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(54) Title: CRYSTAL STRUCTURE OF OX40L AND OX40L COMPLEXED WITH OX40 RECEPTOR

(57) Abstract: The present disclosure provides crystals of and structural coordinates of mOX40L, hOX40L, hOX40 receptor and complexes thereof. The crystals and crystal structures are useful, for example, in the design and synthesis of modulators of mOX40L, hOX40L, and/or hOX40 receptor.



WO 2007/149880 A2

CRYSTAL STRUCTURES OF OX40L AND OX40L COMPLEXED WITH OX40 RECEPTOR

Cross Reference to Related Application

This application is a International Application which claims priority to U.S. Serial
5 No. 60/805,433, filed June 21, 2006, which application is hereby incorporated by reference.

Background of the Invention

Many members of the Tumor Necrosis Factor superfamily (TNFSF) and their
receptors modulate immune system activity either by triggering apoptosis or, conversely, by
acting as growth or survival factors (Locksley et al., *CeH*, 104:487-501 (2001)). OX40
10 (also known as TNFRSF4, ACT35, TXGPIL or CD134) along with TNFRSF family
members 4-1BB, CD27, CD30, and CD40 are co-stimulatory molecules acting at different
stages in T and B cell activation to modulate and control the immune response (Watts,
Annu Rev Immunol. 23:23-68 (2005)). The OX40-OX40L pair function relatively late in T
cell activation. OX40L (also known as TNFSF4, gp34, TXGPI) is expressed on the surface
15 of antigen presenting cells (APCs) approximately 1 to 3 days after initial antigen encounter
and interacts with OX40 expressed on activated T cells (Croft, *Cytokine Growth Factor
Rev*, 14:265-273 (2003)). This interaction results in recruitment of TRAF2 and signals for
T cell survival in a survivin dependent manner (Song et al., *Immunity*, 22:621-631 (2005)).
OX40 activity is implicated in the generation of activated TH1 and TH2 cells as well as the
20 maintenance of memory T cell populations (Croft, cited supra; Weinberg et al., *J Leukoc
Biol*, 75:962-972 (2004)).

The cytokine, TSLP, which has a robust association with TH2 pathologies in human
disease, has recently been shown to trigger OX40L expression on dendritic cells (Ito et al., *J
Exp Med*, 202:1213-1223 (2005)). Additionally, OX40 and OX40L knock-out mice are
25 deficient in TH2 responses suggesting that TH2 polarization is the pathway most influenced
by OX40 signaling (Jember et al., *J Exp Med*, 193:387-392 (2001); Hoshino et al., *Eur J
Immunol*, 33:861-869 (2003)). Consistent with this hypothesis, treatment with anti-OX40L
monoclonal antibodies which block interaction with OX40 results in reduced cytokine
production, antigen specific IgE levels and lung inflammation in murine models of allergic
30 asthma (Hoshino et al., cited supra). Blocking of OX40-OX40L interaction in vivo has been
shown to reduce severity of disease in acute graft vs. host disease, inflammatory bowel
disease, and collagen induced arthritis (Weinberg et al., *Trends in Immunology*, 23:102
(2002)).

Despite their varied biological roles, TNFSF ligands are generally homotrimeric
35 proteins composed of three jelly roll protomers. Each protomer is formed by two β -sheets

which contain strands A'AHCF and B'BGDE. Most TNFSF ligands are type II transmembrane proteins and several, such as FasL, TNF, BAFF, and EDA, have processing sites allowing them to be released from the cell surface to act as soluble factors (Bodmer et al., Trends Biochem Sci, 27:19-26 (2002)). The TNFSF ligands can roughly be divided into
5 three groups based on sequence and structural features: the conventional, the EF-disulfide containing, and the divergent.

The "conventional" TNFSF members include TNF, LTa₁LT₂, Apo2L/TRAIL, TL1A, LIGHT, FasL, RANKL and CD40L. Crystal structures are available for TNF, LTa, Apo2L/TRAIL, RANKL and CD40L. These structures and models indicate that these
10 ligands all have relatively long loops connecting the CD, DE and EF strands giving the trimers a characteristic pyramidal shape. The "conventional" ligands all have, in the DE loop, a conserved hydrophobic residue (generally a tyrosine) which has been shown to be energetically important for receptor binding in several of the family members.

The second TNFSF ligand group, the "EF-disulfide" group, includes APRIL, BAFF, TWEAK and EDA. Crystal structures are available for APRIL, BAFF and EDA (Hymowitz et al. Biochemistry, 39:633-640 (2000); Karpusas et al, J Mol Biol, 315:145-154 (2002); Wallweber et al, J Mol Biol, 343:283-290 (2004)). These ligands all possess a disulfide
15 connecting the E and F strands and are characterized by shorter CD and EF loops resulting in a more globular shape. Receptor binding by this TNFSF group also differs from the conventional ligand group as they lack the conserved hydrophobic residues in the DE loop. In addition, three (APRIL, BAFF and TWEAK) of the these four ligands have been shown to bind very small atypical TNFSF members (BR3, TACI, BCMA, and Fn14) (Bodmer et al, cited supra).

The third "divergent" ligand group includes CD27L, CD30L, GITRL, 4-1BBL, and OX40L. These ligands all have sequences that are very divergent from each other and from
25 either the "conventional" or "EF-disulfide" groups. No structural or mutagenesis data is available to validate if or how these ligands assemble into trimers or interact with receptors. OX40L is an example of this group. It is one of the most divergent members of the TNFSF with only ~10-15% sequence identity to other family members and is also very compact
30 with only 132 residues in the entire extra cellular region of human OX40L. In addition to the lack of sequence homology within the TNF-domain, OX40L also has an unusually short linker between the extracellular TNF homology domain and the transmembrane helix with no discernable proteolytic site and thus is expected to exist only in a membrane bound state (Baum et al, Embo J, 13:3992-4001 (1994); Godfrey et al, J Exp Med, 180:757-762
35 (1994)).

In contrast to the globular ligands, TNFRSF receptors are elongated molecules composed of an extracellular domain of ~40 residue pseudo repeats typically containing 6 cysteines forming 3 disulfide bonds. These modules are termed CRDs (cysteine rich domains) and can be further subdivided into smaller submodules based on the number of cysteines and topology of the cysteine connectivity (Naismith and Sprang, Trends Biochem Sci, 23:74-79 (1998)). A typical CRD is composed of A1 and B2 tandemly linked subdomains. The A1 subdomain contains a single disulfide (the 1-2 disulfide) while the B2 subdomain contains two disulfides which are linked in a 3-5, 4-6 topology. Other subdomain variants exist such as the A2 which contains two disulfides or the B1 which lacks one of the characteristic disulfides. Sequence analysis suggests that, unlike OX40L, OX40 is a relatively conventional member of the TNFRSF. The extracellular ligand binding domain of OX40 is composed of three full CRD and a partial, fourth C-terminal CRD (Godfrey, W. R. et al., cited supra). Both CRD1 and CRD2 have the prototypical A1-B2 linkage while CRD3 is an atypical CRD with the more unusual A1-B1 linkage.

As discussed previously, OX40 is implicated in the generation of TH1 and TH2 cells. The T-helper cell subsets (TH1 and TH2) define 2 pathways of immunity: cell-mediated immunity and humoral immunity. Release profiles of cytokines for TH1 and TH2 subtypes influence selection of effector mechanisms and cytotoxic cells (Mosmann et al., Adv. Immunol., 46:1 11-147 (1989); Mosmann et al., Immunol. Today, 17:138-146 (1996)). TH1 cells, a functional subset of CD4⁺ cells, are characterized by their ability to boost cell-mediated immunity and produce cytokines including 11-2, interferon-gamma, and lymphotoxin beta (Mosmann et al., 1989, 1996, supra). 11-2 and interferon-gamma secreted by TH1 cells activate macrophages and cytotoxic cells. TH2 cells are also CD4⁺ cells, but are distinct from TH1 cells. TH2 cells are characterized by their ability to boost humoral immunity, such as antibody production. TH2 cells produce cytokines, including 11-4, 11-5, and 11-10 (Mosmann et al., 1989, 1996, supra). 11-4, 11-5, and 11-10 secreted by TH2 cells increase production of eosinophils and mast cells, as well as enhance production of antibodies, including IgE, and decrease the function of cytotoxic cells (Powrie et al., Immunol. Today, 14:270 (1993)). Overproduction of cytokines produced by either or both of TH1 and TH2 cells impacts a host of medical disorders. For example, overproduction of TH1 cytokines contributes to pathogenesis of various autoimmune disorders, such as multiple sclerosis and rheumatoid arthritis. Overproduction of TH2 cytokines contributes to pathogenesis of allergic disorders.

There remains a need to develop new therapies useful to treat immune system diseases, autoimmune diseases, allergic disorders, and other diseases associated with TNF receptor signaling such as cancer.

Summary of the Invention

The present disclosure thus includes a crystalline form and a crystal structure of murine OX40L (mOX40L), a crystalline form and a crystal structure of human OX40L (hOX40L) complexed with a human OX40 receptor (hOX40), and a crystalline form and a crystal structure of mOX40L complexed with a hOX40 receptor. In other aspects, the disclosure provides methods of using the crystal structures and structural coordinates to identify homologous proteins and to design or identify agents that can modulate the function of the mOX40L, hOX40L, hOX40 receptor, and combinations thereof. The present disclosure also includes the three-dimensional configuration of points derived from the structure coordinates of at least a portion of a molecule or molecular complex, as well as structurally equivalent configurations, as described below. The three-dimensional configuration includes points derived from structure coordinates representing the locations of at least one or a plurality of the amino acids defining a binding site on mOX40L for a hOX40 receptor, a binding site on hOX40L for the hOX40 receptor, or a binding site on hOX40 receptor for either the mOX40L and/or hOX40L.

In some embodiments, the three-dimensional configuration includes points derived from structure coordinates representing the locations of the backbone atoms of a plurality of amino acids defining a binding site on mOX40L for the hOX40 receptor, a binding site on hOX40L for the hOX40 receptor, or a binding site on hOX40 receptor for either the mOX40L or hOX40L. Alternatively, the three-dimensional configuration includes points derived from structure coordinates representing the locations of the side chain and the backbone atoms (other than hydrogens) of a plurality of the amino acids defining a binding site on mOX40L for the hOX40 receptor, a binding site on hOX40L for the hOX40 receptor, or a binding site on hOX40 receptor for either the mOX40L or hOX40L.

In some embodiments, a crystal comprising a murine OX40L comprising SEQ ID NO: 1, or a fragment of SEQ ID NO: 1 comprising the sequence of amino acids 51 to 198 of SEQ ID NO: 1 is provided. In some embodiments, a crystal of mOX40L diffracts Xrays to a resolution of 5 Å or better. In some embodiments, a crystal of mOX40L diffracts Xrays to a resolution of at least 1.45 to 2.5 Å or better. Also provided herein is a crystal of a fragment of mOX40L having a space group symmetry of $P6_3$ and comprising a unit cell having the dimensions of $a=b$ and are about 74Å, and c is about 48Å. The unit cell dimensions can vary at least about plus or minus about 0.5 Å. The structural coordinates for mOX40L are provided in Table 8. In some embodiments, a composition comprises a crystal of mOX40L. Compositions and crystals of mOX40L may be a useful way to store, deliver or purify mOX40L.

In some embodiments, a cocrystal comprising a murine OX40L comprising SEQ ID NO:1, or a fragment of SEQ ID NO:1 comprising the sequence of amino acids 51 to 198 of SEQ ID NO:1 and hOX40 receptor comprising an amino acid sequence of SEQ ID NO:2 or a fragment of SEQ ID NO:2 comprising the sequence of amino acids 29 to 170 of SEQ ID NO:2 is provided. In some embodiments, a cocrystal of mOX40L-hOX40 receptor diffracts Xrays to a resolution of 5 Å or better. In some embodiments, a cocrystal of mOX40L-hOX40 receptor diffracts Xrays to a resolution of at least 1.45 to 2.5 Å or better. Also provided herein is a cocrystal of a fragment of mOX40L and a fragment of a hOX40 receptor having a space group symmetry of R32 and comprising a unit cell having the dimensions of $a=b$ and are about 105 Å, and c is about 478 Å. The unit cell dimensions can vary at least about plus or minus about 0.5 Å. The structural coordinates for the cocrystal of mOX40L and hOX40L are provided in Table 9. In some embodiments, a composition comprises a cocrystal of mOX40L and hOX40 receptor. Compositions and crystals of mOX40L and hOX40 receptor may be a useful way to store, deliver or purify mOX40L and/or hOX40 receptor.

In some embodiments, a cocrystal comprising a human OX40L comprising SEQ ID NO:3, or a fragment of SEQ ID NO:3 comprising the sequence of amino acids 51 to 183 of SEQ ID NO:3 and hOX40 receptor comprising an amino acids sequence of SEQ ID NO:2 or a fragment of SEQ ID NO:2 comprising the sequence of amino acids 29 to 170 of SEQ ID NO:2 is provided. In some embodiments, a cocrystal of hOX40L-hOX40 receptor diffracts Xrays to a resolution of 5 Å or better. In some embodiments, a cocrystal of hOX40L-hOX40 receptor diffracts Xrays to a resolution of at least 1.45 to 2.5 Å or better. Also provided herein is a cocrystal of a fragment of hOX40L and a fragment of a hOX40 receptor having a space group symmetry of R32 and comprising a unit cell having the dimensions of $a=b$ and are about 112 Å, and c is about 233 Å. The unit cell dimensions can vary at least about plus or minus about 0.5 Å. The structural coordinates for the cocrystal of hOX40L and hOX40L are provided in Table 10. In some embodiments, a composition comprises a cocrystal of hOX40L and hOX40 receptor. Compositions and crystals of hOX40L and hOX40 receptor may be a useful way to store, deliver or purify hOX40L and/or hOX40 receptor.

In another aspect, the disclosure includes mOX40L polypeptides and polynucleotides encoding the polypeptides. The disclosure includes a polynucleotide encoding a polypeptide and/or a polypeptide having at least 90% sequence identity to the polypeptide comprising the amino acid sequence of amino acids 51-198 of SEQ ID NO:1, not including the polypeptide having the amino acid sequence of SEQ ID NO:1 or SEQ ID NO:3, and wherein the polypeptide binds a hOX40 receptor or a hOX40 receptor ligand

binding fragment thereof. Another embodiment, comprises a polynucleotide encoding a polypeptide and/or a polypeptide that comprises the amino acid sequence starting at any one of amino acids 51 to amino acid residue 66 and ending at any one of amino acids 180 to 191 of SEQ ID NO: 1, not including the polypeptide having the amino acid sequence of SEQ ID NO: 1 or SEQ ID NO:3, and wherein the polypeptide binds a hOX40 receptor or a hOX40 receptor ligand binding fragment thereof. In some embodiments, a polynucleotide encoding a polypeptide and/or a polypeptide has at least 90% sequence identity to the polypeptide comprising the amino acid sequence of amino acids 64 to 190 of SEQ ID NO:1, not including the polypeptide having the amino acid sequence of SEQ ID NO: 1 or SEQ ID NO:3, and wherein the polypeptide binds a hOX40 receptor or a hOX40 receptor ligand binding fragment thereof. In some embodiments, a polynucleotide encoding a polypeptide and/or a polypeptide has at least 90% sequence identity to the polypeptide comprising the amino acid sequence of amino acids 99 to 191 of SEQ ID NO:1, not including the polypeptide having the amino acid sequence of SEQ ID NO: 1 or SEQ ID NO:3, and wherein the polypeptide binds a hOX40 receptor or a hOX40 receptor ligand binding fragment thereof. The disclosure also includes a crystalline form of each of these polypeptides.

The present disclosure also includes an isolated polypeptide comprising, consisting essentially of, or consisting of a portion or fragment of the mOX40L. In some embodiments, the polypeptide comprises a binding site for hOX40 receptor. In other embodiments, the polypeptide comprises an extracellular domain of mOX40L. In other embodiments, the polypeptide comprises the trimer interface. In some embodiments, the trimer interface includes amino acid residues corresponding to amino acids 99 to 191 of SEQ. ID NO: 1. An embodiment of a polypeptide comprises, consists essentially of, or consists of an amino acid residue starting from any one of amino acid residue 51 to amino acid residue 66 and ending at amino acid residue 180 to residue 191 or residues corresponding to those positions in the polypeptide comprising SEQ ID NO: 1, excluding the amino acid sequence of SEQ ID NO: 1. An embodiment of a polypeptide comprises, consists essentially of, or consists of an amino acid residues corresponding to amino acid residues 51 to 198 in the polypeptide comprising SEQ ID NO:1, excluding the amino acid sequence of SEQ ID NO:1. An embodiment of a polypeptide comprises, consists essentially of, or consists of an amino acid residues corresponding to amino acid residues 64 to 189 or 190 in the polypeptide comprising SEQ ID NO:1, excluding the amino acid sequence of SEQ ID NO: 1. In some embodiments, the polypeptide has the ability to bind to hOX40 receptor. The disclosure also includes polynucleotides encoding such polypeptides and/or a hOX40

receptor ligand binding fragment thereof. The disclosure also includes a crystalline form of each of these polypeptides.

The disclosure also includes a polynucleotide encoding a polypeptide and/or a polypeptide having at least 90% sequence identity to the polypeptide comprising the amino acid sequence of amino acids 51 to 183 of SEQ ID NO:3, not including the polypeptide having the amino acid sequence of SEQ ID NO:3 or SEQ ID NO: 1, and wherein the polypeptide binds a hOX40 receptor or a hOX40 receptor ligand binding fragment thereof. Another embodiment, comprises a polynucleotide encoding a polypeptide and/or a polypeptide that comprises the amino acid sequence starting at any one of amino acids 51 to amino acid residue 65 and ending at any one of amino acids 180 to 183 of SEQ ID NO:3, not including the polypeptide having the amino acid sequence of SEQ ID NO:3 or SEQ ID NO: 1, and wherein the polypeptide binds a hOX40 receptor a hOX40 receptor ligand binding fragment thereof. In some embodiments, a polynucleotide encoding a polypeptide and/or a polypeptide has at least 90% sequence identity to the polypeptide comprising the amino acid sequence of amino acids 98 to 183 of SEQ ID NO:3, not including the polypeptide having the amino acid sequence of SEQ ID NO:3 or SEQ ID NO:1, and wherein the polypeptide binds a hOX40 receptor a hOX40 receptor ligand binding fragment thereof.. The disclosure also includes a crystalline form of each of these polypeptides.

In another aspect, the disclosure includes hOX40L polypeptides and polynucleotides encoding the polypeptides. The present disclosure also includes an isolated polypeptide comprising, consisting essentially of, or consisting of a portion or fragment of the hOX40L. In some embodiments, the polypeptide comprises a binding site for hOX40 receptor. In other embodiments, the polypeptide comprises the trimer interface. In other embodiments, the polypeptide comprises an extracellular domain of hOX40L. An embodiment of a polypeptide comprises, consists essentially of, or consists of an amino acid residue starting from any one of amino acid residue 51 to amino acid residue 65 and ending at amino acid residue 180 to residue 183 or residues corresponding to those positions in the polypeptide comprising SEQ ID NO:3, excluding the amino acid sequence of SEQ ID NO:3. An embodiment of a polypeptide comprises, consists essentially of, or consists of an amino acid residues corresponding to amino acid residues 58 to 183 in the polypeptide comprising SEQ ID NO:3, excluding the amino acid sequence of SEQ ID NO:3. An embodiment of a polypeptide comprises, consists essentially of, or consists of an amino acid residues corresponding to amino acid residues 65 to 182 in the polypeptide comprising SEQ ID NO:3, excluding the amino acid sequence of SEQ ID NO:3. An embodiment of a polypeptide comprises, consists essentially of, or consists of an amino acid residues corresponding to amino acid residues 98 to 183 in the polypeptide comprising SEQ ID

NO:3, excluding the amino acid sequence of SEQ ID NO:3. In some embodiments, the polypeptide portion has the ability to bind to hOX40 receptor and/or a hOX40 receptor ligand binding fragment thereof. The disclosure also includes polynucleotides encoding such polypeptides. The disclosure also includes a crystalline form of each of these

5 polypeptides.

In another aspect, the disclosure includes hOX40 receptor polypeptides and polynucleotides encoding the polypeptides. The disclosure includes a polynucleotide encoding a polypeptide and/or a polypeptide having at least 90% sequence identity to the polypeptide comprising the amino acid sequence of amino acids 29 to 170 of SEQ ID NO:2,

10 not including the polypeptide having the amino acid sequence of SEQ ED NO:2, and wherein the polypeptide binds hOX40L or a receptor binding fragment thereof. Another embodiment, comprises a polynucleotide encoding a polypeptide and/or a polypeptide that comprises the amino acid sequence starting at any one of amino acids 29 to amino acid residue 42 and ending at any one of amino acids 119 to 170 of SEQ ID NO:2, not including

15 the polypeptide having the amino acid sequence of SEQ ID NO:2, and wherein the polypeptide binds a hOX40L or a receptor binding fragment thereof. In some embodiments, a polynucleotide encoding a polypeptide and/or a polypeptide has at least 90% sequence identity to the polypeptide comprising the amino acid sequence of amino acids 29 to 147 of SEQ DD NO:2, not including the polypeptide having the amino acid sequence of SEQ DD

20 NO:2, and wherein the polypeptide binds a hOX40L or a receptor binding fragment thereof. The disclosure also includes a crystalline form of each of these polypeptides.

In some embodiments, a polynucleotide encoding a polypeptide and/or a polypeptide comprises the amino acid sequence of amino acids 35 to 124 of SEQ ID NO:2, not including the polypeptide having the amino acid sequence of SEQ DD NO:2. In some

25 embodiments, a polynucleotide encoding a polypeptide and/or a polypeptide comprises the amino acid sequence of amino acids 31 to 119 of SEQ DD NO:2, not including the polypeptide having the amino acid sequence of SEQ ID NO:2. The present disclosure also includes an isolated polypeptide comprising, consisting essentially of, or consisting of a portion or fragment of the hOX40 receptor. In some embodiments, the polypeptide

30 comprises a binding site for hOX40L and/or mOX40L. In other embodiments, the polypeptide comprises at least CRD1, CRD2 and CRD3. In other embodiments, the polypeptide comprises an extracellular domain of hOX40 receptor. In some embodiments, the polypeptide binds to hOX40L or a receptor binding fragment thereof. The disclosure also includes a crystalline form of each of these polypeptides.

35 In some embodiments, a mOX40L binding site for hOX40 receptor comprises, consists essentially of, or consists of at least one amino acid residue corresponding to an

amino acid selected from the group consisting of R64, A66, T68, S78, Y80, K81, N82, E83, D99, F111, Q112, H119, R121, N125, P126, S145, L146, A147, F148, K149, D150, L166, Q167, I168, N169, G171, Y182, P185, G187, S188, Y189, H190 of the polypeptide comprising SEQ ID NO:1, and combinations thereof. In some embodiments, a mOX40L binding site for hOX40 receptor comprises, consists essentially of, or consists of at least one amino acid residue corresponding to an amino acid selected from the group consisting of A66, J68, Y80, N82, E83, D99, F111, N125, P126, H119, S145, A147, F148, K149, D150, Q167, I168, N169, G171, Y182, S188, Y189 of the polypeptide comprising SEQ ID NO:1, and combinations thereof. In some embodiments, a mOX40L binding site for hOX40 receptor comprises, consists essentially of, or consists of at least one amino acid residue corresponding to an amino acid selected from the group consisting of A66, Y80, D99, F111, A147, N169, Y182, S188 of the polypeptide comprising SEQ ID NO:1 and combinations thereof. In some embodiments, a mOX40L binding site for hOX40 receptor comprises, consists essentially of, or consists of at least one amino acid residue that has at least about 25% of its surface area buried in crystal structure of mOX40L and hOX40 receptor. The disclosure also includes a crystal comprising a crystal structure defined by the structural coordinates of all or a portion of the binding site of mOX40L for hOX40 receptor, as well as the use of the structural coordinates in the methods disclosed herein.

In some embodiments, a hOX40L binding site for hOX40 receptor comprises, consists essentially of, or consists of at least one amino acid residue corresponding to an amino acid selected from the group consisting of Q65, T67, Q80, E82, D98, Y108, F109, S110, Y119, E123, E124, S142, T144, Y145, K146, D147, D162, H164, V165, N166, G167, F180, V182 of the polypeptide comprising SEQ ID NO:3, and combinations thereof. In some embodiments, a hOX40L binding site for hOX40 receptor comprises, consists essentially of, or consists of at least one amino acid residue corresponding to an amino acid selected from the group consisting of Q65, T67, E82, D98, S110, E123, T144, Y145, K146, D147, D162, H164/V165, N166, G167, F180, V182 of the polypeptide comprising SEQ ID NO:3, and combinations thereof. In some embodiments, a hOX40L binding site for hOX40 receptor comprises, consists essentially of, or consists of at least one amino acid residue corresponding to an amino acid selected from the group consisting of D98, T144, D162, N166, F180 of the polypeptide comprising SEQ ID NO:3, and combinations thereof. In some embodiments, a hOX40L binding site for hOX40 receptor comprises, consists essentially of, or consists of at least one amino acid residue that has at least 25% of its surface area buried in crystal structure of hOX40L and hOX40 receptor. The disclosure also includes a crystal comprising a crystal structure defined by the structural coordinates of all

or a portion of the binding site of hOX40L for hOX40 receptor, as well as the use of the structural coordinates in the methods disclosed herein.

In some embodiments, a hOX40 receptor binding site for hOX40L comprises, consists essentially of, or consists of at least one amino acid residue corresponding to an amino acid selected from the group consisting of T35, Y36, P37, S38, E45, M52, V53, S54, R55, R65, F71, V75, S78, K79, P80, K82, P83, C84, T85, W86, C87, N88, L89, Y119, K120, V123, D124 of the polypeptide comprising SEQ ID NO:2, and combinations thereof. In some embodiments, a hOX40 receptor binding site for hOX40L comprises, consists essentially of, or consists of at least one amino acid residue corresponding to an amino acid selected from the group consisting of Y36, P37, S38, E45, V53, R55, S78, K79, P83, T85, W86, C87, N88, Y119, V123 of the polypeptide comprising SEQ ID NO:2, and combinations thereof. In some embodiments, a hOX40 receptor binding site for hOX40L comprises, consists essentially of, or consists of at least one amino acid residue corresponding to an amino acid selected from the group consisting of, V53, R55, S78, K79, C87, N88 of the polypeptide comprising SEQ ID NO:2, and combinations thereof. In some embodiments, a hOX40 receptor binding site for hOX40L comprises, consists essentially of, or consists of at least one amino acid residue that has at least 25% of its surface area buried in crystal structure of hOX40L and hOX40 receptor. The disclosure also includes a crystal comprising a crystal structure defined by the structural coordinates of all or a portion of the binding site of hOX40 receptor for hOX40L, as well as the use of the structural coordinates in the methods disclosed herein.

In some embodiments, a hOX40 receptor binding site for mOX40L comprises, consists essentially of, or consists of at least one amino acid residue corresponding to an amino acid selected from the group consisting of L29, H30, C31, G33, T35, Y36, P37, S38, E45, M52, V53, S54, R55, F71, V75, S78, K79, P80, C81, P83, C84, T85, W86, C87, N88, R90, Y119, K120, V123 of the polypeptide comprising SEQ ID NO:2, and combinations thereof. In some embodiments, a hOX40 receptor binding site for mOX40L comprises, consists essentially of, or consists of at least one amino acid residue corresponding to an amino acid selected from the group consisting of C31, G33, T35, Y36, P37, S38, E45, M52, V53, S54, R55, F71, S78, K79, P80, P83, C84, W86, N88, Y119 of the polypeptide comprising SEQ ID NO:2, and combinations thereof. In some embodiments, a hOX40 receptor binding site for mOX40L comprises, consists essentially of, or consists of at least one amino acid residue corresponding to an amino acid selected from the group consisting of C31, Y36, P37, M52, R55, and P80 of the polypeptide comprising SEQ ID NO:2, and combinations thereof. In some embodiments, a hOX40 receptor site for mOX40L comprises, consists essentially of, or consists of at least one amino acid residue

that has at least 25% of its surface area buried in crystal structure of mOX40L and hOX40 receptor. The disclosure also includes a crystal comprising a crystal structure defined by the structural coordinates of all or a portion of the binding site of hOX40 receptor for mOX40L, as well as the use of the structural coordinates in the methods disclosed herein.

5 In some embodiments, a hOX40 receptor binding site for FFV comprises, consists essentially of, or consists of at least one amino acid corresponding to an amino acid selected from the group consisting of R58, S59, N61, H44, V63 of the polypeptide comprising the amino acid sequence of SEQ ID NO:2, and combinations thereof.

Another aspect of the disclosure includes a three-dimensional configuration of
10 points wherein at least a portion of the points are derived from structure coordinates of Table 8 or 9 representing locations of the backbone atoms of amino acids defining the mOX40L binding site for hOX40 receptor. Other embodiments include a three-dimensional configuration of points wherein at least a portion of the points are derived from structure coordinates of Table 10 representing locations of the backbone atoms of amino acids
15 defining the hOX40L binding site for hOX40 receptor. Other embodiments include a three-dimensional configuration of points wherein at least a portion of the points are derived from structure coordinates of Table 10 representing locations of the backbone atoms of amino acids defining the binding site on the hOX40 receptor for hOX40L. Other embodiments include a three-dimensional configuration of points wherein at least a portion of the points
20 are derived from structure coordinates of Table 9 representing locations of the backbone atoms of amino acids defining the binding site on the hOX40 receptor for mOX40L. The three-dimensional configuration of points of can be displayed as a holographic image, a stereodiagram, a model, or a computer-displayed image of at least a portion of the points derived from structure coordinates listed in Tables 8, 9, and/or 10.

25 Also provided herein is a machine-readable data storage medium comprising a data storage material encoded with machine-readable data, wherein a machine programmed with instructions for using such data displays a graphical three-dimensional representation of at least one molecule or molecular complex comprising at least a portion of a mOX40L binding site for hOX40 receptor, hOX40L binding site for hOX40 receptor, hOX40 receptor binding
30 site for mOX40L, hOX40 receptor binding site for hOX40L, or the binding site defined by a set of points having a root mean square deviation of less than about 0.05 Å from points representing the atoms of the amino acids as represented by the structure coordinates listed in Tables 8, 9, or 10. In some embodiments, the data comprises all or a portion of the diffraction data and/or structural coordinates of the crystals as described herein. In some
35 embodiments, the invention includes a machine readable data storage medium comprising data storage material encoded with a first set of machine readable data which is combined

with a second set of machine readable data using a machine programmed with instructions for using the first and second sets of data, and which determines at least a portion of the structure coordinates corresponding to the second set of data, wherein the first set of data comprises a Fourier transform of at least a portion of the structural coordinates of Tables 8, 9, and/or 10, and wherein the second set of data comprises an X-ray diffraction pattern of a molecule or molecular complex for which the three dimensional structure is unknown or incompletely known.

Likewise, the disclosure also includes the scalable three-dimensional configuration of points derived from structure coordinates of molecules or molecular complexes that are structurally homologous to mOX40L, hOX40L, hOX40 receptor or combinations thereof as well as structurally equivalent configurations. Structurally homologous molecules or molecular complexes are defined below. Advantageously, structurally homologous molecules can be identified using all or a portion of the structure coordinates of the Tables 8, 9, and/or 10 according to a method of the disclosure.

Another aspect of the invention provides several different methods. In some embodiments, a computer-assisted method for identifying an agent that modulates mOX40L or hOX40L signaling comprising (a) providing a computer modeling application with a set of structure coordinates of any one of Tables 8, 9, and/or 10 defining at least a portion of a mOX40L binding site, hOX40L binding site, hOX40 receptor binding site for mOX40L, hOX40 receptor binding site for hOX40L, or the binding site defined by a set of points having a root mean square deviation of less than about 0.7 Å from points representing the atoms of the amino acids as represented by the structure coordinates listed in any one of Tables 8, 9, and/or 10 ; (b) providing the computer modeling application with a set of structure coordinates for a test agent; and (c) modeling the structure of (a) complexed with (b) to determine if the test agent associates with a binding site is provided. The methods of the disclosure further comprise testing the test agent in an assay for binding and/or modulating activity.

Another embodiment includes a computer-assisted method for designing an agent that binds the mOX40L binding site, hOX40L binding site, hOX40 receptor binding site for mOX40L, hOX40 receptor binding site for hOX40L, or the binding site defined by a set of points having a root mean square deviation of less than about 0.7 Å from points representing the atoms of the amino acids as represented by the structure coordinates listed in Tables 8, 9, and/or 10 comprising (a) providing a computer modeling application with a set of structural coordinates of any one of Tables 8, 9, and/or 10 defining at least a portion of the mOX40L binding site, hOX40L binding site, hOX40 receptor binding site for mOX40L, hOX40 receptor binding site for hOX40L, or the binding site defined by a set of points having a root

mean square deviation of less than about 0.7 Å from points representing the atoms of the amino acids as represented by the structure coordinates listed in of any one of Tables 8, 9, and/or 10 ; and (b) modeling the structural coordinates of (a) to identify an agent that contacts at least one amino acid residue in one of the binding site. The method of the disclosure further comprises testing the agent in an assay for binding to mOX40L, hOX40L, hOX40 receptor binding site for mOX40L, and/or hOX40 receptor binding site for hOX40L.

Another embodiment includes a method of identifying a molecule that mimics mOX40L, hOX40L, or hOX40 receptor comprising a) searching a molecular structure database with all or a portion of the structural coordinates of any one of Tables 8, 9, and/or 10; and selecting a molecule from the database that mimics the structural coordinates of the mOX40L, hOX40L, or an hOX40 receptor. The method of the disclosure further comprises testing the molecule in an assay, for example, binding to mOX40L, hOX40L, hOX40 receptor binding site for mOX40L, and/or hOX40 receptor binding site for hOX40L.

Another embodiment includes a method of identifying agents that are antagonists or agonists of mOX40L, hOX40L, or an hOX40 receptor comprising a) applying at least a portion of the crystallography coordinates of any one of Tables 8, 9, and/or 10 to a computer algorithm that generates a 3 dimensional model of mOX40L, hOX40L, an hOX40 receptor or combinations thereof suitable for designing molecules that are antagonists or agonists; and b) searching a molecular structure database to identify potential antagonists or agonists of mOX40L, hOX40L, hOX40 receptor or combinations thereof. The methods of the disclosure further comprise testing the agent in an assay for inhibiting or enhancing the activity of mOX40L, hOX40L, hOX40 receptor binding site for mOX40L, and/or hOX40 receptor binding site for hOX40L.

Another embodiment includes a method of assessing agents that are antagonists or agonists of mOX40L, hOX40L, or hOX40 receptor, or combinations thereof, comprising: a) contacting a candidate antagonist or agonist with mOX40L, hOX40L, or hOX40 receptor, or combinations thereof, and selecting the antagonist or agonist that modulates the activity of mOX40L, hOX40L, or hOX40 receptor, or combinations thereof; b) identifying the structure of the selected antagonist or agonist and obtaining the structural coordinates of the selected antagonist or agonist's; c) applying at least a portion of the crystallography coordinates of Tables 8, 9, and/or 10 to a computer algorithm that generates a 3 dimensional model of mOX40L, hOX40L, or hOX40 receptor, or combinations thereof, suitable for designing molecules that are antagonists or agonists to the coordinates of the selected antagonist or agonist; and d) designing a modified antagonist or agonist of the selected antagonist or agonist by performing a fitting operation between the structural coordinates for

the selected antagonist or agonist and at least a portion of the structural coordinates of Tables 8, 9, and/or 10. The method of the disclosure further comprises testing the antagonist or agonist in an assay for inhibiting or enhancing the activity of mOX40L, hOX40L, hOX40 receptor binding site for mOX40L, and/or hOX40 receptor binding site for hOX40L.

5 A further embodiment includes a method for evaluating the ability of a chemical agent to associate with a molecule or molecular complex comprising at least one amino acid residue in mOX40L binding site, hOX40L binding site, hOX40 receptor binding site for mOX40L, hOX40 receptor binding site for hOX40L, or the binding site defined by a set of points having a root mean square deviation of less than about 0.7 Å from points representing the atoms of the amino acids as represented by the structure coordinates listed in Tables 8, 9, and/or 10, said method comprising employing computational means to perform a fitting operation between the chemical agent and the structure coordinates of the amino acid residues of the binding site; and analyzing the results of the fitting operation and selecting those chemical agents that associate with the amino acid residue as defined by favorable polar, nonpolar, electrostatic, shape complementarity, or combinations thereof after conformational adjustments to the binding site. The method of the disclosure further comprises testing the chemical agent in an assay, for example, binding to mOX40L, hOX40L, hOX40 receptor binding site for mOX40L, and/or hOX40 receptor binding site for hOX40L.

20 **Brief Description of the Drawings**

Figure 1: The hOX40L trimer differs from other TNFSF members. a) The hOX40L trimers are each rendered as ribbon. Some of the residues along the trimer axis are identified. b) Ribbon rendering of the LT trimer (pdb code: ltnr) labeled similarly to a.). Note the close packing of the protomers along the trimer axis. c.) LT protomer (gray) is superimposed on one of the hOX40L protomers showing that hOX40L has shorter strands but that the protomer structure is conserved. Approximate hOX40L trimer axis is shown as an arrow. d.) LT trimer (gray) superimposed on hOX40L (black) showing that the trimer assemblies differ. Dashed Black arrow, approximate LT trimer axis. Dark Gray arrow, hOX40L trimer axis.

Figure 2: The hOX40-hOX40L complex. hOX40L is shown as a molecular surface. The three protomers forming the trimer are shown as light gray, and dark gray. One copy of hOX40 receptor is shown as a tube with CRD1, CRD2, CRD3, and the vestigial CRD4. Disulfide bonds in OX40 receptor are rendered as sticks with the sulfur atoms shown as spheres. The N(29) and C-termini (168) of the receptor are labeled. The other two copies of OX40 receptor are shown with transparent molecular surfaces. There are 7 residues missing from the N-terminus of the ligand which form a linker connecting to the

ligand transmembrane domain. These residues are disordered in the electron density and are likely flexible. The complex is oriented such that the membranes of the ligand and receptor containing cells would be at the top and bottom of the figure respectively.

Figure 3: Structure-based sequence alignment of representatives from the "divergent" (hOX40L), "conventional" (LT; 11% sequence identity with hOX40L) and "EF-disulfide" (BAFF; 10% sequence identity with hOX40L) TNFSF sub-families. Residues forming β -strands are underlined. hOX40L strands are also shown as arrows above the sequences and labeled. Some of the residues which bury at least 50% of accessible surface area and at least 10 Å² upon binding receptor are shadowed in gray. hOX40L residues which resulted in at least a 10-fold decrease in IC₅₀ are N166 and F180. OX40L residues which resulted in a 3-fold or greater decrease in IC₅₀ include Q80, E123, T144, D162, N166 and F180. In the LT sequence, the hydrophobic residue (Y108) in the DE loop is conserved in the "conventional" ligands.

Figure 4: Sequence alignment of CRDs containing B1 modules. a.) Sequence alignments of B1 modules lacking the 4-6 disulfide. The A and B modules are labeled. TNFR1 CRD3 is included as a reference of a conventional A1, B2 containing CRD which has been structurally characterized. Cysteine residues are underlined, and the connectivity is indicated by lines above the sequences. b.) Sequence alignment of CRDs containing B1 modules lacking the 3-5 disulfide (the "B2-like" B1 modules). Sequences of TNFR1 CRD2, DR5 CRD2, and OX40 CRD2 are included as examples conventional A1, B2 containing CRD which have been structurally characterized. The aromatic/small residue pair replacing the 3-5 disulfide in the B2-like B1 modules is highlighted in bold.

Figure 5: Open book view of the hOX40L-hOX40 interface, a.) hOX40L and one receptor are rendered as molecular surfaces. Some of the residues in the interface are shown by % of accessible surface area buried upon complex formation (1-25%, light gray; 25-50%, darker gray; 50-75%, darker gray; 75-100%, black; See Table 6 for residue identification). Potential glycosylation sites are also shown; N90, N114, N152, and N157. Ligand residues N90 and N114 were mutated to Asp to remove potential glycosylation sites; other glycosylation sites include N152, and N157. Some of the residues of interest are labeled. Underlined residues are identical in murine and human OX40L. b.) hOX40L is rendered as in a.) but with residues with a greater than 10-fold increase or 5-fold increase in IC₅₀ when mutated to alanine colored black and dark gray respectively. Residues which had less than a 5-fold change in IC₅₀ when mutated to alanine have a white background (E123 and T144). c.) shows hOX40 receptor; residues shown with a black background have 75% or greater surface area buried, dark gray have 50% or greater surface area buried. (See Table 6)

Detailed Description of the Preferred Embodiment

Definitions:

The following definitions are used herein, unless otherwise described:

The term "OX40 ligand" or "OX40L", as used herein, refers, unless specifically or contextually indicated otherwise, to any (whether native or synthetic) OX40L polypeptide that is capable of binding to OX40 receptor and/or activating the OX40 receptor under conditions that permit such process to occur. The term "wild type OX40L sequence" generally refers to an amino acid sequence found in naturally occurring OX40L and includes naturally occurring truncated or secreted forms, variant forms (e.g. alternatively spliced forms) and naturally occurring allelic variants. An example of a wild-type murine OX40L is a polypeptide comprising an amino acid sequence of SEQ ID NO:1 in Table 3. An example of a wild-type murine OX40L is a polypeptide comprising an amino acid sequence of amino acids 51-198 of SEQ ID NO:1 in Table 3b. An example of a wild-type human OX40L is a polypeptide comprising an amino acid sequence of SEQ ID NO:3 in Table 5. An example of a wild-type human OX40L is a polypeptide comprising an amino acid sequence of amino acids 51 to 183 of SEQ ID NO:3 in Table 5b. The sequence numbering of mOX40L or hOX40L begins with the methionine shown as the first amino acid in Table 3 or Table 5, respectively.

"OX40L polypeptides" may also include polypeptides that have a different sequence than a reference polypeptide. Polypeptides can have substitutions, additions or deletions. In some embodiments, the reference polypeptide is a OX40L polypeptide comprising SEQ ID NO:1, comprising SEQ ID NO:3, or fragments thereof. In some embodiments, "non-naturally" occurring variant polypeptides are those prepared synthetically or recombinantly with substitutions, deletions or additions as compared to a naturally occurring sequence. In some embodiments, a variant has at least 80% amino acid sequence identity with the amino acid sequence of SEQ ID NO: 1, SEQ ID NO:3, or fragments thereof. In some embodiments, the polypeptides have the biological activity of binding to the hOX40 receptor and/or activating it. In other embodiments, the polypeptide can bind to the hOX40 receptor, but not activate it. Ordinarily, a OX40L polypeptide will have at least 80% sequence identity, more preferably will have at least 81% sequence identity, more preferably will have at least 82% sequence identity, more preferably will have at least 83% sequence identity, more preferably will have at least 84% sequence identity; more preferably will have at least 85% sequence identity, more preferably will have at least 86% sequence identity, more preferably will have at least 87% sequence identity, more preferably will have at least 88% sequence identity, more preferably will have at least 89% sequence identity, more preferably will have at least 90% sequence

- identity, more preferably will have at least 91% sequence identity, more preferably will have at least 92% sequence identity, more preferably will have at least 93% sequence identity, more preferably will have at least 94% sequence identity, more preferably will have at least 95% sequence identity, more preferably will have at least 96% sequence identity, more preferably will have at least 97% sequence identity, more preferably will have at least 98% sequence identity, more preferably will have at least 99% sequence identity with a OX40L polypeptide comprising an amino acid sequence comprising SEQ ID NO:1, comprising SEQ ID NO:3, or fragments thereof. Preferably, the variant polypeptides bind to the hOX40 receptor. Fragments include polypeptides comprising the amino acid sequence of amino acids 51-198 of SEQ ID NO:1 (Table 3b) or comprising the amino acids sequence of amino acids 51-183 of SEQ ID NO:3 (Table 5b). In specific embodiments, a human OX40L polypeptide comprises at least one amino acid substitution such as N90D, N114D, F180A, N166A, Q80A, D162A, T144A, E123A or mixtures thereof.
- The term "OX40 receptor", as used herein, refers to any (whether native or synthetic) OX40 receptor polypeptide that is capable of binding to an OX40L. The term "wild-type OX40 receptor" generally refers to a polypeptide comprising an amino acid sequence found in a naturally occurring receptors and includes naturally occurring truncated or secreted forms, variant forms (e.g. alternatively spliced forms) and naturally occurring allelic variants. An embodiment of the human OX40 receptor has an amino acid sequence of SEQ ID NO:2 shown in Table 4. An embodiment of the human OX40 receptor has an amino acid sequence of amino acid residues of 29 to 170 of SEQ ID NO:2 shown in Table 4b. The sequence numbering of hOX40 receptor begins with the methionine shown as the first amino acid as shown in Table 4.
- "OX40 receptor" also refers to a polypeptide that has a different sequence than a reference polypeptide. In some embodiments, the reference polypeptide is an OX40 receptor comprising SEQ ID NO:2. In some embodiments, "non-naturally" occurring variants include those polypeptides that have substitutions, additions or deletions as compared to a wild-type or naturally occurring sequence. In some embodiments, the polypeptide can bind to the OX40L. Ordinarily, a OX40 receptor polypeptide will have at least 80% sequence identity, more preferably will have at least 81% sequence identity, more preferably will have at least 82% sequence identity, more preferably will have at least 83% sequence identity, more preferably will have at least 84% sequence identity; more preferably will have at least 85% sequence identity, more preferably will have at least 86% sequence identity, more preferably will have at least 87% sequence identity, more preferably will have at least 88% sequence identity, more preferably will have at least 89% sequence

identity, more preferably will have at least 90% sequence identity, more preferably will have at least 91% sequence identity, more preferably will have at least 92% sequence identity, more preferably will have at least 93% sequence identity, more preferably will have at least 94% sequence identity, more preferably will have at least 95% sequence
5 identity, more preferably will have at least 96% sequence identity, more preferably will have at least 96% sequence identity, more preferably will have at least 97% sequence identity, more preferably will have at least 98% sequence identity, more preferably will have at least 99% sequence identity with a OX40 receptor polypeptide comprising an amino acid sequence comprising SEQ ID NO:2 or a fragment thereof.

10 The term "binding site," as used herein, refers to a region of a molecule or molecular complex that, as a result of its shape, distribution of electrostatic charge, presentation of hydrogen-bond acceptors or hydrogen-bond donors, and/or distribution of nonpolar regions, favorably associates with a ligand. Thus, a binding site may include or consist of features such as cavities, surfaces, or interfaces between domains. Ligands that
15 may associate with a binding site include, but are not limited to, cofactors, substrates, receptors, agonists, and antagonists. The term binding site includes a functional binding site and/or a structural binding site. A structural binding site can include "in contact" amino acid residues as determined from examination of a three-dimensional structure. "Contact" can be determined using Van der Waals radii of atoms or by proximity sufficient to exclude
20 solvent, typically water, from the space between the ligand and the molecule or molecular complex. In some embodiments, a OX40L residue in contact with OX40 receptor or other substrate or inhibitor is a residue that has one atom within about 5Å of a hOX40 receptor residue. Alternatively, "in contact" residue may be those that have a loss of solvent accessible surface area of at least about 25% to 100%, more preferably at least about 50% to
25 100%, more preferably about 75% to 100% and/or at least about 10 angstroms squared of surface area is lost. In some embodiments, loss of solvent accessible surface determinations can vary plus or minus 5%. Loss of solvent accessible surface can be determined by the method of Lee & Richards (J Mol Biol, 55(3):379-400 (1971)) and similar algorithms known to those skilled in the art, for instance as found in the SOLV module from C. Broger
30 of F. Hoffman-La Roche in Basel Switzerland.

Some of the "in contact" amino acid residues, if substituted with another amino acid type, may not cause any change in a biochemical assay, a cell-based assay, or an *in vivo* assay used to define a functional binding site but may contribute to the formation of a three dimensional structure. A functional binding site includes amino acid residues that are
35 identified as binding site residues based upon loss or gain of function, for example, loss of binding to ligand upon mutation of the residue. In some embodiments, the amino acid

residues of a functional binding site are a subset of the amino acid residues of the structural binding site.

The term "hOX40L binding site" refers to a region of a human OX40L that can favorably associate with a hOX40 receptor.

5 The term "mOX40L binding site" refers to a region of a murine OX40L that can favorably associate with a hOX40 receptor.

The term "hOX40 receptor binding site" refers to a region of a human OX40 receptor that can favorably associate with a OX40L, such as mOX40L and/or hOX40L.

A structurally equivalent ligand binding site is defined by a root mean square
10 deviation from the structure coordinates of the backbone atoms of the amino acids that make up a binding sites as described herein of at most about 0.70 Å, preferably about 0.5 Å.

"Crystal" as used herein, refers to one form of a solid state of matter in which atoms are arranged in a pattern that repeats periodically in three-dimensions, typically forming a lattice.

15 "Complementary or complement" as used herein, means the fit or relationship between two molecules that permits interaction, including for example, space, charge, three-dimensional configuration, and the like.

The term "corresponding" or "corresponds" refers to an amino acid residue or amino acid sequence that is found at the same position or positions in a sequence when the
20 amino acid position or sequences are aligned with a reference sequence to maximize sequence identity. In some embodiments, the reference sequence is a fragment of the mOX40L having a sequence of amino acids residues 51-198 of SEQ ID NO: 1. In some embodiments, the reference sequence is a fragment of the hOX40 receptor having a sequence of amino acids residues 29-170 of SEQ ID NO:2. In some embodiments, the
25 reference sequence is a fragment of the hOX40L having a sequence of amino acids residues 51-183 of SEQ ID NO:3. It will be appreciated that when the amino acid position or sequence is aligned with the reference sequence the numbering of the amino acids may differ from that of the reference sequence.

"Heavy atom derivative", as used herein, means a derivative produced by
30 chemically modifying a crystal with a heavy atom such as Hg, Au, or a halogen.

"Structural homolog" of OX40L or hOX40 receptor as used herein refers to a protein that contains one or more amino acid substitutions, deletions, additions, or rearrangements with respect to the amino acid sequence of OX40L or hOX40 receptor, but that, when folded into its native conformation, exhibits or is reasonably expected to exhibit
35 at least a portion of the tertiary (three-dimensional) structure of the OX40L or hOX40 receptor.

Tertiary structure can be probed, measured, or confirmed by known analytic or diagnostic methods, for example, X-ray, NMR, circular dichroism, a panel of monoclonal antibodies that recognize OX40L, hOX40 receptor or complexes thereof and like techniques. For example, structurally homologous molecules can have substitutions, deletions or additions of one or more contiguous or noncontiguous amino acids, such as a loop or a domain. Structurally homologous molecules also include "modified" OX40L or hOX40 receptor molecules that have been chemically or enzymatically derivatized at one or more constituent amino acid, including side chain modifications, backbone modifications, and N- and C- terminal modifications including acetylation, hydroxylation, methylation, amidation, and the attachment of carbohydrate or lipid moieties, cofactors, and like modifications.

"Ligand", as used herein, refers to an agent or compound that associates with a binding site on a molecule, for example, OX40L binding sites for hOX40 receptor, and may be an antagonist or agonist of OX40L activity. Ligands include molecules that mimic OX40L binding to hOX40 receptor and in some embodiments, are not capable of activating hOX40 receptor.

"Compound" refers to molecule that associates with the hOX40 receptor, mOX40L, hOX40L, or complexes thereof or a pharmaceutically acceptable salt, ester, amide, prodrug, isomer, or metabolite, thereof. "Pharmaceutically acceptable salt" refers to a formulation of a compound that does not compromise the biological activity and properties of the compound. Pharmaceutical salts can be obtained by reacting a binding-active compound of the disclosure with inorganic or organic acids such as hydrochloric acid, hydrobromic acid, sulfuric acid, nitric acid, phosphoric acid, methanesulfonic acid, ethanesulfonic acid, p-toluenesulfonic acid, salicylic acid and the like. "Prodrug" refers to an agent that is converted into the parent drug in vivo. Prodrugs are often useful because, in some situations, they may be easier to administer than the parent drug. They may, for instance, be bioavailable by oral administration whereas the parent is not. The prodrug may also have improved solubility in pharmaceutical compositions over the parent drug. An example, without limitation, of a prodrug would be a compound which is administered as an ester (the "prodrug") to facilitate transport across a cell membrane where water solubility is detrimental to mobility but which then is metabolically hydrolyzed to the carboxylic acid, the active entity, once inside the cell where water solubility is beneficial. A further example of a prodrug might be a short peptide (polyaminoacid) bonded to an acid group wherein the peptide is metabolized to yield the active moiety.

"Molecular complex", as used herein, refers to a combination of bound substrate or ligand with polypeptide, such as OX40L bound to hOX40 receptor, or a ligand bound to an hOX40 receptor and/or OX40L.

5 "Machine-readable data storage medium", as used herein, means a data storage material encoded with machine-readable data, wherein a machine programmed with instructions for using such data and is capable of displaying data in the desired format, for example, a graphical three-dimensional representation of molecules or molecular complexes.

10 "Scalable," as used herein, means the increasing or decreasing of distances between coordinates (configuration of points) by a scalar factor while keeping the angles essentially the same.

"Space group symmetry", as used herein, means the whole symmetry of the crystal that combines the translational symmetry of a crystalline lattice with the point group symmetry. A space group is designated by a capital letter identifying the lattice type (*P*, *A*, *F*, etc.) followed by the point group symbol in which the rotation and reflection elements are
15 extended to include screw axes and glide planes. Note that the point group symmetry for a given space group can be determined by removing the cell centering symbol of the space group and replacing all screw axes by similar rotation axes and replacing all glide planes with mirror planes. The point group symmetry for a space group describes the true
20 symmetry of its reciprocal lattice.

"Unit cell", as used herein, means the atoms in a crystal that are arranged in a regular repeating pattern, in which the smallest repeating unit is called the unit cell. The entire structure can be reconstructed from knowledge of the unit cell, which is characterized by three lengths (*a*, *b* and *c*) and three angles (α , β and γ). The quantities *a* and *b* are the
25 lengths of the sides of the base of the cell and γ is the angle between these two sides. The quantity *c* is the height of the unit cell. In some embodiments, the unit cell lengths can vary plus or minus 0.5 Å. The angles α and β describe the angles between the base and the vertical sides of the unit cell.

"X-ray diffraction pattern" means the pattern obtained from X-ray scattering of the periodic assembly of molecules or atoms in a crystal. X-ray crystallography is a technique
30 that exploits the fact that X-rays are diffracted by crystals. X-rays have the proper wavelength (in the Angstrom (Å) range, approximately 10^{-8} cm) to be scattered by the electron cloud of an atom of comparable size. Based on the diffraction pattern obtained from X-ray scattering of the periodic assembly of molecules or atoms in the crystal, the
35 electron density can be reconstructed. Additional phase information can be extracted either from the diffraction data or from supplementing diffraction experiments to complete the

reconstruction (the phase problem in crystallography). A model is then progressively built into the experimental electron density, refined against the data to produce an accurate molecular structure.

5 X-ray structure coordinates define a unique configuration of points in space. Those of skill in the art understand that a set of structure coordinates for a protein or a protein/ligand complex, or a portion thereof, define a relative set of points that, in turn, define a configuration in three dimensions. A similar or identical configuration can be defined by an entirely different set of coordinates, provided the distances and angles between coordinates remain essentially the same. In addition, a configuration of points can
10 be defined by increasing or decreasing the distances between coordinates by a scalar factor, while keeping the angles essentially the same.

"Crystal structure" generally refers to the three-dimensional or lattice spacing arrangement of repeating atomic or molecular units in a crystalline material. The crystal structure of a crystalline material can be determined by X-ray crystallographic methods, see
15 for example, "Principles of Protein X-Ray Crystallography," by Jan Drenth, Springer Advanced Texts in Chemistry, Springer Verlag; 2nd ed., February 1999, ISBN: 0387985875, and "Introduction to Macromolecular Crystallography," by Alexander McPherson, Wiley-Liss, October 18, 2002, ISBN: 0471251224.

Modes for Carrying Out the Invention:

20 The present disclosure thus includes a crystalline form and a crystal structure of each of a murine OX40L (mOX40L) and a mOX40L or a hOX40L complexed with a hOX40 receptor. In other aspects, the disclosure provides methods of using the crystal structures and structural coordinates to identify homologous proteins and to design or identify agents that can modulate the function of the OX40L, hOX40 receptor and/or
25 complexes thereof. The present disclosure also includes the three-dimensional configuration of points derived from the structure coordinates of at least a portion of a OX40L molecule, hOX40 receptor or molecular complexes thereof, as well as structurally equivalent configurations, as described below. The three-dimensional configuration includes points derived from structure coordinates representing the locations of one or more
30 of a plurality of the amino acids defining the mOX40L binding site when it is not bound to hOX40 receptor, mOX40L binding site when it is bound to hOX40 receptor, hOX40L binding site when it is bound to hOX40 receptor, hOX40 receptor binding site for hOX40L or mOX40L.

In some embodiments, the three-dimensional configuration includes points derived
35 from structure coordinates representing the locations of the backbone atoms of a plurality of amino acids defining the defining the mOX40L binding site when it is not bound to hOX40

receptor, mOX40L binding site when it is bound to hOX40 receptor, hOX40L binding site when it is bound to hOX40 receptor, and hOX40 receptor binding site for hOX40L or mOX40L. Alternatively, the three-dimensional configuration includes points derived from structure coordinates representing the locations of the side chain and the backbone atoms
5 (other than hydrogens) of a plurality of the amino acids defining the defining the mOX40L binding site when it is not bound to hOX40 receptor, mOX40L binding site when it is bound to hOX40 receptor, hOX40L binding site when it is bound to hOX40 receptor, and hOX40 receptor binding site for hOX40L or mOX40L.

Likewise, the disclosure also includes the scalable three-dimensional configuration
10 of points derived from structure coordinates of molecules or molecular complexes that are structurally homologous to OX40L, hOX40 receptor, or complexes thereof as well as structurally equivalent configurations. Structurally homologous molecules or molecular complexes are defined below. Advantageously, structurally homologous molecules can be identified using the structure coordinates of the OX40L, hOX40 receptor, or complexes
15 thereof according to a method of the disclosure.

The configurations of points in space derived from structure coordinates according to the disclosure can be visualized as, for example, a holographic image, a stereodiagram, a model, or a computer-displayed image, and the disclosure thus includes such images, diagrams or models.

20 The crystal structure and structural coordinates can be used in methods, for example, for obtaining structural information of a related molecule, and for identifying and designing agents that modulate activity or binding of OX40L, hOX40 receptor, or complexes thereof .

The coordinates of mOX40L are provided in Table 8. The coordinates of mOX40L
25 cocrystallized with hOX40 receptor are provided in Table 9. The coordinates of hOX40L cocrystallized with hOX40 receptor are provided in Table 10.

1. **OX40L and hOX40 receptor polypeptides, polynucleotides and variants thereof**

The present disclosure includes OX40L polypeptides and hOX40 receptor
30 polypeptide.

Native or wild-type OX40L are those polypeptides that have a sequence of a polypeptide obtained from nature. Native or wild-type polypeptides include naturally occurring variants, secreted or truncated forms. An embodiment of wild type murine OX40L comprises a sequence of SEQ ID NO:1 shown in Table 3. An embodiment of wild
35 type human OX40L comprises a sequence of SEQ ID NO:3 shown in Table 5.

In some embodiments, a OX40L includes several domains including A, A', B', B, C, D, E, F, G, and H β sheet strands that form jelly roll β sandwich monomer sheets as follows: A'AHCF and B'BGDE. The OX40L forms a flower like trimer with an interface formed by a layer of generally hydrophobic residues along the C strand, F strand, and C
 5 terminal extension (amino acid residues 175-183 in hOX40L and residues 178-191 in mOX40L). The monomers are splayed out and form an angle of about 45° with respect to the trimer axis. The trimer interface is compact with about 2600 Å² accessible surface area buried.

In another aspect, the disclosure includes mOX40L polypeptides and
 10 polynucleotides encoding the polypeptides. The disclosure includes a polynucleotide encoding a polypeptide and/or a polypeptide having at least 90% sequence identity to the polypeptide comprising the amino acid sequence of amino acids 51-198 of SEQ ID NO:1, not including the polypeptide having the amino acid sequence of SEQ ID NO: 1 or SEQ ID NO:3, and wherein the polypeptide is a hOX40 receptor or a hOX40 receptor ligand binding
 15 fragment thereof. Another embodiment, comprises a polynucleotide encoding a polypeptide and/or a polypeptide that comprises the amino acid sequence starting at any one of amino acids 51 to amino acid residue 66 and ending at any one of amino acids 180 to 191 of SEQ ID NO:1, not including the polypeptide having the amino acid sequence of SEQ ID NO: 1 or SEQ ID NO:3, and wherein the polypeptide binds a hOX40 receptor or a hOX40 receptor
 20 ligand binding fragment thereof. In some embodiments, a polynucleotide encoding a polypeptide and/or a polypeptide has at least 90% sequence identity to the polypeptide comprising the amino acid sequence of amino acids 64 to 190 of SEQ ID NO:1, not including the polypeptide having the amino acid sequence of SEQ ID NO:1 or SEQ ID NO:3, and wherein the polypeptide binds a hOX40 receptor or a hOX40 receptor
 25 binding fragment thereof. In some embodiments, a polynucleotide encoding a polypeptide and/or a polypeptide has at least 90% sequence identity to the polypeptide comprising the amino acid sequence of amino acids 99 to 191 of SEQ ID NO:1, not including the polypeptide having the amino acid sequence of SEQ ID NO:1 or SEQ ID NO:3, and wherein the polypeptide binds a hOX40 receptor or a hOX40 receptor ligand binding
 30 fragment thereof. The disclosure also includes a crystalline form of each of these polypeptides.

The present disclosure also includes an isolated polypeptide comprising, consisting essentially of, or consisting of a portion or fragment of the mOX40L. In some
 35 embodiments, the polypeptide comprises a binding site for hOX40 receptor. In some embodiments, the polypeptide comprises an extracellular domain of mOX40L. In other embodiments, the polypeptide comprises the trimer interface. In some embodiments, the

trimer interface includes that amino acid residues corresponding to amino acids 99 to 191 of SEQ. ID NO:1. An embodiment of a polypeptide comprises, consists essentially of, or consists of an amino acid residue starting from any one of amino acid residue 51 to amino acid residue 66 and ending at amino acid residue 180 to residue 191 or residues

5 corresponding to those positions in the polypeptide comprising SEQ ID NO: 1, excluding the amino acid sequence of SEQ ID NO: 1. An embodiment of a polypeptide comprises, consists essentially of, or consists of an amino acid residues corresponding to amino acid residues 51 to 198 in the polypeptide comprising SEQ ID NO:1, excluding the amino acid sequence of SEQ ID NO: 1. An embodiment of a polypeptide comprises, consists essentially

10 of, or consists of an amino acid residues corresponding to amino acid residues 66 to 190 in the polypeptide comprising SEQ ID NO:1, excluding the amino acid sequence of SEQ ID NO:1. An embodiment of a polypeptide comprises, consists essentially of, or consists of an amino acid residues corresponding to amino acid residues 64 to 190 in the polypeptide comprising SEQ ID NO: 1, excluding the amino acid sequence of SEQ ED NO: 1 excluding

15 the amino acid sequence of SEQ ID NO: 1. An embodiment of a polypeptide comprises, consists essentially of, or consists of an amino acid residues corresponding to amino acid residues 66 to 189 in the polypeptide comprising SEQ ID NO:1, excluding the amino acid sequence of SEQ ID NO:1. An embodiment of a polypeptide comprises, consists essentially of, or consists of an amino acid residues corresponding to amino acid residues 99 to 191 in

20 the polypeptide comprising SEQ ID NO: 1, excluding the amino acid sequence of SEQ ED NO: 1. In some embodiments, the polypeptide portion has the ability to bind to hOX40 receptor or a hOX40 receptor ligand binding fragment thereof. The disclosure also includes polynucleotides encoding such polypeptides. The disclosure includes a crystalline form of each of these polypeptides, as well as one structural coordinate and use all or a portion of

25 structural coordinates in the methods described herein.

The disclosure also includes a polynucleotide encoding a polypeptide and/or a polypeptide having at least 90% sequence identity to the polypeptide comprising the amino acid sequence of amino acids 51 to 183 of SEQ ED NO:3, not including the polypeptide having the amino acid sequence of SEQ ED NO:3 or SEQ ED-NO: 1, and wherein the

30 polypeptide binds a hOX40 receptor or a hOX40 receptor ligand binding fragment thereof. Another embodiment, comprises a polynucleotide encoding a polypeptide and/or a polypeptide that comprises the amino acid sequence starting at any one of amino acids 51 to amino acid residue 65 and ending at any one of amino acids 180 to 183 of SEQ ED NO:3, not including the polypeptide having the amino acid sequence of SEQ ED NO:3 or SEQ ID

35 NO: 1, and wherein the polypeptide binds a hOX40 receptor or a hOX40 receptor ligand binding fragment thereof. In some embodiments, a polynucleotide encoding a polypeptide

and/or a polypeptide has at least 90% sequence identity to the polypeptide comprising the amino acid sequence of amino acids 98 to 183 of SEQ ID NO:3, not including the polypeptide having the amino acid sequence of SEQ ID NO:3 or SEQ ID NO:1, and wherein the polypeptide ity binds a hOX40 receptor or a hOX40 receptor ligand binding
5 fragment thereof. In some embodiments, a polynucleotide encoding a polypeptide and/or a polypeptide has at least 90% sequence identity to the polypeptide comprising the amino acid sequence of amino acids 65 to 182 of SEQ ED NO:3, not including the polypeptide having the amino acid sequence of SEQ DD NO:3 or SEQ ED NO:1, and wherein the polypeptide binds a hOX40 receptor or a hOX40 receptor ligand binding fragment thereof. The
10 disclosure also includes a crystalline form of each of these polypeptides.

In another aspect, the disclosure includes hOX40L polypeptides and polynucleotides encoding the polypeptides. The present disclosure also includes an isolated polypeptide comprising, consisting essentially of, or consisting of a portion or fragment of the hOX40L. In some embodiments, the polypeptide comprises a binding site for hOX40
15 receptor. In some embodiments, the polypeptide comprises an extracellular domain of hOX40L. In other embodiments, the polypeptide comprises the trimer interface. In some embodiments, the trimer interface includes amino acid residues corresponding to amino acids 98 to 182 or 183 of the amino acid sequence of SEQ DD NO:3. An embodiment of a polypeptide comprises, consists essentially of, or consists of an amino acid residue starting
20 from any one of amino acid residue 51 to amino acid residue 65 and ending at amino acid residue 180 to residue 183 or residues corresponding to those positions in the polypeptide comprising SEQ DD NO:3, excluding the amino acid sequence of SEQ DD NO:3. An embodiment of a polypeptide comprises, consists essentially of, or consists of an amino acid residues corresponding to amino acid residues 58 to 183 in the polypeptide comprising SEQ
25 ID NO:3, excluding the amino acid sequence of SEQ DD NO:3. An embodiment of a polypeptide comprises, consists essentially of, or consists of an amino acid residues corresponding to amino acid residues 65 to 182 in the polypeptide comprising SEQ DD NO:3, excluding the amino acid sequence of SEQ DD NO:3. An embodiment of a polypeptide comprises, consists essentially of, or consists of an amino acid residues
30 corresponding to amino acid residues 98 to 183 in the polypeptide comprising SEQ DD NO:3, excluding the amino acid sequence of SEQ DD NO:3. In some embodiments, the polypeptide portion has the ability to bind to hOX40 receptor and/or hOX40 receptor ligand binding fragment thereof. The disclosure also includes polynucleotides encoding such polypeptides. The disclosure also includes a crystalline form of each of these polypeptides,
35 as well as the structural coordinates and use of all or portion of the coordinates in the methods described herein.

The present disclosure also includes OX40L polypeptides that have amino acid substitutions, deletions, and additions. Amino acid substitutions can be made for example to replace cysteines and eliminate formation of disulfide bonds. Amino acid substitutions can also be made to change proteolytic cleavage sites or eliminate glycosylation sites. Other
 5 variants can be made at the OX40L binding site for hOX40 receptor. In other embodiments, the OX40L polypeptides bind hOX40 receptor with the same or higher affinity than a wild type OX40L. In specific embodiments, a human OX40L polypeptide comprises at least one amino acid substitution such as N90D, N114D, F180A, N166A, Q80A, D162A, T144A, E123A or mixtures thereof.

10 Native or wild type hOX40 receptors are those polypeptides that have a sequence of a polypeptide obtained from nature. A specific embodiment of a human OX40 receptor comprises a sequence of SEQ ID NO:2 as shown in Table 4.

Wild type OX40 receptors are integral cell surface proteins that are composed of three full CRDs and a partial C-terminal CRD which form a contiguous structure.
 15 Superposition of the three independent copies of hOX40 (two in the mOX40L-hOX40 asymmetric unit and one in the hOX40L-OX40 asymmetric unit) reveals that CRD1 and CRD2 form a rigid unit while there is some rotational freedom between the subdomains of CRD3 and the partial CRD4. CRD3 in hOX40 differs more than CRD1 and CRD2 from its counterpart in TNFR1 or DR5 as it is smaller and lacks one of the canonical disulfides.
 20 CRD3 contains an A1, B1 module rather than the A1, B2 architecture of CRD1 and 2. In the case of OX40, the disulfide formed by the fourth and sixth cysteines in CRD3 (the 4-6 disulfide) is missing. This missing disulfide in hOX40 CRD3 is not replaced by either hydrogen bonds or hydrophobic interactions but rather the entire module is smaller due to shortening and re-arrangement of intervening loops. This re-arrangement causes the
 25 backbone of the remaining 3-5 disulfide to be in an anti-parallel orientation rather than the parallel orientation seen in B2 modules. A long disulfide containing loop follows the B1 module. The connectivity and structure of this loop are compatible with it being an A1 module of a vestigial CRD4.

The present disclosure also includes a polypeptide comprising, consisting
 30 essentially of, or consisting of a portion or fragment of hOX40 receptor. In some embodiments, the polypeptide comprises an extracellular domain of hOX40L receptor. In other embodiments, the polypeptide comprises a binding site for mOX40L and/or hOX40L. Preferably, the polypeptide comprises one or more of the CRD domains, preferably the CRD1, CRD2, and/or CRD3 domains. In some embodiments, CRD1 comprises amino acids
 35 29-65; CRD2 comprises amino acids 66-108; CRD3 comprises amino acids 109-147; of the amino acid sequence of SEQ ID NO:2. In some embodiments, CRD1 includes at least

residues 31-64 including Cys 31, 42, 43, 56, 46 and 64; CRD2 includes at least residues 67-107 including Cys 67, Cys 81, Cys 84, Cys 99, Cys 87 and Cys 107; CRD3 includes at least 109-141 including cys 109, cys 125, cys 128, and cys 141; and CRD4 includes at least residues 147-166 including cys 147 and cys 166 of the amino acid sequence of SEQ ID
5 NO:2.

In another aspect, the disclosure includes hOX40 receptor polypeptides and polynucleotides encoding the polypeptides. The disclosure includes a polynucleotide encoding a polypeptide and/or a polypeptide having at least 90% sequence identity to the polypeptide comprising the amino acid sequence of amino acids 29 to 170 of SEQ ID NO:2,
10 not including the polypeptide having the amino acid sequence of SEQ ED NO:2, and wherein the polypeptide hOX40L, mOX40L, or receptor binding fragment thereof. Another embodiment, comprises a polynucleotide encoding a polypeptide and/or a polypeptide that comprises the amino acid sequence starting at any one of amino acids 29 to amino acid residue 36 and ending at any one of amino acids 119 to 170 of SEQ ED NO:2, not including
15 the polypeptide having the amino acid sequence of SEQ ED NO:2, and wherein the polypeptide binds a hOX40L, mOX40L, or receptor binding fragment thereof. In some embodiments, a polynucleotide encoding a polypeptide and/or a polypeptide has at least 90% sequence identity to the polypeptide comprising the amino acid sequence of amino acids 29 to 147 of SEQ ID NO:2, not including the polypeptide having the amino acid
20 sequence of SEQ ID NO:2, and wherein the polypeptide binds a hOX40L, mOX40L, or receptor binding fragment thereof. The disclosure also includes a crystalline form of each of these polypeptides.

An embodiment of a polypeptide comprises a polypeptide starting at any one of amino acid residues 29 to amino acid residue 36 and ending at any one of amino acid
25 residues 147 to amino acid residue 170 of SEQ ED NO:2, not including the amino acid sequence of SEQ DD NO:2. An embodiment of a polypeptide comprises a polypeptide starting at any one of amino acid residues 31 to amino acid residue 36 and ending at any one of amino acid residues 147 to amino acid residue 170 of SEQ DD NO:2, not including the amino acid sequence of SEQ DD NO:2. An embodiment of a polypeptide comprises a
30 polypeptide starting at any one of amino acid residues 31 to amino acid residue 36 and ending at any one of amino acid residues 119 to amino acid residue 170 of SEQ ED NO:2, not including the amino acid sequence of SEQ ED NO:2. In some embodiments, a polypeptide comprises the amino acid sequence of amino acids 35 to 124 of SEQ ID NO:2, not including the polypeptide having the amino acid sequence of SEQ DD NO:2. In some
35 embodiments, a polypeptide comprises the amino acid sequence of amino acids 31 to 119 of SEQ ED NO:2, not including the polypeptide having the amino acid sequence of SEQ ED

NO:2. The fragment preferably comprises a binding site for mOX40L and/or hOX40L. The disclosure also includes polynucleotides encoding these polypeptides. The disclosure also includes a crystalline form of each of these polypeptides, as well as all or a portion of the structural coordinates for use in the methods described herein.

- 5 The present disclosure also include hOX40 receptor polypeptides that have amino acid substitutions, deletions, and additions. Amino acid substitutions can be made for example to replace cysteines and eliminate formation of disulfide bonds. Amino acid substitutions can also be made to change proteolytic cleavage sites or eliminate glycosylation sites. Other variants can be made at the amino acid residue or residues that
10 bind to hOX40L and/or mOX40L as identified herein.

Fusion Proteins

- OX40L and/or OX40 receptor polypeptides, structural homologs, or portions thereof, may be fused to a heterologous polypeptide or compound. The heterologous polypeptide is a polypeptide that has a different function than that of the OX40L and/or
15 OX40 receptor. Examples of heterologous polypeptide include polypeptides that may act as carriers, may extend half life, may act as epitope tags, provide for secretion, may provide ways to detect or purify the fusion protein. Heterologous polypeptides include KLH, albumin, salvage receptor binding epitopes, immunoglobulin constant regions, and peptide tags. In a specific embodiment, the polypeptides may be fused to the signal peptide of the
20 67 kd envelope glycoprotein of AcNPV baculovirus to provide for secretion from cells. Peptide tags useful for detection or purification include FLAG, gD protein, polyhistidine tags, hemagglutinin from influenza virus, T7 tag, S tag, Strep tag, chloramiphenicol acetyl transferase, biotin, glutathione-S transferase, green fluorescent protein and maltose binding protein. Compounds that can be combined with the OX40L, OX40 receptors, variants or
25 structural homolog or portions thereof, include radioactive labels, protecting groups, and carbohydrate or lipid moieties.

Polynucleotides, Vectors and Host Cells

- OX40L, OX40 receptors, variants or fragments thereof can be prepared by introducing appropriate nucleotide changes into DNA encoding OX40L or OX40 receptor ,
30 or by synthesis of the desired polypeptide variants.

- Polynucleotide sequences encoding mOX40L, hOX40L and hOX40 receptor are known to those of skill in the art and can be obtained from sources such as Genbank and the like. For example, a polynucleotide sequence encoding mOX40L can be found at accession number U12763(gI:551080); an amino acid sequence for mOX40L can be found at
35 accession number P43488; a polynucleotide sequence encoding hOX40L can be found at accession number D90224(gI:219665); an amino acid sequence for hOX40L can be found at

accession number P23510; a polynucleotide sequence encoding hOX40 receptor can be found at accession number X65962(gi:472957);and an amino acid sequence for hOX40 receptor can be found at accession number P42489.

Polynucleotide sequences encoding the polypeptides described herein can be
5 obtained using standard recombinant techniques. Desired polynucleotide sequences may be isolated and sequenced from appropriate source cells. Alternatively, polynucleotides can be synthesized using nucleotide synthesizer or PCR techniques. Once obtained, sequences encoding the polypeptides or variant polypeptides are inserted into a recombinant vector capable of replicating and expressing heterologous polynucleotides in a host cell. Many
10 vectors that are available and known in the art can be used for the purpose of the present invention. Selection of an appropriate vector will depend mainly on the size of the nucleic acids to be inserted into the vector and the particular host cell to be transformed with the vector. Each vector contains various components, depending on its function (amplification or expression of heterologous polynucleotide, or both) and its compatibility with the
15 particular host cell in which it resides. The vector components generally include, but are not limited to: an origin of replication (in particular when the vector is inserted into a prokaryotic cell), a selection marker gene, a promoter, a ribosome binding site (RBS), a signal sequence, the heterologous nucleic acid insert and a transcription termination sequence.

20 In general, plasmid vectors containing replicon and control sequences, which are derived from a species compatible with the host cell are used in connection with these hosts. The vector ordinarily carries a replication site, as well as marking sequences, which are capable of providing phenotypic selection in transformed cells. For example, *E. coli* is typically transformed using pBR322, a plasmid derived from an *E. coli* species. pBR322
25 contains genes encoding ampicillin (Amp) and tetracycline (Tet) resistance and thus provides easy means for identifying transformed cells. pBR322, its derivatives, or other microbial plasmids or bacteriophage may also contain, or be modified to contain, promoters which can be used by the microbial organism for expression of endogenous proteins.

In addition, phage vectors containing replicon and control sequences that are
30 compatible with the host microorganism can be used as transforming vectors in connection with these hosts. For example, bacteriophage such as λ GEM.TM.-I 1 may be utilized in making a recombinant vector which can be used to transform susceptible host cells such as *E. coli* LE392.

Either constitutive or inducible promoters can be used in the present invention, in
35 accordance with the needs of a particular situation, which can be ascertained by one skilled in the art. A large number of promoters recognized by a variety of potential host cells are

well known. The selected promoter can be operably linked to cistron DNA encoding a polypeptide described herein by removing the promoter from the source DNA via restriction enzyme digestion and inserting the isolated promoter sequence into the vector of choice.

Both the native promoter sequence and many heterologous promoters may be used to direct
5 amplification and/or expression of the target genes. However, heterologous promoters are preferred, as they generally permit greater transcription and higher yields of expressed target gene as compared to the native target polypeptide promoter.

Promoters suitable for use with prokaryotic hosts include the PhoA promoter, the β -galactamase and lactose promoter systems, a tryptophan (*trp*) promoter system and hybrid
10 promoters such as the *tac* or the *trc* promoter. However, other promoters that are functional in bacteria (such as other known bacterial or phage promoters) are suitable as well. Their nucleotide sequences have been published, thereby enabling a skilled worker operably to ligate them to cistrons encoding the polypeptides or variant polypeptides (Siebenlist et al., Cell, 20: 269 (1980)) using linkers or adaptors to supply any required restriction sites.

15 In embodiments, each cistron within a recombinant vector comprises a secretion signal sequence component that directs translocation of the expressed polypeptides across a membrane. In general, the signal sequence may be a component of the vector, or it may be a part of the polypeptide encoding DNA that is inserted into the vector. The signal sequence selected for the purpose of this invention should be one that is recognized and processed
20 (i.e. cleaved by a signal peptidase) by the host cell. For prokaryotic host cells that do not recognize and process the signal sequences native to the heterologous polypeptides, the signal sequence is substituted by a prokaryotic signal sequence selected, for example, from the group consisting of the alkaline phosphatase, penicillinase, Ipp, or heat-stable enterotoxin II (STII) leaders, LamB, PhoE, PeIB, OmpA and MBP.

25 Prokaryotic host cells suitable for expressing polypeptides include Archaeobacteria and Eubacteria, such as Gram-negative or Gram-positive organisms. Examples of useful bacteria include Escherichia (e.g., *E. coli*), Bacilli (e.g., *B. subtilis*), Enterobacteria, Pseudomonas species (e.g., *P. aeruginosa*), Salmonella typhimurium, Serratia marcescans, Klebsiella, Proteus, Shigella, Rhizobia, Vitreoscilla, or Paracoccus. Preferably, gram-
30 negative cells are used. Preferably the host cell should secrete minimal amounts of proteolytic enzymes, and additional protease inhibitors may desirably be incorporated in the cell culture.

Besides prokaryotic host cells, eukaryotic host cell systems are also well established in the art. Examples of invertebrate cells include insect cells such as Drosophila S2 and
35 Spodoptera Sf9, as well as plants and plant cells. Examples of useful mammalian host cell lines include Chinese hamster ovary (CHO) and COS cells. More specific examples include

monkey kidney CV1 line transformed by SV40 (COS-7, ATCC CRL 1651); Chinese hamster ovary cells/-DHFR (CHO, Urlaub and Chasin, *Proc. Natl. Acad. Sci. USA*, 77:4216 (1980)); mouse Sertoli cells (TM4, Mather, *Biol. Reprod.*, 23:243-251 (1980)); High Five cells (derived from *Trichopulsia ni* cell line; High Five cells are available from Invitrogen) and mouse mammary tumor (MMT 060562, ATCC CCL5 1).

In a specific embodiment, a baculovirus transfer vector is utilized. Several such transfer vectors are known to those of skill in the art and commercially available. For example, BD Pharmingen has several vectors using sequences from AcPNV baculovirus.

Polypeptide Production

Host cells are transformed or transfected with the above-described expression vectors and cultured in conventional nutrient media modified as appropriate for inducing promoters, selecting transformants, or amplifying the genes encoding the desired sequences.

Transfection refers to the taking up of an expression vector by a host cell whether or not any coding sequences are in fact expressed. Numerous methods of transfection are known to the ordinarily skilled artisan, for example, CaPO_4 precipitation and electroporation. Successful transfection is generally recognized when any indication of the operation of this vector occurs within the host cell.

Transformation means introducing DNA into the prokaryotic host so that the DNA is replicable, either as an extrachromosomal element or by chromosomal integrant. Depending on the host cell used, transformation is done using standard techniques appropriate to such cells. The calcium treatment employing calcium chloride is generally used for bacterial cells that contain substantial cell-wall barriers. Another method for transformation employs polyethylene glycol/DMSO. Yet another technique used is electroporation.

Prokaryotic cells used to produce the polypeptides of the invention are grown in media known in the art and suitable for culture of the selected host cells. Examples of suitable media include luria broth (LB) plus necessary nutrient supplements. In preferred embodiments, the media also contains a selection agent, chosen based on the construction of the expression vector, to selectively permit growth of prokaryotic cells containing the expression vector. For example, ampicillin is added to media for growth of cells expressing ampicillin resistant gene.

Any necessary supplements besides carbon, nitrogen, and inorganic phosphate sources may also be included at appropriate concentrations introduced alone or as a mixture with another supplement or medium such as a complex nitrogen source. Optionally the culture medium may contain one or more reducing agents selected from the group

consisting of glutathione, cysteine, cystamine, thioglycollate, dithioerythritol and dithiothreitol.

The prokaryotic host cells are cultured at suitable temperatures. For *E. coli* growth, for example, the preferred temperature ranges from about 20°C to about 39°C, more preferably from about 25°C to about 37°C, even more preferably at about 30°C. The pH of the medium may be any pH ranging from about 5 to about 9, depending mainly on the host organism. For *E. coli*, the pH is preferably from about 6.8 to about 7.4, and more preferably about 7.0.

If an inducible promoter is used in the expression vector, protein expression is induced under conditions suitable for the activation of the promoter. For example, if a PhoA promoter is used for controlling transcription, the transformed host cells may be cultured in a phosphate-limiting medium for induction. A variety of other inducers may be used, according to the vector construct employed, as is known in the art.

Eukaryotic host cells are cultured under conditions suitable for expression of the OX40L and/or OX40 receptor polypeptides. The host cells used to produce the polypeptides may be cultured in a variety of media. Commercially available media such as Ham's F10 (Sigma), Minimal Essential Medium ((MEM), (Sigma), RPMI-1 640 (Sigma), and Dulbecco's Modified Eagle's Medium ((DMEM), Sigma) are suitable for culturing the host cells. In addition, any of the media described in one or more of Ham et al., Meth. Enz., 58:44 (1979), Barnes et al., Anal. Biochem., 102: 255 (1980), USPN 4,767,704, USPN 4,657,866, USPN 4,927,762, USPN 4,560,655, or USPN 5,122,469, WO 90/103430, WO 87/00195, and USPN Re. 30,985 may be used as culture media for the host cells. Any of these media may be supplemented as necessary with hormones and/or other growth factors (such as insulin, transferrin, or epidermal growth factor), salts (such as sodium chloride, calcium, magnesium, and phosphate), buffers (such as HEPES™), nucleotides (such as adenosine and thymidine), antibiotics (such as GENTAMYCIN™), trace elements (defined as inorganic compounds usually present at final concentrations in the micromolar range), and glucose or an equivalent energy source. Other supplements may also be included at appropriate concentrations that would be known to those skilled in the art. The culture conditions, such as temperature, pH, and the like, are those previously used with the host cell selected for expression, and will be apparent to the ordinarily skilled artisan.

Polypeptides described herein expressed in a host cell may be secreted and/or recovered from the periplasm of the host cells. Protein recovery typically involves disrupting the microorganism, generally by such means as osmotic shock, sonication or lysis. Once cells are disrupted, cell debris or whole cells may be removed by centrifugation or filtration. The proteins may be further purified, for example, by affinity resin

chromatography. Alternatively, proteins can be transported or secreted into the culture media and isolated there from. Cells may be removed from the culture and the culture supernatant filtered and concentrated for further purification of the proteins produced. The expressed polypeptides can be further isolated and identified using commonly known methods such as fractionation on immunoaffinity or ion-exchange columns; ethanol precipitation; reverse phase HPLC; chromatography on silica or on a cation exchange resin such as DEAE; chromatofocusing; SDS-PAGE; ammonium sulfate precipitation; gel filtration using, for example, Sephadex G-75; hydrophobic affinity resins, ligand affinity using a suitable antigen immobilized on a matrix and Western blot assay.

Polypeptides that are produced may be purified to obtain preparations that are substantially homogeneous for further assays and uses. Standard protein purification methods known in the art can be employed. The following procedures are exemplary of suitable purification procedures: fractionation on immunoaffinity or ion-exchange columns, ethanol precipitation, reverse phase HPLC, chromatography on silica or on a cation-exchange resin such as DEAE, chromatofocusing, SDS-PAGE, ammonium sulfate precipitation, and gel filtration using, for example, Sephadex G-75.

2. Crystals and Crystal Structures

The present disclosure provides a crystalline form of and a crystal structure of the mOX40L, and a crystalline form of and the crystal structures of the hOX40 receptor cocrystallized with either mOX40L or hOX40L. The crystals are formed by contacting a mixture of purified OX40L and/or fragment thereof and/or an hOX40 receptor and/or fragment thereof with a precipitant in a buffer. In some embodiments, the precipitant is about 8-10% polyethylene glycol 20,000. In other embodiments, the precipitant is about 1-2M ammonium sulfate.

tnOX40L can be purified and crystallized. In a specific embodiment, mOX40L is a fragment comprising the amino acid sequence of S51 to L198 of SEQ ID NO:1 (Table 3b). The crystals of mOX40L can be diffracted to about 1.45-2.5 Å resolution (Table 1). The crystals belong in space group $P6_3$ with $a=b$ and are about 74 Å, and c about 48 Å. Unit cell volume and molecular weight suggested 1 protomer in the asymmetric unit. When the crystals are resolubilized, the mOX40L has at least one biological activity. Crystals can be combined with a carrier to form a composition. Crystal of mOX40L may also be a useful way to store, concentrate or deliver mOX40L. Constituent amino acids in mOX40L have a set of structural coordinates as provided in Table 8. NAG indicates carbohydrate residues.

The cocrystals of mOX40L and hOX40 receptor diffracted to about 2.00-2.07 Å resolution (Table 1) and the biologically relevant complex contains 3 ligands forming a trimer and 3 receptors. The structural coordinates for the 2 ligand/receptor pairs in the

mOX40L-hOX40 structure are part of two different complexes. In a specific embodiment, mOX40L is a fragment comprising residues S51 to L198 of SEQ ID NO:1 (Table 3b) and hOX40 receptor is a fragment comprising the amino acid sequence of 29-170 of SEQ ID NO:2 (Table 4b).

5 In a specific embodiment, the structure of mOX40L and hOX40 receptor was solved by molecular replacement with the program AMORE (NAVAZA 1994) using the crystal structure of mOX40L alone as search model. The crystals belonged to space group R32 with cell parameters of: $a=b$ and are about 105 Å, and c is about 478 Å. Crystals of the complex can be combined with a carrier to form a composition. Crystals may also be a
10 useful way to store, concentrate or deliver a of mOX40L and/or hOX40 receptor. Constituent amino acids in mOX40L and/or hOX40 receptor complex have a set of structural coordinates as set forth in Table 9. The coordinates of two molecules of each of mOX40L and hOX40 receptor are provided. The structural coordinates for the 2 ligand/receptor pairs in the mOX40L-hOX40 structure are part of two different complexes. The
15 structural coordinates from each of the molecules as shown in Table 9 may be utilized.

The crystals of hOX40L and hOX40 receptor diffracted to about 2.40-2.49 Å resolution (Table 1) and have one (1) full complex containing one trimeric ligand and 1 receptor in the crystallographic asymmetric unit. Crystallographic three-fold symmetry generates the biologically relevant trimers. In a specific embodiment, hOX40L is a
20 fragment comprising residues 51-183 of SEQ ID NO:3 (Table 5b) and hOX40 receptor is a fragment comprising the amino acid sequence of 29-170 of SEQ ID NO:2 (Table 4b). In some embodiments, hOX40L is a fragment comprising residues 51-183 of SEQ ID NO:3 (Table 5b) with an amino acid substitution N90D and N114D.

In a specific embodiment, the structure of hOX40L and hOX40 receptor was solved
25 by molecular replacement with the program AMORE (NAVAZA 1994) using the crystal structure of mOX40L alone as search model. The crystals belonged to space group R32 with cell parameters of: $a=b$ and are about 112 Å, c is about 233 Å. Crystals of the complex can be combined with a carrier to form a composition. Crystals may also be a useful way to store, concentrate or deliver a complex of hOX40L and/or hOX40 receptor.
30 Constituent amino acids in hOX40L and hOX40 receptor complex have a set of structural coordinates as set forth in Table 10.

The term "structure coordinates" refers to Cartesian coordinates derived from mathematical equations related to the patterns obtained on diffraction of a monochromatic beam of X-rays by the atoms (scattering centers) of a mOX40L, mOX40L-hOX40 receptor
35 complex, or hOX40L-hOX40 receptor in crystal form. The diffraction data are used to calculate an electron density map of the repeating unit of the crystal. The electron density

maps are then used to establish the positions of the individual atoms of the mOX40L, mOX40L-hOX40 receptor complex, or hOX40L-hOX40 receptor complex.

Slight variations in structure coordinates can be generated by mathematically manipulating the mOX40L, mOX40L-hOX40 receptor complex, or hOX40L-hOX40
5 receptor complex structure coordinates. For example, the structure coordinates as set forth in Tables 8, 9 and/or 10 could be manipulated by crystallographic permutations of the structure coordinates, fractionalization of the structure coordinates, integer additions or subtractions to sets of the structure coordinates, inversion of the structure coordinates, or any combination of the above. Alternatively, modifications in the crystal structure due to
10 mutations, additions, substitutions, deletions, and combinations thereof, of amino acids, or other changes in any of the components that make up the crystal, could also yield variations in structure coordinates. Such slight variations in the individual coordinates will have little effect on overall shape. If such variations are within an acceptable standard error as compared to the original coordinates, the resulting three-dimensional shape is considered to
15 be structurally equivalent. Structural equivalence is described in more detail below.

It should be noted that slight variations in individual structure coordinates of the mOX40L, mOX40L-OX40 receptor complex, or hOX40L-hOX40 receptor complex would not be expected to significantly alter the nature of chemical entities such as ligands that could associate with a binding site or other structural features of mOX40L, hOX40L, or
20 hOX40 receptor or complexes thereof. In this context, the phrase "associating with" refers to a condition of proximity between a ligand, or portions thereof, and a mOX40L, hOX40L, hOX40 receptor molecule or portions thereof. The association may be non-covalent, wherein the juxtaposition is energetically favored by hydrogen bonding, van der Waals forces, and/or electrostatic interactions, or it may be covalent.

25 In addition, all or a portion of the structural coordinates provided in any of Tables 8, 9, and/or 10 can be utilized to generate nmr assignments. The X-ray coordinates for OX40L-OX40 can be used to assist in determining NMR structures of OX40L, OX40, or complexes thereof with other entities. Briefly, chemical shift information may be obtained from NMR determined chemical shifts (using HSQC, TOCSY, NOESY and other
30 experiments) or may be calculated from the coordinates of OX40, OX40L, or the OX40-OX40L complex using computer programs such as SHIFTS or other custom programs. Comparison of the chemical shifts of free and bound molecules can be used to map binding sites of protein or small molecule ligands on either OX40, OX40L, or the OX40-Ox40L complex. In addition, an expected pattern of through-space proton-proton interactions
35 (NOESY crosspeaks) can be generated from the X-ray coordinated and compared to those measured in an NMR spectra (NOESY) using NMR structure determination programs such

as ATNOS, ARIA, CNS, CCPN or other custom programs. This information may then be used to refine the structures of complexes between OX40, OX40L, OX40-OX40L and other entities.

5 3. **Structurally equivalent crystal structures**

Various computational analyses can be used to determine whether a molecule or portions of the molecule defining structure features are "structurally equivalent," defined in terms of its three-dimensional structure, to all or part of a mOX40L, mOX40L-hOX40 receptor complex, or hOX40L-hOX40 receptor complex. Such analyses may be carried out
10 in current software applications, such as the Molecular Similarity application of QUANTA (Molecular Simulations Inc., San Diego, CA), Version 4.1, and as described in the accompanying User's Guide.

The Molecular Similarity application permits comparisons between different structures, different conformations of the same structure, and different parts of the same
15 structure. A procedure used in Molecular Similarity to compare structures comprises: 1) loading the structures to be compared; 2) defining the atom equivalences in these structures; 3) performing a fitting operation; and 4) analyzing the results.

One structure is identified as the target (i.e., the fixed structure); all remaining structures are working structures (i.e., moving structures). Since atom equivalency within
20 QUANTA is defined by user input, for the purpose of this disclosure equivalent atoms are defined as protein backbone atoms (N, Ca, C, and O) for all conserved residues between the two structures being compared. A conserved residue is defined as a residue that is structurally or functionally equivalent. Only rigid fitting operations are considered.

When a rigid fitting method is used, the working structure is translated and rotated
25 to obtain an optimum fit with the target structure. The fitting operation uses an algorithm that computes the optimum translation and rotation to be applied to the moving structure, such that the root mean square difference of the fit over the specified pairs of equivalent atom is an absolute minimum. This number, given in Angstroms, is reported by QUANTA.

Structurally equivalent crystal structures have portions of the two molecules that are
30 substantially identical, within an acceptable margin of error. The margin of error can be calculated by methods known to those of skill in the art. In some embodiments, any molecule or molecular complex or any portion thereof, that has a root mean square deviation of conserved residue backbone atoms (N, Ca, C, O) of less than about 0.70 Å, preferably 0.5 Å. For example, structurally equivalent molecules or molecular complexes are those
35 that are defined by the entire set of structure coordinates listed in Tables 8, 9, and/or 10 ± a root mean square deviation from the conserved backbone atoms of those amino acids of not

more than 0.70 Å, preferably 0.5 Å. The term "root mean square deviation" means the square root of the arithmetic mean of the squares of the deviations. It is a way to express the deviation or variation from a trend or object. For purposes of this disclosure, the "root mean square deviation" defines the variation in the backbone of a protein from the backbone of
 5 mOX40L, mOX40L-hOX40 receptor complex, or mOX40L-hOX40 receptor complex (as defined by the structure coordinates of the complex as described herein) or a defining structural feature thereof.

4. **Structurally homologous molecules, molecular complexes, and crystal structures**

10

Structure coordinates can be used to aid in obtaining structural information about another crystallized molecule or molecular complex. The method of the disclosure allows determination of at least a portion of the three-dimensional structure of molecules or molecular complexes that contain one or more structural features that are similar to
 15 structural features of at least a portion of the mOX40L, mOX40L-hOX40 receptor complex, or hOX40L-hOX40 receptor complex. These molecules are referred to herein as "structurally homologous" to mOX40L, mOX40L-hOX40 receptor complex, or hOX40L-hOX40 receptor complex. Similar structural features can include, for example, regions of amino acid identity, conserved active site or binding site motifs, and similarly arranged
 20 secondary structural elements.

Structural elements in OX40L include several domains including A, A', B', B, C, D, E, F, G, and H β sheet strands that form jelly roll β sandwich monomer sheets as follows: A'AHCF and B'BGDE. The OX40L forms a flower like trimer with interface formed by a layer of generally hydrophobic residues along the C strand, F strand, and C terminal
 25 extension (amino acid residues 175-183 in hOX40L and residues 178-191 in mOX40L). The monomers are splayed out and form an angle of about 45° with respect to the trimer axis. The trimer interface is compact with about 2600 Å² accessible surface area buried.

In some embodiments, a portion of the three dimensional structure refers to structural domains of the OX40L, including the A, A', B', B, C, D, E, F, G, H β sheets or
 30 the loops connecting the β sheets including amino acid residues corresponding to Q80, E82, D98, S110, Y119, E123, E124, T144, Y145, K146, D147, D162, H164, V165, F180, L183 of the amino acid sequence of SEQ ID NO:3 or combinations thereof. In some embodiments, the structural domains include A and/or H β sheets, and/or amino acids linking β sheets A' to B', B to C, C to D, D to E, F to G, G to H, or combinations thereof. In other
 35 embodiments, the structural domains refer to the amino acids found at the interface of the trimer including amino acids corresponding to those found at positions Q175, L102, L138, or mixtures thereof. The trimer interface may comprise amino acid residues 98 to 183 of the

amino acid sequence of SEQ ID NO:3, or may comprise amino acid residues 99 to 191 of the amino acid sequence of SEQ ID NO:1. In some embodiments, the structural element is the mOX40L and/or hOX40L binding site for hOX40 receptor.

Structural elements in hOX40 receptor include three full CRDs and a partial C-terminal CRD which form a contiguous structure. CRD1 and CRD2 form a rigid unit while there is some rotational freedom between the subdomains of CRD3 and the partial CRD4. CRD3 in hOX40 differs more than CRD1 and CRD2 from its counterpart in TNFR1 or DR5 as it is smaller and lacks one of the canonical disulfides. CRD3 contains an A1, B1 module rather than the A1, B2 architecture of CRD1 and 2. In the case of OX40, the disulfide formed by the fourth and sixth cysteines in CRD3 (the 4-6 disulfide) is missing. This missing disulfide in hOX40 CRD3 is not replaced by either hydrogen bonds or hydrophobic interactions, but rather the entire module smaller due to shortening and re-arrangement of intervening loops. This re-arrangement causes the backbone of the remaining 3-5 disulfide to be in an anti-parallel orientation rather than the parallel orientation seen in B2 modules. A long disulfide containing loop follows the B1 module. The connectivity and structure of this loop are compatible with it being an A1 module of a vestigial CRD4.

In some embodiments, a portion of the three dimensional structure refers to the domains of hOX40 receptor including CRD1, CRD2, CRD3, CRD4, or combinations thereof. In some embodiments, CRD1 comprises amino acids 29-65; CRD2 comprises amino acids 66-108; CRD3 comprises amino acids 109-147; of the amino acid sequence of SEQ ID NO:2. In some embodiments, CRD1 includes at least residues 31-64 including Cys 31, 42, 43, 56, 46 and 64; CRD2 includes at least residues 67-107 including Cys 67, Cys 81, Cys 84, Cys 99, Cys 87 and Cys 107; CRD3 includes at least 109-141 including cys 109, cys 125, cys 128, and cys 141; and CRD4 includes at least residues 147-166 including cys 147 and cys 166 of the amino acid sequence of SEQ ID NO:2. In some embodiments, the structural domain is that of the CRD1, CRD2 or CDRD3. In some embodiments, the structural feature is the binding site on hOX40 receptor for hOX40L or mOX40L. In some embodiments, structurally homologous molecules do not include the CRD2 domain of DR5, or the CRD3 domain of hGITR, hRANK and/or hEDAR.

Optionally, structural homology is determined by aligning the residues of the two amino acid sequences to optimize the number of identical amino acids along the lengths of their sequences; gaps in either or both sequences are permitted in making the alignment in order to optimize the number of identical amino acids, although the amino acids in each sequence must nonetheless remain in their proper order. Two amino acid sequences are compared using the BLAST program, version 2.0.9, of the BLAST 2 search algorithm, as described by Tatusova et al. (56), and available at <http://www.ncbi.nlm.nih.gov/BLAST/>.

Preferably, the default values for all BLAST 2 search parameters are used, including matrix = BLOSUM62; open gap penalty = 11, extension gap penalty = 1, gap x_dropoff = 50, expect = 10, wordsize = 3, and filter on. In the comparison of two amino acid sequences using the BLAST search algorithm, structural similarity is referred to as "identity."

5 In some embodiments, a structurally homologous molecule is a protein that has an amino acid sequence having at least 80% identity with a wild type or recombinant amino acid sequence of mOX40L, hOX40 receptor, or hOX40L having a sequence of SEQ ID NO:1, SEQ ED NO:2, or SEQ ID NO:3, of fragments thereof as described herein respectively. More preferably, a protein that is structurally homologous to mOX40L,
10 hOX40 receptor, or hOX40L includes at least one contiguous stretch of at least 25, 50, or even up to 100 amino acids that have at least 80% amino acid sequence identity with the analogous portion of the wild type or recombinant mOX40L, hOX40 receptor, or hOX40L. Methods for generating structural information about the structurally homologous molecule or molecular complex are well known and include, for example, molecular replacement
15 techniques.

Therefore, in another embodiment this disclosure provides a method of utilizing molecular replacement to obtain structural information about a molecule or molecular complex whose structure is unknown comprising:

(a) generating an X-ray diffraction pattern from a crystallized molecule or
20 molecular complex of unknown or incompletely known structure; and
(b) applying at least a portion of the structural coordinates of mOX40L, mOX40L-hOX40 receptor complex, or hOX40L-hOX40 receptor complex to the X-ray diffraction pattern to generate a three-dimensional electron density map of the molecule or molecular complex whose structure is unknown or incompletely known.

25 By using molecular replacement, all or part of the structure coordinates of mOX40L, mOX40L-hOX40 receptor complex, or hOX40L-hOX40 receptor complex as provided by this disclosure can be used to determine the unsolved structure of a crystallized molecule or molecular complex more quickly and efficiently than attempting to determine such information *ab initio*.

30 Molecular replacement can provide an accurate estimation of the phases for an unknown or incompletely known structure. Phases are one factor in equations that are used to solve crystal structures, and this factor cannot be determined directly. Obtaining accurate values for the phases, by methods other than molecular replacement, can be a time-consuming process that involves iterative cycles of approximations and refinements and
35 greatly hinders the solution of crystal structures. However, when the crystal structure of a protein containing at least a structurally homologous portion has been solved, molecular

replacement using the known structure provide a useful estimate of the phases for the unknown or incompletely known structure.

Thus, this method involves generating a preliminary model of a molecule or molecular complex whose structure coordinates are unknown, by orienting and positioning the relevant portion of the mOX40L, mOX40L-hOX40 receptor complex, or hOX40L-hOX40 receptor complex within the unit cell of the crystal of the unknown molecule or molecular complex. This orientation or positioning is conducted so as best to account for the observed X-ray diffraction pattern of the crystal of the molecule or molecular complex whose structure is unknown. Phases can then be calculated from this model and combined with the observed X-ray diffraction pattern amplitudes to generate an electron density map of the structure. This map, in turn, can be subjected to established and well-known model building and structure refinement techniques to provide a final, accurate structure of the unknown crystallized molecule or molecular complex (see for example, Lattman, Methods in Enzymology, 115:55-77 (1985)).

Structural information about a portion of any crystallized molecule or molecular complex that is sufficiently structurally homologous to a portion of mOX40L, mOX40L-hOX40 receptor complex, or hOX40L-hOX40 receptor complex can be solved by this method. In addition to a molecule that shares one or more structural features with the OX40L, such as the β sandwich monomer sheets and/or trimer interface, and/or OX40 receptor CRD domains described above, a molecule that has similar bioactivity, such as the same catalytic activity, substrate specificity or ligand binding activity as mOX40L, mOX40L-hOX40 receptor complex, or hOX40L-hOX40 receptor complex, may also be sufficiently structurally homologous to a portion of the mOX40L, mOX40L-hOX40 receptor complex, or hOX40L-hOX40 receptor complex to permit use of the structure coordinates of described herein to solve its crystal structure or identify structural features that are similar to those identified in the mOX40L, mOX40L-hOX40 receptor complex, or hOX40L-hOX40 receptor complex. It will be appreciated that amino acid residues in the structurally homologous molecule identified as corresponding to the OX40L or hOX40 receptor structural feature may have different amino acid numbering.

In one embodiment of the disclosure, the method of molecular replacement is utilized to obtain structural information about a molecule or molecular complex, wherein the molecule or molecular complex is homologous to at least one mOX40L, mOX40L-hOX40 receptor complex, or hOX40L-hOX40 receptor complex structural feature or homolog. In the context of the present disclosure, a "structural homolog" of the mOX40L, mOX40L-hOX40 receptor complex, or hOX40L-hOX40 receptor complex is a protein that contains one or more amino acid substitutions, deletions, additions, or rearrangements with respect to

the amino acid sequence of mOX40L, mOX40L-hOX40 receptor complex, or hOX40L-hOX40 receptor complex, but that, when folded into its native conformation, exhibits or is reasonably expected to exhibit at least a portion of the tertiary (three-dimensional) structure of at least a portion of mOX40L, mOX40L-hOX40 receptor complex, or hOX40L-hOX40
5 receptor complex.

A heavy atom derivative of mOX40L, mOX40L-hOX40 receptor complex, or hOX40L-hOX40 receptor complex is a homolog. The term "heavy atom derivative" refers to derivatives of mOX40L, mOX40L-hOX40 receptor complex, or hOX40L-hOX40 receptor complex by chemically modifying a crystal of mOX40L, mOX40L-hOX40
10 receptor complex, or hOX40L-hOX40 receptor complex. In practice, a crystal is soaked in a solution containing heavy metal atom salts, or organometallic compounds, e.g., lead chloride, gold thiomalate, thiomersal or uranyl acetate, which can diffuse through the crystal and bind to the surface of the protein. The location(s) of the bound heavy metal atom(s) can be determined by X-ray diffraction analysis of the soaked crystal. This information, in turn,
15 is used to generate the phase information used to construct three-dimensional structure of the protein (Blundell, et al., 1976, Protein Crystallography, Academic Press, San Diego, CA.).

An isotopically labeled polypeptide of mOX40L, hOX40 receptor complex, or hOX40L complex is a derivative. Isotopic labels include ^{13}C , ^{15}N , ^2H , ^3H , ^{31}P , ^{23}Na , ^{14}N , and
20 /or ^{19}F .

mOX40L, hOX40 receptor, or hOX40L polypeptides may be prepared, for example, by expression of cDNA previously altered in its coding sequence by oligonucleotide-directed mutagenesis as described herein. Polypeptides may also be generated by site-specific incorporation of unnatural amino acids into mOX40L, hOX40 receptor, or hOX40L
25 polypeptides using known biosynthetic methods (Noren, et al., Science, 244: 182-88 (1989)). hOX40L polypeptides with amino acid substitutions have been described herein.

For example, structurally homologous molecules can contain deletions or additions of one or more contiguous or noncontiguous amino acids, such as a loop or a domain. For example, domains and loops of hOX40L are shown in Figure 3 and described herein.
30 Structurally homologous molecules also include "modified" mOX40L, hOX40 receptor, or hOX40L polypeptides molecules that have been chemically or enzymatically derivatized at one or more constituent amino acid, including side chain modifications, backbone modifications, and N- and C- terminal modifications including acetylation, hydroxylation, methylation, amidation, and the attachment of carbohydrate or lipid moieties, cofactors, and
35 like modifications. It will be appreciated that amino acid residues in the structurally

homologous molecule identified as corresponding to mOX40L, hOX40 receptor, or hOX40L polypeptides or other structural feature may have different amino acid numbering.

All of the complexes referred to above may be studied using well-known X-ray diffraction techniques and may be refined versus 1.5-3.5 Å resolution X-ray data to an R-factor of about 0.30 or less using computer software, such as X-PLOR (Yale University, distributed by Molecular Simulations, Inc.) (see, for example, Blundell, et al. 1976. Protein Crystallography, Academic Press, San Diego, CA., and Methods in Enzymology, Vol. 114 & 115, H.W. Wyckoff et al., eds., Academic Press (1985)). This information may thus be used to optimize known mOX40L, hOX40 receptor, or hOX40L modulators, and more importantly, to design new mOX40L, hOX40 receptor, or hOX40L modulators.

In addition, all or a portion of the structural coordinates may be utilized to make nmr assignments of the residues of all or a portion of mOX40L, hOX40L, and/or hOX40 receptor. The X-ray coordinates for OX40L-OX40 can be used to assist in determining NMR structures of OX40L, OX40, or complexes thereof, with other entities. Briefly, chemical shift information may be obtained from NMR determined chemical shifts (using HSQC, TOCSY, NOESY and other experiments) or may be calculated from the coordinates of OX40, OX40L, or the OX40-OX40L complex using computer programs such as SHIFTS or other custom programs. Comparison of the chemical shifts of free and bound molecules can be used to map binding sites of protein or small molecule ligands on either OX40, OX40L, or the OX40-OX40L complex. In addition, an expected pattern of through-space proton-proton interactions (NOESY crosspeaks) can be generated from the X-ray coordinated and compared to those measured in an NMR spectra (NOESY) using NMR structure determination programs such as ATNOS, ARIA, CNS, CCPN or other custom programs. This information may then be used to refine the structures of complexes between OX40, OX40L, OX40-OX40L and other entities.

The disclosure also includes the unique three-dimensional configuration defined by a set of points defined by the structure coordinates for a molecule or molecular complex structurally homologous to mOX40L, hOX40 receptor, or hOX40L polypeptides as determined using the method of the present disclosure, structurally equivalent configurations, configuration of homologous sequences or structures and magnetic storage media including such sets of structure coordinates.

5. Homology modeling

Using homology modeling, a computer model of a homolog of a mOX40L, hOX40 receptor, or hOX40L polypeptides or complexes thereof can be built or refined without crystallizing the homolog. First, a preliminary model of the homolog is created by sequence alignment with mOX40L, hOX40 receptor, or hOX40L polypeptides, secondary structure

prediction, the screening of structural libraries, or any combination of those techniques. Computational software may be used to carry out the sequence alignments and the secondary structure predictions. Structural incoherences, e.g., structural fragments around insertions and deletions, can be modeled by screening a structural library for peptides of the
5 desired length and with a suitable conformation. For prediction of the side chain conformation, a side chain rotamer library may be employed. If the homolog has been crystallized, the final homology model can be used to solve the crystal structure of the homolog by molecular replacement, as described above. Next, the preliminary model is subjected to energy minimization to yield an energy-minimized model. The energy-
10 minimized model may contain regions where stereochemistry restraints are violated, in which case such regions are remodeled to obtain a final homology model. The homology model is positioned according to the results of molecular replacement, and subjected to further refinement including molecular dynamics calculations.

6. **Methods for Identification of Modulators of mOX40L, hOX40L, and/or**
15 **OX40 receptor**

Potent and selective ligands that modulate activity (antagonists and agonists) of mOX40L, hOX40 receptor, or hOX40L polypeptides are identified using the three-dimensional model of the binding site on mOX40L for the hOX40 receptor, or on the binding site on the hOX40L for the hOX40 receptor, or the binding site on hOX40 receptor
20 for mOX40L or hOX40L and/or other structural features produced using all or a portion of the coordinates of Tables 8, 9 and/or Table 10. Using these models, ligands that associate with such a binding site with or without a ligand or inhibitor are identified, and the result of the interactions is modeled. In some embodiments, agents identified as candidate molecules for modulating the activity of mOX40L, hOX40L, and/or hOX40 receptor can be screened
25 against known bioassays. For example, the ability of an agent to inhibit the binding of mOX40L and/or hOX40L to hOX40 receptor can be measured using assays known in the art. Elisa may be used to determine whether agent inhibits of binding of OX40 to OX40L, or vice versa . Bioassays for OX40L antagonist: detect inhibition of OX40-induced NFK/3 signaling, detect inhibition of T cell proliferation using MLR assay. These assays are
30 described in co-owned co-pending USSN 60/751,377 (filed Dec. 16, 2005) and WO2006/029879.

Using the modeling information and the assays described, one can identify agents that possess mOX40L, hOX40L, and/or hOX40 receptor modulating properties.

The methods of the disclosure also include methods of identifying molecules that
35 mimic binding of mOX40L and/or hOX40L to hOX40 receptor, but do not activate the receptor, or mimic binding of hOX40 receptor to mOX40L and/or hOX40L, but do not

activate the OX40 ligand. These molecules can be identified using the three-dimensional model of mOX40L, hOX40L- hOX40 receptor complexes, and/or mOX40L-OX40 receptor complexes using all or a portion of the coordinates of Tables 8, 9, and/or 10. The methods of the disclosure further comprise testing the test agent in an assay for binding and/or

5 modulating activity.

In another embodiment, a candidate modulator can be identified using a biological assay such as binding to hOX40 receptor or receptor activation, or binding to mOX40L or hOX40L. The candidate modulator can then serve as a model to design similar agents and/or to modify the candidate modulator for example, to improve characteristics such as
10 binding to mOX40L, hOX40L, OX40 receptor or complexes thereof. Design or modification of candidate modulators can be accomplished using the crystal structure coordinates and available software.

Binding Site and Other Structural Features

15 Applicants' disclosure provides information inter alia about the shape and structure of the binding site of mOX40L for the hOX40 receptor, hOX40L for the hOX40 receptor, and/or OX40 receptor for mOX40L and/or hOX40L. Binding sites are of significant utility in fields such as drug discovery. The association of ligands or substrates with the binding sites of their corresponding receptors or enzymes is the basis of many biological
20 mechanisms of action. Similarly, many drugs exert their biological effects through association with the binding sites of receptors and enzymes. Such associations may occur with all or any part of the binding site. An understanding of such associations helps lead to the design of drugs having more favorable associations with their target, and thus improved biological effects. Therefore, this information is valuable in designing potential modulators
25 of mOX40L, hOX40L, and/or hOX40 receptor binding sites, as discussed in more detail below.

In some embodiments, a hOX40L binding site for hOX40 receptor comprises, consists essentially of, or consists of at least one amino acid residue corresponding to an amino acid residue selected from the group consisting of Q65, T67, Q80, E82, D98, Y108, F109, S110, Y119, E123, E124, S142, T144, Y145, K146, D147, D162, H164, V165, N166, G167, F180, and V182 of the polypeptide comprising SEQ ID NO:3, and combinations thereof. In some embodiments, a hOX40L binding site for hOX40 receptor comprises, consists essentially of, or consists of at least one amino acid residue corresponding to an amino acid residue selected from the group consisting of Q65, T67, E82, D98, S110, E123, T144, Y145, K146, D147, D162, H164/V165, N166, G167, F180, and V182 of the polypeptide comprising SEQ ID NO:3, and combinations thereof. In some embodiments, a
35

hOX40L binding site for hOX40 receptor comprises, consists essentially of, or consists of at least one amino acid residue corresponding to an amino acid selected from the group consisting of D98, T144, D162, N166, and F180 of the polypeptide comprising SEQ ID NO:3, and combinations thereof. In some embodiments, a hOX40L functional binding site for hOX40 receptor comprises, consists essentially of, or consists of at least one amino acid residue corresponding to an amino acid residue selected from the group consisting of Q80, D162, T144, E123, N166 and F180 of the polypeptide comprising SEQ ID NO:3, and combinations thereof. In some embodiments, a hOX40L binding site for the hOX40 receptor includes 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23 or all of the identified amino acids or combinations thereof. The disclosure includes all or a portion of the crystal structure coordinates for at least one amino acid residue of a hOX40L binding site for hOX40 receptor, such as provided in Table 10.

In some embodiments, a mOX40L binding site for hOX40 receptor comprises, consists essentially of, or consists of at least one amino acid residue corresponding to an amino acid residue selected from the group consisting of R64, A66, T68, S78, Y80, K81, N82, E83, D99, F111, Q112, H119, R121, N125, P126, S145, L146, A147, F148, K149, D150, L166, Q167, I168, N169, G171, Y182, P185, G187, S188, Y189, and H190 of the polypeptide comprising SEQ ID NO:1, and combinations thereof. In some embodiments, a mOX40L binding site for hOX40 receptor comprises, consists essentially of, or consists of at least one amino acid residue corresponding to an amino acid residue selected from the group consisting of A66/T68, Y80, N82, E83, D99, F111, N125, P126, H119, S145, A147, F148, K149, D150, Q167, I168, N169, G171, Y182, S188, and Y189 of the polypeptide comprising SEQ ID NO:1, and combinations thereof. In some embodiments, a mOX40L binding site for hOX40 receptor comprises, consists essentially of, or consists of at least one amino acid residue corresponding to an amino acid residue selected from the group consisting of A66, Y80, D99, F111, A147, N169, Y182, and S188 of the polypeptide comprising SEQ ID NO:1, and combinations thereof. In some embodiments, a mOX40L binding site for the hOX40 receptor includes 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, or all of the identified amino acids, or combinations thereof. The disclosure includes all or a portion of the crystal structure coordinates for at least one amino acid residue of a mOX40L binding site for hOX40 receptor, such as provided in Tables 8 or 9.

In some embodiments, a hOX40 receptor binding site for hOX40L comprises, consists essentially of, or consists of at least one amino acid residue corresponding to an amino acid selected from the group consisting of T35, Y36, P37, S38, E45, M52, V53, S54, R55, R65, F71, V75, S78, K79, P80, K82, P83, C84, T85/W86, C87, N88, L89, Y119,

K120, V123, and D124 of the polypeptide comprising SEQ ED NO:2, and combinations thereof. In some embodiments, a hOX40 receptor binding site for hOX40L comprises, consists essentially of, or consists of at least one amino acid residue corresponding to an amino acid selected from the group consisting of Y36, P37, S38, E45, V53, R55, S78, K79, P83, T85, W86, C87, N88, Y1 19, and V123 of the polypeptide comprising SEQ ID NO:2, and combinations thereof. In some embodiments, a hOX40 receptor binding site for hOX40L comprises, consists essentially of, or consists of at least one amino acid residue corresponding to an amino acid selected from the group consisting of V53, R55, S78, K79, C87, and N88 of the polypeptide comprising SEQ ED NO:2, and combinations thereof. In some embodiments, a hOX40 receptor binding site for the hOX40L includes 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, or all of the identified amino acids or combinations thereof. The disclosure includes all or a portion of the crystal structure coordinates for at least one amino acid residue of a hOX40 receptor binding site for hOX40L, such as provided in Table 10.

In some embodiments, a hOX40 receptor binding site for mOX40L comprises, consists essentially of, or consists of at least one amino acid residue corresponding to an amino acid selected from the group consisting of L29, H30, C31, G33, T35, Y36, P37, S38, E45, M52, V53, S54, R55, F71, V75, S78, K79, P80, C81, P83, C84, T85, W86, C87, N88, R90, Y1 19, K120, and V123 of the polypeptide comprising SEQ ID NO:2, and combinations thereof. In some embodiments, a hOX40 receptor binding site for mOX40L comprises, consists essentially of, or consists of at least one amino acid residue corresponding to an amino acid selected from the group consisting of C31, G33, T35, Y36, P37, S38, E45, M52, V53, S54, R55, F71, S78, K79, P80, P83, C84, W86, N88, and Y1 19 of the polypeptide comprising SEQ ED NO:2, and combinations thereof. In some embodiments, a hOX40 receptor binding site for mOX40L comprises, consists essentially of, or consists of at least one amino acid residue corresponding to an amino acid selected from the group consisting of C31, Y36, P37, M52, R55, and P80 of the polypeptide comprising SEQ ID NO:2, and combinations thereof. In some embodiments, a hOX40 receptor binding site for the mOX40L includes 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, or all of the identified amino acids or combinations thereof. The disclosure includes all or a portion of the crystal structure coordinates for at least one amino acid residue of a hOX40 receptor binding site for mOX40L, such as provided in Table 9.

In some embodiments, a hOX40 receptor binding site for FIV comprises, consists essentially of, or consists of at least one amino acid corresponding to an amino acid selected

from the group consisting of R58, S59, N61, H44, V63 of the polypeptide comprising the amino acid sequence of SEQ ID NO:3, and combinations thereof.

Other structural features include the interface of hOX40L or mOX40L trimers. In some embodiments the interface comprises at least one amino acid or combinations thereof, in a position of OX40L corresponding to L102, L138, or Q175 of the polypeptide comprising the amino acid sequence of SEQ ID NO:3. In some embodiments, the trimer interface includes one or more amino acid residues corresponding to amino acids 98 to 182 or 183 of the amino acid sequence of SEQ ID NO:3. In some embodiments, the trimer interface includes one or more amino acid residues corresponding to amino acids 99 to 191 of SEQ. ID NO: 1. In other embodiments, the interface comprises at least one amino acid corresponding to an amino acid selected from the group consisting of D98, G99, F100, Y101, L102, I103, S104, L105, K106, G107, Y108, F109, S110, S134, V135, N136, S137, L138, M139, V140, A141, S142, L143, Q175, N176, P177, G178, E179, F180, C181, V182, L183 of the polypeptide comprising the amino acid sequence of SEQ ID NO:3, and combinations thereof. In some embodiments, a OX40L trimer interface includes 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32 or all of the identified amino acids, or combinations thereof. The disclosure includes all or a portion of the crystal structure coordinates for at least one amino acid residue of a hOX40L or mOX40L trimer interface.

20 ***Rational drug design***

Computational techniques can be used to screen, identify, select, design ligands, and combinations thereof, capable of associating with mOX40L, hOX40L, and/or hOX40 receptor or structurally homologous molecules. Candidate modulators of mOX40L, hOX40L, and/or hOX40 receptor may be identified using functional assays, such as binding assays, and novel modulators designed based on the structure of the candidate molecules so identified. Knowledge of the structure coordinates for mOX40L, hOX40L, and/or hOX40 receptor or complexes thereof permits, for example, the design, the identification of synthetic compounds, and like processes, and the design, the identification of other molecules and like processes, that have a shape complementary to the conformation of the mOX40L, hOX40L, and/or hOX40 receptor binding sites. The identification or design of modulators can be de novo or based on a known TNF inhibitor.

In particular, computational techniques can be used to identify or design ligands, such as agonists and/or antagonists, that associate with a mOX40L, hOX40L, and/or hOX40 receptor binding site. Antagonists may bind to or interfere with all or a portion of an active site of mOX40L, hOX40L, and/or hOX40 receptor, and can be competitive, non-competitive, or uncompetitive inhibitors. Once identified and screened for biological

activity, these agonists, antagonists, and combinations thereof, may be used therapeutically and/or prophylactically, for example, to block mOX40L, hOX40L, and/or hOX40 receptor activity and thus prevent the onset and/or further progression of diseases associated with mOX40L, hOX40L, and/or hOX40 receptor activity. Structure-activity data for analogues
 5 of ligands that bind to or interfere with mOX40L, hOX40L, and/or hOX40 receptor binding sites can also be obtained computationally.

In some embodiments, agonists or antagonists can be designed to include components that preserve and/ or strengthen the interactions. For example, such antagonists would include components that are able to associate, for example, hydrogen bond with one
 10 or more of Q80, D162, E163, and/or N166, or interact with hydrophobic residues T144 and/or F180 of the hOX40L. In some embodiments, the inhibitor would be designed to be more specific for hOX40L rather than mOX40L by minimizing interactions with one or more residues corresponding to A66, Y80, A147, Y182, S188, and/or F111 of the mOX40L. Such antagonists or agonists may also include components that are able to interact, for
 15 example, with hydrophobic residues A66, A188, and/or F111 of the mOX40L.

In some embodiments, for mOX40L or hOX40L, antagonist or agonist molecules are designed or selected that can associate with at least one or all amino acid residues that comprise, consist essentially of, or consist of at least one amino acid residue corresponding to an amino acid residue in the monomer interface, or mixtures thereof. In some
 20 embodiments, the trimer interface includes amino acid residues corresponding to amino acids 98 to 182 or 183 of the amino acid sequence of SEQ ID NO:3. In some embodiments, the trimer interface includes amino acid residues corresponding to amino acids 99 to 191 of SEQ. ID NO: 1. In some embodiments, the interface comprises at least one amino acid, or combinations thereof, in a position of OX40L corresponding to D98, G99, F100, Y101,
 25 L102, I103, S104, L105, K106, G107, Y108, F109, S110, S134, V135, N136, S137, L138, M139, V140, A141, S142, L143, Q175, N176, P177, G178, E179, F180, C181, V182, or L183 of SEQ ID NO:3. In some embodiments the agonist or antagonist that can bind at the monomer interface can fit into a groove of about 2600 Angstroms.

In other embodiments, another criteria that may be utilized in the design of
 30 modulators is whether the modulator can fit into the binding site on hOX40 receptor. In some embodiments, such antagonists or agonists would include components that are able to associate, for example, hydrogen bond with one or more of R55, K79, N88, C87, or combinations thereof, or associate with one or more of Y36, V53, S78, P83, W86, or combinations thereof, of the hOX40 receptor. The volume of the binding site hOX40
 35 receptor for hOX40L is about 2600 cubic angstroms, split about equally between the hOX40L and hOX40 receptor. The volume of the binding site hOX40 receptor for

mOX40L is about 2600 cubic angstroms, split about equally between the mOX40L and hOX40 receptor. In some embodiments, the volume of the identified or designed modulator may be 2600 angstroms or less. The volume of the cavity can be determined by using a program like GRASP to calculate the volume of those atoms.

5 In some embodiments, the portion of the mOX40L, hOX40L, or hOX40 receptor molecule that binds at the hOX40 receptor binding site or the hOX40L binding site can be used in the initial design of other inhibitors or modulators.

 For example, the present disclosure also includes a polypeptide comprising, consisting essentially of, or consisting of a portion or fragment of the OX40L. An
10 embodiment of a polypeptide fragment comprises, consists essentially of, or consists of an amino acid residue starting from any one of amino acid residue 51 to amino acid residue 65 and ending at amino acid residue 180 to residue 183 or residues corresponding to those positions in the polypeptide comprising SEQ ID NO:3. An embodiment of a polypeptide fragment comprises, consists essentially of, or consists of an amino acid residue starting
15 from any one of amino acid residue 51 to amino acid residue 66 and ending at amino acid residue 185 to residue 198 or residues corresponding to those positions in the polypeptide comprising SEQ ID NO: 1. In some embodiments, the polypeptide portion has the ability to bind to hOX40 receptor. Fragments of the hOX40L or mOX40L that include binding site residues or trimer interface residues may be utilized in the design of peptidomimetics. As
20 discussed previously, it may be desirable in some embodiments to design a modulator having moieties that can hydrogen bond with V53, W86, or C87 of the receptor.

 The present disclosure also includes a polypeptide comprising, consisting essentially of, or consisting of a portion or fragment of a hOX40 receptor. Preferably, the fragment comprises one or more of the CRD domains, preferably the CRD1, CRD2, and/or
25 CRD3 domains. An embodiment of a polypeptide fragment comprises a fragment starting at an amino acid residue 29 to amino acid residue 36 and ending at any one of amino acid residues 147 to amino acid residue 170 of SEQ ID NO:2. The fragment preferably retains the ability to bind to OX40L. As discussed previously, it may be desirable in some embodiments to retain amino acids or other moieties that can hydrogen bond with Q80 or
30 N166, or interact with F180 of the hOX40L. In some embodiments, a modulator may be about 2600 angstroms or less.

 In addition, the designed modulator molecules may also be modeled with other known members of TNFRSF or TNFSF in order to identify features that would enhance the specificity of the modulator for mOX40L, hOX40L, or hOX40 receptor. For example,
35 features may be selected that interact with the smaller trimer interface of hOX40L or that interact with CRD1 residues of hOX40 receptor (such as V53, R55, or Y36).

Other lead compounds that may be utilized to design antagonists or agonists of mOX40L, hOX40L, or hOX40 receptor include already identified classes of small molecule that inhibit TNFRSF or TNFSF. These inhibitors include 6,7-dimethyl-3-[(methyl{2-[methyl({1-[3-(trifluoromethyl)phenyl]-1H-indol-3-yl)methyl}amino)ethyl}amino)methyl]-4h-chromen-4-one and 5-(3-morpholin-4-yl-propyl)-2-(3-nitro-phenyl)-4-thioxo-4,5-dihydro-1-thia-3,5-diaza-cyclopenta[a]pentalen-6-one.

Several databases are available to search and identify compounds that may bind to and/or inhibit mOX40L, hOX40L, or hOX40 receptor. These databases include ACD (Molecular Designs Limited), NCI (National Cancer Institute), CCDC (Cambridge Crystalline Data Center) and DOCK (University of California, San Francisco).

Data stored in a machine-readable storage medium that is capable of displaying a graphical three-dimensional representation of the structure of mOX40L, hOX40L, or hOX40 receptor or a structurally homologous molecule or molecular complex, as identified herein, or portions thereof, may thus be advantageously used for drug discovery. The structure coordinates of the ligand are used to generate a three-dimensional image that can be computationally fit to the three-dimensional image of mOX40L, hOX40L, or hOX40 receptor or a structurally homologous molecule. The three-dimensional molecular structure encoded by the data in the data storage medium can then be computationally evaluated for its ability to associate with ligands. When the molecular structures encoded by the data is displayed in a graphical three-dimensional representation on a computer screen, the protein structure can also be visually inspected for potential association with ligands. The methods of the disclosure further comprise testing the test agent in an assay for binding and/or modulating activity.

One embodiment of the method of drug design involves evaluating the potential association of a candidate ligand with mOX40L, hOX40L, or hOX40 receptor or a structurally homologous molecule or homologous complex, particularly with at least one amino acid residue in a binding site of the mOX40L, hOX40L, or hOX40 receptor or a portion of the binding site. The method of drug design thus includes computationally evaluating the potential of a selected ligand to associate with any of the molecules or molecular complexes set forth above. This method includes the steps of: (a) employing computational means, for example, such as a programmable computer including the appropriate software known in the art or as disclosed herein, to perform a fitting operation between the selected ligand and a ligand binding site or a subsite of the ligand binding site of the molecule or molecular complex; and (b) analyzing the results of the fitting operation to quantify the association between the ligand and the ligand binding site. Optionally, the method further comprises analyzing the ability of the selected ligand to interact with amino acids in the mOX40L,

hOX40L, or hOX40 receptor binding site and/or subsite. The method may also further comprise optimizing the fit of the ligand for the binding site of mOX40L, hOX40L, or hOX40 receptor as compared to other TNFRSF or TNFSFL members. Optionally, the selected ligand can be synthesized, cocrystallized with mOX40L, hOX40L, or hOX40
5 receptor, and further modifications to selected ligand can be made to enhance inhibitory activity or fit in the binding pocket. Other structural features of the mOX40L, hOX40L, or hOX40 receptor such as the monomer interface can also be analyzed in the same manner. The methods of the disclosure further comprise testing the test agent or ligand in an assay for binding and/or modulating activity.

10 In another embodiment, the method of drug design involves computer-assisted design of ligand that associates with mOX40L, hOX40L, or hOX40 receptor, its homologs, or portions thereof. Ligands can be designed in a step-wise fashion, one fragment at a time, or may be designed as a whole or *de novo*. Ligands can be designed based on the structure of molecules that can modulate at least one biological function of mOX40L, hOX40L, or
15 hOX40 receptor. In addition, the inhibitors can be modeled on other known inhibitors of TNFRSF or TNFSFL.

In some embodiments, to be a viable drug candidate, the ligand identified or designed according to the method must be capable of structurally associating with at least part of a mOX40L, hOX40L, or hOX40 receptor binding site, and must be able, sterically
20 and energetically, to assume a conformation that allows it to associate with the mOX40L, hOX40L, or hOX40 receptor binding site. Non-covalent molecular interactions important in this association include hydrogen bonding, van der Waals interactions, hydrophobic interactions, and/or electrostatic interactions. Conformational considerations include the overall three-dimensional structure and orientation of the ligand in relation to the ligand
25 binding site, and the spacing between various functional groups of a ligand that directly interact with the mOX40L, hOX40L, or hOX40 receptor binding site or homologs thereof.

Optionally, the potential binding of a ligand to a mOX40L, hOX40L, or hOX40 receptor binding site is analyzed using computer modeling techniques prior to the actual synthesis and testing of the ligand. If these computational experiments suggest insufficient
30 interaction and association between it and the mOX40L, hOX40L, or hOX40 receptor binding site, testing of the ligand is obviated. However, if computer modeling indicates a strong interaction, the molecule may then be synthesized and tested for its ability to bind to or interfere with a mOX40L, hOX40L, or hOX40 receptor binding site. Assays to determine if a compound actually modulates mOX40L, hOX40L, or hOX40 receptor
35 activity can also be performed and are well known in the art.

Several methods can be used to screen ligands or fragments for the ability to associate with a mOX40L, hOX40L, or hOX40 receptor binding site. This process may begin by visual inspection of, for example, a mOX40L, hOX40L, or hOX40 receptor binding site on the computer screen based on the mOX40L, hOX40L, or hOX40 receptor or
5 complexes thereof structure coordinates or other coordinates which define a similar shape generated from the machine-readable storage medium. Selected ligands may then be positioned in a variety of orientations, or docked, within the binding site. Docking may be accomplished using software such as QUANTA and SYBYL, followed by energy minimization and molecular dynamics with standard molecular mechanics force fields, such
10 as CHARMM and AMBER.

Specialized computer programs may also assist in the process of selecting ligands. Examples include GRID (Hubbard, Nature Struct. Biol., 6:71 1-4 (1999)); MCSS (Miranker et al., Proteins, 11:29-34 (1991)) available from Molecular Simulations, San Diego, CA; AUTODOCK (Goodsell et al., Proteins, 8:195-202 (1990)) available from Scripps Research
15 Institute, La Jolla, CA; and DOCK (Kuntz et al., J. Mol. Biol., 161:269-88 (1982)) available from University of California, San Francisco, CA; Glide (Halgren et al. J. Med. Clin. 47:1750; Flexx, J. Mol. Biol., 261 :470 (1996)) and KM (Abagyan et al., J. Mol. Biol. 235:983 (1999)).

There are many ligand design methods including, without limitation, LUDI (Bohm, J. Comput. Aided Mol. Design, 6:61-78 (1992)) available from Molecular Simulations Inc.,
20 San Diego, CA; LEGEND (Nishibata et al., J. Med. Chem., 36:2921-8 (1993)) available from Molecular Simulations Inc., San Diego, CA; LeapFrog, available from Tripos Associates, St. Louis, MO; and SPROUT (Gillet et al., J. Comput. Aided Mol. Design, 7:127-53 (1993)) available from the University of Leeds, UK.

Useful programs to aid in searching databases to select ligands include, but are not limited to, CAVEAT (In Molecular Recognition in Chemical and Biological Problems, Royal Chem. Soc. 78:82-196 (1989), 3D Database Systems search as MACCS-3D (J. Med. Clin., 35:2145 (1992), HOOK (available from Molecular Simulateous, Burlington, Mass.) and CLIX (Lawrence et al. Proteins, 12:3141 (1992)).
25

Databases include ACD (Molecular Designs Limited), NCI (National Cancer Institute), CCDC (Cambridge Crystaleography Data Center) and DOCK (University of California, San Francisco).
30

Once a compound has been designed or selected by the above methods, the efficiency with which that ligand may bind to or interfere with a mOX40L, hOX40L, or
35 hOX40 receptor binding site may be tested and optimized by computational evaluation. For example, an effective binding site ligand should preferably demonstrate a relatively small

difference in energy between its bound and free states (i.e., a small deformation energy of binding). mOX40L, hOX40L, or hOX40 receptor binding site ligands may interact with the binding site in more than one conformation that is similar in overall binding energy. In those cases, the deformation energy of binding is taken to be the difference between the free
5 energy of the ligand and the average energy of the conformations observed when the ligand binds to the protein. A mOX40L, hOX40L, or hOX40 receptor binding site ligand can also preferably be designed with an IC₅₀ 0.1 to about 100nM, more preferably about 10 to 100 nM, more preferably about 50 to 100nM.

A ligand designed or selected as binding to or interfering with a mOX40L,
10 hOX40L, or hOX40 receptor binding site may be further computationally optimized so that in its bound state it would preferably lack repulsive electrostatic interaction with the receptor or its ligand and with the surrounding water molecules. Such non-complementary electrostatic interactions include repulsive charge-charge, dipole-dipole, and charge-dipole interactions.

15 Specific computer software is available to evaluate compound deformation energy and electrostatic interactions. Examples of programs designed for such uses include: Gaussian 94, revision C (MJ. Frisch, Gaussian, Inc., Pittsburgh, PA); AMBER, version 4.1 (P.A. Kollman, University of California at San Francisco,); QUANTA/CHARMM (Molecular Simulations, Inc., San Diego, CA); Insight II/Discover (Molecular Simulations,
20 Inc., San Diego, CA); DelPhi (Molecular Simulations, Inc., San Diego, CA); and AMSOL (Quantum Chemistry Program Exchange, Indiana University). These programs can be implemented, for instance, using a Silicon Graphics workstation, such as an Indigo2 with IMPACT graphics. Other hardware systems and software packages will be known to those skilled in the art.

25 Another approach encompassed by this disclosure is the computational screening of small molecule databases for ligands or compounds that can bind in whole, or in part, to a mOX40L, hOX40L, or hOX40 receptor. In this screening, the quality of fit of such ligands to the binding site may be judged either by shape complementarity or by estimated interaction energy (Meng et al. *J. Comp. Chem.*, 13:505-24 (1992)). In addition, these small
30 molecule databases can be screened for the ability to interact with the amino acids in the mOX40L, hOX40L, or hOX40 receptor binding site as identified herein.

A compound that is identified or designed as a result of any of these methods can be obtained (or synthesized) and tested for its biological activity, for example, binding and/or inhibition of mOX40L, hOX40L, or hOX40 receptor activity. Any high throughput assay
35 may be utilized, including ELISA, competition assays, array based assays.

A method comprises applying at least a portion of the crystallography coordinates of Tables 8,9,and/or 10 to a computer algorithm that generates a three-dimensional model of mOX40L, hOX40L, or hOX40 receptor suitable for designing molecules that are antagonists or agonists and searching a molecular structure database to identify potential antagonists or agonists. In some embodiments, a portion of the structural coordinates of Tables 8,9,and/or 10 that define a structural feature, for example, all or a portion of a binding site for an inhibitor on mOX40L, hOX40L, or hOX40 receptor may be utilized. The method may further comprise synthesizing or obtaining the agonist or antagonist and contacting the agonist or antagonist with the mOX40L, hOX40L, or hOX40 receptor and selecting the antagonist or agonist that modulates the mOX40L, hOX40L, or hOX40 receptor activity compared to a control without the agonist or antagonists and/or selecting the antagonist or agonist that binds to the mOX40L, hOX40L, or hOX40 receptor.

7. **Machine-readable storage media**

Transformation of the structure coordinates for all or a portion of mOX40L, hOX40L, or hOX40 receptor, or one of its ligand binding sites, or structurally homologous molecules as defined below, or for the structural equivalents of any of these molecules or molecular complexes as defined above, into three-dimensional graphical representations of the molecule or complex can be conveniently achieved through the use of commercially-available software.

The disclosure thus further provides a machine-readable storage medium including a data storage material encoded with machine-readable data wherein a machine programmed with instructions for using said data displays an amino acid sequence, a nucleotide sequence and/or a graphical three-dimensional representation of any of the molecule or molecular complexes of this disclosure that have been described above. In a preferred embodiment, the machine-readable data storage medium includes a data storage material encoded with machine-readable data wherein a machine programmed with instructions for using the abovementioned data displays a graphical three-dimensional representation of a molecule or molecular complex including all or any parts of an mOX40L, hOX40L, or hOX40 receptor. In another preferred embodiment, the machine-readable data storage medium includes a data storage material encoded with machine readable data wherein a machine programmed with instructions for using the data displays a graphical three-dimensional representation of a molecule or molecular complex $\pm$ a root mean square deviation from the atoms of the amino acids of not more than 0.05 Å.

In an alternative embodiment, the machine-readable data storage medium includes a data storage material encoded with a first set of machine readable data which includes the Fourier transform of structure coordinates, and wherein a machine programmed with

instructions for using the data is combined with a second set of machine readable data including the X-ray diffraction pattern of a molecule or molecular complex to determine at least a portion of the structure coordinates corresponding to the second set of machine readable data.

5 Another aspect of the disclosure provides systems, particularly computer based systems, which contain sequence, structure, and/or diffraction data described using such systems are designed to do structure determination of OX40L and/or OX40 receptors or at least one structural feature thereof. A skilled artisan can access this information to model or design a related molecule, structural feature, mimetic or ligand thereof using available
10 software as described herein.

 For example, a system for reading a data storage medium may include a computer based system including a central processing unit ("CPU"), a working memory which may be, for example, RAM (random access memory) or "core" memory, mass storage memory (such as one or more disk drives or CD-ROM drives), one or more display devices (e.g.,
15 cathode-ray tube ("CRT") displays, light emitting diode ("LED") displays, liquid crystal displays ("LCDs"), electroluminescent displays, vacuum fluorescent displays, field emission displays ("FEDs"), plasma displays, projection panels, etc.), one or more user input devices (e.g., keyboards, microphones, mice, track balls, touch pads, etc.), one or more input lines, and one or more output lines, all of which are interconnected by a conventional bidirectional
20 system bus. The system may be a stand-alone computer, or may be networked (e.g., through local area networks, wide area networks, intranets, extranets, or the internet) to other systems (e.g., computers, hosts, servers, etc.). The system may also include additional computer controlled devices such as consumer electronics and appliances.

 Input hardware may be coupled to the computer by input lines and may be
25 implemented in a variety of ways. Machine-readable data of this disclosure may be inputted via the use of a modem or modems connected by a telephone line or dedicated data line. Alternatively or additionally, the input hardware may include CD-ROM drives or disk drives. In conjunction with a display terminal, a keyboard may also be used as an input device.

30 Output hardware may be coupled to the computer by output lines and may similarly be implemented by conventional devices. By way of example, the output hardware may include a display device for displaying a graphical representation of a binding site of this disclosure using a program such as QUANTA as described herein. Output hardware might also include a printer, so that hard copy output may be produced, or a disk drive, to store
35 system output for later use.

In operation, a CPU coordinates the use of the various input and output devices, coordinates data accesses from mass storage devices, accesses to and from working memory, and determines the sequence of data processing steps. A number of programs may be used to process the machine-readable data of this disclosure. Such programs are
5 discussed in reference to the computational methods of drug discovery as described herein. References to components of the hardware system are included as appropriate throughout the following description of the data storage medium.

Machine-readable storage devices useful in the present disclosure include, but are not limited to, magnetic devices, electrical devices, optical devices, and combinations
10 thereof. Examples of such data storage devices include, but are not limited to, hard disk devices, CD devices, digital video disk devices, floppy disk devices, removable hard disk devices, magneto-optic disk devices, magnetic tape devices, flash memory devices, bubble memory devices, holographic storage devices, and any other mass storage peripheral device. It should be understood that these storage devices include necessary hardware (e.g., drives,
15 controllers, power supplies, etc.) as well as any necessary media (e.g., disks, flash cards, etc.) to enable the storage of data.

8. Therapeutic Use

mOX40L, hOX40L, or hOX40 receptor modulator compounds obtained by methods of the invention are useful in a variety of therapeutic settings. For example,
20 mOX40L, hOX40L, or hOX40 receptor antagonists designed or identified using the crystal structure of mOX40L, hOX40L, or hOX40 receptor complexes can be used to treat disorders or conditions, where inhibition or prevention of mOX40L, hOX40L, or hOX40 receptor binding or activity is indicated. Such conditions include conditions associated with TH1 and/or TH2 cells including autoimmune diseases and allergic disorders.

25 Likewise, mOX40L, hOX40L, or hOX40 receptor agonists designed or identified using the crystal structure of the mOX40L, hOX40L, or hOX40 receptor complex can be used to treat disorders or conditions, where induction or stimulation of mOX40L, hOX40L, or hOX40 receptor is indicated, for example, in the treatment of cancer or tumors.

In one aspect, the disclosure provides use of a modulator in the preparation of a
30 medicament for the therapeutic and/or prophylactic treatment of a disorder, such as an immune disorder. In some embodiments the modulator is an antagonist of OX40L and/or hOX40 receptor. In some embodiments, the disorder is an autoimmune disorder. In some embodiments, the disorder is asthma, atopic dermatitis, allergic rhinitis, inflammatory bowel disease, multiple sclerosis, and/or systemic lupus erythematosus. In some embodiments, the
35 disorder is a disease associated with virus, bacteria or other infectious agent. See US 2005/0069548 A1. Disorder can be graft-verses-host disease or transplant rejection.

In some embodiments, the disorder is arthritis (acute and chronic, rheumatoid arthritis including juvenile-onset rheumatoid arthritis and stages such as rheumatoid synovitis, gout or gouty arthritis, acute immunological arthritis, chronic inflammatory arthritis, degenerative arthritis, type II collagen-induced arthritis, infectious arthritis, Lyme

5 arthritis, proliferative arthritis, psoriatic arthritis, Still's disease, vertebral arthritis, osteoarthritis, arthritis chronica progrediente, arthritis deformans, polyarthritis chronica primaria, reactive arthritis, menopausal arthritis, estrogen-depletion arthritis, and ankylosing spondylitis/rheumatoid spondylitis), autoimmune lymphoproliferative disease, inflammatory hyperproliferative skin diseases, psoriasis such as plaque psoriasis, guttate psoriasis,

10 pustular psoriasis, and psoriasis of the nails, atopy including atopic diseases such as hay fever and Job's syndrome, dermatitis including contact dermatitis, chronic contact dermatitis, exfoliative dermatitis, allergic dermatitis, allergic contact dermatitis, hives, dermatitis herpetiformis, nummular dermatitis, seborrheic dermatitis, non-specific dermatitis, primary irritant contact dermatitis, and atopic dermatitis, x-linked hyper IgM

15 syndrome, allergic intraocular inflammatory diseases, urticaria such as chronic allergic urticaria and chronic idiopathic urticaria, including chronic autoimmune urticaria, myositis, polymyositis/dermatomyositis, juvenile dermatomyositis, toxic epidermal necrolysis, scleroderma (including systemic scleroderma), sclerosis such as systemic sclerosis, multiple sclerosis (MS) such as spino-optical MS, primary progressive MS (PPMS), and relapsing

20 remitting MS (RRMS), progressive systemic sclerosis, atherosclerosis, arteriosclerosis, sclerosis disseminata, ataxic sclerosis, neuromyelitis optica (NMO), inflammatory bowel disease (IBD) (for example, Crohn's disease, autoimmune-mediated gastrointestinal diseases, gastrointestinal inflammation, colitis such as ulcerative colitis, colitis ulcerosa, microscopic colitis, collagenous colitis, colitis polyposa, necrotizing enterocolitis, and

25 transmural colitis, and autoimmune inflammatory bowel disease), bowel inflammation, pyoderma gangrenosum, erythema nodosum, primary sclerosing cholangitis, respiratory distress syndrome, including adult or acute respiratory distress syndrome (ARDS), meningitis, inflammation of all or part of the uvea, iritis, choroiditis, an autoimmune hematological disorder, graft-versus-host disease, angioedema such as hereditary

30 angioedema, cranial nerve damage as in meningitis, herpes gestationis, pemphigoid gestationis, pruritis scroti, autoimmune premature ovarian failure, sudden hearing loss due to an autoimmune condition, IgE-mediated diseases such as anaphylaxis and allergic and atopic rhinitis, encephalitis such as Rasmussen's encephalitis and limbic and/or brainstem encephalitis, uveitis, such as anterior uveitis, acute anterior uveitis, granulomatous uveitis,

35 nongranulomatous uveitis, phacoantigenic uveitis, posterior uveitis, or autoimmune uveitis, glomerulonephritis (GN) with and without nephrotic syndrome such as chronic or acute

glomerulonephritis such as primary GN, immune-mediated GN, membranous GN (membranous nephropathy), idiopathic membranous GN or idiopathic membranous nephropathy, membrano- or membranous proliferative GN (MPGN), including Type I and Type II, and rapidly progressive GN (RPGN), proliferative nephritis, autoimmune

5 polyglandular endocrine failure, balanitis including balanitis circumscripta plasmacellularis, balanoposthitis, erythema annulare centrifugum, erythema dyschromicum perstans, erythema multiform, granuloma annulare, lichen nitidus, lichen sclerosus et atrophicus, lichen simplex chronicus, lichen spinulosus, lichen planus, lamellar ichthyosis, epidermolytic hyperkeratosis, premalignant keratosis, pyoderma gangrenosum, allergic conditions and

10 responses, food allergies, drug allergies, insect allergies, rare allergic disorders such as mastocytosis, allergic reaction, eczema including allergic or atopic eczema, asteatotic eczema, dyshidrotic eczema, and vesicular palmoplanar eczema, asthma such as asthma bronchiale, bronchial asthma, auto-immune asthma allergic asthma, and pediatric asthma, conditions involving infiltration of T cells and chronic inflammatory responses, immune

15 reactions against foreign antigens such as fetal A-B-O blood groups during pregnancy, chronic pulmonary inflammatory disease, autoimmune myocarditis, leukocyte adhesion deficiency, lupus, including lupus nephritis, lupus cerebritis, pediatric lupus, non-renal lupus, extra-renal lupus, discoid lupus and discoid lupus erythematosus, alopecia lupus, SLE, such as cutaneous SLE or subacute cutaneous SLE, neonatal lupus syndrome (NLE),

20 and lupus erythematosus disseminatus, juvenile onset (Type I) diabetes mellitus, including pediatric EDDM, adult onset diabetes mellitus (Type II diabetes), autoimmune diabetes, idiopathic diabetes insipidus, diabetic retinopathy, diabetic nephropathy, diabetic colitis, diabetic large-artery disorder, immune responses associated with acute and delayed hypersensitivity mediated by cytokines and T-lymphocytes, tuberculosis, sarcoidosis,

25 granulomatosis including lymphomatoid granulomatosis, Wegener's granulomatosis, agranulocytosis, vasculitides, including vasculitis, large-vessel vasculitis (including polymyalgia rheumatica and giant-cell (Takayasu's) arteritis), medium-vessel vasculitis (including Kawasaki's disease and polyarteritis nodosa/periarteritis nodosa), microscopic polyarteritis, immunovascularitis, CNS vasculitis, cutaneous vasculitis, hypersensitivity

30 vasculitis, necrotizing vasculitis such as systemic necrotizing vasculitis, and ANCA-associated vasculitis, such as Churg-Strauss vasculitis or syndrome (CSS) and ANCA-associated small-vessel vasculitis, temporal arteritis, aplastic anemia, autoimmune aplastic anemia, Coombs positive anemia, Diamond Blackfan anemia, hemolytic anemia or immune hemolytic anemia including autoimmune hemolytic anemia (AIHA), pernicious anemia

35 (anemia perniciosa), Addison's disease, pure red cell anemia or aplasia (PRCA), Factor VIII deficiency, hemophilia A, autoimmune neutropenia(s), cytopenias such as pancytopenia,

leukopenia, diseases involving leukocyte diapedesis, CNS inflammatory disorders, Alzheimer's disease, Parkinson's disease, multiple organ injury syndrome such as those secondary to septicemia, trauma or hemorrhage, antigen-antibody complex-mediated diseases, anti-glomerular basement membrane disease, anti-phospholipid antibody

5 syndrome, motoneuritis, allergic neuritis, Behçet's disease/syndrome, Castleman's syndrome, Goodpasture's syndrome, Raynaud's syndrome, Sjogren's syndrome, Stevens-Johnson syndrome, pemphigoid such as pemphigoid bullous and skin pemphigoid, pemphigus (including pemphigus vulgaris, pemphigus foliaceus, pemphigus mucus-membrane pemphigoid, and pemphigus erythematosus), autoimmune polyendocrinopathies,

10 Reiter's disease or syndrome, thermal injury due to an autoimmune condition, preeclampsia, an immune complex disorder such as immune complex nephritis, antibody-mediated nephritis, neuroinflammatory disorders, polyneuropathies, chronic neuropathy such as IgM polyneuropathies or IgM-mediated neuropathy, thrombocytopenia (as developed by myocardial infarction patients, for example), including thrombotic thrombocytopenic

15 purpura (TTP), post-transfusion purpura (PTP), heparin-induced thrombocytopenia, and autoimmune or immune-mediated thrombocytopenia including, for example, idiopathic thrombocytopenic purpura (ITP) including chronic or acute ITP, scleritis such as idiopathic cerato-scleritis, episcleritis, autoimmune disease of the testis and ovary including autoimmune orchitis and oophoritis, primary hypothyroidism, hypoparathyroidism,

20 autoimmune endocrine diseases including thyroiditis such as autoimmune thyroiditis, Hashimoto's disease, chronic thyroiditis (Hashimoto's thyroiditis), or subacute thyroiditis, autoimmune thyroid disease, idiopathic hypothyroidism, Grave's disease, polyglandular syndromes such as autoimmune polyglandular syndromes, for example, type I (or polyglandular endocrinopathy syndromes), paraneoplastic syndromes, including neurologic

25 paraneoplastic syndromes such as Lambert-Eaton myasthenic syndrome or Eaton-Lambert syndrome, stiff-man or stiff-person syndrome, encephalomyelitis such as allergic encephalomyelitis or encephalomyelitis allergica and experimental allergic encephalomyelitis (EAE), myasthenia gravis such as thymoma-associated myasthenia gravis, cerebellar degeneration, neuromyotonia, opsoclonus or opsoclonus myoclonus

30 syndrome (OMS), and sensory neuropathy, multifocal motor neuropathy, Sheehan's syndrome, autoimmune hepatitis, chronic hepatitis, lupoid hepatitis, giant-cell hepatitis, chronic active hepatitis or autoimmune chronic active hepatitis, pneumonitis such as lymphoid interstitial pneumonitis (LIP), bronchiolitis obliterans (non-transplant) vs NSEP, Guillain-Barre syndrome, Berger's disease (IgA nephropathy), idiopathic IgA nephropathy,

35 linear IgA dermatosis, acute febrile neutrophilic dermatosis, subcorneal pustular dermatosis, transient acantholytic dermatosis, cirrhosis such as primary biliary cirrhosis and

pneumonocirrhosis, autoimmune enteropathy syndrome, Celiac or Coeliac disease, celiac sprue (gluten enteropathy), refractory sprue, idiopathic sprue, cryoglobulinemia such as mixed cryoglobulinemia, amyotrophic lateral sclerosis (ALS; Lou Gehrig's disease), coronary artery disease, autoimmune ear disease such as autoimmune inner ear disease
 5 (AIED), autoimmune hearing loss, polychondritis such as refractory or relapsed or relapsing polychondritis, pulmonary alveolar proteinosis, Cogan's syndrome/nonsyphilitic interstitial keratitis, Bell's palsy, Sweet's disease/syndrome, rosacea autoimmune, zoster-associated pain, amyloidosis, a non-cancerous lymphocytosis, a primary lymphocytosis, which includes monoclonal B cell lymphocytosis (e.g., benign monoclonal gammopathy and
 10 monoclonal gammopathy of undetermined significance, MGUS), peripheral neuropathy, paraneoplastic syndrome, channelopathies such as epilepsy, migraine, arrhythmia, muscular disorders, deafness, blindness, periodic paralysis, and channelopathies of the CNS, autism, inflammatory myopathy, focal or segmental or focal segmental glomerulosclerosis (FSGS), endocrine ophthalmopathy, uveoretinitis, chorioretinitis, autoimmune hepatological
 15 disorder, fibromyalgia, multiple endocrine failure, Schmidt's syndrome, adrenalitis, gastric atrophy, presenile dementia, demyelinating diseases such as autoimmune demyelinating diseases and chronic inflammatory demyelinating polyneuropathy, Dressler's syndrome, alopecia areata, alopecia totalis, CREST syndrome (calcinosis, Raynaud's phenomenon, esophageal dysmotility, sclerodactyly, and telangiectasia), male and female autoimmune
 20 infertility, e.g., due to anti-spermatozoan antibodies, mixed connective tissue disease, Chagas' disease, rheumatic fever, recurrent abortion, farmer's lung, erythema multiforme, post-cardiotomy syndrome, Cushing's syndrome, bird-fancier's lung, allergic granulomatous angiitis, benign lymphocytic angiitis, Alport's syndrome, alveolitis such as allergic alveolitis and fibrosing alveolitis, interstitial lung disease, transfusion reaction, leprosy, malaria,
 25 parasitic diseases such as leishmaniasis, kypanosomiasis, schistosomiasis, ascariasis, aspergillosis, Sampter's syndrome, Caplan's syndrome, dengue, endocarditis, endomyocardial fibrosis, diffuse interstitial pulmonary fibrosis, interstitial lung fibrosis, fibrosing mediastinitis, pulmonary fibrosis, idiopathic pulmonary fibrosis, cystic fibrosis, endophthalmitis, erythema elevatum et diutinum, erythroblastosis fetalis, eosinophilic
 30 faciitis, Shulman's syndrome, Felty's syndrome, flariasis, cyclitis such as chronic cyclitis, heterochrony cyclitis, iridocyclitis (acute or chronic), or Fuch's cyclitis, Henoch-Schonlein purpura, human immunodeficiency virus (HIV) infection, SCID, acquired immune deficiency syndrome (AIDS), echovirus infection, sepsis (systemic inflammatory response syndrome (SIRS)), endotoxemia, pancreatitis, thyroxicosis, parvovirus infection, rubella
 35 virus infection, post-vaccination syndromes, congenital rubella infection, Epstein-Barr virus infection, mumps, Evan's syndrome, autoimmune gonadal failure, Sydenham's chorea, post-

streptococcal nephritis, thromboangitis obliterans, thyrotoxicosis, tabes dorsalis, chorioiditis, giant-cell polymyalgia, chronic hypersensitivity pneumonitis, conjunctivitis, such as vernal catarrh, keratoconjunctivitis sicca, and epidemic keratoconjunctivitis, idiopathic nephritic syndrome, minimal change nephropathy, benign familial and ischemia-reperfusion injury,

5 transplant organ reperfusion, retinal autoimmunity, joint inflammation, bronchitis, chronic obstructive airway/pulmonary disease, silicosis, aphthae, aphthous stomatitis, arteriosclerotic disorders (cerebral vascular insufficiency) such as arteriosclerotic encephalopathy and arteriosclerotic retinopathy, aspermiogenesis, autoimmune hemolysis, Boeck's disease, cryoglobulinemia, Dupuytren's contracture, endophthemia

10 phacoanaphylactica, enteritis allergica, erythema nodosum leprosum, idiopathic facial paralysis, chronic fatigue syndrome, febris rheumatica, Hamman-Rich's disease, sensorineural hearing loss, haemoglobinuria paroxysmatica, hypogonadism, ileitis regionalis, leucopenia, mononucleosis infectiosa, transverse myelitis, primary idiopathic myxedema, nephrosis, ophthalmia sympathica, orchitis granulomatosa, pancreatitis, polyradiculitis acuta,

15 pyoderma gangrenosum, Quervain's thyroiditis, acquired splenic atrophy, non-malignant thymoma, lymphofollicular thymitis, vitiligo, toxic-shock syndrome, food poisoning, conditions involving infiltration of T cells, leukocyte-adhesion deficiency, immune responses associated with acute and delayed hypersensitivity mediated by cytokines and T-lymphocytes, diseases involving leukocyte diapedesis, multiple organ injury syndrome,

20 antigen-antibody complex-mediated diseases, antiglomerular basement membrane disease, autoimmune polyendocrinopathies, oophoritis, primary myxedema, autoimmune atrophic gastritis, sympathetic ophthalmia, rheumatic diseases, mixed connective tissue disease, nephrotic syndrome, insulinitis, polyendocrine failure, autoimmune polyglandular syndromes, including polyglandular syndrome type I, adult-onset idiopathic hypoparathyroidism

25 (AOIH), cardiomyopathy such as dilated cardiomyopathy, epidermolysis bullosa acquisita (EBA), hemochromatosis, myocarditis, nephrotic syndrome, primary sclerosing cholangitis, purulent or nonpurulent sinusitis, acute or chronic sinusitis, ethmoid, frontal, maxillary, or sphenoid sinusitis, allergic sinusitis, an eosinophil-related disorder such as eosinophilia, pulmonary infiltration eosinophilia, eosinophilia-myalgia syndrome, Löffler's syndrome,

30 chronic eosinophilic pneumonia, tropical pulmonary eosinophilia, bronchopneumonic aspergillosis, aspergilloma, or granulomas containing eosinophils, anaphylaxis, spondyloarthropathies, seronegative spondyloarthritides, polyendocrine autoimmune disease, sclerosing cholangitis, sclera, episclera, chronic mucocutaneous candidiasis, Bruton's syndrome, transient hypogammaglobulinemia of infancy, Wiskott-Aldrich

35 syndrome, ataxia telangiectasia syndrome, angiectasis, autoimmune disorders associated with collagen disease, rheumatism such as chronic arthrorheumatism, lymphadenitis,

reduction in blood pressure response, vascular dysfunction, tissue injury, cardiovascular ischemia, hyperalgesia, renal ischemia, cerebral ischemia, and disease accompanying vascularization, allergic hypersensitivity disorders, glomerulonephritides, reperfusion injury, ischemic re-perfusion disorder, reperfusion injury of myocardial or other tissues,

5 lymphomatous tracheobronchitis, inflammatory dermatoses, dermatoses with acute inflammatory components, multiple organ failure, bullous diseases, renal cortical necrosis, acute purulent meningitis or other central nervous system inflammatory disorders, ocular and orbital inflammatory disorders, granulocyte transfusion-associated syndromes, cytokine-induced toxicity, narcolepsy, acute serious inflammation, chronic intractable

10 inflammation, pyelitis, endarterial hyperplasia, peptic ulcer, valvulitis, and endometriosis. Other examples, which in some cases encompass those listed above, include but are not limited to autoimmune rheumatologic disorders (such as, for example, rheumatoid arthritis, Sjogren's syndrome, scleroderma, lupus such as SLE and lupus nephritis, polymyositis/dermatomyositis, cryoglobulinemia, anti-phospholipid antibody syndrome, and

15 psoriatic arthritis), autoimmune gastrointestinal and liver disorders (such as, for example, inflammatory bowel diseases (e.g., ulcerative colitis and Crohn's disease), autoimmune gastritis and pernicious anemia, autoimmune hepatitis, primary biliary cirrhosis, primary sclerosing cholangitis, and celiac disease), vasculitis (such as, for example, ANCA-associated vasculitis, including Churg-Strauss vasculitis, Wegener's granulomatosis, and

20 polyarteritis), autoimmune neurological disorders (such as, for example, multiple sclerosis, opsoclonus myoclonus syndrome, myasthenia gravis, neuromyelitis optica, Parkinson's disease, Alzheimer's disease, and autoimmune polyneuropathies), renal disorders (such as, for example, glomerulonephritis, Goodpasture's syndrome, and Berger's disease), autoimmune dermatologic disorders (such as, for example, psoriasis, urticaria, hives,

25 pemphigus vulgaris, bullous pemphigoid, and cutaneous lupus erythematosus), hematologic disorders (such as, for example, thrombocytopenic purpura, thrombotic thrombocytopenic purpura, post-transfusion purpura, and autoimmune hemolytic anemia), atherosclerosis, uveitis, autoimmune hearing diseases (such as, for example, inner ear disease and hearing loss), Behcet's disease, Raynaud's syndrome, organ transplant, and autoimmune endocrine

30 disorders (such as, for example, diabetic-related autoimmune diseases such as insulin-dependent diabetes mellitus (IDDM), Addison's disease, and autoimmune thyroid disease (e.g., Graves' disease and thyroiditis)). More preferred such diseases include, for example, rheumatoid arthritis, ulcerative colitis, ANCA-associated vasculitis, lupus, multiple sclerosis, Sjogren's syndrome, Graves' disease, IDDM, pernicious anemia, thyroiditis, and

35 glomerulonephritis.

For example, Multiple Sclerosis (MS) is a disorder of the central nervous system that affects the brain and spinal cord. Common signs and symptoms of MS include paresthesias in one or more extremities, in the trunk, or on one side of the face; weakness or clumsiness of a leg or hand; or visual disturbances (such as partial blindness and pain in one
5 eye), dimness of vision, or scotomas. Other common early symptoms are ocular palsy resulting in double vision (diplopia), transient weakness of one or more extremities, slight stiffness or unusual fatigability of a limb, minor gait disturbances, difficulty with bladder control, vertigo, and mild emotional disturbances (Berkow et al. (ed.), 1999, Merck Manual of Diagnosis and Therapy: 17th Ed). Current treatments for MS include corticosteroids,
10 beta interferons (Betaferon, Avonex, Rebif), glatiramer acetate (Copaxone), methotrexate, azathioprine, cyclophosphamide, cladribine, baclofen, tizanidine, amitriptyline, carbamazepine (Berkow et al. (ed.), 1999, supra).

Rheumatoid arthritis (RA) is a chronic autoimmune disorder characterized by synovitis of joints that typically affects small and large joints, leading to their progressive
15 destruction (Berkow et al. (ed.), 1999, supra). Symptoms of RA can include stiffness, tenderness, synovial thickening, flexion contractures, visceral nodules, vasculitis causing leg ulcers or mononeuritis multiplex, pleural or pericardial effusions, and fever (Berkow et al. (ed.), 1999, supra).

Current treatments for RA include non-steroidal anti-inflammatory drugs (including
20 salicylates), gold compounds, methotrexate, hydroxychloroquine, sulfasalazine, penicillamine, corticosteroids, and cytotoxic or immunosuppressive drugs. (Berkow et al. (ed.), 1999, Merck Manual of Diagnosis and Therapy: 17th Ed.).

In one aspect, the invention provides use of an agonist of OX40L and/or receptor in the preparation of a medicament for the therapeutic and/or prophylactic treatment of a
25 disorder in which enhancement of immune function is beneficial, such as cancer. Immune function is enhanced by activating OX40 (in presence or absence of antigen-specific immune stimulation), including enhanced anti-tumor immunity. Increasing the immune response by providing molecules which engage the OX-40 receptor, e.g. during T-cell priming, can markedly increase the resistance of an animal to disease, by boosting T-cell
30 recognition of antigens presented by infectious agents, such as bacteria and viruses, as well as tumor cells. Accordingly, the present disclosure provides among other things the use of an OX-40 receptor binding agent as designed or identified herein, or of a nucleic acid encoding an OX-40 receptor binding agent(if the agent is a polypeptide or can be incorporated into a polypeptide), in the manufacture of a pharmaceutical composition for
35 enhancing immune response against an antigen in a mammal, which is either a tumour antigen, or an antigen for which the composition is administered so as to present the OX-40

receptor binding agent to T-cells of the mammal during or shortly after priming of the T-cells by the antigen.

According to a further aspect of the invention a nucleic acid which encodes an OX-40 receptor binding agent identified as described herein that is localised on the surface of a cell, along with tumor cells from a mammal, can be used in the manufacture of a pharmaceutical composition for stimulating the immune response of a mammal to a tumor in the mammal by (a) removing tumor cells from the mammal; (b) attenuating the removed tumor cells; (c) introducing the nucleic acid into the attenuated tumor cells; and (d) administering the thus-treated attenuated tumor cells containing the nucleic acid molecule to the mammal. The OX-40 receptor binding agent in this aspect can be OX-40L or a hOX40 receptor binding fragment thereof, as well as other molecules designed or identified by the methods described herein. The tumor cells can be attenuated prior to or after introducing the nucleic acid molecule.

In an alternative manner of carrying out the invention, a nucleic acid which encodes an OX-40 receptor binding agent as designed or identified herein (if the agent is a polypeptide or can be incorporated into a polypeptide) that is localised on the surface of a cell can be used, along with T-cells from a mammal, in the manufacture of a pharmaceutical composition for enhancing the immune response of a mammal to an antigen, by removing T-cells from the mammal, incubating the removed T-cells ex vivo with an OX-40 receptor binding agent, and returning the thus-treated T-cells to the mammal. Again, the mammal may have a tumor, and the antigen can be a tumor antigen.

More generally, an OX-40 receptor binding agent or a nucleic acid encoding an OX-40 receptor binding agent as identified or designed herein can be used in the manufacture of a pharmaceutical for enhancing immune response against a tumor in a mammal by increasing the amount of OX-40 receptor binding agent at the tumor site. All types of tumor are potentially amenable to treatment by this approach including, for example, carcinoma of the breast, lung, pancreas, ovary, kidney, colon and bladder, as well as melanomas and sarcomas. Nucleic acid molecules encoding a OX-40 receptor binding agent (if the agent is a polypeptide or can be incorporated into a polypeptide) are incorporated into a vector suitable for expression of the OX-40 receptor binding agent in tumor cells. Suitable vectors include plasmid, cosmid and viral vectors, such as retroviruses, adenoviruses and herpesviruses. Because of the high efficiency with which viral vectors infect mammalian cells, viral vectors are expected to offer advantages over other vector types. In addition to a nucleic acid molecule encoding an OX-40 receptor binding agent, other nucleic acid molecules may also be introduced into the vector to further enhance the immunogenic effect. By way of example, such other nucleic acid molecules include nucleic acids

encoding MHC class II proteins (including .alpha, and .beta. subunits), and other co-stimulatory molecules, such as B7.1 and B7.2. If desired, a nucleic acid molecule encoding a selectable marker may also be introduced into the vector, such that those tumor cells successfully transformed with the vector can be readily selected.

5 All publications, patents, and patent documents are incorporated by reference herein, as though individually incorporated by reference. The disclosure has been described with reference to various specific and preferred embodiments and techniques. However, it should be understood that many variations and modifications can be made while remaining within the spirit and scope of the disclosure.

10 **Example 1**

Analysis of the crystal structure of mOX40L and cocrystals of hOX40L with mOX40 and hOX40L was conducted in order to determine how these members of the TNF family interact with one another. The crystal structure provides information useful in the design of potential modulators.

15 **Materials and Methods:**

Protein Expression:

DNA encoding residues 51-198, 51-183, and 29-170 of murine OX40L (mOX40L), human OX40L (hOX40L), and human OX40 (hOX40) respectively were cloned into a pET 15b expression vector by PCR then subcloned into the baculovirus transfer vector
20 pAcGP67-B (BD Pharmingen) and used for transfection and subsequent viral amplification. To decrease heterogeneity of hOX40L due to glycosylation, residues 90 and 114 were mutated to aspartic acid by site directed mutagenesis (QuickChange mutagenesis kit, Stratagene). Asn to Asp substitutions at positions 152 and 157 severely decreased expression levels and were therefore not pursued.

25 The resulting viral stocks were used for protein expression in High Five cells (available from Invitrogen) Following growth at 27°C for 3 days, cell culture media was harvested by centrifugation, treated with nickel chloride, calcium chloride, and Tris buffer, pH 8.0, then filtered prior to passage over a Ni-NTA column to isolate recombinant proteins. His-Tags were removed by thrombin cleavage overnight and the proteins were
30 subsequently further purified by size exclusion chromatography on an S-75 or S-200 column prior to concentration. An N-terminal amino acid sequence of GSHM that was a part of the viral vector remained present on the polypeptides. Complexes of mOX40L-hOX40 and hOX40L-hOX40 were further purified by size exclusion chromatography. Final buffer conditions were 100 mM NaCl, 20 mM Tris, pH 8.0 for mOX40, and 100mM NaCl, 20mM
35 Tris, pH 8.2 for mOX40-OX40 and hOX40-OX40. All proteins sequences were verified by mass spectrometry and N-terminal sequencing.

Crystallization and Data Collection:

Crystals of mOX40L grew by vapor diffusion after approximately 2 weeks in sitting drops containing 1 μ L protein and 1 μ L well solution consisting of 0.1 M NaAcetate pH 4.5, 2.0 M Ammonium Sulfate at 19 $^{\circ}$ C. Crystals of mOX40L-hOX40 and hOX40L-hOX40 were grown by the same procedure but with well solution of 0.1 M NaCl, 0.1 M Bis Tris pH 6.5, 1.4 M Ammonium Sulfate and 8% PEG 20,000, 0.1 M MES pH 6.5, respectively. Prior to data collections, mOX40L, mOX40L-hOX40, and hOX40L-hOX40 were immersed in artificial mother liquor consisting of the well solution with water replaced by either 20% glycerol (mOX40L) or 20 - 25% ethylene glycol (mOX40L-hOX40, hOX40L-hOX40). For phasing, mOX40L crystals were soaked for 60 s in cryo-protectant solution supplemented with 1.2 M NaBr prior to flash-cooling in liquid nitrogen. A four wavelength Br MAD experiment was collected at beam line 5.0.2 at ALS. Subsequently a 1.45 $\text{\AA}$ native data set was collected at beamline F1 at CHESS (Cornell High Energy Synchrotron Source). Heavy atom location and phase refinement of the mOX40L structure was performed using the program SHARP. (Statistical Heavy Atom Refinement and Phasing available at Center for Structural Biology Core website at Yale University.) Native data sets for mOX40L-hOX40 and hOX40L-hOX40 were collected at beamlines 19ID at ADP (Advanced Photon Source Argonne National Laboratory) and by MXpress at ESRF (European Synchrotron Radiation Facility). All data sets were processed using the HKL package (Otwinowsk and Minor, 1997).

The structures of mOX40L-hOX40 and hOX40L-hOX40 were solved by molecular replacement with the program AMoRe (Navaza, 2001) using the refined mOX40L and mOX40L-hOX40 structures respectively as search models. Refinement of all structures was done using the program REFMAC (Winn et al., 2003). See Table 1 for crystallographic statistics.

Results**Structure of OX40L**

The structure of mOX40L was solved using MAD phasing with NaBr soaked crystals (Table 1). This approach was used after attempts at using molecular replacement to solve either the mOX40L or receptor complexes failed due to the low sequence homology and structural similarity between OX40L and available structures of members of the TNFSF. The refined 1.45 $\text{\AA}$ mOX40L structure was then used to solve the structures of the hOX40-mOX40L and hOX40-hOX40L complexes by molecular replacement (Table 1). These structures show that the OX40L protomer is brick shaped and packs together to form flower-like trimers. These trimers lack the pyramidal shape typical of more conventional TNFSF members such as Apo2L/TRAIL, TNF, or LT (Figure 1). However, despite the

differences in the appearance and assembly of the ligand, hOX40 binds at the monomer-monomer interface as seen in other structures of multi-domain TNFRSF-ligand complexes (Bodmer et al., Trends Biochem Sci 27:19-26 (2002)) (Figure 2).

Human and murine OX40L are less similar to each other than many other TNFSF orthologs with only ~40% sequence identity, yet they share the same distinctive features. Both murine and human OX40L are very compact making OX40L more representative of smaller members of the TNFSF such as GITRL and CD27L. The OX40L TNF homology domain is followed by a C-terminal extension including residues 175-183 in hOX40L and residues 178-191 in mOX40L (Figure 1). In hOX40L the entire extension is ordered and interacts with the BC loop both by backbone-hydrogen bonds as well as via a conserved disulfide between residues 181 and 97. A second disulfide in murine OX40L contacts the AA' loop to the GH loop and is not conserved in hOX40L. In both human and murine OX40L, the strands and loops comprising the jelly-roll B-sandwich monomer sheets (A'AHCF and B'BGDE) are significantly shorter than in other TNFSF members such as TNF or Apo2L/TRAIL. In addition to the compact TNF homology domain, hOX40L has a six residue connection to the N-terminal transmembrane domain. These residues are expected to form a short unstructured linker and are not visible in the electron density.

The trimeric packing of TNFSF members is generally very well conserved even among the more distant family members such as BAFF and EDA. Unexpectedly, the structures of human and murine OX40L show that the protomers assemble differently into a trimer than in other structurally characterized members of the TNFSF (Figure 1). In OX40L, the monomers are splayed out and form an angle of -45° with respect to the trimer axis which differs from other TNFL by -15° rotation of the monomer. For most TNFSF members, as exemplified by LT, the angle between the AHCF sheet and the trimer axis is $25-30^\circ$. This difference in trimer assembly correlates with the lack of sequence conservation between OX40L and other members of the TNFSF (Figure 3) and accounts for the difficulty in generating high quality homology models of the OX40L trimer.

Another unusual aspect of the OX40L trimer is that human OX40L and murine OX40L have much smaller trimer interfaces than other structurally characterized TNF ligands (Figure 1). The hOX40L trimer interface is particularly compact with only $\sim 2600 \text{ \AA}^2$ of accessible surface area buried upon trimer formation in comparison to $12,000 \text{ \AA}^2$ or 5-fold more buried by BAFF and LT (BAFF, LT both $\sim 12000 \text{ \AA}^2$; hOX40L $\sim 2600 \text{ \AA}^2$; mOX40L, $\sim 4000 \text{ \AA}^2$). An additional striking difference between the OX40L and other TNFSF is the absence in OX40L of the characteristic "tiles" of alternating aromatic or hydrophobic residues along the trimer axis first seen in the structure of TNF (Eck and Sprang, 1989; Jones et al., 1992). Instead, the trimer interface of murine and human OX40L

is formed by a very short layer of generally hydrophobic residues from the C-strand (L102), F-strand (L138), and the C-terminal tail (Q175). In murine OX40L, the corresponding residues are 1103, T141 and V175. In addition, L178 from the murine OX40L C-terminal tail also contributes to the trimer interface.

5

Structure of hOX40 receptor

In contrast to the distinctive structure of OX40L, hOX40 is a relatively conventional multi-domain TNFR. It is composed of three full CRDs and a partial C-terminal CRD which form a contiguous structure. Superposition of the three independent copies of hOX40 (two in the mOX40L-hOX40 asymmetric unit and one in the hOX40L-hOX40 asymmetric unit) reveals that CRD1 and CRD2 form a rigid unit while there is some rotational freedom between the subdomains of CRD3 and the partial CRD4. The first and second CRD have the same disulfide connectivity as the corresponding domains of TNFR1, and in the terminology of Naismith et al are composed of A1-B2 modules (Naismith and Sprang, cited supra). As in other TNFR such as DR5, CRD2 is the best conserved structurally with only a 1 residue deletion with respect to TNFR1 and rmsd of 0.9 Å² on all equivalent C-α when superimposed on TNFR1 CRD2 (residues 55-97).

CRD3 in hOX40 differs more than CRD1 and CRD2 from its counterpart in TNFR1 or DR5 as it is smaller and lacks one of the canonical disulfides (Figure 4). CRD3 contains an A1, B1 module rather than the A1, B2 architecture of CRD1 and 2. This structure of hOX40 CRD3 contains the first experimentally determined B1 subdomain. As discussed above, B1 modules are defined in part by their lack of a conserved disulfide (Naismith and Sprang, cited supra). In the case of hOX40, the disulfide formed by the fourth and sixth cysteines in CRD3 (the 4-6 disulfide) is missing. This missing disulfide in hOX40 CRD3 is not replaced by either hydrogen bonds or hydrophobic interactions but rather the entire module is smaller due to shortening and re-arrangement of intervening loops. This re-arrangement causes the backbone of the remaining 3-5 disulfide to be in an anti-parallel orientation rather than the parallel orientation seen in B2 modules. A long disulfide containing loop follows the B1 module. The connectivity and structure of this loop are compatible with it being an A1 module of a vestigial CRD4.

B1 modules have been detected in the sequences of a number of other TNFRSF including OPG, RANK, TNFR2, LT/3-R, HVEM, DcR3, CD30, 4-1BB, GITR, EDAR and RELT. Examining the sequences of these B1 modules along with the structure of the OX40 B1 modules indicates that the B1 modules form two distinct groups based on their size and on which disulfide pair is lacking: a smaller groups consisting of OX40-like B1 modules which lack the 4-6 disulfide and a larger groups of B-I modules that are more B2-like and

lack the 3-5 disulfide (Figure 5). Like OX40, GTR, EDAR (CRD3) and possibly RANK (CRD3) all possess the smaller B1 module lacking the 4-6 disulfide. The second, more B2-like group is defined by having similar sequence and cysteine spacing as B2-modules. In this group, the 3-5 disulfide is replaced by an aromatic/small amino acid pair, most frequently histidine and glycine. Receptors EDAR (CRD2), CD40, DR6, DcR3, LT/3-R, TNFR2, and RANK (CRD2) are all predicted to possess 1 or more of these larger, more B2-like modules.

The hOX40-OX40L complex

Three copies of hOX40 receptor bind to the trimeric ligand to form the hOX40-OX40L complex. Each copy of hOX40 binds at a monomer-monomer interface on OX40L forming an extensive interface (2232 Å² hOX40-hOX40L; 2605 Å² hOX40-mOX40L) (Figure 2, 5). This interface is larger than that seen in either the TNFR1-LT (Banner et al., *Cell*, 73:431-445 (1993)) or DR5-Apo21/TRAIL (Hymowitz et al., *Mol Cell* 4:563-571 (1999); Mongkolsapaya et al., *Nat Struct Biol* 6:1048-1053 (1999)) complexes and is split equally between each monomer (473 Å² for the F180 containing "right" monomer; 640 Å² for the N166 containing "left" monomer). Unexpectedly, hOX40 uses residues from CRD1 (e.g. T35, Y36, P37, S38, E45, V53, and R55) (355 Å²), CRD2 (e.g. S78, K79, P83, T85, W86, C87, and N88) (497 Å²) and CRD3 (e.g. Y119, V123, and D124) (167 Å²) to bind hOX40L.

In contrast, in the structures of TNFR1-LT and DR5-Apo2L, only residues from CRD2 and CRD3 are used with both CRDs making approximately equal contributions in binding ligand. OX40 uses the same general portions of CRD2 (the A1 loop and immediately following residues) and CRD3 (primarily the A1 loop) as used by TNFR1 or DR5 but makes additional contacts using CRD1. The ligand portion of this interface is even more discontinuous. Thirty one hOX40L residues from eleven different secondary structure elements including the unusual C-terminal tail contact receptor.

Overall, the OX40L-hOX40 complex structure spans ~80 Å (Figure 2). This distance, in conjunction with an ~40 amino acid linker between the vestigial CRD4 and the OX40 transmembrane domain, suggests that the complex could connect cells whose surfaces are ~100-150 Å apart. This distance is compatible with the dimensions of other ligand-receptor complexes which extend between antigen presenting cells and T cells such as the MHC-TCR complex and the B7-CD28 costimulatory complex (Schwartz et al., cited supra).

Comparison of the free mOX40L structure and the mOX40L-hOX40 complex indicate that there are no significant alterations in ligand conformation that are attributable to receptor binding. Two loops (the AA' loop and residues 79-85 in the A'B' loop) are

significantly rearranged in the free vs. bound ligand structure; however, both of these loops in the free structure are involved in crystal packing contacts which likely drives the alterations in conformation.

Comparison of the human and murine complex structures helps explain why, despite their lack of high sequence similarity, both mOX40L and hOX40L bind hOX40 (Figure 5). In general the murine and human OX40L surfaces are very distinct; of the 44 residues which bury any surface area in the mOX40L-hOX40 complex, only 26 are also involved in the hOX40L-OX40 interface. (See Tables 6 and 7) Of those twenty-six shared residues, only eleven are identical between mOX40L and hOX40L. The identical residues account for only $\sim 360 \text{ \AA}^2$ of the ligand interface (the total ligand buried surface area is $\sim 1200 \text{ \AA}^2$). Six of the unshared residues are located in the C-terminal tail of mOX40L which is significantly longer in mOX40L than in hOX40L. Nonetheless, two critically important residues, F180 and N166, are conserved between human and murine OX40L and make similar contributions to binding receptor. Mutational analysis has identified both residues as being crucial for receptor affinity (see Example 2).

Discussion

Both the structural and mutagenesis data show that the OX40-OX40L interface is not a contiguous patch with a single "hot-spot" but instead is distributed over the surface of hOX40L in at least two general areas. Mutagenesis data indicates that residues on both sides of the monomer-monomer interface are important for high affinity binding, and, further, that contacts made by three hOX40 CRD contribute to the binding affinity. The importance of F180 which is located in the hOX40L C-terminal tail indicates that this feature which is also present in murine and cyno OX40L sequences, is not just a structural oddity but that it has an important role in hOX40L function (Figure 5b). Despite the extensive interface between hOX40 and hOX40L, the affinity of monomeric hOX40 for hOX40L was found to be $\sim 150 \text{ nM}$ (Table II) which is in good agreement with values reported in the literature measured using other techniques (Al-Shamkhani et al., *J Biol Chem*, 272:5275-5282 (1997)), but is somewhat lower than had been reported for other TNF-multi-domain TNFR interactions. However, since in vivo OX40L is expected to be membrane bound, other phenomena such as local clustering may lead to increased apparent affinity.

Two unusual features distinguish the hOX40-OX40L complex from other TNFSF-TNFRSF complexes: the unusual "open" OX40L trimer interface and the extensive contacts made by hOX40 CRD1 to OX40L (Figure 1,5). These features expand the TNFSF-TNFRSF repertoire of interactions. Until now, TNFSF ligand-multi CRD receptor interactions have all been interpreted using the rubric of the DR5-Apo2L and TNFRI-LT

interactions which implied that only CRD2 and CRD3 were likely to contact ligand. In light of the OX40 complex structures reported here, it is possible that CRD1 plays a more important role in other TNFSF interactions than previously thought. For example, some disease causing mutations in EDA (Ectodysplasin) map to surface residues away from the areas where CRD2 and CRD3 from either EDAR or XEDAR are expected to bind (Hymowitz et al., Structure, 11:1513-1520 (2003)). Interestingly, these changes (A356D, R357P in the EDA BC loop and D298H, G299S in the EDA FG loop) map to areas of the EDA surface analogous to where OX40L contacts OX40 CRD1, indicating that EDAR and XEDAR (the receptors respectively for the EDA-A1 and EDA-A2 splice variants) may also use CRD1 to contact ligand.

The structures of the OX40L-hOX40 receptor complexes may shed new light on findings involving other OX40 interactions. For instance, Feline immunodeficiency virus, FIV, has recently been shown to require feline OX40 as a co-receptor for entry into T cells (de Parseval et al., Proc Natl Acad Sci USA, 101:13044-13049 (2004); Shimojima et al., Science, 303:1192-1195 (2004)). Elders et al have mapped the residues crucial for FIV interactions with feline OX40 to the tip of CRD1. Alteration of five residues in hOX40 CRD1 (H44S, R58G, S59D, N61D, V63K) is sufficient to confer FIV binding equivalent to that of feline OX40 (de Parseval et al., Nat Struct Mol Biol, 12:60-66 (2005)). These residues are distal from the receptor cell membrane and are not involved in binding OX40L consistent with biochemical data that soluble feline OX40L does not compete with FIV for binding feline OX40. However, the ability of feline OX40L to affect binding of FIV to feline OX40 may be different in vivo where OX40L is membrane-bound rather than soluble. The hOX40-hOX40L complex shows that the residues in OX40 CRD1 involved in binding FIV are likely to be very close to the ligand cell membrane (Figures 2). The presence of the ligand cell membrane may sterically hinder FIV binding to OX40 in vivo.

In summary, the structure of the hOX40-OX40L complex shows that the ligand itself as well as the complex are more divergent than had been expected from sequence analysis. The OX40L trimer differs from that of other known TNFSF and distant homologs in its assembly while hOX40 receptor makes more extensive contacts including novel interactions mediated by CRD1 and the OX40L C-terminal tail that have not been seen in other TNFSF members.

Example 2

Mutations were made in the hOX40L to determine the effect of the mutations on binding to the hOX40 receptor. Several residues that were identified in the binding site in the hOX40L were substituted with alanine in order to determine the effect of these

substitutions on the ability of the mutants to compete with wild-type ligand for binding to the receptor.

Materials and Methods

Alanine scanning mutagenesis

5 Single alanine mutations were made in the background of the hOX40L double glycosylate mutant at residues Q65, Q80, E123, T144, K146, D147, D162, H164, N166 and F180 using Quickchange site directed mutagenesis (Stratagene). Mutations at Q65, K146, D147, and H164 resulted in significantly decreased expression levels and were not purified or characterized. The remaining six alanine mutants were expressed and purified
10 from insect cells as described above. Mutations were verified by DNA sequencing and mass spectrometry. Final buffer conditions were 150 mM NaCl, 20 mM Tris, pH 8.0.

Competition ELISA binding experiments:

 hOX40 was dialyzed into PBS and biotinylated using a 4 fold molar excess of biotin-NHS-LC. Serial dilutions of biotinylated hOX40 were then tested for binding to a
15 plate coated with mOX40L. The dilution which gave approximately 50% saturating signal was used in the solution binding assay in which the biotinylated hOX40 was incubated with increasing concentrations of each hOX40L alanine mutant for 1 hour. The solutions were then transferred to mOX40L coated plates for 15 minutes to capture unbound receptor. Biotinylated hOX40 was detected with TMB substrate and the absorbance at 450 nM was
20 measured. IC₅₀ was calculated as the concentration of hOX40L alanine mutant in solution-binding stage that inhibited 50% of the receptor from binding to immobilized mOX40L.

Results

Functional characterization of the OX40L-OX40 complex

25 In order to determine which portions of the hOX40L surface contribute to receptor affinity, ten residues (Q65, Q80, E123, T144, K146, D147, D162, H164, N166 and F180) distributed over the surface were chosen for mutation to alanine in the context of the N90D, N114D double glycosylation mutant. Of these residues, four (Q65, K146, D147, and H164) resulted in severely diminished expression likely due to folding or secretion defects. The
30 remaining six mutant proteins were shown by size exclusion chromatography to be properly assembled trimers.

 The IC₅₀ of these six mutants to compete for hOX40 was assessed in a competition ELISA assay (see Table II, Figure 5b). Two of these substitutions, F180A in the C-terminal extension and N166A in the GH loop strand both resulted in undetectable binding for
35 hOX40. Substitutions at Q80 (AA' loop) and D162 (GH loop) had more moderate effects while the affinity of proteins with mutations at T144 (F strand) and E123 (DE loop) were

essentially unchanged. The four residues which do affect ligand affinity for receptor do not form a compact region but instead are dispersed over the hOX40-hOX40L interface. The two residues F180 and N166 are diagonally at opposite ends of the monomer-monomer interface. F180 interacts with a hydrophobic region on hOX40 CRD1 while N166 forms
5 hydrogen bonds to the backbone of hOX40 residues W86 and C87 at the juncture of CRD2 and 3. F180 and N166 are conserved in murine OX40L (Y182 and N169) and make similar interactions in the hOX40-mOX40L complex. Q80, like F180, interacts with CRD1 but forms hydrogen bonds to the backbone of V53 rather than making hydrophobic contacts. D162 makes van der waals contacts near to where N166 binds. The murine equivalents of
10 Q80 and D162 (N82 and H165) do not make similar interactions.

Discussion

This mutational analysis shows that the binding energy in the hOX40-hOX40L interface is not concentrated in one location but is spread out to at least two areas, similar to what was seen for Apo2L/TRAIL interacting with DR5. However, the OX40-OX40L
15 complex differs from the complexes formed by conventional TNFSF members with regard to the distribution of binding energy and the role of the ligand DE loop. In OX40L, unlike in the Apo2L/TRAIL or LT-receptor complexes, there is no significant hydrophobic contact between the DE loop and the A1 loop of CRD2. The one residue within the ligand DE loop which does extensively contact receptor, E123, does not contribute energetically to binding.

**Table 1. Crystallographic Statistics
Phasing mOX40L**

	Br Peak P6 ₃	Br High	Br Inflec	Br Low
Space Group	P6 ₃			
Unit Cell (A)	a= 75.0 c=47.6			
Wavelength (A)	0.9199	0.9050	0.9202	1.5418
Max. Resolution (A)	2.0	2.2	2.0	2.6
Completeness (%) ^a	99.8 (100)	99.8 (100)	99.8 (100)	99.8 (100)
R _{sym} ^{a, b}	0.065(0.42)	0.067(0.45)	0.047 (0.33)	0.045 (0.20)
Reflections measured ^c	91256	68648	91337	42450
Reflections unique ^c	10438	7858	10452	4990
Resolution for Phasing	2.8	2.8	2.8	2.8
Phasing power iso	0.0	1.7	0.97	1.7
Phasing power anom	1.13	1.3	0.23	0.62
FOM acentric, centric	0.66, 0.62			
Data Collection	mOX40L	mOX40L-hOX40	hOX40L-hOX40	
Space Group	P6 ₃	R32	R32	
Resolution (A) ^a	30-1.45 (1.50-1.45)	30-2.0 (2.07-2.00)	30-2.4 (2.49-2.40)	
Unit cell constants (A)	a = 74.5 c = 49.0	a= 104.7 c =478.2	a= 111.9 c = 233.2	
R _{sym} ^{a, b}	0.068 (0.466)	0.069 (0.272)	0.055 (0.505)	
No. observations	388,637	312,989	135,176	
Unique reflections	27,220	68,124	22,255	
Completeness (%) ^a	100 (100)	98.6 (96.4)	99.8 (100)	
Asymmetric Unit	1 ligand protomer	2 ligand:receptor protomers	1 ligand:receptor protomer	
Refinement				
Resolution (A)	30-1.45	30-2.0	30-2.4	
Final R ^d , R _f _{ree} (%)	16.5, 19.2	22.1, 24.7	20.8, 25.1	
No. solvent atoms	108	181	87	
Rmsd bonds, angles (A, ⁰)	0.007, 1.3	0.007, 1.0	0.007, 1.1	
Ramachandran Plot(%) ^e	90.4 8.7; 0.9; 0	92.1; 7.1; 0.9; 0	90.4 8.7; 0.9; 0	

^a Numbers in parentheses refer to the highest resolution shell.^b $R_{\text{sym}} = \sum |I - \langle I \rangle| / \sum I$, $\langle I \rangle$ is the average intensity of symmetry related observations of a unique reflection.^c Bijvoet reflections are kept separate in the Br statistics^d $R = \sum |F_o - F_c| / \sum F_o$ ^e Percentage of residues in the most favored, additionally allowed, generously allowed, and disallowed regions of a Ramachandran plot.

Table II: Effect of alanine mutations on hOX40L-hOX40 interactions in a competition ELISA. IC50s are the average of three independent measurements. All mutations are in the N90D, N114D background. Fold-change values are relative to the IC50 of hOX40L containing the double mutation (N90D, N114D). Only values

5 >3-fold different from the reference are considered significant. N.D.: no detectable competition.

Protein	IC50 (nM)	Fold-change in IC50 (Mutant/D90D, N114D)
WT	139 ± 43	2.2
N90D, N114D	62 ± 2	1.0
F180A	N.D.	N.D.
N166A	N.D.	N.D.
Q80A	537 ± 111	8.6
D162A	425 ± 73	6.9
T144A	139 ± 14	2.2
E123A	186 ± 5	3.0

Table 3 mOX40L (SEQ ID NO:1)

megegvppld enlengsrpr fkwwkklrlv vsgikgagml lcfiyvclql ssspakdppi
 5 qrlrgavtrc edgqlfissy kneymtmevq nnswikcdg lyiylkgsf fgevkidlhf
 redhnpisip mlndgrrivf twaslafkd kvyltnapd tlcehlqind geliwqltp
 gycapgsyh stvnqvpl
 10

Table 3b (SEQ ID NO:4)

SSSPAKDPPIQRLRGAVTRCEDGQLFISSYKNEYQTMEVQNNSVV π CC
 15 51 64 98
 DGLYIIYLKGSFFQEVKIDLHFRDHNPIPIMLNDGRRIVFTVVASLAFKDKVY
 99 153
 LTVNAPDTLCEHLQINDGELIVVQLTPGYCAPEGSYHSTVNQVPL
 154 185 198
 20

Table 4 hOX40 (SEQ ID NO:2)

MCVGARRLGRGPCAALLLLGLGLSTVTGLHCVGDTYPSNDRCCHECRPGNGMVSRC
 5 RSQNTVCRPCGPGFYNDWSSKPCKPCTWCNLRSGSERKQLCTATQDTVCRCRAGTQP
 LDSYKPGVDCAPCPPGHFSPGDNQACKPWTNCTLAGKHTLQPASNSSDAICEDRDPPAT
 10 QPQETQGPPARPITVQPTEAWPRTSQGPSTRPVEVPGGRAVAAILGLGLVLGLLGPLAIL
 LALYLLRRDQRLPPDAHKKPPGGGSFRTPIQEEQADAHSTLAKI

Table 4b (SEQ ID NO:5)

15 LHCVGDTYPSNDRCCHECRPGNGMVSRCRSQNTVCRPCGPGFYNDW
 29 76
 SSKPCKPCTWCNLRSGSERKQLCTATQDTVCRCRAGTQPLDSYK
 77 120
 20 PGVDCAPCPPGHFSPGDNQACKPWTNCTLAGKHTLQPASNSSDAICEDRD
 121 170

Table 5 hOX40L (SEQ ID NO:3)

5 MERVQPLEENVGNAARPRFERNKLLLVASVIQGLGLLLCFTYICLHFSALQVSHRYPRIQ
 SIKVQFTEYKKEKGFIILTSQKEDEIMKVQNNNSVI INCDFGYLISLKGYSQEVNISLHYQ
 KDEEPLFQLKKVRSVNSLMVASLTYKDKVYLNVTDDNTSLDDFHVNGGELILIHQNPGE
 10 FCVL

Table 5b (SEQ ID NO:6)

15 QVSHRYPRIQSIKVQFTEYKKEKGFIILTSQKEDEIMKVQNNNSVI INCDFGY
 51 58 101
 LISLKGYSQEVNISLHYQKDEEPLFQLKKVR EVNSLMVASLTYKD KVYLNVT
 102 155
 DNTSLDDFHVNGGELILIHQNPGEFCVL
 20 156 183

Table 5c (SEQ ID NO:7)

25 QVSHRYPRIQSIKVQFTEYKKEKGFIILTSQKEDEIMKVQNNNSVI INCDFGY
 51 58 101
 LISLKGYSQEVNISLHYQKDEEPLFQLKKVRSVNSLMVASLTYKDKVYLNVT
 102 155
 DNTSLDDFHVNGGELILIHQNPGEFCVL
 30 156 183

Table 6

Amino Acid	angstroms²	% of surface area buried
hOX40Ligand:		
ASP A 98	28.00	70.00 % of 40.00
TYR A 119	18.00	33.96 % of 53.00
GLN A 120	2.00	2.94 % of 68.00
GLU A 123	63.00	66.32 % of 95.00
GLU A 124	30.00	22.39 % of 134.00
LYS A 130	19.00	13.48 % of 141.00
SER A 142	13.00	28.89 % of 45.00
THR A 144	51.00	76.12 % of 67.00
TYR A 145	42.00	46.15 % of 91.00
LYS A 146	91.00	60.67 % of 150.00
ASP A 147	4.00	66.67 % of 6.00
PHE A 180	85.00	72.03 % of 118.00
CYS A 181	1.00	2.13 % of 47.00
VAL A 182	26.00	48.15 % of 54.00
LYS A1063	14.00	17.72 % of 79.00
GLN A1065	56.00	61.54 % of 91.00
THR A1067	43.00	47.78 % of 90.00
THR A1078	9.00	13.85 % of 65.00
GLN A1080	53.00	43.44 % of 122.00
GLU A1082	63.00	49.22 % of 128.00
ASP A1083	28.00	19.05 % of 147.00
TYR A1108	31.00	29.25 % of 106.00
PHE A1109	2.00	40.00 % of 5.00
SER A1110	30.00	58.82 % of 51.00
ARG A1133	29.00	21.80 % of 133.00
ASP A1162	83.00	74.11 % of 112.00
HIS A1164	64.00	68.09 % of 94.00
VAL A1165	5.00	62.50 % of 8.00
ASN A1166	99.00	90.83 % of 109.00
GLY A1167	29.00	54.72 % of 53.00
GLY A1168	2.00	20.00 % of 10.00
CHAIN A DIFF- AREA:	1113.0	(7.55 % of 14751.0 total AREA for this chain)

Amino Acid	angstroms ²	%Surface Area Buried
hOX40Receptor:		
GLY B 33	8.00	11.59 % of 69.00
THR B 35	12.00	44.44 % of 27.00
TYR B 36	22.00	95.65 % of 23.00
PRO B 37	62.00	68.89 % of 90.00
SER B 38	14.00	51.85 % of 27.00
GLU B 45	27.00	58.70 % of 46.00
MET B 52	11.00	35.48 % of 31.00
VAL B 53	62.00	75.61 % of 82.00
SER B 54	19.00	39.58 % of 48.00
ARG B 55	83.00	72.17 % of 115.00
ARG B 65	35.00	22.44 % of 156.00
PHE B 71	37.00	43.53 % of 85.00
ASP B 74	3.00	4.00 % of 75.00
VAL B 75	17.00	26.56 % of 64.00
SER B 78	24.00	82.76 % of 29.00
LYS B 79	98.00	72.59 % of 135.00
PRO B 80	22.00	23.40 % of 94.00
CYS B 81	6.00	20.00 % of 30.00
LYS B 82	25.00	32.47 % of 77.00
PRO B 83	47.00	65.28 % of 72.00
CYS B 84	5.00	20.83 % of 24.00
THR B 85	4.00	50.00 % of 8.00
TRP B 86	103.00	52.02 % of 198.00
CYS B 87	13.00	72.22 % of 18.00
ASN B 88	57.00	86.36 % of 66.00
LEU B 89	32.00	26.45 % of 121.00
ARG B 90	4.00	1.79 % of 223.00
ASP B 117	20.00	12.50 % of 160.00
TYR B 119	97.00	56.40 % of 172.00
LYS B 120	24.00	30.38 % of 79.00
PRO B 121	3.00	3.12 % of 96.00
VAL B 123	6.00	60.00 % of 10.00
ASP B 124	17.00	41.46 % of 41.00
ASP B 168	0.00	0.00 % of 160.00
CHAIN B DIFF-AREA:	1019.0	(11.05 % of 9218.0 total AREA for this chain)
TOTAL DIFF-AREA:	2132.0	(8.89 % of 23969.0 total AREA over all chains)

Table 6 continued

TABLE 7

Amino Acid	angstroms ²	%Buried Surface Area
MOX40L		
ASP A 99	19.00	86.36 % of 22.00
HIS A 119	13.00	65.00 % of 20.00
PHE A 120	4.00	20.00 % of 20.00
ARG A 121	22.00	27.50 % of 80.00
GLU A 122	12.00	9.52 % of 126.00
ASP A 123	24.00	20.00 % of 120.00
HIS A 124	8.00	14.29 % of 56.00
ASN A 125	69.00	51.49 % of 134.00
PRO A 126	24.00	47.06 % of 51.00
SER A 145	22.00	46.81 % of 47.00
LEU A 146	2.00	40.00 % of 5.00
ALA A 147	32.00	84.21 % of 38.00
PHE A 148	25.00	48.08 % of 52.00
LYS A 149	51.00	61.45 % of 83.00
ASP A 150	14.00	66.67 % of 21.00
TYR A 153	1.00	3.23 % of 31.00
TYR A 182	88.00	77.88 % of 113.00
ALA A 184	1.00	20.00 % of 5.00
PRO A 185	18.00	21.18 % of 85.00
GLY A 187	15.00	20.55 % of 73.00
SER A 188	68.00	91.89 % of 74.00
TYR A 189	53.00	55.21 % of 96.00
HIS A 190	47.00	28.83 % of 163.00
SER A 191	18.00	11.92 % of 151.00
ARG A 1064	16.00	29.63 % of 54.00
ALA A 1066	15.00	100.00 % of 15.00
THR A 1068	54.00	63.53 % of 85.00
ARG A 1069	6.00	5.88 % of 102.00
SER A 1078	19.00	43.18 % of 44.00
TYR A 1080	71.00	78.89 % of 90.00
LYS A 1081	47.00	26.55 % of 177.00
ASN A 1082	55.00	68.75 % of 80.00
GLU A 1083	70.00	46.36 % of 151.00
PHE A 1111	111.00	86.72 % of 128.00
GLN A 1112	22.00	31.43 % of 70.00
LEU A 1166	2.00	25.00 % of 8.00
GLN A 1167	52.00	48.60 % of 107.00
ILE A 1168	5.00	62.50 % of 8.00
ASN A 1169	68.00	82.93 % of 82.00
ASP A 1170	2.00	2.06 % of 97.00
GLY A 1171	7.00	53.85 % of 13.00
CHAIN A DIFF-AREA:	1272.0	(8.69 % of 14633.0 total AREA for this chain)

Amino Acid	angstroms ²	%Buried Surface Area
HOX40 receptor		
LEU B 29	28.00	20.44 % of 137.00
HIS B 30	62.00	38.51 % of 161.00
CYS B 31	28.00	96.55 % of 29.00
VAL B 32	19.00	17.59 % of 108.00
GLY B 33	38.00	55.88 % of 68.00
THR B 35	15.00	46.88 % of 32.00
TYR B 36	17.00	100.00 % of 17.00
PRO B 37	91.00	100.00 % of 91.00
SER B 38	14.00	50.00 % of 28.00
GLU B 45	28.00	57.14 % of 49.00
MET B 52	13.00	86.67 % of 15.00
VAL B 53	64.00	65.31 % of 98.00
SER B 54	21.00	60.00 % of 35.00
ARG B 55	109.00	91.60 % of 119.00
ARG B 65	12.00	7.27 % of 165.00
GLY B 70	3.00	6.98 % of 43.00
PHE B 71	47.00	51.65 % of 91.00
VAL B 75	19.00	24.36 % of 78.00
VAL B 76	15.00	28.30 % of 53.00
SER B 77	1.00	6.67 % of 15.00
SER B 78	18.00	51.43 % of 35.00
LYS B 79	96.00	64.00 % of 150.00
PRO B 80	71.00	74.74 % of 95.00
CYS B 81	11.00	42.31 % of 26.00
LYS B 82	1.00	1.25 % of 80.00
PRO B 83	54.00	62.07 % of 87.00
CYS B 84	13.00	48.15 % of 27.00
THR B 85	13.00	36.11 % of 36.00
TRP B 86	136.00	62.67 % of 217.00
CYS B 87	12.00	44.44 % of 27.00
ASN B 88	34.00	54.84 % of 62.00
LEU B 89	3.00	2.50 % of 120.00
ARG B 90	73.00	31.74 % of 230.00
ASP B 117	13.00	16.46 % of 79.00
TYR B 119	106.00	53.54 % of 198.00
LYS B 120	23.00	29.49 % of 78.00
VAL B 123	7.00	43.75 % of 16.00
ASP B 124	5.00	7.04 % of 71.00
CYS B 166	0.00	0.00 % of 75.00
CHAIN B DIFF-AREA:	1333.0	(14.29 % of 9328.0 total AREA for this chain)
TOTAL DIFF-AREA:	2605.0	(10.87 % of 23961.0 total AREA over all chains)

Table 7 continued

TABLE 8

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5  HEADER      ----                XX-XXX-XX   xxxx
   COMPND     ---
   REMARK      3
   REMARK      3 REFINEMENT.
   REMARK      3   PROGRAM       : REFMAC 5.2.0005
   REMARK      3   AUTHORS        : MURSHUDOV ,VAGIN ,DODSON
10  REMARK      3
   REMARK      3   REFINEMENT TARGET : MAXIMUM LIKELIHOOD
   REMARK      3
   REMARK      3 DATA USED IN REFINEMENT.
   REMARK      3   RESOLUTION RANGE HIGH (ANGSTROMS) : 1.45
15  REMARK      3   RESOLUTION RANGE LOW  (ANGSTROMS) : 30.00
   REMARK      3   DATA CUTOFF          (SIGMA(F)) : NONE
   REMARK      3   COMPLETENESS FOR RANGE (%) : 97.62
   REMARK      3   NUMBER OF REFLECTIONS : 23933
   REMARK      3
20  REMARK      3 FIT TO DATA USED IN REFINEMENT.
   REMARK      3   CROSS-VALIDATION METHOD : THROUGHOUT
   REMARK      3   FREE R VALUE TEST SET SELECTION : RANDOM
   REMARK      3   R VALUE (WORKING + TEST SET) : 0.16765
   REMARK      3   R VALUE (WORKING SET) : 0.16505
25  REMARK      3   FREE R VALUE : 0.19220
   REMARK      3   FREE R VALUE TEST SET SIZE (%) : 9.9
   REMARK      3   FREE R VALUE TEST SET COUNT : 2635
   REMARK      3
   REMARK      3 FIT IN THE HIGHEST RESOLUTION BIN.
30  REMARK      3   TOTAL NUMBER OF BINS USED : 25
   REMARK      3   BIN RESOLUTION RANGE HIGH : 1.450
   REMARK      3   BIN RESOLUTION RANGE LOW : 1.480
   REMARK      3   REFLECTION IN BIN (WORKING SET) : 1466
   REMARK      3   BIN COMPLETENESS (WORKING+TEST) (%) : 100.00
35  REMARK      3   BIN R VALUE (WORKING SET) : 0.159
   REMARK      3   BIN FREE R VALUE SET COUNT : 164
   REMARK      3   BIN FREE R VALUE : 0.226
   REMARK      3
40  REMARK      3 NUMBER OF NON- HYDROGEN ATOMS USED IN REFINEMENT.
   REMARK      3   ALL ATOMS : 1152
   REMARK      3
   REMARK      3 B VALUES .
   REMARK      3   FROM WILSON PLOT (A**2) : NULL
   REMARK      3   MEAN B VALUE (OVERALL, A**2) : 17.786
45  REMARK      3 OVERALL ANISOTROPIC B VALUE.
   REMARK      3   B11 (A**2) : -0..20
   REMARK      3   B22 (A**2) : -0..20
   REMARK      3   B33 (A**2) : 0.30
   REMARK      3   B12 (A**2) : -0..10
50  REMARK      3   B13 (A**2) : 0.00
   REMARK      3   B23 (A**2) : 0.00
   REMARK      3
   REMARK      3 ESTIMATED OVERALL COORDINATE ERROR.
   REMARK      3   ESU BASED ON R VALUE (A) : 0.073
55  REMARK      3   ESU BASED ON FREE R VALUE (A) : 0.064
   REMARK      3   ESU BASED ON MAXIMUM LIKELIHOOD (A) : 0.035
   REMARK      3   ESU FOR B VALUES BASED ON MAXIMUM LIKELIHOOD (A**2) : 1.935
   REMARK      3
   REMARK      3 CORRELATION COEFFICIENTS .
60  REMARK      3   CORRELATION COEFFICIENT FO-FC : 0.969
   REMARK      3   CORRELATION COEFFICIENT FO-FC FREE : 0.962
   REMARK      3
   REMARK      3 RMS DEVIATIONS FROM IDEAL VALUES
   REMARK      3   BOND LENGTHS REFINED ATOMS (A) : 1072 ; 0.007 ; 0.022
65  REMARK      3   BOND LENGTHS OTHERS (A) : 985 ; 0.001 ; 0.020
   REMARK      3   BOND ANGLES REFINED ATOMS (DEGREES) : 1461 ; 1.275 ; 1.981
   REMARK      3   BOND ANGLES OTHERS (DEGREES) : 2288 ; 0.753 ; 3.000
   REMARK      3   TORSION ANGLES, PERIOD 1 (DEGREES) : 127 ; 7.387 ; 5.000
   REMARK      3   TORSION ANGLES, PERIOD 2 (DEGREES) : 49 ; 31.155 ; 24.490
70  REMARK      3   TORSION ANGLES, PERIOD 3 (DEGREES) : 182 ; 12.473 ; 15.000
   REMARK      3   TORSION ANGLES, PERIOD 4 (DEGREES) : 6 ; 16.943 ; 15.000

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REMARK 3 CHIRAL-CENTER RESTRAINTS (A**3) : 174 ; 0.085 ; 0.200
REMARK 3 GENERAL PLANES REFINED ATOMS (A) : 1149 ; 0.004 ; 0.020
REMARK 3 GENERAL PLANES OTHERS (A) : 205 ; 0.001 ; 0.020
5 REMARK 3 NON-BONDED CONTACTS REFINED ATOMS (A) : 152 ; 0.189 ; 0.200
REMARK 3 NON-BONDED CONTACTS OTHERS (A) : 983 ; 0.180 ; 0.200
REMARK 3 NON-BONDED TORSION REFINED ATOMS (A) : 522 ; 0.171 ; 0.200
REMARK 3 NON-BONDED TORSION OTHERS (A) : 663 ; 0.079 ; 0.200
REMARK 3 H-BOND (X...Y) REFINED ATOMS (A) : 76 ; 0.171 ; 0.200
10 REMARK 3 H-BOND (X...Y) OTHERS (A) : 1 ; 0.038 ; 0.200
REMARK 3 SYMMETRY VDW REFINED ATOMS (A) : 14 ; 0.203 ; 0.200
REMARK 3 SYMMETRY VDW OTHERS (A) : 46 ; 0.256 ; 0.200
REMARK 3 SYMMETRY H-BOND REFINED ATOMS (A) : 17 ; 0.207 ; 0.200
REMARK 3
REMARK 3 ISOTROPIC THERMAL FACTOR RESTRAINTS. COUNT RMS WEIGHT
15 REMARK 3 MAIN- CHAIN BOND REFINED ATOMS (A**2) : 838 ; 2.794 ; 2.500
REMARK 3 MAIN- CHAIN BOND OTHER ATOMS (A**2) : 258 ; 1.059 ; 2.500
REMARK 3 MAIN- CHAIN ANGLE REFINED ATOMS (A**2) : 1061 ; 3.295 ; 5.000
REMARK 3 SIDE-CHAIN BOND REFINED ATOMS (A**2) : 486 ; 3.115 ; 2.500
REMARK 3 SIDE-CHAIN ANGLE REFINED ATOMS (A**2) : 400 ; 3.953 ; 5.000
20 REMARK 3
REMARK 3 ANISOTROPIC THERMAL FACTOR RESTRAINTS. COUNT RMS WEIGHT
REMARK 3 RIGID-BOND RESTRAINTS (A**2) : 2436 ; 1.822 ; 3.000
REMARK 3 SPHERICITY; FREE ATOMS (A**2) : 103 ; 7.292 ; 3.000
REMARK 3 SPHERICITY; BONDED ATOMS (A**2) : 2034 ; 2.679 ; 3.000
25 REMARK 3
REMARK 3 NCS RESTRAINTS STATISTICS
REMARK 3 NUMBER OF NCS GROUPS : NULL
REMARK 3
REMARK 3
30 REMARK 3 TLS DETAILS
REMARK 3 NUMBER OF TLS GROUPS : 1
REMARK 3 ATOM RECORD CONTAINS RESIDUAL B FACTORS ONLY
REMARK 3
REMARK 3 TLS GROUP : 1
35 REMARK 3 NUMBER OF COMPONENTS GROUP : 1
REMARK 3 COMPONENTS C SSSEQI TO C SSSEQI
REMARK 3 RESIDUE RANGE : F 58 F 201
REMARK 3 ORIGIN FOR THE GROUP (A) : -8.9097 54.0568 32.7820
REMARK 3 T TENSOR
40 REMARK 3 T11 : -0.0281 T22 : -0.0606
REMARK 3 T33 : -0.0220 T12 : 0.0006
REMARK 3 T13 : -0.0113 T23 : -0.0169
REMARK 3 L TENSOR
REMARK 3 L11 : 1.2563 L22 : 1.8668
45 REMARK 3 L33 : 1.6017 L12 : 0.1382
REMARK 3 L13 : 0.0472 L23 : 1.0084
REMARK 3 S TENSOR
REMARK 3 S11 : 0.0001 S12 : -0.0610 S13 : 0.1595
REMARK 3 S21 : 0.0766 S22 : -0.0924 S23 : 0.1510
50 REMARK 3 S31 : -0.0310 S32 : -0.1332 S33 : 0.0923
REMARK 3
REMARK 3
REMARK 3 BULK SOLVENT MODELLING.
REMARK 3 METHOD USED : MASK
55 REMARK 3 PARAMETERS FOR MASK CALCULATION
REMARK 3 VDW PROBE RADIUS : 1.40
REMARK 3 ION PROBE RADIUS : 0.80
REMARK 3 SHRINKAGE RADIUS : 0.80
REMARK 3
60 REMARK 3 OTHER REFINEMENT REMARKS :
REMARK 3 HYDROGENS HAVE BEEN ADDED IN THE RIDING POSITIONS
REMARK 3
1 CYS F 70 CYS F 163
SSBOND
2 CYS F 98 CYS F 183
SSBOND
65 LINK C1 NAG F 200 1.439 ND2 ASN F 91 NAG-ASN
MODRES NAG F 200 NAG-b-D RENAME
CRYST1 74.149 74.149 48.815 90.00 90.00 120.00 P 63
SCALE1 0.013486 0.007786 0.000000 0.000000
SCALE2 0.000000 0.015573 0.000000 0.000000
70 SCALE3 0.000000 0.000000 0.020486 0.000000
ATOM 1 N PRO F 58 -8.814 50.033 10.354 1.00 34.33 N

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	ANISOU	1	N	PRO	F	58	4296	4377	4371	-79	-109	-33	N
	ATOM	2	CA	PRO	F	58	-8.301	50.948	11.372	1.00	31.11		C
	ANISOU	2	CA	PRO	F	58	3802	4128	3890	-50	-120	59	C
	ATOM	4	CB	PRO	F	58	-9.448	51.015	12.391	1.00	33.84		C
5	ANISOU	4	CB	PRO	F	58	4179	4514	4162	4	-40	-25	C
	ATOM	7	CG	PRO	F	58	-10.672	50.737	11.585	1.00	35.43		C
	ANISOU	7	CG	PRO	F	58	4357	4583	4521	-38	-82	-6	C
	ATOM	10	CD	PRO	F	58	-10.245	49.736	10.549	1.00	36.08		C
10	ANISOU	10	CD	PRO	F	58	4457	4653	4598	-9	-14	3	C
	ATOM	13	C	PRO	F	58	-7.016	50.459	12.046	1.00	28.59		C
	ANISOU	13	C	PRO	F	58	3738	3757	3365	-123	-55	22	C
	ATOM	14	O	PRO	F	58	-6.696	49.268	11.996	1.00	31.80		O
	ANISOU	14	O	PRO	F	58	4229	4050	3803	-258	60	-12	O
	ATOM	17	N	PRO	F	59	-6.284	51.377	12.689	1.00	24.78		N
15	ANISOU	17	N	PRO	F	59	3234	3293	2889	-77	41	234	N
	ATOM	18	CA	PRO	F	59	-5.044	51.002	13.358	1.00	22.83		C
	ANISOU	18	CA	PRO	F	59	3021	3041	2610	-45	-5	142	C
	ATOM	20	CB	PRO	F	59	-4.402	52.353	13.664	1.00	23.26		C
	ANISOU	20	CB	PRO	F	59	3076	2918	2841	-13	78	135	C
20	ATOM	23	CG	PRO	F	59	-5.545	53.283	13.800	1.00	25.77		C
	ANISOU	23	CG	PRO	F	59	3249	3407	3134	-20	152	-11	C
	ATOM	26	CD	PRO	F	59	-6.588	52.809	12.849	1.00	25.39		C
	ANISOU	26	CD	PRO	F	59	3168	3378	3100	29	162	98	C
	ATOM	29	C	PRO	F	59	-5.311	50.248	14.657	1.00	20.93		C
25	ANISOU	29	C	PRO	F	59	2487	3005	2458	-43	1	84	C
	ATOM	30	O	PRO	F	59	-6.440	50.240	15.146	1.00	21.96		O
	ANISOU	30	O	PRO	F	59	2459	3131	2750	-69	-106	127	O
	ATOM	31	N	ILE	F	60	-4.277	49.624	15.214	1.00	18.99		N
	ANISOU	31	N	ILE	F	60	2512	2563	2138	85	86	13	N
30	ATOM	32	CA	ILE	F	60	-4.388	49.070	16.564	1.00	17.63		C
	ANISOU	32	CA	ILE	F	60	2205	2380	2113	-87	-2	27	C
	ATOM	34	CB	ILE	F	60	-3.033	48.528	17.092	1.00	18.26		C
	ANISOU	34	CB	ILE	F	60	2239	2427	2271	-66	-40	-33	C
	ATOM	36	CG1	ILE	F	60	-2.600	47.300	16.276	1.00	19.82		C
35	ANISOU	36	CG1	ILE	F	60	2234	2618	2679	-73	92	50	C
	ATOM	39	CD1	ILE	F	60	-1.163	46.887	16.504	1.00	21.47		C
	ANISOU	39	CD1	ILE	F	60	2570	2920	2665	121	-69	5	C
	ATOM	43	CG2	ILE	F	60	-3.128	48.169	18.578	1.00	19.79		C
	ANISOU	43	CG2	ILE	F	60	2229	2736	2551	54	-203	101	C
40	ATOM	47	C	ILE	F	60	-4.936	50.167	17.473	1.00	16.83		C
	ANISOU	47	C	ILE	F	60	2034	2219	2139	-47	-67	190	C
	ATOM	48	O	ILE	F	60	-4.466	51.307	17.464	1.00	16.48		O
	ANISOU	48	O	ILE	F	60	1992	2292	1976	-175	-121	63	O
	ATOM	50	N	GLN	F	61	-5.944	49.821	18.259	1.00	15.12		N
45	ANISOU	50	N	GLN	F	61	1765	2046	1932	-152	-140	-13	N
	ATOM	51	CA	GLN	F	61	-6.622	50.801	19.088	1.00	14.99		C
	ANISOU	51	CA	GLN	F	61	1933	1818	1942	-43	-92	144	C
	ATOM	53	CB	GLN	F	61	-8.043	50.334	19.367	1.00	15.53		C
	ANISOU	53	CB	GLN	F	61	1899	1959	2040	-93	-33	-47	C
50	ATOM	56	CG	GLN	F	61	-8.874	50.182	18.102	1.00	16.12		C
	ANISOU	56	CG	GLN	F	61	1858	2092	2172	-110	-95	-7	C
	ATOM	59	CD	GLN	F	61	-9.270	51.515	17.503	1.00	16.91		C
	ANISOU	59	CD	GLN	F	61	2061	2320	2041	-8	-173	13	C
	ATOM	60	OE1	GLN	F	61	-10.091	52.231	18.072	1.00	18.23		O
55	ANISOU	60	OE1	GLN	F	61	2087	2270	2566	31	-82	78	O
	ATOM	61	NE2	GLN	F	61	-8.679	51.861	16.365	1.00	17.40		N
	ANISOU	61	NE2	GLN	F	61	1820	2470	2318	0	-39	270	N
	ATOM	64	C	GLN	F	61	-5.864	51.014	20.381	1.00	15.33		C
	ANISOU	64	C	GLN	F	61	1920	1806	2098	-106	31	48	C
60	ATOM	65	O	GLN	F	61	-5.596	50.062	21.102	1.00	16.88		O
	ANISOU	65	O	GLN	F	61	2408	2024	1981	-145	-413	21	O
	ATOM	67	N	ARG	F	62	-5.496	52.261	20.657	1.00	12.95		N
	ANISOU	67	N	ARG	F	62	1542	1660	1718	60	-20	29	N
	ATOM	68	CA	ARG	F	62	-4.871	52.582	21.931	1.00	14.89		C
65	ANISOU	68	CA	ARG	F	62	1667	1891	2099	87	-80	-155	C
	ATOM	70	CB	ARG	F	62	-3.357	52.308	21.931	1.00	16.73		C
	ANISOU	70	CB	ARG	F	62	1869	2191	2295	182	-69	-88	C
	ATOM	73	CG	ARG	F	62	-2.504	53.254	21.113	1.00	18.96		C
	ANISOU	73	CG	ARG	F	62	2050	2603	2549	68	-54	-76	C
70	ATOM	76	CD	ARG	F	62	-2.517	52.895	19.635	1.00	20.68		C
	ANISOU	76	CD	ARG	F	62	2307	2804	2744	44	-65	-9	C

	ATOM	79	NE	ARG	F	62	-1.282	53.303	18.976	1.00	19..35		N
	ANISOU	79	NE	ARG	F	62	2390	2415	2544	399	-117	155	N
	ATOM	81	CZ	ARG	F	62	-0.973	53.011	17.718	1.00	19..21		C
	ANISOU	81	CZ	ARG	F	62	2558	2294	2445	286	22	147	C
5	ATOM	82	NH1	ARG	F	62	-1.782	52.283	16.964	1.00	18..86		N
	ANISOU	82	NH1	ARG	F	62	2168	2446	2550	-88	65	89	N
	ATOM	85	NH2	ARG	F	62	0.176	53.426	17.217	1.00	21.10		N
	ANISOU	85	NH2	ARG	F	62	2316	2781	2918	-64	8	118	N
	ATOM	88	C	ARG	F	62	-5.129	53.999	22.368	1.00	13.29		C
10	ANISOU	88	C	ARG	F	62	1674	1637	1737	-77	-71	-64	C
	ATOM	89	O	ARG	F	62	-5.370	54.904	21.557	1.00	13.99		O
	ANISOU	89	O	ARG	F	62	1759	1734	1820	27	-44	77	O
	ATOM	91	N	LEU	F	63	-5.053	54.174	23.675	1.00	15.59		N
	ANISOU	91	N	LEU	F	63	2245	1874	1803	69	-78	175	N
15	ATOM	92	CA	LEU	F	63	-5.120	55.475	24.284	1.00	15.28		C
	ANISOU	92	CA	LEU	F	63	1992	1862	1949	30	-48	1	C
	ATOM	94	CB	LEU	F	63	-6.566	55.818	24.626	1.00	18.62		C
	ANISOU	94	CB	LEU	F	63	2357	2269	2448	109	-120	-124	C
	ATOM	97	CG	LEU	F	63	-6.689	57.230	25.208	1.00	23.64		C
20	ANISOU	97	CG	LEU	F	63	3058	2953	2970	192	97	-351	C
	ATOM	99	CD1	LEU	F	63	-7.681	58.054	24.427	1.00	26.60		C
	ANISOU	99	CD1	LEU	F	63	3629	3223	3254	193	158	-95	C
	ATOM	103	CD2	LEU	F	63	-6.969	57.208	26.706	1.00	24.00		C
25	ANISOU	103	CD2	LEU	F	63	2990	3066	3062	-117	115	-103	C
	ATOM	107	C	LEU	F	63	-4.268	55.452	25.542	1.00	15.13		C
	ANISOU	107	C	LEU	F	63	2123	1763	1861	-53	-74	-42	C
	ATOM	108	O	LEU	F	63	-4.352	54.512	26.329	1.00	16.78		O
	ANISOU	108	O	LEU	F	63	2495	1960	1919	-75	-28	-36	O
	ATOM	110	N	ARG	F	64	-3.458	56.495	25.735	1.00	14.74		N
30	ANISOU	110	N	ARG	F	64	1891	1800	1910	-64	-39	-104	N
	ATOM	111	CA	ARG	F	64	-2.756	56.693	27.004	1.00	15..20		C
	ANISOU	111	CA	ARG	F	64	1834	2026	1915	-58	-18	84	C
	ATOM	113	CB	ARG	F	64	-1.241	56.637	26.843	1.00	15.87		C
	ANISOU	113	CB	ARG	F	64	1910	2066	2055	-55	129	-23	C
35	ATOM	116	CG	ARG	F	64	-0.478	56.847	28.166	1.00	17.00		C
	ANISOU	116	CG	ARG	F	64	1931	2237	2291	32	86	-80	C
	ATOM	119	CD	ARG	F	64	0.947	56.326	28.083	1.00	18.05		C
	ANISOU	119	CD	ARG	F	64	2150	2349	2356	89	25	77	C
	ATOM	122	NE	ARG	F	64	1.701	57.179	27.181	1.00	17.85		N
40	ANISOU	122	NE	ARG	F	64	2207	2343	2229	198	-73	181	N
	ATOM	124	CZ	ARG	F	64	2.462	58.210	27.535	1.00	15.63		C
	ANISOU	124	CZ	ARG	F	64	1710	2087	2140	350	-94	90	C
	ATOM	125	NH1	ARG	F	64	2.651	58.547	28.802	1.00	18.66		N
45	ANISOU	125	NH1	ARG	F	64	2652	2136	2301	-4	-1	151	N
	ATOM	128	NH2	ARG	F	64	3.066	58.906	26.593	1.00	16.50		N
	ANISOU	128	NH2	ARG	F	64	1955	2149	2162	161	-65	170	N
	ATOM	131	C	ARG	F	64	-3.194	58.044	27.521	1.00	15.62		C
	ANISOU	131	C	ARG	F	64	1719	2141	2073	-42	26	92	C
	ATOM	132	O	ARG	F	64	-2.877	59.066	26.922	1.00	17..48		O
50	ANISOU	132	O	ARG	F	64	2304	1899	2438	13	217	-21	O
	ATOM	134	N	GLY	F	65	-3.961	58.038	28.603	1.00	16.07		N
	ANISOU	134	N	GLY	F	65	2012	1927	2165	18	85	16	N
	ATOM	135	CA	GLY	F	65	-4.540	59.258	29.140	1.00	16.98		C
55	ANISOU	135	CA	GLY	F	65	2195	2107	2148	196	-36	-87	C
	ATOM	138	C	GLY	F	65	-3.985	59.627	30.494	1.00	17.09		C
	ANISOU	138	C	GLY	F	65	2240	2142	2111	181	133	-67	C
	ATOM	139	O	GLY	F	65	-3.574	58.766	31.266	1.00	17.,37		O
	ANISOU	139	O	GLY	F	65	2560	2022	2015	124	-155	-52	O
	ATOM	141	N	ALA	F	66	-4.007	60.916	30.790	1.00	16.38		N
60	ANISOU	141	N	ALA	F	66	2177	2051	1996	87	230	-53	N
	ATOM	142	CA	ALA	F	66	-3.642	61.399	32.106	1.00	16.35		C
	ANISOU	142	CA	ALA	F	66	2001	2182	2029	-114	170	2	C
	ATOM	144	CB	ALA	F	66	-3.226	62.850	32.038	1.00	17.14		C
65	ANISOU	144	CB	ALA	F	66	2346	2093	2073	-81	163	-105	C
	ATOM	148	C	ALA	F	66	-4.859	61.239	32.997	1.00	17..26		C
	ANISOU	148	C	ALA	F	66	2236	2288	2032	93	261	-127	C
	ATOM	149	O	ALA	F	66	-5.966	61.570	32.593	1.00	17.71		O
	ANISOU	149	O	ALA	F	66	2152	2556	2018	18	280	209	O
	ATOM	151	N	VAL	F	67	-4.646	60.733	34.203	1.00	16.06		N
70	ANISOU	151	N	VAL	F	67	1769	2251	2080	158	187	52	N
	ATOM	152	CA	VAL	F	67	-5.707	60.630	35.195	1.00	15.78		C

	ANISOU	152	CA	VAL	F	67	2086	2182	1726	42	186	-8	C
	ATOM	154	CB	VAL	F	67	-5.726	59.239	35.865	1.00	16.98		C
	ANISOU	154	CB	VAL	F	67	2154	2172	2125	-41	-26	-86	C
	ATOM	156	CG1	VAL	F	67	-6.832	59.156	36.887	1.00	18.14		C
5	ANISOU	156	CG1	VAL	F	67	2361	2302	2226	-43	66	-126	C
	ATOM	160	CG2	VAL	F	67	-5.895	58.155	34.811	1.00	17.87		C
	ANISOU	160	CG2	VAL	F	67	2158	2127	2504	-67	174	-53	C
	ATOM	164	C	VAL	F	67	-5.400	61.748	36.175	1.00	16.24		C
	ANISOU	164	C	VAL	F	67	2154	2080	1936	117	163	28	C
10	ATOM	165	O	VAL	F	67	-4.469	61.650	36.961	1.00	16.41		O
	ANISOU	165	O	VAL	F	67	2050	2120	2064	87	174	-73	O
	ATOM	167	N	THR	F	68	-6.176	62.829	36.088	1.00	16.02		N
	ANISOU	167	N	THR	F	68	1925	2093	2066	247	49	-18	N
	ATOM	168	CA	THR	F	68	-5.739	64.134	36.582	1.00	17.34		C
15	ANISOU	168	CA	THR	F	68	2233	2270	2083	99	117	-51	C
	ATOM	170	CB	THR	F	68	-6.168	65.235	35.590	1.00	19.08		C
	ANISOU	170	CB	THR	F	68	2463	2314	2472	34	252	125	C
	ATOM	172	OG1	THR	F	68	-7.584	65.174	35.377	1.00	18.27		O
	ANISOU	172	OG1	THR	F	68	2409	2511	2021	41	22	-6	O
20	ATOM	174	CG2	THR	F	68	-5.461	65.048	34.255	1.00	20.34		C
	ANISOU	174	CG2	THR	F	68	2835	2534	2359	-37	214	-35	C
	ATOM	178	C	THR	F	68	-6.254	64.528	37.962	1.00	16.44		C
	ANISOU	178	C	THR	F	68	2136	2135	1975	-7	74	-63	C
	ATOM	179	O	THR	F	68	-5.555	65.214	38.718	1.00	17.65		O
25	ANISOU	179	O	THR	F	68	1910	2641	2154	-131	-23	-317	O
	ATOM	181	N	ARG	F	69	-7.485	64.131	38.263	1.00	15.75		N
	ANISOU	181	N	ARG	F	69	1971	2115	1895	-74	54	7	N
	ATOM	182	CA	ARG	F	69	-8.193	64.572	39.461	1.00	15.68		C
	ANISOU	182	CA	ARG	F	69	2067	1965	1925	-250	-64	-40	C
30	ATOM	184	CB	ARG	F	69	-8.497	66.070	39.383	1.00	15.93		C
	ANISOU	184	CB	ARG	F	69	1999	2108	1944	29	177	-171	C
	ATOM	187	CG	ARG	F	69	-9.393	66.483	38.214	1.00	18.29		C
	ANISOU	187	CG	ARG	F	69	2342	2234	2373	154	-19	-107	C
	ATOM	190	CD	ARG	F	69	-9.420	68.004	38.018	1.00	22.32		C
35	ANISOU	190	CD	ARG	F	69	3045	2524	2910	133	25	-63	C
	ATOM	193	NE	ARG	F	69	-8.227	68.496	37.313	1.00	28.14		N
	ANISOU	193	NE	ARG	F	69	3503	3635	3555	-28	25	108	N
	ATOM	195	CZ	ARG	F	69	-7.138	69.021	37.881	1.00	28.71		C
	ANISOU	195	CZ	ARG	F	69	3662	3658	3586	-84	18	95	C
40	ATOM	196	NH1	ARG	F	69	-7.042	69.172	39.201	1.00	28.01		N
	ANISOU	196	NH1	ARG	F	69	3677	3453	3511	-56	55	23	N
	ATOM	199	NH2	ARG	F	69	-6.128	69.422	37.112	1.00	28.22		N
	ANISOU	199	NH2	ARG	F	69	3348	3869	3505	-70	98	25	N
	ATOM	202	C	ARG	F	69	-9.492	63.789	39.613	1.00	12.99		C
45	ANISOU	202	C	ARG	F	69	1701	1699	1535	-101	-57	-50	C
	ATOM	203	O	ARG	F	69	-9.860	63.008	38.737	1.00	14.41		O
	ANISOU	203	O	ARG	F	69	2035	1960	1478	-249	39	-192	O
	ATOM	205	N	CYS	F	70	-10.176	64.011	40.733	1.00	13.36		N
	ANISOU	205	N	CYS	F	70	1817	1707	1552	-60	190	-136	N
50	ATOM	206	CA	CYS	F	70	-11.494	63.447	40.992	1.00	13.78		C
	ANISOU	206	CA	CYS	F	70	1946	1716	1572	-176	-136	-180	C
	ATOM	208	CB	CYS	F	70	-11.444	62.572	42.246	1.00	14.09		C
	ANISOU	208	CB	CYS	F	70	1787	1762	1804	-172	-5	36	C
	ATOM	211	SG	CYS	F	70	-12.995	61.712	42.674	1.00	17.48		S
55	ANISOU	211	SG	CYS	F	70	2245	2059	2335	-262	-32	254	S
	ATOM	213	C	CYS	F	70	-12.499	64.579	41.171	1.00	15.06		C
	ANISOU	213	C	CYS	F	70	1820	2084	1816	-239	-5	85	C
	ATOM	214	O	CYS	F	70	-12.214	65.552	41.860	1.00	13.74		O
	ANISOU	214	O	CYS	F	70	1983	1859	1377	-275	56	-6	O
60	ATOM	216	N	GLU	F	71	-13.655	64.460	40.526	1.00	15.36		N
	ANISOU	216	N	GLU	F	71	2187	1974	1675	-193	-182	-93	N
	ATOM	217	CA	GLU	F	71	-14.777	65.355	40.781	1.00	18.85		C
	ANISOU	217	CA	GLU	F	71	2403	2470	2286	-61	-15	-67	C
	ATOM	219	CB	GLU	F	71	-14.849	66.473	39.750	1.00	21.60		C
65	ANISOU	219	CB	GLU	F	71	2970	2684	2552	56	43	-46	C
	ATOM	222	CG	GLU	F	71	-15.948	67.477	40.060	1.00	23.17		C
	ANISOU	222	CG	GLU	F	71	3033	2864	2905	89	-77	38	C
	ATOM	225	CD	GLU	F	71	-16.050	68.564	39.024	1.00	25.93		C
	ANISOU	225	CD	GLU	F	71	3423	3124	3302	54	-11	165	C
70	ATOM	226	OE1	GLU	F	71	-15.053	69.276	38.839	1.00	31.24		O
	ANISOU	226	OE1	GLU	F	71	3853	4035	3982	-171	95	245	O

	ATOM	227	OE2	GLU	F	71	-17.125	68.715	38.407	1.00	30.01		0
	ANISOU	227	OE2	GLU	F	71	3803	3904	3694	-158	-266	191	0
	ATOM	228	C	GLU	F	71	-16.073	64.565	40.751	1.00	18.90		C
	ANISOU	228	C	GLU	F	71	2421	2490	2267	-37	-71	-80	C
5	ATOM	229	O	GLU	F	71	-16.279	63.758	39.850	1.00	17.04		O
	ANISOU	229	O	GLU	F	71	2369	2127	1979	-61	-254	-46	O
	ATOM	231	N	ASP	F	72	-16.935	64.815	41.738	1.00	18.71		N
	ANISOU	231	N	ASP	F	72	2362	2360	2384	75	-20	-60	N
	ATOM	232	CA	ASP	F	72	-18.229	64.142	41.848	1.00	18.22		C
10	ANISOU	232	CA	ASP	F	72	2248	2391	2282	55	50	-59	C
	ATOM	234	CB	ASP	F	72	-19.200	64.689	40.793	1.00	22.83		C
	ANISOU	234	CB	ASP	F	72	2878	2958	2839	231	-50	62	C
	ATOM	237	CG	ASP	F	72	-19.453	66.174	40.947	1.00	27.66		C
	ANISOU	237	CG	ASP	F	72	3556	3426	3525	182	-63	85	C
15	ATOM	238	OD1	ASP	F	72	-19.647	66.632	42.091	1.00	27.57		O
	ANISOU	238	OD1	ASP	F	72	3646	3324	3503	417	-127	0	O
	ATOM	239	OD2	ASP	F	72	-19.459	66.885	39.921	1.00	33.79		O
	ANISOU	239	OD2	ASP	F	72	4439	4194	4204	150	-42	366	O
	ATOM	240	C	ASP	F	72	-18.122	62.616	41.733	1.00	18.15		C
20	ANISOU	240	C	ASP	F	72	2402	2371	2120	34	-50	52	C
	ATOM	241	O	ASP	F	72	-18.972	61.969	41.127	1.00	19.94		O
	ANISOU	241	O	ASP	F	72	2504	2551	2520	46	-139	8	O
	ATOM	243	N	GLY	F	73	-17.073	62.047	42.320	1.00	15.68		N
	ANISOU	243	N	GLY	F	73	1913	2080	1965	-80	16	-156	N
25	ATOM	244	CA	GLY	F	73	-16.909	60.601	42.363	1.00	15.91		C
	ANISOU	244	CA	GLY	F	73	2081	2132	1830	-85	39	-30	C
	ATOM	247	C	GLY	F	73	-16.345	59.957	41.108	1.00	16.51		C
	ANISOU	247	C	GLY	F	73	2323	2096	1851	-52	33	68	C
	ATOM	248	O	GLY	F	73	-16.293	58.738	41.031	1.00	17.61		O
30	ANISOU	248	O	GLY	F	73	2596	2063	2031	-80	145	8	O
	ATOM	250	N	GLN	F	74	-15.919	60.764	40.136	1.00	15.15		N
	ANISOU	250	N	GLN	F	74	1950	2010	1796	56	5	-76	N
	ATOM	251	CA	GLN	F	74	-15.341	60.238	38.905	1.00	14.99		C
	ANISOU	251	CA	GLN	F	74	1804	1931	1958	-88	45	47	C
35	ATOM	253	CB	GLN	F	74	-16.200	60.605	37.692	1.00	16.14		C
	ANISOU	253	CB	GLN	F	74	1978	2257	1897	-64	0	-24	C
	ATOM	256	CG	GLN	F	74	-15.687	59.981	36.395	1.00	17.47		C
	ANISOU	256	CG	GLN	F	74	2310	2346	1980	-97	-49	-49	C
	ATOM	259	CD	GLN	F	74	-16.622	60.159	35.217	1.00	19.11		C
40	ANISOU	259	CD	GLN	F	74	2266	2692	2302	100	-50	8	C
	ATOM	260	OE1	GLN	F	74	-17.592	60.923	35.269	1.00	22.97		O
	ANISOU	260	OE1	GLN	F	74	2743	3171	2811	545	12	51	O
	ATOM	261	NE2	GLN	F	74	-16.324	59.460	34.137	1.00	19.36		N
	ANISOU	261	NE2	GLN	F	74	2670	2499	2186	-89	-190	-262	N
45	ATOM	264	C	GLN	F	74	-13.936	60.793	38.719	1.00	13.87		C
	ANISOU	264	C	GLN	F	74	1754	1856	1660	-66	85	-16	C
	ATOM	265	O	GLN	F	74	-13.695	61.984	38.925	1.00	15.30		O
	ANISOU	265	O	GLN	F	74	2035	1887	1890	13	120	-58	O
	ATOM	267	N	LEU	F	75	-13.014	59.921	38.324	1.00	14.21		N
50	ANISOU	267	N	LEU	F	75	1850	1783	1764	-36	-17	-94	N
	ATOM	268	CA	LEU	F	75	-11.676	60.362	37.957	1.00	13.72		C
	ANISOU	268	CA	LEU	F	75	1720	1821	1673	-199	47	-70	C
	ATOM	270	CB	LEU	F	75	-10.636	59.247	38.069	1.00	15.19		C
	ANISOU	270	CB	LEU	F	75	1795	1828	2146	-344	-107	18	C
55	ATOM	273	CG	LEU	F	75	-10.460	58.632	39.456	1.00	17.99		C
	ANISOU	273	CG	LEU	F	75	2276	2333	2225	-216	55	126	C
	ATOM	275	CD1	LEU	F	75	-9.285	57.694	39.498	1.00	18.25		C
	ANISOU	275	CD1	LEU	F	75	2453	2203	2276	-154	-93	84	C
	ATOM	279	CD2	LEU	F	75	-10.270	59.693	40.500	1.00	20.52		C
60	ANISOU	279	CD2	LEU	F	75	2803	2410	2583	54	-94	40	C
	ATOM	283	C	LEU	F	75	-11.705	60.914	36.552	1.00	14.36		C
	ANISOU	283	C	LEU	F	75	1787	1845	1821	-164	26	-71	C
	ATOM	284	O	LEU	F	75	-12.272	60.311	35.645	1.00	17.12		O
	ANISOU	284	O	LEU	F	75	2202	2555	1746	-562	-69	-366	O
65	ATOM	286	N	PHE	F	76	-11.087	62.072	36.381	1.00	13.68		N
	ANISOU	286	N	PHE	F	76	1751	1688	1755	-195	77	-90	N
	ATOM	287	CA	PHE	F	76	-10.998	62.699	35.074	1.00	13.76		C
	ANISOU	287	CA	PHE	F	76	1601	1934	1691	-96	-38	33	C
	ATOM	289	CB	PHE	F	76	-10.774	64.208	35.220	1.00	18.02		C
70	ANISOU	289	CB	PHE	F	76	2350	2272	2224	-76	-22	19	C
	ATOM	292	CG	PHE	F	76	-12.027	64.986	35.534	1.00	19.08		C

	ANISOU	292	CG	PHE	F	76	2493	2519	2237	-78	-4	-85	C
	ATOM	293	CD1	PHE	F	76	-13.123	64.387	36.150	1.00	19.74		C
	ANISOU	293	CD1	PHE	F	76	2571	2557	2371	96	217	-131	C
	ATOM	295	CE1	PHE	F	76	-14.269	65.124	36.437	1.00	20.29		C
5	ANISOU	295	CE1	PHE	F	76	2514	2723	2471	33	6	-75	C
	ATOM	297	CZ	PHE	F	76	-14.333	66.461	36.106	1.00	20.84		C
	ANISOU	297	CZ	PHE	F	76	2584	2783	2549	180	152	-9	C
	ATOM	299	CE2	PHE	F	76	-13.251	67.075	35.505	1.00	21.35		C
10	ANISOU	299	CE2	PHE	F	76	2701	2604	2807	117	79	164	C
	ATOM	301	CD2	PHE	F	76	-12.104	66.335	35.219	1.00	22.26		C
	ANISOU	301	CD2	PHE	F	76	2860	2808	2787	114	142	59	C
	ATOM	303	C	PHE	F	76	-9.877	62.062	34.267	1.00	15.24		C
	ANISOU	303	C	PHE	F	76	1830	2062	1898	26	-84	-101	C
	ATOM	304	O	PHE	F	76	-8.825	61.708	34.806	1.00	17.61		O
15	ANISOU	304	O	PHE	F	76	2122	2710	1858	159	5	-165	O
	ATOM	305	N	ILE	F	77	-10.128	61.905	32.973	1.00	15.50		N
	ANISOU	306	N	ILE	F	77	1866	2287	1737	84	40	-32	N
	ATOM	307	CA	ILE	F	77	-9.175	61.315	32.048	1.00	15.38		C
20	ANISOU	307	CA	ILE	F	77	1907	2203	1732	99	-7	-43	C
	ATOM	309	CB	ILE	F	77	-9.667	59.966	31.493	1.00	16.87		C
	ANISOU	309	CB	ILE	F	77	2093	2212	2105	64	230	-87	C
	ATOM	311	CG1	ILE	F	77	-9.947	58.986	32.640	1.00	18.70		C
	ANISOU	311	CG1	ILE	F	77	2324	2295	2483	9	155	63	C
	ATOM	314	CD1	ILE	F	77	-10.637	57.701	32.201	1.00	20.04		C
25	ANISOU	314	CD1	ILE	F	77	2607	2412	2594	74	161	-13	C
	ATOM	318	CG2	ILE	F	77	-8.636	59.387	30.506	1.00	18.52		C
	ANISOU	318	CG2	ILE	F	77	2369	2575	2092	109	158	-223	C
	ATOM	322	C	ILE	F	77	-8.991	62.281	30.897	1.00	18.04		C
30	ANISOU	322	C	ILE	F	77	2493	2304	2056	69	166	-77	C
	ATOM	323	O	ILE	F	77	-9.970	62.691	30.271	1.00	19.54		O
	ANISOU	323	O	ILE	F	77	2448	2878	2095	-47	284	11	O
	ATOM	325	N	SER	F	78	-7.734	62.620	30.634	1.00	18.39		N
	ANISOU	325	N	SER	F	78	2444	2418	2123	151	127	-31	N
	ATOM	326	CA	SER	F	78	-7.343	63.575	29.602	1.00	19.51		C
35	ANISOU	326	CA	SER	F	78	2669	2490	2253	204	263	77	C
	ATOM	328	CB	SER	F	78	-6.552	64.719	30.249	1.00	22.44		C
	ANISOU	328	CB	SER	F	78	3169	2579	2778	23	230	90	C
	ATOM	331	OG	SER	F	78	-5.839	65.487	29.293	1.00	24.20		O
40	ANISOU	331	OG	SER	F	78	3196	3167	2832	-76	494	-224	O
	ATOM	333	C	SER	F	78	-6.473	62.879	28.557	1.00	19.75		C
	ANISOU	333	C	SER	F	78	2696	2414	2392	339	251	125	C
	ATOM	334	O	SER	F	78	-5.622	62.068	28.902	1.00	21.81		O
	ANISOU	334	O	SER	F	78	2929	3126	2233	580	189	325	O
	ATOM	336	N	SER	F	79	-6.669	63.206	27.284	1.00	21.32		N
45	ANISOU	336	N	SER	F	79	2696	2833	2569	192	215	-1	N
	ATOM	337	CA	SER	F	79	-5.804	62.674	26.231	1.00	20.00		C
	ANISOU	337	CA	SER	F	79	2538	2708	2352	62	81	-83	C
	ATOM	339	CB	SER	F	79	-6.546	62.644	24.889	1.00	23.79		C
	ANISOU	339	CB	SER	F	79	3073	3405	2561	87	-9	59	C
50	ATOM	342	OG	SER	F	79	-6.843	63.956	24.451	1.00	27.88		O
	ANISOU	342	OG	SER	F	79	3530	3628	3434	-34	-159	-38	O
	ATOM	344	C	SER	F	79	-4.481	63.451	26.087	1.00	19.51		C
	ANISOU	344	C	SER	F	79	2348	2765	2298	68	87	47	C
	ATOM	345	O	SER	F	79	-3.704	63.159	25.176	1.00	18.96		O
55	ANISOU	345	O	SER	F	79	2417	2839	1945	403	-28	186	O
	ATOM	347	N	TYR	F	80	-4.221	64.411	26.986	1.00	18.72		N
	ANISOU	347	N	TYR	F	80	2280	2620	2212	93	232	-9	N
	ATOM	348	CA	TYR	F	80	-2.985	65.209	26.973	1.00	19.32		C
	ANISOU	348	CA	TYR	F	80	2396	2480	2464	65	39	-53	C
60	ATOM	350	CB	TYR	F	80	-3.150	66.523	27.766	1.00	22.20		C
	ANISOU	350	CB	TYR	F	80	2920	2838	2677	-34	61	-72	C
	ATOM	353	CG	TYR	F	80	-1.922	67.434	27.727	1.00	23.19		C
	ANISOU	353	CG	TYR	F	80	2930	3124	2754	-42	28	13	C
	ATOM	354	CD1	TYR	F	80	-1.541	68.083	26.550	1.00	23.18		C
65	ANISOU	354	CD1	TYR	F	80	2967	2935	2903	-35	46	68	C
	ATOM	356	CE1	TYR	F	80	-0.417	68.903	26.511	1.00	22.74		C
	ANISOU	356	CE1	TYR	F	80	2952	3004	2683	0	-2	51	C
	ATOM	358	CZ	TYR	F	80	0.332	69.089	27.657	1.00	23.56		C
	ANISOU	358	CZ	TYR	F	80	2995	3027	2928	-43	-4	46	C
70	ATOM	359	OH	TYR	F	80	1.446	69.895	27.633	1.00	23.19		O
	ANISOU	359	OH	TYR	F	80	2812	3278	2719	-2	8	16	O

	ATOM	361	CE2	TYR	F	80	-0.029	68.459	28.837	1.00	24..58		C
	ANISOU	361	CE2	TYR	F	80	3093	3357	2887	-94	20	39	C
	ATOM	363	CD2	TYR	F	80	-1.147	67.643	28.867	1.00	24.38		C
	ANISOU	363	CD2	TYR	F	80	3111	3155	2996	-111	-38	2	C
5	ATOM	365	C	TYR	F	80	-1.793	64.412	27.493	1.00	20.18		C
	ANISOU	365	C	TYR	F	80	2404	2771	2493	119	40	-80	C
	ATOM	366	O	TYR	F	80	-1.374	64.542	28.651	1.00	22.67		O
	ANISOU	366	O	TYR	F	80	2784	3163	2666	267	103	-224	O
	ATOM	368	N	LYS	F	81	-1.264	63.577	26.611	1.00	18.78		N
10	ANISOU	368	N	LYS	F	81	2140	2723	2273	20	15	-74	N
	ATOM	369	CA	LYS	F	81	-0.049	62.807	26.843	1.00	17..48		C
	ANISOU	369	CA	LYS	F	81	2080	2476	2085	103	-48	-8	C
	ATOM	371	CB	LYS	F	81	-0.382	61.370	27.258	1.00	20.98		C
	ANISOU	371	CB	LYS	F	81	2645	2543	2781	-31	61	-3	C
15	ATOM	374	CG	LYS	F	81	-0.846	61.200	28.699	1.00	22.98		C
	ANISOU	374	CG	LYS	F	81	2883	2871	2976	-113	80	78	C
	ATOM	377	CD	LYS	F	81	0.219	61.676	29.673	1.00	27.09		C
	ANISOU	377	CD	LYS	F	81	3314	3700	3279	33	-17	30	C
	ATOM	380	CE	LYS	F	81	0.115	61.023	31.013	1.00	28..43		C
20	ANISOU	380	CE	LYS	F	81	3449	3820	3530	-54	-30	-22	C
	ATOM	383	NZ	LYS	F	81	1.183	61.575	31.887	1.00	29..24		N
	ANISOU	383	NZ	LYS	F	81	3437	4206	3465	-105	-267	-69	N
	ATOM	387	C	LYS	F	81	0.719	62.769	25.531	1.00	17..08		C
	ANISOU	387	C	LYS	F	81	1825	2641	2021	158	79	227	C
25	ATOM	388	O	LYS	F	81	0.126	62.916	24.449	1.00	16.54		O
	ANISOU	388	O	LYS	F	81	1697	2529	2057	323	45	202	O
	ATOM	390	N	ASN	F	82	2.026	62.536	25.609	1.00	15.86		N
	ANISOU	390	N	ASN	F	82	1644	2454	1925	187	-144	79	N
	ATOM	391	CA	ASN	F	82	2.833	62.369	24.396	1.00	14.60		C
30	ANISOU	391	CA	ASN	F	82	1677	2094	1774	21	-153	153	C
	ATOM	393	CB	ASN	F	82	4.308	62.690	24.648	1.00	14.67		C
	ANISOU	393	CB	ASN	F	82	1742	2087	1745	197	-393	154	C
	ATOM	396	CG	ASN	F	82	4.548	64.168	24.801	1.00	14.07		C
	ANISOU	396	CG	ASN	F	82	1536	2129	1680	39	-39	124	C
35	ATOM	397	OD1	ASN	F	82	4.588	64.903	23.817	1.00	13.53		O
	ANISOU	397	OD1	ASN	F	82	1480	2247	1412	383	-301	261	O
	ATOM	398	ND2	ASN	F	82	4.687	64.623	26.039	1.00	17.71		N
	ANISOU	398	ND2	ASN	F	82	2226	2562	1938	302	-513	-93	N
	ATOM	401	C	ASN	F	82	2.657	60.972	23.832	1.00	16..29		C
40	ANISOU	401	C	ASN	F	82	1919	2245	2024	181	-59	-10	C
	ATOM	402	O	ASN	F	82	3.543	60.120	23.922	1.00	16.92		O
	ANISOU	402	O	ASN	F	82	1894	2273	2262	331	-140	248	O
	ATOM	404	N	GLU	F	83	1.482	60.748	23.254	1.00	15.38		N
45	ANISOU	404	N	GLU	F	83	1768	2167	1908	166	-117	103	N
	ATOM	405	CA	GLU	F	83	1.122	59.460	22.708	1.00	15.56		C
	ANISOU	405	CA	GLU	F	83	1769	2174	1966	66	-121	159	C
	ATOM	407	CB	GLU	F	83	0.323	58.645	23.722	1.00	15.82		C
	ANISOU	407	CB	GLU	F	83	1762	2423	1824	11	-26	114	C
	ATOM	410	CG	GLU	F	83	0.182	57.173	23.361	1.00	17.01		C
50	ANISOU	410	CG	GLU	F	83	2051	2399	2013	71	105	193	C
	ATOM	413	CD	GLU	F	83	1.495	56.439	23.465	1.00	17..47		C
	ANISOU	413	CD	GLU	F	83	2138	2219	2277	143	-323	82	C
	ATOM	414	OE1	GLU	F	83	2.253	56.725	24.420	1.00	18.03		O
	ANISOU	414	OE1	GLU	F	83	2337	2471	2041	238	-378	-102	O
55	ATOM	415	OE2	GLU	F	83	1.785	55.599	22.597	1.00	21.32		O
	ANISOU	415	OE2	GLU	F	83	2568	2753	2778	419	-326	36	O
	ATOM	416	C	GLU	F	83	0.269	59.677	21.484	1.00	15.38		C
	ANISOU	416	C	GLU	F	83	1878	2137	1828	94	-136	122	C
	ATOM	417	O	GLU	F	83	-0.584	60.562	21.469	1.00	16..73		O
60	ANISOU	417	O	GLU	F	83	1909	2141	2305	138	-208	141	O
	ATOM	419	N	TYR	F	84	0.492	58.859	20.465	1.00	16..41		N
	ANISOU	419	N	TYR	F	84	1992	2357	1886	189	-52	50	N
	ATOM	420	CA	TYR	F	84	-0.396	58.829	19.316	1.00	16.91		C
	ANISOU	420	CA	TYR	F	84	2060	2246	2116	27	-164	28	C
65	ATOM	422	CB	TYR	F	84	0.291	58.152	18.129	1.00	23.05		C
	ANISOU	422	CB	TYR	F	84	2813	3058	2886	75	85	-45	C
	ATOM	425	CG	TYR	F	84	-0.627	57.874	16.965	1.00	23..84		C
	ANISOU	425	CG	TYR	F	84	3023	3196	2837	34	-37	-50	C
	ATOM	426	CD1	TYR	F	84	-1.450	58.867	16.445	1.00	27.48		C
70	ANISOU	426	CD1	TYR	F	84	3409	3684	3347	156	-183	-91	C
	ATOM	428	CE1	TYR	F	84	-2.291	58.610	15.373	1.00	27.55		C

	ANISOU	428	CE1	TYR	F	84	3358	3611	3499	100	-175	-223	C
	ATOM	430	CZ	TYR	F	84	-2.308	57.354	14.808	1.00	26.98		C
	ANISOU	430	CZ	TYR	F	84	3366	3519	3363	33	-200	-66	C
	ATOM	431	OH	TYR	F	84	-3.139	57.106	13.738	1.00	28.72		O
5	ANISOU	431	OH	TYR	F	84	3429	3907	3574	39	-251	-342	O
	ATOM	433	CE2	TYR	F	84	-1.494	56.356	15.300	1.00	26.53		C
	ANISOU	433	CE2	TYR	F	84	3240	3581	3259	6	-63	-132	C
	ATOM	435	CD2	TYR	F	84	-0.662	56.619	16.374	1.00	25.57		C
	ANISOU	435	CD2	TYR	F	84	3263	3294	3157	-7	-101	-66	C
10	ATOM	437	C	TYR	F	84	-1.656	58.074	19.738	1.00	15.81		C
	ANISOU	437	C	TYR	F	84	1949	1984	2074	64	-174	148	C
	ATOM	438	O	TYR	F	84	-1.608	56.865	19.994	1.00	17.73		O
	ANISOU	438	O	TYR	F	84	2004	2264	2466	-68	-63	359	O
	ATOM	440	N	GLN	F	85	-2.762	58.808	19.859	1.00	15.47		N
15	ANISOU	440	N	GLN	F	85	1774	1942	2161	-21	-77	213	N
	ATOM	441	CA	GLN	F	85	-4.028	58.250	20.328	1.00	15.86		C
	ANISOU	441	CA	GLN	F	85	2106	2081	1836	-6	-99	167	C
	ATOM	443	CB	GLN	F	85	-4.837	59.281	21.134	1.00	15.93		C
	ANISOU	443	CB	GLN	F	85	2074	1871	2107	89	-153	298	C
20	ATOM	446	CG	GLN	F	85	-4.051	60.140	22.111	1.00	15.25		C
	ANISOU	446	CG	GLN	F	85	1960	2030	1801	110	65	134	C
	ATOM	449	CD	GLN	F	85	-3.591	59.417	23.358	1.00	15.31		C
	ANISOU	449	CD	GLN	F	85	1764	1913	2139	12	-47	106	C
	ATOM	450	OE1	GLN	F	85	-3.505	58.186	23.407	1.00	16.95		O
25	ANISOU	450	OE1	GLN	F	85	2286	2083	2068	-90	125	169	O
	ATOM	451	NE2	GLN	F	85	-3.265	60.195	24.379	1.00	17.03		N
	ANISOU	451	NE2	GLN	F	85	1993	2400	2076	-76	-9	-152	N
	ATOM	454	C	GLN	F	85	-4.845	57.810	19.131	1.00	17.47		C
	ANISOU	454	C	GLN	F	85	2162	2167	2309	-5	-256	65	C
30	ATOM	455	O	GLN	F	85	-4.950	58.540	18.143	1.00	19.66		O
	ANISOU	455	O	GLN	F	85	2443	2432	2593	-138	-275	189	O
	ATOM	457	N	THR	F	86	-5.419	56.616	19.211	1.00	16.44		N
	ANISOU	457	N	THR	F	86	2000	2212	2030	79	-137	114	N
	ATOM	458	CA	THR	F	86	-6.337	56.154	18.169	1.00	15.71		C
35	ANISOU	458	CA	THR	F	86	1971	2054	1942	-95	-200	96	C
	ATOM	460	CB	THR	F	86	-5.783	54.921	17.406	1.00	16.05		C
	ANISOU	460	CB	THR	F	86	1867	2178	2052	-29	-91	117	C
	ATOM	462	OG1	THR	F	86	-5.603	53.827	18.311	1.00	18.47		O
	ANISOU	462	OG1	THR	F	86	2363	2318	2337	126	-141	276	O
40	ATOM	464	CG2	THR	F	86	-4.446	55.264	16.738	1.00	18.52		C
	ANISOU	464	CG2	THR	F	86	2213	2378	2445	122	110	80	C
	ATOM	468	C	THR	F	86	-7.744	55.882	18.709	1.00	17.57		C
	ANISOU	468	C	THR	F	86	2272	2184	2218	-117	150	120	C
	ATOM	469	O	THR	F	86	-8.589	55.374	17.978	1.00	20.26		O
45	ANISOU	469	O	THR	F	86	2405	2889	2401	-372	25	1	O
	ATOM	471	N	MET	F	87	-7.986	56.209	19.980	1.00	18.29		N
	ANISOU	471	N	MET	F	87	2433	2204	2313	-139	-166	-130	N
	ATOM	472	CA	MET	F	87	-9.334	56.211	20.557	1.00	18.67		C
	ANISOU	472	CA	MET	F	87	2318	2348	2427	-105	7	-41	C
50	ATOM	474	CB	MET	F	87	-9.472	55.133	21.641	1.00	20.05		C
	ANISOU	474	CB	MET	F	87	2651	2550	2416	-151	18	-24	C
	ATOM	477	CG	MET	F	87	-9.790	53.746	21.076	1.00	22.62		C
	ANISOU	477	CG	MET	F	87	3160	2630	2805	-39	-21	-62	C
	ATOM	480	SD	MET	F	87	-9.998	52.458	22.327	1.00	22.54		S
55	ANISOU	480	SD	MET	F	87	2591	2900	3072	-207	-164	-72	S
	ATOM	481	CE	MET	F	87	-8.344	52.498	22.842	1.00	13.96		C
	ANISOU	481	CE	MET	F	87	1483	1664	2154	65	89	-285	C
	ATOM	485	C	MET	F	87	-9.654	57.583	21.151	1.00	20.47		C
	ANISOU	485	C	MET	F	87	2614	2627	2536	-168	27	-100	C
60	ATOM	486	O	MET	F	87	-8.753	58.341	21.507	1.00	21.71		O
	ANISOU	486	O	MET	F	87	2614	2715	2917	-288	-223	-253	O
	ATOM	488	N	GLU	F	88	-10.945	57.890	21.253	1.00	19.52		N
	ANISOU	488	N	GLU	F	88	2516	2492	2408	-37	204	-68	N
	ATOM	489	CA	GLU	F	88	-11.405	59.157	21.811	1.00	21.86		C
65	ANISOU	489	CA	GLU	F	88	2867	2754	2683	-54	157	-61	C
	ATOM	491	CB	GLU	F	88	-12.669	59.621	21.094	1.00	24.93		C
	ANISOU	491	CB	GLU	F	88	3198	3254	3018	85	33	86	C
	ATOM	494	CG	GLU	F	88	-12.485	59.874	19.615	1.00	28.91		C
	ANISOU	494	CG	GLU	F	88	3786	3774	3423	-39	13	18	C
70	ATOM	497	CD	GLU	F	88	-13.706	60.513	18.993	1.00	31.58		C
	ANISOU	497	CD	GLU	F	88	3955	4099	3941	91	-49	65	C

	ATOM	498	OE1	GLU	F	88	-14.832	60.213	19.448	1.00	37.75		O
	ANISOU	498	OE1	GLU	F	88	4454	4946	4942	-20	184	-25	O
	ATOM	499	OE2	GLU	F	88	-13.543	61.314	18.048	1.00	36.75		O
	ANISOU	499	OE2	GLU	F	88	4712	4622	4629	-39	219	194	O
5	ATOM	500	C	GLU	F	88	-11.726	59.044	23.292	1.00	18.59		C
	ANISOU	500	C	GLU	F	88	2460	2321	2281	-72	140	-33	C
	ATOM	501	O	GLU	F	88	-12.140	57.991	23.775	1.00	17.20		O
	ANISOU	501	O	GLU	F	88	2405	2141	1987	-262	-124	-117	O
10	ATOM	503	N	VAL	F	89	-11.543	60.149	24.005	1.00	19.38		N
	ANISOU	503	N	VAL	F	89	2513	2304	2545	-113	126	-83	N
	ATOM	504	CA	VAL	F	89	-12.087	60.314	25.344	1.00	20.00		C
	ANISOU	504	CA	VAL	F	89	2726	2343	2529	-75	4	32	C
	ATOM	506	CB	VAL	F	89	-11.063	60.936	26.307	1.00	22.30		C
	ANISOU	506	CB	VAL	F	89	2833	2940	2698	-151	-21	-105	C
15	ATOM	508	CG1	VAL	F	89	-11.701	61.204	27.673	1.00	24.53		C
	ANISOU	508	CG1	VAL	F	89	3212	3157	2949	-81	93	-197	C
	ATOM	512	CG2	VAL	F	89	-9.863	60.035	26.441	1.00	22.17		C
	ANISOU	512	CG2	VAL	F	89	2965	2822	2635	-98	-201	8	C
	ATOM	516	C	VAL	F	89	-13.292	61.245	25.245	1.00	19.55		C
20	ANISOU	516	C	VAL	F	89	2781	2366	2280	18	-185	54	C
	ATOM	517	O	VAL	F	89	-13.207	62.333	24.661	1.00	22.14		O
	ANISOU	517	O	VAL	F	89	3262	2352	2796	-17	272	179	O
	ATOM	519	N	GLN	F	90	-14.410	60.806	25.809	1.00	19.88		N
	ANISOU	519	N	GLN	F	90	2759	2193	2600	86	-78	-35	N
25	ATOM	520	CA	GLN	F	90	-15.640	61.583	25.830	1.00	21.47		C
	ANISOU	520	CA	GLN	F	90	2758	2664	2736	91	-7	-8	C
	ATOM	522	CB	GLN	F	90	-16.658	60.993	24.840	1.00	22.51		C
	ANISOU	522	CB	GLN	F	90	2881	2821	2848	105	-179	35	C
	ATOM	525	CG	GLN	F	90	-18.024	61.681	24.807	1.00	25.97		C
30	ANISOU	525	CG	GLN	F	90	3188	3409	3270	21	-43	-3	C
	ATOM	528	CD	GLN	F	90	-19.057	60.928	23.964	1.00	28.52		C
	ANISOU	528	CD	GLN	F	90	3466	3654	3714	-12	-126	-55	C
	ATOM	529	OE1	GLN	F	90	-18.905	59.736	23.668	1.00	32.21		O
	ANISOU	529	OE1	GLN	F	90	4140	3775	4322	136	-69	-140	O
35	ATOM	530	NE2	GLN	F	90	-20.122	61.625	23.584	1.00	32.15		N
	ANISOU	530	NE2	GLN	F	90	3892	4274	4049	109	-78	122	N
	ATOM	533	C	GLN	F	90	-16.182	61.545	27.253	1.00	18.25		C
	ANISOU	533	C	GLN	F	90	2270	2270	2391	19	-254	-103	C
	ATOM	534	O	GLN	F	90	-16.403	60.470	27.808	1.00	20.71		O
40	ANISOU	534	O	GLN	F	90	2677	2473	2718	-106	-322	-183	O
	ATOM	536	N	ASN	F	91	-16.380	62.720	27.845	1.00	21.03		N
	ANISOU	536	N	ASN	F	91	2701	2600	2689	163	-227	-5	N
	ATOM	537	CA	ASN	F	91	-16.901	62.822	29.201	1.00	21.23		C
	ANISOU	537	CA	ASN	F	91	2707	2676	2684	120	-63	-15	C
45	ATOM	539	CB	ASN	F	91	-18.395	62.477	29.216	1.00	24.57		C
	ANISOU	539	CB	ASN	F	91	2982	3370	2984	17	15	-30	C
	ATOM	542	CG	ASN	F	91	-19.132	63.080	30.409	1.00	25.14		C
	ANISOU	542	CG	ASN	F	91	3083	3293	3176	140	45	-139	C
	ATOM	543	OD1	ASN	F	91	-18.542	63.775	31.240	1.00	27.90		O
50	ANISOU	543	OD1	ASN	F	91	3371	3642	3586	341	-68	-261	O
	ATOM	544	ND2	ASN	F	91	-20.437	62.821	30.483	1.00	28.13		N
	ANISOU	544	ND2	ASN	F	91	3286	3837	3564	13	55	-27	N
	ATOM	547	C	ASN	F	91	-16.132	61.924	30.169	1.00	17.84		C
	ANISOU	547	C	ASN	F	91	2336	2256	2186	-79	-3	-189	C
55	ATOM	548	O	ASN	F	91	-16.724	61.172	30.941	1.00	20.54		O
	ANISOU	548	O	ASN	F	91	2431	2792	2578	-149	31	-80	O
	ATOM	550	N	ASN	F	92	-14.803	61.994	30.091	1.00	16.95		N
	ANISOU	550	N	ASN	F	92	2254	1942	2244	61	109	-10	N
	ATOM	551	CA	ASN	F	92	-13.917	61.260	30.994	1.00	16.49		C
60	ANISOU	551	CA	ASN	F	92	2169	2043	2050	1	45	-83	C
	ATOM	553	CB	ASN	F	92	-14.091	61.767	32.427	1.00	16.52		C
	ANISOU	553	CB	ASN	F	92	2177	1994	2105	73	-19	-74	C
	ATOM	556	CG	ASN	F	92	-13.666	63.204	32.565	1.00	16.31		C
	ANISOU	556	CG	ASN	F	92	2100	2034	2060	-61	-32	-249	C
65	ATOM	557	OD1	ASN	F	92	-12.530	63.541	32.248	1.00	15.71		O
	ANISOU	557	OD1	ASN	F	92	2113	1962	1893	-248	-117	-166	O
	ATOM	558	ND2	ASN	F	92	-14.584	64.070	33.001	1.00	18.63		N
	ANISOU	558	ND2	ASN	F	92	2325	2284	2467	157	72	-302	N
	ATOM	561	C	ASN	F	92	-14.051	59.736	30.915	1.00	16.96		C
70	ANISOU	561	C	ASN	F	92	2471	1982	1991	43	44	-157	C
	ATOM	562	O	ASN	F	92	-13.731	59.020	31.867	1.00	16.93		O

	ANISOU	562	O	ASN	F	92	2433	1937	2061	-66	-44	-59	O
	ATOM	564	N	SER	F	93	-14.492	59.255	29.753	1.00	16..02		N
	ANISOU	564	N	SER	F	93	2430	1981	1673	-129	31	4	N
	ATOM	565	CA	SER	F	93	-14.522	57.828	29.444	1.00	17..15		C
5	ANISOU	565	CA	SER	F	93	2450	1941	2125	8	80	-121	C
	ATOM	567	CB	ASER	F	93	-15.960	57.328	29.295	0.60	18..24		C
	ANISOU	567	CB	ASER	F	93	2542	2171	2217	81	121	-117	C
	ATOM	568	CB	BSER	F	93	-15.959	57.320	29.349	0.40	18..45		C
	ANISOU	568	CB	BSER	F	93	2538	2132	2339	-7	69	-130	C
10	ATOM	573	OG	ASER	F	93	-16.713	57.503	30.481	0.60	21..09		O
	ANISOU	573	OG	ASER	F	93	2523	3186	2302	195	329	313	O
	ATOM	574	OG	BSER	F	93	-16.589	57.777	28.167	0.40	20..44		O
	ANISOU	574	OG	BSER	F	93	2601	2582	2580	-179	-2	22	O
	ATOM	577	C	SER	F	93	-13.798	57.571	28.132	1.00	16..44		C
15	ANISOU	577	C	SER	F	93	2313	1758	2172	-111	40	-99	C
	ATOM	578	O	SER	F	93	-13.916	58.351	27.182	1.00	17..56		O
	ANISOU	578	O	SER	F	93	2498	1968	2203	114	164	-177	O
	ATOM	580	N	VAL	F	94	-13.091	56.448	28.067	1.00	14..99		N
	ANISOU	580	N	VAL	F	94	2056	1645	1993	-160	10	-40	N
20	ATOM	581	CA	VAL	F	94	-12.469	56.017	26.827	1.00	15..91		C
	ANISOU	581	CA	VAL	F	94	2028	1953	2062	-232	32	-205	C
	ATOM	583	CB	VAL	F	94	-11.262	55.102	27.072	1.00	17..06		C
	ANISOU	583	CB	VAL	F	94	2166	2203	2112	-153	-41	-121	C
	ATOM	585	CG1	VAL	F	94	-10.612	54.710	25.754	1.00	17..02		C
25	ANISOU	585	CG1	VAL	F	94	2376	2055	2034	-93	-148	-170	C
	ATOM	589	CG2	VAL	F	94	-10.239	55.793	27.967	1.00	17..60		C
	ANISOU	589	CG2	VAL	F	94	2096	2239	2352	11	-58	-239	C
	ATOM	593	C	VAL	F	94	-13.539	55.278	26.029	1.00	16..36		C
	ANISOU	593	C	VAL	F	94	2165	2098	1950	-249	-120	-94	C
30	ATOM	594	O	VAL	F	94	-14.149	54.330	26.527	1.00	15..62		O
	ANISOU	594	O	VAL	F	94	2223	1965	1747	-276	-85	-170	O
	ATOM	596	N	VAL	F	95	-13.748	55.718	24.791	1.00	16..33		N
	ANISOU	596	N	VAL	F	95	2369	1956	1878	-329	-109	-126	N
	ATOM	597	CA	VAL	F	95	-14.816	55.218	23.935	1.00	16..51		C
35	ANISOU	597	CA	VAL	F	95	2102	2065	2106	61	-154	-32	C
	ATOM	599	CB	VAL	F	95	-15.352	56.361	23.035	1.00	17..65		C
	ANISOU	599	CB	VAL	F	95	2305	2180	2218	96	-161	-110	C
	ATOM	601	CG1	VAL	F	95	-16.417	55.857	22.077	1.00	18..66		C
	ANISOU	601	CG1	VAL	F	95	2410	2469	2210	2	-191	-121	C
40	ATOM	605	CG2	VAL	F	95	-15.870	57.502	23.901	1.00	18..00		C
	ANISOU	605	CG2	VAL	F	95	2447	2025	2367	-9	-72	-62	C
	ATOM	609	C	VAL	F	95	-14.293	54.088	23.062	1.00	15..55		C
	ANISOU	609	C	VAL	F	95	2053	1869	1985	-156	-165	-66	C
	ATOM	610	O	VAL	F	95	-13.435	54.302	22.218	1.00	16..77		O
45	ANISOU	610	O	VAL	F	95	2378	1847	2146	-445	252	-348	O
	ATOM	612	N	ILE	F	96	-14.809	52.881	23.264	1.00	14..81		N
	ANISOU	612	N	ILE	F	96	1952	1828	1845	-73	227	-59	N
	ATOM	613	CA	ILE	F	96	-14.377	51.738	22.468	1.00	13..75		C
	ANISOU	613	CA	ILE	F	96	1847	1715	1661	-96	-56	55	C
50	ATOM	615	CB	ILE	F	96	-14.582	50.406	23.225	1.00	15..36		C
	ANISOU	615	CB	ILE	F	96	2036	1723	2075	-87	-43	60	C
	ATOM	617	CG1	ILE	F	96	-13.895	50.448	24.599	1.00	15..78		C
	ANISOU	617	CG1	ILE	F	96	1916	1970	2108	32	-19	229	C
	ATOM	620	CD1	ILE	F	96	-12.444	50.845	24.546	1.00	17..68		C
55	ANISOU	620	CD1	ILE	F	96	2286	2274	2157	-165	-93	0	C
	ATOM	624	CG2	ILE	F	96	-14.074	49.224	22.388	1.00	14..61		C
	ANISOU	624	CG2	ILE	F	96	1881	1746	1922	-48	7	-109	C
	ATOM	628	C	ILE	F	96	-15.133	51.713	21.146	1.00	13..88		C
	ANISOU	628	C	ILE	F	96	1748	1688	1837	58	-71	-69	C
60	ATOM	629	O	ILE	F	96	-16.361	51.779	21.116	1.00	14..74		O
	ANISOU	629	O	ILE	F	96	1844	1854	1900	9	77	148	O
	ATOM	631	N	LYS	F	97	-14.384	51.615	20.052	1.00	15..75		N
	ANISOU	631	N	LYS	F	97	1996	1969	2019	39	-6	-55	N
	ATOM	632	CA	LYS	F	97	-14.975	51.525	18.721	1.00	17..05		C
65	ANISOU	632	CA	LYS	F	97	2270	2133	2075	63	18	-46	C
	ATOM	634	CB	LYS	F	97	-14.407	52.625	17.820	1.00	22..27		C
	ANISOU	634	CB	LYS	F	97	3079	2686	2696	-63	-28	151	C
	ATOM	637	CG	LYS	F	97	-14.872	54.028	18.198	1.00	24..55		C
	ANISOU	637	CG	LYS	F	97	3224	3124	2979	31	17	-54	C
70	ATOM	640	CD	LYS	F	97	-16.359	54.235	17.898	1.00	27..18		C
	ANISOU	640	CD	LYS	F	97	3459	3456	3410	107	-17	39	C

	ATOM	643	CE	LYS	F	97	-16.651	55.611	17.308	1.00	28.29		C
	ANISOU	643	CE	LYS	F	97	3641	3385	3722	65	18	52	C
	ATOM	646	NZ	LYS	F	97	-17.668	55.520	16.220	1.00	30.77		N
	ANISOU	646	NZ	LYS	F	97	3987	3860	3843	-107	-62	-1	N
5	ATOM	650	C	LYS	F	97	-14.785	50.158	18.073	1.00	15.63		C
	ANISOU	650	C	LYS	F	97	1924	1975	2039	-74	-189	-162	C
	ATOM	651	O	LYS	F	97	-15.608	49.755	17.258	1.00	16.53		O
	ANISOU	651	O	LYS	F	97	1886	2344	2048	102	-110	-255	O
	ATOM	653	N	CYS	F	98	-13.719	49.452	18.447	1.00	14.49		N
10	ANISOU	653	N	CYS	F	98	1987	1772	1745	-55	-163	-110	N
	ATOM	654	CA	CYS	F	98	-13.404	48.148	17.881	1.00	14.80		C
	ANISOU	654	CA	CYS	F	98	2097	1790	1735	-105	-129	18	C
	ATOM	656	CB	CYS	F	98	-12.044	48.175	17.191	1.00	15.14		C
	ANISOU	656	CB	CYS	F	98	2099	1864	1789	-153	-44	-208	C
15	ATOM	659	SG	CYS	F	98	-11.823	49.453	15.946	1.00	18.60		S
	ANISOU	659	SG	CYS	F	98	2388	2251	2428	-324	-20	100	S
	ATOM	661	C	CYS	F	98	-13.377	47.053	18.937	1.00	14.64		C
	ANISOU	661	C	CYS	F	98	1961	1815	1786	75	-10	-1	C
	ATOM	662	O	CYS	F	98	-12.811	47.221	20.012	1.00	15.41		O
20	ANISOU	662	O	CYS	F	98	1894	2019	1940	-69	-316	-91	O
	ATOM	664	N	ASP	F	99	-13.964	45.912	18.604	1.00	13.84		N
	ANISOU	664	N	ASP	F	99	1812	1665	1780	-38	-3	83	N
	ATOM	665	CA	ASP	F	99	-13.924	44.754	19.487	1.00	14.62		C
	ANISOU	665	CA	ASP	F	99	1909	1845	1801	104	78	123	C
25	ATOM	667	CB	ASP	F	99	-14.752	43.601	18.924	1.00	16.18		C
	ANISOU	667	CB	ASP	F	99	1985	2031	2128	-134	-71	178	C
	ATOM	670	CG	ASP	F	99	-16.241	43.904	18.809	1.00	18.10		C
	ANISOU	670	CG	ASP	F	99	2294	2242	2341	96	-159	88	C
	ATOM	671	OD1	ASP	F	99	-16.714	45.016	19.147	1.00	19.14		O
30	ANISOU	671	OD1	ASP	F	99	2294	2629	2349	96	-88	19	O
	ATOM	672	OD2	ASP	F	99	-16.940	42.981	18.353	1.00	22.71		O
	ANISOU	672	OD2	ASP	F	99	2685	2573	3370	-268	-34	33	O
	ATOM	673	C	ASP	F	99	-12.493	44.250	19.624	1.00	14.33		C
	ANISOU	673	C	ASP	F	99	1921	1758	1763	96	0	16	C
35	ATOM	674	O	ASP	F	99	-11.685	44.360	18.704	1.00	14.84		O
	ANISOU	674	O	ASP	F	99	1722	1999	1916	47	-8	334	O
	ATOM	676	N	GLY	F	100	-12.199	43.645	20.760	1.00	14.54		N
	ANISOU	676	N	GLY	F	100	1679	2016	1828	84	51	298	N
	ATOM	677	CA	GLY	F	100	-10.937	42.952	20.933	1.00	15.13		C
40	ANISOU	677	CA	GLY	F	100	1885	1970	1894	0	-81	-69	C
	ATOM	680	C	GLY	F	100	-10.671	42.639	22.386	1.00	12.39		C
	ANISOU	680	C	GLY	F	100	1685	1606	1414	-70	12	6	C
	ATOM	681	O	GLY	F	100	-11.386	43.120	23.289	1.00	14.68		O
	ANISOU	681	O	GLY	F	100	1689	1972	1916	118	98	-14	O
45	ATOM	683	N	LEU	F	101	-9.650	41.820	22.618	1.00	13.67		N
	ANISOU	683	N	LEU	F	101	1637	1873	1683	5	67	-99	N
	ATOM	684	CA	LEU	F	101	-9.042	41.757	23.940	1.00	14.27		C
	ANISOU	684	CA	LEU	F	101	1788	1828	1803	82	28	20	C
	ATOM	686	CB	LEU	F	101	-8.216	40.492	24.125	1.00	14.74		C
50	ANISOU	686	CB	LEU	F	101	1709	1969	1922	275	9	66	C
	ATOM	689	CG	LEU	F	101	-9.027	39.196	24.128	1.00	15.85		C
	ANISOU	689	CG	LEU	F	101	2027	2016	1980	91	-36	188	C
	ATOM	691	CD1	LEU	F	101	-8.103	37.990	24.102	1.00	18.28		C
	ANISOU	691	CD1	LEU	F	101	2583	2219	2143	86	425	-106	C
55	ATOM	695	CD2	LEU	F	101	-9.940	39.126	25.332	1.00	15.70		C
	ANISOU	695	CD2	LEU	F	101	1981	1968	2014	43	-16	102	C
	ATOM	699	C	LEU	F	101	-8.157	42.984	24.075	1.00	13.65		C
	ANISOU	699	C	LEU	F	101	1707	1668	1810	163	-27	-2	C
	ATOM	700	O	LEU	F	101	-7.434	43.331	23.136	1.00	15.01		O
60	ANISOU	700	O	LEU	F	101	1809	2024	1870	-77	112	-11	O
	ATOM	702	N	TYR	F	102	-8.285	43.680	25.199	1.00	13.98		N
	ANISOU	702	N	TYR	F	102	1674	1806	1829	65	141	-26	N
	ATOM	703	CA	TYR	F	102	-7.477	44.854	25.493	1.00	13.82		C
	ANISOU	703	CA	TYR	F	102	1666	1783	1802	-42	-14	-114	C
65	ATOM	705	CB	TYR	F	102	-8.351	46.093	25.606	1.00	14.12		C
	ANISOU	705	CB	TYR	F	102	1784	1789	1789	-19	21	8	C
	ATOM	708	CG	TYR	F	102	-8.928	46.674	24.331	1.00	13.72		C
	ANISOU	708	CG	TYR	F	102	1686	1790	1737	93	69	23	C
	ATOM	709	CD1	TYR	F	102	-9.950	46.035	23.638	1.00	13.32		C
70	ANISOU	709	CD1	TYR	F	102	1720	1636	1704	-37	54	49	C
	ATOM	711	CEL	TYR	F	102	-10.501	46.596	22.478	1.00	14.16		C

	ANISOU	711	CE1	TYR	F	102	1746	1764	1867	6	-204	-70	C
	ATOM	713	CZ	TYR	F	102	-10.035	47.824	22.019	1.00	14.34		C
	ANISOU	713	CZ	TYR	F	102	1774	1847	1826	169	24	91	C
	ATOM	714	OH	TYR	F	102	-10.558	48.425	20.894	1.00	14.98		O
5	ANISOU	714	OH	TYR	F	102	1942	1850	1899	77	-23	-59	O
	ATOM	716	CE2	TYR	F	102	-9.040	48.479	22.708	1.00	14.53		C
	ANISOU	716	CE2	TYR	F	102	1815	1879	1824	-18	174	60	C
	ATOM	718	CD2	TYR	F	102	-8.482	47.900	23.846	1.00	14.28		C
	ANISOU	718	CD2	TYR	F	102	1721	1696	2009	-33	-22	66	C
10	ATOM	720	C	TYR	F	102	-6.790	44.700	26.845	1.00	14.44		C
	ANISOU	720	C	TYR	F	102	1796	1810	1879	39	12	-62	C
	ATOM	721	O	TYR	F	102	-7.348	44.110	27.776	1.00	15.36		O
	ANISOU	721	O	TYR	F	102	1894	2068	1872	-91	-168	-18	O
	ATOM	723	N	ILE	F	103	-5.589	45.254	26.960	1.00	14.20		N
15	ANISOU	723	N	ILE	F	103	1693	1908	1791	-185	-9	-14	N
	ATOM	724	CAA	ILE	F	103	-5.059	45.559	28.291	1.00	15.09		C
	ANISOU	724	CAA	ILE	F	103	1841	1971	1921	-143	74	-102	C
	ATOM	726	CB	AILE	F	103	-3.530	45.684	28.256	0.65	16.66		C
	ANISOU	726	CB	AILE	F	103	1812	2514	2001	-143	193	-9	C
20	ATOM	727	CB	BILE	F	103	-3.508	45.360	28.490	0.35	20.13		C
	ANISOU	727	CB	BILE	F	103	2308	2627	2714	-158	120	-46	C
	ATOM	730	CG1AILE	F	103		-2.894	44.334	27.998	0.65	16.80		C
	ANISOU	730	CG1AILE	F	103		2232	2201	1950	-128	134	-102	C
	ATOM	731	CG1BILE	F	103		-2.690	45.768	27.271	0.35	22.31		C
25	ANISOU	731	CG1BILE	F	103		2726	3013	2738	25	53	-59	C
	ATOM	736	CD1AILE	F	103		-1.391	44.385	27.825	0.65	16.49		C
	ANISOU	736	CD1AILE	F	103		2201	2119	1943	-76	-77	-66	C
	ATOM	737	CD1BILE	F	103		-1.413	44.979	27.058	0.35	22.10		C
	ANISOU	737	CD1BILE	F	103		2616	2909	2870	9	111	-20	C
30	ATOM	744	CG2AILE	F	103		-2.994	46.303	29.568	0.65	17.36		C
	ANISOU	744	CG2AILE	F	103		1852	2710	2031	-227	-11	-408	C
	ATOM	745	CG2BILE	F	103		-3.217	43.921	28.919	0.35	22.16		C
	ANISOU	745	CG2BILE	F	103		2610	2979	2830	-6	14	-20	C
	ATOM	752	C	ILE	F	103	-5.570	46.907	28.744	1.00	14.96		C
35	ANISOU	752	C	ILE	F	103	1976	1823	1884	-34	-85	-26	C
	ATOM	753	O	ILE	F	103	-5.661	47.845	27.956	1.00	16.30		O
	ANISOU	753	O	ILE	F	103	2584	1787	1822	-214	46	-57	O
	ATOM	755	N	ILE	F	104	-5.932	46.969	30.023	1.00	16.20		N
	ANISOU	755	N	ILE	F	104	2179	1947	2027	44	106	9	N
40	ATOM	756	CAA	ILE	F	104	-6.277	48.209	30.699	1.00	16.16		C
	ANISOU	756	CAA	ILE	F	104	2362	1853	1925	-94	-71	-94	C
	ATOM	758	CB	ILE	F	104	-7.738	48.245	31.198	1.00	16.78		C
	ANISOU	758	CB	ILE	F	104	2407	1962	2007	-57	-59	45	C
	ATOM	760	CG1	ILE	F	104	-8.705	48.016	30.025	1.00	17.49		C
45	ANISOU	760	CG1	ILE	F	104	2344	2100	2200	-43	-140	-84	C
	ATOM	763	CD1	ILE	F	104	-10.147	47.800	30.441	1.00	18.65		C
	ANISOU	763	CD1	ILE	F	104	2435	2157	2492	-84	-124	-209	C
	ATOM	767	CG22	ILE	F	104	-8.037	49.586	31.885	1.00	18.46		C
	ANISOU	767	CG22	ILE	F	104	2622	2135	2254	16	59	-10	C
50	ATOM	771	C	ILE	F	104	-5.314	48.280	31.874	1.00	16.48		C
	ANISOU	771	C	ILE	F	104	2422	1921	1918	-111	-232	-72	C
	ATOM	772	O	ILE	F	104	-5.273	47.374	32.704	1.00	18.15		O
	ANISOU	772	O	ILE	F	104	2912	2072	1911	-226	-111	87	O
	ATOM	774	N	TYR	F	105	-4.541	49.357	31.921	1.00	16.16		N
55	ANISOU	774	N	TYR	F	105	2296	1835	2009	-138	-141	-26	N
	ATOM	775	CAA	TYR	F	105	-3.461	49.531	32.876	1.00	15.69		C
	ANISOU	775	CAA	TYR	F	105	2187	1873	1900	14	-73	-34	C
	ATOM	111	CB	TYR	F	105	-2.135	49.460	32.147	1.00	17.36		C
	ANISOU	111	CB	TYR	F	105	2312	2170	2113	78	-30	-152	C
60	ATOM	780	CGG	TYR	F	105	-0.922	49.945	32.892	1.00	17.41		C
	ANISOU	780	CGG	TYR	F	105	2344	2344	1926	146	137	-232	C
	ATOM	781	CD1	TYR	F	105	-0.224	49.104	33.741	1.00	17.51		C
	ANISOU	781	CD1	TYR	F	105	2308	2323	2021	131	378	-223	C
	ATOM	783	CE1	TYR	F	105	0.912	49.538	34.412	1.00	16.94		C
65	ANISOU	783	CE1	TYR	F	105	2033	2492	1908	131	369	-62	C
	ATOM	785	CZ	TYR	F	105	1.376	50.814	34.203	1.00	16.07		C
	ANISOU	785	CZ	TYR	F	105	2123	2185	1796	136	251	-215	C
	ATOM	786	OH	TYR	F	105	2.507	51.259	34.837	1.00	19.21		O
	ANISOU	786	OH	TYR	F	105	2224	2726	2349	145	160	45	O
70	ATOM	788	CE2	TYR	F	105	0.692	51.675	33.355	1.00	17.52		C
	ANISOU	788	CE2	TYR	F	105	2391	2142	2124	97	-46	-109	C

	ATOM	790	CD2	TYR	F	105	-0.444	51.235	32.707	1.00	17.94		C
	ANISOU	790	CD2	TYR	F	105	2291	2275	2250	86	192	-280	C
	ATOM	792	C	TYR	F	105	-3.627	50.883	33.541	1.00	15.73		C
	ANISOU	792	C	TYR	F	105	2114	1863	1998	-21	137	-35	C
5	ATOM	793	O	TYR	F	105	-3.825	51.891	32.863	1.00	15.44		O
	ANISOU	793	O	TYR	F	105	2219	1843	1803	103	-1	-10	O
	ATOM	795	N	LEU	F	106	-3.557	50.893	34.869	1.00	14.76		N
	ANISOU	795	N	LEU	F	106	2184	1700	1724	-42	-40	-63	N
10	ATOM	796	CA	LEU	F	106	-3.658	52.130	35.637	1.00	14.47		C
	ANISOU	796	CA	LEU	F	106	2007	1763	1727	-21	30	-65	C
	ATOM	798	CB	LEU	F	106	-4.920	52.141	36.507	1.00	15.78		C
	ANISOU	798	CB	LEU	F	106	2106	1947	1942	-79	112	34	C
	ATOM	801	CG	LEU	F	106	-5.138	53.402	37.359	1.00	16.76		C
	ANISOU	801	CG	LEU	F	106	2018	2394	1956	52	81	-109	C
15	ATOM	803	CD1	LEU	F	106	-5.375	54.626	36.499	1.00	18.79		C
	ANISOU	803	CD1	LEU	F	106	2287	2381	2470	129	149	-148	C
	ATOM	807	CD2	LEU	F	106	-6.298	53.214	38.317	1.00	18.21		C
	ANISOU	807	CD2	LEU	F	106	2094	2737	2087	115	149	144	C
20	ATOM	811	C	LEU	F	106	-2.442	52.239	36.529	1.00	13.95		C
	ANISOU	811	C	LEU	F	106	1807	1826	1665	11	88	-138	C
	ATOM	812	O	LEU	F	106	-2.086	51.284	37.214	1.00	14.71		O
	ANISOU	812	O	LEU	F	106	1858	1801	1929	176	1	-63	O
	ATOM	814	N	LYS	F	107	-1.829	53.417	36.518	1.00	15.12		N
	ANISOU	814	N	LYS	F	107	1987	1830	1927	67	98	-41	N
25	ATOM	815	CA	LYS	F	107	-0.709	53.736	37.393	1.00	16.76		C
	ANISOU	815	CA	LYS	F	107	2285	1881	2201	129	-144	-206	C
	ATOM	817	CB	LYS	F	107	0.600	53.741	36.583	1.00	22.43		C
	ANISOU	817	CB	LYS	F	107	2744	3101	2675	120	29	-400	C
30	ATOM	820	CG	LYS	F	107	1.791	54.437	37.245	1.00	27.94		C
	ANISOU	820	CG	LYS	F	107	3176	3806	3633	45	-32	-218	C
	ATOM	823	CD	LYS	F	107	3.025	54.394	36.361	1.00	29.70		C
	ANISOU	823	CD	LYS	F	107	3408	4042	3831	-60	105	-44	C
	ATOM	826	CE	LYS	F	107	4.190	55.140	36.995	1.00	32.52		C
	ANISOU	826	CE	LYS	F	107	3751	4374	4228	-162	66	-14	C
35	ATOM	829	NZ	LYS	F	107	5.238	55.507	35.997	1.00	35.68		N
	ANISOU	829	NZ	LYS	F	107	4136	4786	4633	-114	286	84	N
	ATOM	833	C	LYS	F	107	-0.951	55.106	38.002	1.00	15.25		C
	ANISOU	833	C	LYS	F	107	1937	1992	1863	25	-49	-84	C
40	ATOM	834	O	LYS	F	107	-1.480	56.001	37.341	1.00	16.52		O
	ANISOU	834	O	LYS	F	107	2277	2046	1953	93	-171	-186	O
	ATOM	836	N	GLY	F	108	-0.551	55.275	39.254	1.00	15.84		N
	ANISOU	836	N	GLY	F	108	2138	1836	2044	205	26	-188	N
	ATOM	837	CA	GLY	F	108	-0.525	56.604	39.835	1.00	17.05		C
	ANISOU	837	CA	GLY	F	108	2342	1989	2145	176	-225	-150	C
45	ATOM	840	C	GLY	F	108	-0.120	56.573	41.279	1.00	15.99		C
	ANISOU	840	C	GLY	F	108	2090	1904	2080	96	-283	-48	C
	ATOM	841	O	GLY	F	108	-0.146	55.517	41.905	1.00	16.11		O
	ANISOU	841	O	GLY	F	108	2223	1925	1971	79	18	-64	O
50	ATOM	843	N	SER	F	109	0.285	57.740	41.774	1.00	16.46		N
	ANISOU	843	N	SER	F	109	2193	1852	2208	100	-67	-76	N
	ATOM	844	CA	SER	F	109	0.602	57.933	43.169	1.00	16.17		C
	ANISOU	844	CA	SER	F	109	2141	1917	2082	208	113	-123	C
	ATOM	846	CB	SER	F	109	1.926	58.678	43.335	1.00	19.13		C
	ANISOU	846	CB	SER	F	109	2283	2451	2532	14	76	-89	C
55	ATOM	849	OG	SER	F	109	3.013	57.861	42.947	1.00	24.47		O
	ANISOU	849	OG	SER	F	109	2703	3217	3375	242	137	114	O
	ATOM	851	C	SER	F	109	-0.559	58.746	43.718	1.00	16.11		C
	ANISOU	851	C	SER	F	109	2078	1619	2422	154	208	-164	C
60	ATOM	852	O	SER	F	109	-0.820	59.859	43.274	1.00	17.46		O
	ANISOU	852	O	SER	F	109	2260	1772	2603	176	269	68	O
	ATOM	854	N	PHE	F	110	-1.306	58.128	44.615	1.00	19.35		N
	ANISOU	854	N	PHE	F	110	2598	2128	2624	294	602	61	N
	ATOM	855	CA	PHE	F	110	-2.567	58.672	45.091	1.00	20.30		C
	ANISOU	855	CA	PHE	F	110	2498	2378	2836	322	238	1	C
65	ATOM	857	CB	PHE	F	110	-3.706	57.649	44.930	1.00	21.11		C
	ANISOU	857	CB	PHE	F	110	2688	2450	2880	-36	193	19	C
	ATOM	860	CG	PHE	F	110	-4.078	57.364	43.495	1.00	23.82		C
	ANISOU	860	CG	PHE	F	110	2912	2961	3176	-155	161	313	C
	ATOM	861	CD1	PHE	F	110	-3.275	56.561	42.708	1.00	21.47		C
70	ANISOU	861	CD1	PHE	F	110	2723	2365	3066	-196	0	42	C
	ATOM	863	CE1	PHE	F	110	-3.599	56.310	41.385	1.00	23.75		C

	ANISOU	863	CE1	PHE	F	110	2941	2822	3259	-79	-17	0	C
	ATOM	865	CZ	PHE	F	110	-4.759	56.839	40.843	1.00	23.58		C
	ANISOU	865	CZ	PHE	F	110	3021	2755	3181	-45	-27	6	C
	ATOM	867	CE2	PHE	F	110	-5.579	57.625	41.624	1.00	23.62		C
5	ANISOU	867	CE2	PHE	F	110	2961	2895	3119	-42	85	52	C
	ATOM	869	CD2	PHE	F	110	-5.243	57.884	42.942	1.00	21.82		C
	ANISOU	869	CD2	PHE	F	110	2720	2667	2901	-195	-59	9	C
	ATOM	871	C	PHE	F	110	-2.337	58.995	46.546	1.00	20.38		C
	ANISOU	871	C	PHE	F	110	2811	2258	2673	185	215	-269	C
10	ATOM	872	O	PHE	F	110	-1.917	58.137	47.310	1.00	24.51		O
	ANISOU	872	O	PHE	F	110	2919	3076	3316	673	369	-90	O
	ATOM	874	N	PHE	F	111	-2.606	60.238	46.937	1.00	21.82		N
	ANISOU	874	N	PHE	F	111	2857	2287	3145	175	208	-65	N
	ATOM	875	CA	PHE	F	111	-2.237	60.718	48.272	1.00	20.62		C
15	ANISOU	875	CA	PHE	F	111	2578	2571	2682	10	100	-25	C
	ATOM	877	CB	PHE	F	111	-1.686	62.150	48.182	1.00	20.86		C
	ANISOU	877	CB	PHE	F	111	2580	2522	2821	13	96	109	C
	ATOM	880	CG	PHE	F	111	-0.361	62.210	47.512	1.00	18.38		C
	ANISOU	880	CG	PHE	F	111	2274	1883	2824	-71	-12	-63	C
20	ATOM	881	CD1	PHE	F	111	-0.271	62.102	46.131	1.00	20.61		C
	ANISOU	881	CD1	PHE	F	111	2345	2618	2866	-140	21	188	C
	ATOM	883	CE1	PHE	F	111	0.954	62.104	45.500	1.00	21.81		C
	ANISOU	883	CE1	PHE	F	111	2716	2883	2687	-94	94	188	C
	ATOM	885	CZ	PHE	F	111	2.112	62.194	46.249	1.00	20.99		C
25	ANISOU	885	CZ	PHE	F	111	2527	2637	2809	-166	2	142	C
	ATOM	887	CE2	PHE	F	111	2.036	62.280	47.629	1.00	20.15		C
	ANISOU	887	CE2	PHE	F	111	2513	2501	2639	89	73	267	C
	ATOM	889	CD2	PHE	F	111	0.805	62.278	48.256	1.00	18.82		C
	ANISOU	889	CD2	PHE	F	111	2432	2176	2542	-161	-141	56	C
30	ATOM	891	C	PHE	F	111	-3.350	60.583	49.318	1.00	21.22		C
	ANISOU	891	C	PHE	F	111	2654	2449	2960	-3	228	19	C
	ATOM	892	O	PHE	F	111	-3.267	61.148	50.405	1.00	19.63		O
	ANISOU	892	O	PHE	F	111	2495	2107	2854	170	331	129	O
	ATOM	894	N	GLN	F	112	-4.389	59.829	48.972	1.00	21.77		N
35	ANISOU	894	N	GLN	F	112	2871	2548	2850	21	190	31	N
	ATOM	895	CA	GLN	F	112	-5.268	59.221	49.968	1.00	23.59		C
	ANISOU	895	CA	GLN	F	112	2986	2807	3171	-118	157	18	C
	ATOM	897	CB	GLN	F	112	-6.672	59.816	49.903	1.00	24.19		C
	ANISOU	897	CB	GLN	F	112	2973	3039	3177	-96	22	29	C
40	ATOM	900	CG	GLN	F	112	-6.737	61.346	49.907	1.00	23.90		C
	ANISOU	900	CG	GLN	F	112	2972	2968	3140	27	29	83	C
	ATOM	903	CD	GLN	F	112	-8.088	61.879	49.431	1.00	24.82		C
	ANISOU	903	CD	GLN	F	112	3013	3133	3284	22	4	4	C
	ATOM	904	OE1	GLN	F	112	-8.906	61.130	48.888	1.00	25.85		O
45	ANISOU	904	OE1	GLN	F	112	2917	3242	3660	224	76	41	O
	ATOM	905	NE2	GLN	F	112	-8.321	63.180	49.625	1.00	22.82		N
	ANISOU	905	NE2	GLN	F	112	2520	2974	3176	126	198	27	N
	ATOM	908	C	GLN	F	112	-5.323	57.731	49.638	1.00	24.59		C
	ANISOU	908	C	GLN	F	112	3230	3000	3110	-180	-30	-143	C
50	ATOM	909	O	GLN	F	112	-5.178	57.359	48.478	1.00	25.87		O
	ANISOU	909	O	GLN	F	112	3487	2687	3655	-427	486	-360	O
	ATOM	911	N	GLU	F	113	-5.491	56.887	50.654	1.00	25.73		N
	ANISOU	911	N	GLU	F	113	3346	2993	3437	-262	64	-136	N
	ATOM	912	CA	GLU	F	113	-5.797	55.481	50.417	1.00	24.69		C
55	ANISOU	912	CA	GLU	F	113	3077	3072	3231	-44	69	-61	C
	ATOM	914	CB	GLU	F	113	-5.799	54.688	51.719	1.00	27.35		C
	ANISOU	914	CB	GLU	F	113	3470	3414	3506	61	61	39	C
	ATOM	917	CG	GLU	F	113	-5.972	53.190	51.517	1.00	30.11		C
	ANISOU	917	CG	GLU	F	113	3849	3638	3951	-60	60	28	C
60	ATOM	920	CD	GLU	F	113	-4.943	52.370	52.277	1.00	34.01		C
	ANISOU	920	CD	GLU	F	113	4259	4325	4338	70	-46	92	C
	ATOM	921	OE1	GLU	F	113	-4.770	52.599	53.493	1.00	36.98		O
	ANISOU	921	OE1	GLU	F	113	4650	4858	4540	40	55	28	O
	ATOM	922	OE2	GLU	F	113	-4.306	51.494	51.651	1.00	38.16		O
65	ANISOU	922	OE2	GLU	F	113	4708	4736	5055	92	57	24	O
	ATOM	923	C	GLU	F	113	-7.163	55.469	49.762	1.00	22.34		C
	ANISOU	923	C	GLU	F	113	2979	2933	2576	14	55	1	C
	ATOM	924	O	GLU	F	113	-8.122	56.003	50.317	1.00	23.49		O
	ANISOU	924	O	GLU	F	113	2809	2973	3141	28	-170	-196	O
70	ATOM	926	N	VAL	F	114	-7.239	54.891	48.567	1.00	21.67		N
	ANISOU	926	N	VAL	F	114	2753	2686	2792	-2	-45	-73	N

	ATOM	927	CA	VAL	F	114	-8.395	55.079	47.695	1.00	22.38		C
	ANISOU	927	CA	VAL	F	114	2752	2747	3004	-28	10	0	C
	ATOM	929	CB	VAL	F	114	-8.045	55.883	46.403	1.00	22.75		C
	ANISOU	929	CB	VAL	F	114	2860	2826	2956	-53	-58	-29	C
5	ATOM	931	CG1	VAL	F	114	-7.823	57.350	46.731	1.00	25.86		C
	ANISOU	931	CG1	VAL	F	114	3385	3036	3401	18	43	55	C
	ATOM	935	CG2	VAL	F	114	-6.832	55.295	45.684	1.00	23.38		C
	ANISOU	935	CG2	VAL	F	114	2938	2944	2998	-53	61	107	C
	ATOM	939	C	VAL	F	114	-9.012	53.758	47.298	1.00	21.58		C
10	ANISOU	939	C	VAL	F	114	2688	2588	2922	5	-1	-118	C
	ATOM	940	O	VAL	F	114	-8.313	52.746	47.153	1.00	22.59		O
	ANISOU	940	O	VAL	F	114	2493	2867	3219	33	-66	-358	O
	ATOM	942	N	LYS	F	115	-10.332	53.782	47.142	1.00	21.32		N
	ANISOU	942	N	LYS	F	115	2650	2594	2855	15	-198	76	N
15	ATOM	943	CA	LYS	F	115	-11.089	52.668	46.592	1.00	20.88		C
	ANISOU	943	CA	LYS	F	115	2716	2659	2558	-13	-175	32	C
	ATOM	945	CB	LYS	F	115	-12.249	52.295	47.517	1.00	23.20		C
	ANISOU	945	CB	LYS	F	115	2874	2982	2959	-41	-54	-21	C
	ATOM	948	CG	LYS	F	115	-11.598	51.652	48.816	0.00	30.00		C
20	ANISOU	948	CG	LYS	F	115	3799	3799	3799	0	0	0	C
	ATOM	951	CD	LYS	F	115	-11.630	50.122	48.747	0.00	30.00		C
	ANISOU	951	CD	LYS	F	115	3799	3799	3799	0	0	0	C
	ATOM	954	CE	LYS	F	115	-11.035	49.514	50.021	0.00	30.00		C
	ANISOU	954	CE	LYS	F	115	3799	3799	3799	0	0	0	C
25	ATOM	957	NZ	LYS	F	115	-11.067	48.012	49.953	0.00	30.00		N
	ANISOU	957	NZ	LYS	F	115	3799	3799	3799	0	0	0	N
	ATOM	961	C	LYS	F	115	-11.607	53.108	45.229	1.00	20.11		C
	ANISOU	961	C	LYS	F	115	2481	2559	2598	-94	-61	189	C
	ATOM	962	O	LYS	F	115	-12.642	53.778	45.141	1.00	19.68		O
30	ANISOU	962	O	LYS	F	115	2584	2925	1968	23	-78	367	O
	ATOM	964	N	ILE	F	116	-10.860	52.753	44.186	1.00	18.52		N
	ANISOU	964	N	ILE	F	116	2327	2320	2389	-170	-361	-63	N
	ATOM	965	CA	ILE	F	116	-11.212	53.095	42.810	1.00	18.46		C
	ANISOU	965	CA	ILE	F	116	2291	2407	2312	-29	-18	-8	C
35	ATOM	967	CB	ILE	F	116	-9.973	53.528	41.997	1.00	20.49		C
	ANISOU	967	CB	ILE	F	116	2485	2595	2703	-34	84	136	C
	ATOM	969	CG1	ILE	F	116	-9.371	54.798	42.603	1.00	22.40		C
	ANISOU	969	CG1	ILE	F	116	2575	2872	3062	-87	-3	68	C
	ATOM	972	CD1	ILE	F	116	-8.009	55.162	42.049	1.00	23.39		C
40	ANISOU	972	CD1	ILE	F	116	2615	3043	3226	-114	-95	162	C
	ATOM	976	CG2	ILE	F	116	-10.335	53.769	40.537	1.00	21.13		C
	ANISOU	976	CG2	ILE	F	116	2523	2673	2829	-99	-41	78	C
	ATOM	980	C	ILE	F	116	-11.834	51.879	42.131	1.00	17.28		C
	ANISOU	980	C	ILE	F	116	2137	2099	2326	6	-129	-37	C
45	ATOM	981	O	ILE	F	116	-11.321	50.767	42.257	1.00	19.11		O
	ANISOU	981	O	ILE	F	116	2409	2049	2802	-88	-241	-74	O
	ATOM	983	N	ASP	F	117	-12.923	52.108	41.397	1.00	15.31		N
	ANISOU	983	N	ASP	F	117	1992	1784	2040	29	-145	75	N
	ATOM	984	CA	ASP	F	117	-13.569	51.077	40.589	1.00	15.89		C
50	ANISOU	984	CA	ASP	F	117	2136	1999	1902	-20	-90	13	C
	ATOM	986	CB	ASP	F	117	-15.079	51.070	40.835	1.00	17.20		C
	ANISOU	986	CB	ASP	F	117	2144	2302	2086	-79	-46	-35	C
	ATOM	989	CG	ASP	F	117	-15.482	50.312	42.095	1.00	21.32		C
	ANISOU	989	CG	ASP	F	117	2466	3081	2553	40	152	256	C
55	ATOM	990	OD1	ASP	F	117	-14.647	49.603	42.687	1.00	23.05		O
	ANISOU	990	OD1	ASP	F	117	2763	3069	2924	402	437	273	O
	ATOM	991	OD2	ASP	F	117	-16.663	50.425	42.498	1.00	27.77		O
	ANISOU	991	OD2	ASP	F	117	3006	4046	3499	180	230	362	O
	ATOM	992	C	ASP	F	117	-13.319	51.339	39.109	1.00	14.80		C
60	ANISOU	992	C	ASP	F	117	1929	1753	1939	14	-135	31	C
	ATOM	993	O	ASP	F	117	-13.548	52.452	38.622	1.00	15.53		O
	ANISOU	993	O	ASP	F	117	2138	1675	2087	101	-165	-131	O
	ATOM	995	N	LEU	F	118	-12.862	50.303	38.407	1.00	15.66		N
	ANISOU	995	N	LEU	F	118	2097	1943	1909	-5	-126	-167	N
65	ATOM	996	CA	LEU	F	118	-12.700	50.326	36.956	1.00	15.55		C
	ANISOU	996	CA	LEU	F	118	1987	2109	1811	-113	-106	-127	C
	ATOM	998	CB	LEU	F	118	-11.482	49.498	36.529	1.00	16.89		C
	ANISOU	998	CB	LEU	F	118	2118	2084	2215	-111	-218	-72	C
	ATOM	1001	CG	LEU	F	118	-11.319	49.235	35.026	1.00	19.16		C
70	ANISOU	1001	CG	LEU	F	118	2518	2323	2435	92	-52	-212	C
	ATOM	1003	CD1	LEU	F	118	-11.073	50.519	34.280	1.00	19.19		C

	ANISOU	1003	CD1	LEU	F	118	2715	2304	2270	158	-99	-252	C
	ATOM	1007	CD2	LEU	F	118	-10.201	48.240	34.755	1.00	19.16		C
	ANISOU	1007	CD2	LEU	F	118	2220	2707	2353	211	-10	-60	C
	ATOM	1011	C	LEU	F	118	-13.951	49.757	36.283	1.00	15.63		C
5	ANISOU	1011	C	LEU	F	118	1968	1960	2011	-120	-49	-113	C
	ATOM	1012	O	LEU	F	118	-14.297	48.588	36.479	1.00	16.62		O
	ANISOU	1012	O	LEU	F	118	2220	1845	2246	-232	-181	232	O
	ATOM	1014	N	HIS	F	119	-14.616	50.607	35.508	1.00	15.26		N
	ANISOU	1014	N	HIS	F	119	2024	1826	1947	-160	-52	-164	N
10	ATOM	1015	CA	HIS	F	119	-15.784	50.241	34.718	1.00	16.07		C
	ANISOU	1015	CA	HIS	F	119	2081	1929	2095	-81	-61	-156	C
	ATOM	1017	CB	HIS	F	119	-16.842	51.344	34.790	1.00	16.77		C
	ANISOU	1017	CB	HIS	F	119	2040	2250	2080	-77	3	0	C
	ATOM	1020	CG	HIS	F	119	-17.264	51.694	36.183	1.00	16.91		C
15	ANISOU	1020	CG	HIS	F	119	2273	2108	2043	-105	3	28	C
	ATOM	1021	ND1	HIS	F	119	-18.506	51.376	36.686	1.00	21.55		N
	ANISOU	1021	ND1	HIS	F	119	2668	2928	2592	102	-23	2	N
	ATOM	1023	CE1	HIS	F	119	-18.603	51.827	37.926	1.00	21.15		C
	ANISOU	1023	CE1	HIS	F	119	2528	3078	2429	-31	276	-46	C
20	ATOM	1025	NE2	HIS	F	119	-17.471	52.429	38.242	1.00	20.97		N
	ANISOU	1025	NE2	HIS	F	119	2593	3000	2372	209	138	-123	N
	ATOM	1027	CD2	HIS	F	119	-16.614	52.356	37.170	1.00	18.10		C
	ANISOU	1027	CD2	HIS	F	119	2158	2478	2242	3	13	-108	C
	ATOM	1029	C	HIS	F	119	-15.335	50.070	33.276	1.00	17.52		C
25	ANISOU	1029	C	HIS	F	119	2346	2075	2236	-184	86	-131	C
	ATOM	1030	O	HIS	F	119	-14.670	50.942	32.724	1.00	18.05		O
	ANISOU	1030	O	HIS	F	119	2689	2148	2020	-327	-50	-196	O
	ATOM	1032	N	PHE	F	120	-15.694	48.943	32.670	1.00	17.51		N
	ANISOU	1032	N	PHE	F	120	2367	2155	2129	-341	-152	-127	N
30	ATOM	1033	CA	PHE	F	120	-15.238	48.637	31.315	1.00	19.20		C
	ANISOU	1033	CA	PHE	F	120	2464	2367	2462	-184	23	-217	C
	ATOM	1035	CB	PHE	F	120	-14.000	47.720	31.354	1.00	21.14		C
	ANISOU	1035	CB	PHE	F	120	2663	2786	2582	50	1	-352	C
	ATOM	1038	CG	PHE	F	120	-14.225	46.397	32.044	1.00	21.25		C
35	ANISOU	1038	CG	PHE	F	120	2765	2764	2543	251	-76	-256	C
	ATOM	1039	CD1	PHE	F	120	-14.313	46.315	33.431	1.00	25.44		C
	ANISOU	1039	CD1	PHE	F	120	3731	2975	2958	127	54	-59	C
	ATOM	1041	CE1	PHE	F	120	-14.516	45.093	34.067	1.00	26.15		C
	ANISOU	1041	CE1	PHE	F	120	3690	3282	2963	138	-36	-53	C
40	ATOM	1043	CZ	PHE	F	120	-14.620	43.935	33.321	1.00	24.99		C
	ANISOU	1043	CZ	PHE	F	120	3397	3010	3088	57	-14	49	C
	ATOM	1045	CE2	PHE	F	120	-14.517	43.999	31.940	1.00	24.52		C
	ANISOU	1045	CE2	PHE	F	120	3259	3027	3028	185	-70	-138	C
	ATOM	1047	CD2	PHE	F	120	-14.313	45.222	31.310	1.00	21.18		C
45	ANISOU	1047	CD2	PHE	F	120	2475	2657	2912	-108	137	-348	C
	ATOM	1049	C	PHE	F	120	-16.336	48.075	30.408	1.00	18.39		C
	ANISOU	1049	C	PHE	F	120	2541	1987	2459	-113	66	-161	C
	ATOM	1050	O	PHE	F	120	-16.254	48.192	29.187	1.00	19.63		O
	ANISOU	1050	O	PHE	F	120	3020	2039	2400	-209	-51	-333	O
50	ATOM	1052	N	ARG	F	121	-17.368	47.483	30.998	1.00	18.34		N
	ANISOU	1052	N	ARG	F	121	2116	2292	2559	-143	32	-97	N
	ATOM	1053	CA	ARG	F	121	-18.519	47.009	30.228	1.00	17.91		C
	ANISOU	1053	CA	ARG	F	121	2367	2081	2354	-64	-153	-106	C
	ATOM	1055	CB	ARG	F	121	-18.202	45.699	29.480	1.00	19.34		C
55	ANISOU	1055	CB	ARG	F	121	2489	2421	2438	-145	-171	-47	C
	ATOM	1058	CG	ARG	F	121	-17.665	44.578	30.347	1.00	19.62		C
	ANISOU	1058	CG	ARG	F	121	2477	2414	2561	-1	-91	-101	C
	ATOM	1061	CD	ARG	F	121	-17.146	43.411	29.508	1.00	18.19		C
	ANISOU	1061	CD	ARG	F	121	2371	2093	2445	-53	-277	9	C
60	ATOM	1064	NE	ARG	F	121	-18.241	42.661	28.903	1.00	16.81		N
	ANISOU	1064	NE	ARG	F	121	2278	1934	2172	42	-388	208	N
	ATOM	1066	CZ	ARG	F	121	-18.125	41.443	28.380	1.00	16.78		C
	ANISOU	1066	CZ	ARG	F	121	2128	2200	2046	73	-115	55	C
	ATOM	1067	NH1	ARG	F	121	-16.955	40.825	28.312	1.00	17.38		N
65	ANISOU	1067	NH1	ARG	F	121	2363	2172	2065	200	-84	4	N
	ATOM	1070	NH2	ARG	F	121	-19.203	40.857	27.893	1.00	16.24		N
	ANISOU	1070	NH2	ARG	F	121	2206	2001	1964	-66	-256	132	N
	ATOM	1073	C	ARG	F	121	-19.714	46.860	31.166	1.00	19.17		C
	ANISOU	1073	C	ARG	F	121	2496	2394	2393	-53	-40	-94	C
70	ATOM	1074	O	ARG	F	121	-19.580	46.369	32.293	1.00	21.56		O
	ANISOU	1074	O	ARG	F	121	2659	2966	2566	-121	45	30	O

	ATOM	1076	N	GLU	F	122	-20.881	47.297	30.697	1.00	20.01		N
	ANISOU	1076	N	GLU	F	122	2556	2785	2261	167	0	-246	N
	ATOM	1077	CA	GLU	F	122	-22.066	47.418	31.558	1.00	22.57		C
	ANISOU	1077	CA	GLU	F	122	2795	3001	2777	47	194	-95	C
5	ATOM	1079	CB	GLU	F	122	-23.162	48.219	30.848	1.00	28.28		C
	ANISOU	1079	CB	GLU	F	122	3478	3763	3504	157	-3	53	C
	ATOM	1082	CG	GLU	F	122	-22.812	49.678	30.634	1.00	31.86		C
	ANISOU	1082	CG	GLU	F	122	4042	4060	4003	4	30	71	C
	ATOM	1085	CD	GLU	F	122	-23.787	50.504	29.946	0.00	30.00		C
10	ANISOU	1085	CD	GLU	F	122	3799	3799	3799	0	0	0	C
	ATOM	1086	OE1	GLU	F	122	-23.672	51.731	29.866	0.00	30.00		O
	ANISOU	1086	OE1	GLU	F	122	3799	3799	3799	0	0	0	O
	ATOM	1087	OE2	GLU	F	122	-24.764	49.913	29.473	0.00	30.00		O
	ANISOU	1087	OE2	GLU	F	122	3799	3799	3799	0	0	0	O
15	ATOM	1088	C	GLU	F	122	-22.639	46.086	32.040	1.00	21.47		C
	ANISOU	1088	C	GLU	F	122	2819	2759	2579	28	158	-180	C
	ATOM	1089	O	GLU	F	122	-23.363	46.048	33.038	1.00	23.19		O
	ANISOU	1089	O	GLU	F	122	2826	3107	2877	70	392	-151	O
	ATOM	1091	N	ASP	F	123	-22.324	45.004	31.328	1.00	20.73		N
20	ANISOU	1091	N	ASP	F	123	2699	2711	2466	69	123	-210	N
	ATOM	1092	CA	ASP	F	123	-22.806	43.669	31.684	1.00	21.72		C
	ANISOU	1092	CA	ASP	F	123	2711	2895	2645	-83	-30	-89	C
	ATOM	1094	CB	ASP	F	123	-23.075	42.851	30.415	1.00	19.64		C
	ANISOU	1094	CB	ASP	F	123	2516	2535	2411	-111	-38	-124	C
25	ATOM	1097	CG	ASP	F	123	-21.823	42.590	29.593	1.00	19.69		C
	ANISOU	1097	CG	ASP	F	123	2423	2508	2550	-178	-189	-128	C
	ATOM	1098	OD1	ASP	F	123	-20.828	43.344	29.722	1.00	19.73		O
	ANISOU	1098	OD1	ASP	F	123	2087	2711	2698	-161	-271	-264	O
	ATOM	1099	OD2	ASP	F	123	-21.850	41.626	28.803	1.00	20.37		O
30	ANISOU	1099	OD2	ASP	F	123	2411	2743	2586	-31	-196	-280	O
	ATOM	1100	C	ASP	F	123	-21.894	42.883	32.643	1.00	21.81		C
	ANISOU	1100	C	ASP	F	123	2791	2886	2608	-123	-108	-87	C
	ATOM	1101	O	ASP	F	123	-22.178	41.733	32.961	1.00	23.76		O
	ANISOU	1101	O	ASP	F	123	2868	3169	2991	-93	-14	40	O
35	ATOM	1103	N	HIS	F	124	-20.807	43.501	33.101	1.00	21.27		N
	ANISOU	1103	N	HIS	F	124	2558	2862	2660	-224	74	54	N
	ATOM	1104	CA	HIS	F	124	-19.962	42.915	34.148	1.00	22.87		C
	ANISOU	1104	CA	HIS	F	124	3027	2956	2705	-100	-122	-28	C
	ATOM	1106	CB	HIS	F	124	-18.590	42.508	33.595	1.00	23.88		C
40	ANISOU	1106	CB	HIS	F	124	3077	3087	2909	-141	-93	23	C
	ATOM	1109	CG	HIS	F	124	-18.605	41.243	32.790	1.00	25.03		C
	ANISOU	1109	CG	HIS	F	124	3328	3149	3031	65	-22	27	C
	ATOM	1110	ND1	HIS	F	124	-17.926	40.106	33.174	1.00	27.36		N
	ANISOU	1110	ND1	HIS	F	124	3480	3510	3404	165	-131	-266	N
45	ATOM	1112	CE1	HIS	F	124	-18.114	39.155	32.276	1.00	26.40		C
	ANISOU	1112	CE1	HIS	F	124	3096	3487	3447	128	-72	-214	C
	ATOM	1114	NE2	HIS	F	124	-18.889	39.635	31.320	1.00	25.12		N
	ANISOU	1114	NE2	HIS	F	124	3345	3196	3001	52	18	-55	N
	ATOM	1116	CD2	HIS	F	124	-19.210	40.938	31.619	1.00	26.08		C
50	ANISOU	1116	CD2	HIS	F	124	3473	3272	3162	160	-104	-68	C
	ATOM	1118	C	HIS	F	124	-19.787	43.924	35.286	1.00	24.15		C
	ANISOU	1118	C	HIS	F	124	3325	3049	2801	-82	-142	-26	C
	ATOM	1119	O	HIS	F	124	-19.883	45.134	35.077	1.00	24.44		O
	ANISOU	1119	O	HIS	F	124	3541	3043	2701	18	-195	-219	O
55	ATOM	1121	N	ASN	F	125	-19.532	43.423	36.490	1.00	22.84		N
	ANISOU	1121	N	ASN	F	125	3015	3057	2606	-458	-90	78	N
	ATOM	1122	CA	ASN	F	125	-19.267	44.307	37.630	1.00	23.22		C
	ANISOU	1122	CA	ASN	F	125	3101	2938	2783	-129	-63	-70	C
	ATOM	1124	CB	ASN	F	125	-19.168	43.511	38.932	1.00	25.12		C
60	ANISOU	1124	CB	ASN	F	125	3275	3155	3111	-151	-127	12	C
	ATOM	1127	CG	ASN	F	125	-20.496	42.955	39.380	1.00	27.67		C
	ANISOU	1127	CG	ASN	F	125	3473	3577	3462	-21	77	88	C
	ATOM	1128	OD1	ASN	F	125	-21.547	43.556	39.154	1.00	29.94		O
	ANISOU	1128	OD1	ASN	F	125	3587	3936	3851	-15	68	263	O
65	ATOM	1129	ND2	ASN	F	125	-20.458	41.801	40.031	1.00	29.44		N
	ANISOU	1129	ND2	ASN	F	125	3812	3642	3730	30	-23	134	N
	ATOM	1132	C	ASN	F	125	-17.970	45.082	37.425	1.00	21.41		C
	ANISOU	1132	C	ASN	F	125	3061	2603	2469	-88	11	59	C
	ATOM	1133	O	ASN	F	125	-17.053	44.584	36.768	1.00	22.41		O
70	ANISOU	1133	O	ASN	F	125	3000	2525	2991	-157	-114	-172	O
	ATOM	1135	N	PRO	F	126	-17.884	46.304	37.976	1.00	21.91		N

	ANISOU	1135	N	PRO	F	126	2880	2956	2486	-150	-204	99	N
	ATOM	1136	CA	PRO	F	126	-16.601	46.987	37.932	1.00	21.55		C
	ANISOU	1136	CA	PRO	F	126	2696	2855	2637	-22	-41	42	C
	ATOM	1138	CB	PRO	F	126	-16.904	48.364	38.530	1.00	21.93		C
5	ANISOU	1138	CB	PRO	F	126	2831	2772	2727	-75	-137	-48	C
	ATOM	1141	CG	PRO	F	126	-18.115	48.171	39.349	1.00	22.95		C
	ANISOU	1141	CG	PRO	F	126	3148	2703	2866	-36	-16	-112	C
	ATOM	1144	CD	PRO	F	126	-18.912	47.105	38.661	1.00	22.46		C
	ANISOU	1144	CD	PRO	F	126	2737	2938	2857	-104	-154	-31	C
10	ATOM	1147	C	PRO	F	126	-15.575	46.243	38.770	1.00	20.61		C
	ANISOU	1147	C	PRO	F	126	2640	2781	2407	-120	0	-5	C
	ATOM	1148	O	PRO	F	126	-15.939	45.511	39.697	1.00	22.12		O
	ANISOU	1148	O	PRO	F	126	2580	2948	2877	-346	-335	344	O
	ATOM	1149	N	ILE	F	127	-14.307	46.403	38.416	1.00	19.44		N
15	ANISOU	1149	N	ILE	F	127	2446	2507	2433	-97	14	-59	N
	ATOM	1150	CA	ILE	F	127	-13.220	45.797	39.162	1.00	19.46		C
	ANISOU	1150	CA	ILE	F	127	2515	2509	2367	-54	-78	-29	C
	ATOM	1152	CB	ILE	F	127	-12.063	45.354	38.224	1.00	21.19		C
	ANISOU	1152	CB	ILE	F	127	2635	2805	2610	-37	93	-54	C
20	ATOM	1154	CG1	ILE	F	127	-12.529	44.220	37.302	1.00	24.20		C
	ANISOU	1154	CG1	ILE	F	127	2990	3222	2982	-5	66	-98	C
	ATOM	1157	CD1	ILE	F	127	-11.485	43.788	36.261	1.00	23.78		C
	ANISOU	1157	CD1	ILE	F	127	2902	3129	3001	-4	40	-158	C
	ATOM	1161	CG2	ILE	F	127	-10.843	44.918	39.037	1.00	23.11		C
25	ANISOU	1161	CG2	ILE	F	127	2827	2905	3046	82	16	26	C
	ATOM	1165	C	ILE	F	127	-12.718	46.815	40.177	1.00	17.96		C
	ANISOU	1165	C	ILE	F	127	2360	2095	2366	-145	35	26	C
	ATOM	1166	O	ILE	F	127	-12.353	47.932	39.825	1.00	19.11		O
	ANISOU	1166	O	ILE	F	127	2439	2158	2661	-414	-114	76	O
30	ATOM	1168	N	SER	F	128	-12.710	46.422	41.443	1.00	17.99		N
	ANISOU	1168	N	SER	F	128	2182	2285	2366	-70	-99	166	N
	ATOM	1169	CA	SER	F	128	-12.121	47.242	42.496	1.00	17.94		C
	ANISOU	1169	CA	SER	F	128	2311	2011	2494	-2	45	-98	C
	ATOM	1171	CB	ASER	F	128	-12.573	46.740	43.871	0.50	18.69		C
35	ANISOU	1171	CB	ASER	F	128	2311	2400	2386	53	7	-53	C
	ATOM	1172	CB	BSER	F	128	-12.578	46.769	43.874	0.50	18.83		C
	ANISOU	1172	CB	BSER	F	128	2336	2384	2432	19	-2	-51	C
	ATOM	1177	OG	ASER	F	128	-12.022	47.508	44.928	0.50	20.18		O
	ANISOU	1177	OG	ASER	F	128	2515	2689	2464	86	-11	-31	O
40	ATOM	1178	OG	BSER	F	128	-13.976	46.946	44.025	0.50	20.88		O
	ANISOU	1178	OG	BSER	F	128	2440	2648	2845	17	31	35	O
	ATOM	1181	C	SER	F	128	-10.602	47.167	42.379	1.00	18.74		C
	ANISOU	1181	C	SER	F	128	2255	2284	2582	25	3	16	C
	ATOM	1182	O	SER	F	128	-10.024	46.095	42.417	1.00	19.81		O
45	ANISOU	1182	O	SER	F	128	1992	2165	3369	119	-168	-172	O
	ATOM	1184	N	ILE	F	129	-9.960	48.313	42.215	1.00	17.19		N
	ANISOU	1184	N	ILE	F	129	1914	2080	2535	60	-12	-89	N
	ATOM	1185	CA	ILE	F	129	-8.524	48.365	41.959	1.00	17.26		C
	ANISOU	1185	CA	ILE	F	129	2171	2227	2157	32	100	-10	C
50	ATOM	1187	CB	AILE	F	129	-8.150	49.628	41.150	0.40	18.33		C
	ANISOU	1187	CB	AILE	F	129	2259	2280	2422	-29	61	-28	C
	ATOM	1188	CB	BILE	F	129	-8.144	49.613	41.154	0.60	18.29		C
	ANISOU	1188	CB	BILE	F	129	2249	2264	2435	-55	54	-45	C
	ATOM	1191	CG1AILE	F	129		-9.034	49.747	39.903	0.40	18.91		C
55	ANISOU	1191	CG1AILE	F	129		2310	2451	2421	-32	43	-15	C
	ATOM	1192	CG1BILE	F	129		-8.806	49.545	39.777	0.60	18.63		C
	ANISOU	1192	CG1BILE	F	129		2317	2326	2434	-66	-45	2	C
	ATOM	1197	CD1AILE	F	129		-8.915	48.587	38.936	0.40	19.61		C
	ANISOU	1197	CD1AILE	F	129		2370	2597	2484	-18	-15	1	C
60	ATOM	1198	CD1BILE	F	129		-8.632	50.803	38.955	0.60	17.90		C
	ANISOU	1198	CD1BILE	F	129		2211	2415	2174	-140	-71	134	C
	ATOM	1205	CG2AILE	F	129		-6.670	49.607	40.763	0.40	18.88		C
	ANISOU	1205	CG2AILE	F	129		2249	2306	2618	-67	21	-12	C
	ATOM	1206	CG2BILE	F	129		-6.619	49.728	41.029	0.60	19.18		C
65	ANISOU	1206	CG2BILE	F	129		2258	2371	2656	-143	-7	-59	C
	ATOM	1213	C	ILE	F	129	-7.757	48.353	43.277	1.00	18.10		C
	ANISOU	1213	C	ILE	F	129	2183	2428	2264	10	57	138	C
	ATOM	1214	O	ILE	F	129	-7.954	49.233	44.100	1.00	19.43		O
	ANISOU	1214	O	ILE	F	129	2047	2761	2574	118	-108	-239	O
70	ATOM	1216	N	PRO	F	130	-6.864	47.365	43.465	1.00	18.06		N
	ANISOU	1216	N	PRO	F	130	2218	2307	2336	-54	67	94	N

	ATOM	1217	CA	PRO	F	130	-6.051	47.316	44.671	1.00	18.76		C
	ANISOU	1217	CA	PRO	F	130	2258	2406	2464	17	76	-6	C
	ATOM	1219	CB	PRO	F	130	-5.493	45.893	44.645	1.00	20.84		C
	ANISOU	1219	CB	PRO	F	130	2459	2485	2970	59	19	151	C
5	ATOM	1222	CG	PRO	F	130	-5.365	45.600	43.199	1.00	21.00		C
	ANISOU	1222	CG	PRO	F	130	2496	2379	3103	13	6	36	C
	ATOM	1225	CD	PRO	F	130	-6.542	46.252	42.554	1.00	19.45		C
	ANISOU	1225	CD	PRO	F	130	2378	2335	2676	-98	45	17	C
	ATOM	1228	C	PRO	F	130	-4.912	48.321	44.611	1.00	17.79		C
10	ANISOU	1228	C	PRO	F	130	2246	2512	1999	-80	-93	84	C
	ATOM	1229	O	PRO	F	130	-4.418	48.628	43.528	1.00	19.43		O
	ANISOU	1229	O	PRO	F	130	2320	2582	2481	-37	98	-58	O
	ATOM	1230	N	MET	F	131	-4.511	48.832	45.769	1.00	18.34		N
	ANISOU	1230	N	MET	F	131	2210	2273	2485	-35	4	-27	N
15	ATOM	1231	CA	MET	F	131	-3.293	49.614	45.864	1.00	19.95		C
	ANISOU	1231	CA	MET	F	131	2297	2492	2789	90	-61	123	C
	ATOM	1233	CB	MET	F	131	-3.405	50.640	46.980	1.00	19.87		C
	ANISOU	1233	CB	MET	F	131	2308	2650	2588	-4	-44	186	C
	ATOM	1236	CG	MET	F	131	-4.586	51.565	46.820	1.00	22.06		C
20	ANISOU	1236	CG	MET	F	131	2583	2697	3101	89	36	-90	C
	ATOM	1239	SD	MET	F	131	-4.418	53.013	47.851	1.00	21.20		S
	ANISOU	1239	SD	MET	F	131	2225	2683	3145	316	64	-214	S
	ATOM	1240	CE	MET	F	131	-3.384	54.057	46.844	1.00	19.42		C
	ANISOU	1240	CE	MET	F	131	2415	2386	2577	108	-56	-48	C
25	ATOM	1244	C	MET	F	131	-2.133	48.680	46.143	1.00	20.50		C
	ANISOU	1244	C	MET	F	131	2291	2517	2979	125	49	279	C
	ATOM	1245	O	MET	F	131	-2.332	47.550	46.586	1.00	20.30		O
	ANISOU	1245	O	MET	F	131	1867	2450	3395	178	251	343	O
	ATOM	1247	N	LEU	F	132	-0.924	49.153	45.865	1.00	19.46		N
30	ANISOU	1247	N	LEU	F	132	2255	2353	2784	144	-75	382	N
	ATOM	1248	CA	LEU	F	132	0.277	48.450	46.293	1.00	20.50		C
	ANISOU	1248	CA	LEU	F	132	2360	2631	2796	121	76	240	C
	ATOM	1250	CB	LEU	F	132	1.523	49.067	45.646	1.00	21.67		C
	ANISOU	1250	CB	LEU	F	132	2537	2820	2873	56	145	118	C
35	ATOM	1253	CG	LEU	F	132	1.559	49.057	44.106	1.00	21.85		C
	ANISOU	1253	CG	LEU	F	132	2624	2805	2871	9	124	-71	C
	ATOM	1255	CD1	LEU	F	132	2.896	49.578	43.596	1.00	22.50		C
	ANISOU	1255	CD1	LEU	F	132	2703	2764	3080	91	125	-103	C
	ATOM	1259	CD2	LEU	F	132	1.272	47.678	43.516	1.00	23.34		C
40	ANISOU	1259	CD2	LEU	F	132	2869	2950	3049	73	267	-45	C
	ATOM	1263	C	LEU	F	132	0.348	48.510	47.821	1.00	21.98		C
	ANISOU	1263	C	LEU	F	132	2672	2777	2899	104	52	86	C
	ATOM	1264	O	LEU	F	132	-0.370	49.288	48.461	1.00	21.59		O
	ANISOU	1264	O	LEU	F	132	2392	3083	2727	202	126	162	O
45	ATOM	1266	N	ASN	F	133	1.213	47.692	48.408	1.00	23.94		N
	ANISOU	1266	N	ASN	F	133	2854	3087	3154	53	-8	251	N
	ATOM	1267	CA	ASN	F	133	1.246	47.543	49.867	1.00	24.54		C
	ANISOU	1267	CA	ASN	F	133	3069	3208	3046	94	17	184	C
	ATOM	1269	CB	ASN	F	133	2.174	46.393	50.272	1.00	27.81		C
50	ANISOU	1269	CB	ASN	F	133	3420	3430	3714	144	41	164	C
	ATOM	1272	CG	ASN	F	133	1.595	45.030	49.930	1.00	30.45		C
	ANISOU	1272	CG	ASN	F	133	3811	3794	3963	9	-36	61	C
	ATOM	1273	OD1	ASN	F	133	0.442	44.919	49.506	1.00	33.10		O
	ANISOU	1273	OD1	ASN	F	133	4003	4133	4440	58	-36	190	O
55	ATOM	1274	ND2	ASN	F	133	2.391	43.983	50.118	1.00	32.68		N
	ANISOU	1274	ND2	ASN	F	133	3964	4080	4372	116	-13	76	N
	ATOM	1277	C	ASN	F	133	1.601	48.808	50.650	1.00	25.14		C
	ANISOU	1277	C	ASN	F	133	3146	3378	3027	46	-83	110	C
	ATOM	1278	O	ASN	F	133	1.295	48.898	51.840	1.00	27.95		O
60	ANISOU	1278	O	ASN	F	133	3543	3777	3298	106	62	207	O
	ATOM	1280	N	ASP	F	134	2.219	49.789	49.990	1.00	24.82		N
	ANISOU	1280	N	ASP	F	134	3105	3339	2986	46	-174	160	N
	ATOM	1281	CA	ASP	F	134	2.525	51.066	50.638	1.00	25.10		C
	ANISOU	1281	CA	ASP	F	134	3108	3239	3189	77	-3	120	C
65	ATOM	1283	CB	ASP	F	134	3.639	51.832	49.890	1.00	27.25		C
	ANISOU	1283	CB	ASP	F	134	3337	3501	3515	54	54	219	C
	ATOM	1286	CG	ASP	F	134	3.238	52.297	48.487	1.00	28.42		C
	ANISOU	1286	CG	ASP	F	134	3391	3737	3668	-36	-39	144	C
	ATOM	1287	OD1	ASP	F	134	2.086	52.091	48.044	1.00	25.50		O
70	ANISOU	1287	OD1	ASP	F	134	3193	3236	3260	83	-171	182	O
	ATOM	1288	OD2	ASP	F	134	4.113	52.892	47.822	1.00	30.05		O

	ANISOU	1288	0D2	ASP	F	134	3528	3997	3893	-29	-54	443	O
	ATOM	1289	C	ASP	F	134	1.297	51.961	50.878	1.00	24.77		C
	ANISOU	1289	C	ASP	F	134	3113	3208	3088	34	-43	58	C
	ATOM	1290	O	ASP	F	134	1.382	52.933	51.628	1.00	26.84		O
5	ANISOU	1290	O	ASP	F	134	3540	3310	3345	-126	-16	54	O
	ATOM	1292	N	GLY	F	135	0.166	51.630	50.254	1.00	23.76		N
	ANISOU	1292	N	GLY	F	135	3056	3110	2859	127	-54	-71	N
	ATOM	1293	CA	GLY	F	135	-1.070	52.400	50.420	1.00	22.21		C
	ANISOU	1293	CA	GLY	F	135	2933	2970	2535	49	13	-73	C
10	ATOM	1296	C	GLY	F	135	-1.039	53.756	49.735	1.00	22.44		C
	ANISOU	1296	C	GLY	F	135	2803	2862	2861	-2	98	-176	C
	ATOM	1297	O	GLY	F	135	-1.869	54.620	50.027	1.00	22.98		O
	ANISOU	1297	O	GLY	F	135	2823	2760	3148	12	227	-198	O
	ATOM	1299	N	ARG	F	136	-0.094	53.934	48.813	1.00	20.80		N
15	ANISOU	1299	N	ARG	F	136	2657	2716	2528	-83	97	-109	N
	ATOM	1300	CA	ARG	F	136	0.134	55.219	48.150	1.00	21.72		C
	ANISOU	1300	CA	ARG	F	136	2848	2766	2639	137	126	-53	C
	ATOM	1302	CB	ARG	F	136	1.454	55.825	48.633	1.00	23.16		C
	ANISOU	1302	CB	ARG	F	136	2971	2827	3001	11	31	-41	C
20	ATOM	1305	CG	ARG	F	136	1.591	55.896	50.151	1.00	24.12		C
	ANISOU	1305	CG	ARG	F	136	3078	2994	3092	7	-16	-145	C
	ATOM	1308	CD	ARG	F	136	2.729	56.800	50.606	1.00	25.79		C
	ANISOU	1308	CD	ARG	F	136	3154	3192	3453	3	-61	-21	C
	ATOM	1311	NE	ARG	F	136	2.747	56.926	52.062	1.00	27.74		N
25	ANISOU	1311	NE	ARG	F	136	3539	3464	3537	-5	1	-53	N
	ATOM	1313	CZ	ARG	F	136	3.567	57.718	52.754	1.00	30.25		C
	ANISOU	1313	CZ	ARG	F	136	3804	3796	3892	-29	-14	-24	C
	ATOM	1314	NH1	ARG	F	136	4.464	58.478	52.132	1.00	31.93		N
	ANISOU	1314	NH1	ARG	F	136	4022	3995	4112	-43	82	92	N
30	ATOM	1317	NH2	ARG	F	136	3.491	57.752	54.082	1.00	30.74		N
	ANISOU	1317	NH2	ARG	F	136	3831	3888	3957	9	1	66	N
	ATOM	1320	C	ARG	F	136	0.172	55.125	46.626	1.00	19.97		C
	ANISOU	1320	C	ARG	F	136	2738	2422	2427	379	163	-103	C
	ATOM	1321	O	ARG	F	136	-0.018	56.123	45.946	1.00	25.10		O
35	ANISOU	1321	O	ARG	F	136	3861	2732	2943	877	359	-127	O
	ATOM	1323	N	ARG	F	137	0.448	53.942	46.088	1.00	17.28		N
	ANISOU	1323	N	ARG	F	137	2172	2035	2355	144	-97	-162	N
	ATOM	1324	CA	ARG	F	137	0.568	53.768	44.654	1.00	17.46		C
	ANISOU	1324	CA	ARG	F	137	2136	2179	2315	183	-53	5	C
40	ATOM	1326	CB	ARG	F	137	1.992	53.351	44.279	1.00	18.11		C
	ANISOU	1326	CB	ARG	F	137	2237	2243	2401	94	69	-86	C
	ATOM	1329	CG	ARG	F	137	3.034	54.405	44.588	1.00	19.93		C
	ANISOU	1329	CG	ARG	F	137	2338	2487	2747	-36	71	-163	C
	ATOM	1332	CD	ARG	F	137	4.396	54.015	44.052	1.00	23.05		C
45	ANISOU	1332	CD	ARG	F	137	2642	2960	3154	22	109	-15	C
	ATOM	1335	NE	ARG	F	137	4.895	52.793	44.680	1.00	25.64		N
	ANISOU	1335	NE	ARG	F	137	2918	3279	3545	68	130	-50	N
	ATOM	1337	CZ	ARG	F	137	5.604	51.849	44.058	1.00	25.30		C
	ANISOU	1337	CZ	ARG	F	137	3209	2990	3413	19	53	-61	C
50	ATOM	1338	NH1	ARG	F	137	5.895	51.950	42.763	1.00	25.69		N
	ANISOU	1338	NH1	ARG	F	137	3124	2992	3645	270	388	-47	N
	ATOM	1341	NH2	ARG	F	137	6.002	50.787	44.743	1.00	27.37		N
	ANISOU	1341	NH2	ARG	F	137	3164	3347	3888	120	210	-5	N
	ATOM	1344	C	ARG	F	137	-0.395	52.714	44.139	1.00	15.06		C
55	ANISOU	1344	C	ARG	F	137	1802	1925	1994	80	124	-6	C
	ATOM	1345	O	ARG	F	137	-0.763	51.783	44.850	1.00	15.24		O
	ANISOU	1345	O	ARG	F	137	1768	2087	1933	221	152	69	O
	ATOM	1347	N	ILE	F	138	-0.782	52.885	42.882	1.00	14.86		N
	ANISOU	1347	N	ILE	F	138	1987	1888	1769	27	-13	-54	N
60	ATOM	1348	CA	ILE	F	138	-1.470	51.863	42.102	1.00	15.16		C
	ANISOU	1348	CA	ILE	F	138	1815	1885	2058	22	-2	82	C
	ATOM	1350	CB	ILE	F	138	-2.869	52.348	41.656	1.00	15.14		C
	ANISOU	1350	CB	ILE	F	138	1862	1910	1977	66	49	103	C
	ATOM	1352	CG1	ILE	F	138	-3.757	52.532	42.896	1.00	16.80		C
65	ANISOU	1352	CG1	ILE	F	138	2284	2313	1784	104	79	261	C
	ATOM	1355	CD1	ILE	F	138	-5.143	53.056	42.628	1.00	17.39		C
	ANISOU	1355	CD1	ILE	F	138	2039	2233	2332	9	89	173	C
	ATOM	1359	CG2	ILE	F	138	-3.484	51.390	40.629	1.00	16.48		C
	ANISOU	1359	CG2	ILE	F	138	1829	2141	2288	1	62	-12	C
70	ATOM	1363	C	ILE	F	138	-0.618	51.595	40.874	1.00	15.24		C
	ANISOU	1363	C	ILE	F	138	1761	1888	2139	69	133	-104	C

	ATOM	1364	O	ILE	F	138	-0.147	52.531	40.234	1.00	15.00		O
	ANISOU	1364	O	ILE	F	138	1931	1749	2019	145	59	-26	O
	ATOM	1366	N	VAL	F	139	-0.391	50.315	40.583	1.00	15.93		N
	ANISOU	1366	N	VAL	F	139	1992	1837	2223	216	-54	116	N
5	ATOM	1367	CA	VAL	F	139	0.166	49.865	39.302	1.00	16.50		C
	ANISOU	1367	CA	VAL	F	139	2025	1952	2289	-1	-104	16	C
	ATOM	1369	CB	VAL	F	139	1.700	49.603	39.357	1.00	17.84		C
	ANISOU	1369	CB	VAL	F	139	2105	2322	2351	217	-16	28	C
	ATOM	1371	CG1	VAL	F	139	2.220	49.226	37.968	1.00	19.59		C
10	ANISOU	1371	CG1	VAL	F	139	2227	2691	2526	319	187	-62	C
	ATOM	1375	CG2	VAL	F	139	2.462	50.800	39.898	1.00	18.51		C
	ANISOU	1375	CG2	VAL	F	139	2230	2380	2423	40	-13	113	C
	ATOM	1379	C	VAL	F	139	-0.549	48.550	39.000	1.00	16.60		C
	ANISOU	1379	C	VAL	F	139	2030	2037	2239	-104	-169	-33	C
15	ATOM	1380	O	VAL	F	139	-0.175	47.499	39.529	1.00	21.65		O
	ANISOU	1380	O	VAL	F	139	2841	2294	3088	55	-413	96	O
	ATOM	1382	N	PHE	F	140	-1.583	48.619	38.167	1.00	15.70		N
	ANISOU	1382	N	PHE	F	140	2139	1757	2068	135	-92	-51	N
	ATOM	1383	CA	PHE	F	140	-2.560	47.534	38.053	1.00	16.70		C
20	ANISOU	1383	CA	PHE	F	140	2182	1995	2169	3	-89	6	C
	ATOM	1385	CB	PHE	F	140	-3.846	47.938	38.770	1.00	20.87		C
	ANISOU	1385	CB	PHE	F	140	2707	2552	2668	-62	128	-187	C
	ATOM	1388	CG	PHE	F	140	-4.820	46.812	38.954	1.00	20.87		C
	ANISOU	1388	CG	PHE	F	140	2600	2932	2397	-39	369	-398	C
25	ATOM	1389	CD1	PHE	F	140	-4.481	45.702	39.703	1.00	23.86		C
	ANISOU	1389	CD1	PHE	F	140	2897	2676	3490	-282	206	-255	C
	ATOM	1391	CE1	PHE	F	140	-5.393	44.652	39.880	1.00	24.36		C
	ANISOU	1391	CE1	PHE	F	140	3010	2695	3548	-172	125	-41	C
	ATOM	1393	CZ	PHE	F	140	-6.655	44.746	39.321	1.00	22.92		C
30	ANISOU	1393	CZ	PHE	F	140	2876	2734	3095	-227	145	-299	C
	ATOM	1395	CE2	PHE	F	140	-7.004	45.853	38.584	1.00	23.95		C
	ANISOU	1395	CE2	PHE	F	140	2937	3032	3129	-223	207	-348	C
	ATOM	1397	CD2	PHE	F	140	-6.086	46.885	38.405	1.00	22.59		C
	ANISOU	1397	CD2	PHE	F	140	2953	2795	2835	-111	200	-374	C
35	ATOM	1399	C	PHE	F	140	-2.865	47.241	36.596	1.00	15.17		C
	ANISOU	1399	C	PHE	F	140	1902	1969	1891	71	-74	0	C
	ATOM	1400	O	PHE	F	140	-3.092	48.158	35.814	1.00	16.11		O
	ANISOU	1400	O	PHE	F	140	2310	1792	2017	15	-57	-13	O
	ATOM	1402	N	THR	F	141	-2.879	45.958	36.245	1.00	14.78		N
40	ANISOU	1402	N	THR	F	141	1945	1722	1948	-16	81	-95	N
	ATOM	1403	CA	THR	F	141	-3.123	45.500	34.883	1.00	15.54		C
	ANISOU	1403	CA	THR	F	141	1987	1936	1979	-49	1	112	C
	ATOM	1405	CB	ATHR	F	141	-1.877	44.777	34.342	0.65	18.27		C
	ANISOU	1405	CB	ATHR	F	141	2209	2356	2376	-37	50	-138	C
45	ATOM	1406	CB	BTHR	F	141	-1.904	44.765	34.264	0.35	18.01		C
	ANISOU	1406	CB	BTHR	F	141	2183	2342	2315	-27	18	-67	C
	ATOM	1409	OG1ATHR	F	141		-0.728	45.615	34.521	0.65	17.99		O
	ANISOU	1409	OG1ATHR	F	141		2050	2371	2412	40	358	-179	O
	ATOM	1410	OG1BTHR	F	141		-1.481	43.698	35.120	0.35	18.84		O
50	ANISOU	1410	OG1BTHR	F	141		2254	2661	2241	-22	-68	-41	O
	ATOM	1413	CG2ATHR	F	141		-2.044	44.431	32.871	0.65	18.25		C
	ANISOU	1413	CG2ATHR	F	141		2280	2334	2321	-79	113	-267	C
	ATOM	1414	CG2BTHR	F	141		-0.756	45.713	34.039	0.35	18.09		C
	ANISOU	1414	CG2BTHR	F	141		2277	2238	2355	-7	83	-30	C
55	ATOM	1421	C	THR	F	141	-4.309	44.546	34.840	1.00	14.50		C
	ANISOU	1421	C	THR	F	141	1884	1745	1881	34	-19	-149	C
	ATOM	1422	O	THR	F	141	-4.378	43.579	35.613	1.00	15.83		O
	ANISOU	1422	O	THR	F	141	2124	1891	1996	-69	-24	89	O
	ATOM	1424	N	VAL	F	142	-5.212	44.823	33.909	1.00	15.64		N
60	ANISOU	1424	N	VAL	F	142	2108	1947	1886	-16	26	15	N
	ATOM	1425	CA	VAL	F	142	-6.358	43.978	33.614	1.00	16.86		C
	ANISOU	1425	CA	VAL	F	142	2202	2125	2079	-69	-28	51	C
	ATOM	1427	CB	VAL	F	142	-7.671	44.752	33.940	1.00	21.78		C
	ANISOU	1427	CB	VAL	F	142	2611	3217	2444	1	392	-179	C
65	ATOM	1429	CG1	VAL	F	142	-8.903	44.082	33.354	1.00	24.73		C
	ANISOU	1429	CG1	VAL	F	142	2892	3569	2933	227	185	-42	C
	ATOM	1433	CG2	VAL	F	142	-7.807	44.922	35.457	1.00	21.96		C
	ANISOU	1433	CG2	VAL	F	142	2688	3282	2371	-131	99	-202	C
	ATOM	1437	C	VAL	F	142	-6.308	43.639	32.126	1.00	15.68		C
70	ANISOU	1437	C	VAL	F	142	1920	1989	2046	-65	-126	9	C
	ATOM	1438	O	VAL	F	142	-5.833	44.435	31.323	1.00	16.32		O

	ANISOU	1438	O	VAL	F	142	2183	2059	1958	-278	120	-16	O
	ATOM	1440	N	VAL	F	143	-6.767	42.445	31.769	1.00	14.19		N
	ANISOU	1440	N	VAL	F	143	1604	1827	1959	-27	-81	188	N
	ATOM	1441	CA	VAL	F	143	-7.064	42.112	30.388	1.00	14.51		C
5	ANISOU	1441	CA	VAL	F	143	1682	1711	2120	-174	44	-22	C
	ATOM	1443	CB	VAL	F	143	-6.285	40.885	29.895	1.00	16.39		C
	ANISOU	1443	CB	VAL	F	143	1862	1909	2454	-11	0	108	C
	ATOM	1445	CG1	VAL	F	143	-6.573	40.641	28.409	1.00	17.26		C
	ANISOU	1445	CG1	VAL	F	143	2054	1975	2528	85	259	-91	C
10	ATOM	1449	CG2	VAL	F	143	-4.790	41.079	30.144	1.00	18.30		C
	ANISOU	1449	CG2	VAL	F	143	2052	2188	2711	84	103	398	C
	ATOM	1453	C	VAL	F	143	-8.559	41.863	30.302	1.00	14.41		C
	ANISOU	1453	C	VAL	F	143	1728	1782	1965	116	130	56	C
	ATOM	1454	O	VAL	F	143	-9.122	41.164	31.142	1.00	14.67		O
15	ANISOU	1454	O	VAL	F	143	1650	1968	1954	105	-41	335	O
	ATOM	1456	N	ALA	F	144	-9.197	42.459	29.304	1.00	14.30		N
	ANISOU	1456	N	ALA	F	144	1581	2000	1849	-258	33	7	N
	ATOM	1457	CA	ALA	F	144	-10.644	42.392	29.196	1.00	14.71		C
	ANISOU	1457	CA	ALA	F	144	1677	2018	1891	-89	-96	0	C
20	ATOM	1459	CB	ALA	F	144	-11.279	43.580	29.883	1.00	17.42		C
	ANISOU	1459	CB	ALA	F	144	1848	2627	2141	263	-176	-199	C
	ATOM	1463	C	ALA	F	144	-11.088	42.333	27.756	1.00	14.29		C
	ANISOU	1463	C	ALA	F	144	1699	1913	1815	63	-72	164	C
	ATOM	1464	O	ALA	F	144	-10.357	42.738	26.855	1.00	14.98		O
25	ANISOU	1464	O	ALA	F	144	1857	2155	1678	-332	5	43	O
	ATOM	1466	N	SER	F	145	-12.300	41.829	27.563	1.00	14.33		N
	ANISOU	1466	N	SER	F	145	1738	1834	1871	153	-55	95	N
	ATOM	1467	CA	SER	F	145	-12.905	41.711	26.247	1.00	13.12		C
	ANISOU	1467	CA	SER	F	145	1566	1818	1599	93	55	12	C
30	ATOM	1469	CB	SER	F	145	-13.643	40.374	26.146	1.00	14.72		C
	ANISOU	1469	CB	SER	F	145	1784	1935	1871	34	-116	184	C
	ATOM	1472	OG	SER	F	145	-14.234	40.187	24.877	1.00	15.44		O
	ANISOU	1472	OG	SER	F	145	2071	1912	1882	-60	-257	138	O
	ATOM	1474	C	SER	F	145	-13.870	42.874	26.053	1.00	13.64		C
35	ANISOU	1474	C	SER	F	145	1869	1741	1570	49	-41	-59	C
	ATOM	1475	O	SER	F	145	-14.926	42.915	26.670	1.00	15.00		O
	ANISOU	1475	O	SER	F	145	1792	1900	2004	136	-72	293	O
	ATOM	1477	N	LEU	F	146	-13.491	43.809	25.188	1.00	13.65		N
	ANISOU	1477	N	LEU	F	146	1629	1688	1868	87	180	84	N
40	ATOM	1478	CA	LEU	F	146	-14.249	45.029	24.989	1.00	12.77		C
	ANISOU	1478	CA	LEU	F	146	1593	1696	1561	102	-66	9	C
	ATOM	1480	CB	LEU	F	146	-13.355	46.264	25.132	1.00	13.54		C
	ANISOU	1480	CB	LEU	F	146	1786	1624	1733	175	-207	-13	C
	ATOM	1483	CG	LEU	F	146	-12.538	46.359	26.429	1.00	14.27		C
45	ANISOU	1483	CG	LEU	F	146	1684	1857	1881	136	-235	47	C
	ATOM	1485	CD1	LEU	F	146	-11.796	47.662	26.454	1.00	16.12		C
	ANISOU	1485	CD1	LEU	F	146	2009	2116	1997	-182	1	-259	C
	ATOM	1489	CD2	LEU	F	146	-13.405	46.243	27.662	1.00	16.12		C
	ANISOU	1489	CD2	LEU	F	146	2010	2106	2007	84	-173	32	C
50	ATOM	1493	C	LEU	F	146	-14.911	45.015	23.619	1.00	11.76		C
	ANISOU	1493	C	LEU	F	146	1605	1484	1379	82	-97	128	C
	ATOM	1494	O	LEU	F	146	-14.483	44.296	22.708	1.00	13.59		O
	ANISOU	1494	O	LEU	F	146	1777	1813	1573	229	-46	23	O
	ATOM	1496	N	ALA	F	147	-15.966	45.811	23.496	1.00	12.27		N
55	ANISOU	1496	N	ALA	F	147	1728	1551	1382	46	-21	131	N
	ATOM	1497	CA	ALA	F	147	-16.751	45.868	22.273	1.00	12.45		C
	ANISOU	1497	CA	ALA	F	147	1658	1540	1531	89	-130	-37	C
	ATOM	1499	CB	ALA	F	147	-17.961	44.958	22.375	1.00	14.04		C
	ANISOU	1499	CB	ALA	F	147	1903	1898	1532	4	-320	131	C
60	ATOM	1503	C	ALA	F	147	-17.204	47.288	22.018	1.00	13.71		C
	ANISOU	1503	C	ALA	F	147	1922	1649	1638	77	-57	121	C
	ATOM	1504	O	ALA	F	147	-17.252	48.119	22.930	1.00	13.17		O
	ANISOU	1504	O	ALA	F	147	2001	1366	1636	151	-225	131	O
	ATOM	1506	N	PHE	F	148	-17.540	47.554	20.763	1.00	15.34		N
65	ANISOU	1506	N	PHE	F	148	2287	1854	1687	42	-122	57	N
	ATOM	1507	CA	PHE	F	148	-18.155	48.816	20.378	1.00	14.72		C
	ANISOU	1507	CA	PHE	F	148	2143	1621	1828	-27	-159	168	C
	ATOM	1509	CB	PHE	F	148	-18.754	48.676	18.976	1.00	18.27		C
	ANISOU	1509	CB	PHE	F	148	2409	2345	2185	-63	-164	160	C
70	ATOM	1512	CG	PHE	F	148	-19.523	49.885	18.500	1.00	18.22		C
	ANISOU	1512	CG	PHE	F	148	2352	2215	2354	-15	-100	297	C

	ATOM	1513	CD1	PHE	F	148	-18.985	51.166	18.602	1.00	19.45		C
	ANISOU	1513	CD1	PHE	F	148	2628	2239	2523	93	-85	225	C
	ATOM	1515	CE1	PHE	F	148	-19.696	52.272	18.154	1.00	20.71		C
	ANISOU	1515	CE1	PHE	F	148	2676	2495	2698	3	-39	201	C
5	ATOM	1517	CZ	PHE	F	148	-20.940	52.103	17.594	1.00	20.99		C
	ANISOU	1517	CZ	PHE	F	148	2766	2479	2729	-16	-87	201	C
	ATOM	1519	CE2	PHE	F	148	-21.482	50.830	17.473	1.00	19.63		C
	ANISOU	1519	CE2	PHE	F	148	2405	2577	2475	30	-273	259	C
	ATOM	1521	CD2	PHE	F	148	-20.775	49.732	17.919	1.00	20.60		C
10	ANISOU	1521	CD2	PHE	F	148	2659	2513	2654	-142	-23	135	C
	ATOM	1523	C	PHE	F	148	-19.224	49.216	21.385	1.00	15.21		C
	ANISOU	1523	C	PHE	F	148	1955	1934	1891	141	-261	334	C
	ATOM	1524	O	PHE	F	148	-20.058	48.397	21.775	1.00	14.51		O
	ANISOU	1524	O	PHE	F	148	2027	1665	1820	-73	-400	118	O
15	ATOM	1526	N	LYS	F	149	-19.140	50.475	21.823	1.00	16.65		N
	ANISOU	1526	N	LYS	F	149	2472	1908	1943	-84	-160	-23	N
	ATOM	1527	CA	LYS	F	149	-20.077	51.130	22.756	1.00	18.14		C
	ANISOU	1527	CA	LYS	F	149	2651	2070	2169	144	19	-20	C
	ATOM	1529	CB	LYS	F	149	-21.542	50.729	22.530	1.00	19.99		C
20	ANISOU	1529	CB	LYS	F	149	2782	2384	2430	162	-16	-111	C
	ATOM	1532	CG	LYS	F	149	-22.063	51.128	21.155	1.00	23.10		C
	ANISOU	1532	CG	LYS	F	149	3158	2833	2786	136	-79	-18	C
	ATOM	1535	CD	LYS	F	149	-23.566	51.042	21.094	1.00	24.33		C
	ANISOU	1535	CD	LYS	F	149	3169	3101	2972	94	-1	-38	C
25	ATOM	1538	CE	LYS	F	149	-24.111	51.559	19.774	1.00	25.06		C
	ANISOU	1538	CE	LYS	F	149	3276	3269	2978	-29	-104	-14	C
	ATOM	1541	NZ	LYS	F	149	-25.591	51.506	19.775	1.00	26.84		N
	ANISOU	1541	NZ	LYS	F	149	3385	3562	3250	131	-42	65	N
	ATOM	1545	C	LYS	F	149	-19.690	51.009	24.230	1.00	16.78		C
30	ANISOU	1545	C	LYS	F	149	2139	2052	2184	139	-99	0	C
	ATOM	1546	O	LYS	F	149	-20.267	51.696	25.084	1.00	19.16		O
	ANISOU	1546	O	LYS	F	149	2633	2405	2241	135	-290	-364	O
	ATOM	1548	N	ASP	F	150	-18.700	50.167	24.527	1.00	14.59		N
	ANISOU	1548	N	ASP	F	150	2024	1760	1757	41	-97	-203	N
35	ATOM	1549	CA	ASP	F	150	-18.148	50.100	25.871	1.00	14.96		C
	ANISOU	1549	CA	ASP	F	150	2029	1749	1904	-96	-54	-115	C
	ATOM	1551	CB	ASP	F	150	-17.105	48.985	26.004	1.00	14.34		C
	ANISOU	1551	CB	ASP	F	150	1849	1777	1823	-96	-123	-82	C
	ATOM	1554	CG	ASP	F	150	-17.710	47.589	26.119	1.00	14.19		C
40	ANISOU	1554	CG	ASP	F	150	1777	1800	1813	101	63	-103	C
	ATOM	1555	OD1	ASP	F	150	-18.947	47.432	26.300	1.00	15.63		O
	ANISOU	1555	OD1	ASP	F	150	2038	1933	1965	-135	-2	-160	O
	ATOM	1556	OD2	ASP	F	150	-16.915	46.618	26.035	1.00	15.23		O
	ANISOU	1556	OD2	ASP	F	150	2036	2027	1723	177	-21	-250	O
45	ATOM	1557	C	ASP	F	150	-17.480	51.442	26.179	1.00	14.31		C
	ANISOU	1557	C	ASP	F	150	2084	1499	1851	-154	267	19	C
	ATOM	1558	O	ASP	F	150	-16.922	52.085	25.288	1.00	15.78		O
	ANISOU	1558	O	ASP	F	150	2283	1751	1959	-302	131	-245	O
	ATOM	1560	N	LYS	F	151	-17.551	51.838	27.446	1.00	15.98		N
50	ANISOU	1560	N	LYS	F	151	2167	1924	1981	-323	-14	-130	N
	ATOM	1561	CA	LYS	F	151	-16.925	53.057	27.950	1.00	16.95		C
	ANISOU	1561	CA	LYS	F	151	2251	2027	2160	-277	-11	-185	C
	ATOM	1563	CB	LYS	F	151	-17.975	54.052	28.439	1.00	21.98		C
	ANISOU	1563	CB	LYS	F	151	2958	2424	2968	-142	59	-222	C
55	ATOM	1566	CG	LYS	F	151	-19.023	54.433	27.423	1.00	26.42		C
	ANISOU	1566	CG	LYS	F	151	3483	3123	3430	17	16	-147	C
	ATOM	1569	CD	LYS	F	151	-18.438	55.159	26.236	1.00	27.37		C
	ANISOU	1569	CD	LYS	F	151	3482	3342	3573	-86	13	-64	C
	ATOM	1572	CE	LYS	F	151	-19.526	55.875	25.451	1.00	29.75		C
60	ANISOU	1572	CE	LYS	F	151	3941	3676	3686	-84	-57	113	C
	ATOM	1575	NZ	LYS	F	151	-19.113	56.133	24.045	1.00	33.11		N
	ANISOU	1575	NZ	LYS	F	151	4424	4189	3966	-82	165	53	N
	ATOM	1579	C	LYS	F	151	-16.044	52.646	29.118	1.00	16.77		C
	ANISOU	1579	C	LYS	F	151	2090	2122	2159	-129	10	-111	C
65	ATOM	1580	O	LYS	F	151	-16.522	52.036	30.079	1.00	20.57		O
	ANISOU	1580	O	LYS	F	151	2455	2875	2482	-388	-4	-75	O
	ATOM	1582	N	VAL	F	152	-14.757	52.961	29.037	1.00	14.98		N
	ANISOU	1582	N	VAL	F	152	1942	1868	1878	-113	-55	-144	N
	ATOM	1583	CA	VAL	F	152	-13.842	52.651	30.123	1.00	16.07		C
70	ANISOU	1583	CA	VAL	F	152	2182	2084	1839	-107	-110	-193	C
	ATOM	1585	CB	VAL	F	152	-12.464	52.195	29.612	1.00	15.99		C

	ANISOU	1585	CB	VAL	F	152	2210	2014	1850	-50	-34	-43	C
	ATOM	1587	CG1	VAL	F	152	-11.540	51.877	30.784	1.00	17.64		C
	ANISOU	1587	CG1	VAL	F	152	2311	2240	2151	34	-6	-186	C
	ATOM	1591	CG2	VAL	F	152	-12.616	50.982	28.704	1.00	17.84		C
5	ANISOU	1591	CG2	VAL	F	152	2263	2450	2063	139	-138	-137	C
	ATOM	1595	C	VAL	F	152	-13.713	53.907	30.976	1.00	15.13		C
	ANISOU	1595	C	VAL	F	152	2073	1854	1822	-109	-11	-80	C
	ATOM	1596	O	VAL	F	152	-13.307	54.956	30.487	1.00	14.98		O
	ANISOU	1596	O	VAL	F	152	2138	1834	1718	-109	164	-234	O
10	ATOM	1598	N	TYR	F	153	-14.072	53.803	32.251	1.00	15.68		N
	ANISOU	1598	N	TYR	F	153	2222	1825	1908	-217	-96	-279	N
	ATOM	1599	CA	TYR	F	153	-13.977	54.948	33.148	1.00	15.00		C
	ANISOU	1599	CA	TYR	F	153	1923	1963	1809	-189	-28	-244	C
	ATOM	1601	CB	TYR	F	153	-15.224	55.827	33.030	1.00	15.97		C
15	ANISOU	1601	CB	TYR	F	153	2187	1997	1880	-38	-26	-214	C
	ATOM	1604	CG	TYR	F	153	-16.523	55.180	33.432	1.00	17.16		C
	ANISOU	1604	CG	TYR	F	153	2142	2249	2127	-15	-108	-15	C
	ATOM	1605	CD1	TYR	F	153	-17.254	54.422	32.522	1.00	17.94		C
	ANISOU	1605	CD1	TYR	F	153	2168	2350	2296	-125	-165	-112	C
20	ATOM	1607	CE1	TYR	F	153	-18.462	53.838	32.879	1.00	17.94		C
	ANISOU	1607	CE1	TYR	F	153	2240	2410	2165	-143	-136	-23	C
	ATOM	1609	CZ	TYR	F	153	-18.960	54.012	34.156	1.00	17.93		C
	ANISOU	1609	CZ	TYR	F	153	2030	2449	2332	-210	65	187	C
	ATOM	1610	OH	TYR	F	153	-20.164	53.423	34.503	1.00	22.57		O
25	ANISOU	1610	OH	TYR	F	153	2340	3155	3078	-259	-13	304	O
	ATOM	1612	CE2	TYR	F	153	-18.256	54.766	35.076	1.00	19.28		C
	ANISOU	1612	CE2	TYR	F	153	2295	2660	2369	-82	89	99	C
	ATOM	1614	CD2	TYR	F	153	-17.050	55.355	34.707	1.00	18.05		C
	ANISOU	1614	CD2	TYR	F	153	2171	2410	2277	-78	-108	-51	C
30	ATOM	1616	C	TYR	F	153	-13.709	54.504	34.576	1.00	14.39		C
	ANISOU	1616	C	TYR	F	153	1933	1688	1845	-71	-34	-233	C
	ATOM	1617	O	TYR	F	153	-13.726	53.311	34.885	1.00	15.30		O
	ANISOU	1617	O	TYR	F	153	2191	1828	1792	-15	-89	-292	O
	ATOM	1619	N	LEU	F	154	-13.438	55.481	35.438	1.00	14.62		N
35	ANISOU	1619	N	LEU	F	154	2173	1661	1720	-72	-83	-254	N
	ATOM	1620	CA	LEU	F	154	-12.935	55.216	36.776	1.00	14.16		C
	ANISOU	1620	CA	LEU	F	154	1897	1632	1850	-30	-92	-291	C
	ATOM	1622	CB	LEU	F	154	-11.477	55.654	36.868	1.00	15.77		C
	ANISOU	1622	CB	LEU	F	154	1941	1976	2072	-125	55	-20	C
40	ATOM	1625	CG	LEU	F	154	-10.485	54.926	35.958	1.00	16.54		C
	ANISOU	1625	CG	LEU	F	154	1997	2029	2257	-100	-32	-190	C
	ATOM	1627	CD1	LEU	F	154	-9.188	55.718	35.786	1.00	17.99		C
	ANISOU	1627	CD1	LEU	F	154	2064	2485	2286	-21	148	-184	C
	ATOM	1631	CD2	LEU	F	154	-10.199	53.546	36.527	1.00	17.90		C
45	ANISOU	1631	CD2	LEU	F	154	2185	2087	2529	-48	31	-47	C
	ATOM	1635	C	LEU	F	154	-13.763	56.015	37.753	1.00	14.32		C
	ANISOU	1635	C	LEU	F	154	1692	1931	1816	-90	84	-183	C
	ATOM	1636	O	LEU	F	154	-13.955	57.211	37.551	1.00	14.79		O
	ANISOU	1636	O	LEU	F	154	1969	1804	1844	-70	-1	-94	O
50	ATOM	1638	N	THR	F	155	-14.266	55.361	38.795	1.00	14.61		N
	ANISOU	1638	N	THR	F	155	2023	1773	1755	118	-23	-203	N
	ATOM	1639	CA	THR	F	155	-14.992	56.064	39.853	1.00	16.14		C
	ANISOU	1639	CA	THR	F	155	2162	1980	1990	192	142	-103	C
	ATOM	1641	CB	THR	F	155	-16.467	55.639	39.928	1.00	17.47		C
55	ANISOU	1641	CB	THR	F	155	2155	2311	2173	165	88	-150	C
	ATOM	1643	OG1	THR	F	155	-16.559	54.235	40.186	1.00	18.42		O
	ANISOU	1643	OG1	THR	F	155	2302	2289	2405	6	-13	-154	O
	ATOM	1645	CG2	THR	F	155	-17.190	55.960	38.624	1.00	20.08		C
	ANISOU	1645	CG2	THR	F	155	2356	2854	2417	138	-41	-6	C
60	ATOM	1649	C	THR	F	155	-14.332	55.835	41.200	1.00	17.71		C
	ANISOU	1649	C	THR	F	155	2334	2206	2188	191	95	-78	C
	ATOM	1650	O	THR	F	155	-13.578	54.886	41.383	1.00	17.14		O
	ANISOU	1650	O	THR	F	155	2510	2028	1973	258	-227	-336	O
	ATOM	1652	N	VAL	F	156	-14.639	56.726	42.134	1.00	17.18		N
65	ANISOU	1652	N	VAL	F	156	2513	2066	1947	58	-64	-194	N
	ATOM	1653	CA	VAL	F	156	-14.067	56.706	43.471	1.00	20.01		C
	ANISOU	1653	CA	VAL	F	156	2818	2483	2300	94	-1	-69	C
	ATOM	1655	CB	VAL	F	156	-13.322	58.034	43.781	1.00	21.87		C
	ANISOU	1655	CB	VAL	F	156	2835	2825	2647	-44	70	-64	C
70	ATOM	1657	CG1	VAL	F	156	-12.735	58.014	45.188	1.00	23.10		C
	ANISOU	1657	CG1	VAL	F	156	3024	2856	2895	-38	-19	-6	C

	ATOM	1661	CG2	VAL	F	156	-12.225	58.278	42.753	1.00	22.73		C
	ANISOU	1661	CG2	VAL	F	156	2923	2989	2723	77	135	-5	C
	ATOM	1665	C	VAL	F	156	-15.214	56.513	44.445	1.00	22.61		C
	ANISOU	1665	C	VAL	F	156	3012	2820	2758	72	3	25	C
5	ATOM	1666	O	VAL	F	156	-16.205	57.239	44.390	1.00	20.94		O
	ANISOU	1666	O	VAL	F	156	2737	2941	2275	214	308	-190	O
	ATOM	1668	N	ASN	F	157	-15.093	55.506	45.305	1.00	23.72		N
	ANISOU	1668	N	ASN	F	157	3244	2895	2871	-71	-7	-5	N
	ATOM	1669	CA	ASN	F	157	-16.070	55.275	46.347	1.00	23.81		C
10	ANISOU	1669	CA	ASN	F	157	3171	2906	2968	-98	-16	13	C
	ATOM	1671	CB	ASN	F	157	-16.312	53.773	46.542	1.00	27.76		C
	ANISOU	1671	CB	ASN	F	157	3612	3265	3669	-12	-48	62	C
	ATOM	1674	CG	ASN	F	157	-17.725	53.465	47.014	1.00	31.77		C
	ANISOU	1674	CG	ASN	F	157	3978	3960	4131	-61	20	65	C
15	ATOM	1675	OD1	ASN	F	157	-18.299	54.199	47.821	1.00	34.50		O
	ANISOU	1675	OD1	ASN	F	157	4386	4267	4453	0	95	27	O
	ATOM	1676	ND2	ASN	F	157	-18.294	52.379	46.501	1.00	34.88		N
	ANISOU	1676	ND2	ASN	F	157	4636	4068	4549	9	-88	0	N
	ATOM	1679	C	ASN	F	157	-15.543	55.942	47.614	1.00	23.27		C
20	ANISOU	1679	C	ASN	F	157	3216	2884	2742	26	-12	-50	C
	ATOM	1680	O	ASN	F	157	-14.744	55.360	48.352	1.00	25.94		O
	ANISOU	1680	O	ASN	F	157	3555	3123	3178	132	-145	-42	O
	ATOM	1682	N	ALA	F	158	-15.959	57.186	47.828	1.00	21.24		N
	ANISOU	1682	N	ALA	F	158	2834	2610	2624	-101	-82	139	N
25	ATOM	1683	CA	ALA	F	158	-15.507	57.972	48.975	1.00	20.22		C
	ANISOU	1683	CA	ALA	F	158	2540	2532	2611	-86	35	34	C
	ATOM	1685	CB	ALA	F	158	-14.069	58.432	48.774	1.00	21.35		C
	ANISOU	1685	CB	ALA	F	158	2738	2656	2718	18	4	48	C
	ATOM	1689	C	ALA	F	158	-16.406	59.185	49.180	1.00	19.68		C
30	ANISOU	1689	C	ALA	F	158	2372	2430	2674	-258	28	190	C
	ATOM	1690	O	ALA	F	158	-17.081	59.621	48.244	1.00	19.41		O
	ANISOU	1690	O	ALA	F	158	2248	2481	2647	-372	31	311	O
	ATOM	1692	N	PRO	F	159	-16.415	59.740	50.405	1.00	19.80		N
	ANISOU	1692	N	PRO	F	159	2532	2408	2581	-213	-14	106	N
35	ATOM	1693	CA	PRO	F	159	-17.074	61.025	50.630	1.00	20.70		C
	ANISOU	1693	CA	PRO	F	159	2432	2673	2758	-9	95	80	C
	ATOM	1695	CB	PRO	F	159	-16.655	61.394	52.056	1.00	21.14		C
	ANISOU	1695	CB	PRO	F	159	2693	2630	2706	-60	-5	37	C
	ATOM	1698	CG	PRO	F	159	-16.342	60.097	52.712	1.00	21.88		C
40	ANISOU	1698	CG	PRO	F	159	2847	2708	2755	-10	-62	7	C
	ATOM	1701	CD	PRO	F	159	-15.824	59.192	51.639	1.00	21.49		C
	ANISOU	1701	CD	PRO	F	159	2755	2675	2733	-79	-90	57	C
	ATOM	1704	C	PRO	F	159	-16.564	62.062	49.637	1.00	20.20		C
	ANISOU	1704	C	PRO	F	159	2347	2509	2820	-60	171	59	C
45	ATOM	1705	O	PRO	F	159	-15.376	62.051	49.294	1.00	19.76		O
	ANISOU	1705	O	PRO	F	159	2100	2556	2851	-136	298	61	O
	ATOM	1706	N	ASP	F	160	-17.436	62.945	49.164	1.00	23.30		N
	ANISOU	1706	N	ASP	F	160	2724	3078	3052	-104	81	183	N
	ATOM	1707	CA	ASP	F	160	-17.041	63.831	48.071	1.00	23.19		C
50	ANISOU	1707	CA	ASP	F	160	2839	2985	2984	-120	-29	168	C
	ATOM	1709	CB	ASP	F	160	-18.227	64.595	47.485	1.00	26.81		C
	ANISOU	1709	CB	ASP	F	160	3329	3469	3385	-50	-109	199	C
	ATOM	1712	CG	ASP	F	160	-17.985	65.002	46.042	1.00	27.83		C
	ANISOU	1712	CG	ASP	F	160	3508	3637	3427	-13	-54	173	C
55	ATOM	1713	OD1	ASP	F	160	-17.697	64.115	45.206	1.00	31.31		O
	ANISOU	1713	OD1	ASP	F	160	3877	4357	3663	-60	90	195	O
	ATOM	1714	OD2	ASP	F	160	-18.077	66.207	45.745	1.00	31.16		O
	ANISOU	1714	OD2	ASP	F	160	4105	3836	3898	-271	-113	171	O
	ATOM	1715	C	ASP	F	160	-15.915	64.793	48.453	1.00	20.36		C
60	ANISOU	1715	C	ASP	F	160	2656	2601	2479	-51	-18	34	C
	ATOM	1716	O	ASP	F	160	-15.123	65.167	47.597	1.00	19.54		O
	ANISOU	1716	O	ASP	F	160	2178	2879	2366	-29	148	359	O
	ATOM	1718	N	THR	F	161	-15.817	65.177	49.723	1.00	19.03		N
	ANISOU	1718	N	THR	F	161	2359	2502	2367	-39	109	261	N
65	ATOM	1719	CA	THR	F	161	-14.706	66.017	50.162	1.00	18.22		C
	ANISOU	1719	CA	THR	F	161	2314	2310	2299	72	115	133	C
	ATOM	1721	CB	THR	F	161	-14.777	66.306	51.666	1.00	18.72		C
	ANISOU	1721	CB	THR	F	161	2406	2438	2268	42	100	-2	C
	ATOM	1723	OG1	THR	F	161	-16.040	66.906	51.971	1.00	22.22		O
70	ANISOU	1723	OG1	THR	F	161	2621	3053	2767	249	200	172	O
	ATOM	1725	CG2	THR	F	161	-13.655	67.248	52.094	1.00	19.20		C

	ANISOU	1725	CG2	THR	F	161	2429	2516	2349	11	50	57	C
	ATOM	1729	C	THR	F	161	-13.364	65.359	49.847	1.00	16.95		C
	ANISOU	1729	C	THR	F	161	2020	2066	2353	-39	142	286	C
	ATOM	1730	O	THR	F	161	-12.447	66.008	49.339	1.00	13.90		O
5	ANISOU	1730	O	THR	F	161	1604	1620	2057	-200	-65	450	O
	ATOM	1732	N	LEU	F	162	-13.252	64.067	50.141	1.00	15.21		N
	ANISOU	1732	N	LEU	F	162	1861	1915	2000	-90	262	254	N
	ATOM	1733	CA	LEU	F	162	-12.021	63.342	49.847	1.00	16.41		C
	ANISOU	1733	CA	LEU	F	162	2005	2037	2192	-45	25	127	C
10	ATOM	1735	CB	LEU	F	162	-12.078	61.912	50.392	1.00	18.52		C
	ANISOU	1735	CB	LEU	F	162	2341	2134	2561	-51	-16	124	C
	ATOM	1738	CG	LEU	F	162	-12.179	61.779	51.917	1.00	23.62		C
	ANISOU	1738	CG	LEU	F	162	2934	2981	3057	30	33	74	C
	ATOM	1740	CD1	LEU	F	162	-12.185	60.307	52.320	1.00	26.31		C
15	ANISOU	1740	CD1	LEU	F	162	3262	3221	3514	1	12	237	C
	ATOM	1744	CD2	LEU	F	162	-11.051	62.520	52.632	1.00	25.26		C
	ANISOU	1744	CD2	LEU	F	162	3127	3138	3330	-3	-58	128	C
	ATOM	1748	C	LEU	F	162	-11.765	63.338	48.345	1.00	14.91		C
	ANISOU	1748	C	LEU	F	162	1716	1965	1983	-43	-171	414	C
20	ATOM	1749	O	LEU	F	162	-10.637	63.550	47.908	1.00	15.58		O
	ANISOU	1749	O	LEU	F	162	1511	2353	2052	-43	-47	570	O
	ATOM	1751	N	CYS	F	163	-12.814	63.124	47.555	1.00	14.01		N
	ANISOU	1751	N	CYS	F	163	1815	1514	1993	-105	-61	244	N
	ATOM	1752	CA	CYS	F	163	-12.685	63.153	46.100	1.00	13.84		C
25	ANISOU	1752	CA	CYS	F	163	1847	1627	1785	0	31	19	C
	ATOM	1754	CB	CYS	F	163	-14.008	62.795	45.417	1.00	15.00		C
	ANISOU	1754	CB	CYS	F	163	1885	1604	2209	-238	56	335	C
	ATOM	1757	SG	CYS	F	163	-14.100	63.166	43.631	1.00	19.15		S
	ANISOU	1757	SG	CYS	F	163	2439	2478	2358	-273	-194	179	S
30	ATOM	1759	C	CYS	F	163	-12.168	64.493	45.592	1.00	13.67		C
	ANISOU	1759	C	CYS	F	163	1735	1808	1650	64	65	35	C
	ATOM	1760	O	CYS	F	163	-11.195	64.537	44.840	1.00	11.70		O
	ANISOU	1760	O	CYS	F	163	1551	1539	1353	-94	158	165	O
	ATOM	1762	N	GLU	F	164	-12.792	65.586	46.024	1.00	11.33		N
35	ANISOU	1762	N	GLU	F	164	1200	1402	1701	-73	-35	117	N
	ATOM	1763	CA	GLU	F	164	-12.432	66.907	45.497	1.00	13.80		C
	ANISOU	1763	CA	GLU	F	164	1618	1729	1895	-2	0	115	C
	ATOM	1765	CB	GLU	F	164	-13.418	67.978	45.966	1.00	14.55		C
	ANISOU	1765	CB	GLU	F	164	1559	1827	2142	45	-163	130	C
40	ATOM	1768	CG	GLU	F	164	-14.897	67.690	45.658	1.00	18.73		C
	ANISOU	1768	CG	GLU	F	164	1945	2605	2566	58	-126	143	C
	ATOM	1771	CD	GLU	F	164	-15.208	67.549	44.188	1.00	20.53		C
	ANISOU	1771	CD	GLU	F	164	2346	2719	2735	188	-14	128	C
	ATOM	1772	OE1	GLU	F	164	-14.486	68.140	43.362	1.00	24.39		O
45	ANISOU	1772	OE1	GLU	F	164	2497	3728	3041	223	-51	460	O
	ATOM	1773	OE2	GLU	F	164	-16.195	66.851	43.861	1.00	20.87		O
	ANISOU	1773	OE2	GLU	F	164	2599	2872	2460	182	-161	-161	O
	ATOM	1774	C	GLU	F	164	-11.004	67.303	45.862	1.00	13.08		C
	ANISOU	1774	C	GLU	F	164	1606	1632	1732	43	-68	59	C
50	ATOM	1775	O	GLU	F	164	-10.359	68.040	45.119	1.00	12.00		O
	ANISOU	1775	O	GLU	F	164	1514	1878	1164	-6	-181	80	O
	ATOM	1777	N	HIS	F	165	-10.513	66.806	46.996	1.00	11.47		N
	ANISOU	1777	N	HIS	F	165	1305	1392	1660	-97	137	328	N
	ATOM	1778	CA	HIS	F	165	-9.159	67.113	47.467	1.00	12.32		C
55	ANISOU	1778	CA	HIS	F	165	1426	1566	1686	47	-91	258	C
	ATOM	1780	CB	HIS	F	165	-9.138	67.188	48.989	1.00	12.12		C
	ANISOU	1780	CB	HIS	F	165	1504	1367	1733	0	21	381	C
	ATOM	1783	CG	HIS	F	165	-9.621	68.495	49.513	1.00	9.75		C
	ANISOU	1783	CG	HIS	F	165	1249	1295	1160	171	65	315	C
60	ATOM	1784	ND1	HIS	F	165	-10.939	68.731	49.830	1.00	12.58		N
	ANISOU	1784	ND1	HIS	F	165	1758	1386	1634	-117	-123	753	N
	ATOM	1786	CE1	HIS	F	165	-11.063	69.980	50.245	1.00	7.88		C
	ANISOU	1786	CE1	HIS	F	165	1105	874	1013	36	-124	324	C
	ATOM	1788	NE2	HIS	F	165	-9.878	70.558	50.203	1.00	12.14		N
65	ANISOU	1788	NE2	HIS	F	165	1793	1496	1321	347	99	647	N
	ATOM	1790	CD2	HIS	F	165	-8.959	69.653	49.743	1.00	7.82		C
	ANISOU	1790	CD2	HIS	F	165	657	1264	1047	-419	-75	559	C
	ATOM	1792	C	HIS	F	165	-8.082	66.139	46.995	1.00	13.20		C
	ANISOU	1792	C	HIS	F	165	1591	1760	1663	49	-130	58	C
70	ATOM	1793	O	HIS	F	165	-6.903	66.417	47.165	1.00	15.07		O
	ANISOU	1793	O	HIS	F	165	1652	1878	2195	166	-183	-1	O

	ATOM	1795	N	LEU	F	166	-8.481	65.029	46.374	1.00	11.52		N
	ANISOU	1795	N	LEU	F	166	1211	1497	1668	91	230	121	N
	ATOM	1796	CA	LEU	F	166	-7.541	63.974	46.016	1.00	12.78		C
	ANISOU	1796	CA	LEU	F	166	1597	1666	1590	138	52	110	C
5	ATOM	1798	CB	LEU	F	166	-8.290	62.804	45.382	1.00	14.44		C
	ANISOU	1798	CB	LEU	F	166	1777	1764	1946	120	71	-13	C
	ATOM	1801	CG	LEU	F	166	-7.469	61.588	44.947	1.00	15.07		C
	ANISOU	1801	CG	LEU	F	166	1990	1874	1860	173	122	33	C
	ATOM	1803	CD1	LEU	F	166	-6.897	60.873	46.154	1.00	16.42		C
10	ANISOU	1803	CD1	LEU	F	166	2374	1484	2379	-11	-60	6	C
	ATOM	1807	CD2	LEU	F	166	-8.340	60.652	44.141	1.00	17.07		C
	ANISOU	1807	CD2	LEU	F	166	2248	1863	2375	135	24	-45	C
	ATOM	1811	C	LEU	F	166	-6.477	64.472	45.049	1.00	13.67		C
	ANISOU	1811	C	LEU	F	166	1790	1544	1857	-65	-29	122	C
15	ATOM	1812	O	LEU	F	166	-6.800	64.994	43.987	1.00	15.26		O
	ANISOU	1812	O	LEU	F	166	1777	2154	1864	46	27	137	O
	ATOM	1814	N	GLN	F	167	-5.212	64.310	45.441	1.00	13.19		N
	ANISOU	1814	N	GLN	F	167	1565	1676	1771	190	89	208	N
	ATOM	1815	CA	GLN	F	167	-4.076	64.572	44.569	1.00	13.66		C
20	ANISOU	1815	CA	GLN	F	167	1752	1765	1672	65	111	123	C
	ATOM	1817	CB	GLN	F	167	-2.905	65.188	45.344	1.00	14.94		C
	ANISOU	1817	CB	GLN	F	167	1755	1930	1991	-50	205	41	C
	ATOM	1820	CG	GLN	F	167	-1.640	65.423	44.507	1.00	15.01		C
	ANISOU	1820	CG	GLN	F	167	1914	1795	1991	-63	127	136	C
25	ATOM	1823	CD	GLN	F	167	-1.854	66.416	43.368	1.00	17.40		C
	ANISOU	1823	CD	GLN	F	167	2242	2237	2129	-51	-20	58	C
	ATOM	1824	OE1	GLN	F	167	-2.736	67.269	43.431	1.00	20.15		O
	ANISOU	1824	OE1	GLN	F	167	2162	2526	2969	-178	-175	569	O
	ATOM	1825	NE2	GLN	F	167	-1.028	66.317	42.335	1.00	19.20		N
30	ANISOU	1825	NE2	GLN	F	167	2496	2550	2249	-151	203	-22	N
	ATOM	1828	C	GLN	F	167	-3.627	63.267	43.927	1.00	13.05		C
	ANISOU	1828	C	GLN	F	167	1625	1516	1817	153	124	120	C
	ATOM	1829	O	GLN	F	167	-3.421	62.269	44.624	1.00	13.76		O
	ANISOU	1829	O	GLN	F	167	1721	1772	1736	260	85	260	O
35	ATOM	1831	N	ILE	F	168	-3.468	63.291	42.607	1.00	14.87		N
	ANISOU	1831	N	ILE	F	168	1836	1688	2124	55	121	175	N
	ATOM	1832	CA	ILE	F	168	-2.938	62.170	41.853	1.00	14.23		C
	ANISOU	1832	CA	ILE	F	168	1936	1779	1689	-47	176	99	C
	ATOM	1834	CB	ILE	F	168	-3.972	61.644	40.840	1.00	15.94		C
40	ANISOU	1834	CB	ILE	F	168	2066	2020	1969	0	136	39	C
	ATOM	1836	CG1	ILE	F	168	-5.324	61.437	41.534	1.00	16.59		C
	ANISOU	1836	CG1	ILE	F	168	1944	2172	2186	-260	41	47	C
	ATOM	1839	CD1	ILE	F	168	-6.452	61.063	40.606	1.00	18.38		C
	ANISOU	1839	CD1	ILE	F	168	2182	2492	2309	-183	45	51	C
45	ATOM	1843	CG2	ILE	F	168	-3.478	60.345	40.195	1.00	17.40		C
	ANISOU	1843	CG2	ILE	F	168	2314	2265	2031	-177	266	-129	C
	ATOM	1847	C	ILE	F	168	-1.694	62.638	41.110	1.00	15.01		C
	ANISOU	1847	C	ILE	F	168	1943	1926	1833	-57	118	-13	C
	ATOM	1848	O	ILE	F	168	-1.783	63.526	40.258	1.00	16.28		O
50	ANISOU	1848	O	ILE	F	168	2220	2457	1506	144	387	94	O
	ATOM	1850	N	ASN	F	169	-0.545	62.066	41.464	1.00	15.48		N
	ANISOU	1850	N	ASN	F	169	2082	1983	1816	-49	235	10	N
	ATOM	1851	CA	ASN	F	169	0.721	62.367	40.795	1.00	16.64		C
	ANISOU	1851	CA	ASN	F	169	2016	2220	2084	21	24	152	C
55	ATOM	1853	CB	ASN	F	169	1.901	62.353	41.779	1.00	19.99		C
	ANISOU	1853	CB	ASN	F	169	2434	2650	2508	-129	-100	-126	C
	ATOM	1856	CG	ASN	F	169	1.999	63.605	42.611	1.00	23.08		C
	ANISOU	1856	CG	ASN	F	169	2933	2871	2963	-34	71	13	C
	ATOM	1857	OD1	ASN	F	169	1.207	64.538	42.473	1.00	24.26		O
60	ANISOU	1857	OD1	ASN	F	169	3101	2780	3336	-6	286	-33	O
	ATOM	1858	ND2	ASN	F	169	2.993	63.632	43.485	1.00	26.89		N
	ANISOU	1858	ND2	ASN	F	169	3415	3687	3112	-255	-114	70	N
	ATOM	1861	C	ASN	F	169	0.990	61.329	39.730	1.00	16.40		C
	ANISOU	1861	C	ASN	F	169	1896	2179	2155	-119	23	46	C
65	ATOM	1862	O	ASN	F	169	0.919	60.136	40.009	1.00	16.84		O
	ANISOU	1862	O	ASN	F	169	1903	2173	2320	45	78	-183	O
	ATOM	1864	N	ASP	F	170	1.316	61.796	38.529	1.00	19.57		N
	ANISOU	1864	N	ASP	F	170	2391	2553	2491	-136	-12	-24	N
	ATOM	1865	CA	ASP	F	170	1.746	60.936	37.438	1.00	20.03		C
70	ANISOU	1865	CA	ASP	F	170	2571	2590	2447	-161	67	-40	C
	ATOM	1867	CB	ASP	F	170	3.135	60.353	37.744	1.00	23.81		C

	ANISOU	1867	CB	ASP	F	170	2990	3061	2993	81	41	-172	C
	ATOM	1870	CG	ASP	F	170	4.159	61.422	38.117	1.00	31.88		C
	ANISOU	1870	CG	ASP	F	170	3865	4131	4115	-49	33	50	C
	ATOM	1871	OD1	ASP	F	170	4.171	62.495	37.476	1.00	35.54		O
5	ANISOU	1871	OD1	ASP	F	170	4337	4358	4807	-35	238	185	O
	ATOM	1872	OD2	ASP	F	170	4.961	61.190	39.048	1.00	36.73		O
	ANISOU	1872	OD2	ASP	F	170	4486	4840	4628	99	4	176	O
	ATOM	1873	C	ASP	F	170	0.722	59.831	37.167	1.00	19.47		C
	ANISOU	1873	C	ASP	F	170	2331	2555	2511	-4	63	70	C
10	ATOM	1874	O	ASP	F	170	1.079	58.688	36.901	1.00	21.30		O
	ANISOU	1874	O	ASP	F	170	2575	2805	2711	-100	227	-201	O
	ATOM	1876	N	GLY	F	171	-0.556	60.184	37.251	1.00	17.25		N
	ANISOU	1876	N	GLY	F	171	2153	2160	2241	-113	139	-163	N
	ATOM	1877	CA	GLY	F	171	-1.620	59.220	36.995	1.00	15.70		C
15	ANISOU	1877	CA	GLY	F	171	1985	2096	1884	33	26	-160	C
	ATOM	1880	C	GLY	F	171	-1.803	58.999	35.510	1.00	14.75		C
	ANISOU	1880	C	GLY	F	171	1894	1808	1902	-53	123	-6	C
	ATOM	1881	O	GLY	F	171	-1.873	59.962	34.732	1.00	15.81		O
	ANISOU	1881	O	GLY	F	171	2129	1977	1900	79	-31	-53	O
20	ATOM	1883	N	GLU	F	172	-1.886	57.736	35.104	1.00	14.97		N
	ANISOU	1883	N	GLU	F	172	1853	1982	1851	-74	155	-53	N
	ATOM	1884	CA	GLU	F	172	-2.197	57.450	33.718	1.00	15.61		C
	ANISOU	1884	CA	GLU	F	172	1789	2071	2068	20	41	-77	C
	ATOM	1886	CB	GLU	F	172	-0.950	57.477	32.825	1.00	21.74		C
25	ANISOU	1886	CB	GLU	F	172	2547	2967	2744	-137	192	-67	C
	ATOM	1889	CG	GLU	F	172	0.024	56.380	33.056	1.00	22.88		C
	ANISOU	1889	CG	GLU	F	172	2749	2914	3029	-53	234	-86	C
	ATOM	1892	CD	GLU	F	172	1.198	56.398	32.071	1.00	23.85		C
	ANISOU	1892	CD	GLU	F	172	2752	3107	3203	-35	364	110	C
30	ATOM	1893	OE1	GLU	F	172	1.357	57.372	31.298	1.00	24.37		O
	ANISOU	1893	OE1	GLU	F	172	2645	3619	2994	480	232	340	O
	ATOM	1894	OE2	GLU	F	172	1.966	55.422	32.089	1.00	27.42		O
	ANISOU	1894	OE2	GLU	F	172	3083	3424	3910	188	417	15	O
	ATOM	1895	C	GLU	F	172	-2.968	56.159	33.546	1.00	14.33		C
35	ANISOU	1895	C	GLU	F	172	1878	1719	1848	114	116	-41	C
	ATOM	1896	O	GLU	F	172	-2.824	55.212	34.322	1.00	15.78		O
	ANISOU	1896	O	GLU	F	172	2100	1903	1990	139	-77	12	O
	ATOM	1898	N	LEU	F	173	-3.817	56.162	32.527	1.00	15.26		N
	ANISOU	1898	N	LEU	F	173	2026	1804	1967	102	-97	-46	N
40	ATOM	1899	CA	LEU	F	173	-4.612	55.022	32.134	1.00	15.42		C
	ANISOU	1899	CA	LEU	F	173	1840	2063	1956	28	-15	-225	C
	ATOM	1901	CB	LEU	F	173	-6.100	55.378	32.180	1.00	16.05		C
	ANISOU	1901	CB	LEU	F	173	1961	2092	2044	30	90	-148	C
	ATOM	1904	CG	LEU	F	173	-7.060	54.258	31.756	1.00	17.75		C
45	ANISOU	1904	CG	LEU	F	173	2157	2431	2157	79	-162	-413	C
	ATOM	1906	CD1	LEU	F	173	-7.108	53.184	32.806	1.00	18.22		C
	ANISOU	1906	CD1	LEU	F	173	1996	2105	2820	83	36	-327	C
	ATOM	1910	CD2	LEU	F	173	-8.455	54.822	31.504	1.00	20.29		C
	ANISOU	1910	CD2	LEU	F	173	2358	2773	2576	144	-218	-271	C
50	ATOM	1914	C	LEU	F	173	-4.202	54.680	30.711	1.00	17.24		C
	ANISOU	1914	C	LEU	F	173	2379	2024	2147	6	96	-128	C
	ATOM	1915	O	LEU	F	173	-4.208	55.552	29.839	1.00	17.45		O
	ANISOU	1915	O	LEU	F	173	2686	2094	1847	213	28	-94	O
	ATOM	1917	N	ILE	F	174	-3.840	53.422	30.486	1.00	14.95		N
55	ANISOU	1917	N	ILE	F	174	1940	1807	1931	87	23	-78	N
	ATOM	1918	CA	ILE	F	174	-3.501	52.932	29.159	1.00	15.00		C
	ANISOU	1918	CA	ILE	F	174	1848	1886	1963	134	-3	118	C
	ATOM	1920	CB	ILE	F	174	-2.067	52.389	29.092	1.00	15.25		C
	ANISOU	1920	CB	ILE	F	174	1913	2007	1874	274	20	-61	C
60	ATOM	1922	CG1	ILE	F	174	-1.081	53.517	29.431	1.00	17.85		C
	ANISOU	1922	CG1	ILE	F	174	1905	2359	2516	110	-217	213	C
	ATOM	1925	CD1	ILE	F	174	0.398	53.098	29.524	1.00	18.77		C
	ANISOU	1925	CD1	ILE	F	174	1970	2517	2644	171	-13	85	C
	ATOM	1929	CG2	ILE	F	174	-1.788	51.842	27.704	1.00	18.57		C
65	ANISOU	1929	CG2	ILE	F	174	2222	2626	2205	324	-33	-210	C
	ATOM	1933	C	ILE	F	174	-4.486	51.847	28.785	1.00	14.91		C
	ANISOU	1933	C	ILE	F	174	2001	1818	1844	8	-102	-40	C
	ATOM	1934	O	ILE	F	174	-4.676	50.895	29.530	1.00	16.31		O
	ANISOU	1934	O	ILE	F	174	2305	2054	1836	-202	-52	-41	O
70	ATOM	1936	N	VAL	F	175	-5.135	52.029	27.638	1.00	14.84		N
	ANISOU	1936	N	VAL	F	175	2047	1783	1807	-121	-149	61	N

	ATOM	1937	CA	VAL	F	175	-6.032	51.041	27.067	1.00	15.25		C
	ANISOU	1937	CA	VAL	F	175	1981	1876	1934	-193	82	-26	C
	ATOM	1939	CB	VAL	F	175	-7.446	51.607	26.895	1.00	15.72		C
	ANISOU	1939	CB	VAL	F	175	2027	1993	1952	-73	37	16	C
5	ATOM	1941	CG1	VAL	F	175	-8.373	50.549	26.339	1.00	17.65		C
	ANISOU	1941	CG1	VAL	F	175	2272	2195	2236	-116	-74	-24	C
	ATOM	1945	CG2	VAL	F	175	-7.975	52.128	28.229	1.00	16.50		C
	ANISOU	1945	CG2	VAL	F	175	2157	2099	2013	-49	103	-100	C
	ATOM	1949	C	VAL	F	175	-5.455	50.660	25.708	1.00	14.19		C
10	ANISOU	1949	C	VAL	F	175	1742	1777	1873	-80	-8	-147	C
	ATOM	1950	O	VAL	F	175	-5.279	51.524	24.854	1.00	15.82		O
	ANISOU	1950	O	VAL	F	175	2386	1775	1847	-60	55	63	O
	ATOM	1952	N	VAL	F	176	-5.117	49.389	25.519	1.00	14.60		N
	ANISOU	1952	N	VAL	F	176	1944	1777	1824	-104	9	-57	N
15	ATOM	1953	CA	VAL	F	176	-4.452	48.966	24.289	1.00	14.55		C
	ANISOU	1953	CA	VAL	F	176	1886	1793	1846	-115	63	27	C
	ATOM	1955	CB	VAL	F	176	-2.912	48.993	24.431	1.00	16.92		C
	ANISOU	1955	CB	VAL	F	176	2133	2255	2038	-54	-35	61	C
	ATOM	1957	CG1	VAL	F	176	-2.447	48.219	25.603	1.00	19.92		C
20	ANISOU	1957	CG1	VAL	F	176	2358	2567	2642	-121	162	41	C
	ATOM	1961	CG2	VAL	F	176	-2.224	48.549	23.150	1.00	16.21		C
	ANISOU	1961	CG2	VAL	F	176	1751	2303	2102	41	-60	-147	C
	ATOM	1965	C	VAL	F	176	-4.974	47.628	23.781	1.00	13.32		C
	ANISOU	1965	C	VAL	F	176	1559	1698	1801	144	206	-80	C
25	ATOM	1966	O	VAL	F	176	-5.036	46.648	24.513	1.00	14.24		O
	ANISOU	1966	O	VAL	F	176	1786	1820	1802	37	-31	104	O
	ATOM	1968	N	GLN	F	177	-5.335	47.609	22.502	1.00	13.81		N
	ANISOU	1968	N	GLN	F	177	1738	1686	1820	-24	86	69	N
	ATOM	1969	CA	GLN	F	177	-5.921	46.444	21.862	1.00	13.58		C
30	ANISOU	1969	CA	GLN	F	177	1720	1710	1730	25	38	-17	C
	ATOM	1971	CB	GLN	F	177	-6.580	46.891	20.556	1.00	14.37		C
	ANISOU	1971	CB	GLN	F	177	1696	1875	1887	-57	-16	-115	C
	ATOM	1974	CG	GLN	F	177	-7.376	45.845	19.828	1.00	14.39		C
	ANISOU	1974	CG	GLN	F	177	1873	1726	1868	-135	-6	22	C
35	ATOM	1977	CD	GLN	F	177	-7.927	46.370	18.527	1.00	14.67		C
	ANISOU	1977	CD	GLN	F	177	1847	1902	1824	-139	-88	-26	C
	ATOM	1978	OE1	GLN	F	177	-7.303	47.228	17.875	1.00	15.37		O
	ANISOU	1978	OE1	GLN	F	177	1984	1919	1936	-331	-8	1	O
	ATOM	1979	NE2	GLN	F	177	-9.089	45.848	18.118	1.00	15.69		N
40	ANISOU	1979	NE2	GLN	F	177	1737	1936	2288	-228	-15	-30	N
	ATOM	1982	C	GLN	F	177	-4.851	45.393	21.581	1.00	14.62		C
	ANISOU	1982	C	GLN	F	177	1773	1788	1994	67	43	76	C
	ATOM	1983	O	GLN	F	177	-3.795	45.718	21.034	1.00	16.34		O
	ANISOU	1983	O	GLN	F	177	1974	1827	2407	-26	359	160	O
45	ATOM	1985	N	LEU	F	178	-5.141	44.144	21.943	1.00	13.42		N
	ANISOU	1985	N	LEU	F	178	1639	1641	1818	8	185	-54	N
	ATOM	1986	CA	LEU	F	178	-4.253	43.006	21.691	1.00	14.36		C
	ANISOU	1986	CA	LEU	F	178	1740	1740	1974	35	80	-42	C
	ATOM	1988	CB	LEU	F	178	-4.153	42.127	22.931	1.00	14.43		C
50	ANISOU	1988	CB	LEU	F	178	1695	1784	2003	-78	-68	77	C
	ATOM	1991	CG	LEU	F	178	-3.707	42.819	24.208	1.00	14.48		C
	ANISOU	1991	CG	LEU	F	178	1898	1881	1721	17	89	62	C
	ATOM	1993	CD1	LEU	F	178	-3.728	41.823	25.330	1.00	15.93		C
	ANISOU	1993	CD1	LEU	F	178	2077	2299	1675	-125	-105	56	C
55	ATOM	1997	CD2	LEU	F	178	-2.330	43.430	24.054	1.00	16.96		C
	ANISOU	1997	CD2	LEU	F	178	1926	2313	2203	68	-64	52	C
	ATOM	2001	C	LEU	F	178	-4.693	42.117	20.541	1.00	14.89		C
	ANISOU	2001	C	LEU	F	178	1882	1903	1870	27	-147	73	C
	ATOM	2002	O	LEU	F	178	-3.865	41.431	19.948	1.00	15.70		O
60	ANISOU	2002	O	LEU	F	178	1852	2134	1979	160	-42	-27	O
	ATOM	2004	N	THR	F	179	-5.988	42.085	20.260	1.00	13.89		N
	ANISOU	2004	N	THR	F	179	1688	1680	1908	148	-21	-131	N
	ATOM	2005	CA	THR	F	179	-6.506	41.276	19.171	1.00	14.91		C
	ANISOU	2005	CA	THR	F	179	1766	1880	2019	-38	-73	-50	C
65	ATOM	2007	CB	THR	F	179	-7.210	39.995	19.662	1.00	15.23		C
	ANISOU	2007	CB	THR	F	179	1985	1906	1895	-35	100	-103	C
	ATOM	2009	OG1	THR	F	179	-8.342	40.340	20.465	1.00	16.72		O
	ANISOU	2009	OG1	THR	F	179	2092	2059	2201	-136	436	-110	O
	ATOM	2011	CG2	THR	F	179	-6.265	39.158	20.473	1.00	16.64		C
70	ANISOU	2011	CG2	THR	F	179	2385	1915	2022	4	42	-65	C
	ATOM	2015	C	THR	F	179	-7.477	42.106	18.354	1.00	15.55		C

	ANISOU	2015	C	THR	F	179	1987	1949	1971	-162	-114	3	C
	ATOM	2016	O	THR	F	179	-8.160	42.964	18.896	1.00	15.86		O
	ANISOU	2016	O	THR	F	179	1790	1938	2298	-39	-201	-56	O
	ATOM	2018	N	PRO	F	180	-7.531	41.859	17.042	1.00	17.37		N
5	ANISOU	2018	N	PRO	F	180	2350	2131	2117	188	-162	-16	N
	ATOM	2019	CA	PRO	F	180	-8.405	42.622	16.168	1.00	17.80		C
	ANISOU	2019	CA	PRO	F	180	2234	2294	2234	159	-188	-23	C
	ATOM	2021	CB	PRO	F	180	-7.852	42.306	14.780	1.00	20.17		C
10	ANISOU	2021	CB	PRO	F	180	2376	2879	2406	151	-192	76	C
	ATOM	2024	CG	PRO	F	180	-7.323	40.927	14.908	1.00	20.77		C
	ANISOU	2024	CG	PRO	F	180	2704	2823	2362	57	-15	-138	C
	ATOM	2027	CD	PRO	F	180	-6.740	40.864	16.295	1.00	18.87		C
	ANISOU	2027	CD	PRO	F	180	2430	2596	2141	182	205	-156	C
	ATOM	2030	C	PRO	F	180	-9.865	42.193	16.293	1.00	18.44		C
15	ANISOU	2030	C	PRO	F	180	2364	2337	2304	129	-120	56	C
	ATOM	2031	O	PRO	F	180	-10.174	41.097	16.751	1.00	21.99		O
	ANISOU	2031	O	PRO	F	180	2676	2735	2942	287	-278	186	O
	ATOM	2032	N	GLY	F	181	-10.760	43.074	15.882	1.00	19.14		N
	ANISOU	2032	N	GLY	F	181	2262	2461	2547	189	52	63	N
20	ATOM	2033	CA	GLY	F	181	-12.176	42.764	15.893	1.00	17.72		C
	ANISOU	2033	CA	GLY	F	181	2283	2303	2144	1	92	-26	C
	ATOM	2036	C	GLY	F	181	-12.944	43.744	15.046	1.00	18.20		C
	ANISOU	2036	C	GLY	F	181	2174	2281	2458	-16	99	45	C
	ATOM	2037	O	GLY	F	181	-12.377	44.659	14.452	1.00	19.48		O
25	ANISOU	2037	O	GLY	F	181	2159	2484	2757	-102	21	320	O
	ATOM	2039	N	TYR	F	182	-14.247	43.542	14.994	1.00	16.77		N
	ANISOU	2039	N	TYR	F	182	2066	1897	2407	-237	-17	-63	N
	ATOM	2040	CA	TYR	F	182	-15.113	44.415	14.250	1.00	18.04		C
	ANISOU	2040	CA	TYR	F	182	2290	2171	2390	-75	-102	-123	C
30	ATOM	2042	CB	TYR	F	182	-16.559	43.957	14.407	1.00	21.95		C
	ANISOU	2042	CB	TYR	F	182	2637	2756	2943	-170	2	44	C
	ATOM	2045	CG	TYR	F	182	-17.539	44.951	13.873	1.00	22.91		C
	ANISOU	2045	CG	TYR	F	182	2773	2754	3177	-159	90	84	C
	ATOM	2046	CD1	TYR	F	182	-17.898	44.940	12.534	1.00	23.56		C
35	ANISOU	2046	CD1	TYR	F	182	2741	2979	3229	-204	-10	203	C
	ATOM	2048	CE1	TYR	F	182	-18.793	45.863	12.028	1.00	23.27		C
	ANISOU	2048	CE1	TYR	F	182	2824	2842	3173	-56	51	162	C
	ATOM	2050	CZ	TYR	F	182	-19.333	46.811	12.864	1.00	22.67		C
	ANISOU	2050	CZ	TYR	F	182	2774	2857	2981	-168	7	88	C
40	ATOM	2051	OH	TYR	F	182	-20.223	47.720	12.350	1.00	24.51		O
	ANISOU	2051	OH	TYR	F	182	2952	3056	3302	-15	188	237	O
	ATOM	2053	CE2	TYR	F	182	-18.983	46.850	14.205	1.00	24.49		C
	ANISOU	2053	CE2	TYR	F	182	3017	3108	3179	99	89	177	C
	ATOM	2055	CD2	TYR	F	182	-18.089	45.922	14.700	1.00	22.68		C
45	ANISOU	2055	CD2	TYR	F	182	2677	3027	2911	30	28	147	C
	ATOM	2057	C	TYR	F	182	-14.969	45.849	14.751	1.00	17.50		C
	ANISOU	2057	C	TYR	F	182	2436	2036	2178	-63	-147	-38	C
	ATOM	2058	O	TYR	F	182	-14.967	46.075	15.957	1.00	16.98		O
	ANISOU	2058	O	TYR	F	182	2363	2155	1930	-215	-220	197	O
50	ATOM	2060	N	CYS	F	183	-14.855	46.802	13.825	1.00	17.83		N
	ANISOU	2060	N	CYS	F	183	2392	2281	2101	-272	-120	-113	N
	ATOM	2061	CA	CYS	F	183	-14.863	48.226	14.159	1.00	20.04		C
	ANISOU	2061	CA	CYS	F	183	2682	2467	2465	-89	-25	-173	C
	ATOM	2063	CB	CYS	F	183	-13.664	48.942	13.551	1.00	21.00		C
55	ANISOU	2063	CB	CYS	F	183	2866	2599	2514	-233	45	-69	C
	ATOM	2066	SG	CYS	F	183	-12.087	48.424	14.206	1.00	24.51		S
	ANISOU	2066	SG	CYS	F	183	3195	3064	3053	-242	88	108	S
	ATOM	2068	C	CYS	F	183	-16.117	48.875	13.626	1.00	20.52		C
	ANISOU	2068	C	CYS	F	183	2751	2357	2690	-60	4	58	C
60	ATOM	2069	O	CYS	F	183	-16.496	48.636	12.481	1.00	21.28		O
	ANISOU	2069	O	CYS	F	183	3001	2574	2509	-197	56	224	O
	ATOM	2071	N	ALA	F	184	-16.746	49.707	14.452	1.00	21.80		N
	ANISOU	2071	N	ALA	F	184	2904	2794	2584	0	-97	-97	N
	ATOM	2072	CA	ALA	F	184	-17.899	50.493	14.027	1.00	25.91		C
65	ANISOU	2072	CA	ALA	F	184	3239	3284	3319	110	27	-52	C
	ATOM	2074	CB	ALA	F	184	-18.520	51.209	15.221	1.00	27.04		C
	ANISOU	2074	CB	ALA	F	184	3458	3397	3415	148	86	42	C
	ATOM	2078	C	ALA	F	184	-17.472	51.512	12.970	1.00	28.78		C
	ANISOU	2078	C	ALA	F	184	3607	3650	3679	9	81	68	C
70	ATOM	2079	O	ALA	F	184	-16.365	52.051	13.045	1.00	30.99		O
	ANISOU	2079	O	ALA	F	184	3798	3987	3989	-121	-51	119	O

	ATOM	2081	N	PRO	F	185	-18.339	51.774	11.977	1.00	29.74		N
	ANISOU	2081	N	PRO	F	185	3797	3733	3770	16	68	76	N
	ATOM	2082	CA	PRO	F	185	-18.091	52.821	10.978	1.00	30.44		C
	ANISOU	2082	CA	PRO	F	185	3945	3819	3799	16	88	86	C
5	ATOM	2084	CB	PRO	F	185	-19.431	52.925	10.246	1.00	30.69		C
	ANISOU	2084	CB	PRO	F	185	3958	3835	3865	-17	16	30	C
	ATOM	2087	CG	PRO	F	185	-20.040	51.589	10.385	1.00	29.98		C
	ANISOU	2087	CG	PRO	F	185	3813	3743	3832	-4	14	49	C
	ATOM	2090	CD	PRO	F	185	-19.604	51.061	11.714	1.00	29.33		C
10	ANISOU	2090	CD	PRO	F	185	3753	3640	3750	-31	-3	7	C
	ATOM	2093	C	PRO	F	185	-17.717	54.178	11.580	1.00	33.44		C
	ANISOU	2093	C	PRO	F	185	4416	4061	4226	-47	54	-29	C
	ATOM	2094	O	PRO	F	185	-18.101	54.484	12.710	1.00	36.58		O
	ANISOU	2094	O	PRO	F	185	4864	4486	4548	-7	186	-16	O
15	ATOM	2095	Cl	NAG	F	200	-21.028	63.219	31.740	1.00	30.10		C
	ANISOU	2095	Cl	NAG	F	200	3763	3900	3773	79	77	-39	C
	ATOM	2098	C2	NAG	F	200	-22.434	63.530	31.236	1.00	32.17		C
	ANISOU	2098	C2	NAG	F	200	4039	4137	4045	48	-28	35	C
	ATOM	2100	N2	NAG	F	200	-22.442	64.540	30.186	1.00	33.66		N
20	ANISOU	2100	N2	NAG	F	200	4279	4333	4176	20	2	47	N
	ATOM	2102	C7	NAG	F	200	-22.582	64.219	28.898	1.00	34.85		C
	ANISOU	2102	C7	NAG	F	200	4410	4563	4266	-52	9	-9	C
	ATOM	2103	O7	NAG	F	200	-21.706	64.433	28.060	1.00	38.15		O
	ANISOU	2103	O7	NAG	F	200	4794	5087	4611	-225	81	70	O
25	ATOM	2104	C8	NAG	F	200	-23.867	63.563	28.486	1.00	33.97		C
	ANISOU	2104	C8	NAG	F	200	4326	4405	4175	-56	9	-5	C
	ATOM	2108	C3	NAG	F	200	-23.261	63.969	32.432	1.00	32.46		C
	ANISOU	2108	C3	NAG	F	200	4028	4205	4099	63	32	56	C
	ATOM	2110	O3	NAG	F	200	-24.561	64.337	32.019	1.00	34.73		O
30	ANISOU	2110	O3	NAG	F	200	4185	4540	4470	129	-64	148	O
	ATOM	2112	C4	NAG	F	200	-23.349	62.826	33.438	1.00	32.07		C
	ANISOU	2112	C4	NAG	F	200	3989	4144	4052	107	7	31	C
	ATOM	2114	O4	NAG	F	200	-23.864	63.340	34.653	1.00	32.07		O
	ANISOU	2114	O4	NAG	F	200	4103	4211	3868	68	-44	95	O
35	ATOM	2116	C5	NAG	F	200	-22.001	62.134	33.704	1.00	32.25		C
	ANISOU	2116	C5	NAG	F	200	3995	4187	4069	81	53	83	C
	ATOM	2118	C6	NAG	F	200	-22.218	60.673	34.102	1.00	32.38		C
	ANISOU	2118	C6	NAG	F	200	4000	4188	4115	23	8	53	C
	ATOM	2121	O6	NAG	F	200	-22.509	60.569	35.475	1.00	35.19		O
40	ANISOU	2121	O6	NAG	F	200	4485	4698	4189	15	-17	150	O
	ATOM	2123	O5	NAG	F	200	-21.100	62.103	32.604	1.00	31.54		O
	ANISOU	2123	O5	NAG	F	200	3923	4087	3971	40	94	65	O
	ATOM	2124	S	S04	F	201	4.476	61.749	28.616	1.00	17.31		S
	ANISOU	2124	S	S04	F	201	2363	2131	2082	336	-232	432	S
45	ATOM	2125	O1	S04	F	201	4.876	60.864	27.532	1.00	18.13		O
	ANISOU	2125	O1	S04	F	201	2426	2211	2250	545	-306	301	O
	ATOM	2126	O2	S04	F	201	3.472	62.689	28.124	1.00	18.62		O
	ANISOU	2126	O2	S04	F	201	2138	2646	2289	671	-211	354	O
	ATOM	2127	O3	S04	F	201	5.624	62.472	29.139	1.00	20.60		O
50	ANISOU	2127	O3	S04	F	201	2604	2640	2581	66	-289	280	O
	ATOM	2128	O4	S04	F	201	3.892	60.946	29.692	1.00	20.33		O
	ANISOU	2128	O4	S04	F	201	3006	2470	2246	80	-226	479	O
	ATOM	2129	O	HOH	W	102	-1.272	45.036	20.445	1.00	19.51		O
	ANISOU	2129	O	HOH	W	102	2034	1797	3581	92	160	229	O
55	ATOM	2132	O	HOH	W	103	-20.926	47.481	24.342	1.00	22.65		O
	ANISOU	2132	O	HOH	W	103	2402	2974	3228	-266	-773	-607	O
	ATOM	2135	O	HOH	W	104	-13.426	58.236	34.448	1.00	16.92		O
	ANISOU	2135	O	HOH	W	104	2421	1730	2276	-314	-84	-644	O
	ATOM	2138	O	HOH	W	105	-1.818	62.903	22.227	1.00	21.85		O
60	ANISOU	2138	O	HOH	W	105	2615	2679	3008	247	-47	-14	O
	ATOM	2141	O	HOH	W	107	-12.718	55.843	20.134	1.00	22.61		O
	ANISOU	2141	O	HOH	W	107	2911	2872	2805	-112	-567	-91	O
	ATOM	2144	O	HOH	W	108	-11.623	50.947	19.906	1.00	16.14		O
	ANISOU	2144	O	HOH	W	108	2124	1789	2217	-38	-476	-50	O
65	ATOM	2147	O	HOH	W	109	-1.948	48.448	42.204	1.00	19.71		O
	ANISOU	2147	O	HOH	W	109	2800	2090	2595	-30	-29	277	O
	ATOM	2150	O	HOH	W	110	-17.361	47.014	34.149	1.00	25.48		O
	ANISOU	2150	O	HOH	W	110	3026	3201	3451	-999	-238	-489	O
	ATOM	2153	O	HOH	W	111	-9.232	65.632	42.922	1.00	18.09		O
70	ANISOU	2153	O	HOH	W	111	2511	2094	2266	-142	261	-755	O
	ATOM	2156	O	HOH	W	112	-10.785	40.613	33.197	1.00	21.81		O

	ANISOU	2156	0	HOH	W	112	2135	3346	2805	-89	343	57	0
	ATOM	2159	0	HOH	W	113	-10.525	39.753	19.175	1.00	23.82		0
	ANISOU	2159	0	HOH	W	113	2861	3205	2985	-233	-185	-538	0
	ATOM	2162	0	HOH	W	114	4.026	55.134	21.171	1.00	24.30		0
5	ANISOU	2162	0	HOH	W	114	3574	2486	3171	352	107	-182	0
	ATOM	2165	0	HOH	W	115	-11.479	54.725	17.961	1.00	25.20		0
	ANISOU	2165	0	HOH	W	115	3217	2943	3415	184	-131	-1	0
	ATOM	2168	0	HOH	W	116	-4.659	65.575	41.220	1.00	22.14		0
	ANISOU	2168	0	HOH	W	116	3548	2433	2432	52	-340	-517	0
10	ATOM	2171	0	HOH	W	117	-13.802	64.113	28.720	1.00	31.81		0
	ANISOU	2171	0	HOH	W	117	4288	3636	4162	159	-319	130	0
	ATOM	2174	0	HOH	W	118	-1.998	62.708	37.586	1.00	17.07		0
	ANISOU	2174	0	HOH	W	118	2553	1889	2041	-188	-179	-308	0
	ATOM	2177	0	HOH	W	119	2.433	54.015	40.803	1.00	33.43		0
15	ANISOU	2177	0	HOH	W	119	4060	4162	4478	91	21	-241	0
	ATOM	2180	0	HOH	W	120	-7.604	47.458	15.112	1.00	29.94		0
	ANISOU	2180	0	HOH	W	120	4288	4167	2918	-721	244	-132	0
	ATOM	2183	0	HOH	W	121	-8.607	66.352	33.122	1.00	31.41		0
	ANISOU	2183	0	HOH	W	121	3921	4032	3979	66	-216	69	0
20	ATOM	2186	0	HOH	W	122	-19.093	62.559	36.968	1.00	30.39		0
	ANISOU	2186	0	HOH	W	122	3265	4238	4042	459	-119	-644	0
	ATOM	2189	0	HOH	W	123	-18.077	53.250	22.952	1.00	32.72		0
	ANISOU	2189	0	HOH	W	123	3686	4336	4407	-18	-219	-207	0
	ATOM	2192	0	HOH	W	124	3.157	57.818	20.374	1.00	31.42		0
25	ANISOU	2192	0	HOH	W	124	3487	4465	3985	385	129	62	0
	ATOM	2195	0	HOH	W	125	-5.989	48.127	48.178	1.00	36.72		0
	ANISOU	2195	0	HOH	W	125	5025	5169	3755	-106	320	91	0
	ATOM	2198	0	HOH	W	126	-18.812	57.599	42.091	1.00	38.14		0
	ANISOU	2198	0	HOH	W	126	4296	4971	5223	183	479	-380	0
30	ATOM	2201	0	HOH	W	127	-9.787	45.954	15.229	1.00	21.65		0
	ANISOU	2201	0	HOH	W	127	3112	2894	2218	-72	-517	-283	0
	ATOM	2204	0	HOH	W	128	0.414	55.247	20.342	1.00	21.30		0
	ANISOU	2204	0	HOH	W	128	2549	2697	2848	-88	50	54	0
	ATOM	2207	0	HOH	W	129	-7.963	60.952	22.200	1.00	25.36		0
35	ANISOU	2207	0	HOH	W	129	3719	2190	3725	156	-527	31	0
	ATOM	2210	0	HOH	W	130	-8.102	51.819	44.462	1.00	23.55		0
	ANISOU	2210	0	HOH	W	130	3185	2475	3285	39	3	-438	0
	ATOM	2213	0	HOH	W	131	-1.453	50.223	14.260	1.00	29.43		0
	ANISOU	2213	0	HOH	W	131	3173	4383	3623	-157	632	173	0
40	ATOM	2216	0	HOH	W	132	-16.971	40.038	24.996	1.00	20.61		0
	ANISOU	2216	0	HOH	W	132	2298	2606	2926	-216	-222	-378	0
	ATOM	2219	0	HOH	W	133	7.688	54.238	42.249	1.00	31.68		0
	ANISOU	2219	0	HOH	W	133	4315	3951	3770	568	419	-398	0
	ATOM	2222	0	HOH	W	134	-19.445	44.958	18.832	1.00	26.98		0
45	ANISOU	2222	0	HOH	W	134	3270	3364	3616	-241	-109	-222	0
	ATOM	2225	0	HOH	W	135	-6.264	67.507	42.525	1.00	30.67		0
	ANISOU	2225	0	HOH	W	135	3791	3729	4131	-13	-160	-342	0
	ATOM	2228	0	HOH	W	136	4.438	64.688	46.307	1.00	24.99		0
	ANISOU	2228	0	HOH	W	136	3081	2587	3828	-243	275	-181	0
50	ATOM	2231	0	HOH	W	137	-0.433	52.710	13.943	1.00	35.50		0
	ANISOU	2231	0	HOH	W	137	4258	4565	4664	247	2	85	0
	ATOM	2234	0	HOH	W	138	-19.854	50.788	28.894	1.00	32.97		0
	ANISOU	2234	0	HOH	W	138	4468	3827	4231	123	627	-368	0
	ATOM	2237	0	HOH	W	139	-1.455	44.037	38.205	1.00	31.94		0
55	ANISOU	2237	0	HOH	W	139	4513	3796	3824	158	-473	227	0
	ATOM	2240	0	HOH	W	140	-15.747	42.294	36.438	1.00	37.11		0
	ANISOU	2240	0	HOH	W	140	4789	4384	4927	52	-60	0	0
	ATOM	2243	0	HOH	W	141	-14.593	45.948	11.031	1.00	34.46		0
	ANISOU	2243	0	HOH	W	141	4698	4941	3453	-36	-436	-103	0
60	ATOM	2246	0	HOH	W	142	3.026	46.194	47.081	1.00	30.31		0
	ANISOU	2246	0	HOH	W	142	4040	3696	3779	396	127	314	0
	ATOM	2249	0	HOH	W	143	-10.257	62.436	22.662	1.00	27.49		0
	ANISOU	2249	0	HOH	W	143	4475	2149	3821	-156	194	293	0
	ATOM	2252	0	HOH	W	144	-11.773	55.925	48.147	1.00	37.17		0
65	ANISOU	2252	0	HOH	W	144	5025	4647	4450	163	-83	-304	0
	ATOM	2255	0	HOH	W	145	-5.114	46.241	13.538	1.00	49.22		0
	ANISOU	2255	0	HOH	W	145	6244	6477	5981	-67	-13	-4	0
	ATOM	2258	0	HOH	W	146	-9.018	64.821	26.736	1.00	35.18		0
	ANISOU	2258	0	HOH	W	146	4216	4204	4947	226	158	3	0
70	ATOM	2261	0	HOH	W	148	0.002	42.809	21.295	0.33	20.62		0
	ANISOU	2261	0	HOH	W	148	2467	2467	2897	0	0	0	0

	ATOM	2264	0	HOH	W	149	-20.830	48.490	27.934	1.00	23.74	0
	ANISOU	2264	0	HOH	W	149	2862	3179	2979	95	171	-613
	ATOM	2267	0	HOH	W	150	-14.581	41.607	22.420	1.00	23.84	0
	ANISOU	2267	0	HOH	W	150	3791	2062	3204	-201	-131	-224
5	ATOM	2270	0	HOH	W	151	-17.034	53.779	42.672	1.00	28.29	0
	ANISOU	2270	0	HOH	W	151	3875	3593	3279	-242	449	-161
	ATOM	2273	0	HOH	W	153	-0.167	61.931	34.026	1.00	32.11	0
	ANISOU	2273	0	HOH	W	153	4347	3624	4229	-743	-42	348
	ATOM	2276	0	HOH	W	154	-2.805	61.480	18.807	1.00	28.09	0
10	ANISOU	2276	0	HOH	W	154	4258	2391	4021	85	10	886
	ATOM	2279	0	HOH	W	155	-14.660	57.218	18.936	1.00	36.02	0
	ANISOU	2279	0	HOH	W	155	4563	4355	4766	342	-220	0
	ATOM	2282	0	HOH	W	156	-15.297	41.286	16.642	1.00	28.25	0
	ANISOU	2282	0	HOH	W	156	3304	3297	4131	-545	-518	-216
15	ATOM	2285	0	HOH	W	157	-2.243	57.376	49.840	1.00	27.49	0
	ANISOU	2285	0	HOH	W	157	3773	3402	3269	111	-113	-221
	ATOM	2288	0	HOH	W	158	-11.052	65.750	31.721	1.00	30.00	0
	ANISOU	2288	0	HOH	W	158	4377	2979	4041	-36	-73	-204
	ATOM	2291	0	HOH	W	159	-18.733	50.460	31.261	1.00	32.59	0
20	ANISOU	2291	0	HOH	W	159	3598	3681	5101	-233	111	-265
	ATOM	2294	0	HOH	W	160	-17.389	63.326	33.651	1.00	29.08	0
	ANISOU	2294	0	HOH	W	160	3061	3483	4505	731	254	-527
	ATOM	2297	0	HOH	W	163	-2.824	41.746	36.954	1.00	22.98	0
	ANISOU	2297	0	HOH	W	163	3178	2376	3174	-19	236	96
25	ATOM	2300	0	HOH	W	166	-1.347	62.571	51.614	1.00	29.56	0
	ANISOU	2300	0	HOH	W	166	3997	3431	3803	224	80	305
	ATOM	2303	0	HOH	W	167	-17.508	64.604	37.456	1.00	38.73	0
	ANISOU	2303	0	HOH	W	167	5032	5154	4528	35	0	-37
	ATOM	2306	0	HOH	W	168	-10.121	49.371	45.573	1.00	36.68	0
30	ANISOU	2306	0	HOH	W	168	4890	4692	4353	-254	63	-212
	ATOM	2309	0	HOH	W	169	-17.875	59.214	31.890	1.00	39.88	0
	ANISOU	2309	0	HOH	W	169	5220	5114	4815	12	-68	-283
	ATOM	2312	0	HOH	W	170	-11.118	64.605	28.842	1.00	33.58	0
	ANISOU	2312	0	HOH	W	170	4482	4039	4238	135	-163	336
35	ATOM	2315	0	HOH	W	171	2.773	57.449	35.259	1.00	38.57	0
	ANISOU	2315	0	HOH	W	171	4880	4868	4906	-151	60	-120
	ATOM	2318	0	HOH	W	172	-16.223	60.008	45.734	1.00	33.89	0
	ANISOU	2318	0	HOH	W	172	4171	4323	4381	-442	77	-118
	ATOM	2321	0	HOH	W	173	-17.917	64.871	51.915	1.00	40.44	0
40	ANISOU	2321	0	HOH	W	173	4801	5476	5087	121	463	-251
	ATOM	2324	0	HOH	W	176	-18.615	51.603	41.037	1.00	39.91	0
	ANISOU	2324	0	HOH	W	176	4865	5447	4850	9	126	-181
	ATOM	2327	0	HOH	W	177	-2.290	43.463	17.960	1.00	36.57	0
45	ANISOU	2327	0	HOH	W	177	5258	4396	4239	-273	249	108
	ATOM	2330	0	HOH	W	178	-18.592	40.312	37.066	1.00	45.41	0
	ANISOU	2330	0	HOH	W	178	5988	5497	5766	-270	217	-149
	ATOM	2333	0	HOH	W	179	-12.661	50.011	44.964	1.00	38.21	0
	ANISOU	2333	0	HOH	W	179	5534	4642	4341	-9	186	-8
	ATOM	2336	0	HOH	W	180	-15.870	65.334	26.487	1.00	44.98	0
50	ANISOU	2336	0	HOH	W	180	5920	5605	5562	238	-30	71
	ATOM	2339	0	HOH	W	181	-1.497	45.718	42.268	1.00	46.67	0
	ANISOU	2339	0	HOH	W	181	6000	5242	6489	133	-129	145
	ATOM	2342	0	HOH	W	182	-9.007	54.660	15.337	1.00	30.30	0
	ANISOU	2342	0	HOH	W	182	4148	3741	3624	312	-591	636
55	ATOM	2345	0	HOH	W	183	-16.725	68.640	50.051	1.00	35.36	0
	ANISOU	2345	0	HOH	W	183	4154	4188	5092	-368	292	130
	ATOM	2348	0	HOH	W	184	-6.500	62.585	20.455	1.00	38.40	0
	ANISOU	2348	0	HOH	W	184	5138	4120	5332	162	-451	215
	ATOM	2351	0	HOH	W	185	-0.818	63.914	35.532	1.00	42.56	0
60	ANISOU	2351	0	HOH	W	185	5537	5392	5242	-378	57	0
	ATOM	2354	0	HOH	W	186	-19.261	41.968	17.498	1.00	32.55	0
	ANISOU	2354	0	HOH	W	186	4279	3955	4131	-433	-664	-360
	ATOM	2357	0	HOH	W	187	-2.161	54.751	12.443	1.00	51.33	0
	ANISOU	2357	0	HOH	W	187	6555	6548	6400	-207	67	-55
65	ATOM	2360	0	HOH	W	188	8.065	54.660	45.373	1.00	47.00	0
	ANISOU	2360	0	HOH	W	188	5848	5869	6138	67	-16	-106
	ATOM	2363	0	HOH	W	190	8.082	49.232	46.085	1.00	41.83	0
	ANISOU	2363	0	HOH	W	190	5311	5032	5551	175	-35	142
	ATOM	2366	0	HOH	W	193	-7.492	50.820	48.827	1.00	46.76	0
70	ANISOU	2366	0	HOH	W	193	6076	5927	5762	53	179	130
	ATOM	2369	0	HOH	W	195	-13.334	68.992	41.155	1.00	48.46	0

	ANISOU	2369	0	HOH	W	195	6062	6228	6122	21	88	24	0
	ATOM	2372	0	HOH	W	198	-11.210	68.088	40.735	1.00	37.12		0
	ANISOU	2372	0	HOH	W	198	5096	4237	4768	-23	68	-255	0
	ATOM	2375	0	HOH	W	199	-1.209	45.229	45.850	1.00	41.80		0
5	ANISOU	2375	0	HOH	W	199	5122	4864	5894	40	91	-138	0
	ATOM	2378	0	HOH	W	200	-0.209	64.949	31.175	1.00	42.90		0
	ANISOU	2378	0	HOH	W	200	5637	5446	5217	-258	-149	127	0
	ATOM	2381	0	HOH	W	201	-14.698	49.311	46.572	1.00	43.90		0
	ANISOU	2381	0	HOH	W	201	5543	5559	5575	-94	-37	-90	0
10	ATOM	2384	0	HOH	W	202	-5.161	61.193	17.491	1.00	39.45		0
	ANISOU	2384	0	HOH	W	202	5371	4486	5130	-174	-36	376	0
	ATOM	2387	0	HOH	W	206	-3.300	66.537	37.955	1.00	45.17		0
	ANISOU	2387	0	HOH	W	206	5318	5743	6101	-155	41	-79	0
	ATOM	2390	0	HOH	W	207	-20.335	50.000	35.063	1.00	46.13		0
15	ANISOU	2390	0	HOH	W	207	5544	5707	6276	-234	-196	17	0
	ATOM	2393	0	HOH	W	208	-21.010	60.974	28.216	1.00	44.88		0
	ANISOU	2393	0	HOH	W	208	5585	5720	5747	-87	-138	72	0
	ATOM	2396	0	HOH	W	209	-23.773	41.837	41.420	1.00	49.48		0
	ANISOU	2396	0	HOH	W	209	6015	6280	6505	1	-16	63	0
20	ATOM	2399	0	HOH	W	210	0.002	42.809	47.889	0.33	43.16		0
	ANISOU	2399	0	HOH	W	210	5469	5469	5460	0	0	0	0
	ATOM	2402	0	HOH	W	211	-0.940	65.973	39.157	1.00	35.55		0
	ANISOU	2402	0	HOH	W	211	5140	4032	4332	-152	-223	-32	0
	ATOM	2405	0	HOH	W	212	1.186	64.588	38.091	1.00	41.23		0
25	ANISOU	2405	0	HOH	W	212	5243	4868	5551	-229	10	97	0
	ATOM	2408	0	HOH	W	213	-20.041	61.023	38.988	1.00	44.93		0
	ANISOU	2408	0	HOH	W	213	5638	5829	5603	-30	-143	-209	0
	ATOM	2411	0	HOH	W	214	-20.170	55.338	15.170	1.00	51.70		0
	ANISOU	2411	0	HOH	W	214	6589	6588	6465	-21	-68	79	0
30	ATOM	2414	0	HOH	W	215	-17.144	41.072	21.849	1.00	39.18		0
	ANISOU	2414	0	HOH	W	215	5000	5091	4795	74	17	-154	0
	ATOM	2417	0	HOH	W	216	-4.308	61.704	46.630	1.00	42.61		0
	ANISOU	2417	0	HOH	W	216	5390	5469	5330	2	241	-264	0
	ATOM	2420	0	HOH	W	217	-8.078	69.110	44.390	1.00	37.23		0
35	ANISOU	2420	0	HOH	W	217	4457	4659	5029	-81	119	289	0
	ATOM	2423	0	HOH	W	218	3.813	55.462	30.287	1.00	20.17		0
	ANISOU	2423	0	HOH	W	218	3277	2333	2054	957	163	233	0
	ATOM	2426	0	HOH	W	219	5.588	55.956	23.111	1.00	18.62		0
	ANISOU	2426	0	HOH	W	219	2809	1528	2737	-241	-909	182	0
40	ATOM	2429	0	HOH	W	220	4.873	57.326	31.456	1.00	33.95		0
	ANISOU	2429	0	HOH	W	220	3799	4714	4383	1	-56	-174	0
	ATOM	2432	0	HOH	W	221	-2.690	43.167	45.639	1.00	35.10		0
	ANISOU	2432	0	HOH	W	221	4700	4210	4426	39	-39	53	0
	ATOM	2435	0	HOH	W	222	-6.453	68.695	30.899	1.00	46.25		0
45	ANISOU	2435	0	HOH	W	222	6040	5876	5656	167	16	-143	0

TABLE 9

	HEADER	----	XX-XXX-XX	XXXXX
	COMPND	---		
5	REMARK	3		
	REMARK	3	REFINEMENT.	
	REMARK	3	PROGRAM : REFMAC 5.2.0005	
	REMARK	3	AUTHORS : MURSHUDOV ,VAGIN ,DODSON	
	REMARK	3		
10	REMARK	3	REFINEMENT TARGET : MAXIMUM LIKELIHOOD	
	REMARK	3		
	REMARK	3	DATA USED IN REFINEMENT.	
	REMARK	3	RESOLUTION RANGE HIGH (ANGSTROMS) : 2.00	
	REMARK	3	RESOLUTION RANGE LOW (ANGSTROMS) : 30.00	
15	REMARK	3	DATA CUTOFF (SIGMA(F)) : NONE	
	REMARK	3	COMPLETENESS FOR RANGE (%) : 98.82	
	REMARK	3	NUMBER OF REFLECTIONS : 60840	
	REMARK	3		
	REMARK	3	FIT TO DATA USED IN REFINEMENT.	
20	REMARK	3	CROSS-VALIDATION METHOD : THROUGHOUT	
	REMARK	3	FREE R VALUE TEST SET SELECTION : RANDOM	
	REMARK	3	R VALUE (WORKING + TEST SET) : 0.22320	
	REMARK	3	R VALUE (WORKING SET) : 0.22054	
	REMARK	3	FREE R VALUE : 0.24713	
25	REMARK	3	FREE R VALUE TEST SET SIZE (%) : 10.1	
	REMARK	3	FREE R VALUE TEST SET COUNT : 6853	
	REMARK	3		
	REMARK	3	FIT IN THE HIGHEST RESOLUTION BIN.	
	REMARK	3	TOTAL NUMBER OF BINS USED : 25	
30	REMARK	3	BIN RESOLUTION RANGE HIGH : 2.004	
	REMARK	3	BIN RESOLUTION RANGE LOW : 2.045	
	REMARK	3	REFLECTION IN BIN (WORKING SET) : 3505	
	REMARK	3	BIN COMPLETENESS (WORKING+TEST) (%) : 97.12	
	REMARK	3	BIN R VALUE (WORKING SET) : 0.236	
35	REMARK	3	BIN FREE R VALUE SET COUNT : 374	
	REMARK	3	BIN FREE R VALUE : 0.293	
	REMARK	3		
	REMARK	3	NUMBER OF NON-HYDROGEN ATOMS USED IN REFINEMENT.	
	REMARK	3	ALL ATOMS : 4323	
40	REMARK	3		
	REMARK	3	B VALUES .	
	REMARK	3	FROM WILSON PLOT (A**2) : NULL	
	REMARK	3	MEAN B VALUE (OVERALL, A**2) : 34.815	
	REMARK	3	OVERALL ANISOTROPIC B VALUE.	
45	REMARK	3	B11 (A**2) : 1.10	
	REMARK	3	B22 (A**2) : 1.10	
	REMARK	3	B33 (A**2) : -1.65	
	REMARK	3	B12 (A**2) : 0.55	
	REMARK	3	B13 (A**2) : 0.00	
50	REMARK	3	B23 (A**2) : 0.00	
	REMARK	3		
	REMARK	3	ESTIMATED OVERALL COORDINATE ERROR.	
	REMARK	3	ESU BASED ON R VALUE (A) : 0.145	
	REMARK	3	ESU BASED ON FREE R VALUE (A) : 0.137	
55	REMARK	3	ESU BASED ON MAXIMUM LIKELIHOOD (A) : 0.088	
	REMARK	3	ESU FOR B VALUES BASED ON MAXIMUM LIKELIHOOD (A**2) : 5.995	
	REMARK	3		
	REMARK	3	CORRELATION COEFFICIENTS.	
	REMARK	3	CORRELATION COEFFICIENT F0-FC : 0.941	
60	REMARK	3	CORRELATION COEFFICIENT F0-FC FREE : 0.927	
	REMARK	3		
	REMARK	3	RMS DEVIATIONS FROM IDEAL VALUES	COUNT RMS WEIGHT
	REMARK	3	BOND LENGTHS REFINED ATOMS (A) : 4259 ; 0.007 ; 0.022	
	REMARK	3	BOND LENGTHS OTHERS (A) : 3663 ; 0.001 ; 0.020	
65	REMARK	3	BOND ANGLES REFINED ATOMS (DEGREES) : 5799 ; 1.041 ; 1.958	
	REMARK	3	BOND ANGLES OTHERS (DEGREES) : 8587 ; 0.692 ; 3.000	
	REMARK	3	TORSION ANGLES, PERIOD 1 (DEGREES) : 537 ; 5.786 ; 5.000	
	REMARK	3	TORSION ANGLES, PERIOD 2 (DEGREES) : 192 ; 35.940 ; 24.010	
	REMARK	3	TORSION ANGLES, PERIOD 3 (DEGREES) : 668 ; 13.371 ; 15.000	
70	REMARK	3	TORSION ANGLES, PERIOD 4 (DEGREES) : 30 ; 14.820 ; 15.000	
	REMARK	3	CHIRAL-CENTER RESTRAINTS (A**3) : 626 ; 0.067 ; 0.200	

REMARK 3 GENERAL PLANES REFINED ATOMS (A) : 4781 ; 0.003 ; 0.020
REMARK 3 GENERAL PLANES OTHERS (A) : 825 ; 0.001 ; 0.020
REMARK 3 NON -BONDED CONTACTS REFINED ATOM VISS (A) : 672 ; 0.189 ; 0.200
REMARK 3 NON -BONDED CONTACTS OTHERS (A) : 3395 ; 0.173 ; 0.200
5 REMARK 3 NON -BONDED TORSION REFINED ATOMS 3 (A) : 197 7 ; 0.167 ; 0.200
REMARK 3 NON -BONDED TORSION OTHERS (A) : 2518 ; 0.078 ; 0.200
REMARK 3 H-BOND (X... Y) REFINED ATOMS (A) : 168 ; 0.118 ; 0.200
REMARK 3 SYMMETRY VDW REFINED ATOMS (A) : 12 ; 0.110 ; 0.200
REMARK 3 SYMMETRY VDW OTHERS (A) : 89 ; 0.173 ; 0.200
10 REMARK 3 SYMMETRY H-BOND REFINED ATOMS (A) : 14 ; 0.120 ; 0.200
REMARK 3
REMARK 3 ISOTROPIC THERMAL FACTOR RESTRAIN \ITISS... COUNT RMS WEIGHT
REMARK 3 MAIN- CHAIN BOND REFINED ATOMS (A**2) : 3484 ; 2.469 ; 2.500
REMARK 3 MAIN- CHAIN BOND OTHER ATOMS (A**2) : 1087 ; 0.398 ; 2.500
15 REMARK 3 MAIN- CHAIN ANGLE REFINED ATOMS (A**2) : 4384 ; 3.073 ; 5.000
REMARK 3 SIDE-CHAIN BOND REFINED ATOMS (A**2) : 1787 ; 2.335 ; 2.500
REMARK 3 S IDE -CHAIN ANGLE REFINED ATOMS (A**2) : 1415 ; 3.346 ; 5.000
REMARK 3
20 REMARK 3 NCS RESTRAINTS STATISTICS
REMARK 3 NUMBER OF NCS GROUPS : NULL
REMARK 3
REMARK 3
REMARK 3 TLS DETAILS
REMARK 3 NUMBER OF TLS GROUPS : 8
25 REMARK 3 ATOM RECORD CONTAINS RESIDUAL B FACTORS ONLY
REMARK 3
REMARK 3
REMARK 3 TLS GROUP : 1
REMARK 3 NUMBER OF COMPONENTS GROUP : 1
REMARK 3 COMPONENTS C SSSEQI TO C SSSEQI
30 REMARK 3 RESIDUE RANGE : F 57 F 191
REMARK 3 ORIGIN FOR THE GROUP (A) : 43.9142 102.7918 174.8679
REMARK 3 T TENSOR
REMARK 3 T11 : -0.0988 T22 : -0.1296
REMARK 3 T33 : -0.0612 T12 : 0.0227
35 REMARK 3 T13 : 0.0310 T23 : 0.0020
REMARK 3 L TENS 3OR
REMARK 3 L11 : 1.4095 L22 : 2.0527
REMARK 3 L33 : 1.6573 L12 : 0.4989
REMARK 3 L13 : 0.4289 L23 : 0.5244
40 REMARK 3 S TENS 3OR
REMARK 3 S11 : 0.0610 S12 : -0.1507 S13 : 0.2233
REMARK 3 S21 : 0.1403 S22 : -0.0410 S23 : 0.1536
REMARK 3 S31 : -0.2464 S32 : -0.2021 S33 : -0.0199
REMARK 3
45 REMARK 3 TLS GROUP : 2
REMARK 3 NUMBER OF COMPONENTS GROUP : 1
REMARK 3 COMPONENTS C SSSEQI TO C SSSEQI
REMARK 3 RESIDUE RANGE : G 57 G 191
50 REMARK 3 ORIGIN FOR THE GROUP (A) : 14.6102 58.4872 216.4521
REMARK 3 T TENSOR
REMARK 3 T1111 : 0.00095555 T222 : 0.0060000
REMARK 3 T3333 : -0.00663388 T1122 : 0.00116688
REMARK 3 T1133 : -0.00884477 T223 : -0.0027744
REMARK 3 L TENSOR
55 REMARK 3 L11 : 1.6896 L22 : 2.6344
REMARK 3 L33 : 2.0297 L12 : -0.0786
REMARK 3 L13 : 0.1509 L23 : -0.4868
REMARK 3 S TENS 3OR
REMARK 3 S11 : 0.0348 S12 : -0.3010 S13 : -0.0765
60 REMARK 3 S21 : 0.4486 S22 : 0.0609 S23 : -0.3884
REMARK 3 S31 : 0.0253 S32 : 0.3677 S33 : -0.0957
REMARK 3
REMARK 3 TLS GROUP : 3
REMARK 3 NUMBER OF COMPONENTS GROUP : 1
65 REMARK 3 COMPONENTS C SSSEQI TO C SSSEQI
REMARK 3 RESIDUE RANGE : R 29 R 108
REMARK 3 ORIGIN FOR THE GROUP (A) : 25.6686 87.7196 169.9556
REMARK 3 T TENSOR
REMARK 3 T11 : -0.1381 T22 : -0.0932
70 REMARK 3 T33 : -0.0595 T12 : -0.0493
REMARK 3 T13 : -0.0193 T23 : -0.0313

REMARK 3 L TENSOR
REMARK 3 L11 : 1.5922 L22 : 0.6020
REMARK 3 L33 : 5.1978 L12 : 0.4407
REMARK 3 L13 : -0.7141 L23 : -0.8882
5 REMARK 3 S TEN.30R
REMARK 3 S11 : -0.0233 S12 : 0.0770 S13 : 0.1890
REMARK 3 S21 : 0.0376 S22 : -0.0632 S23 : 0.1629
REMARK 3 S31 : -0.1226 S32 : -0.1850 S33 : 0.0865
REMARK 3
10 REMARK 3 TLS GROUP : 4
REMARK 3 NUMBER OF COMPONENTS GROUP : 1
REMARK 3 COMPONENTS C SSSEQI TO C SSSEQI
REMARK 3 RESIDUE RANGE : R 109 R 140
REMARK 3 ORIGIN FOR THE GROUP (A) : 25.3215 93.6141 196.7325
15 REMARK 3 T TENSOR
REMARK 3 T11 : 0.1474 T22 : 0.1342
REMARK 3 T33 : 0.0065 T12 : -0.2101
REMARK 3 T13 : 0.1620 T23 : -0.1749
REMARK 3 L TEN.30R
20 REMARK 3 L11 : 8.3007 L22 : 4.6110
REMARK 3 L33 : 6.6462 L12 : -0.4453
REMARK 3 L13 : -5.4694 L23 : 1.1369
REMARK 3 S TEN.30R
25 REMARK 3 S11 : 0.7103 S12 : -0.8209 S13 : 0.9584
REMARK 3 S21 : 0.1917 S22 : -0.0805 S23 : 0.0379
REMARK 3 S31 : -1.0716 S32 : 0.5838 S33 : -0.6298
REMARK 3
30 REMARK 3 TLS GROUP : 5
REMARK 3 NUMBER OF COMPONENTS GROUP : 1
REMARK 3 COMPONENTS C SSSEQI TO C SSSEQI
REMARK 3 RESIDUE RANGE : R 141 R 166
REMARK 3 ORIGIN FOR THE GROUP (A) : 16.8496 100.8594 213.0094
REMARK 3 T TENSOR
35 REMARK 3 T11 : 0.4924 T22 : 0.2599
REMARK 3 T33 : 0.1608 T12 : -0.1013
REMARK 3 T13 : 0.2358 T23 : -0.2032
REMARK 3 L TENS30R
40 REMARK 3 L11 : 5.4047 L22 : 9.7294
REMARK 3 L33 : 22.1208 L12 : -3.3609
REMARK 3 L13 : -7.1965 L23 : 5.4286
REMARK 3 S TENS50R
45 REMARK 3 S11 : -0.0919 S12 : -0.2657 S13 : 0.4059
REMARK 3 S21 : 0.5516 S22 : 0.4574 S23 : 0.6014
REMARK 3 S31 : -1.2713 S32 : 0.1665 S33 : -0.3654
REMARK 3
50 REMARK 3 TLS GROUP : 6
REMARK 3 NUMBER OF COMPONENTS 5 GROUP : 1
REMARK 3 COMPONENTS C SSSEQI TO C SSSEQI
REMARK 3 RESIDUE RANGE : T 29 T 108
REMARK 3 ORIGIN FOR THE GROUP (A) : 16.2781 81.5721 211.5454
REMARK 3 T TENSOR
55 REMARK 3 T11 : 0.1643 T22 : 0.0992
REMARK 3 T33 : 0.0653 T12 : -0.1703
REMARK 3 T13 : 0.0085 T23 : -0.0648
REMARK 3 L TENS10R
60 REMARK 3 L11 : 1.5274 L22 : 0.8567
REMARK 3 L33 : 8.6339 L12 : -0.2123
REMARK 3 L13 : -2.3410 L23 : -0.0957
REMARK 3 S TENS10R
REMARK 3 S11 : 0.1399 S12 : -0.3521 S13 : 0.1940
REMARK 3 S21 : 0.3353 S22 : -0.0519 S23 : -0.2094
REMARK 3 S31 : -0.7345 S32 : 0.7190 S33 : -0.0880
REMARK 3
65 REMARK 3 TLS GROUP : 7
REMARK 3 NUMBER OF COMPONENTS ; GROUP : 1
REMARK 3 COMPONENTS C SSSEQI TO C SSSEQI
REMARK 3 RESIDUE RANGE : T 109 T 140
REMARK 3 ORIGIN FOR THE GROUP (A) : 18.2096 78.1285 240.9816
70 REMARK 3 T TENSOR
REMARK 3 T11 : 0.4902 T22 : 0.3530
REMARK 3 T33 : 0.0272 T12 : -0.1840

REMARK 3 T13: -0.2380 T23: -0.4636
REMARK 3 L TENSOR
REMARK 3 L11: 3.2040 L22: 4.6424
REMARK 3 L33: 38.8550 L12: -1.8483
5 REMARK 3 L13: 10.3445 L23: -1.5503
REMARK 3 S TENSOR
REMARK 3 S11: -0.3552 S12: 0.6662 S13: -0.7694
REMARK 3 S21: 0.2239 S22: 0.7654 S23: -0.5121
REMARK 3 S31: 0.7250 S32: 2.1475 S33: -0.4102
10 REMARK 3
REMARK 3 TLS GROUP : 8
REMARK 3 NUMBER OF COMPONENTS GROUP : 1
REMARK 3 COMPONENTS C SSSEQI TO C SSSEQI
REMARK 3 RESIDUE RANGE : T 141 T 166
15 REMARK 3 ORIGIN FOR THE GROUP (A): 26.4654 81.7957 256.4784
REMARK 3 T TENSOR
REMARK 3 T11: 0.4382 T22: 0.4983
REMARK 3 T33: 0.2746 T12: 0.1032
REMARK 3 T13: 0.0217 T23: -0.3335
20 REMARK 3 L TENJ30R
REMARK 3 L11: 27.7115 L22: 8.6242
REMARK 3 L33: 32.0119 L12: 0.0615
REMARK 3 L13: 13.4817 L23: 2.4624
REMARK 3 S TENS30R
25 REMARK 3 S11: 0.0981 S12: 0.2481 S13: -0.3615
REMARK 3 S21: -0.1364 S22: 0.4003 S23: -0.0823
REMARK 3 S31: 0.2206 S32: 1.9882 S33: -0.4983
REMARK 3
REMARK 3
30 REMARK 3 BULK SOLVENT MODELLING.
REMARK 3 METHOD USED : MASK
REMARK 3 PARAMETERS FOR MASK CALCULATION
REMARK 3 VDW PROBE RADIUS : 1.40
REMARK 3 ION PROBE RADIUS : 0.80
35 REMARK 3 SHRINKAGE RADIUS : 0.80
REMARK 3
REMARK 3 OTHER REFINEMENT REMARKS :
REMARK 3 HYDROGENS HAVE BEEN ADDED IN THE RIDING POSITIONS
REMARK 3
40 SSBOND 1 CYS F 70 CYS F 163
SSBOND 2 CYS F 98 CYS F 183
SSBOND 3 CYS G 70 CYS G 163
SSBOND 4 CYS G 98 CYS G 183
SSBOND 5 CYS R 31 CYS R 42
45 SSBOND 6 CYS R 43 CYS R 56
SSBOND 7 CYS R 46 CYS R 64
SSBOND 8 CYS R 67 CYS R 81
SSBOND 9 CYS R 87 CYS R 107
SSBOND 10 CYS R 109 CYS R 125
50 SSBOND 11 CYS R 128 CYS R 141
SSBOND 12 CYS T 31 CYS T 42
SSBOND 13 CYS T 43 CYS T 56
SSBOND 14 CYS T 46 CYS T 64
SSBOND 15 CYS T 67 CYS T 81
55 SSBOND 16 CYS T 87 CYS T 107
SSBOND 17 CYS T 109 CYS T 125
LINK ALA T 150 THR T 154 gap
CRYST1 104.729 104.729 478.161 90.00 90.00 120.00 H 3 2
60 SCALE1 0.009548 0.005513 0.000000 0.000000
SCALE2 0.000000 0.011026 0.000000 0.000000
SCALE3 0.000000 0.000000 0.002091 0.000000
ATOM 1 N ASP F 57 44.153 95.412 151.972 1.00 66.84 N
ATOM 2 CA ASP F 57 44.513 96.691 151.280 1.00 62.49 C
ATOM 4 CB ASP F 57 43.323 97.226 150.460 1.00 66.77 C
65 ATOM 7 CG ASP F 57 43.491 98.680 150.054 1.00 68.45 C
ATOM 8 OD1 ASP F 57 44.502 99.002 149.389 1.00 69.74 O
ATOM 9 OD2 ASP F 57 42.604 99.496 150.396 1.00 69.38 O
ATOM 10 C ASP F 57 45.060 97.750 152.255 1.00 59.71 C
ATOM 11 O ASP F 57 46.158 98.267 152.040 1.00 58.36 O
70 ATOM 15 N PRO F 58 44.308 98.078 153.327 1.00 55.23 N
ATOM 16 CA PRO F 58 44.851 99.063 154.268 1.00 50.43 C

5	ATOM	18	CB	PRO	F	58	43.685	99.305	155.240	1.00	52.41	C
	ATOM	21	CG	PRO	F	58	42.472	98.806	154.519	1.00	55.15	C
	ATOM	24	CD	PRO	F	58	42.971	97.628	153.750	1.00	56.20	C
	ATOM	27	C	PRO	F	58	46.086	98.539	155.010	1.00	42.75	C
	ATOM	28	O	PRO	F	58	46.320	97.332	155.035	1.00	38.16	O
10	ATOM	29	N	PRO	F	59	46.877	99.445	155.610	1.00	38.23	N
	ATOM	30	CA	PRO	F	59	48.073	99.007	156.317	1.00	36.33	C
	ATOM	32	CB	PRO	F	59	48.828	100.312	156.568	1.00	37.32	C
	ATOM	35	CG	PRO	F	59	47.768	101.348	156.639	1.00	38.40	C
	ATOM	38	CD	PRO	F	59	46.688	100.902	155.689	1.00	37.89	C
15	ATOM	41	C	PRO	F	59	47.717	98.328	157.638	1.00	33.39	C
	ATOM	42	O	PRO	F	59	46.563	98.381	158.075	1.00	30.88	O
	ATOM	43	N	ILE	F	60	48.705	97.699	158.264	1.00	30.85	N
	ATOM	44	CA	ILE	F	60	48.537	97.170	159.610	1.00	30.27	C
	ATOM	46	CB	ILE	F	60	49.835	96.481	160.126	1.00	30.92	C
20	ATOM	48	CG1	ILE	F	60	50.147	95.243	159.266	1.00	33.39	C
	ATOM	51	CD1	ILE	F	60	51.526	94.640	159.499	1.00	32.58	C
	ATOM	55	CG2	ILE	F	60	49.680	96.093	161.588	1.00	30.54	C
	ATOM	59	C	ILE	F	60	48.131	98.349	160.497	1.00	28.20	C
	ATOM	60	O	ILE	F	60	48.730	99.429	160.437	1.00	28.16	O
25	ATOM	62	N	GLN	F	61	47.094	98.134	161.291	1.00	28.70	N
	ATOM	63	CA	GLN	F	61	46.498	99.182	162.107	1.00	29.25	C
	ATOM	65	CB	GLN	F	61	45.046	98.826	162.445	1.00	28.25	C
	ATOM	68	CG	GLN	F	61	44.132	98.713	161.225	1.00	28.67	C
	ATOM	71	CD	GLN	F	61	43.855	100.050	160.579	1.00	29.94	C
30	ATOM	72	OE1	GLN	F	61	43.066	100.834	161.098	1.00	30.67	O
	ATOM	73	NE2	GLN	F	61	44.500	100.322	159.439	1.00	30.01	N
	ATOM	76	C	GLN	F	61	47.318	99.369	163.374	1.00	28.57	C
	ATOM	77	O	GLN	F	61	47.563	98.415	164.118	1.00	30.22	O
	ATOM	79	N	ARG	F	62	47.773	100.593	163.608	1.00	28.86	N
35	ATOM	80	CA	ARG	F	62	48.503	100.883	164.827	1.00	31.60	C
	ATOM	82	CB	ARG	F	62	49.966	100.474	164.729	1.00	37.58	C
	ATOM	85	CG	ARG	F	62	50.757	101.167	163.685	1.00	37.73	C
	ATOM	88	CD	ARG	F	62	52.121	101.579	164.198	1.00	45.17	C
	ATOM	91	NE	ARG	F	62	52.091	102.810	164.981	1.00	45.40	N
40	ATOM	93	CZ	ARG	F	62	53.165	103.490	165.380	1.00	45.42	C
	ATOM	94	NH1	ARG	F	62	54.384	103.090	165.071	1.00	52.09	N
	ATOM	97	NH2	ARG	F	62	53.018	104.608	166.080	1.00	47.32	N
	ATOM	100	C	ARG	F	62	48.416	102.314	165.287	1.00	28.16	C
	ATOM	101	O	ARG	F	62	48.334	103.261	164.488	1.00	29.23	O
45	ATOM	103	N	LEU	F	63	48.466	102.454	166.605	1.00	31.40	N
	ATOM	104	CA	LEU	F	63	48.422	103.755	167.243	1.00	32.49	C
	ATOM	106	CB	LEU	F	63	46.992	104.144	167.607	1.00	37.07	C
	ATOM	109	CG	LEU	F	63	46.960	105.559	168.213	1.00	38.21	C
	ATOM	111	CD1	LEU	F	63	46.062	106.465	167.432	1.00	43.35	C
50	ATOM	115	CD2	LEU	F	63	46.626	105.538	169.695	1.00	38.93	C
	ATOM	119	C	LEU	F	63	49.264	103.731	168.496	1.00	29.85	C
	ATOM	120	O	LEU	F	63	49.171	102.813	169.292	1.00	30.53	O
	ATOM	122	N	ARG	F	64	50.072	104.764	168.655	1.00	29.53	N
	ATOM	123	CA	ARG	F	64	50.780	105.013	169.891	1.00	29.90	C
55	ATOM	125	CB	ARG	F	64	52.272	104.954	169.622	1.00	28.03	C
	ATOM	128	CG	ARG	F	64	53.133	105.132	170.831	1.00	32.92	C
	ATOM	131	CD	ARG	F	64	54.559	104.905	170.420	1.00	37.46	C
	ATOM	134	NE	ARG	F	64	55.483	105.430	171.397	1.00	44.60	N
	ATOM	136	CZ	ARG	F	64	56.150	106.574	171.300	1.00	38.97	C
60	ATOM	137	NH1	ARG	F	64	56.060	107.371	170.242	1.00	43.86	N
	ATOM	140	NH2	ARG	F	64	56.948	106.913	172.286	1.00	41.09	N
	ATOM	143	C	ARG	F	64	50.384	106.395	170.392	1.00	29.14	C
	ATOM	144	O	ARG	F	64	50.368	107.358	169.619	1.00	29.42	O
	ATOM	146	N	GLY	F	65	50.066	106.485	171.682	1.00	31.17	N
65	ATOM	147	CA	GLY	F	65	49.743	107.761	172.320	1.00	31.68	C
	ATOM	150	C	GLY	F	65	50.371	107.914	173.689	1.00	31.45	C
	ATOM	151	O	GLY	F	65	50.594	106.928	174.405	1.00	33.45	O
	ATOM	153	N	ALA	F	66	50.676	109.154	174.052	1.00	31.26	N
	ATOM	154	CA	ALA	F	66	51.170	109.460	175.386	1.00	30.85	C
70	ATOM	156	CB	ALA	F	66	52.023	110.720	175.379	1.00	32.87	C
	ATOM	160	C	ALA	F	66	49.988	109.620	176.340	1.00	33.24	C
	ATOM	161	O	ALA	F	66	48.892	110.015	175.936	1.00	31.23	O
	ATOM	163	N	VAL	F	67	50.236	109.295	177.606	1.00	35.76	N
	ATOM	164	CA	VAL	F	67	49.267	109.460	178.688	1.00	35.90	C
	ATOM	166	CB	VAL	F	67	48.763	108.080	179.201	1.00	34.68	C

5	ATOM	168	CG1	VAL	F	67	47.646	108.253	180.228	1.00	36.61	C
	ATOM	172	CG2	VAL	F	67	48.271	107.241	178.034	1.00	35.63	C
	ATOM	176	C	VAL	F	67	49.963	110.259	179.800	1.00	35.16	C
	ATOM	177	O	VAL	F	67	50.901	109.777	180.440	1.00	36.77	O
	ATOM	179	N	THR	F	68	49.541	111.504	179.980	1.00	38.98	N
10	ATOM	180	CA	THR	F	68	50.186	112.427	180.923	1.00	39.17	C
	ATOM	182	CB	THR	F	68	50.799	113.635	180.147	1.00	43.00	C
	ATOM	184	OG1	THR	F	68	51.721	113.153	179.157	1.00	46.80	O
	ATOM	186	CG2	THR	F	68	51.539	114.564	181.073	1.00	44.19	C
	ATOM	190	C	THR	F	68	49.213	112.945	182.002	1.00	39.50	C
15	ATOM	191	O	THR	F	68	49.642	113.420	183.065	1.00	37.57	O
	ATOM	193	N	ARG	F	69	47.913	112.846	181.732	1.00	38.51	N
	ATOM	194	CA	ARG	F	69	46.883	113.384	182.629	1.00	38.40	C
	ATOM	196	CB	ARG	F	69	46.705	114.883	182.367	1.00	39.86	C
	ATOM	199	CG	ARG	F	69	46.580	115.250	180.894	1.00	41.83	C
20	ATOM	202	CD	ARG	F	69	46.369	116.743	180.708	1.00	44.43	C
	ATOM	205	NE	ARG	F	69	44.999	117.053	180.298	1.00	46.17	N
	ATOM	207	CZ	ARG	F	69	44.596	117.244	179.042	1.00	45.88	C
	ATOM	208	NH1	ARG	F	69	45.445	117.181	178.019	1.00	46.31	N
	ATOM	211	NH2	ARG	F	69	43.321	117.517	178.808	1.00	46.73	N
25	ATOM	214	C	ARG	F	69	45.548	112.661	182.453	1.00	35.07	C
	ATOM	215	O	ARG	F	69	45.406	111.813	181.569	1.00	35.38	O
	ATOM	217	N	CYS	F	70	44.589	112.995	183.316	1.00	32.36	N
	ATOM	218	CA	CYS	F	70	43.234	112.452	183.276	1.00	35.55	C
	ATOM	220	CB	CYS	F	70	42.866	111.835	184.635	1.00	38.07	C
30	ATOM	223	SG	CYS	F	70	41.159	111.188	184.842	1.00	42.72	S
	ATOM	225	C	CYS	F	70	42.290	113.591	182.929	1.00	37.28	C
	ATOM	226	O	CYS	F	70	42.532	114.745	183.307	1.00	33.85	O
	ATOM	228	N	GLU	F	71	41.221	113.264	182.211	1.00	38.37	N
	ATOM	229	CA	GLU	F	71	40.231	114.255	181.787	1.00	40.11	C
35	ATOM	231	CB	GLU	F	71	40.584	114.771	180.390	1.00	41.97	C
	ATOM	234	CG	GLU	F	71	39.619	115.809	179.833	1.00	45.06	C
	ATOM	237	CD	GLU	F	71	40.062	116.344	178.481	1.00	47.04	C
	ATOM	238	OE1	GLU	F	71	39.818	115.668	177.458	1.00	49.11	O
	ATOM	239	OE2	GLU	F	71	40.643	117.446	178.445	1.00	50.33	O
40	ATOM	240	C	GLU	F	71	38.854	113.610	181.766	1.00	37.40	C
	ATOM	241	O	GLU	F	71	38.656	112.614	181.076	1.00	37.09	O
	ATOM	243	N	ASP	F	72	37.916	114.171	182.524	1.00	36.72	N
	ATOM	244	CA	ASP	F	72	36.539	113.671	182.579	1.00	40.16	C
	ATOM	246	CB	ASP	F	72	35.800	113.970	181.261	1.00	45.47	C
45	ATOM	249	CG	ASP	F	72	35.573	115.457	181.036	1.00	48.82	C
	ATOM	250	OD1	ASP	F	72	34.968	116.111	181.913	1.00	50.23	O
	ATOM	251	OD2	ASP	F	72	35.984	115.969	179.969	1.00	51.56	O
	ATOM	252	C	ASP	F	72	36.480	112.170	182.898	1.00	39.76	C
	ATOM	253	O	ASP	F	72	35.778	111.404	182.229	1.00	37.08	O
50	ATOM	255	N	GLY	F	73	37.230	111.761	183.921	1.00	38.04	N
	ATOM	256	CA	GLY	F	73	37.203	110.380	184.404	1.00	35.82	C
	ATOM	259	C	GLY	F	73	37.906	109.374	183.518	1.00	30.45	C
	ATOM	260	O	GLY	F	73	37.759	108.164	183.718	1.00	30.26	O
	ATOM	262	N	GLN	F	74	38.681	109.858	182.549	1.00	32.17	N
55	ATOM	263	CA	GLN	F	74	39.390	108.997	181.607	1.00	35.21	C
	ATOM	265	CB	GLN	F	74	38.754	109.061	180.216	1.00	38.25	C
	ATOM	268	CG	GLN	F	74	37.283	108.714	180.192	1.00	39.40	C
	ATOM	271	CD	GLN	F	74	36.739	108.444	178.795	1.00	39.13	C
	ATOM	272	OE1	GLN	F	74	35.541	108.211	178.634	1.00	42.87	O
60	ATOM	273	NE2	GLN	F	74	37.607	108.468	177.786	1.00	35.70	N
	ATOM	276	C	GLN	F	74	40.838	109.412	181.484	1.00	33.47	C
	ATOM	277	O	GLN	F	74	41.155	110.599	181.560	1.00	37.31	O
	ATOM	279	N	LEU	F	75	41.718	108.434	181.299	1.00	34.11	N
	ATOM	280	CA	LEU	F	75	43.094	108.720	180.928	1.00	35.05	C
65	ATOM	282	CB	LEU	F	75	43.938	107.442	180.859	1.00	37.04	C
	ATOM	285	CG	LEU	F	75	44.143	106.655	182.167	1.00	38.44	C
	ATOM	287	CD1	LEU	F	75	44.996	105.442	181.923	1.00	40.51	C
	ATOM	291	CD2	LEU	F	75	44.765	107.522	183.248	1.00	41.38	C
	ATOM	295	C	LEU	F	75	43.051	109.428	179.576	1.00	34.62	C
70	ATOM	296	O	LEU	F	75	42.324	109.016	178.667	1.00	33.35	O
	ATOM	298	N	PHE	F	76	43.802	110.517	179.452	1.00	36.91	N
	ATOM	299	CA	PHE	F	76	43.769	111.305	178.226	1.00	35.73	C
	ATOM	301	CB	PHE	F	76	43.981	112.795	178.510	1.00	38.02	C
	ATOM	304	CG	PHE	F	76	43.891	113.648	177.284	1.00	36.39	C
	ATOM	305	CD1	PHE	F	76	42.654	113.991	176.756	1.00	39.22	C

	ATOM	307	CE1	PHE	F	76	42.562	114.766	175.601	1.00	39.33	C
	ATOM	309	CZ	PHE	F	76	43.719	115.196	174.962	1.00	39.59	C
	ATOM	311	CE2	PHE	F	76	44.964	114.852	175.479	1.00	39.17	C
5	ATOM	313	CD2	PHE	F	76	45.043	114.077	176.631	1.00	39.39	C
	ATOM	315	C	PHE	F	76	44.835	110.788	177.266	1.00	32.41	C
	ATOM	316	O	PHE	F	76	46.010	110.739	177.618	1.00	32.71	O
	ATOM	318	N	ILE	F	77	44.417	110.422	176.055	1.00	32.77	N
	ATOM	319	CA	ILE	F	77	45.323	109.882	175.035	1.00	33.31	C
10	ATOM	321	CB	ILE	F	77	44.658	108.709	174.256	1.00	33.72	C
	ATOM	323	CG1	ILE	F	77	44.113	107.648	175.227	1.00	33.14	C
	ATOM	326	CD1	ILE	F	77	43.069	106.717	174.615	1.00	32.80	C
	ATOM	330	CG2	ILE	F	77	45.655	108.072	173.262	1.00	34.01	C
	ATOM	334	C	ILE	F	77	45.746	110.985	174.054	1.00	33.50	C
	ATOM	335	O	ILE	F	77	44.920	111.490	173.297	1.00	35.38	O
15	ATOM	337	N	SER	F	78	47.023	111.375	174.075	1.00	34.73	N
	ATOM	338	CA	SER	F	78	47.544	112.275	173.044	1.00	35.69	C
	ATOM	340	CB	SER	F	78	48.375	113.427	173.625	1.00	40.55	C
	ATOM	343	OG	SER	F	78	49.463	112.965	174.389	1.00	49.39	O
20	ATOM	345	C	SER	F	78	48.326	111.478	171.997	1.00	33.95	C
	ATOM	346	O	SER	F	78	49.422	110.966	172.253	1.00	31.82	O
	ATOM	348	N	SER	F	79	47.724	111.372	170.821	1.00	34.55	N
	ATOM	349	CA	SER	F	79	48.281	110.608	169.730	1.00	34.48	C
	ATOM	351	CB	SER	F	79	47.220	110.363	168.661	1.00	38.17	C
25	ATOM	354	OG	SER	F	79	47.759	109.625	167.576	1.00	43.21	O
	ATOM	356	C	SER	F	79	49.444	111.374	169.128	1.00	30.73	C
	ATOM	357	O	SER	F	79	49.337	112.561	168.854	1.00	29.63	O
	ATOM	359	N	TYR	F	80	50.549	110.680	168.912	1.00	29.49	N
	ATOM	360	CA	TYR	F	80	51.695	111.272	168.234	1.00	32.34	C
30	ATOM	362	CB	TYR	F	80	52.895	110.343	168.353	1.00	31.61	C
	ATOM	365	CG	TYR	F	80	53.440	110.242	169.761	1.00	31.19	C
	ATOM	366	CD1	TYR	F	80	54.246	111.250	170.283	1.00	34.23	C
	ATOM	368	CE1	TYR	F	80	54.753	111.171	171.564	1.00	33.04	C
	ATOM	370	CZ	TYR	F	80	54.469	110.074	172.347	1.00	33.50	C
35	ATOM	371	OH	TYR	F	80	54.998	110.011	173.618	1.00	34.38	O
	ATOM	373	CE2	TYR	F	80	53.672	109.047	171.854	1.00	32.19	C
	ATOM	375	CD2	TYR	F	80	53.163	109.139	170.566	1.00	31.69	C
	ATOM	377	C	TYR	F	80	51.371	111.515	166.765	1.00	31.18	C
	ATOM	378	O	TYR	F	80	50.632	110.749	166.153	1.00	36.84	O
40	ATOM	380	N	LYS	F	81	51.931	112.578	166.210	1.00	35.15	N
	ATOM	381	CA	LYS	F	81	51.785	112.887	164.794	1.00	39.56	C
	ATOM	383	CB	LYS	F	81	51.661	114.401	164.593	1.00	49.16	C
	ATOM	386	CG	LYS	F	81	50.452	115.025	165.298	1.00	53.98	C
	ATOM	389	CD	LYS	F	81	49.136	114.668	164.601	1.00	58.66	C
45	ATOM	392	CE	LYS	F	81	47.915	115.125	165.402	1.00	58.13	C
	ATOM	395	NZ	LYS	F	81	47.548	114.154	166.480	1.00	58.85	N
	ATOM	399	C	LYS	F	81	53.007	112.338	164.070	1.00	36.05	C
	ATOM	400	O	LYS	F	81	54.114	112.857	164.219	1.00	39.95	O
	ATOM	402	N	ASN	F	82	52.802	111.266	163.312	1.00	32.29	N
50	ATOM	403	CA	ASN	F	82	53.898	110.538	162.692	1.00	30.77	C
	ATOM	405	CB	ASN	F	82	54.628	109.685	163.768	1.00	36.31	C
	ATOM	408	CG	ASN	F	82	55.861	108.954	163.225	1.00	38.97	C
	ATOM	409	OD1	ASN	F	82	55.764	107.801	162.828	1.00	42.48	O
	ATOM	410	ND2	ASN	F	82	57.022	109.627	163.210	1.00	36.16	N
55	ATOM	413	C	ASN	F	82	53.342	109.661	161.558	1.00	28.91	C
	ATOM	414	O	ASN	F	82	52.192	109.183	161.620	1.00	27.08	O
	ATOM	416	N	GLU	F	83	54.164	109.461	160.531	1.00	25.96	N
	ATOM	417	CA	GLU	F	83	53.823	108.613	159.380	1.00	26.59	C
	ATOM	419	CB	GLU	F	83	55.005	108.550	158.405	1.00	24.88	C
60	ATOM	422	CG	GLU	F	83	56.242	107.825	158.955	1.00	25.74	C
	ATOM	425	CD	GLU	F	83	57.423	107.866	157.998	1.00	27.29	C
	ATOM	426	OE1	GLU	F	83	57.195	107.921	156.773	1.00	28.83	O
	ATOM	427	OE2	GLU	F	83	58.581	107.869	158.472	1.00	26.92	O
	ATOM	428	C	GLU	F	83	53.411	107.184	159.735	1.00	29.86	C
65	ATOM	429	O	GLU	F	83	52.700	106.535	158.971	1.00	29.60	O
	ATOM	431	N	TYR	F	84	53.870	106.678	160.874	1.00	26.37	N
	ATOM	432	CA	TYR	F	84	53.591	105.303	161.230	1.00	28.42	C
	ATOM	434	CB	TYR	F	84	54.711	104.749	162.118	1.00	29.04	C
	ATOM	437	CG	TYR	F	84	56.069	104.653	161.436	1.00	24.31	C
70	ATOM	438	CD1	TYR	F	84	56.197	104.177	160.134	1.00	25.74	C
	ATOM	440	CE1	TYR	F	84	57.446	104.071	159.524	1.00	26.82	C
	ATOM	442	CZ	TYR	F	84	58.580	104.413	160.232	1.00	26.85	C

5	ATOM	443	OH	TYR	F	84	59.828	104.323	159.646	1.00	24.57	O
	ATOM	445	CE2	TYR	F	84	58.473	104.878	161.527	1.00	27.66	C
	ATOM	447	CD2	TYR	F	84	57.231	104.992	162.120	1.00	30.04	C
	ATOM	449	C	TYR	F	84	52.227	105.102	161.891	1.00	29.64	C
	ATOM	450	O	TYR	F	84	51.778	103.971	162.041	1.00	32.17	O
10	ATOM	452	N	GLN	F	85	51.570	106.193	162.280	1.00	26.50	N
	ATOM	453	CA	GLN	F	85	50.234	106.112	162.875	1.00	27.04	C
	ATOM	455	CB	GLN	F	85	49.885	107.436	163.564	1.00	32.00	C
	ATOM	458	CG	GLN	F	85	50.882	107.869	164.648	1.00	32.59	C
	ATOM	461	CD	GLN	F	85	50.553	107.299	166.025	1.00	35.31	C
15	ATOM	462	OE1	GLN	F	85	50.402	106.098	166.188	1.00	32.90	O
	ATOM	463	NE2	GLN	F	85	50.443	108.170	167.016	1.00	39.36	N
	ATOM	466	C	GLN	F	85	49.220	105.799	161.776	1.00	27.70	C
	ATOM	467	O	GLN	F	85	49.162	106.499	160.765	1.00	28.29	O
	ATOM	469	N	THR	F	86	48.443	104.734	161.943	1.00	30.20	N
20	ATOM	470	CA	THR	F	86	47.437	104.359	160.942	1.00	29.63	C
	ATOM	472	CB	THR	F	86	47.811	103.038	160.214	1.00	29.27	C
	ATOM	474	OG1	THR	F	86	47.926	101.966	161.161	1.00	31.11	O
	ATOM	476	CG2	THR	F	86	49.117	103.189	159.458	1.00	30.95	C
	ATOM	480	C	THR	F	86	46.007	104.237	161.507	1.00	30.59	C
25	ATOM	481	O	THR	F	86	45.116	103.764	160.809	1.00	30.88	O
	ATOM	483	N	MET	F	87	45.799	104.650	162.758	1.00	32.49	N
	ATOM	484	CA	MET	F	87	44.466	104.708	163.363	1.00	33.04	C
	ATOM	486	CB	MET	F	87	44.309	103.665	164.469	1.00	32.57	C
	ATOM	489	CG	MET	F	87	44.247	102.227	163.993	1.00	36.60	C
30	ATOM	492	SD	MET	F	87	43.834	101.052	165.330	1.00	43.06	S
	ATOM	493	CE	MET	F	87	45.373	100.909	166.015	1.00	30.49	C
	ATOM	497	C	MET	F	87	44.239	106.095	163.944	1.00	32.91	C
	ATOM	498	O	MET	F	87	45.198	106.818	164.209	1.00	28.95	O
	ATOM	500	N	GLU	F	88	42.969	106.451	164.144	1.00	32.67	N
35	ATOM	501	CA	GLU	F	88	42.588	107.750	164.707	1.00	32.31	C
	ATOM	503	CB	GLU	F	88	41.406	108.365	163.937	1.00	39.84	C
	ATOM	506	CG	GLU	F	88	41.591	108.523	162.430	1.00	48.31	C
	ATOM	509	CD	GLU	F	88	42.645	109.550	162.040	1.00	55.04	C
	ATOM	510	OE1	GLU	F	88	42.588	110.699	162.529	1.00	57.19	O
40	ATOM	511	OE2	GLU	F	88	43.527	109.206	161.218	1.00	60.26	O
	ATOM	512	C	GLU	F	88	42.176	107.640	166.170	1.00	31.08	C
	ATOM	513	O	GLU	F	88	41.656	106.606	166.616	1.00	29.96	O
	ATOM	515	N	VAL	F	89	42.431	108.719	166.910	1.00	29.46	N
	ATOM	516	CA	VAL	F	89	41.854	108.942	168.225	1.00	33.88	C
45	ATOM	518	CB	VAL	F	89	42.908	109.452	169.232	1.00	34.18	C
	ATOM	520	CG1	VAL	F	89	42.245	109.950	170.527	1.00	35.93	C
	ATOM	524	CG2	VAL	F	89	43.905	108.362	169.535	1.00	34.05	C
	ATOM	528	C	VAL	F	89	40.744	109.978	168.063	1.00	34.40	C
	ATOM	529	O	VAL	F	89	40.971	111.034	167.495	1.00	34.04	O
50	ATOM	531	N	GLN	F	90	39.546	109.658	168.545	1.00	33.43	N
	ATOM	532	CA	GLN	F	90	38.406	110.577	168.508	1.00	36.87	C
	ATOM	534	CB	GLN	F	90	37.469	110.213	167.354	1.00	40.50	C
	ATOM	537	CG	GLN	F	90	38.030	110.550	165.973	1.00	47.27	C
	ATOM	540	CD	GLN	F	90	37.178	110.007	164.833	1.00	49.85	C
55	ATOM	541	OE1	GLN	F	90	35.946	110.033	164.898	1.00	56.89	O
	ATOM	542	NE2	GLN	F	90	37.835	109.510	163.780	1.00	53.34	N
	ATOM	545	C	GLN	F	90	37.665	110.502	169.839	1.00	33.05	C
	ATOM	546	O	GLN	F	90	37.355	109.412	170.313	1.00	33.30	O
	ATOM	548	N	ASN	F	91	37.400	111.654	170.445	1.00	30.67	N
60	ATOM	549	CA	ASN	F	91	36.770	111.725	171.772	1.00	34.21	C
	ATOM	551	CB	ASN	F	91	35.313	111.282	171.699	1.00	37.29	C
	ATOM	554	CG	ASN	F	91	34.498	112.139	170.763	1.00	40.36	C
	ATOM	555	OD1	ASN	F	91	34.723	113.343	170.656	1.00	41.82	O
	ATOM	556	ND2	ASN	F	91	33.549	111.524	170.076	1.00	44.04	N
65	ATOM	559	C	ASN	F	91	37.511	110.904	172.825	1.00	31.42	C
	ATOM	560	O	ASN	F	91	36.896	110.223	173.650	1.00	28.99	O
	ATOM	562	N	ASN	F	92	38.836	110.980	172.772	1.00	31.15	N
	ATOM	563	CA	ASN	F	92	39.710	110.303	173.723	1.00	32.78	C
	ATOM	565	CB	ASN	F	92	39.471	110.839	175.139	1.00	35.47	C
70	ATOM	568	CG	ASN	F	92	40.611	110.516	176.079	1.00	36.48	C
	ATOM	569	OD1	ASN	F	92	41.754	110.399	175.650	1.00	38.20	O
	ATOM	570	ND2	ASN	F	92	40.301	110.342	177.363	1.00	34.17	N
	ATOM	573	C	ASN	F	92	39.591	108.772	173.687	1.00	33.20	C
	ATOM	574	O	ASN	F	92	39.771	108.098	174.703	1.00	35.43	O
	ATOM	576	N	SER	F	93	39.309	108.233	172.504	1.00	32.41	N

	ATOM	577	CA	SER	F	93	39.234	106.787	172.298	1.00	31.44	C
	ATOM	579	CB	SER	F	93	37.777	106.303	172.314	1.00	34.24	C
	ATOM	582	OG	SER	F	93	37.075	106.750	171.172	1.00	35.99	O
	ATOM	584	C	SER	F	93	39.905	106.446	170.972	1.00	30.94	C
5	ATOM	585	O	SER	F	93	39.880	107.242	170.040	1.00	28.84	O
	ATOM	587	N	VAL	F	94	40.534	105.276	170.907	1.00	31.26	N
	ATOM	588	CA	VAL	F	94	41.138	104.796	169.675	1.00	30.70	C
	ATOM	590	CB	VAL	F	94	42.272	103.790	169.946	1.00	30.85	C
	ATOM	592	CG1	VAL	F	94	42.922	103.349	168.633	1.00	32.42	C
10	ATOM	596	CG2	VAL	F	94	43.315	104.389	170.887	1.00	29.31	C
	ATOM	600	C	VAL	F	94	40.033	104.128	168.846	1.00	32.37	C
	ATOM	601	O	VAL	F	94	39.396	103.187	169.314	1.00	31.63	O
	ATOM	603	N	VAL	F	95	39.827	104.617	167.624	1.00	31.16	N
	ATOM	604	CA	VAL	F	95	38.732	104.160	166.766	1.00	30.98	C
15	ATOM	606	CB	VAL	F	95	38.279	105.268	165.789	1.00	32.06	C
	ATOM	608	CG1	VAL	F	95	37.092	104.800	164.940	1.00	33.64	C
	ATOM	612	CG2	VAL	F	95	37.906	106.540	166.552	1.00	32.86	C
	ATOM	616	C	VAL	F	95	39.147	102.905	165.995	1.00	31.81	C
	ATOM	617	O	VAL	F	95	40.138	102.906	165.253	1.00	30.06	O
20	ATOM	619	N	ILE	F	96	38.393	101.827	166.178	1.00	29.04	N
	ATOM	620	CA	ILE	F	96	38.710	100.575	165.507	1.00	32.14	C
	ATOM	622	CB	ILE	F	96	38.375	99.330	166.364	1.00	29.02	C
	ATOM	624	CG1	ILE	F	96	39.087	99.389	167.722	1.00	31.90	C
	ATOM	627	CD1	ILE	F	96	40.635	99.508	167.644	1.00	31.87	C
25	ATOM	631	CG2	ILE	F	96	38.748	98.039	165.626	1.00	29.24	C
	ATOM	635	C	ILE	F	96	37.951	100.556	164.187	1.00	30.25	C
	ATOM	636	O	ILE	F	96	36.724	100.489	164.165	1.00	31.38	O
	ATOM	638	N	LYS	F	97	38.715	100.642	163.099	1.00	30.81	N
	ATOM	639	CA	LYS	F	97	38.206	100.605	161.738	1.00	33.46	C
30	ATOM	641	CB	LYS	F	97	39.077	101.510	160.850	1.00	34.21	C
	ATOM	644	CG	LYS	F	97	38.629	101.605	159.407	1.00	37.93	C
	ATOM	647	CD	LYS	F	97	39.396	102.694	158.635	1.00	40.98	C
	ATOM	650	CE	LYS	F	97	40.757	102.204	158.140	1.00	41.89	C
	ATOM	653	NZ	LYS	F	97	41.608	103.331	157.631	1.00	42.34	N
35	ATOM	657	C	LYS	F	97	38.218	99.184	161.173	1.00	30.79	C
	ATOM	658	O	LYS	F	97	37.384	98.847	160.344	1.00	29.59	O
	ATOM	660	N	CYS	F	98	39.188	98.375	161.594	1.00	31.57	N
	ATOM	661	CA	CYS	F	98	39.398	97.044	161.033	1.00	29.43	C
	ATOM	663	CB	CYS	F	98	40.778	96.936	160.384	1.00	32.50	C
40	ATOM	666	SG	CYS	F	98	41.146	98.189	159.146	1.00	33.96	S
	ATOM	668	C	CYS	F	98	39.278	95.943	162.064	1.00	32.27	C
	ATOM	669	O	CYS	F	98	39.805	96.064	163.176	1.00	33.15	O
	ATOM	671	N	ASP	F	99	38.615	94.854	161.678	1.00	30.84	N
	ATOM	672	CA	ASP	F	99	38.546	93.642	162.503	1.00	27.70	C
45	ATOM	674	CB	ASP	F	99	37.695	92.547	161.845	1.00	29.90	C
	ATOM	677	CG	ASP	F	99	36.210	92.837	161.832	1.00	32.65	C
	ATOM	678	OD1	ASP	F	99	35.751	93.874	162.350	1.00	29.49	O
	ATOM	679	OD2	ASP	F	99	35.481	91.980	161.284	1.00	29.45	O
	ATOM	680	C	ASP	F	99	39.949	93.074	162.631	1.00	30.45	C
50	ATOM	681	O	ASP	F	99	40.766	93.213	161.715	1.00	29.85	O
	ATOM	683	N	GLY	F	100	40.210	92.408	163.753	1.00	32.83	N
	ATOM	684	CA	GLY	F	100	41.456	91.677	163.946	1.00	31.74	C
	ATOM	687	C	GLY	F	100	41.712	91.334	165.399	1.00	30.54	C
	ATOM	688	O	GLY	F	100	40.989	91.784	166.288	1.00	28.92	O
55	ATOM	690	N	LEU	F	101	42.729	90.512	165.631	1.00	29.77	N
	ATOM	691	CA	LEU	F	101	43.342	90.401	166.958	1.00	29.75	C
	ATOM	693	CB	LEU	F	101	44.106	89.091	167.122	1.00	31.87	C
	ATOM	696	CG	LEU	F	101	43.290	87.796	167.046	1.00	32.91	C
	ATOM	698	CD1	LEU	F	101	44.196	86.596	167.260	1.00	33.15	C
60	ATOM	702	CD2	LEU	F	101	42.166	87.823	168.085	1.00	34.94	C
	ATOM	706	C	LEU	F	101	44.303	91.570	167.107	1.00	29.86	C
	ATOM	707	O	LEU	F	101	45.078	91.869	166.183	1.00	29.98	O
	ATOM	709	N	TYR	F	102	44.224	92.235	168.253	1.00	29.08	N
	ATOM	710	CA	TYR	F	102	45.084	93.361	168.573	1.00	29.61	C
65	ATOM	712	CB	TYR	F	102	44.263	94.643	168.701	1.00	29.60	C
	ATOM	715	CG	TYR	F	102	43.726	95.259	167.423	1.00	27.77	C
	ATOM	716	CD1	TYR	F	102	42.613	94.731	166.779	1.00	26.54	C
	ATOM	718	CE1	TYR	F	102	42.087	95.319	165.628	1.00	27.73	C
	ATOM	720	CZ	TYR	F	102	42.662	96.461	165.121	1.00	30.91	C
70	ATOM	721	OH	TYR	F	102	42.149	97.073	163.988	1.00	29.61	O
	ATOM	723	CE2	TYR	F	102	43.759	97.023	165.758	1.00	29.67	C

5	ATOM	725	CD2	TYR	F	102	44 .280	96 .422	166 .906	1 .000	29 .100	C
	ATOM	727	C	TYR	F	102	45.767	93 .125	169 .908	1.00	29.19	C
	ATOM	728	O	TYR	F	102	45.204	92 .495	170 .812	1.00	29.11	O
	ATOM	730	N	ILE	F	103	46.976	93 .655	170 .034	1.00	27.81	N
	ATOM	731	CA	ILE	F	103	47.587	93 .858	171 .329	1.00	30.85	C
10	ATOM	733	CB	ILE	F	103	49.120	93 .760	171 .301	1.00	33.46	C
	ATOM	735	CG1	ILE	F	103	49.558	92 .399	170 .829	1.00	37.09	C
	ATOM	738	CD1	ILE	F	103	51.082	92 .262	170 .725	1.00	38.79	C
	ATOM	742	CG2	ILE	F	103	49.718	94 .038	172 .702	1.00	36.79	C
	ATOM	746	C	ILE	F	103	47.233	95 .257	171 .784	1.00	31.01	C
15	ATOM	747	O	ILE	F	103	47.336	96 .221	171 .014	1.00	31.53	O
	ATOM	749	N	ILE	F	104	46.819	95 .362	173 .039	1.00	30.88	N
	ATOM	750	CA	ILE	F	104	46.702	96 .650	173 .717	1.00	31.77	C
	ATOM	752	CB	ILE	F	104	45 .270	96 .909	174 .191	1.00	34 .45	C
	ATOM	754	CG1	ILE	F	104	44 .320	96 .848	172 .991	1.00	34.38	C
20	ATOM	757	CD1	ILE	F	104	42.917	96 .635	173 .363	1.00	40.10	C
	ATOM	761	CG2	ILE	F	104	45.156	98 .271	174 .871	1.00	35.31	C
	ATOM	765	C	ILE	F	104	47.717	96 .642	174 .870	1.00	31.64	C
	ATOM	766	O	ILE	F	104	47.730	95 .726	175 .718	1.00	30.59	O
	ATOM	768	N	TYR	F	105	48.600	97 .635	174 .851	1.00	28.00	N
25	ATOM	769	CA	TYR	F	105	49.676	97 .765	175 .816	1.00	29.44	C
	ATOM	771	CB	TYR	F	105	51.045	97 .681	175 .133	1.00	36.38	C
	ATOM	774	CG	TYR	F	105	52 .184	97 .634	176 .126	1.00	34.89	C
	ATOM	775	CD1	TYR	F	105	52 .406	96 .488	176 .858	1.00	40.95	C
	ATOM	in	CE1	TYR	F	105	53 .421	96 .404	177 .775	1.00	42.22	C
30	ATOM	779	CZ	TYR	F	105	54 .239	97 .471	177 .987	1 .00	39.23	C
	ATOM	780	OH	TYR	F	105	55.245	97 .309	178 .921	1.00	44 .74	O
	ATOM	782	CE2	TYR	F	105	54 .067	98 .647	177 .277	1.00	38.05	C
	ATOM	784	CD2	TYR	F	105	53 .023	98 .730	176 .345	1.00	41.78	C
	ATOM	786	C	TYR	F	105	49.561	99 .114	176 .517	1.00	28.35	C
35	ATOM	787	O	TYR	F	105	49 .432	100 .142	175 .857	1.00	29.78	O
	ATOM	789	N	LEU	F	106	49.625	99 .101	177 .842	1.00	29.59	N
	ATOM	790	CA	LEU	F	106	49.555	100 .334	178 .646	1.00	27.33	C
	ATOM	792	CB	LEU	F	106	48.207	100 .437	179 .373	1.00	29.18	C
	ATOM	795	CG	LEU	F	106	47.986	101 .676	180 .261	1.00	30.55	C
40	ATOM	797	CD1	LEU	F	106	47.974	102 .952	179 .432	1.00	33.47	C
	ATOM	801	CD2	LEU	F	106	46.700	101 .547	181 .052	1.00	33.66	C
	ATOM	805	C	LEU	F	106	50.671	100 .328	179 .663	1.00	24 .41	C
	ATOM	806	O	LEU	F	106	50.889	99 .327	180 .344	1.00	25.05	O
	ATOM	808	N	LYS	F	107	51.384	101 .446	179 .765	1.00	28.15	N
45	ATOM	809	CA	LYS	F	107	52.314	101 .645	180 .852	1.00	30.42	C
	ATOM	811	CB	LYS	F	107	53 .757	101 .428	180 .390	1.00	36.27	C
	ATOM	814	CG	LYS	F	107	54 .255	102 .445	179 .396	1.00	41 .94	C
	ATOM	817	CD	LYS	F	107	55.678	102 .135	178 .947	1.00	42.96	C
	ATOM	820	CE	LYS	F	107	56.695	102 .527	179 .974	1.00	46.90	C
50	ATOM	823	NZ	LYS	F	107	58.060	102 .093	179 .559	1.00	50.38	N
	ATOM	827	C	LYS	F	107	52 .135	103 .043	181 .411	1.00	28 .87	C
	ATOM	828	O	LYS	F	107	51.698	103 .931	180 .710	1.00	27.30	O
	ATOM	830	N	GLY	F	108	52 .452	103 .209	182 .686	1.00	30.50	N
	ATOM	831	CA	GLY	F	108	52 .399	104 .511	183 .331	1.00	29 .77	C
55	ATOM	834	C	GLY	F	108	52 .904	104 .448	184 .750	1.00	26.93	C
	ATOM	835	O	GLY	F	108	52 .855	103 .393	185 .388	1.00	30.37	O
	ATOM	837	N	SER	F	109	53 .399	105 .581	185 .240	1.00	26.48	N
	ATOM	838	CA	SER	F	109	53 .830	105 .721	186 .617	1.00	30 .15	C
	ATOM	840	CB	SER	F	109	55.329	106 .041	186 .690	1.00	33 .60	C
60	ATOM	843	OG	SER	F	109	56.089	105 .046	186 .017	1.00	36.48	O
	ATOM	845	C	SER	F	109	53 .006	106 .824	187 .274	1.00	29.90	C
	ATOM	846	O	SER	F	109	52.790	107 .892	186 .690	1.00	25.72	O
	ATOM	848	N	PHE	F	110	52 .545	106 .542	188 .485	1.00	28.54	N
	ATOM	849	CA	PHE	F	110	51.640	107 .405	189 .217	1.00	28.31	C
65	ATOM	851	CB	PHE	F	110	50.295	106 .693	189 .397	1.00	31.72	C
	ATOM	854	CG	PHE	F	110	49.648	106 .280	188 .094	1.00	29.50	C
	ATOM	855	CD1	PHE	F	110	50.055	105 .131	187 .434	1.00	33.96	C
	ATOM	857	CE1	PHE	F	110	49.475	104 .754	186 .234	1.00	32 .61	C
	ATOM	859	CZ	PHE	F	110	48.467	105 .528	185 .687	1.00	32.93	C
70	ATOM	861	CE2	PHE	F	110	48.053	106 .679	186 .333	1.00	31.71	C
	ATOM	863	CD2	PHE	F	110	48.642	107 .048	187 .530	1.00	32 .22	C
	ATOM	865	C	PHE	F	110	52 .284	107 .709	190 .560	1.00	30.21	C
	ATOM	866	O	PHE	F	110	53 .246	107 .044	190 .949	1.00	33.59	O
	ATOM	868	N	PHE	F	111	51.774	108 .725	191 .249	1.00	28.68	N
	ATOM	869	CA	PHE	F	111	52 .260	109 .095	192 .582	1.00	28.57	C

5	ATOM	871	CB	PHE	F	111	52.461	110.607	192.691	1.00	28.27	C
	ATOM	874	CG	PHE	F	111	53.390	111.181	191.653	1.00	28.09	C
	ATOM	875	CD1	PHE	F	111	54.613	110.580	191.376	1.00	28.65	C
	ATOM	877	CE1	PHE	F	111	55.472	111.118	190.427	1.00	27.93	C
	ATOM	879	CZ	PHE	F	111	55.120	112.269	189.752	1.00	28.58	C
10	ATOM	881	CE2	PHE	F	111	53.913	112.888	190.022	1.00	29.54	C
	ATOM	883	CD2	PHE	F	111	53.053	112.344	190.973	1.00	30.24	C
	ATOM	885	C	PHE	F	111	51.290	108.630	193.672	1.00	28.64	C
	ATOM	886	O	PHE	F	111	51.479	108.934	194.847	1.00	26.04	O
	ATOM	888	N	GLN	F	112	50.258	107.896	193.273	1.00	30.69	N
15	ATOM	889	CA	GLN	F	112	49.271	107.359	194.204	1.00	34.46	C
	ATOM	891	CB	GLN	F	112	48.232	108.425	194.557	1.00	35.32	C
	ATOM	894	CG	GLN	F	112	47.366	108.852	193.384	1.00	37.97	C
	ATOM	897	CD	GLN	F	112	46.567	110.093	193.671	1.00	39.33	C
	ATOM	898	OE1	GLN	F	112	45.601	110.058	194.434	1.00	44.84	O
20	ATOM	899	NE2	GLN	F	112	46.962	111.209	193.060	1.00	41.29	N
	ATOM	902	C	GLN	F	112	48.600	106.145	193.571	1.00	35.82	C
	ATOM	903	O	GLN	F	112	48.712	105.925	192.357	1.00	31.47	O
	ATOM	905	N	GLU	F	113	47.906	105.360	194.395	1.00	35.40	N
	ATOM	906	CA	GLU	F	113	47.185	104.185	193.911	1.00	35.49	C
25	ATOM	908	CB	GLU	F	113	46.606	103.368	195.078	1.00	41.50	C
	ATOM	911	CG	GLU	F	113	47.628	102.900	196.118	1.00	47.70	C
	ATOM	914	CD	GLU	F	113	48.126	101.485	195.882	1.00	51.05	C
	ATOM	915	OE1	GLU	F	113	47.449	100.526	196.329	1.00	51.35	O
	ATOM	916	OE2	GLU	F	113	49.208	101.338	195.273	1.00	50.12	O
30	ATOM	917	C	GLU	F	113	46.048	104.646	193.009	1.00	29.04	C
	ATOM	918	O	GLU	F	113	45.332	105.592	193.343	1.00	36.71	O
	ATOM	920	N	VAL	F	114	45.890	103.979	191.876	1.00	35.77	N
	ATOM	921	CA	VAL	F	114	44.790	104.246	190.960	1.00	34.63	C
	ATOM	923	CB	VAL	F	114	45.247	105.048	189.699	1.00	31.03	C
35	ATOM	925	CG1	VAL	F	114	45.879	106.377	190.118	1.00	35.12	C
	ATOM	929	CG2	VAL	F	114	46.202	104.241	188.843	1.00	32.85	C
	ATOM	933	C	VAL	F	114	44.163	102.936	190.523	1.00	35.55	C
	ATOM	934	O	VAL	F	114	44.835	101.901	190.474	1.00	36.33	O
	ATOM	936	N	LYS	F	115	42.875	102.996	190.192	1.00	34.61	N
40	ATOM	937	CA	LYS	F	115	42.160	101.868	189.596	1.00	34.20	C
	ATOM	939	CB	LYS	F	115	40.909	101.533	190.414	1.00	35.12	C
	ATOM	942	CG	LYS	F	115	41.198	101.050	191.822	1.00	37.25	C
	ATOM	945	CD	LYS	F	115	39.910	100.867	192.611	1.00	38.64	C
	ATOM	948	CE	LYS	F	115	40.140	100.121	193.916	1.00	40.07	C
45	ATOM	951	NZ	LYS	F	115	38.844	99.810	194.597	1.00	41.65	N
	ATOM	955	C	LYS	F	115	41.771	102.250	188.178	1.00	32.77	C
	ATOM	956	O	LYS	F	115	40.984	103.173	187.977	1.00	33.31	O
	ATOM	958	N	ILE	F	116	42.341	101.555	187.198	1.00	30.22	N
	ATOM	959	CA	ILE	F	116	42.084	101.840	185.799	1.00	31.26	C
50	ATOM	961	CB	ILE	F	116	43.406	102.155	185.052	1.00	33.21	C
	ATOM	963	CG1	ILE	F	116	44.057	103.393	185.684	1.00	37.28	C
	ATOM	966	CD1	ILE	F	116	45.430	103.728	185.182	1.00	39.77	C
	ATOM	970	CG2	ILE	F	116	43.150	102.386	183.569	1.00	30.49	C
	ATOM	974	C	ILE	F	116	41.324	100.679	185.151	1.00	30.44	C
55	ATOM	975	O	ILE	F	116	41.585	99.505	185.441	1.00	31.68	O
	ATOM	977	N	ASP	F	117	40.356	101.029	184.310	1.00	29.80	N
	ATOM	978	CA	ASP	F	117	39.560	100.061	183.556	1.00	29.58	C
	ATOM	980	CB	ASP	F	117	38.069	100.173	183.900	1.00	32.71	C
	ATOM	983	CG	ASP	F	117	37.729	99.675	185.301	1.00	37.22	C
60	ATOM	984	OD1	ASP	F	117	38.305	98.672	185.762	1.00	35.20	O
	ATOM	985	OD2	ASP	F	117	36.844	100.288	185.946	1.00	40.61	O
	ATOM	986	C	ASP	F	117	39.740	100.333	182.071	1.00	30.59	C
	ATOM	987	O	ASP	F	117	39.736	101.488	181.638	1.00	29.98	O
	ATOM	989	N	LEU	F	118	39.886	99.254	181.303	1.00	31.13	N
65	ATOM	990	CA	LEU	F	118	40.043	99.290	179.861	1.00	30.74	C
	ATOM	992	CB	LEU	F	118	41.157	98.316	179.454	1.00	30.83	C
	ATOM	995	CG	LEU	F	118	41.392	98.050	177.967	1.00	32.17	C
	ATOM	997	CD1	LEU	F	118	41.809	99.336	177.249	1.00	31.18	C
	ATOM	1001	CD2	LEU	F	118	42.452	96.974	177.802	1.00	34.09	C
70	ATOM	1005	C	LEU	F	118	38.734	98.868	179.194	1.00	31.68	C
	ATOM	1006	O	LEU	F	118	38.199	97.798	179.487	1.00	29.27	O
	ATOM	1008	N	HIS	F	119	38.244	99.710	178.288	1.00	31.23	N
	ATOM	1009	CA	HIS	F	119	36.951	99.525	177.619	1.00	30.48	C
	ATOM	1011	CB	HIS	F	119	36.047	100.749	177.815	1.00	29.71	C
	ATOM	1014	CG	HIS	F	119	35.796	101.126	179.241	1.00	30.89	C

5	ATOM	1015	ND1	HIS	F	119	34.597	100.879	179.875	1.00	31.76	N
	ATOM	1017	CE1	HIS	F	119	34.651	101.345	181.110	1.00	32.27	C
	ATOM	1019	NE2	HIS	F	119	35.833	101.906	181.294	1.00	31.34	N
	ATOM	1021	CD2	HIS	F	119	36.563	101.794	180.137	1.00	31.42	C
	ATOM	1023	C	HIS	F	119	37.211	99.372	176.126	1.00	30.71	C
10	ATOM	1024	O	HIS	F	119	38.079	100.054	175.577	1.00	29.95	O
	ATOM	1026	N	PHE	F	120	36.474	98.471	175.480	1.00	33.18	N
	ATOM	1027	CA	PHE	F	120	36.547	98.265	174.028	1.00	33.86	C
	ATOM	1029	CB	PHE	F	120	36.601	96.777	173.682	1.00	36.56	C
	ATOM	1032	CG	PHE	F	120	37.809	96.053	174.230	1.00	36.09	C
15	ATOM	1033	CD1	PHE	F	120	39.025	96.703	174.417	1.00	36.43	C
	ATOM	1035	CE1	PHE	F	120	40.120	96.017	174.912	1.00	39.05	C
	ATOM	1037	CZ	PHE	F	120	40.025	94.671	175.199	1.00	38.81	C
	ATOM	1039	CE2	PHE	F	120	38.835	94.006	174.995	1.00	38.01	C
	ATOM	1041	CD2	PHE	F	120	37.736	94.698	174.507	1.00	38.78	C
20	ATOM	1043	C	PHE	F	120	35.354	98.870	173.300	1.00	34.66	C
	ATOM	1044	O	PHE	F	120	35.360	98.970	172.077	1.00	31.76	O
	ATOM	1046	N	ARG	F	121	34.327	99.250	174.049	1.00	35.83	N
	ATOM	1047	CA	ARG	F	121	33.167	99.938	173.495	1.00	39.64	C
	ATOM	1049	CB	ARG	F	121	32.336	99.014	172.589	1.00	39.98	C
25	ATOM	1052	CG	ARG	F	121	31.634	99.766	171.450	1.00	41.10	C
	ATOM	1055	CD	ARG	F	121	31.195	98.855	170.317	1.00	44.27	C
	ATOM	1058	NE	ARG	F	121	30.024	98.058	170.664	1.00	49.02	N
	ATOM	1060	CZ	ARG	F	121	29.283	97.379	169.789	1.00	49.79	C
	ATOM	1061	NH1	ARG	F	121	29.563	97.399	168.487	1.00	49.55	N
30	ATOM	1064	NH2	ARG	F	121	28.239	96.682	170.220	1.00	50.60	N
	ATOM	1067	C	ARG	F	121	32.339	100.433	174.674	1.00	40.52	C
	ATOM	1068	O	ARG	F	121	32.600	100.050	175.814	1.00	38.29	O
	ATOM	1070	N	GLU	F	122	31.352	101.283	174.401	1.00	43.32	N
	ATOM	1071	CA	GLU	F	122	30.535	101.893	175.459	1.00	45.49	C
35	ATOM	1073	CB	GLU	F	122	29.610	102.973	174.880	1.00	51.00	C
	ATOM	1076	CG	GLU	F	122	30.324	104.264	174.458	1.00	55.20	C
	ATOM	1079	CD	GLU	F	122	30.840	104.249	173.019	1.00	60.79	C
	ATOM	1080	OE1	GLU	F	122	31.196	103.164	172.491	1.00	61.68	O
	ATOM	1081	OE2	GLU	F	122	30.895	105.345	172.415	1.00	63.87	O
40	ATOM	1082	C	GLU	F	122	29.714	100.874	176.257	1.00	44.36	C
	ATOM	1083	O	GLU	F	122	29.465	101.073	177.447	1.00	46.14	O
	ATOM	1085	N	ASP	F	123	29.306	99.787	175.607	1.00	43.72	N
	ATOM	1086	CA	ASP	F	123	28.521	98.731	176.266	1.00	46.27	C
	ATOM	1088	CB	ASP	F	123	27.405	98.246	175.329	1.00	48.38	C
45	ATOM	1091	CG	ASP	F	123	27.930	97.760	173.984	1.00	49.94	C
	ATOM	1092	OD1	ASP	F	123	29.164	97.750	173.784	1.00	50.75	O
	ATOM	1093	OD2	ASP	F	123	27.102	97.387	173.126	1.00	50.56	O
	ATOM	1094	C	ASP	F	123	29.362	97.533	176.752	1.00	47.24	C
	ATOM	1095	O	ASP	F	123	28.820	96.575	177.300	1.00	49.69	O
50	ATOM	1097	N	HIS	F	124	30.678	97.597	176.545	1.00	46.31	N
	ATOM	1098	CA	HIS	F	124	31.600	96.517	176.913	1.00	42.87	C
	ATOM	1100	CB	HIS	F	124	32.914	96.716	176.133	1.00	44.77	C
	ATOM	1103	CG	HIS	F	124	34.019	95.779	176.517	1.00	46.09	C
	ATOM	1104	ND1	HIS	F	124	35.171	96.210	177.139	1.00	44.42	N
55	ATOM	1106	CE1	HIS	F	124	35.972	95.179	177.342	1.00	44.95	C
	ATOM	1108	NE2	HIS	F	124	35.379	94.094	176.878	1.00	43.97	N
	ATOM	1110	CD2	HIS	F	124	34.160	94.443	176.348	1.00	46.25	C
	ATOM	1112	C	HIS	F	124	31.846	96.487	178.435	1.00	41.21	C
	ATOM	1113	O	HIS	F	124	32.034	97.533	179.057	1.00	40.22	O
60	ATOM	1115	N	ASN	F	125	31.818	95.291	179.027	1.00	39.98	N
	ATOM	1116	CA	ASN	F	125	32.217	95.091	180.430	1.00	39.41	C
	ATOM	1118	CB	ASN	F	125	31.788	93.702	180.912	1.00	40.85	C
	ATOM	1121	CG	ASN	F	125	31.936	93.513	182.423	1.00	43.60	C
	ATOM	1122	OD1	ASN	F	125	32.229	94.452	183.169	1.00	45.85	O
65	ATOM	1123	ND2	ASN	F	125	31.713	92.286	182.879	1.00	44.49	N
	ATOM	1126	C	ASN	F	125	33.741	95.244	180.534	1.00	38.97	C
	ATOM	1127	O	ASN	F	125	34.479	94.435	179.965	1.00	37.29	O
	ATOM	1129	N	PRO	F	126	34.221	96.280	181.248	1.00	38.29	N
	ATOM	1130	CA	PRO	F	126	35.647	96.612	181.126	1.00	37.18	C
70	ATOM	1132	CB	PRO	F	126	35.741	98.012	181.744	1.00	38.83	C
	ATOM	1135	CG	PRO	F	126	34.566	98.164	182.591	1.00	38.46	C
	ATOM	1138	CD	PRO	F	126	33.517	97.186	182.170	1.00	38.80	C
	ATOM	1141	C	PRO	F	126	36.608	95.660	181.830	1.00	36.04	C
	ATOM	1142	O	PRO	F	126	36.219	94.941	182.748	1.00	35.04	O
	ATOM	1143	N	ILE	F	127	37.864	95.684	181.390	1.00	33.47	N

5	ATOM	1144	CA	ILE	F	127	38.932	94.930	182.029	1.00	33.95	C
	ATOM	1146	CB	ILE	F	127	40.004	94.497	181.000	1.00	33.78	C
	ATOM	1148	CG1	ILE	F	127	39.375	93.605	179.916	1.00	38.57	C
	ATOM	1151	CD1	ILE	F	127	40.238	93.459	178.650	1.00	41.00	C
	ATOM	1155	CG2	ILE	F	127	41.147	93.767	181.694	1.00	33.53	C
10	ATOM	1159	C	ILE	F	127	39.573	95.795	183.116	1.00	33.36	C
	ATOM	1160	O	ILE	F	127	40.049	96.901	182.844	1.00	31.39	O
	ATOM	1162	N	SER	F	128	39.576	95.286	184.342	1.00	27.99	N
	ATOM	1163	CA	SER	F	128	40.252	95.947	185.460	1.00	33.77	C
	ATOM	1165	CB	SER	F	128	39.746	95.389	186.791	1.00	35.44	C
15	ATOM	1168	OG	SER	F	128	40.492	95.881	187.895	1.00	40.27	O
	ATOM	1170	C	SER	F	128	41.756	95.728	185.315	1.00	33.81	C
	ATOM	1171	O	SER	F	128	42.216	94.593	185.300	1.00	31.64	O
	ATOM	1173	N	ILE	F	129	42.516	96.809	185.201	1.00	31.18	N
	ATOM	1174	CA	ILE	F	129	43.962	96.716	184.976	1.00	34.16	C
20	ATOM	1176	CB	ILE	F	129	44.484	97.959	184.202	1.00	32.56	C
	ATOM	1178	CG1	ILE	F	129	43.879	97.975	182.797	1.00	35.35	C
	ATOM	1181	CD1	ILE	F	129	44.259	99.180	181.970	1.00	39.13	C
	ATOM	1185	CG2	ILE	F	129	46.019	97.955	184.132	1.00	33.03	C
	ATOM	1189	C	ILE	F	129	44.718	96.556	186.300	1.00	34.77	C
25	ATOM	1190	O	ILE	F	129	44.594	97.396	187.185	1.00	36.24	O
	ATOM	1192	N	PRO	F	130	45.513	95.479	186.441	1.00	36.07	N
	ATOM	1193	CA	PRO	F	130	46.278	95.334	187.679	1.00	38.75	C
	ATOM	1195	CB	PRO	F	130	46.773	93.887	187.633	1.00	39.27	C
	ATOM	1198	CG	PRO	F	130	46.688	93.468	186.221	1.00	40.09	C
30	ATOM	1201	CD	PRO	F	130	45.745	94.369	185.499	1.00	38.62	C
	ATOM	1204	C	PRO	F	130	47.452	96.306	187.764	1.00	38.29	C
	ATOM	1205	O	PRO	F	130	48.127	96.561	186.767	1.00	36.20	O
	ATOM	1206	N	MET	F	131	47.667	96.856	188.952	1.00	39.61	N
	ATOM	1207	CA	MET	F	131	48.851	97.652	189.239	1.00	44.26	C
35	ATOM	1209	CB	MET	F	131	48.554	98.694	190.322	1.00	47.71	C
	ATOM	1212	CG	MET	F	131	48.597	100.106	189.813	1.00	49.46	C
	ATOM	1215	SD	MET	F	131	48.545	101.349	191.097	1.00	48.37	S
	ATOM	1216	CE	MET	F	131	49.320	102.681	190.193	1.00	49.64	C
	ATOM	1220	C	MET	F	131	49.984	96.745	189.709	1.00	45.81	C
40	ATOM	1221	O	MET	F	131	49.734	95.736	190.369	1.00	43.21	O
	ATOM	1223	N	LEU	F	132	51.222	97.116	189.375	1.00	48.02	N
	ATOM	1224	CA	LEU	F	132	52.401	96.358	189.805	1.00	49.72	C
	ATOM	1226	CB	LEU	F	132	53.685	96.889	189.159	1.00	50.32	C
	ATOM	1229	CG	LEU	F	132	53.913	96.648	187.663	1.00	51.14	C
45	ATOM	1231	CD1	LEU	F	132	55.320	97.066	187.295	1.00	51.30	C
	ATOM	1235	CD2	LEU	F	132	53.688	95.202	187.285	1.00	52.46	C
	ATOM	1239	C	LEU	F	132	52.542	96.429	191.312	1.00	51.72	C
	ATOM	1240	O	LEU	F	132	52.013	97.344	191.944	1.00	51.73	O
	ATOM	1242	N	ASN	F	133	53.283	95.471	191.875	1.00	54.23	N
50	ATOM	1243	CA	ASN	F	133	53.499	95.377	193.324	1.00	53.52	C
	ATOM	1245	CB	ASN	F	133	54.385	94.172	193.661	1.00	56.50	C
	ATOM	1248	CG	ASN	F	133	53.841	92.869	193.094	1.00	57.08	C
	ATOM	1249	OD1	ASN	F	133	52.718	92.824	192.586	1.00	58.74	O
	ATOM	1250	ND2	ASN	F	133	54.640	91.809	193.166	1.00	55.18	N
55	ATOM	1253	C	ASN	F	133	54.121	96.653	193.880	1.00	54.30	C
	ATOM	1254	O	ASN	F	133	54.017	96.942	195.075	1.00	53.43	O
	ATOM	1256	N	ASP	F	134	54.794	97.379	192.989	1.00	54.15	N
	ATOM	1257	CA	ASP	F	134	55.186	98.777	193.174	1.00	55.50	C
	ATOM	1259	CB	ASP	F	134	55.470	99.394	191.784	1.00	56.66	C
60	ATOM	1262	CG	ASP	F	134	56.704	100.262	191.762	1.00	61.23	C
	ATOM	1263	OD1	ASP	F	134	57.701	99.916	192.433	1.00	66.25	O
	ATOM	1264	OD2	ASP	F	134	56.691	101.288	191.049	1.00	64.56	O
	ATOM	1265	C	ASP	F	134	54.118	99.622	193.887	1.00	54.08	C
	ATOM	1266	O	ASP	F	134	54.436	100.428	194.757	1.00	56.90	O
65	ATOM	1268	N	GLY	F	135	52.856	99.440	193.500	1.00	53.84	N
	ATOM	1269	CA	GLY	F	135	51.767	100.315	193.937	1.00	51.79	C
	ATOM	1272	C	GLY	F	135	51.632	101.558	193.058	1.00	52.22	C
	ATOM	1273	O	GLY	F	135	50.600	102.230	193.062	1.00	52.19	O
	ATOM	1275	N	ARG	F	136	52.671	101.849	192.281	1.00	50.66	N
70	ATOM	1276	CA	ARG	F	136	52.781	103.109	191.559	1.00	47.14	C
	ATOM	1278	CB	ARG	F	136	54.094	103.791	191.954	1.00	48.57	C
	ATOM	1281	CG	ARG	F	136	54.170	104.184	193.424	1.00	49.69	C
	ATOM	1284	CD	ARG	F	136	53.239	105.351	193.735	1.00	48.83	C
	ATOM	1287	NE	ARG	F	136	53.213	105.678	195.155	1.00	48.94	N
	ATOM	3289	CZ	ARG	F	136	52.465	105.070	196.075	1.00	48.61	C

	ATOM	1290	NH1	ARG	F	136	51.652	104.070	195.750	1.00	47.33	N
	ATOM	1293	NH2	ARG	F	136	52.535	105.469	197.344	1.00	47.54	N
	ATOM	1296	C	ARG	F	136	52.742	102.947	190.048	1.00	42.89	C
	ATOM	1297	O	ARG	F	136	52.679	103.939	189.330	1.00	36.01	O
5	ATOM	1299	N	ARG	F	137	52.748	101.705	189.565	1.00	41.10	N
	ATOM	1300	CA	ARG	F	137	53.078	101.446	188.176	1.00	38.01	C
	ATOM	1302	CB	ARG	F	137	54.454	100.790	188.095	1.00	41.95	C
	ATOM	1305	CG	ARG	F	137	55.381	101.461	187.126	1.00	48.06	C
	ATOM	1308	CD	ARG	F	137	56.173	100.473	186.305	1.00	48.97	C
10	ATOM	1311	NE	ARG	F	137	57.188	99.779	187.067	1.00	51.07	N
	ATOM	1313	CZ	ARG	F	137	58.211	99.124	186.525	1.00	47.02	C
	ATOM	1314	NH1	ARG	F	137	58.375	99.083	185.204	1.00	43.96	N
	ATOM	1317	NH2	ARG	F	137	59.070	98.518	187.320	1.00	43.53	N
	ATOM	1320	C	ARG	F	137	52.079	100.547	187.468	1.00	32.66	C
15	ATOM	1321	O	ARG	F	137	51.494	99.646	188.075	1.00	31.68	O
	ATOM	1323	N	ILE	F	138	51.915	100.790	186.173	1.00	30.74	N
	ATOM	1324	CA	ILE	F	138	51.198	99.876	185.295	1.00	31.14	C
	ATOM	1326	CB	ILE	F	138	49.959	100.545	184.687	1.00	29.86	C
	ATOM	1328	CG1	ILE	F	138	48.950	100.784	185.812	1.00	32.61	C
20	ATOM	1331	CD1	ILE	F	138	47.735	101.487	185.417	1.00	33.80	C
	ATOM	1335	CG2	ILE	F	138	49.359	99.687	183.561	1.00	28.66	C
	ATOM	1339	C	ILE	F	138	52.139	99.418	184.202	1.00	31.42	C
	ATOM	1340	O	ILE	F	138	52.832	100.224	183.596	1.00	29.29	O
	ATOM	1342	N	VAL	F	139	52.181	98.109	183.992	1.00	29.60	N
25	ATOM	1343	CA	VAL	F	139	52.813	97.501	182.823	1.00	35.14	C
	ATOM	1345	CB	VAL	F	139	54.195	96.897	183.144	1.00	42.11	C
	ATOM	1347	CG1	VAL	F	139	54.832	96.349	181.874	1.00	44.18	C
	ATOM	1351	CG2	VAL	F	139	55.112	97.931	183.776	1.00	42.63	C
	ATOM	1355	C	VAL	F	139	51.865	96.384	182.392	1.00	36.13	C
30	ATOM	1356	O	VAL	F	139	51.858	95.316	182.986	1.00	42.25	O
	ATOM	1358	N	PHE	F	140	51.027	96.658	181.403	1.00	34.44	N
	ATOM	1359	CA	PHE	F	140	49.879	95.795	181.129	1.00	33.21	C
	ATOM	1361	CB	PHE	F	140	48.595	96.485	181.603	1.00	35.89	C
	ATOM	1364	CG	PHE	F	140	47.356	95.668	181.392	1.00	36.81	C
35	ATOM	1365	CD1	PHE	F	140	47.108	94.560	182.184	1.00	36.71	C
	ATOM	1367	CE1	PHE	F	140	45.968	93.801	182.007	1.00	37.36	C
	ATOM	1369	CZ	PHE	F	140	45.069	94.136	181.031	1.00	37.64	C
	ATOM	1371	CE2	PHE	F	140	45.301	95.241	180.217	1.00	39.99	C
	ATOM	1373	CD2	PHE	F	140	46.445	96.001	180.403	1.00	40.03	C
40	ATOM	1375	C	PHE	F	140	49.762	95.448	179.655	1.00	28.19	C
	ATOM	1376	O	PHE	F	140	49.782	96.333	178.804	1.00	28.51	O
	ATOM	1378	N	THR	F	141	49.629	94.159	179.364	1.00	29.73	N
	ATOM	1379	CA	THR	F	141	49.434	93.671	178.003	1.00	31.81	C
	ATOM	1381	CB	THR	F	141	50.598	92.760	177.570	1.00	39.40	C
45	ATOM	1383	OG1	THR	F	141	51.836	93.443	177.758	1.00	39.39	O
	ATOM	1385	CG2	THR	F	141	50.452	92.352	176.104	1.00	40.26	C
	ATOM	1389	C	THR	F	141	48.162	92.832	177.913	1.00	31.07	C
	ATOM	1390	O	THR	F	141	47.933	91.943	178.737	1.00	33.43	O
	ATOM	1392	N	VAL	F	142	47.334	93.126	176.919	1.00	29.06	N
50	ATOM	1393	CA	VAL	F	142	46.192	92.264	176.567	1.00	32.68	C
	ATOM	1395	CB	VAL	F	142	44.825	92.883	177.013	1.00	34.56	C
	ATOM	1397	CG1	VAL	F	142	44.595	94.208	176.401	1.00	41.46	C
	ATOM	1401	CG2	VAL	F	142	43.647	91.952	176.679	1.00	39.57	C
	ATOM	1405	C	VAL	F	142	46.188	91.987	175.064	1.00	29.71	C
55	ATOM	1406	O	VAL	F	142	46.550	92.841	174.271	1.00	30.24	O
	ATOM	1408	N	VAL	F	143	45.783	90.781	174.687	1.00	30.43	N
	ATOM	1409	CA	VAL	F	143	45.454	90.467	173.306	1.00	26.34	C
	ATOM	1411	CB	VAL	F	143	46.202	89.222	172.775	1.00	28.05	C
	ATOM	1413	CG1	VAL	F	143	45.916	89.025	171.288	1.00	28.61	C
60	ATOM	1417	CG2	VAL	F	143	47.688	89.340	173.025	1.00	32.10	C
	ATOM	1421	C	VAL	F	143	43.952	90.234	173.279	1.00	28.54	C
	ATOM	1422	O	VAL	F	143	43.418	89.499	174.117	1.00	29.57	O
	ATOM	1424	N	ALA	F	144	43.283	90.873	172.332	1.00	30.16	N
	ATOM	1425	CA	ALA	F	144	41.828	90.853	172.252	1.00	30.65	C
65	ATOM	1427	CB	ALA	F	144	41.260	92.067	172.987	1.00	32.27	C
	ATOM	1431	C	ALA	F	144	41.357	90.855	170.805	1.00	29.58	C
	ATOM	1432	O	ALA	F	144	42.003	91.443	169.925	1.00	28.90	O
	ATOM	1434	N	SER	F	145	40.221	90.207	170.564	1.00	29.16	N
	ATOM	1435	CA	SER	F	145	39.550	90.279	169.275	1.00	31.00	C
70	ATOM	1437	CB	SER	F	145	38.658	89.055	169.043	1.00	32.81	C
	ATOM	1440	OG	SER	F	145	38.092	89.092	167.747	1.00	36.52	O

5	ATOM	1442	C	SER	F	145	38.699	91.549	169.243	1.00	32.33	C
	ATOM	1443	O	SER	F	145	37.755	91.687	170.013	1.00	32.56	O
	ATOM	1445	N	LEU	F	146	39.062	92.478	168.368	1.00	28.60	N
	ATOM	1446	CA	LEU	F	146	38.328	93.716	168.190	1.00	30.06	C
	ATOM	1448	CB	LEU	F	146	39.243	94.926	168.354	1.00	29.79	C
10	ATOM	1451	CG	LEU	F	146	40.044	95.014	169.659	1.00	29.76	C
	ATOM	1453	CD1	LEU	F	146	40.896	96.283	169.642	1.00	30.68	C
	ATOM	1457	CD2	LEU	F	146	39.129	94.997	170.861	1.00	31.15	C
	ATOM	1461	C	LEU	F	146	37.665	93.748	166.820	1.00	30.65	C
	ATOM	1462	O	LEU	F	146	38.064	93.038	165.901	1.00	30.30	O
15	ATOM	1464	N	ALA	F	147	36.644	94.587	166.701	1.00	29.76	N
	ATOM	1465	CA	ALA	F	147	35.865	94.694	165.471	1.00	31.78	C
	ATOM	1467	CB	ALA	F	147	34.576	93.871	165.588	1.00	31.54	C
	ATOM	1471	C	ALA	F	147	35.533	96.141	165.164	1.00	30.56	C
	ATOM	1472	O	ALA	F	147	35.511	96.981	166.060	1.00	32.11	O
20	ATOM	1474	N	PHE	F	148	35.282	96.430	163.892	1.00	30.23	N
	ATOM	1475	CA	PHE	F	148	34.700	97.714	163.490	1.00	29.13	C
	ATOM	1477	CB	PHE	F	148	34.182	97.636	162.046	1.00	27.59	C
	ATOM	1480	CG	PHE	F	148	33.390	98.837	161.606	1.00	28.92	C
	ATOM	1481	CD1	PHE	F	148	33.914	100.119	161.730	1.00	26.93	C
25	ATOM	1483	CE1	PHE	F	148	33.196	101.218	161.313	1.00	27.53	C
	ATOM	1485	CZ	PHE	F	148	31.946	101.063	160.757	1.00	28.80	C
	ATOM	1487	CE2	PHE	F	148	31.408	99.783	160.608	1.00	29.05	C
	ATOM	1489	CD2	PHE	F	148	32.132	98.685	161.033	1.00	27.28	C
	ATOM	1491	C	PHE	F	148	33.573	98.112	164.445	1.00	30.68	C
30	ATOM	1492	O	PHE	F	148	32.741	97.288	164.812	1.00	32.23	O
	ATOM	1494	N	LYS	F	149	33.569	99.389	164.824	1.00	32.61	N
	ATOM	1495	CA	LYS	F	149	32.645	99.997	165.796	1.00	29.94	C
	ATOM	1497	CB	LYS	F	149	31.214	99.442	165.721	1.00	32.26	C
	ATOM	1500	CG	LYS	F	149	30.525	99.750	164.398	1.00	28.97	C
35	ATOM	1503	CD	LYS	F	149	29.103	99.261	164.367	1.00	29.28	C
	ATOM	1506	CE	LYS	F	149	28.554	99.307	162.956	1.00	30.08	C
	ATOM	1509	NZ	LYS	F	149	27.105	99.022	162.918	1.00	27.52	N
	ATOM	1513	C	LYS	F	149	33.181	99.984	167.231	1.00	32.24	C
	ATOM	1514	O	LYS	F	149	32.651	100.676	168.093	1.00	25.91	O
40	ATOM	1516	N	ASP	F	150	34.240	99.220	167.492	1.00	32.13	N
	ATOM	1517	CA	ASP	F	150	34.862	99.252	168.808	1.00	32.81	C
	ATOM	1519	CB	ASP	F	150	35.824	98.071	169.013	1.00	32.80	C
	ATOM	1522	CG	ASP	F	150	35.102	96.728	169.223	1.00	35.26	C
	ATOM	1523	OD1	ASP	F	150	33.874	96.694	169.474	1.00	33.22	O
45	ATOM	1524	OD2	ASP	F	150	35.785	95.687	169.149	1.00	33.07	O
	ATOM	1525	C	ASP	F	150	35.585	100.594	168.991	1.00	32.78	C
	ATOM	1526	O	ASP	F	150	36.008	101.234	168.022	1.00	30.42	O
	ATOM	1528	N	LYS	F	151	35.683	101.032	170.241	1.00	35.98	N
	ATOM	1529	CA	LYS	F	151	36.393	102.260	170.594	1.00	35.80	C
50	ATOM	1531	CB	LYS	F	151	35.408	103.430	170.742	1.00	39.98	C
	ATOM	1534	CG	LYS	F	151	34.879	103.951	169.400	1.00	41.76	C
	ATOM	1537	CD	LYS	F	151	33.683	104.869	169.554	1.00	43.66	C
	ATOM	1540	CE	LYS	F	151	33.134	105.292	168.194	1.00	43.97	C
	ATOM	1543	NZ	LYS	F	151	31.870	106.082	168.327	1.00	47.14	N
55	ATOM	1547	C	LYS	F	151	37.137	101.983	171.895	1.00	33.57	C
	ATOM	1548	O	LYS	F	151	36.511	101.678	172.909	1.00	33.07	O
	ATOM	1550	N	VAL	F	152	38.468	102.044	171.852	1.00	30.79	N
	ATOM	1551	CA	VAL	F	152	39.304	101.676	172.996	1.00	30.67	C
	ATOM	1553	CB	VAL	F	152	40.643	101.031	172.544	1.00	31.45	C
60	ATOM	1555	CG1	VAL	F	152	41.529	100.687	173.750	1.00	35.17	C
	ATOM	1559	CG2	VAL	F	152	40.379	99.776	171.698	1.00	34.71	C
	ATOM	1563	C	VAL	F	152	39.596	102.904	173.846	1.00	29.54	C
	ATOM	1564	O	VAL	F	152	40.146	103.885	173.348	1.00	30.16	O
	ATOM	1566	N	TYR	F	153	39.222	102.850	175.121	1.00	29.57	N
65	ATOM	1567	CA	TYR	F	153	39.481	103.959	176.043	1.00	30.80	C
	ATOM	1569	CB	TYR	F	153	38.374	105.015	175.957	1.00	31.78	C
	ATOM	1572	CG	TYR	F	153	37.000	104.520	176.331	1.00	31.12	C
	ATOM	1573	CD1	TYR	F	153	36.202	103.857	175.404	1.00	32.46	C
	ATOM	1575	CE1	TYR	F	153	34.931	103.397	175.748	1.00	32.60	C
70	ATOM	1577	CZ	TYR	F	153	34.452	103.612	177.024	1.00	31.96	C
	ATOM	1578	OH	TYR	F	153	33.196	103.168	177.376	1.00	33.94	O
	ATOM	1580	CE2	TYR	F	153	35.227	104.277	177.956	1.00	32.37	C
	ATOM	1582	CD2	TYR	F	153	36.492	104.726	177.606	1.00	30.63	C
	ATOM	1584	C	TYR	F	153	39.680	103.470	177.470	1.00	28.88	C
	ATOM	1585	O	TYR	F	153	39.434	102.303	177.780	1.00	30.97	O

	ATOM	1587	N	LEU	F	154	40.153	104.366	178.329	1.00	27.30	N
	ATOM	1588	CA	LEU	F	154	40.544	104.002	179.680	1.00	29.52	C
	ATOM	1590	CB	LEU	F	154	42.058	104.094	179.809	1.00	31.10	C
5	ATOM	1593	CG	LEU	F	154	42.856	103.153	178.899	1.00	34.02	C
	ATOM	1595	CD1	LEU	F	154	44.076	103.873	178.371	1.00	38.13	C
	ATOM	1599	CD2	LEU	F	154	43.238	101.881	179.632	1.00	35.46	C
	ATOM	1603	C	LEU	F	154	39.889	104.934	180.681	1.00	28.29	C
	ATOM	1604	O	LEU	F	154	40.003	106.141	180.559	1.00	26.74	O
10	ATOM	1606	N	THR	F	155	39.203	104.368	181.670	1.00	27.72	N
	ATOM	1607	CA	THR	F	155	38.606	105.167	182.732	1.00	29.68	C
	ATOM	1609	CB	THR	F	155	37.128	104.794	182.988	1.00	30.42	C
	ATOM	1611	OG1	THR	F	155	37.022	103.397	183.271	1.00	29.41	O
	ATOM	1613	CG2	THR	F	155	36.272	105.130	181.790	1.00	31.00	C
15	ATOM	1617	C	THR	F	155	39.388	105.003	184.027	1.00	30.72	C
	ATOM	1618	O	THR	F	155	40.087	104.009	184.231	1.00	30.95	O
	ATOM	1620	N	VAL	F	156	39.281	106.008	184.885	1.00	31.97	N
	ATOM	1621	CA	VAL	F	156	39.828	105.960	186.227	1.00	37.73	C
	ATOM	1623	CB	VAL	F	156	40.626	107.230	186.541	1.00	41.50	C
20	ATOM	1625	CG1	VAL	F	156	41.135	107.204	187.976	1.00	42.50	C
	ATOM	1629	CG2	VAL	F	156	41.781	107.379	185.549	1.00	40.22	C
	ATOM	1633	C	VAL	F	156	38.648	105.842	187.188	1.00	40.99	C
	ATOM	1634	O	VAL	F	156	37.727	106.662	187.141	1.00	39.99	O
	ATOM	1636	N	ASN	F	157	38.659	104.813	188.036	1.00	42.25	N
25	ATOM	1637	CA	ASN	F	157	37.615	104.651	189.045	1.00	43.66	C
	ATOM	1639	CB	ASN	F	157	37.363	103.167	189.349	1.00	46.30	C
	ATOM	1642	CG	ASN	F	157	35.950	102.906	189.866	1.00	50.35	C
	ATOM	1643	OD1	ASN	F	157	35.192	102.129	189.276	1.00	56.96	O
	ATOM	1644	ND2	ASN	F	157	35.587	103.568	190.959	1.00	50.63	N
30	ATOM	1647	C	ASN	F	157	38.004	105.431	190.305	1.00	43.69	C
	ATOM	1648	O	ASN	F	157	38.716	104.920	191.173	1.00	43.76	O
	ATOM	1650	N	ALA	F	158	37.545	106.678	190.380	1.00	44.97	N
	ATOM	1651	CA	ALA	F	158	37.864	107.570	191.497	1.00	45.39	C
	ATOM	1653	CB	ALA	F	158	39.341	107.942	191.461	1.00	46.60	C
35	ATOM	1657	C	ALA	F	158	37.000	108.835	191.436	1.00	46.23	C
	ATOM	1658	O	ALA	F	158	36.401	109.119	190.396	1.00	43.53	O
	ATOM	1660	N	PRO	F	159	36.934	109.602	192.546	1.00	47.82	N
	ATOM	1661	CA	PRO	F	159	36.196	110.871	192.535	1.00	48.95	C
	ATOM	1663	CB	PRO	F	159	36.365	111.399	193.969	1.00	50.06	C
40	ATOM	1666	CG	PRO	F	159	36.758	110.222	194.786	1.00	49.84	C
	ATOM	1669	CD	PRO	F	159	37.524	109.323	193.869	1.00	49.11	C
	ATOM	1672	C	PRO	F	159	36.752	111.881	191.527	1.00	49.87	C
	ATOM	1673	O	PRO	F	159	37.933	111.823	191.180	1.00	52.64	O
	ATOM	1674	N	ASP	F	160	35.902	112.797	191.070	1.00	49.94	N
45	ATOM	1675	CA	ASP	F	160	36.282	113.794	190.059	1.00	51.49	C
	ATOM	1677	CB	ASP	F	160	35.151	114.817	189.865	1.00	54.24	C
	ATOM	1680	CG	ASP	F	160	33.907	114.210	189.221	1.00	55.84	C
	ATOM	1681	OD1	ASP	F	160	34.044	113.498	188.206	1.00	55.57	O
	ATOM	1682	OD2	ASP	F	160	32.791	114.455	189.730	1.00	56.57	O
50	ATOM	1683	C	ASP	F	160	37.578	114.532	190.413	1.00	51.05	C
	ATOM	1684	O	ASP	F	160	38.418	114.772	189.546	1.00	48.96	O
	ATOM	1686	N	THR	F	161	37.725	114.882	191.689	1.00	51.67	N
	ATOM	1687	CA	THR	F	161	38.886	115.629	192.181	1.00	50.62	C
	ATOM	1689	CB	THR	F	161	38.745	115.919	193.686	1.00	51.31	C
55	ATOM	1691	OG1	THR	F	161	37.591	116.738	193.901	1.00	53.82	O
	ATOM	1693	CG2	THR	F	161	39.977	116.634	194.230	1.00	52.05	C
	ATOM	1697	C	THR	F	161	40.210	114.903	191.947	1.00	48.52	C
	ATOM	1698	O	THR	F	161	41.201	115.528	191.566	1.00	47.96	O
	ATOM	1700	N	LEU	F	162	40.225	113.597	192.199	1.00	47.49	N
60	ATOM	1701	CA	LEU	F	162	41.423	112.786	191.999	1.00	47.25	C
	ATOM	1703	CB	LEU	F	162	41.178	111.336	192.444	1.00	48.04	C
	ATOM	1706	CG	LEU	F	162	42.362	110.349	192.397	1.00	48.96	C
	ATOM	1708	CD1	LEU	F	162	42.208	109.263	193.463	1.00	50.01	C
	ATOM	1712	CD2	LEU	F	162	42.543	109.710	191.022	1.00	49.97	C
65	ATOM	1716	C	LEU	F	162	41.872	112.836	190.536	1.00	46.49	C
	ATOM	1717	O	LEU	F	162	43.059	113.006	190.264	1.00	44.88	O
	ATOM	1719	N	CYS	F	163	40.919	112.692	189.612	1.00	45.37	N
	ATOM	1720	CA	CYS	F	163	41.195	112.747	188.168	1.00	43.21	C
	ATOM	1722	CB	CYS	F	163	39.919	112.450	187.361	1.00	46.10	C
70	ATOM	1725	SG	CYS	F	163	40.066	112.761	185.566	1.00	48.69	S
	ATOM	1727	C	CYS	F	163	41.788	114.087	187.726	1.00	39.68	C
	ATOM	1728	O	CYS	F	163	42.794	114.118	187.027	1.00	36.24	O

	ATOM	1730	N	GLU	F	164	41.183	115.191	188.163	1.00	40.04	N
	ATOM	1731	CA	GLU	F	164	41.630	116.531	187.762	1.00	39.02	C
	ATOM	1733	CB	GLU	F	164	40.729	117.605	188.380	1.00	43.22	C
5	ATOM	1736	CG	GLU	F	164	39.305	117.605	187.857	1.00	45.05	C
	ATOM	1739	CD	GLU	F	164	38.396	118.515	188.654	1.00	46.26	C
	ATOM	1740	OE1	GLU	F	164	38.880	119.557	189.151	1.00	49.45	O
	ATOM	1741	OE2	GLU	F	164	37.195	118.186	188.784	1.00	50.36	O
	ATOM	1742	C	GLU	F	164	43.084	116.822	188.150	1.00	35.83	C
10	ATOM	1743	O	GLU	F	164	43.780	117.563	187.454	1.00	35.73	O
	ATOM	1745	N	HIS	F	165	43.530	116.245	189.263	1.00	32.13	N
	ATOM	1746	CA	HIS	F	165	44.874	116.490	189.783	1.00	32.56	C
	ATOM	1748	CB	HIS	F	165	44.797	116.787	191.282	1.00	33.94	C
	ATOM	1751	CG	HIS	F	165	43.907	117.945	191.617	1.00	32.55	C
15	ATOM	1752	ND1	HIS	F	165	43.965	119.144	190.939	1.00	35.41	N
	ATOM	1754	CE1	HIS	F	165	43.068	119.975	191.441	1.00	36.93	C
	ATOM	1756	NE2	HIS	F	165	42.428	119.355	192.417	1.00	37.11	N
	ATOM	1758	CD2	HIS	F	165	42.931	118.082	192.543	1.00	33.76	C
	ATOM	1760	C	HIS	F	165	45.847	115.333	189.525	1.00	30.15	C
20	ATOM	1761	O	HIS	F	165	47.001	115.400	189.938	1.00	30.52	O
	ATOM	1763	N	LEU	F	166	45.391	114.292	188.832	1.00	30.38	N
	ATOM	1764	CA	LEU	F	166	46.224	113.116	188.566	1.00	30.63	C
	ATOM	1766	CB	LEU	F	166	45.393	111.977	187.958	1.00	32.97	C
	ATOM	1769	CG	LEU	F	166	46.036	110.582	187.972	1.00	34.63	C
25	ATOM	1771	CD1	LEU	F	166	46.438	110.173	189.391	1.00	35.80	C
	ATOM	1775	CD2	LEU	F	166	45.098	109.538	187.370	1.00	35.74	C
	ATOM	1779	C	LEU	F	166	47.391	113.472	187.640	1.00	30.85	C
	ATOM	1780	O	LEU	F	166	47.195	114.091	186.585	1.00	32.27	O
	ATOM	1782	N	GLN	F	167	48.601	113.100	188.060	1.00	26.54	N
30	ATOM	1783	CA	GLN	F	167	49.815	113.323	187.282	1.00	27.54	C
	ATOM	1785	CB	GLN	F	167	50.830	114.132	188.100	1.00	26.85	C
	ATOM	1788	CG	GLN	F	167	50.322	115.517	188.507	1.00	29.90	C
	ATOM	1791	CD	GLN	F	167	51.321	116.311	189.324	1.00	31.20	C
	ATOM	1792	OE1	GLN	F	167	52.256	115.759	189.896	1.00	32.29	O
35	ATOM	1793	NE2	GLN	F	167	51.107	117.617	189.406	1.00	38.56	N
	ATOM	1796	C	GLN	F	167	50.393	111.972	186.879	1.00	30.20	C
	ATOM	1797	O	GLN	F	167	50.560	111.091	187.727	1.00	30.34	O
	ATOM	1799	N	ILE	F	168	50.666	111.797	185.586	1.00	28.45	N
	ATOM	1800	CA	ILE	F	168	51.175	110.528	185.059	1.00	28.43	C
40	ATOM	1802	CB	ILE	F	168	50.156	109.874	184.084	1.00	30.51	C
	ATOM	1804	CG1	ILE	F	168	48.757	109.862	184.724	1.00	33.96	C
	ATOM	1807	CD1	ILE	F	168	47.648	109.447	183.798	1.00	34.62	C
	ATOM	1811	CG2	ILE	F	168	50.607	108.464	183.683	1.00	32.63	C
	ATOM	1815	C	ILE	F	168	52.506	110.756	184.353	1.00	28.48	C
45	ATOM	1816	O	ILE	F	168	52.621	111.653	183.512	1.00	28.72	O
	ATOM	1818	N	ASN	F	169	53.514	109.966	184.732	1.00	26.67	N
	ATOM	1819	CA	ASN	F	169	54.827	109.959	184.082	1.00	29.36	C
	ATOM	1821	CB	ASN	F	169	55.959	110.040	185.115	1.00	28.75	C
	ATOM	1824	CG	ASN	F	169	56.247	111.456	185.586	1.00	27.48	C
50	ATOM	1825	OD1	ASN	F	169	55.914	112.439	184.919	1.00	24.90	O
	ATOM	1826	ND2	ASN	F	169	56.899	111.564	186.741	1.00	23.92	N
	ATOM	1829	C	ASN	F	169	54.981	108.655	183.302	1.00	32.98	C
	ATOM	1830	O	ASN	F	169	54.358	107.654	183.641	1.00	32.59	O
	ATOM	1832	N	ASP	F	170	55.810	108.673	182.263	1.00	38.46	N
55	ATOM	1833	CA	ASP	F	170	56.169	107.451	181.533	1.00	37.00	C
	ATOM	1835	CB	ASP	F	170	57.027	106.559	182.448	1.00	42.36	C
	ATOM	1838	CG	ASP	F	170	57.801	105.484	181.692	1.00	48.69	C
	ATOM	1839	OD1	ASP	F	170	58.112	105.670	180.493	1.00	53.95	O
	ATOM	1840	OD2	ASP	F	170	58.119	104.450	182.322	1.00	54.05	O
60	ATOM	1841	C	ASP	F	170	54.908	106.711	181.065	1.00	37.38	C
	ATOM	1842	O	ASP	F	170	54.829	105.482	181.153	1.00	37.13	O
	ATOM	1844	N	GLY	F	171	53.942	107.485	180.571	1.00	32.70	N
	ATOM	1845	CA	GLY	F	171	52.604	107.012	180.255	1.00	35.98	C
	ATOM	1848	C	GLY	F	171	52.426	106.832	178.761	1.00	37.54	C
65	ATOM	1849	O	GLY	F	171	52.657	107.762	177.987	1.00	38.58	O
	ATOM	1851	N	GLU	F	172	51.999	105.641	178.355	1.00	31.57	N
	ATOM	1852	CA	GLU	F	172	51.922	105.309	176.935	1.00	31.06	C
	ATOM	1854	CB	GLU	F	172	53.299	104.882	176.435	1.00	30.59	C
	ATOM	1857	CG	GLU	F	172	53.346	104.460	174.973	1.00	30.96	C
70	ATOM	1860	CD	GLU	F	172	54.757	104.470	174.441	1.00	35.33	C
	ATOM	1861	OE1	GLU	F	172	55.306	105.572	174.223	1.00	44.00	O
	ATOM	1862	OE2	GLU	F	172	55.329	103.396	174.250	1.00	38.83	O

5	ATOM	1863	C	GLU	F	172	50.918	104.204	176.679	1.00	29.73	C
	ATOM	1864	O	GLU	F	172	50.880	103.208	177.415	1.00	30.04	O
	ATOM	1866	N	LEU	F	173	50.100	104.406	175.646	1.00	29.14	N
	ATOM	1867	CA	LEU	F	173	49.150	103.408	175.174	1.00	30.88	C
	ATOM	1869	CB	LEU	F	173	47.724	103.964	175.181	1.00	30.65	C
10	ATOM	1872	CG	LEU	F	173	46.644	103.054	174.569	1.00	29.85	C
	ATOM	1874	CD1	LEU	F	173	46.356	101.853	175.472	1.00	29.90	C
	ATOM	1878	CD2	LEU	F	173	45.391	103.840	174.285	1.00	31.95	C
	ATOM	1882	C	LEU	F	173	49.532	103.014	173.754	1.00	30.02	C
	ATOM	1883	O	LEU	F	173	49.770	103.877	172.914	1.00	29.62	O
15	ATOM	1885	N	ILE	F	174	49.581	101.709	173.499	1.00	28.44	N
	ATOM	1886	CA	ILE	F	174	49.781	101.185	172.159	1.00	28.40	C
	ATOM	1888	CB	ILE	F	174	51.168	100.505	171.990	1.00	29.47	C
	ATOM	1890	CG1	ILE	F	174	52.271	101.556	172.024	1.00	29.90	C
	ATOM	1893	CD1	ILE	F	174	53.629	101.023	172.282	1.00	30.86	C
20	ATOM	1897	CG2	ILE	F	174	51.256	99.748	170.653	1.00	29.29	C
	ATOM	1901	C	ILE	F	174	48.668	100.202	171.829	1.00	29.87	C
	ATOM	1902	O	ILE	F	174	48.371	99.296	172.610	1.00	28.28	O
	ATOM	1904	N	VAL	F	175	48.044	100.408	170.673	1.00	30.57	N
	ATOM	1905	CA	VAL	F	175	47.079	99.466	170.105	1.00	28.64	C
25	ATOM	1907	CB	VAL	F	175	45.701	100.125	169.925	1.00	29.59	C
	ATOM	1909	CG1	VAL	F	175	44.688	99.126	169.364	1.00	31.05	C
	ATOM	1913	CG2	VAL	F	175	45.207	100.687	171.251	1.00	31.49	C
	ATOM	1917	C	VAL	F	175	47.649	99.046	168.753	1.00	27.88	C
	ATOM	1918	O	VAL	F	175	47.976	99.900	167.934	1.00	30.69	O
30	ATOM	1920	N	VAL	F	176	47.797	97.748	168.522	1.00	28.04	N
	ATOM	1921	CA	VAL	F	176	48.415	97.272	167.285	1.00	28.01	C
	ATOM	1923	CB	VAL	F	176	49.975	97.158	167.424	1.00	31.82	C
	ATOM	1925	CG1	VAL	F	176	50.374	96.271	168.586	1.00	36.26	C
	ATOM	1929	CG2	VAL	F	176	50.619	96.693	166.131	1.00	31.64	C
35	ATOM	1933	C	VAL	F	176	47.790	95.948	166.826	1.00	29.19	C
	ATOM	1934	O	VAL	F	176	47.659	94.998	167.596	1.00	26.77	O
	ATOM	1936	N	GLN	F	177	47.420	95.929	165.550	1.00	28.91	N
	ATOM	1937	CA	GLN	F	177	46.748	94.815	164.912	1.00	28.80	C
	ATOM	1939	CB	GLN	F	177	46.121	95.319	163.616	1.00	29.08	C
40	ATOM	1942	CG	GLN	F	177	45.243	94.336	162.888	1.00	28.32	C
	ATOM	1945	CD	GLN	F	177	44.764	94.877	161.563	1.00	28.02	C
	ATOM	1946	OE1	GLN	F	177	45.455	95.668	160.917	1.00	29.14	O
	ATOM	1947	NE2	GLN	F	177	43.574	94.452	161.144	1.00	32.31	N
	ATOM	1950	C	GLN	F	177	47.737	93.705	164.620	1.00	21.11	C
45	ATOM	1951	O	GLN	F	177	48.826	93.960	164.101	1.00	28.33	O
	ATOM	1953	N	LEU	F	178	47.352	92.471	164.944	1.00	28.40	N
	ATOM	1954	CA	LEU	F	178	48.194	91.296	164.686	1.00	27.25	C
	ATOM	1956	CB	LEU	F	178	48.255	90.403	165.934	1.00	29.56	C
	ATOM	1959	CG	LEU	F	178	48.757	91.034	167.233	1.00	28.94	C
50	ATOM	1961	CD1	LEU	F	178	48.762	89.994	168.350	1.00	29.61	C
	ATOM	1965	CD2	LEU	F	178	50.145	91.655	167.045	1.00	30.23	C
	ATOM	1969	C	LEU	F	178	47.723	90.443	163.499	1.00	30.44	C
	ATOM	1970	O	LEU	F	178	48.526	89.733	162.889	1.00	28.99	O
	ATOM	1972	N	THR	F	179	46.426	90.484	163.201	1.00	29.98	N
55	ATOM	1973	CA	THR	F	179	45.847	89.685	162.126	1.00	29.50	C
	ATOM	1975	CB	THR	F	179	45.109	88.446	162.666	1.00	28.80	C
	ATOM	1977	OG1	THR	F	179	44.073	88.860	163.567	1.00	33.38	O
	ATOM	1979	CG2	THR	F	179	46.065	87.520	163.380	1.00	31.06	C
	ATOM	1983	C	THR	F	179	44.876	90.559	161.315	1.00	31.33	C
60	ATOM	1984	O	THR	F	179	44.242	91.477	161.873	1.00	29.47	O
	ATOM	1986	N	PRO	F	180	44.760	90.287	160.004	1.00	33.42	N
	ATOM	1987	CA	PRO	F	180	43.941	91.145	159.146	1.00	32.56	C
	ATOM	1989	CB	PRO	F	180	44.449	90.813	157.739	1.00	35.67	C
	ATOM	1992	CG	PRO	F	180	44.864	89.393	157.824	1.00	35.88	C
65	ATOM	1995	CD	PRO	F	180	45.378	89.185	159.239	1.00	34.62	C
	ATOM	1998	C	PRO	F	180	42.471	90.828	159.257	1.00	34.06	C
	ATOM	1999	O	PRO	F	180	42.090	89.770	159.753	1.00	31.06	O
	ATOM	2000	N	GLY	F	181	41.641	91.750	158.793	1.00	33.25	N
	ATOM	2001	CA	GLY	F	181	40.218	91.500	158.729	1.00	32.42	C
70	ATOM	2004	C	GLY	F	181	39.503	92.594	157.968	1.00	32.27	C
	ATOM	2005	O	GLY	F	181	40.134	93.483	157.391	1.00	34.40	O
	ATOM	2007	N	TYR	F	182	38.181	92.535	158.003	1.00	31.07	N
	ATOM	2008	CA	TYR	F	182	37.330	93.544	157.389	1.00	30.52	C
	ATOM	2010	CB	TYR	F	182	35.860	93.241	157.719	1.00	27.55	C
	ATOM	2013	CG	TYR	F	182	34.923	94.410	157.530	1.00	26.30	C

5	ATOM	2014	CD1	TYR	F	182	34.365	94.691	156.289	1.00	28.04	C
	ATOM	2016	CE1	TYR	F	182	33.514	95.779	156.117	1.00	26.36	C
	ATOM	2018	CZ	TYR	F	182	33.207	96.582	157.207	1.00	25.16	C
	ATOM	2019	OH	TYR	F	182	32.364	97.658	157.064	1.00	26.19	O
	ATOM	2021	CE2	TYR	F	182	33.742	96.316	158.443	1.00	26.20	C
10	ATOM	2023	CD2	TYR	F	182	34.594	95.241	158.606	1.00	28.29	C
	ATOM	2025	C	TYR	F	182	37.703	94.942	157.867	1.00	29.17	C
	ATOM	2026	O	TYR	F	182	37.928	95.147	159.059	1.00	28.86	O
	ATOM	2028	N	CYS	F	183	37.780	95.894	156.933	1.00	29.79	N
	ATOM	2029	CA	CYS	F	183	37.944	97.316	157.266	1.00	31.56	C
15	ATOM	2031	CB	CYS	F	183	39.256	97.894	156.701	1.00	37.43	C
	ATOM	2034	SG	CYS	F	183	40.812	97.207	157.355	1.00	41.45	S
	ATOM	2036	C	CYS	F	183	36.775	98.102	156.690	1.00	31.70	C
	ATOM	2037	O	CYS	F	183	36.415	97.927	155.525	1.00	27.60	O
	ATOM	2039	N	ALA	F	184	36.178	98.975	157.495	1.00	32.41	N
20	ATOM	2040	CA	ALA	F	184	35.129	99.847	156.999	1.00	32.82	C
	ATOM	2042	CB	ALA	F	184	34.369	100.456	158.148	1.00	30.47	C
	ATOM	2046	C	ALA	F	184	35.764	100.951	156.138	1.00	34.67	C
	ATOM	2047	O	ALA	F	184	36.684	101.615	156.594	1.00	38.14	O
	ATOM	2049	N	PRO	F	185	35.292	101.136	154.890	1.00	38.22	N
25	ATOM	2050	CA	PRO	F	185	35.774	102.271	154.080	1.00	44.15	C
	ATOM	2052	CB	PRO	F	185	34.901	102.205	152.824	1.00	43.58	C
	ATOM	2055	CG	PRO	F	185	34.440	100.801	152.742	1.00	42.96	C
	ATOM	2058	CD	PRO	F	185	34.321	100.308	154.153	1.00	40.11	C
	ATOM	2061	C	PRO	F	185	35.592	103.622	154.784	1.00	48.02	C
30	ATOM	2062	O	PRO	F	185	34.635	103.793	155.544	1.00	48.82	O
	ATOM	2063	N	GLU	F	186	36.504	104.565	154.541	1.00	53.33	N
	ATOM	2064	CA	GLU	F	186	36.439	105.890	155.177	1.00	53.63	C
	ATOM	2066	CB	GLU	F	186	37.654	106.748	154.786	1.00	56.08	C
	ATOM	2069	CG	GLU	F	186	37.724	108.115	155.492	1.00	57.50	C
35	ATOM	2072	CD	GLU	F	186	38.636	109.117	154.785	1.00	59.93	C
	ATOM	2073	OE1	GLU	F	186	39.731	108.727	154.322	1.00	63.98	O
	ATOM	2074	OE2	GLU	F	186	38.256	110.305	154.699	1.00	62.77	O
	ATOM	2075	C	GLU	F	186	35.147	106.624	154.804	1.00	53.10	C
	ATOM	2076	O	GLU	F	186	34.740	106.623	153.640	1.00	52.75	O
40	ATOM	2078	N	GLY	F	187	34.510	107.236	155.803	1.00	52.60	N
	ATOM	2079	CA	GLY	F	187	33.316	108.063	155.594	1.00	52.92	C
	ATOM	2082	C	GLY	F	187	32.066	107.341	155.110	1.00	53.17	C
	ATOM	2083	O	GLY	F	187	31.154	107.977	154.582	1.00	51.26	O
	ATOM	2085	N	SER	F	188	32.007	106.022	155.301	1.00	53.46	N
45	ATOM	2086	CA	SER	F	188	30.895	105.211	154.782	1.00	51.73	C
	ATOM	2088	CB	SER	F	188	31.437	103.989	154.029	1.00	52.30	C
	ATOM	2091	OG	SER	F	188	32.223	103.165	154.879	1.00	54.21	O
	ATOM	2093	C	SER	F	188	29.890	104.763	155.857	1.00	50.13	C
	ATOM	2094	O	SER	F	188	28.907	104.095	155.538	1.00	49.87	O
50	ATOM	2096	N	TYR	F	189	30.127	105.123	157.118	1.00	47.59	N
	ATOM	2097	CA	TYR	F	189	29.200	104.766	158.194	1.00	49.50	C
	ATOM	2099	CB	TYR	F	189	29.617	103.441	158.861	1.00	45.16	C
	ATOM	2102	CG	TYR	F	189	28.726	103.056	160.031	1.00	44.75	C
	ATOM	2103	CD1	TYR	F	189	27.552	102.332	159.831	1.00	44.79	C
55	ATOM	2105	CE1	TYR	F	189	26.721	102.001	160.895	1.00	44.48	C
	ATOM	2107	CZ	TYR	F	189	27.065	102.396	162.176	1.00	43.99	C
	ATOM	2108	OH	TYR	F	189	26.257	102.066	163.238	1.00	43.92	O
	ATOM	2110	CE2	TYR	F	189	28.224	103.114	162.400	1.00	43.97	C
	ATOM	2112	CD2	TYR	F	189	29.044	103.441	161.331	1.00	44.52	C
60	ATOM	2114	C	TYR	F	189	29.085	105.859	159.257	1.00	50.32	C
	ATOM	2115	O	TYR	F	189	30.086	106.460	159.655	1.00	50.46	O
	ATOM	2117	N	HIS	F	190	27.856	106.092	159.717	1.00	51.52	N
	ATOM	2118	CA	HIS	F	190	27.591	106.921	160.895	1.00	56.05	C
	ATOM	2120	CB	HIS	F	190	27.156	108.332	160.485	1.00	61.41	C
65	ATOM	2123	CG	HIS	F	190	28.291	109.208	160.050	1.00	65.11	C
	ATOM	2124	ND1	HIS	F	190	28.611	109.411	158.724	1.00	66.38	N
	ATOM	2126	CE1	HIS	F	190	29.654	110.219	158.643	1.00	67.47	C
	ATOM	2128	NE2	HIS	F	190	30.024	110.545	159.869	1.00	67.73	N
	ATOM	2130	CD2	HIS	F	190	29.189	109.924	160.767	1.00	66.86	C
70	ATOM	2132	C	HIS	F	190	26.520	106.253	161.762	1.00	56.83	C
	ATOM	2133	O	HIS	F	190	25.545	105.699	161.242	1.00	54.36	O
	ATOM	2135	N	SER	F	191	26.707	106.309	163.079	1.00	58.50	N
	ATOM	2136	CA	SER	F	191	25.825	105.617	164.023	1.00	59.71	C
	ATOM	2138	CB	SER	F	191	26.435	105.620	165.429	1.00	61.10	C
	ATOM	2141	OG	SER	F	191	25.772	104.852	166.253	0.00	30.00	O

5	ATOM	2143	C	SER	F	191	24.434	106.237	164.064	1.00	61.29	C
	ATOM	2144	O	SER	F	191	23.469	105.642	163.583	1.00	63.22	O
	ATOM	2146	N	ASP	G	57	8.975	62.479	192.445	1.00	63.34	N
	ATOM	2147	CA	ASP	G	57	9.431	61.070	192.208	1.00	61.45	C
	ATOM	2149	CB	ASP	G	57	10.387	60.983	190.998	1.00	64.19	C
10	ATOM	2152	CG	ASP	G	57	11.700	61.713	191.217	1.00	67.04	C
	ATOM	2153	OD1	ASP	G	57	12.588	61.164	191.903	1.00	69.19	O
	ATOM	2154	OD2	ASP	G	57	11.854	62.832	190.684	1.00	69.86	O
	ATOM	2155	C	ASP	G	57	10.018	60.329	193.430	1.00	59.39	C
	ATOM	2156	O	ASP	G	57	9.882	59.105	193.503	1.00	59.16	O
15	ATOM	2160	N	PRO	G	58	10.672	61.042	194.380	1.00	56.44	N
	ATOM	2161	CA	PRO	G	58	11.139	60.298	195.559	1.00	51.46	C
	ATOM	2163	CB	PRO	G	58	11.890	61.356	196.381	1.00	54.42	C
	ATOM	2166	CG	PRO	G	58	12.185	62.454	195.430	1.00	55.83	C
	ATOM	2169	CD	PRO	G	58	11.043	62.466	194.472	1.00	57.57	C
20	ATOM	2172	C	PRO	G	58	9.981	59.720	196.376	1.00	42.86	C
	ATOM	2173	O	PRO	G	58	8.925	60.348	196.470	1.00	42.33	O
	ATOM	2174	N	PRO	G	59	10.171	58.525	196.958	1.00	38.76	N
	ATOM	2175	CA	PRO	G	59	9.080	57.899	197.706	1.00	38.38	C
	ATOM	2177	CB	PRO	G	59	9.602	56.486	197.970	1.00	39.72	C
25	ATOM	2180	CG	PRO	G	59	11.085	56.616	197.944	1.00	41.19	C
	ATOM	2183	CD	PRO	G	59	11.393	57.701	196.960	1.00	39.53	C
	ATOM	2186	C	PRO	G	59	8.801	58.612	199.021	1.00	31.56	C
	ATOM	2187	O	PRO	G	59	9.623	59.407	199.474	1.00	31.11	O
	ATOM	2188	N	ILE	G	60	7.661	58.308	199.639	1.00	32.04	N
30	ATOM	2189	CA	ILE	G	60	7.366	58.811	200.970	1.00	32.85	C
	ATOM	2191	CB	ILE	G	60	5.966	58.349	201.478	1.00	34.99	C
	ATOM	2193	CG1	ILE	G	60	4.851	58.989	200.646	1.00	36.38	C
	ATOM	2196	CD1	ILE	G	60	3.495	58.361	200.852	1.00	36.97	C
	ATOM	2200	CG2	ILE	G	60	5.771	58.700	202.951	1.00	34.30	C
35	ATOM	2204	C	ILE	G	60	8.486	58.295	201.875	1.00	32.54	C
	ATOM	2205	O	ILE	G	60	8.860	57.116	201.821	1.00	30.77	O
	ATOM	2207	N	GLN	G	61	9.039	59.192	202.683	1.00	32.33	N
	ATOM	2208	CA	GLN	G	61	10.200	58.874	203.502	1.00	33.23	C
	ATOM	2210	CB	GLN	G	61	10.947	60.155	203.876	1.00	33.19	C
40	ATOM	2213	CG	GLN	G	61	11.450	60.920	202.664	1.00	32.42	C
	ATOM	2216	CD	GLN	G	61	12.626	60.243	202.013	1.00	31.12	C
	ATOM	2217	OE1	GLN	G	61	13.752	60.317	202.521	1.00	30.29	O
	ATOM	2218	NE2	GLN	G	61	12.384	59.575	200.884	1.00	30.02	N
	ATOM	2221	C	GLN	G	61	9.751	58.139	204.750	1.00	32.25	C
45	ATOM	2222	O	GLN	G	61	8.879	58.615	205.483	1.00	33.47	O
	ATOM	2224	N	ARG	G	62	10.319	56.966	204.979	1.00	34.65	N
	ATOM	2225	CA	ARG	G	62	9.993	56.216	206.175	1.00	35.57	C
	ATOM	2227	CB	ARG	G	62	8.710	55.403	206.004	1.00	39.53	C
	ATOM	2230	CG	ARG	G	62	8.771	54.245	205.048	1.00	38.60	C
50	ATOM	2233	CD	ARG	G	62	8.120	52.989	205.635	1.00	41.73	C
	ATOM	2236	NE	ARG	G	62	9.075	52.155	206.364	1.00	41.04	N
	ATOM	2238	CZ	ARG	G	62	8.858	50.905	206.789	1.00	41.20	C
	ATOM	2239	NH1	ARG	G	62	7.705	50.291	206.590	1.00	44.67	N
	ATOM	2242	NH2	ARG	G	62	9.823	50.250	207.427	1.00	39.78	N
55	ATOM	2245	C	ARG	G	62	11.128	55.336	206.664	1.00	32.27	C
	ATOM	2246	O	ARG	G	62	11.915	54.796	205.878	1.00	29.33	O
	ATOM	2248	N	LEU	G	63	11.196	55.218	207.984	1.00	33.39	N
	ATOM	2249	CA	LEU	G	63	12.178	54.374	208.641	1.00	32.48	C
	ATOM	2251	CB	LEU	G	63	13.462	55.142	208.964	1.00	36.37	C
60	ATOM	2254	CG	LEU	G	63	14.504	54.229	209.640	1.00	38.06	C
	ATOM	2256	CD1	LEU	G	63	15.826	54.278	208.931	1.00	42.17	C
	ATOM	2260	CD2	LEU	G	63	14.641	54.533	211.126	1.00	39.69	C
	ATOM	2264	C	LEU	G	63	11.599	53.802	209.919	1.00	31.87	C
	ATOM	2265	O	LEU	G	63	10.984	54.515	210.712	1.00	29.73	O
65	ATOM	2267	N	ARG	G	64	11.829	52.509	210.106	1.00	33.15	N
	ATOM	2268	CA	ARG	G	64	11.467	51.803	211.318	1.00	32.44	C
	ATOM	2270	CB	ARG	G	64	10.428	50.737	210.979	1.00	32.19	C
	ATOM	2273	CG	ARG	G	64	9.954	49.883	212.130	1.00	34.41	C
	ATOM	2276	CD	ARG	G	64	9.093	48.766	211.573	1.00	36.89	C
70	ATOM	2279	NE	ARG	G	64	8.650	47.863	212.613	1.00	42.65	N
	ATOM	2281	CZ	ARG	G	64	8.894	46.557	212.673	1.00	40.15	C
	ATOM	2282	NH1	ARG	G	64	9.559	45.906	211.714	1.00	40.83	N
	ATOM	2285	NH2	ARG	G	64	8.425	45.885	213.709	1.00	41.56	N
	ATOM	2288	C	ARG	G	64	12.742	51.172	211.871	1.00	30.62	C
	ATOM	2289	O	ARG	G	64	13.509	50.549	211.131	1.00	30.23	O

5	ATOM	2291	N	GLY	G	65	12.968	51.355	213.167	1.00	27.63	N
	ATOM	2292	CA	GLY	G	65	14.164	50.850	213.822	1.00	31.87	C
	ATOM	2295	C	GLY	G	65	13.849	50.205	215.157	1.00	31.53	C
	ATOM	2296	O	GLY	G	65	12.975	50.674	215.896	1.00	32.78	O
	ATOM	2298	N	ALA	G	66	14.558	49.123	215.463	1.00	31.27	N
10	ATOM	2299	CA	ALA	G	66	14.474	48.496	216.775	1.00	31.67	C
	ATOM	2301	CB	ALA	G	66	14.890	47.037	216.698	1.00	33.23	C
	ATOM	2305	C	ALA	G	66	15.379	49.254	217.742	1.00	34.13	C
	ATOM	2306	O	ALA	G	66	16.432	49.758	217.343	1.00	31.04	O
	ATOM	2308	N	VAL	G	67	14.958	49.330	219.005	1.00	34.89	N
15	ATOM	2309	CA	VAL	G	67	15.756	49.935	220.075	1.00	36.20	C
	ATOM	2311	CB	VAL	G	67	15.114	51.260	220.587	1.00	37.26	C
	ATOM	2313	CG1	VAL	G	67	16.028	51.952	221.588	1.00	39.66	C
	ATOM	2317	CG2	VAL	G	67	14.824	52.203	219.424	1.00	37.92	C
	ATOM	2321	C	VAL	G	67	15.892	48.902	221.212	1.00	34.56	C
20	ATOM	2322	O	VAL	G	67	14.917	48.594	221.902	1.00	31.76	O
	ATOM	2324	N	THR	G	68	17.090	48.345	221.377	1.00	36.57	N
	ATOM	2325	CA	THR	G	68	17.341	47.336	222.421	1.00	37.78	C
	ATOM	2327	CB	THR	G	68	17.781	45.977	221.812	1.00	38.26	C
	ATOM	2329	OG1	THR	G	68	19.046	46.125	221.158	1.00	38.23	O
25	ATOM	2331	CG2	THR	G	68	16.752	45.470	220.807	1.00	38.50	C
	ATOM	2335	C	THR	G	68	18.393	47.746	223.453	1.00	39.29	C
	ATOM	2336	O	THR	G	68	18.407	47.209	224.563	1.00	40.04	O
	ATOM	2338	N	ARG	G	69	19.278	48.672	223.088	1.00	38.78	N
	ATOM	2339	CA	ARG	G	69	20.366	49.080	223.968	1.00	39.85	C
30	ATOM	2341	CB	ARG	G	69	21.605	48.209	223.715	1.00	41.06	C
	ATOM	2344	CG	ARG	G	69	22.199	48.336	222.314	1.00	41.88	C
	ATOM	2347	CD	ARG	G	69	23.584	47.712	222.244	1.00	44.11	C
	ATOM	2350	NE	ARG	G	69	24.276	48.048	221.000	1.00	44.78	N
	ATOM	2352	CZ	ARG	G	69	24.065	47.459	219.824	1.00	47.01	C
35	ATOM	2353	NH1	ARG	G	69	23.169	46.481	219.692	1.00	46.96	N
	ATOM	2356	NH2	ARG	G	69	24.761	47.853	218.763	1.00	47.96	N
	ATOM	2359	C	ARG	G	69	20.709	50.556	223.786	1.00	37.60	C
	ATOM	2360	O	ARG	G	69	20.137	51.236	222.936	1.00	30.53	O
	ATOM	2362	N	CYS	G	70	21.642	51.034	224.605	1.00	37.33	N
40	ATOM	2363	CA	CYS	G	70	22.145	52.401	224.542	1.00	39.49	C
	ATOM	2365	CB	CYS	G	70	21.894	53.104	225.888	1.00	42.65	C
	ATOM	2368	SG	CYS	G	70	22.723	54.713	226.170	1.00	45.86	S
	ATOM	2370	C	CYS	G	70	23.638	52.334	224.224	1.00	39.98	C
	ATOM	2371	O	CYS	G	70	24.341	51.451	224.726	1.00	37.75	O
45	ATOM	2373	N	GLU	G	71	24.115	53.254	223.388	1.00	41.30	N
	ATOM	2374	CA	GLU	G	71	25.536	53.318	223.035	1.00	42.86	C
	ATOM	2376	CB	GLU	G	71	25.799	52.553	221.732	1.00	43.82	C
	ATOM	2379	CG	GLU	G	71	27.233	52.043	221.601	1.00	46.31	C
	ATOM	2382	CD	GLU	G	71	27.545	51.473	220.225	1.00	47.91	C
50	ATOM	2383	OE1	GLU	G	71	26.645	50.883	219.590	1.00	48.78	O
	ATOM	2384	OE2	GLU	G	71	28.707	51.607	219.784	1.00	53.02	O
	ATOM	2385	C	GLU	G	71	25.988	54.776	222.901	1.00	43.03	C
	ATOM	2386	O	GLU	G	71	25.346	55.563	222.201	1.00	43.33	O
	ATOM	2388	N	ASP	G	72	27.084	55.120	223.579	1.00	40.96	N
55	ATOM	2389	CA	ASP	G	72	27.640	56.485	223.589	1.00	40.54	C
	ATOM	2391	CB	ASP	G	72	28.257	56.835	222.221	1.00	43.44	C
	ATOM	2394	CG	ASP	G	72	29.514	56.029	221.913	1.00	46.62	C
	ATOM	2395	OD1	ASP	G	72	30.129	55.471	222.847	1.00	46.67	O
	ATOM	2396	OD2	ASP	G	72	29.893	55.963	220.723	1.00	49.36	O
60	ATOM	2397	C	ASP	G	72	26.627	57.560	224.019	1.00	38.62	C
	ATOM	2398	O	ASP	G	72	26.569	58.648	223.438	1.00	39.45	O
	ATOM	2400	N	GLY	G	73	25.837	57.246	225.044	1.00	35.70	N
	ATOM	2401	CA	GLY	G	73	24.854	58.186	225.588	1.00	34.85	C
	ATOM	2404	C	GLY	G	73	23.612	58.368	224.734	1.00	31.04	C
65	ATOM	2405	O	GLY	G	73	22.847	59.312	224.941	1.00	28.92	O
	ATOM	2407	N	GLN	G	74	23.412	57.466	223.776	1.00	30.10	N
	ATOM	2408	CA	GLN	G	74	22.260	57.517	222.876	1.00	32.77	C
	ATOM	2410	CB	GLN	G	74	22.688	57.974	221.476	1.00	33.58	C
	ATOM	2413	CG	GLN	G	74	23.211	59.408	221.414	1.00	34.38	C
70	ATOM	2416	CD	GLN	G	74	23.616	59.852	220.010	1.00	35.12	C
	ATOM	2417	OE1	GLN	G	74	24.187	60.930	219.833	1.00	35.60	O
	ATOM	2418	NE2	GLN	G	74	23.324	59.027	219.011	1.00	34.58	N
	ATOM	2421	C	GLN	G	74	21.596	56.149	222.776	1.00	32.07	C
	ATOM	2422	O	GLN	G	74	22.268	55.115	222.836	1.00	31.12	O
	ATOM	2424	N	LEU	G	75	20.275	56.146	222.640	1.00	30.91	N

5	ATOM	2425	CA	LEU	G	75	19.551	54.924	222.313	1.00	32.20	C
	ATOM	2427	CB	LEU	G	75	18.038	55.165	222.307	1.00	33.14	C
	ATOM	2430	CG	LEU	G	75	17.418	55.612	223.637	1.00	33.79	C
	ATOM	2432	CD1	LEU	G	75	15.935	55.858	223.462	1.00	35.55	C
	ATOM	2436	CD2	LEU	G	75	17.671	54.580	224.715	1.00	36.74	C
10	ATOM	2440	C	LEU	G	75	20.024	54.458	220.939	1.00	30.90	C
	ATOM	2441	O	LEU	G	75	20.086	55.254	219.999	1.00	30.31	O
	ATOM	2443	N	PHE	G	76	20.381	53.181	220.828	1.00	33.35	N
	ATOM	2444	CA	PHE	G	76	20.899	52.650	219.571	1.00	32.90	C
	ATOM	2446	CB	PHE	G	76	21.833	51.458	219.801	1.00	38.12	C
15	ATOM	2449	CG	PHE	G	76	22.585	51.045	218.567	1.00	37.48	C
	ATOM	2450	CD1	PHE	G	76	23.706	51.753	218.156	1.00	39.99	C
	ATOM	2452	CE1	PHE	G	76	24.398	51.390	217.003	1.00	40.19	C
	ATOM	2454	CZ	PHE	G	76	23.961	50.316	216.244	1.00	40.18	C
	ATOM	2456	CE2	PHE	G	76	22.833	49.608	216.638	1.00	40.03	C
20	ATOM	2458	CD2	PHE	G	76	22.150	49.977	217.794	1.00	39.48	C
	ATOM	2460	C	PHE	G	76	19.745	52.257	218.644	1.00	33.13	C
	ATOM	2461	O	PHE	G	76	18.894	51.443	219.005	1.00	33.12	O
	ATOM	2463	N	ILE	G	77	19.722	52.851	217.456	1.00	32.32	N
	ATOM	2464	CA	ILE	G	77	18.689	52.563	216.457	1.00	32.99	C
25	ATOM	2466	CB	ILE	G	77	18.334	53.810	215.625	1.00	32.56	C
	ATOM	2468	CG1	ILE	G	77	17.933	54.973	216.535	1.00	34.51	C
	ATOM	2471	CD1	ILE	G	77	18.078	56.330	215.870	1.00	36.53	C
	ATOM	2475	CG2	ILE	G	77	17.210	53.488	214.618	1.00	34.75	C
	ATOM	2479	C	ILE	G	77	19.180	51.477	215.507	1.00	32.47	C
30	ATOM	2480	O	ILE	G	77	20.129	51.687	214.747	1.00	32.81	O
	ATOM	2482	N	SER	G	78	18.532	50.318	215.560	1.00	33.80	N
	ATOM	2483	CA	SER	G	78	18.846	49.210	214.669	1.00	35.35	C
	ATOM	2485	CB	SER	G	78	18.867	47.895	215.445	1.00	39.07	C
	ATOM	2488	OG	SER	G	78	19.058	46.799	214.573	1.00	44.44	O
35	ATOM	2490	C	SER	G	78	17.814	49.163	213.537	1.00	35.46	C
	ATOM	2491	O	SER	G	78	16.692	48.679	213.719	1.00	33.39	O
	ATOM	2493	N	SER	G	79	18.210	49.674	212.374	1.00	33.37	N
	ATOM	2494	CA	SER	G	79	17.316	49.801	211.232	1.00	35.99	C
	ATOM	2496	CB	SER	G	79	17.925	50.747	210.194	1.00	38.04	C
40	ATOM	2499	OG	SER	G	79	17.029	50.975	209.122	1.00	42.21	O
	ATOM	2501	C	SER	G	79	17.058	48.428	210.613	1.00	36.83	C
	ATOM	2502	O	SER	G	79	17.993	47.670	210.361	1.00	36.03	O
	ATOM	2504	N	TYR	G	80	15.788	48.106	210.385	1.00	34.22	N
	ATOM	2505	CA	TYR	G	80	15.421	46.839	209.754	1.00	34.82	C
45	ATOM	2507	CB	TYR	G	80	13.913	46.613	209.844	1.00	34.39	C
	ATOM	2510	CG	TYR	G	80	13.442	46.302	211.246	1.00	33.00	C
	ATOM	2511	CD1	TYR	G	80	13.630	45.039	211.793	1.00	33.92	C
	ATOM	2513	CE1	TYR	G	80	13.201	44.742	213.077	1.00	33.97	C
	ATOM	2515	CZ	TYR	G	80	12.583	45.715	213.835	1.00	34.47	C
50	ATOM	2516	OH	TYR	G	80	12.165	45.407	215.107	1.00	34.94	O
	ATOM	2518	CE2	TYR	G	80	12.381	46.980	213.317	1.00	33.88	C
	ATOM	2520	CD2	TYR	G	80	12.811	47.266	212.023	1.00	33.40	C
	ATOM	2522	C	TYR	G	80	15.877	46.789	208.295	1.00	34.25	C
	ATOM	2523	O	TYR	G	80	15.924	47.816	207.619	1.00	36.18	O
55	ATOM	2525	N	LYS	G	81	16.237	45.592	207.838	1.00	35.25	N
	ATOM	2526	CA	LYS	G	81	16.579	45.343	206.435	1.00	35.81	C
	ATOM	2528	CB	LYS	G	81	17.732	44.409	206.304	0.00	30.00	C
	ATOM	2531	CG	LYS	G	81	18.174	44.256	204.849	0.00	30.00	C
	ATOM	2534	CD	LYS	G	81	19.317	43.248	204.742	0.00	30.00	C
60	ATOM	2537	CE	LYS	G	81	19.771	43.107	203.290	0.00	30.00	C
	ATOM	2540	NZ	LYS	G	81	20.882	42.107	203.181	0.00	30.00	N
	ATOM	2544	C	LYS	G	81	15.316	44.914	205.681	1.00	35.07	C
	ATOM	2545	O	LYS	G	81	14.890	43.759	205.776	1.00	37.10	O
	ATOM	2547	N	ASN	G	82	14.721	45.848	204.942	1.00	32.01	N
65	ATOM	2548	CA	ASN	G	82	13.441	45.612	204.275	1.00	31.17	C
	ATOM	2550	CB	ASN	G	82	12.297	45.717	205.306	1.00	34.26	C
	ATOM	2553	CG	ASN	G	82	10.931	45.338	204.728	1.00	35.43	C
	ATOM	2554	OD1	ASN	G	82	10.149	46.207	204.351	1.00	35.57	O
	ATOM	2555	ND2	ASN	G	82	10.645	44.042	204.664	1.00	33.34	N
70	ATOM	2558	C	ASN	G	82	13.224	46.606	203.122	1.00	31.23	C
	ATOM	2559	O	ASN	G	82	13.679	47.752	203.179	1.00	28.31	O
	ATOM	2561	N	GLU	G	83	12.511	46.151	202.091	1.00	28.49	N
	ATOM	2562	CA	GLU	G	83	12.200	46.954	200.896	1.00	29.72	C
	ATOM	2564	CB	GLU	G	83	11.380	46.112	199.896	1.00	29.27	C
	ATOM	2567	CG	GLU	G	83	10.005	45.669	200.428	1.00	27.52	C

5	ATOM	2570	CD	GLU	G	83	9.242	44.789	199.452	1.00	29.63	C
	ATOM	2571	OE1	GLU	G	83	9.424	44.961	198.234	1.00	28.62	O
	ATOM	2572	OE2	GLU	G	83	8.460	43.923	199.906	1.00	26.96	O
	ATOM	2573	C	GLU	G	83	11.458	48.267	201.182	1.00	31.17	C
	ATOM	2574	O	GLU	G	83	11.569	49.222	200.410	1.00	31.63	O
10	ATOM	2576	N	TYR	G	84	10.696	48.315	202.274	1.00	29.16	N
	ATOM	2577	CA	TYR	G	84	9.898	49.500	202.601	1.00	29.45	C
	ATOM	2579	CB	TYR	G	84	8.702	49.109	203.477	1.00	30.73	C
	ATOM	2582	CG	TYR	G	84	7.701	48.184	202.797	1.00	28.86	C
	ATOM	2583	CD1	TYR	G	84	7.252	48.437	201.502	1.00	30.14	C
15	ATOM	2585	CE1	TYR	G	84	6.330	47.605	200.879	1.00	29.91	C
	ATOM	2587	CZ	TYR	G	84	5.831	46.507	201.556	1.00	29.47	C
	ATOM	2588	OH	TYR	G	84	4.919	45.678	200.932	1.00	27.45	O
	ATOM	2590	CE2	TYR	G	84	6.255	46.233	202.844	1.00	30.11	O
	ATOM	2592	CD2	TYR	G	84	7.191	47.069	203.460	1.00	31.27	C
20	ATOM	2594	C	TYR	G	84	10.679	50.637	203.266	1.00	28.70	C
	ATOM	2595	O	TYR	G	84	10.154	51.743	203.415	1.00	30.02	O
	ATOM	2597	N	GLN	G	85	11.924	50.375	203.660	1.00	30.01	N
	ATOM	2598	CA	GLN	G	85	12.772	51.403	204.259	1.00	28.47	C
	ATOM	2600	CB	GLN	G	85	13.966	50.753	204.968	1.00	32.41	C
25	ATOM	2603	CG	GLN	G	85	13.595	49.755	206.063	1.00	30.80	C
	ATOM	2606	CD	GLN	G	85	13.358	50.406	207.409	1.00	32.52	C
	ATOM	2607	OE1	GLN	G	85	12.573	51.339	207.524	1.00	33.54	O
	ATOM	2608	NE2	GLN	G	85	14.047	49.920	208.436	1.00	35.09	N
	ATOM	2611	C	GLN	G	85	13.263	52.369	203.169	1.00	29.95	C
30	ATOM	2612	O	GLN	G	85	13.874	51.940	202.189	1.00	26.27	O
	ATOM	2614	N	THR	G	86	12.986	53.662	203.332	1.00	28.12	N
	ATOM	2615	CA	THR	G	86	13.379	54.674	202.339	1.00	27.66	C
	ATOM	2617	CB	THR	G	86	12.144	55.267	201.620	1.00	26.80	C
	ATOM	2619	OG1	THR	G	86	11.261	55.852	202.578	1.00	29.71	O
35	ATOM	2621	CG2	THR	G	86	11.389	54.185	200.835	1.00	27.57	C
	ATOM	2625	C	THR	G	86	14.220	55.813	202.931	1.00	31.54	C
	ATOM	2626	O	THR	G	86	14.463	56.812	202.256	1.00	29.35	O
	ATOM	2628	N	MET	G	87	14.654	55.662	204.186	1.00	32.94	N
	ATOM	2629	CA	MET	G	87	15.596	56.589	204.820	1.00	33.98	C
40	ATOM	2631	CB	MET	G	87	14.924	57.383	205.938	1.00	34.16	C
	ATOM	2634	CG	MET	G	87	14.033	58.509	205.445	1.00	37.77	C
	ATOM	2637	SD	MET	G	87	13.464	59.574	206.794	1.00	42.70	S
	ATOM	2638	CE	MET	G	87	12.218	58.543	207.441	1.00	32.33	C
	ATOM	2642	C	MET	G	87	16.772	55.813	205.395	1.00	34.94	C
45	ATOM	2643	O	MET	G	87	16.665	54.611	205.663	1.00	35.43	O
	ATOM	2645	N	GLU	G	88	17.884	56.521	205.585	1.00	32.93	N
	ATOM	2646	CA	GLU	G	88	19.118	55.946	206.108	1.00	35.69	C
	ATOM	2648	CB	GLU	G	88	20.309	56.425	205.272	1.00	41.28	C
	ATOM	2651	CG	GLU	G	88	20.350	55.844	203.859	1.00	48.44	C
50	ATOM	2654	CD	GLU	G	88	21.501	54.877	203.650	1.00	54.05	C
	ATOM	2655	OE1	GLU	G	88	22.662	55.342	203.626	1.00	56.38	O
	ATOM	2656	OE2	GLU	G	88	21.246	53.660	203.500	1.00	57.43	O
	ATOM	2657	C	GLU	G	88	19.338	56.338	207.565	1.00	35.58	C
	ATOM	2658	O	GLU	G	88	18.933	57.420	207.999	1.00	31.94	O
55	ATOM	2660	N	VAL	G	89	19.967	55.436	208.314	1.00	34.34	N
	ATOM	2661	CA	VAL	G	89	20.490	55.744	209.637	1.00	35.48	C
	ATOM	2663	CB	VAL	G	89	20.088	54.681	210.697	1.00	36.35	C
	ATOM	2665	CG1	VAL	G	89	20.855	54.884	212.008	1.00	36.55	C
	ATOM	2669	CG2	VAL	G	89	18.592	54.719	210.943	1.00	38.46	C
60	ATOM	2673	C	VAL	G	89	22.003	55.799	209.499	1.00	36.90	C
	ATOM	2674	O	VAL	G	89	22.610	54.860	208.982	1.00	36.19	O
	ATOM	2676	N	GLN	G	90	22.593	56.908	209.939	1.00	37.51	N
	ATOM	2677	CA	GLN	G	90	24.036	57.118	209.898	1.00	38.77	C
	ATOM	2679	CB	GLN	G	90	24.397	58.098	208.778	1.00	40.08	C
65	ATOM	2682	CG	GLN	G	90	25.895	58.204	208.495	1.00	44.38	C
	ATOM	2685	CD	GLN	G	90	26.304	59.535	207.874	1.00	46.83	C
	ATOM	2686	OE1	GLN	G	90	27.440	59.990	208.053	1.00	52.00	O
	ATOM	2687	NE2	GLN	G	90	25.385	60.165	207.145	1.00	48.23	N
	ATOM	2690	C	GLN	G	90	24.470	57.687	211.247	1.00	35.50	C
70	ATOM	2691	O	GLN	G	90	23.825	58.595	211.771	1.00	33.92	O
	ATOM	2693	N	ASN	G	91	25.553	57.152	211.807	1.00	37.28	N
	ATOM	2694	CA	ASN	G	91	26.051	57.579	213.117	1.00	36.91	C
	ATOM	2696	CB	ASN	G	91	26.722	58.955	213.015	1.00	40.43	C
	ATOM	2699	CG	ASN	G	91	28.016	58.919	212.215	1.00	44.77	C
	ATOM	2700	OD1	ASN	G	91	28.790	57.966	212.302	1.00	46.89	O

	ATOM	2701	ND2	ASN	G	91	28.261	59.970	211.440	1.00	48.21	N
	ATOM	2704	C	ASN	G	91	24.945	57.585	214.176	1.00	35.82	C
	ATOM	2705	O	ASN	G	91	24.845	58.508	214.991	1.00	34.98	O
	ATOM	2707	N	ASN	G	92	24.120	56.541	214.140	1.00	33.65	N
5	ATOM	2708	CA	ASN	G	92	23.006	56.357	215.068	1.00	35.02	C
	ATOM	2710	CB	ASN	G	92	23.532	56.101	216.490	1.00	37.01	C
	ATOM	2713	CG	ASN	G	92	22.491	55.462	217.390	1.00	36.62	C
	ATOM	2714	OD1	ASN	G	92	21.617	54.732	216.922	1.00	35.62	O
10	ATOM	2715	ND2	ASN	G	92	22.572	55.742	218.689	1.00	36.66	N
	ATOM	2718	C	ASN	G	92	21.992	57.512	215.050	1.00	33.94	C
	ATOM	2719	O	ASN	G	92	21.452	57.903	216.087	1.00	33.96	O
	ATOM	2721	N	SER	G	93	21.743	58.049	213.858	1.00	34.57	N
	ATOM	2722	CA	SER	G	93	20.694	59.048	213.656	1.00	33.69	C
15	ATOM	2724	CB	SER	G	93	21.277	60.467	213.682	1.00	35.98	C
	ATOM	2727	OG	SER	G	93	22.139	60.703	212.583	1.00	38.49	O
	ATOM	2729	C	SER	G	93	19.971	58.787	212.340	1.00	33.03	C
	ATOM	2730	O	SER	G	93	20.555	58.249	211.402	1.00	29.97	O
	ATOM	2732	N	VAL	G	94	18.693	59.150	212.290	1.00	32.02	N
20	ATOM	2733	CA	VAL	G	94	17.908	59.079	211.065	1.00	32.18	C
	ATOM	2735	CB	VAL	G	94	16.404	58.968	211.363	1.00	31.71	C
	ATOM	2737	CG1	VAL	G	94	15.608	58.881	210.075	1.00	33.15	C
	ATOM	2741	CG2	VAL	G	94	16.131	57.746	212.258	1.00	33.24	C
	ATOM	2745	C	VAL	G	94	18.191	60.337	210.238	1.00	32.39	C
	ATOM	2746	O	VAL	G	94	17.925	61.457	210.683	1.00	30.37	O
25	ATOM	2748	N	VAL	G	95	18.734	60.130	209.042	1.00	30.33	N
	ATOM	2749	CA	VAL	G	95	19.131	61.218	208.151	1.00	30.86	C
	ATOM	2751	CB	VAL	G	95	20.213	60.748	207.160	1.00	32.28	C
	ATOM	2753	CG1	VAL	G	95	20.644	61.891	206.248	1.00	32.89	C
30	ATOM	2757	CG2	VAL	G	95	21.412	60.172	207.913	1.00	32.79	C
	ATOM	2761	C	VAL	G	95	17.929	61.738	207.366	1.00	31.94	C
	ATOM	2762	O	VAL	G	95	17.297	60.989	206.606	1.00	32.36	O
	ATOM	2764	N	ILE	G	96	17.621	63.021	207.547	1.00	29.86	N
	ATOM	2765	CA	ILE	G	96	16.508	63.653	206.836	1.00	31.13	C
35	ATOM	2767	CB	ILE	G	96	15.826	64.762	207.681	1.00	29.87	C
	ATOM	2769	CG1	ILE	G	96	15.391	64.232	209.059	1.00	31.88	C
	ATOM	2772	CD1	ILE	G	96	14.472	63.013	209.018	1.00	31.79	C
	ATOM	2776	CG2	ILE	G	96	14.637	65.366	206.927	1.00	29.46	C
	ATOM	2780	C	ILE	G	96	17.026	64.236	205.519	1.00	30.74	C
40	ATOM	2781	O	ILE	G	96	17.856	65.148	205.511	1.00	28.33	O
	ATOM	2783	N	LYS	G	97	16.547	63.683	204.410	1.00	35.40	N
	ATOM	2784	CA	LYS	G	97	16.905	64.171	203.080	1.00	35.66	C
	ATOM	2786	CB	LYS	G	97	17.234	63.002	202.140	1.00	42.38	C
	ATOM	2789	CG	LYS	G	97	18.564	62.305	202.447	1.00	47.38	C
45	ATOM	2792	CD	LYS	G	97	19.782	63.213	202.209	1.00	47.37	C
	ATOM	2795	CE	LYS	G	97	21.077	62.534	202.608	1.00	48.34	C
	ATOM	2798	NZ	LYS	G	97	22.227	63.491	202.715	1.00	49.53	N
	ATOM	2802	C	LYS	G	97	15.810	65.039	202.468	1.00	33.17	C
	ATOM	2803	O	LYS	G	97	16.101	65.844	201.593	1.00	30.00	O
50	ATOM	2805	N	CYS	G	98	14.563	64.869	202.924	1.00	32.18	N
	ATOM	2806	CA	CYS	G	98	13.425	65.596	202.370	1.00	31.83	C
	ATOM	2808	CB	CYS	G	98	12.415	64.625	201.745	1.00	34.55	C
	ATOM	2811	SG	CYS	G	98	13.092	63.548	200.463	1.00	34.35	S
	ATOM	2813	C	CYS	G	98	12.714	66.436	203.433	1.00	32.93	C
55	ATOM	2814	O	CYS	G	98	12.455	65.960	204.545	1.00	31.21	O
	ATOM	2816	N	ASP	G	99	12.390	67.676	203.072	1.00	29.60	N
	ATOM	2817	CA	ASP	G	99	11.555	68.539	203.896	1.00	28.79	C
	ATOM	2819	CB	ASP	G	99	11.327	69.906	203.235	1.00	29.04	C
	ATOM	2822	CG	ASP	G	99	12.567	70.753	203.150	1.00	31.31	C
60	ATOM	2823	OD1	ASP	G	99	13.649	70.326	203.612	1.00	31.26	O
	ATOM	2824	OD2	ASP	G	99	12.433	71.872	202.615	1.00	29.27	O
	ATOM	2825	C	ASP	G	99	10.175	67.913	204.046	1.00	31.17	C
	ATOM	2826	O	ASP	G	99	9.706	67.210	203.156	1.00	30.40	O
	ATOM	2828	N	GLY	G	100	9.506	68.229	205.149	1.00	33.55	N
65	ATOM	2829	CA	GLY	G	100	8.118	67.840	205.330	1.00	31.26	C
	ATOM	2832	C	GLY	G	100	7.728	67.807	206.788	1.00	31.48	C
	ATOM	2833	O	GLY	G	100	8.570	67.992	207.688	1.00	29.36	O
	ATOM	2835	N	LEU	G	101	6.439	67.595	207.021	1.00	27.92	N
	ATOM	2836	CA	LEU	G	101	5.975	67.217	208.342	1.00	27.87	C
70	ATOM	2838	CB	LEU	G	101	4.511	67.589	208.559	1.00	28.54	C
	ATOM	2841	CG	LEU	G	101	4.152	69.060	208.410	1.00	32.99	C
	ATOM	2843	CD1	LEU	G	101	2.679	69.225	208.701	1.00	35.03	C

5	ATOM	2847	CD2	LEU	G	101	5.000	69.937	209.322	1.00	35.16	C
	ATOM	2851	C	LEU	G	101	6.146	65.714	208.460	1.00	28.81	C
	ATOM	2852	O	LEU	G	101	5.754	64.954	207.553	1.00	30.91	O
	ATOM	2854	N	TYR	G	102	6.733	65.299	209.577	1.00	29.37	N
	ATOM	2855	CA	TYR	G	102	6.951	63.896	209.892	1.00	29.98	C
10	ATOM	2857	CB	TYR	G	102	8.443	63.613	210.048	1.00	30.15	C
	ATOM	2860	CG	TYR	G	102	9.268	63.594	208.783	1.00	29.96	C
	ATOM	2861	CD1	TYR	G	102	9.575	64.765	208.103	1.00	28.76	C
	ATOM	2863	CE1	TYR	G	102	10.351	64.741	206.938	1.00	30.07	C
	ATOM	2865	CZ	TYR	G	102	10.844	63.537	206.475	1.00	31.46	C
15	ATOM	2866	OH	TYR	G	102	11.632	63.485	205.346	1.00	30.76	O
	ATOM	2868	CE2	TYR	G	102	10.565	62.368	207.152	1.00	30.45	C
	ATOM	2870	CD2	TYR	G	102	9.787	62.402	208.296	1.00	30.45	C
	ATOM	2872	C	TYR	G	102	6.308	63.581	211.232	1.00	30.82	C
	ATOM	2873	O	TYR	G	102	6.300	64.426	212.134	1.00	30.44	O
20	ATOM	2875	N	ILE	G	103	5.797	62.364	211.367	1.00	32.88	N
	ATOM	2876	CA	ILE	G	103	5.532	61.794	212.678	1.00	34.26	C
	ATOM	2878	CB	ILE	G	103	4.411	60.741	212.672	1.00	37.22	C
	ATOM	2880	CG1	ILE	G	103	3.112	61.338	212.156	1.00	42.68	C
	ATOM	2883	CD1	ILE	G	103	1.980	60.318	212.013	1.00	43.31	C
25	ATOM	2887	CG2	ILE	G	103	4.215	60.170	214.083	1.00	39.89	C
	ATOM	2891	C	ILE	G	103	6.784	61.092	213.162	1.00	30.82	C
	ATOM	2892	O	ILE	G	103	7.404	60.333	212.418	1.00	31.79	O
	ATOM	2894	N	ILE	G	104	7.150	61.352	214.410	1.00	31.85	N
	ATOM	2895	CA	ILE	G	104	8.167	60.568	215.093	1.00	32.24	C
30	ATOM	2897	CB	ILE	G	104	9.299	61.443	215.659	1.00	32.88	C
	ATOM	2899	CG1	ILE	G	104	10.040	62.161	214.521	1.00	35.22	C
	ATOM	2902	CD1	ILE	G	104	9.700	63.623	214.383	1.00	38.01	C
	ATOM	2906	CG2	ILE	G	104	10.278	60.602	216.481	1.00	34.65	C
	ATOM	2910	C	ILE	G	104	7.443	59.800	216.194	1.00	32.66	C
35	ATOM	2911	O	ILE	G	104	6.713	60.397	216.998	1.00	32.16	O
	ATOM	2913	N	TYR	G	105	7.598	58.477	216.187	1.00	32.24	N
	ATOM	2914	CA	TYR	G	105	6.952	57.614	217.176	1.00	31.00	C
	ATOM	2916	CB	TYR	G	105	5.935	56.683	216.520	1.00	34.53	C
	ATOM	2919	CG	TYR	G	105	5.100	55.947	217.543	1.00	33.22	C
40	ATOM	2920	CD1	TYR	G	105	4.099	56.609	218.235	1.00	35.90	C
	ATOM	2922	CE1	TYR	G	105	3.333	55.962	219.183	1.00	37.56	C
	ATOM	2924	CZ	TYR	G	105	3.569	54.633	219.466	1.00	36.48	C
	ATOM	2925	OH	TYR	G	105	2.775	54.008	220.413	1.00	37.56	O
	ATOM	2927	CE2	TYR	G	105	4.562	53.941	218.797	1.00	33.57	C
45	ATOM	2929	CD2	TYR	G	105	5.331	54.605	217.844	1.00	37.41	C
	ATOM	2931	C	TYR	G	105	7.996	56.785	217.909	1.00	30.39	C
	ATOM	2932	O	TYR	G	105	8.843	56.160	217.274	1.00	29.73	O
	ATOM	2934	N	LEU	G	106	7.931	56.790	219.238	1.00	30.64	N
	ATOM	2935	CA	LEU	G	106	8.886	56.051	220.068	1.00	30.38	C
50	ATOM	2937	CB	LEU	G	106	9.874	57.013	220.738	1.00	30.66	C
	ATOM	2940	CG	LEU	G	106	10.963	56.352	221.592	1.00	32.63	C
	ATOM	2942	CD1	LEU	G	106	11.849	55.457	220.731	1.00	33.08	C
	ATOM	2946	CD2	LEU	G	106	11.786	57.402	222.329	1.00	34.12	C
	ATOM	2950	C	LEU	G	106	8.157	55.250	221.135	1.00	28.09	C
55	ATOM	2951	O	LEU	G	106	7.270	55.771	221.814	1.00	30.21	O
	ATOM	2953	N	LYS	G	107	8.521	53.977	221.265	1.00	31.52	N
	ATOM	2954	CA	LYS	G	107	8.069	53.158	222.381	1.00	32.65	C
	ATOM	2956	CB	LYS	G	107	6.941	52.211	221.968	1.00	35.18	C
	ATOM	2959	CG	LYS	G	107	7.305	51.206	220.882	1.00	38.20	C
60	ATOM	2962	CD	LYS	G	107	6.063	50.490	220.362	1.00	39.36	C
	ATOM	2965	CE	LYS	G	107	5.961	49.063	220.824	1.00	42.07	C
	ATOM	2968	NZ	LYS	G	107	6.641	48.156	219.853	1.00	43.82	N
	ATOM	2972	C	LYS	G	107	9.237	52.372	222.954	1.00	31.70	C
	ATOM	2973	O	LYS	G	107	10.207	52.087	222.258	1.00	28.79	O
65	ATOM	2975	N	GLY	G	108	9.133	52.029	224.228	1.00	30.03	N
	ATOM	2976	CA	GLY	G	108	10.175	51.247	224.889	1.00	33.43	C
	ATOM	2979	C	GLY	G	108	9.827	50.978	226.332	1.00	32.14	C
	ATOM	2980	O	GLY	G	108	9.120	51.769	226.955	1.00	35.13	O
	ATOM	2982	N	SER	G	109	10.309	49.848	226.848	1.00	34.51	N
70	ATOM	2983	CA	SER	G	109	10.148	49.479	228.250	1.00	34.13	C
	ATOM	2985	CB	SER	G	109	9.357	48.178	228.374	1.00	36.14	C
	ATOM	2988	OG	SER	G	109	8.104	48.287	227.718	1.00	38.49	O
	ATOM	2990	C	SER	G	109	11.524	49.311	228.888	1.00	33.56	C
	ATOM	2991	O	SER	G	109	12.417	48.710	228.287	1.00	28.74	O
	ATOM	2993	N	PHE	G	110	11.678	49.842	230.101	1.00	32.10	N

5	ATOM	2994	CA	PHE	G	110	12.960	49.864	230.807	1.00	34.97	C
	ATOM	2996	CB	PHE	G	110	13.438	51.308	231.002	1.00	36.89	C
	ATOM	2999	CG	PHE	G	110	13.644	52.067	229.717	1.00	36.45	C
	ATOM	3000	CD1	PHE	G	110	12.562	52.595	229.025	1.00	37.94	C
	ATOM	3002	CE1	PHE	G	110	12.747	53.298	227.837	1.00	37.66	C
10	ATOM	3004	CZ	PHE	G	110	14.029	53.484	227.339	1.00	37.57	C
	ATOM	3006	CE2	PHE	G	110	15.118	52.968	228.027	1.00	36.83	C
	ATOM	3008	CD2	PHE	G	110	14.921	52.264	229.208	1.00	37.66	C
	ATOM	3010	C	PHE	G	110	12.819	49.198	232.173	1.00	36.05	C
	ATOM	3011	O	PHE	G	110	11.713	49.092	232.709	1.00	35.76	O
15	ATOM	3013	N	PHE	G	111	13.944	48.758	232.731	1.00	36.58	N
	ATOM	3014	CA	PHE	G	111	13.968	48.157	234.062	1.00	36.34	C
	ATOM	3016	CB	PHE	G	111	14.953	46.981	234.103	1.00	36.17	C
	ATOM	3019	CG	PHE	G	111	14.643	45.884	233.114	1.00	36.28	C
	ATOM	3020	CD1	PHE	G	111	13.330	45.469	232.890	1.00	36.63	C
20	ATOM	3022	CE1	PHE	G	111	13.050	44.453	231.988	1.00	36.22	C
	ATOM	3024	CZ	PHE	G	111	14.081	43.834	231.302	1.00	36.23	C
	ATOM	3026	CE2	PHE	G	111	15.387	44.232	231.514	1.00	36.20	C
	ATOM	3028	CD2	PHE	G	111	15.666	45.251	232.419	1.00	36.23	C
	ATOM	3030	C	PHE	G	111	14.331	49.167	235.152	1.00	37.55	C
25	ATOM	3031	O	PHE	G	111	14.256	48.851	236.340	1.00	34.15	O
	ATOM	3033	N	GLN	G	112	14.727	50.373	234.746	1.00	38.25	N
	ATOM	3034	CA	GLN	G	112	15.070	51.434	235.688	1.00	38.92	C
	ATOM	3036	CB	GLN	G	112	16.580	51.453	235.965	1.00	39.42	C
	ATOM	3039	CG	GLN	G	112	17.468	51.552	234.724	1.00	40.30	C
30	ATOM	3042	CD	GLN	G	112	18.945	51.348	235.041	1.00	41.41	C
	ATOM	3043	OE1	GLN	G	112	19.453	51.836	236.055	1.00	41.51	O
	ATOM	3044	NE2	GLN	G	112	19.642	50.624	234.170	1.00	42.05	C
	ATOM	3047	C	GLN	G	112	14.606	52.790	235.172	1.00	38.86	C
	ATOM	3048	O	GLN	G	112	14.369	52.965	233.976	1.00	37.64	O
35	ATOM	3050	N	GLU	G	113	14.469	53.739	236.094	1.00	39.67	N
	ATOM	3051	CA	GLU	G	113	14.054	55.102	235.772	1.00	39.86	C
	ATOM	3053	CB	GLU	G	113	13.941	55.931	237.057	1.00	41.54	C
	ATOM	3056	CG	GLU	G	113	13.501	57.373	236.847	1.00	42.98	C
	ATOM	3059	CD	GLU	G	113	13.225	58.098	238.155	1.00	44.34	C
40	ATOM	3060	OE1	GLU	G	113	13.950	57.858	239.147	1.00	47.27	O
	ATOM	3061	OE2	GLU	G	113	12.280	58.912	238.187	1.00	47.76	O
	ATOM	3062	C	GLU	G	113	15.054	55.750	234.817	1.00	38.51	C
	ATOM	3063	O	GLU	G	113	16.262	55.737	235.068	1.00	35.69	O
	ATOM	3065	N	VAL	G	114	14.545	56.310	233.723	1.00	39.08	N
45	ATOM	3066	CA	VAL	G	114	15.392	56.920	232.701	1.00	39.10	C
	ATOM	3068	CB	VAL	G	114	15.625	55.937	231.514	1.00	39.48	C
	ATOM	3070	CG1	VAL	G	114	14.354	55.738	230.697	1.00	38.87	C
	ATOM	3074	CG2	VAL	G	114	16.760	56.417	230.624	1.00	41.42	C
	ATOM	3078	C	VAL	G	114	14.787	58.236	232.204	1.00	38.45	C
50	ATOM	3079	O	VAL	G	114	13.569	58.420	232.237	1.00	39.60	O
	ATOM	3081	N	LYS	G	115	15.657	59.148	231.772	1.00	37.36	N
	ATOM	3082	CA	LYS	G	115	15.258	60.408	231.148	1.00	37.42	C
	ATOM	3084	CB	LYS	G	115	15.832	61.608	231.915	1.00	38.31	C
	ATOM	3087	CG	LYS	G	115	15.189	61.853	233.278	1.00	39.01	C
55	ATOM	3090	CD	LYS	G	115	15.756	63.093	233.963	1.00	39.29	C
	ATOM	3093	CE	LYS	G	115	15.161	63.281	235.355	1.00	40.26	C
	ATOM	3096	NZ	LYS	G	115	15.782	64.411	236.104	1.00	40.67	N
	ATOM	3100	C	LYS	G	115	15.773	60.407	229.713	1.00	35.77	C
	ATOM	3101	O	LYS	G	115	16.970	60.256	229.479	1.00	36.04	O
60	ATOM	3103	N	ILE	G	116	14.869	60.564	228.752	1.00	35.05	N
	ATOM	3104	CA	ILE	G	116	15.246	60.517	227.339	1.00	35.19	C
	ATOM	3106	CB	ILE	G	116	14.655	59.264	226.646	1.00	35.38	C
	ATOM	3108	CG1	ILE	G	116	15.273	58.008	227.281	1.00	38.41	C
	ATOM	3111	CD1	ILE	G	116	14.609	56.712	226.913	1.00	39.78	C
65	ATOM	3115	CG2	ILE	G	116	14.920	59.306	225.136	1.00	35.79	C
	ATOM	3119	C	ILE	G	116	14.863	61.810	226.615	1.00	33.36	C
	ATOM	3120	O	ILE	G	116	13.793	62.380	226.853	1.00	32.00	O
	ATOM	3122	N	ASP	G	117	15.763	62.267	225.745	1.00	32.93	N
	ATOM	3123	CA	ASP	G	117	15.585	63.504	224.984	1.00	33.14	C
70	ATOM	3125	CB	ASP	G	117	16.655	64.526	225.375	1.00	33.72	C
	ATOM	3128	CG	ASP	G	117	16.573	64.936	226.835	1.00	37.42	C
	ATOM	3129	OD1	ASP	G	117	15.516	65.447	227.255	1.00	38.72	O
	ATOM	3130	OD2	ASP	G	117	17.577	64.758	227.562	1.00	40.90	O
	ATOM	3131	C	ASP	G	117	15.679	63.227	223.487	1.00	32.30	C
	ATOM	3132	O	ASP	G	117	16.507	62.426	223.057	1.00	31.68	O

5	ATOM	3134	N	LEU	G	118	14.837	63.906	222.705	1.00	31.80	N
	ATOM	3135	CA	LEU	G	118	14.768	63.731	221.250	1.00	32.06	C
	ATOM	3137	CB	LEU	G	118	13.306	63.548	220.835	1.00	30.98	C
	ATOM	3140	CG	LEU	G	118	12.973	63.551	219.348	1.00	31.53	C
	ATOM	3142	CD1	LEU	G	118	13.650	62.385	218.652	1.00	27.96	C
10	ATOM	3146	CD2	LEU	G	118	11.469	63.488	219.169	1.00	34.35	C
	ATOM	3150	C	LEU	G	118	15.355	64.949	220.527	1.00	31.71	C
	ATOM	3151	O	LEU	G	118	14.911	66.076	220.752	1.00	32.20	O
	ATOM	3153	N	HIS	G	119	16.343	64.707	219.666	1.00	33.18	N
	ATOM	3154	CA	HIS	G	119	17.034	65.757	218.913	1.00	31.88	C
15	ATOM	3156	CB	HIS	G	119	18.553	65.622	219.064	1.00	31.06	C
	ATOM	3159	CG	HIS	G	119	19.036	65.693	220.477	1.00	32.32	C
	ATOM	3160	ND1	HIS	G	119	18.885	64.652	221.367	1.00	32.89	N
	ATOM	3162	CE1	HIS	G	119	19.413	64.993	222.529	1.00	32.16	C
	ATOM	3164	NE2	HIS	G	119	19.907	66.212	222.422	1.00	32.84	N
20	ATOM	3166	CD2	HIS	G	119	19.689	66.671	221.147	1.00	30.57	C
	ATOM	3168	C	HIS	G	119	16.704	65.647	217.429	1.00	31.85	C
	ATOM	3169	O	HIS	G	119	16.567	64.544	216.903	1.00	31.96	O
	ATOM	3171	N	PHE	G	120	16.591	66.797	216.767	1.00	32.59	N
	ATOM	3172	CA	PHE	G	120	16.357	66.873	215.323	1.00	34.71	C
25	ATOM	3174	CB	PHE	G	120	15.213	67.840	215.000	1.00	37.57	C
	ATOM	3177	CG	PHE	G	120	13.862	67.424	215.552	1.00	36.81	C
	ATOM	3178	CD1	PHE	G	120	13.553	66.092	215.801	1.00	38.42	C
	ATOM	3180	CE1	PHE	G	120	12.307	65.734	216.296	1.00	37.91	C
	ATOM	3182	CZ	PHE	G	120	11.352	66.704	216.535	1.00	37.40	C
30	ATOM	3184	CE2	PHE	G	120	11.638	68.027	216.278	1.00	39.44	C
	ATOM	3186	CD2	PHE	G	120	12.888	68.383	215.782	1.00	38.84	C
	ATOM	3188	C	PHE	G	120	17.612	67.329	214.579	1.00	34.86	C
	ATOM	3189	O	PHE	G	120	17.694	67.207	213.357	1.00	36.36	O
	ATOM	3191	N	ARG	G	121	18.573	67.871	215.316	1.00	36.09	N
35	ATOM	3192	CA	ARG	G	121	19.880	68.205	214.767	1.00	37.40	C
	ATOM	3194	CB	ARG	G	121	19.812	69.450	213.869	1.00	37.23	C
	ATOM	3197	CG	ARG	G	121	20.839	69.434	212.724	1.00	37.55	C
	ATOM	3200	CD	ARG	G	121	20.469	70.373	211.586	1.00	38.24	C
	ATOM	3203	NE	ARG	G	121	20.627	71.770	211.972	1.00	38.58	N
40	ATOM	3205	CZ	ARG	G	121	20.694	72.789	211.119	1.00	39.83	C
	ATOM	3206	NH1	ARG	G	121	20.596	72.593	209.803	1.00	38.47	N
	ATOM	3209	NH2	ARG	G	121	20.853	74.022	211.591	1.00	36.68	N
	ATOM	3212	C	ARG	G	121	20.848	68.415	215.922	1.00	37.87	C
	ATOM	3213	O	ARG	G	121	20.437	68.463	217.088	1.00	33.84	O
45	ATOM	3215	N	GLU	G	122	22.130	68.535	215.594	1.00	41.10	N
	ATOM	3216	CA	GLU	G	122	23.182	68.704	216.599	1.00	42.86	C
	ATOM	3218	CB	GLU	G	122	24.569	68.591	215.946	1.00	47.99	C
	ATOM	3221	CG	GLU	G	122	24.905	67.199	215.390	1.00	51.18	C
	ATOM	3224	CD	GLU	G	122	24.486	66.999	213.929	1.00	54.74	C
50	ATOM	3225	OE1	GLU	G	122	23.344	67.365	213.560	1.00	50.63	O
	ATOM	3226	OE2	GLU	G	122	25.306	66.456	213.154	1.00	58.26	O
	ATOM	3227	C	GLU	G	122	23.064	70.027	217.369	1.00	43.14	C
	ATOM	3228	O	GLU	G	122	23.489	70.113	218.522	1.00	40.39	O
	ATOM	3230	N	ASP	G	123	22.483	71.044	216.729	1.00	43.56	N
55	ATOM	3231	CA	ASP	G	123	22.282	72.365	217.346	1.00	44.30	C
	ATOM	3233	CB	ASP	G	123	22.782	73.471	216.400	1.00	44.22	C
	ATOM	3236	CG	ASP	G	123	22.102	73.445	215.033	1.00	43.48	C
	ATOM	3237	OD1	ASP	G	123	21.149	72.657	214.838	1.00	41.46	O
	ATOM	3238	OD2	ASP	G	123	22.531	74.218	214.148	1.00	42.03	O
60	ATOM	3239	C	ASP	G	123	20.821	72.631	217.767	1.00	45.93	C
	ATOM	3240	O	ASP	G	123	20.450	73.770	218.062	1.00	47.73	O
	ATOM	3242	N	HIS	G	124	20.014	71.570	217.802	1.00	46.41	N
	ATOM	3243	CA	HIS	G	124	18.601	71.634	218.186	1.00	44.93	C
	ATOM	3245	CB	HIS	G	124	17.850	70.482	217.502	1.00	45.45	C
65	ATOM	3248	CG	HIS	G	124	16.412	70.342	217.901	1.00	46.19	C
	ATOM	3249	ND1	HIS	G	124	15.925	69.217	218.531	1.00	45.11	N
	ATOM	3251	CE1	HIS	G	124	14.626	69.353	218.734	1.00	45.05	C
	ATOM	3253	NE2	HIS	G	124	14.251	70.527	218.259	1.00	44.42	N
	ATOM	3255	CD2	HIS	G	124	15.347	71.162	217.722	1.00	46.87	C
70	ATOM	3257	C	HIS	G	124	18.454	71.528	219.703	1.00	45.27	C
	ATOM	3258	O	HIS	G	124	19.131	70.718	220.344	1.00	42.61	O
	ATOM	3260	N	ASN	G	125	17.563	72.339	220.270	1.00	44.79	N
	ATOM	3261	CA	ASN	G	125	17.221	72.219	221.685	1.00	45.80	C
	ATOM	3263	CB	ASN	G	125	16.594	73.512	222.221	1.00	49.79	C
	ATOM	3266	CG	ASN	G	125	17.132	73.892	223.582	1.00	53.63	C

	ATOM	3267	OD1	ASN	G	125	16.424	73.812	224.589	1.00	56.18	O
	ATOM	3268	ND2	ASN	G	125	18.402	74.294	223.626	1.00	54.31	N
	ATOM	3271	C	ASN	G	125	16.261	71.032	221.853	1.00	42.94	C
	ATOM	3272	O	ASN	G	125	15.162	71.050	221.300	1.00	45.72	O
5	ATOM	3274	N	PRO	G	126	16.664	70.006	222.627	1.00	40.72	N
	ATOM	3275	CA	PRO	G	126	15.965	68.721	222.554	1.00	40.30	C
	ATOM	3277	CB	PRO	G	126	16.906	67.755	223.296	1.00	41.72	C
	ATOM	3280	CG	PRO	G	126	18.069	68.555	223.755	1.00	40.81	C
	ATOM	3283	CD	PRO	G	126	17.731	69.988	223.641	1.00	41.40	C
10	ATOM	3286	C	PRO	G	126	14.594	68.714	223.227	1.00	39.13	C
	ATOM	3287	O	PRO	G	126	14.341	69.504	224.140	1.00	35.82	O
	ATOM	3288	N	ILE	G	127	13.725	67.815	222.770	1.00	35.49	N
	ATOM	3289	CA	ILE	G	127	12.432	67.593	223.403	1.00	36.73	C
	ATOM	3291	CB	ILE	G	127	11.385	67.089	222.384	1.00	36.04	C
15	ATOM	3293	CG1	ILE	G	127	11.081	68.181	221.351	1.00	38.10	C
	ATOM	3296	CD1	ILE	G	127	10.501	67.648	220.059	1.00	39.51	C
	ATOM	3300	CG2	ILE	G	127	10.101	66.663	223.089	1.00	36.84	C
	ATOM	3304	C	ILE	G	127	12.588	66.561	224.521	1.00	34.92	C
	ATOM	3305	O	ILE	G	127	13.081	65.464	224.284	1.00	32.62	O
20	ATOM	3307	N	SER	G	128	12.154	66.915	225.729	1.00	34.99	N
	ATOM	3308	CA	SER	G	128	12.102	65.967	226.838	1.00	36.10	C
	ATOM	3310	CB	SER	G	128	11.972	66.703	228.174	1.00	35.99	C
	ATOM	3313	OG	SER	G	128	11.862	65.784	229.251	1.00	35.92	O
	ATOM	3315	C	SER	G	128	10.910	65.038	226.642	1.00	37.07	C
25	ATOM	3316	O	SER	G	128	9.778	65.498	226.563	1.00	37.95	O
	ATOM	3318	N	ILE	G	129	11.165	63.736	226.561	1.00	37.63	N
	ATOM	3319	CA	ILE	G	129	10.102	62.758	226.323	1.00	37.49	C
	ATOM	3321	CB	ILE	G	129	10.658	61.488	225.637	1.00	38.10	C
	ATOM	3323	CG1	ILE	G	129	11.123	61.847	224.221	1.00	38.97	C
30	ATOM	3326	CD1	ILE	G	129	11.640	60.685	223.402	1.00	40.20	C
	ATOM	3330	CG2	ILE	G	129	9.597	60.371	225.604	1.00	37.97	C
	ATOM	3334	C	ILE	G	129	9.392	62.402	227.635	1.00	37.98	C
	ATOM	3335	O	ILE	G	129	10.034	61.909	228.572	1.00	35.37	O
	ATOM	3337	N	PRO	G	130	8.070	62.665	227.719	1.00	37.06	N
35	ATOM	3338	CA	PRO	G	130	7.338	62.271	228.933	1.00	37.60	C
	ATOM	3340	CB	PRO	G	130	5.905	62.761	228.669	1.00	37.90	C
	ATOM	3343	CG	PRO	G	130	6.012	63.740	227.553	1.00	38.22	C
	ATOM	3346	CD	PRO	G	130	7.192	63.336	226.744	1.00	36.72	C
	ATOM	3349	C	PRO	G	130	7.358	60.752	229.128	1.00	37.37	C
40	ATOM	3350	O	PRO	G	130	7.198	59.999	228.161	1.00	34.94	O
	ATOM	3351	N	MET	G	131	7.567	60.319	230.365	1.00	35.20	N
	ATOM	3352	CA	MET	G	131	7.677	58.903	230.683	1.00	37.52	C
	ATOM	3354	CB	MET	G	131	8.933	58.654	231.515	1.00	39.48	C
	ATOM	3357	CG	MET	G	131	10.209	59.246	230.932	1.00	41.69	C
45	ATOM	3360	SD	MET	G	131	10.693	58.440	229.394	1.00	42.71	S
	ATOM	3361	CE	MET	G	131	11.223	56.849	230.035	1.00	43.15	C
	ATOM	3365	C	MET	G	131	6.463	58.435	231.472	1.00	38.41	C
	ATOM	3366	O	MET	G	131	5.844	59.215	232.198	1.00	38.04	O
	ATOM	3368	N	LEU	G	132	6.134	57.154	231.322	1.00	38.69	N
50	ATOM	3369	CA	LEU	G	132	5.124	56.499	232.148	1.00	40.20	C
	ATOM	3371	CB	LEU	G	132	4.128	55.746	231.267	1.00	39.95	C
	ATOM	3374	CG	LEU	G	132	3.375	56.597	230.244	1.00	42.57	C
	ATOM	3376	CD1	LEU	G	132	2.560	55.710	229.312	1.00	43.03	C
	ATOM	3380	CD2	LEU	G	132	2.487	57.625	230.945	1.00	43.96	C
55	ATOM	3384	C	LEU	G	132	5.806	55.529	233.113	1.00	39.89	C
	ATOM	3385	O	LEU	G	132	7.007	55.270	232.995	1.00	35.31	O
	ATOM	3387	N	ASN	G	133	5.035	55.012	234.069	1.00	41.84	N
	ATOM	3388	CA	ASN	G	133	5.500	53.966	234.994	1.00	43.18	C
	ATOM	3390	CB	ASN	G	133	5.754	52.654	234.232	1.00	45.43	C
60	ATOM	3393	CG	ASN	G	133	4.554	52.199	233.423	1.00	47.82	C
	ATOM	3394	OD1	ASN	G	133	3.541	52.892	233.338	1.00	51.00	O
	ATOM	3395	ND2	ASN	G	133	4.667	51.022	232.819	1.00	48.46	N
	ATOM	3398	C	ASN	G	133	6.753	54.351	235.787	1.00	42.84	C
	ATOM	3399	O	ASN	G	133	7.702	53.571	235.874	1.00	43.25	O
65	ATOM	3401	N	ASP	G	134	6.743	55.550	236.366	1.00	43.66	N
	ATOM	3402	CA	ASP	G	134	7.888	56.080	237.125	1.00	43.77	C
	ATOM	3404	CB	ASP	G	134	8.054	55.337	238.461	1.00	45.66	C
	ATOM	3407	CG	ASP	G	134	6.892	55.570	239.415	1.00	47.30	C
	ATOM	3408	OD1	ASP	G	134	6.326	56.684	239.426	1.00	48.54	O
70	ATOM	3409	OD2	ASP	G	134	6.555	54.637	240.170	1.00	48.06	O
	ATOM	3410	C	ASP	G	134	9.198	56.043	236.321	1.00	42.84	C

5	ATOM	3411	O	ASP	G	134	10.247	55.631	236.830	1.00	40.38	O
	ATOM	3413	N	GLY	G	135	9.119	56.477	235.064	1.00	39.79	N
	ATOM	3414	CA	GLY	G	135	10.294	56.602	234.203	1.00	41.20	C
	ATOM	3417	C	GLY	G	135	10.740	55.332	233.493	1.00	40.43	C
	ATOM	3418	O	GLY	G	135	11.877	55.262	233.032	1.00	41.35	O
10	ATOM	3420	N	ARG	G	136	9.855	54.340	233.389	1.00	39.20	N
	ATOM	3421	CA	ARG	G	136	10.216	53.024	232.836	1.00	39.01	C
	ATOM	3423	CB	ARG	G	136	9.993	51.939	233.889	1.00	39.26	C
	ATOM	3426	CG	ARG	G	136	10.952	52.013	235.053	1.00	39.97	C
	ATOM	3429	CD	ARG	G	136	10.806	50.797	235.946	1.00	41.96	C
15	ATOM	3432	NE	ARG	G	136	10.901	51.153	237.359	1.00	44.07	N
	ATOM	3434	CZ	ARG	G	136	10.675	50.314	238.367	1.00	44.99	C
	ATOM	3435	NH1	ARG	G	136	10.345	49.044	238.139	1.00	46.05	N
	ATOM	3438	NH2	ARG	G	136	10.781	50.749	239.615	1.00	45.05	N
	ATOM	3441	C	ARG	G	136	9.479	52.619	231.555	1.00	37.21	C
20	ATOM	3442	O	ARG	G	136	9.785	51.574	230.977	1.00	34.53	O
	ATOM	3444	N	ARG	G	137	8.505	53.411	231.121	1.00	35.93	N
	ATOM	3445	CA	ARG	G	137	7.820	53.132	229.862	1.00	36.46	C
	ATOM	3447	CB	ARG	G	137	6.458	52.479	230.104	1.00	36.52	C
	ATOM	3450	CG	ARG	G	137	5.773	52.060	228.815	1.00	36.06	C
25	ATOM	3453	CD	ARG	G	137	4.401	51.482	229.045	1.00	37.15	C
	ATOM	3456	NE	ARG	G	137	3.816	51.074	227.772	1.00	36.40	N
	ATOM	3458	CZ	ARG	G	137	2.548	50.717	227.590	1.00	36.44	C
	ATOM	3459	NH1	ARG	G	137	1.689	50.688	228.603	1.00	36.26	N
	ATOM	3462	NH2	ARG	G	137	2.145	50.371	226.373	1.00	36.01	N
30	ATOM	3465	C	ARG	G	137	7.645	54.391	229.027	1.00	34.82	C
	ATOM	3466	O	ARG	G	137	7.272	55.445	229.545	1.00	34.17	O
	ATOM	3468	N	ILE	G	138	7.912	54.255	227.731	1.00	34.76	N
	ATOM	3469	CA	ILE	G	138	7.701	55.327	226.764	1.00	35.08	C
	ATOM	3471	CB	ILE	G	138	8.996	55.655	225.997	1.00	35.07	C
35	ATOM	3473	CG1	ILE	G	138	10.096	55.992	227.001	1.00	39.34	C
	ATOM	3476	CD1	ILE	G	138	11.350	56.555	226.395	1.00	40.25	C
	ATOM	3480	CG2	ILE	G	138	8.782	56.825	225.031	1.00	35.04	C
	ATOM	3484	C	ILE	G	138	6.622	54.923	225.776	1.00	31.35	C
	ATOM	3485	O	ILE	G	138	6.633	53.814	225.244	1.00	26.44	O
40	ATOM	3487	N	VAL	G	139	5.668	55.822	225.576	1.00	31.76	N
	ATOM	3488	CA	VAL	G	139	4.780	55.788	224.416	1.00	34.01	C
	ATOM	3490	CB	VAL	G	139	3.380	55.224	224.745	1.00	35.26	C
	ATOM	3492	CG1	VAL	G	139	2.484	55.280	223.499	1.00	37.79	C
	ATOM	3496	CG2	VAL	G	139	3.481	53.806	225.272	1.00	34.86	C
45	ATOM	3500	C	VAL	G	139	4.674	57.245	223.993	1.00	34.42	C
	ATOM	3501	O	VAL	G	139	4.069	58.053	224.695	1.00	35.03	O
	ATOM	3503	N	PHE	G	140	5.302	57.595	222.877	1.00	33.64	N
	ATOM	3504	CA	PHE	G	140	5.494	59.004	222.549	1.00	34.03	C
	ATOM	3506	CB	PHE	G	140	6.897	59.450	222.966	1.00	36.15	C
50	ATOM	3509	CG	PHE	G	140	7.190	60.887	222.658	1.00	35.11	C
	ATOM	3510	CD1	PHE	G	140	6.665	61.896	223.448	1.00	38.14	C
	ATOM	3512	CE1	PHE	G	140	6.932	63.229	223.172	1.00	36.51	C
	ATOM	3514	CZ	PHE	G	140	7.724	63.562	222.098	1.00	37.38	C
	ATOM	3516	CE2	PHE	G	140	8.250	62.569	221.291	1.00	38.45	C
55	ATOM	3518	CD2	PHE	G	140	7.980	61.234	221.571	1.00	37.69	C
	ATOM	3520	C	PHE	G	140	5.285	59.276	221.072	1.00	33.25	C
	ATOM	3521	O	PHE	G	140	5.901	58.629	220.226	1.00	31.37	O
	ATOM	3523	N	THR	G	141	4.413	60.241	220.779	1.00	34.52	N
	ATOM	3524	CA	THR	G	141	4.165	60.690	219.411	1.00	35.25	C
60	ATOM	3526	CB	THR	G	141	2.701	60.449	218.987	1.00	39.10	C
	ATOM	3528	OG1	THR	G	141	2.348	59.080	219.209	1.00	37.71	O
	ATOM	3530	CG2	THR	G	141	2.495	60.791	217.509	1.00	39.26	C
	ATOM	3534	C	THR	G	141	4.450	62.186	219.308	1.00	37.64	C
	ATOM	3535	O	THR	G	141	4.060	62.973	220.185	1.00	36.06	O
65	ATOM	3537	N	VAL	G	142	5.158	62.562	218.248	1.00	37.01	N
	ATOM	3538	CA	VAL	G	142	5.305	63.961	217.870	1.00	34.85	C
	ATOM	3540	CB	VAL	G	142	6.660	64.574	218.350	1.00	37.60	C
	ATOM	3542	CG1	VAL	G	142	7.838	63.836	217.785	1.00	37.01	C
	ATOM	3546	CG2	VAL	G	142	6.752	66.058	217.997	1.00	39.45	C
70	ATOM	3550	C	VAL	G	142	5.151	64.096	216.358	1.00	32.27	C
	ATOM	3551	O	VAL	G	142	5.563	63.216	215.595	1.00	31.32	O
	ATOM	3553	N	VAL	G	143	4.498	65.176	215.947	1.00	30.99	N
	ATOM	3554	CA	VAL	G	143	4.528	65.639	214.581	1.00	29.81	C
	ATOM	3556	CB	VAL	G	143	3.111	65.933	214.044	1.00	32.61	C
	ATOM	3558	CG1	VAL	G	143	3.166	66.272	212.558	1.00	31.79	C

5	ATOM	3562	CG2	VAL	G	143	2.195	64.741	214.295	1.00	31.30	C
	ATOM	3566	C	VAL	G	143	5.373	66.908	214.575	1.00	31.33	C
	ATOM	3567	O	VAL	G	143	5.189	67.783	215.430	1.00	30.24	O
	ATOM	3569	N	ALA	G	144	6.306	66.992	213.631	1.00	31.31	N
	ATOM	3570	CA	ALA	G	144	7.262	68.096	213.587	1.00	33.09	C
10	ATOM	3572	CB	ALA	G	144	8.521	67.736	214.388	1.00	33.45	C
	ATOM	3576	C	ALA	G	144	7.631	68.422	212.153	1.00	33.43	C
	ATOM	3577	O	ALA	G	144	7.631	67.545	211.286	1.00	30.07	O
	ATOM	3579	N	SER	G	145	7.947	69.689	211.909	1.00	33.79	N
	ATOM	3580	CA	SER	G	145	8.485	70.106	210.628	1.00	33.60	C
15	ATOM	3582	CB	SER	G	145	8.234	71.595	210.405	1.00	35.97	C
	ATOM	3585	OG	SER	G	145	8.788	72.006	209.173	1.00	38.46	O
	ATOM	3587	C	SER	G	145	9.983	69.820	210.599	1.00	33.36	C
	ATOM	3588	O	SER	G	145	10.740	70.369	211.396	1.00	32.20	O
	ATOM	3590	N	LEU	G	146	10.396	68.935	209.700	1.00	33.62	N
20	ATOM	3591	CA	LEU	G	146	11.798	68.593	209.527	1.00	32.68	C
	ATOM	3593	CB	LEU	G	146	11.985	67.080	209.647	1.00	32.52	C
	ATOM	3596	CG	LEU	G	146	11.520	66.450	210.971	1.00	31.98	C
	ATOM	3598	CD1	LEU	G	146	11.881	64.981	210.990	1.00	31.72	C
	ATOM	3602	CD2	LEU	G	146	12.147	67.156	212.167	1.00	32.69	C
25	ATOM	3606	C	LEU	G	146	12.284	69.085	208.168	1.00	32.54	C
	ATOM	3607	O	LEU	G	146	11.495	69.257	207.241	1.00	32.09	O
	ATOM	3609	N	ALA	G	147	13.586	69.319	208.059	1.00	32.14	N
	ATOM	3610	CA	ALA	G	147	14.184	69.774	206.810	1.00	31.97	C
	ATOM	3612	CB	ALA	G	147	14.456	71.275	206.878	1.00	29.54	C
30	ATOM	3616	C	ALA	G	147	15.474	69.024	206.504	1.00	32.61	C
	ATOM	3617	O	ALA	G	147	16.140	68.509	207.409	1.00	32.23	O
	ATOM	3619	N	PHE	G	148	15.825	68.977	205.220	1.00	31.06	N
	ATOM	3620	CA	PHE	G	148	17.142	68.515	204.785	1.00	29.92	C
	ATOM	3622	CB	PHE	G	148	17.399	68.980	203.339	1.00	29.49	C
35	ATOM	3625	CG	PHE	G	148	18.801	68.741	202.854	1.00	28.01	C
	ATOM	3626	CD1	PHE	G	148	19.367	67.479	202.926	1.00	28.99	C
	ATOM	3628	CE1	PHE	G	148	20.664	67.253	202.486	1.00	29.38	C
	ATOM	3630	CZ	PHE	G	148	21.407	68.293	201.945	1.00	30.10	C
	ATOM	3632	CE2	PHE	G	148	20.846	69.562	201.857	1.00	31.06	C
40	ATOM	3634	CD2	PHE	G	148	19.548	69.778	202.309	1.00	26.97	C
	ATOM	3636	C	PHE	G	148	18.248	69.017	205.735	1.00	29.03	C
	ATOM	3637	O	PHE	G	148	18.273	70.194	206.100	1.00	28.49	O
	ATOM	3639	N	LYS	G	149	19.137	68.097	206.121	1.00	32.45	N
	ATOM	3640	CA	LYS	G	149	20.263	68.316	207.057	1.00	32.23	C
45	ATOM	3642	CB	LYS	G	149	20.903	69.703	206.926	1.00	32.52	C
	ATOM	3645	CG	LYS	G	149	21.538	69.953	205.571	1.00	32.22	C
	ATOM	3648	CD	LYS	G	149	22.185	71.313	205.516	1.00	32.59	C
	ATOM	3651	CE	LYS	G	149	22.654	71.641	204.113	1.00	33.38	C
	ATOM	3654	NZ	LYS	G	149	23.619	72.768	204.123	1.00	32.22	N
50	ATOM	3658	C	LYS	G	149	19.921	68.009	208.523	1.00	32.79	C
	ATOM	3659	O	LYS	G	149	20.819	67.926	209.363	1.00	29.22	O
	ATOM	3661	N	ASP	G	150	18.641	67.832	208.829	1.00	31.05	N
	ATOM	3662	CA	ASP	G	150	18.249	67.352	210.147	1.00	33.21	C
	ATOM	3664	CB	ASP	G	150	16.731	67.446	210.357	1.00	33.12	C
55	ATOM	3667	CG	ASP	G	150	16.252	68.864	210.622	1.00	34.26	C
	ATOM	3668	OD1	ASP	G	150	17.089	69.761	210.864	1.00	32.00	O
	ATOM	3669	OD2	ASP	G	150	15.018	69.082	210.596	1.00	33.63	O
	ATOM	3670	C	ASP	G	150	18.708	65.906	210.338	1.00	32.31	C
	ATOM	3671	O	ASP	G	150	18.809	65.126	209.381	1.00	31.03	O
60	ATOM	3673	N	LYS	G	151	18.996	65.571	211.589	1.00	32.10	N
	ATOM	3674	CA	LYS	G	151	19.382	64.223	211.975	1.00	34.75	C
	ATOM	3676	CB	LYS	G	151	20.893	64.137	212.137	1.00	37.51	C
	ATOM	3679	CG	LYS	G	151	21.629	64.078	210.810	1.00	39.27	C
	ATOM	3682	CD	LYS	G	151	23.070	64.517	210.927	1.00	41.73	C
65	ATOM	3685	CE	LYS	G	151	23.834	64.219	209.639	1.00	43.98	C
	ATOM	3688	NZ	LYS	G	151	23.008	64.469	208.419	1.00	47.72	N
	ATOM	3692	C	LYS	G	151	18.673	63.878	213.275	1.00	32.64	C
	ATOM	3693	O	LYS	G	151	18.891	64.523	214.297	1.00	33.28	O
	ATOM	3695	N	VAL	G	152	17.814	62.868	213.228	1.00	31.61	N
70	ATOM	3696	CA	VAL	G	152	16.975	62.528	214.373	1.00	32.20	C
	ATOM	3698	CB	VAL	G	152	15.583	62.046	213.928	1.00	33.20	C
	ATOM	3700	CG1	VAL	G	152	14.716	61.693	215.133	1.00	33.07	C
	ATOM	3704	CG2	VAL	G	152	14.911	63.112	213.070	1.00	34.07	C
	ATOM	3708	C	VAL	G	152	17.651	61.477	215.250	1.00	31.20	C
	ATOM	3709	O	VAL	G	152	17.926	60.364	214.801	1.00	28.73	O

	ATOM	3711	N	TYR	G	153	17.923	61.845	216.499	1.00	30.45	N
	ATOM	3712	CA	TYR	G	153	18.533	60.923	217.453	1.00	31.82	C
	ATOM	3714	CB	TYR	G	153	20.061	60.997	217.383	1.00	32.34	C
	ATOM	3717	CG	TYR	G	153	20.663	62.329	217.749	1.00	31.88	C
5	ATOM	3718	CD1	TYR	G	153	20.720	63.369	216.823	1.00	32.51	C
	ATOM	3720	CE1	TYR	G	153	21.293	64.599	217.156	1.00	31.44	C
	ATOM	3722	CZ	TYR	G	153	21.821	64.785	218.420	1.00	32.42	C
	ATOM	3723	OH	TYR	G	153	22.389	65.987	218.761	1.00	32.82	O
	ATOM	3725	CE2	TYR	G	153	21.786	63.764	219.352	1.00	33.70	C
10	ATOM	3727	CD2	TYR	G	153	21.211	62.542	219.012	1.00	32.75	C
	ATOM	3729	C	TYR	G	153	18.037	61.132	218.880	1.00	32.10	C
	ATOM	3730	O	TYR	G	153	17.384	62.132	219.187	1.00	32.35	O
	ATOM	3732	N	LEU	G	154	18.355	60.163	219.736	1.00	32.03	N
	ATOM	3733	CA	LEU	G	154	17.784	60.065	221.071	1.00	31.11	C
15	ATOM	3735	CB	LEU	G	154	16.863	58.846	221.154	1.00	31.78	C
	ATOM	3738	CG	LEU	G	154	15.603	58.880	220.285	1.00	35.07	C
	ATOM	3740	CD1	LEU	G	154	15.169	57.469	219.907	1.00	37.39	C
	ATOM	3744	CD2	LEU	G	154	14.492	59.626	220.997	1.00	34.86	C
	ATOM	3748	C	LEU	G	154	18.904	59.901	222.074	1.00	30.28	C
20	ATOM	3749	O	LEU	G	154	19.659	58.935	221.991	1.00	27.43	O
	ATOM	3751	N	THR	G	155	19.022	60.838	223.013	1.00	30.43	N
	ATOM	3752	CA	THR	G	155	20.010	60.716	224.079	1.00	30.24	C
	ATOM	3754	CB	THR	G	155	20.723	62.041	224.361	1.00	30.52	C
	ATOM	3756	OG1	THR	G	155	19.757	63.025	224.738	1.00	28.71	O
25	ATOM	3758	CG2	THR	G	155	21.506	62.510	223.140	1.00	31.02	C
	ATOM	3762	C	THR	G	155	19.354	60.257	225.374	1.00	31.46	C
	ATOM	3763	O	THR	G	155	18.166	60.494	225.603	1.00	30.61	O
	ATOM	3765	N	VAL	G	156	20.143	59.588	226.207	1.00	32.25	N
	ATOM	3766	CA	VAL	G	156	19.753	59.255	227.562	1.00	38.04	C
30	ATOM	3768	CB	VAL	G	156	20.080	57.787	227.904	1.00	39.96	C
	ATOM	3770	CG1	VAL	G	156	19.763	57.494	229.371	1.00	39.74	C
	ATOM	3774	CG2	VAL	G	156	19.324	56.840	226.974	1.00	39.26	C
	ATOM	3778	C	VAL	G	156	20.554	60.176	228.479	1.00	40.60	C
	ATOM	3779	O	VAL	G	156	21.786	60.110	228.501	1.00	40.10	O
35	ATOM	3781	N	ASN	G	157	19.861	61.045	229.211	1.00	43.59	N
	ATOM	3782	CA	ASN	G	157	20.518	61.919	230.182	1.00	45.58	C
	ATOM	3784	CB	ASN	G	157	19.619	63.115	230.526	1.00	45.61	C
	ATOM	3787	CG	ASN	G	157	20.333	64.179	231.354	1.00	45.86	C
	ATOM	3788	OD1	ASN	G	157	21.518	64.058	231.675	1.00	46.91	O
40	ATOM	3789	ND2	ASN	G	157	19.604	65.233	231.704	1.00	45.70	N
	ATOM	3792	C	ASN	G	157	20.880	61.113	231.435	1.00	48.32	C
	ATOM	3793	O	ASN	G	157	20.052	60.936	232.333	1.00	50.00	O
	ATOM	3795	N	ALA	G	158	22.118	60.619	231.473	1.00	50.32	N
	ATOM	3796	CA	ALA	G	158	22.615	59.813	232.592	1.00	51.05	C
45	ATOM	3798	CB	ALA	G	158	21.931	58.447	232.604	1.00	51.27	C
	ATOM	3802	C	ALA	G	158	24.135	59.638	232.502	1.00	53.29	C
	ATOM	3803	O	ALA	G	158	24.722	59.884	231.446	1.00	54.76	O
	ATOM	3805	N	PRO	G	159	24.781	59.220	233.611	1.00	53.91	N
	ATOM	3806	CA	PRO	G	159	26.200	58.844	233.573	1.00	54.26	C
50	ATOM	3808	CB	PRO	G	159	26.473	58.343	234.999	1.00	54.61	C
	ATOM	3811	CG	PRO	G	159	25.449	59.009	235.841	1.00	54.42	C
	ATOM	3814	CD	PRO	G	159	24.227	59.120	234.975	1.00	54.20	C
	ATOM	3817	C	PRO	G	159	26.516	57.744	232.551	1.00	55.54	C
	ATOM	3818	O	PRO	G	159	25.642	56.943	232.207	1.00	55.54	O
55	ATOM	3819	N	ASP	G	160	27.766	57.711	232.091	1.00	56.10	N
	ATOM	3820	CA	ASP	G	160	28.206	56.787	231.034	1.00	55.53	C
	ATOM	3822	CB	ASP	G	160	29.700	56.984	230.729	1.00	56.97	C
	ATOM	3825	CG	ASP	G	160	30.052	58.427	230.390	1.00	57.52	C
	ATOM	3826	OD1	ASP	G	160	29.480	58.974	229.425	1.00	56.60	O
60	ATOM	3827	OD2	ASP	G	160	30.908	59.008	231.092	1.00	58.18	O
	ATOM	3828	C	ASP	G	160	27.968	55.322	231.406	1.00	55.25	C
	ATOM	3829	O	ASP	G	160	27.533	54.527	230.573	1.00	53.83	O
	ATOM	3831	N	THR	G	161	28.251	54.987	232.665	1.00	55.14	N
	ATOM	3832	CA	THR	G	161	28.188	53.611	233.169	1.00	54.26	C
65	ATOM	3834	CB	THR	G	161	28.501	53.572	234.679	1.00	55.03	C
	ATOM	3836	OG1	THR	G	161	29.751	54.226	234.926	1.00	57.09	O
	ATOM	3838	CG2	THR	G	161	28.560	52.133	235.193	1.00	55.51	C
	ATOM	3842	C	THR	G	161	26.835	52.934	232.961	1.00	52.44	C
	ATOM	3843	O	THR	G	161	26.767	51.788	232.515	1.00	49.87	O
70	ATOM	3845	N	LEU	G	162	25.762	53.641	233.298	1.00	51.41	N
	ATOM	3846	CA	LEU	G	162	24.425	53.061	233.230	1.00	51.38	C

5	ATOM	3848	CB	LEU	G	162	23.431	53.890	234.057	1.00	53.41	C
	ATOM	3851	CG	LEU	G	162	23.629	53.728	235.574	1.00	55.87	C
	ATOM	3853	CD1	LEU	G	162	23.077	54.915	236.353	1.00	56.66	C
	ATOM	3857	CD2	LEU	G	162	23.014	52.424	236.080	1.00	56.38	C
	ATOM	3861	C	LEU	G	162	23.933	52.866	231.791	1.00	49.78	C
10	ATOM	3862	O	LEU	G	162	23.052	52.041	231.559	1.00	50.92	O
	ATOM	3864	N	CYS	G	163	24.511	53.597	230.832	1.00	47.92	N
	ATOM	3865	CA	CYS	G	163	24.146	53.436	229.416	1.00	45.83	C
	ATOM	3867	CB	CYS	G	163	24.712	54.569	228.546	1.00	46.95	C
	ATOM	3870	SG	CYS	G	163	24.632	54.253	226.742	1.00	47.29	S
15	ATOM	3872	C	CYS	G	163	24.566	52.072	228.859	1.00	42.69	C
	ATOM	3873	O	CYS	G	163	23.745	51.383	228.263	1.00	37.97	O
	ATOM	3875	N	GLU	G	164	25.820	51.660	229.066	1.00	42.98	N
	ATOM	3876	CA	GLU	G	164	26.260	50.347	228.548	1.00	42.18	C
	ATOM	3878	CB	GLU	G	164	27.789	50.153	228.592	1.00	44.40	C
20	ATOM	3881	CG	GLU	G	164	28.499	50.581	229.869	1.00	45.32	C
	ATOM	3884	CD	GLU	G	164	29.337	51.842	229.693	1.00	47.32	C
	ATOM	3885	OE1	GLU	G	164	28.909	52.757	228.957	1.00	48.37	O
	ATOM	3886	OE2	GLU	G	164	30.432	51.914	230.297	1.00	47.83	O
	ATOM	3887	C	GLU	G	164	25.545	49.157	229.203	1.00	39.22	C
25	ATOM	3888	O	GLU	G	164	25.567	48.054	228.655	1.00	40.36	O
	ATOM	3890	N	HIS	G	165	24.901	49.381	230.348	1.00	36.80	N
	ATOM	3891	CA	HIS	G	165	24.116	48.337	231.020	1.00	38.28	C
	ATOM	3893	CB	HIS	G	165	24.431	48.318	232.521	1.00	39.92	C
	ATOM	3896	CG	HIS	G	165	25.824	47.868	232.836	1.00	40.60	C
30	ATOM	3897	ND1	HIS	G	165	26.273	46.595	232.558	1.00	40.60	N
	ATOM	3899	CE1	HIS	G	165	27.533	46.482	232.940	1.00	42.21	C
	ATOM	3901	NE2	HIS	G	165	27.917	47.637	233.455	1.00	41.97	N
	ATOM	3903	CD2	HIS	G	165	26.867	48.520	233.404	1.00	41.10	C
	ATOM	3905	C	HIS	G	165	22.604	48.481	230.808	1.00	36.42	C
35	ATOM	3906	O	HIS	G	165	21.833	47.626	231.249	1.00	34.78	O
	ATOM	3908	N	LEU	G	166	22.181	49.548	230.133	1.00	34.82	N
	ATOM	3909	CA	LEU	G	166	20.759	49.793	229.898	1.00	36.67	C
	ATOM	3911	CB	LEU	G	166	20.535	51.199	229.327	1.00	36.79	C
	ATOM	3914	CG	LEU	G	166	19.118	51.763	229.470	1.00	38.00	C
40	ATOM	3916	CD1	LEU	G	166	18.805	52.105	230.925	1.00	39.40	C
	ATOM	3920	CD2	LEU	G	166	18.946	52.988	228.583	1.00	38.65	C
	ATOM	3924	C	LEU	G	166	20.186	48.747	228.937	1.00	35.83	C
	ATOM	3925	O	LEU	G	166	20.756	48.497	227.873	1.00	35.31	O
	ATOM	3927	N	GLN	G	167	19.064	48.144	229.329	1.00	35.66	N
45	ATOM	3928	CA	GLN	G	167	18.389	47.114	228.536	1.00	34.22	C
	ATOM	3930	CB	GLN	G	167	18.357	45.800	229.312	1.00	35.14	C
	ATOM	3933	CG	GLN	G	167	19.734	45.240	229.630	1.00	34.19	C
	ATOM	3936	CD	GLN	G	167	19.686	43.930	230.388	1.00	34.32	C
	ATOM	3937	OE1	GLN	G	167	20.611	43.122	230.300	1.00	39.47	O
50	ATOM	3938	NE2	GLN	G	167	18.618	43.714	231.147	1.00	30.74	N
	ATOM	3941	C	GLN	G	167	16.967	47.557	228.228	1.00	33.04	C
	ATOM	3942	O	GLN	G	167	16.232	47.960	229.131	1.00	29.93	O
	ATOM	3944	N	ILE	G	168	16.580	47.481	226.954	1.00	33.01	N
	ATOM	3945	CA	ILE	G	168	15.281	47.973	226.507	1.00	33.59	C
55	ATOM	3947	CB	ILE	G	168	15.449	49.130	225.493	1.00	34.28	C
	ATOM	3949	CG1	ILE	G	168	16.370	50.205	226.083	1.00	35.48	C
	ATOM	3952	CD1	ILE	G	168	16.866	51.213	225.100	1.00	36.50	C
	ATOM	3956	CG2	ILE	G	168	14.093	49.725	225.126	1.00	34.17	C
	ATOM	3960	C	ILE	G	168	14.463	46.846	225.874	1.00	33.37	C
60	ATOM	3961	O	ILE	G	168	14.953	46.136	224.990	1.00	30.67	O
	ATOM	3963	N	ASN	G	169	13.224	46.690	226.346	1.00	31.91	N
	ATOM	3964	CA	ASN	G	169	12.264	45.744	225.775	1.00	32.58	C
	ATOM	3966	CB	ASN	G	169	11.585	44.917	226.879	1.00	31.65	C
	ATOM	3969	CG	ASN	G	169	12.429	43.737	227.345	1.00	31.00	C
65	ATOM	3970	OD1	ASN	G	169	13.366	43.315	226.663	1.00	28.97	O
	ATOM	3971	ND2	ASN	G	169	12.086	43.187	228.508	1.00	29.46	N
	ATOM	3974	C	ASN	G	169	11.200	46.484	224.968	1.00	32.76	C
	ATOM	3975	O	ASN	G	169	10.857	47.626	225.288	1.00	30.73	O
	ATOM	3977	N	ASP	G	170	10.689	45.830	223.925	1.00	34.94	N
70	ATOM	3978	CA	ASP	G	170	9.603	46.377	223.102	1.00	35.82	C
	ATOM	3980	CB	ASP	G	170	8.287	46.337	223.896	1.00	39.67	C
	ATOM	3983	CG	ASP	G	170	7.046	46.466	223.018	1.00	43.95	C
	ATOM	3984	OD1	ASP	G	170	7.090	46.105	221.817	1.00	47.90	O
	ATOM	3985	OD2	ASP	G	170	6.006	46.926	223.549	1.00	50.00	O
	ATOM	3986	C	ASP	G	170	9.932	47.803	222.637	1.00	35.76	C

	ATOM	3987	O	ASP	G	170	9.093	48.705	222.701	1.00	37.04	O
	ATOM	3989	N	GLY	G	171	11.167	47.991	222.178	1.00	33.06	N
	ATOM	3990	CA	GLY	G	171	11.665	49.300	221.779	1.00	33.21	C
	ATOM	3993	C	GLY	G	171	11.612	49.488	220.277	1.00	34.16	C
5	ATOM	3994	O	GLY	G	171	12.067	48.628	219.519	1.00	32.96	O
	ATOM	3996	N	GLU	G	172	11.065	50.620	219.843	1.00	33.30	N
	ATOM	3997	CA	GLU	G	172	10.918	50.884	218.420	1.00	32.96	C
	ATOM	3999	CB	GLU	G	172	9.667	50.187	217.882	1.00	33.88	C
	ATOM	4002	CG	GLU	G	172	9.429	50.377	216.389	1.00	35.64	C
10	ATOM	4005	CD	GLU	G	172	8.447	49.372	215.835	1.00	38.47	C
	ATOM	4006	OE1	GLU	G	172	8.860	48.215	215.606	1.00	43.84	O
	ATOM	4007	OE2	GLU	G	172	7.268	49.729	215.638	1.00	38.77	O
	ATOM	4008	C	GLU	G	172	10.847	52.371	218.138	1.00	31.04	C
	ATOM	4009	O	GLU	G	172	10.158	53.107	218.846	1.00	31.70	O
15	ATOM	4011	N	LEU	G	173	11.577	52.800	217.109	1.00	30.96	N
	ATOM	4012	CA	LEU	G	173	11.510	54.165	216.601	1.00	30.64	C
	ATOM	4014	CB	LEU	G	173	12.900	54.801	216.558	1.00	31.38	C
	ATOM	4017	CG	LEU	G	173	12.982	56.190	215.912	1.00	30.28	C
	ATOM	4019	CD1	LEU	G	173	12.193	57.218	216.714	1.00	31.20	C
20	ATOM	4023	CD2	LEU	G	173	14.419	56.620	215.755	1.00	33.38	C
	ATOM	4027	C	LEU	G	173	10.946	54.136	215.190	1.00	30.34	C
	ATOM	4028	O	LEU	G	173	11.423	53.368	214.352	1.00	29.59	O
	ATOM	4030	N	ILE	G	174	9.930	54.960	214.936	1.00	30.68	N
	ATOM	4031	CA	ILE	G	174	9.421	55.164	213.583	1.00	30.14	C
25	ATOM	4033	CB	ILE	G	174	7.974	54.624	213.388	1.00	31.16	C
	ATOM	4035	CG1	ILE	G	174	7.971	53.094	213.463	1.00	33.41	C
	ATOM	4038	CD1	ILE	G	174	6.603	52.441	213.438	1.00	34.23	C
	ATOM	4042	CG2	ILE	G	174	7.411	55.088	212.039	1.00	33.28	C
	ATOM	4046	C	ILE	G	174	9.477	56.648	213.243	1.00	30.57	C
30	ATOM	4047	O	ILE	G	174	9.062	57.492	214.033	1.00	29.00	O
	ATOM	4049	N	VAL	G	175	10.009	56.944	212.063	1.00	32.41	N
	ATOM	4050	CA	VAL	G	175	9.982	58.277	211.482	1.00	30.75	C
	ATOM	4052	CB	VAL	G	175	11.408	58.864	211.352	1.00	31.43	C
	ATOM	4054	CG1	VAL	G	175	11.362	60.297	210.808	1.00	33.05	C
35	ATOM	4058	CG2	VAL	G	175	12.125	58.844	212.706	1.00	31.61	C
	ATOM	4062	C	VAL	G	175	9.321	58.146	210.108	1.00	30.19	C
	ATOM	4063	O	VAL	G	175	9.753	57.347	209.279	1.00	32.01	O
	ATOM	4065	N	VAL	G	176	8.258	58.906	209.879	1.00	29.88	N
	ATOM	4066	CA	VAL	G	176	7.494	58.804	208.636	1.00	30.44	C
40	ATOM	4068	CB	VAL	G	176	6.310	57.793	208.767	1.00	34.76	C
	ATOM	4070	CG1	VAL	G	176	5.398	58.144	209.933	1.00	38.16	C
	ATOM	4074	CG2	VAL	G	176	5.521	57.701	207.453	1.00	32.47	C
	ATOM	4078	C	VAL	G	176	7.003	60.179	208.172	1.00	30.80	C
	ATOM	4079	O	VAL	G	176	6.432	60.942	208.952	1.00	31.78	O
45	ATOM	4081	N	GLN	G	177	7.249	60.473	206.896	1.00	29.01	N
	ATOM	4082	CA	GLN	G	177	6.882	61.730	206.264	1.00	28.98	C
	ATOM	4084	CB	GLN	G	177	7.684	61.879	204.977	1.00	29.97	C
	ATOM	4087	CG	GLN	G	177	7.558	63.205	204.250	1.00	30.61	C
	ATOM	4090	CD	GLN	G	177	8.265	63.164	202.914	1.00	31.18	C
50	ATOM	4091	OE1	GLN	G	177	8.364	62.105	202.301	1.00	29.35	O
	ATOM	4092	NE2	GLN	G	177	8.760	64.312	202.454	1.00	31.97	N
	ATOM	4095	C	GLN	G	177	5.385	61.766	205.950	1.00	32.27	C
	ATOM	4096	O	GLN	G	177	4.837	60.794	205.434	1.00	29.85	O
	ATOM	4098	N	LEU	G	178	4.749	62.891	206.280	1.00	30.33	N
55	ATOM	4099	CA	LEU	G	178	3.310	63.121	206.087	1.00	29.78	C
	ATOM	4101	CB	LEU	G	178	2.713	63.750	207.357	1.00	32.52	C
	ATOM	4104	CG	LEU	G	178	2.081	62.851	208.423	1.00	35.40	C
	ATOM	4106	CD1	LEU	G	178	2.670	61.462	208.512	1.00	36.75	C
	ATOM	4110	CD2	LEU	G	178	2.072	63.553	209.770	1.00	34.10	C
60	ATOM	4114	C	LEU	G	178	2.988	64.031	204.899	1.00	30.40	C
	ATOM	4115	O	LEU	G	178	1.918	63.917	204.279	1.00	26.95	O
	ATOM	4117	N	THR	G	179	3.884	64.965	204.613	1.00	31.34	N
	ATOM	4118	CA	THR	G	179	3.689	65.907	203.518	1.00	30.29	C
	ATOM	4120	CB	THR	G	179	3.357	67.309	204.040	1.00	31.21	C
65	ATOM	4122	OG1	THR	G	179	4.396	67.743	204.922	1.00	31.44	O
	ATOM	4124	CG2	THR	G	179	2.026	67.310	204.782	1.00	33.31	C
	ATOM	4128	C	THR	G	179	4.970	65.966	202.693	1.00	32.79	C
	ATOM	4129	O	THR	G	179	6.066	65.818	203.249	1.00	33.43	O
	ATOM	4131	N	PRO	G	180	4.840	66.178	201.372	1.00	32.87	N
70	ATOM	4132	CA	PRO	G	180	6.007	66.184	200.498	1.00	33.28	C
	ATOM	4134	CB	PRO	G	180	5.396	66.019	199.109	1.00	36.99	C

5	ATOM	4137	CG	PRO	G	180	4.081	66.712	199.210	1.00	36.57	C
	ATOM	4140	CD	PRO	G	180	3.596	66.430	200.618	1.00	34.18	C
	ATOM	4143	C	PRO	G	180	6.763	67.497	200.592	1.00	33.62	C
	ATOM	4144	O	PRO	G	180	6.225	68.494	201.077	1.00	32.32	O
	ATOM	4145	N	GLY	G	181	8.006	67.493	200.132	1.00	32.40	N
10	ATOM	4146	CA	GLY	G	181	8.810	68.697	200.133	1.00	31.93	C
	ATOM	4149	C	GLY	G	181	10.079	68.511	199.346	1.00	31.94	C
	ATOM	4150	O	GLY	G	181	10.295	67.463	198.724	1.00	30.76	O
	ATOM	4152	N	TYR	G	182	10.911	69.543	199.381	1.00	30.99	N
	ATOM	4153	CA	TYR	G	182	12.234	69.518	198.769	1.00	30.37	C
15	ATOM	4155	CB	TYR	G	182	12.992	70.796	199.155	1.00	29.05	C
	ATOM	4158	CG	TYR	G	182	14.480	70.724	198.928	1.00	28.96	C
	ATOM	4159	CD1	TYR	G	182	15.034	71.046	197.688	1.00	30.22	C
	ATOM	4161	CE1	TYR	G	182	16.398	70.963	197.476	1.00	28.29	C
	ATOM	4163	CZ	TYR	G	182	17.230	70.559	198.510	1.00	28.04	C
20	ATOM	4164	OH	TYR	G	182	18.592	70.473	198.316	1.00	28.02	O
	ATOM	4166	CE2	TYR	G	182	16.707	70.230	199.738	1.00	28.48	C
	ATOM	4168	CD2	TYR	G	182	15.338	70.319	199.946	1.00	29.33	C
	ATOM	4170	C	TYR	G	182	13.014	68.289	199.223	1.00	30.19	C
	ATOM	4171	O	TYR	G	182	13.049	67.991	200.414	1.00	28.55	O
25	ATOM	4173	N	CYS	G	183	13.614	67.574	198.272	1.00	31.35	N
	ATOM	4174	CA	CYS	G	183	14.551	66.489	198.573	1.00	32.86	C
	ATOM	4176	CB	CYS	G	183	14.069	65.146	198.004	1.00	37.54	C
	ATOM	4179	SG	CYS	G	183	12.511	64.498	198.725	1.00	43.21	S
	ATOM	4181	C	CYS	G	183	15.902	66.830	197.973	1.00	31.59	C
30	ATOM	4182	O	CYS	G	183	15.988	67.251	196.818	1.00	29.27	O
	ATOM	4184	N	ALA	G	184	16.956	66.658	198.762	1.00	31.83	N
	ATOM	4185	CA	ALA	G	184	18.314	66.821	198.266	1.00	32.88	C
	ATOM	4187	CB	ALA	G	184	19.283	66.960	199.424	1.00	31.71	C
	ATOM	4191	C	ALA	G	184	18.655	65.590	197.432	1.00	34.21	C
35	ATOM	4192	O	ALA	G	184	18.550	64.473	197.934	1.00	35.70	O
	ATOM	4194	N	PRO	G	185	19.028	65.781	196.151	1.00	40.34	N
	ATOM	4195	CA	PRO	G	185	19.434	64.650	195.301	1.00	41.97	C
	ATOM	4197	CB	PRO	G	185	19.850	65.325	193.990	1.00	43.06	C
	ATOM	4200	CG	PRO	G	185	19.120	66.614	193.977	1.00	43.53	C
40	ATOM	4203	CD	PRO	G	185	19.060	67.055	195.405	1.00	41.57	C
	ATOM	4206	C	PRO	G	185	20.605	63.847	195.870	1.00	44.95	C
	ATOM	4207	O	PRO	G	185	21.515	64.424	196.467	1.00	45.80	O
	ATOM	4208	N	GLU	G	186	20.576	62.531	195.677	1.00	46.09	N
	ATOM	4209	CA	GLU	G	186	21.618	61.645	196.195	1.00	45.81	C
45	ATOM	4211	CB	GLU	G	186	21.292	60.205	195.965	0.00	30.00	C
	ATOM	4214	CG	GLU	G	186	20.067	59.805	196.785	0.00	30.00	C
	ATOM	4217	CD	GLU	G	186	19.734	58.331	196.563	0.00	30.00	C
	ATOM	4218	OE1	GLU	G	186	20.305	57.716	195.662	0.00	30.00	O
	ATOM	4219	OE2	GLU	G	186	18.900	57.787	197.290	0.00	30.00	O
50	ATOM	4220	C	GLU	G	186	22.989	61.982	195.612	1.00	46.06	C
	ATOM	4221	O	GLU	G	186	23.131	62.118	194.396	1.00	46.72	O
	ATOM	4223	N	GLY	G	187	23.982	62.136	196.488	1.00	46.95	N
	ATOM	4224	CA	GLY	G	187	25.363	62.418	196.082	1.00	47.72	C
	ATOM	4227	C	GLY	G	187	25.687	63.868	195.741	1.00	48.91	C
55	ATOM	4228	O	GLY	G	187	26.772	64.152	195.228	1.00	47.34	O
	ATOM	4230	N	SER	G	188	24.771	64.791	196.042	1.00	49.06	N
	ATOM	4231	CA	SER	G	188	24.924	66.200	195.645	1.00	49.26	C
	ATOM	4233	CB	SER	G	188	23.620	66.713	195.027	1.00	49.38	C
	ATOM	4236	OG	SER	G	188	22.565	66.711	195.977	1.00	50.89	O
60	ATOM	4238	C	SER	G	188	25.358	67.146	196.777	1.00	49.22	C
	ATOM	4239	O	SER	G	188	25.658	68.317	196.518	1.00	46.47	O
	ATOM	4241	N	TYR	G	189	25.375	66.656	198.019	1.00	50.65	N
	ATOM	4242	CA	TYR	G	189	25.810	67.464	199.165	1.00	51.82	C
	ATOM	4244	CB	TYR	G	189	24.608	68.010	199.950	1.00	50.78	C
65	ATOM	4247	CG	TYR	G	189	25.024	68.911	201.098	1.00	50.42	C
	ATOM	4248	CD1	TYR	G	189	25.245	70.271	200.896	1.00	49.87	C
	ATOM	4250	CE1	TYR	G	189	25.651	71.096	201.937	1.00	50.54	C
	ATOM	4252	CZ	TYR	G	189	25.846	70.561	203.201	1.00	51.14	C
	ATOM	4253	OH	TYR	G	189	26.243	71.375	204.239	1.00	50.35	O
70	ATOM	4255	CE2	TYR	G	189	25.635	69.211	203.427	1.00	51.13	C
	ATOM	4257	CD2	TYR	G	189	25.229	68.394	202.377	1.00	50.71	C
	ATOM	4259	C	TYR	G	189	26.723	66.680	200.113	1.00	53.17	C
	ATOM	4260	O	TYR	G	189	26.475	65.507	200.397	1.00	52.31	O
	ATOM	4262	N	HIS	G	190	27.768	67.349	200.603	1.00	54.42	N
	ATOM	4263	CA	HIS	G	190	28.678	66.782	201.603	1.00	56.64	C

5	ATOM	4265	CB	HIS	G	190	29.963	66.278	200.939	1.00	60.60	C
	ATOM	4268	CG	HIS	G	190	29.754	65.097	200.041	1.00	62.76	C
	ATOM	4269	ND1	HIS	G	190	29.933	65.158	198.675	1.00	63.61	N
	ATOM	4271	CE1	HIS	G	190	29.676	63.974	198.147	1.00	64.44	C
	ATOM	4273	NE2	HIS	G	190	29.331	63.149	199.120	1.00	64.84	N
10	ATOM	4275	CD2	HIS	G	190	29.372	63.827	200.315	1.00	63.82	C
	ATOM	4277	C	HIS	G	190	29.018	67.813	202.683	1.00	57.39	C
	ATOM	4278	O	HIS	G	190	29.100	69.014	202.414	1.00	57.33	O
	ATOM	4280	N	LEU	R	29	28.588	105.309	149.054	1.00	46.27	N
	ATOM	4281	CA	LEU	R	29	27.939	104.381	150.031	1.00	43.68	C
15	ATOM	4283	CB	LEU	R	29	28.681	103.039	150.074	1.00	44.65	C
	ATOM	4286	CG	LEU	R	29	28.126	101.970	151.023	1.00	44.57	C
	ATOM	4288	CD1	LEU	R	29	26.685	101.634	150.677	1.00	45.42	C
	ATOM	4292	CD2	LEU	R	29	28.994	100.720	150.991	1.00	43.98	C
	ATOM	4296	C	LEU	R	29	27.906	104.996	151.426	1.00	42.91	C
20	ATOM	4297	O	LEU	R	29	28.923	105.499	151.908	1.00	45.02	O
	ATOM	4301	N	HIS	R	30	26.740	104.957	152.069	1.00	42.60	N
	ATOM	4302	CA	HIS	R	30	26.615	105.416	153.448	1.00	41.72	C
	ATOM	4304	CB	HIS	R	30	26.309	106.908	153.517	1.00	46.72	C
	ATOM	4307	CG	HIS	R	30	26.477	107.479	154.890	1.00	48.60	C
25	ATOM	4308	ND1	HIS	R	30	25.476	107.445	155.837	1.00	51.14	N
	ATOM	4310	CE1	HIS	R	30	25.911	108.002	156.953	1.00	51.61	C
	ATOM	4312	NE2	HIS	R	30	27.160	108.389	156.766	1.00	51.53	N
	ATOM	4314	CD2	HIS	R	30	27.541	108.066	155.487	1.00	50.82	C
	ATOM	4316	C	HIS	R	30	25.559	104.640	154.227	1.00	39.91	C
30	ATOM	4317	O	HIS	R	30	24.370	104.684	153.901	1.00	38.06	O
	ATOM	4319	N	CYS	R	31	26.015	103.957	155.277	1.00	35.54	N
	ATOM	4320	CA	CYS	R	31	25.184	103.060	156.069	1.00	35.67	C
	ATOM	4322	CB	CYS	R	31	25.886	101.707	156.215	1.00	36.19	C
	ATOM	4325	SG	CYS	R	31	26.282	100.928	154.640	1.00	38.52	S
35	ATOM	4327	C	CYS	R	31	24.912	103.647	157.447	1.00	34.00	C
	ATOM	4328	O	CYS	R	31	25.673	104.486	157.936	1.00	34.26	O
	ATOM	4330	N	VAL	R	32	23.824	103.193	158.065	1.00	33.47	N
	ATOM	4331	CA	VAL	R	32	23.439	103.622	159.410	1.00	35.34	C
	ATOM	4333	CB	VAL	R	32	22.363	104.746	159.371	1.00	35.78	C
40	ATOM	4335	CG1	VAL	R	32	22.912	105.984	158.679	1.00	34.85	C
	ATOM	4339	CG2	VAL	R	32	21.078	104.265	158.682	1.00	35.40	C
	ATOM	4343	C	VAL	R	32	22.906	102.440	160.223	1.00	37.00	C
	ATOM	4344	O	VAL	R	32	22.592	101.388	159.669	1.00	37.17	O
	ATOM	4346	N	GLY	R	33	22.811	102.622	161.537	1.00	36.26	N
45	ATOM	4347	CA	GLY	R	33	22.196	101.627	162.417	1.00	36.56	C
	ATOM	4350	C	GLY	R	33	22.966	100.324	162.551	1.00	37.35	C
	ATOM	4351	O	GLY	R	33	24.193	100.327	162.676	1.00	39.86	O
	ATOM	4353	N	ASP	R	34	22.240	99.208	162.505	1.00	34.47	N
	ATOM	4354	CA	ASP	R	34	22.807	97.878	162.735	1.00	33.97	C
50	ATOM	4356	CB	ASP	R	34	21.732	96.953	163.311	1.00	37.54	C
	ATOM	4359	CG	ASP	R	34	21.188	97.439	164.651	1.00	40.50	C
	ATOM	4360	OD1	ASP	R	34	21.905	98.170	165.366	1.00	43.53	O
	ATOM	4361	OD2	ASP	R	34	20.041	97.081	164.991	1.00	41.97	O
	ATOM	4362	C	ASP	R	34	23.374	97.278	161.453	1.00	31.16	C
55	ATOM	4363	O	ASP	R	34	23.125	96.115	161.133	1.00	31.70	O
	ATOM	4365	N	THR	R	35	24.132	98.085	160.717	1.00	29.60	N
	ATOM	4366	CA	THR	R	35	24.695	97.667	159.447	1.00	30.50	C
	ATOM	4368	CB	THR	R	35	23.928	98.297	158.254	1.00	32.36	C
	ATOM	4370	OG1	THR	R	35	24.007	99.722	158.325	1.00	32.83	O
60	ATOM	4372	CG2	THR	R	35	22.456	97.869	158.265	1.00	35.06	C
	ATOM	4376	C	THR	R	35	26.173	98.031	159.345	1.00	28.90	C
	ATOM	4377	O	THR	R	35	26.710	98.762	160.179	1.00	27.73	O
	ATOM	4379	N	TYR	R	36	26.828	97.484	158.332	1.00	27.80	N
	ATOM	4380	CA	TYR	R	36	28.199	97.850	158.024	1.00	27.30	C
65	ATOM	4382	CB	TYR	R	36	29.187	96.882	158.693	1.00	27.22	C
	ATOM	4385	CG	TYR	R	36	29.044	95.435	158.274	1.00	23.58	C
	ATOM	4386	CD1	TYR	R	36	28.102	94.608	158.869	1.00	24.91	C
	ATOM	4388	CE1	TYR	R	36	27.966	93.272	158.490	1.00	27.21	C
	ATOM	4390	CZ	TYR	R	36	28.787	92.751	157.504	1.00	28.43	C
70	ATOM	4391	OH	TYR	R	36	28.657	91.422	157.133	1.00	27.14	O
	ATOM	4393	CE2	TYR	R	36	29.726	93.558	156.891	1.00	28.23	C
	ATOM	4395	CD2	TYR	R	36	29.850	94.899	157.281	1.00	25.45	C
	ATOM	4397	C	TYR	R	36	28.384	97.904	156.515	1.00	27.42	C
	ATOM	4398	O	TYR	R	36	27.771	97.116	155.774	1.00	29.24	O
	ATOM	4400	N	PRO	R	37	29.198	98.861	156.042	1.00	27.68	N

5	ATOM	4401	CA	PRO	R	37	29.415	99.039	154.620	1.00	28.95	C
	ATOM	4403	CB	PRO	R	37	30.003	100.447	154.541	1.00	27.74	C
	ATOM	4406	CG	PRO	R	37	30.698	100.626	155.827	1.00	28.32	C
	ATOM	4409	CD	PRO	R	37	29.945	99.850	156.842	1.00	26.68	C
	ATOM	4412	C	PRO	R	37	30.388	98.006	154.060	1.00	32.41	C
10	ATOM	4413	O	PRO	R	37	31.498	97.856	154.581	1.00	33.45	O
	ATOM	4414	N	SER	R	38	29.969	97.298	153.014	1.00	30.58	N
	ATOM	4415	CA	SER	R	38	30.844	96.344	152.340	1.00	35.75	C
	ATOM	4417	CB	SER	R	38	30.987	95.070	153.185	1.00	39.20	C
	ATOM	4420	OG	SER	R	38	31.989	94.209	152.671	1.00	39.12	O
15	ATOM	4422	C	SER	R	38	30.311	95.996	150.955	1.00	37.47	C
	ATOM	4423	O	SER	R	38	29.096	95.911	150.755	1.00	34.52	O
	ATOM	4425	N	ASN	R	39	31.221	95.817	149.998	1.00	40.27	N
	ATOM	4426	CA	ASN	R	39	30.860	95.366	148.651	1.00	41.01	C
	ATOM	4428	CB	ASN	R	39	30.486	93.875	148.686	1.00	44.45	C
20	ATOM	4431	CG	ASN	R	39	31.670	92.987	149.027	1.00	47.41	C
	ATOM	4432	OD1	ASN	R	39	32.530	92.735	148.182	1.00	51.95	O
	ATOM	4433	ND2	ASN	R	39	31.722	92.510	150.268	1.00	45.84	N
	ATOM	4436	C	ASN	R	39	29.727	96.196	148.025	1.00	41.85	C
	ATOM	4437	O	ASN	R	39	28.777	95.649	147.451	1.00	43.29	O
25	ATOM	4439	N	ASP	R	40	29.835	97.516	148.161	1.00	40.41	N
	ATOM	4440	CA	ASP	R	40	28.860	98.475	147.615	1.00	41.55	C
	ATOM	4442	CB	ASP	R	40	28.826	98.401	146.079	1.00	48.28	C
	ATOM	4445	CG	ASP	R	40	30.151	98.785	145.438	1.00	53.53	C
	ATOM	4446	OD1	ASP	R	40	30.987	99.439	146.100	1.00	56.57	O
30	ATOM	4447	OD2	ASP	R	40	30.348	98.444	144.251	1.00	59.35	O
	ATOM	4448	C	ASP	R	40	27.436	98.356	148.174	1.00	38.17	C
	ATOM	4449	O	ASP	R	40	26.471	98.685	147.488	1.00	38.74	O
	ATOM	4451	N	ARG	R	41	27.302	97.904	149.417	1.00	37.16	N
	ATOM	4452	CA	ARG	R	41	26.000	97.869	150.081	1.00	34.97	C
35	ATOM	4454	CB	ARG	R	41	25.182	96.659	149.612	1.00	37.69	C
	ATOM	4457	CG	ARG	R	41	25.683	95.311	150.106	1.00	36.81	C
	ATOM	4460	CD	ARG	R	41	24.910	94.184	149.448	1.00	38.16	C
	ATOM	4463	NE	ARG	R	41	25.298	92.871	149.966	1.00	37.15	N
	ATOM	4465	CZ	ARG	R	41	24.749	92.270	151.021	1.00	37.68	C
40	ATOM	4466	NH1	ARG	R	41	23.776	92.849	151.717	1.00	36.39	N
	ATOM	4469	NH2	ARG	R	41	25.186	91.075	151.391	1.00	37.68	N
	ATOM	4472	C	ARG	R	41	26.130	97.866	151.598	1.00	33.22	C
	ATOM	4473	O	ARG	R	41	27.238	97.797	152.144	1.00	28.29	O
	ATOM	4475	N	CYS	R	42	24.990	97.957	152.276	1.00	31.23	N
45	ATOM	4476	CA	CYS	R	42	24.958	97.939	153.731	1.00	33.69	C
	ATOM	4478	CB	CYS	R	42	23.982	98.989	154.251	1.00	35.92	C
	ATOM	4481	SG	CYS	R	42	24.452	100.661	153.756	1.00	38.34	S
	ATOM	4483	C	CYS	R	42	24.582	96.551	154.229	1.00	33.48	C
	ATOM	4484	O	CYS	R	42	23.430	96.146	154.149	1.00	31.75	O
50	ATOM	4486	N	CYS	R	43	25.571	95.821	154.734	1.00	32.23	N
	ATOM	4487	CA	CYS	R	43	25.347	94.466	155.217	1.00	31.50	C
	ATOM	4489	CB	CYS	R	43	26.625	93.643	155.087	1.00	33.21	C
	ATOM	4492	SG	CYS	R	43	27.180	93.422	153.366	1.00	35.12	S
	ATOM	4494	C	CYS	R	43	24.825	94.514	156.655	1.00	29.59	C
55	ATOM	4495	O	CYS	R	43	25.019	95.500	157.358	1.00	31.21	O
	ATOM	4497	N	HIS	R	44	24.140	93.457	157.077	1.00	32.52	N
	ATOM	4498	CA	HIS	R	44	23.461	93.440	158.368	1.00	31.47	C
	ATOM	4500	CB	HIS	R	44	22.077	92.812	158.221	1.00	36.17	C
	ATOM	4503	CG	HIS	R	44	21.191	93.552	157.268	1.00	36.62	C
60	ATOM	4504	ND1	HIS	R	44	20.285	94.503	157.681	1.00	41.14	N
	ATOM	4506	CE1	HIS	R	44	19.660	94.999	156.628	1.00	39.90	C
	ATOM	4508	NE2	HIS	R	44	20.139	94.414	155.545	1.00	39.22	N
	ATOM	4510	CD2	HIS	R	44	21.102	93.509	155.918	1.00	38.43	C
	ATOM	4512	C	HIS	R	44	24.267	92.713	159.434	1.00	28.73	C
65	ATOM	4513	O	HIS	R	44	24.907	91.709	159.162	1.00	31.01	O
	ATOM	4515	N	GLU	R	45	24.237	93.245	160.649	1.00	31.29	N
	ATOM	4516	CA	GLU	R	45	24.874	92.599	161.790	1.00	32.85	C
	ATOM	4518	CB	GLU	R	45	25.197	93.627	162.862	1.00	34.07	C
	ATOM	4521	CG	GLU	R	45	26.243	94.638	162.401	1.00	36.23	C
70	ATOM	4524	CD	GLU	R	45	26.469	95.761	163.388	1.00	38.00	C
	ATOM	4525	OE1	GLU	R	45	25.552	96.094	164.153	1.00	42.91	O
	ATOM	4526	OE2	GLU	R	45	27.570	96.332	163.386	1.00	49.67	O
	ATOM	4527	C	GLU	R	45	23.931	91.523	162.311	1.00	32.49	C
	ATOM	4528	O	GLU	R	45	22.776	91.466	161.902	1.00	33.12	O
	ATOM	4530	N	CYS	R	46	24.433	90.655	163.183	1.00	30.35	N

5	ATOM	4531	CA	CYS	R	46	23.642	89.541	163.700	1..00	33.51	C
	ATOM	4533	CB	CYS	R	46	24.561	88.392	164.120	1..00	34.70	C
	ATOM	4536	SG	CYS	R	46	25.551	87.714	162.761	1..00	37.69	S
	ATOM	4538	C	CYS	R	46	22.763	89.970	164.876	1..00	34.47	C
	ATOM	4539	O	CYS	R	46	23.211	90.698	165.753	1..00	37.61	O
10	ATOM	4541	N	ARG	R	47	21.518	89.502	164.882	1..00	33.33	N
	ATOM	4542	CA	ARG	R	47	20.566	89.806	165.947	1..00	36.56	C
	ATOM	4544	CB	ARG	R	47	19.155	89.391	165.529	1..00	40.56	C
	ATOM	4547	CG	ARG	R	47	18.625	90.019	164.241	1..00	45.79	C
	ATOM	4550	CD	ARG	R	47	17.216	89.491	163.939	1..00	49.44	C
15	ATOM	4553	NE	ARG	R	47	17.026	89.162	162.526	1..00	53.43	N
	ATOM	4555	CZ	ARG	R	47	16.643	90.018	161.579	1..00	56.07	C
	ATOM	4556	NH1	ARG	R	47	16.391	91.295	161.861	1..00	57.99	N
	ATOM	4559	NH2	ARG	R	47	16.512	89.591	160.326	1..00	57.41	N
	ATOM	4562	C	ARG	R	47	20.920	89.072	167.248	1..00	34.49	C
20	ATOM	4563	O	ARG	R	47	21.683	88.102	167.236	1..00	31.54	O
	ATOM	4565	N	PRO	R	48	20.348	89.522	168.381	1..00	35.95	N
	ATOM	4566	CA	PRO	R	48	20.495	88.774	169.630	1..00	33.16	C
	ATOM	4568	CB	PRO	R	48	19.507	89.478	170.568	1..00	34.82	C
	ATOM	4571	CG	PRO	R	48	19.479	90.886	170.064	1..00	35.62	C
25	ATOM	4574	CD	PRO	R	48	19.551	90.752	168.574	1..00	35.51	C
	ATOM	4577	C	PRO	R	48	20.138	87.298	169.466	1..00	30.90	C
	ATOM	4578	O	PRO	R	48	19.191	86.971	168.751	1..00	30.07	O
	ATOM	4579	N	GLY	R	49	20.893	86.420	170.119	1..00	28.21	N
	ATOM	4580	CA	GLY	R	49	20.691	84.978	169.995	1..00	29.71	C
30	ATOM	4583	C	GLY	R	49	21.464	84.319	168.867	1..00	30.51	C
	ATOM	4584	O	GLY	R	49	21.421	83.094	168.713	1..00	29.20	O
	ATOM	4586	N	ASN	R	50	22.143	85.141	168.070	1..00	30.48	N
	ATOM	4587	CA	ASN	R	50	23.013	84.698	166.987	1..00	29.74	C
	ATOM	4589	CB	ASN	R	50	22.533	85.232	165.630	1..00	29.26	C
35	ATOM	4592	CG	ASN	R	50	21.296	84.539	165.102	1..00	28.97	C
	ATOM	4593	OD1	ASN	R	50	21.000	83.389	165.431	1..00	28.47	O
	ATOM	4594	ND2	ASN	R	50	20.567	85.247	164.235	1..00	29.84	N
	ATOM	4597	C	ASN	R	50	24.416	85.239	167.207	1..00	30.15	C
	ATOM	4598	O	ASN	R	50	24.603	86.270	167.872	1..00	30.74	O
40	ATOM	4600	N	GLY	R	51	25.395	84.544	166.630	1..00	30.31	N
	ATOM	4601	CA	GLY	R	51	26.769	85.018	166.555	1..00	29.72	C
	ATOM	4604	C	GLY	R	51	27.240	85.102	165.115	1..00	29.68	C
	ATOM	4605	O	GLY	R	51	26.781	84.344	164.259	1..00	29.73	O
	ATOM	4607	N	MET	R	52	28.157	86.026	164.828	1..00	29.58	N
45	ATOM	4608	CA	MET	R	52	28.641	86.191	163.456	1..00	31.58	C
	ATOM	4610	CB	MET	R	52	29.138	87.618	163.166	1..00	32.45	C
	ATOM	4613	CG	MET	R	52	29.282	87.921	161.627	1..00	31.49	C
	ATOM	4616	SD	MET	R	52	29.766	89.608	161.254	1..00	38.14	S
	ATOM	4617	CE	MET	R	52	28.199	90.458	161.291	1..00	36.96	C
50	ATOM	4621	C	MET	R	52	29.738	85.176	163.150	1..00	31.29	C
	ATOM	4622	O	MET	R	52	30.729	85.044	163.888	1..00	30.38	O
	ATOM	4624	N	VAL	R	53	29.534	84.443	162.062	1..00	30.33	N
	ATOM	4625	CA	VAL	R	53	30.502	83.461	161.584	1..00	28.02	C
	ATOM	4627	CB	VAL	R	53	29.782	82.200	161.056	1..00	27.53	C
55	ATOM	4629	CG1	VAL	R	53	30.769	81.189	160.484	1..00	30.81	C
	ATOM	4633	CG2	VAL	R	53	28.948	81.562	162.171	1..00	31.04	C
	ATOM	4637	C	VAL	R	53	31.373	84.102	160.504	1..00	27.05	C
	ATOM	4638	O	VAL	R	53	32.594	83.917	160.480	1..00	27.90	O
	ATOM	4640	N	SER	R	54	30.750	84.861	159.608	1..00	27.21	N
60	ATOM	4641	CA	SER	R	54	31.496	85.538	158.547	1..00	25.29	C
	ATOM	4643	CB	SER	R	54	31.765	84.587	157.376	1..00	27.92	C
	ATOM	4646	OG	SER	R	54	30.563	84.038	156.859	1..00	28.05	O
	ATOM	4648	C	SER	R	54	30.764	86.763	158.045	1..00	28.58	C
	ATOM	4649	O	SER	R	54	29.541	86.755	157.910	1..00	28.69	O
65	ATOM	4651	N	ARG	R	55	31.521	87.818	157.761	1..00	29.09	N
	ATOM	4652	CA	ARG	R	55	30.963	89.014	157.143	1..00	26.28	C
	ATOM	4654	CB	ARG	R	55	31.944	90.172	157.236	1..00	27.77	C
	ATOM	4657	CG	ARG	R	55	32.141	90.668	158.657	1..00	30.02	C
	ATOM	4660	CD	ARG	R	55	32.594	92.065	158.635	1..00	28.05	C
70	ATOM	4663	NE	ARG	R	55	32.967	92.588	159.941	1..00	29.72	N
	ATOM	4665	CZ	ARG	R	55	32.216	93.380	160.705	1..00	27.14	C
	ATOM	4666	NH1	ARG	R	55	30.988	93.720	160.354	1..00	28.65	N
	ATOM	4669	NH2	ARG	R	55	32.703	93.824	161.854	1..00	25.33	N
	ATOM	4672	C	ARG	R	55	30.604	88.741	155.697	1..00	29.87	C
	ATOM	4673	O	ARG	R	55	31.092	87.781	155.100	1..00	31.83	O

5	ATOM	4675	N	CYS	R	56	29.728	89.577	155.144	1.00	29.35	N
	ATOM	4676	CA	CYS	R	56	29.326	89.455	153.755	1.00	29.68	C
	ATOM	4678	CB	CYS	R	56	28.263	90.513	153.389	1.00	31.88	C
	ATOM	4681	SG	CYS	R	56	28.858	92.233	153.470	1.00	37.15	S
	ATOM	4683	C	CYS	R	56	30.555	89.575	152.853	1.00	32.70	C
10	ATOM	4684	O	CYS	R	56	31.551	90.218	153.207	1.00	30.66	O
	ATOM	4686	N	SER	R	57	30.497	88.907	151.709	1.00	30.96	N
	ATOM	4687	CA	SER	R	57	31.517	89.043	150.677	1.00	33.44	C
	ATOM	4689	CB	SER	R	57	32.301	87.740	150.532	1.00	33.76	C
	ATOM	4692	OG	SER	R	57	31.528	86.758	149.855	1.00	32.09	O
15	ATOM	4694	C	SER	R	57	30.812	89.396	149.369	1.00	35.67	C
	ATOM	4695	O	SER	R	57	29.593	89.605	149.341	1.00	34.42	O
	ATOM	4697	N	ARG	R	58	31.577	89.474	148.290	1.00	34.86	N
	ATOM	4698	CA	ARG	R	58	31.010	89.749	146.975	1.00	37.51	C
	ATOM	4700	CB	ARG	R	58	32.118	89.970	145.933	1.00	43.12	C
20	ATOM	4703	CG	ARG	R	58	33.115	88.819	145.791	1.00	49.66	C
	ATOM	4706	CD	ARG	R	58	34.555	89.314	145.917	1.00	55.38	C
	ATOM	4709	NE	ARG	R	58	34.797	89.923	147.231	1.00	58.71	N
	ATOM	4711	CZ	ARG	R	58	35.092	89.260	148.350	1.00	56.44	C
	ATOM	4712	NH1	ARG	R	58	35.201	87.933	148.352	1.00	57.41	N
25	ATOM	4715	NH2	ARG	R	58	35.284	89.934	149.482	1.00	55.87	N
	ATOM	4718	C	ARG	R	58	30.041	88.648	146.523	1.00	35.92	C
	ATOM	4719	O	ARG	R	58	29.094	88.929	145.809	1.00	36.92	O
	ATOM	4721	N	SER	R	59	30.260	87.411	146.966	1.00	33.51	N
	ATOM	4722	CA	SER	R	59	29.434	86.287	146.527	1.00	36.40	C
30	ATOM	4724	CB	SER	R	59	30.325	85.191	145.944	1.00	38.81	C
	ATOM	4727	OG	SER	R	59	31.178	84.651	146.931	1.00	39.42	O
	ATOM	4729	C	SER	R	59	28.538	85.682	147.621	1.00	33.02	C
	ATOM	4730	O	SER	R	59	27.709	84.828	147.322	1.00	32.07	O
	ATOM	4732	N	GLN	R	60	28.689	86.127	148.866	1.00	32.27	N
35	ATOM	4733	CA	GLN	R	60	27.994	85.492	149.993	1.00	32.20	C
	ATOM	4735	CB	GLN	R	60	28.963	84.534	150.687	1.00	33.10	C
	ATOM	4738	CG	GLN	R	60	28.325	83.506	151.575	1.00	35.02	C
	ATOM	4741	CD	GLN	R	60	29.343	82.551	152.165	1.00	35.93	C
	ATOM	4742	OE1	GLN	R	60	29.443	81.401	151.742	1.00	40.27	O
40	ATOM	4743	NE2	GLN	R	60	30.110	83.027	153.141	1.00	29.84	N
	ATOM	4746	C	GLN	R	60	27.458	86.519	150.990	1.00	31.11	C
	ATOM	4747	O	GLN	R	60	28.160	87.468	151.343	1.00	30.64	O
	ATOM	4749	N	ASN	R	61	26.218	86.325	151.448	1.00	28.33	N
	ATOM	4750	CA	ASN	R	61	25.674	87.112	152.571	1.00	28.02	C
45	ATOM	4752	CB	ASN	R	61	24.195	86.779	152.814	1.00	25.78	C
	ATOM	4755	CG	ASN	R	61	23.267	87.323	151.728	1.00	26.40	C
	ATOM	4756	OD1	ASN	R	61	23.635	88.194	150.949	1.00	29.07	O
	ATOM	4757	ND2	ASN	R	61	22.051	86.819	151.697	1.00	25.95	N
	ATOM	4760	C	ASN	R	61	26.440	86.861	153.869	1.00	29.13	C
50	ATOM	4761	O	ASN	R	61	27.146	85.864	154.003	1.00	29.13	O
	ATOM	4763	N	THR	R	62	26.289	87.781	154.822	1.00	27.26	N
	ATOM	4764	CA	THR	R	62	26.685	87.562	156.205	1.00	29.13	C
	ATOM	4766	CB	THR	R	62	26.100	88.659	157.118	1.00	32.11	C
	ATOM	4768	OG1	THR	R	62	26.481	89.946	156.627	1.00	31.13	O
55	ATOM	4770	CG2	THR	R	62	26.574	88.497	158.555	1.00	31.30	C
	ATOM	4774	C	THR	R	62	26.145	86.224	156.693	1.00	28.13	C
	ATOM	4775	O	THR	R	62	24.999	85.877	156.407	1.00	26.55	O
	ATOM	4777	N	VAL	R	63	26.969	85.479	157.418	1.00	28.36	N
	ATOM	4778	CA	VAL	R	63	26.536	84.225	158.037	1.00	28.90	C
60	ATOM	4780	CB	VAL	R	63	27.490	83.053	157.700	1.00	29.70	C
	ATOM	4782	CG1	VAL	R	63	27.002	81.758	158.346	1.00	30.27	C
	ATOM	4786	CG2	VAL	R	63	27.622	82.901	156.207	1.00	31.20	C
	ATOM	4790	C	VAL	R	63	26.476	84.395	159.549	1.00	29.89	C
	ATOM	4791	O	VAL	R	63	27.499	84.628	160.196	1.00	26.01	O
65	ATOM	4793	N	CYS	R	64	25.266	84.277	160.091	1.00	29.40	N
	ATOM	4794	CA	CYS	R	64	24.992	84.305	161.525	1.00	33.15	C
	ATOM	4796	CB	CYS	R	64	23.872	85.307	161.844	1.00	34.63	C
	ATOM	4799	SG	CYS	R	64	24.209	87.037	161.387	1.00	38.55	S
	ATOM	4801	C	CYS	R	64	24.535	82.905	161.931	1.00	31.30	C
70	ATOM	4802	O	CYS	R	64	23.837	82.231	161.166	1.00	30.68	O
	ATOM	4804	N	ARG	R	65	24.921	82.468	163.123	1.00	32.20	N
	ATOM	4805	CA	ARG	R	65	24.578	81.126	163.612	1.00	34.89	C
	ATOM	4807	CB	ARG	R	65	25.832	80.256	163.648	1.00	39.55	C
	ATOM	4810	CG	ARG	R	65	25.607	78.811	164.036	1.00	42.23	C
	ATOM	4813	CD	ARG	R	65	26.917	78.014	164.131	1.00	48.78	C

	ATOM	4816	NE	ARG	R	65	26.647	76.566	164.149	1..00	52.41	N
	ATOM	4818	CZ	ARG	R	65	26.874	75.710	163.147	1..00	54.03	C
	ATOM	4819	NH1	ARG	R	65	27.420	76.104	161.997	1..00	56.08	N
	ATOM	4822	NH2	ARG	R	65	26.568	74.426	163.307	1..00	55.34	N
5	ATOM	4825	C	ARG	R	65	23.982	81.252	165.012	1..00	30.86	C
	ATOM	4826	O	ARG	R	65	24.441	82.085	165.794	1..00	31.67	O
	ATOM	4828	N	PRO	R	66	22.986	80.416	165.351	1..00	28.23	N
	ATOM	4829	CA	PRO	R	66	22.412	80.507	166.697	1..00	31.49	C
	ATOM	4831	CB	PRO	R	66	21.349	79.405	166.717	1..00	30.68	C
10	ATOM	4834	CG	PRO	R	66	21.157	78.988	165.344	1..00	31.07	C
	ATOM	4837	CD	PRO	R	66	22.357	79.347	164.553	1..00	28.62	C
	ATOM	4840	C	PRO	R	66	23.460	80.216	167.755	1..00	30.63	C
	ATOM	4841	O	PRO	R	66	24.316	79.371	167.533	1.00	32.34	O
	ATOM	4842	N	CYS	R	67	23.387	80.895	168.896	1.00	32.88	N
15	ATOM	4843	CA	CYS	R	67	24.317	80.630	169.985	1.00	34.81	C
	ATOM	4845	CB	CYS	R	67	24.110	81.610	171.140	1.00	34.33	C
	ATOM	4848	SG	CYS	R	67	24.385	83.324	170.714	1.00	36.42	S
	ATOM	4850	C	CYS	R	67	24.152	79.191	170.470	1.00	34.59	C
	ATOM	4851	O	CYS	R	67	23.033	78.718	170.680	1.00	36.19	O
20	ATOM	4853	N	GLY	R	68	25.274	78.499	170.625	1.00	36.01	N
	ATOM	4854	CA	GLY	R	68	25.265	77.120	171.099	1.00	38.18	C
	ATOM	4857	C	GLY	R	68	25.040	77.027	172.595	1.00	38.55	C
	ATOM	4858	O	GLY	R	68	24.996	78.052	173.287	1.00	35.06	O
	ATOM	4860	N	PRO	R	69	24.893	75.793	173.111	1.00	40.65	N
25	ATOM	4861	CA	PRO	R	69	24.681	75.597	174.547	1.00	39.03	C
	ATOM	4863	CB	PRO	R	69	24.688	74.070	174.704	1.00	41.74	C
	ATOM	4866	CG	PRO	R	69	24.354	73.537	173.355	1.00	43.58	C
	ATOM	4869	CD	PRO	R	69	24.910	74.516	172.371	1.00	43.21	C
	ATOM	4872	C	PRO	R	69	25.796	76.228	175.373	1.00	33.91	C
30	ATOM	4873	O	PRO	R	69	26.974	76.038	175.066	1.00	33.40	O
	ATOM	4874	N	GLY	R	70	25.423	76.991	176.391	1.00	35.04	N
	ATOM	4875	CA	GLY	R	70	26.398	77.686	177.239	1.00	35.67	C
	ATOM	4878	C	GLY	R	70	26.903	79.011	176.688	1.00	31.97	C
	ATOM	4879	O	GLY	R	70	27.821	79.601	177.253	1.00	31.94	O
35	ATOM	4881	N	PHE	R	71	26.297	79.494	175.602	1.00	31.75	N
	ATOM	4882	CA	PHE	R	71	26.686	80.767	174.986	1.00	33.00	C
	ATOM	4884	CB	PHE	R	71	27.453	80.537	173.674	1.00	34.75	C
	ATOM	4887	CG	PHE	R	71	28.827	79.957	173.865	1.00	33.67	C
	ATOM	4888	CD1	PHE	R	71	28.991	78.607	174.131	1.00	36.06	C
40	ATOM	4890	CE1	PHE	R	71	30.253	78.068	174.326	1.00	38.06	C
	ATOM	4892	CZ	PHE	R	71	31.375	78.884	174.243	1.00	38.56	C
	ATOM	4894	CE2	PHE	R	71	31.226	80.233	173.971	1.00	36.77	C
	ATOM	4896	CD2	PHE	R	71	29.956	80.761	173.782	1.00	36.48	C
	ATOM	4898	C	PHE	R	71	25.468	81.641	174.718	1.00	33.47	C
45	ATOM	4899	O	PHE	R	71	24.358	81.140	174.535	1.00	32.23	O
	ATOM	4901	N	TYR	R	72	25.691	82.952	174.691	1.00	30.53	N
	ATOM	4902	CA	TYR	R	72	24.621	83.925	174.509	1.00	32.63	C
	ATOM	4904	CB	TYR	R	72	24.071	84.381	175.873	1.00	33.63	C
	ATOM	4907	CG	TYR	R	72	24.929	85.427	176.533	1.00	32.43	C
50	ATOM	4908	CD1	TYR	R	72	26.109	85.080	177.187	1.00	32.28	C
	ATOM	4910	CE1	TYR	R	72	26.907	86.050	177.780	1.00	35.41	C
	ATOM	4912	CZ	TYR	R	72	26.532	87.375	177.707	1.00	33.52	C
	ATOM	4913	OH	TYR	R	72	27.311	88.359	178.273	1.00	35.08	O
	ATOM	4915	CE2	TYR	R	72	25.374	87.740	177.064	1.00	35.41	C
55	ATOM	4917	CD2	TYR	R	72	24.574	86.773	176.487	1.00	32.63	C
	ATOM	4919	C	TYR	R	72	25.100	85.143	173.725	1.00	31.76	C
	ATOM	4920	O	TYR	R	72	26.306	85.386	173.577	1.00	30.90	O
	ATOM	4922	N	ASN	R	73	24.130	85.884	173.208	1.00	35.11	N
	ATOM	4923	CA	ASN	R	73	24.365	87.176	172.593	1.00	34.31	C
60	ATOM	4925	CB	ASN	R	73	24.593	87.063	171.086	1.00	36.39	C
	ATOM	4928	CG	ASN	R	73	24.882	88.413	170.448	1.00	43.42	C
	ATOM	4929	OD1	ASN	R	73	25.695	89.175	170.977	1.00	53.93	O
	ATOM	4930	ND2	ASN	R	73	24.217	88.727	169.313	1.00	41.04	N
	ATOM	4933	C	ASN	R	73	23.159	88.047	172.845	1.00	31.14	C
65	ATOM	4934	O	ASN	R	73	22.094	87.808	172.272	1.00	31.98	O
	ATOM	4936	N	ASP	R	74	23.336	89.056	173.695	1.00	31.37	N
	ATOM	4937	CA	ASP	R	74	22.240	89.886	174.168	1.00	35.31	C
	ATOM	4939	CB	ASP	R	74	22.430	90.245	175.658	1.00	38.09	C
	ATOM	4942	CG	ASP	R	74	23.701	91.049	175.936	1.00	40.36	C
70	ATOM	4943	OD1	ASP	R	74	24.747	90.846	175.282	1.00	41.90	O
	ATOM	4944	OD2	ASP	R	74	23.652	91.885	176.850	1.00	47.32	O

5	ATOM	4945	C	ASP	R	74	21.972	91.143	173.336	1.00	35.25	C
	ATOM	4946	O	ASP	R	74	20.925	91.767	173.495	1.00	35.55	O
	ATOM	4948	N	VAL	R	75	22.892	91.505	172.447	1.00	33.35	N
	ATOM	4949	CA	VAL	R	75	22.710	92.683	171.591	1.00	37.93	C
	ATOM	4951	CB	VAL	R	75	23.590	93.873	172.069	1.00	41.35	C
10	ATOM	4953	CG1	VAL	R	75	23.129	94.357	173.430	1.00	44.63	C
	ATOM	4957	CG2	VAL	R	75	25.061	93.484	172.110	1.00	42.94	C
	ATOM	4961	C	VAL	R	75	23.044	92.385	170.135	1.00	36.68	C
	ATOM	4962	O	VAL	R	75	23.574	91.328	169.813	1.00	38.00	O
	ATOM	4964	N	VAL	R	76	22.739	93.333	169.256	1.00	37.93	N
15	ATOM	4965	CA	VAL	R	76	23.156	93.235	167.858	1.00	39.65	C
	ATOM	4967	CB	VAL	R	76	22.598	94.412	167.027	1.00	40.06	C
	ATOM	4969	CG1	VAL	R	76	23.256	94.493	165.672	1.00	41.55	C
	ATOM	4973	CG2	VAL	R	76	21.102	94.265	166.872	1.00	38.76	C
	ATOM	4977	C	VAL	R	76	24.683	93.208	167.839	1.00	39.10	C
20	ATOM	4978	O	VAL	R	76	25.319	93.976	168.553	1.00	38.21	O
	ATOM	4980	N	SER	R	77	25.268	92.320	167.034	1.00	39.48	N
	ATOM	4981	CA	SER	R	77	26.702	92.028	167.127	1.00	38.80	C
	ATOM	4983	CB	SER	R	77	26.912	90.898	168.144	1.00	43.02	C
	ATOM	4986	OG	SER	R	77	28.226	90.383	168.092	1.00	45.90	O
25	ATOM	4988	C	SER	R	77	27.355	91.626	165.803	1.00	36.62	C
	ATOM	4989	O	SER	R	77	26.701	91.090	164.906	1.00	34.04	O
	ATOM	4991	N	SER	R	78	28.659	91.875	165.713	1.00	31.97	N
	ATOM	4992	CA	SER	R	78	29.508	91.392	164.626	1.00	35.38	C
	ATOM	4994	CB	SER	R	78	30.191	92.572	163.927	1.00	40.76	C
30	ATOM	4997	OG	SER	R	78	29.260	93.326	163.181	1.00	46.19	O
	ATOM	4999	C	SER	R	78	30.568	90.430	165.166	1.00	33.73	C
	ATOM	5000	O	SER	R	78	31.628	90.260	164.563	1.00	35.83	O
	ATOM	5002	N	LYS	R	79	30.275	89.793	166.294	1.00	36.23	N
	ATOM	5003	CA	LYS	R	79	31.211	88.882	166.936	1.00	37.39	C
35	ATOM	5005	CB	LYS	R	79	31.814	89.533	168.194	1.00	39.80	C
	ATOM	5008	CG	LYS	R	79	32.760	90.692	167.882	1.00	41.39	C
	ATOM	5011	CD	LYS	R	79	33.318	91.357	169.147	1.00	43.07	C
	ATOM	5014	CE	LYS	R	79	34.464	92.318	168.818	1.00	41.96	C
	ATOM	5017	NZ	LYS	R	79	34.897	93.210	169.954	1.00	42.37	N
40	ATOM	5021	C	LYS	R	79	30.531	87.562	167.280	1.00	34.11	C
	ATOM	5022	O	LYS	R	79	29.305	87.479	167.298	1.00	33.57	O
	ATOM	5024	N	PRO	R	80	31.331	86.509	167.527	1.00	35.25	N
	ATOM	5025	CA	PRO	R	80	30.776	85.246	168.010	1.00	36.23	C
	ATOM	5027	CB	PRO	R	80	32.015	84.373	168.213	1.00	37.14	C
45	ATOM	5030	CG	PRO	R	80	33.055	84.974	167.328	1.00	39.47	C
	ATOM	5033	CD	PRO	R	80	32.792	86.428	167.330	1.00	37.86	C
	ATOM	5036	C	PRO	R	80	30.024	85.418	169.333	1.00	33.74	C
	ATOM	5037	O	PRO	R	80	30.226	86.405	170.033	1.00	30.78	O
	ATOM	5038	N	CYS	R	81	29.159	84.463	169.649	1.00	33.59	N
50	ATOM	5039	CA	CYS	R	81	28.438	84.443	170.923	1.00	35.45	C
	ATOM	5041	CB	CYS	R	81	27.456	83.273	170.957	1.00	37.81	C
	ATOM	5044	SG	CYS	R	81	26.159	83.356	169.692	1.00	39.04	S
	ATOM	5046	C	CYS	R	81	29.421	84.341	172.088	1.00	38.06	C
	ATOM	5047	O	CYS	R	81	30.541	83.870	171.912	1.00	38.03	O
55	ATOM	5049	N	LYS	R	82	28.997	84.811	173.264	1.00	34.71	N
	ATOM	5050	CA	LYS	R	82	29.849	84.883	174.450	1.00	34.60	C
	ATOM	5052	CB	LYS	R	82	29.660	86.228	175.148	1.00	36.54	C
	ATOM	5055	CG	LYS	R	82	29.931	87.434	174.278	1.00	39.68	C
	ATOM	5058	CD	LYS	R	82	29.614	88.730	175.017	1.00	43.55	C
60	ATOM	5061	CE	LYS	R	82	28.131	89.052	174.964	1.00	43.86	C
	ATOM	5064	NZ	LYS	R	82	27.823	90.344	175.657	1.00	42.03	N
	ATOM	5068	C	LYS	R	82	29.505	83.765	175.434	1.00	33.15	C
	ATOM	5069	O	LYS	R	82	28.357	83.357	175.520	1.00	30.25	O
	ATOM	5071	N	PRO	R	83	30.495	83.277	176.196	1.00	34.94	N
65	ATOM	5072	CA	PRO	R	83	30.161	82.222	177.138	1.00	33.35	C
	ATOM	5074	CB	PRO	R	83	31.522	81.699	177.606	1.00	37.58	C
	ATOM	5077	CG	PRO	R	83	32.521	82.701	177.201	1.00	39.69	C
	ATOM	5080	CD	PRO	R	83	31.911	83.675	176.259	1.00	38.22	C
	ATOM	5083	C	PRO	R	83	29.312	82.749	178.299	1.00	32.61	C
70	ATOM	5084	O	PRO	R	83	29.492	83.883	178.745	1.00	32.18	O
	ATOM	5085	N	CYS	R	84	28.366	81.942	178.761	1.00	31.26	N
	ATOM	5086	CA	CYS	R	84	27.512	82.343	179.876	1.00	32.99	C
	ATOM	5088	CB	CYS	R	84	26.368	81.357	180.045	1.00	36.52	C
	ATOM	5091	SG	CYS	R	84	25.289	81.326	178.581	1.00	43.19	S
	ATOM	5093	C	CYS	R	84	28.305	82.432	181.177	1.00	32.63	C

	ATOM	5094	O	CYS	R	84	29.269	81.699	181.377	1.00	29.51	O
	ATOM	5096	N	THR	R	85	27.871	83.328	182.056	1.00	30.21	N
	ATOM	5097	CA	THR	R	85	28.542	83.589	183.326	1.00	30.58	C
	ATOM	5099	CB	THR	R	85	28.244	85.034	183.784	1.00	32.58	C
5	ATOM	5101	OG1	THR	R	85	28.590	85.947	182.727	1.00	33.09	O
	ATOM	5103	CG2	THR	R	85	29.045	85.390	185.029	1.00	34.68	C
	ATOM	5107	C	THR	R	85	28.098	82.633	184.435	1.00	29.84	C
	ATOM	5108	O	THR	R	85	26.916	82.282	184.536	1.00	31.33	O
	ATOM	5110	N	TRP	R	86	29.048	82.234	185.273	1.00	31.33	N
10	ATOM	5111	CA	TRP	R	86	28.755	81.560	186.539	1.00	30.53	C
	ATOM	5113	CB	TRP	R	86	29.928	80.687	186.974	1.00	35.45	C
	ATOM	5116	CG	TRP	R	86	30.353	79.627	186.023	1.00	35.47	C
	ATOM	5117	CD1	TRP	R	86	31.394	79.682	185.155	1.00	36.03	C
	ATOM	5119	NE1	TRP	R	86	31.505	78.497	184.471	1.00	36.99	N
15	ATOM	5121	CE2	TRP	R	86	30.526	77.644	184.901	1.00	35.80	C
	ATOM	5122	CD2	TRP	R	86	29.779	78.325	185.884	1.00	35.33	C
	ATOM	5123	CE3	TRP	R	86	28.704	77.670	186.491	1.00	38.29	C
	ATOM	5125	CZ3	TRP	R	86	28.408	76.365	186.092	1.00	38.82	C
	ATOM	5127	CH2	TRP	R	86	29.167	75.720	185.102	1.00	37.07	C
20	ATOM	5129	CZ2	TRP	R	86	30.227	76.339	184.497	1.00	39.25	C
	ATOM	5131	C	TRP	R	86	28.551	82.601	187.635	1.00	28.82	C
	ATOM	5132	O	TRP	R	86	29.334	83.545	187.755	1.00	29.68	O
	ATOM	5134	N	CYS	R	87	27.538	82.406	188.472	1.00	31.45	N
	ATOM	5135	CA	CYS	R	87	27.371	83.250	189.653	1.00	30.36	C
25	ATOM	5137	CB	CYS	R	87	25.967	83.080	190.248	1.00	29.93	C
	ATOM	5140	SG	CYS	R	87	24.587	83.214	189.068	1.00	33.16	S
	ATOM	5142	C	CYS	R	87	28.442	82.892	190.698	1.00	29.84	C
	ATOM	5143	O	CYS	R	87	28.758	81.714	190.894	1.00	30.21	O
	ATOM	5145	N	ASN	R	88	28.999	83.902	191.363	1.00	32.19	N
30	ATOM	5146	CA	ASN	R	88	29.993	83.680	192.423	1.00	31.85	C
	ATOM	5148	CB	ASN	R	88	30.908	84.900	192.582	1.00	33.21	C
	ATOM	5151	CG	ASN	R	88	32.073	84.651	193.539	1.00	33.14	C
	ATOM	5152	OD1	ASN	R	88	32.122	83.640	194.249	1.00	37.17	O
	ATOM	5153	ND2	ASN	R	88	33.021	85.575	193.553	1.00	35.10	N
35	ATOM	5156	C	ASN	R	88	29.308	83.333	193.748	1.00	33.56	C
	ATOM	5157	O	ASN	R	88	29.074	84.205	194.596	1.00	33.85	O
	ATOM	5159	N	LEU	R	89	29.010	82.046	193.909	1.00	32.16	N
	ATOM	5160	CA	LEU	R	89	28.316	81.514	195.077	1.00	34.67	C
	ATOM	5162	CB	LEU	R	89	28.239	79.991	194.976	1.00	34.99	C
40	ATOM	5165	CG	LEU	R	89	27.400	79.261	196.026	1.00	33.60	C
	ATOM	5167	CD1	LEU	R	89	25.897	79.385	195.721	1.00	35.01	C
	ATOM	5171	CD2	LEU	R	89	27.812	77.794	196.095	1.00	34.74	C
	ATOM	5175	C	LEU	R	89	28.970	81.897	196.406	1.00	36.45	C
	ATOM	5176	O	LEU	R	89	28.287	82.344	197.326	1.00	36.03	O
45	ATOM	5178	N	ARG	R	90	30.286	81.719	196.498	1.00	39.08	N
	ATOM	5179	CA	ARG	R	90	31.030	81.998	197.736	1.00	41.48	C
	ATOM	5181	CB	ARG	R	90	32.503	81.600	197.584	1.00	47.97	C
	ATOM	5184	CG	ARG	R	90	32.752	80.097	197.415	1.00	50.87	C
	ATOM	5187	CD	ARG	R	90	34.176	79.843	196.895	1.00	52.39	C
50	ATOM	5190	NE	ARG	R	90	34.496	78.420	196.734	1.00	54.25	N
	ATOM	5192	CZ	ARG	R	90	34.223	77.680	195.656	1.00	56.23	C
	ATOM	5193	NH1	ARG	R	90	33.599	78.192	194.598	1.00	55.29	N
	ATOM	5196	NH2	ARG	R	90	34.573	76.397	195.641	1.00	57.44	N
	ATOM	5199	C	ARG	R	90	30.941	83.461	198.187	1.00	39.02	C
55	ATOM	5200	O	ARG	R	90	31.070	83.748	199.378	1.00	36.94	O
	ATOM	5202	N	SER	R	91	30.729	84.381	197.246	1.00	36.53	N
	ATOM	5203	CA	SER	R	91	30.575	85.801	197.582	1.00	34.97	C
	ATOM	5205	CB	SER	R	91	30.965	86.680	196.388	1.00	34.58	C
	ATOM	5208	OG	SER	R	91	29.942	86.723	195.406	1.00	32.03	O
60	ATOM	5210	C	SER	R	91	29.160	86.165	198.058	1.00	33.52	C
	ATOM	5211	O	SER	R	91	28.936	87.275	198.540	1.00	34.22	O
	ATOM	5213	N	GLY	R	92	28.214	85.239	197.922	1.00	34.38	N
	ATOM	5214	CA	GLY	R	92	26.822	85.482	198.299	1.00	33.58	C
	ATOM	5217	C	GLY	R	92	25.847	85.553	197.135	1.00	31.97	C
65	ATOM	5218	O	GLY	R	92	24.671	85.864	197.327	1.00	28.82	O
	ATOM	5220	N	SER	R	93	26.329	85.273	195.929	1.00	30.57	N
	ATOM	5221	CA	SER	R	93	25.482	85.267	194.747	1.00	31.84	C
	ATOM	5223	CB	SER	R	93	26.312	85.482	193.478	1.00	32.12	C
	ATOM	5226	OG	SER	R	93	25.476	85.572	192.346	1.00	30.24	O
70	ATOM	5228	C	SER	R	93	24.719	83.949	194.645	1.00	30.80	C
	ATOM	5229	O	SER	R	93	25.158	82.921	195.158	1.00	32.24	O

	ATOM	5231	N	GLU	R	94	23.562	84.001	193.999	1.00	28.20	N
	ATOM	5232	CA	GLU	R	94	22.786	82.804	193.709	1.00	28.68	C
	ATOM	5234	CB	GLU	R	94	21.715	82.594	194.791	1.00	28.68	C
5	ATOM	5237	CG	GLU	R	94	20.923	81.280	194.672	1.00	30.10	C
	ATOM	5240	CD	GLU	R	94	19.753	81.218	195.641	1.00	30.83	C
	ATOM	5241	OE1	GLU	R	94	19.957	80.879	196.827	1.00	30.39	O
	ATOM	5242	OE2	GLU	R	94	18.623	81.511	195.209	1.00	31.37	O
	ATOM	5243	C	GLU	R	94	22.152	82.948	192.327	1.00	29.45	C
10	ATOM	5244	O	GLU	R	94	21.613	83.999	191.988	1.00	27.09	O
	ATOM	5246	N	ARG	R	95	22.215	81.885	191.530	1.00	30.53	N
	ATOM	5247	CA	ARG	R	95	21.600	81.898	190.212	1.00	31.60	C
	ATOM	5249	CB	ARG	R	95	22.039	80.689	189.384	1.00	31.20	C
	ATOM	5252	CG	ARG	R	95	21.537	80.718	187.951	1.00	33.93	C
15	ATOM	5255	CD	ARG	R	95	22.149	79.597	187.136	1.00	36.84	C
	ATOM	5258	NE	ARG	R	95	21.421	78.348	187.290	1.00	41.45	N
	ATOM	5260	CZ	ARG	R	95	21.904	77.141	186.994	1.00	42.48	C
	ATOM	5261	NH1	ARG	R	95	23.143	76.985	186.542	1.00	46.37	N
	ATOM	5264	NH2	ARG	R	95	21.138	76.079	187.173	1.00	43.76	N
20	ATOM	5267	C	ARG	R	95	20.093	81.904	190.341	1.00	30.92	C
	ATOM	5268	O	ARG	R	95	19.521	81.055	191.022	1.00	29.45	O
	ATOM	5270	N	LYS	R	96	19.460	82.874	189.689	1.00	29.39	N
	ATOM	5271	CA	LYS	R	96	18.010	82.939	189.612	1.00	31.01	C
	ATOM	5273	CB	LYS	R	96	17.545	84.395	189.523	1.00	31.86	C
25	ATOM	5276	CG	LYS	R	96	16.039	84.572	189.540	1.00	33.38	C
	ATOM	5279	CD	LYS	R	96	15.659	86.037	189.609	1.00	33.79	C
	ATOM	5282	CE	LYS	R	96	14.153	86.207	189.562	1.00	35.74	C
	ATOM	5285	NZ	LYS	R	96	13.785	87.637	189.689	1.00	38.04	N
	ATOM	5289	C	LYS	R	96	17.529	82.162	188.397	1.00	30.86	C
30	ATOM	5290	O	LYS	R	96	16.619	81.335	188.509	1.00	32.68	O
	ATOM	5292	N	GLN	R	97	18.132	82.443	187.241	1.00	31.11	N
	ATOM	5293	CA	GLN	R	97	17.725	81.859	185.965	1.00	35.00	C
	ATOM	5295	CB	GLN	R	97	16.891	82.861	185.152	1.00	39.06	C
	ATOM	5298	CG	GLN	R	97	15.790	83.559	185.932	1.00	44.63	C
35	ATOM	5301	CD	GLN	R	97	15.034	84.575	185.094	1.00	47.48	C
	ATOM	5302	OE1	GLN	R	97	14.531	84.255	184.018	1.00	52.28	O
	ATOM	5303	NE2	GLN	R	97	14.949	85.810	185.589	1.00	51.58	N
	ATOM	5306	C	GLN	R	97	18.929	81.459	185.123	1.00	34.03	C
	ATOM	5307	O	GLN	R	97	19.935	82.177	185.077	1.00	29.98	O
40	ATOM	5309	N	LEU	R	98	18.798	80.330	184.428	1.00	33.04	N
	ATOM	5310	CA	LEU	R	98	19.792	79.884	183.454	1.00	34.97	C
	ATOM	5312	CB	LEU	R	98	19.383	78.541	182.840	1.00	39.35	C
	ATOM	5315	CG	LEU	R	98	19.609	77.284	183.679	1.00	44.11	C
	ATOM	5317	CD1	LEU	R	98	18.634	76.191	183.274	1.00	46.39	C
45	ATOM	5321	CD2	LEU	R	98	21.049	76.808	183.540	1.00	45.60	C
	ATOM	5325	C	LEU	R	98	19.942	80.895	182.323	1.00	31.37	C
	ATOM	5326	O	LEU	R	98	18.984	81.574	181.951	1.00	27.93	O
	ATOM	5328	N	CYS	R	99	21.144	80.982	181.767	1.00	30.66	N
	ATOM	5329	CA	CYS	R	99	21.353	81.772	180.565	1.00	31.87	C
50	ATOM	5331	CB	CYS	R	99	22.820	81.780	180.174	1.00	42.55	C
	ATOM	5334	SG	CYS	R	99	23.366	80.183	179.597	1.00	53.05	S
	ATOM	5336	C	CYS	R	99	20.547	81.206	179.404	1.00	33.99	C
	ATOM	5337	O	CYS	R	99	20.274	80.000	179.345	1.00	31.15	O
	ATOM	5339	N	THR	R	100	20.145	82.094	178.502	1.00	33.12	N
55	ATOM	5340	CA	THR	R	100	19.486	81.708	177.264	1.00	34.14	C
	ATOM	5342	CB	THR	R	100	18.064	82.308	177.153	1.00	35.64	C
	ATOM	5344	OG1	THR	R	100	18.154	83.714	176.907	1.00	33.56	O
	ATOM	5346	CG2	THR	R	100	17.259	82.061	178.425	1.00	39.29	C
	ATOM	5350	C	THR	R	100	20.348	82.217	176.110	1.00	29.99	C
60	ATOM	5351	O	THR	R	100	21.344	82.917	176.330	1.00	30.86	O
	ATOM	5353	N	ALA	R	101	19.948	81.896	174.884	1.00	32.24	N
	ATOM	5354	CA	ALA	R	101	20.658	82.375	173.693	1.00	31.73	C
	ATOM	5356	CB	ALA	R	101	20.008	81.824	172.427	1.00	34.95	C
	ATOM	5360	C	ALA	R	101	20.716	83.899	173.637	1.00	30.60	C
65	ATOM	5361	O	ALA	R	101	21.653	84.466	173.074	1.00	28.59	O
	ATOM	5363	N	THR	R	102	19.724	84.558	174.235	1.00	31.23	N
	ATOM	5364	CA	THR	R	102	19.596	86.011	174.174	1.00	30.59	C
	ATOM	5366	CB	THR	R	102	18.181	86.417	173.728	1.00	32.66	C
	ATOM	5368	OG1	THR	R	102	17.199	85.842	174.607	1.00	32.09	O
70	ATOM	5370	CG2	THR	R	102	17.917	85.947	172.313	1.00	34.21	C
	ATOM	5374	C	THR	R	102	19.924	86.727	175.487	1.00	31.72	C
	ATOM	5375	O	THR	R	102	19.893	87.948	175.544	1.00	30.88	O

5	ATOM	5377	N	GLN	R	103	20.263	85.981	176.532	1.00	34.68	N
	ATOM	5378	CA	GLN	R	103	20.408	86.572	177.855	1.00	34.55	C
	ATOM	5380	CB	GLN	R	103	19.041	86.627	178.548	1.00	37.38	C
	ATOM	5383	CG	GLN	R	103	18.986	87.556	179.744	1.00	42.14	C
	ATOM	5386	CD	GLN	R	103	17.573	87.757	180.270	1.00	46.68	C
10	ATOM	5387	OE1	GLN	R	103	16.780	86.809	180.357	1.00	50.40	O
	ATOM	5388	NE2	GLN	R	103	17.252	88.996	180.630	1.00	52.65	N
	ATOM	5391	C	GLN	R	103	21.394	85.785	178.698	1.00	32.00	C
	ATOM	5392	O	GLN	R	103	21.285	84.569	178.825	1.00	34.25	O
	ATOM	5394	N	ASP	R	104	22.359	86.488	179.279	1.00	32.62	N
15	ATOM	5395	CA	ASP	R	104	23.301	85.868	180.197	1.00	31.86	C
	ATOM	5397	CB	ASP	R	104	24.370	86.879	180.608	1.00	34.62	C
	ATOM	5400	CG	ASP	R	104	25.624	86.230	181.141	1.00	31.61	C
	ATOM	5401	OD1	ASP	R	104	25.742	84.980	181.117	1.00	32.26	O
	ATOM	5402	OD2	ASP	R	104	26.501	86.987	181.591	1.00	34.77	O
20	ATOM	5403	C	ASP	R	104	22.561	85.344	181.436	1.00	30.54	C
	ATOM	5404	O	ASP	R	104	21.425	85.727	181.705	1.00	28.69	O
	ATOM	5406	N	THR	R	105	23.220	84.453	182.165	1.00	30.75	N
	ATOM	5407	CA	THR	R	105	22.802	84.027	183.503	1.00	31.10	C
	ATOM	5409	CB	THR	R	105	24.009	83.395	184.222	1.00	29.90	C
25	ATOM	5411	OG1	THR	R	105	24.649	82.469	183.336	1.00	29.15	O
	ATOM	5413	CG2	THR	R	105	23.603	82.695	185.483	1.00	30.64	C
	ATOM	5417	C	THR	R	105	22.296	85.187	184.361	1.00	29.39	C
	ATOM	5418	O	THR	R	105	22.909	86.255	184.395	1.00	29.12	O
	ATOM	5420	N	VAL	R	106	21.175	84.978	185.055	1.00	28.36	N
30	ATOM	5421	CA	VAL	R	106	20.680	85.958	186.009	1.00	30.23	C
	ATOM	5423	CB	VAL	R	106	19.147	86.100	185.962	1.00	32.86	C
	ATOM	5425	CG1	VAL	R	106	18.680	87.183	186.937	1.00	34.77	C
	ATOM	5429	CG2	VAL	R	106	18.692	86.420	184.545	1.00	35.80	C
	ATOM	5433	C	VAL	R	106	21.137	85.538	187.404	1.00	31.04	C
35	ATOM	5434	O	VAL	R	106	20.771	84.467	187.883	1.00	28.66	O
	ATOM	5436	N	CYS	R	107	21.952	86.390	188.025	1.00	29.71	N
	ATOM	5437	CA	CYS	R	107	22.520	86.161	189.352	1.00	31.37	C
	ATOM	5439	CB	CYS	R	107	24.044	86.200	189.289	1.00	32.45	C
	ATOM	5442	SG	CYS	R	107	24.809	85.034	188.154	1.00	33.53	S
40	ATOM	5444	C	CYS	R	107	22.066	87.275	190.278	1.00	32.20	C
	ATOM	5445	O	CYS	R	107	22.016	88.433	189.869	1.00	31.22	O
	ATOM	5447	N	ARG	R	108	21.757	86.933	191.524	1.00	31.12	N
	ATOM	5448	CA	ARG	R	108	21.321	87.932	192.508	1.00	31.59	C
	ATOM	5450	CB	ARG	R	108	19.819	87.823	192.742	1.00	29.80	C
45	ATOM	5453	CG	ARG	R	108	18.969	88.126	191.518	1.00	31.23	C
	ATOM	5456	CD	ARG	R	108	18.974	89.596	191.172	1.00	32.30	C
	ATOM	5459	NE	ARG	R	108	18.115	89.884	190.028	1.00	31.10	N
	ATOM	5461	CZ	ARG	R	108	18.530	90.129	188.782	1.00	36.67	C
	ATOM	5462	NH1	ARG	R	108	19.827	90.146	188.459	1.00	36.87	N
50	ATOM	5465	NH2	ARG	R	108	17.625	90.374	187.839	1.00	39.52	N
	ATOM	5468	C	ARG	R	108	22.063	87.791	193.828	1.00	29.67	C
	ATOM	5469	O	ARG	R	108	22.314	86.685	194.297	1.00	29.04	O
	ATOM	5471	N	CYS	R	109	22.402	88.925	194.430	1.00	30.97	N
	ATOM	5472	CA	CYS	R	109	23.082	88.936	195.716	1.00	33.71	C
55	ATOM	5474	CB	CYS	R	109	23.827	90.261	195.915	1.00	33.71	C
	ATOM	5477	SG	CYS	R	109	25.179	90.492	194.745	1.00	36.63	S
	ATOM	5479	C	CYS	R	109	22.079	88.685	196.848	1.00	34.61	C
	ATOM	5480	O	CYS	R	109	20.978	89.241	196.852	1.00	36.09	O
	ATOM	5482	N	ARG	R	110	22.465	87.818	197.783	1.00	34.30	N
60	ATOM	5483	CA	ARG	R	110	21.628	87.475	198.940	1.00	36.90	C
	ATOM	5485	CB	ARG	R	110	22.131	86.187	199.616	1.00	38.35	C
	ATOM	5488	CG	ARG	R	110	23.456	86.323	200.363	1.00	38.87	C
	ATOM	5491	CD	ARG	R	110	23.868	85.038	201.086	1.00	42.34	C
	ATOM	5494	NE	ARG	R	110	24.918	85.330	202.067	1.00	44.29	N
65	ATOM	5496	CZ	ARG	R	110	26.151	84.813	202.098	1.00	47.50	C
	ATOM	5497	NH1	ARG	R	110	26.565	83.903	201.217	1.00	47.46	N
	ATOM	5500	NH2	ARG	R	110	26.987	85.205	203.054	1.00	49.10	N
	ATOM	5503	C	ARG	R	110	21.600	88.613	199.952	1.00	35.72	C
	ATOM	5504	O	ARG	R	110	22.377	89.578	199.851	1.00	33.85	O
70	ATOM	5506	N	ALA	R	111	20.709	88.492	200.935	1.00	34.36	N
	ATOM	5507	CA	ALA	R	111	20.631	89.457	202.029	1.00	34.82	C
	ATOM	5509	CB	ALA	R	111	19.518	89.069	203.018	1.00	34.10	C
	ATOM	5513	C	ALA	R	111	21.969	89.563	202.755	1.00	33.97	C
	ATOM	5514	O	ALA	R	111	22.663	88.565	202.948	1.00	32.06	O
	ATOM	5516	N	GLY	R	112	22.321	90.783	203.153	1.00	33.85	N

	ATOM	5517	CA	GLY	R	112	23.601	91.047	203.801	1.00	34.14	C
	ATOM	5520	C	GLY	R	112	24.734	91.341	202.838	1.00	33.66	C
	ATOM	5521	O	GLY	R	112	25.848	91.648	203.271	1.00	34.08	O
5	ATOM	5523	N	THR	R	113	24.463	91.241	201.536	1.00	34.60	N
	ATOM	5524	CA	THR	R	113	25.455	91.534	200.507	1.00	34.09	C
	ATOM	5526	CB	THR	R	113	26.033	90.241	199.870	1.00	35.49	C
	ATOM	5528	OG1	THR	R	113	25.050	89.613	199.038	1.00	36.76	O
	ATOM	5530	CG2	THR	R	113	26.479	89.256	200.948	1.00	33.94	C
10	ATOM	5534	C	THR	R	113	24.852	92.422	199.422	1.00	33.73	C
	ATOM	5535	O	THR	R	113	23.630	92.542	199.315	1.00	33.16	O
	ATOM	5537	N	GLN	R	114	25.722	93.059	198.638	1.00	34.70	N
	ATOM	5538	CA	GLN	R	114	25.304	93.900	197.518	1.00	34.29	C
	ATOM	5540	CB	GLN	R	114	25.336	95.379	197.914	1.00	33.57	C
15	ATOM	5543	CG	GLN	R	114	26.724	95.890	198.293	1.00	33.79	C
	ATOM	5546	CD	GLN	R	114	26.770	97.389	198.512	1.00	36.08	C
	ATOM	5547	OE1	GLN	R	114	25.819	98.110	198.192	1.00	37.47	O
	ATOM	5548	NE2	GLN	R	114	27.882	97.868	199.067	1.00	34.57	N
	ATOM	5551	C	GLN	R	114	26.217	93.672	196.310	1.00	34.87	C
20	ATOM	5552	O	GLN	R	114	27.356	93.225	196.474	1.00	35.45	O
	ATOM	5554	N	PRO	R	115	25.726	93.986	195.096	1.00	34.42	N
	ATOM	5555	CA	PRO	R	115	26.553	93.834	193.894	1.00	36.54	C
	ATOM	5557	CB	PRO	R	115	25.613	94.271	192.760	1.00	36.34	C
	ATOM	5560	CG	PRO	R	115	24.247	94.168	193.318	1.00	36.76	C
25	ATOM	5563	CD	PRO	R	115	24.380	94.487	194.768	1.00	34.77	C
	ATOM	5566	C	PRO	R	115	27.808	94.712	193.902	1.00	36.97	C
	ATOM	5567	O	PRO	R	115	27.755	95.868	194.333	1.00	36.24	O
	ATOM	5568	N	LEU	R	116	28.921	94.155	193.431	1.00	39.67	N
	ATOM	5569	CA	LEU	R	116	30.180	94.897	193.267	1.00	42.63	C
30	ATOM	5571	CB	LEU	R	116	31.372	93.928	193.214	1.00	43.90	C
	ATOM	5574	CG	LEU	R	116	31.930	93.472	194.567	1.00	45.30	C
	ATOM	5576	CD1	LEU	R	116	32.553	92.086	194.480	1.00	46.21	C
	ATOM	5580	CD2	LEU	R	116	32.945	94.478	195.094	1.00	46.55	C
	ATOM	5584	C	LEU	R	116	30.208	95.796	192.020	1.00	44.97	C
35	ATOM	5585	O	LEU	R	116	30.871	96.840	192.028	1.00	43.90	O
	ATOM	5587	N	ASP	R	117	29.507	95.394	190.958	1.00	47.08	N
	ATOM	5588	CA	ASP	R	117	29.596	96.082	189.658	1.00	46.73	C
	ATOM	5590	CB	ASP	R	117	30.413	95.225	188.676	1.00	51.87	C
	ATOM	5593	CG	ASP	R	117	31.034	96.038	187.543	1.00	53.86	C
40	ATOM	5594	OD1	ASP	R	117	30.803	97.265	187.465	1.00	58.67	O
	ATOM	5595	OD2	ASP	R	117	31.767	95.445	186.719	1.00	59.45	O
	ATOM	5596	C	ASP	R	117	28.217	96.375	189.061	1.00	46.50	C
	ATOM	5597	O	ASP	R	117	27.221	95.742	189.428	1.00	46.99	O
	ATOM	5599	N	SER	R	118	28.173	97.334	188.136	1.00	41.41	N
45	ATOM	5600	CA	SER	R	118	26.935	97.710	187.447	1.00	41.35	C
	ATOM	5602	CB	SER	R	118	26.858	99.232	187.300	1.00	42.18	C
	ATOM	5605	OG	SER	R	118	28.024	99.750	186.683	1.00	42.35	O
	ATOM	5607	C	SER	R	118	26.768	97.050	186.070	1.00	40.03	C
	ATOM	5608	O	SER	R	118	25.680	97.095	185.496	1.00	39.62	O
50	ATOM	5610	N	TYR	R	119	27.827	96.436	185.544	1.00	39.79	N
	ATOM	5611	CA	TYR	R	119	27.783	95.851	184.192	1.00	38.77	C
	ATOM	5613	CB	TYR	R	119	29.185	95.761	183.584	1.00	36.43	C
	ATOM	5616	CG	TYR	R	119	29.701	97.088	183.091	1.00	35.89	C
	ATOM	5617	CD1	TYR	R	119	29.448	97.518	181.789	1.00	35.65	C
55	ATOM	5619	CE1	TYR	R	119	29.920	98.744	181.333	1.00	35.02	C
	ATOM	5621	CZ	TYR	R	119	30.651	99.553	182.187	1.00	35.42	C
	ATOM	5622	OH	TYR	R	119	31.129	100.770	181.750	1.00	35.96	O
	ATOM	5624	CE2	TYR	R	119	30.910	99.145	183.485	1.00	35.55	C
	ATOM	5626	CD2	TYR	R	119	30.436	97.921	183.928	1.00	36.16	C
60	ATOM	5628	C	TYR	R	119	27.121	94.482	184.172	1.00	39.46	C
	ATOM	5629	O	TYR	R	119	26.368	94.168	183.247	1.00	40.37	O
	ATOM	5631	N	LYS	R	120	27.423	93.668	185.180	1.00	37.87	N
	ATOM	5632	CA	LYS	R	120	26.752	92.386	185.380	1.00	38.93	C
	ATOM	5634	CB	LYS	R	120	27.667	91.228	184.980	1.00	40.07	C
65	ATOM	5637	CG	LYS	R	120	27.982	91.187	183.491	1.00	40.92	C
	ATOM	5640	CD	LYS	R	120	28.148	89.758	182.992	1.00	41.07	C
	ATOM	5643	CE	LYS	R	120	28.199	89.694	181.475	1.00	40.99	C
	ATOM	5646	NZ	LYS	R	120	26.841	89.625	180.866	1.00	41.79	N
	ATOM	5650	C	LYS	R	120	26.350	92.275	186.844	1.00	37.40	C
70	ATOM	5651	O	LYS	R	120	26.941	91.496	187.594	1.00	39.96	O
	ATOM	5653	N	PRO	R	121	25.343	93.065	187.260	1.00	37.59	N
	ATOM	5654	CA	PRO	R	121	25.026	93.137	188.687	1.00	35.09	C

	ATOM	5656	CB	PRO	R	121	23.927	94.209	188.778	1.00	36.47	C
	ATOM	5659	CG	PRO	R	121	23.677	94.698	187.412	1.00	38.26	C
	ATOM	5662	CD	PRO	R	121	24.449	93.893	186.431	1.00	37.76	C
5	ATOM	5665	C	PRO	R	121	24.531	91.811	189.240	1.00	33.21	C
	ATOM	5666	O	PRO	R	121	23.612	91.209	188.680	1.00	35.26	O
	ATOM	5667	N	GLY	R	122	25.156	91.352	190.320	1.00	33.34	N
	ATOM	5668	CA	GLY	R	122	24.719	90.144	191.017	1.00	33.71	C
	ATOM	5671	C	GLY	R	122	25.664	88.967	190.910	1.00	33.45	C
10	ATOM	5672	O	GLY	R	122	25.599	88.046	191.724	1.00	34.39	O
	ATOM	5674	N	VAL	R	123	26.538	88.983	189.904	1.00	31.72	N
	ATOM	5675	CA	VAL	R	123	27.501	87.900	189.708	1.00	32.92	C
	ATOM	5677	CB	VAL	R	123	28.280	88.061	188.389	1.00	30.25	C
	ATOM	5679	CG1	VAL	R	123	29.405	87.031	188.280	1.00	31.28	C
15	ATOM	5683	CG2	VAL	R	123	27.331	87.944	187.205	1.00	31.97	C
	ATOM	5687	C	VAL	R	123	28.462	87.823	190.892	1.00	33.11	C
	ATOM	5688	O	VAL	R	123	28.625	86.761	191.499	1.00	30.44	O
	ATOM	5690	N	ASP	R	124	29.090	88.955	191.201	1.00	34.58	N
	ATOM	5691	CA	ASP	R	124	29.994	89.089	192.336	1.00	36.79	C
20	ATOM	5693	CB	ASP	R	124	31.327	89.723	191.920	1.00	38.94	C
	ATOM	5696	CG	ASP	R	124	32.078	88.915	190.876	1.00	43.88	C
	ATOM	5697	OD1	ASP	R	124	32.304	87.705	191.081	1.00	45.60	O
	ATOM	5698	OD2	ASP	R	124	32.475	89.513	189.855	1.00	47.12	O
	ATOM	5699	C	ASP	R	124	29.331	90.001	193.358	1.00	34.55	C
25	ATOM	5700	O	ASP	R	124	28.842	91.082	193.011	1.00	32.54	O
	ATOM	5702	N	CYS	R	125	29.331	89.565	194.613	1.00	35.07	N
	ATOM	5703	CA	CYS	R	125	28.716	90.319	195.699	1.00	34.81	C
	ATOM	5705	CB	CYS	R	125	27.569	89.507	196.297	1.00	33.47	C
	ATOM	5708	SG	CYS	R	125	26.399	88.909	195.059	1.00	33.91	S
30	ATOM	5710	C	CYS	R	125	29.735	90.661	196.783	1.00	33.70	C
	ATOM	5711	O	CYS	R	125	30.794	90.046	196.862	1.00	32.65	O
	ATOM	5713	N	ALA	R	126	29.403	91.649	197.610	1.00	35.35	N
	ATOM	5714	CA	ALA	R	126	30.257	92.051	198.732	1.00	36.56	C
	ATOM	5716	CB	ALA	R	126	31.052	93.289	198.371	1.00	37.14	C
35	ATOM	5720	C	ALA	R	126	29.403	92.313	199.973	1.00	37.30	C
	ATOM	5721	O	ALA	R	126	28.288	92.823	199.848	1.00	37.10	O
	ATOM	5723	N	PRO	R	127	29.921	91.975	201.174	1.00	37.98	N
	ATOM	5724	CA	PRO	R	127	29.147	92.219	202.392	1.00	38.60	C
	ATOM	5726	CB	PRO	R	127	30.081	91.731	203.514	1.00	39.67	C
40	ATOM	5729	CG	PRO	R	127	31.055	90.831	202.858	1.00	40.45	C
	ATOM	5732	CD	PRO	R	127	31.233	91.370	201.474	1.00	39.31	C
	ATOM	5735	C	PRO	R	127	28.836	93.701	202.587	1.00	37.68	C
	ATOM	5736	O	PRO	R	127	29.652	94.553	202.216	1.00	37.62	O
	ATOM	5737	N	CYS	R	128	27.671	94.007	203.155	1.00	35.33	N
45	ATOM	5738	CA	CYS	R	128	27.347	95.391	203.504	1.00	38.24	C
	ATOM	5740	CB	CYS	R	128	25.974	95.502	204.183	1.00	39.95	C
	ATOM	5743	SG	CYS	R	128	24.532	95.413	203.077	1.00	42.04	S
	ATOM	5745	C	CYS	R	128	28.429	95.927	204.438	1.00	36.38	C
	ATOM	5746	O	CYS	R	128	28.931	95.185	205.285	1.00	36.04	O
50	ATOM	5748	N	PRO	R	129	28.815	97.206	204.271	1.00	37.38	N
	ATOM	5749	CA	PRO	R	129	29.808	97.812	205.158	1.00	38.38	C
	ATOM	5751	CB	PRO	R	129	30.158	99.131	204.455	1.00	38.85	C
	ATOM	5754	CG	PRO	R	129	28.993	99.443	203.600	1.00	38.50	C
	ATOM	5757	CD	PRO	R	129	28.339	98.146	203.238	1.00	38.66	C
55	ATOM	5760	C	PRO	R	129	29.218	98.061	206.548	1.00	39.28	C
	ATOM	5761	O	PRO	R	129	28.021	97.828	206.742	1.00	38.85	O
	ATOM	5762	N	PRO	R	130	30.048	98.512	207.513	1.00	39.28	N
	ATOM	5763	CA	PRO	R	130	29.552	98.802	208.861	1.00	39.71	C
	ATOM	5765	CB	PRO	R	130	30.751	99.478	209.544	1.00	38.66	C
60	ATOM	5768	CG	PRO	R	130	31.937	98.982	208.814	1.00	39.18	C
	ATOM	5771	CD	PRO	R	130	31.499	98.762	207.397	1.00	39.87	C
	ATOM	5774	C	PRO	R	130	28.343	99.742	208.863	1.00	40.99	C
	ATOM	5775	O	PRO	R	130	28.358	100.765	208.176	1.00	44.25	O
	ATOM	5776	N	GLY	R	131	27.307	99.383	209.619	1.00	38.86	N
65	ATOM	5777	CA	GLY	R	131	26.138	100.245	209.788	1.00	36.80	C
	ATOM	5780	C	GLY	R	131	25.198	100.310	208.603	1.00	35.88	C
	ATOM	5781	O	GLY	R	131	24.395	101.241	208.498	1.00	35.38	O
	ATOM	5783	N	HIS	R	132	25.285	99.321	207.721	1.00	35.26	N
	ATOM	5784	CA	HIS	R	132	24.432	99.260	206.538	1.00	36.04	C
70	ATOM	5786	CB	HIS	R	132	25.272	99.481	205.274	1.00	36.55	C
	ATOM	5789	CG	HIS	R	132	25.841	100.862	205.169	1.00	38.37	C
	ATOM	5790	ND1	HIS	R	132	26.854	101.315	205.988	1.00	39.83	N

	ATOM	5792	CE1	HIS	R	132	27.143	102.566	205.677	1.00	40.38	C
	ATOM	5794	NE2	HIS	R	132	26.352	102.943	204.689	1.00	40.89	N
	ATOM	5796	CD2	HIS	R	132	25.526	101.897	204.354	1.00	39.73	C
5	ATOM	5798	C	HIS	R	132	23.685	97.932	206.476	1.00	34.75	C
	ATOM	5799	O	HIS	R	132	24.119	96.939	207.076	1.00	34.24	O
	ATOM	5801	N	PHE	R	133	22.546	97.941	205.775	1.00	35.10	N
	ATOM	5802	CA	PHE	R	133	21.748	96.734	205.538	1.00	35.58	C
	ATOM	5804	CB	PHE	R	133	20.478	96.745	206.403	1.00	35.67	C
10	ATOM	5807	CG	PHE	R	133	19.386	97.640	205.874	1.00	35.68	C
	ATOM	5808	CD1	PHE	R	133	19.420	99.012	206.105	1.00	36.17	C
	ATOM	5810	CE1	PHE	R	133	18.416	99.843	205.618	1.00	35.65	C
	ATOM	5812	CZ	PHE	R	133	17.366	99.303	204.889	1.00	36.03	C
	ATOM	5814	CE2	PHE	R	133	17.320	97.937	204.654	1.00	35.75	C
15	ATOM	5816	CD2	PHE	R	133	18.328	97.113	205.144	1.00	35.77	C
	ATOM	5818	C	PHE	R	133	21.345	96.601	204.071	1.00	34.57	C
	ATOM	5819	O	PHE	R	133	21.178	97.599	203.364	1.00	31.08	O
	ATOM	5821	N	SER	R	134	21.174	95.356	203.631	1.00	34.02	N
	ATOM	5822	CA	SER	R	134	20.526	95.066	202.360	1.00	35.43	C
20	ATOM	5824	CB	SER	R	134	21.561	94.850	201.255	1.00	35.12	C
	ATOM	5827	OG	SER	R	134	20.925	94.484	200.040	1.00	36.26	O
	ATOM	5829	C	SER	R	134	19.653	93.820	202.503	1.00	34.91	C
	ATOM	5830	O	SER	R	134	20.082	92.840	203.110	1.00	33.90	O
	ATOM	5832	N	PRO	R	135	18.430	93.847	201.937	1.00	36.45	N
25	ATOM	5833	CA	PRO	R	135	17.590	92.645	201.943	1.00	37.13	C
	ATOM	5835	CB	PRO	R	135	16.175	93.187	201.684	1.00	39.77	C
	ATOM	5838	CG	PRO	R	135	16.333	94.619	201.287	1.00	40.31	C
	ATOM	5841	CD	PRO	R	135	17.778	94.974	201.247	1.00	37.77	C
	ATOM	5844	C	PRO	R	135	17.968	91.627	200.863	1.00	37.11	C
30	ATOM	5845	O	PRO	R	135	17.358	90.560	200.786	1.00	36.05	O
	ATOM	5846	N	GLY	R	136	18.962	91.953	200.040	1.00	37.34	N
	ATOM	5847	CA	GLY	R	136	19.370	91.085	198.940	1.00	37.25	C
	ATOM	5850	C	GLY	R	136	18.628	91.440	197.667	1.00	37.44	C
	ATOM	5851	O	GLY	R	136	18.162	92.573	197.507	1.00	34.77	O
35	ATOM	5853	N	ASP	R	137	18.526	90.461	196.764	1.00	37.68	N
	ATOM	5854	CA	ASP	R	137	17.913	90.642	195.440	1.00	36.12	C
	ATOM	5856	CB	ASP	R	137	16.393	90.817	195.557	1.00	36.83	C
	ATOM	5859	CG	ASP	R	137	15.668	90.564	194.236	1.00	39.67	C
	ATOM	5860	OD1	ASP	R	137	16.147	89.733	193.433	1.00	39.04	O
40	ATOM	5861	OD2	ASP	R	137	14.616	91.197	194.000	1.00	41.55	O
	ATOM	5862	C	ASP	R	137	18.532	91.814	194.664	1.00	33.91	C
	ATOM	5863	O	ASP	R	137	17.844	92.508	193.913	1.00	33.24	O
	ATOM	5865	N	ASN	R	138	19.837	92.004	194.849	1.00	34.54	N
	ATOM	5866	CA	ASN	R	138	20.613	93.076	194.208	1.00	34.80	C
45	ATOM	5868	CB	ASN	R	138	20.511	93.007	192.667	1.00	33.64	C
	ATOM	5871	CG	ASN	R	138	21.447	91.982	192.058	1.00	32.16	C
	ATOM	5872	OD1	ASN	R	138	22.085	91.199	192.761	1.00	31.59	O
	ATOM	5873	ND2	ASN	R	138	21.539	91.991	190.736	1.00	32.02	N
	ATOM	5876	C	ASN	R	138	20.304	94.497	194.695	1.00	35.01	C
50	ATOM	5877	O	ASN	R	138	20.709	95.467	194.057	1.00	32.65	O
	ATOM	5879	N	GLN	R	139	19.610	94.633	195.822	1.00	35.28	N
	ATOM	5880	CA	GLN	R	139	19.386	95.958	196.397	1.00	36.66	C
	ATOM	5882	CB	GLN	R	139	18.236	95.950	197.411	1.00	38.13	C
	ATOM	5885	CG	GLN	R	139	16.866	95.917	196.748	1.00	39.52	C
55	ATOM	5888	CD	GLN	R	139	15.723	95.933	197.738	1.00	41.82	C
	ATOM	5889	OE1	GLN	R	139	15.647	96.804	198.610	1.00	41.21	O
	ATOM	5890	NE2	GLN	R	139	14.816	94.968	197.604	1.00	44.42	N
	ATOM	5893	C	GLN	R	139	20.683	96.465	197.028	1.00	36.29	C
	ATOM	5894	O	GLN	R	139	21.436	95.693	197.630	1.00	34.50	O
60	ATOM	5896	N	ALA	R	140	20.944	97.758	196.852	1.00	37.51	N
	ATOM	5897	CA	ALA	R	140	22.126	98.412	197.415	1.00	37.94	C
	ATOM	5899	CB	ALA	R	140	22.291	99.799	196.814	1.00	38.08	C
	ATOM	5903	C	ALA	R	140	22.026	98.511	198.934	1.00	35.87	C
	ATOM	5904	O	ALA	R	140	20.932	98.701	199.475	1.00	34.33	O
65	ATOM	5906	N	CYS	R	141	23.162	98.370	199.618	1.00	35.36	N
	ATOM	5907	CA	CYS	R	141	23.205	98.551	201.071	1.00	37.17	C
	ATOM	5909	CB	CYS	R	141	24.567	98.146	201.659	1.00	39.09	C
	ATOM	5912	SG	CYS	R	141	25.095	96.413	201.382	1.00	41.32	S
	ATOM	5914	C	CYS	R	141	22.910	100.022	201.391	1.00	37.26	C
70	ATOM	5915	O	CYS	R	141	23.400	100.918	200.699	1.00	35.92	O
	ATOM	5917	N	LYS	R	142	22.096	100.252	202.424	1.00	37.15	N
	ATOM	5918	CA	LYS	R	142	21.697	101.598	202.844	1.00	35.21	C

	ATOM	5920	CB	LYS	R	142	20.197	101.800	202.625	1.00	36.09	C
	ATOM	5923	CG	LYS	R	142	19.759	101.743	201.174	1.00	36.84	C
	ATOM	5926	CD	LYS	R	142	18.258	101.959	201.039	1.00	36.53	C
	ATOM	5929	CE	LYS	R	142	17.882	102.354	199.617	1.00	37.35	C
5	ATOM	5932	NZ	LYS	R	142	16.431	102.665	199.487	1.00	37.92	N
	ATOM	5936	C	LYS	R	142	22.011	101.804	204.322	1.00	33.33	C
	ATOM	5937	O	LYS	R	142	22.080	100.830	205.074	1.00	31.02	O
	ATOM	5939	N	PRO	R	143	22.185	103.073	204.754	1.00	32.67	N
10	ATOM	5940	CA	PRO	R	143	22.446	103.338	206.172	1.00	33.72	C
	ATOM	5942	CB	PRO	R	143	22.622	104.866	206.232	1.00	32.29	C
	ATOM	5945	CG	PRO	R	143	22.805	105.318	204.840	1.00	32.99	C
	ATOM	5948	CD	PRO	R	143	22.143	104.312	203.957	1.00	32.79	C
	ATOM	5951	C	PRO	R	143	21.280	102.923	207.065	1.00	33.07	C
15	ATOM	5952	O	PRO	R	143	20.124	103.103	206.683	1.00	33.29	O
	ATOM	5953	N	TRP	R	144	21.583	102.382	208.244	1.00	35.07	N
	ATOM	5954	CA	TRP	R	144	20.545	102.094	209.241	1.00	36.35	C
	ATOM	5956	CB	TRP	R	144	21.131	101.454	210.506	1.00	39.11	C
	ATOM	5959	CG	TRP	R	144	21.780	100.122	210.313	1.00	39.33	C
20	ATOM	5960	CD1	TRP	R	144	21.534	99.220	209.322	1.00	39.53	C
	ATOM	5962	NE1	TRP	R	144	22.318	98.106	209.490	1.00	39.66	N
	ATOM	5964	CE2	TRP	R	144	23.085	98.267	210.614	1.00	39.70	C
	ATOM	5965	CD2	TRP	R	144	22.766	99.526	211.164	1.00	39.80	C
	ATOM	5966	CE3	TRP	R	144	23.417	99.939	212.335	1.00	40.29	C
25	ATOM	5968	CZ3	TRP	R	144	24.354	99.090	212.912	1.00	39.93	C
	ATOM	5970	CH2	TRP	R	144	24.650	97.841	212.339	1.00	39.77	C
	ATOM	5972	CZ2	TRP	R	144	24.027	97.412	211.194	1.00	39.66	C
	ATOM	5974	C	TRP	R	144	19.836	103.379	209.655	1.00	35.60	C
	ATOM	5975	O	TRP	R	144	20.467	104.432	209.776	1.00	35.43	O
30	ATOM	5977	N	THR	R	145	18.527	103.284	209.873	1.00	35.80	N
	ATOM	5978	CA	THR	R	145	17.755	104.383	210.445	1.00	36.17	C
	ATOM	5980	CB	THR	R	145	16.232	104.119	210.360	1.00	35.41	C
	ATOM	5982	OG1	THR	R	145	15.851	103.943	208.990	1.00	34.30	O
	ATOM	5984	CG2	THR	R	145	15.439	105.280	210.954	1.00	35.74	C
35	ATOM	5988	C	THR	R	145	18.159	104.571	211.908	1.00	36.85	C
	ATOM	5989	O	THR	R	145	18.229	103.603	212.672	1.00	36.30	O
	ATOM	5991	N	ASN	R	146	18.430	105.820	212.282	1.00	37.69	N
	ATOM	5992	CA	ASN	R	146	18.862	106.162	213.637	1.00	37.04	C
	ATOM	5994	CB	ASN	R	146	19.911	107.284	213.585	1.00	38.27	C
40	ATOM	5997	CG	ASN	R	146	20.493	107.617	214.954	1.00	38.84	C
	ATOM	5998	OD1	ASN	R	146	20.484	106.794	215.870	1.00	40.12	O
	ATOM	5999	ND2	ASN	R	146	21.010	108.832	215.092	1.00	39.29	N
	ATOM	6002	C	ASN	R	146	17.669	106.576	214.501	1.00	36.00	C
	ATOM	6003	O	ASN	R	146	17.271	107.744	214.511	1.00	34.48	O
45	ATOM	6005	N	CYS	R	147	17.103	105.603	215.216	1.00	34.89	N
	ATOM	6006	CA	CYS	R	147	15.955	105.838	216.098	1.00	36.41	C
	ATOM	6008	CB	CYS	R	147	15.513	104.530	216.759	1.00	34.05	C
	ATOM	6011	SG	CYS	R	147	15.236	103.175	215.598	1.00	31.53	S
	ATOM	6013	C	CYS	R	147	16.285	106.867	217.177	1.00	36.13	C
50	ATOM	6014	O	CYS	R	147	15.455	107.708	217.520	1.00	33.50	O
	ATOM	6016	N	THR	R	148	17.510	106.788	217.691	1.00	38.64	N
	ATOM	6017	CA	THR	R	148	18.005	107.720	218.695	1.00	40.44	C
	ATOM	6019	CB	THR	R	148	19.060	107.051	219.600	1.00	40.73	C
	ATOM	6021	OG1	THR	R	148	20.239	106.750	218.844	1.00	41.31	O
55	ATOM	6023	CG2	THR	R	148	18.503	105.759	220.187	1.00	40.81	C
	ATOM	6027	C	THR	R	148	18.562	108.950	217.970	1.00	42.88	C
	ATOM	6028	O	THR	R	148	19.737	109.013	217.601	1.00	43.31	O
	ATOM	6030	N	LEU	R	149	17.685	109.928	217.779	1.00	43.91	N
	ATOM	6031	CA	LEU	R	149	17.925	111.043	216.866	1.00	43.30	C
60	ATOM	6033	CB	LEU	R	149	18.763	110.526	215.571	0.00	30.00	C
	ATOM	6036	CG	LEU	R	149	19.176	111.728	214.724	0.00	30.00	C
	ATOM	6038	CD1	LEU	R	149	19.236	112.990	215.582	0.00	30.00	C
	ATOM	6042	CD2	LEU	R	149	20.552	111.453	214.114	0.00	30.00	C
	ATOM	6046	C	LEU	R	149	16.570	111.613	216.445	1.00	43.50	C
65	ATOM	6047	O	LEU	R	149	16.393	112.831	216.365	1.00	42.30	O
	ATOM	6049	N	ALA	R	150	15.621	110.713	216.182	1.00	42.50	N
	ATOM	6050	CA	ALA	R	150	14.216	111.076	215.995	1.00	41.83	C
	ATOM	6052	CB	ALA	R	150	13.555	110.114	215.014	1.00	42.26	C
	ATOM	6056	C	ALA	R	150	13.448	111.086	217.326	1.00	41.20	C
70	ATOM	6057	O	ALA	R	150	12.229	111.267	217.336	1.00	41.99	O
	ATOM	6059	N	GLY	R	151	14.157	110.893	218.439	1.00	39.99	N
	ATOM	6060	CA	GLY	R	151	13.550	110.884	219.769	1.00	39.46	C

	ATOM	6063	C	GLY	R	151	12.732	109.636	220.055	1.00	39.07	C
	ATOM	6064	O	GLY	R	151	11.733	109.699	220.775	1.00	38.53	O
	ATOM	6066	N	LYS	R	152	13.167	108.503	219.502	1.00	38.38	N
5	ATOM	6067	CA	LYS	R	152	12.428	107.242	219.596	1.00	38.47	C
	ATOM	6069	CB	LYS	R	152	11.860	106.856	218.224	1.00	38.26	C
	ATOM	6072	CG	LYS	R	152	11.006	107.929	217.565	1.00	38.69	C
	ATOM	6075	CD	LYS	R	152	10.329	107.401	216.309	1.00	38.61	C
	ATOM	6078	CE	LYS	R	152	9.466	108.465	215.651	1.00	38.81	C
10	ATOM	6081	NZ	LYS	R	152	8.777	107.947	214.437	1.00	38.79	N
	ATOM	6085	C	LYS	R	152	13.313	106.102	220.093	1.00	38.15	C
	ATOM	6086	O	LYS	R	152	14.511	106.065	219.803	1.00	38.22	O
	ATOM	6088	N	HIS	R	153	12.711	105.168	220.830	1.00	36.95	N
	ATOM	6089	CA	HIS	R	153	13.381	103.919	221.195	1.00	35.80	C
15	ATOM	6091	CB	HIS	R	153	12.607	103.173	222.282	1.00	33.88	C
	ATOM	6094	CG	HIS	R	153	12.609	103.861	223.609	1.00	33.93	C
	ATOM	6095	ND1	HIS	R	153	13.770	104.197	224.271	1.00	33.66	N
	ATOM	6097	CE1	HIS	R	153	13.466	104.784	225.416	1.00	32.96	C
	ATOM	6099	NE2	HIS	R	153	12.151	104.831	225.524	1.00	32.81	N
20	ATOM	6101	CD2	HIS	R	153	11.591	104.258	224.408	1.00	32.74	C
	ATOM	6103	C	HIS	R	153	13.507	103.008	219.978	1.00	34.67	C
	ATOM	6104	O	HIS	R	153	12.787	103.175	218.989	1.00	34.28	O
	ATOM	6106	N	THR	R	154	14.415	102.040	220.073	1.00	34.00	N
	ATOM	6107	CA	THR	R	154	14.596	101.020	219.040	1.00	36.10	C
25	ATOM	6109	CB	THR	R	154	16.095	100.742	218.784	1.00	34.32	C
	ATOM	6111	OG1	THR	R	154	16.795	101.984	218.641	1.00	33.32	O
	ATOM	6113	CG2	THR	R	154	16.292	99.911	217.521	1.00	33.62	C
	ATOM	6117	C	THR	R	154	13.899	99.726	219.476	1.00	37.51	C
	ATOM	6118	O	THR	R	154	14.355	99.052	220.402	1.00	38.12	O
30	ATOM	6120	N	LEU	R	155	12.790	99.396	218.815	1.00	38.98	N
	ATOM	6121	CA	LEU	R	155	12.021	98.194	219.147	1.00	39.81	C
	ATOM	6123	CB	LEU	R	155	10.628	98.246	218.510	1.00	40.74	C
	ATOM	6126	CG	LEU	R	155	9.645	97.113	218.842	1.00	41.26	C
	ATOM	6128	CD1	LEU	R	155	9.705	96.691	220.315	1.00	41.60	C
35	ATOM	6132	CD2	LEU	R	155	8.228	97.534	218.471	1.00	41.43	C
	ATOM	6136	C	LEU	R	155	12.751	96.929	218.713	1.00	39.74	C
	ATOM	6137	O	LEU	R	155	12.812	95.960	219.468	1.00	39.19	O
	ATOM	6139	N	GLN	R	156	13.294	96.950	217.494	1.00	41.34	N
	ATOM	6140	CA	GLN	R	156	14.142	95.873	216.981	1.00	41.48	C
40	ATOM	6142	CB	GLN	R	156	13.400	95.061	215.913	1.00	42.42	C
	ATOM	6145	CG	GLN	R	156	14.271	94.031	215.201	1.00	44.19	C
	ATOM	6148	CD	GLN	R	156	13.467	92.985	214.451	1.00	44.98	C
	ATOM	6149	OE1	GLN	R	156	12.735	92.198	215.053	1.00	46.29	O
	ATOM	6150	NE2	GLN	R	156	13.614	92.960	213.131	1.00	48.64	N
45	ATOM	6153	C	GLN	R	156	15.430	96.463	216.394	1.00	40.01	C
	ATOM	6154	O	GLN	R	156	15.367	97.361	215.551	1.00	37.09	O
	ATOM	6156	N	PRO	R	157	16.604	95.965	216.834	1.00	39.73	N
	ATOM	6157	CA	PRO	R	157	17.857	96.476	216.273	1.00	38.78	C
	ATOM	6159	CB	PRO	R	157	18.945	95.755	217.086	1.00	39.02	C
50	ATOM	6162	CG	PRO	R	157	18.262	95.133	218.237	1.00	41.17	C
	ATOM	6165	CD	PRO	R	157	16.839	94.925	217.851	1.00	40.99	C
	ATOM	6168	C	PRO	R	157	18.020	96.146	214.790	1.00	37.84	C
	ATOM	6169	O	PRO	R	157	17.398	95.208	214.286	1.00	35.63	O
	ATOM	6170	N	ALA	R	158	18.859	96.917	214.106	1.00	38.62	N
55	ATOM	6171	CA	ALA	R	158	19.191	96.644	212.715	1.00	37.47	C
	ATOM	6173	CB	ALA	R	158	19.820	97.871	212.066	1.00	38.14	C
	ATOM	6177	C	ALA	R	158	20.143	95.458	212.628	1.00	37.70	C
	ATOM	6178	O	ALA	R	158	20.823	95.115	213.600	1.00	37.32	O
60	ATOM	6180	N	SER	R	159	20.175	94.830	211.456	1.00	37.03	N
	ATOM	6181	CA	SER	R	159	21.139	93.779	211.163	1.00	36.10	C
	ATOM	6183	CB	SER	R	159	20.460	92.406	211.204	1.00	36.14	C
	ATOM	6186	OG	SER	R	159	19.567	92.237	210.113	1.00	34.55	O
	ATOM	6188	C	SER	R	159	21.738	94.046	209.787	1.00	35.53	C
	ATOM	6189	O	SER	R	159	21.440	95.066	209.162	1.00	36.18	O
65	ATOM	6191	N	ASN	R	160	22.583	93.134	209.319	1.00	35.47	N
	ATOM	6192	CA	ASN	R	160	23.112	93.212	207.955	1.00	34.24	C
	ATOM	6194	CB	ASN	R	160	24.248	92.197	207.754	1.00	35.91	C
	ATOM	6197	CG	ASN	R	160	23.792	90.754	207.929	1.00	38.15	C
	ATOM	6198	OD1	ASN	R	160	22.758	90.484	208.544	1.00	41.64	O
70	ATOM	6199	ND2	ASN	R	160	24.568	89.819	207.390	1.00	41.23	N
	ATOM	6202	C	ASN	R	160	22.020	93.024	206.890	1.00	31.94	C
	ATOM	6203	O	ASN	R	160	22.188	93.455	205.749	1.00	32.45	O

	ATOM	6205	N	SER	R	161	20.904	92.399	207.276	1.00	29.55	N
	ATOM	6206	CA	SER	R	161	19.816	92.077	206.354	1.00	30.26	C
	ATOM	6208	CB	SER	R	161	19.448	90.591	206.483	1.00	29.75	C
5	ATOM	6211	OG	SER	R	161	18.950	90.285	207.779	1.00	32.29	O
	ATOM	6213	C	SER	R	161	18.551	92.929	206.524	1.00	29.66	C
	ATOM	6214	O	SER	R	161	17.624	92.810	205.719	1.00	27.80	O
	ATOM	6216	N	SER	R	162	18.495	93.773	207.558	1.00	32.80	N
	ATOM	6217	CA	SER	R	162	17.269	94.525	207.853	1.00	31.16	C
10	ATOM	6219	CB	SER	R	162	16.289	93.641	208.626	1.00	32.12	C
	ATOM	6222	OG	SER	R	162	16.816	93.267	209.888	1.00	32.67	O
	ATOM	6224	C	SER	R	162	17.502	95.826	208.626	1.00	31.42	C
	ATOM	6225	O	SER	R	162	18.462	95.955	209.389	1.00	29.65	O
	ATOM	6227	N	ASP	R	163	16.602	96.783	208.417	1.00	30.71	N
15	ATOM	6228	CA	ASP	R	163	16.691	98.082	209.065	1.00	33.33	C
	ATOM	6230	CB	ASP	R	163	15.872	99.122	208.285	1.00	34.54	C
	ATOM	6233	CG	ASP	R	163	16.332	100.554	208.538	1.00	34.53	C
	ATOM	6234	OD1	ASP	R	163	17.245	100.772	209.365	1.00	33.92	O
	ATOM	6235	OD2	ASP	R	163	15.774	101.469	207.897	1.00	36.35	O
20	ATOM	6236	C	ASP	R	163	16.183	97.984	210.499	1.00	33.66	C
	ATOM	6237	O	ASP	R	163	15.443	97.057	210.847	1.00	33.38	O
	ATOM	6239	N	ALA	R	164	16.595	98.941	211.328	1.00	35.14	N
	ATOM	6240	CA	ALA	R	164	16.078	99.056	212.689	1.00	34.23	C
	ATOM	6242	CB	ALA	R	164	16.912	100.050	213.499	1.00	34.58	C
25	ATOM	6246	C	ALA	R	164	14.618	99.495	212.654	1.00	34.61	C
	ATOM	6247	O	ALA	R	164	14.200	100.210	211.737	1.00	34.60	O
	ATOM	6249	N	ILE	R	165	13.850	99.054	213.649	1.00	33.40	N
	ATOM	6250	CA	ILE	R	165	12.448	99.434	213.791	1.00	34.04	C
	ATOM	6252	CB	ILE	R	165	11.534	98.202	213.981	1.00	34.48	C
30	ATOM	6254	CG1	ILE	R	165	11.845	97.130	212.930	1.00	34.62	C
	ATOM	6257	CD1	ILE	R	165	11.003	95.880	213.056	1.00	35.48	C
	ATOM	6261	CG2	ILE	R	165	10.057	98.604	213.900	1.00	34.33	C
	ATOM	6265	C	ILE	R	165	12.322	100.355	215.004	1.00	33.30	C
	ATOM	6266	O	ILE	R	165	12.823	100.038	216.084	1.00	30.10	O
35	ATOM	6268	N	CYS	R	166	11.661	101.495	214.813	1.00	34.70	N
	ATOM	6269	CA	CYS	R	166	11.457	102.467	215.888	1.00	35.63	C
	ATOM	6271	CB	CYS	R	166	11.245	103.867	215.306	1.00	37.75	C
	ATOM	6274	SG	CYS	R	166	12.531	104.383	214.139	1.00	40.43	S
	ATOM	6276	C	CYS	R	166	10.260	102.072	216.747	1.00	35.93	C
40	ATOM	6277	O	CYS	R	166	9.226	101.648	216.230	1.00	35.11	O
	ATOM	6279	N	LEU	T	29	26.611	67.584	190.236	1.00	45.25	N
	ATOM	6280	CA	LEU	T	29	26.448	68.732	191.185	1.00	45.04	C
	ATOM	6282	CB	LEU	T	29	24.963	69.084	191.357	1.00	44.44	C
	ATOM	6285	CG	LEU	T	29	24.607	70.255	192.280	1.00	44.76	C
45	ATOM	6287	CD1	LEU	T	29	25.231	71.553	191.792	1.00	45.26	C
	ATOM	6291	CD2	LEU	T	29	23.092	70.390	192.386	1.00	45.14	C
	ATOM	6295	C	LEU	T	29	27.073	68.421	192.546	1.00	44.26	C
	ATOM	6296	O	LEU	T	29	26.975	67.297	193.037	1.00	45.64	O
	ATOM	6300	N	HIS	T	30	27.719	69.422	193.137	1.00	44.57	N
50	ATOM	6301	CA	HIS	T	30	28.322	69.299	194.462	1.00	43.88	C
	ATOM	6303	CB	HIS	T	30	29.793	68.900	194.339	1.00	46.90	C
	ATOM	6306	CG	HIS	T	30	30.511	68.812	195.651	1.00	47.92	C
	ATOM	6307	ND1	HIS	T	30	31.710	69.450	195.888	1.00	48.91	N
	ATOM	6309	CE1	HIS	T	30	32.104	69.197	197.124	1.00	49.55	C
55	ATOM	6311	NE2	HIS	T	30	31.201	68.424	197.699	1.00	50.77	N
	ATOM	6313	CD2	HIS	T	30	30.193	68.169	196.800	1.00	49.47	C
	ATOM	6315	C	HIS	T	30	28.193	70.621	195.222	1.00	43.43	C
	ATOM	6316	O	HIS	T	30	28.754	71.638	194.807	1.00	44.57	O
	ATOM	6318	N	CYS	T	31	27.442	70.599	196.322	1.00	39.30	N
60	ATOM	6319	CA	CYS	T	31	27.268	71.770	197.175	1.00	38.29	C
	ATOM	6321	CB	CYS	T	31	25.784	72.149	197.288	1.00	34.77	C
	ATOM	6324	SG	CYS	T	31	24.952	72.541	195.709	1.00	32.97	S
	ATOM	6326	C	CYS	T	31	27.854	71.472	198.558	1.00	38.30	C
	ATOM	6327	O	CYS	T	31	27.789	70.339	199.039	1.00	37.06	O
65	ATOM	6329	N	VAL	T	32	28.432	72.494	199.183	1.00	39.22	N
	ATOM	6330	CA	VAL	T	32	29.041	72.368	200.510	1.00	39.62	C
	ATOM	6332	CB	VAL	T	32	30.595	72.332	200.437	1.00	40.98	C
	ATOM	6334	CG1	VAL	T	32	31.075	71.051	199.762	1.00	40.96	C
	ATOM	6338	CG2	VAL	T	32	31.147	73.564	199.715	1.00	41.68	C
70	ATOM	6342	C	VAL	T	32	28.611	73.528	201.407	1.00	40.80	C
	ATOM	6343	O	VAL	T	32	27.970	74.478	200.945	1.00	41.97	O
	ATOM	6345	N	GLY	T	33	28.962	73.433	202.688	1.00	38.89	N

	ATOM	6346	CA	GLY	T	33	28.724	74.509	203.643	1.00	37.81	C
	ATOM	6349	C	GLY	T	33	27.253	74.820	203.861	1.00	37.92	C
	ATOM	6350	O	GLY	T	33	26.423	73.911	203.998	1.00	37.49	O
5	ATOM	6352	N	ASP	T	34	26.926	76.110	203.879	1.00	34.95	N
	ATOM	6353	CA	ASP	T	34	25.574	76.563	204.203	1.00	33.25	C
	ATOM	6355	CB	ASP	T	34	25.639	77.883	204.982	1.00	34.65	C
	ATOM	6358	CG	ASP	T	34	26.369	77.744	206.318	1.00	37.07	C
	ATOM	6359	OD1	ASP	T	34	26.282	76.669	206.952	1.00	35.96	O
10	ATOM	6360	OD2	ASP	T	34	27.031	78.716	206.735	1.00	39.48	O
	ATOM	6361	C	ASP	T	34	24.719	76.717	202.945	1.00	30.58	C
	ATOM	6362	O	ASP	T	34	23.966	77.685	202.807	1.00	29.05	O
	ATOM	6364	N	THR	T	35	24.834	75.751	202.036	1.00	28.25	N
	ATOM	6365	CA	THR	T	35	24.065	75.755	200.800	1.00	30.36	C
15	ATOM	6367	CB	THR	T	35	24.968	75.983	199.566	1.00	29.95	C
	ATOM	6369	OG1	THR	T	35	25.861	74.876	199.409	1.00	30.62	O
	ATOM	6371	CG2	THR	T	35	25.776	77.280	199.704	1.00	31.09	C
	ATOM	6375	C	THR	T	35	23.313	74.440	200.618	1.00	27.31	C
	ATOM	6376	O	THR	T	35	23.570	73.458	201.322	1.00	26.74	O
20	ATOM	6378	N	TYR	T	36	22.381	74.437	199.671	1.00	25.45	N
	ATOM	6379	CA	TYR	T	36	21.630	73.232	199.321	1.00	28.04	C
	ATOM	6381	CB	TYR	T	36	20.255	73.204	200.011	1.00	27.81	C
	ATOM	6384	CG	TYR	T	36	19.340	74.349	199.639	1.00	27.67	C
	ATOM	6385	CD1	TYR	T	36	19.443	75.576	200.277	1.00	29.75	C
25	ATOM	6387	CE1	TYR	T	36	18.614	76.637	199.937	1.00	29.46	C
	ATOM	6389	CZ	TYR	T	36	17.673	76.474	198.948	1.00	27.01	C
	ATOM	6390	OH	TYR	T	36	16.863	77.531	198.621	1.00	28.38	O
	ATOM	6392	CE2	TYR	T	36	17.544	75.264	198.299	1.00	26.11	O
	ATOM	6394	CD2	TYR	T	36	18.379	74.206	198.643	1.00	27.30	C
30	ATOM	6396	C	TYR	T	36	21.502	73.118	197.799	1.00	26.04	C
	ATOM	6397	O	TYR	T	36	21.409	74.130	197.102	1.00	25.06	O
	ATOM	6399	N	PRO	T	37	21.549	71.883	197.274	1.00	27.52	N
	ATOM	6400	CA	PRO	T	37	21.453	71.632	195.839	1.00	27.78	C
	ATOM	6402	CB	PRO	T	37	22.022	70.216	195.704	1.00	28.36	C
35	ATOM	6405	CG	PRO	T	37	21.717	69.568	197.000	1.00	26.84	C
	ATOM	6408	CD	PRO	T	37	21.760	70.638	198.040	1.00	27.31	C
	ATOM	6411	C	PRO	T	37	20.025	71.695	195.289	1.00	28.89	C
	ATOM	6412	O	PRO	T	37	19.117	71.068	195.843	1.00	28.47	O
	ATOM	6413	N	SER	T	38	19.835	72.441	194.204	1.00	28.14	N
40	ATOM	6414	CA	SER	T	38	18.529	72.528	193.561	1.00	30.24	C
	ATOM	6416	CB	SER	T	38	17.629	73.500	194.337	1.00	31.57	C
	ATOM	6419	OG	SER	T	38	16.276	73.400	193.930	1.00	30.17	O
	ATOM	6421	C	SER	T	38	18.672	72.974	192.109	1.00	30.46	C
	ATOM	6422	O	SER	T	38	19.402	73.919	191.821	1.00	29.55	O
45	ATOM	6424	N	ASN	T	39	17.988	72.274	191.201	1.00	28.90	N
	ATOM	6425	CA	ASN	T	39	17.940	72.632	189.783	1.00	30.97	C
	ATOM	6427	CB	ASN	T	39	17.090	73.897	189.593	1.00	32.78	C
	ATOM	6430	CG	ASN	T	39	15.858	73.911	190.478	1.00	30.17	C
	ATOM	6431	OD1	ASN	T	39	14.903	73.160	190.256	1.00	32.83	O
50	ATOM	6432	ND2	ASN	T	39	15.881	74.750	191.505	1.00	25.86	N
	ATOM	6435	C	ASN	T	39	19.336	72.798	189.152	1.00	31.10	C
	ATOM	6436	O	ASN	T	39	19.575	73.724	188.380	1.00	35.41	O
	ATOM	6438	N	ASP	T	40	20.242	71.888	189.506	1.00	32.75	N
	ATOM	6439	CA	ASP	T	40	21.613	71.837	188.980	1.00	32.55	C
55	ATOM	6441	CB	ASP	T	40	21.611	71.695	187.447	1.00	36.00	C
	ATOM	6444	CG	ASP	T	40	22.965	71.254	186.891	1.00	39.64	C
	ATOM	6445	OD1	ASP	T	40	23.617	70.376	187.499	1.00	43.86	O
	ATOM	6446	OD2	ASP	T	40	23.381	71.788	185.838	1.00	47.17	O
	ATOM	6447	C	ASP	T	40	22.493	73.022	189.406	1.00	31.39	C
60	ATOM	6448	O	ASP	T	40	23.466	73.346	188.726	1.00	29.21	O
	ATOM	6450	N	ARG	T	41	22.152	73.658	190.526	1.00	29.86	N
	ATOM	6451	CA	ARG	T	41	22.999	74.704	191.112	1.00	29.44	C
	ATOM	6453	CB	ARG	T	41	22.717	76.087	190.481	1.00	27.78	C
	ATOM	6456	CG	ARG	T	41	21.272	76.583	190.522	1.00	28.43	C
65	ATOM	6459	CD	ARG	T	41	20.885	77.182	191.874	1.00	26.43	C
	ATOM	6462	NE	ARG	T	41	19.823	78.181	191.763	1.00	25.92	N
	ATOM	6464	CZ	ARG	T	41	18.527	77.901	191.643	1.00	26.98	C
	ATOM	6465	NH1	ARG	T	41	18.111	76.647	191.629	1.00	26.55	N
	ATOM	6468	NH2	ARG	T	41	17.634	78.881	191.550	1.00	27.51	N
70	ATOM	6471	C	ARG	T	41	22.867	74.720	192.637	1.00	27.67	C
	ATOM	6472	O	ARG	T	41	22.093	73.950	193.211	1.00	27.15	O
	ATOM	6474	N	CYS	T	42	23.657	75.565	193.291	1.00	27.93	N

	ATOM	6475	CA	CYS	T	42	23.658	75.639	194.748	1.00	28.67	C
	ATOM	6477	CB	CYS	T	42	25.095	75.597	195.280	1.00	29.86	C
	ATOM	6480	SG	CYS	T	42	26.032	74.072	194.871	1.00	32.16	S
5	ATOM	6482	C	CYS	T	42	22.939	76.906	195.216	1.00	28.39	C
	ATOM	6483	O	CYS	T	42	23.104	77.984	194.635	1.00	27.40	O
	ATOM	6485	N	CYS	T	43	22.144	76.761	196.272	1.00	28.42	N
	ATOM	6486	CA	CYS	T	43	21.329	77.851	196.807	1.00	28.41	C
	ATOM	6488	CB	CYS	T	43	19.851	77.498	196.676	1.00	33.18	C
10	ATOM	6491	SG	CYS	T	43	19.315	77.307	194.956	1.00	34.22	S
	ATOM	6493	C	CYS	T	43	21.697	78.114	198.265	1.00	26.97	C
	ATOM	6494	O	CYS	T	43	22.092	77.201	198.987	1.00	26.47	O
	ATOM	6496	N	HIS	T	44	21.587	79.366	198.688	1.00	27.05	N
	ATOM	6497	CA	HIS	T	44	21.975	79.750	200.039	1.00	28.91	C
15	ATOM	6499	CB	HIS	T	44	22.377	81.220	200.076	1.00	27.22	C
	ATOM	6502	CG	HIS	T	44	23.637	81.520	199.326	1.00	24.93	C
	ATOM	6503	ND1	HIS	T	44	24.871	81.070	199.741	1.00	25.54	N
	ATOM	6505	CE1	HIS	T	44	25.798	81.491	198.899	1.00	27.28	C
	ATOM	6507	NE2	HIS	T	44	25.208	82.201	197.953	1.00	25.52	N
20	ATOM	6509	CD2	HIS	T	44	23.856	82.232	198.196	1.00	23.47	C
	ATOM	6511	C	HIS	T	44	20.857	79.501	201.056	1.00	29.95	C
	ATOM	6512	O	HIS	T	44	19.704	79.863	200.823	1.00	29.36	O
	ATOM	6514	N	GLU	T	45	21.217	78.877	202.176	1.00	29.90	N
	ATOM	6515	CA	GLU	T	45	20.345	78.803	203.347	1.00	34.29	C
25	ATOM	6517	CB	GLU	T	45	20.865	77.765	204.342	1.00	35.37	C
	ATOM	6520	CG	GLU	T	45	20.852	76.343	203.817	1.00	37.60	C
	ATOM	6523	CD	GLU	T	45	21.077	75.328	204.917	1.00	39.59	C
	ATOM	6524	OE1	GLU	T	45	22.219	75.234	205.416	1.00	42.58	O
	ATOM	6525	OE2	GLU	T	45	20.108	74.627	205.286	1.00	43.53	O
30	ATOM	6526	C	GLU	T	45	20.281	80.168	204.030	1.00	33.27	C
	ATOM	6527	O	GLU	T	45	21.146	81.018	203.813	1.00	31.18	O
	ATOM	6529	N	CYS	T	46	19.260	80.368	204.859	1.00	33.32	N
	ATOM	6530	CA	CYS	T	46	19.086	81.627	205.579	1.00	37.24	C
	ATOM	6532	CB	CYS	T	46	17.669	81.746	206.147	1.00	37.21	C
35	ATOM	6535	SG	CYS	T	46	16.330	81.458	204.962	1.00	40.81	S
	ATOM	6537	C	CYS	T	46	20.108	81.748	206.713	1.00	38.88	C
	ATOM	6538	O	CYS	T	46	20.474	80.755	207.346	1.00	39.39	O
	ATOM	6540	N	ARG	T	47	20.557	82.972	206.964	1.00	41.13	N
	ATOM	6541	CA	ARG	T	47	21.533	83.241	208.019	1.00	42.38	C
40	ATOM	6543	CB	ARG	T	47	22.393	84.455	207.636	1.00	49.03	C
	ATOM	6546	CG	ARG	T	47	23.272	84.232	206.404	1.00	51.61	C
	ATOM	6549	CD	ARG	T	47	24.320	83.155	206.663	1.00	55.11	C
	ATOM	6552	NE	ARG	T	47	25.277	83.021	205.567	1.00	56.09	N
	ATOM	6554	CZ	ARG	T	47	26.427	82.349	205.640	1.00	59.65	C
45	ATOM	6555	NH1	ARG	T	47	26.789	81.736	206.766	1.00	60.81	N
	ATOM	6558	NH2	ARG	T	47	27.231	82.293	204.581	1.00	59.12	N
	ATOM	6561	C	ARG	T	47	20.811	83.483	209.344	1.00	41.54	C
	ATOM	6562	O	ARG	T	47	19.590	83.637	209.360	1.00	38.49	O
	ATOM	6564	N	PRO	T	48	21.558	83.490	210.467	1.00	41.28	N
50	ATOM	6565	CA	PRO	T	48	20.964	83.901	211.739	1.00	39.71	C
	ATOM	6567	CB	PRO	T	48	22.177	84.027	212.663	1.00	41.04	C
	ATOM	6570	CG	PRO	T	48	23.155	83.055	212.118	1.00	40.74	C
	ATOM	6573	CD	PRO	T	48	22.967	83.082	210.631	1.00	40.28	C
	ATOM	6576	C	PRO	T	48	20.227	85.235	211.624	1.00	37.36	C
55	ATOM	6577	O	PRO	T	48	20.698	86.145	210.945	1.00	33.57	O
	ATOM	6578	N	GLY	T	49	19.072	85.334	212.272	1.00	36.81	N
	ATOM	6579	CA	GLY	T	49	18.249	86.537	212.195	1.00	37.64	C
	ATOM	6582	C	GLY	T	49	17.273	86.537	211.036	1.00	36.52	C
	ATOM	6583	O	GLY	T	49	16.550	87.514	210.842	1.00	36.20	O
60	ATOM	6585	N	ASN	T	50	17.251	85.447	210.266	1.00	35.60	N
	ATOM	6586	CA	ASN	T	50	16.338	85.296	209.131	1.00	37.14	C
	ATOM	6588	CB	ASN	T	50	17.052	85.604	207.808	1.00	38.58	C
	ATOM	6591	CG	ASN	T	50	17.710	86.975	207.793	1.00	38.00	C
	ATOM	6592	OD1	ASN	T	50	18.847	87.132	208.237	1.00	39.14	O
65	ATOM	6593	ND2	ASN	T	50	17.009	87.967	207.252	1.00	37.25	N
	ATOM	6596	C	ASN	T	50	15.762	83.878	209.064	1.00	35.64	C
	ATOM	6597	O	ASN	T	50	16.420	82.918	209.467	1.00	34.45	O
	ATOM	6599	N	GLY	T	51	14.539	83.758	208.551	1.00	35.93	N
	ATOM	6600	CA	GLY	T	51	13.888	82.457	208.354	1.00	34.79	C
70	ATOM	6603	C	GLY	T	51	13.483	82.259	206.902	1.00	32.95	C
	ATOM	6604	O	GLY	T	51	13.227	83.229	206.192	1.00	32.70	O
	ATOM	6606	N	MET	T	52	13.418	81.008	206.455	1.00	33.33	N

	ATOM	6607	CA	MET	T	52	13.084	80.732	205.052	1.00	35.61	C
	ATOM	6609	CB	MET	T	52	13.680	79.413	204.565	1.00	39.08	C
	ATOM	6612	CG	MET	T	52	13.834	79.383	203.029	1.00	37.86	C
	ATOM	6615	SD	MET	T	52	14.739	77.961	202.481	1.00	45.92	S
5	ATOM	6616	CE	MET	T	52	16.420	78.412	202.871	1.00	40.41	C
	ATOM	6620	C	MET	T	52	11.587	80.729	204.781	1.00	32.52	C
	ATOM	6621	O	MET	T	52	10.804	80.094	205.496	1.00	29.20	O
	ATOM	6623	N	VAL	T	53	11.209	81.443	203.725	1.00	30.65	N
	ATOM	6624	CA	VAL	T	53	9.843	81.453	203.219	1.00	29.99	C
10	ATOM	6626	CB	VAL	T	53	9.471	82.846	202.684	1.00	29.17	C
	ATOM	6628	CG1	VAL	T	53	8.065	82.852	202.098	1.00	29.90	C
	ATOM	6632	CG2	VAL	T	53	9.606	83.886	203.799	1.00	29.24	C
	ATOM	6636	C	VAL	T	53	9.708	80.423	202.100	1.00	30.26	C
	ATOM	6637	O	VAL	T	53	8.728	79.684	202.036	1.00	27.00	O
15	ATOM	6639	N	SER	T	54	10.698	80.375	201.216	1.00	28.75	N
	ATOM	6640	CA	SER	T	54	10.643	79.470	200.082	1.00	28.26	C
	ATOM	6642	CB	SER	T	54	9.778	80.064	198.958	1.00	29.61	C
	ATOM	6645	OG	SER	T	54	10.352	81.247	198.429	1.00	28.78	O
	ATOM	6647	C	SER	T	54	12.037	79.156	199.570	1.00	29.71	C
20	ATOM	6648	O	SER	T	54	12.883	80.044	199.465	1.00	28.78	O
	ATOM	6650	N	ARG	T	55	12.268	77.883	199.258	1.00	32.04	N
	ATOM	6651	CA	ARG	T	55	13.519	77.460	198.657	1.00	29.82	C
	ATOM	6653	CB	ARG	T	55	13.635	75.940	198.678	1.00	29.36	C
	ATOM	6656	CG	ARG	T	55	13.856	75.350	200.060	1.00	29.40	C
25	ATOM	6659	CD	ARG	T	55	14.373	73.956	199.936	1.00	30.06	C
	ATOM	6662	NE	ARG	T	55	14.554	73.290	201.221	1.00	30.89	N
	ATOM	6664	CZ	ARG	T	55	15.646	73.367	201.982	1.00	30.59	C
	ATOM	6665	NH1	ARG	T	55	16.699	74.082	201.610	1.00	30.30	N
	ATOM	6668	NH2	ARG	T	55	15.689	72.694	203.125	1.00	29.56	N
30	ATOM	6671	C	ARG	T	55	13.590	77.956	197.220	1.00	28.31	C
	ATOM	6672	O	ARG	T	55	12.567	78.292	196.616	1.00	26.70	O
	ATOM	6674	N	CYS	T	56	14.800	77.999	196.674	1.00	30.25	N
	ATOM	6675	CA	CYS	T	56	14.984	78.367	195.277	1.00	30.06	C
	ATOM	6677	CB	CYS	T	56	16.476	78.454	194.923	1.00	31.60	C
35	ATOM	6680	SG	CYS	T	56	17.323	76.877	195.055	1.00	33.41	S
	ATOM	6682	C	CYS	T	56	14.263	77.360	194.373	1.00	31.78	C
	ATOM	6683	O	CYS	T	56	13.838	76.279	194.811	1.00	34.15	O
	ATOM	6685	N	SER	T	57	14.077	77.750	193.122	1.00	31.02	N
	ATOM	6686	CA	SER	T	57	13.426	76.901	192.133	1.00	32.12	C
40	ATOM	6688	CB	SER	T	57	11.931	11.211	192.061	1.00	32.64	C
	ATOM	6691	OG	SER	T	57	11.707	78.532	191.595	1.00	33.86	O
	ATOM	6693	C	SER	T	57	14.126	77.125	190.796	1.00	32.36	C
	ATOM	6694	O	SER	T	57	15.181	77.756	190.754	1.00	30.27	O
	ATOM	6696	N	ARG	T	58	13.567	76.592	189.716	1.00	34.30	N
45	ATOM	6697	CA	ARG	T	58	14.218	76.670	188.414	1.00	35.58	C
	ATOM	6699	CB	ARG	T	58	13.404	75.912	187.357	1.00	38.66	C
	ATOM	6702	CG	ARG	T	58	14.107	75.847	186.009	1.00	42.37	C
	ATOM	6705	CD	ARG	T	58	13.631	74.685	185.151	1.00	47.41	C
	ATOM	6708	NE	ARG	T	58	12.320	74.925	184.554	1.00	51.07	N
50	ATOM	6710	CZ	ARG	T	58	11.786	74.188	183.577	1.00	54.07	C
	ATOM	6711	NH1	ARG	T	58	12.443	73.146	183.066	1.00	54.39	N
	ATOM	6714	NH2	ARG	T	58	10.584	74.495	183.101	1.00	53.65	N
	ATOM	6717	C	ARG	T	58	14.472	78.111	187.957	1.00	32.18	C
	ATOM	6718	O	ARG	T	58	15.482	78.383	187.312	1.00	32.39	O
55	ATOM	6720	N	SER	T	59	13.564	79.021	188.294	1.00	29.54	N
	ATOM	6721	CA	SER	T	59	13.653	80.415	187.843	1.00	32.97	C
	ATOM	6723	CB	SER	T	59	12.607	80.663	186.751	1.00	38.07	C
	ATOM	6726	OG	SER	T	59	12.872	79.848	185.621	1.00	41.86	O
	ATOM	6728	C	SER	T	59	13.486	81.444	188.970	1.00	29.09	C
60	ATOM	6729	O	SER	T	59	13.271	82.626	188.700	1.00	28.44	O
	ATOM	6731	N	GLN	T	60	13.600	81.004	190.222	1.00	30.48	N
	ATOM	6732	CA	GLN	T	60	13.478	81.898	191.372	1.00	29.22	C
	ATOM	6734	CB	GLN	T	60	12.106	81.748	192.049	1.00	33.69	C
	ATOM	6737	CG	GLN	T	60	10.894	81.963	191.133	1.00	37.47	C
65	ATOM	6740	CD	GLN	T	60	10.779	83.388	190.608	1.00	40.36	C
	ATOM	6741	OE1	GLN	T	60	11.082	84.352	191.312	1.00	40.60	O
	ATOM	6742	NE2	GLN	T	60	10.332	83.523	189.362	1.00	40.94	N
	ATOM	6745	C	GLN	T	60	14.570	81.621	192.398	1.00	26.24	C
	ATOM	6746	O	GLN	T	60	15.021	80.476	192.553	1.00	27.04	O
70	ATOM	6748	N	ASN	T	61	14.978	82.679	193.095	1.00	24.72	N
	ATOM	6749	CA	ASN	T	61	15.935	82.593	194.194	1.00	27.28	C

5	ATOM	6751	CB	ASN	T	61	16.594	83.958	194.457	1.00	25.19	C
	ATOM	6754	CG	ASN	T	61	17.578	84.365	193.366	1.00	24.89	C
	ATOM	6755	OD1	ASN	T	61	17.427	85.410	192.734	1.00	22.67	O
	ATOM	6756	ND2	ASN	T	61	18.595	83.544	193.150	1.00	25.92	N
	ATOM	6759	C	ASN	T	61	15.275	82.131	195.489	1.00	29.63	C
10	ATOM	6760	O	ASN	T	61	14.054	82.209	195.644	1.00	26.77	O
	ATOM	6762	N	THR	T	62	16.104	81.666	196.418	1.00	31.32	N
	ATOM	6763	CA	THR	T	62	15.687	81.435	197.801	1.00	30.06	C
	ATOM	6765	CB	THR	T	62	16.907	81.062	198.675	1.00	30.83	C
	ATOM	6767	OG1	THR	T	62	17.582	79.939	198.098	1.00	30.36	O
15	ATOM	6769	CG2	THR	T	62	16.489	80.730	200.105	1.00	32.37	C
	ATOM	6773	C	THR	T	62	15.082	82.716	198.373	1.00	32.30	C
	ATOM	6774	O	THR	T	62	15.616	83.802	198.141	1.00	27.58	O
	ATOM	6776	N	VAL	T	63	13.979	82.588	199.114	1.00	29.43	N
	ATOM	6777	CA	VAL	T	63	13.396	83.728	199.830	1.00	32.45	C
20	ATOM	6779	CB	VAL	T	63	11.912	83.971	199.454	1.00	31.19	C
	ATOM	6781	CG1	VAL	T	63	11.348	85.161	200.222	1.00	32.49	C
	ATOM	6785	CG2	VAL	T	63	11.773	84.208	197.957	1.00	31.55	C
	ATOM	6789	C	VAL	T	63	13.515	83.528	201.336	1.00	33.39	C
	ATOM	6790	O	VAL	T	63	12.864	82.647	201.916	1.00	30.03	O
25	ATOM	6792	N	CYS	T	64	14.372	84.340	201.952	1.00	34.36	N
	ATOM	6793	CA	CYS	T	64	14.486	84.426	203.402	1.00	37.87	C
	ATOM	6795	CB	CYS	T	64	15.941	84.263	203.846	1.00	39.41	C
	ATOM	6798	SG	CYS	T	64	16.694	82.686	203.382	1.00	41.51	S
	ATOM	6800	C	CYS	T	64	13.963	85.786	203.851	1.00	38.61	C
30	ATOM	6801	O	CYS	T	64	14.037	86.764	203.104	1.00	37.49	O
	ATOM	6803	N	ARG	T	65	13.423	85.845	205.066	1.00	38.27	N
	ATOM	6804	CA	ARG	T	65	12.914	87.105	205.613	1.00	41.06	C
	ATOM	6806	CB	ARG	T	65	11.383	87.131	205.585	1.00	47.00	C
	ATOM	6809	CG	ARG	T	65	10.782	87.082	204.179	1.00	50.39	C
35	ATOM	6812	CD	ARG	T	65	10.847	88.433	203.464	1.00	52.14	C
	ATOM	6815	NE	ARG	T	65	10.815	88.280	202.008	1.00	51.81	N
	ATOM	6817	CZ	ARG	T	65	10.379	89.199	201.142	1.00	54.95	C
	ATOM	6818	NH1	ARG	T	65	9.914	90.378	201.558	1.00	56.38	N
	ATOM	6821	NH2	ARG	T	65	10.403	88.935	199.836	1.00	54.16	N
40	ATOM	6824	C	ARG	T	65	13.421	87.308	207.038	1.00	38.65	C
	ATOM	6825	O	ARG	T	65	13.521	86.341	207.799	1.00	36.99	O
	ATOM	6827	N	PRO	T	66	13.752	88.565	207.402	1.00	37.95	N
	ATOM	6828	CA	PRO	T	66	14.164	88.870	208.776	1.00	38.35	C
	ATOM	6830	CB	PRO	T	66	14.303	90.396	208.775	1.00	38.69	C
45	ATOM	6833	CG	PRO	T	66	14.516	90.766	207.363	1.00	38.44	C
	ATOM	6836	CD	PRO	T	66	13.765	89.766	206.547	1.00	38.44	C
	ATOM	6839	C	PRO	T	66	13.113	88.439	209.795	1.00	36.37	C
	ATOM	6840	O	PRO	T	66	11.919	88.584	209.535	1.00	34.32	O
	ATOM	6841	N	CYS	T	67	13.555	87.909	210.933	1.00	36.18	N
50	ATOM	6842	CA	CYS	T	67	12.636	87.463	211.975	1.00	38.61	C
	ATOM	6844	CB	CYS	T	67	13.386	86.780	213.127	1.00	38.78	C
	ATOM	6847	SG	CYS	T	67	14.382	85.320	212.691	1.00	39.72	S
	ATOM	6849	C	CYS	T	67	11.856	88.662	212.512	1.00	39.70	C
	ATOM	6850	O	CYS	T	67	12.437	89.712	212.795	1.00	40.88	O
55	ATOM	6852	N	GLY	T	68	10.541	88.504	212.640	1.00	39.56	N
	ATOM	6853	CA	GLY	T	68	9.679	89.577	213.125	1.00	39.84	C
	ATOM	6856	C	GLY	T	68	9.769	89.713	214.632	1.00	38.36	C
	ATOM	6857	O	GLY	T	68	10.444	88.914	215.285	1.00	37.51	O
	ATOM	6859	N	PRO	T	69	9.096	90.733	215.199	1.00	40.96	N
60	ATOM	6860	CA	PRO	T	69	9.055	90.901	216.655	1.00	38.07	C
	ATOM	6862	CB	PRO	T	69	8.104	92.090	216.847	1.00	40.57	C
	ATOM	6865	CG	PRO	T	69	8.163	92.837	215.564	1.00	40.73	C
	ATOM	6868	CD	PRO	T	69	8.353	91.801	214.503	1.00	41.19	C
	ATOM	6871	C	PRO	T	69	8.527	89.659	217.378	1.00	35.48	C
65	ATOM	6872	O	PRO	T	69	7.500	89.103	216.989	1.00	35.12	O
	ATOM	6873	N	GLY	T	70	9.245	89.221	218.408	1.00	34.06	N
	ATOM	6874	CA	GLY	T	70	8.866	88.033	219.171	1.00	34.32	C
	ATOM	6877	C	GLY	T	70	9.373	86.721	218.588	1.00	33.68	C
	ATOM	6878	O	GLY	T	70	9.072	85.658	219.130	1.00	29.88	O
70	ATOM	6880	N	PHE	T	71	10.150	86.795	217.503	1.00	33.14	N
	ATOM	6881	CA	PHE	T	71	10.754	85.613	216.873	1.00	34.86	C
	ATOM	6883	CB	PHE	T	71	10.089	85.318	215.523	1.00	37.04	C
	ATOM	6886	CG	PHE	T	71	8.663	84.869	215.632	1.00	37.24	C
	ATOM	6887	CD1	PHE	T	71	7.637	85.795	215.789	1.00	38.30	C
	ATOM	6889	CE1	PHE	T	71	6.310	85.381	215.890	1.00	38.42	C

5	ATOM	6891	CZ	PHE	T	71	6.002	84.028	215.830	1.00	38.39	C
	ATOM	6893	CE2	PHE	T	71	7.019	83.094	215.670	1.00	37.90	C
	ATOM	6895	CD2	PHE	T	71	8.340	83.517	215.571	1.00	38.44	C
	ATOM	6897	C	PHE	T	71	12.254	85.804	216.651	1.00	35.17	C
	ATOM	6898	O	PHE	T	71	12.736	86.933	216.545	1.00	34.79	O
10	ATOM	6900	N	TYR	T	72	12.978	84.690	216.553	1.00	34.44	N
	ATOM	6901	CA	TYR	T	72	14.427	84.714	216.366	1.00	35.22	C
	ATOM	6903	CB	TYR	T	72	15.129	84.774	217.726	1.00	35.59	C
	ATOM	6906	CG	TYR	T	72	15.234	83.421	218.386	1.00	35.73	C
	ATOM	6907	CD1	TYR	T	72	14.143	82.864	219.050	1.00	34.26	C
15	ATOM	6909	CE1	TYR	T	72	14.226	81.614	219.643	1.00	35.51	C
	ATOM	6911	CZ	TYR	T	72	15.406	80.898	219.566	1.00	35.51	C
	ATOM	6912	OH	TYR	T	72	15.493	79.660	220.157	1.00	35.96	O
	ATOM	6914	CE2	TYR	T	72	16.503	81.425	218.908	1.00	36.24	C
	ATOM	6916	CD2	TYR	T	72	16.412	82.681	218.320	1.00	35.96	C
20	ATOM	6918	C	TYR	T	72	14.938	83.492	215.601	1.00	36.85	C
	ATOM	6919	O	TYR	T	72	14.232	82.490	215.437	1.00	34.10	O
	ATOM	6921	N	ASN	T	73	16.181	83.588	215.143	1.00	38.45	N
	ATOM	6922	CA	ASN	T	73	16.898	82.443	214.597	1.00	37.38	C
	ATOM	6924	CB	ASN	T	73	16.677	82.331	213.086	1.00	39.96	C
25	ATOM	6927	CG	ASN	T	73	17.454	81.181	212.470	1.00	41.43	C
	ATOM	6928	OD1	ASN	T	73	17.481	80.074	213.015	1.00	43.13	O
	ATOM	6929	ND2	ASN	T	73	18.096	81.438	211.331	1.00	42.47	N
	ATOM	6932	C	ASN	T	73	18.388	82.569	214.914	1.00	36.67	C
	ATOM	6933	O	ASN	T	73	19.042	83.500	214.453	1.00	34.57	O
30	ATOM	6935	N	ASP	T	74	18.909	81.625	215.698	1.00	35.89	N
	ATOM	6936	CA	ASP	T	74	20.299	81.671	216.162	1.00	36.94	C
	ATOM	6938	CB	ASP	T	74	20.383	81.257	217.643	1.00	35.94	C
	ATOM	6941	CG	ASP	T	74	19.951	79.818	217.890	1.00	36.88	C
	ATOM	6942	OD1	ASP	T	74	19.087	79.299	217.150	1.00	37.53	O
35	ATOM	6943	OD2	ASP	T	74	20.465	79.208	218.851	1.00	40.14	O
	ATOM	6944	C	ASP	T	74	21.281	80.845	215.314	1.00	36.41	C
	ATOM	6945	O	ASP	T	74	22.488	80.875	215.564	1.00	34.75	O
	ATOM	6947	N	VAL	T	75	20.773	80.135	214.309	1.00	35.84	N
	ATOM	6948	CA	VAL	T	75	21.609	79.282	213.455	1.00	36.04	C
40	ATOM	6950	CB	VAL	T	75	21.427	77.777	213.796	1.00	35.40	C
	ATOM	6952	CG1	VAL	T	75	21.832	77.502	215.238	1.00	36.11	C
	ATOM	6956	CG2	VAL	T	75	19.987	77.318	213.539	1.00	34.73	C
	ATOM	6960	C	VAL	T	75	21.303	79.487	211.974	1.00	37.17	C
	ATOM	6961	O	VAL	T	75	20.328	80.149	211.615	1.00	39.09	O
45	ATOM	6963	N	VAL	T	76	22.147	78.917	211.117	1.00	37.02	N
	ATOM	6964	CA	VAL	T	76	21.871	78.866	209.685	1.00	36.47	C
	ATOM	6966	CB	VAL	T	76	23.127	78.470	208.878	1.00	37.75	C
	ATOM	6968	CG1	VAL	T	76	22.768	78.137	207.428	1.00	38.65	C
	ATOM	6972	CG2	VAL	T	76	24.165	79.583	208.938	1.00	38.43	C
50	ATOM	6976	C	VAL	T	76	20.788	77.817	209.479	1.00	35.92	C
	ATOM	6977	O	VAL	T	76	20.914	76.704	209.986	1.00	34.52	O
	ATOM	6979	N	SER	T	77	19.728	78.160	208.748	1.00	36.66	N
	ATOM	6980	CA	SER	T	77	18.611	77.231	208.587	1.00	35.83	C
	ATOM	6982	CB	SER	T	77	17.664	77.332	209.788	1.00	38.75	C
55	ATOM	6985	OG	SER	T	77	16.791	78.441	209.654	1.00	40.91	O
	ATOM	6987	C	SER	T	77	17.799	77.404	207.304	1.00	33.75	C
	ATOM	6988	O	SER	T	77	17.921	78.394	206.578	1.00	32.41	O
	ATOM	6990	N	SER	T	78	16.969	76.402	207.052	1.00	33.95	N
	ATOM	6991	CA	SER	T	78	15.994	76.420	205.972	1.00	33.65	C
60	ATOM	6993	CB	SER	T	78	16.284	75.281	205.002	1.00	35.05	C
	ATOM	6996	OG	SER	T	78	17.557	75.451	204.401	1.00	38.47	O
	ATOM	6998	C	SER	T	78	14.598	76.285	206.575	1.00	30.99	C
	ATOM	6999	O	SER	T	78	13.702	75.690	205.975	1.00	31.02	O
	ATOM	7001	N	LYS	T	79	14.422	76.857	207.763	1.00	30.65	N
65	ATOM	7002	CA	LYS	T	79	13.141	76.833	208.466	1.00	32.43	C
	ATOM	7004	CB	LYS	T	79	13.249	75.956	209.721	1.00	34.16	C
	ATOM	7007	CG	LYS	T	79	13.583	74.496	209.419	1.00	33.57	C
	ATOM	7010	CD	LYS	T	79	13.189	73.550	210.559	1.00	35.21	C
	ATOM	7013	CE	LYS	T	79	13.813	72.173	210.376	1.00	34.50	C
70	ATOM	7016	NZ	LYS	T	79	13.631	71.272	211.550	1.00	31.45	N
	ATOM	7020	C	LYS	T	79	12.717	78.255	208.849	1.00	32.96	C
	ATOM	7021	O	LYS	T	79	13.556	79.164	208.898	1.00	31.21	O
	ATOM	7023	N	PRO	T	80	11.412	78.464	209.110	1.00	31.23	N
	ATOM	7024	CA	PRO	T	80	10.959	79.749	209.653	1.00	33.72	C
	ATOM	7026	CB	PRO	T	80	9.453	79.530	209.870	1.00	33.31	C

5	ATOM	7029	CG	PRO	T	80	9.094	78.437	208.948	1.00	33.07	C
	ATOM	7032	CD	PRO	T	80	10.286	77.538	208.901	1.00	33.53	C
	ATOM	7035	C	PRO	T	80	11.631	80.083	210.981	1.00	31.68	C
	ATOM	7036	O	PRO	T	80	12.204	79.198	211.621	1.00	28.73	O
	ATOM	7037	N	CYS	T	81	11.566	81.348	211.385	1.00	34.79	N
10	ATOM	7038	CA	CYS	T	81	12.065	81.765	212.701	1.00	36.06	C
	ATOM	7040	CB	CYS	T	81	12.071	83.289	212.828	1.00	37.56	C
	ATOM	7043	SG	CYS	T	81	13.132	84.102	211.616	1.00	40.87	S
	ATOM	7045	C	CYS	T	81	11.217	81.147	213.811	1.00	37.25	C
	ATOM	7046	O	CYS	T	81	10.079	80.747	213.579	1.00	37.93	O
15	ATOM	7048	N	LYS	T	82	11.789	81.071	215.010	1.00	34.02	N
	ATOM	7049	CA	LYS	T	82	11.169	80.393	216.146	1.00	36.28	C
	ATOM	7051	CB	LYS	T	82	12.188	79.464	216.812	1.00	38.79	C
	ATOM	7054	CG	LYS	T	82	12.826	78.461	215.859	1.00	41.73	C
	ATOM	7057	CD	LYS	T	82	13.999	77.738	216.504	1.00	42.70	C
20	ATOM	7060	CE	LYS	T	82	15.266	78.581	216.485	1.00	43.74	C
	ATOM	7063	NZ	LYS	T	82	16.352	77.951	217.287	1.00	44.66	N
	ATOM	7067	C	LYS	T	82	10.682	81.431	217.158	1.00	33.84	C
	ATOM	7068	O	LYS	T	82	11.263	82.509	217.250	1.00	32.50	O
	ATOM	7070	N	PRO	T	83	9.612	81.119	217.911	1.00	33.44	N
25	ATOM	7071	CA	PRO	T	83	9.161	82.078	218.932	1.00	34.44	C
	ATOM	7073	CB	PRO	T	83	7.864	81.456	219.471	1.00	35.09	C
	ATOM	7076	CG	PRO	T	83	7.500	80.365	218.516	1.00	35.63	C
	ATOM	7079	CD	PRO	T	83	8.766	79.914	217.870	1.00	34.07	C
	ATOM	7082	C	PRO	T	83	10.180	82.255	220.060	1.00	33.45	C
30	ATOM	7083	O	PRO	T	83	10.873	81.302	220.424	1.00	31.63	O
	ATOM	7084	N	CYS	T	84	10.269	83.470	220.597	1.00	34.05	N
	ATOM	7085	CA	CYS	T	84	11.143	83.756	221.732	1.00	35.54	C
	ATOM	7087	CB	CYS	T	84	11.298	85.264	221.925	1.00	37.11	C
	ATOM	7090	SG	CYS	T	84	11.837	86.114	220.439	1.00	41.83	S
35	ATOM	7092	C	CYS	T	84	10.589	83.149	223.019	1.00	36.56	C
	ATOM	7093	O	CYS	T	84	9.370	83.028	223.187	1.00	34.52	O
	ATOM	7095	N	THR	T	85	11.493	82.795	223.928	1.00	34.32	N
	ATOM	7096	CA	THR	T	85	11.122	82.188	225.199	1.00	35.41	C
	ATOM	7098	CB	THR	T	85	12.311	81.397	225.795	1.00	35.95	C
40	ATOM	7100	OG1	THR	T	85	12.806	80.474	224.816	1.00	34.26	O
	ATOM	7102	CG2	THR	T	85	11.896	80.630	227.044	1.00	36.36	C
	ATOM	7106	C	THR	T	85	10.670	83.251	226.201	1.00	34.77	C
	ATOM	7107	O	THR	T	85	11.204	84.364	226.215	1.00	35.28	O
	ATOM	7109	N	TRP	T	86	9.675	82.899	227.017	1.00	34.73	N
45	ATOM	7110	CA	TRP	T	86	9.278	83.692	228.189	1.00	35.03	C
	ATOM	7112	CB	TRP	T	86	7.773	83.563	228.460	1.00	39.45	C
	ATOM	7115	CG	TRP	T	86	6.839	83.986	227.353	1.00	39.38	C
	ATOM	7116	CD1	TRP	T	86	6.281	83.183	226.398	1.00	41.17	C
	ATOM	7118	NE1	TRP	T	86	5.459	83.916	225.576	1.00	41.33	N
50	ATOM	7120	CE2	TRP	T	86	5.458	85.219	226.000	1.00	40.59	C
	ATOM	7121	CD2	TRP	T	86	6.313	85.301	227.122	1.00	39.70	C
	ATOM	7122	CE3	TRP	T	86	6.486	86.541	227.750	1.00	40.74	C
	ATOM	7124	CZ3	TRP	T	86	5.810	87.648	227.242	1.00	40.64	C
	ATOM	7126	CH2	TRP	T	86	4.971	87.534	226.122	1.00	40.91	C
55	ATOM	7128	CZ2	TRP	T	86	4.782	86.332	225.488	1.00	41.10	C
	ATOM	7130	C	TRP	T	86	10.018	83.179	229.430	1.00	33.20	C
	ATOM	7131	O	TRP	T	86	10.175	81.969	229.611	1.00	30.39	O
	ATOM	7133	N	CYS	T	87	10.456	84.094	230.295	1.00	31.70	N
	ATOM	7134	CA	CYS	T	87	11.019	83.713	231.593	1.00	32.58	C
60	ATOM	7136	CB	CYS	T	87	11.905	84.834	232.161	1.00	33.42	C
	ATOM	7139	SG	CYS	T	87	13.267	85.411	231.086	1.00	34.91	S
	ATOM	7141	C	CYS	T	87	9.880	83.413	232.569	1.00	30.26	C
	ATOM	7142	O	CYS	T	87	8.871	84.121	232.582	1.00	29.56	O
	ATOM	7144	N	ASN	T	88	10.038	82.364	233.375	1.00	30.25	N
65	ATOM	7145	CA	ASN	T	88	9.044	82.016	234.398	1.00	32.12	C
	ATOM	7147	CB	ASN	T	88	9.155	80.536	234.788	1.00	30.70	C
	ATOM	7150	CG	ASN	T	88	7.979	80.049	235.631	1.00	31.82	C
	ATOM	7151	OD1	ASN	T	88	7.840	78.849	235.864	1.00	32.91	O
	ATOM	7152	ND2	ASN	T	88	7.134	80.972	236.093	1.00	33.44	N
70	ATOM	7155	C	ASN	T	88	9.228	82.914	235.625	1.00	31.84	C
	ATOM	7156	O	ASN	T	88	9.939	82.557	236.567	1.00	31.33	O
	ATOM	7158	N	LEU	T	89	8.562	84.065	235.606	1.00	33.56	N
	ATOM	7159	CA	LEU	T	89	8.757	85.106	236.622	1.00	35.59	C
	ATOM	7161	CB	LEU	T	89	8.017	86.386	236.211	1.00	37.38	C
	ATOM	7164	CG	LEU	T	89	8.442	87.020	234.880	1.00	39.15	C

5	ATOM	7166	CD1	LEU	T	89	7.377	87.991	234.386	1.00	40.53	C
	ATOM	7170	CD2	LEU	T	89	9.791	87.712	235.004	1.00	39.68	C
	ATOM	7174	C	LEU	T	89	8.317	84.683	238.030	1.00	36.14	C
	ATOM	7175	O	LEU	T	89	8.926	85.092	239.023	1.00	35.72	O
	ATOM	7177	N	ARG	T	90	7.267	83.868	238.107	1.00	37.32	N
10	ATOM	7178	CA	ARG	T	90	6.726	83.407	239.387	1.00	39.48	C
	ATOM	7180	CB	ARG	T	90	5.344	82.768	239.192	1.00	43.48	C
	ATOM	7183	CG	ARG	T	90	4.303	83.716	238.607	1.00	45.53	C
	ATOM	7186	CD	ARG	T	90	2.931	83.057	238.448	1.00	46.70	C
	ATOM	7189	NE	ARG	T	90	2.192	83.619	237.311	1.00	48.12	N
15	ATOM	7191	CZ	ARG	T	90	0.862	83.684	237.203	1.00	49.64	C
	ATOM	7192	NH1	ARG	T	90	0.063	83.228	238.167	1.00	50.29	N
	ATOM	7195	NH2	ARG	T	90	0.323	84.224	236.113	1.00	49.28	N
	ATOM	7198	C	ARG	T	90	7.661	82.418	240.085	1.00	37.77	C
	ATOM	7199	O	ARG	T	90	7.713	82.372	241.317	1.00	37.13	O
20	ATOM	7201	N	SER	T	91	8.400	81.637	239.298	1.00	35.78	N
	ATOM	7202	CA	SER	T	91	9.329	80.646	239.843	1.00	36.49	C
	ATOM	7204	CB	SER	T	91	9.668	79.594	238.785	1.00	36.19	C
	ATOM	7207	OG	SER	T	91	10.583	80.097	237.827	1.00	36.85	O
	ATOM	7209	C	SER	T	91	10.622	81.271	240.378	1.00	36.78	C
25	ATOM	7210	O	SER	T	91	11.348	80.633	241.144	1.00	37.36	O
	ATOM	7212	N	GLY	T	92	10.904	82.510	239.973	1.00	36.33	N
	ATOM	7213	CA	GLY	T	92	12.111	83.222	240.400	1.00	35.60	C
	ATOM	7216	C	GLY	T	92	13.012	83.669	239.258	1.00	33.96	C
	ATOM	7217	O	GLY	T	92	14.000	84.364	239.483	1.00	34.12	O
30	ATOM	7219	N	SER	T	93	12.686	83.270	238.030	1.00	35.00	N
	ATOM	7220	CA	SER	T	93	13.448	83.691	236.851	1.00	34.55	C
	ATOM	7222	CB	SER	T	93	12.994	82.894	235.623	1.00	36.29	C
	ATOM	7225	OG	SER	T	93	13.705	83.237	234.439	1.00	33.40	O
	ATOM	7227	C	SER	T	93	13.272	85.192	236.607	1.00	35.84	C
35	ATOM	7228	O	SER	T	93	12.232	85.767	236.937	1.00	37.17	O
	ATOM	7230	N	GLU	T	94	14.304	85.819	236.052	1.00	34.32	N
	ATOM	7231	CA	GLU	T	94	14.264	87.236	235.703	1.00	36.25	C
	ATOM	7233	CB	GLU	T	94	15.067	88.071	236.710	1.00	34.77	C
	ATOM	7236	CG	GLU	T	94	14.536	88.034	238.144	1.00	35.35	C
40	ATOM	7239	CD	GLU	T	94	15.382	88.855	239.117	1.00	35.70	C
	ATOM	7240	OE1	GLU	T	94	16.513	89.243	238.753	1.00	37.77	O
	ATOM	7241	OE2	GLU	T	94	14.917	89.110	240.249	1.00	32.14	O
	ATOM	7242	C	GLU	T	94	14.855	87.406	234.312	1.00	37.24	C
	ATOM	7243	O	GLU	T	94	15.849	86.761	233.976	1.00	37.78	O
45	ATOM	7245	N	ARG	T	95	14.241	88.266	233.503	1.00	39.70	N
	ATOM	7246	CA	ARG	T	95	14.757	88.565	232.171	1.00	40.26	C
	ATOM	7248	CB	ARG	T	95	13.684	89.229	231.308	1.00	40.83	C
	ATOM	7251	CG	ARG	T	95	14.102	89.421	229.853	1.00	39.88	C
	ATOM	7254	CD	ARG	T	95	12.904	89.670	228.955	1.00	40.88	C
50	ATOM	7257	NE	ARG	T	95	12.235	90.934	229.254	1.00	40.49	N
	ATOM	7259	CZ	ARG	T	95	11.127	91.364	228.653	1.00	41.90	C
	ATOM	7260	NH1	ARG	T	95	10.542	90.638	227.703	1.00	43.10	N
	ATOM	7263	NH2	ARG	T	95	10.601	92.535	229.000	1.00	42.48	N
	ATOM	7266	C	ARG	T	95	15.980	89.473	232.274	1.00	41.85	C
55	ATOM	7267	O	ARG	T	95	15.905	90.563	232.846	1.00	43.55	O
	ATOM	7269	N	LYS	T	96	17.101	89.004	231.732	1.00	42.69	N
	ATOM	7270	CA	LYS	T	96	18.345	89.772	231.697	1.00	43.17	C
	ATOM	7272	CB	LYS	T	96	19.559	88.835	231.808	1.00	44.18	C
	ATOM	7275	CG	LYS	T	96	20.896	89.474	231.415	1.00	44.19	C
60	ATOM	7278	CD	LYS	T	96	22.089	88.669	231.926	1.00	44.45	C
	ATOM	7281	CE	LYS	T	96	23.370	89.498	231.917	1.00	45.12	C
	ATOM	7284	NZ	LYS	T	96	24.388	88.985	232.881	1.00	43.79	N
	ATOM	7288	C	LYS	T	96	18.419	90.567	230.401	1.00	42.89	C
	ATOM	7289	O	LYS	T	96	18.561	91.792	230.416	1.00	40.79	O
65	ATOM	7291	N	GLN	T	97	18.322	89.850	229.284	1.00	43.76	N
	ATOM	7292	CA	GLN	T	97	18.467	90.440	227.959	1.00	44.97	C
	ATOM	7294	CB	GLN	T	97	19.736	89.909	227.280	1.00	46.31	C
	ATOM	7297	CG	GLN	T	97	20.527	90.976	226.524	1.00	47.95	C
	ATOM	7300	CD	GLN	T	97	21.634	90.401	225.648	1.00	48.46	C
70	ATOM	7301	OE1	GLN	T	97	21.573	89.249	225.212	1.00	49.32	O
	ATOM	7302	NE2	GLN	T	97	22.650	91.215	225.380	1.00	50.03	N
	ATOM	7305	C	GLN	T	97	17.244	90.110	227.111	1.00	45.40	C
	ATOM	7306	O	GLN	T	97	16.793	88.961	227.077	1.00	43.17	O
	ATOM	7308	N	LEU	T	98	16.712	91.122	226.430	1.00	45.18	N
	ATOM	7309	CA	LEU	T	98	15.594	90.926	225.514	1.00	44.04	C

	ATOM	7311	CB	LEU	T	98	15.128	92.264	224.933	1.00	44.92	C
	ATOM	7314	CG	LEU	T	98	14.505	93.274	225.895	1.00	46.57	C
	ATOM	7316	CD1	LEU	T	98	14.330	94.618	225.203	1.00	46.23	C
5	ATOM	7320	CD2	LEU	T	98	13.177	92.759	226.424	1.00	47.22	C
	ATOM	7324	C	LEU	T	98	15.995	90.001	224.370	1.00	43.11	C
	ATOM	7325	O	LEU	T	98	17.174	89.903	224.011	1.00	40.49	O
	ATOM	7327	N	CYS	T	99	15.010	89.313	223.804	1.00	42.59	N
	ATOM	7328	CA	CYS	T	99	15.243	88.521	222.607	1.00	42.84	C
10	ATOM	7330	CB	CYS	T	99	14.052	87.617	222.314	1.00	42.83	C
	ATOM	7333	SG	CYS	T	99	14.357	86.459	220.973	1.00	45.54	S
	ATOM	7335	C	CYS	T	99	15.485	89.450	221.422	1.00	40.92	C
	ATOM	7336	O	CYS	T	99	14.837	90.495	221.299	1.00	39.42	O
	ATOM	7338	N	THR	T	100	16.433	89.067	220.572	1.00	41.49	N
	ATOM	7339	CA	THR	T	100	16.690	89.758	219.305	1.00	41.88	C
15	ATOM	7341	CB	THR	T	100	18.131	90.328	219.226	1.00	43.92	C
	ATOM	7343	OG1	THR	T	100	18.332	90.961	217.952	1.00	46.89	O
	ATOM	7345	CG2	THR	T	100	19.190	89.238	219.428	1.00	42.33	C
	ATOM	7349	C	THR	T	100	16.442	88.774	218.166	1.00	41.73	C
20	ATOM	7350	O	THR	T	100	16.012	87.650	218.405	1.00	40.39	O
	ATOM	7352	N	ALA	T	101	16.710	89.201	216.935	1.00	41.45	N
	ATOM	7353	CA	ALA	T	101	16.556	88.343	215.763	1.00	40.33	C
	ATOM	7355	CB	ALA	T	101	16.733	89.160	214.486	1.00	41.27	C
	ATOM	7359	C	ALA	T	101	17.527	87.157	215.775	1.00	39.69	C
25	ATOM	7360	O	ALA	T	101	17.175	86.064	215.338	1.00	38.12	O
	ATOM	7362	N	THR	T	102	18.741	87.369	216.282	1.00	37.89	N
	ATOM	7363	CA	THR	T	102	19.786	86.338	216.258	1.00	38.56	C
	ATOM	7365	CB	THR	T	102	21.165	86.960	215.946	1.00	37.78	C
	ATOM	7367	OG1	THR	T	102	21.515	87.903	216.970	1.00	37.14	O
30	ATOM	7369	CG2	THR	T	102	21.146	87.660	214.595	1.00	36.76	C
	ATOM	7373	C	THR	T	102	19.915	85.530	217.557	1.00	38.71	C
	ATOM	7374	O	THR	T	102	20.687	84.573	217.620	1.00	39.91	O
	ATOM	7376	N	GLN	T	103	19.156	85.893	218.585	1.00	39.28	N
	ATOM	7377	CA	GLN	T	103	19.401	85.365	219.923	1.00	39.83	C
35	ATOM	7379	CB	GLN	T	103	20.416	86.261	220.652	1.00	41.15	C
	ATOM	7382	CG	GLN	T	103	21.305	85.530	221.649	1.00	42.91	C
	ATOM	7385	CD	GLN	T	103	22.159	86.475	222.485	1.00	43.06	C
	ATOM	7386	OE1	GLN	T	103	22.584	87.535	222.014	1.00	44.46	O
	ATOM	7387	NE2	GLN	T	103	22.417	86.092	223.730	1.00	43.42	N
40	ATOM	7390	C	GLN	T	103	18.105	85.287	220.717	1.00	38.58	C
	ATOM	7391	O	GLN	T	103	17.311	86.229	220.710	1.00	37.40	O
	ATOM	7393	N	ASP	T	104	17.898	84.164	221.402	1.00	37.64	N
	ATOM	7394	CA	ASP	T	104	16.727	83.989	222.260	1.00	38.66	C
	ATOM	7396	CB	ASP	T	104	16.528	82.504	222.606	1.00	38.21	C
45	ATOM	7399	CG	ASP	T	104	15.114	82.190	223.089	1.00	37.12	C
	ATOM	7400	OD1	ASP	T	104	14.228	83.069	223.005	1.00	33.93	O
	ATOM	7401	OD2	ASP	T	104	14.891	81.055	223.561	1.00	38.27	O
	ATOM	7402	C	ASP	T	104	16.856	84.814	223.546	1.00	38.35	C
	ATOM	7403	O	ASP	T	104	17.953	85.247	223.917	1.00	35.65	O
50	ATOM	7405	N	THR	T	105	15.719	85.032	224.207	1.00	38.28	N
	ATOM	7406	CA	THR	T	105	15.670	85.664	225.520	1.00	39.30	C
	ATOM	7408	CB	THR	T	105	14.264	85.516	226.155	1.00	37.98	C
	ATOM	7410	OG1	THR	T	105	13.255	85.866	225.199	1.00	34.62	O
	ATOM	7412	CG2	THR	T	105	14.127	86.400	227.393	1.00	37.85	C
55	ATOM	7416	C	THR	T	105	16.681	85.030	226.472	1.00	40.61	C
	ATOM	7417	O	THR	T	105	16.863	83.812	226.468	1.00	40.51	O
	ATOM	7419	N	VAL	T	106	17.340	85.867	227.272	1.00	40.18	N
	ATOM	7420	CA	VAL	T	106	18.242	85.400	228.323	1.00	41.65	C
	ATOM	7422	CB	VAL	T	106	19.537	86.246	228.391	1.00	42.10	C
60	ATOM	7424	CG1	VAL	T	106	20.465	85.725	229.485	1.00	40.85	C
	ATOM	7428	CG2	VAL	T	106	20.245	86.240	227.036	1.00	42.75	C
	ATOM	7432	C	VAL	T	106	17.510	85.478	229.660	1.00	40.61	C
	ATOM	7433	O	VAL	T	106	17.122	86.560	230.099	1.00	38.96	O
	ATOM	7435	N	CYS	T	107	17.304	84.319	230.282	1.00	41.34	N
65	ATOM	7436	CA	CYS	T	107	16.630	84.226	231.569	1.00	43.71	C
	ATOM	7438	CB	CYS	T	107	15.432	83.277	231.490	1.00	40.41	C
	ATOM	7441	SG	CYS	T	107	14.120	83.728	230.314	1.00	35.76	S
	ATOM	7443	C	CYS	T	107	17.624	83.701	232.593	1.00	46.38	C
	ATOM	7444	O	CYS	T	107	18.380	82.774	232.308	1.00	45.77	O
70	ATOM	7446	N	ARG	T	108	17.624	84.300	233.779	1.00	49.86	N
	ATOM	7447	CA	ARG	T	108	18.496	83.871	234.867	1.00	52.45	C
	ATOM	7449	CB	ARG	T	108	19.686	84.823	235.003	1.00	54.11	C

	ATOM	7452	CG	ARG	T	108	20.711	84.726	233.878	1.00	54.49	C
	ATOM	7455	CD	ARG	T	108	21.582	83.484	234.012	1.00	55.09	C
	ATOM	7458	NE	ARG	T	108	22.663	83.465	233.025	1.00	55.14	N
5	ATOM	7460	CZ	ARG	T	108	22.551	83.041	231.765	1.00	55.49	C
	ATOM	7461	NH1	ARG	T	108	21.394	82.587	231.292	1.00	55.65	N
	ATOM	7464	NH2	ARG	T	108	23.610	83.074	230.964	1.00	55.40	N
	ATOM	7467	C	ARG	T	108	17.706	83.825	236.169	1.00	53.32	C
	ATOM	7468	O	ARG	T	108	16.776	84.610	236.368	1.00	51.51	O
10	ATOM	7470	N	CYS	T	109	18.078	82.897	237.047	1.00	54.58	N
	ATOM	7471	CA	CYS	T	109	17.429	82.756	238.349	1.00	60.22	C
	ATOM	7473	CB	CYS	T	109	17.622	81.335	238.891	1.00	60.35	C
	ATOM	7476	SG	CYS	T	109	16.918	80.011	237.819	1.00	64.74	S
	ATOM	7478	C	CYS	T	109	17.975	83.795	239.336	1.00	61.34	C
15	ATOM	7479	O	CYS	T	109	19.178	84.048	239.374	1.00	62.81	O
	ATOM	7481	N	ARG	T	110	17.071	84.388	240.117	1.00	64.12	N
	ATOM	7482	CA	ARG	T	110	17.420	85.399	241.121	1.00	65.20	C
	ATOM	7484	CB	ARG	T	110	16.161	86.135	241.608	1.00	67.88	C
	ATOM	7487	CG	ARG	T	110	15.180	85.275	242.419	1.00	69.84	C
20	ATOM	7490	CD	ARG	T	110	14.065	86.103	243.053	1.00	71.53	C
	ATOM	7493	NE	ARG	T	110	13.181	86.700	242.052	1.00	73.16	N
	ATOM	7495	CZ	ARG	T	110	11.989	87.238	242.309	1.00	73.85	C
	ATOM	7496	NH1	ARG	T	110	11.495	87.258	243.544	1.00	74.50	N
	ATOM	7499	NH2	ARG	T	110	11.275	87.755	241.313	1.00	73.76	N
25	ATOM	7502	C	ARG	T	110	18.134	84.770	242.310	1.00	64.78	C
	ATOM	7503	O	ARG	T	110	18.246	83.543	242.403	1.00	65.69	O
	ATOM	7505	N	ALA	T	111	18.608	85.621	243.218	1.00	62.71	N
	ATOM	7506	CA	ALA	T	111	19.181	85.153	244.467	1.00	62.56	C
	ATOM	7508	CB	ALA	T	111	19.792	86.321	245.257	1.00	63.12	C
30	ATOM	7512	C	ALA	T	111	18.078	84.458	245.264	1.00	59.72	C
	ATOM	7513	O	ALA	T	111	16.909	84.867	245.211	1.00	57.89	O
	ATOM	7515	N	GLY	T	112	18.445	83.377	245.953	1.00	58.06	N
	ATOM	7516	CA	GLY	T	112	17.490	82.596	246.741	1.00	58.62	C
	ATOM	7519	C	GLY	T	112	16.776	81.503	245.963	1.00	56.88	C
35	ATOM	7520	O	GLY	T	112	15.934	80.793	246.517	1.00	52.57	O
	ATOM	7522	N	THR	T	113	17.102	81.366	244.679	1.00	56.21	N
	ATOM	7523	CA	THR	T	113	16.545	80.298	243.848	1.00	57.52	C
	ATOM	7525	CB	THR	T	113	15.354	80.792	242.979	1.00	54.77	C
	ATOM	7527	OG1	THR	T	113	15.844	81.558	241.871	1.00	49.72	O
40	ATOM	7529	CG2	THR	T	113	14.384	81.651	243.798	1.00	54.74	C
	ATOM	7533	C	THR	T	113	17.627	79.689	242.948	1.00	57.81	C
	ATOM	7534	O	THR	T	113	18.711	80.255	242.783	1.00	57.08	O
	ATOM	7536	N	GLN	T	114	17.310	78.534	242.367	1.00	58.56	N
	ATOM	7537	CA	GLN	T	114	18.266	77.741	241.596	1.00	58.71	C
45	ATOM	7539	CB	GLN	T	114	18.820	76.634	242.493	1.00	59.14	C
	ATOM	7542	CG	GLN	T	114	19.925	75.787	241.881	1.00	59.82	C
	ATOM	7545	CD	GLN	T	114	20.364	74.649	242.791	1.00	59.58	C
	ATOM	7546	OE1	GLN	T	114	19.730	74.366	243.808	1.00	57.96	O
	ATOM	7547	NE2	GLN	T	114	21.452	73.985	242.420	1.00	61.17	N
50	ATOM	7550	C	GLN	T	114	17.573	77.123	240.367	1.00	57.16	C
	ATOM	7551	O	GLN	T	114	16.429	76.676	240.470	1.00	51.14	O
	ATOM	7553	N	PRO	T	115	18.262	77.086	239.205	1.00	58.01	N
	ATOM	7554	CA	PRO	T	115	17.615	76.551	237.992	1.00	61.65	C
55	ATOM	7556	CB	PRO	T	115	18.651	76.802	236.885	1.00	60.59	C
	ATOM	7559	CG	PRO	T	115	19.653	77.728	237.458	1.00	60.48	C
	ATOM	7562	CD	PRO	T	115	19.643	77.524	238.935	1.00	59.21	C
	ATOM	7565	C	PRO	T	115	17.283	75.058	238.061	1.00	61.12	C
	ATOM	7566	O	PRO	T	115	17.877	74.323	238.851	1.00	58.11	O
	ATOM	7567	N	LEU	T	116	16.345	74.625	237.222	1.00	66.00	N
60	ATOM	7568	CA	LEU	T	116	15.934	73.222	237.168	1.00	68.42	C
	ATOM	7570	CB	LEU	T	116	14.414	73.112	236.985	1.00	69.89	C
	ATOM	7573	CG	LEU	T	116	13.526	73.548	238.154	1.00	70.59	C
	ATOM	7575	CD1	LEU	T	116	12.062	73.497	237.746	1.00	70.65	C
	ATOM	7579	CD2	LEU	T	116	13.769	72.684	239.385	1.00	71.19	C
65	ATOM	7583	C	LEU	T	116	16.643	72.463	236.046	1.00	70.72	C
	ATOM	7584	O	LEU	T	116	17.484	71.601	236.306	1.00	71.34	O
	ATOM	7586	N	ASP	T	117	16.307	72.801	234.803	1.00	72.90	N
	ATOM	7587	CA	ASP	T	117	16.713	72.013	233.633	1.00	72.94	C
	ATOM	7589	CB	ASP	T	117	15.759	72.286	232.464	1.00	73.78	C
70	ATOM	7592	CG	ASP	T	117	14.332	71.850	232.758	1.00	74.03	C
	ATOM	7593	OD1	ASP	T	117	13.958	71.773	233.948	1.00	72.64	O
	ATOM	7594	OD2	ASP	T	117	13.582	71.586	231.792	1.00	74.25	O

	ATOM	7595	C	ASP	T	117	18.163	72.269	233.209	1.00	74.00	C
	ATOM	7596	O	ASP	T	117	18.838	73.139	233.765	1.00	74.71	O
	ATOM	7598	N	SER	T	118	18.626	71.502	232.221	1.00	74.96	N
	ATOM	7599	CA	SER	T	118	20.026	71.523	231.783	1.00	75.09	C
5	ATOM	7601	CB	SER	T	118	20.546	70.088	231.649	1.00	76.20	C
	ATOM	7604	OG	SER	T	118	21.942	70.065	231.401	1.00	76.88	O
	ATOM	7606	C	SER	T	118	20.243	72.268	230.462	1.00	75.03	C
	ATOM	7607	O	SER	T	118	21.176	73.063	230.345	1.00	75.10	O
	ATOM	7609	N	TYR	T	119	19.393	72.003	229.470	1.00	74.86	N
10	ATOM	7610	CA	TYR	T	119	19.572	72.567	228.123	1.00	74.21	C
	ATOM	7612	CB	TYR	T	119	18.791	71.750	227.082	1.00	74.15	C
	ATOM	7615	CG	TYR	T	119	19.421	70.411	226.754	1.00	73.91	C
	ATOM	7616	CD1	TYR	T	119	20.400	70.304	225.769	1.00	74.16	C
	ATOM	7618	CE1	TYR	T	119	20.984	69.078	225.460	1.00	74.21	C
15	ATOM	7620	CZ	TYR	T	119	20.589	67.940	226.142	1.00	74.17	C
	ATOM	7621	OH	TYR	T	119	21.164	66.726	225.837	1.00	73.91	O
	ATOM	7623	CE2	TYR	T	119	19.617	68.020	227.126	1.00	74.07	C
	ATOM	7625	CD2	TYR	T	119	19.038	69.252	227.425	1.00	73.82	C
	ATOM	7627	C	TYR	T	119	19.199	74.053	228.016	1.00	73.95	C
20	ATOM	7628	O	TYR	T	119	19.701	74.751	227.132	1.00	73.99	O
	ATOM	7630	N	LYS	T	120	18.325	74.528	228.905	1.00	73.13	N
	ATOM	7631	CA	LYS	T	120	17.924	75.940	228.938	1.00	71.96	C
	ATOM	7633	CB	LYS	T	120	16.663	76.173	228.129	0.00	30.00	C
	ATOM	7636	CG	LYS	T	120	15.543	75.418	228.842	0.00	30.00	C
25	ATOM	7639	CD	LYS	T	120	14.210	75.643	228.130	0.00	30.00	C
	ATOM	7642	CE	LYS	T	120	13.091	74.888	228.842	0.00	30.00	C
	ATOM	7645	NZ	LYS	T	120	11.782	75.109	228.144	0.00	30.00	N
	ATOM	7649	C	LYS	T	120	17.922	76.490	230.367	1.00	70.28	C
	ATOM	7650	O	LYS	T	120	16.863	76.813	230.910	1.00	66.83	O
30	ATOM	7652	N	PRO	T	121	19.114	76.617	230.974	1.00	70.53	N
	ATOM	7653	CA	PRO	T	121	19.212	76.957	232.394	1.00	71.04	C
	ATOM	7655	CB	PRO	T	121	20.677	76.650	232.724	1.00	71.38	C
	ATOM	7658	CG	PRO	T	121	21.400	76.840	231.441	1.00	71.37	C
	ATOM	7661	CD	PRO	T	121	20.441	76.465	230.347	1.00	70.93	C
35	ATOM	7664	C	PRO	T	121	18.886	78.420	232.699	1.00	69.78	C
	ATOM	7665	O	PRO	T	121	19.455	79.321	232.079	1.00	67.67	O
	ATOM	7666	N	GLY	T	122	17.969	78.638	233.643	1.00	70.28	N
	ATOM	7667	CA	GLY	T	122	17.609	79.982	234.106	1.00	70.66	C
	ATOM	7670	C	GLY	T	122	16.169	80.406	233.819	1.00	70.33	C
40	ATOM	7671	O	GLY	T	122	15.729	81.465	234.253	1.00	76.91	O
	ATOM	7673	N	VAL	T	123	15.423	79.597	233.069	1.00	73.90	N
	ATOM	7674	CA	VAL	T	123	14.031	79.930	232.730	1.00	70.39	C
	ATOM	7676	CB	VAL	T	123	13.601	79.268	231.411	1.00	75.51	C
	ATOM	7678	CG1	VAL	T	123	12.109	79.526	231.132	1.00	72.57	C
45	ATOM	7682	CG2	VAL	T	123	14.469	79.761	230.266	1.00	75.53	C
	ATOM	7686	C	VAL	T	123	13.056	79.481	233.813	1.00	70.92	C
	ATOM	7687	O	VAL	T	123	12.151	80.242	234.231	1.00	82.85	O
	ATOM	7689	N	ASP	T	124	13.207	78.201	234.225	1.00	65.64	N
	ATOM	7690	CA	ASP	T	124	12.446	77.637	235.339	1.00	65.06	C
50	ATOM	7692	CB	ASP	T	124	11.883	76.263	234.969	1.00	65.30	C
	ATOM	7695	CG	ASP	T	124	11.045	75.295	233.709	1.00	63.98	C
	ATOM	7696	OD1	ASP	T	124	10.148	77.159	233.606	1.00	61.67	O
	ATOM	7697	OD2	ASP	T	124	11.283	75.449	232.823	1.00	66.17	O
	ATOM	7698	C	ASP	T	124	13.366	77.492	236.545	1.00	63.63	C
55	ATOM	7699	O	ASP	T	124	14.407	76.830	236.462	1.00	63.46	O
	ATOM	7701	N	CYS	T	125	12.983	78.106	237.662	1.00	61.40	N
	ATOM	7702	CA	CYS	T	125	13.804	78.092	238.869	1.00	59.40	C
	ATOM	7704	CB	CYS	T	125	14.245	79.518	239.202	1.00	58.64	C
	ATOM	7707	SG	CYS	T	125	14.918	80.393	237.749	1.00	58.68	S
60	ATOM	7709	C	CYS	T	125	13.060	77.452	240.040	1.00	57.27	C
	ATOM	7710	O	CYS	T	125	11.850	77.228	239.972	1.00	53.38	O
	ATOM	7712	N	ALA	T	126	13.799	77.151	241.106	1.00	56.21	N
	ATOM	7713	CA	ALA	T	126	13.234	76.533	242.304	1.00	55.90	C
	ATOM	7715	CB	ALA	T	126	13.377	75.023	242.232	1.00	56.15	C
65	ATOM	7719	C	ALA	T	126	13.935	77.077	243.553	1.00	53.90	C
	ATOM	7720	O	ALA	T	126	15.137	77.346	243.509	1.00	49.05	O
	ATOM	7722	N	PRO	T	127	13.194	77.228	244.670	1.00	54.33	N
	ATOM	7723	CA	PRO	T	127	13.775	77.830	245.880	1.00	54.43	C
	ATOM	7725	CB	PRO	T	127	12.589	77.881	246.857	1.00	55.09	C
70	ATOM	7728	CG	PRO	T	127	11.369	77.694	246.025	1.00	55.15	C
	ATOM	7731	CD	PRO	T	127	11.784	76.847	244.877	1.00	54.67	C

	ATOM	7734	C	PRO	T	127	14.921	77.021	246.496	1.00	53.26	C
	ATOM	7735	O	PRO	T	127	14.995	75.808	246.306	1.00	52.32	O
	ATOM	7736	N	CYS	T	128	15.804	77.699	247.228	1.00	54.27	N
	ATOM	7737	CA	CYS	T	128	16.865	77.026	247.979	1.00	53.86	C
5	ATOM	7739	CB	CYS	T	128	17.809	78.040	248.633	1.00	58.25	C
	ATOM	7742	SG	CYS	T	128	18.741	79.095	247.503	1.00	63.91	S
	ATOM	7744	C	CYS	T	128	16.247	76.162	249.077	1.00	51.31	C
	ATOM	7745	O	CYS	T	128	15.248	76.562	249.682	1.00	48.54	O
	ATOM	7747	N	PRO	T	129	16.826	74.973	249.337	1.00	49.59	N
10	ATOM	7748	CA	PRO	T	129	16.378	74.206	250.499	1.00	48.98	C
	ATOM	7750	CB	PRO	T	129	17.129	72.871	250.363	1.00	49.02	C
	ATOM	7753	CG	PRO	T	129	17.633	72.836	248.958	1.00	51.39	C
	ATOM	7756	CD	PRO	T	129	17.874	74.262	248.587	1.00	51.44	C
	ATOM	7759	C	PRO	T	129	16.756	74.910	251.808	1.00	46.65	C
15	ATOM	7760	O	PRO	T	129	17.568	75.839	251.788	1.00	43.55	O
	ATOM	7761	N	PRO	T	130	16.170	74.476	252.939	1.00	46.60	N
	ATOM	7762	CA	PRO	T	130	16.508	75.078	254.229	1.00	46.26	C
	ATOM	7764	CB	PRO	T	130	15.761	74.195	255.236	1.00	45.70	C
	ATOM	7767	CG	PRO	T	130	14.645	73.602	254.471	1.00	45.90	C
20	ATOM	7770	CD	PRO	T	130	15.160	73.411	253.078	1.00	46.51	C
	ATOM	7773	C	PRO	T	130	18.011	75.060	254.512	1.00	46.44	C
	ATOM	7774	O	PRO	T	130	18.652	74.021	254.354	1.00	44.65	O
	ATOM	7775	N	GLY	T	131	18.561	76.205	254.916	1.00	46.37	N
	ATOM	7776	CA	GLY	T	131	19.978	76.310	255.265	1.00	46.88	C
25	ATOM	7779	C	GLY	T	131	20.933	76.459	254.095	1.00	47.32	C
	ATOM	7780	O	GLY	T	131	22.137	76.228	254.242	1.00	46.24	O
	ATOM	7782	N	HIS	T	132	20.400	76.847	252.938	1.00	48.02	N
	ATOM	7783	CA	HIS	T	132	21.206	77.061	251.739	1.00	51.04	C
	ATOM	7785	CB	HIS	T	132	20.825	76.058	250.647	1.00	51.16	C
30	ATOM	7788	CG	HIS	T	132	21.330	74.669	250.891	1.00	52.13	C
	ATOM	7789	ND1	HIS	T	132	22.572	74.413	251.425	1.00	52.59	N
	ATOM	7791	CE1	HIS	T	132	22.755	73.108	251.511	1.00	51.95	C
	ATOM	7793	NE2	HIS	T	132	21.679	72.506	251.041	1.00	52.08	N
	ATOM	7795	CD2	HIS	T	132	20.777	73.460	250.639	1.00	53.04	C
35	ATOM	7797	C	HIS	T	132	21.027	78.478	251.207	1.00	53.10	C
	ATOM	7798	O	HIS	T	132	20.027	79.138	251.499	1.00	55.47	O
	ATOM	7800	N	PHE	T	133	22.004	78.937	250.427	1.00	54.32	N
	ATOM	7801	CA	PHE	T	133	21.909	80.223	249.738	1.00	54.73	C
	ATOM	7803	CB	PHE	T	133	22.795	81.273	250.410	1.00	54.22	C
40	ATOM	7806	CG	PHE	T	133	24.262	81.140	250.090	1.00	54.14	C
	ATOM	7807	CD1	PHE	T	133	25.046	80.191	250.737	1.00	54.02	C
	ATOM	7809	CE1	PHE	T	133	26.400	80.072	250.453	1.00	54.02	C
	ATOM	7811	CZ	PHE	T	133	26.987	80.912	249.518	1.00	54.16	C
	ATOM	7813	CE2	PHE	T	133	26.217	81.870	248.872	1.00	54.19	C
45	ATOM	7815	CD2	PHE	T	133	24.863	81.981	249.161	1.00	53.70	C
	ATOM	7817	C	PHE	T	133	22.293	80.118	248.265	1.00	55.86	C
	ATOM	7818	O	PHE	T	133	22.947	79.164	247.844	1.00	53.63	O
	ATOM	7820	N	SER	T	134	21.875	81.121	247.499	1.00	57.55	N
	ATOM	7821	CA	SER	T	134	22.341	81.317	246.134	1.00	58.72	C
50	ATOM	7823	CB	SER	T	134	21.440	80.578	245.147	1.00	59.31	C
	ATOM	7826	OG	SER	T	134	21.910	80.734	243.819	1.00	59.68	O
	ATOM	7828	C	SER	T	134	22.340	82.813	245.821	1.00	60.73	C
	ATOM	7829	O	SER	T	134	21.340	83.484	246.065	1.00	62.90	O
	ATOM	7831	N	PRO	T	135	23.461	83.347	245.298	1.00	61.16	N
55	ATOM	7832	CA	PRO	T	135	23.454	84.736	244.826	1.00	60.99	C
	ATOM	7834	CB	PRO	T	135	24.934	85.024	244.525	1.00	61.31	C
	ATOM	7837	CG	PRO	T	135	25.702	83.909	245.148	1.00	61.14	C
	ATOM	7840	CD	PRO	T	135	24.790	82.732	245.142	1.00	60.96	C
	ATOM	7843	C	PRO	T	135	22.618	84.959	243.565	1.00	62.40	C
60	ATOM	7844	O	PRO	T	135	22.329	86.109	243.228	1.00	64.14	O
	ATOM	7845	N	GLY	T	136	22.246	83.874	242.881	1.00	60.60	N
	ATOM	7846	CA	GLY	T	136	21.503	83.945	241.629	1.00	60.94	C
	ATOM	7849	C	GLY	T	136	22.429	83.760	240.443	1.00	60.01	C
	ATOM	7850	O	GLY	T	136	23.541	83.244	240.589	1.00	61.56	O
65	ATOM	7852	N	ASP	T	137	21.968	84.195	239.273	1.00	58.33	N
	ATOM	7853	CA	ASP	T	137	22.708	84.051	238.016	1.00	57.86	C
	ATOM	7855	CB	ASP	T	137	23.980	84.913	238.041	1.00	58.76	C
	ATOM	7858	CG	ASP	T	137	24.520	85.214	236.649	1.00	58.58	C
	ATOM	7859	OD1	ASP	T	137	23.715	85.397	235.712	1.00	59.25	O
70	ATOM	7860	OD2	ASP	T	137	25.758	85.280	236.497	1.00	58.95	O
	ATOM	7861	C	ASP	T	137	23.043	82.582	237.722	1.00	56.32	C

	ATOM	7862	O	ASP	T	137	24.155	82.255	237.301	1.00	56.11	O
	ATOM	7864	N	ASN	T	138	22.072	81.703	237.963	1.00	54.25	N
	ATOM	7865	CA	ASN	T	138	22.222	80.277	237.674	1.00	55.50	C
5	ATOM	7867	CB	ASN	T	138	22.449	79.665	236.347	0.00	19.08	C
	ATOM	7870	CG	ASN	T	138	21.185	79.614	235.513	0.00	19.54	C
	ATOM	7871	OD1	ASN	T	138	20.104	79.980	235.967	0.00	18.47	O
	ATOM	7872	ND2	ASN	T	138	21.321	79.148	234.282	0.00	17.88	N
	ATOM	7875	C	ASN	T	138	23.160	79.506	238.605	1.00	55.03	C
10	ATOM	7876	O	ASN	T	138	23.496	78.353	238.327	1.00	56.92	O
	ATOM	7878	N	GLN	T	139	23.572	80.140	239.704	1.00	54.40	N
	ATOM	7879	CA	GLN	T	139	24.492	79.529	240.655	1.00	52.22	C
	ATOM	7881	CB	GLN	T	139	25.334	80.398	241.549	0.00	22.61	C
	ATOM	7884	CG	GLN	T	139	26.540	80.987	240.839	0.00	24.97	C
	ATOM	7887	CD	GLN	T	139	27.338	81.922	241.714	0.00	29.00	C
15	ATOM	7888	OE1	GLN	T	139	27.730	81.563	242.823	0.00	27.17	O
	ATOM	7889	NE2	GLN	T	139	27.584	83.125	241.217	0.00	31.84	N
	ATOM	7892	C	GLN	T	139	23.758	78.508	241.514	1.00	51.18	C
	ATOM	7893	O	GLN	T	139	22.632	78.757	241.956	1.00	50.76	O
	ATOM	7895	N	ALA	T	140	24.397	77.361	241.737	1.00	50.20	N
20	ATOM	7896	CA	ALA	T	140	23.818	76.292	242.550	1.00	48.41	C
	ATOM	7898	CB	ALA	T	140	24.588	74.989	242.344	1.00	48.95	C
	ATOM	7902	C	ALA	T	140	23.797	76.669	244.031	1.00	45.99	C
	ATOM	7903	O	ALA	T	140	24.607	77.480	244.488	1.00	45.62	O
	ATOM	7905	N	CYS	T	141	22.866	76.071	244.771	1.00	43.97	N
25	ATOM	7906	CA	CYS	T	141	22.720	76.325	246.199	1.00	43.13	C
	ATOM	7908	CB	CYS	T	141	21.355	75.840	246.689	1.00	43.11	C
	ATOM	7911	SG	CYS	T	141	19.951	76.627	245.880	1.00	42.95	S
	ATOM	7913	C	CYS	T	141	23.824	75.629	246.989	1.00	41.36	C
	ATOM	7914	O	CYS	T	141	24.165	74.481	246.704	1.00	39.71	O
30	ATOM	7916	N	LYS	T	142	24.369	76.331	247.982	1.00	39.74	N
	ATOM	7917	CA	LYS	T	142	25.455	75.812	248.814	1.00	39.27	C
	ATOM	7919	CB	LYS	T	142	26.747	76.582	248.535	1.00	39.48	C
	ATOM	7922	CG	LYS	T	142	27.247	76.458	247.107	1.00	39.49	C
	ATOM	7925	CD	LYS	T	142	28.626	77.081	246.933	1.00	39.47	C
35	ATOM	7928	CE	LYS	T	142	29.273	76.624	245.629	1.00	40.05	C
	ATOM	7931	NZ	LYS	T	142	30.651	77.165	245.448	1.00	40.15	N
	ATOM	7935	C	LYS	T	142	25.103	75.940	250.297	1.00	37.92	C
	ATOM	7936	O	LYS	T	142	24.443	76.905	250.686	1.00	35.12	O
	ATOM	7938	N	PRO	T	143	25.538	74.968	251.130	1.00	37.46	N
40	ATOM	7939	CA	PRO	T	143	25.329	75.046	252.583	1.00	36.92	C
	ATOM	7941	CB	PRO	T	143	26.148	73.868	253.130	1.00	37.18	C
	ATOM	7944	CG	PRO	T	143	26.333	72.945	252.005	1.00	37.15	C
	ATOM	7947	CD	PRO	T	143	26.240	73.733	250.737	1.00	37.49	C
	ATOM	7950	C	PRO	T	143	25.837	76.354	253.178	1.00	36.09	C
45	ATOM	7951	O	PRO	T	143	26.872	76.863	252.743	1.00	36.46	O
	ATOM	7952	N	TRP	T	144	25.109	76.900	254.151	1.00	35.32	N
	ATOM	7953	CA	TRP	T	144	25.581	78.082	254.869	1.00	34.63	C
	ATOM	7955	CB	TRP	T	144	24.540	78.594	255.873	1.00	32.92	C
	ATOM	7958	CG	TRP	T	144	23.335	79.229	255.262	1.00	32.22	C
50	ATOM	7959	CD1	TRP	T	144	23.246	79.818	254.033	1.00	32.25	C
	ATOM	7961	NE1	TRP	T	144	21.978	80.301	253.831	1.00	32.06	N
	ATOM	7963	CE2	TRP	T	144	21.221	80.043	254.943	1.00	31.60	C
	ATOM	7964	CD2	TRP	T	144	22.047	79.371	255.869	1.00	31.87	C
	ATOM	7965	CE3	TRP	T	144	21.509	78.995	257.105	1.00	32.00	C
55	ATOM	7967	CZ3	TRP	T	144	20.175	79.294	257.372	1.00	32.25	C
	ATOM	7969	CH2	TRP	T	144	19.379	79.961	256.427	1.00	31.91	C
	ATOM	7971	CZ2	TRP	T	144	19.883	80.344	255.212	1.00	32.37	C
	ATOM	7973	C	TRP	T	144	26.861	77.752	255.620	1.00	33.69	C
	ATOM	7974	O	TRP	T	144	26.984	76.676	256.209	1.00	31.62	O
60	ATOM	7976	N	THR	T	145	27.813	78.679	255.584	1.00	35.15	N
	ATOM	7977	CA	THR	T	145	29.010	78.576	256.403	1.00	36.27	C
	ATOM	7979	CB	THR	T	145	30.050	79.655	256.031	1.00	37.26	C
	ATOM	7981	OG1	THR	T	145	30.229	79.682	254.610	1.00	38.70	O
	ATOM	7983	CG2	THR	T	145	31.391	79.373	256.703	1.00	37.30	C
65	ATOM	7987	C	THR	T	145	28.598	78.752	257.863	1.00	36.05	C
	ATOM	7988	O	THR	T	145	28.028	79.779	258.226	1.00	35.93	O
	ATOM	7990	N	ASN	T	146	28.864	77.735	258.679	1.00	36.96	N
	ATOM	7991	CA	ASN	T	146	28.566	77.779	260.107	1.00	37.64	C
	ATOM	7993	CB	ASN	T	146	28.317	76.363	260.644	1.00	37.11	C
70	ATOM	7996	CG	ASN	T	146	27.552	76.357	261.959	1.00	36.74	C
	ATOM	7997	OD1	ASN	T	146	27.968	76.976	262.937	1.00	35.84	O

	ATOM	7998	ND2	ASN	T	146	26.431	75.643	261.988	1.00	36.65	N
	ATOM	8001	C	ASN	T	146	29.718	78.456	260.852	1.00	38.34	C
	ATOM	8002	O	ASN	T	146	30.793	77.874	261.019	1.00	37.86	O
	ATOM	8004	N	CYS	T	147	29.489	79.694	261.281	1.00	39.56	N
5	ATOM	8005	CA	CYS	T	147	30.499	80.472	262.004	1.00	40.67	C
	ATOM	8007	CB	CYS	T	147	30.038	81.924	262.153	1.00	40.90	C
	ATOM	8010	SG	CYS	T	147	29.125	82.554	260.724	1.00	41.14	S
	ATOM	8012	C	CYS	T	147	30.785	79.881	263.384	1.00	40.94	C
10	ATOM	8013	O	CYS	T	147	31.906	79.976	263.889	1.00	40.28	O
	ATOM	8015	N	THR	T	148	29.764	79.264	263.978	1.00	42.22	N
	ATOM	8016	CA	THR	T	148	29.858	78.687	265.316	1.00	43.09	C
	ATOM	8018	CB	THR	T	148	28.500	78.748	266.054	1.00	42.86	C
	ATOM	8020	OG1	THR	T	148	27.573	77.832	265.460	1.00	44.06	O
	ATOM	8022	CG2	THR	T	148	27.921	80.155	265.986	1.00	41.95	C
15	ATOM	8026	C	THR	T	148	30.363	77.247	265.205	1.00	44.36	C
	ATOM	8027	O	THR	T	148	29.627	76.283	265.431	1.00	44.99	O
	ATOM	8029	N	LEU	T	149	31.635	77.129	264.841	1.00	44.84	N
	ATOM	8030	CA	LEU	T	149	32.287	75.839	264.625	1.00	44.50	C
20	ATOM	8032	CB	LEU	T	149	31.800	75.193	263.323	1.00	44.78	C
	ATOM	8035	CG	LEU	T	149	31.976	73.673	263.232	1.00	44.91	C
	ATOM	8037	CD1	LEU	T	149	30.909	72.958	264.051	1.00	45.01	C
	ATOM	8041	CD2	LEU	T	149	31.934	73.206	261.784	1.00	44.87	C
	ATOM	8045	C	LEU	T	149	33.802	76.039	264.581	1.00	44.60	C
	ATOM	8046	O	LEU	T	149	34.550	75.334	265.261	1.00	45.41	O
25	ATOM	8048	N	ALA	T	150	34.240	77.005	263.773	1.00	43.99	N
	ATOM	8049	CA	ALA	T	150	35.644	77.404	263.711	1.00	44.19	C
	ATOM	8051	CB	ALA	T	150	35.858	78.391	262.572	1.00	44.09	C
	ATOM	8055	C	ALA	T	150	36.103	78.019	265.031	1.00	43.90	C
	ATOM	8056	O	ALA	T	150	35.400	78.839	265.623	1.00	43.66	O
30	ATOM	8058	N	THR	T	154	29.358	85.819	264.050	1.00	26.31	N
	ATOM	8059	CA	THR	T	154	28.553	86.131	262.873	1.00	28.57	C
	ATOM	8061	CB	THR	T	154	27.227	85.324	262.872	1.00	29.03	C
	ATOM	8063	OG1	THR	T	154	27.507	83.927	263.035	1.00	28.77	O
	ATOM	8065	CG2	THR	T	154	26.464	85.533	261.571	1.00	28.18	C
35	ATOM	8069	C	THR	T	154	28.242	87.629	262.785	1.00	28.99	C
	ATOM	8070	O	THR	T	154	27.356	88.127	263.481	1.00	30.37	O
	ATOM	8072	N	LEU	T	155	28.979	88.339	261.932	1.00	28.93	N
	ATOM	8073	CA	LEU	T	155	28.745	89.765	261.697	1.00	28.73	C
40	ATOM	8075	CB	LEU	T	155	29.808	90.503	261.060	0.00	30.00	C
	ATOM	8078	CG	LEU	T	155	31.053	90.502	261.946	0.00	30.00	C
	ATOM	8080	CD1	LEU	T	155	32.251	91.061	261.181	0.00	30.00	C
	ATOM	8084	CD2	LEU	T	155	30.783	91.360	263.183	0.00	30.00	C
	ATOM	8088	C	LEU	T	155	27.414	89.993	260.979	1.00	28.71	C
	ATOM	8089	O	LEU	T	155	26.642	90.877	261.356	1.00	27.81	O
45	ATOM	8091	N	GLN	T	156	27.165	89.194	259.940	1.00	28.97	N
	ATOM	8092	CA	GLN	T	156	25.882	89.189	259.233	1.00	29.48	C
	ATOM	8094	CB	GLN	T	156	26.016	89.825	257.844	1.00	30.26	C
	ATOM	8097	CG	GLN	T	156	25.588	91.288	257.802	1.00	30.94	C
	ATOM	8100	CD	GLN	T	156	25.891	91.961	256.475	1.00	31.09	C
50	ATOM	8101	OE1	GLN	T	156	25.928	91.313	255.427	1.00	32.88	O
	ATOM	8102	NE2	GLN	T	156	26.103	93.273	256.514	1.00	31.03	N
	ATOM	8105	C	GLN	T	156	25.349	87.761	259.110	1.00	28.77	C
	ATOM	8106	O	GLN	T	156	26.090	86.858	258.716	1.00	28.10	O
	ATOM	8108	N	PRO	T	157	24.063	87.551	259.448	1.00	28.11	N
55	ATOM	8109	CA	PRO	T	157	23.491	86.211	259.369	1.00	27.91	C
	ATOM	8111	CB	PRO	T	157	22.158	86.352	260.111	1.00	27.94	C
	ATOM	8114	CG	PRO	T	157	21.790	87.778	259.966	1.00	28.02	C
	ATOM	8117	CD	PRO	T	157	23.077	88.546	259.916	1.00	28.09	C
	ATOM	8120	C	PRO	T	157	23.264	85.771	257.925	1.00	27.51	C
60	ATOM	8121	O	PRO	T	157	23.246	86.606	257.016	1.00	27.87	O
	ATOM	8122	N	ALA	T	158	23.106	84.468	257.718	1.00	26.53	N
	ATOM	8123	CA	ALA	T	158	22.831	83.940	256.385	1.00	27.12	C
	ATOM	8125	CB	ALA	T	158	23.194	82.464	256.312	1.00	27.87	C
	ATOM	8129	C	ALA	T	158	21.366	84.143	256.005	1.00	26.16	C
65	ATOM	8130	O	ALA	T	158	20.499	84.269	256.874	1.00	24.55	O
	ATOM	8132	N	SER	T	159	21.111	84.183	254.699	1.00	26.14	N
	ATOM	8133	CA	SER	T	159	19.755	84.261	254.144	1.00	25.62	C
	ATOM	8135	CB	SER	T	159	19.394	85.710	253.817	1.00	26.16	C
	ATOM	8138	OG	SER	T	159	20.210	86.216	252.772	1.00	25.57	O
70	ATOM	8140	C	SER	T	159	19.699	83.421	252.875	1.00	25.53	C
	ATOM	8141	O	SER	T	159	20.713	82.851	252.472	1.00	23.78	O

	ATOM	8143	N	ASN	T	160	18.528	83.349	252.243	1.00	25.37	N
	ATOM	8144	CA	ASN	T	160	18.393	82.630	250.967	1.00	26.15	C
	ATOM	8146	CB	ASN	T	160	16.922	82.562	250.500	1.00	25.49	C
	ATOM	8149	CG	ASN	T	160	16.272	83.940	250.323	1.00	25.82	C
5	ATOM	8150	OD1	ASN	T	160	16.900	84.979	250.538	1.00	27.51	O
	ATOM	8151	ND2	ASN	T	160	14.999	83.943	249.940	1.00	23.50	N
	ATOM	8154	C	ASN	T	160	19.286	83.204	249.859	1.00	26.63	C
	ATOM	8155	O	ASN	T	160	19.781	82.461	249.013	1.00	24.30	O
	ATOM	8157	N	SER	T	161	19.507	84.519	249.891	1.00	27.47	N
10	ATOM	8158	CA	SER	T	161	20.220	85.227	248.821	1.00	28.36	C
	ATOM	8160	CB	SER	T	161	19.539	86.575	248.552	1.00	28.25	C
	ATOM	8163	OG	SER	T	161	19.372	87.313	249.748	1.00	29.60	O
	ATOM	8165	C	SER	T	161	21.722	85.449	249.070	1.00	28.99	C
	ATOM	8166	O	SER	T	161	22.440	85.855	248.153	1.00	29.56	O
15	ATOM	8168	N	SER	T	162	22.198	85.197	250.290	1.00	29.81	N
	ATOM	3169	CA	SER	T	162	23.605	85.456	250.627	1.00	30.17	C
	ATOM	8171	CB	SER	T	162	23.823	86.952	250.891	1.00	30.17	C
	ATOM	8174	OG	SER	T	162	23.028	87.410	251.973	1.00	29.77	O
	ATOM	8176	C	SER	T	162	24.114	84.646	251.823	1.00	30.42	C
20	ATOM	8177	O	SER	T	162	23.342	84.238	252.695	1.00	30.44	O
	ATOM	8179	N	ASP	T	163	25.427	84.431	251.847	1.00	30.81	N
	ATOM	8180	CA	ASP	T	163	26.085	83.661	252.900	1.00	31.76	C
	ATOM	8182	CB	ASP	T	163	27.407	83.084	252.373	1.00	30.27	C
	ATOM	8185	CG	ASP	T	163	27.931	81.924	253.213	1.00	30.14	C
25	ATOM	8186	OD1	ASP	T	163	27.215	81.439	254.116	1.00	29.23	O
	ATOM	8187	OD2	ASP	T	163	29.072	81.487	252.959	1.00	30.39	O
	ATOM	8188	C	ASP	T	163	26.355	84.549	254.116	1.00	32.78	C
	ATOM	8189	O	ASP	T	163	26.437	85.775	253.996	1.00	32.94	O
	ATOM	8191	N	ALA	T	164	26.489	83.922	255.282	1.00	33.65	N
30	ATOM	8192	CA	ALA	T	164	26.854	84.635	256.507	1.00	35.56	C
	ATOM	8194	CB	ALA	T	164	26.635	83.744	257.726	1.00	35.68	C
	ATOM	8198	C	ALA	T	164	28.308	85.109	256.455	1.00	36.88	C
	ATOM	8199	O	ALA	T	164	29.162	84.450	255.851	1.00	36.68	O
	ATOM	8201	N	ILE	T	165	28.573	86.252	257.087	1.00	37.68	N
35	ATOM	8202	CA	ILE	T	165	29.922	86.816	257.181	1.00	37.89	C
	ATOM	8204	CB	ILE	T	165	29.958	88.295	256.711	1.00	37.93	C
	ATOM	8206	CG1	ILE	T	165	29.415	88.416	255.281	1.00	38.14	C
	ATOM	8209	CD1	ILE	T	165	29.190	89.845	254.816	1.00	38.14	C
	ATOM	8213	CG2	ILE	T	165	31.384	88.852	256.786	1.00	37.67	C
40	ATOM	8217	C	ILE	T	165	30.405	86.719	258.629	1.00	38.11	C
	ATOM	8218	O	ILE	T	165	29.613	86.850	259.564	1.00	37.30	O
	ATOM	8220	N	CYS	T	166	31.706	86.493	258.805	1.00	38.75	N
	ATOM	8221	CA	CYS	T	166	32.300	86.302	260.129	1.00	39.81	C
	ATOM	8223	CB	CYS	T	166	33.033	84.964	260.181	1.00	41.59	C
45	ATOM	8226	SG	CYS	T	166	32.030	83.571	259.616	1.00	44.81	S
	ATOM	8228	C	CYS	T	166	33.262	87.434	260.487	1.00	39.70	C
	ATOM	8229	O	CYS	T	166	33.429	88.388	259.725	1.00	39.41	O
	ATOM	8231	S	S04	W	101	23.436	90.519	154.786	1.00	34.98	S
	ATOM	8232	O1	S04	W	101	24.221	91.111	155.861	1.00	35.51	O
50	ATOM	8233	O2	S04	W	101	22.405	89.675	155.374	1.00	39.55	O
	ATOM	8234	O3	S04	W	101	24.308	89.740	153.943	1.00	27.98	O
	ATOM	8235	O4	S04	W	101	22.813	91.573	153.998	1.00	37.81	O
	ATOM	8236	O	HOH	W	102	54.770	107.250	167.229	1.00	18.07	O
	ATOM	8239	O	HOH	W	103	25.783	79.731	188.012	1.00	19.03	O
55	ATOM	8242	O	HOH	W	104	51.166	92.972	163.241	1.00	19.81	O
	ATOM	8245	O	HOH	W	105	10.348	47.286	208.660	1.00	20.45	O
	ATOM	8248	O	HOH	W	106	52.836	101.667	160.751	1.00	28.06	O
	ATOM	8251	O	HOH	W	107	41.023	104.540	163.225	1.00	22.36	O
	ATOM	8254	O	HOH	W	108	20.822	87.787	162.673	1.00	28.40	O
60	ATOM	8257	O	HOH	W	109	41.446	99.657	162.968	1.00	22.67	O
	ATOM	8260	O	HOH	W	110	57.746	103.147	172.937	1.00	24.63	O
	ATOM	8263	O	HOH	W	111	19.283	81.375	168.922	1.00	25.86	O
	ATOM	8266	O	HOH	W	112	29.754	85.296	154.615	1.00	21.18	O
	ATOM	8269	O	HOH	W	113	23.323	79.718	183.259	1.00	27.29	O
65	ATOM	8272	O	HOH	W	114	20.378	79.074	170.287	1.00	29.25	O
	ATOM	8275	O	HOH	W	115	54.352	108.045	175.112	1.00	27.64	O
	ATOM	8278	O	HOH	W	116	-0.552	62.997	204.601	1.00	28.66	O
	ATOM	8281	O	HOH	W	117	42.770	94.541	158.217	1.00	25.15	O
	ATOM	8284	O	HOH	W	118	50.058	91.424	160.988	1.00	27.15	O
70	ATOM	8287	O	HOH	W	119	51.488	99.804	159.890	1.00	25.07	O
	ATOM	8290	O	HOH	W	120	22.574	87.045	156.033	1.00	27.43	O

5	ATOM	8293	0	HOH	W	121	51.410	97.977	157.195	1.00	30.46	O
	ATOM	8296	0	HOH	W	122	19.365	85.192	205.100	1.00	34.57	O
	ATOM	8299	0	HOH	W	123	42.099	103.383	160.947	1.00	33.36	O
	ATOM	8302	0	HOH	W	124	26.180	76.822	192.140	1.00	36.64	O
	ATOM	8305	0	HOH	W	125	14.124	62.157	204.327	1.00	25.15	O
10	ATOM	8308	0	HOH	W	126	20.504	81.744	163.170	1.00	29.14	O
	ATOM	8311	0	HOH	W	127	57.631	109.466	173.328	1.00	35.01	O
	ATOM	8314	0	HOH	W	128	27.008	87.281	169.355	1.00	40.26	O
	ATOM	8317	0	HOH	W	129	7.234	54.883	201.343	1.00	26.63	O
	ATOM	8320	0	HOH	W	130	33.734	90.129	162.692	1.00	34.98	O
15	ATOM	8323	0	HOH	W	131	40.788	107.004	177.231	1.00	28.36	O
	ATOM	8326	0	HOH	W	132	56.672	115.058	167.550	1.00	24.24	O
	ATOM	8329	0	HOH	W	133	9.350	64.811	199.526	1.00	28.91	O
	ATOM	8332	0	HOH	W	134	23.728	79.566	192.471	1.00	27.79	O
	ATOM	8335	0	HOH	W	135	31.380	95.653	163.805	1.00	34.18	O
20	ATOM	8338	0	HOH	W	136	41.350	88.796	175.647	1.00	36.12	O
	ATOM	8341	0	HOH	W	137	58.583	108.754	154.669	1.00	28.17	O
	ATOM	8344	0	HOH	W	138	44.907	114.900	185.320	1.00	31.04	O
	ATOM	8347	0	HOH	W	139	30.997	81.340	156.779	1.00	28.28	O
	ATOM	8350	0	HOH	W	140	57.251	102.563	164.819	1.00	32.60	O
25	ATOM	8353	0	HOH	W	141	6.053	56.262	198.535	1.00	36.10	O
	ATOM	8356	0	HOH	W	142	19.841	57.781	218.581	1.00	33.06	O
	ATOM	8359	0	HOH	W	143	18.890	84.265	181.651	1.00	29.85	O
	ATOM	8362	0	HOH	W	144	32.412	92.346	154.587	1.00	27.81	O
	ATOM	8365	0	HOH	W	145	18.219	78.677	188.227	1.00	31.99	O
30	ATOM	8368	0	HOH	W	146	55.308	101.162	183.952	1.00	26.44	O
	ATOM	8371	0	HOH	W	147	41.971	87.983	161.987	1.00	37.04	O
	ATOM	8374	0	HOH	W	148	32.137	96.404	167.481	1.00	34.32	O
	ATOM	8377	0	HOH	W	149	49.848	110.144	190.055	1.00	30.80	O
	ATOM	8380	0	HOH	W	150	55.676	103.630	183.521	1.00	41.02	O
35	ATOM	8383	0	HOH	W	151	22.226	89.380	179.229	1.00	31.03	O
	ATOM	8386	0	HOH	W	152	42.770	98.607	188.639	1.00	30.68	O
	ATOM	8389	0	HOH	W	153	57.466	98.957	179.802	1.00	36.15	O
	ATOM	8392	0	HOH	W	154	5.028	70.021	204.005	1.00	44.13	O
	ATOM	8395	0	HOH	W	155	59.808	105.621	157.158	1.00	27.98	O
40	ATOM	8398	0	HOH	W	156	44.458	103.036	158.185	1.00	28.58	O
	ATOM	8401	0	HOH	W	157	10.245	83.113	209.503	1.00	36.42	O
	ATOM	8404	0	HOH	W	158	44.142	110.937	165.761	1.00	33.37	O
	ATOM	8407	0	HOH	W	159	7.849	52.554	201.971	1.00	33.60	O
	ATOM	8410	0	HOH	W	160	2.099	61.550	202.373	1.00	30.01	O
45	ATOM	8413	0	HOH	W	161	38.439	92.459	184.732	1.00	32.69	O
	ATOM	8416	0	HOH	W	162	22.985	83.629	158.326	1.00	32.76	O
	ATOM	8419	0	HOH	W	163	31.849	80.837	194.285	1.00	37.65	O
	ATOM	8422	0	HOH	W	164	18.779	72.676	203.893	1.00	47.73	O
	ATOM	8425	0	HOH	W	165	40.121	98.726	188.070	1.00	38.05	O
50	ATOM	8428	0	HOH	W	166	13.071	68.459	195.474	1.00	36.16	O
	ATOM	8431	0	HOH	W	167	17.861	59.243	204.496	1.00	30.52	O
	ATOM	8434	0	HOH	W	168	5.250	48.682	206.105	1.00	38.61	O
	ATOM	8437	0	HOH	W	169	6.131	44.590	198.767	1.00	29.12	O
	ATOM	8440	0	HOH	W	170	52.913	93.472	180.211	1.00	43.87	O
55	ATOM	8443	0	HOH	W	171	42.906	94.798	188.940	1.00	37.25	O
	ATOM	8446	0	HOH	W	172	14.637	74.108	196.014	1.00	36.33	O
	ATOM	8449	0	HOH	W	173	18.074	71.254	208.715	1.00	38.78	O
	ATOM	8452	0	HOH	W	174	41.404	105.303	190.918	1.00	33.98	O
	ATOM	8455	0	HOH	W	175	20.566	95.115	160.531	1.00	49.06	O
60	ATOM	8458	0	HOH	W	176	16.270	59.196	202.257	1.00	31.78	O
	ATOM	8461	0	HOH	W	177	16.598	87.359	194.605	1.00	39.68	O
	ATOM	8464	0	HOH	W	178	16.183	78.973	184.744	1.00	31.10	O
	ATOM	8467	0	HOH	W	179	11.788	81.011	196.129	1.00	30.47	O
	ATOM	8470	0	HOH	W	180	56.277	113.757	165.505	1.00	34.03	O
65	ATOM	8473	0	HOH	W	181	27.916	79.665	170.035	1.00	37.82	O
	ATOM	8476	0	HOH	W	182	40.430	112.933	171.470	1.00	35.13	O
	ATOM	8479	0	HOH	W	183	30.586	90.200	179.381	1.00	63.17	O
	ATOM	8482	0	HOH	W	185	37.611	94.988	154.085	1.00	32.89	O
	ATOM	8485	0	HOH	W	186	22.506	79.494	175.747	1.00	39.27	O
70	ATOM	8488	0	HOH	W	187	48.583	105.727	197.523	1.00	52.75	O
	ATOM	8491	0	HOH	W	188	8.750	62.137	199.368	1.00	41.55	O
	ATOM	8494	0	HOH	W	189	32.671	95.088	171.436	1.00	45.11	O
	ATOM	8497	0	HOH	W	190	11.463	74.312	189.893	1.00	41.06	O
	ATOM	8500	0	HOH	W	191	35.124	102.009	165.479	1.00	34.47	O
	ATOM	8503	0	HOH	W	193	21.896	92.799	197.298	1.00	40.92	O

5	ATOM	8506	0	HOH	W	194	7.314	49.390	225.196	1.00	43.66	0
	ATOM	8509	0	HOH	W	195	32.179	103.988	179.845	1.00	39.44	0
	ATOM	8512	0	HOH	W	196	9.993	43.825	214.884	1.00	39.92	0
	ATOM	8515	0	HOH	W	197	52.368	90.695	164.264	0.33	24.43	0
	ATOM	8518	0	HOH	W	198	0.002	60.464	205.635	0.33	23.11	0
10	ATOM	8521	0	HOH	W	199	52.367	90.695	159.819	0.33	28.10	0
	ATOM	8524	0	HOH	W	200	46.307	100.028	187.959	1.00	45.36	0
	ATOM	8527	0	HOH	W	201	12.425	74.380	204.026	1.00	34.45	0
	ATOM	8530	0	HOH	W	202	59.165	108.588	161.177	1.00	31.50	0
	ATOM	8533	0	HOH	W	203	58.724	108.163	175.517	1.00	40.30	0
15	ATOM	8536	0	HOH	W	204	47.895	91.860	159.377	1.00	37.40	0
	ATOM	8539	0	HOH	W	205	29.501	79.120	157.361	1.00	39.50	0
	ATOM	8542	0	HOH	W	206	35.079	91.104	155.012	1.00	29.96	0
	ATOM	8545	0	HOH	W	207	22.495	77.617	177.306	1.00	50.19	0
	ATOM	8548	0	HOH	W	208	8.337	43.284	202.618	1.00	36.59	0
20	ATOM	8551	0	HOH	W	209	5.442	47.969	214.237	1.00	35.58	0
	ATOM	8554	0	HOH	W	210	0.833	65.609	197.403	1.00	40.43	0
	ATOM	8557	0	HOH	W	211	20.164	65.215	206.995	1.00	43.89	0
	ATOM	8560	0	HOH	W	212	20.074	59.716	203.316	1.00	39.93	0
	ATOM	8563	0	HOH	W	213	27.842	92.430	190.949	1.00	36.03	0
25	ATOM	8566	0	HOH	W	214	18.241	87.493	196.699	1.00	39.37	0
	ATOM	8569	0	HOH	W	215	20.219	83.549	198.012	1.00	33.33	0
	ATOM	8572	0	HOH	W	216	33.512	107.423	176.531	1.00	44.90	0
	ATOM	8575	0	HOH	W	217	14.404	57.827	199.595	1.00	31.83	0
	ATOM	8578	0	HOH	W	218	45.797	107.926	160.727	1.00	47.97	0
30	ATOM	8581	0	HOH	W	219	2.345	56.205	234.550	1.00	42.91	0
	ATOM	8584	0	HOH	W	220	37.657	90.553	165.261	1.00	40.73	0
	ATOM	8587	0	HOH	W	221	52.278	95.771	156.150	1.00	36.34	0
	ATOM	8590	0	HOH	W	222	27.043	89.635	149.322	1.00	46.63	0
	ATOM	8593	0	HOH	W	223	11.645	43.133	223.170	1.00	38.24	0
35	ATOM	8596	0	HOH	W	224	5.644	51.309	225.407	1.00	35.87	0
	ATOM	8599	0	HOH	W	225	11.107	47.101	216.620	1.00	38.48	0
	ATOM	8602	0	HOH	W	226	36.037	108.104	175.082	1.00	41.68	0
	ATOM	8605	0	HOH	W	227	31.887	81.919	181.843	1.00	37.49	0
	ATOM	8608	0	HOH	W	228	24.793	86.884	148.285	1.00	33.64	0
40	ATOM	8611	0	HOH	W	230	13.481	46.239	222.019	1.00	41.95	0
	ATOM	8614	0	HOH	W	232	53.369	111.775	157.875	1.00	39.60	0
	ATOM	8617	0	HOH	W	235	41.200	87.982	157.255	1.00	44.43	0
	ATOM	8620	0	HOH	W	236	16.612	60.703	199.715	1.00	49.63	0
	ATOM	8623	0	HOH	W	238	29.873	95.897	162.001	1.00	37.66	0
45	ATOM	8626	0	HOH	W	239	32.258	100.048	178.534	1.00	38.86	0
	ATOM	8629	0	HOH	W	241	46.356	104.752	156.721	1.00	45.69	0
	ATOM	8632	0	HOH	W	242	37.136	102.994	186.046	1.00	62.70	0
	ATOM	8635	0	HOH	W	243	48.815	112.303	191.146	1.00	42.28	0
	ATOM	8638	0	HOH	W	244	49.861	111.078	162.348	1.00	37.82	0
50	ATOM	8641	0	HOH	W	245	15.180	71.707	187.444	1.00	48.45	0
	ATOM	8644	0	HOH	W	246	12.453	62.230	229.870	1.00	39.77	0
	ATOM	8647	0	HOH	W	247	51.667	112.487	159.789	1.00	47.05	0
	ATOM	8650	0	HOH	W	248	49.601	109.381	160.322	1.00	42.54	0
	ATOM	8653	0	HOH	W	249	43.031	106.103	160.220	1.00	46.86	0
55	ATOM	8656	0	HOH	W	250	39.012	105.745	161.946	1.00	35.16	0
	ATOM	8659	0	HOH	W	251	40.527	106.556	159.585	1.00	52.88	0
	ATOM	8662	0	HOH	W	252	36.784	103.741	161.256	1.00	47.49	0
	ATOM	8665	0	HOH	W	253	31.541	112.141	168.878	1.00	60.98	0
	ATOM	8668	0	HOH	W	254	57.441	100.204	182.407	1.00	35.79	0
60	ATOM	8671	0	HOH	W	255	58.924	102.200	183.026	1.00	46.18	0
	ATOM	8674	0	HOH	W	256	53.323	115.388	192.659	1.00	47.09	0
	ATOM	8677	0	HOH	W	257	31.090	92.765	177.359	1.00	55.44	0
	ATOM	8680	0	HOH	W	258	57.593	105.693	175.608	1.00	42.87	0
	ATOM	8683	0	HOH	W	259	37.393	92.396	153.871	1.00	46.96	0
65	ATOM	8686	0	HOH	W	260	23.675	61.131	226.789	1.00	51.61	0
	ATOM	8689	0	HOH	W	261	17.634	52.195	206.674	1.00	44.40	0
	ATOM	8692	0	HOH	W	262	20.260	52.708	207.200	1.00	37.56	0
	ATOM	8695	0	HOH	W	263	14.074	64.076	229.512	1.00	44.70	0
	ATOM	8698	0	HOH	W	264	9.538	65.041	230.251	1.00	49.75	0
70	ATOM	8701	0	HOH	W	265	3.028	61.888	222.574	1.00	36.43	0
	ATOM	8704	0	HOH	W	266	10.023	71.460	206.573	1.00	47.90	0
	ATOM	8707	0	HOH	W	267	23.371	68.283	210.126	1.00	50.35	0
	ATOM	8710	0	HOH	W	268	22.870	49.531	226.677	1.00	43.65	0
	ATOM	8713	0	HOH	W	269	31.904	99.251	149.957	1.00	52.04	0
	ATOM	8716	0	HOH	W	270	32.801	84.650	150.732	1.00	48.20	0

	ATOM	8719	0	HOH W 271	33.440	84.497	153.363	1.00	49.57	0
	ATOM	8722	0	HOH W 272	24.654	76.881	167.263	1.00	40.34	0
	ATOM	8725	0	HOH W 273	27.291	80.204	167.477	1.00	44.53	0
5	ATOM	8728	0	HOH W 275	20.277	85.533	196.267	1.00	41.93	0
	ATOM	8731	0	HOH W 276	18.279	78.264	178.803	1.00	41.09	0
	ATOM	8734	0	HOH W 277	17.797	79.835	174.353	1.00	39.48	0
	ATOM	8737	0	HOH W 278	21.201	88.456	182.588	1.00	42.99	0
	ATOM	8740	0	HOH W 279	23.028	88.833	186.953	1.00	33.82	0
10	ATOM	8743	0	HOH W 280	25.349	87.591	184.298	1.00	40.23	0
	ATOM	8746	0	HOH W 281	29.258	91.370	189.205	1.00	35.91	0
	ATOM	8749	0	HOH W 282	25.496	80.174	202.241	1.00	46.81	0
	ATOM	8752	0	HOH W 283	20.164	69.464	191.339	1.00	46.09	0
	ATOM	8755	0	HOH W 284	26.981	74.919	190.142	1.00	53.98	0
	ATOM	8758	0	HOH W 285	8.072	82.895	198.325	1.00	37.18	0
15	ATOM	8761	0	HOH W 286	10.593	78.310	189.044	1.00	46.87	0

TABLE 10

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HEADER      ----                      XX-XXX-XX   xxxxx
COMPND      ---
5  REMARK    3
REMARK      3 REFINEMENT.
REMARK      3   PROGRAM      : REFMAC 5.2.0005
REMARK      3   AUTHORS       : MURSHUDOV, VAGIN, DODSON
10 REMARK     3   REFINEMENT TARGET : MAXIMUM LIKELIHOOD
REMARK      3
REMARK      3 DATA USED IN REFINEMENT.
REMARK      3 RESOLUTION RANGE HIGH (ANGSTROMS) : 2.41
REMARK      3 RESOLUTION RANGE LOW  (ANGSTROMS) : 30.00
15 REMARK     3 DATA CUTOFF          (SIGMA(F)) : NONE
REMARK      3 COMPLETENESS FOR RANGE           (%) : 99.86
REMARK      3 NUMBER OF REFLECTIONS              : 19882
REMARK      3
REMARK      3 FIT TO DATA USED IN REFINEMENT.
20 REMARK     3 CROSS-VALIDATION METHOD          : THROUGHOUT
REMARK      3 FREE R VALUE TEST SET SELECTION      : RANDOM
REMARK      3 R VALUE          (WORKING + TEST SET) : 0.21248
REMARK      3 R VALUE          (WORKING SET)        : 0.20825
REMARK      3 FREE R VALUE              : 0.25110
25 REMARK     3 FREE R VALUE TEST SET SIZE      (%) : 10.0
REMARK      3 FREE R VALUE TEST SET COUNT          : 2221
REMARK      3
REMARK      3 FIT IN THE HIGHEST RESOLUTION BIN.
30 REMARK     3 TOTAL NUMBER OF BINS USED                : 25
REMARK      3 BIN RESOLUTION RANGE HIGH                : 2.406
REMARK      3 BIN RESOLUTION RANGE LOW                 : 2.456
REMARK      3 REFLECTION IN BIN (WORKING SET)          : 1144
REMARK      3 BIN COMPLETENESS (WORKING+TEST) (%)      : 99.92
REMARK      3 BIN R VALUE (WORKING SET)                : 0.276
35 REMARK     3 BIN FREE R VALUE SET COUNT                : 133
REMARK      3 BIN FREE R VALUE                        : 0.357
REMARK      3
REMARK      3 NUMBER OF NON-HYDROGEN ATOMS USED IN REFINEMENT.
40 REMARK     3 ALL ATOMS                      : 2175
REMARK      3
REMARK      3 B VALUES .
REMARK      3 FROM WILSON PLOT (A**2) : NULL
REMARK      3 MEAN B VALUE (OVERALL, A**2) : 38.975
REMARK      3 OVERALL ANISOTROPIC B VALUE.
45 REMARK     3 B11 (A**2) : 1.91
REMARK      3 B22 (A**2) : 1.91
REMARK      3 B33 (A**2) : -2.87
REMARK      3 B12 (A**2) : 0.96
REMARK      3 B13 (A**2) : 0.00
50 REMARK     3 B23 (A**2) : 0.00
REMARK      3
REMARK      3 ESTIMATED OVERALL COORDINATE ERROR.
REMARK      3 ESU BASED ON R VALUE (A) : 0.229
REMARK      3 ESU BASED ON FREE R VALUE (A) : 0.207
55 REMARK     3 ESU BASED ON MAXIMUM LIKELIHOOD (A) : 0.136
REMARK      3 ESU FOR B VALUES BASED ON MAXIMUM LIKELIHOOD (A**2) : 11.211
REMARK      3
REMARK      3 CORRELATION COEFFICIENTS .
REMARK      3 CORRELATION COEFFICIENT FO-FC : 0.941
60 REMARK     3 CORRELATION COEFFICIENT FO-FC FREE : 0.913
REMARK      3
REMARK      3 RMS DEVIATIONS FROM IDEAL VALUES
REMARK      3 BOND LENGTHS REFINED ATOMS (A) : 2143 ; 0.007 ; 0.022
REMARK      3 BOND LENGTHS OTHERS (A) : 1831 ; 0.001 ; 0.020
65 REMARK     3 BOND ANGLES REFINED ATOMS (DEGREES) : 2910 ; 1.109 ; 1.974
REMARK      3 BOND ANGLES OTHERS (DEGREES) : 4310 ; 0.694 ; 3.000
REMARK      3 TORSION ANGLES, PERIOD 1 (DEGREES) : 264 ; 5.866 ; 5.000
REMARK      3 TORSION ANGLES, PERIOD 2 (DEGREES) : 96 ; 35.790 ; 25.104
REMARK      3 TORSION ANGLES, PERIOD 3 (DEGREES) : 360 ; 14.019 ; 15.000
70 REMARK     3 TORSION ANGLES, PERIOD 4 (DEGREES) : 10 ; 13.332 ; 15.000
REMARK      3 CHIRAL-CENTER RESTRAINTS (A**3) : 320 ; 0.067 ; 0.200

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REMARK 3 GENERAL PLANES REFINED ATOMS (A) : 2359 ; 0.003 ; 0.020
REMARK 3 GENERAL PLANES OTHERS (A) : 393 ; 0.001 ; 0.020
REMARK 3 NON-BONDED CONTACTS DEFINED ATOMS (A) : 343 ; 0.172 ; 0.200
REMARK 3 NON-BONDED CONTACTS OTHERS (A) : 1692 ; 0.168 ; 0.200
5 REMARK 3 NON-BONDED TORSION REFINED ATOMS (A) : 976 ; 0.170 ; 0.200
REMARK 3 NON-BONDED TORSION OTHERS (A) : 1284 ; 0.080 ; 0.200
REMARK 3 H-BOND (X...Y) REFINED ATOMS (A) : 84 ; 0.155 ; 0.200
REMARK 3 SYMMETRY VDW REFINED ATOMS (A) : 9 ; 0.124 ; 0.200
REMARK 3 SYMMETRY VDW OTHERS (A) : 47 ; 0.158 ; 0.200
10 REMARK 3 SYMMETRY H-BOND REFINED ATOMS (A) : 12 ; 0.328 ; 0.200
REMARK 3
REMARK 3 ISOTROPIC THERMAL FACTOR RESTRAINTS . COUNT RMS WEIGHT
REMARK 3 MAIN-CHAIN BOND REFINED ATOMS (A**2) : 1708 ; 2.242 ; 2.500
REMARK 3 MAIN-CHAIN BOND OTHER ATOMS (A**2) : 537 ; 0.368 ; 2.500
15 REMARK 3 MAIN-CHAIN ANGLE REFINED ATOMS (A**2) : 2155 ; 2.877 ; 5.000
REMARK 3 SIDE-CHAIN BOND REFINED ATOMS (A**2) : 938 ; 1.909 ; 2.500
REMARK 3 SIDE-CHAIN ANGLE REFINED ATOMS (A**2) : 755 ; 2.852 ; 5.000
REMARK 3
REMARK 3 NCS RESTRAINTS STATISTICS
20 REMARK 3 NUMBER OF NCS GROUPS : NULL
REMARK 3
REMARK 3
REMARK 3 TLS DETAILS
REMARK 3 NUMBER OF TLS GROUPS : 4
25 REMARK 3 ATOM RECORD CONTAINS RESIDUAL B FACTORS ONLY
REMARK 3
REMARK 3 TLS GROUP : 1
REMARK 3 NUMBER OF COMPONENTS GROUP : 1
REMARK 3 COMPONENTS C SSSEQUI TO C SSSEQUI
30 REMARK 3 RESIDUE RANGE : F 58 F 200
REMARK 3 ORIGIN FOR THE GROUP (A) : -7.8785 50.6023 72.1994
REMARK 3 T TENSOR
REMARK 3 T11: -0.1062 T22: -0.1850
REMARK 3 T33: -0.0686 T12: 0.0015
35 REMARK 3 T13: 0.0020 T23: -0.0049
REMARK 3 L TENE30R
REMARK 3 L11: 3.8381 L22: 2.1796
REMARK 3 L33: 4.3252 L12: -0.8241
REMARK 3 L13: -2.1881 L23: 0.5823
40 REMARK 3 S TENJ30R
REMARK 3 S11: -0.2276 S12: -0.0799 S13: -0.4435
REMARK 3 S21: 0.1453 S22: 0.0664 S23: 0.2325
REMARK 3 S31: 0.4190 S32: -0.0636 S33: 0.1612
REMARK 3
45 REMARK 3 TLS GROUP : 2
REMARK 3 NUMBER OF COMPONENTS GROUP : 1
REMARK 3 COMPONENTS C SSSEQUI TO C SSSEQUI
REMARK 3 RESIDUE RANGE : R 29 R 108
50 REMARK 3 ORIGIN FOR THE GROUP (A) : 13.7010 41.2586 66.6269
REMARK 3 T TENSOR
REMARK 3 T11: -0.0682 T22: -0.1533
REMARK 3 T33: -0.0925 T12: 0.0389
REMARK 3 T13: 0.0388 T23: 0.0193
REMARK 3 L TENJ30R
55 REMARK 3 L11: 1.9807 L22: 2.6417
REMARK 3 L33: 11.0623 L12: -0.2957
REMARK 3 L13: 2.3891 L23: 1.0837
REMARK 3 S TENS;OR
REMARK 3 S11: 0.1067 S12: 0.2259 S13: -0.2228
60 REMARK 3 S21: -0.2702 S22: -0.2205 S23: -0.0924
REMARK 3 S31: 0.1546 S32: 0.3839 S33: 0.1138
REMARK 3
REMARK 3 TLS GROUP : 3
REMARK 3 NUMBER OF COMPONENTS GROUP : 1
65 REMARK 3 COMPONENTS C SSSEQUI TO C SSSEQUI
REMARK 3 RESIDUE RANGE : R 109 R 140
REMARK 3 ORIGIN FOR THE GROUP (A) : 11.6952 43.2929 95.7162
REMARK 3 T TENSOR
REMARK 3 T11: 0.1892 T22: -0.1001
70 REMARK 3 T33: -0.0550 T12: 0.0496
REMARK 3 T13: 0.0457 T23: 0.0097

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REMARK 3 L TENSOR
REMARK 3 L11 : 3.7438 L22 : 10.2790
REMARK 3 L33 : 17.8915 L12 : 3.7855
REMARK 3 L13 : -2.0543 L23 : -12.4767
5 REMARK 3 S TENSOR
REMARK 3 S11 : 0.3741 S12 : 0.4377 S13 : 0.5374
REMARK 3 S21 : 1.1423 S22 : 0.1023 S23 : 0.4310
REMARK 3 S31 : -1.4776 S32 : -0.6530 S33 : -0.4764
REMARK 3
10 REMARK 3 TLS GROUP : 4
REMARK 3 NUMBER OF COMPONENTS GROUP : 1
REMARK 3 COMPONENTS C SSSEQI TO C SSSEQI
REMARK 3 RESIDUE RANGE : R 141 R 200
REMARK 3 ORIGIN FOR THE GROUP (A) : 8.7716 33.7127 113.0385
15 REMARK 3 T TENSOR
REMARK 3 T11 : 0.3210 T22 : 0.1111
REMARK 3 T33 : -0.1255 T12 : -0.0831
REMARK 3 T13 : 0.0000 T23 : -0.0175
REMARK 3 L TENSOR
20 REMARK 3 L11 : 12.7405 L22 : 12.4875
REMARK 3 L33 : 34.5604 L12 : 2.0421
REMARK 3 L13 : -12.3548 L23 : -14.4159
REMARK 3 S TENSOR
REMARK 3 S11 : 0.1582 S12 : -1.6300 S13 : -0.6502
25 REMARK 3 S21 : 1.3331 S22 : -0.4932 S23 : 0.1028
REMARK 3 S31 : -1.0266 S32 : 1.5312 S33 : 0.3350
REMARK 3
REMARK 3
30 REMARK 3 BULK SOLVENT MODELLING.
REMARK 3 METHOD USED : MASK
REMARK 3 PARAMETERS FOR MASK CALCULATION
REMARK 3 VDW PROBE RADIUS : 1.40
REMARK 3 ION PROBE RADIUS : 0.80
REMARK 3 SHRINKAGE RADIUS : 0.80
35 REMARK 3
REMARK 3 OTHER REFINEMENT REMARKS :
REMARK 3 HYDROGENS HAVE BEEN ADDED IN THE RIDING POSITIONS
REMARK 3
SSBOND 1 CYS F 97 CYS F 181
40 LINK C1 NAG F 200 1.439 ND2 ASN F 152 NAG-
ASN
SSBOND 2 CYS R 31 CYS R 42
SSBOND 3 CYS R 43 CYS R 56
SSBOND 4 CYS R 46 CYS R 64
45 SSBOND 5 CYS R 67 CYS R 81
SSBOND 6 CYS R 84 CYS R 99
SSBOND 7 CYS R 87 CYS R 107
SSBOND 8 CYS R 109 CYS R 125
SSBOND 9 CYS R 128 CYS R 141
50 SSBOND 10 CYS R 147 CYS R 166
LINK C1 NAG R 200 1.439 ND2 ASN R 160 NAG-
ASN
MODRES NAG F 200 NAG-b-D RENAME
MODRES NAG R 200 NAG-b-D RENAME
55 CRYST1 111 .903 111.903 233.238 90.00 90.00 120.00 H 3 2
SCALE1 0.008936 0.005159 0.000000 0.000000
SCALE2 0.000000 0.010319 0.000000 0.000000
SCALE3 0.000000 0.000000 0.004287 0.000000
60 ATOM 1 N ARG F 58 -8.066 59.372 53.307 1.00 58.49 N
ATOM 2 CA ARG F 58 -6.756 58.742 52.936 1.00 56.65 C
ATOM 4 CB ARG F 58 -6.019 59.599 51.900 1.00 58.42 C
ATOM 7 CG ARG F 58 -4.970 58.832 51.105 1.00 61.43 C
ATOM 10 CD ARG F 58 -4.191 59.757 50.175 1.00 64.49 C
ATOM 13 NE ARG F 58 -5.012 60.284 49.084 1.00 65.39 N
65 ATOM 15 CZ ARG F 58 -4.701 61.350 48.342 1.00 68.08 C
ATOM 16 NH1 ARG F 58 -3.580 62.036 48.560 1.00 68.21 N
ATOM 19 NH2 ARG F 58 -5.522 61.739 47.369 1.00 68.35 N
ATOM 22 C ARG F 58 -5.858 58.516 54.153 1.00 51.17 C
ATOM 23 O ARG F 58 -5.102 57.545 54.196 1.00 50.16 O
70 ATOM 27 N ILE F 59 -5.934 59.422 55.128 1.00 47.64 N
ATOM 28 CA ILE F 59 -5.190 59.288 56.381 1.00 47.31 C

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5	ATOM	30	CB	ILE	F	59	-5.233	60.597	57.225	1.00	47.48	C
	ATOM	32	CG1	ILE	F	59	-4.504	61.735	56.493	1.00	49.70	C
	ATOM	35	CD1	ILE	F	59	-3.009	61.526	56.283	1.00	50.48	C
	ATOM	39	CG2	ILE	F	59	-4.638	60.392	58.617	1.00	46.65	C
	ATOM	43	C	ILE	F	59	-5.754	58.132	57.198	1.00	42.96	C
10	ATOM	44	O	ILE	F	59	-6.961	58.015	57.362	1.00	42.46	O
	ATOM	46	N	GLN	F	60	-4.863	57.277	57.695	1.00	42.46	N
	ATOM	47	CA	GLN	F	60	-5.253	56.142	58.520	1.00	40.15	C
	ATOM	49	CB	GLN	F	60	-4.151	55.082	58.527	1.00	37.56	C
	ATOM	52	CG	GLN	F	60	-3.888	54.446	57.174	1.00	37.51	C
15	ATOM	55	CD	GLN	F	60	-4.732	53.211	56.889	1.00	36.17	C
	ATOM	56	OE1	GLN	F	60	-5.080	52.450	57.797	1.00	35.68	O
	ATOM	57	NE2	GLN	F	60	-5.032	52.987	55.610	1.00	32.67	N
	ATOM	60	C	GLN	F	60	-5.557	56.621	59.940	1.00	39.06	C
	ATOM	61	O	GLN	F	60	-4.647	56.944	60.714	1.00	34.97	O
20	ATOM	63	N	SER	F	61	-6.847	56.693	60.262	1.00	38.09	N
	ATOM	64	CA	SER	F	61	-7.284	57.127	61.585	1.00	38.03	C
	ATOM	66	CB	SER	F	61	-7.350	58.659	61.669	1.00	36.83	C
	ATOM	69	OG	SER	F	61	-8.551	59.159	61.115	1.00	36.77	O
	ATOM	71	C	SER	F	61	-8.634	56.525	61.947	1.00	37.56	C
25	ATOM	72	O	SER	F	61	-9.398	56.108	61.072	1.00	38.68	O
	ATOM	74	N	ILE	F	62	-8.911	56.471	63.247	1.00	37.77	N
	ATOM	75	CA	ILE	F	62	-10.161	55.912	63.744	1.00	39.42	C
	ATOM	77	CB	ILE	F	62	-10.074	54.360	63.840	1.00	39.72	C
	ATOM	79	CG1	ILE	F	62	-11.465	53.740	64.025	1.00	41.38	C
30	ATOM	82	CD1	ILE	F	62	-11.472	52.234	63.905	1.00	40.54	C
	ATOM	86	CG2	ILE	F	62	-9.144	53.920	64.956	1.00	39.35	C
	ATOM	90	C	ILE	F	62	-10.530	56.498	65.106	1.00	40.39	C
	ATOM	91	O	ILE	F	62	-9.652	56.785	65.926	1.00	39.04	O
	ATOM	93	N	LYS	F	63	-11.833	56.680	65.319	1.00	41.91	N
35	ATOM	94	CA	LYS	F	63	-12.407	56.956	66.643	1.00	41.77	C
	ATOM	96	CB	LYS	F	63	-13.314	58.175	66.592	1.00	42.73	C
	ATOM	99	CG	LYS	F	63	-13.748	58.699	67.951	1.00	45.72	C
	ATOM	102	CD	LYS	F	63	-14.860	59.732	67.772	1.00	46.90	C
	ATOM	105	CE	LYS	F	63	-14.845	60.802	68.856	1.00	49.93	C
40	ATOM	108	NZ	LYS	F	63	-15.995	61.747	68.699	1.00	51.44	N
	ATOM	112	C	LYS	F	63	-13.214	55.728	67.095	1.00	40.14	C
	ATOM	113	O	LYS	F	63	-14.175	55.325	66.438	1.00	39.40	O
	ATOM	115	N	VAL	F	64	-12.799	55.137	68.207	1.00	38.33	N
	ATOM	116	CA	VAL	F	64	-13.477	53.995	68.804	1.00	40.38	C
45	ATOM	118	CB	VAL	F	64	-12.462	52.848	69.111	1.00	41.99	C
	ATOM	120	CG1	VAL	F	64	-13.034	51.833	70.096	1.00	41.32	C
	ATOM	124	CG2	VAL	F	64	-12.029	52.168	67.820	1.00	42.76	C
	ATOM	128	C	VAL	F	64	-14.183	54.424	70.094	1.00	37.52	C
	ATOM	129	O	VAL	F	64	-13.645	55.208	70.881	1.00	36.68	O
50	ATOM	131	N	GLN	F	65	-15.389	53.907	70.297	1.00	36.59	N
	ATOM	132	CA	GLN	F	65	-16.088	54.045	71.576	1.00	39.52	C
	ATOM	134	CB	GLN	F	65	-17.436	54.755	71.387	1.00	37.77	C
	ATOM	137	CG	GLN	F	65	-17.252	56.218	71.016	1.00	37.67	C
	ATOM	140	CD	GLN	F	65	-18.518	56.920	70.597	1.00	37.85	C
55	ATOM	141	OE1	GLN	F	65	-19.499	56.299	70.188	1.00	38.69	O
	ATOM	142	NE2	GLN	F	65	-18.494	58.236	70.678	1.00	36.91	N
	ATOM	145	C	GLN	F	65	-16.280	52.674	72.198	1.00	40.08	C
	ATOM	146	O	GLN	F	65	-16.169	51.651	71.519	1.00	41.65	O
	ATOM	148	N	PHE	F	66	-16.537	52.664	73.499	1.00	40.06	N
60	ATOM	149	CA	PHE	F	66	-16.828	51.433	74.222	1.00	39.35	C
	ATOM	151	CB	PHE	F	66	-15.537	50.727	74.659	1.00	38.78	C
	ATOM	154	CG	PHE	F	66	-14.565	51.609	75.405	1.00	38.58	C
	ATOM	155	CD1	PHE	F	66	-13.628	52.369	74.721	1.00	38.38	C
	ATOM	157	CE1	PHE	F	66	-12.731	53.176	75.417	1.00	39.28	C
65	ATOM	159	CZ	PHE	F	66	-12.765	53.218	76.822	1.00	37.27	C
	ATOM	161	CE2	PHE	F	66	-13.682	52.461	77.503	1.00	37.24	C
	ATOM	163	CD2	PHE	F	66	-14.577	51.659	76.800	1.00	39.05	C
	ATOM	165	C	PHE	F	66	-17.737	51.737	75.413	1.00	41.76	C
	ATOM	166	O	PHE	F	66	-17.486	52.678	76.179	1.00	40.06	O
70	ATOM	168	N	THR	F	67	-18.822	50.970	75.522	1.00	42.72	N
	ATOM	169	CA	THR	F	67	-19.793	51.128	76.606	1.00	43.44	C
	ATOM	171	CB	THR	F	67	-21.075	51.850	76.116	1.00	44.64	C
	ATOM	173	OG1	THR	F	67	-21.825	50.992	75.244	1.00	45.40	O
	ATOM	175	CG2	THR	F	67	-20.720	53.126	75.364	1.00	47.40	C
	ATOM	179	C	THR	F	67	-20.168	49.786	77.257	1.00	44.06	C

5	ATOM	180	O	THR	F	67	-20.254	49.695	78.481	1.00	44.75	O
	ATOM	182	N	GLU	F	68	-20.387	48.756	76.443	1.00	44.26	N
	ATOM	183	CA	GLU	F	68	-20.831	47.455	76.936	1.00	45.71	C
	ATOM	185	CB	GLU	F	68	-21.557	46.701	75.820	1.00	46.87	C
	ATOM	188	CG	GLU	F	68	-22.364	45.498	76.290	1.00	48.57	C
10	ATOM	191	CD	GLU	F	68	-22.823	44.591	75.152	1.00	50.54	C
	ATOM	192	OE1	GLU	F	68	-22.578	44.919	73.972	1.00	51.01	O
	ATOM	193	OE2	GLU	F	68	-23.433	43.538	75.448	1.00	54.16	O
	ATOM	194	C	GLU	F	68	-19.655	46.615	77.454	1.00	45.18	C
	ATOM	195	O	GLU	F	68	-18.704	46.364	76.728	1.00	45.34	O
15	ATOM	197	N	TYR	F	69	-19.739	46.181	78.708	1.00	44.43	N
	ATOM	198	CA	TYR	F	69	-18.733	45.318	79.321	1.00	46.97	C
	ATOM	200	CB	TYR	F	69	-18.407	45.824	80.729	1.00	43.39	C
	ATOM	203	CG	TYR	F	69	-17.190	45.189	81.380	1.00	43.27	C
	ATOM	204	CD1	TYR	F	69	-15.902	45.527	80.973	1.00	43.51	C
20	ATOM	206	CE1	TYR	F	69	-14.782	44.962	81.577	1.00	43.05	C
	ATOM	208	CZ	TYR	F	69	-14.948	44.058	82.612	1.00	42.56	C
	ATOM	209	OH	TYR	F	69	-13.847	43.495	83.217	1.00	43.08	O
	ATOM	211	CE2	TYR	F	69	-16.215	43.709	83.036	1.00	42.19	C
	ATOM	213	CD2	TYR	F	69	-17.327	44.276	82.424	1.00	43.05	C
25	ATOM	215	C	TYR	F	69	-19.260	43.883	79.383	1.00	48.46	C
	ATOM	216	O	TYR	F	69	-20.242	43.603	80.073	1.00	45.35	O
	ATOM	218	N	LYS	F	70	-18.611	42.986	78.645	1.00	52.61	N
	ATOM	219	CA	LYS	F	70	-18.967	41.568	78.642	1.00	56.94	C
	ATOM	221	CB	LYS	F	70	-18.932	41.012	77.219	1.00	58.20	C
30	ATOM	224	CG	LYS	F	70	-20.142	41.396	76.375	1.00	60.12	C
	ATOM	227	CD	LYS	F	70	-20.294	40.472	75.169	1.00	61.22	C
	ATOM	230	CE	LYS	F	70	-20.930	39.132	75.552	1.00	63.13	C
	ATOM	233	NZ	LYS	F	70	-20.662	38.073	74.533	1.00	62.18	N
	ATOM	237	C	LYS	F	70	-18.018	40.780	79.543	1.00	59.04	C
35	ATOM	238	O	LYS	F	70	-16.821	41.067	79.593	1.00	57.20	O
	ATOM	240	N	LYS	F	71	-18.564	39.781	80.239	1.00	64.32	N
	ATOM	241	CA	LYS	F	71	-17.832	39.027	81.268	1.00	65.32	C
	ATOM	243	CB	LYS	F	71	-18.672	37.837	81.756	1.00	67.52	C
	ATOM	246	CG	LYS	F	71	-18.043	37.043	82.907	1.00	67.88	C
40	ATOM	249	CD	LYS	F	71	-18.702	35.678	83.091	1.00	68.02	C
	ATOM	252	CE	LYS	F	71	-17.885	34.788	84.019	1.00	68.00	C
	ATOM	255	NZ	LYS	F	71	-18.663	33.604	84.481	1.00	67.74	N
	ATOM	259	C	LYS	F	71	-16.457	38.542	80.797	1.00	67.15	C
	ATOM	260	O	LYS	F	71	-15.427	38.988	81.314	1.00	68.33	O
45	ATOM	262	N	GLU	F	72	-16.442	37.643	79.816	1.00	66.64	N
	ATOM	263	CA	GLU	F	72	-15.192	37.049	79.335	1.00	66.21	C
	ATOM	265	CB	GLU	F	72	-15.304	35.518	79.319	1.00	68.61	C
	ATOM	268	CG	GLU	F	72	-15.722	34.931	80.671	1.00	69.08	C
	ATOM	271	CD	GLU	F	72	-15.503	33.433	80.769	1.00	69.95	C
50	ATOM	272	OE1	GLU	F	72	-14.520	32.930	80.181	1.00	72.23	O
	ATOM	273	OE2	GLU	F	72	-16.310	32.758	81.447	1.00	70.17	O
	ATOM	274	C	GLU	F	72	-14.804	37.596	77.961	1.00	64.57	C
	ATOM	275	O	GLU	F	72	-14.531	36.845	77.023	1.00	65.25	O
	ATOM	211	N	LYS	F	73	-14.778	38.920	77.864	1.00	62.67	N
55	ATOM	278	CA	LYS	F	73	-14.353	39.619	76.647	1.00	59.75	C
	ATOM	280	CB	LYS	F	73	-15.445	39.537	75.567	1.00	62.78	C
	ATOM	283	CG	LYS	F	73	-14.977	39.916	74.149	1.00	63.42	C
	ATOM	286	CD	LYS	F	73	-15.953	39.408	73.078	1.00	63.02	C
	ATOM	289	CE	LYS	F	73	-15.671	40.002	71.693	1.00	63.65	C
60	ATOM	292	NZ	LYS	F	73	-14.435	39.461	71.037	1.00	63.28	N
	ATOM	296	C	LYS	F	73	-13.979	41.084	76.924	1.00	55.49	C
	ATOM	297	O	LYS	F	73	-13.140	41.653	76.222	1.00	53.60	O
	ATOM	299	N	GLY	F	74	-14.607	41.689	77.935	1.00	51.53	N
	ATOM	300	CA	GLY	F	74	-14.312	43.066	78.339	1.00	47.77	C
65	ATOM	303	C	GLY	F	74	-15.177	44.063	77.595	1.00	40.13	C
	ATOM	304	O	GLY	F	74	-16.209	43.704	77.041	1.00	36.92	O
	ATOM	306	N	PHE	F	75	-14.752	45.321	77.584	1.00	41.78	N
	ATOM	307	CA	PHE	F	75	-15.457	46.371	76.841	1.00	41.77	C
	ATOM	309	CB	PHE	F	75	-14.864	47.754	77.132	1.00	38.29	C
70	ATOM	312	CG	PHE	F	75	-15.282	48.322	78.464	1.00	38.25	C
	ATOM	313	CD1	PHE	F	75	-16.576	48.796	78.657	1.00	38.72	C
	ATOM	315	CE1	PHE	F	75	-16.974	49.315	79.887	1.00	38.08	C
	ATOM	317	CZ	PHE	F	75	-16.075	49.357	80.937	1.00	38.52	C
	ATOM	319	CE2	PHE	F	75	-14.778	48.883	80.758	1.00	37.82	C
	ATOM	321	CD2	PHE	F	75	-14.391	48.371	79.526	1.00	37.77	C

5	ATOM	323	C	PHE	F	75	-15.469	46.096	75.333	1.00	41.91	C
	ATOM	324	O	PHE	F	75	-14.445	45.734	74.737	1.00	40.98	O
	ATOM	326	N	ILE	F	76	-16.645	46.261	74.735	1.00	42.39	N
	ATOM	327	CA	ILE	F	76	-16.841	46.017	73.308	1.00	41.90	C
	ATOM	329	CB	ILE	F	76	-18.297	45.575	73.000	1.00	41.54	C
10	ATOM	331	CG1	ILE	F	76	-18.687	44.355	73.843	1.00	41.53	C
	ATOM	334	CD1	ILE	F	76	-17.820	43.138	73.635	1.00	42.80	C
	ATOM	338	CG2	ILE	F	76	-18.478	45.281	71.511	1.00	41.15	C
	ATOM	342	C	ILE	F	76	-16.507	47.294	72.545	1.00	39.95	C
	ATOM	343	O	ILE	F	76	-17.090	48.345	72.813	1.00	38.39	O
15	ATOM	345	N	LEU	F	77	-15.564	47.196	71.608	1.00	38.25	N
	ATOM	346	CA	LEU	F	77	-15.127	48.347	70.824	1.00	38.89	C
	ATOM	348	CB	LEU	F	77	-13.690	48.160	70.327	1.00	38.78	C
	ATOM	351	CG	LEU	F	77	-12.561	47.944	71.341	1.00	35.86	C
	ATOM	353	CD1	LEU	F	77	-11.226	48.028	70.622	1.00	35.83	C
20	ATOM	357	CD2	LEU	F	77	-12.611	48.940	72.499	1.00	34.56	C
	ATOM	361	C	LEU	F	77	-16.045	48.568	69.627	1.00	39.58	C
	ATOM	362	O	LEU	F	77	-16.250	47.665	68.820	1.00	39.30	O
	ATOM	364	N	THR	F	78	-16.584	49.783	69.521	1.00	42.21	N
	ATOM	365	CA	THR	F	78	-17.463	50.178	68.422	1.00	40.01	C
25	ATOM	367	CB	THR	F	78	-18.889	50.526	68.940	1.00	39.74	C
	ATOM	369	OG1	THR	F	78	-18.830	51.653	69.823	1.00	41.89	O
	ATOM	371	CG2	THR	F	78	-19.497	49.343	69.697	1.00	37.63	C
	ATOM	375	C	THR	F	78	-16.869	51.370	67.653	1.00	38.43	C
	ATOM	376	O	THR	F	78	-16.140	52.179	68.213	1.00	36.20	O
30	ATOM	378	N	SER	F	79	-17.165	51.436	66.358	1.00	41.65	N
	ATOM	379	CA	SER	F	79	-16.787	52.557	65.502	1.00	44.07	C
	ATOM	381	CB	SER	F	79	-15.357	52.401	64.995	1.00	44.28	C
	ATOM	384	OG	SER	F	79	-15.222	51.262	64.172	1.00	44.96	O
	ATOM	386	C	SER	F	79	-17.746	52.615	64.323	1.00	47.37	C
35	ATOM	387	O	SER	F	79	-18.565	51.716	64.150	1.00	46.09	O
	ATOM	389	N	GLN	F	80	-17.641	53.671	63.515	1.00	51.57	N
	ATOM	390	CA	GLN	F	80	-18.480	53.820	62.316	1.00	49.85	C
	ATOM	392	CB	GLN	F	80	-18.670	55.296	61.965	1.00	49.14	C
	ATOM	395	CG	GLN	F	80	-19.511	55.527	60.715	1.00	51.31	C
40	ATOM	398	CD	GLN	F	80	-19.700	56.996	60.402	1.00	52.92	C
	ATOM	399	OE1	GLN	F	80	-20.142	57.771	61.257	1.00	56.02	O
	ATOM	400	NE2	GLN	F	80	-19.375	57.389	59.168	1.00	50.15	N
	ATOM	403	C	GLN	F	80	-17.862	53.077	61.128	1.00	48.98	C
	ATOM	404	O	GLN	F	80	-16.691	53.274	60.808	1.00	46.25	O
45	ATOM	406	N	LYS	F	81	-18.669	52.250	60.464	1.00	50.59	N
	ATOM	407	CA	LYS	F	81	-18.194	51.402	59.364	1.00	52.32	C
	ATOM	409	CB	LYS	F	81	-18.972	50.077	59.338	1.00	57.01	C
	ATOM	412	CG	LYS	F	81	-19.090	49.381	60.706	1.00	59.64	C
	ATOM	415	CD	LYS	F	81	-17.738	49.227	61.407	1.00	59.75	C
50	ATOM	418	CE	LYS	F	81	-17.887	48.643	62.811	1.00	59.83	C
	ATOM	421	NZ	LYS	F	81	-16.628	48.734	63.622	1.00	58.60	N
	ATOM	425	C	LYS	F	81	-18.279	52.082	57.995	1.00	50.75	C
	ATOM	426	O	LYS	F	81	-17.569	51.691	57.068	1.00	49.69	O
	ATOM	428	N	GLU	F	82	-19.147	53.084	57.868	1.00	49.62	N
55	ATOM	429	CA	GLU	F	82	-19.250	53.857	56.635	1.00	49.12	C
	ATOM	431	CB	GLU	F	82	-20.528	54.700	56.608	1.00	49.43	C
	ATOM	434	CG	GLU	F	82	-21.813	53.899	56.476	1.00	52.96	C
	ATOM	437	CD	GLU	F	82	-22.457	53.566	57.809	1.00	54.62	C
	ATOM	438	OE1	GLU	F	82	-23.699	53.455	57.830	1.00	54.41	O
60	ATOM	439	OE2	GLU	F	82	-21.737	53.423	58.827	1.00	55.37	O
	ATOM	440	C	GLU	F	82	-18.042	54.775	56.477	1.00	45.82	C
	ATOM	441	O	GLU	F	82	-17.730	55.555	57.374	1.00	43.51	O
	ATOM	443	N	ASP	F	83	-17.397	54.687	55.316	1.00	47.86	N
	ATOM	444	CA	ASP	F	83	-16.183	55.449	54.991	1.00	50.62	C
65	ATOM	446	CB	ASP	F	83	-16.423	56.968	55.056	1.00	54.79	C
	ATOM	449	CG	ASP	F	83	-17.686	57.403	54.334	1.00	58.50	C
	ATOM	450	OD1	ASP	F	83	-17.959	56.888	53.227	1.00	58.88	O
	ATOM	451	OD2	ASP	F	83	-18.398	58.276	54.881	1.00	60.11	O
	ATOM	452	C	ASP	F	83	-14.993	55.086	55.885	1.00	47.45	C
70	ATOM	453	O	ASP	F	83	-14.049	55.869	55.998	1.00	48.00	O
	ATOM	455	N	GLU	F	84	-15.020	53.904	56.498	1.00	45.77	N
	ATOM	456	CA	GLU	F	84	-13.957	53.517	57.423	1.00	48.89	C
	ATOM	458	CB	GLU	F	84	-14.390	52.343	58.313	1.00	49.19	C
	ATOM	461	CG	GLU	F	84	-14.338	50.968	57.658	1.00	49.79	C
	ATOM	464	CD	GLU	F	84	-14.811	49.859	58.575	1.00	50.13	C

5	ATOM	465	OE1	GLU	F	84	-14.868	50.077	59.806	1.00	49.46	O
	ATOM	466	OE2	GLU	F	84	-15.116	48.759	58.061	1.00	53.55	O
	ATOM	467	C	GLU	F	84	-12.672	53.182	56.667	1.00	48.42	C
	ATOM	468	O	GLU	F	84	-12.712	52.620	55.574	1.00	47.87	O
	ATOM	470	N	ILE	F	85	-11.537	53.553	57.248	1.00	50.15	N
10	ATOM	471	CA	ILE	F	85	-10.228	53.205	56.681	1.00	50.05	C
	ATOM	473	CB	ILE	F	85	-9.362	54.469	56.397	1.00	53.68	C
	ATOM	475	CG1	ILE	F	85	-8.097	54.080	55.634	1.00	56.23	C
	ATOM	478	CD1	ILE	F	85	-7.302	55.253	55.122	1.00	56.60	C
	ATOM	482	CG2	ILE	F	85	-9.000	55.203	57.674	1.00	55.72	C
15	ATOM	486	C	ILE	F	85	-9.505	52.204	57.585	1.00	47.36	C
	ATOM	487	O	ILE	F	85	-8.795	51.316	57.097	1.00	47.31	O
	ATOM	489	N	MET	F	86	-9.696	52.356	58.895	1.00	45.05	N
	ATOM	490	CA	MET	F	86	-9.250	51.385	59.887	1.00	44.95	C
	ATOM	492	CB	MET	F	86	-8.426	52.063	60.988	1.00	40.72	C
20	ATOM	495	CG	MET	F	86	-7.153	52.745	60.496	1.00	41.06	C
	ATOM	498	SD	MET	F	86	-6.251	53.638	61.782	1.00	41.36	S
	ATOM	499	CE	MET	F	86	-5.497	52.293	62.677	1.00	44.06	C
	ATOM	503	C	MET	F	86	-10.475	50.685	60.489	1.00	45.01	C
	ATOM	504	O	MET	F	86	-11.491	51.318	60.779	1.00	42.88	O
25	ATOM	506	N	LYS	F	87	-10.356	49.374	60.673	1.00	45.98	N
	ATOM	507	CA	LYS	F	87	-11.472	48.529	61.089	1.00	47.85	C
	ATOM	509	CB	LYS	F	87	-11.612	47.347	60.125	1.00	48.40	C
	ATOM	512	CG	LYS	F	87	-11.612	47.755	58.668	1.00	51.87	C
	ATOM	515	CD	LYS	F	87	-12.057	46.624	57.759	1.00	53.25	C
30	ATOM	518	CE	LYS	F	87	-12.035	47.053	56.289	1.00	54.37	C
	ATOM	521	NZ	LYS	F	87	-12.567	45.984	55.380	1.00	53.08	N
	ATOM	525	C	LYS	F	87	-11.291	47.999	62.511	1.00	43.85	C
	ATOM	526	O	LYS	F	87	-10.167	47.914	63.022	1.00	35.73	O
	ATOM	528	N	VAL	F	88	-12.415	47.656	63.136	1.00	42.45	N
35	ATOM	529	CA	VAL	F	88	-12.418	46.890	64.374	1.00	44.24	C
	ATOM	531	CB	VAL	F	88	-13.441	47.432	65.404	1.00	44.22	C
	ATOM	533	CG1	VAL	F	88	-13.551	46.495	66.613	1.00	43.36	C
	ATOM	537	CG2	VAL	F	88	-13.045	48.838	65.852	1.00	45.09	C
	ATOM	541	C	VAL	F	88	-12.736	45.439	64.010	1.00	41.47	C
40	ATOM	542	O	VAL	F	88	-13.716	45.162	63.321	1.00	39.18	O
	ATOM	544	N	GLN	F	89	-11.888	44.528	64.470	1.00	41.70	N
	ATOM	545	CA	GLN	F	89	-12.020	43.114	64.168	1.00	43.90	C
	ATOM	547	CB	GLN	F	89	-11.235	42.785	62.891	1.00	45.86	C
	ATOM	550	CG	GLN	F	89	-11.924	41.790	61.981	1.00	50.07	C
45	ATOM	553	CD	GLN	F	89	-11.014	41.245	60.887	1.00	52.30	C
	ATOM	554	OE1	GLN	F	89	-10.088	41.923	60.424	1.00	53.74	O
	ATOM	555	NE2	GLN	F	89	-11.284	40.009	60.461	1.00	56.24	N
	ATOM	558	C	GLN	F	89	-11.480	42.326	65.364	1.00	40.92	C
	ATOM	559	O	GLN	F	89	-10.417	42.655	65.886	1.00	40.25	O
50	ATOM	561	N	ASP	F	90	-12.216	41.304	65.795	1.00	40.89	N
	ATOM	562	CA	ASP	F	90	-11.901	40.547	67.017	1.00	43.03	C
	ATOM	564	CB	ASP	F	90	-10.654	39.672	66.826	1.00	49.16	C
	ATOM	567	CG	ASP	F	90	-10.765	38.737	65.631	1.00	52.07	C
	ATOM	568	OD1	ASP	F	90	-11.844	38.145	65.423	1.00	51.49	O
55	ATOM	569	OD2	ASP	F	90	-9.761	38.592	64.903	1.00	57.57	O
	ATOM	570	C	ASP	F	90	-11.721	41.469	68.228	1.00	41.24	C
	ATOM	571	O	ASP	F	90	-10.806	41.281	69.035	1.00	40.11	O
	ATOM	573	N	ASN	F	91	-12.608	42.458	68.334	1.00	39.16	N
	ATOM	574	CA	ASN	F	91	-12.598	43.458	69.405	1.00	38.71	C
60	ATOM	576	CB	ASN	F	91	-12.992	42.814	70.738	1.00	39.20	C
	ATOM	579	CG	ASN	F	91	-13.626	43.805	71.697	1.00	39.68	C
	ATOM	580	OD1	ASN	F	91	-14.369	44.691	71.283	1.00	40.03	O
	ATOM	581	ND2	ASN	F	91	-13.338	43.657	72.982	1.00	39.93	N
	ATOM	584	C	ASN	F	91	-11.277	44.219	69.545	1.00	39.16	C
65	ATOM	585	O	ASN	F	91	-10.863	44.589	70.650	1.00	36.99	O
	ATOM	587	N	SER	F	92	-10.627	44.468	68.413	1.00	41.70	N
	ATOM	588	CA	SER	F	92	-9.360	45.187	68.392	1.00	39.32	C
	ATOM	590	CB	SER	F	92	-8.202	44.198	68.523	1.00	39.89	C
	ATOM	593	OG	SER	F	92	-8.016	43.467	67.331	1.00	42.53	O
70	ATOM	595	C	SER	F	92	-9.233	46.012	67.109	1.00	38.46	C
	ATOM	596	O	SER	F	92	-9.865	45.707	66.106	1.00	38.35	O
	ATOM	598	N	VAL	F	93	-8.420	47.063	67.165	1.00	39.14	N
	ATOM	599	CA	VAL	F	93	-8.184	47.940	66.025	1.00	37.98	C
	ATOM	601	CB	VAL	F	93	-7.822	49.370	66.493	1.00	38.25	C
	ATOM	603	CG1	VAL	F	93	-7.409	50.241	65.305	1.00	38.90	C

5	ATOM	607	CG2	VAL	F	93	-8.988	49.998	67.258	1.00	37.55	C
	ATOM	611	C	VAL	F	93	-7.041	47.400	65.157	1.00	36.72	C
	ATOM	612	O	VAL	F	93	-5.888	47.333	65.595	1.00	34.73	O
	ATOM	614	N	ILE	F	94	-7.363	47.064	63.912	1.00	36.49	N
	ATOM	615	CA	ILE	F	94	-6.402	46.467	62.989	1.00	37.34	C
10	ATOM	617	CB	ILE	F	94	-7.128	45.646	61.883	1.00	38.13	C
	ATOM	619	CG1	ILE	F	94	-8.108	44.639	62.507	1.00	38.13	C
	ATOM	622	CD1	ILE	F	94	-7.483	43.674	63.488	1.00	37.39	C
	ATOM	626	CG2	ILE	F	94	-6.124	44.918	60.971	1.00	36.93	C
	ATOM	630	C	ILE	F	94	-5.492	47.544	62.370	1.00	37.38	C
15	ATOM	631	O	ILE	F	94	-5.963	48.471	61.720	1.00	42.04	O
	ATOM	633	N	ILE	F	95	-4.187	47.405	62.584	1.00	36.11	N
	ATOM	634	CA	ILE	F	95	-3.196	48.312	62.011	1.00	37.69	C
	ATOM	636	CB	ILE	F	95	-2.009	48.496	62.970	1.00	41.60	C
	ATOM	638	CG1	ILE	F	95	-2.483	49.305	64.188	1.00	45.37	C
20	ATOM	641	CD1	ILE	F	95	-1.769	48.947	65.412	1.00	50.43	C
	ATOM	645	CG2	ILE	F	95	-0.837	49.218	62.282	1.00	38.97	C
	ATOM	649	C	ILE	F	95	-2.738	47.841	60.627	1.00	37.92	C
	ATOM	650	O	ILE	F	95	-2.242	46.729	60.466	1.00	37.73	O
	ATOM	652	N	ASN	F	96	-2.945	48.714	59.640	1.00	37.94	N
25	ATOM	653	CA	ASN	F	96	-2.704	48.430	58.232	1.00	36.20	C
	ATOM	655	CB	ASN	F	96	-3.769	49.120	57.372	1.00	37.20	C
	ATOM	658	CG	ASN	F	96	-5.179	48.753	57.783	1.00	35.98	C
	ATOM	659	OD1	ASN	F	96	-5.471	47.584	58.027	1.00	37.56	O
	ATOM	660	ND2	ASN	F	96	-6.063	49.751	57.859	1.00	29.93	N
30	ATOM	663	C	ASN	F	96	-1.354	48.941	57.781	1.00	35.53	C
	ATOM	664	O	ASN	F	96	-0.721	48.330	56.916	1.00	35.15	O
	ATOM	666	N	CYS	F	97	-0.933	50.070	58.362	1.00	37.19	N
	ATOM	667	CA	CYS	F	97	0.253	50.802	57.914	1.00	38.30	C
	ATOM	669	CB	CYS	F	97	-0.138	52.180	57.367	1.00	36.39	C
35	ATOM	672	SG	CYS	F	97	-1.366	52.119	56.061	1.00	38.99	S
	ATOM	674	C	CYS	F	97	1.275	50.982	59.029	1.00	36.30	C
	ATOM	675	O	CYS	F	97	0.921	51.304	60.164	1.00	33.31	O
	ATOM	677	N	ASP	F	98	2.542	50.782	58.680	1.00	35.28	N
	ATOM	678	CA	ASP	F	98	3.647	50.977	59.602	1.00	35.43	C
40	ATOM	680	CB	ASP	F	98	4.959	50.469	58.998	1.00	34.00	C
	ATOM	683	CG	ASP	F	98	4.960	48.984	58.754	1.00	33.68	C
	ATOM	684	OD1	ASP	F	98	3.993	48.306	59.155	1.00	32.61	O
	ATOM	685	OD2	ASP	F	98	5.944	48.495	58.159	1.00	32.93	O
	ATOM	686	C	ASP	F	98	3.822	52.449	59.921	1.00	35.77	C
45	ATOM	687	O	ASP	F	98	3.575	53.320	59.083	1.00	35.55	O
	ATOM	689	N	GLY	F	99	4.263	52.723	61.140	1.00	37.33	N
	ATOM	690	CA	GLY	F	99	4.666	54.072	61.507	1.00	35.62	C
	ATOM	693	C	GLY	F	99	4.248	54.419	62.908	1.00	35.92	C
	ATOM	694	O	GLY	F	99	3.818	53.555	63.690	1.00	33.73	O
50	ATOM	696	N	PHE	F	100	4.388	55.701	63.216	1.00	35.54	N
	ATOM	697	CA	PHE	F	100	3.990	56.237	64.497	1.00	35.24	C
	ATOM	699	CB	PHE	F	100	4.676	57.581	64.769	1.00	34.17	C
	ATOM	702	CG	PHE	F	100	6.170	57.500	64.854	1.00	31.96	C
	ATOM	703	CD1	PHE	F	100	6.782	56.746	65.835	1.00	30.75	C
55	ATOM	705	CE1	PHE	F	100	8.168	56.684	65.916	1.00	33.50	C
	ATOM	707	CZ	PHE	F	100	8.946	57.392	65.011	1.00	33.89	C
	ATOM	709	CE2	PHE	F	100	8.344	58.150	64.033	1.00	32.40	C
	ATOM	711	CD2	PHE	F	100	6.966	58.206	63.960	1.00	33.75	C
	ATOM	713	C	PHE	F	100	2.489	56.437	64.480	1.00	35.94	C
60	ATOM	714	O	PHE	F	100	1.905	56.782	63.443	1.00	38.22	O
	ATOM	716	N	TYR	F	101	1.871	56.209	65.634	1.00	36.53	N
	ATOM	717	CA	TYR	F	101	0.453	56.455	65.817	1.00	36.10	C
	ATOM	719	CB	TYR	F	101	-0.314	55.133	65.959	1.00	36.31	C
	ATOM	722	CG	TYR	F	101	-0.537	54.455	64.627	1.00	34.69	C
65	ATOM	723	CD1	TYR	F	101	0.461	53.693	64.036	1.00	35.56	C
	ATOM	725	CE1	TYR	F	101	0.262	53.081	62.799	1.00	36.62	C
	ATOM	727	CZ	TYR	F	101	-0.939	53.253	62.147	1.00	36.30	C
	ATOM	728	OH	TYR	F	101	-1.163	52.672	60.918	1.00	35.42	O
	ATOM	730	CE2	TYR	F	101	-1.937	54.018	62.723	1.00	37.30	C
70	ATOM	732	CD2	TYR	F	101	-1.732	54.614	63.943	1.00	33.54	C
	ATOM	734	C	TYR	F	101	0.269	57.321	67.042	1.00	37.21	C
	ATOM	735	O	TYR	F	101	0.746	56.979	68.121	1.00	36.84	O
	ATOM	737	N	LEU	F	102	-0.397	58.456	66.850	1.00	36.20	N
	ATOM	738	CA	LEU	F	102	-0.878	59.280	67.945	1.00	36.19	C
	ATOM	740	CB	LEU	F	102	-1.182	60.687	67.440	1.00	34.28	C

	ATOM	743	CG	LEU	F	102	-1.729	61.717	68.426	1.00	37.33	C
	ATOM	745	CD1	LEU	F	102	-0.829	61.894	69.663	1.00	37.81	C
	ATOM	749	CD2	LEU	F	102	-1.894	63.031	67.690	1.00	35.94	C
5	ATOM	753	C	LEU	F	102	-2.136	58.628	68.511	1.00	38.38	C
	ATOM	754	O	LEU	F	102	-3.129	58.478	67.796	1.00	36.62	O
	ATOM	756	N	ILE	F	103	-2.086	58.249	69.792	1.00	38.83	N
	ATOM	757	CA	ILE	F	103	-3.161	57.489	70.432	1.00	37.78	C
	ATOM	759	CB	ILE	F	103	-2.675	56.087	70.880	1.00	39.67	C
10	ATOM	761	CG1	ILE	F	103	-2.124	55.306	69.683	1.00	40.77	C
	ATOM	764	CD1	ILE	F	103	-1.476	54.005	70.036	1.00	41.44	C
	ATOM	768	CG2	ILE	F	103	-3.812	55.314	71.550	1.00	39.60	C
	ATOM	772	C	ILE	F	103	-3.704	58.242	71.639	1.00	38.09	C
	ATOM	773	O	ILE	F	103	-2.935	58.646	72.509	1.00	38.29	O
15	ATOM	775	N	SER	F	104	-5.029	58.424	71.672	1.00	40.41	N
	ATOM	776	CA	SER	F	104	-5.748	59.048	72.787	1.00	38.58	C
	ATOM	778	CB	SER	F	104	-6.564	60.250	72.276	1.00	38.71	C
	ATOM	781	OG	SER	F	104	-7.335	60.875	73.301	1.00	35.24	O
	ATOM	783	C	SER	F	104	-6.670	57.990	73.435	1.00	39.78	C
20	ATOM	784	O	SER	F	104	-7.412	57.302	72.734	1.00	35.29	O
	ATOM	786	N	LEU	F	105	-6.592	57.849	74.760	1.00	41.17	N
	ATOM	787	CA	LEU	F	105	-7.488	56.967	75.524	1.00	41.22	C
	ATOM	789	CB	LEU	F	105	-6.713	55.790	76.116	1.00	42.77	C
	ATOM	792	CG	LEU	F	105	-7.493	54.724	76.900	1.00	42.85	C
25	ATOM	794	CD1	LEU	F	105	-8.654	54.127	76.107	1.00	43.00	C
	ATOM	798	CD2	LEU	F	105	-6.535	53.622	77.365	1.00	44.02	C
	ATOM	802	C	LEU	F	105	-8.168	57.763	76.638	1.00	39.88	C
	ATOM	803	O	LEU	F	105	-7.499	58.360	77.473	1.00	36.24	O
	ATOM	805	N	LYS	F	106	-9.499	57.781	76.628	1.00	42.59	N
30	ATOM	806	CA	LYS	F	106	-10.289	58.513	77.623	1.00	42.33	C
	ATOM	808	CB	LYS	F	106	-10.931	59.759	76.995	1.00	43.09	C
	ATOM	811	CG	LYS	F	106	-9.931	60.881	76.719	1.00	46.44	C
	ATOM	814	CD	LYS	F	106	-10.416	61.893	75.690	1.00	45.30	C
	ATOM	817	CE	LYS	F	106	-11.369	62.911	76.287	1.00	48.33	C
35	ATOM	820	NZ	LYS	F	106	-12.022	63.736	75.226	1.00	46.34	N
	ATOM	824	C	LYS	F	106	-11.372	57.607	78.190	1.00	41.92	C
	ATOM	825	O	LYS	F	106	-11.877	56.726	77.502	1.00	42.17	O
	ATOM	827	N	GLY	F	107	-11.744	57.844	79.441	1.00	42.97	N
	ATOM	828	CA	GLY	F	107	-12.864	57.131	80.041	1.00	41.64	C
40	ATOM	831	C	GLY	F	107	-12.995	57.396	81.521	1.00	40.55	C
	ATOM	832	O	GLY	F	107	-11.992	57.536	82.223	1.00	37.90	O
	ATOM	834	N	TYR	F	108	-14.243	57.444	81.987	1.00	41.84	N
	ATOM	835	CA	TYR	F	108	-14.570	57.697	83.392	1.00	42.31	C
	ATOM	837	CB	TYR	F	108	-15.287	59.059	83.532	1.00	49.74	C
45	ATOM	840	CG	TYR	F	108	-14.381	60.155	83.004	1.00	51.76	C
	ATOM	841	CD1	TYR	F	108	-14.291	60.408	81.634	1.00	52.64	C
	ATOM	843	CE1	TYR	F	108	-13.411	61.360	81.121	1.00	52.72	C
	ATOM	845	CZ	TYR	F	108	-12.591	62.071	81.979	1.00	53.84	C
	ATOM	846	OH	TYR	F	108	-11.732	63.016	81.452	1.00	53.30	O
50	ATOM	848	CE2	TYR	F	108	-12.647	61.839	83.352	1.00	53.56	C
	ATOM	850	CD2	TYR	F	108	-13.535	60.868	83.857	1.00	54.68	C
	ATOM	852	C	TYR	F	108	-15.374	56.495	83.900	1.00	38.85	C
	ATOM	853	O	TYR	F	108	-16.499	56.270	83.475	1.00	36.85	O
	ATOM	855	N	PHE	F	109	-14.757	55.707	84.780	1.00	38.98	N
55	ATOM	856	CA	PHE	F	109	-15.309	54.424	85.226	1.00	37.99	C
	ATOM	858	CB	PHE	F	109	-14.192	53.386	85.335	1.00	37.00	C
	ATOM	861	CG	PHE	F	109	-13.470	53.155	84.041	1.00	37.21	C
	ATOM	862	CD1	PHE	F	109	-12.345	53.907	83.716	1.00	36.22	C
	ATOM	864	CE1	PHE	F	109	-11.690	53.714	82.505	1.00	38.76	C
60	ATOM	866	CZ	PHE	F	109	-12.158	52.756	81.603	1.00	37.56	C
	ATOM	868	CE2	PHE	F	109	-13.278	52.004	81.918	1.00	37.37	C
	ATOM	870	CD2	PHE	F	109	-13.931	52.206	83.132	1.00	37.27	C
	ATOM	872	C	PHE	F	109	-16.016	54.585	86.554	1.00	36.21	C
	ATOM	873	O	PHE	F	109	-15.605	55.405	87.365	1.00	37.93	O
65	ATOM	875	N	SER	F	110	-17.071	53.795	86.768	1.00	35.35	N
	ATOM	876	CA	SER	F	110	-17.954	53.941	87.937	1.00	36.90	C
	ATOM	878	CB	SER	F	110	-19.313	53.286	87.670	1.00	37.72	C
	ATOM	881	OG	SER	F	110	-19.175	51.901	87.439	1.00	36.46	O
	ATOM	883	C	SER	F	110	-17.366	53.358	89.213	1.00	37.81	C
70	ATOM	884	O	SER	F	110	-17.838	53.654	90.312	1.00	35.71	O
	ATOM	886	N	GLN	F	111	-16.366	52.496	89.059	1.00	37.46	N
	ATOM	887	CA	GLN	F	111	-15.585	52.011	90.183	1.00	37.79	C

5	ATOM	889	CB	GLN	F	111	-16.162	50.700	90.726	1.00	39.00	C
	ATOM	892	CG	GLN	F	111	-16.070	49.519	89.764	1.00	39.83	C
	ATOM	895	CD	GLN	F	111	-16.944	48.355	90.181	1.00	39.53	C
	ATOM	896	OE1	GLN	F	111	-17.981	48.544	90.817	1.00	42.69	O
	ATOM	897	NE2	GLN	F	111	-16.532	47.142	89.820	1.00	37.36	N
10	ATOM	900	C	GLN	F	111	-14.141	51.843	89.734	1.00	38.94	C
	ATOM	901	O	GLN	F	111	-13.800	52.072	88.568	1.00	38.33	O
	ATOM	903	N	GLU	F	112	-13.294	51.457	90.675	1.00	37.98	N
	ATOM	904	CA	GLU	F	112	-11.861	51.410	90.446	1.00	39.02	C
	ATOM	906	CB	GLU	F	112	-11.161	51.134	91.774	1.00	40.41	C
15	ATOM	909	CG	GLU	F	112	-9.764	51.648	91.876	1.00	42.75	C
	ATOM	912	CD	GLU	F	112	-9.270	51.633	93.301	1.00	43.50	C
	ATOM	913	OE1	GLU	F	112	-8.564	50.670	93.664	1.00	48.34	O
	ATOM	914	OE2	GLU	F	112	-9.613	52.568	94.060	1.00	43.35	O
	ATOM	915	C	GLU	F	112	-11.522	50.337	89.412	1.00	38.71	C
20	ATOM	916	O	GLU	F	112	-12.122	49.262	89.416	1.00	37.43	O
	ATOM	918	N	VAL	F	113	-10.582	50.643	88.516	1.00	38.71	N
	ATOM	919	CA	VAL	F	113	-10.156	49.694	87.485	1.00	38.20	C
	ATOM	921	CB	VAL	F	113	-10.784	49.994	86.094	1.00	37.92	C
	ATOM	923	CG1	VAL	F	113	-12.295	49.971	86.161	1.00	39.45	C
25	ATOM	927	CG2	VAL	F	113	-10.290	51.326	85.528	1.00	39.38	C
	ATOM	931	C	VAL	F	113	-8.641	49.665	87.318	1.00	38.63	C
	ATOM	932	O	VAL	F	113	-7.935	50.583	87.740	1.00	37.29	O
	ATOM	934	N	ASP	F	114	-8.163	48.570	86.730	1.00	39.69	N
	ATOM	935	CA	ASP	F	114	-6.838	48.504	86.123	1.00	40.13	C
30	ATOM	937	CB	ASP	F	114	-6.134	47.189	86.455	1.00	39.72	C
	ATOM	940	CG	ASP	F	114	-5.701	47.110	87.894	1.00	40.27	C
	ATOM	941	OD1	ASP	F	114	-5.822	48.123	88.611	1.00	42.53	O
	ATOM	942	OD2	ASP	F	114	-5.245	46.029	88.314	1.00	40.84	O
	ATOM	943	C	ASP	F	114	-7.067	48.582	84.633	1.00	40.15	C
35	ATOM	944	O	ASP	F	114	-7.960	47.913	84.116	1.00	38.30	O
	ATOM	946	N	ILE	F	115	-6.291	49.414	83.945	1.00	40.64	N
	ATOM	947	CA	ILE	F	115	-6.479	49.596	82.508	1.00	41.32	C
	ATOM	949	CB	ILE	F	115	-7.289	50.884	82.180	1.00	43.28	C
	ATOM	951	CG1	ILE	F	115	-7.383	51.090	80.663	1.00	42.87	C
40	ATOM	954	CD1	ILE	F	115	-8.538	51.958	80.253	1.00	44.46	C
	ATOM	958	CG2	ILE	F	115	-6.692	52.113	82.856	1.00	45.70	C
	ATOM	962	C	ILE	F	115	-5.157	49.556	81.738	1.00	40.93	C
	ATOM	963	O	ILE	F	115	-4.181	50.205	82.111	1.00	41.08	O
	ATOM	965	N	SER	F	116	-5.143	48.778	80.662	1.00	39.89	N
45	ATOM	966	CA	SER	F	116	-3.997	48.724	79.772	1.00	38.85	C
	ATOM	968	CB	SER	F	116	-3.106	47.527	80.109	1.00	36.55	C
	ATOM	971	OG	SER	F	116	-3.864	46.411	80.529	1.00	37.81	O
	ATOM	973	C	SER	F	116	-4.408	48.712	78.295	1.00	37.29	C
	ATOM	974	O	SER	F	116	-5.486	48.246	77.935	1.00	34.01	O
50	ATOM	976	N	LEU	F	117	-3.535	49.261	77.458	1.00	37.98	N
	ATOM	977	CA	LEU	F	117	-3.716	49.258	76.014	1.00	39.62	C
	ATOM	979	CB	LEU	F	117	-3.660	50.695	75.479	1.00	41.92	C
	ATOM	982	CG	LEU	F	117	-4.284	51.013	74.120	1.00	43.27	C
	ATOM	984	CD1	LEU	F	117	-5.782	50.687	74.089	1.00	41.42	C
55	ATOM	988	CD2	LEU	F	117	-4.039	52.488	73.789	1.00	43.71	C
	ATOM	992	C	LEU	F	117	-2.587	48.425	75.446	1.00	37.92	C
	ATOM	993	O	LEU	F	117	-1.433	48.630	75.816	1.00	38.84	O
	ATOM	995	N	HIS	F	118	-2.929	47.466	74.581	1.00	39.17	N
	ATOM	996	CA	HIS	F	118	-1.974	46.498	74.030	1.00	37.52	C
60	ATOM	998	CB	HIS	F	118	-2.358	45.086	74.458	1.00	37.14	C
	ATOM	1001	CG	HIS	F	118	-2.369	44.867	75.938	1.00	33.64	C
	ATOM	1002	ND1	HIS	F	118	-3.399	45.290	76.747	1.00	34.43	N
	ATOM	1004	CE1	HIS	F	118	-3.140	44.944	77.995	1.00	34.60	C
	ATOM	1006	NE2	HIS	F	118	-1.987	44.306	78.023	1.00	33.08	N
65	ATOM	1008	CD2	HIS	F	118	-1.485	44.242	76.748	1.00	34.88	C
	ATOM	1010	C	HIS	F	118	-1.980	46.517	72.508	1.00	37.57	C
	ATOM	1011	O	HIS	F	118	-2.991	46.822	71.905	1.00	39.18	O
	ATOM	1013	N	TYR	F	119	-0.854	46.157	71.901	1.00	41.91	N
	ATOM	1014	CA	TYR	F	119	-0.730	46.035	70.437	1.00	41.70	C
70	ATOM	1016	CB	TYR	F	119	0.334	46.999	69.902	1.00	42.07	C
	ATOM	1019	CG	TYR	F	119	1.752	46.676	70.331	1.00	39.49	C
	ATOM	1020	CD1	TYR	F	119	2.236	47.099	71.561	1.00	38.88	C
	ATOM	1022	CE1	TYR	F	119	3.531	46.818	71.953	1.00	42.24	C
	ATOM	1024	CZ	TYR	F	119	4.356	46.097	71.113	1.00	42.41	C
	ATOM	1025	OH	TYR	F	119	5.641	45.809	71.501	1.00	43.65	O

	ATOM	1027	CE2	TYR	F	119	3.899	45.667	69.885	1.00	40.62	C
	ATOM	1029	CD2	TYR	F	119	2.604	45.965	69.499	1.00	39.35	C
	ATOM	1031	C	TYR	F	119	-0.407	44.616	69.964	1.00	41.14	C
5	ATOM	1032	O	TYR	F	119	-0.639	44.288	68.805	1.00	42.99	O
	ATOM	1034	N	GLN	F	120	0.164	43.799	70.845	1.00	45.37	N
	ATOM	1035	CA	GLN	F	120	0.428	42.384	70.565	1.00	47.68	C
	ATOM	1037	CB	GLN	F	120	1.875	42.174	70.091	1.00	48.74	C
	ATOM	1040	CG	GLN	F	120	2.049	41.196	68.896	1.00	51.02	C
10	ATOM	1043	CD	GLN	F	120	2.153	41.914	67.553	1.00	52.54	C
	ATOM	1044	OE1	GLN	F	120	1.498	41.550	66.582	1.00	47.23	O
	ATOM	1045	NE2	GLN	F	120	2.976	42.953	67.504	1.00	58.26	N
	ATOM	1048	C	GLN	F	120	0.172	41.608	71.856	1.00	48.98	C
	ATOM	1049	O	GLN	F	120	0.377	42.142	72.947	1.00	48.93	O
	ATOM	1051	N	LYS	F	121	-0.260	40.354	71.719	1.00	52.71	N
15	ATOM	1052	CA	LYS	F	121	-0.744	39.533	72.843	1.00	53.36	C
	ATOM	1054	CB	LYS	F	121	-1.189	38.149	72.338	1.00	59.67	C
	ATOM	1057	CG	LYS	F	121	-2.603	38.120	71.754	1.00	63.44	C
	ATOM	1060	CD	LYS	F	121	-3.672	38.041	72.848	1.00	64.88	C
20	ATOM	1063	CE	LYS	F	121	-5.090	38.125	72.279	1.00	64.69	C
	ATOM	1066	NZ	LYS	F	121	-5.622	39.524	72.239	1.00	63.41	N
	ATOM	1070	C	LYS	F	121	0.226	39.344	74.013	1.00	52.18	C
	ATOM	1071	O	LYS	F	121	-0.175	39.461	75.173	1.00	53.77	O
	ATOM	1073	N	ASP	F	122	1.485	39.047	73.710	1.00	50.49	N
25	ATOM	1074	CA	ASP	F	122	2.464	38.666	74.734	1.00	51.93	C
	ATOM	1076	CB	ASP	F	122	3.144	37.359	74.315	1.00	54.64	C
	ATOM	1079	CG	ASP	F	122	2.177	36.183	74.287	1.00	57.10	C
	ATOM	1080	OD1	ASP	F	122	1.529	35.923	75.331	1.00	56.65	O
	ATOM	1081	OD2	ASP	F	122	2.069	35.525	73.224	1.00	56.29	O
30	ATOM	1082	C	ASP	F	122	3.512	39.753	74.991	1.00	49.61	C
	ATOM	1083	O	ASP	F	122	4.520	39.525	75.663	1.00	48.31	O
	ATOM	1085	N	GLU	F	123	3.240	40.943	74.475	1.00	47.41	N
	ATOM	1086	CA	GLU	F	123	4.182	42.045	74.485	1.00	47.94	C
	ATOM	1088	CB	GLU	F	123	4.167	42.707	73.097	1.00	48.69	C
35	ATOM	1091	CG	GLU	F	123	5.534	42.988	72.481	1.00	50.68	C
	ATOM	1094	CD	GLU	F	123	6.401	41.761	72.274	1.00	50.52	C
	ATOM	1095	OE1	GLU	F	123	5.875	40.640	72.100	1.00	55.88	O
	ATOM	1096	OE2	GLU	F	123	7.633	41.925	72.271	1.00	47.66	O
	ATOM	1097	C	GLU	F	123	3.760	43.026	75.586	1.00	47.13	C
40	ATOM	1098	O	GLU	F	123	2.609	43.003	76.042	1.00	46.43	O
	ATOM	1100	N	GLU	F	124	4.684	43.878	76.023	1.00	47.45	N
	ATOM	1101	CA	GLU	F	124	4.361	44.872	77.043	1.00	48.57	C
	ATOM	1103	CB	GLU	F	124	5.613	45.628	77.511	1.00	54.98	C
	ATOM	1106	CG	GLU	F	124	6.636	44.755	78.274	1.00	59.64	C
45	ATOM	1109	CD	GLU	F	124	6.022	44.011	79.451	1.00	61.36	C
	ATOM	1110	OE1	GLU	F	124	5.454	44.669	80.352	1.00	62.77	O
	ATOM	1111	OE2	GLU	F	124	6.098	42.764	79.466	1.00	61.77	O
	ATOM	1112	C	GLU	F	124	3.328	45.854	76.493	1.00	46.56	C
	ATOM	1113	O	GLU	F	124	3.401	46.231	75.327	1.00	43.72	O
50	ATOM	1115	N	PRO	F	125	2.348	46.252	77.326	1.00	43.58	N
	ATOM	1116	CA	PRO	F	125	1.350	47.188	76.831	1.00	44.45	C
	ATOM	1118	CB	PRO	F	125	0.372	47.347	78.013	1.00	45.55	C
	ATOM	1121	CG	PRO	F	125	1.063	46.811	79.199	1.00	45.26	C
	ATOM	1124	CD	PRO	F	125	2.110	45.855	78.726	1.00	43.87	C
55	ATOM	1127	C	PRO	F	125	1.949	48.541	76.431	1.00	42.36	C
	ATOM	1128	O	PRO	F	125	3.025	48.918	76.901	1.00	40.37	O
	ATOM	1129	N	LEU	F	126	1.240	49.235	75.550	1.00	42.49	N
	ATOM	1130	CA	LEU	F	126	1.529	50.614	75.188	1.00	45.49	C
	ATOM	1132	CB	LEU	F	126	0.563	51.080	74.084	1.00	42.67	C
60	ATOM	1135	CG	LEU	F	126	0.571	50.298	72.775	1.00	42.55	C
	ATOM	1137	CD1	LEU	F	126	-0.505	50.815	71.832	1.00	42.26	C
	ATOM	1141	CD2	LEU	F	126	1.951	50.366	72.134	1.00	41.34	C
	ATOM	1145	C	LEU	F	126	1.335	51.532	76.389	1.00	46.32	C
	ATOM	1146	O	LEU	F	126	2.053	52.507	76.558	1.00	48.60	O
65	ATOM	1148	N	PHE	F	127	0.336	51.200	77.200	1.00	46.43	N
	ATOM	1149	CA	PHE	F	127	-0.155	52.052	78.265	1.00	45.87	C
	ATOM	1151	CB	PHE	F	127	-1.286	52.924	77.726	1.00	44.94	C
	ATOM	1154	CG	PHE	F	127	-1.910	53.816	78.758	1.00	44.97	C
	ATOM	1155	CD1	PHE	F	127	-1.283	54.994	79.139	1.00	45.31	C
70	ATOM	1157	CE1	PHE	F	127	-1.856	55.828	80.091	1.00	45.56	C
	ATOM	1159	CZ	PHE	F	127	-3.058	55.480	80.677	1.00	45.67	C
	ATOM	1161	CE2	PHE	F	127	-3.694	54.297	80.313	1.00	45.30	C

	ATOM	1163	CD2	PHE	F	127	-3.120	53.477	79.352	1.00	44.56	C
	ATOM	1165	C	PHE	F	127	-0.684	51.168	79.384	1.00	45.96	C
	ATOM	1166	O	PHE	F	127	-1.339	50.169	79.120	1.00	48.34	O
5	ATOM	1168	N	GLN	F	128	-0.418	51.550	80.630	1.00	49.16	N
	ATOM	1169	CA	GLN	F	128	-0.879	50.780	81.778	1.00	48.72	C
	ATOM	1171	CB	GLN	F	128	0.161	49.710	82.103	1.00	49.23	C
	ATOM	1174	CG	GLN	F	128	-0.332	48.626	83.031	1.00	53.05	C
	ATOM	1177	CD	GLN	F	128	0.641	47.463	83.141	1.00	54.97	C
10	ATOM	1178	OE1	GLN	F	128	1.758	47.504	82.606	1.00	55.66	O
	ATOM	1179	NE2	GLN	F	128	0.218	46.414	83.834	1.00	57.59	N
	ATOM	1182	C	GLN	F	128	-1.136	51.670	83.004	1.00	47.48	C
	ATOM	1183	O	GLN	F	128	-0.282	52.468	83.388	1.00	48.54	O
	ATOM	1185	N	LEU	F	129	-2.320	51.532	83.601	1.00	46.10	N
15	ATOM	1186	CA	LEU	F	129	-2.646	52.191	84.875	1.00	45.55	C
	ATOM	1188	CB	LEU	F	129	-3.575	53.398	84.668	1.00	45.68	C
	ATOM	1191	CG	LEU	F	129	-2.927	54.673	84.116	1.00	46.58	C
	ATOM	1193	CD1	LEU	F	129	-3.965	55.760	83.896	1.00	46.33	C
	ATOM	1197	CD2	LEU	F	129	-1.816	55.165	85.048	1.00	47.46	C
20	ATOM	1201	C	LEU	F	129	-3.307	51.200	85.820	1.00	43.47	C
	ATOM	1202	O	LEU	F	129	-4.074	50.336	85.383	1.00	42.34	O
	ATOM	1204	N	LYS	F	130	-3.013	51.337	87.112	1.00	40.57	N
	ATOM	1205	CA	LYS	F	130	-3.625	50.499	88.133	1.00	43.94	C
	ATOM	1207	CB	LYS	F	130	-2.562	49.645	88.830	1.00	47.05	C
25	ATOM	1210	CG	LYS	F	130	-1.999	48.539	87.939	1.00	49.58	C
	ATOM	1213	CD	LYS	F	130	-0.890	47.769	88.638	1.00	50.12	C
	ATOM	1216	CE	LYS	F	130	-0.477	46.521	87.859	1.00	51.10	C
	ATOM	1219	NZ	LYS	F	130	0.240	45.545	88.751	1.00	50.89	N
	ATOM	1223	C	LYS	F	130	-4.389	51.332	89.157	1.00	42.18	C
30	ATOM	1224	O	LYS	F	130	-3.917	52.385	89.596	1.00	41.30	O
	ATOM	1226	N	LYS	F	131	-5.576	50.847	89.520	1.00	40.68	N
	ATOM	1227	CA	LYS	F	131	-6.397	51.439	90.574	1.00	42.56	C
	ATOM	1229	CB	LYS	F	131	-5.719	51.276	91.942	1.00	43.61	C
	ATOM	1232	CG	LYS	F	131	-5.399	49.836	92.285	1.00	45.79	C
35	ATOM	1235	CD	LYS	F	131	-5.033	49.681	93.750	1.00	46.38	C
	ATOM	1238	CE	LYS	F	131	-5.089	48.229	94.196	1.00	46.61	C
	ATOM	1241	NZ	LYS	F	131	-5.130	48.129	95.683	1.00	46.77	N
	ATOM	1245	C	LYS	F	131	-6.749	52.904	90.305	1.00	39.02	C
	ATOM	1246	O	LYS	F	131	-6.492	53.786	91.126	1.00	38.41	O
40	ATOM	1248	N	VAL	F	132	-7.339	53.144	89.143	1.00	40.86	N
	ATOM	1249	CA	VAL	F	132	-7.779	54.482	88.742	1.00	40.13	C
	ATOM	1251	CB	VAL	F	132	-7.082	54.956	87.435	1.00	39.54	C
	ATOM	1253	CG1	VAL	F	132	-5.594	55.190	87.668	1.00	39.44	C
	ATOM	1257	CG2	VAL	F	132	-7.291	53.963	86.304	1.00	40.16	C
45	ATOM	1261	C	VAL	F	132	-9.297	54.509	88.557	1.00	38.68	C
	ATOM	1262	O	VAL	F	132	-9.935	53.473	88.348	1.00	36.99	O
	ATOM	1264	N	ARG	F	133	-9.872	55.700	88.637	1.00	39.05	N
	ATOM	1265	CA	ARG	F	133	-11.295	55.882	88.363	1.00	38.67	C
	ATOM	1267	CB	ARG	F	133	-11.913	56.786	89.421	1.00	34.90	C
50	ATOM	1270	CG	ARG	F	133	-12.085	56.109	90.780	1.00	33.77	C
	ATOM	1273	CD	ARG	F	133	-13.156	55.024	90.739	1.00	35.64	C
	ATOM	1276	NE	ARG	F	133	-14.408	55.539	90.186	1.00	37.54	N
	ATOM	1278	CZ	ARG	F	133	-15.308	56.252	90.863	1.00	39.09	C
	ATOM	1279	NH1	ARG	F	133	-15.130	56.536	92.151	1.00	39.19	N
55	ATOM	1282	NH2	ARG	F	133	-16.405	56.680	90.250	1.00	39.25	N
	ATOM	1285	C	ARG	F	133	-11.525	56.441	86.959	1.00	40.17	C
	ATOM	1286	O	ARG	F	133	-12.657	56.462	86.468	1.00	41.54	O
	ATOM	1288	N	SER	F	134	-10.449	56.883	86.314	1.00	39.98	N
	ATOM	1289	CA	SER	F	134	-10.539	57.460	84.984	1.00	41.63	C
60	ATOM	1291	CB	SER	F	134	-11.059	58.903	85.051	1.00	43.44	C
	ATOM	1294	OG	SER	F	134	-10.106	59.781	85.621	1.00	42.63	O
	ATOM	1296	C	SER	F	134	-9.199	57.436	84.255	1.00	42.21	C
	ATOM	1297	O	SER	F	134	-8.142	57.201	84.849	1.00	39.06	O
	ATOM	1299	N	VAL	F	135	-9.278	57.677	82.951	1.00	43.98	N
65	ATOM	1300	CA	VAL	F	135	-8.116	57.758	82.079	1.00	40.67	C
	ATOM	1302	CB	VAL	F	135	-7.868	56.423	81.297	1.00	41.31	C
	ATOM	1304	CG1	VAL	F	135	-9.018	56.068	80.390	1.00	40.29	C
	ATOM	1308	CG2	VAL	F	135	-6.575	56.489	80.488	1.00	45.11	C
	ATOM	1312	C	VAL	F	135	-8.331	58.931	81.136	1.00	38.56	C
70	ATOM	1313	O	VAL	F	135	-9.449	59.180	80.691	1.00	36.27	O
	ATOM	1315	N	ASN	F	136	-7.265	59.679	80.883	1.00	41.87	N
	ATOM	1316	CA	ASN	F	136	-7.268	60.750	79.889	1.00	41.04	C

	ATOM	1318	CB	ASN	F	136	-7.867	62.038	80.469	1.00	43.93	C
	ATOM	1321	CG	ASN	F	136	-7.996	63.163	79.429	1.00	43.16	C
	ATOM	1322	OD1	ASN	F	136	-8.179	64.316	79.785	1.00	45.54	O
	ATOM	1323	ND2	ASN	F	136	-7.904	62.822	78.157	1.00	44.48	N
5	ATOM	1326	C	ASN	F	136	-5.835	60.969	79.441	1.00	41.32	C
	ATOM	1327	O	ASN	F	136	-5.124	61.836	79.961	1.00	38.87	O
	ATOM	1329	N	SER	F	137	-5.409	60.148	78.485	1.00	43.08	N
	ATOM	1330	CA	SER	F	137	-4.001	60.064	78.132	1.00	42.60	C
10	ATOM	1332	CB	SER	F	137	-3.387	58.785	78.718	1.00	46.32	C
	ATOM	1335	OG	SER	F	137	-3.283	58.886	80.138	1.00	48.33	O
	ATOM	1337	C	SER	F	137	-3.781	60.130	76.626	1.00	40.64	C
	ATOM	1338	O	SER	F	137	-4.557	59.597	75.838	1.00	36.35	O
	ATOM	1340	N	LEU	F	138	-2.708	60.814	76.254	1.00	40.13	N
	ATOM	1341	CA	LEU	F	138	-2.285	60.944	74.880	1.00	38.99	C
15	ATOM	1343	CB	LEU	F	138	-2.327	62.424	74.494	1.00	39.95	C
	ATOM	1346	CG	LEU	F	138	-2.316	62.793	73.010	1.00	43.27	C
	ATOM	1348	CD1	LEU	F	138	-3.502	62.182	72.287	1.00	43.69	C
	ATOM	1352	CD2	LEU	F	138	-2.301	64.324	72.851	1.00	41.17	C
20	ATOM	1356	C	LEU	F	138	-0.865	60.389	74.805	1.00	36.23	C
	ATOM	1357	O	LEU	F	138	-0.046	60.679	75.662	1.00	34.37	O
	ATOM	1359	N	MET	F	139	-0.575	59.569	73.801	1.00	37.81	N
	ATOM	1360	CA	MET	F	139	0.755	58.980	73.669	1.00	36.78	C
	ATOM	1362	CB	MET	F	139	0.812	57.656	74.441	1.00	37.47	C
25	ATOM	1365	CG	MET	F	139	0.100	56.496	73.740	1.00	39.18	C
	ATOM	1368	SD	MET	F	139	-0.755	55.350	74.824	1.00	42.74	S
	ATOM	1369	CE	MET	F	139	-2.048	56.414	75.490	1.00	43.52	C
	ATOM	1373	C	MET	F	139	1.095	58.762	72.195	1.00	35.47	C
	ATOM	1374	O	MET	F	139	0.226	58.820	71.341	1.00	38.62	O
30	ATOM	1376	N	VAL	F	140	2.369	58.521	71.909	1.00	36.73	N
	ATOM	1377	CA	VAL	F	140	2.809	58.131	70.571	1.00	36.17	C
	ATOM	1379	CB	VAL	F	140	3.755	59.190	69.932	1.00	32.97	C
	ATOM	1381	CG1	VAL	F	140	4.422	58.646	68.685	1.00	30.38	C
	ATOM	1385	CG2	VAL	F	140	2.973	60.453	69.600	1.00	35.43	C
35	ATOM	1389	C	VAL	F	140	3.520	56.787	70.656	1.00	37.01	C
	ATOM	1390	O	VAL	F	140	4.381	56.588	71.520	1.00	35.32	O
	ATOM	1392	N	ALA	F	141	3.160	55.884	69.744	1.00	36.58	N
	ATOM	1393	CA	ALA	F	141	3.733	54.547	69.678	1.00	36.38	C
	ATOM	1395	CB	ALA	F	141	2.747	53.540	70.243	1.00	38.09	C
40	ATOM	1399	C	ALA	F	141	4.094	54.181	68.237	1.00	36.59	C
	ATOM	1400	O	ALA	F	141	3.416	54.581	67.300	1.00	37.75	O
	ATOM	1402	N	SER	F	142	5.173	53.422	68.081	1.00	36.48	N
	ATOM	1403	CA	SER	F	142	5.560	52.834	66.802	1.00	36.74	C
	ATOM	1405	CB	SER	F	142	7.075	52.623	66.753	1.00	32.96	C
45	ATOM	1408	OG	SER	F	142	7.747	53.749	67.271	1.00	39.45	O
	ATOM	1410	C	SER	F	142	4.874	51.484	66.607	1.00	37.19	C
	ATOM	1411	O	SER	F	142	5.135	50.532	67.343	1.00	41.66	O
	ATOM	1413	N	LEU	F	143	4.014	51.402	65.604	1.00	36.82	N
	ATOM	1414	CA	LEU	F	143	3.284	50.173	65.306	1.00	36.42	C
50	ATOM	1416	CB	LEU	F	143	1.786	50.401	65.506	1.00	38.11	C
	ATOM	1419	CG	LEU	F	143	1.369	50.986	66.870	1.00	36.43	C
	ATOM	1421	CD1	LEU	F	143	-0.098	51.315	66.908	1.00	38.19	C
	ATOM	1425	CD2	LEU	F	143	1.720	50.036	68.003	1.00	38.28	C
	ATOM	1429	C	LEU	F	143	3.589	49.718	63.876	1.00	36.46	C
55	ATOM	1430	O	LEU	F	143	4.092	50.491	63.060	1.00	38.32	O
	ATOM	1432	N	THR	F	144	3.320	48.447	63.601	1.00	36.76	N
	ATOM	1433	CA	THR	F	144	3.549	47.855	62.284	1.00	36.34	C
	ATOM	1435	CB	THR	F	144	4.875	47.053	62.225	1.00	36.33	C
	ATOM	1437	OG1	THR	F	144	4.854	45.997	63.190	1.00	36.43	O
60	ATOM	1439	CG2	THR	F	144	6.069	47.950	62.491	1.00	37.74	C
	ATOM	1443	C	THR	F	144	2.398	46.930	61.911	1.00	33.62	C
	ATOM	1444	O	THR	F	144	1.684	46.450	62.779	1.00	30.82	O
	ATOM	1446	N	TYR	F	145	2.223	46.686	60.615	1.00	37.69	N
	ATOM	1447	CA	TYR	F	145	1.212	45.747	60.139	1.00	37.21	C
65	ATOM	1449	CB	TYR	F	145	1.340	45.503	58.625	1.00	37.14	C
	ATOM	1452	CG	TYR	F	145	0.451	44.380	58.137	1.00	36.40	C
	ATOM	1453	CD1	TYR	F	145	-0.930	44.537	58.087	1.00	37.63	C
	ATOM	1455	CE1	TYR	F	145	-1.756	43.503	57.670	1.00	36.79	C
	ATOM	1457	CZ	TYR	F	145	-1.203	42.299	57.304	1.00	38.34	C
70	ATOM	1458	OH	TYR	F	145	-2.016	41.277	56.877	1.00	39.10	O
	ATOM	1460	CE2	TYR	F	145	0.169	42.115	57.350	1.00	37.84	C
	ATOM	1462	CD2	TYR	F	145	0.984	43.152	57.769	1.00	34.93	C

5	ATOM	1464	C	TYR	F	145	1.351	44.436	60.909	1.00	37.43	C
	ATOM	1465	O	TYR	F	145	2.464	43.995	61.155	1.00	39.31	O
	ATOM	1467	N	LYS	F	146	0.206	43.846	61.271	1.00	40.41	N
	ATOM	1468	CA	LYS	F	146	0.059	42.650	62.138	1.00	37.17	C
	ATOM	1470	CB	LYS	F	146	1.202	41.629	62.006	1.00	36.70	C
10	ATOM	1473	CG	LYS	F	146	1.119	40.784	60.755	1.00	37.51	C
	ATOM	1476	CD	LYS	F	146	1.879	39.483	60.902	1.00	37.94	C
	ATOM	1479	CE	LYS	F	146	1.818	38.677	59.624	1.00	36.62	C
	ATOM	1482	NZ	LYS	F	146	2.600	37.414	59.693	1.00	35.64	N
	ATOM	1486	C	LYS	F	146	-0.182	42.984	63.614	1.00	37.43	C
15	ATOM	1487	O	LYS	F	146	-0.666	42.136	64.367	1.00	38.06	O
	ATOM	1489	N	ASP	F	147	0.154	44.205	64.030	1.00	37.60	N
	ATOM	1490	CA	ASP	F	147	-0.247	44.694	65.348	1.00	36.69	C
	ATOM	1492	CB	ASP	F	147	0.412	46.035	65.681	1.00	35.65	C
	ATOM	1495	CG	ASP	F	147	1.911	45.929	65.911	1.00	34.67	C
20	ATOM	1496	OD1	ASP	F	147	2.466	44.815	65.977	1.00	33.49	O
	ATOM	1497	OD2	ASP	F	147	2.540	46.993	66.040	1.00	35.12	O
	ATOM	1498	C	ASP	F	147	-1.760	44.880	65.365	1.00	38.67	C
	ATOM	1499	O	ASP	F	147	-2.370	45.224	64.344	1.00	38.17	O
	ATOM	1501	N	LYS	F	148	-2.356	44.642	66.529	1.00	38.74	N
25	ATOM	1502	CA	LYS	F	148	-3.790	44.832	66.739	1.00	38.13	C
	ATOM	1504	CB	LYS	F	148	-4.547	43.502	66.641	1.00	37.69	C
	ATOM	1507	CG	LYS	F	148	-4.341	42.742	65.330	1.00	39.03	C
	ATOM	1510	CD	LYS	F	148	-4.873	41.323	65.431	1.00	39.83	C
	ATOM	1513	CE	LYS	F	148	-4.769	40.593	64.124	1.00	40.49	C
30	ATOM	1516	NZ	LYS	F	148	-5.369	39.231	64.215	1.00	43.46	N
	ATOM	1520	C	LYS	F	148	-3.969	45.447	68.121	1.00	36.95	C
	ATOM	1521	O	LYS	F	148	-3.579	44.858	69.127	1.00	35.25	O
	ATOM	1523	N	VAL	F	149	-4.551	46.639	68.161	1.00	39.11	N
	ATOM	1524	CA	VAL	F	149	-4.649	47.409	69.397	1.00	38.45	C
35	ATOM	1526	CB	VAL	F	149	-4.502	48.918	69.128	1.00	38.42	C
	ATOM	1528	CG1	VAL	F	149	-4.780	49.738	70.376	1.00	42.66	C
	ATOM	1532	CG2	VAL	F	149	-3.111	49.207	68.631	1.00	39.71	C
	ATOM	1536	C	VAL	F	149	-5.956	47.088	70.105	1.00	38.69	C
	ATOM	1537	O	VAL	F	149	-7.040	47.227	69.543	1.00	41.58	O
40	ATOM	1539	N	TYR	F	150	-5.840	46.615	71.334	1.00	37.40	N
	ATOM	1540	CA	TYR	F	150	-7.002	46.252	72.105	1.00	38.89	C
	ATOM	1542	CB	TYR	F	150	-7.223	44.735	72.104	1.00	35.93	C
	ATOM	1545	CG	TYR	F	150	-6.168	43.914	72.811	1.00	36.31	C
	ATOM	1546	CD1	TYR	F	150	-5.059	43.424	72.123	1.00	37.01	C
45	ATOM	1548	CE1	TYR	F	150	-4.092	42.659	72.770	1.00	35.19	C
	ATOM	1550	CZ	TYR	F	150	-4.242	42.367	74.106	1.00	34.95	C
	ATOM	1551	OH	TYR	F	150	-3.295	41.608	74.744	1.00	38.19	O
	ATOM	1553	CE2	TYR	F	150	-5.339	42.834	74.808	1.00	35.82	C
	ATOM	1555	CD2	TYR	F	150	-6.294	43.598	74.159	1.00	35.91	C
50	ATOM	1557	C	TYR	F	150	-6.888	46.801	73.513	1.00	39.95	C
	ATOM	1558	O	TYR	F	150	-5.802	47.163	73.975	1.00	36.11	O
	ATOM	1560	N	LEU	F	151	-8.042	46.873	74.164	1.00	41.73	N
	ATOM	1561	CA	LEU	F	151	-8.178	47.454	75.480	1.00	42.48	C
	ATOM	1563	CB	LEU	F	151	-9.397	48.366	75.482	1.00	43.47	C
55	ATOM	1566	CG	LEU	F	151	-9.685	49.212	76.709	1.00	44.88	C
	ATOM	1568	CD1	LEU	F	151	-8.617	50.259	76.916	1.00	45.64	C
	ATOM	1572	CD2	LEU	F	151	-11.046	49.844	76.526	1.00	47.81	C
	ATOM	1576	C	LEU	F	151	-8.339	46.330	76.496	1.00	42.46	C
	ATOM	1577	O	LEU	F	151	-8.945	45.299	76.214	1.00	43.13	O
60	ATOM	1579	N	ASN	F	152	-7.790	46.543	77.680	1.00	44.63	N
	ATOM	1580	CA	ASN	F	152	-7.792	45.551	78.741	1.00	45.55	C
	ATOM	1582	CB	ASN	F	152	-6.417	44.872	78.772	1.00	49.23	C
	ATOM	1585	CG	ASN	F	152	-6.305	43.747	79.791	1.00	50.43	C
	ATOM	1586	OD1	ASN	F	152	-7.179	43.539	80.636	1.00	53.00	O
65	ATOM	1587	ND2	ASN	F	152	-5.196	43.010	79.704	1.00	56.41	N
	ATOM	1590	C	ASN	F	152	-8.086	46.305	80.032	1.00	44.78	C
	ATOM	1591	O	ASN	F	152	-7.204	46.957	80.584	1.00	43.50	O
	ATOM	1593	N	VAL	F	153	-9.341	46.256	80.476	1.00	44.89	N
	ATOM	1594	CA	VAL	F	153	-9.713	46.780	81.793	1.00	44.78	C
70	ATOM	1596	CB	VAL	F	153	-10.563	48.112	81.731	1.00	47.24	C
	ATOM	1598	CG1	VAL	F	153	-11.030	48.431	80.319	1.00	50.93	C
	ATOM	1602	CG2	VAL	F	153	-11.723	48.123	82.726	1.00	44.92	C
	ATOM	1606	C	VAL	F	153	-10.329	45.696	82.693	1.00	44.28	C
	ATOM	1607	O	VAL	F	153	-11.247	44.969	82.303	1.00	44.32	O
	ATOM	1609	N	THR	F	154	-9.769	45.581	83.892	1.00	39.88	N

	ATOM	1610	CA	THR	F	154	-10.224	44.631	84.880	1.00	42.98	C
	ATOM	1612	CB	THR	F	154	-9.121	43.605	85.219	1.00	45.60	C
	ATOM	1614	OG1	THR	F	154	-7.945	44.290	85.665	1.00	46.84	O
	ATOM	1616	CG2	THR	F	154	-8.779	42.767	83.992	1.00	45.83	C
5	ATOM	1620	C	THR	F	154	-10.649	45.385	86.137	1.00	40.52	C
	ATOM	1621	O	THR	F	154	-10.124	46.460	86.449	1.00	35.32	O
	ATOM	1623	N	THR	F	155	-11.612	44.812	86.847	1.00	39.29	N
	ATOM	1624	CA	THR	F	155	-12.223	45.485	87.980	1.00	39.79	C
10	ATOM	1626	CB	THR	F	155	-13.408	46.378	87.513	1.00	38.52	C
	ATOM	1628	OG1	THR	F	155	-13.757	47.310	88.542	1.00	39.43	O
	ATOM	1630	CG2	THR	F	155	-14.631	45.544	87.130	1.00	38.27	C
	ATOM	1634	C	THR	F	155	-12.676	44.445	88.987	1.00	39.31	C
	ATOM	1635	O	THR	F	155	-12.491	43.246	88.776	1.00	38.45	O
	ATOM	1637	N	ASP	F	156	-13.250	44.916	90.087	1.00	42.41	N
15	ATOM	1638	CA	ASP	F	156	-13.821	44.043	91.103	1.00	41.26	C
	ATOM	1640	CB	ASP	F	156	-14.253	44.887	92.307	1.00	43.55	C
	ATOM	1643	CG	ASP	F	156	-14.673	44.060	93.504	1.00	43.54	C
	ATOM	1644	OD1	ASP	F	156	-14.681	42.814	93.430	1.00	45.44	O
	ATOM	1645	OD2	ASP	F	156	-14.997	44.681	94.536	1.00	44.53	O
20	ATOM	1646	C	ASP	F	156	-15.009	43.317	90.476	1.00	40.85	C
	ATOM	1647	O	ASP	F	156	-16.057	43.918	90.246	1.00	39.23	O
	ATOM	1649	N	ASN	F	157	-14.827	42.029	90.182	1.00	42.16	N
	ATOM	1650	CA	ASN	F	157	-15.862	41.213	89.532	1.00	42.08	C
	ATOM	1652	CB	ASN	F	157	-15.254	39.916	88.978	1.00	42.43	C
25	ATOM	1655	CG	ASN	F	157	-14.400	40.148	87.735	1.00	42.91	C
	ATOM	1656	OD1	ASN	F	157	-14.785	40.886	86.826	1.00	41.58	O
	ATOM	1657	ND2	ASN	F	157	-13.244	39.496	87.685	1.00	42.16	N
	ATOM	1660	C	ASN	F	157	-17.053	40.885	90.438	1.00	40.86	C
	ATOM	1661	O	ASN	F	157	-18.027	40.276	89.986	1.00	37.98	O
30	ATOM	1663	N	THR	F	158	-16.964	41.277	91.709	1.00	43.69	N
	ATOM	1664	CA	THR	F	158	-18.089	41.193	92.644	1.00	43.92	C
	ATOM	1666	CB	THR	F	158	-17.623	41.457	94.094	1.00	43.82	C
	ATOM	1668	OG1	THR	F	158	-16.826	40.354	94.541	1.00	43.15	O
	ATOM	1670	CG2	THR	F	158	-18.805	41.635	95.043	1.00	45.34	C
35	ATOM	1674	C	THR	F	158	-19.193	42.185	92.277	1.00	45.75	C
	ATOM	1675	O	THR	F	158	-20.370	41.824	92.270	1.00	46.49	O
	ATOM	1677	N	SER	F	159	-18.811	43.430	91.986	1.00	46.33	N
	ATOM	1678	CA	SER	F	159	-19.776	44.466	91.613	1.00	45.13	C
	ATOM	1680	CB	SER	F	159	-19.561	45.742	92.433	1.00	46.86	C
40	ATOM	1683	OG	SER	F	159	-18.232	46.204	92.326	1.00	48.59	O
	ATOM	1685	C	SER	F	159	-19.713	44.770	90.119	1.00	43.03	C
	ATOM	1686	O	SER	F	159	-18.957	45.631	89.675	1.00	43.47	O
	ATOM	1688	N	LEU	F	160	-20.515	44.038	89.354	1.00	42.68	N
	ATOM	1689	CA	LEU	F	160	-20.684	44.283	87.929	1.00	42.18	C
45	ATOM	1691	CB	LEU	F	160	-20.339	43.012	87.145	1.00	41.14	C
	ATOM	1694	CG	LEU	F	160	-18.884	42.539	87.262	1.00	41.56	C
	ATOM	1696	CD1	LEU	F	160	-18.774	41.078	86.874	1.00	43.58	C
	ATOM	1700	CD2	LEU	F	160	-17.935	43.389	86.416	1.00	42.66	C
	ATOM	1704	C	LEU	F	160	-22.109	44.746	87.592	1.00	41.83	C
50	ATOM	1705	O	LEU	F	160	-22.399	45.043	86.432	1.00	42.81	O
	ATOM	1707	N	ASP	F	161	-22.983	44.832	88.597	1.00	40.24	N
	ATOM	1708	CA	ASP	F	161	-24.390	45.183	88.377	1.00	42.77	C
	ATOM	1710	CB	ASP	F	161	-25.193	45.077	89.687	1.00	46.10	C
	ATOM	1713	CG	ASP	F	161	-25.356	43.641	90.161	1.00	50.56	C
55	ATOM	1714	OD1	ASP	F	161	-24.516	42.787	89.791	1.00	52.09	O
	ATOM	1715	OD2	ASP	F	161	-26.325	43.363	90.905	1.00	53.72	O
	ATOM	1716	C	ASP	F	161	-24.573	46.577	87.767	1.00	42.75	C
	ATOM	1717	O	ASP	F	161	-25.483	46.787	86.963	1.00	42.99	O
	ATOM	1719	N	ASP	F	162	-23.721	47.525	88.154	1.00	41.00	N
60	ATOM	1720	CA	ASP	F	162	-23.784	48.884	87.613	1.00	40.35	C
	ATOM	1722	CB	ASP	F	162	-24.499	49.812	88.605	1.00	40.18	C
	ATOM	1725	CG	ASP	F	162	-24.884	51.150	87.991	1.00	41.36	C
	ATOM	1726	OD1	ASP	F	162	-25.686	51.170	87.029	1.00	39.61	O
	ATOM	1727	OD2	ASP	F	162	-24.385	52.185	88.479	1.00	41.96	O
65	ATOM	1728	C	ASP	F	162	-22.378	49.394	87.279	1.00	40.42	C
	ATOM	1729	O	ASP	F	162	-22.045	50.557	87.526	1.00	43.19	O
	ATOM	1731	N	PHE	F	163	-21.556	48.508	86.719	1.00	37.13	N
	ATOM	1732	CA	PHE	F	163	-20.229	48.878	86.254	1.00	36.99	C
	ATOM	1734	CB	PHE	F	163	-19.283	47.669	86.224	1.00	34.56	C
70	ATOM	1737	CG	PHE	F	163	-17.904	47.997	85.704	1.00	33.92	C
	ATOM	1738	CD1	PHE	F	163	-17.172	49.047	86.252	1.00	32.93	C

	ATOM	1740	CE1	PHE	F	163	-15.905	49.364	85.767	1.00	34.65	C
	ATOM	1742	CZ	PHE	F	163	-15.354	48.616	84.735	1.00	34.07	C
	ATOM	1744	CE2	PHE	F	163	-16.073	47.569	84.183	1.00	32.90	C
5	ATOM	1746	CD2	PHE	F	163	-17.339	47.262	84.667	1.00	33.44	C
	ATOM	1748	C	PHE	F	163	-20.342	49.483	84.862	1.00	36.95	C
	ATOM	1749	O	PHE	F	163	-20.815	48.832	83.933	1.00	36.94	O
	ATOM	1751	N	HIS	F	164	-19.906	50.730	84.718	1.00	37.09	N
	ATOM	1752	CA	HIS	F	164	-20.038	51.435	83.450	1.00	35.77	C
10	ATOM	1754	CB	HIS	F	164	-21.398	52.147	83.361	1.00	32.87	C
	ATOM	1757	CG	HIS	F	164	-22.555	51.212	83.173	1.00	30.54	C
	ATOM	1758	ND1	HIS	F	164	-22.752	50.495	82.013	1.00	29.35	N
	ATOM	1760	CE1	HIS	F	164	-23.833	49.747	82.137	1.00	28.11	C
	ATOM	1762	NE2	HIS	F	164	-24.342	49.947	83.338	1.00	26.02	N
15	ATOM	1764	CD2	HIS	F	164	-23.558	50.854	84.010	1.00	28.88	C
	ATOM	1766	C	HIS	F	164	-18.915	52.430	83.246	1.00	37.17	C
	ATOM	1767	O	HIS	F	164	-18.243	52.840	84.189	1.00	35.87	O
	ATOM	1769	N	VAL	F	165	-18.723	52.799	81.987	1.00	38.34	N
	ATOM	1770	CA	VAL	F	165	-17.775	53.829	81.609	1.00	36.95	C
20	ATOM	1772	CB	VAL	F	165	-16.621	53.260	80.730	1.00	36.32	C
	ATOM	1774	CG1	VAL	F	165	-17.134	52.759	79.379	1.00	38.21	C
	ATOM	1778	CG2	VAL	F	165	-15.526	54.301	80.532	1.00	36.28	C
	ATOM	1782	C	VAL	F	165	-18.536	54.943	80.885	1.00	38.26	C
	ATOM	1783	O	VAL	F	165	-19.403	54.676	80.036	1.00	38.14	O
25	ATOM	1785	N	ASN	F	166	-18.238	56.186	81.260	1.00	35.73	N
	ATOM	1786	CA	ASN	F	166	-18.718	57.348	80.533	1.00	35.61	C
	ATOM	1788	CB	ASN	F	166	-19.349	58.362	81.481	1.00	33.13	C
	ATOM	1791	CG	ASN	F	166	-20.704	57.934	81.985	1.00	31.58	C
	ATOM	1792	OD1	ASN	F	166	-21.551	57.464	81.223	1.00	27.56	O
30	ATOM	1793	ND2	ASN	F	166	-20.930	58.120	83.284	1.00	31.50	N
	ATOM	1796	C	ASN	F	166	-17.565	58.007	79.780	1.00	34.95	C
	ATOM	1797	O	ASN	F	166	-16.458	58.128	80.303	1.00	36.96	O
	ATOM	1799	N	GLY	F	167	-17.834	58.434	78.552	1.00	34.63	N
	ATOM	1800	CA	GLY	F	167	-16.824	59.098	77.727	1.00	35.89	C
35	ATOM	1803	C	GLY	F	167	-15.706	58.170	77.284	1.00	35.95	C
	ATOM	1804	O	GLY	F	167	-14.596	58.626	77.007	1.00	41.18	O
	ATOM	1806	N	GLY	F	168	-16.003	56.872	77.223	1.00	34.60	N
	ATOM	1807	CA	GLY	F	168	-15.056	55.859	76.777	1.00	36.43	C
	ATOM	1810	C	GLY	F	168	-14.712	56.046	75.312	1.00	37.81	C
40	ATOM	1811	O	GLY	F	168	-15.562	55.877	74.445	1.00	39.12	O
	ATOM	1813	N	GLU	F	169	-13.456	56.389	75.042	1.00	40.78	N
	ATOM	1814	CA	GLU	F	169	-13.035	56.812	73.715	1.00	38.12	C
	ATOM	1816	CB	GLU	F	169	-13.228	58.315	73.584	1.00	41.40	C
	ATOM	1819	CG	GLU	F	169	-12.997	58.888	72.190	1.00	41.79	C
45	ATOM	1822	CD	GLU	F	169	-13.021	60.393	72.219	1.00	42.87	C
	ATOM	1823	OE1	GLU	F	169	-11.976	61.005	72.540	1.00	40.82	O
	ATOM	1824	OE2	GLU	F	169	-14.095	60.961	71.944	1.00	46.26	O
	ATOM	1825	C	GLU	F	169	-11.579	56.465	73.457	1.00	36.78	C
	ATOM	1826	O	GLU	F	169	-10.705	56.803	74.259	1.00	36.62	O
50	ATOM	1828	N	LEU	F	170	-11.341	55.779	72.337	1.00	35.81	N
	ATOM	1829	CA	LEU	F	170	-10.003	55.439	71.876	1.00	35.89	C
	ATOM	1831	CB	LEU	F	170	-9.784	53.925	71.935	1.00	37.28	C
	ATOM	1834	CG	LEU	F	170	-8.571	53.317	71.213	1.00	36.19	C
	ATOM	1836	CD1	LEU	F	170	-7.275	53.769	71.847	1.00	36.63	C
55	ATOM	1840	CD2	LEU	F	170	-8.662	51.791	71.212	1.00	36.34	C
	ATOM	1844	C	LEU	F	170	-9.822	55.954	70.445	1.00	37.75	C
	ATOM	1845	O	LEU	F	170	-10.513	55.510	69.514	1.00	34.03	O
	ATOM	1847	N	ILE	F	171	-8.901	56.905	70.283	1.00	36.62	N
	ATOM	1848	CA	ILE	F	171	-8.543	57.421	68.971	1.00	37.41	C
60	ATOM	1850	CB	ILE	F	171	-8.624	58.960	68.946	1.00	35.58	C
	ATOM	1852	CG1	ILE	F	171	-10.070	59.424	69.136	1.00	35.28	C
	ATOM	1855	CD1	ILE	F	171	-10.200	60.938	69.389	1.00	35.66	C
	ATOM	1859	CG2	ILE	F	171	-8.030	59.525	67.639	1.00	36.02	C
	ATOM	1863	C	ILE	F	171	-7.124	56.961	68.597	1.00	36.06	C
65	ATOM	1864	O	ILE	F	171	-6.227	56.987	69.434	1.00	38.72	O
	ATOM	1866	N	LEU	F	172	-6.939	56.507	67.357	1.00	36.84	N
	ATOM	1867	CA	LEU	F	172	-5.587	56.336	66.788	1.00	37.28	C
	ATOM	1869	CB	LEU	F	172	-5.221	54.879	66.506	1.00	39.72	C
	ATOM	1872	CG	LEU	F	172	-5.737	53.585	67.146	1.00	41.24	C
70	ATOM	1874	CD1	LEU	F	172	-4.560	52.624	67.209	1.00	42.11	C
	ATOM	1878	CD2	LEU	F	172	-6.362	53.698	68.492	1.00	44.22	C
	ATOM	1882	C	LEU	F	172	-5.440	57.134	65.485	1.00	37.58	C

	ATOM	1883	O	LEU	F	172	-6.347	57.145	64.641	1.00	35.52	O
	ATOM	1885	N	ILE	F	173	-4.302	57.808	65.331	1.00	37.82	N
	ATOM	1886	CA	ILE	F	173	-4.026	58.607	64.131	1.00	36.23	C
	ATOM	1888	CB	ILE	F	173	-4.186	60.120	64.388	1.00	36.94	C
5	ATOM	1890	CG1	ILE	F	173	-5.550	60.438	65.020	1.00	37.84	C
	ATOM	1893	CD1	ILE	F	173	-5.674	61.864	65.563	1.00	36.14	C
	ATOM	1897	CG2	ILE	F	173	-4.006	60.898	63.099	1.00	34.14	C
	ATOM	1901	C	ILE	F	173	-2.608	58.346	63.629	1.00	36.89	C
	ATOM	1902	O	ILE	F	173	-1.628	58.716	64.283	1.00	35.93	O
10	ATOM	1904	N	HIS	F	174	-2.516	57.702	62.465	1.00	38.49	N
	ATOM	1905	CA	HIS	F	174	-1.249	57.450	61.779	1.00	37.86	C
	ATOM	1907	CB	HIS	F	174	-1.535	56.725	60.462	1.00	39.54	C
	ATOM	1910	CG	HIS	F	174	-0.330	56.154	59.783	1.00	39.08	C
	ATOM	1911	ND1	HIS	F	174	-0.203	56.120	58.409	1.00	39.03	N
15	ATOM	1913	CE1	HIS	F	174	0.937	55.536	58.088	1.00	37.60	C
	ATOM	1915	NE2	HIS	F	174	1.555	55.192	59.204	1.00	37.87	N
	ATOM	1917	CD2	HIS	F	174	0.781	55.561	60.278	1.00	36.83	C
	ATOM	1919	C	HIS	F	174	-0.531	58.767	61.516	1.00	37.68	C
	ATOM	1920	O	HIS	F	174	-1.162	59.757	61.129	1.00	35.00	O
20	ATOM	1922	N	GLN	F	175	0.783	58.783	61.740	1.00	37.16	N
	ATOM	1923	CA	GLN	F	175	1.583	59.997	61.547	1.00	37.10	C
	ATOM	1925	CB	GLN	F	175	2.348	60.347	62.831	1.00	38.15	C
	ATOM	1928	CG	GLN	F	175	1.469	60.622	64.042	1.00	37.55	C
	ATOM	1931	CD	GLN	F	175	0.620	61.860	63.880	1.00	36.83	C
25	ATOM	1932	OE1	GLN	F	175	1.133	62.945	63.572	1.00	37.36	O
	ATOM	1933	NE2	GLN	F	175	-0.682	61.716	64.098	1.00	31.75	N
	ATOM	1936	C	GLN	F	175	2.565	59.911	60.379	1.00	35.45	C
	ATOM	1937	O	GLN	F	175	3.261	60.884	60.086	1.00	34.80	O
	ATOM	1939	N	ASN	F	176	2.592	58.773	59.692	1.00	39.05	N
30	ATOM	1940	CA	ASN	F	176	3.566	58.528	58.629	1.00	37.50	C
	ATOM	1942	CB	ASN	F	176	4.561	57.468	59.086	1.00	33.92	C
	ATOM	1945	CG	ASN	F	176	5.372	57.922	60.246	1.00	32.87	C
	ATOM	1946	OD1	ASN	F	176	4.998	57.691	61.387	1.00	33.38	O
	ATOM	1947	ND2	ASN	F	176	6.477	58.618	59.970	1.00	32.08	N
35	ATOM	1950	C	ASN	F	176	2.956	58.090	57.314	1.00	36.45	C
	ATOM	1951	O	ASN	F	176	3.328	57.043	56.796	1.00	33.58	O
	ATOM	1953	N	PRO	F	177	2.049	58.906	56.744	1.00	39.03	N
	ATOM	1954	CA	PRO	F	177	1.533	58.596	55.410	1.00	39.64	C
	ATOM	1956	CB	PRO	F	177	0.744	59.865	55.020	1.00	40.97	C
40	ATOM	1959	CG	PRO	F	177	1.093	60.907	56.034	1.00	39.58	C
	ATOM	1962	CD	PRO	F	177	1.469	60.151	57.277	1.00	40.02	C
	ATOM	1965	C	PRO	F	177	2.655	58.327	54.402	1.00	39.95	C
	ATOM	1966	O	PRO	F	177	3.664	59.034	54.399	1.00	43.14	O
	ATOM	1967	N	GLY	F	178	2.473	57.306	53.572	1.00	40.05	N
45	ATOM	1968	CA	GLY	F	178	3.455	56.923	52.559	1.00	43.05	C
	ATOM	1971	C	GLY	F	178	4.278	55.699	52.937	1.00	44.93	C
	ATOM	1972	O	GLY	F	178	5.001	55.143	52.101	1.00	43.29	O
	ATOM	1974	N	GLU	F	179	4.168	55.279	54.196	1.00	44.71	N
	ATOM	1975	CA	GLU	F	179	4.911	54.127	54.701	1.00	44.56	C
50	ATOM	1977	CB	GLU	F	179	5.015	54.196	56.236	1.00	50.41	C
	ATOM	1980	CG	GLU	F	179	6.416	53.983	56.791	1.00	59.02	C
	ATOM	1983	CD	GLU	F	179	7.362	55.145	56.496	1.00	63.76	C
	ATOM	1984	OE1	GLU	F	179	7.121	56.260	57.000	1.00	70.53	O
	ATOM	1985	OE2	GLU	F	179	8.359	54.943	55.770	1.00	64.40	O
55	ATOM	1986	C	GLU	F	179	4.213	52.838	54.236	1.00	42.08	C
	ATOM	1987	O	GLU	F	179	3.153	52.891	53.614	1.00	43.52	O
	ATOM	1989	N	PHE	F	180	4.810	51.686	54.523	1.00	40.75	N
	ATOM	1990	CA	PHE	F	180	4.231	50.397	54.128	1.00	39.16	C
	ATOM	1992	CB	PHE	F	180	5.093	49.238	54.631	1.00	37.33	C
60	ATOM	1995	CG	PHE	F	180	4.485	47.882	54.372	1.00	38.10	C
	ATOM	1996	CD1	PHE	F	180	4.597	47.286	53.121	1.00	35.59	C
	ATOM	1998	CE1	PHE	F	180	4.025	46.047	52.876	1.00	36.56	C
	ATOM	2000	CZ	PHE	F	180	3.325	45.394	53.881	1.00	35.30	C
	ATOM	2002	CE2	PHE	F	180	3.196	45.980	55.123	1.00	34.78	C
65	ATOM	2004	CD2	PHE	F	180	3.776	47.217	55.368	1.00	34.91	C
	ATOM	2006	C	PHE	F	180	2.811	50.201	54.661	1.00	39.57	C
	ATOM	2007	O	PHE	F	180	2.558	50.418	55.849	1.00	39.17	O
	ATOM	2009	N	CYS	F	181	1.900	49.788	53.776	1.00	36.56	N
	ATOM	2010	CA	CYS	F	181	0.534	49.443	54.152	1.00	39.15	C
70	ATOM	2012	CB	CYS	F	181	-0.468	50.493	53.654	1.00	40.67	C
	ATOM	2015	SG	CYS	F	181	-0.275	52.133	54.349	1.00	42.33	S

5	ATOM	2017	C	CYS	F	181	0.134	48.104	53.569	1.00	38.47	C
	ATOM	2018	O	CYS	F	181	0.686	47.674	52.561	1.00	39.25	O
	ATOM	2020	N	VAL	F	182	-0.822	47.446	54.219	1.00	39.80	N
	ATOM	2021	CA	VAL	F	182	-1.576	46.361	53.594	1.00	42.69	C
	ATOM	2023	CB	VAL	F	182	-1.490	45.034	54.378	1.00	42.73	C
10	ATOM	2025	CG1	VAL	F	182	-2.483	44.019	53.821	1.00	43.26	C
	ATOM	2029	CG2	VAL	F	182	-0.069	44.471	54.330	1.00	43.17	C
	ATOM	2033	C	VAL	F	182	-3.017	46.845	53.515	1.00	43.74	C
	ATOM	2034	O	VAL	F	182	-3.704	46.965	54.531	1.00	41.25	O
	ATOM	2036	N	LEU	F	183	-3.456	47.144	52.300	1.00	47.76	N
15	ATOM	2037	CA	LEU	F	183	-4.773	47.717	52.073	1.00	51.36	C
	ATOM	2039	CB	LEU	F	183	-4.670	48.895	51.089	1.00	53.23	C
	ATOM	2042	CG	LEU	F	183	-3.793	50.065	51.577	1.00	53.38	C
	ATOM	2044	CD1	LEU	F	183	-3.572	51.095	50.473	1.00	53.94	C
	ATOM	2048	CD2	LEU	F	183	-4.386	50.730	52.816	1.00	51.39	C
20	ATOM	2052	C	LEU	F	183	-5.745	46.650	51.569	1.00	53.53	C
	ATOM	2053	O	LEU	F	183	-5.385	45.743	50.815	1.00	51.68	O
	ATOM	2055	OXT	LEU	F	183	-6.922	46.671	51.934	1.00	57.05	O
	ATOM	2056	C1	NAG	F	200	-4.868	42.259	80.901	1.00	61.02	C
	ATOM	2059	C2	NAG	F	200	-3.908	41.258	80.253	1.00	62.06	C
25	ATOM	2061	N2	NAG	F	200	-4.564	40.490	79.199	1.00	61.70	N
	ATOM	2063	C7	NAG	F	200	-4.235	40.539	77.902	1.00	63.68	C
	ATOM	2064	O7	NAG	F	200	-5.075	40.461	77.010	1.00	63.74	O
	ATOM	2065	C8	NAG	F	200	-2.786	40.658	77.524	1.00	65.63	C
	ATOM	2069	C3	NAG	F	200	-3.357	40.322	81.330	1.00	64.43	C
30	ATOM	2071	O3	NAG	F	200	-2.371	39.458	80.797	1.00	62.44	O
	ATOM	2073	C4	NAG	F	200	-2.765	41.109	82.503	1.00	66.42	C
	ATOM	2075	O4	NAG	F	200	-2.493	40.232	83.582	1.00	67.74	O
	ATOM	2077	C5	NAG	F	200	-3.676	42.255	82.966	1.00	65.41	C
	ATOM	2079	C6	NAG	F	200	-2.932	43.179	83.936	1.00	65.22	C
35	ATOM	2082	O6	NAG	F	200	-3.776	43.621	84.979	1.00	64.02	O
	ATOM	2084	O5	NAG	F	200	-4.131	43.011	81.852	1.00	62.60	O
	ATOM	2085	N	LEU	R	29	-4.590	37.427	47.176	1.00	68.49	N
	ATOM	2086	CA	LEU	R	29	-3.361	37.040	47.937	1.00	67.62	C
	ATOM	2088	CB	LEU	R	29	-2.271	38.107	47.782	1.00	67.85	C
40	ATOM	2091	CG	LEU	R	29	-0.922	37.802	48.442	1.00	67.30	C
	ATOM	2093	CD1	LEU	R	29	-0.334	36.496	47.905	1.00	66.86	C
	ATOM	2097	CD2	LEU	R	29	0.035	38.961	48.226	1.00	67.01	C
	ATOM	2101	C	LEU	R	29	-3.658	36.840	49.420	1.00	65.77	C
	ATOM	2102	O	LEU	R	29	-4.113	37.763	50.094	1.00	65.27	O
45	ATOM	2106	N	HIS	R	30	-3.383	35.637	49.920	1.00	64.96	N
	ATOM	2107	CA	HIS	R	30	-3.589	35.318	51.331	1.00	64.21	C
	ATOM	2109	CB	HIS	R	30	-4.815	34.416	51.504	1.00	68.47	C
	ATOM	2112	CG	HIS	R	30	-5.786	34.914	52.529	1.00	71.12	C
	ATOM	2113	ND1	HIS	R	30	-6.976	35.521	52.190	1.00	72.21	N
50	ATOM	2115	CE1	HIS	R	30	-7.622	35.863	53.291	1.00	72.83	C
	ATOM	2117	NE2	HIS	R	30	-6.891	35.505	54.332	1.00	73.27	N
	ATOM	2119	CD2	HIS	R	30	-5.736	34.910	53.883	1.00	72.51	C
	ATOM	2121	C	HIS	R	30	-2.336	34.650	51.896	1.00	62.07	C
	ATOM	2122	O	HIS	R	30	-2.014	33.510	51.546	1.00	60.28	O
55	ATOM	2124	N	CYS	R	31	-1.632	35.379	52.761	1.00	59.01	N
	ATOM	2125	CA	CYS	R	31	-0.369	34.927	53.333	1.00	56.06	C
	ATOM	2127	CB	CYS	R	31	0.576	36.111	53.532	1.00	49.48	C
	ATOM	2130	SG	CYS	R	31	1.007	36.978	52.023	1.00	41.00	S
	ATOM	2132	C	CYS	R	31	-0.614	34.257	54.672	1.00	57.87	C
60	ATOM	2133	O	CYS	R	31	-1.389	34.762	55.489	1.00	60.13	O
	ATOM	2135	N	VAL	R	32	0.058	33.131	54.901	1.00	56.89	N
	ATOM	2136	CA	VAL	R	32	-0.114	32.369	56.136	1.00	54.65	C
	ATOM	2138	CB	VAL	R	32	-0.649	30.941	55.867	1.00	56.56	C
	ATOM	2140	CG1	VAL	R	32	-2.115	31.001	55.461	1.00	57.47	C
65	ATOM	2144	CG2	VAL	R	32	0.185	30.221	54.803	1.00	57.11	C
	ATOM	2148	C	VAL	R	32	1.185	32.284	56.925	1.00	53.50	C
	ATOM	2149	O	VAL	R	32	2.280	32.297	56.355	1.00	51.88	O
	ATOM	2151	N	GLY	R	33	1.047	32.197	58.244	1.00	51.87	N
	ATOM	2152	CA	GLY	R	33	2.192	32.066	59.129	1.00	49.61	C
70	ATOM	2155	C	GLY	R	33	2.946	33.371	59.273	1.00	48.76	C
	ATOM	2156	O	GLY	R	33	2.339	34.428	59.475	1.00	50.34	O
	ATOM	2158	N	ASP	R	34	4.270	33.295	59.145	1.00	45.33	N
	ATOM	2159	CA	ASP	R	34	5.159	33.417	59.450	1.00	41.78	C
	ATOM	2161	CB	ASP	R	34	6.370	33.902	60.212	1.00	39.78	C
	ATOM	2164	CG	ASP	R	34	5.988	33.233	61.517	1.00	41.19	C

	ATOM	2165	OD1	ASP	R	34	5.015	33.661	62.170	1.00	45.29	O
	ATOM	2166	OD2	ASP	R	34	6.672	32.279	61.907	1.00	41.33	O
	ATOM	2167	C	ASP	R	34	5.586	35.181	58.195	1.00	40.52	C
5	ATOM	2168	O	ASP	R	34	6.772	35.414	57.954	1.00	38.72	O
	ATOM	2170	N	THR	R	35	4.585	35.574	57.413	1.00	40.50	N
	ATOM	2171	CA	THR	R	35	4.774	36.348	56.205	1.00	37.48	C
	ATOM	2173	CB	THR	R	35	4.564	35.477	54.934	1.00	37.55	C
	ATOM	2175	OG1	THR	R	35	3.261	34.884	54.956	1.00	36.83	O
10	ATOM	2177	CG2	THR	R	35	5.606	34.368	54.845	1.00	37.16	C
	ATOM	2181	C	THR	R	35	3.781	37.513	56.202	1.00	37.67	C
	ATOM	2182	O	THR	R	35	2.865	37.564	57.029	1.00	34.55	O
	ATOM	2184	N	TYR	R	36	3.983	38.453	55.283	1.00	37.27	N
	ATOM	2185	CA	TYR	R	36	3.035	39.543	55.051	1.00	36.18	C
15	ATOM	2187	CB	TYR	R	36	3.475	40.827	55.757	1.00	34.24	C
	ATOM	2190	CG	TYR	R	36	4.856	41.318	55.379	1.00	33.51	C
	ATOM	2191	CD1	TYR	R	36	5.037	42.233	54.347	1.00	33.30	C
	ATOM	2193	CE1	TYR	R	36	6.306	42.684	54.001	1.00	33.44	C
	ATOM	2195	CZ	TYR	R	36	7.409	42.230	54.702	1.00	33.51	C
20	ATOM	2196	OH	TYR	R	36	8.668	42.676	54.380	1.00	32.68	O
	ATOM	2198	CE2	TYR	R	36	7.255	41.328	55.736	1.00	34.65	C
	ATOM	2200	CD2	TYR	R	36	5.984	40.874	56.068	1.00	34.20	C
	ATOM	2202	C	TYR	R	36	2.921	39.805	53.563	1.00	35.86	C
	ATOM	2203	O	TYR	R	36	3.893	39.604	52.824	1.00	35.42	O
25	ATOM	2205	N	PRO	R	37	1.738	40.265	53.116	1.00	35.59	N
	ATOM	2206	CA	PRO	R	37	1.528	40.542	51.702	1.00	35.78	C
	ATOM	2208	CB	PRO	R	37	-0.001	40.624	51.582	1.00	34.57	C
	ATOM	2211	CG	PRO	R	37	-0.476	41.014	52.909	1.00	33.07	C
	ATOM	2214	CD	PRO	R	37	0.531	40.536	53.917	1.00	34.42	C
30	ATOM	2217	C	PRO	R	37	2.187	41.839	51.240	1.00	34.31	C
	ATOM	2218	O	PRO	R	37	1.989	42.881	51.852	1.00	35.70	O
	ATOM	2219	N	SER	R	38	2.968	41.751	50.168	1.00	37.15	N
	ATOM	2220	CA	SER	R	38	3.566	42.911	49.519	1.00	39.54	C
	ATOM	2222	CB	SER	R	38	4.827	43.353	50.258	1.00	40.87	C
35	ATOM	2225	OG	SER	R	38	5.424	44.482	49.637	1.00	39.37	O
	ATOM	2227	C	SER	R	38	3.921	42.549	48.085	1.00	42.65	C
	ATOM	2228	O	SER	R	38	4.465	41.476	47.832	1.00	44.60	O
	ATOM	2230	N	ASN	R	39	3.600	43.438	47.148	1.00	46.63	N
	ATOM	2231	CA	ASN	R	39	3.961	43.251	45.745	1.00	47.22	C
40	ATOM	2233	CB	ASN	R	39	5.493	43.324	45.583	1.00	49.37	C
	ATOM	2236	CG	ASN	R	39	6.074	44.656	46.046	1.00	50.52	C
	ATOM	2237	OD1	ASN	R	39	6.702	44.747	47.109	1.00	50.59	O
	ATOM	2238	ND2	ASN	R	39	5.867	45.698	45.246	1.00	50.40	N
	ATOM	2241	C	ASN	R	39	3.422	41.932	45.170	1.00	48.67	C
45	ATOM	2242	O	ASN	R	39	4.160	41.181	44.525	1.00	51.24	O
	ATOM	2244	N	ASP	R	40	2.139	41.657	45.414	1.00	47.61	N
	ATOM	2245	CA	ASP	R	40	1.489	40.413	44.958	1.00	49.01	C
	ATOM	2247	CB	ASP	R	40	1.292	40.426	43.432	1.00	50.99	C
	ATOM	2250	CG	ASP	R	40	0.543	41.660	42.938	1.00	54.43	C
50	ATOM	2251	OD1	ASP	R	40	0.115	42.490	43.771	1.00	55.76	O
	ATOM	2252	OD2	ASP	R	40	0.380	41.798	41.702	1.00	56.84	O
	ATOM	2253	C	ASP	R	40	2.264	39.150	45.378	1.00	48.84	C
	ATOM	2254	O	ASP	R	40	2.331	38.172	44.638	1.00	49.49	O
	ATOM	2256	N	ARG	R	41	2.839	39.180	46.576	1.00	49.68	N
55	ATOM	2257	CA	ARG	R	41	3.682	38.097	47.071	1.00	47.71	C
	ATOM	2259	CB	ARG	R	41	5.094	38.224	46.477	1.00	49.94	C
	ATOM	2262	CG	ARG	R	41	6.223	37.532	47.262	1.00	50.35	C
	ATOM	2265	CD	ARG	R	41	7.584	37.754	46.617	1.00	50.24	C
	ATOM	2268	NE	ARG	R	41	7.944	39.176	46.579	1.00	51.57	N
60	ATOM	2270	CZ	ARG	R	41	9.027	39.724	47.131	1.00	49.92	C
	ATOM	2271	NH1	ARG	R	41	9.925	38.999	47.779	1.00	50.09	N
	ATOM	2274	NH2	ARG	R	41	9.224	41.022	47.013	1.00	50.40	N
	ATOM	2277	C	ARG	R	41	3.718	38.158	48.593	1.00	45.51	C
	ATOM	2278	O	ARG	R	41	3.420	39.195	49.176	1.00	43.63	O
65	ATOM	2280	N	CYS	R	42	4.074	37.037	49.219	1.00	42.92	N
	ATOM	2281	CA	CYS	R	42	4.185	36.937	50.663	1.00	40.88	C
	ATOM	2283	CB	CYS	R	42	3.560	35.624	51.132	1.00	40.54	C
	ATOM	2286	SG	CYS	R	42	1.775	35.525	50.830	1.00	41.29	S
	ATOM	2288	C	CYS	R	42	5.642	37.026	51.127	1.00	41.63	C
70	ATOM	2289	O	CYS	R	42	6.403	36.069	50.966	1.00	42.56	O
	ATOM	2291	N	CYS	R	43	6.016	38.172	51.709	1.00	39.71	N
	ATOM	2292	CA	CYS	R	43	7.374	38.396	52.222	1.00	37.60	C

	ATOM	2294	CB	CYS	R	43	7.764	39.863	52.084	1.00	39.25	C
	ATOM	2297	SG	CYS	R	43	7.924	40.486	50.392	1.00	40.36	S
	ATOM	2299	C	CYS	R	43	7.488	37.980	53.691	1.00	37.12	C
	ATOM	2300	O	CYS	R	43	6.491	37.916	54.401	1.00	37.00	O
5	ATOM	2302	N	HIS	R	44	8.710	37.730	54.153	1.00	34.87	N
	ATOM	2303	CA	HIS	R	44	8.914	37.096	55.451	1.00	35.08	C
	ATOM	2305	CB	HIS	R	44	9.999	36.015	55.365	1.00	32.44	C
	ATOM	2308	CG	HIS	R	44	9.522	34.738	54.748	1.00	32.05	C
	ATOM	2309	ND1	HIS	R	44	9.460	34.546	53.387	1.00	31.26	N
10	ATOM	2311	CE1	HIS	R	44	8.996	33.335	53.134	1.00	33.71	C
	ATOM	2313	NE2	HIS	R	44	8.746	32.736	54.284	1.00	33.11	N
	ATOM	2315	CD2	HIS	R	44	9.062	33.594	55.310	1.00	34.02	C
	ATOM	2317	C	HIS	R	44	9.250	38.087	56.558	1.00	39.44	C
	ATOM	2318	O	HIS	R	44	10.018	39.037	56.371	1.00	38.28	O
15	ATOM	2320	N	GLU	R	45	8.655	37.858	57.722	1.00	39.77	N
	ATOM	2321	CA	GLU	R	45	8.992	38.633	58.893	1.00	40.74	C
	ATOM	2323	CB	GLU	R	45	7.917	38.476	59.962	1.00	43.89	C
	ATOM	2326	CG	GLU	R	45	6.616	39.132	59.542	1.00	47.80	C
	ATOM	2329	CD	GLU	R	45	5.579	39.056	60.612	1.00	52.76	C
20	ATOM	2330	OE1	GLU	R	45	5.041	37.939	60.817	1.00	53.75	O
	ATOM	2331	OE2	GLU	R	45	5.319	40.110	61.260	1.00	62.14	O
	ATOM	2332	C	GLU	R	45	10.362	38.229	59.409	1.00	37.15	C
	ATOM	2333	O	GLU	R	45	10.914	37.181	59.040	1.00	32.72	O
	ATOM	2335	N	CYS	R	46	10.930	39.097	60.231	1.00	37.98	N
25	ATOM	2336	CA	CYS	R	46	12.261	38.865	60.750	1.00	39.28	C
	ATOM	2338	CB	CYS	R	46	12.904	40.171	61.238	1.00	41.93	C
	ATOM	2341	SG	CYS	R	46	13.212	41.364	59.891	1.00	40.71	S
	ATOM	2343	C	CYS	R	46	12.170	37.838	61.850	1.00	37.19	C
	ATOM	2344	O	CYS	R	46	11.108	37.639	62.445	1.00	36.08	O
30	ATOM	2346	N	ARG	R	47	13.299	37.185	62.091	1.00	37.01	N
	ATOM	2347	CA	ARG	R	47	13.401	36.094	63.044	1.00	37.38	C
	ATOM	2349	CB	ARG	R	47	14.290	35.012	62.437	1.00	36.98	C
	ATOM	2352	CG	ARG	R	47	13.595	34.301	61.297	1.00	35.26	C
	ATOM	2355	CD	ARG	R	47	12.657	33.302	61.899	1.00	37.58	C
35	ATOM	2358	NE	ARG	R	47	11.292	33.386	61.439	1.00	34.84	N
	ATOM	2360	CZ	ARG	R	47	10.336	32.565	61.852	1.00	34.86	C
	ATOM	2361	NH1	ARG	R	47	10.581	31.608	62.734	1.00	35.21	N
	ATOM	2364	NH2	ARG	R	47	9.117	32.689	61.371	1.00	38.90	N
	ATOM	2367	C	ARG	R	47	13.994	36.583	64.354	1.00	37.63	C
40	ATOM	2368	O	ARG	R	47	14.623	37.635	64.383	1.00	39.92	O
	ATOM	2370	N	PRO	R	48	13.798	35.818	65.449	1.00	38.02	N
	ATOM	2371	CA	PRO	R	48	14.403	36.164	66.730	1.00	37.12	C
	ATOM	2373	CB	PRO	R	48	14.069	34.952	67.604	1.00	38.82	C
	ATOM	2376	CG	PRO	R	48	12.812	34.431	67.026	1.00	37.34	C
45	ATOM	2379	CD	PRO	R	48	12.985	34.592	65.557	1.00	37.25	C
	ATOM	2382	C	PRO	R	48	15.908	36.353	66.606	1.00	36.34	C
	ATOM	2383	O	PRO	R	48	16.554	35.631	65.849	1.00	39.58	O
	ATOM	2384	N	GLY	R	49	16.451	37.329	67.330	1.00	36.52	N
	ATOM	2385	CA	GLY	R	49	17.856	37.708	67.204	1.00	36.12	C
50	ATOM	2388	C	GLY	R	49	18.134	38.623	66.020	1.00	38.32	C
	ATOM	2389	O	GLY	R	49	19.301	38.891	65.692	1.00	35.18	O
	ATOM	2391	N	ASN	R	50	17.067	39.087	65.369	1.00	37.15	N
	ATOM	2392	CA	ASN	R	50	17.171	40.012	64.246	1.00	37.85	C
	ATOM	2394	CB	ASN	R	50	17.044	39.295	62.892	1.00	35.71	C
55	ATOM	2397	CG	ASN	R	50	18.068	38.192	62.700	1.00	34.18	C
	ATOM	2398	OD1	ASN	R	50	19.134	38.404	62.109	1.00	32.50	O
	ATOM	2399	ND2	ASN	R	50	17.741	36.998	63.180	1.00	32.35	N
	ATOM	2402	C	ASN	R	50	16.098	41.097	64.334	1.00	38.00	C
	ATOM	2403	O	ASN	R	50	15.043	40.900	64.939	1.00	39.01	O
60	ATOM	2405	N	GLY	R	51	16.383	42.236	63.713	1.00	37.06	N
	ATOM	2406	CA	GLY	R	51	15.444	43.341	63.642	1.00	37.50	C
	ATOM	2409	C	GLY	R	51	15.237	43.761	62.207	1.00	36.01	C
	ATOM	2410	O	GLY	R	51	16.136	43.624	61.375	1.00	33.03	O
	ATOM	2412	N	MET	R	52	14.043	44.275	61.920	1.00	36.80	N
65	ATOM	2413	CA	MET	R	52	13.700	44.719	60.584	1.00	35.50	C
	ATOM	2415	CB	MET	R	52	12.192	44.681	60.354	1.00	36.97	C
	ATOM	2418	CG	MET	R	52	11.828	44.725	58.868	1.00	36.34	C
	ATOM	2421	SD	MET	R	52	10.079	44.914	58.530	1.00	35.02	S
	ATOM	2422	CE	MET	R	52	9.826	46.642	58.945	1.00	35.14	C
70	ATOM	2426	C	MET	R	52	14.219	46.119	60.332	1.00	35.44	C
	ATOM	2427	O	MET	R	52	13.903	47.047	61.072	1.00	36.41	O

	ATOM	2429	N	VAL	R	53	15.021	46.241	59.274	1.00	36.38	N
	ATOM	2430	CA	VAL	R	53	15.573	47.499	58.816	1.00	35.10	C
	ATOM	2432	CB	VAL	R	53	16.958	47.269	58.135	1.00	37.13	C
	ATOM	2434	CG1	VAL	R	53	17.490	48.557	57.495	1.00	36.05	C
5	ATOM	2438	CG2	VAL	R	53	17.966	46.694	59.139	1.00	37.55	C
	ATOM	2442	C	VAL	R	53	14.595	48.128	57.818	1.00	36.17	C
	ATOM	2443	O	VAL	R	53	14.332	49.330	57.867	1.00	30.66	O
	ATOM	2445	N	SER	R	54	14.084	47.303	56.902	1.00	36.58	N
	ATOM	2446	CA	SER	R	54	13.094	47.740	55.933	1.00	35.77	C
10	ATOM	2448	CB	SER	R	54	13.765	48.460	54.751	1.00	37.90	C
	ATOM	2451	OG	SER	R	54	14.694	47.635	54.073	1.00	38.42	O
	ATOM	2453	C	SER	R	54	12.262	46.564	55.443	1.00	36.21	C
	ATOM	2454	O	SER	R	54	12.689	45.417	55.510	1.00	39.97	O
	ATOM	2456	N	ARG	R	55	11.061	46.868	54.962	1.00	38.21	N
15	ATOM	2457	CA	ARG	R	55	10.186	45.883	54.329	1.00	37.59	C
	ATOM	2459	CB	ARG	R	55	8.799	46.499	54.069	1.00	38.54	C
	ATOM	2462	CG	ARG	R	55	7.976	46.824	55.321	1.00	37.24	C
	ATOM	2465	CD	ARG	R	55	7.220	45.602	55.823	1.00	38.17	C
	ATOM	2468	NE	ARG	R	55	6.392	45.896	56.992	1.00	38.99	N
20	ATOM	2470	CZ	ARG	R	55	5.861	44.982	57.805	1.00	38.46	C
	ATOM	2471	NH1	ARG	R	55	6.051	43.691	57.600	1.00	40.31	N
	ATOM	2474	NH2	ARG	R	55	5.136	45.363	58.844	1.00	39.89	N
	ATOM	2477	C	ARG	R	55	10.781	45.421	53.003	1.00	38.59	C
	ATOM	2478	O	ARG	R	55	11.657	46.070	52.435	1.00	40.77	O
25	ATOM	2480	N	CYS	R	56	10.271	44.308	52.495	1.00	38.66	N
	ATOM	2481	CA	CYS	R	56	10.747	43.752	51.243	1.00	40.38	C
	ATOM	2483	CB	CYS	R	56	10.118	42.386	51.012	1.00	39.15	C
	ATOM	2486	SG	CYS	R	56	8.367	42.445	50.673	1.00	37.51	S
	ATOM	2488	C	CYS	R	56	10.444	44.655	50.043	1.00	43.13	C
30	ATOM	2489	O	CYS	R	56	9.464	45.403	50.040	1.00	42.16	O
	ATOM	2491	N	SER	R	57	11.307	44.565	49.033	1.00	45.93	N
	ATOM	2492	CA	SER	R	57	11.159	45.303	47.775	1.00	46.60	C
	ATOM	2494	CB	SER	R	57	12.531	45.759	47.280	1.00	44.57	C
	ATOM	2497	OG	SER	R	57	13.351	44.642	46.982	1.00	38.85	O
35	ATOM	2499	C	SER	R	57	10.497	44.391	46.741	1.00	48.81	C
	ATOM	2500	O	SER	R	57	9.982	43.330	47.084	1.00	47.48	O
	ATOM	2502	N	ARG	R	58	10.497	44.803	45.480	1.00	50.54	N
	ATOM	2503	CA	ARG	R	58	9.923	43.981	44.419	1.00	51.31	C
	ATOM	2505	CB	ARG	R	58	9.904	44.750	43.110	1.00	54.51	C
40	ATOM	2508	CG	ARG	R	58	9.005	45.972	43.048	1.00	57.59	C
	ATOM	2511	CD	ARG	R	58	9.139	46.667	41.686	1.00	58.60	C
	ATOM	2514	NE	ARG	R	58	8.803	45.769	40.578	1.00	61.06	N
	ATOM	2516	CZ	ARG	R	58	9.648	44.929	39.970	1.00	63.31	C
	ATOM	2517	NH1	ARG	R	58	10.929	44.834	40.336	1.00	63.39	N
45	ATOM	2520	NH2	ARG	R	58	9.206	44.165	38.978	1.00	63.48	N
	ATOM	2523	C	ARG	R	58	10.707	42.691	44.181	1.00	49.28	C
	ATOM	2524	O	ARG	R	58	10.136	41.686	43.757	1.00	51.57	O
	ATOM	2526	N	SER	R	59	12.015	42.736	44.422	1.00	46.83	N
	ATOM	2527	CA	SER	R	59	12.913	41.628	44.097	1.00	49.60	C
50	ATOM	2529	CB	SER	R	59	14.040	42.145	43.211	1.00	53.62	C
	ATOM	2532	OG	SER	R	59	14.675	43.263	43.816	1.00	57.66	O
	ATOM	2534	C	SER	R	59	13.530	40.945	45.314	1.00	47.99	C
	ATOM	2535	O	SER	R	59	13.820	39.749	45.271	1.00	48.35	O
	ATOM	2537	N	GLN	R	60	13.754	41.712	46.376	1.00	45.52	N
55	ATOM	2538	CA	GLN	R	60	14.411	41.216	47.581	1.00	47.39	C
	ATOM	2540	CB	GLN	R	60	15.410	42.254	48.115	1.00	50.40	C
	ATOM	2543	CG	GLN	R	60	16.318	42.891	47.055	1.00	53.71	C
	ATOM	2546	CD	GLN	R	60	17.219	41.884	46.356	1.00	55.99	C
	ATOM	2547	OE1	GLN	R	60	17.641	40.889	46.952	1.00	55.32	O
60	ATOM	2548	NE2	GLN	R	60	17.529	42.145	45.086	1.00	58.04	N
	ATOM	2551	C	GLN	R	60	13.376	40.914	48.659	1.00	46.37	C
	ATOM	2552	O	GLN	R	60	12.260	41.435	48.634	1.00	44.21	O
	ATOM	2554	N	ASN	R	61	13.760	40.069	49.608	1.00	47.09	N
	ATOM	2555	CA	ASN	R	61	12.932	39.792	50.771	1.00	45.68	C
65	ATOM	2557	CB	ASN	R	61	13.236	38.391	51.331	1.00	47.62	C
	ATOM	2560	CG	ASN	R	61	12.043	37.767	52.076	1.00	48.04	C
	ATOM	2561	OD1	ASN	R	61	11.186	38.471	52.610	1.00	44.26	O
	ATOM	2562	ND2	ASN	R	61	11.991	36.434	52.100	1.00	46.39	N
	ATOM	2565	C	ASN	R	61	13.205	40.876	51.812	1.00	43.93	C
70	ATOM	2566	O	ASN	R	61	14.088	41.717	51.636	1.00	43.05	O
	ATOM	2568	N	THR	R	62	12.429	40.851	52.886	1.00	41.64	N

5	ATOM	2569	CA	THR	R	62	12.619	41.730	54.033	1.00	40.65	C
	ATOM	2571	CB	THR	R	62	11.822	41.178	55.233	1.00	38.78	C
	ATOM	2573	OG1	THR	R	62	10.498	40.832	54.799	1.00	37.94	O
	ATOM	2575	CG2	THR	R	62	11.741	42.188	56.358	1.00	39.65	C
	ATOM	2579	C	THR	R	62	14.092	41.864	54.436	1.00	40.08	C
10	ATOM	2580	O	THR	R	62	14.813	40.869	54.502	1.00	42.46	O
	ATOM	2582	N	VAL	R	63	14.533	43.092	54.706	1.00	39.61	N
	ATOM	2583	CA	VAL	R	63	15.892	43.318	55.199	1.00	39.02	C
	ATOM	2585	CB	VAL	R	63	16.489	44.656	54.708	1.00	38.60	C
	ATOM	2587	CG1	VAL	R	63	17.942	44.796	55.166	1.00	37.56	C
15	ATOM	2591	CG2	VAL	R	63	16.409	44.743	53.186	1.00	36.99	C
	ATOM	2595	C	VAL	R	63	15.911	43.238	56.726	1.00	38.44	C
	ATOM	2596	O	VAL	R	63	15.432	44.146	57.424	1.00	35.43	O
	ATOM	2598	N	CYS	R	64	16.453	42.122	57.218	1.00	39.13	N
	ATOM	2599	CA	CYS	R	64	16.574	41.829	58.642	1.00	39.53	C
20	ATOM	2601	CB	CYS	R	64	15.975	40.462	58.962	1.00	37.79	C
	ATOM	2604	SG	CYS	R	64	14.252	40.293	58.509	1.00	37.27	S
	ATOM	2606	C	CYS	R	64	18.042	41.821	59.033	1.00	40.16	C
	ATOM	2607	O	CYS	R	64	18.874	41.248	58.333	1.00	39.46	O
	ATOM	2609	N	ARG	R	65	18.357	42.456	60.155	1.00	41.99	N
25	ATOM	2610	CA	ARG	R	65	19.727	42.558	60.605	1.00	42.37	C
	ATOM	2612	CB	ARG	R	65	20.187	44.015	60.589	1.00	45.50	C
	ATOM	2615	CG	ARG	R	65	21.606	44.201	61.124	1.00	49.03	C
	ATOM	2618	CD	ARG	R	65	22.307	45.373	60.488	1.00	53.50	C
	ATOM	2621	NE	ARG	R	65	21.671	46.643	60.830	1.00	58.11	N
30	ATOM	2623	CZ	ARG	R	65	22.051	47.824	60.345	1.00	59.54	C
	ATOM	2624	NH1	ARG	R	65	23.072	47.908	59.494	1.00	58.91	N
	ATOM	2627	NH2	ARG	R	65	21.406	48.927	60.712	1.00	60.05	N
	ATOM	2630	C	ARG	R	65	19.857	41.966	62.002	1.00	39.31	C
	ATOM	2631	O	ARG	R	65	19.013	42.229	62.867	1.00	37.03	O
35	ATOM	2633	N	PRO	R	66	20.895	41.138	62.220	1.00	35.57	N
	ATOM	2634	CA	PRO	R	66	21.207	40.670	63.570	1.00	39.27	C
	ATOM	2636	CB	PRO	R	66	22.576	40.000	63.406	1.00	36.92	C
	ATOM	2639	CG	PRO	R	66	22.631	39.579	62.001	1.00	37.87	C
	ATOM	2642	CD	PRO	R	66	21.805	40.560	61.214	1.00	37.99	C
40	ATOM	2645	C	PRO	R	66	21.287	41.811	64.586	1.00	37.84	C
	ATOM	2646	O	PRO	R	66	21.848	42.866	64.293	1.00	37.06	O
	ATOM	2647	N	CYS	R	67	20.709	41.601	65.762	1.00	40.43	N
	ATOM	2648	CA	CYS	R	67	20.768	42.590	66.831	1.00	42.28	C
	ATOM	2650	CB	CYS	R	67	19.914	42.148	68.022	1.00	41.98	C
45	ATOM	2653	SG	CYS	R	67	18.151	41.931	67.648	1.00	42.25	S
	ATOM	2655	C	CYS	R	67	22.213	42.792	67.272	1.00	43.23	C
	ATOM	2656	O	CYS	R	67	22.924	41.824	67.554	1.00	45.65	O
	ATOM	2658	N	GLY	R	68	22.648	44.049	67.309	1.00	42.90	N
	ATOM	2659	CA	GLY	R	68	24.007	44.377	67.724	1.00	43.36	C
50	ATOM	2662	C	GLY	R	68	24.134	44.378	69.236	1.00	43.50	C
	ATOM	2663	O	GLY	R	68	23.136	44.240	69.937	1.00	44.94	O
	ATOM	2665	N	PRO	R	69	25.365	44.553	69.750	1.00	45.11	N
	ATOM	2666	CA	PRO	R	69	25.591	44.593	71.196	1.00	44.75	C
	ATOM	2668	CB	PRO	R	69	27.060	45.024	71.311	1.00	45.27	C
55	ATOM	2671	CG	PRO	R	69	27.683	44.596	70.029	1.00	45.52	C
	ATOM	2674	CD	PRO	R	69	26.620	44.739	68.990	1.00	45.92	C
	ATOM	2677	C	PRO	R	69	24.677	45.598	71.902	1.00	45.05	C
	ATOM	2678	O	PRO	R	69	24.506	46.724	71.427	1.00	44.17	O
	ATOM	2679	N	GLY	R	70	24.085	45.177	73.016	1.00	44.10	N
60	ATOM	2680	CA	GLY	R	70	23.156	46.014	73.765	1.00	42.38	C
	ATOM	2683	C	GLY	R	70	21.715	45.915	73.301	1.00	42.40	C
	ATOM	2684	O	GLY	R	70	20.842	46.581	73.866	1.00	43.15	O
	ATOM	2686	N	PHE	R	71	21.455	45.074	72.295	1.00	42.17	N
	ATOM	2687	CA	PHE	R	71	20.109	44.915	71.726	1.00	40.60	C
65	ATOM	2689	CB	PHE	R	71	20.020	45.575	70.346	1.00	42.37	C
	ATOM	2692	CG	PHE	R	71	20.181	47.059	70.384	1.00	42.12	C
	ATOM	2693	CD1	PHE	R	71	21.442	47.631	70.333	1.00	42.57	C
	ATOM	2695	CE1	PHE	R	71	21.599	49.006	70.378	1.00	43.91	C
	ATOM	2697	CZ	PHE	R	71	20.480	49.827	70.483	1.00	44.13	C
70	ATOM	2699	CE2	PHE	R	71	19.215	49.262	70.536	1.00	43.36	C
	ATOM	2701	CD2	PHE	R	71	19.071	47.886	70.488	1.00	42.20	C
	ATOM	2703	C	PHE	R	71	19.715	43.455	71.594	1.00	37.90	C
	ATOM	2704	O	PHE	R	71	20.569	42.582	71.480	1.00	34.21	O
	ATOM	2706	N	TYR	R	72	18.407	43.209	71.589	1.00	39.91	N
	ATOM	2707	CA	TYR	R	72	17.867	41.863	71.481	1.00	40.10	C

	ATOM	2709	CB	TYR	R	72	17.738	41.224	72.874	1.00	38.83	C
	ATOM	2712	CG	TYR	R	72	16.519	41.685	73.627	1.00	39.35	C
	ATOM	2713	CD1	TYR	R	72	15.357	40.926	73.636	1.00	36.50	C
	ATOM	2715	CE1	TYR	R	72	14.230	41.357	74.293	1.00	36.62	C
5	ATOM	2717	CZ	TYR	R	72	14.244	42.563	74.958	1.00	38.29	C
	ATOM	2718	OH	TYR	R	72	13.119	42.979	75.632	1.00	41.35	O
	ATOM	2720	CE2	TYR	R	72	15.378	43.345	74.967	1.00	38.36	C
	ATOM	2722	CD2	TYR	R	72	16.509	42.908	74.294	1.00	40.79	C
10	ATOM	2724	C	TYR	R	72	16.501	41.887	70.796	1.00	40.05	C
	ATOM	2725	O	TYR	R	72	15.868	42.929	70.681	1.00	39.45	O
	ATOM	2727	N	ASN	R	73	16.064	40.721	70.338	1.00	42.29	N
	ATOM	2728	CA	ASN	R	73	14.709	40.543	69.839	1.00	40.30	C
	ATOM	2730	CB	ASN	R	73	14.601	40.917	68.353	1.00	42.10	C
	ATOM	2733	CG	ASN	R	73	13.202	41.378	67.969	1.00	41.89	C
15	ATOM	2734	OD1	ASN	R	73	12.225	41.007	68.611	1.00	44.85	O
	ATOM	2735	ND2	ASN	R	73	13.105	42.203	66.929	1.00	42.23	N
	ATOM	2738	C	ASN	R	73	14.305	39.097	70.077	1.00	40.66	C
	ATOM	2739	O	ASN	R	73	14.922	38.175	69.536	1.00	42.11	O
20	ATOM	2741	N	ASP	R	74	13.285	38.915	70.912	1.00	38.25	N
	ATOM	2742	CA	ASP	R	74	12.869	37.591	71.388	1.00	38.21	C
	ATOM	2744	CB	ASP	R	74	12.357	37.677	72.849	1.00	39.35	C
	ATOM	2747	CG	ASP	R	74	11.301	38.777	73.062	1.00	39.21	C
	ATOM	2748	OD1	ASP	R	74	11.281	39.752	72.297	1.00	39.10	O
	ATOM	2749	OD2	ASP	R	74	10.488	38.669	74.002	1.00	41.38	O
25	ATOM	2750	C	ASP	R	74	11.814	36.909	70.509	1.00	37.47	C
	ATOM	2751	O	ASP	R	74	11.521	35.736	70.709	1.00	40.58	O
	ATOM	2753	N	VAL	R	75	11.261	37.634	69.539	1.00	36.04	N
	ATOM	2754	CA	VAL	R	75	10.142	37.141	68.736	1.00	35.19	C
	ATOM	2756	CB	VAL	R	75	8.791	37.773	69.170	1.00	34.59	C
30	ATOM	2758	CG1	VAL	R	75	8.432	37.340	70.576	1.00	34.10	C
	ATOM	2762	CG2	VAL	R	75	8.828	39.308	69.065	1.00	34.70	C
	ATOM	2766	C	VAL	R	75	10.313	37.398	67.241	1.00	37.15	C
	ATOM	2767	O	VAL	R	75	11.150	38.199	66.813	1.00	39.08	O
	ATOM	2769	N	VAL	R	76	9.500	36.684	66.467	1.00	39.52	N
35	ATOM	2770	CA	VAL	R	76	9.297	36.941	65.047	1.00	36.31	C
	ATOM	2772	CB	VAL	R	76	8.362	35.876	64.423	1.00	33.40	C
	ATOM	2774	CG1	VAL	R	76	8.030	36.208	62.969	1.00	35.65	C
	ATOM	2778	CG2	VAL	R	76	8.980	34.484	64.534	1.00	30.29	C
	ATOM	2782	C	VAL	R	76	8.642	38.313	64.973	1.00	40.52	C
40	ATOM	2783	O	VAL	R	76	7.681	38.576	65.700	1.00	40.07	O
	ATOM	2785	N	SER	R	77	9.161	39.199	64.123	1.00	40.74	N
	ATOM	2786	CA	SER	R	77	8.670	40.571	64.109	1.00	37.38	C
	ATOM	2788	CB	SER	R	77	9.270	41.348	65.289	1.00	39.69	C
	ATOM	2791	OG	SER	R	77	10.562	41.835	64.986	1.00	40.87	O
45	ATOM	2793	C	SER	R	77	8.946	41.337	62.819	1.00	37.15	C
	ATOM	2794	O	SER	R	77	9.726	40.906	61.969	1.00	39.88	O
	ATOM	2796	N	SER	R	78	8.279	42.484	62.702	1.00	33.97	N
	ATOM	2797	CA	SER	R	78	8.552	43.470	61.675	1.00	35.67	C
	ATOM	2799	CB	SER	R	78	7.309	43.689	60.810	1.00	35.00	C
50	ATOM	2802	OG	SER	R	78	6.189	44.071	61.590	1.00	36.65	O
	ATOM	2804	C	SER	R	78	9.012	44.776	62.342	1.00	36.19	C
	ATOM	2805	O	SER	R	78	8.732	45.867	61.859	1.00	38.90	O
	ATOM	2807	N	LYS	R	79	9.753	44.636	63.439	1.00	38.16	N
	ATOM	2808	CA	LYS	R	79	10.214	45.760	64.247	1.00	42.15	C
55	ATOM	2810	CB	LYS	R	79	9.505	45.742	65.608	1.00	41.48	C
	ATOM	2813	CG	LYS	R	79	8.005	45.920	65.516	1.00	41.85	C
	ATOM	2816	CD	LYS	R	79	7.421	46.437	66.820	1.00	42.48	C
	ATOM	2819	CE	LYS	R	79	6.063	47.071	66.604	1.00	41.42	C
	ATOM	2822	NZ	LYS	R	79	5.121	46.109	65.995	1.00	39.74	N
60	ATOM	2826	C	LYS	R	79	11.736	45.692	64.462	1.00	43.20	C
	ATOM	2827	O	LYS	R	79	12.333	44.623	64.335	1.00	41.52	O
	ATOM	2829	N	PRO	R	80	12.366	46.835	64.788	1.00	45.21	N
	ATOM	2830	CA	PRO	R	80	13.787	46.812	65.140	1.00	45.44	C
	ATOM	2832	CB	PRO	R	80	14.164	48.303	65.212	1.00	44.79	C
65	ATOM	2835	CG	PRO	R	80	12.897	49.017	65.452	1.00	45.90	C
	ATOM	2838	CD	PRO	R	80	11.806	48.200	64.829	1.00	47.40	C
	ATOM	2841	C	PRO	R	80	14.064	46.114	66.474	1.00	46.92	C
	ATOM	2842	O	PRO	R	80	13.146	45.875	67.265	1.00	50.69	O
	ATOM	2843	N	CYS	R	81	15.327	45.777	66.708	1.00	45.70	N
70	ATOM	2844	CA	CYS	R	81	15.733	45.164	67.968	1.00	45.17	C
	ATOM	2846	CB	CYS	R	81	17.214	44.809	67.927	1.00	44.25	C

5	ATOM	2849	SG	CYS	R	81	17.635	43.633	66.631	1..00	42.68	S
	ATOM	2851	C	CYS	R	81	15.451	46.081	69.159	1..00	43.72	C
	ATOM	2852	O	CYS	R	81	15.483	47.302	69.032	1..00	42.70	O
	ATOM	2854	N	LYS	R	82	15.162	45.468	70.304	1..00	46.15	N
	ATOM	2855	CA	LYS	R	82	14.873	46.185	71.546	1..00	46.61	C
10	ATOM	2857	CB	LYS	R	82	13.909	45.363	72.409	1..00	47.58	C
	ATOM	2860	CG	LYS	R	82	12.515	45.109	71.817	1..00	46.05	C
	ATOM	2863	CD	LYS	R	82	12.001	43.745	72.291	1..00	46.55	C
	ATOM	2866	CE	LYS	R	82	10.516	43.531	72.066	1..00	46.68	C
	ATOM	2869	NZ	LYS	R	82	10.133	42.105	72.377	1..00	45.06	N
15	ATOM	2873	C	LYS	R	82	16.171	46.411	72.332	1..00	46.68	C
	ATOM	2874	O	LYS	R	82	17.091	45.594	72.260	1..00	42.48	O
	ATOM	2876	N	PRO	R	83	16.254	47.506	73.103	1..00	49.15	N
	ATOM	2877	CA	PRO	R	83	17.467	47.685	73.908	1..00	47.77	C
	ATOM	2879	CB	PRO	R	83	17.429	49.172	74.302	1..00	49.53	C
20	ATOM	2882	CG	PRO	R	83	16.221	49.757	73.599	1..00	52.66	C
	ATOM	2885	CD	PRO	R	83	15.310	48.614	73.300	1..00	52.40	C
	ATOM	2888	C	PRO	R	83	17.460	46.800	75.155	1..00	44.49	C
	ATOM	2889	O	PRO	R	83	16.410	46.593	75.767	1..00	38.12	O
	ATOM	2890	N	CYS	R	84	18.631	46.288	75.516	1..00	44.36	N
25	ATOM	2891	CA	CYS	R	84	18.766	45.441	76.692	1..00	44.02	C
	ATOM	2893	CB	CYS	R	84	20.160	44.816	76.748	1..00	46.59	C
	ATOM	2896	SG	CYS	R	84	20.503	43.692	75.365	1..00	48.61	S
	ATOM	2898	C	CYS	R	84	18.492	46.234	77.960	1..00	40.25	C
	ATOM	2899	O	CYS	R	84	18.765	47.432	78.036	1..00	38.27	O
30	ATOM	2901	N	THR	R	85	17.927	45.551	78.947	1..00	40.84	N
	ATOM	2902	CA	THR	R	85	17.519	46.169	80.197	1..00	40.07	C
	ATOM	2904	CB	THR	R	85	16.345	45.381	80.822	1.00	41.59	C
	ATOM	2906	OG1	THR	R	85	15.223	45.417	79.932	1.00	44.86	O
	ATOM	2908	CG2	THR	R	85	15.940	45.956	82.169	1.00	41.37	C
35	ATOM	2912	C	THR	R	85	18.680	46.166	81.171	1.00	39.20	C
	ATOM	2913	O	THR	R	85	19.388	45.175	81.281	1.00	40.74	O
	ATOM	2915	N	TRP	R	86	18.863	47.277	81.878	1.00	40.33	N
	ATOM	2916	CA	TRP	R	86	19.834	47.364	82.966	1.00	37.17	C
	ATOM	2918	CB	TRP	R	86	20.589	48.694	82.913	1.00	34.79	C
40	ATOM	2921	CG	TRP	R	86	21.508	48.798	81.750	1.00	33.82	C
	ATOM	2922	CD1	TRP	R	86	21.207	49.282	80.516	1.00	34.21	C
	ATOM	2924	NE1	TRP	R	86	22.313	49.219	79.697	1.00	34.87	N
	ATOM	2926	CE2	TRP	R	86	23.356	48.676	80.401	1.00	37.09	C
	ATOM	2927	CD2	TRP	R	86	22.884	48.394	81.702	1.00	33.40	C
45	ATOM	2928	CE3	TRP	R	86	23.765	47.831	82.635	1.00	33.66	C
	ATOM	2930	CZ3	TRP	R	86	25.065	47.562	82.246	1.00	33.79	C
	ATOM	2932	CH2	TRP	R	86	25.510	47.854	80.939	1.00	34.60	C
	ATOM	2934	CZ2	TRP	R	86	24.674	48.411	80.006	1.00	35.25	C
	ATOM	2936	C	TRP	R	86	19.132	47.223	84.303	1.00	37.98	C
50	ATOM	2937	O	TRP	R	86	18.145	47.915	84.578	1.00	39.84	O
	ATOM	2939	N	CYS	R	87	19.643	46.318	85.132	1.00	41.68	N
	ATOM	2940	CA	CYS	R	87	19.132	46.127	86.484	1.00	37.84	C
	ATOM	2942	CB	CYS	R	87	19.639	44.803	87.066	1.00	36.52	C
	ATOM	2945	SG	CYS	R	87	19.458	43.326	86.002	1.00	38.06	S
55	ATOM	2947	C	CYS	R	87	19.601	47.302	87.342	1.00	36.84	C
	ATOM	2948	O	CYS	R	87	20.706	47.813	87.140	1.00	36.37	O
	ATOM	2950	N	ASN	R	88	18.759	47.743	88.274	1.00	37.04	N
	ATOM	2951	CA	ASN	R	88	19.134	48.795	89.225	1.00	37.77	C
	ATOM	2953	CB	ASN	R	88	17.908	49.629	89.625	1.00	38.23	C
60	ATOM	2956	CG	ASN	R	88	18.278	50.949	90.311	1.00	37.84	C
	ATOM	2957	OD1	ASN	R	88	19.341	51.083	90.911	1.00	39.59	O
	ATOM	2958	ND2	ASN	R	88	17.386	51.925	90.223	1.00	37.33	N
	ATOM	2961	C	ASN	R	88	19.807	48.165	90.447	1.00	39.72	C
	ATOM	2962	O	ASN	R	88	19.165	47.889	91.460	1.00	40.55	O
65	ATOM	2964	N	LEU	R	89	21.114	47.949	90.331	1.00	41.13	N
	ATOM	2965	CA	LEU	R	89	21.906	47.253	91.345	1.00	39.41	C
	ATOM	2967	CB	LEU	R	89	23.370	47.177	90.903	1.00	40.73	C
	ATOM	2970	CG	LEU	R	89	23.661	46.576	89.524	1.00	41.79	C
	ATOM	2972	CD1	LEU	R	89	25.159	46.615	89.245	1.00	40.59	C
70	ATOM	2976	CD2	LEU	R	89	23.118	45.149	89.411	1.00	42.79	C
	ATOM	2980	C	LEU	R	89	21.841	47.895	92.730	1.00	41.24	C
	ATOM	2981	O	LEU	R	89	21.783	47.194	93.745	1.00	41.16	O
	ATOM	2983	N	ARG	R	90	21.866	49.223	92.768	1.00	41.88	N
	ATOM	2984	CA	ARG	R	90	21.842	49.970	94.029	1.00	40.28	C
	ATOM	2986	CB	ARG	R	90	22.157	51.355	93.876	0.00	30.00	C

	ATOM	2989	CG	ARG	R	90	22.292	52.046	95.234	0.00	30.00	C
	ATOM	2992	CD	ARG	R	90	23.534	51.545	95.969	0.00	30.00	C
	ATOM	2995	NE	ARG	R	90	23.664	52.208	97.274	0.00	30.00	N
	ATOM	2997	CZ	ARG	R	90	24.681	51.939	98.115	0.00	30.00	C
5	ATOM	2998	NH1	ARG	R	90	25.632	51.045	97.803	0.00	30.00	N
	ATOM	3001	NH2	ARG	R	90	24.745	52.580	99.296	0.00	30.00	N
	ATOM	3004	C	ARG	R	90	20.605	49.634	94.858	1.00	39.42	C
	ATOM	3005	O	ARG	R	90	20.684	49.511	96.081	1.00	42.72	O
	ATOM	3007	N	SER	R	91	19.474	49.464	94.179	1.00	37.94	N
10	ATOM	3008	CA	SER	R	91	18.204	49.148	94.832	1.00	38.19	C
	ATOM	3010	CB	SER	R	91	17.049	49.421	93.863	1.00	35.54	C
	ATOM	3013	OG	SER	R	91	17.054	48.532	92.762	1.00	35.81	O
	ATOM	3015	C	SER	R	91	18.103	47.708	95.396	1.00	39.30	C
	ATOM	3016	O	SER	R	91	17.198	47.418	96.179	1.00	37.67	O
15	ATOM	3018	N	GLY	R	92	19.038	46.832	95.019	1.00	39.53	N
	ATOM	3019	CA	GLY	R	92	19.028	45.419	95.434	1.00	38.40	C
	ATOM	3022	C	GLY	R	92	18.712	44.451	94.294	1.00	38.13	C
	ATOM	3023	O	GLY	R	92	18.579	43.242	94.517	1.00	39.48	O
	ATOM	3025	N	SER	R	93	18.592	44.983	93.078	1.00	34.70	N
20	ATOM	3026	CA	SER	R	93	18.355	44.186	91.871	1.00	39.05	C
	ATOM	3028	CB	SER	R	93	17.880	45.088	90.716	1.00	40.03	C
	ATOM	3031	OG	SER	R	93	17.480	44.340	89.579	1.00	39.62	O
	ATOM	3033	C	SER	R	93	19.640	43.482	91.467	1.00	38.65	C
	ATOM	3034	O	SER	R	93	20.710	44.077	91.474	1.00	37.25	O
25	ATOM	3036	N	GLU	R	94	19.524	42.212	91.108	1.00	42.11	N
	ATOM	3037	CA	GLU	R	94	20.674	41.405	90.726	1.00	42.41	C
	ATOM	3039	CB	GLU	R	94	20.764	40.214	91.674	1.00	45.66	C
	ATOM	3042	CG	GLU	R	94	21.798	39.157	91.322	1.00	48.13	C
	ATOM	3045	CD	GLU	R	94	21.755	37.984	92.285	1.00	51.61	C
30	ATOM	3046	OE1	GLU	R	94	21.047	38.094	93.315	1.00	54.93	O
	ATOM	3047	OE2	GLU	R	94	22.422	36.960	92.010	1.00	53.86	O
	ATOM	3048	C	GLU	R	94	20.522	40.935	89.286	1.00	38.20	C
	ATOM	3049	O	GLU	R	94	19.449	40.483	88.891	1.00	33.53	O
	ATOM	3051	N	ARG	R	95	21.591	41.039	88.502	1.00	38.29	N
35	ATOM	3052	CA	ARG	R	95	21.564	40.549	87.131	1.00	39.34	C
	ATOM	3054	CB	ARG	R	95	22.578	41.266	86.248	1.00	39.19	C
	ATOM	3057	CG	ARG	R	95	22.535	40.782	84.795	1.00	40.92	C
	ATOM	3060	CD	ARG	R	95	23.322	41.684	83.869	1.00	41.14	C
	ATOM	3063	NE	ARG	R	95	24.733	41.735	84.242	1.00	41.41	N
40	ATOM	3065	CZ	ARG	R	95	25.646	42.496	83.643	1.00	43.25	C
	ATOM	3066	NH1	ARG	R	95	25.316	43.283	82.617	1.00	45.91	N
	ATOM	3069	NH2	ARG	R	95	26.901	42.462	84.065	1.00	41.35	N
	ATOM	3072	C	ARG	R	95	21.850	39.063	87.131	1.00	39.90	C
	ATOM	3073	O	ARG	R	95	22.992	38.645	87.330	1.00	41.04	O
45	ATOM	3075	N	LYS	R	96	20.810	38.270	86.899	1.00	40.23	N
	ATOM	3076	CA	LYS	R	96	20.924	36.815	86.923	1.00	41.08	C
	ATOM	3078	CB	LYS	R	96	19.590	36.195	87.342	1.00	40.24	C
	ATOM	3081	CG	LYS	R	96	19.157	36.575	88.754	1.00	40.56	C
	ATOM	3084	CD	LYS	R	96	20.021	35.928	89.844	1.00	40.66	C
50	ATOM	3087	CE	LYS	R	96	19.837	34.409	89.889	1.00	42.22	C
	ATOM	3090	NZ	LYS	R	96	20.235	33.829	91.212	1.00	42.40	N
	ATOM	3094	C	LYS	R	96	21.378	36.242	85.583	1.00	41.82	C
	ATOM	3095	O	LYS	R	96	21.974	35.175	85.542	1.00	40.66	O
	ATOM	3097	N	GLN	R	97	21.085	36.943	84.488	1.00	45.91	N
55	ATOM	3098	CA	GLN	R	97	21.542	36.531	83.159	1.00	46.83	C
	ATOM	3100	CB	GLN	R	97	20.480	35.700	82.438	1.00	50.23	C
	ATOM	3103	CG	GLN	R	97	20.107	34.413	83.121	1.00	55.48	C
	ATOM	3106	CD	GLN	R	97	19.104	33.609	82.323	1.00	57.47	C
	ATOM	3107	OE1	GLN	R	97	19.115	33.630	81.088	1.00	60.38	O
60	ATOM	3108	NE2	GLN	R	97	18.232	32.880	83.027	1.00	61.22	N
	ATOM	3111	C	GLN	R	97	21.859	37.733	82.286	1.00	43.79	C
	ATOM	3112	O	GLN	R	97	21.193	38.758	82.366	1.00	39.90	O
	ATOM	3114	N	LEU	R	98	22.863	37.571	81.431	1.00	42.86	N
	ATOM	3115	CA	LEU	R	98	23.208	38.563	80.436	1.00	42.17	C
65	ATOM	3117	CB	LEU	R	98	24.602	38.280	79.863	1.00	42.73	C
	ATOM	3120	CG	LEU	R	98	25.797	38.426	80.811	1.00	43.29	C
	ATOM	3122	CD1	LEU	R	98	27.077	38.025	80.096	1.00	43.48	C
	ATOM	3126	CD2	LEU	R	98	25.902	39.846	81.343	1.00	43.89	C
	ATOM	3130	C	LEU	R	98	22.183	38.572	79.307	1.00	41.40	C
70	ATOM	3131	O	LEU	R	98	21.573	37.555	78.981	1.00	42.32	O
	ATOM	3133	N	CYS	R	99	21.991	39.748	78.732	1.00	42.90	N

	ATOM	3134	CA	CYS	R	99	21.200	39.915	77.531	1.00	41.33	C
	ATOM	3136	CB	CYS	R	99	21.099	41.405	77.192	1.00	43.88	C
	ATOM	3139	SG	CYS	R	99	19.831	41.900	76.004	1.00	46.86	S
5	ATOM	3141	C	CYS	R	99	21.936	39.192	76.423	1.00	40.18	C
	ATOM	3142	O	CYS	R	99	23.168	39.224	76.373	1.00	38.68	O
	ATOM	3144	N	THR	R	100	21.185	38.507	75.567	1.00	39.85	N
	ATOM	3145	CA	THR	R	100	21.717	37.978	74.321	1.00	41.13	C
	ATOM	3147	CB	THR	R	100	21.639	36.446	74.287	1.00	40.68	C
10	ATOM	3149	OG1	THR	R	100	20.269	36.046	74.265	1.00	38.28	O
	ATOM	3151	CG2	THR	R	100	22.326	35.845	75.502	1.00	39.23	C
	ATOM	3155	C	THR	R	100	20.910	38.555	73.156	1.00	40.69	C
	ATOM	3156	O	THR	R	100	19.959	39.303	73.362	1.00	38.84	O
	ATOM	3158	N	ALA	R	101	21.287	38.201	71.935	1.00	40.91	N
15	ATOM	3159	CA	ALA	R	101	20.567	38.653	70.750	1.00	41.08	C
	ATOM	3161	CB	ALA	R	101	21.245	38.108	69.482	1.00	38.94	C
	ATOM	3165	C	ALA	R	101	19.079	38.268	70.775	1.00	40.12	C
	ATOM	3166	O	ALA	R	101	18.261	38.955	70.180	1.00	42.14	O
	ATOM	3168	N	THR	R	102	18.733	37.189	71.475	1.00	41.49	N
20	ATOM	3169	CA	THR	R	102	17.372	36.650	71.464	1.00	43.28	C
	ATOM	3171	CB	THR	R	102	17.384	35.158	71.096	1.00	42.17	C
	ATOM	3173	OG1	THR	R	102	18.099	34.431	72.100	1.00	44.61	O
	ATOM	3175	CG2	THR	R	102	18.049	34.943	69.736	1.00	40.58	C
	ATOM	3179	C	THR	R	102	16.587	36.809	72.779	1.00	44.45	C
25	ATOM	3180	O	THR	R	102	15.405	36.456	72.834	1.00	42.84	O
	ATOM	3182	N	GLN	R	103	17.223	37.322	73.832	1.00	45.06	N
	ATOM	3183	CA	GLN	R	103	16.511	37.571	75.095	1.00	46.85	C
	ATOM	3185	CB	GLN	R	103	16.426	36.294	75.937	1.00	48.63	C
	ATOM	3188	CG	GLN	R	103	17.758	35.661	76.194	1.00	52.01	C
30	ATOM	3191	CD	GLN	R	103	17.647	34.242	76.709	1.00	53.48	C
	ATOM	3192	OE1	GLN	R	103	16.977	33.987	77.712	1.00	56.52	O
	ATOM	3193	NE2	GLN	R	103	18.322	33.311	76.033	1.00	52.37	N
	ATOM	3196	C	GLN	R	103	17.106	38.703	75.928	1.00	44.63	C
	ATOM	3197	O	GLN	R	103	18.293	39.006	75.843	1.00	49.16	O
35	ATOM	3199	N	ASP	R	104	16.251	39.318	76.735	1.00	40.34	N
	ATOM	3200	CA	ASP	R	104	16.640	40.436	77.569	1.00	41.70	C
	ATOM	3202	CB	ASP	R	104	15.391	41.205	78.034	1.00	40.47	C
	ATOM	3205	CG	ASP	R	104	15.689	42.645	78.441	1.00	41.52	C
	ATOM	3206	OD1	ASP	R	104	16.836	43.119	78.290	1.00	39.21	O
40	ATOM	3207	OD2	ASP	R	104	14.754	43.313	78.915	1.00	40.42	O
	ATOM	3208	C	ASP	R	104	17.426	39.951	78.789	1.00	41.49	C
	ATOM	3209	O	ASP	R	104	17.373	38.779	79.176	1.00	40.19	O
	ATOM	3211	N	THR	R	105	18.167	40.883	79.375	1.00	42.77	N
	ATOM	3212	CA	THR	R	105	18.724	40.742	80.711	1.00	40.70	C
45	ATOM	3214	CB	THR	R	105	19.139	42.127	81.222	1.00	38.83	C
	ATOM	3216	OG1	THR	R	105	19.813	42.831	80.164	1.00	33.82	O
	ATOM	3218	CG2	THR	R	105	20.033	42.025	82.446	1.00	38.20	C
	ATOM	3222	C	THR	R	105	17.656	40.169	81.635	1.00	41.30	C
	ATOM	3223	O	THR	R	105	16.480	40.478	81.478	1.00	41.61	O
50	ATOM	3225	N	VAL	R	106	18.054	39.314	82.573	1.00	42.93	N
	ATOM	3226	CA	VAL	R	106	17.146	38.854	83.623	1.00	40.98	C
	ATOM	3228	CB	VAL	R	106	17.104	37.312	83.756	1.00	41.63	C
	ATOM	3230	CG1	VAL	R	106	16.229	36.902	84.936	1.00	42.13	C
	ATOM	3234	CG2	VAL	R	106	16.577	36.674	82.471	1.00	41.41	C
55	ATOM	3238	C	VAL	R	106	17.605	39.502	84.924	1.00	41.13	C
	ATOM	3239	O	VAL	R	106	18.742	39.310	85.346	1.00	38.65	O
	ATOM	3241	N	CYS	R	107	16.713	40.300	85.514	1.00	43.12	N
	ATOM	3242	CA	CYS	R	107	16.957	41.042	86.745	1.00	37.37	C
	ATOM	3244	CB	CYS	R	107	16.609	42.515	86.551	1.00	38.65	C
60	ATOM	3247	SG	CYS	R	107	17.545	43.356	85.281	1.00	38.44	S
	ATOM	3249	C	CYS	R	107	16.049	40.474	87.813	1.00	36.44	C
	ATOM	3250	O	CYS	R	107	14.868	40.263	87.557	1.00	37.02	O
	ATOM	3252	N	ARG	R	108	16.589	40.232	89.006	1.00	36.58	N
	ATOM	3253	CA	ARG	R	108	15.811	39.681	90.104	1.00	35.09	C
65	ATOM	3255	CB	ARG	R	108	16.038	38.173	90.210	1.00	35.87	C
	ATOM	3258	CG	ARG	R	108	15.418	37.360	89.072	1.00	36.29	C
	ATOM	3261	CD	ARG	R	108	13.894	37.296	89.175	1.00	35.60	C
	ATOM	3264	NE	ARG	R	108	13.317	36.495	88.094	1.00	32.85	N
	ATOM	3266	CZ	ARG	R	108	12.989	36.961	86.892	1.00	33.36	C
70	ATOM	3267	NH1	ARG	R	108	13.158	38.239	86.584	1.00	32.00	N
	ATOM	3270	NH2	ARG	R	108	12.484	36.139	85.982	1.00	35.99	N
	ATOM	3273	C	ARG	R	108	16.172	40.366	91.409	1.00	36.22	C

	ATOM	3274	O	ARG	R	108	17.340	40.626	91.676	1.00	38.57	O
	ATOM	3276	N	CYS	R	109	15.163	40.668	92.221	1.00	38.83	N
	ATOM	3277	CA	CYS	R	109	15.389	41.334	93.501	1.00	38.85	C
	ATOM	3279	CB	CYS	R	109	14.102	41.976	94.006	1.00	38.93	C
5	ATOM	3282	SG	CYS	R	109	13.525	43.340	92.990	1.00	40.16	S
	ATOM	3284	C	CYS	R	109	15.935	40.350	94.533	1.00	36.92	C
	ATOM	3285	O	CYS	R	109	15.488	39.213	94.608	1.00	38.83	O
	ATOM	3287	N	ARG	R	110	16.906	40.800	95.319	1.00	40.22	N
	ATOM	3288	CA	ARG	R	110	17.593	39.936	96.283	1.00	41.24	C
10	ATOM	3290	CB	ARG	R	110	18.930	40.553	96.704	1.00	43.64	C
	ATOM	3293	CG	ARG	R	110	19.979	40.567	95.603	1.00	46.93	C
	ATOM	3296	CD	ARG	R	110	21.185	41.406	96.013	1.00	48.16	C
	ATOM	3299	NE	ARG	R	110	22.151	41.592	94.925	1.00	48.54	N
	ATOM	3301	CZ	ARG	R	110	23.066	40.696	94.547	1.00	51.36	C
15	ATOM	3302	NH1	ARG	R	110	23.160	39.508	95.145	1.00	51.80	N
	ATOM	3305	NH2	ARG	R	110	23.899	40.987	93.554	1.00	51.84	N
	ATOM	3308	C	ARG	R	110	16.749	39.676	97.523	1.00	39.27	C
	ATOM	3309	O	ARG	R	110	15.732	40.332	97.754	1.00	39.00	O
	ATOM	3311	N	ALA	R	111	17.188	38.707	98.318	1.00	38.68	N
20	ATOM	3312	CA	ALA	R	111	16.599	38.453	99.621	1.00	38.43	C
	ATOM	3314	CB	ALA	R	111	17.378	37.359	100.348	1.00	39.35	C
	ATOM	3318	C	ALA	R	111	16.602	39.739	100.435	1.00	37.64	C
	ATOM	3319	O	ALA	R	111	17.577	40.498	100.400	1.00	39.53	O
	ATOM	3321	N	GLY	R	112	15.503	39.987	101.146	1.00	35.96	N
25	ATOM	3322	CA	GLY	R	112	15.348	41.196	101.952	1.00	37.19	C
	ATOM	3325	C	GLY	R	112	14.764	42.373	101.197	1.00	38.74	C
	ATOM	3326	O	GLY	R	112	14.507	43.424	101.784	1.00	40.74	O
	ATOM	3328	N	THR	R	113	14.568	42.209	99.891	1.00	41.61	N
	ATOM	3329	CA	THR	R	113	13.972	43.247	99.062	1.00	40.63	C
30	ATOM	3331	CB	THR	R	113	15.011	43.897	98.105	1.00	39.77	C
	ATOM	3333	OG1	THR	R	113	15.276	43.027	96.997	1.00	36.97	O
	ATOM	3335	CG2	THR	R	113	16.313	44.197	98.836	1.00	40.04	C
	ATOM	3339	C	THR	R	113	12.836	42.646	98.244	1.00	41.92	C
	ATOM	3340	O	THR	R	113	12.714	41.423	98.136	1.00	39.87	O
35	ATOM	3342	N	GLN	R	114	12.004	43.522	97.688	1.00	42.78	N
	ATOM	3343	CA	GLN	R	114	10.927	43.126	96.789	1.00	41.54	C
	ATOM	3345	CB	GLN	R	114	9.579	43.144	97.518	1.00	41.16	C
	ATOM	3348	CG	GLN	R	114	9.171	44.517	98.056	1.00	41.55	C
	ATOM	3351	CD	GLN	R	114	7.796	44.526	98.725	1.00	42.44	C
40	ATOM	3352	OE1	GLN	R	114	7.060	43.538	98.689	1.00	41.58	O
	ATOM	3353	NE2	GLN	R	114	7.450	45.655	99.338	1.00	39.24	N
	ATOM	3356	C	GLN	R	114	10.874	44.079	95.597	1.00	41.33	C
	ATOM	3357	O	GLN	R	114	11.330	45.228	95.694	1.00	38.51	O
	ATOM	3359	N	PRO	R	115	10.295	43.617	94.473	1.00	42.37	N
45	ATOM	3360	CA	PRO	R	115	10.124	44.496	93.311	1.00	42.04	C
	ATOM	3362	CB	PRO	R	115	9.512	43.574	92.249	1.00	39.19	C
	ATOM	3365	CG	PRO	R	115	9.654	42.211	92.747	1.00	39.88	C
	ATOM	3368	CD	PRO	R	115	9.768	42.264	94.225	1.00	39.73	C
	ATOM	3371	C	PRO	R	115	9.178	45.672	93.566	1.00	43.79	C
50	ATOM	3372	O	PRO	R	115	8.096	45.482	94.118	1.00	44.59	O
	ATOM	3373	N	LEU	R	116	9.596	46.872	93.170	1.00	45.69	N
	ATOM	3374	CA	LEU	R	116	8.696	48.021	93.096	1.00	47.91	C
	ATOM	3376	CB	LEU	R	116	9.474	49.330	93.267	1.00	49.98	C
	ATOM	3379	CG	LEU	R	116	10.102	49.611	94.636	1.00	50.77	C
55	ATOM	3381	CD1	LEU	R	116	11.060	50.801	94.540	1.00	50.97	C
	ATOM	3385	CD2	LEU	R	116	9.019	49.859	95.684	1.00	51.64	C
	ATOM	3389	C	LEU	R	116	8.011	48.014	91.734	1.00	49.03	C
	ATOM	3390	O	LEU	R	116	8.396	47.250	90.852	1.00	50.67	O
	ATOM	3392	N	ASP	R	117	6.990	48.852	91.565	1.00	51.13	N
60	ATOM	3393	CA	ASP	R	117	6.452	49.125	90.230	1.00	51.41	C
	ATOM	3395	CB	ASP	R	117	5.222	50.037	90.278	1.00	53.66	C
	ATOM	3398	CG	ASP	R	117	3.976	49.318	90.774	1.00	56.60	C
	ATOM	3399	OD1	ASP	R	117	4.101	48.212	91.347	1.00	57.65	O
	ATOM	3400	OD2	ASP	R	117	2.866	49.869	90.596	1.00	59.57	O
65	ATOM	3401	C	ASP	R	117	7.575	49.778	89.440	1.00	52.66	C
	ATOM	3402	O	ASP	R	117	8.174	50.758	89.887	1.00	55.22	O
	ATOM	3404	N	SER	R	118	7.869	49.213	88.275	1.00	51.03	N
	ATOM	3405	CA	SER	R	118	9.129	49.474	87.600	1.00	46.65	C
	ATOM	3407	CB	SER	R	118	10.174	48.480	88.116	1.00	46.26	C
70	ATOM	3410	OG	SER	R	118	11.447	48.708	87.546	1.00	47.94	O
	ATOM	3412	C	SER	R	118	8.983	49.342	86.091	1.00	45.14	C

	ATOM	3413	O	SER	R	118	7.909	49.002	85.586	1.00	44.62	O
	ATOM	3415	N	TYR	R	119	10.071	49.640	85.385	1.00	41.44	N
	ATOM	3416	CA	TYR	R	119	10.175	49.417	83.947	1.00	40.02	C
5	ATOM	3418	CB	TYR	R	119	11.580	49.792	83.483	1.00	34.27	C
	ATOM	3421	CG	TYR	R	119	11.814	49.565	82.017	1.00	36.02	C
	ATOM	3422	CD1	TYR	R	119	11.270	50.429	81.066	1.00	30.33	C
	ATOM	3424	CE1	TYR	R	119	11.475	50.225	79.723	1.00	31.18	C
	ATOM	3426	CZ	TYR	R	119	12.234	49.146	79.304	1.00	31.70	C
10	ATOM	3427	OH	TYR	R	119	12.445	48.947	77.962	1.00	33.04	O
	ATOM	3429	CE2	TYR	R	119	12.784	48.271	80.218	1.00	32.38	C
	ATOM	3431	CD2	TYR	R	119	12.571	48.481	81.573	1.00	34.09	C
	ATOM	3433	C	TYR	R	119	9.872	47.951	83.593	1.00	39.25	C
	ATOM	3434	O	TYR	R	119	9.048	47.667	82.717	1.00	37.35	O
15	ATOM	3436	N	LYS	R	120	10.560	47.039	84.276	1.00	39.97	N
	ATOM	3437	CA	LYS	R	120	10.263	45.605	84.229	1.00	40.94	C
	ATOM	3439	CB	LYS	R	120	11.210	44.874	83.270	1.00	42.17	C
	ATOM	3442	CG	LYS	R	120	10.866	45.033	81.796	1.00	42.73	C
	ATOM	3445	CD	LYS	R	120	11.579	43.992	80.939	1.00	42.27	C
20	ATOM	3448	CE	LYS	R	120	11.275	44.179	79.460	1.00	44.21	C
	ATOM	3451	NZ	LYS	R	120	11.699	42.998	78.652	1.00	45.04	N
	ATOM	3455	C	LYS	R	120	10.395	45.036	85.644	1.00	40.61	C
	ATOM	3456	O	LYS	R	120	11.159	45.568	86.447	1.00	39.91	O
	ATOM	3458	N	PRO	R	121	9.644	43.963	85.958	1.00	41.51	N
25	ATOM	3459	CA	PRO	R	121	9.652	43.400	87.314	1.00	41.84	C
	ATOM	3461	CB	PRO	R	121	8.506	42.382	87.289	1.00	41.28	C
	ATOM	3464	CG	PRO	R	121	8.313	42.049	85.852	1.00	41.20	C
	ATOM	3467	CD	PRO	R	121	8.739	43.231	85.054	1.00	40.87	C
	ATOM	3470	C	PRO	R	121	10.980	42.732	87.674	1.00	42.82	C
30	ATOM	3471	O	PRO	R	121	11.333	41.693	87.105	1.00	45.56	O
	ATOM	3472	N	GLY	R	122	11.695	43.336	88.619	1.00	40.11	N
	ATOM	3473	CA	GLY	R	122	13.010	42.869	89.035	1.00	39.04	C
	ATOM	3476	C	GLY	R	122	14.091	43.906	88.802	1.00	38.40	C
	ATOM	3477	O	GLY	R	122	15.181	43.795	89.354	1.00	38.91	O
35	ATOM	3479	N	VAL	R	123	13.794	44.909	87.975	1.00	38.74	N
	ATOM	3480	CA	VAL	R	123	14.752	45.970	87.660	1.00	38.19	C
	ATOM	3482	CB	VAL	R	123	14.313	46.805	86.444	1.00	37.05	C
	ATOM	3484	CG1	VAL	R	123	15.228	48.020	86.270	1.00	36.90	C
	ATOM	3488	CG2	VAL	R	123	14.293	45.949	85.181	1.00	35.50	C
40	ATOM	3492	C	VAL	R	123	14.946	46.901	88.847	1.00	36.70	C
	ATOM	3493	O	VAL	R	123	16.074	47.238	89.181	1.00	35.93	O
	ATOM	3495	N	ASP	R	124	13.840	47.326	89.454	1.00	38.39	N
	ATOM	3496	CA	ASP	R	124	13.866	48.181	90.640	1.00	39.46	C
	ATOM	3498	CB	ASP	R	124	13.088	49.481	90.412	1.00	41.95	C
45	ATOM	3501	CG	ASP	R	124	13.919	50.542	89.725	1.00	42.46	C
	ATOM	3502	OD1	ASP	R	124	14.977	50.905	90.272	1.00	45.49	O
	ATOM	3503	OD2	ASP	R	124	13.518	51.016	88.647	1.00	43.59	O
	ATOM	3504	C	ASP	R	124	13.285	47.439	91.823	1.00	38.81	C
	ATOM	3505	O	ASP	R	124	12.237	46.806	91.713	1.00	39.49	O
50	ATOM	3507	N	CYS	R	125	13.986	47.535	92.951	1.00	40.26	N
	ATOM	3508	CA	CYS	R	125	13.659	46.800	94.160	1.00	40.24	C
	ATOM	3510	CB	CYS	R	125	14.701	45.709	94.415	1.00	37.84	C
	ATOM	3513	SG	CYS	R	125	15.052	44.684	92.969	1.00	35.41	S
	ATOM	3515	C	CYS	R	125	13.638	47.772	95.328	1.00	41.20	C
55	ATOM	3516	O	CYS	R	125	14.193	48.865	95.240	1.00	40.62	O
	ATOM	3518	N	ALA	R	126	12.985	47.362	96.412	1.00	41.96	N
	ATOM	3519	CA	ALA	R	126	12.943	48.137	97.648	1.00	39.78	C
	ATOM	3521	CB	ALA	R	126	11.652	48.927	97.733	1.00	40.65	C
	ATOM	3525	C	ALA	R	126	13.046	47.181	98.820	1.00	39.05	C
60	ATOM	3526	O	ALA	R	126	12.542	46.064	98.742	1.00	39.57	O
	ATOM	3528	N	PRO	R	127	13.688	47.618	99.918	1.00	41.87	N
	ATOM	3529	CA	PRO	R	127	13.786	46.744	101.083	1.00	42.01	C
	ATOM	3531	CB	PRO	R	127	14.644	47.552	102.071	1.00	42.41	C
	ATOM	3534	CG	PRO	R	127	14.530	48.969	101.629	1.00	42.56	C
65	ATOM	3537	CD	PRO	R	127	14.336	48.925	100.145	1.00	42.28	C
	ATOM	3540	C	PRO	R	127	12.412	46.432	101.676	1.00	43.42	C
	ATOM	3541	O	PRO	R	127	11.463	47.212	101.500	1.00	43.33	O
	ATOM	3542	N	CYS	R	128	12.309	45.287	102.346	1.00	41.22	N
	ATOM	3543	CA	CYS	R	128	11.083	44.911	103.043	1.00	42.35	C
70	ATOM	3545	CB	CYS	R	128	11.167	43.476	103.583	1.00	42.90	C
	ATOM	3548	SG	CYS	R	128	11.166	42.184	102.330	1.00	45.69	S
	ATOM	3550	C	CYS	R	128	10.860	45.862	104.211	1.00	42.23	C

	ATOM	3551	O	CYS	R	128	11.804	46.143	104.955	1.00	41.17	O
	ATOM	3553	N	PRO	R	129	9.614	46.350	104.385	1.00	41.88	N
	ATOM	3554	CA	PRO	R	129	9.280	47.143	105.567	1.00	40.30	C
5	ATOM	3556	CB	PRO	R	129	7.758	47.296	105.472	1.00	40.62	C
	ATOM	3559	CG	PRO	R	129	7.430	47.108	104.048	1.00	40.80	C
	ATOM	3562	CD	PRO	R	129	8.457	46.188	103.483	1.00	40.98	C
	ATOM	3565	C	PRO	R	129	9.647	46.427	106.872	1.00	40.12	C
	ATOM	3566	O	PRO	R	129	9.878	45.210	106.864	1.00	38.40	O
10	ATOM	3567	N	PRO	R	130	9.685	47.170	107.994	1.00	38.10	N
	ATOM	3568	CA	PRO	R	130	9.993	46.551	109.282	1.00	38.42	C
	ATOM	3570	CB	PRO	R	130	9.680	47.662	110.287	1.00	38.90	C
	ATOM	3573	CG	PRO	R	130	9.841	48.919	109.518	1.00	38.43	C
	ATOM	3576	CD	PRO	R	130	9.420	48.613	108.123	1.00	37.59	C
15	ATOM	3579	C	PRO	R	130	9.115	45.332	109.556	1.00	36.74	C
	ATOM	3580	O	PRO	R	130	7.926	45.345	109.230	1.00	37.44	O
	ATOM	3581	N	GLY	R	131	9.699	44.286	110.128	1.00	35.10	N
	ATOM	3582	CA	GLY	R	131	8.946	43.080	110.461	1.00	35.95	C
	ATOM	3585	C	GLY	R	131	8.398	42.299	109.274	1.00	37.04	C
20	ATOM	3586	O	GLY	R	131	7.451	41.524	109.428	1.00	37.03	O
	ATOM	3588	N	HIS	R	132	8.985	42.502	108.091	1.00	37.84	N
	ATOM	3589	CA	HIS	R	132	8.619	41.751	106.884	1.00	37.23	C
	ATOM	3591	CB	HIS	R	132	8.063	42.679	105.795	1.00	35.37	C
	ATOM	3594	CG	HIS	R	132	6.665	43.145	106.053	1.00	34.92	C
25	ATOM	3595	ND1	HIS	R	132	6.337	43.972	107.106	1.00	37.51	N
	ATOM	3597	CE1	HIS	R	132	5.038	44.215	107.084	1.00	37.56	C
	ATOM	3599	NE2	HIS	R	132	4.513	43.576	106.053	1.00	37.50	N
	ATOM	3601	CD2	HIS	R	132	5.510	42.903	105.390	1.00	34.76	C
	ATOM	3603	C	HIS	R	132	9.835	41.009	106.352	1.00	38.32	C
30	ATOM	3604	O	HIS	R	132	10.972	41.410	106.606	1.00	39.01	O
	ATOM	3606	N	PHE	R	133	9.588	39.924	105.622	1.00	39.09	N
	ATOM	3607	CA	PHE	R	133	10.663	39.142	105.008	1.00	37.71	C
	ATOM	3609	CB	PHE	R	133	10.876	37.817	105.761	1.00	35.63	C
	ATOM	3612	CG	PHE	R	133	9.915	36.719	105.364	1.00	34.86	C
35	ATOM	3613	CD1	PHE	R	133	8.625	36.691	105.872	1.00	34.36	C
	ATOM	3615	CE1	PHE	R	133	7.738	35.680	105.506	1.00	36.41	C
	ATOM	3617	CZ	PHE	R	133	8.144	34.688	104.625	1.00	33.54	C
	ATOM	3619	CE2	PHE	R	133	9.433	34.704	104.117	1.00	32.03	C
	ATOM	3621	CD2	PHE	R	133	10.309	35.713	104.482	1.00	33.23	C
40	ATOM	3623	C	PHE	R	133	10.375	38.857	103.541	1.00	38.63	C
	ATOM	3624	O	PHE	R	133	9.219	38.806	103.128	1.00	38.95	O
	ATOM	3626	N	SER	R	134	11.442	38.686	102.765	1.00	39.15	N
	ATOM	3627	CA	SER	R	134	11.364	38.102	101.433	1.00	38.45	C
	ATOM	3629	CB	SER	R	134	11.173	39.160	100.353	1.00	37.72	C
45	ATOM	3632	OG	SER	R	134	11.217	38.544	99.069	1.00	36.41	O
	ATOM	3634	C	SER	R	134	12.654	37.345	101.142	1.00	39.67	C
	ATOM	3635	O	SER	R	134	13.742	37.894	101.330	1.00	38.74	O
	ATOM	3637	N	PRO	R	135	12.539	36.091	100.666	1.00	38.81	N
	ATOM	3638	CA	PRO	R	135	13.725	35.318	100.289	1.00	41.45	C
50	ATOM	3640	CB	PRO	R	135	13.214	33.872	100.269	1.00	39.21	C
	ATOM	3643	CG	PRO	R	135	11.758	33.967	100.070	1.00	38.65	C
	ATOM	3646	CD	PRO	R	135	11.293	35.326	100.478	1.00	38.21	C
	ATOM	3649	C	PRO	R	135	14.342	35.701	98.929	1.00	41.66	C
	ATOM	3650	O	PRO	R	135	15.348	35.116	98.522	1.00	41.87	O
55	ATOM	3651	N	GLY	R	136	13.747	36.669	98.243	1.00	41.50	N
	ATOM	3652	CA	GLY	R	136	14.290	37.167	96.993	1.00	39.28	C
	ATOM	3655	C	GLY	R	136	13.666	36.483	95.802	1.00	38.37	C
	ATOM	3656	O	GLY	R	136	12.591	35.890	95.908	1.00	37.47	O
	ATOM	3658	N	ASP	R	137	14.364	36.577	94.671	1.00	36.94	N
60	ATOM	3659	CA	ASP	R	137	13.882	36.129	93.372	1.00	37.31	C
	ATOM	3661	CB	ASP	R	137	13.929	34.606	93.257	1.00	37.83	C
	ATOM	3664	CG	ASP	R	137	14.088	34.134	91.825	1.00	36.77	C
	ATOM	3665	OD1	ASP	R	137	14.909	34.715	91.078	1.00	39.27	O
	ATOM	3666	OD2	ASP	R	137	13.402	33.172	91.436	1.00	36.00	O
65	ATOM	3667	C	ASP	R	137	12.490	36.668	93.063	1.00	36.94	C
	ATOM	3668	O	ASP	R	137	11.603	35.930	92.633	1.00	37.76	O
	ATOM	3670	N	ASN	R	138	12.330	37.971	93.287	1.00	36.22	N
	ATOM	3671	CA	ASN	R	138	11.114	38.731	92.956	1.00	38.59	C
	ATOM	3673	CB	ASN	R	138	10.785	38.627	91.455	1.00	37.92	C
70	ATOM	3676	CG	ASN	R	138	11.579	39.607	90.620	1.00	36.63	C
	ATOM	3677	OD1	ASN	R	138	12.536	40.229	91.097	1.00	34.49	O
	ATOM	3678	ND2	ASN	R	138	11.185	39.754	89.364	1.00	35.73	N

	ATOM	3681	C	ASN	R	138	9.877	38.446	93.806	1.00	39.02	C
	ATOM	3682	O	ASN	R	138	8.805	38.999	93.545	1.00	39.34	O
	ATOM	3684	N	GLN	R	139	10.029	37.629	94.845	1.00	41.14	N
5	ATOM	3685	CA	GLN	R	139	8.921	37.344	95.754	1.00	39.94	C
	ATOM	3687	CB	GLN	R	139	9.258	36.158	96.667	1.00	39.35	C
	ATOM	3690	CG	GLN	R	139	9.219	34.817	95.956	1.00	40.12	C
	ATOM	3693	CD	GLN	R	139	9.736	33.681	96.817	1.00	42.94	C
	ATOM	3694	OE1	GLN	R	139	8.956	32.922	97.405	1.00	44.07	O
10	ATOM	3695	NE2	GLN	R	139	11.058	33.558	96.898	1.00	42.85	N
	ATOM	3698	C	GLN	R	139	8.605	38.597	96.571	1.00	38.77	C
	ATOM	3699	O	GLN	R	139	9.513	39.320	96.977	1.00	40.35	O
	ATOM	3701	N	ALA	R	140	7.317	38.859	96.785	1.00	41.14	N
	ATOM	3702	CA	ALA	R	140	6.877	40.005	97.582	1.00	40.41	C
15	ATOM	3704	CB	ALA	R	140	5.379	40.214	97.412	1.00	41.01	C
	ATOM	3708	C	ALA	R	140	7.207	39.787	99.055	1.00	40.86	C
	ATOM	3709	O	ALA	R	140	7.257	38.651	99.517	1.00	43.34	O
	ATOM	3711	N	CYS	R	141	7.432	40.877	99.785	1.00	40.40	N
	ATOM	3712	CA	CYS	R	141	7.644	40.810	101.227	1.00	40.41	C
20	ATOM	3714	CB	CYS	R	141	8.141	42.157	101.766	1.00	41.14	C
	ATOM	3717	SG	CYS	R	141	9.691	42.763	101.034	1.00	39.82	S
	ATOM	3719	C	CYS	R	141	6.345	40.405	101.935	1.00	41.01	C
	ATOM	3720	O	CYS	R	141	5.258	40.740	101.466	1.00	41.62	O
	ATOM	3722	N	LYS	R	142	6.461	39.679	103.048	1.00	40.34	N
25	ATOM	3723	CA	LYS	R	142	5.297	39.248	103.834	1.00	41.12	C
	ATOM	3725	CB	LYS	R	142	4.986	37.766	103.587	1.00	43.48	C
	ATOM	3728	CG	LYS	R	142	4.707	37.397	102.133	1.00	44.52	C
	ATOM	3731	CD	LYS	R	142	3.355	37.905	101.638	1.00	45.78	C
	ATOM	3734	CE	LYS	R	142	3.233	37.756	100.120	1.00	45.68	C
30	ATOM	3737	NZ	LYS	R	142	1.826	37.613	99.656	1.00	44.97	N
	ATOM	3741	C	LYS	R	142	5.550	39.472	105.329	1.00	41.97	C
	ATOM	3742	O	LYS	R	142	6.702	39.453	105.766	1.00	43.45	O
	ATOM	3744	N	PRO	R	143	4.478	39.683	106.120	1.00	40.81	N
35	ATOM	3745	CA	PRO	R	143	4.662	39.890	107.564	1.00	42.56	C
	ATOM	3747	CB	PRO	R	143	3.236	40.159	108.083	1.00	41.51	C
	ATOM	3750	CG	PRO	R	143	2.411	40.449	106.892	1.00	42.05	C
	ATOM	3753	CD	PRO	R	143	3.059	39.753	105.731	1.00	42.03	C
	ATOM	3756	C	PRO	R	143	5.250	38.670	108.271	1.00	44.65	C
	ATOM	3757	O	PRO	R	143	4.960	37.533	107.886	1.00	46.62	O
40	ATOM	3758	N	TRP	R	144	6.069	38.905	109.295	1.00	44.51	N
	ATOM	3759	CA	TRP	R	144	6.599	37.812	110.093	1.00	42.77	C
	ATOM	3761	CB	TRP	R	144	7.599	38.303	111.145	1.00	42.23	C
	ATOM	3764	CG	TRP	R	144	8.873	38.894	110.618	1.00	42.65	C
	ATOM	3765	CD1	TRP	R	144	9.416	38.723	109.373	1.00	43.34	C
45	ATOM	3767	NE1	TRP	R	144	10.603	39.413	109.278	1.00	43.26	N
	ATOM	3769	CE2	TRP	R	144	10.859	40.028	110.476	1.00	40.70	C
	ATOM	3770	CD2	TRP	R	144	9.794	39.717	111.347	1.00	41.04	C
	ATOM	3771	CE3	TRP	R	144	9.814	40.232	112.651	1.00	41.45	C
	ATOM	3773	CZ3	TRP	R	144	10.885	41.035	113.038	1.00	41.91	C
50	ATOM	3775	CH2	TRP	R	144	11.929	41.325	112.148	1.00	42.29	C
	ATOM	3777	CZ2	TRP	R	144	11.935	40.832	110.866	1.00	41.85	C
	ATOM	3779	C	TRP	R	144	5.446	37.132	110.817	1.00	44.64	C
	ATOM	3780	O	TRP	R	144	4.491	37.793	111.247	1.00	42.53	O
55	ATOM	3782	N	THR	R	145	5.534	35.812	110.950	1.00	44.76	N
	ATOM	3783	CA	THR	R	145	4.658	35.084	111.856	1.00	43.71	C
	ATOM	3785	CB	THR	R	145	4.771	33.560	111.660	1.00	44.06	C
	ATOM	3787	OG1	THR	R	145	4.455	33.229	110.299	1.00	47.36	O
	ATOM	3789	CG2	THR	R	145	3.818	32.817	112.592	1.00	43.31	C
	ATOM	3793	C	THR	R	145	5.052	35.453	113.286	1.00	43.22	C
60	ATOM	3794	O	THR	R	145	6.211	35.290	113.680	1.00	41.08	O
	ATOM	3796	N	ASN	R	146	4.091	35.983	114.039	1.00	42.64	N
	ATOM	3797	CA	ASN	R	146	4.267	36.224	115.463	1.00	43.24	C
	ATOM	3799	CB	ASN	R	146	3.344	37.359	115.937	1.00	44.73	C
	ATOM	3802	CG	ASN	R	146	3.729	37.905	117.307	1.00	44.33	C
65	ATOM	3803	OD1	ASN	R	146	4.306	37.203	118.140	1.00	44.55	O
	ATOM	3804	ND2	ASN	R	146	3.401	39.170	117.544	1.00	45.73	N
	ATOM	3807	C	ASN	R	146	3.961	34.922	116.206	1.00	42.81	C
	ATOM	3808	O	ASN	R	146	2.796	34.558	116.385	1.00	40.36	O
	ATOM	3810	N	CYS	R	147	5.014	34.221	116.621	1.00	42.12	N
70	ATOM	3811	CA	CYS	R	147	4.869	32.937	117.307	1.00	40.42	C
	ATOM	3813	CB	CYS	R	147	6.236	32.282	117.509	1.00	38.67	C
	ATOM	3816	SG	CYS	R	147	7.079	31.813	115.981	1.00	34.09	S

	ATOM	3818	C	CYS	R	147	4.161	33.068	118.652	1.00	41.13	C
	ATOM	3819	O	CYS	R	147	3.353	32.207	119.005	1.00	41.35	O
	ATOM	3821	N	THR	R	148	4.467	34.138	119.391	1.00	40.48	N
5	ATOM	3822	CA	THR	R	148	3.833	34.416	120.689	1.00	40.71	C
	ATOM	3824	CB	THR	R	148	4.416	35.695	121.350	1.00	41.10	C
	ATOM	3826	OG1	THR	R	148	5.816	35.518	121.596	1.00	42.62	O
	ATOM	3828	CG2	THR	R	148	3.719	36.005	122.670	1.00	40.79	C
	ATOM	3832	C	THR	R	148	2.316	34.579	120.576	1.00	39.73	C
10	ATOM	3833	O	THR	R	148	1.569	34.029	121.387	1.00	38.53	O
	ATOM	3835	N	LEU	R	149	1.877	35.334	119.572	1.00	40.44	N
	ATOM	3836	CA	LEU	R	149	0.453	35.614	119.349	1.00	41.77	C
	ATOM	3838	CB	LEU	R	149	0.271	36.504	118.108	1.00	41.66	C
	ATOM	3841	CG	LEU	R	149	-1.106	37.140	117.886	1.00	41.83	C
15	ATOM	3843	CD1	LEU	R	149	-1.391	38.205	118.937	1.00	41.84	C
	ATOM	3847	CD2	LEU	R	149	-1.200	37.735	116.488	1.00	42.65	C
	ATOM	3851	C	LEU	R	149	-0.374	34.335	119.196	1.00	41.84	C
	ATOM	3852	O	LEU	R	149	-1.528	34.285	119.628	1.00	41.45	O
	ATOM	3854	N	ALA	R	150	0.223	33.308	118.591	1.00	42.38	N
20	ATOM	3855	CA	ALA	R	150	-0.442	32.019	118.390	1.00	43.11	C
	ATOM	3857	CB	ALA	R	150	-0.041	31.431	117.042	1.00	44.51	C
	ATOM	3861	C	ALA	R	150	-0.159	31.013	119.513	1.00	44.05	C
	ATOM	3862	O	ALA	R	150	-0.392	29.817	119.340	1.00	46.97	O
	ATOM	3864	N	GLY	R	151	0.330	31.491	120.657	1.00	43.36	N
25	ATOM	3865	CA	GLY	R	151	0.579	30.632	121.818	1.00	42.94	C
	ATOM	3868	C	GLY	R	151	1.696	29.626	121.610	1.00	43.06	C
	ATOM	3869	O	GLY	R	151	1.607	28.490	122.076	1.00	42.12	O
	ATOM	3871	N	LYS	R	152	2.749	30.051	120.912	1.00	43.51	N
	ATOM	3872	CA	LYS	R	152	3.898	29.196	120.600	1.00	43.33	C
30	ATOM	3874	CB	LYS	R	152	3.900	28.834	119.109	1.00	43.47	C
	ATOM	3877	CG	LYS	R	152	2.754	27.931	118.679	1.00	43.78	C
	ATOM	3880	CD	LYS	R	152	2.758	27.715	117.175	1.00	43.72	C
	ATOM	3883	CE	LYS	R	152	1.692	26.720	116.739	1.00	44.14	C
	ATOM	3886	NZ	LYS	R	152	1.904	26.267	115.331	1.00	44.91	N
35	ATOM	3890	C	LYS	R	152	5.209	29.898	120.952	1.00	43.03	C
	ATOM	3891	O	LYS	R	152	5.271	31.128	121.010	1.00	42.11	O
	ATOM	3893	N	HIS	R	153	6.253	29.109	121.191	1.00	43.26	N
	ATOM	3894	CA	HIS	R	153	7.599	29.653	121.369	1.00	43.07	C
	ATOM	3896	CB	HIS	R	153	8.438	28.769	122.301	1.00	43.57	C
40	ATOM	3899	CG	HIS	R	153	8.086	28.917	123.750	1.00	44.38	C
	ATOM	3900	ND1	HIS	R	153	8.256	30.099	124.439	1.00	44.13	N
	ATOM	3902	CE1	HIS	R	153	7.869	29.935	125.692	1.00	45.41	C
	ATOM	3904	NE2	HIS	R	153	7.455	28.689	125.842	1.00	44.67	N
	ATOM	3906	CD2	HIS	R	153	7.581	28.031	124.643	1.00	45.16	C
45	ATOM	3908	C	HIS	R	153	8.270	29.792	120.008	1.00	41.54	C
	ATOM	3909	O	HIS	R	153	7.887	29.121	119.050	1.00	40.10	O
	ATOM	3911	N	THR	R	154	9.267	30.669	119.932	1.00	41.95	N
	ATOM	3912	CA	THR	R	154	10.006	30.898	118.695	1.00	42.63	C
	ATOM	3914	CB	THR	R	154	10.419	32.381	118.553	1.00	42.68	C
50	ATOM	3916	OG1	THR	R	154	9.249	33.209	118.572	1.00	42.70	O
	ATOM	3918	CG2	THR	R	154	11.178	32.620	117.245	1.00	42.48	C
	ATOM	3922	C	THR	R	154	11.254	30.016	118.629	1.00	42.39	C
	ATOM	3923	O	THR	R	154	12.181	30.176	119.423	1.00	38.85	O
	ATOM	3925	N	LEU	R	155	11.268	29.096	117.667	1.00	44.83	N
55	ATOM	3926	CA	LEU	R	155	12.427	28.240	117.408	1.00	46.06	C
	ATOM	3928	CB	LEU	R	155	12.023	27.046	116.527	1.00	47.02	C
	ATOM	3931	CG	LEU	R	155	12.654	25.694	116.855	1.00	47.55	C
	ATOM	3933	CD1	LEU	R	155	12.021	25.138	118.108	1.00	47.32	C
	ATOM	3937	CD2	LEU	R	155	12.494	24.717	115.690	1.00	47.77	C
60	ATOM	3941	C	LEU	R	155	13.528	29.054	116.716	1.00	46.82	C
	ATOM	3942	O	LEU	R	155	14.638	29.180	117.240	1.00	45.93	O
	ATOM	3944	N	GLN	R	156	13.192	29.609	115.546	1.00	46.72	N
	ATOM	3945	CA	GLN	R	156	14.112	30.408	114.729	1.00	46.66	C
	ATOM	3947	CB	GLN	R	156	14.175	29.864	113.294	1.00	47.19	C
65	ATOM	3950	CG	GLN	R	156	14.437	28.359	113.168	1.00	47.78	C
	ATOM	3953	CD	GLN	R	156	15.911	28.004	113.106	1.00	47.55	C
	ATOM	3954	OE1	GLN	R	156	16.652	28.518	112.265	1.00	47.82	O
	ATOM	3955	NE2	GLN	R	156	16.339	27.103	113.984	1.00	46.18	N
	ATOM	3958	C	GLN	R	156	13.614	31.853	114.677	1.00	46.30	C
70	ATOM	3959	O	GLN	R	156	12.457	32.087	114.334	1.00	45.60	O
	ATOM	3961	N	PRO	R	157	14.467	32.828	115.044	1.00	47.61	N
	ATOM	3962	CA	PRO	R	157	14.087	34.227	114.837	1.00	46.46	C

	ATOM	3964	CB	PRO	R	157	15.285	35.009	115.396	1.00	47.25	C
	ATOM	3967	CG	PRO	R	157	15.985	34.064	116.298	1.00	48.32	C
	ATOM	3970	CD	PRO	R	157	15.779	32.709	115.706	1.00	48.43	C
	ATOM	3973	C	PRO	R	157	13.864	34.579	113.360	1.00	47.30	C
5	ATOM	3974	O	PRO	R	157	14.564	34.067	112.476	1.00	47.60	O
	ATOM	3975	N	ALA	R	158	12.889	35.447	113.108	1.00	45.44	N
	ATOM	3976	CA	ALA	R	158	12.627	35.945	111.765	1.00	43.40	C
	ATOM	3978	CB	ALA	R	158	11.289	36.666	111.718	1.00	40.55	C
10	ATOM	3982	C	ALA	R	158	13.751	36.885	111.338	1.00	44.62	C
	ATOM	3983	O	ALA	R	158	14.354	37.564	112.179	1.00	47.19	O
	ATOM	3985	N	SER	R	159	14.042	36.899	110.039	1.00	42.68	N
	ATOM	3986	CA	SER	R	159	15.047	37.805	109.467	1.00	42.78	C
	ATOM	3988	CB	SER	R	159	16.297	37.028	109.031	1.00	40.46	C
	ATOM	3991	OG	SER	R	159	16.044	36.225	107.887	1.00	38.69	O
15	ATOM	3993	C	SER	R	159	14.417	38.527	108.284	1.00	43.06	C
	ATOM	3994	O	SER	R	159	13.224	38.370	108.035	1.00	45.34	O
	ATOM	3996	N	ASN	R	160	15.201	39.324	107.560	1.00	44.08	N
	ATOM	3997	CA	ASN	R	160	14.692	39.973	106.342	1.00	43.32	C
20	ATOM	3999	CB	ASN	R	160	15.569	41.169	105.920	1.00	44.24	C
	ATOM	4002	CG	ASN	R	160	16.989	40.773	105.504	1.00	45.15	C
	ATOM	4003	OD1	ASN	R	160	17.238	39.658	105.034	1.00	44.63	O
	ATOM	4004	ND2	ASN	R	160	17.923	41.718	105.657	1.00	45.43	N
	ATOM	4007	C	ASN	R	160	14.488	38.990	105.175	1.00	41.69	C
25	ATOM	4008	O	ASN	R	160	13.734	39.279	104.251	1.00	40.07	O
	ATOM	4010	N	SER	R	161	15.156	37.836	105.237	1.00	41.10	N
	ATOM	4011	CA	SER	R	161	15.111	36.834	104.170	1.00	40.06	C
	ATOM	4013	CB	SER	R	161	16.536	36.395	103.792	1.00	40.18	C
	ATOM	4016	OG	SER	R	161	17.204	35.759	104.869	1.00	39.54	O
30	ATOM	4018	C	SER	R	161	14.258	35.610	104.507	1.00	38.95	C
	ATOM	4019	O	SER	R	161	13.970	34.798	103.630	1.00	44.04	O
	ATOM	4021	N	SER	R	162	13.857	35.464	105.765	1.00	39.95	N
	ATOM	4022	CA	SER	R	162	13.050	34.315	106.166	1.00	39.08	C
	ATOM	4024	CB	SER	R	162	13.942	33.106	106.465	1.00	39.18	C
35	ATOM	4027	OG	SER	R	162	14.923	33.423	107.434	1.00	40.71	O
	ATOM	4029	C	SER	R	162	12.155	34.608	107.361	1.00	38.75	C
	ATOM	4030	O	SER	R	162	12.400	35.528	108.136	1.00	39.38	O
	ATOM	4032	N	ASP	R	163	11.108	33.802	107.489	1.00	41.71	N
	ATOM	4033	CA	ASP	R	163	10.136	33.934	108.566	1.00	41.19	C
40	ATOM	4035	CB	ASP	R	163	8.796	33.331	108.125	1.00	41.36	C
	ATOM	4038	CG	ASP	R	163	7.620	33.843	108.929	1.00	43.13	C
	ATOM	4039	OD1	ASP	R	163	7.793	34.771	109.750	1.00	44.94	O
	ATOM	4040	OD2	ASP	R	163	6.507	33.309	108.747	1.00	43.35	O
	ATOM	4041	C	ASP	R	163	10.646	33.207	109.801	1.00	42.61	C
45	ATOM	4042	O	ASP	R	163	11.543	32.355	109.711	1.00	42.49	O
	ATOM	4044	N	ALA	R	164	10.082	33.561	110.954	1.00	42.18	N
	ATOM	4045	CA	ALA	R	164	10.307	32.814	112.184	1.00	41.34	C
	ATOM	4047	CB	ALA	R	164	9.727	33.561	113.388	1.00	39.51	C
	ATOM	4051	C	ALA	R	164	9.680	31.426	112.078	1.00	39.87	C
50	ATOM	4052	O	ALA	R	164	8.655	31.238	111.420	1.00	38.54	O
	ATOM	4054	N	ILE	R	165	10.309	30.452	112.723	1.00	42.44	N
	ATOM	4055	CA	ILE	R	165	9.721	29.122	112.851	1.00	42.23	C
	ATOM	4057	CB	ILE	R	165	10.682	28.013	112.357	1.00	42.14	C
	ATOM	4059	CG1	ILE	R	165	11.005	28.246	110.870	1.00	42.01	C
55	ATOM	4062	CD1	ILE	R	165	11.934	27.228	110.243	1.00	40.75	C
	ATOM	4066	CG2	ILE	R	165	10.057	26.631	112.573	1.00	42.08	C
	ATOM	4070	C	ILE	R	165	9.320	28.935	114.313	1.00	41.00	C
	ATOM	4071	O	ILE	R	165	10.107	29.222	115.216	1.00	38.53	O
	ATOM	4073	N	CYS	R	166	8.078	28.498	114.529	1.00	41.63	N
60	ATOM	4074	CA	CYS	R	166	7.542	28.271	115.874	1.00	40.25	C
	ATOM	4076	CB	CYS	R	166	6.136	28.874	116.010	1.00	36.60	C
	ATOM	4079	SG	CYS	R	166	5.823	30.442	115.133	1.00	35.73	S
	ATOM	4081	C	CYS	R	166	7.472	26.773	116.179	1.00	40.69	C
	ATOM	4082	O	CYS	R	166	7.720	25.938	115.310	1.00	40.17	O
65	ATOM	4084	N	GLU	R	167	7.135	26.451	117.426	1.00	44.50	N
	ATOM	4085	CA	GLU	R	167	6.860	25.077	117.849	1.00	44.93	C
	ATOM	4087	CB	GLU	R	167	8.151	24.372	118.282	1.00	45.04	C
	ATOM	4090	CG	GLU	R	167	7.972	22.906	118.691	1.00	44.95	C
	ATOM	4093	CD	GLU	R	167	9.225	22.293	119.289	1.00	45.34	C
70	ATOM	4094	OE1	GLU	R	167	10.329	22.577	118.776	1.00	40.92	O
	ATOM	4095	OE2	GLU	R	167	9.102	21.517	120.273	1.00	47.99	O
	ATOM	4096	C	GLU	R	167	5.865	25.121	119.004	1.00	47.65	C

	ATOM	4097	O	GLU	R	167	5.782	26.127	119.711	1.00	49.69	O
	ATOM	4099	N	ASP	R	168	5.114	24.035	119.192	1.00	49.16	N
	ATOM	4100	CA	ASP	R	168	4.136	23.945	120.280	1.00	48.85	C
5	ATOM	4102	CB	ASP	R	168	3.139	22.811	120.018	1.00	50.72	C
	ATOM	4105	CG	ASP	R	168	2.174	23.131	118.886	1.00	52.34	C
	ATOM	4106	OD1	ASP	R	168	2.637	23.492	117.784	1.00	53.71	O
	ATOM	4107	OD2	ASP	R	168	0.949	23.020	119.096	1.00	54.20	O
	ATOM	4108	C	ASP	R	168	4.808	23.753	121.639	1.00	49.72	C
10	ATOM	4109	O	ASP	R	168	5.737	22.957	121.781	1.00	50.73	O
	ATOM	4111	C1	NAG	R	200	19.280	41.261	105.448	1.00	49.92	C
	ATOM	4114	C2	NAG	R	200	19.879	42.650	105.162	1.00	50.89	C
	ATOM	4116	N2	NAG	R	200	19.329	43.233	103.933	1.00	48.22	N
	ATOM	4118	C7	NAG	R	200	19.970	43.309	102.766	1.00	49.18	C
15	ATOM	4119	O7	NAG	R	200	21.108	43.764	102.636	1.00	51.17	O
	ATOM	4120	C8	NAG	R	200	19.219	42.833	101.558	1.00	48.74	C
	ATOM	4124	C3	NAG	R	200	21.414	42.622	105.228	1.00	52.36	C
	ATOM	4126	O3	NAG	R	200	21.973	43.919	105.134	1.00	52.44	O
	ATOM	4128	C4	NAG	R	200	21.881	41.968	106.522	1.00	53.18	C
20	ATOM	4130	O4	NAG	R	200	23.290	41.862	106.507	1.00	55.04	O
	ATOM	4132	C5	NAG	R	200	21.228	40.595	106.668	1.00	52.74	C
	ATOM	4134	C6	NAG	R	200	21.645	39.856	107.944	1.00	52.41	C
	ATOM	4137	O6	NAG	R	200	22.679	40.524	108.636	1.00	51.52	O
	ATOM	4139	O5	NAG	R	200	19.817	40.741	106.654	1.00	52.42	O
25	ATOM	4140	O	HOH	W	1	0.003	64.605	62.043	0.33	24.72	O
	ATOM	4143	O	HOH	W	2	-9.605	59.559	73.200	1.00	26.68	O
	ATOM	4146	O	HOH	W	3	-8.140	58.184	89.102	1.00	31.94	O
	ATOM	4149	O	HOH	W	4	-7.063	63.539	74.010	1.00	25.66	O
	ATOM	4152	O	HOH	W	5	-4.723	59.253	82.512	1.00	37.75	O
30	ATOM	4155	O	HOH	W	6	-3.376	51.621	59.948	1.00	30.82	O
	ATOM	4158	O	HOH	W	7	-21.301	47.919	89.797	1.00	45.00	O
	ATOM	4161	O	HOH	W	8	17.454	35.093	91.847	1.00	36.98	O
	ATOM	4164	O	HOH	W	9	-11.544	54.737	60.091	1.00	35.28	O
	ATOM	4167	O	HOH	W	10	11.517	34.054	89.321	1.00	38.62	O
35	ATOM	4170	O	HOH	W	11	15.538	37.329	60.314	1.00	40.16	O
	ATOM	4173	O	HOH	W	12	-2.071	57.563	57.100	1.00	30.60	O
	ATOM	4176	O	HOH	W	13	-14.156	51.778	61.686	1.00	43.45	O
	ATOM	4179	O	HOH	W	14	9.646	34.836	59.126	1.00	30.31	O
	ATOM	4182	O	HOH	W	15	21.142	46.286	66.627	1.00	46.45	O
40	ATOM	4185	O	HOH	W	16	-10.386	45.662	73.129	1.00	33.78	O
	ATOM	4188	O	HOH	W	17	-16.511	59.613	72.079	1.00	31.04	O
	ATOM	4191	O	HOH	W	18	23.071	41.631	72.861	1.00	44.59	O
	ATOM	4194	O	HOH	W	19	16.837	33.637	100.166	1.00	41.27	O
	ATOM	4197	O	HOH	W	20	-14.217	62.821	74.196	1.00	32.88	O
45	ATOM	4200	O	HOH	W	21	-14.670	40.569	64.129	1.00	41.83	O
	ATOM	4203	O	HOH	W	22	-18.656	59.058	85.064	1.00	49.03	O
	ATOM	4206	O	HOH	W	23	15.806	33.463	88.496	1.00	37.42	O
	ATOM	4209	O	HOH	W	25	12.189	39.742	64.884	1.00	45.26	O
	ATOM	4212	O	HOH	W	26	-8.792	47.345	90.359	1.00	46.94	O
50	ATOM	4215	O	HOH	W	27	-2.885	42.079	69.492	1.00	30.23	O
	ATOM	4218	O	HOH	W	28	6.726	51.739	63.231	1.00	36.36	O
	ATOM	4221	O	HOH	W	29	-2.489	44.580	61.826	1.00	31.20	O
	ATOM	4224	O	HOH	W	30	3.671	43.621	63.911	1.00	29.09	O
	ATOM	4227	O	HOH	W	31	6.639	55.364	72.156	1.00	26.88	O
55	ATOM	4230	O	HOH	W	32	-20.935	57.981	68.149	1.00	56.53	O
	ATOM	4233	O	HOH	W	33	-5.708	40.662	69.409	1.00	40.78	O
	ATOM	4236	O	HOH	W	34	-18.463	55.317	77.193	1.00	33.89	O
	ATOM	4239	O	HOH	W	35	24.111	41.732	89.693	1.00	41.89	O
	ATOM	4242	O	HOH	W	37	-7.192	51.146	54.815	1.00	42.35	O
60	ATOM	4245	O	HOH	W	38	7.353	30.448	54.395	1.00	36.83	O
	ATOM	4248	O	HOH	W	39	-1.856	47.579	49.816	1.00	49.91	O
	ATOM	4251	O	HOH	W	40	1.022	45.075	74.032	1.00	31.65	O
	ATOM	4254	O	HOH	W	41	-13.675	56.719	63.083	1.00	30.98	O
	ATOM	4257	O	HOH	W	42	4.184	56.101	74.625	1.00	37.55	O
65	ATOM	4260	O	HOH	W	43	6.021	49.653	70.667	1.00	45.68	O
	ATOM	4263	O	HOH	W	44	10.849	37.414	49.625	1.00	46.96	O
	ATOM	4266	O	HOH	W	45	7.908	39.387	73.942	1.00	47.08	O
	ATOM	4269	O	HOH	W	46	17.232	35.188	60.295	1.00	37.63	O
	ATOM	4272	O	HOH	W	47	7.163	43.073	82.513	1.00	45.08	O
70	ATOM	4275	O	HOH	W	48	7.348	53.460	70.376	1.00	39.99	O
	ATOM	4278	O	HOH	W	49	-22.392	53.200	86.801	1.00	35.43	O
	ATOM	4281	O	HOH	W	50	-15.839	55.952	64.302	1.00	36.96	O

	ATOM	4284	0	HOH	W	51	-1.641	62.755	78.227	1.00	46.06	O
	ATOM	4287	0	HOH	W	52	18.525	50.453	86.037	1.00	38.49	O
	ATOM	4290	0	HOH	W	53	-20.729	51.556	80.247	1.00	36.50	O
5	ATOM	4293	0	HOH	W	54	9.596	48.525	62.029	1.00	35.06	O
	ATOM	4296	0	HOH	W	55	21.406	37.333	65.920	1.00	37.87	O
	ATOM	4299	0	HOH	W	56	5.766	51.736	71.089	1.00	49.98	O
	ATOM	4302	0	HOH	W	58	10.804	31.713	105.358	1.00	42.64	O
	ATOM	4305	0	HOH	W	59	-4.355	45.593	56.651	1.00	42.50	O
10	ATOM	4308	0	HOH	W	61	-27.365	49.332	86.072	1.00	36.03	O
	ATOM	4311	0	HOH	W	62	-18.249	58.520	67.105	1.00	40.31	O
	ATOM	4314	0	HOH	W	65	13.450	36.678	57.611	1.00	37.99	O
	ATOM	4317	0	HOH	W	67	22.014	45.061	84.064	1.00	34.03	O
	ATOM	4320	0	HOH	W	68	-26.144	48.249	84.250	1.00	31.91	O
15	ATOM	4323	0	HOH	W	70	9.027	35.753	50.589	1.00	49.17	O
	ATOM	4326	0	HOH	W	71	13.615	37.382	54.874	1.00	43.95	O
	ATOM	4329	0	HOH	W	72	-15.933	56.390	59.505	1.00	42.61	O
	ATOM	4332	0	HOH	W	73	-19.841	50.436	89.715	1.00	42.47	O
	ATOM	4335	0	HOH	W	74	-19.837	48.747	73.481	1.00	41.87	O
20	ATOM	4338	0	HOH	W	76	1.873	53.977	81.007	1.00	42.67	O
	ATOM	4341	0	HOH	W	77	-11.971	45.719	75.394	1.00	41.21	O
	ATOM	4344	0	HOH	W	78	-1.236	62.638	60.793	1.00	39.38	O
	ATOM	4347	0	HOH	W	79	17.280	46.618	64.398	1.00	36.58	O
	ATOM	4350	0	HOH	W	80	17.929	49.358	66.877	1.00	62.41	O
25	ATOM	4353	0	HOH	W	81	22.466	51.650	91.599	1.00	71.88	O
	ATOM	4356	0	HOH	W	82	19.089	36.624	79.306	1.00	44.88	O
	ATOM	4359	0	HOH	W	83	13.496	38.415	76.625	1.00	38.69	O
	ATOM	4362	0	HOH	W	84	13.005	35.737	76.139	1.00	45.40	O
	ATOM	4365	0	HOH	W	85	7.425	45.305	89.345	1.00	45.36	O
30	ATOM	4368	0	HOH	W	86	13.958	41.378	84.076	1.00	42.15	O
	ATOM	4371	0	HOH	W	87	12.886	31.526	103.743	1.00	47.81	O
	ATOM	4374	0	HOH	W	88	7.844	35.098	92.726	1.00	49.59	O
	ATOM	4377	0	HOH	W	89	-18.830	48.613	65.744	1.00	52.05	O
	ATOM	4380	0	HOH	W	90	-14.910	48.132	61.613	1.00	47.14	O
35	ATOM	4383	0	HOH	W	91	-13.808	51.473	93.782	1.00	49.41	O
	ATOM	4386	0	HOH	W	92	-18.040	53.288	92.965	1.00	47.90	O
	ATOM	4389	0	HOH	W	93	-14.768	58.203	87.005	1.00	34.70	O
	ATOM	4392	0	HOH	W	94	2.625	54.056	73.796	1.00	38.73	O
	ATOM	4395	0	HOH	W	95	-26.673	53.342	85.864	1.00	39.34	O
40	ATOM	4398	0	HOH	W	96	-22.448	52.552	89.977	1.00	57.76	O

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WE CLAM:

1. An isolated polypeptide having at least 90% sequence identity to the polypeptide comprising the amino acid sequence of amino acids 51-198 of SEQ ID NO:1, not including the polypeptide having the amino acid sequence of SEQ ID NO:1, and wherein the polypeptide binds a hOX40 receptor or a hOX40 receptor ligand binding fragment thereof.
2. An isolated polypeptide comprising the amino acid sequence starting at any one of amino acids 51 to amino acid residue 66 and ending at any one of amino acids 180 to 191 of SEQ ID NO: 1, not including the polypeptide having the amino acid sequence of SEQ ID NO:1, and wherein the polypeptide binds a hOX40 receptor or a hOX40 receptor ligand binding fragment thereof .
3. A isolated polypeptide having at least 90% sequence identity to the polypeptide comprising the amino acid sequence of amino acids 99 to 191 of SEQ ID NO: 1, not including the polypeptide having the amino acid sequence of SEQ ID NO: 1, and wherein the polypeptide binds a hOX40 receptor or a hOX40 receptor ligand binding fragment thereof .
4. A crystalline form of any one of the polypeptides of claims 1-3.
5. A crystal comprising a mOX40L comprising SEQ ID NO: 1, or a fragment of SEQ ID NO:1 comprising the sequence of amino acids 51-198 of SEQ ID NO:1.
6. A crystal of a fragment of mOX40L having a space group symmetry of $P6_3$ and comprising a unit cell having the dimensions of $a=b$ and are about 74 Å, and c is about 48 Å.
7. A crystal of mOX40L having the structural coordinates of Table 8.
8. A composition comprising a crystal of any of claims 4-7, and a carrier.
9. A heavy atom derivative of a crystal of any of claims 4-7.
10. A crystal comprising a mOX40L obtainable by the method of

- a) contacting isolated mOX40L of any of claims 1-3 with a precipitant and a buffer to form a mixture; and
- b) incubating the mixture until a crystal is formed.

11. A crystal of any one of claims 4 to 10 comprising a crystal structure defined by at least one structural coordinate of at least one amino acid residue corresponding to an amino acid residue selected from the group consisting of A66, T68, Y80, N82, E83, D99, F11, N125, P126, H119, S145, A147, F148, K149, D150, Q167, I168, N169, G171, Y182, S188, and Y189 of the polypeptide comprising SEQ ID NO:1, and combinations thereof, according to Table 8 or Table 9, or the structural coordinates of any of the amino acid residues defined by a set of points having a root mean square deviation of less than about 0.70 Å from points representing the backbone atoms of the amino acids as represented by the structure coordinates listed in Tables 8 or 9.

12. The crystal of any one of claims 4-11 further comprising a ligand, wherein said ligand binds to the mOX40L binding site for hOX40 receptor.

13. The crystal of claim 12, wherein the ligand comprises a polypeptide comprising the amino acid sequence of amino acids 29 to 170 of SEQ ID NO:2.

14. A molecule or molecular complex comprising at least a portion of an mOX40L binding site, wherein the binding site comprises at least one amino acid residue corresponding to an amino acid residue selected from the group consisting of A66, T68, Y80, N82, E83, D99, F11, N125, P126, H119, S145, A147, F148, K149, D150, Q167, I168, N169, G171, Y182, S188, Y189 of the polypeptide comprising SEQ ID NO:1, and combinations thereof.

15. A three-dimensional configuration of points wherein at least a portion of the points are derived from structure coordinates of Table 8 or 9 representing locations of the backbone atoms of amino acids defining the mOX40L binding site.

16. The three-dimensional configuration of points of claim 15 displayed as a holographic image, a stereodiagram, a model, or a computer-displayed image.

17. A machine-readable data storage medium comprising a data storage material encoded with machine-readable data, wherein the data comprises at least a portion

of the diffraction data of a crystal of any one of claims 4-13, wherein the machine is programmed with instructions for using such data to display a graphical three-dimensional representation of at least one molecule or molecular complex comprising at least a portion of a mOX40L binding site or the binding site defined by a set of points having a root mean square deviation of less than about 0.05 Å from points representing the atoms of the amino acids as represented by the structure coordinates listed in Table 8 or 9.

18. The machine of claim 17, wherein the data comprises at least one structural coordinate for at least one amino acid residue corresponding to an amino acid selected from the group consisting of A66.T68, Y80, N82, E83, D99, F111, N125, P126, H119, S145 A147, F148, K149, D150, Q167, I168, N169, G171 Y182, S188, and Y189 of the polypeptide comprising SEQ ID NO:1, and combinations thereof, according to Tables 8 or 9, or the amino acids defined by a set of points having a root mean square deviation of less than about 0.05 Å from points representing the atoms of the amino acids as represented by the structure coordinates listed in Table 8 or 9.

19. A machine-readable data storage medium comprising a crystal structure defined by at least a portion of the structural coordinates of a crystal of any one of claims 4-13, wherein the machine is programmed with instructions for using such data to display a graphical three-dimensional representation of at least one molecule or molecular complex comprising at least a portion of a mOX40L binding site, the binding site defined by a set of points having a root mean square deviation of less than about 0.05 Å from points representing the atoms of the amino acids as represented by the structure coordinates listed in Table 8 or 9.

20. The machine of claim 19, wherein the structural coordinates comprise the structural coordinates of at least one amino acid residue corresponding to an amino acid selected from the group consisting of A66.T68, Y80, N82, E83, D99, F111, N125, P126, H119, S145 A147, F148, K149, D150, Q167, I168, N169, G171 Y182, S188, and Y189 of the polypeptide comprising SEQ ID NO:1, and combinations thereof, according to Tables 8 or 9, or the amino acids defined by a set of points having a root mean square deviation of less than about 0.05 Å from points representing the atoms of the amino acids as represented by the structure coordinates listed in Table 8 or 9.

21. A method for obtaining structural information about a molecule or molecular complex comprising application of at least a portion of the mOX40L structure

coordinates listed in Table 8 or 9 to an X-ray diffraction pattern of the molecule or molecular complex's crystal structure to generate a three-dimensional electron density map of at least a portion of the molecule or molecular complex.

22. The method of claim 26, wherein the molecule or molecular complex comprises an antagonist of at least one biological activity of mOX40L.

23. A computer-assisted method for identifying an agent that modulates mOX40L activity comprising:

- (a) providing a computer modeling application with a set of structure coordinates of Table 8 or 9 defining at least a portion of a mOX40L binding site;
- (b) providing the computer modeling application with a set of structure coordinates for a test agent; and
- (c) modeling the structure of (a) complexed with (b) to determine if the test agent associates with the mOX40L binding site and optionally determining if the test agent modulates binding or activity of mOX40L.

24. A computer-assisted method for designing an agent that binds the mOX40L binding site, comprising:

- (a) providing a computer modeling application with a set of structural coordinates of Table 8 or 9 defining at least a portion of the mOX40L binding site; and
- (b) modeling the structural coordinates of (a) to identify an agent that contacts at least one amino acid residue in the mOX40L binding site and optionally determining if the test agent modulates binding or activity of mOX40L.

25. A method of identifying a molecule that mimics mOX40L comprising:

- a) searching a molecular structure database with the structural coordinates of Table 8 or 9; and
- b) selecting a molecule from the database that mimics the structural coordinates of the mOX40L and optionally determining if the molecule modulates binding or activity of mOX40L.

26. A method of assessing agents that are antagonists or agonists of mOX40L comprising:

- a) applying at least a portion of the crystallography coordinates of Table 8 or 9 to a computer algorithm that generates a 3 dimensional model of mOX40L or mOX40L complexed hOX40 receptor suitable for designing molecules that are antagonists or agonists; and
- b) searching a molecular structure database to identify potential antagonists or agonists of mOX40L and optionally determining if the antagonist or agonist modulates binding or activity of mOX40L and/or hOX40 receptor.

27. The method of claim 26, further comprising:

- a) synthesizing or obtaining the antagonist or agonist;
- b) contacting the antagonist or agonist with mOX40L and selecting the antagonist or agonist that modulates the activity or binding of mOX40L.

28. The method of any one of claims 21-27, wherein the structural coordinates comprise the structural coordinates for at least one amino acid corresponding to an amino acid selected from the group consisting of A66/T68, Y80, N82, E83, D99, F111, N125, P126, H119, S145, A147, F148, K149, D150, Q167, I168, N169, G171, Y182, S188, and Y189 of the polypeptide comprising SEQ ID NO:1 and combinations thereof.

29. A polypeptide having at least 90% sequence identity to the polypeptide comprising the amino acid sequence of amino acids 51-183 of SEQ ID NO:3, not including the polypeptide having the amino acid sequence of SEQ ID NO:3, and wherein the polypeptide binds a hOX40 receptor or a hOX40 receptor ligand binding fragment thereof.

30. A polypeptide comprising the amino acid sequence starting at any one of amino acids 51 to amino acid residue 65 and ending at any one of amino acids 180 to 183 of SEQ ID NO:3, not including the polypeptide having the amino acid sequence of SEQ ID NO:3, and wherein the polypeptide binds a hOX40 receptor or a hOX40 receptor ligand binding fragment thereof.

31. A polypeptide having at least 90% sequence identity to the polypeptide comprising the amino acid sequence of amino acids 98 to 183 of SEQ ID NO:3, not including the polypeptide having the amino acid sequence of SEQ ID NO:3, and wherein the polypeptide binds a hOX40 receptor or a hOX40 receptor ligand binding fragment thereof.

32. A crystalline form of any one of the polypeptides of claims 29-31.
33. A cocrystal comprising a hOX40L comprising a polypeptide comprising the amino acid sequence of SEQ ID NO:3, or a fragment comprising the sequence of amino acids 51-183 of SEQ ID NO:3. and a hOX40 receptor comprising a polypeptide comprising the amino acid sequence of SEQ ED NO:2 or a fragment of SEQ ID NO:2 comprising the amino acid sequence of amino acids 29-170 of SEQ DD NO:2.
34. The cocrystal of claim 33 having a space group symmetry of R32 and comprising a unit cell having the dimensions of a=b and are about 112 Å, and c is about 233 Å.
35. A cocrystal of hOX40L and hOX40 receptor having the structural coordinates of Table 10.
36. A composition comprising a crystal of any of claims 32-35, and a carrier.
37. A heavy atom derivative of a crystal of any of claims 32-35.
38. A cocrystal comprising a hOX40L and hOX40 receptor obtainable by the method of
- contacting an isolated hOX40L of any of claims 29-31 and hOX40 receptor with a precipitant and a buffer to form a mixture; and
 - incubating the mixture until a crystal is formed.
39. A crystal of any one of claims 32-38 comprising a crystal structure defined by one or more structural coordinates of at least one amino acid residue corresponding to an amino acid residue selected from the group consisting of Q65, T67, E82, D98, S110, E123, T144, Y145, K146, D147, D162, H164, V165, N166, G167, F180, and V182 of the polypeptide comprising SEQ DD NO:3, and combinations thereof. according to Table 10, or the structural coordinates of any of the amino acid residues defined by a set of points having a root mean square deviation of less than about 0.70 Å from points representing the backbone atoms of the amino acids as represented by the structure coordinates listed in Table 10.

40. A molecule or molecular complex comprising at least a portion of an hOX40L binding site, wherein the binding site comprises at least one amino acid residue corresponding to an amino acid residue selected from the group consisting of Q65, T67, E82, D98, S110, E123, T144, Y145, K146, D147, D162, H164, V165, N166, G167, F180, V182 of the polypeptide comprising SEQ ID NO:3, and combinations thereof.

41. A three-dimensional configuration of points wherein at least a portion of the points are derived from structure coordinates of Table 10 representing locations of the backbone atoms of amino acids defining the hOX40L binding site.

42. The three-dimensional configuration of points of claim 41 displayed as a holographic image, a stereodiagram, a model, or a computer-displayed image.

43. A machine-readable data storage medium comprising a data storage material encoded with machine-readable data, wherein the data comprises at least a portion of the diffraction data of a crystal of any one of claims 32-39, wherein the machine is programmed with instructions for using such data to display a graphical three-dimensional representation of at least one molecule or molecular complex comprising at least a portion of a hOX40L binding site or the binding site defined by a set of points having a root mean square deviation of less than about 0.05 Å from points representing the atoms of the amino acids as represented by the structure coordinates listed in Table 10.

44. The machine of claim 43, wherein the data comprises the structural coordinates for at least one amino acid residue corresponding to an amino acid selected from the group consisting of Q65, T67, E82, D98, S110, E123, T144, Y145, K146, D147, D162, H164, V165, N166, G167, F180, V182 of the polypeptide comprising SEQ ID NO:3, and combinations thereof, according to Table 10, or the amino acids defined by a set of points having a root mean square deviation of less than about 0.05 Å from points representing the atoms of the amino acids as represented by the structure coordinates listed in Table 10.

45. A method for obtaining structural information about a molecule or molecular complex comprising application of at least a portion of the hOX40L structure coordinates listed in Table 10 to an X-ray diffraction pattern of the molecule or molecular complex's crystal structure to generate a three-dimensional electron density map of at least a portion of the molecule or molecular complex.

46. The method of claim 45, wherein the molecule or molecular complex comprises an antagonist of at least one biological activity of hOX40L.

47. A computer-assisted method for identifying an agent that modulates hOX40L activity comprising:

- (a) providing a computer modeling application with a set of structure coordinates of Table 10 defining at least a portion of a hOX40L binding site;
- (b) providing the computer modeling application with a set of structure coordinates for a test agent; and
- (c) modeling the structure of (a) complexed with (b) to determine if the test agent associates with the hOX40L binding site and optionally determining if the test agent modulates binding or activity of hOX40L.

48. A computer-assisted method for designing an agent that binds the hOX40L binding site, comprising:

- (a) providing a computer modeling application with a set of structural coordinates of Table 10 defining at least a portion of the hOX40L binding site; and
- (b) modeling the structural coordinates of (a) to identify an agent that contacts at least one amino acid residue in the hOX40L binding site and optionally determining if the test agent modulates binding or activity of hOX40L.

49. A method of identifying a molecule that mimics hOX40L comprising:

- a) searching a molecular structure database with the structural coordinates of Table 10; and
- b) selecting a molecule from the database that mimics the structural coordinates of the hOX40L and optionally determining if the molecule modulates binding or activity of hOX40L.

50. A method of assessing agents that are antagonists or agonists of hOX40L comprising:

- a) applying at least a portion of the crystallography coordinates of Table 10 to a computer algorithm that generates a 3 dimensional model of hOX40L or hOX40L complexed hOX40 receptor suitable for designing molecules that are antagonists or agonists; and

b) searching a molecular structure database to identify potential antagonists or agonists of hOX40L and optionally determining if the agonist or antagonist modulates binding or activity of hOX40L.

51. The method of claim 50, further comprising:

a) synthesizing or obtaining the antagonist or agonist;
b) contacting the antagonist or agonist with hOX40L and selecting the antagonist or agonist that modulates the activity of hOX40L.

52. The method of any one of claims 45-51, wherein the structural coordinates comprise the structural coordinates for at least one amino acid corresponding to an amino acid selected from the group consisting of Q65, T67, E82, D98, S110, E123, T144, Y145, K146, D147, D162, H164, V165, N166, G167, F180, V182 of the polypeptide comprising SEQ ID NO:3, and combinations thereof.

53. A polypeptide having at least 90% sequence identity to the polypeptide comprising the amino acid sequence of amino acids 29-170 of SEQ ID NO:2, not including the polypeptide having the amino acid sequence of SEQ ID NO:2, and wherein the polypeptide binds hOX40L or a receptor binding fragment thereof.

54. A polypeptide comprising the amino acid sequence starting at any one of amino acids 29 to amino acid 42 and ending at any one of amino acids 119 to 170 of SEQ ID NO:2, not including the polypeptide having the amino acid sequence of SEQ ID NO:2, and wherein the polypeptide binds hOX40L or a receptor binding fragment thereof.

55. A crystalline form of any one of the polypeptides of claims 53-54.

56. A cocrystal comprising a mOX40L comprising a polypeptide comprising the amino acid sequence of SEQ ID NO:1, or a fragment of SEQ ID NO:1 comprising the sequence of amino acids 51-198 of SEQ ID NO:1, and a hOX40 receptor comprising a polypeptide comprising the amino acid sequence of SEQ ID NO:2 or a fragment of SEQ ID NO:2 comprising the amino acid sequence of amino acids 29-170 of SEQ ID NO:2.

57. A cocrystal of claim 56 having a space group symmetry of R32 and comprising a unit cell having the dimensions of a=b and are about 105 Å, and c is about 478 Å.

58. A cocrystal of mOX40L and hOX40 receptor having the structural coordinates of Table 9.
59. A composition comprising a crystal of any of claims 55-58, and a carrier.
60. A heavy atom derivative of a crystal of any of claims 55-58.
61. A cocrystal comprising a mOX40L and hOX40 receptor obtainable by the method of
- contacting an isolated mOX40L of any of claims 1-3 and hOX40 receptor with a precipitant and a buffer to form a mixture; and
 - incubating the mixture until a crystal is formed.
62. A crystal of any one of claims 33-35 comprising a crystal structure defined by one or more structural coordinates of at least one amino acid residue in a binding site on hOX40 receptor for hOX40L corresponding to an amino acid residue selected from the group consisting of Y36, P37, S38, E45, V53, R55, S78, K79, P83, T85, W86, C87, N88.Y1 19, and V123 of the polypeptide comprising SEQ ID NO:2, and combinations thereof, according to table 10, or the structural coordinates of any of the amino acid residues defined by a set of points having a root mean square deviation of less than about 0.70 Å from points representing the backbone atoms of the amino acids as represented by the structure coordinates listed in Table 10.
63. A molecule or molecular complex comprising at least a portion of an hOX40 receptor binding site for hOX40L, wherein the binding site comprises at least one amino acid residue corresponding to an amino acid residue selected from the group consisting of Y36, P37, S38, E45, V53, R55, S78, K79, P83, T85, W86, C87, N88.Y1 19, and V 123 of the polypeptide comprising SEQ ID NO:2, and combinations thereof.
64. A three-dimensional configuration of points wherein at least a portion of the points are derived from structure coordinates of Table 10 representing locations of the backbone atoms of amino acids defining the hOX40 receptor binding site for hOX40L.
65. The three-dimensional configuration of points of claim 64 displayed as a holographic image, a stereodiagram, a model, or a computer-displayed image.

66. A machine-readable data storage medium comprising a data storage material encoded with machine-readable data, wherein the data comprises at least a portion of the diffraction data of a crystal of any one of claims 33-35, wherein the machine is programmed with instructions for using such data to display a graphical three-dimensional representation of at least one molecule or molecular complex comprising at least a portion of a hOX40 receptor binding site for hOX40L or the binding site defined by a set of points having a root mean square deviation of less than about 0.05 Å from points representing the atoms of the amino acids as represented by the structure coordinates listed in Table 10.

67. The machine of claim 66, wherein the data comprises the structural coordinates for at least one amino acid residue corresponding to an amino acid selected from the group consisting of Y36, P37, S38, E45, V53, R55, S78, K79, P83, T85, W86, C87, N88, Y119, and V123 of the polypeptide comprising SEQ ID NO:2, and combinations thereof, according to Table 10, or the amino acids defined by a set of points having a root mean square deviation of less than about 0.05 Å from points representing the atoms of the amino acids as represented by the structure coordinates listed in Table 10.

68. A method for obtaining structural information about a molecule or molecular complex comprising application of at least a portion of the hOX40 receptor structure coordinates listed in Table 10 to an X-ray diffraction pattern of the molecule or molecular complex's crystal structure to generate a three-dimensional electron density map of at least a portion of the molecule or molecular complex.

69. The method of claim 68, wherein the molecule or molecular complex comprises an antagonist of at least one biological activity of hOX40 receptor.

70. A computer-assisted method for identifying an agent that modulates hOX40 receptor activity comprising:

- (a) providing a computer modeling application with a set of structure coordinates of Table 10 defining at least a portion of a hOX40 receptor binding site for hOX40L;
- (b) providing the computer modeling application with a set of structure coordinates for a test agent; and

(c) modeling the structure of (a) complexed with (b) to determine if the test agent associates with the hOX40 receptor binding site and optionally determining if the testagent modulates binding or activity of hOX40 receptor.

71. A computer-assisted method for designing an agent that binds the hOX40 receptor binding site, comprising:

(a) providing a computer modeling application with a set of structural coordinates of Table 10 defining at least a portion of the hOX40 receptor binding site for hOX40L; and

(b) modeling the structural coordinates of (a) to identify an agent that contacts at least one amino acid residue in the hOX40 receptor binding site and optionally determining if the testagent modulates binding or activity of hOX40 receptor.

72. A method of identifying a molecule that mimics the hOX40 receptor comprising:

a) searching a molecular structure database with the structural coordinates of Table 10; and

b) selecting a molecule from the database that mimics the structural coordinates of the hOX40 receptor and optionally determining if the molecule modulates binding or activity of hOX40 receptor.

73. A method of assessing agents that are antagonists or agonists of hOX40 receptor comprising:

a) applying at least a portion of the crystallography coordinates of Table 10 to a computer algorithm that generates a 3 dimensional model of hOX40 receptor or hOX40L complexed with hOX40 receptor suitable for designing molecules that are antagonists or agonists; and

b) searching a molecular structure database to identify potential antagonists or agonists of hOX40 receptor.

74. The method of claim 73, further comprising:

a) synthesizing or obtaining the antagonist or agonist;

b) contacting the antagonist or agonist with hOX40 receptor and selecting the antagonist or agonist that modulates the activity of hOX40 receptor.

75. The method of any one of claims 68-74, wherein the structural coordinates comprise the structural coordinates for at least one amino acid corresponding to an amino acid selected from the group consisting of Y36, P37, S38, E45, V53, R55, S78, K79, P83, T85, W86, C87, N88, Y119, V123 of the polypeptide comprising SEQ ID NO:2, and combinations thereof.

76. A crystal of any one of claims 56 to 58 comprising a crystal structure defined by one or more structural coordinates of at least one amino acid residue in a binding site on hOX40 receptor for mOX40L corresponding to an amino acid residue selected from the group consisting of C31, G33, T35, Y36, P37, S38, E45, M52, V53, S54, R55, F71, S78, K79, P80, P83, C84, W86, N88, and Y119 of the polypeptide comprising SEQ ID NO:2, and combinations thereof, according to tables 8 or 9, or the structural coordinates of any of the amino acid residues defined by a set of points having a root mean square deviation of less than about 0.70 Å from points representing the backbone atoms of the amino acids as represented by the structure coordinates listed in Table 8 or 9.

77. A molecule or molecular complex comprising at least a portion of an hOX40 receptor binding site for mOX40L, wherein the binding site comprises at least one amino acid residue corresponding to an amino acid residue selected from the group consisting of C31, G33, T35, Y36, P37, S38, E45, M52, V53, S54, R55, F71, S78, K79, P80, P83, C84, W86, N88, Y119 of the polypeptide comprising SEQ ID NO:2, and combinations thereof.

78. A three-dimensional configuration of points wherein at least a portion of the points are derived from structure coordinates of Table 9 representing locations of the backbone atoms of amino acids defining the hOX40 receptor binding site for mOX40L.

79. The three-dimensional configuration of points of claim 78 displayed as a holographic image, a stereodiagram, a model, or a computer-displayed image.

80. A machine-readable data storage medium comprising a data storage material encoded with machine-readable data, wherein the data comprises at least a portion of the diffraction data of a crystal of any one of claims 56-58, wherein the machine is programmed with instructions for using such data to display a graphical three-dimensional representation of at least one molecule or molecular complex comprising at least a portion of a hOX40 receptor binding site for mOX40L or the binding site defined by a set of points

having a root mean square deviation of less than about 0.05 Å from points representing the atoms of the amino acids as represented by the structure coordinates listed in Table 9.

81. The machine of claim 80, wherein the data comprises the structural coordinates for at least one amino acid residue corresponding to an amino acid selected from the group consisting of C31, G33, T35, Y36, P37, S38, E45, M52, V53, S54, R55, F71, S78, K79, P80, P83, C84, W86, N88, Y119 of the polypeptide comprising SEQ ID NO:2, and combinations thereof, according to Table 9, or the amino acids defined by a set of points having a root mean square deviation of less than about 0.05 Å from points representing the atoms of the amino acids as represented by the structure coordinates listed in Table 9.

82. A method for obtaining structural information about a molecule or molecular complex comprising application of at least a portion of the hOX40 receptor structure coordinates listed in Table 9 to an X-ray diffraction pattern of the molecule or molecular complex's crystal structure to generate a three-dimensional electron density map of at least a portion of the molecule or molecular complex.

83. The method of claim 82, wherein the molecule or molecular complex comprises an antagonist of at least one biological activity of hOX40 receptor.

84. A computer-assisted method for identifying an agent that modulates hOX40 receptor activity comprising:

- (a) providing a computer modeling application with a set of structure coordinates of Table 9 defining at least a portion of a hOX40 receptor binding site for mOX40L;
- (b) providing the computer modeling application with a set of structure coordinates for a test agent; and
- (c) modeling the structure of (a) complexed with (b) to determine if the test agent associates with the hOX40 receptor binding site and optionally determining whether the test agent modulates the activity of hOX40 receptor.

85. A computer-assisted method for designing an agent that binds the hOX40 receptor binding site, comprising:

- (a) providing a computer modeling application with a set of structural coordinates of Table 9 defining at least a portion of the hOX40 receptor binding site for mOX40L; and

(b) modeling the structural coordinates of (a) to identify an agent that contacts at least one amino acid residue in the hOX40 receptor binding site and optionally determining whether the test agent modulates the activity of hOX40 receptor.

86. A method of identifying a molecule that mimics the hOX40 receptor comprising:

- a) searching a molecular structure database with the structural coordinates of Table 9; and
- b) selecting a molecule from the database that mimics the structural coordinates of the hOX40 receptor and optionally determining whether the molecule modulates the activity of hOX40 receptor.

87. A method of assessing agents that are antagonists or agonists of hOX40 receptor comprising:

- a) applying at least a portion of the crystallography coordinates of Table 9 to a computer algorithm that generates a 3 dimensional model of hOX40 receptor or mOX40L complexed with hOX40 receptor suitable for designing molecules that are antagonists or agonists; and
- b) searching a molecular structure database to identify potential antagonists or agonists of hOX40 receptor and optionally determining whether the agonist or antagonist modulates the activity of hOX40 receptor.

88. The method of claim 87, further comprising:

- a) synthesizing or obtaining the antagonist or agonist;
- b) contacting the antagonist or agonist with hOX40 receptor and selecting the antagonist or agonist that modulates the activity of hOX40 receptor.

89. The method of any one of claims 82-87, wherein the structural coordinates comprise the structural coordinates for at least one amino acid corresponding to an amino acid selected from the group consisting of C31, G33, T35, Y36, P37, S38, E45, M52, V53, S54, R55, F71, S78, K79, P80, P83, C84, W86, N88, Y119 of the polypeptide comprising SEQ ID NO:2, and combinations thereof.

Figure 1

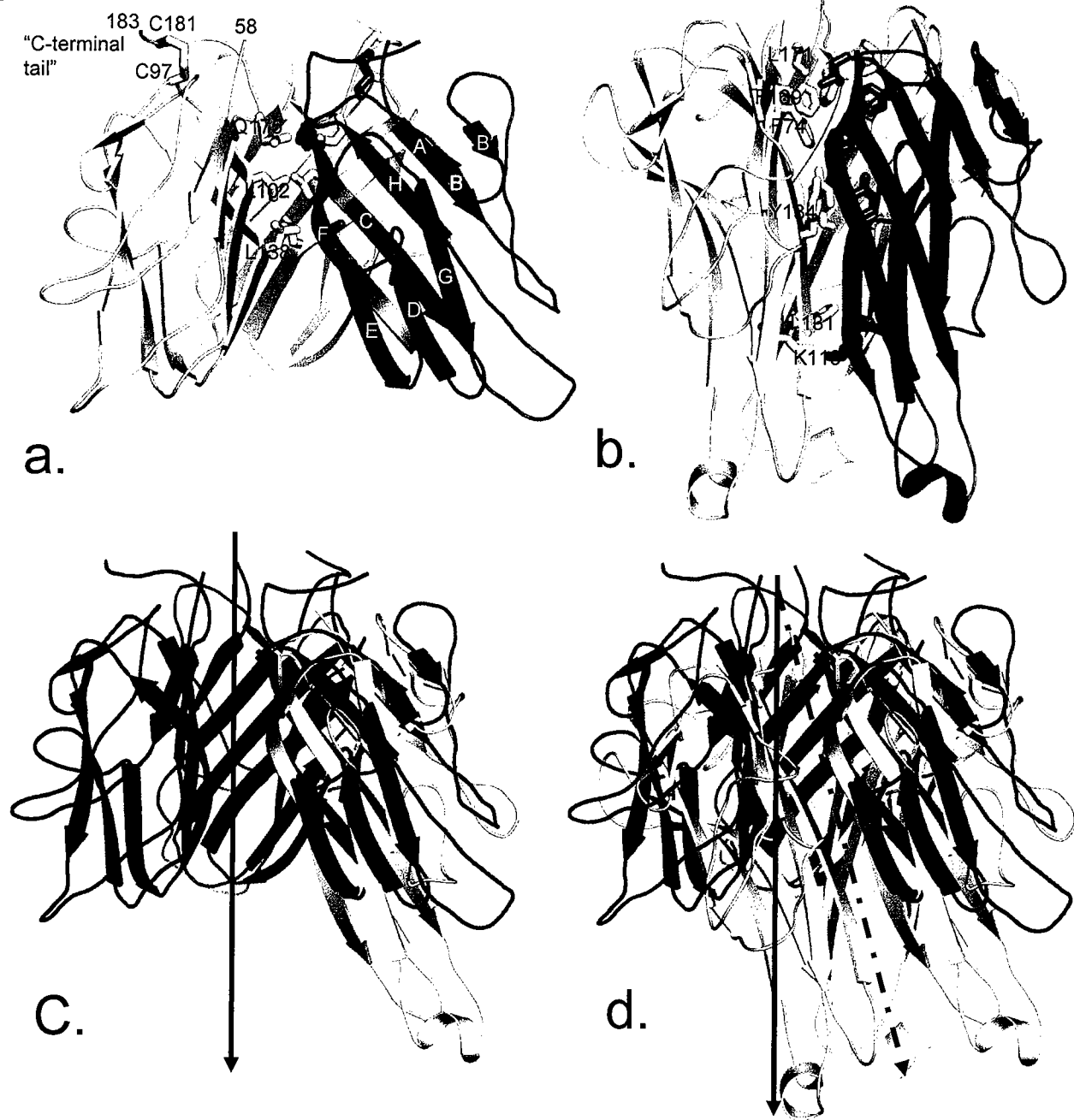


Figure 2

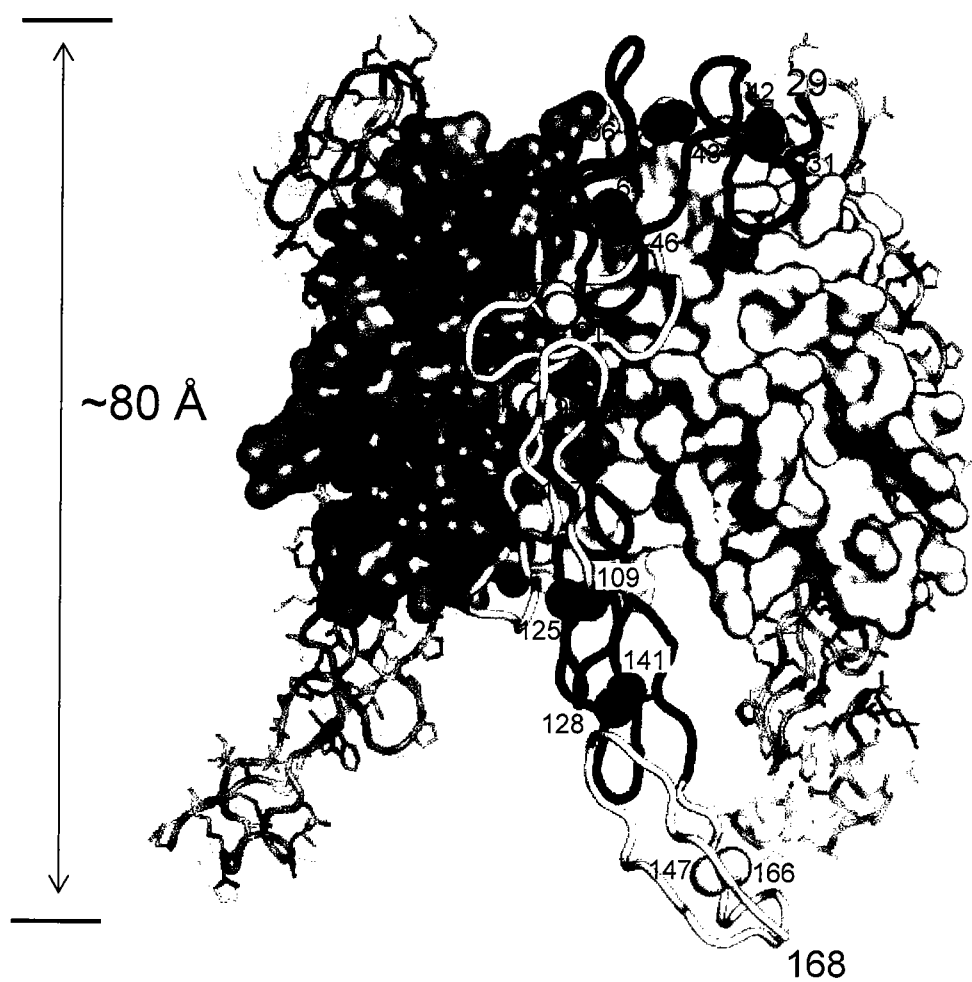


Figure 3 (green became italic with shadow, orange became outlined, yellow became bold)

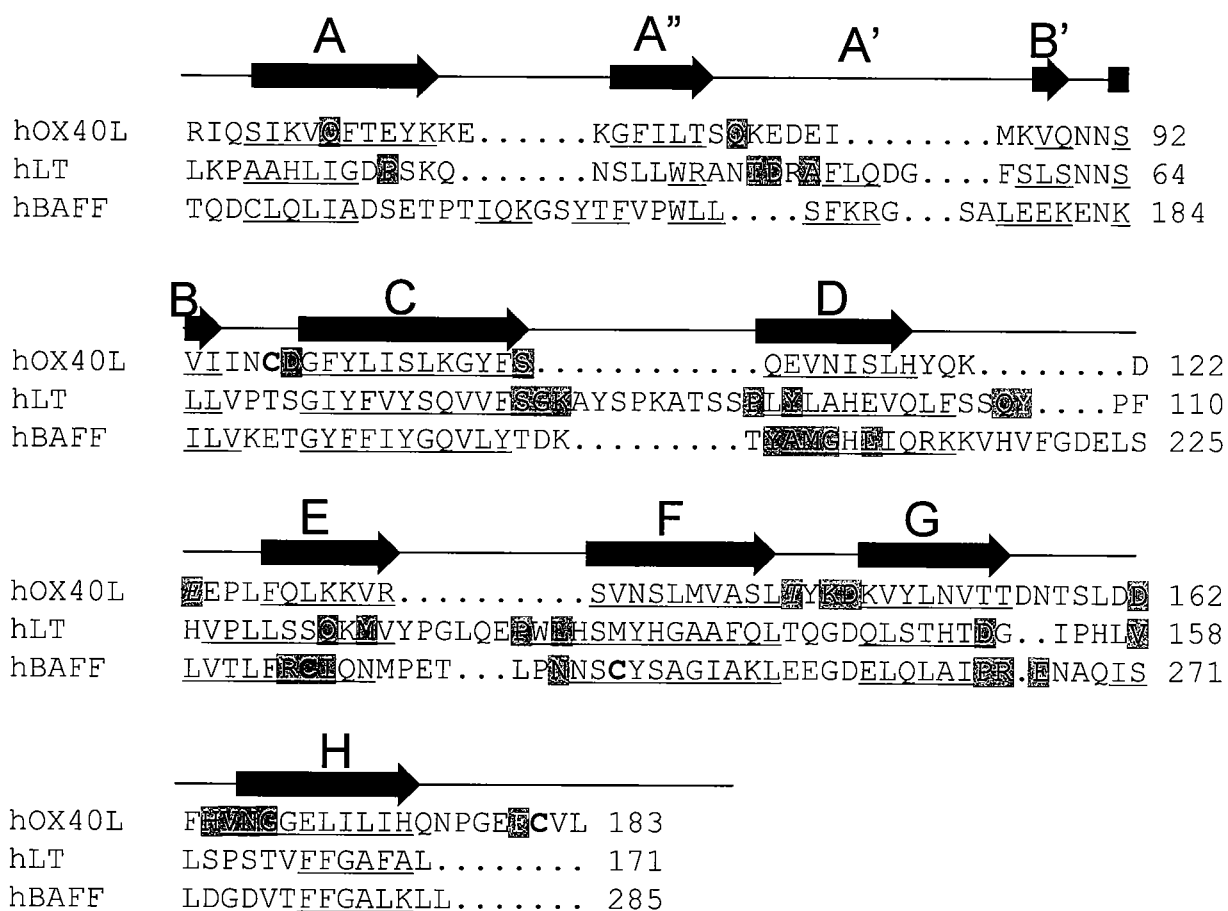
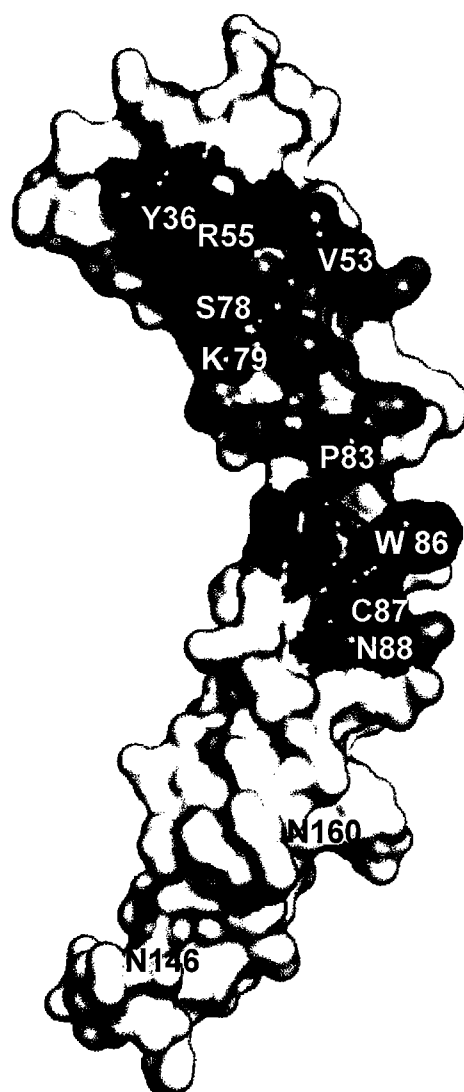
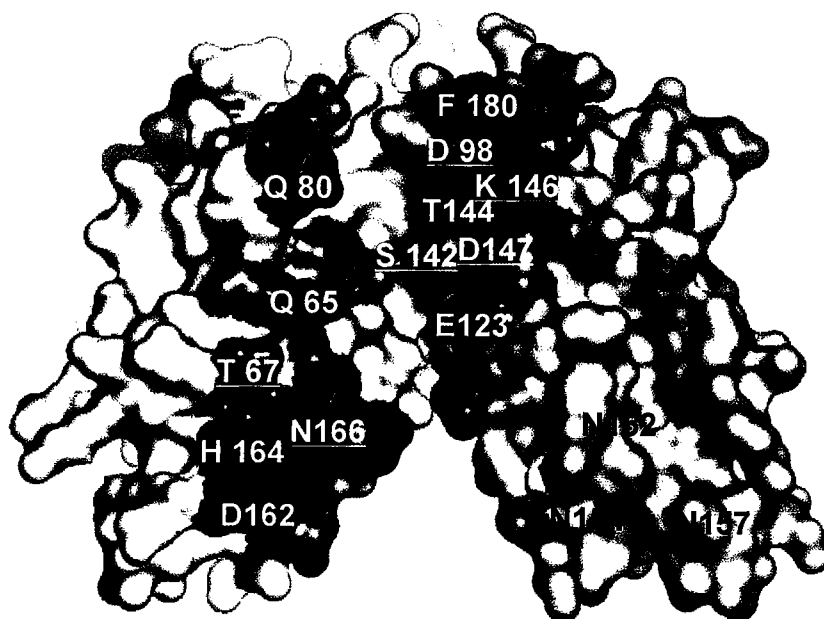


Fig 4

		A1	B1 or B2
a.			
hTNFR1_CRD3		CRKNQYRHYW...SENLFQCFNCSLCLNGT...VHLSCQEKQNTVC	
hOX40_CRD3		CRAG...TQPLDSYKPGVDCAPCPPGHFSPG...DNQACKPWTN...	
hGITR_CRDX		CPPGQ.GVQSQGKFSFGFQCIDCASGTFSGG...HEGHCKPWTD...	
hRANK_CRD3		CAPGL.GAQHPLQLNKDTVCKPCLAGYFSDAFSSTDKCRPWTN...	
hEDAR_CRD3		CLPGYYMLENRPRNIYGMVCYSCLLAPP.....NTKECVGATS...	
b.		A1 or A2	B1 or B2
hOX40_CRD2		CGPG.FYNDVV...SSK.PCKPCTWCNLAGSERKQLCTATQDTV	
hDR5_CRD2		CKYGQDYSTHW...NDLLFCLRCTRCDS...GEVELSPCTTTTRNTVC	
hTNFR1_CRD2		CESG.SFTASE...NHLRHCLSCSKCRKEMGQVEISSCTVDRDTC	
hEDAR_CRD2		CPAE.KFSKG....GYQICRRHKDCGFFRATVLTPGDMENDAEC	
hCD40_CRD2		CGES.EFLDTW...NRETHCHQHKYCDPNLGLRVQQKGTSETDTIC	
hRANK_CRD2		CGPD.EYLDSW...NEEDKCLLHKVCDTGKALVAVVAGNSTTPRR	
hDR6_CRD3		CPPG.MF.....QSNATCAPHTVCPV...GWGVRKKGTETEDVRC	
hTNFR2_CRD3		CRPG.WYCALSKQEGCRLCAPLRKCRP...GFGVARPGTETS DVVC	
hCD40_CRD3		CEEG.WHCT...SEACECVLHRSCSP...GFGVKQIATGVSDTIC	
hDCR3_CRD3		CRTG.FF.....AHAGFCLEHASCPP...GAGVIAPGTPSQNTQC	
hOPG_CRD3		CKEG.RY.....LEIEFCLKHRSCPP...GFGVVQAGTPERN TVC	
hCD40_CRD4		CPVG.FFSN...VSSAFEKCHPWTSCTET.KDLVVQQAGTNKTDVVC	
hDR6_CRD4		CARG.TFSD...VPSSVMCKKAYTDCLS.QNLVVIKPGTKETDNVC	
hLTb_CRD4		CKAG.HFQN...TSSPSARCQPHTRCEN.QGLVEAAPGTAQSDTTC	
hDCR3_CRD4		CPPG.TFSA...SSSSSEQCQPHRNCTAL.GLALNVPGSSSHDTLC	
hTNFR2_CRD4		CAPG.TFSN...TTSSTDICRPHQICN.....VVAIPGNASRDAVC	
hOPG_CRD4		CPDG.FFSN...ETSSKAPCRKHTNC SV.FGLLLTQKGNATHDNIC	

Figure 5
a.



b.

