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[54] CRYSTALLIZED N-TERMINAL DOMAIN OF INFLUENZA VIRUS MATRIX PROTEIN M1 AND METHOD OF DETERMINING AND USING SAME

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Related U.S. Application Data

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[51] Int. Cl.⁷ C12N 7/00; C12N 7/04;
C07K 14/11; C12Q 1/70

[52] U.S. Cl. 435/235.1; 435/236; 435/239;
435/5; 530/350; 378/74; 378/73; 424/204.1;
424/206.1

[58] Field of Search 530/350; 435/5,
435/235.1, 236-239; 378/73, 74; 424/204.1,
206.1

[56] References Cited

PUBLICATIONS

YE et al., Journal of Virology, 1987, vol. 61, No. 2, pp. 239-246, 1987.

Sha et al., Nature Structural Biology, Mar. 1997, vol. 4, No. 3, pp. 239-244, Mar. 1997.

Helenius, A., Unpacking the incoming influenza virus, Cell 69:577-578 (1992).

Zhirnov., O.P., Isolation of matrix protein M1 from influenza virus by acid-dependent extraction with nonionic detergent, Virology 186:324-330 (1992).

Martin, K. and Helenius, A., Transport of incoming influenza virus nucleocapsids into the nucleus, J. Virology 65:232-244 (1991).

Martin, K. and Helenius, A., Nuclear transport of influenza virus ribonucleoproteins: the viral matrix protein (m1) promotes export and inhibits import, Cell 67:117-130 (1991).

Zhirnov., O.P., Solubilization of matrix protein M1/M from virions occurs at different pH for Orthomyxo-and Paramyxoviruses, Virology 176:274-279 (1990).

Hankins et al., Monoclonal antibody analysis of influenza virus matrix protein epitopes involved in transcription inhibition, Virus Genes. 3(2):111-126, (1989).

Ye et al., Transcription-inhibition and RNA-binding domains of influenza A virus matrix protein mapped with anti-idiotypic antibodies and synthetic peptides, J. Virol. 63:3586-3594 (1989).

Wakefield, L. and Brownlee, G.G., RNA-binding properties of influenza A virus matrix protein M1, Nucleic Acids Res. 17:8569-8580 (1989).

Ye et al., Functional and antigenic domains of the matrix (M1) protein of influenza A virus, J. Virol. 61:239-246 (1987).

Winter, G. and Fields, S., The structure of the gene enclosing the nucleoprotein of human influenza virus A/PR/8/34, Virology 114:423-428 (1981).

Winter, G. and Fields, S., Cloning of influenza cDNA into M13: the sequence of the RNA segment encoding the A/PR/8/34 matrix protein, Nucleic Acids Res. 8:1965-1974 (1980).

Bucher et al., Incorporation of influenza virus M-protein into liposomes, J. Virol. 36:586-590 (1980).

Pons et al., Isolation and characterization of the ribonucleoprotein of influenza virus, Virology 39:250-259 (1969).

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[57] ABSTRACT

The matrix protein, M1, of influenza virus strain A/PR/8/34 has been purified from virions and crystallized. The crystals consist of a stable fragment (18 Kd) of the M1 protein. X-ray diffraction studies indicated that the crystals have a space group of P3₁21 or P3₂21. Vm calculations showed that there are two monomers in an asymmetric unit. A crystallized N-terminal domain of M1, wherein the N-terminal domain of M1 is crystallized such that the three dimensional structure of the crystallized N-terminal domain of M1 can be determined to a resolution of about 2.1 Å or better, and wherein the three dimensional structure of the uncrystallized N-terminal domain of M1 cannot be determined to a resolution of about 2.1 Å or better. A method of purifying M1 and a method of crystallizing M1. A method of using the three-dimensional crystal structure of M1 to screen for antiviral, influenza virus treating or preventing compounds. A method of using the three-dimensional crystal structure of M1 to screen for improved binding to or inhibition of influenza virus M1. The use of the three-dimensional crystal structure of the M1 protein of influenza virus in the manufacture of an inhibitor of influenza virus M1. The use of the three-dimensional crystal structure of the M1 protein of influenza virus in the screening of candidates for inhibition of influenza virus M1.

18 Claims, 8 Drawing Sheets

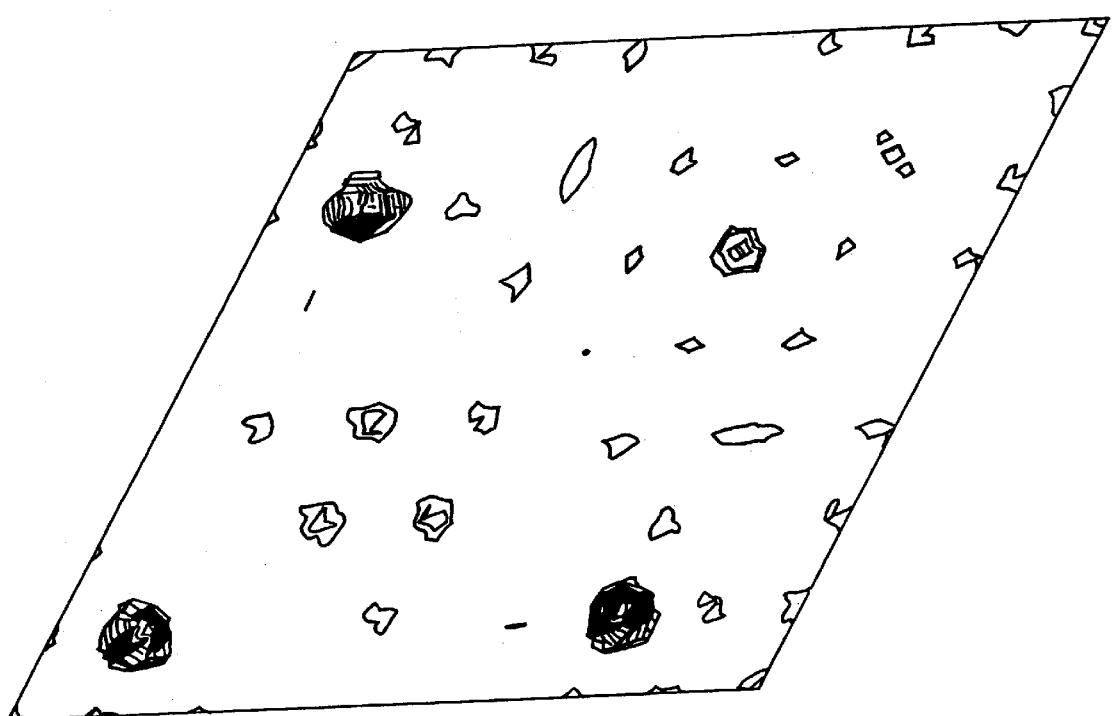


FIG. 1a

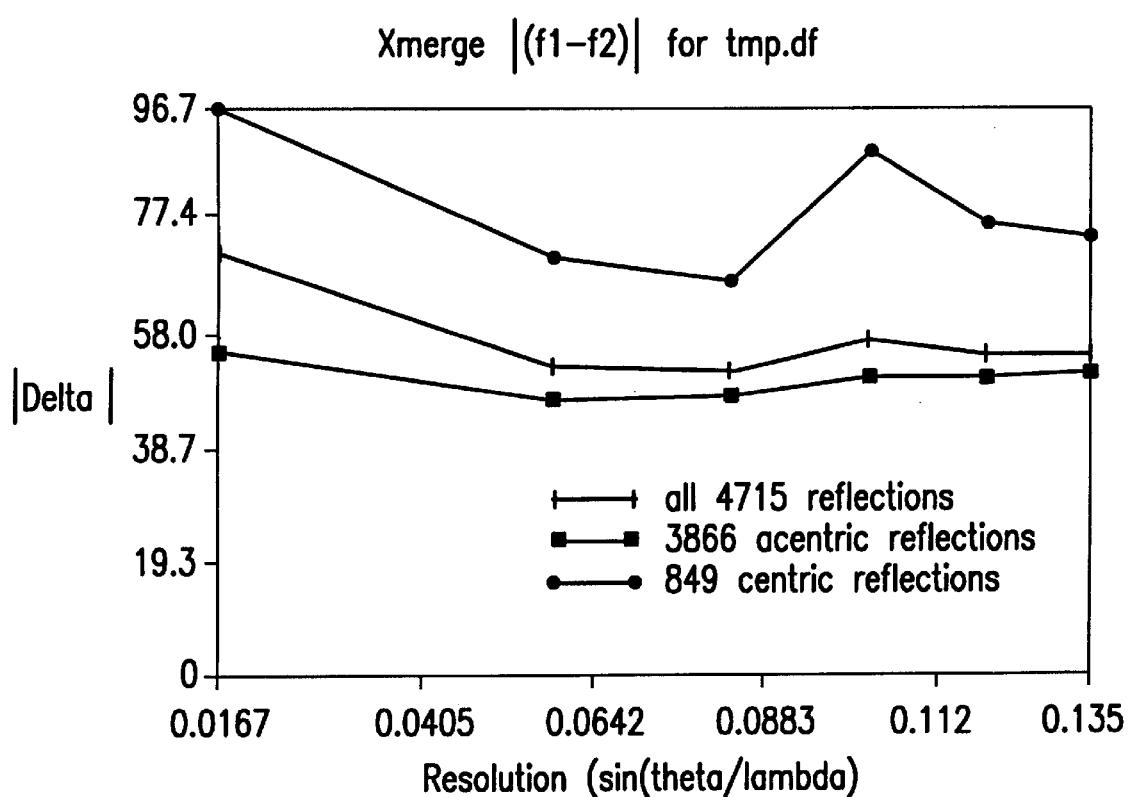


FIG.1b

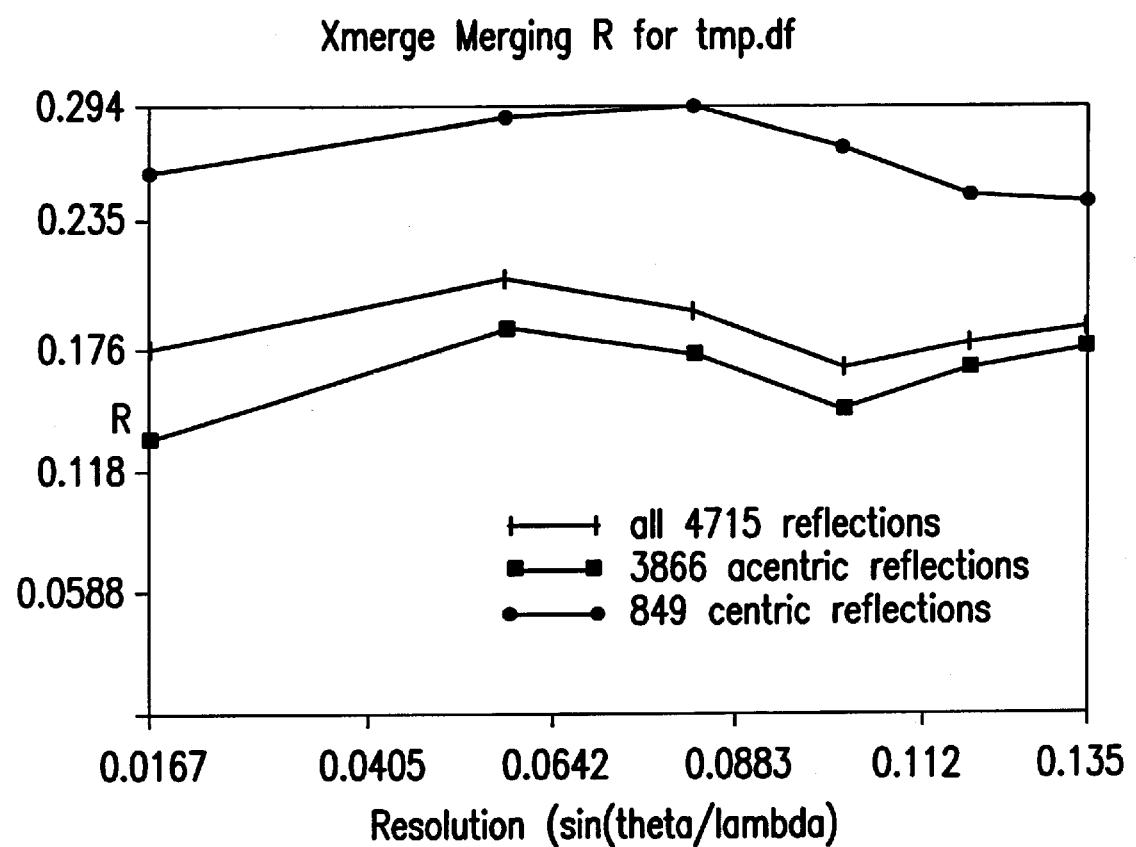


FIG. 1c

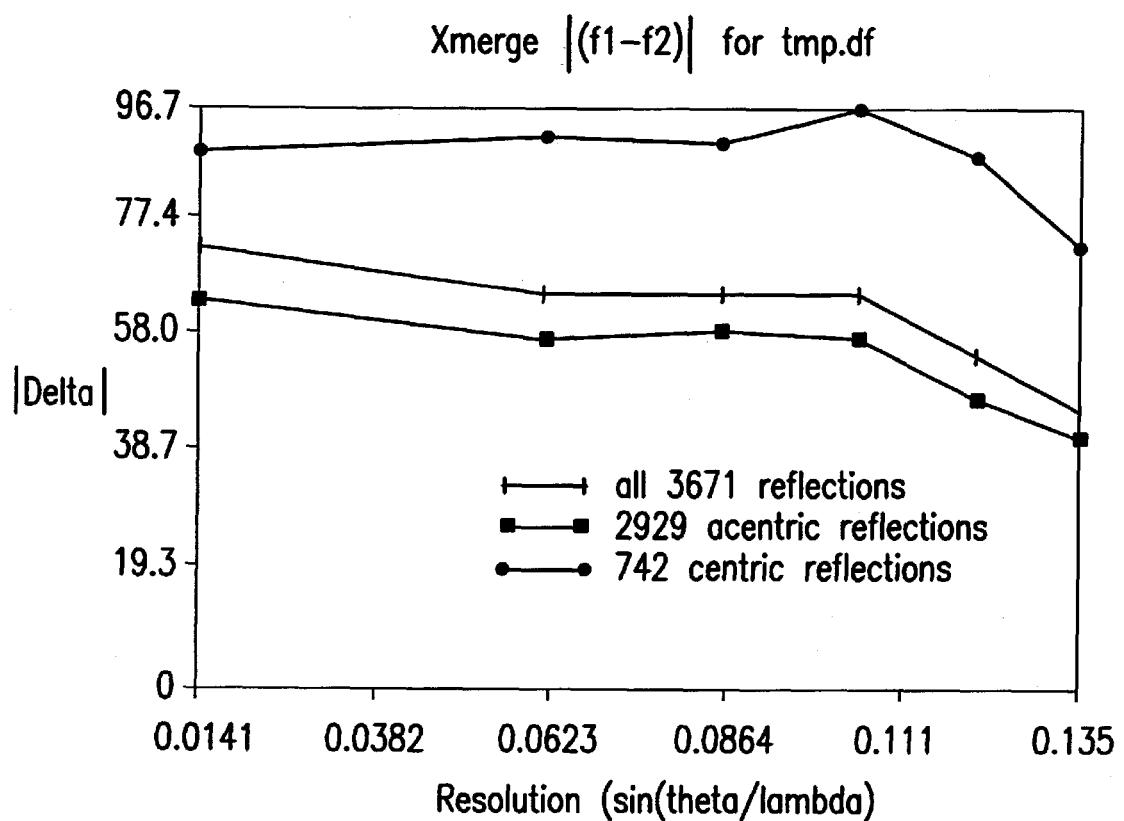


FIG.2a

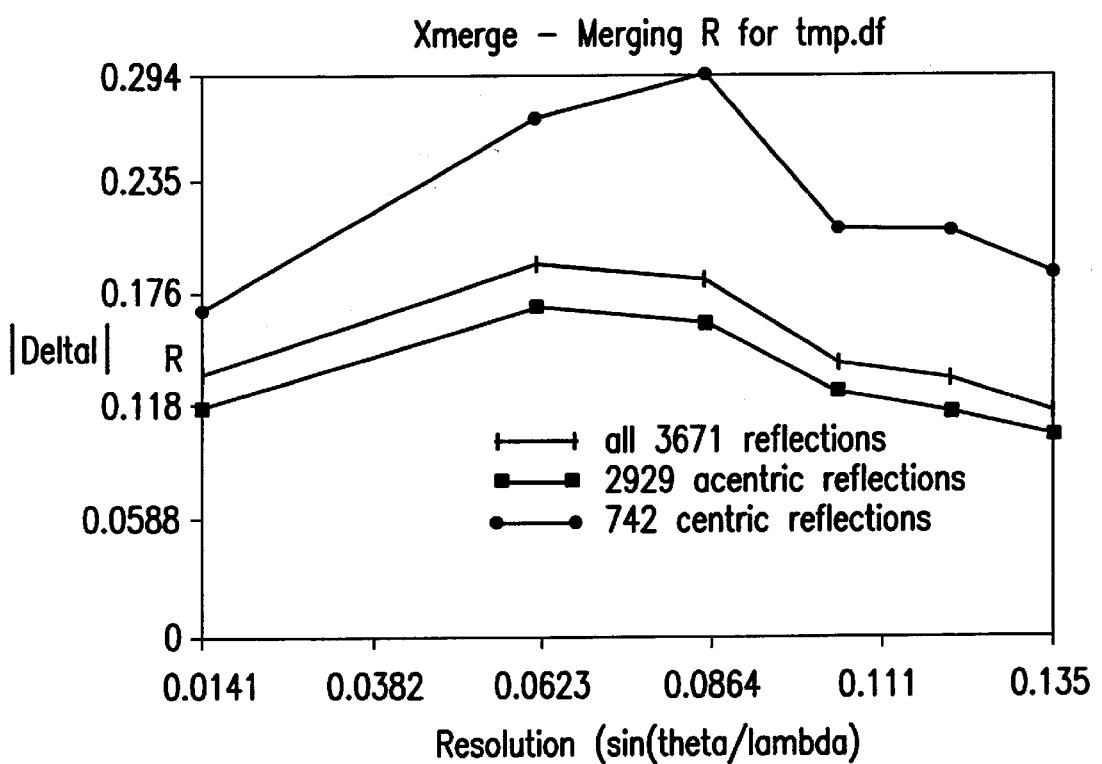


FIG.2b

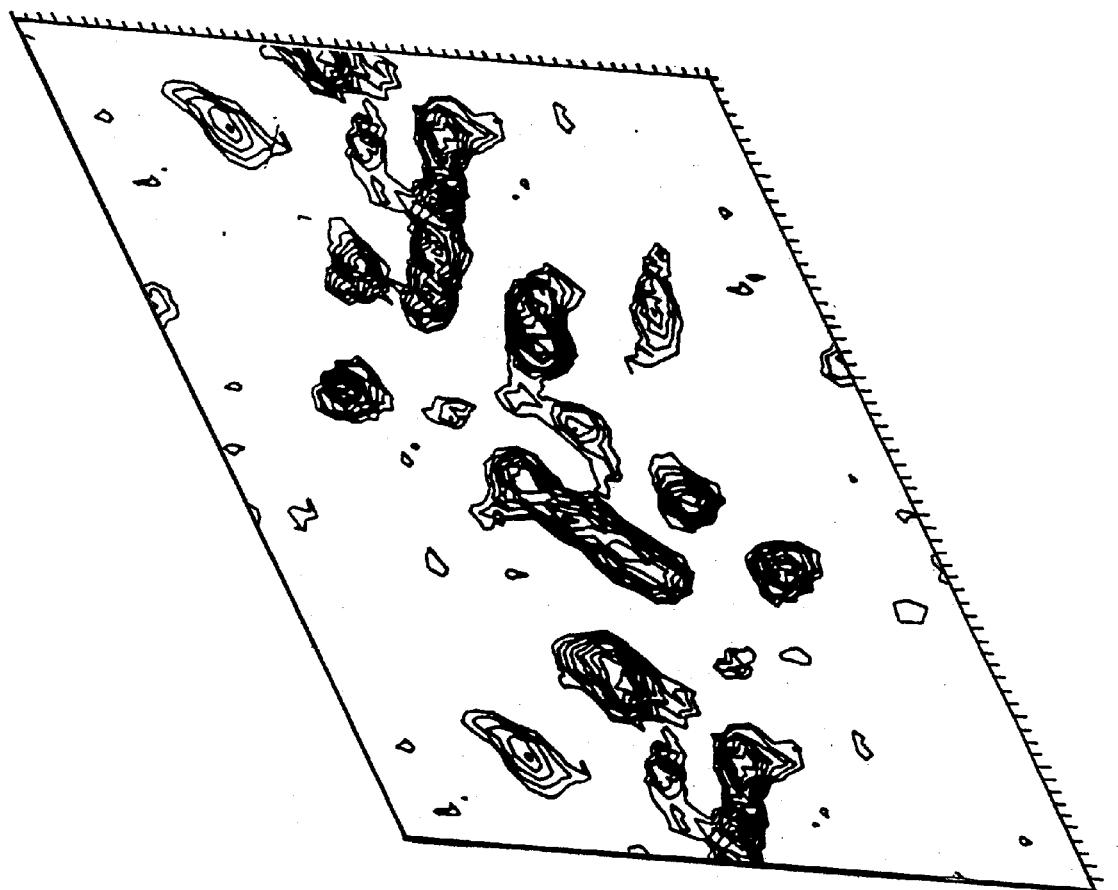


FIG. 2c



FIG. 2d

Res. limits (Å)	I/sigma (I)	Rsymm %	% of observations	Observations/ reflections
25.00	3.78	44.1	2.7	95.4
3.78	3.00	42.4	3.9	96.0
3.00	2.62	33.0	5.4	95.9
2.62	2.38	24.6	7.8	96.0
2.38	2.21	18.5	10.2	95.9
2.21	2.08	9.1	17.5	88.6
All	33.7	4.6	94.7	2.9
Space group: P3 ₁ 21, a=b=67.17Å, c=135.30Å				

FIG. 3

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**CRYSTALLIZED N-TERMINAL DOMAIN OF
INFLUENZA VIRUS MATRIX PROTEIN M1
AND METHOD OF DETERMINING AND
USING SAME**

BACKGROUND OF THE INVENTION

This application claims benefit, pursuant to 35 U.S.C. § 119, of applicants' provisional U.S. Ser. No. 60/023,564, filed Aug. 7, 1996, the contents of which are hereby incorporated by reference.

This application was supported, in part, by a grant from NASA (NAGW-819).

FIELD OF THE INVENTION

The present invention relates to the field of crystallography and, particularly, to the characterization of the structure of matrix protein M1 of influenza virus neuraminidase and, specifically, the determination of the crystal structure of the N-terminal domain of M1, the domain itself, the crystallized domain, methods of purifying and crystallographically determining the three-dimensional structure of that domain, and methods of using the crystal structure of N-terminal domain of M1 to design pharmaceuticals.

BACKGROUND OF THE INVENTION

Influenza virus is an enveloped virus which contains eight separate segments of negative-stranded RNA genome. There are two spike glycoproteins on the surface of the viral membrane envelope, the receptor binding hemagglutinin (HA), and the neuraminidase (NA). The core ribonucleoprotein (RNP) encapsulated in the viral membrane envelope is composed of an RNA polymerase and RNA-binding nucleoproteins (NP) (1). The interaction of RNPs with the membrane is mediated by the matrix protein M1 (252 amino acids, Mr=27 kd), which are tightly associated with the RNP cores while interacting with the cytoplasmic tails of the spike glycoprotein and the viral membrane (2). Through the binding of hydrophobic domains to the virion lipid envelope, M1 maintains the structural integrity of the virus particle (3,4). On the other hand, the interaction of M1 with RNP cores is mostly electrostatic at neutral pH (5,6). The M1 can easily be dissociated from the RNP cores by low pH treatment (7,8).

In addition to packaging the RNP cores during virion assembly, M1 also directs the transportation of RNPs into or out of the nucleus (9,10). Upon entry of the virus into the new host cell, M1 is dissociated from RNPs as the result of reducing pH in the fusion endosome, allowing the RNPs to enter the nucleus. When progeny viral RNPs are produced, newly synthesized M1 escort the RNPs out of nucleus and target them to the assembly site on the cellular membrane where HA and NA are located. It is therefore highly desirable to provide a method of deducing the crystal structure of M1 and of providing a method of using this structure provide antiviral candidates and M1 inhibitors.

SUMMARY OF THE INVENTION

The present invention provides a crystallized N-terminal domain of M1, wherein the N-terminal domain of M1 is crystallized such that the three dimensional structure of the crystallized N-terminal domain of M1 can be determined to a resolution of 2.1 Å or better, and wherein the three-dimensional structure of the uncrystallized N-terminal domain of M1 cannot be determined to a resolution of 2.1 Å or better.

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In an alternate embodiment, the present invention provides a method of extracting the M1 protein of influenza virus comprising stripping the membrane proteins from influenza virus, removing the stripped membrane proteins, thereby leaving the M1-RNP complex, and releasing M1 from the M1-RNP complex by suspending the complex in a solution comprising NaH₂PO₄, Benzamidine, and NaN₃, at a pH of from 3 to 5, preferably about 4.0. In a further embodiment, the released M1 is purified.

In yet another embodiment, the present invention provides a method of extracting the N-terminal domain of the M1 protein of influenza virus comprising stripping the membrane proteins from influenza virus, removing the stripped membrane proteins, thereby leaving the M1-RNP complex, releasing M1 from the M1-RNP complex by suspending the complex in a solution comprising NaH₂PO₄, Benzamidine, and NaN₃, at a pH of from 3.0 to 5.0, more preferably about 4.0, purifying the released M1, concentrating the purified M1 to a concentration of from about 3 to about 20 mg/ml, more preferably from about 4 to about 10 mg/ml, and most preferably about 5 mg/ml and after a period of time sufficient for the formation of an 18 kd protein fragment corresponding to the N-terminal domain of M1, collecting the 18 kd polypeptide corresponding to the N-terminal domain of M1. In a further embodiment, the method also includes crystallizing the 18 kd polypeptide corresponding to the N-terminal domain of M1 in hanging drops (which is one crystal formation method, see elsewhere herein for others) using the vapor diffusion method to a resolution of less than about 2.1 Å, wherein the N-terminal domain of M1 is present at a concentration of from 3 to 20 mg/ml, preferably 5 mg/ml, and the crystallization takes place at 4 to 32° C. over 20% PEG 3350, to thereby obtain crystals of space group P3₂1 or P3₁21 with approximate a=68.0 Å and approximate c=136.57 Å.

In yet another embodiment, the present invention provides a method for determining the three dimensional structure of the crystallized N-terminal domain of the M1 protein of influenza virus to a resolution of 2.1 Å or better comprising the steps of crystallizing the N-terminal domain of M1 in hanging drops using the vapor diffusion method to a resolution of less than about 2.1 Å, wherein the N-terminal domain of M1 is present at a concentration of about 3 to about 20 mg/ml and the crystallization takes place at from about 4 to about 32° C. over 20% PEG 3350, to thereby obtain crystals of space group P3₂1 or P3₁21 with approximate a=68.0 Å and approximate c=136.57 Å, and then analyzing the N-terminal domain of M1 to determine the three-dimensional structure of the crystallized N-terminal domain of M1. In a further embodiment, the invention provides the crystallized N-terminal domain of M1 produced by this process.

In yet another embodiment, the present invention provides a method for designing an antiviral compound for the prevention or treatment of influenza virus infection, comprising evaluating the three dimensional structure of the crystallized N-terminal domain of M1 produced by crystallizing a purified N-terminal domain of M1 in hanging drops using the vapor diffusion method to a resolution of less than about 2.1 Å, wherein the N-terminal domain of M1 is present at a concentration of about 3 to about 20 mg/ml and the crystallization takes place at from about 4 to about 32° C. over 20% PEG 3350, to thereby obtain crystals of space group P3₂1 or P3₁21 with approximate a=68.0 Å and approximate c=136.57 Å, and synthesizing an antiviral compound based on the three-dimensional crystal structure of the crystallized N-terminal domain of M1, wherein the

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antiviral compound can be screened for having improved binding to M1.

In yet another embodiment, the present invention provides a purified N-terminal domain of M1. In a further embodiment, the present invention provides this purified N-terminal domain of M1, comprising the amino acid sequence of SEQ. ID. NO. 1 (see below). In one embodiment, "N-terminal domain" means the amino acid sequence of SEQ. ID. NO. 1. One of skill in the art would recognize that various amino acid substitutions could be made to this polypeptide. Such modifications, so long as the basic and novel utility of the present invention is not disturbed, are understood to be within the scope of the present invention. For instance, a polypeptide could be constructed containing the first 150 amino acids, from position 1 (perhaps by cleavage of some of the amino acids and addition at the N-terminal end). Such a polypeptide is intended to be within the scope of the present invention. To the extent that the crystal structures of such analogous polypeptides are similar to the structure set forth herein, such structures fall within the scope of the present invention.

In yet another embodiment, the present invention provides a method for designing a candidate compound for screening for improved binding to or inhibition of influenza virus M1, comprising evaluating the three dimensional structure of the crystallized N-terminal domain of M1, and synthesizing a candidate binding compound based on the three-dimensional crystal structure of the crystallized N-terminal domain of M1 for improved binding to M1.

In a further embodiment, the present invention provides the three-dimensional crystal structure of influenza virus protein M1 as set forth elsewhere herein. In a further embodiment, the present invention provides a crystallized polypeptide having that three-dimensional crystal structure.

In yet another embodiment, the invention provides a method for designing a candidate compound for screening as an antiviral for the prevention or treatment of influenza virus infection, comprising evaluating the three-dimensional crystal structure set forth elsewhere herein, and synthesizing a candidate compound based on the three-dimensional crystal structure. Moreover, the present invention provides for the use of the three-dimensional crystal structure as set forth herein for screening candidate compounds for inhibition of influenza virus M1.

In a further embodiment, the present invention also provides for the use of the N-terminal domain of M1 for screening candidate compounds for inhibition of influenza virus M1.

Finally, the present invention provides a crystallized N-terminal domain of M1.

BRIEF DESCRIPTION OF THE DRAWINGS

FIG. 1a shows the Harker section (Z=1/3) of the difference Pattern of Os derivative of M1 crystals.

FIG. 1b shows the structure factor amplitude difference between native and Os derivative data sets versus resolution. From top to bottom, the curves are for all reflections, acentric reflections and centric reflections, respectively.

FIG. 1c shows the merging R-factor between native and Os derivative data sets versus resolution. From top to bottom, the curves are for all reflections, acentric reflections and centric reflections, respectively.

FIG. 2a shows the structure factor amplitude difference between native and Pt derivative data sets versus resolution. From top to bottom, the curves are for all reflections, acentric reflections and centric reflections, respectively.

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FIG. 2b shows the merging R-factor between native and Pt derivative data sets versus resolution. From top to bottom, the curves are for all reflections, acentric reflections and centric reflections, respectively.

FIG. 2c shows a section of solvent flattened map (FOM=0.89) at 5 Å resolution.

FIG. 2d shows a slice of electron density map at 3.5 Å resolution corresponding to an alpha-helix.

FIG. 3 shows atomic coordinates of the three dimensional crystal structure of influenza virus protein M1.

DETAILED DESCRIPTION OF THE PREFERRED EMBODIMENTS

The present invention may be understood more readily by reference to the following detailed description of preferred embodiments of the invention and the Figures.

Before the present methods and structures are disclosed and described, it is to be understood that the terminology used herein is for the purpose of describing particular embodiments only and is not intended to be limiting. It must be noted that, as used in the specification and the appended claims, the singular forms "a," "an" and "the" include plural referents unless the context clearly dictates otherwise.

Throughout this application, where publications are referenced, the disclosures of these publications in their entireties are hereby incorporated by reference into this application in order to more fully describe the state of the art to which this invention pertains. Publications have been referenced herein by placing the number in parentheses.

These publications are listed according to their respective numbers in the "Reference" section hereinbelow.

The present invention therefore provides a crystallized N-terminal domain of M1, wherein the N-terminal domain of M1 is crystallized such that the three dimensional structure of the crystallized N-terminal domain of M1 can be determined to a resolution of 2.1 Å or better, and wherein the three dimensional structure of the uncrystallized N-terminal domain of M1 cannot be determined to a resolution of 2.1 Å or better.

In a further embodiment, the present invention provides a method of extracting the M1 protein of influenza virus comprising stripping the membrane proteins from influenza virus, removing the stripped membrane proteins, thereby leaving the M1-RNP complex, and releasing M1 from the M1-RNP complex by suspending the complex in a solution comprising NaH₂PO₄, Benzamidine, and NaN₃. In a preferred embodiment, the solution has a pH of from about 3 to about 5, more preferably about 4.0. In a further embodiment, this method is extended to include purifying the released M1.

In yet another embodiment, the present invention provides a method of extracting the N-terminal domain of the M1 protein of influenza virus comprising stripping the membrane proteins from influenza virus, removing the stripped membrane proteins, thereby leaving the M1-RNP complex, releasing M1 from the M1-RNP complex by suspending the complex in a solution comprising NaH₂PO₄, Benzamidine, and NaN₃, purifying the released M1, concentrating the purified M1 to a concentration of from about 3 to about 20 mg/ml, more preferably from about 4 to about 10 mg/ml, and most preferably about 5 mg/ml, and after a period of time sufficient for the formation of an 18 kd protein fragment corresponding to the N-terminal domain of M1, collecting the 18 kd polypeptide corresponding to the N-terminal domain of M1. In a further embodiment, the time period is approximately fourteen days. In yet another embodiment, this method further comprises crystallizing the 18 kd polypeptide corresponding to the N-terminal domain

of M1 to a resolution of less than about 2.1 Å, wherein the N-terminal domain of M1 is present at a concentration of about 3 to about 20 mg/ml, more preferably from about 4 to about 10 mg/ml and most preferably about 5 mg/ml, and the crystallization takes place at from 4 to 32° C., more preferably from 10 to 26° C., even more preferably at about 16 to about 24° C., and even more preferably 20° C., to thereby obtain crystals of space group P3₂1 or P3₁21. The crystals may have an approximate *a*=68.0 Å and approximate *c*=136.57 Å. The crystallization, in one embodiment, may occur using hanging drops and the vapor diffusion method. Alternatively, other crystallization methods may be used. For instance, a temperature variation may be used to produce crystals, or crystallization in space may be used to improve resolution. The crystallization, in another embodiment, may occur over 20% PEG 3350. In addition, other chemicals can be used in the place of PEG3350. For instance, organic chemicals (e.g. isopropanol), inorganic chemicals (e.g. (NH₄)₂SO₄, NaH₂PO₄), and other molecular weight PEG (from MPD to PEG20,000) may be used.

In yet another embodiment, the present invention provides a method for determining the three dimensional structure of the crystallized N-terminal domain of the M1 protein of influenza virus to a resolution of 2.1 Å or better comprising the steps of crystallizing the N-terminal domain of M1 to a resolution of less than about 2.1 Å, wherein the N-terminal domain of M1 is present at a concentration of about 3 to about 20 mg/ml, more preferably about 4 to about 10 mg/ml, even more preferably about 5 mg/ml and the crystallization takes place at from about 4 to about 32° C., more preferably from 10 to 26° C., even more preferably at about 16 to about 24° C., and even more preferably 20° C., to thereby obtain crystals of space group P3₂1 or P3₁21, and then analyzing the N-terminal domain of M1 to determine the three dimensional structure of the crystallized N-terminal domain of M1. In a preferred embodiment, the analyzing is by x-ray diffraction. The crystallization, in one embodiment, may occur over 20% PEG 3350. The crystallization, in one embodiment, may occur using hanging drops and the vapor diffusion method. Alternatively, other crystallization methods may be used. For instance, a temperature variation method may be used to produce crystals, or crystallization in outer space may be used to improve resolution.

In yet another embodiment, the present invention provides a crystallized N-terminal domain of M1 produced by the process described above.

In yet another embodiment, the present invention provides a method for designing an antiviral compound for the prevention or treatment of influenza virus infection, comprising evaluating the three dimensional structure of the crystallized N-terminal domain of M1 produced by crystallizing a purified N-terminal domain of M1 to a resolution of less than about 2.1 Å, wherein the N-terminal domain of M1 is present at a concentration of about 3 to about 20 mg/ml, more preferably about 4 to about 10 mg/ml, even more preferably about 5 mg/ml and the crystallization takes place at from about 4 to about 32° C., more preferably from 10 to 26° C., even more preferably at about 16 to about 24° C., and even more preferably 20° C., to thereby obtain crystals of space group P3₂1 or P3₁21, and synthesizing an antiviral compound based on the three-dimensional crystal structure of the crystallized N-terminal domain of M1, wherein the antiviral compound can be screened for having improved binding to M1. In a further embodiment, the antiviral compound is a peptide or polypeptide. The crystallization, in one embodiment, may occur using hanging drops and the vapor diffusion method. Alternatively, other crystallization methods may be used. For instance, a temperature variation may be used to produce crystals, or crystallization in space may be used to improve resolution.

In yet another embodiment, the present invention provides a purified N-terminal domain of M1. In a further embodiment, the invention provides that purified N-terminal domain of M1, comprising the amino acid sequence of SEQ. ID. NO. 1.

In yet another embodiment, the present invention provides a method for designing a candidate compound for screening for improved binding to or inhibition of influenza virus M1, comprising evaluating the three dimensional structure of the crystallized N-terminal domain of M1, and synthesizing a candidate binding compound based on the three-dimensional crystal structure of the crystallized N-terminal domain of M1 for improved binding to M1. In a further embodiment, the candidate compound is a peptide or polypeptide.

In yet another embodiment, the present invention provides the three-dimensional crystal structure of influenza virus protein M1 as set forth in the following table (see also FIG. 3):

CRYST1	67.170	67.170	135.300	90.00	90.00	120.00	
SCALE1	0.014888	0.008595	0.000000	0.000000			
SCALE2	0.000000	0.017194	0.000000	0.000000			
SCALE3	0.000000	0.000000	0.007391	0.000000			
ATOM 1	CB	SER	2	26.695	28.292	28.613	1.00 22.72
ATOM 2	O	SER	2	26.267	29.344	29.471	1.00 24.24
ATOM 3	HG	SER	2	25.482	29.760	29.123	1.00 0.00
ATOM 4	C	SER	2	24.953	27.000	29.814	1.00 23.15
ATOM 5	O	SER	2	23.851	27.524	30.005	1.00 19.52
ATOM 6	HT1	SER	2	24.182	27.440	27.702	1.00 0.00
ATOM 7	HT2	SER	2	23.938	26.815	27.350	1.00 0.00
ATOM 8	N	SER	2	24.659	27.548	27.417	1.00 23.47
ATOM 9	HT3	SER	2	25.138	27.701	26.518	1.00 0.00
ATOM 10	CA	SER	2	25.657	27.183	28.472	1.00 23.46
ATOM 11	N	LEU	3	25.592	26.298	30.751	1.00 20.35
ATOM 12	H	LEU	3	26.490	25.933	30.576	1.00 0.00
ATOM 13	CA	LEU	3	24.979	26.088	32.062	1.00 17.46
ATOM 14	CB	LEU	3	25.781	25.075	32.898	1.00 19.31
ATOM 15	CG	LEU	3	25.374	24.879	34.379	1.00 19.41
ATOM 16	CD1	LEU	3	23.898	24.508	34.496	1.00 11.43
ATOM 17	CD2	LEU	3	26.260	23.802	35.023	1.00 18.23
ATOM 18	C	LEU	3	24.896	27.407	32.816	1.00 16.36
ATOM 19	O	LEU	3	23.860	27.768	33.371	1.00 15.18
ATOM 20	N	LEU	4	25.987	28.152	32.772	1.00 14.87
ATOM 21	H	LEU	4	26.761	27.849	32.251	1.00 0.00
ATOM 22	CA	LEU	4	26.062	29.401	33.484	1.00 15.53
ATOM 23	CB	LEU	4	27.461	29.999	33.343	1.00 15.39
ATOM 24	CG	LEU	4	28.520	29.077	33.971	1.00 13.82
ATOM 25	CD1	LEU	4	29.923	29.582	33.704	1.00 11.19
ATOM 26	CD2	LEU	4	28.271	28.971	35.466	1.00 17.28
ATOM 27	C	LEU	4	24.955	30.378	33.123	1.00 18.38
ATOM 28	O	LEU	4	24.512	31.149	33.973	1.00 18.56
ATOM 29	N	THR	5	24.466	30.323	31.890	1.00 19.71
ATOM 30	H	THR	5	24.836	26.692	31.523	1.00 0.00
ATOM 31	CA	THR	5	23.384	31.217	31.509	1.00 22.15
ATOM 32	CB	THR	5	23.228	31.339	29.983	1.00 26.89
ATOM 33	OG1	THR	5	22.981	30.054	29.406	1.00 34.75
ATOM 34	HG1	THR	5	23.680	29.463	29.624	1.00 0.00
ATOM 35	CG2	THR	5	24.488	31.891	29.383	1.00 23.91
ATOM 36	C	THR	5	22.084	30.763	32.179	1.00 20.11
ATOM 37	O	THR	5	21.277	31.602	32.588	1.00 21.65
ATOM 38	N	GLU	6	21.914	29.444	32.337	1.00 22.06
ATOM 39	H	GLU	6	22.587	28.831	31.988	1.00 0.00
ATOM 40	CA	GLU	6	20.736	28.883	33.013	1.00 17.17
ATOM 41	CB	GLU	6	20.752	27.364	32.989	1.00 19.28
ATOM 42	CG	GLU	6	20.517	26.705	31.662	1.00 23.44
ATOM 43	CD	GLU	6	20.397	25.192	31.809	1.00 26.59
ATOM 44	OE1	GLU	6	19.417	24.719	32.428	1.00 27.73
ATOM 45	OE2	GLU	6	21.300	24.474	31.333	1.00 30.79
ATOM 46	C	GLU	6	20.802	29.326	24.473	1.00 18.78

-continued

ATOM 47 O GLU 6 19.805 27.786 35.043 1.00 18.66	ATOM 119 CG1 ILE 14 16.909 35.761 43.609 1.00 19.30
ATOM 48 N VAL 7 21.981 29.160 35.077 1.00 17.63	ATOM 120 CD1 ILE 14 17.602 35.203 44.827 1.00 14.33
ATOM 49 H VAL 7 22.719 28.754 34.576 1.00 0.00	ATOM 121 C ILE 14 15.019 38.078 42.794 1.00 15.86
ATOM 50 CA VAL 7 22.207 29.570 36.463 1.00 15.32	ATOM 122 O ILE 14 14.594 38.629 43.799 1.00 15.25
ATOM 51 CB VAL 7 23.703 29.406 36.877 1.00 12.34	ATOM 123 N ILE 15 15.729 38.734 41.883 1.00 21.19
ATOM 52 CG1 VAL 7 23.963 30.032 38.218 1.00 10.28	ATOM 124 H ILE 15 16.019 38.276 41.067 1.00 0.00
ATOM 53 CG2 VAL 7 24.076 27.957 36.927 1.00 10.34	ATOM 125 CA ILE 15 16.050 40.154 42.060 1.00 23.81
ATOM 54 C VAL 7 21.809 31.041 36.593 1.00 17.63	ATOM 126 CB ILE 15 17.309 40.584 41.266 1.00 24.86
ATOM 55 O VAL 7 21.111 31.415 37.534 1.00 17.77	ATOM 127 CG2 ILE 15 17.785 41.967 41.749 1.00 26.57
ATOM 56 N GLU 8 22.200 31.856 35.611 1.00 16.16	ATOM 128 CG1 ILE 15 18.437 39.554 41.400 1.00 25.02
ATOM 57 H GLU 8 22.713 31.489 34.861 1.00 0.00	ATOM 129 CD1 ILE 15 18.931 39.359 42.800 1.00 31.18
ATOM 58 CA GLU 8 21.882 33.279 35.635 1.00 17.04	ATOM 130 C ILE 15 14.907 41.038 41.559 1.00 28.51
ATOM 59 CB GLU 8 22.546 34.032 34.483 1.00 18.28	ATOM 131 O ILE 15 14.289 40.739 40.542 1.00 30.32
ATOM 60 CG GLU 8 22.355 35.540 34.622 1.00 18.53	ATOM 132 N PRO 16 14.567 42.104 42.301 1.00 31.91
ATOM 61 CD GLU 8 22.846 36.345 33.442 1.00 21.27	ATOM 133 CD PRO 16 14.958 42.504 43.666 1.00 33.48
ATOM 62 OE1 GLU 8 23.311 35.767 32.450 1.00 19.23	ATOM 134 CA PRO 16 13.477 42.946 41.793 1.00 34.20
ATOM 63 OE2 GLU 8 22.771 37.583 33.512 1.00 28.23	ATOM 135 CB PRO 16 13.204 43.898 42.968 1.00 32.63
ATOM 64 C GLU 8 20.395 33.599 35.633 1.00 13.86	ATOM 136 CG PRO 16 14.516 43.939 43.715 1.00 35.14
ATOM 65 O GLU 8 19.967 34.512 36.320 1.00 14.68	ATOM 137 C PRO 16 13.924 43.689 40.519 1.00 32.66
ATOM 66 N THR 9 19.611 32.876 34.851 1.00 13.26	ATOM 138 O PRO 16 15.072 44.139 40.425 1.00 30.48
ATOM 67 H THR 9 19.988 32.164 34.294 1.00 0.00	ATOM 139 N SER 17 13.035 43.769 39.529 1.00 34.68
ATOM 68 CA THR 9 18.179 33.148 34.813 1.00 19.26	ATOM 140 H SER 17 12.158 43.369 39.649 1.00 0.00
ATOM 69 CB THR 9 17.437 32.302 33.713 1.00 16.47	ATOM 141 CA SER 17 13.341 44.449 38.264 1.00 37.99
ATOM 70 OG1 THR 9 17.316 30.939 34.137 1.00 30.32	ATOM 142 CB SER 17 12.143 44.377 37.311 1.00 39.60
ATOM 71 HG1 THR 9 18.193 30.560 34.274 1.00 0.00	ATOM 143 OG SER 17 11.717 43.032 37.120 1.00 47.68
ATOM 72 CG2 THR 9 18.219 32.307 32.421 1.00 11.87	ATOM 144 HG SER 17 11.462 42.649 37.957 1.00 0.00
ATOM 73 C THR 9 17.584 32.895 32.216 1.00 19.01	ATOM 145 C SER 17 13.737 45.908 38.498 1.00 38.06
ATOM 74 O THR 9 16.838 33.731 36.742 1.00 19.66	ATOM 146 O SER 17 13.101 46.623 39.273 1.00 38.78
ATOM 75 N TYR 10 17.948 31.768 36.831 1.00 17.18	ATOM 147 N GLY 18 14.807 46.339 37.842 1.00 38.35
ATOM 76 H TYR 10 18.569 31.150 36.382 1.00 0.00	ATOM 148 H GLY 18 15.299 45.731 37.253 1.00 0.00
ATOM 77 CA TYR 10 17.460 31.438 38.167 1.00 15.38	ATOM 149 CA GLY 18 15.271 47.701 38.006 1.00 34.14
ATOM 78 CB TYR 10 17.984 30.087 38.617 1.00 15.57	ATOM 150 C GLY 18 16.717 47.805 37.585 1.00 34.09
ATOM 79 CG TYR 10 17.205 28.941 38.055 1.00 13.50	ATOM 151 O GLY 18 17.293 46.822 37.117 1.00 36.02
ATOM 80 CD1 TYR 10 17.708 28.193 37.003 1.00 11.74	ATOM 152 N PRO 19 17.347 48.969 37.789 1.00 34.46
ATOM 81 CE1 TYR 10 16.972 27.154 36.440 1.00 16.51	ATOM 153 CD PRO 19 16.738 50.089 38.528 1.00 35.80
ATOM 82 CD2 TYR 10 15.943 28.626 38.552 1.00 17.02	ATOM 154 CA PRO 19 18.743 49.266 37.447 1.00 33.74
ATOM 83 CE2 TYR 10 15.193 27.589 38.004 1.00 19.98	ATOM 155 CB PRO 19 18.889 50.724 37.879 1.00 36.63
ATOM 84 CZ TYR 10 15.710 26.856 36.942 1.00 21.89	ATOM 156 CG PRO 19 17.946 50.819 39.056 1.00 37.03
ATOM 85 OH TYR 10 14.955 25.847 36.362 1.00 22.73	ATOM 157 C PRO 19 19.734 48.374 38.187 1.00 35.10
ATOM 86 HH TYR 10 14.113 25.788 36.803 1.00 0.00	ATOM 158 O PRO 19 20.744 47.958 37.621 1.00 35.49
ATOM 87 C TYR 10 17.856 32.466 39.197 1.00 13.97	ATOM 159 N LEU 20 19.437 48.094 39.456 1.00 36.74
ATOM 88 O TYR 10 17.067 32.822 40.068 1.00 16.11	ATOM 160 H LEU 20 18.629 48.478 39.844 1.00 0.00
ATOM 89 N VAL 11 19.085 32.947 39.098 1.00 14.44	ATOM 161 CA LEU 20 20.281 47.245 40.301 1.00 32.44
ATOM 90 H VAL 11 19.671 32.632 38.374 1.00 0.00	ATOM 162 CB LEU 20 19.670 47.111 41.703 1.00 32.72
ATOM 91 CA VAL 11 19.583 33.923 40.046 1.00 13.86	ATOM 163 CG LEU 20 20.579 47.103 42.937 1.00 33.61
ATOM 92 CB VAL 11 21.097 34.098 39.909 1.00 17.09	ATOM 164 CD1 LEU 20 19.784 46.663 44.144 1.00 31.90
ATOM 93 CG1 VAL 11 21.569 35.203 40.816 1.00 16.86	ATOM 165 CD2 LEU 20 21.760 46.182 42.732 1.00 33.95
ATOM 94 CG2 VAL 11 21.804 32.790 40.243 1.00 15.07	ATOM 166 C LEU 20 20.352 45.869 39.646 1.00 28.85
ATOM 95 C VAL 11 18.881 35.256 39.879 1.00 16.92	ATOM 167 O LEU 20 21.430 45.284 39.507 1.00 30.02
ATOM 96 O VAL 11 18.487 35.886 40.860 1.00 15.65	ATOM 168 N LYS 21 16.198 45.378 39.216 1.00 23.41
ATOM 97 N LEU 12 18.693 35.666 38.627 1.00 18.12	ATOM 169 H LYS 21 18.377 45.891 39.336 1.00 0.00
ATOM 98 H LEU 12 19.004 35.103 37.887 1.00 0.00	ATOM 170 CA LYS 21 19.125 44.088 38.569 1.00 21.47
ATOM 99 CA LEU 12 18.030 36.927 38.331 1.00 16.98	ATOM 171 CB LYS 21 17.669 43.736 38.289 1.00 16.66
ATOM 100 CB LEU 12 18.198 37.312 36.854 1.00 14.73	ATOM 172 CG LYS 21 17.433 42.316 37.808 1.00 14.92
ATOM 101 CG LEU 12 19.625 37.688 36.466 1.00 13.13	ATOM 173 CD LYS 21 15.961 42.053 37.717 1.00 10.55
ATOM 102 CD1 LEU 12 19.624 38.200 35.069 1.00 15.19	ATOM 174 CE LYS 21 15.681 40.611 37.453 1.00 15.68
ATOM 103 CD2 LEU 12 20.180 38.764 37.406 1.00 13.68	ATOM 175 NZ LYS 21 14.257 40.283 37.718 1.00 16.95
ATOM 104 C LEU 12 16.562 36.886 38.692 1.00 15.90	ATOM 176 HZ1 LYS 21 13.651 40.851 37.094 1.00 0.00
ATOM 105 O LEU 12 16.009 37.895 39.118 1.00 20.74	ATOM 177 HZ2 LYS 21 14.033 40.481 38.706 1.00 0.00
ATOM 106 N SER 13 15.953 35.709 38.599 1.00 16.34	ATOM 178 HZ3 LYS 21 14.100 39.270 37.520 1.00 0.00
ATOM 107 H SER 13 16.462 34.926 38.318 1.00 0.00	ATOM 179 C LYS 21 19.966 44.123 37.276 1.00 25.28
ATOM 108 CA SER 13 14.539 35.558 38.906 1.00 16.50	ATOM 180 O LYS 21 20.514 43.093 36.841 1.00 26.00
ATOM 109 CB SER 13 14.089 34.111 38.690 1.00 19.68	ATOM 181 N ALA 22 22.210.7 43.309 36.688 1.00 19.79
ATOM 110 OG SER 13 14.485 33.248 39.752 1.00 20.41	ATOM 182 H ALA 22 19.661 46.088 37.066 1.00 0.00
ATOM 111 HG SER 13 15.416 33.255 39.842 1.00 0.00	ATOM 183 CA ALA 22 20.910 45.452 35.481 1.00 20.93
ATOM 112 C SER 13 14.135 36.034 40.306 1.00 19.26	ATOM 184 CB ALA 22 20.651 46.796 34.812 1.00 19.38
ATOM 113 O SER 13 12.968 36.301 40.552 1.00 21.35	ATOM 185 C ALA 22 22.374 45.331 35.868 1.00 17.57
ATOM 114 NILE 14 15.087 36.152 41.223 1.00 20.06	ATOM 186 O ALA 22 23.144 44.658 35.194 1.00 22.09
ATOM 115 HILE 14 16.017 35.952 40.997 1.00 0.00	ATOM 187 N GLU 23 22.761 45.992 36.950 1.00 20.96
ATOM 116 CAILE 14 14.736 36.601 42.555 1.00 16.72	ATOM 188 H GLU 23 22.111 46.531 37.443 1.00 0.00
ATOM 117 CBILE 14 15.384 35.704 43.672 1.00 17.84	ATOM 189 CAGLU 23 24.139 45.933 37.427 1.00 23.81
ATOM 118 CG2ILE 14 14.876 34.283 43.560 1.00 13.91	ATOM 190 CBGLU 23 24.305 46.812 38.648 1.00 25.77
ATOM 119 CGLU 23 24.154 48.273 38.351 1.00 33.59	ATOM 191 CD2ASP 30 31.728 40.580 33.792 1.00 23.63
ATOM 120 CDGLU 23 23.522 49.014 39.496 1.00 38.59	ATOM 192 CGASP 30 31.319 41.686 32.816 1.00 26.58
ATOM 121 OE1GLU 23 22.567 49.780 39.247 1.00 44.81	ATOM 193 OD1ASP 30 31.497 42.873 33.158 1.00 27.51
ATOM 122 OE2GLU 23 23.964 48.818 40.650 1.00 49.94	ATOM 194 OD2ASP 30 30.820 41.377 31.713 1.00 25.65
ATOM 123 CGLU 23 24.549 44.509 37.781 1.00 25.74	ATOM 195 CASP 30 32.192 38.125 34.037 1.00 20.66
ATOM 124 OGLU 23 25.607 44.047 37.365 1.00 29.16	ATOM 196 OASP 30 33.245 37.692 33.550 1.00 21.87
ATOM 125 NVAL 23 24.723 43.832 38.577 1.00 23.09	ATOM 197 NVAL 31 31.741 37.701 35.221 1.00 16.91

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ATOM 198 H ILE 24 22.928 44.282 38.918 1.00 0.00	ATOM 270 H VAL 31 30.922 38.070 35.613 1.00 0.00
ATOM 199 CA ILE 24 23.974 42.447 38.978 1.00 20.14	ATOM 271 CA VAL 31 32.508 36.669 35.917 1.00 16.50
ATOM 200 CB ILE 24 22.815 41.924 39.877 1.00 21.29	ATOM 272 CB VAL 31 32.073 36.385 37.405 1.00 18.56
ATOM 201 CG2 ILE 24 22.876 40.025 40.025 1.00 19.58	ATOM 273 CG1 VAL 31 32.236 37.621 38.246 1.00 22.25
ATOM 202 CG1 ILE 24 22.847 42.644 41.234 1.00 23.57	ATOM 274 CG2 VAL 31 30.662 35.883 37.489 1.00 20.05
ATOM 203 CD1 ILE 24 21.648 42.367 42.133 1.00 21.62	ATOM 275 C VAL 31 32.370 35.399 35.118 1.00 14.17
ATOM 204 C ILE 24 24.154 41.535 37.752 1.00 17.46	ATOM 276 O VAL 31 33.360 34.704 34.894 1.00 14.10
ATOM 205 O ILE 24 25.147 40.813 37.664 1.00 20.13	ATOM 277 N PHE 32 31.163 35.155 34.604 1.00 10.67
ATOM 206 N ALA 25 23.230 41.611 36.794 1.00 16.90	ATOM 278 H PHE 32 30.444 35.785 34.763 1.00 0.00
ATOM 207 H ALA 25 22.478 42.235 36.916 1.00 0.00	ATOM 279 CA PHE 32 30.889 33.949 33.824 1.00 17.93
ATOM 208 CA ALA 25 23.288 40.803 35.572 1.00 18.54	ATOM 280 CB PHE 32 29.412 33.860 33.424 1.00 16.59
ATOM 209 CB ALA 25 22.120 41.113 34.671 1.00 17.95	ATOM 281 CG PHE 32 28.483 33.579 34.568 1.00 20.17
ATOM 210 C ALA 25 24.584 40.994 34.804 1.00 18.47	ATOM 282 CD1 PHE 32 27.108 33.608 34.378 1.00 20.46
ATOM 211 O ALA 25 25.140 40.038 34.273 1.00 19.08	ATOM 283 CD2 PHE 32 28.973 33.288 35.830 1.00 20.31
ATOM 212 N GLN 26 25.038 42.240 34.716 1.00 22.49	ATOM 284 CE1 PHE 32 26.240 33.354 35.424 1.00 21.08
ATOM 213 H GLN 26 24.526 42.964 35.143 1.00 0.00	ATOM 285 CE2 PHE 32 28.106 33.032 36.887 1.00 24.55
ATOM 214 CA GLN 26 26.271 42.564 34.025 1.00 19.66	ATOM 286 CZ PHE 32 26.735 33.065 36.681 1.00 21.99
ATOM 215 CB GLN 26 26.467 44.072 33.982 1.00 23.24	ATOM 287 C PHE 32 31.759 33.849 32.582 1.00 21.13
ATOM 216 CG GLN 26 27.762 44.518 33.307 1.00 32.72	ATOM 288 O PHE 32 32.179 32.752 32.201 1.00 20.61
ATOM 217 CD GLN 26 27.870 44.059 31.866 1.00 39.27	ATOM 289 N ALA 33 32.023 35.003 31.968 1.00 21.59
ATOM 218 OE1 GLN 26 28.827 43.383 31.493 1.00 44.74	ATOM 290 H ALA 33 31.637 35.820 32.334 1.00 0.00
ATOM 219 NE2 GLN 26 28.898 44.441 31.041 1.00 45.96	ATOM 291 CA ALA 33 32.842 35.081 30.775 1.00 21.27
ATOM 220 HE21 GLN 26 26.167 44.993 31.384 1.00 0.00	ATOM 292 CB ALA 33 32.540 36.349 30.019 1.00 21.72
ATOM 221 HE22 GLN 26 26.952 44.147 30.111 1.00 0.00	ATOM 293 C ALA 33 34.314 35.009 31.138 1.00 24.38
ATOM 222 C GLN 26 27.441 41.932 34.747 1.00 19.36	ATOM 294 O ALA 33 35.182 35.033 30.272 1.00 25.88
ATOM 223 O GLN 26 28.319 41.349 34.109 1.00 20.52	ATOM 295 N GLY 34 34.601 35.007 32.427 1.00 24.57
ATOM 224 N ARG 27 27.464 42.067 36.073 1.00 17.79	ATOM 296 H GLY 34 33.895 35.089 33.093 1.00 0.00
ATOM 225 H ARG 27 26.739 42.558 36.517 1.00 0.00	ATOM 297 CA GLY 34 35.974 34.881 32.840 1.00 30.55
ATOM 226 CA ARG 27 28.535 41.492 36.905 1.00 18.48	ATOM 298 C GLY 34 36.733 36.101 33.296 1.00 34.76
ATOM 227 CB ARG 27 28.359 41.861 38.384 1.00 19.92	ATOM 299 O GLY 34 37.888 35.953 33.696 1.00 36.73
ATOM 228 CG ARG 27 28.698 43.315 38.643 1.00 22.05	ATOM 300 N LYS 35 36.146 37.292 33.237 1.00 40.49
ATOM 229 CD ARG 27 28.146 43.828 39.942 1.00 28.72	ATOM 301 H LYS 35 35.233 37.373 32.882 1.00 0.00
ATOM 230 NE ARG 27 28.161 45.289 39.964 1.00 33.96	ATOM 302 CB LYS 35 36.877 38.481 33.706 1.00 47.46
ATOM 231 HE ARG 27 27.384 45.753 39.603 1.00 0.00	ATOM 303 CB LYS 35 36.123 39.777 33.374 1.00 46.18
ATOM 232 CZ ARG 27 29.158 46.030 40.440 1.00 40.38	ATOM 304 CG LYS 35 35.330 39.758 32.073 1.00 47.13
ATOM 233 NH1 ARG 27 30.250 45.459 40.951 1.00 43.63	ATOM 305 CD LYS 35 36.198 39.538 30.855 1.00 50.64
ATOM 234 HH11 ARG 27 30.337 44.463 40.979 1.00 0.00	ATOM 306 CE LYS 35 35.364 39.660 29.592 1.00 50.86
ATOM 235 HH12 ARG 27 30.997 46.029 41.306 1.00 0.00	ATOM 307 NZ LYS 35 34.644 40.963 29.571 1.00 48.30
ATOM 236 NH2 ARG 27 29.058 47.354 40.414 1.00 39.68	ATOM 308 HZ1 LYS 35 35.348 41.744 29.595 1.00 0.00
ATOM 237 HH21 ARG 27 28.238 47.784 40.045 1.00 0.00	ATOM 309 HZ2 LYS 35 34.027 41.041 30.395 1.00 0.00
ATOM 238 HH22 ARG 27 29.803 47.918 40.775 1.00 0.00	ATOM 310 HZ3 LYS 35 34.092 41.044 28.696 1.00 0.00
ATOM 239 C ARG 27 28.595 39.988 36.754 1.00 17.75	ATOM 311 C LYS 35 37.075 38.374 35.237 1.00 51.34
ATOM 240 H ARG 27 29.681 39.431 36.571 1.00 22.76	ATOM 312 O LYS 35 36.108 38.526 36.009 1.00 50.56
ATOM 241 N LEU 28 27.433 39.340 36.783 1.00 13.74	ATOM 313 N ASN 36 38.305 38.057 35.668 1.00 55.49
ATOM 242 H LEU 28 26.606 39.845 36.910 1.00 0.00	ATOM 314 H ASN 36 39.008 37.883 35.012 1.00 0.00
ATOM 243 CA LEU 28 27.381 37.895 36.629 1.00 16.11	ATOM 315 CA ASN 36 38.605 37.926 37.102 1.00 57.00
ATOM 244 CB LEU 28 25.952 37.368 36.757 1.00 13.10	ATOM 316 CB ASN 36 40.051 37.476 37.404 1.00 57.80
ATOM 245 CG LEU 28 25.339 37.219 38.151 1.00 17.27	ATOM 317 CG ASN 36 40.297 37.232 38.928 1.00 59.89
ATOM 246 CD1 LEU 28 23.847 36.918 38.035 1.00 14.43	ATOM 318 OD1 ASN 36 39.374 36.893 39.690 1.00 53.37
ATOM 247 CD2 LEU 28 26.039 36.111 38.911 1.00 14.44	ATOM 319 ND2 ASN 36 41.546 37.390 39.357 1.00 58.78
ATOM 248 C LEU 28 27.961 37.494 35.287 1.00 17.24	ATOM 320 HD1 ASN 36 42.246 37.643 38.738 1.00 0.00
ATOM 249 O LEU 28 28.904 36.704 35.234 1.00 19.78	ATOM 321 HD2 ASN 36 41.720 37.237 40.314 1.00 0.00
ATOM 250 N GLU 29 27.423 38.078 34.214 1.00 19.33	ATOM 322 C ASN 36 38.338 39.233 37.798 1.00 54.68
ATOM 251 H GLU 29 26.702 38.275 34.347 1.00 0.00	ATOM 323 O ASN 36 38.985 40.251 37.528 1.00 55.96
ATOM 252 CA GLU 29 27.862 37.795 32.850 1.00 18.96	ATOM 324 N THR 37 37.341 39.201 38.664 1.00 51.87
ATOM 253 CB GLU 29 27.115 38.689 31.859 1.00 19.98	ATOM 325 H THR 37 36.859 38.364 38.824 1.00 0.00
ATOM 254 CG GLU 29 25.660 38.295 31.684 1.00 23.80	ATOM 326 CA THR 37 36.972 40.379 39.393 1.00 48.77
ATOM 255 CD GLU 29 24.758 39.443 31.245 1.00 28.55	ATOM 327 CB THR 37 35.446 40.580 39.355 1.00 51.89
ATOM 256 OE1 GLU 29 25.183 40.613 31.316 1.00 35.86	ATOM 328 OG1 THR 37 34.951 40.258 38.047 1.00 52.86
ATOM 257 OE2 GLU 29 23.601 39.179 30.852 1.00 31.38	ATOM 329 HG1 THR 37 35.154 39.344 37.827 1.00 0.00
ATOM 258 C GLU 29 29.372 37.936 32.686 1.00 19.46	ATOM 330 CG2 THR 37 35.095 42.039 39.677 1.00 54.40
ATOM 259 O GLU 29 30.010 37.104 32.029 1.00 18.46	ATOM 331 C THR 37 37.469 40.246 40.823 1.00 43.38
ATOM 260 N ASP 30 29.945 38.959 33.316 1.00 19.80	ATOM 332 O THR 37 37.812 39.152 41.285 1.00 44.42
ATOM 261 H ASP 30 29.379 39.584 33.819 1.00 0.00	ATOM 333 N ASP 38 37.604 41.386 41.484 1.00 37.50
ATOM 262 CA ASP 30 31.388 39.183 33.274 1.00 19.46	ATOM 334 H ASP 38 37.411 42.224 41.013 1.00 0.00
ATOM 335 CA ASP 38 38.027 41.426 42.862 1.00 30.75	ATOM 407 HE1 TRP 45 27.028 49.009 42.977 1.00 0.00
ATOM 336 CB ASP 38 38.503 42.823 43.230 1.00 31.44	ATOM 408 CZ2 TRP 45 25.715 46.613 42.153 1.00 15.30
ATOM 337 CG ASP 38 39.239 42.869 44.550 1.00 33.99	ATOM 409 CZ3 TRP 45 26.092 44.275 42.712 1.00 22.34
ATOM 338 OD1 ASP 38 39.127 41.910 45.349 1.00 32.32	ATOM 410 CH2 TRP 45 25.380 45.291 42.022 1.00 22.84
ATOM 339 OD2 ASP 38 39.942 43.872 44.790 1.00 36.56	ATOM 411 C TRP 45 27.816 45.516 47.200 1.00 20.98
ATOM 340 C ASP 38 36.794 41.057 43.681 1.00 26.79	ATOM 412 O TRP 45 26.875 46.202 47.580 1.00 22.52
ATOM 341 O ASP 38 35.874 41.870 43.844 1.00 22.79	ATOM 413 N LEU 46 27.740 44.197 47.134 1.00 20.45
ATOM 342 N LEU 39 36.772 39.814 44.158 1.00 22.33	ATOM 414 H LEU 46 28.526 43.684 46.854 1.00 0.00
ATOM 343 H LEU 39 37.499 39.191 43.943 1.00 0.00	ATOM 415 CA LEU 46 26.505 43.494 47.456 1.00 19.83
ATOM 344 CA LEU 39 35.661 39.320 44.964 1.00 18.89	ATOM 416 CB LEU 46 26.717 41.988 47.349 1.00 20.94
ATOM 345 CB LEU 39 35.921 37.864 45.397 1.00 13.81	ATOM 417 CG LEU 46 26.554 41.283 46.020 1.00 24.92
ATOM 346 CG LEU 39 34.889 37.153 46.291 1.00 11.86	ATOM 418 CD1 LEU 46 26.923 39.833 46.239 1.00 24.33
ATOM 347 CD1 LEU 39 33.552 37.013 45.571 1.00 11.90	ATOM 419 CD2 LEU 46 25.113 41.417 45.542 1.00 24.55
ATOM 348 CD2 LEU 39 35.410 35.805 46.694 1.00 10.47	ATOM 420 C LEU 46 26.039 43.788 48.879 1.00 18.43

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ATOM 349 C LEU 39 35.444 40.225 46.183 1.00 18.68	ATOM 421 O LEU 46 24.865 44.073 49.128 1.00 20.04
ATOM 350 O LEU 39 34.308 40.498 46.565 1.00 21.12	ATOM 422 N LYS 47 26.963 43.631 49.812 1.00 15.42
ATOM 351 N GLU 40 36.533 40.726 46.753 1.00 19.42	ATOM 423 H LYS 47 27.866 43.367 49.542 1.00 0.00
ATOM 352 H GLU 40 37.410 40.497 46.396 1.00 0.00	ATOM 424 CA LYS 47 26.681 43.841 51.200 1.00 15.05
ATOM 353 CA GLU 40 36.451 41.591 47.921 1.00 23.60	ATOM 425 CB LYS 47 27.967 43.847 51.999 1.00 16.25
ATOM 354 CB GLU 40 37.843 42.023 48.366 1.00 27.21	ATOM 426 CG LYS 47 27.679 44.043 53.455 1.00 20.69
ATOM 355 CG GLU 40 37.842 42.938 49.584 1.00 44.74	ATOM 427 CD LYS 47 28.919 44.064 54.292 1.00 28.23
ATOM 356 CD GLU 40 39.230 43.454 49.927 1.00 53.90	ATOM 428 CE LYS 47 28.513 44.194 55.746 1.00 30.70
ATOM 357 OE1 GLU 40 39.937 42.784 50.718 1.00 59.32	ATOM 429 NZ LYS 47 29.654 44.501 56.646 1.00 35.92
ATOM 358 OE2 GLU 40 39.613 44.529 49.402 1.00 60.65	ATOM 430 HZ1 LYS 47 30.090 45.401 56.366 1.00 0.00
ATOM 359 C GLU 40 35.623 42.814 47.595 1.00 24.31	ATOM 431 HZ2 LYS 47 30.354 43.736 56.590 1.00 0.00
ATOM 360 O GLU 40 34.833 43.278 48.412 1.00 23.52	ATOM 432 HZ1 LYS 47 29.306 44.578 57.627 1.00 0.00
ATOM 361 N VAL 41 35.817 43.333 46.389 1.00 26.71	ATOM 433 C LYS 47 25.963 45.158 51.408 1.00 20.22
ATOM 362 H VAL 41 36.456 42.906 45.793 1.00 0.00	ATOM 434 O LYS 47 24.957 45.207 52.096 1.00 18.90
ATOM 363 CA VAL 41 35.092 44.510 45.918 1.00 30.42	ATOM 435 N THR 48 26.489 46.216 50.793 1.00 25.04
ATOM 364 CB VAL 41 35.772 45.094 44.648 1.00 35.26	ATOM 436 H THR 48 27.289 46.088 50.235 1.00 0.00
ATOM 365 CG1 VAL 41 34.909 46.192 44.025 1.00 38.11	ATOM 437 CA THR 48 25.927 47.561 50.904 1.00 23.95
ATOM 366 CG2 VAL 41 37.153 45.640 45.004 1.00 32.38	ATOM 438 CB THR 48 27.028 48.613 50.714 1.00 20.88
ATOM 367 C VAL 41 33.629 44.159 45.636 1.00 24.47	ATOM 439 OG1 THR 48 27.693 48.387 49.468 1.00 25.10
ATOM 368 O VAL 41 32.714 44.851 46.074 1.00 26.21	ATOM 440 HG1 THR 48 28.095 47.517 49.462 1.00 0.00
ATOM 369 N LEU 42 33.424 43.060 44.928 1.00 24.20	ATOM 441 CG2 THR 48 28.042 48.521 51.822 1.00 19.81
ATOM 370 H LEU 42 34.197 42.554 44.617 1.00 0.00	ATOM 442 C THR 48 24.747 47.912 49.978 1.00 23.98
ATOM 371 CA LEU 42 32.096 42.576 44.588 1.00 20.29	ATOM 443 O THR 48 24.254 49.031 50.010 1.00 25.61
ATOM 372 CB LEU 42 32.219 41.216 43.904 1.00 24.03	ATOM 444 N ARG 49 24.265 46.970 49.180 1.00 27.77
ATOM 373 CG LEU 42 31.611 41.062 42.525 1.00 26.40	ATOM 445 H ARG 49 24.663 46.074 49.180 1.00 0.00
ATOM 374 CD1 LEU 42 31.964 39.715 41.965 1.00 25.94	ATOM 446 CA ARG 49 23.147 47.274 48.283 1.00 31.32
ATOM 375 CD2 LEU 42 30.116 41.247 42.629 1.00 32.20	ATOM 447 AB ARG 49 22.961 46.196 47.194 1.00 30.53
ATOM 376 C LEU 42 31.261 42.414 45.846 1.00 17.94	ATOM 448 CG ARG 49 24.007 46.144 46.076 1.00 28.56
ATOM 377 O LEU 42 30.172 42.479 45.961 1.00 18.69	ATOM 449 CD ARG 49 24.323 47.528 45.510 1.00 30.84
ATOM 378 N MET 43 31.801 41.656 46.797 1.00 15.65	ATOM 450 NE ARG 49 25.396 48.175 46.267 1.00 31.36
ATOM 379 H MET 43 32.682 41.284 46.645 1.00 0.00	ATOM 451 HE ARG 49 25.898 47.636 46.892 1.00 0.00
ATOM 380 CA MET 43 31.133 41.364 48.064 1.00 17.70	ATOM 452 CZ ARG 49 25.725 49.460 46.179 1.00 31.53
ATOM 381 CB MET 43 31.999 40.434 48.918 1.00 15.00	ATOM 453 NH1 ARG 49 25.068 50.272 45.359 1.00 33.61
ATOM 382 CG MET 43 32.195 39.058 48.311 1.00 15.30	ATOM 454 HH11 ARG 49 24.321 49.918 44.792 1.00 0.00
ATOM 383 SD MET 43 30.702 38.017 48.215 1.00 17.90	ATOM 455 HH12 ARG 49 25.326 51.236 45.287 1.00 0.00
ATOM 384 CE MET 43 30.226 38.195 46.576 1.00 22.51	ATOM 456 NH2 ARG 49 26.718 49.931 46.916 1.00 31.78
ATOM 385 C MET 43 30.722 42.593 48.866 1.00 16.98	ATOM 457 HH21 ARG 49 27.214 49.324 47.530 1.00 0.00
ATOM 386 O MET 43 29.612 42.649 49.382 1.00 17.31	ATOM 458 HH22 ARG 49 26.973 50.898 46.847 1.00 0.00
ATOM 387 N GLU 44 31.612 43.575 48.955 1.00 20.26	ATOM 459 C ARG 49 21.805 47.488 48.986 1.00 35.36
ATOM 388 H GLU 44 32.483 43.463 48.514 1.00 0.00	ATOM 460 O ARG 49 21.366 46.667 49.791 1.00 34.08
ATOM 389 CA GLU 44 31.343 44.813 49.671 1.00 23.74	ATOM 461 N PRO 50 21.128 48.586 48.673 1.00 39.27
ATOM 390 CB GLU 44 32.612 45.681 49.752 1.00 25.41	ATOM 462 CD PRO 50 21.530 49.640 47.723 1.00 41.19
ATOM 391 CG GLU 44 32.467 46.983 50.563 1.00 31.31	ATOM 463 CA PRO 50 19.826 48.877 49.274 1.00 39.02
ATOM 392 CD GLU 44 31.832 46.774 51.941 1.00 35.92	ATOM 464 CB PRO 50 19.621 50.337 48.904 1.00 42.38
ATOM 393 OE1 GLU 44 32.195 45.800 52.643 1.00 36.04	ATOM 465 CG PRO 50 20.238 50.390 47.501 1.00 44.74
ATOM 394 OE2 GLU 44 30.950 47.583 52.314 1.00 39.72	ATOM 466 C PRO 50 18.787 47.995 48.575 1.00 38.81
ATOM 395 C GLU 44 30.201 45.561 48.993 1.00 24.64	ATOM 467 O PRO 50 19.075 47.393 47.539 1.00 34.20
ATOM 396 O GLU 44 29.306 46.122 49.658 1.00 24.29	ATOM 468 N ILE 51 17.575 47.970 49.125 1.00 39.84
ATOM 397 N TRP 45 30.208 45.510 47.662 1.00 22.97	ATOM 469 H ILE 51 17.435 48.506 49.931 1.00 0.00
ATOM 398 H TRP 45 30.934 45.032 47.207 1.00 0.00	ATOM 470 CA ILE 51 16.434 47.191 48.621 1.00 41.44
ATOM 399 CA TRP 45 29.176 46.150 46.857 1.00 23.59	ATOM 471 CB ILE 51 15.861 47.734 47.253 1.00 45.38
ATOM 400 CB TRP 45 29.517 46.000 45.367 1.00 20.89	ATOM 472 CG2 ILE 51 15.891 47.273 47.224 1.00 47.02
ATOM 401 CG TRP 45 28.525 46.618 44.456 1.00 20.23	ATOM 473 CG1 ILE 51 16.608 47.137 46.055 1.00 50.71
ATOM 402 CD2 TRP 45 27.518 45.936 43.700 1.00 19.85	ATOM 474 CD1 ILE 51 16.119 47.630 44.696 1.00 54.88
ATOM 403 CE2 TRP 45 26.785 46.926 42.996 1.00 20.46	ATOM 475 C ILE 51 16.578 45.655 48.577 1.00 37.85
ATOM 404 CE3 TRP 45 27.155 45.588 43.549 1.00 17.73	ATOM 476 I OLE 51 15.584 44.945 48.738 1.00 39.23
ATOM 405 CD1 TRP 45 28.378 47.946 44.189 1.00 18.89	ATOM 477 N LEU 52 17.789 45.141 48.366 1.00 31.60
ATOM 406 NE1 TRP 45 27.335 48.138 43.316 1.00 18.48	ATOM 478 H LEU 52 18.552 45.723 48.238 1.00 0.00
ATOM 479 CA LEU 52 17.992 43.695 48.323 1.00 26.68	ATOM 551 CD1 LEU 60 22.417 39.325 44.150 1.00 17.25
ATOM 480 CB LEU 52 19.393 43.333 47.818 1.00 21.97	ATOM 552 CD2 LEU 60 23.183 37.358 42.846 1.00 13.12
ATOM 481 CG LEU 52 19.742 43.661 46.367 1.00 20.21	ATOM 553 C LEU 60 25.783 36.158 45.860 1.00 12.78
ATOM 482 CD1 LEU 52 21.136 43.140 46.057 1.00 19.41	ATOM 554 O LEU 60 26.713 35.935 45.074 1.00 13.84
ATOM 483 CD2 LEU 52 18.727 43.041 45.428 1.00 20.03	ATOM 555 N GLY 61 25.938 36.315 47.172 1.00 9.31
ATOM 484 C LEU 52 17.801 43.115 49.716 1.00 25.06	ATOM 556 H GLY 61 25.163 36.524 47.724 1.00 0.00
ATOM 485 O LEU 52 18.287 43.664 50.705 1.00 23.98	ATOM 557 CA GLY 61 27.238 36.195 47.802 1.00 9.25
ATOM 486 N SER 53 17.066 42.018 49.798 1.00 23.37	ATOM 558 C GLY 61 27.792 34.818 47.511 1.00 10.59
ATOM 487 H SER 53 16.651 41.647 48.993 1.00 0.00	ATOM 559 O GLY 61 28.934 34.676 47.077 1.00 11.56
ATOM 488 CA SER 53 16.844 41.377 51.080 1.00 23.35	ATOM 560 N PHE 62 26.698 33.800 47.716 1.00 10.85
ATOM 489 CB SER 53 15.750 40.308 50.956 1.00 25.31	ATOM 561 H PHE 62 26.071 33.988 48.054 1.00 0.00
ATOM 490 OG SER 53 16.201 39.183 50.210 1.00 24.71	ATOM 562 CA PHE 62 27.346 32.407 47.450 1.00 12.29
ATOM 491 HG SER 53 16.954 38.795 50.638 1.00 0.00	ATOM 563 CB PHE 52 26.156 31.517 47.818 1.00 10.34
ATOM 492 C SER 53 18.137 40.693 51.482 1.00 20.63	ATOM 564 CG PHE 62 26.394 30.045 47.647 1.00 16.08
ATOM 493 O SER 53 18.962 40.362 50.622 1.00 21.92	ATOM 565 CD1 PHE 62 26.812 29.276 48.716 1.00 13.97
ATOM 494 N PRO 54 18.326 40.460 52.789 1.00 20.64	ATOM 566 CD2 PHE 62 26.111 29.409 46.437 1.00 20.52
ATOM 495 CD PRO 54 17.556 41.025 53.910 1.00 20.93	ATOM 567 CE1 PHE 62 26.941 27.898 48.595 1.00 16.42
ATOM 496 CA PRO 54 19.534 39.788 53.279 1.00 16.81	ATOM 568 CE2 PHE 62 26.237 28.026 46.306 1.00 20.64
ATOM 497 CB PRO 54 19.295 39.751 54.780 1.00 20.34	ATOM 569 CZ PHE 62 26.655 27.271 47.394 1.00 19.89
ATOM 498 CG PRO 54 18.574 41.048 55.017 1.00 22.23	ATOM 570 C PHE 62 27.739 32.204 45.957 1.00 12.39
ATOM 499 C PRO 54 19.663 38.372 52.678 1.00 13.03	ATOM 571 O PHE 62 28.817 31.672 45.643 1.00 9.64

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ATOM 500 O PRO 54 20.766 37.906 52.405 1.00 9.38	ATOM 572 N VAL 63 26.859 32.632 45.051 1.00 12.11
ATOM 501 N LEU 55 18.534 37.717 52.418 1.00 12.84	ATOM 573 H VAL 63 26.030 33.048 45.363 1.00 0.00
ATOM 502 H LEU 55 17.676 38.141 52.613 1.00 0.00	ATOM 574 CA VAL 63 27.086 32.507 43.611 1.00 14.15
ATOM 503 CA LEU 55 18.561 36.375 51.847 1.00 14.56	ATOM 575 CB VAL 63 25.945 33.160 42.787 1.00 16.96
ATOM 504 CB LEU 55 17.162 35.796 51.762 1.00 17.02	ATOM 576 CG1 VAL 63 26.214 32.989 41.295 1.00 15.72
ATOM 505 CG LEU 55 16.970 34.283 51.921 1.00 21.28	ATOM 577 CG2 VAL 63 24.609 32.535 43.150 1.00 14.32
ATOM 506 CD1 LEU 55 15.619 33.906 51.335 1.00 25.89	ATOM 578 C VAL 63 28.409 33.130 43.195 1.00 11.36
ATOM 507 CD2 LEU 55 18.057 33.485 51.254 1.00 17.96	ATOM 579 O VAL 63 29.227 32.489 42.548 1.00 12.16
ATOM 508 C LEU 55 19.126 36.459 50.445 1.00 15.67	ATOM 580 N PHE 64 28.621 34.373 43.594 1.00 11.64
ATOM 509 O LEU 55 20.019 35.698 50.068 1.00 18.05	ATOM 581 H PHE 64 27.932 34.829 44.117 1.00 0.00
ATOM 510 N THR 56 18.579 37.381 49.669 1.00 15.34	ATOM 582 CA PHE 64 29.844 34.078 43.267 1.00 12.42
ATOM 511 H THR 56 17.859 37.924 50.002 1.00 0.00	ATOM 583 CB PHE 64 29.766 36.526 43.729 1.00 12.23
ATOM 512 CA THR 56 19.018 37.602 48.297 1.00 16.13	ATOM 584 CG PHE 64 28.960 37.386 42.813 1.00 19.72
ATOM 513 CB THR 56 18.258 38.790 47.693 1.00 15.71	ATOM 585 CD1 PHE 64 28.005 38.256 43.308 1.00 21.00
ATOM 514 OG1 THR 56 16.900 38.403 47.495 1.00 17.76	ATOM 586 CD2 PHE 64 29.153 37.315 41.429 1.00 20.33
ATOM 515 HG1 THR 56 16.415 39.120 47.104 1.00 0.00	ATOM 587 CE1 PHE 64 27.251 39.052 42.431 1.00 26.47
ATOM 516 CG2 THR 56 18.869 39.232 46.367 1.00 13.57	ATOM 588 CE2 PHE 64 28.409 38.105 40.549 1.00 24.02
ATOM 517 C THR 56 20.526 37.862 48.228 1.00 15.56	ATOM 589 CZ PHE 64 27.454 38.976 41.049 1.00 22.91
ATOM 518 O THR 56 21.230 37.338 47.349 1.00 13.64	ATOM 590 C PHE 64 31.122 34.432 43.739 1.00 12.20
ATOM 519 N LYS 57 21.002 38.694 49.149 1.00 12.96	ATOM 591 O PHE 64 32.090 34.385 42.982 1.00 10.58
ATOM 520 H LYS 57 20.380 39.096 49.786 1.00 0.00	ATOM 592 N THR 64 31.136 33.896 44.958 1.00 15.46
ATOM 521 CA LYS 57 22.414 39.031 49.236 1.00 15.26	ATOM 593 H THR 65 30.331 33.930 45.527 1.00 0.00
ATOM 522 CB LYS 57 22.626 40.115 50.292 1.00 16.39	ATOM 594 CA THR 65 32.353 33.256 45.458 1.00 15.26
ATOM 523 CG LYS 57 22.043 41.458 49.935 1.00 15.74	ATOM 595 CB THR 65 32.276 32.889 46.968 1.00 15.45
ATOM 524 CD LYS 57 22.365 42.457 51.034 1.00 18.06	ATOM 596 OG1 THR 65 31.493 31.709 47.141 1.00 30.54
ATOM 525 CE LYS 57 22.042 43.870 50.593 1.00 20.25	ATOM 597 HG1 THR 65 31.874 30.971 46.666 1.00 0.00
ATOM 526 NZ LYS 57 22.223 44.831 51.705 1.00 23.31	ATOM 598 CG2 THR 65 31.643 33.994 47.749 1.00 11.88
ATOM 527 HZ1 LYS 57 23.200 44.804 52.032 1.00 0.00	ATOM 599 C THR 65 32.613 31.987 44.665 1.00 13.68
ATOM 528 HZ2 LYS 57 21.589 44.571 52.494 1.00 0.00	ATOM 600 O THR 65 33.753 31.627 44.389 1.00 17.47
ATOM 529 HZ3 LYS 57 21.983 45.791 51.386 1.00 0.00	ATOM 601 N LEU 66 31.535 31.330 44.272 1.00 14.36
ATOM 530 C LYS 57 23.288 37.814 49.569 1.00 14.09	ATOM 602 H LEU 66 30.645 31.700 44.486 1.00 0.00
ATOM 531 O LYS 57 24.448 37.740 49.129 1.00 12.70	ATOM 603 CA LEU 66 31.619 30.090 43.530 1.00 16.09
ATOM 532 N GLY 58 22.733 36.387 50.358 1.00 15.03	ATOM 604 CB LEU 66 30.234 29.444 43.494 1.00 19.06
ATOM 533 H GLY 58 21.826 37.028 50.701 1.00 0.00	ATOM 605 CG LEU 66 30.034 28.010 43.971 1.00 26.72
ATOM 534 CA GLY 58 23.446 35.676 50.741 1.00 14.02	ATOM 606 CD1 LEU 66 30.297 27.917 45.486 1.00 33.43
ATOM 535 C GLY 58 23.603 34.745 49.555 1.00 14.16	ATOM 607 CD2 LEU 66 28.604 27.604 43.665 1.00 29.53
ATOM 536 O GLY 58 24.673 34.168 49.331 1.00 14.13	ATOM 608 C LEU 66 32.095 30.238 42.084 1.00 18.82
ATOM 537 N ILE 59 22.526 34.620 48.781 1.00 16.19	ATOM 609 O LEU 66 32.762 29.347 41.554 1.00 19.11
ATOM 538 H ILE 59 21.715 35.105 49.041 1.00 0.00	ATOM 610 N THR 67 31.697 31.335 41.446 1.00 15.33
ATOM 539 CA ILE 59 22.494 33.791 47.576 1.00 12.32	ATOM 611 H THR 67 31.183 32.009 41.937 1.00 0.00
ATOM 540 CB ILE 59 21.055 33.722 46.991 1.00 11.19	ATOM 612 CA THR 67 31.982 31.563 40.042 1.00 14.14
ATOM 541 CG2 ILE 59 21.037 33.034 45.605 1.00 3.54	ATOM 613 CB THR 67 30.722 32.041 39.345 1.00 8.38
ATOM 542 CG1 ILE 59 20.148 33.005 47.997 1.00 9.06	ATOM 614 OG1 THR 67 30.300 33.287 39.916 1.00 11.18
ATOM 543 CD1 ILE 59 18.712 32.824 47.543 1.00 15.78	ATOM 615 HG1 THR 67 30.109 33.172 40.848 1.00 0.00
ATOM 544 C ILE 59 23.489 34.354 46.548 1.00 15.16	ATOM 616 CG2 THR 67 29.620 31.016 39.528 1.00 5.37
ATOM 545 O ILE 59 24.337 33.621 46.036 1.00 15.23	ATOM 617 C THR 67 33.141 32.486 39.705 1.00 18.23
ATOM 546 N LEU 60 23.436 35.658 46.301 1.00 12.86	ATOM 618 O THR 67 33.656 32.455 38.583 1.00 17.80
ATOM 547 H LEU 60 22.768 36.214 46.753 1.00 0.00	ATOM 619 N VAL 68 33.564 33.281 40.683 1.00 17.46
ATOM 548 CA LEU 60 24.361 36.269 45.358 1.00 14.47	ATOM 620 H VAL 68 33.109 33.265 41.538 1.00 0.00
ATOM 549 CB LEU 60 24.009 37.730 45.132 1.00 16.93	ATOM 621 CA VAL 68 34.678 34.197 40.506 1.00 19.37
ATOM 550 CG LEU 60 22.813 37.877 44.211 1.00 14.49	ATOM 622 CB VAL 68 34.813 35.092 41.760 1.00 22.10
ATOM 623 CG1 VAL 68 35.816 34.536 42.738 1.00 15.19	ATOM 695 N ARG 76 35.411 33.893 54.533 1.00 16.95
ATOM 624 CG2 VAL 68 35.058 36.356 41.370 1.00 19.51	ATOM 696 H ARG 76 35.828 33.225 55.110 1.00 0.00
ATOM 625 C VAL 68 35.920 33.315 40.245 1.00 22.98	ATOM 697 CA ARG 76 33.983 33.805 54.245 1.00 16.24
ATOM 626 O VAL 68 36.066 32.260 40.873 1.00 22.77	ATOM 698 CB ARG 76 33.377 32.548 54.883 1.00 16.94
ATOM 627 N PRO 69 36.813 33.724 39.307 1.00 23.51	ATOM 699 CG ARG 76 33.854 31.233 54.254 1.00 18.42
ATOM 628 CD PRO 69 36.816 34.956 38.492 1.00 20.60	ATOM 700 CD ARG 76 33.766 31.366 52.751 1.00 20.49
ATOM 629 CA PRO 69 37.991 32.879 39.046 1.00 25.71	ATOM 701 NE ARG 76 33.596 30.103 52.052 1.00 23.98
ATOM 630 CB PRO 69 38.733 33.598 37.908 1.00 25.24	ATOM 702 HE ARG 76 33.195 29.370 52.536 1.00 0.00
ATOM 631 CG PRO 69 38.157 34.946 37.880 1.00 25.82	ATOM 703 CZ ARG 76 34.006 29.895 50.807 1.00 19.60
ATOM 632 C PRO 69 38.842 32.622 40.281 1.00 29.88	ATOM 704 NH1 ARG 76 34.618 30.867 50.151 1.00 21.93
ATOM 633 O PRO 69 39.172 31.465 40.570 1.00 31.71	ATOM 705 HH11 ARG 76 34.764 31.756 50.588 1.00 0.00
ATOM 634 N SER 70 39.147 33.675 41.038 1.00 28.74	ATOM 706 HH12 ARG 76 34.916 30.727 49.205 1.00 0.00
ATOM 635 H SER 70 38.847 34.569 40.767 1.00 0.00	ATOM 707 NH2 ARG 76 33.766 28.741 50.211 1.00 16.37
ATOM 636 CA SER 70 39.929 33.521 42.268 1.00 31.02	ATOM 708 HH21 ARG 76 33.286 28.016 50.700 1.00 0.00
ATOM 637 CB SER 70 41.386 33.994 44.585 1.00 32.48	ATOM 709 HH22 ARG 76 34.074 28.595 49.269 1.00 0.00
ATOM 638 OG SER 70 41.530 34.878 49.881 1.00 41.24	ATOM 710 C ARG 76 33.339 35.062 54.822 1.00 14.95
ATOM 639 HG SER 70 40.971 35.653 41.103 1.00 0.00	ATOM 711 O ARG 76 33.810 35.591 55.823 1.00 19.14
ATOM 640 C SER 70 39.298 34.244 43.449 1.00 26.93	ATOM 712 N ARG 77 32.285 35.559 54.192 1.00 14.43
ATOM 641 O SER 70 38.832 35.380 43.318 1.00 25.63	ATOM 713 H ARG 77 31.937 35.107 53.402 1.00 0.00
ATOM 642 N GLU 71 39.237 33.554 44.585 1.00 24.01	ATOM 714 CA ARG 77 31.639 36.776 54.673 1.00 16.84
ATOM 643 H GLU 71 39.537 32.625 44.607 1.00 0.00	ATOM 715 CB ARG 77 31.101 37.592 53.497 1.00 16.48
ATOM 644 CA GLU 71 38.702 34.141 45.811 1.00 23.36	ATOM 716 CG ARG 77 32.186 38.079 52.557 1.00 19.55
ATOM 645 CB GLU 71 38.264 33.066 46.797 1.00 26.79	ATOM 717 CD ARG 77 32.801 39.413 52.993 1.00 25.33
ATOM 646 CG GLU 71 37.087 32.247 46.346 1.00 36.00	ATOM 718 NE ARG 77 34.043 39.317 53.765 1.00 32.73
ATOM 647 CD GLU 71 36.736 31.171 47.339 1.00 39.09	ATOM 719 HE ARG 77 34.052 39.719 54.654 1.00 0.00
ATOM 648 OE1 GLU 71 36.170 30.147 46.911 1.00 41.16	ATOM 720 CZ ARG 77 35.158 38.697 53.374 1.00 37.18
ATOM 649 OE2 GLU 71 37.020 31.347 48.545 1.00 46.63	ATOM 721 NH1 ARG 77 35.217 38.075 52.206 1.00 45.18
ATOM 650 C GLU 71 39.797 34.970 46.459 1.00 22.23	ATOM 722 HH11 ARG 77 34.443 38.091 51.580 1.00 0.00

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ATOM 651 O GLU 71 39.527 35.732 47.376 1.00 20.81	ATOM 723 HH12 ARG 77 36.082 37.653 51.907 1.00 0.00
ATOM 652 N ARG 72 41.040 34.766 46.021 1.00 18.01	ATOM 724 NH2 ARG 77 36.251 38.750 54.125 1.00 35.27
ATOM 653 H ARG 72 41.187 34.083 45.337 1.00 0.00	ATOM 725 HH21 ARG 77 36.239 39.253 54.988 1.00 0.00
ATOM 654 CA ARG 72 42.184 35.508 46.541 1.00 18.63	ATOM 726 HH22 ARG 77 37.096 38.304 53.821 1.00 0.00
ATOM 655 CB ARG 72 45.059 36.987 46.162 1.00 22.88	ATOM 727 C ARG 77 30.539 36.567 55.700 1.00 18.14
ATOM 656 CG ARG 72 41.640 37.218 44.712 1.00 22.96	ATOM 728 O ARG 77 29.620 35.763 55.512 1.00 16.53
ATOM 657 CD ARG 72 41.631 38.703 44.344 1.00 23.05	ATOM 729 N ARG 78 30.615 37.345 56.772 1.00 21.45
ATOM 658 NE ARG 72 41.397 38.868 42.909 1.00 29.61	ATOM 730 H ARG 78 31.375 37.957 56.846 1.00 0.00
ATOM 659 HE ARG 72 41.165 30.067 42.396 1.00 0.00	ATOM 731 CA ARG 78 29.638 37.303 57.859 1.00 19.61
ATOM 660 CZ ARG 72 41.470 40.024 42.253 1.00 27.27	ATOM 732 CB ARG 78 30.008 38.375 58.888 1.00 25.10
ATOM 661 NH1 ARG 72 41.776 41.135 42.901 1.00 25.95	ATOM 733 CG ARG 78 28.959 38.634 59.928 1.00 35.74
ATOM 662 HH11 ARG 72 41.955 41.107 43.899 1.00 0.00	ATOM 734 CD ARG 78 29.425 39.673 60.914 1.00 47.69
ATOM 663 HH12 ARG 72 41.838 42.002 42.414 1.00 0.00	ATOM 735 NE ARG 78 28.454 29.822 61.996 1.00 62.90
ATOM 664 NH2 ARG 72 41.212 40.069 40.951 1.00 23.28	ATOM 736 HE ARG 78 28.6321 39.351 62.837 1.00 0.00
ATOM 665 HH21 ARG 72 40.977 39.232 40.462 1.00 0.00	ATOM 737 CZ ARG 78 27.351 40.564 61.917 1.00 67.36
ATOM 666 HH22 ARG 72 41.283 40.938 40.465 1.00 0.00	ATOM 738 NH1 ARG 78 27.083 41.242 60.804 1.00 72.55
ATOM 667 C ARG 72 42.363 35.369 48.061 1.00 20.31	ATOM 739 HH11 ARG 78 27.712 41.191 60.025 1.00 0.00
ATOM 668 O ARG 72 42.750 36.319 48.738 1.00 15.15	ATOM 740 HH12 ARG 78 26.257 41.797 60.740 1.00 0.00
ATOM 669 N GLY 73 42.059 34.186 48.583 1.00 18.99	ATOM 741 NH2 ARG 78 26.491 40.587 62.929 1.00 67.11
ATOM 670 H GLY 73 41.643 33.504 48.071 1.00 0.00	ATOM 742 HH21 ARG 78 26.677 40.051 63.752 1.00 0.00
ATOM 671 CA GLY 73 42.192 33.927 50.000 1.00 20.88	ATOM 743 HH22 ARG 78 25.666 41.146 62.868 1.00 0.00
ATOM 672 C GLY 73 41.330 34.797 50.894 1.00 21.37	ATOM 744 C ARG 78 28.189 37.495 57.348 1.00 15.98
ATOM 673 O GLY 73 41.711 35.087 52.033 1.00 25.47	ATOM 745 O ARG 78 27.284 36.770 57.761 1.00 16.16
ATOM 674 N LEU 74 40.181 35.238 50.396 1.00 21.12	ATOM 746 N PHE 79 27.972 38.425 56.411 1.00 16.65
ATOM 675 H LEU 74 39.922 35.014 49.482 1.00 0.00	ATOM 747 H PHE 79 28.714 38.951 56.083 1.00 0.00
ATOM 676 CA LEU 74 39.921 36.063 51.212 1.00 21.29	ATOM 748 CA PHE 79 26.613 38.662 55.881 1.00 11.51
ATOM 677 CB LEU 74 38.303 36.834 50.345 1.00 21.15	ATOM 749 CB PHE 79 26.499 39.986 55.062 1.00 11.25
ATOM 678 CG LEU 74 38.927 37.751 49.304 1.00 29.09	ATOM 750 CG PHE 79 27.070 39.937 53.648 1.00 12.26
ATOM 679 CD1 LEU 74 37.802 38.397 48.561 1.00 32.52	ATOM 751 CD1 PHE 79 26.234 39.670 52.549 1.00 12.23
ATOM 680 CD2 LEU 74 39.872 38.802 49.919 1.00 27.60	ATOM 752 CD2 PHE 79 28.416 40.218 53.408 1.00 9.84
ATOM 681 C LEU 74 38.522 35.181 52.190 1.00 20.91	ATOM 753 CE1 PHE 79 26.731 39.685 51.233 1.00 12.52
ATOM 682 O LEU 74 38.114 34.070 51.841 1.00 17.35	ATOM 754 CD2 PHE 79 28.925 40.239 52.089 1.00 11.33
ATOM 683 N GLN 75 38.363 35.664 53.422 1.00 21.46	ATOM 755 CZ PHE 79 28.078 39.972 51.007 1.00 8.90
ATOM 684 H GLN 75 38.752 36.530 53.638 1.00 0.00	ATOM 756 C PHE 79 26.044 37.458 55.143 1.00 8.21
ATOM 685 CA GLN 75 37.631 34.928 54.450 1.00 19.45	ATOM 757 O PHE 79 24.850 37.185 55.196 1.00 8.94
ATOM 686 CB GLN 75 37.782 35.631 55.807 1.00 19.60	ATOM 758 N VAL 80 36.923 36.676 54.534 1.00 7.83
ATOM 687 CG GLN 75 39.215 35.713 56.358 1.00 17.96	ATOM 759 H VAL 80 27.874 36.883 54.578 1.00 0.00
ATOM 688 CD GLN 75 36.866 34.358 56.592 1.00 15.76	ATOM 760 CA VAL 80 26.488 35.494 53.824 1.00 9.30
ATOM 689 OE1 GLN 75 39.189 33.326 56.691 1.00 15.14	ATOM 761 CB VAL 80 27.509 35.071 52.743 1.00 8.14
ATOM 690 NE2 GLN 75 41.197 34.351 56.669 1.00 16.91	ATOM 762 CG1 VAL 80 27.013 33.862 52.004 1.00 6.78
ATOM 691 HE21 GLN 75 41.683 35.196 56.567 1.00 0.00	ATOM 763 CG2 VAL 80 27.702 36.197 51.741 1.00 11.62
ATOM 692 HE22 GLN 75 41.626 33.501 56.803 1.00 0.00	ATOM 764 C VAL 80 26.247 34.351 54.818 1.00 9.86
ATOM 693 C GLN 75 36.151 34.888 54.053 1.00 17.46	ATOM 765 O VAL 80 25.236 33.659 54.741 1.00 9.66
ATOM 694 O GLN 75 35.709 35.720 53.268 1.00 17.50	ATOM 766 N GLN 81 27.158 34.171 55.766 1.00 10.87
ATOM 697 H GLN 81 27.939 34.755 55.800 1.00 0.00	ATOM 769 CB ASP 89 15.664 26.240 62.397 1.00 11.39
ATOM 768 CA GLN 81 27.010 33.111 56.751 1.00 10.72	ATOM 804 CG ASP 89 14.532 25.309 62.766 1.00 17.46
ATOM 769 CB GLN 81 28.179 33.124 57.729 1.00 9.85	ATOM 841 OD1 ASP 89 13.987 25.419 63.885 1.00 20.46
ATOM 770 CG GLN 81 29.516 32.805 57.081 1.00 11.05	ATOM 842 OD2 ASP 89 14.166 24.464 61.936 1.00 19.66
ATOM 771 CD GLN 81 30.666 32.915 58.063 1.00 18.77	ATOM 843 C ASP 89 17.455 24.544 62.930 1.00 14.77
ATOM 772 OE1 GLN 81 30.843 33.949 58.711 1.00 15.83	ATOM 844 O ASP 89 17.798 24.208 61.798 1.00 13.18
ATOM 773 NE2 GLN 81 31.450 31.841 58.192 1.00 16.43	ATOM 845 N PRO 90 17.445 23.677 63.972 1.00 17.07
ATOM 774 HE21 GLN 81 31.254 31.037 57.660 1.00 0.00	ATOM 846 CD PRO 90 16.998 24.000 65.343 1.00 11.50
ATOM 775 HE22 GLN 81 32.194 31.896 58.821 1.00 0.00	ATOM 847 CA PRO 90 17.911 22.281 63.906 1.00 14.78
ATOM 776 C GLN 81 25.710 33.305 57.505 1.00 11.63	ATOM 848 CB PRO 90 17.706 21.776 65.335 1.00 12.18
ATOM 777 O GLN 81 24.981 32.341 57.750 1.00 13.10	ATOM 849 CG PRO 90 17.796 23.018 66.161 1.00 12.39
ATOM 778 N ASN 82 25.399 34.557 57.838 1.00 12.35	ATOM 850 C PRO 90 17.161 21.416 62.890 1.00 14.07
ATOM 779 H ASN 82 26.007 35.283 57.589 1.00 0.00	ATOM 851 O PRO 90 17.749 20.536 62.266 1.00 15.58
ATOM 780 CA ASN 82 24.177 34.871 58.564 1.00 13.80	ATOM 852 N ASN 91 15.867 21.654 62.717 1.00 14.18
ATOM 781 CB ASN 82 24.262 36.279 59.150 1.00 16.03	ATOM 853 H ASN 91 15.430 22.353 63.236 1.00 0.00
ATOM 782 CG ASN 82 25.135 36.330 60.397 1.00 17.96	ATOM 854 CA ASN 91 15.105 20.883 61.749 1.00 16.21
ATOM 783 OD1 ASN 82 25.202 35.357 61.149 1.00 11.67	ATOM 855 CB ASN 91 13.619 21.115 61.936 1.00 24.97
ATOM 784 ND2 ASN 82 25.806 37.453 60.615 1.00 14.22	ATOM 856 CG ASN 91 12.907 19.885 62.454 1.00 35.60
ATOM 785 HD1 ASN 82 25.720 38.191 59.981 1.00 0.00	ATOM 857 OD1 ASN 91 11.990 19.376 61.815 1.00 42.50
ATOM 786 HD2 ASN 82 26.370 37.486 61.411 1.00 0.00	ATOM 858 ND2 ASN 91 13.322 19.400 62.620 1.00 40.50
ATOM 787 C ASN 82 22.922 34.683 57.719 1.00 17.66	ATOM 859 HD2 ASN 91 14.052 19.830 64.095 1.00 0.00
ATOM 788 O ASN 82 21.896 34.205 58.217 1.00 18.68	ATOM 860 HD2 ASN 91 12.848 18.612 63.957 1.00 0.00
ATOM 789 N ALA 83 23.022 34.980 56.424 1.00 15.35	ATOM 861 C ASN 91 15.543 21.210 60.319 1.00 15.13
ATOM 790 H ALA 83 23.868 35.332 56.076 1.00 0.00	ATOM 862 O ASN 91 15.691 20.316 59.483 1.00 13.21
ATOM 791 CA ALA 83 21.893 34.810 55.504 1.00 15.30	ATOM 863 N ASN 92 15.787 22.488 60.056 1.00 11.44
ATOM 792 CB ALA 83 22.160 35.579 54.199 1.00 16.37	ATOM 864 H ASN 92 15.647 23.155 60.749 1.00 0.00
ATOM 793 C ALA 83 21.602 33.339 55.180 1.00 16.18	ATOM 865 CA ASN 92 16.259 22.916 58.744 1.00 8.74
ATOM 794 O ALA 83 20.448 32.937 55.039 1.00 18.70	ATOM 866 CB ASN 92 16.399 24.435 58.678 1.00 4.08
ATOM 795 N LEU 84 22.649 32.528 55.095 1.00 15.97	ATOM 867 CG ASN 92 15.053 25.140 58.526 1.00 9.59
ATOM 796 H LEU 84 23.548 32.880 55.267 1.00 0.00	ATOM 868 OD1 ASN 92 14.0052 24.508 58.211 1.00 10.61
ATOM 797 CA LEU 84 22.496 31.121 57.757 1.00 14.89	ATOM 869 ND2 ASN 92 15.031 26.445 58.746 1.00 5.11
ATOM 798 CB LEU 84 23.579 30.726 53.739 1.00 12.49	ATOM 870 HD2 ASN 92 15.856 26.910 58.994 1.00 0.00
ATOM 799 CG LEU 84 23.696 31.532 52.433 1.00 9.46	ATOM 871 HD2 ASN 92 14.166 26.896 58.644 1.00 0.00
ATOM 800 CD1 LEU 84 24.793 30.962 51.574 1.00 4.78	ATOM 872 C ASN 92 17.615 22.305 58.508 1.00 7.66
ATOM 801 CD2 LEU 84 22.360 31.529 51.673 1.00 7.79	ATOM 873 O ASN 92 17.862 21.705 57.472 1.00 12.10

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ATOM 802 C LEU 84 22.539 30.173 55.966 1.00 16.23	ATOM 874 N MET 93 18.483 22.420 59.505 1.00 9.04
ATOM 803 O LEU 84 22.945 29.021 55.845 1.00 15.18	ATOM 875 H MET 93 18.203 22.880 60.322 1.00 0.00
ATOM 804 N ASN 85 22.083 60.622 57.125 1.00 17.83	ATOM 876 CA MET 93 19.844 21.888 59.425 1.00 12.35
ATOM 805 H ASN 85 21.729 34.533 57.210 1.00 0.00	ATOM 877 CB MET 93 20.623 22.316 60.671 1.00 12.66
ATOM 806 CA ASN 85 22.139 29.747 58.283 1.00 19.32	ATOM 878 CG MET 93 20.642 23.835 60.897 1.00 18.15
ATOM 807 CB ASN 85 22.730 30.478 59.478 1.00 16.43	ATOM 879 SD MET 93 21.107 24.283 62.597 1.00 21.04
ATOM 808 CB ASN 85 21.807 31.497 60.037 1.00 19.25	ATOM 880 CE MET 93 22.720 23.827 62.582 1.00 8.29
ATOM 809 OD1 ASN 85 20.632 31.559 59.670 1.00 22.86	ATOM 881 C MET 93 19.854 20.361 59.267 1.00 13.02
ATOM 810 ND2 ASN 85 22.323 32.328 60.921 1.00 23.33	ATOM 882 O MET 93 20.702 19.794 58.587 1.00 13.82
ATOM 811 HD21 ASN 85 23.280 32.238 61.168 1.00 0.00	ATOM 883 N ASP 94 18.872 19.708 59.878 1.00 14.47
ATOM 812 HD22 ASN 85 21.744 33.010 61.298 1.00 0.00	ATOM 884 H ASP 94 18.231 20.204 60.404 1.00 0.00
ATOM 813 C ASN 85 20.845 29.032 58.679 1.00 22.92	ATOM 885 CA ASP 94 18.747 18.266 59.792 1.00 13.72
ATOM 814 O ASN 85 20.788 28.420 59.753 1.00 23.44	ATOM 886 CB ASP 94 17.654 17.764 60.764 1.00 16.17
ATOM 815 N GLY 86 19.814 29.109 57.827 1.00 21.89	ATOM 887 CG ASP 94 17.359 16.247 60.607 1.00 17.39
ATOM 816 H GLY 86 19.940 29.596 56.986 1.00 0.00	ATOM 888 OD1 ASP 94 18.338 15.435 60.773 1.00 23.05
ATOM 817 CA GLY 86 18.533 28.447 58.096 1.00 18.54	ATOM 889 OD2 ASP 94 16.220 15.888 60.287 1.00 25.15
ATOM 818 C GLY 86 17.884 28.809 59.431 1.00 17.54	ATOM 890 C ASP 94 18.398 17.880 58.363 1.00 12.80
ATOM 819 O GLY 86 17.151 28.004 60.013 1.00 14.35	ATOM 891 O ASP 94 18.976 16.932 57.818 1.00 10.22
ATOM 820 N ASN 87 18.141 30.036 59.891 1.00 19.78	ATOM 892 N LYS 95 17.440 18.588 57.770 1.00 10.60
ATOM 821 H ASN 87 18.711 30.625 59.355 1.00 0.00	ATOM 893 H LYS 95 17.014 19.325 58.265 1.00 0.00
ATOM 822 CA ASN 87 17.632 30.565 61.169 1.00 23.22	ATOM 894 CA LYS 95 17.019 18.306 56.400 1.00 10.58
ATOM 823 CB ASN 87 16.105 30.476 61.252 1.00 27.67	ATOM 895 CB LYS 95 15.782 19.112 56.043 1.00 14.37
ATOM 824 CG ASN 87 15.423 31.253 60.163 1.00 36.30	ATOM 896 CG LYS 95 14.571 18.826 56.894 1.00 21.95
ATOM 825 OD1 ASN 87 15.759 32.409 59.924 1.00 44.79	ATOM 897 CD LYS 95 14.133 17.395 56.745 1.00 34.60
ATOM 826 ND2 ASN 87 14.468 30.627 59.485 1.00 36.18	ATOM 898 CE LYS 95 12.747 17.186 57.358 1.00 43.52
ATOM 827 HD21 ASN 87 14.227 29.712 59.733 1.00 0.00	ATOM 899 NZ LYS 95 12.570 17.755 58.717 1.00 45.28
ATOM 828 HD22 ASN 87 14.003 31.146 58.797 1.00 0.00	ATOM 900 HZ1 LYS 95 12.928 18.670 58.895 1.00 0.00
ATOM 829 C ASN 87 18.223 29.804 62.349 1.00 23.72	ATOM 901 HZ2 LYS 95 13.245 17.272 59.157 1.00 0.00
ATOM 830 O ASN 87 17.704 29.890 63.466 1.00 23.99	ATOM 902 HZ3 LYS 95 11.741 17.465 59.222 1.00 0.00
ATOM 831 N GLY 88 19.299 29.059 62.090 1.00 19.60	ATOM 903 C LYS 95 18.130 16.647 55.248 1.00 9.18
ATOM 832 H GLY 88 19.679 29.052 61.194 1.00 0.00	ATOM 904 O LYS 95 18.330 17.928 54.461 1.00 10.80
ATOM 833 CA GLY 88 19.929 28.255 63.122 1.00 18.58	ATOM 905 N ALA 96 18.857 19.731 55.718 1.00 9.15
ATOM 834 C GLY 88 18.962 27.204 63.628 1.00 15.03	ATOM 906 H ALA 96 18.629 20.237 56.527 1.00 0.00
ATOM 835 O GLY 88 19.108 26.685 64.725 1.00 15.92	ATOM 907 CA ALA 96 19.975 20.204 54.898 1.00 11.98
ATOM 836 N ASP 89 17.956 26.911 62.824 1.00 14.80	ATOM 908 CB ALA 96 20.547 21.497 55.455 1.00 7.21
ATOM 837 H ASP 89 17.892 27.352 61.958 1.00 0.00	ATOM 909 C ALA 96 21.068 19.159 54.830 1.00 13.36
ATOM 838 CA ASP 89 16.941 25.953 63.185 1.00 12.89	ATOM 910 O ALA 96 21.662 18.956 53.772 1.00 15.09
ATOM 911 N VAL 97 21.348 18.514 55.963 1.00 10.71	ATOM 983 C LYS 102 22.722 13.710 47.218 1.00 13.82
ATOM 912 H VAL 97 20.857 18.752 56.779 1.00 0.00	ATOM 984 O LYS 102 23.048 13.145 46.180 1.00 13.50
ATOM 913 CA VAL 97 22.361 17.469 56.018 1.00 8.78	ATOM 985 N LEU 103 22.997 14.991 47.467 1.00 13.29
ATOM 914 CB VAL 97 22.651 17.066 57.489 1.00 9.36	ATOM 986 H LEU 103 22.713 15.380 48.316 1.00 0.00
ATOM 915 CG1 VAL 97 23.413 15.745 57.563 1.00 9.31	ATOM 987 CA LEU 103 23.708 15.828 46.506 1.00 12.21
ATOM 916 CG2 VAL 97 23.430 18.165 58.164 1.00 3.88	ATOM 988 CB LEU 103 23.791 17.295 56.951 1.00 7.85
ATOM 917 C VAL 97 21.892 16.267 55.193 1.00 7.98	ATOM 989 CG LEU 103 22.526 18.146 46.922 1.00 8.47
ATOM 918 O VAL 97 22.684 15.608 54.514 1.00 8.85	ATOM 990 CD1 LEU 103 22.919 19.595 47.119 1.00 7.33
ATOM 919 N LYS 98 20.593 16.015 55.215 1.00 7.81	ATOM 991 CD2 LEU 103 21.801 17.977 45.599 1.00 10.39
ATOM 920 H LYS 98 20.001 16.577 55.764 1.00 0.00	ATOM 992 C LEU 103 25.099 15.300 46.232 1.00 15.80
ATOM 921 CA LYS 98 20.024 14.904 54.455 1.00 12.54	ATOM 993 O LEU 103 25.624 15.484 45.130 1.00 20.24
ATOM 922 CB LYS 98 18.572 14.655 54.872 1.00 8.12	ATOM 994 N LYS 104 25.702 14.654 47.222 1.00 14.57
ATOM 923 CG LYS 98 18.498 13.903 56.173 1.00 10.36	ATOM 995 H LYS 104 25.253 14.573 48.089 1.00 0.00
ATOM 924 CD LYS 98 17.145 14.029 56.837 1.00 13.11	ATOM 996 CA LYS 104 27.024 14.064 47.048 1.00 16.23
ATOM 925 CE LYS 98 17.122 13.169 58.077 1.00 12.15	ATOM 997 CB LYS 104 27.551 13.495 48.367 1.00 17.01
ATOM 926 NZ LYS 98 15.820 13.292 58.758 1.00 15.93	ATOM 998 CG LYS 104 28.432 14.446 49.132 1.00 22.33
ATOM 927 HZ1 LYS 98 15.061 12.984 58.126 1.00 0.00	ATOM 999 CD1 LYS 104 29.206 13.692 50.185 1.00 26.94
ATOM 928 HZ2 LYS 98 15.667 14.285 59.035 1.00 0.00	ATOM 1000 CE LYS 104 30.608 14.242 50.306 1.00 28.25
ATOM 929 HZ2 LYS 98 15.824 12.701 59.617 1.00 0.00	ATOM 1001 NZ LYS 104 31.378 13.464 51.316 1.00 34.09
ATOM 930 C LYS 98 20.123 15.186 52.960 1.00 12.23	ATOM 1002 HZ1 LYS 104 31.433 12.467 51.038 1.00 0.00
ATOM 931 O LYS 98 20.495 14.301 52.184 1.00 13.83	ATOM 1003 HZ2 LYS 104 30.904 13.537 52.245 1.00 0.00
ATOM 932 N LEU 99 19.807 16.417 52.565 1.00 7.09	ATOM 1004 HZ3 LYS 104 32.342 13.853 51.405 1.00 0.00
ATOM 933 H LEU 99 19.503 17.075 53.224 1.00 0.00	ATOM 1005 C LYS 104 27.011 12.946 45.999 1.00 16.92
ATOM 934 CA LEU 99 19.906 16.801 51.168 1.00 8.07	ATOM 1006 O LYS 104 28.037 12.651 45.400 1.00 20.96
ATOM 935 CB LEU 99 19.427 18.250 50.959 1.00 7.14	ATOM 1007 N ARG 105 25.854 12.327 47.790 1.00 17.39
ATOM 936 CG LEU 99 19.967 18.878 49.578 1.00 5.05	ATOM 1008 H ARG 105 25.072 12.599 46.306 1.00 0.00
ATOM 937 CD1 LEU 99 19.136 17.982 48.436 1.00 7.40	ATOM 1009 CA ARG 105 25.715 11.245 44.815 1.00 17.76
ATOM 938 CD2 LEU 99 18.993 20.232 49.534 1.00 6.20	ATOM 1010 CB ARG 105 24.648 10.263 45.284 1.00 22.55
ATOM 939 C LEU 99 21.358 16.653 50.721 1.00 7.22	ATOM 1011 CG ARG 105 24.920 9.587 46.609 1.00 35.04
ATOM 940 O LEU 99 21.647 16.056 49.482 1.00 9.37	ATOM 1012 CD ARG 105 23.658 8.879 47.073 1.00 44.94
ATOM 941 N TYR 100 22.265 17.176 51.531 1.00 5.02	ATOM 1013 NE ARG 105 23.766 8.360 48.436 1.00 57.02
ATOM 942 H TYR 100 21.967 17.631 52.345 1.00 0.00	ATOM 1014 HE ARG 105 24.630 7.998 48.727 1.00 0.00
ATOM 943 CA TYR 100 23.684 17.117 51.251 1.00 6.66	ATOM 1015 CZ ARG 105 22.772 8.365 49.321 1.00 58.01
ATOM 944 CB TYR 100 24.464 17.708 52.438 1.00 5.94	ATOM 1016 NH1 ARG 105 21.588 8.875 48.996 1.00 56.95
ATOM 945 CG TYR 100 25.959 17.489 52.397 1.00 7.46	ATOM 1017 HH11 ARG 105 21.437 9.249 48.082 1.00 0.00
ATOM 946 CD1 TYR 100 26.713 17.860 51.281 1.00 9.91	ATOM 1018 HH12 ARG 105 20.839 8.860 49.653 1.00 0.00
ATOM 947 CE1 TYR 100 28.087 17.605 51.214 1.00 10.47	ATOM 1019 NH2 ARG 105 22.949 7.817 50.516 1.00 61.23
ATOM 948 CD2 TYR 100 26.622 16.867 53.463 1.00 8.23	ATOM 1020 HH21 ARG 105 23.826 7.408 50.756 1.00 0.00
ATOM 949 CE2 TYR 100 28.005 16.617 53.407 1.00 9.35	ATOM 1021 HH22 ARG 105 22.196 7.815 51.179 1.00 0.00
ATOM 950 CZ TYR 100 28.724 16.984 52.274 1.00 12.51	ATOM 1022 C ARG 105 25.297 11.748 43.437 1.00 18.60
ATOM 951 OH TYR 100 30.067 16.708 52.172 1.00 10.26	ATOM 1023 O ARG 105 25.125 10.955 42.504 1.00 23.60
ATOM 952 HH TYR 100 30.354 16.259 52.970 1.00 0.00	ATOM 1024 N GLU 106 25.013 13.041 43.345 1.00 15.40

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ATOM 953 C TYR 100 24.146 15.700 50.915 1.00 9.97	ATOM 1025 H GLU 106 25.099 13.604 44.137 1.00 0.00
ATOM 954 O TYR 100 24.884 15.497 49.947 1.00 8.51	ATOM 1026 CA GLU 106 24.588 13.650 42.104 1.00 13.48
ATOM 955 N ARG 101 23.696 14.717 51.697 1.00 12.95	ATOM 1027 CB GLU 106 23.639 14.802 42.405 1.00 10.05
ATOM 956 H ARG 101 23.108 14.936 52.453 1.00 0.00	ATOM 1028 CG GLU 106 22.364 14.351 43.053 1.00 14.28
ATOM 957 CA ARG 101 24.077 13.325 51.462 1.00 12.96	ATOM 1029 CD GLU 106 21.611 13.377 42.175 1.00 22.12
ATOM 958 CB ARG 101 23.419 12.396 52.492 1.00 13.49	ATOM 1030 OE1 GLU 106 21.330 13.700 41.000 1.00 23.22
ATOM 959 CG ARG 101 23.793 10.921 52.328 1.00 14.43	ATOM 1031 OE2 GLU 106 21.299 12.273 42.646 1.00 23.74
ATOM 960 CD ARG 101 23.137 10.023 53.381 1.00 11.92	ATOM 1032 C GLU 106 25.793 14.130 41.303 1.00 12.12
ATOM 961 NE ARG 101 23.671 10.254 54.726 1.00 16.66	ATOM 1033 O GLU 106 26.832 14.451 41.862 1.00 11.30
ATOM 962 HE ARG 101 25.545 9.853 54.943 1.00 0.00	ATOM 1034 N ILE 107 25.652 14.180 39.989 1.00 13.18
ATOM 963 CZ ARG 101 23.055 10.945 55.686 1.00 18.57	ATOM 1035 H ILE 107 24.806 13.903 39.587 1.00 0.00
ATOM 964 NH1 ARG 101 21.863 11.496 55.473 1.00 13.14	ATOM 1036 CA ILE 107 26.758 14.617 39.147 1.00 15.12
ATOM 965 HH1 ARG 101 21.428 11.384 54.574 1.00 0.00	ATOM 1037 CB ILE 107 27.479 13.374 38.500 1.00 14.49
ATOM 966 HH12 ARG 101 21.406 12.002 56.188 1.00 0.00	ATOM 1038 CG2 ILE 107 26.531 12.628 37.579 1.00 13.70
ATOM 967 NH2 ARG 101 23.633 11.074 56.871 1.00 13.67	ATOM 1039 CG1 ILE 107 28.789 13.770 37.809 1.00 14.83
ATOM 968 HH21 ARG 101 24.528 10.664 57.044 1.00 0.00	ATOM 1040 CD1 ILE 107 29.835 14.405 38.728 1.00 8.99
ATOM 969 HH22 ARG 101 23.172 11.591 57.593 1.00 0.00	ATOM 1041 C ILE 107 26.303 15.650 38.107 1.00 16.00
ATOM 970 C ARG 101 23.680 12.909 50.041 1.00 14.49	ATOM 1042 O ILE 107 27.120 16.312 37.484 1.00 19.84
ATOM 971 O ARG 101 24.464 12.272 49.327 1.00 12.43	ATOM 1043 N THR 108 24.998 15.872 38.004 1.00 17.53
ATOM 972 N LYS 102 22.462 13.262 49.643 1.00 12.41	ATOM 1044 H THR 108 24.380 15.392 38.587 1.00 0.00
ATOM 973 H LYS 102 21.888 13.773 50.253 1.00 0.00	ATOM 1045 CA THR 108 24.484 16.836 37.037 1.00 14.06
ATOM 974 CA LYS 102 21.971 12.937 48.302 1.00 14.14	ATOM 1046 CB THR 108 23.548 16.172 35.968 1.00 15.28
ATOM 975 CB LYS 102 20.484 13.233 48.175 1.00 10.90	ATOM 1047 OG1 THR 108 22.448 15.532 36.625 1.00 17.64
ATOM 976 CG LYS 102 19.601 12.387 49.047 1.00 10.43	ATOM 1048 HG1 THR 108 21.948 16.185 37.099 1.00 0.00
ATOM 977 CD LYS 102 18.187 12.883 48.941 1.00 12.57	ATOM 1049 CG2 THR 108 24.297 15.130 35.142 1.00 13.09
ATOM 978 CE LYS 102 17.245 12.032 49.758 1.00 16.49	ATOM 1050 C THR 108 23.715 17.945 37.731 1.00 15.45
ATOM 979 NZ LYS 102 15.842 12.523 49.654 1.00 20.07	ATOM 1051 O THR 108 23.231 17.779 38.857 1.00 10.14
ATOM 980 HZ1 LYS 102 15.545 12.498 48.662 1.00 0.00	ATOM 1052 N PHE 109 23.560 19.043 37.000 1.00 9.08
ATOM 981 HZ2 LYS 102 15.809 13.505 50.005 1.00 0.00	ATOM 1053 H PHE 109 23.958 19.059 36.111 1.00 0.00
ATOM 982 HZ3 LYS 102 15.227 11.926 50.233 1.00 0.00	ATOM 1054 CA PHE 109 22.861 20.225 37.447 1.00 9.80
ATOM 1055 CB PHE 109 23.050 21.293 36.382 1.00 8.07	ATOM 1127 O SER 116 14.950 20.960 47.227 1.00 11.86
ATOM 1056 CG PHE 109 22.144 22.454 36.520 1.00 12.25	ATOM 1128 N LEU 117 14.654 20.651 45.019 1.00 12.30
ATOM 1057 CD1 PHE 109 22.320 23.372 37.550 1.00 9.93	ATOM 1129 H LEU 117 15.027 20.299 44.178 1.00 0.00
ATOM 1058 CD2 PHE 109 21.091 22.626 35.630 1.00 12.66	ATOM 1130 CA LEU 117 13.294 21.208 45.021 1.00 15.69
ATOM 1059 CE1 PHE 109 21.456 24.444 37.702 1.00 13.89	ATOM 1131 CB LEU 117 12.720 21.296 43.594 1.00 12.52
ATOM 1060 CE2 PHE 109 20.215 23.699 35.769 1.00 16.94	ATOM 1132 CG LEU 117 13.208 22.443 42.702 1.00 12.20
ATOM 1061 CZ PHE 109 20.397 24.613 36.810 1.00 15.71	ATOM 1133 CD1 LEU 117 12.781 22.194 41.230 1.00 12.94
ATOM 1062 C PHE 109 21.373 19.937 37.687 1.00 16.19	ATOM 1134 CD2 LEU 117 12.679 23.774 43.224 1.00 7.95
ATOM 1063 O PHE 109 20.809 20.304 38.727 1.00 16.01	ATOM 1135 C LEU 117 12.321 20.456 45.939 1.00 12.60
ATOM 1064 N HIS 110 20.736 19.278 36.719 1.00 15.98	ATOM 1136 O LEU 117 11.234 20.949 46.230 1.00 15.03
ATOM 1065 H HIS 110 21.235 19.018 35.931 1.00 0.00	ATOM 1137 N SER 118 12.696 19.258 46.375 1.00 14.56
ATOM 1066 CA HIS 110 19.323 18.948 36.821 1.00 14.96	ATOM 1138 H SER 118 13.557 18.876 46.094 1.00 0.00
ATOM 1067 CB HIS 110 18.750 18.574 35.451 1.00 16.50	ATOM 1139 CA SER 118 11.837 18.492 47.270 1.00 14.85
ATOM 1068 CG HIS 110 18.493 19.757 34.578 1.00 20.40	ATOM 1140 CB SER 118 12.098 16.991 47.140 1.00 11.99
ATOM 1069 CD2 HIS 110 17.485 20.661 34.567 1.00 22.83	ATOM 1141 OG SER 118 13.376 16.632 47.651 1.00 19.51
ATOM 1070 ND1 HIS 110 19.378 20.168 33.603 1.00 25.49	ATOM 1142 HG SER 118 13.402 16.843 48.592 1.00 0.00
ATOM 1071 HD1 HIS 110 20.191 19.712 33.331 1.00 0.00	ATOM 1143 C SER 118 12.051 18.935 48.724 1.00 13.49
ATOM 1072 CE1 HIS 110 18.926 21.276 33.034 1.00 25.22	ATOM 1144 O SER 118 11.454 18.378 49.639 1.00 11.93
ATOM 1073 NE2 HIS 110 17.778 21.591 33.608 1.00 30.14	ATOM 1145 N TYR 119 12.916 19.920 48.932 1.00 12.03
ATOM 1074 HE2 HIS 110 17.232 22.393 33.401 1.00 0.00	ATOM 1146 H TYR 119 13.375 20.336 48.173 1.00 0.00
ATOM 1075 C HIS 110 18.989 17.890 37.864 1.00 12.85	ATOM 1147 CA TYR 119 13.193 20.408 50.271 1.00 9.11
ATOM 1076 O HIS 110 17.955 17.972 38.497 1.00 14.45	ATOM 1148 CB TYR 119 14.700 20.353 50.570 1.00 0.00
ATOM 1077 N GLY 111 19.840 16.886 38.022 1.00 9.71	ATOM 1149 CG TYR 119 15.237 18.950 50.797 1.00 10.85
ATOM 1078 H GLY 111 20.628 16.828 37.470 1.00 0.00	ATOM 1150 CD1 TYR 119 15.611 18.139 49.718 1.00 9.48
ATOM 1079 CA GLY 111 19.583 15.866 39.029 1.00 12.89	ATOM 1151 CE1 TYR 119 16.043 16.828 49.912 1.00 8.37
ATOM 1080 C GLY 111 19.614 16.517 40.408 1.00 15.28	ATOM 1152 CD2 TYR 119 15.324 18.408 52.088 1.00 11.10
ATOM 1081 O GLY 111 18.755 16.296 41.261 1.00 14.53	ATOM 1153 CE2 TYR 119 15.765 17.080 52.295 1.00 8.45
ATOM 1082 N ALA 112 20.594 17.386 40.587 1.00 12.94	ATOM 1154 CZ TYR 119 16.114 16.306 51.201 1.00 7.77
ATOM 1083 H ALA 112 21.220 17.557 39.857 1.00 0.00	ATOM 1155 OH TYR 119 16.521 15.008 51.373 1.00 10.04
ATOM 1084 CA ALA 112 20.775 18.096 41.823 1.00 9.74	ATOM 1156 HH TYR 119 16.514 14.774 52.314 1.00 0.00
ATOM 1085 CB ALA 112 22.064 18.885 41.767 1.00 13.72	ATOM 1157 C TYR 119 12.664 21.819 50.441 1.00 9.59
ATOM 1086 C ALA 112 19.609 19.028 42.031 1.00 11.07	ATOM 1158 O TYR 119 12.523 22.566 49.475 1.00 11.29
ATOM 1087 O ALA 112 19.055 19.091 43.123 1.00 15.67	ATOM 1159 N SER 120 12.352 22.171 51.680 1.00 10.84
ATOM 1088 N LYS 113 19.230 19.768 40.997 1.00 8.32	ATOM 1160 H SER 120 12.469 21.523 52.398 1.00 0.00
ATOM 1089 H LYS 113 19.692 19.688 40.144 1.00 0.00	ATOM 1161 CA SER 120 11.843 23.485 51.990 1.00 12.68
ATOM 1090 CA LYS 113 18.145 20.701 41.137 1.00 8.53	ATOM 1162 CB SER 120 11.317 23.512 53.429 1.00 18.92
ATOM 1091 CB LYS 113 17.987 21.626 39.918 1.00 10.67	ATOM 1163 OG SER 120 12.284 23.052 54.365 1.00 22.03
ATOM 1092 CG LYS 113 16.964 22.735 40.104 1.00 7.70	ATOM 1164 HG SER 120 12.495 22.136 54.145 1.00 0.00
ATOM 1093 CD LYS 113 16.939 23.720 38.939 1.00 12.62	ATOM 1165 C SER 120 12.926 24.535 51.811 1.00 12.21
ATOM 1094 CE LYS 113 16.476 23.066 37.640 1.00 13.25	ATOM 1166 O SER 120 14.104 24.213 51.844 1.00 12.23
ATOM 1095 NZ LYS 113 15.141 22.417 37.758 1.00 19.14	ATOM 1167 N ALA 121 12.518 25.792 51.651 1.00 12.76
ATOM 1096 HZ1 LYS 113 14.428 23.131 38.031 1.00 0.00	ATOM 1168 H ALA 121 11.556 25.972 51.644 1.00 0.00
ATOM 1097 HZ2 LYS 113 15.169 21.679 38.496 1.00 0.00	ATOM 1169 CA ALA 121 13.441 26.914 51.486 1.00 13.79
ATOM 1098 HZ3 LYS 113 14.866 21.988 36.854 1.00 0.00	ATOM 1170 CB ALA 121 12.663 28.203 51.273 1.00 9.93
ATOM 1099 C LYS 113 16.803 19.988 41.424 1.00 9.66	ATOM 1171 C ALA 121 14.415 27.084 52.666 1.00 15.83
ATOM 1100 O LYS 113 16.016 20.454 42.234 1.00 11.59	ATOM 1172 O ALA 121 15.554 27.506 52.463 1.00 18.89
ATOM 1101 N GLU 114 16.578 18.850 40.784 1.00 11.24	ATOM 1173 N GLY 122 13.962 26.792 53.889 1.00 14.13
ATOM 1102 H GLU 114 17.231 18.529 40.141 1.00 0.00	ATOM 1174 H GLY 122 13.040 26.488 54.008 1.00 0.00
ATOM 1103 CA GLU 114 15.369 18.081 41.009 1.00 16.90	ATOM 1175 CA GLY 122 14.821 26.921 55.059 1.00 9.48

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ATOM 1104 CB LGU 114 15.333 16.851 40.110 1.00 24.56	ATOM 1176 C GLY 122 15.946 25.902 55.039 1.00 8.10
ATOM 1105 CG GLU 114 14.960 17.113 38.673 1.00 43.69	ATOM 1177 O GLY 122 17.100 26.236 55.336 1.00 11.50
ATOM 1106 CD GLU 114 15.300 15.930 37.759 1.00 54.79	ATOM 1178 N ALA 123 15.603 24.662 54.680 1.00 6.93
ATOM 1107 OE1 GLU 114 15.628 16.176 36.571 1.00 60.55	ATOM 1179 H ALA 123 14.660 24.480 54.491 1.00 0.00
ATOM 1108 OE2 GLU 114 15.249 14.763 38.227 1.00 58.35	ATOM 1180 CA ALA 123 16.551 23.544 54.575 1.00 9.25
ATOM 1109 C GLU 114 15.276 17.625 42.465 1.00 15.80	ATOM 1181 CB ALA 123 15.803 22.246 54.325 1.00 6.69
ATOM 1110 O GLU 114 14.244 17.810 43.107 1.00 13.65	ATOM 1182 C ALA 123 17.526 23.777 53.437 1.00 10.15
ATOM 1111 N ILE 115 16.337 17.033 43.004 1.00 15.64	ATOM 1183 O ALA 123 18.701 23.431 53.536 1.00 10.03
ATOM 1112 H ILE 115 17.150 16.882 42.469 1.00 0.00	ATOM 1184 N LEU 124 17.011 24.318 52.335 1.00 10.82
ATOM 1113 CA ILE 115 16.255 16.586 44.392 1.00 16.89	ATOM 1185 H LEU 124 16.052 24.510 52.299 1.00 0.00
ATOM 1114 CB ILE 115 17.397 15.623 44.819 1.00 21.22	ATOM 1186 CA LEU 124 17.836 24.613 51.167 1.00 12.02
ATOM 1115 CG2 ILE 115 17.563 14.496 43.815 1.00 21.57	ATOM 1187 CB LEU 124 16.990 25.058 49.962 1.00 11.24
ATOM 1116 CG1 ILE 115 18.711 16.364 44.988 1.00 20.64	ATOM 1188 CG LEU 124 16.325 23.982 49.101 1.00 14.10
ATOM 1117 CD1 ILE 115 19.734 15.522 45.686 1.00 29.19	ATOM 1189 CD1 LEU 124 15.593 24.623 47.938 1.00 17.23
ATOM 1118 C ILE 115 16.156 17.727 45.389 1.00 14.46	ATOM 1190 CD2 LEU 124 17.351 23.015 48.587 1.00 10.37
ATOM 1119 O ILE 115 15.472 17.604 46.407 1.00 14.58	ATOM 1191 C LEU 124 18.855 25.676 51.479 1.00 5.00
ATOM 1120 N SER 116 16.818 18.843 45.102 1.00 11.91	ATOM 1192 O LEU 124 20.022 25.531 51.122 1.00 5.96
ATOM 1121 H SER 116 17.334 18.909 44.269 1.00 0.00	ATOM 1193 N ALA 125 18.421 26.735 52.159 1.00 8.88
ATOM 1122 CA SER 116 16.783 19.989 46.014 1.00 11.85	ATOM 1194 H ALA 125 17.479 26.790 52.419 1.00 0.00
ATOM 1123 CB SER 116 17.802 21.065 45.595 1.00 13.41	ATOM 1195 CA ALA 125 19.324 27.837 52.511 1.00 8.18
ATOM 1124 OG SER 116 19.140 20.570 45.629 1.00 11.32	ATOM 1196 CB ALA 125 18.549 29.018 53.405 1.00 7.28
ATOM 1125 HG SER 116 19.214 19.817 45.010 1.00 0.00	ATOM 1197 C ALA 125 20.369 27.344 53.485 1.00 8.63
ATOM 1126 C SER 116 15.381 20.589 46.133 1.00 12.95	ATOM 1198 O ALA 125 21.541 27.738 53.422 1.00 9.42
ATOM 1199 N SER 126 19.935 26.499 54.412 1.00 10.67	ATOM 1271 N ARG 134 32.044 25.285 53.886 1.00 12.45
ATOM 1200 H SER 126 18.989 26.257 54.447 1.00 0.00	ATOM 1272 H ARG 134 31.389 25.519 53.205 1.00 0.00
ATOM 1201 CA SER 126 20.850 25.942 55.388 1.00 12.02	ATOM 1273 CA ARG 134 32.891 24.120 53.657 1.00 9.53
ATOM 1202 CB SER 126 20.067 25.160 56.449 1.00 14.88	ATOM 1274 CB ARG 134 34.363 24.527 53.513 1.00 10.66
ATOM 1203 OG SER 126 20.917 26.641 57.470 1.00 22.88	ATOM 1275 CG ARG 134 34.705 25.392 52.285 1.00 19.69
ATOM 1204 HG SER 126 21.565 24.046 57.075 1.00 0.00	ATOM 1276 CD ARG 134 36.223 25.622 52.219 1.00 27.89
ATOM 1205 C SER 126 21.876 25.051 54.668 1.00 7.89	ATOM 1277 NE ARG 134 36.693 26.537 51.168 1.00 25.68
ATOM 1206 O SER 126 23.053 25.071 54.983 1.00 10.56	ATOM 1278 HE ARG 134 36.899 26.153 50.297 1.00 0.00
ATOM 1207 N CYS 127 21.426 24.276 53.688 1.00 9.41	ATOM 1279 CZ ARG 134 36.874 27.853 51.323 1.00 29.12
ATOM 1208 H CYS 127 20.478 24.291 53.455 1.00 0.00	ATOM 1280 NH1 ARG 134 36.603 28.446 52.481 1.00 25.56
ATOM 1209 CA CYS 127 22.331 23.407 52.948 1.00 6.08	ATOM 1281 HH11 ARG 134 36.263 27.920 53.223 1.00 0.00
ATOM 1210 CB CYS 127 21.539 22.557 51.957 1.00 4.91	ATOM 1282 HH12 ARG 134 36.739 29.431 52.593 1.00 0.00
ATOM 1211 SG CYS 127 22.497 21.234 51.199 1.00 10.63	ATOM 1283 NH2 ARG 134 37.443 28.569 50.354 1.00 25.85
ATOM 1212 C CYS 127 23.383 24.279 52.247 1.00 7.67	ATOM 1284 HH21 ARG 134 37.733 28.125 49.511 1.00 0.00
ATOM 1213 O CYS 127 24.580 23.977 52.284 1.00 11.04	ATOM 1285 HH22 ARG 134 37.574 29.556 50.473 1.00 0.00
ATOM 1214 N MET 128 22.948 25.395 51.661 1.00 5.72	ATOM 1286 C ARG 134 32.734 23.012 54.710 1.00 11.97
ATOM 1215 H MET 128 21.991 25.610 51.675 1.00 0.00	ATOM 1287 O ARG 134 33.682 22.310 55.041 1.00 12.26
ATOM 1216 CA MET 128 23.869 26.305 50.992 1.00 7.03	ATOM 1288 N MET 135 31.549 22.895 55.289 1.00 10.32
ATOM 1217 CB MET 128 23.119 27.473 50.327 1.00 5.99	ATOM 1289 H MET 135 30.838 23.533 55.085 1.00 0.00
ATOM 1218 CG MET 128 22.413 27.133 48.981 1.00 8.59	ATOM 1290 CA MET 135 31.304 21.812 56.228 1.00 13.20
ATOM 1219 SD MET 128 21.495 28.555 48.317 1.00 11.63	ATOM 1291 CB MET 135 30.159 22.159 57.172 1.00 9.31
ATOM 1220 CE MET 128 22.764 29.725 48.392 1.00 13.39	ATOM 1292 CG MET 135 30.484 23.321 58.095 1.00 16.72
ATOM 1221 C MET 128 24.880 26.836 51.999 1.00 9.78	ATOM 1293 SD MET 135 29.594 23.266 59.649 1.00 18.85
ATOM 1222 O MET 128 26.051 27.000 51.677 1.00 12.00	ATOM 1294 CE MET 135 30.752 22.203 30.639 1.00 7.14
ATOM 1223 N GLY 129 24.431 27.138 53.211 1.00 9.57	ATOM 1295 C MET 135 30.956 20.577 55.386 1.00 16.58
ATOM 1224 H GLY 129 23.483 27.039 53.433 1.00 0.00	ATOM 1296 O MET 135 30.794 19.473 55.908 1.00 18.62
ATOM 1225 CA GLY 129 25.363 27.615 54.217 1.00 12.54	ATOM 1297 N GLY 136 30.788 20.789 54.081 1.00 13.75
ATOM 1226 C GLY 129 26.402 26.546 54.541 1.00 15.15	ATOM 1298 H GLY 136 30.868 21.694 53.723 1.00 0.00
ATOM 1227 O GLY 129 27.584 26.824 54.699 1.00 15.41	ATOM 1299 CA GLY 136 30.497 19.698 53.168 1.00 9.23
ATOM 1228 N LEU 130 25.958 25.298 54.583 1.00 16.07	ATOM 1300 C GLY 136 30.952 20.130 51.786 1.00 9.05
ATOM 1229 H LEU 130 25.003 25.137 54.414 1.00 0.00	ATOM 1301 O GLY 136 31.220 21.312 51.595 1.00 10.44
ATOM 1230 CA LEU 130 26.815 24.165 54.874 1.00 14.53	ATOM 1302 N ALA 137 31.084 19.199 50.841 1.00 8.78
ATOM 1231 CB LEU 130 25.933 22.928 54.933 1.00 13.30	ATOM 1303 H ALA 137 30.881 18.270 51.062 1.00 0.00
ATOM 1232 CG LEU 130 26.499 21.651 55.501 1.00 19.80	ATOM 1304 CA ALA 137 31.502 19.538 49.478 1.00 7.06
ATOM 1233 CD1 LEU 130 25.340 20.802 55.983 1.00 20.50	ATOM 1305 CB ALA 137 33.003 19.352 49.309 1.00 7.32
ATOM 1234 CD2 LEU 130 27.298 20.934 54.411 1.00 19.97	ATOM 1306 C ALA 137 30.771 18.725 48.432 1.00 7.65
ATOM 1235 C LEU 130 27.939 24.019 53.830 1.00 14.41	ATOM 1307 O ALA 137 30.471 17.556 48.655 1.00 11.86
ATOM 1236 O LEU 130 29.094 23.766 54.166 1.00 11.24	ATOM 1308 N VAL 138 30.430 19.380 47.318 1.00 12.92
ATOM 1237 N ILE 131 27.587 24.165 52.561 1.00 12.46	ATOM 1309 H VAL 138 30.650 20.336 47.254 1.00 0.00
ATOM 1238 H ILE 131 26.645 24.335 52.344 1.00 0.00	ATOM 1310 CA VAL 138 29.747 18.761 46.169 1.00 10.65
ATOM 1239 CA ILE 131 28.564 24.077 51.486 1.00 13.33	ATOM 1311 CB VAL 138 28.233 19.106 46.136 1.00 7.32
ATOM 1240 CB ILE 131 27.865 23.949 50.094 1.00 10.82	ATOM 1312 CG1 VAL 138 27.493 18.422 47.301 1.00 4.42
ATOM 1241 CG2 ILE 131 28.915 23.970 48.988 1.00 17.49	ATOM 1313 CG2 VAL 138 27.999 20.624 46.176 1.00 3.67
ATOM 1242 CG1 ILE 131 27.041 22.660 50.003 1.00 7.85	ATOM 1314 C VAL 138 30.418 19.307 44.894 1.00 12.61
ATOM 1243 CD1 ILE 131 27.848 24.107 50.068 1.00 10.42	ATOM 1315 O VAL 138 31.216 20.247 44.964 1.00 13.30
ATOM 1244 C ILE 131 29.438 25.351 51.500 1.00 11.32	ATOM 1316 N THR 139 30.145 18.712 43.739 1.00 12.53
ATOM 1245 O ILE 131 30.660 25.288 51.398 1.00 9.76	ATOM 1317 H THR 139 29.567 17.932 43.720 1.00 0.00
ATOM 1246 N TYR 132 28.802 26.507 51.661 1.00 11.05	ATOM 1318 CA THR 139 30.736 19.226 42.501 1.00 11.01
ATOM 1247 H TYR 132 27.836 26.500 51.763 1.00 0.00	ATOM 1319 CB THR 139 30.513 18.262 41.344 1.00 9.71
ATOM 1248 CA TYR 132 29.512 27.778 51.688 1.00 13.75	ATOM 1320 OG1 THR 139 29.132 17.898 41.284 1.00 11.98
ATOM 1249 CB TYR 132 28.529 28.913 51.985 1.00 13.06	ATOM 1321 HG1 THR 139 28.888 17.482 42.106 1.00 0.00
ATOM 1250 CG TYR 132 29.177 30.277 51.998 1.00 14.32	ATOM 1322 CG2 THR 139 31.336 17.015 41.535 1.00 13.10
ATOM 1251 CD1 TYR 132 29.758 30.824 50.833 1.00 8.32	ATOM 1323 C THR 139 30.085 20.574 42.189 1.00 8.25
ATOM 1252 CE1 TYR 132 30.405 32.063 50.869 1.00 7.98	ATOM 1324 O THR 139 28.966 20.822 42.616 1.00 10.07
ATOM 1253 CD2 TYR 132 29.258 31.002 53.183 1.00 9.90	ATOM 1325 N THR 140 30.767 21.419 41.422 1.00 8.47
ATOM 1254 CE2 TYR 132 29.893 32.218 53.230 1.00 8.74	ATOM 1326 H THR 140 31.639 21.135 41.069 1.00 0.00

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ATOM 1255 CZ TYR 132 30.464 32.752 52.088 1.00 10.10	ATOM 1327 CA THR 140 30.278 22.754 41.072 1.00 10.58
ATOM 1256 OH TYR 132 31.066 33.981 52.240 1.00 10.50	ATOM 1328 CB THR 140 31.245 23.459 40.094 1.00 11.37
ATOM 1257 HH TYR 132 31.388 34.204 51.423 1.00 0.00	ATOM 1329 OG1 THR 140 32.573 23.362 40.589 1.00 19.59
ATOM 1258 C TYR 132 30.618 27.792 52.735 1.00 14.84	ATOM 1330 HG1 THR 140 32.634 23.764 41.459 1.00 0.00
ATOM 1259 O TYR 132 31.732 28.260 52.487 1.00 12.02	ATOM 1331 CG2 THR 140 30.933 24.928 39.970 1.00 11.42
ATOM 1260 N ASN 133 30.275 27.294 53.917 1.00 16.11	ATOM 1332 C THR 140 28.886 22.814 40.458 1.00 9.63
ATOM 1261 H ASN 133 29.374 26.944 54.032 1.00 0.00	ATOM 1333 O THR 140 28.068 23.645 80.844 1.00 9.01
ATOM 1262 CA ASN 133 31.187 27.235 55.041 1.00 14.06	ATOM 1334 N GLU 141 28.627 21.954 39.483 1.00 8.40
ATOM 1263 CB ASN 133 30.401 27.245 56.347 1.00 10.32	ATOM 1335 H GLU 141 29.300 21.295 39.233 1.00 0.00
ATOM 1264 CG ASN 133 29.832 28.617 56.664 1.00 13.22	ATOM 1336 CA GLU 141 27.336 21.948 38.800 1.00 10.65
ATOM 1265 OD1 ASN 133 30.543 26.609 56.630 1.00 14.06	ATOM 1337 CB GLU 141 27.426 21.090 37.530 1.00 13.62
ATOM 1266 ND2 ASN 133 28.541 28.676 56.968 1.00 12.50	ATOM 1338 CG GLU 141 28.579 21.501 36.566 1.00 10.12
ATOM 1267 HD21 ASN 133 28.008 27.858 56.963 1.00 0.00	ATOM 1339 CD GLU 141 29.953 21.031 37.030 1.00 10.60
ATOM 1268 HD22 ASN 133 28.172 29.568 57.155 1.00 0.00	ATOM 1340 OE1 GLU 141 30.046 19.981 37.684 1.00 16.76
ATOM 1269 C ASN 133 32.130 26.043 57.976 1.00 11.53	ATOM 1341 OE2 GLU 141 30.952 21.713 36.755 1.00 17.34
ATOM 1270 O ASN 133 32.919 25.824 55.887 1.00 12.37	ATOM 1342 C GLU 141 26.188 21.494 39.722 1.00 9.83
ATOM 1343 O GLU 141 25.043 21.915 39.564 1.00 7.25	ATOM 1415 H CYS 151 17.337 29.032 44.202 1.00 0.00
ATOM 1344 N VAL 142 26.520 20.640 40.689 1.00 10.61	ATOM 1416 CA CYS 151 15.981 30.618 43.803 1.00 11.02
ATOM 1345 H VAL 142 27.444 20.317 40.736 1.00 0.00	ATOM 1417 CB CYS 151 16.856 30.947 42.605 1.00 8.67
ATOM 1346 CA VAL 142 25.561 20.153 41.672 1.00 8.00	ATOM 1418 SG CYS 151 18.366 31.666 43.084 1.00 15.75
ATOM 1347 CB VAL 142 26.127 18.894 42.411 1.00 7.01	ATOM 1419 C CYS 151 14.603 30.340 43.285 1.00 11.21
ATOM 1348 CG1 VAL 142 25.362 18.605 43.682 1.00 9.50	ATOM 1420 O CYS 151 13.723 31.167 43.379 1.00 15.23
ATOM 1349 CG2 VAL 142 26.025 17.685 41.521 1.00 6.00	ATOM 1421 N GLU 152 14.445 29.179 42.676 1.00 12.23
ATOM 1350 C VAL 142 25.260 21.332 42.625 1.00 9.83	ATOM 1422 H GLU 152 15.206 28.570 42.595 1.00 0.00
ATOM 1351 O VAL 142 24.101 21.575 42.982 1.00 11.75	ATOM 1423 CA GLU 152 13.170 28.772 42.138 1.00 17.47
ATOM 1352 N ALA 143 23.293 22.110 42.967 1.00 9.16	ATOM 1424 CB GLU 152 13.330 27.415 41.456 1.00 15.93
ATOM 1353 H ALA 143 27.180 21.895 42.609 1.00 0.00	ATOM 1425 CG GLU 152 12.115 26.929 40.717 1.00 21.04
ATOM 1354 CA ALA 143 26.137 23.270 43.840 1.00 6.52	ATOM 1426 CD GLU 152 12.413 25.747 39.816 1.00 24.99
ATOM 1355 CB ALA 143 27.502 23.882 44.171 1.00 5.45	ATOM 1427 OE1 GLU 152 13.578 25.306 39.752 1.00 25.94
ATOM 1356 C ALA 143 25.255 24.296 43.129 1.00 11.05	ATOM 1428 OE2 GLU 152 11.476 25.259 39.155 1.00 32.48
ATOM 1357 O ALA 143 24.456 24.986 43.763 1.00 12.06	ATOM 1429 C GLU 152 12.116 28.737 43.266 1.00 22.62
ATOM 1358 N PHE 144 25.403 24.402 41.807 1.00 12.68	ATOM 1430 O GLU 152 11.021 29.287 43.106 1.00 21.98
ATOM 1359 H PHE 144 26.066 23.849 41.353 1.00 0.00	ATOM 1431 N GLN 153 12.457 28.143 44.414 1.00 22.64
ATOM 1360 CA PHE 144 24.598 25.333 41.020 1.00 6.76	ATOM 1432 H GLN 153 13.345 27.752 44.504 1.00 0.00
ATOM 1361 CB PHE 144 25.059 25.377 39.551 1.00 7.23	ATOM 1433 CA GLN 153 11.522 28.077 45.539 1.00 22.96
ATOM 1362 CG PHE 144 26.392 26.061 39.325 1.00 8.19	ATOM 1434 CB GLN 153 12.133 27.336 46.735 1.00 25.41
ATOM 1363 CD1 PHE 144 27.163 25.735 38.222 1.00 9.21	ATOM 1435 CG GLN 153 12.473 25.881 46.509 1.00 26.48
ATOM 1364 CD2 PHE 144 26.857 27.048 40.189 1.00 11.80	ATOM 1436 CD GLN 153 11.257 24.984 46.406 1.00 26.11
ATOM 1365 CE1 PHE 144 28.379 26.382 37.979 1.00 8.34	ATOM 1437 OE1 GLN 153 10.402 25.159 45.530 1.00 30.11
ATOM 1366 CE2 PHE 144 28.073 27.697 39.954 1.00 10.30	ATOM 1438 NE2 GLN 153 11.210 23.971 47.249 1.00 24.58
ATOM 1367 CZ PHE 144 28.829 27.366 38.850 1.00 10.79	ATOM 1439 HE21 GLN 153 11.947 23.833 47.892 1.00 0.00
ATOM 1368 C PHE 144 23.133 24.890 41.083 1.00 6.24	ATOM 1440 HE22 GLN 153 10.447 23.371 47.205 1.00 0.00
ATOM 1369 O PHE 144 22.243 25.718 41.224 1.00 10.40	ATOM 1441 C GLN 153 11.135 29.483 45.990 1.00 23.13
ATOM 1370 N GLY 145 22.889 23.588 40.944 1.00 7.95	ATOM 1442 O GLN 153 9.957 29.789 46.153 1.00 27.09
ATOM 1371 H GLY 145 23.638 22.971 40.806 1.00 0.00	ATOM 1443 N ILE 154 12.134 30.341 46.158 1.00 23.64
ATOM 1372 CA GLY 145 21.532 23.064 41.007 1.00 9.52	ATOM 1444 H ILE 154 13.048 30.044 45.970 1.00 0.00
ATOM 1373 C GLY 145 20.878 23.367 42.360 1.00 13.71	ATOM 1445 CA ILE 154 11.931 31.713 46.646 1.00 24.34
ATOM 1374 O GLY 145 19.689 23.669 42.440 1.00 16.36	ATOM 1446 CB ILE 154 13.286 32.426 46.899 1.00 26.55
ATOM 1375 N LEU 146 21.654 23.283 43.435 1.00 11.72	ATOM 1447 CG2 ILE 154 13.046 33.849 47.393 1.00 29.89
ATOM 1376 H LEU 146 22.592 23.012 43.323 1.00 0.00	ATOM 1448 CG1 ILE 154 14.092 31.664 47.948 1.00 26.58
ATOM 1377 CA LEU 146 21.155 23.588 44.768 1.00 9.87	ATOM 1449 CD1 ILE 154 15.382 32.348 48.310 1.00 27.39
ATOM 1378 CB LEU 146 22.230 23.268 45.821 1.00 6.53	ATOM 1450 C ILE 154 11.147 32.565 45.630 1.00 23.64
ATOM 1379 CG LEU 146 22.049 23.850 47.227 1.00 3.71	ATOM 1451 O ILE 154 10.274 33.345 46.018 1.00 23.27
ATOM 1380 CD1 LEU 146 20.866 23.208 47.910 1.00 4.97	ATOM 1452 N ALA 155 11.486 32.445 44.357 1.00 22.50
ATOM 1381 CD2 LEU 146 23.301 23.644 48.048 1.00 6.08	ATOM 1453 H ALA 155 12.197 31.832 44.107 1.00 0.00
ATOM 1382 C LEU 146 20.759 25.079 44.853 1.00 12.57	ATOM 1454 CA ALA 155 10.816 33.216 43.326 1.00 24.60
ATOM 1383 O LEU 146 19.643 25.416 45.281 1.00 12.75	ATOM 1455 CB ALA 155 11.469 32.957 41.959 1.00 15.01
ATOM 1384 N VAL 147 21.656 25.983 44.457 1.00 12.23	ATOM 1456 C ALA 155 9.330 32.867 43.303 1.00 25.67
ATOM 1385 H VAL 147 22.537 25.704 44.130 1.00 0.00	ATOM 1457 O ALA 155 8.488 33.752 43.229 1.00 26.42
ATOM 1386 CA VAL 147 21.300 27.398 44.534 1.00 12.12	ATOM 1458 N ASP 156 9.019 31.583 43.458 1.00 30.93
ATOM 1387 CB VAL 147 22.516 28.366 44.375 1.00 14.02	ATOM 1459 H ASP 156 9.740 30.926 43.585 1.00 0.00
ATOM 1388 CG1 VAL 147 23.239 28.131 43.103 1.00 13.40	ATOM 1460 CA ASP 156 7.634 31.118 43.445 1.00 36.44
ATOM 1389 CG2 VAL 147 22.054 29.816 44.466 1.00 14.74	ATOM 1461 CB ASP 156 7.753 29.600 43.310 1.00 42.76
ATOM 1390 C VAL 147 20.158 27.731 43.590 1.00 13.59	ATOM 1462 CG ASP 156 8.105 29.112 41.959 1.00 49.60
ATOM 1391 O VAL 147 19.328 28.573 43.917 1.00 13.65	ATOM 1463 OD1 ASP 156 8.003 29.818 40.946 1.00 54.15
ATOM 1392 N CYS 148 20.075 27.044 42.445 1.00 12.84	ATOM 1464 OD2 ASP 156 8.647 28.010 41.874 1.00 53.52
ATOM 1393 H CYS 148 20.752 26.372 42.236 1.00 0.00	ATOM 1465 C ASP 156 6.820 31.577 44.642 1.00 37.91
ATOM 1394 CA CYS 148 19.877 27.292 41.496 1.00 13.53	ATOM 1466 O ASP 156 5.595 31.622 44.567 1.00 38.75
ATOM 1395 CB CYS 148 19.293 26.725 40.106 1.00 6.40	ATOM 1467 N SER 157 7.487 31.906 45.746 1.00 36.87
ATOM 1396 SG CYS 148 20.564 27.738 39.334 1.00 11.77	ATOM 1468 H SER 157 8.453 31.806 45.770 1.00 0.00
ATOM 1397 C CYS 148 17.617 26.812 42.018 1.00 12.91	ATOM 1469 CA SER 157 6.788 32.397 46.939 1.00 36.20
ATOM 1398 O CYS 148 16.601 27.460 41.790 1.00 15.45	ATOM 1470 CB SER 157 7.691 32.313 48.184 1.00 30.91
ATOM 1399 N ALA 149 17.604 25.684 42.726 1.00 17.88	ATOM 1471 OG SER 157 8.608 33.394 48.273 1.00 16.54
ATOM 1400 H ALA 149 18.438 25.186 42.845 1.00 0.00	ATOM 1472 HG SER 157 9.181 33.403 47.503 1.00 0.00
ATOM 1401 CA ALA 149 16.380 25.156 43.329 1.00 15.13	ATOM 1473 C SER 157 6.347 33.854 46.696 1.00 41.61
ATOM 1402 CB ALA 149 16.648 23.807 43.981 1.00 9.57	ATOM 1474 O SER 157 5.419 34.354 47.344 1.00 38.48
ATOM 1403 C ALA 149 15.904 26.160 44.386 1.00 15.41	ATOM 1475 N GLN 158 7.050 34.525 45.783 1.00 47.31
ATOM 1404 O ALA 149 14.718 26.471 44.472 1.00 17.40	ATOM 1476 H GLN 158 7.786 34.078 45.331 1.00 0.00
ATOM 1405 N THR 150 16.843 26.687 45.167 1.00 14.69	ATOM 1477 CA GLN 158 6.771 35.909 45.409 1.00 52.71

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ATOM 1406 H THR 150 17.780 26.411 45.057 1.00 0.00	ATOM 1478 CB GLN 158 8.006 36.526 44.739 1.00 51.04
ATOM 1407 CA THR 150 16.516 27.672 46.198 1.00 15.98	ATOM 1479 CG GLN 158 9.288 36.477 45.567 1.00 49.19
ATOM 1408 CB THR 150 17.751 28.068 47.011 1.00 13.74	ATOM 1480 CD GLN 158 10.540 36.886 44.779 1.00 48.92
ATOM 1409 OG1 THR 150 18.472 26.881 47.370 1.00 15.40	ATOM 1481 OE1 GLN 158 10.489 37.188 43.583 1.00 46.55
ATOM 1410 HG1 THR 150 17.908 26.319 47.899 1.00 0.00	ATOM 1482 NE2 GLN 158 11.672 36.891 45.459 1.00 48.60
ATOM 1411 CG2 THR 150 17.330 28.823 48.286 1.00 18.44	ATOM 1483 HE21 GLN 158 11.666 36.647 46.402 1.00 0.00
ATOM 1412 C THR 150 15.895 28.920 45.585 1.00 14.15	ATOM 1484 HE22 GLN 158 12.481 37.152 44.965 1.00 0.00
ATOM 1413 O THR 150 14.891 29.408 46.083 1.00 18.21	ATOM 1485 C GLN 158 5.558 36.009 44.455 1.00 58.48
ATOM 1414 N CYS 151 16.501 29.443 44.518 1.00 14.47	ATOM 1486 O GLN 158 4.951 37.104 44.376 1.00 61.29
ATOM 1487 OT GLN 158 5.217 35.003 43.784 1.00 62.85	ATOM 1559 CG2 THR 209 42.205 23.739 85.218 1.00 23.14
ATOM 1488 CB SER 202 36.503 31.482 88.093 1.00 45.76	ATOM 1560 C THR 209 41.763 22.320 81.650 1.00 15.53
ATOM 1489 OG SER 202 37.808 31.091 87.693 1.00 43.89	ATOM 1561 O THR 209 42.573 21.507 81.209 1.00 19.41
ATOM 1490 HG SER 202 38.263 30.678 88.441 1.00 0.00	ATOM 1562 N TYR 210 40.511 22.370 81.214 1.00 13.91
ATOM 1491 C SER 202 35.492 29.342 87.320 1.00 42.83	ATOM 1563 H TYR 210 39.880 23.019 81.592 1.00 0.00
ATOM 1492 O SER 202 36.292 28.427 87.125 1.00 40.83	ATOM 1564 CA TYR 210 40.092 21.444 80.173 1.00 12.82
ATOM 1493 HT1 SER 202 37.295 29.247 89.283 1.00 0.00	ATOM 1565 CB TYR 210 38.594 21.556 79.899 1.00 13.43
ATOM 1494 HT2 SER 202 35.803 28.722 89.898 1.00 0.00	ATOM 1566 CG TYR 210 37.728 20.773 80.845 1.00 11.53
ATOM 1495 N SER 202 36.367 29.547 89.639 1.00 45.24	ATOM 1567 CD1 TYR 210 37.038 21.412 81.883 1.00 12.85
ATOM 1496 HT3 SER 202 36.479 30.200 90.432 1.00 0.00	ATOM 1568 CE1 TYR 210 36.185 20.686 82.735 1.00 11.80
ATOM 1497 CA SER 202 35.672 30.268 88.522 1.00 44.26	ATOM 1569 CD2 TYR 210 37.559 19.392 80.678 1.00 10.21
ATOM 1498 N LEU 203 34.479 29.616 86.490 1.00 39.07	ATOM 1570 CE2 TYR 210 36.712 18.657 81.516 1.00 7.26
ATOM 1499 H LEU 203 33.890 30.381 86.690 1.00 0.00	ATOM 1571 CZ TYR 210 36.025 19.310 82.539 1.00 7.27
ATOM 1500 CA LEU 203 34.231 28.798 85.311 1.00 34.20	ATOM 1572 OH TYR 210 35.154 18.589 83.325 1.00 7.76
ATOM 1501 CB LEU 203 32.999 29.288 84.556 1.00 33.82	ATOM 1573 HH TYR 210 34.749 19.169 83.973 1.00 0.00
ATOM 1502 CG LEU 203 32.147 28.180 83.921 1.00 33.57	ATOM 1574 C TYR 210 40.861 21.792 78.907 1.00 12.95
ATOM 1503 CD1 LEU 203 31.308 28.746 82.779 1.00 30.93	ATOM 1575 O TYR 210 41.433 20.925 78.261 1.00 13.94
ATOM 1504 CD2 LEU 203 33.024 27.039 43.413 1.00 37.57	ATOM 1576 N VAL 211 40.890 23.069 78.561 1.00 15.03
ATOM 1505 C LEU 203 35.441 28.890 84.388 1.00 31.19	ATOM 1577 H VAL 211 40.443 23.706 79.118 1.00 0.00
ATOM 1506 O LEU 203 35.972 27.873 83.940 1.00 30.08	ATOM 1578 CA VAL 211 41.589 23.509 77.362 1.00 16.63
ATOM 1507 N LEU 204 35.909 30.117 84.174 1.00 27.77	ATOM 1579 CB VAL 211 41.417 25.043 77.137 1.00 16.75
ATOM 1508 H LEU 204 35.472 30.881 84.586 1.00 0.00	ATOM 1580 CG1 VAL 211 42.283 25.522 75.999 1.00 13.39
ATOM 1509 CA LEU 204 37.053 30.373 83.311 1.00 26.50	ATOM 1581 CG2 VAL 211 39.966 25.651 78.801 1.00 6.94
ATOM 1510 CB LEU 204 37.363 31.872 83.243 1.00 27.74	ATOM 1582 C VAL 211 43.061 23.090 77.356 1.00 18.10
ATOM 1511 CG LEU 204 36.361 32.735 82.450 1.00 33.57	ATOM 1583 O VAL 211 43.530 22.481 76.384 1.00 19.38
ATOM 1512 CD1 LEU 204 36.818 34.183 82.453 1.00 34.61	ATOM 1584 N LEU 212 43.765 23.321 78.463 1.00 16.58
ATOM 1513 CD2 LEU 204 36.201 32.240 80.998 1.00 30.17	ATOM 1585 H LEU 212 43.332 23.744 79.224 1.00 0.00
ATOM 1514 C LEU 204 38.286 29.571 83.692 1.00 24.23	ATOM 1586 CA LEU 212 45.176 22.958 78.540 1.00 12.67
ATOM 1515 O LEU 204 39.069 29.190 82.823 1.00 24.00	ATOM 1587 CB LEU 212 45.816 23.527 79.804 1.00 17.11
ATOM 1516 N THR 205 38.432 29.260 84.975 1.00 22.66	ATOM 1588 CG LEU 212 45.843 25.052 79.896 1.00 21.80
ATOM 1517 H THR 205 37.771 29.545 85.623 1.00 0.00	ATOM 1589 CD1 LEU 212 46.459 25.467 81.212 1.00 23.26
ATOM 1518 CA THR 205 39.574 28.467 85.416 1.00 22.80	ATOM 1590 CD2 LEU 212 46.636 25.630 78.739 1.00 21.56
ATOM 1519 CB THR 205 39.830 28.604 86.927 1.00 23.16	ATOM 1591 C LEU 212 45.435 21.471 78.472 1.00 12.30
ATOM 1520 OG1 THR 205 40.291 29.933 87.211 1.00 27.63	ATOM 1592 O LEU 212 46.508 21.056 78.063 1.00 17.88
ATOM 1521 HG1 THR 205 39.637 30.576 86.910 1.00 0.00	ATOM 1593 N SER 213 44.450 20.655 78.815 1.00 14.49
ATOM 1522 CG2 THR 205 40.868 27.601 87.402 1.00 21.83	ATOM 1594 H SER 213 43.577 21.018 79.074 1.00 0.00
ATOM 1523 C THR 205 39.338 27.015 85.046 1.00 21.86	ATOM 1595 CA SER 213 44.648 19.209 78.799 1.00 14.39
ATOM 1524 O THR 205 40.260 26.308 74.638 1.00 21.85	ATOM 1596 CB SER 213 43.479 18.495 79.472 1.00 13.96
ATOM 1525 N GLU 206 38.086 26.588 85.126 1.00 22.68	ATOM 1597 OG SER 213 42.325 18.512 78.665 1.00 18.43
ATOM 1526 H GLU 206 37.373 27.199 85.410 1.00 0.00	ATOM 1598 HG SER 213 42.078 19.380 78.505 1.00 0.00
ATOM 1527 CA GLU 206 37.752 25.220 84.780 1.00 21.05	ATOM 1599 C SER 213 44.916 18.585 77.437 1.00 15.86
ATOM 1528 CB GLU 206 36.322 24.908 85.166 1.00 21.51	ATOM 1600 O SER 213 45.407 17.464 77.363 1.00 15.00
ATOM 1529 CG GLU 206 35.980 23.454 84.934 1.00 19.38	ATOM 1601 N ILE 214 44.562 19.274 76.357 1.00 18.77
ATOM 1530 CD GLU 206 34.672 23.065 85.548 1.00 21.06	ATOM 1602 H ILE 214 44.136 20.152 76.455 1.00 0.00
ATOM 1531 OE1 GLU 206 34.314 21.880 85.431 1.00 23.08	ATOM 1603 CA ILE 214 44.815 18.717 75.026 1.00 21.44
ATOM 1532 OE2 GLU 206 33.996 23.942 86.144 1.00 26.46	ATOM 1604 CB ILE 214 43.693 19.069 74.001 1.00 19.51
ATOM 1533 C GLU 206 37.930 24.992 83.296 1.00 21.34	ATOM 1605 CG2 ILE 214 42.354 18.547 74.470 1.00 14.52
ATOM 1534 O GLU 206 38.400 23.934 82.868 1.00 21.36	ATOM 1606 CG1 ILE 214 43.663 20.575 73.733 1.00 17.72
ATOM 1535 N VAL 207 37.530 25.990 82.517 1.00 22.28	ATOM 1607 CD1 ILE 214 42.710 20.977 72.639 1.00 16.15
ATOM 1536 H VAL 207 37.142 26.781 82.937 1.00 0.00	ATOM 1608 C ILE 214 46.175 19.162 74.448 1.00 23.04
ATOM 1537 CA VAL 207 37.637 25.953 81.068 1.00 17.29	ATOM 1609 O ILE 214 46.624 18.639 73.427 1.00 27.72
ATOM 1538 CB VAL 207 37.037 27.236 80.453 1.00 19.23	ATOM 1610 N ILE 215 46.810 20.139 75.083 1.00 23.66
ATOM 1539 CG1 VAL 207 37.363 27.324 78.956 1.00 18.06	ATOM 1611 H ILE 215 46.413 20.518 75.891 1.00 0.00
ATOM 1540 CG2 VAL 207 35.528 27.266 80.681 1.00 20.90	ATOM 1612 CA ILE 215 48.099 20.662 74.628 1.00 25.79
ATOM 1541 C VAL 207 39.110 25.868 80.706 1.00 17.78	ATOM 1613 CB ILE 215 48.234 22.168 74.995 1.00 25.29
ATOM 1542 O VAL 207 39.523 25.052 79.887 1.00 21.08	ATOM 1614 CG2 ILE 215 49.524 22.736 74.453 1.00 27.20
ATOM 1543 N GLU 208 39.919 26.681 81.366 1.00 18.92	ATOM 1615 CG1 ILE 215 47.052 22.950 74.429 1.00 23.49
ATOM 1544 H GLU 208 39.557 27.293 82.038 1.00 0.00	ATOM 1616 CD1 ILE 215 46.488 24.287 75.039 1.00 23.80
ATOM 1545 CA GLU 208 41.340 26.686 81.086 1.00 17.84	ATOM 1617 C ILE 215 49.264 19.872 75.248 1.00 29.29
ATOM 1546 CB GLU 208 42.036 27.785 81.880 1.00 17.11	ATOM 1618 O ILE 215 49.320 19.665 76.472 1.00 26.95
ATOM 1547 CG GLU 208 43.503 27.882 81.589 1.00 18.26	ATOM 1619 N PRO 216 50.188 19.377 74.405 1.00 32.63
ATOM 1548 CD GLU 208 44.211 28.873 82.481 1.00 22.55	ATOM 1620 CD PRO 216 50.265 19.472 72.935 1.00 36.17
ATOM 1549 OE1 GLU 208 43.533 29.622 83.224 1.00 26.35	ATOM 1621 CA PRO 216 51.321 18.621 74.943 1.00 32.44
ATOM 1550 OE2 GLU 208 45.460 28.899 82.434 1.00 25.84	ATOM 1622 CB PRO 216 52.023 18.113 73.683 1.00 33.48
ATOM 1551 C GLU 208 41.987 25.332 81.348 10.00 17.60	ATOM 1623 CG PRO 216 51.726 19.190 72.673 1.00 35.65
ATOM 1552 O GLU 208 42.847 24.906 80.570 1.00 21.38	ATOM 1624 C PRO 216 52.202 19.545 75.777 1.00 29.89
ATOM 1553 N THR 209 41.588 24.645 82.423 1.00 18.97	ATOM 1625 O PRO 216 52.264 20.762 75.544 1.00 26.07
ATOM 1554 H THR 209 40.914 25.022 83.023 1.00 0.00	ATOM 1626 N SER 217 52.848 18.965 76.775 1.00 28.39
ATOM 1555 CA THR 209 42.173 23.327 82.716 1.00 19.28	ATOM 1627 H SER 217 52.747 18.009 76.917 1.00 0.00
ATOM 1556 CB THR 209 41.799 22.770 84.123 1.00 22.75	ATOM 1628 CA SER 217 53.694 19.728 77.670 1.00 31.83

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ATOM 1557 OG1 THR 209 40.389 22.550 84.200 1.00 33.54	ATOM 1629 CB SER 217 54.173 18.811 78.787 1.00 36.74
ATOM 1558 HG1 THR 209 39.924 23.378 84.048 1.00 0.00	ATOM 1630 OG SER 217 53.051 18.155 79.361 1.00 43.62
ATOM 1631 HG SER 217 52.588 17.645 78.708 1.00 0.00	ATOM 1703 CG GLN 226 50.933 34.857 80.100 1.00 56.06
ATOM 1632 C SER 217 54.858 20.434 76.973 1.00 31.11	ATOM 1704 CD GLN 226 50.740 35.034 81.608 1.00 65.41
ATOM 1633 O SER 217 55.455 19.895 76.042 1.00 29.48	ATOM 1705 OE1 GLN 226 51.682 34.873 82.389 1.00 71.36
ATOM 1634 N GLY 218 55.162 21.653 77.413 1.00 31.19	ATOM 1706 NE2 GLN 226 49.521 35.380 82.019 1.00 69.24
ATOM 1635 H GLY 218 54.650 22.057 78.150 1.00 0.00	ATOM 1707 HE21 GLN 226 48.811 35.506 81.360 1.00 0.00
ATOM 1636 CA GLY 218 56.242 22.399 76.798 1.00 31.10	ATOM 1708 HE22 GLN 226 49.396 35.496 82.982 1.00 0.00
ATOM 1637 C GLY 218 56.119 23.905 76.949 1.00 33.16	ATOM 1709 C GLN 226 48.358 33.721 79.040 1.00 26.90
ATOM 1638 O GLY 218 55.185 24.185 77.598 1.00 32.64	ATOM 1710 O GLN 226 47.762 34.651 79.586 1.00 26.58
ATOM 1639 N PRO 219 57.047 24.672 76.344 1.00 33.29	ATOM 1711 N ARG 227 48.230 33.430 77.746 1.00 28.46
ATOM 1640 CD PRO 219 58.239 24.177 75.628 1.00 30.91	ATOM 1712 H ARG 227 48.774 32.706 77.369 1.00 0.00
ATOM 1641 CA PRO 219 57.055 26.135 76.413 1.00 33.69	ATOM 1713 CA ARG 227 47.301 34.156 76.868 1.00 28.40
ATOM 1642 CB PRO 219 58.365 26.502 75.716 1.00 33.20	ATOM 1714 CB ARG 227 47.482 33.742 75.419 1.00 29.43
ATOM 1643 CG PRO 219 58.620 25.357 74.807 1.00 32.73	ATOM 1715 CG ARG 227 48.691 34.349 74.796 1.00 28.83
ATOM 1644 C PRO 219 55.855 26.808 75.772 1.00 36.42	ATOM 1716 CD ARG 227 49.207 33.479 73.692 1.00 35.73
ATOM 1645 O PRO 219 55.382 27.835 76.264 1.00 38.04	ATOM 1717 NE ARG 227 50.642 33.666 73.540 1.00 41.05
ATOM 1646 N LEU 220 53.355 26.221 74.688 1.00 37.44	ATOM 1718 HE ARG 227 51.220 32.889 73.649 1.00 0.00
ATOM 1647 H LEU 220 55.767 25.403 74.349 1.00 0.00	ATOM 1719 CZ ARG 227 51.211 34.829 73.252 1.00 42.98
ATOM 1648 CA LEU 220 54.202 26.775 73.984 1.00 36.21	ATOM 1720 NH1 ARG 227 50.460 35.910 73.072 1.00 47.92
ATOM 1649 CB LEU 220 54.025 26.095 72.623 1.00 41.05	ATOM 1721 HH11 ARG 227 49.463 35.860 73.153 1.00 0.00
ATOM 1650 CG LEU 220 53.027 26.676 71.610 1.00 43.93	ATOM 1722 HH12 ARG 227 50.888 36.792 72.859 1.00 0.00
ATOM 1651 CD1 LEU 220 53.099 28.216 72.577 1.00 42.74	ATOM 1723 NH2 ARG 227 52.532 34.924 73.195 1.00 44.69
ATOM 1652 CD2 LEU 220 53.308 26.064 70.228 1.00 43.21	ATOM 1724 HH21 ARG 227 53.090 34.116 73.359 1.00 0.00
ATOM 1653 C LEU 220 52.955 26.627 74.836 1.00 33.18	ATOM 1725 HH22 ARG 227 52.957 35.802 72.974 1.00 0.00
ATOM 1654 O LEU 220 52.096 27.505 74.844 1.00 31.72	ATOM 1726 C ARG 227 45.867 33.905 77.289 1.00 28.89
ATOM 1655 N LYS 221 52.895 25.540 75.599 1.00 32.75	ATOM 1727 O ARG 227 45.042 34.827 77.269 1.00 30.98
ATOM 1656 H LYS 221 53.622 24.890 75.550 1.00 0.00	ATOM 1728 N LEU 228 45.572 32.658 77.652 1.00 27.57
ATOM 1657 CA LYS 221 51.764 25.288 76.487 1.00 32.53	ATOM 1729 H LEU 228 46.254 31.979 77.605 1.00 0.00
ATOM 1658 CB LYS 221 51.914 23.923 77.173 1.00 31.53	ATOM 1730 CA LEU 228 44.244 32.302 78.131 1.00 27.07
ATOM 1659 CG LYS 221 50.728 23.519 78.040 1.00 29.82	ATOM 1731 CB LEU 228 44.144 30.806 78.458 1.00 26.14
ATOM 1660 CD LYS 221 50.778 22.048 78.391 1.00 28.10	ATOM 1732 CG LEU 228 43.930 29.847 77.287 1.00 26.19
ATOM 1661 CE LYS 221 49.564 21.636 79.198 1.00 21.91	ATOM 1733 CD1 LEU 228 43.862 28.428 77.813 1.00 22.88
ATOM 1662 NZ LYS 221 49.367 20.165 79.180 1.00 18.88	ATOM 1734 CD2 LEU 228 42.657 30.211 76.513 1.00 23.61
ATOM 1663 HZ1 LYS 221 50.205 19.703 79.595 1.00 0.00	ATOM 1735 C LEU 228 43.958 33.127 79.380 1.00 23.46
ATOM 1664 HZ2 LYS 221 49.241 19.843 78.212 1.00 0.00	ATOM 1736 O LEU 228 42.938 33.793 79.461 1.00 23.05
ATOM 1665 HZ3 LYS 221 48.529 19.921 79.742 1.00 0.00	ATOM 1737 N GLU 229 44.886 33.122 80.329 1.00 25.86
ATOM 1666 C LYS 221 51.717 26.403 77.527 1.00 33.59	ATOM 1738 H GLU 229 45.702 32.595 80.200 1.00 0.00
ATOM 1667 O LYS 221 50.643 26.869 77.928 1.00 31.97	ATOM 1739 CA GLU 229 44.712 33.881 81.556 1.00 26.46
ATOM 1668 N ALA 222 52.902 26.850 77.930 1.00 35.55	ATOM 1740 CB GLU 229 45.858 33.592 52.506 1.00 29.02
ATOM 1669 H ALA 222 53.711 26.447 77.562 1.00 0.00	ATOM 1741 CG GLU 229 45.736 32.220 83.117 1.00 35.68
ATOM 1670 CA ALA 222 53.035 27.918 78.915 1.00 36.45	ATOM 1742 CD GLU 229 47.055 31.639 83.590 1.00 42.02
ATOM 1671 CB ALA 222 54.493 28.048 79.348 1.00 38.57	ATOM 1743 OE1 GLU 229 47.020 30.587 84.257 1.00 47.25
ATOM 1672 C ALA 222 52.541 29.235 78.329 1.00 34.13	ATOM 1744 OE2 GLU 229 48.128 32.208 83.290 1.00 48.22
ATOM 1673 A ALA 222 51.845 30.012 78.996 1.00 32.40	ATOM 1745 C GLU 229 44.567 35.380 81.295 1.00 28.97
ATOM 1674 N GLU 223 52.902 29.470 77.072 1.00 31.05	ATOM 1746 O GLU 229 43.705 36.036 81.889 1.00 28.12
ATOM 1675 H GLU 223 53.452 28.804 76.611 1.00 0.00	ATOM 1747 N ASP 230 45.367 35.907 80.371 1.00 30.33
ATOM 1676 CA GLU 223 52.517 30.681 76.374 1.00 31.88	ATOM 1748 H ASP 230 46.005 35.330 79.913 1.00 0.00
ATOM 1677 CB GLU 223 53.179 30.713 75.010 1.00 33.98	ATOM 1749 CA ASP 230 45.309 37.322 80.020 1.00 31.37
ATOM 1678 CG GLU 223 54.682 30.818 75.116 1.00 40.16	ATOM 1750 CB ASP 230 46.459 37.705 79.096 1.00 34.93
ATOM 1679 CD GLU 223 55.380 30.540 73.804 1.00 46.19	ATOM 1751 CG ASP 230 47.790 37.849 79.830 1.00 43.53
ATOM 1680 OE1 GLU 223 54.721 30.653 72.749 1.00 46.69	ATOM 1752 OD1 ASP 230 47.814 37.851 81.088 1.00 42.08
ATOM 1681 OE2 GLU 223 56.584 30.191 73.830 1.00 49.10	ATOM 1753 OD2 ASP 230 48.826 37.965 79.131 1.00 47.31
ATOM 1682 C GLU 223 51.010 30.774 76.253 1.00 29.27	ATOM 1754 C ASP 230 43.998 37.697 79.352 1.00 33.84
ATOM 1683 O GLU 223 50.418 31.770 76.657 1.00 27.55	ATOM 1755 O ASP 230 43.461 38.778 79.608 1.00 35.17
ATOM 1684 N ILE 224 50.387 29.700 75.775 1.00 28.64	ATOM 1756 N VAL 231 43.518 36.847 78.446 1.00 31.08
ATOM 1685 H ILE 224 50.919 28.919 75.518 1.00 0.00	ATOM 1757 H VAL 231 44.005 36.027 78.242 1.00 0.00
ATOM 1686 CA ILE 224 48.932 29.653 75.627 1.00 24.57	ATOM 1758 CA VAL 231 42.256 37.117 77.761 1.00 32.04
ATOM 1687 CB ILE 224 48.475 28.322 75.026 1.00 22.57	ATOM 1759 CB VAL 231 42.030 36.166 76.550 1.00 29.32
ATOM 1688 CG2 ILE 224 46.965 28.283 74.940 1.00 20.95	ATOM 1760 CG1 VAL 231 40.688 36.435 75.898 1.00 27.10
ATOM 1689 CG1 ILE 224 49.095 28.140 73.642 1.00 25.41	ATOM 1761 CG2 VAL 231 43.133 36.337 75.535 1.00 25.64
ATOM 1690 CD1 ILE 224 49.068 26.710 73.156 1.00 30.02	ATOM 1762 C VAL 231 41.093 36.990 78.754 1.00 36.60
ATOM 1691 C ILE 224 48.265 29.851 76.980 1.00 23.70	ATOM 1763 O VAL 231 40.191 37.832 78.764 1.00 40.64
ATOM 1692 O ILE 224 47.323 30.640 77.105 1.00 24.41	ATOM 1764 N PHE 232 41.157 35.984 79.632 1.00 34.95
ATOM 1693 N ALA 225 48.765 29.150 77.996 1.00 22.80	ATOM 1765 H PHE 232 41.928 35.385 79.603 1.00 0.00
ATOM 1694 H ALA 225 49.508 28.532 77.830 1.00 0.00	ATOM 1766 CA PHE 232 40.106 35.745 80.632 1.00 38.18
ATOM 1695 CA ALA 225 48.230 29.273 79.348 1.00 21.66	ATOM 1767 CB PHE 232 40.330 34.414 81.378 1.00 33.30
ATOM 1696 CB ALA 225 49.125 28.538 80.327 1.00 26.49	ATOM 1768 CG PHE 232 40.068 33.181 80.538 1.00 28.81
ATOM 1697 C ALA 225 48.153 30.739 79.729 1.00 21.34	ATOM 1769 CD1 PHE 232 40.559 31.945 80.939 1.00 25.79
ATOM 1698 O ALA 225 47.103 31.228 80.144 1.00 21.30	ATOM 1770 CD2 PHE 232 39.329 33.254 79.356 1.00 25.06
ATOM 1699 N GLN 226 49.254 31.453 79.508 1.00 25.01	ATOM 1771 CE1 PHE 232 40.319 30.794 80.178 1.00 27.90
ATOM 1700 H GLN 226 50.037 31.011 79.110 1.00 0.00	ATOM 1772 CE2 PHE 232 39.084 32.112 78.588 1.00 25.66
ATOM 1701 CA GLN 226 49.333 32.875 79.837 1.00 30.14	ATOM 1773 CZ PHE 232 39.575 30.882 78.994 1.00 26.36
ATOM 1702 CB GLN 226 50.751 33.411 79.639 1.00 40.36	ATOM 1774 C PHE 232 40.023 36.896 81.625 1.00 39.58
ATOM 1703 CG GLN 226 50.125 32.875 80.327 1.00 26.49	ATOM 1784 O GLU 240 45.378 38.202 64.693 1.00 25.96
ATOM 1704 CD GLN 226 50.125 32.875 80.327 1.00 26.49	ATOM 1784 N VAL 241 45.514 39.825 66.246 1.00 24.78
ATOM 1705 OE1 GLN 226 50.125 32.875 80.327 1.00 26.49	ATOM 1784 H VAL 241 45.050 40.549 66.715 1.00 0.00
ATOM 1706 NE2 GLN 226 50.125 32.875 80.327 1.00 26.49	ATOM 1785 CA VAL 241 46.898 39.456 66.603 1.00 25.87
ATOM 1707 HE21 GLN 226 48.811 35.506 81.360 1.00 0.00	ATOM 17851 CB VAL 241 47.459 40.657 67.517 1.00 28.94

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ATOM 1780 C ALA 233 40.834 39.932 82.108 1.00 43.84	ATOM 1852 CG1 VAL 241 48.651 40.155 68.319 1.00 31.40
ATOM 1781 O ALA 233 40.844 41.002 82.706 1.00 45.83	ATOM 1853 CG2 VAL 241 47.869 41.846 66.670 1.00 29.28
ATOM 1782 N GLY 234 40.498 39.822 80.827 1.00 48.25	ATOM 1854 C VAL 241 46.991 38.185 67.291 1.00 25.79
ATOM 1783 H GLY 234 40.497 39.951 80.388 1.00 0.00	ATOM 1855 O VAL 241 47.911 37.402 67.023 1.00 28.70
ATOM 1784 CA GLY 234 40.091 40.984 80.061 1.00 53.20	ATOM 1856 N LEU 242 46.008 37.899 68.141 1.00 25.00
ATOM 1785 C GLY 234 41.249 41.931 79.800 1.00 57.49	ATOM 1857 H LEU 242 45.319 38.580 68.298 1.00 0.00
ATOM 1786 O GLY 234 41.044 43.082 79.406 1.00 58.25	ATOM 1858 CA LEU 242 45.916 36.633 68.868 1.00 22.95
ATOM 1787 N LYS 235 42.468 41.466 80.053 1.00 60.31	ATOM 1859 CB LEU 242 44.715 36.682 69.810 1.00 25.74
ATOM 1788 H LYS 235 42.573 40.558 80.384 1.00 0.00	ATOM 1860 CG LEU 242 44.994 36.696 71.303 1.00 25.17
ATOM 1789 CA LYS 235 43.648 42.289 79.825 1.00 63.78	ATOM 1861 CD1 LEU 242 43.666 36.756 72.033 1.00 21.02
ATOM 1790 CB LYS 235 44.803 41.862 80.741 1.00 71.11	ATOM 1862 CD2 LEU 242 45.802 35.448 71.674 1.00 28.21
ATOM 1791 CG LYS 235 46.143 42.567 80.460 1.00 82.93	ATOM 1863 C LEU 242 45.737 35.443 67.920 1.00 19.00
ATOM 1792 CD LYS 235 46.041 44.109 80.405 1.00 89.87	ATOM 1864 O LEU 242 46.388 34.411 68.067 1.00 16.60
ATOM 1793 CE LYS 235 45.721 44.735 81.759 1.00 93.76	ATOM 1865 N MET 243 44.830 35.600 66.961 1.00 17.56
ATOM 1794 NZ LYS 235 45.539 46.209 81.649 1.00 94.59	ATOM 1866 H MET 243 44.357 36.445 66.905 1.00 0.00
ATOM 1795 HZ1 LYS 235 44.758 46.419 81.005 1.00 0.00	ATOM 1867 CA MET 243 44.524 34.568 65.983 1.00 17.74
ATOM 1796 HZ2 LYS 235 46.418 46.640 81.293 1.00 0.00	ATOM 1868 CB MET 243 43.225 34.917 65.255 1.00 15.78
ATOM 1797 HZ3 LYS 235 45.331 46.600 82.594 1.00 0.00	ATOM 1869 CG MET 243 42.001 34.952 66.157 1.00 13.77
ATOM 1798 C LYS 235 44.053 42.184 78.363 1.00 61.62	ATOM 1870 SD MET 243 41.528 33.366 66.919 1.00 15.74
ATOM 1799 O LYS 235 44.314 43.194 77.705 1.00 63.55	ATOM 1871 CE MET 243 40.733 32.532 65.613 1.00 10.67
ATOM 1800 N ASN 236 44.129 40.957 77.865 1.00 58.43	ATOM 1872 C MET 243 45.672 34.286 65.000 1.00 16.07
ATOM 1801 H ASN 236 43.918 40.198 78.433 1.00 0.00	ATOM 1873 O MET 243 45.918 33.139 64.630 1.00 17.62
ATOM 1802 CA ASN 236 44.486 40.736 76.472 1.00 55.59	ATOM 1874 N GLU 244 46.395 35.322 64.600 1.00 21.04
ATOM 1803 CB ASN 236 45.045 39.320 76.270 1.00 52.40	ATOM 1875 H GLU 244 46.156 36.224 64.896 1.00 0.00
ATOM 1804 CG ASN 236 45.805 39.163 74.954 1.00 50.33	ATOM 1876 CA GLU 244 47.534 35.139 63.700 1.00 22.88
ATOM 1805 OD1 ASN 236 45.523 39.848 73.972 1.00 48.03	ATOM 1877 CB GLU 244 48.030 36.496 63.172 1.00 26.39
ATOM 1806 ND2 ASN 236 46.775 38.249 74.934 1.00 45.67	ATOM 1878 CG GLU 244 49.197 36.408 62.174 1.00 31.05
ATOM 1807 HD21 ASN 236 46.951 37.720 75.736 1.00 0.00	ATOM 1879 CD GLU 244 48.894 35.527 60.955 1.00 33.63
ATOM 1808 HD22 ASN 236 47.261 38.136 74.093 1.00 0.00	ATOM 1880 OE1 GLU 244 49.749 34.680 60.623 1.00 33.84
ATOM 1809 C ASN 236 43.251 40.958 75.593 1.00 55.63	ATOM 1881 OE2 GLU 244 47.812 35.679 60.334 1.00 35.83
ATOM 1810 O ASN 236 42.097 40.813 76.032 1.00 55.31	ATOM 1882 C GLU 244 48.655 34.393 64.430 1.00 21.16
ATOM 1811 N THR 237 43.511 41.376 74.366 1.00 53.25	ATOM 1883 O GLU 244 49.289 33.514 63.854 1.00 21.96
ATOM 1812 H THR 237 44.441 41.499 74.082 1.00 0.00	ATOM 1884 N TRP 245 48.875 34.733 65.701 1.00 21.45
ATOM 1813 CA THR 237 42.468 41.620 73.403 1.00 51.23	ATOM 1885 H TRP 245 48.340 35.455 66.101 1.00 0.00
ATOM 1814 CB THR 237 41.707 42.919 73.725 1.00 51.31	ATOM 1886 CA TRP 245 49.901 34.076 66.514 1.00 24.48
ATOM 1815 OG1 THR 237 40.687 43.138 72.741 1.00 57.93	ATOM 1887 CB TRP 245 49.914 34.661 67.941 1.00 27.17
ATOM 1816 HG1 THR 237 40.072 42.398 72.749 1.00 0.00	ATOM 1888 CG TRP 245 50.932 34.013 68.893 1.00 30.61
ATOM 1817 CG2 THR 237 42.652 44.102 73.786 1.00 51.40	ATOM 1889 CD2 TRP 245 50.681 32.971 69.853 1.00 32.76
ATOM 1818 C THR 237 43.129 41.633 72.028 1.00 49.50	ATOM 1890 CE2 TRP 245 51.919 32.674 70.480 1.00 33.63
ATOM 1819 O THR 237 44.216 41.078 71.868 1.00 51.84	ATOM 1891 CE3 TRP 245 49.545 32.254 70.246 1.00 34.69
ATOM 1820 N ASP 238 42.509 42.293 71.057 1.00 46.73	ATOM 1892 CD1 TRP 245 52.267 34.298 68.892 1.00 32.07
ATOM 1821 H ASP 238 41.648 42.972 71.255 1.00 0.00	ATOM 1893 NE1 TRP 245 52.864 33.497 69.928 1.00 31.38
ATOM 1822 CA ASP 238 43.005 42.337 69.674 1.00 44.41	ATOM 1894 HE1 TRP 245 53.819 33.516 70.159 1.00 0.00
ATOM 1823 CB ASP 238 44.355 43.032 69.519 1.00 46.32	ATOM 1895 CZ2 TRP 245 52.043 31.689 71.477 1.00 36.30
ATOM 1824 CG ASP 238 44.526 43.648 68.139 1.00 50.54	ATOM 1896 CZ3 TRP 245 49.675 31.265 71.247 1.00 38.55
ATOM 1825 OD1 ASP 238 45.580 43.438 67.522 1.00 53.28	ATOM 1897 CH2 TRP 245 50.916 30.999 71.844 1.00 33.06
ATOM 1826 OD2 ASP 238 43.601 44.348 67.667 1.00 53.75	ATOM 1898 C TRP 245 49.583 32.588 66.576 1.00 24.04
ATOM 1827 C ASP 238 43.071 40.913 69.154 1.00 39.10	ATOM 1899 O TRP 245 50.438 31.731 66.337 1.00 20.97
ATOM 1828 O ASP 238 44.140 40.306 69.006 1.00 35.55	ATOM 1900 N LEU 246 48.325 32.296 66.879 1.00 24.79
ATOM 1829 N LEU 239 41.874 40.404 68.898 1.00 32.36	ATOM 1901 H LEU 246 47.699 33.031 67.048 1.00 0.00
ATOM 1830 H LEU 239 41.096 40.974 69.054 1.00 0.00	ATOM 1902 CA LEU 246 47.848 30.924 66.985 1.00 25.07
ATOM 1831 CA LEU 239 41.648 39.073 68.413 1.00 28.63	ATOM 1903 CB LEU 246 46.351 30.912 67.291 1.00 24.89
ATOM 1832 CB LEU 239 40.165 38.916 68.102 1.00 23.74	ATOM 1904 CG LEU 246 45.853 30.275 68.585 1.00 26.05
ATOM 1833 CG LEU 239 39.718 37.501 67.798 1.00 20.81	ATOM 1905 CD1 LEU 246 44.356 30.340 68.547 1.00 18.05
ATOM 1834 CD1 LEU 239 40.158 36.576 68.937 1.00 18.50	ATOM 1906 CD2 LEU 246 46.330 28.829 68.700 1.00 23.56
ATOM 1835 CD2 LEU 239 38.218 37.515 67.603 1.00 14.34	ATOM 1907 C LEU 246 48.089 30.174 65.688 1.00 24.91
ATOM 1836 C LEU 239 42.480 38.753 67.184 1.00 31.22	ATOM 1908 O LEU 246 48.650 29.084 65.690 1.00 26.81
ATOM 1837 O LEU 239 42.986 37.639 67.063 1.00 32.51	ATOM 1909 N LYS 247 47.651 30.777 64.588 1.00 24.06
ATOM 1838 N GLU 240 42.661 39.734 66.301 1.00 32.13	ATOM 1910 H LYS 247 47.209 31.648 64.678 1.00 0.00
ATOM 1839 H GLU 240 42.293 40.611 66.483 1.00 0.00	ATOM 1911 CA LYS 247 47.783 30.202 63.250 1.00 24.97
ATOM 1840 CA GLU 240 43.423 39.516 65.070 1.00 33.79	ATOM 1912 CB LYS 247 47.290 31.214 62.214 1.00 21.42
ATOM 1841 CB GLU 240 43.322 40.728 64.129 1.00 41.79	ATOM 1913 CG LYS 247 47.163 30.688 60.806 1.00 24.96
ATOM 1842 CG GLU 240 43.896 42.032 64.658 1.00 58.76	ATOM 1914 CD LYS 247 46.689 31.805 59.889 1.00 26.54
ATOM 1843 CD GLU 240 45.250 42.392 64.046 1.00 68.00	ATOM 1915 CE LYS 247 46.554 31.341 58.446 1.00 33.16
ATOM 1844 OE1 GLU 240 45.852 43.403 64.488 1.00 72.93	ATOM 1916 NZ LYS 247 46.058 32.427 57.534 1.00 33.41
ATOM 1845 OE2 GLU 240 45.710 41.676 63.124 1.00 71.76	ATOM 1917 HZ1 LYS 247 46.728 33.223 57.547 1.00 0.00
ATOM 1846 C GLU 240 44.867 39.126 65.321 1.00 26.92	ATOM 1918 HZ2 LYS 247 45.123 32.759 57.854 1.00 0.00
ATOM 1849 HZ1 LYS 247 45.978 32.058 56.566 1.00 0.00	ATOM 1919 CB LEU 255 42.116 19.306 65.998 1.00 17.29
ATOM 1850 HZ2 LYS 247 45.978 32.058 56.566 1.00 0.00	ATOM 1920 CG LEU 255 40.734 18.824 66.457 1.00 22.10
ATOM 1851 HZ3 LYS 247 45.978 32.058 56.566 1.00 0.00	ATOM 1921 CD1 LEU 255 40.913 18.124 67.786 1.00 21.22
ATOM 1852 HZ4 LYS 247 45.978 32.058 56.566 1.00 0.00	ATOM 1922 CD2 LEU 255 39.689 19.923 66.533 1.00 10.32
ATOM 1853 HZ5 LYS 247 45.978 32.058 56.566 1.00 0.00	ATOM 1923 C LEU 255 42.551 21.554 67.079 1.00 16.96
ATOM 1854 HZ6 LYS 247 45.978 32.058 56.566 1.00 0.00	ATOM 1924 CA LYS 247 45.981 21.923 66.533 1.00 10.32
ATOM 1855 HZ7 LYS 247 45.978 32.058 56.566 1.00 0.00	ATOM 1925 C LEU 255 42.551 21.554 67.079 1.00 16.96
ATOM 1856 HZ8 LYS 247 45.978 32.058 56.566 1.00 0.00	ATOM 1926 CA LYS 247 45.981 21.923 66.533 1.00 10.32
ATOM 1857 HZ9 LYS 247 45.978 32.058 56.566 1.00 0.00	ATOM 1927 C LEU 255 42.551 21.554 67.079 1.00 16.96
ATOM 1858 HZ10 LYS 247 45.978 32.058 56.566 1.00 0.00	ATOM 1928 CA LYS 247 45.981 21.923 66.533 1.00 10.32
ATOM 1859 HZ11 LYS 247 45.978 32.058 56.566 1.00 0.00	ATOM 1929 C LEU 255 42.551 21.554 67.079 1.00 16.96
ATOM 1860 HZ12 LYS 247 45.978 32.058 56.566 1.00 0.00	ATOM 1930 C LEU 255 42.551 21.554 67.079 1.00 16.96
ATOM 1861 HZ13 LYS 247 45.978 32.058 56.566 1.00 0.00	ATOM 1931 C LEU 255 42.551 21.554 67.079 1.00 16.96
ATOM 1862 HZ14 LYS 247 45.978 32.058 56.566 1.00 0.00	ATOM 1932 C LEU 255 42.551 21.554 67.079 1.00 16.96
ATOM 1863 HZ15 LYS 247 45.978 32.058 56.566 1.00 0.00	ATOM 1933 C LEU 255 42.551 21.554 67.079 1.00 16.96
ATOM 1864 HZ16 LYS 247 45.978 32.058 56.566 1.00 0.00	ATOM 1934 C LEU 255 42.551 21.554 67.079 1.00 16.96
ATOM 1865 HZ17 LYS 247 45.978 32.058 56.566 1.00 0.00	ATOM 1935 C LEU 255 42.551 21.554 67.079 1.00 16.96
ATOM 1866 HZ18 LYS 247 45.978 32.058 56.566 1.00 0.00	ATOM 1936 C LEU 255 42.551 21.554 67.079 1.00 16.96
ATOM 1867 HZ19 LYS 247 45.978 32.058 56.566 1.00 0.00	ATOM 1937 C LEU 255 42.551 21.554 67.079 1.00 16.96
ATOM 1868 HZ20 LYS 247 45.978 32.058 56.566 1.00 0.00	ATOM 1938 C LEU 255 42.551 21.554 67.079 1.00 16.96
ATOM 1869 HZ21 LYS 247 45.978 32.058 56.566 1.00 0.00	ATOM 1939 C LEU 255 42.551 21.554 67.079 1.00 16.96
ATOM 1870 HZ22 LYS 247 45.978 32.058 56.566 1.00 0.00	ATOM 1940 C LEU 255 42.551 21.554 67.079 1.00 16.96
ATOM 1871 HZ23 LYS 247 45.978 32.058 56.566 1.00 0.00	ATOM 1941 C LEU 255 42.551 21.554 67.079 1.00 16.96
ATOM 1872 HZ24 LYS 247 45.978 32.058 56.566 1.00 0.00	ATOM 1942 C LEU 255 42.551 21.554 67.079 1.00 16.96
ATOM 1873 HZ25 LYS 247 45.978 32.058 56.566 1.00 0.00	ATOM 1943 C LEU 255 42.551 21.554 67.079 1.00 16.96
ATOM 1874 HZ26 LYS 247 45.978 32.058 56.566 1.00 0.00	ATOM 1944 C LEU 255 42.551 21.554 67.079 1.00 16.96
ATOM 1875 HZ27 LYS 247 45.978 32.058 56.566 1.00 0.00	ATOM 1945 C LEU 255 42.551 21.554 67.079 1.00 16.96
ATOM 1876 HZ28 LYS 247 45.978 32.058 56.566 1.00 0.00	ATOM 1946 C LEU 255 42.551 21.554 67.079 1.00 16.96
ATOM 1877 HZ29 LYS 247 45.978 32.058 56.566 1.00 0.00	ATOM 1947 C LEU 255 42.551 21.554 67.079 1.00 16.96
ATOM 1878 HZ30 LYS 247 45.978 32.058 56.566 1.00 0.00	ATOM 1948 C LEU 255 42.551 21.554 67.079 1.00 16.96
ATOM 1879 HZ31 LYS 247 45.978 32.058 56.566 1.00 0.00	ATOM 1949 C LEU 255 42.551 21.554 67.079 1.00 16.96
ATOM 1880 HZ32 LYS 247 45.978 32.058 56.566 1.00 0.00	ATOM 1950 C LEU 255 42.551 21.554 67.079 1.00 16.96
ATOM 1881 HZ33 LYS 247 45.978 32.058 56.566 1.00 0.00	ATOM 1951 C LEU 255 42.551 21.554 67.079 1.00 16.96
ATOM 1882 HZ34 LYS 247 45.978 32.058 56.566 1.00 0.00	ATOM 1952 C LEU 255 42.551 21.554 67.079 1.00 16.96
ATOM 1883 HZ35 LYS 247 45.978 32.058 56.566 1.00 0.00	ATOM 1953 C LEU 255 42.551 21.554 67.079 1.00 16.96
ATOM 1884 HZ36 LYS 247 45.978 32.058 56.566 1.00 0.00	ATOM 1954 C LEU 255 42.551 21.554 67.079 1.00 16.96
ATOM 1885 HZ37 LYS 247 45.978 32.058 56.566 1.00 0.00	ATOM 1955 C LEU 255 42.551 21.554 67.079 1.00 16.96
ATOM 1886 HZ38 LYS 247 45.978 32.058 56.566 1.00 0.00	ATOM 1956 C LEU 255 42.551 21.554 67.079 1.00 16.96
ATOM 1887 HZ39 LYS 247 45.978 32.058 56.566 1.00 0.00	ATOM 1957 C LEU 255 42.551 21.554 67.079 1.00 16.96
ATOM 1888 HZ40 LYS 247 45.978 32.058 56.566 1.00 0.00	ATOM 1958 C LEU 255 42.551 21.554 67

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ATOM 1931 N ARG 249 51.801 29.007 65.139 1.00 33.40	ATOM 2003 CG2 THR 256 45.230 20.292 69.895 1.00 12.01
ATOM 1932 H ARG 249 50.843 29.187 65.282 1.00 0.00	ATOM 2004 C THR 256 43.899 23.738 68.578 1.00 20.08
ATOM 1933 CA ARG 249 52.513 28.152 66.107 1.00 31.70	ATOM 2005 O THR 256 43.388 24.576 69.328 1.00 22.98
ATOM 1934 CB ARG 249 51.264 27.826 67.313 1.00 27.94	ATOM 2006 N LYS 257 44.414 24.055 67.386 1.00 19.49
ATOM 1935 CG ARG 249 51.202 29.005 68.146 1.00 28.39	ATOM 2007 H LYS 257 44.782 23.352 66.815 1.00 0.00
ATOM 1936 CD ARG 249 52.394 29.831 68.538 1.00 29.29	ATOM 2008 CA LYS 257 44.440 25.443 66.916 1.00 16.20
ATOM 1937 NE ARG 249 52.783 30.729 67.461 1.00 33.71	ATOM 2009 CB LYS 257 45.227 25.580 65.608 1.00 18.79
ATOM 1938 HE ARG 249 52.182 30.821 66.692 1.00 0.00	ATOM 2010 CG LYS 257 46.730 25.614 65.807 1.00 19.72
ATOM 1939 CZ ARG 249 53.907 31.436 67.449 1.00 38.58	ATOM 2011 CD LYS 257 47.458 25.681 64.480 1.00 21.43
ATOM 1940 NH1 ARG 249 54.763 31.340 68.458 1.00 41.62	ATOM 2012 CE LYS 257 48.960 25.713 64.707 1.00 23.03
ATOM 1941 HH11 ARG 249 54.557 30.736 69.227 1.00 0.00	ATOM 2013 NZ LYS 257 49.754 26.153 63.517 1.00 20.57
ATOM 1942 HH12 ARG 249 55.605 31.876 68.452 1.00 0.00	ATOM 2014 HZ1 LYS 257 49.457 27.108 63.239 1.00 0.00
ATOM 1943 NH2 ARG 249 54.144 32.287 66.459 1.00 39.18	ATOM 2015 HZ2 LYS 257 49.572 25.492 62.733 1.00 0.00
ATOM 1944 HH21 ARG 249 53.475 32.406 65.725 1.00 0.00	ATOM 2016 HZ3 LYS 257 50.760 26.149 63.750 1.00 0.00
ATOM 1945 HH22 ARG 249 54.988 32.827 66.456 1.00 0.00	ATOM 2017 C LYS 257 43.012 25.932 66.726 1.00 12.86
ATOM 1946 C ARG 249 52.966 26.826 65.523 1.00 34.57	ATOM 2018 O LYS 257 42.669 27.034 67.141 1.00 14.09
ATOM 1947 O ARG 249 52.158 26.069 64.993 1.00 38.65	ATOM 2019 N GLY 258 42.170 25.084 66.154 1.00 12.55
ATOM 1948 N PRO 250 54.262 26.508 65.619 1.00 37.16	ATOM 2020 H GLY 258 42.490 24.214 65.855 1.00 0.00
ATOM 1949 CD PRO 250 55.426 27.207 66.175 1.00 38.70	ATOM 2021 CA GLY 258 40.778 25.446 65.956 1.00 15.35
ATOM 1950 CA PRO 250 54.647 25.214 65.051 1.00 38.55	ATOM 2022 C GLY 258 40.050 25.691 67.273 1.00 15.50
ATOM 1951 CB PRO 250 56.181 25.283 65.033 1.00 39.31	ATOM 2023 O GLY 258 39.320 26.682 67.431 1.00 13.67
ATOM 1952 CG PRO 250 56.502 26.765 65.223 1.00 40.46	ATOM 2024 N ILE 259 40.259 24.784 68.224 1.00 16.64
ATOM 1953 C PRO 250 54.161 24.175 66.058 1.00 41.32	ATOM 2025 H ILE 259 40.852 24.025 68.031 1.00 0.00
ATOM 1954 O PRO 250 53.760 24.533 67.174 1.00 39.81	ATOM 2026 CA ILE 259 39.636 27.878 69.542 1.00 14.17
ATOM 1955 N ILE 251 54.221 22.903 65.676 1.00 43.38	ATOM 2027 CB ILE 259 39.859 23.571 70.356 1.00 15.52
ATOM 1956 H ILE 251 54.559 22.703 64.787 1.00 0.00	ATOM 2028 CG2 ILE 259 39.512 23.757 71.850 1.00 11.02
ATOM 1957 CA ILE 251 53.805 21.769 66.523 1.00 46.51	ATOM 2029 CG1 ILE 259 39.014 22.464 69.731 1.00 6.64
ATOM 1958 CB ILE 251 54.707 21.566 67.821 1.00 49.95	ATOM 2030 CD1 ILE 259 39.381 21.073 70.183 1.00 10.73
ATOM 1959 CG2 ILE 251 56.187 21.729 67.472 1.00 49.50	ATOM 2031 C ILE 259 40.084 26.130 70.292 1.00 10.91
ATOM 1960 CG1 ILE 251 54.277 22.493 68.972 1.00 53.08	ATOM 2032 O ILE 259 39.255 26.836 70.838 1.00 13.73
ATOM 1961 CD1 ILE 251 54.997 22.250 70.291 1.00 56.61	ATOM 2033 N LEU 260 41.373 26.443 70.281 1.00 12.18
ATOM 1962 C ILE 251 52.316 21.655 66.898 1.00 41.74	ATOM 2034 H LEU 260 42.014 25.865 69.823 1.00 0.00
ATOM 1963 O ILE 251 51.756 20.555 66.831 1.00 42.72	ATOM 2035 CA LEU 260 41.847 27.650 70.960 1.00 11.32
ATOM 1964 N LEU 252 51.684 22.754 67.309 1.00 37.22	ATOM 2036 CB LEU 260 43.369 27.694 71.023 1.00 13.90
ATOM 1965 H LEU 252 52.163 23.600 67.371 1.00 0.00	ATOM 2037 CG LEU 260 44.033 26.747 72.013 1.00 18.17
ATOM 1966 CA LEU 252 50.265 22.718 67.671 1.00 32.33	ATOM 2038 CD1 LEU 260 45.426 26.426 71.518 1.00 16.80
ATOM 1967 CB LEU 252 49.724 24.125 67.908 1.00 28.03	ATOM 2039 CD2 LEU 260 44.034 27.359 73.421 1.00 13.15
ATOM 1968 CG LEU 252 50.062 24.767 69.243 1.00 27.67	ATOM 2040 C LEU 260 41.345 28.867 70.220 1.00 11.32
ATOM 1969 CD1 LEU 252 49.149 25.950 69.450 1.00 23.50	ATOM 2041 O LEU 260 41.007 29.873 70.833 1.00 13.99
ATOM 1970 CD2 LEU 252 49.888 23.745 70.370 1.00 30.62	ATOM 2042 N GLY 261 41.305 28.773 68.893 1.00 13.68
ATOM 1971 C LEU 252 49.445 22.061 66.571 1.00 29.96	ATOM 2043 H GLY 261 41.626 27.962 68.455 1.00 0.00
ATOM 1972 O LEU 252 49.441 22.511 65.426 1.00 33.29	ATOM 2044 CA GLY 261 40.806 29.878 68.088 1.00 12.10
ATOM 1973 N SER 253 48.760 20.974 66.894 1.00 28.11	ATOM 2045 C GLY 261 39.359 30.142 68.439 1.00 6.12
ATOM 1974 H SER 253 48.787 20.641 67.806 1.00 0.00	ATOM 2046 O GLY 261 38.939 31.273 68.618 1.00 8.51
ATOM 1975 CA SER 253 47.954 20.317 65.884 1.00 25.46	ATOM 2047 N PHE 262 38.589 29.073 68.540 1.00 9.67
ATOM 1976 CB SER 253 47.342 19.016 66.407 1.00 26.72	ATOM 2048 H PHE 262 38.970 28.200 68.359 1.00 0.00
ATOM 1977 OG SER 253 46.147 19.250 67.128 1.00 27.57	ATOM 2049 CA PHE 262 37.183 29.170 68.912 1.00 12.77
ATOM 1978 HG SER 253 45.795 18.417 67.447 1.00 0.00	ATOM 2050 CB PHE 262 36.538 27.782 68.856 1.00 10.75
ATOM 1979 C SER 253 46.855 21.277 65.430 1.00 23.91	ATOM 2051 CG PHE 262 35.095 27.751 69.278 1.00 10.80
ATOM 1980 O SER 253 46.395 22.137 66.194 1.00 20.03	ATOM 2052 CD1 PHE 262 34.102 27.451 68.349 1.00 8.33
ATOM 1981 N PRO 254 46.402 21.121 64.185 1.00 22.83	ATOM 2053 CD2 PHE 262 34.729 27.961 70.612 1.00 9.95
ATOM 1982 CD PRO 254 46.762 20.032 63.254 1.00 24.06	ATOM 2054 CE1 PHE 262 32.772 27.357 68.728 1.00 9.19
ATOM 1983 CA PRO 254 45.351 21.967 63.614 1.00 24.41	ATOM 2055 CE2 PHE 262 33.401 27.871 71.009 1.00 11.23
ATOM 1984 CB PRO 254 45.041 21.255 62.285 1.00 25.78	ATOM 2056 CZ PHE 262 32.413 27.566 70.060 1.00 11.72
ATOM 1985 CG PRO 254 46.354 20.601 61.934 1.00 24.32	ATOM 2057 C PHE 262 37.071 29.766 70.316 1.00 11.12
ATOM 1986 C PRO 254 44.087 22.042 64.502 1.00 23.16	ATOM 2058 O PHE 262 36.273 30.659 70.531 1.00 16.33
ATOM 1987 O PRO 254 43.546 23.121 64.754 1.00 19.45	ATOM 2059 N VAL 263 37.884 29.298 71.264 1.00 13.36
ATOM 1988 N LEU 255 43.625 20.880 64.953 1.00 20.07	ATOM 2060 H VAL 263 38.522 28.589 71.039 1.00 0.00
ATOM 1989 H LEU 255 44.105 20.062 64.726 1.00 0.00	ATOM 2061 CA VAL 263 37.835 29.823 72.639 1.00 15.47
ATOM 1990 CA LEU 255 42.427 20.780 65.765 1.00 19.36	ATOM 2062 CB VAL 263 38.723 28.976 73.600 1.00 17.93
ATOM 2063 CG1 VAL 263 38.886 29.672 74.947 1.00 17.24	ATOM 2135 OE1 GLU 271 33.591 37.125 66.168 1.00 48.54
ATOM 2064 CG2 VAL 263 38.079 27.609 73.822 1.00 15.21	ATOM 2136 OE2 GLU 271 32.192 38.148 67.537 1.00 53.65
ATOM 2065 C VAL 263 38.180 31.321 72.732 1.00 15.07	ATOM 2137 C GLU 271 33.516 47.789 66.791 1.00 56.14
ATOM 2066 O VAL 263 37.462 32.096 73.375 1.00 15.34	ATOM 2138 O GLU 271 37.376 41.683 65.921 1.00 56.73
ATOM 2067 N PHE 264 39.250 31.731 82.055 1.00 18.90	ATOM 2139 N ARG 272 35.817 42.907 67.005 1.00 58.86
ATOM 2068 H PHE 264 39.774 31.076 75.557 1.00 0.00	ATOM 2140 H ARG 272 35.131 42.903 67.700 1.00 0.00
ATOM 2069 CA PHE 264 39.669 33.133 72.031 1.00 21.09	ATOM 2141 CA ARG 272 36.035 44.158 66.273 1.00 61.83
ATOM 2070 CB PHE 264 40.975 33.309 71.245 1.00 21.53	ATOM 2142 CB PHE 272 37.466 44.684 66.496 1.00 66.96
ATOM 2071 CG PHE 264 42.197 32.825 71.974 1.00 24.83	ATOM 2143 CG ARG 272 37.927 44.727 67.953 1.00 78.06
ATOM 2072 CD1 PHE 264 43.274 32.288 71.266 1.00 24.52	ATOM 2144 CD ARG 272 39.442 44.981 68.089 1.00 85.70
ATOM 2073 CD2 PHE 264 42.278 32.912 73.367 1.00 22.79	ATOM 2145 NE ARG 272 40.254 44.110 37.231 1.00 93.83
ATOM 2074 CE1 PHE 264 44.405 31.848 71.940 0.00 26.06	ATOM 2146 HE ARG 272 40.797 44.536 66.532 1.00 0.00
ATOM 2075 CE2 PHE 264 43.404 21.478 74.048 1.00 21.09	ATOM 2147 CZ ARG 272 40.322 42.782 67.330 1.00 95.55
ATOM 2076 CZ PHE 264 44.466 31.946 37.343 1.00 21.31	ATOM 2148 NH1 ARG 272 39.630 42.134 68.259 1.00 96.47
ATOM 2077 C PHE 264 38.607 34.044 71.416 1.00 21.61	ATOM 2149 HH11 ARG 272 39.059 42.641 68.899 1.00 0.00
ATOM 2078 O PHE 264 38.416 35.172 71.876 1.00 19.64	ATOM 2150 HH12 ARG 272 39.694 41.143 68.323 1.00 0.00
ATOM 2079 N THR 265 37.894 33.559 70.399 1.00 20.39	ATOM 2151 NH2 ARG 272 41.063 42.095 66.470 1.00 96.37
ATOM 2080 H THR 265 38.052 32.647 70.081 1.00 0.00	ATOM 2152 HH21 ARG 272 41.576 42.569 65.754 1.00 0.00
ATOM 2081 CA THR 265 36.881 34.398 69.768 1.00 18.63	ATOM 2153 HH22 ARG 272 41.118 41.098 66.541 1.00 0.00

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ATOM 2082 CB THR 265 36.498 33.895 68.327 1.00 19.30	ATOM 2154 C ARG 272 35.780 44.004 64.770 1.00 60.35
ATOM 2083 OG1 THR 265 35.599 32.793 68.407 1.00 33.53	ATOM 2155 O ARG 272 36.385 44.703 63.959 1.00 62.79
ATOM 2084 HG1 THR 265 36.008 32.055 68.896 1.00 0.00	ATOM 2156 N GLY 273 34.888 43.091 64.395 1.00 55.94
ATOM 2085 CG2 THR 265 37.704 33.409 67.602 1.00 13.43	ATOM 2157 H GLY 273 34.429 42.558 65.070 1.00 0.00
ATOM 2086 C THR 265 35.651 34.566 70.656 1.00 17.69	ATOM 2158 CA GLY 273 34.595 42.894 62.982 1.00 51.40
ATOM 2087 O THR 265 34.974 35.589 70.602 1.00 18.30	ATOM 2159 C GLY 273 35.535 41.975 62.206 1.00 48.56
ATOM 2088 N LEU 266 35.435 33.593 71.538 1.00 20.96	ATOM 2160 O GLY 273 35.579 42.007 60.970 1.00 48.16
ATOM 2089 H LEU 266 36.057 32.840 71.566 1.00 0.00	ATOM 2161 N LEU 274 36.285 41.150 62.927 1.00 43.81
ATOM 2090 CA LEU 266 34.300 33.579 72.470 1.00 19.74	ATOM 2162 H LEU 274 36.219 41.166 62.898 1.00 0.00
ATOM 2091 CB LEU 266 34.068 32.130 72.973 1.00 18.59	ATOM 2163 CA LEU 274 37.211 40.215 62.312 1.00 37.25
ATOM 2092 CG LEU 266 32.903 31.615 73.755 1.00 16.93	ATOM 2164 CB LEU 274 38.187 39.675 63.368 1.00 33.69
ATOM 2093 CD1 LEU 266 31.609 31.566 72.964 1.00 16.73	ATOM 2165 CG LEU 274 39.310 38.767 62.689 1.00 33.59
ATOM 2094 CD2 LEU 266 33.269 30.208 74.169 1.00 23.03	ATOM 2166 CD1 LEU 274 40.366 39.624 62.218 1.00 33.98
ATOM 2095 C LEU 266 34.580 34.447 73.691 1.00 19.29	ATOM 2167 CD2 LEU 274 39.919 37.969 64.005 1.00 33.40
ATOM 2096 O LEU 266 33.709 35.164 74.184 1.00 18.02	ATOM 2168 C LEU 274 36.407 39.060 61.725 1.00 33.64
ATOM 2097 N THR 267 35.811 34.361 74.175 1.00 22.16	ATOM 2169 O LEU 274 35.660 38.393 62.444 1.00 32.62
ATOM 2098 H THR 267 36.455 33.791 73.722 1.00 0.00	ATOM 2170 N GLN 275 36.528 38.832 60.421 1.00 30.31
ATOM 2099 CA THR 267 36.230 35.087 75.356 1.00 22.07	ATOM 2171 H GLN 275 37.100 39.403 59.880 1.00 0.00
ATOM 2100 CB THR 267 37.300 34.303 76.090 1.00 17.69	ATOM 2172 CA GLN 275 35.805 37.720 59.808 1.00 25.26
ATOM 2101 OG1 THR 267 38.380 34.019 75.198 1.00 16.60	ATOM 2173 CB GLN 275 36.086 37.628 58.298 1.00 19.14
ATOM 2102 HG1 THR 267 38.051 33.496 74.464 1.00 0.00	ATOM 2174 CG GLN 275 35.616 38.829 57.480 1.00 19.44
ATOM 2103 CG2 THR 267 36.727 32.995 76.593 1.00 17.07	ATOM 2175 CD GLN 275 34.103 39.057 57.506 1.00 16.85
ATOM 2104 C THR 267 36.699 36.518 75.151 1.00 28.83	ATOM 2176 OE1 GLN 275 33.316 38.130 57.676 1.00 23.53
ATOM 2105 O THR 267 36.531 37.355 76.036 1.00 32.54	ATOM 2177 NE2 GLN 275 33.696 40.294 57.319 1.00 15.80
ATOM 2106 N VAL 268 37.302 36.811 74.005 1.00 32.30	ATOM 2178 HE21 GLN 275 34.357 41.007 57.184 1.00 0.00
ATOM 2107 H VAL 268 37.429 36.117 73.331 1.00 0.00	ATOM 2179 HE22 GLN 275 32.739 40.465 57.338 1.00 0.00
ATOM 2108 CA VAL 268 37.789 38.163 73.745 1.00 36.85	ATOM 2180 C GLN 275 36.303 36.451 60.494 1.00 24.15
ATOM 2109 CB VAL 268 38.437 38.528 72.326 1.00 36.24	ATOM 2181 O GLN 275 37.432 36.412 60.993 1.00 26.83
ATOM 2110 CG1 VAL 268 37.415 38.714 71.275 1.00 30.68	ATOM 2182 N ARG 276 35.451 35.440 60.570 1.00 21.69
ATOM 2111 CG2 VAL 268 39.691 39.115 72.357 1.00 27.04	ATOM 2183 H ARG 276 34.548 35.536 60.213 1.00 0.00
ATOM 2112 C VAL 268 36.627 39.156 73.898 1.00 43.33	ATOM 2184 CA ARG 276 35.838 34.164 61.167 1.00 19.65
ATOM 2113 O VAL 268 35.847 38.847 73.545 1.00 43.53	ATOM 2185 CB ARG 276 34.647 33.192 61.111 1.00 17.59
ATOM 2114 N PRO 269 36.887 40.337 74.489 1.00 48.08	ATOM 2186 CG ARG 276 33.468 33.638 62.002 1.00 15.00
ATOM 2115 CD PRO 269 38.152 40.854 75.035 1.00 51.38	ATOM 2187 CD ARG 276 33.857 33.488 63.474 1.00 14.70
ATOM 2116 CA PRO 269 35.816 41.321 74.659 1.00 52.01	ATOM 2188 NE ARG 276 33.091 34.297 64.418 1.00 12.83
ATOM 2117 CB PRO 269 36.545 42.530 75.529 1.00 50.38	ATOM 2189 HE ARG 276 33.399 35.210 64.577 1.00 0.00
ATOM 2118 CG PRO 269 37.971 42.331 74.848 1.00 52.06	ATOM 2190 CZ ARG 276 31.999 33.886 65.065 1.00 18.90
ATOM 2119 C PRO 269 35.162 41.648 73.322 1.00 54.55	ATOM 2191 NH1 ARG 276 31.499 32.668 64.883 1.00 19.00
ATOM 2120 O PRO 269 33.935 41.638 73.194 1.00 55.57	ATOM 2192 HH11 ARG 276 31.935 32.030 64.261 1.00 0.00
ATOM 2121 N SER 270 35.983 41.898 72.311 1.00 56.02	ATOM 2193 HH12 ARG 276 30.673 32.393 65.386 1.00 0.00
ATOM 2122 H SER 270 36.951 41.870 72.440 1.00 0.00	ATOM 2194 NH2 ARG 276 31.422 34.687 65.948 1.00 18.90
ATOM 2123 CA SER 270 35.433 42.204 71.010 1.00 55.44	ATOM 2195 HH21 ARG 276 31.812 35.596 66.119 1.00 0.00
ATOM 2124 CB SER 270 35.222 44.313 70.850 1.00 59.59	ATOM 2196 HH22 ARG 276 30.603 34.397 66.434 1.00 0.00
ATOM 2125 OG SER 270 34.455 44.000 69.687 1.00 63.26	ATOM 2197 C ARG 276 37.059 33.661 60.369 1.00 19.56
ATOM 2126 HG SER 270 33.591 43.592 69.782 1.00 0.00	ATOM 2198 O ARG 276 37.226 34.020 59.203 1.00 18.15
ATOM 2127 C SER 270 36.269 41.663 69.866 1.00 53.06	ATOM 2199 N ARG 277 37.906 32.846 60.988 1.00 15.03
ATOM 2128 O SER 270 37.502 41.682 69.900 1.00 48.03	ATOM 2200 H ARG 277 37.712 32.558 61.903 1.00 0.00
ATOM 2129 N GLU 270 35.556 41.139 68.876 1.00 53.04	ATOM 2201 CA ARG 277 39.131 32.373 60.341 1.00 17.54
ATOM 2130 H GLU 271 34.585 41.106 68.983 1.00 0.00	ATOM 2202 CB ARG 277 40.292 32.406 61.347 1.00 16.22
ATOM 2131 CA GLU 271 36.147 40.597 67.667 1.00 54.48	ATOM 2203 CG ARG 277 40.521 33.775 62.033 1.00 19.01
ATOM 2131 CB GLU 271 35.123 39.725 66.938 1.00 54.93	ATOM 2204 CD ARG 277 41.174 34.832 61.126 1.00 19.17
ATOM 2133 CG GLU 271 34.516 38.613 67.795 1.00 54.99	ATOM 2205 NE ARG 277 40.214 35.788 60.564 1.00 26.26
ATOM 2134 CD GLU 271 33.349 37.911 67.114 1.00 52.97	ATOM 2206 HE ARG 277 39.293 35.742 60.887 1.00 0.00
ATOM 2207 CZ ARG 277 40.511 36.715 59.646 1.00 24.81	ATOM 2207 CB ALA 283 40.798 23.264 63.007 1.00 18.53
ATOM 2208 NH1 ARG 277 41.741 36.830 59.166 1.00 26.15	ATOM 2208 C ALA 283 38.766 21.855 62.555 1.00 16.97
ATOM 2209 HH11 ARG 277 42.464 36.211 59.491 1.00 0.00	ATOM 2209 O ALA 283 38.775 20.702 62.988 1.00 14.00
ATOM 2210 HH12 ARG 277 41.951 37.512 58.472 1.00 0.00	ATOM 2209 N LEU 284 37.695 22.632 62.611 1.00 15.85
ATOM 2211 NH2 ARG 277 39.573 37.528 59.195 1.00 26.84	ATOM 2209 H LEU 284 37.747 23.542 62.250 1.00 0.00
ATOM 2212 HH21 ARG 277 38.640 37.451 59.538 1.00 0.00	ATOM 2209 CA LEU 284 36.454 22.165 63.202 1.00 16.34
ATOM 2213 HH22 ARG 277 39.803 38.208 58.500 1.00 0.00	ATOM 2209 CB ALA 283 40.798 23.264 63.007 1.00 18.53
ATOM 2214 C ARG 277 39.086 31.009 59.646 1.00 17.93	ATOM 2209 CG LEU 284 36.690 23.937 65.073 1.00 8.16
ATOM 2215 O ARG 277 38.617 30.034 60.207 1.00 17.46	ATOM 2209 CD1 LEU 284 36.018 25.180 65.567 1.00 8.60
ATOM 2216 N ARG 278 39.616 30.941 58.431 1.00 17.74	ATOM 2209 CD2 LEU 284 36.938 22.963 66.204 1.00 5.36
ATOM 2217 H ARG 278 39.984 31.756 58.032 1.00 0.00	ATOM 2209 C LEU 284 35.423 21.544 62.250 1.00 20.99
ATOM 2218 CA ARG 278 39.638 29.695 57.669 1.00 19.27	ATOM 2209 O LEU 284 34.694 20.633 62.657 1.00 23.47
ATOM 2219 CB ARG 278 40.315 29.913 56.302 1.00 26.70	ATOM 2209 N ASN 285 35.363 22.006 60.999 1.00 20.31
ATOM 2220 CG ARG 278 40.541 28.655 55.424 1.00 30.07	ATOM 2209 H ASN 285 35.985 22.707 60.724 1.00 0.00
ATOM 2221 CD ARG 278 39.279 28.146 54.708 1.00 33.95	ATOM 2209 CA ASN 285 34.378 21.494 60.024 1.00 26.25
ATOM 2222 NE ARG 278 39.490 26.851 54.037 1.00 38.49	ATOM 2209 CB ASN 285 34.666 21.980 58.605 1.00 21.03
ATOM 2223 HE ARG 278 39.252 26.054 54.517 1.00 0.00	ATOM 2209 CG ASN 285 34.267 23.431 58.407 1.00 21.30
ATOM 2224 CZ ARG 278 39.961 26.681 52.795 1.00 38.09	ATOM 2209 OD1 ASN 285 33.589 24.020 59.255 1.00 22.55
ATOM 2225 NH1 ARG 278 40.283 37.726 52.039 1.00 35.69	ATOM 2209 ND2 ASN 285 34.698 24.022 57.304 1.00 19.92
ATOM 2226 HH11 ARG 278 40.179 28.651 52.402 1.00 0.00	ATOM 2209 HD21 ASN 285 35.246 23.532 56.665 1.00 0.00
ATOM 2227 HH12 ARG 278 40.648 27.595 51.119 1.00 0.00	ATOM 2209 HD21 ASN 285 34.444 24.968 57.168 1.00 0.00
ATOM 2228 NH2 ARG 278 40.121 25.452 52.312 1.00 33.68	ATOM 2209 C ASN 285 34.068 20.007 60.040 1.00 28.14
ATOM 2229 HH21 ARG 278 39.871 24.660 52.860 1.00 0.00	ATOM 2209 O ASN 285 32.906 19.631 59.964 1.00 28.81
ATOM 2230 HH22 ARG 278 40.472 25.329 51.380 1.00 0.00	ATOM 2209 N GLY 286 35.088 19.156 60.051 1.00 34.18
ATOM 2231 C ARG 278 40.352 28.582 58.416 1.00 17.18	ATOM 2209 H GLY 286 36.000 19.483 60.013 1.00 0.00
ATOM 2232 O ARG 278 39.894 27.448 58.396 1.00 19.40	ATOM 2209 CA GLY 286 34.821 17.727 60.158 1.00 39.04

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ATOM 2233 N PHE 279 41.461 28.895 59.087 1.00 17.77	ATOM 2305 C GLY 286 34.957 16.711 59.036 1.00 39.96
ATOM 2234 H PHE 279 41.786 29.820 59.100 1.00 0.00	ATOM 2306 O GLY 286 34.456 15.589 59.201 1.00 45.42
ATOM 2235 CA PHE 279 42.198 27.853 59.796 1.00 13.89	ATOM 2307 N ASN 287 35.625 17.078 57.937 1.00 34.10
ATOM 2236 CB PHE 279 43.552 28.347 60.342 1.00 14.71	ATOM 2308 H ASN 287 35.974 17.984 57.918 1.00 0.00
ATOM 2237 CG PHE 279 43.484 29.183 61.607 1.00 15.65	ATOM 2309 CA ASN 287 35.861 16.211 56.761 1.00 29.60
ATOM 2238 CD1 PHE 279 43.717 28.594 62.858 1.00 18.80	ATOM 2310 CB ASN 287 36.539 14.865 57.139 1.00 34.52
ATOM 2239 CD2 PHE 279 43.341 30.571 61.542 1.00 15.68	ATOM 2311 CG ASN 287 35.548 13.700 57.352 1.00 40.80
ATOM 2240 CE1 PHE 279 43.823 29.369 64.033 1.00 13.51	ATOM 2312 OD1 ASN 287 34.322 13.886 57.421 1.00 43.97
ATOM 2241 CE2 PHE 279 43.447 31.359 62.710 1.00 19.29	ATOM 2313 ND2 ASN 287 36.094 12.484 57.464 1.00 36.28
ATOM 2242 CZ PHE 279 43.691 30.750 63.958 1.00 14.33	ATOM 2314 HD21 ASN 287 37.057 12.835 57.409 1.00 0.00
ATOM 2243 C PHE 279 41.365 27.191 60.865 1.00 14.00	ATOM 2315 HD22 ASN 287 35.475 11.736 57.596 1.00 0.00
ATOM 2244 O PHE 279 41.463 25.985 61.082 1.00 13.69	ATOM 2316 C ASN 287 34.737 16.009 55.741 1.00 25.40
ATOM 2245 N VAL 280 40.511 27.979 61.503 1.00 16.14	ATOM 2317 O ASN 287 34.931 15.338 54.730 1.00 22.82
ATOM 2246 H VAL 280 40.460 28.923 61.263 1.00 0.00	ATOM 2318 N GLY 288 33.576 16.602 55.991 1.00 19.10
ATOM 2247 CA VAL 280 39.635 27.464 62.543 1.00 14.61	ATOM 2319 H GLY 288 33.455 17.110 56.808 1.00 0.00
ATOM 2248 CB VAL 280 39.015 28.620 63.371 1.00 16.28	ATOM 2320 CA GLY 288 32.475 16.497 55.048 1.00 18.41
ATOM 2249 CG1 VAL 280 37.946 28.083 64.339 1.00 12.84	ATOM 2321 C GLY 288 31.564 15.295 55.133 1.00 17.17
ATOM 2250 CG2 VAL 280 40.118 29.344 64.129 1.00 12.25	ATOM 2322 O GLY 288 30.639 15.168 54.342 1.00 14.79
ATOM 2251 C VAL 280 38.543 26.653 61.872 1.00 12.07	ATOM 2323 N ASP 289 31.823 14.404 56.079 1.00 19.90
ATOM 2252 O VAL 280 38.233 25.531 62.294 1.00 15.69	ATOM 2324 H ASP 289 32.585 14.563 56.676 1.00 0.00
ATOM 2253 N GLN 281 38.003 27.202 60.791 1.00 12.46	ATOM 2325 CA ASP 289 31.015 13.208 56.269 1.00 17.92
ATOM 2254 H GLN 281 38.323 28.080 60.492 1.00 0.00	ATOM 2326 CB ASP 289 31.700 12.331 57.328 1.00 24.19
ATOM 2255 CA GLN 281 36.946 26.541 60.046 1.00 12.48	ATOM 2327 CG ASP 289 31.065 10.951 57.479 1.00 27.47
ATOM 2256 CB GLN 281 36.460 27.428 58.890 1.00 12.05	ATOM 2328 OD1 ASP 289 30.310 10.489 56.596 1.00 32.15
ATOM 2257 CG GLN 281 35.85 28.769 59.325 1.00 15.34	ATOM 2329 OD2 ASP 289 31.352 10.310 58.507 1.00 37.02
ATOM 2258 CD GLN 281 35.847 29.820 58.199 1.00 18.27	ATOM 2330 C ASP 289 29.614 13.609 56.745 1.00 19.07
ATOM 2259 OE1 GLN 281 36.473 29.640 57.151 1.00 21.65	ATOM 2331 O ASP 289 29.464 14.189 57.829 1.00 17.44
ATOM 2260 NE2 GLN 281 35.182 30.939 58.442 1.00 16.98	ATOM 2332 N PRO 290 28.566 13.315 55.950 1.00 16.17
ATOM 2261 HE21 GLN 281 34.726 31.050 59.312 1.00 0.00	ATOM 2333 CD PRO 290 28.532 12.778 54.573 1.00 14.59
ATOM 2262 HE22 GLN 281 35.161 31.610 57.734 1.00 0.00	ATOM 2334 CA PRO 290 27.221 13.689 56.397 1.00 14.74
ATOM 2263 C GLN 281 37.437 25.197 59.522 1.00 13.34	ATOM 2335 CB PRO 290 26.333 13.334 55.195 1.00 12.58
ATOM 2264 O GLN 281 36.746 24.192 59.640 1.00 16.51	ATOM 2336 CG PRO 290 27.116 12.282 54.458 1.00 13.57
ATOM 2265 N ASN 282 38.656 25.149 59.010 1.00 14.65	ATOM 2337 C PRO 290 26.771 12.973 57.670 1.00 16.11
ATOM 2266 H ASN 282 39.205 25.937 58.997 1.00 0.00	ATOM 2338 O PRO 290 25.947 13.495 58.423 1.00 17.73
ATOM 2267 CA ASN 282 39.175 23.897 58.493 1.00 13.22	ATOM 2339 N ASN 291 27.316 11.784 57.919 1.00 15.95
ATOM 2268 CB ASN 282 40.482 24.125 57.766 1.00 22.94	ATOM 2340 H ASN 291 27.977 11.429 57.290 1.00 0.00
ATOM 2269 CG ASN 282 40.298 24.887 56.482 1.00 26.80	ATOM 2341 CA ASN 291 26.934 11.010 59.098 1.00 15.36
ATOM 2270 OD1 ASN 282 39.206 24.902 55.902 1.00 26.92	ATOM 2342 CB ASN 291 27.544 9.607 59.045 1.00 20.14
ATOM 2271 ND2 ASN 282 41.366 25.534 56.025 1.00 29.37	ATOM 2343 CG ASN 291 26.957 8.751 57.914 1.00 29.95
ATOM 2272 HD21 ASN 282 42.201 25.499 56.524 1.00 0.00	ATOM 2344 OD1 ASN 291 25.764 8.840 57.603 1.00 27.64
ATOM 2273 HD22 ASN 282 41.250 26.042 55.195 1.00 0.00	ATOM 2345 ND2 ASN 291 27.800 7.926 57.287 1.00 35.21
ATOM 2274 C ASN 282 39.381 22.867 59.575 1.00 16.97	ATOM 2346 HD21 ASN 291 28.743 7.888 57.559 1.00 0.00
ATOM 2275 O ASN 282 39.181 21.676 59.346 1.00 15.36	ATOM 2347 HD22 ASN 291 27.439 7.374 56.563 1.00 0.00
ATOM 2276 N ALA 283 39.770 23.335 60.758 1.00 17.24	ATOM 2348 C ASN 291 27.338 11.725 60.376 1.00 15.24
ATOM 2277 H ALA 283 39.905 24.298 60.854 1.00 0.00	ATOM 2349 O ASN 291 26.555 11.838 61.326 1.00 14.36
ATOM 2278 CA ALA 283 40.023 22.474 61.927 1.00 20.01	ATOM 2350 N ASN 292 28.562 12.227 60.383 1.00 13.11
ATOM 2251 H ASN 292 29.154 12.105 59.616 1.00 0.00	ATOM 2342 CG LEU 299 26.056 18.212 70.751 1.00 5.81
ATOM 2252 CA ASN 292 29.087 12.956 61.516 1.00 13.18	ATOM 2424 CD1 LEU 299 25.444 17.859 72.104 1.00 5.01
ATOM 2253 CB ASN 292 30.596 13.107 61.355 1.00 19.78	ATOM 2425 CD2 LEU 299 27.537 17.895 70.753 1.00 3.65
ATOM 2254 CG ASN 292 31.211 14.071 62.302 1.00 28.71	ATOM 2426 C LEU 299 23.402 19.024 69.742 1.00 9.73
ATOM 2255 OD1 ASN 292 31.514 15.209 61.938 1.00 29.73	ATOM 2427 O LEU 299 22.973 19.451 70.808 1.00 13.20
ATOM 2256 ND2 ASN 292 31.412 13.630 63.545 1.00 34.11	ATOM 2428 CG TYR 300 23.510 19.781 68.653 1.00 10.11
ATOM 2257 HD21 ASN 292 31.183 12.741 63.846 1.00 0.00	ATOM 2429 H TYR 300 23.872 19.379 67.834 1.00 0.00
ATOM 2258 HD22 ASN 292 31.760 14.303 64.150 1.00 0.00	ATOM 2430 CA TYR 300 23.122 21.186 68.629 1.00 9.02
ATOM 2259 C ASN 292 28.362 14.309 61.643 1.00 13.32	ATOM 2431 CB TYR 300 23.367 21.785 67.241 1.00 7.95
ATOM 2260 O ASN 292 28.010 14.731 62.741 1.00 15.59	ATOM 2432 CG TYR 300 22.788 23.158 67.068 1.00 10.20
ATOM 2261 N MET 293 28.057 14.946 60.514 1.00 14.57	ATOM 2433 CD1 TYR 300 23.295 24.238 67.779 1.00 16.87
ATOM 2262 H MET 293 28.334 14.557 59.661 1.00 0.00	ATOM 2434 CE1 TYR 300 22.747 25.512 67.643 1.00 15.45
ATOM 2263 CA MET 293 27.336 16.222 60.527 1.00 11.47	ATOM 2435 CD2 TYR 300 21.717 23.379 66.210 1.00 9.46
ATOM 2264 CB MET 293 27.230 16.798 59.111 1.00 11.95	ATOM 2436 CE2 TYR 300 21.162 24.646 66.059 1.00 8.57
ATOM 2265 CG MET 293 28.489 17.469 58.600 1.00 17.06	ATOM 2437 CZ TYR 300 21.680 25.704 66.774 1.00 14.54
ATOM 2266 SD MET 293 29.105 18.779 59.711 1.00 21.66	ATOM 2438 OH TYR 300 21.169 26.969 66.597 1.00 17.24
ATOM 2267 CE MET 293 27.790 20.093 59.487 1.00 17.21	ATOM 2439 HH TYR 300 21.605 27.561 67.185 1.00 0.00
ATOM 2268 C MET 293 25.928 16.047 61.119 1.00 11.57	ATOM 2440 C TYR 300 21.660 21.374 69.014 1.00 6.78
ATOM 2269 O MET 293 25.407 16.938 61.809 1.00 13.99	ATOM 2441 O TYR 300 21.318 22.323 69.072 1.00 11.35
ATOM 2270 N ASP 294 25.319 14.894 60.842 1.00 11.64	ATOM 2442 N ARG 301 20.796 20.490 68.542 1.00 5.73
ATOM 2271 H ASP 294 25.785 14.237 60.287 1.00 0.00	ATOM 2443 H ARG 301 21.109 19.768 67.960 1.00 0.00
ATOM 2272 CA ASP 294 23.984 14.571 61.326 1.00 11.13	ATOM 2444 CA ARG 301 19.384 20.569 68.865 1.00 7.64
ATOM 2273 CB ASP 294 23.558 13.193 60.804 1.00 11.26	ATOM 2445 CB ARG 301 18.647 19.416 68.174 1.00 8.01
ATOM 2274 CG ASP 294 22.290 12.661 61.475 1.00 12.41	ATOM 2446 CG ARG 301 17.181 19.168 68.563 1.00 14.79
ATOM 2275 OD1 ASP 294 21.227 13.331 61.454 1.00 12.07	ATOM 2447 CD ARG 301 16.339 18.583 67.379 1.00 20.64
ATOM 2276 OD2 ASP 294 22.363 11.541 62.023 1.00 14.66	ATOM 2448 NE ARG 301 17.140 17.736 66.487 1.00 28.98
ATOM 2277 C ASP 294 24.031 14.572 62.842 1.00 11.54	ATOM 2449 HE ARG 301 17.909 17.271 66.872 1.00 0.00
ATOM 2278 O ASP 294 23.175 15.168 53.493 1.00 10.58	ATOM 2450 CZ ARG 301 16.905 17.539 65.186 1.00 31.08
ATOM 2279 N LYS 295 25.073 13.947 63.385 1.00 9.77	ATOM 2451 NH1 ARG 301 15.867 18.122 64.590 1.00 20.46
ATOM 2280 H LYS 295 25.736 13.544 62.788 1.00 0.00	ATOM 2452 HH11 ARG 301 15.253 18.717 65.106 1.00 0.00
ATOM 2281 CA LYS 295 25.274 13.844 64.820 1.00 11.01	ATOM 2453 HH12 ARG 301 15.702 17.971 63.611 1.00 0.00
ATOM 2282 CB LYS 295 26.405 12.861 65.132 1.00 12.17	ATOM 2454 NH2 ARG 301 17.736 16.769 64.470 1.00 29.91
ATOM 2283 CG LYS 295 26.112 11.414 64.721 1.00 15.92	ATOM 2455 HH21 ARG 301 18.524 16.341 64.906 1.00 0.00

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ATOM 2384 CD LYS 295 24.745 10.935 65.238 1.00 26.08	ATOM 2456 HH22 ARG 301 17.561 16.620 63.493 1.00 0.00
ATOM 2385 CE LYS 295 24.650 10.986 66.779 1.00 32.27	ATOM 2457 C ARG 301 19.255 20.508 70.392 1.00 11.97
ATOM 2386 NZ LYS 295 23.340 10.508 67.328 1.00 35.24	ATOM 2458 O ARG 301 18.539 21.306 71.008 1.00 8.66
ATOM 2387 HZ1 LYS 295 23.187 9.519 67.040 1.00 0.00	ATOM 2459 N LYS 302 20.032 19.621 71.005 1.00 12.43
ATOM 2388 HZ2 LYS 295 22.568 11.098 66.951 1.00 0.00	ATOM 2460 H LYS 302 20.624 19.048 70.476 1.00 0.00
ATOM 2389 HZ3 LYS 295 23.355 10.573 68.362 1.00 0.00	ATOM 2461 CA LYS 302 20.001 19.473 72.456 1.00 13.80
ATOM 2390 C LYS 295 25.576 15.194 65.449 1.00 9.04	ATOM 2462 CB LYS 302 20.659 18.163 72.872 1.00 11.66
ATOM 2391 O LYS 295 25.142 15.478 66.568 1.00 10.34	ATOM 2463 CG LYS 302 19.857 16.963 72.470 1.00 10.77
ATOM 2392 N ALA 296 26.345 16.017 64.746 1.00 7.72	ATOM 2464 CD LYS 302 20.610 15.694 72.793 1.00 10.43
ATOM 2393 H ALA 296 26.690 15.740 63.873 1.00 0.00	ATOM 2465 CE LYS 302 19.802 14.507 72.347 1.00 11.53
ATOM 2394 CA ALA 296 26.671 17.333 65.621 1.00 5.19	ATOM 2466 NZ LYS 302 20.469 13.216 72.662 1.00 13.56
ATOM 2395 CB ALA 296 27.715 18.004 64.381 1.00 6.61	ATOM 2467 HZ1 LYS 302 20.601 13.136 73.690 1.00 0.00
ATOM 2396 C ALA 296 25.392 18.172 65.358 1.00 6.09	ATOM 2468 HZ2 LYS 302 21.393 13.174 81.187 1.00 0.00
ATOM 2397 O ALA 296 25.250 18.972 66.277 1.00 8.56	ATOM 2469 HZ3 LYS 302 19.871 12.432 72.327 1.00 0.00
ATOM 2398 N VAL 297 24.444 17.955 64.434 1.00 10.76	ATOM 2470 C LYS 302 20.615 20.659 73.195 1.00 10.42
ATOM 2399 H VAL 297 24.613 17.284 63.743 1.00 0.00	ATOM 2471 O LYS 302 20.032 21.158 74.153 1.00 10.98
ATOM 2400 CA VAL 297 23.162 18.673 64.415 1.00 7.41	ATOM 2472 N LEU 303 21.766 21.128 72.730 1.00 6.22
ATOM 2401 CB VAL 297 22.457 18.528 63.038 1.00 8.39	ATOM 2473 H LEU 303 22.179 20.704 71.953 1.00 0.00
ATOM 2402 CG1 VAL 297 21.046 19.133 63.088 1.00 8.02	ATOM 2474 CA LEU 303 22.419 22.262 73.349 1.00 10.05
ATOM 2403 CG2 VAL 297 23.293 19.198 61.971 1.00 3.74	ATOM 2475 CB LEU 303 23.755 22.554 72.689 1.00 7.08
ATOM 2404 C VAL 297 22.226 18.206 65.526 1.00 5.23	ATOM 2476 CG LEU 303 24.884 21.545 72.876 1.00 10.45
ATOM 2405 O VAL 297 21.463 18.982 66.087 1.00 8.24	ATOM 2477 CD1 LEU 303 26.131 22.045 72.162 1.00 10.81
ATOM 2406 N LYS 298 22.247 16.917 65.800 1.00 6.55	ATOM 2478 CD2 LEU 303 25.193 21.339 74.328 1.00 6.09
ATOM 2407 H LYS 298 22.817 16.323 65.271 1.00 0.00	ATOM 2479 C LEU 303 21.571 23.524 73.310 1.00 16.52
ATOM 2408 CA LYS 298 21.442 16.349 66.869 1.00 7.19	ATOM 2480 O LEU 303 21.736 24.392 74.168 1.00 18.88
ATOM 2409 CB LYS 298 21.566 14.828 66.867 1.00 7.37	ATOM 2481 N LYS 304 20.659 23.607 72.336 1.00 18.39
ATOM 2410 CG LYS 298 20.667 14.133 65.879 1.00 15.04	ATOM 2482 H LYS 304 20.588 22.865 71.696 1.00 0.00
ATOM 2411 CD LYS 298 21.327 12.896 65.347 1.00 20.63	ATOM 2483 CA LYS 304 19.769 34.766 72.150 1.00 20.75
ATOM 2412 CE LYS 298 20.322 12.005 64.644 1.00 28.28	ATOM 2484 CB LYS 304 18.923 25.594 70.882 1.00 23.75
ATOM 2413 NZ LYS 298 19.194 12.789 63.771 1.00 37.61	ATOM 2485 CG LYS 304 19.216 25.550 69.747 1.00 31.46
ATOM 2414 HZ1 LYS 298 19.980 13.301 63.063 1.00 0.00	ATOM 2486 CD LYS 304 18.784 26.980 70.060 1.00 44.15
ATOM 2415 HZ2 LYS 298 18.901 13.478 64.358 1.00 0.00	ATOM 2487 CE LYS 304 18.941 27.875 68.834 1.00 45.35
ATOM 2416 HZ3 LYS 298 18.748 12.155 63.304 1.00 0.00	ATOM 2488 NZ LYS 304 18.712 29.306 69.151 1.00 51.31
ATOM 2417 C LYS 298 21.943 16.907 68.204 1.00 7.36	ATOM 2489 HZ1 LYS 304 19.398 29.618 69.868 1.00 0.00
ATOM 2418 O LYS 298 21.145 17.190 69.089 1.00 9.72	ATOM 2490 HZ2 LYS 304 17.747 29.434 69.514 1.00 0.00
ATOM 2419 N LEU 299 23.263 16.984 68.376 1.00 7.00	ATOM 2491 HZ3 LYS 304 18.836 29.875 68.287 1.00 0.00
ATOM 2420 H LEU 299 23.858 16.644 67.676 1.00 0.00	ATOM 2492 C LYS 304 18.824 24.907 73.324 1.00 18.42
ATOM 2421 CA LEU 299 23.831 17.556 69.599 1.00 7.71	ATOM 2493 O LYS 304 18.238 25.961 73.549 1.00 22.41
ATOM 2422 CB LEU 299 23.353 17.473 69.593 1.00 3.79	ATOM 2494 N ARG 305 18.639 23.822 74.048 1.00 16.95
ATOM 2495 H ARG 305 19.098 22.988 73.807 1.00 0.00	ATOM 2495 C GLY 311 24.602 20.545 80.033 1.00 8.82
ATOM 2496 CA ARG 305 17.757 23.842 75.188 1.00 19.62	ATOM 2496 O GLY 311 24.465 19.471 79.423 1.00 9.64
ATOM 2497 CB ARG 305 16.964 22.546 75.230 1.00 21.07	ATOM 2499 N ALA 312 25.191 21.615 79.522 1.00 8.08
ATOM 2498 CG ARG 305 16.172 22.311 73.957 1.00 25.07	ATOM 2500 H ALA 312 25.250 22.428 80.063 1.00 0.00
ATOM 2499 CD ARG 305 15.393 21.039 74.043 1.00 26.97	ATOM 2501 CA ALA 312 25.769 21.630 78.189 1.00 8.48
ATOM 2500 NE ARG 305 14.736 20.740 72.777 1.00 31.36	ATOM 2502 CB ALA 312 26.292 23.023 77.873 1.00 8.53
ATOM 2501 HE ARG 305 14.150 21.425 72.388 1.00 0.00	ATOM 2503 C ALA 312 26.895 20.598 78.093 1.00 9.64
ATOM 2502 CZ ARG 305 14.889 19.604 72.109 1.00 32.19	ATOM 2504 H ALA 312 26.918 19.772 77.172 1.00 9.55
ATOM 2503 NH1 ARG 305 15.691 18.651 72.579 1.00 34.71	ATOM 2505 N LYS 313 27.817 20.623 79.050 1.00 5.87
ATOM 2504 HH11 ARG 305 16.176 18.789 73.443 1.00 0.00	ATOM 2506 H LYS 313 27.749 21.278 79.766 1.00 0.00
ATOM 2505 HH12 ARG 305 15.793 17.791 72.082 1.00 0.00	ATOM 2507 CA LYS 313 28.919 19.672 79.049 1.00 6.70
ATOM 2506 NH2 ARG 305 14.199 19.400 70.993 1.00 32.82	ATOM 2508 CB LYS 313 29.931 20.006 80.169 1.00 7.83
ATOM 2507 HH21 ARG 305 13.576 20.106 70.656 1.00 0.00	ATOM 2509 CG LYS 313 31.208 19.156 80.129 1.00 8.27
ATOM 2508 HH22 ARG 305 14.306 18.543 70.489 1.00 0.00	ATOM 2510 CD LYS 313 32.274 19.689 81.073 1.00 6.98
ATOM 2509 C ARG 305 18.505 24.039 76.499 1.00 21.81	ATOM 2511 CE LYS 313 31.776 19.685 82.508 1.00 9.13
ATOM 2510 O ARG 305 17.892 24.305 77.530 1.00 24.20	ATOM 2512 HZ1 LYS 313 31.522 18.308 83.035 1.00 10.81
ATOM 2511 N GLU 306 19.828 23.922 76.470 1.00 18.02	ATOM 2513 HZ2 LYS 313 32.413 17.764 83.005 1.00 0.00
ATOM 2512 H GLU 306 20.281 23.767 75.617 1.00 0.00	ATOM 2514 HZ3 LYS 313 30.815 17.835 82.440 1.00 0.00
ATOM 2513 CA GLU 306 20.615 24.068 77.691 1.00 11.09	ATOM 2515 HZ1 LYS 313 31.184 18.363 84.013 1.00 0.00
ATOM 2514 CB GLU 306 21.958 23.344 77.541 1.00 9.94	ATOM 2516 HZ2 LYS 313 31.252 18.225 79.184 1.00 9.48
ATOM 2515 CG GLU 306 21.874 21.910 77.107 1.00 6.81	ATOM 2517 HZ3 LYS 313 31.243 17.764 83.005 1.00 10.99
ATOM 2516 CD GLU 306 21.317 21.009 78.175 1.00 14.41	ATOM 2518 HZ1 LYS 313 31.243 17.764 83.005 1.00 0.00
ATOM 2517 OE1 GLU 306 21.414 21.345 79.370 1.00 16.53	ATOM 2519 HZ2 LYS 313 30.815 17.835 82.440 1.00 0.00
ATOM 2518 OE2 GLU 306 20.761 19.955 77.827 1.00 22.60	ATOM 2520 HZ3 LYS 313 31.184 18.363 84.013 1.00 0.00
ATOM 2519 C GLU 306 20.917 25.517 77.799 1.00 10.43	ATOM 2521 HZ1 LYS 313 31.243 17.764 83.005 1.00 10.30
ATOM 2520 O GLU 306 21.054 26.301 77.044 1.00 8.17	ATOM 2522 HZ2 LYS 313 31.243 17.764 83.005 1.00 13.21
ATOM 2521 N ILE 307 21.023 25.874 79.244 1.00 12.01	ATOM 2523 HZ3 LYS 313 31.243 17.764 83.005 1.00 17.97
ATOM 2522 H ILE 307 20.833 25.217 79.940 1.00 0.00	ATOM 2524 HZ1 LYS 313 31.243 17.764 83.005 1.00 21.28
ATOM 2523 CA ILE 307 21.403 27.237 79.616 1.00 12.96	ATOM 2525 HZ2 LYS 313 31.243 17.764 83.005 1.00 13.39
ATOM 2524 CB ILE 307 20.236 28.095 80.236 1.00 12.97	ATOM 2526 HZ3 LYS 313 31.243 17.764 83.005 1.00 10.09
ATOM 2525 CG2 ILE 307 19.125 28.303 79.199 1.00 15.84	ATOM 2527 HZ1 LYS 313 31.243 17.764 83.005 1.00 10.37
ATOM 2526 CG1 ILE 307 19.679 27.440 51.509 1.00 11.68	ATOM 2528 HZ2 LYS 313 31.243 17.764 83.005 1.00 12.08
ATOM 2527 CD1 ILE 307 18.792 28.362 82.351 1.00 8.49	ATOM 2529 HZ3 LYS 313 31.243 17.764 83.005 1.00 0.00
ATOM 2528 C ILE 307 22.576 27.199 80.591 1.00 11.34	ATOM 2530 HZ1 LYS 313 31.243 17.764 83.005 1.00 0.00
ATOM 2529 O ILE 307 23.133 28.239 80.920 1.00 13.88	ATOM 2531 HZ2 LYS 313 31.243 17.764 83.005 1.00 0.00
ATOM 2530 N THR 308 22.968 26.013 81.053 1.00 9.66	ATOM 2532 HZ3 LYS 313 31.243 17.764 83.005 1.00 0.00
ATOM 2531 H THR 308 22.518 25.209 80.757 1.00 0.00	ATOM 2533 HZ1 LYS 313 31.243 17.764 83.005 1.00 0.00
ATOM 2532 CA THR 308 24.082 25.925 81.998 1.00 9.42	ATOM 2534 HZ2 LYS 313 31.243 17.764 83.005 1.00 0.00
ATOM 2533 CB THR 308 23.683 25.241 83.373 1.00 10.90	ATOM 2535 HZ3 LYS 313 31.243 17.764 83.005 1.00 0.00
ATOM 2534 OG1 THR 308 23.318 23.864 83.160 1.00 17.40	ATOM 2536 HZ1 LYS 313 31.243 17.764 83.005 1.00 0.00
ATOM 2537 HZ2 LYS 313 31.243 17.764 83.005 1.00 0.00	ATOM 2538 HZ3 LYS 313 31.243 17.764 83.005 1.00 0.00
ATOM 2539 HZ1 LYS 313 31.243 17.764 83.005 1.00 0.00	ATOM 2539 HZ2 LYS 313 31.243 17.764 83.005 1.00 0.00
ATOM 2540 HZ3 LYS 313 31.243 17.764 83.005 1.00 0.00	ATOM 2541 HZ1 LYS 313 31.243 17.764 83.005 1.00 0.00
ATOM 2541 HZ2 LYS 313 31.243 17.764 83.005 1.00 0.00	ATOM 2542 HZ3 LYS 313 31.243 17.764 83.005 1.00 0.00
ATOM 2542 HZ1 LYS 313 31.243 17.764 83.005 1.00 0.00	ATOM 2543 HZ2 LYS 313 31.243 17.764 83.005 1.00 0.00
ATOM 2543 HZ2 LYS 313 31.243 17.764 83.005 1.00 0.00	ATOM 2544 HZ3 LYS 313 31.243 17.764 83.005 1.00 0.00
ATOM 2544 HZ1 LYS 313 31.243 17.764 83.005 1.00 0.00	ATOM 2545 HZ2 LYS 313 31.243 17.764 83.005 1.00 0.00
ATOM 2545 HZ2 LYS 313 31.243 17.764 83.005 1.00 0.00	ATOM 2546 HZ3 LYS 313 31.243 17.764 83.005 1.00 0.00
ATOM 2546 HZ1 LYS 313 31.243 17.764 83.005 1.00 0.00	ATOM 2547 HZ2 LYS 313 31.243 17.764 83.005 1.00 0.00
ATOM 2547 HZ2 LYS 313 31.243 17.764 83.005 1.00 0.00	ATOM 2548 HZ3 LYS 313 31.243 17.764 83.005 1.00 0.00
ATOM 2548 HZ1 LYS 313 31.243 17.764 83.005 1.00 0.00	ATOM 2549 HZ2 LYS 313 31.243 17.764 83.005 1.00 0.00
ATOM 2549 HZ2 LYS 313 31.243 17.764 83.005 1.00 0.00	ATOM 2550 HZ3 LYS 313 31.243 17.764 83.005 1.00 0.00
ATOM 2550 HZ1 LYS 313 31.243 17.764 83.005 1.00 0.00	ATOM 2551 HZ2 LYS 313 31.243 17.764 83.005 1.00 0.00
ATOM 2551 HZ2 LYS 313 31.243 17.764 83.005 1.00 0.00	ATOM 2552 HZ3 LYS 313 31.243 17.764 83.005 1.00 0.00
ATOM 2552 HZ1 LYS 313 31.243 17.764 83.005 1.00 0.00	ATOM 2553 HZ2 LYS 313 31.243 17.764 83.005 1.00 0.00
ATOM 2553 HZ2 LYS 313 31.243 17.764 83.005 1.00 0.00	ATOM 2554 HZ3 LYS 313 31.243 17.764 83.005 1.00 0.00
ATOM 2554 HZ1 LYS 313 31.243 17.764 83.005 1.00 0.00	ATOM 2555 HZ2 LYS 313 31.243 17.764 83.005 1.00 0.00
ATOM 2555 HZ2 LYS 313 31.243 17.764 83.005 1.00 0.00	ATOM 2556 HZ3 LYS 313 31.243 17.764 83.005 1.00 0.00
ATOM 2556 HZ1 LYS 313 31.243 17.764 83.005 1.00 0.00	ATOM 2557 HZ2 LYS 313 31.243 17.764 83.005 1.00 0.00
ATOM 2557 HZ2 LYS 313 31.243 17.764 83.005 1.00 0.00	ATOM 2558 HZ3 LYS 313 31.243 17.764 83.005 1.00 0.00
ATOM 2558 HZ1 LYS 313 31.243 17.764 83.005 1.00 0.00	ATOM 2559 HZ2 LYS 313 31.243 17.764 83.005 1.00 0.00
ATOM 2559 HZ2 LYS 313 31.243 17.764 83.005 1.00 0.00	ATOM 2560 HZ3 LYS 313 31.243 17.764 83.005 1.00 0.00
ATOM 2560 HZ1 LYS 313 31.243 17.764 83.005 1.00 0.00	ATOM 2561 HZ2 LYS 313 31.243 17.764 83.005 1.00 0.00
ATOM 2561 HZ2 LYS 313 31.243 17.764 83.005 1.00 0.00	ATOM 2562 HZ3 LYS 313 31.243 17.764 83.005 1.00 0.00
ATOM 2562 HZ1 LYS 313 31.243 17.764 83.005 1.00 0.00	ATOM 2563 HZ2 LYS 313 31.243 17.764 83.005 1.00 0.00
ATOM 2563 HZ2 LYS 313 31.243 17.764 83.005 1.00 0.00	ATOM 2564 HZ3 LYS 313 31.243 17.764 83.005 1.00 0.00
ATOM 2564 HZ1 LYS 313 31.243 17.764 83.005 1.00 0.00	ATOM 2565 HZ2 LYS 313 31.243 17.764 83.005 1.00 0.00
ATOM 2565 HZ2 LYS 313 31.243 17.764 83.005 1.00 0.00	ATOM 2566 HZ3 LYS 313 31.243 17.764 83.005 1.00 0.00

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ATOM 2535 HG1 THR 308 22.532 23.846 82.591 1.00 0.00	ATOM 2607 N SER 316 26.893 16.779 75.886 1.00 7.34
ATOM 2536 CG2 THR 308 22.530 26.007 84.095 1.00 9.88	ATOM 2608 H SER 316 26.880 17.534 76.517 1.00 0.00
ATOM 2537 C THR 308 25.291 25.186 81.431 1.00 7.68	ATOM 2609 CA SER 316 27.990 16.696 74.926 1.00 6.45
ATOM 2538 O THR 308 25.154 24.314 80.573 1.00 12.31	ATOM 2610 CB SER 316 28.904 17.911 75.066 1.00 6.72
ATOM 2539 N PHE 309 26.463 25.534 81.954 1.00 7.15	ATOM 2611 OG SER 316 28.229 19.094 74.683 1.00 8.15
ATOM 2540 H PHE 309 36.474 26.251 82.627 1.00 0.00	ATOM 2612 HG SER 316 28.813 19.846 74.799 1.00 0.00
ATOM 2541 CA PHE 309 27.741 24.941 81.583 1.00 10.36	ATOM 2613 C SER 316 28.794 15.412 75.118 1.00 12.37
ATOM 2542 CB PHE 309 28.853 25.564 82.435 1.00 4.51	ATOM 2614 O SER 316 29.350 14.863 74.165 1.00 11.95
ATOM 2543 CG PHE 309 30.163 24.838 82.339 1.00 7.97	ATOM 2615 N LEU 317 28.826 14.921 76.356 1.00 13.97
ATOM 2544 CD1 PHE 309 31.010 25.052 81.246 1.00 9.69	ATOM 2616 H LEU 317 28.344 15.396 77.071 1.00 0.00
ATOM 2545 CD2 PHE 309 30.538 23.911 83.319 1.00 7.03	ATOM 2617 CA LEU 317 29.552 13.705 76.694 1.00 11.99
ATOM 2546 CE1 PHE 309 21.193 24.345 81.109 1.00 6.61	ATOM 2618 CB LEU 317 29.611 13.538 78.216 1.00 12.81
ATOM 2547 CE2 PHE 309 31.728 23.189 83.196 1.00 6.73	ATOM 2619 CG LEU 317 30.431 14.580 79.001 1.00 17.31
ATOM 2548 CZ PHE 309 32.561 23.411 82.086 1.00 7.86	ATOM 2620 CD1 LEU 317 30.330 14.316 80.504 1.00 15.91
ATOM 2549 C PHE 309 27.719 23.444 81.823 1.00 11.68	ATOM 2621 CD2 LEU 317 31.899 14.563 78.550 1.00 17.80
ATOM 2550 O PHE 309 28.121 22.656 80.968 1.00 13.44	ATOM 2622 C LEU 317 28.960 12.457 76.029 1.00 15.63
ATOM 2551 N HIS 310 27.261 23.053 83.006 1.00 13.27	ATOM 2623 O LEU 317 29.594 11.394 76.005 1.00 16.20
ATOM 2552 H HIS 310 26.947 23.720 83.648 1.00 0.00	ATOM 2624 N SER 318 27.739 12.562 75.506 1.00 15.11
ATOM 2553 CA HIS 310 27.217 21.655 83.351 1.00 11.98	ATOM 2625 H SER 318 27.236 13.398 75.579 1.00 0.00
ATOM 2554 CB HIS 310 26.860 21.462 84.815 1.00 15.73	ATOM 2626 CA SER 318 27.137 11.419 74.826 1.00 11.86
ATOM 2555 CG HIS 310 26.676 20.034 85.184 1.00 11.24	ATOM 2627 CB SER 318 25.613 11.385 75.008 1.00 15.54
ATOM 2556 CD2 HIS 310 27.599 19.060 85.464 1.00 9.87	ATOM 2628 OG SER 318 24.998 12.546 74.482 1.00 22.77
ATOM 2557 ND1 HIS 310 25.470 19.400 85.146 1.00 16.13	ATOM 2629 HG SER 318 25.307 13.306 74.918 1.00 0.00
ATOM 2558 HD1 HIS 310 24.598 19.834 84.991 1.00 0.00	ATOM 2630 C SER 318 27.505 11.405 73.339 1.00 15.03
ATOM 2559 CE1 HIS 310 25.616 18.113 85.362 1.00 15.93	ATOM 2631 O SER 318 27.091 10.509 72.606 1.00 17.55
ATOM 2560 NE2 HIS 310 26.914 17.885 85.558 1.00 16.87	ATOM 2632 N TYR 319 28.389 12.313 72.926 1.00 14.09
ATOM 2561 HE2 HIS 310 27.314 17.005 85.735 1.00 0.00	ATOM 2633 H TYR 319 28.766 12.947 73.568 1.00 0.00
ATOM 2562 C HIS 310 26.248 20.860 82.481 1.00 12.95	ATOM 2634 CA TYR 319 28.806 12.403 71.525 1.00 12.76
ATOM 2563 O HIS 310 26.558 19.734 82.077 1.00 12.90	ATOM 2635 CB TYR 319 28.375 13.755 70.930 1.00 10.14
ATOM 2564 N GLY 311 25.060 21.414 52.258 1.00 10.96	ATOM 2636 CG TYR 319 26.875 13.856 70.761 1.00 12.67
ATOM 2565 H GLY 311 24.844 22.285 82.645 1.00 0.00	ATOM 2637 CD1 TYR 319 26.060 14.251 71.824 1.00 6.01
ATOM 2566 CA GLY 311 24.073 20.734 81.438 1.00 11.14	ATOM 2638 CE1 TYR 319 24.677 14.283 71.697 1.00 7.18
ATOM 2569 CD2 TYR 319 26.261 13.497 69.551 1.00 10.75	ATOM 2711 H GLY 329 32.095 22.695 65.112 1.00 0.00
ATOM 2640 CE2 TYR 319 24.877 13.527 69.411 1.00 8.24	ATOM 2712 CA GLY 329 32.109 24.286 63.733 1.00 10.69
ATOM 2641 CZ TYR 319 24.090 13.918 70.489 1.00 10.13	ATOM 2713 C GLY 329 30.796 24.936 63.316 1.00 10.39
ATOM 2642 OH TYR 319 22.712 13.926 70.364 1.00 12.82	ATOM 2714 O GLY 329 30.808 26.032 62.776 1.00 12.00
ATOM 2643 HH TYR 319 22.469 13.627 69.495 1.00 0.00	ATOM 2715 N LEU 330 29.669 24.278 63.570 1.00 4.79
ATOM 2644 C TYR 319 30.303 12.183 71.337 1.00 16.52	ATOM 2716 H LEU 330 29.719 23.386 63.968 1.00 0.00
ATOM 2645 O TYR 319 31.097 12.447 72.244 1.00 16.79	ATOM 2717 CA LEU 330 28.367 24.841 63.253 1.00 8.84
ATOM 2646 N SER 320 30.687 11.661 70.172 1.00 13.62	ATOM 2718 CB LEU 330 27.246 23.969 63.812 1.00 6.31
ATOM 2647 H SER 320 30.000 11.455 69.505 1.00 0.00	ATOM 2719 CG LEU 330 26.997 22.592 63.224 1.00 10.14
ATOM 2648 CA SER 320 32.087 11.391 69.892 1.00 14.04	ATOM 2720 CD1 LEU 330 23.580 21.945 63.971 1.00 11.07
ATOM 2649 CB SER 320 32.220 10.526 68.638 1.00 18.38	ATOM 2721 CD2 LEU 330 26.662 22.706 61.744 1.00 14.61
ATOM 2650 OG SER 320 31.901 11.267 67.471 1.00 21.74	ATOM 2722 C LEU 330 28.257 26.208 63.905 1.00 8.14
ATOM 2651 HG SER 320 30.999 11.575 67.521 1.00 0.00	ATOM 2723 O LEU 330 27.894 27.190 63.266 1.00 14.59
ATOM 2652 C SER 320 32.838 12.680 69.670 1.00 13.69	ATOM 2724 N ILE 331 28.569 26.258 65.190 1.00 10.75
ATOM 2653 O SER 320 32.246 13.688 69.321 1.00 17.20	ATOM 2725 H ILE 331 28.831 25.426 65.637 1.00 0.00
ATOM 2654 N ALA 321 34.159 12.615 69.781 1.00 14.55	ATOM 2726 CA ILE 331 28.518 29.491 65.973 1.00 8.61
ATOM 2655 H ALA 321 34.567 11.579 70.020 1.00 0.00	ATOM 2727 CB ILE 331 28.724 27.154 67.486 1.00 14.63
ATOM 2656 CA ALA 321 35.029 13.771 69.580 1.00 14.54	ATOM 2728 CG2 ILE 331 28.877 28.412 68.303 1.00 15.69
ATOM 2657 CB ALA 321 36.489 13.352 69.735 1.00 17.29	ATOM 2729 CG1 ILE 331 27.514 26.371 68.020 1.00 11.64
ATOM 2658 C ALA 321 34.821 14.383 68.200 1.00 12.07	ATOM 2730 CD1 ILE 331 27.776 25.653 69.307 1.00 13.02
ATOM 2659 O ALA 321 35.033 15.582 67.998 1.00 13.71	ATOM 2731 C ILE 331 29.512 28.555 65.472 1.00 9.88
ATOM 2660 N GLY 322 34.454 13.538 67.248 1.00 13.47	ATOM 2732 O ILE 331 29.152 29.714 65.260 1.00 9.23
ATOM 2661 H GLY 322 34.317 12.593 67.463 1.00 0.00	ATOM 2733 N TYR 332 30.741 28.150 65.183 1.00 8.51
ATOM 2662 CA GLY 322 34.237 13.993 65.887 1.00 15.49	ATOM 2734 H TYR 332 30.985 27.208 65.317 1.00 0.00
ATOM 2663 C GLY 322 32.976 14.818 65.732 1.00 14.78	ATOM 2735 CA TYR 332 31.742 29.089 64.696 1.00 9.89
ATOM 2664 O GLY 322 32.968 15.810 64.991 1.00 16.40	ATOM 2736 CB TYR 332 33.102 28.404 64.633 1.00 7.30
ATOM 2665 N ALA 323 31.881 14.342 66.327 1.00 11.91	ATOM 2737 CG TYR 332 34.244 29.357 64.406 1.00 10.37
ATOM 2666 H ALA 323 31.946 13.536 66.881 1.00 0.00	ATOM 2738 CD1 TYR 332 34.724 30.164 65.439 1.00 9.94
ATOM 2667 CA ALA 323 30.608 15.041 66.250 1.00 11.53	ATOM 2739 CE1 TYR 332 35.792 30.038 65.229 1.00 7.63
ATOM 2668 CB ALA 323 29.495 14.171 66.754 1.00 5.28	ATOM 2740 CD2 TYR 332 34.858 29.447 63.155 1.00 11.58
ATOM 2669 C ALA 323 30.692 16.319 67.057 1.00 12.61	ATOM 2741 CE2 TYR 332 35.921 30.311 62.934 1.00 14.42
ATOM 2670 O ALA 323 30.058 17.326 66.720 1.00 13.81	ATOM 2742 CZ TYR 332 36.385 13.103 63.972 1.00 13.17
ATOM 2671 N LEU 324 31.515 16.279 68.100 1.00 9.94	ATOM 2743 OH TYR 332 37.445 31.938 63.710 1.00 13.95
ATOM 2672 H LEU 324 31.994 14.452 68.301 1.00 0.00	ATOM 2744 HH TYR 332 37.652 32.429 64.514 1.00 0.00
ATOM 2673 CA LEU 324 31.720 17.421 68.973 1.00 8.79	ATOM 2745 C TYR 332 31.383 29.638 63.318 1.00 11.07
ATOM 2674 CB LEU 324 32.497 16.994 70.218 1.00 13.93	ATOM 2746 O TYR 332 31.773 30.746 62.966 1.00 11.27
ATOM 2675 CG LEU 324 31.761 16.143 71.253 1.00 14.65	ATOM 2747 N ASN 333 30.643 28.849 62.538 1.00 12.83
ATOM 2676 CD1 LEU 324 32.776 15.501 72.188 1.00 21.09	ATOM 2748 H ASN 333 30.374 27.972 62.880 1.00 0.00
ATOM 2677 CD2 LEU 324 30.761 16.980 72.023 1.00 13.81	ATOM 2749 CA ASN 333 30.241 29.232 61.184 1.00 10.24
ATOM 2678 LEU 324 32.462 18.555 68.262 1.00 10.41	ATOM 2750 CB ASN 333 30.038 27.987 60.338 1.00 4.03
ATOM 2679 O LEU 324 32.078 19.723 68.371 1.00 11.89	ATOM 2751 CG ASN 333 31.323 27.336 59.965 1.00 9.06
ATOM 2680 N ALA 325 33.515 18.215 67.525 1.00 10.43	ATOM 2752 OD1 ASN 333 32.375 27.954 60.020 1.00 9.53
ATOM 2681 H ALA 325 33.783 17.276 67.480 1.00 0.00	ATOM 2753 ND2 ASN 333 31.262 26.074 59.605 1.00 9.96
ATOM 2682 CA ALA 325 34.296 19.221 66.802 1.00 8.57	ATOM 2754 HD21 ASN 333 30.405 25.605 59.610 1.00 0.00
ATOM 2683 CB ALA 325 35.519 18.587 66.160 1.00 10.40	ATOM 2755 HD22 ASN 333 32.111 25.625 59.373 1.00 0.00
ATOM 2684 C ALA 325 33.430 19.877 65.746 1.00 4.56	ATOM 2756 C ASN 333 28.960 30.041 61.163 1.00 14.77
ATOM 2685 O ALA 325 33.418 21.088 65.618 1.00 11.53	ATOM 2757 O ASN 333 28.474 30.406 60.088 1.00 14.34

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ATOM 2686 N SER 326 32.662 19.080 65.016 1.00 8.36	ATOM 2758 N ARG 334 28.379 30.251 62.347 1.00 15.99
ATOM 2687 H SER 326 32.685 18.114 65.163 1.00 0.00	ATOM 2759 H ARG 334 28.811 29.886 63.152 1.00 0.00
ATOM 2688 CA SER 326 31.800 19.638 63.987 1.00 10.75	ATOM 2760 CA ARG 334 27.132 31.006 62.527 1.00 14.30
ATOM 2689 CB SER 326 31.294 18.537 63.064 1.00 6.06	ATOM 2761 CB ARG 334 27.201 32.385 61.860 1.00 12.13
ATOM 2690 OG SER 326 32.399 17.399 62.357 1.00 13.88	ATOM 2762 CG ARG 334 28.467 33.159 62.160 1.00 12.54
ATOM 2691 HG SER 326 33.012 17.638 62.982 1.00 0.00	ATOM 2763 CD ARG 334 28.415 35.548 61.550 1.00 14.86
ATOM 2692 C SER 326 30.667 20.478 64.591 1.00 12.64	ATOM 2764 NE ARG 334 29.745 35.121 61.408 1.00 13.78
ATOM 2693 O SER 326 30.231 21.464 63.992 1.00 11.71	ATOM 2765 HE ARG 334 30.288 34.824 60.652 1.00 0.00
ATOM 2694 N CYS 327 30.205 20.118 65.788 1.00 12.50	ATOM 2766 CZ ARG 334 30.276 36.016 62.232 1.00 18.36
ATOM 2695 H CYS 327 30.543 19.307 66.224 1.00 0.00	ATOM 2767 NH1 ARG 334 29.596 36.451 63.275 1.00 22.12
ATOM 2696 CA CYS 327 29.173 20.922 66.443 1.00 9.23	ATOM 2768 HH1 ARG 334 28.674 36.108 63.453 1.00 0.00
ATOM 2697 CB CYS 327 28.634 20.233 67.695 1.00 4.17	ATOM 2769 HH1 ARG 334 30.001 37.126 63.894 1.00 0.00
ATOM 2698 SG CYS 327 27.219 21.118 68.396 1.00 11.27	ATOM 2770 NH2 ARG 334 31.478 36.511 61.983 1.00 17.96
ATOM 2699 C CYS 327 29.791 22.298 66.783 1.00 8.75	ATOM 2771 HH1 ARG 334 31.988 36.217 61.178 1.00 0.00
ATOM 2700 O CYS 327 29.138 23.326 66.688 1.00 9.40	ATOM 2772 HH2 ARG 334 31.876 37.188 62.607 1.00 0.00
ATOM 2701 N MET 328 31.066 22.316 67.153 1.00 6.97	ATOM 2773 C ARG 334 25.940 30.245 61.991 1.00 15.31
ATOM 2702 H MET 328 31.558 21.471 67.239 1.00 0.00	ATOM 2774 O ARG 334 24.923 30.840 61.653 1.00 18.76
ATOM 2703 CA MET 328 31.742 23.567 67.443 1.00 5.18	ATOM 2775 N MET 335 26.083 28.928 61.884 1.00 15.35
ATOM 2703 CB MET 328 33.145 23.305 67.996 1.00 4.83	ATOM 2776 H MET 335 26.933 28.524 62.148 1.00 0.00
ATOM 2705 CG MET 328 33.175 22.929 69.500 1.00 7.46	ATOM 2777 CA MET 335 25.020 28.066 61.382 1.00 15.46
ATOM 2706 SD MET 328 34.824 22.610 70.205 1.00 10.23	ATOM 2778 CB MET 335 25.613 26.792 60.817 1.00 13.01
ATOM 2707 CE MET 328 35.534 24.168 70.112 1.00 2.00	ATOM 2779 CG MET 335 26.576 27.059 59.698 1.00 17.95
ATOM 2708 C MET 328 31.838 24.373 66.159 1.00 7.71	ATOM 2780 SD MET 335 27.318 25.562 59.112 1.00 33.34
ATOM 2709 O MET 328 31.787 25.596 66.184 1.00 7.55	ATOM 2781 CE MET 335 25.814 24.584 58.716 1.00 30.01
ATOM 2710 N GLY 329 32.015 23.668 65.045 1.00 11.52	ATOM 2782 C MET 335 24.046 27.736 62.497 1.00 16.27
ATOM 2783 O MET 335 22.914 27.375 62.243 1.00 21.65	ATOM 2855 C PHE 344 31.895 25.092 77.548 1.00 10.59
ATOM 2784 N GLY 336 24.535 27.800 63.727 1.00 17.39	ATOM 2856 O PHE 344 32.887 24.363 77.560 1.00 14.02
ATOM 2785 H GLY 336 25.486 28.002 63.847 1.00 0.00	ATOM 2857 N GLY 345 30.676 24.663 77.880 1.00 9.18
ATOM 2786 CA GLY 336 23.728 27.561 64.906 1.00 16.17	ATOM 2858 H GLY 345 29.932 25.305 77.905 1.00 0.00
ATOM 2787 C GLY 336 24.244 28.549 65.937 1.00 17.50	ATOM 2859 CA GLY 345 30.431 23.265 78.193 1.00 7.24
ATOM 2788 O GLY 336 25.339 29.101 65.758 1.00 17.86	ATOM 2860 C GLY 345 30.816 22.355 77.028 1.00 10.74
ATOM 2789 N ALA 337 23.471 28.816 66.987 1.00 15.82	ATOM 2861 O GLY 345 31.500 21.346 77.232 1.00 8.67
ATOM 2790 H ALA 337 22.613 28.390 67.070 1.00 0.00	ATOM 2862 N LEU 346 30.369 22.693 75.813 1.00 11.73
ATOM 2791 CA ALA 337 23.896 29.751 68.025 1.00 13.47	ATOM 2863 H LEU 346 29.793 23.487 75.736 1.00 0.00
ATOM 2792 CB ALA 337 23.237 31.104 67.855 1.00 16.73	ATOM 2864 CA LEU 346 30.703 21.925 74.593 1.00 8.91
ATOM 2793 C ALA 337 23.577 29.195 69.389 1.00 14.36	ATOM 2865 CB LEU 346 30.090 22.594 73.341 1.00 7.42
ATOM 2794 O ALA 337 22.557 28.547 69.578 1.00 17.81	ATOM 2866 CG LEU 346 30.508 22.120 71.930 1.00 6.63
ATOM 2795 N VAL 338 24.410 29.539 70.361 1.00 14.94	ATOM 2867 CD1 LEU 346 30.113 20.665 71.722 1.00 2.85
ATOM 2796 H VAL 338 25.141 30.163 70.181 1.00 0.00	ATOM 2868 CD2 LEU 346 29.846 22.974 70.851 1.00 5.26
ATOM 2797 CA VAL 338 24.262 29.037 71.723 1.00 16.42	ATOM 2869 C LEU 346 32.223 21.831 74.402 1.00 6.21
ATOM 2798 CB VAL 338 25.041 27.691 71.770 1.00 16.57	ATOM 2870 O LEU 346 32.743 20.760 74.134 1.00 7.04
ATOM 2799 CG1 VAL 338 26.444 27.873 72.284 1.00 15.56	ATOM 2871 N VAL 347 32.908 22.967 74.518 1.00 6.57
ATOM 2800 CG2 VAL 338 24.273 26.643 72.459 1.00 1.00	ATOM 2872 H VAL 347 32.407 23.793 74.703 1.00 0.00
ATOM 2801 C VAL 338 24.845 30.105 72.962 1.00 17.49	ATOM 2873 CA VAL 347 34.363 23.056 74.368 1.00 7.97
ATOM 2802 O VAL 338 25.582 30.994 72.236 1.00 16.55	ATOM 2874 CB VAL 347 34.862 24.498 74.642 1.00 11.21
ATOM 2803 N THR 339 24.494 30.060 73.980 1.00 17.19	ATOM 2875 CG1 VAL 347 34.363 24.512 74.879 1.00 13.97
ATOM 2804 H THR 339 23.867 29.360 74.300 1.00 0.00	ATOM 2876 CG2 VAL 347 34.495 25.437 73.495 1.00 7.51
ATOM 2805 CA THR 339 25.030 31.037 74.962 1.00 16.56	ATOM 2877 C VAL 347 35.073 22.120 75.341 1.00 10.24
ATOM 2806 CB THR 339 24.249 31.079 76.321 1.00 14.23	ATOM 2878 O VAL 337 36.029 21.433 74.973 1.00 9.62
ATOM 2807 OG1 THR 339 24.423 29.853 77.040 1.00 17.38	ATOM 2879 N CYS 348 34.586 22.079 76.582 1.00 11.21
ATOM 2808 HG1 THR 339 25.328 29.719 77.234 1.00 0.00	ATOM 2880 H CYS 348 33.810 22.636 76.811 1.00 0.00
ATOM 2809 CG2 THR 339 22.763 31.303 76.083 1.00 19.66	ATOM 2881 CA CYS 348 35.187 21.241 77.620 1.00 8.37
ATOM 2810 C THR 339 26.480 30.704 75.255 1.00 12.10	ATOM 2882 CB CYS 348 34.715 21.692 78.994 1.00 8.63
ATOM 2811 O THR 339 26.881 29.559 75.149 1.00 13.55	ATOM 2883 SG CYS 348 35.450 23.266 79.481 1.00 16.28
ATOM 2812 N THR 340 27.251 31.695 75.658 1.00 11.94	ATOM 2884 C CYS 348 34.957 19.759 77.427 1.00 7.38
ATOM 2813 H THR 340 26.864 32.596 75.770 1.00 0.00	ATOM 2885 O CYS 348 35.823 18.936 77.746 1.00 9.09
ATOM 2814 CA THR 340 28.665 31.495 75.946 1.00 15.32	ATOM 2886 N ALA 349 33.791 19.399 76.908 1.00 8.67
ATOM 2815 CB THR 340 29.319 32.822 76.381 1.00 19.16	ATOM 2887 H ALA 349 33.109 20.076 76.695 1.00 0.00
ATOM 2816 OG1 THR 340 29.006 33.827 75.415 1.00 20.58	ATOM 2888 CA ALA 349 33.535 17.994 76.652 1.00 7.20
ATOM 2817 HG1 THR 340 29.371 33.550 75.478 1.00 0.00	ATOM 2889 CB ALA 349 32.081 17.777 76.294 1.00 6.86
ATOM 2818 CG2 THR 340 30.827 32.684 76.466 1.00 19.52	ATOM 2890 C ALA 349 34.448 17.557 75.508 1.00 8.04
ATOM 2819 C THR 340 28.948 30.399 76.972 1.00 12.71	ATOM 2891 O ALA 349 35.072 16.504 75.594 1.00 12.59
ATOM 2820 O THR 340 29.887 29.632 76.807 1.00 12.19	ATOM 2892 N THR 350 34.572 18.387 74.463 1.00 13.57
ATOM 2821 N GLU 341 28.100 30.295 77.990 1.00 10.08	ATOM 2893 H THR 350 34.084 19.240 74.461 1.00 0.00
ATOM 2822 H GLU 341 27.344 30.917 78.031 1.00 0.00	ATOM 2894 CA THR 350 35.423 18.056 73.309 1.00 12.48
ATOM 2823 CA GLU 341 28.243 29.283 79.043 1.00 13.73	ATOM 2895 CB THR 350 35.302 19.079 72.119 1.00 11.62
ATOM 2824 CB GLU 341 27.184 29.525 80.149 1.00 18.89	ATOM 2896 OG1 THR 350 36.073 20.238 72.399 1.00 25.07
ATOM 2825 CG GLU 341 27.208 30.952 80.818 1.00 35.09	ATOM 2897 HG1 THR 350 36.995 20.003 72.503 1.00 0.00
ATOM 2826 CD GLU 341 26.251 32.032 80.178 1.00 38.66	ATOM 2898 CG2 THR 350 33.888 19.526 71.940 1.00 3.73
ATOM 2827 OE1 GLU 341 25.190 32.386 80.797 1.00 31.21	ATOM 2899 C THR 350 36.879 17.956 73.755 1.00 10.28
ATOM 2828 OE2 GLU 341 36.596 32.565 79.087 1.00 31.75	ATOM 2900 O THR 350 37.589 17.027 73.382 1.00 14.11
ATOM 2829 C GLU 341 28.085 27.856 78.463 1.00 13.64	ATOM 2901 N CYS 351 37.342 18.917 74.540 1.00 11.19
ATOM 2830 O GLU 341 28.824 26.921 78.807 1.00 11.29	ATOM 2902 H CYS 351 36.766 19.665 74.800 1.00 0.00
ATOM 2831 N VAL 342 27.068 27.694 77.625 1.00 12.75	ATOM 2903 CA CYS 351 38.717 18.850 75.025 1.00 13.10
ATOM 2832 H VAL 342 26.480 28.445 77.448 1.00 0.00	ATOM 2904 CB CYS 351 29.052 20.064 75.878 1.00 7.05
ATOM 2833 CA VAL 342 26.784 26.431 76.959 1.00 9.60	ATOM 2905 SG CYS 351 39.198 21.617 74.987 1.00 12.54
ATOM 2834 CB VAL 342 25.456 26.534 76.154 1.00 9.98	ATOM 2906 C CYS 351 38.927 17.571 75.852 1.00 16.59
ATOM 2835 CG1 VAL 342 25.147 25.230 75.462 1.00 9.26	ATOM 2907 O CYS 351 39.894 16.8839 75.635 1.00 15.17
ATOM 2836 CG2 VAL 342 24.316 26.930 77.061 1.00 9.74	ATOM 2908 N GLU 352 37.994 17.275 76.760 1.00 16.15

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ATOM 2837 C VAL 342 27.947 26.138 75.993 1.00 11.29	ATOM 2909 H GLU 352 37.217 17.857 76.863 1.00 0.00
ATOM 2838 O VAL 342 28.403 24.999 75.883 1.00 12.19	ATOM 2910 CA GLU 352 38.123 16.084 77.600 1.00 14.25
ATOM 2839 N ALA 343 28.404 27.167 75.274 1.00 10.18	ATOM 2911 CB GLU 352 36.929 15.969 78.578 1.00 14.59
ATOM 2840 H ALA 343 27.980 28.036 75.376 1.00 0.00	ATOM 2912 CG GLU 352 37.173 14.954 79.709 1.00 13.70
ATOM 2841 CA ALA 343 29.524 27.028 74.337 1.00 10.07	ATOM 2913 CD GLU 352 37.031 13.498 79.276 1.00 13.27
ATOM 2842 CB ALA 343 29.837 28.384 73.706 1.00 9.90	ATOM 2914 OE1 GLU 352 36.108 13.206 78.486 1.00 12.42
ATOM 2843 C ALA 343 30.736 26.490 75.120 1.00 12.16	ATOM 2915 OE2 GLU 352 37.807 12.638 79.755 1.00 16.07
ATOM 2844 O ALA 343 31.438 25.589 74.650 1.00 10.31	ATOM 2916 C GLU 352 38.188 14.844 76.731 1.00 13.50
ATOM 2845 N PHE 344 30.943 27.017 76.331 1.00 12.47	ATOM 2917 O GLU 352 39.051 13.992 76.937 1.00 12.79
ATOM 2846 H PHE 344 30.340 27.719 76.645 1.00 0.00	ATOM 2918 N GLN 353 37.291 14.747 75.753 1.00 12.33
ATOM 2847 CA PHE 344 32.033 26.582 77.214 1.00 13.30	ATOM 2919 H GLN 353 36.644 15.467 75.626 1.00 0.00
ATOM 2848 CB PHE 344 32.016 27.372 78.533 1.00 18.23	ATOM 2920 CA GLN 353 37.270 13.599 74.857 1.00 15.93
ATOM 2849 CG PHE 344 32.678 28.724 78.460 1.00 21.49	ATOM 2921 CB GLN 353 36.091 13.712 73.880 1.00 20.18
ATOM 2850 CD1 PHE 344 32.308 29.730 79.349 1.00 25.39	ATOM 2922 CG GLN 353 34.706 13.664 74.552 1.00 23.36
ATOM 2851 CD2 PHE 344 33.675 28.989 77.523 1.00 23.26	ATOM 2923 CD GLN 353 34.161 12.251 74.710 1.00 29.07
ATOM 2852 CE1 PHE 344 32.927 30.991 79.310 1.00 28.66	ATOM 2924 OE1 GLN 353 34.862 11.343 75.164 1.00 32.63
ATOM 2853 CE2 PHE 344 34.301 30.241 77.474 1.00 26.03	ATOM 2925 NE2 GLN 353 32.909 12.059 74.337 1.00 27.25
ATOM 2854 CZ PHE 344 33.927 31.242 78.363 1.00 27.84	ATOM 2926 HE21 GLN 353 32.399 12.824 73.976 1.00 0.00
ATOM 2927 HE22 GLN 353 32.549 11.182 74.446 1.00 0.00	ATOM 2999 O1 HOH 509 35.509 34.054 50.366 1.00 28.21
ATOM 2928 C GLN 353 38.600 13.409 74.101 1.00 15.86	ATOM 3000 H1 HOH 509 36.107 34.284 51.088 1.00 0.00
ATOM 2929 O GLN 353 39.115 12.303 74.004 1.00 17.10	ATOM 3001 H2 HOH 509 36.024 33.534 49.772 1.00 0.00
ATOM 2930 N ILE 354 39.165 14.495 73.600 1.00 16.42	ATOM 3002 O1 HOH 510 34.933 29.155 39.816 1.00 17.84
ATOM 2931 H ILE 354 38.178 15.358 73.723 1.00 0.00	ATOM 3003 H1 HOH 510 34.218 29.305 40.439 1.00 0.00
ATOM 2932 CA ILE 354 40.419 14.448 72.865 1.00 15.89	ATOM 3004 H2 HOH 510 34.758 28.333 39.412 1.00 0.00
ATOM 2933 CB ILE 354 40.734 15.828 72.264 1.00 15.56	ATOM 3005 O1 HOH 511 32.156 31.380 36.574 1.00 7.04
ATOM 2934 CG2 ILE 354 42.126 15.823 71.624 1.00 13.85	ATOM 3006 H1 HOH 511 31.929 30.636 37.023 1.00 0.00
ATOM 2935 CG1 ILE 354 39.629 16.204 71.258 1.00 16.39	ATOM 3007 H2 HOH 511 31.780 31.315 35.697 1.00 0.00
ATOM 2936 CD1 ILE 354 39.605 17.672 70.824 1.00 15.26	ATOM 3008 O1 HOH 512 36.121 30.620 43.066 1.00 21.42
ATOM 2937 C ILE 354 41.547 14.032 73.795 1.00 18.65	ATOM 3009 H1 HOH 512 35.422 30.730 43.712 1.00 0.00
ATOM 2938 O ILE 354 42.322 13.123 73.490 1.00 17.76	ATOM 3010 H2 HOH 512 35.887 31.294 42.397 1.00 0.00
ATOM 2939 N ALA 355 41.628 14.714 74.931 1.00 18.52	ATOM 3011 O1 HOH 513 32.964 30.772 33.972 1.00 14.70
ATOM 2940 H ALA 355 40.978 15.420 75.103 1.00 0.00	ATOM 3012 H1 HOH 513 32.633 31.248 33.208 1.00 0.00
ATOM 2941 CA ALA 355 42.644 14.446 75.923 1.00 16.17	ATOM 3013 H2 HOH 513 32.875 29.849 33.758 1.00 0.00
ATOM 2942 CB ALA 355 42.456 15.374 77.101 1.00 18.27	ATOM 3014 O1 HOH 514 40.740 31.037 44.455 1.00 23.55
ATOM 2943 C ALA 355 42.540 12.996 76.376 1.00 16.93	ATOM 3015 H1 HOH 514 40.322 31.620 43.854 1.00 0.00
ATOM 2944 O ALA 355 43.540 12.298 76.507 1.00 16.12	ATOM 3016 H2 HOH 514 40.840 30.227 43.965 1.00 0.00
ATOM 2945 N ASP 356 41.315 12.532 76.566 1.00 14.46	ATOM 3017 O1 HOH 515 37.112 31.979 55.782 1.00 13.43
ATOM 2946 H ASP 356 40.554 13.108 76.386 1.00 0.00	ATOM 3018 H1 HOH 515 36.492 31.236 55.780 1.00 0.00
ATOM 2947 CA ASP 356 41.089 11.168 77.012 1.00 16.37	ATOM 3019 H2 HOH 515 37.691 31.766 56.528 1.00 0.00
ATOM 2948 CB ASP 356 39.607 10.963 77.351 1.00 12.46	ATOM 3020 O1 HOH 516 34.932 33.743 57.726 1.00 16.34
ATOM 2949 CG ASP 356 39.386 9.811 78.302 1.00 9.76	ATOM 3021 H1 HOH 516 35.651 34.371 57.865 1.00 0.00
ATOM 2950 OD1 ASP 356 40.259 9.602 79.156 1.00 12.73	ATOM 3022 H2 HOH 516 35.135 33.039 58.319 1.00 0.00
ATOM 2951 OD2 ASP 356 38.367 9.098 78.200 1.00 13.11	ATOM 3023 O1 HOH 517 32.992 35.898 59.122 1.00 13.65
ATOM 2952 C ASP 356 41.559 10.109 76.004 1.00 18.28	ATOM 3024 H1 HOH 517 32.337 36.031 58.412 1.00 0.00
ATOM 2953 O ASP 356 41.825 8.969 76.375 1.00 16.16	ATOM 3025 H2 HOH 517 33.543 36.652 59.040 1.00 0.00
ATOM 2954 N SER 357 41.629 10.478 74.731 1.00 25.77	ATOM 3026 O1 HOH 518 14.064 17.135 60.635 1.00 55.52
ATOM 2955 H SER 357 41.388 11.394 74.485 1.00 0.00	ATOM 3027 H1 HOH 518 14.963 16.813 60.568 1.00 0.00
ATOM 2956 CA SER 357 42.053 9.553 73.678 1.00 30.13	ATOM 3028 H2 HOH 518 13.906 16.402 59.956 1.00 0.00
ATOM 2957 CB SER 357 41.483 9.982 72.321 1.00 33.88	ATOM 3029 O1 HOH 519 12.446 20.018 54.033 1.00 15.26
ATOM 2958 OG SER 357 40.076 9.818 72.244 1.00 43.35	ATOM 3030 H1 HOH 519 12.575 20.616 54.773 1.00 0.00
ATOM 2959 HG SER 357 39.849 8.907 72.419 1.00 0.00	ATOM 3031 H2 HOH 519 12.614 19.150 54.431 1.00 0.00
ATOM 2960 C SER 357 43.567 9.452 73.549 1.00 30.70	ATOM 3032 O1 HOH 520 20.474 15.871 62.473 1.00 11.21
ATOM 2961 O SER 357 44.079 8.479 73.009 1.00 32.33	ATOM 3033 H1 HOH 520 21.285 15.847 62.978 1.00 0.00
ATOM 2962 N GLN 358 44.260 10.504 73.966 1.00 35.85	ATOM 3034 H2 HOH 520 20.056 16.690 62.676 1.00 0.00
ATOM 2963 H GLN 358 43.785 11.252 74.373 1.00 0.00	ATOM 3035 O1 HOH 521 20.705 14.732 59.125 1.00 12.83
ATOM 2964 CA GLN 358 45.712 10.572 73.895 1.00 39.48	ATOM 3036 H1 HOH 521 21.403 14.640 58.502 1.00 0.00
ATOM 2965 CB GLN 358 46.154 12.034 73.938 1.00 40.72	ATOM 3037 H2 HOH 521 20.067 15.324 58.723 1.00 0.00
ATOM 2966 CG GLN 358 45.553 12.900 72.842 1.00 42.43	ATOM 3038 O1 HOH 522 21.233 12.291 57.983 1.00 12.36
ATOM 2967 CD GLN 358 45.689 14.388 73.136 1.00 48.68	ATOM 3039 H1 HOH 522 20.778 12.810 57.348 1.00 0.00
ATOM 2968 OE1 GLN 358 45.967 14.793 74.269 1.00 51.49	ATOM 3040 H2 HOH 522 21.565 11.520 57.533 1.00 0.00
ATOM 2969 NE2 GLN 358 45.481 15.213 72.115 1.00 51.68	ATOM 3041 O1 HOH 523 15.613 13.306 53.673 1.00 20.29
ATOM 2970 HE21 GLN 358 45.256 18.841 71.243 1.00 0.00	ATOM 3042 H1 HOH 523 14.912 13.680 53.140 1.00 0.00
ATOM 2971 HE22 GLN 358 45.575 16.170 72.298 1.00 0.00	ATOM 3043 H2 HOH 523 15.145 12.776 54.328 1.00 0.00
ATOM 2972 C GLN 358 46.398 9.792 75.017 1.00 41.97	ATOM 3044 O1 HOH 524 14.552 10.615 51.652 1.00 29.13
ATOM 2973 O GLN 358 47.610 9.493 74.853 1.00 44.23	ATOM 3045 H1 HOH 524 13.775 10.065 51.586 1.00 0.00
ATOM 2974 OT GLN 358 45.729 9.503 76.042 1.00 39.09	ATOM 3046 H2 HOH 524 15.267 10.000 51.866 1.00 0.00
ATOM 2975 O1 HOH 501 21.113 21.834 31.125 1.00 34.11	ATOM 3047 O1 HOH 525 26.412 10.425 50.161 1.00 21.16
ATOM 2976 H1 HOH 501 20.569 22.495 31.526 1.00 0.00	ATOM 3048 H1 HOH 525 27.168 10.793 50.610 1.00 0.00
ATOM 2977 H2 HOH 501 21.864 22.333 30.772 1.00 0.00	ATOM 3049 H2 HOH 525 25.871 11.187 49.943 1.00 0.00
ATOM 2978 O1 HOH 502 16.027 23.882 32.958 1.00 19.80	ATOM 3050 O1 HOH 526 28.657 16.318 44.297 1.00 10.28
ATOM 2979 H1 HOH 502 16.158 23.419 32.150 1.00 0.00	ATOM 3051 H1 HOH 526 28.391 16.679 43.468 1.00 0.00
ATOM 2980 H2 HOH 502 15.086 23.733 33.200 1.00 0.00	ATOM 3052 H2 HOH 526 27.806 16.001 44.665 1.00 0.00
ATOM 2981 O1 HOH 503 14.494 37.841 36.012 1.00 26.64	ATOM 3053 O1 HOH 527 28.310 18.186 38.834 1.00 11.71
ATOM 2982 H1 HOH 503 14.011 37.975 35.200 1.00 0.00	ATOM 3054 H1 HOH 527 28.155 17.321 39.222 1.00 0.00
ATOM 2983 H2 HOH 503 14.861 36.932 35.880 1.00 0.00	ATOM 3055 H2 HOH 527 27.936 18.078 37.943 1.00 0.00
ATOM 2984 O1 HOH 504 24.785 43.283 29.843 1.00 41.72	ATOM 3056 O1 HOH 528 23.160 13.587 38.766 1.00 11.23
ATOM 2985 H1 HOH 504 24.046 42.664 29.813 1.00 0.00	ATOM 3057 H1 HOH 528 23.349 13.948 37.885 1.00 0.00
ATOM 2986 H2 HOH 504 24.485 44.028 29.328 1.00 0.00	ATOM 3058 H2 HOH 528 22.372 14.053 39.041 1.00 0.00
ATOM 2987 O1 HOH 505 24.609 34.687 30.302 1.00 29.71	ATOM 3059 O1 HOH 529 9.507 21.350 48.406 1.00 23.08

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ATOM 2988 H1 HOH 505 24.843 35.356 29.653 1.00 0.00	ATOM 3060 H1 HOH 529 10.286 21.320 47.818 1.00 0.00
ATOM 2989 H2 HOH 505 24.190 35.172 30.968 1.00 0.00	ATOM 3061 H2 HOH 529 8.828 20.950 47.880 1.00 0.00
ATOM 2990 O1 HOH 506 35.336 38.962 49.998 1.00 23.91	ATOM 3062 O1 HOH 530 35.924 27.794 54.972 1.00 14.10
ATOM 2991 H1 HOH 506 35.753 39.055 50.828 1.00 0.00	ATOM 3063 H1 HOH 530 36.607 28.458 55.108 1.00 0.00
ATOM 2992 H2 HOH 506 35.012 38.056 49.955 1.00 0.00	ATOM 3064 H2 HOH 530 36.124 27.392 54.150 1.00 0.00
ATOM 2993 O1 HOH 507 30.302 40.821 56.153 1.00 2.00	ATOM 3065 O1 HOH 531 31.190 23.605 44.871 1.00 22.64
ATOM 2994 H1 HOH 507 29.583 40.377 55.722 1.00 0.00	ATOM 2066 H1 HOH 531 30.810 24.408 44.486 1.00 0.00
ATOM 2995 H2 HOH 507 30.902 40.142 56.438 1.00 0.00	ATOM 2067 H2 HOH 531 30.729 22.895 44.415 1.00 0.00
ATOM 2996 O1 HOH 508 32.683 35.011 50.212 1.00 9.76	ATOM 2068 O1 HOH 532 8.072 35.577 49.772 1.00 9.91
ATOM 2997 H1 HOH 508 31.900 34.649 50.413 1.00 0.00	ATOM 2069 H1 HOH 532 8.548 36.077 50.422 1.00 0.00
ATOM 2998 H2 HOH 508 32.600 35.145 49.303 1.00 0.00	ATOM 2070 H2 HOH 532 7.247 35.987 49.656 1.00 0.00
ATOM 3071 O1 HOH 533 45.213 20.999 82.495 1.00 23.69	ATOM 3143 O1 HOH 557 24.340 26.762 57.198 1.00 29.86
ATOM 3072 H1 HOH 533 45.907 20.881 81.842 1.00 0.00	ATOM 3144 H1 HOH 557 23.871 27.500 56.759 1.00 0.00
ATOM 3073 H2 HOH 533 44.415 21.134 81.969 1.00 0.00	ATOM 3145 H2 HOH 557 24.760 27.183 57.934 1.00 0.00
ATOM 3074 O1 HOH 534 47.201 19.833 81.157 1.00 17.76	ATOM 3146 O1 HOH 558 26.379 30.155 58.148 1.00 10.16
ATOM 3075 H1 HOH 534 46.964 19.911 80.228 1.00 0.00	ATOM 3147 H1 HOH 558 26.928 29.399 58.399 1.00 0.00
ATOM 3076 H2 HOH 534 47.549 20.689 81.401 1.00 0.00	ATOM 3148 H2 HOH 558 26.723 30.844 58.725 1.00 0.00
ATOM 3077 O1 HOH 535 48.572 15.906 76.182 1.00 29.31	ATOM 3149 O1 HOH 559 13.369 12.800 56.988 1.00 40.74
ATOM 3078 H1 HOH 535 48.443 16.537 76.895 1.00 0.00	ATOM 3150 H1 HOH 559 12.635 12.453 56.463 1.00 0.00
ATOM 3079 H2 HOH 535 47.657 15.791 75.836 1.00 0.00	ATOM 3151 H2 HOH 559 14.077 12.176 56.830 1.00 0.00
ATOM 3080 O1 HOH 536 55.029 34.083 73.481 1.00 40.49	ATOM 3152 O1 HOH 560 53.861 23.078 74.598 1.00 47.23
ATOM 3081 H1 HOH 536 55.819 33.750 73.902 1.00 0.00	ATOM 3153 H1 HOH 560 53.956 23.050 75.549 1.00 0.00
ATOM 3082 H2 HOH 536 54.617 33.307 73.094 1.00 0.00	ATOM 3154 H2 HOH 560 53.274 22.301 74.446 1.00 0.00
ATOM 3083 O1 HOH 537 50.980 36.933 65.633 1.00 44.62	ATOM 3155 O1 HOH 561 48.624 20.162 69.741 1.00 19.26
ATOM 3084 H1 HOH 537 51.900 37.081 65.437 1.00 0.00	ATOM 3156 H1 HOH 561 49.369 19.604 69.997 1.00 0.00
ATOM 3085 H2 HOH 537 50.746 36.133 65.175 1.00 0.00	ATOM 3157 H2 HOH 561 48.182 19.644 69.059 1.00 0.00
ATOM 3086 O1 HOH 538 43.014 31.670 58.158 1.00 3.46	ATOM 3158 O1 HOH 562 37.820 34.373 64.745 1.00 15.33
ATOM 3087 H1 HOH 538 42.583 32.266 57.558 1.00 0.00	ATOM 3159 H1 HOH 562 37.850 33.656 65.323 1.00 0.00
ATOM 3088 H2 HOH 538 43.956 31.791 57.967 1.00 0.00	ATOM 3160 H2 HOH 562 37.975 35.155 65.301 1.00 0.00
ATOM 3089 O1 HOH 539 28.529 10.869 68.204 1.00 10.19	ATOM 3161 O1 HOH 563 26.510 28.479 82.830 1.00 20.91
ATOM 3090 H1 HOH 539 29.270 10.962 67.620 1.00 0.00	ATOM 3162 H1 HOH 563 26.501 29.397 82.536 1.00 0.00
ATOM 3091 H2 HOH 539 27.777 10.817 67.594 1.00 0.00	ATOM 3163 H2 HOH 563 25.698 28.133 82.465 1.00 0.00
ATOM 3092 O1 HOH 540 18.863 15.829 69.006 1.00 11.06	ATOM 3164 O1 HOH 564 35.083 17.450 63.254 1.00 28.49
ATOM 3093 H1 HOH 540 18.641 14.930 69.228 1.00 0.00	ATOM 3165 H1 HOH 564 34.249 17.114 63.557 1.00 0.00
ATOM 3094 H2 HOH 540 19.791 15.910 69.192 1.00 0.00	ATOM 3166 H2 HOH 564 34.874 18.055 62.539 1.00 0.00
ATOM 3095 O1 HOH 541 16.474 15.926 70.889 1.00 13.53	ATOM 3167 O1 HOH 565 34.570 32.464 85.654 1.00 38.87
ATOM 3096 H1 HOH 541 15.831 15.250 71.030 1.00 0.00	ATOM 3168 H1 HOH 565 34.239 31.595 85.561 1.00 0.00
ATOM 3097 H2 HOH 541 16.083 16.738 71.204 1.00 0.00	ATOM 3169 H2 HOH 565 35.383 32.452 86.127 1.00 0.00
ATOM 3098 O1 HOH 542 24.752 9.611 61.454 1.00 34.29	ATOM 3170 O1 HOH 566 27.590 32.106 29.612 1.00 29.25
ATOM 3099 H1 HOH 542 24.372 10.478 61.588 1.00 0.00	ATOM 3171 H1 HOH 566 26.708 32.450 29.591 1.00 0.00
ATOM 3100 H2 HOH 542 25.681 9.801 61.309 1.00 0.00	ATOM 3172 H2 HOH 566 27.517 31.161 29.565 1.00 0.00
ATOM 3101 O1 HOH 543 19.120 19.082 75.742 1.00 31.85	ATOM 3173 O1 HOH 567 35.194 34.042 36.435 1.00 26.99
ATOM 3102 H1 HOH 543 18.979 18.494 76.468 1.00 0.00	ATOM 3174 H1 HOH 567 35.566 34.492 35.707 1.00 0.00
ATOM 3103 H2 HOH 543 19.758 19.728 76.057 1.00 0.00	ATOM 3175 H2 HOH 567 35.900 33.706 36.949 1.00 0.00
ATOM 3104 O1 HOH 544 20.890 23.564 81.292 1.00 7.35	ATOM 3176 O1 HOH 568 16.603 20.218 77.754 1.00 33.83
ATOM 3105 H1 HOH 544 21.473 22.863 80.979 1.00 0.00	ATOM 3177 H1 HOH 568 16.886 19.313 77.800 1.00 0.00
ATOM 3106 H2 HOH 544 20.108 23.467 80.725 1.00 0.00	ATOM 3178 H2 HOH 568 15.639 20.159 77.731 1.00 0.00
ATOM 3107 O1 HOH 545 23.258 30.530 79.524 1.00 24.15	ATOM 3179 O1 HOH 569 44.260 42.711 49.744 1.00 49.42
ATOM 3108 H1 HOH 545 23.170 29.756 80.060 1.00 0.00	ATOM 3180 H1 HOH 569 43.569 42.272 50.249 1.00 0.00
ATOM 3109 H2 HOH 545 22.877 31.208 80.059 1.00 0.00	ATOM 3181 H2 HOH 569 45.049 42.209 49.943 1.00 0.00
ATOM 3110 O1 HOH 546 28.803 17.795 82.962 1.00 11.68	ATOM 3182 O1 HOH 570 21.872 48.032 53.264 1.00 41.45
ATOM 3111 H1 HOH 546 29.360 17.056 83.227 1.00 0.00	ATOM 3183 H1 HOH 570 22.620 48.612 53.236 1.00 0.00
ATOM 3112 H2 HOH 546 27.954 17.405 82.768 1.00 0.00	ATOM 3184 H2 HOH 570 21.783 47.696 52.361 1.00 0.00
ATOM 3113 O1 HOH 547 30.182 20.906 85.733 1.00 23.69	ATOM 3185 O1 HOH 571 12.792 32.834 61.142 1.00 21.34
ATOM 3114 H1 HOH 547 29.256 20.762 85.836 1.00 0.00	ATOM 3186 H1 HOH 571 11.962 32.850 61.572 1.00 0.00
ATOM 3115 H2 HOH 547 30.305 21.821 86.021 1.00 0.00	ATOM 3187 H2 HOH 571 13.363 32.323 61.709 1.00 0.00
ATOM 3116 O1 HOH 548 22.573 11.792 73.330 1.00 29.86	ATOM 3188 O1 HOH 572 17.695 12.090 61.460 1.00 25.70
ATOM 3117 H1 HOH 548 22.027 11.157 73.769 1.00 0.00	ATOM 3189 H1 HOH 572 17.582 13.022 61.236 1.00 0.00
ATOM 3118 H2 HOH 548 22.105 12.046 72.546 1.00 0.00	ATOM 3190 H2 HOH 572 16.812 11.737 61.464 1.00 0.00
ATOM 3119 O1 HOH 549 26.762 31.362 66.476 1.00 19.77	ATOM 3191 O1 HOH 573 19.834 11.716 53.122 1.00 21.51
ATOM 3120 H1 HOH 549 27.481 30.835 66.104 1.00 0.00	ATOM 3192 H1 HOH 573 19.651 12.580 52.717 1.00 0.00
ATOM 3121 H2 HOH 549 25.999 30.809 66.387 1.00 0.00	ATOM 3193 H2 HOH 573 20.774 11.693 53.217 1.00 0.00
ATOM 3122 O1 HOH 550 36.271 10.655 77.620 1.00 12.01	ATOM 3194 O1 HOH 574 21.268 11.375 45.183 1.00 26.95
ATOM 3123 H1 HOH 550 36.338 11.487 77.960 1.00 0.00	ATOM 3195 H1 HOH 574 21.824 11.796 45.845 1.00 0.00
ATOM 3124 H2 HOH 550 35.441 10.668 77.127 1.00 0.00	ATOM 3196 H2 HOH 574 21.467 11.858 44.429 1.00 0.00
ATOM 3125 O1 HOH 551 15.409 35.471 35.400 1.00 21.53	ATOM 3197 O1 HOH 575 31.324 22.466 47.474 1.00 15.68
ATOM 3126 H1 HOH 551 15.910 35.092 36.113 1.00 0.00	ATOM 3198 H1 HOH 575 31.326 22.189 46.553 1.00 0.00
ATOM 3127 H2 HOH 551 15.393 34.800 34.719 1.00 0.00	ATOM 3199 H2 HOH 575 31.377 23.423 47.421 1.00 0.00
ATOM 3128 O1 HOH 552 11.203 40.791 44.564 1.00 45.20	ATOM 3200 O1 HOH 576 33.771 20.240 41.075 1.00 19.98
ATOM 3129 H1 HOH 552 12.144 40.650 44.489 1.00 0.00	ATOM 3201 H1 HOH 576 34.128 20.649 40.260 1.00 0.00
ATOM 3130 H2 HOH 552 10.822 39.934 44.337 1.00 0.00	ATOM 3202 H2 HOH 576 34.195 19.384 41.088 1.00 0.00
ATOM 3131 O1 HOH 553 15.641 41.263 47.151 1.00 18.63	ATOM 3203 O1 HOH 577 6.251 37.204 48.560 1.00 24.53
ATOM 3132 H1 HOH 553 15.949 40.445 47.518 1.00 0.00	ATOM 3204 H1 HOH 577 5.978 36.403 48.041 1.00 0.00
ATOM 3133 H2 HOH 553 15.775 41.187 46.203 1.00 0.00	ATOM 3205 H2 HOH 577 6.452 36.906 49.406 1.00 0.00
ATOM 3134 O1 HOH 554 18.730 37.027 57.126 1.00 27.98	ATOM 3206 O1 HOH 578 3.214 32.888 43.239 1.00 32.15
ATOM 3135 H1 HOH 554 18.564 36.463 56.358 1.00 0.00	ATOM 3207 H1 HOH 578 4.089 32.749 43.668 1.00 0.00
ATOM 3136 H2 HOH 554 19.443 36.558 57.577 1.00 0.00	ATOM 3208 H2 HOH 578 3.258 33.840 43.082 1.00 0.00
ATOM 3137 O1 HOH 555 16.938 39.005 58.568 1.00 38.75	ATOM 3209 O1 HOH 579 56.568 34.393 67.441 1.00 49.59
ATOM 3138 H1 HOH 555 17.197 39.899 58.352 1.00 0.00	ATOM 3210 H1 HOH 579 56.311 34.641 66.555 1.00 0.00

-continued

ATOM 3139 H2 HOH 555 17.772 38.497 58.439 1.00 0.00	ATOM 3211 H2 HOH 579 57.351 34.920 67.636 1.00 0.00
ATOM 3140 O1 HOH 556 18.892 30.925 56.057 1.00 23.90	ATOM 3212 O1 HOH 580 58.741 36.148 68.590 1.00 32.81
ATOM 3141 H1 HOH 556 18.795 30.584 56.919 1.00 0.00	ATOM 3213 H1 HOH 580 58.738 37.120 68.606 1.00 0.00
ATOM 3142 H2 HOH 556 19.544 31.632 56.110 1.00 0.00	ATOM 3214 H2 HOH 580 58.745 35.930 67.671 1.00 0.00
ATOM 3215 O1 HOH 581 39.287 14.270 67.499 1.00 27.97	ATOM 3287 O1 HOH 605 36.759 26.472 88.853 1.00 37.02
ATOM 3216 H1 HOH 581 39.735 13.617 68.033 1.00 0.00	ATOM 3288 H1 HOH 605 37.215 27.264 89.016 1.00 0.00
ATOM 3217 H2 HOH 581 38.408 14.341 67.837 1.00 0.00	ATOM 3289 H2 HOH 605 37.052 25.865 89.547 1.00 0.00
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ATOM 3219 H1 HOH 582 29.020 30.472 72.403 1.00 0.00	ATOM 3291 H1 HOH 606 46.668 13.027 78.263 1.00 0.00
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ATOM 3223 H2 HOH 583 26.463 31.287 70.130 1.00 0.00	ATOM 3295 H2 HOH 607 32.538 23.517 49.481 1.00 0.00
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ATOM 3225 H1 HOH 584 28.746 33.818 73.377 1.00 0.00	ATOM 3297 H1 HOH 608 34.171 26.367 47.165 1.00 0.00
ATOM 3226 H2 HOH 584 29.077 34.230 71.971 1.00 0.00	ATOM 3298 H2 HOH 608 34.253 26.192 48.656 1.00 0.00
ATOM 3227 O1 HOH 585 31.452 31.259 68.561 1.00 18.22	ATOM 3299 O1 HOH 609 22.027 49.801 35.605 1.00 36.28
ATOM 3228 H1 HOH 585 34.169 31.848 68.460 1.00 0.00	ATOM 3300 H1 HOH 609 21.466 49.284 35.038 1.00 0.00
ATOM 3229 H2 HOH 585 32.798 31.604 67.959 1.00 0.00	ATOM 3301 H2 HOH 609 22.457 50.431 35.038 1.00 0.00
ATOM 3230 O1 HOH 586 38.431 40.677 59.022 1.00 29.80	ATOM 3302 O1 HOH 610 34.267 19.550 45.395 1.00 41.99
ATOM 3231 H1 HOH 586 39.024 41.173 58.436 1.00 0.00	ATOM 3303 H1 HOH 610 34.071 20.126 44.666 1.00 0.00
ATOM 3232 H2 HOH 586 38.787 39.792 59.006 1.00 0.00	ATOM 3304 H2 HOH 610 35.224 19.450 45.388 1.00 0.00
ATOM 3233 O1 HOH 587 14.214 22.425 34.386 1.00 33.05	ATOM 3305 O1 HOH 611 52.119 25.683 61.288 1.00 41.57
ATOM 3234 H1 HOH 587 13.445 21.830 34.508 1.00 0.00	ATOM 3306 H1 HOH 611 51.694 26.226 61.981 1.00 0.00
ATOM 3235 H2 HOH 587 14.727 21.982 33.728 1.00 0.00	ATOM 3307 H2 HOH 611 52.670 25.093 61.763 1.00 0.00
ATOM 3236 O1 HOH 588 11.513 23.667 35.426 1.00 42.66	ATOM 3308 O1 HOH 612 37.621 20.380 57.482 1.00 34.82
ATOM 3237 H1 HOH 588 12.378 23.931 35.082 1.00 0.00	ATOM 3309 H1 HOH 612 38.060 19.607 57.100 1.00 0.00
ATOM 3238 H2 HOH 588 11.508 24.024 36.320 1.00 0.00	ATOM 3310 H2 HOH 612 36.838 20.510 56.991 1.00 0.00
ATOM 3239 O1 HOH 589 13.301 30.707 39.584 1.00 29.17	
ATOM 3240 H1 HOH 589 13.479 30.983 40.491 1.00 0.00	
ATOM 3241 H2 HOH 589 13.621 31.461 39.079 1.00 0.00	
ATOM 3242 O1 HOH 590 19.672 44.315 53.325 1.00 41.86	
ATOM 3243 H1 HOH 590 19.608 44.468 52.368 1.00 0.00	
ATOM 3244 H2 HOH 590 19.001 43.668 53.491 1.00 0.00	
ATOM 3245 O1 HOH 591 39.643 38.244 53.938 1.00 27.16	
ATOM 3246 H1 HOH 591 39.900 39.085 54.329 1.00 0.00	
ATOM 3247 H2 HOH 591 38.704 38.198 54.058 1.00 0.00	
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ATOM 3249 H1 HOH 592 18.946 32.662 57.857 1.00 0.00	
ATOM 3250 H2 HOH 592 17.664 32.568 58.686 1.00 0.00	
ATOM 3251 O1 HOH 593 17.303 10.921 54.069 1.00 26.92	
ATOM 3252 H1 HOH 593 18.237 10.758 54.241 1.00 0.00	
ATOM 3253 H2 HOH 593 17.350 11.747 53.536 1.00 0.00	
ATOM 3254 O1 HOH 594 20.129 9.475 51.235 1.00 24.40	
ATOM 3255 H1 HOH 594 20.501 8.710 50.822 1.00 0.00	
ATOM 3256 H2 HOH 594 20.735 10.190 51.037 1.00 0.00	
ATOM 3257 O1 HOH 595 9.777 26.290 50.831 1.00 37.95	
ATOM 3258 H1 HOH 595 8.909 26.442 50.397 1.00 0.00	
ATOM 3259 H2 HOH 595 9.816 27.023 51.445 1.00 0.00	
ATOM 3260 O1 HOH 596 50.629 25.842 82.360 1.00 59.98	
ATOM 3261 H1 HOH 596 50.530 25.393 83.200 1.00 0.00	
ATOM 3262 H2 HOH 596 50.950 26.712 52.589 1.00 0.00	
ATOM 3263 O1 HOH 597 48.511 43.589 61.934 1.00 37.97	
ATOM 3264 H1 HOH 597 47.854 43.556 62.597 1.00 0.00	
ATOM 3265 H2 HOH 597 48.406 42.811 61.392 1.00 0.00	
ATOM 3266 O1 HOH 598 36.392 36.630 64.471 1.00 18.46	
ATOM 3267 H1 HOH 598 35.592 37.143 64.368 1.00 0.00	
ATOM 3268 H2 HOH 598 36.881 36.849 63.658 1.00 0.00	
ATOM 3269 O1 HOH 599 32.970 38.963 63.176 1.00 36.80	
ATOM 3279 H1 HOH 599 32.057 39.224 63.225 1.00 0.00	
ATOM 3271 H2 HOH 599 33.135 38.453 63.965 1.00 0.00	
ATOM 3272 O1 HOH 600 33.301 30.677 60.530 1.00 29.65	
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ATOM 3274 H2 HOH 600 32.913 30.997 61.360 1.00 0.00	
ATOM 3275 O1 HOH 601 32.209 18.034 57.926 1.00 16.83	
ATOM 3276 H1 HOH 601 32.571 18.189 58.807 1.00 0.00	
ATOM 3277 H2 HOH 601 32.293 17.089 57.803 1.00 0.00	
ATOM 3278 O1 HOH 602 42.025 13.710 67.531 1.00 41.72	
ATOM 3279 H1 HOH 602 42.000 13.498 68.453 1.00 0.00	
ATOM 3280 H2 HOH 602 42.530 14.512 67.456 1.00 0.00	
ATOM 3281 O1 HOH 603 32.784 8.013 66.048 1.00 31.46	
ATOM 3282 H1 HOH 603 33.139 7.169 65.772 1.00 0.00	
ATOM 3283 H2 HOH 603 33.424 8.293 66.718 1.00 0.00	
ATOM 3284 O1 HOH 604 42.347 32.216 46.922 1.00 26.11	
ATOM 3285 H1 HOH 604 42.468 33.068 47.176 1.00 0.00	
ATOM 3286 H2 HOH 604 43.218 31.862 47.060 1.00 0.00	

In yet a further embodiment, the present invention provides a crystallized polypeptide having the three-dimensional crystal structure set forth in the previous table. The present invention also provides a method for designing a candidate compound for screening as an antiviral for the prevention or treatment of influenza virus infection, comprising evaluating the three-dimensional crystal structure set forth in the previous table and synthesizing a candidate compound based on the three-dimensional crystal structure. In a further embodiment, the candidate compound is a peptide. In yet another embodiment, the present invention provides for the use of the three-dimensional crystal structure as set forth in the previous table for screening candidate compounds for inhibition of influenza virus M1.

In a further embodiment, the present invention provides for the use of the N-terminal domain of M1 as described herein for screening candidate compounds for inhibition of influenza virus M1.

The present invention also provides a crystallized N-terminal domain of M1.

The use of the crystal structure to design candidate antivirals may be accomplished in the following fashion. Once the crystal structure of the target (e.g., the N-terminal domain of M1) is determined, computer modeling is conducted (using such as programs DOCK or Multiple Copy Simultaneous Search (MCSS)) to construct candidate inhibitor compounds based on the crystal structure. These compounds are chemically synthesized and their biological activity is assayed. For those compounds which show activity, they are associated or complexed with the crystal for further X-ray diffraction analysis to map the interactions of the compound with the crystal structure.

From the resulting inhibitor-target crystal structure, one of ordinary skill in the art could construct further improved candidate compounds. The steps set forth in the preceding paragraph are repeated and refined as desired.

With this in mind, examples using the preferred embodiments of the above-described methods and structures are set forth hereinbelow. Other features of the invention will become apparent from the following examples, which are for illustrative purposes only and are not intended as a limitation upon the present invention.

EXAMPLE I

Virus Preparation

Since M1 constitutes 40% of the total protein in the influenza virus, intact virions were used as the source for purification of the M1 protein. This also ensures that the M1 protein under study is authentic. Attempts to express the whole protein or M1 fragments in *E. coli* failed to produce any useful protein. Influenza virus strain A/PR/8/34 was inoculated in 11-day-old embryonated eggs (Hyvac Lab, Iowa) followed by incubation at 34.5° C. for 48 hours. The allantoic fluid was harvested at the end of incubation, and was centrifuged at 8,000 rpm in a Beckman JA10 rotor for 20 minutes at 4° C. Virus which stayed in the supernatant was concentrated by about 15 fold through an Amicon concentrator in a 4° C. cold room. The virus was pelleted in a Beckman Ti 45 rotor at 20K rpm for three hours at 4° C. The virus pellet was then soaked in Ca⁺⁺Mg⁺⁺-Saline (0.2 mM CaCl₂, 0.8 mM MgCl₂, 0.15 M NaCl) solution overnight. The softened pellet was resuspended by pipetting gently to complete suspension. The virus solution was then subjected to centrifugation on a 10%-40% linear sucrose gradient in a Beckman SW28 rotor at 17K rpm for 40

minutes at 4° C. The virus band was collected from the upper middle area, and was pelleted again in a Beckman SW28 rotor at 25K rpm for three hours at 4° C. Finally, the virus was resuspended in Ca⁺⁺Mg⁺⁺-Saline solution for storage.

EXAMPLE II

Protein Extraction and Purification

In order to strip off the lipid membrane and the membrane embedded surface proteins, 1 M1 of the purified virus preparation was loaded on a three-step sucrose gradient (8). The gradient consisted of, from bottom to top, 3 M1 32% sucrose and 5 M1 17% sucrose in 0.15 M NaCl, 10 mM Hepes (pH 7.2) containing 1% of nonionic detergent NP40, and 2 M1 10% sucrose in 0.15 M NaCl, 10 mM Hepes (pH 7.2) without detergent. After centrifugation in a Beckman SW41 rotor at 21 K rpm for three hours at 4° C., the M1-RNP complex was pelleted to the bottom of the centrifuge tube whereas the membrane associated proteins stayed in the gradient solution. The pellet of the M1-RNP complex was resuspended in 1 M1 of 50 mM NaH₂PO₄ 50 mM, 5 mM Benzamidine and 0.02% NaN₃ (pH of from 3.0 to 5.0, preferably 4.0) to release the M1 protein from the M1-RNP complex (8). The RNP cores (lacking M1) were removed by centrifugation in a Beckman SW55 rotor at 22K rpm for one hour at 4° C.

The M1 protein was further purified by gel filtration in a column of Superdex 75 (Pharmacia) mounted on a Pharmacia FPLC system. The M1 protein was pooled about 62 minutes after sample injection at a flow rate of 1 M1/min. Compared with the molecular weights of the protein standards, the apparent molecular weight of the eluted M1 protein was about 50 kd. Because the molecular weight of M1 monomer derived from its amino acid sequence was expected to be 27 kd (11), the M1 protein appears to form a dimer in solution at acidic pH.

However, the M1 protein was not stable when concentrated to 5 mg/ml prior to crystallization. A stable fragment of 18 Kd was identified after two week storage of the concentrated protein sample at room temperature. Dot-blotting showed that this major fragment of the M1 protein was still recognized by rabbit anti-M1 polyclonal antibodies. The molecular weight of the fragment was determined by Mass Spectrum (PE Sciex API III) to be 18,230 dalton. The M1 fragment remained soluble after transfer of the concentrated protein into a buffer with pH 7.2. The soluble fragment, at pH 7.2, was then incubated with M1-free RNP cores obtained during M1 purification. The mixture was pelleted and analyzed by SDS-PAGE gel. The gel showed that, similar to the native M1 protein, the M1 fragment was still able to bind RNP cores at neutral pH.

Since this fragment can still bind to RNP cores, M1 can be conceptualized as a two-domain protein. The C-terminal domain binds the RNP cores through hydrophilic interactions which can be interrupted by reducing the pH. The N-terminal domain binds the membrane. Without wishing to be bound by theory, the N-terminal domain probably has hydrophobic properties because the intact M1 protein aggregates at neutral pH while the C-terminal domain binds the RNP cores through hydrophilic interactions which can be interrupted by reducing the pH. The N-terminal end thus binds the membrane. The concept of a two domain protein is consistent with the function of M1. During virus production, M1 is synthesized and transported to the nucleus as a dimer where it binds to RNP cores by the C-terminal domain. This is consistent with the RNA binding and anti-transcriptase activity data which were mapped by

monoclonal antibodies to be within the amino acid sequence at from position 90 to position 164. The association of M1 with RNP cores signals, perhaps through a conformational change of M1, the transportation of the M1-RNP complex to the assembly site on the cellular membrane. Only the RNP-associated M1 N-terminal domain can bind to the membrane and the C-terminal tails of the spike glycoproteins, HA and NAA. This completes the function of M1 during virion assembly. During virion entry, the C-terminal domain of M1 is dissociated from the RNP cores due to the low pH of the fusion endosome while the N-terminal domain remains associated with the membrane and the spike glycoprotein tails by hydrophobic interactions. The dissociation of M1 releases naked RNP cores and uncovers the signal for nucleus targeting carried by RNP cores. The virion M1 could not block the transportation of entering RNP cores into the nucleus because of conformational changes induced by low pH. Unlike the matrix protein of human immunodeficiency virus (HIV) and simian immunodeficiency virus (SIV), which are single domain proteins forming a trimer, the M1 protein is a two domain protein functioning as a dimer. The membrane anchoring of M1 occurs through an entirely separate N-terminal protein domain, rather than a covalent myristoyl modification, as found in HIV and SIV matrix proteins.

EXAMPLE III

Crystallization, Data Collection and Processing

Crystallization was carried out in hanging drops by the vapor diffusion method. However, one of skill in the art would recognize that other crystallization methods may be used. For instance, a temperature variation method may be used to produce crystals, while crystallization in outer space may be used to improve resolution. Nonetheless, for the hanging drop method, the protein concentration was about 5 mg/ml. Large crystals (0.05 mm×0.05 mm×0.3 mm) of the 18 kd M1 protein fragment could be grown at 20° C. over 20% PEG 3350 in two months. X-ray diffraction data were collected at the Brookhaven National Laboratory on beamline X-12C. 60 frames from two crystals were collected and the data were processed by the HKL package. The crystals were classified as belonging to space group P3₁21 or P3₂21 with a =68.74 Å, c=136.57 Å. The data were about 56% complete to 2.35 Å resolution and the R_{symm} was 0.11 when reflections with 1>2*sigma(1) were included in the statistics. The V_m value is 2.50 for two monomers per asymmetric unit, which is within the range of normal protein crystals. A further native data set (to 2.1 Å resolution) was collected at NSLS under cryo conditions and the statistics are shown in Table 1.

TABLE 1

The Native Data from NSLS Synchrotron					
Res. limits (Å)	I/sigma (I)	R _{symm} %	% of observations	Observations/ reflections	
25.00	3.78	44.1	2.7	95.4	2.8
3.78	3.00	42.4	3.9	96.0	3.0
3.00	2.62	33.0	5.4	95.9	3.0
2.62	2.38	24.6	7.8	96.0	3.0
2.38	2.21	18.5	10.2	95.9	3.0
2.21	2.08	9.11	17.5	88.6	2.6
All		33.7	4.6	94.7	2.9
Space group: P3 ₁ 21, a = b = 67.17 Å, c=135.30 Å					

Because there are no reported homologous structures to M1, the structural solution relies on the conventional multiple isomorphous replacement method. Three data sets were

collected under identical conditions from a SIEMENS High-star multiwire detector, mounted on a Rigaku rotating anode source with the Oxford cryo system. These three data sets are a new native and two derivative data sets. The statistics are shown in Table 2.

TABLE 2

Refinement of heavy Atom Parameters			
	Native	K ₂ PtCl ₆	K ₂ O ₈ FCl ₆
Resolution	3.5 Å	3.5 Å	3.5 Å
Completeness	96.2%	94.4%	75.9%
R _{symm}	4.2%	4.7%	3.1%
R _{clulis}		0.77	0.76
Phasing power		1.19	1.89
Position	.577, .385, .439	.514, .115, .477	
		FOM = 0.52	

The Harker section of the difference patterns of the Os and Pt derivatives are shown in FIGS. 1a, 1b, 1c, 1d, 2a, 2b, 2c and 2d. The amplitude difference and merging R factors versus resolution for the two derivatives are shown also shown in FIGS. 1a, 1b, 1c, 1d, 2a, 2b, 2c and 2d. Finally, a section of solvent flattened map (FOM=0.89) at 5 Å resolution is shown in FIG. 2c, and a region corresponding to an α-helix at 3.5 Å is shown in FIG. 2d.

REFERENCES

- The following references are incorporated in their entirety herein by this reference:
1. Pons, M. W., Schulze, I. T., Hirst, G. K. and Hauser, R., *Isolation and characterization of the ribonucleoprotein of influenza virus*, VIROLOGY 39:250–259 (1969).
 2. Helenius, A., *Unpacking the incoming influenza virus*, CELL 69:577–578 (1992).
 3. Ye, Z., Pal, R., Fox, W. and Wagner, R. R., *Functional and antigenic domains of the matrix (M1) protein of influenza A virus*, J. VIROL. 61:239–246 (1987).
 4. Bucher, D. J., Kharitonov, I. G., Zakomirdin, J. A., Grigoriev, V. B., Klimenko, S. M. and Davis, J. F., *Incorporation of influenza virus M-protein into liposomes*, J. VIROL. 36:586–590 (1980).
 5. Wakefield, L. and Brownlee, G. G., *RNA-binding properties of influenza A virus matrix protein M1*, NUCLEIC ACIDS RES. 17:8569–8580 (1989).
 6. Winter, G. and Fields, S., *The structure of the gene enclosing the nucleoprotein of human influenza virus A/PR/8/34*, VIROLOGY 114:423–428 (1981).
 7. Zhirnov, O. P., *Solubilization of matrixprotein M1/M from virions occurs at different pH for Orthomyxo- and Paramyxoviruses*, VIROLOGY 176:274–279 (1990).
 8. Zhirnov, O. P., *Isolation of matrix protein M1 from influenza virus by acid-dependent extraction with non-ionic detergent*, VIROLOGY 186:324–330 (1992).
 9. Martin, K. and Helenius, A., *Transport of incoming influenza virus nucleocapsids into the nucleus*, J. VIROLOGY 65:232–244 (1991).
 10. Martin, K. and Helenius, A., *Nuclear transport of influenza virus ribonucleoproteins: the viral matrix protein (ml) promotes export and inhibits import*, CELL 67:117–130 (1991).
 11. Winter, G. and Fields, S., *Cloning of influenza cDNA into M13: the sequence of the RNA segment encoding the A/PR/8/34 matrix protein*, NUCLEIC ACIDS RES. 8:1965–1974 (1980).
 12. Otwinowski, Z. and Minor, W., *An oscillation data processing suite for macromolecular crystallography*, (1995).

13. Matthews, B. W., *Solvent content of protein crystals*, J. MOL. BIO. 33:491-497 (1968).
14. Ye, Z., Baylor, N. W. and Wagner, R. R., *Transcription-inhibition and RNA-binding domains of influenza A virus*

specification and practice of the invention disclosed herein. It is intended that the specification and examples be considered as exemplary only, with the true scope and spirit of the invention being indicated by the following claims.

SEQUENCE LISTING

<160> NUMBER OF SEQ ID NOS: 1

<210> SEQ ID NO 1
<211> LENGTH: 163
<212> TYPE: PRT
<213> ORGANISM: Influenza Virus

<400> SEQUENCE: 1

Ser	Leu	Leu	Thr	Glu	Val	Glu	Thr	Tyr	Val	Leu	Ser	Ile	Ile	Pro	Ser
1					5				10					15	
Gly	Pro	Leu	Lys	Ala	Glu	Ile	Ala	Gln	Arg	Leu	Glu	Asp	Val	Phe	Ala
						20			25				30		
Gly	Lys	Asn	Thr	Asp	Leu	Glu	Val	Leu	Met	Glu	Trp	Lys	Thr	Arg	
						35			40			45			
Pro	Ile	Leu	Ser	Pro	Leu	Thr	Lys	Gly	Ile	Leu	Gly	Phe	Val	Phe	Thr
	50					55						60			
Leu	Thr	Val	Pro	Ser	Glu	Arg	Gly	Leu	Gln	Arg	Arg	Arg	Phe	Val	Gln
					65				70		75		80		
Asn	Ala	Leu	Asn	Gly	Asn	Gly	Asp	Pro	Asn	Asn	Met	Asp	Lys	Ala	Val
					85				90			95			
Lys	Leu	Tyr	Arg	Lys	Leu	Lys	Arg	Glu	Ile	Thr	Phe	His	Gly	Ala	Lys
					100				105			110			
Glu	Ile	Ser	Leu	Ser	Tyr	Ser	Ala	Gly	Ala	Leu	Ala	Ser	Cys	Met	Gly
	115					120						125			
Leu	Ile	Tyr	Asn	Arg	Met	Gly	Ala	Val	Thr	Thr	Glu	Val	Ala	Phe	Gly
	130				135						140				
Leu	Val	Cys	Ala	Thr	Cys	Glu	Gln	Ile	Ala	Asp	Ser	Gln	His	Arg	Ser
	145				150				155			160			
His Arg Gln															

matrix protein mapped with anti-idiotypic antibodies and synthetic peptides, J. VIROL. 63:3586-3594 (1989).

15. Hankins, R. W., Nagata, K., Bucher, D. J., Popple, S. and Ishihama, A., *Monoclonal antibody analysis of influenza virus matrix protein epitopes involved in transcription inhibition*, VIRUS GENES. 3(2):111-126, (1989).

Sequence Listing

SEQ. ID. NO. 1 represents amino acids 2-164 of the N-terminal domain of influenza virus matrix protein M1:

SEQ. ID. NO.1: SLLTEVETYVLSIIPS- GPLKAE- IAQRLED VFAGKNTDLEVLMWLKTR- PILSPLT- KGILGFVF TLTVPSER GLQRRRFVQNAL- NGNGDPNNMDKAVKLYRKLKREIT1F- 60 H GAKEISL SY SAG ALAS CMGLIYNRM- GAVTTEVAFGLVCATCEQIADSQHRSRQ

It will be apparent to those skilled in the art that various modifications and variations can be made in the present invention without departing from the scope or spirit of the invention. Other embodiments of the invention will be apparent to those skilled in the art from consideration of the

What is claimed is:

1. A crystallized N-terminal domain of the M1 protein of influenza virus comprising the amino acid sequence set forth in the Sequence Listing as SEQ ID NO:1, wherein the N-terminal domain of M1 is crystallized to obtain crystals of space group P3₂1 or P3₁21 with approximate $a=68.0 \text{ \AA}$ and approximate $c=136.57 \text{ \AA}$ such that the three dimensional structure of the crystallized N-terminal domain of M1 can be determined to a resolution of about 2.1 \AA or better.
2. A method of extracting and purifying the M1 protein of influenza virus comprising:
 - a) stripping the membrane proteins from influenza virus;
 - b) removing the stripped membrane proteins, thereby leaving the M1-RNP complex;
 - c) releasing M1 from the M1-RNP complex by suspending the complex in a solution comprising NaH_2PO_4 , Benzamidine, and NaN_3 ; and
 - d) purifying the released M1 by FPLC chromatography.
3. A method of extracting the N-terminal domain of the M1 protein of influenza virus comprising the amino acid sequence set forth in the Sequence Listing as SEQ ID NO:1 comprising:

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- a) stripping the membrane proteins from influenza virus;
 - b) removing the stripped membrane proteins, thereby leaving the M1-RNP complex;
 - c) releasing M1 from the M1-RNP complex by suspending the complex in a solution comprising NaH₂PO₄, Benzamidine, and NaN₃;
 - d) purifying the released M1;
 - e) concentrating the purified M1 to a concentration of from 3 mg/ml to 20 mg/ml; and
 - f) after a period of time sufficient for the formation of an 18 kd protein fragment corresponding to the N-terminal domain of M1, collecting the 18 kd polypeptide corresponding to the N-terminal domain of M1.
4. The method of claim 3, wherein the time period is from 7 to 21 days.

5. The method of claim 3, further comprising crystallizing the 18 kd polypeptide corresponding to the N-terminal domain of M1 to a resolution of less than about 2.1 Å, wherein the N-terminal domain of M1 is present at a concentration of from 3 to 20 mg/ml and the crystallization takes place at from 4 to 32° C. to thereby obtain crystals of space group P3₂1 or P3₁21.

6. The method of claim 3, wherein the pH of the solution of step c) is from 3.0 to 5.0.

7. The method of claim 5, wherein the crystallization occurs in hanging drops using the vapor diffusion method.

8. A method for determining the three dimensional structure of the crystallized N-terminal domain of the M1 protein of influenza virus comprising the amino acid sequence set forth in the Sequence Listing as SEQ ID NO:1 to a resolution of about 2.1 Å or better comprising the steps of crystallizing the N-terminal domain of M1 to a resolution of about 2.1 Å, wherein the N-terminal domain of M1 is present at a concentration of from 3 to 20 mg/ml and the crystallization takes place at from 4 to 32° C., to thereby obtain crystals of space group P3₂1 or P3₁21, and then analyzing the N-terminal domain of M1 to determine the three-dimensional structure of the crystallized N-terminal domain of M1.

9. The method of claim 8, wherein the analyzing is by x-ray diffraction.

10. The method of claim 8, wherein the crystallization occurs in hanging drops using the vapor diffusion method.

11. The crystallized N-terminal domain of M1 produced by the process of claim 5.

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12. A method for designing a potential antiviral compound for the prevention or treatment of influenza virus infection, comprising:

- a. obtaining crystals of the N-terminal domain of M1, wherein the crystals have the space group P3₂1 or P3₁21 with approximate $a=68.0 \text{ \AA}$ and approximate $c=136.57 \text{ \AA}$ such that the three dimensional structure of the crystallized N-terminal domain of M1 can be determined to a resolution of about 2.1 Å or better,
- b. evaluating the three dimensional structure of the crystallized N-terminal domain of M1;
- c) synthesizing the potential antiviral compound based on the three-dimensional crystal structure of the crystallized N-terminal domain of M1;
- d) contacting an influenza virus or an influenza viral protein with the potential antiviral compound; and
- e) assaying the influenza virus for infectivity or monitoring the influenza viral protein for activity, or both, whereby a decrease in the infectivity of the influenza virus or a change in the activity of the influenza virus protein indicates the compound may be used for the prevention or treatment of influenza virus infection.

13. The method of claim 12, wherein the antiviral compound is a peptide or polypeptide.

14. The method of claim 12, wherein the crystallization occurs in hanging drops using the vapor diffusion method.

15. The method of claim 12, wherein the crystal has the three dimensional crystal structure of influenza virus protein M1 as set forth in FIG. 3.

16. The method of claim 12, wherein the influenza viral protein comprises M1.

17. A method for designing a candidate compound for screening for binding to or inhibition of influenza virus M1, comprising:

- a) utilizing the three dimensional structure of a crystallized N-terminal domain of M1 which is defined by the atomic coordinates in FIG. 3; and
- b) designing a candidate binding compound based on the three-dimensional crystal structure of the crystallized N-terminal domain of M1 for binding to M1.

18. The method of claim 17, wherein the candidate compound is a peptide or polypeptide.

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