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Crystallization and Structure of a Plant Peptide Deformylase

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(54) **CRYSTALLIZATION AND STRUCTURE OF A PLANT PEPTIDE DEFORMYLASE**

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C12N 9/78 (2006.01)
G01N 31/00 (2006.01)

(52) **U.S. Cl.** **435/227**; 436/4

(58) **Field of Classification Search** ..... None
See application file for complete search history.

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(57) **ABSTRACT**

This invention relates to the crystal structure of a plant peptide deformylase polypeptide and methods of using the structure to design compounds that modulate the activity of the polypeptide.

4 Claims, 15 Drawing Sheets

Figure 1A

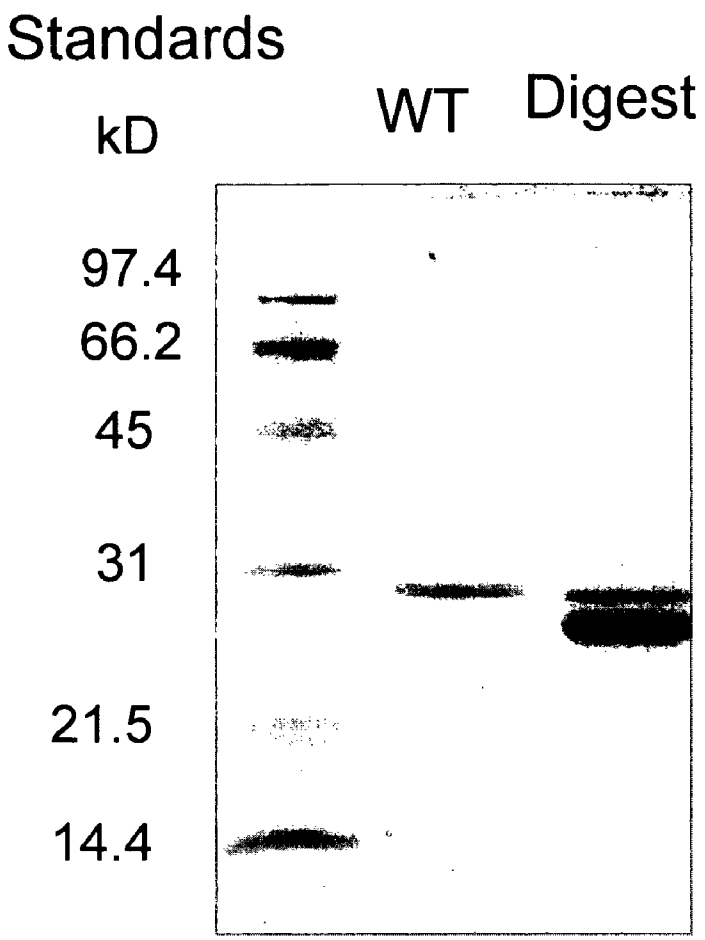


Figure 1B

```
      70         80         90        100        110        120
   KDDKVA SATDVQFETP LKIVEYPDPI LRAKNKRIDI FDENLKNLVD AMFDVMYKTD

     130        140        150        160        170        180
GIGLSAPQVG LNVQLMVFNP AGEPGEGKEI VLVNPKIKKY SDKLVPFDEG CLSFPGIYAE

     190        200        210        220        230        240
VVRPQSVKID ARDITGERFS ISLSRLPARI FQHEYDHLEG VLFFDRMTDQ VLDSIREELE

     250    257
ALEKKYEEKT GLPSPER
```

Figure 2A

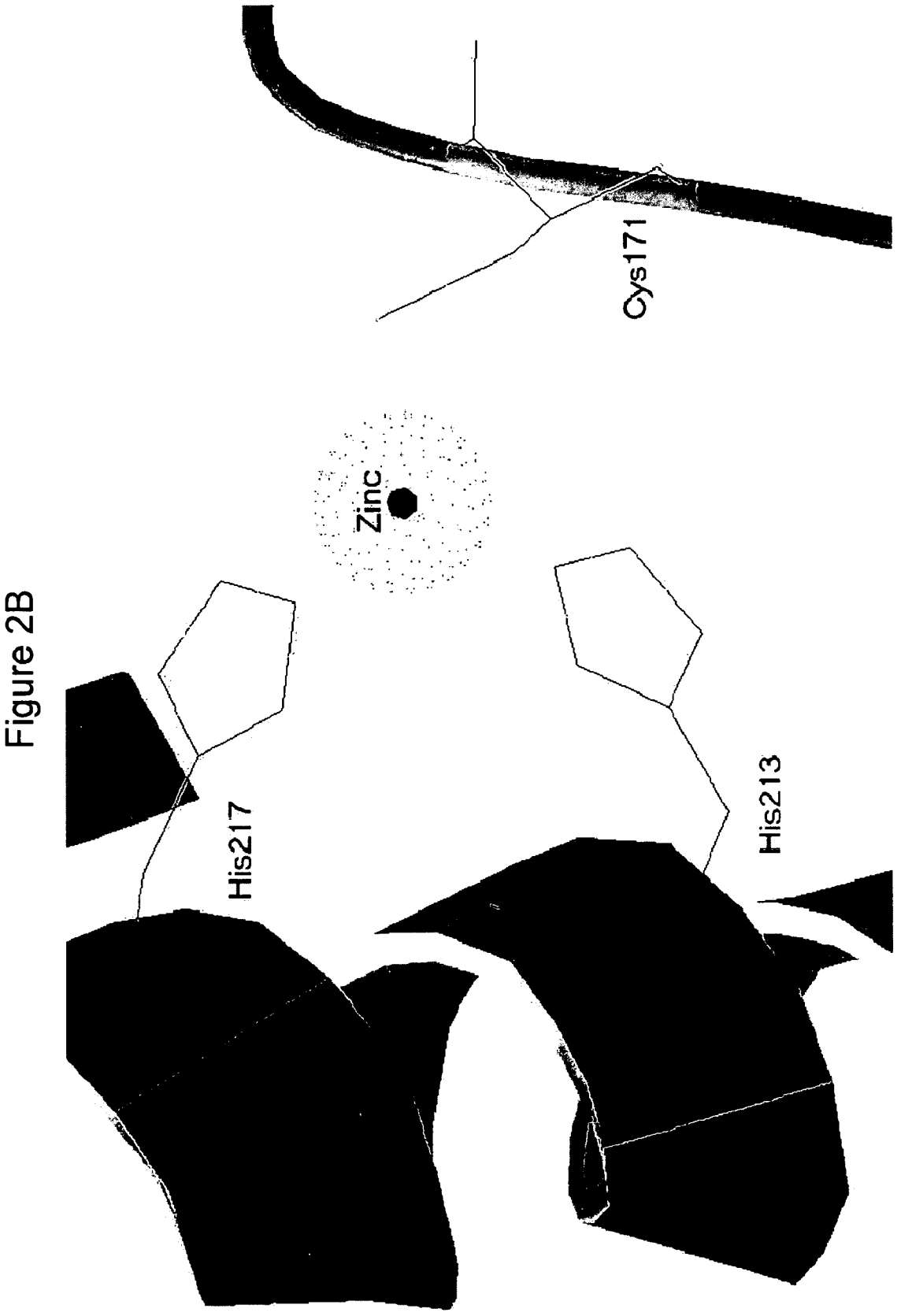
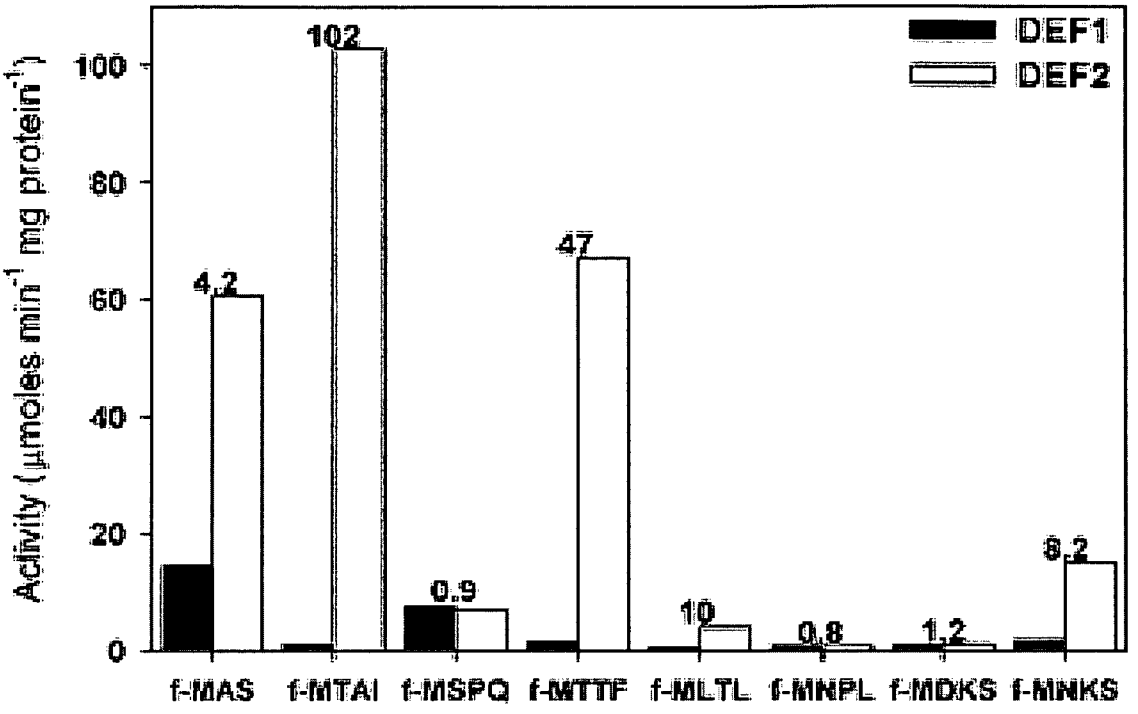


Figure 2B

Figure 3


DEF1
DEF2
Activity (μmoles min-1 mg protein-1)
0
20
40
60
80
100
4.2
102
0.9
47
1.0
0.8
1.2
8.2
f-MAS
f-MTAI
f-MSPQ
f-MTTF
f-MLTL
f-MNPL
f-MDKS
f-MNKS

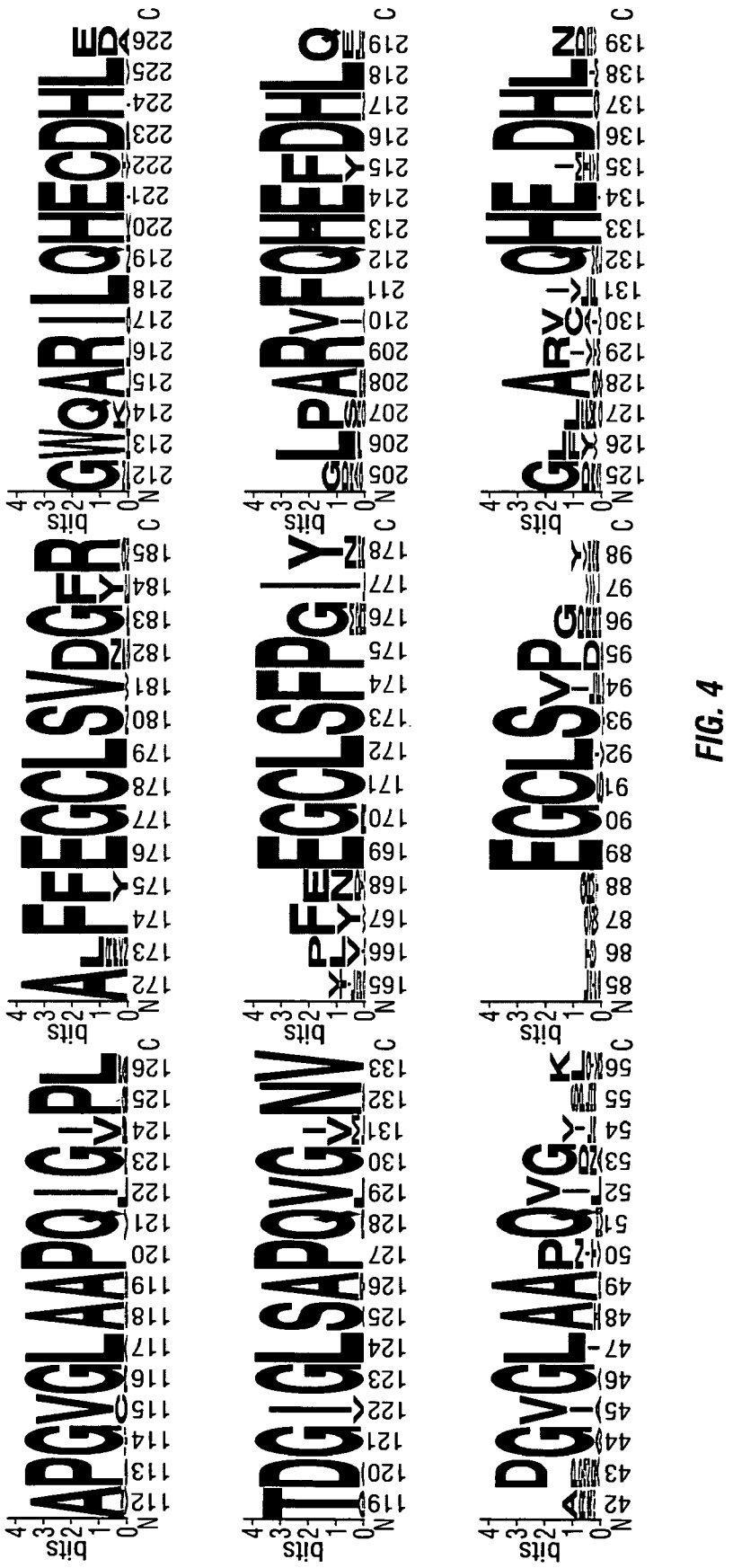
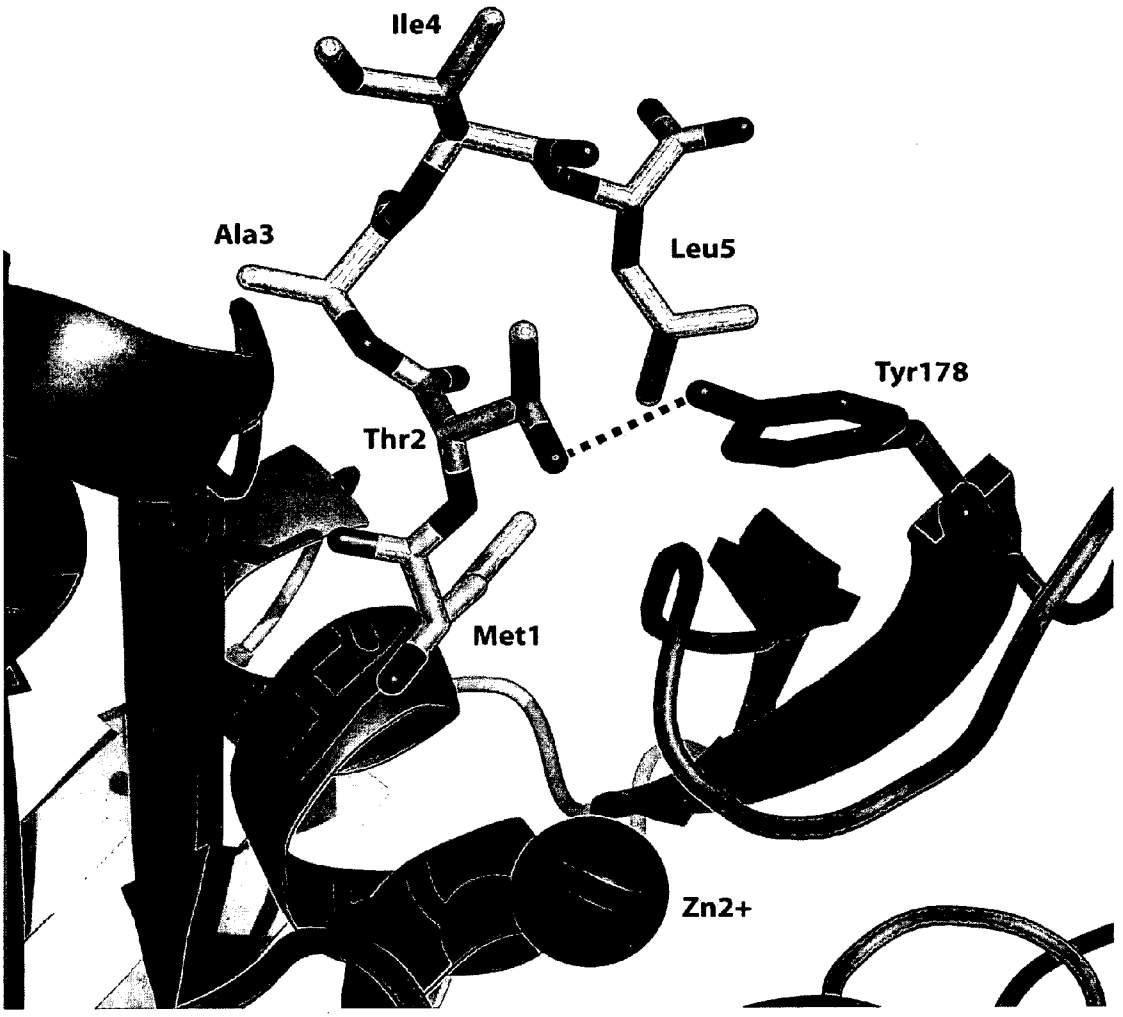


FIG. 4

Figure 5



Motif I

		AtDEF1 sequence															
		44 sequence alignment															
	residue numbering of the sequence is difficult because of different translational start sites, however going with the METLFR as start, numbering is as follows:																
	#:		112	113	114	115	116	117	118	119	120	121	122	123	124	125	126	
	1ZXZ RESIDUE#		45	46	47	48	49	50	51	52	53	54	55	56	57	58	59	
		Number of sequences aligned at this residue:																
			34	34	34	34	31	31	31	31	31	31	31	31	32	33	34	
	R	L	A	P	G	V	G	L	A	A	P	Q	I	G	V	P	L	R
A			31						31	31								
C						5												
D			1															
E															1			
F															1		2	
G					32		31							31				
H																		
I													28		16			
K																		
L					1			31					3		1		30	
M																		
N																		
P				33		1					31					30	1	
Q												31						
R					1													
S			1			1										2	1	
T																		
V			1			27									13	1		
W																		
Y																		
SUM CHECK			34	34	34	34	31	31	31	31	31	31	31	31	32	33	34	

FIG. 6, PANEL A

Motif II

		AtDEF1 sequence															
		44 sequence alignment															
	residue numbering of the sequence is difficult because of different translational start sites, however going with the METLFR as start, numbering is as follows:																
	#:		172	173	174	175	176	177	178	179	180	181	182	183	184	185	186	
	1ZXZ RESIDUE#		105	106	107	108	109	110	111	112	113	114	115	116	117	118	119	
		Number of sequences aligned at this residue:																
			41	42	42	42	43	43	43	43	41	41	40	40	40	39	39	

	K	K	A	L	F	F	E	G	C	L	S	V	D	G	F	R	A	A
A			41															
C				2					42			1	1					
D													31		1			
E							42	1			1							
F				7	41	33				1					24			
G							1	41						39				
H																		
I						1												
K				3				1										
L				21	1					41					1			
M																		
N											1		6			1		
P													2	1				
Q				2														
R				6												36		
S									1		39					2		
T																		
V				1								39						
W												1						
Y						8				1					14			
SUM CHECK			41	42	42	42	43	43	43	43	41	41	40	40	40	39	0	

FIG. 6, PANEL B

Motif III

		AtDEF1 sequence															
		44 sequence alignment															
	residue numbering of the sequence is difficult because of different translational start sites, however going with the METLFR as start, numbering is as follows:																
	#:		212	213	214	215	216	217	218	219	220	221	222	223	224	225	226	
	1ZXZ RESIDUE#		145	146	147	148	149	150	151	152	153	154	155	156	157	158	159	
		Number of sequences aligned at this residue:																
			35	35	35	34	34	34	33	33	33	32	31	30	30	29	29	

	A	S	G	W	Q	A	R	I	L	Q	H	E	C	D	H	L	D	G
A						33											4	
C													3					
D														29			12	
E											1	31					13	
F																		
G			33															
H				1							32				29			
I								33				1			1			
K					5													
L						1	1		33							28		
M																		
N			1							1								
P			1											1				
Q					29					32								
R							33											
S								1										
T													1					
V																		
W				34												1		
Y					1								27					
SUM CHECK			35	35	35	34	34	34	33	33	33	32	31	30	30	29	29	

FIG. 6, PANEL C

Motif I

		AtDEF2 sequence																
		52 sequence alignment																
	RESIDUE#	119	120	121	122	123	124	125	126	127	128	129	130	131	132	133	134	1
		Number of sequences aligned at this residue:																
		42	42	42	42	42	42	43	43	43	44	44	44	44	44	44		
	K	T	O	G	I	G	L	S	A	P	Q	V	G	L	N	V	Q	L
A		1	1					1	41									
C																		
D		1	41						1									
E																		
F																		
G				42		42							44					
H											1							
I					37									17				
K																		
L							42					5		3				
M														8				
N															43			
P										43								
Q											43							
R																		
S								42							1			
T		40							1									
V					5							39		16		44		
W																		
Y																		
SUM CHECK	0	42	42	42	42	42	42	43	43	43	44	44	44	44	44	44	0	

FIG. 7, PANEL A

Motif II

		AtDEF2 sequence																
		52 sequence alignment																
	RESIDUE#	165	166	167	168	169	170	171	172	173	174	175	176	177	178	179	180	1
		Number of sequences aligned at this residue:																
		43	43	42	43	43	43	43	43	43	42	41	41	40	40			

	L	V	P	F	D	E	G	C	L	S	F	P	G	I	V	A	E	V
A																		
C								43										
D			1		4								2					
E		4			18	42							2					
F				28							42							
G				1			42						33					
H															2			
I		6	2											39				
K						1												
L		6	13						43					1				
M													3					
N					17										7			
P			15									41						
Q																		
R		4					1						1		2			
S		3			1					43								
T		7			3													
V		13	12															
W																		
Y				13											29			
SUM CHECK	0	43	43	42	43	43	43	43	43	43	42	41	41	40	40	0	0	

FIG. 7, PANEL B

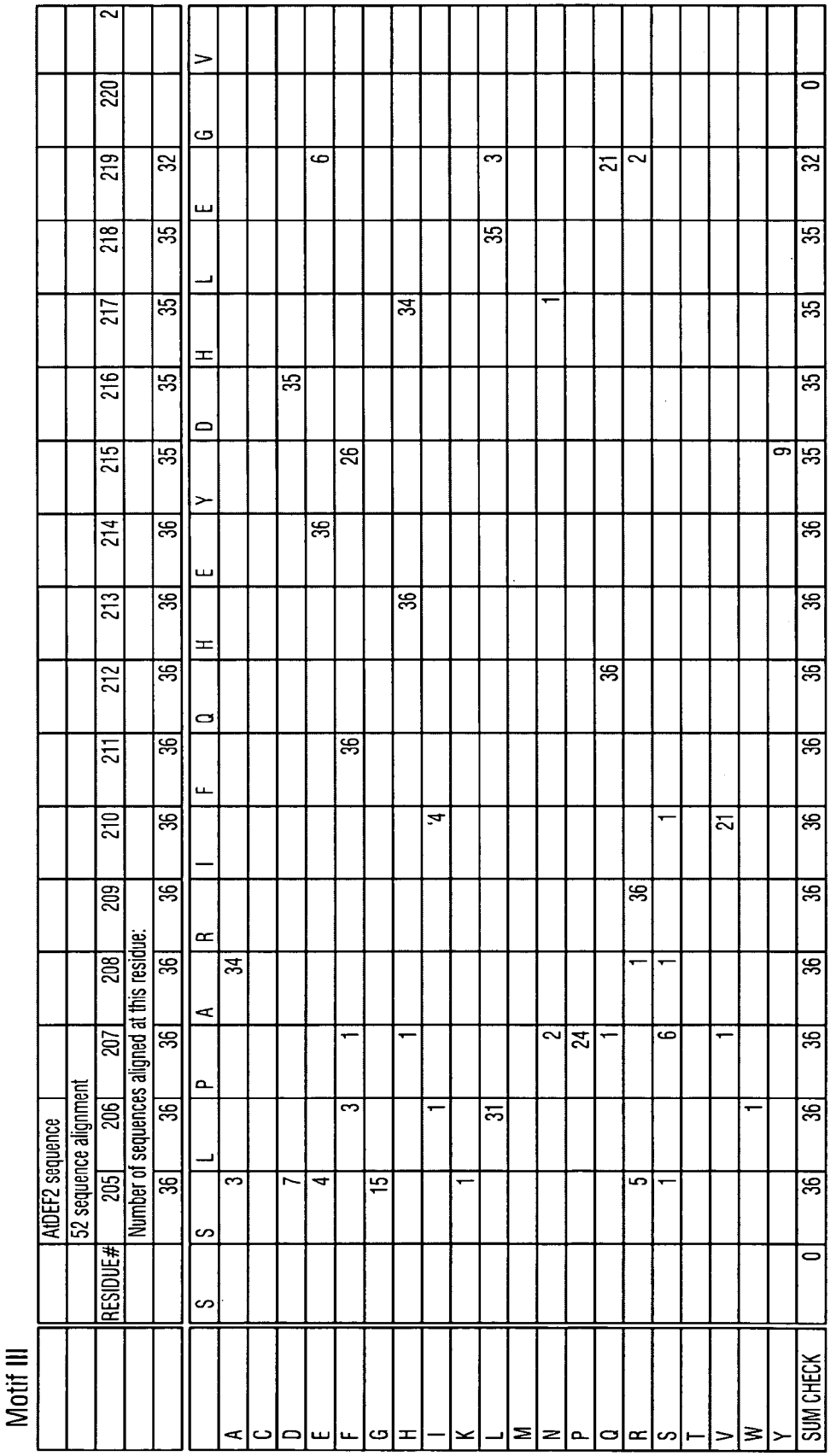

Motif III
AtDEF2 sequence
52 sequence alignment
RESIDUE#
205 206 207 208 209 210 211 212 213 214 215 216 217 218 219 220
Number of sequences aligned at this residue:
36 36 36 36 36 36 36 36 36 36 35 35 35 35 35 2
S S L P A R I F Q H E Y D H L E G V
A 3 34
C
D 7 35
E 4 36 6
F 3 1 36 26
G 15
H 1 36 34
I 1 4
K 1
L 31 35 3
M
N 2 1
P 24
Q 1 36 21
R 5 1 36 2
S 1 6 1 1
T
V 1 21
W 1
Y 9
SUM CHECK 0 36 36 36 36 36 36 36 36 36 36 35 35 35 35 32 0

FIG. 7, PANEL C

Motif I

	Q2VP16_ECOLI	(Also #age for the most part because mostly 100 sequences in the determination)																							
	100 sequence alignment: Blasted E coli and then from the list returned, removed all below the first non-DEF protein, removed all DEFs with number other than 1 and with precuror assignment																								
	Q2VP16 RESIDUE#	41	42	43	44	45	46	47	48	49	50	51	52	53	54	55	56								
	Number of sequences aligned at this residue:																								
		97	98	99	99	100	100	100	100	100	100	100	100	100	100	100	100								
	Y	A	E	K	G	I	G	L	A	A	T	Q	V	D	I	H	Q	R							
A			43			4	8	3		92	97	1			6		1								
C					2					2						3									
D				16											14		5								
E			7	10												5	3	4							
F			2																						
G				4	94		97			1	2				70		5								
H			3	1									4			2	8								
I			5	2		33		14			10			41		30		6							
K			2	9												1	2	41							
L			18					85						13		14	15	29							
M			1									2				1									
N			4	9								16			10	1	6								
P				20								57					21								
Q			2	1									94			4	1	10							
R				26												3		4							
S			7							1	1	1				1	27								
T			2	1						4		10					4								
V						59		1				5		45		31		6							
W																1	2								
Y			3											1		3									
SUM CHECK		0	0	99	99	100	100	100	100	100	100	100	100	100	100	100	100	100							

FIG. 8, PANEL A

Motif II

	Q2VP16_ECOLI	(A so #age for the most part because mostly 100 sequences in the determination)																
	100 sequence alignment: Blasted E coli and then from the list returned, removed all below the first non-DEF protein, removed all DEFs with number other than 1 and with precuror assignment																	
	Q2VP16 RESIDUE#	84	85	86	87	88	89	90	91	92	93	94	95	96	97	98	99	10
		Number of sequences aligned at this residue:																
			99	99	99	100	100	100	100	100	100	100	100	100	100	100		
	G	E	T	G	I	E	E	G	C	L	S	I	P	E	Q	R	A	L
A			5	3	6									1	2	4		
C			4		2				92									
D			8	2	15	3							20	17		1		
E			9	7	7	22	100							14	3	7		
F					9	2						9			9	4		
G			2	6	19	23		99					1	43		2		
H			1		4									2	3	4		
I			11	4	3	2				5		30	1	2	11			
K			2	3		5							2	2	2	2		
L			21	1		3				90		10		2	10			
M			2	4	2					1		4		1	2			
N			1	3	1	7								10		1		
P				5	1	3							76	1		9		
Q			11	3	1	12								1	4	11		
R				2		6									4	13		
S			9	18	4			1	8		98					8		
T			2	22	4	3					2			1	1	2		
V			9	13	2	2				4		47		3	32	1		
W				1	2	5									1			
Y			2	2	17	2									16	31		
SUM CHECK	0	0	99	99	99	100	100	100	100	100	100	100	100	100	100	100	0	

FIG. 8, PANEL B

Motif III

	Q2VP16_ECOLI	(A so #age for the most part because mostly 100 sequences in the determination)																
	100 sequence alignment: Blasted E coli and then from the list returned, removed all below the first non-DEF protein, removed all DEFs with number other than 1 and with precuror assignment																	
	Q2VP16 RESIDUE#	124	125	126	127	128	129	130	131	132	133	134	135	136	137	138	139	14
		Number of sequences aligned at this residue:																
			100	100	100	100	100	100	100	100	100	100	100	100	100	100	100	
	A	D	G	L	L	A	I	C	I	Q	H	E	M	D	H	L	V	G
A			1		2	90	1	13										
C								33	1	3			4					
D			11	3										95			22	
E			7		1							97		1			7	
F				26	8				14				7			1		
G			75			3								4				
H					4				2		100				92		6	
I				3	2		26	11	43			2	46			8	2	
K					1		2										2	
L				36	44				17	3			3			86		
M				1	8		3	6	2	4			15			2	1	
N			3		5								3		1	1	48	
P					15													
Q					1		1			90					6		5	
R					1		46											
S			3			7											2	
T				1	3		7						13			2	1	
V					3		14	37	20				2				3	
W				7					1									
Y				23	2								7		1		1	
SUM CHECK	0	0	100	100	100	100	100	100	100	100	100	100	100	100	100	100	100	

FIG. 8, PANEL C

CRYSTALLIZATION AND STRUCTURE OF A PLANT PEPTIDE DEFORMYLASE

CROSS REFERENCE TO RELATED APPLICATIONS

This application claims priority to U.S. Provisional Application Ser. No. 60/835,823 filed Aug. 4, 2006, the disclosure of which is incorporated herein by reference.

STATEMENTS REGARDING FEDERALLY SPONSORED RESEARCH

The invention was funded in part by Grant No. MCB-MCB-0240165 awarded by the National Science Foundation (NSF). The government may have certain rights in the invention.

TECHNICAL FIELD

This invention relates to the crystallization and structure of plant peptide deformylase and methods of using the structure.

BACKGROUND

Peptide deformylase (DEF; EC 3.5.1.88) is a metallopeptidase that catalyzes the removal of an N-formyl group from N-formyl methionine, which is the initiating amino acid residue for prokaryotically translated proteins. DEF is an essential enzyme and mutations, deletions, or insertions in the DEF gene, or inhibition of enzymatic activity, are lethal to prokaryotic organisms. For decades DEF was believed to be exclusively restricted to prokaryotes because protein translation in eukaryotic organisms initiates with an unformylated methionine residue. The restriction to prokaryotic organisms and the essentiality of DEF have made this enzyme the molecular target of many research efforts directed towards the development of broad-spectrum antibiotics, which would have little or no mammalian toxicity. In 2000 the existence of DEF in the chloroplasts of higher plants was reported, and it was also discovered that actinonin, a potent inhibitor of DEF, was phytotoxic to all plant species. The lethality of actinonin to a wide range of plants, including many agriculturally significant weed species, suggests that DEF is an essential and highly conserved enzyme in plants, and inhibitors targeting this enzyme could potentially serve as a new class of broad-spectrum herbicides as well as selectable markers.

Accordingly, plant peptide deformylase (DEF) polypeptides provide an attractive target for crystallization and structural studies which can lead to the identification and synthesis of new broad-spectrum herbicides and selectable markers with high specificity towards plant DEF.

SUMMARY

Provided herein are crystalline forms of a peptide deformylase, and atomic coordinates derived therefrom, useful for designing and identifying compounds that modulate the activity of the peptide deformylase. Accordingly, in one embodiment, a crystalline form of a polypeptide comprising the amino acid residues of SEQ ID NO:1, is provided. In some aspects, the crystalline form includes a structure characterized by tetragonal space group symmetry $P4_12_12$ and unit cell of dimensions a, b, and c. In some aspects, a is about 40 Å to about 60 Å, b is about 40 Å to about 60 Å, and c is about 120 Å to about 160 Å. In other aspects, $\alpha=\beta=\gamma=90°$. In some aspects, the polypeptide is a peptide deformylase isolated from *Arabidopsis thaliana*.

In some embodiments, the crystalline form includes a coordinated metal ion selected from the group of consisting of Fe, Zn, and Ni, and any combination thereof. In one aspect, the metal ion is coordinated by amino acid residues Cys171, His213, and His217 of SEQ ID NO:1.

In another embodiment, a crystalline form of a polypeptide including a structure defined by one or more structure coordinates of *Arabidopsis thaliana* peptide deformylase amino acid residues Gly121, Gly123, Leu124, Gln128, Glu169, Gly170, Cys171, Leu172, His213, Glu214, His217, and Tyr178 according to Table 1, is provided. In general, structures derived from these crystalline forms encompass structures having coordinates that differ by a root mean square deviation of less than about 1.5 Å, 0.75 Å, or 0.35 Å, or any deviation in this range, when superimposed on the non-hydrogen atom positions of the corresponding atomic coordinates of Table 1. In some aspects, amino acid residues Gly121, Gly123, Leu124, Gln128, Glu169, Gly170, Cys171, Leu172, His213, Glu214, His217, and Tyr178 include the active site of the peptide deformylase. In some aspects, the polypeptide includes an amino acid sequence having at least 75%, at least 85%, or at least 95%, or any percent in this range, amino acid sequence identity to SEQ ID NO:1.

In other embodiments, a crystalline form of a polypeptide provided herein also includes a ligand complexed with the polypeptide. In some aspects, the ligand is a small molecule.

In another embodiment, a crystalline form of a polypeptide that includes the amino acid residues of SEQ ID NO:1 and an atomic structure characterized by the coordinates of Table 1, is provided.

In yet another embodiment, a machine-readable medium embedded with information that corresponds to a three-dimensional structural representation of a crystalline form of a polypeptide as provided herein.

In one embodiment, a computer system including a database containing information on the three dimensional structure of a crystalline form of an *Arabidopsis thaliana* peptide deformylase polypeptide and a user interface to view the information, is provided. In some aspects, the computer system includes information related to diffraction data obtained from a crystalline form comprising SEQ ID NO:1. In other aspects, the computer system of includes information related to an electron density map of a crystal comprising SEQ ID NO:1.

In another aspect, a computer system provided herein includes information related to the structure coordinates of Table 1 or homologous structure coordinates for the amino acid residues of SEQ ID NO:1 that have a root mean square deviation of non-hydrogen atoms of less than about 1.5 Å, 0.75 Å, 0.35 Å, or any percent in this range, when superimposed on the non-hydrogen atom positions of the corresponding atomic coordinates of Table 1.

In other aspects, a computer system provided herein includes information related to the structure coordinates for one or more amino acid residues Gly121, Gly123, Leu124, Gln128, Glu169, Gly170, Cys171, Leu172, His213, Glu214, His217, and Tyr178 according to Table 1, or similar structure coordinates for the amino acids including a root mean square deviation of non-hydrogen atoms of less than about 1.5 Å, 0.75 Å, 0.35 Å, or any percent in this range, when superimposed on the non-hydrogen atom positions of the corresponding atomic coordinates of Table 1.

In another embodiment, a method of identifying a candidate compound that binds to the active site of *Arabidopsis thaliana* peptide deformylase polypeptide, is provided. The method includes comparing the atomic structure of the compound with a three-dimensional structure of a crystalline

form of an *Arabidopsis thaliana* peptide deformylase polypeptide and computationally identifying a candidate compound for an ability to bind to the *Arabidopsis thaliana* peptide deformylase. In some aspects, the candidate compound binds to the active site of the *Arabidopsis thaliana* peptide deformylase. In other aspects, comparing the atomic structure of the compound with a three-dimensional structure of a crystalline form of an *Arabidopsis thaliana* peptide deformylase polypeptide includes employing a computational means to perform a fitting operation between the compound and at least one binding site of the peptide deformylase.

In some embodiments, the candidate compound identified by a computational method provided herein can be synthesized and screened for the ability to bind a plant peptide deformylase in vitro or in vivo. In some aspects, the compound is an herbicide.

In another embodiment, a method of identifying a candidate compound that binds to the active site of *Arabidopsis thaliana* peptide deformylase polypeptide, is provided. The method includes comparing the atomic structure of the compound with a three-dimensional structural representation of a crystalline form provided herein and computationally identifying a candidate compound for an ability to bind to the active site of *Arabidopsis thaliana* peptide deformylase.

In yet another embodiment, a method of computationally designing a candidate compound that binds to *Arabidopsis thaliana* peptide deformylase polypeptide, is provided. The method includes comparing the atomic structure of chemical entities, or fragments thereof, with a three-dimensional structural representation of a crystalline form of a polypeptide provided herein; identifying chemical entities capable of associating with the three-dimensional structural representation of a crystalline form of a polypeptide; and assembling the chemical entities, or fragments thereof, into a single molecule to provide the structure of the candidate compound. In some aspects, the candidate compound binds to the active site of *Arabidopsis thaliana* peptide deformylase.

In another embodiment, a method of identifying a region of *Arabidopsis thaliana* peptide deformylase polypeptide that contacts a compound, is provided. The method includes obtaining X-ray diffraction data for a crystal of *Arabidopsis thaliana* peptide deformylase; obtaining X-ray diffraction data for a complex of a *Arabidopsis thaliana* peptide deformylase and the compound; subtracting the X-ray diffraction data from the peptide deformylase with the X-ray diffraction data obtained from the complex to obtain the difference in the X-ray diffraction data; obtaining phases that correspond to X-ray diffraction data obtained for the peptide deformylase; correlating the data to generate a difference Fourier image of the compound; and locating the region of *Arabidopsis thaliana* peptide deformylase contacted by the compound. In some aspects, the compound is actinonin.

In another embodiment, a method of modifying an inhibitor of *Arabidopsis thaliana* peptide deformylase activity, is provided. The method includes obtaining a crystal including an *Arabidopsis thaliana* peptide deformylase polypeptide and an inhibitor; obtaining the atomic coordinates of the crystal; correlating the atomic coordinate data with one or more molecular modeling techniques; identifying at least one modification predicted to effect the interaction of the inhibitor with the polypeptide; and modifying the inhibitor based on the prediction. In one aspect, the modification is a computer generated modification. In other aspects, the modification is a physical modification made to the structure of the inhibitor. In one aspect, the crystal comprises the amino acid residues of SEQ ID NO:1.

In other aspects, the one or more molecular modeling techniques are selected from the group consisting of graphic molecular modeling and computational chemistry. In another aspect, obtaining the atomic coordinates of the crystal includes detecting the interaction of the inhibitor to one or more amino acid residues Gly121, Gly123, Leu124, Gln128, Glu169, Gly170, Cys171, Leu172, His213, Glu214, His217, and Tyr178 of SEQ ID NO:1.

The details of one or more embodiments of the disclosure are set forth in the accompanying drawings and the description below. Other features, objects, and advantages will be apparent from the description and drawings, and from the claims.

BRIEF DESCRIPTION OF DRAWINGS

FIG. **1**A depicts a polyacrylamide gel showing that limited trypsinolysis creates a core protein that retained activity and remained soluble in the absence of high salt concentrations.

FIG. **1**B depicts the amino acid sequence of the AtDEF peptide (SEQ ID NO: 1).

FIG. **2**A depicts a ribbon representation of crystallized AtDEF2. The cylinders represent helices and the arrows represent sheets.

FIG. **2**B depicts a slab view of the ribbon representation of trypsinolyzed AtDEF2 highlighting the active-site-metal binding ligands (1 Cys and 2 His) from motifs II and III, respectively (EGCLS and QHEXXH) (SEQ ID NOS 15-16).

FIG. **3** depicts a graph of substrate specificity comparison of AtDEF1 and AtDEF2.

FIG. **4** depicts a comparison of amino acid sequence conservation of the three motifs in AtDEF1 and 2 and bacterial DEFs (SEQ ID NOS 2-5).

FIG. **5** depicts a molecular model of the N-terminal residues from the D1 polypeptide docked into the active site of *Arabidopsis thaliana* peptide deformylase.

FIG. **6** depicts a phylogenetic analyses comparing Motif 1 (SEQ ID NO: 6), Motif 2 (SEQ ID NO: 7) and Motif 3 (SEQ ID NO: 8) of plant AtDEF1 peptide deformylase with the amino acid sequence of other peptide deformylase sequences.

FIG. **7** depicts a phylogenetic analyses comparing Motif 1 (SEQ ID NO: 9), Motif 2 (SEQ ID NO: 10) and Motif 3 (SEQ ID NO: 11) of plant AtDEF2 peptide deformylase with the amino acid sequence of other peptide deformylase sequences.

FIG. **8** depicts a phylogenetic analyses comparing Motif 1 (SEQ ID NO: 12), Motif 2 (SEQ ID NO: 13) and Motif 3 (SEQ ID NO: 14) of various peptide deformylase amino acid sequences.

Like reference symbols in the various drawings indicate like elements.

DETAILED DESCRIPTION

Provided herein are novel crystalline forms of peptide deformylase polypeptides and atomic coordinate information related to such crystals. Also provided are methods of using such information to identify, design and/or modify compounds that modulate the activity of a peptide deformylase. In addition, computer systems that include such information are provided. The crystal structures and information derived therefrom are suitable for designing and identifying, for example, broad spectrum herbicides. Such herbicides can be used, for example, to inhibit or prevent the growth of undesirable vegetation.

The crystal structure is based, at least in part, on the discovery of a plant nuclear gene that encodes a chloroplast targeted peptide deformylase polypeptide. The gene has sub-

stantial homology to bacterial peptide deformylase. The deduced translation of this nucleic acid sequence reveals the presence of three conserved protein motifs associated with prokaryotic peptide deformylase (see e.g., FIGS. **6**, **7**, and **8**). Nucleic acid and amino acid sequences for plant peptide deformylases are disclosed in U.S. Pat. No. 6,730,634, issued May 4, 2004, and U.S. Patent Application Publication No. 20040088755, the contents of which are incorporated herein by reference.

It is to be understood that the crystalline form of a plant peptide deformylase from which the atomic structure coordinates of the invention can be obtained is not limited to wild-type *Arabidopsis thaliana* peptide deformylase polypeptide, or a truncated form of the polypeptide (see e.g., SEQ ID NO:1) as provided herein. Indeed, the crystals may comprise mutants of wild-type *Arabidopsis thaliana* peptide deformylase or the sequence of amino acids set forth in SEQ ID NO:1. Mutants can be obtained by replacing at least one amino acid residue in the sequence of the wild-type *Arabidopsis thaliana* peptide deformylase or the sequence of amino acids set forth in SEQ ID NO:1 with a different amino acid residue, or by adding or deleting one or more amino acid residues within the wild-type sequence and/or at the N- and/or C-terminus of the wild-type *Arabidopsis thaliana* peptide deformylase or the sequence of amino acids set forth in SEQ ID NO:1. Preferably, such mutants will crystallize under crystallization conditions that are substantially similar to those used to crystallize the wild-type *Arabidopsis thaliana* peptide deformylase or the sequence of amino acids set forth in SEQ ID NO:1.

The types of mutants contemplated by this invention include conservative mutants, non-conservative mutants, deletion mutants, truncated mutants, extended mutants, methionine mutants, selenomethionine mutants, cysteine mutants and selenocysteine mutants. A mutant may have, but need not have, *Arabidopsis thaliana* peptide deformylase activity. Preferably, a mutant displays biological activity that is substantially similar to that of the wild-type polypeptide or that of SEQ ID NO:1.

It will be recognized by one of skill in the art that the types of mutants contemplated herein are not mutually exclusive; that is, for example, a polypeptide having a conservative mutation in one amino acid may in addition have a truncation of residues at the N-terminus.

In addition, conservative or non-conservative amino acid substitutions can be made to amino acids of wild-type *Arabidopsis thaliana* peptide deformylase or the sequence of amino acids set forth in SEQ ID NO:1 that are implicated in the active site of the polypeptide (e.g., amino acid residues Gly121, Gly123, Leu124, Gln128, Glu169, Gly170, Cys171, Leu172, His213, Glu214, His217, and Tyr178 of SEQ ID NO:1). Such conservative or non-conservative substitutions can affect, e.g., the affinity with which wild-type *Arabidopsis thaliana* peptide deformylase or the sequence of amino acids set forth in SEQ ID NO:1 binds to a substrate. In certain embodiments, the conservative or non-conservative amino acid substitutions can increase the affinity with which wild-type *Arabidopsis thaliana* peptide deformylase or the sequence of amino acids set forth in SEQ ID NO:1 binds to a substrate.

Conservative amino acid substitutions are well-known in the art, and include substitutions made on the basis of a similarity in polarity, charge, solubility, hydrophobicity and/or the hydrophilicity of the amino acid residues involved. Typical conservative substitutions are those in which the amino acid is substituted with a different amino acid that is a member of the same class or category, as those classes are defined herein. Thus, typical conservative substitutions include aromatic to aromatic, apolar to apolar, aliphatic to aliphatic, acidic to acidic, basic to basic, polar to polar, etc. Other conservative amino acid substitutions are well known in the art. It will be recognized by those of skill in the art that generally, a total of about 20% or fewer, typically about 10% or fewer, most usually about 5% or fewer, of the amino acids in the wild-type polypeptide sequence can be conservatively substituted with other amino acids without deleteriously affecting the biological activity and/or three-dimensional structure of the molecule, provided that such substitutions do not involve residues that are critical for activity. The following abbreviations are used for amino acids throughout this disclosure: A=Ala=Alanine, T=Thr=Threonine, V=Val=Valine, C=Cys=Cysteine, L=Leu=Leucine, Y=Tyr=Tyrosine, I=Ile=Isoleucine, N=Asn=Asparagine, P=Pro=Proline, Q=Gln=Glutamine, F=Phe=Phenylalanine, D=Asp=Aspartic Acid, W=Trp=Tryptophan, E=Glu=Glutamic Acid, M=Met=Methionine, K=Lys=Lysine, G=Gly=Glycine, R=Arg=Arginine, S=Ser=Serine, H=His=Histidine.

In some embodiments, it may be desirable to make mutations in the active site of a polypeptide, e.g., to reduce or completely eliminate deformylase activity. Mutations that will reduce or completely eliminate the activity of a particular protein will be apparent to those of skill in the art. For example, the amino acids identified in Table 1 could be mutated in order to reduce or eliminate the binding activity of wild-type *Arabidopsis thaliana* peptide deformylase or the sequence of amino acids set forth in SEQ ID NO:1.

The amino acid residue Cys (C) is unusual in that it can form disulfide bridges with other Cys (C) residues or other sulfhydryl-containing amino acids ("cysteine-like amino acids"). The ability of Cys (C) residues and other cysteine-like amino acids to exist in a polypeptide in either the reduced free —SH or oxidized disulfide-bridged form affects whether Cys (C) residues contribute net hydrophobic or hydrophilic character to a polypeptide.

While in most instances the amino acids of wild-type *Arabidopsis thaliana* peptide deformylase or the sequence of amino acids set forth in SEQ ID NO:1 will be substituted with genetically-encoded amino acids, in certain circumstances mutants may include genetically non-encoded amino acids. Alternatively, in instances where the mutant will be prepared in whole or in part by chemical synthesis, virtually any non-encoded amino acids may be used, ranging from D-isomers of the genetically encoded amino acids to non-encoded naturally-occurring natural and synthetic amino acids.

Conservative amino acid substitutions for many of the commonly known non-genetically encoded amino acids are well known in the art. Conservative substitutions for other non-encoded amino acids can be determined based on their physical properties as compared to the properties of the genetically encoded amino acids.

In some instances, it may be particularly advantageous or convenient to substitute, delete from and/or add amino acid residues to wild-type *Arabidopsis thaliana* peptide deformylase or the sequence of amino acids set forth in SEQ ID NO:1 in order to provide convenient cloning sites in cDNA encoding the polypeptide, to aid in purification of the polypeptide, etc. Such substitutions, deletions and/or additions that do not substantially alter the three dimensional structure of the native *Arabidopsis thaliana* peptide deformylase or the sequence of amino acids set forth in SEQ ID NO:1 will be apparent to those having skills in the art. These substitutions, deletions and/or additions include, but are not limited to, His tags, BirA tags, intein-containing self-cleaving tags, maltose binding protein fusions, glutathione S-transferase protein

fusions, antibody fusions, green fluorescent protein fusions, signal peptide fusions, biotin accepting peptide fusions, and the like.

Mutations may also be introduced into a polypeptide sequence where there are residues, e.g., cysteine residues, that interfere with crystallization. Such cysteine residues can be substituted with an appropriate amino acid that does not readily form covalent bonds with other amino acid residues under crystallization conditions; e.g., by substituting the cysteine with Ala, Ser or Gly. Any cysteine located in a non-helical or non-beta-stranded segment, based on secondary structure assignments, are good candidates for replacement.

It should be noted that the mutants contemplated herein need not exhibit deformylase activity. Indeed, amino acid substitutions, additions or deletions that interfere with the binding activity of wild-type *Arabidopsis thaliana* peptide deformylase or the sequence of amino acids set forth in SEQ ID NO:1 are specifically contemplated by the invention. Such crystalline polypeptides, or the atomic structure coordinates obtained therefrom, can be used to provide phase information to aid the determination of the three-dimensional X-ray structures of other related or non-related crystalline polypeptides.

Also contemplated are homologs of the *Arabidopsis thaliana* peptide deformylase. The present invention provides a computer-assisted method for homology modeling an *Arabidopsis thaliana* peptide deformylase homolog including: aligning the amino acid sequence of an *Arabidopsis thaliana* peptide deformylase homolog with the amino acid sequence of *Arabidopsis thaliana* peptide deformylase SEQ ID NO:1 and incorporating the sequence of the *Arabidopsis thaliana* peptide deformylase homolog into a model of *Arabidopsis thaliana* peptide deformylase derived from structure coordinates set forth in Table 1 to yield a preliminary model of the *Arabidopsis thaliana* peptide deformylase homolog; subjecting the preliminary model to energy minimization to yield an energy minimized model; remodeling regions of the energy minimized model where stereochemistry restraints are violated to yield a final model of the *Arabidopsis thaliana* peptide deformylase homolog.

As used herein, the term "homolog" refers to the polypeptide molecule or the nucleic acid molecule which encodes the polypeptide, or a functional domain from said polypeptide from a first source having at least about 30%, 40% or 50% sequence identity, or at least about 60%, 70% or 75% sequence identity, or at least about 80% sequence identity, or more preferably at least about 85% sequence identity, or even more preferably at least about 90% sequence identity, and most preferably at least about 95%, 97% or 99% amino acid or nucleotide sequence identity, with the polypeptide, encoding nucleic acid molecule or any functional domain thereof, from a second source. The second source may be a version of the molecule from the first source that has been genetically altered by any available means to change the primary amino acid or nucleotide sequence or may be from the same or a different species than that of the first source. Homology modeling is further discussed below.

Accordingly, provided herein are crystalline forms of a plant peptide deformylase. Referring to FIG. **1**A, limited trypsinolysis creates a core protein that retained activity and remained soluble in the absence of high salt concentrations. Analysis of wild-type and proteolyzed AtDEF2 on an 8-16% gradient SDS-PAGE. Trypsinolysis produces a truncated DEF2 with a mobility shift corresponding to a 3 kDa loss in molecular mass from AtDEF2, a 24.598 kDa enzyme. The truncated DEF2, which loses its hexahistidyl sequence, was subsequently separated from undigested DEF2 by loading the digested sample onto a HiTrap® affinity column (Amersham Pharmacia) and collecting the flowthrough. Undigested DEF2 remained bound to the column. Referring to FIG. **1**B, the amino acid sequence of the truncated DEF2 polypeptide is provided.

It is understood that the term "crystalline form" includes a polypeptide associated with a plant peptide deformylase can include just the polypeptide, or the polypeptide complexed with a metal, a ligand, or any other chemical entity suitable for crystallization with the polypeptide. An exemplary polypeptide includes *Arabidopsis thaliana* peptide deformylase, or fragments thereof, suitable for crystallization. Such fragments include optionally, the crystal may include a coordinated metal ion selected from the group of consisting of Fe, Zn, Ni, or combinations thereof. Thus, "crystalline form" and "crystal" refer to a composition comprising a polypeptide complex in crystalline form. The term "crystal" includes native crystals, heavy-atom derivative crystals and poly-crystals. "Native Crystal" refers to a crystal wherein the polypeptide complex is substantially pure.

Referring to FIG. **2**A, the crystal structure of DEF2 was determined by molecular replacement and refined to a resolution of 2.7 Å. "Molecular Replacement" refers to the method of calculating initial phases for a new crystal of a polypeptide whose structure coordinates are unknown by orienting and positioning a polypeptide whose structure coordinates are known within the unit cell of the new crystal so as to best account for the observed diffraction pattern of the new crystal. Phases are then calculated from the oriented and positioned polypeptide and combined with observed amplitudes to provide an approximate Fourier synthesis of the structure of the polypeptides comprising the new crystal (Jones et al., 1991, Acta Crystallogr. 47:753-70; Brunger et al., 1998, Acta Crystallogr. D. Biol. Crystallogr. 54:905-21).

The overall fold of the enzyme resembles the $\alpha+\beta$ conformation of known bacterial peptide deformylases, with an r.m.s deviation of about 1.04 Å on main chain atoms relative to the *E. coli* enzyme. The largest differences occur in the orientation of the C-terminal helix (helix 3) and the conformation of the loop between β strands 2 and 3, which form part of the five-stranded central sheet. Motif I, II and III are colored blue, green and pink, respectively. The active site metal, modeled as zinc due to the conditions of crystallization, is a space-filled sphere in the middle of the structure. Referring to FIG. **2**B, a slab view of the ribbon representation of trypsinolyzed AtDEF2 highlighting the active-site-metal binding ligands (1 Cys and 2 His) from motifs II and III, respectively (EGCLS (SEQ ID NO: 2) and QHEXXH (SEQ ID NO: 3) is provided. As used herein, the term "active site" refers to regions on a protein or a structural motif of a protein that are directly involved in the function or activity of the peptide deformylase.

As used herein, the terms "binding site" or "binding pocket" refer to a region of a polypeptide or a molecular complex comprising the polypeptide that, as a result of the primary amino acid sequence of the polypeptide and/or its three-dimensional shape, favorably associates with another chemical entity or compound including ligands or inhibitors.

The crystalline form can include the tetragonal space group symmetry $P4_12_12$ and includes a unit cell having dimensions a, b, and c; wherein a is about 40 Å to about 60 Å, b is about 40 Å to about 60 Å, and c is about 120 Å to about 160 Å; and wherein alpha=beta=gamma=90 degree. In some aspects, a is about 49 Å to about 52 Å, b is about 49 Å to about 52 Å, and c is about 143 Å to about 147 Å.

"Unit Cell" refers to the smallest and simplest volume element (i.e., parallel piped-shaped block) of a crystal that is completely representative of the unit or pattern of the crystal,

such that the entire crystal can be generated by translation of the unit cell. The dimensions of the unit cell are defined by six numbers: dimensions a, b and c and angles α, β and γ (Blundel et al., 1976, Protein Crystallography, Academic Press). A crystal is an efficiently packed array of many unit cells. "Tetragonal Unit Cell" refers to a unit cell in which a≠b≠c; and α=β=γ90°. "Crystal lattice" refers to the array of points defined by the vertices of packed unit cells. "Space group" refers to the set of symmetry operations of a unit cell. In a space group designation (e.g., C_2) the capital letter indicates the lattice type and the other symbols represent symmetry operations that can be carried out on the unit cell without changing its appearance. "Asymmetric Unit" refers to the largest aggregate of molecules in the unit cell that possesses no symmetry elements that are part of the space group symmetry, but that can be juxtaposed on other identical entities by symmetry operations.

When a crystal is placed in an X-ray beam, the incident X-rays interact with the electron cloud of the molecules that make up the crystal, resulting in X-ray scatter. The combination of X-ray scatter with the lattice of the crystal gives rise to nonuniformity of the scatter; areas of high intensity are called diffracted X-rays. The angle at which diffracted beams emerge from the crystal can be computed by treating diffraction as if it were reflection from sets of equivalent, parallel planes of atoms in a crystal (Bragg's Law). The most obvious sets of planes in a crystal lattice are those that are parallel to the faces of the unit cell. These and other sets of planes can be drawn through the lattice points. Each set of planes is identified by three indices, hkl. The h index gives the number of parts into which the a edge of the unit cell is cut, the k index gives the number of parts into which the b edge of the unit cell is cut, and the l index gives the number of parts into which the c edge of the unit cell is cut by the set of hkl planes. Thus, for example, the 235 planes cut the a edge of each unit cell into halves, the b edge of each unit cell into thirds, and the c edge of each unit cell into fifths. Planes that are parallel to the bc face of the unit cell are the 100 planes; planes that are parallel to the ac face of the unit cell are the 010 planes; and planes that are parallel to the ab face of the unit cell are the 001 planes.

When a detector is placed in the path of the diffracted X-rays, in effect cutting into the sphere of diffraction, a series of spots, or reflections, are recorded to produce a "still" diffraction pattern. Each reflection is the result of X-rays reflecting off one set of parallel planes, and is characterized by an intensity, which is related to the distribution of molecules in the unit cell, and hkl indices, which correspond to the parallel planes from which the beam producing that spot was reflected. If the crystal is rotated about an axis perpendicular to the X-ray beam, a large number of reflections is recorded on the detector, resulting in a diffraction pattern.

The unit cell dimensions and space group of a crystal can be determined from its diffraction pattern. First, the spacing of reflections is inversely proportional to the lengths of the edges of the unit cell. Therefore, if a diffraction pattern is recorded when the X-ray beam is perpendicular to a face of the unit cell, two of the unit cell dimensions may be deduced from the spacing of the reflections in the x and y directions of the detector, the crystal-to-detector distance, and the wavelength of the X-rays. Those of skill in the art will appreciate that, in order to obtain all three unit cell dimensions, the crystal can be rotated such that the X-ray beam is perpendicular to another face of the unit cell. Second, the angles of a unit cell can be determined by the angles between lines of spots on the diffraction pattern. Third, the absence of certain reflections and the repetitive nature of the diffraction pattern, which may be evident by visual inspection, indicate the internal symmetry, or space group, of the crystal. Therefore, a crystal may be characterized by its unit cell and space group, as well as by its diffraction pattern.

Once the dimensions of the unit cell are determined, the likely number of polypeptides in the asymmetric unit can be deduced from the size of the polypeptide, the density of the average protein, and the typical solvent content of a protein crystal, which is usually in the range of 30-70% of the unit cell volume (Matthews, 1968, J. Mol. Biol. 33:491-497).

The diffraction pattern of a crystal is related to the three-dimensional shape of the molecules that constitute the crystal by a Fourier transform. It has been established that diffraction patterns of a crystal can result from X-ray diffraction as well as Laue, electron or neutron diffraction. X-ray diffraction has been the most widely used methods for determining macromolecular structures. It is therefore used by way of illustration to discuss the processes of diffraction data collection and subsequent structure determination. The scope of the present invention is, however, by no means limited only to X-ray diffraction analyses of crystalline forms of polypeptides. After enough diffraction data are collected for a crystal, the process of determining the solution is in essence a re-focusing of the diffracted X-rays to produce a three-dimensional image of the molecule in the crystal. Since lenses capable of focusing X-ray radiation do not yet exist, the structure determination can be done via mathematical operations that simulate the re-focusing process.

"X-ray Diffraction" refers to a type of wave interference created when high energy X-ray radiation interacts with any obstruction in its traveling path. The obstruction is often in the form of a crystal of protein, nucleic acid, or inorganic compound. The electrons that surround the atoms in the crystal, rather than the atomic nuclei, are the entities which physically interact with the incoming X-ray photons. When X-ray radiation hits the atoms in a crystal, they make the electronic clouds of the atoms move as does any electromagnetic wave. The re-emitted X-ray radiation gives rise to constructive or destructive interferences. This phenomenon is called X-ray diffraction. In X-ray crystallography, the X-ray diffraction patterns of closely spaced lattices of atoms in the crystal are recorded and then analyzed to reveal the structural nature of the crystal. For example, the spacing between the crystal lattices can be determined using Bragg's law. X-ray diffraction is widely used in chemistry and biochemistry to determine the structures of an immense variety of molecules, including inorganic compounds, DNA and proteins. X-ray diffraction is commonly carried out using single crystals of a material, but if these are not available, microcrystalline powdered samples may also be used, although this requires different equipment. A detailed discussion on X-ray diffraction may be found in Chapter 4 in "Principles of Protein X-ray Crystallography" by Drenth, second edition 1999, Springer-Verlag Inc.

"Bragg's Law" refers to the principle that defines the diffraction conditions that give rise to constructive interferences. When the phase shift of the incident radiation is proportional to 2π, the condition can be expressed as: $n\lambda=2d\sin(\theta)$, where n is an integer; λ is the wavelength of the X-ray radiation, or radiations caused by moving electrons, protons and neutrons; d is the spacing between the planes in the atomic lattice, and θ is the angle between the incident ray and the scattering planes.

"Crystallization" in the context of protein X-ray crystallography refers to the processes during which soluble proteins are transformed into their crystalline forms. Crystals of a protein can be grown out of its solution state under experimental conditions that allow controlled phase transition. Such

experimental conditions include a mixture of multiple solutions that often contain an aqueous solution of the target protein, a solution of one or a mixture of precipitants, and one or more compounds that contribute to the overall pH or ionic strength of the final mixture.

Provided herein are crystalline forms of a plant peptide deformylase polyepeptide, or a deformylase complexed with other molecules or chemical entities. Analysis of such crystalline forms of a polypeptide provides data in the form of structure coordinates. Exemplary structure coordinates for *Arabidopsis thaliana* peptide deformylase polypeptide are provided in Table 1. As used herein, the term "atomic coordinates" or "structure coordinates" refers to mathematical coordinates that describe the positions of atoms in crystals of a plant peptide deformylase in Protein Data Bank (PDB) format, including X, Y, Z and B, for each atom. The diffraction data obtained from the crystals are used to calculate an electron density map of the repeating unit of the crystal. The electron density maps may be used to establish the positions (i.e., coordinates X, Y and Z) of the individual atoms within the crystal. Those of skill in the art understand that a set of structure coordinates determined by X-ray crystallography is not without standard error. For the purpose of this invention, any set of structure coordinates for a plant peptide deformylse from any source having a root mean square deviation (r.m.s.d) of non-hydrogen atoms of less than about 1.5 Å when superimposed on the non-hydrogen atom positions of the corresponding atomic coordinates of Table 1 are considered substantially identical or homologous. Moreover, any set of structure coordinates for plant peptide deformylse from any source having a root mean square deviation of non-hydrogen atoms of less than about 0.75 Å when superimposed on the non-hydrogen atom positions of the corresponding atomic coordinates of Table 1 are considered substantially identical or homologous.

The term "root mean square deviation" means the square root of the arithmetic mean of the squares of the deviations. It is a way to express the deviation or variation from a trend or object. For purposes of this invention, the "root mean square deviation" defines the variation in the backbone of a protein from the backbone of a *Arabidopsis thaliana* peptide deformylase polypeptide or an active site portion thereof, as defined by the structure coordinates described herein. "Having substantially the same three-dimensional structure" refers to a polypeptide that is characterized by a set of atomic structure coordinates that have a root mean square deviation (r.m.s.d.) of less than or equal to about 1.5 Å when superimposed onto the atomic structure coordinates of Table 1 when at least about 50% to 100% of the C α atoms of the coordinates are included in the superposition.

Slight variations in structure coordinates can be generated by mathematically manipulating the plant peptide deformylase structure coordinates provided herein. For example, the structure coordinates set forth in Table 1 could be manipulated by crystallographic permutations of the structure coordinates, fractionalization of the structure coordinates, integer additions or subtractions to sets of the structure coordinates, inversion of the structure coordinates or any combination of the above. Alternatively, modifications in the crystal structure due to mutations, additions, substitutions, and/or deletions of amino acids, or other changes in any of the components that make up the crystal, could also yield variations in structure coordinates. Such slight variations in the individual coordinates will have little effect on overall shape. If such variations are within an acceptable standard error as compared to the original coordinates, the resulting three-dimensional shape is considered to be structurally equivalent. Thus, for the purpose of the structures provided herein, any active site, binding site or binding pocket defined by a set of structure coordinates for a polypeptide or for a homolog of a polypeptide from any source having a root mean square deviation of non-hydrogen atoms of less than about 1.5 Å when superimposed on the non-hydrogen atom positions of the corresponding atomic coordinates of Table 1, are considered substantially identical or homologous.

Active sites are of significant utility in the identification of compounds that specifically interact with, and modulate the activity of, a particular polypeptide. The association of natural ligands or substrates with the active sites of their corresponding receptors or enzymes is the basis of many biological mechanisms of action. Similarly, many compounds exert their biological effects through association with the active sites of receptors and enzymes. Such associations may occur with all or any parts of the active site. An understanding of such associations helps lead to the design of compounds that modulate the activity of their target. Therefore, this information is valuable in designing potential modifiers of plant peptide deformylase activity, as discussed in more detail below. For example, the structure of a substrate utilized by a particular deformylase can be used to design compounds that bind to an active site of a peptide deformylase. Referring to FIG. **3**, substrate specificities for plant peptide deformylase AtDEF1 and AtDEF2 are shown. AtDEF1 and 2 activities are influenced by peptide substrate sequence. Peptide mimics of the N-termini of chloroplast-translated proteins, ribosomal protein S18 (f-MDKS), Rubisco LS (f-MSPQ), D1(f-MTAI), PSI-I (f-MTTF), PSII-I (f-MLTL), and ATPase subunit III (f-MNPL) were tested as substrates. In addition to a control substrate for the assay (f-MAS), the formate-dehydrogenase-linked assay was performed with 4 mM substrate and either 1.2 mg AtDEF1 or 0.2 mg AtDEF2. The numbers above the grouped bars represent the ratio of AtDEF2 to AtDEF1 activities. (Dirk et al., Arch Biochem Biophys 406:135-141).

The term "active site (or binding pocket)," as used herein, refers to a region of a molecule or molecular complex, that, as a result of its shape, favorably associates with another chemical entity or compound. Thus, an active site may include or consist of features such as interfaces between domains. Chemical entities or compounds that may associate with an active site include, but are not limited to, compounds, ligands, cofactors, substrates, inhibitors, agonists, antagonists, etc.

An exemplary active site for a plant peptide deformylase is provided by amino acid residues Gly121, Gly123, Leu124, Gln128, Glu169, Gly170, Cys171, Leu172, His213, Glu214, His217, and Tyr178 of SEQ ID NO:1 and as shown in Table 1. Referring to FIG. **5**, a model of the D1 N-terminus in AtDEF2's active site is provided. Potential H-bond highlighted between the Thr in the P_2 position of the polypeptide substrate and a conserved AtDEF2 Tyr178 just carboxy terminal to motif II. The model was generated by taking a snapshot from a molecular dynamics simulation using AMBER. The total length of the simulation was 1 ns, and this snapshot is at 126 ps.

In general, the exemplary active site is defined by a set of points having a root mean square deviation of less than about 0.35 Å from points representing the backbone atoms of amino acids as represented by structure coordinates listed in Table 1. As noted above, the crystalline form optionally includes additional molecules such as a coordinated metal ion selected from the group of metals consisting of Fe, Zn, Ni and combinations thereof. In some aspects, the metal ion is coordinated by the amino acids Cys171, His213, and His217.

Also provided are scalable three-dimensional configuration of points, at least a portion of said points derived from

structure coordinates of at least a portion of an *Arabidopsis thaliana* peptide deformylase molecule or molecular complex listed in Table 1 and having a root mean square deviation of about 1.04 Å from said structure coordinates. Preferably, at least a portion of the points are derived from the *Arabidopsis thaliana* peptide deformylase structure coordinates derived from structure coordinates representing the locations of at least the backbone atoms of a plurality of the amino acids defining at least one *Arabidopsis thaliana* peptide deformylase or *Arabidopsis thaliana* peptide deformylase-like active site, the active site including amino acids Gly121, Gly123, Leu124, Gln128, Glu169, Gly170, Cys171, Leu172, His213, Glu214, His217, and Tyr178.

The structure coordinates generated for a plant peptide deformylase, or an active site thereof, as shown in Table 1 define a unique configuration of points in space. Those of skill in the art understand that a set of structure coordinates for a polypeptide, or a polypeptide complexed with a chemical entity, or a portion thereof, define a relative set of points that, in turn, define a configuration in three dimensions. A similar or identical configuration can be defined by an entirely different set of coordinates, provided the distances and angles between coordinates remain essentially the same. Accordingly, the coordinates provided in Table 1 provide a "scalable" configuration of points that can be modified by increasing or decreasing the distances between coordinates by a scalar factor while keeping the angles essentially the same.

The atomic structure coordinates provided herein can be used in molecular modeling and design, as described more fully below. The present invention encompasses the structure coordinates and other information, e.g., amino acid sequence, connectivity tables, vector-based representations, temperature factors, etc., used to generate the three-dimensional structure of the plant peptide deformylase polypeptide for use in the software programs described below and other software programs.

The invention encompasses machine-readable media embedded with the three-dimensional structure of the model described herein, or with portions thereof. As used herein, "machine-readable medium" refers to any medium that can be read and accessed directly by a computer or scanner. Such media include, but are not limited to: magnetic storage media, such as floppy discs, hard disc storage medium and magnetic tape; optical storage media such as optical discs or CD-ROM; electrical storage media such as RAM or ROM; and hybrids of these categories such as magnetic/optical storage media. Such media further include paper on which is recorded a representation of the atomic structure coordinates, e.g., Cartesian coordinates, that can be read by a scanning device and converted into a three-dimensional structure with an OCR.

A variety of data storage structures are available to a skilled artisan for creating a computer readable medium having recorded thereon the atomic structure coordinates of the invention or portions thereof and/or X-ray diffraction data. The choice of the data storage structure will generally be based on the means chosen to access the stored information. In addition, a variety of data processor programs and formats can be used to store the sequence and X-ray data information on a computer readable medium. Such formats include, but are not limited to, Protein Data Bank ("PDB") format (Research Collaboratory for Structural Bioinformatics; Cambridge Crystallographic Data Centre format; Structure-data ("SD") file format (MDL Information Systems, Inc.; Dalby et al., 1992, J. Chem. Inf. Comp. Sci. 32:244-255), and line-notation, e.g., as used in SMILES (Weininger, 1988, J. Chem. Inf. Comp. Sci. 28:31-36). Methods of converting between various formats read by different computer software will be readily apparent to those of skill in the art, e.g., BABEL (v. 1.06, Walters & Stahl, .COPYRGT.1992, 1993, 1994). All format representations of the polypeptide coordinates described herein, or portions thereof, are contemplated by the present invention. By providing computer readable medium having stored thereon the atomic coordinates of the invention, one of skill in the art can routinely access the atomic coordinates of the invention, or portions thereof, and related information for use in modeling and design programs, described in detail below.

While Cartesian coordinates are important and convenient representations of the three-dimensional structure of a polypeptide, those of skill in the art will readily recognize that other representations of the structure are also useful. Therefore, the three-dimensional structure of a polypeptide, as discussed herein, includes not only the Cartesian coordinate representation, but also all alternative representations of the three-dimensional distribution of atoms. For example, atomic coordinates may be represented as a Z-matrix, wherein a first atom of the protein is chosen, a second atom is placed at a defined distance from the first atom, a third atom is placed at a defined distance from the second atom so that it makes a defined angle with the first atom. Each subsequent atom is placed at a defined distance from a previously placed atom with a specified angle with respect to the third atom, and at a specified torsion angle with respect to a fourth atom. Atomic coordinates may also be represented as a Patterson function, wherein all interatomic vectors are drawn and are then placed with their tails at the origin. This representation is particularly useful for locating heavy atoms in a unit cell. In addition, atomic coordinates may be represented as a series of vectors having magnitude and direction and drawn from a chosen origin to each atom in the polypeptide structure. Furthermore, the positions of atoms in a three-dimensional structure may be represented as fractions of the unit cell (fractional coordinates), or in spherical polar coordinates.

Additional information, such as thermal parameters, which measure the motion of each atom in the structure, chain identifiers, which identify the particular chain of a multi-chain protein in which an atom is located, and connectivity information, which indicates to which atoms a particular atom is bonded, is also useful for representing a three-dimensional molecular structure.

Accordingly, also provided herein is a machine-readable data storage medium including a data storage material encoded with machine readable data which, when using a machine programmed with instructions for using the data, displays a graphical three-dimensional representation of at least one molecule or molecular complex selected from the group consisting of (i) a molecule or molecular complex including at least a portion of an *Arabidopsis thaliana* peptide deformylase or an *Arabidopsis thaliana* peptide deformylase-like active site including amino acids Gly121, Gly123, Leu124, Gln128, Glu169, Gly170, Cys171, Leu172, His213, Glu214, His217, and Tyr178 the active site being defined by a set of points having a root mean square deviation of less than about 1.5 Å from points representing the backbone atoms of the amino acids as represented by structure coordinates listed in Table 1.

Structure information, typically in the form of the atomic structure coordinates, can be used in a variety of computational or computer-based methods to, for example, design, screen for and/or identify compounds that bind the crystallized polypeptide or a portion or fragment thereof, or to intelligently design mutants that have altered biological properties, and the like. Three-dimensional modeling may be performed using the experimentally determined coordinates

derived from X-ray diffraction patterns, such as those in Table 1, for example, wherein such modeling includes, but is not limited to, drawing pictures of the actual structures, building physical models of the actual structures, and determining the structures of related subunits and /ligand and subunit/ligand complexes using the coordinates. Such molecular modeling can utilize known X-ray diffraction molecular modeling algorithms or molecular modeling software to generate atomic coordinates corresponding to the three-dimensional structure of a plant peptide deformylase.

As described above, molecular modeling involves the use of computational methods, preferably computer assisted methods, to build realistic models of molecules that are identifiably related in sequence to the known crystal structure. It also involves modeling new small molecule inhibitors bound to a plant peptide deformylase starting with the structures of deformylase alone or complexed with known ligands or inhibitors. The methods utilized in ligand modeling range from molecular graphics (i.e., 3D representations) to computational chemistry (i.e., calculations of the physical and chemical properties) to make predictions about the binding of ligands or activities of ligands; to design new ligands; and to predict novel molecules, including ligands such as compounds that inhibit the activity of a plant deformylase. Such compounds may be useful as herbicides, for example.

One approach to rational design of a compound is to search for known molecular structures that might bind to an active site. Using molecular modeling, rational design programs can look at a range of different molecular structures of compounds that may fit into the active site of an enzyme or protein, and by moving them in a three-dimensional environment it can be decided which structures actually fit the site well. An alternate but related rational compound design approach starts with the known structure of a complex with a small molecule ligand and models modifications of that small molecule in an effort to make additional favorable interactions with peptide deformylase polypeptides, and/or the active site of such polypeptides.

The present invention includes the use of molecular and computer modeling techniques to design and select ligands, such as small molecule agonists or antagonists or other compounds that interact with peptide deformylase polypeptides. Such compounds include, but are not limited to, actinonin and derivatives thereof.

This invention also includes the design of compounds that act as uncompetitive inhibitors of at least one function of peptide deformylase polypeptides. These inhibitors may bind to all, or a portion of, the active sites or other regions of the polypeptide already bound to a ligand and may be more potent and less non-specific than competitive inhibitors that compete for active sites. Similarly, non-competitive inhibitors that bind to and inhibit at least one function of peptide deformylase polypeptides whether or not it is bound to another chemical entity, such as a natural ligand, for example, may be designed using the atomic coordinates of the chimeras or complexes comprising the chimeras of this invention.

The atomic coordinates of the present invention also provide the needed information to probe a crystal of a peptide deformylase polypeptide with molecules composed of a variety of different chemical features to determine optimal sites for interaction between candidate inhibitors and/or activators. For example, high resolution X-ray diffraction data collected from crystals saturated with solvent allows the determination of where each type of solvent molecule sticks. Small molecules that bind to those sites can then be designed and synthesized and tested for their inhibitory activity (Travis, J., Science 262:1374 (1993)).

The present invention also includes methods for computationally screening small molecule databases and libraries for chemical entities, agents, ligands, or compounds that can bind in whole, or in part, to peptide deformylase polypeptides. In this screening, the quality of fit of such entities or compounds to the binding site or sites may be judged either by shape complementarity or by estimated interaction energy (Meng, E. C. et al., J. Comp. Chem. 13:505-524 (1992)).

The design of compounds that bind to, promote or inhibit the functional activity of peptide deformylase polypeptides according to this invention generally involves consideration of two factors. First, the compound must be capable of physically and structurally associating with the peptide deformylase polypeptide. Non-covalent molecular interactions important in the association of the peptide deformylase polypeptide with the compound include hydrogen bonding, van der Waals and hydrophobic interactions. Second, the compound must be able to assume a conformation that allows it to associate with a peptide deformylase polypeptide. Although certain portions of the compound may not directly participate in the association with peptide deformylase polypeptide, those portions may still influence the overall conformation of the molecule. This, in turn, may have a significant impact on binding affinities and potency. Such conformational requirements include the overall three-dimensional structure and orientation of the chemical entity or compound in relation to all or a portion of the active site or other region of a peptide deformylase polypeptide, or the spacing between functional groups of a compound comprising several chemical entities that directly interact with a peptide deformylase polypeptide.

The potential, predicted, inhibitory agonist, antagonist or binding effect of a ligand or other compound on a peptide deformylase polypeptide may be analyzed prior to its actual synthesis and testing by the use of computer modeling techniques. If the theoretical structure of the given compound suggests insufficient interaction and association between it and the peptide deformylase polypeptide, synthesis and testing of the compound may be obviated. However, if computer modeling indicates a strong interaction, the molecule may then be synthesized and tested for its ability to interact with a peptide deformylase polypeptide. In this manner, synthesis of inoperative compounds may be avoided. In some cases, inactive compounds are synthesized predicted on modeling and then tested to develop a SAR (structure-activity relationship) for compounds interacting with a specific region of a peptide deformylase polypeptide.

One skilled in the art may use one of several methods to screen chemical entities fragments, compounds, or agents for their ability to associate with a peptide deformylase polypeptide and more particularly with the individual binding pockets or active sites of the peptide deformylase polypeptide. This process may begin by visual inspection of, for example, the active site based on the atomic coordinates of the polypeptide or the polypeptide complexed with a ligand. Selected chemical entities, compounds, or agents may then be positioned in a variety of orientations, or docked within an individual binding pocket of the peptide deformylase polypeptide. Docking may be accomplished using software-such as Quanta and Sybyl, followed by energy minimization and molecular dynamics with standard molecular mechanics forcefields, such as CHARMM and AMBER.

Specialized computer programs may also assist in the process of selecting chemical entities. These include but are not limited to: GRID (Goodford, P. J., "A Computational Procedure for Determining Energetically Favorable Binding Sites on Biologically Important Macromolecules," J. Med. Chem.

28:849-857 (1985), available from Oxford University, Oxford, UK); MCSS (Miranker, A. and M. Karplus, "Functionality Maps of Binding Sites: A Multiple Copy Simultaneous Search Method." Proteins: Structure, Function and Genetics 11: 29-34 (1991), available from Molecular Simulations, Burlington, Mass.); AUTODOCK (Goodsell, D. S. and A. J. Olsen, "Automated Docking of Substrates to Proteins by Simulated Annealing" Proteins: Structure. Function, and Genetics 8:195-202 (1990), available from Scripps Research Institute, La Jolla, Calif.); DOCK (Kuntz, I. D. et al., "A Geometric Approach to Macromolecule-Ligand Interactions," J. Mol. Biol. 161:269-288 (1982), available from University of California, San Francisco, Calif.); Gold (Jones, G. et al., "Development and validation of a genetic algorithm for flexible docking." J. Mol. Biol. 267: 727-748 (1997)); Glide (Halgren, T. A. et al., "Glide: a new approach for rapid, accurate docking and scoring. 2. Enrichment factors in database screening." J Med Chem, 47:1750-1759 (2004), Friesner, R. A. et al., "Glide: a new approach for rapid, accurate docking and scoring. 1. Method and assessment of docking accuracy." J Med Chem, 47:1739-1749 (2004)); FlexX (Rarey, M. et al., "A fast flexible docking method using an incremental construction algorithm." J. Mol. Biol. 261: 470-489 (1996)); and ICM (Abagyan, R. A. and Totrov, M. M., J. Mol. Biol. 235: 983-1002 (1994)).

The use of software such as GRID, a program that determines probable interaction sites between probes with various functional group characteristics and the macromolecular surface, is used to analyze the surface sites to determine structures of similar inhibiting proteins or compounds. The GRID calculations, with suitable inhibiting groups on molecules (e.g., protonated primary amines) as the probe, are used to identify potential hotspots around accessible positions at suitable energy contour levels. The program DOCK may be used to analyze an active site or ligand binding site and suggest ligands with complementary steric properties. See also, See, also, Kellenberger, P. N et al., "Recovering the true targets of specific ligands by virtual screening of the protein data bank," Proteins 54(4):671-80 (2004); Oldfield, T., "Applications for macromolecular map interpretation: X-AUTOFIT, X-POWERFIT, X-BUILD, X-LIGAND, and X-SOLVATE," Methods Enzymol. 374:271-300 (2003); Richardson, J. S. et al., "New tools and data for improving structures, using all-atom contacts," Methods Enzymol. 374: 385-412 (2003); Terwilliger, T. C., "Improving macromolecular atomic models at moderate resolution by automated iterative model building, statistical density modification and refinement," Acta Crystallogr D Biol Crystallogr. 59(Pt 7): 1174-82 (2003); Toerger, T. C. and Sacchettini, J. C., "TEXTAL system: artificial intelligence techniques for automated protein model building," Methods Enzymol. 374:244-70 (2003); von Grotthuss, M. et al., "Predicting protein structures accurately," Science 304 (5677):1597-9 (2004); Rajakiannan, V. et al., "The use of ACORN in solving a 39.5 kDa macromolecule with 1.9 Å resolution laboratory source data," J Synchrotron Radiat. 11(Pt 4):358-62 (2004); Claude, J. B. et al., "CaspR: a web server for automated molecular replacement using homology modeling," Nucleic Acids Res. 32(Web Server issue): W606-9 (2004); Suhre, K. and Sanejouand, Y. H., "ElNemo: a normal mode web server for protein movement analysis and the generation of templates for molecular replacement," Nucleic Acids Res. 32(Web Server issue):W610-4 (2004).

Once suitable chemical entities, compounds, or agents have been selected, they can be assembled into a single ligand or compound or inhibitor or activator. Assembly may proceed by visual inspection of the relationship of the fragments to each other on the three-dimensional image. This may be followed by manual model building using software such as Quanta or Sybyl.

Useful programs to aid in connecting the individual chemical entities, compounds, or agents include but are not limited to: CAVEAT (Bartlett, P. A. et al., "CAVEAT: A Program to Facilitate the Structure-Derived Design of Biologically Active Molecules." In Molecular Recognition in Chemical and Biological, Problems, Special Pub., Royal Chem. Soc., 78, pp. 82-196 (1989)); 3D Database systems such as MACCS-3D (MDL Information Systems, San Leandro, C A and Martin, Y. C., "3D Database Searching in Drug Design," J. Med. Chem. 35: 2145-2154 (1992); and HOOK (available from Molecular Simulations, Burlington, Mass.).

Several methodologies for searching three-dimensional databases to test hypotheses and select compounds for screening are available. These include the program CAVEAT (Bacon et al., J. Mol. Biol. 225:849-858 (1992)). For instance, CAVEAT uses databases of cyclic compounds which can act as "spacers" to connect any number of chemical fragments already positioned in the active site. This allows one skilled in the art to quickly generate hundreds of possible ways to connect the fragments already known or suspected to be necessary for tight binding.

Instead of proceeding to build an inhibitor activator, agonist or antagonist of a peptide deformylase polypeptide in a step-wise fashion one chemical entity at a time as described above, such compounds may be designed as a whole or "de novo" using either an empty active site or optionally including some portion(s) of a known molecules. These methods include: LUDI (Bohm, H.-J., "The Computer Program LUDI: A New Method for the De Novo Design of Enzyme Inhibitors", J. Comp. Aid. Molec. Design, 6, pp. 61-78 (1992), available from Biosym Technologies, San Diego, Calif.); LEGEND (Nishibata, Y. and A. Itai, Tetrahedron 47:8985 (1991), available from Molecular Simulations, Burlington, Mass.); and LeapFrog (available from Tripos Associates, St. Louis, Mo.).

For instance, the program LUDI can determine a list of interaction sites into which to place both hydrogen bonding and hydrophobic fragments. LUDI then uses a library of linkers to connect up to four different interaction sites into fragments. Then smaller "bridging" groups such as —CH2— and —COO— are used to connect these fragments.

Once a compound has been designed or selected by the above methods, the affinity with which that compound may bind or associate with a peptide deformylase polypeptide may be tested and optimized by computational evaluation and/or by testing biological activity after synthesizing the compound. Inhibitors or compounds may interact with the deformylase in more than one conformation that is similar in overall binding energy. In those cases, the deformation energy of binding is taken to be the difference between the energy of the free compound and the average energy of the conformations observed when the compound binds to a peptide deformylase polypeptide.

A compound designed or selected as binding or associating with a plant peptide deformylase may be further computationally optimized so that in its bound state it would preferably lack repulsive electrostatic interaction with the protein. Such non-complementary (e.g., electrostatic) interactions include repulsive charge-charge, dipole-dipole and charge-dipole interactions. Specifically, the sum of all electrostatic interactions between the inhibitor and the chimera when the inhibitor is bound, preferably make a neutral or favorable

contribution to the enthalpy of binding. Weak binding compounds will also be designed by these methods so as to determine SAR.

Specific computer software is available in the art to evaluate compound deformation energy and electrostatic interaction. Examples of programs designed for such uses include: Gaussian 92, revision C (M. J. Frisch, Gaussian, Inc., Pittsburgh, Pa., COPYRGT 1992); AMBER, version 4.0 (P. A. Kollman, University of California at San Francisco, COPYRGT 1994); QUANTA/CHARMM (Molecular Simulations, Inc., Burlington, Mass. COPYRGT 1994); Insight II/Discover (Biosysm Technologies Inc., San Diego, Calif. COPYRGT. 1994); and Delphi (A. Nicholls and B. Honig "A rapid finite difference algorithm, utilizing successive over-relaxation to solve the Poisson-Boltzman equation" J. Comp. Chem. 12: 435-445 (1991), M. K. Gilson and B. Honig. "Calculation of the total electrostatic energy of a macromolecular system: Solvation energies, binding energies and conformation analysis" Proteins 4: 7-18 (1988), M. K. Gilson et al., "Calculating the electrostatic potential of molecules in solution: Method and error assessment" J Comp. Chem 9: 327-335 (1987)). Other hardware systems and software packages will be known to those skilled in the art.

Once a compound that associates with the peptide deformylase polypeptide has been optimally selected or designed, as described above, substitutions may then be made in some of its atoms or side groups in order to improve or modify its binding properties. Generally, initial substitutions are conservative, i.e., the replacement group will have approximately the same size, shape, hydrophobicity and charge as the original group. It should, of course, be understood that components known in the art to alter conformation may be avoided. Such substituted chemical compounds may then be analyzed for efficiency of fit to a peptide deformylase polypeptide by the same computer methods described in detail, above.

Accordingly, as described above the present invention provides a computer-assisted method for obtaining structural information about a molecule or a molecular complex of unknown structure including: crystallizing the molecule or molecular complex; generating an x-ray diffraction pattern from the crystallized molecule or molecular complex; applying at least a portion of the structure coordinates set forth in Table 1 to the x-ray diffraction pattern to generate a three-dimensional electron density map of at least a portion of the molecule or molecular complex whose structure is unknown.

In another aspect, the present invention provides a computer-assisted method for homology modeling an *Arabidopsis thaliana* peptide deformylase homolog including: aligning the amino acid sequence of an *Arabidopsis thaliana* peptide deformylase homolog with the amino acid sequence of *Arabidopsis thaliana* peptide deformylase SEQ ID NO:1 and incorporating the sequence of the *Arabidopsis thaliana* peptide deformylase homolog into a model of *Arabidopsis thaliana* peptide deformylase derived from structure coordinates set forth in Table 1 to yield a preliminary model of the *Arabidopsis thaliana* peptide deformylase homolog; subjecting the preliminary model to energy minimization to yield an energy minimized model; remodeling regions of the energy minimized model where stereochemistry restraints are violated to yield a final model of the *Arabidopsis thaliana* peptide deformylase homolog.

Domains of peptide deformylase polypeptides retain sequence and structural conservation. Accordingly, these conserved regions can be used to model deformylase homologs. Referring to FIG. **4**, conservation of the three motifs in AtDEF1 and 2 and bacterial DEFs are shown. AtDEF1- and 2-like sequences were identified with a tblastn (BLAST) search of plant EST databases, aligned around the indicated motifs, and submitted for analysis by WebLogo. For the bacterial DEF alignment, the first 100 bacterial sequences from a blastp using the SwissProt database with Q2VP16 (*E. coli*) as query were used for the similarity analyses. Sequence conservation is represented by WebLogo images by the overall height of the stack and relative frequency of the amino acid at the position within the sequence is represented by the height of its symbol (Crooks et al., Genome Res. 14:1188-1190; Schneider and Stephens, Nucl. Acids Res. 18:6097-6100).

Due to the nature of the sequences used for the plant DEFs, different numbers of sequences were used for each motif in the generation of FIG. **4**. For motif I, there were 34, 42 and 100 sequences for 1, 2 and bacterial DEFs, respectively; whereas, there were 36, 40, and 100 for motif II and 40, 32, and 100 for motif II.

In addition, referring to FIGS. **6**, **7** and **8**, a phylogenetic analyses of the distribution of amino acid substitutions throughout the available collection of peptide deformylase sequences from plants compared with bacterial deformylase is provided. The results are presented as a comparison of both the number and percentage of substitutions found at any location within the sequence of peptide deformylase 1 & 2 from plants as well as *E. coli*. There are a number of residue changes which suggest selection pressure in the evolution of peptide deformylase specifically adapted to plants. Thus, these changes are indicative of specific sites where residue changes are likely to affect peptide deformylase activity and/or specificity without adversely affecting enzyme stability and are useful as targets for mutational changes.

Thus, the structure coordinates set forth in Table 1 can be used to aid in obtaining structural information about another crystallized molecule or molecular complex. A "molecular complex" means a protein in covalent or non-covalent association with a chemical entity or compound. The method of the invention allows determination of at least a portion of the three-dimensional structure of molecules or molecular complexes which contain one or more structural features that are similar to structural features of *Arabidopsis thaliana* peptide deformylase. These molecules are referred to herein as "structurally homologous" to *Arabidopsis thaliana* peptide deformylase. Similar structural features can include, for example, regions of amino acid identity, conserved active site or binding site motifs, and similarly arranged secondary structural elements (e.g., α helices and β sheets). Optionally, structural homology is determined by aligning the residues of the two amino acid sequences to optimize the number of identical amino acids along the lengths of their sequences; gaps in either or both sequences are permitted in making the alignment in order to optimize the number of identical amino acids, although the amino acids in each sequence must nonetheless remain in their proper order. Preferably, two amino acid sequences are compared using the Blastp program, version 2.0.9, of the BLAST 2 search algorithm, as described by Tatusova et al., FEMS Microbiol Lett., 174:247-50 (1999). Preferably, the default values for all BLAST 2 search parameters are used, including matrix=BLOSUM62; open gap penalty=11, extension gap penalty=1, gap x_dropoff=50, expect=10, wordsize=3, and filter on. In the comparison of two amino acid sequences using the BLAST search algorithm, structural similarity is referred to as "identity." Preferably, a structurally homologous molecule is a protein that has an amino acid sequence sharing at least 65% identity with the amino acid sequence of *Arabidopsis thaliana* peptide deformylase. Methods for generating structural information

about the structurally homologous molecule or molecular complex are well-known and include, for example, molecular replacement techniques. By using molecular replacement, all or part of the structure coordinates of *Arabidopsis thaliana* peptide deformylase (and set forth in Table 1) can be used to determine the structure of a crystallized molecule or molecular complex whose structure is unknown more quickly and efficiently than attempting to determine such information ab initio.

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

Thus, this method involves generating a preliminary model of a molecule or molecular complex whose structure coordinates are unknown, by orienting and positioning the relevant portion of *Arabidopsis thaliana* peptide deformylase according to Table 1 within the unit cell of the crystal of the unknown molecule or molecular complex so as best to account for the observed x-ray diffraction pattern of the crystal of the molecule or molecular complex whose structure is unknown. Phases can then be calculated from this model and combined with the observed x-ray diffraction pattern amplitudes to generate an electron density map of the structure whose coordinates are unknown. This, in turn, can be subjected to any well-known model building and structure refinement techniques to provide a final, accurate structure of the unknown crystallized molecule or molecular complex (E. Lattman, "Use of the Rotation and Translation Functions," in Meth. Enzymol., 115:55-77 (1985); M. G. Rossman, ed., "The Molecular Replacement Method," Int. Sci. Rev. Ser., No. 13, Gordon & Breach, New York (1972)).

Structural information about a portion of any crystallized molecule or molecular complex that is sufficiently structurally homologous to a portion of *Arabidopsis thaliana* peptide deformylase can be resolved by this method. In addition to a molecule that shares one or more structural features with *Arabidopsis thaliana* peptide deformylase as described above, a molecule that has similar bioactivity, such as the same catalytic activity, substrate specificity or ligand binding activity as *Arabidopsis thaliana* peptide deformylase, may also be sufficiently structurally homologous to *Arabidopsis thaliana* peptide deformylase to permit use of the structure coordinates of *Arabidopsis thaliana* peptide deformylase to solve its crystal structure.

In addition, using homology modeling, a computer model of an *Arabidopsis thaliana* peptide deformylase homolog can be built or refined without crystallizing the homolog. First, a preliminary model of the *Arabidopsis thaliana* peptide deformylase homolog is created by sequence alignment with *Arabidopsis thaliana* peptide deformylase, secondary structure prediction, the screening of structural libraries, or any combination of those techniques. Computational software may be used to carry out the sequence alignments and the secondary structure predictions. Structural incoherences, e.g., structural fragments around insertions and deletions, can be modeled by screening a structural library for peptides of the desired length and with a suitable conformation. For prediction of the side chain conformation, a side chain rotamer library may be employed. Where the *Arabidopsis thaliana* peptide deformylase homolog has been crystallized, the final homology model can be used to solve the crystal structure of the homolog by molecular replacement, as described above. Next, the preliminary model is subjected to energy minimization to yield an energy minimized model. The energy minimized model may contain regions where stereochemistry restraints are violated, in which case such regions are remodeled to obtain a final homology model. The homology model is positioned according to the results of molecular replacement, and subjected to further refinement including molecular dynamics calculations.

In another aspect, the present invention provides a computer-assisted method for designing a potential modifier of *Arabidopsis thaliana* peptide deformylase activity including: supplying a computer modeling application with a set of structure coordinates of a molecule or molecular complex, the molecule or molecular complex including at least a portion of at least one *Arabidopsis thaliana* peptide deformylase or *Arabidopsis thaliana* peptide deformylase-like active site, the active site including amino acids Gly121, Gly123, Leu124, Gln128, Glu169, Gly170, Cys171, Leu172, His213, Glu214, His217, and Tyr178; supplying the computer modeling application with a set of structure coordinates for a chemical entity; evaluating the potential binding interactions between the chemical entity and active site of the molecule or molecular complex; structurally modifying the chemical entity to yield a set of structure coordinates for a modified chemical entity; and determining whether the modified chemical entity is expected to bind to the molecule or molecular complex, wherein binding to the molecule or molecular complex is indicative of potential modification of *Arabidopsis thaliana* peptide deformylase activity.

The present invention also provides a computer-assisted method for designing a potential modifier of *Arabidopsis thaliana* peptide deformylase activity de novo including: supplying a computer modeling application with a set of structure coordinates of a molecule or molecular complex, the molecule or molecular complex including at least a portion of at least one *Arabidopsis thaliana* peptide deformylase or *Arabidopsis thaliana* peptide deformylase like active site, wherein the active site includes amino acids Gly121, Gly123, Leu124, Gln128, Glu169, Gly170, Cys171, Leu172, His213, Glu214, His217, and Tyr178; forming a chemical entity represented by set of structure coordinates; and determining whether the chemical entity is expected to bind to the molecule or molecular complex, wherein binding to the molecule or molecular complex is indicative of potential modification of *Arabidopsis thaliana* peptide deformylase activity.

In another aspect, the present invention provides a method for making a potential modifier of *Arabidopsis thaliana* peptide deformylase activity, the method including chemically or enzymatically synthesizing a chemical entity to yield a potential modifier of *Arabidopsis thaliana* peptide deformylase activity, the chemical entity having been identified during a computer-assisted process including supplying a computer modeling application with a set of structure coordinates of a molecule or molecular complex, the molecule or molecular complex including at least a portion of a *Arabidopsis thaliana* peptide deformylase or *Arabidopsis thaliana* peptide deformylase-like active site; supplying the computer modeling application with a set of structure coordinates of a chemical entity; and determining whether the chemical entity is expected to bind to the molecule or molecular complex at the active site, wherein binding to the molecule or molecular complex is indicative of potential modification of *Arabidopsis thaliana* peptide deformylase activity.

In another aspect, the present invention provides a method for making a potential modifier of *Arabidopsis thaliana* peptide deformylase activity, the method including chemically or enzymatically synthesizing a chemical entity to yield a potential modifier of *Arabidopsis thaliana* peptide deformylase activity, the chemical entity having been designed during a computer-assisted process including supplying a computer modeling application with a set of structure coordinates of a molecule or molecular complex, the molecule or molecular complex including at least a portion of a *Arabidopsis thaliana* peptide deformylase or *Arabidopsis thaliana* peptide deformylase-like active site; supplying the computer modeling application with a set of structure coordinates for a chemical entity; evaluating the potential binding interactions between the chemical entity and the active site of the molecule or molecular complex; structurally modifying the chemical entity to yield a set of structure coordinates for a modified chemical entity; and determining whether the chemical entity is expected to bind to the molecule or molecular complex at the active site, wherein binding to the molecule or molecular complex is indicative of potential modification of *Arabidopsis thaliana* peptide deformylase activity.

In general, methods for making a potential modifier of a plant peptide deformylase activity are provided herein. Such methods include chemically or enzymatically synthesizing a chemical entity to yield a potential modifier of plant peptide deformylase activity. Those skilled in the art of crystallography will understand that the atomic coordinates provided herein can be used to design a chemical entity during a computer-assisted process that includes supplying a computer modeling application with a set of structure coordinates of a molecule or molecular complex, the molecule or molecular complex including at least a portion of a plant peptide deformylase or *Arabidopsis thaliana* peptide deformylase-like active site; forming a chemical entity represented by set of structure coordinates; and determining whether the chemical entity is expected to bind to the molecule or molecular complex at the active site. Binding to the molecule or molecular complex is indicative of potential modification of *Arabidopsis thaliana* peptide deformylase activity.

FIGS. **6-8** contain phylogenetic analyses of the distribution of amino acid substitutions throughout the available collection of peptide deformylase sequences from plants compared with bacteria. The results are presented as a comparison of both the number and percentage of substitutions found at any location within the sequence of peptide deformylase 1 & 2 from plants as well as *E. coli*. There are a number of residue changes which suggest selection pressure in the evolution of peptide deformylase specifically adapted to plants. Thus, these changes are indicative of specific sites where residue changes are likely to affect peptide deformylase activity and/or specificity without adversely affecting enzyme stability and are useful as targets for mutational changes.

AtDEF2 is an essential plant enzyme responsible for the co-translational processing of chloroplast translated proteins. Although biochemically characterized, no structure exists for AtDEF2 in part because of a requirement for 0.5 M NaCl for solubility. The dependency on sodium chloride for solubility was removed by limited tryptic proteolysis and crystals of AtDEF2 were obtained. The structure was determined by molecular replacement and refined to a resolution of 2.7 Å. The overall fold of the enzyme closely resembles the alpha+beta conformation of known bacterial peptide deformylases, with an r.m.s deviation of 1.04 Å on main chain atoms relative to the *E. coli* enzyme. The largest differences occur in the orientation of the C-terminal helix (helix 3) and the conformation of the loop between beta strands 2 and 3, which form part of the five-stranded central sheet. Modeling the preferred substrate for AtDEF2 (the N-termini of the D1 polypeptide from photosystem II), in both chloroplast protein structures can be used to elucidate the mechanism underlying the 102-fold greater activity of AtDEF2 on this sequence (see FIG. **3**). Structural comparison can also be accomplished with the known eubacterial peptide deformylase structures to determine approaches for designing specific inhibitors against the chloroplast enzyme. Specific AtDEF2 inhibitors could potentially be used as broad-spectrum herbicides without impact on soil microorganisms.

The *Arabidopsis thaliana* DEF2 protein was over-expressed and purified from *E. coli*. Limited tryptic proteolysis yielded a form of *Arabidopsis thaliana* DEF2 (see FIG. **1**B, SEQ ID NO:1) which readily crystallized. The useful crystals all belong to the tetragonal space group. The unit cell parameters were a, b, and c; wherein a is about 40 Å to about 60 Å, b is about 40 Å to about 60 Å, and c is about 120 Å to about 160 Å.

Crystals of the truncated peptide deformylase construct are grown by hanging drop vapor diffusion in 24 well plates with well solutions containing 15-18% peg monomethyl ester 550, 28-70 mM $ZnSO_4$, and 70 mM MES pH 6.5. Protein solution at approximately 5 mg/ml is mixed 1:1 with well solution to a final volume of 2-5 microliters for the crystallization drops. Crystals form in several days to several weeks. To prepare the crystals for data collection, they were briefly placed into a solution containing the same components as the well solution in addition to 20% glycerol, mounted in nylon or mylar loops, and flash-cooled by plunging into liquid nitrogen.

Table 1 lists the atomic structure coordinates for the *Arabidopsis thaliana* peptide deformylase (*A. thaliana* DEF2) molecule as derived by x-ray diffraction from a crystal of the protein. The following abbreviations are used in Table 1. "Atom type" refers to the element whose coordinates are measured. The first letter in the column defines the element. "X, Y, Z" crystallographically define the atomic position of the element measured. "B" is a thermal factor that measures movement of the atom around its atomic center. "Occ" is an occupancy factor that refers to the fraction of the molecules in which each atom occupies the position specified by the coordinates. A value of "1" indicates that each atom has the same conformation, i.e., the same position, in all molecules of the crystal.

Table 1 is provided below:

REMARK coordinates from simulated annealing refinement
REMARK refinement resolution: 500.0–2.4 A
REMARK starting r = 0.2407 free_r = 0.2946
REMARK final r = 0.2352 free_r = 0.2983
REMARK rmsd bonds = 0.007053 rmsd angles = 1.33915
REMARK wa_initial = 2.77981 wa_dynamics = 3.30373 wa_final = 2.90342
REMARK target = mlf md-method = torsion annealing schedule = slowcool
REMARK starting temperature = 2500 total md steps = 100 * 6

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REMARK  sg = P4(1)2(1)2 a = 50.902 b = 50.902 c = 144.783 alpha = 90 beta = 90 gamma = 90
REMARK  parameter file 1  :  CNS_TOPPAR:protein_rep_cis.param
REMARK  parameter file 2  :  CNS_TOPPAR:ion.param
REMARK  parameter file 3  :  CNS_TOPPAR:water_rep.param
REMARK  molecular structure file: generate_r8h.mtf
REMARK  input coordinates: generate_r8h.pdb
REMARK  reflection file = pepdef1_p41212_cv.cns
REMARK  ncs = none
REMARK  B-correction resolution: 6.0–2.4
REMARK  initial B-factor correction applied to fobs:
REMARK  B11 =     1.447 B22 =     1.447 B33 =    −2.893
REMARK  B12 =     0.000 B13 =     0.000 B23 =     0.000
REMARK  B-factor correction applied to coordinate array B:     1.092
REMARK  bulk solvent: density level = 0.398841 e/A^3, B-factor = 39.902 A^2
REMARK  reflections with |Fobs|/sigma_F < 0.0 rejected
REMARK  reflections with |Fobs| > 10000 * rms(Fobs) rejected
REMARK  theoretical total number of refl. in resol. range:          8021 (   100.0%)
REMARK  number of unobserved reflections (no entry or |F| = 0):        5 (     0.1%)
REMARK  number of reflections rejected:                                0 (     0.0%)
REMARK  total number of reflections used:                           8016 (    99.9%)
REMARK  number of reflections in working set:                       7166 (    89.3%)
REMARK  number of reflections in test set:                           850 (    10.6%)
CRYST1   50.902   50.902  144.783  90.00  90.00  90.00  P 41 21 2
REMARK  FILENAME = "anneal_pepdef1_r8h_1.pdb"
REMARK  DATE: 28-Apr-05 13:49:32
REMARK  VERSION: 1.0
ATOM      1  CB  ASP  A   74      39.005  −3.139  −26.015  1.00  40.08  A
ATOM      2  CG  ASP  A   74      37.793  −3.950  −25.591  1.00  39.52  A
ATOM      3  OD1 ASP  A   74      37.991  −5.048  −25.026  1.00  39.78  A
ATOM      4  OD2 ASP  A   74      36.651  −3.487  −25.804  1.00  37.24  A
ATOM      5  C   ASP  A   74      39.677  −4.292  −28.136  1.00  39.44  A
ATOM      6  O   ASP  A   74      38.789  −5.104  −28.382  1.00  40.59  A
ATOM      7  N   ASP  A   74      41.403  −3.315  −26.608  1.00  40.71  A
ATOM      8  CA  ASP  A   74      40.079  −3.996  −26.689  1.00  40.00  A
ATOM      9  N   VAL  A   75      40.329  −3.631  −29.089  1.00  36.98  A
ATOM     10  CA  VAL  A   75      40.043  −3.850  −30.503  1.00  34.57  A
ATOM     11  CB  VAL  A   75      38.952  −2.881  −31.027  1.00  35.15  A
ATOM     12  CG1 VAL  A   75      37.610  −3.228  −30.407  1.00  35.82  A
ATOM     13  CG2 VAL  A   75      39.323  −1.440  −30.706  1.00  35.83  A
ATOM     14  C   VAL  A   75      41.294  −3.686  −31.367  1.00  33.70  A
ATOM     15  O   VAL  A   75      41.849  −2.591  −31.473  1.00  31.73  A
ATOM     16  N   GLN  A   76      41.744  −4.785  −31.968  1.00  32.36  A
ATOM     17  CA  GLN  A   76      42.917  −4.752  −32.834  1.00  31.43  A
ATOM     18  CB  GLN  A   76      43.809  −5.977  −32.597  1.00  30.15  A
ATOM     19  CG  GLN  A   76      43.948  −6.377  −31.146  1.00  32.55  A
ATOM     20  CD  GLN  A   76      45.062  −7.391  −30.900  1.00  33.57  A
ATOM     21  OE1 GLN  A   76      45.222  −8.363  −31.647  1.00  30.76  A
ATOM     22  NE2 GLN  A   76      45.832  −7.169  −29.835  1.00  32.62  A
ATOM     23  C   GLN  A   76      42.442  −4.747  −34.284  1.00  30.41  A
ATOM     24  O   GLN  A   76      41.713  −5.642  −34.714  1.00  32.15  A
ATOM     25  N   PHE  A   77      42.843  −3.737  −35.042  1.00  29.07  A
ATOM     26  CA  PHE  A   77      42.442  −3.672  −36.437  1.00  29.03  A
ATOM     27  CB  PHE  A   77      41.147  −2.871  −36.582  1.00  26.50  A
ATOM     28  CG  PHE  A   77      41.287  −1.426  −36.198  1.00  25.67  A
ATOM     29  CD1 PHE  A   77      41.416  −0.442  −37.172  1.00  25.19  A
ATOM     30  CD2 PHE  A   77      41.317  −1.050  −34.858  1.00  24.82  A
ATOM     31  CE1 PHE  A   77      41.572   0.895  −36.818  1.00  23.61  A
ATOM     32  CE2 PHE  A   77      41.473   0.283  −34.497  1.00  24.11  A
ATOM     33  CZ  PHE  A   77      41.600   1.258  −35.483  1.00  23.48  A
ATOM     34  C   PHE  A   77      43.523  −3.035  −37.287  1.00  30.55  A
ATOM     35  O   PHE  A   77      44.372  −2.293  −36.789  1.00  28.47  A
ATOM     36  N   GLU  A   78      43.487  −3.355  −38.576  1.00  33.02  A
ATOM     37  CA  GLU  A   78      44.418  −2.797  −39.542  1.00  34.82  A
ATOM     38  CB  GLU  A   78      44.965  −3.876  −40.491  1.00  35.56  A
ATOM     39  CG  GLU  A   78      45.913  −4.906  −39.860  1.00  35.90  A
ATOM     40  CD  GLU  A   78      45.187  −5.934  −39.001  1.00  37.85  A
ATOM     41  OE1 GLU  A   78      44.210  −6.534  −39.493  1.00  39.60  A
ATOM     42  OE2 GLU  A   78      45.590  −6.152  −37.841  1.00  37.63  A
ATOM     43  C   GLU  A   78      43.580  −1.814  −40.339  1.00  35.67  A
ATOM     44  O   GLU  A   78      42.386  −2.030  −40.543  1.00  34.84  A
ATOM     45  N   THR  A   79      44.184  −0.713  −40.755  1.00  36.81  A
ATOM     46  CA  THR  A   79      43.448   0.241  −41.556  1.00  37.92  A
ATOM     47  CB  THR  A   79      43.983   1.662  −41.389  1.00  39.37  A
ATOM     48  OG1 THR  A   79      45.378   1.684  −41.710  1.00  42.97  A
ATOM     49  CG2 THR  A   79      43.770   2.143  −39.953  1.00  41.38  A
ATOM     50  C   THR  A   79      43.700  −0.247  −42.965  1.00  37.15  A
ATOM     51  O   THR  A   79      44.299  −1.298  −43.159  1.00  40.94  A
ATOM     52  N   CPR  A   80      43.288   0.520  −43.969  1.00  34.90  A
ATOM     53  CD  CPR  A   80      44.233   0.907  −45.032  1.00  33.68  A
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ATOM	54	CA	CPR	A	80	41.941	0.367	−44.515	1.00	31.75	A
ATOM	55	CB	CPR	A	80	42.189	0.321	−46.016	1.00	32.26	A
ATOM	56	CG	CPR	A	80	43.316	1.267	−46.177	1.00	34.32	A
ATOM	57	C	CPR	A	80	41.207	−0.880	−44.023	1.00	29.73	A
ATOM	58	O	CPR	A	80	41.726	−1.994	−44.105	1.00	28.01	A
ATOM	59	N	LEU	A	81	40.000	−0.684	−43.504	1.00	26.29	A
ATOM	60	CA	LEU	A	81	39.187	−1.805	−43.067	1.00	24.35	A
ATOM	61	CB	LEU	A	81	38.007	−1.326	−42.218	1.00	20.43	A
ATOM	62	CG	LEU	A	81	38.345	−0.696	−40.868	1.00	18.48	A
ATOM	63	CD1	LEU	A	81	37.074	−0.120	−40.242	1.00	10.91	A
ATOM	64	CD2	LEU	A	81	39.000	−1.749	−39.969	1.00	15.22	A
ATOM	65	C	LEU	A	81	38.660	−2.430	−44.352	1.00	24.72	A
ATOM	66	O	LEU	A	81	38.610	−1.772	−45.392	1.00	22.96	A
ATOM	67	N	LYS	A	82	38.276	−3.698	−44.281	1.00	26.20	A
ATOM	68	CA	LYS	A	82	37.738	−4.402	−45.441	1.00	26.69	A
ATOM	69	CB	LYS	A	82	38.682	−5.540	−45.852	1.00	28.51	A
ATOM	70	CG	LYS	A	82	38.188	−6.384	−47.022	1.00	34.36	A
ATOM	71	CD	LYS	A	82	39.217	−7.445	−47.429	1.00	37.34	A
ATOM	72	CE	LYS	A	82	38.722	−8.278	−48.609	1.00	39.22	A
ATOM	73	NZ	LYS	A	82	39.762	−9.208	−49.129	1.00	41.01	A
ATOM	74	C	LYS	A	82	36.366	−4.955	−45.059	1.00	25.07	A
ATOM	75	O	LYS	A	82	36.169	−5.422	−43.940	1.00	25.23	A
ATOM	76	N	ILE	A	83	35.417	−4.896	−45.986	1.00	22.76	A
ATOM	77	CA	ILE	A	83	34.074	−5.387	−45.713	1.00	20.03	A
ATOM	78	CB	ILE	A	83	33.061	−4.820	−46.717	1.00	17.56	A
ATOM	79	CG2	ILE	A	83	31.687	−5.395	−46.443	1.00	14.23	A
ATOM	80	CG1	ILE	A	83	33.050	−3.292	−46.642	1.00	14.83	A
ATOM	81	CD1	ILE	A	83	32.504	−2.738	−45.351	1.00	18.36	A
ATOM	82	C	ILE	A	83	34.007	−6.905	−45.770	1.00	19.27	A
ATOM	83	O	ILE	A	83	34.519	−7.520	−46.697	1.00	20.95	A
ATOM	84	N	VAL	A	84	33.369	−7.498	−44.770	1.00	18.88	A
ATOM	85	CA	VAL	A	84	33.209	−8.943	−44.689	1.00	18.55	A
ATOM	86	CB	VAL	A	84	33.199	−9.409	−43.220	1.00	18.38	A
ATOM	87	CG1	VAL	A	84	32.826	−10.874	−43.136	1.00	17.47	A
ATOM	88	CG2	VAL	A	84	34.566	−9.166	−42.593	1.00	16.32	A
ATOM	89	C	VAL	A	84	31.877	−9.299	−45.343	1.00	19.91	A
ATOM	90	O	VAL	A	84	30.832	−8.759	−44.972	1.00	21.19	A
ATOM	91	N	GLU	A	85	31.912	−10.210	−46.311	1.00	19.07	A
ATOM	92	CA	GLU	A	85	30.700	−10.597	−47.022	1.00	18.15	A
ATOM	93	CB	GLU	A	85	30.957	−10.620	−48.535	1.00	19.75	A
ATOM	94	CG	GLU	A	85	31.242	−9.268	−49.179	1.00	20.83	A
ATOM	95	CD	GLU	A	85	31.658	−9.413	−50.642	1.00	24.60	A
ATOM	96	OE1	GLU	A	85	31.043	−10.251	−51.350	1.00	24.61	A
ATOM	97	OE2	GLU	A	85	32.587	−8.691	−51.086	1.00	23.72	A
ATOM	98	C	GLU	A	85	30.144	−11.948	−46.615	1.00	16.54	A
ATOM	99	O	GLU	A	85	30.891	−12.871	−46.289	1.00	15.61	A
ATOM	100	N	TYR	A	86	28.816	−12.040	−46.642	1.00	14.81	A
ATOM	101	CA	TYR	A	86	28.086	−13.273	−46.342	1.00	13.38	A
ATOM	102	CB	TYR	A	86	26.585	−13.045	−46.614	1.00	13.37	A
ATOM	103	CG	TYR	A	86	25.740	−14.294	−46.671	1.00	11.64	A
ATOM	104	CD1	TYR	A	86	25.387	−14.988	−45.508	1.00	12.48	A
ATOM	105	CE1	TYR	A	86	24.653	−16.180	−45.576	1.00	9.76	A
ATOM	106	CD2	TYR	A	86	25.330	−14.815	−47.900	1.00	10.58	A
ATOM	107	CE2	TYR	A	86	24.602	−15.993	−47.979	1.00	7.91	A
ATOM	108	CZ	TYR	A	86	24.271	−16.676	−46.821	1.00	9.19	A
ATOM	109	OH	TYR	A	86	23.624	−17.891	−46.923	1.00	9.80	A
ATOM	110	C	TYR	A	86	28.660	−14.288	−47.326	1.00	11.79	A
ATOM	111	O	TYR	A	86	29.028	−13.922	−48.443	1.00	9.00	A
ATOM	112	N	PRO	A	87	28.737	−15.571	−46.940	1.00	13.07	A
ATOM	113	CD	PRO	A	87	29.187	−16.597	−47.904	1.00	12.32	A
ATOM	114	CA	PRO	A	87	28.335	−16.193	−45.672	1.00	14.67	A
ATOM	115	CB	PRO	A	87	27.876	−17.563	−46.122	1.00	13.93	A
ATOM	116	CG	PRO	A	87	28.972	−17.908	−47.144	1.00	13.84	A
ATOM	117	C	PRO	A	87	29.449	−16.289	−44.612	1.00	16.37	A
ATOM	118	O	PRO	A	87	29.415	−17.176	−43.751	1.00	16.16	A
ATOM	119	N	ASP	A	88	30.433	−15.396	−44.676	1.00	14.88	A
ATOM	120	CA	ASP	A	88	31.529	−15.427	−43.708	1.00	16.94	A
ATOM	121	CB	ASP	A	88	32.374	−14.155	−43.811	1.00	17.27	A
ATOM	122	CG	ASP	A	88	33.647	−14.237	−42.991	1.00	20.01	A
ATOM	123	OD1	ASP	A	88	33.564	−14.530	−41.779	1.00	22.56	A
ATOM	124	OD2	ASP	A	88	34.734	−14.005	−43.559	1.00	22.48	A
ATOM	125	C	ASP	A	88	30.964	−15.563	−42.286	1.00	17.02	A
ATOM	126	O	ASP	A	88	30.111	−14.771	−41.864	1.00	14.24	A
ATOM	127	N	PRO	A	89	31.454	−16.562	−41.528	1.00	17.30	A
ATOM	128	CD	PRO	A	89	32.572	−17.414	−41.972	1.00	17.85	A
ATOM	129	CA	PRO	A	89	31.063	−16.896	−40.148	1.00	16.77	A
ATOM	130	CB	PRO	A	89	32.039	−18.014	−39.769	1.00	17.99	A
ATOM	131	CG	PRO	A	89	32.412	−18.623	−41.091	1.00	19.05	A
ATOM	132	C	PRO	A	89	31.102	−15.742	−39.141	1.00	17.05	A

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ATOM	133	O	PRO	A	89	30.343	−15.737	−38.167	1.00	14.98 A
ATOM	134	N	ILE	A	90	31.997	−14.781	−39.371	1.00	16.08 A
ATOM	135	CA	ILE	A	90	32.138	−13.624	−38.489	1.00	15.58 A
ATOM	136	CB	ILE	A	90	33.228	−12.657	−39.019	1.00	14.80 A
ATOM	137	CG2	ILE	A	90	33.261	−11.394	−38.178	1.00	12.19 A
ATOM	138	CG1	ILE	A	90	34.596	−13.344	−38.983	1.00	15.77 A
ATOM	139	CD1	ILE	A	90	35.729	−12.544	−39.637	1.00	14.96 A
ATOM	140	C	ILE	A	90	30.823	−12.853	−38.332	1.00	15.25 A
ATOM	141	O	ILE	A	90	30.595	−12.190	−37.318	1.00	13.85 A
ATOM	142	N	LEU	A	91	29.951	−12.960	−39.329	1.00	13.85 A
ATOM	143	CA	LEU	A	91	28.679	−12.262	−39.295	1.00	12.86 A
ATOM	144	CB	LEU	A	91	28.124	−12.129	−40.709	1.00	8.77 A
ATOM	145	CG	LEU	A	91	29.118	−11.425	−41.639	1.00	8.91 A
ATOM	146	CD1	LEU	A	91	28.533	−11.337	−43.034	1.00	9.63 A
ATOM	147	CD2	LEU	A	91	29.460	−10.035	−41.096	1.00	7.28 A
ATOM	148	C	LEU	A	91	27.666	−12.934	−38.383	1.00	14.00 A
ATOM	149	O	LEU	A	91	26.585	−12.392	−38.147	1.00	15.75 A
ATOM	150	N	ARG	A	92	28.024	−14.102	−37.856	1.00	14.41 A
ATOM	151	CA	ARG	A	92	27.142	−14.841	−36.946	1.00	16.37 A
ATOM	152	CB	ARG	A	92	26.771	−16.202	−37.541	1.00	17.16 A
ATOM	153	CG	ARG	A	92	26.132	−16.163	−38.904	1.00	17.07 A
ATOM	154	CD	ARG	A	92	24.720	−15.650	−38.825	1.00	17.49 A
ATOM	155	NE	ARG	A	92	23.973	−15.900	−40.058	1.00	16.77 A
ATOM	156	CZ	ARG	A	92	22.704	−15.549	−40.237	1.00	15.33 A
ATOM	157	NH1	ARG	A	92	22.042	−14.928	−39.263	1.00	15.95 A
ATOM	158	NH2	ARG	A	92	22.093	−15.828	−41.378	1.00	15.85 A
ATOM	159	C	ARG	A	92	27.832	−15.099	−35.609	1.00	16.73 A
ATOM	160	O	ARG	A	92	27.185	−15.475	−34.636	1.00	16.22 A
ATOM	161	N	ALA	A	93	29.142	−14.874	−35.582	1.00	18.23 A
ATOM	162	CA	ALA	A	93	30.006	−15.132	−34.425	1.00	22.48 A
ATOM	163	CB	ALA	A	93	31.457	−14.786	−34.797	1.00	23.31 A
ATOM	164	C	ALA	A	93	29.726	−14.602	−33.015	1.00	24.67 A
ATOM	165	O	ALA	A	93	30.506	−14.902	−32.106	1.00	28.53 A
ATOM	166	N	LYS	A	94	28.665	−13.833	−32.799	1.00	24.09 A
ATOM	167	CA	LYS	A	94	28.384	−13.346	−31.439	1.00	24.96 A
ATOM	168	CB	LYS	A	94	28.436	−14.500	−30.437	1.00	25.30 A
ATOM	169	CG	LYS	A	94	28.341	−14.049	−29.000	1.00	29.01 A
ATOM	170	CD	LYS	A	94	29.295	−14.836	−28.131	1.00	32.16 A
ATOM	171	CE	LYS	A	94	29.502	−14.124	−26.805	1.00	33.93 A
ATOM	172	NZ	LYS	A	94	29.929	−12.709	−27.033	1.00	34.32 A
ATOM	173	C	LYS	A	94	29.371	−12.256	−31.016	1.00	22.46 A
ATOM	174	O	LYS	A	94	30.581	−12.475	−30.959	1.00	21.86 A
ATOM	175	N	ASN	A	95	28.832	−11.093	−30.673	1.00	21.41 A
ATOM	176	CA	ASN	A	95	29.657	−9.946	−30.341	1.00	22.01 A
ATOM	177	CB	ASN	A	95	29.187	−8.774	−31.208	1.00	20.42 A
ATOM	178	CG	ASN	A	95	28.983	−9.187	−32.651	1.00	19.92 A
ATOM	179	OD1	ASN	A	95	27.859	−9.463	−33.085	1.00	18.30 A
ATOM	180	ND2	ASN	A	95	30.081	−9.268	−33.397	1.00	20.07 A
ATOM	181	C	ASN	A	95	29.774	−9.517	−28.884	1.00	21.39 A
ATOM	182	O	ASN	A	95	28.777	−9.287	−28.199	1.00	20.41 A
ATOM	183	N	LYS	A	96	31.019	−9.395	−28.434	1.00	23.00 A
ATOM	184	CA	LYS	A	96	31.334	−8.989	−27.071	1.00	23.73 A
ATOM	185	CB	LYS	A	96	32.779	−9.351	−26.732	1.00	25.32 A
ATOM	186	CG	LYS	A	96	33.051	−10.845	−26.646	1.00	26.59 A
ATOM	187	CD	LYS	A	96	34.537	−11.110	−26.428	1.00	30.79 A
ATOM	188	CE	LYS	A	96	34.831	−12.599	−26.255	1.00	32.28 A
ATOM	189	NZ	LYS	A	96	36.296	−12.888	−26.289	1.00	32.84 A
ATOM	190	C	LYS	A	96	31.135	−7.492	−26.874	1.00	25.90 A
ATOM	191	O	LYS	A	96	31.421	−6.686	−27.769	1.00	25.26 A
ATOM	192	N	ARG	A	97	30.642	−7.134	−25.692	1.00	26.74 A
ATOM	193	CA	ARG	A	97	30.402	−5.743	−25.336	1.00	27.69 A
ATOM	194	CB	ARG	A	97	29.702	−5.662	−23.979	1.00	28.92 A
ATOM	195	CG	ARG	A	97	28.317	−6.287	−23.952	1.00	33.87 A
ATOM	196	CD	ARG	A	97	27.813	−6.493	−22.525	1.00	37.61 A
ATOM	197	NE	ARG	A	97	28.062	−5.314	−21.706	1.00	39.27 A
ATOM	198	CZ	ARG	A	97	29.170	−5.119	−20.999	1.00	40.73 A
ATOM	199	NH1	ARG	A	97	30.132	−6.035	−20.995	1.00	41.21 A
ATOM	200	NH2	ARG	A	97	29.334	−3.987	−20.330	1.00	40.81 A
ATOM	201	C	ARG	A	97	31.730	−5.009	−25.262	1.00	27.45 A
ATOM	202	O	ARG	A	97	32.773	−5.619	−25.014	1.00	27.82 A
ATOM	203	N	ILE	A	98	31.689	−3.702	−25.487	1.00	25.11 A
ATOM	204	CA	ILE	A	98	32.889	−2.888	−25.426	1.00	24.66 A
ATOM	205	CB	ILE	A	98	32.866	−1.803	−26.529	1.00	24.88 A
ATOM	206	CG2	ILE	A	98	33.965	−0.767	−26.301	1.00	20.36 A
ATOM	207	CG1	ILE	A	98	33.044	−2.485	−27.891	1.00	24.66 A
ATOM	208	CD1	ILE	A	98	33.092	−1.538	−29.061	1.00	28.24 A
ATOM	209	C	ILE	A	98	32.997	−2.267	−24.035	1.00	24.19 A
ATOM	210	O	ILE	A	98	32.093	−1.571	−23.581	1.00	24.25 A
ATOM	211	N	ASP	A	99	34.104	−2.549	−23.359	1.00	23.56 A

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ATOM	212	CA	ASP	A	99	34.339	−2.053	−22.008	1.00	23.39 A
ATOM	213	CB	ASP	A	99	34.250	−3.214	−21.018	1.00	23.94 A
ATOM	214	CG	ASP	A	99	35.163	−4.366	−21.394	1.00	24.05 A
ATOM	215	OD1	ASP	A	99	35.055	−5.439	−20.766	1.00	24.51 A
ATOM	216	OD2	ASP	A	99	35.991	−4.196	−22.318	1.00	23.12 A
ATOM	217	C	ASP	A	99	35.699	−1.370	−21.880	1.00	23.34 A
ATOM	218	O	ASP	A	99	36.285	−1.317	−20.800	1.00	21.90 A
ATOM	219	N	ILE	A	100	36.204	−0.875	−23.002	1.00	22.91 A
ATOM	220	CA	ILE	A	100	37.469	−0.161	−23.033	1.00	22.92 A
ATOM	221	CB	ILE	A	100	38.647	−1.068	−23.461	1.00	21.59 A
ATOM	222	CG2	ILE	A	100	39.872	−0.209	−23.780	1.00	21.34 A
ATOM	223	CG1	ILE	A	100	38.960	−2.072	−22.342	1.00	20.46 A
ATOM	224	CD1	ILE	A	100	40.247	−2.845	−22.530	1.00	16.61 A
ATOM	225	C	ILE	A	100	37.292	0.975	−24.026	1.00	23.77 A
ATOM	226	O	ILE	A	100	37.268	0.767	−25.243	1.00	22.69 A
ATOM	227	N	PHE	A	101	37.145	2.179	−23.489	1.00	23.83 A
ATOM	228	CA	PHE	A	101	36.934	3.360	−24.308	1.00	24.41 A
ATOM	229	CB	PHE	A	101	35.788	4.175	−23.705	1.00	23.98 A
ATOM	230	CG	PHE	A	101	34.559	3.343	−23.419	1.00	24.14 A
ATOM	231	CD1	PHE	A	101	34.480	2.567	−22.261	1.00	25.77 A
ATOM	232	CD2	PHE	A	101	33.517	3.274	−24.339	1.00	23.97 A
ATOM	233	CE1	PHE	A	101	33.379	1.729	−22.025	1.00	26.25 A
ATOM	234	CE2	PHE	A	101	32.413	2.444	−24.115	1.00	24.68 A
ATOM	235	CZ	PHE	A	101	32.344	1.669	−22.958	1.00	24.94 A
ATOM	236	C	PHE	A	101	38.227	4.152	−24.398	1.00	24.03 A
ATOM	237	O	PHE	A	101	38.514	5.009	−23.565	1.00	24.43 A
ATOM	238	N	ASP	A	102	39.002	3.840	−25.435	1.00	23.26 A
ATOM	239	CA	ASP	A	102	40.301	4.458	−25.658	1.00	22.30 A
ATOM	240	CB	ASP	A	102	41.408	3.437	−25.360	1.00	22.09 A
ATOM	241	CG	ASP	A	102	41.328	2.199	−26.256	1.00	20.92 A
ATOM	242	OD1	ASP	A	102	40.445	2.141	−27.143	1.00	18.72 A
ATOM	243	OD2	ASP	A	102	42.158	1.279	−26.072	1.00	20.13 A
ATOM	244	C	ASP	A	102	40.495	4.990	−27.066	1.00	21.70 A
ATOM	245	O	ASP	A	102	39.567	5.025	−27.868	1.00	22.38 A
ATOM	246	N	GLU	A	103	41.728	5.398	−27.349	1.00	22.47 A
ATOM	247	CA	GLU	A	103	42.108	5.927	−28.653	1.00	21.29 A
ATOM	248	CB	GLU	A	103	43.610	6.188	−28.705	1.00	19.68 A
ATOM	249	CG	GLU	A	103	43.965	7.635	−28.642	1.00	21.47 A
ATOM	250	CD	GLU	A	103	43.305	8.423	−29.741	1.00	21.50 A
ATOM	251	OE1	GLU	A	103	42.668	9.445	−29.427	1.00	20.68 A
ATOM	252	OE2	GLU	A	103	43.427	8.020	−30.914	1.00	22.92 A
ATOM	253	C	GLU	A	103	41.764	4.954	−29.754	1.00	20.91 A
ATOM	254	O	GLU	A	103	41.172	5.331	−30.767	1.00	19.57 A
ATOM	255	N	ASN	A	104	42.172	3.705	−29.550	1.00	21.14 A
ATOM	256	CA	ASN	A	104	41.937	2.639	−30.507	1.00	22.17 A
ATOM	257	CB	ASN	A	104	42.341	1.299	−29.897	1.00	26.29 A
ATOM	258	CG	ASN	A	104	43.312	0.541	−30.766	1.00	29.79 A
ATOM	259	OD1	ASN	A	104	43.027	0.261	−31.930	1.00	33.45 A
ATOM	260	ND2	ASN	A	104	44.473	0.204	−30.208	1.00	30.61 A
ATOM	261	C	ASN	A	104	40.473	2.593	−30.920	1.00	22.03 A
ATOM	262	O	ASN	A	104	40.160	2.479	−32.108	1.00	21.05 A
ATOM	263	N	LEU	A	105	39.581	2.684	−29.934	1.00	19.85 A
ATOM	264	CA	LEU	A	105	38.150	2.657	−30.199	1.00	19.86 A
ATOM	265	CB	LEU	A	105	37.358	2.735	−28.886	1.00	21.38 A
ATOM	266	CG	LEU	A	105	35.919	2.188	−28.821	1.00	21.48 A
ATOM	267	CD1	LEU	A	105	35.056	3.165	−28.032	1.00	21.52 A
ATOM	268	CD2	LEU	A	105	35.341	1.980	−30.207	1.00	21.83 A
ATOM	269	C	LEU	A	105	37.771	3.830	−31.102	1.00	19.11 A
ATOM	270	O	LEU	A	105	36.987	3.668	−32.036	1.00	19.29 A
ATOM	271	N	LYS	A	106	38.328	5.008	−30.820	1.00	17.86 A
ATOM	272	CA	LYS	A	106	38.051	6.194	−31.627	1.00	18.70 A
ATOM	273	CB	LYS	A	106	38.639	7.449	−30.974	1.00	18.90 A
ATOM	274	CG	LYS	A	106	38.329	8.737	−31.744	1.00	21.08 A
ATOM	275	CD	LYS	A	106	38.916	9.962	−31.051	1.00	20.57 A
ATOM	276	CE	LYS	A	106	40.425	10.037	−31.200	1.00	19.98 A
ATOM	277	NZ	LYS	A	106	41.013	11.166	−30.404	1.00	18.10 A
ATOM	278	C	LYS	A	106	38.597	6.061	−33.058	1.00	18.80 A
ATOM	279	O	LYS	A	106	37.914	6.413	−34.023	1.00	18.37 A
ATOM	280	N	ASN	A	107	39.822	5.556	−33.190	1.00	17.20 A
ATOM	281	CA	ASN	A	107	40.431	5.370	−34.506	1.00	18.47 A
ATOM	282	CB	ASN	A	107	41.857	4.814	−34.363	1.00	21.05 A
ATOM	283	CG	ASN	A	107	42.777	5.725	−33.544	1.00	24.77 A
ATOM	284	OD1	ASN	A	107	43.803	5.275	−33.021	1.00	26.42 A
ATOM	285	ND2	ASN	A	107	42.423	7.005	−33.441	1.00	23.25 A
ATOM	286	C	ASN	A	107	39.587	4.394	−35.332	1.00	17.56 A
ATOM	287	O	ASN	A	107	39.453	4.543	−36.545	1.00	17.37 A
ATOM	288	N	LEU	A	108	39.008	3.401	−34.659	1.00	18.87 A
ATOM	289	CA	LEU	A	108	38.182	2.393	−35.315	1.00	18.66 A
ATOM	290	CB	LEU	A	108	37.754	1.318	−34.310	1.00	17.82 A

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ATOM	291	CG	LEU	A	108	37.452	−0.094	−34.834	1.00	18.20	A
ATOM	292	CD1	LEU	A	108	36.611	−0.846	−33.809	1.00	14.71	A
ATOM	293	CD2	LEU	A	108	36.712	−0.033	−36.137	1.00	16.41	A
ATOM	294	C	LEU	A	108	36.938	3.025	−35.936	1.00	19.55	A
ATOM	295	O	LEU	A	108	36.669	2.851	−37.127	1.00	20.36	A
ATOM	296	N	VAL	A	109	36.183	3.752	−35.117	1.00	19.78	A
ATOM	297	CA	VAL	A	109	34.961	4.412	−35.567	1.00	20.39	A
ATOM	298	CB	VAL	A	109	34.391	5.350	−34.460	1.00	20.97	A
ATOM	299	CG1	VAL	A	109	33.245	6.201	−35.014	1.00	18.35	A
ATOM	300	CG2	VAL	A	109	33.908	4.514	−33.282	1.00	18.10	A
ATOM	301	C	VAL	A	109	35.207	5.218	−36.841	1.00	21.06	A
ATOM	302	O	VAL	A	109	34.448	5.104	−37.815	1.00	20.21	A
ATOM	303	N	ASP	A	110	36.268	6.021	−36.833	1.00	19.90	A
ATOM	304	CA	ASP	A	110	36.609	6.834	−37.993	1.00	19.28	A
ATOM	305	CB	ASP	A	110	37.787	7.760	−37.665	1.00	21.34	A
ATOM	306	CG	ASP	A	110	38.385	8.412	−38.904	1.00	23.52	A
ATOM	307	OD1	ASP	A	110	39.280	7.805	−39.525	1.00	23.06	A
ATOM	308	OD2	ASP	A	110	37.950	9.526	−39.264	1.00	25.77	A
ATOM	309	C	ASP	A	110	36.954	5.948	−39.187	1.00	18.12	A
ATOM	310	O	ASP	A	110	36.606	6.260	−40.326	1.00	16.99	A
ATOM	311	N	ALA	A	111	37.640	4.842	−38.928	1.00	17.77	A
ATOM	312	CA	ALA	A	111	38.007	3.934	−40.014	1.00	18.12	A
ATOM	313	CB	ALA	A	111	38.991	2.879	−39.517	1.00	17.41	A
ATOM	314	C	ALA	A	111	36.747	3.265	−40.559	1.00	18.06	A
ATOM	315	O	ALA	A	111	36.688	2.909	−41.735	1.00	17.71	A
ATOM	316	N	MET	A	112	35.741	3.093	−39.700	1.00	16.57	A
ATOM	317	CA	MET	A	112	34.493	2.476	−40.131	1.00	16.68	A
ATOM	318	CB	MET	A	112	33.625	2.094	−38.932	1.00	16.96	A
ATOM	319	CG	MET	A	112	34.095	0.844	−38.224	1.00	15.01	A
ATOM	320	SD	MET	A	112	33.117	0.488	−36.768	1.00	19.27	A
ATOM	321	CE	MET	A	112	31.718	−0.406	−37.514	1.00	17.01	A
ATOM	322	C	MET	A	112	33.729	3.421	−41.036	1.00	16.16	A
ATOM	323	O	MET	A	112	33.206	3.009	−42.072	1.00	16.11	A
ATOM	324	N	PHE	A	113	33.661	4.688	−40.643	1.00	16.28	A
ATOM	325	CA	PHE	A	113	32.965	5.674	−41.458	1.00	18.18	A
ATOM	326	CB	PHE	A	113	32.955	7.054	−40.770	1.00	16.66	A
ATOM	327	CG	PHE	A	113	31.803	7.259	−39.806	1.00	14.71	A
ATOM	328	CD1	PHE	A	113	30.482	7.154	−40.239	1.00	14.21	A
ATOM	329	CD2	PHE	A	113	32.041	7.552	−38.457	1.00	15.65	A
ATOM	330	CE1	PHE	A	113	29.406	7.334	−39.341	1.00	12.91	A
ATOM	331	CE2	PHE	A	113	30.979	7.735	−37.554	1.00	13.65	A
ATOM	332	CZ	PHE	A	113	29.658	7.624	−38.001	1.00	13.65	A
ATOM	333	C	PHE	A	113	33.674	5.763	−42.813	1.00	19.19	A
ATOM	334	O	PHE	A	113	33.036	5.966	−43.848	1.00	20.51	A
ATOM	335	N	ASP	A	114	34.993	5.593	−42.809	1.00	19.06	A
ATOM	336	CA	ASP	A	114	35.752	5.671	−44.050	1.00	19.17	A
ATOM	337	CB	ASP	A	114	37.258	5.516	−43.800	1.00	19.27	A
ATOM	338	CG	ASP	A	114	37.847	6.649	−42.972	1.00	18.16	A
ATOM	339	OD1	ASP	A	114	37.388	7.798	−43.112	1.00	18.34	A
ATOM	340	OD2	ASP	A	114	38.792	6.383	−42.194	1.00	16.95	A
ATOM	341	C	ASP	A	114	35.328	4.601	−45.047	1.00	20.74	A
ATOM	342	O	ASP	A	114	34.948	4.905	−46.178	1.00	22.18	A
ATOM	343	N	VAL	A	115	35.402	3.343	−44.635	1.00	19.76	A
ATOM	344	CA	VAL	A	115	35.051	2.271	−45.541	1.00	20.05	A
ATOM	345	CB	VAL	A	115	35.421	0.882	−44.952	1.00	18.79	A
ATOM	346	CG1	VAL	A	115	34.508	0.535	−43.781	1.00	19.87	A
ATOM	347	CG2	VAL	A	115	35.348	−0.179	−46.047	1.00	18.66	A
ATOM	348	C	VAL	A	115	33.570	2.319	−45.888	1.00	20.92	A
ATOM	349	O	VAL	A	115	33.172	1.900	−46.976	1.00	21.72	A
ATOM	350	N	MET	A	116	32.756	2.843	−44.975	1.00	20.52	A
ATOM	351	CA	MET	A	116	31.324	2.928	−45.225	1.00	20.64	A
ATOM	352	CB	MET	A	116	30.574	3.419	−43.975	1.00	21.83	A
ATOM	353	CG	MET	A	116	29.047	3.419	−44.133	1.00	21.70	A
ATOM	354	SD	MET	A	116	28.146	4.174	−42.758	1.00	25.32	A
ATOM	355	CE	MET	A	116	28.020	5.885	−43.298	1.00	22.79	A
ATOM	356	C	MET	A	116	31.107	3.896	−46.387	1.00	21.10	A
ATOM	357	O	MET	A	116	30.475	3.544	−47.389	1.00	18.06	A
ATOM	358	N	TYR	A	117	31.652	5.106	−46.247	1.00	21.03	A
ATOM	359	CA	TYR	A	117	31.537	6.135	−47.275	1.00	20.92	A
ATOM	360	CB	TYR	A	117	32.175	7.448	−46.809	1.00	20.51	A
ATOM	361	CG	TYR	A	117	31.419	8.154	−45.709	1.00	18.43	A
ATOM	362	CD1	TYR	A	117	30.033	8.240	−45.744	1.00	17.94	A
ATOM	363	CE1	TYR	A	117	29.328	8.917	−44.754	1.00	18.18	A
ATOM	364	CD2	TYR	A	117	32.089	8.765	−44.652	1.00	17.61	A
ATOM	365	CE2	TYR	A	117	31.391	9.450	−43.655	1.00	17.47	A
ATOM	366	CZ	TYR	A	117	30.011	9.518	−43.719	1.00	16.23	A
ATOM	367	OH	TYR	A	117	29.301	10.186	−42.759	1.00	18.52	A
ATOM	368	C	TYR	A	117	32.212	5.700	−48.563	1.00	22.73	A
ATOM	369	O	TYR	A	117	31.717	5.976	−49.653	1.00	22.10	A

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ATOM	370	N	LYS	A	118	33.356	5.034	−48.434	1.00	24.25 A
ATOM	371	CA	LYS	A	118	34.091	4.576	−49.602	1.00	25.84 A
ATOM	372	CB	LYS	A	118	35.328	3.776	−49.188	1.00	26.26 A
ATOM	373	CG	LYS	A	118	36.230	3.407	−50.364	1.00	30.30 A
ATOM	374	CD	LYS	A	118	37.218	2.273	−50.035	1.00	31.07 A
ATOM	375	CE	LYS	A	118	36.496	0.934	−49.841	1.00	32.32 A
ATOM	376	NZ	LYS	A	118	37.410	−0.253	−49.726	1.00	29.48 A
ATOM	377	C	LYS	A	118	33.189	3.687	−50.446	1.00	27.75 A
ATOM	378	O	LYS	A	118	33.102	3.836	−51.667	1.00	27.33 A
ATOM	379	N	THR	A	119	32.510	2.765	−49.774	1.00	28.14 A
ATOM	380	CA	THR	A	119	31.637	1.814	−50.438	1.00	28.42 A
ATOM	381	CB	THR	A	119	31.617	0.480	−49.649	1.00	28.33 A
ATOM	382	OG1	THR	A	119	31.330	0.739	−48.269	1.00	29.06 A
ATOM	383	CG2	THR	A	119	32.975	−0.211	−49.738	1.00	27.56 A
ATOM	384	C	THR	A	119	30.223	2.354	−50.631	1.00	29.80 A
ATOM	385	O	THR	A	119	29.297	1.607	−50.955	1.00	28.97 A
ATOM	386	N	ASP	A	120	30.078	3.665	−50.454	1.00	31.38 A
ATOM	387	CA	ASP	A	120	28.790	4.333	−50.605	1.00	32.18 A
ATOM	388	CB	ASP	A	120	28.401	4.406	−52.092	1.00	34.50 A
ATOM	389	CG	ASP	A	120	29.104	5.544	−52.828	1.00	38.27 A
ATOM	390	OD1	ASP	A	120	28.855	6.724	−52.478	1.00	40.42 A
ATOM	391	OD2	ASP	A	120	29.905	5.266	−53.752	1.00	38.92 A
ATOM	392	C	ASP	A	120	27.724	3.599	−49.800	1.00	30.66 A
ATOM	393	O	ASP	A	120	26.683	3.199	−50.323	1.00	31.17 A
ATOM	394	N	GLY	A	121	28.012	3.415	−48.517	1.00	28.44 A
ATOM	395	CA	GLY	A	121	27.087	2.734	−47.634	1.00	26.11 A
ATOM	396	C	GLY	A	121	26.363	3.735	−46.755	1.00	25.00 A
ATOM	397	O	GLY	A	121	26.607	4.944	−46.837	1.00	22.88 A
ATOM	398	N	ILE	A	122	25.484	3.240	−45.894	1.00	23.50 A
ATOM	399	CA	ILE	A	122	24.730	4.131	−45.032	1.00	23.79 A
ATOM	400	CB	ILE	A	122	23.255	4.131	−45.452	1.00	24.10 A
ATOM	401	CG2	ILE	A	122	22.460	3.154	−44.612	1.00	23.83 A
ATOM	402	CG1	ILE	A	122	22.721	5.555	−45.390	1.00	23.51 A
ATOM	403	CD1	ILE	A	122	23.404	6.457	−46.381	1.00	22.10 A
ATOM	404	C	ILE	A	122	24.852	3.766	−43.568	1.00	22.35 A
ATOM	405	O	ILE	A	122	24.598	4.585	−42.685	1.00	21.65 A
ATOM	406	N	GLY	A	123	25.240	2.521	−43.329	1.00	21.64 A
ATOM	407	CA	GLY	A	123	25.405	2.018	−41.980	1.00	20.23 A
ATOM	408	C	GLY	A	123	26.421	0.892	−41.999	1.00	20.31 A
ATOM	409	O	GLY	A	123	26.645	0.250	−43.032	1.00	21.53 A
ATOM	410	N	LEU	A	124	27.051	0.647	−40.860	1.00	19.19 A
ATOM	411	CA	LEU	A	124	28.049	−0.405	−40.784	1.00	18.26 A
ATOM	412	CB	LEU	A	124	29.366	0.095	−41.390	1.00	16.37 A
ATOM	413	CG	LEU	A	124	30.540	−0.878	−41.504	1.00	18.75 A
ATOM	414	CD1	LEU	A	124	30.236	−1.928	−42.573	1.00	20.38 A
ATOM	415	CD2	LEU	A	124	31.803	−0.101	−41.868	1.00	17.41 A
ATOM	416	C	LEU	A	124	28.264	−0.824	−39.336	1.00	17.38 A
ATOM	417	O	LEU	A	124	28.340	0.014	−38.440	1.00	17.30 A
ATOM	418	N	SER	A	125	28.352	−2.128	−39.113	1.00	16.59 A
ATOM	419	CA	SER	A	125	28.578	−2.656	−37.782	1.00	15.38 A
ATOM	420	CB	SER	A	125	27.498	−3.672	−37.429	1.00	15.89 A
ATOM	421	OG	SER	A	125	27.537	−4.772	−38.323	1.00	20.69 A
ATOM	422	C	SER	A	125	29.949	−3.324	−37.790	1.00	14.95 A
ATOM	423	O	SER	A	125	30.388	−3.824	−38.819	1.00	13.32 A
ATOM	424	N	ALA	A	126	30.616	−3.319	−36.641	1.00	13.72 A
ATOM	425	CA	ALA	A	126	31.942	−3.903	−36.498	1.00	14.24 A
ATOM	426	CB	ALA	A	126	32.362	−3.878	−35.034	1.00	13.11 A
ATOM	427	C	ALA	A	126	32.089	−5.318	−37.060	1.00	14.55 A
ATOM	428	O	ALA	A	126	33.113	−5.640	−37.663	1.00	16.65 A
ATOM	429	N	PRO	A	127	31.083	−6.188	−36.859	1.00	15.05 A
ATOM	430	CD	PRO	A	127	29.881	−6.062	−36.012	1.00	13.21 A
ATOM	431	CA	PRO	A	127	31.205	−7.549	−37.395	1.00	14.59 A
ATOM	432	CB	PRO	A	127	29.837	−8.155	−37.104	1.00	15.34 A
ATOM	433	CG	PRO	A	127	29.489	−7.513	−35.782	1.00	14.66 A
ATOM	434	C	PRO	A	127	31.522	−7.518	−38.885	1.00	15.75 A
ATOM	435	O	PRO	A	127	32.242	−8.382	−39.400	1.00	12.00 A
ATOM	436	N	GLN	A	128	30.993	−6.498	−39.559	1.00	15.65 A
ATOM	437	CA	GLN	A	128	31.191	−6.323	−40.993	1.00	17.40 A
ATOM	438	CB	GLN	A	128	30.180	−5.316	−41.542	1.00	16.39 A
ATOM	439	CG	GLN	A	128	28.812	−5.917	−41.778	1.00	18.40 A
ATOM	440	CD	GLN	A	128	27.801	−4.891	−42.228	1.00	20.84 A
ATOM	441	OE1	GLN	A	128	27.428	−4.002	−41.458	1.00	22.13 A
ATOM	442	NE2	GLN	A	128	27.350	−4.999	−43.482	1.00	18.66 A
ATOM	443	C	GLN	A	128	32.603	−5.912	−41.396	1.00	19.05 A
ATOM	444	O	GLN	A	128	32.919	−5.860	−42.584	1.00	20.10 A
ATOM	445	N	VAL	A	129	33.448	−5.608	−40.418	1.00	19.63 A
ATOM	446	CA	VAL	A	129	34.828	−5.241	−40.712	1.00	20.04 A
ATOM	447	CB	VAL	A	129	35.152	−3.775	−40.284	1.00	20.18 A
ATOM	448	CG1	VAL	A	129	34.404	−2.805	−41.161	1.00	18.05 A

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ATOM	449	CG2	VAL	A	129	34.780	−3.546	−38.829	1.00	19.45	A
ATOM	450	C	VAL	A	129	35.773	−6.216	−40.002	1.00	21.14	A
ATOM	451	O	VAL	A	129	36.959	−5.944	−39.844	1.00	21.90	A
ATOM	452	N	GLY	A	130	35.228	−7.348	−39.561	1.00	22.19	A
ATOM	453	CA	GLY	A	130	36.035	−8.368	−38.907	1.00	20.21	A
ATOM	454	C	GLY	A	130	36.113	−8.351	−37.390	1.00	19.73	A
ATOM	455	O	GLY	A	130	36.776	−9.201	−36.790	1.00	18.88	A
ATOM	456	N	LEU	A	131	35.445	−7.396	−36.758	1.00	17.97	A
ATOM	457	CA	LEU	A	131	35.488	−7.307	−35.305	1.00	16.71	A
ATOM	458	CB	LEU	A	131	35.860	−5.890	−34.878	1.00	17.61	A
ATOM	459	CG	LEU	A	131	37.335	−5.519	−35.060	1.00	19.78	A
ATOM	460	CD1	LEU	A	131	37.765	−5.704	−36.509	1.00	21.35	A
ATOM	461	CD2	LEU	A	131	37.539	−4.091	−34.629	1.00	17.99	A
ATOM	462	C	LEU	A	131	34.175	−7.717	−34.662	1.00	16.20	A
ATOM	463	O	LEU	A	131	33.110	−7.171	−34.979	1.00	16.20	A
ATOM	464	N	ASN	A	132	34.249	−8.687	−33.758	1.00	15.11	A
ATOM	465	CA	ASN	A	132	33.049	−9.158	−33.092	1.00	14.07	A
ATOM	466	CB	ASN	A	132	33.109	−10.675	−32.904	1.00	14.53	A
ATOM	467	CG	ASN	A	132	32.921	−11.420	−34.221	1.00	15.08	A
ATOM	468	OD1	ASN	A	132	33.885	−11.786	−34.882	1.00	17.92	A
ATOM	469	ND2	ASN	A	132	31.673	−11.611	−34.617	1.00	13.68	A
ATOM	470	C	ASN	A	132	32.768	−8.444	−31.780	1.00	13.50	A
ATOM	471	O	ASN	A	132	32.749	−9.050	−30.708	1.00	13.65	A
ATOM	472	N	VAL	A	133	32.549	−7.138	−31.890	1.00	12.59	A
ATOM	473	CA	VAL	A	133	32.242	−6.307	−30.741	1.00	13.93	A
ATOM	474	CB	VAL	A	133	33.409	−5.347	−30.416	1.00	10.85	A
ATOM	475	CG1	VAL	A	133	34.607	−6.149	−29.931	1.00	10.23	A
ATOM	476	CG2	VAL	A	133	33.784	−4.544	−31.638	1.00	10.25	A
ATOM	477	C	VAL	A	133	30.971	−5.513	−31.018	1.00	13.57	A
ATOM	478	O	VAL	A	133	30.563	−5.364	−32.162	1.00	13.60	A
ATOM	479	N	GLN	A	134	30.353	−5.002	−29.963	1.00	15.90	A
ATOM	480	CA	GLN	A	134	29.111	−4.246	−30.100	1.00	17.13	A
ATOM	481	CB	GLN	A	134	28.276	−4.439	−28.831	1.00	15.99	A
ATOM	482	CG	GLN	A	134	27.851	−5.906	−28.679	1.00	17.43	A
ATOM	483	CD	GLN	A	134	27.161	−6.217	−27.368	1.00	19.77	A
ATOM	484	OE1	GLN	A	134	26.439	−5.386	−26.822	1.00	23.84	A
ATOM	485	NE2	GLN	A	134	27.359	−7.433	−26.866	1.00	18.29	A
ATOM	486	C	GLN	A	134	29.324	−2.771	−30.423	1.00	16.76	A
ATOM	487	O	GLN	A	134	29.182	−1.900	−29.566	1.00	16.52	A
ATOM	488	N	LEU	A	135	29.672	−2.515	−31.682	1.00	15.24	A
ATOM	489	CA	LEU	A	135	29.928	−1.162	−32.172	1.00	15.82	A
ATOM	490	CB	LEU	A	135	31.436	−0.933	−32.344	1.00	14.00	A
ATOM	491	CG	LEU	A	135	31.828	0.460	−32.840	1.00	15.40	A
ATOM	492	CD1	LEU	A	135	31.450	1.490	−31.775	1.00	14.23	A
ATOM	493	CD2	LEU	A	135	33.322	0.508	−33.163	1.00	12.52	A
ATOM	494	C	LEU	A	135	29.218	−0.931	−33.502	1.00	14.99	A
ATOM	495	O	LEU	A	135	29.251	−1.773	−34.400	1.00	15.49	A
ATOM	496	N	MET	A	136	28.608	0.235	−33.638	1.00	16.04	A
ATOM	497	CA	MET	A	136	27.859	0.561	−34.841	1.00	18.35	A
ATOM	498	CB	MET	A	136	26.396	0.180	−34.588	1.00	19.43	A
ATOM	499	CG	MET	A	136	25.375	0.880	−35.438	1.00	23.19	A
ATOM	500	SD	MET	A	136	23.777	0.872	−34.619	1.00	26.18	A
ATOM	501	CE	MET	A	136	23.640	−0.872	−34.190	1.00	22.49	A
ATOM	502	C	MET	A	136	27.967	2.039	−35.255	1.00	19.14	A
ATOM	503	O	MET	A	136	28.119	2.934	−34.408	1.00	18.03	A
ATOM	504	N	VAL	A	137	27.904	2.284	−36.563	1.00	18.64	A
ATOM	505	CA	VAL	A	137	27.941	3.643	−37.094	1.00	19.57	A
ATOM	506	CB	VAL	A	137	29.354	4.075	−37.558	1.00	21.08	A
ATOM	507	CG1	VAL	A	137	30.374	3.826	−36.451	1.00	20.89	A
ATOM	508	CG2	VAL	A	137	29.723	3.356	−38.854	1.00	20.49	A
ATOM	509	C	VAL	A	137	27.018	3.757	−38.301	1.00	20.02	A
ATOM	510	O	VAL	A	137	26.667	2.754	−38.933	1.00	18.78	A
ATOM	511	N	PHE	A	138	26.621	4.985	−38.614	1.00	20.79	A
ATOM	512	CA	PHE	A	138	25.771	5.225	−39.762	1.00	22.08	A
ATOM	513	CB	PHE	A	138	24.451	4.446	−39.629	1.00	23.84	A
ATOM	514	CG	PHE	A	138	23.535	4.947	−38.549	1.00	22.93	A
ATOM	515	CD1	PHE	A	138	22.588	5.926	−38.822	1.00	25.45	A
ATOM	516	CD2	PHE	A	138	23.584	4.405	−37.268	1.00	25.82	A
ATOM	517	CE1	PHE	A	138	21.692	6.357	−37.832	1.00	24.76	A
ATOM	518	CE2	PHE	A	138	22.697	4.829	−36.271	1.00	25.19	A
ATOM	519	CZ	PHE	A	138	21.748	5.807	−36.558	1.00	24.73	A
ATOM	520	C	PHE	A	138	25.511	6.705	−39.982	1.00	23.31	A
ATOM	521	O	PHE	A	138	25.671	7.530	−39.071	1.00	21.01	A
ATOM	522	N	ASN	A	139	25.137	7.026	−41.216	1.00	24.83	A
ATOM	523	CA	ASN	A	139	24.838	8.388	−41.622	1.00	26.78	A
ATOM	524	CB	ASN	A	139	26.104	9.080	−42.113	1.00	28.84	A
ATOM	525	CG	ASN	A	139	25.919	10.574	−42.268	1.00	31.35	A
ATOM	526	OD1	ASN	A	139	24.951	11.031	−42.876	1.00	29.99	A
ATOM	527	ND2	ASN	A	139	26.850	11.346	−41.717	1.00	31.87	A

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ATOM	528	C	ASN	A	139	23.826	8.305	−42.762	1.00	27.67 A
ATOM	529	O	ASN	A	139	24.147	7.834	−43.850	1.00	26.38 A
ATOM	530	N	PRO	A	140	22.587	8.762	−42.522	1.00	28.57 A
ATOM	531	CD	PRO	A	140	22.108	9.409	−41.288	1.00	27.09 A
ATOM	532	CA	PRO	A	140	21.525	8.733	−43.531	1.00	29.40 A
ATOM	533	CB	PRO	A	140	20.451	9.626	−42.923	1.00	27.26 A
ATOM	534	CG	PRO	A	140	20.606	9.366	−41.472	1.00	28.54 A
ATOM	535	C	PRO	A	140	21.976	9.231	−44.892	1.00	29.84 A
ATOM	536	O	PRO	A	140	21.655	8.635	−45.914	1.00	30.11 A
ATOM	537	N	ALA	A	141	22.716	10.332	−44.897	1.00	31.08 A
ATOM	538	CA	ALA	A	141	23.200	10.921	−46.138	1.00	33.10 A
ATOM	539	CB	ALA	A	141	23.945	12.207	−45.838	1.00	32.04 A
ATOM	540	C	ALA	A	141	24.095	9.969	−46.928	1.00	34.75 A
ATOM	541	O	ALA	A	141	23.899	9.777	−48.129	1.00	34.87 A
ATOM	542	N	GLY	A	142	25.079	9.380	−46.253	1.00	36.61 A
ATOM	543	CA	GLY	A	142	25.989	8.461	−46.916	1.00	38.38 A
ATOM	544	C	GLY	A	142	27.181	9.178	−47.519	1.00	39.97 A
ATOM	545	O	GLY	A	142	28.022	8.559	−48.175	1.00	40.45 A
ATOM	546	N	GLU	A	143	27.248	10.487	−47.293	1.00	41.61 A
ATOM	547	CA	GLU	A	143	28.327	11.321	−47.808	1.00	43.02 A
ATOM	548	CB	GLU	A	143	27.765	12.402	−48.737	1.00	44.16 A
ATOM	549	CG	GLU	A	143	26.697	11.917	−49.707	1.00	47.41 A
ATOM	550	CD	GLU	A	143	27.262	11.131	−50.874	1.00	49.37 A
ATOM	551	OE1	GLU	A	143	28.046	10.183	−50.645	1.00	50.56 A
ATOM	552	OE2	GLU	A	143	26.914	11.463	−52.027	1.00	51.60 A
ATOM	553	C	GLU	A	143	29.014	12.000	−46.630	1.00	43.65 A
ATOM	554	O	GLU	A	143	28.353	12.483	−45.710	1.00	42.94 A
ATOM	555	N	PRO	A	144	30.351	12.046	−46.639	1.00	44.50 A
ATOM	556	CD	PRO	A	144	31.298	11.494	−47.620	1.00	44.64 A
ATOM	557	CA	PRO	A	144	31.062	12.690	−45.535	1.00	45.86 A
ATOM	558	CB	PRO	A	144	32.525	12.567	−45.947	1.00	44.41 A
ATOM	559	CG	PRO	A	144	32.539	11.336	−46.788	1.00	44.69 A
ATOM	560	C	PRO	A	144	30.624	14.146	−45.431	1.00	47.73 A
ATOM	561	O	PRO	A	144	30.269	14.765	−46.437	1.00	49.56 A
ATOM	562	N	GLY	A	145	30.639	14.684	−44.216	1.00	48.72 A
ATOM	563	CA	GLY	A	145	30.260	16.070	−44.010	1.00	50.25 A
ATOM	564	C	GLY	A	145	29.010	16.538	−44.735	1.00	51.98 A
ATOM	565	O	GLY	A	145	28.889	17.719	−45.063	1.00	51.37 A
ATOM	566	N	GLU	A	146	28.074	15.625	−44.986	1.00	53.56 A
ATOM	567	CA	GLU	A	146	26.834	15.989	−45.664	1.00	54.37 A
ATOM	568	CB	GLU	A	146	26.947	15.734	−47.175	1.00	56.97 A
ATOM	569	CG	GLU	A	146	25.797	16.333	−47.990	1.00	61.12 A
ATOM	570	CD	GLU	A	146	25.915	16.063	−49.483	1.00	64.36 A
ATOM	571	OE1	GLU	A	146	25.957	14.876	−49.877	1.00	65.64 A
ATOM	572	OE2	GLU	A	146	25.961	17.040	−50.263	1.00	66.22 A
ATOM	573	C	GLU	A	146	25.640	15.224	−45.099	1.00	52.66 A
ATOM	574	O	GLU	A	146	24.731	14.850	−45.833	1.00	53.40 A
ATOM	575	N	GLY	A	147	25.646	14.994	−43.790	1.00	51.08 A
ATOM	576	CA	GLY	A	147	24.546	14.281	−43.167	1.00	48.20 A
ATOM	577	C	GLY	A	147	24.567	14.368	−41.652	1.00	46.60 A
ATOM	578	O	GLY	A	147	24.767	15.442	−41.080	1.00	46.48 A
ATOM	579	N	LYS	A	148	24.361	13.230	−40.997	1.00	44.44 A
ATOM	580	CA	LYS	A	148	24.353	13.171	−39.541	1.00	42.17 A
ATOM	581	CB	LYS	A	148	22.908	13.167	−39.032	1.00	44.06 A
ATOM	582	CG	LYS	A	148	22.653	13.989	−37.773	1.00	44.66 A
ATOM	583	CD	LYS	A	148	23.184	13.323	−36.515	1.00	46.34 A
ATOM	584	CE	LYS	A	148	22.674	14.052	−35.271	1.00	47.35 A
ATOM	585	NZ	LYS	A	148	23.051	13.382	−33.995	1.00	48.38 A
ATOM	586	C	LYS	A	148	25.064	11.889	−39.126	1.00	40.11 A
ATOM	587	O	LYS	A	148	24.509	10.799	−39.251	1.00	39.43 A
ATOM	588	N	GLU	A	149	26.297	12.020	−38.646	1.00	37.37 A
ATOM	589	CA	GLU	A	149	27.062	10.853	−38.227	1.00	35.24 A
ATOM	590	CB	GLU	A	149	28.559	11.133	−38.288	1.00	33.46 A
ATOM	591	CG	GLU	A	149	29.049	11.512	−39.662	1.00	33.59 A
ATOM	592	CD	GLU	A	149	30.535	11.306	−39.810	1.00	32.30 A
ATOM	593	OE1	GLU	A	149	31.252	11.517	−38.809	1.00	29.90 A
ATOM	594	OE2	GLU	A	149	30.982	10.943	−40.923	1.00	31.18 A
ATOM	595	C	GLU	A	149	26.692	10.414	−36.823	1.00	33.65 A
ATOM	596	O	GLU	A	149	26.843	11.169	−35.863	1.00	33.30 A
ATOM	597	N	ILE	A	150	26.210	9.180	−36.715	1.00	31.34 A
ATOM	598	CA	ILE	A	150	25.808	8.622	−35.434	1.00	28.27 A
ATOM	599	CB	ILE	A	150	24.303	8.325	−35.411	1.00	28.74 A
ATOM	600	CG2	ILE	A	150	23.948	7.564	−34.138	1.00	27.91 A
ATOM	601	CG1	ILE	A	150	23.518	9.634	−35.538	1.00	29.27 A
ATOM	602	CD1	ILE	A	150	22.030	9.449	−35.777	1.00	31.15 A
ATOM	603	C	ILE	A	150	26.541	7.326	−35.156	1.00	26.22 A
ATOM	604	O	ILE	A	150	26.504	6.400	−35.965	1.00	27.50 A
ATOM	605	N	VAL	A	151	27.218	7.265	−34.017	1.00	22.94 A
ATOM	606	CA	VAL	A	151	27.931	6.057	−33.629	1.00	21.78 A

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ATOM	607	CB	VAL	A	151	29.468	6.322	−33.492	1.00	21.52	A
ATOM	608	CG1	VAL	A	151	29.748	7.803	−33.617	1.00	20.75	A
ATOM	609	CG2	VAL	A	151	30.001	5.774	−32.182	1.00	19.13	A
ATOM	610	C	VAL	A	151	27.319	5.577	−32.316	1.00	20.78	A
ATOM	611	O	VAL	A	151	26.936	6.390	−31.473	1.00	22.39	A
ATOM	612	N	LEU	A	152	27.196	4.264	−32.152	1.00	19.13	A
ATOM	613	CA	LEU	A	152	26.600	3.716	−30.938	1.00	19.50	A
ATOM	614	CB	LEU	A	152	25.161	3.260	−31.223	1.00	19.10	A
ATOM	615	CG	LEU	A	152	24.193	4.305	−31.798	1.00	24.16	A
ATOM	616	CD1	LEU	A	152	23.081	3.618	−32.569	1.00	24.32	A
ATOM	617	CD2	LEU	A	152	23.618	5.156	−30.677	1.00	24.79	A
ATOM	618	C	LEU	A	152	27.392	2.545	−30.353	1.00	17.69	A
ATOM	619	O	LEU	A	152	27.678	1.571	−31.049	1.00	16.33	A
ATOM	620	N	VAL	A	153	27.742	2.641	−29.073	1.00	15.12	A
ATOM	621	CA	VAL	A	153	28.466	1.563	−28.409	1.00	14.13	A
ATOM	622	CB	VAL	A	153	29.672	2.096	−27.611	1.00	13.29	A
ATOM	623	CG1	VAL	A	153	30.442	0.939	−26.997	1.00	12.78	A
ATOM	624	CG2	VAL	A	153	30.578	2.901	−28.514	1.00	14.26	A
ATOM	625	C	VAL	A	153	27.498	0.843	−27.457	1.00	15.36	A
ATOM	626	O	VAL	A	153	26.748	1.491	−26.719	1.00	12.91	A
ATOM	627	N	ASN	A	154	27.530	−0.492	−27.480	1.00	15.63	A
ATOM	628	CA	ASN	A	154	26.653	−1.334	−26.658	1.00	16.94	A
ATOM	629	CB	ASN	A	154	27.180	−1.448	−25.225	1.00	15.99	A
ATOM	630	CG	ASN	A	154	28.646	−1.828	−25.171	1.00	17.69	A
ATOM	631	OD1	ASN	A	154	29.097	−2.698	−25.915	1.00	17.61	A
ATOM	632	ND2	ASN	A	154	29.398	−1.182	−24.282	1.00	15.37	A
ATOM	633	C	ASN	A	154	25.216	−0.801	−26.632	1.00	17.66	A
ATOM	634	O	ASN	A	154	24.666	−0.510	−25.571	1.00	17.48	A
ATOM	635	N	PRO	A	155	24.588	−0.677	−27.814	1.00	18.56	A
ATOM	636	CD	PRO	A	155	25.183	−0.907	−29.138	1.00	18.26	A
ATOM	637	CA	PRO	A	155	23.215	−0.181	−27.950	1.00	18.44	A
ATOM	638	CB	PRO	A	155	23.056	0.004	−29.459	1.00	17.65	A
ATOM	639	CG	PRO	A	155	24.458	0.102	−29.966	1.00	19.09	A
ATOM	640	C	PRO	A	155	22.173	−1.157	−27.412	1.00	18.75	A
ATOM	641	O	PRO	A	155	22.277	−2.365	−27.606	1.00	19.82	A
ATOM	642	N	LYS	A	156	21.162	−0.622	−26.745	1.00	20.00	A
ATOM	643	CA	LYS	A	156	20.082	−1.441	−26.221	1.00	20.87	A
ATOM	644	CB	LYS	A	156	20.150	−1.499	−24.701	1.00	21.41	A
ATOM	645	CG	LYS	A	156	21.482	−1.949	−24.167	1.00	26.83	A
ATOM	646	CD	LYS	A	156	21.488	−1.995	−22.637	1.00	30.30	A
ATOM	647	CE	LYS	A	156	21.449	−0.601	−22.030	1.00	34.64	A
ATOM	648	NZ	LYS	A	156	21.678	−0.636	−20.551	1.00	36.85	A
ATOM	649	C	LYS	A	156	18.751	−0.824	−26.653	1.00	21.39	A
ATOM	650	O	LYS	A	156	18.532	0.388	−26.514	1.00	19.74	A
ATOM	651	N	ILE	A	157	17.869	−1.649	−27.198	1.00	22.00	A
ATOM	652	CA	ILE	A	157	16.571	−1.148	−27.616	1.00	24.95	A
ATOM	653	CB	ILE	A	157	15.983	−1.978	−28.781	1.00	24.61	A
ATOM	654	CG2	ILE	A	157	14.540	−1.559	−29.045	1.00	24.26	A
ATOM	655	CG1	ILE	A	157	16.834	−1.779	−30.038	1.00	24.91	A
ATOM	656	CD1	ILE	A	157	16.258	−2.433	−31.290	1.00	25.22	A
ATOM	657	C	ILE	A	157	15.634	−1.204	−26.422	1.00	26.62	A
ATOM	658	O	ILE	A	157	15.236	−2.284	−25.988	1.00	25.35	A
ATOM	659	N	LYS	A	158	15.306	−0.035	−25.879	1.00	30.00	A
ATOM	660	CA	LYS	A	158	14.411	0.052	−24.732	1.00	32.44	A
ATOM	661	CB	LYS	A	158	14.584	1.393	−24.009	1.00	34.21	A
ATOM	662	CG	LYS	A	158	15.822	1.460	−23.114	1.00	36.80	A
ATOM	663	CD	LYS	A	158	15.721	0.464	−21.965	1.00	37.85	A
ATOM	664	CE	LYS	A	158	17.089	0.107	−21.389	1.00	40.17	A
ATOM	665	NZ	LYS	A	158	17.827	1.271	−20.817	1.00	40.51	A
ATOM	666	C	LYS	A	158	12.969	−0.119	−25.170	1.00	32.94	A
ATOM	667	O	LYS	A	158	12.183	−0.765	−24.486	1.00	34.80	A
ATOM	668	N	LYS	A	159	12.623	0.456	−26.314	1.00	33.25	A
ATOM	669	CA	LYS	A	159	11.269	0.349	−26.834	1.00	34.87	A
ATOM	670	CB	LYS	A	159	10.367	1.438	−26.235	1.00	37.06	A
ATOM	671	CG	LYS	A	159	10.126	1.305	−24.736	1.00	40.70	A
ATOM	672	CD	LYS	A	159	9.057	2.265	−24.239	1.00	42.38	A
ATOM	673	CE	LYS	A	159	8.687	1.963	−22.787	1.00	44.63	A
ATOM	674	NZ	LYS	A	159	7.473	2.710	−22.322	1.00	46.12	A
ATOM	675	C	LYS	A	159	11.269	0.495	−28.340	1.00	34.89	A
ATOM	676	O	LYS	A	159	12.135	1.161	−28.903	1.00	35.59	A
ATOM	677	N	TYR	A	160	10.311	−0.147	−28.996	1.00	35.44	A
ATOM	678	CA	TYR	A	160	10.187	−0.025	−30.439	1.00	36.62	A
ATOM	679	CB	TYR	A	160	10.842	−1.208	−31.162	1.00	42.19	A
ATOM	680	CG	TYR	A	160	10.445	−2.569	−30.673	1.00	47.11	A
ATOM	681	CD1	TYR	A	160	9.143	−3.037	−30.838	1.00	50.34	A
ATOM	682	CE1	TYR	A	160	8.776	−4.314	−30.407	1.00	53.27	A
ATOM	683	CD2	TYR	A	160	11.381	−3.405	−30.062	1.00	49.07	A
ATOM	684	CE2	TYR	A	160	11.030	−4.677	−29.626	1.00	52.79	A
ATOM	685	CZ	TYR	A	160	9.723	−5.129	−29.802	1.00	54.17	A

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ATOM	686	OH	TYR	A	160	9.363	−6.395	−29.381	1.00	56.97 A
ATOM	687	C	TYR	A	160	8.718	0.129	−30.812	1.00	33.35 A
ATOM	688	O	TYR	A	160	7.833	−0.296	−30.077	1.00	33.80 A
ATOM	689	N	SER	A	161	8.469	0.770	−31.945	1.00	28.83 A
ATOM	690	CA	SER	A	161	7.117	1.037	−32.406	1.00	25.47 A
ATOM	691	CB	SER	A	161	7.175	1.761	−33.756	1.00	25.05 A
ATOM	692	OG	SER	A	161	5.877	2.039	−34.248	1.00	25.20 A
ATOM	693	C	SER	A	161	6.227	−0.194	−32.525	1.00	24.00 A
ATOM	694	O	SER	A	161	6.699	−1.310	−32.736	1.00	25.13 A
ATOM	695	N	ASP	A	162	4.927	0.016	−32.377	1.00	20.81 A
ATOM	696	CA	ASP	A	162	3.988	−1.078	−32.512	1.00	18.67 A
ATOM	697	CB	ASP	A	162	2.924	−1.012	−31.404	1.00	17.74 A
ATOM	698	CG	ASP	A	162	2.043	0.224	−31.491	1.00	20.48 A
ATOM	699	OD1	ASP	A	162	2.411	1.197	−32.193	1.00	19.28 A
ATOM	700	OD2	ASP	A	162	0.974	0.216	−30.832	1.00	20.44 A
ATOM	701	C	ASP	A	162	3.361	−1.031	−33.917	1.00	17.19 A
ATOM	702	O	ASP	A	162	2.405	−1.748	−34.214	1.00	16.88 A
ATOM	703	N	LYS	A	163	3.922	−0.185	−34.778	1.00	13.19 A
ATOM	704	CA	LYS	A	163	3.458	−0.060	−36.157	1.00	14.42 A
ATOM	705	CB	LYS	A	163	3.063	1.392	−36.465	1.00	17.11 A
ATOM	706	CG	LYS	A	163	2.008	1.943	−35.516	1.00	21.55 A
ATOM	707	CD	LYS	A	163	1.511	3.321	−35.933	1.00	25.69 A
ATOM	708	CE	LYS	A	163	0.470	3.836	−34.942	1.00	26.67 A
ATOM	709	NZ	LYS	A	163	−0.163	5.115	−35.373	1.00	30.99 A
ATOM	710	C	LYS	A	163	4.563	−0.515	−37.114	1.00	14.12 A
ATOM	711	O	LYS	A	163	5.709	−0.067	−37.029	1.00	11.38 A
ATOM	712	N	LEU	A	164	4.207	−1.405	−38.032	1.00	14.88 A
ATOM	713	CA	LEU	A	164	5.167	−1.934	−38.987	1.00	15.75 A
ATOM	714	CB	LEU	A	164	4.933	−3.430	−39.182	1.00	16.05 A
ATOM	715	CG	LEU	A	164	5.202	−4.299	−37.953	1.00	17.46 A
ATOM	716	CD1	LEU	A	164	4.720	−5.716	−38.219	1.00	15.64 A
ATOM	717	CD2	LEU	A	164	6.696	−4.269	−37.617	1.00	16.61 A
ATOM	718	C	LEU	A	164	5.153	−1.251	−40.340	1.00	17.09 A
ATOM	719	O	LEU	A	164	4.097	−0.893	−40.865	1.00	17.75 A
ATOM	720	N	VAL	A	165	6.343	−1.066	−40.900	1.00	17.38 A
ATOM	721	CA	VAL	A	165	6.466	−0.457	−42.209	1.00	18.26 A
ATOM	722	CB	VAL	A	165	6.899	1.017	−42.118	1.00	16.51 A
ATOM	723	CG1	VAL	A	165	5.763	1.841	−41.511	1.00	16.42 A
ATOM	724	CG2	VAL	A	165	8.172	1.145	−41.290	1.00	17.21 A
ATOM	725	C	VAL	A	165	7.469	−1.243	−43.045	1.00	19.14 A
ATOM	726	O	VAL	A	165	8.433	−1.808	−42.518	1.00	20.01 A
ATOM	727	N	PRO	A	166	7.234	−1.316	−44.362	1.00	19.02 A
ATOM	728	CD	PRO	A	166	5.982	−0.965	−45.062	1.00	18.32 A
ATOM	729	CA	PRO	A	166	8.137	−2.047	−45.251	1.00	20.65 A
ATOM	730	CB	PRO	A	166	7.195	−2.543	−46.340	1.00	20.89 A
ATOM	731	CG	PRO	A	166	6.284	−1.350	−46.503	1.00	19.48 A
ATOM	732	C	PRO	A	166	9.222	−1.132	−45.805	1.00	21.42 A
ATOM	733	O	PRO	A	166	9.073	0.087	−45.803	1.00	21.01 A
ATOM	734	N	PHE	A	167	10.312	−1.728	−46.275	1.00	23.28 A
ATOM	735	CA	PHE	A	167	11.405	−0.966	−46.859	1.00	25.18 A
ATOM	736	CB	PHE	A	167	12.141	−0.176	−45.779	1.00	28.27 A
ATOM	737	CG	PHE	A	167	13.095	0.840	−46.325	1.00	33.26 A
ATOM	738	CD1	PHE	A	167	12.637	2.083	−46.751	1.00	35.31 A
ATOM	739	CD2	PHE	A	167	14.450	0.540	−46.459	1.00	36.84 A
ATOM	740	CE1	PHE	A	167	13.514	3.022	−47.308	1.00	37.46 A
ATOM	741	CE2	PHE	A	167	15.341	1.468	−47.014	1.00	38.88 A
ATOM	742	CZ	PHE	A	167	14.870	2.714	−47.440	1.00	38.07 A
ATOM	743	C	PHE	A	167	12.375	−1.919	−47.547	1.00	24.62 A
ATOM	744	O	PHE	A	167	12.677	−2.981	−47.010	1.00	24.38 A
ATOM	745	N	ASP	A	168	12.837	−1.562	−48.745	1.00	25.04 A
ATOM	746	CA	ASP	A	168	13.791	−2.414	−49.456	1.00	25.00 A
ATOM	747	CB	ASP	A	168	13.804	−2.116	−50.958	1.00	27.03 A
ATOM	748	CG	ASP	A	168	12.478	−2.418	−51.629	1.00	28.34 A
ATOM	749	OD1	ASP	A	168	11.679	−3.193	−51.063	1.00	30.93 A
ATOM	750	OD2	ASP	A	168	12.239	−1.890	−52.736	1.00	31.05 A
ATOM	751	C	ASP	A	168	15.155	−2.113	−48.861	1.00	24.01 A
ATOM	752	O	ASP	A	168	15.679	−1.010	−49.002	1.00	23.88 A
ATOM	753	N	GLU	A	169	15.723	−3.095	−48.182	1.00	23.69 A
ATOM	754	CA	GLU	A	169	17.011	−2.908	−47.532	1.00	23.00 A
ATOM	755	CB	GLU	A	169	16.997	−3.555	−46.149	1.00	23.01 A
ATOM	756	CG	GLU	A	169	16.073	−2.907	−45.142	1.00	24.80 A
ATOM	757	CD	GLU	A	169	16.034	−3.679	−43.833	1.00	25.40 A
ATOM	758	OE1	GLU	A	169	17.108	−4.145	−43.398	1.00	24.55 A
ATOM	759	OE2	GLU	A	169	14.940	−3.814	−43.240	1.00	25.14 A
ATOM	760	C	GLU	A	169	18.182	−3.478	−48.305	1.00	21.78 A
ATOM	761	O	GLU	A	169	18.068	−4.495	−48.979	1.00	21.39 A
ATOM	762	N	GLY	A	170	19.312	−2.797	−48.196	1.00	20.18 A
ATOM	763	CA	GLY	A	170	20.526	−3.262	−48.826	1.00	19.41 A
ATOM	764	C	GLY	A	170	21.488	−3.541	−47.684	1.00	19.42 A

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ATOM	765	O	GLY	A	170	21.205	−3.179	−46.533	1.00	18.09 A
ATOM	766	N	CYS	A	171	22.609	−4.189	−47.983	1.00	17.85 A
ATOM	767	CA	CYS	A	171	23.617	−4.495	−46.973	1.00	17.78 A
ATOM	768	CB	CYS	A	171	23.274	−5.793	−46.222	1.00	17.35 A
ATOM	769	SG	CYS	A	171	24.482	−6.273	−44.946	1.00	17.05 A
ATOM	770	C	CYS	A	171	24.956	−4.644	−47.667	1.00	17.66 A
ATOM	771	O	CYS	A	171	25.051	−5.264	−48.731	1.00	18.62 A
ATOM	772	N	LEU	A	172	25.988	−4.071	−47.060	1.00	18.65 A
ATOM	773	CA	LEU	A	172	27.337	−4.120	−47.607	1.00	17.51 A
ATOM	774	CB	LEU	A	172	28.268	−3.218	−46.780	1.00	18.35 A
ATOM	775	CG	LEU	A	172	28.433	−1.739	−47.177	1.00	18.16 A
ATOM	776	CD1	LEU	A	172	27.382	−1.317	−48.180	1.00	19.26 A
ATOM	777	CD2	LEU	A	172	28.373	−0.875	−45.930	1.00	17.19 A
ATOM	778	C	LEU	A	172	27.895	−5.537	−47.672	1.00	17.16 A
ATOM	779	O	LEU	A	172	28.819	−5.811	−48.438	1.00	19.43 A
ATOM	780	N	SER	A	173	27.335	−6.442	−46.879	1.00	15.56 A
ATOM	781	CA	SER	A	173	27.807	−7.822	−46.880	1.00	15.09 A
ATOM	782	CB	SER	A	173	27.627	−8.438	−45.498	1.00	13.35 A
ATOM	783	OG	SER	A	173	28.432	−7.766	−44.542	1.00	13.38 A
ATOM	784	C	SER	A	173	27.077	−8.668	−47.920	1.00	16.25 A
ATOM	785	O	SER	A	173	27.318	−9.872	−48.037	1.00	16.75 A
ATOM	786	N	PHE	A	174	26.180	−8.029	−48.664	1.00	16.57 A
ATOM	787	CA	PHE	A	174	25.396	−8.688	−49.709	1.00	17.10 A
ATOM	788	CB	PHE	A	174	23.954	−8.905	−49.235	1.00	18.18 A
ATOM	789	CG	PHE	A	174	23.819	−9.875	−48.085	1.00	17.61 A
ATOM	790	CD1	PHE	A	174	23.432	−11.196	−48.313	1.00	17.43 A
ATOM	791	CD2	PHE	A	174	24.047	−9.461	−46.775	1.00	18.73 A
ATOM	792	CE1	PHE	A	174	23.267	−12.091	−47.253	1.00	16.70 A
ATOM	793	CE2	PHE	A	174	23.887	−10.352	−45.703	1.00	19.19 A
ATOM	794	CZ	PHE	A	174	23.495	−11.670	−45.946	1.00	18.29 A
ATOM	795	C	PHE	A	174	25.413	−7.748	−50.916	1.00	16.80 A
ATOM	796	O	PHE	A	174	24.402	−7.142	−51.276	1.00	16.00 A
ATOM	797	N	PRO	A	175	26.576	−7.627	−51.562	1.00	18.42 A
ATOM	798	CD	PRO	A	175	27.766	−8.470	−51.335	1.00	17.82 A
ATOM	799	CA	PRO	A	175	26.771	−6.762	−52.728	1.00	19.70 A
ATOM	800	CB	PRO	A	175	28.048	−7.317	−53.350	1.00	20.05 A
ATOM	801	CG	PRO	A	175	28.826	−7.755	−52.138	1.00	18.23 A
ATOM	802	C	PRO	A	175	25.617	−6.700	−53.716	1.00	20.20 A
ATOM	803	O	PRO	A	175	25.240	−7.710	−54.312	1.00	20.33 A
ATOM	804	N	GLY	A	176	25.059	−5.497	−53.866	1.00	21.23 A
ATOM	805	CA	GLY	A	176	23.968	−5.260	−54.800	1.00	19.68 A
ATOM	806	C	GLY	A	176	22.669	−6.019	−54.598	1.00	18.84 A
ATOM	807	O	GLY	A	176	21.826	−6.065	−55.498	1.00	16.30 A
ATOM	808	N	ILE	A	177	22.487	−6.621	−53.430	1.00	18.40 A
ATOM	809	CA	ILE	A	177	21.256	−7.355	−53.186	1.00	19.40 A
ATOM	810	CB	ILE	A	177	21.547	−8.683	−52.450	1.00	19.34 A
ATOM	811	CG2	ILE	A	177	20.250	−9.372	−52.066	1.00	20.31 A
ATOM	812	CG1	ILE	A	177	22.398	−9.584	−53.352	1.00	20.29 A
ATOM	813	CD1	ILE	A	177	22.776	−10.927	−52.735	1.00	18.41 A
ATOM	814	C	ILE	A	177	20.278	−6.498	−52.391	1.00	19.23 A
ATOM	815	O	ILE	A	177	20.642	−5.904	−51.378	1.00	18.56 A
ATOM	816	N	TYR	A	178	19.043	−6.408	−52.878	1.00	20.54 A
ATOM	817	CA	TYR	A	178	18.014	−5.624	−52.199	1.00	22.95 A
ATOM	818	CB	TYR	A	178	17.813	−4.266	−52.879	1.00	24.10 A
ATOM	819	CG	TYR	A	178	19.064	−3.420	−52.962	1.00	27.38 A
ATOM	820	CD1	TYR	A	178	20.069	−3.721	−53.888	1.00	26.85 A
ATOM	821	CE1	TYR	A	178	21.235	−2.962	−53.962	1.00	27.02 A
ATOM	822	CD2	TYR	A	178	19.258	−2.330	−52.106	1.00	26.90 A
ATOM	823	CE2	TYR	A	178	20.431	−1.560	−52.176	1.00	28.14 A
ATOM	824	CZ	TYR	A	178	21.414	−1.888	−53.111	1.00	28.84 A
ATOM	825	OH	TYR	A	178	22.577	−1.147	−53.210	1.00	30.05 A
ATOM	826	C	TYR	A	178	16.680	−6.352	−52.154	1.00	22.69 A
ATOM	827	O	TYR	A	178	16.192	−6.839	−53.175	1.00	23.47 A
ATOM	828	N	ALA	A	179	16.095	−6.430	−50.965	1.00	21.13 A
ATOM	829	CA	ALA	A	179	14.801	−7.085	−50.800	1.00	21.16 A
ATOM	830	CB	ALA	A	179	14.991	−8.557	−50.478	1.00	20.57 A
ATOM	831	C	ALA	A	179	14.021	−6.390	−49.697	1.00	21.14 A
ATOM	832	O	ALA	A	179	14.597	−5.699	−48.855	1.00	21.11 A
ATOM	833	N	GLU	A	180	12.706	−6.569	−49.706	1.00	21.61 A
ATOM	834	CA	GLU	A	180	11.842	−5.929	−48.721	1.00	22.07 A
ATOM	835	CB	GLU	A	180	10.399	−5.943	−49.230	1.00	24.22 A
ATOM	836	CG	GLU	A	180	9.437	−5.163	−48.352	1.00	27.20 A
ATOM	837	CD	GLU	A	180	8.021	−5.150	−48.893	1.00	27.70 A
ATOM	838	OE1	GLU	A	180	7.245	−6.075	−48.568	1.00	27.79 A
ATOM	839	OE2	GLU	A	180	7.691	−4.210	−49.649	1.00	27.64 A
ATOM	840	C	GLU	A	180	11.880	−6.526	−47.306	1.00	20.52 A
ATOM	841	O	GLU	A	180	11.805	−7.736	−47.124	1.00	20.89 A
ATOM	842	N	VAL	A	181	11.993	−5.664	−46.304	1.00	19.74 A
ATOM	843	CA	VAL	A	181	11.995	−6.112	−44.916	1.00	20.39 A

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ATOM	844	CB	VAL	A	181	13.399	−5.964	−44.264	1.00	20.82 A
ATOM	845	CG1	VAL	A	181	13.372	−6.508	−42.840	1.00	20.17 A
ATOM	846	CG2	VAL	A	181	14.450	−6.708	−45.089	1.00	18.51 A
ATOM	847	C	VAL	A	181	10.984	−5.268	−44.136	1.00	20.46 A
ATOM	848	O	VAL	A	181	10.877	−4.063	−44.352	1.00	20.70 A
ATOM	849	N	VAL	A	182	10.224	−5.901	−43.248	1.00	20.35 A
ATOM	850	CA	VAL	A	182	9.235	−5.183	−42.443	1.00	19.16 A
ATOM	851	CB	VAL	A	182	7.881	−5.935	−42.419	1.00	20.20 A
ATOM	852	CG1	VAL	A	182	6.865	−5.168	−41.587	1.00	19.98 A
ATOM	853	CG2	VAL	A	182	7.365	−6.120	−43.841	1.00	20.58 A
ATOM	854	C	VAL	A	182	9.738	−5.020	−41.011	1.00	17.95 A
ATOM	855	O	VAL	A	182	10.083	−6.001	−40.353	1.00	18.95 A
ATOM	856	N	ARG	A	183	9.789	−3.781	−40.531	1.00	16.50 A
ATOM	857	CA	ARG	A	183	10.257	−3.516	−39.169	1.00	14.82 A
ATOM	858	CB	ARG	A	183	11.713	−3.036	−39.167	1.00	15.48 A
ATOM	859	CG	ARG	A	183	12.749	−3.901	−39.862	1.00	12.14 A
ATOM	860	CD	ARG	A	183	14.098	−3.199	−39.730	1.00	13.95 A
ATOM	861	NE	ARG	A	183	15.172	−3.826	−40.492	1.00	14.27 A
ATOM	862	CZ	ARG	A	183	15.907	−4.844	−40.062	1.00	14.82 A
ATOM	863	NH1	ARG	A	183	15.687	−5.361	−38.856	1.00	13.88 A
ATOM	864	NH2	ARG	A	183	16.863	−5.342	−40.845	1.00	10.27 A
ATOM	865	C	ARG	A	183	9.436	−2.421	−38.502	1.00	15.01 A
ATOM	866	O	ARG	A	183	8.731	−1.658	−39.172	1.00	13.85 A
ATOM	867	N	PRO	A	184	9.512	−2.332	−37.161	1.00	14.58 A
ATOM	868	CD	PRO	A	184	10.141	−3.264	−36.206	1.00	13.75 A
ATOM	869	CA	PRO	A	184	8.764	−1.285	−36.458	1.00	14.05 A
ATOM	870	CB	PRO	A	184	9.171	−1.496	−35.001	1.00	13.48 A
ATOM	871	CG	PRO	A	184	9.379	−2.981	−34.926	1.00	13.61 A
ATOM	872	C	PRO	A	184	9.287	0.035	−37.030	1.00	13.54 A
ATOM	873	O	PRO	A	184	10.463	0.123	−37.394	1.00	12.47 A
ATOM	874	N	GLN	A	185	8.437	1.052	−37.121	1.00	14.24 A
ATOM	875	CA	GLN	A	185	8.867	2.326	−37.703	1.00	16.35 A
ATOM	876	CB	GLN	A	185	7.647	3.160	−38.144	1.00	16.49 A
ATOM	877	CG	GLN	A	185	6.647	3.488	−37.053	1.00	18.19 A
ATOM	878	CD	GLN	A	185	5.486	4.339	−37.562	1.00	20.93 A
ATOM	879	OE1	GLN	A	185	5.126	4.276	−38.735	1.00	22.48 A
ATOM	880	NE2	GLN	A	185	4.886	5.126	−36.672	1.00	19.77 A
ATOM	881	C	GLN	A	185	9.783	3.191	−36.843	1.00	16.52 A
ATOM	882	O	GLN	A	185	10.467	4.071	−37.358	1.00	16.86 A
ATOM	883	N	SER	A	186	9.804	2.951	−35.540	1.00	17.54 A
ATOM	884	CA	SER	A	186	10.642	3.749	−34.655	1.00	17.28 A
ATOM	885	CB	SER	A	186	9.888	4.984	−34.193	1.00	16.83 A
ATOM	886	OG	SER	A	186	8.814	4.597	−33.365	1.00	16.18 A
ATOM	887	C	SER	A	186	11.087	2.963	−33.433	1.00	18.56 A
ATOM	888	O	SER	A	186	10.483	1.948	−33.072	1.00	17.15 A
ATOM	889	N	VAL	A	187	12.145	3.454	−32.794	1.00	18.41 A
ATOM	890	CA	VAL	A	187	12.707	2.812	−31.614	1.00	17.19 A
ATOM	891	CB	VAL	A	187	13.880	1.875	−31.990	1.00	16.71 A
ATOM	892	CG1	VAL	A	187	13.376	0.651	−32.717	1.00	14.52 A
ATOM	893	CG2	VAL	A	187	14.868	2.629	−32.869	1.00	16.52 A
ATOM	894	C	VAL	A	187	13.257	3.845	−30.643	1.00	19.68 A
ATOM	895	O	VAL	A	187	13.471	5.012	−30.991	1.00	17.36 A
ATOM	896	N	LYS	A	188	13.488	3.379	−29.422	1.00	22.44 A
ATOM	897	CA	LYS	A	188	14.041	4.170	−28.333	1.00	24.50 A
ATOM	898	CB	LYS	A	188	13.044	4.223	−27.175	1.00	27.86 A
ATOM	899	CG	LYS	A	188	13.634	4.704	−25.858	1.00	32.55 A
ATOM	900	CD	LYS	A	188	12.604	4.645	−24.724	1.00	37.24 A
ATOM	901	CE	LYS	A	188	11.438	5.613	−24.952	1.00	39.23 A
ATOM	902	NZ	LYS	A	188	10.474	5.621	−23.803	1.00	40.21 A
ATOM	903	C	LYS	A	188	15.291	3.399	−27.925	1.00	24.24 A
ATOM	904	O	LYS	A	188	15.202	2.222	−27.574	1.00	25.34 A
ATOM	905	N	ILE	A	189	16.449	4.049	−27.976	1.00	25.02 A
ATOM	906	CA	ILE	A	189	17.707	3.382	−27.648	1.00	25.74 A
ATOM	907	CB	ILE	A	189	18.677	3.413	−28.853	1.00	25.43 A
ATOM	908	CG2	ILE	A	189	19.959	2.665	−28.520	1.00	27.70 A
ATOM	909	CG1	ILE	A	189	18.010	2.801	−30.084	1.00	25.02 A
ATOM	910	CD1	ILE	A	189	17.209	3.794	−30.886	1.00	26.73 A
ATOM	911	C	ILE	A	189	18.476	3.936	−26.452	1.00	26.55 A
ATOM	912	O	ILE	A	189	18.340	5.098	−26.080	1.00	28.56 A
ATOM	913	N	ASP	A	190	19.296	3.071	−25.867	1.00	26.77 A
ATOM	914	CA	ASP	A	190	20.167	3.398	−24.745	1.00	25.30 A
ATOM	915	CB	ASP	A	190	19.769	2.591	−23.506	1.00	27.91 A
ATOM	916	CG	ASP	A	190	19.126	3.447	−22.425	1.00	29.11 A
ATOM	917	OD1	ASP	A	190	18.312	4.335	−22.757	1.00	32.09 A
ATOM	918	OD2	ASP	A	190	19.428	3.220	−21.235	1.00	31.65 A
ATOM	919	C	ASP	A	190	21.527	2.930	−25.249	1.00	23.53 A
ATOM	920	O	ASP	A	190	21.631	1.846	−25.814	1.00	25.23 A
ATOM	921	N	ALA	A	191	22.564	3.735	−25.073	1.00	20.98 A
ATOM	922	CA	ALA	A	191	23.889	3.339	−25.536	1.00	19.22 A

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ATOM	923	CB	ALA	A	191	23.975	3.501	−27.052	1.00	16.43 A
ATOM	924	C	ALA	A	191	24.961	4.179	−24.869	1.00	16.73 A
ATOM	925	O	ALA	A	191	24.659	5.021	−24.031	1.00	14.46 A
ATOM	926	N	ARG	A	192	26.215	3.932	−25.241	1.00	17.62 A
ATOM	927	CA	ARG	A	192	27.344	4.701	−24.719	1.00	16.89 A
ATOM	928	CB	ARG	A	192	28.344	3.813	−23.983	1.00	14.64 A
ATOM	929	CG	ARG	A	192	27.849	3.112	−22.736	1.00	16.43 A
ATOM	930	CD	ARG	A	192	28.933	2.152	−22.266	1.00	14.30 A
ATOM	931	NE	ARG	A	192	28.564	1.361	−21.099	1.00	17.12 A
ATOM	932	CZ	ARG	A	192	28.434	1.847	−19.868	1.00	17.79 A
ATOM	933	NH1	ARG	A	192	28.638	3.137	−19.629	1.00	18.41 A
ATOM	934	NH2	ARG	A	192	28.116	1.035	−18.869	1.00	16.93 A
ATOM	935	C	ARG	A	192	28.060	5.305	−25.921	1.00	16.09 A
ATOM	936	O	ARG	A	192	27.943	4.800	−27.029	1.00	14.43 A
ATOM	937	N	ASP	A	193	28.808	6.378	−25.691	1.00	17.73 A
ATOM	938	CA	ASP	A	193	29.574	7.023	−26.750	1.00	19.68 A
ATOM	939	CB	ASP	A	193	29.559	8.543	−26.557	1.00	21.17 A
ATOM	940	CG	ASP	A	193	30.420	8.997	−25.394	1.00	22.73 A
ATOM	941	OD1	ASP	A	193	30.523	8.270	−24.381	1.00	23.37 A
ATOM	942	OD2	ASP	A	193	30.991	10.101	−25.493	1.00	26.89 A
ATOM	943	C	ASP	A	193	30.997	6.462	−26.634	1.00	19.97 A
ATOM	944	O	ASP	A	193	31.235	5.571	−25.815	1.00	17.40 A
ATOM	945	N	ILE	A	194	31.937	6.971	−27.430	1.00	20.45 A
ATOM	946	CA	ILE	A	194	33.304	6.451	−27.385	1.00	21.45 A
ATOM	947	CB	ILE	A	194	34.173	6.962	−28.554	1.00	21.84 A
ATOM	948	CG2	ILE	A	194	33.679	6.381	−29.862	1.00	22.88 A
ATOM	949	CG1	ILE	A	194	34.180	8.488	−28.592	1.00	22.27 A
ATOM	950	CD1	ILE	A	194	35.136	9.058	−29.644	1.00	23.29 A
ATOM	951	C	ILE	A	194	34.057	6.732	−26.093	1.00	22.29 A
ATOM	952	O	ILE	A	194	35.073	6.098	−25.824	1.00	23.35 A
ATOM	953	N	THR	A	195	33.574	7.676	−25.292	1.00	21.53 A
ATOM	954	CA	THR	A	195	34.248	7.978	−24.035	1.00	22.32 A
ATOM	955	CB	THR	A	195	34.119	9.478	−23.636	1.00	21.72 A
ATOM	956	OG1	THR	A	195	32.741	9.811	−23.418	1.00	18.57 A
ATOM	957	CG2	THR	A	195	34.694	10.370	−24.723	1.00	20.26 A
ATOM	958	C	THR	A	195	33.632	7.118	−22.941	1.00	22.63 A
ATOM	959	O	THR	A	195	34.074	7.143	−21.791	1.00	21.86 A
ATOM	960	N	GLY	A	196	32.601	6.363	−23.313	1.00	23.03 A
ATOM	961	CA	GLY	A	196	31.930	5.493	−22.365	1.00	23.21 A
ATOM	962	C	GLY	A	196	30.759	6.147	−21.660	1.00	24.01 A
ATOM	963	O	GLY	A	196	30.146	5.535	−20.792	1.00	23.82 A
ATOM	964	N	GLU	A	197	30.445	7.389	−22.019	1.00	26.36 A
ATOM	965	CA	GLU	A	197	29.325	8.080	−21.391	1.00	27.87 A
ATOM	966	CB	GLU	A	197	29.437	9.598	−21.558	1.00	30.06 A
ATOM	967	CG	GLU	A	197	30.667	10.225	−20.908	1.00	35.75 A
ATOM	968	CD	GLU	A	197	30.787	9.923	−19.420	1.00	39.16 A
ATOM	969	OE1	GLU	A	197	31.824	10.299	−18.825	1.00	42.10 A
ATOM	970	OE2	GLU	A	197	29.857	9.312	−18.844	1.00	39.72 A
ATOM	971	C	GLU	A	197	28.037	7.593	−22.020	1.00	27.80 A
ATOM	972	O	GLU	A	197	27.955	7.420	−23.236	1.00	28.26 A
ATOM	973	N	ARG	A	198	27.031	7.365	−21.189	1.00	28.14 A
ATOM	974	CA	ARG	A	198	25.753	6.885	−21.682	1.00	28.82 A
ATOM	975	CB	ARG	A	198	24.991	6.185	−20.561	1.00	32.41 A
ATOM	976	CG	ARG	A	198	25.853	5.255	−19.720	1.00	37.31 A
ATOM	977	CD	ARG	A	198	25.068	4.036	−19.282	1.00	42.63 A
ATOM	978	NE	ARG	A	198	24.541	3.322	−20.444	1.00	46.58 A
ATOM	979	CZ	ARG	A	198	24.024	2.100	−20.403	1.00	48.75 A
ATOM	980	NH1	ARG	A	198	23.964	1.445	−19.247	1.00	48.98 A
ATOM	981	NH2	ARG	A	198	23.564	1.535	−21.518	1.00	48.98 A
ATOM	982	C	ARG	A	198	24.900	8.016	−22.243	1.00	27.54 A
ATOM	983	O	ARG	A	198	25.071	9.189	−21.891	1.00	27.87 A
ATOM	984	N	PHE	A	199	23.986	7.653	−23.132	1.00	25.20 A
ATOM	985	CA	PHE	A	199	23.079	8.613	−23.728	1.00	23.21 A
ATOM	986	CB	PHE	A	199	23.769	9.393	−24.858	1.00	21.17 A
ATOM	987	CG	PHE	A	199	24.088	8.572	−26.084	1.00	19.11 A
ATOM	988	CD1	PHE	A	199	23.124	8.359	−27.070	1.00	17.06 A
ATOM	989	CD2	PHE	A	199	25.373	8.049	−26.273	1.00	18.18 A
ATOM	990	CE1	PHE	A	199	23.437	7.639	−28.232	1.00	17.14 A
ATOM	991	CE2	PHE	A	199	25.698	7.328	−27.425	1.00	14.22 A
ATOM	992	CZ	PHE	A	199	24.731	7.124	−28.407	1.00	16.27 A
ATOM	993	C	PHE	A	199	21.859	7.871	−24.243	1.00	23.72 A
ATOM	994	O	PHE	A	199	21.898	6.659	−24.450	1.00	21.75 A
ATOM	995	N	SER	A	200	20.769	8.600	−24.431	1.00	25.35 A
ATOM	996	CA	SER	A	200	19.541	8.000	−24.915	1.00	26.06 A
ATOM	997	CB	SER	A	200	18.551	7.844	−23.767	1.00	26.35 A
ATOM	998	OG	SER	A	200	19.115	7.060	−22.732	1.00	29.16 A
ATOM	999	C	SER	A	200	18.941	8.867	−25.996	1.00	26.17 A
ATOM	1000	O	SER	A	200	18.994	10.092	−25.915	1.00	27.31 A
ATOM	1001	N	ILE	A	201	18.376	8.226	−27.013	1.00	26.58 A

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ATOM	1002	CA	ILE	A	201	17.756	8.942	−28.118	1.00	26.23 A
ATOM	1003	CB	ILE	A	201	18.762	9.214	−29.250	1.00	28.26 A
ATOM	1004	CG2	ILE	A	201	19.813	10.216	−28.790	1.00	29.33 A
ATOM	1005	CG1	ILE	A	201	19.394	7.895	−29.701	1.00	28.98 A
ATOM	1006	CD1	ILE	A	201	20.230	8.010	−30.962	1.00	31.66 A
ATOM	1007	C	ILE	A	201	16.593	8.152	−28.709	1.00	25.11 A
ATOM	1008	O	ILE	A	201	16.418	6.958	−28.434	1.00	23.45 A
ATOM	1009	N	SER	A	202	15.796	8.833	−29.522	1.00	24.09 A
ATOM	1010	CA	SER	A	202	14.657	8.209	−30.180	1.00	23.76 A
ATOM	1011	CB	SER	A	202	13.356	8.918	−29.802	1.00	23.27 A
ATOM	1012	OG	SER	A	202	13.018	8.677	−28.447	1.00	26.12 A
ATOM	1013	C	SER	A	202	14.864	8.297	−31.676	1.00	22.76 A
ATOM	1014	O	SER	A	202	15.181	9.357	−32.205	1.00	20.95 A
ATOM	1015	N	LEU	A	203	14.708	7.178	−32.364	1.00	22.93 A
ATOM	1016	CA	LEU	A	203	14.871	7.193	−33.804	1.00	23.93 A
ATOM	1017	CB	LEU	A	203	16.005	6.257	−34.237	1.00	23.48 A
ATOM	1018	CG	LEU	A	203	17.387	6.575	−33.669	1.00	23.22 A
ATOM	1019	CD1	LEU	A	203	18.414	5.669	−34.321	1.00	23.21 A
ATOM	1020	CD2	LEU	A	203	17.727	8.039	−33.914	1.00	21.89 A
ATOM	1021	C	LEU	A	203	13.585	6.795	−34.498	1.00	23.86 A
ATOM	1022	O	LEU	A	203	12.781	6.024	−33.966	1.00	24.42 A
ATOM	1023	N	SER	A	204	13.396	7.350	−35.685	1.00	25.11 A
ATOM	1024	CA	SER	A	204	12.237	7.060	−36.514	1.00	27.28 A
ATOM	1025	CB	SER	A	204	11.111	8.051	−36.236	1.00	28.55 A
ATOM	1026	OG	SER	A	204	11.482	9.351	−36.658	1.00	30.10 A
ATOM	1027	C	SER	A	204	12.741	7.248	−37.934	1.00	27.55 A
ATOM	1028	O	SER	A	204	13.933	7.502	−38.137	1.00	27.70 A
ATOM	1029	N	ARG	A	205	11.845	7.133	−38.910	1.00	28.31 A
ATOM	1030	CA	ARG	A	205	12.221	7.315	−40.307	1.00	28.06 A
ATOM	1031	CB	ARG	A	205	12.594	8.777	−40.569	1.00	31.86 A
ATOM	1032	CG	ARG	A	205	11.428	9.756	−40.709	1.00	36.98 A
ATOM	1033	CD	ARG	A	205	11.988	11.169	−40.867	1.00	40.88 A
ATOM	1034	NE	ARG	A	205	11.122	12.070	−41.621	1.00	44.32 A
ATOM	1035	CZ	ARG	A	205	11.423	13.343	−41.879	1.00	47.87 A
ATOM	1036	NH1	ARG	A	205	12.568	13.861	−41.442	1.00	48.05 A
ATOM	1037	NH2	ARG	A	205	10.583	14.107	−42.573	1.00	48.10 A
ATOM	1038	C	ARG	A	205	13.396	6.424	−40.706	1.00	25.68 A
ATOM	1039	O	ARG	A	205	13.523	5.293	−40.235	1.00	24.48 A
ATOM	1040	N	LEU	A	206	14.261	6.958	−41.563	1.00	21.87 A
ATOM	1041	CA	LEU	A	206	15.413	6.219	−42.057	1.00	19.85 A
ATOM	1042	CB	LEU	A	206	16.115	7.006	−43.166	1.00	20.52 A
ATOM	1043	CG	LEU	A	206	17.278	6.277	−43.856	1.00	23.37 A
ATOM	1044	CD1	LEU	A	206	16.765	5.016	−44.565	1.00	20.22 A
ATOM	1045	CD2	LEU	A	206	17.951	7.217	−44.853	1.00	22.79 A
ATOM	1046	C	LEU	A	206	16.420	5.854	−40.974	1.00	18.21 A
ATOM	1047	O	LEU	A	206	16.921	4.727	−40.953	1.00	16.21 A
ATOM	1048	N	PRO	A	207	16.742	6.799	−40.069	1.00	16.71 A
ATOM	1049	CD	PRO	A	207	16.439	8.245	−40.087	1.00	17.35 A
ATOM	1050	CA	PRO	A	207	17.709	6.487	−39.008	1.00	17.46 A
ATOM	1051	CB	PRO	A	207	17.795	7.794	−38.217	1.00	16.29 A
ATOM	1052	CG	PRO	A	207	17.588	8.828	−39.283	1.00	16.84 A
ATOM	1053	C	PRO	A	207	17.264	5.305	−38.154	1.00	16.91 A
ATOM	1054	O	PRO	A	207	18.084	4.484	−37.747	1.00	18.14 A
ATOM	1055	N	ALA	A	208	15.963	5.212	−37.896	1.00	16.46 A
ATOM	1056	CA	ALA	A	208	15.437	4.106	−37.104	1.00	15.91 A
ATOM	1057	CB	ALA	A	208	13.967	4.344	−36.780	1.00	16.38 A
ATOM	1058	C	ALA	A	208	15.597	2.800	−37.883	1.00	14.15 A
ATOM	1059	O	ALA	A	208	15.932	1.763	−37.320	1.00	14.30 A
ATOM	1060	N	ARG	A	209	15.357	2.862	−39.187	1.00	14.77 A
ATOM	1061	CA	ARG	A	209	15.473	1.686	−40.041	1.00	14.78 A
ATOM	1062	CB	ARG	A	209	14.910	1.999	−41.434	1.00	16.76 A
ATOM	1063	CG	ARG	A	209	14.841	0.804	−42.360	1.00	18.33 A
ATOM	1064	CD	ARG	A	209	14.418	−0.437	−41.596	1.00	22.27 A
ATOM	1065	NE	ARG	A	209	13.889	−1.463	−42.480	1.00	25.66 A
ATOM	1066	CZ	ARG	A	209	12.611	−1.556	−42.834	1.00	28.46 A
ATOM	1067	NH1	ARG	A	209	11.709	−0.687	−42.377	1.00	27.84 A
ATOM	1068	NH2	ARG	A	209	12.235	−2.516	−43.659	1.00	28.08 A
ATOM	1069	C	ARG	A	209	16.934	1.210	−40.145	1.00	14.81 A
ATOM	1070	O	ARG	A	209	17.224	0.025	−40.001	1.00	12.46 A
ATOM	1071	N	ILE	A	210	17.854	2.137	−40.389	1.00	13.90 A
ATOM	1072	CA	ILE	A	210	19.261	1.774	−40.482	1.00	13.38 A
ATOM	1073	CB	ILE	A	210	20.138	3.010	−40.830	1.00	14.75 A
ATOM	1074	CG2	ILE	A	210	21.620	2.649	−40.768	1.00	13.71 A
ATOM	1075	CG1	ILE	A	210	19.775	3.526	−42.229	1.00	12.89 A
ATOM	1076	CD1	ILE	A	210	20.449	4.828	−42.600	1.00	11.08 A
ATOM	1077	C	ILE	A	210	19.709	1.200	−39.140	1.00	14.16 A
ATOM	1078	O	ILE	A	210	20.444	0.210	−39.092	1.00	12.22 A
ATOM	1079	N	PHE	A	211	19.247	1.816	−38.050	1.00	13.33 A
ATOM	1080	CA	PHE	A	211	19.622	1.358	−36.718	1.00	13.42 A

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ATOM	1081	CB	PHE	A	211	18.978	2.221	−35.634	1.00	13.55	A
ATOM	1082	CG	PHE	A	211	19.137	1.642	−34.261	1.00	10.76	A
ATOM	1083	CD1	PHE	A	211	20.323	1.815	−33.555	1.00	10.51	A
ATOM	1084	CD2	PHE	A	211	18.145	0.827	−33.719	1.00	11.87	A
ATOM	1085	CE1	PHE	A	211	20.522	1.175	−32.328	1.00	11.75	A
ATOM	1086	CE2	PHE	A	211	18.338	0.179	−32.489	1.00	9.24	A
ATOM	1087	CZ	PHE	A	211	19.527	0.355	−31.797	1.00	8.29	A
ATOM	1088	C	PHE	A	211	19.275	−0.107	−36.421	1.00	13.34	A
ATOM	1089	O	PHE	A	211	20.108	−0.863	−35.901	1.00	12.59	A
ATOM	1090	N	GLN	A	212	18.039	−0.495	−36.721	1.00	11.92	A
ATOM	1091	CA	GLN	A	212	17.590	−1.860	−36.468	1.00	13.18	A
ATOM	1092	CB	GLN	A	212	16.084	−1.968	−36.702	1.00	12.41	A
ATOM	1093	CG	GLN	A	212	15.287	−1.129	−35.730	1.00	14.52	A
ATOM	1094	CD	GLN	A	212	13.820	−1.126	−36.049	1.00	16.44	A
ATOM	1095	OE1	GLN	A	212	13.102	−2.070	−35.732	1.00	18.15	A
ATOM	1096	NE2	GLN	A	212	13.362	−0.067	−36.698	1.00	17.06	A
ATOM	1097	C	GLN	A	212	18.341	−2.887	−37.313	1.00	13.31	A
ATOM	1098	O	GLN	A	212	18.689	−3.976	−36.823	1.00	12.33	A
ATOM	1099	N	HIS	A	213	18.584	−2.543	−38.574	1.00	12.02	A
ATOM	1100	CA	HIS	A	213	19.326	−3.421	−39.470	1.00	13.70	A
ATOM	1101	CB	HIS	A	213	19.485	−2.754	−40.845	1.00	15.78	A
ATOM	1102	CG	HIS	A	213	20.385	−3.497	−41.785	1.00	16.70	A
ATOM	1103	CD2	HIS	A	213	21.733	−3.494	−41.917	1.00	18.08	A
ATOM	1104	ND1	HIS	A	213	19.914	−4.410	−42.704	1.00	19.47	A
ATOM	1105	CE1	HIS	A	213	20.932	−4.939	−43.361	1.00	18.40	A
ATOM	1106	NE2	HIS	A	213	22.047	−4.401	−42.901	1.00	18.23	A
ATOM	1107	C	HIS	A	213	20.712	−3.679	−38.856	1.00	13.57	A
ATOM	1108	O	HIS	A	213	21.184	−4.822	−38.832	1.00	13.81	A
ATOM	1109	N	GLU	A	214	21.347	−2.621	−38.346	1.00	11.88	A
ATOM	1110	CA	GLU	A	214	22.686	−2.741	−37.750	1.00	13.61	A
ATOM	1111	CB	GLU	A	214	23.372	−1.374	−37.656	1.00	13.71	A
ATOM	1112	CG	GLU	A	214	23.547	−0.614	−38.972	1.00	14.63	A
ATOM	1113	CD	GLU	A	214	24.277	−1.403	−40.055	1.00	17.21	A
ATOM	1114	OE1	CLU	A	214	25.122	−2.266	−39.730	1.00	15.04	A
ATOM	1115	OE2	GLU	A	214	24.015	−1.132	−41.250	1.00	21.39	A
ATOM	1116	C	GLU	A	214	22.671	−3.376	−36.361	1.00	14.65	A
ATOM	1117	O	GLU	A	214	23.628	−4.041	−35.957	1.00	14.69	A
ATOM	1118	N	TYR	A	215	21.594	−3.155	−35.620	1.00	16.18	A
ATOM	1119	CA	TYR	A	215	21.488	−3.742	−34.298	1.00	15.85	A
ATOM	1120	CB	TYR	A	215	20.218	−3.261	−33.587	1.00	17.67	A
ATOM	1121	CG	TYR	A	215	20.067	−3.844	−32.196	1.00	21.32	A
ATOM	1122	CD1	TYR	A	215	20.887	−3.421	−31.148	1.00	19.48	A
ATOM	1123	CE1	TYR	A	215	20.798	−4.003	−29.883	1.00	20.09	A
ATOM	1124	CD2	TYR	A	215	19.143	−4.866	−31.940	1.00	20.98	A
ATOM	1125	CE2	TYR	A	215	19.046	−5.452	−30.680	1.00	20.75	A
ATOM	1126	CZ	TYR	A	215	19.879	−5.020	−29.654	1.00	21.44	A
ATOM	1127	OH	TYR	A	215	19.821	−5.626	−28.413	1.00	18.89	A
ATOM	1128	C	TYR	A	215	21.452	−5.260	−34.472	1.00	14.58	A
ATOM	1129	O	TYR	A	215	22.055	−6.007	−33.689	1.00	14.06	A
ATOM	1130	N	ASP	A	216	20.750	−5.710	−35.506	1.00	13.46	A
ATOM	1131	CA	ASP	A	216	20.657	−7.135	−35.787	1.00	14.06	A
ATOM	1132	CB	ASP	A	216	19.780	−7.388	−37.008	1.00	13.61	A
ATOM	1133	CG	ASP	A	216	18.308	−7.427	−36.671	1.00	13.64	A
ATOM	1134	OD1	ASP	A	216	17.957	−7.402	−35.475	1.00	12.49	A
ATOM	1135	OD2	ASP	A	216	17.495	−7.489	−37.611	1.00	15.97	A
ATOM	1136	C	ASP	A	216	22.041	−7.720	−36.031	1.00	15.02	A
ATOM	1137	O	ASP	A	216	22.353	−8.823	−35.557	1.00	16.95	A
ATOM	1138	N	HIS	A	217	22.863	−6.988	−36.779	1.00	13.44	A
ATOM	1139	CA	HIS	A	217	24.218	−7.433	−37.065	1.00	13.38	A
ATOM	1140	CB	HIS	A	217	25.011	−6.350	−37.810	1.00	13.13	A
ATOM	1141	CG	HIS	A	217	24.825	−6.370	−39.293	1.00	14.65	A
ATOM	1142	CD2	HIS	A	217	24.458	−5.397	−40.160	1.00	16.14	A
ATOM	1143	ND1	HIS	A	217	25.054	−7.495	−40.056	1.00	14.89	A
ATOM	1144	CE1	HIS	A	217	24.836	−7.214	−41.328	1.00	14.42	A
ATOM	1145	NE2	HIS	A	217	24.473	−5.948	−41.418	1.00	17.14	A
ATOM	1146	C	HIS	A	217	24.906	−7.717	−35.736	1.00	14.40	A
ATOM	1147	O	HIS	A	217	25.659	−8.684	−35.604	1.00	12.69	A
ATOM	1148	N	LEU	A	218	24.644	−6.864	−34.750	1.00	14.83	A
ATOM	1149	CA	LEU	A	218	25.255	−7.037	−33.445	1.00	14.51	A
ATOM	1150	CB	LEU	A	218	25.053	−5.766	−32.611	1.00	12.54	A
ATOM	1151	CG	LEU	A	218	25.713	−4.539	−33.285	1.00	17.61	A
ATOM	1152	CD1	LEU	A	218	25.643	−3.309	−32.390	1.00	16.94	A
ATOM	1153	CD2	LEU	A	218	27.180	−4.856	−33.619	1.00	14.59	A
ATOM	1154	C	LEU	A	218	24.727	−8.291	−32.741	1.00	15.91	A
ATOM	1155	O	LEU	A	218	25.375	−8.827	−31.846	1.00	17.34	A
ATOM	1156	N	GLU	A	219	23.564	−8.774	−33.164	1.00	15.63	A
ATOM	1157	CA	GLU	A	219	22.994	−9.983	−32.586	1.00	18.38	A
ATOM	1158	CB	GLU	A	219	21.467	−9.865	−32.462	1.00	22.20	A
ATOM	1159	CG	GLU	A	219	20.962	−8.892	−31.401	1.00	27.10	A

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ATOM	1160	CD	GLU	A	219	21.262	−9.346	−29.987	1.00	30.86 A
ATOM	1161	OE1	GLU	A	219	21.025	−10.535	−29.673	1.00	33.62 A
ATOM	1162	OE2	GLU	A	219	21.723	−8.510	−29.183	1.00	34.35 A
ATOM	1163	C	GLU	A	219	23.327	−11.184	−33.477	1.00	17.11 A
ATOM	1164	O	GLU	A	219	22.786	−12.272	−33.283	1.00	17.19 A
ATOM	1165	N	GLY	A	220	24.220	−10.983	−34.444	1.00	14.72 A
ATOM	1166	CA	GLY	A	220	24.580	−12.056	−35.356	1.00	12.31 A
ATOM	1167	C	GLY	A	220	23.423	−12.355	−36.302	1.00	15.10 A
ATOM	1168	O	GLY	A	220	23.401	−13.389	−36.979	1.00	14.67 A
ATOM	1169	N	VAL	A	221	22.456	−11.437	−36.347	1.00	14.21 A
ATOM	1170	CA	VAL	A	221	21.278	−11.581	−37.191	1.00	14.18 A
ATOM	1171	CB	VAL	A	221	20.023	−11.047	−36.462	1.00	17.59 A
ATOM	1172	CG1	VAL	A	221	18.802	−11.120	−37.377	1.00	17.23 A
ATOM	1173	CG2	VAL	A	221	19.791	−11.844	−35.182	1.00	15.15 A
ATOM	1174	C	VAL	A	221	21.418	−10.848	−38.529	1.00	14.45 A
ATOM	1175	O	VAL	A	221	21.732	−9.657	−38.568	1.00	11.29 A
ATOM	1176	N	LEU	A	222	21.176	−11.571	−39.620	1.00	13.92 A
ATOM	1177	CA	LEU	A	222	21.269	−11.004	−40.965	1.00	15.74 A
ATOM	1178	CB	LEU	A	222	21.972	−12.000	−41.893	1.00	13.26 A
ATOM	1179	CG	LEU	A	222	23.492	−11.841	−42.001	1.00	13.73 A
ATOM	1180	CD1	LEU	A	222	24.070	−11.302	−40.699	1.00	13.62 A
ATOM	1181	CD2	LEU	A	222	24.119	−13.182	−42.379	1.00	12.93 A
ATOM	1182	C	LEU	A	222	19.886	−10.639	−41.496	1.00	15.93 A
ATOM	1183	O	LEU	A	222	18.906	−11.326	−41.198	1.00	16.25 A
ATOM	1184	N	PHE	A	223	19.811	−9.579	−42.302	1.00	17.16 A
ATOM	1185	CA	PHE	A	223	18.529	−9.097	−42.815	1.00	15.87 A
ATOM	1186	CB	PHE	A	223	18.722	−7.817	−43.661	1.00	17.74 A
ATOM	1187	CG	PHE	A	223	19.229	−8.044	−45.073	1.00	18.05 A
ATOM	1188	CD1	PHE	A	223	20.177	−9.023	−45.361	1.00	19.74 A
ATOM	1189	CD2	PHE	A	223	18.803	−7.207	−46.109	1.00	18.79 A
ATOM	1190	CE1	PHE	A	223	20.694	−9.161	−46.658	1.00	17.18 A
ATOM	1191	CE2	PHE	A	223	19.312	−7.333	−47.407	1.00	14.65 A
ATOM	1192	CZ	PHE	A	223	20.259	−8.311	−47.680	1.00	18.55 A
ATOM	1193	C	PHE	A	223	17.635	−10.089	−43.539	1.00	17.30 A
ATOM	1194	O	PHE	A	223	16.408	−9.948	−43.493	1.00	16.29 A
ATOM	1195	N	PHE	A	224	18.207	−11.103	−44.187	1.00	16.43 A
ATOM	1196	CA	PHE	A	224	17.341	−12.058	−44.861	1.00	15.78 A
ATOM	1197	CB	PHE	A	224	18.116	−12.898	−45.906	1.00	14.49 A
ATOM	1198	CG	PHE	A	224	19.045	−13.945	−45.331	1.00	12.96 A
ATOM	1199	CD1	PHE	A	224	18.548	−15.152	−44.854	1.00	11.77 A
ATOM	1200	CD2	PHE	A	224	20.430	−13.742	−45.334	1.00	12.30 A
ATOM	1201	CE1	PHE	A	224	19.421	−16.150	−44.392	1.00	12.19 A
ATOM	1202	CE2	PHE	A	224	21.314	−14.720	−44.877	1.00	7.51 A
ATOM	1203	CZ	PHE	A	224	20.812	−15.930	−44.405	1.00	13.32 A
ATOM	1204	C	PHE	A	224	16.636	−12.923	−43.818	1.00	17.87 A
ATOM	1205	O	PHE	A	224	15.608	−13.541	−44.115	1.00	16.51 A
ATOM	1206	N	ASP	A	225	17.175	−12.930	−42.592	1.00	17.97 A
ATOM	1207	CA	ASP	A	225	16.586	−13.692	−41.484	1.00	17.66 A
ATOM	1208	CB	ASP	A	225	17.426	−13.586	−40.186	1.00	16.43 A
ATOM	1209	CG	ASP	A	225	18.781	−14.305	−40.260	1.00	18.04 A
ATOM	1210	OD1	ASP	A	225	18.941	−15.266	−41.040	1.00	16.53 A
ATOM	1211	OD2	ASP	A	225	19.697	−13.911	−39.504	1.00	17.05 A
ATOM	1212	C	ASP	A	225	15.182	−13.151	−41.163	1.00	18.56 A
ATOM	1213	O	ASP	A	225	14.311	−13.894	−40.713	1.00	18.42 A
ATOM	1214	N	ARG	A	226	14.969	−11.858	−41.386	1.00	18.50 A
ATOM	1215	CA	ARG	A	226	13.681	−11.240	−41.072	1.00	21.41 A
ATOM	1216	CB	ARG	A	226	13.915	−9.901	−40.360	1.00	22.31 A
ATOM	1217	CG	ARG	A	226	14.890	−10.019	−39.186	1.00	25.19 A
ATOM	1218	CD	ARG	A	226	15.206	−8.683	−38.564	1.00	28.37 A
ATOM	1219	NE	ARG	A	226	14.317	−8.367	−37.451	1.00	32.73 A
ATOM	1220	CZ	ARG	A	226	14.361	−8.965	−36.264	1.00	35.61 A
ATOM	1221	NH1	ARG	A	226	15.258	−9.916	−36.031	1.00	38.22 A
ATOM	1222	NH2	ARG	A	226	13.503	−8.621	−35.310	1.00	35.12 A
ATOM	1223	C	ARG	A	226	12.758	−11.044	−42.279	1.00	21.52 A
ATOM	1224	O	ARG	A	226	11.689	−10.447	−42.165	1.00	21.42 A
ATOM	1225	N	MET	A	227	13.166	−11.559	−43.433	1.00	20.50 A
ATOM	1226	CA	MET	A	227	12.345	−11.432	−44.628	1.00	20.39 A
ATOM	1227	CB	MET	A	227	13.202	−11.585	−45.884	1.00	18.95 A
ATOM	1228	CG	MET	A	227	14.359	−10.619	−45.971	1.00	18.23 A
ATOM	1229	SD	MET	A	227	15.261	−10.828	−47.512	1.00	16.76 A
ATOM	1230	CE	MET	A	227	16.117	−9.282	−47.571	1.00	16.68 A
ATOM	1231	C	MET	A	227	11.275	−12.515	−44.620	1.00	19.32 A
ATOM	1232	O	MET	A	227	11.432	−13.547	−43.969	1.00	17.02 A
ATOM	1233	N	THR	A	228	10.180	−12.271	−45.324	1.00	19.28 A
ATOM	1234	CA	THR	A	228	9.129	−13.269	−45.401	1.00	23.61 A
ATOM	1235	CB	THR	A	228	7.854	−12.705	−46.062	1.00	23.79 A
ATOM	1236	OG1	THR	A	228	8.189	−12.120	−47.327	1.00	22.17 A
ATOM	1237	CG2	THR	A	228	7.213	−11.645	−45.165	1.00	20.55 A
ATOM	1238	C	THR	A	228	9.671	−14.415	−46.247	1.00	26.65 A

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ATOM	1239	O	THR	A	228	10.715	−14.282	−46.899	1.00	25.82 A
ATOM	1240	N	ASP	A	229	8.977	−15.544	−46.232	1.00	29.30 A
ATOM	1241	CA	ASP	A	229	9.418	−16.689	−47.014	1.00	32.65 A
ATOM	1242	CB	ASP	A	229	8.494	−17.890	−46.756	1.00	38.87 A
ATOM	1243	CG	ASP	A	229	8.284	−18.172	−45.259	1.00	45.09 A
ATOM	1244	OD1	ASP	A	229	7.796	−17.274	−44.534	1.00	48.75 A
ATOM	1245	OD2	ASP	A	229	8.600	−19.298	−44.806	1.00	45.52 A
ATOM	1246	C	ASP	A	229	9.401	−16.310	−48.503	1.00	32.03 A
ATOM	1247	O	ASP	A	229	10.309	−16.660	−49.258	1.00	31.02 A
ATOM	1248	N	GLN	A	230	8.374	−15.572	−48.913	1.00	31.00 A
ATOM	1249	CA	GLN	A	230	8.238	−15.162	−50.305	1.00	31.22 A
ATOM	1250	CB	GLN	A	230	6.884	−14.487	−50.533	1.00	32.85 A
ATOM	1251	CG	GLN	A	230	5.709	−15.456	−50.531	1.00	37.00 A
ATOM	1252	CD	GLN	A	230	4.364	−14.754	−50.639	1.00	38.18 A
ATOM	1253	OE1	GLN	A	230	4.100	−14.024	−51.601	1.00	38.74 A
ATOM	1254	NE2	GLN	A	230	3.502	−14.976	−49.650	1.00	37.86 A
ATOM	1255	C	GLN	A	230	9.348	−14.243	−50.787	1.00	29.78 A
ATOM	1256	O	GLN	A	230	9.902	−14.453	−51.869	1.00	29.39 A
ATOM	1257	N	VAL	A	231	9.665	−13.217	−50.005	1.00	27.08 A
ATOM	1258	CA	VAL	A	231	10.726	−12.303	−50.401	1.00	26.16 A
ATOM	1259	CB	VAL	A	231	10.801	−11.080	−49.469	1.00	26.30 A
ATOM	1260	CG1	VAL	A	231	9.551	−10.231	−49.610	1.00	25.48 A
ATOM	1261	CG2	VAL	A	231	10.936	−11.536	−48.055	1.00	27.95 A
ATOM	1262	C	VAL	A	231	12.050	−13.056	−50.371	1.00	25.45 A
ATOM	1263	O	VAL	A	231	12.949	−12.789	−51.172	1.00	25.65 A
ATOM	1264	N	LEU	A	232	12.162	−14.014	−49.456	1.00	24.04 A
ATOM	1265	CA	LEU	A	232	13.379	−14.804	−49.345	1.00	22.95 A
ATOM	1266	CB	LEU	A	232	13.304	−15.753	−48.148	1.00	23.20 A
ATOM	1267	CG	LEU	A	232	14.562	−16.605	−47.940	1.00	24.20 A
ATOM	1268	CD1	LEU	A	232	15.782	−15.692	−47.782	1.00	25.17 A
ATOM	1269	CD2	LEU	A	232	14.390	−17.490	−46.718	1.00	25.41 A
ATOM	1270	C	LEU	A	232	13.614	−15.606	−50.621	1.00	24.32 A
ATOM	1271	O	LEU	A	232	14.745	−15.687	−51.113	1.00	23.37 A
ATOM	1272	N	ASP	A	233	12.554	−16.206	−51.156	1.00	24.48 A
ATOM	1273	CA	ASP	A	233	12.688	−16.974	−52.386	1.00	25.90 A
ATOM	1274	CB	ASP	A	233	11.348	−17.582	−52.826	1.00	27.95 A
ATOM	1275	CG	ASP	A	233	10.871	−18.694	−51.902	1.00	31.23 A
ATOM	1276	OD1	ASP	A	233	11.721	−19.352	−51.261	1.00	31.77 A
ATOM	1277	OD2	ASP	A	233	9.642	−18.922	−51.831	1.00	33.39 A
ATOM	1278	C	ASP	A	233	13.209	−16.065	−53.490	1.00	24.49 A
ATOM	1279	O	ASP	A	233	14.045	−16.477	−54.288	1.00	23.31 A
ATOM	1280	N	SER	A	234	12.728	−14.822	−53.519	1.00	23.93 A
ATOM	1281	CA	SER	A	234	13.144	−13.867	−54.546	1.00	24.19 A
ATOM	1282	CB	SER	A	234	12.434	−12.522	−54.357	1.00	24.54 A
ATOM	1283	OG	SER	A	234	13.044	−11.745	−53.341	1.00	26.38 A
ATOM	1284	C	SER	A	234	14.655	−13.624	−54.609	1.00	24.31 A
ATOM	1285	O	SER	A	234	15.154	−13.082	−55.591	1.00	26.53 A
ATOM	1286	N	ILE	A	235	15.388	−14.006	−53.570	1.00	23.33 A
ATOM	1287	CA	ILE	A	235	16.830	−13.808	−53.596	1.00	21.51 A
ATOM	1288	CB	ILE	A	235	17.262	−12.641	−52.663	1.00	20.78 A
ATOM	1289	CG2	ILE	A	235	16.624	−11.329	−53.138	1.00	14.94 A
ATOM	1290	CG1	ILE	A	235	16.879	−12.964	−51.216	1.00	18.91 A
ATOM	1291	CD1	ILE	A	235	17.392	−11.968	−50.211	1.00	18.32 A
ATOM	1292	C	ILE	A	235	17.616	−15.061	−53.215	1.00	22.26 A
ATOM	1293	O	ILE	A	235	18.810	−14.983	−52.919	1.00	22.63 A
ATOM	1294	N	ARG	A	236	16.958	−16.217	−53.229	1.00	22.15 A
ATOM	1295	CA	ARG	A	236	17.637	−17.459	−52.882	1.00	23.00 A
ATOM	1296	CB	ARG	A	236	16.685	−18.648	−53.003	1.00	24.18 A
ATOM	1297	CG	ARG	A	236	15.802	−18.852	−51.786	1.00	28.66 A
ATOM	1298	CD	ARG	A	236	14.937	−20.104	−51.903	1.00	30.02 A
ATOM	1299	NE	ARG	A	236	14.181	−20.349	−50.678	1.00	31.89 A
ATOM	1300	CZ	ARG	A	236	14.710	−20.823	−49.552	1.00	33.51 A
ATOM	1301	NH1	ARG	A	236	16.003	−21.115	−49.490	1.00	33.19 A
ATOM	1302	NH2	ARG	A	236	13.947	−20.989	−48.480	1.00	35.80 A
ATOM	1303	C	ARG	A	236	18.865	−17.704	−53.758	1.00	24.86 A
ATOM	1304	O	ARG	A	236	19.946	−18.026	−53.248	1.00	24.45 A
ATOM	1305	N	GLU	A	237	18.698	−17.556	−55.073	1.00	23.40 A
ATOM	1306	CA	GLU	A	237	19.802	−17.775	−55.996	1.00	22.38 A
ATOM	1307	CB	GLU	A	237	19.339	−17.613	−57.450	1.00	21.86 A
ATOM	1308	CG	GLU	A	237	18.187	−18.534	−57.832	1.00	26.01 A
ATOM	1309	CD	GLU	A	237	18.347	−19.954	−57.284	1.00	28.79 A
ATOM	1310	OE1	GLU	A	237	19.326	−20.640	−57.649	1.00	31.36 A
ATOM	1311	OE2	GLU	A	237	17.487	−20.387	−56.479	1.00	31.54 A
ATOM	1312	C	GLU	A	237	20.931	−16.803	−55.683	1.00	19.80 A
ATOM	1313	O	GLU	A	237	22.102	−17.174	−55.709	1.00	18.95 A
ATOM	1314	N	GLU	A	238	20.570	−15.567	−55.362	1.00	17.58 A
ATOM	1315	CA	GLU	A	238	21.557	−14.546	−55.035	1.00	16.50 A
ATOM	1316	CB	GLU	A	238	20.848	−13.219	−54.729	1.00	16.60 A
ATOM	1317	CG	GLU	A	238	20.357	−12.449	−55.972	1.00	15.75 A

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ATOM	1318	CD	GLU	A	238	19.198	−13.120	−56.712	1.00	16.05 A
ATOM	1319	OE1	GLU	A	238	18.860	−12.653	−57.817	1.00	15.84 A
ATOM	1320	OE2	GLU	A	238	18.613	−14.097	−56.199	1.00	19.07 A
ATOM	1321	C	GLU	A	238	22.449	−14.961	−53.851	1.00	16.83 A
ATOM	1322	O	GLU	A	238	23.677	−14.877	−53.925	1.00	14.90 A
ATOM	1323	N	LEU	A	239	21.820	−15.405	−52.764	1.00	15.47 A
ATOM	1324	CA	LEU	A	239	22.542	−15.836	−51.574	1.00	16.39 A
ATOM	1325	CB	LEU	A	239	21.553	−16.095	−50.428	1.00	14.91 A
ATOM	1326	CG	LEU	A	239	20.700	−14.891	−50.006	1.00	17.17 A
ATOM	1327	CD1	LEU	A	239	19.828	−15.234	−48.796	1.00	15.12 A
ATOM	1328	CD2	LEU	A	239	21.617	−13.734	−49.679	1.00	15.57 A
ATOM	1329	C	LEU	A	239	23.344	−17.100	−51.874	1.00	16.05 A
ATOM	1330	O	LEU	A	239	24.430	−17.316	−51.331	1.00	14.99 A
ATOM	1331	N	GLU	A	240	22.800	−17.927	−52.756	1.00	17.95 A
ATOM	1332	CA	GLU	A	240	23.444	−19.169	−53.149	1.00	21.35 A
ATOM	1333	CB	GLU	A	240	22.492	−19.969	−54.037	1.00	25.83 A
ATOM	1334	CG	GLU	A	240	22.635	−21.471	−53.966	1.00	31.74 A
ATOM	1335	CD	GLU	A	240	21.535	−22.176	−54.753	1.00	36.90 A
ATOM	1336	OE1	GLU	A	240	20.349	−21.810	−54.566	1.00	37.59 A
ATOM	1337	OE2	GLU	A	240	21.853	−23.092	−55.549	1.00	39.47 A
ATOM	1338	C	GLU	A	240	24.740	−18.854	−53.903	1.00	19.90 A
ATOM	1339	O	GLU	A	240	25.748	−19.548	−53.743	1.00	20.76 A
ATOM	1340	N	ALA	A	241	24.711	−17.798	−54.710	1.00	18.49 A
ATOM	1341	CA	ALA	A	241	25.887	−17.396	−55.480	1.00	18.34 A
ATOM	1342	CB	ALA	A	241	25.515	−16.306	−56.483	1.00	19.10 A
ATOM	1343	C	ALA	A	241	27.007	−16.905	−54.566	1.00	17.84 A
ATOM	1344	O	ALA	A	241	28.183	−17.073	−54.881	1.00	17.32 A
ATOM	1345	N	LEU	A	242	26.642	−16.289	−53.441	1.00	17.42 A
ATOM	1346	CA	LEU	A	242	27.641	−15.794	−52.494	1.00	17.40 A
ATOM	1347	CB	LEU	A	242	27.005	−14.800	−51.517	1.00	14.72 A
ATOM	1348	CG	LEU	A	242	26.611	−13.447	−52.119	1.00	13.60 A
ATOM	1349	CD1	LEU	A	242	25.823	−12.653	−51.105	1.00	13.80 A
ATOM	1350	CD2	LEU	A	242	27.848	−12.675	−52.532	1.00	10.81 A
ATOM	1351	C	LEU	A	242	28.267	−16.965	−51.730	1.00	18.23 A
ATOM	1352	O	LEU	A	242	29.445	−16.925	−51.375	1.00	16.99 A
ATOM	1353	N	GLU	A	243	27.472	−18.007	−51.494	1.00	19.15 A
ATOM	1354	CA	GLU	A	243	27.941	−19.197	−50.792	1.00	20.79 A
ATOM	1355	CB	GLU	A	243	26.770	−20.140	−50.507	1.00	21.06 A
ATOM	1356	CG	CLU	A	243	25.848	−19.685	−49.378	1.00	19.76 A
ATOM	1357	CD	GLU	A	243	24.475	−20.318	−49.474	1.00	20.44 A
ATOM	1358	OE1	GLU	A	243	24.357	−21.358	−50.150	1.00	22.37 A
ATOM	1359	OE2	GLU	A	243	23.518	−19.784	−48.873	1.00	20.73 A
ATOM	1360	C	GLU	A	243	28.975	−19.912	−51.649	1.00	22.94 A
ATOM	1361	O	GLU	A	243	29.983	−20.410	−51.143	1.00	22.58 A
ATOM	1362	N	LYS	A	244	28.717	−19.963	−52.951	1.00	23.02 A
ATOM	1363	CA	LYS	A	244	29.637	−20.601	−53.879	1.00	24.52 A
ATOM	1364	CB	LYS	A	244	28.966	−20.798	−55.242	1.00	25.82 A
ATOM	1365	CG	LYS	A	244	27.699	−21.650	−55.171	1.00	31.89 A
ATOM	1366	CD	LYS	A	244	27.998	−23.064	−54.652	1.00	34.68 A
ATOM	1367	CE	LYS	A	244	26.751	−23.745	−54.097	1.00	35.93 A
ATOM	1368	NZ	LYS	A	244	26.233	−23.064	−52.871	1.00	36.31 A
ATOM	1369	C	LYS	A	244	30.884	−19.735	−54.024	1.00	24.80 A
ATOM	1370	O	LYS	A	244	32.005	−20.239	−53.979	1.00	24.15 A
ATOM	1371	N	LYS	A	245	30.686	−18.431	−54.194	1.00	23.61 A
ATOM	1372	CA	LYS	A	245	31.805	−17.503	−54.330	1.00	23.86 A
ATOM	1373	CB	LYS	A	245	31.276	−16.075	−54.482	1.00	24.85 A
ATOM	1374	CG	LYS	A	245	32.325	−14.977	−54.377	1.00	27.82 A
ATOM	1375	CD	LYS	A	245	33.472	−15.174	−55.357	1.00	30.16 A
ATOM	1376	CE	LYS	A	245	33.044	−14.966	−56.803	1.00	32.00 A
ATOM	1377	NZ	LYS	A	245	34.179	−15.225	−57.737	1.00	29.90 A
ATOM	1378	C	LYS	A	245	32.715	−17.609	−53.105	1.00	23.77 A
ATOM	1379	O	LYS	A	245	33.938	−17.506	−53.207	1.00	21.14 A
ATOM	1380	N	TYR	A	246	32.098	−17.827	−51.949	1.00	23.97 A
ATOM	1381	CA	TYR	A	246	32.823	−17.966	−50.694	1.00	23.96 A
ATOM	1382	CB	TYR	A	246	31.845	−18.110	−49.531	1.00	23.71 A
ATOM	1383	CG	TYR	A	246	32.520	−18.412	−48.219	1.00	24.55 A
ATOM	1384	CD1	TYR	A	246	33.192	−17.415	−47.518	1.00	23.26 A
ATOM	1385	CE1	TYR	A	246	33.847	−17.697	−46.323	1.00	23.72 A
ATOM	1386	CD2	TYR	A	246	32.517	−19.705	−47.692	1.00	25.41 A
ATOM	1387	CE2	TYR	A	246	33.172	−19.998	−46.497	1.00	24.58 A
ATOM	1388	CZ	TYR	A	246	33.835	−18.986	−45.821	1.00	24.76 A
ATOM	1389	OH	TYR	A	246	34.501	−19.257	−44.647	1.00	25.79 A
ATOM	1390	C	TYR	A	246	33.688	−19.210	−50.751	1.00	24.29 A
ATOM	1391	O	TYR	A	246	34.864	−19.187	−50.386	1.00	23.22 A
ATOM	1392	N	GLU	A	247	33.077	−20.302	−51.193	1.00	24.70 A
ATOM	1393	CA	GLU	A	247	33.767	−21.569	−51.302	1.00	26.80 A
ATOM	1394	CB	GLU	A	247	32.783	−22.658	−51.732	1.00	25.70 A
ATOM	1395	CG	GLU	A	247	31.852	−23.115	−50.617	1.00	26.11 A
ATOM	1396	CD	GLU	A	247	30.768	−24.069	−51.098	1.00	26.88 A

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ATOM	1397	OE1	GLU	A	247	31.094	−25.045	−51.804	1.00	27.71 A
ATOM	1398	OE2	GLU	A	247	29.584	−23.848	−50.764	1.00	28.44 A
ATOM	1399	C	GLU	A	247	34.916	−21.461	−52.297	1.00	27.97 A
ATOM	1400	O	GLU	A	247	36.018	−21.937	−52.033	1.00	29.90 A
ATOM	1401	N	GLU	A	248	34.660	−20.816	−53.428	1.00	29.20 A
ATOM	1402	CA	GLU	A	248	35.675	−20.654	−54.460	1.00	31.97 A
ATOM	1403	CB	GLU	A	248	35.073	−20.025	−55.726	1.00	34.39 A
ATOM	1404	CG	GLU	A	248	35.868	−20.328	−57.004	1.00	40.86 A
ATOM	1405	CD	GLU	A	248	35.930	−19.154	−57.983	1.00	44.67 A
ATOM	1406	OE1	GLU	A	248	34.864	−18.578	−58.313	1.00	47.37 A
ATOM	1407	OE2	GLU	A	248	37.052	−18.813	−58.432	1.00	44.21 A
ATOM	1408	C	GLU	A	248	36.829	−19.780	−53.976	1.00	31.88 A
ATOM	1409	O	GLU	A	248	37.993	−20.072	−54.255	1.00	31.42 A
ATOM	1410	N	LYS	A	249	36.509	−18.708	−53.254	1.00	31.46 A
ATOM	1411	CA	LYS	A	249	37.546	−17.803	−52.769	1.00	31.64 A
ATOM	1412	CB	LYS	A	249	36.948	−16.456	−52.340	1.00	31.29 A
ATOM	1413	CG	LYS	A	249	37.985	−15.524	−51.731	1.00	33.88 A
ATOM	1414	CD	LYS	A	249	37.443	−14.145	−51.384	1.00	36.01 A
ATOM	1415	CE	LYS	A	249	38.546	−13.266	−50.777	1.00	38.28 A
ATOM	1416	NZ	LYS	A	249	38.102	−11.882	−50.419	1.00	39.36 A
ATOM	1417	C	LYS	A	249	38.372	−18.371	−51.618	1.00	31.30 A
ATOM	1418	O	LYS	A	249	39.598	−18.353	−51.672	1.00	31.00 A
ATOM	1419	N	THR	A	250	37.708	−18.877	−50.584	1.00	30.44 A
ATOM	1420	CA	THR	A	250	38.418	−19.414	−49.428	1.00	31.23 A
ATOM	1421	CB	THR	A	250	37.555	−19.338	−48.148	1.00	31.86 A
ATOM	1422	OG1	THR	A	250	36.507	−20.314	−48.214	1.00	34.34 A
ATOM	1423	CG2	THR	A	250	36.941	−17.952	−48.001	1.00	34.00 A
ATOM	1424	C	THR	A	250	38.892	−20.857	−49.586	1.00	30.95 A
ATOM	1425	O	THR	A	250	39.942	−21.223	−49.065	1.00	29.91 A
ATOM	1426	N	GLY	A	251	38.125	−21.668	−50.306	1.00	30.20 A
ATOM	1427	CA	GLY	A	251	38.491	−23.064	−50.475	1.00	30.06 A
ATOM	1428	C	GLY	A	251	37.843	−23.878	−49.365	1.00	30.74 A
ATOM	1429	O	GLY	A	251	38.060	−25.083	−49.238	1.00	31.77 A
ATOM	1430	N	LEU	A	252	37.030	−23.193	−48.564	1.00	29.90 A
ATOM	1431	CA	LEU	A	252	36.323	−23.790	−47.440	1.00	27.62 A
ATOM	1432	CB	LEU	A	252	36.561	−22.942	−46.191	1.00	27.01 A
ATOM	1433	CG	LEU	A	252	38.024	−22.633	−45.872	1.00	25.71 A
ATOM	1434	CD1	LEU	A	252	38.102	−21.489	−44.875	1.00	25.85 A
ATOM	1435	CD2	LEU	A	252	38.701	−23.888	−45.330	1.00	24.69 A
ATOM	1436	C	LEU	A	252	34.823	−23.840	−47.736	1.00	27.80 A
ATOM	1437	O	LEU	A	252	34.306	−23.006	−48.480	1.00	27.40 A
ATOM	1438	N	PRO	A	253	34.109	−24.822	−47.159	1.00	27.39 A
ATOM	1439	CD	PRO	A	253	34.659	−25.921	−46.355	1.00	27.81 A
ATOM	1440	CA	PRO	A	253	32.663	−24.994	−47.344	1.00	28.16 A
ATOM	1441	CB	PRO	A	253	32.399	−26.394	−46.784	1.00	28.26 A
ATOM	1442	CG	PRO	A	253	33.756	−27.045	−46.736	1.00	28.79 A
ATOM	1443	C	PRO	A	253	31.954	−23.931	−46.506	1.00	29.29 A
ATOM	1444	O	PRO	A	253	32.331	−23.707	−45.355	1.00	30.16 A
ATOM	1445	N	SER	A	254	30.931	−23.283	−47.054	1.00	30.59 A
ATOM	1446	CA	SER	A	254	30.231	−22.248	−46.286	1.00	32.13 A
ATOM	1447	CB	SER	A	254	29.629	−21.192	−47.219	1.00	31.94 A
ATOM	1448	OG	SER	A	254	28.478	−21.688	−47.880	1.00	30.37 A
ATOM	1449	C	SER	A	254	29.114	−22.815	−45.423	1.00	32.34 A
ATOM	1450	O	SER	A	254	28.543	−23.851	−45.742	1.00	30.85 A
ATOM	1451	N	PRO	A	255	28.808	−22.150	−44.299	1.00	34.62 A
ATOM	1452	CD	PRO	A	255	29.704	−21.193	−43.627	1.00	33.82 A
ATOM	1453	CA	PRO	A	255	27.736	−22.594	−43.393	1.00	35.62 A
ATOM	1454	CB	PRO	A	255	28.082	−21.906	−42.079	1.00	36.32 A
ATOM	1455	CG	PRO	A	255	29.590	−21.635	−42.200	1.00	35.07 A
ATOM	1456	C	PRO	A	255	26.410	−22.096	−43.984	1.00	38.43 A
ATOM	1457	O	PRO	A	255	25.564	−21.528	−43.295	1.00	37.08 A
ATOM	1458	N	GLU	A	256	26.273	−22.334	−45.287	1.00	42.39 A
ATOM	1459	CA	GLU	A	256	25.139	−21.942	−46.124	1.00	45.09 A
ATOM	1460	CB	GLU	A	256	25.419	−22.388	−47.564	1.00	48.71 A
ATOM	1461	CG	GLU	A	256	24.872	−23.776	−47.940	1.00	51.06 A
ATOM	1462	CD	GLU	A	256	25.525	−24.911	−47.177	1.00	54.43 A
ATOM	1463	OE1	GLU	A	256	26.723	−25.180	−47.422	1.00	54.78 A
ATOM	1464	OE2	GLU	A	256	24.840	−25.533	−46.334	1.00	54.37 A
ATOM	1465	C	GLU	A	256	23.721	−22.388	−45.759	1.00	45.88 A
ATOM	1466	O	GLU	A	256	23.420	−22.700	−44.607	1.00	46.95 A
ATOM	1467	N	ARG	A	257	22.875	−22.396	−46.795	1.00	47.40 A
ATOM	1468	CA	ARG	A	257	21.458	−22.766	−46.768	1.00	48.03 A
ATOM	1469	CB	ARG	A	257	21.166	−23.841	−45.708	1.00	49.00 A
ATOM	1470	CG	ARG	A	257	19.673	−24.239	−45.527	1.00	49.58 A
ATOM	1471	CD	ARG	A	257	18.926	−24.462	−46.845	1.00	50.25 A
ATOM	1472	NE	ARG	A	257	18.716	−23.197	−47.542	1.00	50.22 A
ATOM	1473	CZ	ARG	A	257	19.098	−22.961	−48.791	1.00	51.01 A
ATOM	1474	NH1	ARG	A	257	19.705	−23.913	−49.485	1.00	51.87 A
ATOM	1475	NH2	ARG	A	257	18.900	−21.767	−49.332	1.00	51.93 A

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ATOM	1476	C	ARG	A	257	20.576	−21.545	−46.548	1.00	48.27 A
ATOM	1477	O	ARG	A	257	19.959	−21.445	−45.465	1.00	48.75 A
ATOM	1478	OXT	ARG	A	257	20.517	−20.700	−47.471	1.00	47.21 A
ATOM	1479	S	SO4	L	1	26.750	−1.543	−20.726	1.00	38.59 L
ATOM	1480	O1	SO4	L	1	26.466	−2.892	−21.261	1.00	36.34 L
ATOM	1481	O2	SO4	L	1	25.516	−0.950	−20.178	1.00	38.18 L
ATOM	1482	O3	SO4	L	1	27.748	−1.640	−19.643	1.00	39.55 L
ATOM	1483	O4	SO4	L	1	27.270	−0.687	−21.812	1.00	36.64 L
ATOM	1484	ZN + 2	ZN2	M	1	24.054	−4.948	−43.032	1.00	17.46 M
ATOM	1485	ZN + 2	ZN2	M	2	39.953	7.918	−41.358	1.00	25.22 M
ATOM	1486	ZN + 2	ZN2	M	3	36.946	−5.734	−22.999	1.00	22.38 M
ATOM	1487	ZN + 2	ZN2	M	4	19.157	−22.594	−56.610	0.50	43.08 M
ATOM	1488	ZN + 2	ZN2	M	5	21.794	−10.556	−27.675	0.40	29.27 M
ATOM	1489	ZN + 2	ZN2	M	6	−0.285	1.757	−30.184	0.50	36.10 M
ATOM	1490	OH2	TIP	S	1	25.969	−2.074	−44.807	1.00	14.25 S
ATOM	1491	OH2	TIP	S	2	3.811	2.346	−30.357	1.00	14.25 S
ATOM	1492	OH2	TIP	S	3	−0.051	0.258	−28.134	1.00	14.25 S
ATOM	1493	OH2	TIP	S	4	10.090	−8.668	−43.625	1.00	15.50 S
ATOM	1494	OH2	TIP	S	5	24.192	−17.873	−42.585	1.00	9.05 S
ATOM	1495	OH2	TIP	S	6	26.335	−9.687	−38.091	1.00	2.09 S
ATOM	1496	OH2	TIP	S	7	42.910	−1.393	−27.043	1.00	40.60 S
ATOM	1497	OH2	TIP	S	8	22.287	−8.014	−43.054	1.00	3.78 S
ATOM	1498	OH2	TIP	S	9	22.996	−4.825	−50.565	1.00	6.81 S
ATOM	1499	OH2	TIP	S	10	9.921	−9.608	−46.068	1.00	10.87 S
ATOM	1500	OH2	TIP	S	11	21.456	−25.782	−55.836	1.00	28.41 S
ATOM	1501	OH2	TIP	S	12	31.066	7.682	−53.311	1.00	21.03 S
ATOM	1502	OH2	TIP	S	13	11.349	−7.646	−52.115	1.00	13.10 S
ATOM	1503	OH2	TIP	S	14	24.496	−4.224	−28.092	1.00	23.20 S
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ATOM	1505	OH2	TIP	S	16	27.530	−14.722	−42.923	1.00	9.87 S
ATOM	1506	OH2	TIP	S	17	9.342	6.275	−38.471	1.00	18.89 S
ATOM	1507	OH2	TIP	S	18	5.984	−3.364	−30.710	1.00	11.90 S
ATOM	1508	OH2	TIP	S	19	19.793	−0.210	−46.871	1.00	26.54 S
ATOM	1509	OH2	TIP	S	20	28.046	−17.680	−41.836	1.00	10.88 S
ATOM	1510	OH2	TIP	S	23	21.557	−7.309	−40.376	1.00	14.41 S
ATOM	1511	OH2	TIP	S	24	12.004	1.128	−39.615	1.00	16.43 S
ATOM	1512	OH2	TIP	S	25	30.777	−14.876	−50.134	1.00	11.00 S
ATOM	1513	OH2	TIP	S	26	−1.303	−0.882	−25.776	1.00	38.49 S
ATOM	1514	OH2	TIP	S	28	13.901	−4.350	−36.733	1.00	17.30 S
ATOM	1515	OH2	TIP	S	30	28.137	−11.377	−35.724	1.00	13.45 S
ATOM	1516	OH2	TIP	S	32	10.937	−8.045	−38.922	1.00	19.04 S
ATOM	1517	OH2	TIP	S	33	32.844	−9.803	−54.314	1.00	43.74 S
ATOM	1518	OH2	TIP	S	34	36.191	−3.234	−48.811	1.00	43.05 S
ATOM	1519	OH2	TIP	S	36	16.139	−16.545	−56.285	1.00	35.15 S
ATOM	1520	OH2	TIP	S	37	33.130	11.162	−16.863	1.00	27.08 S
ATOM	1521	OH2	TIP	S	38	13.131	−19.278	−54.777	1.00	21.83 S
ATOM	1522	OH2	TIP	S	39	26.597	−10.167	−54.360	1.00	17.41 S
ATOM	1523	OH2	TIP	S	40	12.308	−8.028	−32.094	1.00	23.20 S
ATOM	1524	OH2	TIP	S	41	23.225	−15.656	−35.045	1.00	28.13 S
ATOM	1525	OH2	TIP	S	42	24.923	−2.981	−42.626	1.00	13.51 S
ATOM	1526	OH2	TIP	S	43	44.298	−1.798	−33.197	1.00	17.76 S
ATOM	1527	OH2	TIP	S	44	20.680	−0.619	−44.292	1.00	14.01 S
ATOM	1528	OH2	TIP	S	45	5.896	−15.409	−44.351	1.00	22.87 S
ATOM	1529	OH2	TIP	S	46	23.233	−24.442	−53.915	1.00	39.19 S
ATOM	1530	OH2	TIP	S	47	14.208	−10.403	−32.245	1.00	18.95 S
ATOM	1531	OH2	TIP	S	48	38.832	−0.501	−27.020	1.00	14.49 S
ATOM	1532	OH2	TIP	S	49	18.236	−0.002	−44.579	1.00	27.51 S
ATOM	1533	OH2	TIP	S	50	36.434	8.748	−34.776	1.00	11.42 S
ATOM	1534	OH2	TIP	S	51	27.579	14.569	−38.647	1.00	28.40 S
ATOM	1535	OH2	TIP	S	52	38.153	2.185	−20.385	1.00	15.38 S
ATOM	1536	OH2	TIP	S	54	29.121	−17.432	−57.522	1.00	14.06 S
ATOM	1537	OH2	TIP	S	55	28.554	−19.346	−40.014	1.00	37.78 S
ATOM	1538	OH2	TIP	S	56	22.082	−22.880	−50.314	1.00	24.72 S
ATOM	1539	OH2	TIP	S	59	35.171	−10.112	−50.196	1.00	27.04 S
ATOM	1540	OH2	TIP	S	61	9.233	−20.875	−49.991	1.00	31.75 S
ATOM	1541	OH2	TIP	S	62	18.870	−7.844	−55.461	1.00	34.62 S
ATOM	1542	OH2	TIP	S	63	11.323	3.689	−39.850	1.00	18.17 S
ATOM	1543	OH2	TIP	S	64	35.403	9.921	−37.907	1.00	26.55 S
ATOM	1544	OH2	TIP	S	65	8.090	14.529	−43.710	1.00	30.17 S
ATOM	1545	OH2	TIP	S	66	38.045	−0.048	−19.192	1.00	30.52 S
ATOM	1546	OH2	TIP	S	67	33.352	−13.694	−29.289	1.00	33.68 S
ATOM	1547	OH2	TIP	S	69	35.976	−15.780	−40.760	1.00	13.56 S

The examples set forth above are provided to give those of ordinary skill in the art a complete disclosure and description of how to make and use the embodiments of the devices, systems and methods of the invention, and are not intended to limit the scope of what the inventors regard as their invention. Modifications of the above-described modes for carrying out the invention that are obvious to persons of skill in the art are intended to be within the scope of the following claims. All patents and publications mentioned in the specification are indicative of the levels of skill of those skilled in the art to which the invention pertains. All references cited in this disclosure are incorporated by reference to the same extent as if each reference had been incorporated by reference in its entirety individually.

In addition, it is understood that the terminology used herein is for the purpose of describing particular embodiments only, and is not intended to be limiting. As used in this specification and the appended claims, the singular forms "a," "an," and "the" include plural referents unless the content clearly dictates otherwise. Unless defined otherwise, all technical and scientific terms used herein have the same meaning as commonly understood by one of ordinary skill in the art to which the invention pertains. Although any methods and materials similar or equivalent to those described herein can be used in the practice for testing of the invention(s), specific examples of appropriate materials and methods are described herein.

A number of embodiments of the invention have been described. Nevertheless, it will be understood that various modifications may be made without departing from the spirit and scope of the invention. Accordingly, other embodiments are within the scope of the following claims.

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Phe Asp Val Met Tyr Lys Thr Asp Gly Ile Gly Leu Ser Ala Pro Gln
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Ser Asp Lys Leu Val Pro Phe Asp Glu Gly Cys Leu Ser Phe Pro Gly
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<400> SEQUENCE: 11

Ser Ser Leu Pro Ala Arg Ile Phe Gln His Glu Tyr Asp His Leu Glu
1 5 10 15

Gly Val

<210> SEQ ID NO 12
<211> LENGTH: 18
<212> TYPE: PRT
<213> ORGANISM: Escherichia coli

<400> SEQUENCE: 12

Tyr Ala Glu Lys Gly Ile Gly Leu Ala Ala Thr Gln Val Asp Ile His
1 5 10 15

Gln Arg

<210> SEQ ID NO 13
<211> LENGTH: 18
<212> TYPE: PRT
<213> ORGANISM: Escherichia coli

<400> SEQUENCE: 13

Gly Glu Thr Gly Ile Glu Glu Gly Cys Leu Ser Ile Pro Glu Gln Arg
1 5 10 15

Ala Leu

<210> SEQ ID NO 14
<211> LENGTH: 18
<212> TYPE: PRT
<213> ORGANISM: Escherichia coli

<400> SEQUENCE: 14

Ala Asp Gly Leu Leu Ala Ile Cys Ile Gln His Glu Met Asp His Leu
1 5 10 15

Val Gly

<210> SEQ ID NO 15
<211> LENGTH: 5
<212> TYPE: PRT
<213> ORGANISM: Arabidopsis thaliana

<400> SEQUENCE: 15

Glu Gly Cys Leu Ser
1 5

<210> SEQ ID NO 16
<211> LENGTH: 6
<212> TYPE: PRT
<213> ORGANISM: Arabidopsis thaliana
<220> FEATURE:
<221> NAME/KEY: MOD_RES

-continued

<222> LOCATION: (4)..(5)
<223> OTHER INFORMATION: variable residue

<400> SEQUENCE: 16

Gln His Glu Xaa Xaa His
1 5

What is claimed is:

1. A crystalline form of a polypeptide consisting of the amino acid sequence of SEQ ID NO:1 complexed with Zn^{2+}, wherein said crystalline form has the space group symmetry $P4_12_12$; unit cell dimensions of a=about 49 angstroms to about 52 angstroms, b=about 49 angstroms to about 52 angstroms, and c=about 143 angstroms to about 147 angstroms and alpha=beta=gamma=90 degrees.

2. The crystalline form of claim **1**, wherein said crystalline form produces the structural coordinates as set forth Table 1 upon X-ray diffraction pattern analysis.

3. The crystalline form of claim **1**, wherein said crystalline form diffracts X-rays to a resolution of 2.4 angstroms.

4. The crystalline form of claim **1**, wherein said unit cell dimensions are a=50.902 angstroms, b=50.902 angstroms, and c=144.783 angstroms.

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