01	50.85	10.89
161	ASN	OD1	-24.80	-21.22	51.35	14.49
161	ASN	ND2	-24.21	-22.56	49.67	16.31
161	ASN	C	-23.56	-22.29	53.92	12.43
161	ASN	O	-23.02	-21.20	54.14	13.86
162	HIS	N	-24.62	-22.69	54.60	11.27
162	HIS	CA	-25.19	-21.85	55.64	10.37
162	HIS	CB	-26.13	-20.82	55.00	5.69
162	HIS	CG	-26.80	-19.89	55.96	6.06
162	HIS	CD2	-28.10	-19.79	56.33	6.15
162	HIS	ND1	-26.14	-18.85	56.61	11.02
162	HIS	CE1	-27.01	-18.16	57.33	5.27
162	HIS	NE2	-28.20	-18.71	57.17	6.68
162	HIS	C	-25.92	-22.76	56.61	11.99
162	HIS	O	-26.68	-23.63	56.20	15.71
163	ALA	N	-25.59	-22.65	57.89	14.09
163	ALA	CA	-26.22	-23.48	58.91	10.89
163	ALA	CB	-25.26	-23.79	60.01	12.33
163	ALA	C	-27.38	-22.67	59.43	8.08
163	ALA	O	-27.24	-21.48	59.69	7.93
164	VAL	N	-28.52	-23.33	59.61	8.61
164	VAL	CA	-29.73	-22.67	60.06	9.19
164	VAL	CB	-30.58	-22.36	58.82	13.42
164	VAL	CG1	-31.55	-23.51	58.50	8.48
164	VAL	CG2	-31.22	-21.00	58.93	12.71
164	VAL	C	-30.45	-23.60	61.06	9.94
164	VAL	O	-29.95	-24.69	61.35	11.85

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165	LEU	N	-31.59	-23.20	61.61	5.74
165	LEU	CA	-32.29	-24.07	62.58	6.61
165	LEU	CB	-32.27	-23.43	63.97	3.31
165	LEU	CG	-32.85	-24.20	65.15	2.00
165	LEU	CD1	-31.81	-25.14	65.69	3.91
165	LEU	CD2	-33.27	-23.20	66.22	3.66
165	LEU	C	-33.71	-24.47	62.20	8.12
165	LEU	O	-34.52	-23.62	61.80	12.38
166	ALA	N	-34.04	-25.75	62.36	6.76
166	ALA	CA	-35.37	-26.25	62.02	6.92
166	ALA	CB	-35.28	-27.67	61.50	5.38
166	ALA	C	-36.29	-26.20	63.24	9.15
166	ALA	O	-36.23	-27.07	64.10	12.12
167	VAL	N	-37.15	-25.19	63.30	10.50
167	VAL	CA	-38.06	-25.06	64.42	10.11
167	VAL	CB	-38.16	-23.60	64.93	9.38
167	VAL	CG1	-36.79	-23.07	65.35	2.39
167	VAL	CG2	-38.82	-22.71	63.88	7.39
167	VAL	C	-39.47	-25.56	64.11	10.07
167	VAL	O	-40.44	-25.13	64.73	12.94
168	GLY	N	-39.60	-26.47	63.16	9.76
168	GLY	CA	-40.93	-26.97	62.85	7.51
168	GLY	C	-41.09	-27.55	61.46	8.86
168	GLY	O	-40.11	-27.88	60.80	7.84
169	TYR	N	-42.34	-27.71	61.06	10.03
169	TYR	CA	-42.70	-28.24	59.76	12.55
169	TYR	CB	-42.20	-29.67	59.56	12.27
169	TYR	CG	-42.79	-30.71	60.51	12.03
169	TYR	CD1	-44.13	-31.06	60.43	9.03
169	TYR	CE1	-44.67	-32.02	61.26	9.87
169	TYR	CD2	-42.00	-31.35	61.45	11.40
169	TYR	CE2	-42.54	-32.31	62.30	8.77
169	TYR	CZ	-43.87	-32.64	62.19	6.67
169	TYR	OH	-44.45	-33.58	63.00	8.74
169	TYR	C	-44.21	-28.15	59.68	15.32
169	TYR	O	-44.88	-28.12	60.72	19.66
170	GLY	N	-44.77	-28.10	58.47	15.75
170	GLY	CA	-46.21	-28.00	58.36	13.53
170	GLY	C	-46.70	-28.03	56.94	14.99
170	GLY	O	-46.13	-28.72	56.09	14.31
171	ILE	N	-47.70	-27.21	56.66	17.47
171	ILE	CA	-48.28	-27.14	55.33	23.06

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171	ILE	CB	-49.37	-28.23	55.17	25.40
171	ILE	CG2	-50.56	-27.93	56.06	30.02
171	ILE	CG1	-49.86	-28.31	53.73	33.16
171	ILE	CD1	-49.86	-29.73	53.19	37.53
171	ILE	C	-48.86	-25.75	55.07	21.85
171	ILE	O	-49.14	-25.02	56.01	26.83
172	GLN	N	-48.95	-25.33	53.81	24.21
172	GLN	CA	-49.52	-24.03	53.46	24.63
172	GLN	CB	-48.53	-22.88	53.66	22.98
172	GLN	CG	-49.13	-21.50	53.34	24.04
172	GLN	CD	-48.15	-20.35	53.49	25.53
172	GLN	OE1	-47.37	-20.30	54.45	30.09
172	GLN	NE2	-48.17	-19.42	52.55	28.42
172	GLN	C	-50.02	-24.03	52.02	25.83
172	GLN	O	-49.24	-24.28	51.09	28.71
173	LYS	N	-51.32	-23.80	51.83	23.80
173	LYS	CA	-51.91	-23.78	50.49	22.33
173	LYS	CB	-51.58	-22.46	49.78	22.26
173	LYS	CG	-52.35	-21.23	50.29	26.56
173	LYS	CD	-53.81	-21.23	49.80	30.52
173	LYS	CE	-54.48	-19.85	49.89	29.44
173	LYS	NZ	-54.64	-19.30	51.27	28.52
173	LYS	C	-51.45	-24.98	49.66	21.89
173	LYS	O	-51.02	-24.84	48.52	22.66
174	GLY	N	-51.49	-26.16	50.27	21.87
174	GLY	CA	-51.08	-27.38	49.61	20.01
174	GLY	C	-49.59	-27.70	49.71	19.12
174	GLY	O	-49.18	-28.85	49.49	14.08
175	ASN	N	-48.79	-26.71	50.06	19.25
175	ASN	CA	-47.34	-26.90	50.16	22.03
175	ASN	CB	-46.59	-25.65	49.70	23.43
175	ASN	CG	-47.13	-25.08	48.40	26.87
175	ASN	OD1	-46.80	-25.56	47.31	24.31
175	ASN	ND2	-47.96	-24.04	48.52	27.46
175	ASN	C	-46.85	-27.30	51.56	22.36
175	ASN	O	-46.95	-26.52	52.51	22.73
176	LYS	N	-46.34	-28.52	51.69	18.82
176	LYS	CA	-45.79	-28.98	52.95	18.15
176	LYS	CB	-45.64	-30.50	52.97	19.27
176	LYS	CG	-46.95	-31.32	53.07	21.41
176	LYS	CD	-46.63	-32.84	52.96	17.01
176	LYS	CE	-47.83	-33.72	53.27	21.32

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176	LYS	NZ	-48.07	-33.97	54.73	17.44
176	LYS	C	-44.42	-28.30	53.03	20.70
176	LYS	O	-43.56	-28.53	52.17	21.72
177	HIS	N	-44.19	-27.51	54.08	18.91
177	HIS	CA	-42.93	-26.78	54.26	13.73
177	HIS	CB	-43.18	-25.28	54.19	16.90
177	HIS	CG	-44.04	-24.76	55.30	17.13
177	HIS	CD2	-43.77	-24.55	56.62	20.36
177	HIS	ND1	-45.37	-24.39	55.13	20.15
177	HIS	CE1	-45.87	-23.99	56.28	21.57
177	HIS	NE2	-44.92	-24.08	57.20	21.14
177	HIS	C	-42.20	-27.08	55.56	13.57
177	HIS	O	-42.71	-27.80	56.42	15.98
178	TRP	N	-41.05	-26.45	55.74	11.27
178	TRP	CA	-40.27	-26.56	56.97	10.08
178	TRP	CB	-38.80	-26.95	56.72	13.29
178	TRP	CG	-38.53	-28.36	56.29	9.82
178	TRP	CD2	-38.48	-29.53	57.12	13.57
178	TRP	CE2	-38.10	-30.61	56.30	13.92
178	TRP	CE3	-38.73	-29.77	58.48	15.49
178	TRP	CD1	-38.19	-28.77	55.04	12.10
178	TRP	NE1	-37.93	-30.12	55.03	13.58
178	TRP	CZ2	-37.95	-31.92	56.79	14.49
178	TRP	CZ3	-38.58	-31.07	58.97	16.39
178	TRP	CH2	-38.19	-32.13	58.12	16.81
178	TRP	C	-40.31	-25.13	57.51	10.66
178	TRP	O	-40.55	-24.19	56.75	11.76
179	ILE	N	-40.13	-24.95	58.82	11.11
179	ILE	CA	-40.11	-23.61	59.41	9.30
179	ILE	CB	-40.99	-23.50	60.66	11.02
179	ILE	CG2	-40.96	-22.10	61.21	3.09
179	ILE	CG1	-42.44	-23.88	60.33	9.87
179	ILE	CD1	-43.38	-23.79	61.52	10.20
179	ILE	C	-38.66	-23.46	59.79	10.91
179	ILE	O	-38.13	-24.27	60.55	13.14
180	ILE	N	-38.01	-22.45	59.23	12.47
180	ILE	CA	-36.60	-22.25	59.48	10.39
180	ILE	CB	-35.84	-22.35	58.14	4.50
180	ILE	CG2	-34.41	-21.90	58.27	4.54
180	ILE	CG1	-35.91	-23.78	57.61	6.63
180	ILE	CD1	-35.21	-24.85	58.48	10.08
180	ILE	C	-36.27	-20.95	60.18	12.35

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180	ILE	O	-36.73	-19.88	59.76	18.36
181	LYS	N	-35.50	-21.05	61.27	9.02
181	LYS	CA	-35.06	-19.88	62.03	6.93
181	LYS	CB	-34.92	-20.19	63.52	8.20
181	LYS	CG	-34.55	-18.99	64.39	4.18
181	LYS	CD	-34.21	-19.41	65.80	5.00
181	LYS	CE	-33.83	-18.23	66.69	2.00
181	LYS	NZ	-33.38	-18.69	68.03	2.00
181	LYS	C	-33.71	-19.45	61.47	6.56
181	LYS	O	-32.76	-20.23	61.51	9.50
182	ASN	N	-33.63	-18.25	60.93	6.31
182	ASN	CA	-32.38	-17.79	60.36	7.51
182	ASN	CB	-32.62	-17.18	58.97	12.34
182	ASN	CG	-31.37	-17.16	58.12	13.66
182	ASN	OD1	-30.38	-17.83	58.43	13.80
182	ASN	ND2	-31.40	-16.41	57.03	14.20
182	ASN	C	-31.67	-16.80	61.27	8.95
182	ASN	O	-32.29	-16.18	62.12	9.35
183	SER	N	-30.37	-16.65	61.07	12.23
183	SER	CA	-29.55	-15.74	61.87	12.33
183	SER	CB	-28.41	-16.50	62.54	11.14
183	SER	OG	-27.51	-17.06	61.60	2.83
183	SER	C	-29.03	-14.56	61.05	17.18
183	SER	O	-27.84	-14.23	61.12	14.11
184	TRP	N	-29.92	-13.92	60.30	20.03
184	TRP	CA	-29.59	-12.77	59.45	17.75
184	TRP	CB	-29.94	-13.03	57.99	17.44
184	TRP	CG	-28.96	-13.87	57.26	11.74
184	TRP	CD2	-29.09	-14.40	55.93	10.49
184	TRP	CE2	-27.91	-15.11	55.65	11.82
184	TRP	CE3	-30.09	-14.34	54.96	7.76
184	TRP	CD1	-27.75	-14.27	57.71	13.64
184	TRP	NE1	-27.11	-15.01	56.76	18.22
184	TRP	CZ2	-27.70	-15.76	54.44	8.06
184	TRP	CZ3	-29.88	-14.99	53.75	8.86
184	TRP	CH2	-28.70	-15.69	53.50	6.44
184	TRP	C	-30.30	-11.51	59.91	18.70
184	TRP	O	-30.21	-10.47	59.27	18.61
185	GLY	N	-31.05	-11.62	61.01	19.92
185	GLY	CA	-31.75	-10.48	61.55	17.99
185	GLY	C	-33.25	-10.62	61.47	21.34
185	GLY	O	-33.78	-11.41	60.68	24.20

TABLE VII

186	GLU	N	-33.94	-9.85	62.30	25.86
186	GLU	CA	-35.39	-9.85	62.34	28.63
186	GLU	CB	-35.92	-9.06	63.55	33.72
186	GLU	CG	-37.35	-9.41	64.01	33.62
186	GLU	CD	-37.39	-10.59	64.97	33.61
186	GLU	OE1	-36.64	-10.57	65.96	35.89
186	GLU	OE2	-38.18	-11.54	64.74	33.82
186	GLU	C	-35.93	-9.26	61.04	27.44
186	GLU	O	-37.08	-9.48	60.68	29.63
187	ASN	N	-35.09	-8.50	60.33	28.18
187	ASN	CA	-35.54	-7.88	59.08	30.53
187	ASN	CB	-35.10	-6.41	58.99	33.02
187	ASN	CG	-36.04	-5.57	58.12	36.45
187	ASN	OD1	-35.65	-4.51	57.62	41.13
187	ASN	ND2	-37.28	-6.03	57.95	34.46
187	ASN	C	-35.20	-8.65	57.79	29.17
187	ASN	O	-35.12	-8.08	56.69	26.38
188	TRP	N	-34.95	-9.94	57.93	26.78
188	TRP	CA	-34.69	-10.76	56.76	22.32
188	TRP	CB	-33.39	-11.54	56.84	20.90
188	TRP	CG	-33.28	-12.47	55.69	18.19
188	TRP	CD2	-33.78	-13.82	55.64	20.16
188	TRP	CE2	-33.53	-14.30	54.34	16.93
188	TRP	CE3	-34.43	-14.65	56.56	15.73
188	TRP	CD1	-32.75	-12.21	54.46	12.09
188	TRP	NE1	-32.90	-13.31	53.64	17.84
188	TRP	CZ2	-33.90	-15.58	53.94	18.81
188	TRP	CZ3	-34.79	-15.92	56.17	18.58
188	TRP	CH2	-34.53	-16.38	54.87	19.87
188	TRP	C	-35.87	-11.70	56.68	21.57
188	TRP	O	-36.40	-12.11	57.72	19.48
189	GLY	N	-36.28	-12.04	55.46	22.26
189	GLY	CA	-37.41	-12.93	55.26	19.03
189	GLY	C	-38.59	-12.53	56.12	16.83
189	GLY	O	-38.70	-11.37	56.51	16.64
190	ASN	N	-39.44	-13.48	56.47	19.64
190	ASN	CA	-40.60	-13.17	57.30	21.04
190	ASN	CB	-41.76	-14.13	57.02	18.69
190	ASN	CG	-43.09	-13.58	57.49	20.80
190	ASN	OD1	-43.14	-12.58	58.20	25.63
190	ASN	ND2	-44.18	-14.23	57.09	16.08
190	ASN	C	-40.20	-13.18	58.78	20.26

TABLE VII

190	ASN	O	-40.08	-14.23	59.39	21.80
191	LYS	N	-39.91	-11.99	59.31	19.09
191	LYS	CA	-39.51	-11.81	60.71	17.89
191	LYS	CB	-40.69	-11.99	61.66	19.60
191	LYS	CG	-41.88	-11.07	61.39	20.04
191	LYS	CD	-43.02	-11.37	62.36	17.35
191	LYS	CE	-44.34	-10.84	61.84	16.88
191	LYS	NZ	-45.47	-11.13	62.77	17.42
191	LYS	C	-38.33	-12.71	61.12	14.97
191	LYS	O	-38.28	-13.22	62.23	11.80
192	GLY	N	-37.38	-12.87	60.20	16.54
192	GLY	CA	-36.20	-13.67	60.47	10.79
192	GLY	C	-36.40	-15.14	60.19	12.10
192	GLY	O	-35.53	-15.94	60.52	14.29
193	TYR	N	-37.53	-15.50	59.59	15.02
193	TYR	CA	-37.82	-16.91	59.26	15.85
193	TYR	CB	-39.02	-17.45	60.08	19.04
193	TYR	CG	-38.75	-17.68	61.55	20.49
193	TYR	CD1	-38.79	-16.64	62.45	23.39
193	TYR	CE1	-38.52	-16.84	63.79	24.79
193	TYR	CD2	-38.43	-18.95	62.02	21.17
193	TYR	CE2	-38.15	-19.17	63.36	22.23
193	TYR	CZ	-38.19	-18.11	64.24	24.79
193	TYR	OH	-37.88	-18.29	65.56	25.50
193	TYR	C	-38.11	-17.13	57.77	14.84
193	TYR	O	-38.58	-16.22	57.07	11.51
194	ILE	N	-37.90	-18.36	57.33	16.12
194	ILE	CA	-38.16	-18.78	55.96	14.70
194	ILE	CB	-36.84	-18.88	55.15	17.12
194	ILE	CG2	-35.85	-19.82	55.81	13.78
194	ILE	CG1	-37.11	-19.29	53.70	15.67
194	ILE	CD1	-35.97	-18.96	52.77	13.44
194	ILE	C	-38.92	-20.12	55.97	12.70
194	ILE	O	-38.59	-21.02	56.73	11.58
195	LEU	N	-39.99	-20.21	55.18	12.52
195	LEU	CA	-40.79	-21.43	55.09	12.23
195	LEU	CB	-42.27	-21.12	54.93	12.99
195	LEU	CG	-42.88	-20.23	55.99	16.19
195	LEU	CD1	-44.36	-20.05	55.68	16.70
195	LEU	CD2	-42.69	-20.87	57.36	17.95
195	LEU	C	-40.36	-22.30	53.93	10.25
195	LEU	O	-41.15	-22.59	53.05	15.85

TABLE VII

196	MET	N	-39.12	-22.76	53.96	9.10
196	MET	CA	-38.58	-23.59	52.89	9.39
196	MET	CB	-37.15	-23.99	53.20	8.97
196	MET	CG	-36.23	-22.80	53.29	8.78
196	MET	SD	-34.62	-23.28	53.80	18.24
196	MET	CE	-33.88	-23.71	52.24	8.14
196	MET	C	-39.43	-24.79	52.52	10.25
196	MET	O	-40.21	-25.27	53.33	13.91
197	ALA	N	-39.26	-25.28	51.30	11.72
197	ALA	CA	-40.03	-26.42	50.82	12.43
197	ALA	CB	-39.92	-26.52	49.30	7.27
197	ALA	C	-39.62	-27.73	51.49	13.38
197	ALA	O	-38.45	-27.92	51.85	11.55
198	ARG	N	-40.58	-28.64	51.65	11.95
198	ARG	CA	-40.38	-29.92	52.30	13.06
198	ARG	CB	-41.05	-29.94	53.69	14.09
198	ARG	CG	-41.05	-31.27	54.39	5.88
198	ARG	CD	-41.44	-31.09	55.84	6.02
198	ARG	NE	-42.82	-30.68	56.02	3.48
198	ARG	CZ	-43.85	-31.52	56.05	6.84
198	ARG	NH1	-43.64	-32.82	55.89	2.00
198	ARG	NH2	-45.07	-31.08	56.35	2.52
198	ARG	C	-40.94	-31.02	51.43	12.96
198	ARG	O	-41.97	-30.84	50.78	15.58
199	ASN	N	-40.29	-32.18	51.47	12.90
199	ASN	CA	-40.66	-33.34	50.66	13.45
199	ASN	CB	-42.17	-33.57	50.63	17.26
199	ASN	CG	-42.69	-34.17	51.91	22.47
199	ASN	OD1	-42.08	-35.09	52.47	20.71
199	ASN	ND2	-43.83	-33.68	52.36	26.83
199	ASN	C	-40.12	-33.20	49.24	12.34
199	ASN	O	-39.63	-34.18	48.69	12.85
200	LYS	N	-40.22	-32.00	48.68	10.89
200	LYS	CA	-39.73	-31.64	47.34	8.22
200	LYS	CB	-39.86	-30.13	47.11	8.55
200	LYS	CG	-41.26	-29.57	47.04	5.90
200	LYS	CD	-41.97	-30.04	45.79	9.80
200	LYS	CE	-43.07	-29.09	45.40	9.34
200	LYS	NZ	-42.51	-27.88	44.72	10.27
200	LYS	C	-38.29	-32.09	47.02	7.56
200	LYS	O	-37.43	-31.27	46.71	5.62
201	ASN	N	-38.05	-33.39	47.07	9.28

TABLE VII

201	ASN	CA	-36.76	-33.99	46.79	10.44
201	ASN	CB	-36.58	-34.11	45.28	12.24
201	ASN	CG	-37.80	-34.72	44.61	16.00
201	ASN	OD1	-38.18	-35.86	44.91	12.64
201	ASN	ND2	-38.47	-33.93	43.78	14.00
201	ASN	C	-35.55	-33.38	47.47	10.11
201	ASN	O	-34.60	-32.95	46.82	11.93
202	ASN	N	-35.59	-33.36	48.80	11.90
202	ASN	CA	-34.50	-32.83	49.61	9.85
202	ASN	CB	-33.31	-33.79	49.55	13.31
202	ASN	CG	-32.38	-33.63	50.72	13.23
202	ASN	OD1	-32.82	-33.40	51.84	16.24
202	ASN	ND2	-31.09	-33.81	50.47	7.73
202	ASN	C	-34.09	-31.43	49.19	10.35
202	ASN	O	-32.90	-31.12	49.17	13.84
203	ALA	N	-35.05	-30.59	48.88	15.00
203	ALA	H	-35.55	-31.01	49.01	15.00
203	ALA	CA	-34.83	-29.22	48.41	15.00
203	ALA	CB	-35.54	-28.63	48.10	15.00
203	ALA	C	-33.66	-28.58	49.16	15.00
203	ALA	O	-33.48	-28.72	50.36	18.81
204	CYS	N	-32.82	-27.85	48.40	16.60
204	CYS	CA	-31.68	-27.12	48.94	13.11
204	CYS	C	-30.69	-27.92	49.78	13.70
204	CYS	O	-29.77	-27.35	50.36	13.59
204	CYS	CB	-32.14	-25.88	49.70	11.09
204	CYS	SG	-32.81	-24.55	48.65	21.00
205	GLY	N	-30.86	-29.23	49.82	15.46
205	GLY	CA	-29.96	-30.07	50.60	17.31
205	GLY	C	-30.16	-29.87	52.09	18.03
205	GLY	O	-29.21	-29.94	52.87	16.28
206	ILE	N	-31.42	-29.72	52.49	18.33
206	ILE	CA	-31.76	-29.48	53.88	18.94
206	ILE	CB	-33.23	-28.93	54.04	19.06
206	ILE	CG2	-34.22	-29.85	53.34	18.93
206	ILE	CG1	-33.59	-28.78	55.52	14.65
206	ILE	CD1	-34.76	-27.88	55.75	16.36
206	ILE	C	-31.52	-30.66	54.82	21.37
206	ILE	O	-31.03	-30.47	55.94	21.08
207	ALA	N	-31.79	-31.88	54.34	20.23
207	ALA	CA	-31.63	-33.08	55.16	19.58
207	ALA	CB	-32.79	-34.05	54.92	20.40

TABLE VII

207	ALA	C	-30.29	-33.82	55.03	17.00
207	ALA	O	-30.18	-34.98	55.38	15.14
208	ASN	N	-29.26	-33.13	54.55	17.17
208	ASN	CA	-27.97	-33.79	54.42	16.44
208	ASN	CB	-27.26	-33.40	53.11	16.56
208	ASN	CG	-27.95	-33.93	51.86	12.14
208	ASN	OD1	-28.79	-34.83	51.91	6.67
208	ASN	ND2	-27.58	-33.36	50.72	12.22
208	ASN	C	-27.01	-33.56	55.59	16.20
208	ASN	O	-26.14	-34.39	55.83	19.88
209	LEU	N	-27.14	-32.44	56.30	11.98
209	LEU	CA	-26.22	-32.16	57.40	12.42
209	LEU	CB	-25.19	-31.10	56.96	11.33
209	LEU	CG	-23.81	-31.03	57.61	6.60
209	LEU	CD1	-23.24	-32.42	57.81	6.26
209	LEU	CD2	-22.89	-30.23	56.73	6.70
209	LEU	C	-26.87	-31.77	58.73	14.26
209	LEU	O	-26.32	-30.96	59.48	15.18
210	ALA	N	-27.99	-32.44	59.08	15.00
210	ALA	H	-28.41	-32.84	58.30	15.00
210	ALA	CA	-28.76	-32.10	60.27	15.00
210	ALA	CB	-30.25	-32.37	60.06	15.00
210	ALA	C	-28.31	-32.97	61.45	15.00
210	ALA	O	-28.07	-34.16	61.40	11.82
211	SER	N	-28.32	-32.32	62.66	12.69
211	SER	CA	-27.97	-33.00	63.90	11.35
211	SER	CB	-26.47	-33.22	64.03	10.79
211	SER	OG	-25.80	-32.01	64.32	5.14
211	SER	C	-28.50	-32.25	65.11	11.89
211	SER	O	-28.51	-31.01	65.14	11.91
212	PHE	N	-28.97	-32.99	66.09	12.57
212	PHE	CA	-29.47	-32.38	67.31	11.64
212	PHE	CB	-30.95	-32.69	67.51	12.77
212	PHE	CG	-31.27	-34.12	67.44	11.84
212	PHE	CD1	-31.61	-34.70	66.24	10.42
212	PHE	CD2	-31.23	-34.91	68.58	14.45
212	PHE	CE1	-31.91	-36.03	66.17	16.06
212	PHE	CE2	-31.53	-36.24	68.53	15.41
212	PHE	CZ	-31.87	-36.81	67.32	16.55
212	PHE	C	-28.61	-32.83	68.48	12.10
212	PHE	O	-27.91	-33.85	68.41	12.03
213	PRO	N	-28.60	-32.05	69.57	12.99

TABLE VII

213	PRO	CD	-29.24	-30.73	69.77	10.69
213	PRO	CA	-27.79	-32.41	70.74	12.29
213	PRO	CB	-27.41	-31.05	71.29	11.67
213	PRO	CG	-28.70	-30.29	71.12	14.62
213	PRO	C	-28.56	-33.23	71.75	12.17
213	PRO	O	-29.78	-33.11	71.88	2.00
214	LYS	N	-27.82	-34.09	72.45	14.45
214	LYS	CA	-28.39	-34.94	73.50	19.77
214	LYS	CB	-27.80	-36.34	73.46	20.65
214	LYS	CG	-28.06	-37.08	72.17	24.16
214	LYS	CD	-27.54	-38.52	72.24	29.93
214	LYS	CE	-26.02	-38.57	72.40	33.14
214	LYS	NZ	-25.49	-39.97	72.44	35.37
214	LYS	C	-28.15	-34.26	74.84	21.45
214	LYS	O	-27.02	-33.92	75.20	16.74
215	MET	N	-29.23	-34.05	75.57	22.65
215	MET	CA	-29.16	-33.38	76.85	25.38
215	MET	CB	-30.04	-32.13	76.79	27.81
215	MET	CG	-29.77	-31.09	77.85	26.22
215	MET	SD	-30.44	-29.54	77.29	25.84
215	MET	CE	-28.92	-28.76	76.63	23.17
215	MET	C	-29.56	-34.30	77.99	25.33
215	MET	OT1	-28.65	-34.77	78.71	27.00
215	MET	OT2	-30.77	-34.58	78.12	23.48
216	HOH	OH2	-31.11	-16.42	65.02	14.43
217	HOH	OH2	-29.30	-20.25	62.17	18.73
218	HOH	OH2	-10.67	-12.22	63.70	43.10
219	HOH	OH2	-16.45	-12.20	72.96	5.87
220	HOH	OH2	-35.12	-23.55	69.64	9.44
221	HOH	OH2	-24.01	-30.97	61.16	4.73
222	HOH	OH2	-13.01	-8.39	61.94	32.49
223	HOH	OH2	-14.66	-21.66	66.41	2.00
224	HOH	OH2	-43.65	-26.52	48.92	29.00
225	HOH	OH2	-45.60	-35.43	55.56	13.84
226	HOH	OH2	-40.92	-17.45	68.90	12.03
227	HOH	OH2	-43.72	-25.26	44.65	38.82
228	HOH	OH2	-24.12	-5.83	68.94	43.50
229	HOH	OH2	-30.71	-18.60	67.86	32.89
230	HOH	OH2	-35.05	-26.71	51.39	30.11
231	HOH	OH2	-36.74	-24.80	49.94	8.69
232	HOH	OH2	-46.77	-33.25	57.36	12.67
233	HOH	OH2	-28.91	-10.19	75.44	15.32

TABLE VII

234	HOH	OH2	-36.31	-14.76	75.60	16.14
235	HOH	OH2	-16.18	-4.92	68.62	27.92
236	HOH	OH2	-16.52	-8.98	75.02	28.63
237	HOH	OH2	-10.50	-18.37	70.18	39.29
238	HOH	OH2	-9.29	-19.89	78.20	29.36
239	HOH	OH2	-45.95	-16.45	54.42	32.47
240	HOH	OH2	-33.98	-29.86	44.88	32.74
241	HOH	OH2	-36.55	-38.18	52.42	11.87
242	HOH	OH2	-41.73	-34.84	55.47	18.73
243	HOH	OH2	-41.21	-19.79	71.20	12.36
244	HOH	OH2	-47.90	-19.78	72.76	27.97
245	HOH	OH2	-42.20	-14.92	70.78	34.65
246	HOH	OH2	-26.14	-8.98	67.92	37.03
247	HOH	OH2	-32.81	-7.84	63.95	35.20
248	HOH	OH2	-19.95	-7.54	63.08	32.69
249	HOH	OH2	-16.19	-10.67	61.92	30.22
250	HOH	OH2	-35.01	-39.74	65.90	10.75
251	HOH	OH2	-13.63	-24.17	76.67	16.76
252	HOH	OH2	-8.21	-25.68	60.56	19.27
253	HOH	OH2	-20.14	-27.62	51.69	32.97
254	HOH	OH2	-25.01	-33.27	60.23	25.95
255	HOH	OH2	-13.56	-29.77	72.49	36.07
256	HOH	OH2	-33.43	-40.03	63.75	25.23
257	HOH	OH2	-20.84	-23.81	87.06	28.06
258	HOH	OH2	-13.50	-12.46	62.97	41.75
259	HOH	OH2	-28.41	-30.03	56.55	11.99
260	HOH	OH2	-28.87	-16.56	42.17	23.76
261	HOH	OH2	-25.56	-19.23	42.44	8.60
262	HOH	OH2	-32.08	-33.98	47.05	47.25
263	HOH	OH2	-22.35	-31.23	43.22	18.34
264	HOH	OH2	-32.62	-28.89	42.32	42.83
265	HOH	OH2	-38.09	-30.05	50.12	38.26

TABLE VIII

Table of the orthogonal three dimensional coordinates in Ångstroms and B factors ($Å^2$) for the cathepsin K complex with inhibitor 4-[N-[(4-pyridylmethoxy)carbonyl]-L-leucyl]-1-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-3-pyrrolidinone.

Residue	Atom	X	Y	Z	B
1	ALA CB	-46.30	-38.07	64.13	15.00
1	ALA C	-48.64	-37.16	64.46	15.00
1	ALA O	-49.53	-37.68	63.79	15.00
1	ALA N	-48.10	-39.41	65.31	15.00
1	ALA CA	-47.55	-38.03	65.08	15.00
2	PRO N	-48.69	-35.88	64.81	15.00
2	PRO CD	-48.06	-35.33	66.02	15.00
2	PRO CA	-49.67	-34.93	64.29	15.00
2	PRO CB	-49.53	-33.73	65.24	15.00
2	PRO CG	-48.13	-33.85	65.77	15.00
2	PRO C	-49.42	-34.53	62.86	15.00
2	PRO O	-48.34	-34.77	62.28	15.00
3	ASP N	-50.40	-33.85	62.30	15.00
3	ASP CA	-50.29	-33.37	60.93	15.00
3	ASP CB	-51.65	-33.42	60.27	15.00
3	ASP CG	-52.12	-34.84	60.00	15.00
3	ASP OD1	-52.02	-35.30	58.84	15.00
3	ASP OD2	-52.59	-35.51	60.95	15.00
3	ASP C	-49.76	-31.93	61.01	15.00
3	ASP O	-49.44	-31.32	59.99	15.00
4	SER N	-49.58	-31.45	62.24	15.00
4	SER CA	-49.13	-30.09	62.51	15.00
4	SER CB	-50.32	-29.14	62.52	15.00
4	SER OG	-50.86	-29.02	61.20	15.00
4	SER C	-48.39	-29.96	63.84	15.00
4	SER O	-48.74	-30.63	64.84	15.00
5	VAL N	-47.34	-29.15	63.84	15.00
5	VAL CA	-46.50	-28.91	64.99	15.00
5	VAL CB	-45.35	-29.97	65.11	15.00
5	VAL CG1	-44.17	-29.43	65.89	15.00
5	VAL CG2	-45.84	-31.21	65.74	15.00
5	VAL C	-45.86	-27.57	64.80	15.00

TABLE VIII

5	VAL	O	-45.37	-27.25	63.70	15.00
6	ASP	N	-45.84	-26.80	65.89	15.00
6	ASP	CA	-45.22	-25.50	65.92	15.00
6	ASP	CB	-46.16	-24.37	65.46	15.00
6	ASP	CG	-45.40	-23.07	65.15	15.00
6	ASP	OD1	-44.21	-22.96	65.51	15.00
6	ASP	OD2	-45.98	-22.17	64.51	15.00
6	ASP	C	-44.81	-25.27	67.34	15.00
6	ASP	O	-45.65	-24.96	68.17	15.00
7	TYR	N	-43.51	-25.35	67.61	15.00
7	TYR	CA	-43.00	-25.14	68.94	15.00
7	TYR	CB	-41.63	-25.80	69.13	15.00
7	TYR	CG	-41.68	-27.30	69.31	15.00
7	TYR	CD1	-41.55	-27.88	70.57	15.00
7	TYR	CE1	-41.60	-29.29	70.74	15.00
7	TYR	CD2	-41.86	-28.14	68.22	15.00
7	TYR	CE2	-41.91	-29.55	68.38	15.00
7	TYR	CZ	-41.79	-30.10	69.64	15.00
7	TYR	OH	-41.91	-31.46	69.83	15.00
7	TYR	C	-42.85	-23.70	69.30	15.00
7	TYR	O	-42.16	-23.39	70.26	15.00
8	ARG	N	-43.40	-22.80	68.50	15.00
8	ARG	CA	-43.31	-21.39	68.80	15.00
8	ARG	CB	-43.55	-20.55	67.56	15.00
8	ARG	CG	-42.37	-20.55	66.60	15.00
8	ARG	CD	-42.57	-19.68	65.38	15.00
8	ARG	NE	-43.64	-20.20	64.53	15.00
8	ARG	CZ	-43.88	-19.78	63.29	15.00
8	ARG	NH1	-43.09	-18.84	62.77	15.00
8	ARG	NH2	-44.92	-20.26	62.60	15.00
8	ARG	C	-44.37	-21.14	69.84	15.00
8	ARG	O	-44.09	-20.64	70.93	15.00
9	LYS	N	-45.58	-21.65	69.54	15.00
9	LYS	CA	-46.73	-21.55	70.42	15.00
9	LYS	CB	-47.95	-22.19	69.75	15.00
9	LYS	CG	-48.42	-21.37	68.55	15.00
9	LYS	CD	-48.71	-22.24	67.29	15.00
9	LYS	CE	-49.41	-21.46	66.17	15.00
9	LYS	NZ	-50.87	-21.36	66.45	15.00
9	LYS	C	-46.44	-22.17	71.79	15.00
9	LYS	O	-46.36	-21.45	72.77	15.00
10	LYS	N	-46.15	-23.46	71.83	15.00

TABLE VIII

10	LYS	CA	-45.85	-24.13	73.10	15.00
10	LYS	CB	-45.43	-25.57	72.86	15.00
10	LYS	CG	-46.52	-26.39	72.25	15.00
10	LYS	CD	-46.05	-27.76	71.89	15.00
10	LYS	CE	-46.89	-28.35	70.81	15.00
10	LYS	NZ	-48.31	-27.94	70.92	15.00
10	LYS	C	-44.81	-23.41	73.94	15.00
10	LYS	O	-44.74	-23.62	75.14	15.00
11	GLY	N	-43.95	-22.63	73.30	15.00
11	GLY	CA	-42.94	-21.90	74.05	15.00
11	GLY	C	-41.53	-22.43	74.01	15.00
11	GLY	O	-40.78	-22.24	74.97	15.00
12	TYR	N	-41.13	-23.07	72.91	15.00
12	TYR	CA	-39.76	-23.60	72.84	15.00
12	TYR	CB	-39.78	-24.98	72.15	15.00
12	TYR	CG	-40.42	-26.09	72.97	15.00
12	TYR	CD1	-41.76	-26.06	73.35	15.00
12	TYR	CE1	-42.34	-27.10	74.13	15.00
12	TYR	CD2	-39.66	-27.18	73.39	15.00
12	TYR	CE2	-40.21	-28.21	74.17	15.00
12	TYR	CZ	-41.55	-28.17	74.53	15.00
12	TYR	OH	-42.10	-29.21	75.25	15.00
12	TYR	C	-38.82	-22.68	72.08	15.00
12	TYR	O	-37.64	-22.97	71.90	15.00
13	VAL	N	-39.37	-21.59	71.56	15.00
13	VAL	CA	-38.56	-20.71	70.75	15.00
13	VAL	CB	-39.14	-20.70	69.33	15.00
13	VAL	CG1	-38.15	-20.04	68.35	15.00
13	VAL	CG2	-39.49	-22.09	68.92	15.00
13	VAL	C	-38.31	-19.27	71.23	15.00
13	VAL	O	-39.24	-18.52	71.45	15.00
14	THR	N	-37.03	-18.90	71.32	15.00
14	THR	CA	-36.64	-17.56	71.76	15.00
14	THR	CB	-35.17	-17.57	72.25	15.00
14	THR	OG1	-34.33	-18.03	71.18	15.00
14	THR	CG2	-35.01	-18.43	73.50	15.00
14	THR	C	-36.70	-16.58	70.60	15.00
14	THR	O	-37.20	-16.92	69.53	15.00
15	PRO	N	-36.27	-15.32	70.83	15.00
15	PRO	CD	-36.21	-14.64	72.14	15.00
15	PRO	CA	-36.29	-14.32	69.76	15.00
15	PRO	CB	-35.98	-13.04	70.49	15.00

TABLE VIII

15	PRO	CG	-36.64	-13.24	71.83	15.00
15	PRO	C	-35.23	-14.60	68.72	15.00
15	PRO	O	-34.20	-15.21	69.02	15.00
16	VAL	N	-35.48	-14.05	67.52	15.00
16	VAL	CA	-34.61	-14.19	66.36	15.00
16	VAL	CB	-35.37	-13.74	65.10	15.00
16	VAL	CG1	-34.43	-13.61	63.92	15.00
16	VAL	CG2	-36.44	-14.72	64.78	15.00
16	VAL	C	-33.40	-13.33	66.56	15.00
16	VAL	O	-33.47	-12.33	67.23	15.00
17	LYS	N	-32.24	-13.78	66.10	15.00
17	LYS	CA	-31.04	-12.97	66.26	15.00
17	LYS	CB	-29.96	-13.71	67.06	15.00
17	LYS	CG	-30.45	-14.44	68.35	15.00
17	LYS	CD	-30.63	-13.52	69.54	15.00
17	LYS	CE	-30.89	-14.30	70.82	15.00
17	LYS	NZ	-32.14	-15.10	70.83	15.00
17	LYS	C	-30.46	-12.58	64.91	15.00
17	LYS	O	-31.06	-12.84	63.87	15.00
18	ASN	N	-29.30	-11.94	64.94	15.00
18	ASN	CA	-28.58	-11.48	63.75	15.00
18	ASN	CB	-28.58	-9.96	63.69	15.00
18	ASN	CG	-29.93	-9.39	63.96	15.00
18	ASN	OD1	-30.89	-9.75	63.32	15.00
18	ASN	ND2	-30.02	-8.56	64.97	15.00
18	ASN	C	-27.16	-11.93	63.99	15.00
18	ASN	O	-26.58	-11.59	65.03	15.00
19	GLN	N	-26.59	-12.69	63.06	15.00
19	GLN	CA	-25.22	-13.13	63.22	15.00
19	GLN	CB	-24.96	-14.41	62.43	15.00
19	GLN	CG	-25.34	-14.25	60.98	15.00
19	GLN	CD	-25.10	-15.49	60.16	15.00
19	GLN	OE1	-26.04	-16.20	59.82	15.00
19	GLN	NE2	-23.86	-15.72	59.77	15.00
19	GLN	C	-24.24	-12.02	62.83	15.00
19	GLN	O	-23.05	-12.15	63.08	15.00
20	GLY	N	-24.72	-11.01	62.11	15.00
20	GLY	CA	-23.86	-9.91	61.69	15.00
20	GLY	C	-22.83	-10.31	60.65	15.00
20	GLY	O	-23.08	-11.26	59.94	15.00
21	GLN	N	-21.69	-9.61	60.49	15.00
21	GLN	CA	-20.72	-10.02	59.43	15.00

TABLE VIII

21	GLN	CB	-20.01	-8.83	58.75	15.00
21	GLN	CG	-20.87	-8.13	57.66	15.00
21	GLN	CD	-21.58	-9.06	56.63	15.00
21	GLN	OE1	-20.99	-10.02	56.16	15.00
21	GLN	NE2	-22.84	-8.74	56.29	15.00
21	GLN	C	-19.72	-11.10	59.87	15.00
21	GLN	O	-18.50	-11.01	59.66	15.00
22	CYS	N	-20.32	-12.22	60.26	15.00
22	CYS	CA	-19.59	-13.37	60.72	15.00
22	CYS	C	-20.26	-14.68	60.30	15.00
22	CYS	O	-21.48	-14.80	60.28	15.00
22	CYS	CB	-19.48	-13.22	62.25	15.00
22	CYS	SG	-19.02	-14.67	63.24	15.00
23	GLY	N	-19.45	-15.65	59.90	15.00
23	GLY	CA	-20.01	-16.93	59.52	15.00
23	GLY	C	-20.27	-17.81	60.75	15.00
23	GLY	O	-19.73	-18.91	60.83	15.00
24	SER	N	-21.20	-17.40	61.61	15.00
24	SER	CA	-21.49	-18.12	62.84	15.00
24	SER	CB	-21.32	-17.21	64.08	15.00
24	SER	OG	-22.22	-16.10	64.07	15.00
24	SER	C	-22.89	-18.73	62.86	15.00
24	SER	O	-23.44	-19.03	63.90	15.00
25	CYS	N	-23.46	-18.96	61.69	15.00
25	CYS	CA	-24.78	-19.55	61.56	15.00
25	CYS	CB	-25.18	-19.59	60.07	15.00
25	CYS	SG	-24.19	-20.73	59.02	15.00
25	CYS	C	-24.80	-20.92	62.24	15.00
25	CYS	O	-25.77	-21.25	62.88	15.00
25	INH	C1	-14.75	-27.52	59.81	15.00
25	INH	C2	-15.58	-26.77	58.94	15.00
25	INH	C3	-15.24	-25.44	58.65	15.00
25	INH	C4	-14.06	-24.88	59.25	15.00
25	INH	C5	-13.21	-25.64	60.14	15.00
25	INH	C6	-13.57	-26.96	60.42	15.00
25	INH	C7	-16.11	-24.63	57.72	15.00
25	INH	O8	-17.39	-25.29	57.48	15.00
25	INH	C9	-18.43	-24.53	57.00	15.00
25	INH	O10	-18.33	-23.63	56.17	15.00
25	INH	N11	-19.57	-24.86	57.54	15.00
25	INH	C12	-20.88	-24.22	57.23	15.00
25	INH	C13	-21.31	-23.29	58.42	15.00

TABLE VIII

25	INH	N14	-21.06	-21.86	58.16	15.00
25	INH	C15	-21.68	-21.41	56.87	15.00
25	INH	C16	-21.59	-21.00	59.27	15.00
25	INH	C17	-22.57	-20.07	58.55	15.00
25	INH	C18	-22.15	-19.99	57.10	15.00
25	INH	C19	-21.87	-25.40	57.01	15.00
25	INH	C20	-22.73	-25.74	58.21	15.00
25	INH	C21	-22.94	-27.22	58.28	15.00
25	INH	C22	-24.00	-25.01	57.98	15.00
25	INH	N23	-23.18	-19.45	56.18	15.00
25	INH	C24	-23.12	-18.15	55.84	15.00
25	INH	O25	-22.20	-17.42	56.28	15.00
25	INH	C26	-24.25	-17.59	54.91	15.00
25	INH	C27	-24.00	-18.05	53.43	15.00
25	INH	C28	-25.22	-18.05	52.51	15.00
25	INH	C29	-25.14	-19.24	51.66	15.00
25	INH	C30	-25.25	-16.77	51.69	15.00
25	INH	N31	-24.30	-16.10	54.92	15.00
25	INH	C32	-24.85	-15.34	55.87	15.00
25	INH	O33	-25.40	-15.84	56.83	15.00
25	INH	O34	-24.72	-13.96	55.64	15.00
25	INH	C35	-24.74	-13.12	56.80	15.00
25	INH	C36	-25.68	-11.91	56.62	15.00
25	INH	C37	-25.21	-10.60	56.86	15.00
25	INH	C38	-26.09	-9.52	56.74	15.00
25	INH	N39	-27.37	-9.73	56.40	15.00
25	INH	C40	-27.85	-10.96	56.16	15.00
25	INH	C41	-27.03	-12.08	56.26	15.00
25	INH	O42	-22.66	-18.72	58.88	15.00
26	TRP	N	-23.72	-21.69	62.15	15.00
26	TRP	CA	-23.64	-23.01	62.85	15.00
26	TRP	CB	-22.30	-23.65	62.59	15.00
26	TRP	CG	-21.18	-22.75	63.06	15.00
26	TRP	CD2	-20.40	-22.85	64.28	15.00
26	TRP	CE2	-19.44	-21.79	64.22	15.00
26	TRP	CE3	-20.41	-23.71	65.38	15.00
26	TRP	CD1	-20.71	-21.70	62.39	15.00
26	TRP	NE1	-19.66	-21.12	63.05	15.00
26	TRP	CZ2	-18.49	-21.56	65.24	15.00
26	TRP	CZ3	-19.48	-23.49	66.41	15.00
26	TRP	CH2	-18.52	-22.41	66.33	15.00
26	TRP	C	-23.72	-22.83	64.40	15.00

TABLE VIII

26	TRP	O	-23.97	-23.79	65.16	15.00
27	ALA	N	-23.39	-21.64	64.91	15.00
27	ALA	CA	-23.50	-21.43	66.36	15.00
27	ALA	CB	-22.70	-20.24	66.80	15.00
27	ALA	C	-24.98	-21.21	66.72	15.00
27	ALA	O	-25.52	-21.89	67.60	15.00
28	PHE	N	-25.63	-20.27	66.03	15.00
28	PHE	CA	-27.02	-19.90	66.31	15.00
28	PHE	CB	-27.46	-18.71	65.44	15.00
28	PHE	CG	-26.88	-17.40	65.85	15.00
28	PHE	CD1	-25.73	-16.87	65.27	15.00
28	PHE	CD2	-27.47	-16.73	66.88	15.00
28	PHE	CE1	-25.16	-15.71	65.70	15.00
28	PHE	CE2	-26.92	-15.57	67.33	15.00
28	PHE	CZ	-25.75	-15.04	66.75	15.00
28	PHE	C	-27.93	-21.09	66.06	15.00
28	PHE	O	-29.08	-21.05	66.44	15.00
29	SER	N	-27.44	-22.09	65.33	15.00
29	SER	CA	-28.24	-23.28	65.05	15.00
29	SER	CB	-27.74	-23.99	63.81	15.00
29	SER	OG	-28.44	-25.21	63.58	15.00
29	SER	C	-28.13	-24.15	66.27	15.00
29	SER	O	-29.14	-24.63	66.79	15.00
30	SER	N	-26.90	-24.31	66.76	15.00
30	SER	CA	-26.64	-25.13	67.94	15.00
30	SER	CB	-25.14	-25.24	68.21	15.00
30	SER	OG	-24.40	-25.67	67.06	15.00
30	SER	C	-27.29	-24.63	69.21	15.00
30	SER	O	-27.66	-25.40	70.08	15.00
31	VAL	N	-27.31	-23.32	69.35	15.00
31	VAL	CA	-27.89	-22.67	70.51	15.00
31	VAL	CB	-27.39	-21.19	70.58	15.00
31	VAL	CG1	-28.13	-20.34	71.59	15.00
31	VAL	CG2	-25.91	-21.19	70.86	15.00
31	VAL	C	-29.41	-22.80	70.55	15.00
31	VAL	O	-30.02	-22.96	71.63	15.00
32	GLY	N	-29.99	-22.81	69.35	15.00
32	GLY	CA	-31.43	-22.91	69.21	15.00
32	GLY	C	-31.90	-24.26	69.66	15.00
32	GLY	O	-32.81	-24.39	70.47	15.00
33	ALA	N	-31.22	-25.29	69.17	15.00
33	ALA	CA	-31.51	-26.66	69.53	15.00

TABLE VIII

33	ALA	CB	-30.58	-27.55	68.80	15.00
33	ALA	C	-31.38	-26.86	71.06	15.00
33	ALA	O	-32.23	-27.54	71.68	15.00
34	LEU	N	-30.29	-26.34	71.63	15.00
34	LEU	CA	-30.03	-26.45	73.05	15.00
34	LEU	CB	-28.72	-25.82	73.41	15.00
34	LEU	CG	-27.43	-26.58	73.17	15.00
34	LEU	CD1	-26.28	-25.63	73.53	15.00
34	LEU	CD2	-27.38	-27.85	74.05	15.00
34	LEU	C	-31.12	-25.73	73.83	15.00
34	LEU	O	-31.65	-26.29	74.80	15.00
35	GLU	N	-31.47	-24.51	73.44	15.00
35	GLU	CA	-32.54	-23.76	74.12	15.00
35	GLU	CB	-32.78	-22.42	73.41	15.00
35	GLU	CG	-31.67	-21.39	73.64	15.00
35	GLU	CD	-31.63	-20.29	72.57	15.00
35	GLU	OE1	-32.41	-20.37	71.57	15.00
35	GLU	OE2	-30.81	-19.35	72.71	15.00
35	GLU	C	-33.83	-24.57	74.20	15.00
35	GLU	O	-34.34	-24.83	75.31	15.00
36	GLY	N	-34.26	-25.10	73.05	15.00
36	GLY	CA	-35.48	-25.91	72.99	15.00
36	GLY	C	-35.58	-27.11	73.93	15.00
36	GLY	O	-36.67	-27.47	74.37	15.00
37	GLN	N	-34.44	-27.72	74.24	15.00
37	GLN	CA	-34.40	-28.87	75.12	15.00
37	GLN	CB	-33.06	-29.60	74.95	15.00
37	GLN	CG	-32.79	-30.19	73.58	15.00
37	GLN	CD	-33.83	-31.19	73.19	15.00
37	GLN	OE1	-33.99	-32.23	73.84	15.00
37	GLN	NE2	-34.56	-30.89	72.11	15.00
37	GLN	C	-34.52	-28.38	76.55	15.00
37	GLN	O	-35.01	-29.10	77.43	15.00
38	LEU	N	-33.98	-27.18	76.79	15.00
38	LEU	CA	-34.03	-26.60	78.12	15.00
38	LEU	CB	-33.30	-25.26	78.14	15.00
38	LEU	CG	-33.24	-24.54	79.47	15.00
38	LEU	CD1	-32.61	-25.51	80.46	15.00
38	LEU	CD2	-32.41	-23.30	79.36	15.00
38	LEU	C	-35.46	-26.45	78.60	15.00
38	LEU	O	-35.86	-27.10	79.58	15.00
39	LYS	N	-36.26	-25.70	77.84	15.00

TABLE VIII

39	LYS	CA	-37.68	-25.45	78.15	15.00
39	LYS	CB	-38.34	-24.71	76.97	15.00
39	LYS	CG	-39.49	-23.74	77.33	15.00
39	LYS	CD	-40.74	-24.43	77.83	15.00
39	LYS	CE	-41.85	-23.45	78.12	15.00
39	LYS	NZ	-41.65	-22.78	79.42	15.00
39	LYS	C	-38.42	-26.78	78.46	15.00
39	LYS	O	-39.33	-26.82	79.30	15.00
40	LYS	N	-38.04	-27.84	77.77	15.00
40	LYS	CA	-38.66	-29.14	77.99	15.00
40	LYS	CB	-38.41	-30.07	76.81	15.00
40	LYS	CG	-39.57	-31.02	76.53	15.00
40	LYS	CD	-39.10	-32.29	75.82	15.00
40	LYS	CE	-40.02	-32.72	74.68	15.00
40	LYS	NZ	-40.21	-31.65	73.65	15.00
40	LYS	C	-38.08	-29.74	79.27	15.00
40	LYS	O	-38.79	-30.27	80.12	15.00
41	LYS	N	-36.77	-29.60	79.41	15.00
41	LYS	CA	-36.05	-30.13	80.55	15.00
41	LYS	CB	-34.53	-29.93	80.33	15.00
41	LYS	CG	-33.63	-30.86	81.11	15.00
41	LYS	CD	-33.79	-32.26	80.55	15.00
41	LYS	CE	-33.13	-33.31	81.42	15.00
41	LYS	NZ	-33.45	-34.68	80.86	15.00
41	LYS	C	-36.49	-29.45	81.84	15.00
41	LYS	O	-37.34	-29.97	82.61	15.00
42	THR	N	-35.96	-28.25	82.04	15.00
42	THR	CA	-36.22	-27.48	83.24	15.00
42	THR	CB	-34.87	-26.94	83.78	15.00
42	THR	OG1	-34.35	-25.91	82.92	15.00
42	THR	CG2	-33.86	-28.07	83.79	15.00
42	THR	C	-37.16	-26.30	83.02	15.00
42	THR	O	-36.86	-25.20	83.45	15.00
43	GLY	N	-38.28	-26.52	82.34	15.00
43	GLY	CA	-39.26	-25.47	82.12	15.00
43	GLY	C	-38.87	-24.03	81.79	15.00
43	GLY	O	-39.77	-23.21	81.54	15.00
44	LYS	N	-37.56	-23.75	81.75	15.00
44	LYS	CA	-37.02	-22.41	81.49	15.00
44	LYS	CB	-35.84	-22.13	82.44	15.00
44	LYS	CG	-36.25	-21.41	83.72	15.00
44	LYS	CD	-35.09	-21.25	84.67	15.00

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44	LYS	CE	-35.50	-20.36	85.86	15.00
44	LYS	NZ	-36.56	-20.99	86.66	15.00
44	LYS	C	-36.56	-22.13	80.06	15.00
44	LYS	O	-35.71	-22.83	79.51	15.00
45	LEU	N	-37.07	-21.04	79.50	15.00
45	LEU	CA	-36.70	-20.66	78.14	15.00
45	LEU	CB	-37.93	-20.08	77.46	15.00
45	LEU	CG	-38.06	-19.92	75.94	15.00
45	LEU	CD1	-37.93	-21.25	75.26	15.00
45	LEU	CD2	-39.40	-19.29	75.63	15.00
45	LEU	C	-35.66	-19.57	78.35	15.00
45	LEU	O	-36.00	-18.46	78.71	15.00
46	LEU	N	-34.40	-19.94	78.29	15.00
46	LEU	CA	-33.30	-18.99	78.50	15.00
46	LEU	CB	-32.23	-19.62	79.41	15.00
46	LEU	CG	-31.90	-18.84	80.70	15.00
46	LEU	CD1	-32.48	-19.56	81.88	15.00
46	LEU	CD2	-30.35	-18.72	80.89	15.00
46	LEU	C	-32.68	-18.70	77.13	15.00
46	LEU	O	-32.93	-19.45	76.19	15.00
47	ASN	N	-31.92	-17.61	76.99	15.00
47	ASN	CA	-31.23	-17.30	75.73	15.00
47	ASN	CB	-31.29	-15.79	75.44	15.00
47	ASN	CG	-32.61	-15.36	74.77	15.00
47	ASN	OD1	-32.68	-15.24	73.55	15.00
47	ASN	ND2	-33.63	-15.06	75.58	15.00
47	ASN	C	-29.74	-17.70	75.90	15.00
47	ASN	O	-29.01	-16.99	76.58	15.00
48	LEU	N	-29.28	-18.80	75.29	15.00
48	LEU	CA	-27.88	-19.20	75.45	15.00
48	LEU	CB	-27.67	-20.68	75.16	15.00
48	LEU	CG	-28.05	-21.69	76.27	15.00
48	LEU	CD1	-27.81	-21.07	77.65	15.00
48	LEU	CD2	-29.49	-22.12	76.12	15.00
48	LEU	C	-26.85	-18.34	74.73	15.00
48	LEU	O	-27.20	-17.31	74.23	15.00
49	SER	N	-25.58	-18.70	74.74	15.00
49	SER	CA	-24.59	-17.83	74.11	15.00
49	SER	CB	-23.51	-17.50	75.14	15.00
49	SER	OG	-22.32	-17.09	74.51	15.00
49	SER	C	-23.93	-18.37	72.87	15.00
49	SER	O	-23.08	-19.27	72.98	15.00

TABLE VIII

50	PRO	N	-24.29	-17.86	71.67	15.00
50	PRO	CD	-25.31	-16.83	71.34	15.00
50	PRO	CA	-23.66	-18.36	70.45	15.00
50	PRO	CB	-24.47	-17.67	69.35	15.00
50	PRO	CG	-24.96	-16.44	69.97	15.00
50	PRO	C	-22.18	-17.94	70.44	15.00
50	PRO	O	-21.36	-18.62	69.86	15.00
51	GLN	N	-21.82	-16.87	71.13	15.00
51	GLN	CA	-20.43	-16.41	71.17	15.00
51	GLN	CB	-20.39	-14.98	71.74	15.00
51	GLN	CG	-19.02	-14.25	71.69	15.00
51	GLN	CD	-18.76	-13.61	70.35	15.00
51	GLN	OE1	-19.65	-12.97	69.76	15.00
51	GLN	NE2	-17.54	-13.79	69.84	15.00
51	GLN	C	-19.46	-17.34	71.94	15.00
51	GLN	O	-18.31	-17.50	71.53	15.00
52	ASN	N	-19.90	-17.99	73.02	15.00
52	ASN	CA	-19.02	-18.91	73.78	15.00
52	ASN	CB	-19.79	-19.58	74.91	15.00
52	ASN	CG	-18.92	-20.56	75.72	15.00
52	ASN	OD1	-19.45	-21.25	76.60	15.00
52	ASN	ND2	-17.61	-20.58	75.49	15.00
52	ASN	C	-18.54	-19.96	72.80	15.00
52	ASN	O	-17.34	-20.22	72.69	15.00
53	LEU	N	-19.50	-20.50	72.05	15.00
53	LEU	CA	-19.28	-21.52	71.00	15.00
53	LEU	CB	-20.62	-21.86	70.33	15.00
53	LEU	CG	-21.43	-23.10	70.69	15.00
53	LEU	CD1	-21.19	-23.59	72.12	15.00
53	LEU	CD2	-22.91	-22.80	70.38	15.00
53	LEU	C	-18.28	-21.04	69.94	15.00
53	LEU	O	-17.34	-21.76	69.60	15.00
54	VAL	N	-18.48	-19.82	69.46	15.00
54	VAL	CA	-17.63	-19.27	68.44	15.00
54	VAL	CB	-18.01	-17.82	68.09	15.00
54	VAL	CG1	-16.94	-17.17	67.25	15.00
54	VAL	CG2	-19.32	-17.76	67.40	15.00
54	VAL	C	-16.18	-19.32	68.84	15.00
54	VAL	O	-15.36	-19.90	68.11	15.00
55	ASP	N	-15.88	-18.75	70.02	15.00
55	ASP	CA	-14.53	-18.65	70.58	15.00
55	ASP	CB	-14.49	-17.73	71.81	15.00

TABLE VIII

55	ASP	CG	-14.86	-16.30	71.52	15.00
55	ASP	OD1	-14.87	-15.89	70.35	15.00
55	ASP	OD2	-15.13	-15.56	72.49	15.00
55	ASP	C	-13.87	-19.93	71.08	15.00
55	ASP	O	-12.65	-20.14	70.82	15.00
56	CYS	N	-14.62	-20.75	71.81	15.00
56	CYS	CA	-14.06	-21.94	72.42	15.00
56	CYS	C	-14.14	-23.23	71.62	15.00
56	CYS	O	-13.36	-24.15	71.85	15.00
56	CYS	CB	-14.74	-22.17	73.76	15.00
56	CYS	SG	-14.67	-20.81	74.99	15.00
57	VAL	N	-15.00	-23.30	70.62	15.00
57	VAL	CA	-15.09	-24.53	69.88	15.00
57	VAL	CB	-16.51	-24.71	69.30	15.00
57	VAL	CG1	-16.66	-26.03	68.70	15.00
57	VAL	CG2	-17.56	-24.53	70.42	15.00
57	VAL	C	-13.92	-24.66	68.88	15.00
57	VAL	O	-14.05	-24.47	67.68	15.00
58	SER	N	-12.79	-25.08	69.43	15.00
58	SER	CA	-11.51	-25.26	68.71	15.00
58	SER	CB	-10.43	-25.78	69.66	15.00
58	SER	OG	-9.18	-25.96	68.99	15.00
58	SER	C	-11.53	-26.13	67.45	15.00
58	SER	O	-10.66	-26.01	66.58	15.00
59	GLU	N	-12.54	-26.98	67.36	15.00
59	GLU	CA	-12.67	-27.86	66.21	15.00
59	GLU	CB	-13.47	-29.12	66.60	15.00
59	GLU	CG	-13.12	-29.70	68.00	15.00
59	GLU	CD	-14.02	-29.15	69.13	15.00
59	GLU	OE1	-15.16	-29.68	69.29	15.00
59	GLU	OE2	-13.56	-28.20	69.84	15.00
59	GLU	C	-13.30	-27.07	65.05	15.00
59	GLU	O	-13.21	-27.46	63.91	15.00
60	ASN	N	-13.91	-25.93	65.35	15.00
60	ASN	CA	-14.50	-25.14	64.28	15.00
60	ASN	CB	-15.92	-24.71	64.63	15.00
60	ASN	CG	-16.96	-25.87	64.48	15.00
60	ASN	OD1	-17.94	-25.95	65.23	15.00
60	ASN	ND2	-16.75	-26.74	63.50	15.00
60	ASN	C	-13.60	-23.94	63.89	15.00
60	ASN	O	-12.43	-23.91	64.25	15.00
61	ASP	N	-14.11	-23.06	63.02	15.00

TABLE VIII

61	ASP	CA	-13.36	-21.90	62.53	15.00
61	ASP	CB	-13.29	-21.96	61.02	15.00
61	ASP	CG	-11.96	-22.46	60.52	15.00
61	ASP	OD1	-11.41	-23.42	61.13	15.00
61	ASP	OD2	-11.48	-21.91	59.50	15.00
61	ASP	C	-13.89	-20.55	62.98	15.00
61	ASP	O	-13.38	-19.49	62.62	15.00
62	GLY	N	-14.94	-20.59	63.77	15.00
62	GLY	CA	-15.48	-19.35	64.30	15.00
62	GLY	C	-16.16	-18.55	63.21	15.00
62	GLY	O	-17.14	-19.03	62.59	15.00
63	CYS	N	-15.70	-17.33	62.93	15.00
63	CYS	CA	-16.40	-16.58	61.91	15.00
63	CYS	C	-16.18	-17.07	60.50	15.00
63	CYS	O	-16.75	-16.57	59.55	15.00
63	CYS	CB	-16.13	-15.11	62.08	15.00
63	CYS	SG	-17.00	-14.35	63.54	15.00
64	GLY	N	-15.46	-18.19	60.41	15.00
64	GLY	CA	-15.19	-18.79	59.11	15.00
64	GLY	C	-16.12	-19.97	58.83	15.00
64	GLY	O	-16.19	-20.49	57.72	15.00
65	GLY	N	-16.79	-20.46	59.86	15.00
65	GLY	CA	-17.70	-21.56	59.62	15.00
65	GLY	C	-17.39	-22.81	60.42	15.00
65	GLY	O	-16.24	-23.13	60.74	15.00
66	GLY	N	-18.43	-23.62	60.61	15.00
66	GLY	CA	-18.29	-24.85	61.37	15.00
66	GLY	C	-19.48	-25.78	61.43	15.00
66	GLY	O	-20.57	-25.37	61.00	15.00
67	TYR	N	-19.31	-26.94	62.06	15.00
67	TYR	CA	-20.37	-27.91	62.16	15.00
67	TYR	CB	-19.83	-29.31	61.82	15.00
67	TYR	CG	-19.28	-29.38	60.43	15.00
67	TYR	CD1	-20.08	-29.14	59.33	15.00
67	TYR	CE1	-19.54	-29.09	58.03	15.00
67	TYR	CD2	-17.93	-29.57	60.21	15.00
67	TYR	CE2	-17.39	-29.52	58.91	15.00
67	TYR	CZ	-18.20	-29.27	57.84	15.00
67	TYR	OH	-17.70	-29.21	56.59	15.00
67	TYR	C	-21.11	-27.86	63.49	15.00
67	TYR	O	-20.55	-27.52	64.52	15.00
68	MET	N	-22.40	-28.13	63.48	15.00

TABLE VIII

68	MET	CA	-23.12	-28.14	64.76	15.00
68	MET	CB	-24.62	-28.23	64.56	15.00
68	MET	CG	-25.11	-27.02	63.82	15.00
68	MET	SD	-24.76	-27.31	62.04	15.00
68	MET	CE	-26.39	-28.14	61.56	15.00
68	MET	C	-22.66	-29.31	65.63	15.00
68	MET	O	-22.63	-29.21	66.83	15.00
69	THR	N	-22.32	-30.42	64.99	15.00
69	THR	CA	-21.87	-31.57	65.74	15.00
69	THR	CB	-21.55	-32.78	64.81	15.00
69	THR	OG1	-20.68	-32.38	63.72	15.00
69	THR	CG2	-22.82	-33.41	64.29	15.00
69	THR	C	-20.65	-31.21	66.61	15.00
69	THR	O	-20.61	-31.62	67.76	15.00
70	ASN	N	-19.74	-30.38	66.11	15.00
70	ASN	CA	-18.56	-30.05	66.91	15.00
70	ASN	CB	-17.53	-29.28	66.07	15.00
70	ASN	CG	-16.83	-30.17	65.02	15.00
70	ASN	OD1	-17.07	-31.39	64.94	15.00
70	ASN	ND2	-16.02	-29.55	64.17	15.00
70	ASN	C	-18.99	-29.22	68.11	15.00
70	ASN	O	-18.59	-29.49	69.21	15.00
71	ALA	N	-19.95	-28.33	67.87	15.00
71	ALA	CA	-20.42	-27.44	68.91	15.00
71	ALA	CB	-21.27	-26.35	68.33	15.00
71	ALA	C	-21.15	-28.13	70.05	15.00
71	ALA	O	-21.13	-27.69	71.20	15.00
72	PHE	N	-21.84	-29.22	69.71	15.00
72	PHE	CA	-22.53	-29.99	70.74	15.00
72	PHE	CB	-23.59	-30.93	70.13	15.00
72	PHE	CG	-24.75	-30.22	69.47	15.00
72	PHE	CD1	-25.59	-29.41	70.21	15.00
72	PHE	CD2	-25.05	-30.41	68.12	15.00
72	PHE	CE1	-26.70	-28.82	69.63	15.00
72	PHE	CE2	-26.16	-29.82	67.55	15.00
72	PHE	CZ	-26.97	-29.03	68.31	15.00
72	PHE	C	-21.49	-30.80	71.51	15.00
72	PHE	O	-21.54	-30.91	72.73	15.00
73	GLN	N	-20.55	-31.39	70.78	15.00
73	GLN	CA	-19.50	-32.16	71.39	15.00
73	GLN	CB	-18.48	-32.63	70.34	15.00
73	GLN	CG	-17.59	-33.74	70.84	15.00

TABLE VIII

73	GLN	CD	-17.19	-34.69	69.73	15.00
73	GLN	OE1	-17.48	-35.89	69.78	15.00
73	GLN	NE2	-16.52	-34.16	68.72	15.00
73	GLN	C	-18.81	-31.26	72.43	15.00
73	GLN	O	-18.64	-31.64	73.59	15.00
74	TYR	N	-18.39	-30.06	72.02	15.00
74	TYR	CA	-17.70	-29.17	72.97	15.00
74	TYR	CB	-17.27	-27.85	72.29	15.00
74	TYR	CG	-17.25	-26.64	73.21	15.00
74	TYR	CD1	-16.09	-26.24	73.83	15.00
74	TYR	CE1	-16.11	-25.21	74.74	15.00
74	TYR	CD2	-18.43	-25.98	73.51	15.00
74	TYR	CE2	-18.46	-24.94	74.43	15.00
74	TYR	CZ	-17.30	-24.57	75.05	15.00
74	TYR	OH	-17.27	-23.57	76.01	15.00
74	TYR	C	-18.51	-28.95	74.27	15.00
74	TYR	O	-18.01	-29.19	75.35	15.00
75	VAL	N	-19.77	-28.61	74.13	15.00
75	VAL	CA	-20.68	-28.40	75.27	15.00
75	VAL	CB	-22.10	-28.09	74.67	15.00
75	VAL	CG1	-23.21	-28.24	75.71	15.00
75	VAL	CG2	-22.09	-26.67	74.09	15.00
75	VAL	C	-20.70	-29.59	76.29	15.00
75	VAL	O	-21.29	-29.50	77.38	15.00
76	GLN	N	-20.09	-30.71	75.88	15.00
76	GLN	CA	-20.03	-31.93	76.68	15.00
76	GLN	CB	-20.30	-33.15	75.77	15.00
76	GLN	CG	-20.03	-34.52	76.35	15.00
76	GLN	CD	-20.70	-35.58	75.54	15.00
76	GLN	OE1	-21.76	-36.09	75.93	15.00
76	GLN	NE2	-20.15	-35.88	74.37	15.00
76	GLN	C	-18.70	-32.10	77.39	15.00
76	GLN	O	-18.66	-32.13	78.61	15.00
77	LYS	N	-17.61	-32.20	76.65	15.00
77	LYS	CA	-16.31	-32.37	77.28	15.00
77	LYS	CB	-15.24	-32.65	76.24	15.00
77	LYS	CG	-15.60	-33.84	75.35	15.00
77	LYS	CD	-14.38	-34.57	74.81	15.00
77	LYS	CE	-13.52	-33.71	73.91	15.00
77	LYS	NZ	-12.57	-34.54	73.09	15.00
77	LYS	C	-15.94	-31.16	78.15	15.00
77	LYS	O	-15.31	-31.32	79.19	15.00

TABLE VIII

78	ASN	N	-16.35	-29.96	77.75	15.00
78	ASN	CA	-16.09	-28.77	78.57	15.00
78	ASN	CB	-16.09	-27.49	77.72	15.00
78	ASN	CG	-16.13	-26.22	78.58	15.00
78	ASN	OD1	-15.14	-25.84	79.17	15.00
78	ASN	ND2	-17.32	-25.64	78.72	15.00
78	ASN	C	-17.17	-28.68	79.66	15.00
78	ASN	O	-17.18	-27.77	80.49	15.00
79	ARG	N	-18.08	-29.64	79.64	15.00
79	ARG	CA	-19.18	-29.69	80.60	15.00
79	ARG	CB	-18.69	-30.15	81.98	15.00
79	ARG	CG	-18.36	-31.63	82.12	15.00
79	ARG	CD	-17.79	-31.93	83.52	15.00
79	ARG	NE	-16.63	-32.84	83.47	15.00
79	ARG	CZ	-15.39	-32.46	83.15	15.00
79	ARG	NH1	-15.15	-31.19	82.86	15.00
79	ARG	NH2	-14.38	-33.34	83.16	15.00
79	ARG	C	-20.00	-28.40	80.78	15.00
79	ARG	O	-20.27	-27.99	81.91	15.00
80	GLY	N	-20.32	-27.70	79.70	15.00
80	GLY	CA	-21.14	-26.50	79.88	15.00
80	GLY	C	-21.02	-25.34	78.91	15.00
80	GLY	O	-19.94	-25.13	78.31	15.00
81	ILE	N	-22.13	-24.60	78.78	15.00
81	ILE	CA	-22.27	-23.43	77.92	15.00
81	ILE	CB	-23.18	-23.77	76.69	15.00
81	ILE	CG2	-24.60	-24.14	77.13	15.00
81	ILE	CG1	-23.28	-22.57	75.76	15.00
81	ILE	CD1	-24.04	-22.84	74.48	15.00
81	ILE	C	-22.91	-22.32	78.75	15.00
81	ILE	O	-23.73	-22.62	79.63	15.00
82	ASP	N	-22.58	-21.05	78.48	15.00
82	ASP	CA	-23.13	-19.92	79.28	15.00
82	ASP	CB	-22.13	-18.77	79.29	15.00
82	ASP	CG	-20.88	-19.11	80.02	15.00
82	ASP	OD1	-19.80	-18.87	79.48	15.00
82	ASP	OD2	-20.96	-19.62	81.14	15.00
82	ASP	C	-24.47	-19.36	78.83	15.00
82	ASP	O	-25.10	-19.90	77.94	15.00
83	SER	N	-24.92	-18.31	79.51	15.00
83	SER	CA	-26.12	-17.57	79.18	15.00
83	SER	CB	-26.70	-16.97	80.48	15.00

TABLE VIII

83	SER	OG	-25.68	-16.38	81.28	15.00
83	SER	C	-25.55	-16.45	78.27	15.00
83	SER	O	-24.33	-16.24	78.28	15.00
84	GLU	N	-26.35	-15.82	77.39	15.00
84	GLU	CA	-25.85	-14.72	76.54	15.00
84	GLU	CB	-27.00	-13.88	75.94	15.00
84	GLU	CG	-27.12	-13.72	74.39	15.00
84	GLU	CD	-25.97	-12.97	73.70	15.00
84	GLU	OE1	-25.80	-11.74	73.90	15.00
84	GLU	OE2	-25.23	-13.64	72.93	15.00
84	GLU	C	-25.15	-13.79	77.53	15.00
84	GLU	O	-24.00	-13.44	77.37	15.00
85	ASP	N	-25.85	-13.43	78.61	15.00
85	ASP	CA	-25.31	-12.53	79.65	15.00
85	ASP	CB	-26.08	-12.68	80.98	15.00
85	ASP	CG	-27.48	-12.06	80.94	15.00
85	ASP	OD1	-28.41	-12.76	81.40	15.00
85	ASP	OD2	-27.63	-10.90	80.45	15.00
85	ASP	C	-23.80	-12.67	79.97	15.00
85	ASP	O	-23.07	-11.67	80.00	15.00
86	ALA	N	-23.36	-13.90	80.22	15.00
86	ALA	CA	-21.96	-14.21	80.59	15.00
86	ALA	CB	-21.89	-15.55	81.31	15.00
86	ALA	C	-21.00	-14.20	79.40	15.00
86	ALA	O	-19.76	-14.22	79.57	15.00
87	TYR	N	-21.55	-14.11	78.20	15.00
87	TYR	CA	-20.74	-14.13	76.99	15.00
87	TYR	CB	-20.41	-15.60	76.66	15.00
87	TYR	CG	-18.96	-15.90	76.36	15.00
87	TYR	CD1	-18.23	-15.14	75.50	15.00
87	TYR	CE1	-16.93	-15.44	75.21	15.00
87	TYR	CD2	-18.34	-16.98	76.94	15.00
87	TYR	CE2	-17.04	-17.27	76.65	15.00
87	TYR	CZ	-16.35	-16.52	75.79	15.00
87	TYR	OH	-15.09	-16.87	75.41	15.00
87	TYR	C	-21.57	-13.50	75.86	15.00
87	TYR	O	-21.88	-14.19	74.89	15.00
88	PRO	N	-21.98	-12.22	75.98	15.00
88	PRO	CD	-21.70	-11.28	77.08	15.00
88	PRO	CA	-22.78	-11.57	74.93	15.00
88	PRO	CB	-22.84	-10.11	75.41	15.00
88	PRO	CG	-22.78	-10.21	76.93	15.00

TABLE VIII

88 PRO C	-22.14	-11.72	73.54	15.00
88 PRO O	-20.91	-11.95	73.44	15.00
89 TYR N	-22.97	-11.62	72.49	15.00
89 TYR CA	-22.50	-11.76	71.11	15.00
89 TYR CB	-23.64	-12.25	70.22	15.00
89 TYR CG	-23.22	-12.67	68.82	15.00
89 TYR CD1	-22.42	-13.82	68.64	15.00
89 TYR CE1	-22.03	-14.24	67.35	15.00
89 TYR CD2	-23.62	-11.92	67.68	15.00
89 TYR CE2	-23.24	-12.31	66.41	15.00
89 TYR CZ	-22.44	-13.47	66.24	15.00
89 TYR OH	-22.00	-13.78	64.96	15.00
89 TYR C	-21.91	-10.45	70.58	15.00
89 TYR O	-22.53	-9.40	70.70	15.00
90 VAL N	-20.67	-10.51	70.08	15.00
90 VAL CA	-19.98	-9.36	69.50	15.00
90 VAL CB	-18.74	-8.92	70.32	15.00
90 VAL CG1	-19.17	-8.55	71.75	15.00
90 VAL CG2	-17.66	-9.99	70.28	15.00
90 VAL C	-19.58	-9.60	68.03	15.00
90 VAL O	-18.77	-8.86	67.47	15.00
91 GLY N	-20.12	-10.65	67.43	15.00
91 GLY CA	-19.85	-10.97	66.03	15.00
91 GLY C	-18.40	-10.89	65.56	15.00
91 GLY O	-18.09	-10.75	64.36	15.00
92 GLN N	-17.49	-11.02	66.50	15.00
92 GLN CA	-16.08	-10.99	66.22	15.00
92 GLN CB	-15.44	-9.73	66.78	15.00
92 GLN CG	-14.07	-9.49	66.26	15.00
92 GLN CD	-13.74	-8.01	66.30	15.00
92 GLN OE1	-13.84	-7.29	65.30	15.00
92 GLN NE2	-13.35	-7.54	67.49	15.00
92 GLN C	-15.63	-12.18	67.00	15.00
92 GLN O	-16.16	-12.45	68.08	15.00
93 GLU N	-14.75	-12.96	66.42	15.00
93 GLU CA	-14.27	-14.11	67.13	15.00
93 GLU CB	-13.67	-15.14	66.19	15.00
93 GLU CG	-13.54	-16.51	66.82	15.00
93 GLU CD	-12.31	-17.23	66.33	15.00
93 GLU OE1	-11.79	-18.11	67.03	15.00
93 GLU OE2	-11.86	-16.90	65.23	15.00
93 GLU C	-13.17	-13.56	68.00	15.00

TABLE VIII

93	GLU	O	-12.58	-12.52	67.67	15.00
94	GLU	N	-12.98	-14.19	69.17	15.00
94	GLU	CA	-11.95	-13.83	70.12	15.00
94	GLU	CB	-12.45	-12.76	71.08	15.00
94	GLU	CG	-13.44	-11.78	70.55	15.00
94	GLU	CD	-13.36	-10.49	71.28	15.00
94	GLU	OE1	-12.35	-9.77	71.16	15.00
94	GLU	OE2	-14.28	-10.18	72.03	15.00
94	GLU	C	-11.52	-15.03	70.95	15.00
94	GLU	O	-12.21	-16.05	71.03	15.00
95	SER	N	-10.46	-14.79	71.73	15.00
95	SER	CA	-9.89	-15.79	72.60	15.00
95	SER	CB	-8.61	-15.24	73.23	15.00
95	SER	OG	-7.71	-14.80	72.23	15.00
95	SER	C	-10.92	-16.24	73.63	15.00
95	SER	O	-11.66	-15.42	74.18	15.00
96	CYS	N	-10.99	-17.55	73.82	15.00
96	CYS	CA	-11.94	-18.19	74.74	15.00
96	CYS	C	-11.83	-17.70	76.17	15.00
96	CYS	O	-10.75	-17.73	76.79	15.00
96	CYS	CB	-11.80	-19.73	74.68	15.00
96	CYS	SG	-12.78	-20.81	75.78	15.00
97	MET	N	-12.97	-17.26	76.69	15.00
97	MET	CA	-13.10	-16.73	78.03	15.00
97	MET	CB	-13.17	-15.20	78.02	15.00
97	MET	CG	-12.67	-14.49	79.27	15.00
97	MET	SD	-10.82	-14.26	79.19	15.00
97	MET	CE	-10.31	-15.40	80.50	15.00
97	MET	C	-14.34	-17.32	78.74	15.00
97	MET	O	-15.06	-16.60	79.42	15.00
98	TYR	N	-14.60	-18.61	78.59	15.00
98	TYR	CA	-15.74	-19.28	79.24	15.00
98	TYR	CB	-15.63	-20.78	79.00	15.00
98	TYR	CG	-16.63	-21.59	79.77	15.00
98	TYR	CD1	-17.98	-21.47	79.50	15.00
98	TYR	CE1	-18.91	-22.15	80.24	15.00
98	TYR	CD2	-16.22	-22.44	80.82	15.00
98	TYR	CE2	-17.15	-23.16	81.58	15.00
98	TYR	CZ	-18.51	-22.99	81.27	15.00
98	TYR	OH	-19.51	-23.63	81.97	15.00
98	TYR	C	-15.85	-19.00	80.73	15.00
98	TYR	O	-14.85	-18.70	81.38	15.00

TABLE VIII

99	ASN	N	-17.06	-19.08	81.26	15.00
99	ASN	CA	-17.25	-18.79	82.67	15.00
99	ASN	CB	-17.77	-17.37	82.86	15.00
99	ASN	CG	-17.78	-16.95	84.33	15.00
99	ASN	OD1	-18.62	-17.40	85.11	15.00
99	ASN	ND2	-16.82	-16.11	84.70	15.00
99	ASN	C	-18.13	-19.73	83.47	15.00
99	ASN	O	-19.36	-19.70	83.36	15.00
100	PRO	N	-17.51	-20.60	84.28	15.00
100	PRO	CD	-16.06	-20.90	84.34	15.00
100	PRO	CA	-18.26	-21.55	85.10	15.00
100	PRO	CB	-17.25	-21.89	86.20	15.00
100	PRO	CG	-15.98	-22.00	85.45	15.00
100	PRO	C	-19.56	-21.03	85.71	15.00
100	PRO	O	-20.61	-21.68	85.55	15.00
101	THR	N	-19.48	-19.89	86.41	15.00
101	THR	CA	-20.63	-19.30	87.10	15.00
101	THR	CB	-20.18	-18.20	88.13	15.00
101	THR	OG1	-19.04	-17.45	87.66	15.00
101	THR	CG2	-19.82	-18.87	89.46	15.00
101	THR	C	-21.77	-18.86	86.17	15.00
101	THR	O	-22.95	-18.78	86.56	15.00
102	GLY	N	-21.40	-18.68	84.91	15.00
102	GLY	CA	-22.35	-18.33	83.88	15.00
102	GLY	C	-23.27	-19.50	83.58	15.00
102	GLY	O	-24.47	-19.30	83.42	15.00
103	LYS	N	-22.68	-20.69	83.38	15.00
103	LYS	CA	-23.39	-21.95	83.13	15.00
103	LYS	CB	-22.95	-23.01	84.16	15.00
103	LYS	CG	-23.73	-24.31	84.12	15.00
103	LYS	CD	-23.11	-25.38	85.05	15.00
103	LYS	CE	-21.69	-25.76	84.61	15.00
103	LYS	NZ	-21.01	-26.68	85.56	15.00
103	LYS	C	-24.90	-21.82	83.20	15.00
103	LYS	O	-25.45	-21.45	84.23	15.00
104	ALA	N	-25.58	-22.16	82.10	15.00
104	ALA	CA	-27.05	-22.11	82.04	15.00
104	ALA	CB	-27.54	-20.84	81.26	15.00
104	ALA	C	-27.64	-23.39	81.42	15.00
104	ALA	O	-28.85	-23.61	81.42	15.00
105	ALA	N	-26.79	-24.26	80.92	15.00
105	ALA	CA	-27.24	-25.50	80.30	15.00

TABLE VIII

105	ALA	CB	-28.05	-25.22	79.03	15.00
105	ALA	C	-26.03	-26.35	79.97	15.00
105	ALA	O	-24.88	-25.90	80.04	15.00
106	LYS	N	-26.32	-27.59	79.60	15.00
106	LYS	CA	-25.32	-28.57	79.25	15.00
106	LYS	CB	-24.74	-29.13	80.55	15.00
106	LYS	CG	-23.71	-30.22	80.42	15.00
106	LYS	CD	-23.54	-30.96	81.75	15.00
106	LYS	CE	-24.85	-31.60	82.15	15.00
106	LYS	NZ	-24.61	-32.90	82.82	15.00
106	LYS	C	-26.09	-29.63	78.43	15.00
106	LYS	O	-27.32	-29.62	78.34	15.00
107	CYS	N	-25.36	-30.51	77.77	15.00
107	CYS	CA	-26.00	-31.54	76.97	15.00
107	CYS	CB	-26.06	-31.11	75.50	15.00
107	CYS	SG	-24.54	-31.49	74.55	15.00
107	CYS	C	-25.07	-32.72	77.10	15.00
107	CYS	O	-23.85	-32.54	77.25	15.00
108	ARG	N	-25.62	-33.92	77.06	15.00
108	ARG	CA	-24.80	-35.12	77.17	15.00
108	ARG	CB	-25.28	-36.03	78.28	15.00
108	ARG	CG	-25.35	-35.42	79.64	15.00
108	ARG	CD	-25.75	-36.49	80.66	15.00
108	ARG	NE	-27.18	-36.72	80.71	15.00
108	ARG	CZ	-27.75	-37.86	81.09	15.00
108	ARG	NH1	-27.00	-38.90	81.43	15.00
108	ARG	NH2	-29.07	-37.94	81.22	15.00
108	ARG	C	-24.85	-35.89	75.85	15.00
108	ARG	O	-25.59	-36.87	75.72	15.00
109	GLY	N	-24.11	-35.40	74.87	15.00
109	GLY	CA	-24.05	-36.03	73.57	15.00
109	GLY	C	-24.99	-35.44	72.55	15.00
109	GLY	O	-25.58	-34.38	72.78	15.00
110	TYR	N	-25.00	-36.06	71.36	15.00
110	TYR	CA	-25.86	-35.67	70.23	15.00
110	TYR	CB	-25.19	-34.54	69.43	15.00
110	TYR	CG	-23.92	-34.95	68.76	15.00
110	TYR	CD1	-22.72	-34.87	69.39	15.00
110	TYR	CE1	-21.60	-35.34	68.80	15.00
110	TYR	CD2	-23.95	-35.49	67.52	15.00
110	TYR	CE2	-22.82	-35.97	66.92	15.00
110	TYR	CZ	-21.64	-35.90	67.55	15.00

TABLE VIII

115 GLU CD	-26.48	-39.24	53.21	15.00
115 GLU OE1	-26.78	-40.40	52.85	15.00
115 GLU OE2	-25.33	-38.75	53.12	15.00
115 GLU C	-30.20	-38.50	54.78	15.00
115 GLU O	-30.37	-39.53	54.16	15.00
116 GLY N	-30.90	-37.40	54.58	15.00
116 GLY CA	-31.88	-37.30	53.52	15.00
116 GLY C	-33.29	-37.78	53.79	15.00
116 GLY O	-34.11	-37.73	52.87	15.00
117 ASN N	-33.56	-38.25	55.01	15.00
117 ASN CA	-34.89	-38.73	55.36	15.00
117 ASN CB	-34.76	-40.00	56.22	15.00
117 ASN CG	-36.06	-40.77	56.33	15.00
117 ASN OD1	-37.13	-40.29	55.89	15.00
117 ASN ND2	-35.99	-41.96	56.91	15.00
117 ASN C	-35.76	-37.69	56.07	15.00
117 ASN O	-35.55	-37.38	57.23	15.00
118 GLU N	-36.72	-37.13	55.34	15.00
118 GLU CA	-37.65	-36.15	55.89	15.00
118 GLU CB	-38.29	-35.34	54.78	15.00
118 GLU CG	-37.31	-34.44	54.07	15.00
118 GLU CD	-38.00	-33.61	53.01	15.00
118 GLU OE1	-38.09	-34.08	51.85	15.00
118 GLU OE2	-38.48	-32.51	53.32	15.00
118 GLU C	-38.73	-36.78	56.75	15.00
118 GLU O	-39.42	-36.09	57.50	15.00
119 LYS N	-38.84	-38.11	56.68	15.00
119 LYS CA	-39.82	-38.82	57.49	15.00
119 LYS CB	-40.11	-40.20	56.91	15.00
119 LYS CG	-40.84	-41.15	57.86	15.00
119 LYS CD	-41.21	-42.46	57.19	15.00
119 LYS CE	-39.98	-43.29	56.80	15.00
119 LYS NZ	-38.99	-43.60	57.92	15.00
119 LYS C	-39.24	-38.95	58.88	15.00
119 LYS O	-39.97	-38.92	59.86	15.00
120 ALA N	-37.92	-39.06	58.95	15.00
120 ALA CA	-37.26	-39.21	60.24	15.00
120 ALA CB	-35.86	-39.73	60.05	15.00
120 ALA C	-37.20	-37.84	60.87	15.00
120 ALA O	-37.26	-37.70	62.09	15.00
121 LEU N	-37.08	-36.82	60.03	15.00
121 LEU CA	-36.98	-35.45	60.51	15.00

TABLE VIII

121 LEU CB	-36.44	-34.53	59.41	15.00
121 LEU CG	-36.17	-33.05	59.73	15.00
121 LEU CD1	-35.09	-32.86	60.74	15.00
121 LEU CD2	-35.74	-32.40	58.46	15.00
121 LEU C	-38.30	-34.95	61.07	15.00
121 LEU O	-38.33	-34.36	62.16	15.00
122 LYS N	-39.40	-35.27	60.39	15.00
122 LYS CA	-40.71	-34.88	60.89	15.00
122 LYS CB	-41.80	-35.31	59.90	15.00
122 LYS CG	-43.25	-35.03	60.34	15.00
122 LYS CD	-44.28	-35.77	59.47	15.00
122 LYS CE	-45.67	-35.70	60.08	15.00
122 LYS NZ	-46.60	-36.58	59.32	15.00
122 LYS C	-40.88	-35.54	62.26	15.00
122 LYS O	-41.33	-34.90	63.22	15.00
123 ARG N	-40.48	-36.81	62.38	15.00
123 ARG CA	-40.58	-37.50	63.65	15.00
123 ARG CB	-40.25	-38.98	63.52	15.00
123 ARG CG	-41.30	-39.84	62.88	15.00
123 ARG CD	-41.30	-41.21	63.51	15.00
123 ARG NE	-39.95	-41.78	63.60	15.00
123 ARG CZ	-39.25	-42.23	62.56	15.00
123 ARG NH1	-39.75	-42.19	61.32	15.00
123 ARG NH2	-38.05	-42.77	62.77	15.00
123 ARG C	-39.70	-36.88	64.73	15.00
123 ARG O	-40.18	-36.62	65.83	15.00
124 ALA N	-38.45	-36.57	64.41	15.00
124 ALA CA	-37.57	-35.99	65.43	15.00
124 ALA CB	-36.19	-35.74	64.86	15.00
124 ALA C	-38.12	-34.71	66.02	15.00
124 ALA O	-38.00	-34.46	67.22	15.00
125 VAL N	-38.77	-33.92	65.17	15.00
125 VAL CA	-39.36	-32.62	65.52	15.00
125 VAL CB	-39.54	-31.74	64.24	15.00
125 VAL CG1	-40.40	-30.50	64.54	15.00
125 VAL CG2	-38.15	-31.36	63.70	15.00
125 VAL C	-40.70	-32.75	66.24	15.00
125 VAL O	-41.14	-31.81	66.92	15.00
126 ALA N	-41.40	-33.85	66.02	15.00
126 ALA CA	-42.67	-34.05	66.68	15.00
126 ALA CB	-43.57	-35.00	65.86	15.00
126 ALA C	-42.42	-34.59	68.08	15.00

TABLE VIII

126 ALA O	-42.99	-34.11	69.06	15.00
127 ARG N	-41.47	-35.52	68.18	15.00
127 ARG CA	-41.15	-36.15	69.47	15.00
127 ARG CB	-40.71	-37.61	69.26	15.00
127 ARG CG	-41.77	-38.56	68.76	15.00
127 ARG CD	-42.88	-38.82	69.77	15.00
127 ARG NE	-43.75	-39.92	69.33	15.00
127 ARG CZ	-44.83	-40.35	69.98	15.00
127 ARG NH1	-45.54	-41.36	69.47	15.00
127 ARG NH2	-45.21	-39.78	71.13	15.00
127 ARG C	-40.13	-35.44	70.36	15.00
127 ARG O	-40.28	-35.42	71.58	15.00
128 VAL N	-39.07	-34.89	69.76	15.00
128 VAL CA	-37.97	-34.24	70.49	15.00
128 VAL CB	-36.63	-34.58	69.81	15.00
128 VAL CG1	-35.45	-34.03	70.61	15.00
128 VAL CG2	-36.48	-36.07	69.66	15.00
128 VAL C	-38.10	-32.73	70.56	15.00
128 VAL O	-37.92	-32.12	71.63	15.00
129 GLY N	-38.44	-32.14	69.42	15.00
129 GLY CA	-38.57	-30.70	69.33	15.00
129 GLY C	-37.60	-30.09	68.33	15.00
129 GLY O	-37.12	-30.79	67.45	15.00
130 PRO N	-37.31	-28.77	68.42	15.00
130 PRO CD	-37.83	-27.89	69.47	15.00
130 PRO CA	-36.40	-28.02	67.54	15.00
130 PRO CB	-36.13	-26.77	68.34	15.00
130 PRO CG	-37.40	-26.52	68.98	15.00
130 PRO C	-35.13	-28.78	67.19	15.00
130 PRO O	-34.38	-29.24	68.05	15.00
131 VAL N	-34.91	-28.91	65.89	15.00
131 VAL CA	-33.78	-29.63	65.37	15.00
131 VAL CB	-34.27	-30.83	64.56	15.00
131 VAL CG1	-33.10	-31.52	63.87	15.00
131 VAL CG2	-35.02	-31.76	65.47	15.00
131 VAL C	-32.91	-28.75	64.48	15.00
131 VAL O	-33.43	-28.02	63.65	15.00
132 SER N	-31.60	-28.85	64.68	15.00
132 SER CA	-30.59	-28.13	63.91	15.00
132 SER CB	-29.21	-28.32	64.54	15.00
132 SER OG	-28.89	-27.37	65.52	15.00
132 SER C	-30.50	-28.73	62.50	15.00

TABLE VIII

132 SER O	-30.34	-29.94	62.34	15.00
133 VAL N	-30.47	-27.87	61.50	15.00
133 VAL CA	-30.38	-28.36	60.13	15.00
133 VAL CB	-31.75	-28.35	59.45	15.00
133 VAL CG1	-32.73	-29.24	60.17	15.00
133 VAL CG2	-32.30	-26.98	59.41	15.00
133 VAL C	-29.52	-27.41	59.35	15.00
133 VAL O	-29.29	-26.29	59.79	15.00
134 ALA N	-29.14	-27.85	58.15	15.00
134 ALA CA	-28.32	-27.08	57.22	15.00
134 ALA CB	-26.99	-27.75	56.97	15.00
134 ALA C	-29.14	-27.06	55.95	15.00
134 ALA O	-29.99	-27.92	55.71	15.00
135 ILE N	-28.79	-26.11	55.09	15.00
135 ILE CA	-29.49	-25.93	53.83	15.00
135 ILE CB	-30.82	-25.12	54.04	15.00
135 ILE CG2	-31.90	-26.00	54.64	15.00
135 ILE CG1	-30.57	-23.83	54.85	15.00
135 ILE CD1	-31.76	-22.91	54.86	15.00
135 ILE C	-28.69	-25.16	52.82	15.00
135 ILE O	-27.58	-24.73	53.10	15.00
136 ASP N	-29.20	-25.10	51.61	15.00
136 ASP CA	-28.56	-24.32	50.56	15.00
136 ASP CB	-28.74	-24.95	49.18	15.00
136 ASP CG	-28.23	-24.06	48.08	15.00
136 ASP OD1	-28.28	-24.45	46.91	15.00
136 ASP OD2	-27.73	-22.96	48.35	15.00
136 ASP C	-29.32	-23.01	50.62	15.00
136 ASP O	-30.51	-22.93	50.35	15.00
137 ALA N	-28.59	-21.94	50.84	15.00
137 ALA CA	-29.23	-20.64	50.97	15.00
137 ALA CB	-29.22	-20.22	52.43	15.00
137 ALA C	-28.65	-19.55	50.07	15.00
137 ALA O	-28.89	-18.38	50.30	15.00
138 SER N	-27.97	-19.97	49.00	15.00
138 SER CA	-27.34	-19.06	48.03	15.00
138 SER CB	-26.28	-19.80	47.23	15.00
138 SER OG	-26.71	-21.14	47.02	15.00
138 SER C	-28.32	-18.41	47.07	15.00
138 SER O	-28.09	-17.29	46.57	15.00
139 LEU N	-29.42	-19.14	46.81	15.00
139 LEU CA	-30.44	-18.68	45.87	15.00

TABLE VIII

139 LEU CB	-31.60	-19.68	45.83	15.00
139 LEU CG	-31.57	-20.77	44.76	15.00
139 LEU CD1	-31.68	-20.14	43.39	15.00
139 LEU CD2	-30.29	-21.58	44.84	15.00
139 LEU C	-30.95	-17.30	46.25	15.00
139 LEU O	-31.39	-17.09	47.37	15.00
140 THR N	-30.99	-16.39	45.28	15.00
140 THR CA	-31.41	-15.04	45.54	15.00
140 THR CB	-31.16	-14.10	44.30	15.00
140 THR OG1	-30.83	-14.87	43.13	15.00
140 THR CG2	-30.00	-13.22	44.59	15.00
140 THR C	-32.86	-14.97	46.00	15.00
140 THR O	-33.25	-14.00	46.66	15.00
141 SER N	-33.65	-15.99	45.68	15.00
141 SER CA	-35.05	-16.03	46.09	15.00
141 SER CB	-35.80	-17.14	45.35	15.00
141 SER OG	-34.95	-18.27	45.17	15.00
141 SER C	-35.15	-16.16	47.60	15.00
141 SER O	-35.95	-15.48	48.25	15.00
142 PHE N	-34.23	-16.95	48.15	15.00
142 PHE CA	-34.11	-17.19	49.58	15.00
142 PHE CB	-32.92	-18.13	49.84	15.00
142 PHE CG	-32.94	-18.73	51.21	15.00
142 PHE CD1	-33.41	-20.03	51.41	15.00
142 PHE CD2	-32.54	-17.97	52.34	15.00
142 PHE CE1	-33.50	-20.55	52.67	15.00
142 PHE CE2	-32.63	-18.49	53.60	15.00
142 PHE CZ	-33.10	-19.77	53.78	15.00
142 PHE C	-33.90	-15.87	50.34	15.00
142 PHE O	-34.57	-15.60	51.33	15.00
143 GLN N	-33.02	-15.01	49.84	15.00
143 GLN CA	-32.74	-13.74	50.49	15.00
143 GLN CB	-31.45	-13.14	49.95	15.00
143 GLN CG	-30.34	-14.15	49.75	15.00
143 GLN CD	-29.07	-13.49	49.24	15.00
143 GLN OE1	-29.02	-12.26	49.08	15.00
143 GLN NE2	-28.02	-14.29	49.00	15.00
143 GLN C	-33.90	-12.76	50.35	15.00
143 GLN O	-34.20	-12.02	51.29	15.00
144 PHE N	-34.58	-12.77	49.20	15.00
144 PHE CA	-35.72	-11.87	49.00	15.00
144 PHE CB	-35.76	-11.31	47.56	15.00

TABLE VIII

144 PHE CG	-34.56	-10.48	47.21	15.00
144 PHE CD1	-34.12	-9.49	48.08	15.00
144 PHE CD2	-33.89	-10.69	46.02	15.00
144 PHE CE1	-33.03	-8.71	47.77	15.00
144 PHE CE2	-32.80	-9.92	45.68	15.00
144 PHE CZ	-32.36	-8.93	46.55	15.00
144 PHE C	-37.07	-12.48	49.36	15.00
144 PHE O	-38.09	-11.81	49.24	15.00
145 TYR N	-37.08	-13.74	49.80	15.00
145 TYR CA	-38.31	-14.45	50.22	15.00
145 TYR CB	-37.94	-15.77	50.96	15.00
145 TYR CG	-39.07	-16.36	51.80	15.00
145 TYR CD1	-39.94	-17.34	51.29	15.00
145 TYR CE1	-41.00	-17.82	52.05	15.00
145 TYR CD2	-39.30	-15.88	53.10	15.00
145 TYR CE2	-40.33	-16.32	53.86	15.00
145 TYR CZ	-41.19	-17.29	53.34	15.00
145 TYR OH	-42.25	-17.67	54.16	15.00
145 TYR C	-39.14	-13.55	51.14	15.00
145 TYR O	-38.60	-12.81	51.97	15.00
146 SER N	-40.45	-13.64	51.02	15.00
146 SER CA	-41.31	-12.83	51.88	15.00
146 SER CB	-41.74	-11.55	51.16	15.00
146 SER OG	-40.94	-10.40	51.51	15.00
146 SER C	-42.53	-13.55	52.45	15.00
146 SER O	-42.89	-13.33	53.61	15.00
147 LYS N	-43.15	-14.44	51.68	15.00
147 LYS CA	-44.33	-15.12	52.17	15.00
147 LYS CB	-45.53	-14.22	51.94	15.00
147 LYS CG	-45.80	-13.23	53.02	15.00
147 LYS CD	-46.76	-12.13	52.55	15.00
147 LYS CE	-47.91	-12.66	51.67	15.00
147 LYS NZ	-48.65	-13.77	52.35	15.00
147 LYS C	-44.63	-16.41	51.41	15.00
147 LYS O	-44.45	-16.45	50.20	15.00
148 GLY N	-45.09	-17.43	52.10	15.00
148 GLY CA	-45.45	-18.66	51.42	15.00
148 GLY C	-44.53	-19.82	51.65	15.00
148 GLY O	-43.56	-19.73	52.41	15.00
149 VAL N	-44.79	-20.91	50.92	15.00
149 VAL CA	-43.99	-22.13	50.98	15.00
149 VAL CB	-44.85	-23.39	50.69	15.00

TABLE VIII

149 VAL CG1	-43.98	-24.66	50.78	15.00
149 VAL CG2	-45.98	-23.43	51.62	15.00
149 VAL C	-42.91	-22.02	49.90	15.00
149 VAL O	-43.22	-22.06	48.72	15.00
150 TYR N	-41.68	-21.79	50.34	15.00
150 TYR CA	-40.49	-21.66	49.49	15.00
150 TYR CB	-39.31	-21.17	50.33	15.00
150 TYR CG	-38.07	-21.02	49.48	15.00
150 TYR CD1	-37.90	-19.91	48.65	15.00
150 TYR CE1	-36.75	-19.75	47.90	15.00
150 TYR CD2	-37.05	-21.97	49.52	15.00
150 TYR CE2	-35.89	-21.82	48.77	15.00
150 TYR CZ	-35.75	-20.71	47.97	15.00
150 TYR OH	-34.59	-20.55	47.26	15.00
150 TYR C	-40.04	-22.89	48.73	15.00
150 TYR O	-39.72	-23.95	49.29	15.00
151 TYR N	-39.88	-22.68	47.44	15.00
151 TYR CA	-39.46	-23.73	46.54	15.00
151 TYR CB	-40.63	-24.64	46.18	15.00
151 TYR CG	-40.18	-25.91	45.48	15.00
151 TYR CD1	-39.56	-26.99	46.24	15.00
151 TYR CE1	-39.05	-28.12	45.59	15.00
151 TYR CD2	-40.31	-25.99	44.05	15.00
151 TYR CE2	-39.83	-27.07	43.37	15.00
151 TYR CZ	-39.19	-28.15	44.13	15.00
151 TYR OH	-38.66	-29.25	43.41	15.00
151 TYR C	-38.86	-23.09	45.29	15.00
151 TYR O	-39.45	-22.21	44.68	15.00
152 ASP N	-37.66	-23.52	44.96	15.00
152 ASP CA	-36.90	-23.04	43.81	15.00
152 ASP CB	-35.90	-21.97	44.26	15.00
152 ASP CG	-35.26	-21.25	43.08	15.00
152 ASP OD1	-35.42	-20.01	42.99	15.00
152 ASP OD2	-34.63	-21.92	42.23	15.00
152 ASP C	-36.16	-24.28	43.31	15.00
152 ASP O	-35.56	-25.00	44.09	15.00
153 GLU N	-36.16	-24.49	42.00	15.00
153 GLU CA	-35.56	-25.67	41.38	15.00
153 GLU CB	-36.09	-25.74	39.97	15.00
153 GLU CG	-35.94	-24.42	39.26	15.00
153 GLU CD	-36.44	-24.48	37.83	15.00
153 GLU OE1	-35.63	-24.12	36.94	15.00

TABLE VIII

153 GLU OE2	-37.62	-24.87	37.62	15.00
153 GLU C	-34.04	-25.70	41.31	15.00
153 GLU O	-33.47	-26.73	40.99	15.00
154 SER N	-33.39	-24.59	41.60	15.00
154 SER CA	-31.95	-24.48	41.56	15.00
154 SER CB	-31.59	-23.07	41.09	15.00
154 SER OG	-32.22	-22.78	39.85	15.00
154 SER C	-31.28	-24.79	42.91	15.00
154 SER O	-30.07	-24.67	43.03	15.00
155 CYS N	-32.08	-25.19	43.90	15.00
155 CYS CA	-31.55	-25.49	45.23	15.00
155 CYS C	-30.88	-26.84	45.21	15.00
155 CYS O	-31.52	-27.87	45.08	15.00
155 CYS CB	-32.63	-25.43	46.33	15.00
155 CYS SG	-32.25	-24.44	47.82	15.00
156 ASN N	-29.57	-26.79	45.39	15.00
156 ASN CA	-28.70	-27.97	45.38	15.00
156 ASN CB	-27.30	-27.52	44.99	15.00
156 ASN CG	-26.51	-28.59	44.35	15.00
156 ASN OD1	-26.70	-29.78	44.62	15.00
156 ASN ND2	-25.58	-28.18	43.51	15.00
156 ASN C	-28.63	-28.71	46.72	15.00
156 ASN O	-28.12	-28.19	47.70	15.00
157 SER N	-29.09	-29.96	46.73	15.00
157 SER CA	-29.09	-30.77	47.95	15.00
157 SER CB	-29.77	-32.11	47.70	15.00
157 SER OG	-31.03	-31.95	47.10	15.00
157 SER C	-27.68	-31.08	48.43	15.00
157 SER O	-27.48	-31.52	49.54	15.00
158 ASP N	-26.71	-30.93	47.55	15.00
158 ASP CA	-25.34	-31.23	47.91	15.00
158 ASP CB	-24.69	-32.07	46.78	15.00
158 ASP CG	-25.32	-33.44	46.67	15.00
158 ASP OD1	-26.15	-33.63	45.75	15.00
158 ASP OD2	-25.05	-34.30	47.55	15.00
158 ASP C	-24.46	-30.07	48.28	15.00
158 ASP O	-23.27	-30.25	48.57	15.00
159 ASN N	-25.05	-28.88	48.29	15.00
159 ASN CA	-24.30	-27.69	48.61	15.00
159 ASN CB	-24.34	-26.74	47.42	15.00
159 ASN CG	-23.51	-25.49	47.62	15.00
159 ASN OD1	-22.35	-25.55	48.00	15.00

TABLE VIII

159 ASN ND2	-24.12	-24.33	47.38	15.00
159 ASN C	-24.93	-27.03	49.82	15.00
159 ASN O	-25.67	-26.05	49.68	15.00
160 LEU N	-24.68	-27.59	50.99	15.00
160 LEU CA	-25.16	-27.07	52.24	15.00
160 LEU CB	-25.06	-28.15	53.29	15.00
160 LEU CG	-25.72	-29.45	52.83	15.00
160 LEU CD1	-25.24	-30.64	53.62	15.00
160 LEU CD2	-27.22	-29.26	52.91	15.00
160 LEU C	-24.22	-25.95	52.63	15.00
160 LEU O	-23.06	-26.21	52.92	15.00
161 ASN N	-24.73	-24.74	52.74	15.00
161 ASN CA	-23.91	-23.58	53.10	15.00
161 ASN CB	-23.61	-22.78	51.83	15.00
161 ASN CG	-24.84	-22.55	50.93	15.00
161 ASN OD1	-25.71	-21.74	51.22	15.00
161 ASN ND2	-24.92	-23.31	49.84	15.00
161 ASN C	-24.42	-22.67	54.23	15.00
161 ASN O	-23.75	-21.70	54.59	15.00
162 HIS N	-25.60	-22.96	54.76	15.00
162 HIS CA	-26.13	-22.19	55.86	15.00
162 HIS CB	-27.12	-21.15	55.35	15.00
162 HIS CG	-27.63	-20.21	56.41	15.00
162 HIS CD2	-28.89	-19.99	56.84	15.00
162 HIS ND1	-26.82	-19.39	57.16	15.00
162 HIS CE1	-27.56	-18.68	57.99	15.00
162 HIS NE2	-28.82	-19.03	57.82	15.00
162 HIS C	-26.80	-23.11	56.86	15.00
162 HIS O	-27.41	-24.10	56.49	15.00
163 ALA N	-26.61	-22.84	58.14	15.00
163 ALA CA	-27.27	-23.63	59.17	15.00
163 ALA CB	-26.35	-23.90	60.32	15.00
163 ALA C	-28.47	-22.85	59.65	15.00
163 ALA O	-28.43	-21.62	59.83	15.00
164 VAL N	-29.53	-23.57	59.97	15.00
164 VAL CA	-30.75	-22.92	60.40	15.00
164 VAL CB	-31.54	-22.58	59.10	15.00
164 VAL CG1	-32.42	-23.71	58.68	15.00
164 VAL CG2	-32.27	-21.27	59.22	15.00
164 VAL C	-31.49	-23.77	61.47	15.00
164 VAL O	-31.01	-24.81	61.87	15.00
165 LEU N	-32.64	-23.32	61.97	15.00

TABLE VIII

165 LEU CA	-33.33	-24.10	62.98	15.00
165 LEU CB	-33.27	-23.41	64.32	15.00
165 LEU CG	-33.72	-24.12	65.58	15.00
165 LEU CD1	-32.59	-24.89	66.21	15.00
165 LEU CD2	-34.18	-23.05	66.52	15.00
165 LEU C	-34.76	-24.44	62.63	15.00
165 LEU O	-35.55	-23.56	62.28	15.00
166 ALA N	-35.05	-25.73	62.66	15.00
166 ALA CA	-36.37	-26.25	62.37	15.00
166 ALA CB	-36.25	-27.61	61.71	15.00
166 ALA C	-37.09	-26.35	63.69	15.00
166 ALA O	-36.63	-27.02	64.62	15.00
167 VAL N	-38.24	-25.69	63.76	15.00
167 VAL CA	-39.08	-25.64	64.97	15.00
167 VAL CB	-39.16	-24.22	65.61	15.00
167 VAL CG1	-37.79	-23.68	65.96	15.00
167 VAL CG2	-39.89	-23.25	64.67	15.00
167 VAL C	-40.52	-26.07	64.76	15.00
167 VAL O	-41.40	-25.61	65.46	15.00
168 GLY N	-40.78	-26.91	63.77	15.00
168 GLY CA	-42.15	-27.34	63.56	15.00
168 GLY C	-42.35	-27.62	62.09	15.00
168 GLY O	-41.42	-27.58	61.31	15.00
169 TYR N	-43.58	-27.95	61.73	15.00
169 TYR CA	-43.99	-28.29	60.36	15.00
169 TYR CB	-43.51	-29.71	59.99	15.00
169 TYR CG	-44.07	-30.82	60.89	15.00
169 TYR CD1	-45.33	-31.41	60.61	15.00
169 TYR CE1	-45.86	-32.39	61.43	15.00
169 TYR CD2	-43.34	-31.27	62.02	15.00
169 TYR CE2	-43.88	-32.28	62.86	15.00
169 TYR CZ	-45.12	-32.81	62.55	15.00
169 TYR OH	-45.63	-33.71	63.41	15.00
169 TYR C	-45.53	-28.26	60.32	15.00
169 TYR O	-46.20	-28.25	61.37	15.00
170 GLY N	-46.09	-28.23	59.12	15.00
170 GLY CA	-47.54	-28.17	58.95	15.00
170 GLY C	-47.93	-28.06	57.48	15.00
170 GLY O	-47.12	-28.35	56.61	15.00
171 ILE N	-49.14	-27.61	57.17	15.00
171 ILE CA	-49.55	-27.54	55.77	15.00
171 ILE CB	-50.30	-28.85	55.41	15.00

TABLE VIII

171 ILE CG2	-51.37	-29.17	56.40	15.00
171 ILE CG1	-50.79	-28.82	53.99	15.00
171 ILE CD1	-51.11	-30.20	53.45	15.00
171 ILE C	-50.38	-26.29	55.43	15.00
171 ILE O	-51.37	-26.02	56.10	15.00
172 GLN N	-49.93	-25.52	54.44	15.00
172 GLN CA	-50.64	-24.31	54.01	15.00
172 GLN CB	-49.68	-23.10	54.05	15.00
172 GLN CG	-50.30	-21.69	53.87	15.00
172 GLN CD	-49.27	-20.56	53.75	15.00
172 GLN OE1	-48.07	-20.77	53.89	15.00
172 GLN NE2	-49.74	-19.35	53.49	15.00
172 GLN C	-51.25	-24.41	52.63	15.00
172 GLN O	-50.56	-24.19	51.64	15.00
173 LYS N	-52.55	-24.75	52.57	15.00
173 LYS CA	-53.33	-24.85	51.32	15.00
173 LYS CB	-53.40	-23.48	50.61	15.00
173 LYS CG	-54.16	-22.39	51.36	15.00
173 LYS CD	-53.57	-22.02	52.75	15.00
173 LYS CE	-54.37	-22.65	53.92	15.00
173 LYS NZ	-54.04	-22.06	55.23	15.00
173 LYS C	-52.85	-25.93	50.36	15.00
173 LYS O	-52.73	-25.69	49.15	15.00
174 GLY N	-52.61	-27.11	50.90	15.00
174 GLY CA	-52.15	-28.21	50.08	15.00
174 GLY C	-50.64	-28.26	50.03	15.00
174 GLY O	-50.08	-29.23	49.53	15.00
175 ASN N	-49.97	-27.25	50.58	15.00
175 ASN CA	-48.52	-27.27	50.57	15.00
175 ASN CB	-47.92	-26.00	49.95	15.00
175 ASN CG	-48.48	-25.73	48.57	15.00
175 ASN OD1	-48.53	-26.61	47.73	15.00
175 ASN ND2	-48.96	-24.51	48.37	15.00
175 ASN C	-47.94	-27.50	51.94	15.00
175 ASN O	-48.04	-26.66	52.86	15.00
176 LYS N	-47.37	-28.69	52.07	15.00
176 LYS CA	-46.71	-29.13	53.27	15.00
176 LYS CB	-46.28	-30.61	53.08	15.00
176 LYS CG	-47.40	-31.59	52.68	15.00
176 LYS CD	-47.20	-32.92	53.41	15.00
176 LYS CE	-48.36	-33.85	53.17	15.00
176 LYS NZ	-48.49	-34.80	54.30	15.00

TABLE VIII

176 LYS C	-45.51	-28.18	53.48	15.00
176 LYS O	-45.12	-27.49	52.55	15.00
177 HIS N	-44.94	-28.15	54.68	15.00
177 HIS CA	-43.82	-27.26	54.97	15.00
177 HIS CB	-44.23	-25.79	54.78	15.00
177 HIS CG	-45.19	-25.25	55.82	15.00
177 HIS CD2	-45.07	-25.11	57.17	15.00
177 HIS ND1	-46.37	-24.62	55.49	15.00
177 HIS CE1	-46.93	-24.11	56.58	15.00
177 HIS NE2	-46.16	-24.40	57.61	15.00
177 HIS C	-43.08	-27.42	56.30	15.00
177 HIS O	-43.62	-27.92	57.28	15.00
178 TRP N	-41.81	-27.01	56.29	15.00
178 TRP CA	-40.97	-27.01	57.48	15.00
178 TRP CB	-39.52	-27.41	57.16	15.00
178 TRP CG	-39.34	-28.83	56.89	15.00
178 TRP CD2	-39.46	-29.91	57.82	15.00
178 TRP CE2	-39.29	-31.11	57.09	15.00
178 TRP CE3	-39.70	-29.97	59.20	15.00
178 TRP CD1	-39.09	-29.39	55.68	15.00
178 TRP NE1	-39.07	-30.76	55.78	15.00
178 TRP CZ2	-39.34	-32.38	57.67	15.00
178 TRP CZ3	-39.76	-31.22	59.78	15.00
178 TRP CH2	-39.58	-32.42	59.01	15.00
178 TRP C	-41.00	-25.55	57.95	15.00
178 TRP O	-41.12	-24.64	57.14	15.00
179 ILE N	-41.04	-25.34	59.26	15.00
179 ILE CA	-41.05	-23.98	59.78	15.00
179 ILE CB	-41.99	-23.89	60.97	15.00
179 ILE CG2	-41.90	-22.54	61.61	15.00
179 ILE CG1	-43.42	-24.18	60.51	15.00
179 ILE CD1	-44.37	-24.29	61.63	15.00
179 ILE C	-39.62	-23.75	60.20	15.00
179 ILE O	-39.07	-24.45	61.07	15.00
180 ILE N	-38.99	-22.78	59.57	15.00
180 ILE CA	-37.58	-22.52	59.86	15.00
180 ILE CB	-36.79	-22.59	58.57	15.00
180 ILE CG2	-35.36	-22.38	58.83	15.00
180 ILE CG1	-36.99	-23.93	57.91	15.00
180 ILE CD1	-36.41	-25.01	58.75	15.00
180 ILE C	-37.25	-21.18	60.52	15.00
180 ILE O	-37.82	-20.13	60.17	15.00

TABLE VIII

181 LYS N	-36.35	-21.19	61.49	15.00
181 LYS CA	-35.97	-19.95	62.16	15.00
181 LYS CB	-35.83	-20.19	63.65	15.00
181 LYS CG	-35.49	-18.92	64.45	15.00
181 LYS CD	-35.36	-19.25	65.93	15.00
181 LYS CE	-35.01	-18.04	66.76	15.00
181 LYS NZ	-34.86	-18.51	68.16	15.00
181 LYS C	-34.64	-19.50	61.61	15.00
181 LYS O	-33.72	-20.32	61.54	15.00
182 ASN N	-34.49	-18.23	61.27	15.00
182 ASN CA	-33.22	-17.79	60.71	15.00
182 ASN CB	-33.45	-17.10	59.34	15.00
182 ASN CG	-32.32	-17.37	58.34	15.00
182 ASN OD1	-31.30	-18.02	58.65	15.00
182 ASN ND2	-32.53	-16.89	57.09	15.00
182 ASN C	-32.54	-16.84	61.68	15.00
182 ASN O	-33.16	-16.31	62.60	15.00
183 SER N	-31.25	-16.64	61.45	15.00
183 SER CA	-30.40	-15.74	62.23	15.00
183 SER CB	-29.16	-16.50	62.75	15.00
183 SER OG	-28.52	-17.33	61.76	15.00
183 SER C	-29.95	-14.52	61.41	15.00
183 SER O	-28.81	-14.06	61.56	15.00
184 TRP N	-30.82	-13.98	60.55	15.00
184 TRP CA	-30.50	-12.82	59.71	15.00
184 TRP CB	-30.71	-13.10	58.22	15.00
184 TRP CG	-29.79	-14.06	57.58	15.00
184 TRP CD2	-29.90	-14.58	56.26	15.00
184 TRP CE2	-28.80	-15.45	56.05	15.00
184 TRP CE3	-30.82	-14.38	55.22	15.00
184 TRP CD1	-28.66	-14.61	58.11	15.00
184 TRP NE1	-28.06	-15.46	57.20	15.00
184 TRP CZ2	-28.59	-16.14	54.84	15.00
184 TRP CZ3	-30.63	-15.04	54.04	15.00
184 TRP CH2	-29.52	-15.92	53.84	15.00
184 TRP C	-31.34	-11.59	60.02	15.00
184 TRP O	-31.41	-10.70	59.18	15.00
185 GLY N	-31.95	-11.51	61.20	15.00
185 GLY CA	-32.75	-10.34	61.52	15.00
185 GLY C	-34.24	-10.61	61.41	15.00
185 GLY O	-34.63	-11.61	60.82	15.00
186 GLU N	-35.09	-9.75	61.96	15.00

TABLE VIII

186 GLU CA	-36.52	-10.00	61.83	15.00
186 GLU CB	-37.32	-9.44	63.01	15.00
186 GLU CG	-36.65	-9.45	64.34	15.00
186 GLU CD	-37.34	-8.56	65.32	15.00
186 GLU OE1	-36.68	-8.08	66.25	15.00
186 GLU OE2	-38.55	-8.32	65.21	15.00
186 GLU C	-36.99	-9.30	60.56	15.00
186 GLU O	-38.10	-9.52	60.08	15.00
187 ASN N	-36.14	-8.44	60.02	15.00
187 ASN CA	-36.46	-7.68	58.83	15.00
187 ASN CB	-35.60	-6.42	58.79	15.00
187 ASN CG	-35.84	-5.51	59.97	15.00
187 ASN OD1	-34.92	-4.82	60.44	15.00
187 ASN ND2	-37.10	-5.46	60.45	15.00
187 ASN C	-36.21	-8.52	57.60	15.00
187 ASN O	-36.21	-8.00	56.49	15.00
188 TRP N	-35.89	-9.79	57.81	15.00
188 TRP CA	-35.66	-10.68	56.68	15.00
188 TRP CB	-34.39	-11.49	56.84	15.00
188 TRP CG	-34.20	-12.53	55.78	15.00
188 TRP CD2	-34.69	-13.89	55.77	15.00
188 TRP CE2	-34.21	-14.49	54.59	15.00
188 TRP CE3	-35.48	-14.67	56.67	15.00
188 TRP CD1	-33.48	-12.37	54.63	15.00
188 TRP NE1	-33.48	-13.54	53.91	15.00
188 TRP CZ2	-34.50	-15.83	54.26	15.00
188 TRP CZ3	-35.76	-15.96	56.35	15.00
188 TRP CH2	-35.28	-16.55	55.16	15.00
188 TRP C	-36.80	-11.63	56.71	15.00
188 TRP O	-37.29	-11.96	57.78	15.00
189 GLY N	-37.22	-12.09	55.53	15.00
189 GLY CA	-38.30	-13.05	55.42	15.00
189 GLY C	-39.53	-12.66	56.18	15.00
189 GLY O	-39.85	-11.50	56.32	15.00
190 ASN N	-40.23	-13.64	56.73	15.00
190 ASN CA	-41.43	-13.31	57.46	15.00
190 ASN CB	-42.42	-14.44	57.30	15.00
190 ASN CG	-43.81	-14.05	57.76	15.00
190 ASN OD1	-44.10	-12.89	58.14	15.00
190 ASN ND2	-44.72	-15.00	57.62	15.00
190 ASN C	-41.04	-13.20	58.90	15.00
190 ASN O	-40.92	-14.22	59.57	15.00

TABLE VIII

191 LYS N	-40.80	-11.98	59.38	15.00
191 LYS CA	-40.39	-11.79	60.76	15.00
191 LYS CB	-41.62	-11.71	61.67	15.00
191 LYS CG	-42.53	-10.45	61.51	15.00
191 LYS CD	-43.64	-10.73	60.48	15.00
191 LYS CE	-44.65	-9.57	60.22	15.00
191 LYS NZ	-44.60	-8.96	58.86	15.00
191 LYS C	-39.36	-12.83	61.26	15.00
191 LYS O	-39.58	-13.50	62.27	15.00
192 GLY N	-38.25	-12.96	60.52	15.00
192 GLY CA	-37.17	-13.89	60.87	15.00
192 GLY C	-37.47	-15.35	60.56	15.00
192 GLY O	-36.64	-16.20	60.86	15.00
193 TYR N	-38.59	-15.63	59.91	15.00
193 TYR CA	-38.89	-17.04	59.63	15.00
193 TYR CB	-40.12	-17.53	60.44	15.00
193 TYR CG	-39.91	-17.72	61.94	15.00
193 TYR CD1	-39.96	-16.63	62.83	15.00
193 TYR CE1	-39.79	-16.81	64.19	15.00
193 TYR CD2	-39.69	-18.99	62.47	15.00
193 TYR CE2	-39.52	-19.20	63.79	15.00
193 TYR CZ	-39.56	-18.12	64.67	15.00
193 TYR OH	-39.33	-18.34	66.03	15.00
193 TYR C	-39.11	-17.29	58.14	15.00
193 TYR O	-39.23	-16.35	57.35	15.00
194 ILE N	-39.08	-18.56	57.75	15.00
194 ILE CA	-39.32	-18.92	56.37	15.00
194 ILE CB	-37.98	-18.83	55.52	15.00
194 ILE CG2	-36.90	-19.78	56.01	15.00
194 ILE CG1	-38.23	-19.04	54.02	15.00
194 ILE CD1	-36.98	-19.00	53.22	15.00
194 ILE C	-39.99	-20.30	56.33	15.00
194 ILE O	-39.67	-21.15	57.18	15.00
195 LEU N	-41.01	-20.45	55.48	15.00
195 LEU CA	-41.71	-21.72	55.30	15.00
195 LEU CB	-43.20	-21.48	55.00	15.00
195 LEU CG	-43.96	-20.94	56.22	15.00
195 LEU CD1	-45.35	-20.46	55.85	15.00
195 LEU CD2	-44.03	-22.03	57.28	15.00
195 LEU C	-41.08	-22.46	54.14	15.00
195 LEU O	-41.24	-22.03	52.99	15.00
196 MET N	-40.38	-23.55	54.41	15.00

TABLE VIII

196 MET CA	-39.73	-24.28	53.34	15.00
196 MET CB	-38.30	-24.61	53.74	15.00
196 MET CG	-37.40	-23.37	53.79	15.00
196 MET SD	-35.72	-23.74	54.33	15.00
196 MET CE	-35.19	-24.86	53.02	15.00
196 MET C	-40.45	-25.54	52.91	15.00
196 MET O	-40.92	-26.29	53.76	15.00
197 ALA N	-40.52	-25.77	51.61	15.00
197 ALA CA	-41.19	-26.95	51.06	15.00
197 ALA CB	-40.98	-26.99	49.58	15.00
197 ALA C	-40.77	-28.28	51.69	15.00
197 ALA O	-39.59	-28.51	51.93	15.00
198 ARG N	-41.77	-29.13	51.96	15.00
198 ARG CA	-41.53	-30.45	52.55	15.00
198 ARG CB	-42.18	-30.53	53.94	15.00
198 ARG CG	-42.26	-31.94	54.56	15.00
198 ARG CD	-42.45	-31.86	56.05	15.00
198 ARG NE	-43.59	-31.03	56.41	15.00
198 ARG CZ	-44.85	-31.46	56.47	15.00
198 ARG NH1	-45.11	-32.72	56.19	15.00
198 ARG NH2	-45.84	-30.65	56.84	15.00
198 ARG C	-42.05	-31.55	51.67	15.00
198 ARG O	-43.07	-31.41	50.99	15.00
199 ASN N	-41.39	-32.69	51.77	15.00
199 ASN CA	-41.70	-33.89	51.02	15.00
199 ASN CB	-43.17	-34.27	51.14	15.00
199 ASN CG	-43.54	-34.74	52.54	15.00
199 ASN OD1	-42.66	-34.97	53.39	15.00
199 ASN ND2	-44.84	-34.86	52.79	15.00
199 ASN C	-41.32	-33.73	49.56	15.00
199 ASN O	-41.24	-34.72	48.84	15.00
200 LYS N	-41.04	-32.51	49.14	15.00
200 LYS CA	-40.66	-32.31	47.77	15.00
200 LYS CB	-40.98	-30.88	47.33	15.00
200 LYS CG	-42.41	-30.50	47.40	15.00
200 LYS CD	-42.69	-29.14	46.77	15.00
200 LYS CE	-42.63	-29.16	45.28	15.00
200 LYS NZ	-43.85	-29.82	44.77	15.00
200 LYS C	-39.20	-32.67	47.45	15.00
200 LYS O	-38.40	-31.81	47.09	15.00
201 ASN N	-38.85	-33.95	47.62	15.00
201 ASN CA	-37.50	-34.49	47.34	15.00

TABLE VIII

201 ASN CB	-37.30	-34.62	45.82	15.00
201 ASN CG	-38.27	-35.59	45.16	15.00
201 ASN OD1	-37.88	-36.36	44.27	15.00
201 ASN ND2	-39.56	-35.52	45.54	15.00
201 ASN C	-36.34	-33.71	47.95	15.00
201 ASN O	-35.58	-33.08	47.22	15.00
202 ASN N	-36.22	-33.75	49.28	15.00
202 ASN CA	-35.14	-33.08	50.02	15.00
202 ASN CB	-33.88	-33.93	49.92	15.00
202 ASN CG	-33.05	-33.91	51.18	15.00
202 ASN OD1	-33.57	-33.92	52.30	15.00
202 ASN ND2	-31.73	-33.90	51.01	15.00
202 ASN C	-34.85	-31.68	49.53	15.00
202 ASN O	-33.72	-31.35	49.20	15.00
203 ALA N	-35.85	-30.82	49.54	15.00
203 ALA H	-36.60	-31.08	50.11	15.00
203 ALA CA	-35.72	-29.46	49.02	15.00
203 ALA CB	-36.91	-28.60	49.43	15.00
203 ALA C	-34.46	-28.80	49.61	15.00
203 ALA O	-34.31	-28.70	50.79	15.00
204 CYS N	-33.59	-28.31	48.74	15.00
204 CYS CA	-32.40	-27.62	49.21	15.00
204 CYS C	-31.47	-28.47	50.07	15.00
204 CYS O	-30.40	-28.02	50.45	15.00
204 CYS CB	-32.76	-26.38	50.00	15.00
204 CYS SG	-33.64	-25.09	49.12	15.00
205 GLY N	-31.91	-29.64	50.49	15.00
205 GLY CA	-31.04	-30.48	51.28	15.00
205 GLY C	-31.30	-30.32	52.77	15.00
205 GLY O	-30.40	-30.54	53.58	15.00
206 ILE N	-32.52	-29.94	53.13	15.00
206 ILE CA	-32.90	-29.75	54.52	15.00
206 ILE CB	-34.33	-29.12	54.62	15.00
206 ILE CG2	-35.41	-30.09	54.17	15.00
206 ILE CG1	-34.60	-28.70	56.06	15.00
206 ILE CD1	-35.73	-27.69	56.23	15.00
206 ILE C	-32.75	-31.00	55.45	15.00
206 ILE O	-32.59	-30.85	56.66	15.00
207 ALA N	-32.81	-32.22	54.92	15.00
207 ALA CA	-32.67	-33.38	55.79	15.00
207 ALA CB	-33.80	-34.33	55.58	15.00
207 ALA C	-31.34	-34.09	55.63	15.00

TABLE VIII

207 ALA O	-31.17	-35.20	56.13	15.00
208 ASN N	-30.36	-33.45	55.00	15.00
208 ASN CA	-29.04	-34.07	54.76	15.00
208 ASN CB	-28.34	-33.45	53.52	15.00
208 ASN CG	-28.78	-34.07	52.18	15.00
208 ASN OD1	-29.25	-35.21	52.11	15.00
208 ASN ND2	-28.60	-33.31	51.12	15.00
208 ASN C	-28.08	-34.01	55.94	15.00
208 ASN O	-27.28	-34.93	56.15	15.00
209 LEU N	-28.08	-32.88	56.64	15.00
209 LEU CA	-27.19	-32.64	57.78	15.00
209 LEU CB	-26.07	-31.64	57.40	15.00
209 LEU CG	-24.73	-31.69	58.15	15.00
209 LEU CD1	-24.11	-33.07	58.09	15.00
209 LEU CD2	-23.76	-30.66	57.52	15.00
209 LEU C	-27.97	-32.12	59.02	15.00
209 LEU O	-27.72	-30.99	59.50	15.00
210 ALA N	-28.79	-32.99	59.65	15.00
210 ALA H	-29.19	-33.47	58.90	15.00
210 ALA CA	-29.59	-32.51	60.77	15.00
210 ALA CB	-31.08	-32.79	60.54	15.00
210 ALA C	-29.19	-33.24	62.06	15.00
210 ALA O	-28.91	-34.44	62.09	15.00
211 SER N	-29.24	-32.48	63.17	15.00
211 SER CA	-28.94	-33.06	64.47	15.00
211 SER CB	-27.44	-33.22	64.70	15.00
211 SER OG	-26.78	-31.96	64.75	15.00
211 SER C	-29.57	-32.31	65.62	15.00
211 SER O	-30.17	-31.24	65.41	15.00
212 PHE N	-29.43	-32.92	66.81	15.00
212 PHE CA	-29.96	-32.40	68.07	15.00
212 PHE CB	-31.46	-32.75	68.27	15.00
212 PHE CG	-31.78	-34.22	68.27	15.00
212 PHE CD1	-32.33	-34.84	67.14	15.00
212 PHE CD2	-31.61	-34.97	69.41	15.00
212 PHE CE1	-32.71	-36.19	67.17	15.00
212 PHE CE2	-31.98	-36.30	69.45	15.00
212 PHE CZ	-32.54	-36.91	68.33	15.00
212 PHE C	-29.16	-32.88	69.27	15.00
212 PHE O	-28.56	-33.95	69.23	15.00
213 PRO N	-29.11	-32.06	70.33	15.00
213 PRO CD	-29.69	-30.71	70.50	15.00

TABLE VIII

213 PRO CA	-28.36	-32.43	71.53	15.00
213 PRO CB	-28.14	-31.08	72.20	15.00
213 PRO CG	-29.45	-30.47	72.01	15.00
213 PRO C	-29.19	-33.38	72.46	15.00
213 PRO O	-30.42	-33.47	72.36	15.00
214 LYS N	-28.53	-34.16	73.30	15.00
214 LYS CA	-29.24	-35.05	74.22	15.00
214 LYS CB	-28.57	-36.43	74.20	15.00
214 LYS CG	-28.79	-37.24	72.91	15.00
214 LYS CD	-28.01	-38.56	72.92	15.00
214 LYS CE	-28.46	-39.53	71.81	15.00
214 LYS NZ	-27.39	-40.57	71.71	15.00
214 LYS C	-29.05	-34.34	75.56	15.00
214 LYS O	-27.98	-33.76	75.79	15.00
215 MET N	-30.08	-34.35	76.41	15.00
215 MET CA	-29.99	-33.65	77.70	15.00
215 MET CB	-31.12	-32.61	77.90	15.00
215 MET CG	-30.96	-31.28	77.20	15.00
215 MET SD	-29.93	-30.01	77.96	15.00
215 MET CE	-31.16	-28.81	78.53	15.00
215 MET C	-29.93	-34.56	78.90	15.00
215 MET OT1	-28.98	-34.44	79.69	15.00
215 MET OT2	-30.83	-35.40	79.08	15.00
216 HOH OH2	-32.26	-16.46	65.37	15.00
217 HOH OH2	-29.10	-19.91	62.23	15.00
218 HOH OH2	-10.46	-12.34	64.01	15.00
219 HOH OH2	-16.64	-12.04	73.86	15.00
220 HOH OH2	-35.65	-23.61	70.00	15.00
221 HOH OH2	-30.42	-35.41	58.75	15.00
222 HOH OH2	-31.55	-20.39	66.10	15.00
223 HOH OH2	-25.68	-31.53	62.01	15.00
224 HOH OH2	-12.63	-8.84	62.20	15.00
225 HOH OH2	-14.75	-22.14	66.35	15.00
226 HOH OH2	-44.50	-27.54	49.50	15.00
227 HOH OH2	-46.66	-35.25	56.37	15.00
228 HOH OH2	-41.69	-17.81	69.13	15.00
229 HOH OH2	-31.65	-20.57	63.48	15.00
230 HOH OH2	-19.45	-17.08	56.43	15.00
231 HOH OH2	-14.47	-31.20	62.15	15.00
232 HOH OH2	-44.49	-25.37	44.32	15.00
233 HOH OH2	-23.11	-31.07	62.02	15.00
234 HOH OH2	-24.80	-4.69	68.36	15.00

TABLE VIII

235	HOH	OH2	-31.22	-18.66	68.39	15.00
236	HOH	OH2	-37.21	-27.28	51.82	15.00
237	HOH	OH2	-37.54	-25.42	49.65	15.00
238	HOH	OH2	-48.22	-33.37	57.46	15.00
239	HOH	OH2	-29.06	-10.11	76.59	15.00
240	HOH	OH2	-35.53	-14.09	77.20	15.00
241	HOH	OH2	-16.66	-4.74	70.29	15.00
242	HOH	OH2	-17.42	-8.40	75.32	15.00
243	HOH	OH2	-10.92	-18.14	70.16	15.00
244	HOH	OH2	-9.58	-20.04	78.06	15.00
245	HOH	OH2	-46.35	-17.06	54.42	15.00
246	HOH	OH2	-34.19	-29.40	45.76	15.00
247	HOH	OH2	-36.78	-37.90	52.62	15.00
248	HOH	OH2	-42.43	-35.18	56.19	15.00
249	HOH	OH2	-41.62	-19.52	71.38	15.00
250	HOH	OH2	-48.81	-19.01	73.95	15.00
251	HOH	OH2	-41.55	-15.71	71.06	15.00
252	HOH	OH2	-26.21	-9.24	68.97	15.00
253	HOH	OH2	-33.78	-8.96	64.11	15.00
254	HOH	OH2	-20.04	-8.25	62.53	15.00
255	HOH	OH2	-17.20	-6.33	64.20	15.00
256	HOH	OH2	-35.58	-40.12	65.37	15.00
257	HOH	OH2	-13.46	-24.38	76.78	15.00
258	HOH	OH2	-8.00	-25.77	61.24	15.00
259	HOH	OH2	-21.06	-27.44	51.53	15.00
260	HOH	OH2	-25.94	-34.05	61.10	15.00
261	HOH	OH2	-12.35	-29.04	72.99	15.00
262	HOH	OH2	-33.29	-40.38	63.87	15.00
263	HOH	OH2	-20.24	-23.70	87.14	15.00
264	HOH	OH2	-13.21	-12.02	62.79	15.00
265	HOH	OH2	-21.34	-33.08	61.27	15.00
266	HOH	OH2	-29.60	-16.68	41.72	15.00
267	HOH	OH2	-25.80	-19.25	42.13	15.00
268	HOH	OH2	-32.98	-34.45	47.05	15.00
269	HOH	OH2	-23.16	-31.07	42.89	15.00
270	HOH	OH2	-34.03	-29.11	42.28	15.00
271	HOH	OH2	-36.71	-26.01	46.91	15.00

TABLE IX

Table of the orthogonal three dimensional coordinates in Ångstroms and B factors ($Å^2$) for the cathepsin K complex with inhibitor 4-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-1-N[N-(methyl)-L-leucyl)]-3-pyrrolidinone.

Residue	Atom	X	Y	Z	B
1	ALA CB	-54.23	-33.20	65.64	15.00
1	ALA C	-53.54	-33.00	63.24	15.00
1	ALA O	-52.73	-33.83	62.79	15.00
1	ALA N	-54.89	-34.90	63.97	15.00
1	ALA CA	-54.65	-33.45	64.19	15.00
2	PRO N	-53.49	-31.70	62.91	15.00
2	PRO CD	-54.26	-30.56	63.46	15.00
2	PRO CA	-52.44	-31.22	62.00	15.00
2	PRO CB	-52.58	-29.69	62.07	15.00
2	PRO CG	-53.25	-29.45	63.41	15.00
2	PRO C	-51.07	-31.68	62.50	15.00
2	PRO O	-50.74	-31.50	63.67	15.00
3	ASP N	-50.31	-32.35	61.64	15.00
3	ASP CA	-48.98	-32.84	62.01	15.00
3	ASP CB	-48.55	-33.98	61.08	15.00
3	ASP CG	-47.66	-35.01	61.77	15.00
3	ASP OD1	-46.52	-34.66	62.18	15.00
3	ASP OD2	-48.10	-36.17	61.89	15.00
3	ASP C	-48.00	-31.68	61.94	15.00
3	ASP O	-47.13	-31.65	61.06	15.00
4	SER N	-48.12	-30.72	62.85	15.00
4	SER CA	-47.23	-29.56	62.86	15.00
4	SER CB	-47.87	-28.37	62.15	15.00
4	SER OG	-49.05	-27.95	62.82	15.00
4	SER C	-46.76	-29.14	64.25	15.00
4	SER O	-47.54	-29.19	65.22	15.00
5	VAL N	-45.50	-28.70	64.35	15.00
5	VAL CA	-44.91	-28.26	65.61	15.00
5	VAL CB	-43.77	-29.21	66.10	15.00
5	VAL CG1	-43.35	-28.82	67.51	15.00
5	VAL CG2	-44.19	-30.65	66.04	15.00
5	VAL C	-44.29	-26.87	65.45	15.00
5	VAL O	-43.47	-26.65	64.55	15.00

TABLE IX

6	ASP	N	-44.64	-25.95	66.33	15.00
6	ASP	CA	-44.10	-24.60	66.28	15.00
6	ASP	CB	-45.17	-23.57	65.90	15.00
6	ASP	CG	-44.59	-22.26	65.40	15.00
6	ASP	OD1	-43.41	-21.95	65.68	15.00
6	ASP	OD2	-45.34	-21.52	64.73	15.00
6	ASP	C	-43.52	-24.32	67.66	15.00
6	ASP	O	-44.20	-23.78	68.53	15.00
7	TYR	N	-42.27	-24.69	67.85	15.00
7	TYR	CA	-41.62	-24.50	69.13	15.00
7	TYR	CB	-40.20	-25.08	69.12	15.00
7	TYR	CG	-40.20	-26.58	69.20	15.00
7	TYR	CD1	-40.68	-27.24	70.33	15.00
7	TYR	CE1	-40.76	-28.62	70.38	15.00
7	TYR	CD2	-39.81	-27.36	68.11	15.00
7	TYR	CE2	-39.89	-28.74	68.15	15.00
7	TYR	CZ	-40.37	-29.36	69.29	15.00
7	TYR	OH	-40.51	-30.72	69.31	15.00
7	TYR	C	-41.63	-23.07	69.62	15.00
7	TYR	O	-41.57	-22.84	70.83	15.00
8	ARG	N	-41.74	-22.11	68.70	15.00
8	ARG	CA	-41.77	-20.68	69.08	15.00
8	ARG	CB	-41.86	-19.77	67.84	15.00
8	ARG	CG	-40.77	-19.98	66.80	15.00
8	ARG	CD	-41.01	-19.12	65.58	15.00
8	ARG	NE	-42.34	-19.33	65.02	15.00
8	ARG	CZ	-42.70	-18.96	63.80	15.00
8	ARG	NH1	-41.83	-18.36	63.00	15.00
8	ARG	NH2	-43.94	-19.18	63.38	15.00
8	ARG	C	-42.94	-20.39	70.02	15.00
8	ARG	O	-42.79	-19.67	71.02	15.00
9	LYS	N	-44.10	-20.98	69.72	15.00
9	LYS	CA	-45.29	-20.80	70.53	15.00
9	LYS	CB	-46.53	-21.26	69.78	15.00
9	LYS	CG	-46.84	-20.43	68.56	15.00
9	LYS	CD	-48.15	-20.86	67.92	15.00
9	LYS	CE	-48.39	-20.11	66.62	15.00
9	LYS	NZ	-49.58	-20.62	65.88	15.00
9	LYS	C	-45.18	-21.53	71.85	15.00
9	LYS	O	-45.95	-21.29	72.77	15.00
10	LYS	N	-44.18	-22.40	71.95	15.00
10	LYS	CA	-43.99	-23.17	73.16	15.00

TABLE IX

10 LYS CB	-43.71	-24.63	72.80	15.00
10 LYS CG	-44.67	-25.19	71.78	15.00
10 LYS CD	-44.34	-26.64	71.49	15.00
10 LYS CE	-44.42	-27.48	72.76	15.00
10 LYS NZ	-45.74	-27.26	73.43	15.00
10 LYS C	-42.92	-22.65	74.11	15.00
10 LYS O	-42.70	-23.25	75.15	15.00
11 GLY N	-42.24	-21.57	73.73	15.00
11 GLY CA	-41.21	-21.00	74.58	15.00
11 GLY C	-39.83	-21.65	74.47	15.00
11 GLY O	-38.92	-21.31	75.21	15.00
12 TYR N	-39.68	-22.56	73.52	15.00
12 TYR CA	-38.41	-23.26	73.31	15.00
12 TYR CB	-38.63	-24.56	72.54	15.00
12 TYR CG	-39.27	-25.70	73.30	15.00
12 TYR CD1	-40.37	-25.50	74.13	15.00
12 TYR CE1	-40.97	-26.57	74.82	15.00
12 TYR CD2	-38.78	-27.00	73.17	15.00
12 TYR CE2	-39.37	-28.07	73.84	15.00
12 TYR CZ	-40.45	-27.85	74.66	15.00
12 TYR OH	-41.02	-28.91	75.33	15.00
12 TYR C	-37.36	-22.43	72.56	15.00
12 TYR O	-36.22	-22.86	72.46	15.00
13 VAL N	-37.76	-21.27	72.03	15.00
13 VAL CA	-36.86	-20.43	71.23	15.00
13 VAL CB	-37.38	-20.33	69.78	15.00
13 VAL CG1	-36.34	-19.72	68.89	15.00
13 VAL CG2	-37.75	-21.69	69.26	15.00
13 VAL C	-36.62	-19.00	71.75	15.00
13 VAL O	-37.55	-18.32	72.18	15.00
14 THR N	-35.38	-18.53	71.67	15.00
14 THR CA	-35.04	-17.18	72.11	15.00
14 THR CB	-33.58	-17.11	72.54	15.00
14 THR OG1	-32.76	-17.76	71.55	15.00
14 THR CG2	-33.39	-17.76	73.88	15.00
14 THR C	-35.25	-16.15	70.99	15.00
14 THR O	-35.59	-16.51	69.86	15.00
15 PRO N	-35.10	-14.85	71.31	15.00
15 PRO CD	-35.02	-14.21	72.63	15.00
15 PRO CA	-35.29	-13.83	70.27	15.00
15 PRO CB	-35.03	-12.54	71.03	15.00
15 PRO CG	-35.58	-12.84	72.37	15.00

TABLE IX

15 PRO C	-34.27	-14.02	69.14	15.00
15 PRO O	-33.20	-14.57	69.36	15.00
16 VAL N	-34.63	-13.62	67.92	15.00
16 VAL CA	-33.72	-13.74	66.79	15.00
16 VAL CB	-34.41	-13.41	65.45	15.00
16 VAL CG1	-33.40	-13.43	64.31	15.00
16 VAL CG2	-35.52	-14.40	65.18	15.00
16 VAL C	-32.53	-12.82	67.01	15.00
16 VAL O	-32.69	-11.69	67.46	15.00
17 LYS N	-31.34	-13.30	66.69	15.00
17 LYS CA	-30.16	-12.50	66.88	15.00
17 LYS CB	-29.27	-13.11	67.95	15.00
17 LYS CG	-29.97	-13.18	69.30	15.00
17 LYS CD	-29.17	-13.95	70.33	15.00
17 LYS CE	-29.96	-14.12	71.61	15.00
17 LYS NZ	-31.23	-14.87	71.36	15.00
17 LYS C	-29.41	-12.30	65.58	15.00
17 LYS O	-29.51	-13.11	64.66	15.00
18 ASN N	-28.68	-11.18	65.51	15.00
18 ASN CA	-27.89	-10.84	64.33	15.00
18 ASN CB	-28.01	-9.37	63.99	15.00
18 ASN CG	-27.30	-9.03	62.72	15.00
18 ASN OD1	-27.10	-9.90	61.88	15.00
18 ASN ND2	-26.89	-7.78	62.57	15.00
18 ASN C	-26.42	-11.21	64.52	15.00
18 ASN O	-25.77	-10.70	65.43	15.00
19 GLN N	-25.89	-12.04	63.63	15.00
19 GLN CA	-24.50	-12.46	63.73	15.00
19 GLN CB	-24.24	-13.75	62.96	15.00
19 GLN CG	-24.32	-13.63	61.47	15.00
19 GLN CD	-24.07	-14.96	60.80	15.00
19 GLN OE1	-25.01	-15.66	60.43	15.00
19 GLN NE2	-22.81	-15.32	60.65	15.00
19 GLN C	-23.48	-11.40	63.36	15.00
19 GLN O	-22.32	-11.48	63.76	15.00
20 GLY N	-23.90	-10.40	62.59	15.00
20 GLY CA	-22.99	-9.33	62.22	15.00
20 GLY C	-21.93	-9.72	61.22	15.00
20 GLY O	-22.06	-10.71	60.52	15.00
21 GLN N	-20.86	-8.94	61.15	15.00
21 GLN CA	-19.79	-9.22	60.22	15.00
21 GLN CB	-19.10	-7.92	59.77	15.00

TABLE IX

21	GLN	CG	-20.08	-6.82	59.31	15.00
21	GLN	CD	-21.21	-7.35	58.42	15.00
21	GLN	OE1	-20.98	-7.83	57.31	15.00
21	GLN	NE2	-22.44	-7.28	58.92	15.00
21	GLN	C	-18.81	-10.21	60.83	15.00
21	GLN	O	-17.67	-9.87	61.14	15.00
22	CYS	N	-19.29	-11.45	61.00	15.00
22	CYS	CA	-18.53	-12.54	61.60	15.00
22	CYS	C	-19.20	-13.84	61.19	15.00
22	CYS	O	-20.43	-13.93	61.23	15.00
22	CYS	CB	-18.48	-12.40	63.13	15.00
22	CYS	SG	-18.13	-13.92	64.07	15.00
23	GLY	N	-18.42	-14.83	60.76	15.00
23	GLY	CA	-19.01	-16.09	60.33	15.00
23	GLY	C	-19.33	-17.04	61.47	15.00
23	GLY	O	-18.80	-18.16	61.54	15.00
24	SER	N	-20.21	-16.60	62.36	15.00
24	SER	CA	-20.58	-17.40	63.52	15.00
24	SER	CB	-20.34	-16.63	64.80	15.00
24	SER	OG	-21.04	-15.40	64.76	15.00
24	SER	C	-22.00	-17.93	63.45	15.00
24	SER	O	-22.68	-18.02	64.46	15.00
25	CYS	N	-22.46	-18.32	62.28	15.00
25	CYS	CA	-23.80	-18.84	62.17	15.00
25	CYS	CB	-24.25	-18.85	60.71	15.00
25	CYS	SG	-23.19	-19.72	59.59	15.00
25	CYS	C	-23.89	-20.22	62.84	15.00
25	CYS	O	-24.95	-20.62	63.34	15.00
25	INH	C1	-26.58	-9.77	58.47	15.00
25	INH	C2	-26.25	-10.40	57.28	15.00
25	INH	C3	-25.06	-11.13	57.18	15.00
25	INH	C4	-24.20	-11.22	58.27	15.00
25	INH	C5	-24.54	-10.58	59.46	15.00
25	INH	C6	-25.72	-9.86	59.56	15.00
25	INH	C7	-22.95	-12.04	58.18	15.00
25	INH	O8	-22.93	-12.74	56.96	15.00
25	INH	C9	-23.31	-14.09	56.78	15.00
25	INH	O10	-24.36	-14.56	57.24	15.00
25	INH	C11	-22.67	-16.23	55.81	15.00
25	INH	C12	-22.36	-16.56	54.34	15.00
25	INH	C13	-23.44	-17.20	53.45	15.00
25	INH	C14	-24.11	-18.35	54.17	15.00

TABLE IX

25	INH	C15	-24.46	-16.19	52.94	15.00
25	INH	C16	-21.76	-17.01	56.78	15.00
25	INH	O17	-20.87	-16.42	57.43	15.00
25	INH	N18	-21.99	-18.32	56.91	15.00
25	INH	C19	-21.15	-18.98	57.84	15.00
25	INH	N20	-22.45	-14.81	56.08	15.00
25	INH	C21	-20.81	-20.41	57.54	15.00
25	INH	C22	-21.63	-18.99	59.30	15.00
25	INH	O23	-21.62	-17.88	59.81	15.00
25	INH	C24	-17.90	-23.12	57.09	15.00
25	INH	C25	-20.20	-23.31	57.89	15.00
25	INH	C26	-21.15	-24.49	58.06	15.00
25	INH	C27	-21.28	-25.45	56.87	15.00
25	INH	C28	-19.93	-25.80	56.26	15.00
25	INH	C29	-22.00	-26.71	57.30	15.00
25	INH	C30	-20.37	-22.34	59.06	15.00
25	INH	O31	-20.24	-22.76	60.20	15.00
25	INH	N32	-20.66	-21.04	58.80	15.00
25	INH	C33	-20.82	-20.11	59.89	15.00
25	INH	N34	-18.81	-23.74	57.85	15.00
26	TRP	N	-22.76	-20.93	62.89	15.00
26	TRP	CA	-22.67	-22.24	63.53	15.00
26	TRP	CB	-21.35	-22.95	63.19	15.00
26	TRP	CG	-20.14	-22.22	63.67	15.00
26	TRP	CD2	-19.45	-22.41	64.92	15.00
26	TRP	CE2	-18.44	-21.43	65.00	15.00
26	TRP	CE3	-19.61	-23.30	65.99	15.00
26	TRP	CD1	-19.51	-21.18	63.05	15.00
26	TRP	NE1	-18.50	-20.70	63.84	15.00
26	TRP	CZ2	-17.59	-21.32	66.10	15.00
26	TRP	CZ3	-18.76	-23.19	67.08	15.00
26	TRP	CH2	-17.76	-22.21	67.13	15.00
26	TRP	C	-22.83	-22.09	65.05	15.00
26	TRP	O	-23.50	-22.90	65.69	15.00
27	ALA	N	-22.22	-21.05	65.60	15.00
27	ALA	CA	-22.28	-20.76	67.03	15.00
27	ALA	CB	-21.34	-19.64	67.37	15.00
27	ALA	C	-23.71	-20.40	67.41	15.00
27	ALA	O	-24.15	-20.67	68.53	15.00
28	PHE	N	-24.44	-19.79	66.48	15.00
28	PHE	CA	-25.83	-19.42	66.72	15.00
28	PHE	CB	-26.28	-18.29	65.81	15.00

TABLE IX

28	PHE	CG	-25.77	-16.95	66.24	15.00
28	PHE	CD1	-24.53	-16.50	65.83	15.00
28	PHE	CD2	-26.52	-16.16	67.11	15.00
28	PHE	CE1	-24.03	-15.31	66.28	15.00
28	PHE	CE2	-26.02	-14.96	67.56	15.00
28	PHE	CZ	-24.78	-14.53	67.15	15.00
28	PHE	C	-26.76	-20.62	66.63	15.00
28	PHE	O	-27.71	-20.74	67.40	15.00
29	SER	N	-26.51	-21.50	65.67	15.00
29	SER	CA	-27.33	-22.69	65.53	15.00
29	SER	CB	-26.88	-23.54	64.35	15.00
29	SER	OG	-27.59	-24.76	64.31	15.00
29	SER	C	-27.22	-23.49	66.82	15.00
29	SER	O	-28.20	-23.61	67.54	15.00
30	SER	N	-26.01	-23.95	67.12	15.00
30	SER	CA	-25.70	-24.75	68.32	15.00
30	SER	CB	-24.19	-24.86	68.50	15.00
30	SER	OG	-23.53	-25.04	67.27	15.00
30	SER	C	-26.34	-24.24	69.61	15.00
30	SER	O	-26.97	-25.00	70.37	15.00
31	VAL	N	-26.15	-22.96	69.88	15.00
31	VAL	CA	-26.71	-22.32	71.06	15.00
31	VAL	CB	-26.23	-20.85	71.13	15.00
31	VAL	CG1	-27.15	-20.01	71.98	15.00
31	VAL	CG2	-24.83	-20.81	71.69	15.00
31	VAL	C	-28.23	-22.44	71.03	15.00
31	VAL	O	-28.86	-22.74	72.04	15.00
32	GLY	N	-28.82	-22.26	69.85	15.00
32	GLY	CA	-30.26	-22.36	69.72	15.00
32	GLY	C	-30.78	-23.75	70.03	15.00
32	GLY	O	-31.86	-23.89	70.62	15.00
33	ALA	N	-30.07	-24.78	69.61	15.00
33	ALA	CA	-30.50	-26.14	69.90	15.00
33	ALA	CB	-29.65	-27.14	69.16	15.00
33	ALA	C	-30.37	-26.36	71.40	15.00
33	ALA	O	-31.29	-26.85	72.05	15.00
34	LEU	N	-29.24	-25.92	71.96	15.00
34	LEU	CA	-28.96	-26.04	73.40	15.00
34	LEU	CB	-27.57	-25.50	73.75	15.00
34	LEU	CG	-26.28	-26.23	73.40	15.00
34	LEU	CD1	-25.11	-25.32	73.73	15.00
34	LEU	CD2	-26.17	-27.53	74.19	15.00

TABLE IX

34 LEU C	-30.00	-25.35	74.28	15.00
34 LEU O	-30.28	-25.81	75.38	15.00
35 GLU N	-30.49	-24.21	73.82	15.00
35 GLU CA	-31.50	-23.44	74.55	15.00
35 GLU CB	-31.65	-22.02	74.01	15.00
35 GLU CG	-30.41	-21.16	74.08	15.00
35 GLU CD	-30.48	-19.98	73.14	15.00
35 GLU OE1	-31.23	-20.04	72.14	15.00
35 GLU OE2	-29.79	-18.98	73.39	15.00
35 GLU C	-32.84	-24.14	74.47	15.00
35 GLU O	-33.60	-24.12	75.44	15.00
36 GLY N	-33.13	-24.71	73.31	15.00
36 GLY CA	-34.38	-25.43	73.12	15.00
36 GLY C	-34.45	-26.58	74.11	15.00
36 GLY O	-35.47	-26.75	74.79	15.00
37 GLN N	-33.35	-27.32	74.22	15.00
37 GLN CA	-33.25	-28.43	75.15	15.00
37 GLN CB	-32.05	-29.31	74.83	15.00
37 GLN CG	-32.27	-30.21	73.64	15.00
37 GLN CD	-33.50	-31.08	73.81	15.00
37 GLN OE1	-33.74	-31.63	74.88	15.00
37 GLN NE2	-34.28	-31.20	72.75	15.00
37 GLN C	-33.22	-27.96	76.60	15.00
37 GLN O	-33.78	-28.61	77.48	15.00
38 LEU N	-32.60	-26.81	76.84	15.00
38 LEU CA	-32.52	-26.23	78.19	15.00
38 LEU CB	-31.72	-24.94	78.20	15.00
38 LEU CG	-31.57	-24.25	79.55	15.00
38 LEU CD1	-30.61	-25.04	80.42	15.00
38 LEU CD2	-31.08	-22.82	79.38	15.00
38 LEU C	-33.94	-26.00	78.70	15.00
38 LEU O	-34.27	-26.33	79.83	15.00
39 LYS N	-34.78	-25.42	77.86	15.00
39 LYS CA	-36.17	-25.16	78.19	15.00
39 LYS CB	-36.85	-24.36	77.08	15.00
39 LYS CG	-38.38	-24.43	77.06	15.00
39 LYS CD	-39.03	-23.68	78.21	15.00
39 LYS CE	-40.52	-23.93	78.24	15.00
39 LYS NZ	-41.17	-23.27	79.40	15.00
39 LYS C	-36.89	-26.48	78.42	15.00
39 LYS O	-37.73	-26.59	79.30	15.00
40 LYS N	-36.56	-27.49	77.63	15.00

TABLE IX

40	LYS	CA	-37.20	-28.78	77.78	15.00
40	LYS	CB	-36.83	-29.73	76.64	15.00
40	LYS	CG	-37.74	-30.93	76.59	15.00
40	LYS	CD	-37.39	-31.91	75.51	15.00
40	LYS	CE	-38.47	-32.98	75.42	15.00
40	LYS	NZ	-38.17	-34.02	74.40	15.00
40	LYS	C	-36.89	-29.42	79.13	15.00
40	LYS	O	-37.79	-29.93	79.80	15.00
41	LYS	N	-35.62	-29.36	79.53	15.00
41	LYS	CA	-35.17	-29.95	80.79	15.00
41	LYS	CB	-33.65	-30.16	80.81	15.00
41	LYS	CG	-33.08	-30.87	79.59	15.00
41	LYS	CD	-33.91	-32.09	79.21	15.00
41	LYS	CE	-33.34	-32.77	77.99	15.00
41	LYS	NZ	-34.29	-33.81	77.44	15.00
41	LYS	C	-35.59	-29.16	82.02	15.00
41	LYS	O	-36.42	-29.61	82.81	15.00
42	THR	N	-35.01	-27.98	82.17	15.00
42	THR	CA	-35.26	-27.11	83.32	15.00
42	THR	CB	-34.10	-26.13	83.49	15.00
42	THR	OG1	-34.11	-25.20	82.40	15.00
42	THR	CG2	-32.77	-26.87	83.51	15.00
42	THR	C	-36.58	-26.34	83.35	15.00
42	THR	O	-36.92	-25.75	84.37	15.00
43	GLY	N	-37.30	-26.30	82.24	15.00
43	GLY	CA	-38.56	-25.58	82.19	15.00
43	GLY	C	-38.44	-24.08	82.03	15.00
43	GLY	O	-39.45	-23.39	81.86	15.00
44	LYS	N	-37.22	-23.56	82.10	15.00
44	LYS	CA	-36.96	-22.13	81.97	15.00
44	LYS	CB	-36.42	-21.56	83.28	15.00
44	LYS	CG	-37.47	-21.47	84.38	15.00
44	LYS	CD	-36.85	-21.18	85.72	15.00
44	LYS	CE	-36.08	-22.36	86.23	15.00
44	LYS	NZ	-37.00	-23.52	86.37	15.00
44	LYS	C	-35.99	-21.90	80.82	15.00
44	LYS	O	-35.12	-22.73	80.57	15.00
45	LEU	N	-36.16	-20.79	80.10	15.00
45	LEU	CA	-35.31	-20.46	78.95	15.00
45	LEU	CB	-36.19	-20.14	77.73	15.00
45	LEU	CG	-35.60	-19.92	76.34	15.00
45	LEU	CD1	-35.30	-21.23	75.64	15.00

TABLE IX

45	LEU	CD2	-36.62	-19.13	75.55	15.00
45	LEU	C	-34.32	-19.32	79.23	15.00
45	LEU	O	-34.65	-18.34	79.89	15.00
46	LEU	N	-33.11	-19.46	78.68	15.00
46	LEU	CA	-32.02	-18.47	78.83	15.00
46	LEU	CB	-30.97	-18.94	79.82	15.00
46	LEU	CG	-30.95	-18.53	81.29	15.00
46	LEU	CD1	-29.80	-19.23	81.98	15.00
46	LEU	CD2	-30.80	-17.02	81.38	15.00
46	LEU	C	-31.33	-18.24	77.48	15.00
46	LEU	O	-31.36	-19.10	76.62	15.00
47	ASN	N	-30.68	-17.09	77.32	15.00
47	ASN	CA	-29.95	-16.81	76.10	15.00
47	ASN	CB	-29.88	-15.32	75.78	15.00
47	ASN	CG	-31.23	-14.72	75.46	15.00
47	ASN	OD1	-31.79	-13.96	76.25	15.00
47	ASN	ND2	-31.74	-15.03	74.28	15.00
47	ASN	C	-28.56	-17.33	76.35	15.00
47	ASN	O	-27.87	-16.81	77.23	15.00
48	LEU	N	-28.16	-18.41	75.67	15.00
48	LEU	CA	-26.81	-18.95	75.85	15.00
48	LEU	CB	-26.75	-20.44	75.51	15.00
48	LEU	CG	-27.61	-21.41	76.33	15.00
48	LEU	CD1	-27.10	-22.82	76.11	15.00
48	LEU	CD2	-27.55	-21.06	77.80	15.00
48	LEU	C	-25.82	-18.14	75.02	15.00
48	LEU	O	-26.22	-17.32	74.19	15.00
49	SER	N	-24.53	-18.38	75.23	15.00
49	SER	CA	-23.48	-17.62	74.55	15.00
49	SER	CB	-22.43	-17.16	75.56	15.00
49	SER	OG	-21.36	-16.51	74.91	15.00
49	SER	C	-22.77	-18.19	73.33	15.00
49	SER	O	-21.87	-19.03	73.46	15.00
50	PRO	N	-23.11	-17.69	72.12	15.00
50	PRO	CD	-24.26	-16.83	71.79	15.00
50	PRO	CA	-22.46	-18.17	70.90	15.00
50	PRO	CB	-23.32	-17.56	69.80	15.00
50	PRO	CG	-23.89	-16.34	70.43	15.00
50	PRO	C	-21.01	-17.66	70.85	15.00
50	PRO	O	-20.16	-18.22	70.16	15.00
51	GLN	N	-20.74	-16.59	71.61	15.00
51	GLN	CA	-19.41	-15.98	71.71	15.00

TABLE IX

51 GLN CB	-19.50	-14.57	72.29	15.00
51 GLN CG	-18.18	-13.80	72.34	15.00
51 GLN CD	-17.66	-13.43	70.96	15.00
51 GLN OE1	-18.33	-12.73	70.19	15.00
51 GLN NE2	-16.45	-13.88	70.65	15.00
51 GLN C	-18.50	-16.86	72.56	15.00
51 GLN O	-17.27	-16.82	72.42	15.00
52 ASN N	-19.11	-17.64	73.44	15.00
52 ASN CA	-18.38	-18.58	74.30	15.00
52 ASN CB	-19.35	-19.26	75.26	15.00
52 ASN CG	-18.67	-20.14	76.30	15.00
52 ASN OD1	-18.91	-19.99	77.51	15.00
52 ASN ND2	-17.88	-21.11	75.85	15.00
52 ASN C	-17.74	-19.57	73.32	15.00
52 ASN O	-16.55	-19.90	73.41	15.00
53 LEU N	-18.55	-20.00	72.36	15.00
53 LEU CA	-18.11	-20.96	71.35	15.00
53 LEU CB	-19.32	-21.52	70.61	15.00
53 LEU CG	-20.38	-22.09	71.55	15.00
53 LEU CD1	-21.65	-22.44	70.79	15.00
53 LEU CD2	-19.83	-23.30	72.25	15.00
53 LEU C	-17.06	-20.37	70.39	15.00
53 LEU O	-15.94	-20.89	70.28	15.00
54 VAL N	-17.43	-19.27	69.73	15.00
54 VAL CA	-16.55	-18.58	68.78	15.00
54 VAL CB	-17.06	-17.14	68.52	15.00
54 VAL CG1	-16.12	-16.40	67.60	15.00
54 VAL CG2	-18.46	-17.18	67.91	15.00
54 VAL C	-15.12	-18.49	69.29	15.00
54 VAL O	-14.16	-18.68	68.55	15.00
55 ASP N	-15.00	-18.21	70.58	15.00
55 ASP CA	-13.71	-18.08	71.23	15.00
55 ASP CB	-13.82	-17.19	72.49	15.00
55 ASP CG	-14.16	-15.76	72.16	15.00
55 ASP OD1	-13.98	-15.35	71.00	15.00
55 ASP OD2	-14.62	-15.03	73.06	15.00
55 ASP C	-13.05	-19.41	71.60	15.00
55 ASP O	-11.98	-19.76	71.08	15.00
56 CYS N	-13.74	-20.18	72.43	15.00
56 CYS CA	-13.21	-21.42	72.96	15.00
56 CYS C	-13.19	-22.70	72.14	15.00
56 CYS O	-12.40	-23.59	72.45	15.00

TABLE IX

56 CYS CB	-13.84	-21.68	74.32	15.00
56 CYS SG	-14.09	-20.14	75.26	15.00
57 VAL N	-14.06	-22.83	71.15	15.00
57 VAL CA	-14.11	-24.04	70.33	15.00
57 VAL CB	-15.47	-24.21	69.61	15.00
57 VAL CG1	-15.58	-25.61	69.01	15.00
57 VAL CG2	-16.61	-23.97	70.58	15.00
57 VAL C	-12.98	-24.06	69.30	15.00
57 VAL O	-13.18	-23.78	68.12	15.00
58 SER N	-11.80	-24.45	69.76	15.00
58 SER CA	-10.60	-24.55	68.94	15.00
58 SER CB	-9.45	-25.07	69.79	15.00
58 SER OG	-9.53	-24.53	71.10	15.00
58 SER C	-10.73	-25.37	67.67	15.00
58 SER O	-9.99	-25.17	66.72	15.00
59 GLU N	-11.61	-26.36	67.70	15.00
59 GLU CA	-11.83	-27.23	66.55	15.00
59 GLU CB	-12.73	-28.41	66.92	15.00
59 GLU CG	-12.20	-29.30	68.03	15.00
59 GLU CD	-12.38	-28.71	69.41	15.00
59 GLU OE1	-13.54	-28.51	69.82	15.00
59 GLU OE2	-11.37	-28.43	70.06	15.00
59 GLU C	-12.41	-26.48	65.37	15.00
59 GLU O	-12.37	-26.95	64.23	15.00
60 ASN N	-13.03	-25.34	65.65	15.00
60 ASN CA	-13.65	-24.52	64.62	15.00
60 ASN CB	-15.10	-24.18	64.99	15.00
60 ASN CG	-16.04	-25.37	64.87	15.00
60 ASN OD1	-17.24	-25.24	65.03	15.00
60 ASN ND2	-15.49	-26.53	64.55	15.00
60 ASN C	-12.83	-23.26	64.38	15.00
60 ASN O	-11.82	-23.03	65.05	15.00
61 ASP N	-13.28	-22.43	63.44	15.00
61 ASP CA	-12.56	-21.22	63.09	15.00
61 ASP CB	-12.53	-21.05	61.57	15.00
61 ASP CG	-11.12	-20.82	61.03	15.00
61 ASP OD1	-10.18	-20.65	61.83	15.00
61 ASP OD2	-10.96	-20.82	59.79	15.00
61 ASP C	-13.09	-19.95	63.76	15.00
61 ASP O	-12.67	-18.85	63.43	15.00
62 GLY N	-14.00	-20.09	64.72	15.00
62 GLY CA	-14.55	-18.91	65.36	15.00

TABLE IX

62	GLY	C	-15.40	-18.19	64.33	15.00
62	GLY	O	-16.39	-18.75	63.85	15.00
63	CYS	N	-14.98	-16.99	63.94	15.00
63	CYS	CA	-15.70	-16.19	62.94	15.00
63	CYS	C	-15.40	-16.66	61.53	15.00
63	CYS	O	-15.88	-16.07	60.57	15.00
63	CYS	CB	-15.39	-14.70	63.02	15.00
63	CYS	SG	-16.14	-13.86	64.44	15.00
64	GLY	N	-14.57	-17.68	61.40	15.00
64	GLY	CA	-14.26	-18.20	60.08	15.00
64	GLY	C	-15.21	-19.31	59.69	15.00
64	GLY	O	-15.23	-19.74	58.53	15.00
65	GLY	N	-15.99	-19.80	60.65	15.00
65	GLY	CA	-16.93	-20.87	60.37	15.00
65	GLY	C	-16.62	-22.14	61.14	15.00
65	GLY	O	-15.48	-22.38	61.54	15.00
66	GLY	N	-17.64	-22.95	61.35	15.00
66	GLY	CA	-17.45	-24.19	62.08	15.00
66	GLY	C	-18.56	-25.20	61.92	15.00
66	GLY	O	-19.38	-25.12	61.00	15.00
67	TYR	N	-18.56	-26.18	62.81	15.00
67	TYR	CA	-19.55	-27.25	62.80	15.00
67	TYR	CB	-18.89	-28.59	62.62	15.00
67	TYR	CG	-18.09	-28.77	61.37	15.00
67	TYR	CD1	-18.68	-28.65	60.11	15.00
67	TYR	CE1	-17.97	-28.95	58.95	15.00
67	TYR	CD2	-16.77	-29.18	61.44	15.00
67	TYR	CE2	-16.05	-29.48	60.30	15.00
67	TYR	CZ	-16.65	-29.37	59.06	15.00
67	TYR	OH	-15.93	-29.71	57.94	15.00
67	TYR	C	-20.31	-27.25	64.11	15.00
67	TYR	O	-19.73	-26.97	65.15	15.00
68	MET	N	-21.60	-27.57	64.06	15.00
68	MET	CA	-22.40	-27.64	65.27	15.00
68	MET	CB	-23.88	-27.79	64.94	15.00
68	MET	CG	-24.47	-26.62	64.20	15.00
68	MET	SD	-23.93	-26.55	62.51	15.00
68	MET	CE	-25.32	-27.25	61.69	15.00
68	MET	C	-21.91	-28.78	66.17	15.00
68	MET	O	-21.81	-28.64	67.39	15.00
69	THR	N	-21.56	-29.90	65.54	15.00
69	THR	CA	-21.07	-31.07	66.27	15.00

TABLE IX

69	THR	CB	-20.66	-32.20	65.31	15.00
69	THR	OG1	-19.57	-31.77	64.48	15.00
69	THR	CG2	-21.84	-32.58	64.45	15.00
69	THR	C	-19.91	-30.70	67.18	15.00
69	THR	O	-19.94	-31.00	68.37	15.00
70	ASN	N	-18.92	-30.00	66.64	15.00
70	ASN	CA	-17.77	-29.54	67.42	15.00
70	ASN	CB	-16.75	-28.84	66.55	15.00
70	ASN	CG	-15.86	-29.80	65.85	15.00
70	ASN	OD1	-15.33	-30.72	66.46	15.00
70	ASN	ND2	-15.68	-29.61	64.55	15.00
70	ASN	C	-18.17	-28.63	68.60	15.00
70	ASN	O	-17.53	-28.66	69.66	15.00
71	ALA	N	-19.20	-27.82	68.40	15.00
71	ALA	CA	-19.67	-26.91	69.44	15.00
71	ALA	CB	-20.66	-25.91	68.86	15.00
71	ALA	C	-20.33	-27.72	70.55	15.00
71	ALA	O	-20.26	-27.37	71.72	15.00
72	PHE	N	-20.96	-28.83	70.16	15.00
72	PHE	CA	-21.61	-29.70	71.13	15.00
72	PHE	CB	-22.57	-30.66	70.43	15.00
72	PHE	CG	-23.73	-29.98	69.79	15.00
72	PHE	CD1	-24.28	-28.84	70.36	15.00
72	PHE	CD2	-24.29	-30.48	68.63	15.00
72	PHE	CE1	-25.35	-28.21	69.79	15.00
72	PHE	CE2	-25.37	-29.87	68.04	15.00
72	PHE	CZ	-25.91	-28.72	68.62	15.00
72	PHE	C	-20.59	-30.46	71.96	15.00
72	PHE	O	-20.79	-30.69	73.15	15.00
73	GLN	N	-19.48	-30.82	71.33	15.00
73	GLN	CA	-18.43	-31.54	72.03	15.00
73	GLN	CB	-17.46	-32.17	71.04	15.00
73	GLN	CG	-16.71	-33.36	71.59	15.00
73	GLN	CD	-16.83	-34.56	70.67	15.00
73	GLN	OE1	-17.35	-35.61	71.07	15.00
73	GLN	NE2	-16.37	-34.41	69.44	15.00
73	GLN	C	-17.70	-30.62	72.99	15.00
73	GLN	O	-17.18	-31.07	74.02	15.00
74	TYR	N	-17.64	-29.34	72.65	15.00
74	TYR	CA	-16.96	-28.38	73.52	15.00
74	TYR	CB	-16.74	-27.03	72.81	15.00
74	TYR	CG	-16.38	-25.93	73.78	15.00

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74	TYR	CD1	-15.16	-25.95	74.45	15.00
74	TYR	CE1	-14.87	-25.02	75.40	15.00
74	TYR	CD2	-17.30	-24.94	74.11	15.00
74	TYR	CE2	-17.01	-24.00	75.07	15.00
74	TYR	CZ	-15.79	-24.05	75.71	15.00
74	TYR	OH	-15.47	-23.11	76.67	15.00
74	TYR	C	-17.69	-28.17	74.84	15.00
74	TYR	O	-17.07	-28.14	75.89	15.00
75	VAL	N	-19.00	-27.98	74.77	15.00
75	VAL	CA	-19.82	-27.78	75.97	15.00
75	VAL	CB	-21.29	-27.47	75.58	15.00
75	VAL	CG1	-22.13	-27.23	76.82	15.00
75	VAL	CG2	-21.34	-26.25	74.67	15.00
75	VAL	C	-19.73	-29.01	76.87	15.00
75	VAL	O	-19.82	-28.91	78.10	15.00
76	GLN	N	-19.47	-30.16	76.26	15.00
76	GLN	CA	-19.33	-31.42	76.97	15.00
76	GLN	CB	-19.57	-32.58	76.01	15.00
76	GLN	CG	-19.54	-33.95	76.62	15.00
76	GLN	CD	-19.67	-35.03	75.58	15.00
76	GLN	OE1	-20.73	-35.62	75.41	15.00
76	GLN	NE2	-18.60	-35.28	74.86	15.00
76	GLN	C	-17.96	-31.55	77.68	15.00
76	GLN	O	-17.91	-31.76	78.89	15.00
77	LYS	N	-16.87	-31.41	76.94	15.00
77	LYS	CA	-15.53	-31.51	77.53	15.00
77	LYS	CB	-14.43	-31.56	76.46	15.00
77	LYS	CG	-14.07	-30.18	75.87	15.00
77	LYS	CD	-12.80	-30.21	75.01	15.00
77	LYS	CE	-13.01	-30.90	73.67	15.00
77	LYS	NZ	-14.16	-30.32	72.90	15.00
77	LYS	C	-15.26	-30.36	78.49	15.00
77	LYS	O	-14.45	-30.49	79.41	15.00
78	ASN	N	-15.89	-29.22	78.22	15.00
78	ASN	CA	-15.73	-28.04	79.05	15.00
78	ASN	CB	-16.05	-26.77	78.27	15.00
78	ASN	CG	-15.64	-25.51	79.00	15.00
78	ASN	OD1	-14.49	-25.35	79.40	15.00
78	ASN	ND2	-16.57	-24.59	79.14	15.00
78	ASN	C	-16.64	-28.15	80.26	15.00
78	ASN	O	-16.46	-27.45	81.25	15.00
79	ARG	N	-17.63	-29.04	80.16	15.00

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79	ARG	CA	-18.61	-29.26	81.22	15.00
79	ARG	CB	-17.95	-29.71	82.54	15.00
79	ARG	CG	-17.19	-31.05	82.52	15.00
79	ARG	CD	-18.12	-32.28	82.55	15.00
79	ARG	NE	-18.94	-32.34	83.76	15.00
79	ARG	CZ	-20.14	-32.92	83.84	15.00
79	ARG	NH1	-20.69	-33.51	82.78	15.00
79	ARG	NH2	-20.82	-32.88	84.99	15.00
79	ARG	C	-19.47	-28.02	81.44	15.00
79	ARG	O	-19.86	-27.74	82.57	15.00
80	GLY	N	-19.75	-27.27	80.38	15.00
80	GLY	CA	-20.58	-26.08	80.52	15.00
80	GLY	C	-20.38	-24.97	79.49	15.00
80	GLY	O	-19.36	-24.93	78.78	15.00
81	ILE	N	-21.37	-24.08	79.41	15.00
81	ILE	CA	-21.35	-22.92	78.50	15.00
81	ILE	CB	-22.14	-23.20	77.17	15.00
81	ILE	CG2	-23.59	-23.57	77.46	15.00
81	ILE	CG1	-22.11	-21.97	76.25	15.00
81	ILE	CD1	-22.75	-22.19	74.90	15.00
81	ILE	C	-22.00	-21.76	79.25	15.00
81	ILE	O	-22.86	-21.98	80.11	15.00
82	ASP	N	-21.56	-20.54	78.96	15.00
82	ASP	CA	-22.09	-19.34	79.61	15.00
82	ASP	CB	-21.08	-18.20	79.59	15.00
82	ASP	CG	-19.89	-18.44	80.48	15.00
82	ASP	OD1	-18.82	-17.87	80.21	15.00
82	ASP	OD2	-20.03	-19.18	81.47	15.00
82	ASP	C	-23.40	-18.85	79.02	15.00
82	ASP	O	-23.89	-19.36	78.02	15.00
83	SER	N	-23.96	-17.84	79.68	15.00
83	SER	CA	-25.19	-17.20	79.27	15.00
83	SER	CB	-26.03	-16.83	80.49	15.00
83	SER	OG	-25.19	-16.35	81.52	15.00
83	SER	C	-24.76	-15.96	78.49	15.00
83	SER	O	-23.59	-15.58	78.53	15.00
84	GLU	N	-25.68	-15.29	77.81	15.00
84	GLU	CA	-25.29	-14.13	77.03	15.00
84	GLU	CB	-26.39	-13.59	76.13	15.00
84	GLU	CG	-25.83	-12.69	75.03	15.00
84	GLU	CD	-24.85	-13.42	74.11	15.00
84	GLU	OE1	-25.26	-13.79	72.99	15.00

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84	GLU	OE2	-23.68	-13.64	74.49	15.00
84	GLU	C	-24.73	-13.05	77.92	15.00
84	GLU	O	-23.52	-12.84	77.90	15.00
85	ASP	N	-25.56	-12.36	78.69	15.00
85	ASP	CA	-25.00	-11.32	79.55	15.00
85	ASP	CB	-26.06	-10.32	80.06	15.00
85	ASP	CG	-25.45	-8.93	80.42	15.00
85	ASP	OD1	-26.14	-8.14	81.10	15.00
85	ASP	OD2	-24.30	-8.62	80.02	15.00
85	ASP	C	-24.32	-12.06	80.68	15.00
85	ASP	O	-24.91	-12.29	81.73	15.00
86	ALA	N	-23.11	-12.51	80.37	15.00
86	ALA	CA	-22.20	-13.27	81.22	15.00
86	ALA	CB	-22.80	-14.62	81.60	15.00
86	ALA	C	-20.96	-13.46	80.33	15.00
86	ALA	O	-19.83	-13.52	80.81	15.00
87	TYR	N	-21.21	-13.59	79.03	15.00
87	TYR	CA	-20.18	-13.73	78.00	15.00
87	TYR	CB	-19.74	-15.19	77.86	15.00
87	TYR	CG	-18.39	-15.40	77.19	15.00
87	TYR	CD1	-17.78	-14.38	76.45	15.00
87	TYR	CE1	-16.54	-14.59	75.84	15.00
87	TYR	CD2	-17.73	-16.61	77.31	15.00
87	TYR	CE2	-16.49	-16.82	76.72	15.00
87	TYR	CZ	-15.90	-15.80	75.98	15.00
87	TYR	OH	-14.67	-15.99	75.42	15.00
87	TYR	C	-20.88	-13.21	76.73	15.00
87	TYR	O	-21.25	-13.98	75.86	15.00
88	PRO	N	-21.07	-11.89	76.64	15.00
88	PRO	CD	-20.61	-10.92	77.65	15.00
88	PRO	CA	-21.72	-11.18	75.54	15.00
88	PRO	CB	-21.69	-9.73	76.00	15.00
88	PRO	CG	-21.61	-9.83	77.49	15.00
88	PRO	C	-21.11	-11.32	74.15	15.00
88	PRO	O	-19.90	-11.51	74.00	15.00
89	TYR	N	-21.95	-11.12	73.14	15.00
89	TYR	CA	-21.55	-11.21	71.74	15.00
89	TYR	CB	-22.75	-11.61	70.87	15.00
89	TYR	CG	-22.36	-12.04	69.48	15.00
89	TYR	CD1	-21.49	-13.11	69.29	15.00
89	TYR	CE1	-21.07	-13.47	68.02	15.00
89	TYR	CD2	-22.82	-11.36	68.36	15.00

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89	TYR	CE2	-22.41	-11.72	67.10	15.00
89	TYR	CZ	-21.53	-12.77	66.94	15.00
89	TYR	OH	-21.09	-13.11	65.69	15.00
89	TYR	C	-20.90	-9.91	71.24	15.00
89	TYR	O	-21.59	-8.91	71.03	15.00
90	VAL	N	-19.58	-9.92	71.08	15.00
90	VAL	CA	-18.87	-8.73	70.61	15.00
90	VAL	CB	-17.41	-8.68	71.09	15.00
90	VAL	CG1	-17.35	-8.79	72.60	15.00
90	VAL	CG2	-16.59	-9.77	70.43	15.00
90	VAL	C	-18.89	-8.68	69.08	15.00
90	VAL	O	-18.82	-7.61	68.49	15.00
91	GLY	N	-18.98	-9.84	68.45	15.00
91	GLY	CA	-19.04	-9.87	67.01	15.00
91	GLY	C	-17.71	-10.16	66.36	15.00
91	GLY	O	-17.56	-9.93	65.16	15.00
92	GLN	N	-16.76	-10.69	67.13	15.00
92	GLN	CA	-15.43	-11.01	66.62	15.00
92	GLN	CB	-14.62	-9.75	66.38	15.00
92	GLN	CG	-14.24	-9.09	67.68	15.00
92	GLN	CD	-13.83	-7.66	67.52	15.00
92	GLN	OE1	-12.91	-7.19	68.19	15.00
92	GLN	NE2	-14.53	-6.93	66.64	15.00
92	GLN	C	-14.67	-11.92	67.58	15.00
92	GLN	O	-14.91	-11.91	68.79	15.00
93	GLU	N	-13.72	-12.66	67.02	15.00
93	GLU	CA	-12.89	-13.59	67.78	15.00
93	GLU	CB	-11.95	-14.35	66.85	15.00
93	GLU	CG	-12.64	-15.06	65.69	15.00
93	GLU	CD	-11.68	-15.45	64.57	15.00
93	GLU	OE1	-10.56	-15.94	64.87	15.00
93	GLU	OE2	-12.03	-15.24	63.39	15.00
93	GLU	C	-12.11	-12.86	68.86	15.00
93	GLU	O	-11.54	-11.79	68.61	15.00
94	GLU	N	-12.08	-13.46	70.05	15.00
94	GLU	CA	-11.38	-12.93	71.22	15.00
94	GLU	CB	-12.31	-12.19	72.16	15.00
94	GLU	CG	-12.77	-10.82	71.71	15.00
94	GLU	CD	-13.69	-10.18	72.74	15.00
94	GLU	OE1	-13.59	-8.95	72.97	15.00
94	GLU	OE2	-14.50	-10.92	73.33	15.00
94	GLU	C	-10.77	-14.12	71.96	15.00

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94	GLU	O	-11.15	-15.26	71.71	15.00
95	SER	N	-9.87	-13.85	72.90	15.00
95	SER	CA	-9.24	-14.91	73.69	15.00
95	SER	CB	-8.09	-14.36	74.52	15.00
95	SER	OG	-8.52	-13.24	75.28	15.00
95	SER	C	-10.32	-15.52	74.59	15.00
95	SER	O	-11.03	-14.78	75.28	15.00
96	CYS	N	-10.42	-16.84	74.58	15.00
96	CYS	CA	-11.43	-17.54	75.38	15.00
96	CYS	C	-11.55	-17.08	76.82	15.00
96	CYS	O	-10.69	-17.37	77.66	15.00
96	CYS	CB	-11.24	-19.06	75.31	15.00
96	CYS	SG	-12.40	-19.98	76.37	15.00
97	MET	N	-12.60	-16.32	77.10	15.00
97	MET	CA	-12.86	-15.80	78.44	15.00
97	MET	CB	-13.16	-14.29	78.41	15.00
97	MET	CG	-11.97	-13.37	78.13	15.00
97	MET	SD	-12.05	-12.55	76.50	15.00
97	MET	CE	-13.66	-11.72	76.66	15.00
97	MET	C	-13.99	-16.57	79.13	15.00
97	MET	O	-14.93	-15.96	79.66	15.00
98	TYR	N	-13.91	-17.90	79.15	15.00
98	TYR	CA	-14.96	-18.68	79.80	15.00
98	TYR	CB	-14.79	-20.17	79.54	15.00
98	TYR	CG	-15.85	-21.01	80.24	15.00
98	TYR	CD1	-17.20	-20.84	79.95	15.00
98	TYR	CE1	-18.17	-21.59	80.59	15.00
98	TYR	CD2	-15.50	-21.96	81.19	15.00
98	TYR	CE2	-16.48	-22.73	81.83	15.00
98	TYR	CZ	-17.80	-22.53	81.53	15.00
98	TYR	OH	-18.77	-23.27	82.16	15.00
98	TYR	C	-15.11	-18.42	81.29	15.00
98	TYR	O	-14.28	-18.80	82.11	15.00
99	ASN	N	-16.21	-17.74	81.62	15.00
99	ASN	CA	-16.59	-17.38	82.98	15.00
99	ASN	CB	-17.52	-16.16	82.93	15.00
99	ASN	CG	-17.93	-15.66	84.29	15.00
99	ASN	OD1	-17.61	-16.27	85.32	15.00
99	ASN	ND2	-18.65	-14.53	84.32	15.00
99	ASN	C	-17.30	-18.62	83.57	15.00
99	ASN	O	-18.50	-18.81	83.35	15.00
100	PRO	N	-16.59	-19.46	84.35	15.00

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TABLE IX

100 PRO CD	-15.20	-19.31	84.81	15.00
100 PRO CA	-17.20	-20.67	84.94	15.00
100 PRO CB	-16.06	-21.26	85.77	15.00
100 PRO CG	-14.82	-20.73	85.09	15.00
100 PRO C	-18.40	-20.36	85.82	15.00
100 PRO O	-19.33	-21.16	85.93	15.00
101 THR N	-18.37	-19.19	86.44	15.00
101 THR CA	-19.44	-18.75	87.32	15.00
101 THR CB	-19.06	-17.44	88.03	15.00
101 THR OG1	-17.64	-17.23	87.93	15.00
101 THR CG2	-19.46	-17.51	89.50	15.00
101 THR C	-20.74	-18.53	86.56	15.00
101 THR O	-21.82	-18.83	87.07	15.00
102 GLY N	-20.64	-18.01	85.35	15.00
102 GLY CA	-21.85	-17.75	84.58	15.00
102 GLY C	-22.38	-18.91	83.77	15.00
102 GLY O	-23.27	-18.70	82.94	15.00
103 LYS N	-21.85	-20.12	83.98	15.00
103 LYS CA	-22.32	-21.28	83.21	15.00
103 LYS CB	-21.62	-22.56	83.63	15.00
103 LYS CG	-22.20	-23.22	84.86	15.00
103 LYS CD	-21.67	-24.63	85.01	15.00
103 LYS CE	-22.02	-25.45	83.79	15.00
103 LYS NZ	-23.49	-25.45	83.60	15.00
103 LYS C	-23.83	-21.40	83.35	15.00
103 LYS O	-24.37	-21.25	84.45	15.00
104 ALA N	-24.51	-21.65	82.24	15.00
104 ALA CA	-25.96	-21.74	82.28	15.00
104 ALA CB	-26.57	-20.48	81.67	15.00
104 ALA C	-26.55	-22.97	81.62	15.00
104 ALA O	-27.76	-23.22	81.72	15.00
105 ALA N	-25.70	-23.76	80.97	15.00
105 ALA CA	-26.17	-24.96	80.31	15.00
105 ALA CB	-26.66	-24.65	78.91	15.00
105 ALA C	-25.10	-26.02	80.24	15.00
105 ALA O	-23.91	-25.72	80.09	15.00
106 LYS N	-25.53	-27.26	80.40	15.00
106 LYS CA	-24.65	-28.41	80.36	15.00
106 LYS CB	-24.77	-29.23	81.64	15.00
106 LYS CG	-24.05	-28.65	82.83	15.00
106 LYS CD	-22.56	-28.96	82.80	15.00
106 LYS CE	-22.28	-30.46	82.89	15.00

TABLE IX

106 LYS NZ	-22.56	-31.21	81.62	15.00
106 LYS C	-25.08	-29.23	79.17	15.00
106 LYS O	-26.18	-29.04	78.65	15.00
107 CYS N	-24.23	-30.15	78.76	15.00
107 CYS CA	-24.52	-31.01	77.62	15.00
107 CYS CB	-24.00	-30.36	76.33	15.00
107 CYS SG	-24.10	-31.36	74.81	15.00
107 CYS C	-23.81	-32.31	77.94	15.00
107 CYS O	-22.94	-32.34	78.81	15.00
108 ARG N	-24.23	-33.40	77.30	15.00
108 ARG CA	-23.60	-34.70	77.51	15.00
108 ARG CB	-24.27	-35.46	78.66	15.00
108 ARG CG	-25.67	-35.93	78.35	15.00
108 ARG CD	-26.16	-36.95	79.38	15.00
108 ARG NE	-27.36	-37.64	78.90	15.00
108 ARG CZ	-27.34	-38.78	78.20	15.00
108 ARG NH1	-26.18	-39.37	77.92	15.00
108 ARG NH2	-28.48	-39.29	77.75	15.00
108 ARG C	-23.57	-35.53	76.23	15.00
108 ARG O	-23.71	-36.76	76.27	15.00
109 GLY N	-23.37	-34.87	75.10	15.00
109 GLY CA	-23.30	-35.59	73.85	15.00
109 GLY C	-24.02	-34.85	72.75	15.00
109 GLY O	-24.50	-33.73	72.95	15.00
110 TYR N	-24.10	-35.48	71.59	15.00
110 TYR CA	-24.77	-34.92	70.44	15.00
110 TYR CB	-23.91	-33.89	69.74	15.00
110 TYR CG	-22.68	-34.45	69.05	15.00
110 TYR CD1	-21.45	-34.47	69.70	15.00
110 TYR CE1	-20.31	-34.89	69.04	15.00
110 TYR CD2	-22.74	-34.88	67.73	15.00
110 TYR CE2	-21.61	-35.30	67.07	15.00
110 TYR CZ	-20.39	-35.30	67.72	15.00
110 TYR OH	-19.24	-35.68	67.05	15.00
110 TYR C	-25.16	-36.02	69.48	15.00
110 TYR O	-24.41	-36.99	69.31	15.00
111 ARG N	-26.32	-35.87	68.86	15.00
111 ARG CA	-26.83	-36.84	67.91	15.00
111 ARG CB	-28.14	-37.43	68.41	15.00
111 ARG CG	-28.01	-38.15	69.74	15.00
111 ARG CD	-28.52	-39.57	69.65	15.00
111 ARG NE	-27.97	-40.28	68.49	15.00

TABLE IX

111 ARG CZ	-28.38	-41.48	68.10	15.00
111 ARG NH1	-27.83	-42.06	67.03	15.00
111 ARG NH2	-29.32	-42.12	68.78	15.00
111 ARG C	-27.01	-36.25	66.52	15.00
111 ARG O	-27.32	-35.07	66.39	15.00
112 GLU N	-26.81	-37.06	65.50	15.00
112 GLU CA	-26.94	-36.62	64.12	15.00
112 GLU CB	-25.68	-36.90	63.30	15.00
112 GLU CG	-24.42	-36.10	63.68	15.00
112 GLU CD	-23.23	-36.42	62.77	15.00
112 GLU OE1	-22.07	-36.07	63.13	15.00
112 GLU OE2	-23.44	-37.01	61.69	15.00
112 GLU C	-28.14	-37.26	63.44	15.00
112 GLU O	-28.60	-38.33	63.84	15.00
113 ILE N	-28.61	-36.60	62.39	15.00
113 ILE CA	-29.74	-37.06	61.60	15.00
113 ILE CB	-30.51	-35.84	61.05	15.00
113 ILE CG2	-31.61	-36.25	60.09	15.00
113 ILE CG1	-31.10	-35.06	62.22	15.00
113 ILE CD1	-32.01	-35.89	63.07	15.00
113 ILE C	-29.15	-37.84	60.43	15.00
113 ILE O	-28.13	-37.44	59.88	15.00
114 PRO N	-29.74	-38.99	60.08	15.00
114 PRO CD	-30.93	-39.67	60.65	15.00
114 PRO CA	-29.19	-39.76	58.95	15.00
114 PRO CB	-30.23	-40.86	58.75	15.00
114 PRO CG	-30.78	-41.07	60.12	15.00
114 PRO C	-29.18	-38.82	57.75	15.00
114 PRO O	-30.23	-38.35	57.30	15.00
115 GLU N	-27.98	-38.53	57.25	15.00
115 GLU CA	-27.81	-37.64	56.11	15.00
115 GLU CB	-26.36	-37.71	55.63	15.00
115 GLU CG	-26.00	-38.96	54.84	15.00
115 GLU CD	-26.11	-38.74	53.34	15.00
115 GLU OE1	-26.79	-39.55	52.65	15.00
115 GLU OE2	-25.52	-37.74	52.85	15.00
115 GLU C	-28.81	-37.80	54.96	15.00
115 GLU O	-28.93	-38.86	54.37	15.00
116 GLY N	-29.54	-36.73	54.67	15.00
116 GLY CA	-30.51	-36.71	53.59	15.00
116 GLY C	-31.88	-37.25	53.92	15.00
116 GLY O	-32.76	-37.31	53.05	15.00

TABLE IX

117	ASN	N	-32.09	-37.61	55.18	15.00
117	ASN	CA	-33.37	-38.18	55.61	15.00
117	ASN	CB	-33.13	-39.38	56.52	15.00
117	ASN	CG	-34.42	-40.02	57.01	15.00
117	ASN	OD1	-35.53	-39.60	56.65	15.00
117	ASN	ND2	-34.28	-41.06	57.83	15.00
117	ASN	C	-34.32	-37.19	56.27	15.00
117	ASN	O	-34.40	-37.10	57.50	15.00
118	GLU	N	-35.10	-36.50	55.45	15.00
118	GLU	CA	-36.05	-35.52	55.96	15.00
118	GLU	CB	-36.81	-34.85	54.83	15.00
118	GLU	CG	-36.06	-33.74	54.15	15.00
118	GLU	CD	-36.96	-32.95	53.26	15.00
118	GLU	OE1	-37.20	-33.39	52.11	15.00
118	GLU	OE2	-37.46	-31.91	53.72	15.00
118	GLU	C	-37.03	-36.09	56.96	15.00
118	GLU	O	-37.48	-35.39	57.88	15.00
119	LYS	N	-37.39	-37.36	56.79	15.00
119	LYS	CA	-38.33	-37.99	57.71	15.00
119	LYS	CB	-38.85	-39.30	57.15	15.00
119	LYS	CG	-40.37	-39.34	57.05	15.00
119	LYS	CD	-40.95	-38.10	56.34	15.00
119	LYS	CE	-42.47	-38.10	56.44	15.00
119	LYS	NZ	-43.07	-36.84	55.99	15.00
119	LYS	C	-37.71	-38.16	59.09	15.00
119	LYS	O	-38.36	-37.86	60.09	15.00
120	ALA	N	-36.45	-38.57	59.15	15.00
120	ALA	CA	-35.77	-38.75	60.44	15.00
120	ALA	CB	-34.45	-39.45	60.27	15.00
120	ALA	C	-35.56	-37.40	61.08	15.00
120	ALA	O	-35.41	-37.31	62.30	15.00
121	LEU	N	-35.52	-36.34	60.26	15.00
121	LEU	CA	-35.37	-34.98	60.78	15.00
121	LEU	CB	-34.93	-33.98	59.69	15.00
121	LEU	CG	-34.71	-32.55	60.19	15.00
121	LEU	CD1	-33.44	-32.47	61.03	15.00
121	LEU	CD2	-34.62	-31.58	59.02	15.00
121	LEU	C	-36.70	-34.57	61.37	15.00
121	LEU	O	-36.77	-34.00	62.45	15.00
122	LYS	N	-37.77	-34.88	60.65	15.00
122	LYS	CA	-39.12	-34.58	61.09	15.00
122	LYS	CB	-40.14	-35.16	60.12	15.00

TABLE IX

122 LYS CG	-41.58	-34.91	60.49	15.00
122 LYS CD	-42.51	-35.55	59.48	15.00
122 LYS CE	-43.96	-35.15	59.73	15.00
122 LYS NZ	-44.83	-35.53	58.58	15.00
122 LYS C	-39.29	-35.19	62.48	15.00
122 LYS O	-39.68	-34.50	63.42	15.00
123 ARG N	-38.95	-36.47	62.59	15.00
123 ARG CA	-39.04	-37.19	63.86	15.00
123 ARG CB	-38.64	-38.65	63.70	15.00
123 ARG CG	-39.66	-39.49	62.94	15.00
123 ARG CD	-39.69	-40.93	63.45	15.00
123 ARG NE	-38.49	-41.71	63.12	15.00
123 ARG CZ	-38.54	-42.87	62.47	15.00
123 ARG NH1	-39.71	-43.37	62.09	15.00
123 ARG NH2	-37.42	-43.54	62.20	15.00
123 ARG C	-38.19	-36.51	64.93	15.00
123 ARG O	-38.63	-36.34	66.05	15.00
124 ALA N	-36.98	-36.12	64.57	15.00
124 ALA CA	-36.09	-35.45	65.50	15.00
124 ALA CB	-34.77	-35.16	64.86	15.00
124 ALA C	-36.70	-34.15	66.00	15.00
124 ALA O	-36.77	-33.93	67.21	15.00
125 VAL N	-37.14	-33.31	65.08	15.00
125 VAL CA	-37.72	-32.03	65.45	15.00
125 VAL CB	-38.13	-31.20	64.21	15.00
125 VAL CG1	-38.87	-29.94	64.63	15.00
125 VAL CG2	-36.90	-30.81	63.41	15.00
125 VAL C	-38.90	-32.21	66.39	15.00
125 VAL O	-39.02	-31.48	67.36	15.00
126 ALA N	-39.75	-33.20	66.13	15.00
126 ALA CA	-40.92	-33.43	66.99	15.00
126 ALA CB	-41.96	-34.25	66.25	15.00
126 ALA C	-40.58	-34.09	68.33	15.00
126 ALA O	-41.09	-33.68	69.38	15.00
127 ARG N	-39.75	-35.12	68.30	15.00
127 ARG CA	-39.38	-35.83	69.52	15.00
127 ARG CB	-38.82	-37.21	69.20	15.00
127 ARG CG	-39.74	-38.08	68.36	15.00
127 ARG CD	-39.22	-39.50	68.39	15.00
127 ARG NE	-39.68	-40.36	67.30	15.00
127 ARG CZ	-40.95	-40.55	66.96	15.00
127 ARG NH1	-41.25	-41.36	65.96	15.00

TABLE IX

127 ARG NH2	-41.92	-39.90	67.59	15.00
127 ARG C	-38.41	-35.07	70.40	15.00
127 ARG O	-38.63	-34.94	71.60	15.00
128 VAL N	-37.33	-34.58	69.81	15.00
128 VAL CA	-36.30	-33.85	70.54	15.00
128 VAL CB	-34.95	-33.96	69.83	15.00
128 VAL CG1	-33.89	-33.20	70.59	15.00
128 VAL CG2	-34.56	-35.42	69.68	15.00
128 VAL C	-36.62	-32.39	70.77	15.00
128 VAL O	-36.73	-31.94	71.90	15.00
129 GLY N	-36.70	-31.64	69.68	15.00
129 GLY CA	-36.98	-30.21	69.76	15.00
129 GLY C	-36.20	-29.51	68.66	15.00
129 GLY O	-35.93	-30.12	67.63	15.00
130 PRO N	-35.81	-28.24	68.86	15.00
130 PRO CD	-36.15	-27.39	70.00	15.00
130 PRO CA	-35.06	-27.48	67.86	15.00
130 PRO CB	-34.77	-26.18	68.58	15.00
130 PRO CG	-36.00	-26.00	69.41	15.00
130 PRO C	-33.78	-28.20	67.49	15.00
130 PRO O	-32.98	-28.51	68.37	15.00
131 VAL N	-33.60	-28.46	66.19	15.00
131 VAL CA	-32.42	-29.16	65.69	15.00
131 VAL CB	-32.80	-30.40	64.82	15.00
131 VAL CG1	-31.55	-31.10	64.33	15.00
131 VAL CG2	-33.66	-31.37	65.60	15.00
131 VAL C	-31.54	-28.26	64.83	15.00
131 VAL O	-32.02	-27.54	63.96	15.00
132 SER N	-30.24	-28.35	65.05	15.00
132 SER CA	-29.27	-27.55	64.31	15.00
132 SER CB	-27.93	-27.54	65.04	15.00
132 SER OG	-28.09	-27.80	66.43	15.00
132 SER C	-29.11	-28.11	62.90	15.00
132 SER O	-28.80	-29.29	62.74	15.00
133 VAL N	-29.34	-27.29	61.88	15.00
133 VAL CA	-29.20	-27.74	60.49	15.00
133 VAL CB	-30.57	-27.83	59.76	15.00
133 VAL CG1	-31.29	-29.10	60.15	15.00
133 VAL CG2	-31.42	-26.63	60.06	15.00
133 VAL C	-28.26	-26.86	59.67	15.00
133 VAL O	-27.82	-25.81	60.14	15.00
134 ALA N	-27.93	-27.29	58.46	15.00

TABLE IX

134 ALA CA	-27.05	-26.53	57.59	15.00
134 ALA CB	-25.65	-27.10	57.62	15.00
134 ALA C	-27.62	-26.60	56.18	15.00
134 ALA O	-27.92	-27.68	55.69	15.00
135 ILE N	-27.80	-25.44	55.56	15.00
135 ILE CA	-28.36	-25.36	54.21	15.00
135 ILE CB	-29.74	-24.70	54.21	15.00
135 ILE CG2	-30.76	-25.58	54.87	15.00
135 ILE CG1	-29.64	-23.31	54.87	15.00
135 ILE CD1	-30.91	-22.52	54.84	15.00
135 ILE C	-27.51	-24.50	53.29	15.00
135 ILE O	-26.46	-23.99	53.67	15.00
136 ASP N	-28.04	-24.32	52.09	15.00
136 ASP CA	-27.44	-23.50	51.05	15.00
136 ASP CB	-27.56	-24.20	49.70	15.00
136 ASP CG	-27.01	-23.38	48.56	15.00
136 ASP OD1	-27.62	-23.39	47.48	15.00
136 ASP OD2	-25.96	-22.75	48.73	15.00
136 ASP C	-28.17	-22.15	51.05	15.00
136 ASP O	-29.30	-22.07	50.57	15.00
137 ALA N	-27.56	-21.12	51.62	15.00
137 ALA CA	-28.19	-19.81	51.68	15.00
137 ALA CB	-28.23	-19.33	53.12	15.00
137 ALA C	-27.52	-18.76	50.80	15.00
137 ALA O	-27.74	-17.56	50.97	15.00
138 SER N	-26.72	-19.22	49.84	15.00
138 SER CA	-26.00	-18.34	48.92	15.00
138 SER CB	-24.80	-19.07	48.33	15.00
138 SER OG	-25.20	-20.25	47.66	15.00
138 SER C	-26.85	-17.71	47.82	15.00
138 SER O	-26.50	-16.66	47.27	15.00
139 LEU N	-27.96	-18.36	47.45	15.00
139 LEU CA	-28.85	-17.84	46.42	15.00
139 LEU CB	-29.97	-18.82	46.10	15.00
139 LEU CG	-29.63	-20.08	45.32	15.00
139 LEU CD1	-30.91	-20.89	45.13	15.00
139 LEU CD2	-29.04	-19.71	43.97	15.00
139 LEU C	-29.45	-16.51	46.85	15.00
139 LEU O	-29.82	-16.33	48.00	15.00
140 THR N	-29.61	-15.59	45.90	15.00
140 THR CA	-30.17	-14.28	46.20	15.00
140 THR CB	-29.95	-13.25	45.03	15.00

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TABLE IX

140	THR	OG1	-29.88	-13.93	43.77	15.00
140	THR	CG2	-28.67	-12.47	45.23	15.00
140	THR	C	-31.65	-14.34	46.59	15.00
140	THR	O	-32.12	-13.52	47.37	15.00
141	SER	N	-32.37	-15.35	46.10	15.00
141	SER	CA	-33.79	-15.49	46.43	15.00
141	SER	CB	-34.47	-16.53	45.55	15.00
141	SER	OG	-33.70	-17.71	45.45	15.00
141	SER	C	-34.00	-15.80	47.91	15.00
141	SER	O	-34.99	-15.38	48.50	15.00
142	PHE	N	-33.07	-16.54	48.49	15.00
142	PHE	CA	-33.13	-16.89	49.91	15.00
142	PHE	CB	-32.01	-17.88	50.28	15.00
142	PHE	CG	-31.93	-18.18	51.75	15.00
142	PHE	CD1	-32.67	-19.22	52.31	15.00
142	PHE	CD2	-31.12	-17.42	52.59	15.00
142	PHE	CE1	-32.62	-19.48	53.68	15.00
142	PHE	CE2	-31.06	-17.68	53.95	15.00
142	PHE	CZ	-31.81	-18.71	54.51	15.00
142	PHE	C	-33.00	-15.60	50.70	15.00
142	PHE	O	-33.80	-15.30	51.59	15.00
143	GLN	N	-32.00	-14.81	50.30	15.00
143	GLN	CA	-31.67	-13.54	50.93	15.00
143	GLN	CB	-30.35	-13.03	50.36	15.00
143	GLN	CG	-29.20	-13.96	50.70	15.00
143	GLN	CD	-27.93	-13.71	49.91	15.00
143	GLN	OE1	-27.22	-12.73	50.12	15.00
143	GLN	NE2	-27.63	-14.63	49.01	15.00
143	GLN	C	-32.77	-12.47	50.94	15.00
143	GLN	O	-32.99	-11.82	51.97	15.00
144	PHE	N	-33.47	-12.27	49.82	15.00
144	PHE	CA	-34.54	-11.27	49.79	15.00
144	PHE	CB	-34.55	-10.47	48.49	15.00
144	PHE	CG	-34.68	-11.30	47.25	15.00
144	PHE	CD1	-33.69	-11.28	46.28	15.00
144	PHE	CD2	-35.81	-12.07	47.03	15.00
144	PHE	CE1	-33.82	-12.00	45.10	15.00
144	PHE	CE2	-35.95	-12.79	45.85	15.00
144	PHE	CZ	-34.95	-12.76	44.89	15.00
144	PHE	C	-35.92	-11.84	50.10	15.00
144	PHE	O	-36.95	-11.28	49.70	15.00
145	TYR	N	-35.94	-12.99	50.77	15.00

TABLE IX

145	TYR	CA	-37.17	-13.65	51.15	15.00
145	TYR	CB	-36.88	-15.04	51.74	15.00
145	TYR	CG	-38.04	-15.65	52.51	15.00
145	TYR	CD1	-38.88	-16.58	51.91	15.00
145	TYR	CE1	-39.95	-17.13	52.62	15.00
145	TYR	CD2	-38.29	-15.28	53.83	15.00
145	TYR	CE2	-39.35	-15.82	54.53	15.00
145	TYR	CZ	-40.17	-16.74	53.93	15.00
145	TYR	OH	-41.23	-17.25	54.64	15.00
145	TYR	C	-37.88	-12.76	52.15	15.00
145	TYR	O	-37.25	-12.09	52.96	15.00
146	SER	N	-39.21	-12.78	52.12	15.00
146	SER	CA	-40.01	-12.00	53.04	15.00
146	SER	CB	-40.30	-10.61	52.47	15.00
146	SER	OG	-40.96	-10.71	51.22	15.00
146	SER	C	-41.29	-12.72	53.43	15.00
146	SER	O	-41.83	-12.48	54.51	15.00
147	LYS	N	-41.76	-13.63	52.58	15.00
147	LYS	CA	-42.98	-14.39	52.86	15.00
147	LYS	CB	-44.22	-13.50	52.79	15.00
147	LYS	CG	-44.61	-13.04	51.39	15.00
147	LYS	CD	-45.75	-12.03	51.44	15.00
147	LYS	CE	-45.98	-11.35	50.09	15.00
147	LYS	NZ	-47.01	-10.28	50.19	15.00
147	LYS	C	-43.16	-15.60	51.95	15.00
147	LYS	O	-42.49	-15.70	50.92	15.00
148	GLY	N	-44.05	-16.50	52.36	15.00
148	GLY	CA	-44.34	-17.71	51.60	15.00
148	GLY	C	-43.51	-18.90	52.07	15.00
148	GLY	O	-42.99	-18.90	53.18	15.00
149	VAL	N	-43.43	-19.92	51.22	15.00
149	VAL	CA	-42.66	-21.12	51.51	15.00
149	VAL	CB	-43.53	-22.39	51.40	15.00
149	VAL	CG1	-42.69	-23.64	51.56	15.00
149	VAL	CG2	-44.62	-22.35	52.45	15.00
149	VAL	C	-41.53	-21.16	50.47	15.00
149	VAL	O	-41.75	-21.48	49.30	15.00
150	TYR	N	-40.33	-20.80	50.90	15.00
150	TYR	CA	-39.19	-20.78	50.01	15.00
150	TYR	CB	-37.96	-20.25	50.75	15.00
150	TYR	CG	-36.72	-20.12	49.90	15.00
150	TYR	CD1	-36.64	-19.13	48.91	15.00

TABLE IX

150 TYR CE1	-35.51	-19.02	48.09	15.00
150 TYR CD2	-35.64	-20.99	50.05	15.00
150 TYR CE2	-34.51	-20.89	49.24	15.00
150 TYR CZ	-34.45	-19.91	48.26	15.00
150 TYR OH	-33.36	-19.82	47.42	15.00
150 TYR C	-38.89	-22.11	49.33	15.00
150 TYR O	-38.81	-23.15	49.98	15.00
151 TYR N	-38.77	-22.06	48.01	15.00
151 TYR CA	-38.39	-23.22	47.21	15.00
151 TYR CB	-39.55	-24.11	46.79	15.00
151 TYR CG	-39.06	-25.31	45.98	15.00
151 TYR CD1	-37.99	-26.08	46.43	15.00
151 TYR CE1	-37.47	-27.12	45.66	15.00
151 TYR CD2	-39.60	-25.61	44.73	15.00
151 TYR CE2	-39.09	-26.64	43.95	15.00
151 TYR CZ	-38.02	-27.39	44.43	15.00
151 TYR OH	-37.46	-28.37	43.65	15.00
151 TYR C	-37.65	-22.71	45.98	15.00
151 TYR O	-38.13	-21.81	45.29	15.00
152 ASP N	-36.50	-23.30	45.71	15.00
152 ASP CA	-35.69	-22.88	44.58	15.00
152 ASP CB	-34.92	-21.62	44.94	15.00
152 ASP CG	-34.31	-20.95	43.75	15.00
152 ASP OD1	-33.30	-21.46	43.24	15.00
152 ASP OD2	-34.83	-19.90	43.34	15.00
152 ASP C	-34.74	-24.00	44.16	15.00
152 ASP O	-33.67	-24.16	44.74	15.00
153 GLU N	-35.12	-24.77	43.14	15.00
153 GLU CA	-34.30	-25.88	42.66	15.00
153 GLU CB	-34.99	-26.68	41.55	15.00
153 GLU CG	-35.86	-25.85	40.61	15.00
153 GLU CD	-35.20	-24.55	40.21	15.00
153 GLU OE1	-35.85	-23.49	40.40	15.00
153 GLU OE2	-34.05	-24.58	39.73	15.00
153 GLU C	-32.88	-25.53	42.24	15.00
153 GLU O	-32.12	-26.41	41.84	15.00
154 SER N	-32.56	-24.24	42.24	15.00
154 SER CA	-31.21	-23.81	41.87	15.00
154 SER CB	-31.23	-22.38	41.29	15.00
154 SER OG	-29.99	-22.04	40.68	15.00
154 SER C	-30.32	-23.92	43.11	15.00
154 SER O	-29.08	-23.86	43.03	15.00

TABLE IX

155 CYS N	-30.95	-24.11	44.26	15.00
155 CYS CA	-30.25	-24.27	45.52	15.00
155 CYS C	-29.46	-25.57	45.44	15.00
155 CYS O	-30.01	-26.60	45.04	15.00
155 CYS CB	-31.24	-24.29	46.67	15.00
155 CYS SG	-30.52	-24.05	48.32	15.00
156 ASN N	-28.18	-25.54	45.80	15.00
156 ASN CA	-27.32	-26.73	45.73	15.00
156 ASN CB	-25.94	-26.34	45.18	15.00
156 ASN CG	-25.00	-27.52	45.10	15.00
156 ASN OD1	-25.41	-28.68	45.25	15.00
156 ASN ND2	-23.72	-27.24	44.86	15.00
156 ASN C	-27.17	-27.54	47.03	15.00
156 ASN O	-26.43	-27.15	47.94	15.00
157 SER N	-27.79	-28.71	47.05	15.00
157 SER CA	-27.75	-29.59	48.22	15.00
157 SER CB	-28.54	-30.87	47.97	15.00
157 SER OG	-29.86	-30.55	47.53	15.00
157 SER C	-26.34	-29.93	48.65	15.00
157 SER O	-26.09	-30.17	49.82	15.00
158 ASP N	-25.42	-29.97	47.69	15.00
158 ASP CA	-24.04	-30.32	47.98	15.00
158 ASP CB	-23.39	-30.98	46.77	15.00
158 ASP CG	-24.30	-32.01	46.10	15.00
158 ASP OD1	-25.16	-31.59	45.30	15.00
158 ASP OD2	-24.16	-33.22	46.38	15.00
158 ASP C	-23.23	-29.12	48.47	15.00
158 ASP O	-22.07	-29.26	48.88	15.00
159 ASN N	-23.84	-27.94	48.44	15.00
159 ASN CA	-23.16	-26.74	48.87	15.00
159 ASN CB	-23.23	-25.65	47.79	15.00
159 ASN CG	-22.43	-24.40	48.16	15.00
159 ASN OD1	-21.20	-24.43	48.25	15.00
159 ASN ND2	-23.13	-23.30	48.37	15.00
159 ASN C	-23.72	-26.25	50.20	15.00
159 ASN O	-24.52	-25.31	50.24	15.00
160 LEU N	-23.32	-26.89	51.29	15.00
160 LEU CA	-23.78	-26.48	52.62	15.00
160 LEU CB	-23.80	-27.66	53.59	15.00
160 LEU CG	-24.71	-28.86	53.26	15.00
160 LEU CD1	-24.59	-29.92	54.34	15.00
160 LEU CD2	-26.15	-28.43	53.10	15.00

TABLE IX

160 LEU C	-22.89	-25.34	53.12	15.00
160 LEU O	-21.71	-25.55	53.43	15.00
161 ASN N	-23.46	-24.15	53.23	15.00
161 ASN CA	-22.70	-22.98	53.65	15.00
161 ASN CB	-22.49	-22.04	52.46	15.00
161 ASN CG	-23.80	-21.60	51.80	15.00
161 ASN OD1	-24.62	-20.89	52.40	15.00
161 ASN ND2	-24.02	-22.04	50.57	15.00
161 ASN C	-23.24	-22.19	54.82	15.00
161 ASN O	-22.50	-21.41	55.44	15.00
162 HIS N	-24.50	-22.38	55.16	15.00
162 HIS CA	-25.09	-21.63	56.25	15.00
162 HIS CB	-26.09	-20.60	55.70	15.00
162 HIS CG	-26.36	-19.45	56.63	15.00
162 HIS CD2	-27.52	-18.88	57.02	15.00
162 HIS ND1	-25.35	-18.74	57.27	15.00
162 HIS CE1	-25.89	-17.79	58.01	15.00
162 HIS NE2	-27.20	-17.85	57.88	15.00
162 HIS C	-25.73	-22.52	57.32	15.00
162 HIS O	-26.57	-23.36	57.03	15.00
163 ALA N	-25.29	-22.33	58.56	15.00
163 ALA CA	-25.82	-23.08	59.68	15.00
163 ALA CB	-24.83	-23.11	60.82	15.00
163 ALA C	-27.09	-22.35	60.10	15.00
163 ALA O	-27.17	-21.12	60.04	15.00
164 VAL N	-28.07	-23.10	60.57	15.00
164 VAL CA	-29.33	-22.51	60.95	15.00
164 VAL CB	-30.15	-22.28	59.67	15.00
164 VAL CG1	-30.99	-23.50	59.31	15.00
164 VAL CG2	-30.94	-21.02	59.76	15.00
164 VAL C	-30.02	-23.41	62.00	15.00
164 VAL O	-29.40	-24.32	62.53	15.00
165 LEU N	-31.28	-23.14	62.31	15.00
165 LEU CA	-31.97	-23.95	63.31	15.00
165 LEU CB	-31.89	-23.27	64.69	15.00
165 LEU CG	-32.54	-23.86	65.94	15.00
165 LEU CD1	-31.64	-24.89	66.56	15.00
165 LEU CD2	-32.80	-22.75	66.92	15.00
165 LEU C	-33.42	-24.23	62.94	15.00
165 LEU O	-34.17	-23.31	62.68	15.00
166 ALA N	-33.78	-25.51	62.87	15.00
166 ALA CA	-35.16	-25.91	62.55	15.00

TABLE IX

166 ALA CB	-35.20	-27.32	62.01	15.00
166 ALA C	-35.95	-25.80	63.83	15.00
166 ALA O	-35.67	-26.47	64.81	15.00
167 VAL N	-36.93	-24.91	63.82	15.00
167 VAL CA	-37.77	-24.62	64.97	15.00
167 VAL CB	-37.87	-23.05	65.10	15.00
167 VAL CG1	-39.11	-22.60	65.81	15.00
167 VAL CG2	-36.64	-22.53	65.82	15.00
167 VAL C	-39.14	-25.30	64.88	15.00
167 VAL O	-39.98	-25.17	65.77	15.00
168 GLY N	-39.36	-26.05	63.81	15.00
168 GLY CA	-40.63	-26.73	63.66	15.00
168 GLY C	-40.88	-27.11	62.23	15.00
168 GLY O	-39.96	-27.09	61.41	15.00
169 TYR N	-42.12	-27.45	61.92	15.00
169 TYR CA	-42.52	-27.84	60.57	15.00
169 TYR CB	-41.99	-29.24	60.21	15.00
169 TYR CG	-42.49	-30.37	61.09	15.00
169 TYR CD1	-43.82	-30.80	61.01	15.00
169 TYR CE1	-44.30	-31.81	61.82	15.00
169 TYR CD2	-41.66	-30.99	62.01	15.00
169 TYR CE2	-42.13	-32.01	62.83	15.00
169 TYR CZ	-43.46	-32.41	62.73	15.00
169 TYR OH	-43.96	-33.41	63.53	15.00
169 TYR C	-44.03	-27.76	60.48	15.00
169 TYR O	-44.71	-27.65	61.49	15.00
170 GLY N	-44.57	-27.80	59.26	15.00
170 GLY CA	-46.01	-27.72	59.11	15.00
170 GLY C	-46.48	-27.54	57.68	15.00
170 GLY O	-45.85	-28.04	56.75	15.00
171 ILE N	-47.55	-26.79	57.50	15.00
171 ILE CA	-48.11	-26.53	56.18	15.00
171 ILE CB	-49.30	-27.48	55.85	15.00
171 ILE CG2	-48.79	-28.88	55.55	15.00
171 ILE CG1	-50.29	-27.53	57.02	15.00
171 ILE CD1	-51.40	-26.48	56.97	15.00
171 ILE C	-48.63	-25.10	56.07	15.00
171 ILE O	-48.87	-24.44	57.08	15.00
172 GLN N	-48.75	-24.62	54.84	15.00
172 GLN CA	-49.27	-23.28	54.60	15.00
172 GLN CB	-48.22	-22.34	54.00	15.00
172 GLN CG	-48.63	-20.86	53.96	15.00

TABLE IX

172 GLN CD	-47.49	-19.92	54.36	15.00
172 GLN OE1	-47.54	-19.28	55.40	15.00
172 GLN NE2	-46.46	-19.83	53.52	15.00
172 GLN C	-50.46	-23.45	53.67	15.00
172 GLN O	-51.49	-24.00	54.07	15.00
173 LYS N	-50.30	-23.07	52.41	15.00
173 LYS CA	-51.38	-23.21	51.46	15.00
173 LYS CB	-51.36	-22.10	50.42	15.00
173 LYS CG	-51.38	-20.70	51.04	15.00
173 LYS CD	-52.68	-20.45	51.78	15.00
173 LYS CE	-53.81	-20.28	50.78	15.00
173 LYS NZ	-53.58	-19.10	49.88	15.00
173 LYS C	-51.15	-24.57	50.86	15.00
173 LYS O	-50.84	-24.70	49.68	15.00
174 GLY N	-51.19	-25.57	51.73	15.00
174 GLY CA	-50.98	-26.94	51.31	15.00
174 GLY C	-49.52	-27.32	51.13	15.00
174 GLY O	-49.20	-28.49	50.87	15.00
175 ASN N	-48.63	-26.35	51.27	15.00
175 ASN CA	-47.21	-26.62	51.11	15.00
175 ASN CB	-46.45	-25.42	50.56	15.00
175 ASN CG	-47.23	-24.69	49.49	15.00
175 ASN OD1	-48.07	-23.83	49.80	15.00
175 ASN ND2	-46.97	-25.03	48.24	15.00
175 ASN C	-46.60	-27.05	52.42	15.00
175 ASN O	-46.82	-26.41	53.46	15.00
176 LYS N	-45.87	-28.16	52.38	15.00
176 LYS CA	-45.20	-28.68	53.57	15.00
176 LYS CB	-44.69	-30.10	53.34	15.00
176 LYS CG	-45.74	-31.11	52.86	15.00
176 LYS CD	-46.88	-31.26	53.85	15.00
176 LYS CE	-47.97	-32.21	53.34	15.00
176 LYS NZ	-48.80	-31.66	52.19	15.00
176 LYS C	-44.05	-27.71	53.76	15.00
176 LYS O	-43.63	-27.08	52.80	15.00
177 HIS N	-43.57	-27.54	54.99	15.00
177 HIS CA	-42.45	-26.64	55.21	15.00
177 HIS CB	-42.88	-25.18	54.99	15.00
177 HIS CG	-43.82	-24.66	56.02	15.00
177 HIS CD2	-43.66	-24.45	57.35	15.00
177 HIS ND1	-45.10	-24.21	55.71	15.00
177 HIS CE1	-45.67	-23.75	56.81	15.00

TABLE IX

177	HIS	NE2	-44.82	-23.88	57.81	15.00
177	HIS	C	-41.71	-26.78	56.53	15.00
177	HIS	O	-42.23	-27.35	57.50	15.00
178	TRP	N	-40.49	-26.24	56.54	15.00
178	TRP	CA	-39.60	-26.23	57.69	15.00
178	TRP	CB	-38.19	-26.64	57.31	15.00
178	TRP	CG	-37.99	-28.06	56.96	15.00
178	TRP	CD2	-38.07	-29.18	57.84	15.00
178	TRP	CE2	-37.75	-30.33	57.09	15.00
178	TRP	CE3	-38.38	-29.33	59.20	15.00
178	TRP	CD1	-37.64	-28.56	55.74	15.00
178	TRP	NE1	-37.49	-29.92	55.81	15.00
178	TRP	CZ2	-37.73	-31.61	57.65	15.00
178	TRP	CZ3	-38.37	-30.60	59.76	15.00
178	TRP	CH2	-38.05	-31.72	58.98	15.00
178	TRP	C	-39.54	-24.81	58.28	15.00
178	TRP	O	-39.17	-23.88	57.58	15.00
179	ILE	N	-39.90	-24.63	59.55	15.00
179	ILE	CA	-39.78	-23.31	60.15	15.00
179	ILE	CB	-40.56	-23.19	61.47	15.00
179	ILE	CG2	-40.42	-21.80	62.04	15.00
179	ILE	CG1	-42.03	-23.55	61.26	15.00
179	ILE	CD1	-42.83	-23.54	62.53	15.00
179	ILE	C	-38.30	-23.20	60.48	15.00
179	ILE	O	-37.76	-24.02	61.22	15.00
180	ILE	N	-37.61	-22.23	59.88	15.00
180	ILE	CA	-36.18	-22.05	60.12	15.00
180	ILE	CB	-35.39	-22.09	58.78	15.00
180	ILE	CG2	-33.93	-21.75	58.98	15.00
180	ILE	CG1	-35.49	-23.48	58.17	15.00
180	ILE	CD1	-35.01	-24.57	59.10	15.00
180	ILE	C	-35.91	-20.73	60.84	15.00
180	ILE	O	-36.58	-19.74	60.60	15.00
181	LYS	N	-34.98	-20.76	61.79	15.00
181	LYS	CA	-34.59	-19.57	62.52	15.00
181	LYS	CB	-34.57	-19.82	64.03	15.00
181	LYS	CG	-34.13	-18.62	64.86	15.00
181	LYS	CD	-33.87	-19.01	66.30	15.00
181	LYS	CE	-33.59	-17.80	67.13	15.00
181	LYS	NZ	-33.32	-18.14	68.55	15.00
181	LYS	C	-33.19	-19.24	62.02	15.00
181	LYS	O	-32.27	-20.05	62.15	15.00

TABLE IX

182 ASN N	-33.04	-18.08	61.38	15.00
182 ASN CA	-31.75	-17.66	60.85	15.00
182 ASN CB	-31.93	-16.90	59.53	15.00
182 ASN CG	-30.71	-16.97	58.64	15.00
182 ASN OD1	-29.58	-17.07	59.11	15.00
182 ASN ND2	-30.94	-16.92	57.33	15.00
182 ASN C	-31.07	-16.80	61.91	15.00
182 ASN O	-31.52	-16.75	63.05	15.00
183 SER N	-29.98	-16.13	61.55	15.00
183 SER CA	-29.28	-15.27	62.49	15.00
183 SER CB	-28.10	-16.00	63.13	15.00
183 SER OG	-27.27	-16.59	62.15	15.00
183 SER C	-28.83	-13.99	61.81	15.00
183 SER O	-27.65	-13.66	61.82	15.00
184 TRP N	-29.77	-13.30	61.17	15.00
184 TRP CA	-29.49	-12.05	60.48	15.00
184 TRP CB	-29.61	-12.22	58.96	15.00
184 TRP CG	-28.60	-13.15	58.37	15.00
184 TRP CD2	-28.66	-13.78	57.08	15.00
184 TRP CE2	-27.49	-14.55	56.94	15.00
184 TRP CE3	-29.60	-13.77	56.03	15.00
184 TRP CD1	-27.43	-13.56	58.93	15.00
184 TRP NE1	-26.76	-14.39	58.08	15.00
184 TRP CZ2	-27.22	-15.31	55.78	15.00
184 TRP CZ3	-29.33	-14.53	54.89	15.00
184 TRP CH2	-28.15	-15.29	54.78	15.00
184 TRP C	-30.42	-10.97	61.00	15.00
184 TRP O	-30.89	-10.12	60.25	15.00
185 GLY N	-30.70	-11.03	62.30	15.00
185 GLY CA	-31.58	-10.07	62.94	15.00
185 GLY C	-33.02	-10.33	62.57	15.00
185 GLY O	-33.31	-11.05	61.62	15.00
186 GLU N	-33.94	-9.76	63.35	15.00
186 GLU CA	-35.36	-9.93	63.07	15.00
186 GLU CB	-36.22	-9.59	64.28	15.00
186 GLU CG	-36.03	-8.21	64.80	15.00
186 GLU CD	-36.84	-7.96	66.04	15.00
186 GLU OE1	-37.97	-8.49	66.13	15.00
186 GLU OE2	-36.35	-7.22	66.93	15.00
186 GLU C	-35.77	-9.12	61.86	15.00
186 GLU O	-36.90	-9.24	61.38	15.00
187 ASN N	-34.84	-8.32	61.36	15.00

TABLE IX

187	ASN	CA	-35.06	-7.47	60.20	15.00
187	ASN	CB	-34.05	-6.32	60.16	15.00
187	ASN	CG	-34.41	-5.27	59.11	15.00
187	ASN	OD1	-35.57	-5.16	58.70	15.00
187	ASN	ND2	-33.41	-4.49	58.69	15.00
187	ASN	C	-35.00	-8.26	58.91	15.00
187	ASN	O	-35.44	-7.79	57.86	15.00
188	TRP	N	-34.42	-9.46	58.97	15.00
188	TRP	CA	-34.30	-10.30	57.80	15.00
188	TRP	CB	-33.01	-11.12	57.86	15.00
188	TRP	CG	-32.84	-11.99	56.71	15.00
188	TRP	CD2	-33.26	-13.36	56.60	15.00
188	TRP	CE2	-32.96	-13.77	55.29	15.00
188	TRP	CE3	-33.86	-14.26	57.48	15.00
188	TRP	CD1	-32.32	-11.65	55.51	15.00
188	TRP	NE1	-32.39	-12.71	54.64	15.00
188	TRP	CZ2	-33.24	-15.07	54.83	15.00
188	TRP	CZ3	-34.15	-15.55	57.02	15.00
188	TRP	CH2	-33.84	-15.94	55.72	15.00
188	TRP	C	-35.50	-11.21	57.63	15.00
188	TRP	O	-36.05	-11.71	58.61	15.00
189	GLY	N	-35.92	-11.43	56.38	15.00
189	GLY	CA	-37.05	-12.30	56.10	15.00
189	GLY	C	-38.29	-11.99	56.92	15.00
189	GLY	O	-38.61	-10.83	57.20	15.00
190	ASN	N	-39.01	-13.04	57.31	15.00
190	ASN	CA	-40.21	-12.85	58.11	15.00
190	ASN	CB	-41.21	-13.98	57.90	15.00
190	ASN	CG	-42.58	-13.65	58.45	15.00
190	ASN	OD1	-42.74	-12.81	59.33	15.00
190	ASN	ND2	-43.60	-14.32	57.92	15.00
190	ASN	C	-39.77	-12.74	59.56	15.00
190	ASN	O	-39.83	-13.72	60.30	15.00
191	LYS	N	-39.24	-11.59	59.94	15.00
191	LYS	CA	-38.80	-11.39	61.31	15.00
191	LYS	CB	-40.02	-11.23	62.23	15.00
191	LYS	CG	-40.86	-10.00	61.87	15.00
191	LYS	CD	-42.05	-9.79	62.79	15.00
191	LYS	CE	-43.16	-10.79	62.51	15.00
191	LYS	NZ	-43.76	-10.63	61.14	15.00
191	LYS	C	-37.83	-12.46	61.81	15.00
191	LYS	O	-38.02	-13.08	62.86	15.00

TABLE IX

192	GLY	N	-36.77	-12.65	61.03	15.00
192	GLY	CA	-35.73	-13.62	61.37	15.00
192	GLY	C	-35.96	-15.05	60.91	15.00
192	GLY	O	-35.00	-15.80	60.72	15.00
193	TYR	N	-37.21	-15.43	60.71	15.00
193	TYR	CA	-37.53	-16.78	60.30	15.00
193	TYR	CB	-38.71	-17.32	61.10	15.00
193	TYR	CG	-38.44	-17.47	62.58	15.00
193	TYR	CD1	-38.48	-16.39	63.44	15.00
193	TYR	CE1	-38.21	-16.54	64.79	15.00
193	TYR	CD2	-38.12	-18.72	63.11	15.00
193	TYR	CE2	-37.84	-18.88	64.46	15.00
193	TYR	CZ	-37.89	-17.79	65.29	15.00
193	TYR	OH	-37.62	-17.95	66.63	15.00
193	TYR	C	-37.78	-16.91	58.82	15.00
193	TYR	O	-38.05	-15.93	58.14	15.00
194	ILE	N	-37.72	-18.14	58.33	15.00
194	ILE	CA	-37.95	-18.43	56.92	15.00
194	ILE	CB	-36.63	-18.38	56.07	15.00
194	ILE	CG2	-35.63	-19.42	56.55	15.00
194	ILE	CG1	-36.94	-18.61	54.60	15.00
194	ILE	CD1	-35.75	-18.49	53.69	15.00
194	ILE	C	-38.57	-19.82	56.79	15.00
194	ILE	O	-38.12	-20.78	57.42	15.00
195	LEU	N	-39.65	-19.91	56.03	15.00
195	LEU	CA	-40.34	-21.17	55.80	15.00
195	LEU	CB	-41.84	-20.95	55.67	15.00
195	LEU	CG	-42.72	-21.15	56.90	15.00
195	LEU	CD1	-42.11	-20.50	58.14	15.00
195	LEU	CD2	-44.10	-20.59	56.59	15.00
195	LEU	C	-39.79	-21.84	54.56	15.00
195	LEU	O	-40.17	-21.50	53.45	15.00
196	MET	N	-38.86	-22.76	54.75	15.00
196	MET	CA	-38.25	-23.48	53.63	15.00
196	MET	CB	-36.83	-23.91	53.98	15.00
196	MET	CG	-35.91	-22.73	54.21	15.00
196	MET	SD	-34.18	-23.17	54.37	15.00
196	MET	CE	-33.94	-24.05	52.84	15.00
196	MET	C	-39.13	-24.66	53.22	15.00
196	MET	O	-40.03	-25.06	53.97	15.00
197	ALA	N	-38.87	-25.24	52.05	15.00
197	ALA	CA	-39.67	-26.35	51.54	15.00

TABLE IX

197 ALA CB	-39.50	-26.46	50.04	15.00
197 ALA C	-39.40	-27.70	52.18	15.00
197 ALA O	-38.26	-28.15	52.25	15.00
198 ARG N	-40.47	-28.36	52.62	15.00
198 ARG CA	-40.35	-29.67	53.24	15.00
198 ARG CB	-41.11	-29.71	54.57	15.00
198 ARG CG	-41.08	-31.06	55.27	15.00
198 ARG CD	-41.32	-30.93	56.75	15.00
198 ARG NE	-42.61	-30.32	57.06	15.00
198 ARG CZ	-43.76	-30.98	57.14	15.00
198 ARG NH1	-43.79	-32.29	56.95	15.00
198 ARG NH2	-44.88	-30.33	57.45	15.00
198 ARG C	-40.82	-30.77	52.30	15.00
198 ARG O	-41.91	-30.70	51.73	15.00
199 ASN N	-39.97	-31.76	52.12	15.00
199 ASN CA	-40.27	-32.90	51.25	15.00
199 ASN CB	-41.62	-33.54	51.63	15.00
199 ASN CG	-41.53	-34.36	52.90	15.00
199 ASN OD1	-42.42	-34.31	53.75	15.00
199 ASN ND2	-40.45	-35.13	53.05	15.00
199 ASN C	-40.21	-32.59	49.76	15.00
199 ASN O	-40.78	-33.32	48.94	15.00
200 LYS N	-39.48	-31.54	49.41	15.00
200 LYS CA	-39.31	-31.17	48.01	15.00
200 LYS CB	-39.31	-29.66	47.81	15.00
200 LYS CG	-40.70	-29.02	47.77	15.00
200 LYS CD	-41.37	-29.23	46.42	15.00
200 LYS CE	-42.76	-28.59	46.37	15.00
200 LYS NZ	-42.73	-27.14	46.73	15.00
200 LYS C	-37.98	-31.78	47.60	15.00
200 LYS O	-37.11	-31.09	47.06	15.00
201 ASN N	-37.81	-33.06	47.93	15.00
201 ASN CA	-36.58	-33.78	47.62	15.00
201 ASN CB	-36.41	-33.93	46.11	15.00
201 ASN CG	-37.15	-35.13	45.56	15.00
201 ASN OD1	-36.68	-35.78	44.63	15.00
201 ASN ND2	-38.32	-35.42	46.13	15.00
201 ASN C	-35.33	-33.22	48.27	15.00
201 ASN O	-34.27	-33.16	47.66	15.00
202 ASN N	-35.46	-32.84	49.54	15.00
202 ASN CA	-34.37	-32.30	50.35	15.00
202 ASN CB	-33.25	-33.34	50.49	15.00

TABLE IX

202 ASN CG	-32.20	-32.93	51.48	15.00
202 ASN OD1	-32.51	-32.44	52.56	15.00
202 ASN ND2	-30.94	-33.14	51.13	15.00
202 ASN C	-33.83	-30.96	49.85	15.00
202 ASN O	-32.62	-30.77	49.68	15.00
203 ALA N	-34.73	-30.00	49.69	15.00
203 ALA H	-35.60	-30.20	50.07	15.00
203 ALA CA	-34.39	-28.68	49.18	15.00
203 ALA CB	-35.57	-27.74	49.24	15.00
203 ALA C	-33.27	-28.06	50.04	15.00
203 ALA O	-33.33	-28.03	51.26	15.00
204 CYS N	-32.23	-27.56	49.35	15.00
204 CYS CA	-31.11	-26.89	50.02	15.00
204 CYS C	-30.29	-27.71	51.00	15.00
204 CYS O	-29.50	-27.14	51.76	15.00
204 CYS CB	-31.58	-25.60	50.69	15.00
204 CYS SG	-32.12	-24.29	49.55	15.00
205 GLY N	-30.43	-29.03	50.98	15.00
205 GLY CA	-29.68	-29.88	51.90	15.00
205 GLY C	-30.10	-29.71	53.35	15.00
205 GLY O	-29.31	-29.92	54.27	15.00
206 ILE N	-31.37	-29.38	53.54	15.00
206 ILE CA	-31.95	-29.16	54.85	15.00
206 ILE CB	-33.46	-28.92	54.73	15.00
206 ILE CG2	-34.13	-30.13	54.12	15.00
206 ILE CG1	-34.06	-28.55	56.10	15.00
206 ILE CD1	-33.76	-27.15	56.54	15.00
206 ILE C	-31.71	-30.29	55.85	15.00
206 ILE O	-31.47	-30.04	57.03	15.00
207 ALA N	-31.79	-31.54	55.38	15.00
207 ALA CA	-31.58	-32.69	56.25	15.00
207 ALA CB	-32.72	-33.68	56.08	15.00
207 ALA C	-30.25	-33.35	55.94	15.00
207 ALA O	-30.15	-34.57	55.95	15.00
208 ASN N	-29.24	-32.54	55.67	15.00
208 ASN CA	-27.91	-33.04	55.33	15.00
208 ASN CB	-27.41	-32.42	54.03	15.00
208 ASN CG	-27.70	-33.30	52.84	15.00
208 ASN OD1	-28.85	-33.50	52.47	15.00
208 ASN ND2	-26.65	-33.86	52.26	15.00
208 ASN C	-26.85	-32.89	56.41	15.00
208 ASN O	-25.80	-33.53	56.35	15.00

TABLE IX

209 LEU N	-27.08	-32.00	57.36	15.00
209 LEU CA	-26.10	-31.82	58.42	15.00
209 LEU CB	-25.07	-30.77	58.03	15.00
209 LEU CG	-23.69	-31.04	58.63	15.00
209 LEU CD1	-23.08	-32.21	57.88	15.00
209 LEU CD2	-22.82	-29.81	58.52	15.00
209 LEU C	-26.77	-31.46	59.73	15.00
209 LEU O	-26.25	-30.66	60.51	15.00
210 ALA N	-27.91	-32.08	59.97	15.00
210 ALA H	-27.81	-31.90	59.38	15.00
210 ALA CA	-28.67	-31.80	61.19	15.00
210 ALA CB	-29.27	-31.17	61.33	15.00
210 ALA C	-28.06	-32.58	62.37	15.00
210 ALA O	-27.58	-33.69	62.23	15.00
211 SER N	-28.08	-31.93	63.53	15.00
211 SER CA	-27.60	-32.53	64.76	15.00
211 SER CB	-26.07	-32.52	64.86	15.00
211 SER OG	-25.53	-31.21	64.89	15.00
211 SER C	-28.25	-31.80	65.93	15.00
211 SER O	-28.68	-30.65	65.78	15.00
212 PHE N	-28.44	-32.51	67.03	15.00
212 PHE CA	-29.04	-31.94	68.23	15.00
212 PHE CB	-30.53	-32.29	68.37	15.00
212 PHE CG	-30.81	-33.77	68.41	15.00
212 PHE CD1	-31.04	-34.48	67.24	15.00
212 PHE CD2	-30.85	-34.45	69.62	15.00
212 PHE CE1	-31.30	-35.84	67.27	15.00
212 PHE CE2	-31.11	-35.82	69.67	15.00
212 PHE CZ	-31.33	-36.51	68.48	15.00
212 PHE C	-28.22	-32.41	69.43	15.00
212 PHE O	-27.54	-33.43	69.36	15.00
213 PRO N	-28.19	-31.63	70.50	15.00
213 PRO CD	-28.56	-30.21	70.63	15.00
213 PRO CA	-27.41	-32.07	71.65	15.00
213 PRO CB	-26.98	-30.75	72.28	15.00
213 PRO CG	-28.17	-29.90	72.06	15.00
213 PRO C	-28.21	-32.91	72.65	15.00
213 PRO O	-29.45	-32.81	72.72	15.00
214 LYS N	-27.50	-33.77	73.38	15.00
214 LYS CA	-28.12	-34.59	74.42	15.00
214 LYS CB	-27.50	-35.97	74.52	15.00
214 LYS CG	-28.01	-37.00	73.53	15.00

TABLE IX

214 LYS CD	-27.20	-38.28	73.68	15.00
214 LYS CE	-27.79	-39.45	72.93	15.00
214 LYS NZ	-27.00	-40.67	73.21	15.00
214 LYS C	-27.86	-33.84	75.70	15.00
214 LYS O	-26.73	-33.45	75.98	15.00
215 MET N	-28.90	-33.63	76.49	15.00
215 MET CA	-28.73	-32.91	77.73	15.00
215 MET CB	-29.47	-31.58	77.67	15.00
215 MET CG	-28.62	-30.45	78.17	15.00
215 MET SD	-29.49	-28.92	78.17	15.00
215 MET CE	-30.02	-28.81	79.89	15.00
215 MET C	-29.15	-33.74	78.95	15.00
215 MET OT1	-30.12	-34.53	78.84	15.00
215 MET OT2	-28.49	-33.59	80.01	15.00
216 HOH OH2	-28.59	-18.05	86.43	15.00
217 HOH OH2	-24.24	-33.32	82.08	15.00
218 HOH OH2	-30.97	-16.19	65.69	15.00
219 HOH OH2	-30.10	-20.71	63.47	15.00
220 HOH OH2	-13.66	-11.12	63.10	15.00
221 HOH OH2	-9.67	-9.48	64.25	15.00
222 HOH OH2	-34.55	-23.08	70.24	15.00
223 HOH OH2	-14.15	-32.13	69.51	15.00
224 HOH OH2	-11.90	-8.52	62.51	15.00
225 HOH OH2	-24.25	-30.66	62.17	15.00
226 HOH OH2	-10.58	-2.52	79.25	15.00
227 HOH OH2	-14.05	-21.32	67.22	15.00
228 HOH OH2	-44.68	-30.63	50.04	15.00
229 HOH OH2	-45.38	-36.05	56.05	15.00
230 HOH OH2	-39.65	-13.31	65.32	15.00
231 HOH OH2	-35.12	-36.60	49.29	15.00
232 HOH OH2	-17.36	-34.13	65.07	15.00
233 HOH OH2	-30.35	-19.53	65.73	15.00
234 HOH OH2	-27.89	-19.53	62.51	15.00
235 HOH OH2	-21.85	-29.55	62.34	15.00
236 HOH OH2	-30.14	3.73	67.17	15.00
237 HOH OH2	-40.50	-29.62	80.16	15.00
238 HOH OH2	-27.85	-23.15	86.33	15.00
239 HOH OH2	-38.29	-13.95	44.87	15.00
240 HOH OH2	-36.58	-24.59	50.05	15.00
241 HOH OH2	-46.68	-34.18	57.37	15.00
242 HOH OH2	-26.77	-6.82	59.79	15.00
243 HOH OH2	-43.58	-17.40	60.45	15.00

TABLE IX

244	HOH	OH2	-23.22	-6.13	61.38	15.00
245	HOH	OH2	-33.13	-28.30	71.09	15.00
246	HOH	OH2	-46.57	-25.22	78.97	15.00
247	HOH	OH2	-14.51	-7.76	88.79	15.00
248	HOH	OH2	-3.26	-20.73	74.76	15.00
249	HOH	OH2	0.44	-15.91	75.31	15.00
250	HOH	OH2	-19.71	-34.82	58.63	15.00
251	HOH	OH2	-34.91	-11.28	53.79	15.00
252	HOH	OH2	-32.46	-28.27	46.13	15.00
253	HOH	OH2	-38.20	-15.68	37.93	15.00
254	HOH	OH2	-41.44	-34.28	56.30	15.00
255	HOH	OH2	-46.93	-13.62	73.92	15.00
256	HOH	OH2	-32.58	-13.60	60.68	15.00
257	HOH	OH2	-35.46	-6.38	55.50	15.00
258	HOH	OH2	-24.79	-7.91	66.67	15.00
259	HOH	OH2	-32.06	-6.48	63.77	15.00
260	HOH	OH2	-17.19	-5.30	66.67	15.00
261	HOH	OH2	-33.68	-20.47	70.17	15.00
262	HOH	OH2	-13.42	-23.06	78.55	15.00
263	HOH	OH2	-8.54	-20.70	73.58	15.00
264	HOH	OH2	-8.22	-29.32	76.42	15.00
265	HOH	OH2	-25.08	-33.76	60.84	15.00
266	HOH	OH2	-23.92	-37.99	66.66	15.00
267	HOH	OH2	-14.04	-33.08	66.81	15.00
268	HOH	OH2	-12.79	-27.03	71.88	15.00
269	HOH	OH2	-18.55	-42.19	77.34	15.00
270	HOH	OH2	-22.19	-37.43	71.34	15.00
271	HOH	OH2	-3.79	-11.43	71.45	15.00
272	HOH	OH2	-10.91	-19.86	67.02	15.00
273	HOH	OH2	-30.22	-20.12	49.07	15.00
274	HOH	OH2	-25.88	-18.93	42.52	15.00
275	HOH	OH2	-36.21	-36.23	51.70	15.00
276	HOH	OH2	-20.20	-20.55	47.99	15.00
277	HOH	OH2	-38.35	-31.19	41.44	15.00
278	HOH	OH2	-37.29	-30.41	51.12	15.00

TABLE X

Table of the orthogonal three dimensional coordinates in Ångstroms and B factors ($Å^2$) for the cathepsin K complex with inhibitor 1-N-(N-imidazole acetyl-leucinyl)-amino-3-N-(4-phenoxy-phenyl-sulfonyl)-amino-propan-2-one.

Residue	Atom	X	Y	Z	B
1	ALA CB	-8.26	15.35	87.29	15.00
1	ALA C	-6.43	14.73	88.90	15.00
1	ALA O	-6.17	15.27	89.97	15.00
1	ALA N	-8.92	14.74	89.58	15.00
1	ALA CA	-7.91	14.50	88.49	15.00
2	PRO N	-5.47	14.25	88.09	15.00
2	PRO CD	-5.62	13.29	86.98	15.00
2	PRO CA	-4.05	14.45	88.44	15.00
2	PRO CB	-3.32	13.49	87.50	15.00
2	PRO CG	-4.27	13.38	86.30	15.00
2	PRO C	-3.55	15.87	88.27	15.00
2	PRO O	-4.33	16.79	88.21	15.00
3	ASP N	-2.23	16.02	88.20	15.00
3	ASP CA	-1.59	17.30	88.03	15.00
3	ASP CB	-0.07	17.14	88.15	15.00
3	ASP CG	0.45	17.62	89.50	15.00
3	ASP OD1	-0.04	17.07	90.52	15.00
3	ASP OD2	1.29	18.57	89.55	15.00
3	ASP C	-1.90	18.00	86.73	15.00
3	ASP O	-1.71	17.44	85.64	15.00
4	SER N	-2.32	19.26	86.85	15.00
4	SER CA	-2.67	20.16	85.75	15.00
4	SER CB	-3.63	19.49	84.75	15.00
4	SER OG	-4.80	19.03	85.40	15.00
4	SER C	-3.32	21.45	86.30	15.00
4	SER O	-3.83	21.46	87.42	15.00
5	VAL N	-3.30	22.53	85.53	15.00
5	VAL CA	-3.93	23.80	85.94	15.00
5	VAL CB	-3.00	24.65	86.90	15.00
5	VAL CG1	-1.73	25.13	86.17	15.00
5	VAL CG2	-3.76	25.89	87.45	15.00
5	VAL C	-4.21	24.62	84.69	15.00
5	VAL O	-3.43	24.58	83.75	15.00

TABLE X

6	ASP	N	-5.38	25.23	84.60	15.00
6	ASP	CA	-5.68	26.09	83.46	15.00
6	ASP	CB	-6.83	25.51	82.64	15.00
6	ASP	CG	-7.00	26.20	81.28	15.00
6	ASP	OD1	-6.01	26.77	80.80	15.00
6	ASP	OD2	-8.12	26.17	80.72	15.00
6	ASP	C	-6.08	27.42	84.03	15.00
6	ASP	O	-7.06	27.49	84.72	15.00
7	TYR	N	-5.27	28.45	83.88	15.00
7	TYR	CA	-5.62	29.77	84.41	15.00
7	TYR	CB	-4.36	30.64	84.56	15.00
7	TYR	CG	-3.46	30.18	85.71	15.00
7	TYR	CD1	-3.91	30.31	87.05	15.00
7	TYR	CE1	-3.20	29.78	88.07	15.00
7	TYR	CD2	-2.23	29.50	85.46	15.00
7	TYR	CE2	-1.52	28.98	86.45	15.00
7	TYR	CZ	-2.00	29.10	87.79	15.00
7	TYR	OH	-1.35	28.46	88.84	15.00
7	TYR	C	-6.71	30.50	83.66	15.00
7	TYR	O	-7.24	31.48	84.14	15.00
8	ARG	N	-7.05	29.98	82.49	15.00
8	ARG	CA	-8.10	30.59	81.68	15.00
8	ARG	CB	-8.09	30.02	80.26	15.00
8	ARG	CG	-6.79	30.28	79.56	15.00
8	ARG	CD	-6.68	29.59	78.25	15.00
8	ARG	NE	-6.70	28.13	78.38	15.00
8	ARG	CZ	-6.78	27.29	77.36	15.00
8	ARG	NH1	-6.85	27.73	76.13	15.00
8	ARG	NH2	-6.72	25.99	77.58	15.00
8	ARG	C	-9.44	30.40	82.35	15.00
8	ARG	O	-10.24	31.34	82.45	15.00
9	LYS	N	-9.68	29.21	82.87	15.00
9	LYS	CA	-10.94	28.95	83.54	15.00
9	LYS	CB	-11.17	27.45	83.73	15.00
9	LYS	CG	-11.06	26.59	82.48	15.00
9	LYS	CD	-11.19	25.12	82.85	15.00
9	LYS	CE	-11.10	24.18	81.67	15.00
9	LYS	NZ	-11.53	22.81	82.08	15.00
9	LYS	C	-10.96	29.61	84.91	15.00
9	LYS	O	-12.02	29.58	85.59	15.00
10	LYS	N	-9.86	30.26	85.31	15.00
10	LYS	CA	-9.84	30.86	86.64	15.00

TABLE X

10	LYS	CB	-8.57	30.42	87.38	15.00
10	LYS	CG	-8.45	28.89	87.51	15.00
10	LYS	CD	-7.03	28.46	87.81	15.00
10	LYS	CE	-6.43	29.14	89.04	15.00
10	LYS	NZ	-7.24	28.91	90.30	15.00
10	LYS	C	-9.98	32.40	86.61	15.00
10	LYS	O	-10.16	33.04	87.64	15.00
11	GLY	N	-9.85	32.98	85.41	15.00
11	GLY	CA	-9.94	34.41	85.22	15.00
11	GLY	C	-8.63	35.17	85.27	15.00
11	GLY	O	-8.61	36.39	85.26	15.00
12	TYR	N	-7.54	34.42	85.20	15.00
12	TYR	CA	-6.21	34.98	85.26	15.00
12	TYR	CB	-5.24	33.95	85.84	15.00
12	TYR	CG	-5.32	33.72	87.35	15.00
12	TYR	CD1	-6.52	33.50	87.99	15.00
12	TYR	CE1	-6.58	33.26	89.37	15.00
12	TYR	CD2	-4.18	33.66	88.13	15.00
12	TYR	CE2	-4.23	33.42	89.47	15.00
12	TYR	CZ	-5.42	33.23	90.06	15.00
12	TYR	OH	-5.43	33.02	91.43	15.00
12	TYR	C	-5.68	35.43	83.90	15.00
12	TYR	O	-4.68	36.17	83.83	15.00
13	VAL	N	-6.34	35.06	82.81	15.00
13	VAL	CA	-5.82	35.45	81.50	15.00
13	VAL	CB	-5.54	34.18	80.66	15.00
13	VAL	CG1	-4.93	34.52	79.31	15.00
13	VAL	CG2	-4.58	33.24	81.42	15.00
13	VAL	C	-6.76	36.37	80.72	15.00
13	VAL	O	-7.95	36.17	80.78	15.00
14	THR	N	-6.24	37.41	80.08	15.00
14	THR	CA	-7.06	38.29	79.27	15.00
14	THR	CB	-6.41	39.67	79.12	15.00
14	THR	OG1	-5.06	39.53	78.69	15.00
14	THR	CG2	-6.48	40.43	80.39	15.00
14	THR	C	-7.20	37.68	77.89	15.00
14	THR	O	-6.41	36.81	77.48	15.00
15	PRO	N	-8.14	38.18	77.09	15.00
15	PRO	CD	-9.11	39.26	77.34	15.00
15	PRO	CA	-8.33	37.64	75.75	15.00
15	PRO	CB	-9.51	38.47	75.23	15.00
15	PRO	CG	-9.35	39.77	75.97	15.00

TABLE X

15	PRO	C	-7.09	37.85	74.89	15.00
15	PRO	O	-6.26	38.73	75.17	15.00
16	VAL	N	-6.96	37.00	73.87	15.00
16	VAL	CA	-5.81	37.05	73.00	15.00
16	VAL	CB	-5.74	35.80	72.11	15.00
16	VAL	CG1	-4.42	35.77	71.35	15.00
16	VAL	CG2	-5.84	34.56	72.97	15.00
16	VAL	C	-5.76	38.30	72.12	15.00
16	VAL	O	-6.70	38.61	71.37	15.00
17	LYS	N	-4.58	38.91	72.12	15.00
17	LYS	CA	-4.36	40.08	71.32	15.00
17	LYS	CB	-3.75	41.20	72.15	15.00
17	LYS	CG	-4.73	42.01	72.95	15.00
17	LYS	CD	-5.27	41.23	74.12	15.00
17	LYS	CE	-5.71	42.11	75.23	15.00
17	LYS	NZ	-5.93	41.40	76.53	15.00
17	LYS	C	-3.45	39.72	70.16	15.00
17	LYS	O	-2.83	38.63	70.16	15.00
18	ASN	N	-3.32	40.68	69.24	15.00
18	ASN	CA	-2.51	40.54	68.03	15.00
18	ASN	CB	-3.37	40.84	66.84	15.00
18	ASN	CG	-2.76	40.33	65.56	15.00
18	ASN	OD1	-1.57	40.56	65.29	15.00
18	ASN	ND2	-3.55	39.60	64.78	15.00
18	ASN	C	-1.33	41.51	68.00	15.00
18	ASN	O	-1.50	42.73	67.86	15.00
19	GLN	N	-0.15	40.93	68.03	15.00
19	GLN	CA	1.12	41.67	68.01	15.00
19	GLN	CB	2.23	40.66	67.93	15.00
19	GLN	CG	3.64	41.21	67.96	15.00
19	GLN	CD	4.65	40.13	68.03	15.00
19	GLN	OE1	4.35	39.00	68.42	15.00
19	GLN	NE2	5.86	40.47	67.64	15.00
19	GLN	C	1.22	42.69	66.88	15.00
19	GLN	O	1.75	43.75	67.04	15.00
20	GLY	N	0.66	42.38	65.74	15.00
20	GLY	CA	0.66	43.27	64.59	15.00
20	GLY	C	1.84	42.90	63.73	15.00
20	GLY	O	1.98	41.74	63.33	15.00
21	GLN	N	2.67	43.89	63.43	15.00
21	GLN	CA	3.88	43.70	62.61	15.00
21	GLN	CB	3.90	44.62	61.39	15.00

TABLE X

21	GLN	CG	2.90	44.23	60.27	15.00
21	GLN	CD	3.33	43.03	59.44	15.00
21	GLN	OE1	4.25	43.10	58.59	15.00
21	GLN	NE2	2.58	41.95	59.58	15.00
21	GLN	C	5.05	44.09	63.52	15.00
21	GLN	O	6.20	43.88	63.19	15.00
22	CYS	N	4.74	44.77	64.60	15.00
22	CYS	CA	5.74	45.22	65.53	15.00
22	CYS	C	6.26	44.01	66.35	15.00
22	CYS	O	5.48	43.07	66.60	15.00
22	CYS	CB	5.08	46.25	66.43	15.00
22	CYS	SG	6.07	46.62	67.91	15.00
23	GLY	N	7.57	43.99	66.68	15.00
23	GLY	CA	8.16	42.91	67.47	15.00
23	GLY	C	8.07	43.16	68.96	15.00
23	GLY	O	9.08	43.15	69.68	15.00
24	SER	N	6.82	43.29	69.42	15.00
24	SER	CA	6.47	43.55	70.79	15.00
24	SER	CB	5.45	44.66	70.86	15.00
24	SER	OG	4.31	44.30	70.15	15.00
24	SER	C	5.97	42.28	71.46	15.00
24	SER	O	5.26	42.34	72.45	15.00
25	CYS	N	6.43	41.13	70.98	15.00
25	CYS	CA	6.06	39.87	71.53	15.00
25	CYS	CB	6.61	38.78	70.65	15.00
25	CYS	SG	8.41	38.83	70.46	15.00
25	CYS	C	6.49	39.79	73.01	15.00
25	CYS	O	5.74	39.28	73.84	15.00
25	INH	C1	3.24	39.22	63.40	15.00
25	INH	C2	2.86	38.72	62.13	15.00
25	INH	C3	1.57	38.27	61.89	15.00
25	INH	C4	0.62	38.31	62.90	15.00
25	INH	C5	0.94	38.79	64.16	15.00
25	INH	C6	2.25	39.24	64.42	15.00
25	INH	O7	4.57	39.75	63.63	15.00
25	INH	C8	5.72	39.02	63.91	15.00
25	INH	C9	5.62	38.42	65.17	15.00
25	INH	C10	6.58	37.50	65.60	15.00
25	INH	C11	7.65	37.17	64.78	15.00
25	INH	C12	7.79	37.78	63.51	15.00
25	INH	C13	6.82	38.71	63.08	15.00
25	INH	S14	8.67	35.93	65.55	15.00

TABLE X

25 INH O15	7.93	34.70	65.54	15.00
25 INH O16	9.92	35.97	64.82	15.00
25 INH N17	8.95	36.39	67.18	15.00
25 INH C18	9.50	37.70	67.57	15.00
25 INH C19	9.05	38.78	68.64	15.00
25 INH O20	8.53	39.68	67.70	15.00
25 INH C21	10.52	39.34	69.16	15.00
25 INH N22	11.16	38.50	70.20	15.00
25 INH C23	12.14	38.91	71.00	15.00
25 INH O24	12.59	40.07	70.97	15.00
25 INH C25	12.61	37.92	72.07	15.00
25 INH C26	11.69	38.19	73.25	15.00
25 INH C27	11.80	37.33	74.48	15.00
25 INH C28	12.06	35.90	74.03	15.00
25 INH C29	12.95	37.84	75.32	15.00
25 INH N30	14.03	38.09	72.47	15.00
25 INH C31	14.92	37.10	72.44	15.00
25 INH O32	14.63	35.96	72.06	15.00
25 INH C33	16.36	37.38	72.94	15.00
25 INH C34	17.21	36.17	73.26	15.00
25 INH C35	17.54	35.58	74.44	15.00
25 INH N36	18.35	34.51	74.16	15.00
25 INH C37	18.52	34.43	72.85	15.00
25 INH N38	17.85	35.42	72.28	15.00
26 TRP N	7.57	40.50	73.34	15.00
26 TRP CA	8.08	40.58	74.69	15.00
26 TRP CB	9.55	41.06	74.66	15.00
26 TRP CG	9.72	42.45	74.12	15.00
26 TRP CD2	9.74	43.67	74.85	15.00
26 TRP CE2	9.80	44.74	73.89	15.00
26 TRP CE3	9.72	43.99	76.22	15.00
26 TRP CD1	9.78	42.79	72.83	15.00
26 TRP NE1	9.82	44.15	72.67	15.00
26 TRP CZ2	9.83	46.10	74.25	15.00
26 TRP CZ3	9.75	45.31	76.58	15.00
26 TRP CH2	9.81	46.37	75.59	15.00
26 TRP C	7.21	41.51	75.60	15.00
26 TRP O	7.08	41.27	76.81	15.00
27 ALA N	6.58	42.54	75.01	15.00
27 ALA CA	5.77	43.48	75.79	15.00
27 ALA CB	5.51	44.71	74.96	15.00
27 ALA C	4.47	42.75	76.05	15.00

TABLE X

27	ALA	O	3.88	42.85	77.12	15.00
28	PHE	N	4.07	41.90	75.13	15.00
28	PHE	CA	2.81	41.20	75.33	15.00
28	PHE	CB	2.29	40.66	73.99	15.00
28	PHE	CG	1.55	41.68	73.15	15.00
28	PHE	CD1	2.23	42.39	72.20	15.00
28	PHE	CD2	0.19	41.92	73.31	15.00
28	PHE	CE1	1.57	43.34	71.43	15.00
28	PHE	CE2	-0.46	42.87	72.55	15.00
28	PHE	CZ	0.23	43.58	71.61	15.00
28	PHE	C	2.87	40.12	76.46	15.00
28	PHE	O	1.92	39.99	77.26	15.00
29	SER	N	3.97	39.39	76.54	15.00
29	SER	CA	4.16	38.37	77.55	15.00
29	SER	CB	5.40	37.55	77.18	15.00
29	SER	OG	5.72	36.66	78.21	15.00
29	SER	C	4.28	38.96	78.94	15.00
29	SER	O	3.68	38.47	79.91	15.00
30	SER	N	5.04	40.05	79.02	15.00
30	SER	CA	5.25	40.76	80.28	15.00
30	SER	CB	6.13	41.95	80.06	15.00
30	SER	OG	7.38	41.52	79.59	15.00
30	SER	C	3.96	41.22	80.96	15.00
30	SER	O	3.72	40.99	82.17	15.00
31	VAL	N	3.13	41.85	80.14	15.00
31	VAL	CA	1.83	42.35	80.51	15.00
31	VAL	CB	1.33	43.26	79.35	15.00
31	VAL	CG1	-0.15	43.27	79.23	15.00
31	VAL	CG2	1.86	44.66	79.52	15.00
31	VAL	C	0.91	41.16	80.90	15.00
31	VAL	O	0.02	41.32	81.77	15.00
32	GLY	N	1.16	39.98	80.31	15.00
32	GLY	CA	0.35	38.81	80.61	15.00
32	GLY	C	0.70	38.25	81.97	15.00
32	GLY	O	-0.17	37.79	82.70	15.00
33	ALA	N	1.98	38.30	82.34	15.00
33	ALA	CA	2.47	37.84	83.63	15.00
33	ALA	CB	3.98	37.93	83.67	15.00
33	ALA	C	1.84	38.86	84.60	15.00
33	ALA	O	1.09	38.48	85.52	15.00
34	LEU	N	2.09	40.15	84.37	15.00
34	LEU	CA	1.54	41.22	85.20	15.00

TABLE X

34	LEU	CB	1.88	42.56	84.56	15.00
34	LEU	CG	3.30	43.17	84.66	15.00
34	LEU	CD1	3.26	44.56	84.13	15.00
34	LEU	CD2	3.76	43.24	86.11	15.00
34	LEU	C	0.02	41.13	85.45	15.00
34	LEU	O	-0.47	41.28	86.60	15.00
35	GLU	N	-0.70	40.80	84.39	15.00
35	GLU	CA	-2.16	40.62	84.49	15.00
35	GLU	CB	-2.77	40.37	83.11	15.00
35	GLU	CG	-2.92	41.61	82.27	15.00
35	GLU	CD	-3.06	41.33	80.78	15.00
35	GLU	OE1	-2.97	40.14	80.38	15.00
35	GLU	OE2	-3.31	42.29	80.00	15.00
35	GLU	C	-2.60	39.51	85.47	15.00
35	GLU	O	-3.31	39.78	86.45	15.00
36	GLY	N	-2.11	38.29	85.24	15.00
36	GLY	CA	-2.42	37.14	86.06	15.00
36	GLY	C	-2.20	37.38	87.56	15.00
36	GLY	O	-2.96	36.89	88.40	15.00
37	GLN	N	-1.13	38.09	87.89	15.00
37	GLN	CA	-0.78	38.39	89.27	15.00
37	GLN	CB	0.64	38.96	89.35	15.00
37	GLN	CG	1.72	37.92	89.12	15.00
37	GLN	CD	1.50	36.73	90.00	15.00
37	GLN	OE1	1.69	36.81	91.20	15.00
37	GLN	NE2	1.12	35.61	89.42	15.00
37	GLN	C	-1.78	39.38	89.83	15.00
37	GLN	O	-2.30	39.19	90.94	15.00
38	LEU	N	-2.10	40.38	89.02	15.00
38	LEU	CA	-3.04	41.41	89.38	15.00
38	LEU	CB	-3.28	42.29	88.15	15.00
38	LEU	CG	-4.10	43.56	88.33	15.00
38	LEU	CD1	-3.72	44.25	89.66	15.00
38	LEU	CD2	-3.95	44.48	87.16	15.00
38	LEU	C	-4.32	40.75	89.82	15.00
38	LEU	O	-4.90	41.05	90.86	15.00
39	LYS	N	-4.75	39.78	89.04	15.00
39	LYS	CA	-5.95	39.07	89.36	15.00
39	LYS	CB	-6.29	38.15	88.20	15.00
39	LYS	CG	-7.34	37.13	88.56	15.00
39	LYS	CD	-8.65	37.80	88.80	15.00
39	LYS	CE	-9.71	36.74	88.86	15.00

TABLE X

39	LYS	NZ	-10.82	37.33	89.61	15.00
39	LYS	C	-5.78	38.28	90.67	15.00
39	LYS	O	-6.62	38.34	91.53	15.00
40	LYS	N	-4.66	37.59	90.83	15.00
40	LYS	CA	-4.40	36.83	92.03	15.00
40	LYS	CB	-3.01	36.20	91.96	15.00
40	LYS	CG	-2.68	35.31	93.16	15.00
40	LYS	CD	-1.38	34.53	93.00	15.00
40	LYS	CE	-1.10	33.63	94.23	15.00
40	LYS	NZ	-0.27	32.41	93.89	15.00
40	LYS	C	-4.50	37.71	93.27	15.00
40	LYS	O	-5.26	37.42	94.20	15.00
41	LYS	N	-3.86	38.87	93.18	15.00
41	LYS	CA	-3.77	39.84	94.28	15.00
41	LYS	CB	-2.31	40.32	94.41	15.00
41	LYS	CG	-1.28	39.21	94.20	15.00
41	LYS	CD	-0.04	39.35	95.07	15.00
41	LYS	CE	0.68	38.01	95.15	15.00
41	LYS	NZ	-0.14	36.86	95.66	15.00
41	LYS	C	-4.64	41.07	94.09	15.00
41	LYS	O	-4.15	42.18	94.26	15.00
42	THR	N	-5.91	40.88	93.78	15.00
42	THR	CA	-6.80	42.01	93.60	15.00
42	THR	CB	-6.50	42.75	92.28	15.00
42	THR	OG1	-5.17	43.26	92.28	15.00
42	THR	CG2	-7.48	43.85	92.07	15.00
42	THR	C	-8.22	41.47	93.50	15.00
42	THR	O	-9.17	42.02	94.07	15.00
43	GLY	N	-8.37	40.40	92.74	15.00
43	GLY	CA	-9.67	39.80	92.56	15.00
43	GLY	C	-10.28	40.20	91.22	15.00
43	GLY	O	-11.22	39.57	90.74	15.00
44	LYS	N	-9.65	41.19	90.58	15.00
44	LYS	CA	-10.13	41.70	89.32	15.00
44	LYS	CB	-10.71	43.10	89.52	15.00
44	LYS	CG	-11.95	43.16	90.39	15.00
44	LYS	CD	-12.36	44.57	90.76	15.00
44	LYS	CE	-11.43	45.21	91.78	15.00
44	LYS	NZ	-11.50	44.47	93.08	15.00
44	LYS	C	-9.02	41.76	88.30	15.00
44	LYS	O	-7.91	42.20	88.61	15.00
45	LEU	N	-9.35	41.40	87.07	15.00

TABLE X

45	LEU	CA	-8.38	41.39	85.99	15.00
45	LEU	CB	-8.61	40.14	85.13	15.00
45	LEU	CG	-7.85	39.77	83.85	15.00
45	LEU	CD1	-6.47	39.23	84.16	15.00
45	LEU	CD2	-8.67	38.72	83.14	15.00
45	LEU	C	-8.55	42.68	85.16	15.00
45	LEU	O	-9.55	43.36	85.27	15.00
46	LEU	N	-7.57	43.04	84.37	15.00
46	LEU	CA	-7.65	44.23	83.55	15.00
46	LEU	CB	-7.27	45.46	84.35	15.00
46	LEU	CG	-7.82	46.76	83.83	15.00
46	LEU	CD1	-9.28	46.67	83.92	15.00
46	LEU	CD2	-7.33	47.91	84.71	15.00
46	LEU	C	-6.63	44.03	82.45	15.00
46	LEU	O	-5.67	43.30	82.61	15.00
47	ASN	N	-6.80	44.76	81.36	15.00
47	ASN	CA	-5.90	44.66	80.25	15.00
47	ASN	CB	-6.61	45.08	78.95	15.00
47	ASN	CG	-7.47	43.98	78.39	15.00
47	ASN	OD1	-7.52	42.88	78.93	15.00
47	ASN	ND2	-8.19	44.28	77.33	15.00
47	ASN	C	-4.77	45.63	80.52	15.00
47	ASN	O	-5.02	46.82	80.64	15.00
48	LEU	N	-3.54	45.17	80.66	15.00
48	LEU	CA	-2.44	46.13	80.87	15.00
48	LEU	CB	-1.29	45.54	81.75	15.00
48	LEU	CG	-1.76	45.23	83.19	15.00
48	LEU	CD1	-0.62	44.99	84.10	15.00
48	LEU	CD2	-2.69	46.29	83.75	15.00
48	LEU	C	-1.96	46.66	79.51	15.00
48	LEU	O	-2.40	46.14	78.46	15.00
49	SER	N	-1.12	47.70	79.52	15.00
49	SER	CA	-0.63	48.29	78.28	15.00
49	SER	CB	-0.70	49.82	78.41	15.00
49	SER	OG	0.06	50.46	77.43	15.00
49	SER	C	0.75	47.87	77.84	15.00
49	SER	O	1.75	48.29	78.43	15.00
50	PRO	N	0.81	47.08	76.75	15.00
50	PRO	CD	-0.34	46.48	76.03	15.00
50	PRO	CA	2.10	46.61	76.22	15.00
50	PRO	CB	1.68	45.45	75.34	15.00
50	PRO	CG	0.33	45.96	74.79	15.00

TABLE X

50 PRO C	2.77	47.79	75.45	15.00
50 PRO O	3.99	47.96	75.47	15.00
51 GLN N	1.96	48.67	74.86	15.00
51 GLN CA	2.48	49.87	74.18	15.00
51 GLN CB	1.37	50.77	73.66	15.00
51 GLN CG	2.00	51.92	72.85	15.00
51 GLN CD	2.33	51.51	71.46	15.00
51 GLN OE1	1.83	50.49	70.97	15.00
51 GLN NE2	3.19	52.26	70.81	15.00
51 GLN C	3.29	50.70	75.17	15.00
51 GLN O	4.21	51.38	74.79	15.00
52 ASN N	2.93	50.65	76.45	15.00
52 ASN CA	3.62	51.40	77.47	15.00
52 ASN CB	2.96	51.15	78.82	15.00
52 ASN CG	3.52	52.04	79.91	15.00
52 ASN OD1	4.31	52.93	79.64	15.00
52 ASN ND2	3.09	51.81	81.14	15.00
52 ASN C	5.04	50.91	77.52	15.00
52 ASN O	5.98	51.71	77.54	15.00
53 LEU N	5.19	49.60	77.57	15.00
53 LEU CA	6.53	49.05	77.64	15.00
53 LEU CB	6.40	47.59	77.98	15.00
53 LEU CG	5.80	47.51	79.34	15.00
53 LEU CD1	5.66	46.07	79.79	15.00
53 LEU CD2	6.65	48.34	80.33	15.00
53 LEU C	7.25	49.26	76.30	15.00
53 LEU O	8.43	49.52	76.27	15.00
54 VAL N	6.53	49.17	75.19	15.00
54 VAL CA	7.19	49.34	73.89	15.00
54 VAL CB	6.25	49.16	72.69	15.00
54 VAL CG1	6.98	49.50	71.41	15.00
54 VAL CG2	5.83	47.75	72.63	15.00
54 VAL C	7.89	50.66	73.74	15.00
54 VAL O	9.06	50.71	73.32	15.00
55 ASP N	7.28	51.70	74.27	15.00
55 ASP CA	7.87	53.05	74.15	15.00
55 ASP CB	6.76	54.08	73.93	15.00
55 ASP CG	5.70	53.58	72.94	15.00
55 ASP OD1	5.95	52.76	72.00	15.00
55 ASP OD2	4.60	54.09	73.02	15.00
55 ASP C	8.68	53.42	75.33	15.00
55 ASP O	9.58	54.23	75.23	15.00

TABLE X

56	CYS	N	8.38	52.90	76.50	15.00
56	CYS	CA	9.13	53.37	77.67	15.00
56	CYS	C	10.33	52.59	78.21	15.00
56	CYS	O	11.25	53.15	78.82	15.00
56	CYS	CB	8.16	53.80	78.81	15.00
56	CYS	SG	6.73	54.73	78.24	15.00
57	VAL	N	10.39	51.31	77.97	15.00
57	VAL	CA	11.49	50.47	78.46	15.00
57	VAL	CB	11.10	48.99	78.38	15.00
57	VAL	CG1	12.15	48.16	78.95	15.00
57	VAL	CG2	9.83	48.77	79.11	15.00
57	VAL	C	12.66	50.67	77.55	15.00
57	VAL	O	12.94	49.87	76.66	15.00
58	SER	N	13.40	51.73	77.79	15.00
58	SER	CA	14.54	52.04	76.91	15.00
58	SER	CB	15.13	53.44	77.26	15.00
58	SER	OG	15.02	53.68	78.65	15.00
58	SER	C	15.61	50.98	76.86	15.00
58	SER	O	16.39	50.92	75.91	15.00
59	GLU	N	15.66	50.15	77.91	15.00
59	GLU	CA	16.66	49.07	78.00	15.00
59	GLU	CB	16.59	48.34	79.35	15.00
59	GLU	CG	16.98	49.19	80.58	15.00
59	GLU	CD	15.98	50.33	80.88	15.00
59	GLU	OE1	14.75	50.10	80.81	15.00
59	GLU	OE2	16.46	51.46	81.17	15.00
59	GLU	C	16.48	48.04	76.89	15.00
59	GLU	O	17.36	47.20	76.67	15.00
60	ASN	N	15.31	48.07	76.27	15.00
60	ASN	CA	15.00	47.16	75.19	15.00
60	ASN	CB	13.64	46.51	75.47	15.00
60	ASN	CG	13.69	45.49	76.59	15.00
60	ASN	OD1	12.76	45.39	77.36	15.00
60	ASN	ND2	14.76	44.68	76.63	15.00
60	ASN	C	14.98	47.89	73.85	15.00
60	ASN	O	15.26	49.09	73.79	15.00
61	ASP	N	14.67	47.16	72.79	15.00
61	ASP	CA	14.64	47.72	71.44	15.00
61	ASP	CB	15.38	46.80	70.48	15.00
61	ASP	CG	16.10	47.57	69.36	15.00
61	ASP	OD1	16.04	48.81	69.34	15.00
61	ASP	OD2	16.76	46.92	68.52	15.00

TABLE X

61 ASP C	13.28	48.07	70.81	15.00
61 ASP O	13.13	48.13	69.60	15.00
62 GLY N	12.31	48.40	71.63	15.00
62 GLY CA	10.98	48.67	71.11	15.00
62 GLY C	10.49	47.51	70.24	15.00
62 GLY O	10.64	46.38	70.57	15.00
63 CYS N	9.98	47.80	69.05	15.00
63 CYS CA	9.47	46.79	68.11	15.00
63 CYS C	10.61	45.95	67.62	15.00
63 CYS O	10.41	45.05	66.81	15.00
63 CYS CB	8.71	47.45	66.95	15.00
63 CYS SG	7.16	48.19	67.39	15.00
64 GLY N	11.82	46.25	68.06	15.00
64 GLY CA	12.94	45.47	67.59	15.00
64 GLY C	13.32	44.36	68.55	15.00
64 GLY O	14.37	43.74	68.40	15.00
65 GLY N	12.48	44.12	69.55	15.00
65 GLY CA	12.76	43.06	70.49	15.00
65 GLY C	13.11	43.58	71.88	15.00
65 GLY O	13.33	44.80	72.13	15.00
66 GLY N	13.21	42.63	72.80	15.00
66 GLY CA	13.50	43.00	74.18	15.00
66 GLY C	13.34	41.82	75.15	15.00
66 GLY O	12.91	40.73	74.72	15.00
67 TYR N	13.65	42.02	76.42	15.00
67 TYR CA	13.55	40.94	77.37	15.00
67 TYR CB	14.85	40.83	78.19	15.00
67 TYR CG	16.13	40.41	77.42	15.00
67 TYR CD1	16.31	39.16	76.96	15.00
67 TYR CE1	17.51	38.78	76.29	15.00
67 TYR CD2	17.13	41.25	77.20	15.00
67 TYR CE2	18.32	40.83	76.53	15.00
67 TYR CZ	18.49	39.61	76.08	15.00
67 TYR OH	19.63	39.12	75.47	15.00
67 TYR C	12.41	41.24	78.31	15.00
67 TYR O	12.00	42.40	78.46	15.00
68 MET N	11.84	40.20	78.88	15.00
68 MET CA	10.72	40.40	79.78	15.00
68 MET CB	10.01	39.09	80.00	15.00
68 MET CG	9.14	38.63	78.85	15.00
68 MET SD	10.15	37.92	77.61	15.00
68 MET CE	10.37	36.10	78.19	15.00

TABLE X

68	MET	C	11.20	41.05	81.10	15.00
68	MET	O	10.55	41.92	81.68	15.00
69	THR	N	12.33	40.56	81.59	15.00
69	THR	CA	12.91	41.02	82.85	15.00
69	THR	CB	14.24	40.26	83.21	15.00
69	THR	OG1	15.16	40.38	82.12	15.00
69	THR	CG2	13.99	38.77	83.56	15.00
69	THR	C	13.15	42.55	82.80	15.00
69	THR	O	13.15	43.20	83.83	15.00
70	ASN	N	13.42	43.10	81.63	15.00
70	ASN	CA	13.61	44.55	81.51	15.00
70	ASN	CB	14.23	44.95	80.15	15.00
70	ASN	CG	15.73	44.64	80.08	15.00
70	ASN	OD1	16.28	44.44	78.98	15.00
70	ASN	ND2	16.41	44.61	81.22	15.00
70	ASN	C	12.27	45.27	81.66	15.00
70	ASN	O	12.24	46.42	82.08	15.00
71	ALA	N	11.20	44.62	81.19	15.00
71	ALA	CA	9.84	45.13	81.24	15.00
71	ALA	CB	8.96	44.17	80.50	15.00
71	ALA	C	9.39	45.23	82.69	15.00
71	ALA	O	8.79	46.23	83.13	15.00
72	PHE	N	9.72	44.17	83.43	15.00
72	PHE	CA	9.39	44.09	84.87	15.00
72	PHE	CB	9.67	42.66	85.39	15.00
72	PHE	CG	8.80	41.59	84.75	15.00
72	PHE	CD1	7.52	41.87	84.33	15.00
72	PHE	CD2	9.28	40.32	84.57	15.00
72	PHE	CE1	6.73	40.91	83.73	15.00
72	PHE	CE2	8.50	39.35	83.98	15.00
72	PHE	CZ	7.23	39.64	83.56	15.00
72	PHE	C	10.19	45.09	85.71	15.00
72	PHE	O	9.73	45.60	86.72	15.00
73	GLN	N	11.41	45.38	85.28	15.00
73	GLN	CA	12.27	46.36	85.97	15.00
73	GLN	CB	13.74	46.30	85.47	15.00
73	GLN	CG	14.74	46.94	86.38	15.00
73	GLN	CD	14.58	46.42	87.78	15.00
73	GLN	OE1	14.18	45.26	87.96	15.00
73	GLN	NE2	14.76	47.28	88.79	15.00
73	GLN	C	11.74	47.79	85.84	15.00
73	GLN	O	11.83	48.57	86.78	15.00

TABLE X

74	TYR	N	11.23	48.14	84.67	15.00
74	TYR	CA	10.67	49.45	84.41	15.00
74	TYR	CB	10.48	49.62	82.93	15.00
74	TYR	CG	9.52	50.72	82.59	15.00
74	TYR	CD1	9.90	51.97	82.44	15.00
74	TYR	CE1	8.98	53.00	82.06	15.00
74	TYR	CD2	8.25	50.50	82.38	15.00
74	TYR	CE2	7.39	51.55	82.01	15.00
74	TYR	CZ	7.74	52.77	81.85	15.00
74	TYR	OH	6.87	53.67	81.39	15.00
74	TYR	C	9.35	49.64	85.16	15.00
74	TYR	O	9.04	50.74	85.58	15.00
75	VAL	N	8.60	48.58	85.39	15.00
75	VAL	CA	7.35	48.70	86.13	15.00
75	VAL	CB	6.46	47.47	85.92	15.00
75	VAL	CG1	5.15	47.64	86.74	15.00
75	VAL	CG2	6.10	47.32	84.44	15.00
75	VAL	C	7.63	48.95	87.62	15.00
75	VAL	O	6.92	49.76	88.26	15.00
76	GLN	N	8.69	48.31	88.13	15.00
76	GLN	CA	9.12	48.47	89.51	15.00
76	GLN	CB	10.10	47.35	89.89	15.00
76	GLN	CG	10.55	47.31	91.38	15.00
76	GLN	CD	11.76	46.41	91.65	15.00
76	GLN	OE1	12.14	46.22	92.80	15.00
76	GLN	NE2	12.37	45.85	90.59	15.00
76	GLN	C	9.78	49.88	89.59	15.00
76	GLN	O	9.37	50.72	90.39	15.00
77	LYS	N	10.72	50.19	88.69	15.00
77	LYS	CA	11.40	51.49	88.72	15.00
77	LYS	CB	12.56	51.50	87.72	15.00
77	LYS	CG	13.20	52.85	87.44	15.00
77	LYS	CD	14.22	52.70	86.33	15.00
77	LYS	CE	15.18	51.56	86.62	15.00
77	LYS	NZ	16.20	51.34	85.56	15.00
77	LYS	C	10.51	52.71	88.55	15.00
77	LYS	O	10.73	53.76	89.17	15.00
78	ASN	N	9.50	52.55	87.70	15.00
78	ASN	CA	8.51	53.59	87.37	15.00
78	ASN	CB	7.84	53.25	86.04	15.00
78	ASN	CG	7.15	54.42	85.42	15.00
78	ASN	OD1	7.70	55.49	85.36	15.00

TABLE X

78 ASN ND2	5.93	54.22	84.95	15.00
78 ASN C	7.44	53.69	88.42	15.00
78 ASN O	6.89	54.77	88.64	15.00
79 ARG N	7.15	52.56	89.05	15.00
79 ARG CA	6.14	52.48	90.08	15.00
79 ARG CB	6.27	53.65	91.07	15.00
79 ARG CG	7.58	53.69	91.85	15.00
79 ARG CD	7.76	55.00	92.63	15.00
79 ARG NE	6.66	55.34	93.55	15.00
79 ARG CZ	6.30	54.65	94.63	15.00
79 ARG NH1	6.95	53.54	94.96	15.00
79 ARG NH2	5.21	55.01	95.31	15.00
79 ARG C	4.77	52.46	89.43	15.00
79 ARG O	3.80	52.99	90.00	15.00
80 GLY N	4.66	51.78	88.30	15.00
80 GLY CA	3.39	51.70	87.64	15.00
80 GLY C	3.39	51.50	86.16	15.00
80 GLY O	4.32	51.90	85.43	15.00
81 ILE N	2.30	50.87	85.73	15.00
81 ILE CA	2.03	50.55	84.34	15.00
81 ILE CB	2.38	49.06	83.98	15.00
81 ILE CG2	1.41	48.10	84.64	15.00
81 ILE CG1	2.48	48.88	82.46	15.00
81 ILE CD1	2.67	47.47	82.00	15.00
81 ILE C	0.57	50.92	84.01	15.00
81 ILE O	-0.33	50.73	84.82	15.00
82 ASP N	0.35	51.53	82.85	15.00
82 ASP CA	-1.01	51.93	82.43	15.00
82 ASP CB	-0.91	52.93	81.27	15.00
82 ASP CG	-0.45	54.32	81.71	15.00
82 ASP OD1	0.52	54.88	81.14	15.00
82 ASP OD2	-1.08	54.84	82.64	15.00
82 ASP C	-1.87	50.76	82.00	15.00
82 ASP O	-1.39	49.64	81.87	15.00
83 SER N	-3.16	51.03	81.87	15.00
83 SER CA	-4.11	50.02	81.42	15.00
83 SER CB	-5.54	50.23	82.00	15.00
83 SER OG	-5.97	51.58	81.87	15.00
83 SER C	-4.14	50.20	79.91	15.00
83 SER O	-3.48	51.11	79.34	15.00
84 GLU N	-4.79	49.26	79.24	15.00
84 GLU CA	-4.92	49.33	77.79	15.00

TABLE X

84 GLU CB	-5.77	48.16	77.25	15.00
84 GLU CG	-5.57	47.95	75.77	15.00
84 GLU CD	-4.09	47.91	75.42	15.00
84 GLU OE1	-3.52	48.88	74.89	15.00
84 GLU OE2	-3.46	46.90	75.73	15.00
84 GLU C	-5.65	50.62	77.45	15.00
84 GLU O	-5.13	51.48	76.76	15.00
85 ASP N	-6.84	50.77	78.03	15.00
85 ASP CA	-7.68	51.96	77.78	15.00
85 ASP CB	-9.03	51.85	78.51	15.00
85 ASP CG	-9.94	53.12	78.30	15.00
85 ASP OD1	-10.32	53.78	79.30	15.00
85 ASP OD2	-10.26	53.46	77.15	15.00
85 ASP C	-7.01	53.27	78.08	15.00
85 ASP O	-7.29	54.29	77.43	15.00
86 ALA N	-6.11	53.26	79.05	15.00
86 ALA CA	-5.41	54.47	79.38	15.00
86 ALA CB	-4.88	54.38	80.80	15.00
86 ALA C	-4.27	54.73	78.39	15.00
86 ALA O	-4.00	55.89	78.07	15.00
87 TYR N	-3.69	53.66	77.83	15.00
87 TYR CA	-2.57	53.78	76.88	15.00
87 TYR CB	-1.24	53.68	77.66	15.00
87 TYR CG	0.04	54.14	77.00	15.00
87 TYR CD1	0.10	54.44	75.56	15.00
87 TYR CE1	1.32	54.83	74.98	15.00
87 TYR CD2	1.21	54.26	77.84	15.00
87 TYR CE2	2.42	54.65	77.33	15.00
87 TYR CZ	2.49	54.94	75.86	15.00
87 TYR OH	3.71	55.29	75.29	15.00
87 TYR C	-2.68	52.66	75.83	15.00
87 TYR O	-2.00	51.63	75.92	15.00
88 PRO N	-3.51	52.90	74.79	15.00
88 PRO CD	-4.53	53.97	74.75	15.00
88 PRO CA	-3.75	51.94	73.71	15.00
88 PRO CB	-4.87	52.62	72.90	15.00
88 PRO CG	-5.64	53.31	73.98	15.00
88 PRO C	-2.52	51.62	72.84	15.00
88 PRO O	-1.59	52.42	72.70	15.00
89 TYR N	-2.58	50.42	72.24	15.00
89 TYR CA	-1.54	49.87	71.38	15.00
89 TYR CB	-1.64	48.34	71.47	15.00

TABLE X

89 TYR CG	-0.54	47.59	70.84	15.00
89 TYR CD1	0.79	47.78	71.31	15.00
89 TYR CE1	1.83	47.13	70.72	15.00
89 TYR CD2	-0.80	46.69	69.76	15.00
89 TYR CE2	0.20	46.03	69.15	15.00
89 TYR CZ	1.53	46.24	69.61	15.00
89 TYR OH	2.55	45.63	68.93	15.00
89 TYR C	-1.73	50.30	69.92	15.00
89 TYR O	-2.81	50.16	69.38	15.00
90 VAL N	-0.65	50.73	69.28	15.00
90 VAL CA	-0.69	51.22	67.88	15.00
90 VAL CB	-0.15	52.67	67.77	15.00
90 VAL CG1	-0.81	53.58	68.80	15.00
90 VAL CG2	-1.34	52.68	67.96	15.00
90 VAL C	0.11	50.36	66.90	15.00
90 VAL O	-0.09	50.40	65.68	15.00
91 GLY N	1.05	49.58	67.43	15.00
91 GLY CA	1.85	48.75	66.55	15.00
91 GLY C	3.14	49.42	66.11	15.00
91 GLY O	3.81	48.92	65.19	15.00
92 GLN N	3.51	50.52	66.75	15.00
92 GLN CA	4.75	51.17	66.39	15.00
92 GLN CB	4.53	52.11	65.23	15.00
92 GLN CG	3.31	52.97	65.48	15.00
92 GLN CD	3.44	54.31	64.81	15.00
92 GLN OE1	2.68	54.64	63.92	15.00
92 GLN NE2	4.41	55.10	65.25	15.00
92 GLN C	5.34	51.97	67.53	15.00
92 GLN O	4.72	52.25	68.53	15.00
93 GLU N	6.57	52.40	67.30	15.00
93 GLU CA	7.33	53.20	68.25	15.00
93 GLU CB	8.81	53.08	67.91	15.00
93 GLU CG	9.33	51.65	68.15	15.00
93 GLU CD	10.59	51.29	67.38	15.00
93 GLU OE1	10.87	51.94	66.34	15.00
93 GLU OE2	11.31	50.35	67.80	15.00
93 GLU C	6.85	54.66	68.26	15.00
93 GLU O	6.48	55.24	67.24	15.00
94 GLU N	6.79	55.20	69.46	15.00
94 GLU CA	6.36	56.56	69.67	15.00
94 GLU CB	4.83	56.70	69.62	15.00
94 GLU CG	4.07	55.48	70.04	15.00

TABLE X

94 GLU CD	2.76	55.78	70.70	15.00
94 GLU OE1	1.99	56.60	70.14	15.00
94 GLU OE2	2.51	55.26	71.81	15.00
94 GLU C	6.86	56.98	71.01	15.00
94 GLU O	7.15	56.12	71.84	15.00
95 SER N	6.98	58.29	71.23	15.00
95 SER CA	7.47	58.78	72.52	15.00
95 SER CB	7.26	60.29	72.63	15.00
95 SER OG	6.14	60.73	71.85	15.00
95 SER C	6.78	58.06	73.70	15.00
95 SER O	5.61	57.59	73.59	15.00
96 CYS N	7.52	57.90	74.80	15.00
96 CYS CA	6.93	57.30	75.96	15.00
96 CYS C	5.80	58.23	76.33	15.00
96 CYS O	6.00	59.44	76.37	15.00
96 CYS CB	7.95	57.27	77.09	15.00
96 CYS SG	7.32	56.63	78.67	15.00
97 MET N	4.58	57.73	76.42	15.00
97 MET CA	3.46	58.59	76.84	15.00
97 MET CB	2.40	58.64	75.75	15.00
97 MET CG	2.95	58.79	74.35	15.00
97 MET SD	1.74	59.21	73.09	15.00
97 MET CE	0.27	58.48	73.83	15.00
97 MET C	2.79	58.10	78.14	15.00
97 MET O	1.57	58.06	78.24	15.00
98 TYR N	3.59	57.79	79.15	15.00
98 TYR CA	3.09	57.31	80.45	15.00
98 TYR CB	4.25	56.91	81.37	15.00
98 TYR CG	3.71	56.31	82.64	15.00
98 TYR CD1	2.99	55.13	82.59	15.00
98 TYR CE1	2.42	54.60	83.75	15.00
98 TYR CD2	3.86	56.96	83.88	15.00
98 TYR CE2	3.30	56.45	85.03	15.00
98 TYR CZ	2.59	55.27	84.95	15.00
98 TYR OH	1.99	54.70	86.05	15.00
98 TYR C	2.17	58.29	81.19	15.00
98 TYR O	2.56	59.42	81.48	15.00
99 ASN N	0.97	57.85	81.49	15.00
99 ASN CA	-0.01	58.66	82.21	15.00
99 ASN CB	-1.39	58.64	81.52	15.00
99 ASN CG	-2.41	59.49	82.25	15.00
99 ASN OD1	-2.15	59.98	83.35	15.00

TABLE X

99	ASN	ND2	-3.60	59.65	81.65	15.00
99	ASN	C	-0.17	58.09	83.63	15.00
99	ASN	O	-0.87	57.05	83.81	15.00
100	PRO	N	0.31	58.84	84.66	15.00
100	PRO	CD	0.81	60.23	84.63	15.00
100	PRO	CA	0.20	58.38	86.04	15.00
100	PRO	CB	0.80	59.53	86.83	15.00
100	PRO	CG	1.64	60.28	85.79	15.00
100	PRO	C	-1.25	58.14	86.50	15.00
100	PRO	O	-1.49	57.37	87.41	15.00
101	THR	N	-2.22	58.73	85.82	15.00
101	THR	CA	-3.61	58.53	86.23	15.00
101	THR	CB	-4.58	59.63	85.74	15.00
101	THR	OG1	-5.12	59.28	84.45	15.00
101	THR	CG2	-3.91	60.96	85.67	15.00
101	THR	C	-4.09	57.21	85.69	15.00
101	THR	O	-5.05	56.64	86.24	15.00
102	GLY	N	-3.50	56.77	84.58	15.00
102	GLY	CA	-3.90	55.51	83.98	15.00
102	GLY	C	-3.31	54.30	84.66	15.00
102	GLY	O	-3.63	53.16	84.25	15.00
103	LYS	N	-2.50	54.52	85.70	15.00
103	LYS	CA	-1.87	53.41	86.40	15.00
103	LYS	CB	-1.06	53.93	87.58	15.00
103	LYS	CG	-0.26	52.86	88.29	15.00
103	LYS	CD	-0.09	53.20	89.77	15.00
103	LYS	CE	-1.41	52.95	90.56	15.00
103	LYS	NZ	-1.62	51.48	90.82	15.00
103	LYS	C	-2.90	52.38	86.85	15.00
103	LYS	O	-3.84	52.70	87.56	15.00
104	ALA	N	-2.70	51.13	86.45	15.00
104	ALA	CA	-3.60	50.03	86.82	15.00
104	ALA	CB	-4.23	49.45	85.59	15.00
104	ALA	C	-2.81	48.95	87.53	15.00
104	ALA	O	-3.37	48.03	88.10	15.00
105	ALA	N	-1.49	49.07	87.52	15.00
105	ALA	CA	-0.72	48.05	88.20	15.00
105	ALA	CB	-0.65	46.80	87.34	15.00
105	ALA	C	0.66	48.46	88.70	15.00
105	ALA	O	1.21	49.47	88.26	15.00
106	LYS	N	1.18	47.64	89.63	15.00
106	LYS	CA	2.49	47.81	90.27	15.00

TABLE X

106 LYS CB	2.33	48.37	91.70	15.00
106 LYS CG	1.94	49.82	91.78	15.00
106 LYS CD	2.39	50.49	93.08	15.00
106 LYS CE	3.90	50.73	93.15	15.00
106 LYS NZ	4.68	49.45	93.03	15.00
106 LYS C	3.31	46.52	90.33	15.00
106 LYS O	2.78	45.42	90.25	15.00
107 CYS N	4.58	46.66	90.67	15.00
107 CYS CA	5.44	45.50	90.73	15.00
107 CYS CB	5.96	45.28	89.31	15.00
107 CYS SG	7.11	43.91	89.12	15.00
107 CYS C	6.58	45.74	91.71	15.00
107 CYS O	7.13	46.84	91.75	15.00
108 ARG N	6.93	44.73	92.50	15.00
108 ARG CA	8.03	44.94	93.42	15.00
108 ARG CB	7.57	44.79	94.87	15.00
108 ARG CG	7.03	43.41	95.26	15.00
108 ARG CD	6.66	43.37	96.77	15.00
108 ARG NE	6.16	42.05	97.15	15.00
108 ARG CZ	6.83	40.90	96.99	15.00
108 ARG NH1	8.05	40.88	96.47	15.00
108 ARG NH2	6.25	39.76	97.31	15.00
108 ARG C	9.24	44.06	93.14	15.00
108 ARG O	9.94	43.63	94.07	15.00
109 GLY N	9.47	43.78	91.85	15.00
109 GLY CA	10.58	42.92	91.49	15.00
109 GLY C	10.15	41.85	90.50	15.00
109 GLY O	9.05	41.91	89.95	15.00
110 TYR N	10.97	40.81	90.37	15.00
110 TYR CA	10.68	39.71	89.47	15.00
110 TYR CB	10.79	40.15	88.01	15.00
110 TYR CG	12.20	40.50	87.61	15.00
110 TYR CD1	12.66	41.85	87.79	15.00
110 TYR CE1	13.95	42.21	87.41	15.00
110 TYR CD2	13.08	39.49	87.02	15.00
110 TYR CE2	14.35	39.80	86.64	15.00
110 TYR CZ	14.80	41.19	86.83	15.00
110 TYR OH	16.07	41.57	86.47	15.00
110 TYR C	11.67	38.57	89.72	15.00
110 TYR O	12.72	38.78	90.34	15.00
111 ARG N	11.36	37.37	89.26	15.00
111 ARG CA	12.26	36.23	89.43	15.00

TABLE X

111 ARG CB	11.86	35.41	90.67	15.00
111 ARG CG	11.78	36.26	91.94	15.00
111 ARG CD	12.04	35.36	93.15	15.00
111 ARG NE	13.43	34.92	93.18	15.00
111 ARG CZ	13.89	33.89	93.89	15.00
111 ARG NH1	15.19	33.60	93.83	15.00
111 ARG NH2	13.04	33.14	94.59	15.00
111 ARG C	12.24	35.31	88.24	15.00
111 ARG O	11.17	35.05	87.66	15.00
112 GLU N	13.43	34.83	87.90	15.00
112 GLU CA	13.63	33.90	86.82	15.00
112 GLU CB	15.09	33.97	86.40	15.00
112 GLU CG	15.46	35.25	85.64	15.00
112 GLU CD	15.38	35.07	84.12	15.00
112 GLU OE1	14.25	35.12	83.56	15.00
112 GLU OE2	16.47	34.88	83.50	15.00
112 GLU C	13.36	32.48	87.30	15.00
112 GLU O	13.00	32.27	88.44	15.00
113 ILE N	13.55	31.53	86.41	15.00
113 ILE CA	13.36	30.12	86.72	15.00
113 ILE CB	12.20	29.54	85.92	15.00
113 ILE CG2	12.22	28.02	85.90	15.00
113 ILE CG1	10.91	30.06	86.51	15.00
113 ILE CD1	9.69	29.82	85.68	15.00
113 ILE C	14.68	29.49	86.33	15.00
113 ILE O	15.33	29.97	85.44	15.00
114 PRO N	15.20	28.55	87.13	15.00
114 PRO CD	14.60	28.07	88.38	15.00
114 PRO CA	16.49	27.87	86.88	15.00
114 PRO CB	16.38	26.62	87.77	15.00
114 PRO CG	15.73	27.17	88.97	15.00
114 PRO C	16.69	27.54	85.40	15.00
114 PRO O	15.93	26.78	84.83	15.00
115 GLU N	17.71	28.13	84.80	15.00
115 GLU CA	18.03	28.00	83.38	15.00
115 GLU CB	19.41	28.59	83.11	15.00
115 GLU CG	19.58	29.05	81.64	15.00
115 GLU CD	20.85	29.87	81.42	15.00
115 GLU OE1	20.80	31.11	81.48	15.00
115 GLU OE2	21.91	29.28	81.19	15.00
115 GLU C	17.96	26.62	82.77	15.00
115 GLU O	18.99	25.96	82.65	15.00

TABLE X

116 GLY N	16.78	26.24	82.28	15.00
116 GLY CA	16.64	24.93	81.66	15.00
116 GLY C	15.95	23.89	82.52	15.00
116 GLY O	15.82	22.73	82.13	15.00
117 ASN N	15.49	24.30	83.70	15.00
117 ASN CA	14.84	23.38	84.61	15.00
117 ASN CB	15.29	23.66	86.03	15.00
117 ASN CG	14.55	22.85	87.06	15.00
117 ASN OD1	13.47	22.36	86.81	15.00
117 ASN ND2	15.14	22.73	88.25	15.00
117 ASN C	13.34	23.50	84.47	15.00
117 ASN O	12.71	24.37	85.05	15.00
118 GLU N	12.78	22.55	83.74	15.00
118 GLU CA	11.35	22.52	83.45	15.00
118 GLU CB	11.10	21.52	82.33	15.00
118 GLU CG	10.04	21.91	81.37	15.00
118 GLU CD	9.94	20.95	80.16	15.00
118 GLU OE1	8.82	20.50	79.88	15.00
118 GLU OE2	10.96	20.58	79.52	15.00
118 GLU C	10.45	22.18	84.64	15.00
118 GLU O	9.30	22.61	84.67	15.00
119 LYS N	10.97	21.46	85.63	15.00
119 LYS CA	10.15	21.13	86.77	15.00
119 LYS CB	10.74	19.95	87.52	15.00
119 LYS CG	9.69	19.04	88.07	15.00
119 LYS CD	8.84	18.47	86.94	15.00
119 LYS CE	7.78	17.54	87.45	15.00
119 LYS NZ	7.03	17.08	86.28	15.00
119 LYS C	10.02	22.33	87.69	15.00
119 LYS O	9.02	22.45	88.42	15.00
120 ALA N	11.01	23.22	87.66	15.00
120 ALA CA	10.99	24.43	88.48	15.00
120 ALA CB	12.36	25.05	88.46	15.00
120 ALA C	9.95	25.39	87.87	15.00
120 ALA O	9.39	26.27	88.57	15.00
121 LEU N	9.79	25.27	86.55	15.00
121 LEU CA	8.83	26.05	85.78	15.00
121 LEU CB	9.06	25.87	84.28	15.00
121 LEU CG	8.06	26.54	83.31	15.00
121 LEU CD1	8.05	28.02	83.54	15.00
121 LEU CD2	8.42	26.24	81.90	15.00
121 LEU C	7.43	25.59	86.13	15.00

TABLE X

121 LEU O	6.59	26.43	86.46	15.00
122 LYS N	7.17	24.28	86.10	15.00
122 LYS CA	5.83	23.74	86.40	15.00
122 LYS CB	5.81	22.20	86.25	15.00
122 LYS CG	4.49	21.54	86.59	15.00
122 LYS CD	4.61	20.10	86.92	15.00
122 LYS CE	5.26	19.90	88.29	15.00
122 LYS NZ	5.14	18.48	88.78	15.00
122 LYS C	5.34	24.13	87.78	15.00
122 LYS O	4.13	24.20	87.99	15.00
123 ARG N	6.27	24.36	88.71	15.00
123 ARG CA	5.90	24.76	90.06	15.00
123 ARG CB	6.95	24.36	91.07	15.00
123 ARG CG	7.05	22.94	91.45	15.00
123 ARG CD	8.15	22.86	92.43	15.00
123 ARG NE	9.44	23.25	91.82	15.00
123 ARG CZ	10.56	23.53	92.50	15.00
123 ARG NH1	10.58	23.50	93.81	15.00
123 ARG NH2	11.71	23.76	91.85	15.00
123 ARG C	5.71	26.25	90.17	15.00
123 ARG O	5.12	26.72	91.13	15.00
124 ALA N	6.31	27.00	89.25	15.00
124 ALA CA	6.16	28.42	89.30	15.00
124 ALA CB	7.22	29.12	88.43	15.00
124 ALA C	4.78	28.73	88.81	15.00
124 ALA O	4.06	29.46	89.47	15.00
125 VAL N	4.37	28.09	87.72	15.00
125 VAL CA	3.06	28.41	87.21	15.00
125 VAL CB	2.82	27.94	85.72	15.00
125 VAL CG1	4.09	27.54	85.00	15.00
125 VAL CG2	1.70	26.88	85.60	15.00
125 VAL C	2.03	27.82	88.15	15.00
125 VAL O	0.89	28.28	88.17	15.00
126 ALA N	2.42	26.86	88.98	15.00
126 ALA CA	1.47	26.25	89.89	15.00
126 ALA CB	1.94	24.91	90.29	15.00
126 ALA C	1.32	27.11	91.12	15.00
126 ALA O	0.22	27.27	91.63	15.00
127 ARG N	2.42	27.71	91.55	15.00
127 ARG CA	2.42	28.50	92.77	15.00
127 ARG CB	3.67	28.22	93.60	15.00
127 ARG CG	3.74	26.79	94.07	15.00

TABLE X

127 ARG CD	5.07	26.45	94.67	15.00
127 ARG NE	5.02	25.01	94.96	15.00
127 ARG CZ	6.03	24.24	95.34	15.00
127 ARG NH1	5.84	22.94	95.55	15.00
127 ARG NH2	7.24	24.73	95.54	15.00
127 ARG C	2.30	29.98	92.61	15.00
127 ARG O	2.15	30.68	93.60	15.00
128 VAL N	2.46	30.47	91.38	15.00
128 VAL CA	2.37	31.91	91.11	15.00
128 VAL CB	3.70	32.49	90.59	15.00
128 VAL CG1	3.62	33.98	90.47	15.00
128 VAL CG2	4.87	32.10	91.53	15.00
128 VAL C	1.29	32.25	90.10	15.00
128 VAL O	-0.47	33.10	90.36	15.00
129 GLY N	1.30	31.60	88.94	15.00
129 GLY CA	0.31	31.85	87.91	15.00
129 GLY C	1.10	32.00	86.61	15.00
129 GLY O	2.27	31.60	86.57	15.00
130 PRO N	0.52	32.56	85.53	15.00
130 PRO CD	-0.89	32.96	85.30	15.00
130 PRO CA	1.27	32.70	84.30	15.00
130 PRO CB	0.38	33.61	83.50	15.00
130 PRO CG	-0.98	33.09	83.81	15.00
130 PRO C	2.68	33.24	84.44	15.00
130 PRO O	2.93	34.17	85.20	15.00
131 VAL N	3.59	32.56	83.75	15.00
131 VAL CA	5.01	32.88	83.76	15.00
131 VAL CB	5.79	31.64	84.27	15.00
131 VAL CG1	7.25	31.88	84.32	15.00
131 VAL CG2	5.29	31.20	85.62	15.00
131 VAL C	5.46	33.28	82.34	15.00
131 VAL O	4.93	32.82	81.36	15.00
132 SER N	6.29	34.30	82.27	15.00
132 SER CA	6.77	34.75	80.98	15.00
132 SER CB	7.15	36.24	81.04	15.00
132 SER OG	5.98	36.98	81.39	15.00
132 SER C	7.92	33.89	80.48	15.00
132 SER O	9.01	33.83	81.08	15.00
133 VAL N	7.65	33.20	79.38	15.00
133 VAL CA	8.65	32.34	78.76	15.00
133 VAL CB	8.09	30.90	78.61	15.00
133 VAL CG1	7.58	30.35	79.92	15.00

TABLE X

133 VAL CG2	6.97	30.91	77.61	15.00
133 VAL C	9.05	32.84	77.37	15.00
133 VAL O	8.48	33.81	76.85	15.00
134 ALA N	10.08	32.21	76.81	15.00
134 ALA CA	10.60	32.51	75.49	15.00
134 ALA CB	11.89	33.29	75.59	15.00
134 ALA C	10.85	31.16	74.84	15.00
134 ALA O	11.46	30.30	75.47	15.00
135 ILE N	10.35	30.97	73.62	15.00
135 ILE CA	10.52	29.73	72.86	15.00
135 ILE CB	9.18	28.95	72.80	15.00
135 ILE CG2	8.71	28.60	74.21	15.00
135 ILE CG1	8.13	29.80	72.09	15.00
135 ILE CD1	6.78	29.14	72.00	15.00
135 ILE C	11.04	30.04	71.44	15.00
135 ILE O	11.30	31.20	71.08	15.00
136 ASP N	11.28	28.98	70.67	15.00
136 ASP CA	11.71	29.13	69.30	15.00
136 ASP CB	12.68	28.01	68.94	15.00
136 ASP CG	13.21	28.11	67.50	15.00
136 ASP OD1	13.77	27.12	67.00	15.00
136 ASP OD2	13.08	29.18	66.88	15.00
136 ASP C	10.45	28.94	68.51	15.00
136 ASP O	9.90	27.82	68.48	15.00
137 ALA N	9.98	30.01	67.87	15.00
137 ALA CA	8.78	29.93	67.06	15.00
137 ALA CB	7.74	30.91	67.56	15.00
137 ALA C	9.09	30.18	65.58	15.00
137 ALA O	8.27	30.79	64.88	15.00
138 SER N	10.22	29.67	65.10	15.00
138 SER CA	10.66	29.83	63.72	15.00
138 SER CB	12.18	29.81	63.63	15.00
138 SER OG	12.67	28.54	64.01	15.00
138 SER C	10.15	28.77	62.77	15.00
138 SER O	9.81	29.07	61.62	15.00
139 LEU N	10.12	27.53	63.26	15.00
139 LEU CA	9.66	26.42	62.45	15.00
139 LEU CB	9.74	25.13	63.29	15.00
139 LEU CG	11.05	24.33	63.34	15.00
139 LEU CD1	12.24	25.24	63.67	15.00
139 LEU CD2	10.92	23.21	64.38	15.00
139 LEU C	8.24	26.59	61.88	15.00

TABLE X

139 LEU O	7.32	26.95	62.60	15.00
140 THR N	8.08	26.30	60.58	15.00
140 THR CA	6.80	26.39	59.88	15.00
140 THR CB	6.88	25.76	58.50	15.00
140 THR OG1	8.18	25.97	57.94	15.00
140 THR CG2	5.86	26.37	57.60	15.00
140 THR C	5.76	25.62	60.67	15.00
140 THR O	4.67	26.12	60.88	15.00
141 SER N	6.13	24.45	61.17	15.00
141 SER CA	5.20	23.63	61.94	15.00
141 SER CB	5.79	22.28	62.28	15.00
141 SER OG	7.00	22.40	62.97	15.00
141 SER C	4.65	24.28	63.18	15.00
141 SER O	3.60	23.89	63.66	15.00
142 PHE N	5.35	25.26	63.72	15.00
142 PHE CA	4.82	25.94	64.90	15.00
142 PHE CB	5.94	26.71	65.64	15.00
142 PHE CG	5.46	27.49	66.86	15.00
142 PHE CD1	5.60	26.99	68.12	15.00
142 PHE CD2	4.89	28.74	66.71	15.00
142 PHE CE1	5.15	27.76	69.25	15.00
142 PHE CE2	4.46	29.49	67.82	15.00
142 PHE CZ	4.59	29.00	69.07	15.00
142 PHE C	3.74	26.88	64.42	15.00
142 PHE O	2.63	26.88	64.93	15.00
143 GLN N	4.08	27.58	63.36	15.00
143 GLN CA	3.24	28.59	62.73	15.00
143 GLN CB	4.04	29.36	61.69	15.00
143 GLN CG	5.38	29.87	62.23	15.00
143 GLN CD	6.19	30.64	61.16	15.00
143 GLN OE1	5.83	31.75	60.75	15.00
143 GLN NE2	7.25	30.01	60.64	15.00
143 GLN C	1.95	28.10	62.12	15.00
143 GLN O	0.99	28.86	62.08	15.00
144 PHE N	1.91	26.90	61.55	15.00
144 PHE CA	0.61	26.44	61.01	15.00
144 PHE CB	0.73	25.77	59.63	15.00
144 PHE CG	1.72	24.62	59.58	15.00
144 PHE CD1	2.76	24.61	58.69	15.00
144 PHE CD2	1.58	23.50	60.36	15.00
144 PHE CE1	3.60	23.51	58.60	15.00
144 PHE CE2	2.47	22.41	60.22	15.00

TABLE X

144 PHE CZ	3.44	22.44	59.35	15.00
144 PHE C	-0.14	25.50	61.98	15.00
144 PHE O	-1.10	24.82	61.59	15.00
145 TYR N	0.31	25.47	63.24	15.00
145 TYR CA	-0.31	24.65	64.26	15.00
145 TYR CB	0.32	24.91	65.65	15.00
145 TYR CG	-0.47	24.34	66.81	15.00
145 TYR CD1	-0.26	23.01	67.22	15.00
145 TYR CE1	-0.98	22.48	68.28	15.00
145 TYR CD2	-1.42	25.12	67.48	15.00
145 TYR CE2	-2.15	24.61	68.54	15.00
145 TYR CZ	-1.93	23.28	68.94	15.00
145 TYR OH	-2.67	22.83	70.02	15.00
145 TYR C	-1.80	24.98	64.30	15.00
145 TYR O	-2.24	26.10	64.03	15.00
146 SER N	-2.60	24.00	64.69	15.00
146 SER CA	-4.06	24.19	64.77	15.00
146 SER CB	-4.67	23.67	63.48	15.00
146 SER OG	-4.29	22.33	63.27	15.00
146 SER C	-4.67	23.42	65.95	15.00
146 SER O	-5.59	23.89	66.62	15.00
147 LYS N	-4.20	22.20	66.13	15.00
147 LYS CA	-4.67	21.36	67.20	15.00
147 LYS CB	-5.96	20.64	66.83	15.00
147 LYS CG	-5.81	19.47	65.90	15.00
147 LYS CD	-7.06	18.58	65.92	15.00
147 LYS CE	-6.91	17.41	64.96	15.00
147 LYS NZ	-8.13	16.56	64.99	15.00
147 LYS C	-3.60	20.36	67.62	15.00
147 LYS O	-2.62	20.16	66.90	15.00
148 GLY N	-3.82	19.73	68.78	15.00
148 GLY CA	-2.88	18.75	69.30	15.00
148 GLY C	-1.76	19.26	70.20	15.00
148 GLY O	-1.75	20.39	70.59	15.00
149 VAL N	-0.79	18.40	70.52	15.00
149 VAL CA	0.33	18.81	71.35	15.00
149 VAL CB	0.58	17.89	72.57	15.00
149 VAL CG1	1.74	18.42	73.41	15.00
149 VAL CG2	-0.68	17.75	73.42	15.00
149 VAL C	1.59	18.86	70.48	15.00
149 VAL O	2.06	17.84	69.96	15.00
150 TYR N	2.13	20.07	70.35	15.00

TABLE X

150 TYR CA	3.32	20.33	69.53	15.00
150 TYR CB	3.50	21.83	69.29	15.00
150 TYR CG	4.59	22.21	68.31	15.00
150 TYR CD1	4.47	22.01	66.95	15.00
150 TYR CE1	5.48	22.37	66.04	15.00
150 TYR CD2	5.74	22.78	68.72	15.00
150 TYR CE2	6.75	23.13	67.81	15.00
150 TYR CZ	6.61	22.93	66.48	15.00
150 TYR OH	7.57	23.30	65.60	15.00
150 TYR C	4.60	19.72	70.12	15.00
150 TYR O	4.76	19.60	71.37	15.00
151 TYR N	5.44	19.24	69.21	15.00
151 TYR CA	6.74	18.68	69.55	15.00
151 TYR CB	6.62	17.30	70.22	15.00
151 TYR CG	7.96	16.61	70.42	15.00
151 TYR CD1	9.15	17.34	70.60	15.00
151 TYR CE1	10.41	16.67	70.84	15.00
151 TYR CD2	8.02	15.21	70.47	15.00
151 TYR CE2	9.24	14.52	70.71	15.00
151 TYR CZ	10.43	15.27	70.89	15.00
151 TYR OH	11.60	14.61	71.14	15.00
151 TYR C	7.38	18.53	68.19	15.00
151 TYR O	6.82	17.86	67.31	15.00
152 ASP N	8.47	19.26	67.98	15.00
152 ASP CA	9.18	19.22	66.71	15.00
152 ASP CB	8.83	20.40	65.81	15.00
152 ASP CG	9.30	20.18	64.37	15.00
152 ASP OD1	10.54	20.06	64.18	15.00
152 ASP OD2	8.42	20.06	63.48	15.00
152 ASP C	10.69	19.18	66.97	15.00
152 ASP O	11.34	20.21	67.14	15.00
153 GLU N	11.24	17.97	66.94	15.00
153 GLU CA	12.64	17.77	67.18	15.00
153 GLU CB	13.00	16.30	66.88	15.00
153 GLU CG	12.45	15.71	65.61	15.00
153 GLU CD	11.10	15.02	65.83	15.00
153 GLU OE1	11.10	13.96	66.53	15.00
153 GLU OE2	10.06	15.52	65.30	15.00
153 GLU C	13.60	18.73	66.48	15.00
153 GLU O	14.75	18.90	66.91	15.00
154 SER N	13.17	19.30	65.35	15.00
154 SER CA	14.02	20.24	64.60	15.00

TABLE X

154 SER CB	13.49	20.49	63.17	15.00
154 SER OG	13.06	19.29	62.54	15.00
154 SER C	14.13	21.57	65.34	15.00
154 SER O	14.95	22.40	65.00	15.00
155 CYS N	13.37	21.72	66.43	15.00
155 CYS CA	13.33	22.98	67.21	15.00
155 CYS C	14.64	23.18	67.97	15.00
155 CYS O	15.25	22.21	68.44	15.00
155 CYS CB	12.15	22.99	68.17	15.00
155 CYS SG	11.63	24.66	68.64	15.00
156 ASN N	15.04	24.44	68.16	15.00
156 ASN CA	16.31	24.74	68.81	15.00
156 ASN CB	17.20	25.46	67.80	15.00
156 ASN CG	18.46	26.05	68.41	15.00
156 ASN OD1	18.80	25.83	69.59	15.00
156 ASN ND2	19.18	26.80	67.59	15.00
156 ASN C	16.22	25.55	70.11	15.00
156 ASN O	16.12	26.80	70.09	15.00
157 SER N	16.27	24.83	71.22	15.00
157 SER CA	16.22	25.44	72.55	15.00
157 SER CB	16.51	24.37	73.60	15.00
157 SER OG	15.49	23.40	73.56	15.00
157 SER C	17.22	26.59	72.72	15.00
157 SER O	16.99	27.51	73.49	15.00
158 ASP N	18.35	26.52	72.02	15.00
158 ASP CA	19.40	27.52	72.06	15.00
158 ASP CB	20.71	26.91	71.57	15.00
158 ASP CG	20.91	25.47	72.03	15.00
158 ASP OD1	21.16	24.60	71.16	15.00
158 ASP OD2	20.81	25.18	73.26	15.00
158 ASP C	19.05	28.77	71.26	15.00
158 ASP O	19.69	29.81	71.37	15.00
159 ASN N	18.04	28.67	70.40	15.00
159 ASN CA	17.64	29.82	69.62	15.00
159 ASN CB	17.77	29.53	68.12	15.00
159 ASN CG	17.54	30.78	67.23	15.00
159 ASN OD1	17.33	30.67	66.00	15.00
159 ASN ND2	17.63	31.96	67.83	15.00
159 ASN C	16.22	30.27	69.99	15.00
159 ASN O	15.23	29.87	69.36	15.00
160 LEU N	16.12	31.10	71.03	15.00
160 LEU CA	14.84	31.64	71.49	15.00

TABLE X

160 LEU CB	14.88	31.87	73.00	15.00
160 LEU CG	15.40	30.70	73.88	15.00
160 LEU CD1	15.23	31.09	75.33	15.00
160 LEU CD2	14.68	29.38	73.59	15.00
160 LEU C	14.66	32.96	70.75	15.00
160 LEU O	15.56	33.76	70.75	15.00
161 ASN N	13.52	33.17	70.11	15.00
161 ASN CA	13.28	34.40	69.36	15.00
161 ASN CB	13.53	34.18	67.85	15.00
161 ASN CG	12.91	32.90	67.32	15.00
161 ASN OD1	11.68	32.70	67.33	15.00
161 ASN ND2	13.78	32.01	66.83	15.00
161 ASN C	11.86	34.98	69.54	15.00
161 ASN O	11.57	36.09	69.09	15.00
162 HIS N	10.99	34.28	70.26	15.00
162 HIS CA	9.66	34.79	70.41	15.00
162 HIS CB	8.74	34.04	69.45	15.00
162 HIS CG	7.37	34.62	69.35	15.00
162 HIS CD2	6.94	35.88	69.10	15.00
162 HIS ND1	6.24	33.84	69.45	15.00
162 HIS CE1	5.17	34.59	69.25	15.00
162 HIS NE2	5.57	35.83	69.03	15.00
162 HIS C	9.28	34.53	71.85	15.00
162 HIS O	9.61	33.48	72.39	15.00
163 ALA N	8.70	35.56	72.47	15.00
163 ALA CA	8.26	35.51	73.85	15.00
163 ALA CB	8.50	36.80	74.53	15.00
163 ALA C	6.78	35.24	73.87	15.00
163 ALA O	6.02	35.80	73.09	15.00
164 VAL N	6.39	34.38	74.78	15.00
164 VAL CA	5.01	34.03	74.97	15.00
164 VAL CB	4.69	32.69	74.29	15.00
164 VAL CG1	4.67	32.84	72.75	15.00
164 VAL CG2	5.73	31.64	74.69	15.00
164 VAL C	4.72	33.94	76.48	15.00
164 VAL O	5.55	34.42	77.30	15.00
165 LEU N	3.60	33.31	76.85	15.00
165 LEU CA	3.27	33.21	78.26	15.00
165 LEU CB	2.31	34.36	78.60	15.00
165 LEU CG	1.52	34.51	79.93	15.00
165 LEU CD1	2.25	35.21	81.00	15.00
165 LEU CD2	0.26	35.25	79.65	15.00

TABLE X

165 LEU C	2.65	31.88	78.63	15.00
165 LEU O	1.68	31.50	77.98	15.00
166 ALA N	3.25	31.15	79.57	15.00
166 ALA CA	2.73	29.85	80.03	15.00
166 ALA CB	3.79	29.05	80.72	15.00
166 ALA C	1.57	30.12	80.98	15.00
166 ALA O	1.76	30.63	82.05	15.00
167 VAL N	0.38	29.73	80.56	15.00
167 VAL CA	-0.88	29.95	81.26	15.00
167 VAL CB	-1.94	30.48	80.19	15.00
167 VAL CG1	-3.36	30.02	80.45	15.00
167 VAL CG2	-1.88	32.03	80.10	15.00
167 VAL C	-1.36	28.70	82.03	15.00
167 VAL O	-2.35	28.75	82.70	15.00
168 GLY N	-0.67	27.57	81.88	15.00
168 GLY CA	-1.07	26.35	82.56	15.00
168 GLY C	-0.36	25.13	82.00	15.00
168 GLY O	0.52	25.29	81.17	15.00
169 TYR N	-0.68	23.94	82.49	15.00
169 TYR CA	-0.03	22.73	81.98	15.00
169 TYR CB	1.33	22.45	82.69	15.00
169 TYR CG	1.24	22.33	84.21	15.00
169 TYR CD1	0.66	21.21	84.82	15.00
169 TYR CE1	0.51	21.16	86.19	15.00
169 TYR CD2	1.67	23.36	85.02	15.00
169 TYR CE2	1.53	23.30	86.36	15.00
169 TYR CZ	0.94	22.20	86.95	15.00
169 TYR OH	0.76	22.18	88.32	15.00
169 TYR C	-0.97	21.62	82.29	15.00
169 TYR O	-1.89	21.79	83.08	15.00
170 GLY N	-0.71	20.47	81.70	15.00
170 GLY CA	-1.54	19.31	81.93	15.00
170 GLY C	-1.19	18.20	80.97	15.00
170 GLY O	-0.05	18.05	80.56	15.00
171 ILE N	-2.19	17.42	80.63	15.00
171 ILE CA	-1.99	16.31	79.71	15.00
171 ILE CB	-1.71	14.98	80.49	15.00
171 ILE CG2	-2.84	14.65	81.48	15.00
171 ILE CG1	-1.47	13.80	79.57	15.00
171 ILE CD1	-1.37	12.49	80.30	15.00
171 ILE C	-3.23	16.19	78.81	15.00
171 ILE O	-4.29	16.77	79.10	15.00

TABLE X

172 GLN N	-3.09	15.50	77.69	15.00
172 GLN CA	-4.21	15.35	76.77	15.00
172 GLN CB	-3.96	16.16	75.48	15.00
172 GLN CG	-5.15	16.20	74.49	15.00
172 GLN CD	-5.05	17.33	73.50	15.00
172 GLN OE1	-4.76	18.47	73.87	15.00
172 GLN NE2	-5.27	17.03	72.22	15.00
172 GLN C	-4.51	13.86	76.49	15.00
172 GLN O	-5.23	13.22	77.27	15.00
173 LYS N	-4.00	13.30	75.41	15.00
173 LYS CA	-4.27	11.89	75.22	15.00
173 LYS CB	-4.76	11.64	73.81	15.00
173 LYS CG	-6.07	12.36	73.52	15.00
173 LYS CD	-6.45	12.30	72.03	15.00
173 LYS CE	-5.44	13.01	71.15	15.00
173 LYS NZ	-5.85	12.96	69.72	15.00
173 LYS C	-2.97	11.18	75.51	15.00
173 LYS O	-2.29	10.72	74.59	15.00
174 GLY N	-2.59	11.22	76.78	15.00
174 GLY CA	-1.36	10.60	77.21	15.00
174 GLY C	-0.18	11.54	77.14	15.00
174 GLY O	0.88	11.27	77.72	15.00
175 ASN N	-0.34	12.66	76.42	15.00
175 ASN CA	0.75	13.62	76.27	15.00
175 ASN CB	0.84	14.07	74.82	15.00
175 ASN CG	1.30	12.97	73.90	15.00
175 ASN OD1	2.46	12.52	73.96	15.00
175 ASN ND2	0.38	12.50	73.05	15.00
175 ASN C	0.75	14.84	77.17	15.00
175 ASN O	-0.24	15.61	77.23	15.00
176 LYS N	1.91	15.07	77.78	15.00
176 LYS CA	2.12	16.20	78.66	15.00
176 LYS CB	3.36	15.99	79.53	15.00
176 LYS CG	3.19	14.86	80.52	15.00
176 LYS CD	4.24	14.85	81.66	15.00
176 LYS CE	4.17	13.51	82.41	15.00
176 LYS NZ	2.95	13.37	83.28	15.00
176 LYS C	2.25	17.46	77.85	15.00
176 LYS O	2.71	17.42	76.71	15.00
177 HIS N	1.74	18.56	78.38	15.00
177 HIS CA	1.85	19.81	77.66	15.00
177 HIS CB	0.73	19.92	76.63	15.00

TABLE X

177 HIS CG	-0.62	20.17	77.21	15.00
177 HIS CD2	-1.20	21.32	77.65	15.00
177 HIS ND1	-1.56	19.18	77.38	15.00
177 HIS CE1	-2.67	19.70	77.89	15.00
177 HIS NE2	-2.47	21.00	78.06	15.00
177 HIS C	1.83	21.03	78.53	15.00
177 HIS O	1.38	20.97	79.68	15.00
178 TRP N	2.20	22.13	77.89	15.00
178 TRP CA	2.21	23.47	78.45	15.00
178 TRP CB	3.57	24.15	78.26	15.00
178 TRP CG	4.71	23.55	78.98	15.00
178 TRP CD2	4.98	23.62	80.41	15.00
178 TRP CE2	6.14	22.88	80.64	15.00
178 TRP CE3	4.33	24.22	81.52	15.00
178 TRP CD1	5.70	22.82	78.45	15.00
178 TRP NE1	6.56	22.40	79.44	15.00
178 TRP CZ2	6.67	22.72	81.91	15.00
178 TRP CZ3	4.86	24.05	82.77	15.00
178 TRP CH2	6.01	23.31	82.96	15.00
178 TRP C	1.18	24.24	77.64	15.00
178 TRP O	1.14	24.11	76.42	15.00
179 ILE N	0.33	25.01	78.30	15.00
179 ILE CA	-0.64	25.81	77.55	15.00
179 ILE CB	-1.90	26.08	78.34	15.00
179 ILE CG2	-2.77	27.07	77.61	15.00
179 ILE CG1	-2.54	24.73	78.71	15.00
179 ILE CD1	-3.79	24.79	79.53	15.00
179 ILE C	0.03	27.14	77.31	15.00
179 ILE O	0.36	27.82	78.27	15.00
180 ILE N	0.23	27.49	76.05	15.00
180 ILE CA	0.89	28.72	75.68	15.00
180 ILE CB	2.09	28.49	74.78	15.00
180 ILE CG2	2.73	29.81	74.51	15.00
180 ILE CG1	3.09	27.57	75.46	15.00
180 ILE CD1	3.92	28.26	76.47	15.00
180 ILE C	-0.04	29.69	75.03	15.00
180 ILE O	-0.88	29.33	74.22	15.00
181 LYS N	0.06	30.94	75.44	15.00
181 LYS CA	-0.80	31.95	74.91	15.00
181 LYS CB	-1.26	32.84	76.03	15.00
181 LYS CG	-1.94	34.09	75.52	15.00
181 LYS CD	-2.47	34.90	76.67	15.00

TABLE X

181 LYS CE	-2.92	36.22	76.11	15.00
181 LYS NZ	-3.47	37.09	77.17	15.00
181 LYS C	0.15	32.72	74.03	15.00
181 LYS O	1.19	33.15	74.52	15.00
182 ASN N	-0.15	32.81	72.75	15.00
182 ASN CA	0.73	33.49	71.81	15.00
182 ASN CB	0.96	32.61	70.59	15.00
182 ASN CG	1.97	33.17	69.65	15.00
182 ASN OD1	2.31	34.34	69.73	15.00
182 ASN ND2	2.42	32.35	68.71	15.00
182 ASN C	0.01	34.76	71.38	15.00
182 ASN O	-1.21	34.83	71.39	15.00
183 SER N	0.75	35.80	71.01	15.00
183 SER CA	-0.09	37.03	70.61	15.00
183 SER CB	0.81	38.23	71.20	15.00
183 SER OG	2.19	38.09	71.04	15.00
183 SER C	-0.09	37.18	69.10	15.00
183 SER O	0.19	38.25	68.56	15.00
184 TRP N	-0.58	36.16	68.41	15.00
184 TRP CA	-0.73	36.29	66.97	15.00
184 TRP CB	0.00	35.18	66.21	15.00
184 TRP CG	1.47	35.38	66.20	15.00
184 TRP CD2	2.44	34.39	65.92	15.00
184 TRP CE2	3.69	35.01	65.97	15.00
184 TRP CE3	2.38	33.02	65.61	15.00
184 TRP CD1	2.13	36.54	66.41	15.00
184 TRP NE1	3.47	36.33	66.27	15.00
184 TRP CZ2	4.88	34.32	65.74	15.00
184 TRP CZ3	3.56	32.33	65.37	15.00
184 TRP CH2	4.79	32.98	65.44	15.00
184 TRP C	-2.17	36.42	66.57	15.00
184 TRP O	-2.53	36.20	65.42	15.00
185 GLY N	-2.97	36.92	67.51	15.00
185 GLY CA	-4.37	37.14	67.23	15.00
185 GLY C	-5.06	35.83	67.50	15.00
185 GLY O	-4.46	34.76	67.64	15.00
186 GLU N	-6.37	35.94	67.57	15.00
186 GLU CA	-7.23	34.80	67.84	15.00
186 GLU CB	-8.63	35.32	68.26	15.00
186 GLU CG	-9.57	34.27	68.68	15.00
186 GLU CD	-10.89	34.86	69.09	15.00
186 GLU OE1	-11.68	35.25	68.20	15.00

TABLE X

186 GLU OE2	-11.14	34.91	70.31	15.00
186 GLU C	-7.36	33.76	66.75	15.00
186 GLU O	-7.74	32.62	67.03	15.00
187 ASN N	-7.00	34.14	65.52	15.00
187 ASN CA	-7.11	33.25	64.36	15.00
187 ASN CB	-7.33	34.07	63.08	15.00
187 ASN CG	-8.45	33.50	62.21	15.00
187 ASN OD1	-8.22	33.17	61.07	15.00
187 ASN ND2	-9.66	33.42	62.75	15.00
187 ASN C	-5.92	32.36	64.14	15.00
187 ASN O	-5.90	31.63	63.13	15.00
188 TRP N	-4.89	32.50	64.96	15.00
188 TRP CA	-3.73	31.66	64.83	15.00
188 TRP CB	-2.53	32.41	65.32	15.00
188 TRP CG	-1.34	31.51	65.25	15.00
188 TRP CD2	-0.66	30.87	66.35	15.00
188 TRP CE2	0.34	30.12	65.83	15.00
188 TRP CE3	-0.81	30.87	67.72	15.00
188 TRP CD1	-0.72	31.11	64.13	15.00
188 TRP NE1	0.30	30.26	64.46	15.00
188 TRP CZ2	1.18	29.39	66.64	15.00
188 TRP CZ3	0.04	30.13	68.52	15.00
188 TRP CH2	0.98	29.43	68.01	15.00
188 TRP C	-3.93	30.46	65.72	15.00
188 TRP O	-4.69	30.59	66.69	15.00
189 GLY N	-3.29	29.33	65.40	15.00
189 GLY CA	-3.42	28.14	66.22	15.00
189 GLY C	-4.80	27.88	66.77	15.00
189 GLY O	-5.82	28.15	66.15	15.00
190 ASN N	-4.87	27.38	67.98	15.00
190 ASN CA	-6.16	27.08	68.58	15.00
190 ASN CB	-6.04	25.89	69.53	15.00
190 ASN CG	-7.37	25.28	69.86	15.00
190 ASN OD1	-8.42	25.95	69.81	15.00
190 ASN ND2	-7.34	24.00	70.23	15.00
190 ASN C	-6.70	28.34	69.26	15.00
190 ASN O	-6.57	28.50	70.46	15.00
191 LYS N	-7.23	29.26	68.47	15.00
191 LYS CA	-7.79	30.49	68.99	15.00
191 LYS CB	-9.10	30.17	69.71	15.00
191 LYS CG	-10.01	29.28	68.87	15.00
191 LYS CD	-10.50	29.93	67.53	15.00

TABLE X

191 LYS CE	-9.41	30.19	66.45	15.00
191 LYS NZ	-8.63	28.95	66.03	15.00
191 LYS C	-6.81	31.27	69.84	15.00
191 LYS O	-7.13	31.73	70.96	15.00
192 GLY N	-5.60	31.43	69.30	15.00
192 GLY CA	-4.58	32.18	70.01	15.00
192 GLY C	-3.63	31.36	70.87	15.00
192 GLY O	-2.54	31.86	71.19	15.00
193 TYR N	-4.03	30.16	71.27	15.00
193 TYR CA	-3.20	29.32	72.12	15.00
193 TYR CB	-4.03	28.72	73.28	15.00
193 TYR CG	-4.53	29.79	74.21	15.00
193 TYR CD1	-5.69	30.50	73.91	15.00
193 TYR CE1	-6.13	31.53	74.73	15.00
193 TYR CD2	-3.81	30.13	75.36	15.00
193 TYR CE2	-4.22	31.14	76.20	15.00
193 TYR CZ	-5.37	31.84	75.89	15.00
193 TYR OH	-5.74	32.89	76.71	15.00
193 TYR C	-2.54	28.21	71.35	15.00
193 TYR O	-2.85	27.94	70.17	15.00
194 ILE N	-1.68	27.50	72.06	15.00
194 ILE CA	-0.99	26.35	71.50	15.00
194 ILE CB	0.26	26.72	70.64	15.00
194 ILE CG2	1.18	27.65	71.44	15.00
194 ILE CG1	1.03	25.47	70.15	15.00
194 ILE CD1	2.16	25.76	69.14	15.00
194 ILE C	-0.54	25.54	72.70	15.00
194 ILE O	-0.28	26.08	73.75	15.00
195 LEU N	-0.56	24.23	72.57	15.00
195 LEU CA	-0.12	23.30	73.59	15.00
195 LEU CB	-1.11	22.15	73.67	15.00
195 LEU CG	-2.34	22.29	74.58	15.00
195 LEU CD1	-2.88	23.70	74.67	15.00
195 LEU CD2	-3.41	21.38	74.05	15.00
195 LEU C	1.21	22.81	73.09	15.00
195 LEU O	1.31	22.26	71.99	15.00
196 MET N	2.25	23.13	73.83	15.00
196 MET CA	3.58	22.69	73.45	15.00
196 MET CB	4.57	23.83	73.65	15.00
196 MET CG	4.29	24.99	72.69	15.00
196 MET SD	5.56	26.26	72.94	15.00
196 MET CE	7.08	25.68	71.98	15.00

TABLE X

196 MET C	3.97	21.45	74.27	15.00
196 MET O	3.31	21.15	75.28	15.00
197 ALA N	4.97	20.70	73.81	15.00
197 ALA CA	5.38	19.48	74.52	15.00
197 ALA CB	6.32	18.63	73.67	15.00
197 ALA C	6.01	19.71	75.90	15.00
197 ALA O	6.93	20.50	76.02	15.00
198 ARG N	5.56	19.01	76.94	15.00
198 ARG CA	6.13	19.21	78.27	15.00
198 ARG CB	5.05	19.61	79.26	15.00
198 ARG CG	5.46	19.52	80.76	15.00
198 ARG CD	4.45	20.21	81.65	15.00
198 ARG NE	3.20	19.48	81.76	15.00
198 ARG CZ	3.00	18.51	82.64	15.00
198 ARG NH1	3.99	18.18	83.47	15.00
198 ARG NH2	1.80	17.95	82.78	15.00
198 ARG C	6.82	17.93	78.72	15.00
198 ARG O	6.19	16.88	78.82	15.00
199 ASN N	8.13	18.02	78.90	15.00
199 ASN CA	8.99	16.89	79.34	15.00
199 ASN CB	8.28	15.93	80.33	15.00
199 ASN CG	8.26	16.47	81.77	15.00
199 ASN OD1	7.22	16.83	82.31	15.00
199 ASN ND2	9.45	16.55	82.38	15.00
199 ASN C	9.79	16.12	78.28	15.00
199 ASN O	10.49	15.17	78.61	15.00
200 LYS N	9.77	16.62	77.05	15.00
200 LYS CA	10.56	16.06	75.94	15.00
200 LYS CB	9.83	16.23	74.61	15.00
200 LYS CG	8.82	15.14	74.28	15.00
200 LYS CD	7.48	15.29	74.99	15.00
200 LYS CE	6.27	15.00	74.07	15.00
200 LYS NZ	6.29	13.60	73.43	15.00
200 LYS C	11.87	16.86	75.92	15.00
200 LYS O	12.15	17.61	74.99	15.00
201 ASN N	12.64	16.70	76.99	15.00
201 ASN CA	13.91	17.41	77.22	15.00
201 ASN CB	15.14	16.71	76.60	15.00
201 ASN CG	15.48	15.43	77.29	15.00
201 ASN OD1	15.33	14.36	76.70	15.00
201 ASN ND2	15.91	15.52	78.56	15.00
201 ASN C	13.91	18.86	76.81	15.00

TABLE X

201 ASN O	14.74	19.28	76.01	15.00
202 ASN N	13.02	19.62	77.41	15.00
202 ASN CA	12.87	21.05	77.17	15.00
202 ASN CB	13.98	21.82	77.88	15.00
202 ASN CG	13.66	23.27	78.07	15.00
202 ASN OD1	12.53	23.63	78.38	15.00
202 ASN ND2	14.63	24.12	77.83	15.00
202 ASN C	12.73	21.47	75.69	15.00
202 ASN O	13.48	22.28	75.16	15.00
203 ALA N	11.66	21.00	75.05	15.00
203 ALA H	11.06	20.52	75.65	15.00
203 ALA CA	11.34	21.22	73.64	15.00
203 ALA CB	10.03	20.53	73.27	15.00
203 ALA C	11.16	22.72	73.38	15.00
203 ALA O	10.25	23.38	73.78	15.00
204 CYS N	11.98	23.21	72.42	15.00
204 CYS CA	12.00	24.60	72.00	15.00
204 CYS C	12.56	25.58	73.01	15.00
204 CYS O	12.50	26.79	72.81	15.00
204 CYS CB	10.64	25.06	71.56	15.00
204 CYS SG	10.05	24.34	69.96	15.00
205 GLY N	13.03	25.04	74.13	15.00
205 GLY CA	13.63	25.86	75.14	15.00
205 GLY C	12.69	26.61	76.01	15.00
205 GLY O	13.03	27.59	76.63	15.00
206 ILE N	11.50	26.08	76.12	15.00
206 ILE CA	10.47	26.69	76.92	15.00
206 ILE CB	9.30	25.69	77.08	15.00
206 ILE CG2	9.78	24.44	77.78	15.00
206 ILE CG1	8.15	26.33	77.87	15.00
206 ILE CD1	7.20	27.12	77.00	15.00
206 ILE C	10.95	27.11	78.33	15.00
206 ILE O	10.50	28.12	78.86	15.00
207 ALA N	11.85	26.34	78.95	15.00
207 ALA CA	12.32	26.67	80.30	15.00
207 ALA CB	12.30	25.45	81.18	15.00
207 ALA C	13.68	27.35	80.43	15.00
207 ALA O	14.20	27.46	81.56	15.00
208 ASN N	14.21	27.84	79.31	15.00
208 ASN CA	15.51	28.52	79.26	15.00
208 ASN CB	16.13	28.39	77.88	15.00
208 ASN CG	16.75	27.01	77.59	15.00

TABLE X

208 ASN OD1	16.26	25.96	78.00	15.00
208 ASN ND2	17.86	27.03	76.88	15.00
208 ASN C	15.37	30.02	79.55	15.00
208 ASN O	16.37	30.73	79.73	15.00
209 LEU N	14.16	30.55	79.48	15.00
209 LEU CA	13.97	31.98	79.73	15.00
209 LEU CB	14.05	32.79	78.43	15.00
209 LEU CG	14.45	34.26	78.52	15.00
209 LEU CD1	15.95	34.30	78.78	15.00
209 LEU CD2	14.12	35.06	77.23	15.00
209 LEU C	12.71	32.35	80.51	15.00
209 LEU O	12.13	33.44	80.31	15.00
210 ALA N	12.37	31.55	81.52	15.00
210 ALA H	12.79	30.67	81.51	15.00
210 ALA CA	11.14	31.81	82.27	15.00
210 ALA CB	10.61	30.53	82.92	15.00
210 ALA C	11.43	32.81	83.41	15.00
210 ALA O	12.41	32.78	84.11	15.00
211 SER N	10.44	33.74	83.58	15.00
211 SER CA	10.44	34.68	84.69	15.00
211 SER CB	11.25	35.95	84.38	15.00
211 SER OG	10.66	36.74	83.37	15.00
211 SER C	8.97	35.02	85.03	15.00
211 SER O	8.07	34.77	84.22	15.00
212 PHE N	8.74	35.50	86.25	15.00
212 PHE CA	7.44	35.96	86.75	15.00
212 PHE CB	6.68	34.87	87.53	15.00
212 PHE CG	7.43	34.30	88.72	15.00
212 PHE CD1	8.34	33.31	88.54	15.00
212 PHE CD2	7.26	34.79	90.01	15.00
212 PHE CE1	9.08	32.83	89.64	15.00
212 PHE CE2	8.00	34.30	91.08	15.00
212 PHE CZ	8.90	33.33	90.90	15.00
212 PHE C	7.65	37.23	87.63	15.00
212 PHE O	8.64	37.35	88.34	15.00
213 PRO N	6.79	38.23	87.46	15.00
213 PRO CD	5.64	38.27	86.55	15.00
213 PRO CA	6.88	39.49	88.23	15.00
213 PRO CB	6.03	40.48	87.41	15.00
213 PRO CG	4.96	39.59	87.00	15.00
213 PRO C	6.30	39.32	89.66	15.00
213 PRO O	5.25	38.68	89.88	15.00

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TABLE X

214 LYS N	6.99	39.82	90.67	15.00
214 LYS CA	6.40	39.71	92.01	15.00
214 LYS CB	7.46	39.54	93.11	15.00
214 LYS CG	8.31	38.28	92.90	15.00
214 LYS CD	8.81	37.72	94.19	15.00
214 LYS CE	9.63	38.73	94.95	15.00
214 LYS NZ	10.60	39.41	94.05	15.00
214 LYS C	5.57	40.96	92.27	15.00
214 LYS O	5.99	42.07	91.94	15.00
215 MET N	4.33	40.78	92.72	15.00
215 MET CA	3.47	41.93	92.99	15.00
215 MET CB	2.11	41.74	92.32	15.00
215 MET CG	1.57	43.08	91.85	15.00
215 MET SD	-0.31	43.10	90.56	15.00
215 MET CE	-1.09	43.67	91.53	15.00
215 MET C	3.31	42.16	94.50	15.00
215 MET OT1	3.48	41.21	95.29	15.00
215 MET OT2	3.17	43.33	94.89	15.00
216 HOH OH2	8.87	46.84	97.48	15.00
217 HOH OH2	-2.18	37.97	73.56	15.00
218 HOH OH2	1.71	36.04	75.21	15.00
219 HOH OH2	9.44	52.65	61.91	15.00
220 HOH OH2	0.80	56.90	67.17	15.00
221 HOH OH2	-2.51	36.41	82.35	15.00
222 HOH OH2	17.40	43.23	83.47	15.00
223 HOH OH2	-1.57	52.44	64.46	15.00
224 HOH OH2	12.41	35.91	80.62	15.00
225 HOH OH2	11.65	62.93	58.36	15.00
226 HOH OH2	11.38	48.93	74.41	15.00
227 HOH OH2	5.00	12.95	78.69	15.00
228 HOH OH2	4.86	15.66	86.17	15.00
229 HOH OH2	-9.01	32.96	72.96	15.00
230 HOH OH2	14.02	19.79	82.02	15.00
231 HOH OH2	18.09	36.59	88.86	15.00
232 HOH OH2	0.22	37.62	76.69	15.00
233 HOH OH2	3.45	36.52	73.19	15.00
234 HOH OH2	13.53	38.17	80.00	15.00
235 HOH OH2	-15.93	48.59	69.63	15.00
236 HOH OH2	-5.38	44.85	97.00	15.00
237 HOH OH2	-7.89	45.15	89.13	15.00
238 HOH OH2	2.43	19.39	65.70	15.00
239 HOH OH2	7.43	21.65	71.07	15.00

TABLE X

240	HOH	OH2	2.41	16.41	85.78	15.00
241	HOH	OH2	-0.33	36.99	59.82	15.00
242	HOH	OH2	-7.54	26.54	72.89	15.00
243	HOH	OH2	-3.03	44.85	65.86	15.00
244	HOH	OH2	0.80	35.69	86.28	15.00
245	HOH	OH2	-9.57	36.85	95.54	15.00
246	HOH	OH2	-1.06	62.37	83.93	15.00
247	HOH	OH2	7.72	62.09	69.81	15.00
248	HOH	OH2	4.95	60.85	80.90	15.00
249	HOH	OH2	14.51	30.92	83.13	15.00
250	HOH	OH2	-1.50	28.47	63.31	15.00
251	HOH	OH2	15.32	22.32	71.31	15.00
252	HOH	OH2	-1.00	14.71	55.75	15.00
253	HOH	OH2	-6.77	18.87	84.05	15.00
254	HOH	OH2	-9.65	32.88	79.27	15.00
255	HOH	OH2	-2.32	34.26	69.09	15.00
256	HOH	OH2	-11.12	32.20	64.94	15.00
257	HOH	OH2	-3.80	45.19	72.07	15.00
258	HOH	OH2	-7.43	38.35	65.10	15.00
259	HOH	OH2	1.41	46.77	63.08	15.00
260	HOH	OH2	-3.18	37.41	80.05	15.00
261	HOH	OH2	7.12	59.13	81.53	15.00
262	HOH	OH2	9.18	59.65	79.58	15.00
263	HOH	OH2	8.43	57.49	83.56	15.00
264	HOH	OH2	22.06	33.25	80.24	15.00
265	HOH	OH2	20.66	27.84	95.17	15.00
266	HOH	OH2	17.09	49.08	84.72	15.00
267	HOH	OH2	12.06	54.25	84.82	15.00
268	HOH	OH2	9.93	50.78	92.92	15.00
269	HOH	OH2	13.59	41.50	91.19	15.00
270	HOH	OH2	11.18	49.64	64.47	15.00
271	HOH	OH2	12.14	55.71	75.81	15.00
272	HOH	OH2	9.07	26.37	66.15	15.00
273	HOH	OH2	24.27	24.31	64.11	15.00
274	HOH	OH2	18.35	21.16	79.19	15.00
275	HOH	OH2	20.62	28.49	61.87	15.00
276	HOH	OH2	13.58	15.19	72.83	15.00
277	HOH	OH2	9.33	19.74	77.14	15.00

TABLE XI

Table of angles between atoms of the inhibitor and protein for all protein atoms within 5 Ångstroms of the inhibitor 3(S)-3-[(N-benzyloxycarbonyl)-L-leucinyl]amino-5-methyl-1-(1-propoxy)-2-hexanone.

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
242OH2	25C1	18OD1	69.66	242OH2	25C1	18ND2	48.33
242OH2	25C1	184O	82.25	242OH2	25C1	18CG	62.66
242OH2	25C1	184C	92.20	18OD1	25C1	184CA	78.01
18OD1	25C1	18ND2	33.84	18OD1	25C1	184O	82.68
18OD1	25C1	184CD1	97.11	18OD1	25C1	18CG	16.91
18OD1	25C1	184C	73.04	18OD1	25C1	20O	60.56
184CB	25C1	184CA	23.31	184CB	25C1	18ND2	93.14
184CB	25C1	184O	42.27	184CB	25C1	184CG	22.32
184CB	25C1	184CD1	38.40	184CB	25C1	18CG	92.58
184CB	25C1	184C	36.61	184CB	25C1	184CD2	32.79
184CB	25C1	184NE1	49.18	184CA	25C1	18ND2	72.65
184CA	25C1	184O	35.91	184CA	25C1	184CG	38.24
184CA	25C1	184CD1	44.79	184CA	25C1	18CG	69.61
184CA	25C1	184C	21.48	184CA	25C1	184CD2	52.43
184CA	25C1	184NE1	58.86	18ND2	25C1	184O	58.28
18ND2	25C1	18CG	18.49	18ND2	25C1	184C	56.82
18ND2	25C1	20O	92.88	184O	25C1	184CG	64.55
184O	25C1	184CD1	78.02	184O	25C1	18CG	67.10
184O	25C1	184C	17.17	184O	25C1	184CD2	73.76
184O	25C1	184NE1	90.68	184CG	25C1	184CD1	19.59
184CG	25C1	184C	56.91	184CG	25C1	184CD2	15.07
184CG	25C1	184NE1	27.32	184CD1	25C1	18CG	99.42
184CD1	25C1	184C	66.13	184CD1	25C1	184CD2	27.32
184CD1	25C1	184NE1	14.36	184CD1	25C1	20O	86.22
18CG	25C1	184C	59.85	18CG	25C1	20O	77.46
184C	25C1	184CD2	69.30	184C	25C1	184NE1	80.01
184CD2	25C1	184NE1	26.78	184NE1	25C1	20O	80.98
18OD1	25C2	184CA	93.13	18OD1	25C2	18CG	18.16
18OD1	25C2	20N	42.62	18OD1	25C2	18ND2	35.44
18OD1	25C2	242OH2	68.83	18OD1	25C2	20O	79.33
18OD1	25C2	183O	73.73	18OD1	25C2	184C	80.63
18OD1	25C2	19CG	85.64	18OD1	25C2	20CA	45.72
18OD1	25C2	19N	47.90	18OD1	25C2	184O	85.52
18OD1	25C2	20C	65.28	18OD1	25C2	184N	90.71

TABLE XI

18OD1	25C2	19C	49.49	18OD1	25C2	18CB	22.83
18OD1	25C2	183C	82.72	18OD1	25C2	18CA	34.96
18OD1	25C2	18C	34.23	18OD1	25C2	19CA	54.26
184CD1	25C2	184CA	49.90	184CD1	25C2	184CB	40.27
184CD1	25C2	184CG	20.32	184CD1	25C2	183O	55.01
184CD1	25C2	184C	70.22	184CD1	25C2	19CG	61.53
184CD1	25C2	19N	85.18	184CD1	25C2	184O	78.11
184CD1	25C2	184NE1	15.62	184CD1	25C2	184N	44.48
184CD1	25C2	183C	47.20	184CD1	25C2	18CA	94.36
184CD1	25C2	18C	95.90	184CD1	25C2	184CD2	23.77
184CD1	25C2	19CA	87.00	184CA	25C2	18CG	78.59
184CA	25C2	18ND2	76.16	184CA	25C2	184CB	23.25
184CA	25C2	184CG	39.72	184CA	25C2	183O	40.92
184CA	25C2	184C	20.77	184CA	25C2	19CG	86.38
184CA	25C2	19N	76.16	184CA	25C2	184O	33.25
184CA	25C2	184NE1	65.31	184CA	25C2	184N	13.46
184CA	25C2	18CB	70.34	184CA	25C2	183C	28.93
184CA	25C2	18CA	61.99	184CA	25C2	18C	75.30
184CA	25C2	184CD2	51.97	184CA	25C2	19CA	89.58
18CG	25C2	20N	59.81	18CG	25C2	18ND2	20.07
18CG	25C2	184CB	99.39	18CG	25C2	242OH2	62.04
18CG	25C2	20O	97.48	18CG	25C2	183O	69.32
18CG	25C2	184C	63.66	18CG	25C2	19CG	95.51
18CG	25C2	20CA	63.78	18CG	25C2	19N	54.69
18CG	25C2	184O	67.41	18CG	25C2	20C	83.28
18CG	25C2	184N	79.10	18CG	25C2	19C	65.07
18CG	25C2	18CB	12.54	18CG	25C2	183C	75.08
18CG	25C2	18CA	30.58	18CG	25C2	18C	39.48
18CG	25C2	19CA	65.54	20N	25C2	18ND2	78.04
20N	25C2	20O	42.02	20N	25C2	183O	74.98
20N	25C2	19CG	52.80	20N	25C2	20CA	19.88
20N	25C2	19N	37.71	20N	25C2	20C	32.71
20N	25C2	19C	11.44	20N	25C2	18CB	58.04
20N	25C2	183C	87.83	20N	25C2	18CA	55.70
20N	25C2	18C	39.13	20N	25C2	19CA	28.06
18ND2	25C2	184CB	92.26	18ND2	25C2	242OH2	45.09
18ND2	25C2	183O	80.83	18ND2	25C2	184C	57.03
18ND2	25C2	20CA	77.75	18ND2	25C2	19N	73.94
18ND2	25C2	184O	55.05	18ND2	25C2	20C	96.02
18ND2	25C2	184N	81.33	18ND2	25C2	19C	84.52
18ND2	25C2	18CB	29.48	18ND2	25C2	183C	82.74
18ND2	25C2	18CA	46.57	18ND2	25C2	18C	58.80

TABLE XI

18ND2	25C2	19CA	85.56	184CB	25C2	184CG	22.40
184CB	25C2	183O	59.35	184CB	25C2	184C	36.03
184CB	25C2	19CG	94.64	184CB	25C2	19N	96.61
184CB	25C2	184O	38.77	184CB	25C2	184NE1	52.96
184CB	25C2	184N	31.46	184CB	25C2	18CB	92.63
184CB	25C2	183C	46.49	184CB	25C2	18CA	85.24
184CB	25C2	18C	97.95	184CB	25C2	184CD2	31.97
242OH2	25C2	184C	81.46	242OH2	25C2	20CA	87.88
242OH2	25C2	184O	68.50	242OH2	25C2	20C	95.83
242OH2	25C2	18CB	73.69	242OH2	25C2	18CA	91.46
184CG	25C2	183O	61.89	184CG	25C2	184C	57.17
184CG	25C2	19CG	81.07	184CG	25C2	19N	97.59
184CG	25C2	184O	61.14	184CG	25C2	184NE1	30.80
184CG	25C2	184N	40.66	184CG	25C2	183C	50.54
184CG	25C2	18CA	97.12	184CG	25C2	184CD2	12.85
20O	25C2	19CG	59.65	20O	25C2	20CA	33.80
20O	25C2	19N	73.93	20O	25C2	184NE1	98.68
20O	25C2	20C	15.00	20O	25C2	19C	44.20
20O	25C2	18CB	98.94	20O	25C2	18CA	97.51
20O	25C2	18C	80.19	20O	25C2	19CA	58.60
183O	25C2	184C	52.11	183O	25C2	19CG	50.15
183O	25C2	20CA	94.61	183O	25C2	19N	37.44
183O	25C2	184O	68.46	183O	25C2	184NE1	67.20
183O	25C2	184N	28.51	183O	25C2	19C	66.39
183O	25C2	18CB	56.86	183O	25C2	183C	12.86
183O	25C2	18CA	39.61	183O	25C2	18C	42.74
183O	25C2	184CD2	73.55	183O	25C2	19CA	48.97
184C	25C2	19N	79.88	184C	25C2	184O	16.37
184C	25C2	184NE1	85.33	184C	25C2	184N	31.43
184C	25C2	18CB	58.56	184C	25C2	183C	43.26
184C	25C2	18CA	56.66	184C	25C2	18C	73.56
184C	25C2	184CD2	67.95	184C	25C2	19CA	95.56
19CG	25C2	20CA	68.54	19CG	25C2	19N	41.00
19CG	25C2	184NE1	59.71	19CG	25C2	20C	65.93
19CG	25C2	184N	72.99	19CG	25C2	19C	41.61
19CG	25C2	18CB	85.55	19CG	25C2	183C	58.81
19CG	25C2	18CA	69.73	19CG	25C2	18C	56.16
19CG	25C2	184CD2	84.49	19CG	25C2	19CA	31.40
20CA	25C2	19N	57.18	20CA	25C2	20C	19.60
20CA	25C2	19C	30.27	20CA	25C2	18CB	66.65
20CA	25C2	18CA	70.02	20CA	25C2	18C	55.87
20CA	25C2	19CA	47.75	19N	25C2	184O	94.75

TABLE XI

19N	25C2	184NE1	91.69	19N	25C2	20C	69.08
19N	25C2	184N	65.26	19N	25C2	19C	30.47
19N	25C2	18CB	44.60	19N	25C2	183C	50.23
19N	25C2	18CA	30.19	19N	25C2	18C	15.21
19N	25C2	19CA	16.11	184O	25C2	184NE1	91.68
184O	25C2	184N	45.89	184O	25C2	18CB	65.91
184O	25C2	183C	59.15	184O	25C2	18CA	68.65
184O	25C2	18C	86.43	184O	25C2	184CD2	69.23
184NE1	25C2	184N	60.01	184NE1	25C2	183C	61.27
184NE1	25C2	184CD2	26.96	184NE1	25C2	19CA	89.32
20C	25C2	19C	38.71	20C	25C2	18CB	86.12
20C	25C2	18CA	87.75	20C	25C2	18C	71.80
20C	25C2	19CA	55.73	184N	25C2	19C	94.86
184N	25C2	18CB	68.81	184N	25C2	183C	15.92
184N	25C2	18CA	56.71	184N	25C2	18C	67.03
184N	25C2	184CD2	53.50	184N	25C2	19CA	77.48
19C	25C2	18CB	60.71	19C	25C2	183C	79.19
19C	25C2	18CA	54.22	19C	25C2	18C	36.38
19C	25C2	19CA	17.76	18CB	25C2	183C	63.21
18CB	25C2	18CA	18.13	18CB	25C2	18C	29.64
18CB	25C2	19CA	57.42	183C	25C2	18CA	47.76
183C	25C2	18C	54.26	183C	25C2	184CD2	62.80
183C	25C2	19CA	61.67	18CA	25C2	18C	17.97
18CA	25C2	19CA	45.40	18C	25C2	19CA	28.26
20O	25C3	19CG	77.70	20O	25C3	20N	48.86
20O	25C3	18OD1	82.41	20O	25C3	20C	15.02
20O	25C3	20CA	36.52	20O	25C3	19CD	82.71
20O	25C3	19C	49.69	20O	25C3	19N	81.60
20O	25C3	19CB	69.52	20O	25C3	18CG	93.56
20O	25C3	19OE1	97.10	20O	25C3	19CA	66.55
184CD1	25C3	19CG	70.95	184CD1	25C3	184NE1	20.32
184CD1	25C3	184CG	17.18	184CD1	25C3	19CD	63.15
184CD1	25C3	19N	84.37	184CD1	25C3	184CA	41.74
184CD1	25C3	183O	51.08	184CD1	25C3	19CB	82.21
184CD1	25C3	184CB	33.05	184CD1	25C3	18CG	99.94
184CD1	25C3	19OE1	48.60	184CD1	25C3	19CA	92.55
184CD1	25C3	184CE2	24.46	19CG	25C3	20N	60.87
19CG	25C3	18OD1	86.79	19CG	25C3	20C	80.83
19CG	25C3	184NE1	70.80	19CG	25C3	20CA	78.71
19CG	25C3	184CG	86.74	19CG	25C3	19CD	19.15
19CG	25C3	19C	46.56	19CG	25C3	19N	42.15
19CG	25C3	184CA	83.50	19CG	25C3	183O	50.42

TABLE XI

19CG	25C3	19CB	14.34	19CG	25C3	184CB	93.55
19CG	25C3	18CG	90.03	19CG	25C3	19OE1	29.89
19CG	25C3	19CA	32.74	19CG	25C3	184CE2	83.95
20N	25C3	18OD1	40.95	20N	25C3	20C	38.02
20N	25C3	20CA	21.15	20N	25C3	19CD	78.19
20N	25C3	19C	14.72	20N	25C3	19N	36.90
20N	25C3	184CA	98.63	20N	25C3	183O	71.83
20N	25C3	19CB	46.57	20N	25C3	18CG	51.19
20N	25C3	19OE1	90.75	20N	25C3	19CA	30.28
20N	25C3	242OH2	86.06	18OD1	25C3	20C	67.75
18OD1	25C3	20CA	45.89	18OD1	25C3	19C	52.30
18OD1	25C3	19N	45.18	18OD1	25C3	184CA	70.04
18OD1	25C3	183O	62.55	18OD1	25C3	19CB	74.34
18OD1	25C3	184CB	86.92	18OD1	25C3	18CG	11.19
18OD1	25C3	19CA	55.77	18OD1	25C3	242OH2	51.35
20C	25C3	20CA	22.11	20C	25C3	19CD	90.19
20C	25C3	19C	43.18	20C	25C3	19N	73.89
20C	25C3	19CB	69.80	20C	25C3	18CG	78.83
20C	25C3	19CA	61.77	20C	25C3	242OH2	89.06
184NE1	25C3	184CG	32.04	184NE1	25C3	19CD	56.99
184NE1	25C3	19N	96.67	184NE1	25C3	184CA	61.92
184NE1	25C3	183O	67.54	184NE1	25C3	19CB	84.48
184NE1	25C3	184CB	50.65	184NE1	25C3	19OE1	42.30
184NE1	25C3	19CA	99.57	184NE1	25C3	184CE2	13.16
20CA	25C3	19CD	93.68	20CA	25C3	19C	32.85
20CA	25C3	19N	57.68	20CA	25C3	183O	91.89
20CA	25C3	19CB	64.99	20CA	25C3	18CG	57.06
20CA	25C3	19CA	50.80	20CA	25C3	242OH2	76.89
184CG	25C3	19CD	80.27	184CG	25C3	19N	91.72
184CG	25C3	184CA	34.06	184CG	25C3	183O	56.45
184CG	25C3	19CB	96.63	184CG	25C3	184CB	18.84
184CG	25C3	18CG	93.58	184CG	25C3	19OE1	65.78
184CG	25C3	184CE2	28.26	184CG	25C3	242OH2	94.95
19CD	25C3	19C	63.50	19CD	25C3	19N	60.85
19CD	25C3	184CA	88.20	19CD	25C3	183O	60.91
19CD	25C3	19CB	32.82	19CD	25C3	184CB	92.35
19CD	25C3	19OE1	14.96	19CD	25C3	19CA	51.66
19CD	25C3	184CE2	69.81	19C	25C3	19N	31.91
19C	25C3	184CA	98.36	19C	25C3	183O	66.62
19C	25C3	19CB	32.43	19C	25C3	18CG	61.26
19C	25C3	19OE1	76.35	19C	25C3	19CA	18.84
19N	25C3	184CA	66.70	19N	25C3	183O	35.29

TABLE XI

19N	25C3	19CB	31.75	19N	25C3	184CB	85.03
19N	25C3	18CG	47.94	19N	25C3	19OE1	67.18
19N	25C3	19CA	17.97	19N	25C3	242OH2	95.18
184CA	25C3	183O	35.33	184CA	25C3	19CB	86.05
184CA	25C3	184CB	19.26	184CA	25C3	18CG	59.77
184CA	25C3	19OE1	78.16	184CA	25C3	19CA	83.25
184CA	25C3	184CE2	61.84	184CA	25C3	242OH2	75.15
183O	25C3	19CB	50.84	183O	25C3	184CB	51.32
183O	25C3	18CG	57.48	183O	25C3	19OE1	57.08
183O	25C3	19CA	49.31	183O	25C3	184CE2	75.42
183O	25C3	242OH2	96.01	19CB	25C3	184CB	99.69
19CB	25C3	18CG	79.10	19CB	25C3	19OE1	44.22
19CB	25C3	19CA	18.92	19CB	25C3	184CE2	97.58
184CB	25C3	18CG	76.03	184CB	25C3	19OE1	79.22
184CB	25C3	184CE2	46.73	184CB	25C3	242OH2	78.05
18CG	25C3	19CA	61.53	18CG	25C3	242OH2	47.27
19OE1	25C3	19CA	62.05	19OE1	25C3	184CE2	55.29
20O	25C4	20C	10.43	20O	25C4	19CG	62.30
20O	25C4	20N	35.25	20O	25C4	20CA	26.32
20O	25C4	19CD	71.57	20O	25C4	21NE2	50.82
20O	25C4	18OD1	61.89	184CD1	25C4	184NE1	20.27
184CD1	25C4	19CG	57.56	184CD1	25C4	184CG	16.41
184CD1	25C4	184CE2	28.68	184CD1	25C4	20N	90.35
184CD1	25C4	19CD	54.84	184CD1	25C4	18OD1	81.65
184CD1	25C4	184CD2	25.56	184NE1	25C4	19CG	61.65
184NE1	25C4	184CG	29.79	184NE1	25C4	184CE2	15.87
184NE1	25C4	19CD	51.78	184NE1	25C4	184CD2	25.93
20C	25C4	19CG	66.50	20C	25C4	20N	31.03
20C	25C4	20CA	17.90	20C	25C4	19CD	78.21
20C	25C4	21NE2	44.60	20C	25C4	18OD1	53.90
19CG	25C4	184CG	72.66	19CG	25C4	184CE2	77.52
19CG	25C4	20N	46.19	19CG	25C4	20CA	61.94
19CG	25C4	19CD	18.17	19CG	25C4	18OD1	63.67
19CG	25C4	184CD2	82.38	184CG	25C4	184CE2	28.98
184CG	25C4	20N	98.65	184CG	25C4	19CD	71.23
184CG	25C4	18OD1	82.35	184CG	25C4	184CD2	16.48
184CE2	25C4	19CD	67.12	184CE2	25C4	184CD2	16.42
20N	25C4	20CA	17.47	20N	25C4	19CD	63.14
20N	25C4	21NE2	68.18	20N	25C4	18OD1	30.69
20CA	25C4	19CD	77.50	20CA	25C4	21NE2	50.79
20CA	25C4	18OD1	36.03	19CD	25C4	18OD1	81.70
19CD	25C4	184CD2	76.27	21NE2	25C4	18OD1	71.09

TABLE XI

18OD1	25C4	184CD2	98.63	184CD1	25C5	20O	89.99
184CD1	25C5	184NE1	17.97	184CD1	25C5	184CG	17.29
184CD1	25C5	184CE2	27.88	184CD1	25C5	242OH2	99.26
184CD1	25C5	184CD2	27.37	20O	25C5	184NE1	92.08
20O	25C5	242OH2	86.50	20O	25C5	21NE2	47.88
184NE1	25C5	184CG	28.79	184NE1	25C5	184CE2	16.62
184NE1	25C5	184CD2	27.40	184CG	25C5	184CE2	28.30
184CG	25C5	242OH2	92.08	184CG	25C5	184CD2	17.13
184CE2	25C5	184CD2	16.84	242OH2	25C5	21NE2	65.12
242OH2	25C6	184CB	96.30	242OH2	25C6	184CA	83.88
242OH2	25C6	18OD1	51.77	242OH2	25C6	184O	63.15
184CG	25C6	184CD1	17.92	184CG	25C6	184CB	19.89
184CG	25C6	184CD2	17.11	184CG	25C6	184NE1	27.45
184CG	25C6	184CA	31.62	184CG	25C6	18OD1	84.34
184CG	25C6	184O	53.51	184CD1	25C6	184CB	33.90
184CD1	25C6	184CD2	27.70	184CD1	25C6	184NE1	16.02
184CD1	25C6	184CA	37.26	184CD1	25C6	18OD1	76.75
184CD1	25C6	184O	64.28	184CB	25C6	184CD2	32.92
184CB	25C6	184NE1	46.79	184CB	25C6	184CA	18.16
184CB	25C6	18OD1	76.20	184CB	25C6	184O	33.78
184CD2	25C6	184NE1	26.79	184CD2	25C6	184CA	47.98
184CD2	25C6	184O	65.87	184NE1	25C6	184CA	53.03
184NE1	25C6	18OD1	88.79	184NE1	25C6	184O	79.21
184CA	25C6	18OD1	58.04	184CA	25C6	184O	28.15
18OD1	25C6	184O	61.50	20O	25C7	20C	4.43
20O	25C7	19CG	62.28	20O	25C7	19CD	77.38
20O	25C7	19NE2	74.82	20O	25C7	19OE1	90.67
184NE1	25C7	19CG	59.54	184NE1	25C7	19CD	53.46
184NE1	25C7	184CD1	17.49	184NE1	25C7	19NE2	66.80
184NE1	25C7	19OE1	40.08	184NE1	25C7	184CE2	14.60
20C	25C7	19CG	65.46	20C	25C7	19CD	81.18
20C	25C7	19NE2	79.11	20C	25C7	19OE1	94.22
19CG	25C7	19CD	19.72	19CG	25C7	184CD1	52.93
19CG	25C7	19NE2	30.67	19CG	25C7	19OE1	29.47
19CG	25C7	184CE2	74.12	19CD	25C7	184CD1	53.97
19CD	25C7	19NE2	16.35	19CD	25C7	19OE1	14.31
19CD	25C7	184CE2	67.37	184CD1	25C7	19NE2	69.74
184CD1	25C7	19OE1	43.73	184CD1	25C7	184CE2	26.87
19NE2	25C7	19OE1	26.90	19NE2	25C7	184CE2	79.58
19OE1	25C7	184CE2	53.50	184NE1	25O8	19CD	69.28
184NE1	25O8	19NE2	88.26	184NE1	25O8	19OE1	52.70
184NE1	25O8	19CG	72.15	184NE1	25O8	184CD1	18.62

TABLE XI

184NE1	25O8	184CE2	15.78	184NE1	25O8	184CZ2	30.82
19CD	25O8	19NE2	21.45	19CD	25O8	19OE1	19.40
19CD	25O8	19CG	23.73	19CD	25O8	20O	83.60
19CD	25O8	184CD1	65.36	19CD	25O8	184CE2	84.12
19CD	25O8	22O	53.07	19CD	25O8	184CZ2	93.15
19NE2	25O8	19OE1	35.59	19NE2	25O8	19CG	38.13
19NE2	25O8	20O	82.17	19NE2	25O8	184CD1	86.56
19NE2	25O8	22O	36.04	19OE1	25O8	19CG	37.46
19OE1	25O8	184CD1	53.61	19OE1	25O8	184CE2	66.40
19OE1	25O8	22O	70.80	19OE1	25O8	184CZ2	73.99
19CG	25O8	20O	63.71	19CG	25O8	184CD1	60.70
19CG	25O8	184CE2	87.89	19CG	25O8	22O	54.69
20O	25O8	22O	57.31	184CD1	25O8	184CE2	30.67
184CD1	25O8	184CZ2	47.47	184CE2	25O8	184CZ2	16.93
19NE2	25C9	184NE1	78.75	19NE2	25C9	19CD	19.52
19NE2	25C9	19OE1	33.07	19NE2	25C9	184CE2	94.10
19NE2	25C9	19CG	30.70	19NE2	25C9	184CD1	73.44
19NE2	25C9	22O	33.46	184NE1	25C9	19CD	59.66
184NE1	25C9	19OE1	47.23	184NE1	25C9	184CE2	16.38
184NE1	25C9	184CZ2	33.08	184NE1	25C9	19CG	58.24
184NE1	25C9	184CD1	12.56	19CD	25C9	19OE1	17.75
19CD	25C9	184CE2	75.46	19CD	25C9	184CZ2	89.07
19CD	25C9	19CG	17.50	19CD	25C9	184CD1	53.92
19CD	25C9	22O	48.71	19OE1	25C9	184CE2	61.55
19OE1	25C9	184CZ2	73.08	19OE1	25C9	19CG	30.61
19OE1	25C9	184CD1	45.28	19OE1	25C9	22O	65.42
184CE2	25C9	184CZ2	17.56	184CE2	25C9	19CG	74.59
184CE2	25C9	184CD1	26.94	184CZ2	25C9	19CG	90.93
184CZ2	25C9	184CD1	44.43	19CG	25C9	184CD1	48.87
19CG	25C9	22O	48.21	184CD1	25C9	22O	97.02
19NE2	25O10	23CA	53.09	19NE2	25O10	19CD	16.71
19NE2	25O10	22O	36.83	19NE2	25O10	23N	57.66
19NE2	25O10	19OE1	28.25	19NE2	25O10	22C	50.13
23CA	25O10	19CD	69.80	23CA	25O10	22O	36.05
23CA	25O10	23N	17.68	23CA	25O10	19OE1	79.02
23CA	25O10	22C	29.83	19CD	25O10	22O	49.55
19CD	25O10	23N	73.42	19CD	25O10	19OE1	15.11
19CD	25O10	22C	63.87	22O	25O10	23N	27.96
22O	25O10	19OE1	63.96	22O	25O10	22C	14.56
23N	25O10	19OE1	85.79	23N	25O10	22C	15.87
19OE1	25O10	22C	77.94	162ND1	25C11	184CZ2	63.39
162ND1	25C11	162CE1	16.78	162ND1	25C11	184NE1	61.01

TABLE XI

162ND1	25C11	184CE2	62.72	162ND1	25C11	162CG	15.67
162ND1	25C11	184CH2	68.93	162ND1	25C11	162CB	30.11
184CZ2	25C11	162CE1	53.21	184CZ2	25C11	184NE1	33.69
184CZ2	25C11	184CE2	16.65	184CZ2	25C11	162CG	59.25
184CZ2	25C11	184CH2	12.22	184CZ2	25C11	162CB	70.77
162CE1	25C11	184NE1	44.59	162CE1	25C11	184CE2	48.65
162CE1	25C11	162CG	27.93	162CE1	25C11	184CH2	61.58
162CE1	25C11	162CB	44.93	184NE1	25C11	184CE2	17.24
184NE1	25C11	162CG	67.01	184NE1	25C11	184CH2	45.73
184NE1	25C11	162CB	83.92	184CE2	25C11	162CG	63.63
184CE2	25C11	184CH2	28.52	184CE2	25C11	162CB	78.45
162CG	25C11	184CH2	61.52	162CG	25C11	162CB	17.47
184CH2	25C11	162CB	69.67	138OG	25C15	138CB	12.25
138OG	25C15	138CA	28.90	138OG	25C15	161OD1	38.49
138CB	25C15	138CA	18.42	138CB	25C15	161OD1	45.39
138CA	25C15	161OD1	48.24	162ND1	25C16	161O	83.50
162ND1	25C16	162CG	18.14	162ND1	25C16	162CE1	16.51
162ND1	25C16	162CB	37.71	162ND1	25C16	25SG	53.12
162ND1	25C16	162CA	45.79	162ND1	25C16	161C	76.59
162ND1	25C16	184CZ2	58.80	162ND1	25C16	25CB	44.47
162ND1	25C16	162N	61.56	162ND1	25C16	19OE1	54.44
161O	25C16	162CG	73.87	161O	25C16	162CE1	99.61
161O	25C16	162CB	55.47	161O	25C16	25SG	68.22
161O	25C16	162CA	38.54	161O	25C16	161C	12.03
161O	25C16	25CB	87.95	161O	25C16	162N	25.97
162CG	25C16	162CE1	32.06	162CG	25C16	162CB	21.17
162CG	25C16	25SG	64.52	162CG	25C16	162CA	35.58
162CG	25C16	161C	64.63	162CG	25C16	184CZ2	58.11
162CG	25C16	25CB	60.75	162CG	25C16	162N	48.98
162CG	25C16	19OE1	71.80	162CE1	25C16	162CB	53.00
162CE1	25C16	25SG	57.54	162CE1	25C16	162CA	62.27
162CE1	25C16	161C	93.08	162CE1	25C16	184CZ2	50.19
162CE1	25C16	25CB	42.26	162CE1	25C16	162N	78.06
162CE1	25C16	19OE1	40.00	162CB	25C16	25SG	70.05
162CB	25C16	162CA	20.87	162CB	25C16	161C	44.96
162CB	25C16	184CZ2	71.73	162CB	25C16	25CB	73.86
162CB	25C16	162N	29.56	162CB	25C16	19OE1	92.15
25SG	25C16	162CA	56.57	25SG	25C16	161C	72.16
25SG	25C16	25CB	21.35	25SG	25C16	162N	67.66
25SG	25C16	19OE1	58.28	162CA	25C16	161C	30.81
162CA	25C16	184CZ2	91.78	162CA	25C16	25CB	67.26
162CA	25C16	162N	16.41	162CA	25C16	19OE1	95.96

TABLE XI

161C	25C16	25CB	89.77	161C	25C16	162N	15.65
184CZ2	25C16	25CB	89.70	184CZ2	25C16	19OE1	64.53
25CB	25C16	162N	81.65	25CB	25C16	19OE1	37.30
162ND1	25O17	162CB	53.19	162ND1	25O17	162CG	26.33
162ND1	25O17	162CA	63.48	162ND1	25O17	162N	85.18
162ND1	25O17	162CE1	12.84	162ND1	25O17	25SG	56.41
162ND1	25O17	162CD2	24.16	162ND1	25O17	162C	54.50
162ND1	25O17	162NE2	14.17	162ND1	25O17	184CZ2	59.71
162ND1	25O17	163N	47.86	162ND1	25O17	25CB	41.51
162CB	25O17	161O	76.56	162CB	25O17	162CG	28.45
162CB	25O17	162CA	28.85	162CB	25O17	161C	60.68
162CB	25O17	162N	40.36	162CB	25O17	162CE1	64.12
162CB	25O17	25SG	83.81	162CB	25O17	161OD1	58.91
162CB	25O17	162CD2	36.23	162CB	25O17	162C	31.62
162CB	25O17	162NE2	52.83	162CB	25O17	184CZ2	81.36
162CB	25O17	163N	44.40	162CB	25O17	25CB	83.22
162CB	25O17	161CA	66.51	162CB	25O17	161CB	74.63
161O	25O17	162CA	52.04	161O	25O17	161C	18.10
161O	25O17	162N	36.49	161O	25O17	25SG	77.20
161O	25O17	161OD1	60.19	161O	25O17	162C	58.32
161O	25O17	163N	63.78	161O	25O17	25CB	97.03
161O	25O17	161CA	21.34	161O	25O17	161CB	35.39
162CG	25O17	162CA	48.03	162CG	25O17	161C	86.77
162CG	25O17	162N	66.31	162CG	25O17	162CE1	35.94
162CG	25O17	25SG	73.55	162CG	25O17	161OD1	84.63
162CG	25O17	162CD2	9.57	162CG	25O17	162C	43.30
162CG	25O17	162NE2	24.46	162CG	25O17	184CZ2	61.90
162CG	25O17	163N	46.12	162CG	25O17	25CB	64.34
162CG	25O17	161CA	94.08	162CA	25O17	161C	40.53
162CA	25O17	162N	22.22	162CA	25O17	162CE1	76.31
162CA	25O17	25SG	66.07	162CA	25O17	161OD1	63.93
162CA	25O17	162CD2	57.57	162CA	25O17	162C	11.05
162CA	25O17	162NE2	70.12	162CA	25O17	163N	26.62
162CA	25O17	25CB	74.60	162CA	25O17	161CA	50.08
162CA	25O17	161CB	64.72	161C	25O17	162N	20.53
161C	25O17	25SG	84.94	161C	25O17	161OD1	45.99
161C	25O17	162CD2	95.86	161C	25O17	162C	49.50
161C	25O17	163N	59.81	161C	25O17	161CA	11.07
161C	25O17	161CB	28.61	162N	25O17	162CE1	97.92
162N	25O17	25SG	81.29	162N	25O17	161OD1	46.28
162N	25O17	162CD2	75.34	162N	25O17	162C	32.79
162N	25O17	162NE2	90.12	162N	25O17	163N	46.59

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TABLE XI

162N	25O17	25CB	94.05	162N	25O17	161CA	28.47
162N	25O17	161CB	42.50	162CE1	25O17	25SG	60.41
162CE1	25O17	162CD2	30.63	162CE1	25O17	162C	67.29
162CE1	25O17	162NE2	14.05	162CE1	25O17	184CZ2	50.87
162CE1	25O17	163N	59.73	162CE1	25O17	25CB	42.09
25SG	25O17	162CD2	77.38	25SG	25O17	162C	56.56
25SG	25O17	162NE2	70.26	25SG	25O17	163N	40.80
25SG	25O17	25CB	20.52	25SG	25O17	161CA	94.97
161OD1	25O17	162CD2	88.85	161OD1	25O17	162C	74.74
161OD1	25O17	163N	90.55	161OD1	25O17	161CA	38.88
161OD1	25O17	161CB	28.90	162CD2	25O17	162C	52.76
162CD2	25O17	162NE2	17.33	162CD2	25O17	184CZ2	52.52
162CD2	25O17	163N	54.44	162CD2	25O17	25CB	65.18
162C	25O17	162NE2	62.89	162C	25O17	163N	16.06
162C	25O17	25CB	63.70	162C	25O17	161CA	59.72
162C	25O17	161CB	75.18	162NE2	25O17	184CZ2	46.51
162NE2	25O17	163N	59.43	162NE2	25O17	25CB	53.98
184CZ2	25O17	25CB	88.90	163N	25O17	25CB	48.07
163N	25O17	161CA	70.75	163N	25O17	161CB	87.59
161CA	25O17	161CB	17.64	25SG	25N18	162ND1	54.05
25SG	25N18	161O	72.12	25SG	25N18	25CB	22.85
25SG	25N18	19NE2	68.04	25SG	25N18	23CA	83.69
25SG	25N18	162CE1	55.83	25SG	25N18	162CA	54.53
25SG	25N18	19OE1	61.94	25SG	25N18	162CG	59.80
25SG	25N18	162CB	64.56	162ND1	25N18	161O	73.75
162ND1	25N18	25CB	47.82	162ND1	25N18	19NE2	80.11
162ND1	25N18	162CE1	14.94	162ND1	25N18	162CA	39.62
162ND1	25N18	19OE1	53.76	162ND1	25N18	162CG	12.62
162ND1	25N18	162CB	29.54	161O	25N18	25CB	91.76
161O	25N18	162CE1	88.51	161O	25N18	162CA	34.27
161O	25N18	162CG	63.44	161O	25N18	162CB	47.06
25CB	25N18	19NE2	48.54	25CB	25N18	23CA	78.61
25CB	25N18	162CE1	42.68	25CB	25N18	162CA	66.30
25CB	25N18	19OE1	39.11	25CB	25N18	162CG	58.13
25CB	25N18	162CB	69.62	19NE2	25N18	23CA	48.32
19NE2	25N18	162CE1	66.29	19NE2	25N18	19OE1	27.62
19NE2	25N18	162CG	92.70	23CA	25N18	19OE1	75.78
162CE1	25N18	162CA	54.27	162CE1	25N18	19OE1	39.27
162CE1	25N18	162CG	26.90	162CE1	25N18	162CB	44.19
162CA	25N18	19OE1	90.56	162CA	25N18	162CG	30.46
162CA	25N18	162CB	17.73	19OE1	25N18	162CG	66.12
19OE1	25N18	162CB	83.30	162CG	25N18	162CB	17.35

TABLE XI

25SG	25C19	161O	94.77	25SG	25C19	162ND1	55.31
25SG	25C19	25CB	20.96	25SG	25C19	162CA	63.69
25SG	25C19	161C	89.52	25SG	25C19	23CA	94.30
25SG	25C19	23O	76.83	25SG	25C19	23C	78.19
25SG	25C19	162N	77.13	25SG	25C19	25N	39.34
25SG	25C19	19NE2	66.56	25SG	25C19	163N	35.68
25SG	25C19	162CE1	52.07	25SG	25C19	162CB	68.67
161O	25C19	162ND1	77.82	161O	25C19	162CA	38.27
161O	25C19	161C	6.45	161O	25C19	162N	21.62
161O	25C19	163N	59.92	161O	25C19	162CE1	90.20
161O	25C19	162CB	47.78	162ND1	25C19	25CB	49.17
162ND1	25C19	162CA	42.28	162ND1	25C19	161C	71.68
162ND1	25C19	162N	57.38	162ND1	25C19	25N	77.84
162ND1	25C19	19NE2	72.32	162ND1	25C19	163N	45.25
162ND1	25C19	162CE1	12.42	162ND1	25C19	162CB	30.12
25CB	25C19	162CA	73.53	25CB	25C19	23CA	82.52
25CB	25C19	23O	74.24	25CB	25C19	23C	70.22
25CB	25C19	162N	89.39	25CB	25C19	25N	30.03
25CB	25C19	19NE2	46.97	25CB	25C19	163N	50.32
25CB	25C19	162CE1	41.12	25CB	25C19	162CB	72.32
162CA	25C19	161C	31.82	162CA	25C19	162N	16.65
162CA	25C19	163N	29.20	162CA	25C19	162CE1	53.97
162CA	25C19	162CB	17.00	161C	25C19	162N	15.17
161C	25C19	163N	54.26	161C	25C19	162CE1	84.02
161C	25C19	162CB	41.75	23CA	25C19	23O	29.88
23CA	25C19	23C	18.55	23CA	25C19	25N	55.13
23CA	25C19	19NE2	45.62	23O	25C19	23C	14.86
23O	25C19	25N	44.51	23O	25C19	19NE2	58.93
23C	25C19	25N	40.60	23C	25C19	19NE2	45.52
162N	25C19	163N	41.46	162N	25C19	162CE1	69.54
162N	25C19	162CB	28.25	25N	25C19	19NE2	36.78
25N	25C19	163N	74.96	25N	25C19	162CE1	67.79
19NE2	25C19	163N	96.25	19NE2	25C19	162CE1	59.92
163N	25C19	162CE1	51.59	163N	25C19	162CB	39.57
162CE1	25C19	162CB	42.53	161O	25C20	25SG	71.78
161O	25C20	161C	1.07	25SG	25C20	23CA	80.86
25SG	25C20	23O	69.40	25SG	25C20	23C	68.41
25SG	25C20	161C	71.72	23CA	25C20	23O	30.94
23CA	25C20	23C	18.34	23O	25C20	23C	14.77
161O	25C21	161C	6.69	161O	25C22	161C	13.34
161O	25C22	161CA	34.90	161O	25C22	161CB	44.27
161C	25C22	161CA	21.77	161C	25C22	161CB	34.39

TABLE XI

161CA	25C22	161CB	20.42	184NE1	25N24	184CZ2	42.68
184NE1	25N24	184CE2	21.38	184NE1	25N24	19OE1	49.07
184NE1	25N24	162ND1	68.83	184NE1	25N24	162CE1	51.55
184NE1	25N24	19CD	58.30	184NE1	25N24	19NE2	75.34
184NE1	25N24	184CD1	9.07	184NE1	25N24	184CH2	51.38
184CZ2	25N24	184CE2	21.94	184CZ2	25N24	19OE1	85.09
184CZ2	25N24	162ND1	64.71	184CZ2	25N24	162CE1	57.67
184CZ2	25N24	19CD	98.31	184CZ2	25N24	184CD1	50.33
184CZ2	25N24	184CH2	9.57	184CE2	25N24	19OE1	68.35
184CE2	25N24	162ND1	68.77	184CE2	25N24	162CE1	55.33
184CE2	25N24	19CD	79.25	184CE2	25N24	19NE2	96.20
184CE2	25N24	184CD1	28.46	184CE2	25N24	184CH2	30.12
19OE1	25N24	162ND1	58.04	19OE1	25N24	162CE1	44.62
19OE1	25N24	19CD	16.03	19OE1	25N24	19NE2	29.68
19OE1	25N24	184CD1	47.21	19OE1	25N24	184CH2	94.65
162ND1	25N24	162CE1	18.14	162ND1	25N24	19CD	72.35
162ND1	25N24	19NE2	76.87	162ND1	25N24	184CD1	75.84
162ND1	25N24	184CH2	69.90	162CE1	25N24	19CD	60.33
162CE1	25N24	19NE2	69.25	162CE1	25N24	184CD1	58.03
162CE1	25N24	184CH2	65.20	19CD	25N24	19NE2	17.04
19CD	25N24	184CD1	53.84	19NE2	25N24	184CD1	70.73
184CD1	25N24	184CH2	58.50	25SG	25C25	25CB	32.75
25SG	25C25	25N	68.12	25SG	25C25	25CA	46.11
25SG	25C25	19NE2	91.26	25SG	25C25	162ND1	50.45
25SG	25C25	161O	83.98	25SG	25C25	26N	50.26
25SG	25C25	25C	39.24	25SG	25C25	24C	75.91
25SG	25C25	163N	26.06	25SG	25C25	19OE1	68.77
25SG	25C25	162CA	52.77	25SG	25C25	162CE1	48.87
25SG	25C25	24CA	93.64	25SG	25C25	19CD	79.92
25CB	25C25	25N	43.75	25CB	25C25	25CA	22.80
25CB	25C25	23C	96.85	25CB	25C25	19NE2	58.71
25CB	25C25	162ND1	52.80	25CB	25C25	24N	79.85
25CB	25C25	26N	49.57	25CB	25C25	25C	32.45
25CB	25C25	24C	53.95	25CB	25C25	163N	56.86
25CB	25C25	19OE1	39.72	25CB	25C25	162CA	76.70
25CB	25C25	162CE1	41.55	25CB	25C25	24CA	71.02
25CB	25C25	19CD	48.30	25N	25C25	23O	61.20
25N	25C25	25CA	22.53	25N	25C25	23C	54.87
25N	25C25	23CA	71.33	25N	25C25	19NE2	46.58
25N	25C25	162ND1	94.33	25N	25C25	24N	38.82
25N	25C25	26N	37.62	25N	25C25	25C	32.96
25N	25C25	24C	10.58	25N	25C25	163N	94.01

TABLE XI

25N	25C25	19OE1	53.89	25N	25C25	162CE1	80.69
25N	25C25	24CA	27.34	25N	25C25	19CD	48.28
23O	25C25	25CA	82.78	23O	25C25	23C	18.78
23O	25C25	23CA	35.84	23O	25C25	19NE2	73.70
23O	25C25	24N	31.06	23O	25C25	26N	72.39
23O	25C25	25C	83.36	23O	25C25	24C	51.02
23O	25C25	19OE1	99.77	23O	25C25	24CA	34.14
23O	25C25	19CD	86.19	25CA	25C25	23C	77.38
25CA	25C25	23CA	92.63	25CA	25C25	19NE2	55.22
25CA	25C25	162ND1	75.50	25CA	25C25	24N	61.07
25CA	25C25	26N	33.30	25CA	25C25	25C	18.88
25CA	25C25	24C	31.91	25CA	25C25	163N	72.17
25CA	25C25	19OE1	48.70	25CA	25C25	162CA	96.87
25CA	25C25	162CE1	63.50	25CA	25C25	24CA	49.61
25CA	25C25	19CD	50.26	23C	25C25	23CA	22.22
23C	25C25	19NE2	55.76	23C	25C25	24N	17.04
23C	25C25	26N	77.83	23C	25C25	25C	83.98
23C	25C25	24C	46.58	23C	25C25	19OE1	82.85
23C	25C25	24CA	28.93	23C	25C25	19CD	68.78
23CA	25C25	19NE2	53.36	23CA	25C25	24N	33.27
23CA	25C25	26N	99.45	23CA	25C25	24C	65.16
23CA	25C25	19OE1	80.77	23CA	25C25	24CA	48.92
23CA	25C25	19CD	66.76	19NE2	25C25	162ND1	78.91
19NE2	25C25	24N	43.72	19NE2	25C25	26N	83.54
19NE2	25C25	25C	73.61	19NE2	25C25	24C	50.86
19NE2	25C25	19OE1	27.88	19NE2	25C25	162CE1	65.60
19NE2	25C25	24CA	51.46	19NE2	25C25	19CD	13.57
162ND1	25C25	161O	66.11	162ND1	25C25	26N	97.49
162ND1	25C25	25C	81.90	162ND1	25C25	163N	47.00
162ND1	25C25	19OE1	52.01	162ND1	25C25	162CA	38.64
162ND1	25C25	162CE1	14.60	162ND1	25C25	19CD	65.91
161O	25C25	163N	58.15	161O	25C25	162CA	33.71
161O	25C25	162CE1	80.71	24N	25C25	26N	67.35
24N	25C25	25C	70.00	24N	25C25	24C	31.89
24N	25C25	19OE1	68.76	24N	25C25	24CA	16.51
24N	25C25	19CD	55.45	26N	25C25	25C	17.11
26N	25C25	24C	37.71	26N	25C25	163N	70.13
26N	25C25	19OE1	81.99	26N	25C25	162CA	99.71
26N	25C25	162CE1	89.75	26N	25C25	24CA	50.94
26N	25C25	19CD	82.06	25C	25C25	24C	38.11
25C	25C25	163N	63.33	25C	25C25	19OE1	66.63
25C	25C25	162CA	91.85	25C	25C25	162CE1	73.03

TABLE XI

25C	25C25	24CA	55.12	25C	25C25	19CD	69.13
24C	25C25	19OE1	62.72	24C	25C25	162CE1	91.22
24C	25C25	24CA	17.90	24C	25C25	19CD	55.23
163N	25C25	19OE1	86.02	163N	25C25	162CA	29.58
163N	25C25	162CE1	53.83	163N	25C25	19CD	99.46
19OE1	25C25	162CA	90.22	19OE1	25C25	162CE1	38.06
19OE1	25C25	24CA	71.30	19OE1	25C25	19CD	14.33
162CA	25C25	162CE1	52.16	162CE1	25C25	19CD	52.25
24CA	25C25	19CD	60.28	25SG	25O26	25N	75.08
25SG	25O26	25CB	37.30	25SG	25O26	25CA	54.02
25SG	25O26	24C	86.45	25SG	25O26	19CD	97.95
25SG	25O26	19OE1	82.42	25SG	25O26	25C	45.95
25SG	25O26	26N	51.16	25SG	25O26	162ND1	46.91
25SG	25O26	162CE1	52.51	25N	25O26	23C	71.27
25N	25O26	25CB	49.91	25N	25O26	23CA	95.71
25N	25O26	19NE2	63.43	25N	25O26	23O	74.28
25N	25O26	24N	51.65	25N	25O26	25CA	24.00
25N	25O26	24C	13.92	25N	25O26	19CD	63.32
25N	25O26	19OE1	66.78	25N	25O26	24CA	35.47
25N	25O26	23N	92.49	25N	25O26	22O	75.23
25N	25O26	25C	29.57	25N	25O26	26N	34.00
25N	25O26	162ND1	97.43	25N	25O26	22C	83.38
25N	25O26	162CE1	86.18	23C	25O26	23CA	29.24
23C	25O26	19NE2	77.74	23C	25O26	23O	22.63
23C	25O26	24N	23.28	23C	25O26	25CA	95.23
23C	25O26	24C	57.44	23C	25O26	19CD	92.50
23C	25O26	24CA	35.81	23C	25O26	23N	31.40
23C	25O26	22O	45.44	23C	25O26	25C	94.92
23C	25O26	26N	85.14	23C	25O26	22C	36.80
25CB	25O26	19NE2	75.38	25CB	25O26	25CA	26.07
25CB	25O26	24C	63.79	25CB	25O26	19CD	62.61
25CB	25O26	19OE1	50.03	25CB	25O26	24CA	85.37
25CB	25O26	25C	32.00	25CB	25O26	26N	48.03
25CB	25O26	162ND1	48.42	25CB	25O26	162CE1	40.75
23CA	25O26	19NE2	74.13	23CA	25O26	23O	44.84
23CA	25O26	24N	44.10	23CA	25O26	24C	82.84
23CA	25O26	19CD	89.48	23CA	25O26	24CA	61.85
23CA	25O26	23N	7.91	23CA	25O26	22O	37.03
23CA	25O26	22C	22.99	19NE2	25O26	23O	99.02
19NE2	25O26	24N	59.57	19NE2	25O26	25CA	69.12
19NE2	25O26	24C	64.61	19NE2	25O26	19CD	15.61
19NE2	25O26	19OE1	33.20	19NE2	25O26	24CA	66.27

TABLE XI

19NE2	25O26	23N	66.26	19NE2	25O26	22O	37.24
19NE2	25O26	25C	85.04	19NE2	25O26	26N	96.39
19NE2	25O26	162ND1	87.10	19NE2	25O26	22C	51.16
19NE2	25O26	162CE1	72.58	23O	25O26	24N	40.19
23O	25O26	25CA	95.80	23O	25O26	24C	61.05
23O	25O26	24CA	42.72	23O	25O26	23N	49.93
23O	25O26	22O	68.06	23O	25O26	25C	89.22
23O	25O26	26N	75.10	23O	25O26	22C	58.63
24N	25O26	25CA	75.32	24N	25O26	24C	38.83
24N	25O26	19CD	72.68	24N	25O26	19OE1	88.39
24N	25O26	24CA	19.05	24N	25O26	23N	41.71
24N	25O26	22O	37.44	24N	25O26	25C	79.23
24N	25O26	26N	74.55	24N	25O26	22C	37.15
25CA	25O26	24C	37.79	25CA	25O26	19CD	62.07
25CA	25O26	19OE1	57.50	25CA	25O26	24CA	59.43
25CA	25O26	22O	92.92	25CA	25O26	25C	16.48
25CA	25O26	26N	31.94	25CA	25O26	162ND1	74.28
25CA	25O26	162CE1	64.77	24C	25O26	19CD	68.53
24C	25O26	19OE1	75.73	24C	25O26	24CA	21.65
24C	25O26	23N	80.40	24C	25O26	22O	67.31
24C	25O26	25C	40.54	24C	25O26	26N	39.44
24C	25O26	22C	73.15	24C	25O26	162CE1	99.55
19CD	25O26	19OE1	17.61	19CD	25O26	24CA	75.72
19CD	25O26	23N	81.58	19CD	25O26	22O	52.77
19CD	25O26	25C	78.56	19CD	25O26	26N	92.72
19CD	25O26	162ND1	71.98	19CD	25O26	22C	66.59
19CD	25O26	162CE1	57.18	19OE1	25O26	24CA	87.94
19OE1	25O26	23N	98.65	19OE1	25O26	22O	70.22
19OE1	25O26	25C	73.17	19OE1	25O26	26N	89.43
19OE1	25O26	162ND1	54.76	19OE1	25O26	22C	83.88
19OE1	25O26	162CE1	39.72	24CA	25O26	23N	60.38
24CA	25O26	22O	54.26	24CA	25O26	25C	60.91
24CA	25O26	26N	55.50	24CA	25O26	22C	56.01
23N	25O26	22O	29.27	23N	25O26	22C	15.20
22O	25O26	22C	14.07	25C	25O26	26N	16.90
25C	25O26	162ND1	78.47	25C	25O26	162CE1	72.68
26N	25O26	162ND1	91.53	26N	25O26	162CE1	88.05
162ND1	25O26	162CE1	15.41	25SG	25C27	25N	57.08
25SG	25C27	25CB	21.02	25SG	25C27	26N	58.38
25SG	25C27	25CA	39.38	25SG	25C27	24N	91.00
25SG	25C27	24C	70.32	25SG	25C27	25C	43.75
25SG	25C27	161O	68.95	25SG	25C27	26CB	82.20

TABLE XI

25SG	25C27	24CA	87.49	25SG	25C27	26CG	96.26
23O	25C27	23C	18.46	23O	25C27	25N	62.85
23O	25C27	65CA	58.88	23O	25C27	25CB	97.75
23O	25C27	26CD1	56.83	23O	25C27	26N	82.95
23O	25C27	23CA	34.44	23O	25C27	25CA	81.88
23O	25C27	24N	28.16	23O	25C27	24C	51.85
23O	25C27	25C	88.07	23O	25C27	65N	46.70
23O	25C27	26CB	86.79	23O	25C27	66N	79.07
23O	25C27	24CA	33.37	23O	25C27	26CG	69.96
23O	25C27	65C	66.97	23C	25C27	25N	53.34
23C	25C27	65CA	76.45	23C	25C27	25CB	84.25
23C	25C27	26CD1	70.76	23C	25C27	26N	83.38
23C	25C27	23CA	21.08	23C	25C27	25CA	72.15
23C	25C27	24N	15.52	23C	25C27	24C	46.42
23C	25C27	25C	83.42	23C	25C27	65N	62.90
23C	25C27	26CB	96.45	23C	25C27	66N	97.46
23C	25C27	24CA	29.98	23C	25C27	26CG	81.94
23C	25C27	65C	85.36	25N	25C27	25CB	36.48
25N	25C27	26CD1	68.71	25N	25C27	26N	39.49
25N	25C27	23CA	66.25	25N	25C27	25CA	19.15
25N	25C27	24N	37.84	25N	25C27	24C	14.42
25N	25C27	25C	31.97	25N	25C27	26CB	68.32
25N	25C27	24CA	30.42	25N	25C27	26CG	67.30
65CA	25C27	26CD1	53.12	65CA	25C27	23CA	82.66
65CA	25C27	24N	86.51	65CA	25C27	24C	98.45
65CA	25C27	65N	15.90	65CA	25C27	26CB	77.82
65CA	25C27	66N	30.25	65CA	25C27	24CA	84.16
65CA	25C27	26CG	63.87	65CA	25C27	65C	14.85
25CB	25C27	26CD1	96.07	25CB	25C27	26N	48.98
25CB	25C27	23CA	88.62	25CB	25C27	25CA	20.65
25CB	25C27	24N	70.19	25CB	25C27	24C	50.31
25CB	25C27	25C	32.85	25CB	25C27	161O	88.13
25CB	25C27	26CB	78.77	25CB	25C27	24CA	66.76
25CB	25C27	26CG	88.03	26CD1	25C27	26N	49.41
26CD1	25C27	23CA	90.70	26CD1	25C27	25CA	76.35
26CD1	25C27	24N	67.23	26CD1	25C27	24C	55.82
26CD1	25C27	25C	64.70	26CD1	25C27	65N	58.91
26CD1	25C27	26CB	32.69	26CD1	25C27	66N	42.33
26CD1	25C27	24CA	52.50	26CD1	25C27	26CG	14.60
26CD1	25C27	65C	44.57	26N	25C27	25CA	33.28
26N	25C27	24N	69.36	26N	25C27	24C	38.31
26N	25C27	25C	16.13	26N	25C27	26CB	31.48

TABLE XI

26N	25C27	66N	83.54	26N	25C27	24CA	53.43
26N	25C27	26CG	39.23	26N	25C27	65C	91.88
23CA	25C27	25CA	82.90	23CA	25C27	24N	32.54
23CA	25C27	24C	63.47	23CA	25C27	25C	98.17
23CA	25C27	65N	67.00	23CA	25C27	24CA	49.60
23CA	25C27	65C	95.04	25CA	25C27	24N	56.77
25CA	25C27	24C	31.07	25CA	25C27	25C	19.16
25CA	25C27	26CB	64.76	25CA	25C27	24CA	48.93
25CA	25C27	26CG	70.17	24N	25C27	24C	31.48
24N	25C27	25C	68.08	24N	25C27	65N	74.86
24N	25C27	26CB	87.15	24N	25C27	24CA	17.56
24N	25C27	26CG	75.54	24N	25C27	65C	92.54
24C	25C27	25C	37.23	24C	25C27	65N	93.14
24C	25C27	26CB	61.81	24C	25C27	66N	98.06
24C	25C27	24CA	18.48	24C	25C27	26CG	56.79
24C	25C27	65C	96.78	25C	25C27	26CB	46.70
25C	25C27	66N	99.53	25C	25C27	24CA	55.28
25C	25C27	26CG	55.30	65N	25C27	26CB	88.24
65N	25C27	66N	45.67	65N	25C27	24CA	76.36
65N	25C27	26CG	72.00	65N	25C27	65C	30.06
26CB	25C27	66N	53.44	26CB	25C27	24CA	69.63
26CB	25C27	26CG	18.09	26CB	25C27	65C	64.59
66N	25C27	24CA	91.56	66N	25C27	26CG	45.61
66N	25C27	65C	15.61	24CA	25C27	26CG	58.92
24CA	25C27	65C	85.96	26CG	25C27	65C	52.65
25SG	25O28	161O	76.60	25SG	25O28	23O	80.25
25SG	25O28	26CD1	87.41	25SG	25O28	26N	47.59
25SG	25O28	26CB	75.36	25SG	25O28	161C	77.06
25SG	25O28	25CB	9.94	25SG	25O28	163N	39.01
65CA	25O28	23O	50.13	65CA	25O28	66N	33.41
65CA	25O28	66O	67.54	65CA	25O28	26CD1	48.79
65CA	25O28	65C	17.37	65CA	25O28	26N	90.83
65CA	25O28	26CB	76.12	161O	25O28	161C	10.43
161O	25O28	25CB	85.93	161O	25O28	163N	57.90
23O	25O28	66N	73.33	23O	25O28	66O	98.34
23O	25O28	26CD1	46.36	23O	25O28	65C	62.14
23O	25O28	26N	63.88	23O	25O28	26CB	73.66
23O	25O28	25CB	70.99	66N	25O28	66O	34.18
66N	25O28	26CD1	42.77	66N	25O28	65C	16.09
66N	25O28	26N	80.82	66N	25O28	26CB	55.05
66O	25O28	26CD1	53.93	66O	25O28	65C	50.27
66O	25O28	26N	71.20	66O	25O28	26CB	41.80

TABLE XI

66O	25O28	163N	96.32	26CD1	25O28	65C	44.16
26CD1	25O28	26N	42.70	26CD1	25O28	26CB	31.40
26CD1	25O28	25CB	78.43	65C	25O28	26N	86.36
65C	25O28	26CB	65.21	26N	25O28	26CB	29.67
26N	25O28	25CB	40.69	26N	25O28	163N	65.13
26CB	25O28	25CB	69.78	26CB	25O28	163N	79.13
161C	25O28	25CB	86.86	161C	25O28	163N	52.19
25CB	25O28	163N	47.47	66O	25C29	66N	48.91
66O	25C29	65CA	91.41	66O	25C29	65C	68.29
66O	25C29	66C	13.27	66O	25C29	26CD1	67.50
66O	25C29	66CA	34.11	66O	25C29	26CB	50.71
66O	25C29	26CG	54.55	66O	25C29	65N	99.08
66O	25C29	65O	66.95	66O	25C29	26N	80.09
66N	25C29	65CA	42.87	66N	25C29	65C	19.38
66N	25C29	66C	36.24	66N	25C29	26CD1	51.44
66N	25C29	66CA	15.57	66N	25C29	26CB	68.44
66N	25C29	26CG	54.31	66N	25C29	23O	78.55
66N	25C29	65N	50.66	66N	25C29	65O	18.11
66N	25C29	26N	91.42	65CA	25C29	65C	23.73
65CA	25C29	66C	79.07	65CA	25C29	26CD1	55.65
65CA	25C29	66CA	58.35	65CA	25C29	26CB	89.86
65CA	25C29	26CG	70.46	65CA	25C29	23O	47.25
65CA	25C29	65N	7.81	65CA	25C29	65O	25.70
65CA	25C29	26N	94.75	65C	25C29	66C	55.59
65C	25C29	26CD1	52.52	65C	25C29	66CA	34.70
65C	25C29	26CB	79.47	65C	25C29	26CG	61.82
65C	25C29	23O	65.09	65C	25C29	65N	31.53
65C	25C29	65O	2.78	65C	25C29	26N	95.49
66C	25C29	26CD1	64.26	66C	25C29	66CA	21.04
66C	25C29	26CB	56.28	66C	25C29	26CG	54.75
66C	25C29	65N	86.84	66C	25C29	65O	54.09
66C	25C29	26N	86.08	26CD1	25C29	66CA	57.66
26CD1	25C29	26CB	35.62	26CD1	25C29	25SG	81.23
26CD1	25C29	26CG	17.23	26CD1	25C29	23O	45.73
26CD1	25C29	65N	58.39	26CD1	25C29	65O	54.62
26CD1	25C29	26N	42.97	66CA	25C29	26CB	64.36
66CA	25C29	26CG	54.97	66CA	25C29	23O	92.04
66CA	25C29	65N	66.15	66CA	25C29	65O	33.08
66CA	25C29	26N	91.66	26CB	25C29	25SG	73.09
26CB	25C29	26CG	19.41	26CB	25C29	23O	74.83
26CB	25C29	65N	93.60	26CB	25C29	65O	80.55
26CB	25C29	26N	29.84	25SG	25C29	26CG	81.03

TABLE XI

25SG	25C29	23O	65.42	25SG	25C29	161O	57.72
25SG	25C29	26N	44.40	26CG	25C29	23O	61.35
26CG	25C29	65N	74.27	26CG	25C29	65O	63.28
26CG	25C29	26N	37.32	23O	25C29	65N	42.49
23O	25C29	65O	67.82	23O	25C29	26N	59.60
65N	25C29	65O	33.46	65N	25C29	26N	94.60
65O	25C29	26N	97.54	66O	25C30	66N	43.16
66O	25C30	66C	13.69	66O	25C30	65CA	74.47
66O	25C30	66CA	31.15	66O	25C30	65C	58.33
66N	25C30	66C	35.28	66N	25C30	65CA	33.44
66N	25C30	66CA	17.60	66N	25C30	65C	15.22
66C	25C30	65CA	68.55	66C	25C30	66CA	19.80
66C	25C30	65C	50.23	65CA	25C30	66CA	50.69
65CA	25C30	65C	19.75	66CA	25C30	65C	31.38
66O	25C31	66C	9.16	66O	25C31	66N	30.51
66O	25C31	163CB	81.88	161O	25C31	161C	15.04
161O	25C31	163CB	81.82	161O	25C31	160O	59.31
66C	25C31	66N	28.88	66C	25C31	163CB	90.84
161C	25C31	163CB	80.88	161C	25C31	160O	48.22
66N	25C31	163CB	97.56				

TABLE XII

Table of angles between atoms of the inhibitor and protein for all protein atoms within 5 Ångstroms of the inhibitor bis-(Cbz-leucinyl)-1,3-diamino-propan-2-one

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
184CB	25C1	184CG	21.22	184CB	25C1	18OD1	72.94
184CB	25C1	184CD1	35.50	184CB	25C1	184CA	19.59
184CB	25C1	184CD2	33.67	184CB	25C1	184O	34.28
184CB	25C1	184C	30.67	184CG	25C1	18OD1	81.92
184CG	25C1	184CD1	18.31	184CG	25C1	184CA	34.17
184CG	25C1	184CD2	16.99	184CG	25C1	184O	55.47
184CG	25C1	184C	50.07	18OD1	25C1	184CD1	74.79
18OD1	25C1	184CA	53.36	18OD1	25C1	184CD2	98.79
18OD1	25C1	184O	61.42	18OD1	25C1	184C	50.27
184CD1	25C1	184CA	39.83	184CD1	25C1	184CD2	28.30
184CD1	25C1	184O	67.35	184CD1	25C1	184C	57.99
184CA	25C1	184CD2	50.19	184CA	25C1	184O	29.82
184CA	25C1	184C	18.22	184CD2	25C1	184O	66.46
184CD2	25C1	184C	64.29	184O	25C1	184C	14.58
18OD1	25C2	184CD1	93.56	18OD1	25C2	184CB	85.20
18OD1	25C2	184CA	63.93	18OD1	25C2	184CG	97.27
18OD1	25C2	18CG	7.95	18OD1	25C2	20O	82.27
18OD1	25C2	20N	45.49	18OD1	25C2	184C	56.77
18OD1	25C2	18ND2	22.89	18OD1	25C2	20CA	55.50
18OD1	25C2	184O	66.85	18OD1	25C2	20C	72.94
18OD1	25C2	19CG	66.66	184CD1	25C2	184CB	36.96
184CD1	25C2	184CA	43.35	184CD1	25C2	184CG	19.17
184CD1	25C2	20O	93.58	184CD1	25C2	20N	91.27
184CD1	25C2	184C	62.15	184CD1	25C2	184NE1	14.42
184CD1	25C2	184O	68.85	184CD1	25C2	19CG	47.81
184CB	25C2	184CA	21.51	184CB	25C2	184CG	20.93
184CB	25C2	18CG	90.69	184CB	25C2	184C	32.58
184CB	25C2	184NE1	48.17	184CB	25C2	184O	33.58
184CB	25C2	19CG	75.81	184CA	25C2	184CG	35.93
184CA	25C2	18CG	69.84	184CA	25C2	20N	91.24
184CA	25C2	184C	19.09	184CA	25C2	18ND2	85.37
184CA	25C2	184NE1	57.50	184CA	25C2	184O	29.61
184CA	25C2	19CG	65.69	184CG	25C2	184C	51.91
184CG	25C2	184NE1	27.66	184CG	25C2	184O	54.51
184CG	25C2	19CG	65.63	18CG	25C2	20O	83.37

TABLE XII

18CG	25C2	20N	47.67	18CG	25C2	184C	60.57
18CG	25C2	18ND2	15.73	18CG	25C2	20CA	54.96
18CG	25C2	184O	69.03	18CG	25C2	20C	72.82
18CG	25C2	19CG	73.59	20O	25C2	20N	37.03
20O	25C2	18ND2	77.52	20O	25C2	20CA	29.71
20O	25C2	184NE1	87.40	20O	25C2	20C	13.14
20O	25C2	19CG	52.69	20N	25C2	184C	94.70
20N	25C2	18ND2	46.43	20N	25C2	20CA	17.58
20N	25C2	184NE1	94.15	20N	25C2	20C	29.99
20N	25C2	19CG	44.09	184C	25C2	18ND2	74.66
184C	25C2	184NE1	76.04	184C	25C2	184O	14.64
184C	25C2	19CG	80.33	18ND2	25C2	20CA	47.82
18ND2	25C2	184O	81.12	18ND2	25C2	20C	65.32
18ND2	25C2	19CG	81.86	20CA	25C2	20C	17.90
20CA	25C2	19CG	58.30	184NE1	25C2	184O	81.39
184NE1	25C2	20C	98.78	184NE1	25C2	19CG	50.29
184O	25C2	19CG	94.21	20C	25C2	19CG	58.17
20O	25C3	18OD1	94.92	20O	25C3	20C	14.93
20O	25C3	20N	45.22	20O	25C3	20CA	34.91
20O	25C3	19CG	67.31	20O	25C3	18CG	90.10
20O	25C3	19C	44.11	20O	25C3	19CD	68.85
18OD1	25C3	20C	83.09	18OD1	25C3	20N	50.73
18OD1	25C3	184CD1	86.70	18OD1	25C3	20CA	61.59
18OD1	25C3	19CG	73.40	18OD1	25C3	184CG	83.83
18OD1	25C3	18CG	7.01	18OD1	25C3	184CB	69.00
18OD1	25C3	184CA	52.51	18OD1	25C3	19C	56.82
18OD1	25C3	19CD	89.80	20C	25C3	20N	36.79
20C	25C3	20CA	21.55	20C	25C3	19CG	72.42
20C	25C3	18CG	77.56	20C	25C3	19C	39.99
20C	25C3	19CD	77.92	20N	25C3	20CA	20.57
20N	25C3	19CG	52.06	20N	25C3	18CG	47.19
20N	25C3	184CA	88.94	20N	25C3	19C	12.18
20N	25C3	19CD	65.92	184CD1	25C3	19CG	54.41
184CD1	25C3	184CG	17.14	184CD1	25C3	184NE1	17.22
184CD1	25C3	18CG	93.47	184CD1	25C3	184CB	32.16
184CD1	25C3	184CA	38.24	184CD1	25C3	19C	92.25
184CD1	25C3	19CD	49.63	20CA	25C3	19CG	69.55
20CA	25C3	18CG	56.01	20CA	25C3	19C	29.66
20CA	25C3	19CD	80.70	19CG	25C3	184CG	69.80
19CG	25C3	184NE1	57.02	19CG	25C3	18CG	76.04
19CG	25C3	184CB	76.30	19CG	25C3	184CA	66.22
19CG	25C3	19C	40.46	19CG	25C3	19CD	16.92

TABLE XII

184CG	25C3	184NE1	28.96	184CG	25C3	18CG	90.83
184CG	25C3	184CB	18.06	184CG	25C3	184CA	31.35
184CG	25C3	19CD	66.65	184NE1	25C3	184CB	46.68
184NE1	25C3	184CA	55.31	184NE1	25C3	19C	97.43
184NE1	25C3	19CD	46.53	18CG	25C3	184CB	75.84
18CG	25C3	184CA	59.51	18CG	25C3	19C	54.70
18CG	25C3	19CD	92.81	184CB	25C3	184CA	18.20
184CB	25C3	19CD	77.96	184CA	25C3	19C	86.12
184CA	25C3	19CD	72.78	19C	25C3	19CD	53.79
20O	25C4	20C	9.86	20O	25C4	19CG	57.67
20O	25C4	18OD1	69.35	20O	25C4	20N	32.43
184CD1	25C4	184NE1	18.35	184CD1	25C4	184CG	15.96
184CD1	25C4	19CG	48.28	184CD1	25C4	184CE2	26.62
184CD1	25C4	18OD1	68.05	184CD1	25C4	20N	82.80
184NE1	25C4	184CG	27.99	184NE1	25C4	19CG	53.65
184NE1	25C4	184CE2	15.20	184NE1	25C4	18OD1	85.79
184NE1	25C4	20N	94.26	20C	25C4	19CG	62.70
20C	25C4	18OD1	63.89	20C	25C4	20N	29.77
184CG	25C4	19CG	62.53	184CG	25C4	184CE2	27.11
184CG	25C4	18OD1	67.71	184CG	25C4	20N	91.33
19CG	25C4	184CE2	68.70	19CG	25C4	18OD1	57.18
19CG	25C4	20N	42.85	184CE2	25C4	18OD1	93.39
18OD1	25C4	20N	37.93	184CD1	25C5	184NE1	17.38
184CD1	25C5	20O	82.23	184CD1	25C5	184CG	16.75
184CD1	25C5	184CE2	27.59	184CD1	25C5	184CD2	27.17
184NE1	25C5	20O	86.19	184NE1	25C5	184CG	27.91
184NE1	25C5	184CE2	16.68	184NE1	25C5	184CD2	27.27
20O	25C5	184CG	96.36	184CG	25C5	184CE2	27.86
184CG	25C5	184CD2	16.99	184CE2	25C5	184CD2	16.85
184CG	25C6	184CD1	17.30	184CG	25C6	184CD2	18.02
184CG	25C6	184CB	18.64	184CG	25C6	184NE1	27.34
184CG	25C6	184CE2	27.75	184CD1	25C6	184CD2	28.13
184CD1	25C6	184CB	32.10	184CD1	25C6	184NE1	16.25
184CD1	25C6	184CE2	26.86	184CD2	25C6	184CB	32.59
184CD2	25C6	184NE1	27.14	184CD2	25C6	184CE2	16.75
184CB	25C6	184NE1	45.42	184CB	25C6	184CE2	45.85
184NE1	25C6	184CE2	16.05	20O	25C7	20C	5.96
20O	25C7	21CA	34.09	20O	25C7	19CD	73.49
20O	25C7	19CG	60.92	20O	25C7	21OE1	66.16
20O	25C7	21N	17.58	20O	25C7	19OE1	87.57
20O	25C7	19NE2	69.26	20C	25C7	21CA	31.76
20C	25C7	19CD	79.31	20C	25C7	19CG	66.28

TABLE XII

20C	25C7	21OE1	60.89	20C	25C7	21N	14.18
20C	25C7	19OE1	93.30	20C	25C7	19NE2	75.21
184NE1	25C7	19CD	47.01	184NE1	25C7	19CG	52.85
184NE1	25C7	184CD1	16.44	184NE1	25C7	19OE1	33.68
184NE1	25C7	19NE2	59.90	21CA	25C7	19CD	96.04
21CA	25C7	19CG	89.60	21CA	25C7	21OE1	41.39
21CA	25C7	21N	17.76	21CA	25C7	19NE2	85.25
19CD	25C7	19CG	18.31	19CD	25C7	21N	88.09
19CD	25C7	184CD1	47.08	19CD	25C7	19OE1	14.53
19CD	25C7	19NE2	15.43	19CG	25C7	21N	77.54
19CG	25C7	184CD1	46.14	19CG	25C7	19OE1	28.58
19CG	25C7	19NE2	28.52	21OE1	25C7	21N	49.85
21N	25C7	19NE2	80.92	184CD1	25C7	19OE1	37.45
184CD1	25C7	19NE2	62.12	19OE1	25C7	19NE2	26.24
20O	25O8	19CD	90.86	20O	25O8	19NE2	87.53
20O	25O8	19CG	72.09	20O	25O8	20C	2.00
20O	25O8	22O	62.72	20O	25O8	19CB	63.81
19CD	25O8	19OE1	19.87	19CD	25O8	19NE2	21.15
19CD	25O8	19CG	23.15	19CD	25O8	184NE1	60.87
19CD	25O8	184CD1	58.07	19CD	25O8	20C	89.41
19CD	25O8	22O	57.75	19CD	25O8	184CE2	73.67
19CD	25O8	19CB	27.32	19OE1	25O8	19NE2	35.82
19OE1	25O8	19CG	37.30	19OE1	25O8	184NE1	43.39
19OE1	25O8	184CD1	45.88	19OE1	25O8	22O	74.89
19OE1	25O8	184CE2	55.38	19OE1	25O8	19CB	45.39
19NE2	25O8	19CG	37.34	19NE2	25O8	184NE1	79.21
19NE2	25O8	184CD1	78.91	19NE2	25O8	20C	85.68
19NE2	25O8	22O	39.13	19NE2	25O8	184CE2	91.05
19NE2	25O8	19CB	33.61	19CG	25O8	184NE1	65.75
19CG	25O8	184CD1	54.97	19CG	25O8	20C	71.02
19CG	25O8	22O	61.28	19CG	25O8	184CE2	78.82
19CG	25O8	19CB	12.33	184NE1	25O8	184CD1	18.60
184NE1	25O8	184CE2	13.25	184NE1	25O8	19CB	77.87
184CD1	25O8	184CE2	27.58	184CD1	25O8	19CB	67.24
20C	25O8	22O	60.75	20C	25O8	19CB	62.46
22O	25O8	19CB	49.98	184CE2	25O8	19CB	91.01
19OE1	25C9	19NE2	33.38	19OE1	25C9	19CD	18.07
19OE1	25C9	184NE1	40.26	19OE1	25C9	20O	84.29
19OE1	25C9	19CG	30.18	19OE1	25C9	22O	69.67
19OE1	25C9	184CE2	53.38	19OE1	25C9	184CD1	39.42
19NE2	25C9	19CD	19.36	19NE2	25C9	184NE1	73.02
19NE2	25C9	20O	69.77	19NE2	25C9	19CG	30.40

TABLE XII

19NE2	25C9	22O	36.73	19NE2	25C9	184CE2	86.66
19NE2	25C9	184CD1	68.70	19CD	25C9	184NE1	54.70
19CD	25C9	20O	69.22	19CD	25C9	19CG	17.06
19CD	25C9	22O	53.02	19CD	25C9	184CE2	68.86
19CD	25C9	184CD1	49.36	184NE1	25C9	20O	95.14
184NE1	25C9	19CG	55.54	184NE1	25C9	184CE2	14.51
184NE1	25C9	184CD1	14.36	20O	25C9	19CG	54.13
20O	25C9	22O	54.06	20O	25C9	184CD1	80.80
19CG	25C9	22O	53.71	19CG	25C9	184CE2	69.95
19CG	25C9	184CD1	45.63	22O	25C9	184CD1	99.26
184CE2	25C9	184CD1	26.16	19NE2	25O10	20O	62.12
19NE2	25O10	22O	35.56	19NE2	25O10	19CD	15.61
19NE2	25O10	19OE1	26.78	20O	25O10	22O	52.61
20O	25O10	19CD	59.60	20O	25O10	19OE1	70.63
22O	25O10	19CD	48.47	22O	25O10	19OE1	61.86
19CD	25O10	19OE1	14.34	162ND1	25C11	184CZ2	66.42
162ND1	25C11	184NE1	66.34	162ND1	25C11	162CE1	17.78
162ND1	25C11	19OE1	57.83	162ND1	25C11	184CE2	67.52
162ND1	25C11	162CG	14.11	162ND1	25C11	19NE2	72.38
162ND1	25C11	19CD	68.15	184CZ2	25C11	184NE1	34.50
184CZ2	25C11	162CE1	56.59	184CZ2	25C11	19OE1	69.19
184CZ2	25C11	184CE2	17.54	184CZ2	25C11	162CG	60.04
184CZ2	25C11	19NE2	95.66	184CZ2	25C11	19CD	80.47
184NE1	25C11	162CE1	49.27	184NE1	25C11	19OE1	37.54
184NE1	25C11	184CE2	17.27	184NE1	25C11	162CG	68.99
184NE1	25C11	19NE2	62.26	184NE1	25C11	19CD	46.90
162CE1	25C11	19OE1	42.46	162CE1	25C11	184CE2	53.20
162CE1	25C11	162CG	26.53	162CE1	25C11	19NE2	62.11
162CE1	25C11	19CD	54.33	19OE1	25C11	184CE2	53.84
19OE1	25C11	162CG	68.94	19OE1	25C11	19NE2	26.94
19OE1	25C11	19CD	13.30	184CE2	25C11	162CG	65.59
184CE2	25C11	19NE2	79.38	184CE2	25C11	19CD	64.03
162CG	25C11	19NE2	86.02	162CG	25C11	19CD	80.39
19NE2	25C11	19CD	15.36	184CZ2	25C15	184CH2	16.48
184CZ2	25C15	143OE1	72.66	184CZ2	25C15	137O	75.04
184CH2	25C15	143OE1	58.91	184CH2	25C15	137O	61.89
143OE1	25C15	137O	63.98	162ND1	25C16	162CE1	19.73
162ND1	25C16	162CG	16.60	162ND1	25C16	25SG	47.39
162ND1	25C16	161O	72.64	162ND1	25C16	19OE1	62.63
162ND1	25C16	162CB	33.51	162ND1	25C16	162CA	39.24
162ND1	25C16	162NE2	20.67	162ND1	25C16	19NE2	81.12
162ND1	25C16	184CZ2	64.44	162ND1	25C16	25CB	44.50

TABLE XII

162ND1	25C16	184NE1	64.44	162ND1	25C16	162CD2	17.81
162CE1	25C16	162CG	32.31	162CE1	25C16	25SG	53.22
162CE1	25C16	161O	91.93	162CE1	25C16	19OE1	44.18
162CE1	25C16	162CB	51.51	162CE1	25C16	162CA	58.97
162CE1	25C16	162NE2	11.09	162CE1	25C16	19NE2	66.33
162CE1	25C16	184CZ2	53.67	162CE1	25C16	25CB	41.27
162CE1	25C16	184NE1	46.11	162CE1	25C16	162CD2	24.34
162CG	25C16	25SG	59.98	162CG	25C16	161O	66.72
162CG	25C16	19OE1	76.48	162CG	25C16	162CB	19.50
162CG	25C16	162CA	32.20	162CG	25C16	162NE2	27.13
162CG	25C16	19NE2	97.24	162CG	25C16	184CZ2	60.98
162CG	25C16	25CB	60.57	162CG	25C16	184NE1	70.16
162CG	25C16	162CD2	12.90	25SG	25C16	161O	62.69
25SG	25C16	19OE1	65.19	25SG	25C16	162CB	65.02
25SG	25C16	162CA	52.80	25SG	25C16	162NE2	62.49
25SG	25C16	19NE2	61.43	25SG	25C16	25CB	20.75
25SG	25C16	184NE1	91.34	25SG	25C16	162CD2	65.19
161O	25C16	162CB	50.15	161O	25C16	162CA	34.64
161O	25C16	162NE2	92.16	161O	25C16	25CB	82.66
161O	25C16	162CD2	79.61	19OE1	25C16	162CB	95.63
19OE1	25C16	162CA	99.99	19OE1	25C16	162NE2	51.09
19OE1	25C16	19NE2	27.38	19OE1	25C16	184CZ2	62.46
19OE1	25C16	25CB	44.47	19OE1	25C16	184NE1	33.86
19OE1	25C16	162CD2	67.06	162CB	25C16	162CA	18.75
162CB	25C16	162NE2	46.53	162CB	25C16	184CZ2	73.28
162CB	25C16	25CB	72.45	162CB	25C16	184NE1	88.17
162CB	25C16	162CD2	31.28	162CA	25C16	162NE2	57.73
162CA	25C16	184CZ2	91.31	162CA	25C16	25CB	65.83
162CA	25C16	162CD2	45.08	162NE2	25C16	19NE2	75.48
162NE2	25C16	184CZ2	45.32	162NE2	25C16	25CB	52.16
162NE2	25C16	184NE1	44.44	162NE2	25C16	162CD2	16.02
19NE2	25C16	184CZ2	88.09	19NE2	25C16	25CB	44.94
19NE2	25C16	184NE1	58.55	19NE2	25C16	162CD2	90.64
184CZ2	25C16	25CB	91.81	184CZ2	25C16	184NE1	29.55
184CZ2	25C16	162CD2	49.38	25CB	25C16	184NE1	71.82
25CB	25C16	162CD2	60.66	184NE1	25C16	162CD2	57.37
162ND1	25O17	162CG	25.38	162ND1	25O17	162CB	48.94
162ND1	25O17	162CE1	18.45	162ND1	25O17	161O	93.58
162ND1	25O17	162CA	54.76	162ND1	25O17	25SG	48.39
162ND1	25O17	161C	89.31	162ND1	25O17	162CD2	25.71
162ND1	25O17	162N	73.99	162ND1	25O17	162NE2	21.11
162ND1	25O17	184CZ2	69.27	162ND1	25O17	137CB	75.37

TABLE XII

162CG	25O17	162CB	26.64	162CG	25O17	162CE1	38.41
162CG	25O17	161O	86.53	162CG	25O17	162CA	42.50
162CG	25O17	25SG	67.49	162CG	25O17	161C	76.51
162CG	25O17	162CD2	13.63	162CG	25O17	162N	58.79
162CG	25O17	162NE2	29.02	162CG	25O17	161OD1	79.16
162CG	25O17	184CZ2	67.73	162CG	25O17	137CB	51.32
162CB	25O17	162CE1	64.60	162CB	25O17	161O	65.36
162CB	25O17	162CA	24.38	162CB	25O17	25SG	76.49
162CB	25O17	161C	52.48	162CB	25O17	162CD2	38.18
162CB	25O17	162N	34.58	162CB	25O17	162NE2	55.49
162CB	25O17	161OD1	54.52	162CB	25O17	184CZ2	85.85
162CB	25O17	137CB	42.56	162CE1	25O17	162CA	73.15
162CE1	25O17	25SG	55.22	162CE1	25O17	162CD2	31.50
162CE1	25O17	162N	92.28	162CE1	25O17	162NE2	14.96
162CE1	25O17	184CZ2	56.06	162CE1	25O17	137CB	81.03
161O	25O17	162CA	44.07	161O	25O17	25SG	69.63
161O	25O17	161C	15.96	161O	25O17	162N	31.46
161O	25O17	161OD1	56.32	161O	25O17	137CB	91.92
162CA	25O17	25SG	61.24	162CA	25O17	161C	35.13
162CA	25O17	162CD2	56.09	162CA	25O17	162N	19.37
162CA	25O17	162NE2	69.58	162CA	25O17	161OD1	58.28
162CA	25O17	137CB	64.45	25SG	25O17	161C	77.58
25SG	25O17	162CD2	73.41	25SG	25O17	162N	74.60
25SG	25O17	162NE2	67.15	161C	25O17	162CD2	89.68
161C	25O17	162N	17.96	161C	25O17	161OD1	42.82
161C	25O17	137CB	75.96	162CD2	25O17	162N	71.80
162CD2	25O17	162NE2	18.45	162CD2	25O17	161OD1	86.33
162CD2	25O17	184CZ2	54.40	162CD2	25O17	137CB	50.73
162N	25O17	162NE2	87.31	162N	25O17	161OD1	42.68
162N	25O17	137CB	63.55	162NE2	25O17	184CZ2	48.21
162NE2	25O17	137CB	66.23	161OD1	25O17	137CB	44.42
184CZ2	25O17	137CB	61.47	25SG	25N18	162ND1	50.41
25SG	25N18	162CE1	53.56	25SG	25N18	161O	67.92
25SG	25N18	19NE2	71.90	25SG	25N18	19OE1	69.62
25SG	25N18	25CB	22.82	25SG	25N18	23CA	87.13
25SG	25N18	162CG	56.99	25SG	25N18	19CD	72.29
162ND1	25N18	162CE1	17.36	162ND1	25N18	161O	69.09
162ND1	25N18	19NE2	84.51	162ND1	25N18	19OE1	59.48
162ND1	25N18	25CB	49.58	162ND1	25N18	162CG	11.34
162ND1	25N18	19CD	72.69	162CE1	25N18	161O	86.28
162CE1	25N18	19NE2	68.55	162CE1	25N18	19OE1	42.23
162CE1	25N18	25CB	43.96	162CE1	25N18	162CG	27.38

TABLE XII

162CE1	25N18	19CD	55.80	161O	25N18	25CB	89.34
161O	25N18	162CG	61.14	19NE2	25N18	19OE1	29.63
19NE2	25N18	25CB	50.72	19NE2	25N18	23CA	55.49
19NE2	25N18	162CG	95.57	19NE2	25N18	19CD	15.35
19OE1	25N18	25CB	47.37	19OE1	25N18	23CA	85.11
19OE1	25N18	162CG	69.47	19OE1	25N18	19CD	14.61
25CB	25N18	23CA	81.33	25CB	25N18	162CG	59.74
25CB	25N18	19CD	49.52	23CA	25N18	19CD	70.70
162CG	25N18	19CD	83.18	25SG	25C19	161O	92.47
25SG	25C19	162ND1	54.14	25SG	25C19	25CB	20.86
25SG	25C19	162CA	62.74	25SG	25C19	161C	88.58
25SG	25C19	162CE1	51.71	25SG	25C19	23CA	97.99
25SG	25C19	25N	41.07	25SG	25C19	23C	82.10
25SG	25C19	23O	81.30	25SG	25C19	162CG	59.31
25SG	25C19	19NE2	69.11	25SG	25C19	162CB	67.82
25SG	25C19	162N	76.57	161O	25C19	162ND1	78.79
161O	25C19	162CA	38.01	161O	25C19	161C	7.13
161O	25C19	162CE1	93.42	161O	25C19	162CG	66.49
161O	25C19	162CB	49.06	161O	25C19	162N	21.75
162ND1	25C19	25CB	52.62	162ND1	25C19	162CA	42.73
162ND1	25C19	161C	71.68	162ND1	25C19	162CE1	14.66
162ND1	25C19	25N	83.32	162ND1	25C19	162CG	12.47
162ND1	25C19	19NE2	75.83	162ND1	25C19	162CB	30.03
162ND1	25C19	162N	57.42	25CB	25C19	162CA	76.45
25CB	25C19	162CE1	44.02	25CB	25C19	23CA	85.20
25CB	25C19	25N	31.12	25CB	25C19	23C	72.96
25CB	25C19	23O	77.28	25CB	25C19	162CG	62.09
25CB	25C19	19NE2	48.58	25CB	25C19	162CB	75.75
25CB	25C19	162N	92.17	162CA	25C19	161C	31.40
162CA	25C19	162CE1	56.83	162CA	25C19	162CG	31.62
162CA	25C19	162CB	17.87	162CA	25C19	162N	16.50
161C	25C19	162CE1	86.32	161C	25C19	162CG	59.37
161C	25C19	162CB	41.93	161C	25C19	162N	14.94
162CE1	25C19	25N	72.85	162CE1	25C19	162CG	27.09
162CE1	25C19	19NE2	61.17	162CE1	25C19	162CB	44.66
162CE1	25C19	162N	71.95	23CA	25C19	25N	56.99
23CA	25C19	23C	18.49	23CA	25C19	23O	29.45
23CA	25C19	19NE2	51.58	25N	25C19	23C	42.38
25N	25C19	23O	46.35	25N	25C19	162CG	93.20
25N	25C19	19NE2	42.58	23C	25C19	23O	14.74
23C	25C19	19NE2	52.68	23O	25C19	19NE2	66.29
162CG	25C19	19NE2	88.25	162CG	25C19	162CB	17.57

TABLE XII

162CG	25C19	162N	45.36	162CB	25C19	162N	28.45
184NE1	25N20	19OE1	48.31	184NE1	25N20	19CD	61.42
184NE1	25N20	184CE2	19.07	184NE1	25N20	19NE2	80.38
184NE1	25N20	184CZ2	38.30	184NE1	25N20	162CE1	53.42
184NE1	25N20	184CD1	12.98	184NE1	25N20	162ND1	68.69
184NE1	25N20	19CG	57.21	19OE1	25N20	19CD	18.12
19OE1	25N20	184CE2	65.80	19OE1	25N20	19NE2	33.85
19OE1	25N20	184CZ2	80.73	19OE1	25N20	162CE1	45.71
19OE1	25N20	184CD1	44.65	19OE1	25N20	162ND1	59.71
19OE1	25N20	19CG	26.58	19CD	25N20	184CE2	80.19
19CD	25N20	19NE2	19.18	19CD	25N20	184CZ2	97.13
19CD	25N20	162CE1	62.24	19CD	25N20	184CD1	54.10
19CD	25N20	162ND1	74.29	19CD	25N20	19CG	14.62
184CE2	25N20	19NE2	98.89	184CE2	25N20	184CZ2	20.04
184CE2	25N20	162CE1	56.95	184CE2	25N20	184CD1	30.00
184CE2	25N20	162ND1	68.56	184CE2	25N20	19CG	76.21
19NE2	25N20	162CE1	69.93	19NE2	25N20	184CD1	73.25
19NE2	25N20	162ND1	77.40	19NE2	25N20	19CG	29.26
184CZ2	25N20	162CE1	57.21	184CZ2	25N20	184CD1	49.98
184CZ2	25N20	162ND1	63.26	184CZ2	25N20	19CG	95.28
162CE1	25N20	184CD1	61.93	162CE1	25N20	162ND1	16.79
162CE1	25N20	19CG	72.21	184CD1	25N20	162ND1	78.20
184CD1	25N20	19CG	47.15	162ND1	25N20	19CG	86.13
25SG	25C21	25CB	34.64	25SG	25C21	25N	72.39
25SG	25C21	25CA	49.66	25SG	25C21	162ND1	48.43
25SG	25C21	19NE2	93.26	25SG	25C21	26N	53.17
25SG	25C21	161O	82.24	25SG	25C21	25C	43.41
25SG	25C21	24C	80.54	25SG	25C21	162CE1	48.10
25SG	25C21	19OE1	73.78	25SG	25C21	24CA	98.55
25SG	25C21	163N	27.76	25SG	25C21	162CA	50.66
25SG	25C21	19CD	82.46	25SG	25C21	26CD1	90.92
25CB	25C21	25N	45.83	25CB	25C21	25CA	23.90
25CB	25C21	162ND1	58.24	25CB	25C21	19NE2	60.12
25CB	25C21	26N	51.36	25CB	25C21	24N	83.08
25CB	25C21	25C	33.89	25CB	25C21	24C	55.62
25CB	25C21	162CE1	46.38	25CB	25C21	19OE1	47.87
25CB	25C21	24CA	73.29	25CB	25C21	163N	62.27
25CB	25C21	162CA	80.47	25CB	25C21	19CD	51.61
25CB	25C21	26CD1	90.22	25N	25C21	25CA	23.31
25N	25C21	23O	62.57	25N	25C21	23C	56.71
25N	25C21	23CA	72.88	25N	25C21	19NE2	53.88
25N	25C21	26N	39.27	25N	25C21	24N	40.31

TABLE XII

25N	25C21	25C	33.06	25N	25C21	24C	9.89
25N	25C21	162CE1	88.84	25N	25C21	19OE1	66.88
25N	25C21	24CA	27.62	25N	25C21	163N	97.26
25N	25C21	19CD	57.91	25N	25C21	26CD1	57.03
25CA	25C21	23O	85.08	25CA	25C21	23C	79.97
25CA	25C21	162ND1	82.14	25CA	25C21	23CA	94.92
25CA	25C21	19NE2	59.55	25CA	25C21	26N	34.96
25CA	25C21	24N	63.21	25CA	25C21	25C	19.25
25CA	25C21	24C	32.60	25CA	25C21	162CE1	69.83
25CA	25C21	19OE1	60.15	25CA	25C21	24CA	50.80
25CA	25C21	163N	75.98	25CA	25C21	19CD	57.10
25CA	25C21	26CD1	68.81	23O	25C21	23C	18.23
23O	25C21	23CA	34.62	23O	25C21	19NE2	81.51
23O	25C21	26N	74.70	23O	25C21	24N	31.37
23O	25C21	25C	84.83	23O	25C21	24C	52.77
23O	25C21	24CA	35.38	23O	25C21	19CD	94.62
23O	25C21	26CD1	42.49	23C	25C21	23CA	21.54
23C	25C21	19NE2	63.77	23C	25C21	26N	80.57
23C	25C21	24N	17.67	23C	25C21	25C	85.73
23C	25C21	24C	48.08	23C	25C21	19OE1	91.44
23C	25C21	24CA	30.02	23C	25C21	19CD	77.14
23C	25C21	26CD1	56.82	162ND1	25C21	19NE2	82.13
162ND1	25C21	161O	66.39	162ND1	25C21	25C	86.84
162ND1	25C21	162CE1	16.39	162ND1	25C21	19OE1	54.45
162ND1	25C21	163N	49.87	162ND1	25C21	162CA	38.64
162ND1	25C21	19CD	68.76	23CA	25C21	19NE2	59.28
23CA	25C21	24N	33.06	23CA	25C21	24C	65.84
23CA	25C21	19OE1	85.51	23CA	25C21	24CA	49.18
23CA	25C21	19CD	72.54	23CA	25C21	26CD1	76.75
19NE2	25C21	26N	91.47	19NE2	25C21	24N	51.72
19NE2	25C21	25C	78.62	19NE2	25C21	24C	57.38
19NE2	25C21	162CE1	66.80	19NE2	25C21	19OE1	27.71
19NE2	25C21	24CA	59.21	19NE2	25C21	19CD	13.58
26N	25C21	24N	70.38	26N	25C21	25C	17.60
26N	25C21	24C	40.64	26N	25C21	162CE1	94.63
26N	25C21	19OE1	94.99	26N	25C21	24CA	53.42
26N	25C21	163N	67.59	26N	25C21	162CA	96.43
26N	25C21	19CD	91.55	26N	25C21	26CD1	40.50
24N	25C21	25C	71.62	24N	25C21	24C	32.79
24N	25C21	19OE1	78.31	24N	25C21	24CA	16.97
24N	25C21	19CD	64.11	24N	25C21	26CD1	58.21
161O	25C21	162CE1	82.76	161O	25C21	163N	55.62

TABLE XII

161O	25C21	162CA	33.90	25C	25C21	24C	38.87
25C	25C21	162CE1	78.56	25C	25C21	19OE1	78.01
25C	25C21	24CA	55.90	25C	25C21	163N	64.97
25C	25C21	162CA	92.64	25C	25C21	19CD	76.23
25C	25C21	26CD1	56.82	24C	25C21	162CE1	98.56
24C	25C21	19OE1	74.12	24C	25C21	24CA	18.29
24C	25C21	19CD	63.65	24C	25C21	26CD1	49.92
162CE1	25C21	19OE1	39.16	162CE1	25C21	163N	58.96
162CE1	25C21	162CA	54.05	162CE1	25C21	19CD	53.25
19OE1	25C21	24CA	82.23	19OE1	25C21	163N	94.60
19OE1	25C21	162CA	93.01	19OE1	25C21	19CD	14.34
24CA	25C21	19CD	69.26	24CA	25C21	26CD1	46.30
163N	25C21	162CA	28.85	163N	25C21	26CD1	94.44
25SG	25O22	25N	77.15	25SG	25O22	25CB	38.56
25SG	25O22	25CA	56.15	25SG	25O22	24C	89.30
25SG	25O22	19OE1	86.57	25SG	25O22	162ND1	43.24
25SG	25O22	25C	48.29	25SG	25O22	26N	51.24
25SG	25O22	162CE1	50.40	25SG	25O22	24O	83.26
25N	25O22	25CB	51.87	25N	25O22	19NE2	73.58
25N	25O22	23C	71.81	25N	25O22	23CA	95.33
25N	25O22	25CA	24.89	25N	25O22	24N	52.99
25N	25O22	23O	73.36	25N	25O22	24C	13.57
25N	25O22	19CD	75.82	25N	25O22	19OE1	83.34
25N	25O22	24CA	35.40	25N	25O22	22O	81.27
25N	25O22	25C	29.02	25N	25O22	26N	34.61
25N	25O22	23N	91.35	25N	25O22	162CE1	94.53
25N	25O22	22C	85.32	25N	25O22	24O	6.50
25CB	25O22	19NE2	77.77	25CB	25O22	25CA	27.03
25CB	25O22	24C	65.38	25CB	25O22	19CD	66.62
25CB	25O22	19OE1	58.82	25CB	25O22	24CA	87.22
25CB	25O22	162ND1	52.46	25CB	25O22	25C	32.94
25CB	25O22	26N	48.44	25CB	25O22	162CE1	44.82
25CB	25O22	24O	58.22	19NE2	25O22	23C	87.29
19NE2	25O22	23CA	80.68	19NE2	25O22	25CA	75.11
19NE2	25O22	24N	70.11	19NE2	25O22	24C	73.32
19NE2	25O22	19CD	15.53	19NE2	25O22	19OE1	32.76
19NE2	25O22	24CA	76.24	19NE2	25O22	22O	41.66
19NE2	25O22	162ND1	90.29	19NE2	25O22	25C	91.32
19NE2	25O22	23N	70.60	19NE2	25O22	162CE1	74.46
19NE2	25O22	22C	55.07	19NE2	25O22	24O	72.58
23C	25O22	23CA	27.25	23C	25O22	25CA	96.67
23C	25O22	24N	23.18	23C	25O22	23O	20.52

TABLE XII

23C	25O22	24C	58.32	23C	25O22	24CA	36.50
23C	25O22	22O	49.90	23C	25O22	25C	95.16
23C	25O22	26N	86.14	23C	25O22	23N	30.10
23C	25O22	22C	39.20	23C	25O22	24O	65.47
23CA	25O22	24N	42.37	23CA	25O22	23O	41.32
23CA	25O22	24C	81.90	23CA	25O22	19CD	95.72
23CA	25O22	24CA	60.58	23CA	25O22	22O	39.10
23CA	25O22	23N	10.12	23CA	25O22	22C	25.72
23CA	25O22	24O	88.84	25CA	25O22	24N	77.38
25CA	25O22	23O	96.24	25CA	25O22	24C	38.44
25CA	25O22	19CD	70.44	25CA	25O22	19OE1	70.91
25CA	25O22	24CA	60.28	25CA	25O22	22O	98.08
25CA	25O22	162ND1	79.49	25CA	25O22	25C	16.40
25CA	25O22	26N	32.82	25CA	25O22	162CE1	70.84
25CA	25O22	24O	31.31	24N	25O22	23O	38.32
24N	25O22	24C	39.66	24N	25O22	19CD	83.95
24N	25O22	24CA	19.43	24N	25O22	22O	42.54
24N	25O22	25C	80.28	24N	25O22	26N	76.76
24N	25O22	23N	39.05	24N	25O22	22C	38.22
24N	25O22	24O	46.50	23O	25O22	24C	61.42
23O	25O22	24CA	42.50	23O	25O22	22O	70.35
23O	25O22	25C	89.16	23O	25O22	26N	75.88
23O	25O22	23N	47.63	23O	25O22	22C	59.10
23O	25O22	24O	68.00	24C	25O22	19CD	79.18
24C	25O22	19OE1	89.99	24C	25O22	24CA	21.85
24C	25O22	22O	71.83	24C	25O22	25C	41.07
24C	25O22	26N	42.17	24C	25O22	23N	78.42
24C	25O22	22C	73.88	24C	25O22	24O	7.15
19CD	25O22	19OE1	17.46	19CD	25O22	24CA	86.98
19CD	25O22	22O	56.95	19CD	25O22	162ND1	74.94
19CD	25O22	25C	86.74	19CD	25O22	23N	85.73
19CD	25O22	162CE1	58.96	19CD	25O22	22C	70.31
19CD	25O22	24O	76.60	19OE1	25O22	22O	73.26
19OE1	25O22	162ND1	57.54	19OE1	25O22	25C	85.88
19OE1	25O22	162CE1	41.81	19OE1	25O22	22C	86.38
19OE1	25O22	24O	85.82	24CA	25O22	22O	59.15
24CA	25O22	25C	61.20	24CA	25O22	26N	57.49
24CA	25O22	23N	58.31	24CA	25O22	22C	57.09
24CA	25O22	24O	29.00	22O	25O22	23N	28.99
22O	25O22	22C	13.41	22O	25O22	24O	76.18
162ND1	25O22	25C	81.58	162ND1	25O22	26N	91.32
162ND1	25O22	162CE1	16.64	25C	25O22	26N	17.25

TABLE XII

25C	25O22	162CE1	77.24	25C	25O22	24O	34.98
26N	25O22	162CE1	90.62	26N	25O22	24O	38.49
23N	25O22	22C	15.60	23N	25O22	24O	84.97
22C	25O22	24O	79.45	160O	25C23	160CB	36.76
67OH	25C23	67CE1	30.78	160O	25C24	160CB	45.57
160O	25C24	160C	10.69	160O	25C24	160CA	28.84
160O	25C24	160N	35.35	160CB	25C24	160C	34.90
160CB	25C24	209CD2	74.30	160CB	25C24	160CA	18.76
160CB	25C24	160N	30.63	160C	25C24	209CD2	96.30
160C	25C24	160CA	18.91	160C	25C24	160N	29.27
67CE1	25C24	209CD2	57.14	67CE1	25C24	67OH	30.07
209CD2	25C24	160CA	90.67	209CD2	25C24	67OH	85.98
160CA	25C24	160N	17.56	160O	25C25	160C	5.82
160O	25C25	160CB	36.39	160C	25C25	160CB	31.49
67CE1	25C25	67OH	30.77	67CE1	25C25	67CZ	16.04
67OH	25C25	67CZ	16.48	67OH	25C26	67CE1	31.37
67OH	25C26	67CZ	16.61	67CE1	25C26	67CZ	17.15
67OH	25C27	67CZ	14.42	67OH	25C27	67CE1	29.64
67CZ	25C27	67CE1	16.82	67CE1	25C27	160O	94.55
67OH	25C28	67CE1	29.88	67OH	25C28	67CZ	13.63
67CE1	25C28	67CZ	16.55	275OH2	25O30	161CA	92.49
160O	25O30	161CA	34.81	160O	25C31	161CA	41.59
160O	25C31	161O	73.41	160O	25C31	161C	57.25
160O	25C31	160C	11.02	160O	25C31	161N	26.54
160O	25C31	161CB	50.31	161CA	25C31	161O	34.32
161CA	25C31	161C	20.25	161CA	25C31	160C	31.39
161CA	25C31	161N	15.77	161CA	25C31	161CB	16.64
161O	25C31	275OH2	83.79	161O	25C31	161C	16.21
161O	25C31	160C	62.41	161O	25C31	161N	47.12
161O	25C31	161CB	38.54	275OH2	25C31	161C	97.89
275OH2	25C31	161CB	91.47	161C	25C31	160C	46.24
161C	25C31	161N	31.16	161C	25C31	161CB	30.39
160C	25C31	161N	15.86	160C	25C31	161CB	42.23
161N	25C31	161CB	29.11	160O	25O32	161CA	58.97
160O	25O32	161C	79.84	160O	25O32	160C	17.38
160O	25O32	161N	38.10	160O	25O32	161CB	67.22
160O	25O32	162N	74.42	160O	25O32	160CA	13.85
161CA	25O32	161O	45.01	161CA	25O32	161C	27.02
161CA	25O32	160C	43.17	161CA	25O32	161N	22.39
161CA	25O32	161CB	19.73	161CA	25O32	162N	31.22
161CA	25O32	160CA	49.48	161O	25O32	161C	21.40
161O	25O32	160C	83.84	161O	25O32	161N	63.21

TABLE XII

161O	25O32	161CB	49.30	161O	25O32	162N	29.81
161O	25O32	160CA	88.75	161O	25O32	275OH2	81.22
161C	25O32	160C	62.49	161C	25O32	161N	42.18
161C	25O32	161CB	39.00	161C	25O32	162N	12.22
161C	25O32	160CA	67.34	160C	25O32	161N	21.25
160C	25O32	161CB	55.00	160C	25O32	162N	57.22
160C	25O32	160CA	6.68	161N	25O32	161CB	37.70
161N	25O32	162N	39.25	161N	25O32	160CA	27.25
161CB	25O32	162N	47.45	161CB	25O32	160CA	61.67
161CB	25O32	275OH2	93.88	162N	25O32	160CA	61.00
161O	25C33	161C	15.17	161O	25C33	275OH2	81.48
161O	25C33	161CA	29.19	66O	25C33	66N	37.60
66O	25C33	65CA	66.72	161C	25C33	275OH2	91.71
161C	25C33	161CA	18.22	66N	25C33	275OH2	84.36
66N	25C33	65CA	29.78	275OH2	25C33	161CA	86.95
275OH2	25C33	65CA	56.91	66O	25C34	66C	9.95
66O	25C34	66N	42.43	66O	25C34	26CB	47.74
66O	25C34	66CA	25.52	66O	25C34	67N	13.89
66O	25C34	26CG	42.21	66O	25C34	163CB	91.47
66C	25C34	66N	36.15	66C	25C34	26CB	56.11
66C	25C34	66CA	18.24	66C	25C34	67N	11.90
66C	25C34	26CG	48.09	66N	25C34	26CB	65.07
66N	25C34	66CA	17.98	66N	25C34	67N	47.31
66N	25C34	26CG	48.82	26CB	25C34	66CA	60.10
26CB	25C34	67N	60.76	26CB	25C34	26CG	17.03
26CB	25C34	163CB	52.12	66CA	25C34	67N	29.36
66CA	25C34	26CG	46.86	161O	25C34	163CB	78.29
67N	25C34	26CG	56.10	67N	25C34	163CB	99.58
26CG	25C34	163CB	68.12	66O	25C35	163CB	89.09
66O	25C35	66C	7.53	66O	25C35	67CD1	63.13
66O	25C35	68SD	68.36	66O	25C35	26CB	39.72
209CD2	25C35	134CB	51.38	209CD2	25C35	67CD1	51.16
209CD2	25C35	68SD	69.83	209CD2	25C35	160O	84.17
134CB	25C35	163CB	64.65	134CB	25C35	163N	61.10
134CB	25C35	68SD	66.71	134CB	25C35	160O	74.73
134CB	25C35	161O	92.07	163CB	25C35	66C	96.13
163CB	25C35	163N	30.24	163CB	25C35	68SD	45.97
163CB	25C35	26CB	50.88	163CB	25C35	161O	80.11
66C	25C35	67CD1	56.50	66C	25C35	68SD	71.94
66C	25C35	26CB	47.21	67CD1	25C35	68SD	80.40
67CD1	25C35	26CB	97.36	163N	25C35	68SD	74.50
163N	25C35	160O	89.86	163N	25C35	26CB	73.24

TABLE XII

163N	25C35 161O	52.41	68SD	25C35 26CB	52.35
160O	25C35 161O	56.45	26CB	25C35 161O	98.49
161C	25C36 161O	18.57	161C	25C36 162N	20.01
161C	25C36 160O	62.57	161C	25C36 163N	67.45
161C	25C36 161CA	21.83	161C	25C36 162C	54.00
161C	25C36 160C	53.82	161C	25C36 161N	36.26
161C	25C36 162CA	34.07	161C	25C36 163CA	85.21
161C	25C36 163CB	99.05	161C	25C36 162O	59.74
161C	25C36 160CB	80.93	161C	25C36 134CA	96.31
161O	25C36 162N	33.64	161O	25C36 160O	74.48
161O	25C36 163N	66.90	161O	25C36 161CA	34.96
161O	25C36 162C	59.06	161O	25C36 160C	69.44
161O	25C36 161N	53.14	161O	25C36 162CA	38.64
161O	25C36 163CA	85.32	161O	25C36 163CB	94.16
161O	25C36 162O	69.06	161O	25C36 160CB	98.55
162N	25C36 134CB	89.78	162N	25C36 160O	71.09
162N	25C36 163N	52.42	162N	25C36 161CA	35.49
162N	25C36 162C	36.12	162N	25C36 160C	57.50
162N	25C36 161N	39.78	162N	25C36 162CA	19.47
162N	25C36 163CA	68.57	162N	25C36 163CB	85.10
162N	25C36 162O	39.89	162N	25C36 160CB	76.82
162N	25C36 134CA	77.09	134CB	25C36 160O	94.70
134CB	25C36 163N	73.72	134CB	25C36 162C	70.42
134CB	25C36 160C	84.32	134CB	25C36 161N	89.08
134CB	25C36 162CA	87.63	134CB	25C36 163CA	61.39
134CB	25C36 163CB	69.69	134CB	25C36 162O	57.00
134CB	25C36 209CD2	50.87	134CB	25C36 160CB	57.37
134CB	25C36 134CA	14.58	160O	25C36 161CA	40.90
160O	25C36 160C	17.14	160O	25C36 161N	31.70
160O	25C36 162CA	90.56	160O	25C36 162O	96.89
160O	25C36 209CD2	91.01	160O	25C36 160CB	37.47
160O	25C36 134CA	97.11	163N	25C36 161CA	87.43
163N	25C36 162C	18.84	163N	25C36 161N	90.13
163N	25C36 162CA	33.77	163N	25C36 163CA	18.45
163N	25C36 163CB	32.69	163N	25C36 162O	29.16
163N	25C36 134CA	60.25	161CA	25C36 162C	71.59
161CA	25C36 160C	34.60	161CA	25C36 161N	20.18
161CA	25C36 162CA	53.69	161CA	25C36 162O	73.10
161CA	25C36 160CB	64.88	161CA	25C36 134CA	99.89
162C	25C36 160C	86.67	162C	25C36 161N	71.72
162C	25C36 162CA	20.71	162C	25C36 163CA	32.55
162C	25C36 163CB	50.28	162C	25C36 162O	14.79

TABLE XII

162C	25C36	160CB	91.85	162C	25C36	134CA	55.85
160C	25C36	161N	18.17	160C	25C36	162CA	76.54
160C	25C36	162O	79.80	160C	25C36	209CD2	94.97
160C	25C36	160CB	31.31	160C	25C36	134CA	83.64
161N	25C36	162CA	59.12	161N	25C36	162O	67.84
161N	25C36	160CB	45.47	161N	25C36	134CA	83.93
162CA	25C36	163CA	51.16	162CA	25C36	163CB	66.24
162CA	25C36	162O	30.96	162CA	25C36	160CB	91.92
162CA	25C36	134CA	73.28	163CA	25C36	163CB	19.41
163CA	25C36	162O	35.58	163CA	25C36	134CA	50.10
163CA	25C36	66O	93.58	163CB	25C36	162O	54.97
163CB	25C36	209CD2	96.16	163CB	25C36	134CA	62.02
163CB	25C36	66O	74.19	162O	25C36	160CB	79.17
162O	25C36	134CA	42.49	209CD2	25C36	160CB	65.91
209CD2	25C36	134CA	65.34	209CD2	25C36	66O	80.01
160CB	25C36	134CA	61.85	209CD2	25C37	67CD1	67.58
209CD2	25C37	67CE1	72.61	209CD2	25C37	67CG	78.13
209CD2	25C37	160O	97.02	209CD2	25C37	67CZ	85.11
209CD2	25C37	134CB	51.48	209CD2	25C37	67CA	84.67
209CD2	25C37	209CG	2.50	67CD1	25C37	67CE1	21.97
67CD1	25C37	66O	73.49	67CD1	25C37	67CG	14.24
67CD1	25C37	67CZ	29.56	67CD1	25C37	66C	63.11
67CD1	25C37	67CA	43.36	67CD1	25C37	209CG	66.09
67CE1	25C37	66O	88.74	67CE1	25C37	67CG	32.18
67CE1	25C37	67CZ	12.63	67CE1	25C37	66C	77.14
67CE1	25C37	67CA	63.67	67CE1	25C37	209CG	72.01
66O	25C37	67CG	59.39	66O	25C37	67CZ	84.53
66O	25C37	66C	11.85	66O	25C37	67CA	35.08
67CG	25C37	67CZ	34.96	67CG	25C37	66C	48.87
67CG	25C37	67CA	31.56	67CG	25C37	209CG	76.30
160O	25C37	134CB	73.49	160O	25C37	209CG	99.48
67CZ	25C37	66C	72.68	67CZ	25C37	67CA	65.61
67CZ	25C37	209CG	84.57	66C	25C37	67CA	29.50
134CB	25C37	209CG	52.27	67CA	25C37	209CG	82.22
65CA	25C38	66N	35.46	65CA	25C38	66O	74.46
65CA	25C38	26CD1	58.84	65CA	25C38	275OH2	67.35
65CA	25C38	65C	19.07	65CA	25C38	23O	55.20
65CA	25C38	26CB	86.32	65CA	25C38	26CG	69.11
65CA	25C38	64O	33.75	65CA	25C38	65N	11.94
161O	25C38	25SG	65.22	161O	25C38	275OH2	84.21
161O	25C38	161C	10.24	66N	25C38	66O	39.10
66N	25C38	26CD1	49.39	66N	25C38	275OH2	95.80

TABLE XII

66N	25C38	65C	16.72	66N	25C38	23O	75.10
66N	25C38	26CB	62.01	66N	25C38	26CG	49.74
66N	25C38	64O	67.28	66N	25C38	65N	46.94
66O	25C38	26CD1	55.62	66O	25C38	65C	55.45
66O	25C38	23O	98.46	66O	25C38	26CB	41.40
66O	25C38	26CG	43.32	66O	25C38	65N	85.60
26CD1	25C38	25SG	77.15	26CD1	25C38	65C	49.46
26CD1	25C38	23O	44.41	26CD1	25C38	26CB	32.56
26CD1	25C38	26CG	15.85	26CD1	25C38	64O	87.10
26CD1	25C38	65N	61.51	25SG	25C38	23O	70.52
25SG	25C38	26CB	68.80	25SG	25C38	26CG	76.92
25SG	25C38	161C	68.97	275OH2	25C38	65C	83.85
275OH2	25C38	23O	87.47	275OH2	25C38	64O	35.10
275OH2	25C38	161C	89.52	275OH2	25C38	65N	61.32
65C	25C38	23O	62.91	65C	25C38	26CB	71.13
65C	25C38	26CG	55.52	65C	25C38	64O	52.20
65C	25C38	65N	30.26	23O	25C38	26CB	73.10
23O	25C38	26CG	59.68	23O	25C38	64O	61.47
23O	25C38	65N	47.46	26CB	25C38	26CG	17.91
26CB	25C38	65N	91.96	26CG	25C38	65N	74.13
64O	25C38	65N	26.26	65CA	25O39	66N	45.40
65CA	25O39	65C	23.65	65CA	25O39	275OH2	89.27
65CA	25O39	64O	46.55	65CA	25O39	65N	17.11
65CA	25O39	26CD1	69.73	65CA	25O39	23O	68.59
65CA	25O39	64C	33.21	65CA	25O39	66O	84.46
65CA	25O39	66CA	54.04	65CA	25O39	65O	20.83
65CA	25O39	26CG	77.43	65CA	25O39	26NE1	55.20
65CA	25O39	66C	71.68	66N	25O39	65C	22.01
66N	25O39	64O	89.22	66N	25O39	65N	62.07
66N	25O39	26CD1	54.96	66N	25O39	23O	90.19
66N	25O39	64C	78.37	66N	25O39	66O	39.27
66N	25O39	66CA	8.76	66N	25O39	65O	25.54
66N	25O39	26CG	51.40	66N	25O39	26NE1	49.00
66N	25O39	66C	26.33	65C	25O39	64O	69.28
65C	25O39	65N	40.08	65C	25O39	26CD1	57.43
65C	25O39	23O	76.91	65C	25O39	64C	56.85
65C	25O39	66O	60.83	65C	25O39	66CA	30.50
65C	25O39	65O	3.97	65C	25O39	26CG	60.36
65C	25O39	26NE1	45.73	65C	25O39	66C	48.13
275OH2	25O39	64O	44.70	275OH2	25O39	65N	79.36
275OH2	25O39	64C	61.39	275OH2	25O39	161O	78.76
64O	25O39	65N	34.67	64O	25O39	23O	76.69

TABLE XII

64O	25O39	64C	16.94	64O	25O39	66CA	97.89
64O	25O39	65O	67.08	64O	25O39	26NE1	93.96
65N	25O39	26CD1	75.00	65N	25O39	23O	58.94
65N	25O39	64C	18.53	65N	25O39	66CA	70.56
65N	25O39	65O	36.76	65N	25O39	26CG	85.84
65N	25O39	26NE1	60.15	65N	25O39	66C	88.15
26CD1	25O39	23O	49.08	26CD1	25O39	64C	91.52
26CD1	25O39	66O	56.07	26CD1	25O39	66CA	53.07
26CD1	25O39	65O	56.44	26CD1	25O39	26CG	14.63
26CD1	25O39	26NE1	14.91	26CD1	25O39	66C	54.99
23O	25O39	64C	64.20	23O	25O39	66CA	93.33
23O	25O39	65O	73.30	23O	25O39	26CG	63.07
23O	25O39	26NE1	44.74	64C	25O39	66CA	87.09
64C	25O39	65O	53.98	64C	25O39	26NE1	77.02
66O	25O39	66CA	30.52	66O	25O39	65O	63.93
66O	25O39	26CG	42.81	66O	25O39	26NE1	62.05
66O	25O39	66C	13.06	66CA	25O39	65O	33.85
66CA	25O39	26CG	47.00	66CA	25O39	26NE1	49.86
66CA	25O39	66C	17.64	65O	25O39	26CG	60.51
65O	25O39	26NE1	44.00	65O	25O39	66C	51.39
26CG	25O39	26NE1	26.93	26CG	25O39	66C	44.17
26NE1	25O39	66C	57.23	25SG	25N40	161O	83.77
25SG	25N40	26CD1	96.23	25SG	25N40	26N	54.32
25SG	25N40	23O	88.72	25SG	25N40	26CB	85.40
25SG	25N40	163N	48.48	25SG	25N40	25CB	12.78
25SG	25N40	26CG	93.55	25SG	25N40	161C	83.44
25SG	25N40	25N	43.46	25SG	25N40	162CA	55.83
25SG	25N40	26CA	67.26	25SG	25N40	23C	77.46
25SG	25N40	163CB	56.68	25SG	25N40	25CA	30.38
25SG	25N40	25C	40.47	161O	25N40	163N	62.30
161O	25N40	25CB	96.42	161O	25N40	161C	9.97
161O	25N40	162CA	34.15	161O	25N40	163CB	90.03
26CD1	25N40	26N	45.97	26CD1	25N40	23O	47.29
26CD1	25N40	26CB	34.59	26CD1	25N40	25CB	83.86
26CD1	25N40	26CG	16.42	26CD1	25N40	25N	56.97
26CD1	25N40	65CA	53.52	26CD1	25N40	66O	51.90
26CD1	25N40	26CA	42.89	26CD1	25N40	66N	44.25
26CD1	25N40	23C	56.28	26CD1	25N40	163CB	84.60
26CD1	25N40	25CA	66.03	26CD1	25N40	25C	58.27
26N	25N40	23O	70.59	26N	25N40	26CB	33.25
26N	25N40	163N	70.68	26N	25N40	25CB	44.21
26N	25N40	26CG	39.40	26N	25N40	25N	34.54

TABLE XII

26N	25N40	65CA	99.36	26N	25N40	66O	73.26
26N	25N40	162CA	97.09	26N	25N40	26CA	16.76
26N	25N40	66N	85.93	26N	25N40	23C	69.38
26N	25N40	163CB	48.13	26N	25N40	25CA	29.29
26N	25N40	25C	13.85	23O	25N40	26CB	79.60
23O	25N40	25CB	77.95	23O	25N40	26CG	63.18
23O	25N40	25N	49.38	23O	25N40	65CA	52.49
23O	25N40	66O	94.81	23O	25N40	26CA	79.46
23O	25N40	66N	70.07	23O	25N40	23C	13.03
23O	25N40	25CA	66.29	23O	25N40	25C	73.80
26CB	25N40	163N	81.30	26CB	25N40	25CB	76.86
26CB	25N40	26CG	18.52	26CB	25N40	25N	64.46
26CB	25N40	65CA	80.54	26CB	25N40	66O	40.01
26CB	25N40	26CA	18.15	26CB	25N40	66N	57.97
26CB	25N40	23C	85.39	26CB	25N40	163CB	51.83
26CB	25N40	25CA	62.52	26CB	25N40	25C	46.36
163N	25N40	25CB	57.29	163N	25N40	26CG	99.16
163N	25N40	161C	55.09	163N	25N40	25N	84.86
163N	25N40	66O	96.57	163N	25N40	162CA	29.80
163N	25N40	26CA	70.11	163N	25N40	163CB	29.52
163N	25N40	25CA	67.98	163N	25N40	25C	62.99
25CB	25N40	26CG	82.58	25CB	25N40	161C	96.21
25CB	25N40	25N	30.92	25CB	25N40	162CA	68.31
25CB	25N40	26CA	58.91	25CB	25N40	23C	67.68
25CB	25N40	163CB	58.44	25CB	25N40	25CA	17.83
25CB	25N40	25C	30.57	26CG	25N40	25N	61.46
26CG	25N40	65CA	64.22	26CG	25N40	66O	41.69
26CG	25N40	26CA	30.63	26CG	25N40	66N	46.53
26CG	25N40	23C	71.01	26CG	25N40	163CB	69.91
26CG	25N40	25CA	65.57	26CG	25N40	25C	53.15
161C	25N40	162CA	29.49	161C	25N40	163CB	81.51
25N	25N40	65CA	97.53	25N	25N40	162CA	99.23
25N	25N40	26CA	50.89	25N	25N40	23C	41.97
25N	25N40	163CB	74.65	25N	25N40	25CA	16.92
25N	25N40	25C	28.88	65CA	25N40	66O	62.01
65CA	25N40	26CA	94.78	65CA	25N40	66N	28.94
65CA	25N40	23C	64.73	66O	25N40	26CA	57.46
66O	25N40	66N	33.09	66O	25N40	163CB	72.28
66O	25N40	25C	86.11	162CA	25N40	26CA	99.40
162CA	25N40	163CB	59.22	162CA	25N40	25CA	84.50
162CA	25N40	25C	86.43	26CA	25N40	66N	75.24
26CA	25N40	23C	81.32	26CA	25N40	163CB	42.44

TABLE XII

26CA	25N40	25CA	45.63	26CA	25N40	25C	28.66
66N	25N40	23C	83.06	66N	25N40	25C	99.63
23C	25N40	25CA	58.57	23C	25N40	25C	69.36
163CB	25N40	25CA	59.45	163CB	25N40	25C	46.39
25CA	25N40	25C	17.68	25SG	25C41	25N	62.70
25SG	25C41	26N	62.65	25SG	25C41	25CB	23.96
25SG	25C41	25CA	43.98	25SG	25C41	24N	98.96
25SG	25C41	24C	76.68	25SG	25C41	25C	48.95
25SG	25C41	26CB	86.53	25SG	25C41	24CA	95.08
25SG	25C41	161O	70.41	25SG	25C41	26CA	70.68
23O	25C41	25N	69.35	23O	25C41	23C	19.72
23O	25C41	26CD1	58.41	23O	25C41	26N	90.56
23O	25C41	25CA	89.48	23O	25C41	23CA	34.94
23O	25C41	24N	31.63	23O	25C41	24C	57.25
23O	25C41	25C	94.72	23O	25C41	26CB	91.35
23O	25C41	26CG	73.21	23O	25C41	24CA	37.60
23O	25C41	65CA	57.07	23O	25C41	26NE1	46.32
23O	25C41	26CA	94.04	25N	25C41	23C	58.58
25N	25C41	26CD1	71.53	25N	25C41	26N	42.84
25N	25C41	25CB	39.04	25N	25C41	25CA	20.25
25N	25C41	23CA	71.04	25N	25C41	24N	41.24
25N	25C41	24C	14.76	25N	25C41	25C	33.26
25N	25C41	26CB	72.91	25N	25C41	26CG	71.59
25N	25C41	24CA	32.43	25N	25C41	26NE1	71.77
25N	25C41	26CA	57.10	23C	25C41	26CD1	72.85
23C	25C41	26N	90.94	23C	25C41	25CB	91.53
23C	25C41	25CA	78.46	23C	25C41	23CA	20.98
23C	25C41	24N	17.34	23C	25C41	24C	50.23
23C	25C41	25C	89.47	23C	25C41	26CG	86.15
23C	25C41	24CA	32.48	23C	25C41	65CA	75.78
23C	25C41	26NE1	61.91	23C	25C41	26CA	99.05
26CD1	25C41	26N	51.41	26CD1	25C41	25CA	79.66
26CD1	25C41	23CA	92.59	26CD1	25C41	24N	70.00
26CD1	25C41	24C	58.88	26CD1	25C41	25C	66.43
26CD1	25C41	26CB	34.11	26CD1	25C41	26CG	15.31
26CD1	25C41	24CA	54.83	26CD1	25C41	65CA	55.19
26CD1	25C41	26NE1	12.42	26CD1	25C41	26CA	44.47
26N	25C41	25CB	51.65	26N	25C41	25CA	35.77
26N	25C41	24N	75.80	26N	25C41	24C	42.85
26N	25C41	25C	16.65	26N	25C41	26CB	33.09
26N	25C41	26CG	41.38	26N	25C41	24CA	58.47
26N	25C41	26NE1	60.33	26N	25C41	26CA	14.86

TABLE XII

25CB	25C41	25CA	22.08	25CB	25C41	23CA	94.98
25CB	25C41	24N	75.58	25CB	25C41	24C	53.42
25CB	25C41	25C	35.13	25CB	25C41	26CB	82.86
25CB	25C41	26CG	92.88	25CB	25C41	24CA	71.25
25CB	25C41	161O	93.68	25CB	25C41	26CA	64.25
25CA	25C41	23CA	88.69	25CA	25C41	24N	61.20
25CA	25C41	24C	32.93	25CA	25C41	25C	20.29
25CA	25C41	26CB	68.87	25CA	25C41	26CG	74.42
25CA	25C41	24CA	52.13	25CA	25C41	26NE1	83.73
25CA	25C41	26CA	50.39	23CA	25C41	24N	33.53
23CA	25C41	24C	66.67	23CA	25C41	24CA	51.61
23CA	25C41	65CA	80.98	23CA	25C41	26NE1	80.92
24N	25C41	24C	33.63	24N	25C41	25C	72.54
24N	25C41	26CB	93.33	24N	25C41	26CG	80.45
24N	25C41	24CA	18.67	24N	25C41	65CA	88.30
24N	25C41	26NE1	61.55	24N	25C41	26CA	85.94
24C	25C41	25C	39.29	24C	25C41	26CB	67.28
24C	25C41	26CG	61.65	24C	25C41	24CA	19.66
24C	25C41	26NE1	57.67	24C	25C41	26CA	54.90
25C	25C41	26CB	49.26	25C	25C41	26CG	57.75
25C	25C41	24CA	58.24	25C	25C41	26NE1	73.78
25C	25C41	26CA	30.51	26CB	25C41	26CG	18.80
26CB	25C41	24CA	74.83	26CB	25C41	65CA	78.82
26CB	25C41	26NE1	46.51	26CB	25C41	26CA	18.80
26CG	25C41	24CA	63.20	26CG	25C41	65CA	65.01
26CG	25C41	26NE1	27.72	26CG	25C41	26CA	31.31
24CA	25C41	65CA	87.25	24CA	25C41	26NE1	48.94
24CA	25C41	26CA	67.55	65CA	25C41	26NE1	49.22
65CA	25C41	26CA	95.86	26NE1	25C41	26CA	55.54
275OH2	25N42	161O	84.19	275OH2	25N42	66N	91.61
275OH2	25N42	65CA	62.05	275OH2	25N42	161C	94.32
275OH2	25N42	161CA	94.57	161O	25N42	161C	13.86
161O	25N42	160O	61.38	161O	25N42	161CA	29.35
66N	25N42	66O	34.84	66N	25N42	65CA	29.86
66O	25N42	65CA	63.11	161C	25N42	160O	47.97
161C	25N42	161CA	17.98	160O	25N42	161CA	33.22

TABLE XIII

Table of angles between atoms of the inhibitor and protein for all protein atoms within 5 Ångstroms of the inhibitor 2,2'-N,N'-bis-benzyloxycarbonyl-L-leucinylcarbohydrazide.

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
184CB	25C1	184O	38.19	184CB	25C1	184CG	19.52
184CB	25C1	184CD2	33.79	184CB	25C1	184CE3	43.09
184CB	25C1	188CD1	58.81	184O	25C1	184CG	56.83
184O	25C1	184CD2	71.93	184O	25C1	184CE3	78.59
184O	25C1	188CD1	69.71	184CG	25C1	184CD2	17.68
184CG	25C1	184CE3	32.58	184CG	25C1	188CD1	65.18
184CD2	25C1	184CE3	17.04	184CD2	25C1	188CD1	58.90
184CE3	25C1	188CD1	45.42	184O	25C2	184CB	44.21
184O	25C2	18OD1	53.44	184O	25C2	184C	13.95
184O	25C2	184CA	33.42	184O	25C2	184CG	63.00
184CB	25C2	18OD1	67.91	184CB	25C2	184C	34.94
184CB	25C2	184CA	20.32	184CB	25C2	184CG	19.43
18OD1	25C2	184C	45.96	18OD1	25C2	184CA	48.12
18OD1	25C2	184CG	73.56	184C	25C2	184CA	20.19
184C	25C2	184CG	52.12	184CA	25C2	184CG	33.37
18OD1	25C3	184CB	80.07	18OD1	25C3	184O	59.68
18OD1	25C3	184CA	57.15	18OD1	25C3	184CG	89.66
18OD1	25C3	184C	51.33	18OD1	25C3	184CD1	82.13
18OD1	25C3	18CG	11.24	18OD1	25C3	18ND2	27.16
18OD1	25C3	20O	73.60	184CB	25C3	184O	44.39
184CB	25C3	184CA	22.92	184CB	25C3	184CG	22.24
184CB	25C3	184C	36.34	184CB	25C3	184CD1	37.05
184CB	25C3	18CG	84.56	184CB	25C3	18ND2	96.50
184CB	25C3	184CD2	33.32	184O	25C3	184CA	36.38
184O	25C3	184CG	66.41	184O	25C3	184C	16.67
184O	25C3	184CD1	77.34	184O	25C3	18CG	56.51
184O	25C3	18ND2	60.61	184O	25C3	184CD2	76.89
184CA	25C3	184CG	37.43	184CA	25C3	184C	21.29
184CA	25C3	184CD1	42.36	184CA	25C3	18CG	62.14
184CA	25C3	18ND2	75.37	184CA	25C3	184CD2	52.39

TABLE XIII

184CG	25C3	184C	56.26	184CG	25C3	184CD1	18.80
184CG	25C3	18CG	97.29	184CG	25C3	184CD2	15.81
184CG	25C3	20O	99.33	184C	25C3	184CD1	63.60
184C	25C3	18CG	51.80	184C	25C3	18ND2	61.00
184C	25C3	184CD2	69.50	184CD1	25C3	18CG	91.92
184CD1	25C3	184CD2	27.91	184CD1	25C3	20O	80.68
18CG	25C3	18ND2	16.43	18CG	25C3	20O	80.57
18ND2	25C3	20O	85.65	184CG	25C4	184CD1	22.16
184CG	25C4	184CB	23.25	184CG	25C4	184NE1	33.38
184CG	25C4	184CD2	20.04	184CG	25C4	184CA	36.56
184CG	25C4	18OD1	84.23	184CG	25C4	184CE2	31.43
184CG	25C4	184O	59.49	184CG	25C4	184CE3	31.14
184CG	25C4	184C	50.73	184CD1	25C4	184CB	40.60
184CD1	25C4	184NE1	19.22	184CD1	25C4	184CD2	33.07
184CD1	25C4	184CA	43.38	184CD1	25C4	18OD1	80.63
184CD1	25C4	184CE2	30.49	184CD1	25C4	20O	96.73
184CD1	25C4	184O	72.55	184CD1	25C4	184CE3	47.65
184CD1	25C4	184C	60.18	184CB	25C4	184NE1	55.95
184CB	25C4	184CD2	38.71	184CB	25C4	184CA	20.96
184CB	25C4	18OD1	69.40	184CB	25C4	184CE2	54.07
184CB	25C4	184O	36.44	184CB	25C4	184CE3	42.67
184CB	25C4	184C	29.74	184NE1	25C4	184CD2	31.83
184NE1	25C4	184CA	62.30	184NE1	25C4	18OD1	97.90
184NE1	25C4	184CE2	18.20	184NE1	25C4	20O	93.72
184NE1	25C4	184O	90.55	184NE1	25C4	184CE3	45.60
184NE1	25C4	184C	78.96	184CD2	25C4	184CA	55.86
184CD2	25C4	184CE2	18.77	184CD2	25C4	184O	74.24
184CD2	25C4	184CE3	14.78	184CD2	25C4	184C	68.30
184CA	25C4	18OD1	49.23	184CA	25C4	184CE2	67.15
184CA	25C4	184O	30.22	184CA	25C4	184CE3	62.73
184CA	25C4	184C	16.85	18OD1	25C4	20O	73.28
18OD1	25C4	184O	46.75	18OD1	25C4	184C	42.18
184CE2	25C4	184O	90.51	184CE2	25C4	184CE3	29.58
184CE2	25C4	184C	82.12	184O	25C4	184CE3	73.98
184O	25C4	184C	14.33	184CE3	25C4	184C	71.72
184CG	25C5	184CD2	22.73	184CG	25C5	184CD1	20.69
184CG	25C5	184CE2	35.01	184CG	25C5	184NE1	33.46

TABLE XIII

184CG	25C5	184CB	21.39	184CG	25C5	184CE3	38.46
184CG	25C5	184CZ2	50.35	184CG	25C5	184CZ3	51.39
184CG	25C5	184CA	29.48	184CD2	25C5	184CD1	34.47
184CD2	25C5	184CE2	21.03	184CD2	25C5	184NE1	33.32
184CD2	25C5	184CB	39.17	184CD2	25C5	184CE3	19.36
184CD2	25C5	184CZ2	31.82	184CD2	25C5	184CZ3	29.20
184CD2	25C5	184CA	51.36	184CD1	25C5	184CE2	33.24
184CD1	25C5	184NE1	19.76	184CD1	25C5	184CB	37.53
184CD1	25C5	184CE3	53.61	184CD1	25C5	184CZ2	49.12
184CD1	25C5	184CZ3	62.53	184CD1	25C5	184CA	36.61
184CE2	25C5	184NE1	19.71	184CE2	25C5	184CB	55.77
184CE2	25C5	184CE3	34.70	184CE2	25C5	184CZ2	16.25
184CE2	25C5	184CZ3	34.98	184CE2	25C5	184CA	63.76
184NE1	25C5	184CB	54.14	184NE1	25C5	184CE3	51.39
184NE1	25C5	184CZ2	32.74	184NE1	25C5	184CZ3	54.44
184NE1	25C5	184CA	56.07	184CB	25C5	184CE3	47.44
184CB	25C5	184CZ2	70.15	184CB	25C5	184CZ3	62.99
184CB	25C5	184CA	16.19	184CE3	25C5	184CZ2	37.12
184CE3	25C5	184CZ3	15.81	184CE3	25C5	184CA	62.73
184CZ2	25C5	184CZ3	29.69	184CZ2	25C5	184CA	79.60
184CZ3	25C5	184CA	77.85	184CD2	25C6	184CE3	19.98
184CD2	25C6	184CG	20.21	184CD2	25C6	184CB	36.83
184CD2	25C6	184CE2	17.00	184CD2	25C6	184CZ3	30.72
184CD2	25C6	184CD1	27.90	184CE3	25C6	184CG	37.11
184CE3	25C6	184CB	46.74	184CE3	25C6	184CE2	31.55
184CE3	25C6	184CZ3	16.21	184CE3	25C6	184CD1	47.70
184CG	25C6	184CB	20.58	184CG	25C6	184CE2	29.67
184CG	25C6	184CZ3	50.48	184CG	25C6	184CD1	15.71
184CB	25C6	184CE2	49.78	184CB	25C6	184CZ3	62.65
184CB	25C6	184CD1	32.55	184CE2	25C6	184CZ3	34.33
184CE2	25C6	184CD1	27.45	184CZ3	25C6	184CD1	57.71
20O	25C7	19CG	65.72	20O	25C7	20C	13.67
20O	25C7	20N	42.52	20O	25C7	18OD1	88.27
20O	25C7	19CD	74.17	20O	25C7	20CA	32.34
20O	25C7	19NE2	65.37	20O	25C7	19OE1	87.32
20O	25C7	19C	42.11	184CD1	25C7	19CG	67.76
184CD1	25C7	184NE1	21.55	184CD1	25C7	184CG	19.86

TABLE XIII

184CD1	25C7	18OD1	84.02	184CD1	25C7	19CD	60.66
184CD1	25C7	184CE2	29.40	184CD1	25C7	184CB	34.91
184CD1	25C7	19NE2	73.46	184CD1	25C7	184CD2	28.08
184CD1	25C7	184CA	40.17	184CD1	25C7	183O	43.72
184CD1	25C7	19OE1	47.61	184CD1	25C7	19C	99.25
19CG	25C7	184NE1	69.79	19CG	25C7	184CG	86.16
19CG	25C7	20C	70.46	19CG	25C7	20N	50.72
19CG	25C7	18OD1	75.31	19CG	25C7	19CD	20.77
19CG	25C7	20CA	67.17	19CG	25C7	184CE2	86.39
19CG	25C7	184CB	91.37	19CG	25C7	19NE2	32.57
19CG	25C7	184CD2	94.84	19CG	25C7	184CA	78.19
19CG	25C7	183O	44.08	19CG	25C7	19OE1	28.49
19CG	25C7	19C	38.77	184NE1	25C7	184CG	34.11
184NE1	25C7	19CD	55.36	184NE1	25C7	184CE2	16.60
184NE1	25C7	184CB	52.97	184NE1	25C7	19NE2	62.84
184NE1	25C7	184CD2	29.31	184NE1	25C7	184CA	61.52
184NE1	25C7	183O	60.91	184NE1	25C7	19OE1	42.84
184CG	25C7	18OD1	81.09	184CG	25C7	19CD	80.51
184CG	25C7	184CE2	31.09	184CG	25C7	184CB	19.37
184CG	25C7	19NE2	92.98	184CG	25C7	184CD2	17.53
184CG	25C7	184CA	33.64	184CG	25C7	183O	53.42
184CG	25C7	19OE1	67.47	20C	25C7	20N	35.03
20C	25C7	18OD1	76.84	20C	25C7	19CD	82.78
20C	25C7	20CA	20.30	20C	25C7	19NE2	76.56
20C	25C7	183O	97.75	20C	25C7	19OE1	95.52
20C	25C7	19C	38.85	20N	25C7	18OD1	48.08
20N	25C7	19CD	70.24	20N	25C7	20CA	19.43
20N	25C7	19NE2	74.34	20N	25C7	184CA	87.18
20N	25C7	183O	63.69	20N	25C7	19OE1	79.16
20N	25C7	19C	12.46	18OD1	25C7	19CD	94.22
18OD1	25C7	20CA	56.55	18OD1	25C7	184CB	64.46
18OD1	25C7	184CD2	98.02	18OD1	25C7	184CA	47.47
18OD1	25C7	183O	48.16	18OD1	25C7	19OE1	93.80
18OD1	25C7	19C	55.42	19CD	25C7	20CA	84.64
19CD	25C7	184CE2	71.23	19CD	25C7	184CB	91.94
19CD	25C7	19NE2	17.10	19CD	25C7	184CD2	83.77
19CD	25C7	184CA	84.58	19CD	25C7	183O	54.34

TABLE XIII

19CD	25C7	19OE1	13.19	19CD	25C7	19C	57.87
20CA	25C7	19NE2	84.21	20CA	25C7	183O	82.52
20CA	25C7	19OE1	95.40	20CA	25C7	19C	28.93
184CE2	25C7	184CB	50.04	184CE2	25C7	19NE2	76.55
184CE2	25C7	184CD2	18.00	184CE2	25C7	184CA	64.00
184CE2	25C7	183O	72.92	184CE2	25C7	19OE1	59.12
184CB	25C7	184CD2	34.04	184CB	25C7	184CA	19.42
184CB	25C7	183O	50.23	184CB	25C7	19OE1	79.91
19NE2	25C7	184CD2	92.14	19NE2	25C7	183O	71.31
19NE2	25C7	19OE1	27.20	19NE2	25C7	19C	62.12
184CD2	25C7	184CA	50.81	184CD2	25C7	183O	69.19
184CD2	25C7	19OE1	70.74	184CA	25C7	183O	34.36
184CA	25C7	19OE1	74.90	184CA	25C7	19C	87.64
183O	25C7	19OE1	48.64	183O	25C7	19C	59.18
19OE1	25C7	19C	67.25	20O	25O8	20C	10.26
20O	25O8	19CG	58.52	20O	25O8	19NE2	68.66
20O	25O8	19CD	71.25	20O	25O8	20CA	23.15
20O	25O8	20N	31.47	20O	25O8	21N	16.79
20O	25O8	21CA	28.59	20C	25O8	19CG	64.70
20C	25O8	19NE2	78.30	20C	25O8	19CD	79.37
20C	25O8	20CA	16.86	20C	25O8	20N	30.40
20C	25O8	21N	12.70	20C	25O8	21CA	28.94
184NE1	25O8	184CD1	18.63	184NE1	25O8	19CG	59.96
184NE1	25O8	19NE2	61.10	184NE1	25O8	19CD	50.56
184NE1	25O8	184CE2	16.07	184NE1	25O8	20N	95.41
184NE1	25O8	184CG	27.36	184CD1	25O8	19CG	54.74
184CD1	25O8	19NE2	67.50	184CD1	25O8	19CD	52.79
184CD1	25O8	184CE2	28.00	184CD1	25O8	20CA	98.14
184CD1	25O8	20N	81.88	184CD1	25O8	184CG	15.43
19CG	25O8	19NE2	32.50	19CG	25O8	19CD	19.73
19CG	25O8	184CE2	76.01	19CG	25O8	20CA	58.57
19CG	25O8	20N	42.57	19CG	25O8	184CG	68.67
19CG	25O8	21N	75.23	19CG	25O8	21CA	84.51
19NE2	25O8	19CD	17.06	19NE2	25O8	184CE2	74.74
19NE2	25O8	20CA	80.50	19NE2	25O8	20N	68.75
19NE2	25O8	184CG	82.83	19NE2	25O8	21N	83.53
19NE2	25O8	21CA	83.71	19CD	25O8	184CE2	66.00

TABLE XIII

19CD	25O8	20CA	76.51	19CD	25O8	20N	61.57
19CD	25O8	184CG	68.20	19CD	25O8	21N	87.76
19CD	25O8	21CA	92.52	184CE2	25O8	184CG	27.48
20CA	25O8	20N	17.27	20CA	25O8	21N	28.61
20CA	25O8	21CA	45.46	20N	25O8	184CG	88.95
20N	25O8	21N	43.10	20N	25O8	21CA	58.85
21N	25O8	21CA	16.97	20O	25C9	19NE2	82.43
20O	25C9	19CD	79.79	20O	25C9	19CG	60.88
20O	25C9	20C	3.58	20O	25C9	22O	59.91
20O	25C9	184CD1	98.95	20O	25C9	19OE1	91.12
20O	25C9	22N	39.58	20O	25C9	21CA	31.39
20O	25C9	21OE1	65.02	19NE2	25C9	19CD	19.36
19NE2	25C9	19CG	36.33	19NE2	25C9	184NE1	69.05
19NE2	25C9	20C	86.00	19NE2	25C9	22O	36.71
19NE2	25C9	184CD1	71.62	19NE2	25C9	19OE1	26.23
19NE2	25C9	22N	69.60	19NE2	25C9	184CE2	82.17
19NE2	25C9	21CA	96.36	19CD	25C9	19CG	21.85
19CD	25C9	184NE1	54.74	19CD	25C9	20C	83.26
19CD	25C9	22O	50.79	19CD	25C9	184CD1	53.82
19CD	25C9	19OE1	12.53	19CD	25C9	22N	79.86
19CD	25C9	184CE2	69.35	19CG	25C9	184NE1	61.67
19CG	25C9	20C	64.10	19CG	25C9	22O	53.24
19CG	25C9	184CD1	53.39	19CG	25C9	19OE1	30.83
19CG	25C9	22N	72.73	19CG	25C9	184CE2	76.64
19CG	25C9	21CA	87.99	184NE1	25C9	184CD1	16.96
184NE1	25C9	19OE1	43.53	184NE1	25C9	184CE2	15.12
20C	25C9	22O	62.84	20C	25C9	19OE1	94.48
20C	25C9	22N	40.82	20C	25C9	21CA	29.72
20C	25C9	21OE1	62.22	22O	25C9	19OE1	61.50
22O	25C9	22N	33.67	22O	25C9	21CA	61.98
22O	25C9	21OE1	90.36	184CD1	25C9	19OE1	45.59
184CD1	25C9	184CE2	27.01	19OE1	25C9	22N	92.00
19OE1	25C9	184CE2	57.64	22N	25C9	21CA	28.69
22N	25C9	21OE1	58.53	21CA	25C9	21OE1	36.88
20O	25O10	22O	85.43	20O	25O10	19CD	97.70
20O	25O10	19CG	73.17	20O	25O10	22N	56.64
20O	25O10	20C	5.18	20O	25O10	22C	86.37

TABLE XIII

20O	25O10	21CA	39.27	20O	25O10	21C	51.49
20O	25O10	21N	20.36	20O	25O10	22CA	70.79
20O	25O10	19CB	67.40	20O	25O10	20N	28.18
20O	25O10	20CA	10.76	20O	25O10	21OE1	68.78
19NE2	25O10	22O	52.26	19NE2	25O10	19CD	20.65
19NE2	25O10	19CG	42.35	19NE2	25O10	22N	96.61
19NE2	25O10	22C	66.07	19NE2	25O10	19OE1	22.91
19NE2	25O10	22CA	82.67	19NE2	25O10	19CB	43.12
19NE2	25O10	20N	84.11	19NE2	25O10	23N	64.93
19NE2	25O10	184NE1	62.68	19NE2	25O10	23CA	53.12
22O	25O10	19CD	65.17	22O	25O10	19CG	68.00
22O	25O10	22N	45.38	22O	25O10	20C	81.85
22O	25O10	22C	15.92	22O	25O10	21CA	79.66
22O	25O10	21C	61.19	22O	25O10	21N	79.35
22O	25O10	19OE1	72.72	22O	25O10	22CA	30.41
22O	25O10	19CB	55.31	22O	25O10	20N	77.38
22O	25O10	23N	24.55	22O	25O10	20CA	82.51
22O	25O10	23CA	30.74	19CD	25O10	19CG	24.88
19CD	25O10	20C	99.46	19CD	25O10	22C	80.69
19CD	25O10	19OE1	10.13	19CD	25O10	22CA	93.93
19CD	25O10	19CB	31.83	19CD	25O10	20N	69.77
19CD	25O10	23N	82.79	19CD	25O10	20CA	87.09
19CD	25O10	184NE1	49.90	19CD	25O10	23CA	72.96
19CG	25O10	22N	93.59	19CG	25O10	20C	75.37
19CG	25O10	22C	83.51	19CG	25O10	21N	89.04
19CG	25O10	19OE1	32.51	19CG	25O10	22CA	89.71
19CG	25O10	19CB	14.55	19CG	25O10	20N	45.05
19CG	25O10	23N	91.20	19CG	25O10	20CA	62.46
19CG	25O10	184NE1	58.10	19CG	25O10	23CA	87.28
22N	25O10	20C	51.51	22N	25O10	22C	36.02
22N	25O10	21CA	34.76	22N	25O10	21C	15.90
22N	25O10	21N	40.79	22N	25O10	22CA	16.92
22N	25O10	19CB	79.30	22N	25O10	20N	69.27
22N	25O10	23N	46.59	22N	25O10	20CA	61.11
22N	25O10	21OE1	66.06	22N	25O10	23CA	63.27
20C	25O10	22C	81.89	20C	25O10	21CA	35.03
20C	25O10	21C	46.40	20C	25O10	21N	15.83

TABLE XIII

20C	25O10	22CA	65.90	20C	25O10	19CB	68.42
20C	25O10	20N	30.90	20C	25O10	23N	95.35
20C	25O10	20CA	14.07	20C	25O10	21OE1	66.77
22C	25O10	21CA	70.57	22C	25O10	21C	50.65
22C	25O10	21N	75.18	22C	25O10	19OE1	87.67
22C	25O10	22CA	19.15	22C	25O10	19CB	70.26
22C	25O10	20N	85.66	22C	25O10	23N	14.18
22C	25O10	20CA	86.38	22C	25O10	21OE1	94.63
22C	25O10	23CA	28.51	21CA	25O10	21C	20.23
21CA	25O10	21N	19.26	21CA	25O10	22CA	51.43
21CA	25O10	19CB	95.98	21CA	25O10	20N	65.09
21CA	25O10	23N	79.47	21CA	25O10	20CA	49.07
21CA	25O10	21OE1	39.22	21CA	25O10	23CA	96.32
21C	25O10	21N	32.16	21C	25O10	22CA	31.67
21C	25O10	19CB	90.80	21C	25O10	20N	71.25
21C	25O10	23N	59.25	21C	25O10	20CA	58.84
21C	25O10	21OE1	50.69	21C	25O10	23CA	76.11
21N	25O10	22CA	57.03	21N	25O10	19CB	80.04
21N	25O10	20N	45.98	21N	25O10	23N	87.15
21N	25O10	20CA	29.82	21N	25O10	21OE1	54.21
19OE1	25O10	19CB	41.46	19OE1	25O10	20N	77.43
19OE1	25O10	23N	87.76	19OE1	25O10	20CA	94.86
19OE1	25O10	184NE1	41.58	19OE1	25O10	23CA	75.81
22CA	25O10	19CB	75.23	22CA	25O10	20N	77.28
22CA	25O10	23N	30.13	22CA	25O10	20CA	73.19
22CA	25O10	21OE1	78.69	22CA	25O10	23CA	46.56
19CB	25O10	20N	41.01	19CB	25O10	23N	79.42
19CB	25O10	20CA	57.32	19CB	25O10	184NE1	72.38
19CB	25O10	23CA	78.47	20N	25O10	23N	99.51
20N	25O10	20CA	17.43	20N	25O10	184NE1	88.50
20N	25O10	21OE1	96.89	23N	25O10	21OE1	95.90
23N	25O10	23CA	16.87	20CA	25O10	21OE1	79.48
19NE2	25C11	19CD	13.29	19NE2	25C11	184NE1	59.74
19NE2	25C11	22O	32.16	19CD	25C11	184NE1	46.55
19CD	25C11	22O	44.12	184NE1	25C11	22O	89.70
19NE2	25C12	22O	39.61	19NE2	25C12	23CA	60.70
19NE2	25C12	22C	55.91	19NE2	25C12	23N	65.25

TABLE XIII

19NE2	25C12	224OH2	93.02	19NE2	25C12	22N	67.68
19NE2	25C12	19CD	8.19	19NE2	25C12	20O	56.75
22O	25C12	23CA	39.57	22O	25C12	22C	16.82
22O	25C12	23N	31.30	22O	25C12	224OH2	75.08
22O	25C12	22N	34.48	22O	25C12	19CD	46.01
22O	25C12	20O	50.49	23CA	25C12	22C	33.54
23CA	25C12	23N	19.76	23CA	25C12	224OH2	36.28
23CA	25C12	22N	62.96	23CA	25C12	19CD	68.87
23CA	25C12	20Q	89.77	22C	25C12	23N	17.94
22C	25C12	224OH2	64.69	22C	25C12	22N	29.81
22C	25C12	19CD	62.67	22C	25C12	20O	58.58
23N	25C12	224OH2	46.80	23N	25C12	22N	44.68
23N	25C12	19CD	73.05	23N	25C12	20O	76.44
224OH2	25C12	22N	89.06	22N	25C12	19CD	71.05
22N	25C12	20O	37.38	19CD	25C12	20O	54.60
21OE1	25C13	22N	66.00	21OE1	25C13	22C	95.57
21OE1	25C13	22O	97.18	21OE1	25C13	21C	51.73
22N	25C13	22C	29.65	22N	25C13	23N	43.65
22N	25C13	22O	33.57	22N	25C13	21C	15.61
22N	25C13	23CA	58.56	22C	25C13	23N	16.28
22C	25C13	22O	14.98	22C	25C13	21C	44.10
22C	25C13	23CA	29.00	23N	25C13	22O	27.57
23N	25C13	21C	56.18	23N	25C13	23CA	17.03
22O	25C13	21C	49.18	22O	25C13	23CA	33.12
21C	25C13	23CA	72.30	22N	25C14	21C	21.24
22N	25C14	22C	38.14	22N	25C14	21OE1	82.54
22N	25C14	23N	56.21	22N	25C14	22CA	22.02
22N	25C14	21CA	36.01	22N	25C14	21O	33.22
22N	25C14	22O	40.42	22N	25C14	23CA	70.62
22N	25C14	20O	41.05	22N	25C14	21CB	49.85
22N	25C14	21CD	75.68	21C	25C14	22C	58.12
21C	25C14	21OE1	65.17	21C	25C14	23N	74.13
21C	25C14	22CA	37.70	21C	25C14	21CA	21.82
21C	25C14	21O	17.02	21C	25C14	22O	61.64
21C	25C14	23CA	90.21	21C	25C14	20O	46.27
21C	25C14	21CB	30.54	21C	25C14	21CD	59.45
22C	25C14	23N	20.02	22C	25C14	22CA	22.87

TABLE XIII

22C	25C14	21CA	73.72	22C	25C14	21O	63.62
22C	25C14	22O	16.99	22C	25C14	23CA	32.48
22C	25C14	20O	63.32	22C	25C14	21CB	87.93
21OE1	25C14	21CA	46.55	21OE1	25C14	21O	68.11
21OE1	25C14	20O	64.41	21OE1	25C14	21CB	34.92
21OE1	25C14	21CD	7.92	23N	25C14	22CA	36.43
23N	25C14	21CA	92.21	23N	25C14	21O	75.11
23N	25C14	22O	32.42	23N	25C14	23CA	17.87
23N	25C14	20O	82.87	22CA	25C14	21CA	56.88
22CA	25C14	21O	40.83	22CA	25C14	22O	34.41
22CA	25C14	23CA	53.03	22CA	25C14	20O	60.12
22CA	25C14	21CB	68.24	22CA	25C14	21CD	96.45
21CA	25C14	21O	34.25	21CA	25C14	22O	71.57
21CA	25C14	20O	35.31	21CA	25C14	21CB	17.17
21CA	25C14	21CD	39.72	21O	25C14	22O	71.78
21O	25C14	23CA	92.77	21O	25C14	20O	63.21
21O	25C14	21CB	34.50	21O	25C14	21CD	64.40
22O	25C14	23CA	37.01	22O	25C14	20O	51.83
22O	25C14	21CB	88.01	23CA	25C14	20O	88.32
20O	25C14	21CB	50.65	20O	25C14	21CD	56.60
21CB	25C14	21CD	30.13	21OE1	25C15	21CD	12.20
21OE1	25C15	21NE2	26.50	21OE1	25C15	21CA	39.20
21OE1	25C15	20O	65.35	21CD	25C15	21NE2	16.43
21CD	25C15	21CA	39.53	21CD	25C15	20O	59.46
21NE2	25C15	21CA	53.49	21NE2	25C15	20O	65.84
21CA	25C15	20O	32.72	19NE2	25C16	19CD	16.53
19NE2	25C16	162ND1	88.72	19NE2	25C16	19OE1	31.45
19NE2	25C16	162CE1	76.13	19NE2	25C16	184NE1	68.38
19NE2	25C16	184CE2	84.59	19NE2	25C16	25SG	70.09
19NE2	25C16	23CA	54.01	19NE2	25C16	22O	29.07
19CD	25C16	162ND1	77.07	19CD	25C16	19OE1	16.88
19CD	25C16	162CE1	62.31	19CD	25C16	184NE1	52.74
19CD	25C16	184CZ2	85.13	19CD	25C16	184CE2	69.00
19CD	25C16	25SG	69.54	19CD	25C16	23CA	69.33
19CD	25C16	22O	45.46	162ND1	25C16	19OE1	60.33
162ND1	25C16	162CE1	17.92	162ND1	25C16	184NE1	63.79
162ND1	25C16	184CZ2	60.49	162ND1	25C16	184CE2	63.53

TABLE XIII

162ND1	25C16	25SG	43.67	19OE1	25C16	162CE1	45.48
19OE1	25C16	184NE1	45.86	19OE1	25C16	184CZ2	75.36
19OE1	25C16	184CE2	61.18	19OE1	25C16	25SG	59.93
19OE1	25C16	23CA	78.49	19OE1	25C16	22O	60.19
162CE1	25C16	184NE1	47.41	162CE1	25C16	184CZ2	52.59
162CE1	25C16	184CE2	50.53	162CE1	25C16	25SG	51.17
184NE1	25C16	184CZ2	32.85	184NE1	25C16	184CE2	16.26
184NE1	25C16	25SG	93.75	184NE1	25C16	22O	94.69
184CZ2	25C16	184CE2	17.00	25SG	25C16	23CA	63.45
25SG	25C16	22O	79.20	23CA	25C16	22O	32.47
19NE2	25O17	184NE1	87.64	19NE2	25O17	162CE1	97.12
19NE2	25O17	19OE1	40.11	19NE2	25O17	19CD	22.12
19NE2	25O17	184CD1	77.66	19NE2	25O17	25CB	62.38
19NE2	25O17	25SG	74.14	19NE2	25O17	19CG	26.63
184NE1	25O17	162CE1	65.10	184NE1	25O17	162ND1	86.13
184NE1	25O17	19OE1	60.63	184NE1	25O17	19CD	67.63
184NE1	25O17	184CZ2	42.58	184NE1	25O17	184CE2	20.97
184NE1	25O17	162NE2	55.54	184NE1	25O17	162CG	83.50
184NE1	25O17	184CD1	10.23	184NE1	25O17	25CB	94.14
184NE1	25O17	19CG	61.07	184NE1	25O17	162CD2	67.31
184NE1	25O17	184CH2	48.57	162CE1	25O17	162ND1	23.08
162CE1	25O17	19OE1	59.61	162CE1	25O17	19CD	80.14
162CE1	25O17	184CZ2	69.34	162CE1	25O17	184CE2	67.58
162CE1	25O17	162NE2	14.63	162CE1	25O17	162CG	29.19
162CE1	25O17	184CD1	69.18	162CE1	25O17	25CB	46.12
162CE1	25O17	25SG	57.25	162CE1	25O17	19CG	86.83
162CE1	25O17	162CD2	22.83	162CE1	25O17	184CH2	73.20
162ND1	25O17	19OE1	77.34	162ND1	25O17	19CD	96.95
162ND1	25O17	184CZ2	77.78	162ND1	25O17	184CE2	83.59
162ND1	25O17	162NE2	30.71	162ND1	25O17	162CG	13.98
162ND1	25O17	184CD1	91.47	162ND1	25O17	25CB	47.42
162ND1	25O17	25SG	46.98	162ND1	25O17	162CD2	23.75
162ND1	25O17	184CH2	79.38	19OE1	25O17	19CD	20.54
19OE1	25O17	184CZ2	99.66	19OE1	25O17	184CE2	80.49
19OE1	25O17	162NE2	66.69	19OE1	25O17	162CG	88.06
19OE1	25O17	184CD1	53.52	19OE1	25O17	25CB	44.71
19OE1	25O17	25SG	67.03	19OE1	25O17	19CG	28.75

TABLE XIII

19OE1	25O17	162CD2	81.23	19CD	25O17	184CE2	88.60
19CD	25O17	162NE2	86.77	19CD	25O17	184CD1	58.23
19CD	25O17	25CB	57.61	19CD	25O17	25SG	76.46
19CD	25O17	19CG	12.28	184CZ2	25O17	184CE2	21.82
184CZ2	25O17	162NE2	54.71	184CZ2	25O17	162CG	66.69
184CZ2	25O17	184CD1	52.41	184CZ2	25O17	162CD2	54.17
184CZ2	25O17	184CH2	6.39	184CE2	25O17	162NE2	54.32
184CE2	25O17	162CG	76.31	184CE2	25O17	184CD1	30.61
184CE2	25O17	19CG	81.59	184CE2	25O17	162CD2	60.79
184CE2	25O17	184CH2	27.64	162NE2	25O17	162CG	29.72
162NE2	25O17	184CD1	61.67	162NE2	25O17	25CB	60.57
162NE2	25O17	25SG	71.37	162NE2	25O17	19CG	90.84
162NE2	25O17	162CD2	15.82	162NE2	25O17	184CH2	58.64
162CG	25O17	184CD1	90.78	162CG	25O17	25CB	61.39
162CG	25O17	25SG	59.43	162CG	25O17	162CD2	16.23
162CG	25O17	184CH2	67.39	184CD1	25O17	25CB	91.37
184CD1	25O17	19CG	51.04	184CD1	25O17	162CD2	74.86
184CD1	25O17	184CH2	58.22	25CB	25O17	25SG	23.19
25CB	25O17	19CG	69.56	25CB	25O17	162CD2	65.94
25SG	25O17	19CG	88.74	25SG	25O17	162CD2	70.29
162CD2	25O17	184CH2	56.25	19NE2	25N18	25SG	74.49
19NE2	25N18	162ND1	81.92	19NE2	25N18	23CA	57.55
19NE2	25N18	224OH2	93.53	19NE2	25N18	162CE1	67.31
19NE2	25N18	19CD	12.59	19NE2	25N18	25CB	55.64
19NE2	25N18	19OE1	26.71	25SG	25N18	162ND1	48.92
25SG	25N18	161O	67.41	25SG	25N18	23CA	74.24
25SG	25N18	224OH2	87.02	25SG	25N18	162CE1	53.82
25SG	25N18	19CD	69.72	25SG	25N18	25CB	21.75
25SG	25N18	19OE1	60.33	162ND1	25N18	161O	62.58
162ND1	25N18	162CE1	16.19	162ND1	25N18	19CD	69.87
162ND1	25N18	25CB	43.26	162ND1	25N18	19OE1	55.30
161O	25N18	224OH2	98.16	161O	25N18	162CE1	78.73
161O	25N18	25CB	84.03	23CA	25N18	224OH2	36.29
23CA	25N18	19CD	68.30	23CA	25N18	25CB	74.55
23CA	25N18	19OE1	77.72	224OH2	25N18	25CB	98.57
162CE1	25N18	19CD	54.91	162CE1	25N18	25CB	40.63
162CE1	25N18	19OE1	40.66	19CD	25N18	25CB	48.94

TABLE XIII

19CD	25N18	19OE1	14.63	25CB	25N18	19OE1	38.63
25SG	25N19	162ND1	68.67	25SG	25N19	161O	97.88
25SG	25N19	25CB	26.20	25SG	25N19	162CE1	69.25
25SG	25N19	162CA	69.30	25SG	25N19	162CG	76.89
25SG	25N19	19NE2	81.47	25SG	25N19	162CB	81.47
25SG	25N19	161C	91.20	25SG	25N19	23CA	80.48
25SG	25N19	162N	79.54	25SG	25N19	19OE1	67.38
25SG	25N19	224OH2	96.97	162ND1	25N19	161O	84.02
162ND1	25N19	25CB	55.97	162ND1	25N19	162CE1	17.34
162ND1	25N19	162CA	46.46	162ND1	25N19	162CG	15.15
162ND1	25N19	19NE2	86.65	162ND1	25N19	162CB	34.28
162ND1	25N19	161C	76.02	162ND1	25N19	162N	61.82
162ND1	25N19	19OE1	59.63	161O	25N19	162CA	41.35
161O	25N19	162CG	69.81	161O	25N19	162CB	49.97
161O	25N19	161C	8.90	161O	25N19	162N	24.76
25CB	25N19	162CE1	49.59	25CB	25N19	162CA	78.03
25CB	25N19	162CG	68.95	25CB	25N19	19NE2	60.40
25CB	25N19	162CB	81.67	25CB	25N19	23CA	80.10
25CB	25N19	162N	92.77	25CB	25N19	19OE1	41.65
162CE1	25N19	162CA	63.58	162CE1	25N19	162CG	31.41
162CE1	25N19	19NE2	69.42	162CE1	25N19	162CB	51.18
162CE1	25N19	161C	93.28	162CE1	25N19	162N	79.16
162CE1	25N19	19OE1	42.84	162CA	25N19	162CG	35.79
162CA	25N19	162CB	20.40	162CA	25N19	161C	32.47
162CA	25N19	162N	16.68	162CG	25N19	162CB	19.86
162CG	25N19	161C	62.27	162CG	25N19	162N	49.28
162CG	25N19	19OE1	74.24	19NE2	25N19	23CA	51.93
19NE2	25N19	19OE1	27.73	19NE2	25N19	224OH2	83.06
162CB	25N19	161C	42.44	162CB	25N19	162N	30.28
162CB	25N19	19OE1	93.88	161C	25N19	162N	15.85
23CA	25N19	19OE1	74.91	23CA	25N19	224OH2	33.48
19NE2	25N20	184NE1	66.71	19NE2	25N20	19CD	16.40
19NE2	25N20	20O	61.92	19NE2	25N20	184CE2	83.41
19NE2	25N20	184CZ2	92.74	19NE2	25N20	184CD1	65.86
19NE2	25N20	19OE1	25.29	19NE2	25N20	19CG	28.13
184NE1	25N20	19CD	51.81	184NE1	25N20	20O	92.93
184NE1	25N20	184CE2	17.64	184NE1	25N20	184CZ2	33.11

TABLE XIII

184NE1	25N20	184CD1	14.57	184NE1	25N20	19OE1	41.63
184NE1	25N20	19CG	54.80	19CD	25N20	20O	61.53
19CD	25N20	184CE2	69.14	19CD	25N20	184CZ2	80.93
19CD	25N20	184CD1	49.60	19CD	25N20	19OE1	13.44
19CD	25N20	19CG	17.37	20O	25N20	184CD1	79.82
20O	25N20	19OE1	74.00	20O	25N20	19CG	46.41
184CE2	25N20	184CZ2	17.72	184CE2	25N20	184CD1	27.30
184CE2	25N20	19OE1	58.12	184CE2	25N20	19CG	72.23
184CZ2	25N20	184CD1	44.82	184CZ2	25N20	19OE1	68.30
184CZ2	25N20	19CG	87.39	184CD1	25N20	19OE1	43.08
184CD1	25N20	19CG	47.27	19OE1	25N20	19CG	27.95
25SG	25C21	25CB	34.16	25SG	25C21	25N	59.13
25SG	25C21	162ND1	63.16	25SG	25C21	23O	95.53
25SG	25C21	25CA	41.14	25SG	25C21	161O	90.20
25SG	25C21	162CE1	64.32	25SG	25C21	24N	94.43
25SG	25C21	19OE1	78.34	25SG	25C21	162CA	58.84
25SG	25C21	19CD	91.01	25SG	25C21	26N	32.55
25SG	25C21	25C	28.93	25SG	25C21	24C	64.37
25SG	25C21	162CG	63.81	25SG	25C21	163N	30.18
25CB	25C21	25N	41.43	25CB	25C21	162ND1	57.90
25CB	25C21	23C	92.08	25CB	25C21	23O	94.39
25CB	25C21	25CA	20.31	25CB	25C21	19NE2	70.68
25CB	25C21	162CE1	48.50	25CB	25C21	24N	77.34
25CB	25C21	19OE1	44.80	25CB	25C21	162CA	77.90
25CB	25C21	19CD	56.86	25CB	25C21	26N	42.39
25CB	25C21	25C	26.69	25CB	25C21	24C	49.86
25CB	25C21	162CG	64.53	25CB	25C21	163N	55.35
25N	25C21	162ND1	98.16	25N	25C21	23CA	69.54
25N	25C21	23C	50.81	25N	25C21	23O	54.24
25N	25C21	25CA	21.67	25N	25C21	19NE2	62.10
25N	25C21	162CE1	85.44	25N	25C21	24N	37.13
25N	25C21	19OE1	55.93	25N	25C21	19CD	56.26
25N	25C21	26N	35.66	25N	25C21	25C	30.32
25N	25C21	24C	8.74	25N	25C21	163N	88.85
162ND1	25C21	25CA	78.14	162ND1	25C21	19NE2	84.09
162ND1	25C21	161O	65.36	162ND1	25C21	162CE1	16.67
162ND1	25C21	19OE1	59.98	162ND1	25C21	162CA	39.67

TABLE XIII

162ND1	25C21	19CD	72.99	162ND1	25C21	26N	92.87
162ND1	25C21	25C	80.82	162ND1	25C21	162CG	9.83
162ND1	25C21	163N	47.12	23CA	25C21	23C	22.59
23CA	25C21	23O	35.84	23CA	25C21	25CA	90.84
23CA	25C21	19NE2	61.29	23CA	25C21	224OH2	38.65
23CA	25C21	24N	32.44	23CA	25C21	19OE1	87.52
23CA	25C21	19CD	73.32	23CA	25C21	26N	93.91
23CA	25C21	25C	97.86	23CA	25C21	24C	62.65
23C	25C21	23O	18.06	23C	25C21	25CA	72.44
23C	25C21	19NE2	67.14	23C	25C21	224OH2	52.52
23C	25C21	24N	16.23	23C	25C21	19OE1	85.86
23C	25C21	19CD	74.76	23C	25C21	26N	71.38
23C	25C21	25C	76.60	23C	25C21	24C	42.81
23O	25C21	25CA	74.11	23O	25C21	19NE2	84.69
23O	25C21	224OH2	51.69	23O	25C21	24N	29.95
23O	25C21	19CD	90.88	23O	25C21	26N	63.28
23O	25C21	25C	72.90	23O	25C21	24C	45.50
25CA	25C21	19NE2	68.27	25CA	25C21	162CE1	67.59
25CA	25C21	24N	58.61	25CA	25C21	19OE1	50.41
25CA	25C21	162CA	95.22	25CA	25C21	19CD	57.40
25CA	25C21	26N	30.73	25CA	25C21	25C	16.57
25CA	25C21	24C	29.77	25CA	25C21	162CG	84.82
25CA	25C21	163N	69.11	19NE2	25C21	162CE1	68.48
19NE2	25C21	224OH2	93.44	19NE2	25C21	24N	55.94
19NE2	25C21	19OE1	29.51	19NE2	25C21	19CD	14.63
19NE2	25C21	26N	96.37	19NE2	25C21	25C	84.76
19NE2	25C21	24C	64.60	19NE2	25C21	162CG	93.25
161O	25C21	162CE1	81.61	161O	25C21	162CA	35.10
161O	25C21	162CG	55.78	161O	25C21	163N	60.78
162CE1	25C21	19OE1	43.32	162CE1	25C21	162CA	55.76
162CE1	25C21	19CD	56.63	162CE1	25C21	26N	88.80
162CE1	25C21	25C	74.35	162CE1	25C21	24C	94.10
162CE1	25C21	162CG	26.49	162CE1	25C21	163N	57.15
224OH2	25C21	24N	67.70	224OH2	25C21	24C	94.80
24N	25C21	19OE1	70.64	24N	25C21	19CD	60.95
24N	25C21	26N	64.52	24N	25C21	25C	65.81
24N	25C21	24C	30.33	19OE1	25C21	162CA	98.48

TABLE XIII

19OE1	25C21	19CD	15.08	19OE1	25C21	26N	81.12
19OE1	25C21	25C	66.02	19OE1	25C21	24C	62.63
19OE1	25C21	162CG	69.79	19OE1	25C21	163N	90.46
162CA	25C21	26N	89.91	162CA	25C21	25C	87.29
162CA	25C21	162CG	30.51	162CA	25C21	163N	28.80
19CD	25C21	26N	87.36	19CD	25C21	25C	73.91
19CD	25C21	24C	60.95	19CD	25C21	162CG	82.63
26N	25C21	25C	15.95	26N	25C21	24C	37.06
26N	25C21	162CG	95.38	26N	25C21	163N	61.27
25C	25C21	24C	35.55	25C	25C21	162CG	85.16
25C	25C21	163N	58.98	24C	25C21	163N	94.51
162CG	25C21	163N	42.83	25SG	25O22	25CB	38.49
25SG	25O22	25N	68.14	25SG	25O22	25CA	51.61
25SG	25O22	23O	92.70	25SG	25O22	19OE1	92.24
25SG	25O22	162ND1	54.00	25SG	25O22	24C	76.75
25SG	25O22	162CE1	62.63	25SG	25O22	24CA	92.42
25SG	25O22	25C	41.17	25SG	25O22	26N	39.32
19NE2	25O22	25CB	90.81	19NE2	25O22	23CA	83.72
19NE2	25O22	25N	82.91	19NE2	25O22	23C	90.92
19NE2	25O22	25CA	85.84	19NE2	25O22	24N	75.03
19NE2	25O22	19CD	18.29	19NE2	25O22	19OE1	36.86
19NE2	25O22	22O	40.88	19NE2	25O22	162ND1	93.79
19NE2	25O22	24C	82.04	19NE2	25O22	23N	71.12
19NE2	25O22	162CE1	77.66	19NE2	25O22	24CA	80.86
19NE2	25O22	22C	54.65	19NE2	25O22	25C	99.55
25CB	25O22	25N	47.57	25CB	25O22	25CA	24.14
25CB	25O22	24N	93.92	25CB	25O22	19CD	72.69
25CB	25O22	19OE1	55.94	25CB	25O22	162ND1	53.00
25CB	25O22	24C	58.84	25CB	25O22	162CE1	47.93
25CB	25O22	24CA	78.52	25CB	25O22	25C	26.37
25CB	25O22	26N	39.92	23CA	25O22	25N	86.84
23CA	25O22	23C	27.45	23CA	25O22	24N	40.92
23CA	25O22	23O	40.51	23CA	25O22	19CD	98.21
23CA	25O22	22O	43.20	23CA	25O22	24C	75.56
23CA	25O22	23N	12.75	23CA	25O22	224OH2	38.92
23CA	25O22	24CA	55.88	23CA	25O22	22C	29.08
25N	25O22	23C	61.42	25N	25O22	25CA	23.44

TABLE XIII

25N	25O22	24N	46.54	25N	25O22	23O	61.31
25N	25O22	19CD	72.72	25N	25O22	19OE1	69.34
25N	25O22	22O	78.77	25N	25O22	24C	11.28
25N	25O22	23N	87.24	25N	25O22	162CE1	91.85
25N	25O22	24CA	30.96	25N	25O22	22C	83.18
25N	25O22	25C	27.52	25N	25O22	26N	31.88
23C	25O22	25CA	84.51	23C	25O22	24N	21.22
23C	25O22	23O	19.47	23C	25O22	19CD	98.72
23C	25O22	22O	52.92	23C	25O22	24C	50.34
23C	25O22	23N	34.26	23C	25O22	224OH2	55.48
23C	25O22	24CA	31.37	23C	25O22	22C	43.43
23C	25O22	25C	83.00	23C	25O22	26N	74.42
25CA	25O22	24N	69.81	25CA	25O22	23O	81.49
25CA	25O22	19CD	70.36	25CA	25O22	19OE1	59.53
25CA	25O22	22O	96.17	25CA	25O22	162ND1	76.96
25CA	25O22	24C	34.73	25CA	25O22	162CE1	69.68
25CA	25O22	24CA	54.41	25CA	25O22	25C	13.77
25CA	25O22	26N	28.59	24N	25O22	23O	35.89
24N	25O22	19CD	79.36	24N	25O22	19OE1	90.36
24N	25O22	22O	44.09	24N	25O22	24C	35.42
24N	25O22	23N	40.92	24N	25O22	224OH2	75.53
24N	25O22	24CA	16.33	24N	25O22	22C	41.01
24N	25O22	25C	72.48	24N	25O22	26N	69.02
23O	25O22	22O	72.38	23O	25O22	24C	51.99
23O	25O22	23N	50.70	23O	25O22	224OH2	53.17
23O	25O22	24CA	37.85	23O	25O22	22C	62.29
23O	25O22	25C	75.63	23O	25O22	26N	63.41
19CD	25O22	19OE1	19.08	19CD	25O22	22O	55.19
19CD	25O22	162ND1	80.93	19CD	25O22	24C	75.07
19CD	25O22	23N	86.19	19CD	25O22	162CE1	63.77
19CD	25O22	24CA	80.05	19CD	25O22	22C	69.54
19CD	25O22	25C	84.09	19CD	25O22	26N	98.42
19OE1	25O22	22O	73.71	19OE1	25O22	162ND1	64.15
19OE1	25O22	24C	75.30	19OE1	25O22	162CE1	46.77
19OE1	25O22	24CA	86.24	19OE1	25O22	22C	88.09
19OE1	25O22	25C	72.43	19OE1	25O22	26N	87.99
22O	25O22	24C	70.73	22O	25O22	23N	31.00

TABLE XIII

22O	25O22	224OH2	78.01	22O	25O22	24CA	57.51
22O	25O22	22C	14.38	162ND1	25O22	162CE1	17.38
162ND1	25O22	25C	77.53	162ND1	25O22	26N	86.27
24C	25O22	23N	76.28	24C	25O22	24CA	19.68
24C	25O22	22C	73.43	24C	25O22	25C	37.56
24C	25O22	26N	38.26	23N	25O22	224OH2	48.26
23N	25O22	24CA	57.15	23N	25O22	22C	16.66
162CE1	25O22	25C	74.28	162CE1	25O22	26N	86.57
224OH2	25O22	24CA	86.57	224OH2	25O22	22C	63.94
24CA	25O22	22C	56.72	24CA	25O22	25C	56.18
24CA	25O22	26N	53.14	25C	25O22	26N	15.75
61OD1	25C23	59O	92.71	61OD1	25C23	264OH2	51.41
61OD1	25C23	61CG	13.18	61OD1	25C23	61OD2	26.94
61OD1	25C23	59C	87.40	59O	25C23	67CD2	91.32
59O	25C23	264OH2	79.96	59O	25C23	61CG	79.93
59O	25C23	61OD2	71.08	59O	25C23	59C	5.39
67CE2	25C23	67CD2	18.11	67CD2	25C23	59C	92.59
264OH2	25C23	61CG	46.02	264OH2	25C23	61OD2	33.75
264OH2	25C23	59C	77.27	61CG	25C23	61OD2	15.44
61CG	25C23	59C	74.68	61OD2	25C23	59C	66.25
59O	25C24	60ND2	58.48	59O	25C24	60CA	44.55
59O	25C24	59C	9.80	59O	25C24	61CG	88.32
59O	25C24	60C	54.30	59O	25C24	61N	71.19
59O	25C24	60N	26.62	59O	25C24	70OD1	52.26
59O	25C24	61OD2	75.43	59O	25C24	60CG	60.01
59O	25C24	60CB	55.47	59O	25C24	67N	96.69
61OD1	25C24	60CA	80.24	61OD1	25C24	59C	97.84
61OD1	25C24	61CG	15.04	61OD1	25C24	66CA	87.60
61OD1	25C24	60C	61.23	61OD1	25C24	61N	50.12
61OD1	25C24	60N	89.60	61OD1	25C24	61OD2	27.04
61OD1	25C24	60CB	87.33	61OD1	25C24	65O	55.48
67CD2	25C24	60ND2	70.35	67CD2	25C24	67CE2	21.12
67CD2	25C24	66CA	60.05	67CD2	25C24	70OD1	65.25
67CD2	25C24	60CG	77.71	67CD2	25C24	60CB	94.80
67CD2	25C24	67N	38.69	67CD2	25C24	66C	42.86
67CD2	25C24	65O	91.74	67CD2	25C24	67CG	7.62
60ND2	25C24	67CE2	91.22	60ND2	25C24	60CA	41.72

TABLE XIII

60ND2	25C24	59C	52.47	60ND2	25C24	66CA	51.12
60ND2	25C24	60C	59.58	60ND2	25C24	61N	66.53
60ND2	25C24	60N	44.60	60ND2	25C24	70OD1	41.24
60ND2	25C24	60CG	12.36	60ND2	25C24	60CB	29.62
60ND2	25C24	67N	38.69	60ND2	25C24	66C	49.79
60ND2	25C24	65O	68.79	60ND2	25C24	67CG	64.10
67CE2	25C24	66CA	70.56	67CE2	25C24	70OD1	82.90
67CE2	25C24	60CG	97.67	67CE2	25C24	67N	56.69
67CE2	25C24	66C	55.71	67CE2	25C24	65O	96.69
67CE2	25C24	67CG	28.20	60CA	25C24	59C	34.75
60CA	25C24	61CG	65.91	60CA	25C24	66CA	65.63
60CA	25C24	60C	19.12	60CA	25C24	61N	32.35
60CA	25C24	60N	17.94	60CA	25C24	70OD1	70.97
60CA	25C24	61OD2	62.09	60CA	25C24	60CG	32.72
60CA	25C24	60CB	16.35	60CA	25C24	67N	73.13
60CA	25C24	66C	76.33	60CA	25C24	65O	56.57
59C	25C24	61CG	83.18	59C	25C24	66CA	96.04
59C	25C24	60C	45.42	59C	25C24	61N	62.28
59C	25C24	60N	16.82	59C	25C24	70OD1	54.54
59C	25C24	61OD2	71.72	59C	25C24	60CG	52.21
59C	25C24	60CB	46.02	59C	25C24	67N	91.16
59C	25C24	65O	91.18	61CG	25C24	66CA	85.83
61CG	25C24	60C	46.79	61CG	25C24	61N	37.73
61CG	25C24	60N	74.56	61CG	25C24	61OD2	15.30
61CG	25C24	60CG	92.19	61CG	25C24	60CB	74.64
61CG	25C24	65O	52.44	66CA	25C24	60C	69.53
66CA	25C24	61N	60.35	66CA	25C24	60N	81.05
66CA	25C24	70OD1	85.92	66CA	25C24	61OD2	97.05
66CA	25C24	60CG	45.49	66CA	25C24	60CB	50.81
66CA	25C24	67N	29.45	66CA	25C24	66C	17.50
66CA	25C24	65O	33.39	66CA	25C24	67CG	60.31
60C	25C24	61N	16.90	60C	25C24	60N	31.03
60C	25C24	70OD1	89.71	60C	25C24	61OD2	43.83
60C	25C24	60CG	49.02	60C	25C24	60CB	30.73
60C	25C24	67N	85.40	60C	25C24	66C	84.14
60C	25C24	65O	49.16	61N	25C24	60N	47.32
61N	25C24	61OD2	41.00	61N	25C24	60CG	54.47

TABLE XIII

61N	25C24	60CB	37.23	61N	25C24	67N	82.57
61N	25C24	66C	77.02	61N	25C24	65O	34.06
60N	25C24	70OD1	61.08	60N	25C24	61OD2	66.32
60N	25C24	60CG	40.42	60N	25C24	60CB	30.28
60N	25C24	67N	81.86	60N	25C24	66C	88.80
60N	25C24	65O	74.46	70OD1	25C24	60CG	53.02
70OD1	25C24	60CB	66.53	70OD1	25C24	67N	60.32
70OD1	25C24	66C	75.88	70OD1	25C24	67CG	57.76
61OD2	25C24	60CG	92.66	61OD2	25C24	60CB	74.33
61OD2	25C24	65O	64.27	60CG	25C24	60CB	18.33
60CG	25C24	67N	41.67	60CG	25C24	66C	48.95
60CG	25C24	65O	57.71	60CG	25C24	67CG	72.33
60CB	25C24	67N	56.95	60CB	25C24	66C	60.17
60CB	25C24	65O	49.72	60CB	25C24	67CG	90.00
67N	25C24	66C	15.58	67N	25C24	65O	62.20
67N	25C24	67CG	35.72	66C	25C24	65O	50.68
66C	25C24	67CG	42.81	65O	25C24	67CG	93.15
66CA	25C25	67CD2	74.47	66CA	25C25	67CE2	88.53
66CA	25C25	60ND2	59.31	66CA	25C25	66N	21.62
66CA	25C25	65O	44.29	66CA	25C25	66C	21.53
66CA	25C25	65C	36.30	66CA	25C25	60CA	74.60
66CA	25C25	61N	73.02	66CA	25C25	67N	33.98
66CA	25C25	60C	79.39	66CA	25C25	60CG	50.06
66CA	25C25	66O	28.68	66CA	25C25	60CB	56.47
66CA	25C25	61CB	88.35	66CA	25C25	67CG	69.03
66CA	25C25	67CZ	89.74	61OD1	25C25	66N	99.44
61OD1	25C25	65O	70.37	61OD1	25C25	65C	80.66
61OD1	25C25	60CA	81.54	61OD1	25C25	61CG	15.19
61OD1	25C25	61N	55.29	61OD1	25C25	59O	88.76
61OD1	25C25	60C	62.96	61OD1	25C25	60CB	93.30
61OD1	25C25	61CB	28.06	61OD1	25C25	61OD2	23.60
67CD2	25C25	67CE2	22.80	67CD2	25C25	60ND2	71.72
67CD2	25C25	66N	86.08	67CD2	25C25	66C	52.97
67CD2	25C25	59O	98.99	67CD2	25C25	67N	45.03
67CD2	25C25	60CG	81.76	67CD2	25C25	66O	50.77
67CD2	25C25	67CG	6.70	67CD2	25C25	67CZ	27.35
67CE2	25C25	60ND2	94.29	67CE2	25C25	66N	93.17

TABLE XIII

67CE2	25C25	66C	67.80	67CE2	25C25	67N	64.98
67CE2	25C25	66O	60.61	67CE2	25C25	67CG	29.23
67CE2	25C25	67CZ	4.94	60ND2	25C25	66N	80.00
60ND2	25C25	65O	81.55	60ND2	25C25	66C	58.26
60ND2	25C25	65C	87.34	60ND2	25C25	60CA	40.17
60ND2	25C25	61N	69.84	60ND2	25C25	59O	49.72
60ND2	25C25	67N	43.92	60ND2	25C25	60C	58.97
60ND2	25C25	60CG	15.02	60ND2	25C25	66O	71.48
60ND2	25C25	60CB	31.11	60ND2	25C25	67CG	65.78
60ND2	25C25	61OD2	99.69	60ND2	25C25	67CZ	99.01
66N	25C25	65O	33.95	66N	25C25	66C	36.67
66N	25C25	65C	19.02	66N	25C25	60CA	86.34
66N	25C25	61CG	95.07	66N	25C25	61N	72.60
66N	25C25	67N	53.18	66N	25C25	60C	84.37
66N	25C25	60CG	68.93	66N	25C25	66O	35.32
66N	25C25	60CB	70.27	66N	25C25	61CB	77.27
66N	25C25	67CG	82.14	66N	25C25	67CZ	92.55
65O	25C25	66C	65.47	65O	25C25	65C	17.60
65O	25C25	60CA	65.59	65O	25C25	61CG	62.59
65O	25C25	61N	40.94	65O	25C25	67N	77.29
65O	25C25	60C	55.85	65O	25C25	60CG	66.65
65O	25C25	66O	68.27	65O	25C25	60CB	56.61
65O	25C25	61CB	44.60	65O	25C25	61OD2	71.81
66C	25C25	65C	54.91	66C	25C25	60CA	86.39
66C	25C25	61N	92.94	66C	25C25	67N	17.99
66C	25C25	60C	96.20	66C	25C25	60CG	55.13
66C	25C25	66O	13.59	66C	25C25	60CB	68.10
66C	25C25	67CG	47.70	66C	25C25	67CZ	69.56
65C	25C25	60CA	80.60	65C	25C25	61CG	76.13
65C	25C25	61N	58.52	65C	25C25	67N	70.10
65C	25C25	60C	73.03	65C	25C25	60CG	73.62
65C	25C25	66O	54.32	65C	25C25	60CB	68.42
65C	25C25	61CB	58.45	65C	25C25	61OD2	86.99
60CA	25C25	61CG	66.63	60CA	25C25	61N	34.12
60CA	25C25	59O	39.03	60CA	25C25	67N	78.67
60CA	25C25	60C	19.48	60CA	25C25	60CG	33.49
60CA	25C25	66O	99.43	60CA	25C25	60CB	18.48

TABLE XIII

60CA	25C25	61CB	63.35	60CA	25C25	61OD2	59.93
61CG	25C25	61N	40.61	61CG	25C25	59O	78.90
61CG	25C25	60C	47.83	61CG	25C25	60CG	96.99
61CG	25C25	60CB	78.15	61CG	25C25	61CB	17.99
61CG	25C25	61OD2	13.48	61N	25C25	59O	66.77
61N	25C25	67N	95.02	61N	25C25	60C	16.92
61N	25C25	60CG	57.64	61N	25C25	60CB	39.04
61N	25C25	61CB	30.85	61N	25C25	61OD2	41.41
59O	25C25	67N	92.29	59O	25C25	60C	49.98
59O	25C25	60CG	56.13	59O	25C25	60CB	52.99
59O	25C25	61CB	86.68	59O	25C25	67CG	96.56
59O	25C25	61OD2	66.16	67N	25C25	60C	93.00
67N	25C25	60CG	45.25	67N	25C25	66O	28.92
67N	25C25	60CB	62.00	67N	25C25	67CG	38.59
67N	25C25	67CZ	68.17	60C	25C25	60CG	49.75
60C	25C25	60CB	31.34	60C	25C25	61CB	44.00
60C	25C25	61OD2	43.11	60CG	25C25	66O	68.70
60CG	25C25	60CB	18.86	60CG	25C25	61CB	88.11
60CG	25C25	67CG	75.30	60CG	25C25	61OD2	92.65
66O	25C25	60CB	81.00	66O	25C25	67CG	47.02
66O	25C25	67CZ	61.34	60CB	25C25	61CB	69.79
60CB	25C25	67CG	94.15	60CB	25C25	61OD2	74.45
61CB	25C25	61OD2	28.84	67CG	25C25	67CZ	33.62
61OD1	25C26	65O	71.36	61OD1	25C26	65C	85.76
61OD1	25C26	61CG	11.35	61OD1	25C26	61CB	26.51
61OD1	25C26	61N	48.33	61OD1	25C26	65CA	84.59
61OD1	25C26	61OD2	15.64	67CE2	25C26	66CA	78.50
67CE2	25C26	66N	89.75	67CE2	25C26	67CD2	19.87
67CE2	25C26	66C	60.32	67CE2	25C26	67CZ	10.65
67CE2	25C26	66O	56.85	66CA	25C26	66N	21.30
66CA	25C26	65O	40.66	66CA	25C26	65C	35.52
66CA	25C26	67CD2	62.19	66CA	25C26	61CG	97.24
66CA	25C26	66C	18.45	66CA	25C26	61CB	83.20
66CA	25C26	61N	61.53	66CA	25C26	67CZ	84.37
66CA	25C26	65CA	50.10	66CA	25C26	66O	28.03
66N	25C26	65O	32.82	66N	25C26	65C	19.16
66N	25C26	67CD2	77.48	66N	25C26	61CG	94.77

TABLE XIII

66N	25C26	66C	32.67	66N	25C26	61CB	77.42
66N	25C26	61N	65.23	66N	25C26	67CZ	92.40
66N	25C26	65CA	29.97	66N	25C26	66O	32.92
65O	25C26	65C	17.65	65O	25C26	61CG	61.95
65O	25C26	66C	58.76	65O	25C26	61CB	44.89
65O	25C26	61N	36.15	65O	25C26	65CA	29.75
65O	25C26	61OD2	69.17	65O	25C26	66O	64.19
65C	25C26	67CD2	96.05	65C	25C26	61CG	77.55
65C	25C26	66C	50.78	65C	25C26	61CB	59.53
65C	25C26	61N	53.71	65C	25C26	65CA	16.87
65C	25C26	61OD2	85.83	65C	25C26	66O	52.07
67CD2	25C26	66C	45.30	67CD2	25C26	67CZ	29.89
67CD2	25C26	66O	46.56	61CG	25C26	61CB	18.38
61CG	25C26	61N	36.98	61CG	25C26	65CA	79.04
61CG	25C26	61OD2	11.28	66C	25C26	61N	78.34
66C	25C26	67CZ	65.93	66C	25C26	65CA	62.43
66C	25C26	66O	14.16	61CB	25C26	61N	29.95
61CB	25C26	65CA	60.78	61CB	25C26	61OD2	28.51
61N	25C26	65CA	64.34	61N	25C26	61OD2	38.83
61N	25C26	66O	89.56	67CZ	25C26	66O	59.87
65CA	25C26	61OD2	89.18	65CA	25C26	66O	59.63
61OD1	25C27	61CG	5.16	61OD1	25C27	61OD2	15.09
67CE2	25C27	67CD2	15.74	67CE2	25C27	67OH	28.29
61CG	25C27	61OD2	12.69	67CD2	25C27	67OH	44.01
61OD1	25C28	61CG	9.27	61OD1	25C28	264OH2	52.17
61OD1	25C28	61OD2	23.20	67CE2	25C28	67CD2	15.49
61CG	25C28	264OH2	46.24	61CG	25C28	61OD2	14.74
264OH2	25C28	61OD2	33.06	66N	25C29	65C	24.86
66N	25C29	65O	39.60	66N	25C29	66CA	24.12
66N	25C29	65CA	41.74	66N	25C29	67CE2	94.22
66N	25C29	64O	81.94	66N	25C29	66C	34.73
66N	25C29	66O	37.60	66N	25C29	65N	53.80
66N	25C29	67CD2	79.01	66N	25C29	61CG	98.70
66N	25C29	64C	70.01	66N	25C29	61CB	84.65
65C	25C29	65O	20.60	65C	25C29	66CA	42.11
65C	25C29	65CA	24.93	65C	25C29	61OD1	91.42
65C	25C29	64O	61.11	65C	25C29	66C	58.05

TABLE XIII

65C	25C29	66O	62.45	65C	25C29	65N	31.53
65C	25C29	61CG	79.83	65C	25C29	64C	47.67
65C	25C29	61CB	63.17	65O	25C29	66CA	46.14
65O	25C29	65CA	39.66	65O	25C29	61OD1	71.78
65O	25C29	64O	64.40	65O	25C29	66C	65.45
65O	25C29	66O	74.94	65O	25C29	65N	37.56
65O	25C29	61CG	60.19	65O	25C29	64C	50.20
65O	25C29	61CB	45.06	66CA	25C29	65CA	64.24
66CA	25C29	67CE2	75.91	66CA	25C29	66C	19.63
66CA	25C29	66O	32.86	66CA	25C29	65N	73.62
66CA	25C29	67CD2	59.00	66CA	25C29	61CG	93.56
66CA	25C29	64C	89.77	66CA	25C29	61CB	85.67
65CA	25C29	61OD1	97.52	65CA	25C29	64O	40.31
65CA	25C29	66C	76.17	65CA	25C29	66O	74.54
65CA	25C29	65N	15.70	65CA	25C29	61CG	87.20
65CA	25C29	64C	29.78	65CA	25C29	61CB	68.64
61OD1	25C29	64O	78.88	61OD1	25C29	65N	83.10
61OD1	25C29	61CG	11.60	61OD1	25C29	64C	76.76
61OD1	25C29	61CB	29.29	67CE2	25C29	66C	59.68
67CE2	25C29	66O	59.54	67CE2	25C29	67CD2	17.43
64O	25C29	65N	29.62	64O	25C29	61CG	73.88
64O	25C29	64C	14.26	64O	25C29	61CB	59.65
66C	25C29	66O	16.37	66C	25C29	65N	88.46
66C	25C29	67CD2	44.33	66O	25C29	65N	89.10
66O	25C29	67CD2	48.06	65N	25C29	61CG	73.50
65N	25C29	64C	16.31	65N	25C29	61CB	55.08
61CG	25C29	64C	69.32	61CG	25C29	61CB	18.57
64C	25C29	61CB	52.55	66N	25O30	67CE2	95.44
66N	25O30	65C	20.14	66N	25O30	66O	41.64
66N	25O30	66CA	20.76	66N	25O30	65CA	36.46
66N	25O30	66C	35.12	66N	25O30	67CD2	78.01
66N	25O30	65O	28.77	66N	25O30	64O	70.26
67CE2	25O30	66O	66.02	67CE2	25O30	66CA	75.33
67CE2	25O30	66C	62.32	67CE2	25O30	67CD2	17.44
67CE2	25O30	67CZ	17.35	67CE2	25O30	67OH	32.31
65C	25O30	66O	61.78	65C	25O30	66CA	35.78
65C	25O30	65CA	21.92	65C	25O30	66C	54.08

TABLE XIII

65C	25O30	67CD2	93.11	65C	25O30	65O	13.87
65C	25O30	64O	51.57	66O	25O30	66CA	34.58
66O	25O30	65CA	74.20	66O	25O30	66C	16.71
66O	25O30	67CD2	51.17	66O	25O30	67CZ	70.40
66O	25O30	67OH	86.34	66O	25O30	65O	68.48
66CA	25O30	65CA	55.92	66CA	25O30	66C	20.67
66CA	25O30	67CD2	58.02	66CA	25O30	67CZ	88.15
66CA	25O30	65O	36.77	66CA	25O30	64O	87.19
65CA	25O30	66C	71.35	65CA	25O30	65O	31.68
65CA	25O30	64O	35.13	66C	25O30	67CD2	45.28
66C	25O30	67CZ	71.68	66C	25O30	67OH	89.19
66C	25O30	65O	57.23	67CD2	25O30	67CZ	31.46
67CD2	25O30	67OH	48.52	67CD2	25O30	65O	89.19
67CZ	25O30	67OH	17.73	65O	25O30	64O	52.71
66N	25C31	65CA	39.43	66N	25C31	65C	19.88
66N	25C31	66O	41.44	66N	25C31	66CA	16.42
66N	25C31	64O	73.76	66N	25C31	66C	31.86
66N	25C31	65O	24.99	66N	25C31	67CE2	78.02
66N	25C31	65N	48.58	65CA	25C31	65C	22.92
65CA	25C31	66O	78.51	65CA	25C31	66CA	54.89
65CA	25C31	64O	37.80	65CA	25C31	66C	71.14
65CA	25C31	65O	28.31	65CA	25C31	65N	10.41
65C	25C31	66O	61.32	65C	25C31	66CA	33.07
65C	25C31	64O	54.01	65C	25C31	66C	51.04
65C	25C31	65O	9.78	65C	25C31	67CE2	90.50
65C	25C31	65N	30.23	66O	25C31	66CA	32.38
66O	25C31	66C	14.52	66O	25C31	65O	65.09
66O	25C31	67CE2	56.24	66O	25C31	65N	88.60
66CA	25C31	64O	86.14	66CA	25C31	66C	19.15
66CA	25C31	65O	33.97	66CA	25C31	67CE2	61.64
66CA	25C31	65N	63.22	64O	25C31	65O	52.33
64O	25C31	65N	27.39	66C	25C31	65O	53.03
66C	25C31	67CE2	52.59	66C	25C31	65N	80.44
65O	25C31	67CE2	85.62	65O	25C31	65N	32.85
65CA	25O32	64O	42.64	65CA	25O32	66N	34.36
65CA	25O32	65C	19.66	65CA	25O32	64C	30.83
65CA	25O32	65N	14.60	64O	25O32	66N	73.09

TABLE XIII

64O	25O32	65C	55.36	64O	25O32	64C	12.34
64O	25O32	65N	28.48	66N	25O32	65C	17.74
66N	25O32	64C	63.03	66N	25O32	65N	48.15
65C	25O32	64C	45.59	65C	25O32	65N	31.63
64C	25O32	65N	16.37	66O	25C33	66N	39.03
66O	25C33	65CA	71.47	66O	25C33	25SG	98.45
66O	25C33	65C	53.71	66O	25C33	66C	9.09
66N	25C33	65CA	32.53	66N	25C33	25SG	95.78
66N	25C33	65C	14.69	66N	25C33	66C	30.21
161O	25C33	161C	15.33	161O	25C33	25SG	60.66
65CA	25C33	25SG	88.64	65CA	25C33	65C	18.08
65CA	25C33	66C	62.73	161C	25C33	25SG	68.01
25SG	25C33	65C	94.64	65C	25C33	66C	44.83
66O	25C34	163CB	85.75	66O	25C34	66N	32.40
161C	25C34	161O	16.73	161C	25C34	162N	17.83
161C	25C34	163N	62.24	161C	25C34	162CA	31.39
161C	25C34	162C	47.88	161C	25C34	25SG	73.05
161C	25C34	161CA	18.94	161C	25C34	163CB	92.63
161O	25C34	162N	30.34	161O	25C34	163N	65.51
161O	25C34	162CA	35.76	161O	25C34	162C	54.67
161O	25C34	25SG	62.53	161O	25C34	161CA	30.82
161O	25C34	163CB	95.27	162N	25C34	163N	46.66
162N	25C34	162CA	18.35	162N	25C34	162C	31.03
162N	25C34	25SG	69.25	162N	25C34	161CA	31.09
162N	25C34	163CB	76.34	163N	25C34	162CA	31.03
163N	25C34	162C	16.65	163N	25C34	25SG	45.82
163N	25C34	161CA	77.75	163N	25C34	163CB	30.49
162CA	25C34	162C	19.01	162CA	25C34	25SG	52.46
162CA	25C34	161CA	48.32	162CA	25C34	163CB	61.52
162C	25C34	25SG	55.74	162C	25C34	161CA	61.81
162C	25C34	163CB	45.32	25SG	25C34	161CA	91.65
25SG	25C34	163CB	53.96	25SG	25C34	66N	87.39
66O	25C35	66C	2.57	66O	25C35	163CB	96.66
66O	25C35	26CB	46.90	66O	25C35	66N	29.09
66O	25C35	67CA	31.24	66O	25C35	68SD	77.53
66O	25C35	67CD1	62.23	66O	25C35	67CE1	72.23
66C	25C35	163CB	98.61	66C	25C35	26CB	49.23

TABLE XIII

66C	25C35	66N	30.32	66C	25C35	67CA	29.98
66C	25C35	68SD	78.11	66C	25C35	67CD1	59.82
66C	25C35	67CE1	69.68	163CB	25C35	26CB	51.66
163CB	25C35	67CA	90.92	163CB	25C35	209CD2	95.04
163CB	25C35	68SD	41.03	26CB	25C35	66N	52.74
26CB	25C35	67CA	56.99	26CB	25C35	68SD	53.93
26CB	25C35	67CD1	97.81	66N	25C35	67CA	60.27
66N	25C35	67CD1	84.58	66N	25C35	67CE1	89.12
67CA	25C35	209CD2	76.21	67CA	25C35	68SD	56.79
67CA	25C35	67CD1	40.85	67CA	25C35	67CE1	55.83
209CD2	25C35	68SD	66.55	209CD2	25C35	67CD1	48.98
209CD2	25C35	67CE1	49.09	68SD	25C35	67CD1	78.05
68SD	25C35	67CE1	92.43	67CD1	25C35	67CE1	16.13
66O	25C36	68SD	96.83	66O	25C36	26CB	52.43
66O	25C36	66C	6.57	66O	25C36	67CA	36.71
66O	25C36	26CX	70.05	68SD	25C36	163CB	57.33
68SD	25C36	163CA	70.03	68SD	25C36	134CB	84.74
68SD	25C36	163N	89.11	68SD	25C36	26CB	67.27
68SD	25C36	68CE	22.41	68SD	25C36	209CD2	84.13
68SD	25C36	66C	90.48	68SD	25C36	67CA	67.81
68SD	25C36	162C	99.30	68SD	25C36	26CX	59.77
163CB	25C36	163CA	20.06	163CB	25C36	134CB	81.47
163CB	25C36	163N	34.18	163CB	25C36	26CB	62.38
163CB	25C36	68CE	60.98	163CB	25C36	162C	48.31
163CB	25C36	26CX	44.78	163CA	25C36	134CB	65.51
163CA	25C36	163N	19.48	163CA	25C36	26CB	80.86
163CA	25C36	68CE	65.92	163CA	25C36	162C	30.24
163CA	25C36	26CX	63.59	134CB	25C36	163N	69.86
134CB	25C36	68CE	62.66	134CB	25C36	209CD2	53.95
134CB	25C36	162C	59.74	163N	25C36	26CB	84.29
163N	25C36	68CE	85.05	163N	25C36	162C	15.50
163N	25C36	26CX	69.23	26CB	25C36	68CE	88.83
26CB	25C36	66C	50.37	26CB	25C36	67CA	61.54
26CB	25C36	162C	98.98	26CB	25C36	26CX	17.62
68CE	25C36	209CD2	68.72	68CE	25C36	67CA	82.83
68CE	25C36	162C	90.28	68CE	25C36	26CX	78.81
209CD2	25C36	67CA	82.71	66C	25C36	67CA	30.72

TABLE XIII

66C	25C36	26CX	67.86	67CA	25C36	26CX	75.01
162C	25C36	26CX	84.54	66O	25C37	67CE1	76.69
66O	25C37	67CZ	72.75	66O	25C37	67CD1	64.04
66O	25C37	67OH	86.40	66O	25C37	67CE2	57.39
66O	25C37	67CG	48.64	67CE1	25C37	209CD2	60.17
67CE1	25C37	67CZ	18.76	67CE1	25C37	67CD1	18.19
67CE1	25C37	67OH	31.37	67CE1	25C37	67CE2	29.99
67CE1	25C37	67CG	29.19	209CD2	25C37	67CZ	78.42
209CD2	25C37	67CD1	57.12	209CD2	25C37	67OH	84.22
209CD2	25C37	67CE2	89.26	209CD2	25C37	134CB	51.72
209CD2	25C37	67CG	70.82	67CZ	25C37	67CD1	31.75
67CZ	25C37	67OH	17.50	67CZ	25C37	67CE2	16.32
67CZ	25C37	67CG	34.21	67CD1	25C37	67OH	47.81
67CD1	25C37	67CE2	34.53	67CD1	25C37	67CG	15.87
67OH	25C37	160O	98.96	67OH	25C37	67CE2	29.39
67OH	25C37	67CG	51.71	160O	25C37	134CB	78.01
67CE2	25C37	67CG	28.65	65CA	25C38	66N	37.26
65CA	25C38	66O	76.23	65CA	25C38	26CD1	57.25
65CA	25C38	65C	19.78	65CA	25C38	23O	54.21
65CA	25C38	224OH2	55.95	65CA	25C38	26CB	85.45
65CA	25C38	65N	11.58	65CA	25C38	26CG	68.24
25SG	25C38	26CD1	77.09	25SG	25C38	23O	67.47
25SG	25C38	161O	68.31	25SG	25C38	224OH2	89.14
25SG	25C38	26CB	70.06	25SG	25C38	26CG	76.35
66N	25C38	66O	39.10	66N	25C38	26CD1	47.09
66N	25C38	65C	17.53	66N	25C38	23O	72.97
66N	25C38	224OH2	92.76	66N	25C38	26CB	59.41
66N	25C38	65N	48.17	66N	25C38	26CG	48.12
66O	25C38	26CD1	61.41	66O	25C38	65C	56.61
66O	25C38	26CB	46.70	66O	25C38	65N	87.28
66O	25C38	26CG	50.49	26CD1	25C38	65C	48.65
26CD1	25C38	23O	40.99	26CD1	25C38	224OH2	85.80
26CD1	25C38	26CB	32.92	26CD1	25C38	65N	59.48
26CD1	25C38	26CG	15.33	65C	25C38	23O	62.21
65C	25C38	224OH2	75.31	65C	25C38	26CB	70.46
65C	25C38	65N	30.67	65C	25C38	26CG	55.38
23O	25C38	224OH2	47.84	23O	25C38	26CB	69.70

TABLE XIII

23O	25C38	65N	46.94	23O	25C38	26CG	55.26
161O	25C38	224OH2	93.60	224OH2	25C38	65N	44.65
26CB	25C38	65N	90.52	26CB	25C38	26CG	18.20
65N	25C38	26CG	72.50	66N	25O39	26CD1	65.73
66N	25O39	65CA	47.24	66N	25O39	65C	22.10
66N	25O39	66O	47.99	66N	25O39	23O	95.16
66N	25O39	26CG	65.86	66N	25O39	26CB	78.81
66N	25O39	26NE1	58.35	66N	25O39	66CA	14.64
66N	25O39	66C	34.63	66N	25O39	65N	57.39
66N	25O39	65O	22.72	66N	25O39	26CX	95.35
66N	25O39	26CD2	57.58	26CD1	25O39	65CA	77.50
26CD1	25O39	65C	65.28	26CD1	25O39	66O	80.81
26CD1	25O39	23O	52.52	26CD1	25O39	26CG	20.44
26CD1	25O39	26CB	42.80	26CD1	25O39	25SG	91.26
26CD1	25O39	26NE1	14.54	26CD1	25O39	66CA	62.36
26CD1	25O39	66C	69.41	26CD1	25O39	65N	74.38
26CD1	25O39	26N	49.70	26CD1	25O39	65O	61.20
26CD1	25O39	23C	59.40	26CD1	25O39	26CX	47.75
26CD1	25O39	224OH2	98.62	26CD1	25O39	26CD2	17.11
65CA	25O39	65C	25.89	65CA	25O39	66O	94.13
65CA	25O39	23O	66.29	65CA	25O39	26CG	92.00
65CA	25O39	26NE1	63.11	65CA	25O39	66CA	61.64
65CA	25O39	66C	81.81	65CA	25O39	65N	12.36
65CA	25O39	65O	27.30	65CA	25O39	23C	72.79
65CA	25O39	224OH2	56.03	65CA	25O39	26CD2	82.72
65C	25O39	66O	70.06	65C	25O39	23O	78.02
65C	25O39	26CG	73.56	65C	25O39	26CB	92.36
65C	25O39	26NE1	53.27	65C	25O39	66CA	36.02
65C	25O39	66C	56.60	65C	25O39	65N	35.32
65C	25O39	65O	4.12	65C	25O39	23C	86.65
65C	25O39	224OH2	81.45	65C	25O39	26CD2	64.11
66O	25O39	26CG	65.04	66O	25O39	26CB	58.06
66O	25O39	26NE1	84.63	66O	25O39	66CA	35.35
66O	25O39	66C	15.25	66O	25O39	26N	91.09
66O	25O39	65O	70.58	66O	25O39	26CX	73.00
66O	25O39	26CD2	63.97	23O	25O39	26CG	71.55
23O	25O39	26CB	88.75	23O	25O39	25SG	73.57

TABLE XIII

23O	25O39	26NE1	46.88	23O	25O39	65N	54.73
23O	25O39	26N	69.90	23O	25O39	65O	75.20
23O	25O39	23C	9.35	23O	25O39	26CX	82.73
23O	25O39	224OH2	48.87	23O	25O39	26CD2	69.59
26CG	25O39	26CB	23.44	26CG	25O39	25SG	90.54
26CG	25O39	26NE1	33.09	26CG	25O39	66CA	57.23
26CG	25O39	66C	56.85	26CG	25O39	65N	91.62
26CG	25O39	26N	42.86	26CG	25O39	65O	69.92
26CG	25O39	23C	77.26	26CG	25O39	26CX	33.37
26CG	25O39	26CD2	9.50	26CB	25O39	25SG	80.06
26CB	25O39	26NE1	56.36	26CB	25O39	66CA	66.31
26CB	25O39	66C	56.61	26CB	25O39	26N	34.26
26CB	25O39	65O	89.29	26CB	25O39	23C	92.00
26CB	25O39	26CX	17.14	26CB	25O39	26CD2	31.88
25SG	25O39	26N	48.14	25SG	25O39	23C	65.56
25SG	25O39	26CX	62.98	25SG	25O39	224OH2	85.27
25SG	25O39	26CD2	98.66	26NE1	25O39	66CA	58.87
26NE1	25O39	66C	71.02	26NE1	25O39	65N	59.89
26NE1	25O39	26N	63.22	26NE1	25O39	65O	49.16
26NE1	25O39	23C	55.32	26NE1	25O39	26CX	62.29
26NE1	25O39	224OH2	88.14	26NE1	25O39	26CD2	26.49
66CA	25O39	66C	20.82	66CA	25O39	65N	71.23
66CA	25O39	26N	98.43	66CA	25O39	65O	35.79
66CA	25O39	26CX	83.32	66CA	25O39	26CD2	50.40
66C	25O39	65N	91.92	66C	25O39	26N	90.87
66C	25O39	65O	56.59	66C	25O39	26CX	73.34
66C	25O39	26CD2	53.53	65N	25O39	65O	35.54
65N	25O39	23C	60.74	65N	25O39	224OH2	46.37
65N	25O39	26CD2	82.99	26N	25O39	23C	68.72
26N	25O39	26CX	18.10	26N	25O39	26CD2	51.68
65O	25O39	23C	84.01	65O	25O39	224OH2	81.91
65O	25O39	26CD2	60.44	23C	25O39	26CX	83.51
23C	25O39	224OH2	45.98	23C	25O39	26CD2	76.48
26CX	25O39	26CD2	42.86	25SG	25N40	161O	86.06
25SG	25N40	23O	74.10	25SG	25N40	161C	85.73
25SG	25N40	23C	68.83	25SG	25N40	23CA	76.96
25SG	25N40	162CA	56.65	25SG	25N40	25CB	6.53

TABLE XIII

25SG	25N40	26CD1	72.41	161O	25N40	161C	12.75
161O	25N40	162CA	33.97	161O	25N40	25CB	90.20
224OH2	25N40	23O	52.97	224OH2	25N40	65CA	57.51
224OH2	25N40	23C	49.02	224OH2	25N40	23CA	35.43
224OH2	25N40	26CD1	85.10	23O	25N40	65CA	51.31
23O	25N40	23C	13.96	23O	25N40	23CA	29.87
23O	25N40	25CB	68.50	23O	25N40	26CD1	37.36
65CA	25N40	23C	62.89	65CA	25N40	23CA	68.80
65CA	25N40	26CD1	48.33	161C	25N40	162CA	29.53
161C	25N40	25CB	90.88	23C	25N40	23CA	18.22
23C	25N40	25CB	62.59	23C	25N40	26CD1	49.62
23CA	25N40	25CB	70.43	23CA	25N40	26CD1	67.09
162CA	25N40	25CB	62.21	25CB	25N40	26CD1	70.23
25SG	25N41	23C	99.66	25SG	25N41	25CB	18.83
25SG	25N41	25N	49.91	25SG	25N41	24N	86.40
25SG	25N41	161O	75.97	25SG	25N41	26CD1	82.58
25SG	25N41	25CA	32.30	25SG	25N41	26N	41.60
23O	25N41	224OH2	68.49	23O	25N41	23C	20.89
23O	25N41	23CA	42.41	23O	25N41	25CB	89.72
23O	25N41	25N	55.16	23O	25N41	24N	28.91
23O	25N41	65CA	55.11	23O	25N41	26CD1	40.72
23O	25N41	25CA	71.69	23O	25N41	26N	66.61
23O	25N41	23N	44.84	224OH2	25N41	23C	65.79
224OH2	25N41	23CA	48.09	224OH2	25N41	24N	78.14
224OH2	25N41	65CA	60.11	224OH2	25N41	26CD1	98.71
224OH2	25N41	23N	46.92	23C	25N41	23CA	25.44
23C	25N41	25CB	82.83	23C	25N41	25N	49.85
23C	25N41	24N	13.60	23C	25N41	65CA	73.03
23C	25N41	26CD1	59.09	23C	25N41	25CA	67.43
23C	25N41	26N	73.57	23C	25N41	23N	27.92
23CA	25N41	25CB	95.07	23CA	25N41	25N	68.21
23CA	25N41	24N	33.15	23CA	25N41	65CA	80.89
23CA	25N41	26CD1	83.00	23CA	25N41	25CA	84.37
23CA	25N41	26N	97.47	23CA	25N41	23N	2.51
25CB	25N41	25N	34.64	25CB	25N41	24N	69.27
25CB	25N41	161O	90.28	25CB	25N41	26CD1	80.97
25CB	25N41	25CA	18.50	25CB	25N41	26N	41.33

TABLE XIII

25CB	25N41	23N	95.93	25N	25N41	24N	36.95
25N	25N41	26CD1	57.65	25N	25N41	25CA	17.61
25N	25N41	26N	34.79	25N	25N41	23N	69.91
24N	25N41	65CA	83.83	24N	25N41	26CD1	59.64
24N	25N41	25CA	54.36	24N	25N41	26N	64.38
24N	25N41	23N	35.31	65CA	25N41	26CD1	50.18
65CA	25N41	26N	90.57	65CA	25N41	23N	82.10
26CD1	25N41	25CA	64.68	26CD1	25N41	26N	41.23
26CD1	25N41	23N	85.46	25CA	25N41	26N	29.42
25CA	25N41	23N	85.82	26N	25N41	23N	99.68
66O	25N42	66N	49.20	66O	25N42	65CA	85.32
66O	25N42	66C	14.31	66O	25N42	65C	66.36
66O	25N42	66CA	34.57	66O	25N42	67CE2	59.50
66N	25N42	65CA	37.29	66N	25N42	66C	37.91
66N	25N42	65C	17.17	66N	25N42	66CA	18.36
66N	25N42	67CE2	79.25	65CA	25N42	66C	75.14
65CA	25N42	65C	21.61	65CA	25N42	66CA	55.24
66C	25N42	65C	54.69	66C	25N42	66CA	21.22
66C	25N42	67CE2	55.45	65C	25N42	66CA	34.04
65C	25N42	67CE2	88.07	66CA	25N42	67CE2	63.12

TABLE XIV

Table of angles between atoms of the inhibitor and protein for all protein atoms within 5 Ångstroms of the inhibitor (1S)-N-[2-[(1-benzyloxycarbonylamino)-3-methylbutyl]thiazol-4-ylcarbonyl]-N'-(N-benzyloxycarbonyl-L-leucinyl)hydrazide.

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
184CB	25C1	184CG	19.63	184CB	25C1	184O	37.95
184CB	25C1	184CD2	33.99	184CB	25C1	184CE3	43.05
184CB	25C1	188CD1	60.59	184CG	25C1	184O	56.47
184CG	25C1	184CD2	18.11	184CG	25C1	184CE3	33.19
184CG	25C1	188CD1	68.63	184O	25C1	184CD2	71.92
184O	25C1	184CE3	78.39	184O	25C1	188CD1	69.15
184CD2	25C1	184CE3	17.41	184CD2	25C1	188CD1	62.78
184CE3	25C1	188CD1	48.96	184O	25C2	184CB	47.37
184O	25C2	184C	14.60	184O	25C2	184CG	67.03
184O	25C2	184CA	35.09	184O	25C2	184CD2	79.86
184O	25C2	184CD1	72.22	184O	25C2	18ND2	51.81
184CB	25C2	184C	37.41	184CB	25C2	184CG	20.57
184CB	25C2	184CA	21.23	184CB	25C2	184CD2	32.66
184CB	25C2	184CD1	31.54	184CB	25C2	18ND2	83.90
184C	25C2	184CG	55.27	184C	25C2	184CA	21.27
184C	25C2	184CD2	69.82	184C	25C2	184CD1	58.47
184C	25C2	18ND2	51.06	184CG	25C2	184CA	35.04
184CG	25C2	184CD2	16.66	184CG	25C2	184CD1	15.49
184CG	25C2	18ND2	93.96	184CA	25C2	184CD2	50.81
184CA	25C2	184CD1	37.24	184CA	25C2	18ND2	62.72
184CD2	25C2	184CD1	26.96	184CD1	25C2	18ND2	86.49
184O	25C3	184CB	45.92	184O	25C3	184CA	37.85
184O	25C3	184C	17.54	184O	25C3	18OD1	72.66
184O	25C3	184CG	67.51	184O	25C3	184CD1	78.54
184O	25C3	18ND2	59.83	184O	25C3	18CG	62.25
184O	25C3	184CD2	77.25	184CB	25C3	184CA	23.15
184CB	25C3	184C	38.05	184CB	25C3	18OD1	86.49
184CB	25C3	184CG	21.78	184CB	25C3	184CD1	36.65
184CB	25C3	18ND2	94.41	184CB	25C3	18CG	86.35
184CB	25C3	184CD2	32.23	184CA	25C3	184C	22.46
184CA	25C3	18OD1	63.82	184CA	25C3	184CG	37.27
184CA	25C3	184CD1	42.13	184CA	25C3	18ND2	72.53
184CA	25C3	18CG	63.26	184CA	25C3	184CD2	51.60

TABLE XIV

184C	25C3	18OD1	61.36	184C	25C3	184CG	57.47
184C	25C3	184CD1	64.57	184C	25C3	18ND2	57.87
184C	25C3	18CG	54.50	184C	25C3	184CD2	70.12
18OD1	25C3	184CG	91.25	18OD1	25C3	184CD1	79.96
18OD1	25C3	18ND2	31.05	18OD1	25C3	18CG	15.09
184CG	25C3	184CD1	18.78	184CG	25C3	18CG	96.39
184CG	25C3	184CD2	15.20	184CD1	25C3	18CG	88.85
184CD1	25C3	184CD2	27.59	18ND2	25C3	18CG	16.95
184CD1	25C4	184CG	19.46	184CD1	25C4	184CB	35.62
184CD1	25C4	18OD1	77.64	184CD1	25C4	20O	86.16
184CD1	25C4	184CA	39.47	184CD1	25C4	184NE1	16.76
184CD1	25C4	184CD2	28.36	184CD1	25C4	184O	68.14
184CD1	25C4	184CE2	25.97	184CG	25C4	184CB	20.21
184CG	25C4	18OD1	84.29	184CG	25C4	184CA	33.31
184CG	25C4	184NE1	29.37	184CG	25C4	184CD2	16.86
184CG	25C4	184O	56.12	184CG	25C4	184CE2	26.96
184CB	25C4	18OD1	74.62	184CB	25C4	184CA	19.60
184CB	25C4	184NE1	48.98	184CB	25C4	184CD2	33.22
184CB	25C4	184O	36.02	184CB	25C4	184CE2	46.70
18OD1	25C4	20O	64.59	18OD1	25C4	184CA	55.04
18OD1	25C4	184NE1	91.09	18OD1	25C4	184O	58.00
20O	25C4	184NE1	82.83	20O	25C4	184CE2	96.86
184CA	25C4	184NE1	55.98	184CA	25C4	184CD2	49.56
184CA	25C4	184O	30.00	184CA	25C4	184CE2	59.49
184NE1	25C4	184CD2	27.93	184NE1	25C4	184O	83.70
184NE1	25C4	184CE2	15.77	184CD2	25C4	184O	68.31
184CD2	25C4	184CE2	16.44	184O	25C4	184CE2	82.69
184CG	25C5	184CD1	18.11	184CG	25C5	184CD2	18.49
184CG	25C5	184NE1	28.96	184CG	25C5	184CE2	29.05
184CG	25C5	184CB	17.96	184CD1	25C5	184CD2	29.17
184CD1	25C5	184NE1	17.37	184CD1	25C5	184CE2	28.25
184CD1	25C5	184CB	32.12	184CD2	25C5	184NE1	28.48
184CD2	25C5	184CE2	17.52	184CD2	25C5	184CB	32.46
184NE1	25C5	184CE2	16.92	184NE1	25C5	184CB	46.34
184CE2	25C5	184CB	46.48	184CD2	25C6	184CG	18.41
184CD2	25C6	184CE3	17.57	184CD2	25C6	184CB	32.70
184CD2	25C6	184CE2	16.35	184CD2	25C6	184CD1	26.98
184CG	25C6	184CE3	33.10	184CG	25C6	184CB	18.26
184CG	25C6	184CE2	27.66	184CG	25C6	184CD1	15.78
184CE3	25C6	184CB	40.99	184CE3	25C6	143OE1	88.61
184CE3	25C6	184CE2	29.17	184CE3	25C6	184CD1	44.38
184CB	25C6	184CE2	45.38	184CB	25C6	184CD1	30.55

TABLE XIV

184CE2	25C6	184CD1	26.20	20O	25C7	20C	19.21
20O	25C7	20CA	39.07	20O	25C7	20N	45.05
20O	25C7	18OD1	87.05	20O	25C7	19CG	55.64
20O	25C7	21NE2	74.51	20O	25C7	21N	24.68
20O	25C7	18CG	94.59	20O	25C7	19C	40.56
20C	25C7	20CA	23.55	20C	25C7	20N	38.22
20C	25C7	18OD1	77.28	20C	25C7	19CG	67.04
20C	25C7	21NE2	71.32	20C	25C7	21N	11.95
20C	25C7	18CG	83.17	20C	25C7	19C	38.66
20CA	25C7	20N	21.87	20CA	25C7	18OD1	54.50
20CA	25C7	19CG	66.31	20CA	25C7	21NE2	87.33
20CA	25C7	21N	31.76	20CA	25C7	18CG	59.80
20CA	25C7	19C	28.41	20N	25C7	18OD1	42.02
20N	25C7	184CD1	96.35	20N	25C7	19CG	47.93
20N	25C7	21N	49.41	20N	25C7	18CG	49.82
20N	25C7	19C	10.08	20N	25C7	184CA	86.28
18OD1	25C7	184CD1	83.02	18OD1	25C7	19CG	66.42
18OD1	25C7	21N	86.24	18OD1	25C7	184NE1	98.06
18OD1	25C7	184CG	83.82	18OD1	25C7	18CG	8.98
18OD1	25C7	19C	48.05	18OD1	25C7	184CA	54.56
184CD1	25C7	19CG	55.25	184CD1	25C7	184NE1	16.81
184CD1	25C7	184CG	16.56	184CD1	25C7	18CG	85.33
184CD1	25C7	19C	89.88	184CD1	25C7	184CA	36.29
19CG	25C7	21N	77.73	19CG	25C7	184NE1	56.16
19CG	25C7	184CG	70.76	19CG	25C7	18CG	74.86
19CG	25C7	19C	38.66	19CG	25C7	184CA	68.46
21NE2	25C7	21N	59.46	21N	25C7	18CG	91.06
21N	25C7	19C	50.55	184NE1	25C7	184CG	28.00
184NE1	25C7	19C	94.36	184NE1	25C7	184CA	52.97
184CG	25C7	18CG	83.54	184CG	25C7	184CA	30.15
18CG	25C7	19C	56.53	18CG	25C7	184CA	53.47
19C	25C7	184CA	85.50	20O	25O8	19CG	74.18
20O	25O8	20C	14.24	20O	25O8	20N	45.16
20O	25O8	19CD	84.08	20O	25O8	20CA	33.67
20O	25O8	18OD1	81.17	20O	25O8	19C	43.87
20O	25O8	21N	14.62	20O	25O8	19CB	65.10
20O	25O8	19NE2	73.97	19CG	25O8	184CD1	71.14
19CG	25O8	20C	79.40	19CG	25O8	184NE1	74.25
19CG	25O8	20N	55.59	19CG	25O8	19CD	22.00
19CG	25O8	20CA	73.82	19CG	25O8	19OE1	34.44
19CG	25O8	184CG	85.17	19CG	25O8	18OD1	70.42
19CG	25O8	184CE2	88.06	19CG	25O8	19C	42.61

TABLE XIV

19CG	25O8	21N	87.25	19CG	25O8	19CB	11.43
19CG	25O8	19NE2	28.77	19CG	25O8	183O	42.56
19CG	25O8	184CD2	93.05	184CD1	25O8	184NE1	21.99
184CD1	25O8	19CD	64.82	184CD1	25O8	19OE1	49.70
184CD1	25O8	184CG	15.65	184CD1	25O8	18OD1	83.93
184CD1	25O8	184CE2	27.56	184CD1	25O8	19CB	80.03
184CD1	25O8	19NE2	77.46	184CD1	25O8	183O	43.29
184CD1	25O8	184CD2	22.85	20C	25O8	20N	37.96
20C	25O8	19CD	93.27	20C	25O8	20CA	21.59
20C	25O8	18OD1	70.08	20C	25O8	19C	41.74
20C	25O8	21N	10.44	20C	25O8	19CB	68.90
20C	25O8	19NE2	85.00	184NE1	25O8	19CD	59.98
184NE1	25O8	19OE1	43.21	184NE1	25O8	184CG	31.35
184NE1	25O8	184CE2	13.82	184NE1	25O8	19CB	85.19
184NE1	25O8	19NE2	69.30	184NE1	25O8	183O	60.22
184NE1	25O8	184CD2	24.73	20N	25O8	19CD	76.55
20N	25O8	20CA	20.72	20N	25O8	19OE1	89.93
20N	25O8	18OD1	38.33	20N	25O8	19C	14.64
20N	25O8	21N	48.38	20N	25O8	19CB	44.35
20N	25O8	19NE2	76.55	20N	25O8	183O	65.49
19CD	25O8	20CA	92.98	19CD	25O8	19OE1	16.77
19CD	25O8	184CG	80.43	19CD	25O8	18OD1	91.12
19CD	25O8	184CE2	73.34	19CD	25O8	19C	62.65
19CD	25O8	21N	98.59	19CD	25O8	19CB	32.44
19CD	25O8	19NE2	14.03	19CD	25O8	183O	53.18
19CD	25O8	184CD2	82.97	20CA	25O8	18OD1	48.49
20CA	25O8	19C	31.25	20CA	25O8	21N	31.00
20CA	25O8	19CB	62.39	20CA	25O8	19NE2	89.43
20CA	25O8	183O	85.40	19OE1	25O8	184CG	65.32
19OE1	25O8	18OD1	95.73	19OE1	25O8	184CE2	56.63
19OE1	25O8	19C	77.00	19OE1	25O8	19CB	45.84
19OE1	25O8	19NE2	27.83	19OE1	25O8	183O	50.05
19OE1	25O8	184CD2	66.42	184CG	25O8	18OD1	81.85
184CG	25O8	184CE2	29.41	184CG	25O8	19CB	92.98
184CG	25O8	19NE2	93.11	184CG	25O8	183O	51.14
184CG	25O8	184CD2	15.78	18OD1	25O8	19C	48.36
18OD1	25O8	21N	79.10	18OD1	25O8	19CB	63.32
18OD1	25O8	19NE2	98.90	18OD1	25O8	183O	49.03
18OD1	25O8	184CD2	97.37	184CE2	25O8	19CB	98.94
184CE2	25O8	19NE2	81.67	184CE2	25O8	183O	70.16
184CE2	25O8	184CD2	16.41	19C	25O8	21N	51.75
19C	25O8	19CB	31.18	19C	25O8	19NE2	61.93

TABLE XIV

19C	25O8	183O	62.03	21N	25O8	19CB	77.34
21N	25O8	19NE2	88.58	19CB	25O8	19NE2	35.99
19CB	25O8	183O	45.66	19NE2	25O8	183O	66.29
19NE2	25O8	184CD2	93.54	183O	25O8	184CD2	64.88
20O	25C9	19CG	60.67	20O	25C9	19CD	76.38
20O	25C9	19OE1	92.50	20O	25C9	20C	7.58
20O	25C9	19NE2	72.45	20O	25C9	21NE2	67.37
184NE1	25C9	184CD1	20.97	184NE1	25C9	19CG	68.64
184NE1	25C9	19CD	59.83	184NE1	25C9	19OE1	43.65
184NE1	25C9	184CE2	16.49	184NE1	25C9	19NE2	71.84
184NE1	25C9	184CG	26.81	184NE1	25C9	184CZ2	28.68
184CD1	25C9	19CG	60.92	184CD1	25C9	19CD	60.57
184CD1	25C9	19OE1	48.05	184CD1	25C9	184CE2	31.05
184CD1	25C9	19NE2	75.62	184CD1	25C9	184CG	13.88
184CD1	25C9	184CZ2	46.32	19CG	25C9	19CD	21.52
19CG	25C9	19OE1	33.58	19CG	25C9	20C	65.19
19CG	25C9	184CE2	85.10	19CG	25C9	19NE2	31.33
19CG	25C9	184CG	73.53	19CG	25C9	184CZ2	95.37
19CD	25C9	19OE1	16.79	19CD	25C9	20C	82.31
19CD	25C9	184CE2	75.59	19CD	25C9	19NE2	15.81
19CD	25C9	184CG	74.44	19CD	25C9	184CZ2	81.71
19OE1	25C9	20C	97.96	19OE1	25C9	184CE2	59.01
19OE1	25C9	19NE2	28.56	19OE1	25C9	184CG	61.65
19OE1	25C9	184CZ2	65.02	20C	25C9	19NE2	79.44
20C	25C9	21NE2	62.11	184CE2	25C9	19NE2	86.32
184CE2	25C9	184CG	28.77	184CE2	25C9	184CZ2	15.52
19NE2	25C9	184CG	89.47	19NE2	25C9	184CZ2	89.08
184CG	25C9	184CZ2	43.90	184NE1	25O10	184CE2	19.56
184NE1	25O10	184CD1	19.15	184NE1	25O10	20O	98.89
184NE1	25O10	184CZ2	34.13	184NE1	25O10	184CD2	27.67
184NE1	25O10	184CG	27.32	184CE2	25O10	184CD1	31.59
184CE2	25O10	184CZ2	18.04	184CE2	25O10	184CD2	16.51
184CE2	25O10	184CG	28.75	184CD1	25O10	20O	88.35
184CD1	25O10	184CZ2	49.32	184CD1	25O10	184CD2	28.37
184CD1	25O10	184CG	15.83	20O	25O10	184CG	99.14
20O	25O10	21NE2	63.32	184CZ2	25O10	184CD2	30.98
184CZ2	25O10	184CG	46.20	184CD2	25O10	184CG	17.35
19NE2	25C11	22O	38.20	19NE2	25C11	19CD	17.94
19NE2	25C11	20O	68.83	19NE2	25C11	19OE1	29.76
19NE2	25C11	184NE1	67.70	19NE2	25C11	22C	51.21
19NE2	25C11	23CA	50.68	19NE2	25C11	19CG	29.78
19NE2	25C11	22N	68.31	19NE2	25C11	23N	56.54

TABLE XIV

22O	25C11	19CD	51.52	22O	25C11	20O	54.51
22O	25C11	19OE1	66.66	22O	25C11	22C	14.40
22O	25C11	23CA	34.19	22O	25C11	19CG	50.00
22O	25C11	22N	32.97	22O	25C11	23N	26.65
19CD	25C11	20O	64.43	19CD	25C11	19OE1	15.96
19CD	25C11	184NE1	51.25	19CD	25C11	22C	65.67
19CD	25C11	23CA	68.61	19CD	25C11	19CG	17.66
19CD	25C11	22N	76.34	19CD	25C11	23N	73.36
20O	25C11	19OE1	76.37	20O	25C11	184NE1	85.38
20O	25C11	22C	60.00	20O	25C11	23CA	87.97
20O	25C11	19CG	47.41	20O	25C11	22N	38.68
20O	25C11	23N	75.19	19OE1	25C11	184NE1	38.17
19OE1	25C11	22C	80.44	19OE1	25C11	23CA	78.31
19OE1	25C11	19CG	29.35	19OE1	25C11	22N	92.26
19OE1	25C11	23N	86.19	184NE1	25C11	19CG	53.83
22C	25C11	23CA	29.04	22C	25C11	19CG	64.17
22C	25C11	22N	28.19	22C	25C11	23N	15.42
23CA	25C11	19CG	76.14	23CA	25C11	22N	56.58
23CA	25C11	23N	16.87	19CG	25C11	22N	66.36
19CG	25C11	23N	75.77	22N	25C11	23N	40.54
22O	25C12	22C	17.89	22O	25C12	22N	39.45
22O	25C12	23N	32.43	22O	25C12	23CA	38.69
22O	25C12	20O	56.27	22O	25C12	21C	55.84
22O	25C12	22CA	31.37	22O	25C12	21CA	67.07
22O	25C12	19NE2	35.21	22C	25C12	22N	34.05
22C	25C12	23N	18.76	22C	25C12	23CA	33.51
22C	25C12	20O	65.66	22C	25C12	21C	49.03
22C	25C12	22CA	18.77	22C	25C12	21CA	64.80
22C	25C12	19NE2	51.68	22N	25C12	23N	49.61
22N	25C12	23CA	67.28	22N	25C12	20O	43.43
22N	25C12	21C	16.39	22N	25C12	22CA	18.17
22N	25C12	21OE1	71.11	22N	25C12	21CA	30.79
22N	25C12	19NE2	70.87	23N	25C12	23CA	19.64
23N	25C12	20O	84.42	23N	25C12	21C	62.12
23N	25C12	22CA	31.69	23N	25C12	21CA	79.89
23N	25C12	19NE2	58.72	23CA	25C12	20O	94.95
23CA	25C12	21C	81.09	23CA	25C12	22CA	50.18
23CA	25C12	21CA	98.06	23CA	25C12	19NE2	50.86
20O	25C12	21C	45.48	20O	25C12	22CA	58.80
20O	25C12	21OE1	66.04	20O	25C12	21CA	35.16
20O	25C12	19NE2	63.11	21C	25C12	22CA	30.96
21C	25C12	21OE1	55.27	21C	25C12	21CA	18.83

TABLE XIV

21C	25C12	19NE2	86.29	22CA	25C12	21OE1	85.66
22CA	25C12	21CA	48.22	22CA	25C12	19NE2	66.48
21OE1	25C12	21CA	42.41	21CA	25C12	19NE2	90.68
21OE1	25C13	21CD	12.45	21OE1	25C13	21CA	47.08
21OE1	25C13	22N	76.49	21OE1	25C13	21C	61.27
21OE1	25C13	20O	69.05	21OE1	25C13	21NE2	23.98
21CD	25C13	21CA	41.21	21CD	25C13	22N	71.61
21CD	25C13	21C	58.15	21CD	25C13	20O	57.98
21CD	25C13	21NE2	14.96	21CA	25C13	22N	30.42
21CA	25C13	21C	18.99	21CA	25C13	20O	33.62
21CA	25C13	21NE2	51.09	22N	25C13	21C	16.45
22N	25C13	20O	38.35	22N	25C13	21NE2	80.82
21C	25C13	20O	42.37	21C	25C13	21NE2	69.53
20O	25C13	21NE2	58.27	21OE1	25C14	21C	80.26
21OE1	25C14	21CA	58.86	21OE1	25C14	22N	95.27
21OE1	25C14	21CD	11.97	21OE1	25C14	21O	83.12
21OE1	25C14	21CB	43.94	21OE1	25C14	21CG	26.08
21OE1	25C14	21NE2	17.70	21OE1	25C14	20O	71.89
21C	25C14	21CA	23.60	21C	25C14	22N	19.79
21C	25C14	21CD	70.89	21C	25C14	21O	18.03
21C	25C14	21CB	37.30	21C	25C14	22CA	32.39
21C	25C14	21CG	54.18	21C	25C14	22C	48.65
21C	25C14	21NE2	78.83	21C	25C14	23N	61.74
21C	25C14	20O	44.43	21CA	25C14	22N	36.47
21CA	25C14	21CD	48.38	21CA	25C14	21O	36.17
21CA	25C14	21CB	21.86	21CA	25C14	22CA	53.26
21CA	25C14	21CG	33.45	21CA	25C14	22C	65.81
21CA	25C14	21NE2	55.36	21CA	25C14	23N	80.87
21CA	25C14	20O	33.68	22N	25C14	21CD	84.38
22N	25C14	21O	33.19	22N	25C14	21CB	55.22
22N	25C14	22CA	17.77	22N	25C14	21CG	69.86
22N	25C14	22C	29.90	22N	25C14	21NE2	89.31
22N	25C14	23N	44.46	22N	25C14	20O	39.38
21CD	25C14	21O	76.50	21CD	25C14	21CB	36.73
21CD	25C14	21CG	18.01	21CD	25C14	21NE2	12.68
21CD	25C14	20O	60.03	21O	25C14	21CB	39.79
21O	25C14	22CA	37.66	21O	25C14	21CG	58.51
21O	25C14	22C	56.26	21O	25C14	21NE2	86.99
21O	25C14	23N	65.51	21O	25C14	20O	62.32
21CB	25C14	22CA	69.70	21CB	25C14	21CG	18.72
21CB	25C14	22C	85.11	21CB	25C14	21NE2	47.76
21CB	25C14	23N	98.97	21CB	25C14	20O	53.00

TABLE XIV

22CA	25C14	21CG	86.05	22CA	25C14	22C	18.65
22CA	25C14	23N	29.45	22CA	25C14	20O	54.92
21CG	25C14	22C	99.21	21CG	25C14	21NE2	29.49
21CG	25C14	20O	54.91	22C	25C14	23N	15.74
22C	25C14	20O	55.72	21NE2	25C14	20O	58.56
23N	25C14	20O	70.69	21OE1	25C15	21CD	18.02
21OE1	25C15	21NE2	36.11	21OE1	25C15	21CA	45.66
21OE1	25C15	20O	74.47	21OE1	25C15	21CG	20.94
21CD	25C15	21NE2	20.43	21CD	25C15	21CA	42.29
21CD	25C15	20O	63.32	21CD	25C15	21CG	11.31
21NE2	25C15	21CA	56.77	21NE2	25C15	20O	66.57
21NE2	25C15	21CG	29.05	21CA	25C15	20O	33.79
21CA	25C15	21CG	31.00	20O	25C15	21CG	54.47
19NE2	25C16	19OE1	34.42	19NE2	25C16	19CD	19.70
19NE2	25C16	23CA	57.42	19NE2	25C16	184NE1	74.14
19NE2	25C16	22O	38.47	19NE2	25C16	162ND1	77.08
19NE2	25C16	19CG	27.65	19NE2	25C16	23N	58.92
19NE2	25C16	22C	50.59	19OE1	25C16	19CD	18.10
19OE1	25C16	23CA	91.00	19OE1	25C16	184NE1	41.37
19OE1	25C16	22O	70.27	19OE1	25C16	162ND1	54.22
19OE1	25C16	19CG	28.11	19OE1	25C16	23N	93.23
19OE1	25C16	22C	83.37	19OE1	25C16	184CZ2	67.06
19CD	25C16	23CA	76.87	19CD	25C16	184NE1	54.73
19CD	25C16	22O	52.37	19CD	25C16	162ND1	70.37
19CD	25C16	19CG	14.40	19CD	25C16	23N	76.48
19CD	25C16	22C	65.58	19CD	25C16	184CZ2	83.17
23CA	25C16	22O	36.36	23CA	25C16	19CG	79.64
23CA	25C16	23N	16.38	23CA	25C16	22C	28.95
184NE1	25C16	162ND1	56.55	184NE1	25C16	19CG	54.16
184NE1	25C16	184CZ2	30.24	22O	25C16	19CG	48.64
22O	25C16	23N	26.88	22O	25C16	22C	13.31
162ND1	25C16	19CG	82.32	162ND1	25C16	184CZ2	51.21
19CG	25C16	23N	75.10	19CG	25C16	22C	61.77
19CG	25C16	184CZ2	84.32	23N	25C16	22C	15.32
162ND1	25S17	184CZ2	72.20	162ND1	25S17	184NE1	73.37
162ND1	25S17	162CE1	19.38	162ND1	25S17	19OE1	64.03
162ND1	25S17	184CE2	73.12	162ND1	25S17	162CG	16.82
162ND1	25S17	19CD	76.25	162ND1	25S17	19NE2	80.24
162ND1	25S17	162CB	31.46	162ND1	25S17	184CH2	75.04
162ND1	25S17	162NE2	24.22	162ND1	25S17	184CD1	76.19
184CZ2	25S17	184NE1	40.35	184CZ2	25S17	162CE1	61.98
184CZ2	25S17	19OE1	82.50	184CZ2	25S17	184CE2	20.39

TABLE XIV

184CZ2	25S17	162CG	64.57	184CZ2	25S17	19CD	94.35
184CZ2	25S17	162CB	73.92	184CZ2	25S17	184CH2	9.57
184CZ2	25S17	162NE2	50.06	184CZ2	25S17	184CD1	46.22
184NE1	25S17	162CE1	54.53	184NE1	25S17	19OE1	45.35
184NE1	25S17	184CE2	20.06	184NE1	25S17	162CG	77.66
184NE1	25S17	19CD	54.83	184NE1	25S17	19NE2	71.53
184NE1	25S17	162CB	94.60	184NE1	25S17	184CH2	49.77
184NE1	25S17	162NE2	51.06	184NE1	25S17	184CD1	6.15
162CE1	25S17	19OE1	48.96	162CE1	25S17	184CE2	57.43
162CE1	25S17	162CG	30.44	162CE1	25S17	19CD	62.94
162CE1	25S17	19NE2	71.39	162CE1	25S17	162CB	48.22
162CE1	25S17	184CH2	67.56	162CE1	25S17	162NE2	13.10
162CE1	25S17	184CD1	56.98	19OE1	25S17	184CE2	64.06
19OE1	25S17	162CG	78.89	19OE1	25S17	19CD	14.86
19OE1	25S17	19NE2	29.15	19OE1	25S17	162CB	95.48
19OE1	25S17	184CH2	91.95	19OE1	25S17	162NE2	57.76
19OE1	25S17	184CD1	41.33	184CE2	25S17	162CG	71.43
184CE2	25S17	19CD	74.69	184CE2	25S17	19NE2	91.37
184CE2	25S17	162CB	85.35	184CE2	25S17	184CH2	29.73
184CE2	25S17	162NE2	48.91	184CE2	25S17	184CD1	25.84
162CG	25S17	19CD	92.05	162CG	25S17	19NE2	97.02
162CG	25S17	162CB	18.20	162CG	25S17	184CH2	64.89
162CG	25S17	162NE2	27.13	162CG	25S17	184CD1	81.91
19CD	25S17	19NE2	16.70	19CD	25S17	162NE2	72.44
19CD	25S17	184CD1	49.68	19NE2	25S17	162NE2	82.84
19NE2	25S17	184CD1	66.32	162CB	25S17	184CH2	71.34
162CB	25S17	162NE2	45.10	162CB	25S17	184CD1	99.30
184CH2	25S17	162NE2	54.91	184CH2	25S17	184CD1	55.56
162NE2	25S17	184CD1	54.94	19NE2	25N18	23CA	73.04
19NE2	25N18	19CD	18.20	19NE2	25N18	22O	43.17
19NE2	25N18	19OE1	33.64	19NE2	25N18	23C	62.17
19NE2	25N18	25SG	78.34	19NE2	25N18	23N	70.88
19NE2	25N18	22C	57.87	19NE2	25N18	25CB	58.17
19NE2	25N18	24N	45.44	19NE2	25N18	162ND1	81.06
19NE2	25N18	25N	41.89	19NE2	25N18	23O	71.35
23CA	25N18	19CD	90.63	23CA	25N18	22O	43.03
23CA	25N18	23C	19.70	23CA	25N18	25SG	84.26
23CA	25N18	23N	17.82	23CA	25N18	22C	32.08
23CA	25N18	25CB	90.92	23CA	25N18	24N	31.17
23CA	25N18	25N	62.49	23CA	25N18	23O	26.79
19CD	25N18	22O	55.64	19CD	25N18	19OE1	17.64
19CD	25N18	23C	80.36	19CD	25N18	25SG	84.40

TABLE XIV

19CD	25N18	23N	86.18	19CD	25N18	22C	71.10
19CD	25N18	25CB	60.97	19CD	25N18	24N	63.63
19CD	25N18	162ND1	70.54	19CD	25N18	25N	54.63
19CD	25N18	23O	89.15	22O	25N18	19OE1	73.27
22O	25N18	23C	46.87	22O	25N18	23N	31.78
22O	25N18	22C	15.47	22O	25N18	25CB	93.37
22O	25N18	24N	37.57	22O	25N18	25N	64.91
22O	25N18	23O	60.03	19OE1	25N18	23C	93.60
19OE1	25N18	25SG	78.94	19OE1	25N18	22C	88.73
19OE1	25N18	25CB	54.74	19OE1	25N18	24N	77.36
19OE1	25N18	162ND1	53.80	19OE1	25N18	25N	59.44
19OE1	25N18	23O	99.98	23C	25N18	25SG	66.71
23C	25N18	23N	34.39	23C	25N18	22C	42.39
23C	25N18	25CB	71.24	23C	25N18	24N	16.74
23C	25N18	25N	43.13	23C	25N18	23O	13.17
25SG	25N18	25CB	24.23	25SG	25N18	24N	67.84
25SG	25N18	162ND1	54.04	25SG	25N18	25N	40.11
25SG	25N18	23O	57.50	23N	25N18	22C	17.29
23N	25N18	24N	39.13	23N	25N18	25N	73.32
23N	25N18	23O	44.07	22C	25N18	24N	39.37
22C	25N18	25N	71.95	22C	25N18	23O	54.65
25CB	25N18	24N	64.90	25CB	25N18	162ND1	43.82
25CB	25N18	25N	30.73	25CB	25N18	23O	66.97
24N	25N18	25N	34.26	24N	25N18	23O	27.47
162ND1	25N18	25N	73.32	25N	25N18	23O	43.35
25SG	25C19	25CB	30.95	25SG	25C19	19NE2	87.88
25SG	25C19	162ND1	72.09	25SG	25C19	23CA	92.18
25SG	25C19	19OE1	90.53	25SG	25C19	161O	75.25
25SG	25C19	19CD	92.51	25SG	25C19	25N	44.77
25SG	25C19	23C	73.06	25SG	25C19	162CE1	76.49
25SG	25C19	25CA	36.53	25SG	25C19	23O	62.97
25SG	25C19	162CG	75.04	25SG	25C19	24N	71.77
25SG	25C19	162CA	61.03	25CB	25C19	19NE2	64.00
25CB	25C19	162ND1	55.38	25CB	25C19	23CA	96.18
25CB	25C19	19OE1	59.77	25CB	25C19	161O	94.40
25CB	25C19	19CD	63.98	25CB	25C19	25N	33.81
25CB	25C19	23C	76.97	25CB	25C19	162CE1	52.78
25CB	25C19	25CA	15.71	25CB	25C19	23O	73.90
25CB	25C19	162CG	63.84	25CB	25C19	24N	67.67
25CB	25C19	162CA	66.83	19NE2	25C19	162ND1	88.64
19NE2	25C19	23CA	60.82	19NE2	25C19	19OE1	31.76
19NE2	25C19	19CD	16.34	19NE2	25C19	25N	44.95

TABLE XIV

19NE2	25C19	23C	56.12	19NE2	25C19	162CE1	73.67
19NE2	25C19	25CA	52.15	19NE2	25C19	23O	68.16
19NE2	25C19	24N	41.52	162ND1	25C19	19OE1	59.55
162ND1	25C19	161O	71.43	162ND1	25C19	19CD	75.22
162ND1	25C19	25N	86.60	162ND1	25C19	162CE1	15.59
162ND1	25C19	25CA	68.74	162ND1	25C19	162CG	12.11
162ND1	25C19	162CA	39.22	23CA	25C19	19OE1	92.31
23CA	25C19	19CD	76.28	23CA	25C19	25N	62.61
23CA	25C19	23C	19.89	23CA	25C19	25CA	81.01
23CA	25C19	23O	29.74	23CA	25C19	24N	29.49
19OE1	25C19	19CD	16.09	19OE1	25C19	25N	61.21
19OE1	25C19	23C	87.07	19OE1	25C19	162CE1	43.98
19OE1	25C19	25CA	56.66	19OE1	25C19	23O	97.48
19OE1	25C19	162CG	70.72	19OE1	25C19	24N	71.88
19OE1	25C19	162CA	98.02	161O	25C19	162CE1	86.98
161O	25C19	162CG	60.30	161O	25C19	162CA	34.11
19CD	25C19	25N	54.73	19CD	25C19	23C	72.44
19CD	25C19	162CE1	59.74	19CD	25C19	25CA	56.11
19CD	25C19	23O	84.17	19CD	25C19	162CG	86.63
19CD	25C19	24N	57.70	25N	25C19	23C	44.11
25N	25C19	162CE1	79.19	25N	25C19	25CA	18.40
25N	25C19	23O	44.87	25N	25C19	162CG	96.59
25N	25C19	24N	33.86	25N	25C19	162CA	99.25
23C	25C19	25CA	62.33	23C	25C19	23O	14.57
23C	25C19	24N	15.37	162CE1	25C19	25CA	63.05
162CE1	25C19	162CG	26.96	162CE1	25C19	162CA	54.63
25CA	25C19	23O	61.33	25CA	25C19	162CG	78.31
25CA	25C19	24N	52.11	25CA	25C19	162CA	82.37
23O	25C19	24N	26.74	162CG	25C19	162CA	30.21
20O	25N20	19CD	87.74	20O	25N20	19NE2	89.20
20O	25N20	19CG	65.65	20O	25N20	22O	66.51
20O	25N20	20C	2.25	20O	25N20	184CD1	99.19
20O	25N20	22N	43.43	20O	25N20	22C	67.94
20O	25N20	21CA	31.81	20O	25N20	19CB	59.50
19CD	25N20	19NE2	20.94	19CD	25N20	19CG	24.17
19CD	25N20	19OE1	18.66	19CD	25N20	22O	59.53
19CD	25N20	184NE1	61.57	19CD	25N20	20C	89.98
19CD	25N20	184CD1	58.87	19CD	25N20	22N	90.16
19CD	25N20	22C	72.14	19CD	25N20	184CE2	73.87
19CD	25N20	19CB	28.25	19NE2	25N20	19CG	38.17
19NE2	25N20	19OE1	34.54	19NE2	25N20	22O	42.18
19NE2	25N20	184NE1	79.08	19NE2	25N20	20C	91.23

TABLE XIV

19NE2	25N20	184CD1	79.14	19NE2	25N20	22N	76.95
19NE2	25N20	22C	53.71	19NE2	25N20	184CE2	90.08
19NE2	25N20	19CB	35.63	19CG	25N20	19OE1	37.15
19CG	25N20	22O	61.25	19CG	25N20	184NE1	67.75
19CG	25N20	20C	67.89	19CG	25N20	184CD1	57.44
19CG	25N20	22N	80.74	19CG	25N20	22C	74.00
19CG	25N20	21CA	93.39	19CG	25N20	184CE2	80.81
19CG	25N20	19CB	11.02	19OE1	25N20	22O	76.29
19OE1	25N20	184NE1	44.61	19OE1	25N20	184CD1	46.08
19OE1	25N20	22C	88.22	19OE1	25N20	184CE2	56.16
19OE1	25N20	19CB	44.63	22O	25N20	20C	67.58
22O	25N20	22N	36.33	22O	25N20	22C	13.03
22O	25N20	21CA	65.40	22O	25N20	19CB	51.11
184NE1	25N20	184CD1	17.40	184NE1	25N20	184CE2	13.10
184NE1	25N20	19CB	78.62	20C	25N20	22N	43.20
20C	25N20	22C	68.49	20C	25N20	21CA	30.05
20C	25N20	19CB	61.74	184CD1	25N20	184CE2	27.05
184CD1	25N20	19CB	68.40	22N	25N20	22C	29.81
22N	25N20	21CA	29.53	22N	25N20	19CB	69.93
22C	25N20	21CA	59.18	22C	25N20	19CB	63.62
21CA	25N20	19CB	84.67	184CE2	25N20	19CB	91.71
162ND1	25C21	25SG	76.59	162ND1	25C21	162CE1	18.63
162ND1	25C21	162CG	18.63	162ND1	25C21	161O	88.59
162ND1	25C21	25CB	58.66	162ND1	25C21	162CB	39.41
162ND1	25C21	19OE1	66.84	162ND1	25C21	162CA	48.39
162ND1	25C21	19NE2	91.07	162ND1	25C21	19CD	80.09
162ND1	25C21	162NE2	16.42	162ND1	25C21	161C	78.48
162ND1	25C21	184CZ2	60.80	162ND1	25C21	162CD2	15.86
162ND1	25C21	184NE1	63.09	162ND1	25C21	162N	62.96
25SG	25C21	162CE1	82.30	25SG	25C21	162CG	85.48
25SG	25C21	161O	75.19	25SG	25C21	25CB	27.93
25SG	25C21	162CB	86.01	25SG	25C21	19OE1	84.07
25SG	25C21	162CA	67.62	25SG	25C21	19NE2	71.84
25SG	25C21	19CD	81.26	25SG	25C21	162NE2	89.59
25SG	25C21	161C	76.87	25SG	25C21	162CD2	91.13
25SG	25C21	162N	73.63	162CE1	25C21	162CG	34.59
162CE1	25C21	25CB	58.15	162CE1	25C21	162CB	56.62
162CE1	25C21	19OE1	49.16	162CE1	25C21	162CA	67.01
162CE1	25C21	19NE2	75.88	162CE1	25C21	19CD	63.04
162CE1	25C21	162NE2	10.76	162CE1	25C21	161C	97.04
162CE1	25C21	184CZ2	52.78	162CE1	25C21	162CD2	25.92
162CE1	25C21	184NE1	46.57	162CE1	25C21	162N	81.54

TABLE XIV

162CG	25C21	161O	74.86	162CG	25C21	25CB	73.56
162CG	25C21	162CB	22.12	162CG	25C21	19OE1	83.74
162CG	25C21	162CA	37.08	162CG	25C21	19CD	97.60
162CG	25C21	162NE2	27.00	162CG	25C21	161C	64.13
162CG	25C21	184CZ2	58.58	162CG	25C21	162CD2	11.67
162CG	25C21	184NE1	71.27	162CG	25C21	162N	49.24
161O	25C21	25CB	96.45	161O	25C21	162CB	53.58
161O	25C21	162CA	40.31	161O	25C21	161C	10.85
161O	25C21	162CD2	86.16	161O	25C21	162N	25.81
25CB	25C21	162CB	84.13	25CB	25C21	19OE1	58.32
25CB	25C21	162CA	73.26	25CB	25C21	19NE2	55.61
25CB	25C21	19CD	59.29	25CB	25C21	162NE2	67.37
25CB	25C21	161C	94.34	25CB	25C21	162CD2	74.51
25CB	25C21	184NE1	89.62	25CB	25C21	162N	85.19
162CB	25C21	162CA	21.46	162CB	25C21	162NE2	48.98
162CB	25C21	161C	42.74	162CB	25C21	184CZ2	70.53
162CB	25C21	162CD2	32.77	162CB	25C21	184NE1	90.36
162CB	25C21	162N	28.88	19OE1	25C21	19NE2	30.01
19OE1	25C21	19CD	14.42	19OE1	25C21	162NE2	57.58
19OE1	25C21	184CZ2	67.32	19OE1	25C21	162CD2	74.15
19OE1	25C21	184NE1	37.69	162CA	25C21	162NE2	62.57
162CA	25C21	161C	30.75	162CA	25C21	184CZ2	91.75
162CA	25C21	162CD2	48.73	162CA	25C21	162N	15.49
19NE2	25C21	19CD	16.41	19NE2	25C21	162NE2	85.63
19NE2	25C21	184CZ2	94.21	19NE2	25C21	184NE1	63.87
19CD	25C21	162NE2	71.85	19CD	25C21	184CZ2	78.23
19CD	25C21	162CD2	88.39	19CD	25C21	184NE1	47.85
162NE2	25C21	161C	91.07	162NE2	25C21	184CZ2	46.06
162NE2	25C21	162CD2	16.57	162NE2	25C21	184NE1	47.02
162NE2	25C21	162N	75.95	161C	25C21	162CD2	75.36
161C	25C21	162N	15.54	184CZ2	25C21	162CD2	49.06
184CZ2	25C21	184NE1	30.38	184CZ2	25C21	162N	97.18
162CD2	25C21	184NE1	59.61	162CD2	25C21	162N	60.72
25SG	25C22	25CB	34.32	25SG	25C22	25N	58.23
25SG	25C22	23O	96.62	25SG	25C22	25CA	41.06
25SG	25C22	161O	88.83	25SG	25C22	19NE2	94.39
25SG	25C22	24N	94.80	25SG	25C22	162ND1	67.14
25SG	25C22	26N	28.02	25SG	25C22	24C	63.81
25SG	25C22	25C	28.81	25SG	25C22	162CA	61.80
25SG	25C22	26CD1	59.67	25CB	25C22	25N	41.88
25CB	25C22	23C	94.72	25CB	25C22	23O	97.61
25CB	25C22	25CA	20.48	25CB	25C22	19NE2	62.01

TABLE XIV

25CB	25C22	24N	79.22	25CB	25C22	162ND1	50.87
25CB	25C22	26N	40.24	25CB	25C22	24C	51.06
25CB	25C22	25C	25.68	25CB	25C22	162CA	70.19
25CB	25C22	26CD1	77.04	25N	25C22	23CA	72.11
25N	25C22	23C	53.07	25N	25C22	23O	56.89
25N	25C22	25CA	21.75	25N	25C22	19NE2	46.70
25N	25C22	24N	38.64	25N	25C22	162ND1	88.45
25N	25C22	26N	36.83	25N	25C22	24C	9.50
25N	25C22	25C	29.43	25N	25C22	26CD1	53.68
23CA	25C22	23C	23.35	23CA	25C22	23O	37.19
23CA	25C22	25CA	93.17	23CA	25C22	19NE2	58.05
23CA	25C22	24N	33.59	23CA	25C22	26N	99.96
23CA	25C22	24C	64.82	23CA	25C22	26CD1	78.54
23C	25C22	23O	18.81	23C	25C22	25CA	74.82
23C	25C22	19NE2	57.79	23C	25C22	24N	16.66
23C	25C22	26N	76.83	23C	25C22	24C	44.46
23C	25C22	25C	78.94	23C	25C22	26CD1	57.31
23O	25C22	25CA	77.22	23O	25C22	19NE2	74.75
23O	25C22	24N	30.81	23O	25C22	26N	69.15
23O	25C22	24C	47.40	23O	25C22	25C	76.13
23O	25C22	26CD1	41.43	25CA	25C22	19NE2	54.59
25CA	25C22	24N	60.09	25CA	25C22	162ND1	70.00
25CA	25C22	26N	30.49	25CA	25C22	24C	30.68
25CA	25C22	25C	15.62	25CA	25C22	162CA	89.97
25CA	25C22	26CD1	62.21	161O	25C22	162ND1	66.24
161O	25C22	162CA	34.26	19NE2	25C22	24N	44.06
19NE2	25C22	162ND1	75.31	19NE2	25C22	26N	82.03
19NE2	25C22	24C	49.24	19NE2	25C22	25C	69.71
19NE2	25C22	26CD1	96.23	24N	25C22	26N	68.47
24N	25C22	24C	31.27	24N	25C22	25C	66.84
24N	25C22	26CD1	59.64	162ND1	25C22	26N	88.16
162ND1	25C22	24C	97.87	162ND1	25C22	25C	75.88
162ND1	25C22	162CA	38.60	26N	25C22	24C	39.22
26N	25C22	25C	15.72	26N	25C22	162CA	89.81
26N	25C22	26CD1	37.42	24C	25C22	25C	35.57
24C	25C22	26CD1	47.97	25C	25C22	162CA	86.23
25C	25C22	26CD1	51.39	25SG	25O23	25N	74.67
25SG	25O23	25CB	38.15	25SG	25O23	25CA	54.63
25SG	25O23	24C	85.79	25SG	25O23	26N	43.64
25SG	25O23	25C	46.38	25SG	25O23	19OE1	92.56
25SG	25O23	26CD1	68.54	25SG	25O23	162ND1	54.77
25SG	25O23	24O	79.70	23C	25O23	25N	73.70

TABLE XIV

23C	25O23	23CA	31.55	23C	25O23	23O	24.72
23C	25O23	24N	24.08	23C	25O23	19NE2	78.98
23C	25O23	25CA	97.79	23C	25O23	24C	59.01
23C	25O23	24CA	36.52	23C	25O23	23N	33.47
23C	25O23	22O	48.06	23C	25O23	19CD	90.90
23C	25O23	26N	92.04	23C	25O23	25C	96.56
23C	25O23	26CD1	66.16	23C	25O23	22C	38.64
23C	25O23	24O	64.99	25N	25O23	23O	75.80
25N	25O23	25CB	50.26	25N	25O23	24N	53.76
25N	25O23	19NE2	61.26	25N	25O23	25CA	24.14
25N	25O23	24C	14.83	25N	25O23	24CA	37.18
25N	25O23	23N	97.04	25N	25O23	22O	79.60
25N	25O23	19CD	63.80	25N	25O23	26N	37.49
25N	25O23	25C	28.32	25N	25O23	19OE1	68.00
25N	25O23	26CD1	60.48	25N	25O23	22C	87.54
25N	25O23	162ND1	89.51	25N	25O23	24O	9.64
23CA	25O23	23O	48.80	23CA	25O23	24N	46.69
23CA	25O23	19NE2	77.35	23CA	25O23	24C	86.89
23CA	25O23	24CA	64.88	23CA	25O23	23N	7.95
23CA	25O23	22O	38.18	23CA	25O23	19CD	87.87
23CA	25O23	26CD1	93.73	23CA	25O23	22C	23.48
23CA	25O23	24O	93.16	23O	25O23	24N	42.48
23O	25O23	25CA	97.01	23O	25O23	24C	61.75
23O	25O23	24CA	43.63	23O	25O23	23N	53.76
23O	25O23	22O	72.77	23O	25O23	26N	79.20
23O	25O23	25C	89.58	23O	25O23	26CD1	44.93
23O	25O23	22C	62.49	23O	25O23	24O	66.16
25CB	25O23	19NE2	75.63	25CB	25O23	25CA	26.15
25CB	25O23	24C	64.94	25CB	25O23	24CA	87.43
25CB	25O23	19CD	67.69	25CB	25O23	26N	43.69
25CB	25O23	25C	31.03	25CB	25O23	19OE1	57.73
25CB	25O23	26CD1	83.37	25CB	25O23	162ND1	43.20
25CB	25O23	24O	59.04	24N	25O23	19NE2	59.02
24N	25O23	25CA	77.52	24N	25O23	24C	40.38
24N	25O23	24CA	19.70	24N	25O23	23N	44.10
24N	25O23	22O	40.11	24N	25O23	19CD	70.43
24N	25O23	26N	81.70	24N	25O23	25C	80.42
24N	25O23	19OE1	85.06	24N	25O23	26CD1	70.58
24N	25O23	22C	39.18	24N	25O23	24O	46.65
19NE2	25O23	25CA	66.95	19NE2	25O23	24C	63.26
19NE2	25O23	24CA	65.23	19NE2	25O23	23N	69.48
19NE2	25O23	22O	39.17	19NE2	25O23	19CD	11.94

TABLE XIV

19NE2	25O23	26N	96.41	19NE2	25O23	25C	81.46
19NE2	25O23	19OE1	27.37	19NE2	25O23	22C	53.87
19NE2	25O23	162ND1	76.87	19NE2	25O23	24O	65.05
25CA	25O23	24C	38.79	25CA	25O23	24CA	61.29
25CA	25O23	22O	96.77	25CA	25O23	19CD	63.98
25CA	25O23	26N	31.96	25CA	25O23	25C	15.29
25CA	25O23	19OE1	61.11	25CA	25O23	26CD1	68.99
25CA	25O23	162ND1	67.28	25CA	25O23	24O	32.93
24C	25O23	24CA	22.55	24C	25O23	23N	84.41
24C	25O23	22O	71.79	24C	25O23	19CD	68.91
24C	25O23	26N	44.17	24C	25O23	25C	40.07
24C	25O23	19OE1	76.59	24C	25O23	26CD1	54.93
24C	25O23	22C	77.02	24C	25O23	24O	6.27
24CA	25O23	23N	63.29	24CA	25O23	22O	57.79
24CA	25O23	19CD	74.68	24CA	25O23	26N	62.01
24CA	25O23	25C	61.72	24CA	25O23	19OE1	86.76
24CA	25O23	26CD1	55.98	24CA	25O23	22C	58.75
24CA	25O23	24O	28.67	23N	25O23	22O	30.31
23N	25O23	19CD	79.92	23N	25O23	19OE1	93.90
23N	25O23	26CD1	98.39	23N	25O23	22C	15.63
23N	25O23	24O	90.66	22O	25O23	19CD	49.86
22O	25O23	19OE1	64.43	22O	25O23	22C	14.70
22O	25O23	24O	77.07	19CD	25O23	26N	95.38
19CD	25O23	25C	79.18	19CD	25O23	19OE1	15.44
19CD	25O23	22C	64.49	19CD	25O23	162ND1	64.94
19CD	25O23	24O	69.44	26N	25O23	25C	16.77
26N	25O23	19OE1	92.94	26N	25O23	26CD1	39.94
26N	25O23	162ND1	84.95	26N	25O23	24O	38.78
25C	25O23	19OE1	76.17	25C	25O23	26CD1	55.41
25C	25O23	162ND1	74.20	25C	25O23	24O	33.82
19OE1	25O23	22C	78.82	19OE1	25O23	162ND1	49.50
19OE1	25O23	24O	75.54	26CD1	25O23	24O	54.16
22C	25O23	24O	82.96	162ND1	25O23	24O	99.10
64O	25C24	61OD1	49.69	64O	25C25	61OD1	65.86
64O	25C25	64C	4.04	64O	25C25	65CA	36.03
64O	25C25	61CG	60.48	64O	25C25	65N	18.55
61OD1	25C25	64C	66.57	61OD1	25C25	65CA	65.57
61OD1	25C25	61CG	12.80	61OD1	25C25	65N	65.27
64C	25C25	65CA	32.21	64C	25C25	61CG	62.08
64C	25C25	65N	14.69	65CA	25C25	61CG	68.81
65CA	25C25	65N	17.52	61CG	25C25	65N	64.30
64O	25C26	61OD1	75.97	64O	25C26	65CA	46.13

TABLE XIV

64O	25C26	65C	60.97	64O	25C26	64C	10.65
64O	25C26	66N	77.86	64O	25C26	61CG	67.54
64O	25C26	65N	27.99	64O	25C26	65O	58.42
64O	25C26	61CB	50.52	61OD1	25C26	65CA	81.67
61OD1	25C26	65C	66.87	61OD1	25C26	64C	74.15
61OD1	25C26	66N	75.37	61OD1	25C26	61CG	10.88
61OD1	25C26	65N	75.81	61OD1	25C26	65O	51.81
61OD1	25C26	61CB	25.47	65CA	25C26	65C	22.26
65CA	25C26	64C	35.83	65CA	25C26	66N	33.99
65CA	25C26	61CG	80.84	65CA	25C26	65N	18.46
65CA	25C26	65O	32.38	65CA	25C26	61CB	65.67
65C	25C26	64C	50.43	65C	25C26	66N	17.99
65C	25C26	61CG	69.56	65C	25C26	65N	34.42
65C	25C26	65O	15.34	65C	25C26	61CB	58.96
64C	25C26	66N	67.22	64C	25C26	61CG	67.20
64C	25C26	65N	17.48	64C	25C26	65O	48.92
64C	25C26	61CB	49.45	66N	25C26	61CG	80.82
66N	25C26	65N	50.23	66N	25C26	65O	29.57
66N	25C26	61CB	73.71	61CG	25C26	65N	71.80
61CG	25C26	65O	54.22	61CG	25C26	61CB	17.81
65N	25C26	65O	36.92	65N	25C26	61CB	54.59
65O	25C26	61CB	44.43	61OD1	25C27	64O	56.92
61OD1	25C27	66N	69.33	61OD1	25C27	65C	57.67
61OD1	25C27	65CA	66.06	61OD1	25C27	61CG	5.76
64O	25C27	66N	63.73	64O	25C27	65C	48.11
64O	25C27	65CA	35.11	64O	25C27	61CG	54.18
66N	25C27	67CE2	75.89	66N	25C27	65C	16.74
66N	25C27	65CA	30.26	66N	25C27	61CG	73.19
66N	25C27	67OH	95.43	67CE2	25C27	65C	91.10
67CE2	25C27	67OH	29.04	65C	25C27	65CA	18.79
65C	25C27	61CG	60.50	65CA	25C27	61CG	67.06
61OD1	25C28	67CE2	87.37	67OH	25C28	67CE2	29.20
67CE2	25C30	66CA	87.59	67CE2	25C30	67CD2	20.16
67CE2	25C30	67CZ	18.73	67CE2	25C30	67OH	34.56
67CE2	25C30	66C	70.31	67CE2	25C30	66O	70.72
67CE2	25C30	67CG	25.18	66N	25C30	61OD1	77.24
66N	25C30	66CA	21.80	66N	25C30	67CD2	87.09
66N	25C30	65C	18.44	66N	25C30	66C	34.83
66N	25C30	66O	37.41	66N	25C30	65O	28.55
66N	25C30	65CA	30.87	66N	25C30	67CG	79.90
61OD1	25C30	66CA	79.21	61OD1	25C30	65C	61.19
61OD1	25C30	66C	99.06	61OD1	25C30	65O	48.69

TABLE XIV

61OD1	25C30	65CA	65.35	66CA	25C30	67CD2	68.10
66CA	25C30	67CZ	95.64	66CA	25C30	65C	34.85
66CA	25C30	66C	20.50	66CA	25C30	66O	32.31
66CA	25C30	65O	36.26	66CA	25C30	65CA	51.45
66CA	25C30	67CG	63.14	67CD2	25C30	67CZ	35.10
67CD2	25C30	67OH	53.38	67CD2	25C30	66C	52.50
67CD2	25C30	66O	56.67	67CD2	25C30	67CG	11.66
67CZ	25C30	67OH	19.01	67CZ	25C30	66C	75.82
67CZ	25C30	66O	70.92	67CZ	25C30	67CG	34.09
65C	25C30	66C	52.09	65C	25C30	66O	55.84
65C	25C30	65O	14.76	65C	25C30	65CA	18.69
65C	25C30	67CG	97.10	67OH	25C30	66C	93.31
67OH	25C30	66O	85.90	67OH	25C30	67CG	53.10
66C	25C30	66O	15.93	66C	25C30	65O	56.33
66C	25C30	65CA	65.39	66C	25C30	67CG	45.14
66O	25C30	65O	64.17	66O	25C30	65CA	64.29
66O	25C30	67CG	46.61	65O	25C30	65CA	29.99
65O	25C30	67CG	98.82	67CE2	25O31	67CZ	25.44
67CE2	25O31	67OH	43.21	67CE2	25O31	67CD2	21.71
67CE2	25O31	66O	86.23	67CE2	25O31	66C	79.23
67CE2	25O31	66CA	90.96	67CE2	25O31	67CE1	36.09
67CE2	25O31	67CG	31.92	67CE2	25O31	67CD1	36.21
67CE2	25O31	67N	65.41	67CZ	25O31	67OH	23.53
67CZ	25O31	67CD2	40.63	67CZ	25O31	66O	90.28
67CZ	25O31	66C	90.73	67CZ	25O31	67CE1	17.83
67CZ	25O31	67CG	39.73	67CZ	25O31	67CD1	30.41
67CZ	25O31	67N	78.58	67OH	25O31	67CD2	62.56
67OH	25O31	67CE1	36.02	67OH	25O31	67CG	63.25
67OH	25O31	67CD1	52.26	67CD2	25O31	66O	66.16
67CD2	25O31	66N	90.96	67CD2	25O31	66C	57.61
67CD2	25O31	66CA	69.91	67CD2	25O31	67CE1	41.91
67CD2	25O31	67CG	16.99	67CD2	25O31	67CD1	31.58
67CD2	25O31	67N	43.75	66O	25O31	66N	42.55
66O	25O31	66C	18.09	66O	25O31	66CA	35.81
66O	25O31	67CE1	75.32	66O	25O31	67CG	54.80
66O	25O31	65C	57.68	66O	25O31	67CD1	59.89
66O	25O31	67N	27.36	66O	25O31	65CA	66.84
66N	25O31	66C	37.22	66N	25O31	66CA	21.24
66N	25O31	67CG	88.11	66N	25O31	65C	15.16
66N	25O31	67CD1	99.35	66N	25O31	67N	49.30
66N	25O31	65CA	28.53	66C	25O31	66CA	21.98
66C	25O31	67CE1	79.50	66C	25O31	67CG	51.32

TABLE XIV

66C	25O31	65C	51.46	66C	25O31	67CD1	62.32
66C	25O31	67N	13.91	66C	25O31	65CA	65.42
66CA	25O31	67CE1	99.90	66CA	25O31	67CG	68.85
66CA	25O31	65C	32.23	66CA	25O31	67CD1	82.55
66CA	25O31	67N	30.44	66CA	25O31	65CA	48.87
67CE1	25O31	67CG	33.08	67CE1	25O31	67CD1	17.35
67CE1	25O31	67N	69.51	67CG	25O31	67CD1	17.79
67CG	25O31	67N	38.86	65C	25O31	67N	62.38
65C	25O31	65CA	17.93	67CD1	25O31	67N	52.17
67N	25O31	65CA	77.82	66O	25C32	66N	41.03
66O	25C32	67CZ	76.35	66O	25C32	67OH	95.33
66O	25C32	67CE2	69.48	66O	25C32	66C	15.10
66O	25C32	66CA	31.92	66O	25C32	65CA	69.81
66O	25C32	65C	56.36	66O	25C32	67CE1	66.82
66O	25C32	67CD2	53.70	66N	25C32	67CE2	87.72
66N	25C32	66C	33.67	66N	25C32	66CA	17.88
66N	25C32	65CA	31.90	66N	25C32	65C	15.39
66N	25C32	67CD2	73.68	67CZ	25C32	67OH	19.19
67CZ	25C32	67CE2	19.23	67CZ	25C32	66C	73.63
67CZ	25C32	66CA	85.66	67CZ	25C32	67CE1	16.63
67CZ	25C32	67CD2	30.02	67OH	25C32	67CE2	33.49
67OH	25C32	66C	92.69	67OH	25C32	67CE1	30.65
67OH	25C32	67CD2	47.69	67CE2	25C32	66C	62.32
67CE2	25C32	66CA	70.20	67CE2	25C32	65C	96.55
67CE2	25C32	67CE1	30.87	67CE2	25C32	67CD2	16.03
66C	25C32	66CA	19.46	66C	25C32	65CA	65.30
66C	25C32	65C	48.62	66C	25C32	67CE1	68.20
66C	25C32	67CD2	46.37	66CA	25C32	65CA	49.19
66CA	25C32	65C	30.83	66CA	25C32	67CE1	84.10
66CA	25C32	67CD2	55.84	65CA	25C32	65C	19.14
65C	25C32	67CD2	84.41	67CE1	25C32	67CD2	33.97
67OH	25O33	67CZ	16.87	67OH	25O33	66N	97.69
67OH	25O33	67CE2	28.97	67OH	25O33	160O	89.11
67CZ	25O33	66N	81.70	67CZ	25O33	67CE2	16.30
67CZ	25O33	160O	93.56	66N	25O33	67CE2	69.22
66O	25C34	66N	39.13	66O	25C34	65CA	71.17
66O	25C34	25SG	87.16	66O	25C34	65C	53.66
66O	25C34	66C	9.91	66N	25C34	65CA	32.59
66N	25C34	25SG	85.90	66N	25C34	65C	14.62
66N	25C34	66C	30.25	161O	25C34	161C	15.14
161O	25C34	25SG	60.22	161O	25C34	160O	61.47
65CA	25C34	25SG	79.10	65CA	25C34	65C	18.14

TABLE XIV

65CA	25C34 66C	62.76	161C	25C34 25SG	68.39
161C	25C34 160O	48.09	25SG	25C34 65C	84.17
25SG	25C34 66C	90.62	65C	25C34 66C	44.86
161O	25C35 160O	72.48	161O	25C35 161C	18.16
161O	25C35 162N	31.48	161O	25C35 161CA	33.51
161O	25C35 163N	64.70	161O	25C35 160C	64.27
161O	25C35 25SG	63.17	161O	25C35 162CA	35.94
161O	25C35 161N	48.76	161O	25C35 162C	54.37
160O	25C35 161C	58.42	160O	25C35 162N	63.10
160O	25C35 161CA	39.04	160O	25C35 160C	13.43
160O	25C35 162CA	80.67	160O	25C35 161N	27.44
160O	25C35 162C	86.34	161C	25C35 162N	17.93
161C	25C35 161CA	20.68	161C	25C35 163N	61.49
161C	25C35 160C	48.25	161C	25C35 25SG	75.24
161C	25C35 162CA	31.05	161C	25C35 161N	32.29
161C	25C35 162C	47.54	66O	25C35 25SG	85.01
162N	25C35 161CA	32.91	162N	25C35 163N	45.91
162N	25C35 160C	50.42	162N	25C35 25SG	71.74
162N	25C35 162CA	17.88	162N	25C35 161N	35.87
162N	25C35 162C	30.79	161CA	25C35 163N	78.80
161CA	25C35 160C	31.32	161CA	25C35 25SG	95.35
161CA	25C35 162CA	49.73	161CA	25C35 161N	17.33
161CA	25C35 162C	63.45	163N	25C35 160C	88.14
163N	25C35 25SG	47.65	163N	25C35 162CA	30.56
163N	25C35 161N	77.99	163N	25C35 162C	15.86
160C	25C35 162CA	67.69	160C	25C35 161N	15.98
160C	25C35 162C	72.94	25SG	25C35 162CA	55.42
25SG	25C35 162C	57.22	162CA	25C35 161N	53.66
162CA	25C35 162C	18.43	161N	25C35 162C	62.17
66O	25C36 163CB	99.95	66O	25C36 66C	0.80
66O	25C36 25SG	91.26	66O	25C36 68SD	70.79
66O	25C36 26CB	44.37	163CB	25C36 163N	35.50
163CB	25C36 163CA	19.65	163CB	25C36 134CB	72.59
163CB	25C36 162C	49.56	163CB	25C36 25SG	58.45
163CB	25C36 68SD	45.87	163CB	25C36 162N	79.29
163CB	25C36 161C	92.40	163CB	25C36 26CB	57.89
163N	25C36 163CA	19.24	163N	25C36 134CB	72.07
163N	25C36 162C	15.66	163N	25C36 25SG	48.74
163N	25C36 160O	94.75	163N	25C36 68SD	80.23
163N	25C36 162N	44.07	163N	25C36 161C	56.92
163N	25C36 26CB	84.19	163CA	25C36 134CB	63.35
163CA	25C36 162C	30.81	163CA	25C36 25SG	59.31

TABLE XIV

163CA	25C36	68SD	61.48	163CA	25C36	162N	60.75
163CA	25C36	161C	74.90	163CA	25C36	26CB	76.21
134CB	25C36	162C	66.02	134CB	25C36	160O	71.49
134CB	25C36	68SD	70.15	134CB	25C36	162N	74.57
134CB	25C36	161C	86.37	162C	25C36	25SG	57.47
162C	25C36	160O	79.13	162C	25C36	68SD	91.74
162C	25C36	162N	29.94	162C	25C36	161C	44.33
162C	25C36	26CB	99.68	66C	25C36	25SG	91.85
66C	25C36	68SD	71.28	66C	25C36	26CB	45.17
25SG	25C36	68SD	94.27	25SG	25C36	162N	65.87
25SG	25C36	161C	65.98	25SG	25C36	26CB	58.75
160O	25C36	162N	52.97	160O	25C36	161C	46.61
68SD	25C36	26CB	51.40	162N	25C36	161C	15.56
66O	25C37	67CD1	72.85	66O	25C37	67CE1	84.55
66O	25C37	66C	7.48	66O	25C37	67CG	55.90
66O	25C37	67CZ	77.27	66O	25C37	67CA	36.66
66O	25C37	68SD	75.55	66O	25C37	163CB	87.96
66O	25C37	68CE	96.44	66O	25C37	67N	20.80
67CD1	25C37	67CE1	21.00	67CD1	25C37	209CD2	54.83
67CD1	25C37	66C	65.41	67CD1	25C37	67CG	16.96
67CD1	25C37	67CZ	32.06	67CD1	25C37	67CA	45.91
67CD1	25C37	68SD	86.51	67CD1	25C37	68CE	88.92
67CD1	25C37	67N	53.96	67CE1	25C37	209CD2	57.96
67CE1	25C37	66C	77.24	67CE1	25C37	67CG	32.77
67CE1	25C37	67CZ	16.58	67CE1	25C37	67CA	64.93
67CE1	25C37	67N	69.10	209CD2	25C37	134CB	54.20
209CD2	25C37	67CG	69.67	209CD2	25C37	67CZ	74.22
209CD2	25C37	67CA	82.39	209CD2	25C37	68SD	72.35
209CD2	25C37	68CE	57.34	209CD2	25C37	67N	98.27
209CD2	25C37	160O	99.57	66C	25C37	67CG	48.46
66C	25C37	67CZ	70.63	66C	25C37	67CA	31.49
66C	25C37	68SD	76.55	66C	25C37	163CB	93.59
66C	25C37	68CE	96.76	66C	25C37	67N	14.69
134CB	25C37	68SD	73.29	134CB	25C37	163CB	66.42
134CB	25C37	68CE	52.90	134CB	25C37	160O	70.87
67CG	25C37	67CZ	36.23	67CG	25C37	67CA	32.41
67CG	25C37	68SD	83.13	67CG	25C37	68CE	91.57
67CG	25C37	67N	37.47	67CZ	25C37	67CA	67.51
67CZ	25C37	67N	66.38	67CZ	25C37	160O	95.75
67CA	25C37	68SD	57.53	67CA	25C37	163CB	92.22
67CA	25C37	68CE	73.28	67CA	25C37	67N	17.05
68SD	25C37	163CB	43.37	68SD	25C37	68CE	21.25

TABLE XIV

68SD	25C37	67N	68.73	163CB	25C37	68CE	46.72
163CB	25C37	67N	95.05	68CE	25C37	67N	87.13
66O	25C38	26CB	65.13	66O	25C38	66C	6.46
66O	25C38	26CA	86.69	66O	25C38	26N	98.55
66O	25C38	68SD	86.25	66O	25C38	26CG	59.16
66O	25C38	26CD1	64.07	66O	25C38	66N	34.26
66O	25C38	67CA	29.20	66O	25C38	67N	14.41
66O	25C38	66CA	18.99	163CB	25C38	26CB	81.15
163CB	25C38	25SG	73.30	163CB	25C38	163N	37.84
163CB	25C38	26CA	60.80	163CB	25C38	26N	60.85
163CB	25C38	163CA	18.86	163CB	25C38	68SD	54.22
163CB	25C38	26CG	95.41	163CB	25C38	162C	48.20
26CB	25C38	25SG	80.09	26CB	25C38	66C	58.81
26CB	25C38	26CA	21.77	26CB	25C38	26N	35.93
26CB	25C38	163CA	98.31	26CB	25C38	68SD	66.22
26CB	25C38	26CG	18.06	26CB	25C38	26CD1	34.61
26CB	25C38	66N	65.47	26CB	25C38	67CA	61.54
26CB	25C38	67N	56.77	26CB	25C38	66CA	58.47
25SG	25C38	163N	55.98	25SG	25C38	26CA	68.25
25SG	25C38	26N	47.87	25SG	25C38	163CA	68.75
25SG	25C38	26CG	73.64	25SG	25C38	26CD1	61.85
25SG	25C38	66N	91.11	25SG	25C38	162C	60.63
163N	25C38	26CA	87.46	163N	25C38	26N	76.37
163N	25C38	163CA	20.53	163N	25C38	68SD	89.44
163N	25C38	162C	12.27	66C	25C38	26CA	80.45
66C	25C38	26N	92.09	66C	25C38	68SD	84.88
66C	25C38	26CG	52.75	66C	25C38	26CD1	58.32
66C	25C38	66N	32.59	66C	25C38	67CA	29.60
66C	25C38	67N	12.87	66C	25C38	66CA	15.91
26CA	25C38	26N	20.39	26CA	25C38	163CA	77.00
26CA	25C38	68SD	62.23	26CA	25C38	26CG	34.72
26CA	25C38	26CD1	45.79	26CA	25C38	66N	84.74
26CA	25C38	67CA	78.68	26CA	25C38	67N	77.24
26CA	25C38	66CA	79.85	26CA	25C38	162C	99.66
26N	25C38	163CA	72.27	26N	25C38	68SD	79.71
26N	25C38	26CG	39.78	26N	25C38	26CD1	42.14
26N	25C38	66N	85.55	26N	25C38	67CA	97.07
26N	25C38	67N	92.29	26N	25C38	66CA	86.55
26N	25C38	162C	87.67	163CA	25C38	68SD	68.96
163CA	25C38	162C	29.60	68SD	25C38	26CG	83.61
68SD	25C38	67CA	57.57	68SD	25C38	67N	72.28
68SD	25C38	66CA	98.54	68SD	25C38	162C	96.25

TABLE XIV

26CG	25C38	26CD1	17.49	26CG	25C38	66N	50.02
26CG	25C38	67CA	65.74	26CG	25C38	67N	55.48
26CG	25C38	66CA	47.14	26CD1	25C38	66N	43.47
26CD1	25C38	67CA	78.32	26CD1	25C38	67N	64.92
26CD1	25C38	66CA	47.51	66N	25C38	67CA	62.18
66N	25C38	67N	45.30	66N	25C38	66CA	17.02
67CA	25C38	67N	17.03	67CA	25C38	66CA	45.35
67N	25C38	66CA	28.38	65CA	25C39	66N	38.23
65CA	25C39	66O	77.80	65CA	25C39	65C	20.22
65CA	25C39	26CD1	57.59	65CA	25C39	65N	12.86
65CA	25C39	23O	51.79	65CA	25C39	66CA	49.23
25SG	25C39	161O	71.00	25SG	25C39	26CD1	64.51
25SG	25C39	161C	75.18	25SG	25C39	23O	59.23
66N	25C39	66O	39.58	66N	25C39	65C	18.09
66N	25C39	26CD1	47.02	66N	25C39	65N	50.53
66N	25C39	23O	71.29	66N	25C39	66CA	11.02
66O	25C39	65C	57.60	66O	25C39	26CD1	57.39
66O	25C39	65N	89.89	66O	25C39	23O	96.66
66O	25C39	66CA	28.57	161O	25C39	161C	12.79
65C	25C39	26CD1	48.36	65C	25C39	65N	32.45
65C	25C39	23O	59.69	65C	25C39	66CA	29.05
26CD1	25C39	65N	60.85	26CD1	25C39	23O	40.56
26CD1	25C39	66CA	47.30	65N	25C39	23O	44.53
65N	25C39	66CA	61.43	23O	25C39	66CA	77.82
66N	25O40	65CA	49.46	66N	25O40	26CD1	65.76
66N	25O40	65C	23.27	66N	25O40	66O	49.28
66N	25O40	66CA	14.40	66N	25O40	26CG	63.42
66N	25O40	65N	61.07	66N	25O40	26NE1	58.78
66N	25O40	66C	34.93	66N	25O40	23O	92.25
66N	25O40	26CB	74.00	66N	25O40	65O	24.57
65CA	25O40	26CD1	79.08	65CA	25O40	65C	27.14
65CA	25O40	66O	98.43	65CA	25O40	66CA	63.57
65CA	25O40	26CG	90.14	65CA	25O40	65N	13.53
65CA	25O40	26NE1	63.17	65CA	25O40	66C	84.39
65CA	25O40	23O	63.91	65CA	25O40	65O	28.53
26CD1	25O40	65C	65.35	26CD1	25O40	25SG	80.06
26CD1	25O40	66O	75.51	26CD1	25O40	66CA	61.87
26CD1	25O40	26CG	17.43	26CD1	25O40	65N	76.84
26CD1	25O40	26NE1	16.20	26CD1	25O40	66C	66.92
26CD1	25O40	23O	50.44	26CD1	25O40	26CB	36.73
26CD1	25O40	65O	60.57	26CD1	25O40	26N	42.40
65C	25O40	66O	72.49	65C	25O40	66CA	36.77

TABLE XIV

65C	25O40	26CG	70.55	65C	25O40	65N	37.88
65C	25O40	26NE1	52.57	65C	25O40	66C	57.85
65C	25O40	23O	74.40	65C	25O40	26CB	86.99
65C	25O40	65O	4.93	25SG	25O40	26CG	82.32
25SG	25O40	26NE1	89.52	25SG	25O40	23O	68.61
25SG	25O40	26CB	75.26	25SG	25O40	26N	44.90
66O	25O40	66CA	36.06	66O	25O40	26CG	60.15
66O	25O40	26NE1	82.09	66O	25O40	66C	15.20
66O	25O40	26CB	51.97	66O	25O40	65O	73.07
66O	25O40	26N	81.84	66CA	25O40	26CG	55.19
66CA	25O40	65N	74.60	66CA	25O40	26NE1	59.26
66CA	25O40	66C	21.11	66CA	25O40	23O	98.28
66CA	25O40	26CB	62.10	66CA	25O40	65O	37.02
66CA	25O40	26N	91.86	26CG	25O40	65N	90.75
26CG	25O40	26NE1	31.46	26CG	25O40	66C	54.19
26CG	25O40	23O	67.47	26CG	25O40	26CB	20.67
26CG	25O40	65O	66.40	26CG	25O40	26N	38.44
65N	25O40	26NE1	60.66	65N	25O40	66C	95.71
65N	25O40	23O	52.18	65N	25O40	65O	37.84
26NE1	25O40	66C	70.37	26NE1	25O40	23O	42.57
26NE1	25O40	26CB	51.93	26NE1	25O40	65O	47.64
26NE1	25O40	26N	57.31	66C	25O40	26CB	52.36
66C	25O40	65O	58.10	66C	25O40	26N	83.81
23O	25O40	26CB	83.39	23O	25O40	65O	70.59
23O	25O40	26N	67.33	26CB	25O40	65O	83.51
26CB	25O40	26N	31.46	25SG	25N41	161O	86.79
25SG	25N41	161C	87.19	25SG	25N41	23O	62.77
25SG	25N41	66N	93.69	161O	25N41	161C	11.62
65CA	25N41	23O	51.79	65CA	25N41	65N	15.59
65CA	25N41	66N	29.14	23O	25N41	65N	44.44
23O	25N41	66N	64.51	65N	25N41	66N	44.25
25SG	25N42	23O	85.08	25SG	25N42	23CA	98.91
25SG	25N42	23C	83.87	25SG	25N42	161O	78.66
25SG	25N42	25CB	15.26	25SG	25N42	25N	39.74
25SG	25N42	26CD1	63.71	25SG	25N42	24N	72.85
23O	25N42	23CA	37.86	23O	25N42	23C	18.24
23O	25N42	65CA	60.94	23O	25N42	25CB	79.36
23O	25N42	65N	52.05	23O	25N42	25N	48.33
23O	25N42	26CD1	43.36	23O	25N42	24N	25.15
23CA	25N42	23C	22.71	23CA	25N42	65CA	87.12
23CA	25N42	25CB	85.89	23CA	25N42	65N	70.74
23CA	25N42	25N	60.69	23CA	25N42	26CD1	80.64

TABLE XIV

23CA	25N42	24N	29.02	23C	25N42	65CA	77.61
23C	25N42	25CB	74.03	23C	25N42	65N	65.78
23C	25N42	25N	44.16	23C	25N42	26CD1	58.52
23C	25N42	24N	11.74	65CA	25N42	65N	18.58
65CA	25N42	25N	98.97	65CA	25N42	26CD1	51.99
65CA	25N42	24N	86.08	161O	25N42	25CB	84.39
25CB	25N42	25N	31.12	25CB	25N42	26CD1	68.91
25CB	25N42	24N	62.41	65N	25N42	25N	97.62
65N	25N42	26CD1	59.56	65N	25N42	24N	76.12
25N	25N42	26CD1	50.78	25N	25N42	24N	33.18
26CD1	25N42	24N	57.77	66O	25N43	66N	50.46
66O	25N43	66C	15.63	66O	25N43	66CA	35.78
66O	25N43	65CA	83.97	66O	25N43	65C	66.03
66O	25N43	67CZ	75.44	66O	25N43	67CE2	67.55
66O	25N43	67CE1	68.04	66O	25N43	67N	16.30
66N	25N43	66C	39.54	66N	25N43	66CA	19.49
66N	25N43	65CA	35.70	66N	25N43	65C	15.67
66N	25N43	67CE2	84.94	66N	25N43	67N	47.36
66C	25N43	66CA	21.89	66C	25N43	65CA	75.04
66C	25N43	65C	55.08	66C	25N43	67CZ	72.67
66C	25N43	67CE2	61.03	66C	25N43	67CE1	69.65
66C	25N43	67N	8.63	66CA	25N43	65CA	54.94
66CA	25N43	65C	34.13	66CA	25N43	67CZ	83.41
66CA	25N43	67CE2	68.23	66CA	25N43	67CE1	85.39
66CA	25N43	67N	28.69	65CA	25N43	65C	21.08
65CA	25N43	67N	83.04	65C	25N43	67CE2	93.39
65C	25N43	67N	62.65	67CZ	25N43	67CE2	16.72
67CZ	25N43	67CE1	16.22	67CZ	25N43	67N	64.53
67CE2	25N43	67CE1	28.45	67CE2	25N43	67N	53.83
67CE1	25N43	67N	61.03				

TABLE XV

Table of angles between atoms of the inhibitor and protein for all protein atoms within 5 Ångstroms of the inhibitor 2-[N-(3-benzyloxybenzoyl)]-2'-[N'-(N-benzyloxycarbonyl-L-leucinyl)]carbohydrazide.

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
184CD1	25C1	184CB	39.64	184CD1	25C1	184CG	20.72
184CD1	25C1	184O	79.67	184CD1	25C1	18OD1	92.08
184CD1	25C1	184CA	45.35	184CD1	25C1	184C	65.97
184CD1	25C1	18CG	95.35	184CD1	25C1	20O	95.11
184CD1	25C1	184NE1	15.46	184CD1	25C1	184CD2	28.37
184CB	25C1	184CG	22.78	184CB	25C1	184O	43.71
184CB	25C1	18OD1	91.44	184CB	25C1	184CA	22.80
184CB	25C1	18ND2	86.39	184CB	25C1	184C	35.31
184CB	25C1	18CG	84.04	184CB	25C1	184NE1	51.55
184CB	25C1	184CD2	34.26	184CG	25C1	184O	66.36
184CG	25C1	184CA	38.32	184CG	25C1	184C	56.18
184CG	25C1	18CG	98.73	184CG	25C1	184NE1	29.35
184CG	25C1	184CD2	15.76	184O	25C1	18OD1	69.22
184O	25C1	184CA	35.76	184O	25C1	18ND2	48.03
184O	25C1	184C	16.21	184O	25C1	18CG	54.71
184O	25C1	184NE1	93.86	184O	25C1	184CD2	77.07
18OD1	25C1	184CA	68.65	18OD1	25C1	18ND2	32.37
18OD1	25C1	184C	63.21	18OD1	25C1	18CG	16.11
18OD1	25C1	20O	62.46	184CA	25C1	18ND2	67.26
184CA	25C1	184C	20.72	184CA	25C1	18CG	62.00
184CA	25C1	184NE1	60.54	184CA	25C1	184CD2	53.33
18ND2	25C1	184C	51.16	18ND2	25C1	18CG	17.75
18ND2	25C1	20O	89.83	184C	25C1	18CG	51.58
184C	25C1	184NE1	80.98	184C	25C1	184CD2	69.47
18CG	25C1	20O	77.96	20O	25C1	184NE1	90.38
184NE1	25C1	184CD2	28.12	18OD1	25C2	184CA	82.66
18OD1	25C2	20O	82.02	18OD1	25C2	18CG	17.46
18OD1	25C2	20N	42.19	18OD1	25C2	18ND2	35.11
18OD1	25C2	184O	74.48	18OD1	25C2	19CG	79.73

TABLE XV

18OD1	25C2	184C	70.99	18OD1	25C2	183O	67.05
18OD1	25C2	20CA	48.76	18OD1	25C2	20C	68.51
18OD1	25C2	19N	41.49	18OD1	25C2	184N	80.79
18OD1	25C2	19C	47.40	18OD1	25C2	183C	74.42
18OD1	25C2	18CB	20.67	184CD1	25C2	184CA	49.69
184CD1	25C2	184CG	20.47	184CD1	25C2	184CB	40.02
184CD1	25C2	184O	80.18	184CD1	25C2	19CG	63.56
184CD1	25C2	184C	69.76	184CD1	25C2	184NE1	15.99
184CD1	25C2	183O	53.74	184CD1	25C2	19N	85.37
184CD1	25C2	184N	44.38	184CD1	25C2	184CD2	23.21
184CD1	25C2	183C	46.49	184CA	25C2	18CG	70.97
184CA	25C2	184CG	39.55	184CA	25C2	18ND2	72.06
184CA	25C2	184CB	22.96	184CA	25C2	184O	35.00
184CA	25C2	19CG	83.11	184CA	25C2	184C	20.65
184CA	25C2	184NE1	65.57	184CA	25C2	183O	40.23
184CA	25C2	19N	70.98	184CA	25C2	184N	13.04
184CA	25C2	184CD2	51.91	184CA	25C2	183C	28.28
184CA	25C2	18CB	62.55	20O	25C2	18CG	98.28
20O	25C2	20N	45.78	20O	25C2	19CG	69.54
20O	25C2	20CA	33.26	20O	25C2	20C	13.52
20O	25C2	19N	80.94	20O	25C2	241OH2	94.87
20O	25C2	19C	50.12	18CG	25C2	20N	59.60
18CG	25C2	18ND2	19.96	18CG	25C2	184CB	91.12
18CG	25C2	184O	57.44	18CG	25C2	19CG	91.35
18CG	25C2	184C	56.05	18CG	25C2	183O	66.77
18CG	25C2	20CA	65.32	18CG	25C2	20C	84.82
18CG	25C2	19N	51.19	18CG	25C2	184N	72.42
18CG	25C2	19C	64.04	18CG	25C2	183C	70.48
18CG	25C2	18CB	11.35	184CG	25C2	184CB	22.17
184CG	25C2	184O	63.20	184CG	25C2	19CG	82.47
184CG	25C2	184C	56.51	184CG	25C2	184NE1	31.65
184CG	25C2	183O	60.77	184CG	25C2	19N	95.86
184CG	25C2	184N	40.46	184CG	25C2	184CD2	12.76
184CG	25C2	183C	49.79	20N	25C2	18ND2	76.27
20N	25C2	19CG	52.54	20N	25C2	183O	72.94
20N	25C2	20CA	19.39	20N	25C2	20C	34.03
20N	25C2	19N	38.18	20N	25C2	184N	99.39

TABLE XV

20N	25C2	19C	11.58	20N	25C2	183C	85.38
20N	25C2	18CB	59.41	18ND2	25C2	184CB	87.16
18ND2	25C2	184O	47.43	18ND2	25C2	184C	52.81
18ND2	25C2	183O	80.93	18ND2	25C2	20CA	77.11
18ND2	25C2	20C	94.81	18ND2	25C2	19N	70.92
18ND2	25C2	184N	77.97	18ND2	25C2	241OH2	87.90
18ND2	25C2	19C	82.49	18ND2	25C2	183C	81.11
18ND2	25C2	18CB	28.59	184CB	25C2	184O	41.08
184CB	25C2	19CG	93.42	184CB	25C2	184C	35.36
184CB	25C2	184NE1	53.47	184CB	25C2	183O	58.06
184CB	25C2	19N	92.03	184CB	25C2	184N	30.81
184CB	25C2	241OH2	98.67	184CB	25C2	184CD2	32.23
184CB	25C2	183C	45.37	184CB	25C2	18CB	84.11
184O	25C2	184C	16.82	184O	25C2	184NE1	94.48
184O	25C2	183O	69.02	184O	25C2	19N	87.53
184O	25C2	184N	47.05	184O	25C2	241OH2	86.44
184O	25C2	184CD2	71.78	184O	25C2	183C	59.90
184O	25C2	18CB	55.54	19CG	25C2	184C	97.61
19CG	25C2	184NE1	62.79	19CG	25C2	183O	45.36
19CG	25C2	20CA	67.99	19CG	25C2	20C	68.52
19CG	25C2	19N	40.19	19CG	25C2	184N	70.06
19CG	25C2	19C	41.14	19CG	25C2	184CD2	86.47
19CG	25C2	183C	55.31	19CG	25C2	18CB	82.88
184C	25C2	184NE1	85.37	184C	25C2	183O	52.27
184C	25C2	19N	73.95	184C	25C2	184N	31.18
184C	25C2	184CD2	67.55	184C	25C2	183C	43.16
184C	25C2	18CB	50.40	184NE1	25C2	183O	65.82
184NE1	25C2	19N	93.08	184NE1	25C2	184N	60.22
184NE1	25C2	184CD2	27.19	184NE1	25C2	183C	60.67
183O	25C2	20CA	92.25	183O	25C2	19N	35.35
183O	25C2	184N	28.06	183O	25C2	19C	63.84
183O	25C2	184CD2	71.98	183O	25C2	183C	12.70
183O	25C2	18CB	55.43	20CA	25C2	20C	19.77
20CA	25C2	19N	57.18	20CA	25C2	19C	29.86
20CA	25C2	18CB	69.00	20C	25C2	19N	71.24
20C	25C2	241OH2	99.96	20C	25C2	19C	40.54
20C	25C2	18CB	88.76	19N	25C2	184N	61.22

TABLE XV

19N	25C2	19C	30.91	19N	25C2	183C	47.43
19N	25C2	18CB	42.94	184N	25C2	19C	91.32
184N	25C2	184CD2	53.18	184N	25C2	183C	15.60
184N	25C2	18CB	62.40	241OH2	25C2	184CD2	94.01
19C	25C2	183C	76.51	19C	25C2	18CB	61.35
184CD2	25C2	183C	61.73	183C	25C2	18CB	59.34
20O	25C3	19CG	91.80	20O	25C3	20N	53.46
20O	25C3	18OD1	84.67	20O	25C3	20C	13.71
20O	25C3	20CA	35.80	20O	25C3	19CD	97.07
20O	25C3	19C	58.10	20O	25C3	19N	89.89
20O	25C3	19CB	82.19	20O	25C3	18CG	93.78
20O	25C3	19CA	76.43	20O	25C3	19NE2	84.73
20O	25C3	21N	7.78	184CD1	25C3	19CG	71.43
184CD1	25C3	184NE1	19.86	184CD1	25C3	19CD	64.18
184CD1	25C3	184CG	15.82	184CD1	25C3	183O	49.75
184CD1	25C3	19N	83.17	184CD1	25C3	184CA	39.91
184CD1	25C3	19CB	82.78	184CD1	25C3	18CG	94.02
184CD1	25C3	19CA	92.64	184CD1	25C3	19NE2	76.30
184CD1	25C3	184CB	30.78	184CD1	25C3	19OE1	50.83
184CD1	25C3	184CE2	22.67	19CG	25C3	20N	61.01
19CG	25C3	18OD1	81.71	19CG	25C3	20C	85.09
19CG	25C3	184NE1	72.26	19CG	25C3	20CA	79.11
19CG	25C3	19CD	19.52	19CG	25C3	184CG	85.19
19CG	25C3	19C	46.68	19CG	25C3	183O	45.20
19CG	25C3	19N	40.95	19CG	25C3	184CA	79.09
19CG	25C3	19CB	14.28	19CG	25C3	18CG	86.69
19CG	25C3	19CA	32.54	19CG	25C3	19NE2	29.74
19CG	25C3	184CB	89.69	19CG	25C3	19OE1	27.37
19CG	25C3	21N	86.08	19CG	25C3	184CE2	83.99
20N	25C3	18OD1	41.77	20N	25C3	20C	39.98
20N	25C3	20CA	21.31	20N	25C3	19CD	78.54
20N	25C3	19C	14.86	20N	25C3	183O	71.47
20N	25C3	19N	37.66	20N	25C3	184CA	95.61
20N	25C3	19CB	46.74	20N	25C3	18CG	52.23
20N	25C3	19CA	30.40	20N	25C3	19NE2	78.92
20N	25C3	19OE1	88.38	20N	25C3	21N	45.77
18OD1	25C3	20C	71.90	18OD1	25C3	20CA	50.00

TABLE XV

18OD1	25C3	184CG	95.90	18OD1	25C3	19C	51.61
18OD1	25C3	183O	58.74	18OD1	25C3	19N	40.87
18OD1	25C3	184CA	63.14	18OD1	25C3	19CB	70.42
18OD1	25C3	18CG	10.53	18OD1	25C3	19CA	52.41
18OD1	25C3	184CB	79.52	18OD1	25C3	21N	78.64
20C	25C3	20CA	22.29	20C	25C3	19CD	94.40
20C	25C3	19C	46.10	20C	25C3	19N	77.00
20C	25C3	19CB	73.57	20C	25C3	18CG	81.47
20C	25C3	19CA	64.92	20C	25C3	19NE2	84.78
20C	25C3	21N	6.74	184NE1	25C3	19CD	58.87
184NE1	25C3	184CG	31.08	184NE1	25C3	183O	64.98
184NE1	25C3	19N	95.87	184NE1	25C3	184CA	59.73
184NE1	25C3	19CB	85.90	184NE1	25C3	19NE2	66.72
184NE1	25C3	184CB	48.57	184NE1	25C3	19OE1	46.24
184NE1	25C3	184CE2	11.83	20CA	25C3	19CD	94.19
20CA	25C3	19C	33.03	20CA	25C3	183O	92.18
20CA	25C3	19N	58.66	20CA	25C3	19CB	65.28
20CA	25C3	18CG	59.95	20CA	25C3	19CA	51.05
20CA	25C3	19NE2	90.04	20CA	25C3	21N	28.97
19CD	25C3	184CG	79.74	19CD	25C3	19C	63.74
19CD	25C3	183O	55.90	19CD	25C3	19N	60.04
19CD	25C3	184CA	84.73	19CD	25C3	19CB	32.93
19CD	25C3	19CA	51.74	19CD	25C3	19NE2	15.91
19CD	25C3	184CB	89.68	19CD	25C3	19OE1	13.39
19CD	25C3	21N	93.33	19CD	25C3	184CE2	70.59
184CG	25C3	183O	54.91	184CG	25C3	19N	88.52
184CG	25C3	184CA	32.83	184CG	25C3	19CB	95.04
184CG	25C3	18CG	87.10	184CG	25C3	19NE2	92.12
184CG	25C3	184CB	17.79	184CG	25C3	19OE1	66.46
184CG	25C3	184CE2	27.27	19C	25C3	183O	65.15
19C	25C3	19N	32.44	19C	25C3	184CA	94.94
19C	25C3	19CB	32.53	19C	25C3	18CG	61.42
19C	25C3	19CA	18.94	19C	25C3	19NE2	64.39
19C	25C3	19OE1	73.97	19C	25C3	21N	50.41
183O	25C3	19N	33.87	183O	25C3	184CA	35.08
183O	25C3	19CB	47.01	183O	25C3	18CG	56.73
183O	25C3	19CA	47.13	183O	25C3	19NE2	71.34

TABLE XV

183O	25C3	184CB	50.06	183O	25C3	19OE1	50.42
183O	25C3	184CE2	72.00	19N	25C3	184CA	62.75
19N	25C3	19CB	31.18	19N	25C3	18CG	46.02
19N	25C3	19CA	17.94	19N	25C3	19NE2	69.90
19N	25C3	184CB	80.68	19N	25C3	19OE1	63.48
19N	25C3	21N	82.11	184CA	25C3	19CB	82.09
184CA	25C3	18CG	54.80	184CA	25C3	19CA	79.48
184CA	25C3	184CB	18.58	184CA	25C3	19OE1	74.55
184CA	25C3	184CE2	59.43	19CB	25C3	18CG	76.90
19CB	25C3	19CA	18.91	19CB	25C3	19NE2	39.32
19CB	25C3	184CB	95.96	19CB	25C3	19OE1	41.65
19CB	25C3	21N	75.62	19CB	25C3	184CE2	97.49
18CG	25C3	19CA	59.97	18CG	25C3	184CB	70.15
18CG	25C3	21N	88.18	19CA	25C3	19NE2	57.54
19CA	25C3	184CB	96.61	19CA	25C3	19OE1	59.34
19CA	25C3	21N	68.88	19NE2	25C3	19OE1	26.89
19NE2	25C3	21N	82.33	19NE2	25C3	184CE2	77.62
184CB	25C3	19OE1	77.28	184CB	25C3	184CE2	44.87
19OE1	25C3	184CE2	58.06	20O	25C4	20C	5.29
20O	25C4	19CG	73.30	20O	25C4	20N	37.40
20O	25C4	20CA	22.70	20O	25C4	19CD	84.35
20O	25C4	18OD1	61.35	20O	25C4	19NE2	78.63
184CD1	25C4	184NE1	19.87	184CD1	25C4	19CG	58.10
184CD1	25C4	20N	90.23	184CD1	25C4	184CG	14.72
184CD1	25C4	19CD	55.97	184CD1	25C4	184CE2	27.01
184CD1	25C4	18OD1	75.63	184CD1	25C4	19NE2	69.64
184NE1	25C4	19CG	63.14	184NE1	25C4	184CG	28.26
184NE1	25C4	19CD	53.91	184NE1	25C4	184CE2	14.23
184NE1	25C4	18OD1	94.59	184NE1	25C4	19NE2	63.81
20C	25C4	19CG	69.98	20C	25C4	20N	32.25
20C	25C4	20CA	17.47	20C	25C4	19CD	82.18
20C	25C4	18OD1	56.22	20C	25C4	19NE2	77.77
19CG	25C4	20N	46.51	19CG	25C4	184CG	71.25
19CG	25C4	20CA	62.49	19CG	25C4	19CD	18.45
19CG	25C4	184CE2	77.31	19CG	25C4	18OD1	59.85
19CG	25C4	19NE2	29.19	20N	25C4	184CG	96.60
20N	25C4	20CA	17.63	20N	25C4	19CD	63.68

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TABLE XV

20N	25C4	18OD1	30.95	20N	25C4	19NE2	67.31
184CG	25C4	19CD	70.61	184CG	25C4	184CE2	27.62
184CG	25C4	18OD1	75.70	184CG	25C4	241OH2	87.84
184CG	25C4	19NE2	84.36	20CA	25C4	19CD	78.25
20CA	25C4	18OD1	38.85	20CA	25C4	241OH2	97.61
20CA	25C4	19NE2	78.54	19CD	25C4	184CE2	67.82
19CD	25C4	18OD1	78.00	19CD	25C4	19NE2	15.45
184CE2	25C4	241OH2	99.63	184CE2	25C4	19NE2	76.63
18OD1	25C4	241OH2	82.91	18OD1	25C4	19NE2	87.95
20O	25C5	184CD1	97.18	184CD1	25C5	184NE1	18.35
184CD1	25C5	184CG	16.64	184CD1	25C5	184CE2	27.73
184CD1	25C5	184CD2	26.39	184NE1	25C5	184CG	28.44
184NE1	25C5	184CE2	16.30	184NE1	25C5	184CD2	26.54
184CG	25C5	184CE2	27.87	184CG	25C5	184CD2	16.56
184CE2	25C5	184CD2	16.34	184CD1	25C6	184CG	18.54
184CD1	25C6	184CB	33.62	184CD1	25C6	184NE1	17.14
184CD1	25C6	20O	88.08	184CD1	25C6	184CD2	28.33
184CD1	25C6	184CE2	26.95	184CG	25C6	184CB	19.13
184CG	25C6	184NE1	29.00	184CG	25C6	184CD2	17.43
184CG	25C6	184CE2	27.74	184CB	25C6	184NE1	47.54
184CB	25C6	184CD2	32.76	184CB	25C6	184CE2	46.38
184NE1	25C6	20O	88.62	184NE1	25C6	184CD2	27.82
184NE1	25C6	184CE2	16.20	184CD2	25C6	184CE2	16.68
20O	25C7	20C	5.94	20O	25C7	19NE2	91.02
20O	25C7	19CG	72.12	20O	25C7	19CD	89.31
20O	25C7	21CA	34.14	20O	25C7	22O	65.12
20O	25C7	21N	17.69	20O	25C7	21C	46.47
20C	25C7	19NE2	86.13	20C	25C7	19CG	69.33
20C	25C7	19CD	85.63	20C	25C7	21CA	31.54
20C	25C7	22O	59.23	20C	25C7	21N	14.16
20C	25C7	21C	42.01	19NE2	25C7	19CG	32.17
19NE2	25C7	184NE1	66.44	19NE2	25C7	19CD	17.05
19NE2	25C7	21CA	93.37	19NE2	25C7	22O	37.10
19NE2	25C7	184CD1	69.09	19NE2	25C7	21N	87.99
19NE2	25C7	21C	79.11	19CG	25C7	184NE1	58.99
19CG	25C7	19CD	19.56	19CG	25C7	21CA	91.19
19CG	25C7	22O	50.36	19CG	25C7	184CD1	52.04

TABLE XV

19CG	25C7	21N	77.89	19CG	25C7	21C	84.98
184NE1	25C7	19CD	53.40	184NE1	25C7	184CD1	16.66
19CD	25C7	22O	49.22	19CD	25C7	184CD1	53.17
19CD	25C7	21N	91.50	19CD	25C7	21C	90.15
21CA	25C7	22O	56.87	21CA	25C7	21N	17.50
21CA	25C7	21C	18.03	22O	25C7	21N	55.41
22O	25C7	21C	42.02	21N	25C7	21C	28.94
19NE2	25O8	19CD	20.48	19NE2	25O8	184NE1	81.39
19NE2	25O8	20O	89.30	19NE2	25O8	19CG	35.60
19NE2	25O8	19OE1	30.68	19NE2	25O8	22O	40.85
19NE2	25O8	184CD1	79.20	19NE2	25O8	184CE2	92.69
19CD	25O8	184NE1	63.10	19CD	25O8	20O	86.55
19CD	25O8	19CG	21.39	19CD	25O8	19OE1	15.46
19CD	25O8	22O	55.33	19CD	25O8	184CD1	58.99
19CD	25O8	184CE2	75.44	184NE1	25O8	19CG	65.39
184NE1	25O8	19OE1	50.75	184NE1	25O8	184CD1	16.57
184NE1	25O8	184CE2	13.19	20O	25O8	19CG	66.59
20O	25O8	19OE1	99.26	20O	25O8	22O	62.20
20O	25O8	184CD1	90.68	19CG	25O8	19OE1	32.68
19CG	25O8	22O	53.93	19CG	25O8	184CD1	54.99
19CG	25O8	184CE2	78.58	19OE1	25O8	22O	69.68
19OE1	25O8	184CD1	50.54	19OE1	25O8	184CE2	62.13
184CD1	25O8	184CE2	26.99	19NE2	25C9	184NE1	68.02
19NE2	25C9	19CD	15.81	184NE1	25C9	19CD	52.53
162ND1	25C11	184CZ2	58.70	162ND1	25C11	162CE1	15.57
184CZ2	25C11	162CE1	49.86	162ND1	25C14	162CG	20.80
162ND1	25C14	162CB	38.90	162ND1	25C14	162CE1	17.70
162ND1	25C14	162CA	43.05	162ND1	25C14	161O	71.97
162ND1	25C14	184CZ2	66.72	162ND1	25C14	162CD2	25.28
162ND1	25C14	161OD1	87.80	162ND1	25C14	162N	60.63
162ND1	25C14	162NE2	23.20	162ND1	25C14	161C	71.88
162ND1	25C14	25SG	43.89	162CG	25C14	162CB	21.88
162CG	25C14	162CE1	32.41	162CG	25C14	162CA	35.32
162CG	25C14	161O	70.65	162CG	25C14	184CZ2	61.27
162CG	25C14	162CD2	14.29	162CG	25C14	161OD1	69.93
162CG	25C14	162N	50.52	162CG	25C14	162NE2	26.85
162CG	25C14	161C	65.13	162CG	25C14	25SG	60.65

TABLE XV

162CB	25C14	162CE1	53.68	162CB	25C14	162CA	20.45
162CB	25C14	161O	55.44	162CB	25C14	184CZ2	75.70
162CB	25C14	162CD2	33.63	162CB	25C14	161OD1	49.02
162CB	25C14	162N	30.67	162CB	25C14	162NE2	48.52
162CB	25C14	161C	46.38	162CB	25C14	25SG	66.67
162CE1	25C14	162CA	60.62	162CE1	25C14	161O	88.83
162CE1	25C14	184CZ2	55.07	162CE1	25C14	162CD2	27.92
162CE1	25C14	162N	78.11	162CE1	25C14	162NE2	14.38
162CE1	25C14	161C	89.56	162CE1	25C14	25SG	51.14
162CA	25C14	161O	35.99	162CA	25C14	184CZ2	94.99
162CA	25C14	162CD2	49.43	162CA	25C14	161OD1	50.42
162CA	25C14	162N	17.63	162CA	25C14	162NE2	60.81
162CA	25C14	161C	30.12	162CA	25C14	25SG	53.36
161O	25C14	162CD2	84.93	161O	25C14	161OD1	54.15
161O	25C14	162N	27.79	161O	25C14	162NE2	93.77
161O	25C14	161C	14.72	161O	25C14	25SG	53.31
184CZ2	25C14	162CD2	47.18	184CZ2	25C14	161OD1	98.34
184CZ2	25C14	162NE2	43.71	162CD2	25C14	161OD1	77.69
162CD2	25C14	162N	63.80	162CD2	25C14	162NE2	16.69
162CD2	25C14	161C	78.91	162CD2	25C14	25SG	69.06
161OD1	25C14	162N	36.11	161OD1	25C14	162NE2	94.34
161OD1	25C14	161C	39.94	162N	25C14	162NE2	77.07
162N	25C14	161C	15.92	162N	25C14	25SG	64.86
162NE2	25C14	161C	90.92	162NE2	25C14	25SG	64.04
161C	25C14	25SG	63.90	162CB	25O15	162ND1	47.26
162CB	25O15	162CG	27.43	162CB	25O15	161OD1	63.34
162CB	25O15	162CA	23.06	162CB	25O15	162CE1	60.10
162CB	25O15	162CD2	40.37	162CB	25O15	162N	35.92
162CB	25O15	184CZ2	91.76	162CB	25O15	162NE2	55.17
162CB	25O15	161C	52.53	162CB	25O15	161O	60.45
162CB	25O15	137CB	54.06	162CB	25O15	161CG	69.17
162CB	25O15	137O	87.23	162CB	25O15	161CB	73.81
162CB	25O15	184CH2	88.25	162ND1	25O15	162CG	25.12
162ND1	25O15	162CA	49.83	162ND1	25O15	162CE1	16.98
162ND1	25O15	162CD2	32.89	162ND1	25O15	162N	70.32
162ND1	25O15	184CZ2	74.09	162ND1	25O15	162NE2	26.96
162ND1	25O15	161C	78.97	162ND1	25O15	161O	74.28

TABLE XV

162ND1	25O15	137CB	88.45	162ND1	25O15	184CH2	81.61
162CG	25O15	161OD1	90.25	162CG	25O15	162CA	41.57
162CG	25O15	162CE1	33.66	162CG	25O15	162CD2	17.25
162CG	25O15	162N	60.35	162CG	25O15	184CZ2	70.97
162CG	25O15	162NE2	28.08	162CG	25O15	161C	74.63
162CG	25O15	161O	77.02	162CG	25O15	137CB	63.77
162CG	25O15	161CG	96.60	162CG	25O15	137O	97.22
162CG	25O15	184CH2	72.59	161OD1	25O15	162CA	61.62
161OD1	25O15	162CD2	98.29	161OD1	25O15	162N	43.32
161OD1	25O15	161C	45.80	161OD1	25O15	161O	60.74
161OD1	25O15	137CB	55.90	161OD1	25O15	161CG	11.21
161OD1	25O15	137O	59.03	161OD1	25O15	161CB	28.61
162CA	25O15	162CE1	66.36	162CA	25O15	162CD2	58.17
162CA	25O15	162N	20.56	162CA	25O15	162NE2	68.37
162CA	25O15	161C	33.06	162CA	25O15	161O	37.86
162CA	25O15	137CB	73.81	162CA	25O15	161CG	62.82
162CA	25O15	161CB	60.45	162CE1	25O15	162CD2	31.95
162CE1	25O15	162N	86.92	162CE1	25O15	184CZ2	59.12
162CE1	25O15	162NE2	17.11	162CE1	25O15	161C	95.94
162CE1	25O15	161O	90.42	162CE1	25O15	137CB	90.07
162CE1	25O15	184CH2	68.68	162CD2	25O15	162N	75.70
162CD2	25O15	184CZ2	53.94	162CD2	25O15	162NE2	17.99
162CD2	25O15	161C	91.05	162CD2	25O15	161O	94.26
162CD2	25O15	137CB	58.26	162CD2	25O15	137O	88.29
162CD2	25O15	184CH2	55.47	162N	25O15	162NE2	88.07
162N	25O15	161C	17.35	162N	25O15	161O	30.00
162N	25O15	137CB	72.58	162N	25O15	161CG	42.77
162N	25O15	137O	95.02	162N	25O15	161CB	40.21
184CZ2	25O15	162NE2	47.88	184CZ2	25O15	137CB	69.04
184CZ2	25O15	137O	71.73	184CZ2	25O15	184CH2	14.31
162NE2	25O15	161O	99.69	162NE2	25O15	137CB	74.12
162NE2	25O15	184CH2	54.65	161C	25O15	161O	15.92
161C	25O15	137CB	87.40	161C	25O15	161CG	40.49
161C	25O15	161CB	30.37	161O	25O15	161CG	53.91
161O	25O15	161CB	39.98	137CB	25O15	161CG	67.10
137CB	25O15	137O	34.26	137CB	25O15	161CB	84.07
137CB	25O15	184CH2	56.32	161CG	25O15	137O	67.49

TABLE XV

161CG	25O15	161CB	17.89	137O	25O15	161CB	84.60
137O	25O15	184CH2	57.69	162ND1	25N16	25SG	57.00
162ND1	25N16	161O	81.16	162ND1	25N16	162CE1	17.28
162ND1	25N16	162CG	17.24	162ND1	25N16	162CA	44.41
162ND1	25N16	162CB	35.55	162ND1	25N16	161C	76.08
162ND1	25N16	25CB	47.59	162ND1	25N16	162N	61.35
162ND1	25N16	19NE2	78.00	25SG	25N16	161O	66.73
25SG	25N16	162CE1	60.44	25SG	25N16	162CG	69.41
25SG	25N16	162CA	62.55	25SG	25N16	162CB	74.95
25SG	25N16	161C	75.51	25SG	25N16	25CB	22.32
25SG	25N16	162N	74.12	25SG	25N16	19NE2	65.05
161O	25N16	162CE1	97.79	161O	25N16	162CG	74.22
161O	25N16	162CA	38.96	161O	25N16	162CB	57.51
161O	25N16	161C	14.31	161O	25N16	25CB	86.73
161O	25N16	162N	28.02	162CE1	25N16	162CG	31.36
162CE1	25N16	162CA	61.69	162CE1	25N16	162CB	51.34
162CE1	25N16	161C	93.35	162CE1	25N16	25CB	44.14
162CE1	25N16	162N	78.58	162CE1	25N16	19NE2	62.97
162CG	25N16	162CA	35.27	162CG	25N16	162CB	20.22
162CG	25N16	161C	65.76	162CG	25N16	25CB	63.85
162CG	25N16	162N	49.75	162CG	25N16	19NE2	94.18
162CA	25N16	162CB	20.52	162CA	25N16	161C	31.69
162CA	25N16	25CB	71.57	162CA	25N16	162N	17.61
162CB	25N16	161C	47.01	162CB	25N16	25CB	76.68
162CB	25N16	162N	30.74	161C	25N16	25CB	92.93
161C	25N16	162N	16.27	25CB	25N16	162N	87.03
25CB	25N16	19NE2	47.50	25SG	25N17	162ND1	74.24
25SG	25N17	162CA	87.90	25SG	25N17	162CG	86.46
25SG	25N17	162CB	97.30	25SG	25N17	25CB	24.15
25SG	25N17	162CE1	70.19	25SG	25N17	163N	54.13
25SG	25N17	162C	71.67	25SG	25N17	162CD2	84.79
161O	25N17	162CA	52.13	161O	25N17	161C	16.50
161O	25N17	162CG	92.62	161O	25N17	162CB	71.30
161O	25N17	162N	34.71	161O	25N17	163N	65.25
161O	25N17	162C	55.77	161O	25N17	161CA	17.53
162ND1	25N17	162CA	56.42	162ND1	25N17	161C	95.91
162ND1	25N17	162CG	18.78	162ND1	25N17	162CB	41.07

TABLE XV

162ND1	25N17	162N	76.00	162ND1	25N17	25CB	57.57
162ND1	25N17	162CE1	14.79	162ND1	25N17	163N	54.56
162ND1	25N17	162C	55.20	162ND1	25N17	162CD2	12.12
162CA	25N17	161C	40.29	162CA	25N17	162CG	41.09
162CA	25N17	162CB	23.23	162CA	25N17	162N	21.53
162CA	25N17	25CB	91.56	162CA	25N17	162CE1	71.02
162CA	25N17	163N	33.82	162CA	25N17	162C	16.39
162CA	25N17	161CA	50.27	162CA	25N17	162CD2	49.51
161C	25N17	162CG	78.57	161C	25N17	162CB	56.40
161C	25N17	162N	19.96	161C	25N17	163N	62.31
161C	25N17	162C	48.62	161C	25N17	161CA	10.96
161C	25N17	162CD2	87.05	162CG	25N17	162CB	22.57
162CG	25N17	162N	58.64	162CG	25N17	25CB	73.95
162CG	25N17	162CE1	33.00	162CG	25N17	163N	51.02
162CG	25N17	162C	44.96	162CG	25N17	161CA	86.42
162CG	25N17	162CD2	8.55	162CB	25N17	162N	36.69
162CB	25N17	25CB	91.50	162CB	25N17	162CE1	55.54
162CB	25N17	163N	48.31	162CB	25N17	162C	34.62
162CB	25N17	161CA	63.87	162CB	25N17	162CD2	30.83
162N	25N17	162CE1	90.79	162N	25N17	163N	50.48
162N	25N17	162C	33.85	162N	25N17	161CA	29.03
162N	25N17	162CD2	67.15	25CB	25N17	162CE1	49.52
25CB	25N17	163N	61.60	25CB	25N17	162C	77.64
25CB	25N17	162CD2	69.50	162CE1	25N17	163N	64.51
162CE1	25N17	162C	68.30	162CE1	25N17	162CD2	25.14
163N	25N17	162C	17.55	163N	25N17	161CA	73.19
163N	25N17	162CD2	56.08	162C	25N17	161CA	59.51
162C	25N17	162CD2	52.20	161CA	25N17	162CD2	94.68
184NE1	25C18	19NE2	72.19	184NE1	25C18	184CZ2	34.15
184NE1	25C18	162ND1	64.76	184NE1	25C18	162CE1	49.26
184NE1	25C18	19CD	55.65	184NE1	25C18	19OE1	48.22
184NE1	25C18	184CE2	16.77	19NE2	25C18	162ND1	74.92
19NE2	25C18	162CE1	65.60	19NE2	25C18	19CD	16.66
19NE2	25C18	19OE1	29.19	19NE2	25C18	184CE2	88.46
184CZ2	25C18	162ND1	61.13	184CZ2	25C18	162CE1	54.08
184CZ2	25C18	19CD	87.16	184CZ2	25C18	19OE1	75.81
184CZ2	25C18	184CE2	17.74	162ND1	25C18	162CE1	17.06

TABLE XV

162ND1	25C18	19CD	67.56	162ND1	25C18	19OE1	52.95
162ND1	25C18	184CE2	64.20	162CE1	25C18	19CD	54.80
162CE1	25C18	19OE1	39.41	162CE1	25C18	184CE2	52.06
19CD	25C18	19OE1	15.45	19CD	25C18	184CE2	71.81
19OE1	25C18	184CE2	62.64	25SG	25C19	25CB	30.92
25SG	25C19	161O	96.60	25SG	25C19	162ND1	68.37
25SG	25C19	25N	49.94	25SG	25C19	25CA	32.83
25SG	25C19	23O	90.89	25SG	25C19	162CE1	65.52
25SG	25C19	162CA	73.52	25SG	25C19	19NE2	86.96
25SG	25C19	23C	92.63	25SG	25C19	163N	42.91
25SG	25C19	161C	94.64	25SG	25C19	162CG	71.57
25SG	25C19	19OE1	68.21	25SG	25C19	25C	20.12
25SG	25C19	26N	28.60	25CB	25C19	162ND1	59.73
25CB	25C19	25N	36.66	25CB	25C19	25CA	17.74
25CB	25C19	23O	86.02	25CB	25C19	162CE1	48.75
25CB	25C19	162CA	86.55	25CB	25C19	19NE2	56.95
25CB	25C19	23C	79.82	25CB	25C19	163N	62.99
25CB	25C19	23CA	90.53	25CB	25C19	162CG	68.32
25CB	25C19	19OE1	37.70	25CB	25C19	25C	26.97
25CB	25C19	26N	42.42	161O	25C19	162ND1	80.02
161O	25C19	162CE1	96.21	161O	25C19	162CA	38.78
161O	25C19	163N	57.58	161O	25C19	161C	9.12
161O	25C19	162CG	68.74	162ND1	25C19	25N	95.15
162ND1	25C19	25CA	77.47	162ND1	25C19	162CE1	16.21
162ND1	25C19	162CA	42.69	162ND1	25C19	19NE2	79.46
162ND1	25C19	163N	49.40	162ND1	25C19	161C	71.09
162ND1	25C19	162CG	11.30	162ND1	25C19	19OE1	54.54
162ND1	25C19	25C	81.37	162ND1	25C19	26N	95.47
25N	25C19	25CA	20.26	25N	25C19	23O	49.36
25N	25C19	162CE1	81.63	25N	25C19	19NE2	50.17
25N	25C19	23C	44.73	25N	25C19	163N	92.43
25N	25C19	23CA	59.48	25N	25C19	19OE1	52.21
25N	25C19	25C	30.33	25N	25C19	26N	33.58
25CA	25C19	23O	69.09	25CA	25C19	162CE1	66.04
25CA	25C19	19NE2	56.58	25CA	25C19	23C	64.91
25CA	25C19	163N	73.45	25CA	25C19	23CA	78.58
25CA	25C19	162CG	85.89	25CA	25C19	19OE1	46.47

TABLE XV

25CA	25C19	25C	17.28	25CA	25C19	26N	29.70
23O	25C19	19NE2	67.81	23O	25C19	23C	15.74
23O	25C19	23CA	30.61	23O	25C19	19OE1	88.93
23O	25C19	25C	71.99	23O	25C19	26N	63.05
162CE1	25C19	162CA	58.48	162CE1	25C19	19NE2	63.81
162CE1	25C19	163N	59.21	162CE1	25C19	161C	87.29
162CE1	25C19	162CG	27.50	162CE1	25C19	19OE1	38.34
162CE1	25C19	25C	73.76	162CE1	25C19	26N	89.08
162CA	25C19	163N	31.32	162CA	25C19	161C	30.71
162CA	25C19	162CG	31.93	162CA	25C19	19OE1	96.39
162CA	25C19	25C	93.49	162CA	25C19	26N	99.54
19NE2	25C19	23C	52.36	19NE2	25C19	23CA	47.51
19NE2	25C19	162CG	90.36	19NE2	25C19	19OE1	27.54
19NE2	25C19	25C	73.76	19NE2	25C19	26N	82.78
23C	25C19	23CA	18.96	23C	25C19	19OE1	75.13
23C	25C19	25C	72.57	23C	25C19	26N	67.65
163N	25C19	161C	53.30	163N	25C19	162CG	44.32
163N	25C19	19OE1	88.05	163N	25C19	25C	63.02
163N	25C19	26N	68.23	23CA	25C19	19OE1	74.37
23CA	25C19	25C	89.19	23CA	25C19	26N	86.09
161C	25C19	162CG	59.79	162CG	25C19	19OE1	65.83
162CG	25C19	25C	87.18	162CG	25C19	26N	99.91
19OE1	25C19	25C	62.33	19OE1	25C19	26N	76.16
25C	25C19	26N	15.58	25SG	25O20	25CB	34.29
25SG	25O20	25N	58.41	25SG	25O20	23O	94.11
25SG	25O20	162ND1	57.05	25SG	25O20	25CA	42.72
25SG	25O20	19OE1	79.03	25SG	25O20	19CD	92.36
25SG	25O20	24N	95.32	25SG	25O20	162CE1	62.12
25SG	25O20	161O	62.41	25SG	25O20	24C	65.93
25CB	25O20	19NE2	70.39	25CB	25O20	23C	93.15
25CB	25O20	25N	40.44	25CB	25O20	23O	94.44
25CB	25O20	162ND1	54.11	25CB	25O20	25CA	19.78
25CB	25O20	19OE1	46.09	25CB	25O20	19CD	58.16
25CB	25O20	24N	78.39	25CB	25O20	162CE1	47.36
25CB	25O20	161O	92.37	25CB	25O20	24C	49.33
19NE2	25O20	23CA	63.45	19NE2	25O20	23C	67.92
19NE2	25O20	25N	61.15	19NE2	25O20	23O	85.94

TABLE XV

19NE2	25O20	162ND1	88.31	19NE2	25O20	25CA	65.49
19NE2	25O20	19OE1	31.85	19NE2	25O20	19CD	15.16
19NE2	25O20	24N	55.12	19NE2	25O20	162CE1	71.33
19NE2	25O20	24C	60.20	19NE2	25O20	23N	58.44
23CA	25O20	23C	24.00	23CA	25O20	25N	73.06
23CA	25O20	23O	37.74	23CA	25O20	25CA	93.15
23CA	25O20	19OE1	94.06	23CA	25O20	19CD	77.95
23CA	25O20	24N	33.98	23CA	25O20	24C	64.37
23CA	25O20	23N	6.16	23C	25O20	25N	52.77
23C	25O20	23O	18.86	23C	25O20	25CA	73.50
23C	25O20	19OE1	92.10	23C	25O20	19CD	79.18
23C	25O20	24N	16.93	23C	25O20	24C	43.85
23C	25O20	23N	28.31	25N	25O20	23O	55.74
25N	25O20	162ND1	94.17	25N	25O20	25CA	20.73
25N	25O20	19OE1	59.69	25N	25O20	19CD	59.03
25N	25O20	24N	39.08	25N	25O20	162CE1	84.24
25N	25O20	24C	8.93	25N	25O20	23N	74.25
23O	25O20	25CA	75.11	23O	25O20	19CD	95.79
23O	25O20	24N	31.46	23O	25O20	24C	47.72
23O	25O20	23N	43.41	162ND1	25O20	25CA	73.82
162ND1	25O20	19OE1	58.12	162ND1	25O20	19CD	73.91
162ND1	25O20	162CE1	17.08	162ND1	25O20	161O	63.55
25CA	25O20	19OE1	51.34	25CA	25O20	19CD	57.52
25CA	25O20	24N	59.36	25CA	25O20	162CE1	65.59
25CA	25O20	24C	29.65	25CA	25O20	23N	93.68
19OE1	25O20	19CD	16.69	19OE1	25O20	24N	75.92
19OE1	25O20	162CE1	41.10	19OE1	25O20	24C	64.20
19OE1	25O20	23N	89.60	19CD	25O20	24N	64.32
19CD	25O20	162CE1	56.83	19CD	25O20	24C	60.79
19CD	25O20	23N	73.22	24N	25O20	24C	30.42
24N	25O20	23N	35.59	162CE1	25O20	161O	80.58
162CE1	25O20	24C	92.22	24C	25O20	23N	65.85
160CD1	25C21	158O	97.34	160CD1	25C21	160CG	23.97
160CD1	25C21	160CB	37.71	160CD1	25C21	160N	66.46
160CD1	25C21	158C	87.61	160CD1	25C21	160CA	53.04
158O	25C21	160CG	75.13	158O	25C21	160CB	77.51
158O	25C21	160N	47.16	158O	25C21	158C	10.74

TABLE XV

158O	25C21	160CA	63.99	160CG	25C21	160CB	22.63
160CG	25C21	160N	43.47	160CG	25C21	158C	66.36
160CG	25C21	160CA	33.10	160CB	25C21	160N	33.28
160CB	25C21	158C	71.92	160CB	25C21	160CA	16.60
160N	25C21	158C	44.97	160N	25C21	160CA	17.43
158C	25C21	160CA	60.36	160CD1	25C22	160CG	21.04
160CD1	25C22	160CB	35.29	160CD1	25C22	209CD2	57.75
160CD1	25C22	209CD1	70.22	160CD1	25C22	158O	76.29
160CG	25C22	160CB	20.86	160CG	25C22	209CD2	73.30
160CG	25C22	209CD1	90.52	160CG	25C22	158O	57.61
160CB	25C22	209CD2	69.60	160CB	25C22	209CD1	94.36
160CB	25C22	158O	61.33	209CD2	25C22	209CD1	29.68
160CD1	25C23	209CD2	57.43	160CD1	25C23	160CB	34.09
160CD1	25C23	160O	71.45	160CD1	25C23	160CG	18.98
209CD2	25C23	67CE1	66.23	209CD2	25C23	160CB	73.03
209CD2	25C23	160O	88.66	209CD2	25C23	67OH	97.28
209CD2	25C23	160CG	72.08	209CD2	25C23	67CZ	81.22
67CE1	25C23	67OH	31.06	67CE1	25C23	67CZ	15.09
160CB	25C23	160O	37.90	160CB	25C23	160CG	19.32
160O	25C23	160CG	56.76	67OH	25C23	67CZ	16.25
160O	25C24	160CB	44.46	160O	25C24	160C	11.63
160O	25C24	160CA	31.06	160O	25C24	160N	41.50
160O	25C24	160CD1	75.56	160O	25C24	160CG	62.09
160CB	25C24	160C	34.19	160CB	25C24	160CA	18.85
160CB	25C24	160N	32.07	160CB	25C24	160CD1	32.04
160CB	25C24	160CG	18.03	160C	25C24	160CA	19.45
160C	25C24	160N	31.04	160C	25C24	160CD1	66.04
160C	25C24	160CG	51.26	160CA	25C24	160N	18.21
160CA	25C24	160CD1	50.13	160CA	25C24	160CG	33.24
160N	25C24	160CD1	57.42	160N	25C24	160CG	38.76
160CD1	25C24	160CG	18.66	67CE1	25C24	67OH	28.53
160O	25C25	160N	52.68	160O	25C25	160CB	48.40
160O	25C25	160CA	37.54	160O	25C25	160C	16.03
160O	25C25	160CG	68.51	160O	25C25	160CD1	77.48
160O	25C25	159C	58.15	160O	25C25	159CA	73.59
160O	25C25	158C	96.27	160N	25C25	160CB	39.49
160N	25C25	158O	51.80	160N	25C25	160CA	21.57

TABLE XV

160N	25C25	160C	36.87	160N	25C25	160CG	45.04
160N	25C25	160CD1	63.96	160N	25C25	159C	10.14
160N	25C25	159CA	27.45	160N	25C25	158C	43.72
160CB	25C25	158O	77.37	160CB	25C25	160CA	22.69
160CB	25C25	160C	37.96	160CB	25C25	160CG	20.22
160CB	25C25	160CD1	31.90	160CB	25C25	159C	49.57
160CB	25C25	159CA	65.68	160CB	25C25	158C	69.44
158O	25C25	160CA	71.03	158O	25C25	160C	88.59
158O	25C25	160CG	65.33	158O	25C25	160CD1	77.45
158O	25C25	159C	46.06	158O	25C25	159CA	33.23
158O	25C25	158C	8.40	160CA	25C25	160C	22.25
160CA	25C25	160CG	37.31	160CA	25C25	160CD1	53.48
160CA	25C25	159C	31.20	160CA	25C25	159CA	48.92
160CA	25C25	158C	62.65	160C	25C25	160CG	56.85
160C	25C25	160CD1	69.51	160C	25C25	159C	43.18
160C	25C25	159CA	59.72	160C	25C25	158C	80.59
160CG	25C25	160CD1	19.02	160CG	25C25	159C	53.50
160CG	25C25	159CA	65.18	160CG	25C25	158C	58.66
160CD1	25C25	159C	72.53	160CD1	25C25	159CA	83.50
160CD1	25C25	158C	72.33	159C	25C25	159CA	17.81
159C	25C25	158C	38.66	159CA	25C25	158C	27.96
158O	25C26	160N	61.78	158O	25C26	160CB	92.43
158O	25C26	160CG	82.57	158O	25C26	158C	10.10
158O	25C26	160CA	80.14	158O	25C26	160CD1	98.52
158O	25C26	159C	50.29	158O	25C26	159CA	34.65
158O	25C26	160C	92.37	158O	25C26	159N	20.44
158O	25C26	158CA	18.72	160N	25C26	160CB	40.08
160N	25C26	160CG	50.16	160N	25C26	158C	54.73
160N	25C26	160CA	20.14	160N	25C26	160CD1	70.80
160N	25C26	160O	45.75	160N	25C26	159C	12.46
160N	25C26	159CA	31.73	160N	25C26	160C	31.11
160N	25C26	159N	41.35	160N	25C26	158CA	65.61
160CB	25C26	160CG	23.66	160CB	25C26	158C	82.75
160CB	25C26	160CA	21.78	160CB	25C26	160CD1	36.20
160CB	25C26	160O	42.04	160CB	25C26	159C	51.71
160CB	25C26	159CA	70.60	160CB	25C26	160C	32.83
160CB	25C26	159N	74.02	160CB	25C26	158CA	86.07

TABLE XV

160CG	25C26	158C	72.51	160CG	25C26	160CA	39.22
160CG	25C26	160CD1	21.40	160CG	25C26	160O	65.66
160CG	25C26	159C	58.12	160CG	25C26	159CA	73.32
160CG	25C26	160C	55.17	160CG	25C26	159N	69.08
160CG	25C26	158CA	70.57	158C	25C26	160CA	71.90
158C	25C26	160CD1	88.97	158C	25C26	160O	99.96
158C	25C26	159C	44.20	158C	25C26	159CA	31.81
158C	25C26	160C	85.81	158C	25C26	159N	14.55
158C	25C26	158CA	15.01	160CA	25C26	160CD1	56.75
160CA	25C26	160O	33.81	160CA	25C26	159C	32.58
160CA	25C26	159CA	51.87	160CA	25C26	160C	19.16
160CA	25C26	159N	59.89	160CA	25C26	158CA	80.10
160CD1	25C26	160O	74.72	160CD1	25C26	159C	79.44
160CD1	25C26	159CA	94.53	160CD1	25C26	160C	68.62
160CD1	25C26	159N	88.47	160CD1	25C26	158CA	83.00
160O	25C26	159C	55.78	160O	25C26	159CA	71.36
160O	25C26	160C	15.23	160O	25C26	159N	85.80
159C	25C26	159CA	19.31	159C	25C26	160C	42.08
159C	25C26	159N	30.09	159C	25C26	158CA	56.63
159CA	25C26	160C	59.37	159CA	25C26	159N	17.84
159CA	25C26	158CA	46.52	160C	25C26	159N	72.10
160C	25C26	158CA	96.40	159N	25C26	158CA	28.80
160O	25C27	160C	5.58	160O	25C27	160CB	36.45
67OH	25C27	67CE1	31.65	67OH	25C27	67CZ	17.00
67CE1	25C27	67CZ	17.03	160C	25C27	160CB	31.24
160O	25O28	160C	3.01	160O	25O28	161CA	33.47
160O	25O28	160CB	35.39	160O	25O28	161N	15.24
160O	25O28	160CA	17.00	160O	25O28	161O	59.68
160O	25O28	161C	45.54	160C	25O28	161CA	33.37
160C	25O28	160CB	34.06	160C	25O28	161N	14.62
160C	25O28	160CA	16.50	160C	25O28	161O	58.60
160C	25O28	161C	44.40	161CA	25O28	160CB	65.80
161CA	25O28	161N	18.92	161CA	25O28	160CA	49.84
161CA	25O28	161O	28.96	161CA	25O28	161C	17.13
160CB	25O28	161N	47.18	160CB	25O28	160CA	19.23
160CB	25O28	161O	84.88	160CB	25O28	161C	71.68
161N	25O28	160CA	30.98	161N	25O28	161O	44.50

TABLE XV

161N	25O28	161C	30.43	160CA	25O28	161O	73.79
160CA	25O28	161C	59.64	161O	25O28	161C	14.21
160O	25C29	160C	8.30	160O	25C29	161O	64.77
160O	25C29	161CA	35.29	160O	25C29	161C	50.76
160O	25C29	161N	20.86	160C	25C29	161O	58.92
160C	25C29	161CA	30.98	160C	25C29	161C	44.50
160C	25C29	161N	14.62	161O	25C29	161CA	30.36
161O	25C29	161C	14.65	161O	25C29	66O	98.33
161O	25C29	161N	44.35	161CA	25C29	161C	18.41
161CA	25C29	161N	17.07	161C	25C29	161N	30.04
66O	25C29	67CE1	67.43	67CE1	25O30	66O	85.21
67CE1	25O30	67CD1	18.89	67CE1	25O30	67CZ	18.55
67CE1	25O30	66C	76.83	67CE1	25O30	67OH	30.56
67CE1	25O30	67CG	30.00	67CE1	25O30	67CE2	29.39
66O	25O30	67CD1	68.13	66O	25O30	67CZ	86.99
66O	25O30	66C	13.74	66O	25O30	67CG	55.33
66O	25O30	67CE2	73.81	67CD1	25O30	67CZ	32.19
67CD1	25O30	66C	61.85	67CD1	25O30	67OH	47.68
67CD1	25O30	67CG	16.18	67CD1	25O30	67CE2	34.38
67CZ	25O30	66C	75.55	67CZ	25O30	67OH	16.91
67CZ	25O30	67CG	34.81	67CZ	25O30	67CE2	15.93
66C	25O30	67OH	90.11	66C	25O30	67CG	47.06
66C	25O30	67CE2	61.38	67OH	25O30	67CG	51.72
67OH	25O30	67CE2	28.75	67CG	25O30	67CE2	28.79
161O	25C31	161C	15.89	161O	25C31	163CB	92.78
161O	25C31	163N	61.31	161O	25C31	25SG	64.02
161O	25C31	160O	63.87	161O	25C31	161CA	29.15
161O	25C31	162N	24.80	161O	25C31	162C	50.12
161O	25C31	162CA	32.14	161C	25C31	163CB	90.31
161C	25C31	163N	58.98	161C	25C31	25SG	74.60
161C	25C31	160O	51.49	161C	25C31	161CA	18.45
161C	25C31	162N	14.50	161C	25C31	162C	44.52
161C	25C31	162CA	29.60	66O	25C31	163CB	84.58
66O	25C31	25SG	96.91	163CB	25C31	163N	31.73
163CB	25C31	25SG	54.53	163CB	25C31	162N	76.07
163CB	25C31	162C	45.95	163CB	25C31	162CA	61.61
163N	25C31	25SG	46.05	163N	25C31	160O	95.54

TABLE XV

163N	25C31	161CA	75.21	163N	25C31	162N	45.16
163N	25C31	162C	16.28	163N	25C31	162CA	29.89
25SG	25C31	161CA	92.28	25SG	25C31	162N	68.65
25SG	25C31	162C	56.25	25SG	25C31	162CA	53.18
160O	25C31	161CA	34.72	160O	25C31	162N	58.12
160O	25C31	162C	79.70	160O	25C31	162CA	74.94
161CA	25C31	162N	30.24	161CA	25C31	162C	59.56
161CA	25C31	162CA	47.15	162N	25C31	162C	30.15
162N	25C31	162CA	17.36	162C	25C31	162CA	18.28
66O	25C32	66C	6.90	66O	25C32	26CB	47.54
66O	25C32	66N	33.71	66O	25C32	67CA	32.46
66O	25C32	67N	16.73	66O	25C32	68SD	78.15
66O	25C32	66CA	18.01	66C	25C32	26CB	54.44
66C	25C32	66N	33.07	66C	25C32	67CA	31.49
66C	25C32	67N	13.91	66C	25C32	68SD	82.32
66C	25C32	66CA	15.84	163CB	25C32	26CB	63.43
163CB	25C32	161O	78.07	163CB	25C32	68SD	47.45
26CB	25C32	66N	59.39	26CB	25C32	67CA	62.90
26CB	25C32	67N	59.03	26CB	25C32	68SD	57.55
26CB	25C32	66CA	57.10	66N	25C32	67CA	64.54
66N	25C32	67N	46.76	66N	25C32	66CA	17.45
67CA	25C32	67N	17.89	67CA	25C32	68SD	59.36
67CA	25C32	66CA	47.17	67N	25C32	68SD	73.47
67N	25C32	66CA	29.33	68SD	25C32	66CA	96.00
66O	25C33	68SD	88.15	66O	25C33	67CA	38.20
66O	25C33	66C	8.09	66O	25C33	67CD1	67.84
66O	25C33	26CB	42.16	68SD	25C33	163CB	58.04
68SD	25C33	209CD2	90.24	68SD	25C33	68CE	24.67
68SD	25C33	134CB	82.77	68SD	25C33	67CA	68.81
68SD	25C33	66C	87.57	68SD	25C33	67CD1	97.64
68SD	25C33	163CA	69.15	68SD	25C33	26CB	61.04
68SD	25C33	163N	85.62	163CB	25C33	68CE	66.68
163CB	25C33	134CB	76.70	163CB	25C33	163CA	16.69
163CB	25C33	26CB	62.05	163CB	25C33	163N	28.80
209CD2	25C33	68CE	67.71	209CD2	25C33	134CB	48.90
209CD2	25C33	67CA	91.59	209CD2	25C33	67CD1	58.37
68CE	25C33	134CB	60.70	68CE	25C33	67CA	80.55

TABLE XV

68CE	25C33	67CD1	93.40	68CE	25C33	163CA	71.10
68CE	25C33	26CB	85.68	68CE	25C33	163N	88.13
134CB	25C33	163CA	63.97	134CB	25C33	163N	69.60
67CA	25C33	66C	31.31	67CA	25C33	67CD1	43.75
67CA	25C33	26CB	61.06	66C	25C33	67CD1	59.98
66C	25C33	26CB	47.92	163CA	25C33	26CB	77.85
163CA	25C33	163N	17.21	26CB	25C33	163N	81.08
134CB	25C34	163CB	98.21	134CB	25C34	209CD2	58.87
134CB	25C34	134CA	20.10	134CB	25C34	163CA	84.05
134CB	25C34	163N	93.22	134CB	25C34	68SD	90.66
134CB	25C34	162O	68.42	134CB	25C34	162C	84.53
134CB	25C34	68CE	68.29	134CB	25C34	160O	90.59
134CB	25C34	133O	48.20	134CB	25C34	134C	23.47
134CB	25C34	134N	22.08	163CB	25C34	134CA	80.28
163CB	25C34	163CA	22.29	163CB	25C34	163N	35.89
163CB	25C34	68SD	54.05	163CB	25C34	162O	61.05
163CB	25C34	162C	53.04	163CB	25C34	68CE	66.68
163CB	25C34	161O	82.47	163CB	25C34	66O	82.69
163CB	25C34	161C	87.58	163CB	25C34	133O	51.04
163CB	25C34	134C	88.38	163CB	25C34	134N	76.48
209CD2	25C34	134CA	78.36	209CD2	25C34	68SD	85.07
209CD2	25C34	68CE	68.09	209CD2	25C34	160O	89.46
209CD2	25C34	66O	98.98	209CD2	25C34	133O	91.98
209CD2	25C34	134C	80.67	209CD2	25C34	134N	73.48
134CA	25C34	163CA	64.27	134CA	25C34	163N	73.36
134CA	25C34	68SD	87.47	134CA	25C34	162O	50.99
134CA	25C34	162C	66.34	134CA	25C34	68CE	68.94
134CA	25C34	160O	96.11	134CA	25C34	161C	93.44
134CA	25C34	133O	34.17	134CA	25C34	134C	14.63
134CA	25C34	134N	13.38	163CA	25C34	163N	20.60
163CA	25C34	68SD	71.18	163CA	25C34	162O	39.10
163CA	25C34	162C	33.94	163CA	25C34	68CE	76.73
163CA	25C34	161O	73.90	163CA	25C34	161C	74.17
163CA	25C34	133O	43.83	163CA	25C34	134C	69.19
163CA	25C34	134N	64.70	163N	25C34	68SD	89.44
163N	25C34	162O	30.77	163N	25C34	162C	17.88
163N	25C34	68CE	97.26	163N	25C34	160O	97.64

TABLE XV

163N	25C34	161O	53.38	163N	25C34	161C	53.96
163N	25C34	133O	61.87	163N	25C34	134C	73.07
163N	25C34	134N	77.98	68SD	25C34	68CE	23.41
68SD	25C34	66O	65.12	68SD	25C34	133O	57.26
68SD	25C34	134N	74.79	162O	25C34	162C	16.36
162O	25C34	160O	80.07	162O	25C34	161O	57.49
162O	25C34	161C	48.98	162O	25C34	133O	57.78
162O	25C34	134C	45.59	162O	25C34	134N	60.64
162C	25C34	160O	82.14	162C	25C34	161O	46.60
162C	25C34	161C	42.17	162C	25C34	133O	66.02
162C	25C34	134C	61.91	162C	25C34	134N	74.59
68CE	25C34	66O	84.63	68CE	25C34	133O	46.00
68CE	25C34	134C	83.30	68CE	25C34	134N	55.59
160O	25C34	161O	52.91	160O	25C34	161C	45.36
160O	25C34	134C	81.68	161O	25C34	66O	93.09
161O	25C34	161C	14.42	161O	25C34	134C	94.94
161C	25C34	134C	81.60	133O	25C34	134C	47.42
133O	25C34	134N	26.12	134C	25C34	134N	27.76
209CD2	25C35	67CD1	84.45	209CD2	25C35	67CE1	80.21
209CD2	25C35	68SD	97.07	209CD2	25C35	209CG	14.43
209CD2	25C35	68CE	73.57	209CD2	25C35	234OH2	69.51
209CD2	25C35	134CB	48.83	209CD2	25C35	67CZ	91.21
67CD1	25C35	66O	85.63	67CD1	25C35	67CA	57.17
67CD1	25C35	67CE1	19.94	67CD1	25C35	67CG	19.64
67CD1	25C35	67CB	37.21	67CD1	25C35	209CG	80.87
67CD1	25C35	66C	72.49	67CD1	25C35	234OH2	56.52
67CD1	25C35	67N	60.31	67CD1	25C35	68N	77.14
67CD1	25C35	67C	68.08	67CD1	25C35	67CZ	24.12
67CD1	25C35	67CD2	23.57	66O	25C35	67CA	43.70
66O	25C35	67CE1	93.34	66O	25C35	67CG	67.30
66O	25C35	67CB	61.47	66O	25C35	68SD	79.58
66O	25C35	66C	13.35	66O	25C35	234OH2	97.49
66O	25C35	67N	29.17	66O	25C35	68N	61.59
66O	25C35	67C	49.59	66O	25C35	67CZ	83.31
66O	25C35	67CD2	62.47	67CA	25C35	67CE1	74.54
67CA	25C35	67CG	38.46	67CA	25C35	67CB	21.40
67CA	25C35	68SD	71.28	67CA	25C35	68CE	86.07

TABLE XV

67CA	25C35	66C	33.51	67CA	25C35	234OH2	54.58
67CA	25C35	67N	17.55	67CA	25C35	68N	31.22
67CA	25C35	67C	15.46	67CA	25C35	67CZ	70.81
67CA	25C35	67CD2	42.99	67CE1	25C35	67CG	36.15
67CE1	25C35	67CB	56.18	67CE1	25C35	209CG	81.63
67CE1	25C35	66C	81.58	67CE1	25C35	234OH2	73.50
67CE1	25C35	67N	73.49	67CE1	25C35	68N	96.98
67CE1	25C35	67C	86.96	67CE1	25C35	67CZ	11.55
67CE1	25C35	67CD2	33.63	67CG	25C35	67CB	21.11
67CG	25C35	209CG	95.25	67CG	25C35	66C	53.96
67CG	25C35	234OH2	55.92	67CG	25C35	67N	40.77
67CG	25C35	68N	62.93	67CG	25C35	67C	51.10
67CG	25C35	67CZ	34.20	67CG	25C35	67CD2	11.75
67CB	25C35	68SD	84.13	67CB	25C35	209CG	94.85
67CB	25C35	68CE	92.04	67CB	25C35	66C	49.06
67CB	25C35	234OH2	43.66	67CB	25C35	67N	32.31
67CB	25C35	68N	41.83	67CB	25C35	67C	30.89
67CB	25C35	67CZ	55.30	67CB	25C35	67CD2	30.26
68SD	25C35	209CG	86.31	68SD	25C35	68CE	23.56
68SD	25C35	66C	84.14	68SD	25C35	234OH2	65.58
68SD	25C35	67N	81.24	68SD	25C35	134CB	74.35
68SD	25C35	68N	42.38	68SD	25C35	67C	56.14
209CG	25C35	68CE	63.48	209CG	25C35	234OH2	55.92
209CG	25C35	134CB	53.71	209CG	25C35	68N	92.87
209CG	25C35	67CZ	93.16	68CE	25C35	234OH2	58.89
68CE	25C35	67N	99.75	68CE	25C35	134CB	57.04
68CE	25C35	68N	54.84	68CE	25C35	67C	70.76
66C	25C35	234OH2	88.09	66C	25C35	67N	16.98
66C	25C35	68N	57.38	66C	25C35	67C	42.97
66C	25C35	67CZ	72.32	66C	25C35	67CD2	49.60
234OH2	25C35	67N	71.60	234OH2	25C35	134CB	98.59
234OH2	25C35	68N	41.88	234OH2	25C35	67C	48.67
234OH2	25C35	67CZ	80.56	234OH2	25C35	67CD2	67.67
67N	25C35	68N	46.13	67N	25C35	67C	30.25
67N	25C35	67CZ	66.52	67N	25C35	67CD2	39.87
68N	25C35	67C	16.06	68N	25C35	67CZ	97.13
68N	25C35	67CD2	71.07	67C	25C35	67CZ	84.80

TABLE XV

67C	25C35	67CD2	57.44	67CZ	25C35	67CD2	27.90
161O	25C36	25SG	73.45	161O	25C36	161C	9.23
161O	25C36	163N	54.83	25SG	25C36	161C	78.40
25SG	25C36	65CA	99.90	25SG	25C36	26CD1	71.50
25SG	25C36	163N	45.03	25SG	25C36	26CB	68.53
66O	25C36	66N	37.32	66O	25C36	65CA	68.43
66O	25C36	26CD1	49.39	66O	25C36	26CB	39.54
161C	25C36	163N	52.99	66N	25C36	65CA	31.50
66N	25C36	26CD1	39.27	66N	25C36	26CB	55.35
65CA	25C36	26CD1	45.88	65CA	25C36	26CB	73.66
26CD1	25C36	26CB	29.63	163N	25C36	26CB	78.56
66N	25O37	65CA	42.38	66N	25O37	66O	46.15
66N	25O37	65C	19.40	66N	25O37	66CA	14.20
66N	25O37	66C	33.73	66N	25O37	26CD1	46.03
66N	25O37	65N	50.68	66N	25O37	64O	71.48
66N	25O37	26CB	60.88	66N	25O37	26CG	47.75
65CA	25O37	66O	87.59	65CA	25O37	65C	23.08
65CA	25O37	66CA	56.55	65CA	25O37	66C	75.97
65CA	25O37	26CD1	55.04	65CA	25O37	65N	8.31
65CA	25O37	64O	33.61	65CA	25O37	26CB	84.88
65CA	25O37	26CG	67.58	66O	25O37	65C	65.32
66O	25O37	66CA	32.98	66O	25O37	66C	13.52
66O	25O37	26CD1	56.53	66O	25O37	65N	95.80
66O	25O37	26CB	40.45	66O	25O37	26CG	44.04
65C	25O37	66CA	33.51	65C	25O37	66C	53.13
65C	25O37	26CD1	48.33	65C	25O37	65N	31.35
65C	25O37	64O	52.95	65C	25O37	26CB	72.24
65C	25O37	26CG	56.09	161O	25O37	25SG	57.00
66CA	25O37	66C	19.92	66CA	25O37	26CD1	50.28
66CA	25O37	65N	64.84	66CA	25O37	64O	84.47
66CA	25O37	26CB	56.17	66CA	25O37	26CG	47.05
66C	25O37	26CD1	55.02	66C	25O37	65N	84.27
66C	25O37	26CB	47.54	66C	25O37	26CG	45.65
26CD1	25O37	25SG	70.87	26CD1	25O37	65N	59.66
26CD1	25O37	64O	86.49	26CD1	25O37	26CB	31.10
26CD1	25O37	26CG	15.01	25SG	25O37	26CB	64.40
25SG	25O37	26CG	71.37	65N	25O37	64O	27.18

TABLE XV

65N	25O37	26CB	90.35	65N	25O37	26CG	73.15
26CB	25O37	26CG	17.30	161O	25N38	161C	6.07
161O	25N38	162CA	37.32	161O	25N38	163N	66.42
161O	25N38	162N	19.53	161O	25N38	162C	50.16
161O	25N38	161CA	13.58	161O	25N38	163CB	91.46
25SG	25N38	162CA	69.08	25SG	25N38	163N	53.99
25SG	25N38	162N	87.78	25SG	25N38	25CB	2.51
25SG	25N38	162C	65.56	25SG	25N38	163CB	56.74
161C	25N38	162CA	34.04	161C	25N38	163N	61.45
161C	25N38	162N	15.39	161C	25N38	162C	45.21
161C	25N38	161CA	14.75	161C	25N38	163CB	85.67
162CA	25N38	163N	32.71	162CA	25N38	162N	18.81
162CA	25N38	25CB	71.19	162CA	25N38	162C	18.79
162CA	25N38	161CA	48.73	162CA	25N38	163CB	62.05
163N	25N38	162N	47.03	163N	25N38	25CB	56.49
163N	25N38	162C	16.27	163N	25N38	161CA	74.28
163N	25N38	163CB	29.78	162N	25N38	25CB	89.84
162N	25N38	162C	30.82	162N	25N38	161CA	29.96
162N	25N38	163CB	73.48	25CB	25N38	162C	68.00
25CB	25N38	163CB	58.75	162C	25N38	161CA	58.33
162C	25N38	163CB	43.86	161CA	25N38	163CB	95.28
25SG	25N39	161O	88.31	25SG	25N39	23O	88.64
25SG	25N39	25CB	14.83	25SG	25N39	23C	82.58
25SG	25N39	161C	85.92	25SG	25N39	25N	41.66
25SG	25N39	23CA	91.29	25SG	25N39	25CA	24.80
25SG	25N39	162CA	58.01	161O	25N39	25CB	99.78
161O	25N39	161C	3.40	161O	25N39	162CA	31.86
23O	25N39	25CB	77.70	23O	25N39	23C	14.66
23O	25N39	65CA	50.70	23O	25N39	25N	47.04
23O	25N39	23CA	29.83	23O	25N39	25CA	63.85
25CB	25N39	23C	69.66	25CB	25N39	161C	97.02
25CB	25N39	25N	31.35	25CB	25N39	23CA	76.81
25CB	25N39	25CA	16.71	25CB	25N39	162CA	68.20
23C	25N39	65CA	64.77	23C	25N39	25N	41.89
23C	25N39	23CA	18.46	23C	25N39	25CA	58.51
161C	25N39	162CA	28.91	65CA	25N39	25N	88.24
65CA	25N39	23CA	73.18	25N	25N39	23CA	54.84

TABLE XV

25N	25N39	25CA	16.92	25N	25N39	162CA	99.14
23CA	25N39	25CA	69.81	25CA	25N39	162CA	82.61
160O	25N40	161O	83.18	160O	25N40	161C	65.67
160O	25N40	161CA	44.84	160O	25N40	160C	14.22
160O	25N40	161N	30.23	160O	25N40	162N	67.90
161O	25N40	161C	19.36	161O	25N40	161CA	38.54
161O	25N40	160C	72.40	161O	25N40	161N	54.55
161O	25N40	162N	26.72	161C	25N40	161CA	23.35
161C	25N40	160C	53.79	161C	25N40	161N	35.96
161C	25N40	162N	13.14	161CA	25N40	160C	35.76
161CA	25N40	161N	19.52	161CA	25N40	162N	31.98
160C	25N40	161N	17.87	160C	25N40	162N	54.39
161N	25N40	162N	37.86				

TABLE XVI

Table of angles between atoms of the inhibitor and protein for all protein atoms within 5 Ångstroms of the inhibitor 4-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-1-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-3-pyrrolidinone.

Atom 1	Atom 2	Atom 3	Angle in degrees
184O	25C1	184CD1	70.91
184O	25C1	184CG	59.71
184O	25C1	184CB	40.07
184O	25C1	184CA	32.41
184O	25C1	18OD1	51.11
184O	25C1	184C	14.14
184O	25C1	184NE1	85.23
184O	25C1	184CD2	70.75
184CD1	25C1	184CG	18.26
184CD1	25C1	184CB	34.36
184CD1	25C1	184CA	39.63
184CD1	25C1	18OD1	88.02
184CD1	25C1	184C	58.65
184CD1	25C1	184NE1	15.36
184CD1	25C1	184CD2	26.43
184CG	25C1	184CB	19.78
184CG	25C1	184CA	33.68
184CG	25C1	18OD1	90.72
184CG	25C1	184C	50.19
184CG	25C1	184NE1	27.27
184CG	25C1	184CD2	15.55
184CB	25C1	184CA	19.99
184CB	25C1	18OD1	77.76
184CB	25C1	184C	31.92
184CB	25C1	184NE1	46.53
184CB	25C1	184CD2	31.52
184CA	25C1	18OD1	58.36
184CA	25C1	184C	19.14
184CA	25C1	184NE1	54.76
184CA	25C1	184CD2	48.54
18OD1	25C1	184C	48.87
184C	25C1	184NE1	73.60
184C	25C1	184CD2	63.42

TABLE XVI

184NE1	25C1	184CD2	26.12
20O	25C2	20C	16.36
20O	25C2	21NE2	67.96
20O	25C2	20N	38.80
20O	25C2	20CA	32.93
20O	25C2	19CG	52.37
20O	25C2	18OD1	81.91
20C	25C2	21NE2	65.02
20C	25C2	20N	33.58
20C	25C2	20CA	20.23
20C	25C2	19CG	62.24
20C	25C2	18OD1	73.06
21NE2	25C2	20N	97.72
21NE2	25C2	20CA	79.83
184CD1	25C2	20N	95.12
184CD1	25C2	19CG	55.67
184CD1	25C2	18OD1	86.02
184CD1	25C2	184NE1	16.52
184CD1	25C2	184CG	16.21
184CD1	25C2	184CA	36.11
20N	25C2	20CA	19.09
20N	25C2	19CG	44.54
20N	25C2	18OD1	43.33
20N	25C2	184CA	81.17
20CA	25C2	19CG	60.59
20CA	25C2	18OD1	53.05
20CA	25C2	184CA	98.88
19CG	25C2	18OD1	66.67
19CG	25C2	184NE1	60.03
19CG	25C2	184CG	69.53
19CG	25C2	184CA	62.53
18OD1	25C2	184CG	83.94
18OD1	25C2	184CA	53.91
184NE1	25C2	184CG	27.27
184NE1	25C2	184CA	52.47
184CG	25C2	184CA	30.07
20O	25C3	21NE2	68.98
20O	25C3	20C	12.74
20O	25C3	19CG	52.30
20O	25C3	19CD	62.76
184CD1	25C3	184NE1	19.43
184CD1	25C3	19CG	57.07

TABLE XVI

184CD1	25C3	184CG	15.46
184CD1	25C3	184CE2	27.70
184CD1	25C3	19CD	51.26
184NE1	25C3	19CG	64.69
184NE1	25C3	184CG	28.26
184NE1	25C3	184CE2	15.28
184NE1	25C3	19CD	52.93
21NE2	25C3	20C	62.81
20C	25C3	19CG	59.85
20C	25C3	19CD	72.69
19CG	25C3	184CG	69.91
19CG	25C3	184CE2	79.68
19CG	25C3	19CD	17.58
184CG	25C3	184CE2	27.82
184CG	25C3	19CD	66.23
184CE2	25C3	19CD	68.19
184NE1	25C4	184CD1	21.40
184NE1	25C4	184CE2	20.66
184NE1	25C4	184CG	31.78
184NE1	25C4	184CD2	31.15
184NE1	25C4	184CZ2	34.27
184CD1	25C4	184CE2	34.03
184CD1	25C4	184CG	18.28
184CD1	25C4	184CD2	31.27
184CD1	25C4	184CZ2	51.25
184CE2	25C4	184CG	32.35
184CE2	25C4	184CD2	18.86
184CE2	25C4	184CZ2	17.60
184CG	25C4	184CD2	19.32
184CG	25C4	184CZ2	49.25
184CD2	25C4	184CZ2	32.53
184CE2	25C5	184NE1	21.44
184CE2	25C5	184CD2	21.99
184CE2	25C5	184CD1	35.25
184CE2	25C5	184CG	36.03
184CE2	25C5	184CZ2	17.88
184CE2	25C5	184CE3	33.85
184CE2	25C5	184CB	53.93
184CE2	25C5	184CH2	28.11
184CE2	25C5	184CZ3	34.04
184NE1	25C5	184CD2	35.23
184NE1	25C5	184CD1	21.39

TABLE XVI

184NE1	25C5	184CG	35.13
184NE1	25C5	184CZ2	35.43
184NE1	25C5	184CE3	51.78
184NE1	25C5	184CB	52.94
184NE1	25C5	184CH2	48.87
184NE1	25C5	184CZ3	55.18
184CD2	25C5	184CD1	35.19
184CD2	25C5	184CG	22.35
184CD2	25C5	184CZ2	34.58
184CD2	25C5	184CE3	17.91
184CD2	25C5	184CB	36.19
184CD2	25C5	184CH2	34.79
184CD2	25C5	184CZ3	28.60
184CD1	25C5	184CG	21.04
184CD1	25C5	184CZ2	52.70
184CD1	25C5	184CE3	52.87
184CD1	25C5	184CB	34.98
184CD1	25C5	184CH2	62.57
184CD1	25C5	184CZ3	62.67
184CG	25C5	184CZ2	53.00
184CG	25C5	184CE3	36.87
184CG	25C5	184CB	18.54
184CG	25C5	184CH2	56.68
184CG	25C5	184CZ3	50.46
184CZ2	25C5	184CE3	38.17
184CZ2	25C5	184CB	69.96
184CZ2	25C5	184CH2	15.84
184CZ2	25C5	184CZ3	29.77
184CE3	25C5	184CB	44.40
184CE3	25C5	184CH2	29.96
184CE3	25C5	184CZ3	16.03
184CB	25C5	184CH2	70.55
184CB	25C5	184CZ3	60.21
184CH2	25C5	184CZ3	16.60
184CG	25C6	184CD1	20.02
184CG	25C6	184CB	21.95
184CG	25C6	184CD2	20.42
184CG	25C6	184O	61.94
184CG	25C6	184NE1	30.53
184CG	25C6	184CE2	30.58
184CG	25C6	184CA	33.96
184CG	25C6	184CE3	33.66

TABLE XVI

184CG	25C6	184C	50.16
184CD1	25C6	184CB	37.32
184CD1	25C6	184CD2	32.14
184CD1	25C6	184O	71.19
184CD1	25C6	184NE1	17.93
184CD1	25C6	184CE2	29.87
184CD1	25C6	184CA	39.85
184CD1	25C6	184CE3	48.53
184CD1	25C6	184C	57.95
184CB	25C6	184CD2	37.74
184CB	25C6	184O	40.76
184CB	25C6	184NE1	51.79
184CB	25C6	184CE2	51.93
184CB	25C6	184CA	19.22
184CB	25C6	184CE3	43.86
184CB	25C6	184C	30.42
184CD2	25C6	184O	78.21
184CD2	25C6	184NE1	30.21
184CD2	25C6	184CE2	18.12
184CD2	25C6	184CA	53.55
184CD2	25C6	184CE3	16.59
184CD2	25C6	184C	68.06
184O	25C6	184NE1	88.69
184O	25C6	184CE2	92.47
184O	25C6	184CA	31.36
184O	25C6	184CE3	80.46
184O	25C6	184C	13.35
184NE1	25C6	184CE2	17.71
184NE1	25C6	184CA	57.51
184NE1	25C6	184CE3	45.78
184NE1	25C6	184C	75.58
184CE2	25C6	184CA	63.83
184CE2	25C6	184CE3	30.35
184CE2	25C6	184C	80.70
184CA	25C6	184CE3	62.43
184CA	25C6	184C	18.09
184CE3	25C6	184C	73.23
184NE1	25C7	184CE2	21.08
184NE1	25C7	184CZ2	38.55
184NE1	25C7	184CD1	16.84
184NE1	25C7	184CD2	27.78
184NE1	25C7	184CH2	48.97

TABLE XVI

184NE1	25C7	184CG	24.53
184CE2	25C7	184CZ2	20.61
184CE2	25C7	184CD1	31.07
184CE2	25C7	184CD2	15.35
184CE2	25C7	184CH2	28.47
184CE2	25C7	184CG	26.62
184CZ2	25C7	184CD1	51.38
184CZ2	25C7	184CD2	31.85
184CZ2	25C7	184CH2	13.39
184CZ2	25C7	184CG	46.61
184CD1	25C7	184CD2	28.53
184CD1	25C7	184CH2	59.02
184CD1	25C7	184CG	15.12
184CD2	25C7	184CH2	33.93
184CD2	25C7	184CG	16.91
184CH2	25C7	184CG	50.64
184NE1	25O8	184CE2	19.75
184NE1	25O8	184CZ2	37.94
184NE1	25O8	184CD1	15.31
184NE1	25O8	19NE2	71.47
184NE1	25O8	19CD	57.15
184CE2	25O8	184CZ2	19.95
184CE2	25O8	184CD1	31.02
184CE2	25O8	19NE2	90.51
184CE2	25O8	19CD	76.72
184CZ2	25O8	184CD1	50.82
184CZ2	25O8	19CD	92.06
184CD1	25O8	19NE2	67.22
184CD1	25O8	19CD	51.55
19NE2	25O8	19CD	15.86
184NE1	25C9	184CZ2	42.18
184NE1	25C9	184CE2	21.04
184NE1	25C9	162ND1	65.62
184NE1	25C9	162CE1	48.16
184NE1	25C9	184CD1	10.29
184NE1	25C9	19NE2	73.80
184NE1	25C9	19OE1	48.69
184NE1	25C9	19CD	57.90
184NE1	25C9	184CH2	49.13
184CZ2	25C9	184CE2	21.63
184CZ2	25C9	162ND1	65.18
184CZ2	25C9	162CE1	57.30

TABLE XVI

184CZ2	25C9	184CD1	51.49
184CZ2	25C9	19OE1	86.41
184CZ2	25C9	19CD	98.49
184CZ2	25C9	184CH2	7.78
184CE2	25C9	162ND1	66.81
184CE2	25C9	162CE1	52.84
184CE2	25C9	184CD1	29.90
184CE2	25C9	19NE2	94.57
184CE2	25C9	19OE1	68.42
184CE2	25C9	19CD	78.74
184CE2	25C9	184CH2	28.19
162ND1	25C9	162CE1	18.04
162ND1	25C9	184CD1	72.19
162ND1	25C9	19NE2	76.32
162ND1	25C9	19OE1	58.44
162ND1	25C9	19CD	71.67
162ND1	25C9	184CH2	70.09
162CE1	25C9	184CD1	54.22
162CE1	25C9	19NE2	69.37
162CE1	25C9	19OE1	46.03
162CE1	25C9	19CD	60.55
162CE1	25C9	184CH2	63.87
184CD1	25C9	19NE2	66.83
184CD1	25C9	19OE1	44.17
184CD1	25C9	19CD	50.99
184CD1	25C9	184CH2	58.03
19NE2	25C9	19OE1	27.69
19NE2	25C9	19CD	15.92
19OE1	25C9	19CD	14.75
19OE1	25C9	184CH2	94.16
184NE1	25O10	162ND1	90.68
184NE1	25O10	162CE1	67.15
184NE1	25O10	184CE2	23.02
184NE1	25O10	184CZ2	46.79
184NE1	25O10	19OE1	64.53
184NE1	25O10	184CD1	12.02
184NE1	25O10	19NE2	90.63
184NE1	25O10	19CD	72.30
184NE1	25O10	162CG	91.69
184NE1	25O10	162NE2	63.41
184NE1	25O10	184CD2	16.34
184NE1	25O10	184CH2	50.63

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TABLE XVI

184NE1	25O10	162CD2	76.58
184NE1	25O10	184CG	0.86
162ND1	25O10	162CE1	25.39
162ND1	25O10	184CE2	85.65
162ND1	25O10	184CZ2	80.71
162ND1	25O10	19OE1	79.25
162ND1	25O10	184CD1	93.79
162ND1	25O10	19NE2	99.71
162ND1	25O10	19CD	94.77
162ND1	25O10	162CG	11.75
162ND1	25O10	162NE2	27.28
162ND1	25O10	184CD2	87.44
162ND1	25O10	184CH2	80.29
162ND1	25O10	162CD2	17.27
162ND1	25O10	162CB	25.40
162ND1	25O10	25CB	48.85
162ND1	25O10	184CG	91.42
162ND1	25O10	25SG	48.57
162CE1	25O10	184CE2	67.89
162CE1	25O10	184CZ2	72.02
162CE1	25O10	19OE1	61.36
162CE1	25O10	184CD1	68.78
162CE1	25O10	19NE2	90.18
162CE1	25O10	19CD	78.77
162CE1	25O10	162CG	32.27
162CE1	25O10	162NE2	9.58
162CE1	25O10	184CD2	67.64
162CE1	25O10	184CH2	73.24
162CE1	25O10	162CD2	21.07
162CE1	25O10	162CB	48.98
162CE1	25O10	25CB	50.48
162CE1	25O10	184CG	67.80
162CE1	25O10	25SG	61.27
184CE2	25O10	184CZ2	23.77
184CE2	25O10	19OE1	85.64
184CE2	25O10	184CD1	35.04
184CE2	25O10	19CD	95.11
184CE2	25O10	162CG	82.23
184CE2	25O10	162NE2	60.72
184CE2	25O10	184CD2	6.70
184CE2	25O10	184CH2	27.61
184CE2	25O10	162CD2	68.81

TABLE XVI

184CE2	25O10	162CB	92.97
184CE2	25O10	184CG	23.63
184CZ2	25O10	184CD1	58.81
184CZ2	25O10	162CG	73.16
184CZ2	25O10	162NE2	62.79
184CZ2	25O10	184CD2	30.47
184CZ2	25O10	184CH2	3.84
184CZ2	25O10	162CD2	63.78
184CZ2	25O10	162CB	78.57
184CZ2	25O10	184CG	47.41
19OE1	25O10	184CD1	54.02
19OE1	25O10	19NE2	33.65
19OE1	25O10	19CD	17.62
19OE1	25O10	162CG	90.23
19OE1	25O10	162NE2	68.58
19OE1	25O10	184CD2	79.62
19OE1	25O10	162CD2	82.33
19OE1	25O10	25CB	46.49
19OE1	25O10	184CG	64.24
19OE1	25O10	25SG	67.15
184CD1	25O10	19NE2	78.67
184CD1	25O10	19CD	60.49
184CD1	25O10	162CG	97.06
184CD1	25O10	162NE2	67.08
184CD1	25O10	184CD2	28.35
184CD1	25O10	184CH2	62.64
184CD1	25O10	162CD2	81.91
184CD1	25O10	25CB	94.29
184CD1	25O10	184CG	11.41
19NE2	25O10	19CD	18.97
19NE2	25O10	162NE2	98.89
19NE2	25O10	25CB	52.31
19NE2	25O10	184CG	90.06
19NE2	25O10	25SG	64.08
19CD	25O10	162NE2	86.19
19CD	25O10	184CD2	88.53
19CD	25O10	162CD2	99.61
19CD	25O10	25CB	54.29
19CD	25O10	184CG	71.79
19CD	25O10	25SG	71.77
162CG	25O10	162NE2	30.49
162CG	25O10	184CD2	85.26

TABLE XVI

162CG	25O10	184CH2	72.15
162CG	25O10	162CD2	15.20
162CG	25O10	162CB	16.86
162CG	25O10	25CB	60.05
162CG	25O10	184CG	92.50
162CG	25O10	25SG	56.96
162NE2	25O10	184CD2	61.36
162NE2	25O10	184CH2	63.86
162NE2	25O10	162CD2	16.25
162NE2	25O10	162CB	47.22
162NE2	25O10	25CB	59.84
162NE2	25O10	184CG	64.14
162NE2	25O10	25SG	69.18
184CD2	25O10	184CH2	34.30
184CD2	25O10	162CD2	71.14
184CD2	25O10	162CB	97.22
184CD2	25O10	184CG	16.94
184CH2	25O10	162CD2	63.64
184CH2	25O10	162CB	76.54
184CH2	25O10	184CG	51.24
162CD2	25O10	162CB	31.36
162CD2	25O10	25CB	62.62
162CD2	25O10	184CG	77.38
162CD2	25O10	25SG	65.53
162CB	25O10	25CB	66.47
162CB	25O10	25SG	56.57
25CB	25O10	25SG	21.55
161O	25C11	162ND1	77.52
161O	25C11	162CB	48.77
161O	25C11	162CG	66.44
161O	25C11	161C	9.16
161O	25C11	161OD1	44.79
161O	25C11	162CE1	89.91
161O	25C11	162CA	34.68
162ND1	25C11	162CB	36.88
162ND1	25C11	162CG	18.06
162ND1	25C11	184CZ2	57.93
162ND1	25C11	161C	73.11
162ND1	25C11	161OD1	88.11
162ND1	25C11	162CE1	12.39
162ND1	25C11	162CA	43.39
162CB	25C11	162CG	20.08

TABLE XVI

162CB	25C11	184CZ2	75.16
162CB	25C11	161C	41.40
162CB	25C11	161OD1	51.91
162CB	25C11	162CE1	47.69
162CB	25C11	162CA	18.23
162CG	25C11	184CZ2	60.65
162CG	25C11	161C	60.17
162CG	25C11	161OD1	70.16
162CG	25C11	162CE1	27.75
162CG	25C11	162CA	32.09
184CZ2	25C11	161OD1	96.89
184CZ2	25C11	162CE1	48.52
184CZ2	25C11	162CA	91.88
161C	25C11	161OD1	38.12
161C	25C11	162CE1	85.41
161C	25C11	162CA	29.74
161OD1	25C11	162CE1	97.18
161OD1	25C11	162CA	54.92
162CE1	25C11	162CA	55.72
161O	25C12	161OD1	53.96
161O	25C12	161CG	50.90
161O	25C12	161C	12.09
161O	25C12	162CB	45.66
161O	25C12	161CB	38.06
161O	25C12	162ND1	64.70
161OD1	25C12	161CG	14.06
161OD1	25C12	161C	42.27
161OD1	25C12	162CB	55.80
161OD1	25C12	161CB	30.86
161OD1	25C12	162ND1	86.96
161CG	25C12	161C	40.85
161CG	25C12	162CB	65.21
161CG	25C12	161CB	19.00
161CG	25C12	162ND1	96.52
161C	25C12	162CB	40.99
161C	25C12	161CB	31.65
161C	25C12	162ND1	65.80
162CB	25C12	161CB	67.55
162CB	25C12	162ND1	31.38
161CB	25C12	162ND1	96.34
161OD1	25C13	137O	81.25
161OD1	25C13	137C	63.73

TABLE XVI

161OD1	25C13	138N	56.48
161OD1	25C13	138CA	69.03
161OD1	25C13	137CB	63.42
161OD1	25C13	161CG	11.19
161OD1	25C13	161O	44.97
161OD1	25C13	162CB	53.52
161OD1	25C13	137CA	54.88
137O	25C13	137C	17.61
137O	25C13	138N	31.56
137O	25C13	184CZ2	73.45
137O	25C13	138CA	38.68
137O	25C13	137CB	38.26
137O	25C13	143NE2	53.14
137O	25C13	161CG	88.09
137O	25C13	184CH2	57.10
137O	25C13	162CB	89.51
137O	25C13	137CA	30.26
137C	25C13	138N	18.18
137C	25C13	184CZ2	85.16
137C	25C13	138CA	33.43
137C	25C13	137CB	33.67
137C	25C13	143NE2	68.48
137C	25C13	161CG	70.50
137C	25C13	184CH2	70.29
137C	25C13	162CB	80.53
137C	25C13	137CA	17.92
138N	25C13	138CA	19.51
138N	25C13	137CB	49.22
138N	25C13	143NE2	71.83
138N	25C13	161CG	60.17
138N	25C13	184CH2	87.76
138N	25C13	162CB	88.70
138N	25C13	137CA	30.79
184CZ2	25C13	137CB	62.75
184CZ2	25C13	143NE2	73.88
184CZ2	25C13	184CH2	16.99
184CZ2	25C13	162CB	71.91
184CZ2	25C13	137CA	79.40
138CA	25C13	137CB	66.92
138CA	25C13	143NE2	60.03
138CA	25C13	161CG	69.26
138CA	25C13	184CH2	94.51

TABLE XVI

138CA	25C13	137CA	49.37
137CB	25C13	143NE2	87.28
137CB	25C13	161CG	74.16
137CB	25C13	161O	86.27
137CB	25C13	184CH2	53.95
137CB	25C13	162CB	51.39
137CB	25C13	137CA	18.78
143NE2	25C13	184CH2	61.44
143NE2	25C13	137CA	83.39
161CG	25C13	161O	44.82
161CG	25C13	162CB	62.01
161CG	25C13	137CA	64.10
161O	25C13	162CB	40.52
161O	25C13	137CA	89.27
184CH2	25C13	162CB	78.30
184CH2	25C13	137CA	67.80
162CB	25C13	137CA	62.63
143NE2	25C14	184CZ2	89.78
143NE2	25C14	137O	59.02
143NE2	25C14	184CH2	73.23
143NE2	25C14	143CD	7.66
143NE2	25C14	137C	70.92
143NE2	25C14	138CA	63.43
143NE2	25C14	138N	72.92
184CZ2	25C14	137O	73.56
184CZ2	25C14	184CH2	18.41
184CZ2	25C14	143CD	82.48
184CZ2	25C14	137C	80.26
184CZ2	25C14	138N	95.58
137O	25C14	184CH2	58.32
137O	25C14	143CD	59.13
137O	25C14	137C	14.37
137O	25C14	138CA	35.52
137O	25C14	138N	26.67
184CH2	25C14	143CD	66.37
184CH2	25C14	137C	67.66
184CH2	25C14	138CA	93.75
184CH2	25C14	138N	83.05
143CD	25C14	137C	72.08
143CD	25C14	138CA	68.38
143CD	25C14	138N	76.11
137C	25C14	138CA	29.93

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TABLE XVI

137C	25C14	138N	15.47
138CA	25C14	138N	17.13
161OD1	25C15	138CA	95.49
161OD1	25C15	138N	74.59
161OD1	25C15	137C	77.97
161OD1	25C15	138CB	88.03
161OD1	25C15	137O	95.93
161OD1	25C15	161CG	16.54
161OD1	25C15	137CA	62.55
161OD1	25C15	161ND2	28.48
161OD1	25C15	137N	44.50
161OD1	25C15	137CB	65.90
161OD1	25C15	138OG	75.32
161OD1	25C15	161CB	26.73
161OD1	25C15	161O	41.09
138CA	25C15	138N	26.47
138CA	25C15	137C	42.87
138CA	25C15	138CB	25.16
138CA	25C15	137O	47.79
138CA	25C15	161CG	93.95
138CA	25C15	137CA	58.55
138CA	25C15	161ND2	78.54
138CA	25C15	137N	64.03
138CA	25C15	138C	11.03
138CA	25C15	137CB	75.54
138CA	25C15	143NE2	66.87
138CA	25C15	138OG	29.01
138CA	25C15	138O	24.54
138N	25C15	137C	22.54
138N	25C15	138CB	42.08
138N	25C15	137O	37.92
138N	25C15	161CG	78.54
138N	25C15	137CA	33.52
138N	25C15	161ND2	66.91
138N	25C15	137N	37.71
138N	25C15	138C	32.59
138N	25C15	137CB	52.24
138N	25C15	143NE2	80.31
138N	25C15	138OG	36.11
138N	25C15	161CB	95.16
138N	25C15	138O	46.34
137C	25C15	138CB	63.59

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TABLE XVI

137C	25C15 137O	19.93
137C	25C15 161CG	87.64
137C	25C15 137CA	18.45
137C	25C15 161ND2	80.75
137C	25C15 137N	33.66
137C	25C15 138C	43.43
137C	25C15 137CB	32.73
137C	25C15 143NE2	72.28
137C	25C15 138OG	58.64
137C	25C15 138O	53.23
138CB	25C15 137O	72.42
138CB	25C15 161CG	80.25
138CB	25C15 137CA	75.11
138CB	25C15 161ND2	63.55
138CB	25C15 137N	73.01
138CB	25C15 138C	33.69
138CB	25C15 137CB	94.23
138CB	25C15 143NE2	84.72
138CB	25C15 138OG	13.06
138CB	25C15 161CB	92.07
138CB	25C15 138O	41.98
137O	25C15 137CA	33.44
137O	25C15 137N	51.60
137O	25C15 138C	43.03
137O	25C15 137CB	37.73
137O	25C15 143NE2	53.68
137O	25C15 138OG	71.49
137O	25C15 138O	46.98
161CG	25C15 137CA	74.83
161CG	25C15 161ND2	16.70
161CG	25C15 137N	56.04
161CG	25C15 137CB	81.22
161CG	25C15 138OG	68.77
161CG	25C15 161CB	16.63
161CG	25C15 161O	45.51
137CA	25C15 161ND2	72.19
137CA	25C15 137N	18.82
137CA	25C15 138C	61.01
137CA	25C15 137CB	19.45
137CA	25C15 143NE2	86.99
137CA	25C15 138OG	66.83
137CA	25C15 161CB	89.10

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TABLE XVI

137CA	25C15 138O	71.60
137CA	25C15 161O	90.57
161ND2	25C15 137N	54.06
161ND2	25C15 138C	89.54
161ND2	25C15 137CB	83.68
161ND2	25C15 138OG	52.25
161ND2	25C15 161CB	30.53
161ND2	25C15 161O	62.17
137N	25C15 138C	69.92
137N	25C15 137CB	31.11
137N	25C15 138OG	61.80
137N	25C15 161CB	70.66
137N	25C15 138O	82.86
137N	25C15 161O	77.59
138C	25C15 137CB	75.69
138C	25C15 143NE2	55.85
138C	25C15 138OG	39.61
138C	25C15 138O	14.34
137CB	25C15 143NE2	85.14
137CB	25C15 138OG	86.28
137CB	25C15 161CB	91.92
137CB	25C15 138O	83.44
137CB	25C15 161O	82.09
143NE2	25C15 138OG	94.34
143NE2	25C15 138O	43.49
138OG	25C15 161CB	82.00
138OG	25C15 138O	50.85
161CB	25C15 161O	34.58
161O	25C16 162ND1	76.53
161O	25C16 161C	3.98
161O	25C16 162CB	45.40
161O	25C16 25SG	72.69
161O	25C16 162CA	34.24
161O	25C16 162CG	62.41
161O	25C16 162N	17.52
162ND1	25C16 161C	72.86
162ND1	25C16 162CB	33.34
162ND1	25C16 25SG	49.81
162ND1	25C16 162CA	43.06
162ND1	25C16 162CG	15.65
162ND1	25C16 162N	59.06
161C	25C16 162CB	41.47

TABLE XVI

161C	25C16	25SG	71.63
161C	25C16	162CA	30.96
161C	25C16	162CG	58.58
161C	25C16	162N	14.06
162CB	25C16	25SG	60.72
162CB	25C16	162CA	19.06
162CB	25C16	162CG	17.85
162CB	25C16	162N	29.15
25SG	25C16	162CA	49.45
25SG	25C16	162CG	54.90
25SG	25C16	162N	61.48
162CA	25C16	162CG	30.90
162CA	25C16	162N	16.94
162CG	25C16	162N	45.31
161O	25O17	161C	2.40
161O	25N18	25SG	94.42
161O	25N18	162ND1	86.25
161O	25N18	162CA	41.79
161O	25N18	162CB	49.55
161O	25N18	161C	8.51
161O	25N18	162CG	69.44
161O	25N18	162CE1	97.59
161O	25N18	162N	24.49
25SG	25N18	162ND1	65.37
25SG	25N18	162CA	62.23
25SG	25N18	162CB	74.73
25SG	25N18	161C	86.60
25SG	25N18	162CG	67.87
25SG	25N18	25CB	21.50
25SG	25N18	162CE1	64.64
25SG	25N18	162N	73.85
25SG	25N18	19NE2	67.61
25SG	25N18	23CA	79.71
162ND1	25N18	162CA	50.07
162ND1	25N18	162CB	36.70
162ND1	25N18	161C	79.92
162ND1	25N18	162CG	16.82
162ND1	25N18	25CB	53.33
162ND1	25N18	162CE1	11.34
162ND1	25N18	162N	65.85
162ND1	25N18	19NE2	73.54
162CA	25N18	162CB	21.06

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TABLE XVI

162CA	25N18	161C	33.62
162CA	25N18	162CG	34.82
162CA	25N18	25CB	70.27
162CA	25N18	162CE1	60.64
162CA	25N18	162N	17.53
162CB	25N18	161C	43.55
162CB	25N18	162CG	19.91
162CB	25N18	25CB	75.42
162CB	25N18	162CE1	48.04
162CB	25N18	162N	31.25
161C	25N18	162CG	63.15
161C	25N18	162CE1	91.21
161C	25N18	162N	16.15
162CG	25N18	25CB	61.89
162CG	25N18	162CE1	28.15
162CG	25N18	162N	49.49
162CG	25N18	19NE2	89.96
25CB	25N18	162CE1	48.89
25CB	25N18	162N	85.68
25CB	25N18	19NE2	49.72
25CB	25N18	23CA	76.32
162CE1	25N18	162N	76.89
162CE1	25N18	19NE2	62.43
19NE2	25N18	23CA	47.71
25SG	25C19	161O	93.76
25SG	25C19	23CA	98.71
25SG	25C19	25CB	19.06
25SG	25C19	162ND1	55.42
25SG	25C19	23C	83.02
25SG	25C19	162CA	57.95
25SG	25C19	161C	85.45
25SG	25C19	23O	84.21
25SG	25C19	25N	39.84
161O	25C19	162ND1	68.34
161O	25C19	162CA	36.84
161O	25C19	161C	9.82
23CA	25C19	25CB	86.55
23CA	25C19	23C	19.53
23CA	25C19	23O	30.41
23CA	25C19	25N	58.86
25CB	25C19	162ND1	49.56
25CB	25C19	23C	74.71

TABLE XVI

25CB	25C19	162CA	67.81
25CB	25C19	161C	97.94
25CB	25C19	23O	80.56
25CB	25C19	25N	30.79
162ND1	25C19	162CA	42.46
162ND1	25C19	161C	67.39
162ND1	25C19	25N	78.08
23C	25C19	23O	15.10
23C	25C19	25N	44.37
162CA	25C19	161C	30.60
162CA	25C19	25N	96.99
23O	25C19	25N	49.95
184CZ2	25N20	162ND1	57.46
184CZ2	25N20	184NE1	33.66
184CZ2	25N20	184CE2	16.92
184CZ2	25N20	162CE1	48.47
162ND1	25N20	184NE1	53.53
162ND1	25N20	184CE2	56.14
162ND1	25N20	162CE1	14.39
184NE1	25N20	184CE2	17.07
184NE1	25N20	162CE1	39.26
184CE2	25N20	162CE1	43.67
161O	25C21	25SG	97.39
161O	25C21	161C	15.35
161O	25C21	162CA	39.27
161O	25C21	162N	27.81
161O	25C21	161CA	24.14
161O	25C21	25CB	98.96
25SG	25C21	161C	94.07
25SG	25C21	162CA	60.19
25SG	25C21	162N	78.17
25SG	25C21	65CA	98.56
25SG	25C21	25CB	7.84
161C	25C21	162CA	33.93
161C	25C21	162N	16.70
161C	25C21	161CA	15.71
161C	25C21	25CB	97.60
162CA	25C21	162N	19.15
162CA	25C21	161CA	48.75
162CA	25C21	25CB	63.75
162N	25C21	161CA	30.04
162N	25C21	25CB	82.42

TABLE XVI

65CA	25C21	25CB	98.99
25SG	25C22	25CB	34.66
25SG	25C22	25N	70.64
25SG	25C22	25CA	48.75
25SG	25C22	19NE2	98.64
25SG	25C22	24C	78.81
25SG	25C22	162ND1	56.90
25SG	25C22	26N	47.65
25SG	25C22	25C	40.82
25SG	25C22	161O	81.68
25SG	25C22	24CA	97.30
25SG	25C22	162CA	49.19
25SG	25C22	163N	21.43
25SG	25C22	26CD1	82.19
25CB	25C22	25N	45.70
25CB	25C22	25CA	23.52
25CB	25C22	24N	85.13
25CB	25C22	19NE2	64.70
25CB	25C22	24C	56.87
25CB	25C22	162ND1	56.29
25CB	25C22	26N	47.43
25CB	25C22	25C	31.07
25CB	25C22	24CA	75.01
25CB	25C22	162CA	74.58
25CB	25C22	163N	53.55
25CB	25C22	26CD1	84.62
25N	25C22	25CA	23.10
25N	25C22	23C	59.53
25N	25C22	23CA	76.19
25N	25C22	23O	65.52
25N	25C22	24N	41.74
25N	25C22	19NE2	55.79
25N	25C22	24C	11.64
25N	25C22	162ND1	98.55
25N	25C22	26N	37.79
25N	25C22	25C	31.73
25N	25C22	24CA	29.34
25N	25C22	163N	92.04
25N	25C22	26CD1	53.86
25CA	25C22	23C	82.62
25CA	25C22	23CA	98.07
25CA	25C22	23O	87.79

TABLE XVI

25CA	25C22	24N	64.51
25CA	25C22	19NE2	62.14
25CA	25C22	24C	33.67
25CA	25C22	162ND1	79.26
25CA	25C22	26N	32.62
25CA	25C22	25C	17.41
25CA	25C22	24CA	52.26
25CA	25C22	162CA	95.54
25CA	25C22	163N	70.10
25CA	25C22	26CD1	64.67
23C	25C22	23CA	22.66
23C	25C22	23O	17.69
23C	25C22	24N	19.11
23C	25C22	19NE2	64.93
23C	25C22	24C	49.94
23C	25C22	26N	82.64
23C	25C22	25C	87.50
23C	25C22	24CA	31.15
23C	25C22	26CD1	58.43
23CA	25C22	23O	35.06
23CA	25C22	24N	35.02
23CA	25C22	19NE2	59.32
23CA	25C22	24C	68.76
23CA	25C22	24CA	51.14
23CA	25C22	26CD1	80.22
23O	25C22	24N	32.37
23O	25C22	19NE2	82.31
23O	25C22	24C	54.24
23O	25C22	26N	77.95
23O	25C22	25C	87.44
23O	25C22	24CA	36.53
23O	25C22	26CD1	46.14
24N	25C22	19NE2	52.35
24N	25C22	24C	33.74
24N	25C22	26N	70.95
24N	25C22	25C	71.93
24N	25C22	24CA	17.11
24N	25C22	26CD1	57.95
19NE2	25C22	24C	60.62
19NE2	25C22	162ND1	74.96
19NE2	25C22	26N	91.86
19NE2	25C22	25C	79.36

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TABLE XVI

19NE2	25C22	24CA	60.80
24C	25C22	26N	39.04
24C	25C22	25C	38.21
24C	25C22	24CA	18.87
24C	25C22	163N	99.80
24C	25C22	26CD1	45.21
162ND1	25C22	26N	99.77
162ND1	25C22	25C	85.70
162ND1	25C22	161O	61.42
162ND1	25C22	162CA	41.62
162ND1	25C22	163N	51.67
26N	25C22	25C	16.78
26N	25C22	24CA	53.95
26N	25C22	162CA	94.45
26N	25C22	163N	65.37
26N	25C22	26CD1	38.29
25C	25C22	24CA	56.48
25C	25C22	162CA	90.01
25C	25C22	163N	61.59
25C	25C22	26CD1	53.65
161O	25C22	162CA	33.51
161O	25C22	163N	60.45
24CA	25C22	26CD1	44.43
162CA	25C22	163N	29.15
163N	25C22	26CD1	93.88
25SG	25O23	25N	73.79
25SG	25O23	25CB	39.28
25SG	25O23	25CA	55.31
25SG	25O23	24C	83.85
25SG	25O23	19OE1	93.34
25SG	25O23	162ND1	57.67
25SG	25O23	25C	46.54
25SG	25O23	26N	46.32
25SG	25O23	162CE1	63.52
25N	25O23	25CB	50.74
25N	25O23	19NE2	75.64
25N	25O23	23CA	93.95
25N	25O23	23C	70.21
25N	25O23	24N	51.30
25N	25O23	25CA	24.54
25N	25O23	23O	71.33
25N	25O23	24C	13.19

TABLE XVI

25N	25O23	19CD	72.43
25N	25O23	19OE1	71.68
25N	25O23	24CA	34.54
25N	25O23	22O	81.27
25N	25O23	23N	91.47
25N	25O23	25C	27.51
25N	25O23	26N	31.41
25N	25O23	22C	85.55
25N	25O23	162CE1	95.76
25CB	25O23	19NE2	84.85
25CB	25O23	25CA	26.21
25CB	25O23	24C	63.90
25CB	25O23	19CD	71.92
25CB	25O23	19OE1	57.57
25CB	25O23	24CA	85.27
25CB	25O23	162ND1	56.16
25CB	25O23	25C	29.27
25CB	25O23	26N	43.07
25CB	25O23	162CE1	50.07
19NE2	25O23	23CA	79.80
19NE2	25O23	23C	86.33
19NE2	25O23	24N	70.00
19NE2	25O23	25CA	78.56
19NE2	25O23	24C	75.95
19NE2	25O23	19CD	14.24
19NE2	25O23	19OE1	31.36
19NE2	25O23	24CA	76.27
19NE2	25O23	22O	39.90
19NE2	25O23	162ND1	87.36
19NE2	25O23	23N	69.25
19NE2	25O23	25C	92.00
19NE2	25O23	22C	53.68
19NE2	25O23	162CE1	73.60
23CA	25O23	23C	26.89
23CA	25O23	24N	42.72
23CA	25O23	23O	37.90
23CA	25O23	24C	81.01
23CA	25O23	19CD	93.90
23CA	25O23	24CA	59.79
23CA	25O23	22O	39.98
23CA	25O23	23N	10.55
23CA	25O23	22C	26.16

TABLE XVI

23C	25O23	24N	23.21
23C	25O23	25CA	94.66
23C	25O23	23O	17.05
23C	25O23	24C	57.02
23C	25O23	19CD	98.07
23C	25O23	24CA	35.84
23C	25O23	22O	50.35
23C	25O23	23N	31.08
23C	25O23	25C	92.95
23C	25O23	26N	83.85
23C	25O23	22C	39.73
24N	25O23	25CA	75.53
24N	25O23	23O	35.32
24N	25O23	24C	38.60
24N	25O23	19CD	79.21
24N	25O23	19OE1	91.96
24N	25O23	24CA	18.27
24N	25O23	22O	43.58
24N	25O23	23N	40.76
24N	25O23	25C	77.49
24N	25O23	26N	73.33
24N	25O23	22C	39.68
25CA	25O23	23O	94.04
25CA	25O23	24C	37.72
25CA	25O23	19CD	69.69
25CA	25O23	19OE1	61.67
25CA	25O23	24CA	59.08
25CA	25O23	22O	98.54
25CA	25O23	162ND1	81.63
25CA	25O23	25C	13.70
25CA	25O23	26N	29.03
25CA	25O23	162CE1	73.11
23O	25O23	24C	58.97
23O	25O23	24CA	40.61
23O	25O23	22O	67.32
23O	25O23	23N	45.18
23O	25O23	25C	88.46
23O	25O23	26N	76.05
23O	25O23	22C	56.12
24C	25O23	19CD	76.06
24C	25O23	19OE1	79.00
24C	25O23	24CA	21.38

TABLE XVI

24C	25O23	22O	72.85
24C	25O23	23N	79.21
24C	25O23	25C	39.06
24C	25O23	26N	38.39
24C	25O23	22C	74.96
19CD	25O23	19OE1	17.16
19CD	25O23	24CA	81.63
19CD	25O23	22O	53.92
19CD	25O23	162ND1	75.34
19CD	25O23	23N	83.37
19CD	25O23	25C	83.39
19CD	25O23	26N	97.86
19CD	25O23	22C	67.74
19CD	25O23	162CE1	60.88
19OE1	25O23	24CA	90.13
19OE1	25O23	22O	71.06
19OE1	25O23	162ND1	60.32
19OE1	25O23	25C	74.84
19OE1	25O23	26N	90.69
19OE1	25O23	22C	84.88
19OE1	25O23	162CE1	45.33
24CA	25O23	22O	59.13
24CA	25O23	23N	58.89
24CA	25O23	25C	59.55
24CA	25O23	26N	55.16
24CA	25O23	22C	57.43
22O	25O23	23N	29.49
22O	25O23	22C	13.82
162ND1	25O23	25C	84.77
162ND1	25O23	26N	95.34
162ND1	25O23	162CE1	15.15
23N	25O23	22C	15.68
25C	25O23	26N	16.15
25C	25O23	162CE1	79.30
26N	25O23	162CE1	92.61
59O	25C24	61OD2	91.98
59O	25C24	60CA	42.04
59O	25C24	61N	69.68
59O	25C24	60ND2	53.63
59O	25C24	60C	52.10
59O	25C24	59C	9.13
59O	25C24	67CD2	94.90

TABLE XVI

59O	25C24	61CB	94.67
59O	25C24	60N	25.18
59O	25C24	65O	98.75
59O	25C24	66CA	92.74
59O	25C24	61CG	94.59
61OD2	25C24	60CA	80.40
61OD2	25C24	61N	53.38
61OD2	25C24	60C	60.45
61OD2	25C24	59C	89.44
61OD2	25C24	61CB	30.44
61OD2	25C24	60N	85.15
61OD2	25C24	65O	70.09
61OD2	25C24	61CG	12.52
60CA	25C24	61N	33.63
60CA	25C24	60ND2	37.06
60CA	25C24	60C	20.13
60CA	25C24	59C	32.92
60CA	25C24	67CD2	94.92
60CA	25C24	61CB	64.63
60CA	25C24	60N	16.87
60CA	25C24	65O	56.77
60CA	25C24	66CA	57.08
60CA	25C24	61CG	74.69
61N	25C24	60ND2	64.13
61N	25C24	60C	17.58
61N	25C24	59C	61.42
61N	25C24	61CB	31.27
61N	25C24	60N	47.40
61N	25C24	65O	35.46
61N	25C24	66CA	57.56
61N	25C24	61CG	44.25
60ND2	25C24	60C	56.24
60ND2	25C24	67CE2	75.32
60ND2	25C24	59C	47.84
60ND2	25C24	67CD2	57.88
60ND2	25C24	61CB	93.87
60ND2	25C24	60N	39.84
60ND2	25C24	65O	66.16
60ND2	25C24	66CA	42.71
60C	25C24	59C	43.92
60C	25C24	61CB	46.05
60C	25C24	60N	30.63

TABLE XVI

60C	25C24	65O	50.56
60C	25C24	66CA	64.32
60C	25C24	61CG	54.63
67CE2	25C24	67CD2	17.47
67CE2	25C24	66CA	72.97
59C	25C24	67CD2	95.05
59C	25C24	61CB	88.03
59C	25C24	60N	16.05
59C	25C24	65O	89.64
59C	25C24	66CA	84.79
59C	25C24	61CG	90.22
67CD2	25C24	60N	94.87
67CD2	25C24	65O	94.21
67CD2	25C24	66CA	61.75
61CB	25C24	60N	76.56
61CB	25C24	65O	39.70
61CB	25C24	66CA	72.80
61CB	25C24	61CG	18.05
60N	25C24	65O	73.63
60N	25C24	66CA	70.86
60N	25C24	61CG	82.69
65O	25C24	66CA	33.53
65O	25C24	61CG	57.60
66CA	25C24	61CG	90.84
61OD2	25C25	61CB	42.75
61OD2	25C25	61N	69.21
61OD2	25C25	61CG	18.75
61OD2	25C25	65O	92.92
61OD2	25C25	60C	73.08
61OD2	25C25	61CA	51.10
61OD2	25C25	59O	97.68
61OD2	25C25	60CA	92.69
61OD2	25C25	61OD1	17.96
61OD2	25C25	60O	63.26
61CB	25C25	61N	40.79
61CB	25C25	61CG	24.59
61CB	25C25	65O	50.21
61CB	25C25	60C	55.95
61CB	25C25	61CA	21.34
61CB	25C25	60CA	75.07
61CB	25C25	61OD1	27.44
61CB	25C25	65C	60.47

TABLE XVI

61CB	25C25	60O	54.86
61CB	25C25	66CA	83.99
61N	25C25	61CG	58.00
61N	25C25	65O	42.60
61N	25C25	60C	18.61
61N	25C25	61CA	20.61
61N	25C25	59O	69.42
61N	25C25	60CA	34.61
61N	25C25	61OD1	62.35
61N	25C25	65C	54.60
61N	25C25	60O	25.90
61N	25C25	66CA	60.64
61CG	25C25	65O	74.72
61CG	25C25	60C	67.35
61CG	25C25	61CA	37.75
61CG	25C25	60CA	88.04
61CG	25C25	61OD1	4.51
61CG	25C25	65C	84.40
61CG	25C25	60O	60.77
65O	25C25	60C	58.12
65O	25C25	61CA	47.61
65O	25C25	60CA	61.97
65O	25C25	61OD1	77.08
65O	25C25	65C	12.55
65O	25C25	60O	68.17
65O	25C25	66CA	34.76
60C	25C25	61CA	34.62
60C	25C25	59O	51.04
60C	25C25	60CA	20.69
60C	25C25	61OD1	71.85
60C	25C25	65C	68.94
60C	25C25	60O	12.51
60C	25C25	66CA	66.29
61CA	25C25	59O	84.06
61CA	25C25	60CA	53.97
61CA	25C25	61OD1	41.99
61CA	25C25	65C	60.01
61CA	25C25	60O	34.68
61CA	25C25	66CA	75.36
59O	25C25	60CA	38.70
59O	25C25	60O	49.63
59O	25C25	66CA	83.86

TABLE XVI

60CA	25C25	61OD1	92.54
60CA	25C25	65C	69.48
60CA	25C25	60O	29.48
60CA	25C25	66CA	56.22
61OD1	25C25	65C	86.17
61OD1	25C25	60O	65.14
65C	25C25	60O	79.72
65C	25C25	66CA	29.00
60O	25C25	66CA	78.80
61CB	25C26	65O	57.98
61CB	25C26	61OD2	40.43
61CB	25C26	61CG	23.23
61CB	25C26	61N	39.07
61CB	25C26	65C	73.35
61CB	25C26	61CA	18.97
61CB	25C26	64O	64.81
61CB	25C26	66N	88.64
61CB	25C26	66CA	94.09
61CB	25C26	60C	49.39
61CB	25C26	65CA	72.50
61CB	25C26	64C	54.69
61CB	25C26	61OD1	25.08
61CB	25C26	60CA	66.90
65O	25C26	61OD2	96.74
65O	25C26	61CG	81.20
65O	25C26	61N	45.23
65O	25C26	65C	17.69
65O	25C26	61CA	49.81
65O	25C26	64O	56.41
65O	25C26	66N	30.68
65O	25C26	66CA	39.57
65O	25C26	60C	55.87
65O	25C26	65CA	28.89
65O	25C26	64C	44.41
65O	25C26	61OD1	82.28
65O	25C26	60CA	58.71
61OD2	25C26	61CG	19.08
61OD2	25C26	61N	60.79
61OD2	25C26	61CA	47.71
61OD2	25C26	64O	94.75
61OD2	25C26	60C	60.86
61OD2	25C26	64C	89.54

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TABLE XVI

61OD2	25C26	61OD1	23.61
61OD2	25C26	60CA	75.67
61CG	25C26	61N	54.13
61CG	25C26	65C	96.40
61CG	25C26	61CA	36.24
61CG	25C26	64O	76.97
61CG	25C26	60C	59.38
61CG	25C26	65CA	93.65
61CG	25C26	64C	70.68
61CG	25C26	61OD1	7.62
61CG	25C26	60CA	76.74
61N	25C26	65C	62.37
61N	25C26	61CA	20.12
61N	25C26	64O	88.15
61N	25C26	66N	69.41
61N	25C26	66CA	64.66
61N	25C26	60C	13.98
61N	25C26	65CA	73.06
61N	25C26	64C	74.50
61N	25C26	61OD1	59.89
61N	25C26	60CA	28.83
65C	25C26	61CA	67.25
65C	25C26	64O	51.79
65C	25C26	66N	17.38
65C	25C26	66CA	33.55
65C	25C26	60C	71.82
65C	25C26	65CA	17.23
65C	25C26	64C	43.45
65C	25C26	61OD1	96.15
65C	25C26	60CA	71.11
61CA	25C26	64O	76.04
61CA	25C26	66N	79.28
61CA	25C26	66CA	79.89
61CA	25C26	60C	31.02
61CA	25C26	65CA	72.24
61CA	25C26	64C	63.54
61CA	25C26	61OD1	40.94
61CA	25C26	60CA	48.15
64O	25C26	66N	65.51
64O	25C26	66CA	84.31
64O	25C26	65CA	35.23
64O	25C26	64C	13.78

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TABLE XVI

64O	25C26	61OD1	71.21
66N	25C26	66CA	19.09
66N	25C26	60C	75.28
66N	25C26	65CA	30.56
66N	25C26	64C	59.39
66N	25C26	60CA	69.05
66CA	25C26	60C	66.08
66CA	25C26	65CA	49.11
66CA	25C26	64C	76.99
66CA	25C26	60CA	55.34
60C	25C26	65CA	84.60
60C	25C26	64C	88.43
60C	25C26	61OD1	66.22
60C	25C26	60CA	17.82
65CA	25C26	64C	29.29
65CA	25C26	61OD1	91.21
65CA	25C26	60CA	86.87
64C	25C26	61OD1	66.22
64C	25C26	60CA	98.77
61OD1	25C26	60CA	83.78
65O	25C27	65C	19.69
65O	25C27	66N	35.95
65O	25C27	66CA	44.75
65O	25C27	65CA	32.29
65O	25C27	64O	53.20
65O	25C27	61CB	45.32
65O	25C27	66C	62.38
65O	25C27	61N	36.43
65O	25C27	61OD2	72.86
65O	25C27	66O	66.33
65C	25C27	66N	20.59
65C	25C27	66CA	38.16
65C	25C27	65CA	18.27
65C	25C27	64O	50.92
65C	25C27	61CB	62.98
65C	25C27	66C	52.26
65C	25C27	61N	55.57
65C	25C27	61OD2	91.46
65C	25C27	66O	51.89
66N	25C27	66CA	22.16
66N	25C27	65CA	32.66
66N	25C27	64O	68.31

TABLE XVI

67CE2	25C28	66C	86.92
67CE2	25C28	67CG	33.10
67CE2	25C28	67N	73.57
67CE2	25C28	67CE1	29.88
67CE2	25C28	60ND2	85.55
67CE2	25C28	66O	85.99
67CE2	25C28	67CD1	33.21
67CD2	25C28	67CZ	38.76
67CD2	25C28	66CA	84.93
67CD2	25C28	67OH	56.87
67CD2	25C28	66C	66.69
67CD2	25C28	67CG	16.19
67CD2	25C28	67N	51.42
67CD2	25C28	67CE1	37.73
67CD2	25C28	60ND2	63.64
67CD2	25C28	66O	69.45
67CD2	25C28	67CD1	28.35
67CZ	25C28	67OH	19.51
67CZ	25C28	66C	88.11
67CZ	25C28	67CG	39.85
67CZ	25C28	67N	79.74
67CZ	25C28	67CE1	15.82
67CZ	25C28	66O	82.16
67CZ	25C28	67CD1	29.69
66CA	25C28	66C	21.36
66CA	25C28	66N	20.18
66CA	25C28	67CG	73.95
66CA	25C28	65O	39.39
66CA	25C28	67N	33.53
66CA	25C28	65C	33.20
66CA	25C28	67CE1	94.77
66CA	25C28	60ND2	46.84
66CA	25C28	66O	30.13
66CA	25C28	67CD1	79.87
67OH	25C28	67CG	59.35
67OH	25C28	67N	98.79
67OH	25C28	67CE1	31.87
67OH	25C28	66O	96.91
67OH	25C28	67CD1	48.13
66C	25C28	66N	33.87
66C	25C28	67CG	53.83
66C	25C28	65O	60.02

TABLE XVI

66C	25C28	67N	17.65
66C	25C28	65C	50.69
66C	25C28	67CE1	73.54
66C	25C28	60ND2	49.87
66C	25C28	66O	14.26
66C	25C28	67CD1	58.53
66N	25C28	67CG	86.97
66N	25C28	65O	30.60
66N	25C28	67N	50.32
66N	25C28	65C	17.37
66N	25C28	67CE1	99.34
66N	25C28	60ND2	66.19
66N	25C28	66O	33.91
66N	25C28	67CD1	87.99
67CG	25C28	67N	41.20
67CG	25C28	67CE1	31.84
67CG	25C28	60ND2	64.79
67CG	25C28	66O	54.35
67CG	25C28	67CD1	16.69
65O	25C28	67N	72.54
65O	25C28	65C	16.08
65O	25C28	60ND2	67.97
65O	25C28	66O	63.89
67N	25C28	65C	66.13
67N	25C28	67CE1	67.52
67N	25C28	60ND2	39.36
67N	25C28	66O	28.39
67N	25C28	67CD1	50.73
65C	25C28	60ND2	73.05
65C	25C28	66O	51.14
67CE1	25C28	60ND2	96.62
67CE1	25C28	66O	66.57
67CE1	25C28	67CD1	17.05
60ND2	25C28	66O	64.03
60ND2	25C28	67CD1	80.40
66O	25C28	67CD1	54.11
67CE2	25C29	67CD2	24.48
67CE2	25C29	60ND2	95.45
67CE2	25C29	67CZ	15.31
67CE2	25C29	66CA	94.75
67CE2	25C29	67CG	30.54
67CE2	25C29	67OH	29.52

TABLE XVI

67CE2	25C29	67N	69.16
67CE2	25C29	66C	76.62
67CE2	25C29	70OD1	69.19
67CD2	25C29	60ND2	70.99
67CD2	25C29	67CZ	35.94
67CD2	25C29	66CA	77.68
67CD2	25C29	67CG	11.52
67CD2	25C29	67OH	52.86
67CD2	25C29	67N	48.30
67CD2	25C29	66C	59.66
67CD2	25C29	70OD1	48.35
60ND2	25C29	59O	51.92
60ND2	25C29	66CA	47.48
60ND2	25C29	67CG	67.53
60ND2	25C29	67N	39.60
60ND2	25C29	60CA	34.92
60ND2	25C29	66C	48.58
60ND2	25C29	70OD1	36.76
60ND2	25C29	65O	66.66
59O	25C29	66CA	91.68
59O	25C29	67N	91.44
59O	25C29	60CA	36.13
59O	25C29	66C	99.32
59O	25C29	70OD1	57.47
59O	25C29	65O	87.31
67CZ	25C29	66CA	92.71
67CZ	25C29	67CG	37.70
67CZ	25C29	67OH	17.56
67CZ	25C29	67N	72.63
67CZ	25C29	66C	75.91
67CZ	25C29	70OD1	83.35
66CA	25C29	67CG	67.01
66CA	25C29	67N	30.81
66CA	25C29	60CA	57.52
66CA	25C29	66C	18.31
66CA	25C29	70OD1	76.75
66CA	25C29	65O	34.30
67CG	25C29	67OH	55.25
67CG	25C29	67N	38.92
67CG	25C29	66C	48.79
67CG	25C29	70OD1	52.17
67OH	25C29	67N	88.91

TABLE XVI

67OH	25C29	66C	89.71
67OH	25C29	70OD1	98.59
67N	25C29	60CA	68.41
67N	25C29	66C	16.09
67N	25C29	70OD1	52.40
67N	25C29	65O	64.97
60CA	25C29	66C	69.66
60CA	25C29	70OD1	64.85
60CA	25C29	65O	52.85
66C	25C29	70OD1	68.06
66C	25C29	65O	51.98
65C	25C30	66N	22.36
65C	25C30	65O	19.60
65C	25C30	65CA	24.11
65C	25C30	64O	60.69
65C	25C30	66CA	37.47
65C	25C30	64C	47.70
65C	25C30	65N	31.97
65C	25C30	66C	52.44
65C	25C30	66O	56.13
66N	25C30	65O	36.76
66N	25C30	65CA	39.03
66N	25C30	64O	81.12
66N	25C30	66CA	20.96
66N	25C30	64C	68.55
66N	25C30	65N	51.94
66N	25C30	66C	31.15
66N	25C30	66O	33.85
65O	25C30	65CA	37.88
65O	25C30	64O	60.09
65O	25C30	66CA	42.53
65O	25C30	64C	47.65
65O	25C30	65N	37.00
65O	25C30	66C	60.78
65O	25C30	66O	69.10
65CA	25C30	64O	43.45
65CA	25C30	66CA	58.77
65CA	25C30	64C	32.33
65CA	25C30	65N	16.26
65CA	25C30	66C	69.64
65CA	25C30	66O	67.50
64O	25C30	66CA	98.08

TABLE XVI

64O	25C30	64C	13.08
64O	25C30	65N	29.19
66CA	25C30	64C	85.02
66CA	25C30	65N	69.41
66CA	25C30	66C	18.61
66CA	25C30	66O	30.64
64C	25C30	65N	16.80
64C	25C30	66C	99.65
64C	25C30	66O	99.64
65N	25C30	66C	83.08
65N	25C30	66O	82.93
66C	25C30	66O	15.25
66N	25O31	65C	17.32
66N	25O31	67CZ	97.91
66N	25O31	65CA	31.08
66N	25O31	64O	62.95
66N	25O31	66CA	17.26
66N	25O31	66O	33.20
66N	25O31	67CE1	92.81
66N	25O31	67CE2	86.83
66N	25O31	65O	26.88
66N	25O31	66C	29.04
65C	25O31	65CA	19.09
65C	25O31	64O	46.34
65C	25O31	66CA	30.23
65C	25O31	66O	50.48
65C	25O31	67CE2	97.89
65C	25O31	65O	13.61
65C	25O31	66C	45.49
67OH	25O31	67CZ	17.55
67OH	25O31	66CA	98.18
67OH	25O31	66O	90.84
67OH	25O31	67CE1	29.52
67OH	25O31	67CE2	29.04
67OH	25O31	66C	87.47
67CZ	25O31	66CA	81.60
67CZ	25O31	66O	73.49
67CZ	25O31	67CE1	16.52
67CZ	25O31	67CE2	16.35
67CZ	25O31	66C	69.99
65CA	25O31	64O	34.51
65CA	25O31	66CA	47.38

TABLE XVI

65CA	25O31	66O	60.33
65CA	25O31	65O	28.52
65CA	25O31	66C	59.78
64O	25O31	66CA	76.15
64O	25O31	66O	94.57
64O	25O31	65O	44.97
64O	25O31	66C	91.77
66CA	25O31	66O	28.82
66CA	25O31	67CE1	78.69
66CA	25O31	67CE2	69.71
66CA	25O31	65O	33.12
66CA	25O31	66C	17.65
66O	25O31	67CE1	63.44
66O	25O31	67CE2	68.73
66O	25O31	65O	58.85
66O	25O31	66C	14.31
67CE1	25O31	67CE2	28.45
67CE1	25O31	66C	63.77
67CE2	25O31	65O	93.08
67CE2	25O31	66C	61.53
65O	25O31	66C	50.53
66O	25C32	66N	36.46
66O	25C32	65CA	64.42
66O	25C32	65C	52.71
66O	25C32	67CE1	69.47
66O	25C32	66C	14.32
66O	25C32	67CZ	76.69
66O	25C32	66CA	29.45
66O	25C32	67OH	92.97
66N	25C32	65CA	31.01
66N	25C32	65C	16.26
66N	25C32	67CE1	96.14
66N	25C32	66C	30.68
66N	25C32	67CZ	95.21
66N	25C32	66CA	16.64
65CA	25C32	65C	18.68
65CA	25C32	66C	61.49
65CA	25C32	66CA	46.86
65C	25C32	66C	46.16
65C	25C32	66CA	29.55
67CE1	25C32	66C	67.09
67CE1	25C32	67CZ	16.76

TABLE XVI

67CE1	25C32	66CA	79.83
67CE1	25C32	67OH	29.00
66C	25C32	67CZ	70.31
66C	25C32	66CA	18.10
66C	25C32	67OH	85.85
67CZ	25C32	66CA	78.64
67CZ	25C32	67OH	16.35
66CA	25C32	67OH	92.05
67CE1	25O33	67CZ	18.11
67CE1	25O33	67OH	32.18
67CE1	25O33	66O	70.79
67CE1	25O33	67CD1	16.55
67CE1	25O33	253OH2	91.77
67CZ	25O33	67OH	17.82
67CZ	25O33	66O	76.31
67CZ	25O33	67CD1	30.29
67CZ	25O33	253OH2	94.53
67OH	25O33	66O	93.31
67OH	25O33	67CD1	47.11
67OH	25O33	253OH2	82.17
66O	25O33	67CD1	55.11
253OH2	25O33	160O	32.53
66O	25C34	66N	39.24
66O	25C34	65CA	72.10
66O	25C34	65C	54.84
66O	25C34	25SG	98.30
66O	25C34	66C	10.30
66N	25C34	65CA	33.35
66N	25C34	65C	15.62
66N	25C34	25SG	96.34
66N	25C34	66C	31.01
65CA	25C34	65C	18.75
65CA	25C34	25SG	85.74
65CA	25C34	66C	64.35
65C	25C34	25SG	95.57
65C	25C34	66C	46.29
25SG	25C34	161O	60.31
25SG	25C34	161C	66.90
161O	25C34	161C	14.93
66O	25C35	66C	7.49
66O	25C35	68CE	57.46
66O	25C35	66N	35.66

TABLE XVI

66O	25C35 163CB	89.86
66O	25C35 66CA	21.29
66C	25C35 68CE	64.25
66C	25C35 66N	32.33
66C	25C35 163CB	97.34
66C	25C35 66CA	16.42
68CE	25C35 66N	88.65
68CE	25C35 163CB	42.93
68CE	25C35 163N	71.03
68CE	25C35 66CA	78.09
66N	25C35 66CA	16.42
163CB	25C35 163N	28.84
66O	25C36 68CE	48.64
66O	25C36 67CD1	56.25
66O	25C36 67CE1	67.39
134CB	25C36 209CD2	53.33
134CB	25C36 68CE	70.27
134CB	25C36 160O	87.04
134CB	25C36 162N	72.66
134CB	25C36 160C	74.39
134CB	25C36 161C	86.84
134CB	25C36 161CA	88.42
134CB	25C36 161N	74.11
134CB	25C36 160CB	54.87
209CD2	25C36 68CE	80.58
209CD2	25C36 160O	88.38
209CD2	25C36 160C	87.02
209CD2	25C36 67CD1	54.52
209CD2	25C36 67CE1	55.35
209CD2	25C36 161N	98.98
209CD2	25C36 160CB	57.71
68CE	25C36 67CD1	70.75
68CE	25C36 67CE1	87.36
160O	25C36 162N	60.06
160O	25C36 160C	14.84
160O	25C36 161C	52.10
160O	25C36 161CA	34.02
160O	25C36 161N	27.16
160O	25C36 160CB	35.85
162N	25C36 160C	49.38
162N	25C36 161C	15.90
162N	25C36 161CA	29.60

TABLE XVI

162N	25C36 161N	33.75
162N	25C36 160CB	69.36
160C	25C36 161C	45.30
160C	25C36 161CA	29.33
160C	25C36 161N	15.76
160C	25C36 160CB	29.68
161C	25C36 161CA	18.21
161C	25C36 161N	30.25
161C	25C36 160CB	71.28
161CA	25C36 161N	17.23
161CA	25C36 160CB	58.05
67CD1	25C36 67CE1	16.61
67CE1	25C36 160CB	96.33
161N	25C36 160CB	41.59
162N	25C37 162C	38.77
162N	25C37 163N	55.65
162N	25C37 162O	43.88
162N	25C37 161C	19.66
162N	25C37 161N	43.11
162N	25C37 162CA	20.61
162N	25C37 161CA	36.42
162N	25C37 160C	61.64
162N	25C37 163CA	72.52
162N	25C37 163CB	88.83
162N	25C37 160O	71.57
162N	25C37 160CB	86.86
162N	25C37 134CA	86.74
162N	25C37 161O	27.40
162N	25C37 160CA	69.38
134CB	25C37 162C	80.90
134CB	25C37 163N	83.96
134CB	25C37 162O	64.46
134CB	25C37 161N	96.15
134CB	25C37 162CA	99.27
134CB	25C37 160C	92.07
134CB	25C37 163CA	69.42
134CB	25C37 163CB	75.64
134CB	25C37 160CB	64.54
134CB	25C37 134CA	17.37
134CB	25C37 160CA	74.76
134CB	25C37 68CE	75.20
134CB	25C37 209CD2	53.65

TABLE XVI

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162C	25C37 163N	20.04
162C	25C37 162O	18.39
162C	25C37 161C	56.63
162C	25C37 161N	77.75
162C	25C37 162CA	22.08
162C	25C37 161CA	75.17
162C	25C37 160C	94.90
162C	25C37 163CA	33.93
162C	25C37 163CB	51.74
162C	25C37 134CA	63.54
162C	25C37 161O	57.80
162C	25C37 160CA	95.14
162C	25C37 68CE	93.53
163N	25C37 162O	33.61
163N	25C37 161C	70.64
163N	25C37 161N	97.07
163N	25C37 162CA	35.65
163N	25C37 161CA	91.41
163N	25C37 163CA	19.33
163N	25C37 163CB	33.19
163N	25C37 134CA	67.66
163N	25C37 161O	67.69
163N	25C37 68CE	75.10
162O	25C37 161C	63.53
162O	25C37 161N	73.01
162O	25C37 162CA	34.99
162O	25C37 161CA	77.20
162O	25C37 160C	87.26
162O	25C37 163CA	38.61
162O	25C37 163CB	58.25
162O	25C37 160CB	91.83
162O	25C37 134CA	47.36
162O	25C37 161O	68.76
162O	25C37 160CA	82.84
162O	25C37 68CE	96.46
161C	25C37 161N	37.46
161C	25C37 162CA	35.43
161C	25C37 161CA	21.87
161C	25C37 160C	54.49
161C	25C37 163CA	89.14
161C	25C37 160O	59.67
161C	25C37 160CB	85.75

TABLE XVI

161C	25C37 161O	13.22
161C	25C37 160CA	67.48
161N	25C37 162CA	63.61
161N	25C37 161CA	20.70
161N	25C37 160C	18.54
161N	25C37 160O	30.38
161N	25C37 160CB	48.33
161N	25C37 134CA	92.03
161N	25C37 161O	49.54
161N	25C37 160CA	30.13
162CA	25C37 161CA	55.77
162CA	25C37 160C	82.09
162CA	25C37 163CA	53.72
162CA	25C37 163CB	68.64
162CA	25C37 160O	92.06
162CA	25C37 134CA	82.32
162CA	25C37 161O	35.74
162CA	25C37 160CA	88.24
161CA	25C37 160C	34.21
161CA	25C37 160O	37.80
161CA	25C37 160CB	67.22
161CA	25C37 161O	31.20
161CA	25C37 160CA	49.65
160C	25C37 160O	15.98
160C	25C37 160CB	33.38
160C	25C37 134CA	93.50
160C	25C37 161O	65.32
160C	25C37 160CA	17.61
160C	25C37 209CD2	89.23
163CA	25C37 163CB	19.64
163CA	25C37 134CA	55.20
163CA	25C37 161O	86.98
163CA	25C37 68CE	59.96
163CB	25C37 134CA	65.55
163CB	25C37 161O	97.16
163CB	25C37 68CE	41.99
160O	25C37 160CB	38.98
160O	25C37 161O	67.69
160O	25C37 160CA	29.34
160O	25C37 209CD2	86.31
160CB	25C37 134CA	72.65
160CB	25C37 161O	97.76

TABLE XVI

160CB	25C37	160CA	18.30
160CB	25C37	209CD2	58.20
134CA	25C37	160CA	77.94
134CA	25C37	68CE	77.56
134CA	25C37	209CD2	71.01
161O	25C37	160CA	79.66
160CA	25C37	209CD2	76.48
68CE	25C37	209CD2	74.72
209CD2	25C38	67CD1	74.87
209CD2	25C38	67CE1	73.16
209CD2	25C38	134CB	65.56
209CD2	25C38	209CG	16.73
209CD2	25C38	67CG	84.81
67CD1	25C38	67CE1	20.70
67CD1	25C38	68CE	89.96
67CD1	25C38	66O	66.53
67CD1	25C38	209CG	75.95
67CD1	25C38	67CG	12.21
67CD1	25C38	67CA	42.12
67CE1	25C38	66O	77.82
67CE1	25C38	209CG	80.22
67CE1	25C38	67CG	30.41
67CE1	25C38	67CA	60.82
68CE	25C38	134CB	80.62
68CE	25C38	66O	53.63
68CE	25C38	209CG	90.75
68CE	25C38	67CG	80.08
68CE	25C38	67CA	50.64
134CB	25C38	209CG	59.36
66O	25C38	67CG	54.73
66O	25C38	67CA	34.43
209CG	25C38	67CG	83.39
209CG	25C38	67CA	92.38
67CG	25C38	67CA	30.58
65CA	25C39	66N	39.58
65CA	25C39	66O	81.69
65CA	25C39	26CD1	58.77
65CA	25C39	65C	21.13
65CA	25C39	26CB	87.77
65CA	25C39	26CG	70.14
65CA	25C39	66C	70.43
65CA	25C39	65N	10.50

TABLE XVI

65CA	25C39	26N	97.84
65CA	25C39	66CA	51.95
65CA	25C39	23O	44.24
25SG	25C39	26CD1	80.82
25SG	25C39	26CB	77.99
25SG	25C39	26CG	82.69
25SG	25C39	26N	48.23
25SG	25C39	23O	74.80
25SG	25C39	161O	65.02
66N	25C39	66O	42.13
66N	25C39	26CD1	49.89
66N	25C39	65C	18.53
66N	25C39	26CB	61.31
66N	25C39	26CG	50.14
66N	25C39	66C	30.88
66N	25C39	65N	49.74
66N	25C39	26N	85.92
66N	25C39	66CA	12.40
66N	25C39	23O	70.96
66O	25C39	26CD1	64.20
66O	25C39	65C	60.58
66O	25C39	26CB	46.66
66O	25C39	26CG	51.76
66O	25C39	66C	11.26
66O	25C39	65N	91.86
66O	25C39	26N	76.72
66O	25C39	66CA	29.74
26CD1	25C39	65C	52.77
26CD1	25C39	26CB	33.76
26CD1	25C39	26CG	16.02
26CD1	25C39	66C	59.08
26CD1	25C39	65N	61.27
26CD1	25C39	26N	40.34
26CD1	25C39	66CA	52.43
26CD1	25C39	23O	46.03
65C	25C39	26CB	74.04
65C	25C39	26CG	59.01
65C	25C39	66C	49.32
65C	25C39	65N	31.45
65C	25C39	26N	92.79
65C	25C39	66CA	30.85
65C	25C39	23O	58.16

TABLE XVI

26CB	25C39	26CG	18.51
26CB	25C39	66C	48.81
26CB	25C39	65N	92.88
26CB	25C39	26N	30.42
26CB	25C39	66CA	55.33
26CB	25C39	23O	78.36
26CG	25C39	66C	49.18
26CG	25C39	65N	74.55
26CG	25C39	26N	35.79
26CG	25C39	66CA	48.23
26CG	25C39	23O	61.96
66C	25C39	65N	80.62
66C	25C39	26N	79.15
66C	25C39	66CA	18.48
66C	25C39	23O	96.37
65N	25C39	26N	97.76
65N	25C39	66CA	62.14
65N	25C39	23O	37.19
26N	25C39	66CA	83.19
26N	25C39	23O	67.94
66CA	25C39	23O	81.21
66N	25O40	66O	55.03
66N	25O40	26CD1	68.97
66N	25O40	65CA	46.68
66N	25O40	26CB	85.08
66N	25O40	26CG	70.07
66N	25O40	65C	21.06
66N	25O40	66C	40.07
66N	25O40	66CA	17.56
66N	25O40	26NE1	58.94
66N	25O40	65N	53.77
66N	25O40	23O	82.65
66N	25O40	26CD2	60.09
66N	25O40	65O	19.20
66N	25O40	26CE2	54.44
66O	25O40	26CD1	89.64
66O	25O40	26CB	63.20
66O	25O40	26CG	71.47
66O	25O40	65C	75.92
66O	25O40	66C	15.74
66O	25O40	66CA	38.45
66O	25O40	26N	99.32

TABLE XVI

66O	25O40	26NE1	91.06
66O	25O40	26CA	79.34
66O	25O40	26CD2	68.55
66O	25O40	65O	74.21
66O	25O40	68CE	47.85
66O	25O40	26CE2	78.85
26CD1	25O40	65CA	74.34
26CD1	25O40	26CB	46.12
26CD1	25O40	26CG	22.72
26CD1	25O40	65C	67.94
26CD1	25O40	66C	79.23
26CD1	25O40	66CA	69.49
26CD1	25O40	25SG	92.07
26CD1	25O40	26N	50.30
26CD1	25O40	26NE1	14.37
26CD1	25O40	26CA	50.84
26CD1	25O40	65N	70.61
26CD1	25O40	23O	51.41
26CD1	25O40	26CD2	21.35
26CD1	25O40	65O	66.27
26CD1	25O40	68CE	92.41
26CD1	25O40	26CE2	14.76
26CD1	25O40	25N	52.65
65CA	25O40	26CG	91.43
65CA	25O40	65C	25.75
65CA	25O40	66C	86.58
65CA	25O40	66CA	64.21
65CA	25O40	26NE1	60.05
65CA	25O40	65N	8.97
65CA	25O40	23O	48.18
65CA	25O40	26CD2	82.47
65CA	25O40	65O	27.92
65CA	25O40	26CE2	67.12
65CA	25O40	25N	97.61
26CB	25O40	26CG	24.84
26CB	25O40	65C	97.95
26CB	25O40	66C	63.62
26CB	25O40	66CA	72.60
26CB	25O40	25SG	89.79
26CB	25O40	26N	37.46
26CB	25O40	26NE1	58.62
26CB	25O40	26CA	19.07

TABLE XVI

26CB	25O40	23O	95.25
26CB	25O40	26CD2	33.11
26CB	25O40	65O	95.49
26CB	25O40	68CE	46.43
26CB	25O40	26CE2	49.00
26CB	25O40	25N	67.75
26CG	25O40	65C	77.41
26CG	25O40	66C	64.77
26CG	25O40	66CA	63.32
26CG	25O40	25SG	97.02
26CG	25O40	26N	44.89
26CG	25O40	26NE1	33.94
26CG	25O40	26CA	35.84
26CG	25O40	65N	89.76
26CG	25O40	23O	74.03
26CG	25O40	26CD2	10.27
26CG	25O40	65O	75.16
26CG	25O40	68CE	70.18
26CG	25O40	26CE2	24.36
26CG	25O40	25N	62.89
65C	25O40	66C	61.12
65C	25O40	66CA	38.51
65C	25O40	26NE1	54.62
65C	25O40	65N	32.73
65C	25O40	23O	65.00
65C	25O40	26CD2	67.24
65C	25O40	65O	2.52
65C	25O40	26CE2	55.73
66C	25O40	66CA	22.95
66C	25O40	26NE1	78.03
66C	25O40	26CA	81.98
66C	25O40	65N	93.83
66C	25O40	26CD2	59.43
66C	25O40	65O	59.25
66C	25O40	68CE	60.81
66C	25O40	26CE2	66.69
66CA	25O40	26NE1	63.40
66CA	25O40	26CA	91.57
66CA	25O40	65N	71.07
66CA	25O40	23O	96.11
66CA	25O40	26CD2	54.65
66CA	25O40	65O	36.50

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TABLE XVI

66CA	25O40	68CE	82.71
66CA	25O40	26CE2	54.95
25SG	25O40	26N	53.76
25SG	25O40	26CA	70.74
25SG	25O40	23O	76.38
25SG	25O40	68CE	91.56
25SG	25O40	25N	39.87
26N	25O40	26NE1	64.06
26N	25O40	26CA	19.99
26N	25O40	23O	77.54
26N	25O40	26CD2	54.76
26N	25O40	68CE	65.32
26N	25O40	26CE2	62.82
26N	25O40	25N	33.74
26NE1	25O40	26CA	65.10
26NE1	25O40	65N	56.73
26NE1	25O40	23O	44.12
26NE1	25O40	26CD2	28.39
26NE1	25O40	65O	53.18
26NE1	25O40	26CE2	12.89
26NE1	25O40	25N	60.41
26CA	25O40	23O	91.40
26CA	25O40	26CD2	45.97
26CA	25O40	68CE	49.24
26CA	25O40	26CE2	59.06
26CA	25O40	25N	53.14
65N	25O40	23O	39.46
65N	25O40	26CD2	81.69
65N	25O40	65O	34.59
65N	25O40	26CE2	65.52
65N	25O40	25N	89.01
23O	25O40	26CD2	71.57
23O	25O40	65O	65.65
23O	25O40	26CE2	57.01
23O	25O40	25N	49.58
26CD2	25O40	65O	64.96
26CD2	25O40	68CE	75.92
26CD2	25O40	26CE2	16.58
26CD2	25O40	25N	69.33
65O	25O40	26CE2	53.78
68CE	25O40	26CE2	92.46
68CE	25O40	25N	97.92

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TABLE XVI

26CE2	25O40	25N	67.27
25SG	25N41	161O	80.59
25SG	25N41	23O	90.56
25SG	25N41	26CD1	82.77
25SG	25N41	25CB	9.91
25SG	25N41	23C	79.09
25SG	25N41	25N	40.23
25SG	25N41	161C	80.64
25SG	25N41	26N	46.58
25SG	25N41	162CA	52.67
25SG	25N41	163N	39.29
65CA	25N41	23O	48.79
65CA	25N41	26CD1	53.27
65CA	25N41	66N	31.72
65CA	25N41	23C	63.36
65CA	25N41	65N	14.93
65CA	25N41	65C	15.53
65CA	25N41	25N	93.22
65CA	25N41	26N	91.88
161O	25N41	25CB	89.53
161O	25N41	161C	13.63
161O	25N41	162CA	33.89
161O	25N41	163N	62.20
23O	25N41	26CD1	48.03
23O	25N41	66N	68.57
23O	25N41	25CB	80.86
23O	25N41	23C	14.88
23O	25N41	65N	39.21
23O	25N41	65C	57.67
23O	25N41	25N	51.81
23O	25N41	26N	71.06
26CD1	25N41	66N	42.24
26CD1	25N41	25CB	74.76
26CD1	25N41	23C	56.38
26CD1	25N41	65N	58.93
26CD1	25N41	65C	46.09
26CD1	25N41	25N	50.77
26CD1	25N41	26N	38.61
26CD1	25N41	163N	98.70
66N	25N41	23C	82.86
66N	25N41	65N	46.23
66N	25N41	65C	16.19

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TABLE XVI

66N	25N41	25N	92.91
66N	25N41	26N	75.02
25CB	25N41	23C	69.90
25CB	25N41	25N	30.33
25CB	25N41	161C	90.33
25CB	25N41	26N	40.90
25CB	25N41	162CA	62.56
25CB	25N41	163N	48.01
23C	25N41	65N	52.61
23C	25N41	65C	72.52
23C	25N41	25N	43.58
23C	25N41	26N	69.77
65N	25N41	65C	30.16
65N	25N41	25N	89.00
65N	25N41	26N	96.17
65C	25N41	25N	93.25
65C	25N41	26N	83.49
25N	25N41	26N	33.34
25N	25N41	162CA	92.88
25N	25N41	163N	75.53
161C	25N41	162CA	28.77
161C	25N41	163N	54.46
26N	25N41	162CA	89.00
26N	25N41	163N	62.08
162CA	25N41	163N	28.61
25SG	25C42	25N	61.47
25SG	25C42	25CB	23.02
25SG	25C42	24N	99.07
25SG	25C42	26N	58.96
25SG	25C42	25CA	42.76
25SG	25C42	24C	76.26
25SG	25C42	24CA	95.01
25SG	25C42	25C	46.56
25SG	25C42	26CG	94.70
25SG	25C42	26CB	80.63
23O	25C42	23C	20.90
23O	25C42	25N	72.70
23O	25C42	26CD1	61.41
23O	25C42	65CA	57.62
23O	25C42	23CA	37.29
23O	25C42	24N	34.67
23O	25C42	26N	92.67

TABLE XVI

23O	25C42	25CA	92.41
23O	25C42	24C	59.75
23O	25C42	24CA	39.73
23O	25C42	65N	43.51
23O	25C42	26NE1	46.24
23O	25C42	25C	96.61
23O	25C42	26CG	73.49
23O	25C42	66N	75.31
23O	25C42	65C	62.99
23O	25C42	26CB	90.54
23C	25C42	25N	60.95
23C	25C42	26CD1	74.34
23C	25C42	65CA	77.95
23C	25C42	25CB	94.36
23C	25C42	23CA	22.31
23C	25C42	24N	19.02
23C	25C42	26N	92.21
23C	25C42	25CA	80.52
23C	25C42	24C	52.38
23C	25C42	24CA	33.67
23C	25C42	65N	62.45
23C	25C42	26NE1	61.04
23C	25C42	25C	90.42
23C	25C42	26CG	85.04
23C	25C42	66N	95.80
23C	25C42	65C	83.89
25N	25C42	26CD1	66.35
25N	25C42	25CB	38.84
25N	25C42	23CA	73.38
25N	25C42	24N	41.94
25N	25C42	26N	41.41
25N	25C42	25CA	19.88
25N	25C42	24C	16.17
25N	25C42	24CA	33.54
25N	25C42	26NE1	68.49
25N	25C42	25C	31.76
25N	25C42	26CG	65.77
25N	25C42	26CB	67.36
26CD1	25C42	65CA	59.61
26CD1	25C42	25CB	93.02
26CD1	25C42	23CA	96.28
26CD1	25C42	24N	69.60

TABLE XVI

26CD1	25C42	26N	46.05
26CD1	25C42	25CA	73.18
26CD1	25C42	24C	52.84
26CD1	25C42	24CA	52.35
26CD1	25C42	65N	66.14
26CD1	25C42	26NE1	15.58
26CD1	25C42	25C	60.30
26CD1	25C42	26CG	12.37
26CD1	25C42	66N	42.73
26CD1	25C42	65C	47.92
26CD1	25C42	26CB	29.69
65CA	25C42	23CA	85.42
65CA	25C42	24N	91.42
65CA	25C42	24CA	88.16
65CA	25C42	65N	17.82
65CA	25C42	26NE1	51.70
65CA	25C42	26CG	67.28
65CA	25C42	66N	29.94
65CA	25C42	65C	14.64
65CA	25C42	26CB	78.77
25CB	25C42	23CA	97.37
25CB	25C42	24N	76.40
25CB	25C42	26N	48.95
25CB	25C42	25CA	21.77
25CB	25C42	24C	54.30
25CB	25C42	24CA	72.26
25CB	25C42	25C	33.23
25CB	25C42	26CG	86.02
25CB	25C42	26CB	76.81
23CA	25C42	24N	35.27
23CA	25C42	25CA	90.57
23CA	25C42	24C	69.58
23CA	25C42	24CA	53.60
23CA	25C42	65N	67.73
23CA	25C42	26NE1	82.24
23CA	25C42	65C	95.61
24N	25C42	26N	75.74
24N	25C42	25CA	61.52
24N	25C42	24C	34.63
24N	25C42	24CA	19.12
24N	25C42	65N	78.18
24N	25C42	26NE1	60.00

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TABLE XVI

24N	25C42	25C	71.96
24N	25C42	26CG	77.77
24N	25C42	65C	93.70
24N	25C42	26CB	89.98
26N	25C42	25CA	34.07
26N	25C42	24C	41.33
26N	25C42	24CA	58.54
26N	25C42	26NE1	58.48
26N	25C42	25C	16.06
26N	25C42	26CG	37.28
26N	25C42	66N	80.08
26N	25C42	65C	91.09
26N	25C42	26CB	29.32
25CA	25C42	24C	33.53
25CA	25C42	24CA	52.86
25CA	25C42	26NE1	80.09
25CA	25C42	25C	18.89
25CA	25C42	26CG	68.25
25CA	25C42	26CB	63.36
24C	25C42	24CA	20.14
24C	25C42	65N	97.32
24C	25C42	26NE1	52.89
24C	25C42	25C	38.23
24C	25C42	26CG	54.87
24C	25C42	66N	95.24
24C	25C42	65C	96.26
24C	25C42	26CB	60.96
24CA	25C42	65N	79.58
24CA	25C42	26NE1	45.69
24CA	25C42	25C	58.08
24CA	25C42	26CG	59.27
24CA	25C42	66N	89.86
24CA	25C42	65C	85.80
24CA	25C42	26CB	70.86
65N	25C42	26NE1	54.04
65N	25C42	26CG	76.36
65N	25C42	66N	46.51
65N	25C42	65C	30.57
65N	25C42	26CB	90.76
26NE1	25C42	25C	70.82
26NE1	25C42	26CG	27.95
26NE1	25C42	66N	44.28

TABLE XVI

26NE1	25C42	65C	43.42
26NE1	25C42	26CB	45.27
25C	25C42	26CG	52.79
25C	25C42	66N	96.14
25C	25C42	26CB	45.17
26CG	25C42	66N	44.88
26CG	25C42	65C	53.98
26CG	25C42	26CB	17.32
66N	25C42	65C	15.94
66N	25C42	26CB	51.51
65C	25C42	26CB	64.35
66N	25N43	65CA	39.20
66N	25N43	66O	42.83
66N	25N43	65C	19.66
66N	25N43	66C	33.44
66N	25N43	66CA	16.52
66N	25N43	64O	67.91
66N	25N43	65O	24.48
66N	25N43	65N	47.82
65CA	25N43	66O	79.74
65CA	25N43	65C	22.72
65CA	25N43	66C	72.52
65CA	25N43	66CA	54.97
65CA	25N43	64O	35.80
65CA	25N43	65O	27.77
65CA	25N43	65N	9.59
66O	25N43	65C	62.50
66O	25N43	66C	14.75
66O	25N43	66CA	32.80
66O	25N43	65O	66.04
66O	25N43	65N	89.14
65C	25N43	66C	52.38
65C	25N43	66CA	33.37
65C	25N43	64O	48.27
65C	25N43	65O	9.39
65C	25N43	65N	29.76
66C	25N43	66CA	19.82
66C	25N43	64O	99.32
66C	25N43	65O	54.13
66C	25N43	65N	81.27
66CA	25N43	64O	79.51
66CA	25N43	65O	34.33

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TABLE XVI

66CA	25N43	65N	62.98
64O	25N43	65O	45.20
64O	25N43	65N	26.86
65O	25N43	65N	32.42

TABLE XVII

Table of angles between atoms of the inhibitor and protein for all protein atoms within 5 Ångstroms of the inhibitor 4-[N-[(4-pyridylmethoxy)carbonyl]-L-leucyl]-1-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-3-pyrrolidinone.

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
67CE2	25C1	67CD2	21.66	67CE2	25C1	60ND2	88.40
67CE2	25C1	67CZ	15.07	67CE2	25C1	231OH2	72.49
67CE2	25C1	67OH	28.98	67CE2	25C1	66CA	80.69
67CE2	25C1	67CG	26.79	67CE2	25C1	70ND2	78.17
67CD2	25C1	60ND2	67.38	67CD2	25C1	67CZ	33.45
67CD2	25C1	231OH2	62.87	67CD2	25C1	67OH	49.60
67CD2	25C1	66CA	68.97	67CD2	25C1	67CG	10.46
67CD2	25C1	70ND2	58.29	60ND2	25C1	67CZ	95.36
60ND2	25C1	59O	49.64	60ND2	25C1	231OH2	73.76
60ND2	25C1	66CA	42.03	60ND2	25C1	65O	60.94
60ND2	25C1	67CG	61.96	60ND2	25C1	70ND2	36.62
67CZ	25C1	231OH2	87.30	67CZ	25C1	67OH	16.70
67CZ	25C1	66CA	77.40	67CZ	25C1	67CG	34.47
67CZ	25C1	70ND2	91.66	59O	25C1	231OH2	59.15
59O	25C1	66CA	86.93	59O	25C1	65O	85.11
59O	25C1	70ND2	43.49	231OH2	25C1	67OH	96.03
231OH2	25C1	67CG	71.00	231OH2	25C1	70ND2	37.14
67OH	25C1	66CA	87.65	67OH	25C1	67CG	51.17
66CA	25C1	65O	33.94	66CA	25C1	67CG	58.73
66CA	25C1	70ND2	75.50	65O	25C1	67CG	92.09
65O	25C1	70ND2	97.34	67CG	25C1	70ND2	60.11
67CE2	25C2	67CZ	20.70	67CE2	25C2	67CD2	20.73
67CE2	25C2	67OH	36.29	67CE2	25C2	66CA	91.85
67CE2	25C2	67CE1	28.15	67CE2	25C2	60ND2	82.91
67CE2	25C2	66C	74.08	67CE2	25C2	67CG	28.19
67CE2	25C2	67N	63.54	67CZ	25C2	67CD2	36.53
67CZ	25C2	67OH	19.80	67CZ	25C2	66CA	91.39
67CZ	25C2	66N	97.52	67CZ	25C2	67CE1	14.08
67CZ	25C2	60ND2	96.48	67CZ	25C2	66C	73.78

TABLE XVII

67CZ	25C2	67CG	36.08	67CZ	25C2	67N	68.45
67CD2	25C2	67OH	55.27	67CD2	25C2	66CA	75.10
67CD2	25C2	66N	89.93	67CD2	25C2	67CE1	35.97
67CD2	25C2	60ND2	62.30	67CD2	25C2	66C	58.50
67CD2	25C2	67CG	13.99	67CD2	25C2	67N	45.40
67OH	25C2	67CE1	30.01	67OH	25C2	66C	90.02
67OH	25C2	67CG	55.88	67OH	25C2	67N	87.15
66CA	25C2	65O	39.05	66CA	25C2	66N	18.31
66CA	25C2	65C	31.60	66CA	25C2	67CE1	77.85
66CA	25C2	60ND2	42.40	66CA	25C2	66C	17.99
66CA	25C2	67CG	63.85	66CA	25C2	67N	29.89
65O	25C2	66N	29.44	65O	25C2	65C	15.02
65O	25C2	60ND2	62.06	65O	25C2	66C	56.82
65O	25C2	67N	68.16	66N	25C2	65C	16.65
66N	25C2	67CE1	83.45	66N	25C2	60ND2	59.05
66N	25C2	66C	31.58	66N	25C2	67CG	77.19
66N	25C2	67N	46.44	65C	25C2	67CE1	99.01
65C	25C2	60ND2	65.42	65C	25C2	66C	47.55
65C	25C2	67CG	93.66	65C	25C2	67N	61.39
67CE1	25C2	60ND2	88.93	67CE1	25C2	66C	60.58
67CE1	25C2	67CG	29.84	67CE1	25C2	67N	57.26
60ND2	25C2	66C	44.34	60ND2	25C2	67CG	60.48
60ND2	25C2	67N	35.75	66C	25C2	67CG	46.38
66C	25C2	67N	15.93	67CG	25C2	67N	35.42
65O	25C3	65C	17.88	65O	25C3	66CA	41.69
65O	25C3	66N	32.43	65O	25C3	61CB	43.31
65O	25C3	65CA	28.80	65O	25C3	61CG	61.48
65O	25C3	61OD1	68.40	65C	25C3	66CA	35.13
65C	25C3	66N	18.49	65C	25C3	61CB	59.01
65C	25C3	65CA	16.90	65C	25C3	61CG	77.19
65C	25C3	61OD1	85.63	66CA	25C3	66N	20.18
66CA	25C3	67CE2	75.24	66CA	25C3	61CB	82.37
66CA	25C3	65CA	50.05	66CA	25C3	61CG	99.19
66CA	25C3	67CZ	76.99	66CA	25C3	67OH	90.94
66N	25C3	67CE2	90.18	66N	25C3	61CB	75.69
66N	25C3	65CA	30.59	66N	25C3	61CG	93.89
66N	25C3	67CZ	87.56	66N	25C3	67OH	98.55

TABLE XVII

67CE2	25C3	67CZ	16.06	67CE2	25C3	67OH	28.37
61CB	25C3	65CA	59.68	61CB	25C3	61CG	18.24
61CB	25C3	61OD1	28.38	65CA	25C3	61CG	76.44
65CA	25C3	61OD1	88.03	61CG	25C3	61OD1	14.65
67CZ	25C3	67OH	15.78	65O	25C4	61CG	81.72
65O	25C4	61CB	56.74	65O	25C4	61OD1	92.04
65O	25C4	61OD2	90.06	65O	25C4	65C	13.06
65O	25C4	61N	47.80	65O	25C4	61CA	52.82
65O	25C4	66CA	34.06	65O	25C4	66N	23.80
65O	25C4	60C	59.87	65O	25C4	65CA	23.94
61CG	25C4	61CB	24.99	61CG	25C4	61OD1	20.63
61CG	25C4	61OD2	17.88	61CG	25C4	65C	91.97
61CG	25C4	61N	50.91	61CG	25C4	61CA	33.78
61CG	25C4	60C	56.14	61CG	25C4	65CA	87.08
61CB	25C4	61OD1	39.37	61CB	25C4	61OD2	36.30
61CB	25C4	65C	67.18	61CB	25C4	61N	35.38
61CB	25C4	61CA	16.65	61CB	25C4	66CA	87.99
61CB	25C4	66N	80.49	61CB	25C4	60C	47.22
61CB	25C4	65CA	64.13	61OD1	25C4	61OD2	33.84
61OD1	25C4	61N	49.82	61OD1	25C4	61CA	39.25
61OD1	25C4	60C	48.15	61OD2	25C4	65C	97.59
61OD2	25C4	61N	67.70	61OD2	25C4	61CA	49.40
61OD2	25C4	60C	73.98	61OD2	25C4	65CA	88.32
65C	25C4	61N	60.83	65C	25C4	61CA	65.24
65C	25C4	66CA	30.77	65C	25C4	66N	15.04
65C	25C4	60C	72.43	65C	25C4	65CA	16.09
61N	25C4	61CA	19.04	61N	25C4	66CA	65.40
61N	25C4	66N	67.36	61N	25C4	60C	15.56
61N	25C4	65CA	68.40	61CA	25C4	66CA	78.91
61CA	25C4	66N	75.90	61CA	25C4	60C	30.75
61CA	25C4	65CA	67.27	66CA	25C4	66N	17.65
66CA	25C4	60C	69.36	66CA	25C4	65CA	45.82
66N	25C4	60C	75.84	66N	25C4	65CA	28.52
60C	25C4	65CA	82.21	61OD1	25C5	61CG	21.34
61OD1	25C5	61CB	38.98	61OD1	25C5	61N	54.59
61OD1	25C5	65O	86.61	61OD1	25C5	60C	57.24
61OD1	25C5	61OD2	31.11	61OD1	25C5	59O	91.41

TABLE XVII

61OD1	25C5	60CA	77.36	61OD1	25C5	61CA	39.29
61OD1	25C5	60O	47.14	61CG	25C5	61CB	23.42
61CG	25C5	61N	53.21	61CG	25C5	65O	71.11
61CG	25C5	60C	63.55	61CG	25C5	61OD2	15.46
61CG	25C5	60CA	84.04	61CG	25C5	61CA	34.30
61CG	25C5	60O	58.88	61CB	25C5	61N	36.38
61CB	25C5	65O	48.37	61CB	25C5	60C	52.26
61CB	25C5	61OD2	34.12	61CB	25C5	60CA	70.23
61CB	25C5	61CA	19.16	61CB	25C5	60O	54.58
61CB	25C5	60ND2	92.51	61N	25C5	65O	46.30
61N	25C5	60C	18.83	61N	25C5	61OD2	67.79
61N	25C5	59O	68.18	61N	25C5	60CA	33.92
61N	25C5	61CA	19.02	61N	25C5	60O	29.73
61N	25C5	60ND2	59.73	65O	25C5	60C	62.13
65O	25C5	61OD2	76.92	65O	25C5	59O	97.98
65O	25C5	60CA	63.97	65O	25C5	61CA	50.38
65O	25C5	60O	75.74	65O	25C5	60ND2	60.02
60C	25C5	61OD2	79.00	60C	25C5	59O	50.32
60C	25C5	60CA	20.70	60C	25C5	61CA	33.16
60C	25C5	60O	15.46	60C	25C5	60ND2	54.15
61OD2	25C5	60CA	99.43	61OD2	25C5	61CA	48.77
61OD2	25C5	60O	73.92	59O	25C5	60CA	36.41
59O	25C5	61CA	83.15	59O	25C5	60O	49.36
59O	25C5	60ND2	45.49	60CA	25C5	61CA	51.88
60CA	25C5	60O	31.33	60CA	25C5	60ND2	34.90
61CA	25C5	60O	36.38	61CA	25C5	60ND2	78.49
60O	25C5	60ND2	66.22	59O	25C6	61OD1	84.33
59O	25C6	60CA	37.74	59O	25C6	60ND2	52.70
59O	25C6	60C	49.43	59O	25C6	59C	7.16
59O	25C6	231OH2	61.67	59O	25C6	65O	96.01
59O	25C6	61N	65.44	59O	25C6	61CG	94.50
61OD1	25C6	60CA	67.00	61OD1	25C6	60C	47.52
61OD1	25C6	59C	79.80	61OD1	25C6	65O	65.95
61OD1	25C6	61N	43.14	61OD1	25C6	61CG	14.44
60CA	25C6	60ND2	38.07	60CA	25C6	60C	19.60
60CA	25C6	59C	30.68	60CA	25C6	231OH2	90.52
60CA	25C6	65O	58.49	60CA	25C6	61N	31.11

TABLE XVII

60CA	25C6	61CG	70.16	60ND2	25C6	60C	55.78
60ND2	25C6	59C	49.33	60ND2	25C6	231OH2	69.41
60ND2	25C6	65O	60.19	60ND2	25C6	61N	59.59
60ND2	25C6	67CE2	71.07	60C	25C6	59C	42.53
60C	25C6	65O	53.64	60C	25C6	61N	16.42
60C	25C6	61CG	50.89	59C	25C6	231OH2	67.54
59C	25C6	65O	89.09	59C	25C6	61N	58.40
59C	25C6	61CG	89.02	231OH2	25C6	67CE2	58.91
65O	25C6	61N	38.82	65O	25C6	61CG	54.53
65O	25C6	67CE2	90.16	61N	25C6	61CG	41.32
65O	25C7	65C	20.61	65O	25C7	66N	35.57
65O	25C7	65CA	37.59	65O	25C7	64O	63.61
65O	25C7	66CA	40.23	65O	25C7	65N	36.78
65O	25C7	64C	50.16	65C	25C7	66N	20.13
65C	25C7	65CA	22.56	65C	25C7	64O	58.37
65C	25C7	66CA	34.64	65C	25C7	65N	30.89
65C	25C7	64C	46.81	66N	25C7	65CA	35.80
66N	25C7	64O	74.14	66N	25C7	66CA	19.87
66N	25C7	65N	48.83	66N	25C7	64C	64.44
65CA	25C7	64O	38.35	65CA	25C7	66CA	54.61
65CA	25C7	65N	16.17	65CA	25C7	64C	29.70
64O	25C7	66CA	92.52	64O	25C7	65N	28.03
64O	25C7	64C	13.53	66CA	25C7	65N	65.51
66CA	25C7	64C	81.44	66CA	25C7	67OH	89.07
65N	25C7	64C	15.93	66N	25O8	65C	20.16
66N	25O8	66CA	21.24	66N	25O8	65O	33.23
66N	25O8	65CA	33.75	66N	25O8	67CE1	98.44
66N	25O8	67CE2	98.98	66N	25O8	66C	34.36
66N	25O8	66O	36.02	66N	25O8	64O	65.86
65C	25O8	66CA	35.77	65C	25O8	65O	17.66
65C	25O8	65CA	20.48	65C	25O8	66C	52.97
65C	25O8	66O	56.18	65C	25O8	64O	48.74
66CA	25O8	65O	39.76	66CA	25O8	67CZ	88.60
66CA	25O8	65CA	53.75	66CA	25O8	67CE1	82.16
66CA	25O8	67CE2	78.01	66CA	25O8	66C	19.45
66CA	25O8	66O	29.94	66CA	25O8	64O	84.46
67OH	25O8	67CZ	19.19	67OH	25O8	67CE1	31.81

TABLE XVII

67OH	25O8	67CE2	31.82	67OH	25O8	66C	93.01
67OH	25O8	66O	95.44	65O	25O8	65CA	33.40
65O	25O8	66C	59.16	65O	25O8	66O	66.79
65O	25O8	64O	51.69	67CZ	25O8	67CE1	17.96
67CZ	25O8	67CE2	17.62	67CZ	25O8	66C	73.92
67CZ	25O8	66O	77.47	65CA	25O8	66C	67.93
65CA	25O8	66O	66.32	65CA	25O8	64O	32.46
67CE1	25O8	67CE2	30.82	67CE1	25O8	66C	64.46
67CE1	25O8	66O	64.18	67CE2	25O8	66C	67.34
67CE2	25O8	66O	75.18	66C	25O8	66O	15.05
66O	25O8	64O	98.36	66N	25C9	65C	19.56
66N	25C9	65CA	35.74	66N	25C9	66CA	18.50
66N	25C9	65O	29.44	66N	25C9	66O	37.27
66N	25C9	64O	68.91	66N	25C9	66C	32.34
66N	25C9	67CE1	91.45	66N	25C9	67CZ	94.14
65C	25C9	65CA	21.89	65C	25C9	66CA	33.21
65C	25C9	65O	14.71	65C	25C9	66O	56.83
65C	25C9	64O	50.85	65C	25C9	66C	50.46
65CA	25C9	66CA	53.09	65CA	25C9	65O	31.99
65CA	25C9	66O	69.79	65CA	25C9	64O	34.59
65CA	25C9	66C	67.96	66CA	25C9	65O	35.79
66CA	25C9	66O	30.43	66CA	25C9	64O	83.99
66CA	25C9	66C	18.68	66CA	25C9	67OH	90.57
66CA	25C9	67CE1	74.02	66CA	25C9	67CZ	75.67
65O	25C9	66O	64.42	65O	25C9	64O	51.51
65O	25C9	66C	54.47	65O	25C9	67CZ	97.86
66O	25C9	66C	15.18	66O	25C9	67OH	88.11
66O	25C9	67CE1	62.23	66O	25C9	67CZ	72.01
66C	25C9	67OH	81.72	66C	25C9	67CE1	59.79
66C	25C9	67CZ	65.61	67OH	25C9	67CE1	28.34
67OH	25C9	67CZ	16.24	67CE1	25C9	67CZ	16.27
65CA	25O10	64O	37.93	65CA	25O10	65C	19.98
65CA	25O10	66N	32.25	64O	25O10	65C	52.12
64O	25O10	66N	68.39	65C	25O10	66N	17.19
66N	25N11	66O	46.02	66N	25N11	66C	38.85
66N	25N11	66CA	20.73	66N	25N11	65C	17.46
66N	25N11	65CA	33.59	66N	25N11	67CD1	91.49

TABLE XVII

66N	25N11	65O	24.15	66N	25N11	67N	48.38
66O	25N11	66C	17.87	66O	25N11	66CA	35.52
66O	25N11	65C	63.48	66O	25N11	67CE1	75.71
66O	25N11	65CA	76.62	66O	25N11	67CZ	83.40
66O	25N11	67CD1	58.50	66O	25N11	67OH	99.66
66O	25N11	65O	67.57	66O	25N11	67N	24.87
66C	25N11	66CA	21.72	66C	25N11	65C	54.97
66C	25N11	67CE1	70.15	66C	25N11	65CA	72.37
66C	25N11	67CZ	73.23	66C	25N11	67CD1	54.55
66C	25N11	67OH	88.69	66C	25N11	65O	55.57
66C	25N11	67N	11.56	66CA	25N11	65C	34.29
66CA	25N11	67CE1	83.75	66CA	25N11	65CA	53.45
66CA	25N11	67CZ	81.15	66CA	25N11	67CD1	71.00
66CA	25N11	67OH	93.79	66CA	25N11	65O	33.86
66CA	25N11	67N	28.86	65C	25N11	65CA	20.50
65C	25N11	65O	12.17	65C	25N11	67N	63.15
67CE1	25N11	67CZ	16.97	67CE1	25N11	67CD1	17.33
67CE1	25N11	67OH	28.98	67CE1	25N11	67N	58.73
65CA	25N11	65O	29.33	65CA	25N11	67N	81.90
67CZ	25N11	67CD1	29.85	67CZ	25N11	67OH	16.29
67CZ	25N11	65O	95.29	67CZ	25N11	67N	61.81
67CD1	25N11	67OH	44.88	67CD1	25N11	65O	98.49
67CD1	25N11	67N	43.62	67OH	25N11	67N	77.48
65O	25N11	67N	61.50	66O	25C12	66N	39.81
66O	25C12	66C	13.28	66O	25C12	65CA	68.49
66O	25C12	66CA	28.41	66O	25C12	65C	53.90
66N	25C12	66C	32.53	66N	25C12	65CA	30.03
66N	25C12	66CA	16.05	66N	25C12	65C	14.10
161O	25C12	161C	14.53	66C	25C12	65CA	62.55
66C	25C12	66CA	17.90	66C	25C12	65C	45.95
65CA	25C12	66CA	45.67	65CA	25C12	65C	17.89
66CA	25C12	65C	28.39	66O	25C13	66N	46.61
66O	25C13	65CA	81.12	66O	25C13	26CB	42.40
66O	25C13	66C	12.53	66O	25C13	26CD1	59.74
66O	25C13	65C	61.86	66O	25C13	66CA	31.09
66O	25C13	26CG	46.38	66O	25C13	26N	73.59
66N	25C13	65CA	34.83	66N	25C13	26CB	65.68

TABLE XVII

66N	25C13	66C	35.92	66N	25C13	26CD1	50.75
66N	25C13	65C	15.26	66N	25C13	66CA	16.54
66N	25C13	26CG	52.33	66N	25C13	26N	87.54
25SG	25C13	26CB	74.78	25SG	25C13	26CD1	73.77
25SG	25C13	26CG	78.01	25SG	25C13	26N	43.94
25SG	25C13	161O	62.15	65CA	25C13	26CB	87.36
65CA	25C13	66C	70.75	65CA	25C13	26CD1	57.53
65CA	25C13	65C	20.04	65CA	25C13	66CA	51.26
65CA	25C13	26CG	69.09	65CA	25C13	26N	94.25
26CB	25C13	66C	51.08	26CB	25C13	26CD1	34.05
26CB	25C13	65C	76.87	26CB	25C13	66CA	59.32
26CB	25C13	26CG	18.75	26CB	25C13	26N	31.21
66C	25C13	26CD1	60.72	66C	25C13	65C	50.94
66C	25C13	66CA	19.59	66C	25C13	26CG	50.32
66C	25C13	26N	81.92	26CD1	25C13	65C	54.60
26CD1	25C13	66CA	55.37	26CD1	25C13	26CG	16.44
26CD1	25C13	26N	38.73	65C	25C13	66CA	31.37
65C	25C13	26CG	60.91	65C	25C13	26N	93.30
66CA	25C13	26CG	51.05	66CA	25C13	26N	86.68
26CG	25C13	26N	35.89	25SG	25N14	23O	84.00
25SG	25N14	26CD1	79.14	25SG	25N14	161O	68.92
25SG	25N14	26N	43.55	25SG	25N14	23C	74.81
25SG	25N14	26CB	70.46	25SG	25N14	26CG	77.79
65CA	25N14	66N	36.05	65CA	25N14	23O	53.08
65CA	25N14	26CD1	61.64	65CA	25N14	65C	18.94
65CA	25N14	66O	73.48	65CA	25N14	65N	12.48
65CA	25N14	26N	99.87	65CA	25N14	23C	64.69
65CA	25N14	26CB	84.32	65CA	25N14	26CG	69.23
66N	25N14	23O	73.08	66N	25N14	26CD1	49.53
66N	25N14	65C	17.28	66N	25N14	66O	37.50
66N	25N14	65N	47.78	66N	25N14	26N	82.41
66N	25N14	23C	86.05	66N	25N14	26CB	56.95
66N	25N14	26CG	48.25	23O	25N14	26CD1	46.64
23O	25N14	65C	63.98	23O	25N14	66O	96.33
23O	25N14	65N	44.52	23O	25N14	26N	67.73
23O	25N14	23C	13.02	23O	25N14	26CB	76.26
23O	25N14	26CG	60.45	26CD1	25N14	65C	55.15

TABLE XVII

26CD1	25N14	66O	52.89	26CD1	25N14	65N	64.11
26CD1	25N14	26N	38.34	26CD1	25N14	23C	54.90
26CD1	25N14	26CB	30.70	26CD1	25N14	26CG	13.86
65C	25N14	66O	54.77	65C	25N14	65N	31.08
65C	25N14	26N	92.32	65C	25N14	23C	76.79
65C	25N14	26CB	70.71	65C	25N14	26CG	58.49
66O	25N14	65N	84.80	66O	25N14	26N	64.25
66O	25N14	26CB	35.42	66O	25N14	26CG	41.33
65N	25N14	23C	54.87	65N	25N14	26CB	90.63
65N	25N14	26CG	74.10	26N	25N14	23C	67.48
26N	25N14	26CB	29.19	26N	25N14	26CG	34.32
23C	25N14	26CB	82.14	23C	25N14	26CG	68.17
26CB	25N14	26CG	17.47	161O	25C15	25SG	89.42
161O	25C15	161C	13.49	161O	25C15	162CA	34.91
161O	25C15	162N	23.43	161O	25C15	161CA	23.63
25SG	25C15	161C	88.53	25SG	25C15	162CA	57.17
25SG	25C15	162N	74.53	161C	25C15	162CA	31.37
161C	25C15	162N	14.79	161C	25C15	161CA	16.28
162CA	25C15	162N	17.76	162CA	25C15	161CA	46.94
162N	25C15	161CA	29.37	65CA	25C15	230OH2	72.79
25SG	25C16	26N	61.11	25SG	25C16	25N	59.97
25SG	25C16	25CB	23.02	25SG	25C16	25CA	42.42
25SG	25C16	26CB	88.58	25SG	25C16	24N	92.96
25SG	25C16	25C	48.34	25SG	25C16	24C	74.43
25SG	25C16	26CA	71.25	25SG	25C16	24CA	91.58
23O	25C16	26CD1	61.77	23O	25C16	26N	94.53
23O	25C16	25N	67.24	23O	25C16	23C	18.20
23O	25C16	65CA	58.52	23O	25C16	25CA	87.06
23O	25C16	26CG	77.13	23O	25C16	26NE1	47.29
23O	25C16	26CB	97.08	23O	25C16	66N	79.63
23O	25C16	24N	30.53	23O	25C16	23CA	32.27
23O	25C16	25C	94.82	23O	25C16	24C	56.19
23O	25C16	26CA	99.54	23O	25C16	24CA	36.83
23O	25C16	65C	67.39	23O	25C16	65N	45.21
26CD1	25C16	26N	51.13	26CD1	25C16	25N	68.54
26CD1	25C16	23C	73.51	26CD1	25C16	65CA	68.04
26CD1	25C16	25CB	97.25	26CD1	25C16	25CA	76.12

TABLE XVII

26CD1	25C16	26CG	15.44	26CD1	25C16	26NE1	15.45
26CD1	25C16	26CB	35.76	26CD1	25C16	66N	52.08
26CD1	25C16	24N	69.01	26CD1	25C16	23CA	92.69
26CD1	25C16	25C	63.96	26CD1	25C16	24C	55.05
26CD1	25C16	26CA	44.91	26CD1	25C16	24CA	52.83
26CD1	25C16	65C	56.87	26CD1	25C16	66O	54.10
26CD1	25C16	65N	69.48	26N	25C16	25N	44.67
26N	25C16	23C	93.12	26N	25C16	25CB	51.34
26N	25C16	25CA	35.79	26N	25C16	26CG	42.62
26N	25C16	26NE1	63.79	26N	25C16	26CB	34.80
26N	25C16	66N	93.89	26N	25C16	24N	77.38
26N	25C16	25C	16.11	26N	25C16	24C	44.64
26N	25C16	26CA	16.33	26N	25C16	24CA	61.13
26N	25C16	66O	70.60	25N	25C16	23C	56.44
25N	25C16	25CB	37.16	25N	25C16	25CA	19.86
25N	25C16	26CG	71.75	25N	25C16	26NE1	70.29
25N	25C16	26CB	75.60	25N	25C16	24N	39.16
25N	25C16	23CA	68.19	25N	25C16	25C	33.83
25N	25C16	24C	15.28	25N	25C16	26CA	60.18
25N	25C16	24CA	31.81	23C	25C16	65CA	74.98
23C	25C16	25CB	86.20	23C	25C16	25CA	75.86
23C	25C16	26CG	87.97	23C	25C16	26NE1	60.92
23C	25C16	66N	97.84	23C	25C16	24N	17.30
23C	25C16	23CA	19.93	23C	25C16	25C	88.48
23C	25C16	24C	49.42	23C	25C16	24CA	32.05
23C	25C16	65C	85.33	23C	25C16	65N	60.76
65CA	25C16	26CG	76.49	65CA	25C16	26NE1	57.92
65CA	25C16	26CB	90.45	65CA	25C16	66N	33.37
65CA	25C16	24N	89.01	65CA	25C16	23CA	76.80
65CA	25C16	24CA	90.04	65CA	25C16	65C	17.45
65CA	25C16	66O	68.34	65CA	25C16	65N	14.75
25CB	25C16	25CA	21.65	25CB	25C16	26CG	93.09
25CB	25C16	26CB	85.06	25CB	25C16	24N	70.81
25CB	25C16	23CA	89.00	25CB	25C16	25C	35.50
25CB	25C16	24C	52.00	25CB	25C16	26CA	65.90
25CB	25C16	24CA	68.59	25CA	25C16	26CG	73.95
25CA	25C16	26NE1	82.49	25CA	25C16	26CB	70.49

TABLE XVII

25CA	25C16	24N	58.71	25CA	25C16	23CA	85.38
25CA	25C16	25C	20.38	25CA	25C16	24C	32.49
25CA	25C16	26CA	52.03	25CA	25C16	24CA	51.06
26CG	25C16	26NE1	30.69	26CG	25C16	26CB	20.39
26CG	25C16	66N	52.82	26CG	25C16	24N	81.30
26CG	25C16	25C	57.74	26CG	25C16	24C	60.85
26CG	25C16	26CA	32.36	26CG	25C16	24CA	63.73
26CG	25C16	65C	62.21	26CG	25C16	66O	43.58
26CG	25C16	65N	80.99	26NE1	25C16	26CB	51.09
26NE1	25C16	66N	51.16	26NE1	25C16	24N	59.98
26NE1	25C16	23CA	79.09	26NE1	25C16	25C	74.44
26NE1	25C16	24C	55.27	26NE1	25C16	26CA	59.77
26NE1	25C16	24CA	46.88	26NE1	25C16	65C	50.71
26NE1	25C16	66O	63.77	26NE1	25C16	65N	56.44
26CB	25C16	66N	60.55	26CB	25C16	24N	96.31
26CB	25C16	25C	50.81	26CB	25C16	24C	69.20
26CB	25C16	26CA	19.18	26CB	25C16	24CA	77.92
26CB	25C16	65C	73.91	26CB	25C16	66O	36.73
26CB	25C16	65N	98.03	66N	25C16	26CA	79.58
66N	25C16	24CA	97.14	66N	25C16	65C	16.15
66N	25C16	66O	35.16	66N	25C16	65N	46.29
24N	25C16	23CA	32.77	24N	25C16	25C	71.39
24N	25C16	24C	32.88	24N	25C16	26CA	88.94
24N	25C16	24CA	18.41	24N	25C16	65C	96.24
24N	25C16	65N	75.67	23CA	25C16	24C	65.31
23CA	25C16	24CA	50.41	23CA	25C16	65C	91.28
23CA	25C16	65N	62.12	25C	25C16	24C	39.37
25C	25C16	26CA	31.92	25C	25C16	24CA	58.36
25C	25C16	66O	85.95	24C	25C16	26CA	57.54
24C	25C16	24CA	19.36	24C	25C16	65N	97.77
26CA	25C16	24CA	71.17	26CA	25C16	65C	92.26
26CA	25C16	66O	54.28	24CA	25C16	65C	91.93
24CA	25C16	65N	79.37	65C	25C16	66O	51.31
65C	25C16	65N	30.19	66O	25C16	65N	81.41
25SG	25C17	25CB	33.36	25SG	25C17	25N	69.53
25SG	25C17	25CA	47.13	25SG	25C17	26N	51.70
25SG	25C17	25C	42.10	25SG	25C17	161O	81.99

TABLE XVII

25SG	25C17	162ND1	45.09	25SG	25C17	24C	78.33
25SG	25C17	26CD1	91.04	25SG	25C17	19NE2	91.40
25SG	25C17	24CA	96.69	25SG	25C17	163N	23.29
25SG	25C17	162CA	48.75	25CB	25C17	25N	43.65
25CB	25C17	25CA	23.36	25CB	25C17	23C	97.56
25CB	25C17	26N	52.35	25CB	25C17	24N	79.60
25CB	25C17	25C	34.92	25CB	25C17	162ND1	47.80
25CB	25C17	24C	54.50	25CB	25C17	26CD1	89.27
25CB	25C17	19NE2	59.46	25CB	25C17	24CA	71.68
25CB	25C17	163N	55.20	25CB	25C17	162CA	73.99
25N	25C17	25CA	22.58	25N	25C17	23O	63.36
25N	25C17	23C	56.78	25N	25C17	26N	42.10
25N	25C17	23CA	72.74	25N	25C17	24N	39.75
25N	25C17	25C	33.56	25N	25C17	162ND1	89.46
25N	25C17	24C	11.07	25N	25C17	26CD1	57.00
25N	25C17	19NE2	52.78	25N	25C17	24CA	28.26
25N	25C17	163N	92.62	25CA	25C17	23O	85.24
25CA	25C17	23C	79.30	25CA	25C17	26N	36.07
25CA	25C17	23CA	93.96	25CA	25C17	24N	61.96
25CA	25C17	25C	19.74	25CA	25C17	162ND1	71.14
25CA	25C17	24C	32.47	25CA	25C17	26CD1	67.46
25CA	25C17	19NE2	60.34	25CA	25C17	24CA	50.61
25CA	25C17	163N	70.36	25CA	25C17	162CA	94.23
23O	25C17	23C	18.25	23O	25C17	26N	78.82
23O	25C17	23CA	34.40	23O	25C17	24N	31.56
23O	25C17	25C	86.35	23O	25C17	24C	52.82
23O	25C17	26CD1	45.95	23O	25C17	19NE2	76.58
23O	25C17	23OOH2	65.85	23O	25C17	24CA	35.23
23C	25C17	26N	84.24	23C	25C17	23CA	21.57
23C	25C17	24N	17.96	23C	25C17	25C	86.44
23C	25C17	24C	48.18	23C	25C17	26CD1	59.52
23C	25C17	19NE2	58.61	23C	25C17	23OOH2	60.40
23C	25C17	24CA	30.09	26N	25C17	24N	73.12
26N	25C17	25C	17.65	26N	25C17	162ND1	93.89
26N	25C17	24C	42.62	26N	25C17	26CD1	40.31
26N	25C17	19NE2	93.61	26N	25C17	24CA	56.29
26N	25C17	163N	67.72	26N	25C17	162CA	96.10

TABLE XVII

23CA	25C17	24N	33.68	23CA	25C17	24C	66.27
23CA	25C17	26CD1	79.75	23CA	25C17	19NE2	53.84
23CA	25C17	230OH2	40.17	23CA	25C17	24CA	49.58
24N	25C17	25C	71.51	24N	25C17	24C	32.59
24N	25C17	26CD1	59.47	24N	25C17	19NE2	47.60
24N	25C17	230OH2	73.74	24N	25C17	24CA	16.96
25C	25C17	162ND1	79.14	25C	25C17	24C	38.92
25C	25C17	26CD1	55.45	25C	25C17	19NE2	79.80
25C	25C17	24CA	56.38	25C	25C17	163N	62.85
25C	25C17	162CA	90.50	161O	25C17	162ND1	62.06
161O	25C17	230OH2	90.45	161O	25C17	163N	60.08
161O	25C17	162CA	33.46	162ND1	25C17	19NE2	71.55
162ND1	25C17	163N	44.58	162ND1	25C17	162CA	38.78
24C	25C17	26CD1	48.36	24C	25C17	19NE2	57.22
24C	25C17	24CA	18.38	26CD1	25C17	24CA	46.21
19NE2	25C17	230OH2	73.47	19NE2	25C17	24CA	57.12
230OH2	25C17	24CA	89.69	163N	25C17	162CA	28.44
25SG	25C18	161O	91.87	25SG	25C18	25CB	20.14
25SG	25C18	23CA	98.61	25SG	25C18	161C	85.38
25SG	25C18	23O	83.74	25SG	25C18	23C	83.16
25SG	25C18	162ND1	47.66	25SG	25C18	162CA	57.49
25SG	25C18	25N	40.60	161O	25C18	161C	8.04
161O	25C18	162ND1	67.18	161O	25C18	162CA	35.14
230OH2	25C18	23CA	43.13	230OH2	25C18	23O	66.88
230OH2	25C18	23C	61.23	25CB	25C18	23CA	84.02
25CB	25C18	161C	98.23	25CB	25C18	23O	77.59
25CB	25C18	23C	72.21	25CB	25C18	162ND1	43.49
25CB	25C18	162CA	68.17	25CB	25C18	25N	30.01
23CA	25C18	23O	30.55	23CA	25C18	23C	19.20
23CA	25C18	25N	58.06	161C	25C18	162ND1	65.74
161C	25C18	162CA	30.20	23O	25C18	23C	15.25
23O	25C18	25N	47.60	23C	25C18	25N	43.17
162ND1	25C18	162CA	39.32	162ND1	25C18	25N	72.26
162CA	25C18	25N	96.88	66O	25C19	67CE1	68.17
66O	25C19	67CD1	54.92	160O	25C19	161C	52.84
160O	25C19	161CA	35.03	160O	25C19	161O	63.95
160O	25C19	162N	57.36	67CE1	25C19	67CD1	17.17

TABLE XVII

161C	25C19	161CA	18.68	161C	25C19	161O	14.83
161C	25C19	162N	15.27	161CA	25C19	161O	29.02
161CA	25C19	162N	28.85	161O	25C19	162N	26.37
66O	25C20	67CD1	61.25	66O	25C20	163CB	94.46
66O	25C20	66C	9.87	66O	25C20	68SD	69.49
66O	25C20	67CE1	71.63	66O	25C20	26CB	36.33
67CD1	25C20	66C	52.72	67CD1	25C20	68SD	78.08
67CD1	25C20	67CE1	17.64	67CD1	25C20	26CB	92.78
163CB	25C20	68SD	53.55	163CB	25C20	163N	29.80
163CB	25C20	134CB	65.83	163CB	25C20	26CB	58.92
66C	25C20	68SD	74.07	66C	25C20	67CE1	62.03
66C	25C20	26CB	46.18	68SD	25C20	67CE1	95.08
68SD	25C20	163N	82.16	68SD	25C20	134CB	71.67
68SD	25C20	26CB	55.82	163N	25C20	134CB	62.79
163N	25C20	26CB	80.06	67CD1	25C21	209CD2	74.52
67CD1	25C21	67CE1	21.15	67CD1	25C21	66O	65.47
67CD1	25C21	68SD	94.26	67CD1	25C21	67CA	41.35
67CD1	25C21	67CG	10.50	67CD1	25C21	209CG	78.82
67CD1	25C21	66C	53.86	209CD2	25C21	67CE1	74.15
209CD2	25C21	68SD	93.95	209CD2	25C21	134CB	66.63
209CD2	25C21	67CA	99.15	209CD2	25C21	67CG	80.75
209CD2	25C21	209CG	13.43	209CD2	25C21	68CE	78.53
67CE1	25C21	66O	75.62	67CE1	25C21	67CA	60.36
67CE1	25C21	67CG	30.58	67CE1	25C21	209CG	82.83
67CE1	25C21	66C	64.25	66O	25C21	68SD	70.26
66O	25C21	67CA	36.25	66O	25C21	67CG	56.88
66O	25C21	68CE	92.80	66O	25C21	66C	11.70
68SD	25C21	134CB	81.96	68SD	25C21	67CA	59.58
68SD	25C21	67CG	85.39	68SD	25C21	209CG	80.91
68SD	25C21	68CE	22.58	68SD	25C21	66C	74.79
134CB	25C21	209CG	61.74	134CB	25C21	68CE	60.74
67CA	25C21	67CG	30.85	67CA	25C21	209CG	95.15
67CA	25C21	68CE	78.69	67CA	25C21	66C	29.16
67CG	25C21	209CG	82.94	67CG	25C21	68CE	99.01
67CG	25C21	66C	45.56	209CG	25C21	68CE	65.12
68CE	25C21	66C	97.17	163N	25C22	163CB	41.38
163N	25C22	162C	21.72	163N	25C22	163CA	22.86

TABLE XVII

163N	25C22 162O	35.18	163N	25C22 162CA	35.98
163N	25C22 162N	54.90	163N	25C22 134CB	83.08
163N	25C22 25SG	48.42	163N	25C22 161C	68.41
163N	25C22 68SD	98.47	163N	25C22 161O	68.27
163N	25C22 134CA	66.14	163CB	25C22 162C	60.85
163CB	25C22 163CA	23.53	163CB	25C22 162O	65.54
163CB	25C22 162CA	77.32	163CB	25C22 162N	96.04
163CB	25C22 134CB	83.53	163CB	25C22 25SG	60.46
163CB	25C22 66O	95.09	163CB	25C22 68SD	58.15
163CB	25C22 134CA	68.94	162C	25C22 163CA	38.46
162C	25C22 162O	18.52	162C	25C22 162CA	21.19
162C	25C22 162N	35.80	162C	25C22 134CB	73.18
162C	25C22 25SG	61.51	162C	25C22 161C	51.73
162C	25C22 161O	56.33	162C	25C22 134CA	58.55
163CA	25C22 162O	42.12	163CA	25C22 162CA	57.32
163CA	25C22 162N	74.25	163CA	25C22 134CB	72.12
163CA	25C22 25SG	61.97	163CA	25C22 161C	89.59
163CA	25C22 68SD	76.50	163CA	25C22 161O	90.96
163CA	25C22 134CA	55.19	162O	25C22 162CA	34.60
162O	25C22 162N	40.22	162O	25C22 134CB	54.86
162O	25C22 25SG	79.79	162O	25C22 161C	57.52
162O	25C22 161O	66.63	162O	25C22 134CA	41.20
162CA	25C22 162N	20.16	162CA	25C22 134CB	87.29
162CA	25C22 25SG	55.65	162CA	25C22 161C	32.48
162CA	25C22 161O	35.17	162CA	25C22 134CA	75.53
162N	25C22 134CB	81.91	162N	25C22 25SG	71.75
162N	25C22 161C	17.31	162N	25C22 161O	28.19
162N	25C22 134CA	75.24	134CB	25C22 161C	94.20
134CB	25C22 68SD	76.86	134CB	25C22 134CA	17.24
25SG	25C22 161C	71.58	25SG	25C22 66O	87.43
25SG	25C22 161O	59.61	161C	25C22 161O	14.91
161C	25C22 134CA	90.49	66O	25C22 68SD	61.09
68SD	25C22 134CA	77.47	161O	25N23 25SG	96.69
161O	25N23 162ND1	87.98	161O	25N23 161C	7.60
161O	25N23 162CA	42.67	161O	25N23 162CB	53.10
161O	25N23 162N	24.12	161O	25N23 162CG	72.20
161O	25N23 162CE1	99.02	25SG	25N23 162ND1	58.85

TABLE XVII

25SG	25N23	161C	90.78	25SG	25N23	162CA	65.10
25SG	25N23	162CB	74.63	25SG	25N23	25CB	22.39
25SG	25N23	162N	78.71	25SG	25N23	162CG	65.53
25SG	25N23	162CE1	56.82	162ND1	25N23	161C	80.81
162ND1	25N23	162CA	47.69	162ND1	25N23	162CB	35.43
162ND1	25N23	25CB	47.77	162ND1	25N23	162N	64.92
162ND1	25N23	162CG	16.11	162ND1	25N23	162CE1	11.08
161C	25N23	162CA	35.07	161C	25N23	162CB	46.35
161C	25N23	162N	16.53	161C	25N23	162CG	65.21
161C	25N23	162CE1	91.80	162CA	25N23	162CB	20.44
162CA	25N23	25CB	73.45	162CA	25N23	162N	18.55
162CA	25N23	162CG	33.95	162CA	25N23	162CE1	58.16
162CB	25N23	25CB	75.17	162CB	25N23	162N	31.96
162CB	25N23	162CG	19.34	162CB	25N23	162CE1	46.49
25CB	25N23	162N	90.62	25CB	25N23	162CG	59.94
25CB	25N23	162CE1	41.59	162N	25N23	162CG	49.81
162N	25N23	162CE1	75.77	162CG	25N23	162CE1	27.14
161O	25C24	162ND1	71.20	161O	25C24	25SG	68.87
161O	25C24	25CB	86.70	161O	25C24	162CE1	84.02
161O	25C24	161C	5.61	161O	25C24	162CG	60.27
230OH2	25C24	19NE2	82.86	230OH2	25C24	23CA	39.21
162ND1	25C24	25SG	49.38	162ND1	25C24	19NE2	75.30
162ND1	25C24	25CB	42.32	162ND1	25C24	162CE1	12.89
162ND1	25C24	161C	66.20	162ND1	25C24	162CG	13.50
25SG	25C24	19NE2	69.24	25SG	25C24	25CB	21.54
25SG	25C24	162CE1	51.86	25SG	25C24	161C	67.93
25SG	25C24	23CA	75.54	25SG	25C24	162CG	55.53
19NE2	25C24	25CB	50.50	19NE2	25C24	162CE1	63.30
19NE2	25C24	23CA	49.37	19NE2	25C24	162CG	88.70
25CB	25C24	162CE1	38.82	25CB	25C24	161C	84.51
25CB	25C24	23CA	72.33	25CB	25C24	162CG	53.33
162CE1	25C24	161C	79.07	162CE1	25C24	162CG	25.60
161C	25C24	162CG	54.95	230OH2	25O25	23CA	52.31
230OH2	25O25	22O	74.89	230OH2	25O25	23N	49.81
230OH2	25O25	23C	64.37	23CA	25O25	19NE2	59.20
23CA	25O25	25SG	80.98	23CA	25O25	22O	33.94
23CA	25O25	23N	14.51	23CA	25O25	23C	15.82

TABLE XVII

19NE2	25O25	25SG	68.80	19NE2	25O25	22O	32.41
19NE2	25O25	23N	57.42	19NE2	25O25	23C	55.28
25SG	25O25	22O	87.84	25SG	25O25	161O	56.79
25SG	25O25	23N	93.48	25SG	25O25	23C	65.16
22O	25O25	23N	26.63	22O	25O25	23C	39.45
23N	25O25	23C	29.23	162ND1	25C26	161O	70.33
162ND1	25C26	162CG	16.51	162ND1	25C26	184CZ2	61.61
162ND1	25C26	162CB	33.57	162ND1	25C26	162CE1	14.30
162ND1	25C26	184NE1	54.26	161O	25C26	162CG	62.73
161O	25C26	162CB	46.80	161O	25C26	162CE1	84.49
162CG	25C26	184CZ2	58.73	162CG	25C26	162CB	18.91
162CG	25C26	162CE1	27.71	162CG	25C26	184NE1	61.32
184CZ2	25C26	162CB	69.73	184CZ2	25C26	162CE1	53.77
184CZ2	25C26	184NE1	30.35	162CB	25C26	162CE1	46.35
162CB	25C26	184NE1	78.86	162CE1	25C26	184NE1	40.84
161O	25C27	161OD1	53.78	161O	25C27	161C	11.71
161O	25C27	162CB	46.13	161O	25C27	162ND1	62.87
161OD1	25C27	161C	42.77	161OD1	25C27	162CB	55.70
161OD1	25C27	162ND1	86.16	161C	25C27	162CB	40.57
161C	25C27	162ND1	63.10	162CB	25C27	162ND1	30.49
161OD1	25C28	137O	69.81	161OD1	25C28	161O	54.98
161OD1	25C28	137C	53.96	161OD1	25C28	137CB	55.92
161OD1	25C28	162CB	61.51	161OD1	25C28	161CG	11.62
161OD1	25C28	138N	47.36	161OD1	25C28	161C	42.86
137O	25C28	137C	15.86	137O	25C28	184CZ2	70.21
137O	25C28	137CB	37.24	137O	25C28	162CB	85.15
137O	25C28	161CG	80.00	137O	25C28	138N	27.64
137O	25C28	184CH2	55.56	161O	25C28	137CB	84.76
161O	25C28	162CB	45.37	161O	25C28	161CG	49.97
161O	25C28	161C	13.42	137C	25C28	184CZ2	81.49
137C	25C28	137CB	32.38	137C	25C28	162CB	78.21
137C	25C28	161CG	64.18	137C	25C28	138N	15.77
137C	25C28	184CH2	68.22	137C	25C28	161C	90.09
184CZ2	25C28	137CB	63.63	184CZ2	25C28	162CB	70.10
184CZ2	25C28	138N	96.79	184CZ2	25C28	184CH2	15.72
137CB	25C28	162CB	47.93	137CB	25C28	161CG	67.40
137CB	25C28	138N	45.63	137CB	25C28	184CH2	56.70

TABLE XVII

137CB	25C28 161C	73.01	162CB	25C28 161CG	66.72
162CB	25C28 138N	87.00	162CB	25C28 184CH2	76.56
162CB	25C28 161C	39.92	161CG	25C28 138N	55.54
161CG	25C28 161C	39.76	138N	25C28 184CH2	82.84
138N	25C28 161C	88.57	161OD1	25C29 161CG	17.77
161OD1	25C29 161CB	38.20	161OD1	25C29 137C	69.75
161OD1	25C29 138N	63.36	161OD1	25C29 161O	67.46
161OD1	25C29 137O	86.87	161OD1	25C29 138CA	77.48
161OD1	25C29 137CB	66.56	161OD1	25C29 161C	51.63
161OD1	25C29 137CA	57.43	161OD1	25C29 137N	38.54
161OD1	25C29 161ND2	20.78	161OD1	25C29 162CB	69.24
161OD1	25C29 138CB	70.48	161OD1	25C29 161CA	39.44
161OD1	25C29 162N	49.70	161CG	25C29 161CB	23.57
161CG	25C29 137C	84.96	161CG	25C29 138N	74.84
161CG	25C29 161O	62.41	161CG	25C29 138CA	84.52
161CG	25C29 137CB	84.24	161CG	25C29 161C	49.09
161CG	25C29 137CA	74.70	161CG	25C29 137N	55.87
161CG	25C29 161ND2	11.82	161CG	25C29 162CB	78.89
161CG	25C29 138CB	72.41	161CG	25C29 161CA	31.89
161CG	25C29 162N	53.19	161CB	25C29 138N	98.38
161CB	25C29 161O	43.85	161CB	25C29 137CB	99.44
161CB	25C29 161C	35.43	161CB	25C29 137CA	94.94
161CB	25C29 137N	76.23	161CB	25C29 161ND2	33.15
161CB	25C29 162CB	75.97	161CB	25C29 138CB	91.71
161CB	25C29 161CA	16.99	161CB	25C29 162N	46.28
137C	25C29 138N	19.59	137C	25C29 137O	17.39
137C	25C29 138CA	35.03	137C	25C29 137CB	35.61
137C	25C29 137CA	20.11	137C	25C29 137N	34.13
137C	25C29 161ND2	78.64	137C	25C29 162CB	84.64
137C	25C29 138CB	50.91	137C	25C29 162N	96.62
138N	25C29 137O	32.46	138N	25C29 138CA	20.27
138N	25C29 137CB	52.67	138N	25C29 137CA	33.41
138N	25C29 137N	37.77	138N	25C29 161ND2	65.96
138N	25C29 162CB	98.96	138N	25C29 138CB	32.14
161O	25C29 137CB	93.41	161O	25C29 161C	16.38
161O	25C29 137N	91.81	161O	25C29 161ND2	74.07
161O	25C29 162CB	47.11	161O	25C29 161CA	30.52

TABLE XVII

161O	25C29 162N	27.28	137O	25C29 138CA	39.55
137O	25C29 137CB	39.61	137O	25C29 137CA	32.50
137O	25C29 137N	49.84	137O	25C29 161ND2	95.83
137O	25C29 162CB	87.74	137O	25C29 138CB	58.44
138CA	25C29 137CB	70.56	138CA	25C29 137CA	52.71
138CA	25C29 137N	57.82	138CA	25C29 161ND2	73.59
138CA	25C29 138CB	19.26	137CB	25C29 161C	82.69
137CB	25C29 137CA	20.23	137CB	25C29 137N	32.22
137CB	25C29 161ND2	84.94	137CB	25C29 162CB	49.44
137CB	25C29 138CB	84.72	137CB	25C29 161CA	89.09
137CB	25C29 162N	67.71	161C	25C29 137CA	89.83
161C	25C29 137N	76.15	161C	25C29 161ND2	60.90
161C	25C29 162CB	43.16	161C	25C29 161CA	18.88
161C	25C29 162N	15.26	137CA	25C29 137N	18.89
137CA	25C29 161ND2	71.91	137CA	25C29 162CB	66.00
137CA	25C29 138CB	65.00	137CA	25C29 161CA	89.85
137CA	25C29 162N	76.62	137N	25C29 161ND2	53.90
137N	25C29 162CB	64.20	137N	25C29 138CB	63.74
137N	25C29 161CA	72.67	137N	25C29 162N	65.28
161ND2	25C29 162CB	88.34	161ND2	25C29 138CB	60.67
161ND2	25C29 161CA	43.56	161ND2	25C29 162N	64.33
162CB	25C29 161CA	59.23	162CB	25C29 162N	29.75
161CA	25C29 162N	29.47	137O	25C30 143NE2	59.46
137O	25C30 184CZ2	69.76	137O	25C30 137C	14.57
137O	25C30 138CA	35.79	137O	25C30 184CH2	56.99
137O	25C30 138N	26.64	143NE2	25C30 184CZ2	83.66
143NE2	25C30 137C	71.37	143NE2	25C30 138CA	63.07
143NE2	25C30 184CH2	68.61	143NE2	25C30 138N	72.68
184CZ2	25C30 137C	78.03	184CZ2	25C30 184CH2	16.45
184CZ2	25C30 138N	93.46	137C	25C30 138CA	30.17
137C	25C30 184CH2	67.67	137C	25C30 138N	15.43
138CA	25C30 184CH2	92.20	138CA	25C30 138N	17.17
184CH2	25C30 138N	82.69	184CZ2	25N31 184NE1	33.41
184CZ2	25N31 184CE2	17.32	184CZ2	25N31 162ND1	57.89
184CZ2	25N31 19NE2	96.35	184NE1	25N31 184CE2	16.98
184NE1	25N31 162ND1	53.50	184NE1	25N31 19NE2	63.65
184CE2	25N31 162ND1	57.86	184CE2	25N31 19NE2	80.63

TABLE XVII

162ND1	25N31	19NE2	68.39	184NE1	25C32	184CE2	19.92
184NE1	25C32	184CZ2	38.87	184NE1	25C32	19NE2	81.55
184NE1	25C32	19OE1	51.17	184NE1	25C32	19CD	64.02
184NE1	25C32	184CD1	13.69	184NE1	25C32	162ND1	58.56
184NE1	25C32	162CE1	44.43	184CE2	25C32	184CZ2	20.46
184CE2	25C32	19OE1	70.66	184CE2	25C32	19CD	83.94
184CE2	25C32	184CD1	29.80	184CE2	25C32	162ND1	62.83
184CE2	25C32	162CE1	52.80	184CZ2	25C32	19OE1	86.31
184CZ2	25C32	184CD1	50.14	184CZ2	25C32	162ND1	60.09
184CZ2	25C32	162CE1	56.05	19NE2	25C32	19OE1	31.34
19NE2	25C32	19CD	17.91	19NE2	25C32	184CD1	75.00
19NE2	25C32	162ND1	75.92	19NE2	25C32	162CE1	69.31
19OE1	25C32	19CD	16.54	19OE1	25C32	184CD1	47.47
19OE1	25C32	162ND1	56.39	19OE1	25C32	162CE1	44.21
19CD	25C32	184CD1	57.09	19CD	25C32	162ND1	70.79
19CD	25C32	162CE1	60.09	184CD1	25C32	162ND1	69.23
184CD1	25C32	162CE1	53.91	162ND1	25C32	162CE1	16.00
184NE1	25O33	19OE1	71.37	184NE1	25O33	19CD	86.43
184NE1	25O33	184CE2	20.79	184NE1	25O33	184CD1	17.17
184NE1	25O33	162CE1	60.07	184NE1	25O33	184CZ2	41.79
184NE1	25O33	162ND1	76.01	184NE1	25O33	19CG	80.45
184NE1	25O33	184CD2	16.63	184NE1	25O33	162NE2	50.59
184NE1	25O33	184CG	13.72	184NE1	25O33	162CG	72.21
184NE1	25O33	25CB	93.48	19OE1	25O33	19NE2	40.72
19OE1	25O33	19CD	21.44	19OE1	25O33	184CE2	91.61
19OE1	25O33	184CD1	61.45	19OE1	25O33	162CE1	59.41
19OE1	25O33	162ND1	74.45	19OE1	25O33	19CG	30.46
19OE1	25O33	184CD2	87.26	19OE1	25O33	162NE2	64.69
19OE1	25O33	184CG	72.71	19OE1	25O33	162CG	83.38
19OE1	25O33	25CB	44.37	19NE2	25O33	19CD	22.85
19NE2	25O33	184CD1	95.28	19NE2	25O33	162CE1	91.27
19NE2	25O33	162ND1	97.51	19NE2	25O33	19CG	32.33
19NE2	25O33	25CB	55.21	19CD	25O33	184CD1	72.73
19CD	25O33	162CE1	79.91	19CD	25O33	162ND1	92.65
19CD	25O33	19CG	15.53	19CD	25O33	162NE2	85.98
19CD	25O33	184CG	83.64	19CD	25O33	25CB	55.10
184CE2	25O33	184CD1	35.82	184CE2	25O33	162CE1	66.09

TABLE XVII

184CE2	25O33	184CZ2	21.88	184CE2	25O33	162ND1	76.32
184CE2	25O33	184CD2	10.76	184CE2	25O33	162NE2	54.99
184CE2	25O33	184CG	26.75	184CE2	25O33	162CG	68.94
184CD1	25O33	162CE1	68.79	184CD1	25O33	184CZ2	57.65
184CD1	25O33	162ND1	87.29	184CD1	25O33	19CG	64.62
184CD1	25O33	184CD2	27.61	184CD1	25O33	162NE2	61.38
184CD1	25O33	184CG	11.29	184CD1	25O33	162CG	85.74
184CD1	25O33	25CB	93.60	162CE1	25O33	184CZ2	67.50
162CE1	25O33	162ND1	20.07	162CE1	25O33	19CG	89.40
162CE1	25O33	184CD2	72.00	162CE1	25O33	162NE2	11.22
162CE1	25O33	184CG	72.92	162CE1	25O33	162CG	25.06
162CE1	25O33	25CB	41.49	184CZ2	25O33	162ND1	70.13
184CZ2	25O33	184CD2	31.61	184CZ2	25O33	162NE2	56.74
184CZ2	25O33	184CG	48.49	184CZ2	25O33	162CG	60.18
162ND1	25O33	184CD2	84.61	162ND1	25O33	162NE2	25.95
162ND1	25O33	184CG	89.59	162ND1	25O33	162CG	11.10
162ND1	25O33	25CB	42.38	19CG	25O33	184CD2	91.76
19CG	25O33	162NE2	93.17	19CG	25O33	184CG	74.56
19CG	25O33	25CB	70.08	184CD2	25O33	162NE2	61.34
184CD2	25O33	184CG	17.21	184CD2	25O33	162CG	78.20
162NE2	25O33	184CG	63.94	162NE2	25O33	162CG	26.05
162NE2	25O33	25CB	52.56	184CG	25O33	162CG	85.93
162CG	25O33	25CB	53.49	184NE1	25O34	184CE2	18.11
184NE1	25O34	184CZ2	33.70	184NE1	25O34	19NE2	70.03
184NE1	25O34	184CD1	15.57	184NE1	25O34	19CD	56.05
184NE1	25O34	19OE1	43.11	184CE2	25O34	184CZ2	18.11
184CE2	25O34	19NE2	87.63	184CE2	25O34	184CD1	28.12
184CE2	25O34	19CD	74.10	184CE2	25O34	19OE1	60.83
184CZ2	25O34	19NE2	97.82	184CZ2	25O34	184CD1	46.02
184CZ2	25O34	19CD	86.79	184CZ2	25O34	19OE1	72.54
19NE2	25O34	184CD1	68.22	19NE2	25O34	19CD	16.05
19NE2	25O34	19OE1	26.92	184CD1	25O34	19CD	52.52
184CD1	25O34	19OE1	42.67	19CD	25O34	19OE1	14.42
20O	25C35	19NE2	68.42	20O	25C35	19CD	70.46
20O	25C35	19CG	55.17	20O	25C35	19OE1	84.98
20O	25C35	21NE2	59.84	20O	25C35	21OE1	59.50
19NE2	25C35	184NE1	74.82	19NE2	25C35	19CD	18.63

TABLE XVII

19NE2	25C35	19CG	33.10	19NE2	25C35	184CD1	76.03
19NE2	25C35	19OE1	29.73	19NE2	25C35	184CE2	89.27
184NE1	25C35	19CD	61.33	184NE1	25C35	19CG	69.26
184NE1	25C35	184CD1	18.20	184NE1	25C35	19OE1	46.19
184NE1	25C35	184CE2	15.64	19CD	25C35	19CG	20.18
19CD	25C35	184CD1	59.00	19CD	25C35	19OE1	15.55
19CD	25C35	184CE2	76.79	19CG	25C35	184CD1	60.31
19CG	25C35	19OE1	31.00	19CG	25C35	184CE2	84.62
184CD1	25C35	19OE1	46.45	184CD1	25C35	184CE2	27.90
19OE1	25C35	184CE2	61.48	21NE2	25C35	21OE1	26.73
21NE2	25C36	20O	62.73	21NE2	25C36	21CD	14.08
20O	25C36	19CG	49.13	20O	25C36	21CD	53.84
184CD1	25C36	184NE1	18.40	184CD1	25C36	184CG	16.42
184CD1	25C36	184CE2	27.92	184CD1	25C36	19CG	56.22
184NE1	25C36	184CG	28.30	184NE1	25C36	184CE2	16.44
184NE1	25C36	19CG	61.95	184CG	25C36	184CE2	27.91
184CG	25C36	19CG	70.47	184CE2	25C36	19CG	78.31
21NE2	25C37	20O	79.74	21NE2	25C37	21CD	16.72
21NE2	25C37	21OE1	29.73	21NE2	25C37	20C	72.88
20O	25C37	21CD	66.28	20O	25C37	21OE1	66.79
20O	25C37	20C	14.00	21CD	25C37	21OE1	16.17
21CD	25C37	20C	62.16	21OE1	25C37	20C	66.88
21NE2	25C38	21CD	9.90	21NE2	25C38	20O	63.92
21CD	25C38	20O	54.43	184CG	25C40	184CB	20.90
184CG	25C40	184CD2	19.97	184CG	25C40	184CD1	18.76
184CG	25C40	184CE2	29.83	184CG	25C40	184NE1	29.07
184CG	25C40	184CE3	34.09	184CG	25C40	184O	55.54
184CG	25C40	184CA	32.20	184CB	25C40	184CD2	36.24
184CB	25C40	184CD1	35.47	184CB	25C40	184CE2	50.10
184CB	25C40	184NE1	49.38	184CB	25C40	184CE3	43.19
184CB	25C40	184O	34.81	184CB	25C40	184CA	17.73
184CD2	25C40	184CD1	30.80	184CD2	25C40	184CE2	17.77
184CD2	25C40	184NE1	29.02	184CD2	25C40	184CE3	17.34
184CD2	25C40	184O	69.94	184CD2	25C40	184CA	51.16
184CD1	25C40	184CE2	28.86	184CD1	25C40	184NE1	17.14
184CD1	25C40	184CE3	47.95	184CD1	25C40	184O	66.59
184CD1	25C40	184CA	38.47	184CE2	25C40	184NE1	17.07

TABLE XVII

184CE2	25C40	184CE3	30.61	184CE2	25C40	184O	84.89
184CE2	25C40	184CA	61.54	184NE1	25C40	184CE3	45.35
184NE1	25C40	184O	82.69	184NE1	25C40	184CA	55.30
184CE3	25C40	184O	71.49	184CE3	25C40	184CA	60.55
184O	25C40	184CA	28.85	184CD1	25C41	184CG	21.77
184CD1	25C41	184NE1	21.97	184CD1	25C41	184CD2	35.07
184CD1	25C41	184CE2	34.98	184CD1	25C41	184CB	36.36
184CD1	25C41	184CE3	51.22	184CD1	25C41	184CZ2	50.86
184CD1	25C41	184CA	37.30	184CG	25C41	184NE1	35.87
184CG	25C41	184CD2	21.86	184CG	25C41	184CE2	35.60
184CG	25C41	184CB	19.28	184CG	25C41	184CE3	34.71
184CG	25C41	184CZ2	50.97	184CG	25C41	184CA	30.15
184NE1	25C41	184CD2	34.95	184NE1	25C41	184CE2	20.95
184NE1	25C41	184CB	54.49	184NE1	25C41	184CE3	50.02
184NE1	25C41	184CZ2	33.28	184NE1	25C41	184CA	58.90
184CD2	25C41	184CE2	21.45	184CD2	25C41	184CB	36.52
184CD2	25C41	184CE3	16.39	184CD2	25C41	184CZ2	32.78
184CD2	25C41	184CA	51.13	184CE2	25C41	184CB	54.20
184CE2	25C41	184CE3	32.31	184CE2	25C41	184CZ2	16.30
184CE2	25C41	184CA	65.12	184CB	25C41	184CE3	43.07
184CB	25C41	184CZ2	68.63	184CB	25C41	184CA	17.27
184CE3	25C41	184CZ2	36.53	184CE3	25C41	184CA	59.94
184CZ2	25C41	184CA	80.95	25SG	25O42	25CB	38.64
25SG	25O42	25N	73.56	25SG	25O42	25CA	53.59
25SG	25O42	24C	84.78	25SG	25O42	19OE1	88.63
25SG	25O42	25C	44.83	25SG	25O42	26N	45.60
25SG	25O42	162ND1	49.49	25SG	25O42	162CE1	54.51
25SG	25O42	26CD1	74.03	25CB	25O42	25N	49.39
25CB	25O42	19NE2	81.36	25CB	25O42	24N	99.21
25CB	25O42	25CA	25.75	25CB	25O42	24C	62.76
25CB	25O42	24CA	84.14	25CB	25O42	19CD	66.86
25CB	25O42	19OE1	53.70	25CB	25O42	25C	31.71
25CB	25O42	26N	46.47	25CB	25O42	162ND1	47.29
25CB	25O42	162CE1	39.19	25CB	25O42	26CD1	82.79
25N	25O42	23C	70.38	25N	25O42	23CA	94.53
25N	25O42	19NE2	73.90	25N	25O42	24N	51.16
25N	25O42	25CA	23.79	25N	25O42	23O	72.18

TABLE XVII

25N	25O42	24C	13.37	25N	25O42	24CA	34.78
25N	25O42	19CD	67.53	25N	25O42	19OE1	67.99
25N	25O42	22O	80.77	25N	25O42	25C	28.88
25N	25O42	26N	36.19	25N	25O42	162ND1	95.82
25N	25O42	23N	91.99	25N	25O42	22C	85.72
25N	25O42	162CE1	84.41	25N	25O42	26CD1	52.11
23C	25O42	23CA	27.54	23C	25O42	19NE2	81.75
23C	25O42	24N	23.31	23C	25O42	25CA	94.12
23C	25O42	23O	20.23	23C	25O42	24C	57.01
23C	25O42	24CA	35.64	23C	25O42	19CD	92.20
23C	25O42	22O	49.02	23C	25O42	230OH2	70.61
23C	25O42	25C	93.36	23C	25O42	26N	86.51
23C	25O42	23N	31.08	23C	25O42	22C	39.18
23C	25O42	26CD1	57.51	23CA	25O42	19NE2	75.36
23CA	25O42	24N	43.40	23CA	25O42	23O	40.93
23CA	25O42	24C	81.51	23CA	25O42	24CA	60.46
23CA	25O42	19CD	89.50	23CA	25O42	22O	38.60
23CA	25O42	230OH2	46.00	23CA	25O42	23N	9.62
23CA	25O42	22C	25.11	23CA	25O42	26CD1	82.64
19NE2	25O42	24N	65.75	19NE2	25O42	25CA	78.16
19NE2	25O42	24C	73.53	19NE2	25O42	24CA	73.72
19NE2	25O42	19CD	14.86	19NE2	25O42	19OE1	30.78
19NE2	25O42	22O	36.84	19NE2	25O42	230OH2	94.24
19NE2	25O42	25C	94.02	19NE2	25O42	162ND1	84.58
19NE2	25O42	23N	65.76	19NE2	25O42	22C	50.27
19NE2	25O42	162CE1	71.88	24N	25O42	25CA	74.59
24N	25O42	23O	38.03	24N	25O42	24C	38.35
24N	25O42	24CA	18.53	24N	25O42	19CD	72.99
24N	25O42	19OE1	86.24	24N	25O42	22O	42.70
24N	25O42	230OH2	89.40	24N	25O42	25C	78.15
24N	25O42	26N	76.91	24N	25O42	23N	41.41
24N	25O42	22C	39.81	24N	25O42	26CD1	59.70
25CA	25O42	23O	93.85	25CA	25O42	24C	37.14
25CA	25O42	24CA	58.56	25CA	25O42	19CD	66.70
25CA	25O42	19OE1	60.00	25CA	25O42	22O	97.56
25CA	25O42	25C	16.18	25CA	25O42	26N	32.48
25CA	25O42	162ND1	72.81	25CA	25O42	162CE1	62.96

TABLE XVII

25CA	25O42	26CD1	63.86	23O	25O42	24C	59.84
23O	25O42	24CA	41.50	23O	25O42	22O	69.15
23O	25O42	230OH2	73.61	23O	25O42	25C	87.62
23O	25O42	26N	76.22	23O	25O42	23N	47.69
23O	25O42	22C	58.56	23O	25O42	26CD1	41.93
24C	25O42	24CA	21.42	24C	25O42	19CD	70.59
24C	25O42	19OE1	74.79	24C	25O42	22O	72.25
24C	25O42	25C	40.11	24C	25O42	26N	42.88
24C	25O42	23N	79.63	24C	25O42	22C	75.07
24C	25O42	162CE1	96.91	24C	25O42	26CD1	47.33
24CA	25O42	19CD	76.47	24CA	25O42	19OE1	85.89
24CA	25O42	22O	59.12	24CA	25O42	25C	60.08
24CA	25O42	26N	58.46	24CA	25O42	23N	59.62
24CA	25O42	22C	58.07	24CA	25O42	26CD1	46.49
19CD	25O42	19OE1	16.46	19CD	25O42	22O	50.92
19CD	25O42	25C	82.87	19CD	25O42	26N	98.50
19CD	25O42	162ND1	72.56	19CD	25O42	23N	79.96
19CD	25O42	22C	64.41	19CD	25O42	162CE1	58.81
19OE1	25O42	22O	67.33	19OE1	25O42	25C	75.67
19OE1	25O42	26N	92.41	19OE1	25O42	162ND1	56.82
19OE1	25O42	23N	96.37	19OE1	25O42	22C	80.82
19OE1	25O42	162CE1	42.61	22O	25O42	230OH2	68.87
22O	25O42	23N	29.05	22O	25O42	22C	13.49
230OH2	25O42	23N	49.64	230OH2	25O42	22C	59.44
25C	25O42	26N	16.85	25C	25O42	162ND1	77.20
25C	25O42	162CE1	70.85	25C	25O42	26CD1	51.53
26N	25O42	162ND1	87.91	26N	25O42	162CE1	84.47
26N	25O42	26CD1	36.52	162ND1	25O42	162CE1	15.10
23N	25O42	22C	15.56	23N	25O42	26CD1	88.32
22C	25O42	26CD1	95.66				

TABLE XVIII

Table of angles between atoms of the inhibitor and protein for all protein atoms within 5 Ångstroms of the inhibitor 4-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-1-N[N-(methyl)-L-leucyl)]-3-pyrrolidinone.

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
242OH2	25C1	18OD1	67.89	242OH2	25C1	18CG	56.00
242OH2	25C1	18ND2	40.01	242OH2	25C1	184O	81.97
242OH2	25C1	184C	88.17	242OH2	25C1	21NE2	62.78
242OH2	25C1	20N	79.06	18OD1	25C1	184CD1	79.40
18OD1	25C1	184CB	74.81	18OD1	25C1	184CG	85.32
18OD1	25C1	184CA	53.47	18OD1	25C1	18CG	11.94
18OD1	25C1	18ND2	28.26	18OD1	25C1	184NE1	92.34
18OD1	25C1	184O	58.92	18OD1	25C1	184C	49.03
18OD1	25C1	21NE2	93.14	18OD1	25C1	20N	41.90
184CD1	25C1	184CB	38.10	184CD1	25C1	184CG	19.94
184CD1	25C1	184CA	42.92	184CD1	25C1	18CG	90.87
184CD1	25C1	184NE1	15.56	184CD1	25C1	184O	71.50
184CD1	25C1	184CD2	27.97	184CD1	25C1	184C	61.10
184CD1	25C1	20N	84.09	184CB	25C1	184CG	21.98
184CB	25C1	184CA	21.35	184CB	25C1	18CG	81.80
184CB	25C1	18ND2	96.18	184CB	25C1	184NE1	50.19
184CB	25C1	184O	36.35	184CB	25C1	184CD2	33.73
184CB	25C1	184C	32.01	184CG	25C1	184CA	36.19
184CG	25C1	18CG	95.04	184CG	25C1	184NE1	28.76
184CG	25C1	184O	58.26	184CG	25C1	184CD2	15.95
184CG	25C1	184C	51.91	184CA	25C1	18CG	60.97
184CA	25C1	18ND2	76.21	184CA	25C1	184NE1	58.19
184CA	25C1	184O	30.82	184CA	25C1	184CD2	51.40
184CA	25C1	184C	18.27	184CA	25C1	20N	84.75
18CG	25C1	18ND2	16.83	18CG	25C1	184O	59.45
18CG	25C1	184C	52.65	18CG	25C1	21NE2	87.86
18CG	25C1	20N	45.88	18ND2	25C1	184O	68.25
18ND2	25C1	184C	65.08	18ND2	25C1	21NE2	75.52
18ND2	25C1	20N	49.20	184NE1	25C1	184O	85.54
184NE1	25C1	184CD2	27.58	184NE1	25C1	184C	76.21
184NE1	25C1	20N	87.93	184O	25C1	184CD2	69.09
184O	25C1	184C	14.96	184CD2	25C1	184C	65.57
184C	25C1	20N	87.94	21NE2	25C1	20N	61.73
184CD1	25C2	184CG	20.80	184CD1	25C2	184NE1	19.39

TABLE XVIII

184CD1	25C2	184CD2	32.31	184CD1	25C2	184CB	37.15
184CD1	25C2	184CE2	30.89	184CD1	25C2	18OD1	66.60
184CD1	25C2	184CA	37.97	184CD1	25C2	184CE3	47.14
184CG	25C2	184NE1	32.65	184CG	25C2	184CD2	20.10
184CG	25C2	184CB	20.97	184CG	25C2	184CE2	31.76
184CG	25C2	18OD1	71.61	184CG	25C2	184CA	31.32
184CG	25C2	184CE3	31.69	184NE1	25C2	184CD2	31.41
184NE1	25C2	184CB	52.95	184NE1	25C2	184CE2	18.36
184NE1	25C2	18OD1	83.70	184NE1	25C2	184CA	57.03
184NE1	25C2	184CE3	45.36	184CD2	25C2	184CB	36.72
184CD2	25C2	184CE2	18.93	184CD2	25C2	18OD1	91.69
184CD2	25C2	184CA	50.71	184CD2	25C2	184CE3	15.04
184CB	25C2	184CE2	52.15	184CB	25C2	242OH2	91.69
184CB	25C2	18OD1	60.47	184CB	25C2	184CA	17.64
184CB	25C2	184CE3	41.82	184CE2	25C2	18OD1	97.37
184CE2	25C2	184CA	62.35	184CE2	25C2	184CE3	29.53
242OH2	25C2	18OD1	48.28	242OH2	25C2	184CA	79.74
18OD1	25C2	184CA	43.08	184CA	25C2	184CE3	58.53
184NE1	25C3	184CD1	20.69	184NE1	25C3	184CE2	18.79
184NE1	25C3	184CG	31.66	184NE1	25C3	184CD2	29.94
184NE1	25C3	184CZ2	30.27	184CD1	25C3	184CE2	31.79
184CD1	25C3	184CG	18.43	184CD1	25C3	184CD2	29.94
184CD1	25C3	20O	97.66	184CD1	25C3	184CZ2	46.78
184CE2	25C3	184CG	31.39	184CE2	25C3	184CD2	18.34
184CE2	25C3	184CZ2	15.37	184CG	25C3	184CD2	18.68
184CG	25C3	184CZ2	46.08	184CD2	25C3	184CZ2	30.03
20O	25C3	21NE2	47.07	20O	25C4	19CG	63.08
20O	25C4	20C	13.93	20O	25C4	21NE2	58.24
20O	25C4	20N	38.94	20O	25C4	19CD	73.49
20O	25C4	20CA	29.58	20O	25C4	21OE1	64.57
20O	25C4	18OD1	80.18	20O	25C4	21CD	55.60
20O	25C4	19NE2	66.42	20O	25C4	21N	18.83
19CG	25C4	20C	69.89	19CG	25C4	184CD1	59.97
19CG	25C4	184NE1	63.38	19CG	25C4	20N	48.04
19CG	25C4	19CD	19.27	19CG	25C4	20CA	64.22
19CG	25C4	184CG	73.51	19CG	25C4	18OD1	63.24
19CG	25C4	184CE2	77.80	19CG	25C4	19NE2	28.95
19CG	25C4	21N	80.44	20C	25C4	21NE2	47.51
20C	25C4	20N	34.03	20C	25C4	19CD	83.36
20C	25C4	20CA	19.08	20C	25C4	21OE1	60.05
20C	25C4	18OD1	71.76	20C	25C4	21CD	48.39
20C	25C4	19NE2	78.43	20C	25C4	21N	11.83

TABLE XVIII

184CD1	25C4	184NE1	19.36	184CD1	25C4	20N	90.20
184CD1	25C4	19CD	56.87	184CD1	25C4	184CG	14.62
184CD1	25C4	18OD1	63.59	184CD1	25C4	184CE2	26.99
184CD1	25C4	19NE2	70.60	184NE1	25C4	19CD	53.18
184NE1	25C4	184CG	27.61	184NE1	25C4	18OD1	82.57
184NE1	25C4	184CE2	14.41	184NE1	25C4	19NE2	63.56
21NE2	25C4	20N	70.04	21NE2	25C4	20CA	52.20
21NE2	25C4	21OE1	28.00	21NE2	25C4	18OD1	83.21
21NE2	25C4	21CD	15.16	21NE2	25C4	21N	39.44
20N	25C4	19CD	66.67	20N	25C4	20CA	18.60
20N	25C4	21OE1	91.11	20N	25C4	184CG	96.83
20N	25C4	18OD1	41.94	20N	25C4	21CD	77.35
20N	25C4	19NE2	70.35	20N	25C4	21N	45.53
19CD	25C4	20CA	81.50	19CD	25C4	184CG	71.48
19CD	25C4	18OD1	79.99	19CD	25C4	184CE2	66.85
19CD	25C4	19NE2	15.24	19CD	25C4	21N	92.20
20CA	25C4	21OE1	72.56	20CA	25C4	18OD1	52.69
20CA	25C4	21CD	58.76	20CA	25C4	19NE2	81.60
20CA	25C4	21N	28.99	21OE1	25C4	21CD	14.61
21OE1	25C4	21N	48.49	184CG	25C4	18OD1	62.90
184CG	25C4	184CE2	27.32	184CG	25C4	19NE2	85.13
18OD1	25C4	184CE2	89.23	18OD1	25C4	21CD	97.26
18OD1	25C4	19NE2	92.18	18OD1	25C4	21N	80.98
184CE2	25C4	19NE2	75.84	21CD	25C4	21N	37.64
19NE2	25C4	21N	85.10	20O	25C5	20N	55.48
20O	25C5	20C	21.07	20O	25C5	20CA	44.11
20O	25C5	19CG	71.84	20O	25C5	21NE2	66.85
20O	25C5	19C	51.82	20O	25C5	21N	24.93
20O	25C5	19CD	75.35	20O	25C5	19N	84.18
20O	25C5	19CA	67.21	20O	25C5	19CB	67.59
20O	25C5	21CD	58.45	20O	25C5	19O	39.96
20O	25C5	21OE1	62.69	20N	25C5	20C	45.30
20N	25C5	20CA	25.13	20N	25C5	18OD1	58.18
20N	25C5	19CG	59.77	20N	25C5	21NE2	88.80
20N	25C5	19C	15.04	20N	25C5	21N	55.27
20N	25C5	242OH2	88.85	20N	25C5	18CG	53.24
20N	25C5	19CD	75.42	20N	25C5	19N	36.29
20N	25C5	19CA	29.03	20N	25C5	19CB	45.65
20N	25C5	21CD	91.99	20N	25C5	18ND2	55.37
20N	25C5	19O	20.80	20N	25C5	183O	72.28
20C	25C5	20CA	26.08	20C	25C5	18OD1	98.89
20C	25C5	19CG	82.87	20C	25C5	21NE2	55.09

TABLE XVIII

20C	25C5	19C	48.39	20C	25C5	21N	11.08
20C	25C5	242OH2	97.88	20C	25C5	18CG	90.40
20C	25C5	19CD	90.83	20C	25C5	19N	80.24
20C	25C5	19CA	66.78	20C	25C5	19CB	74.20
20C	25C5	21CD	51.59	20C	25C5	18ND2	83.45
20C	25C5	19O	38.43	20C	25C5	21OE1	61.08
20CA	25C5	18OD1	72.87	20CA	25C5	19CG	80.41
20CA	25C5	21NE2	63.95	20CA	25C5	19C	35.76
20CA	25C5	21N	33.35	20CA	25C5	242OH2	81.51
20CA	25C5	18CG	64.36	20CA	25C5	19CD	93.94
20CA	25C5	19N	61.13	20CA	25C5	19CA	53.26
20CA	25C5	19CB	67.53	20CA	25C5	21CD	66.97
20CA	25C5	18ND2	58.72	20CA	25C5	19O	32.23
20CA	25C5	183O	97.26	20CA	25C5	21OE1	79.78
18OD1	25C5	19CG	80.27	18OD1	25C5	19C	65.37
18OD1	25C5	184CD1	74.17	18OD1	25C5	242OH2	54.74
18OD1	25C5	18CG	10.85	18OD1	25C5	19CD	93.30
18OD1	25C5	184NE1	90.85	18OD1	25C5	19N	40.79
18OD1	25C5	19CA	57.69	18OD1	25C5	19CB	70.95
18OD1	25C5	18ND2	26.15	18OD1	25C5	19O	76.52
18OD1	25C5	184CG	70.18	18OD1	25C5	183O	49.64
19CG	25C5	19C	45.54	19CG	25C5	184CD1	61.26
19CG	25C5	21N	92.85	19CG	25C5	18CG	85.81
19CG	25C5	19CD	16.55	19CG	25C5	184NE1	60.42
19CG	25C5	19N	42.09	19CG	25C5	19CA	32.92
19CG	25C5	19CB	14.39	19CG	25C5	18ND2	99.14
19CG	25C5	19O	48.69	19CG	25C5	184CG	74.77
19CG	25C5	183O	42.29	21NE2	25C5	19C	99.03
21NE2	25C5	21N	44.87	21NE2	25C5	242OH2	63.97
21NE2	25C5	18CG	97.62	21NE2	25C5	21CD	14.03
21NE2	25C5	18ND2	81.87	21NE2	25C5	19O	91.86
21NE2	25C5	21OE1	25.97	19C	25C5	184CD1	99.04
19C	25C5	21N	59.38	19C	25C5	18CG	62.98
19C	25C5	19CD	60.71	19C	25C5	19N	32.80
19C	25C5	19CA	18.65	19C	25C5	19CB	31.95
19C	25C5	21CD	99.25	19C	25C5	18ND2	68.17
19C	25C5	19O	11.87	19C	25C5	183O	65.75
184CD1	25C5	18CG	85.01	184CD1	25C5	19CD	55.30
184CD1	25C5	184NE1	16.94	184CD1	25C5	19N	71.72
184CD1	25C5	19CA	80.51	184CD1	25C5	19CB	70.19
184CD1	25C5	18ND2	99.06	184CD1	25C5	184CG	14.35
184CD1	25C5	183O	35.61	21N	25C5	242OH2	94.26

TABLE XVIII

21N	25C5	18CG	95.93	21N	25C5	19CD	99.24
21N	25C5	19N	90.87	21N	25C5	19CA	77.83
21N	25C5	19CB	84.96	21N	25C5	21CD	40.54
21N	25C5	18ND2	86.56	21N	25C5	19O	49.51
21N	25C5	21OE1	50.14	242OH2	25C5	18CG	48.98
242OH2	25C5	19N	93.10	242OH2	25C5	21CD	77.70
242OH2	25C5	18ND2	37.02	242OH2	25C5	184CG	92.59
242OH2	25C5	21OE1	85.45	18CG	25C5	19N	44.21
18CG	25C5	19CA	59.10	18CG	25C5	19CB	74.72
18CG	25C5	18ND2	15.95	18CG	25C5	19O	73.12
18CG	25C5	184CG	80.57	18CG	25C5	183O	59.45
19CD	25C5	184NE1	49.55	19CD	25C5	19N	57.74
19CD	25C5	19CA	49.44	19CD	25C5	19CB	30.83
19CD	25C5	19O	61.72	19CD	25C5	184CG	69.64
19CD	25C5	183O	48.36	184NE1	25C5	19N	82.36
184NE1	25C5	19CA	86.84	184NE1	25C5	19CB	72.47
184NE1	25C5	184CG	26.82	184NE1	25C5	183O	47.92
19N	25C5	19CA	18.06	19N	25C5	19CB	30.56
19N	25C5	18ND2	57.06	19N	25C5	19O	44.42
19N	25C5	184CG	78.07	19N	25C5	183O	36.14
19CA	25C5	19CB	18.64	19CA	25C5	18ND2	69.26
19CA	25C5	19O	28.69	19CA	25C5	184CG	89.98
19CA	25C5	183O	47.24	19CB	25C5	18ND2	86.66
19CB	25C5	19O	37.11	19CB	25C5	184CG	82.34
19CB	25C5	183O	43.36	21CD	25C5	18ND2	94.92
21CD	25C5	19O	90.00	21CD	25C5	21OE1	14.31
18ND2	25C5	19O	76.17	18ND2	25C5	184CG	92.52
18ND2	25C5	183O	75.40	19O	25C5	183O	75.72
19O	25C5	21OE1	98.98	184CG	25C5	183O	42.87
18OD1	25C6	242OH2	77.61	18OD1	25C6	20N	62.12
18OD1	25C6	18CG	14.65	18OD1	25C6	18ND2	34.76
18OD1	25C6	20CA	76.78	18OD1	25C6	184CD1	84.66
18OD1	25C6	20C	97.24	18OD1	25C6	19CG	77.43
18OD1	25C6	184CA	51.93	18OD1	25C6	184CG	83.75
18OD1	25C6	184CB	70.76	18OD1	25C6	19N	38.61
18OD1	25C6	19C	62.85	18OD1	25C6	183O	51.93
18OD1	25C6	244OH2	87.25	18OD1	25C6	184NE1	97.99
242OH2	25C6	18CG	65.17	242OH2	25C6	18ND2	48.30
242OH2	25C6	20CA	92.93	242OH2	25C6	21NE2	71.65
242OH2	25C6	184CA	99.99	242OH2	25C6	244OH2	54.20
20N	25C6	18CG	61.40	20N	25C6	18ND2	64.85
20N	25C6	20CA	22.20	20N	25C6	20O	43.67

TABLE XVIII

20N	25C6	20C	36.81	20N	25C6	21NE2	80.01
20N	25C6	19CG	49.35	20N	25C6	19N	37.08
20N	25C6	19C	10.50	20N	25C6	183O	71.86
20N	25C6	244OH2	62.38	18CG	25C6	18ND2	20.14
18CG	25C6	20CA	71.10	18CG	25C6	184CD1	99.10
18CG	25C6	20C	92.50	18CG	25C6	19CG	87.70
18CG	25C6	184CA	64.20	18CG	25C6	184CG	96.81
18CG	25C6	184CB	82.01	18CG	25C6	19N	47.68
18CG	25C6	19C	65.05	18CG	25C6	183O	66.43
18CG	25C6	244OH2	73.82	18ND2	25C6	20CA	66.38
18ND2	25C6	20C	86.96	18ND2	25C6	21NE2	91.35
18ND2	25C6	184CA	81.21	18ND2	25C6	184CB	96.97
18ND2	25C6	19N	63.62	18ND2	25C6	19C	71.84
18ND2	25C6	183O	86.52	18ND2	25C6	244OH2	56.34
20CA	25C6	20O	36.02	20CA	25C6	20C	21.45
20CA	25C6	21NE2	58.02	20CA	25C6	19CG	66.36
20CA	25C6	19N	58.93	20CA	25C6	19C	31.05
20CA	25C6	183O	94.02	20CA	25C6	244OH2	42.94
20O	25C6	20C	17.19	20O	25C6	21NE2	55.96
20O	25C6	19CG	53.96	20O	25C6	19N	73.45
20O	25C6	19C	43.47	20O	25C6	183O	95.13
20O	25C6	244OH2	65.82	20O	25C6	184NE1	94.22
184CD1	25C6	19CG	55.80	184CD1	25C6	184CA	40.42
184CD1	25C6	184CG	17.20	184CD1	25C6	184CB	33.57
184CD1	25C6	19N	72.31	184CD1	25C6	19C	91.74
184CD1	25C6	183O	36.78	184CD1	25C6	184NE1	14.58
20C	25C6	21NE2	47.89	20C	25C6	19CG	64.56
20C	25C6	19N	72.48	20C	25C6	19C	41.10
20C	25C6	244OH2	49.53	21NE2	25C6	19C	87.32
21NE2	25C6	244OH2	35.45	19CG	25C6	184CA	76.21
19CG	25C6	184CG	72.47	19CG	25C6	184CB	83.57
19CG	25C6	19N	40.03	19CG	25C6	19C	38.92
19CG	25C6	183O	42.08	19CG	25C6	184NE1	53.94
184CA	25C6	184CG	32.82	184CA	25C6	184CB	19.38
184CA	25C6	19N	63.55	184CA	25C6	19C	94.44
184CA	25C6	183O	34.70	184CA	25C6	184NE1	54.88
184CG	25C6	184CB	18.90	184CG	25C6	19N	82.27
184CG	25C6	183O	45.36	184CG	25C6	184NE1	27.16
184CB	25C6	19N	80.80	184CB	25C6	183O	46.93
184CB	25C6	184NE1	45.74	19N	25C6	19C	31.43
19N	25C6	183O	36.92	19N	25C6	244OH2	93.07
19N	25C6	184NE1	79.67	19C	25C6	183O	63.42

TABLE XVIII

19C	25C6	244OH2	72.61	19C	25C6	184NE1	92.57
183O	25C6	184NE1	47.52	20O	25C7	19CG	66.72
20O	25C7	20C	8.16	20O	25C7	19CD	83.83
20O	25C7	19NE2	82.44	20O	25C7	22O	56.54
20O	25C7	22N	36.30	20O	25C7	21CA	31.83
20O	25C7	19OE1	95.92	20O	25C7	21OE1	66.65
20O	25C7	21N	17.17	20O	25C7	20N	30.97
20O	25C7	21NE2	51.64	20O	25C7	20CA	19.21
19CG	25C7	20C	71.45	19CG	25C7	19CD	21.67
19CG	25C7	19NE2	34.92	19CG	25C7	22O	55.96
19CG	25C7	184NE1	60.44	19CG	25C7	22N	79.46
19CG	25C7	21CA	96.64	19CG	25C7	19OE1	30.14
19CG	25C7	21N	83.86	19CG	25C7	184CD1	53.93
19CG	25C7	20N	45.16	19CG	25C7	20CA	61.57
20C	25C7	19CD	89.91	20C	25C7	19NE2	89.95
20C	25C7	22O	64.63	20C	25C7	22N	42.08
20C	25C7	21CA	30.95	20C	25C7	21OE1	60.76
20C	25C7	21N	13.74	20C	25C7	20N	31.22
20C	25C7	21NE2	43.84	20C	25C7	20CA	15.80
19CD	25C7	19NE2	18.60	19CD	25C7	22O	53.43
19CD	25C7	184NE1	53.45	19CD	25C7	22N	85.40
19CD	25C7	19OE1	13.55	19CD	25C7	184CD1	54.25
19CD	25C7	20N	66.44	19CD	25C7	20CA	82.18
19NE2	25C7	22O	38.61	19NE2	25C7	184NE1	67.89
19NE2	25C7	22N	73.27	19NE2	25C7	19OE1	28.20
19NE2	25C7	21N	97.49	19NE2	25C7	184CD1	71.68
19NE2	25C7	20N	74.18	19NE2	25C7	20CA	86.96
22O	25C7	22N	35.17	22O	25C7	21CA	64.61
22O	25C7	19OE1	65.85	22O	25C7	21N	66.20
22O	25C7	20N	67.78	22O	25C7	20CA	70.65
184NE1	25C7	19OE1	40.45	184NE1	25C7	184CD1	16.51
184NE1	25C7	20N	91.81	22N	25C7	21CA	29.87
22N	25C7	19OE1	98.77	22N	25C7	21OE1	70.75
22N	25C7	21N	36.58	22N	25C7	20N	63.54
22N	25C7	21NE2	72.49	22N	25C7	20CA	55.44
21CA	25C7	21OE1	42.69	21CA	25C7	21N	17.64
21CA	25C7	20N	61.95	21CA	25C7	21NE2	43.40
21CA	25C7	20CA	46.53	19OE1	25C7	184CD1	43.68
19OE1	25C7	20N	74.85	19OE1	25C7	20CA	91.61
21OE1	25C7	21N	49.78	21OE1	25C7	20N	86.97
21OE1	25C7	21NE2	27.10	21OE1	25C7	20CA	70.13
21N	25C7	20N	44.95	21N	25C7	21NE2	38.79

TABLE XVIII

21N	25C7	20CA	28.96	184CD1	25C7	20N	77.27
184CD1	25C7	20CA	92.17	20N	25C7	21NE2	62.89
20N	25C7	20CA	17.26	21NE2	25C7	20CA	47.61
20O	25O8	184NE1	98.56	20O	25O8	19NE2	64.94
20O	25O8	19CD	64.80	20O	25O8	19CG	49.58
20O	25O8	184CD1	86.05	20O	25O8	19OE1	77.25
184NE1	25O8	19NE2	65.95	184NE1	25O8	19CD	51.39
184NE1	25O8	19CG	55.21	184NE1	25O8	184CE2	15.43
184NE1	25O8	184CD1	14.81	184NE1	25O8	19OE1	39.31
19NE2	25O8	19CD	16.73	19NE2	25O8	19CG	29.82
19NE2	25O8	184CE2	79.52	19NE2	25O8	184CD1	66.86
19NE2	25O8	19OE1	26.64	19CD	25O8	19CG	18.32
19CD	25O8	184CE2	66.04	19CD	25O8	184CD1	50.50
19CD	25O8	19OE1	13.90	19CG	25O8	184CE2	70.62
19CG	25O8	184CD1	48.50	19CG	25O8	19OE1	28.11
184CE2	25O8	184CD1	26.04	184CE2	25O8	19OE1	53.16
184CD1	25O8	19OE1	41.64	184NE1	25C9	19NE2	75.95
184NE1	25C9	19CD	58.34	184NE1	25C9	184CE2	18.51
184NE1	25C9	184CZ2	36.32	184NE1	25C9	19OE1	46.11
184NE1	25C9	162CE1	47.88	184NE1	25C9	184CD1	13.15
184NE1	25C9	19CG	58.03	19NE2	25C9	19CD	18.37
19NE2	25C9	184CE2	93.09	19NE2	25C9	19OE1	30.69
19NE2	25C9	162CE1	65.23	19NE2	25C9	184CD1	73.02
19NE2	25C9	19CG	30.00	19CD	25C9	184CE2	76.16
19CD	25C9	184CZ2	89.88	19CD	25C9	19OE1	16.50
19CD	25C9	162CE1	58.87	19CD	25C9	184CD1	54.66
19CD	25C9	19CG	17.52	184CE2	25C9	184CZ2	19.20
184CE2	25C9	19OE1	62.52	184CE2	25C9	162CE1	49.95
184CE2	25C9	184CD1	28.40	184CE2	25C9	19CG	76.51
184CZ2	25C9	19OE1	74.32	184CZ2	25C9	162CE1	47.31
184CZ2	25C9	184CD1	47.47	184CZ2	25C9	19CG	93.64
19OE1	25C9	162CE1	43.44	19OE1	25C9	184CD1	46.14
19OE1	25C9	19CG	29.61	162CE1	25C9	184CD1	58.96
162CE1	25C9	19CG	72.86	184CD1	25C9	19CG	50.05
184NE1	25O10	184CE2	25.08	184NE1	25O10	184CZ2	48.91
184NE1	25O10	19OE1	62.37	184NE1	25O10	19CD	75.84
184NE1	25O10	184CD1	15.34	184NE1	25O10	162CE1	66.14
184NE1	25O10	19NE2	95.76	184NE1	25O10	162ND1	81.12
184NE1	25O10	19CG	70.87	184NE1	25O10	184CD2	22.23
184NE1	25O10	162NE2	52.65	184NE1	25O10	184CH2	53.72
184NE1	25O10	184CG	14.63	184CE2	25O10	184CZ2	25.03
184CE2	25O10	19OE1	84.37	184CE2	25O10	184CD1	37.35

TABLE XVIII

184CE2	25O10	162CE1	66.88	184CE2	25O10	162ND1	77.00
184CE2	25O10	19CG	95.89	184CE2	25O10	184CD2	10.58
184CE2	25O10	162NE2	51.22	184CE2	25O10	184CH2	28.91
184CE2	25O10	184CG	26.65	184CZ2	25O10	19OE1	99.91
184CZ2	25O10	184CD1	62.29	184CZ2	25O10	162CE1	61.92
184CZ2	25O10	162ND1	65.32	184CZ2	25O10	184CD2	33.91
184CZ2	25O10	162NE2	48.17	184CZ2	25O10	184CH2	7.17
184CZ2	25O10	184CG	51.50	19OE1	25O10	19CD	19.97
19OE1	25O10	184CD1	59.90	19OE1	25O10	162CE1	56.15
19OE1	25O10	19NE2	35.40	19OE1	25O10	162ND1	68.84
19OE1	25O10	19CG	33.29	19OE1	25O10	184CD2	84.51
19OE1	25O10	162NE2	60.20	19OE1	25O10	184CG	72.32
19CD	25O10	184CD1	68.82	19CD	25O10	162CE1	74.19
19CD	25O10	19NE2	20.25	19CD	25O10	162ND1	84.51
19CD	25O10	19CG	19.19	19CD	25O10	184CD2	97.71
19CD	25O10	162NE2	79.91	19CD	25O10	184CG	82.24
184CD1	25O10	162CE1	78.10	184CD1	25O10	19NE2	89.03
184CD1	25O10	162ND1	94.07	184CD1	25O10	19CG	59.77
184CD1	25O10	184CD2	30.63	184CD1	25O10	162NE2	66.09
184CD1	25O10	184CH2	66.12	184CD1	25O10	184CG	13.45
162CE1	25O10	19NE2	78.81	162CE1	25O10	162ND1	16.74
162CE1	25O10	19CG	89.36	162CE1	25O10	184CD2	75.74
162CE1	25O10	162NE2	15.66	162CE1	25O10	184CH2	68.07
162CE1	25O10	184CG	80.42	19NE2	25O10	162ND1	83.89
19NE2	25O10	19CG	33.67	19NE2	25O10	162NE2	89.03
162ND1	25O10	184CD2	86.96	162ND1	25O10	162NE2	28.50
162ND1	25O10	184CH2	70.03	162ND1	25O10	184CG	94.80
19CG	25O10	184CD2	90.39	19CG	25O10	162NE2	91.46
19CG	25O10	184CG	72.81	184CD2	25O10	162NE2	60.21
184CD2	25O10	184CH2	36.32	184CD2	25O10	184CG	18.11
162NE2	25O10	184CH2	54.84	162NE2	25O10	184CG	66.33
184CH2	25O10	184CG	54.39	162ND1	25C11	162CE1	18.33
162ND1	25C11	184CZ2	57.54	162ND1	25C11	19NE2	74.67
162ND1	25C11	162CG	12.31	162CE1	25C11	184CZ2	47.54
162CE1	25C11	19NE2	62.12	162CE1	25C11	162CG	26.24
184CZ2	25C11	19NE2	86.59	184CZ2	25C11	162CG	53.23
19NE2	25C11	162CG	86.37	162ND1	25C12	161O	52.69
161OD1	25C13	162ND1	77.53	161OD1	25C13	161CG	13.50
161OD1	25C13	161O	49.60	161OD1	25C13	162CB	47.00
161OD1	25C13	162CG	64.44	161OD1	25C13	137O	63.21
162ND1	25C13	161CG	86.85	162ND1	25C13	161O	55.29
162ND1	25C13	184CZ2	52.94	162ND1	25C13	162CB	31.13

TABLE XVIII

162ND1	25C13	162CG	16.56	162ND1	25C13	137O	91.79
161CG	25C13	161O	48.18	161CG	25C13	162CB	57.82
161CG	25C13	162CG	75.53	161CG	25C13	137O	72.06
161O	25C13	162CB	45.12	161O	25C13	162CG	55.63
184CZ2	25C13	162CB	67.90	184CZ2	25C13	162CG	52.88
184CZ2	25C13	137O	65.96	162CB	25C13	162CG	17.71
162CB	25C13	137O	73.09	162CG	25C13	137O	76.90
161OD1	25C14	162CB	67.52	161OD1	25C14	162CG	91.93
161OD1	25C14	161O	65.79	161OD1	25C14	161C	49.33
161OD1	25C14	162CA	65.70	161OD1	25C14	161CG	13.81
161OD1	25C14	162N	48.26	161OD1	25C14	137CB	61.84
161OD1	25C14	161CB	32.59	161OD1	25C14	162CD2	97.90
161OD1	25C14	137C	54.56	161OD1	25C14	161CA	38.35
161OD1	25C14	137O	68.99	161OD1	25C14	137CA	49.42
162ND1	25C14	162CB	44.41	162ND1	25C14	162CG	23.28
162ND1	25C14	161O	75.37	162ND1	25C14	161C	79.50
162ND1	25C14	162CA	48.35	162ND1	25C14	162N	68.54
162ND1	25C14	162CE1	14.58	162ND1	25C14	137CB	81.24
162ND1	25C14	162CD2	28.11	162ND1	25C14	184CZ2	60.58
162ND1	25C14	162NE2	21.94	162ND1	25C14	161CA	95.48
162ND1	25C14	137CA	97.09	162CB	25C14	162CG	25.05
162CB	25C14	161O	62.89	162CB	25C14	161C	53.94
162CB	25C14	162CA	21.95	162CB	25C14	161CG	76.82
162CB	25C14	162N	35.96	162CB	25C14	162CE1	55.50
162CB	25C14	137CB	53.40	162CB	25C14	161CB	80.35
162CB	25C14	162CD2	35.20	162CB	25C14	184CZ2	83.43
162CB	25C14	137C	81.05	162CB	25C14	162NE2	49.18
162CB	25C14	161CA	65.39	162CB	25C14	137O	88.14
162CB	25C14	137CA	63.27	162CG	25C14	161O	77.15
162CG	25C14	161C	73.93	162CG	25C14	162CA	38.93
162CG	25C14	162N	57.98	162CG	25C14	162CE1	31.20
162CG	25C14	137CB	59.50	162CG	25C14	162CD2	13.71
162CG	25C14	184CZ2	62.16	162CG	25C14	137C	90.53
162CG	25C14	162NE2	24.37	162CG	25C14	161CA	87.82
162CG	25C14	137O	91.83	162CG	25C14	137CA	74.49
161O	25C14	161C	17.83	161O	25C14	162CA	41.16
161O	25C14	161CG	59.81	161O	25C14	162N	32.33
161O	25C14	162CE1	89.00	161O	25C14	161CB	43.28
161O	25C14	162CD2	90.86	161O	25C14	162NE2	95.79
161O	25C14	161CA	28.30	161C	25C14	162CA	35.01
161C	25C14	161CG	45.86	161C	25C14	162N	18.49
161C	25C14	162CE1	94.05	161C	25C14	137CB	91.74

TABLE XVIII

161C	25C14	161CB	34.16	161C	25C14	162CD2	87.05
161C	25C14	162NE2	96.49	161C	25C14	161CA	16.14
161C	25C14	137CA	88.79	162CA	25C14	161CG	70.29
162CA	25C14	162N	20.32	162CA	25C14	162CE1	62.52
162CA	25C14	137CB	73.16	162CA	25C14	161CB	66.66
162CA	25C14	162CD2	52.11	162CA	25C14	137C	96.91
162CA	25C14	162NE2	62.05	162CA	25C14	161CA	49.32
162CA	25C14	137CA	79.58	161CG	25C14	162N	50.67
161CG	25C14	137CB	75.47	161CG	25C14	161CB	20.44
161CG	25C14	137C	64.73	161CG	25C14	161CA	31.54
161CG	25C14	137O	78.60	161CG	25C14	137CA	62.23
162N	25C14	162CE1	82.81	162N	25C14	137CB	75.61
162N	25C14	161CB	46.58	162N	25C14	162CD2	70.31
162N	25C14	137C	90.94	162N	25C14	162NE2	81.86
162N	25C14	161CA	29.89	162N	25C14	137CA	76.03
162CE1	25C14	137CB	81.53	162CE1	25C14	162CD2	28.99
162CE1	25C14	184CZ2	47.31	162CE1	25C14	162NE2	14.94
162CE1	25C14	137CA	98.37	137CB	25C14	161CB	93.78
137CB	25C14	162CD2	53.66	137CB	25C14	184CZ2	66.27
137CB	25C14	137C	31.04	137CB	25C14	162NE2	66.78
137CB	25C14	161CA	91.93	137CB	25C14	137O	34.84
137CB	25C14	137CA	16.94	161CB	25C14	137C	85.13
161CB	25C14	161CA	18.06	161CB	25C14	137O	98.82
161CB	25C14	137CA	82.01	162CD2	25C14	184CZ2	49.12
162CD2	25C14	137C	84.06	162CD2	25C14	162NE2	16.33
162CD2	25C14	137O	82.53	162CD2	25C14	137CA	70.12
184CZ2	25C14	137C	79.92	184CZ2	25C14	162NE2	40.56
184CZ2	25C14	137O	67.98	184CZ2	25C14	137CA	79.44
137C	25C14	162NE2	95.36	137C	25C14	161CA	92.71
137C	25C14	137O	14.52	137C	25C14	137CA	17.79
162NE2	25C14	137O	90.59	162NE2	25C14	137CA	83.69
161CA	25C14	137CA	84.51	137O	25C14	137CA	28.01
137O	25C15	184CZ2	82.18	137O	25C15	184CH2	65.00
137O	25C15	137C	15.27	137O	25C15	161OD1	65.35
137O	25C15	138CA	35.59	137O	25C15	138N	27.26
137O	25C15	137CB	35.12	184CZ2	25C15	184CH2	18.93
184CZ2	25C15	137C	89.79	184CZ2	25C15	137CB	65.87
184CH2	25C15	137C	74.80	184CH2	25C15	138N	90.34
184CH2	25C15	137CB	56.59	137C	25C15	161OD1	50.24
137C	25C15	138CA	30.23	137C	25C15	138N	15.68
137C	25C15	137CB	30.32	161OD1	25C15	138CA	56.67
161OD1	25C15	138N	45.35	161OD1	25C15	137CB	48.96

TABLE XVIII

138CA	25C15	138N	17.26	138CA	25C15	137CB	59.96
138N	25C15	137CB	43.35	162ND1	25C16	25SG	47.96
162ND1	25C16	19NE2	81.02	162ND1	25C16	162CE1	17.42
162ND1	25C16	161O	59.00	25SG	25C16	19NE2	64.48
25SG	25C16	162CE1	51.01	25SG	25C16	23CA	79.30
25SG	25C16	161O	61.60	19NE2	25C16	162CE1	65.94
19NE2	25C16	23CA	51.63	162CE1	25C16	161O	76.23
23CA	25O17	19NE2	63.28	23CA	25O17	23C	18.00
23CA	25O17	23N	16.04	23CA	25O17	22O	36.68
23CA	25O17	25SG	86.81	23CA	25O17	22C	27.89
23CA	25O17	19CD	75.23	23CA	25O17	23O	26.79
23CA	25O17	24N	26.12	19NE2	25O17	23C	56.89
19NE2	25O17	23N	63.52	19NE2	25O17	22O	37.86
19NE2	25O17	25SG	64.03	19NE2	25O17	22C	51.98
19NE2	25O17	19CD	12.01	19NE2	25O17	23O	67.69
19NE2	25O17	24N	42.39	23C	25O17	23N	32.96
23C	25O17	22O	43.34	23C	25O17	25SG	68.82
23C	25O17	22C	40.37	23C	25O17	19CD	68.57
23C	25O17	23O	13.76	23C	25O17	24N	14.50
23N	25O17	22O	28.82	23N	25O17	22C	15.59
23N	25O17	19CD	74.62	23N	25O17	23O	42.84
23N	25O17	24N	36.39	22O	25O17	25SG	92.75
22O	25O17	22C	14.54	22O	25O17	19CD	47.50
22O	25O17	23O	57.03	22O	25O17	24N	35.11
25SG	25O17	19CD	63.67	25SG	25O17	23O	64.10
25SG	25O17	24N	64.69	22C	25O17	19CD	61.99
22C	25O17	23O	52.87	22C	25O17	24N	37.51
19CD	25O17	23O	78.75	19CD	25O17	24N	54.07
23O	25O17	24N	26.33	25SG	25N18	162ND1	59.84
25SG	25N18	161O	84.84	25SG	25N18	162CE1	58.94
25SG	25N18	25CB	19.83	25SG	25N18	162CG	65.68
25SG	25N18	161C	84.84	25SG	25N18	162CA	63.77
25SG	25N18	162CB	72.00	25SG	25N18	19NE2	64.56
162ND1	25N18	161O	77.72	162ND1	25N18	162CE1	17.48
162ND1	25N18	25CB	52.80	162ND1	25N18	162CG	12.09
162ND1	25N18	161C	70.93	162ND1	25N18	162CA	42.08
162ND1	25N18	162CB	29.83	162ND1	25N18	19NE2	80.21
161O	25N18	162CE1	95.07	161O	25N18	162CG	66.81
161O	25N18	161C	7.83	161O	25N18	162CA	36.26
161O	25N18	162CB	49.33	162CE1	25N18	25CB	45.72
162CE1	25N18	162CG	29.21	162CE1	25N18	161C	88.39
162CE1	25N18	162CA	59.10	162CE1	25N18	162CB	47.16

TABLE XVIII

162CE1	25N18	19NE2	63.44	25CB	25N18	162CG	62.19
25CB	25N18	161C	98.68	25CB	25N18	162CA	72.18
25CB	25N18	162CB	74.19	25CB	25N18	19NE2	48.00
162CG	25N18	161C	59.70	162CG	25N18	162CA	32.47
162CG	25N18	162CB	17.97	162CG	25N18	19NE2	92.29
161C	25N18	162CA	30.47	161C	25N18	162CB	41.99
162CA	25N18	162CB	18.49	25SG	25C19	161O	87.86
25SG	25C19	25CB	17.43	25SG	25C19	162ND1	51.44
25SG	25C19	23O	85.01	25SG	25C19	23C	84.49
25SG	25C19	25N	40.23	25SG	25C19	161C	84.17
25SG	25C19	162CE1	48.33	25SG	25C19	19NE2	65.89
161O	25C19	162ND1	65.41	161O	25C19	161C	3.96
161O	25C19	162CE1	79.95	25CB	25C19	162ND1	50.53
25CB	25C19	23CA	87.26	25CB	25C19	23O	79.49
25CB	25C19	23C	74.66	25CB	25C19	25N	31.30
25CB	25C19	161C	97.21	25CB	25C19	162CE1	42.12
25CB	25C19	19NE2	48.60	162ND1	25C19	25N	81.01
162ND1	25C19	161C	61.89	162ND1	25C19	162CE1	14.54
162ND1	25C19	19NE2	72.57	23CA	25C19	23O	31.62
23CA	25C19	23C	19.66	23CA	25C19	25N	60.25
23CA	25C19	19NE2	49.27	23O	25C19	23C	15.91
23O	25C19	25N	48.22	23O	25C19	19NE2	64.33
23C	25C19	25N	44.48	23C	25C19	19NE2	49.75
25N	25C19	162CE1	70.28	25N	25C19	19NE2	41.94
161C	25C19	162CE1	76.42	162CE1	25C19	19NE2	58.03
19NE2	25N20	184NE1	61.55	19NE2	25N20	184CZ2	88.39
19NE2	25N20	162CE1	59.51	19NE2	25N20	19CD	15.18
184NE1	25N20	184CZ2	30.44	184NE1	25N20	162CE1	42.35
184NE1	25N20	19CD	46.54	184CZ2	25N20	162CE1	43.21
184CZ2	25N20	19CD	74.46	162CE1	25N20	19CD	52.22
161O	25C21	25SG	96.09	161O	25C21	161C	6.24
161O	25C21	162CA	33.10	161O	25C21	162N	17.36
161O	25C21	162ND1	61.84	161O	25C21	25CB	99.78
161O	25C21	163N	59.11	25SG	25C21	161C	94.55
25SG	25C21	162CA	63.31	25SG	25C21	162N	80.59
25SG	25C21	162ND1	43.09	25SG	25C21	25CB	6.39
25SG	25C21	163N	44.50	161C	25C21	162CA	31.26
161C	25C21	162N	14.07	161C	25C21	162ND1	63.41
161C	25C21	25CB	98.77	161C	25C21	163N	55.24
162CA	25C21	162N	17.54	162CA	25C21	162ND1	37.75
162CA	25C21	25CB	67.54	162CA	25C21	163N	28.93
162N	25C21	162ND1	52.75	162N	25C21	25CB	85.01

TABLE XVIII

162N	25C21	163N	41.75	162ND1	25C21	25CB	43.42
162ND1	25C21	163N	45.75	25CB	25C21	163N	50.47
25SG	25C22	25CB	32.60	25SG	25C22	25N	72.57
25SG	25C22	25CA	49.33	25SG	25C22	19NE2	93.81
25SG	25C22	26N	55.18	25SG	25C22	162ND1	47.43
25SG	25C22	24C	82.40	25SG	25C22	25C	44.53
25SG	25C22	162CE1	48.15	25SG	25C22	161O	75.53
25SG	25C22	26CD1	94.13	25SG	25C22	19OE1	68.36
25SG	25C22	19CD	81.56	25CB	25C22	25N	46.75
25CB	25C22	25CA	24.63	25CB	25C22	19NE2	63.05
25CB	25C22	24N	85.73	25CB	25C22	26N	52.12
25CB	25C22	162ND1	56.93	25CB	25C22	24C	57.01
25CB	25C22	25C	34.57	25CB	25C22	162CE1	46.25
25CB	25C22	24CA	75.71	25CB	25C22	26CD1	92.36
25CB	25C22	19OE1	41.24	25CB	25C22	19CD	51.95
25N	25C22	25CA	23.55	25N	25C22	23O	65.42
25N	25C22	23C	60.13	25N	25C22	23CA	77.28
25N	25C22	19NE2	54.87	25N	25C22	24N	43.20
25N	25C22	26N	39.45	25N	25C22	24C	10.31
25N	25C22	25C	33.15	25N	25C22	162CE1	88.28
25N	25C22	24CA	29.39	25N	25C22	26CD1	58.64
25N	25C22	19OE1	57.16	25N	25C22	19CD	54.20
25CA	25C22	23O	88.34	25CA	25C22	23C	83.54
25CA	25C22	23CA	99.22	25CA	25C22	19NE2	61.73
25CA	25C22	24N	66.05	25CA	25C22	26N	35.11
25CA	25C22	162ND1	81.55	25CA	25C22	24C	33.75
25CA	25C22	25C	19.23	25CA	25C22	162CE1	69.99
25CA	25C22	24CA	52.91	25CA	25C22	26CD1	70.42
25CA	25C22	19OE1	50.96	25CA	25C22	19CD	55.14
23O	25C22	23C	19.26	23O	25C22	23CA	35.89
23O	25C22	19NE2	79.72	23O	25C22	24N	32.92
23O	25C22	26N	78.15	23O	25C22	24C	55.15
23O	25C22	25C	88.29	23O	25C22	24CA	36.77
23O	25C22	26CD1	45.35	23O	25C22	19CD	90.80
23C	25C22	23CA	22.09	23C	25C22	19NE2	61.06
23C	25C22	24N	18.52	23C	25C22	26N	84.89
23C	25C22	24C	50.29	23C	25C22	25C	89.80
23C	25C22	24CA	31.49	23C	25C22	26CD1	60.86
23C	25C22	19OE1	86.44	23C	25C22	19CD	72.74
23CA	25C22	19NE2	57.32	23CA	25C22	24N	34.39
23CA	25C22	24C	68.55	23CA	25C22	24CA	51.33
23CA	25C22	26CD1	81.00	23CA	25C22	19OE1	84.42

TABLE XVIII

23CA	25C22	19CD	70.13	19NE2	25C22	24N	48.45
19NE2	25C22	26N	93.13	19NE2	25C22	162ND1	81.54
19NE2	25C22	24C	55.55	19NE2	25C22	25C	80.63
19NE2	25C22	162CE1	65.93	19NE2	25C22	24CA	57.12
19NE2	25C22	19OE1	27.13	19NE2	25C22	19CD	12.81
24N	25C22	26N	74.25	24N	25C22	24C	34.17
24N	25C22	25C	75.06	24N	25C22	24CA	17.99
24N	25C22	26CD1	62.40	24N	25C22	19OE1	70.97
24N	25C22	19CD	58.41	26N	25C22	24C	43.27
26N	25C22	25C	17.72	26N	25C22	162CE1	96.42
26N	25C22	24CA	56.30	26N	25C22	26CD1	41.56
26N	25C22	19OE1	86.07	26N	25C22	19CD	89.17
162ND1	25C22	25C	87.29	162ND1	25C22	162CE1	16.50
162ND1	25C22	161O	57.76	162ND1	25C22	19OE1	57.61
162ND1	25C22	19CD	70.43	24C	25C22	25C	40.95
24C	25C22	162CE1	97.34	24C	25C22	24CA	19.17
24C	25C22	26CD1	53.28	24C	25C22	19OE1	63.13
24C	25C22	19CD	57.60	25C	25C22	162CE1	79.88
25C	25C22	24CA	58.50	25C	25C22	26CD1	58.12
25C	25C22	19OE1	69.35	25C	25C22	19CD	74.36
162CE1	25C22	161O	74.20	162CE1	25C22	19OE1	41.17
162CE1	25C22	19CD	54.32	24CA	25C22	26CD1	49.39
24CA	25C22	19OE1	73.34	24CA	25C22	19CD	63.76
19OE1	25C22	19CD	14.35	25SG	25O23	25N	75.69
25SG	25O23	25CB	37.11	25SG	25O23	25CA	54.99
25SG	25O23	24C	90.69	25SG	25O23	19OE1	83.77
25SG	25O23	25C	48.15	25SG	25O23	26N	51.79
25SG	25O23	162ND1	44.43	25SG	25O23	162CE1	52.19
25SG	25O23	24O	85.50	25N	25O23	25CB	51.43
25N	25O23	19NE2	75.55	25N	25O23	23C	76.45
25N	25O23	24N	57.15	25N	25O23	23O	76.49
25N	25O23	25CA	24.40	25N	25O23	24C	15.43
25N	25O23	24CA	38.06	25N	25O23	19CD	72.15
25N	25O23	19OE1	71.82	25N	25O23	22O	86.12
25N	25O23	25C	27.77	25N	25O23	26N	33.20
25N	25O23	23N	97.97	25N	25O23	162CE1	94.44
25N	25O23	24O	9.85	25N	25O23	22C	91.69
25CB	25O23	19NE2	80.56	25CB	25O23	25CA	27.06
25CB	25O23	24C	66.23	25CB	25O23	24CA	89.22
25CB	25O23	19CD	67.04	25CB	25O23	19OE1	52.55
25CB	25O23	25C	33.18	25CB	25O23	26N	48.61
25CB	25O23	162ND1	52.03	25CB	25O23	162CE1	45.88

TABLE XVIII

25CB	25O23	24O	59.52	19NE2	25O23	23C	84.54
19NE2	25O23	24N	66.47	19NE2	25O23	23CA	78.32
19NE2	25O23	25CA	77.61	19NE2	25O23	24C	71.54
19NE2	25O23	24CA	74.20	19NE2	25O23	19CD	14.67
19NE2	25O23	19OE1	32.03	19NE2	25O23	22O	39.73
19NE2	25O23	25C	93.21	19NE2	25O23	23N	68.79
19NE2	25O23	162ND1	89.64	19NE2	25O23	162CE1	73.89
19NE2	25O23	24O	69.92	19NE2	25O23	22C	53.32
23C	25O23	24N	24.58	23C	25O23	23CA	28.13
23C	25O23	23O	21.76	23C	25O23	24C	61.59
23C	25O23	24CA	38.61	23C	25O23	19CD	97.49
23C	25O23	22O	49.19	23C	25O23	25C	99.27
23C	25O23	26N	90.14	23C	25O23	23N	30.80
23C	25O23	24O	68.35	23C	25O23	22C	39.19
24N	25O23	23CA	44.35	24N	25O23	23O	40.46
24N	25O23	25CA	80.66	24N	25O23	24C	41.72
24N	25O23	24CA	20.87	24N	25O23	19CD	77.11
24N	25O23	19OE1	91.57	24N	25O23	22O	41.76
24N	25O23	25C	83.71	24N	25O23	26N	80.39
24N	25O23	23N	41.16	24N	25O23	24O	47.80
24N	25O23	22C	39.24	23CA	25O23	23O	43.14
23CA	25O23	24C	85.95	23CA	25O23	24CA	63.70
23CA	25O23	19CD	92.98	23CA	25O23	22O	38.70
23CA	25O23	23N	9.54	23CA	25O23	24O	92.15
23CA	25O23	22C	25.05	23O	25O23	25CA	99.19
23O	25O23	24C	64.48	23O	25O23	24CA	44.29
23O	25O23	22O	70.90	23O	25O23	25C	91.92
23O	25O23	26N	78.46	23O	25O23	23N	49.19
23O	25O23	24O	71.18	23O	25O23	22C	60.24
25CA	25O23	24C	39.48	25CA	25O23	24CA	62.38
25CA	25O23	19CD	68.41	25CA	25O23	19OE1	60.76
25CA	25O23	25C	15.95	25CA	25O23	26N	32.35
25CA	25O23	162ND1	79.08	25CA	25O23	162CE1	71.50
25CA	25O23	24O	32.98	24C	25O23	24CA	22.98
24C	25O23	19CD	72.19	24C	25O23	19OE1	76.64
24C	25O23	22O	73.41	24C	25O23	25C	42.54
24C	25O23	26N	44.02	24C	25O23	23N	82.66
24C	25O23	24O	6.88	24C	25O23	22C	77.34
24CA	25O23	19CD	80.54	24CA	25O23	19OE1	90.57
24CA	25O23	22O	60.20	24CA	25O23	25C	63.31
24CA	25O23	26N	59.62	24CA	25O23	23N	61.69
24CA	25O23	24O	29.75	24CA	25O23	22C	59.80

TABLE XVIII

19CD	25O23	19OE1	17.43	19CD	25O23	22O	54.37
19CD	25O23	25C	84.36	19CD	25O23	26N	99.96
19CD	25O23	23N	83.45	19CD	25O23	162ND1	76.89
19CD	25O23	162CE1	60.68	19CD	25O23	24O	68.84
19CD	25O23	22C	67.98	19OE1	25O23	22O	71.76
19OE1	25O23	25C	76.10	19OE1	25O23	26N	93.05
19OE1	25O23	162ND1	60.98	19OE1	25O23	162CE1	44.53
19OE1	25O23	24O	71.61	19OE1	25O23	22C	85.33
22O	25O23	23N	29.15	22O	25O23	24O	76.62
22O	25O23	22C	13.64	25C	25O23	26N	17.16
25C	25O23	162ND1	82.30	25C	25O23	162CE1	78.86
25C	25O23	24O	37.62	26N	25O23	162ND1	92.78
26N	25O23	162CE1	92.75	26N	25O23	24O	41.67
23N	25O23	24O	88.33	23N	25O23	22C	15.51
162ND1	25O23	162CE1	16.46	24O	25O23	22C	81.85
65CA	25C24	66N	33.46	65CA	25C24	65C	20.36
65CA	25C24	64O	36.58	65CA	25C24	66O	68.87
66N	25C24	65C	17.64	66N	25C24	64O	67.62
66N	25C24	66O	36.45	65C	25C24	64O	50.58
65C	25C24	66O	53.76	66O	25C25	66N	40.06
66O	25C25	66C	8.90	66O	25C25	65CA	70.27
161O	25C25	161CA	28.19	161O	25C25	161C	14.86
66N	25C25	66C	31.52	66N	25C25	25SG	60.39
66N	25C25	25SG	91.38	66N	25C25	65CA	30.22
161C	25C25	161CA	17.63	161C	25C25	65C	14.24
66C	25C25	65CA	61.71	66C	25C25	25SG	69.22
65CA	25C25	25SG	82.36	65CA	25C25	65C	44.80
161CA	25C25	25SG	86.68	25SG	25C25	65C	17.73
66O	25C26	66C	3.30	66O	25C25	65C	92.33
161O	25C26	161C	15.84	161O	25C26	163CB	87.58
161O	25C26	160O	61.70	161O	25C26	163N	56.85
161O	25C26	162N	27.01	161O	25C26	163CB	84.35
161C	25C26	163N	55.26	161C	25C26	161CA	28.97
161C	25C26	163CB	84.79	161C	25C26	160O	50.24
161C	25C26	161CA	17.79	163N	25C26	162N	15.32
163N	25C26	163CB	29.64	163N	25C26	160O	95.75
163N	25C26	161CA	71.03	66C	25C26	162N	42.53
160O	25C26	162N	56.11	160O	25C26	163CB	89.72
163CB	25C26	162N	72.06	162N	25C26	161CA	33.06
160O	25C27	160C	16.28	160O	25C27	161CA	28.56
160O	25C27	161C	59.69	160O	25C27	161N	39.86
							29.94

TABLE XVIII

160O	25C27	161O	70.88	160O	25C27	160CB	39.29
160O	25C27	134CB	91.77	160O	25C27	162N	65.04
160C	25C27	161CA	33.56	160C	25C27	161C	50.71
160C	25C27	161N	17.29	160C	25C27	161O	64.68
160C	25C27	160CB	32.70	160C	25C27	134CB	77.93
160C	25C27	162N	52.23	161CA	25C27	161C	20.25
161CA	25C27	161N	19.14	161CA	25C27	161O	31.54
161CA	25C27	160CB	64.50	161CA	25C27	134CB	90.77
161CA	25C27	162N	30.47	161C	25C27	161N	33.69
161C	25C27	161O	15.99	161C	25C27	160CB	77.36
161C	25C27	134CB	85.39	161C	25C27	162N	15.75
161N	25C27	161O	48.38	161N	25C27	160CB	45.58
161N	25C27	134CB	77.13	161N	25C27	162N	35.42
161O	25C27	160CB	93.10	161O	25C27	134CB	96.47
161O	25C27	162N	27.78	66O	25C27	209CD2	83.62
160CB	25C27	134CB	56.56	160CB	25C27	162N	71.89
160CB	25C27	209CD2	69.27	134CB	25C27	162N	69.95
134CB	25C27	209CD2	49.25	160O	25C28	160C	11.12
160O	25C28	161CA	34.92	160O	25C28	161N	22.64
160C	25C28	161CA	30.68	160C	25C28	161N	14.74
67CE1	25C28	66O	57.93	67CE1	25C28	67CD1	16.20
161CA	25C28	161N	17.22	66O	25C28	67CD1	44.47
209CD2	25C29	134CB	68.69	209CD2	25C29	160CB	90.30
209CD2	25C29	67CD1	65.58	209CD2	25C29	66O	98.85
209CD2	25C29	209CG	7.93	209CD2	25C29	67CE1	70.23
134CB	25C29	160CB	68.29	134CB	25C29	160C	85.31
134CB	25C29	209CG	62.21	160O	25C29	160CB	42.09
160O	25C29	160C	15.52	160CB	25C29	160C	33.72
160CB	25C29	209CG	83.59	67CD1	25C29	66O	45.57
67CD1	25C29	209CG	73.48	67CD1	25C29	67CE1	16.51
66O	25C29	67CE1	56.12	209CG	25C29	67CE1	77.57
66O	25C30	66N	46.15	66O	25C30	65CA	82.36
66O	25C30	26CD1	69.05	66O	25C30	26CB	54.83
66O	25C30	65C	61.73	66O	25C30	66C	12.32
66O	25C30	66CA	31.12	66O	25C30	26CG	57.20
66O	25C30	26N	86.09	66O	25C30	163CB	86.18
66N	25C30	65CA	36.68	66N	25C30	26CD1	45.40
66N	25C30	26CB	62.49	66N	25C30	65C	16.57
66N	25C30	66C	34.22	66N	25C30	66CA	15.04
66N	25C30	26CG	48.20	66N	25C30	26N	85.31
25SG	25C30	26CD1	80.34	25SG	25C30	26CB	78.23
25SG	25C30	161O	67.14	25SG	25C30	26CG	83.17

TABLE XVIII

25SG	25C30	26N	47.19	25SG	25C30	163CB	52.42
25SG	25C30	163N	44.84	65CA	25C30	26CD1	53.97
65CA	25C30	26CB	86.07	65CA	25C30	65C	20.64
65CA	25C30	66C	70.78	65CA	25C30	66CA	51.58
65CA	25C30	26CG	67.39	65CA	25C30	26N	93.38
26CD1	25C30	26CB	34.81	26CD1	25C30	65C	49.80
26CD1	25C30	66C	59.13	26CD1	25C30	66CA	50.39
26CD1	25C30	26CG	17.00	26CD1	25C30	26N	42.15
26CD1	25C30	163CB	83.57	26CB	25C30	65C	74.87
26CB	25C30	66C	51.73	26CB	25C30	66CA	56.97
26CB	25C30	26CG	18.84	26CB	25C30	26N	31.41
26CB	25C30	163CB	54.44	26CB	25C30	163N	82.52
65C	25C30	66C	50.25	65C	25C30	66CA	31.10
65C	25C30	26CG	58.02	65C	25C30	26N	91.94
161O	25C30	163CB	83.35	161O	25C30	163N	54.69
66C	25C30	66CA	19.22	66C	25C30	26CG	49.60
66C	25C30	26N	82.89	66C	25C30	163CB	92.24
66CA	25C30	26CG	47.25	66CA	25C30	26N	84.74
26CG	25C30	26N	37.73	26CG	25C30	163CB	71.86
26CG	25C30	163N	98.68	26N	25C30	163CB	44.77
26N	25C30	163N	65.10	163CB	25C30	163N	28.72
66O	25O31	66N	61.37	66O	25O31	26CB	77.21
66O	25O31	26CD1	95.50	66O	25O31	66C	18.26
66O	25O31	26CG	80.22	66O	25O31	66CA	41.13
66O	25O31	65C	76.22	66O	25O31	65CA	98.52
66O	25O31	26CA	93.42	66O	25O31	26NE1	92.30
66O	25O31	67N	17.71	66O	25O31	26CD2	73.43
66O	25O31	65O	71.00	66N	25O31	26CB	86.34
66N	25O31	26CD1	59.28	66N	25O31	66C	45.73
66N	25O31	26CG	65.50	66N	25O31	66CA	21.43
66N	25O31	65C	16.23	66N	25O31	65CA	39.07
66N	25O31	26NE1	49.90	66N	25O31	67N	52.44
66N	25O31	26CD2	57.23	66N	25O31	65O	11.55
26CB	25O31	26CD1	45.93	26CB	25O31	66C	70.12
26CB	25O31	26CG	25.17	26CB	25O31	66CA	76.25
26CB	25O31	65C	96.29	26CB	25O31	26N	36.99
26CB	25O31	26CA	18.87	26CB	25O31	25SG	86.19
26CB	25O31	26NE1	53.75	26CB	25O31	67N	63.56
26CB	25O31	163CB	61.81	26CB	25O31	26CD2	30.74
26CB	25O31	65O	94.86	26CD1	25O31	66C	78.62
26CD1	25O31	26CG	22.75	26CD1	25O31	66CA	65.15
26CD1	25O31	65C	60.18	26CD1	25O31	65CA	62.48

TABLE XVIII

26CD1	25O31	26N	50.53	26CD1	25O31	26CA	52.01
26CD1	25O31	25SG	86.23	26CD1	25O31	26NE1	10.06
26CD1	25O31	67N	77.85	26CD1	25O31	163CB	97.88
26CD1	25O31	26CD2	24.53	26CD1	25O31	65O	61.57
66C	25O31	26CG	66.43	66C	25O31	66CA	24.43
66C	25O31	65C	61.60	66C	25O31	65CA	84.54
66C	25O31	26CA	88.49	66C	25O31	26NE1	74.51
66C	25O31	67N	8.31	66C	25O31	26CD2	58.54
66C	25O31	65O	56.49	26CG	25O31	66CA	61.97
26CG	25O31	65C	72.65	26CG	25O31	65CA	81.58
26CG	25O31	26N	45.87	26CG	25O31	26CA	37.48
26CG	25O31	25SG	92.89	26CG	25O31	26NE1	29.02
26CG	25O31	67N	62.96	26CG	25O31	163CB	84.79
26CG	25O31	26CD2	9.01	26CG	25O31	65O	72.10
66CA	25O31	65C	37.55	66CA	25O31	65CA	60.47
66CA	25O31	26CA	94.80	66CA	25O31	26NE1	58.06
66CA	25O31	67N	31.03	66CA	25O31	26CD2	52.97
66CA	25O31	65O	32.59	65C	25O31	65CA	22.96
65C	25O31	26NE1	50.12	65C	25O31	67N	68.57
65C	25O31	26CD2	65.66	65C	25O31	65O	5.21
65CA	25O31	26NE1	53.45	65CA	25O31	67N	91.50
65CA	25O31	26CD2	77.14	65CA	25O31	65O	28.05
26N	25O31	26CA	20.41	26N	25O31	25SG	49.78
26N	25O31	26NE1	60.51	26N	25O31	163CB	48.83
26N	25O31	26CD2	54.87	26CA	25O31	25SG	67.76
26CA	25O31	26NE1	61.63	26CA	25O31	67N	81.48
26CA	25O31	163CB	47.51	26CA	25O31	26CD2	45.43
25SG	25O31	26NE1	93.17	25SG	25O31	163CB	52.44
26NE1	25O31	67N	75.15	26NE1	25O31	26CD2	27.61
26NE1	25O31	65O	51.59	67N	25O31	26CD2	55.84
67N	25O31	65O	63.57	163CB	25O31	26CD2	92.09
26CD2	25O31	65O	64.59	25SG	25N32	161O	82.28
25SG	25N32	23O	84.49	25SG	25N32	26CD1	88.80
25SG	25N32	26N	50.25	25SG	25N32	25CB	9.66
25SG	25N32	25N	39.55	25SG	25N32	163N	46.38
25SG	25N32	26CB	79.05	25SG	25N32	161C	82.48
25SG	25N32	23C	74.25	161O	25N32	25CB	91.92
161O	25N32	163N	57.92	161O	25N32	161C	9.03
65CA	25N32	66N	32.94	65CA	25N32	23O	48.76
65CA	25N32	26CD1	52.31	65CA	25N32	26N	94.41
65CA	25N32	25N	92.40	65CA	25N32	65C	17.26
65CA	25N32	66O	67.39	65CA	25N32	26CB	78.37

TABLE XVIII

65CA	25N32	23C	60.93	66N	25N32	23O	68.51
66N	25N32	26CD1	41.20	66N	25N32	26N	79.04
66N	25N32	25N	94.92	66N	25N32	65C	15.81
66N	25N32	66O	35.14	66N	25N32	26CB	53.15
66N	25N32	23C	81.78	23O	25N32	26CD1	46.25
23O	25N32	26N	67.84	23O	25N32	25CB	76.13
23O	25N32	25N	47.96	23O	25N32	65C	59.32
23O	25N32	66O	99.28	23O	25N32	26CB	75.73
23O	25N32	23C	13.32	26CD1	25N32	26N	42.44
26CD1	25N32	25CB	79.55	26CD1	25N32	25N	54.01
26CD1	25N32	65C	45.85	26CD1	25N32	66O	57.60
26CD1	25N32	26CB	31.68	26CD1	25N32	23C	55.94
26N	25N32	25CB	42.72	26N	25N32	25N	33.34
26N	25N32	65C	87.61	26N	25N32	66O	74.76
26N	25N32	163N	67.13	26N	25N32	26CB	30.37
26N	25N32	23C	68.06	25CB	25N32	25N	30.07
25CB	25N32	163N	53.14	25CB	25N32	26CB	72.55
25CB	25N32	161C	92.10	25CB	25N32	23C	66.78
25N	25N32	65C	95.38	25N	25N32	163N	80.01
25N	25N32	26CB	60.55	25N	25N32	23C	41.68
65C	25N32	66O	50.19	65C	25N32	26CB	65.71
65C	25N32	23C	72.49	66O	25N32	163N	92.86
66O	25N32	26CB	44.71	163N	25N32	26CB	78.55
163N	25N32	161C	52.17	26CB	25N32	23C	82.47
25SG	25C33	25N	62.03	25SG	25C33	26N	67.44
25SG	25C33	25CB	22.53	25SG	25C33	25CA	44.14
25SG	25C33	25C	51.85	25SG	25C33	24N	94.55
25SG	25C33	24C	75.69	25SG	25C33	26CB	94.29
25SG	25C33	24CA	93.12	25SG	25C33	26CA	77.03
25SG	25C33	161O	66.31	23O	25C33	25N	68.18
23O	25C33	26CD1	60.30	23O	25C33	26N	92.61
23O	25C33	23C	18.66	23O	25C33	25CA	89.03
23O	25C33	65CA	56.48	23O	25C33	25C	96.38
23O	25C33	24N	30.61	23O	25C33	24C	56.80
23O	25C33	26CG	75.69	23O	25C33	26CB	94.54
23O	25C33	23CA	32.16	23O	25C33	66N	77.02
23O	25C33	24CA	37.25	23O	25C33	26CA	97.15
23O	25C33	26NE1	47.95	23O	25C33	65C	65.17
23O	25C33	65N	43.20	25N	25C33	26CD1	73.26
25N	25C33	26N	44.51	25N	25C33	25CB	39.50
25N	25C33	23C	57.79	25N	25C33	25CA	20.88
25N	25C33	25C	34.96	25N	25C33	24N	40.75

TABLE XVIII

25N	25C33	24C	13.79	25N	25C33	26CG	73.79
25N	25C33	26CB	75.59	25N	25C33	23CA	69.58
25N	25C33	24CA	31.77	25N	25C33	26CA	59.60
25N	25C33	26NE1	73.01	26CD1	25C33	26N	53.40
26CD1	25C33	23C	74.18	26CD1	25C33	25CA	82.03
26CD1	25C33	65CA	58.73	26CD1	25C33	25C	69.11
26CD1	25C33	24N	71.72	26CD1	25C33	24C	61.69
26CD1	25C33	26CG	15.97	26CD1	25C33	26CB	35.58
26CD1	25C33	23CA	91.94	26CD1	25C33	66N	43.00
26CD1	25C33	24CA	56.83	26CD1	25C33	26CA	46.45
26CD1	25C33	26NE1	12.72	26CD1	25C33	65C	47.83
26CD1	25C33	65N	61.48	26N	25C33	25CB	53.84
26N	25C33	23C	92.65	26N	25C33	25CA	37.01
26N	25C33	25C	17.36	26N	25C33	24N	77.69
26N	25C33	24C	45.23	26N	25C33	26CG	43.00
26N	25C33	26CB	34.40	26N	25C33	66N	88.08
26N	25C33	24CA	60.35	26N	25C33	26CA	15.70
26N	25C33	26NE1	62.43	26N	25C33	65C	98.83
25CB	25C33	23C	89.77	25CB	25C33	25CA	22.60
25CB	25C33	25C	36.53	25CB	25C33	24N	74.40
25CB	25C33	24C	53.16	25CB	25C33	26CG	96.54
25CB	25C33	26CB	86.56	25CB	25C33	23CA	92.73
25CB	25C33	24CA	70.80	25CB	25C33	26CA	67.26
25CB	25C33	161O	88.61	23C	25C33	25CA	78.15
23C	25C33	65CA	73.62	23C	25C33	25C	90.88
23C	25C33	24N	17.05	23C	25C33	24C	49.66
23C	25C33	26CG	88.11	23C	25C33	23CA	19.27
23C	25C33	66N	95.67	23C	25C33	24CA	32.32
23C	25C33	26NE1	62.90	23C	25C33	65C	83.62
23C	25C33	65N	59.43	25CA	25C33	25C	21.13
25CA	25C33	24N	61.20	25CA	25C33	24C	33.01
25CA	25C33	26CG	76.92	25CA	25C33	26CB	71.41
25CA	25C33	23CA	87.72	25CA	25C33	24CA	52.23
25CA	25C33	26CA	52.44	25CA	25C33	26NE1	85.76
65CA	25C33	24N	87.00	65CA	25C33	26CG	69.63
65CA	25C33	26CB	84.46	65CA	25C33	23CA	76.25
65CA	25C33	66N	32.22	65CA	25C33	24CA	88.00
65CA	25C33	26NE1	51.85	65CA	25C33	65C	16.56
65CA	25C33	65N	14.77	25C	25C33	24N	74.16
25C	25C33	24C	41.26	25C	25C33	26CG	60.10
25C	25C33	26CB	51.20	25C	25C33	24CA	59.94
25C	25C33	26CA	31.86	25C	25C33	26NE1	76.48

TABLE XVIII

24N	25C33	24C	33.23	24N	25C33	26CG	82.78
24N	25C33	26CB	96.28	24N	25C33	23CA	32.00
24N	25C33	24CA	18.67	24N	25C33	26CA	88.81
24N	25C33	26NE1	62.87	24N	25C33	65C	93.98
24N	25C33	65N	73.77	24C	25C33	26CG	64.93
24C	25C33	26CB	70.95	24C	25C33	23CA	64.79
24C	25C33	24CA	19.55	24C	25C33	26CA	58.29
24C	25C33	26NE1	59.98	24C	25C33	65N	96.26
26CG	25C33	26CB	19.61	26CG	25C33	66N	46.12
26CG	25C33	24CA	65.68	26CG	25C33	26CA	32.66
26CG	25C33	26NE1	28.68	26CG	25C33	65C	55.83
26CG	25C33	65N	75.10	26CB	25C33	66N	55.47
26CB	25C33	24CA	77.83	26CB	25C33	26CA	19.41
26CB	25C33	26NE1	48.27	26CB	25C33	65C	68.78
26CB	25C33	65N	92.50	23CA	25C33	24CA	50.00
23CA	25C33	26NE1	79.91	23CA	25C33	65C	89.99
23CA	25C33	65N	61.53	66N	25C33	24CA	94.59
66N	25C33	26CA	74.61	66N	25C33	26NE1	44.61
66N	25C33	65C	15.82	66N	25C33	65N	45.20
24CA	25C33	26CA	70.41	24CA	25C33	26NE1	50.59
24CA	25C33	65C	89.84	24CA	25C33	65N	77.59
26CA	25C33	26NE1	57.80	26CA	25C33	65C	87.10
26NE1	25C33	65C	44.55	26NE1	25C33	65N	51.65
65C	25C33	65N	29.48	66O	25N34	66N	45.23
66O	25N34	65CA	78.78	66O	25N34	65C	62.40
66O	25N34	66C	13.36	66O	25N34	66CA	32.35
66N	25N34	65CA	34.26	66N	25N34	65C	17.63
66N	25N34	66C	35.00	66N	25N34	66CA	17.78
65CA	25N34	65C	20.48	65CA	25N34	66C	69.25
65CA	25N34	66CA	51.09	65C	25N34	66C	51.11
65C	25N34	66CA	31.81	66C	25N34	66CA	19.75

TABLE XIX

Table of angles between atoms of the inhibitor and protein for all protein atoms within 5 Angstroms of the inhibitor 1-N-(N-imidazole acetyl-leucinyl)-amino-3-N-(4-phenoxy-phenyl-sulfonyl)-amino-propan-2-one.

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
20O	25C1	20C	8.55	20O	25C1	21CA	35.54
20O	25C1	20N	33.52	20O	25C1	21N	19.74
20O	25C1	21NE2	53.30	20O	25C1	19CB	70.43
20O	25C1	19CD	89.13	20O	25C1	20CA	16.45
20O	25C1	19CG	72.65	20C	25C1	21CA	32.39
20C	25C1	20N	30.42	20C	25C1	21N	14.60
20C	25C1	21NE2	58.84	20C	25C1	19CB	64.58
20C	25C1	19CD	81.24	20C	25C1	20CA	14.64
20C	25C1	19CG	65.09	184NE1	25C1	184CD1	18.88
184NE1	25C1	20N	99.03	184NE1	25C1	19CB	64.29
184NE1	25C1	19CD	56.93	184NE1	25C1	184CE2	13.44
184NE1	25C1	19CG	68.65	184CD1	25C1	20N	85.82
184CD1	25C1	19CB	57.54	184CD1	25C1	19CD	61.12
184CD1	25C1	184CE2	26.51	184CD1	25C1	19CG	67.61
21CA	25C1	20N	60.42	21CA	25C1	21N	18.12
21CA	25C1	21NE2	47.16	21CA	25C1	19CB	84.18
21CA	25C1	19CD	86.47	21CA	25C1	20CA	46.79
21CA	25C1	19CG	75.79	20N	25C1	21N	42.62
20N	25C1	21NE2	86.39	20N	25C1	19CB	39.01
20N	25C1	19CD	64.17	20N	25C1	20CA	17.07
20N	25C1	19CG	47.30	21N	25C1	21NE2	54.26
21N	25C1	19CB	71.03	21N	25C1	19CD	81.02
21N	25C1	20CA	28.72	21N	25C1	19CG	66.90
21NE2	25C1	20CA	69.50	19CB	25C1	19CD	29.32
19CB	25C1	20CA	54.83	19CB	25C1	184CE2	77.66
19CB	25C1	19CG	17.68	19CD	25C1	20CA	76.69
19CD	25C1	184CE2	69.09	19CD	25C1	19CG	17.08
20CA	25C1	19CG	59.66	184CE2	25C1	19CG	81.78
20O	25C2	21NE2	59.99	20O	25C2	20C	2.48

TABLE XIX

20O	25C2	184NE1	99.98	20O	25C2	184CD1	92.85
21NE2	25C2	241OH2	86.01	21NE2	25C2	20C	59.23
20C	25C2	184CD1	93.86	184NE1	25C2	184CD1	16.12
241OH2	25C3	21NE2	97.71	20O	25C3	21NE2	54.27
20O	25C3	184CD1	87.74	20O	25C3	20C	3.17
21NE2	25C3	20C	54.18	184CD1	25C3	20C	88.87
241OH2	25C4	184O	97.32	20O	25C4	18OD1	66.74
20O	25C4	184CD1	99.13	20O	25C4	18CG	78.46
20O	25C4	18ND2	91.26	20O	25C4	20C	7.41
20O	25C4	184NE1	94.68	20O	25C4	20N	34.24
18OD1	25C4	184CD1	86.06	18OD1	25C4	184CG	91.60
18OD1	25C4	184O	62.83	18OD1	25C4	184CB	82.77
18OD1	25C4	184CA	64.10	18OD1	25C4	18CG	12.46
18OD1	25C4	18ND2	28.21	18OD1	25C4	20C	59.47
18OD1	25C4	184NE1	97.79	18OD1	25C4	20N	35.84
18OD1	25C4	184C	57.15	184CD1	25C4	184CG	17.48
184CD1	25C4	184O	65.93	184CD1	25C4	184CB	33.13
184CD1	25C4	184CA	37.60	184CD1	25C4	18CG	88.07
184CD1	25C4	18ND2	95.74	184CD1	25C4	20C	99.37
184CD1	25C4	184NE1	15.35	184CD1	25C4	20N	82.14
184CD1	25C4	184C	55.11	184CG	25C4	184O	54.64
184CG	25C4	184CB	18.72	184CG	25C4	184CA	31.21
184CG	25C4	18CG	89.91	184CG	25C4	18ND2	92.98
184CG	25C4	184NE1	27.12	184CG	25C4	20N	96.33
184CG	25C4	184C	46.92	184O	25C4	184CB	36.11
184O	25C4	184CA	29.52	184O	25C4	18CG	52.77
184O	25C4	18ND2	45.59	184O	25C4	184NE1	80.28
184O	25C4	20N	93.80	184O	25C4	184C	13.81
184CB	25C4	184CA	18.71	184CB	25C4	18CG	77.83
184CB	25C4	18ND2	77.39	184CB	25C4	184NE1	45.48
184CB	25C4	20N	98.33	184CB	25C4	184C	30.19
184CA	25C4	18CG	59.86	184CA	25C4	18ND2	61.77
184CA	25C4	184NE1	52.74	184CA	25C4	20N	81.89
184CA	25C4	184C	17.52	18CG	25C4	18ND2	16.14
18CG	25C4	20C	71.10	18CG	25C4	20N	48.30
18CG	25C4	184C	49.48	18ND2	25C4	20C	83.86
18ND2	25C4	20N	63.67	18ND2	25C4	184C	47.21

TABLE XIX

20C	25C4	184NE1	96.84	20C	25C4	20N	28.14
184NE1	25C4	20N	86.08	184NE1	25C4	184C	70.17
20N	25C4	184C	83.78	20O	25C5	18OD1	80.82
20O	25C5	20N	45.03	20O	25C5	20C	11.42
20O	25C5	18CG	91.75	20O	25C5	19CB	74.81
20O	25C5	20CA	30.47	20O	25C5	19N	82.23
20O	25C5	19C	51.72	20O	25C5	19CA	69.30
18OD1	25C5	20N	46.49	18OD1	25C5	184CA	77.31
18OD1	25C5	20C	70.82	18OD1	25C5	18CG	11.80
18OD1	25C5	184CB	96.95	18OD1	25C5	19CB	72.36
18OD1	25C5	183O	66.28	18OD1	25C5	184O	67.87
18OD1	25C5	20CA	51.82	18OD1	25C5	19N	42.94
18OD1	25C5	184C	64.99	18OD1	25C5	18ND2	27.18
18OD1	25C5	19C	53.47	18OD1	25C5	19CA	55.00
184CD1	25C5	184CG	18.87	184CD1	25C5	184NE1	17.79
184CD1	25C5	184CA	44.65	184CD1	25C5	184CB	36.67
184CD1	25C5	19CB	67.07	184CD1	25C5	183O	47.98
184CD1	25C5	184O	72.91	184CD1	25C5	19N	80.31
184CD1	25C5	184C	63.25	184CD1	25C5	19C	98.13
184CD1	25C5	19CA	81.55	184CD1	25C5	184CD2	22.19
20N	25C5	20C	33.70	20N	25C5	18CG	58.10
20N	25C5	19CB	44.66	20N	25C5	183O	72.78
20N	25C5	20CA	18.20	20N	25C5	19N	38.00
20N	25C5	18ND2	73.36	20N	25C5	19C	13.46
20N	25C5	19CA	30.03	184CG	25C5	184NE1	31.64
184CG	25C5	184CA	35.78	184CG	25C5	184CB	20.39
184CG	25C5	19CB	83.44	184CG	25C5	183O	54.59
184CG	25C5	184O	58.05	184CG	25C5	19N	89.86
184CG	25C5	184C	51.94	184CG	25C5	19CA	95.52
184CG	25C5	184CD2	13.48	184NE1	25C5	184CA	62.33
184NE1	25C5	184CB	51.80	184NE1	25C5	19CB	68.57
184NE1	25C5	183O	61.84	184NE1	25C5	184O	89.24
184NE1	25C5	19N	89.54	184NE1	25C5	184C	80.74
184NE1	25C5	19C	99.19	184NE1	25C5	19CA	85.71
184NE1	25C5	184CD2	26.19	184CA	25C5	18CG	69.03
184CA	25C5	184CB	20.92	184CA	25C5	19CB	77.96
184CA	25C5	183O	36.00	184CA	25C5	184O	31.59

TABLE XIX

184CA	25C5	19N	66.93	184CA	25C5	184C	18.86
184CA	25C5	18ND2	67.71	184CA	25C5	19C	97.51
184CA	25C5	19CA	80.33	184CA	25C5	184CD2	49.00
20C	25C5	18CG	82.15	20C	25C5	19CB	67.05
20C	25C5	20CA	19.43	20C	25C5	19N	71.23
20C	25C5	18ND2	92.73	20C	25C5	19C	41.28
20C	25C5	19CA	59.31	18CG	25C5	184CB	87.50
18CG	25C5	19CB	79.43	18CG	25C5	183O	64.87
18CG	25C5	184O	56.38	18CG	25C5	20CA	63.40
18CG	25C5	19N	48.70	18CG	25C5	184C	54.85
18CG	25C5	18ND2	16.71	18CG	25C5	19C	64.20
18CG	25C5	19CA	63.20	184CB	25C5	19CB	90.65
184CB	25C5	183O	52.34	184CB	25C5	184O	37.66
184CB	25C5	19N	86.29	184CB	25C5	184C	32.87
184CB	25C5	18ND2	82.52	184CB	25C5	19CA	97.44
184CB	25C5	241OH2	93.49	184CB	25C5	184CD2	31.41
19CB	25C5	183O	42.37	19CB	25C5	20CA	60.88
19CB	25C5	19N	30.92	19CB	25C5	184C	88.12
19CB	25C5	18ND2	95.45	19CB	25C5	19C	31.26
19CB	25C5	19CA	18.10	19CB	25C5	184CD2	89.12
183O	25C5	184O	61.91	183O	25C5	20CA	90.84
183O	25C5	19N	35.42	183O	25C5	184C	46.49
183O	25C5	18ND2	74.22	183O	25C5	19C	63.18
183O	25C5	19CA	45.18	183O	25C5	184CD2	66.30
184O	25C5	19N	81.26	184O	25C5	184C	15.43
184O	25C5	18ND2	46.67	184O	25C5	19CA	98.50
184O	25C5	241OH2	80.65	184O	25C5	184CD2	68.07
20CA	25C5	19N	55.69	20CA	25C5	18ND2	75.55
20CA	25C5	19C	30.17	20CA	25C5	19CA	47.94
19N	25C5	184C	68.55	19N	25C5	18ND2	64.53
19N	25C5	19C	31.12	19N	25C5	19CA	17.72
184C	25C5	18ND2	50.25	184C	25C5	19C	99.32
184C	25C5	19CA	85.02	184C	25C5	241OH2	95.85
184C	25C5	184CD2	64.13	18ND2	25C5	19C	80.57
18ND2	25C5	19CA	79.75	18ND2	25C5	241OH2	86.00
19C	25C5	19CA	18.28	241OH2	25C5	184CD2	93.94
20O	25C6	20C	12.91	20O	25C6	20N	48.34

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TABLE XIX

20O	25C6	19CB	91.47	20O	25C6	18OD1	72.52
20O	25C6	19CG	86.64	20O	25C6	20CA	29.66
20O	25C6	19C	58.59	20O	25C6	19CA	78.30
20O	25C6	19N	85.64	20O	25C6	21N	15.81
20O	25C6	19NE2	96.10	184CD1	25C6	184NE1	21.76
184CD1	25C6	19CB	75.50	184CD1	25C6	18OD1	95.54
184CD1	25C6	19CG	83.68	184CD1	25C6	184CG	14.32
184CD1	25C6	19CD	72.31	184CD1	25C6	19CA	87.17
184CD1	25C6	19OE1	56.50	184CD1	25C6	19N	79.17
184CD1	25C6	184CE2	25.40	184CD1	25C6	183O	45.26
184CD1	25C6	184CA	35.59	184CD1	25C6	184CB	27.68
184CD1	25C6	19NE2	80.74	184NE1	25C6	19CB	80.25
184NE1	25C6	19CG	80.79	184NE1	25C6	184CG	30.82
184NE1	25C6	19CD	64.39	184NE1	25C6	19CA	96.31
184NE1	25C6	19OE1	49.89	184NE1	25C6	19N	93.83
184NE1	25C6	184CE2	11.71	184NE1	25C6	183O	62.24
184NE1	25C6	184CA	57.31	184NE1	25C6	184CB	47.06
184NE1	25C6	19NE2	68.19	20C	25C6	20N	37.04
20C	25C6	19CB	78.57	20C	25C6	18OD1	67.96
20C	25C6	19CG	74.74	20C	25C6	20CA	19.73
20C	25C6	19C	45.89	20C	25C6	19CD	90.64
20C	25C6	19CA	65.64	20C	25C6	19N	74.27
20C	25C6	21N	11.50	20C	25C6	19NE2	87.59
20N	25C6	19CB	50.10	20N	25C6	18OD1	42.87
20N	25C6	19CG	57.53	20N	25C6	20CA	19.02
20N	25C6	19C	16.56	20N	25C6	19CD	76.93
20N	25C6	19CA	32.67	20N	25C6	19OE1	86.01
20N	25C6	19N	37.35	20N	25C6	183O	71.42
20N	25C6	21N	45.38	20N	25C6	184CA	93.41
20N	25C6	19NE2	82.82	19CB	25C6	18OD1	71.17
19CB	25C6	19CG	20.52	19CB	25C6	184CG	87.09
19CB	25C6	20CA	67.16	19CB	25C6	19C	34.76
19CB	25C6	19CD	33.99	19CB	25C6	19CA	18.63
19CB	25C6	19OE1	37.17	19CB	25C6	19N	30.79
19CB	25C6	184CE2	91.78	19CB	25C6	183O	42.56
19CB	25C6	21N	80.11	19CB	25C6	184CA	74.81
19CB	25C6	184CB	88.09	19CB	25C6	19NE2	46.70

TABLE XIX

18OD1	25C6	19CG	88.69	18OD1	25C6	184CG	91.56
18OD1	25C6	20CA	49.91	18OD1	25C6	19C	53.85
18OD1	25C6	19CA	54.76	18OD1	25C6	19N	40.79
18OD1	25C6	183O	58.55	18OD1	25C6	21N	79.33
18OD1	25C6	184CA	61.28	18OD1	25C6	184CB	76.32
19CG	25C6	184CG	97.34	19CG	25C6	20CA	70.01
19CG	25C6	19C	41.04	19CG	25C6	19CD	19.41
19CG	25C6	19CA	33.94	19CG	25C6	19OE1	31.04
19CG	25C6	19N	50.11	19CG	25C6	184CE2	92.31
19CG	25C6	183O	60.89	19CG	25C6	21N	72.24
19CG	25C6	184CA	92.44	19CG	25C6	19NE2	28.22
184CG	25C6	19CD	86.63	184CG	25C6	19CA	96.09
184CG	25C6	19OE1	70.82	184CG	25C6	19N	84.76
184CG	25C6	184CE2	28.58	184CG	25C6	183O	51.08
184CG	25C6	184CA	30.50	184CG	25C6	184CB	16.46
184CG	25C6	19NE2	94.82	20CA	25C6	19C	32.41
20CA	25C6	19CD	88.73	20CA	25C6	19CA	50.99
20CA	25C6	19N	56.06	20CA	25C6	183O	89.93
20CA	25C6	21N	30.16	20CA	25C6	19NE2	90.65
19C	25C6	19CD	60.43	19C	25C6	19CA	19.75
19C	25C6	19OE1	69.63	19C	25C6	19N	32.09
19C	25C6	183O	64.40	19C	25C6	21N	50.78
19C	25C6	184CA	92.13	19C	25C6	19NE2	67.14
19CD	25C6	19CA	51.19	19CD	25C6	19OE1	15.82
19CD	25C6	19N	64.65	19CD	25C6	184CE2	75.35
19CD	25C6	183O	64.06	19CD	25C6	21N	85.72
19CD	25C6	184CA	91.40	19CD	25C6	184CB	96.57
19CD	25C6	19NE2	14.56	19CA	25C6	19OE1	55.80
19CA	25C6	19N	18.35	19CA	25C6	183O	45.71
19CA	25C6	21N	70.13	19CA	25C6	184CA	75.80
19CA	25C6	184CB	92.14	19CA	25C6	19NE2	62.13
19OE1	25C6	19N	64.68	19OE1	25C6	184CE2	61.31
19OE1	25C6	183O	54.29	19OE1	25C6	184CA	77.83
19OE1	25C6	184CB	81.20	19OE1	25C6	19NE2	26.71
19N	25C6	183O	34.10	19N	25C6	21N	81.52
19N	25C6	184CA	60.05	19N	25C6	184CB	77.37
19N	25C6	19NE2	77.44	184CE2	25C6	183O	69.91

TABLE XIX

184CE2	25C6	184CA	58.41	184CE2	25C6	184CB	44.79
184CE2	25C6	19NE2	77.70	183O	25C6	184CA	32.25
183O	25C6	184CB	46.82	183O	25C6	19NE2	78.49
21N	25C6	19NE2	80.31	184CA	25C6	184CB	17.72
20O	25O7	21CA	42.87	20O	25O7	20C	13.38
20O	25O7	21C	58.81	20O	25O7	19CD	93.04
20O	25O7	21O	73.65	20O	25O7	22O	77.10
20O	25O7	21N	27.93	20O	25O7	19CG	74.84
20O	25O7	19OE1	98.59	20O	25O7	184CD1	93.22
20O	25O7	19CB	66.24	21CA	25O7	20C	34.50
21CA	25O7	19NE2	96.98	21CA	25O7	21C	20.45
21CA	25O7	19CD	99.50	21CA	25O7	21O	32.06
21CA	25O7	22O	59.78	21CA	25O7	21N	18.66
21CA	25O7	19CG	84.02	21CA	25O7	19CB	87.69
20C	25O7	19NE2	92.76	20C	25O7	21C	47.32
20C	25O7	19CD	85.47	20C	25O7	21O	62.79
20C	25O7	22O	64.15	20C	25O7	21N	16.77
20C	25O7	19CG	67.03	20C	25O7	19OE1	93.62
20C	25O7	184CD1	98.91	20C	25O7	19CB	62.11
19NE2	25O7	21C	79.95	19NE2	25O7	19CD	17.34
19NE2	25O7	184NE1	69.42	19NE2	25O7	21O	80.15
19NE2	25O7	22O	37.30	19NE2	25O7	21N	90.94
19NE2	25O7	19CG	30.25	19NE2	25O7	19OE1	27.55
19NE2	25O7	184CD1	74.17	19NE2	25O7	19CB	45.70
21C	25O7	19CD	86.46	21C	25O7	21O	15.78
21C	25O7	22O	43.07	21C	25O7	21N	30.95
21C	25O7	19CG	74.61	21C	25O7	19CB	83.86
19CD	25O7	184NE1	58.81	19CD	25O7	21O	90.75
19CD	25O7	22O	44.18	19CD	25O7	21N	88.47
19CD	25O7	19CG	18.45	19CD	25O7	19OE1	14.37
19CD	25O7	184CD1	60.00	19CD	25O7	19CB	29.83
184NE1	25O7	19CG	69.06	184NE1	25O7	19OE1	44.47
184NE1	25O7	184CD1	15.81	184NE1	25O7	19CB	60.87
21O	25O7	22O	46.84	21O	25O7	21N	46.16
21O	25O7	19CG	82.83	21O	25O7	19CB	95.13
22O	25O7	21N	56.64	22O	25O7	19CG	37.32
22O	25O7	19OE1	58.55	22O	25O7	19CB	52.98

TABLE XIX

21N	25O7	19CG	70.99	21N	25O7	19OE1	99.59
21N	25O7	19CB	71.16	19CG	25O7	19OE1	28.77
19CG	25O7	184CD1	65.14	19CG	25O7	19CB	17.77
19OE1	25O7	184CD1	46.81	19OE1	25O7	19CB	32.36
184CD1	25O7	19CB	52.79	19NE2	25C8	184NE1	74.20
19NE2	25C8	19CD	17.18	19NE2	25C8	20O	86.21
19NE2	25C8	19OE1	28.35	19NE2	25C8	22O	35.57
19NE2	25C8	21O	77.21	19NE2	25C8	184CE2	85.22
184NE1	25C8	19CD	60.55	184NE1	25C8	20O	90.70
184NE1	25C8	19OE1	46.23	184NE1	25C8	184CE2	14.61
19CD	25C8	20O	76.90	19CD	25C8	19OE1	15.08
19CD	25C8	22O	42.30	19CD	25C8	21O	84.98
19CD	25C8	184CE2	73.32	20O	25C8	19OE1	83.60
20O	25C8	22O	62.93	20O	25C8	21O	59.11
19OE1	25C8	22O	57.39	19OE1	25C8	184CE2	58.44
22O	25C8	21O	42.86	184NE1	25C9	19CD	81.47
184NE1	25C9	19OE1	63.24	184NE1	25C9	184CE2	17.78
184NE1	25C9	184CD1	15.24	184NE1	25C9	184CZ2	36.54
184NE1	25C9	19CG	84.02	184NE1	25C9	162NE2	48.91
184NE1	25C9	162CD2	64.08	184NE1	25C9	19CB	68.93
19NE2	25C9	19CD	22.29	19NE2	25C9	19OE1	38.48
19NE2	25C9	184CD1	96.98	19NE2	25C9	19CG	31.33
19NE2	25C9	162NE2	73.61	19NE2	25C9	22O	33.83
19NE2	25C9	162CD2	72.04	19NE2	25C9	19CB	48.00
19CD	25C9	19OE1	20.30	19CD	25C9	184CE2	96.87
19CD	25C9	184CD1	75.05	19CD	25C9	19CG	16.69
19CD	25C9	162NE2	65.70	19CD	25C9	22O	43.91
19CD	25C9	162CD2	70.64	19CD	25C9	19CB	28.29
19OE1	25C9	184CE2	77.36	19OE1	25C9	184CD1	59.86
19OE1	25C9	184CZ2	88.34	19OE1	25C9	19CG	32.36
19OE1	25C9	162NE2	47.50	19OE1	25C9	22O	64.20
19OE1	25C9	162CD2	55.96	19OE1	25C9	19CB	33.06
184CE2	25C9	184CD1	31.58	184CE2	25C9	184CZ2	19.41
184CE2	25C9	162NE2	49.67	184CE2	25C9	162CD2	61.51
184CE2	25C9	19CB	86.67	184CD1	25C9	184CZ2	50.94
184CD1	25C9	19CG	73.85	184CD1	25C9	162NE2	59.35
184CD1	25C9	162CD2	75.48	184CD1	25C9	19CB	57.22

TABLE XIX

184CZ2	25C9	162NE2	48.81	184CZ2	25C9	162CD2	55.09
19CG	25C9	162NE2	79.83	19CG	25C9	22O	36.66
19CG	25C9	162CD2	86.65	19CG	25C9	19CB	17.77
162NE2	25C9	162CD2	16.38	162NE2	25C9	19CB	77.35
22O	25C9	19CB	51.74	162CD2	25C9	19CB	88.41
184NE1	25C10	184CZ2	41.93	184NE1	25C10	19NE2	89.55
184NE1	25C10	184CE2	20.67	184NE1	25C10	162CD2	76.32
184NE1	25C10	19OE1	57.76	184NE1	25C10	162NE2	56.54
184NE1	25C10	19CD	70.87	184NE1	25C10	184CD1	8.43
184NE1	25C10	162CG	77.88	184NE1	25C10	184CH2	49.27
184NE1	25C10	162CE1	51.80	184CZ2	25C10	184CE2	21.41
184CZ2	25C10	162CD2	68.85	184CZ2	25C10	19OE1	92.45
184CZ2	25C10	162NE2	58.15	184CZ2	25C10	184CD1	50.03
184CZ2	25C10	162CG	61.13	184CZ2	25C10	184CH2	7.67
184CZ2	25C10	162CE1	46.19	19NE2	25C10	162CD2	81.68
19NE2	25C10	19OE1	34.40	19NE2	25C10	162NE2	79.07
19NE2	25C10	19CD	18.69	19NE2	25C10	184CD1	83.31
19NE2	25C10	162CG	94.78	19NE2	25C10	162CE1	90.70
184CE2	25C10	162CD2	73.19	184CE2	25C10	19OE1	75.46
184CE2	25C10	162NE2	56.50	184CE2	25C10	19CD	90.32
184CE2	25C10	184CD1	28.64	184CE2	25C10	162CG	70.03
184CE2	25C10	184CH2	28.62	184CE2	25C10	162CE1	47.27
162CD2	25C10	19OE1	63.96	162CD2	25C10	162NE2	20.18
162CD2	25C10	19CD	77.09	162CD2	25C10	184CD1	81.08
162CD2	25C10	162CG	13.20	162CD2	25C10	184CH2	71.00
162CD2	25C10	162CE1	25.99	19OE1	25C10	162NE2	52.28
19OE1	25C10	19CD	17.69	19OE1	25C10	184CD1	53.34
19OE1	25C10	162CG	76.09	19OE1	25C10	184CH2	99.88
19OE1	25C10	162CE1	61.59	162NE2	25C10	19CD	68.59
162NE2	25C10	184CD1	60.95	162NE2	25C10	162CG	26.84
162NE2	25C10	184CH2	62.65	162NE2	25C10	162CE1	12.34
19CD	25C10	184CD1	64.80	19CD	25C10	162CG	90.03
19CD	25C10	162CE1	78.73	184CD1	25C10	162CG	84.10
184CD1	25C10	184CH2	57.23	184CD1	25C10	162CE1	57.81
162CG	25C10	184CH2	61.82	162CG	25C10	162CE1	26.29
184CH2	25C10	162CE1	50.38	184CZ2	25C11	184NE1	33.44
184CZ2	25C11	162CD2	58.33	184CZ2	25C11	184CE2	16.76

TABLE XIX

184CZ2	25C11	19NE2	94.98	184CZ2	25C11	162NE2	47.17
184NE1	25C11	162CD2	59.46	184NE1	25C11	184CE2	17.00
184NE1	25C11	19NE2	65.09	184NE1	25C11	162NE2	43.40
162CD2	25C11	184CE2	59.69	162CD2	25C11	19NE2	64.20
162CD2	25C11	162NE2	16.09	184CE2	25C11	19NE2	81.10
184CE2	25C11	162NE2	45.09	19NE2	25C11	162NE2	60.40
162CD2	25S14	184CZ2	63.39	162CD2	25S14	162CG	18.68
162CD2	25S14	162CB	36.19	162CD2	25S14	161O	65.32
162CD2	25S14	162NE2	15.75	162CD2	25S14	161OD1	86.18
162CD2	25S14	184CH2	70.43	184CZ2	25S14	162CG	63.65
184CZ2	25S14	162CB	78.78	184CZ2	25S14	162NE2	49.18
184CZ2	25S14	184CH2	14.76	162CG	25S14	162CB	20.04
162CG	25S14	161O	60.62	162CG	25S14	162NE2	28.04
162CG	25S14	161OD1	69.44	162CG	25S14	184CH2	65.75
162CB	25S14	161O	46.23	162CB	25S14	162NE2	47.97
162CB	25S14	161OD1	50.06	162CB	25S14	184CH2	76.80
161O	25S14	162NE2	81.07	161O	25S14	161OD1	48.28
162NE2	25S14	161OD1	97.37	162NE2	25S14	184CH2	58.34
161OD1	25S14	184CH2	95.88	184CZ2	25O15	184CH2	22.20
184CZ2	25O15	162CG	77.78	184CZ2	25O15	162CD2	73.98
184CZ2	25O15	137O	88.43	184CZ2	25O15	162CB	96.58
184CZ2	25O15	184CE2	11.44	184CZ2	25O15	137CB	79.42
184CZ2	25O15	162ND1	62.04	184CZ2	25O15	162NE2	56.17
184CZ2	25O15	162CE1	49.68	184CZ2	25O15	137C	97.15
184CZ2	25O15	184NE1	27.38	184CZ2	25O15	184CZ3	22.14
184CH2	25O15	162CG	83.63	184CH2	25O15	162CD2	86.91
184CH2	25O15	137O	66.28	184CH2	25O15	162CB	97.10
184CH2	25O15	184CE2	33.64	184CH2	25O15	137CB	63.34
184CH2	25O15	162ND1	65.67	184CH2	25O15	162NE2	70.78
184CH2	25O15	162CE1	59.07	184CH2	25O15	137C	75.65
184CH2	25O15	184NE1	49.58	184CH2	25O15	184CZ3	0.44
162CG	25O15	162CD2	20.14	162CG	25O15	137O	98.89
162CG	25O15	162CB	21.58	162CG	25O15	184CE2	75.94
162CG	25O15	137CB	60.62	162CG	25O15	162ND1	18.08
162CG	25O15	162NE2	30.14	162CG	25O15	161OD1	74.08
162CG	25O15	162CE1	28.30	162CG	25O15	137C	90.40
162CG	25O15	184NE1	73.88	162CG	25O15	184CZ3	84.03

TABLE XIX

162CD2	25O15	162CB	38.15	162CD2	25O15	184CE2	68.37
162CD2	25O15	137CB	79.85	162CD2	25O15	162ND1	30.08
162CD2	25O15	162NE2	17.97	162CD2	25O15	161OD1	89.07
162CD2	25O15	162CE1	28.23	162CD2	25O15	184NE1	61.40
162CD2	25O15	184CZ3	87.22	137O	25O15	162CB	88.99
137O	25O15	184CE2	99.87	137O	25O15	137CB	38.31
137O	25O15	162ND1	89.22	137O	25O15	161OD1	64.44
137O	25O15	162CE1	99.08	137O	25O15	137C	13.71
137O	25O15	184CZ3	66.38	162CB	25O15	184CE2	96.47
162CB	25O15	137CB	53.88	162CB	25O15	162ND1	34.56
162CB	25O15	162NE2	51.49	162CB	25O15	161OD1	52.55
162CB	25O15	162CE1	48.77	162CB	25O15	137C	77.54
162CB	25O15	184NE1	95.45	162CB	25O15	184CZ3	97.53
184CE2	25O15	137CB	88.43	184CE2	25O15	162ND1	62.44
184CE2	25O15	162NE2	50.44	184CE2	25O15	162CE1	47.79
184CE2	25O15	184NE1	15.94	184CE2	25O15	184CZ3	33.57
137CB	25O15	162ND1	52.03	137CB	25O15	162NE2	80.03
137CB	25O15	161OD1	58.03	137CB	25O15	162CE1	64.80
137CB	25O15	137C	32.11	137CB	25O15	184CZ3	63.70
162ND1	25O15	162NE2	28.43	162ND1	25O15	161OD1	83.20
162ND1	25O15	162CE1	16.55	162ND1	25O15	137C	84.06
162ND1	25O15	184NE1	64.50	162ND1	25O15	184CZ3	66.08
162NE2	25O15	162CE1	16.59	162NE2	25O15	184NE1	44.67
162NE2	25O15	184CZ3	71.04	161OD1	25O15	162CE1	99.43
161OD1	25O15	137C	51.29	162CE1	25O15	137C	96.68
162CE1	25O15	184NE1	48.13	162CE1	25O15	184CZ3	59.41
137C	25O15	184CZ3	75.83	184NE1	25O15	184CZ3	49.51
161OD1	25O16	161O	49.89	161OD1	25O16	161CG	14.03
161O	25O16	161CG	47.85	162CD2	25N17	162CG	24.82
162CD2	25N17	161O	98.82	162CD2	25N17	162CB	49.71
162CD2	25N17	162CA	57.32	162CD2	25N17	162NE2	15.00
162CD2	25N17	161C	92.83	162CD2	25N17	25SG	58.11
162CD2	25N17	162N	75.97	162CD2	25N17	162ND1	25.66
162CD2	25N17	162CE1	19.01	162CD2	25N17	184CZ2	61.54
162CD2	25N17	25CB	41.82	162CG	25N17	161O	86.86
162CG	25N17	162CB	26.56	162CG	25N17	162CA	42.37
162CG	25N17	162NE2	34.27	162CG	25N17	161C	76.28

TABLE XIX

162CG	25N17	25SG	73.91	162CG	25N17	162N	58.18
162CG	25N17	162ND1	11.86	162CG	25N17	161OD1	80.11
162CG	25N17	162CE1	24.71	162CG	25N17	184CZ2	63.21
162CG	25N17	25CB	63.12	161O	25N17	162CB	64.87
161O	25N17	162CA	44.51	161O	25N17	161C	15.53
161O	25N17	25SG	72.13	161O	25N17	162N	31.00
161O	25N17	162ND1	97.99	161O	25N17	161OD1	55.13
161O	25N17	25CB	90.74	162CB	25N17	162CA	24.47
162CB	25N17	162NE2	60.78	162CB	25N17	161C	51.89
162CB	25N17	25SG	82.14	162CB	25N17	162N	34.09
162CB	25N17	162ND1	34.92	162CB	25N17	161OD1	55.89
162CB	25N17	162CE1	50.58	162CB	25N17	184CZ2	81.16
162CB	25N17	25CB	79.93	162CA	25N17	162NE2	71.74
162CA	25N17	161C	35.58	162CA	25N17	25SG	65.34
162CA	25N17	162N	19.04	162CA	25N17	162ND1	53.71
162CA	25N17	161OD1	60.49	162CA	25N17	162CE1	66.39
162CA	25N17	25CB	71.10	162NE2	25N17	25SG	65.94
162NE2	25N17	162N	89.98	162NE2	25N17	162ND1	29.38
162NE2	25N17	162CE1	14.46	162NE2	25N17	184CZ2	48.97
162NE2	25N17	25CB	46.17	161C	25N17	25SG	80.41
161C	25N17	162N	18.12	161C	25N17	162ND1	86.43
161C	25N17	161OD1	42.82	161C	25N17	25CB	95.81
25SG	25N17	162N	77.28	25SG	25N17	162ND1	81.39
25SG	25N17	162CE1	76.71	25SG	25N17	25CB	21.56
162N	25N17	162ND1	68.34	162N	25N17	161OD1	45.06
162N	25N17	162CE1	82.88	162N	25N17	25CB	87.52
162ND1	25N17	161OD1	83.28	162ND1	25N17	162CE1	16.35
162ND1	25N17	184CZ2	51.35	162ND1	25N17	25CB	67.28
161OD1	25N17	162CE1	99.02	161OD1	25N17	184CZ2	99.72
162CE1	25N17	184CZ2	43.80	162CE1	25N17	25CB	58.69
184CZ2	25N17	25CB	91.04	161O	25C18	25SG	88.17
161O	25C18	162CD2	89.98	161O	25C18	162CA	40.67
161O	25C18	161C	9.73	161O	25C18	162CG	74.76
161O	25C18	162CB	55.30	161O	25C18	162N	24.42
25SG	25C18	162CD2	63.21	25SG	25C18	162CA	69.19
25SG	25C18	161C	89.73	25SG	25C18	162CG	72.88
25SG	25C18	162CB	81.01	25SG	25C18	25CB	22.17

TABLE XIX

25SG	25C18	19NE2	60.90	25SG	25C18	162NE2	64.84
25SG	25C18	162N	81.28	162CD2	25C18	162CA	49.41
162CD2	25C18	161C	82.11	162CD2	25C18	162CG	17.90
162CD2	25C18	162CB	38.19	162CD2	25C18	25CB	48.19
162CD2	25C18	19NE2	74.06	162CD2	25C18	162NE2	11.85
162CD2	25C18	162N	65.91	162CA	25C18	161C	33.66
162CA	25C18	162CG	35.77	162CA	25C18	162CB	21.19
162CA	25C18	25CB	73.11	162CA	25C18	162NE2	61.26
162CA	25C18	162N	17.67	161C	25C18	162CG	66.10
161C	25C18	162CB	46.17	161C	25C18	162NE2	93.83
161C	25C18	162N	16.25	162CG	25C18	162CB	20.62
162CG	25C18	25CB	62.56	162CG	25C18	19NE2	91.91
162CG	25C18	162NE2	28.46	162CG	25C18	162N	50.34
162CB	25C18	25CB	77.17	162CB	25C18	162NE2	49.07
162CB	25C18	162N	31.21	25CB	25C18	19NE2	46.45
25CB	25C18	162NE2	46.22	25CB	25C18	162N	89.13
19NE2	25C18	162NE2	63.90	162NE2	25C18	162N	77.68
25SG	25C19	25CB	31.14	25SG	25C19	162CD2	72.89
25SG	25C19	161O	97.36	25SG	25C19	19NE2	87.55
25SG	25C19	25N	42.09	25SG	25C19	25CA	29.35
25SG	25C19	23CA	99.22	25SG	25C19	162CA	71.95
25SG	25C19	23O	76.04	25SG	25C19	23C	80.42
25SG	25C19	162CG	75.66	25SG	25C19	162NE2	71.54
25SG	25C19	19CD	78.54	25SG	25C19	19OE1	73.25
25SG	25C19	161C	92.06	25SG	25C19	162CB	81.06
25CB	25C19	162CD2	57.89	25CB	25C19	19NE2	60.82
25CB	25C19	25N	33.86	25CB	25C19	25CA	15.34
25CB	25C19	23CA	90.78	25CB	25C19	162CA	81.46
25CB	25C19	23O	81.85	25CB	25C19	23C	77.61
25CB	25C19	162CG	67.35	25CB	25C19	162NE2	50.15
25CB	25C19	19CD	49.61	25CB	25C19	19OE1	42.26
25CB	25C19	162CB	81.00	162CD2	25C19	161O	78.28
162CD2	25C19	19NE2	84.27	162CD2	25C19	25N	90.80
162CD2	25C19	25CA	73.23	162CD2	25C19	162CA	45.80
162CD2	25C19	162CG	13.99	162CD2	25C19	162NE2	13.84
162CD2	25C19	19CD	72.50	162CD2	25C19	19OE1	57.48
162CD2	25C19	161C	71.45	162CD2	25C19	162CB	32.02

TABLE XIX

161O	25C19	162CA	36.90	161O	25C19	162CG	64.31
161O	25C19	162NE2	92.09	161O	25C19	161C	7.56
161O	25C19	162CB	46.27	19NE2	25C19	25N	50.87
19NE2	25C19	25CA	58.20	19NE2	25C19	23CA	48.05
19NE2	25C19	23O	68.25	19NE2	25C19	23C	52.78
19NE2	25C19	162CG	98.10	19NE2	25C19	162NE2	70.55
19NE2	25C19	19CD	13.21	19NE2	25C19	19OE1	27.94
25N	25C19	25CA	19.24	25N	25C19	23CA	59.89
25N	25C19	23O	48.33	25N	25C19	23C	44.21
25N	25C19	162NE2	80.81	25N	25C19	19CD	47.37
25N	25C19	19OE1	51.79	25CA	25C19	23CA	78.48
25CA	25C19	162CA	93.16	25CA	25C19	23O	66.60
25CA	25C19	23C	63.45	25CA	25C19	162CG	82.49
25CA	25C19	162NE2	65.00	25CA	25C19	19CD	49.86
25CA	25C19	19OE1	47.62	25CA	25C19	162CB	95.23
23CA	25C19	23O	31.44	23CA	25C19	23C	19.68
23CA	25C19	19CD	59.89	23CA	25C19	19OE1	75.03
162CA	25C19	162CG	32.75	162CA	25C19	162NE2	59.16
162CA	25C19	161C	29.34	162CA	25C19	162CB	18.30
23O	25C19	23C	15.83	23O	25C19	19CD	75.71
23O	25C19	19OE1	88.43	23C	25C19	19CD	61.25
23C	25C19	19OE1	74.96	162CG	25C19	162NE2	27.82
162CG	25C19	19CD	86.48	162CG	25C19	19OE1	71.46
162CG	25C19	161C	57.47	162CG	25C19	162CB	18.04
162NE2	25C19	19CD	58.67	162NE2	25C19	19OE1	43.65
162NE2	25C19	161C	85.29	162NE2	25C19	162CB	45.84
19CD	25C19	19OE1	15.17	19OE1	25C19	162CB	89.49
161C	25C19	162CB	39.48	19NE2	25O20	25SG	93.68
19NE2	25O20	23CA	67.16	19NE2	25O20	25CB	65.25
19NE2	25O20	23C	68.09	19NE2	25O20	19CD	11.46
19NE2	25O20	23O	84.29	19NE2	25O20	25N	55.54
19NE2	25O20	19OE1	27.77	19NE2	25O20	24N	52.93
19NE2	25O20	162CD2	84.48	19NE2	25O20	23N	61.60
19NE2	25O20	25CA	59.16	19NE2	25O20	22O	33.73
25SG	25O20	25CB	29.49	25SG	25O20	23C	86.92
25SG	25O20	19CD	84.98	25SG	25O20	23O	77.98
25SG	25O20	25N	47.84	25SG	25O20	19OE1	75.69

TABLE XIX

25SG	25O20	24N	81.49	25SG	25O20	162CD2	54.46
25SG	25O20	25CA	35.73	25SG	25O20	161O	62.50
23CA	25O20	23C	23.99	23CA	25O20	19CD	77.34
23CA	25O20	23O	36.67	23CA	25O20	25N	69.78
23CA	25O20	19OE1	93.50	23CA	25O20	24N	33.03
23CA	25O20	23N	10.73	23CA	25O20	25CA	87.65
23CA	25O20	22O	36.27	25CB	25O20	23C	83.77
25CB	25O20	19CD	55.78	25CB	25O20	23O	83.59
25CB	25O20	25N	34.83	25CB	25O20	19OE1	46.44
25CB	25O20	24N	71.21	25CB	25O20	162CD2	47.80
25CB	25O20	25CA	16.76	25CB	25O20	22O	91.65
25CB	25O20	161O	85.05	23C	25O20	19CD	75.06
23C	25O20	23O	17.82	23C	25O20	25N	49.05
23C	25O20	19OE1	88.41	23C	25O20	24N	16.95
23C	25O20	23N	33.23	23C	25O20	25CA	67.04
23C	25O20	22O	47.64	19CD	25O20	23O	89.75
19CD	25O20	25N	52.63	19CD	25O20	19OE1	16.53
19CD	25O20	24N	58.75	19CD	25O20	162CD2	73.33
19CD	25O20	23N	72.54	19CD	25O20	25CA	52.30
19CD	25O20	22O	45.08	23O	25O20	25N	51.85
23O	25O20	24N	31.38	23O	25O20	23N	47.25
23O	25O20	25CA	68.11	23O	25O20	22O	65.37
25N	25O20	19OE1	55.38	25N	25O20	24N	36.84
25N	25O20	162CD2	82.30	25N	25O20	23N	74.87
25N	25O20	25CA	18.06	25N	25O20	22O	66.79
19OE1	25O20	24N	71.53	19OE1	25O20	162CD2	56.81
19OE1	25O20	23N	89.05	19OE1	25O20	25CA	48.64
19OE1	25O20	22O	61.51	24N	25O20	23N	38.39
24N	25O20	25CA	54.62	24N	25O20	22O	40.31
162CD2	25O20	25CA	64.39	162CD2	25O20	161O	59.56
23N	25O20	25CA	92.03	23N	25O20	22O	28.59
25CA	25O20	22O	79.45	25CA	25O20	161O	97.28
25SG	25C21	161O	94.20	25SG	25C21	23O	80.20
25SG	25C21	25CB	11.32	25SG	25C21	23C	74.97
25SG	25C21	161C	90.47	25SG	25C21	23CA	85.24
25SG	25C21	162CA	61.66	25SG	25C21	25N	34.26
25SG	25C21	162CD2	42.75	161O	25C21	25CB	99.42

TABLE XIX

161O	25C21	161C	6.02	161O	25C21	162CA	32.54
161O	25C21	162CD2	63.74	23O	25C21	25CB	75.76
23O	25C21	23C	15.44	23O	25C21	65CA	51.45
23O	25C21	23CA	31.46	23O	25C21	25N	46.40
25CB	25C21	23C	68.05	25CB	25C21	161C	96.56
25CB	25C21	23CA	75.96	25CB	25C21	162CA	67.42
25CB	25C21	25N	29.59	25CB	25C21	162CD2	41.05
23C	25C21	65CA	65.91	23C	25C21	23CA	19.15
23C	25C21	25N	41.03	65CA	25C21	23CA	74.18
65CA	25C21	25N	90.25	161C	25C21	162CA	29.15
161C	25C21	162CD2	63.15	23CA	25C21	25N	54.22
23CA	25C21	162CD2	99.59	162CA	25C21	25N	95.84
162CA	25C21	162CD2	38.23	25N	25C21	162CD2	69.67
161O	25N22	161C	14.11	161O	25N22	162CA	41.10
161O	25N22	162N	27.68	161O	25N22	163N	72.60
161O	25N22	162C	56.36	161O	25N22	161CA	21.99
25SG	25N22	162CA	74.63	25SG	25N22	162N	94.42
25SG	25N22	163N	59.02	25SG	25N22	25CB	3.31
25SG	25N22	162C	70.77	161C	25N22	162CA	35.66
161C	25N22	162N	17.48	161C	25N22	163N	63.91
161C	25N22	162C	47.46	161C	25N22	161CA	15.87
162CA	25N22	162N	19.79	162CA	25N22	163N	32.40
162CA	25N22	25CB	71.33	162CA	25N22	162C	17.88
162CA	25N22	161CA	50.91	162N	25N22	163N	46.46
162N	25N22	25CB	91.12	162N	25N22	162C	29.99
162N	25N22	161CA	31.55	163N	25N22	25CB	56.10
163N	25N22	162C	16.47	163N	25N22	161CA	76.35
25CB	25N22	162C	67.57	162C	25N22	161CA	60.36
161O	25C23	25SG	74.84	161O	25C23	161C	14.77
161O	25C23	162N	24.77	161O	25C23	162CA	32.09
161O	25C23	161CA	26.81	25SG	25C23	161C	82.13
25SG	25C23	65CA	98.69	25SG	25C23	162N	73.79
25SG	25C23	162CA	57.15	25SG	25C23	26CD1	66.11
25SG	25C23	161CA	99.24	25SG	25C23	26CB	66.49
161C	25C23	162N	14.87	161C	25C23	162CA	29.26
161C	25C23	161CA	17.21	66O	25C23	65CA	69.84
66O	25C23	66N	37.37	66O	25C23	65C	52.20

TABLE XIX

66O	25C23	26CD1	54.29	66O	25C23	26CB	42.11
65CA	25C23	66N	32.68	65CA	25C23	65C	17.67
65CA	25C23	26CD1	48.54	65CA	25C23	26CB	74.99
66N	25C23	65C	15.04	66N	25C23	26CD1	43.34
66N	25C23	26CB	56.16	162N	25C23	162CA	17.00
162N	25C23	161CA	29.22	162CA	25C23	161CA	45.57
65C	25C23	26CD1	42.77	65C	25C23	26CB	63.55
26CD1	25C23	26CB	29.73	65CA	25O24	66N	44.96
65CA	25O24	65C	24.04	65CA	25O24	66O	88.80
65CA	25O24	65N	11.32	65CA	25O24	26CD1	59.03
65CA	25O24	66CA	56.76	65CA	25O24	66C	76.00
65CA	25O24	64O	31.19	65CA	25O24	23O	51.20
65CA	25O24	26CG	69.83	65CA	25O24	26CB	87.37
65CA	25O24	65O	23.39	65CA	25O24	64C	20.95
66N	25O24	65C	20.92	66N	25O24	66O	44.37
66N	25O24	65N	56.05	66N	25O24	26CD1	51.61
66N	25O24	66CA	11.81	66N	25O24	66C	31.20
66N	25O24	64O	68.01	66N	25O24	23O	77.65
66N	25O24	26CG	49.90	66N	25O24	26CB	61.70
66N	25O24	65O	21.59	66N	25O24	64C	64.08
65C	25O24	66O	65.02	65C	25O24	65N	35.18
65C	25O24	26CD1	51.98	65C	25O24	66CA	32.73
65C	25O24	66C	52.03	65C	25O24	64O	49.51
65C	25O24	23O	64.02	65C	25O24	26CG	57.07
65C	25O24	26CB	72.88	65C	25O24	65O	0.87
65C	25O24	64C	43.58	66O	25O24	65N	99.41
66O	25O24	26CD1	61.59	66O	25O24	66CA	32.76
66O	25O24	66C	13.43	66O	25O24	26CG	47.99
66O	25O24	26CB	43.51	66O	25O24	65O	65.76
65N	25O24	26CD1	62.12	65N	25O24	66CA	67.82
65N	25O24	66C	86.89	65N	25O24	64O	27.80
65N	25O24	23O	45.06	65N	25O24	26CG	74.86
65N	25O24	26CB	92.41	65N	25O24	65O	34.57
65N	25O24	64C	14.20	26CD1	25O24	25SG	67.04
26CD1	25O24	66CA	53.75	26CD1	25O24	66C	58.39
26CD1	25O24	64O	89.45	26CD1	25O24	23O	41.01
26CD1	25O24	26CG	15.28	26CD1	25O24	26CB	31.14

TABLE XIX

26CD1	25O24	65O	52.64	26CD1	25O24	64C	76.32
25SG	25O24	161O	59.11	25SG	25O24	23O	57.25
25SG	25O24	26CG	69.72	25SG	25O24	26CB	63.45
66CA	25O24	66C	19.46	66CA	25O24	64O	78.88
66CA	25O24	23O	85.60	66CA	25O24	26CG	48.11
66CA	25O24	26CB	56.41	66CA	25O24	65O	33.40
66CA	25O24	64C	75.76	66C	25O24	64O	97.72
66C	25O24	23O	96.86	66C	25O24	26CG	47.34
66C	25O24	26CB	48.38	66C	25O24	65O	52.74
66C	25O24	64C	95.21	64O	25O24	23O	69.05
64O	25O24	65O	48.66	64O	25O24	64C	14.27
23O	25O24	26CG	55.76	23O	25O24	26CB	67.79
23O	25O24	65O	64.06	23O	25O24	64C	55.23
26CG	25O24	26CB	17.62	26CG	25O24	65O	57.87
26CG	25O24	64C	88.94	26CB	25O24	65O	73.72
65O	25O24	64C	42.81	161O	25C25	161C	18.10
161O	25C25	162N	30.50	161O	25C25	161CA	32.52
161O	25C25	163N	64.43	161O	25C25	25SG	63.34
161O	25C25	162CA	35.10	161O	25C25	162C	53.40
161O	25C25	163CB	93.18	66O	25C25	25SG	99.66
66O	25C25	66N	34.44	66O	25C25	163CB	83.50
161C	25C25	162N	17.33	161C	25C25	161CA	19.80
161C	25C25	163N	60.64	161C	25C25	25SG	75.44
161C	25C25	162CA	30.92	161C	25C25	162C	46.09
161C	25C25	163CB	89.51	162N	25C25	161CA	32.24
162N	25C25	163N	44.92	162N	25C25	25SG	71.34
162N	25C25	162CA	18.08	162N	25C25	162C	29.44
162N	25C25	163CB	73.04	161CA	25C25	163N	77.08
161CA	25C25	25SG	94.58	161CA	25C25	162CA	49.19
161CA	25C25	162C	61.23	163N	25C25	25SG	49.61
163N	25C25	162CA	30.25	163N	25C25	162C	16.24
163N	25C25	163CB	29.19	25SG	25C25	162CA	54.70
25SG	25C25	162C	58.88	25SG	25C25	66N	88.50
25SG	25C25	163CB	57.12	162CA	25C25	162C	18.49
162CA	25C25	163CB	59.44	162C	25C25	163CB	43.61
66O	25C26	26CB	56.41	66O	25C26	66C	2.37
66O	25C26	26CA	74.83	66O	25C26	68SD	74.84

TABLE XIX

66O	25C26	66N	33.64	66O	25C26	26N	86.28
66O	25C26	26CG	50.23	66O	25C26	26CD1	56.63
163CB	25C26	26CB	71.13	163CB	25C26	163N	35.96
163CB	25C26	25SG	68.31	163CB	25C26	163CA	18.75
163CB	25C26	26CA	53.74	163CB	25C26	162C	49.97
163CB	25C26	68SD	50.69	163CB	25C26	161O	96.76
163CB	25C26	26N	55.09	163CB	25C26	26CG	85.31
163CB	25C26	162CA	65.37	163CB	25C26	161C	92.67
163CB	25C26	162N	78.07	163CB	25C26	26CD1	92.73
26CB	25C26	163N	98.44	26CB	25C26	25SG	73.00
26CB	25C26	163CA	88.50	26CB	25C26	66C	55.68
26CB	25C26	26CA	18.86	26CB	25C26	68SD	60.85
26CB	25C26	66N	60.69	26CB	25C26	26N	31.12
26CB	25C26	26CG	15.82	26CB	25C26	26CD1	29.79
163N	25C26	25SG	54.34	163N	25C26	163CA	19.23
163N	25C26	26CA	79.60	163N	25C26	162C	16.17
163N	25C26	68SD	84.27	163N	25C26	161O	61.07
163N	25C26	26N	71.27	163N	25C26	162CA	29.41
163N	25C26	161C	57.02	163N	25C26	162N	43.18
25SG	25C26	163CA	65.77	25SG	25C26	26CA	61.96
25SG	25C26	162C	61.73	25SG	25C26	161O	58.28
25SG	25C26	66N	92.45	25SG	25C26	26N	44.25
25SG	25C26	26CG	71.07	25SG	25C26	162CA	54.19
25SG	25C26	161C	68.75	25SG	25C26	162N	67.87
25SG	25C26	26CD1	61.51	163CA	25C26	26CA	70.22
163CA	25C26	162C	31.46	163CA	25C26	68SD	65.05
163CA	25C26	161O	79.96	163CA	25C26	26N	67.43
163CA	25C26	162CA	47.86	163CA	25C26	161C	74.37
163CA	25C26	162N	59.50	66C	25C26	26CA	74.25
66C	25C26	68SD	76.55	66C	25C26	66N	31.36
66C	25C26	26N	85.17	66C	25C26	26CG	48.83
66C	25C26	26CD1	54.70	26CA	25C26	162C	95.72
26CA	25C26	68SD	58.01	26CA	25C26	66N	77.90
26CA	25C26	26N	17.81	26CA	25C26	26CG	31.59
26CA	25C26	26CD1	40.72	162C	25C26	68SD	93.90
162C	25C26	161O	49.88	162C	25C26	26N	86.44
162C	25C26	162CA	18.09	162C	25C26	161C	42.92

TABLE XIX

162C	25C26	162N	28.10	68SD	25C26	26N	73.74
68SD	25C26	26CG	75.07	68SD	25C26	26CD1	90.33
161O	25C26	162CA	32.21	161O	25C26	161C	14.49
161O	25C26	162N	26.44	66N	25C26	26N	79.75
66N	25C26	26CG	46.31	66N	25C26	26CD1	41.21
26N	25C26	26CG	36.93	26N	25C26	162CA	89.41
26N	25C26	26CD1	38.63	26CG	25C26	26CD1	15.55
162CA	25C26	161C	28.03	162CA	25C26	162N	16.67
161C	25C26	162N	15.37	163CB	25C27	68SD	63.80
163CB	25C27	163CA	20.61	163CB	25C27	163N	36.17
163CB	25C27	68CE	66.45	163CB	25C27	134CB	82.27
163CB	25C27	26CB	68.13	163CB	25C27	162C	50.98
163CB	25C27	162O	55.96	163CB	25C27	26CA	50.39
68SD	25C27	66O	85.83	68SD	25C27	163CA	78.97
68SD	25C27	163N	98.79	68SD	25C27	68CE	27.50
68SD	25C27	134CB	86.61	68SD	25C27	209CD2	77.07
68SD	25C27	26CB	65.47	68SD	25C27	66C	82.65
68SD	25C27	26CA	60.55	68SD	25C27	67CA	62.19
66O	25C27	26CB	49.09	66O	25C27	66C	4.22
66O	25C27	26CA	66.81	66O	25C27	67CA	32.70
163CA	25C27	163N	20.52	163CA	25C27	68CE	72.92
163CA	25C27	134CB	68.04	163CA	25C27	26CB	86.68
163CA	25C27	162C	32.08	163CA	25C27	162O	35.38
163CA	25C27	26CA	69.20	163N	25C27	68CE	93.00
163N	25C27	134CB	74.40	163N	25C27	26CB	90.05
163N	25C27	162C	16.34	163N	25C27	162O	27.46
163N	25C27	26CA	74.74	68CE	25C27	134CB	59.27
68CE	25C27	209CD2	56.93	68CE	25C27	26CB	92.20
68CE	25C27	162C	98.29	68CE	25C27	162O	89.77
68CE	25C27	26CA	84.17	68CE	25C27	67CA	79.42
134CB	25C27	209CD2	45.82	134CB	25C27	162C	65.01
134CB	25C27	162O	50.58	209CD2	25C27	162O	95.82
209CD2	25C27	67CA	79.47	26CB	25C27	66C	50.07
26CB	25C27	26CA	17.74	26CB	25C27	67CA	62.22
162C	25C27	162O	14.47	162C	25C27	26CA	90.70
66C	25C27	26CA	67.64	66C	25C27	67CA	28.48
26CA	25C27	67CA	76.24	134CB	25C28	163CB	94.94

TABLE XIX

134CB	25C28	163N	95.08	134CB	25C28	162C	86.92
134CB	25C28	162O	68.97	134CB	25C28	163CA	83.27
134CB	25C28	209CD2	54.77	134CB	25C28	134CA	19.96
134CB	25C28	162N	96.63	134CB	25C28	68CE	62.89
134CB	25C28	68SD	87.41	134CB	25C28	134C	23.58
134CB	25C28	161N	87.00	163CB	25C28	163N	38.06
163CB	25C28	162C	57.44	163CB	25C28	162O	66.17
163CB	25C28	163CA	22.67	163CB	25C28	134CA	78.61
163CB	25C28	162N	88.44	163CB	25C28	162CA	69.97
163CB	25C28	68CE	60.09	163CB	25C28	68SD	51.61
163CB	25C28	161C	98.14	163CB	25C28	66O	84.86
163CB	25C28	134C	88.60	163CB	25C28	161O	91.88
163N	25C28	162C	20.41	163N	25C28	162O	35.09
163N	25C28	163CA	22.12	163N	25C28	134CA	75.15
163N	25C28	162N	50.53	163N	25C28	162CA	32.37
163N	25C28	68CE	93.09	163N	25C28	68SD	89.55
163N	25C28	161C	62.08	163N	25C28	134C	76.23
163N	25C28	161O	59.80	163N	25C28	161N	83.44
162C	25C28	162O	18.65	162C	25C28	163CA	37.49
162C	25C28	134CA	68.48	162C	25C28	162N	33.45
162C	25C28	162CA	18.81	162C	25C28	161C	48.13
162C	25C28	134C	64.60	162C	25C28	161O	50.86
162C	25C28	161N	64.31	162O	25C28	163CA	43.61
162O	25C28	134CA	51.60	162O	25C28	162N	38.24
162O	25C28	162CA	32.12	162O	25C28	161C	54.89
162O	25C28	134C	46.14	162O	25C28	161O	62.22
162O	25C28	161N	60.29	163CA	25C28	134CA	64.10
163CA	25C28	162N	70.64	163CA	25C28	162CA	53.50
163CA	25C28	68CE	71.06	163CA	25C28	68SD	70.42
163CA	25C28	161C	83.69	163CA	25C28	134C	70.58
163CA	25C28	161O	81.89	209CD2	25C28	134CA	73.08
209CD2	25C28	68CE	56.44	209CD2	25C28	68SD	70.67
209CD2	25C28	66O	90.11	209CD2	25C28	134C	77.77
134CA	25C28	162N	84.78	134CA	25C28	162CA	83.66
134CA	25C28	68CE	63.87	134CA	25C28	68SD	86.25
134CA	25C28	161C	99.94	134CA	25C28	134C	14.94
134CA	25C28	161N	85.92	162N	25C28	162CA	18.62

TABLE XIX

162N	25C28	161C	16.67	162N	25C28	134C	73.76
162N	25C28	161O	26.48	162N	25C28	161N	33.69
162CA	25C28	161C	30.27	162CA	25C28	134C	76.50
162CA	25C28	161O	32.09	162CA	25C28	161N	52.27
68CE	25C28	68SD	24.56	68CE	25C28	66O	83.70
68CE	25C28	134C	78.45	68SD	25C28	66O	61.76
161C	25C28	134C	87.61	161C	25C28	161O	14.08
161C	25C28	161N	30.20	66O	25C28	161O	96.95
134C	25C28	161N	71.12	161O	25C28	161N	43.13
66O	25C29	68SD	95.60	66O	25C29	67CA	46.15
66O	25C29	67CD1	76.62	66O	25C29	66C	11.19
66O	25C29	67N	28.20	66O	25C29	68N	68.80
66O	25C29	67C	53.21	66O	25C29	67CB	59.40
66O	25C29	67CG	63.57	66O	25C29	234OH2	97.74
66O	25C29	26CB	45.24	66O	25C29	67CE1	81.98
209CD2	25C29	68SD	86.14	209CD2	25C29	67CD1	76.20
209CD2	25C29	68CE	61.12	209CD2	25C29	68N	93.85
209CD2	25C29	67CB	92.20	209CD2	25C29	67CG	87.96
209CD2	25C29	134CB	44.39	209CD2	25C29	234OH2	59.00
209CD2	25C29	67CE1	74.42	68SD	25C29	67CA	76.30
68SD	25C29	66C	94.73	68SD	25C29	68CE	26.92
68SD	25C29	67N	86.90	68SD	25C29	68N	44.21
68SD	25C29	67C	58.54	68SD	25C29	67CB	85.01
68SD	25C29	163CB	50.89	68SD	25C29	134CB	79.09
68SD	25C29	234OH2	57.89	68SD	25C29	26CB	61.09
67CA	25C29	67CD1	50.51	67CA	25C29	66C	35.89
67CA	25C29	68CE	93.88	67CA	25C29	67N	18.53
67CA	25C29	68N	33.04	67CA	25C29	67C	17.87
67CA	25C29	67CB	18.28	67CA	25C29	67CG	34.89
67CA	25C29	234OH2	51.94	67CA	25C29	26CB	68.39
67CA	25C29	67CE1	64.72	67CD1	25C29	66C	66.65
67CD1	25C29	67N	56.05	67CD1	25C29	68N	72.69
67CD1	25C29	67C	65.26	67CD1	25C29	67CB	33.63
67CD1	25C29	67CG	15.94	67CD1	25C29	234OH2	57.55
67CD1	25C29	67CE1	15.80	66C	25C29	67N	17.49
66C	25C29	68N	61.93	66C	25C29	67C	45.45
66C	25C29	67CB	48.27	66C	25C29	67CG	52.89

TABLE XIX

66C	25C29	234OH2	87.82	66C	25C29	26CB	52.23
66C	25C29	67CE1	73.67	68CE	25C29	68N	61.24
68CE	25C29	67C	77.92	68CE	25C29	67CB	95.69
68CE	25C29	163CB	55.77	68CE	25C29	134CB	54.85
68CE	25C29	234OH2	55.46	68CE	25C29	26CB	86.35
67N	25C29	68N	47.83	67N	25C29	67C	30.97
67N	25C29	67CB	31.65	67N	25C29	67CG	40.58
67N	25C29	234OH2	70.44	67N	25C29	26CB	60.08
67N	25C29	67CE1	66.83	68N	25C29	67C	16.87
68N	25C29	67CB	41.26	68N	25C29	67CG	60.50
68N	25C29	163CB	90.93	68N	25C29	234OH2	36.37
68N	25C29	26CB	64.40	68N	25C29	67CE1	88.49
67C	25C29	67CB	31.65	67C	25C29	67CG	50.66
67C	25C29	163CB	99.57	67C	25C29	234OH2	46.71
67C	25C29	26CB	59.86	67C	25C29	67CE1	80.48
67CB	25C29	67CG	19.43	67CB	25C29	234OH2	44.01
67CB	25C29	26CB	86.67	67CB	25C29	67CE1	48.89
67CG	25C29	234OH2	54.79	67CG	25C29	67CE1	29.95
163CB	25C29	134CB	64.77	163CB	25C29	26CB	55.99
134CB	25C29	234OH2	92.26	234OH2	25C29	67CE1	70.61
66O	25N30	66N	36.00	66O	25N30	66C	10.42
66N	25N30	66C	31.15	161O	25N30	161C	14.88
161O	25N30	161CA	29.27	161O	25N30	160O	61.86
161C	25N30	161CA	18.36	161C	25N30	160O	49.77
161CA	25N30	160O	32.60	160O	25C31	161CA	38.22
160O	25C31	160C	13.90	160O	25C31	161C	56.07
160O	25C31	161N	27.07	160O	25C31	161O	68.03
161CA	25C31	160C	31.81	161CA	25C31	161C	19.14
161CA	25C31	161N	17.82	161CA	25C31	161O	29.81
160C	25C31	161C	46.85	160C	25C31	161N	16.04
160C	25C31	161O	60.44	161C	25C31	161N	30.84
161C	25C31	161O	14.70	66O	25C31	67CE1	65.45
161N	25C31	161O	44.68	160O	25O32	160C	20.78
160O	25O32	161CA	51.99	160O	25O32	161N	38.37
160O	25O32	161C	74.30	160O	25O32	160CB	45.78
160O	25O32	161O	86.34	160O	25O32	160CA	28.59
160O	25O32	162N	77.29	160O	25O32	161CB	49.03

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TABLE XIX

160C	25O32	161CA	42.82	160C	25O32	161N	21.72
160C	25O32	161C	61.05	160C	25O32	160CB	36.54
160C	25O32	161O	75.94	160C	25O32	160CA	16.12
160C	25O32	162N	59.68	160C	25O32	161CB	45.43
161CA	25O32	161N	24.13	161CA	25O32	161C	23.46
161CA	25O32	160CB	75.84	161CA	25O32	161O	34.47
161CA	25O32	160CA	57.38	161CA	25O32	162N	33.92
161CA	25O32	161CB	11.93	161N	25O32	161C	39.41
161N	25O32	160CB	51.73	161N	25O32	161O	54.76
161N	25O32	160CA	34.01	161N	25O32	162N	39.00
161N	25O32	161CB	31.34	161C	25O32	160CB	86.66
161C	25O32	161O	16.47	161C	25O32	160CA	72.47
161C	25O32	162N	16.93	161C	25O32	161CB	32.27
160CB	25O32	160CA	20.46	160CB	25O32	162N	76.70
160CB	25O32	161CB	81.15	161O	25O32	160CA	88.45
161O	25O32	162N	29.70	161O	25O32	161CB	38.78
160CA	25O32	162N	66.95	160CA	25O32	161CB	61.27
162N	25O32	161CB	45.15	67CE1	25C33	67CZ	16.24
67CE1	25C33	67CD1	18.33	67CE1	25C33	67OH	30.78
67CZ	25C33	67CD1	31.64	67CZ	25C33	67OH	17.77
67CD1	25C33	67OH	48.37	160O	25C34	160C	9.85
160O	25C34	160CB	38.05	67CE1	25C34	67OH	31.14
67CE1	25C34	67CZ	15.25	67CE1	25C34	67CD1	15.11
67OH	25C34	67CZ	17.26	67OH	25C34	67CD1	45.96
67CZ	25C34	67CD1	29.18	160C	25C34	160CB	29.90
67CE1	25C35	67OH	32.70	67CE1	25C35	209CD2	77.34
67CE1	25C35	67CZ	14.99	67CE1	25C35	67CD1	16.08
67CE1	25C35	209CD1	77.10	67OH	25C35	67CZ	17.98
67OH	25C35	67CD1	48.74	67OH	25C35	209CD1	99.59
209CD2	25C35	67CZ	92.22	209CD2	25C35	67CD1	62.32
209CD2	25C35	160O	97.37	209CD2	25C35	160CB	70.82
209CD2	25C35	209CD1	31.32	67CZ	25C35	67CD1	30.87
67CZ	25C35	209CD1	88.81	67CD1	25C35	209CD1	67.63
160O	25C35	160CB	37.56	160CB	25C35	209CD1	83.17
160O	25N36	160CB	39.26	160O	25N36	160CD1	70.13
160O	25N36	160CG	56.11	160CB	25N36	160CD1	30.89
160CB	25N36	160CG	18.76	160CD1	25N36	160CG	18.07

TABLE XIX

67CE1	25N36	67OH	27.00	160O	25C37	160CB	42.20
160O	25C37	160N	37.40	160O	25C37	160C	10.47
160O	25C37	160CA	28.50	160O	25C37	160CG	58.56
160O	25C37	158O	81.42	160CB	25C37	160N	31.80
160CB	25C37	160C	31.91	160CB	25C37	160CA	18.43
160CB	25C37	160CG	17.89	160CB	25C37	158O	70.66
160N	25C37	160C	30.12	160N	25C37	160CA	17.61
160N	25C37	160CG	36.16	160N	25C37	158O	47.06
160C	25C37	160CA	18.39	160C	25C37	160CG	48.09
160C	25C37	158O	76.49	160CA	25C37	160CG	31.12
160CA	25C37	158O	63.78	160CG	25C37	158O	60.96
160O	25N38	160C	7.90	160O	25N38	160CB	39.77
160O	25N38	160N	32.65	160O	25N38	160CA	24.13
160C	25N38	160CB	32.02	160C	25N38	160N	29.52
160C	25N38	160CA	17.57	160CB	25N38	160N	29.89
160CB	25N38	160CA	18.19	160N	25N38	160CA	17.29

019786

TABLE XX

Table of distances in Ångstroms between atoms of the inhibitor and protein for all protein atoms within 5 Ångstroms of the inhibitor 3(S)-3-[(N-benzyloxycarbonyl)-L-leucinyl]amino-5-methyl-1-(1-propoxy)-2-hexanone.

Atom 1	Atom 2	Dist.	Atom 1	Atom 2	Dist.	Atom 1	Atom 2	Dist.
25C1	242OH2	3.097	25C1	18OD1	3.745	25C1	184CB	3.754
25C1	184CA	3.830	25C1	18ND2	3.916	25C1	184O	3.932
25C1	184CG	3.975	25C1	184CD1	4.022	25C1	18CG	4.158
25C1	184C	4.165	25C1	184CD2	4.830	25C1	184NE1	4.840
25C1	20O	4.895	25C2	18OD1	2.946	25C2	184CD1	3.510
25C2	184CA	3.592	25C2	18CG	3.620	25C2	20N	3.785
25C2	18ND2	3.842	25C2	184CB	3.886	25C2	242OH2	3.894
25C2	184CG	3.897	25C2	20O	3.948	25C2	183O	4.106
25C2	184C	4.198	25C2	19CG	4.207	25C2	20CA	4.229
25C2	19N	4.334	25C2	184O	4.367	25C2	184NE1	4.377
25C2	20C	4.510	25C2	184N	4.678	25C2	19C	4.809
25C2	18CB	4.827	25C2	183C	4.828	25C2	18CA	4.864
25C2	18C	4.870	25C2	184CD2	4.940	25C2	19CA	4.979
25C3	20O	2.991	25C3	184CD1	3.420	25C3	19CG	3.460
25C3	20N	3.592	25C3	18OD1	3.738	25C3	20C	3.852
25C3	184NE1	3.896	25C3	20CA	4.002	25C3	184CG	4.180
25C3	19CD	4.295	25C3	19C	4.443	25C3	19N	4.455
25C3	184CA	4.500	25C3	183O	4.509	25C3	19CB	4.596
25C3	184CB	4.635	25C3	18CG	4.662	25C3	19OE1	4.690
25C3	19CA	4.707	25C3	184CE2	4.837	25C3	242OH2	4.986
25C4	20O	3.250	25C4	184CD1	3.862	25C4	184NE1	3.932
25C4	20C	4.284	25C4	19CG	4.378	25C4	184CG	4.519
25C4	184CE2	4.630	25C4	20N	4.702	25C4	20CA	4.823
25C4	19CD	4.851	25C4	21NE2	4.914	25C4	18OD1	4.958
25C4	184CD2	4.971	25C5	184CD1	4.323	25C5	20O	4.342
25C5	184NE1	4.439	25C5	184CG	4.577	25C5	184CE2	4.766
25C5	242OH2	4.835	25C5	184CD2	4.858	25C5	21NE2	4.951

TABLE XX

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25C6	242OH2	3.703	25C6	184CG	4.325	25C6	184CD1	4.403
25C6	184CB	4.414	25C6	184CD2	4.792	25C6	184NE1	4.871
25C6	184CA	4.873	25C6	18OD1	4.955	25C6	184O	4.967
25C7	20O	3.169	25C7	184NE1	4.191	25C7	20C	4.372
25C7	19CG	4.412	25C7	19CD	4.508	25C7	184CD1	4.544
25C7	19NE2	4.715	25C7	19OE1	4.899	25C7	184CE2	4.927
25O8	184NE1	3.443	25O8	19CD	3.459	25O8	19NE2	3.624
25O8	19OE1	3.712	25O8	19CG	3.802	25O8	20O	3.894
25O8	184CD1	4.085	25O8	184CE2	4.312	25O8	22O	4.666
25O8	184CZ2	4.747	25C9	19NE2	3.833	25C9	184NE1	3.925
25C9	19CD	3.963	25C9	19OE1	4.023	25C9	184CE2	4.572
25C9	184CZ2	4.604	25C9	19CG	4.740	25C9	184CD1	4.906
25C9	22O	4.956	25O10	19NE2	3.975	25O10	23CA	4.264
25O10	19CD	4.483	25O10	22O	4.554	25O10	23N	4.718
25O10	19OE1	4.724	25O10	22C	4.857	25C11	162ND1	3.919
25C11	184CZ2	3.933	25C11	162CE1	4.435	25C11	184NE1	4.520
25C11	184CE2	4.600	25C11	162CG	4.656	25C11	184CH2	4.932
25C11	162CB	4.962	25C13	138OG	4.932	25C15	138OG	3.572
25C15	138CB	4.696	25C15	138CA	4.824	25C15	161OD1	4.950
25C16	162ND1	3.171	25C16	161O	3.822	25C16	162CG	3.975
25C16	162CE1	4.007	25C16	162CB	4.112	25C16	25SG	4.187
25C16	162CA	4.258	25C16	161C	4.677	25C16	184CZ2	4.751
25C16	25CB	4.882	25C16	162N	4.893	25C16	19OE1	4.906
25O17	162ND1	2.637	25O17	162CB	2.951	25O17	161O	3.023
25O17	162CG	3.092	25O17	162CA	3.124	25O17	161C	3.669
25O17	162N	3.731	25O17	162CE1	3.755	25O17	25SG	4.071
25O17	161OD1	4.274	25O17	162CD2	4.298	25O17	162C	4.467
25O17	162NE2	4.594	25O17	184CZ2	4.770	25O17	163N	4.786
25O17	25CB	4.931	25O17	161CA	4.957	25O17	161CB	4.964
25N18	25SG	3.671	25N18	162ND1	3.834	25N18	161O	3.966
25N18	25CB	4.503	25N18	19NE2	4.507	25N18	23CA	4.510
25N18	162CE1	4.582	25N18	162CA	4.791	25N18	19OE1	4.810
25N18	162CG	4.836	25N18	162CB	4.998	25C19	25SG	2.829
25C19	161O	3.274	25C19	162ND1	4.108	25C19	25CB	4.147
25C19	162CA	4.350	25C19	161C	4.428	25C19	23CA	4.502

TABLE XX

25C19	23O	4.704	25C19	23C	4.758	25C19	162N	4.907
25C19	25N	4.915	25C19	19NE2	4.957	25C19	163N	4.992
25C19	162CE1	4.994	25C19	162CB	4.997	25C20	161O	3.580
25C20	25SG	4.069	25C20	23CA	4.393	25C20	23O	4.523
25C20	23C	4.786	25C20	161C	4.808	25C21	161O	3.316
25C21	161C	4.462	25C22	161O	2.892	25C22	161C	3.848
25C22	161CA	4.121	25C22	161CB	4.359	25C23	64O	4.590
25C23	161O	4.811	25N24	184NE1	3.412	25N24	184CZ2	3.492
25N24	184CE2	3.750	25N24	19OE1	4.106	25N24	162ND1	4.147
25N24	162CE1	4.221	25N24	19CD	4.432	25N24	19NE2	4.515
25N24	184CD1	4.633	25N24	184CH2	4.684	25C25	25SG	1.822
25C25	25CB	3.054	25C25	25N	3.471	25C25	23O	3.687
25C25	25CA	3.792	25C25	23C	3.793	25C25	23CA	3.994
25C25	19NE2	4.214	25C25	162ND1	4.271	25C25	161O	4.312
25C25	24N	4.350	25C25	26N	4.445	25C25	25C	4.500
25C25	24C	4.578	25C25	163N	4.693	25C25	19OE1	4.797
25C25	162CA	4.833	25C25	162CE1	4.899	25C25	24CA	4.928
25C25	19CD	4.983	25O26	25SG	2.496	25O26	25N	2.842
25O26	23C	2.922	25O26	25CB	2.985	25O26	23CA	3.053
25O26	19NE2	3.071	25O26	23O	3.183	25O26	24N	3.337
25O26	25CA	3.477	25O26	24C	3.898	25O26	19CD	3.997
25O26	19OE1	4.054	25O26	24CA	4.110	25O26	23N	4.413
25O26	22O	4.471	25O26	25C	4.502	25O26	26N	4.555
25O26	162ND1	4.591	25O26	22C	4.912	25O26	162CE1	4.933
25C27	25SG	2.646	25C27	23O	3.049	25C27	23C	3.646
25C27	25N	3.830	25C27	65CA	3.894	25C27	25CB	4.015
25C27	26CD1	4.040	25C27	26N	4.152	25C27	23CA	4.158
25C27	25CA	4.348	25C27	24N	4.411	25C27	24C	4.634
25C27	25C	4.654	25C27	161O	4.714	25C27	65N	4.725
25C27	26CB	4.746	25C27	66N	4.758	25C27	24CA	4.780
25C27	26CG	4.815	25C27	65C	4.906	25O28	25SG	3.234
25O28	65CA	3.931	25O28	161O	3.970	25O28	23O	4.277
25O28	66N	4.333	25O28	66O	4.402	25O28	26CD1	4.553
25O28	65C	4.712	25O28	26N	4.830	25O28	26CB	4.858
25O28	161C	4.903	25O28	25CB	4.910	25O28	163N	4.929

TABLE XX

25C29	66O	3.071	25C29	66N	3.131	25C29	65CA	3.415
25C29	65C	3.768	25C29	66C	4.000	25C29	26CD1	4.084
25C29	66CA	4.184	25C29	26CB	4.278	25C29	25SG	4.306
25C29	26CG	4.529	25C29	23O	4.746	25C29	65N	4.756
25C29	161O	4.948	25C29	65O	4.978	25C29	26N	4.985
25C30	66O	3.147	25C30	66N	3.696	25C30	66C	4.040
25C30	65CA	4.366	25C30	66CA	4.428	25C30	65C	4.461
25C30	161O	4.799	25C31	66O	3.488	25C31	161O	4.535
25C31	66C	4.544	25C31	161C	4.739	25C31	66N	4.865
25C31	163CB	4.886	25C31	160O	4.980			

TABLE XXI

Table of distances in Ångstroms between atoms of the inhibitor and protein for all protein atoms within 5 Ångstroms of the inhibitor bis-(Cbz-leucinyl)-1,3-diamino-propan-2-one.

Atom 1	Atom 2	Dist.	Atom 1	Atom 2	Dist.	Atom 1	Atom 2	Dist.
25C1	184CB	3.966	25C1	184CG	4.092	25C1	18OD1	4.178
25C1	184CD1	4.335	25C1	184CA	4.489	25C1	184CD2	4.689
25C1	184O	4.748	25C1	184C	4.857	25C2	18OD1	3.023
25C2	184CD1	4.012	25C2	184CB	4.046	25C2	184CA	4.130
25C2	184CG	4.135	25C2	18CG	4.154	25C2	20O	4.291
25C2	20N	4.526	25C2	184C	4.608	25C2	18ND2	4.696
25C2	20CA	4.804	25C2	184NE1	4.825	25C2	184O	4.835
25C2	20C	4.924	25C2	19CG	4.976	25C3	20O	3.073
25C3	18OD1	3.568	25C3	20C	3.908	25C3	20N	3.934
25C3	184CD1	3.954	25C3	20CA	4.129	25C3	19CG	4.226
25C3	184CG	4.484	25C3	184NE1	4.490	25C3	18CG	4.696
25C3	184CB	4.795	25C3	184CA	4.856	25C3	19C	4.885
25C3	19CD	4.898	25C4	20O	3.345	25C4	184CD1	4.222
25C4	184NE1	4.344	25C4	20C	4.381	25C4	184CG	4.772
25C4	19CG	4.838	25C4	184CE2	4.948	25C4	18OD1	4.956
25C4	20N	4.984	25C5	184CD1	4.521	25C5	184NE1	4.550
25C5	20O	4.685	25C5	184CG	4.727	25C5	184CE2	4.764
25C5	184CD2	4.873	25C6	184CG	4.403	25C6	184CD1	4.580
25C6	184CD2	4.609	25C6	184CB	4.657	25C6	184NE1	4.884
25C6	184CE2	4.906	25C7	20O	2.849	25C7	20C	4.026
25C7	184NE1	4.648	25C7	21CA	4.664	25C7	19CD	4.697
25C7	19CG	4.714	25C7	21OE1	4.738	25C7	21N	4.799
25C7	184CD1	4.844	25C7	19OE1	4.907	25C7	19NE2	4.961
25O8	20O	3.212	25O8	19CD	3.453	25O8	19OE1	3.622
25O8	19NE2	3.664	25O8	19CG	3.806	25O8	184NE1	3.870
25O8	184CD1	4.265	25O8	20C	4.432	25O8	22O	4.540
25O8	184CE2	4.808	25O8	19CB	4.983	25C9	19OE1	3.889
25C9	19NE2	3.915	25C9	19CD	3.947	25C9	184NE1	4.155
25C9	20O	4.391	25C9	19CG	4.723	25C9	22O	4.796

TABLE XXI

25C9	184CE2	4.909	25C9	184CD1	4.929	25O10	19NE2	4.578
25O10	20O	4.660	25O10	22O	4.792	25O10	19CD	4.890
25O10	19OE1	4.963	25C11	162ND1	4.101	25C11	184CZ2	4.175
25C11	184NE1	4.284	25C11	162CE1	4.319	25C11	19OE1	4.351
25C11	184CE2	4.593	25C11	162CG	4.929	25C11	19NE2	4.945
25C11	19CD	4.953	25C15	184CZ2	4.332	25C15	184CH2	4.756
25C15	143OE1	4.901	25C15	137O	4.938	25C16	162ND1	3.174
25C16	162CE1	3.757	25C16	162CG	4.082	25C16	25SG	4.189
25C16	161O	4.344	25C16	19OE1	4.427	25C16	162CB	4.457
25C16	162CA	4.770	25C16	162NE2	4.792	25C16	19NE2	4.868
25C16	184CZ2	4.883	25C16	25CB	4.955	25C16	184NE1	4.957
25C16	162CD2	4.977	25O17	162ND1	2.574	25O17	162CG	3.155
25O17	162CB	3.298	25O17	162CE1	3.479	25O17	161O	3.597
25O17	162CA	3.711	25O17	25SG	4.141	25O17	161C	4.187
25O17	162CD2	4.194	25O17	162N	4.282	25O17	162NE2	4.329
25O17	161OD1	4.530	25O17	184CZ2	4.752	25O17	137CB	4.842
25N18	25SG	3.590	25N18	162ND1	3.689	25N18	162CE1	4.248
25N18	161O	4.291	25N18	19NE2	4.292	25N18	19OE1	4.452
25N18	25CB	4.467	25N18	23CA	4.557	25N18	162CG	4.791
25N18	19CD	4.816	25C19	25SG	2.732	25C19	161O	3.385
25C19	162ND1	3.772	25C19	25CB	4.081	25C19	162CA	4.451
25C19	161C	4.513	25C19	162CE1	4.560	25C19	23CA	4.589
25C19	25N	4.775	25C19	23C	4.776	25C19	23O	4.793
25C19	162CG	4.797	25C19	19NE2	4.876	25C19	162CB	4.935
25C19	162N	4.994	25N20	184NE1	3.387	25N20	19OE1	3.405
25N20	19CD	3.866	25N20	184CE2	4.004	25N20	19NE2	4.021
25N20	184CZ2	4.036	25N20	162CE1	4.357	25N20	184CD1	4.441
25N20	162ND1	4.565	25N20	19CG	4.876	25C21	25SG	1.768
25C21	25CB	2.961	25C21	25N	3.320	25C21	25CA	3.665
25C21	23O	3.874	25C21	23C	3.876	25C21	162ND1	3.978
25C21	23CA	4.127	25C21	19NE2	4.215	25C21	26N	4.241
25C21	24N	4.308	25C21	161O	4.319	25C21	25C	4.400
25C21	24C	4.472	25C21	162CE1	4.510	25C21	19OE1	4.818
25C21	24CA	4.852	25C21	163N	4.871	25C21	162CA	4.898
25C21	19CD	4.974	25C21	26CD1	4.991	25O22	25SG	2.461
25O22	25N	2.747	25O22	25CB	2.888	25O22	19NE2	3.089

TABLE XXI

25O22	23C	3.118	25O22	23CA	3.281	25O22	25CA	3.369
25O22	24N	3.372	25O22	23O	3.479	25O22	24C	3.834
25O22	19CD	4.008	25O22	19OE1	4.090	25O22	24CA	4.106
25O22	22O	4.311	25O22	162ND1	4.396	25O22	25C	4.432
25O22	26N	4.446	25O22	23N	4.563	25O22	162CE1	4.605
25O22	22C	4.909	25O22	24O	4.940	25C23	160O	4.313
25C23	67OH	4.425	25C23	67CE1	4.574	25C23	160CB	4.873
25C24	160O	3.278	25C24	160CB	4.082	25C24	160C	4.283
25C24	67CE1	4.352	25C24	209CD2	4.555	25C24	160CA	4.652
25C24	67OH	4.750	25C24	160N	4.847	25C25	160O	3.120
25C25	160C	4.287	25C25	67CE1	4.346	25C25	67OH	4.617
25C25	160CB	4.802	25C25	67CZ	4.867	25C26	160O	4.072
25C26	67OH	4.149	25C26	67CE1	4.572	25C26	67CZ	4.684
25C27	67OH	3.768	25C27	67CZ	4.663	25C27	67CE1	4.776
25C27	160O	4.939	25C28	67OH	3.920	25C28	67CE1	4.781
25C28	67CZ	4.836	25C29	160O	4.671	25C29	67OH	4.760
25O30	275OH2	4.167	25O30	160O	4.205	25O30	161CA	4.860
25C31	160O	3.769	25C31	161CA	4.036	25C31	161O	4.057
25C31	275OH2	4.224	25C31	161C	4.371	25C31	160C	4.689
25C31	161N	4.855	25C31	161CB	4.868	25O32	160O	2.767
25O32	161CA	2.883	25O32	161O	3.281	25O32	161C	3.329
25O32	160C	3.543	25O32	161N	3.634	25O32	161CB	3.892
25O32	162N	4.376	25O32	160CA	4.974	25O32	275OH2	4.982
25C33	161O	3.671	25C33	66O	4.037	25C33	161C	4.309
25C33	66N	4.440	25C33	275OH2	4.717	25C33	161CA	4.785
25C33	65CA	4.801	25C34	66O	2.806	25C34	66C	3.890
25C34	66N	4.077	25C34	26CB	4.273	25C34	66CA	4.590
25C34	161O	4.797	25C34	67N	4.862	25C34	26CG	4.869
25C34	163CB	4.955	25C35	66O	3.565	25C35	209CD2	4.310
25C35	134CB	4.451	25C35	163CB	4.577	25C35	66C	4.668
25C35	67CD1	4.755	25C35	163N	4.786	25C35	68SD	4.819
25C35	160O	4.923	25C35	26CB	4.937	25C35	161O	4.979
25C36	161C	3.690	25C36	161O	3.856	25C36	162N	3.868
25C36	134CB	3.869	25C36	160O	3.882	25C36	163N	3.971
25C36	161CA	4.066	25C36	162C	4.114	25C36	160C	4.145
25C36	161N	4.238	25C36	162CA	4.327	25C36	163CA	4.508

TABLE XXI

25C36	163CB	4.528	25C36	162O	4.616	25C36	209CD2	4.772
25C36	160CB	4.841	25C36	134CA	4.905	25C36	66O	4.996
25C37	209CD2	3.499	25C37	67CD1	3.574	25C37	67CE1	3.696
25C37	66O	3.889	25C37	67CG	4.551	25C37	160O	4.714
25C37	67CZ	4.732	25C37	66C	4.737	25C37	134CB	4.814
25C37	67CA	4.821	25C37	209CG	4.994	25C38	65CA	3.869
25C38	161O	3.955	25C38	66N	4.001	25C38	66O	4.219
25C38	26CD1	4.264	25C38	25SG	4.271	25C38	275OH2	4.287
25C38	65C	4.487	25C38	23O	4.627	25C38	26CB	4.655
25C38	26CG	4.792	25C38	64O	4.873	25C38	161C	4.899
25C38	65N	4.993	25O39	65CA	2.703	25O39	66N	3.332
25O39	65C	3.531	25O39	275OH2	3.677	25O39	64O	3.733
25O39	65N	3.795	25O39	26CD1	4.043	25O39	23O	4.088
25O39	64C	4.155	25O39	66O	4.358	25O39	66CA	4.647
25O39	65O	4.732	25O39	26CG	4.801	25O39	26NE1	4.806
25O39	161O	4.910	25O39	66C	4.976	25N40	25SG	2.943
25N40	161O	3.660	25N40	26CD1	4.126	25N40	26N	4.248
25N40	23O	4.287	25N40	26CB	4.350	25N40	163N	4.551
25N40	25CB	4.560	25N40	26CG	4.646	25N40	161C	4.657
25N40	25N	4.685	25N40	65CA	4.705	25N40	66O	4.809
25N40	162CA	4.847	25N40	26CA	4.856	25N40	66N	4.876
25N40	23C	4.933	25N40	163CB	4.949	25N40	25CA	4.979
25N40	25C	4.984	25C41	25SG	2.569	25C41	23O	3.094
25C41	25N	3.498	25C41	23C	3.558	25C41	26CD1	3.732
25C41	26N	3.810	25C41	25CB	3.828	25C41	25CA	4.081
25C41	23CA	4.144	25C41	24N	4.195	25C41	24C	4.371
25C41	25C	4.413	25C41	26CB	4.509	25C41	26CG	4.528
25C41	24CA	4.533	25C41	161O	4.584	25C41	65CA	4.716
25C41	26NE1	4.762	25C41	26CA	4.764	25N42	275OH2	3.989
25N42	161O	4.257	25N42	66N	4.573	25N42	66O	4.641
25N42	65CA	4.726	25N42	161C	4.818	25N42	160O	4.862
25N42	161CA	4.871						

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TABLE XXII

Table of distances in Ångstroms between atoms of the inhibitor and protein for all protein atoms within 5 Ångstroms of the inhibitor 2,2'-N,N'-bis-benzyloxycarbonyl-L-leucinylcarbohydrazide.

Atom 1	Atom 2	Dist.	Atom 1	Atom 2	Dist.	Atom 1	Atom 2	Dist.
25C1	184CB	4.217	25C1	184O	4.458	25C1	184CG	4.534
25C1	184CD2	4.719	25C1	184CE3	4.742	25C1	188CD1	4.982
25C2	184O	3.589	25C2	184CB	3.931	25C2	18OD1	4.344
25C2	184C	4.365	25C2	184CA	4.384	25C2	184CG	4.474
25C3	18OD1	3.467	25C3	184CB	3.731	25C3	184O	3.805
25C3	184CA	3.925	25C3	184CG	4.004	25C3	184C	4.224
25C3	184CD1	4.243	25C3	18CG	4.424	25C3	18ND2	4.653
25C3	184CD2	4.783	25C3	20O	4.954	25C4	184CG	3.557
25C4	184CD1	3.557	25C4	184CB	3.839	25C4	184NE1	4.069
25C4	184CD2	4.096	25C4	184CA	4.267	25C4	18OD1	4.278
25C4	184CE2	4.376	25C4	20O	4.406	25C4	184O	4.793
25C4	184CE3	4.895	25C4	184C	4.990	25C5	184CG	3.622
25C5	184CD2	3.653	25C5	184CD1	3.870	25C5	184CE2	3.925
25C5	184NE1	4.046	25C5	184CB	4.116	25C5	184CE3	4.153
25C5	184CZ2	4.632	25C5	184CZ3	4.798	25C5	184CA	4.969
25C6	184CD2	4.011	25C6	184CE3	4.065	25C6	184CG	4.134
25C6	184CB	4.303	25C6	184CE2	4.616	25C6	184CZ3	4.700
25C6	184CD1	4.765	25C7	20O	3.159	25C7	184CD1	3.353
25C7	19CG	3.702	25C7	184NE1	3.716	25C7	184CG	3.910
25C7	20C	4.053	25C7	20N	4.098	25C7	18OD1	4.206
25C7	19CD	4.236	25C7	20CA	4.370	25C7	184CE2	4.426
25C7	184CB	4.474	25C7	19NE2	4.497	25C7	184CD2	4.546
25C7	184CA	4.592	25C7	183O	4.805	25C7	19OE1	4.886
25C7	19C	4.994	25O8	20O	2.990	25O8	20C	4.056
25O8	184NE1	4.178	25O8	184CD1	4.264	25O8	19CG	4.312
25O8	19NE2	4.344	25O8	19CD	4.511	25O8	184CE2	4.748
25O8	20CA	4.839	25O8	20N	4.842	25O8	184CG	4.873
25O8	21N	4.938	25O8	21CA	4.989	25C9	20O	3.137

TABLE XXII

25C9	19NE2	3.361	25C9	19CD	3.886	25C9	19CG	4.087
25C9	184NE1	4.190	25C9	20C	4.350	25C9	22O	4.421
25C9	184CD1	4.624	25C9	19OE1	4.690	25C9	22N	4.828
25C9	184CE2	4.870	25C9	21CA	4.905	25C9	21OE1	4.986
25O10	20O	2.532	25O10	19NE2	2.700	25O10	22O	3.220
25O10	19CD	3.446	25O10	19CG	3.596	25O10	22N	3.702
25O10	20C	3.735	25O10	22C	3.951	25O10	21CA	4.210
25O10	21C	4.416	25O10	21N	4.441	25O10	19OE1	4.463
25O10	22CA	4.519	25O10	19CB	4.714	25O10	20N	4.734
25O10	23N	4.741	25O10	20CA	4.838	25O10	184NE1	4.848
25O10	21OE1	4.906	25O10	23CA	4.996	25C11	19NE2	3.727
25C11	19CD	4.636	25C11	184NE1	4.779	25C11	22O	4.911
25C12	19NE2	3.752	25C12	22O	4.028	25C12	23CA	4.150
25C12	22C	4.246	25C12	23N	4.275	25C12	224OH2	4.684
25C12	22N	4.779	25C12	19CD	4.925	25C12	20O	4.975
25C13	21OE1	4.156	25C13	22N	4.627	25C13	22C	4.667
25C13	23N	4.712	25C13	22O	4.742	25C13	21C	4.914
25C13	23CA	4.953	25C14	22N	3.473	25C14	21C	3.659
25C14	22C	3.759	25C14	21OE1	3.793	25C14	23N	3.863
25C14	22CA	3.868	25C14	21CA	4.095	25C14	21O	4.118
25C14	22O	4.147	25C14	23CA	4.513	25C14	20O	4.765
25C14	21CB	4.851	25C14	21CD	4.885	25C15	21OE1	3.260
25C15	21CD	4.221	25C15	21NE2	4.650	25C15	21CA	4.882
25C15	20O	4.924	25C16	19NE2	3.267	25C16	19CD	4.074
25C16	162ND1	4.145	25C16	19OE1	4.238	25C16	162CE1	4.291
25C16	184NE1	4.295	25C16	184CZ2	4.540	25C16	184CE2	4.778
25C16	25SG	4.792	25C16	23CA	4.932	25C16	22O	4.976
25O17	19NE2	3.075	25O17	184NE1	3.183	25O17	162CE1	3.232
25O17	162ND1	3.349	25O17	19OE1	3.394	25O17	19CD	3.490
25O17	184CZ2	3.632	25O17	184CE2	3.732	25O17	162NE2	4.167
25O17	162CG	4.366	25O17	184CD1	4.379	25O17	25CB	4.553
25O17	25SG	4.612	25O17	19CG	4.742	25O17	162CD2	4.779
25O17	184CH2	4.923	25N18	19NE2	3.859	25N18	25SG	4.056
25N18	162ND1	4.100	25N18	161O	4.319	25N18	23CA	4.407
25N18	224OH2	4.562	25N18	162CE1	4.601	25N18	19CD	4.788
25N18	25CB	4.834	25N18	19OE1	4.862	25N19	25SG	2.787

TABLE XXII

25N19	162ND1	3.174	25N19	161O	3.363	25N19	25CB	3.873
25N19	162CE1	3.953	25N19	162CA	4.146	25N19	162CG	4.165
25N19	19NE2	4.334	25N19	162CB	4.414	25N19	161C	4.448
25N19	23CA	4.774	25N19	162N	4.806	25N19	19OE1	4.807
25N19	224OH2	4.923	25N20	19NE2	3.800	25N20	184NE1	4.071
25N20	19CD	4.420	25N20	20O	4.457	25N20	184CE2	4.475
25N20	184CZ2	4.573	25N20	184CD1	4.849	25N20	19OE1	4.977
25N20	19CG	4.982	25C21	25SG	1.799	25C21	25CB	3.030
25C21	25N	3.707	25C21	162ND1	3.784	25C21	23CA	3.850
25C21	23C	3.907	25C21	23O	3.946	25C21	25CA	3.958
25C21	19NE2	4.007	25C21	161O	4.284	25C21	162CE1	4.379
25C21	224OH2	4.436	25C21	24N	4.507	25C21	19OE1	4.543
25C21	162CA	4.728	25C21	19CD	4.730	25C21	26N	4.758
25C21	25C	4.830	25C21	24C	4.870	25C21	162CG	4.947
25C21	163N	4.989	25O22	25SG	2.443	25O22	19NE2	2.871
25O22	25CB	2.954	25O22	23CA	3.128	25O22	25N	3.144
25O22	23C	3.258	25O22	25CA	3.641	25O22	24N	3.649
25O22	23O	3.656	25O22	19CD	3.696	25O22	19OE1	3.727
25O22	22O	4.038	25O22	162ND1	4.175	25O22	24C	4.265
25O22	23N	4.327	25O22	162CE1	4.422	25O22	224OH2	4.423
25O22	24CA	4.529	25O22	22C	4.622	25O22	25C	4.800
25O22	26N	4.898	25C23	61OD1	3.673	25C23	59O	3.735
25C23	67CE2	4.205	25C23	67CD2	4.463	25C23	264OH2	4.473
25C23	61CG	4.499	25C23	61OD2	4.706	25C23	59C	4.887
25C24	59O	3.179	25C24	61OD1	3.691	25C24	67CD2	3.717
25C24	60ND2	3.736	25C24	67CE2	3.832	25C24	60CA	3.942
25C24	59C	4.226	25C24	61CG	4.362	25C24	66CA	4.399
25C24	60C	4.521	25C24	61N	4.525	25C24	60N	4.567
25C24	70OD1	4.595	25C24	61OD2	4.702	25C24	60CG	4.710
25C24	60CB	4.837	25C24	67N	4.915	25C24	66C	4.929
25C24	65O	4.975	25C24	67CG	4.986	25C25	66CA	3.301
25C25	61OD1	3.379	25C25	67CD2	3.477	25C25	67CE2	3.538
25C25	60ND2	3.834	25C25	66N	3.859	25C25	65O	3.860
25C25	66C	3.977	25C25	65C	4.082	25C25	60CA	4.110
25C25	61CG	4.139	25C25	61N	4.153	25C25	59O	4.235
25C25	67N	4.302	25C25	60C	4.526	25C25	60CG	4.585

TABLE XXII

25C25	66O	4.675	25C25	60CB	4.701	25C25	61CB	4.755
25C25	67CG	4.785	25C25	61OD2	4.825	25C25	67CZ	4.879
25C26	61OD1	3.031	25C26	67CE2	3.662	25C26	66CA	3.882
25C26	66N	3.954	25C26	65O	4.020	25C26	65C	4.027
25C26	67CD2	4.058	25C26	61CG	4.066	25C26	66C	4.566
25C26	61CB	4.672	25C26	61N	4.764	25C26	67CZ	4.811
25C26	65CA	4.818	25C26	61OD2	4.956	25C26	66O	4.959
25C27	61OD1	3.004	25C27	67CE2	4.045	25C27	61CG	4.208
25C27	67CD2	4.744	25C27	61OD2	4.951	25C27	67OH	4.988
25C28	61OD1	3.343	25C28	67CE2	4.306	25C28	61CG	4.423
25C28	264OH2	4.506	25C28	61OD2	4.829	25C28	67CD2	4.927
25C29	66N	3.077	25C29	65C	3.103	25C29	65O	3.481
25C29	66CA	3.531	25C29	65CA	3.578	25C29	61OD1	3.662
25C29	67CE2	4.189	25C29	64O	4.192	25C29	66C	4.265
25C29	66O	4.382	25C29	65N	4.522	25C29	67CD2	4.589
25C29	61CG	4.593	25C29	64C	4.738	25C29	61CB	4.762
25O30	66N	3.458	25O30	67CE2	3.803	25O30	65C	3.840
25O30	66O	4.008	25O30	66CA	4.009	25O30	65CA	4.053
25O30	66C	4.287	25O30	67CD2	4.421	25O30	67CZ	4.431
25O30	67OH	4.470	25O30	65O	4.551	25O30	64O	4.750
25C31	66N	3.498	25C31	65CA	3.654	25C31	65C	3.885
25C31	66O	4.018	25C31	66CA	4.416	25C31	64O	4.463
25C31	66C	4.608	25C31	65O	4.872	25C31	67CE2	4.874
25C31	65N	4.883	25O32	65CA	3.690	25O32	64O	3.833
25O32	66N	4.273	25O32	65C	4.343	25O32	64C	4.667
25O32	65N	4.681	25C33	66O	3.876	25C33	66N	4.173
25C33	161O	4.383	25C33	65CA	4.417	25C33	161C	4.670
25C33	25SG	4.802	25C33	65C	4.843	25C33	66C	4.902
25C34	66O	3.833	25C34	161C	4.228	25C34	161O	4.287
25C34	162N	4.305	25C34	163N	4.452	25C34	162CA	4.613
25C34	162C	4.644	25C34	25SG	4.656	25C34	161CA	4.669
25C34	163CB	4.789	25C34	66N	4.994	25C35	66O	2.981
25C35	66C	4.208	25C35	163CB	4.767	25C35	26CB	4.871
25C35	66N	4.887	25C35	67CA	4.934	25C35	209CD2	4.958
25C35	68SD	4.962	25C35	67CD1	4.992	25C35	67CE1	5.000
25C36	66O	3.430	25C36	68SD	3.532	25C36	163CB	3.585

TABLE XXII

25C36	163CA	4.250	25C36	134CB	4.328	25C36	163N	4.364
25C36	26CB	4.411	25C36	68CE	4.444	25C36	209CD2	4.518
25C36	66C	4.580	25C36	67CA	4.718	25C36	162C	4.845
25C36	26CX	4.975	25C37	66O	3.900	25C37	67CE1	4.120
25C37	209CD2	4.133	25C37	67CZ	4.304	25C37	67CD1	4.472
25C37	67OH	4.559	25C37	160O	4.722	25C37	67CE2	4.812
25C37	134CB	4.928	25C37	67CG	4.960	25C38	65CA	3.685
25C38	25SG	3.703	25C38	66N	3.862	25C38	66O	4.169
25C38	26CD1	4.241	25C38	65C	4.328	25C38	23O	4.331
25C38	161O	4.500	25C38	224OH2	4.706	25C38	26CB	4.746
25C38	65N	4.855	25C38	26CG	4.876	25O39	66N	2.954
25O39	26CD1	3.044	25O39	65CA	3.072	25O39	65C	3.468
25O39	66O	3.555	25O39	23O	3.635	25O39	26CG	3.715
25O39	26CB	3.796	25O39	25SG	3.860	25O39	26NE1	4.093
25O39	66CA	4.102	25O39	66C	4.239	25O39	65N	4.292
25O39	26N	4.359	25O39	65O	4.668	25O39	23C	4.669
25O39	26CX	4.689	25O39	224OH2	4.850	25O39	26CD2	4.970
25N40	25SG	3.113	25N40	161O	3.678	25N40	224OH2	4.045
25N40	23O	4.202	25N40	65CA	4.334	25N40	161C	4.525
25N40	23C	4.779	25N40	23CA	4.821	25N40	162CA	4.878
25N40	25CB	4.902	25N40	26CD1	4.925	25N41	25SG	2.621
25N41	23O	3.122	25N41	224OH2	3.404	25N41	23C	3.447
25N41	23CA	3.458	25N41	25CB	4.118	25N41	25N	4.161
25N41	24N	4.403	25N41	65CA	4.453	25N41	161O	4.531
25N41	26CD1	4.572	25N41	25CA	4.709	25N41	26N	4.861
25N41	23N	4.898	25N42	66O	3.140	25N42	66N	3.340
25N42	65CA	3.978	25N42	66C	4.005	25N42	65C	4.084
25N42	66CA	4.168	25N42	67CE2	4.883			

TABLE XXIII

Table of distances in Ångstroms between atoms of the inhibitor and protein for all protein atoms within 5 Ångstroms of the inhibitor (1S)-N-[2-[(1-benzyloxycarbonylamino)-3-methylbutyl]thiazol-4-ylcarbonyl]-N'-(N-benzyloxycarbonyl-L-leucinyl)hydrazide.

Atom 1	Atom 2	Dist.	Atom 1	Atom 2	Dist.	Atom 1	Atom 2	Dist.
25C1	184CB	4.236	25C1	184CG	4.418	25C1	184O	4.425
25C1	184CD2	4.593	25C1	184CE3	4.660	25C1	188CD1	4.721
25C2	184O	3.268	25C2	184CB	3.689	25C2	184C	4.080
25C2	184CG	4.182	25C2	184CA	4.182	25C2	184CD2	4.784
25C2	184CD1	4.821	25C2	18ND2	4.999	25C3	184O	3.481
25C3	184CB	3.729	25C3	184CA	3.863	25C3	184C	3.967
25C3	18OD1	4.001	25C3	184CG	4.006	25C3	184CD1	4.249
25C3	18ND2	4.280	25C3	18CG	4.516	25C3	184CD2	4.834
25C4	184CD1	4.005	25C4	184CG	4.080	25C4	184CB	4.302
25C4	18OD1	4.440	25C4	20O	4.528	25C4	184CA	4.558
25C4	184NE1	4.584	25C4	184CD2	4.705	25C4	184O	4.729
25C4	184CE2	4.985	25C5	184CG	4.312	25C5	184CD1	4.376
25C5	184CD2	4.504	25C5	184NE1	4.612	25C5	184CE2	4.694
25C5	184CB	4.766	25C5	21NE2	4.820	25C6	184CD2	4.450
25C6	184CG	4.480	25C6	184CE3	4.643	25C6	184CB	4.744
25C6	143OE1	4.804	25C6	184CE2	4.925	25C6	184CD1	4.935
25C7	20O	3.040	25C7	20C	3.594	25C7	20CA	3.795
25C7	20N	3.853	25C7	18OD1	3.864	25C7	184CD1	4.135
25C7	19CG	4.463	25C7	21NE2	4.595	25C7	21N	4.617
25C7	184NE1	4.641	25C7	184CG	4.659	25C7	18CG	4.887
25C7	19C	4.937	25C7	184CA	4.958	25O8	20O	2.667
25O8	19CG	3.422	25O8	184CD1	3.450	25O8	20C	3.631
25O8	184NE1	3.675	25O8	20N	3.871	25O8	19CD	3.993
25O8	20CA	4.102	25O8	19OE1	4.232	25O8	184CG	4.325
25O8	18OD1	4.411	25O8	184CE2	4.622	25O8	19C	4.642
25O8	21N	4.725	25O8	19CB	4.727	25O8	19NE2	4.771
25O8	183O	4.826	25O8	184CD2	4.974	25C9	20O	3.188

TABLE XXIII

25C9	184NE1	3.536	25C9	184CD1	3.844	25C9	19CG	4.035
25C9	19CD	4.106	25C9	19OE1	4.229	25C9	20C	4.321
25C9	184CE2	4.325	25C9	19NE2	4.650	25C9	184CG	4.743
25C9	184CZ2	4.957	25C9	21NE2	4.999	25O10	184NE1	3.675
25O10	184CE2	4.068	25O10	184CD1	4.137	25O10	20O	4.244
25O10	184CZ2	4.481	25O10	184CD2	4.713	25O10	184CG	4.754
25O10	21NE2	4.824	25C11	19NE2	4.159	25C11	22O	4.229
25C11	19CD	4.273	25C11	20O	4.296	25C11	19OE1	4.447
25C11	184NE1	4.589	25C11	22C	4.735	25C11	23CA	4.867
25C11	19CG	4.868	25C11	22N	4.974	25C11	23N	4.979
25C12	22O	3.890	25C12	22C	3.995	25C12	22N	4.110
25C12	23N	4.111	25C12	23CA	4.306	25C12	20O	4.346
25C12	21C	4.588	25C12	22CA	4.594	25C12	21OE1	4.629
25C12	21CA	4.715	25C12	19NE2	4.762	25C13	21OE1	3.498
25C13	21CD	4.390	25C13	21CA	4.587	25C13	22N	4.615
25C13	21C	4.659	25C13	20O	4.898	25C13	21NE2	4.928
25C14	21OE1	2.922	25C14	21C	3.654	25C14	21CA	3.785
25C14	22N	3.919	25C14	21CD	3.931	25C14	21O	3.962
25C14	21CB	4.117	25C14	22CA	4.561	25C14	21CG	4.659
25C14	22C	4.749	25C14	21NE2	4.841	25C14	23N	4.886
25C14	20O	4.941	25C15	21OE1	2.917	25C15	21CD	3.612
25C15	21NE2	3.794	25C15	21CA	4.698	25C15	20O	4.791
25C15	21CG	4.892	25C16	19NE2	3.649	25C16	19OE1	3.851
25C16	19CD	3.913	25C16	23CA	4.390	25C16	184NE1	4.396
25C16	22O	4.401	25C16	162ND1	4.744	25C16	19CG	4.960
25C16	23N	4.963	25C16	22C	4.981	25C16	184CZ2	4.990
25S17	162ND1	3.565	25S17	184CZ2	3.585	25S17	184NE1	3.699
25S17	162CE1	3.945	25S17	19OE1	3.950	25S17	184CE2	3.994
25S17	162CG	4.327	25S17	19CD	4.502	25S17	19NE2	4.573
25S17	162CB	4.756	25S17	184CH2	4.771	25S17	162NE2	4.811
25S17	184CD1	4.996	25N18	19NE2	3.269	25N18	23CA	3.310
25N18	19CD	3.941	25N18	22O	3.976	25N18	19OE1	4.019
25N18	23C	4.156	25N18	25SG	4.177	25N18	23N	4.187
25N18	22C	4.455	25N18	25CB	4.460	25N18	24N	4.557
25N18	162ND1	4.710	25N18	25N	4.758	25N18	23O	4.840
25C19	25SG	3.024	25C19	25CB	3.565	25C19	19NE2	3.784

TABLE XXIII

25C19	162ND1	3.801	25C19	23CA	3.948	25C19	19OE1	4.215
25C19	161O	4.243	25C19	19CD	4.411	25C19	25N	4.416
25C19	23C	4.434	25C19	162CE1	4.494	25C19	25CA	4.626
25C19	23O	4.822	25C19	162CG	4.842	25C19	24N	4.896
25C19	162CA	4.932	25N20	20O	3.090	25N20	19CD	3.488
25N20	19NE2	3.690	25N20	19CG	3.707	25N20	19OE1	3.805
25N20	22O	3.918	25N20	184NE1	3.976	25N20	20C	4.316
25N20	184CD1	4.488	25N20	22N	4.551	25N20	22C	4.673
25N20	21CA	4.853	25N20	184CE2	4.906	25N20	19CB	4.997
25C21	162ND1	2.861	25C21	25SG	3.627	25C21	162CE1	3.661
25C21	162CG	3.744	25C21	161O	3.811	25C21	25CB	3.895
25C21	162CB	3.972	25C21	19OE1	4.135	25C21	162CA	4.169
25C21	19NE2	4.408	25C21	19CD	4.664	25C21	162NE2	4.724
25C21	161C	4.759	25C21	184CZ2	4.788	25C21	162CD2	4.789
25C21	184NE1	4.807	25C21	162N	4.963	25C22	25SG	1.806
25C22	25CB	3.017	25C22	25N	3.658	25C22	23CA	3.756
25C22	23C	3.777	25C22	23O	3.783	25C22	25CA	3.942
25C22	161O	4.202	25C22	19NE2	4.263	25C22	24N	4.389
25C22	162ND1	4.411	25C22	26N	4.767	25C22	24C	4.797
25C22	25C	4.896	25C22	162CA	4.914	25C22	26CD1	4.985
25O23	25SG	2.263	25O23	23C	2.724	25O23	25N	2.817
25O23	23CA	2.863	25O23	23O	2.953	25O23	25CB	2.966
25O23	24N	3.216	25O23	19NE2	3.371	25O23	25CA	3.468
25O23	24C	3.844	25O23	24CA	4.001	25O23	23N	4.229
25O23	22O	4.346	25O23	19CD	4.418	25O23	26N	4.527
25O23	25C	4.570	25O23	19OE1	4.594	25O23	26CD1	4.647
25O23	22C	4.750	25O23	162ND1	4.926	25O23	24O	4.984
25C24	64O	4.232	25C24	61OD1	4.886	25C25	64O	2.914
25C25	61OD1	4.012	25C25	64C	4.121	25C25	65CA	4.508
25C25	61CG	4.803	25C25	65N	4.812	25C26	64O	3.004
25C26	61OD1	3.284	25C26	65CA	3.778	25C26	65C	4.006
25C26	64C	4.052	25C26	66N	4.292	25C26	61CG	4.320
25C26	65N	4.406	25C26	65O	4.498	25C26	61CB	4.929
25C27	61OD1	3.654	25C27	64O	4.372	25C27	66N	4.515
25C27	67CE2	4.579	25C27	65C	4.592	25C27	65CA	4.693
25C27	61CG	4.839	25C27	67OH	4.900	25C28	61OD1	4.602

TABLE XXIII

25C28	67OH	4.614	25C28	67CE2	4.849	25C30	67CE2	3.326
25C30	66N	3.711	25C30	61OD1	3.817	25C30	66CA	3.888
25C30	67CD2	3.908	25C30	67CZ	4.039	25C30	65C	4.143
25C30	67OH	4.216	25C30	66C	4.303	25C30	66O	4.459
25C30	65O	4.648	25C30	65CA	4.662	25C30	67CG	4.980
25O31	67CE2	2.958	25O31	67CZ	3.233	25O31	67OH	3.437
25O31	67CD2	3.606	25O31	66O	3.722	25O31	66N	3.758
25O31	66C	3.942	25O31	66CA	3.994	25O31	67CE1	4.053
25O31	67CG	4.365	25O31	65C	4.521	25O31	67CD1	4.543
25O31	67N	4.754	25O31	65CA	4.909	25C32	66O	3.869
25C32	66N	3.875	25C32	67CZ	4.120	25C32	67OH	4.127
25C32	67CE2	4.188	25C32	66C	4.431	25C32	66CA	4.512
25C32	65CA	4.559	25C32	65C	4.577	25C32	67CE1	4.683
25C32	67CD2	4.797	25O33	67OH	4.349	25O33	67CZ	4.706
25O33	66N	4.896	25O33	67CE2	4.948	25O33	160O	4.987
25C34	66O	3.926	25C34	66N	4.154	25C34	161O	4.291
25C34	65CA	4.393	25C34	161C	4.680	25C34	25SG	4.728
25C34	160O	4.762	25C34	65C	4.835	25C34	66C	4.889
25C35	161O	3.923	25C35	160O	3.934	25C35	161C	3.950
25C35	66O	4.195	25C35	162N	4.296	25C35	161CA	4.330
25C35	163N	4.545	25C35	160C	4.652	25C35	25SG	4.661
25C35	162CA	4.717	25C35	161N	4.821	25C35	162C	4.844
25C36	66O	3.516	25C36	163CB	3.928	25C36	163N	4.123
25C36	163CA	4.451	25C36	134CB	4.614	25C36	162C	4.695
25C36	66C	4.739	25C36	25SG	4.777	25C36	160O	4.790
25C36	68SD	4.793	25C36	162N	4.890	25C36	161C	4.930
25C36	26CB	4.984	25C37	66O	3.229	25C37	67CD1	3.782
25C37	67CE1	3.814	25C37	209CD2	4.109	25C37	66C	4.351
25C37	134CB	4.449	25C37	67CG	4.461	25C37	67CZ	4.520
25C37	67CA	4.594	25C37	68SD	4.609	25C37	163CB	4.822
25C37	68CE	4.913	25C37	67N	4.944	25C37	160O	4.999
25C38	66O	2.883	25C38	163CB	3.258	25C38	26CB	3.517
25C38	25SG	3.915	25C38	163N	4.010	25C38	66C	4.045
25C38	26CA	4.069	25C38	26N	4.161	25C38	163CA	4.178
25C38	68SD	4.184	25C38	26CG	4.396	25C38	26CD1	4.512
25C38	66N	4.558	25C38	67CA	4.916	25C38	67N	4.916

TABLE XXIII

25C38	66CA	4.920	25C38	162C	4.937	25C39	65CA	3.532
25C39	25SG	3.557	25C39	66N	3.788	25C39	66O	4.161
25C39	161O	4.207	25C39	65C	4.218	25C39	26CD1	4.481
25C39	65N	4.664	25C39	161C	4.925	25C39	23O	4.951
25C39	66CA	4.972	25O40	66N	2.864	25O40	65CA	2.895
25O40	26CD1	3.289	25O40	65C	3.326	25O40	25SG	3.487
25O40	66O	3.497	25O40	66CA	4.034	25O40	26CG	4.074
25O40	65N	4.098	25O40	26NE1	4.177	25O40	66C	4.186
25O40	23O	4.205	25O40	26CB	4.291	25O40	65O	4.516
25O40	26N	4.644	25N41	25SG	3.236	25N41	161O	3.370
25N41	65CA	4.079	25N41	161C	4.343	25N41	23O	4.777
25N41	65N	4.879	25N41	66N	4.926	25N42	25SG	2.820
25N42	23O	3.597	25N42	23CA	3.792	25N42	23C	3.925
25N42	65CA	4.086	25N42	161O	4.156	25N42	25CB	4.397
25N42	65N	4.514	25N42	25N	4.705	25N42	26CD1	4.802
25N42	24N	4.905	25N43	66O	3.027	25N43	66N	3.312
25N43	66C	3.828	25N43	66CA	4.057	25N43	65CA	4.128
25N43	65C	4.171	25N43	67CZ	4.741	25N43	67CE2	4.807
25N43	67CE1	4.973	25N43	67N	4.980			

TABLE XXIV

Table of distances in Ångstroms between atoms of the inhibitor and protein for all protein atoms within 5 Ångstroms of the inhibitor 2-[N-(3-benzyloxybenzoyl)]-2'-[N'-(N-benzyloxycarbonyl-L-leucinyl)]carbohydrazide.

Atom 1	Atom 2	Dist.	Atom 1	Atom 2	Dist.	Atom 1	Atom 2	Dist.
25C1	241OH2	3.570	25C1	184CD1	3.752	25C1	184CB	3.771
25C1	184CG	3.795	25C1	184O	3.855	25C1	18OD1	3.918
25C1	184CA	3.940	25C1	18ND2	4.077	25C1	184C	4.295
25C1	18CG	4.335	25C1	20O	4.526	25C1	184NE1	4.545
25C1	184CD2	4.638	25C2	18OD1	2.991	25C2	184CD1	3.364
25C2	184CA	3.673	25C2	20O	3.682	25C2	18CG	3.691
25C2	184CG	3.828	25C2	20N	3.856	25C2	18ND2	3.872
25C2	184CB	3.927	25C2	184O	4.146	25C2	19CG	4.202
25C2	184C	4.236	25C2	184NE1	4.236	25C2	183O	4.241
25C2	20CA	4.325	25C2	20C	4.444	25C2	19N	4.506
25C2	184N	4.779	25C2	241OH2	4.781	25C2	19C	4.859
25C2	184CD2	4.882	25C2	183C	4.942	25C2	18CB	4.966
25C3	20O	2.766	25C3	184CD1	3.449	25C3	19CG	3.485
25C3	20N	3.566	25C3	18OD1	3.700	25C3	20C	3.715
25C3	184NE1	3.945	25C3	20CA	3.980	25C3	19CD	4.274
25C3	184CG	4.298	25C3	19C	4.413	25C3	183O	4.573
25C3	19N	4.586	25C3	184CA	4.627	25C3	19CB	4.636
25C3	18CG	4.663	25C3	19CA	4.734	25C3	19NE2	4.739
25C3	184CB	4.805	25C3	19OE1	4.890	25C3	21N	4.941
25C3	184CE2	4.965	25C4	20O	2.926	25C4	184CD1	3.912
25C4	184NE1	3.991	25C4	20C	4.103	25C4	19CG	4.382
25C4	20N	4.662	25C4	184CG	4.708	25C4	20CA	4.787
25C4	19CD	4.799	25C4	184CE2	4.822	25C4	18OD1	4.987
25C4	241OH2	4.989	25C4	19NE2	4.989	25C5	241OH2	3.832
25C5	20O	3.929	25C5	184CD1	4.241	25C5	184NE1	4.312
25C5	184CG	4.671	25C5	184CE2	4.778	25C5	184CD2	4.987
25C6	241OH2	2.940	25C6	184CD1	4.176	25C6	184CG	4.243
25C6	184CB	4.555	25C6	184NE1	4.583	25C6	20O	4.631

TABLE XXIV

25C6	184CD2	4.694	25C6	184CE2	4.889	25C7	20O	2.932
25C7	20C	4.097	25C7	19NE2	4.319	25C7	19CG	4.452
25C7	184NE1	4.478	25C7	19CD	4.533	25C7	21CA	4.627
25C7	22O	4.737	25C7	184CD1	4.756	25C7	21N	4.840
25C7	21C	4.925	25O8	19NE2	3.416	25O8	19CD	3.782
25O8	184NE1	3.951	25O8	20O	4.046	25O8	19CG	4.180
25O8	19OE1	4.351	25O8	22O	4.445	25O8	184CD1	4.559
25O8	184CE2	4.877	25C9	19NE2	4.211	25C9	184NE1	4.403
25C9	19CD	4.724	25C11	162ND1	4.502	25C11	184CZ2	4.687
25C11	162CE1	4.868	25C14	162ND1	3.357	25C14	162CG	3.831
25C14	162CB	4.001	25C14	162CE1	4.036	25C14	162CA	4.368
25C14	161O	4.489	25C14	184CZ2	4.614	25C14	162CD2	4.682
25C14	161OD1	4.720	25C14	162N	4.758	25C14	162NE2	4.766
25C14	161C	4.794	25C14	25SG	4.940	25O15	162CB	3.130
25O15	162ND1	3.165	25O15	162CG	3.174	25O15	161OD1	3.790
25O15	162CA	3.794	25O15	162CE1	3.969	25O15	162CD2	4.004
25O15	162N	4.125	25O15	184CZ2	4.191	25O15	162NE2	4.407
25O15	161C	4.425	25O15	161O	4.436	25O15	137CB	4.597
25O15	161CG	4.704	25O15	137O	4.758	25O15	161CB	4.862
25O15	184CH2	4.953	25N16	162ND1	3.293	25N16	25SG	3.828
25N16	161O	3.898	25N16	162CE1	4.030	25N16	162CG	4.119
25N16	162CA	4.252	25N16	162CB	4.323	25N16	161C	4.537
25N16	25CB	4.583	25N16	162N	4.723	25N16	19NE2	4.776
25N17	25SG	2.713	25N17	161O	2.829	25N17	162ND1	2.962
25N17	162CA	3.321	25N17	161C	3.640	25N17	162CG	3.800
25N17	162CB	3.840	25N17	162N	3.876	25N17	25CB	3.878
25N17	162CE1	3.946	25N17	163N	4.346	25N17	162C	4.395
25N17	161CA	4.922	25N17	162CD2	4.988	25C18	184NE1	4.080
25C18	19NE2	4.103	25C18	184CZ2	4.414	25C18	162ND1	4.448
25C18	162CE1	4.452	25C18	19CD	4.549	25C18	19OE1	4.597
25C18	184CE2	4.604	25C19	25SG	1.793	25C19	25CB	3.071
25C19	161O	3.652	25C19	162ND1	3.659	25C19	25N	4.072
25C19	25CA	4.137	25C19	23O	4.303	25C19	162CE1	4.350
25C19	162CA	4.352	25C19	19NE2	4.435	25C19	23C	4.511
25C19	163N	4.621	25C19	23CA	4.646	25C19	161C	4.687
25C19	162CG	4.766	25C19	19OE1	4.843	25C19	25C	4.879

TABLE XXIV

25C19	26N	4.949	25O20	25SG	2.529	25O20	25CB	3.171
25O20	19NE2	3.371	25O20	23CA	3.588	25O20	23C	3.681
25O20	25N	3.725	25O20	23O	3.770	25O20	162ND1	4.071
25O20	25CA	4.076	25O20	19OE1	4.231	25O20	19CD	4.248
25O20	24N	4.306	25O20	162CE1	4.450	25O20	161O	4.781
25O20	24C	4.875	25O20	23N	4.969	25C21	160CD1	3.590
25C21	158O	3.615	25C21	160CG	3.707	25C21	160CB	3.983
25C21	160N	4.442	25C21	158C	4.580	25C21	160CA	4.835
25C22	160CD1	3.593	25C22	160CG	4.157	25C22	160CB	4.282
25C22	209CD2	4.511	25C22	209CD1	4.980	25C22	158O	4.986
25C23	160CD1	4.157	25C23	209CD2	4.159	25C23	67CE1	4.205
25C23	160CB	4.279	25C23	160O	4.519	25C23	67OH	4.588
25C23	160CG	4.625	25C23	67CZ	4.894	25C24	160O	3.474
25C24	160CB	3.993	25C24	160C	4.419	25C24	160CA	4.596
25C24	160N	4.617	25C24	160CD1	4.665	25C24	160CG	4.704
25C24	67CE1	4.808	25C24	67OH	4.862	25C25	160O	3.271
25C25	160N	3.593	25C25	160CB	3.664	25C25	158O	3.952
25C25	160CA	3.958	25C25	160C	3.985	25C25	160CG	4.302
25C25	160CD1	4.653	25C25	159C	4.710	25C25	159CA	4.972
25C25	158C	4.995	25C26	158O	2.899	25C26	160N	3.477
25C26	160CB	3.661	25C26	160CG	3.791	25C26	158C	3.973
25C26	160CA	4.096	25C26	160CD1	4.159	25C26	160O	4.202
25C26	159C	4.497	25C26	159CA	4.565	25C26	160C	4.606
25C26	159N	4.714	25C26	158CA	4.955	25C27	160O	3.338
25C27	67OH	4.363	25C27	67CE1	4.376	25C27	160C	4.512
25C27	67CZ	4.684	25C27	160CB	4.754	25O28	160O	2.420
25O28	160C	3.644	25O28	161CA	4.394	25O28	160CB	4.473
25O28	161N	4.476	25O28	160CA	4.624	25O28	161O	4.916
25O28	161C	4.988	25C29	160O	3.266	25C29	160C	4.372
25C29	161O	4.438	25C29	161CA	4.632	25C29	161C	4.791
25C29	66O	4.888	25C29	67CE1	4.893	25C29	161N	4.959
25O30	67CE1	3.985	25O30	66O	4.035	25O30	67CD1	4.256
25O30	67CZ	4.313	25O30	160O	4.446	25O30	66C	4.682
25O30	67OH	4.687	25O30	67CG	4.823	25O30	67CE2	4.858
25C31	161O	3.206	25C31	161C	3.941	25C31	66O	3.994
25C31	163CB	4.458	25C31	163N	4.486	25C31	25SG	4.527

TABLE XXIV

25C31	160	4.531	25C31	161CA	4.598	25C31	162N	4.697
25C31	162C	4.753	25C31	162CA	4.857	25C32	66O	2.742
25C32	66C	3.901	25C32	163CB	4.205	25C32	26CB	4.317
25C32	66N	4.512	25C32	67CA	4.651	25C32	161O	4.691
25C32	67N	4.724	25C32	68SD	4.771	25C32	66CA	4.830
25C33	66O	3.447	25C33	68SD	3.722	25C33	163CB	3.798
25C33	209CD2	4.102	25C33	68CE	4.212	25C33	134CB	4.330
25C33	67CA	4.465	25C33	66C	4.538	25C33	67CD1	4.678
25C33	163CA	4.689	25C33	26CB	4.751	25C33	163N	4.950
25C34	134CB	3.099	25C34	163CB	3.583	25C34	209CD2	3.879
25C34	134CA	3.973	25C34	163CA	3.984	25C34	163N	4.154
25C34	68SD	4.317	25C34	162O	4.344	25C34	162C	4.346
25C34	68CE	4.364	25C34	160O	4.704	25C34	161O	4.819
25C34	66O	4.910	25C34	161C	4.924	25C34	133O	4.972
25C34	134C	4.977	25C34	134N	4.991	25C35	209CD2	3.174
25C35	67CD1	3.240	25C35	66O	3.588	25C35	67CA	3.813
25C35	67CE1	3.871	25C35	67CG	3.924	25C35	67CB	4.168
25C35	68SD	4.179	25C35	209CG	4.360	25C35	68CE	4.389
25C35	66C	4.393	25C35	234OH2	4.424	25C35	67N	4.535
25C35	134CB	4.642	25C35	68N	4.661	25C35	67C	4.803
25C35	67CZ	4.930	25C35	67CD2	4.976	25C36	161O	3.232
25C36	25SG	3.829	25C36	66O	4.065	25C36	161C	4.303
25C36	66N	4.338	25C36	65CA	4.529	25C36	26CD1	4.948
25C36	163N	4.963	25C36	26CB	5.000	25O37	66N	3.256
25O37	65CA	3.411	25O37	66O	3.590	25O37	65C	3.845
25O37	161O	4.314	25O37	66CA	4.368	25O37	66C	4.383
25O37	26CD1	4.400	25O37	25SG	4.578	25O37	65N	4.736
25O37	64O	4.804	25O37	26CB	4.911	25O37	26CG	4.987
25N38	161O	2.583	25N38	25SG	2.797	25N38	161C	3.765
25N38	162CA	4.301	25N38	163N	4.348	25N38	162N	4.497
25N38	25CB	4.579	25N38	162C	4.720	25N38	161CA	4.814
25N38	163CB	4.921	25N39	25SG	2.623	25N39	161O	3.421
25N39	23O	3.947	25N39	25CB	4.194	25N39	23C	4.527
25N39	161C	4.625	25N39	65CA	4.670	25N39	25N	4.673
25N39	23CA	4.780	25N39	25CA	4.961	25N39	162CA	4.964
25N40	160	3.177	25N40	161O	3.216	25N40	161C	3.641

TABLE XXIV

25N40 161CA	3.804	25N40 160C	4.036	25N40 161N	4.304
25N40 162N	4.578	25N40 66O	4.918		

TABLE XXV

Table of distances in Ångstroms between atoms of the inhibitor and protein for all protein atoms within 5 Ångstroms of the inhibitor 4-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-1-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-3-pyrrolidinone.

Atom 1	Atom 2	Dist.	Atom 1	Atom 2	Dist.	Atom 1	Atom 2	Dist.
25C1	184O	4.017	25C1	184CD1	4.233	25C1	184CG	4.294
25C1	184CB	4.338	25C1	184CA	4.431	25C1	18OD1	4.581
25C1	184C	4.634	25C1	184NE1	4.872	25C1	184CD2	4.992
25C2	20O	3.689	25C2	20C	4.194	25C2	21NE2	4.254
25C2	184CD1	4.266	25C2	20N	4.386	25C2	20CA	4.394
25C2	19CG	4.696	25C2	18OD1	4.707	25C2	184NE1	4.731
25C2	184CG	4.742	25C2	184CA	4.975	25C3	20O	3.755
25C3	184CD1	4.039	25C3	184NE1	4.087	25C3	21NE2	4.111
25C3	20C	4.569	25C3	19CG	4.678	25C3	184CG	4.714
25C3	184CE2	4.790	25C3	19CD	4.992	25C4	184NE1	3.514
25C4	184CD1	3.761	25C4	184CE2	3.871	25C4	184CG	4.236
25C4	184CD2	4.302	25C4	184CZ2	4.446	25C4	21NE2	4.858
25C5	184CE2	3.679	25C5	184NE1	3.687	25C5	184CD2	3.688
25C5	184CD1	3.704	25C5	184CG	3.711	25C5	184CZ2	4.317
25C5	184CE3	4.332	25C5	184CB	4.417	25C5	184CH2	4.847
25C5	184CZ3	4.856	25C6	184CG	3.747	25C6	184CD1	3.955
25C6	184CB	3.964	25C6	184CD2	4.101	25C6	184O	4.262
25C6	184NE1	4.395	25C6	184CE2	4.487	25C6	184CA	4.531
25C6	184CE3	4.701	25C6	184C	4.882	25C7	184NE1	3.584
25C7	184CE2	3.808	25C7	184CZ2	3.945	25C7	184CD1	4.327
25C7	184CD2	4.651	25C7	184CH2	4.855	25C7	184CG	4.925
25O8	184NE1	3.393	25O8	184CE2	3.944	25O8	184CZ2	4.069
25O8	184CD1	4.312	25O8	19NE2	4.602	25O8	19CD	4.825
25C9	184NE1	3.291	25C9	184CZ2	3.627	25C9	184CE2	3.765
25C9	162ND1	3.949	25C9	162CE1	4.256	25C9	184CD1	4.478
25C9	19NE2	4.492	25C9	19OE1	4.778	25C9	19CD	4.791
25C9	184CH2	4.870	25O10	184NE1	2.688	25O10	162ND1	2.878
25O10	162CE1	3.073	25O10	184CE2	3.353	25O10	184CZ2	3.407
25O10	19OE1	3.804	25O10	184CD1	3.882	25O10	19NE2	3.911
25O10	19CD	4.053	25O10	162CG	4.083	25O10	162NE2	4.247
25O10	184CD2	4.680	25O10	184CH2	4.748	25O10	162CD2	4.767
25O10	162CB	4.822	25O10	25CB	4.894	25O10	184CG	4.921

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TABLE XXV

25O10	25SG	4.959	25C11	161O	3.603	25C11	162ND1	3.785
25C11	162CB	4.170	25C11	162CG	4.352	25C11	184CZ2	4.547
25C11	161C	4.651	25C11	161OD1	4.678	25C11	162CE1	4.739
25C11	162CA	4.759	25C12	161O	3.598	25C12	161OD1	3.692
25C12	161CG	4.426	25C12	161C	4.497	25C12	162CB	4.500
25C12	161CB	4.644	25C12	162ND1	4.828	25C13	161OD1	3.668
25C13	137O	3.927	25C13	137C	4.080	25C13	138N	4.272
25C13	184CZ2	4.318	25C13	138CA	4.377	25C13	137CB	4.500
25C13	143NE2	4.527	25C13	161CG	4.603	25C13	161O	4.651
25C13	184CH2	4.656	25C13	162CB	4.732	25C13	137CA	4.757
25C14	143NE2	3.452	25C14	184CZ2	4.059	25C14	137O	4.191
25C14	184CH2	4.327	25C14	143CD	4.676	25C14	137C	4.726
25C14	138CA	4.757	25C14	138N	4.988	25C15	161OD1	3.025
25C15	138CA	3.182	25C15	138N	3.231	25C15	137C	3.477
25C15	138CB	3.598	25C15	137O	3.616	25C15	161CG	3.781
25C15	137CA	4.362	25C15	161ND2	4.367	25C15	137N	4.495
25C15	138C	4.523	25C15	137CB	4.599	25C15	143NE2	4.610
25C15	138OG	4.662	25C15	161CB	4.679	25C15	138O	4.905
25C15	161O	4.924	25C16	161O	3.101	25C16	162ND1	4.231
25C16	161C	4.310	25C16	162CB	4.562	25C16	25SG	4.612
25C16	162CA	4.657	25C16	162CG	4.876	25C16	162N	4.992
25O17	161O	3.437	25O17	161C	4.661	25N18	161O	3.143
25N18	25SG	3.301	25N18	162ND1	3.608	25N18	162CA	4.088
25N18	162CB	4.239	25N18	161C	4.252	25N18	162CG	4.379
25N18	25CB	4.462	25N18	162CE1	4.653	25N18	162N	4.681
25N18	19NE2	4.948	25N18	23CA	4.995	25C19	25SG	2.850
25C19	161O	3.592	25C19	23CA	4.261	25C19	25CB	4.284
25C19	162ND1	4.530	25C19	23C	4.535	25C19	162CA	4.545
25C19	161C	4.613	25C19	23O	4.725	25C19	25N	4.814
25N20	184CZ2	4.159	25N20	162ND1	4.342	25N20	184NE1	4.452
25N20	184CE2	4.669	25N20	162CE1	4.970	25C21	161O	3.074
25C21	25SG	3.220	25C21	161C	3.894	25C21	162CA	4.288
25C21	162N	4.439	25C21	65CA	4.747	25C21	161CA	4.860
25C21	25CB	4.980	25C22	25SG	1.762	25C22	25CB	2.996
25C22	25N	3.317	25C22	25CA	3.720	25C22	23C	3.769
25C22	23CA	3.914	25C22	23O	4.043	25C22	24N	4.052
25C22	19NE2	4.196	25C22	24C	4.394	25C22	162ND1	4.399
25C22	26N	4.510	25C22	25C	4.601	25C22	161O	4.652
25C22	24CA	4.697	25C22	162CA	4.792	25C22	163N	4.837
25C22	26CD1	4.881	25O23	25SG	2.430	25O23	25N	2.866
25O23	25CB	2.896	25O23	19NE2	3.003	25O23	23CA	3.259

TABLE XXV

25O23	23C	3.263	25O23	24N	3.328	25O23	25CA	3.459
25O23	23O	3.894	25O23	24C	3.945	25O23	19CD	4.004
25O23	19OE1	4.163	25O23	24CA	4.166	25O23	22O	4.360
25O23	162ND1	4.426	25O23	23N	4.535	25O23	25C	4.653
25O23	26N	4.784	25O23	22C	4.908	25O23	162CE1	4.912
25C24	59O	3.356	25C24	61OD2	4.112	25C24	60CA	4.139
25C24	61N	4.252	25C24	60ND2	4.327	25C24	60C	4.397
25C24	67CE2	4.413	25C24	59C	4.424	25C24	67CD2	4.649
25C24	61CB	4.711	25C24	60N	4.781	25C24	65O	4.810
25C24	66CA	4.888	25C24	61CG	4.890	25C25	61OD2	2.979
25C25	61CB	3.456	25C25	61N	3.582	25C25	61CG	3.623
25C25	65O	4.058	25C25	60C	4.074	25C25	61CA	4.084
25C25	59O	4.120	25C25	60CA	4.277	25C25	61OD1	4.827
25C25	65C	4.828	25C25	60O	4.832	25C25	66CA	4.907
25C26	61CB	3.331	25C26	65O	3.342	25C26	61OD2	3.552
25C26	61CG	3.818	25C26	61N	3.860	25C26	65C	3.890
25C26	61CA	4.226	25C26	64O	4.287	25C26	66N	4.362
25C26	66CA	4.392	25C26	60C	4.694	25C26	65CA	4.697
25C26	64C	4.855	25C26	61OD1	4.925	25C26	60CA	4.944
25C27	65O	3.537	25C27	65C	3.661	25C27	66N	3.764
25C27	66CA	3.789	25C27	67CE2	4.460	25C27	65CA	4.463
25C27	64O	4.501	25C27	61CB	4.521	25C27	66C	4.533
25C27	61N	4.713	25C27	67CD2	4.833	25C27	67CZ	4.873
25C27	61OD2	4.935	25C27	66O	4.986	25C28	67CE2	3.131
25C28	67CD2	3.493	25C28	67CZ	3.739	25C28	66CA	3.757
25C28	67OH	4.121	25C28	66C	4.151	25C28	66N	4.180
25C28	67CG	4.339	25C28	65O	4.368	25C28	67N	4.383
25C28	65C	4.453	25C28	67CE1	4.537	25C28	60ND2	4.576
25C28	66O	4.719	25C28	67CD1	4.789	25C29	67CE2	3.099
25C29	67CD2	3.367	25C29	60ND2	4.065	25C29	59O	4.096
25C29	67CZ	4.107	25C29	66CA	4.348	25C29	67CG	4.510
25C29	67OH	4.532	25C29	67N	4.689	25C29	60CA	4.697
25C29	66C	4.785	25C29	70OD1	4.794	25C29	65O	4.942
25C30	65C	3.364	25C30	66N	3.477	25C30	65O	3.676
25C30	65CA	3.705	25C30	64O	3.715	25C30	66CA	3.996
25C30	64C	4.521	25C30	65N	4.571	25C30	66C	4.606
25C30	66O	4.690	25O31	66N	4.304	25O31	65C	4.471
25O31	67OH	4.497	25O31	67CZ	4.562	25O31	65CA	4.615
25O31	64O	4.643	25O31	66CA	4.801	25O31	66O	4.804
25O31	67CE1	4.862	25O31	67CE2	4.899	25O31	65O	4.995
25O31	66C	4.998	25C32	66O	4.210	25C32	66N	4.247

TABLE XXV

25C32	65CA	4.648	25C32	65C	4.675	25C32	67CE1	4.683
25C32	66C	4.745	25C32	67CZ	4.797	25C32	66CA	4.862
25C32	67OH	4.906	25O33	67CE1	4.116	25O33	67CZ	4.445
25O33	67OH	4.485	25O33	66O	4.628	25O33	67CD1	4.718
25O33	253OH2	4.812	25O33	160O	4.869	25C34	66O	3.728
25C34	66N	4.086	25C34	65CA	4.283	25C34	65C	4.685
25C34	25SG	4.701	25C34	66C	4.710	25C34	161O	4.715
25C34	161C	4.780	25C35	66O	3.094	25C35	66C	4.237
25C35	68CE	4.248	25C35	66N	4.449	25C35	163CB	4.779
25C35	163N	4.929	25C35	66CA	4.993	25C36	66O	4.248
25C36	134CB	4.455	25C36	209CD2	4.608	25C36	68CE	4.627
25C36	160O	4.689	25C36	162N	4.700	25C36	160C	4.804
25C36	161C	4.832	25C36	161CA	4.852	25C36	67CD1	4.855
25C36	67CE1	4.866	25C36	161N	4.905	25C36	160CB	4.964
25C37	162N	3.453	25C37	134CB	3.566	25C37	162C	3.722
25C37	163N	3.858	25C37	162O	3.881	25C37	161C	3.888
25C37	161N	4.019	25C37	162CA	4.040	25C37	161CA	4.109
25C37	160C	4.197	25C37	163CA	4.335	25C37	163CB	4.414
25C37	160O	4.461	25C37	160CB	4.479	25C37	134CA	4.485
25C37	161O	4.643	25C37	160CA	4.832	25C37	68CE	4.842
25C37	209CD2	4.996	25C38	209CD2	3.377	25C38	67CD1	3.746
25C38	67CE1	3.972	25C38	68CE	4.019	25C38	134CB	4.063
25C38	66O	4.117	25C38	209CG	4.387	25C38	67CG	4.813
25C38	67CA	4.927	25C39	65CA	3.495	25C39	25SG	3.606
25C39	66N	3.612	25C39	66O	3.741	25C39	26CD1	4.029
25C39	65C	4.099	25C39	26CB	4.554	25C39	26CG	4.652
25C39	66C	4.666	25C39	65N	4.740	25C39	26N	4.747
25C39	66CA	4.755	25C39	23O	4.898	25C39	161O	4.941
25O40	66N	2.789	25O40	66O	2.930	25O40	26CD1	2.937
25O40	65CA	3.211	25O40	26CB	3.444	25O40	26CG	3.455
25O40	65C	3.479	25O40	66C	3.767	25O40	66CA	3.842
25O40	25SG	3.892	25O40	26N	3.999	25O40	26NE1	4.011
25O40	26CA	4.273	25O40	65N	4.534	25O40	23O	4.581
25O40	26CD2	4.697	25O40	65O	4.703	25O40	68CE	4.926
25O40	26CE2	4.943	25O40	25N	4.988	25N41	25SG	2.879
25N41	65CA	3.789	25N41	161O	4.253	25N41	23O	4.382
25N41	26CD1	4.417	25N41	66N	4.577	25N41	25CB	4.611
25N41	23C	4.734	25N41	65N	4.734	25N41	65C	4.774
25N41	25N	4.800	25N41	161C	4.855	25N41	26N	4.870
25N41	162CA	4.874	25N41	163N	4.932	25C42	25SG	2.470
25C42	23O	3.257	25C42	23C	3.448	25C42	25N	3.529

TABLE XXV

25C42	26CD1	3.714	25C42	65CA	3.771	25C42	25CB	3.843
25C42	23CA	3.956	25C42	24N	3.966	25C42	26N	4.147
25C42	25CA	4.156	25C42	24C	4.282	25C42	24CA	4.390
25C42	65N	4.469	25C42	26NE1	4.524	25C42	25C	4.662
25C42	26CG	4.728	25C42	66N	4.771	25C42	65C	4.825
25C42	26CB	4.981	25N43	66N	3.501	25N43	65CA	3.665
25N43	66O	3.722	25N43	65C	3.917	25N43	66C	4.394
25N43	66CA	4.413	25N43	64O	4.690	25N43	65O	4.923
25N43	65N	4.930						

TABLE XXVI

Table of distances in Ångstroms between atoms of the inhibitor and protein for all protein atoms within 5 Ångstroms of the inhibitor 4-[N-[(4-pyridylmethoxy)carbonyl]-L-leucyl]-1-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-3-pyrrolidinone.

Atom 1	Atom 2	Dist.	Atom 1	Atom 2	Dist.	Atom 1	Atom 2	Dist.
25C1	242OH2	3.241	25C1	18OD1	3.446	25C1	184CD1	3.907
25C1	184CB	3.929	25C1	184CG	3.941	25C1	184CA	4.202
25C1	18CG	4.369	25C1	18ND2	4.563	25C1	184NE1	4.640
25C1	184O	4.676	25C1	184CD2	4.729	25C1	184C	4.752
25C1	21NE2	4.852	25C1	20N	4.956	25C2	184CD1	3.751
25C2	184CG	3.778	25C2	184NE1	4.100	25C2	184CD2	4.156
25C2	184CB	4.179	25C2	184CE2	4.339	25C2	242OH2	4.411
25C2	18OD1	4.705	25C2	184CA	4.841	25C2	184CE3	4.910
25C3	184NE1	3.789	25C3	184CD1	3.817	25C3	184CE2	4.203
25C3	184CG	4.246	25C3	184CD2	4.475	25C3	20O	4.505
25C3	184CZ2	4.908	25C3	21NE2	4.969	25C4	20O	3.140
25C4	19CG	4.004	25C4	20C	4.011	25C4	184CD1	4.042
25C4	184NE1	4.079	25C4	21NE2	4.367	25C4	20N	4.403
25C4	19CD	4.509	25C4	20CA	4.543	25C4	21OE1	4.778
25C4	184CG	4.809	25C4	18OD1	4.811	25C4	184CE2	4.867
25C4	21CD	4.895	25C4	19NE2	4.938	25C4	21N	4.965
25C5	20O	2.695	25C5	20N	3.202	25C5	20C	3.263
25C5	20CA	3.407	25C5	18OD1	3.589	25C5	19CG	3.659
25C5	21NE2	3.950	25C5	19C	4.127	25C5	184CD1	4.183
25C5	21N	4.369	25C5	242OH2	4.392	25C5	18CG	4.548
25C5	19CD	4.599	25C5	184NE1	4.619	25C5	19N	4.620
25C5	19CA	4.668	25C5	19CB	4.730	25C5	21CD	4.753
25C5	18ND2	4.801	25C5	19O	4.927	25C5	184CG	4.931
25C5	183O	4.975	25C5	21OE1	4.987	25C6	18OD1	2.695
25C6	242OH2	3.232	25C6	20N	3.572	25C6	18CG	3.627
25C6	18ND2	3.837	25C6	20CA	3.842	25C6	20O	3.869
25C6	184CD1	4.122	25C6	20C	4.133	25C6	21NE2	4.219
25C6	19CG	4.448	25C6	184CA	4.454	25C6	184CG	4.538

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25C6	184CB	4.595	25C6	19N	4.613	25C6	19C	4.668
25C6	183O	4.825	25C6	244OH2	4.841	25C6	184NE1	4.878
25C7	20O	2.832	25C7	19CG	3.901	25C7	20C	3.960
25C7	19CD	4.075	25C7	19NE2	4.108	25C7	22O	4.387
25C7	184NE1	4.479	25C7	22N	4.658	25C7	21CA	4.703
25C7	19OE1	4.733	25C7	21OE1	4.734	25C7	21N	4.779
25C7	184CD1	4.791	25C7	20N	4.797	25C7	21NE2	4.850
25C7	20CA	4.870	25O8	20O	4.185	25O8	184NE1	4.318
25O8	19NE2	4.505	25O8	19CD	4.575	25O8	19CG	4.801
25O8	184CE2	4.904	25O8	184CD1	4.980	25O8	19OE1	4.989
25C9	184NE1	3.701	25C9	19NE2	4.091	25C9	19CD	4.179
25C9	184CE2	4.209	25C9	184CZ2	4.214	25C9	19OE1	4.322
25C9	162CE1	4.669	25C9	184CD1	4.680	25C9	19CG	4.819
25O10	184NE1	2.553	25O10	184CE2	3.148	25O10	184CZ2	3.297
25O10	19OE1	3.438	25O10	19CD	3.591	25O10	184CD1	3.650
25O10	162CE1	3.653	25O10	19NE2	3.822	25O10	162ND1	4.295
25O10	19CG	4.332	25O10	184CD2	4.379	25O10	162NE2	4.393
25O10	184CH2	4.579	25O10	184CG	4.611	25C11	162ND1	3.950
25C11	162CE1	4.196	25C11	184CZ2	4.648	25C11	19NE2	4.924
25C11	162CG	4.968	25C12	162ND1	4.717	25C12	161O	4.982
25C13	161OD1	4.017	25C13	162ND1	4.533	25C13	161CG	4.712
25C13	161O	4.749	25C13	184CZ2	4.831	25C13	162CB	4.860
25C13	162CG	4.864	25C13	137O	4.980	25C14	161OD1	3.145
25C14	162ND1	3.354	25C14	162CB	3.366	25C14	162CG	3.508
25C14	161O	3.685	25C14	161C	3.990	25C14	162CA	4.004
25C14	161CG	4.037	25C14	162N	4.168	25C14	162CE1	4.261
25C14	137CB	4.367	25C14	161CB	4.378	25C14	162CD2	4.476
25C14	184CZ2	4.641	25C14	137C	4.815	25C14	162NE2	4.847
25C14	161CA	4.867	25C14	137O	4.907	25C14	137CA	5.000
25C15	137O	4.063	25C15	184CZ2	4.064	25C15	184CH2	4.220
25C15	137C	4.530	25C15	161OD1	4.738	25C15	138CA	4.806
25C15	138N	4.887	25C15	137CB	4.908	25C16	162ND1	4.014
25C16	25SG	4.159	25C16	19NE2	4.348	25C16	162CE1	4.375
25C16	23CA	4.579	25C16	161O	4.665	25O17	23CA	3.462
25O17	19NE2	3.921	25O17	23C	4.371	25O17	23N	4.429
25O17	22O	4.568	25O17	25SG	4.579	25O17	22C	4.858

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25O17	19CD	4.877	25O17	23O	4.921	25O17	24N	4.983
25N18	25SG	3.257	25N18	162ND1	3.402	25N18	161O	3.468
25N18	162CE1	4.081	25N18	25CB	4.457	25N18	162CG	4.523
25N18	161C	4.569	25N18	162CA	4.582	25N18	162CB	4.845
25N18	19NE2	4.859	25C19	25SG	2.794	25C19	161O	3.684
25C19	25CB	4.234	25C19	162ND1	4.247	25C19	23CA	4.366
25C19	23O	4.457	25C19	23C	4.497	25C19	25N	4.673
25C19	161C	4.876	25C19	162CE1	4.889	25C19	19NE2	4.898
25N20	19NE2	4.613	25N20	184NE1	4.773	25N20	184CZ2	4.805
25N20	162CE1	4.936	25N20	19CD	4.991	25C21	161O	2.879
25C21	25SG	3.218	25C21	161C	4.048	25C21	162CA	4.631
25C21	162N	4.811	25C21	65CA	4.831	25C21	162ND1	4.843
25C21	25CB	4.939	25C21	163N	4.976	25C22	25SG	1.746
25C22	25CB	2.980	25C22	25N	3.156	25C22	25CA	3.592
25C22	23O	3.702	25C22	23C	3.712	25C22	23CA	4.038
25C22	19NE2	4.077	25C22	24N	4.130	25C22	26N	4.232
25C22	162ND1	4.246	25C22	24C	4.298	25C22	25C	4.374
25C22	162CE1	4.608	25C22	24CA	4.620	25C22	161O	4.649
25C22	26CD1	4.828	25C22	19OE1	4.874	25C22	19CD	4.942
25O23	25SG	2.426	25O23	25N	2.644	25O23	25CB	2.944
25O23	19NE2	2.944	25O23	23C	2.957	25O23	24N	3.189
25O23	23CA	3.211	25O23	23O	3.326	25O23	25CA	3.349
25O23	24C	3.666	25O23	24CA	3.882	25O23	19CD	3.941
25O23	19OE1	4.099	25O23	22O	4.365	25O23	25C	4.451
25O23	26N	4.481	25O23	23N	4.525	25O23	162ND1	4.590
25O23	162CE1	4.629	25O23	24O	4.773	25O23	22C	4.910
25C24	65CA	4.095	25C24	66N	4.264	25C24	65C	4.356
25C24	64O	4.547	25C24	66O	4.628	25C25	66O	3.688
25C25	161O	3.862	25C25	66N	4.313	25C25	161C	4.458
25C25	66C	4.741	25C25	65CA	4.778	25C25	161CA	4.939
25C25	25SG	4.963	25C25	65C	4.974	25C26	66O	3.481
25C26	161O	4.269	25C26	161C	4.491	25C26	163N	4.695
25C26	66C	4.696	25C26	160O	4.785	25C26	163CB	4.799
25C26	162N	4.915	25C26	161CA	4.923	25C27	160O	3.472
25C27	160C	4.089	25C27	161CA	4.307	25C27	161C	4.320
25C27	161N	4.440	25C27	161O	4.452	25C27	66O	4.548

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25C27	160CB	4.699	25C27	134CB	4.734	25C27	162N	4.770
25C27	209CD2	4.918	25C28	160O	3.351	25C28	160C	4.338
25C28	67CE1	4.588	25C28	161CA	4.739	25C28	66O	4.818
25C28	161N	4.934	25C28	67CD1	4.955	25C29	209CD2	3.439
25C29	134CB	3.686	25C29	160O	4.049	25C29	160CB	4.234
25C29	160C	4.490	25C29	67CD1	4.759	25C29	66O	4.795
25C29	209CG	4.839	25C29	67CE1	4.896	25C30	66O	3.533
25C30	66N	3.616	25C30	25SG	3.883	25C30	65CA	3.972
25C30	26CD1	4.246	25C30	26CB	4.295	25C30	65C	4.296
25C30	161O	4.302	25C30	66C	4.432	25C30	66CA	4.591
25C30	26CG	4.623	25C30	26N	4.737	25C30	163CB	4.852
25C30	163N	4.940	25O31	66O	2.635	25O31	66N	2.846
25O31	26CB	3.199	25O31	26CD1	3.340	25O31	66C	3.423
25O31	26CG	3.516	25O31	66CA	3.653	25O31	65C	3.792
25O31	65CA	3.821	25O31	26N	4.122	25O31	26CA	4.160
25O31	25SG	4.278	25O31	26NE1	4.531	25O31	67N	4.618
25O31	163CB	4.642	25O31	26CD2	4.797	25O31	65O	4.959
25N32	25SG	2.963	25N32	161O	3.860	25N32	65CA	4.049
25N32	66N	4.382	25N32	23O	4.384	25N32	26CD1	4.398
25N32	26N	4.601	25N32	25CB	4.628	25N32	25N	4.764
25N32	65C	4.790	25N32	66O	4.806	25N32	163N	4.815
25N32	26CB	4.836	25N32	161C	4.880	25N32	23C	4.985
25C33	25SG	2.418	25C33	23O	3.256	25C33	25N	3.403
25C33	26CD1	3.587	25C33	26N	3.672	25C33	25CB	3.751
25C33	23C	3.758	25C33	25CA	3.959	25C33	65CA	3.999
25C33	25C	4.264	25C33	24N	4.334	25C33	24C	4.346
25C33	26CG	4.388	25C33	26CB	4.392	25C33	23CA	4.425
25C33	66N	4.510	25C33	24CA	4.531	25C33	26CA	4.616
25C33	26NE1	4.621	25C33	65C	4.831	25C33	65N	4.901
25C33	161O	4.934	25N34	66O	3.486	25N34	66N	3.771
25N34	65CA	4.261	25N34	65C	4.264	25N34	66C	4.330
25N34	66CA	4.464	25N34	161O	4.991			

TABLE XXVII

Table of distances in Ångstroms between atoms of the inhibitor and protein for all protein atoms within 5 Ångstroms of the inhibitor 4-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-1-N[N-(methyl)-L-leucyl)]-3-pyrrolidinone.

Atom 1	Atom 2	Dist.	Atom 1	Atom 2	Dist.	Atom 1	Atom 2	Dist.
25C1	242OH2	3.241	25C1	18OD1	3.446	25C1	184CD1	3.907
25C1	184CB	3.929	25C1	184CG	3.941	25C1	184CA	4.202
25C1	18CG	4.369	25C1	18ND2	4.563	25C1	184NE1	4.640
25C1	184O	4.676	25C1	184CD2	4.729	25C1	184C	4.752
25C1	21NE2	4.852	25C1	20N	4.956	25C2	184CD1	3.751
25C2	184CG	3.778	25C2	184NE1	4.100	25C2	184CD2	4.156
25C2	184CB	4.179	25C2	184CE2	4.339	25C2	242OH2	4.411
25C2	18OD1	4.705	25C2	184CA	4.841	25C2	184CE3	4.910
25C3	184NE1	3.789	25C3	184CD1	3.817	25C3	184CE2	4.203
25C3	184CG	4.246	25C3	184CD2	4.475	25C3	20O	4.505
25C3	184CZ2	4.908	25C3	21NE2	4.969	25C4	20O	3.140
25C4	19CG	4.004	25C4	20C	4.011	25C4	184CD1	4.042
25C4	184NE1	4.079	25C4	21NE2	4.367	25C4	20N	4.403
25C4	19CD	4.509	25C4	20CA	4.543	25C4	21OE1	4.778
25C4	184CG	4.809	25C4	18OD1	4.811	25C4	184CE2	4.867
25C4	21CD	4.895	25C4	19NE2	4.938	25C4	21N	4.965
25C5	20O	2.695	25C5	20N	3.202	25C5	20C	3.263
25C5	20CA	3.407	25C5	18OD1	3.589	25C5	19CG	3.659
25C5	21NE2	3.950	25C5	19C	4.127	25C5	184CD1	4.183
25C5	21N	4.369	25C5	242OH2	4.392	25C5	18CG	4.548
25C5	19CD	4.599	25C5	184NE1	4.619	25C5	19N	4.620
25C5	19CA	4.668	25C5	19CB	4.730	25C5	21CD	4.753
25C5	18ND2	4.801	25C5	19O	4.927	25C5	184CG	4.931
25C5	183O	4.975	25C5	21OE1	4.987	25C6	18OD1	2.695
25C6	242OH2	3.232	25C6	20N	3.572	25C6	18CG	3.627
25C6	18ND2	3.837	25C6	20CA	3.842	25C6	20O	3.869
25C6	184CD1	4.122	25C6	20C	4.133	25C6	21NE2	4.219
25C6	19CG	4.448	25C6	184CA	4.454	25C6	184CG	4.538

TABLE XXVII

25C6	184CB	4.595	25C6	19N	4.613	25C6	19C	4.668
25C6	183O	4.825	25C6	244OH2	4.841	25C6	184NE1	4.878
25C7	20O	2.832	25C7	19CG	3.901	25C7	20C	3.960
25C7	19CD	4.075	25C7	19NE2	4.108	25C7	22O	4.387
25C7	184NE1	4.479	25C7	22N	4.658	25C7	21CA	4.703
25C7	19OE1	4.733	25C7	21OE1	4.734	25C7	21N	4.779
25C7	184CD1	4.791	25C7	20N	4.797	25C7	21NE2	4.850
25C7	20CA	4.870	25O8	20O	4.185	25O8	184NE1	4.318
25O8	19NE2	4.505	25O8	19CD	4.575	25O8	19CG	4.801
25O8	184CE2	4.904	25O8	184CD1	4.980	25O8	19OE1	4.989
25C9	184NE1	3.701	25C9	19NE2	4.091	25C9	19CD	4.179
25C9	184CE2	4.209	25C9	184CZ2	4.214	25C9	19OE1	4.322
25C9	162CE1	4.669	25C9	184CD1	4.680	25C9	19CG	4.819
25O10	184NE1	2.553	25O10	184CE2	3.148	25O10	184CZ2	3.297
25O10	19OE1	3.438	25O10	19CD	3.591	25O10	184CD1	3.650
25O10	162CE1	3.653	25O10	19NE2	3.822	25O10	162ND1	4.295
25O10	19CG	4.332	25O10	184CD2	4.379	25O10	162NE2	4.393
25O10	184CH2	4.579	25O10	184CG	4.611	25C11	162ND1	3.950
25C11	162CE1	4.196	25C11	184CZ2	4.648	25C11	19NE2	4.924
25C11	162CG	4.968	25C12	162ND1	4.717	25C12	161O	4.982
25C13	161OD1	4.017	25C13	162ND1	4.533	25C13	161CG	4.712
25C13	161O	4.749	25C13	184CZ2	4.831	25C13	162CB	4.860
25C13	162CG	4.864	25C13	137O	4.980	25C14	161OD1	3.145
25C14	162ND1	3.354	25C14	162CB	3.366	25C14	162CG	3.508
25C14	161O	3.685	25C14	161C	3.990	25C14	162CA	4.004
25C14	161CG	4.037	25C14	162N	4.168	25C14	162CE1	4.261
25C14	137CB	4.367	25C14	161CB	4.378	25C14	162CD2	4.476
25C14	184CZ2	4.641	25C14	137C	4.815	25C14	162NE2	4.847
25C14	161CA	4.867	25C14	137O	4.907	25C14	137CA	5.000
25C15	137O	4.063	25C15	184CZ2	4.064	25C15	184CH2	4.220
25C15	137C	4.530	25C15	161OD1	4.738	25C15	138CA	4.806
25C15	138N	4.887	25C15	137CB	4.908	25C16	162ND1	4.014
25C16	25SG	4.159	25C16	19NE2	4.348	25C16	162CE1	4.375
25C16	23CA	4.579	25C16	161O	4.665	25O17	23CA	3.462
25O17	19NE2	3.921	25O17	23C	4.371	25O17	23N	4.429
25O17	22O	4.568	25O17	25SG	4.579	25O17	22C	4.858

TABLE XXVII

25O17	19CD	4.877	25O17	23O	4.921	25O17	24N	4.983
25N18	25SG	3.257	25N18	162ND1	3.402	25N18	161O	3.468
25N18	162CE1	4.081	25N18	25CB	4.457	25N18	162CG	4.523
25N18	161C	4.569	25N18	162CA	4.582	25N18	162CB	4.845
25N18	19NE2	4.859	25C19	25SG	2.794	25C19	161O	3.684
25C19	25CB	4.234	25C19	162ND1	4.247	25C19	23CA	4.366
25C19	23O	4.457	25C19	23C	4.497	25C19	25N	4.673
25C19	161C	4.876	25C19	162CE1	4.889	25C19	19NE2	4.898
25N20	19NE2	4.613	25N20	184NE1	4.773	25N20	184CZ2	4.805
25N20	162CE1	4.936	25N20	19CD	4.991	25C21	161O	2.879
25C21	25SG	3.218	25C21	161C	4.048	25C21	162CA	4.631
25C21	162N	4.811	25C21	65CA	4.831	25C21	162ND1	4.843
25C21	25CB	4.939	25C21	163N	4.976	25C22	25SG	1.746
25C22	25CB	2.980	25C22	25N	3.156	25C22	25CA	3.592
25C22	23O	3.702	25C22	23C	3.712	25C22	23CA	4.038
25C22	19NE2	4.077	25C22	24N	4.130	25C22	26N	4.232
25C22	162ND1	4.246	25C22	24C	4.298	25C22	25C	4.374
25C22	162CE1	4.608	25C22	24CA	4.620	25C22	161O	4.649
25C22	26CD1	4.828	25C22	19OE1	4.874	25C22	19CD	4.942
25O23	25SG	2.426	25O23	25N	2.644	25O23	25CB	2.944
25O23	19NE2	2.944	25O23	23C	2.957	25O23	24N	3.189
25O23	23CA	3.211	25O23	23O	3.326	25O23	25CA	3.349
25O23	24C	3.666	25O23	24CA	3.882	25O23	19CD	3.941
25O23	19OE1	4.099	25O23	22O	4.365	25O23	25C	4.451
25O23	26N	4.481	25O23	23N	4.525	25O23	162ND1	4.590
25O23	162CE1	4.629	25O23	24O	4.773	25O23	22C	4.910
25C24	65CA	4.095	25C24	66N	4.264	25C24	65C	4.356
25C24	64O	4.547	25C24	66O	4.628	25C25	66O	3.688
25C25	161O	3.862	25C25	66N	4.313	25C25	161C	4.458
25C25	66C	4.741	25C25	65CA	4.778	25C25	161CA	4.939
25C25	25SG	4.963	25C25	65C	4.974	25C26	66O	3.481
25C26	161O	4.269	25C26	161C	4.491	25C26	163N	4.695
25C26	66C	4.696	25C26	160O	4.785	25C26	163CB	4.799
25C26	162N	4.915	25C26	161CA	4.923	25C27	160O	3.472
25C27	160C	4.089	25C27	161CA	4.307	25C27	161C	4.320
25C27	161N	4.440	25C27	161O	4.452	25C27	66O	4.548

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25C27	160CB	4.699	25C27	134CB	4.734	25C27	162N	4.770
25C27	209CD2	4.918	25C28	160O	3.351	25C28	160C	4.338
25C28	67CE1	4.588	25C28	161CA	4.739	25C28	66O	4.818
25C28	161N	4.934	25C28	67CD1	4.955	25C29	209CD2	3.439
25C29	134CB	3.686	25C29	160O	4.049	25C29	160CB	4.234
25C29	160C	4.490	25C29	67CD1	4.759	25C29	66O	4.795
25C29	209CG	4.839	25C29	67CE1	4.896	25C30	66O	3.533
25C30	66N	3.616	25C30	25SG	3.883	25C30	65CA	3.972
25C30	26CD1	4.246	25C30	26CB	4.295	25C30	65C	4.296
25C30	161O	4.302	25C30	66C	4.432	25C30	66CA	4.591
25C30	26CG	4.623	25C30	26N	4.737	25C30	163CB	4.852
25C30	163N	4.940	25O31	66O	2.635	25O31	66N	2.846
25O31	26CB	3.199	25O31	26CD1	3.340	25O31	66C	3.423
25O31	26CG	3.516	25O31	66CA	3.653	25O31	65C	3.792
25O31	65CA	3.821	25O31	26N	4.122	25O31	26CA	4.160
25O31	25SG	4.278	25O31	26NE1	4.531	25O31	67N	4.618
25O31	163CB	4.642	25O31	26CD2	4.797	25O31	65O	4.959
25N32	25SG	2.963	25N32	161O	3.860	25N32	65CA	4.049
25N32	66N	4.382	25N32	23O	4.384	25N32	26CD1	4.398
25N32	26N	4.601	25N32	25CB	4.628	25N32	25N	4.764
25N32	65C	4.790	25N32	66O	4.806	25N32	163N	4.815
25N32	26CB	4.836	25N32	161C	4.880	25N32	23C	4.985
25C33	25SG	2.418	25C33	23O	3.256	25C33	25N	3.403
25C33	26CD1	3.587	25C33	26N	3.672	25C33	25CB	3.751
25C33	23C	3.758	25C33	25CA	3.959	25C33	65CA	3.999
25C33	25C	4.264	25C33	24N	4.334	25C33	24C	4.346
25C33	26CG	4.388	25C33	26CB	4.392	25C33	23CA	4.425
25C33	66N	4.510	25C33	24CA	4.531	25C33	26CA	4.616
25C33	26NE1	4.621	25C33	65C	4.831	25C33	65N	4.901
25C33	161O	4.934	25N34	66O	3.486	25N34	66N	3.771
25N34	65CA	4.261	25N34	65C	4.264	25N34	66C	4.330
25N34	66CA	4.464	25N34	161O	4.991			

TABLE XXVIII

Table of distances in Ångstroms between atoms of the inhibitor and protein for all protein atoms within 5 Ångstroms of the inhibitor 1-N-(N-imidazole acetyl-leucinyl)-amino-3-N-(4-phenoxy-phenyl-sulfonyl)-amino-propan-2-one.

Atom 1	Atom 2	Dist.	Atom 1	Atom 2	Dist.	Atom 1	Atom 2	Dist.
25C1	20O	2.824	25C1	20C	3.956	25C1	184NE1	4.078
25C1	184CD1	4.178	25C1	21CA	4.600	25C1	20N	4.704
25C1	21N	4.706	25C1	21NE2	4.738	25C1	19CB	4.859
25C1	19CD	4.929	25C1	20CA	4.947	25C1	184CE2	4.949
25C1	19CG	4.998	25C2	20O	3.367	25C2	21NE2	4.119
25C2	241OH2	4.309	25C2	20C	4.592	25C2	184NE1	4.819
25C2	184CD1	4.860	25C3	241OH2	3.093	25C3	20O	3.775
25C3	21NE2	4.450	25C3	184CD1	4.878	25C3	20C	4.988
25C4	241OH2	3.480	25C4	20O	3.717	25C4	18OD1	3.947
25C4	184CD1	4.219	25C4	184CG	4.493	25C4	184O	4.549
25C4	184CB	4.602	25C4	184CA	4.747	25C4	18CG	4.754
25C4	18ND2	4.754	25C4	20C	4.826	25C4	184NE1	4.840
25C4	20N	4.964	25C4	184C	4.980	25C5	20O	3.239
25C5	18OD1	3.271	25C5	184CD1	3.400	25C5	20N	3.933
25C5	184CG	4.002	25C5	184NE1	4.111	25C5	184CA	4.118
25C5	20C	4.232	25C5	18CG	4.245	25C5	184CB	4.256
25C5	19CB	4.402	25C5	183O	4.499	25C5	184O	4.503
25C5	20CA	4.510	25C5	19N	4.552	25C5	184C	4.587
25C5	18ND2	4.606	25C5	19C	4.765	25C5	19CA	4.817
25C5	241OH2	4.867	25C5	184CD2	4.968	25C6	20O	2.740
25C6	184CD1	3.361	25C6	184NE1	3.660	25C6	20C	3.746
25C6	20N	3.761	25C6	19CB	3.788	25C6	18OD1	4.136
25C6	19CG	4.290	25C6	184CG	4.321	25C6	20CA	4.335
25C6	19C	4.361	25C6	19CD	4.428	25C6	19CA	4.488
25C6	19OE1	4.526	25C6	19N	4.653	25C6	184CE2	4.729
25C6	183O	4.737	25C6	21N	4.769	25C6	184CA	4.918
25C6	184CB	4.981	25C6	19NE2	4.990	25O7	20O	3.287
25O7	21CA	4.138	25O7	20C	4.173	25O7	19NE2	4.269

TABLE XXVIII

25O7	21C	4.370	25O7	19CD	4.416	25O7	184NE1	4.459
25O7	21O	4.466	25O7	22O	4.540	25O7	21N	4.558
25O7	19CG	4.663	25O7	19OE1	4.850	25O7	184CD1	4.897
25O7	19CB	4.977	25C8	19NE2	4.003	25C8	184NE1	4.235
25C8	19CD	4.404	25C8	20O	4.665	25C8	19OE1	4.715
25C8	22O	4.861	25C8	21O	4.937	25C8	184CE2	4.948
25C9	184NE1	3.199	25C9	19NE2	3.212	25C9	19CD	3.472
25C9	19OE1	3.533	25C9	184CE2	4.000	25C9	184CD1	4.152
25C9	184CZ2	4.206	25C9	19CG	4.414	25C9	162NE2	4.653
25C9	22O	4.860	25C9	162CD2	4.867	25C9	19CB	4.910
25C10	184NE1	3.388	25C10	184CZ2	3.605	25C10	19NE2	3.666
25C10	184CE2	3.828	25C10	162CD2	3.878	25C10	19OE1	3.887
25C10	162NE2	3.948	25C10	19CD	4.067	25C10	184CD1	4.615
25C10	162CG	4.799	25C10	184CH2	4.859	25C10	162CE1	4.873
25C11	184CZ2	4.084	25C11	184NE1	4.519	25C11	162CD2	4.567
25C11	184CE2	4.664	25C11	19NE2	4.718	25C11	162NE2	4.920
25C13	19NE2	4.978	25S14	162CD2	3.947	25S14	184CZ2	4.113
25S14	162CG	4.222	25S14	162CB	4.332	25S14	161O	4.574
25S14	162NE2	4.657	25S14	161OD1	4.760	25S14	184CH2	4.865
25O15	184CZ2	3.079	25O15	184CH2	3.580	25O15	162CG	3.856
25O15	162CD2	3.881	25O15	137O	3.985	25O15	162CB	4.051
25O15	184CE2	4.275	25O15	137CB	4.300	25O15	162ND1	4.343
25O15	162NE2	4.364	25O15	161OD1	4.610	25O15	162CE1	4.620
25O15	137C	4.663	25O15	184NE1	4.807	25O15	184CZ3	4.973
25O16	161OD1	4.484	25O16	161O	4.575	25O16	161CG	4.963
25N17	162CD2	2.828	25N17	162CG	3.217	25N17	161O	3.256
25N17	162CB	3.276	25N17	162CA	3.672	25N17	162NE2	3.893
25N17	161C	4.006	25N17	25SG	4.125	25N17	162N	4.251
25N17	162ND1	4.353	25N17	161OD1	4.593	25N17	162CE1	4.665
25N17	184CZ2	4.778	25N17	25CB	4.819	25C18	161O	3.031
25C18	25SG	3.290	25C18	162CD2	3.499	25C18	162CA	4.069
25C18	161C	4.107	25C18	162CG	4.151	25C18	162CB	4.188
25C18	25CB	4.359	25C18	19NE2	4.573	25C18	162NE2	4.594
25C18	162N	4.597	25C19	25SG	1.931	25C19	25CB	3.158
25C19	162CD2	3.616	25C19	161O	3.716	25C19	19NE2	3.740
25C19	25N	4.227	25C19	25CA	4.306	25C19	23CA	4.380

TABLE XXVIII

25C19	162CA	4.405	25C19	23O	4.494	25C19	23C	4.496
25C19	162CG	4.541	25C19	162NE2	4.577	25C19	19CD	4.643
25C19	19OE1	4.705	25C19	161C	4.813	25C19	162CB	4.819
25O20	19NE2	2.778	25O20	25SG	2.890	25O20	23CA	3.251
25O20	25CB	3.629	25O20	23C	3.723	25O20	19CD	3.918
25O20	23O	4.030	25O20	25N	4.152	25O20	19OE1	4.290
25O20	24N	4.342	25O20	162CD2	4.356	25O20	23N	4.524
25O20	25CA	4.566	25O20	22O	4.681	25O20	161O	4.912
25C21	25SG	2.532	25C21	161O	3.420	25C21	23O	4.107
25C21	25CB	4.220	25C21	23C	4.540	25C21	65CA	4.542
25C21	161C	4.578	25C21	23CA	4.599	25C21	162CA	4.793
25C21	25N	4.822	25C21	162CD2	4.980	25N22	161O	2.689
25N22	25SG	2.783	25N22	161C	3.649	25N22	162CA	4.003
25N22	162N	4.221	25N22	163N	4.453	25N22	25CB	4.578
25N22	162C	4.691	25N22	161CA	4.693	25N22	65CA	4.839
25C23	161O	3.461	25C23	25SG	3.771	25C23	161C	4.205
25C23	66O	4.217	25C23	65CA	4.220	25C23	66N	4.268
25C23	162N	4.828	25C23	162CA	4.844	25C23	65C	4.845
25C23	26CD1	4.890	25C23	161CA	4.937	25C23	26CB	4.974
25O24	65CA	3.024	25O24	66N	3.208	25O24	65C	3.657
25O24	66O	3.830	25O24	65N	4.287	25O24	26CD1	4.326
25O24	25SG	4.394	25O24	66CA	4.437	25O24	161O	4.526
25O24	66C	4.595	25O24	64O	4.818	25O24	23O	4.843
25O24	26CG	4.879	25O24	26CB	4.888	25O24	65O	4.923
25O24	64C	4.972	25C25	161O	3.652	25C25	66O	3.880
25C25	161C	3.949	25C25	162N	4.375	25C25	161CA	4.493
25C25	163N	4.584	25C25	25SG	4.592	25C25	162CA	4.608
25C25	162C	4.759	25C25	66N	4.805	25C25	163CB	4.922
25C26	66O	3.186	25C26	163CB	3.703	25C26	26CB	3.850
25C26	163N	4.052	25C26	25SG	4.357	25C26	163CA	4.390
25C26	66C	4.421	25C26	26CA	4.561	25C26	162C	4.598
25C26	68SD	4.628	25C26	161O	4.666	25C26	66N	4.721
25C26	26N	4.729	25C26	26CG	4.770	25C26	162CA	4.869
25C26	161C	4.907	25C26	162N	4.970	25C26	26CD1	4.999
25C27	163CB	3.337	25C27	68SD	3.583	25C27	66O	3.590
25C27	163CA	4.029	25C27	163N	4.096	25C27	68CE	4.156

TABLE XXVIII

25C27	134CB	4.190	25C27	209CD2	4.248	25C27	26CB	4.361
25C27	162C	4.597	25C27	66C	4.797	25C27	162O	4.893
25C27	26CA	4.943	25C27	67CA	4.946	25C28	134CB	3.049
25C28	163CB	3.699	25C28	163N	3.714	25C28	162C	3.789
25C28	162O	3.807	25C28	163CA	3.820	25C28	209CD2	3.901
25C28	134CA	3.967	25C28	162N	4.239	25C28	162CA	4.478
25C28	68CE	4.498	25C28	68SD	4.535	25C28	161C	4.582
25C28	66O	4.956	25C28	134C	4.964	25C28	161O	4.966
25C28	161N	4.992	25C29	66O	2.949	25C29	209CD2	3.567
25C29	68SD	3.617	25C29	67CA	3.759	25C29	67CD1	3.963
25C29	66C	3.998	25C29	68CE	4.231	25C29	67N	4.370
25C29	68N	4.410	25C29	67C	4.555	25C29	67CB	4.556
25C29	67CG	4.589	25C29	163CB	4.636	25C29	134CB	4.685
25C29	234OH2	4.722	25C29	26CB	4.726	25C29	67CE1	4.755
25N30	66O	3.644	25N30	66N	4.623	25N30	161O	4.640
25N30	66C	4.640	25N30	161C	4.793	25N30	161CA	4.888
25N30	160O	4.908	25C31	160O	3.792	25C31	161CA	4.412
25C31	160C	4.476	25C31	161C	4.719	25C31	66O	4.743
25C31	161N	4.777	25C31	161O	4.849	25C31	67CE1	4.934
25O32	160O	2.720	25O32	160C	3.270	25O32	161CA	3.397
25O32	161N	3.577	25O32	161C	3.869	25O32	160CB	4.202
25O32	161O	4.268	25O32	160CA	4.363	25O32	162N	4.395
25O32	161CB	4.698	25C33	67CE1	3.801	25C33	160O	4.307
25C33	67CZ	4.397	25C33	67CD1	4.397	25C33	67OH	4.480
25C34	160O	3.849	25C34	67CE1	4.011	25C34	67OH	4.411
25C34	67CZ	4.629	25C34	160C	4.805	25C34	67CD1	4.850
25C34	160CB	4.898	25C35	67CE1	3.694	25C35	67OH	4.238
25C35	209CD2	4.447	25C35	67CZ	4.449	25C35	67CD1	4.551
25C35	160O	4.567	25C35	160CB	4.790	25C35	209CD1	4.791
25N36	160O	4.470	25N36	160CB	4.515	25N36	160CD1	4.774
25N36	160CG	4.825	25N36	67CE1	4.846	25N36	67OH	4.964
25C37	160O	3.691	25C37	160CB	4.458	25C37	160N	4.495
25C37	160C	4.634	25C37	160CA	4.822	25C37	160CG	4.973
25C37	158O	4.994	25N38	160O	3.211	25N38	160C	4.305
25N38	160CB	4.681	25N38	160N	4.817	25N38	160CA	4.898

TABLE XXIX

Active site amino acid residues for Cathepsin K

ASN	18	GLN	19	GLY	20	GLN	21
CYS	22	GLY	23	SER	24	CYS	25
TRP	26	ALA	27	PHE	28	SER	29
GLU	59	ASN	60	ASP	61	GLY	64
GLY	65	GLY	66	TYR	67	MET	68
ASN	70	ALA	134	ALA	137	SER	138
GLN	143	ASP	158	ASN	159	LEU	160
ASN	161	HIS	162	ALA	163	SER	183
TRP	184	TRP	188	LEU	209		

WHAT IS CLAIMED IS:

1. A method of inhibiting cathepsin K which comprises administering to a mammal in need thereof a compound that fits spatially into the active site of cathepsin K, said compound comprising any two of the following:

(i) an electrophilic carbon atom that binds to the side chain sulfur atom of cysteine 25 wherein said electrophilic carbon atom is 1.7-4.0Å from said sulfur atom;

(ii) a hydrophobic group that interacts with tryptophan 184 wherein the distance between the centroid of said hydrophobic group and the centroid of the side chain atoms of tryptophan 184 is 4.10-7.10Å;

(iii) a hydrophobic group that interacts with tyrosine 67, methionine 68, alanine 134, leucine 160, and leucine 209, creating a hydrophobic pocket, and has distance ranges between the centroid of said hydrophobic group and the centroids of the side chain atoms of the amino acid residues of said hydrophobic pocket which are tyrosine 67: 4.91- 5.91Å, methionine 68: 5.74-6.74Å, alanine 134: 4.15-5.15Å, leucine 160: 6.18-7.18Å, and leucine 209: 5.71-6.71Å;

(iv) a hydrophobic group that interacts with tyrosine 67 wherein the distance between the centroid of said hydrophobic group and the centroid of the side chain atoms of tyrosine 67 is 4.10-7.10Å;

(v) an amino group with a pKa of less than 7 or an oxygen atom, each of which interacts with a hydrogen atom donated by the amide nitrogen of glycine 66 wherein the distance between these two atoms is 2.7-3.5Å;

(vi) a hydrophobic group that interacts with the main chain atoms of glutamine 21, cysteine 22 and glycine 23 wherein the distance between the centroid of said hydrophobic group and the centroids of glutamine 21 , cysteine 22 and glycine 23 are 3.7-5.4, 4.9-5.7 and 5.4-6.7Å, respectively; or

(vii) a hydrophobic group that interacts with the side chain atoms of glutamine 143 and asparagine 161 and the main chain of alanine 137 and serine 138 wherein the distance between the centroid of the hydrophobic group and the centroids of glutamine 143, asparagine 161, alanine 137, and serine 138 are 7.9-9.6Å, 4.7-5.4Å, 4.2-5.5Å, and 4.6-6.4Å, respectively.

2. A method of inhibiting cathepsin K which comprises administering to a mammal in need thereof a compound that fits spatially into the active site of cathepsin K, said compound comprising any three or more of the following:

(i) an electrophilic carbon atom that binds to the side chain sulfur atom of cysteine 25 wherein said electrophilic carbon atom is 1.7-4.0Å from said sulfur atom;

(ii) a hydrophobic group that interacts with tryptophan 184 wherein the distance between the centroid of said hydrophobic group and the centroid of the side chain atoms of tryptophan 184 is 4.10-7.10Å;

(iii) a hydrophobic group that interacts with tyrosine 67, methionine 68, alanine 134, leucine 160, and leucine 209, creating a hydrophobic pocket, and has distance ranges between the centroid of said hydrophobic group and the centroids of the side chain atoms of the amino acid residues of said hydrophobic pocket which are tyrosine 67: 4.91- 5.91Å, methionine 68: 5.74-6.74Å, alanine 134: 4.15-5.15Å, leucine 160: 6.18-7.18Å, and leucine 209: 5.71-6.71Å;

(iv) a hydrophobic group that interacts with tyrosine 67 wherein the distance between the centroid of said hydrophobic group and the centroid of the side chain atoms of tyrosine 67 is 4.10-7.10Å;

(v) an amino group with a pKa of less than 7 or an oxygen atom, each of which interacts with a hydrogen atom donated by the amide nitrogen of glycine 66 wherein the distance between these two atoms is 2.7-3.5Å;

(vi) a hydrophobic group that interacts with the main chain atoms of glutamine 21, cysteine 22 and glycine 23 wherein the distance between the centroid of said hydrophobic group and the centroids of glutamine 21 , cysteine 22 and glycine 23 are 3.7-5.4, 4.9-5.7 and 5.4-6.7Å, respectively; or

(vii) a hydrophobic group that interacts with the side chain atoms of glutamine 143 and asparagine 161 and the main chain of alanine 137 and serine 138 wherein the distance between the centroid of the hydrophobic group and the centroids of glutamine 143, asparagine 161, alanine 137, and serine 138 are 7.9-9.6Å, 4.7-5.4Å, 4.2-5.5Å, and 4.6-6.4Å, respectively.

3. A method of inhibiting cathepsin K which comprises administering to a mammal in need thereof a compound that fits spatially into the active site of cathepsin K, said compound comprising:

(i) an electrophilic carbon atom that binds to the side chain sulfur atom of cysteine 25 wherein said electrophilic carbon atom is 1.7-4.0Å from said sulfur atom; and

(ii) a hydrophobic group that interacts with tryptophan 184 wherein the distance between the centroid of said hydrophobic group and the centroid of the side chain atoms of tryptophan 184 is 4.10-7.10Å.

4. The method of claim 3 wherein said hydrophobic group that interacts with tryptophan 184 is an aromatic group.

5. The method of claim 4 wherein the centroid of said aromatic group that interacts with tryptophan 184 is 9.24-11.24Å from the centroid of said electrophilic carbon that binds to the side chain sulfur atom of cysteine 25.

6. The method of claim 3 wherein said electrophilic carbon that binds to the side chain sulfur atom of cysteine 25 is a carbonyl carbon.

7. The method of claim 3 wherein the compound further comprises a hydrophobic group that:

has a centroid which is 5.44-6.94Å from said electrophilic carbon;

interacts with tyrosine 67, methionine 68, alanine 134, leucine 160, and leucine 209, creating a hydrophobic pocket; and

has distance ranges between the centroid of said hydrophobic group and the centroids of the side chain atoms of the amino acid residues of said hydrophobic pocket which are tyrosine 67: 4.91- 5.91Å, methionine 68: 5.74-6.74Å, alanine 134: 4.15-5.15Å, leucine 160: 6.18-7.18Å, and leucine 209: 5.71-6.71Å.

8. The method of claim 7 wherein said hydrophobic group that interacts with said hydrophobic pocket is an isobutyl group.

9. The method of claim 3 wherein the compound further comprises a hydrophobic group that interacts with tyrosine 67 wherein the distance between the centroid of said hydrophobic group and the centroid of the side chain atoms of tyrosine 67 is 4.10-7.10Å.

10. The method of claim 9 wherein said hydrophobic group that interacts with tyrosine 67 is an aromatic group.

11. The method of claim 3 wherein the compound further comprises an amino group with a pKa of less than 7 or an oxygen atom, each of which interacts with a hydrogen atom donated by the amide nitrogen of glycine 66 wherein the distance between these two atoms is 2.7-3.5Å.

12. The method of claim 3 wherein the compound further comprises a hydrophobic group that interacts with the main chain atoms of glutamine 21, cysteine 22 and glycine 23 wherein the distance between the centroid of said hydrophobic group and the centroids of glutamine 21 , cysteine 22 and glycine 23 are 3.7-5.4, 4.9-5.7 and 5.4-6.7Å, respectively.

13. The method of claim 12 wherein said hydrophobic group that interacts with glutamine 21, cysteine 22 and glycine 23 is an isobutyl group.

14. The method of claim 3 wherein the compound further comprises a hydrophobic group that interacts with the side chain atoms of glutamine 143 and asparagine 161 and the main chain of alanine 137 and serine 138 wherein the distance between the centroid of the hydrophobic group and the centroids of glutamine 143, asparagine 161, alanine 137, and serine 138 are 7.9-9.6Å, 4.7-5.4Å, 4.2-5.5Å, and 4.6-6.4Å, respectively.

15. The method of claim 1 wherein the compound is:

3(S)-3-[(N-benzyloxycarbonyl)-L-leucinyl]amino-5-methyl-1-(1-propoxy)-2-hexanone;

4-[N-[(4-pyridylmethoxy)carbonyl]-L-leucyl]-1-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-3-pyrrolidinone;

4-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-1-N-[N-(methyl)-L-leucyl)]-3-pyrrolidinone;

4-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-1-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-3-pyrrolidinone;

bis-(Cbz-leucinyl)-1,3-diamino-propan-2-one;

2-[N-(3-benzyloxybenzoyl)]-2'-[N'-(N-benzyloxycarbonyl-L-leucinyl)]carbohydrazide;

(1S)-N-[2-[(1-benzyloxycarbonylamino)-3-methylbutyl]thiazol-4-ylcarbonyl]-N'-(N-benzyloxycarbonyl-L-leucinyl)hydrazide;

1-N-(N-imidazole acetyl-leucinyl)-amino-3-N-(4-phenoxy-phenyl-sulfonyl)-amino-propan-2-one; or

2,2'-N,N'-bis-benzyloxycarbonyl-L-leucinylcarbohydrazide;

or a pharmaceutically acceptable salt thereof.

16. A composition comprising cathepsin K in crystalline form.

17. The composition according to claim 16 wherein cathepsin K has an active site cavity formed by the amino acids in Table XXIX.

18. The composition of claim 17 wherein said active site is characterized by the coordinates selected from the group consisting of the coordinates of Tables I-X.

19. A cathepsin K crystal.

20. An isolated, properly folded cathepsin K molecule or fragment thereof having a conformation comprising a catalytically active site formed by the residues listed in Table XXIX, said active site defined by the protein coordinates of Table I.

21. A peptide, peptidomimetic or synthetic molecule which binds with the active site cavity of cathepsin K according to claim 17.

22. A method of identifying an inhibitor compound capable of binding to, and inhibiting the proteolytic activity of, cathepsin K, said method comprising:

introducing into a suitable computer program information defining an active site conformation of a cathepsin K molecule comprising a catalytically active site formed by the residues listed in Table XXIX, said active site defined by the protein coordinates of Table I, wherein said program displays the three-dimensional structure thereof;

FIGURE 1

```
                                1                                                  50
CatK        .......... .MWGLKVLLL PVVSF....A .LYPEEILDT HWELWKKTHR KQ.YNNKVDE ISRRLIWEKN LKYISIHNLE ASLGVHTYEL
CatS        .......... MKRLVCVLLV CSSAV....A QLHKDPTLDH HWHLWKKTYG KQ.YKEKNEE AVRRLIWEKN LKFVMLHNLE HSMGMHSYDL
CatL        .......... ...MNPTLIL AAFCLGIASA TLTFDHSLEA QWTKWKAMHN RL.Y.GMNEE GWRRAVWEKN MKMIELHNQE YREGKHSFTM
Papain      .......... .......... .......... .......... .......... .......... .......... .......... ..........
Actinidin   MGLPKSFVSM SLLFFSTLLI LSLAFNAKNL TQRTNDEVKA MYESWLIKYG KS.YNSLGEW ERRFEIFKET LRFIDEHNAD ...TNRSYKV
CatH        .......MWA TLPLLCAGAW LLGVPVCGAA ELSVNSLEKF HFKSWMSKHR KT.Y.STEEY HHRLQTFASN WRKINAHN.. ..NGNHTFKM
CatB        .......... .......... .......... .......... MWQLWASLCC LLVLANARSR PSFHPVSDEL VNYVNKRNTT WQAGHNFYNV

                                100                                                150
CatK        AMNHLGDMTS EEVVQKMTGL KVPLSHSRSN DTLYIPEWEG RAPDSVDYRK KG.YVTPVKN QGQCGSCWAF SSVGALEGQL KKKTGKLLN.
CatS        GMNHLGDMTS EEVMSLTSSL RVP.SQWQRN IT.YKSNPNR ILPDSVDWRE KG.CVTEVKY QGSCGACWAF SAVGALEAQL KLKTGKLVT.
CatL        AMNAFGDMTS EEFRQVMNGF Q...NRKPRK GKVFQEPLFY EAPRSVDWRE KG.YVTPVKN QGQCGSCWAF SATGALEGQM FRKTGRLIS.
Papain      .......... .......... .......... .......... .IPEYVDWRQ KG.AVTPVKN QGSCGSCWAF SAVVTIEGII KIRTGNLNQ.
Actinidin   GLNQFADLTD EEFRSTYLGF .TSGSNKTKV SNRYEPRFGQ VLPSYVDWRS AG.AVVDIKS QGECGGCWAF SAIATVEGIN KIVTGVLIS.
CatH        ALNQFSDMSF AEIKHK...Y LWSEPQNCSA TKSNYLRGTG PYPPSVDWRK KGNFVSPVKN QGACGSCWTF STTGALESAI AIATGKMLS.
CatB        DMSYLKRLCG TFLGGPKPPQ RVMFTEDLKL PASFDAR... ......EQWP QCPTIKEIRD QGSCGSCWAF GAVEAISDRI CIHTNAHVSV

                                200                                                250
CatK        .LSPQNLVDC VSE...NDGC GGGYMTNAFQ YVQKNRGIDS EDAY...... .......... .......PYV GQEESCM... .....YNPTG
CatS        .LSAQNLVDC STEKYGNKGC NGGFMTTAFQ YIIDNKGIDS DASY...... .......... .......PYK AMDQKCQ... .....YDSKY
CatL        .LSEQNLVDC SGPQ.GNEGC NGGLMDYAFQ YVQDNGGLDS EESY...... .......... .......PYE ATEESCK... .....YNPKY
Papain      .YSEQELLDC DR..RSY.GC NGGYPWSALQ LVAQY.GIHY RNTY...... .......... .......PYE GVQRYCR... .....SREKG
Actinidin   .LSEQELIDC GRTQNTR.GC NGGYITDGFQ FIINNGGINT EENY...... .......... .......PYT AQDGECN... .....LDLQN
CatH        .LAEQQLVDC A.QDFNNYGC QGGLPSQAFE YILYNKGIMG EDTY...... .......... .......PYQ GKDGYCK... .....FQP.G
CatB        EVSAEDLLTC CGSMCG.DGC NGGYPAEAWN F.WTRKGLVS GGLYESHVGC RPYSIPPCEH HVNGSRPPCT GEGDTPKCSK ICEPGYSPTY
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FIGURE 1 (Cont.)

```
                                        300                                                                  350
CatK        K.AAKCRGYR EIPEGNEKAL KRAVARVGPV SVAIDASLTS FQFYSKGVYY DESC..NSDN LNHAVLAVGY G....IQKGN KHWIIKNSWG
CatS        R.AATCSKYT ELPYGREDVL KEAVANKGPV SVGVDARHPS FFLYRSGVYY EPSC...TQN VNHGVLVVGY G....DLNGK EYWLVKNSWG
CatL        S.VANDTGFV DIP.KQEKAL MKAVATVGPI SVAIDAGHES FLFYKEGIYF EPDC..SSED MDHGVLVVGY GFESTESDNN KYWLVKNSWG
Papain      PYAAKTDGVR QVQPYNQGAL LYSIAN.QPV SVVLQAAGKD FQLYRGGIFV GPC....GNK VDHAVAAVGY G....P.... NYILIKNSWG
Actinidin   EKYVTIDTYE NVPYNNEWAL QTAVTY.QPV SVALDAAGDA FKHYSSGIFT GPC....GTA IDHAVTIVGY G....TEGGI DYWIVKNSWD
CatH        KAIGFVKDVA NITIYDEEAM VEAVALYNPV SFAFEVTQD. FMMYRTGIYS STSCHKTPDK VNHAVLAVGY G....EKNGI PYWIVKNSWG
CatB        KQDKHYGYNS V:::NSEKDI MAEIYKNGPV EGAFSV.YSD FLLYKSGVYQ HVTGEMMG.. .GHAIRILGW G....VENGT PYWLVANSWN

                                        400                                                                  430
CatK        ENWGNKGYIL MARNKNNA.. .CGIANLASF PKM..... ..... ..... .....
CatS        HNFGEEGYIR MARNKGNH.. .CGIASFPSY PEI..... ..... ..... .....
CatL        EEWGMGGYVK MAKDRRNH.. .CGIASAASY PTV..... ..... ..... .....
Papain      TGWGENGYIR IKRGTGNSYG VCGLYTSSFY PVKN..... ..... ..... .....
Actinidin   TTWGEEGYMR ILRNVGGA.G TCGIATMPSY PVKYNNQNHP KPYSSLINPP AFSMSKDGPV GVDDGQRYSA
CatH        PQWGMNGYFL IERGKN.... MCGLAACASY PIPLV..... ..... ..... .....
CatB        TDWGDNGFFK ILRGQDHCGI ESEVVAGIPR TDQYWEKI.. ..... ..... .....
```

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FIGURE 2

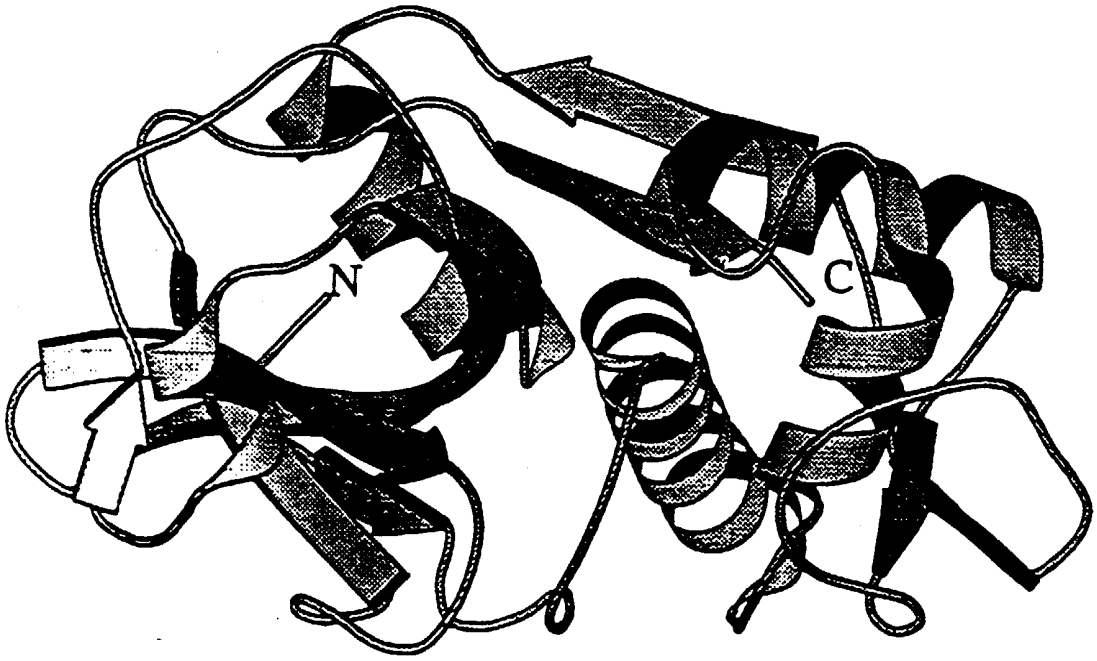


FIGURE 3

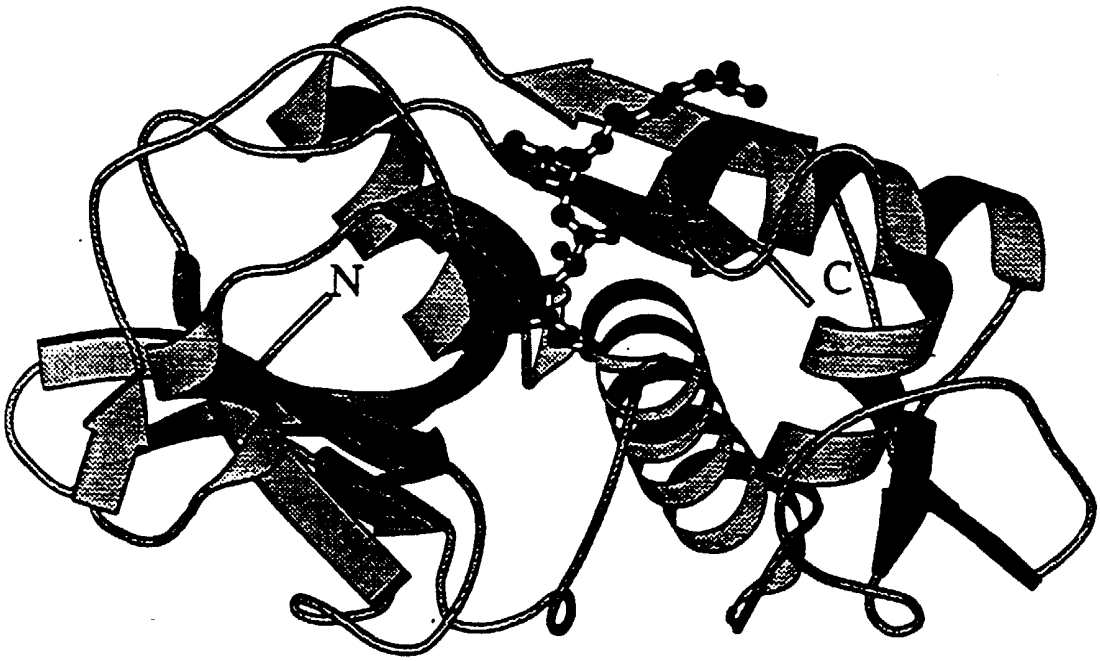
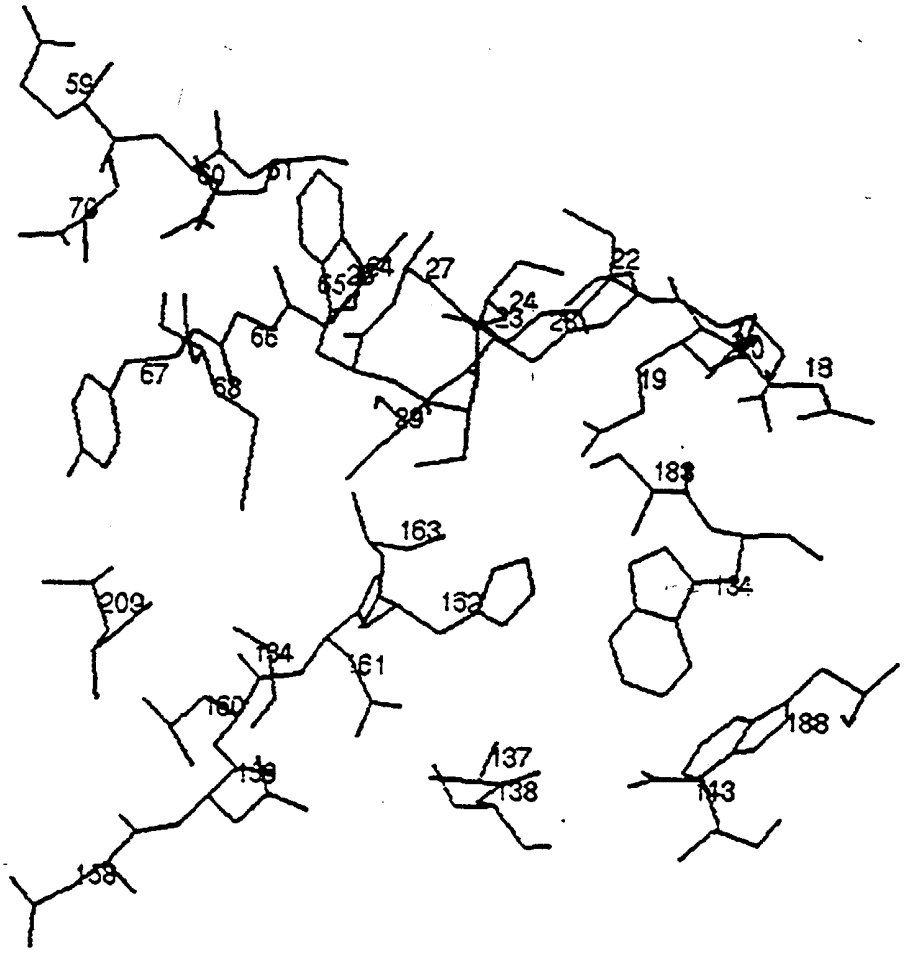


FIGURE 4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158

FIGURE 5

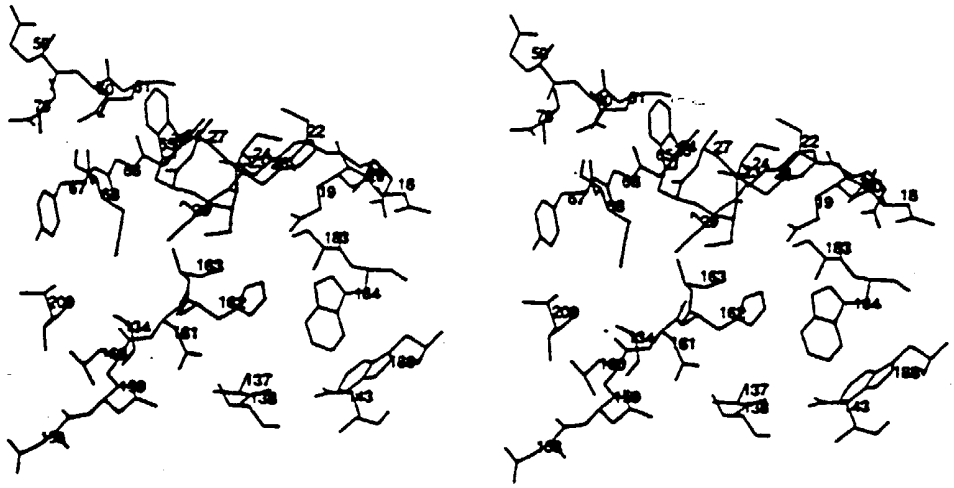


FIGURE 6

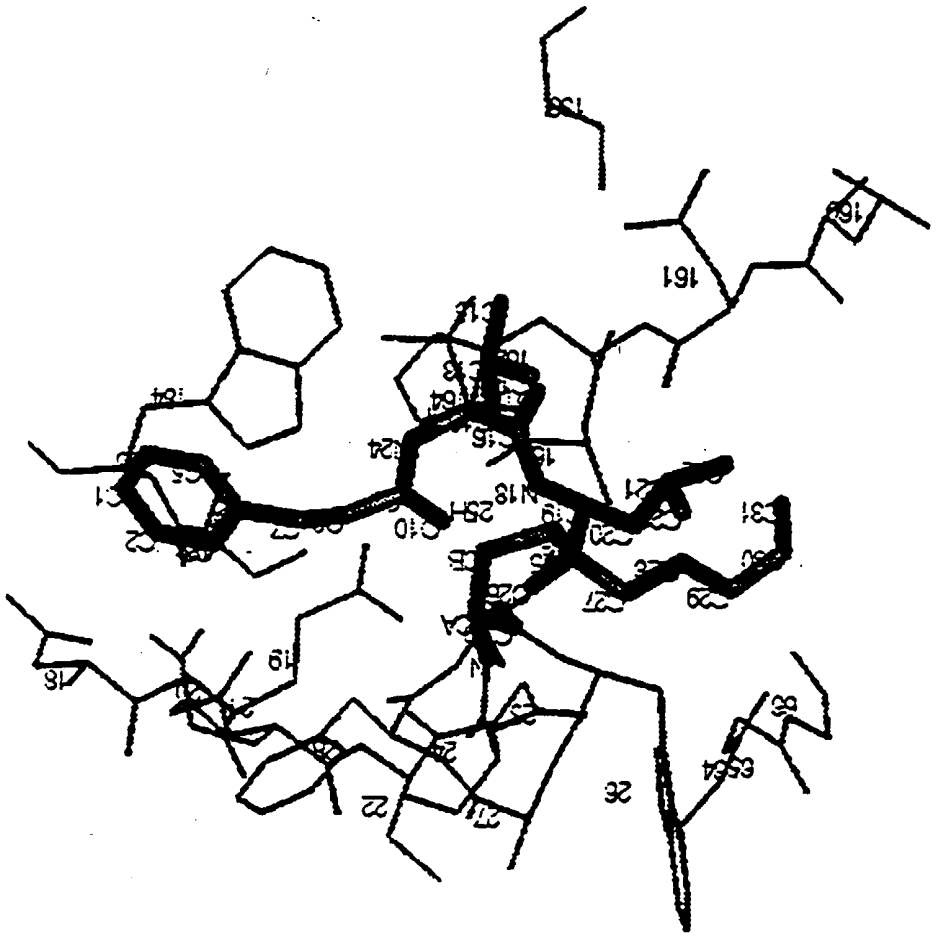


FIGURE 7

FIGURE 8

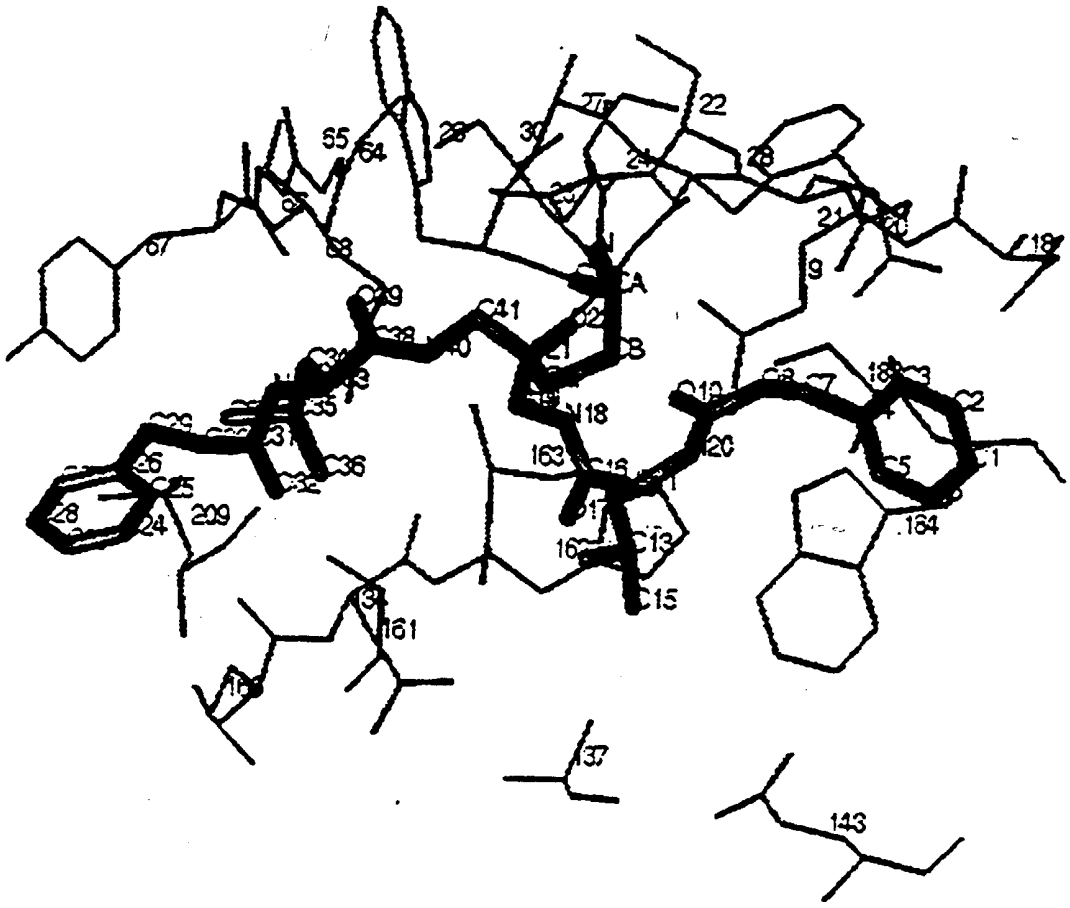


FIGURE 9

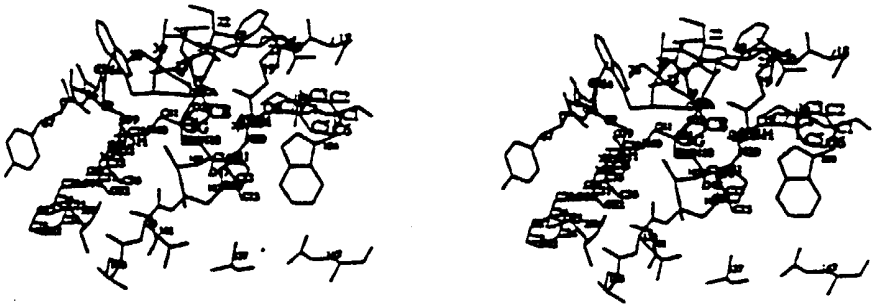
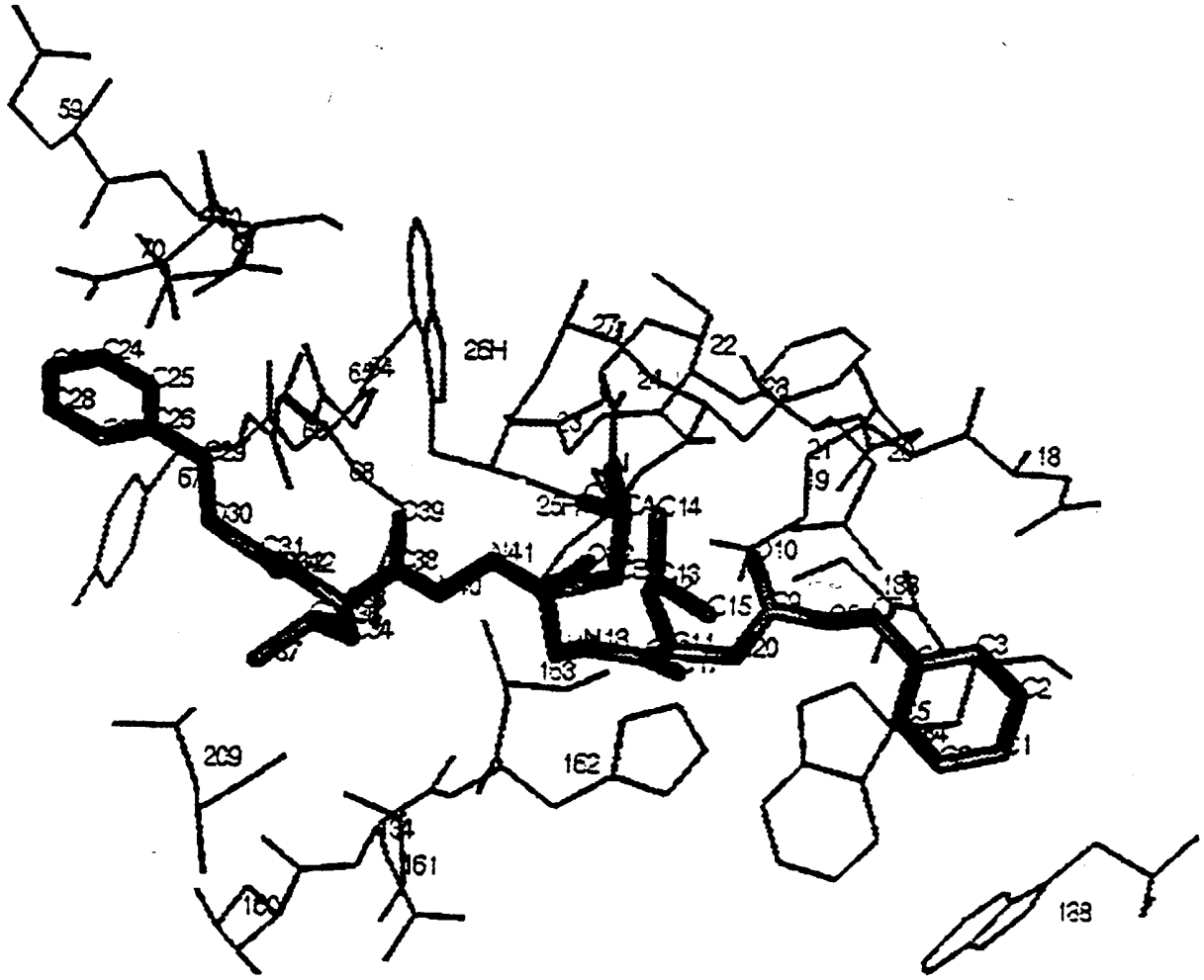


FIGURE 10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C28
C26
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C30
C31
C39
C38
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26H
27
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24
23
21
19
18
25H
C14
C13
C15
C10
20
153
162
209
161
160
188
C3
C2
C1

FIGURE 11

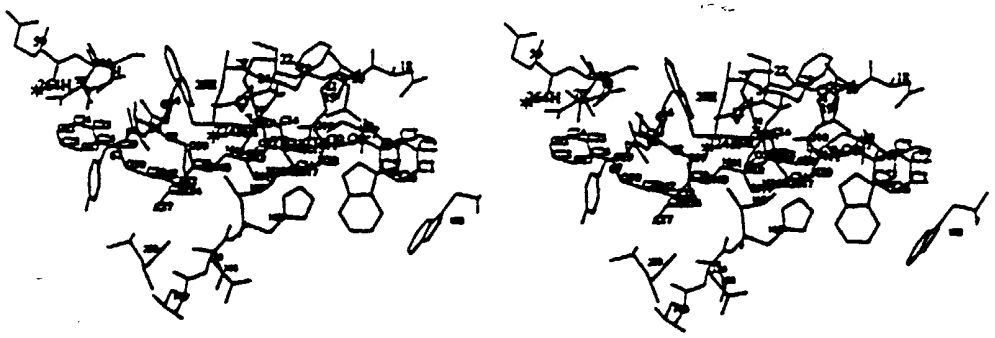


FIGURE 12

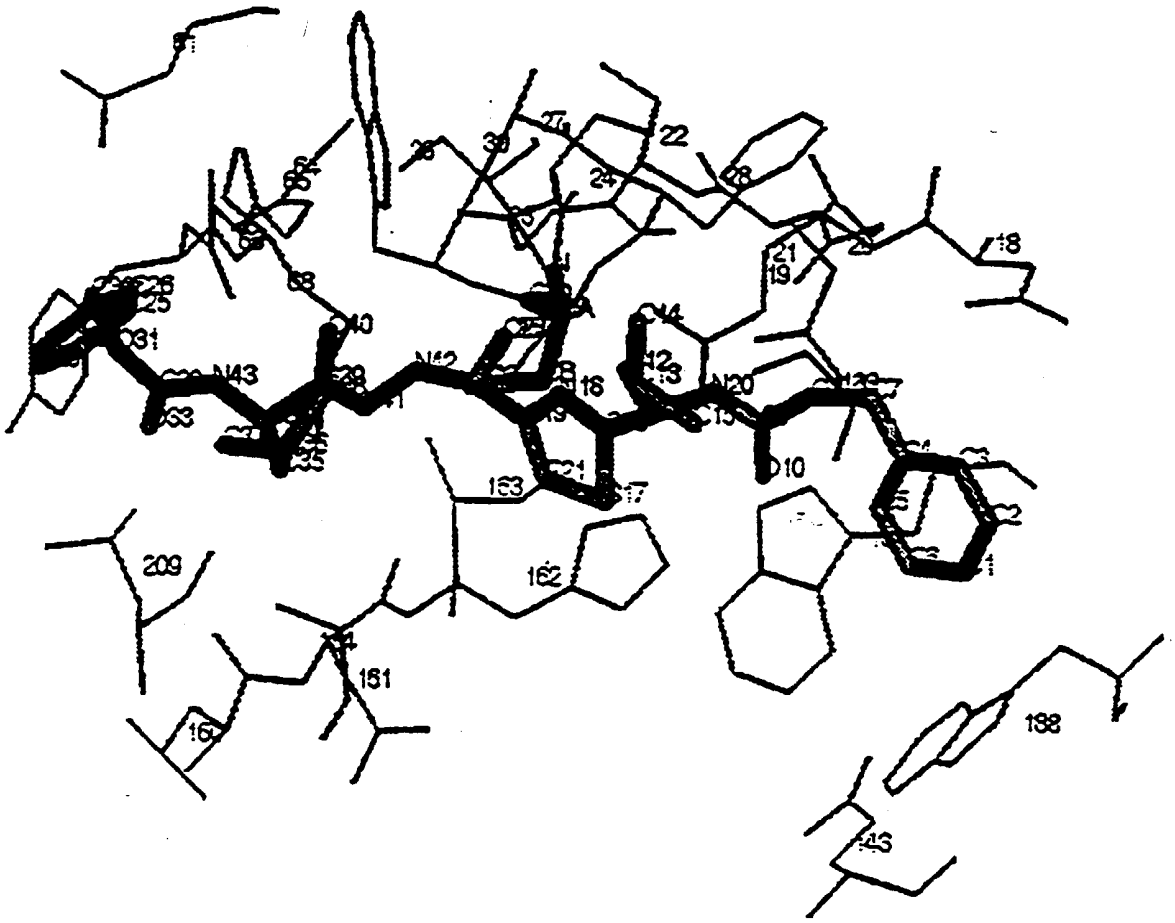


FIGURE 13

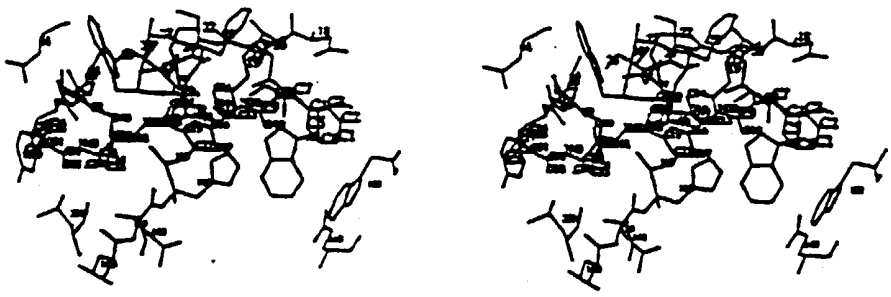


FIGURE 14

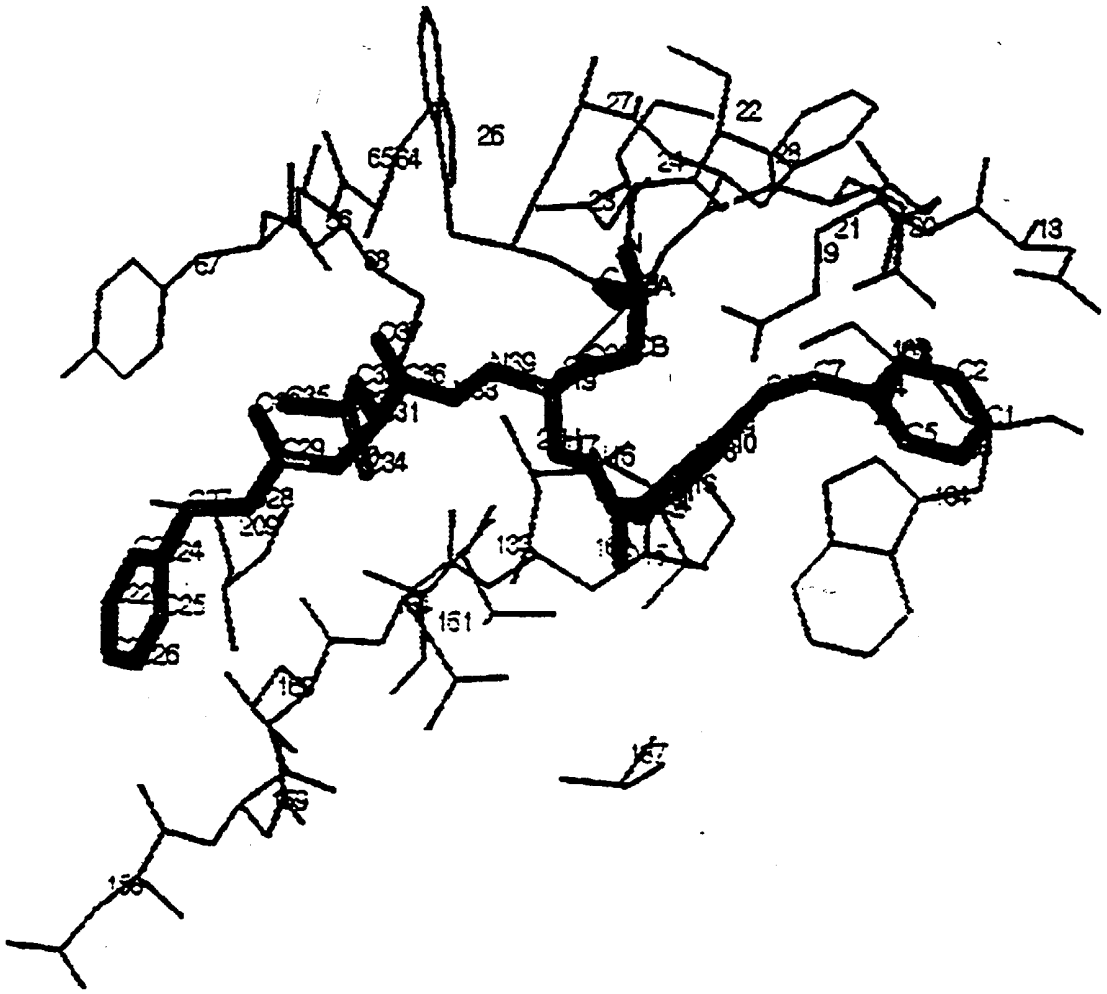


FIGURE 15

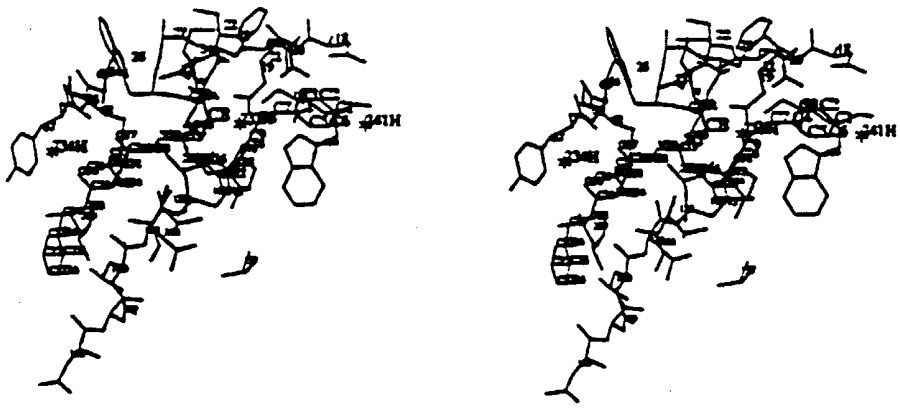
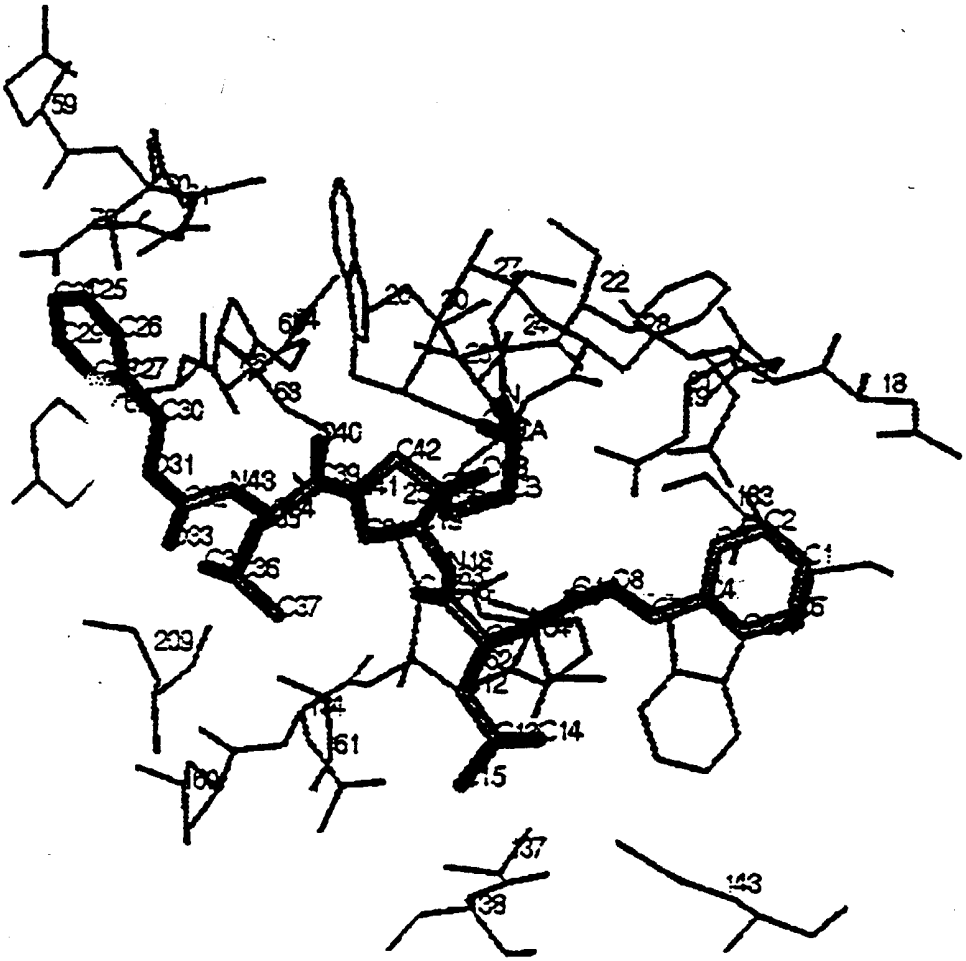


FIGURE 16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C37
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18
C2
C1
C14
137
38
143

FIGURE 17

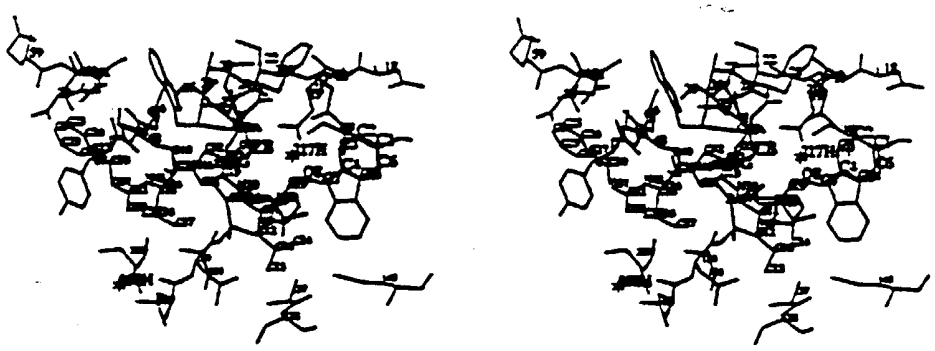
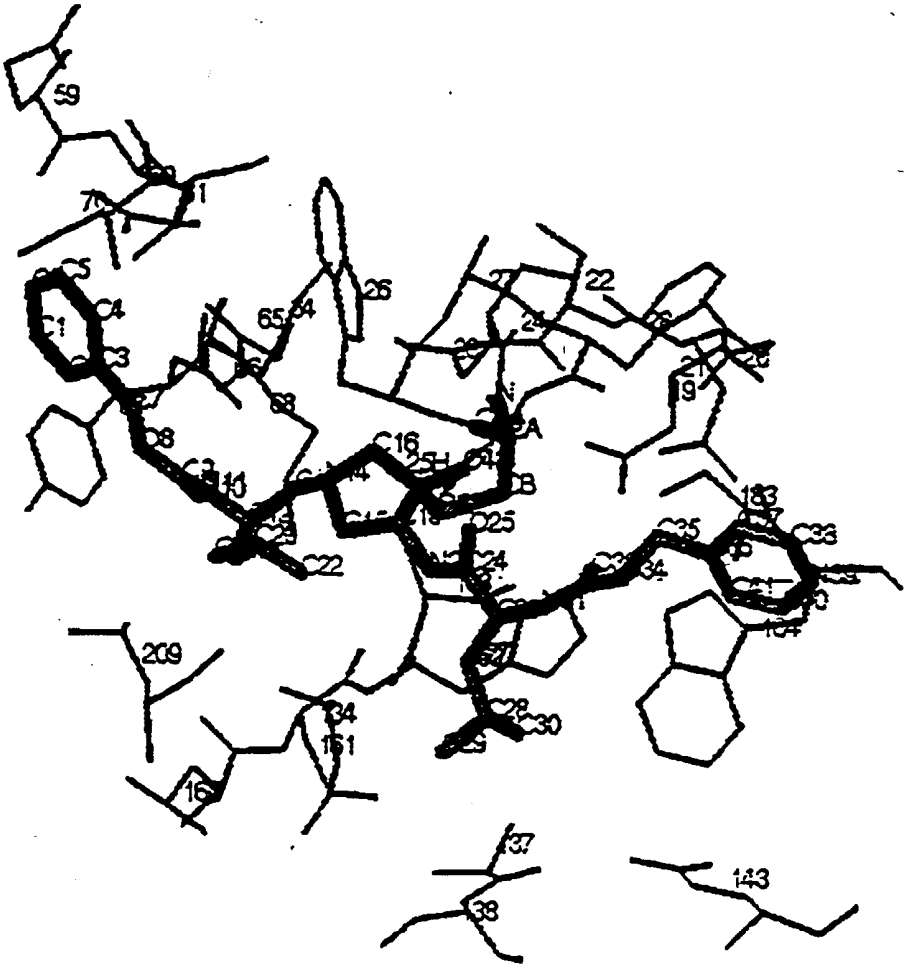


FIGURE 18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C4
C1
C3
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22
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19
C16
C22
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C24
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C28
C30
137
38
143

FIGURE 19

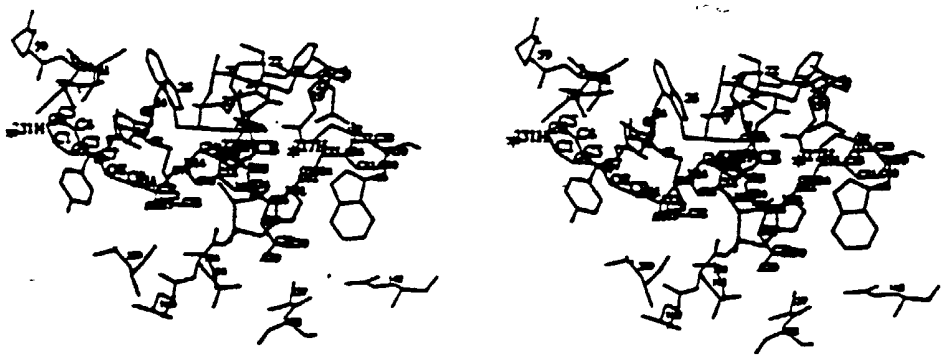

FIGURE 20

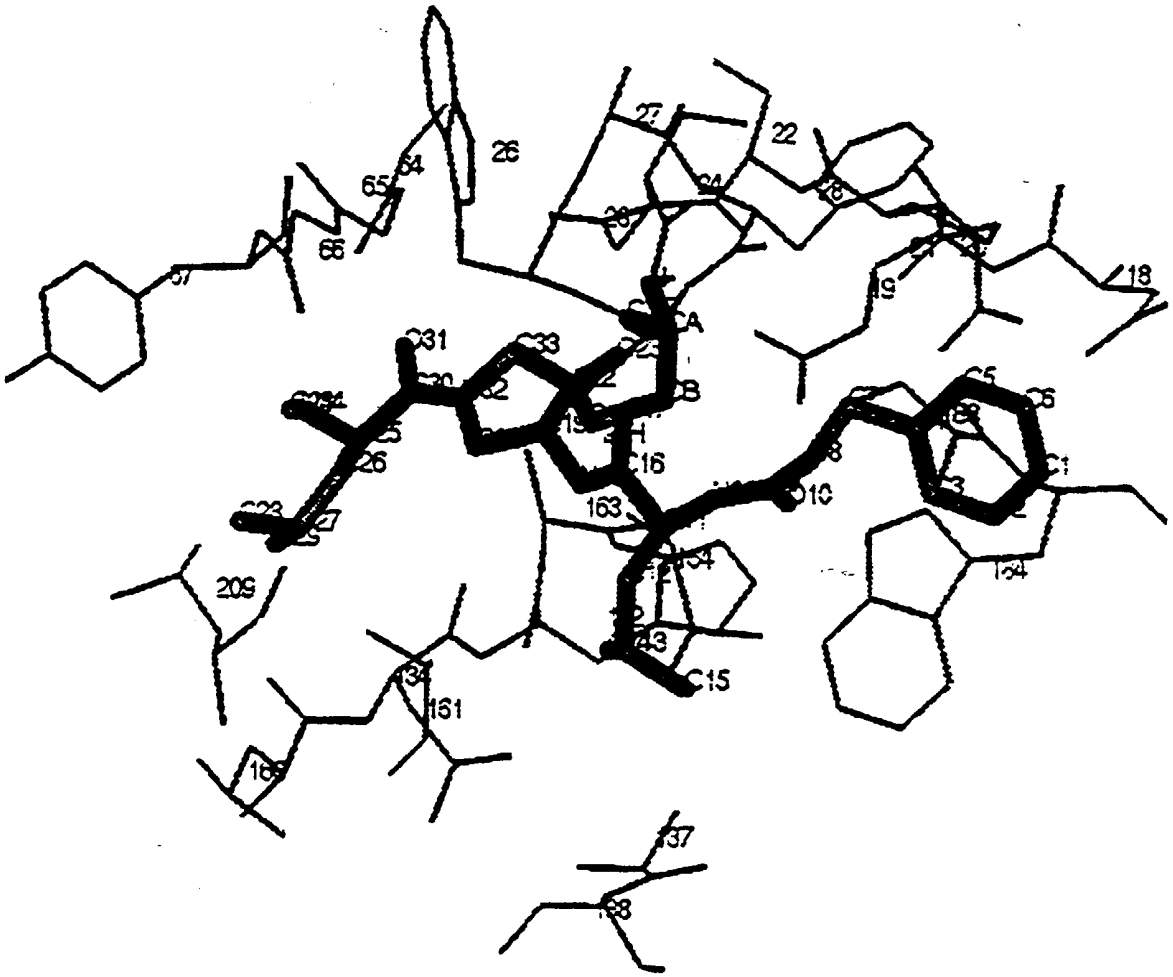

FIGURE 21

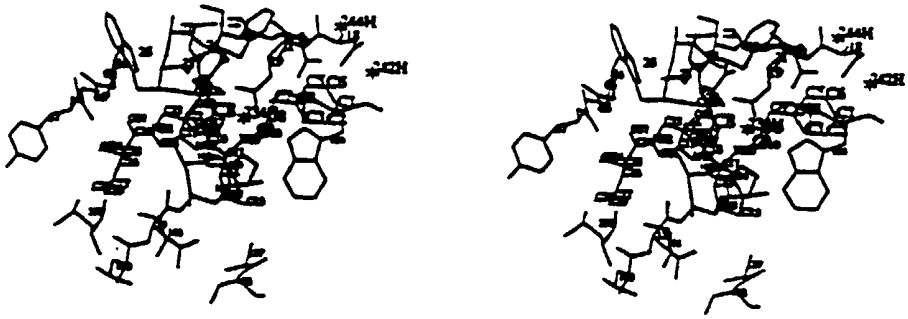

FIGURE 22

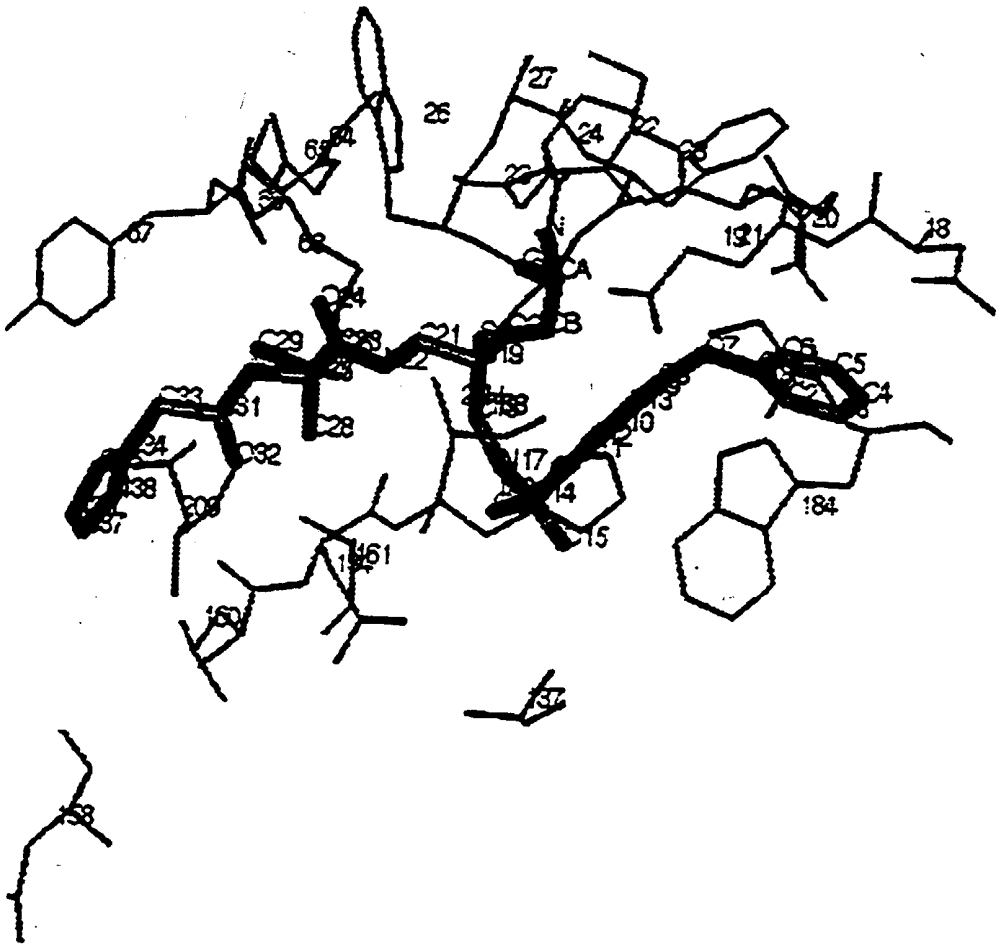

FIGURE 23