



## Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 11:12 PM UTC

PDB ID : 9HZN / pdb\_00009hzn  
EMDB ID : EMD-52527  
Title : 250 A SynPspA H1-5 rod after incubation with EPL  
Authors : Hudina, E.; Junglas, B.; Sachse, C.  
Deposited on : 2025-01-14  
Resolution : 3.80 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

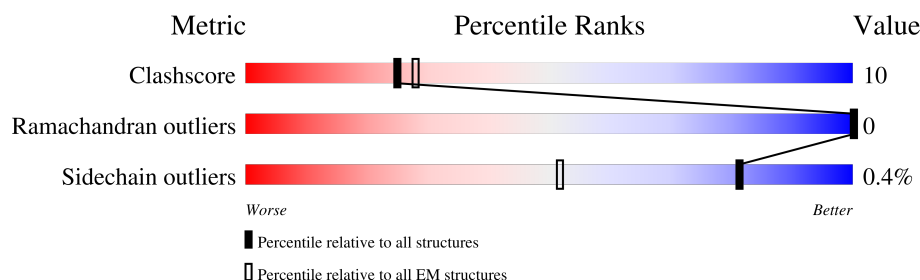
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.
















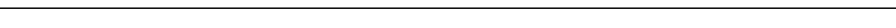











Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	0	223	67% 19% 13%
1	1	223	67% 20% 13%
1	2	223	67% 19% 13%
1	3	223	66% 21% 13%
1	4	223	68% 18% 13%
1	5	223	69% 17% 13%
1	6	223	68% 19% 13%
1	7	223	67% 19% 13%
1	A	223	69% 18% 13%


























Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	B	223	
1	C	223	
1	D	223	
1	E	223	
1	F	223	
1	G	223	
1	H	223	
1	I	223	
1	J	223	
1	K	223	
1	L	223	
1	M	223	
1	N	223	
1	O	223	
1	P	223	
1	Q	223	
1	R	223	
1	S	223	
1	T	223	
1	U	223	
1	V	223	
1	W	223	
1	X	223	
1	Y	223	
1	Z	223	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	a	223	
1	b	223	
1	c	223	
1	d	223	
1	e	223	
1	f	223	
1	g	223	
1	h	223	
1	i	223	
1	j	223	
1	k	223	
1	l	223	
1	m	223	
1	n	223	
1	o	223	
1	p	223	
1	q	223	
1	r	223	
1	s	223	
1	t	223	
1	u	223	
1	v	223	
1	w	223	
1	x	223	
1	y	223	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	z	223	 65% 22% 13%

## 2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 188940 atoms, of which 95400 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Chloroplast membrane-associated 30 kD protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	0	194	Total	C	H	N	O	S	0	0
			3149	968	1590	286	303	2		
1	1	194	Total	C	H	N	O	S	0	0
			3149	968	1590	286	303	2		
1	2	194	Total	C	H	N	O	S	0	0
			3149	968	1590	286	303	2		
1	3	194	Total	C	H	N	O	S	0	0
			3149	968	1590	286	303	2		
1	4	194	Total	C	H	N	O	S	0	0
			3149	968	1590	286	303	2		
1	5	194	Total	C	H	N	O	S	0	0
			3149	968	1590	286	303	2		
1	6	194	Total	C	H	N	O	S	0	0
			3149	968	1590	286	303	2		
1	7	194	Total	C	H	N	O	S	0	0
			3149	968	1590	286	303	2		
1	A	194	Total	C	H	N	O	S	0	0
			3149	968	1590	286	303	2		
1	B	194	Total	C	H	N	O	S	0	0
			3149	968	1590	286	303	2		
1	C	194	Total	C	H	N	O	S	0	0
			3149	968	1590	286	303	2		
1	D	194	Total	C	H	N	O	S	0	0
			3149	968	1590	286	303	2		
1	E	194	Total	C	H	N	O	S	0	0
			3149	968	1590	286	303	2		
1	F	194	Total	C	H	N	O	S	0	0
			3149	968	1590	286	303	2		
1	G	194	Total	C	H	N	O	S	0	0
			3149	968	1590	286	303	2		
1	H	194	Total	C	H	N	O	S	0	0
			3149	968	1590	286	303	2		
1	I	194	Total	C	H	N	O	S	0	0
			3149	968	1590	286	303	2		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms						AltConf	Trace
1	J	194	Total 3149	C 968	H 1590	N 286	O 303	S 2	0	0
1	K	194	Total 3149	C 968	H 1590	N 286	O 303	S 2	0	0
1	L	194	Total 3149	C 968	H 1590	N 286	O 303	S 2	0	0
1	M	194	Total 3149	C 968	H 1590	N 286	O 303	S 2	0	0
1	N	194	Total 3149	C 968	H 1590	N 286	O 303	S 2	0	0
1	O	194	Total 3149	C 968	H 1590	N 286	O 303	S 2	0	0
1	P	194	Total 3149	C 968	H 1590	N 286	O 303	S 2	0	0
1	Q	194	Total 3149	C 968	H 1590	N 286	O 303	S 2	0	0
1	R	194	Total 3149	C 968	H 1590	N 286	O 303	S 2	0	0
1	S	194	Total 3149	C 968	H 1590	N 286	O 303	S 2	0	0
1	T	194	Total 3149	C 968	H 1590	N 286	O 303	S 2	0	0
1	U	194	Total 3149	C 968	H 1590	N 286	O 303	S 2	0	0
1	V	194	Total 3149	C 968	H 1590	N 286	O 303	S 2	0	0
1	W	194	Total 3149	C 968	H 1590	N 286	O 303	S 2	0	0
1	X	194	Total 3149	C 968	H 1590	N 286	O 303	S 2	0	0
1	Y	194	Total 3149	C 968	H 1590	N 286	O 303	S 2	0	0
1	Z	194	Total 3149	C 968	H 1590	N 286	O 303	S 2	0	0
1	a	194	Total 3149	C 968	H 1590	N 286	O 303	S 2	0	0
1	b	194	Total 3149	C 968	H 1590	N 286	O 303	S 2	0	0
1	c	194	Total 3149	C 968	H 1590	N 286	O 303	S 2	0	0
1	d	194	Total 3149	C 968	H 1590	N 286	O 303	S 2	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms						AltConf	Trace
1	e	194	Total	C	H	N	O	S	0	0
			3149	968	1590	286	303	2		
1	f	194	Total	C	H	N	O	S	0	0
			3149	968	1590	286	303	2		
1	g	194	Total	C	H	N	O	S	0	0
			3149	968	1590	286	303	2		
1	h	194	Total	C	H	N	O	S	0	0
			3149	968	1590	286	303	2		
1	i	194	Total	C	H	N	O	S	0	0
			3149	968	1590	286	303	2		
1	j	194	Total	C	H	N	O	S	0	0
			3149	968	1590	286	303	2		
1	k	194	Total	C	H	N	O	S	0	0
			3149	968	1590	286	303	2		
1	l	194	Total	C	H	N	O	S	0	0
			3149	968	1590	286	303	2		
1	m	194	Total	C	H	N	O	S	0	0
			3149	968	1590	286	303	2		
1	n	194	Total	C	H	N	O	S	0	0
			3149	968	1590	286	303	2		
1	o	194	Total	C	H	N	O	S	0	0
			3149	968	1590	286	303	2		
1	p	194	Total	C	H	N	O	S	0	0
			3149	968	1590	286	303	2		
1	q	194	Total	C	H	N	O	S	0	0
			3149	968	1590	286	303	2		
1	r	194	Total	C	H	N	O	S	0	0
			3149	968	1590	286	303	2		
1	s	194	Total	C	H	N	O	S	0	0
			3149	968	1590	286	303	2		
1	t	194	Total	C	H	N	O	S	0	0
			3149	968	1590	286	303	2		
1	u	194	Total	C	H	N	O	S	0	0
			3149	968	1590	286	303	2		
1	v	194	Total	C	H	N	O	S	0	0
			3149	968	1590	286	303	2		
1	w	194	Total	C	H	N	O	S	0	0
			3149	968	1590	286	303	2		
1	x	194	Total	C	H	N	O	S	0	0
			3149	968	1590	286	303	2		
1	y	194	Total	C	H	N	O	S	0	0
			3149	968	1590	286	303	2		

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms						AltConf	Trace
1	z	194	Total	C	H	N	O	S	0	0
			3149	968	1590	286	303	2		

There are 1380 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	1	MET	-	initiating methionine	UNP P74717
0	2	GLY	-	expression tag	UNP P74717
0	3	SER	-	expression tag	UNP P74717
0	4	SER	-	expression tag	UNP P74717
0	5	HIS	-	expression tag	UNP P74717
0	6	HIS	-	expression tag	UNP P74717
0	7	HIS	-	expression tag	UNP P74717
0	8	HIS	-	expression tag	UNP P74717
0	9	HIS	-	expression tag	UNP P74717
0	10	HIS	-	expression tag	UNP P74717
0	11	SER	-	expression tag	UNP P74717
0	12	SER	-	expression tag	UNP P74717
0	13	SER	-	expression tag	UNP P74717
0	14	ALA	-	expression tag	UNP P74717
0	15	ALA	-	expression tag	UNP P74717
0	16	LEU	-	expression tag	UNP P74717
0	17	GLU	-	expression tag	UNP P74717
0	18	VAL	-	expression tag	UNP P74717
0	19	LEU	-	expression tag	UNP P74717
0	20	PHE	-	expression tag	UNP P74717
0	21	GLN	-	expression tag	UNP P74717
0	22	GLY	-	expression tag	UNP P74717
0	23	PRO	-	expression tag	UNP P74717
1	1	MET	-	initiating methionine	UNP P74717
1	2	GLY	-	expression tag	UNP P74717
1	3	SER	-	expression tag	UNP P74717
1	4	SER	-	expression tag	UNP P74717
1	5	HIS	-	expression tag	UNP P74717
1	6	HIS	-	expression tag	UNP P74717
1	7	HIS	-	expression tag	UNP P74717
1	8	HIS	-	expression tag	UNP P74717
1	9	HIS	-	expression tag	UNP P74717
1	10	HIS	-	expression tag	UNP P74717
1	11	SER	-	expression tag	UNP P74717
1	12	SER	-	expression tag	UNP P74717
1	13	SER	-	expression tag	UNP P74717

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
1	14	ALA	-	expression tag	UNP P74717
1	15	ALA	-	expression tag	UNP P74717
1	16	LEU	-	expression tag	UNP P74717
1	17	GLU	-	expression tag	UNP P74717
1	18	VAL	-	expression tag	UNP P74717
1	19	LEU	-	expression tag	UNP P74717
1	20	PHE	-	expression tag	UNP P74717
1	21	GLN	-	expression tag	UNP P74717
1	22	GLY	-	expression tag	UNP P74717
1	23	PRO	-	expression tag	UNP P74717
2	1	MET	-	initiating methionine	UNP P74717
2	2	GLY	-	expression tag	UNP P74717
2	3	SER	-	expression tag	UNP P74717
2	4	SER	-	expression tag	UNP P74717
2	5	HIS	-	expression tag	UNP P74717
2	6	HIS	-	expression tag	UNP P74717
2	7	HIS	-	expression tag	UNP P74717
2	8	HIS	-	expression tag	UNP P74717
2	9	HIS	-	expression tag	UNP P74717
2	10	HIS	-	expression tag	UNP P74717
2	11	SER	-	expression tag	UNP P74717
2	12	SER	-	expression tag	UNP P74717
2	13	SER	-	expression tag	UNP P74717
2	14	ALA	-	expression tag	UNP P74717
2	15	ALA	-	expression tag	UNP P74717
2	16	LEU	-	expression tag	UNP P74717
2	17	GLU	-	expression tag	UNP P74717
2	18	VAL	-	expression tag	UNP P74717
2	19	LEU	-	expression tag	UNP P74717
2	20	PHE	-	expression tag	UNP P74717
2	21	GLN	-	expression tag	UNP P74717
2	22	GLY	-	expression tag	UNP P74717
2	23	PRO	-	expression tag	UNP P74717
3	1	MET	-	initiating methionine	UNP P74717
3	2	GLY	-	expression tag	UNP P74717
3	3	SER	-	expression tag	UNP P74717
3	4	SER	-	expression tag	UNP P74717
3	5	HIS	-	expression tag	UNP P74717
3	6	HIS	-	expression tag	UNP P74717
3	7	HIS	-	expression tag	UNP P74717
3	8	HIS	-	expression tag	UNP P74717
3	9	HIS	-	expression tag	UNP P74717

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
3	10	HIS	-	expression tag	UNP P74717
3	11	SER	-	expression tag	UNP P74717
3	12	SER	-	expression tag	UNP P74717
3	13	SER	-	expression tag	UNP P74717
3	14	ALA	-	expression tag	UNP P74717
3	15	ALA	-	expression tag	UNP P74717
3	16	LEU	-	expression tag	UNP P74717
3	17	GLU	-	expression tag	UNP P74717
3	18	VAL	-	expression tag	UNP P74717
3	19	LEU	-	expression tag	UNP P74717
3	20	PHE	-	expression tag	UNP P74717
3	21	GLN	-	expression tag	UNP P74717
3	22	GLY	-	expression tag	UNP P74717
3	23	PRO	-	expression tag	UNP P74717
4	1	MET	-	initiating methionine	UNP P74717
4	2	GLY	-	expression tag	UNP P74717
4	3	SER	-	expression tag	UNP P74717
4	4	SER	-	expression tag	UNP P74717
4	5	HIS	-	expression tag	UNP P74717
4	6	HIS	-	expression tag	UNP P74717
4	7	HIS	-	expression tag	UNP P74717
4	8	HIS	-	expression tag	UNP P74717
4	9	HIS	-	expression tag	UNP P74717
4	10	HIS	-	expression tag	UNP P74717
4	11	SER	-	expression tag	UNP P74717
4	12	SER	-	expression tag	UNP P74717
4	13	SER	-	expression tag	UNP P74717
4	14	ALA	-	expression tag	UNP P74717
4	15	ALA	-	expression tag	UNP P74717
4	16	LEU	-	expression tag	UNP P74717
4	17	GLU	-	expression tag	UNP P74717
4	18	VAL	-	expression tag	UNP P74717
4	19	LEU	-	expression tag	UNP P74717
4	20	PHE	-	expression tag	UNP P74717
4	21	GLN	-	expression tag	UNP P74717
4	22	GLY	-	expression tag	UNP P74717
4	23	PRO	-	expression tag	UNP P74717
5	1	MET	-	initiating methionine	UNP P74717
5	2	GLY	-	expression tag	UNP P74717
5	3	SER	-	expression tag	UNP P74717
5	4	SER	-	expression tag	UNP P74717
5	5	HIS	-	expression tag	UNP P74717

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
5	6	HIS	-	expression tag	UNP P74717
5	7	HIS	-	expression tag	UNP P74717
5	8	HIS	-	expression tag	UNP P74717
5	9	HIS	-	expression tag	UNP P74717
5	10	HIS	-	expression tag	UNP P74717
5	11	SER	-	expression tag	UNP P74717
5	12	SER	-	expression tag	UNP P74717
5	13	SER	-	expression tag	UNP P74717
5	14	ALA	-	expression tag	UNP P74717
5	15	ALA	-	expression tag	UNP P74717
5	16	LEU	-	expression tag	UNP P74717
5	17	GLU	-	expression tag	UNP P74717
5	18	VAL	-	expression tag	UNP P74717
5	19	LEU	-	expression tag	UNP P74717
5	20	PHE	-	expression tag	UNP P74717
5	21	GLN	-	expression tag	UNP P74717
5	22	GLY	-	expression tag	UNP P74717
5	23	PRO	-	expression tag	UNP P74717
6	1	MET	-	initiating methionine	UNP P74717
6	2	GLY	-	expression tag	UNP P74717
6	3	SER	-	expression tag	UNP P74717
6	4	SER	-	expression tag	UNP P74717
6	5	HIS	-	expression tag	UNP P74717
6	6	HIS	-	expression tag	UNP P74717
6	7	HIS	-	expression tag	UNP P74717
6	8	HIS	-	expression tag	UNP P74717
6	9	HIS	-	expression tag	UNP P74717
6	10	HIS	-	expression tag	UNP P74717
6	11	SER	-	expression tag	UNP P74717
6	12	SER	-	expression tag	UNP P74717
6	13	SER	-	expression tag	UNP P74717
6	14	ALA	-	expression tag	UNP P74717
6	15	ALA	-	expression tag	UNP P74717
6	16	LEU	-	expression tag	UNP P74717
6	17	GLU	-	expression tag	UNP P74717
6	18	VAL	-	expression tag	UNP P74717
6	19	LEU	-	expression tag	UNP P74717
6	20	PHE	-	expression tag	UNP P74717
6	21	GLN	-	expression tag	UNP P74717
6	22	GLY	-	expression tag	UNP P74717
6	23	PRO	-	expression tag	UNP P74717
7	1	MET	-	initiating methionine	UNP P74717

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
7	2	GLY	-	expression tag	UNP P74717
7	3	SER	-	expression tag	UNP P74717
7	4	SER	-	expression tag	UNP P74717
7	5	HIS	-	expression tag	UNP P74717
7	6	HIS	-	expression tag	UNP P74717
7	7	HIS	-	expression tag	UNP P74717
7	8	HIS	-	expression tag	UNP P74717
7	9	HIS	-	expression tag	UNP P74717
7	10	HIS	-	expression tag	UNP P74717
7	11	SER	-	expression tag	UNP P74717
7	12	SER	-	expression tag	UNP P74717
7	13	SER	-	expression tag	UNP P74717
7	14	ALA	-	expression tag	UNP P74717
7	15	ALA	-	expression tag	UNP P74717
7	16	LEU	-	expression tag	UNP P74717
7	17	GLU	-	expression tag	UNP P74717
7	18	VAL	-	expression tag	UNP P74717
7	19	LEU	-	expression tag	UNP P74717
7	20	PHE	-	expression tag	UNP P74717
7	21	GLN	-	expression tag	UNP P74717
7	22	GLY	-	expression tag	UNP P74717
7	23	PRO	-	expression tag	UNP P74717
A	1	MET	-	initiating methionine	UNP P74717
A	2	GLY	-	expression tag	UNP P74717
A	3	SER	-	expression tag	UNP P74717
A	4	SER	-	expression tag	UNP P74717
A	5	HIS	-	expression tag	UNP P74717
A	6	HIS	-	expression tag	UNP P74717
A	7	HIS	-	expression tag	UNP P74717
A	8	HIS	-	expression tag	UNP P74717
A	9	HIS	-	expression tag	UNP P74717
A	10	HIS	-	expression tag	UNP P74717
A	11	SER	-	expression tag	UNP P74717
A	12	SER	-	expression tag	UNP P74717
A	13	SER	-	expression tag	UNP P74717
A	14	ALA	-	expression tag	UNP P74717
A	15	ALA	-	expression tag	UNP P74717
A	16	LEU	-	expression tag	UNP P74717
A	17	GLU	-	expression tag	UNP P74717
A	18	VAL	-	expression tag	UNP P74717
A	19	LEU	-	expression tag	UNP P74717
A	20	PHE	-	expression tag	UNP P74717

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	GLN	-	expression tag	UNP P74717
A	22	GLY	-	expression tag	UNP P74717
A	23	PRO	-	expression tag	UNP P74717
B	1	MET	-	initiating methionine	UNP P74717
B	2	GLY	-	expression tag	UNP P74717
B	3	SER	-	expression tag	UNP P74717
B	4	SER	-	expression tag	UNP P74717
B	5	HIS	-	expression tag	UNP P74717
B	6	HIS	-	expression tag	UNP P74717
B	7	HIS	-	expression tag	UNP P74717
B	8	HIS	-	expression tag	UNP P74717
B	9	HIS	-	expression tag	UNP P74717
B	10	HIS	-	expression tag	UNP P74717
B	11	SER	-	expression tag	UNP P74717
B	12	SER	-	expression tag	UNP P74717
B	13	SER	-	expression tag	UNP P74717
B	14	ALA	-	expression tag	UNP P74717
B	15	ALA	-	expression tag	UNP P74717
B	16	LEU	-	expression tag	UNP P74717
B	17	GLU	-	expression tag	UNP P74717
B	18	VAL	-	expression tag	UNP P74717
B	19	LEU	-	expression tag	UNP P74717
B	20	PHE	-	expression tag	UNP P74717
B	21	GLN	-	expression tag	UNP P74717
B	22	GLY	-	expression tag	UNP P74717
B	23	PRO	-	expression tag	UNP P74717
C	1	MET	-	initiating methionine	UNP P74717
C	2	GLY	-	expression tag	UNP P74717
C	3	SER	-	expression tag	UNP P74717
C	4	SER	-	expression tag	UNP P74717
C	5	HIS	-	expression tag	UNP P74717
C	6	HIS	-	expression tag	UNP P74717
C	7	HIS	-	expression tag	UNP P74717
C	8	HIS	-	expression tag	UNP P74717
C	9	HIS	-	expression tag	UNP P74717
C	10	HIS	-	expression tag	UNP P74717
C	11	SER	-	expression tag	UNP P74717
C	12	SER	-	expression tag	UNP P74717
C	13	SER	-	expression tag	UNP P74717
C	14	ALA	-	expression tag	UNP P74717
C	15	ALA	-	expression tag	UNP P74717
C	16	LEU	-	expression tag	UNP P74717

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
C	17	GLU	-	expression tag	UNP P74717
C	18	VAL	-	expression tag	UNP P74717
C	19	LEU	-	expression tag	UNP P74717
C	20	PHE	-	expression tag	UNP P74717
C	21	GLN	-	expression tag	UNP P74717
C	22	GLY	-	expression tag	UNP P74717
C	23	PRO	-	expression tag	UNP P74717
D	1	MET	-	initiating methionine	UNP P74717
D	2	GLY	-	expression tag	UNP P74717
D	3	SER	-	expression tag	UNP P74717
D	4	SER	-	expression tag	UNP P74717
D	5	HIS	-	expression tag	UNP P74717
D	6	HIS	-	expression tag	UNP P74717
D	7	HIS	-	expression tag	UNP P74717
D	8	HIS	-	expression tag	UNP P74717
D	9	HIS	-	expression tag	UNP P74717
D	10	HIS	-	expression tag	UNP P74717
D	11	SER	-	expression tag	UNP P74717
D	12	SER	-	expression tag	UNP P74717
D	13	SER	-	expression tag	UNP P74717
D	14	ALA	-	expression tag	UNP P74717
D	15	ALA	-	expression tag	UNP P74717
D	16	LEU	-	expression tag	UNP P74717
D	17	GLU	-	expression tag	UNP P74717
D	18	VAL	-	expression tag	UNP P74717
D	19	LEU	-	expression tag	UNP P74717
D	20	PHE	-	expression tag	UNP P74717
D	21	GLN	-	expression tag	UNP P74717
D	22	GLY	-	expression tag	UNP P74717
D	23	PRO	-	expression tag	UNP P74717
E	1	MET	-	initiating methionine	UNP P74717
E	2	GLY	-	expression tag	UNP P74717
E	3	SER	-	expression tag	UNP P74717
E	4	SER	-	expression tag	UNP P74717
E	5	HIS	-	expression tag	UNP P74717
E	6	HIS	-	expression tag	UNP P74717
E	7	HIS	-	expression tag	UNP P74717
E	8	HIS	-	expression tag	UNP P74717
E	9	HIS	-	expression tag	UNP P74717
E	10	HIS	-	expression tag	UNP P74717
E	11	SER	-	expression tag	UNP P74717
E	12	SER	-	expression tag	UNP P74717

*Continued on next page...*



*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
E	13	SER	-	expression tag	UNP P74717
E	14	ALA	-	expression tag	UNP P74717
E	15	ALA	-	expression tag	UNP P74717
E	16	LEU	-	expression tag	UNP P74717
E	17	GLU	-	expression tag	UNP P74717
E	18	VAL	-	expression tag	UNP P74717
E	19	LEU	-	expression tag	UNP P74717
E	20	PHE	-	expression tag	UNP P74717
E	21	GLN	-	expression tag	UNP P74717
E	22	GLY	-	expression tag	UNP P74717
E	23	PRO	-	expression tag	UNP P74717
F	1	MET	-	initiating methionine	UNP P74717
F	2	GLY	-	expression tag	UNP P74717
F	3	SER	-	expression tag	UNP P74717
F	4	SER	-	expression tag	UNP P74717
F	5	HIS	-	expression tag	UNP P74717
F	6	HIS	-	expression tag	UNP P74717
F	7	HIS	-	expression tag	UNP P74717
F	8	HIS	-	expression tag	UNP P74717
F	9	HIS	-	expression tag	UNP P74717
F	10	HIS	-	expression tag	UNP P74717
F	11	SER	-	expression tag	UNP P74717
F	12	SER	-	expression tag	UNP P74717
F	13	SER	-	expression tag	UNP P74717
F	14	ALA	-	expression tag	UNP P74717
F	15	ALA	-	expression tag	UNP P74717
F	16	LEU	-	expression tag	UNP P74717
F	17	GLU	-	expression tag	UNP P74717
F	18	VAL	-	expression tag	UNP P74717
F	19	LEU	-	expression tag	UNP P74717
F	20	PHE	-	expression tag	UNP P74717
F	21	GLN	-	expression tag	UNP P74717
F	22	GLY	-	expression tag	UNP P74717
F	23	PRO	-	expression tag	UNP P74717
G	1	MET	-	initiating methionine	UNP P74717
G	2	GLY	-	expression tag	UNP P74717
G	3	SER	-	expression tag	UNP P74717
G	4	SER	-	expression tag	UNP P74717
G	5	HIS	-	expression tag	UNP P74717
G	6	HIS	-	expression tag	UNP P74717
G	7	HIS	-	expression tag	UNP P74717
G	8	HIS	-	expression tag	UNP P74717

*Continued on next page...*



*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
G	9	HIS	-	expression tag	UNP P74717
G	10	HIS	-	expression tag	UNP P74717
G	11	SER	-	expression tag	UNP P74717
G	12	SER	-	expression tag	UNP P74717
G	13	SER	-	expression tag	UNP P74717
G	14	ALA	-	expression tag	UNP P74717
G	15	ALA	-	expression tag	UNP P74717
G	16	LEU	-	expression tag	UNP P74717
G	17	GLU	-	expression tag	UNP P74717
G	18	VAL	-	expression tag	UNP P74717
G	19	LEU	-	expression tag	UNP P74717
G	20	PHE	-	expression tag	UNP P74717
G	21	GLN	-	expression tag	UNP P74717
G	22	GLY	-	expression tag	UNP P74717
G	23	PRO	-	expression tag	UNP P74717
H	1	MET	-	initiating methionine	UNP P74717
H	2	GLY	-	expression tag	UNP P74717
H	3	SER	-	expression tag	UNP P74717
H	4	SER	-	expression tag	UNP P74717
H	5	HIS	-	expression tag	UNP P74717
H	6	HIS	-	expression tag	UNP P74717
H	7	HIS	-	expression tag	UNP P74717
H	8	HIS	-	expression tag	UNP P74717
H	9	HIS	-	expression tag	UNP P74717
H	10	HIS	-	expression tag	UNP P74717
H	11	SER	-	expression tag	UNP P74717
H	12	SER	-	expression tag	UNP P74717
H	13	SER	-	expression tag	UNP P74717
H	14	ALA	-	expression tag	UNP P74717
H	15	ALA	-	expression tag	UNP P74717
H	16	LEU	-	expression tag	UNP P74717
H	17	GLU	-	expression tag	UNP P74717
H	18	VAL	-	expression tag	UNP P74717
H	19	LEU	-	expression tag	UNP P74717
H	20	PHE	-	expression tag	UNP P74717
H	21	GLN	-	expression tag	UNP P74717
H	22	GLY	-	expression tag	UNP P74717
H	23	PRO	-	expression tag	UNP P74717
I	1	MET	-	initiating methionine	UNP P74717
I	2	GLY	-	expression tag	UNP P74717
I	3	SER	-	expression tag	UNP P74717
I	4	SER	-	expression tag	UNP P74717

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
I	5	HIS	-	expression tag	UNP P74717
I	6	HIS	-	expression tag	UNP P74717
I	7	HIS	-	expression tag	UNP P74717
I	8	HIS	-	expression tag	UNP P74717
I	9	HIS	-	expression tag	UNP P74717
I	10	HIS	-	expression tag	UNP P74717
I	11	SER	-	expression tag	UNP P74717
I	12	SER	-	expression tag	UNP P74717
I	13	SER	-	expression tag	UNP P74717
I	14	ALA	-	expression tag	UNP P74717
I	15	ALA	-	expression tag	UNP P74717
I	16	LEU	-	expression tag	UNP P74717
I	17	GLU	-	expression tag	UNP P74717
I	18	VAL	-	expression tag	UNP P74717
I	19	LEU	-	expression tag	UNP P74717
I	20	PHE	-	expression tag	UNP P74717
I	21	GLN	-	expression tag	UNP P74717
I	22	GLY	-	expression tag	UNP P74717
I	23	PRO	-	expression tag	UNP P74717
J	1	MET	-	initiating methionine	UNP P74717
J	2	GLY	-	expression tag	UNP P74717
J	3	SER	-	expression tag	UNP P74717
J	4	SER	-	expression tag	UNP P74717
J	5	HIS	-	expression tag	UNP P74717
J	6	HIS	-	expression tag	UNP P74717
J	7	HIS	-	expression tag	UNP P74717
J	8	HIS	-	expression tag	UNP P74717
J	9	HIS	-	expression tag	UNP P74717
J	10	HIS	-	expression tag	UNP P74717
J	11	SER	-	expression tag	UNP P74717
J	12	SER	-	expression tag	UNP P74717
J	13	SER	-	expression tag	UNP P74717
J	14	ALA	-	expression tag	UNP P74717
J	15	ALA	-	expression tag	UNP P74717
J	16	LEU	-	expression tag	UNP P74717
J	17	GLU	-	expression tag	UNP P74717
J	18	VAL	-	expression tag	UNP P74717
J	19	LEU	-	expression tag	UNP P74717
J	20	PHE	-	expression tag	UNP P74717
J	21	GLN	-	expression tag	UNP P74717
J	22	GLY	-	expression tag	UNP P74717
J	23	PRO	-	expression tag	UNP P74717

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
K	1	MET	-	initiating methionine	UNP P74717
K	2	GLY	-	expression tag	UNP P74717
K	3	SER	-	expression tag	UNP P74717
K	4	SER	-	expression tag	UNP P74717
K	5	HIS	-	expression tag	UNP P74717
K	6	HIS	-	expression tag	UNP P74717
K	7	HIS	-	expression tag	UNP P74717
K	8	HIS	-	expression tag	UNP P74717
K	9	HIS	-	expression tag	UNP P74717
K	10	HIS	-	expression tag	UNP P74717
K	11	SER	-	expression tag	UNP P74717
K	12	SER	-	expression tag	UNP P74717
K	13	SER	-	expression tag	UNP P74717
K	14	ALA	-	expression tag	UNP P74717
K	15	ALA	-	expression tag	UNP P74717
K	16	LEU	-	expression tag	UNP P74717
K	17	GLU	-	expression tag	UNP P74717
K	18	VAL	-	expression tag	UNP P74717
K	19	LEU	-	expression tag	UNP P74717
K	20	PHE	-	expression tag	UNP P74717
K	21	GLN	-	expression tag	UNP P74717
K	22	GLY	-	expression tag	UNP P74717
K	23	PRO	-	expression tag	UNP P74717
L	1	MET	-	initiating methionine	UNP P74717
L	2	GLY	-	expression tag	UNP P74717
L	3	SER	-	expression tag	UNP P74717
L	4	SER	-	expression tag	UNP P74717
L	5	HIS	-	expression tag	UNP P74717
L	6	HIS	-	expression tag	UNP P74717
L	7	HIS	-	expression tag	UNP P74717
L	8	HIS	-	expression tag	UNP P74717
L	9	HIS	-	expression tag	UNP P74717
L	10	HIS	-	expression tag	UNP P74717
L	11	SER	-	expression tag	UNP P74717
L	12	SER	-	expression tag	UNP P74717
L	13	SER	-	expression tag	UNP P74717
L	14	ALA	-	expression tag	UNP P74717
L	15	ALA	-	expression tag	UNP P74717
L	16	LEU	-	expression tag	UNP P74717
L	17	GLU	-	expression tag	UNP P74717
L	18	VAL	-	expression tag	UNP P74717
L	19	LEU	-	expression tag	UNP P74717

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
L	20	PHE	-	expression tag	UNP P74717
L	21	GLN	-	expression tag	UNP P74717
L	22	GLY	-	expression tag	UNP P74717
L	23	PRO	-	expression tag	UNP P74717
M	1	MET	-	initiating methionine	UNP P74717
M	2	GLY	-	expression tag	UNP P74717
M	3	SER	-	expression tag	UNP P74717
M	4	SER	-	expression tag	UNP P74717
M	5	HIS	-	expression tag	UNP P74717
M	6	HIS	-	expression tag	UNP P74717
M	7	HIS	-	expression tag	UNP P74717
M	8	HIS	-	expression tag	UNP P74717
M	9	HIS	-	expression tag	UNP P74717
M	10	HIS	-	expression tag	UNP P74717
M	11	SER	-	expression tag	UNP P74717
M	12	SER	-	expression tag	UNP P74717
M	13	SER	-	expression tag	UNP P74717
M	14	ALA	-	expression tag	UNP P74717
M	15	ALA	-	expression tag	UNP P74717
M	16	LEU	-	expression tag	UNP P74717
M	17	GLU	-	expression tag	UNP P74717
M	18	VAL	-	expression tag	UNP P74717
M	19	LEU	-	expression tag	UNP P74717
M	20	PHE	-	expression tag	UNP P74717
M	21	GLN	-	expression tag	UNP P74717
M	22	GLY	-	expression tag	UNP P74717
M	23	PRO	-	expression tag	UNP P74717
N	1	MET	-	initiating methionine	UNP P74717
N	2	GLY	-	expression tag	UNP P74717
N	3	SER	-	expression tag	UNP P74717
N	4	SER	-	expression tag	UNP P74717
N	5	HIS	-	expression tag	UNP P74717
N	6	HIS	-	expression tag	UNP P74717
N	7	HIS	-	expression tag	UNP P74717
N	8	HIS	-	expression tag	UNP P74717
N	9	HIS	-	expression tag	UNP P74717
N	10	HIS	-	expression tag	UNP P74717
N	11	SER	-	expression tag	UNP P74717
N	12	SER	-	expression tag	UNP P74717
N	13	SER	-	expression tag	UNP P74717
N	14	ALA	-	expression tag	UNP P74717
N	15	ALA	-	expression tag	UNP P74717

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
N	16	LEU	-	expression tag	UNP P74717
N	17	GLU	-	expression tag	UNP P74717
N	18	VAL	-	expression tag	UNP P74717
N	19	LEU	-	expression tag	UNP P74717
N	20	PHE	-	expression tag	UNP P74717
N	21	GLN	-	expression tag	UNP P74717
N	22	GLY	-	expression tag	UNP P74717
N	23	PRO	-	expression tag	UNP P74717
O	1	MET	-	initiating methionine	UNP P74717
O	2	GLY	-	expression tag	UNP P74717
O	3	SER	-	expression tag	UNP P74717
O	4	SER	-	expression tag	UNP P74717
O	5	HIS	-	expression tag	UNP P74717
O	6	HIS	-	expression tag	UNP P74717
O	7	HIS	-	expression tag	UNP P74717
O	8	HIS	-	expression tag	UNP P74717
O	9	HIS	-	expression tag	UNP P74717
O	10	HIS	-	expression tag	UNP P74717
O	11	SER	-	expression tag	UNP P74717
O	12	SER	-	expression tag	UNP P74717
O	13	SER	-	expression tag	UNP P74717
O	14	ALA	-	expression tag	UNP P74717
O	15	ALA	-	expression tag	UNP P74717
O	16	LEU	-	expression tag	UNP P74717
O	17	GLU	-	expression tag	UNP P74717
O	18	VAL	-	expression tag	UNP P74717
O	19	LEU	-	expression tag	UNP P74717
O	20	PHE	-	expression tag	UNP P74717
O	21	GLN	-	expression tag	UNP P74717
O	22	GLY	-	expression tag	UNP P74717
O	23	PRO	-	expression tag	UNP P74717
P	1	MET	-	initiating methionine	UNP P74717
P	2	GLY	-	expression tag	UNP P74717
P	3	SER	-	expression tag	UNP P74717
P	4	SER	-	expression tag	UNP P74717
P	5	HIS	-	expression tag	UNP P74717
P	6	HIS	-	expression tag	UNP P74717
P	7	HIS	-	expression tag	UNP P74717
P	8	HIS	-	expression tag	UNP P74717
P	9	HIS	-	expression tag	UNP P74717
P	10	HIS	-	expression tag	UNP P74717
P	11	SER	-	expression tag	UNP P74717

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
P	12	SER	-	expression tag	UNP P74717
P	13	SER	-	expression tag	UNP P74717
P	14	ALA	-	expression tag	UNP P74717
P	15	ALA	-	expression tag	UNP P74717
P	16	LEU	-	expression tag	UNP P74717
P	17	GLU	-	expression tag	UNP P74717
P	18	VAL	-	expression tag	UNP P74717
P	19	LEU	-	expression tag	UNP P74717
P	20	PHE	-	expression tag	UNP P74717
P	21	GLN	-	expression tag	UNP P74717
P	22	GLY	-	expression tag	UNP P74717
P	23	PRO	-	expression tag	UNP P74717
Q	1	MET	-	initiating methionine	UNP P74717
Q	2	GLY	-	expression tag	UNP P74717
Q	3	SER	-	expression tag	UNP P74717
Q	4	SER	-	expression tag	UNP P74717
Q	5	HIS	-	expression tag	UNP P74717
Q	6	HIS	-	expression tag	UNP P74717
Q	7	HIS	-	expression tag	UNP P74717
Q	8	HIS	-	expression tag	UNP P74717
Q	9	HIS	-	expression tag	UNP P74717
Q	10	HIS	-	expression tag	UNP P74717
Q	11	SER	-	expression tag	UNP P74717
Q	12	SER	-	expression tag	UNP P74717
Q	13	SER	-	expression tag	UNP P74717
Q	14	ALA	-	expression tag	UNP P74717
Q	15	ALA	-	expression tag	UNP P74717
Q	16	LEU	-	expression tag	UNP P74717
Q	17	GLU	-	expression tag	UNP P74717
Q	18	VAL	-	expression tag	UNP P74717
Q	19	LEU	-	expression tag	UNP P74717
Q	20	PHE	-	expression tag	UNP P74717
Q	21	GLN	-	expression tag	UNP P74717
Q	22	GLY	-	expression tag	UNP P74717
Q	23	PRO	-	expression tag	UNP P74717
R	1	MET	-	initiating methionine	UNP P74717
R	2	GLY	-	expression tag	UNP P74717
R	3	SER	-	expression tag	UNP P74717
R	4	SER	-	expression tag	UNP P74717
R	5	HIS	-	expression tag	UNP P74717
R	6	HIS	-	expression tag	UNP P74717
R	7	HIS	-	expression tag	UNP P74717

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
R	8	HIS	-	expression tag	UNP P74717
R	9	HIS	-	expression tag	UNP P74717
R	10	HIS	-	expression tag	UNP P74717
R	11	SER	-	expression tag	UNP P74717
R	12	SER	-	expression tag	UNP P74717
R	13	SER	-	expression tag	UNP P74717
R	14	ALA	-	expression tag	UNP P74717
R	15	ALA	-	expression tag	UNP P74717
R	16	LEU	-	expression tag	UNP P74717
R	17	GLU	-	expression tag	UNP P74717
R	18	VAL	-	expression tag	UNP P74717
R	19	LEU	-	expression tag	UNP P74717
R	20	PHE	-	expression tag	UNP P74717
R	21	GLN	-	expression tag	UNP P74717
R	22	GLY	-	expression tag	UNP P74717
R	23	PRO	-	expression tag	UNP P74717
S	1	MET	-	initiating methionine	UNP P74717
S	2	GLY	-	expression tag	UNP P74717
S	3	SER	-	expression tag	UNP P74717
S	4	SER	-	expression tag	UNP P74717
S	5	HIS	-	expression tag	UNP P74717
S	6	HIS	-	expression tag	UNP P74717
S	7	HIS	-	expression tag	UNP P74717
S	8	HIS	-	expression tag	UNP P74717
S	9	HIS	-	expression tag	UNP P74717
S	10	HIS	-	expression tag	UNP P74717
S	11	SER	-	expression tag	UNP P74717
S	12	SER	-	expression tag	UNP P74717
S	13	SER	-	expression tag	UNP P74717
S	14	ALA	-	expression tag	UNP P74717
S	15	ALA	-	expression tag	UNP P74717
S	16	LEU	-	expression tag	UNP P74717
S	17	GLU	-	expression tag	UNP P74717
S	18	VAL	-	expression tag	UNP P74717
S	19	LEU	-	expression tag	UNP P74717
S	20	PHE	-	expression tag	UNP P74717
S	21	GLN	-	expression tag	UNP P74717
S	22	GLY	-	expression tag	UNP P74717
S	23	PRO	-	expression tag	UNP P74717
T	1	MET	-	initiating methionine	UNP P74717
T	2	GLY	-	expression tag	UNP P74717
T	3	SER	-	expression tag	UNP P74717

*Continued on next page...*



*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
T	4	SER	-	expression tag	UNP P74717
T	5	HIS	-	expression tag	UNP P74717
T	6	HIS	-	expression tag	UNP P74717
T	7	HIS	-	expression tag	UNP P74717
T	8	HIS	-	expression tag	UNP P74717
T	9	HIS	-	expression tag	UNP P74717
T	10	HIS	-	expression tag	UNP P74717
T	11	SER	-	expression tag	UNP P74717
T	12	SER	-	expression tag	UNP P74717
T	13	SER	-	expression tag	UNP P74717
T	14	ALA	-	expression tag	UNP P74717
T	15	ALA	-	expression tag	UNP P74717
T	16	LEU	-	expression tag	UNP P74717
T	17	GLU	-	expression tag	UNP P74717
T	18	VAL	-	expression tag	UNP P74717
T	19	LEU	-	expression tag	UNP P74717
T	20	PHE	-	expression tag	UNP P74717
T	21	GLN	-	expression tag	UNP P74717
T	22	GLY	-	expression tag	UNP P74717
T	23	PRO	-	expression tag	UNP P74717
U	1	MET	-	initiating methionine	UNP P74717
U	2	GLY	-	expression tag	UNP P74717
U	3	SER	-	expression tag	UNP P74717
U	4	SER	-	expression tag	UNP P74717
U	5	HIS	-	expression tag	UNP P74717
U	6	HIS	-	expression tag	UNP P74717
U	7	HIS	-	expression tag	UNP P74717
U	8	HIS	-	expression tag	UNP P74717
U	9	HIS	-	expression tag	UNP P74717
U	10	HIS	-	expression tag	UNP P74717
U	11	SER	-	expression tag	UNP P74717
U	12	SER	-	expression tag	UNP P74717
U	13	SER	-	expression tag	UNP P74717
U	14	ALA	-	expression tag	UNP P74717
U	15	ALA	-	expression tag	UNP P74717
U	16	LEU	-	expression tag	UNP P74717
U	17	GLU	-	expression tag	UNP P74717
U	18	VAL	-	expression tag	UNP P74717
U	19	LEU	-	expression tag	UNP P74717
U	20	PHE	-	expression tag	UNP P74717
U	21	GLN	-	expression tag	UNP P74717
U	22	GLY	-	expression tag	UNP P74717

*Continued on next page...*



*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
U	23	PRO	-	expression tag	UNP P74717
V	1	MET	-	initiating methionine	UNP P74717
V	2	GLY	-	expression tag	UNP P74717
V	3	SER	-	expression tag	UNP P74717
V	4	SER	-	expression tag	UNP P74717
V	5	HIS	-	expression tag	UNP P74717
V	6	HIS	-	expression tag	UNP P74717
V	7	HIS	-	expression tag	UNP P74717
V	8	HIS	-	expression tag	UNP P74717
V	9	HIS	-	expression tag	UNP P74717
V	10	HIS	-	expression tag	UNP P74717
V	11	SER	-	expression tag	UNP P74717
V	12	SER	-	expression tag	UNP P74717
V	13	SER	-	expression tag	UNP P74717
V	14	ALA	-	expression tag	UNP P74717
V	15	ALA	-	expression tag	UNP P74717
V	16	LEU	-	expression tag	UNP P74717
V	17	GLU	-	expression tag	UNP P74717
V	18	VAL	-	expression tag	UNP P74717
V	19	LEU	-	expression tag	UNP P74717
V	20	PHE	-	expression tag	UNP P74717
V	21	GLN	-	expression tag	UNP P74717
V	22	GLY	-	expression tag	UNP P74717
V	23	PRO	-	expression tag	UNP P74717
W	1	MET	-	initiating methionine	UNP P74717
W	2	GLY	-	expression tag	UNP P74717
W	3	SER	-	expression tag	UNP P74717
W	4	SER	-	expression tag	UNP P74717
W	5	HIS	-	expression tag	UNP P74717
W	6	HIS	-	expression tag	UNP P74717
W	7	HIS	-	expression tag	UNP P74717
W	8	HIS	-	expression tag	UNP P74717
W	9	HIS	-	expression tag	UNP P74717
W	10	HIS	-	expression tag	UNP P74717
W	11	SER	-	expression tag	UNP P74717
W	12	SER	-	expression tag	UNP P74717
W	13	SER	-	expression tag	UNP P74717
W	14	ALA	-	expression tag	UNP P74717
W	15	ALA	-	expression tag	UNP P74717
W	16	LEU	-	expression tag	UNP P74717
W	17	GLU	-	expression tag	UNP P74717
W	18	VAL	-	expression tag	UNP P74717

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
W	19	LEU	-	expression tag	UNP P74717
W	20	PHE	-	expression tag	UNP P74717
W	21	GLN	-	expression tag	UNP P74717
W	22	GLY	-	expression tag	UNP P74717
W	23	PRO	-	expression tag	UNP P74717
X	1	MET	-	initiating methionine	UNP P74717
X	2	GLY	-	expression tag	UNP P74717
X	3	SER	-	expression tag	UNP P74717
X	4	SER	-	expression tag	UNP P74717
X	5	HIS	-	expression tag	UNP P74717
X	6	HIS	-	expression tag	UNP P74717
X	7	HIS	-	expression tag	UNP P74717
X	8	HIS	-	expression tag	UNP P74717
X	9	HIS	-	expression tag	UNP P74717
X	10	HIS	-	expression tag	UNP P74717
X	11	SER	-	expression tag	UNP P74717
X	12	SER	-	expression tag	UNP P74717
X	13	SER	-	expression tag	UNP P74717
X	14	ALA	-	expression tag	UNP P74717
X	15	ALA	-	expression tag	UNP P74717
X	16	LEU	-	expression tag	UNP P74717
X	17	GLU	-	expression tag	UNP P74717
X	18	VAL	-	expression tag	UNP P74717
X	19	LEU	-	expression tag	UNP P74717
X	20	PHE	-	expression tag	UNP P74717
X	21	GLN	-	expression tag	UNP P74717
X	22	GLY	-	expression tag	UNP P74717
X	23	PRO	-	expression tag	UNP P74717
Y	1	MET	-	initiating methionine	UNP P74717
Y	2	GLY	-	expression tag	UNP P74717
Y	3	SER	-	expression tag	UNP P74717
Y	4	SER	-	expression tag	UNP P74717
Y	5	HIS	-	expression tag	UNP P74717
Y	6	HIS	-	expression tag	UNP P74717
Y	7	HIS	-	expression tag	UNP P74717
Y	8	HIS	-	expression tag	UNP P74717
Y	9	HIS	-	expression tag	UNP P74717
Y	10	HIS	-	expression tag	UNP P74717
Y	11	SER	-	expression tag	UNP P74717
Y	12	SER	-	expression tag	UNP P74717
Y	13	SER	-	expression tag	UNP P74717
Y	14	ALA	-	expression tag	UNP P74717

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
Y	15	ALA	-	expression tag	UNP P74717
Y	16	LEU	-	expression tag	UNP P74717
Y	17	GLU	-	expression tag	UNP P74717
Y	18	VAL	-	expression tag	UNP P74717
Y	19	LEU	-	expression tag	UNP P74717
Y	20	PHE	-	expression tag	UNP P74717
Y	21	GLN	-	expression tag	UNP P74717
Y	22	GLY	-	expression tag	UNP P74717
Y	23	PRO	-	expression tag	UNP P74717
Z	1	MET	-	initiating methionine	UNP P74717
Z	2	GLY	-	expression tag	UNP P74717
Z	3	SER	-	expression tag	UNP P74717
Z	4	SER	-	expression tag	UNP P74717
Z	5	HIS	-	expression tag	UNP P74717
Z	6	HIS	-	expression tag	UNP P74717
Z	7	HIS	-	expression tag	UNP P74717
Z	8	HIS	-	expression tag	UNP P74717
Z	9	HIS	-	expression tag	UNP P74717
Z	10	HIS	-	expression tag	UNP P74717
Z	11	SER	-	expression tag	UNP P74717
Z	12	SER	-	expression tag	UNP P74717
Z	13	SER	-	expression tag	UNP P74717
Z	14	ALA	-	expression tag	UNP P74717
Z	15	ALA	-	expression tag	UNP P74717
Z	16	LEU	-	expression tag	UNP P74717
Z	17	GLU	-	expression tag	UNP P74717
Z	18	VAL	-	expression tag	UNP P74717
Z	19	LEU	-	expression tag	UNP P74717
Z	20	PHE	-	expression tag	UNP P74717
Z	21	GLN	-	expression tag	UNP P74717
Z	22	GLY	-	expression tag	UNP P74717
Z	23	PRO	-	expression tag	UNP P74717
a	1	MET	-	initiating methionine	UNP P74717
a	2	GLY	-	expression tag	UNP P74717
a	3	SER	-	expression tag	UNP P74717
a	4	SER	-	expression tag	UNP P74717
a	5	HIS	-	expression tag	UNP P74717
a	6	HIS	-	expression tag	UNP P74717
a	7	HIS	-	expression tag	UNP P74717
a	8	HIS	-	expression tag	UNP P74717
a	9	HIS	-	expression tag	UNP P74717
a	10	HIS	-	expression tag	UNP P74717

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
a	11	SER	-	expression tag	UNP P74717
a	12	SER	-	expression tag	UNP P74717
a	13	SER	-	expression tag	UNP P74717
a	14	ALA	-	expression tag	UNP P74717
a	15	ALA	-	expression tag	UNP P74717
a	16	LEU	-	expression tag	UNP P74717
a	17	GLU	-	expression tag	UNP P74717
a	18	VAL	-	expression tag	UNP P74717
a	19	LEU	-	expression tag	UNP P74717
a	20	PHE	-	expression tag	UNP P74717
a	21	GLN	-	expression tag	UNP P74717
a	22	GLY	-	expression tag	UNP P74717
a	23	PRO	-	expression tag	UNP P74717
b	1	MET	-	initiating methionine	UNP P74717
b	2	GLY	-	expression tag	UNP P74717
b	3	SER	-	expression tag	UNP P74717
b	4	SER	-	expression tag	UNP P74717
b	5	HIS	-	expression tag	UNP P74717
b	6	HIS	-	expression tag	UNP P74717
b	7	HIS	-	expression tag	UNP P74717
b	8	HIS	-	expression tag	UNP P74717
b	9	HIS	-	expression tag	UNP P74717
b	10	HIS	-	expression tag	UNP P74717
b	11	SER	-	expression tag	UNP P74717
b	12	SER	-	expression tag	UNP P74717
b	13	SER	-	expression tag	UNP P74717
b	14	ALA	-	expression tag	UNP P74717
b	15	ALA	-	expression tag	UNP P74717
b	16	LEU	-	expression tag	UNP P74717
b	17	GLU	-	expression tag	UNP P74717
b	18	VAL	-	expression tag	UNP P74717
b	19	LEU	-	expression tag	UNP P74717
b	20	PHE	-	expression tag	UNP P74717
b	21	GLN	-	expression tag	UNP P74717
b	22	GLY	-	expression tag	UNP P74717
b	23	PRO	-	expression tag	UNP P74717
c	1	MET	-	initiating methionine	UNP P74717
c	2	GLY	-	expression tag	UNP P74717
c	3	SER	-	expression tag	UNP P74717
c	4	SER	-	expression tag	UNP P74717
c	5	HIS	-	expression tag	UNP P74717
c	6	HIS	-	expression tag	UNP P74717

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
c	7	HIS	-	expression tag	UNP P74717
c	8	HIS	-	expression tag	UNP P74717
c	9	HIS	-	expression tag	UNP P74717
c	10	HIS	-	expression tag	UNP P74717
c	11	SER	-	expression tag	UNP P74717
c	12	SER	-	expression tag	UNP P74717
c	13	SER	-	expression tag	UNP P74717
c	14	ALA	-	expression tag	UNP P74717
c	15	ALA	-	expression tag	UNP P74717
c	16	LEU	-	expression tag	UNP P74717
c	17	GLU	-	expression tag	UNP P74717
c	18	VAL	-	expression tag	UNP P74717
c	19	LEU	-	expression tag	UNP P74717
c	20	PHE	-	expression tag	UNP P74717
c	21	GLN	-	expression tag	UNP P74717
c	22	GLY	-	expression tag	UNP P74717
c	23	PRO	-	expression tag	UNP P74717
d	1	MET	-	initiating methionine	UNP P74717
d	2	GLY	-	expression tag	UNP P74717
d	3	SER	-	expression tag	UNP P74717
d	4	SER	-	expression tag	UNP P74717
d	5	HIS	-	expression tag	UNP P74717
d	6	HIS	-	expression tag	UNP P74717
d	7	HIS	-	expression tag	UNP P74717
d	8	HIS	-	expression tag	UNP P74717
d	9	HIS	-	expression tag	UNP P74717
d	10	HIS	-	expression tag	UNP P74717
d	11	SER	-	expression tag	UNP P74717
d	12	SER	-	expression tag	UNP P74717
d	13	SER	-	expression tag	UNP P74717
d	14	ALA	-	expression tag	UNP P74717
d	15	ALA	-	expression tag	UNP P74717
d	16	LEU	-	expression tag	UNP P74717
d	17	GLU	-	expression tag	UNP P74717
d	18	VAL	-	expression tag	UNP P74717
d	19	LEU	-	expression tag	UNP P74717
d	20	PHE	-	expression tag	UNP P74717
d	21	GLN	-	expression tag	UNP P74717
d	22	GLY	-	expression tag	UNP P74717
d	23	PRO	-	expression tag	UNP P74717
e	1	MET	-	initiating methionine	UNP P74717
e	2	GLY	-	expression tag	UNP P74717

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
e	3	SER	-	expression tag	UNP P74717
e	4	SER	-	expression tag	UNP P74717
e	5	HIS	-	expression tag	UNP P74717
e	6	HIS	-	expression tag	UNP P74717
e	7	HIS	-	expression tag	UNP P74717
e	8	HIS	-	expression tag	UNP P74717
e	9	HIS	-	expression tag	UNP P74717
e	10	HIS	-	expression tag	UNP P74717
e	11	SER	-	expression tag	UNP P74717
e	12	SER	-	expression tag	UNP P74717
e	13	SER	-	expression tag	UNP P74717
e	14	ALA	-	expression tag	UNP P74717
e	15	ALA	-	expression tag	UNP P74717
e	16	LEU	-	expression tag	UNP P74717
e	17	GLU	-	expression tag	UNP P74717
e	18	VAL	-	expression tag	UNP P74717
e	19	LEU	-	expression tag	UNP P74717
e	20	PHE	-	expression tag	UNP P74717
e	21	GLN	-	expression tag	UNP P74717
e	22	GLY	-	expression tag	UNP P74717
e	23	PRO	-	expression tag	UNP P74717
f	1	MET	-	initiating methionine	UNP P74717
f	2	GLY	-	expression tag	UNP P74717
f	3	SER	-	expression tag	UNP P74717
f	4	SER	-	expression tag	UNP P74717
f	5	HIS	-	expression tag	UNP P74717
f	6	HIS	-	expression tag	UNP P74717
f	7	HIS	-	expression tag	UNP P74717
f	8	HIS	-	expression tag	UNP P74717
f	9	HIS	-	expression tag	UNP P74717
f	10	HIS	-	expression tag	UNP P74717
f	11	SER	-	expression tag	UNP P74717
f	12	SER	-	expression tag	UNP P74717
f	13	SER	-	expression tag	UNP P74717
f	14	ALA	-	expression tag	UNP P74717
f	15	ALA	-	expression tag	UNP P74717
f	16	LEU	-	expression tag	UNP P74717
f	17	GLU	-	expression tag	UNP P74717
f	18	VAL	-	expression tag	UNP P74717
f	19	LEU	-	expression tag	UNP P74717
f	20	PHE	-	expression tag	UNP P74717
f	21	GLN	-	expression tag	UNP P74717

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
f	22	GLY	-	expression tag	UNP P74717
f	23	PRO	-	expression tag	UNP P74717
g	1	MET	-	initiating methionine	UNP P74717
g	2	GLY	-	expression tag	UNP P74717
g	3	SER	-	expression tag	UNP P74717
g	4	SER	-	expression tag	UNP P74717
g	5	HIS	-	expression tag	UNP P74717
g	6	HIS	-	expression tag	UNP P74717
g	7	HIS	-	expression tag	UNP P74717
g	8	HIS	-	expression tag	UNP P74717
g	9	HIS	-	expression tag	UNP P74717
g	10	HIS	-	expression tag	UNP P74717
g	11	SER	-	expression tag	UNP P74717
g	12	SER	-	expression tag	UNP P74717
g	13	SER	-	expression tag	UNP P74717
g	14	ALA	-	expression tag	UNP P74717
g	15	ALA	-	expression tag	UNP P74717
g	16	LEU	-	expression tag	UNP P74717
g	17	GLU	-	expression tag	UNP P74717
g	18	VAL	-	expression tag	UNP P74717
g	19	LEU	-	expression tag	UNP P74717
g	20	PHE	-	expression tag	UNP P74717
g	21	GLN	-	expression tag	UNP P74717
g	22	GLY	-	expression tag	UNP P74717
g	23	PRO	-	expression tag	UNP P74717
h	1	MET	-	initiating methionine	UNP P74717
h	2	GLY	-	expression tag	UNP P74717
h	3	SER	-	expression tag	UNP P74717
h	4	SER	-	expression tag	UNP P74717
h	5	HIS	-	expression tag	UNP P74717
h	6	HIS	-	expression tag	UNP P74717
h	7	HIS	-	expression tag	UNP P74717
h	8	HIS	-	expression tag	UNP P74717
h	9	HIS	-	expression tag	UNP P74717
h	10	HIS	-	expression tag	UNP P74717
h	11	SER	-	expression tag	UNP P74717
h	12	SER	-	expression tag	UNP P74717
h	13	SER	-	expression tag	UNP P74717
h	14	ALA	-	expression tag	UNP P74717
h	15	ALA	-	expression tag	UNP P74717
h	16	LEU	-	expression tag	UNP P74717
h	17	GLU	-	expression tag	UNP P74717

*Continued on next page...*



*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
h	18	VAL	-	expression tag	UNP P74717
h	19	LEU	-	expression tag	UNP P74717
h	20	PHE	-	expression tag	UNP P74717
h	21	GLN	-	expression tag	UNP P74717
h	22	GLY	-	expression tag	UNP P74717
h	23	PRO	-	expression tag	UNP P74717
i	1	MET	-	initiating methionine	UNP P74717
i	2	GLY	-	expression tag	UNP P74717
i	3	SER	-	expression tag	UNP P74717
i	4	SER	-	expression tag	UNP P74717
i	5	HIS	-	expression tag	UNP P74717
i	6	HIS	-	expression tag	UNP P74717
i	7	HIS	-	expression tag	UNP P74717
i	8	HIS	-	expression tag	UNP P74717
i	9	HIS	-	expression tag	UNP P74717
i	10	HIS	-	expression tag	UNP P74717
i	11	SER	-	expression tag	UNP P74717
i	12	SER	-	expression tag	UNP P74717
i	13	SER	-	expression tag	UNP P74717
i	14	ALA	-	expression tag	UNP P74717
i	15	ALA	-	expression tag	UNP P74717
i	16	LEU	-	expression tag	UNP P74717
i	17	GLU	-	expression tag	UNP P74717
i	18	VAL	-	expression tag	UNP P74717
i	19	LEU	-	expression tag	UNP P74717
i	20	PHE	-	expression tag	UNP P74717
i	21	GLN	-	expression tag	UNP P74717
i	22	GLY	-	expression tag	UNP P74717
i	23	PRO	-	expression tag	UNP P74717
j	1	MET	-	initiating methionine	UNP P74717
j	2	GLY	-	expression tag	UNP P74717
j	3	SER	-	expression tag	UNP P74717
j	4	SER	-	expression tag	UNP P74717
j	5	HIS	-	expression tag	UNP P74717
j	6	HIS	-	expression tag	UNP P74717
j	7	HIS	-	expression tag	UNP P74717
j	8	HIS	-	expression tag	UNP P74717
j	9	HIS	-	expression tag	UNP P74717
j	10	HIS	-	expression tag	UNP P74717
j	11	SER	-	expression tag	UNP P74717
j	12	SER	-	expression tag	UNP P74717
j	13	SER	-	expression tag	UNP P74717

*Continued on next page...*



*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
j	14	ALA	-	expression tag	UNP P74717
j	15	ALA	-	expression tag	UNP P74717
j	16	LEU	-	expression tag	UNP P74717
j	17	GLU	-	expression tag	UNP P74717
j	18	VAL	-	expression tag	UNP P74717
j	19	LEU	-	expression tag	UNP P74717
j	20	PHE	-	expression tag	UNP P74717
j	21	GLN	-	expression tag	UNP P74717
j	22	GLY	-	expression tag	UNP P74717
j	23	PRO	-	expression tag	UNP P74717
k	1	MET	-	initiating methionine	UNP P74717
k	2	GLY	-	expression tag	UNP P74717
k	3	SER	-	expression tag	UNP P74717
k	4	SER	-	expression tag	UNP P74717
k	5	HIS	-	expression tag	UNP P74717
k	6	HIS	-	expression tag	UNP P74717
k	7	HIS	-	expression tag	UNP P74717
k	8	HIS	-	expression tag	UNP P74717
k	9	HIS	-	expression tag	UNP P74717
k	10	HIS	-	expression tag	UNP P74717
k	11	SER	-	expression tag	UNP P74717
k	12	SER	-	expression tag	UNP P74717
k	13	SER	-	expression tag	UNP P74717
k	14	ALA	-	expression tag	UNP P74717
k	15	ALA	-	expression tag	UNP P74717
k	16	LEU	-	expression tag	UNP P74717
k	17	GLU	-	expression tag	UNP P74717
k	18	VAL	-	expression tag	UNP P74717
k	19	LEU	-	expression tag	UNP P74717
k	20	PHE	-	expression tag	UNP P74717
k	21	GLN	-	expression tag	UNP P74717
k	22	GLY	-	expression tag	UNP P74717
k	23	PRO	-	expression tag	UNP P74717
l	1	MET	-	initiating methionine	UNP P74717
l	2	GLY	-	expression tag	UNP P74717
l	3	SER	-	expression tag	UNP P74717
l	4	SER	-	expression tag	UNP P74717
l	5	HIS	-	expression tag	UNP P74717
l	6	HIS	-	expression tag	UNP P74717
l	7	HIS	-	expression tag	UNP P74717
l	8	HIS	-	expression tag	UNP P74717
l	9	HIS	-	expression tag	UNP P74717

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
l	10	HIS	-	expression tag	UNP P74717
l	11	SER	-	expression tag	UNP P74717
l	12	SER	-	expression tag	UNP P74717
l	13	SER	-	expression tag	UNP P74717
l	14	ALA	-	expression tag	UNP P74717
l	15	ALA	-	expression tag	UNP P74717
l	16	LEU	-	expression tag	UNP P74717
l	17	GLU	-	expression tag	UNP P74717
l	18	VAL	-	expression tag	UNP P74717
l	19	LEU	-	expression tag	UNP P74717
l	20	PHE	-	expression tag	UNP P74717
l	21	GLN	-	expression tag	UNP P74717
l	22	GLY	-	expression tag	UNP P74717
l	23	PRO	-	expression tag	UNP P74717
m	1	MET	-	initiating methionine	UNP P74717
m	2	GLY	-	expression tag	UNP P74717
m	3	SER	-	expression tag	UNP P74717
m	4	SER	-	expression tag	UNP P74717
m	5	HIS	-	expression tag	UNP P74717
m	6	HIS	-	expression tag	UNP P74717
m	7	HIS	-	expression tag	UNP P74717
m	8	HIS	-	expression tag	UNP P74717
m	9	HIS	-	expression tag	UNP P74717
m	10	HIS	-	expression tag	UNP P74717
m	11	SER	-	expression tag	UNP P74717
m	12	SER	-	expression tag	UNP P74717
m	13	SER	-	expression tag	UNP P74717
m	14	ALA	-	expression tag	UNP P74717
m	15	ALA	-	expression tag	UNP P74717
m	16	LEU	-	expression tag	UNP P74717
m	17	GLU	-	expression tag	UNP P74717
m	18	VAL	-	expression tag	UNP P74717
m	19	LEU	-	expression tag	UNP P74717
m	20	PHE	-	expression tag	UNP P74717
m	21	GLN	-	expression tag	UNP P74717
m	22	GLY	-	expression tag	UNP P74717
m	23	PRO	-	expression tag	UNP P74717
n	1	MET	-	initiating methionine	UNP P74717
n	2	GLY	-	expression tag	UNP P74717
n	3	SER	-	expression tag	UNP P74717
n	4	SER	-	expression tag	UNP P74717
n	5	HIS	-	expression tag	UNP P74717

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
n	6	HIS	-	expression tag	UNP P74717
n	7	HIS	-	expression tag	UNP P74717
n	8	HIS	-	expression tag	UNP P74717
n	9	HIS	-	expression tag	UNP P74717
n	10	HIS	-	expression tag	UNP P74717
n	11	SER	-	expression tag	UNP P74717
n	12	SER	-	expression tag	UNP P74717
n	13	SER	-	expression tag	UNP P74717
n	14	ALA	-	expression tag	UNP P74717
n	15	ALA	-	expression tag	UNP P74717
n	16	LEU	-	expression tag	UNP P74717
n	17	GLU	-	expression tag	UNP P74717
n	18	VAL	-	expression tag	UNP P74717
n	19	LEU	-	expression tag	UNP P74717
n	20	PHE	-	expression tag	UNP P74717
n	21	GLN	-	expression tag	UNP P74717
n	22	GLY	-	expression tag	UNP P74717
n	23	PRO	-	expression tag	UNP P74717
o	1	MET	-	initiating methionine	UNP P74717
o	2	GLY	-	expression tag	UNP P74717
o	3	SER	-	expression tag	UNP P74717
o	4	SER	-	expression tag	UNP P74717
o	5	HIS	-	expression tag	UNP P74717
o	6	HIS	-	expression tag	UNP P74717
o	7	HIS	-	expression tag	UNP P74717
o	8	HIS	-	expression tag	UNP P74717
o	9	HIS	-	expression tag	UNP P74717
o	10	HIS	-	expression tag	UNP P74717
o	11	SER	-	expression tag	UNP P74717
o	12	SER	-	expression tag	UNP P74717
o	13	SER	-	expression tag	UNP P74717
o	14	ALA	-	expression tag	UNP P74717
o	15	ALA	-	expression tag	UNP P74717
o	16	LEU	-	expression tag	UNP P74717
o	17	GLU	-	expression tag	UNP P74717
o	18	VAL	-	expression tag	UNP P74717
o	19	LEU	-	expression tag	UNP P74717
o	20	PHE	-	expression tag	UNP P74717
o	21	GLN	-	expression tag	UNP P74717
o	22	GLY	-	expression tag	UNP P74717
o	23	PRO	-	expression tag	UNP P74717
p	1	MET	-	initiating methionine	UNP P74717

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
p	2	GLY	-	expression tag	UNP P74717
p	3	SER	-	expression tag	UNP P74717
p	4	SER	-	expression tag	UNP P74717
p	5	HIS	-	expression tag	UNP P74717
p	6	HIS	-	expression tag	UNP P74717
p	7	HIS	-	expression tag	UNP P74717
p	8	HIS	-	expression tag	UNP P74717
p	9	HIS	-	expression tag	UNP P74717
p	10	HIS	-	expression tag	UNP P74717
p	11	SER	-	expression tag	UNP P74717
p	12	SER	-	expression tag	UNP P74717
p	13	SER	-	expression tag	UNP P74717
p	14	ALA	-	expression tag	UNP P74717
p	15	ALA	-	expression tag	UNP P74717
p	16	LEU	-	expression tag	UNP P74717
p	17	GLU	-	expression tag	UNP P74717
p	18	VAL	-	expression tag	UNP P74717
p	19	LEU	-	expression tag	UNP P74717
p	20	PHE	-	expression tag	UNP P74717
p	21	GLN	-	expression tag	UNP P74717
p	22	GLY	-	expression tag	UNP P74717
p	23	PRO	-	expression tag	UNP P74717
q	1	MET	-	initiating methionine	UNP P74717
q	2	GLY	-	expression tag	UNP P74717
q	3	SER	-	expression tag	UNP P74717
q	4	SER	-	expression tag	UNP P74717
q	5	HIS	-	expression tag	UNP P74717
q	6	HIS	-	expression tag	UNP P74717
q	7	HIS	-	expression tag	UNP P74717
q	8	HIS	-	expression tag	UNP P74717
q	9	HIS	-	expression tag	UNP P74717
q	10	HIS	-	expression tag	UNP P74717
q	11	SER	-	expression tag	UNP P74717
q	12	SER	-	expression tag	UNP P74717
q	13	SER	-	expression tag	UNP P74717
q	14	ALA	-	expression tag	UNP P74717
q	15	ALA	-	expression tag	UNP P74717
q	16	LEU	-	expression tag	UNP P74717
q	17	GLU	-	expression tag	UNP P74717
q	18	VAL	-	expression tag	UNP P74717
q	19	LEU	-	expression tag	UNP P74717
q	20	PHE	-	expression tag	UNP P74717

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
q	21	GLN	-	expression tag	UNP P74717
q	22	GLY	-	expression tag	UNP P74717
q	23	PRO	-	expression tag	UNP P74717
r	1	MET	-	initiating methionine	UNP P74717
r	2	GLY	-	expression tag	UNP P74717
r	3	SER	-	expression tag	UNP P74717
r	4	SER	-	expression tag	UNP P74717
r	5	HIS	-	expression tag	UNP P74717
r	6	HIS	-	expression tag	UNP P74717
r	7	HIS	-	expression tag	UNP P74717
r	8	HIS	-	expression tag	UNP P74717
r	9	HIS	-	expression tag	UNP P74717
r	10	HIS	-	expression tag	UNP P74717
r	11	SER	-	expression tag	UNP P74717
r	12	SER	-	expression tag	UNP P74717
r	13	SER	-	expression tag	UNP P74717
r	14	ALA	-	expression tag	UNP P74717
r	15	ALA	-	expression tag	UNP P74717
r	16	LEU	-	expression tag	UNP P74717
r	17	GLU	-	expression tag	UNP P74717
r	18	VAL	-	expression tag	UNP P74717
r	19	LEU	-	expression tag	UNP P74717
r	20	PHE	-	expression tag	UNP P74717
r	21	GLN	-	expression tag	UNP P74717
r	22	GLY	-	expression tag	UNP P74717
r	23	PRO	-	expression tag	UNP P74717
s	1	MET	-	initiating methionine	UNP P74717
s	2	GLY	-	expression tag	UNP P74717
s	3	SER	-	expression tag	UNP P74717
s	4	SER	-	expression tag	UNP P74717
s	5	HIS	-	expression tag	UNP P74717
s	6	HIS	-	expression tag	UNP P74717
s	7	HIS	-	expression tag	UNP P74717
s	8	HIS	-	expression tag	UNP P74717
s	9	HIS	-	expression tag	UNP P74717
s	10	HIS	-	expression tag	UNP P74717
s	11	SER	-	expression tag	UNP P74717
s	12	SER	-	expression tag	UNP P74717
s	13	SER	-	expression tag	UNP P74717
s	14	ALA	-	expression tag	UNP P74717
s	15	ALA	-	expression tag	UNP P74717
s	16	LEU	-	expression tag	UNP P74717

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
s	17	GLU	-	expression tag	UNP P74717
s	18	VAL	-	expression tag	UNP P74717
s	19	LEU	-	expression tag	UNP P74717
s	20	PHE	-	expression tag	UNP P74717
s	21	GLN	-	expression tag	UNP P74717
s	22	GLY	-	expression tag	UNP P74717
s	23	PRO	-	expression tag	UNP P74717
t	1	MET	-	initiating methionine	UNP P74717
t	2	GLY	-	expression tag	UNP P74717
t	3	SER	-	expression tag	UNP P74717
t	4	SER	-	expression tag	UNP P74717
t	5	HIS	-	expression tag	UNP P74717
t	6	HIS	-	expression tag	UNP P74717
t	7	HIS	-	expression tag	UNP P74717
t	8	HIS	-	expression tag	UNP P74717
t	9	HIS	-	expression tag	UNP P74717
t	10	HIS	-	expression tag	UNP P74717
t	11	SER	-	expression tag	UNP P74717
t	12	SER	-	expression tag	UNP P74717
t	13	SER	-	expression tag	UNP P74717
t	14	ALA	-	expression tag	UNP P74717
t	15	ALA	-	expression tag	UNP P74717
t	16	LEU	-	expression tag	UNP P74717
t	17	GLU	-	expression tag	UNP P74717
t	18	VAL	-	expression tag	UNP P74717
t	19	LEU	-	expression tag	UNP P74717
t	20	PHE	-	expression tag	UNP P74717
t	21	GLN	-	expression tag	UNP P74717
t	22	GLY	-	expression tag	UNP P74717
t	23	PRO	-	expression tag	UNP P74717
u	1	MET	-	initiating methionine	UNP P74717
u	2	GLY	-	expression tag	UNP P74717
u	3	SER	-	expression tag	UNP P74717
u	4	SER	-	expression tag	UNP P74717
u	5	HIS	-	expression tag	UNP P74717
u	6	HIS	-	expression tag	UNP P74717
u	7	HIS	-	expression tag	UNP P74717
u	8	HIS	-	expression tag	UNP P74717
u	9	HIS	-	expression tag	UNP P74717
u	10	HIS	-	expression tag	UNP P74717
u	11	SER	-	expression tag	UNP P74717
u	12	SER	-	expression tag	UNP P74717

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
u	13	SER	-	expression tag	UNP P74717
u	14	ALA	-	expression tag	UNP P74717
u	15	ALA	-	expression tag	UNP P74717
u	16	LEU	-	expression tag	UNP P74717
u	17	GLU	-	expression tag	UNP P74717
u	18	VAL	-	expression tag	UNP P74717
u	19	LEU	-	expression tag	UNP P74717
u	20	PHE	-	expression tag	UNP P74717
u	21	GLN	-	expression tag	UNP P74717
u	22	GLY	-	expression tag	UNP P74717
u	23	PRO	-	expression tag	UNP P74717
v	1	MET	-	initiating methionine	UNP P74717
v	2	GLY	-	expression tag	UNP P74717
v	3	SER	-	expression tag	UNP P74717
v	4	SER	-	expression tag	UNP P74717
v	5	HIS	-	expression tag	UNP P74717
v	6	HIS	-	expression tag	UNP P74717
v	7	HIS	-	expression tag	UNP P74717
v	8	HIS	-	expression tag	UNP P74717
v	9	HIS	-	expression tag	UNP P74717
v	10	HIS	-	expression tag	UNP P74717
v	11	SER	-	expression tag	UNP P74717
v	12	SER	-	expression tag	UNP P74717
v	13	SER	-	expression tag	UNP P74717
v	14	ALA	-	expression tag	UNP P74717
v	15	ALA	-	expression tag	UNP P74717
v	16	LEU	-	expression tag	UNP P74717
v	17	GLU	-	expression tag	UNP P74717
v	18	VAL	-	expression tag	UNP P74717
v	19	LEU	-	expression tag	UNP P74717
v	20	PHE	-	expression tag	UNP P74717
v	21	GLN	-	expression tag	UNP P74717
v	22	GLY	-	expression tag	UNP P74717
v	23	PRO	-	expression tag	UNP P74717
w	1	MET	-	initiating methionine	UNP P74717
w	2	GLY	-	expression tag	UNP P74717
w	3	SER	-	expression tag	UNP P74717
w	4	SER	-	expression tag	UNP P74717
w	5	HIS	-	expression tag	UNP P74717
w	6	HIS	-	expression tag	UNP P74717
w	7	HIS	-	expression tag	UNP P74717
w	8	HIS	-	expression tag	UNP P74717

*Continued on next page...*



*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
w	9	HIS	-	expression tag	UNP P74717
w	10	HIS	-	expression tag	UNP P74717
w	11	SER	-	expression tag	UNP P74717
w	12	SER	-	expression tag	UNP P74717
w	13	SER	-	expression tag	UNP P74717
w	14	ALA	-	expression tag	UNP P74717
w	15	ALA	-	expression tag	UNP P74717
w	16	LEU	-	expression tag	UNP P74717
w	17	GLU	-	expression tag	UNP P74717
w	18	VAL	-	expression tag	UNP P74717
w	19	LEU	-	expression tag	UNP P74717
w	20	PHE	-	expression tag	UNP P74717
w	21	GLN	-	expression tag	UNP P74717
w	22	GLY	-	expression tag	UNP P74717
w	23	PRO	-	expression tag	UNP P74717
x	1	MET	-	initiating methionine	UNP P74717
x	2	GLY	-	expression tag	UNP P74717
x	3	SER	-	expression tag	UNP P74717
x	4	SER	-	expression tag	UNP P74717
x	5	HIS	-	expression tag	UNP P74717
x	6	HIS	-	expression tag	UNP P74717
x	7	HIS	-	expression tag	UNP P74717
x	8	HIS	-	expression tag	UNP P74717
x	9	HIS	-	expression tag	UNP P74717
x	10	HIS	-	expression tag	UNP P74717
x	11	SER	-	expression tag	UNP P74717
x	12	SER	-	expression tag	UNP P74717
x	13	SER	-	expression tag	UNP P74717
x	14	ALA	-	expression tag	UNP P74717
x	15	ALA	-	expression tag	UNP P74717
x	16	LEU	-	expression tag	UNP P74717
x	17	GLU	-	expression tag	UNP P74717
x	18	VAL	-	expression tag	UNP P74717
x	19	LEU	-	expression tag	UNP P74717
x	20	PHE	-	expression tag	UNP P74717
x	21	GLN	-	expression tag	UNP P74717
x	22	GLY	-	expression tag	UNP P74717
x	23	PRO	-	expression tag	UNP P74717
y	1	MET	-	initiating methionine	UNP P74717
y	2	GLY	-	expression tag	UNP P74717
y	3	SER	-	expression tag	UNP P74717
y	4	SER	-	expression tag	UNP P74717

*Continued on next page...*



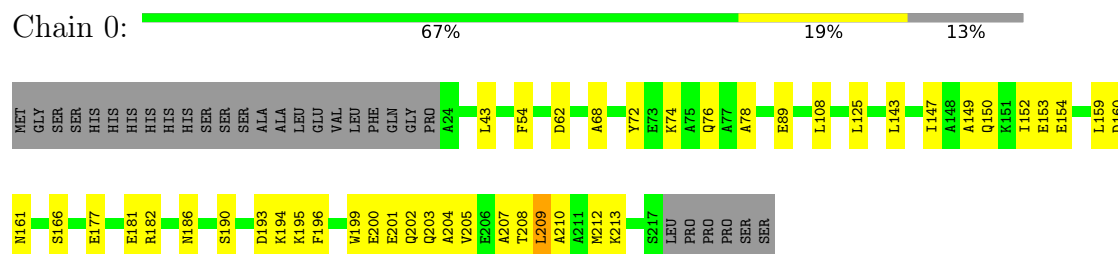
*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
y	5	HIS	-	expression tag	UNP P74717
y	6	HIS	-	expression tag	UNP P74717
y	7	HIS	-	expression tag	UNP P74717
y	8	HIS	-	expression tag	UNP P74717
y	9	HIS	-	expression tag	UNP P74717
y	10	HIS	-	expression tag	UNP P74717
y	11	SER	-	expression tag	UNP P74717
y	12	SER	-	expression tag	UNP P74717
y	13	SER	-	expression tag	UNP P74717
y	14	ALA	-	expression tag	UNP P74717
y	15	ALA	-	expression tag	UNP P74717
y	16	LEU	-	expression tag	UNP P74717
y	17	GLU	-	expression tag	UNP P74717
y	18	VAL	-	expression tag	UNP P74717
y	19	LEU	-	expression tag	UNP P74717
y	20	PHE	-	expression tag	UNP P74717
y	21	GLN	-	expression tag	UNP P74717
y	22	GLY	-	expression tag	UNP P74717
y	23	PRO	-	expression tag	UNP P74717
z	1	MET	-	initiating methionine	UNP P74717
z	2	GLY	-	expression tag	UNP P74717
z	3	SER	-	expression tag	UNP P74717
z	4	SER	-	expression tag	UNP P74717
z	5	HIS	-	expression tag	UNP P74717
z	6	HIS	-	expression tag	UNP P74717
z	7	HIS	-	expression tag	UNP P74717
z	8	HIS	-	expression tag	UNP P74717
z	9	HIS	-	expression tag	UNP P74717
z	10	HIS	-	expression tag	UNP P74717
z	11	SER	-	expression tag	UNP P74717
z	12	SER	-	expression tag	UNP P74717
z	13	SER	-	expression tag	UNP P74717
z	14	ALA	-	expression tag	UNP P74717
z	15	ALA	-	expression tag	UNP P74717
z	16	LEU	-	expression tag	UNP P74717
z	17	GLU	-	expression tag	UNP P74717
z	18	VAL	-	expression tag	UNP P74717
z	19	LEU	-	expression tag	UNP P74717
z	20	PHE	-	expression tag	UNP P74717
z	21	GLN	-	expression tag	UNP P74717
z	22	GLY	-	expression tag	UNP P74717
z	23	PRO	-	expression tag	UNP P74717

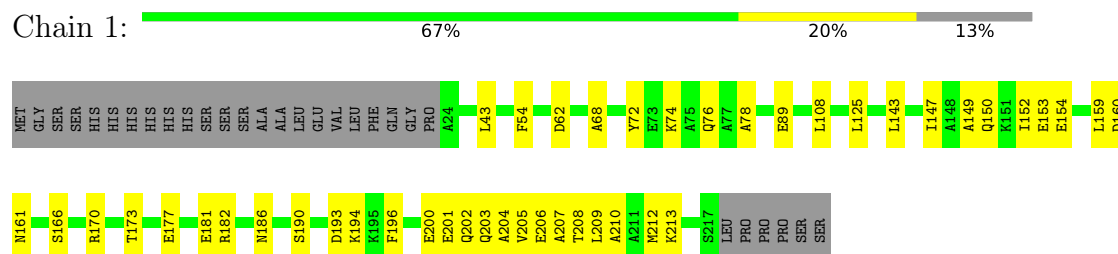
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

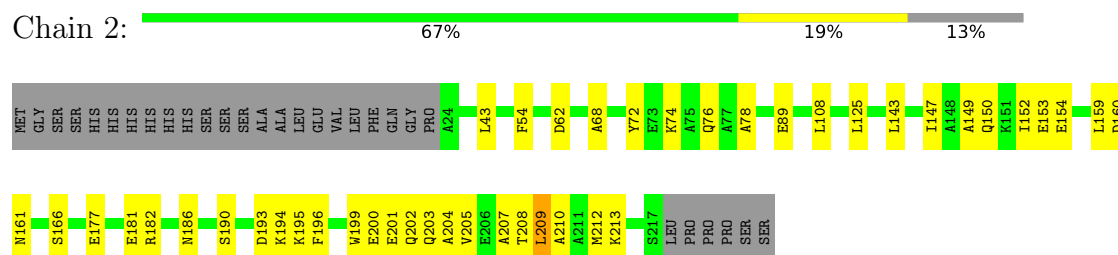
- Molecule 1: Chloroplast membrane-associated 30 kD protein



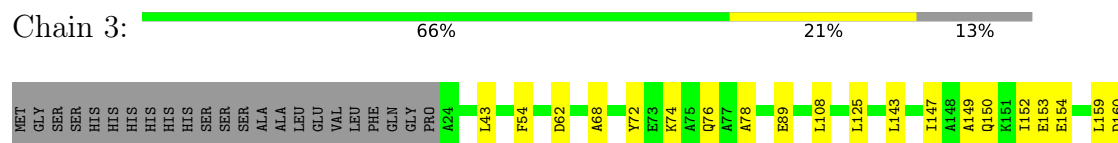
- Molecule 1: Chloroplast membrane-associated 30 kD protein



- Molecule 1: Chloroplast membrane-associated 30 kD protein

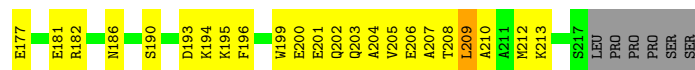


- Molecule 1: Chloroplast membrane-associated 30 kD protein

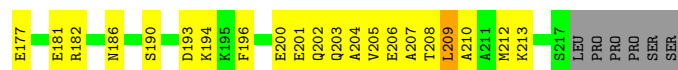




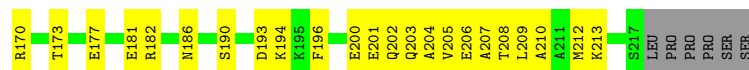
- Molecule 1: Chloroplast membrane-associated 30 kD protein



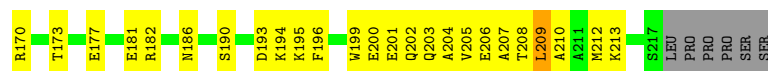
- Molecule 1: Chloroplast membrane-associated 30 kD protein



- Molecule 1: Chloroplast membrane-associated 30 kD protein

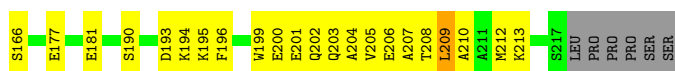


- Molecule 1: Chloroplast membrane-associated 30 kD protein



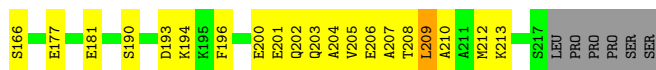
- Molecule 1: Chloroplast membrane-associated 30 kD protein





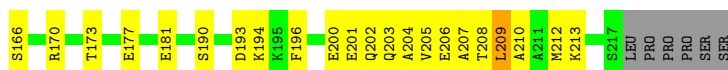
- Molecule 1: Chloroplast membrane-associated 30 kD protein

Chain B: 70% 17% 13%



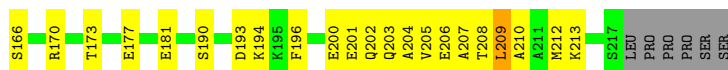
- Molecule 1: Chloroplast membrane-associated 30 kD protein

Chain C: 69% 18% 13%



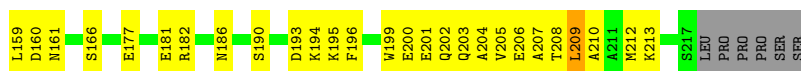
- Molecule 1: Chloroplast membrane-associated 30 kD protein

Chain D: 69% 18% 13%



- Molecule 1: Chloroplast membrane-associated 30 kD protein

Chain E: 66% 20% 13%



- Molecule 1: Chloroplast membrane-associated 30 kD protein

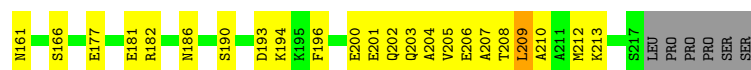
Chain F: 67% 19% 13%





- Molecule 1: Chloroplast membrane-associated 30 kD protein

Chain G: 68% 19% 13%



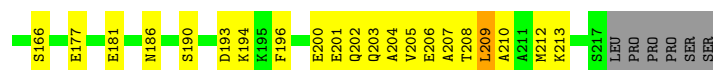
- Molecule 1: Chloroplast membrane-associated 30 kD protein

Chain H: 68% 19% 13%



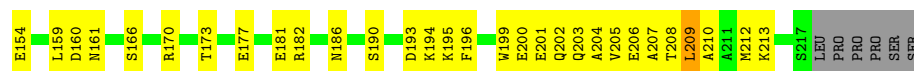
- Molecule 1: Chloroplast membrane-associated 30 kD protein

Chain I: 69% 18% 13%



- Molecule 1: Chloroplast membrane-associated 30 kD protein

Chain J: 65% 22% 13%



- Molecule 1: Chloroplast membrane-associated 30 kD protein

Chain K: 67% 20% 13%







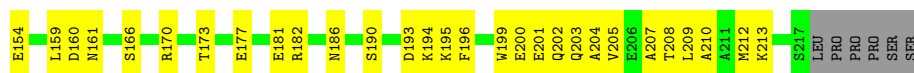
- Molecule 1: Chloroplast membrane-associated 30 kD protein

Chain Q: 66% 21% 13%



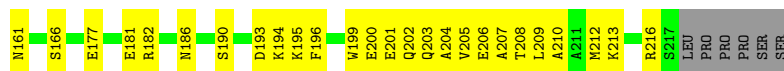
- Molecule 1: Chloroplast membrane-associated 30 kD protein

Chain R: 65% 22% 13%



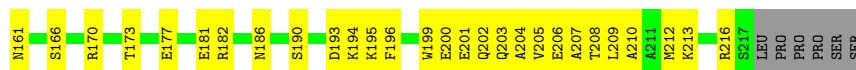
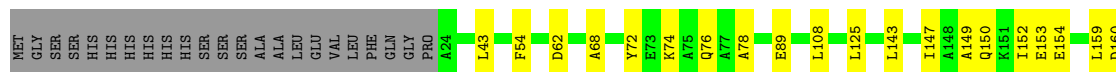
- Molecule 1: Chloroplast membrane-associated 30 kD protein

Chain S: 66% 21% 13%



- Molecule 1: Chloroplast membrane-associated 30 kD protein

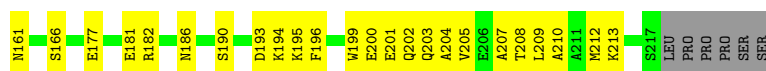
Chain T: 65% 22% 13%



- Molecule 1: Chloroplast membrane-associated 30 kD protein

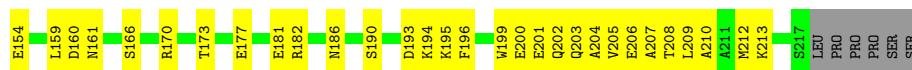
Chain U: 67% 20% 13%





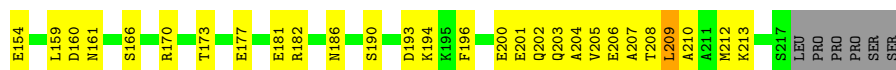
- Molecule 1: Chloroplast membrane-associated 30 kD protein

Chain V: 65% 22% 13%



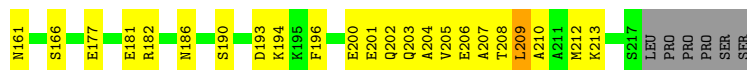
- Molecule 1: Chloroplast membrane-associated 30 kD protein

Chain W: 66% 21% 13%



- Molecule 1: Chloroplast membrane-associated 30 kD protein

Chain X: 68% 19% 13%



- Molecule 1: Chloroplast membrane-associated 30 kD protein

Chain Y: 67% 19% 13%



- Molecule 1: Chloroplast membrane-associated 30 kD protein

Chain Z: 67% 19% 13%

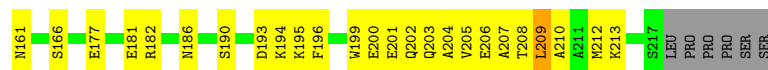






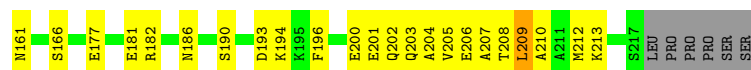
- Molecule 1: Chloroplast membrane-associated 30 kD protein

Chain a: 67% 20% 13%



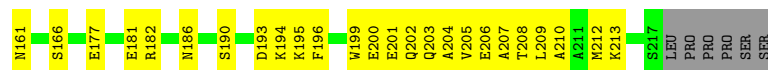
- Molecule 1: Chloroplast membrane-associated 30 kD protein

Chain b: 68% 19% 13%



- Molecule 1: Chloroplast membrane-associated 30 kD protein

Chain c: 67% 20% 13%



- Molecule 1: Chloroplast membrane-associated 30 kD protein

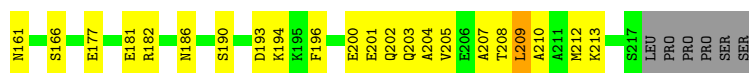
Chain d: 68% 19% 13%



- Molecule 1: Chloroplast membrane-associated 30 kD protein

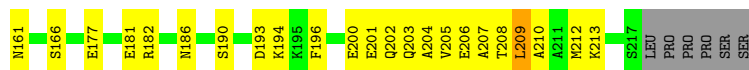
Chain e: 68% 18% 13%





- Molecule 1: Chloroplast membrane-associated 30 kD protein

Chain f: 68% 19% 13%



- Molecule 1: Chloroplast membrane-associated 30 kD protein

Chain g: 67% 20% 13%



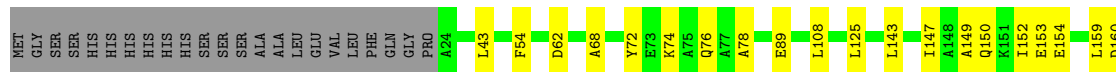
- Molecule 1: Chloroplast membrane-associated 30 kD protein

Chain h: 67% 20% 13%



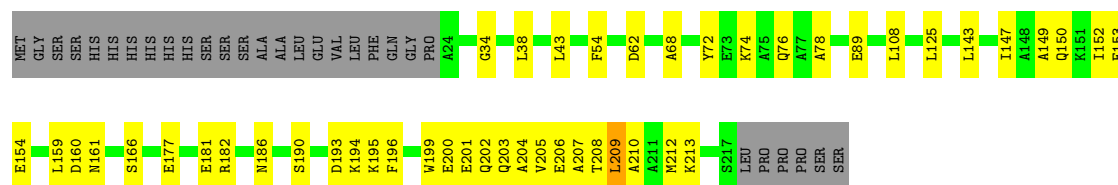
- Molecule 1: Chloroplast membrane-associated 30 kD protein

Chain i: 67% 20% 13%

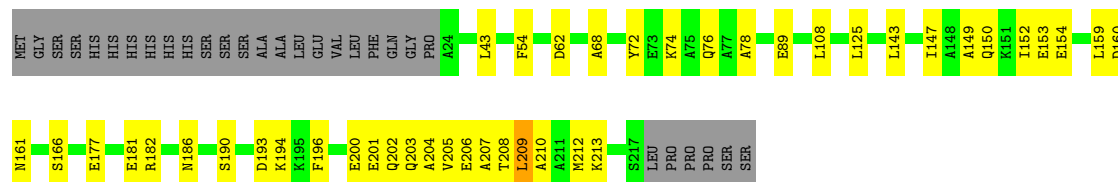


- Molecule 1: Chloroplast membrane-associated 30 kD protein

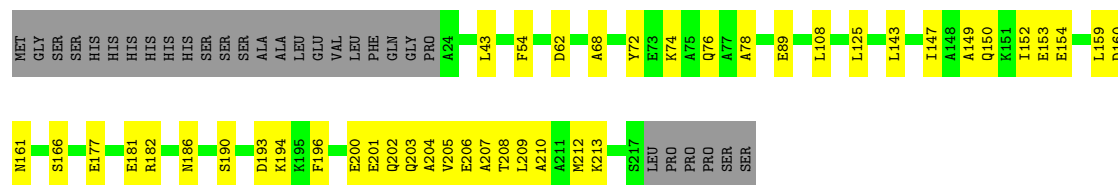
Chain j: 66% 21% 13%



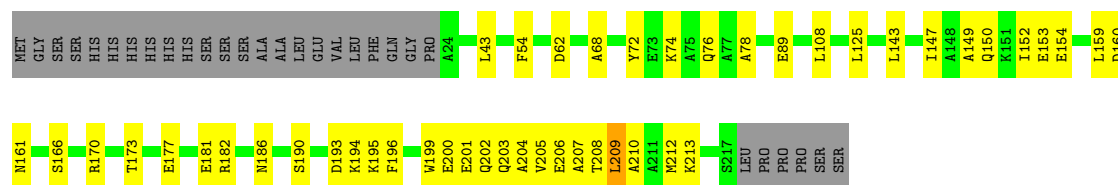
- Molecule 1: Chloroplast membrane-associated 30 kD protein



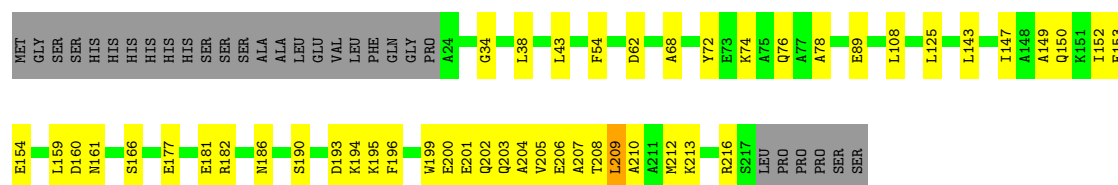
- Molecule 1: Chloroplast membrane-associated 30 kD protein



- Molecule 1: Chloroplast membrane-associated 30 kD protein

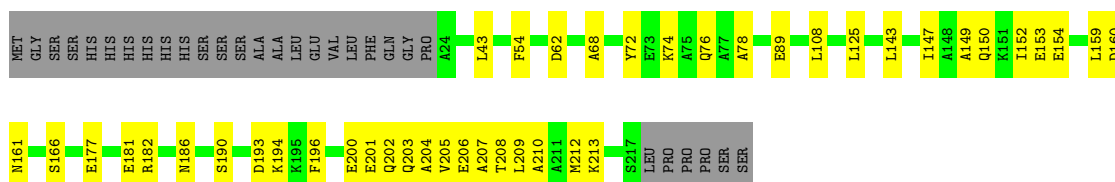


- Molecule 1: Chloroplast membrane-associated 30 kD protein



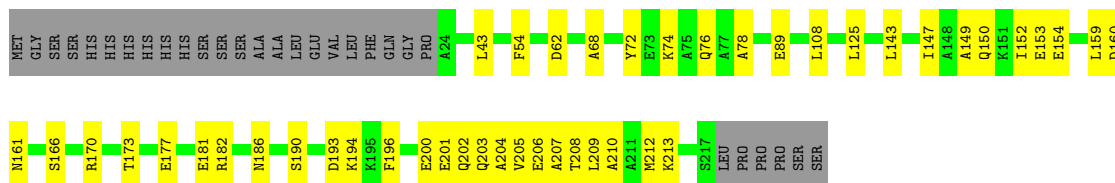
- Molecule 1: Chloroplast membrane-associated 30 kD protein





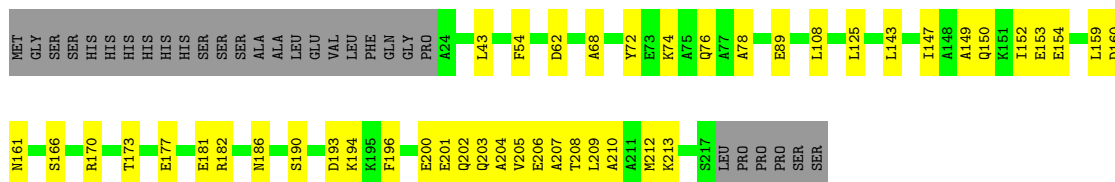
- Molecule 1: Chloroplast membrane-associated 30 kD protein

Chain p: 67% 20% 13%



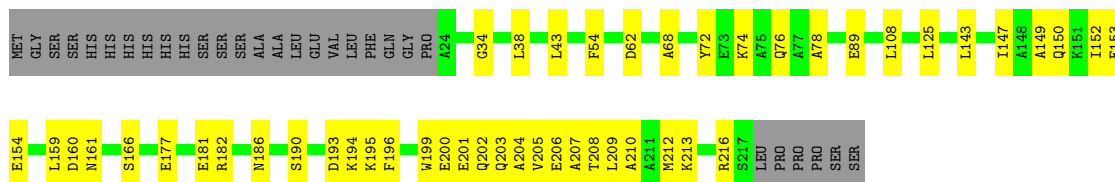
- Molecule 1: Chloroplast membrane-associated 30 kD protein

Chain q: 67% 20% 13%



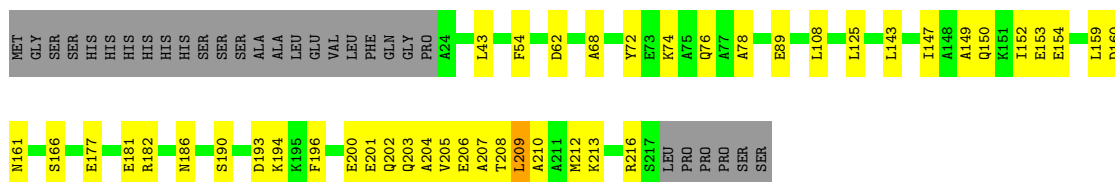
- Molecule 1: Chloroplast membrane-associated 30 kD protein

Chain r: 65% 22% 13%



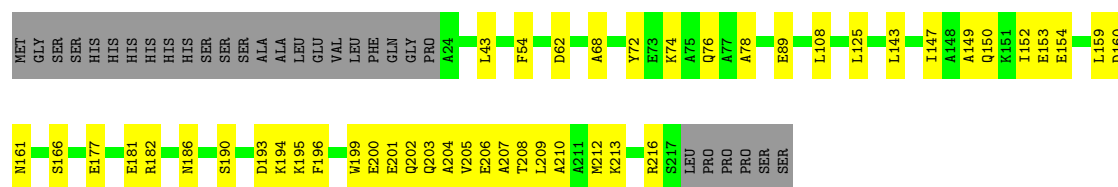
- Molecule 1: Chloroplast membrane-associated 30 kD protein

Chain s: 67% 19% 13%



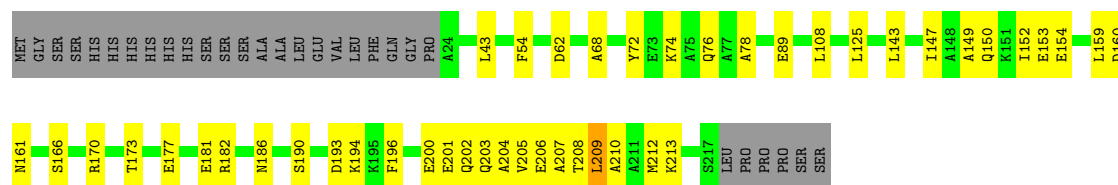
- Molecule 1: Chloroplast membrane-associated 30 kD protein

Chain t:  66% 21% 13%



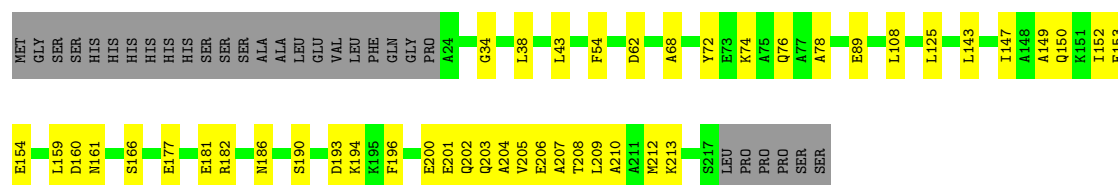
- Molecule 1: Chloroplast membrane-associated 30 kD protein

Chain u:  67% 20% 13%



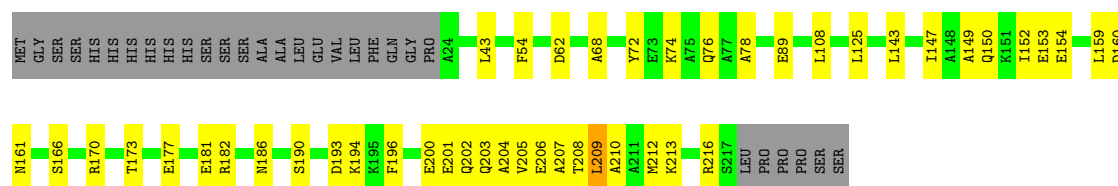
- Molecule 1: Chloroplast membrane-associated 30 kD protein

Chain v:  67% 20% 13%



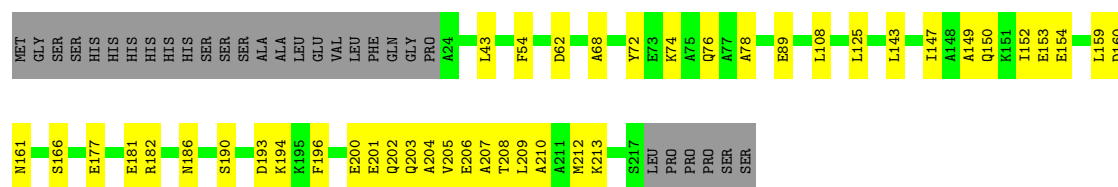
- Molecule 1: Chloroplast membrane-associated 30 kD protein

Chain w:  66% 20% 13%

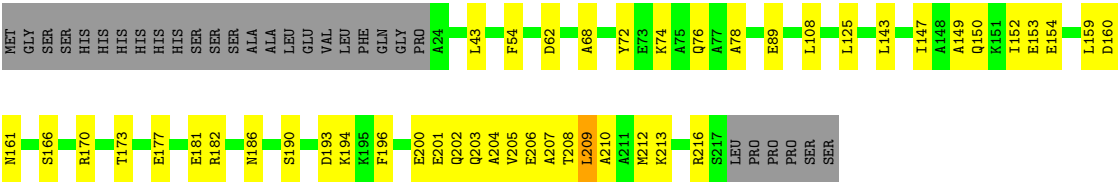
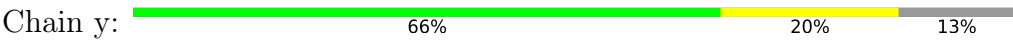


- Molecule 1: Chloroplast membrane-associated 30 kD protein

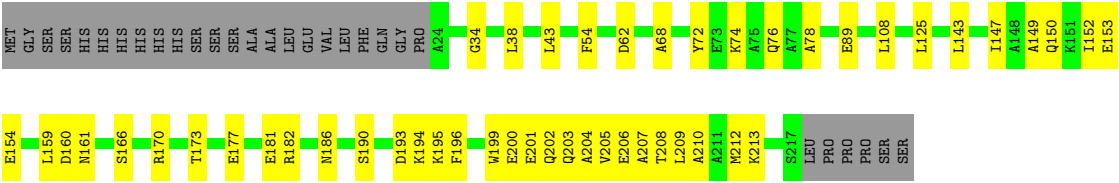
Chain x:  68% 19% 13%



- Molecule 1: Chloroplast membrane-associated 30 kD protein



● Molecule 1: Chloroplast membrane-associated 30 kD protein



## 4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-83.6°, rise=2.10 Å, axial sym=C1	Depositor
Number of segments used	1405435	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	44	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor

## 5 Model quality

### 5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	0	0.11	0/1575	0.26	0/2114
1	1	0.11	0/1575	0.26	0/2114
1	2	0.11	0/1575	0.26	0/2114
1	3	0.11	0/1575	0.26	0/2114
1	4	0.11	0/1575	0.26	0/2114
1	5	0.11	0/1575	0.26	0/2114
1	6	0.11	0/1575	0.26	0/2114
1	7	0.11	0/1575	0.26	0/2114
1	A	0.11	0/1575	0.26	0/2114
1	B	0.11	0/1575	0.26	0/2114
1	C	0.11	0/1575	0.26	0/2114
1	D	0.11	0/1575	0.26	0/2114
1	E	0.11	0/1575	0.25	0/2114
1	F	0.11	0/1575	0.26	0/2114
1	G	0.11	0/1575	0.26	0/2114
1	H	0.11	0/1575	0.26	0/2114
1	I	0.11	0/1575	0.26	0/2114
1	J	0.11	0/1575	0.26	0/2114
1	K	0.11	0/1575	0.26	0/2114
1	L	0.11	0/1575	0.26	0/2114
1	M	0.11	0/1575	0.26	0/2114
1	N	0.11	0/1575	0.26	0/2114
1	O	0.11	0/1575	0.26	0/2114
1	P	0.11	0/1575	0.26	0/2114
1	Q	0.11	0/1575	0.26	0/2114
1	R	0.11	0/1575	0.26	0/2114
1	S	0.11	0/1575	0.26	0/2114
1	T	0.11	0/1575	0.26	0/2114
1	U	0.11	0/1575	0.25	0/2114
1	V	0.11	0/1575	0.26	0/2114
1	W	0.11	0/1575	0.26	0/2114
1	X	0.11	0/1575	0.26	0/2114
1	Y	0.11	0/1575	0.26	0/2114
1	Z	0.11	0/1575	0.26	0/2114



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	a	0.11	0/1575	0.26	0/2114
1	b	0.11	0/1575	0.25	0/2114
1	c	0.11	0/1575	0.26	0/2114
1	d	0.11	0/1575	0.26	0/2114
1	e	0.11	0/1575	0.26	0/2114
1	f	0.11	0/1575	0.26	0/2114
1	g	0.11	0/1575	0.26	0/2114
1	h	0.11	0/1575	0.26	0/2114
1	i	0.11	0/1575	0.26	0/2114
1	j	0.11	0/1575	0.26	0/2114
1	k	0.11	0/1575	0.26	0/2114
1	l	0.11	0/1575	0.26	0/2114
1	m	0.11	0/1575	0.26	0/2114
1	n	0.11	0/1575	0.26	0/2114
1	o	0.11	0/1575	0.26	0/2114
1	p	0.11	0/1575	0.26	0/2114
1	q	0.11	0/1575	0.26	0/2114
1	r	0.11	0/1575	0.26	0/2114
1	s	0.11	0/1575	0.26	0/2114
1	t	0.11	0/1575	0.26	0/2114
1	u	0.11	0/1575	0.26	0/2114
1	v	0.11	0/1575	0.26	0/2114
1	w	0.11	0/1575	0.26	0/2114
1	x	0.11	0/1575	0.26	0/2114
1	y	0.11	0/1575	0.26	0/2114
1	z	0.11	0/1575	0.26	0/2114
All	All	0.11	0/94500	0.26	0/126840

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	1559	1590	1589	37	0
1	1	1559	1590	1589	38	0
1	2	1559	1590	1589	36	0
1	3	1559	1590	1589	37	0
1	4	1559	1590	1589	33	0
1	5	1559	1590	1589	34	0
1	6	1559	1590	1589	32	0
1	7	1559	1590	1589	33	0
1	A	1559	1590	1589	34	0
1	B	1559	1590	1589	34	0
1	C	1559	1590	1589	33	0
1	D	1559	1590	1589	33	0
1	E	1559	1590	1589	35	0
1	F	1559	1590	1589	37	0
1	G	1559	1590	1589	36	0
1	H	1559	1590	1589	35	0
1	I	1559	1590	1589	34	0
1	J	1559	1590	1589	40	0
1	K	1559	1590	1589	37	0
1	L	1559	1590	1589	36	0
1	M	1559	1590	1589	37	0
1	N	1559	1590	1589	39	0
1	O	1559	1590	1589	38	0
1	P	1559	1590	1589	36	0
1	Q	1559	1590	1589	39	0
1	R	1559	1590	1589	38	0
1	S	1559	1590	1589	38	0
1	T	1559	1590	1589	40	0
1	U	1559	1590	1589	37	0
1	V	1559	1590	1589	39	0
1	W	1559	1590	1589	38	0
1	X	1559	1590	1589	37	0
1	Y	1559	1590	1589	38	0
1	Z	1559	1590	1589	37	0
1	a	1559	1590	1589	37	0
1	b	1559	1590	1589	38	0
1	c	1559	1590	1589	36	0
1	d	1559	1590	1589	35	0
1	e	1559	1590	1589	34	0
1	f	1559	1590	1589	38	0
1	g	1559	1590	1589	37	0
1	h	1559	1590	1589	36	0
1	i	1559	1590	1589	36	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	j	1559	1590	1589	39	0
1	k	1559	1590	1589	35	0
1	l	1559	1590	1589	35	0
1	m	1559	1590	1589	37	0
1	n	1559	1590	1589	39	0
1	o	1559	1590	1589	37	0
1	p	1559	1590	1589	36	0
1	q	1559	1590	1589	38	0
1	r	1559	1590	1589	40	0
1	s	1559	1590	1589	38	0
1	t	1559	1590	1589	38	0
1	u	1559	1590	1589	38	0
1	v	1559	1590	1589	37	0
1	w	1559	1590	1589	37	0
1	x	1559	1590	1589	37	0
1	y	1559	1590	1589	39	0
1	z	1559	1590	1589	39	0
All	All	93540	95400	95340	1979	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (1979) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:GLN:O	1:B:207:ALA:N	2.00	0.95
1:2:203:GLN:O	1:2:207:ALA:N	2.00	0.95
1:F:203:GLN:O	1:F:207:ALA:N	2.00	0.95
1:Y:203:GLN:O	1:Y:207:ALA:N	2.00	0.95
1:y:203:GLN:O	1:y:207:ALA:N	2.00	0.95
1:5:203:GLN:O	1:5:207:ALA:N	2.00	0.95
1:b:203:GLN:O	1:b:207:ALA:N	2.00	0.95
1:f:203:GLN:O	1:f:207:ALA:N	2.00	0.95
1:1:203:GLN:O	1:1:207:ALA:N	2.00	0.95
1:C:203:GLN:O	1:C:207:ALA:N	2.00	0.95
1:E:203:GLN:O	1:E:207:ALA:N	2.00	0.95
1:c:203:GLN:O	1:c:207:ALA:N	2.00	0.95
1:z:203:GLN:O	1:z:207:ALA:N	2.00	0.95
1:U:203:GLN:O	1:U:207:ALA:N	2.00	0.95
1:e:203:GLN:O	1:e:207:ALA:N	2.00	0.95
1:X:203:GLN:O	1:X:207:ALA:N	2.00	0.95

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:203:GLN:O	1:Z:207:ALA:N	2.00	0.95
1:4:203:GLN:O	1:4:207:ALA:N	2.00	0.95
1:6:203:GLN:O	1:6:207:ALA:N	2.00	0.95
1:V:203:GLN:O	1:V:207:ALA:N	2.00	0.95
1:q:203:GLN:O	1:q:207:ALA:N	2.00	0.94
1:x:203:GLN:O	1:x:207:ALA:N	2.00	0.94
1:G:203:GLN:O	1:G:207:ALA:N	2.00	0.94
1:N:203:GLN:O	1:N:207:ALA:N	2.00	0.94
1:Q:203:GLN:O	1:Q:207:ALA:N	2.00	0.94
1:g:203:GLN:O	1:g:207:ALA:N	2.00	0.94
1:i:203:GLN:O	1:i:207:ALA:N	2.00	0.94
1:n:203:GLN:O	1:n:207:ALA:N	2.00	0.94
1:w:203:GLN:O	1:w:207:ALA:N	2.00	0.94
1:H:203:GLN:O	1:H:207:ALA:N	2.00	0.94
1:A:203:GLN:O	1:A:207:ALA:N	2.00	0.94
1:J:203:GLN:O	1:J:207:ALA:N	2.00	0.94
1:W:203:GLN:O	1:W:207:ALA:N	2.00	0.94
1:v:203:GLN:O	1:v:207:ALA:N	2.00	0.94
1:h:203:GLN:O	1:h:207:ALA:N	2.00	0.94
1:k:203:GLN:O	1:k:207:ALA:N	2.00	0.94
1:P:203:GLN:O	1:P:207:ALA:N	2.00	0.94
1:3:203:GLN:O	1:3:207:ALA:N	2.00	0.94
1:I:203:GLN:O	1:I:207:ALA:N	2.00	0.94
1:K:203:GLN:O	1:K:207:ALA:N	2.00	0.94
1:M:203:GLN:O	1:M:207:ALA:N	2.00	0.94
1:T:203:GLN:O	1:T:207:ALA:N	2.00	0.94
1:o:203:GLN:O	1:o:207:ALA:N	2.00	0.94
1:t:203:GLN:O	1:t:207:ALA:N	2.00	0.94
1:S:203:GLN:O	1:S:207:ALA:N	2.00	0.94
1:p:203:GLN:O	1:p:207:ALA:N	2.00	0.94
1:u:203:GLN:O	1:u:207:ALA:N	2.00	0.94
1:L:203:GLN:O	1:L:207:ALA:N	2.00	0.94
1:O:203:GLN:O	1:O:207:ALA:N	2.00	0.94
1:a:203:GLN:O	1:a:207:ALA:N	2.00	0.94
1:l:203:GLN:O	1:l:207:ALA:N	2.00	0.94
1:s:203:GLN:O	1:s:207:ALA:N	2.00	0.94
1:r:203:GLN:O	1:r:207:ALA:N	2.00	0.94
1:j:203:GLN:O	1:j:207:ALA:N	2.00	0.93
1:7:203:GLN:O	1:7:207:ALA:N	2.00	0.93
1:m:203:GLN:O	1:m:207:ALA:N	2.00	0.93
1:d:203:GLN:O	1:d:207:ALA:N	2.00	0.93

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:203:GLN:O	1:R:207:ALA:N	2.00	0.93
1:O:203:GLN:O	1:O:207:ALA:N	2.00	0.93
1:D:203:GLN:O	1:D:207:ALA:N	2.00	0.93
1:J:204:ALA:O	1:J:208:THR:OG1	1.96	0.84
1:N:204:ALA:O	1:N:208:THR:OG1	1.96	0.84
1:j:204:ALA:O	1:j:208:THR:OG1	1.96	0.84
1:n:204:ALA:O	1:n:208:THR:OG1	1.96	0.84
1:i:204:ALA:O	1:i:208:THR:OG1	1.96	0.84
1:F:204:ALA:O	1:F:208:THR:OG1	1.96	0.83
1:K:204:ALA:O	1:K:208:THR:OG1	1.96	0.83
1:m:204:ALA:O	1:m:208:THR:OG1	1.96	0.83
1:5:204:ALA:O	1:5:208:THR:OG1	1.96	0.83
1:I:204:ALA:O	1:I:208:THR:OG1	1.96	0.83
1:O:204:ALA:O	1:O:208:THR:OG1	1.96	0.83
1:R:204:ALA:O	1:R:208:THR:OG1	1.96	0.83
1:f:204:ALA:O	1:f:208:THR:OG1	1.96	0.83
1:o:204:ALA:O	1:o:208:THR:OG1	1.96	0.83
1:k:204:ALA:O	1:k:208:THR:OG1	1.96	0.83
1:r:204:ALA:O	1:r:208:THR:OG1	1.96	0.83
1:M:204:ALA:O	1:M:208:THR:OG1	1.96	0.83
1:e:204:ALA:O	1:e:208:THR:OG1	1.96	0.83
1:4:204:ALA:O	1:4:208:THR:OG1	1.96	0.83
1:E:204:ALA:O	1:E:208:THR:OG1	1.96	0.83
1:G:204:ALA:O	1:G:208:THR:OG1	1.96	0.83
1:q:204:ALA:O	1:q:208:THR:OG1	1.96	0.83
1:s:204:ALA:O	1:s:208:THR:OG1	1.96	0.83
1:B:204:ALA:O	1:B:208:THR:OG1	1.96	0.83
1:Q:204:ALA:O	1:Q:208:THR:OG1	1.96	0.83
1:S:204:ALA:O	1:S:208:THR:OG1	1.96	0.83
1:b:204:ALA:O	1:b:208:THR:OG1	1.96	0.83
1:g:204:ALA:O	1:g:208:THR:OG1	1.96	0.83
1:l:204:ALA:O	1:l:208:THR:OG1	1.96	0.83
1:C:204:ALA:O	1:C:208:THR:OG1	1.96	0.83
1:V:204:ALA:O	1:V:208:THR:OG1	1.96	0.83
1:v:204:ALA:O	1:v:208:THR:OG1	1.96	0.83
1:6:204:ALA:O	1:6:208:THR:OG1	1.96	0.83
1:u:204:ALA:O	1:u:208:THR:OG1	1.96	0.83
1:A:204:ALA:O	1:A:208:THR:OG1	1.96	0.82
1:U:204:ALA:O	1:U:208:THR:OG1	1.96	0.82
1:c:204:ALA:O	1:c:208:THR:OG1	1.96	0.82
1:Y:204:ALA:O	1:Y:208:THR:OG1	1.96	0.82

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:204:ALA:O	1:a:208:THR:OG1	1.96	0.82
1:0:204:ALA:O	1:0:208:THR:OG1	1.96	0.82
1:2:204:ALA:O	1:2:208:THR:OG1	1.96	0.82
1:y:204:ALA:O	1:y:208:THR:OG1	1.96	0.82
1:w:204:ALA:O	1:w:208:THR:OG1	1.96	0.82
1:W:204:ALA:O	1:W:208:THR:OG1	1.96	0.82
1:X:204:ALA:O	1:X:208:THR:OG1	1.96	0.82
1:x:204:ALA:O	1:x:208:THR:OG1	1.96	0.82
1:z:204:ALA:O	1:z:208:THR:OG1	1.96	0.82
1:Z:204:ALA:O	1:Z:208:THR:OG1	1.96	0.82
1:3:204:ALA:O	1:3:208:THR:OG1	1.96	0.81
1:t:204:ALA:O	1:t:208:THR:OG1	1.96	0.81
1:7:204:ALA:O	1:7:208:THR:OG1	1.96	0.81
1:D:204:ALA:O	1:D:208:THR:OG1	1.96	0.81
1:T:204:ALA:O	1:T:208:THR:OG1	1.96	0.81
1:d:204:ALA:O	1:d:208:THR:OG1	1.96	0.81
1:P:204:ALA:O	1:P:208:THR:OG1	1.96	0.81
1:h:204:ALA:O	1:h:208:THR:OG1	1.96	0.81
1:p:204:ALA:O	1:p:208:THR:OG1	1.96	0.81
1:H:204:ALA:O	1:H:208:THR:OG1	1.96	0.81
1:L:204:ALA:O	1:L:208:THR:OG1	1.96	0.81
1:l:204:ALA:O	1:l:208:THR:OG1	1.96	0.81
1:f:89:GLU:OE1	1:f:89:GLU:N	2.21	0.74
1:o:89:GLU:N	1:o:89:GLU:OE1	2.21	0.74
1:x:89:GLU:OE1	1:x:89:GLU:N	2.21	0.74
1:6:89:GLU:OE1	1:6:89:GLU:N	2.21	0.74
1:B:89:GLU:OE1	1:B:89:GLU:N	2.21	0.74
1:K:89:GLU:OE1	1:K:89:GLU:N	2.21	0.74
1:T:89:GLU:N	1:T:89:GLU:OE1	2.21	0.74
1:C:89:GLU:OE1	1:C:89:GLU:N	2.21	0.74
1:W:89:GLU:N	1:W:89:GLU:OE1	2.21	0.74
1:0:89:GLU:OE1	1:0:89:GLU:N	2.21	0.74
1:F:89:GLU:OE1	1:F:89:GLU:N	2.20	0.74
1:O:89:GLU:N	1:O:89:GLU:OE1	2.21	0.74
1:X:89:GLU:OE1	1:X:89:GLU:N	2.21	0.74
1:c:89:GLU:OE1	1:c:89:GLU:N	2.21	0.74
1:5:89:GLU:OE1	1:5:89:GLU:N	2.21	0.74
1:g:89:GLU:N	1:g:89:GLU:OE1	2.21	0.74
1:L:89:GLU:N	1:L:89:GLU:OE1	2.21	0.74
1:N:89:GLU:OE1	1:N:89:GLU:N	2.21	0.74
1:w:89:GLU:N	1:w:89:GLU:OE1	2.21	0.74

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:l:89:GLU:OE1	1:l:89:GLU:N	2.21	0.74
1:p:89:GLU:OE1	1:p:89:GLU:N	2.21	0.74
1:r:89:GLU:N	1:r:89:GLU:OE1	2.21	0.74
1:1:89:GLU:N	1:1:89:GLU:OE1	2.21	0.74
1:s:89:GLU:OE1	1:s:89:GLU:N	2.21	0.74
1:b:89:GLU:N	1:b:89:GLU:OE1	2.21	0.73
1:j:89:GLU:N	1:j:89:GLU:OE1	2.21	0.73
1:k:89:GLU:OE1	1:k:89:GLU:N	2.21	0.73
1:n:89:GLU:OE1	1:n:89:GLU:N	2.21	0.73
1:t:89:GLU:OE1	1:t:89:GLU:N	2.20	0.73
1:H:89:GLU:OE1	1:H:89:GLU:N	2.20	0.73
1:S:89:GLU:OE1	1:S:89:GLU:N	2.21	0.73
1:a:89:GLU:OE1	1:a:89:GLU:N	2.20	0.73
1:E:89:GLU:OE1	1:E:89:GLU:N	2.21	0.73
1:w:74:LYS:O	1:w:78:ALA:N	2.21	0.73
1:J:74:LYS:O	1:J:78:ALA:N	2.21	0.73
1:J:89:GLU:OE1	1:J:89:GLU:N	2.21	0.73
1:W:74:LYS:O	1:W:78:ALA:N	2.21	0.73
1:f:74:LYS:O	1:f:78:ALA:N	2.21	0.73
1:i:89:GLU:OE1	1:i:89:GLU:N	2.20	0.73
1:u:89:GLU:N	1:u:89:GLU:OE1	2.21	0.73
1:2:89:GLU:OE1	1:2:89:GLU:N	2.21	0.73
1:U:89:GLU:OE1	1:U:89:GLU:N	2.21	0.73
1:a:74:LYS:O	1:a:78:ALA:N	2.21	0.73
1:y:89:GLU:OE1	1:y:89:GLU:N	2.20	0.73
1:0:74:LYS:O	1:0:78:ALA:N	2.21	0.73
1:3:89:GLU:OE1	1:3:89:GLU:N	2.20	0.73
1:D:74:LYS:O	1:D:78:ALA:N	2.21	0.73
1:1:74:LYS:O	1:1:78:ALA:N	2.21	0.73
1:B:74:LYS:O	1:B:78:ALA:N	2.21	0.73
1:F:74:LYS:O	1:F:78:ALA:N	2.21	0.73
1:N:74:LYS:O	1:N:78:ALA:N	2.21	0.73
1:O:74:LYS:O	1:O:78:ALA:N	2.21	0.73
1:Q:74:LYS:O	1:Q:78:ALA:N	2.21	0.73
1:Q:89:GLU:OE1	1:Q:89:GLU:N	2.21	0.73
1:R:89:GLU:N	1:R:89:GLU:OE1	2.21	0.73
1:S:74:LYS:O	1:S:78:ALA:N	2.21	0.73
1:h:74:LYS:O	1:h:78:ALA:N	2.21	0.73
1:o:74:LYS:O	1:o:78:ALA:N	2.21	0.73
1:y:74:LYS:O	1:y:78:ALA:N	2.21	0.73
1:7:74:LYS:O	1:7:78:ALA:N	2.21	0.73

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:GLU:OE2	1:E:186:ASN:ND2	2.21	0.73
1:G:89:GLU:N	1:G:89:GLU:OE1	2.21	0.73
1:L:74:LYS:O	1:L:78:ALA:N	2.21	0.73
1:Z:89:GLU:N	1:Z:89:GLU:OE1	2.21	0.73
1:e:89:GLU:OE1	1:e:89:GLU:N	2.21	0.73
1:n:74:LYS:O	1:n:78:ALA:N	2.21	0.73
1:r:74:LYS:O	1:r:78:ALA:N	2.21	0.73
1:u:74:LYS:O	1:u:78:ALA:N	2.22	0.73
1:4:89:GLU:N	1:4:89:GLU:OE1	2.21	0.73
1:I:89:GLU:OE1	1:I:89:GLU:N	2.20	0.73
1:P:89:GLU:OE1	1:P:89:GLU:N	2.21	0.73
1:p:74:LYS:O	1:p:78:ALA:N	2.21	0.73
1:q:74:LYS:O	1:q:78:ALA:N	2.21	0.73
1:M:74:LYS:O	1:M:78:ALA:N	2.21	0.73
1:U:74:LYS:O	1:U:78:ALA:N	2.21	0.73
1:Y:74:LYS:O	1:Y:78:ALA:N	2.21	0.73
1:d:89:GLU:OE1	1:d:89:GLU:N	2.20	0.73
1:j:74:LYS:O	1:j:78:ALA:N	2.21	0.73
1:s:74:LYS:O	1:s:78:ALA:N	2.21	0.73
1:3:74:LYS:O	1:3:78:ALA:N	2.21	0.72
1:5:74:LYS:O	1:5:78:ALA:N	2.21	0.72
1:A:89:GLU:OE1	1:A:89:GLU:N	2.21	0.72
1:H:74:LYS:O	1:H:78:ALA:N	2.21	0.72
1:X:74:LYS:O	1:X:78:ALA:N	2.21	0.72
1:Y:89:GLU:OE1	1:Y:89:GLU:N	2.21	0.72
1:d:74:LYS:O	1:d:78:ALA:N	2.21	0.72
1:e:74:LYS:O	1:e:78:ALA:N	2.21	0.72
1:A:74:LYS:O	1:A:78:ALA:N	2.21	0.72
1:K:74:LYS:O	1:K:78:ALA:N	2.21	0.72
1:k:74:LYS:O	1:k:78:ALA:N	2.22	0.72
1:4:74:LYS:O	1:4:78:ALA:N	2.22	0.72
1:6:74:LYS:O	1:6:78:ALA:N	2.21	0.72
1:7:89:GLU:N	1:7:89:GLU:OE1	2.21	0.72
1:c:74:LYS:O	1:c:78:ALA:N	2.21	0.72
1:m:74:LYS:O	1:m:78:ALA:N	2.21	0.72
1:m:89:GLU:OE1	1:m:89:GLU:N	2.21	0.72
1:v:89:GLU:OE1	1:v:89:GLU:N	2.21	0.72
1:z:74:LYS:O	1:z:78:ALA:N	2.21	0.72
1:z:89:GLU:N	1:z:89:GLU:OE1	2.21	0.72
1:C:74:LYS:O	1:C:78:ALA:N	2.21	0.72
1:E:74:LYS:O	1:E:78:ALA:N	2.21	0.72

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:h:89:GLU:OE1	1:h:89:GLU:N	2.21	0.72
1:x:74:LYS:O	1:x:78:ALA:N	2.21	0.72
1:2:74:LYS:O	1:2:78:ALA:N	2.21	0.72
1:V:89:GLU:OE1	1:V:89:GLU:N	2.20	0.72
1:G:74:LYS:O	1:G:78:ALA:N	2.21	0.72
1:P:74:LYS:O	1:P:78:ALA:N	2.21	0.72
1:g:74:LYS:O	1:g:78:ALA:N	2.21	0.72
1:q:89:GLU:OE1	1:q:89:GLU:N	2.21	0.72
1:V:74:LYS:O	1:V:78:ALA:N	2.21	0.72
1:Z:74:LYS:O	1:Z:78:ALA:N	2.21	0.72
1:T:74:LYS:O	1:T:78:ALA:N	2.21	0.72
1:i:74:LYS:O	1:i:78:ALA:N	2.21	0.72
1:l:74:LYS:O	1:l:78:ALA:N	2.21	0.72
1:D:89:GLU:N	1:D:89:GLU:OE1	2.20	0.72
1:M:89:GLU:OE1	1:M:89:GLU:N	2.21	0.72
1:b:74:LYS:O	1:b:78:ALA:N	2.21	0.72
1:t:74:LYS:O	1:t:78:ALA:N	2.21	0.72
1:R:74:LYS:O	1:R:78:ALA:N	2.21	0.71
1:v:74:LYS:O	1:v:78:ALA:N	2.21	0.71
1:I:74:LYS:O	1:I:78:ALA:N	2.21	0.71
1:6:212:MET:HA	1:6:212:MET:HE3	1.75	0.69
1:p:212:MET:HA	1:p:212:MET:HE3	1.75	0.69
1:g:212:MET:HA	1:g:212:MET:HE3	1.75	0.68
1:y:212:MET:HA	1:y:212:MET:HE3	1.75	0.68
1:L:212:MET:HA	1:L:212:MET:HE3	1.75	0.68
1:P:212:MET:HE3	1:P:212:MET:HA	1.75	0.68
1:X:212:MET:HE3	1:X:212:MET:HA	1.75	0.68
1:G:212:MET:HA	1:G:212:MET:HE3	1.75	0.68
1:U:212:MET:HA	1:U:212:MET:HE3	1.75	0.68
1:C:212:MET:HA	1:C:212:MET:HE3	1.75	0.68
1:x:212:MET:HA	1:x:212:MET:HE3	1.75	0.68
1:D:212:MET:HA	1:D:212:MET:HE3	1.75	0.68
1:Y:212:MET:HA	1:Y:212:MET:HE3	1.75	0.68
1:7:212:MET:HA	1:7:212:MET:HE3	1.75	0.68
1:d:212:MET:HA	1:d:212:MET:HE3	1.75	0.68
1:o:212:MET:HA	1:o:212:MET:HE3	1.75	0.68
1:O:212:MET:HA	1:O:212:MET:HE3	1.75	0.68
1:l:212:MET:HA	1:l:212:MET:HE3	1.75	0.68
1:1:212:MET:HA	1:1:212:MET:HE3	1.75	0.68
1:c:212:MET:HE3	1:c:212:MET:HA	1.75	0.68
1:h:212:MET:HA	1:h:212:MET:HE3	1.75	0.68

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:u:212:MET:HA	1:u:212:MET:HE3	1.75	0.67
1:M:212:MET:HA	1:M:212:MET:HE3	1.75	0.67
1:0:153:GLU:OE2	1:4:186:ASN:ND2	2.28	0.67
1:3:186:ASN:ND2	1:z:153:GLU:OE2	2.28	0.67
1:e:153:GLU:OE2	1:i:186:ASN:ND2	2.28	0.67
1:f:212:MET:HA	1:f:212:MET:HE3	1.75	0.67
1:h:153:GLU:OE2	1:l:186:ASN:ND2	2.28	0.67
1:0:186:ASN:ND2	1:w:153:GLU:OE2	2.28	0.67
1:2:186:ASN:ND2	1:y:153:GLU:OE2	2.28	0.67
1:J:153:GLU:OE2	1:N:186:ASN:ND2	2.28	0.67
1:L:153:GLU:OE2	1:P:186:ASN:ND2	2.28	0.67
1:N:153:GLU:OE2	1:R:186:ASN:ND2	2.28	0.67
1:f:153:GLU:OE2	1:j:186:ASN:ND2	2.28	0.67
1:F:212:MET:HA	1:F:212:MET:HE3	1.75	0.67
1:I:153:GLU:OE2	1:M:186:ASN:ND2	2.28	0.67
1:M:153:GLU:OE2	1:Q:186:ASN:ND2	2.28	0.67
1:d:153:GLU:OE2	1:h:186:ASN:ND2	2.28	0.67
1:k:212:MET:HE3	1:k:212:MET:HA	1.75	0.67
1:q:212:MET:HA	1:q:212:MET:HE3	1.75	0.67
1:v:153:GLU:OE2	1:z:186:ASN:ND2	2.28	0.67
1:H:153:GLU:OE2	1:L:186:ASN:ND2	2.28	0.67
1:O:153:GLU:OE2	1:S:186:ASN:ND2	2.28	0.67
1:T:212:MET:HA	1:T:212:MET:HE3	1.75	0.67
1:e:212:MET:HA	1:e:212:MET:HE3	1.75	0.67
1:j:153:GLU:OE2	1:n:186:ASN:ND2	2.28	0.67
1:r:212:MET:HA	1:r:212:MET:HE3	1.75	0.67
1:s:212:MET:HE3	1:s:212:MET:HA	1.75	0.67
1:t:212:MET:HA	1:t:212:MET:HE3	1.75	0.67
1:u:153:GLU:OE2	1:y:186:ASN:ND2	2.28	0.67
1:4:212:MET:HA	1:4:212:MET:HE3	1.75	0.67
1:Q:153:GLU:OE2	1:U:186:ASN:ND2	2.28	0.67
1:S:153:GLU:OE2	1:W:186:ASN:ND2	2.28	0.67
1:V:212:MET:HA	1:V:212:MET:HE3	1.75	0.67
1:a:153:GLU:OE2	1:e:186:ASN:ND2	2.28	0.67
1:c:153:GLU:OE2	1:g:186:ASN:ND2	2.28	0.67
1:i:153:GLU:OE2	1:m:186:ASN:ND2	2.28	0.67
1:m:212:MET:HA	1:m:212:MET:HE3	1.75	0.67
1:3:153:GLU:OE2	1:7:186:ASN:ND2	2.28	0.67
1:Y:153:GLU:OE2	1:c:186:ASN:ND2	2.28	0.67
1:t:153:GLU:OE2	1:x:186:ASN:ND2	2.28	0.67
1:5:212:MET:HE3	1:5:212:MET:HA	1.75	0.67

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:MET:HA	1:A:212:MET:HE3	1.75	0.67
1:B:153:GLU:OE2	1:F:186:ASN:ND2	2.28	0.67
1:E:212:MET:HA	1:E:212:MET:HE3	1.75	0.67
1:H:212:MET:HE3	1:H:212:MET:HA	1.75	0.67
1:R:212:MET:HA	1:R:212:MET:HE3	1.75	0.67
1:o:153:GLU:OE2	1:s:186:ASN:ND2	2.28	0.67
1:r:153:GLU:OE2	1:v:186:ASN:ND2	2.28	0.67
1:1:153:GLU:OE2	1:5:186:ASN:ND2	2.28	0.67
1:2:212:MET:HA	1:2:212:MET:HE3	1.75	0.67
1:3:212:MET:HA	1:3:212:MET:HE3	1.75	0.67
1:C:153:GLU:OE2	1:G:186:ASN:ND2	2.28	0.67
1:N:212:MET:HA	1:N:212:MET:HE3	1.75	0.67
1:R:153:GLU:OE2	1:V:186:ASN:ND2	2.28	0.67
1:X:153:GLU:OE2	1:b:186:ASN:ND2	2.28	0.67
1:Z:153:GLU:OE2	1:d:186:ASN:ND2	2.28	0.67
1:n:212:MET:HA	1:n:212:MET:HE3	1.75	0.67
1:0:212:MET:HA	1:0:212:MET:HE3	1.75	0.66
1:2:153:GLU:OE2	1:6:186:ASN:ND2	2.28	0.66
1:G:153:GLU:OE2	1:K:186:ASN:ND2	2.28	0.66
1:J:212:MET:HA	1:J:212:MET:HE3	1.75	0.66
1:K:212:MET:HA	1:K:212:MET:HE3	1.75	0.66
1:T:153:GLU:OE2	1:X:186:ASN:ND2	2.28	0.66
1:W:212:MET:HA	1:W:212:MET:HE3	1.75	0.66
1:k:153:GLU:OE2	1:o:186:ASN:ND2	2.28	0.66
1:p:153:GLU:OE2	1:t:186:ASN:ND2	2.28	0.66
1:Q:212:MET:HA	1:Q:212:MET:HE3	1.75	0.66
1:a:212:MET:HA	1:a:212:MET:HE3	1.75	0.66
1:l:153:GLU:OE2	1:p:186:ASN:ND2	2.28	0.66
1:z:212:MET:HA	1:z:212:MET:HE3	1.75	0.66
1:1:186:ASN:ND2	1:x:153:GLU:OE2	2.28	0.66
1:I:212:MET:HA	1:I:212:MET:HE3	1.75	0.66
1:b:212:MET:HA	1:b:212:MET:HE3	1.76	0.66
1:j:212:MET:HA	1:j:212:MET:HE3	1.75	0.66
1:m:153:GLU:OE2	1:q:186:ASN:ND2	2.28	0.66
1:w:212:MET:HA	1:w:212:MET:HE3	1.75	0.66
1:F:153:GLU:OE2	1:J:186:ASN:ND2	2.28	0.66
1:i:212:MET:HA	1:i:212:MET:HE3	1.75	0.66
1:v:212:MET:HE3	1:v:212:MET:HA	1.75	0.66
1:B:212:MET:HA	1:B:212:MET:HE3	1.75	0.66
1:U:153:GLU:OE2	1:Y:186:ASN:ND2	2.28	0.66
1:q:153:GLU:OE2	1:u:186:ASN:ND2	2.28	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:212:MET:HA	1:Z:212:MET:HE3	1.75	0.66
1:D:153:GLU:OE2	1:H:186:ASN:ND2	2.28	0.66
1:P:153:GLU:OE2	1:T:186:ASN:ND2	2.28	0.66
1:V:153:GLU:OE2	1:Z:186:ASN:ND2	2.28	0.66
1:n:153:GLU:OE2	1:r:186:ASN:ND2	2.28	0.66
1:W:153:GLU:OE2	1:a:186:ASN:ND2	2.28	0.66
1:b:153:GLU:OE2	1:f:186:ASN:ND2	2.28	0.66
1:s:153:GLU:OE2	1:w:186:ASN:ND2	2.28	0.66
1:S:212:MET:HA	1:S:212:MET:HE3	1.75	0.66
1:g:153:GLU:OE2	1:k:186:ASN:ND2	2.28	0.66
1:K:153:GLU:OE2	1:O:186:ASN:ND2	2.28	0.66
1:E:153:GLU:OE2	1:I:186:ASN:ND2	2.29	0.65
1:A:150:GLN:NE2	1:A:154:GLU:OE2	2.30	0.65
1:J:150:GLN:NE2	1:J:154:GLU:OE2	2.30	0.65
1:M:190:SER:N	1:M:193:ASP:OD2	2.30	0.65
1:Y:150:GLN:NE2	1:Y:154:GLU:OE2	2.30	0.65
1:n:150:GLN:NE2	1:n:154:GLU:OE2	2.30	0.65
1:p:150:GLN:NE2	1:p:154:GLU:OE2	2.30	0.65
1:4:150:GLN:NE2	1:4:154:GLU:OE2	2.30	0.65
1:H:150:GLN:NE2	1:H:154:GLU:OE2	2.30	0.65
1:H:190:SER:N	1:H:193:ASP:OD2	2.30	0.65
1:V:190:SER:N	1:V:193:ASP:OD2	2.30	0.65
1:W:150:GLN:NE2	1:W:154:GLU:OE2	2.30	0.65
1:c:150:GLN:NE2	1:c:154:GLU:OE2	2.30	0.65
1:e:150:GLN:NE2	1:e:154:GLU:OE2	2.30	0.65
1:l:150:GLN:NE2	1:l:154:GLU:OE2	2.30	0.65
1:q:190:SER:N	1:q:193:ASP:OD2	2.30	0.65
1:6:150:GLN:NE2	1:6:154:GLU:OE2	2.30	0.65
1:C:150:GLN:NE2	1:C:154:GLU:OE2	2.30	0.65
1:Q:190:SER:N	1:Q:193:ASP:OD2	2.30	0.65
1:U:150:GLN:NE2	1:U:154:GLU:OE2	2.30	0.65
1:d:150:GLN:NE2	1:d:154:GLU:OE2	2.30	0.65
1:h:190:SER:N	1:h:193:ASP:OD2	2.30	0.65
1:m:150:GLN:NE2	1:m:154:GLU:OE2	2.30	0.65
1:u:150:GLN:NE2	1:u:154:GLU:OE2	2.30	0.65
1:v:150:GLN:NE2	1:v:154:GLU:OE2	2.30	0.65
1:v:190:SER:N	1:v:193:ASP:OD2	2.30	0.65
1:w:150:GLN:NE2	1:w:154:GLU:OE2	2.30	0.65
1:z:190:SER:N	1:z:193:ASP:OD2	2.30	0.65
1:4:190:SER:N	1:4:193:ASP:OD2	2.30	0.64
1:D:190:SER:N	1:D:193:ASP:OD2	2.30	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:150:GLN:NE2	1:L:154:GLU:OE2	2.30	0.64
1:O:190:SER:N	1:O:193:ASP:OD2	2.30	0.64
1:R:150:GLN:NE2	1:R:154:GLU:OE2	2.30	0.64
1:R:190:SER:N	1:R:193:ASP:OD2	2.30	0.64
1:S:150:GLN:NE2	1:S:154:GLU:OE2	2.30	0.64
1:T:150:GLN:NE2	1:T:154:GLU:OE2	2.30	0.64
1:a:150:GLN:NE2	1:a:154:GLU:OE2	2.30	0.64
1:l:190:SER:N	1:l:193:ASP:OD2	2.30	0.64
1:s:150:GLN:NE2	1:s:154:GLU:OE2	2.30	0.64
1:s:190:SER:N	1:s:193:ASP:OD2	2.30	0.64
1:2:150:GLN:NE2	1:2:154:GLU:OE2	2.30	0.64
1:5:150:GLN:NE2	1:5:154:GLU:OE2	2.30	0.64
1:7:150:GLN:NE2	1:7:154:GLU:OE2	2.30	0.64
1:B:150:GLN:NE2	1:B:154:GLU:OE2	2.30	0.64
1:I:150:GLN:NE2	1:I:154:GLU:OE2	2.30	0.64
1:K:190:SER:N	1:K:193:ASP:OD2	2.30	0.64
1:O:150:GLN:NE2	1:O:154:GLU:OE2	2.30	0.64
1:T:190:SER:N	1:T:193:ASP:OD2	2.30	0.64
1:V:150:GLN:NE2	1:V:154:GLU:OE2	2.30	0.64
1:a:190:SER:N	1:a:193:ASP:OD2	2.30	0.64
1:i:150:GLN:NE2	1:i:154:GLU:OE2	2.30	0.64
1:u:190:SER:N	1:u:193:ASP:OD2	2.30	0.64
1:x:190:SER:N	1:x:193:ASP:OD2	2.30	0.64
1:y:150:GLN:NE2	1:y:154:GLU:OE2	2.30	0.64
1:A:190:SER:N	1:A:193:ASP:OD2	2.30	0.64
1:E:150:GLN:NE2	1:E:154:GLU:OE2	2.30	0.64
1:F:150:GLN:NE2	1:F:154:GLU:OE2	2.30	0.64
1:K:150:GLN:NE2	1:K:154:GLU:OE2	2.30	0.64
1:M:150:GLN:NE2	1:M:154:GLU:OE2	2.30	0.64
1:S:190:SER:N	1:S:193:ASP:OD2	2.30	0.64
1:e:190:SER:N	1:e:193:ASP:OD2	2.30	0.64
1:f:150:GLN:NE2	1:f:154:GLU:OE2	2.30	0.64
1:k:150:GLN:NE2	1:k:154:GLU:OE2	2.30	0.64
1:o:190:SER:N	1:o:193:ASP:OD2	2.30	0.64
1:t:190:SER:N	1:t:193:ASP:OD2	2.30	0.64
1:x:150:GLN:NE2	1:x:154:GLU:OE2	2.30	0.64
1:z:150:GLN:NE2	1:z:154:GLU:OE2	2.30	0.64
1:1:150:GLN:NE2	1:1:154:GLU:OE2	2.30	0.64
1:1:190:SER:N	1:1:193:ASP:OD2	2.30	0.64
1:3:150:GLN:NE2	1:3:154:GLU:OE2	2.30	0.64
1:Q:150:GLN:NE2	1:Q:154:GLU:OE2	2.30	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:190:SER:N	1:X:193:ASP:OD2	2.30	0.64
1:b:150:GLN:NE2	1:b:154:GLU:OE2	2.30	0.64
1:m:190:SER:N	1:m:193:ASP:OD2	2.30	0.64
1:r:150:GLN:NE2	1:r:154:GLU:OE2	2.30	0.64
1:t:150:GLN:NE2	1:t:154:GLU:OE2	2.30	0.64
1:w:190:SER:N	1:w:193:ASP:OD2	2.30	0.64
1:P:190:SER:N	1:P:193:ASP:OD2	2.30	0.64
1:g:150:GLN:NE2	1:g:154:GLU:OE2	2.30	0.64
1:o:150:GLN:NE2	1:o:154:GLU:OE2	2.30	0.64
1:0:190:SER:N	1:0:193:ASP:OD2	2.30	0.64
1:D:150:GLN:NE2	1:D:154:GLU:OE2	2.30	0.64
1:I:190:SER:N	1:I:193:ASP:OD2	2.30	0.64
1:L:190:SER:N	1:L:193:ASP:OD2	2.30	0.64
1:N:150:GLN:NE2	1:N:154:GLU:OE2	2.30	0.64
1:P:150:GLN:NE2	1:P:154:GLU:OE2	2.30	0.64
1:Z:190:SER:N	1:Z:193:ASP:OD2	2.30	0.64
1:c:190:SER:N	1:c:193:ASP:OD2	2.30	0.64
1:j:150:GLN:NE2	1:j:154:GLU:OE2	2.30	0.64
1:0:150:GLN:NE2	1:0:154:GLU:OE2	2.30	0.64
1:7:190:SER:N	1:7:193:ASP:OD2	2.30	0.64
1:C:190:SER:N	1:C:193:ASP:OD2	2.30	0.64
1:J:190:SER:N	1:J:193:ASP:OD2	2.30	0.64
1:M:177:GLU:O	1:M:181:GLU:N	2.31	0.64
1:h:150:GLN:NE2	1:h:154:GLU:OE2	2.30	0.64
1:k:190:SER:N	1:k:193:ASP:OD2	2.30	0.64
1:6:190:SER:N	1:6:193:ASP:OD2	2.30	0.64
1:7:177:GLU:O	1:7:181:GLU:N	2.31	0.64
1:D:177:GLU:O	1:D:181:GLU:N	2.31	0.64
1:F:190:SER:N	1:F:193:ASP:OD2	2.30	0.64
1:G:190:SER:N	1:G:193:ASP:OD2	2.30	0.64
1:W:190:SER:N	1:W:193:ASP:OD2	2.30	0.64
1:Y:190:SER:N	1:Y:193:ASP:OD2	2.30	0.64
1:Z:150:GLN:NE2	1:Z:154:GLU:OE2	2.30	0.64
1:j:190:SER:N	1:j:193:ASP:OD2	2.30	0.64
1:q:177:GLU:O	1:q:181:GLU:N	2.31	0.64
1:2:190:SER:N	1:2:193:ASP:OD2	2.30	0.64
1:3:190:SER:N	1:3:193:ASP:OD2	2.30	0.64
1:V:177:GLU:O	1:V:181:GLU:N	2.31	0.64
1:d:190:SER:N	1:d:193:ASP:OD2	2.30	0.64
1:g:190:SER:N	1:g:193:ASP:OD2	2.30	0.64
1:n:190:SER:N	1:n:193:ASP:OD2	2.30	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:p:190:SER:N	1:p:193:ASP:OD2	2.30	0.64
1:q:150:GLN:NE2	1:q:154:GLU:OE2	2.30	0.64
1:y:177:GLU:O	1:y:181:GLU:N	2.31	0.64
1:z:177:GLU:O	1:z:181:GLU:N	2.31	0.64
1:5:190:SER:N	1:5:193:ASP:OD2	2.30	0.64
1:G:150:GLN:NE2	1:G:154:GLU:OE2	2.30	0.64
1:N:190:SER:N	1:N:193:ASP:OD2	2.30	0.64
1:U:177:GLU:O	1:U:181:GLU:N	2.31	0.64
1:b:190:SER:N	1:b:193:ASP:OD2	2.30	0.64
1:d:177:GLU:O	1:d:181:GLU:N	2.31	0.64
1:f:177:GLU:O	1:f:181:GLU:N	2.31	0.64
1:r:190:SER:N	1:r:193:ASP:OD2	2.30	0.64
1:E:190:SER:N	1:E:193:ASP:OD2	2.30	0.63
1:h:177:GLU:O	1:h:181:GLU:N	2.31	0.63
1:o:177:GLU:O	1:o:181:GLU:N	2.31	0.63
1:B:177:GLU:O	1:B:181:GLU:N	2.31	0.63
1:O:177:GLU:O	1:O:181:GLU:N	2.31	0.63
1:U:190:SER:N	1:U:193:ASP:OD2	2.30	0.63
1:m:177:GLU:O	1:m:181:GLU:N	2.31	0.63
1:B:190:SER:N	1:B:193:ASP:OD2	2.30	0.63
1:K:177:GLU:O	1:K:181:GLU:N	2.31	0.63
1:L:177:GLU:O	1:L:181:GLU:N	2.31	0.63
1:W:177:GLU:O	1:W:181:GLU:N	2.31	0.63
1:X:150:GLN:NE2	1:X:154:GLU:OE2	2.30	0.63
1:X:177:GLU:O	1:X:181:GLU:N	2.31	0.63
1:f:190:SER:N	1:f:193:ASP:OD2	2.30	0.63
1:i:190:SER:N	1:i:193:ASP:OD2	2.30	0.63
1:E:177:GLU:O	1:E:181:GLU:N	2.31	0.63
1:F:177:GLU:O	1:F:181:GLU:N	2.31	0.63
1:x:177:GLU:O	1:x:181:GLU:N	2.31	0.63
1:1:177:GLU:O	1:1:181:GLU:N	2.31	0.63
1:5:177:GLU:O	1:5:181:GLU:N	2.31	0.63
1:w:177:GLU:O	1:w:181:GLU:N	2.31	0.63
1:y:190:SER:N	1:y:193:ASP:OD2	2.30	0.63
1:0:177:GLU:O	1:0:181:GLU:N	2.31	0.63
1:Y:177:GLU:O	1:Y:181:GLU:N	2.31	0.63
1:Z:177:GLU:O	1:Z:181:GLU:N	2.31	0.63
1:g:177:GLU:O	1:g:181:GLU:N	2.31	0.63
1:i:177:GLU:O	1:i:181:GLU:N	2.31	0.63
1:s:177:GLU:O	1:s:181:GLU:N	2.31	0.63
1:n:177:GLU:O	1:n:181:GLU:N	2.31	0.63

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:u:177:GLU:O	1:u:181:GLU:N	2.31	0.63
1:v:177:GLU:O	1:v:181:GLU:N	2.31	0.63
1:C:177:GLU:O	1:C:181:GLU:N	2.31	0.63
1:I:177:GLU:O	1:I:181:GLU:N	2.31	0.63
1:Q:177:GLU:O	1:Q:181:GLU:N	2.31	0.63
1:S:177:GLU:O	1:S:181:GLU:N	2.31	0.63
1:l:177:GLU:O	1:l:181:GLU:N	2.31	0.63
1:J:177:GLU:O	1:J:181:GLU:N	2.31	0.62
1:N:177:GLU:O	1:N:181:GLU:N	2.31	0.62
1:T:177:GLU:O	1:T:181:GLU:N	2.31	0.62
1:j:177:GLU:O	1:j:181:GLU:N	2.31	0.62
1:6:177:GLU:O	1:6:181:GLU:N	2.31	0.62
1:G:177:GLU:O	1:G:181:GLU:N	2.31	0.62
1:3:177:GLU:O	1:3:181:GLU:N	2.31	0.62
1:b:177:GLU:O	1:b:181:GLU:N	2.31	0.62
1:2:177:GLU:O	1:2:181:GLU:N	2.31	0.62
1:H:177:GLU:O	1:H:181:GLU:N	2.31	0.62
1:p:177:GLU:O	1:p:181:GLU:N	2.31	0.62
1:A:177:GLU:O	1:A:181:GLU:N	2.31	0.62
1:P:177:GLU:O	1:P:181:GLU:N	2.31	0.62
1:e:177:GLU:O	1:e:181:GLU:N	2.31	0.62
1:k:177:GLU:O	1:k:181:GLU:N	2.31	0.62
1:r:177:GLU:O	1:r:181:GLU:N	2.31	0.62
1:t:177:GLU:O	1:t:181:GLU:N	2.31	0.62
1:a:177:GLU:O	1:a:181:GLU:N	2.31	0.62
1:c:177:GLU:O	1:c:181:GLU:N	2.31	0.62
1:R:177:GLU:O	1:R:181:GLU:N	2.31	0.61
1:4:177:GLU:O	1:4:181:GLU:N	2.31	0.61
1:Y:196:PHE:O	1:Y:200:GLU:N	2.26	0.60
1:o:196:PHE:O	1:o:200:GLU:N	2.26	0.59
1:L:196:PHE:O	1:L:200:GLU:N	2.26	0.59
1:p:196:PHE:O	1:p:200:GLU:N	2.26	0.59
1:X:196:PHE:O	1:X:200:GLU:N	2.26	0.59
1:u:196:PHE:O	1:u:200:GLU:N	2.26	0.59
1:1:196:PHE:O	1:1:200:GLU:N	2.26	0.59
1:b:196:PHE:O	1:b:200:GLU:N	2.26	0.59
1:6:196:PHE:O	1:6:200:GLU:N	2.26	0.59
1:B:196:PHE:O	1:B:200:GLU:N	2.26	0.59
1:P:196:PHE:O	1:P:200:GLU:N	2.26	0.59
1:g:196:PHE:O	1:g:200:GLU:N	2.26	0.59
1:G:196:PHE:O	1:G:200:GLU:N	2.26	0.59

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:x:196:PHE:O	1:x:200:GLU:N	2.26	0.59
1:y:62:ASP:OD2	1:y:62:ASP:N	2.36	0.59
1:D:62:ASP:OD2	1:D:62:ASP:N	2.36	0.59
1:Y:62:ASP:OD2	1:Y:62:ASP:N	2.36	0.59
1:7:62:ASP:OD2	1:7:62:ASP:N	2.36	0.58
1:C:196:PHE:O	1:C:200:GLU:N	2.26	0.58
1:d:62:ASP:OD2	1:d:62:ASP:N	2.36	0.58
1:2:196:PHE:O	1:2:200:GLU:N	2.26	0.58
1:U:62:ASP:OD2	1:U:62:ASP:N	2.36	0.58
1:h:62:ASP:OD2	1:h:62:ASP:N	2.36	0.58
1:M:62:ASP:OD2	1:M:62:ASP:N	2.36	0.58
1:P:62:ASP:N	1:P:62:ASP:OD2	2.36	0.58
1:p:62:ASP:OD2	1:p:62:ASP:N	2.36	0.58
1:3:62:ASP:OD2	1:3:62:ASP:N	2.36	0.58
1:K:196:PHE:O	1:K:200:GLU:N	2.26	0.58
1:2:62:ASP:OD2	1:2:62:ASP:N	2.36	0.58
1:H:62:ASP:N	1:H:62:ASP:OD2	2.36	0.58
1:c:196:PHE:O	1:c:200:GLU:N	2.26	0.58
1:m:62:ASP:OD2	1:m:62:ASP:N	2.36	0.58
1:5:196:PHE:O	1:5:200:GLU:N	2.26	0.58
1:d:196:PHE:O	1:d:200:GLU:N	2.26	0.58
1:k:196:PHE:O	1:k:200:GLU:N	2.26	0.58
1:l:196:PHE:O	1:l:200:GLU:N	2.26	0.58
1:t:62:ASP:OD2	1:t:62:ASP:N	2.36	0.58
1:u:62:ASP:OD2	1:u:62:ASP:N	2.36	0.58
1:q:62:ASP:OD2	1:q:62:ASP:N	2.36	0.58
1:I:62:ASP:OD2	1:I:62:ASP:N	2.36	0.58
1:L:62:ASP:OD2	1:L:62:ASP:N	2.36	0.57
1:T:196:PHE:O	1:T:200:GLU:N	2.26	0.57
1:t:196:PHE:O	1:t:200:GLU:N	2.26	0.57
1:c:62:ASP:N	1:c:62:ASP:OD2	2.36	0.57
1:G:62:ASP:OD2	1:G:62:ASP:N	2.36	0.57
1:V:62:ASP:OD2	1:V:62:ASP:N	2.36	0.57
1:g:62:ASP:OD2	1:g:62:ASP:N	2.36	0.57
1:Q:62:ASP:OD2	1:Q:62:ASP:N	2.36	0.57
1:T:62:ASP:OD2	1:T:62:ASP:N	2.36	0.57
1:Z:62:ASP:OD2	1:Z:62:ASP:N	2.36	0.57
1:v:62:ASP:N	1:v:62:ASP:OD2	2.36	0.57
1:6:62:ASP:OD2	1:6:62:ASP:N	2.36	0.57
1:U:196:PHE:O	1:U:200:GLU:N	2.26	0.57
1:f:196:PHE:O	1:f:200:GLU:N	2.26	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:k:62:ASP:N	1:k:62:ASP:OD2	2.36	0.57
1:l:62:ASP:OD2	1:l:62:ASP:N	2.36	0.57
1:R:62:ASP:OD2	1:R:62:ASP:N	2.36	0.57
1:i:62:ASP:OD2	1:i:62:ASP:N	2.36	0.57
1:s:196:PHE:O	1:s:200:GLU:N	2.26	0.57
1:C:62:ASP:OD2	1:C:62:ASP:N	2.36	0.57
1:1:62:ASP:OD2	1:1:62:ASP:N	2.36	0.57
1:K:62:ASP:OD2	1:K:62:ASP:N	2.36	0.57
1:A:62:ASP:OD2	1:A:62:ASP:N	2.36	0.56
1:z:62:ASP:OD2	1:z:62:ASP:N	2.36	0.56
1:F:196:PHE:O	1:F:200:GLU:N	2.26	0.56
1:v:196:PHE:O	1:v:200:GLU:N	2.26	0.56
1:4:62:ASP:OD2	1:4:62:ASP:N	2.36	0.56
1:a:62:ASP:OD2	1:a:62:ASP:N	2.36	0.56
1:b:62:ASP:OD2	1:b:62:ASP:N	2.36	0.56
1:e:62:ASP:OD2	1:e:62:ASP:N	2.36	0.56
1:E:62:ASP:OD2	1:E:62:ASP:N	2.36	0.56
1:r:62:ASP:OD2	1:r:62:ASP:N	2.36	0.56
1:s:62:ASP:N	1:s:62:ASP:OD2	2.36	0.56
1:J:62:ASP:OD2	1:J:62:ASP:N	2.36	0.56
1:M:196:PHE:O	1:M:200:GLU:N	2.26	0.56
1:S:62:ASP:N	1:S:62:ASP:OD2	2.36	0.56
1:W:62:ASP:OD2	1:W:62:ASP:N	2.36	0.56
1:B:62:ASP:OD2	1:B:62:ASP:N	2.36	0.56
1:D:196:PHE:O	1:D:200:GLU:N	2.26	0.56
1:j:62:ASP:OD2	1:j:62:ASP:N	2.36	0.56
1:w:62:ASP:OD2	1:w:62:ASP:N	2.36	0.56
1:A:196:PHE:O	1:A:200:GLU:N	2.26	0.56
1:x:62:ASP:OD2	1:x:62:ASP:N	2.36	0.56
1:0:62:ASP:N	1:0:62:ASP:OD2	2.36	0.56
1:5:62:ASP:N	1:5:62:ASP:OD2	2.36	0.56
1:n:62:ASP:OD2	1:n:62:ASP:N	2.36	0.56
1:o:62:ASP:OD2	1:o:62:ASP:N	2.36	0.55
1:N:62:ASP:OD2	1:N:62:ASP:N	2.36	0.55
1:V:196:PHE:O	1:V:200:GLU:N	2.26	0.55
1:y:196:PHE:O	1:y:200:GLU:N	2.26	0.55
1:f:62:ASP:OD2	1:f:62:ASP:N	2.36	0.55
1:7:196:PHE:O	1:7:200:GLU:N	2.26	0.54
1:X:62:ASP:OD2	1:X:62:ASP:N	2.36	0.54
1:O:196:PHE:O	1:O:200:GLU:N	2.26	0.54
1:4:196:PHE:O	1:4:200:GLU:N	2.26	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:j:196:PHE:O	1:j:200:GLU:N	2.26	0.54
1:O:62:ASP:OD2	1:O:62:ASP:N	2.36	0.54
1:F:62:ASP:OD2	1:F:62:ASP:N	2.36	0.53
1:J:200:GLU:O	1:J:204:ALA:N	2.34	0.53
1:J:196:PHE:O	1:J:200:GLU:N	2.26	0.53
1:R:194:LYS:HE2	1:R:194:LYS:HA	1.91	0.53
1:g:194:LYS:HE2	1:g:194:LYS:HA	1.91	0.53
1:h:200:GLU:O	1:h:204:ALA:N	2.34	0.53
1:i:194:LYS:HE2	1:i:194:LYS:HA	1.91	0.53
1:z:200:GLU:O	1:z:204:ALA:N	2.34	0.53
1:P:194:LYS:HE2	1:P:194:LYS:HA	1.91	0.53
1:6:194:LYS:HE2	1:6:194:LYS:HA	1.91	0.53
1:I:194:LYS:HE2	1:I:194:LYS:HA	1.91	0.53
1:X:194:LYS:HE2	1:X:194:LYS:HA	1.91	0.53
1:Y:194:LYS:HE2	1:Y:194:LYS:HA	1.91	0.53
1:Z:194:LYS:HE2	1:Z:194:LYS:HA	1.91	0.53
1:a:194:LYS:HE2	1:a:194:LYS:HA	1.91	0.53
1:e:196:PHE:O	1:e:200:GLU:N	2.26	0.53
1:p:194:LYS:HE2	1:p:194:LYS:HA	1.91	0.53
1:q:194:LYS:HA	1:q:194:LYS:HE2	1.91	0.53
1:r:194:LYS:HE2	1:r:194:LYS:HA	1.91	0.53
1:0:194:LYS:HA	1:0:194:LYS:HE2	1.91	0.53
1:E:200:GLU:O	1:E:204:ALA:N	2.34	0.53
1:G:194:LYS:HE2	1:G:194:LYS:HA	1.91	0.53
1:O:194:LYS:HE2	1:O:194:LYS:HA	1.91	0.53
1:Q:194:LYS:HE2	1:Q:194:LYS:HA	1.91	0.53
1:h:194:LYS:HE2	1:h:194:LYS:HA	1.91	0.53
1:A:194:LYS:HE2	1:A:194:LYS:HA	1.91	0.53
1:E:125:LEU:HD13	1:I:152:ILE:HD11	1.91	0.53
1:H:194:LYS:HA	1:H:194:LYS:HE2	1.91	0.53
1:y:194:LYS:HA	1:y:194:LYS:HE2	1.91	0.53
1:z:194:LYS:HE2	1:z:194:LYS:HA	1.91	0.53
1:4:160:ASP:OD1	1:4:161:ASN:N	2.42	0.52
1:F:194:LYS:HE2	1:F:194:LYS:HA	1.91	0.52
1:x:194:LYS:HE2	1:x:194:LYS:HA	1.91	0.52
1:0:160:ASP:OD1	1:0:161:ASN:N	2.42	0.52
1:1:194:LYS:HE2	1:1:194:LYS:HA	1.91	0.52
1:A:160:ASP:OD1	1:A:161:ASN:N	2.42	0.52
1:J:194:LYS:HE2	1:J:194:LYS:HA	1.91	0.52
1:a:160:ASP:OD1	1:a:161:ASN:N	2.42	0.52
1:j:194:LYS:HE2	1:j:194:LYS:HA	1.91	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:o:194:LYS:HE2	1:o:194:LYS:HA	1.91	0.52
1:s:194:LYS:HE2	1:s:194:LYS:HA	1.91	0.52
1:3:194:LYS:HA	1:3:194:LYS:HE2	1.91	0.52
1:4:194:LYS:HE2	1:4:194:LYS:HA	1.91	0.52
1:W:196:PHE:O	1:W:200:GLU:N	2.26	0.52
1:e:160:ASP:OD1	1:e:161:ASN:N	2.42	0.52
1:q:196:PHE:O	1:q:200:GLU:N	2.26	0.52
1:2:194:LYS:HE2	1:2:194:LYS:HA	1.91	0.52
1:7:194:LYS:HE2	1:7:194:LYS:HA	1.91	0.52
1:C:194:LYS:HA	1:C:194:LYS:HE2	1.91	0.52
1:v:194:LYS:HA	1:v:194:LYS:HE2	1.91	0.52
1:E:160:ASP:OD1	1:E:161:ASN:N	2.42	0.52
1:F:160:ASP:OD1	1:F:161:ASN:N	2.42	0.52
1:Y:200:GLU:O	1:Y:204:ALA:N	2.34	0.52
1:f:194:LYS:HA	1:f:194:LYS:HE2	1.91	0.52
1:E:194:LYS:HE2	1:E:194:LYS:HA	1.91	0.52
1:J:160:ASP:OD1	1:J:161:ASN:N	2.42	0.52
1:L:194:LYS:HE2	1:L:194:LYS:HA	1.91	0.52
1:S:194:LYS:HA	1:S:194:LYS:HE2	1.91	0.52
1:X:200:GLU:O	1:X:204:ALA:N	2.34	0.52
1:Y:160:ASP:OD1	1:Y:161:ASN:N	2.42	0.52
1:h:196:PHE:O	1:h:200:GLU:N	2.26	0.52
1:j:160:ASP:OD1	1:j:161:ASN:N	2.42	0.52
1:u:194:LYS:HE2	1:u:194:LYS:HA	1.91	0.52
1:0:209:LEU:O	1:0:213:LYS:N	2.41	0.52
1:1:125:LEU:HD13	1:5:152:ILE:HD11	1.92	0.52
1:1:170:ARG:O	1:1:173:THR:OG1	2.26	0.52
1:B:160:ASP:OD1	1:B:161:ASN:N	2.42	0.52
1:N:194:LYS:HE2	1:N:194:LYS:HA	1.91	0.52
1:W:194:LYS:HE2	1:W:194:LYS:HA	1.91	0.52
1:f:160:ASP:OD1	1:f:161:ASN:N	2.42	0.52
1:m:194:LYS:HE2	1:m:194:LYS:HA	1.91	0.52
1:s:200:GLU:O	1:s:204:ALA:N	2.34	0.52
1:t:194:LYS:HE2	1:t:194:LYS:HA	1.91	0.52
1:D:194:LYS:HE2	1:D:194:LYS:HA	1.91	0.52
1:N:196:PHE:O	1:N:200:GLU:N	2.26	0.52
1:Q:200:GLU:O	1:Q:204:ALA:N	2.34	0.52
1:g:200:GLU:O	1:g:204:ALA:N	2.34	0.52
1:i:160:ASP:OD1	1:i:161:ASN:N	2.42	0.52
1:k:194:LYS:HA	1:k:194:LYS:HE2	1.91	0.52
1:5:160:ASP:OD1	1:5:161:ASN:N	2.42	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:125:LEU:HD13	1:b:152:ILE:HD11	1.92	0.52
1:b:125:LEU:HD13	1:f:152:ILE:HD11	1.92	0.52
1:b:194:LYS:HE2	1:b:194:LYS:HA	1.91	0.52
1:f:125:LEU:HD13	1:j:152:ILE:HD11	1.92	0.52
1:h:209:LEU:O	1:h:213:LYS:N	2.41	0.52
1:j:125:LEU:HD13	1:n:152:ILE:HD11	1.92	0.52
1:t:160:ASP:OD1	1:t:161:ASN:N	2.42	0.52
1:7:160:ASP:OD1	1:7:161:ASN:N	2.42	0.52
1:I:160:ASP:OD1	1:I:161:ASN:N	2.42	0.52
1:J:125:LEU:HD13	1:N:152:ILE:HD11	1.92	0.52
1:Z:200:GLU:O	1:Z:204:ALA:N	2.34	0.52
1:b:160:ASP:OD1	1:b:161:ASN:N	2.42	0.52
1:k:159:LEU:O	1:k:166:SER:OG	2.28	0.52
1:n:125:LEU:HD13	1:r:152:ILE:HD11	1.92	0.52
1:n:200:GLU:O	1:n:204:ALA:N	2.34	0.52
1:1:152:ILE:HD11	1:x:125:LEU:HD13	1.92	0.51
1:B:125:LEU:HD13	1:F:152:ILE:HD11	1.92	0.51
1:M:194:LYS:HE2	1:M:194:LYS:HA	1.91	0.51
1:T:125:LEU:HD13	1:X:152:ILE:HD11	1.92	0.51
1:T:194:LYS:HE2	1:T:194:LYS:HA	1.91	0.51
1:n:160:ASP:OD1	1:n:161:ASN:N	2.42	0.51
1:r:125:LEU:HD13	1:v:152:ILE:HD11	1.92	0.51
1:r:209:LEU:O	1:r:213:LYS:N	2.41	0.51
1:z:160:ASP:OD1	1:z:161:ASN:N	2.42	0.51
1:z:196:PHE:O	1:z:200:GLU:N	2.26	0.51
1:5:194:LYS:HE2	1:5:194:LYS:HA	1.91	0.51
1:F:125:LEU:HD13	1:J:152:ILE:HD11	1.92	0.51
1:K:194:LYS:HA	1:K:194:LYS:HE2	1.91	0.51
1:N:160:ASP:OD1	1:N:161:ASN:N	2.42	0.51
1:U:194:LYS:HE2	1:U:194:LYS:HA	1.91	0.51
1:g:159:LEU:O	1:g:166:SER:OG	2.28	0.51
1:l:194:LYS:HE2	1:l:194:LYS:HA	1.91	0.51
1:t:125:LEU:HD13	1:x:152:ILE:HD11	1.92	0.51
1:2:209:LEU:O	1:2:213:LYS:N	2.41	0.51
1:N:125:LEU:HD13	1:R:152:ILE:HD11	1.92	0.51
1:a:209:LEU:O	1:a:213:LYS:N	2.41	0.51
1:e:194:LYS:HE2	1:e:194:LYS:HA	1.91	0.51
1:j:209:LEU:O	1:j:213:LYS:N	2.41	0.51
1:v:125:LEU:HD13	1:z:152:ILE:HD11	1.92	0.51
1:x:159:LEU:O	1:x:166:SER:OG	2.28	0.51
1:1:160:ASP:OD1	1:1:161:ASN:N	2.42	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:200:GLU:O	1:H:204:ALA:N	2.34	0.51
1:S:200:GLU:O	1:S:204:ALA:N	2.34	0.51
1:V:194:LYS:HA	1:V:194:LYS:HE2	1.91	0.51
1:W:125:LEU:HD13	1:a:152:ILE:HD11	1.92	0.51
1:Z:160:ASP:OD1	1:Z:161:ASN:N	2.42	0.51
1:c:194:LYS:HA	1:c:194:LYS:HE2	1.91	0.51
1:d:194:LYS:HE2	1:d:194:LYS:HA	1.91	0.51
1:h:160:ASP:OD1	1:h:161:ASN:N	2.42	0.51
1:n:194:LYS:HA	1:n:194:LYS:HE2	1.91	0.51
1:s:159:LEU:O	1:s:166:SER:OG	2.28	0.51
1:t:159:LEU:O	1:t:166:SER:OG	2.28	0.51
1:1:159:LEU:O	1:1:166:SER:OG	2.28	0.51
1:3:152:ILE:HD11	1:z:125:LEU:HD13	1.92	0.51
1:3:160:ASP:OD1	1:3:161:ASN:N	2.42	0.51
1:6:170:ARG:O	1:6:173:THR:OG1	2.26	0.51
1:E:196:PHE:O	1:E:200:GLU:N	2.26	0.51
1:O:125:LEU:HD13	1:S:152:ILE:HD11	1.92	0.51
1:P:200:GLU:O	1:P:204:ALA:N	2.34	0.51
1:R:125:LEU:HD13	1:V:152:ILE:HD11	1.92	0.51
1:a:125:LEU:HD13	1:e:152:ILE:HD11	1.92	0.51
1:e:125:LEU:HD13	1:i:152:ILE:HD11	1.92	0.51
1:y:209:LEU:O	1:y:213:LYS:N	2.41	0.51
1:O:125:LEU:HD13	1:4:152:ILE:HD11	1.92	0.51
1:2:160:ASP:OD1	1:2:161:ASN:N	2.42	0.51
1:A:125:LEU:HD13	1:E:152:ILE:HD11	1.93	0.51
1:J:209:LEU:O	1:J:213:LYS:N	2.41	0.51
1:K:125:LEU:HD13	1:O:152:ILE:HD11	1.92	0.51
1:S:125:LEU:HD13	1:W:152:ILE:HD11	1.92	0.51
1:T:160:ASP:OD1	1:T:161:ASN:N	2.42	0.51
1:V:125:LEU:HD13	1:Z:152:ILE:HD11	1.92	0.51
1:b:159:LEU:O	1:b:166:SER:OG	2.28	0.51
1:f:159:LEU:O	1:f:166:SER:OG	2.28	0.51
1:p:125:LEU:HD13	1:t:152:ILE:HD11	1.92	0.51
1:w:194:LYS:HE2	1:w:194:LYS:HA	1.91	0.51
1:B:194:LYS:HE2	1:B:194:LYS:HA	1.91	0.51
1:G:125:LEU:HD13	1:K:152:ILE:HD11	1.92	0.51
1:I:125:LEU:HD13	1:M:152:ILE:HD11	1.92	0.51
1:P:125:LEU:HD13	1:T:152:ILE:HD11	1.92	0.51
1:X:160:ASP:OD1	1:X:161:ASN:N	2.42	0.51
1:m:160:ASP:OD1	1:m:161:ASN:N	2.42	0.51
1:S:209:LEU:O	1:S:213:LYS:N	2.41	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:i:125:LEU:HD13	1:m:152:ILE:HD11	1.92	0.51
1:s:125:LEU:HD13	1:w:152:ILE:HD11	1.92	0.51
1:0:152:ILE:HD11	1:w:125:LEU:HD13	1.92	0.51
1:6:209:LEU:O	1:6:213:LYS:N	2.41	0.51
1:G:200:GLU:O	1:G:204:ALA:N	2.34	0.51
1:M:160:ASP:OD1	1:M:161:ASN:N	2.42	0.51
1:N:200:GLU:O	1:N:204:ALA:N	2.34	0.51
1:P:209:LEU:O	1:P:213:LYS:N	2.41	0.51
1:Z:125:LEU:HD13	1:d:152:ILE:HD11	1.92	0.51
1:Z:196:PHE:O	1:Z:200:GLU:N	2.26	0.51
1:2:159:LEU:O	1:2:166:SER:OG	2.28	0.51
1:3:125:LEU:HD13	1:7:152:ILE:HD11	1.92	0.51
1:G:159:LEU:O	1:G:166:SER:OG	2.28	0.51
1:H:160:ASP:OD1	1:H:161:ASN:N	2.42	0.51
1:L:125:LEU:HD13	1:P:152:ILE:HD11	1.92	0.51
1:L:209:LEU:O	1:L:213:LYS:N	2.41	0.51
1:d:160:ASP:OD1	1:d:161:ASN:N	2.42	0.51
1:l:125:LEU:HD13	1:p:152:ILE:HD11	1.92	0.51
1:l:159:LEU:O	1:l:166:SER:OG	2.28	0.51
1:o:125:LEU:HD13	1:s:152:ILE:HD11	1.92	0.51
1:r:160:ASP:OD1	1:r:161:ASN:N	2.42	0.51
1:x:160:ASP:OD1	1:x:161:ASN:N	2.42	0.51
1:1:200:GLU:O	1:1:204:ALA:N	2.34	0.50
1:M:209:LEU:O	1:M:213:LYS:N	2.41	0.50
1:R:160:ASP:OD1	1:R:161:ASN:N	2.42	0.50
1:d:125:LEU:HD13	1:h:152:ILE:HD11	1.92	0.50
1:w:209:LEU:O	1:w:213:LYS:N	2.41	0.50
1:C:125:LEU:HD13	1:G:152:ILE:HD11	1.92	0.50
1:C:209:LEU:O	1:C:213:LYS:N	2.41	0.50
1:M:125:LEU:HD13	1:Q:152:ILE:HD11	1.92	0.50
1:h:125:LEU:HD13	1:l:152:ILE:HD11	1.92	0.50
1:y:159:LEU:O	1:y:166:SER:OG	2.28	0.50
1:5:209:LEU:O	1:5:213:LYS:N	2.41	0.50
1:D:125:LEU:HD13	1:H:152:ILE:HD11	1.92	0.50
1:D:160:ASP:OD1	1:D:161:ASN:N	2.42	0.50
1:H:125:LEU:HD13	1:L:152:ILE:HD11	1.92	0.50
1:O:160:ASP:OD1	1:O:161:ASN:N	2.42	0.50
1:c:160:ASP:OD1	1:c:161:ASN:N	2.42	0.50
1:f:209:LEU:O	1:f:213:LYS:N	2.41	0.50
1:g:125:LEU:HD13	1:k:152:ILE:HD11	1.92	0.50
1:k:125:LEU:HD13	1:o:152:ILE:HD11	1.92	0.50

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:m:125:LEU:HD13	1:q:152:ILE:HD11	1.92	0.50
1:B:209:LEU:O	1:B:213:LYS:N	2.41	0.50
1:C:170:ARG:O	1:C:173:THR:OG1	2.26	0.50
1:K:159:LEU:O	1:K:166:SER:OG	2.28	0.50
1:K:160:ASP:OD1	1:K:161:ASN:N	2.42	0.50
1:T:209:LEU:O	1:T:213:LYS:N	2.41	0.50
1:d:209:LEU:O	1:d:213:LYS:N	2.41	0.50
1:i:200:GLU:O	1:i:204:ALA:N	2.34	0.50
1:O:209:LEU:O	1:O:213:LYS:N	2.41	0.50
1:S:196:PHE:O	1:S:200:GLU:N	2.26	0.50
1:c:125:LEU:HD13	1:g:152:ILE:HD11	1.92	0.50
1:g:209:LEU:O	1:g:213:LYS:N	2.41	0.50
1:k:209:LEU:O	1:k:213:LYS:N	2.41	0.50
1:l:209:LEU:O	1:l:213:LYS:N	2.41	0.50
1:F:202:GLN:HA	1:F:205:VAL:HG12	1.94	0.50
1:S:160:ASP:OD1	1:S:161:ASN:N	2.42	0.50
1:S:202:GLN:HA	1:S:205:VAL:HG12	1.94	0.50
1:W:159:LEU:O	1:W:166:SER:OG	2.28	0.50
1:e:202:GLN:HA	1:e:205:VAL:HG12	1.94	0.50
1:o:160:ASP:OD1	1:o:161:ASN:N	2.42	0.50
1:q:160:ASP:OD1	1:q:161:ASN:N	2.42	0.50
1:w:202:GLN:HA	1:w:205:VAL:HG12	1.94	0.50
1:Q:125:LEU:HD13	1:U:152:ILE:HD11	1.92	0.50
1:R:196:PHE:O	1:R:200:GLU:N	2.26	0.50
1:R:202:GLN:HA	1:R:205:VAL:HG12	1.94	0.50
1:Y:125:LEU:HD13	1:c:152:ILE:HD11	1.92	0.50
1:Y:159:LEU:O	1:Y:166:SER:OG	2.28	0.50
1:f:202:GLN:HA	1:f:205:VAL:HG12	1.94	0.50
1:q:125:LEU:HD13	1:u:152:ILE:HD11	1.92	0.50
1:r:202:GLN:HA	1:r:205:VAL:HG12	1.94	0.50
1:u:159:LEU:O	1:u:166:SER:OG	2.28	0.50
1:z:209:LEU:O	1:z:213:LYS:N	2.41	0.50
1:G:160:ASP:OD1	1:G:161:ASN:N	2.42	0.50
1:P:159:LEU:O	1:P:166:SER:OG	2.28	0.50
1:Q:160:ASP:OD1	1:Q:161:ASN:N	2.42	0.50
1:i:196:PHE:O	1:i:200:GLU:N	2.26	0.50
1:n:159:LEU:O	1:n:166:SER:OG	2.28	0.50
1:n:196:PHE:O	1:n:200:GLU:N	2.26	0.50
1:o:209:LEU:O	1:o:213:LYS:N	2.41	0.50
1:s:160:ASP:OD1	1:s:161:ASN:N	2.42	0.50
1:A:202:GLN:HA	1:A:205:VAL:HG12	1.94	0.50

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:202:GLN:HA	1:E:205:VAL:HG12	1.94	0.50
1:F:159:LEU:O	1:F:166:SER:OG	2.28	0.50
1:H:159:LEU:O	1:H:166:SER:OG	2.28	0.50
1:O:159:LEU:O	1:O:166:SER:OG	2.28	0.50
1:P:160:ASP:OD1	1:P:161:ASN:N	2.42	0.50
1:Q:196:PHE:O	1:Q:200:GLU:N	2.26	0.50
1:U:125:LEU:HD13	1:Y:152:ILE:HD11	1.92	0.50
1:c:209:LEU:O	1:c:213:LYS:N	2.41	0.50
1:i:209:LEU:O	1:i:213:LYS:N	2.41	0.50
1:j:202:GLN:HA	1:j:205:VAL:HG12	1.94	0.50
1:k:160:ASP:OD1	1:k:161:ASN:N	2.42	0.50
1:v:202:GLN:HA	1:v:205:VAL:HG12	1.94	0.50
1:2:200:GLU:O	1:2:204:ALA:N	2.34	0.49
1:4:202:GLN:HA	1:4:205:VAL:HG12	1.94	0.49
1:A:209:LEU:O	1:A:213:LYS:N	2.41	0.49
1:D:159:LEU:O	1:D:166:SER:OG	2.28	0.49
1:H:209:LEU:O	1:H:213:LYS:N	2.41	0.49
1:L:159:LEU:O	1:L:166:SER:OG	2.28	0.49
1:R:209:LEU:O	1:R:213:LYS:N	2.41	0.49
1:l:160:ASP:OD1	1:l:161:ASN:N	2.42	0.49
1:p:160:ASP:OD1	1:p:161:ASN:N	2.42	0.49
1:s:202:GLN:HA	1:s:205:VAL:HG12	1.94	0.49
1:u:209:LEU:O	1:u:213:LYS:N	2.41	0.49
1:w:196:PHE:O	1:w:200:GLU:N	2.26	0.49
1:2:125:LEU:HD13	1:6:152:ILE:HD11	1.92	0.49
1:2:152:ILE:HD11	1:y:125:LEU:HD13	1.92	0.49
1:7:159:LEU:O	1:7:166:SER:OG	2.28	0.49
1:C:160:ASP:OD1	1:C:161:ASN:N	2.42	0.49
1:L:160:ASP:OD1	1:L:161:ASN:N	2.42	0.49
1:M:202:GLN:HA	1:M:205:VAL:HG12	1.94	0.49
1:X:202:GLN:HA	1:X:205:VAL:HG12	1.94	0.49
1:u:125:LEU:HD13	1:y:152:ILE:HD11	1.92	0.49
1:v:160:ASP:OD1	1:v:161:ASN:N	2.42	0.49
1:x:209:LEU:O	1:x:213:LYS:N	2.41	0.49
1:B:202:GLN:HA	1:B:205:VAL:HG12	1.94	0.49
1:K:202:GLN:HA	1:K:205:VAL:HG12	1.94	0.49
1:N:202:GLN:HA	1:N:205:VAL:HG12	1.94	0.49
1:W:202:GLN:HA	1:W:205:VAL:HG12	1.94	0.49
1:b:200:GLU:O	1:b:204:ALA:N	2.34	0.49
1:h:159:LEU:O	1:h:166:SER:OG	2.28	0.49
1:i:202:GLN:HA	1:i:205:VAL:HG12	1.94	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:k:202:GLN:HA	1:k:205:VAL:HG12	1.94	0.49
1:3:202:GLN:HA	1:3:205:VAL:HG12	1.94	0.49
1:C:209:LEU:HD23	1:C:209:LEU:C	2.38	0.49
1:X:209:LEU:O	1:X:213:LYS:N	2.41	0.49
1:Z:202:GLN:HA	1:Z:205:VAL:HG12	1.94	0.49
1:q:202:GLN:HA	1:q:205:VAL:HG12	1.94	0.49
1:u:209:LEU:C	1:u:209:LEU:HD23	2.38	0.49
1:5:202:GLN:HA	1:5:205:VAL:HG12	1.94	0.49
1:7:68:ALA:O	1:7:72:TYR:N	2.45	0.49
1:H:196:PHE:O	1:H:200:GLU:N	2.26	0.49
1:H:209:LEU:HD23	1:H:209:LEU:C	2.38	0.49
1:K:209:LEU:O	1:K:213:LYS:N	2.41	0.49
1:T:209:LEU:HD23	1:T:209:LEU:C	2.38	0.49
1:U:160:ASP:OD1	1:U:161:ASN:N	2.42	0.49
1:V:160:ASP:OD1	1:V:161:ASN:N	2.42	0.49
1:a:202:GLN:HA	1:a:205:VAL:HG12	1.94	0.49
1:c:200:GLU:O	1:c:204:ALA:N	2.34	0.49
1:d:209:LEU:HD23	1:d:209:LEU:C	2.38	0.49
1:g:160:ASP:OD1	1:g:161:ASN:N	2.42	0.49
1:p:209:LEU:HD23	1:p:209:LEU:C	2.38	0.49
1:r:196:PHE:O	1:r:200:GLU:N	2.26	0.49
1:u:160:ASP:OD1	1:u:161:ASN:N	2.42	0.49
1:w:160:ASP:OD1	1:w:161:ASN:N	2.42	0.49
1:x:209:LEU:C	1:x:209:LEU:HD23	2.38	0.49
1:0:159:LEU:O	1:0:166:SER:OG	2.28	0.49
1:1:202:GLN:HA	1:1:205:VAL:HG12	1.94	0.49
1:2:209:LEU:HD23	1:2:209:LEU:C	2.38	0.49
1:3:159:LEU:O	1:3:166:SER:OG	2.28	0.49
1:5:200:GLU:O	1:5:204:ALA:N	2.34	0.49
1:6:209:LEU:HD23	1:6:209:LEU:C	2.38	0.49
1:C:200:GLU:O	1:C:204:ALA:N	2.34	0.49
1:D:68:ALA:O	1:D:72:TYR:N	2.45	0.49
1:G:202:GLN:HA	1:G:205:VAL:HG12	1.94	0.49
1:J:202:GLN:HA	1:J:205:VAL:HG12	1.94	0.49
1:K:209:LEU:HD23	1:K:209:LEU:C	2.38	0.49
1:R:159:LEU:O	1:R:166:SER:OG	2.28	0.49
1:W:160:ASP:OD1	1:W:161:ASN:N	2.42	0.49
1:Y:209:LEU:HD23	1:Y:209:LEU:C	2.38	0.49
1:c:209:LEU:HD23	1:c:209:LEU:C	2.38	0.49
1:d:68:ALA:O	1:d:72:TYR:N	2.45	0.49
1:e:159:LEU:O	1:e:166:SER:OG	2.28	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:w:200:GLU:O	1:w:204:ALA:N	2.34	0.49
1:x:202:GLN:HA	1:x:205:VAL:HG12	1.94	0.49
1:7:209:LEU:C	1:7:209:LEU:HD23	2.38	0.49
1:D:209:LEU:HD23	1:D:209:LEU:C	2.38	0.49
1:M:68:ALA:O	1:M:72:TYR:N	2.45	0.49
1:N:159:LEU:O	1:N:166:SER:OG	2.28	0.49
1:V:202:GLN:HA	1:V:205:VAL:HG12	1.94	0.49
1:g:209:LEU:HD23	1:g:209:LEU:C	2.38	0.49
1:h:68:ALA:O	1:h:72:TYR:N	2.45	0.49
1:k:209:LEU:HD23	1:k:209:LEU:C	2.38	0.49
1:m:68:ALA:O	1:m:72:TYR:N	2.45	0.49
1:m:202:GLN:HA	1:m:205:VAL:HG12	1.94	0.49
1:4:209:LEU:O	1:4:213:LYS:N	2.41	0.49
1:A:143:LEU:O	1:A:147:ILE:HG22	2.13	0.49
1:M:159:LEU:O	1:M:166:SER:OG	2.28	0.49
1:M:209:LEU:HD23	1:M:209:LEU:C	2.38	0.49
1:O:143:LEU:O	1:O:147:ILE:HG22	2.13	0.49
1:O:202:GLN:HA	1:O:205:VAL:HG12	1.94	0.49
1:Q:209:LEU:HD23	1:Q:209:LEU:C	2.38	0.49
1:S:143:LEU:O	1:S:147:ILE:HG22	2.13	0.49
1:W:143:LEU:O	1:W:147:ILE:HG22	2.13	0.49
1:d:202:GLN:HA	1:d:205:VAL:HG12	1.94	0.49
1:h:209:LEU:HD23	1:h:209:LEU:C	2.38	0.49
1:m:209:LEU:C	1:m:209:LEU:HD23	2.38	0.49
1:q:68:ALA:O	1:q:72:TYR:N	2.45	0.49
1:s:143:LEU:O	1:s:147:ILE:HG22	2.13	0.49
1:y:209:LEU:HD23	1:y:209:LEU:C	2.38	0.49
1:0:202:GLN:HA	1:0:205:VAL:HG12	1.94	0.49
1:3:209:LEU:HD23	1:3:209:LEU:C	2.38	0.49
1:6:160:ASP:OD1	1:6:161:ASN:N	2.42	0.49
1:F:209:LEU:O	1:F:213:LYS:N	2.41	0.49
1:I:159:LEU:O	1:I:166:SER:OG	2.28	0.49
1:I:200:GLU:O	1:I:204:ALA:N	2.34	0.49
1:K:143:LEU:O	1:K:147:ILE:HG22	2.13	0.49
1:P:209:LEU:HD23	1:P:209:LEU:C	2.38	0.49
1:U:68:ALA:O	1:U:72:TYR:N	2.45	0.49
1:V:159:LEU:O	1:V:166:SER:OG	2.28	0.49
1:W:209:LEU:O	1:W:213:LYS:N	2.41	0.49
1:a:143:LEU:O	1:a:147:ILE:HG22	2.13	0.49
1:b:209:LEU:C	1:b:209:LEU:HD23	2.38	0.49
1:b:209:LEU:O	1:b:213:LYS:N	2.41	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:l:209:LEU:HD23	1:l:209:LEU:C	2.38	0.49
1:n:209:LEU:O	1:n:213:LYS:N	2.41	0.49
1:o:143:LEU:O	1:o:147:ILE:HG22	2.13	0.49
1:o:202:GLN:HA	1:o:205:VAL:HG12	1.94	0.49
1:q:159:LEU:O	1:q:166:SER:OG	2.28	0.49
1:w:143:LEU:O	1:w:147:ILE:HG22	2.13	0.49
1:z:209:LEU:HD23	1:z:209:LEU:C	2.38	0.49
1:4:143:LEU:O	1:4:147:ILE:HG22	2.13	0.49
1:E:143:LEU:O	1:E:147:ILE:HG22	2.13	0.49
1:I:68:ALA:O	1:I:72:TYR:N	2.45	0.49
1:Q:159:LEU:O	1:Q:166:SER:OG	2.28	0.49
1:V:209:LEU:HD23	1:V:209:LEU:C	2.38	0.49
1:Y:68:ALA:O	1:Y:72:TYR:N	2.45	0.49
1:e:143:LEU:O	1:e:147:ILE:HG22	2.13	0.49
1:m:196:PHE:O	1:m:200:GLU:N	2.26	0.49
1:r:143:LEU:O	1:r:147:ILE:HG22	2.13	0.49
1:y:68:ALA:O	1:y:72:TYR:N	2.45	0.49
1:z:202:GLN:HA	1:z:205:VAL:HG12	1.94	0.49
1:E:209:LEU:HD23	1:E:209:LEU:C	2.38	0.48
1:F:143:LEU:O	1:F:147:ILE:HG22	2.13	0.48
1:M:205:VAL:O	1:M:209:LEU:HD13	2.13	0.48
1:O:72:TYR:O	1:O:76:GLN:N	2.44	0.48
1:Q:202:GLN:HA	1:Q:205:VAL:HG12	1.94	0.48
1:X:209:LEU:HD23	1:X:209:LEU:C	2.38	0.48
1:j:143:LEU:O	1:j:147:ILE:HG22	2.13	0.48
1:k:143:LEU:O	1:k:147:ILE:HG22	2.13	0.48
1:m:205:VAL:O	1:m:209:LEU:HD13	2.13	0.48
1:n:143:LEU:O	1:n:147:ILE:HG22	2.13	0.48
1:n:202:GLN:HA	1:n:205:VAL:HG12	1.94	0.48
1:q:205:VAL:O	1:q:209:LEU:HD13	2.13	0.48
1:t:209:LEU:O	1:t:213:LYS:N	2.41	0.48
1:v:143:LEU:O	1:v:147:ILE:HG22	2.13	0.48
1:y:160:ASP:OD1	1:y:161:ASN:N	2.42	0.48
1:0:143:LEU:O	1:0:147:ILE:HG22	2.13	0.48
1:3:68:ALA:O	1:3:72:TYR:N	2.45	0.48
1:3:200:GLU:O	1:3:204:ALA:N	2.34	0.48
1:G:143:LEU:O	1:G:147:ILE:HG22	2.13	0.48
1:G:209:LEU:C	1:G:209:LEU:HD23	2.38	0.48
1:H:202:GLN:HA	1:H:205:VAL:HG12	1.94	0.48
1:I:143:LEU:O	1:I:147:ILE:HG22	2.13	0.48
1:I:196:PHE:O	1:I:200:GLU:N	2.26	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:143:LEU:O	1:J:147:ILE:HG22	2.13	0.48
1:L:209:LEU:HD23	1:L:209:LEU:C	2.38	0.48
1:P:202:GLN:HA	1:P:205:VAL:HG12	1.94	0.48
1:Q:205:VAL:O	1:Q:209:LEU:HD13	2.14	0.48
1:T:202:GLN:HA	1:T:205:VAL:HG12	1.94	0.48
1:V:68:ALA:O	1:V:72:TYR:N	2.45	0.48
1:V:143:LEU:O	1:V:147:ILE:HG22	2.13	0.48
1:Y:209:LEU:O	1:Y:213:LYS:N	2.41	0.48
1:i:205:VAL:O	1:i:209:LEU:HD13	2.13	0.48
1:k:200:GLU:O	1:k:204:ALA:N	2.34	0.48
1:r:159:LEU:O	1:r:166:SER:OG	2.28	0.48
1:s:205:VAL:O	1:s:209:LEU:HD13	2.13	0.48
1:u:200:GLU:O	1:u:204:ALA:N	2.34	0.48
1:v:68:ALA:O	1:v:72:TYR:N	2.45	0.48
1:z:68:ALA:O	1:z:72:TYR:N	2.45	0.48
1:z:143:LEU:O	1:z:147:ILE:HG22	2.13	0.48
1:0:205:VAL:O	1:0:209:LEU:HD13	2.13	0.48
1:1:209:LEU:HD23	1:1:209:LEU:C	2.38	0.48
1:5:143:LEU:O	1:5:147:ILE:HG22	2.13	0.48
1:6:159:LEU:O	1:6:166:SER:OG	2.28	0.48
1:A:209:LEU:HD23	1:A:209:LEU:C	2.38	0.48
1:C:202:GLN:HA	1:C:205:VAL:HG12	1.94	0.48
1:E:159:LEU:O	1:E:166:SER:OG	2.28	0.48
1:H:143:LEU:O	1:H:147:ILE:HG22	2.13	0.48
1:I:202:GLN:HA	1:I:205:VAL:HG12	1.94	0.48
1:I:205:VAL:O	1:I:209:LEU:HD13	2.14	0.48
1:N:143:LEU:O	1:N:147:ILE:HG22	2.13	0.48
1:R:143:LEU:O	1:R:147:ILE:HG22	2.13	0.48
1:U:159:LEU:O	1:U:166:SER:OG	2.28	0.48
1:U:202:GLN:HA	1:U:205:VAL:HG12	1.94	0.48
1:U:209:LEU:C	1:U:209:LEU:HD23	2.38	0.48
1:a:209:LEU:HD23	1:a:209:LEU:C	2.38	0.48
1:b:202:GLN:HA	1:b:205:VAL:HG12	1.94	0.48
1:c:202:GLN:HA	1:c:205:VAL:HG12	1.94	0.48
1:g:143:LEU:O	1:g:147:ILE:HG22	2.13	0.48
1:h:202:GLN:HA	1:h:205:VAL:HG12	1.94	0.48
1:i:143:LEU:O	1:i:147:ILE:HG22	2.13	0.48
1:l:143:LEU:O	1:l:147:ILE:HG22	2.13	0.48
1:p:202:GLN:HA	1:p:205:VAL:HG12	1.94	0.48
1:q:209:LEU:HD23	1:q:209:LEU:C	2.38	0.48
1:s:209:LEU:O	1:s:213:LYS:N	2.41	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:s:209:LEU:HD23	1:s:209:LEU:C	2.38	0.48
1:t:200:GLU:O	1:t:204:ALA:N	2.34	0.48
1:w:205:VAL:O	1:w:209:LEU:HD13	2.14	0.48
1:y:202:GLN:HA	1:y:205:VAL:HG12	1.94	0.48
1:z:159:LEU:O	1:z:166:SER:OG	2.28	0.48
1:0:209:LEU:HD23	1:0:209:LEU:C	2.38	0.48
1:2:202:GLN:HA	1:2:205:VAL:HG12	1.94	0.48
1:4:205:VAL:O	1:4:209:LEU:HD13	2.14	0.48
1:5:209:LEU:HD23	1:5:209:LEU:C	2.38	0.48
1:B:200:GLU:O	1:B:204:ALA:N	2.34	0.48
1:B:205:VAL:O	1:B:209:LEU:HD13	2.13	0.48
1:C:143:LEU:O	1:C:147:ILE:HG22	2.13	0.48
1:E:205:VAL:O	1:E:209:LEU:HD13	2.13	0.48
1:F:72:TYR:O	1:F:76:GLN:N	2.44	0.48
1:I:209:LEU:HD23	1:I:209:LEU:C	2.38	0.48
1:L:202:GLN:HA	1:L:205:VAL:HG12	1.94	0.48
1:R:68:ALA:O	1:R:72:TYR:N	2.45	0.48
1:W:209:LEU:HD23	1:W:209:LEU:C	2.38	0.48
1:Y:202:GLN:HA	1:Y:205:VAL:HG12	1.94	0.48
1:a:196:PHE:O	1:a:200:GLU:N	2.26	0.48
1:a:205:VAL:O	1:a:209:LEU:HD13	2.13	0.48
1:e:205:VAL:O	1:e:209:LEU:HD13	2.13	0.48
1:f:143:LEU:O	1:f:147:ILE:HG22	2.13	0.48
1:h:143:LEU:O	1:h:147:ILE:HG22	2.13	0.48
1:i:209:LEU:HD23	1:i:209:LEU:C	2.38	0.48
1:o:209:LEU:HD23	1:o:209:LEU:C	2.38	0.48
1:t:209:LEU:HD23	1:t:209:LEU:C	2.38	0.48
1:u:205:VAL:O	1:u:209:LEU:HD13	2.13	0.48
1:w:209:LEU:HD23	1:w:209:LEU:C	2.38	0.48
1:1:72:TYR:O	1:1:76:GLN:N	2.43	0.48
1:2:68:ALA:O	1:2:72:TYR:N	2.45	0.48
1:4:209:LEU:HD23	1:4:209:LEU:C	2.38	0.48
1:6:202:GLN:HA	1:6:205:VAL:HG12	1.94	0.48
1:A:205:VAL:O	1:A:209:LEU:HD13	2.13	0.48
1:O:205:VAL:O	1:O:209:LEU:HD13	2.13	0.48
1:R:205:VAL:O	1:R:209:LEU:HD13	2.13	0.48
1:S:159:LEU:O	1:S:166:SER:OG	2.28	0.48
1:S:205:VAL:O	1:S:209:LEU:HD13	2.14	0.48
1:W:205:VAL:O	1:W:209:LEU:HD13	2.14	0.48
1:X:205:VAL:O	1:X:209:LEU:HD13	2.13	0.48
1:b:205:VAL:O	1:b:209:LEU:HD13	2.13	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:143:LEU:O	1:c:147:ILE:HG22	2.13	0.48
1:j:205:VAL:O	1:j:209:LEU:HD13	2.13	0.48
1:l:202:GLN:HA	1:l:205:VAL:HG12	1.94	0.48
1:m:143:LEU:O	1:m:147:ILE:HG22	2.13	0.48
1:r:209:LEU:C	1:r:209:LEU:HD23	2.38	0.48
1:1:143:LEU:O	1:1:147:ILE:HG22	2.13	0.48
1:F:209:LEU:HD23	1:F:209:LEU:C	2.38	0.48
1:H:68:ALA:O	1:H:72:TYR:N	2.45	0.48
1:M:143:LEU:O	1:M:147:ILE:HG22	2.13	0.48
1:T:205:VAL:O	1:T:209:LEU:HD13	2.14	0.48
1:U:205:VAL:O	1:U:209:LEU:HD13	2.14	0.48
1:V:170:ARG:O	1:V:173:THR:OG1	2.26	0.48
1:W:200:GLU:O	1:W:204:ALA:N	2.34	0.48
1:Z:143:LEU:O	1:Z:147:ILE:HG22	2.13	0.48
1:Z:159:LEU:O	1:Z:166:SER:OG	2.28	0.48
1:g:202:GLN:HA	1:g:205:VAL:HG12	1.94	0.48
1:j:209:LEU:C	1:j:209:LEU:HD23	2.38	0.48
1:o:205:VAL:O	1:o:209:LEU:HD13	2.14	0.48
1:t:205:VAL:O	1:t:209:LEU:HD13	2.13	0.48
1:1:205:VAL:O	1:1:209:LEU:HD13	2.13	0.48
1:2:143:LEU:O	1:2:147:ILE:HG22	2.13	0.48
1:3:143:LEU:O	1:3:147:ILE:HG22	2.13	0.48
1:6:143:LEU:O	1:6:147:ILE:HG22	2.13	0.48
1:7:202:GLN:HA	1:7:205:VAL:HG12	1.94	0.48
1:C:159:LEU:O	1:C:166:SER:OG	2.28	0.48
1:D:143:LEU:O	1:D:147:ILE:HG22	2.13	0.48
1:G:209:LEU:O	1:G:213:LYS:N	2.41	0.48
1:J:159:LEU:O	1:J:166:SER:OG	2.28	0.48
1:L:68:ALA:O	1:L:72:TYR:N	2.45	0.48
1:N:209:LEU:HD23	1:N:209:LEU:C	2.38	0.48
1:O:209:LEU:C	1:O:209:LEU:HD23	2.38	0.48
1:Q:68:ALA:O	1:Q:72:TYR:N	2.45	0.48
1:S:209:LEU:HD23	1:S:209:LEU:C	2.38	0.48
1:Z:209:LEU:C	1:Z:209:LEU:HD23	2.38	0.48
1:b:143:LEU:O	1:b:147:ILE:HG22	2.13	0.48
1:e:209:LEU:C	1:e:209:LEU:HD23	2.38	0.48
1:i:159:LEU:O	1:i:166:SER:OG	2.28	0.48
1:p:68:ALA:O	1:p:72:TYR:N	2.45	0.48
1:r:200:GLU:O	1:r:204:ALA:N	2.34	0.48
1:r:205:VAL:O	1:r:209:LEU:HD13	2.13	0.48
1:t:202:GLN:HA	1:t:205:VAL:HG12	1.94	0.48

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:u:68:ALA:O	1:u:72:TYR:N	2.45	0.48
1:u:202:GLN:HA	1:u:205:VAL:HG12	1.94	0.48
1:x:205:VAL:O	1:x:209:LEU:HD13	2.14	0.48
1:4:159:LEU:O	1:4:166:SER:OG	2.28	0.48
1:B:143:LEU:O	1:B:147:ILE:HG22	2.13	0.48
1:B:209:LEU:C	1:B:209:LEU:HD23	2.38	0.48
1:D:202:GLN:HA	1:D:205:VAL:HG12	1.94	0.48
1:F:205:VAL:O	1:F:209:LEU:HD13	2.14	0.48
1:J:205:VAL:O	1:J:209:LEU:HD13	2.14	0.48
1:P:68:ALA:O	1:P:72:TYR:N	2.45	0.48
1:P:205:VAL:O	1:P:209:LEU:HD13	2.14	0.48
1:X:143:LEU:O	1:X:147:ILE:HG22	2.13	0.48
1:Y:143:LEU:O	1:Y:147:ILE:HG22	2.13	0.48
1:Z:68:ALA:O	1:Z:72:TYR:N	2.45	0.48
1:f:205:VAL:O	1:f:209:LEU:HD13	2.13	0.48
1:i:68:ALA:O	1:i:72:TYR:N	2.45	0.48
1:l:200:GLU:O	1:l:204:ALA:N	2.34	0.48
1:q:143:LEU:O	1:q:147:ILE:HG22	2.13	0.48
1:x:143:LEU:O	1:x:147:ILE:HG22	2.13	0.48
1:3:196:PHE:O	1:3:200:GLU:N	2.26	0.48
1:5:205:VAL:O	1:5:209:LEU:HD13	2.13	0.48
1:7:143:LEU:O	1:7:147:ILE:HG22	2.13	0.48
1:L:143:LEU:O	1:L:147:ILE:HG22	2.13	0.48
1:Q:143:LEU:O	1:Q:147:ILE:HG22	2.13	0.48
1:d:143:LEU:O	1:d:147:ILE:HG22	2.13	0.48
1:d:159:LEU:O	1:d:166:SER:OG	2.28	0.48
1:p:205:VAL:O	1:p:209:LEU:HD13	2.14	0.48
1:3:72:TYR:O	1:3:76:GLN:N	2.43	0.48
1:4:68:ALA:O	1:4:72:TYR:N	2.45	0.48
1:A:68:ALA:O	1:A:72:TYR:N	2.45	0.48
1:K:205:VAL:O	1:K:209:LEU:HD13	2.13	0.48
1:L:205:VAL:O	1:L:209:LEU:HD13	2.14	0.48
1:Y:205:VAL:O	1:Y:209:LEU:HD13	2.14	0.48
1:e:68:ALA:O	1:e:72:TYR:N	2.45	0.48
1:l:205:VAL:O	1:l:209:LEU:HD13	2.14	0.48
1:u:72:TYR:O	1:u:76:GLN:N	2.44	0.48
1:u:143:LEU:O	1:u:147:ILE:HG22	2.13	0.48
1:v:205:VAL:O	1:v:209:LEU:HD13	2.14	0.48
1:y:205:VAL:O	1:y:209:LEU:HD13	2.13	0.48
1:U:143:LEU:O	1:U:147:ILE:HG22	2.13	0.47
1:k:205:VAL:O	1:k:209:LEU:HD13	2.14	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:l:68:ALA:O	1:l:72:TYR:N	2.45	0.47
1:s:72:TYR:O	1:s:76:GLN:N	2.44	0.47
1:y:143:LEU:O	1:y:147:ILE:HG22	2.13	0.47
1:7:205:VAL:O	1:7:209:LEU:HD13	2.14	0.47
1:A:159:LEU:O	1:A:166:SER:OG	2.28	0.47
1:V:205:VAL:O	1:V:209:LEU:HD13	2.13	0.47
1:p:143:LEU:O	1:p:147:ILE:HG22	2.13	0.47
1:t:68:ALA:O	1:t:72:TYR:N	2.45	0.47
1:t:143:LEU:O	1:t:147:ILE:HG22	2.13	0.47
1:v:209:LEU:HD23	1:v:209:LEU:C	2.38	0.47
1:G:72:TYR:O	1:G:76:GLN:N	2.44	0.47
1:R:209:LEU:C	1:R:209:LEU:HD23	2.38	0.47
1:T:143:LEU:O	1:T:147:ILE:HG22	2.13	0.47
1:a:68:ALA:O	1:a:72:TYR:N	2.45	0.47
1:n:209:LEU:HD23	1:n:209:LEU:C	2.38	0.47
1:r:68:ALA:O	1:r:72:TYR:N	2.45	0.47
1:2:205:VAL:O	1:2:209:LEU:HD13	2.13	0.47
1:3:205:VAL:O	1:3:209:LEU:HD13	2.14	0.47
1:G:205:VAL:O	1:G:209:LEU:HD13	2.13	0.47
1:H:205:VAL:O	1:H:209:LEU:HD13	2.14	0.47
1:N:205:VAL:O	1:N:209:LEU:HD13	2.14	0.47
1:c:68:ALA:O	1:c:72:TYR:N	2.45	0.47
1:h:205:VAL:O	1:h:209:LEU:HD13	2.14	0.47
1:m:159:LEU:O	1:m:166:SER:OG	2.28	0.47
1:n:205:VAL:O	1:n:209:LEU:HD13	2.13	0.47
1:p:209:LEU:O	1:p:213:LYS:N	2.41	0.47
1:v:159:LEU:O	1:v:166:SER:OG	2.28	0.47
1:6:200:GLU:O	1:6:204:ALA:N	2.34	0.47
1:E:68:ALA:O	1:E:72:TYR:N	2.45	0.47
1:Z:205:VAL:O	1:Z:209:LEU:HD13	2.14	0.47
1:g:205:VAL:O	1:g:209:LEU:HD13	2.13	0.47
1:j:72:TYR:O	1:j:76:GLN:N	2.44	0.47
1:C:68:ALA:O	1:C:72:TYR:N	2.45	0.47
1:D:205:VAL:O	1:D:209:LEU:HD13	2.14	0.47
1:D:209:LEU:O	1:D:213:LYS:N	2.41	0.47
1:G:68:ALA:O	1:G:72:TYR:N	2.45	0.47
1:P:143:LEU:O	1:P:147:ILE:HG22	2.13	0.47
1:d:205:VAL:O	1:d:209:LEU:HD13	2.13	0.47
1:f:209:LEU:HD23	1:f:209:LEU:C	2.38	0.47
1:g:68:ALA:O	1:g:72:TYR:N	2.45	0.47
1:l:72:TYR:O	1:l:76:GLN:N	2.44	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:209:LEU:HD23	1:O:210:ALA:N	2.30	0.47
1:5:209:LEU:HD23	1:5:210:ALA:N	2.30	0.47
1:7:170:ARG:O	1:7:173:THR:OG1	2.26	0.47
1:A:209:LEU:HD23	1:A:210:ALA:N	2.30	0.47
1:D:200:GLU:O	1:D:204:ALA:N	2.34	0.47
1:F:209:LEU:HD23	1:F:210:ALA:N	2.30	0.47
1:I:209:LEU:O	1:I:213:LYS:N	2.41	0.47
1:J:209:LEU:C	1:J:209:LEU:HD23	2.38	0.47
1:K:200:GLU:O	1:K:204:ALA:N	2.34	0.47
1:N:209:LEU:HD23	1:N:210:ALA:N	2.30	0.47
1:S:209:LEU:HD23	1:S:210:ALA:N	2.30	0.47
1:Z:209:LEU:O	1:Z:213:LYS:N	2.41	0.47
1:a:72:TYR:O	1:a:76:GLN:N	2.44	0.47
1:c:205:VAL:O	1:c:209:LEU:HD13	2.14	0.47
1:e:209:LEU:HD23	1:e:210:ALA:N	2.30	0.47
1:i:72:TYR:O	1:i:76:GLN:N	2.44	0.47
1:j:209:LEU:HD23	1:j:210:ALA:N	2.30	0.47
1:n:68:ALA:O	1:n:72:TYR:N	2.45	0.47
1:o:209:LEU:HD23	1:o:210:ALA:N	2.30	0.47
1:s:209:LEU:HD23	1:s:210:ALA:N	2.30	0.47
1:z:205:VAL:O	1:z:209:LEU:HD13	2.13	0.47
1:C:205:VAL:O	1:C:209:LEU:HD13	2.14	0.47
1:J:68:ALA:O	1:J:72:TYR:N	2.45	0.47
1:K:209:LEU:HD23	1:K:210:ALA:N	2.30	0.47
1:O:209:LEU:HD23	1:O:210:ALA:N	2.30	0.47
1:c:159:LEU:O	1:c:166:SER:OG	2.28	0.47
1:q:209:LEU:O	1:q:213:LYS:N	2.41	0.47
1:t:72:TYR:O	1:t:76:GLN:N	2.44	0.47
1:w:209:LEU:HD23	1:w:210:ALA:N	2.30	0.47
1:5:201:GLU:O	1:5:205:VAL:HG12	2.15	0.47
1:6:205:VAL:O	1:6:209:LEU:HD13	2.14	0.47
1:B:209:LEU:HD23	1:B:210:ALA:N	2.30	0.47
1:J:201:GLU:O	1:J:205:VAL:HG12	2.15	0.47
1:W:209:LEU:HD23	1:W:210:ALA:N	2.30	0.47
1:b:209:LEU:HD23	1:b:210:ALA:N	2.30	0.47
1:e:201:GLU:O	1:e:205:VAL:HG12	2.15	0.47
1:n:201:GLU:O	1:n:205:VAL:HG12	2.15	0.47
1:v:209:LEU:HD23	1:v:210:ALA:N	2.30	0.47
1:w:201:GLU:O	1:w:205:VAL:HG12	2.15	0.47
1:O:196:PHE:O	1:O:200:GLU:N	2.26	0.47
1:6:68:ALA:O	1:6:72:TYR:N	2.45	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:GLU:O	1:A:205:VAL:HG12	2.15	0.47
1:N:68:ALA:O	1:N:72:TYR:N	2.45	0.47
1:R:200:GLU:O	1:R:204:ALA:N	2.34	0.47
1:T:200:GLU:O	1:T:204:ALA:N	2.34	0.47
1:V:201:GLU:O	1:V:205:VAL:HG12	2.15	0.47
1:X:209:LEU:HD23	1:X:210:ALA:N	2.30	0.47
1:d:72:TYR:O	1:d:76:GLN:N	2.44	0.47
1:k:68:ALA:O	1:k:72:TYR:N	2.45	0.47
1:r:209:LEU:HD23	1:r:210:ALA:N	2.30	0.47
1:z:201:GLU:O	1:z:205:VAL:HG12	2.15	0.47
1:0:68:ALA:O	1:0:72:TYR:N	2.45	0.46
1:B:201:GLU:O	1:B:205:VAL:HG12	2.15	0.46
1:J:209:LEU:HD23	1:J:210:ALA:N	2.30	0.46
1:R:72:TYR:O	1:R:76:GLN:N	2.43	0.46
1:R:209:LEU:HD23	1:R:210:ALA:N	2.30	0.46
1:T:68:ALA:O	1:T:72:TYR:N	2.45	0.46
1:a:209:LEU:HD23	1:a:210:ALA:N	2.30	0.46
1:j:68:ALA:O	1:j:72:TYR:N	2.45	0.46
1:k:209:LEU:HD23	1:k:210:ALA:N	2.30	0.46
1:n:209:LEU:HD23	1:n:210:ALA:N	2.30	0.46
1:4:209:LEU:HD23	1:4:210:ALA:N	2.30	0.46
1:H:72:TYR:O	1:H:76:GLN:N	2.44	0.46
1:I:72:TYR:O	1:I:76:GLN:N	2.44	0.46
1:M:201:GLU:O	1:M:205:VAL:HG12	2.15	0.46
1:N:201:GLU:O	1:N:205:VAL:HG12	2.15	0.46
1:R:201:GLU:O	1:R:205:VAL:HG12	2.15	0.46
1:S:201:GLU:O	1:S:205:VAL:HG12	2.16	0.46
1:U:72:TYR:O	1:U:76:GLN:N	2.44	0.46
1:W:201:GLU:O	1:W:205:VAL:HG12	2.15	0.46
1:b:201:GLU:O	1:b:205:VAL:HG12	2.15	0.46
1:d:200:GLU:O	1:d:204:ALA:N	2.34	0.46
1:j:54:PHE:HE1	1:j:108:LEU:HD21	1.81	0.46
1:x:209:LEU:HD23	1:x:210:ALA:N	2.30	0.46
1:A:54:PHE:HE1	1:A:108:LEU:HD21	1.81	0.46
1:E:201:GLU:O	1:E:205:VAL:HG12	2.15	0.46
1:F:201:GLU:O	1:F:205:VAL:HG12	2.15	0.46
1:G:209:LEU:HD23	1:G:210:ALA:N	2.30	0.46
1:I:209:LEU:HD23	1:I:210:ALA:N	2.30	0.46
1:U:209:LEU:O	1:U:213:LYS:N	2.41	0.46
1:V:209:LEU:HD23	1:V:210:ALA:N	2.30	0.46
1:X:68:ALA:O	1:X:72:TYR:N	2.45	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:n:195:LYS:O	1:n:199:TRP:N	2.34	0.46
1:v:200:GLU:O	1:v:204:ALA:N	2.34	0.46
1:0:201:GLU:O	1:0:205:VAL:HG12	2.15	0.46
1:1:68:ALA:O	1:1:72:TYR:N	2.45	0.46
1:7:209:LEU:O	1:7:213:LYS:N	2.41	0.46
1:F:54:PHE:HE1	1:F:108:LEU:HD21	1.81	0.46
1:F:68:ALA:O	1:F:72:TYR:N	2.45	0.46
1:K:201:GLU:O	1:K:205:VAL:HG12	2.15	0.46
1:O:54:PHE:HE1	1:O:108:LEU:HD21	1.81	0.46
1:U:200:GLU:O	1:U:204:ALA:N	2.34	0.46
1:a:54:PHE:HE1	1:a:108:LEU:HD21	1.81	0.46
1:f:201:GLU:O	1:f:205:VAL:HG12	2.15	0.46
1:q:201:GLU:O	1:q:205:VAL:HG12	2.15	0.46
1:r:201:GLU:O	1:r:205:VAL:HG12	2.15	0.46
1:s:68:ALA:O	1:s:72:TYR:N	2.45	0.46
1:z:209:LEU:HD23	1:z:210:ALA:N	2.30	0.46
1:0:54:PHE:HE1	1:0:108:LEU:HD21	1.81	0.46
1:4:54:PHE:HE1	1:4:108:LEU:HD21	1.81	0.46
1:4:201:GLU:O	1:4:205:VAL:HG12	2.16	0.46
1:D:170:ARG:O	1:D:173:THR:OG1	2.26	0.46
1:J:54:PHE:HE1	1:J:108:LEU:HD21	1.81	0.46
1:S:68:ALA:O	1:S:72:TYR:N	2.45	0.46
1:i:209:LEU:HD23	1:i:210:ALA:N	2.30	0.46
1:j:201:GLU:O	1:j:205:VAL:HG12	2.15	0.46
1:k:201:GLU:O	1:k:205:VAL:HG12	2.15	0.46
1:m:72:TYR:O	1:m:76:GLN:N	2.44	0.46
1:o:54:PHE:HE1	1:o:108:LEU:HD21	1.81	0.46
1:s:54:PHE:HE1	1:s:108:LEU:HD21	1.81	0.46
1:v:54:PHE:HE1	1:v:108:LEU:HD21	1.81	0.46
1:3:209:LEU:HD23	1:3:210:ALA:N	2.30	0.46
1:C:209:LEU:HD23	1:C:210:ALA:N	2.30	0.46
1:X:54:PHE:HE1	1:X:108:LEU:HD21	1.81	0.46
1:Z:209:LEU:HD23	1:Z:210:ALA:N	2.30	0.46
1:a:201:GLU:O	1:a:205:VAL:HG12	2.15	0.46
1:b:68:ALA:O	1:b:72:TYR:N	2.45	0.46
1:c:72:TYR:O	1:c:76:GLN:N	2.43	0.46
1:f:209:LEU:HD23	1:f:210:ALA:N	2.30	0.46
1:g:209:LEU:HD23	1:g:210:ALA:N	2.30	0.46
1:k:72:TYR:O	1:k:76:GLN:N	2.44	0.46
1:o:201:GLU:O	1:o:205:VAL:HG12	2.15	0.46
1:v:201:GLU:O	1:v:205:VAL:HG12	2.15	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:v:209:LEU:O	1:v:213:LYS:N	2.41	0.46
1:w:68:ALA:O	1:w:72:TYR:N	2.45	0.46
1:7:72:TYR:O	1:7:76:GLN:N	2.44	0.46
1:O:68:ALA:O	1:O:72:TYR:N	2.45	0.46
1:R:54:PHE:HE1	1:R:108:LEU:HD21	1.81	0.46
1:e:54:PHE:HE1	1:e:108:LEU:HD21	1.81	0.46
1:e:209:LEU:O	1:e:213:LYS:N	2.41	0.46
1:m:201:GLU:O	1:m:205:VAL:HG12	2.15	0.46
1:s:201:GLU:O	1:s:205:VAL:HG12	2.16	0.46
1:t:209:LEU:HD23	1:t:210:ALA:N	2.30	0.46
1:x:54:PHE:HE1	1:x:108:LEU:HD21	1.81	0.46
1:5:68:ALA:O	1:5:72:TYR:N	2.45	0.46
1:D:201:GLU:O	1:D:205:VAL:HG12	2.15	0.46
1:L:54:PHE:HE1	1:L:108:LEU:HD21	1.81	0.46
1:N:209:LEU:O	1:N:213:LYS:N	2.41	0.46
1:P:209:LEU:HD23	1:P:210:ALA:N	2.30	0.46
1:V:54:PHE:HE1	1:V:108:LEU:HD21	1.81	0.46
1:W:68:ALA:O	1:W:72:TYR:N	2.45	0.46
1:Z:201:GLU:O	1:Z:205:VAL:HG12	2.15	0.46
1:i:201:GLU:O	1:i:205:VAL:HG12	2.16	0.46
1:l:54:PHE:HE1	1:l:108:LEU:HD21	1.81	0.46
1:1:209:LEU:HD23	1:1:210:ALA:N	2.30	0.46
1:4:72:TYR:O	1:4:76:GLN:N	2.44	0.46
1:O:201:GLU:O	1:O:205:VAL:HG12	2.15	0.46
1:Q:54:PHE:HE1	1:Q:108:LEU:HD21	1.81	0.46
1:S:54:PHE:HE1	1:S:108:LEU:HD21	1.81	0.46
1:d:209:LEU:HD23	1:d:210:ALA:N	2.30	0.46
1:f:54:PHE:HE1	1:f:108:LEU:HD21	1.81	0.46
1:h:201:GLU:O	1:h:205:VAL:HG12	2.15	0.46
1:q:209:LEU:HD23	1:q:210:ALA:N	2.30	0.46
1:t:201:GLU:O	1:t:205:VAL:HG12	2.15	0.46
1:4:195:LYS:O	1:4:199:TRP:N	2.34	0.46
1:6:209:LEU:HD23	1:6:210:ALA:N	2.30	0.46
1:7:209:LEU:HD23	1:7:210:ALA:N	2.30	0.46
1:D:209:LEU:HD23	1:D:210:ALA:N	2.30	0.46
1:E:209:LEU:HD23	1:E:210:ALA:N	2.30	0.46
1:G:201:GLU:O	1:G:205:VAL:HG12	2.16	0.46
1:G:208:THR:O	1:G:212:MET:HG2	2.16	0.46
1:K:68:ALA:O	1:K:72:TYR:N	2.45	0.46
1:K:208:THR:O	1:K:212:MET:HG2	2.17	0.46
1:L:72:TYR:O	1:L:76:GLN:N	2.44	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:208:THR:O	1:O:212:MET:HG2	2.17	0.46
1:P:208:THR:O	1:P:212:MET:HG2	2.16	0.46
1:T:201:GLU:O	1:T:205:VAL:HG12	2.15	0.46
1:U:209:LEU:HD23	1:U:210:ALA:N	2.30	0.46
1:f:200:GLU:O	1:f:204:ALA:N	2.34	0.46
1:h:209:LEU:HD23	1:h:210:ALA:N	2.30	0.46
1:l:209:LEU:HD23	1:l:210:ALA:N	2.30	0.46
1:p:54:PHE:HE1	1:p:108:LEU:HD21	1.81	0.46
1:x:68:ALA:O	1:x:72:TYR:N	2.45	0.46
1:1:54:PHE:HE1	1:1:108:LEU:HD21	1.81	0.45
1:2:201:GLU:O	1:2:205:VAL:HG12	2.15	0.45
1:7:201:GLU:O	1:7:205:VAL:HG12	2.15	0.45
1:F:208:THR:O	1:F:212:MET:HG2	2.16	0.45
1:H:209:LEU:HD23	1:H:210:ALA:N	2.30	0.45
1:M:54:PHE:HE1	1:M:108:LEU:HD21	1.81	0.45
1:Q:201:GLU:O	1:Q:205:VAL:HG12	2.15	0.45
1:S:208:THR:O	1:S:212:MET:HG2	2.17	0.45
1:T:208:THR:O	1:T:212:MET:HG2	2.17	0.45
1:c:209:LEU:HD23	1:c:210:ALA:N	2.30	0.45
1:m:209:LEU:HD23	1:m:210:ALA:N	2.30	0.45
1:q:54:PHE:HE1	1:q:108:LEU:HD21	1.81	0.45
1:r:54:PHE:HE1	1:r:108:LEU:HD21	1.81	0.45
1:1:201:GLU:O	1:1:205:VAL:HG12	2.15	0.45
1:3:201:GLU:O	1:3:205:VAL:HG12	2.15	0.45
1:6:208:THR:O	1:6:212:MET:HG2	2.16	0.45
1:C:54:PHE:HE1	1:C:108:LEU:HD21	1.81	0.45
1:H:54:PHE:HE1	1:H:108:LEU:HD21	1.81	0.45
1:H:201:GLU:O	1:H:205:VAL:HG12	2.15	0.45
1:I:201:GLU:O	1:I:205:VAL:HG12	2.15	0.45
1:J:208:THR:O	1:J:212:MET:HG2	2.16	0.45
1:L:201:GLU:O	1:L:205:VAL:HG12	2.15	0.45
1:P:201:GLU:O	1:P:205:VAL:HG12	2.15	0.45
1:T:54:PHE:HE1	1:T:108:LEU:HD21	1.81	0.45
1:T:209:LEU:HD23	1:T:210:ALA:N	2.30	0.45
1:Y:201:GLU:O	1:Y:205:VAL:HG12	2.15	0.45
1:l:201:GLU:O	1:l:205:VAL:HG12	2.15	0.45
1:m:54:PHE:HE1	1:m:108:LEU:HD21	1.81	0.45
1:m:200:GLU:O	1:m:204:ALA:N	2.34	0.45
1:p:201:GLU:O	1:p:205:VAL:HG12	2.15	0.45
1:p:209:LEU:HD23	1:p:210:ALA:N	2.30	0.45
1:r:72:TYR:O	1:r:76:GLN:N	2.44	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:u:54:PHE:HE1	1:u:108:LEU:HD21	1.81	0.45
1:x:201:GLU:O	1:x:205:VAL:HG12	2.15	0.45
1:y:72:TYR:O	1:y:76:GLN:N	2.44	0.45
1:0:208:THR:O	1:0:212:MET:HG2	2.16	0.45
1:5:54:PHE:HE1	1:5:108:LEU:HD21	1.81	0.45
1:5:208:THR:O	1:5:212:MET:HG2	2.17	0.45
1:6:54:PHE:HE1	1:6:108:LEU:HD21	1.81	0.45
1:B:54:PHE:HE1	1:B:108:LEU:HD21	1.81	0.45
1:B:208:THR:O	1:B:212:MET:HG2	2.16	0.45
1:C:208:THR:O	1:C:212:MET:HG2	2.17	0.45
1:E:54:PHE:HE1	1:E:108:LEU:HD21	1.81	0.45
1:L:200:GLU:O	1:L:204:ALA:N	2.34	0.45
1:L:208:THR:O	1:L:212:MET:HG2	2.17	0.45
1:L:209:LEU:HD23	1:L:210:ALA:N	2.30	0.45
1:M:209:LEU:HD23	1:M:210:ALA:N	2.30	0.45
1:N:54:PHE:HE1	1:N:108:LEU:HD21	1.81	0.45
1:U:54:PHE:HE1	1:U:108:LEU:HD21	1.81	0.45
1:X:208:THR:O	1:X:212:MET:HG2	2.17	0.45
1:b:72:TYR:O	1:b:76:GLN:N	2.44	0.45
1:c:54:PHE:HE1	1:c:108:LEU:HD21	1.81	0.45
1:d:201:GLU:O	1:d:205:VAL:HG12	2.15	0.45
1:n:54:PHE:HE1	1:n:108:LEU:HD21	1.81	0.45
1:0:200:GLU:O	1:0:204:ALA:N	2.34	0.45
1:1:208:THR:O	1:1:212:MET:HG2	2.17	0.45
1:2:209:LEU:HD23	1:2:210:ALA:N	2.30	0.45
1:B:68:ALA:O	1:B:72:TYR:N	2.45	0.45
1:K:54:PHE:HE1	1:K:108:LEU:HD21	1.81	0.45
1:P:54:PHE:HE1	1:P:108:LEU:HD21	1.81	0.45
1:U:208:THR:O	1:U:212:MET:HG2	2.16	0.45
1:X:201:GLU:O	1:X:205:VAL:HG12	2.15	0.45
1:Y:208:THR:O	1:Y:212:MET:HG2	2.17	0.45
1:f:68:ALA:O	1:f:72:TYR:N	2.45	0.45
1:h:54:PHE:HE1	1:h:108:LEU:HD21	1.81	0.45
1:l:209:LEU:O	1:l:213:LYS:N	2.41	0.45
1:y:209:LEU:HD23	1:y:210:ALA:N	2.30	0.45
1:2:54:PHE:HE1	1:2:108:LEU:HD21	1.81	0.45
1:4:208:THR:O	1:4:212:MET:HG2	2.17	0.45
1:6:72:TYR:O	1:6:76:GLN:N	2.44	0.45
1:I:208:THR:O	1:I:212:MET:HG2	2.16	0.45
1:W:54:PHE:HE1	1:W:108:LEU:HD21	1.81	0.45
1:W:208:THR:O	1:W:212:MET:HG2	2.17	0.45

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:209:LEU:HD23	1:Y:210:ALA:N	2.30	0.45
1:b:208:THR:O	1:b:212:MET:HG2	2.17	0.45
1:g:54:PHE:HE1	1:g:108:LEU:HD21	1.81	0.45
1:z:54:PHE:HE1	1:z:108:LEU:HD21	1.81	0.45
1:2:208:THR:O	1:2:212:MET:HG2	2.17	0.45
1:A:208:THR:O	1:A:212:MET:HG2	2.17	0.45
1:G:54:PHE:HE1	1:G:108:LEU:HD21	1.81	0.45
1:I:54:PHE:HE1	1:I:108:LEU:HD21	1.81	0.45
1:M:195:LYS:O	1:M:199:TRP:N	2.34	0.45
1:N:72:TYR:O	1:N:76:GLN:N	2.44	0.45
1:b:54:PHE:HE1	1:b:108:LEU:HD21	1.81	0.45
1:c:201:GLU:O	1:c:205:VAL:HG12	2.15	0.45
1:c:208:THR:O	1:c:212:MET:HG2	2.17	0.45
1:o:68:ALA:O	1:o:72:TYR:N	2.45	0.45
1:t:54:PHE:HE1	1:t:108:LEU:HD21	1.81	0.45
1:u:201:GLU:O	1:u:205:VAL:HG12	2.15	0.45
1:v:72:TYR:O	1:v:76:GLN:N	2.44	0.45
1:x:208:THR:O	1:x:212:MET:HG2	2.17	0.45
1:7:54:PHE:HE1	1:7:108:LEU:HD21	1.81	0.45
1:A:195:LYS:O	1:A:199:TRP:N	2.34	0.45
1:M:208:THR:O	1:M:212:MET:HG2	2.16	0.45
1:Z:208:THR:O	1:Z:212:MET:HG2	2.16	0.45
1:d:208:THR:O	1:d:212:MET:HG2	2.17	0.45
1:v:208:THR:O	1:v:212:MET:HG2	2.17	0.45
1:y:201:GLU:O	1:y:205:VAL:HG12	2.15	0.45
1:7:200:GLU:O	1:7:204:ALA:N	2.34	0.45
1:H:208:THR:O	1:H:212:MET:HG2	2.16	0.45
1:N:208:THR:O	1:N:212:MET:HG2	2.17	0.45
1:Q:209:LEU:HD23	1:Q:210:ALA:N	2.30	0.45
1:f:208:THR:O	1:f:212:MET:HG2	2.17	0.45
1:g:201:GLU:O	1:g:205:VAL:HG12	2.15	0.45
1:h:208:THR:O	1:h:212:MET:HG2	2.17	0.45
1:w:208:THR:O	1:w:212:MET:HG2	2.17	0.45
1:z:195:LYS:O	1:z:199:TRP:N	2.34	0.45
1:6:201:GLU:O	1:6:205:VAL:HG12	2.15	0.45
1:C:201:GLU:O	1:C:205:VAL:HG12	2.15	0.45
1:D:72:TYR:O	1:D:76:GLN:N	2.44	0.45
1:E:208:THR:O	1:E:212:MET:HG2	2.17	0.45
1:S:72:TYR:O	1:S:76:GLN:N	2.44	0.45
1:h:195:LYS:O	1:h:199:TRP:N	2.34	0.45
1:o:159:LEU:O	1:o:166:SER:OG	2.28	0.45

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:t:208:THR:O	1:t:212:MET:HG2	2.16	0.45
1:z:208:THR:O	1:z:212:MET:HG2	2.17	0.45
1:T:72:TYR:O	1:T:76:GLN:N	2.44	0.45
1:U:201:GLU:O	1:U:205:VAL:HG12	2.15	0.45
1:V:200:GLU:O	1:V:204:ALA:N	2.34	0.45
1:W:170:ARG:O	1:W:173:THR:OG1	2.26	0.45
1:Z:54:PHE:HE1	1:Z:108:LEU:HD21	1.81	0.45
1:e:208:THR:O	1:e:212:MET:HG2	2.16	0.45
1:g:208:THR:O	1:g:212:MET:HG2	2.17	0.45
1:k:54:PHE:HE1	1:k:108:LEU:HD21	1.81	0.45
1:m:208:THR:O	1:m:212:MET:HG2	2.17	0.45
1:r:208:THR:O	1:r:212:MET:HG2	2.17	0.45
1:u:208:THR:O	1:u:212:MET:HG2	2.17	0.45
1:u:209:LEU:HD23	1:u:210:ALA:N	2.30	0.45
1:w:54:PHE:HE1	1:w:108:LEU:HD21	1.81	0.45
1:D:54:PHE:HE1	1:D:108:LEU:HD21	1.81	0.44
1:M:72:TYR:O	1:M:76:GLN:N	2.44	0.44
1:Q:208:THR:O	1:Q:212:MET:HG2	2.17	0.44
1:Y:54:PHE:HE1	1:Y:108:LEU:HD21	1.81	0.44
1:i:195:LYS:O	1:i:199:TRP:N	2.34	0.44
1:p:72:TYR:O	1:p:76:GLN:N	2.44	0.44
1:q:208:THR:O	1:q:212:MET:HG2	2.17	0.44
1:s:208:THR:O	1:s:212:MET:HG2	2.17	0.44
1:C:72:TYR:O	1:C:76:GLN:N	2.44	0.44
1:J:72:TYR:O	1:J:76:GLN:N	2.44	0.44
1:R:195:LYS:O	1:R:199:TRP:N	2.34	0.44
1:V:208:THR:O	1:V:212:MET:HG2	2.16	0.44
1:Z:170:ARG:O	1:Z:173:THR:OG1	2.26	0.44
1:d:54:PHE:HE1	1:d:108:LEU:HD21	1.81	0.44
1:i:54:PHE:HE1	1:i:108:LEU:HD21	1.81	0.44
1:k:208:THR:O	1:k:212:MET:HG2	2.16	0.44
1:l:208:THR:O	1:l:212:MET:HG2	2.17	0.44
1:p:159:LEU:O	1:p:166:SER:OG	2.28	0.44
1:y:54:PHE:HE1	1:y:108:LEU:HD21	1.81	0.44
1:i:208:THR:O	1:i:212:MET:HG2	2.17	0.44
1:3:54:PHE:HE1	1:3:108:LEU:HD21	1.81	0.44
1:F:200:GLU:O	1:F:204:ALA:N	2.34	0.44
1:J:195:LYS:O	1:J:199:TRP:N	2.34	0.44
1:a:208:THR:O	1:a:212:MET:HG2	2.17	0.44
1:n:208:THR:O	1:n:212:MET:HG2	2.16	0.44
1:o:208:THR:O	1:o:212:MET:HG2	2.17	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:y:208:THR:O	1:y:212:MET:HG2	2.17	0.44
1:3:208:THR:O	1:3:212:MET:HG2	2.17	0.44
1:D:208:THR:O	1:D:212:MET:HG2	2.17	0.44
1:j:208:THR:O	1:j:212:MET:HG2	2.17	0.44
1:5:72:TYR:O	1:5:76:GLN:N	2.44	0.44
1:R:208:THR:O	1:R:212:MET:HG2	2.17	0.44
1:e:200:GLU:O	1:e:204:ALA:N	2.34	0.44
1:m:209:LEU:O	1:m:213:LYS:N	2.41	0.44
1:p:208:THR:O	1:p:212:MET:HG2	2.17	0.44
1:z:170:ARG:O	1:z:173:THR:OG1	2.26	0.44
1:0:72:TYR:O	1:0:76:GLN:N	2.44	0.44
1:7:208:THR:O	1:7:212:MET:HG2	2.17	0.44
1:A:72:TYR:O	1:A:76:GLN:N	2.44	0.44
1:a:200:GLU:O	1:a:204:ALA:N	2.34	0.44
1:o:200:GLU:O	1:o:204:ALA:N	2.34	0.44
1:x:72:TYR:O	1:x:76:GLN:N	2.44	0.44
1:y:170:ARG:O	1:y:173:THR:OG1	2.26	0.44
1:V:72:TYR:O	1:V:76:GLN:N	2.44	0.43
1:W:72:TYR:O	1:W:76:GLN:N	2.44	0.43
1:h:72:TYR:O	1:h:76:GLN:N	2.44	0.43
1:j:159:LEU:O	1:j:166:SER:OG	2.28	0.43
1:q:72:TYR:O	1:q:76:GLN:N	2.44	0.43
1:T:108:LEU:HD23	1:T:108:LEU:C	2.44	0.43
1:r:108:LEU:C	1:r:108:LEU:HD23	2.44	0.43
1:4:108:LEU:C	1:4:108:LEU:HD23	2.44	0.43
1:K:72:TYR:O	1:K:76:GLN:N	2.44	0.43
1:a:195:LYS:O	1:a:199:TRP:N	2.34	0.43
1:q:170:ARG:O	1:q:173:THR:OG1	2.26	0.43
1:z:108:LEU:C	1:z:108:LEU:HD23	2.44	0.43
1:1:108:LEU:HD23	1:1:108:LEU:C	2.44	0.43
1:3:209:LEU:O	1:3:213:LYS:N	2.41	0.43
1:A:108:LEU:HD23	1:A:108:LEU:C	2.44	0.43
1:K:108:LEU:HD23	1:K:108:LEU:C	2.44	0.43
1:c:108:LEU:HD23	1:c:108:LEU:C	2.44	0.43
1:e:108:LEU:C	1:e:108:LEU:HD23	2.44	0.43
1:g:72:TYR:O	1:g:76:GLN:N	2.44	0.43
1:g:108:LEU:HD23	1:g:108:LEU:C	2.44	0.43
1:m:108:LEU:C	1:m:108:LEU:HD23	2.44	0.43
1:p:108:LEU:HD23	1:p:108:LEU:C	2.44	0.43
1:w:72:TYR:O	1:w:76:GLN:N	2.44	0.43
1:5:108:LEU:HD23	1:5:108:LEU:C	2.44	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:108:LEU:HD23	1:I:108:LEU:C	2.44	0.43
1:M:200:GLU:O	1:M:204:ALA:N	2.34	0.43
1:N:170:ARG:O	1:N:173:THR:OG1	2.26	0.43
1:Q:195:LYS:O	1:Q:199:TRP:N	2.34	0.43
1:w:108:LEU:HD23	1:w:108:LEU:C	2.44	0.43
1:7:108:LEU:C	1:7:108:LEU:HD23	2.44	0.43
1:B:108:LEU:C	1:B:108:LEU:HD23	2.44	0.43
1:D:108:LEU:HD23	1:D:108:LEU:C	2.44	0.43
1:N:108:LEU:HD23	1:N:108:LEU:C	2.44	0.43
1:V:108:LEU:HD23	1:V:108:LEU:C	2.44	0.43
1:Y:72:TYR:O	1:Y:76:GLN:N	2.44	0.43
1:a:159:LEU:O	1:a:166:SER:OG	2.28	0.43
1:j:108:LEU:C	1:j:108:LEU:HD23	2.44	0.43
1:l:108:LEU:HD23	1:l:108:LEU:C	2.44	0.43
1:y:108:LEU:HD23	1:y:108:LEU:C	2.44	0.43
1:A:43:LEU:HD22	1:E:149:ALA:HB2	2.01	0.43
1:B:72:TYR:O	1:B:76:GLN:N	2.44	0.43
1:F:108:LEU:HD23	1:F:108:LEU:C	2.44	0.43
1:G:108:LEU:C	1:G:108:LEU:HD23	2.44	0.43
1:Q:108:LEU:HD23	1:Q:108:LEU:C	2.44	0.43
1:X:108:LEU:HD23	1:X:108:LEU:C	2.44	0.43
1:u:108:LEU:C	1:u:108:LEU:HD23	2.44	0.43
1:x:200:GLU:O	1:x:204:ALA:N	2.34	0.43
1:z:72:TYR:O	1:z:76:GLN:N	2.44	0.43
1:2:108:LEU:HD23	1:2:108:LEU:C	2.44	0.43
1:A:150:GLN:HA	1:E:182:ARG:NH1	2.33	0.43
1:A:200:GLU:O	1:A:204:ALA:N	2.34	0.43
1:E:209:LEU:O	1:E:213:LYS:N	2.41	0.43
1:O:108:LEU:C	1:O:108:LEU:HD23	2.44	0.43
1:R:108:LEU:C	1:R:108:LEU:HD23	2.44	0.43
1:S:195:LYS:O	1:S:199:TRP:N	2.34	0.43
1:W:108:LEU:C	1:W:108:LEU:HD23	2.44	0.43
1:d:108:LEU:HD23	1:d:108:LEU:C	2.44	0.43
1:o:72:TYR:O	1:o:76:GLN:N	2.44	0.43
1:s:108:LEU:HD23	1:s:108:LEU:C	2.44	0.43
1:H:108:LEU:HD23	1:H:108:LEU:C	2.44	0.43
1:P:108:LEU:HD23	1:P:108:LEU:C	2.44	0.43
1:f:72:TYR:O	1:f:76:GLN:N	2.44	0.43
1:n:72:TYR:O	1:n:76:GLN:N	2.44	0.43
1:3:195:LYS:O	1:3:199:TRP:N	2.34	0.43
1:Q:209:LEU:O	1:Q:213:LYS:N	2.41	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:108:LEU:HD23	1:S:108:LEU:C	2.44	0.43
1:Z:108:LEU:C	1:Z:108:LEU:HD23	2.44	0.43
1:h:108:LEU:HD23	1:h:108:LEU:C	2.44	0.43
1:i:108:LEU:HD23	1:i:108:LEU:C	2.44	0.43
1:q:200:GLU:O	1:q:204:ALA:N	2.34	0.43
1:r:195:LYS:O	1:r:199:TRP:N	2.34	0.43
1:t:108:LEU:HD23	1:t:108:LEU:C	2.44	0.43
1:u:170:ARG:O	1:u:173:THR:OG1	2.26	0.43
1:J:108:LEU:C	1:J:108:LEU:HD23	2.44	0.42
1:o:108:LEU:HD23	1:o:108:LEU:C	2.44	0.42
1:O:200:GLU:O	1:O:204:ALA:N	2.34	0.42
1:T:159:LEU:O	1:T:166:SER:OG	2.28	0.42
1:a:108:LEU:HD23	1:a:108:LEU:C	2.44	0.42
1:Y:108:LEU:HD23	1:Y:108:LEU:C	2.44	0.42
1:f:108:LEU:HD23	1:f:108:LEU:C	2.44	0.42
1:j:195:LYS:O	1:j:199:TRP:N	2.34	0.42
1:q:108:LEU:HD23	1:q:108:LEU:C	2.44	0.42
1:4:200:GLU:O	1:4:204:ALA:N	2.34	0.42
1:E:108:LEU:HD23	1:E:108:LEU:C	2.44	0.42
1:U:108:LEU:HD23	1:U:108:LEU:C	2.44	0.42
1:X:72:TYR:O	1:X:76:GLN:N	2.44	0.42
1:x:108:LEU:HD23	1:x:108:LEU:C	2.44	0.42
1:L:108:LEU:HD23	1:L:108:LEU:C	2.44	0.42
1:M:108:LEU:HD23	1:M:108:LEU:C	2.44	0.42
1:V:209:LEU:O	1:V:213:LYS:N	2.41	0.42
1:e:72:TYR:O	1:e:76:GLN:N	2.44	0.42
1:k:108:LEU:HD23	1:k:108:LEU:C	2.44	0.42
1:0:108:LEU:HD23	1:0:108:LEU:C	2.44	0.42
1:6:108:LEU:HD23	1:6:108:LEU:C	2.44	0.42
1:P:72:TYR:O	1:P:76:GLN:N	2.44	0.42
1:b:108:LEU:C	1:b:108:LEU:HD23	2.44	0.42
1:n:108:LEU:HD23	1:n:108:LEU:C	2.44	0.42
1:v:108:LEU:HD23	1:v:108:LEU:C	2.44	0.42
1:0:150:GLN:HA	1:4:182:ARG:NH1	2.35	0.42
1:3:108:LEU:HD23	1:3:108:LEU:C	2.44	0.42
1:F:150:GLN:HA	1:J:182:ARG:NH1	2.35	0.42
1:Y:150:GLN:HA	1:c:182:ARG:NH1	2.35	0.42
1:H:150:GLN:HA	1:L:182:ARG:NH1	2.35	0.42
1:N:150:GLN:HA	1:R:182:ARG:NH1	2.35	0.42
1:W:150:GLN:HA	1:a:182:ARG:NH1	2.35	0.42
1:c:43:LEU:HD22	1:g:149:ALA:HB2	2.02	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:u:150:GLN:HA	1:y:182:ARG:NH1	2.35	0.42
1:1:149:ALA:HB2	1:x:43:LEU:HD22	2.02	0.42
1:C:108:LEU:HD23	1:C:108:LEU:C	2.44	0.42
1:C:150:GLN:HA	1:G:182:ARG:NH1	2.35	0.42
1:G:150:GLN:HA	1:K:182:ARG:NH1	2.35	0.42
1:K:150:GLN:HA	1:O:182:ARG:NH1	2.35	0.42
1:O:150:GLN:HA	1:S:182:ARG:NH1	2.35	0.42
1:Q:150:GLN:HA	1:U:182:ARG:NH1	2.35	0.42
1:Y:43:LEU:HD22	1:c:149:ALA:HB2	2.02	0.42
1:e:150:GLN:HA	1:i:182:ARG:NH1	2.35	0.42
1:k:150:GLN:HA	1:o:182:ARG:NH1	2.35	0.42
1:m:195:LYS:O	1:m:199:TRP:N	2.34	0.42
1:o:43:LEU:HD22	1:s:149:ALA:HB2	2.02	0.42
1:o:150:GLN:HA	1:s:182:ARG:NH1	2.35	0.42
1:p:150:GLN:HA	1:t:182:ARG:NH1	2.35	0.42
1:s:150:GLN:HA	1:w:182:ARG:NH1	2.35	0.42
1:t:43:LEU:HD22	1:x:149:ALA:HB2	2.02	0.42
1:y:200:GLU:O	1:y:204:ALA:N	2.34	0.42
1:2:43:LEU:HD22	1:6:149:ALA:HB2	2.02	0.42
1:2:72:TYR:O	1:2:76:GLN:N	2.44	0.42
1:3:150:GLN:HA	1:7:182:ARG:NH1	2.35	0.42
1:B:43:LEU:HD22	1:F:149:ALA:HB2	2.02	0.42
1:H:43:LEU:HD22	1:L:149:ALA:HB2	2.02	0.42
1:K:43:LEU:HD22	1:O:149:ALA:HB2	2.02	0.42
1:O:170:ARG:O	1:O:173:THR:OG1	2.26	0.42
1:P:43:LEU:HD22	1:T:149:ALA:HB2	2.02	0.42
1:f:43:LEU:HD22	1:j:149:ALA:HB2	2.02	0.42
1:h:150:GLN:HA	1:l:182:ARG:NH1	2.35	0.42
1:j:150:GLN:HA	1:n:182:ARG:NH1	2.35	0.42
1:m:150:GLN:HA	1:q:182:ARG:NH1	2.35	0.42
1:w:170:ARG:O	1:w:173:THR:OG1	2.26	0.42
1:0:195:LYS:O	1:0:199:TRP:N	2.34	0.41
1:1:182:ARG:NH1	1:x:150:GLN:HA	2.35	0.41
1:2:150:GLN:HA	1:6:182:ARG:NH1	2.35	0.41
1:E:195:LYS:O	1:E:199:TRP:N	2.34	0.41
1:G:43:LEU:HD22	1:K:149:ALA:HB2	2.02	0.41
1:O:43:LEU:HD22	1:S:149:ALA:HB2	2.02	0.41
1:S:150:GLN:HA	1:W:182:ARG:NH1	2.35	0.41
1:T:43:LEU:HD22	1:X:149:ALA:HB2	2.02	0.41
1:b:43:LEU:HD22	1:f:149:ALA:HB2	2.02	0.41
1:b:150:GLN:HA	1:f:182:ARG:NH1	2.35	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:g:150:GLN:HA	1:k:182:ARG:NH1	2.35	0.41
1:h:43:LEU:HD22	1:l:149:ALA:HB2	2.02	0.41
1:k:43:LEU:HD22	1:o:149:ALA:HB2	2.02	0.41
1:l:43:LEU:HD22	1:p:149:ALA:HB2	2.02	0.41
1:p:170:ARG:O	1:p:173:THR:OG1	2.26	0.41
1:t:150:GLN:HA	1:x:182:ARG:NH1	2.35	0.41
1:v:150:GLN:HA	1:z:182:ARG:NH1	2.35	0.41
1:0:149:ALA:HB2	1:w:43:LEU:HD22	2.02	0.41
1:1:43:LEU:HD22	1:5:149:ALA:HB2	2.02	0.41
1:1:150:GLN:HA	1:5:182:ARG:NH1	2.35	0.41
1:2:149:ALA:HB2	1:y:43:LEU:HD22	2.02	0.41
1:F:43:LEU:HD22	1:J:149:ALA:HB2	2.02	0.41
1:P:150:GLN:HA	1:T:182:ARG:NH1	2.35	0.41
1:Q:43:LEU:HD22	1:U:149:ALA:HB2	2.02	0.41
1:Q:170:ARG:O	1:Q:173:THR:OG1	2.26	0.41
1:S:43:LEU:HD22	1:W:149:ALA:HB2	2.02	0.41
1:W:43:LEU:HD22	1:a:149:ALA:HB2	2.02	0.41
1:c:150:GLN:HA	1:g:182:ARG:NH1	2.35	0.41
1:n:150:GLN:HA	1:r:182:ARG:NH1	2.35	0.41
1:u:43:LEU:HD22	1:y:149:ALA:HB2	2.02	0.41
1:0:43:LEU:HD22	1:4:149:ALA:HB2	2.02	0.41
1:0:182:ARG:NH1	1:w:150:GLN:HA	2.35	0.41
1:D:43:LEU:HD22	1:H:149:ALA:HB2	2.02	0.41
1:I:150:GLN:HA	1:M:182:ARG:NH1	2.35	0.41
1:J:43:LEU:HD22	1:N:149:ALA:HB2	2.02	0.41
1:L:43:LEU:HD22	1:P:149:ALA:HB2	2.02	0.41
1:L:150:GLN:HA	1:P:182:ARG:NH1	2.35	0.41
1:T:150:GLN:HA	1:X:182:ARG:NH1	2.35	0.41
1:V:150:GLN:HA	1:Z:182:ARG:NH1	2.35	0.41
1:V:195:LYS:O	1:V:199:TRP:N	2.34	0.41
1:X:43:LEU:HD22	1:b:149:ALA:HB2	2.02	0.41
1:X:150:GLN:HA	1:b:182:ARG:NH1	2.35	0.41
1:d:150:GLN:HA	1:h:182:ARG:NH1	2.35	0.41
1:n:43:LEU:HD22	1:r:149:ALA:HB2	2.02	0.41
1:p:43:LEU:HD22	1:t:149:ALA:HB2	2.02	0.41
1:r:150:GLN:HA	1:v:182:ARG:NH1	2.35	0.41
1:s:43:LEU:HD22	1:w:149:ALA:HB2	2.02	0.41
1:1:202:GLN:O	1:1:206:GLU:N	2.54	0.41
1:2:182:ARG:NH1	1:y:150:GLN:HA	2.35	0.41
1:3:43:LEU:HD22	1:7:149:ALA:HB2	2.02	0.41
1:C:43:LEU:HD22	1:G:149:ALA:HB2	2.02	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:202:GLN:O	1:T:206:GLU:N	2.54	0.41
1:U:195:LYS:O	1:U:199:TRP:N	2.34	0.41
1:V:202:GLN:O	1:V:206:GLU:N	2.54	0.41
1:Z:43:LEU:HD22	1:d:149:ALA:HB2	2.02	0.41
1:d:202:GLN:O	1:d:206:GLU:N	2.54	0.41
1:g:43:LEU:HD22	1:k:149:ALA:HB2	2.02	0.41
1:j:43:LEU:HD22	1:n:149:ALA:HB2	2.02	0.41
1:l:150:GLN:HA	1:p:182:ARG:NH1	2.35	0.41
1:o:202:GLN:O	1:o:206:GLU:N	2.54	0.41
1:q:43:LEU:HD22	1:u:149:ALA:HB2	2.02	0.41
1:3:170:ARG:O	1:3:173:THR:OG1	2.26	0.41
1:G:202:GLN:O	1:G:206:GLU:N	2.54	0.41
1:I:43:LEU:HD22	1:M:149:ALA:HB2	2.02	0.41
1:I:202:GLN:O	1:I:206:GLU:N	2.54	0.41
1:N:43:LEU:HD22	1:R:149:ALA:HB2	2.02	0.41
1:U:43:LEU:HD22	1:Y:149:ALA:HB2	2.02	0.41
1:Z:150:GLN:HA	1:d:182:ARG:NH1	2.35	0.41
1:d:43:LEU:HD22	1:h:149:ALA:HB2	2.02	0.41
1:e:43:LEU:HD22	1:i:149:ALA:HB2	2.02	0.41
1:f:150:GLN:HA	1:j:182:ARG:NH1	2.35	0.41
1:f:202:GLN:O	1:f:206:GLU:N	2.54	0.41
1:s:202:GLN:O	1:s:206:GLU:N	2.54	0.41
1:K:202:GLN:O	1:K:206:GLU:N	2.54	0.41
1:P:202:GLN:O	1:P:206:GLU:N	2.54	0.41
1:Q:202:GLN:O	1:Q:206:GLU:N	2.54	0.41
1:U:150:GLN:HA	1:Y:182:ARG:NH1	2.35	0.41
1:X:159:LEU:O	1:X:166:SER:OG	2.28	0.41
1:q:202:GLN:O	1:q:206:GLU:N	2.54	0.41
1:x:202:GLN:O	1:x:206:GLU:N	2.54	0.41
1:B:150:GLN:HA	1:F:182:ARG:NH1	2.35	0.41
1:M:43:LEU:HD22	1:Q:149:ALA:HB2	2.02	0.41
1:O:194:LYS:O	1:O:194:LYS:HD3	2.21	0.41
1:Q:72:TYR:O	1:Q:76:GLN:N	2.44	0.41
1:R:43:LEU:HD22	1:V:149:ALA:HB2	2.02	0.41
1:a:43:LEU:HD22	1:e:149:ALA:HB2	2.02	0.41
1:a:150:GLN:HA	1:e:182:ARG:NH1	2.35	0.41
1:b:194:LYS:O	1:b:194:LYS:HD3	2.21	0.41
1:c:202:GLN:O	1:c:206:GLU:N	2.54	0.41
1:i:43:LEU:HD22	1:m:149:ALA:HB2	2.02	0.41
1:i:202:GLN:O	1:i:206:GLU:N	2.54	0.41
1:z:202:GLN:O	1:z:206:GLU:N	2.54	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:182:ARG:NH1	1:z:150:GLN:HA	2.35	0.41
1:5:194:LYS:HD3	1:5:194:LYS:O	2.21	0.41
1:7:202:GLN:O	1:7:206:GLU:N	2.54	0.41
1:B:194:LYS:O	1:B:194:LYS:HD3	2.21	0.41
1:B:202:GLN:O	1:B:206:GLU:N	2.54	0.41
1:N:202:GLN:O	1:N:206:GLU:N	2.54	0.41
1:R:150:GLN:HA	1:V:182:ARG:NH1	2.35	0.41
1:S:202:GLN:O	1:S:206:GLU:N	2.54	0.41
1:V:43:LEU:HD22	1:Z:149:ALA:HB2	2.02	0.41
1:W:202:GLN:O	1:W:206:GLU:N	2.54	0.41
1:f:194:LYS:O	1:f:194:LYS:HD3	2.21	0.41
1:j:200:GLU:O	1:j:204:ALA:N	2.34	0.41
1:j:202:GLN:O	1:j:206:GLU:N	2.54	0.41
1:m:43:LEU:HD22	1:q:149:ALA:HB2	2.02	0.41
1:p:200:GLU:O	1:p:204:ALA:N	2.34	0.41
1:r:43:LEU:HD22	1:v:149:ALA:HB2	2.02	0.41
1:v:43:LEU:HD22	1:z:149:ALA:HB2	2.02	0.41
1:0:194:LYS:O	1:0:194:LYS:HD3	2.21	0.41
1:1:194:LYS:O	1:1:194:LYS:HD3	2.21	0.41
1:3:149:ALA:HB2	1:z:43:LEU:HD22	2.02	0.41
1:3:202:GLN:O	1:3:206:GLU:N	2.54	0.41
1:4:202:GLN:O	1:4:206:GLU:N	2.54	0.41
1:5:202:GLN:O	1:5:206:GLU:N	2.54	0.41
1:6:202:GLN:O	1:6:206:GLU:N	2.54	0.41
1:A:202:GLN:O	1:A:206:GLU:N	2.54	0.41
1:C:202:GLN:O	1:C:206:GLU:N	2.54	0.41
1:D:150:GLN:HA	1:H:182:ARG:NH1	2.35	0.41
1:D:202:GLN:O	1:D:206:GLU:N	2.54	0.41
1:F:194:LYS:O	1:F:194:LYS:HD3	2.21	0.41
1:J:150:GLN:HA	1:N:182:ARG:NH1	2.35	0.41
1:M:150:GLN:HA	1:Q:182:ARG:NH1	2.35	0.41
1:W:194:LYS:O	1:W:194:LYS:HD3	2.21	0.41
1:X:194:LYS:O	1:X:194:LYS:HD3	2.21	0.41
1:b:202:GLN:O	1:b:206:GLU:N	2.54	0.41
1:c:195:LYS:O	1:c:199:TRP:N	2.34	0.41
1:j:194:LYS:O	1:j:194:LYS:HD3	2.21	0.41
1:l:202:GLN:O	1:l:206:GLU:N	2.54	0.41
1:q:150:GLN:HA	1:u:182:ARG:NH1	2.35	0.41
1:s:194:LYS:O	1:s:194:LYS:HD3	2.21	0.41
1:7:195:LYS:O	1:7:199:TRP:N	2.34	0.41
1:J:194:LYS:HD3	1:J:194:LYS:O	2.21	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:202:GLN:O	1:J:206:GLU:N	2.54	0.41
1:L:195:LYS:O	1:L:199:TRP:N	2.34	0.41
1:T:170:ARG:O	1:T:173:THR:OG1	2.26	0.41
1:Y:202:GLN:O	1:Y:206:GLU:N	2.54	0.41
1:Z:72:TYR:O	1:Z:76:GLN:N	2.44	0.41
1:a:202:GLN:O	1:a:206:GLU:N	2.54	0.41
1:b:190:SER:O	1:b:194:LYS:HB3	2.21	0.41
1:g:170:ARG:O	1:g:173:THR:OG1	2.26	0.41
1:g:202:GLN:O	1:g:206:GLU:N	2.54	0.41
1:i:150:GLN:HA	1:m:182:ARG:NH1	2.35	0.41
1:n:194:LYS:HD3	1:n:194:LYS:O	2.21	0.41
1:o:154:GLU:OE1	1:o:154:GLU:N	2.46	0.41
1:o:194:LYS:O	1:o:194:LYS:HD3	2.21	0.41
1:t:195:LYS:O	1:t:199:TRP:N	2.34	0.41
1:v:202:GLN:O	1:v:206:GLU:N	2.54	0.41
1:y:202:GLN:O	1:y:206:GLU:N	2.54	0.41
1:1:190:SER:O	1:1:194:LYS:HB3	2.22	0.40
1:2:195:LYS:O	1:2:199:TRP:N	2.34	0.40
1:5:159:LEU:O	1:5:166:SER:OG	2.28	0.40
1:B:154:GLU:OE1	1:B:154:GLU:N	2.46	0.40
1:B:159:LEU:O	1:B:166:SER:OG	2.28	0.40
1:K:154:GLU:OE1	1:K:154:GLU:N	2.46	0.40
1:Q:194:LYS:O	1:Q:194:LYS:HD3	2.21	0.40
1:T:190:SER:O	1:T:194:LYS:HB3	2.21	0.40
1:X:190:SER:O	1:X:194:LYS:HB3	2.22	0.40
1:X:202:GLN:O	1:X:206:GLU:N	2.54	0.40
1:k:202:GLN:O	1:k:206:GLU:N	2.54	0.40
1:m:202:GLN:O	1:m:206:GLU:N	2.54	0.40
1:r:202:GLN:O	1:r:206:GLU:N	2.54	0.40
1:u:190:SER:O	1:u:194:LYS:HB3	2.21	0.40
1:w:159:LEU:O	1:w:166:SER:OG	2.28	0.40
1:w:202:GLN:O	1:w:206:GLU:N	2.54	0.40
1:x:190:SER:O	1:x:194:LYS:HB3	2.22	0.40
1:5:190:SER:O	1:5:194:LYS:HB3	2.21	0.40
1:A:190:SER:O	1:A:194:LYS:HB3	2.21	0.40
1:B:190:SER:O	1:B:194:LYS:HB3	2.22	0.40
1:D:194:LYS:O	1:D:194:LYS:HD3	2.21	0.40
1:J:190:SER:O	1:J:194:LYS:HB3	2.21	0.40
1:L:202:GLN:O	1:L:206:GLU:N	2.54	0.40
1:N:194:LYS:O	1:N:194:LYS:HD3	2.21	0.40
1:U:190:SER:O	1:U:194:LYS:HB3	2.21	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:190:SER:O	1:V:194:LYS:HB3	2.21	0.40
1:a:190:SER:O	1:a:194:LYS:HB3	2.21	0.40
1:h:194:LYS:O	1:h:194:LYS:HD3	2.21	0.40
1:j:190:SER:O	1:j:194:LYS:HB3	2.21	0.40
1:p:202:GLN:O	1:p:206:GLU:N	2.54	0.40
1:r:194:LYS:O	1:r:194:LYS:HD3	2.21	0.40
1:u:194:LYS:HD3	1:u:194:LYS:O	2.21	0.40
1:x:194:LYS:HD3	1:x:194:LYS:O	2.21	0.40
1:y:190:SER:O	1:y:194:LYS:HB3	2.21	0.40
1:0:190:SER:O	1:0:194:LYS:HB3	2.21	0.40
1:5:154:GLU:OE1	1:5:154:GLU:N	2.46	0.40
1:E:72:TYR:O	1:E:76:GLN:N	2.44	0.40
1:F:190:SER:O	1:F:194:LYS:HB3	2.21	0.40
1:G:194:LYS:O	1:G:194:LYS:HD3	2.21	0.40
1:H:202:GLN:O	1:H:206:GLU:N	2.54	0.40
1:J:170:ARG:O	1:J:173:THR:OG1	2.26	0.40
1:M:194:LYS:HD3	1:M:194:LYS:O	2.21	0.40
1:M:202:GLN:O	1:M:206:GLU:N	2.54	0.40
1:Q:190:SER:O	1:Q:194:LYS:HB3	2.21	0.40
1:R:190:SER:O	1:R:194:LYS:HB3	2.21	0.40
1:Y:190:SER:O	1:Y:194:LYS:HB3	2.22	0.40
1:Z:190:SER:O	1:Z:194:LYS:HB3	2.22	0.40
1:f:154:GLU:OE1	1:f:154:GLU:N	2.46	0.40
1:f:190:SER:O	1:f:194:LYS:HB3	2.22	0.40
1:m:170:ARG:O	1:m:173:THR:OG1	2.26	0.40
1:q:190:SER:O	1:q:194:LYS:HB3	2.21	0.40
1:t:190:SER:O	1:t:194:LYS:HB3	2.21	0.40
1:u:202:GLN:O	1:u:206:GLU:N	2.54	0.40
1:4:190:SER:O	1:4:194:LYS:HB3	2.21	0.40
1:E:202:GLN:O	1:E:206:GLU:N	2.54	0.40
1:J:34:GLY:O	1:J:38:LEU:HD23	2.22	0.40
1:N:212:MET:HE2	1:N:216:ARG:HH21	1.87	0.40
1:O:202:GLN:O	1:O:206:GLU:N	2.54	0.40
1:P:195:LYS:O	1:P:199:TRP:N	2.34	0.40
1:R:34:GLY:O	1:R:38:LEU:HD23	2.22	0.40
1:T:194:LYS:HD3	1:T:194:LYS:O	2.21	0.40
1:T:195:LYS:O	1:T:199:TRP:N	2.34	0.40
1:T:212:MET:HE2	1:T:216:ARG:HH21	1.87	0.40
1:U:194:LYS:HD3	1:U:194:LYS:O	2.21	0.40
1:V:34:GLY:O	1:V:38:LEU:HD23	2.22	0.40
1:W:34:GLY:O	1:W:38:LEU:HD23	2.22	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:154:GLU:OE1	1:b:154:GLU:N	2.46	0.40
1:g:194:LYS:O	1:g:194:LYS:HD3	2.21	0.40
1:j:34:GLY:O	1:j:38:LEU:HD23	2.22	0.40
1:n:34:GLY:O	1:n:38:LEU:HD23	2.22	0.40
1:n:202:GLN:O	1:n:206:GLU:N	2.54	0.40
1:n:212:MET:HE2	1:n:216:ARG:HH21	1.87	0.40
1:q:194:LYS:O	1:q:194:LYS:HD3	2.21	0.40
1:r:34:GLY:O	1:r:38:LEU:HD23	2.22	0.40
1:s:190:SER:O	1:s:194:LYS:HB3	2.21	0.40
1:s:212:MET:HE2	1:s:216:ARG:HH21	1.87	0.40
1:v:190:SER:O	1:v:194:LYS:HB3	2.21	0.40
1:y:194:LYS:HD3	1:y:194:LYS:O	2.21	0.40
1:z:34:GLY:O	1:z:38:LEU:HD23	2.22	0.40
1:z:190:SER:O	1:z:194:LYS:HB3	2.22	0.40
1:2:190:SER:O	1:2:194:LYS:HB3	2.21	0.40
1:A:194:LYS:HD3	1:A:194:LYS:O	2.21	0.40
1:C:190:SER:O	1:C:194:LYS:HB3	2.21	0.40
1:E:34:GLY:O	1:E:38:LEU:HD23	2.22	0.40
1:F:34:GLY:O	1:F:38:LEU:HD23	2.22	0.40
1:I:190:SER:O	1:I:194:LYS:HB3	2.21	0.40
1:K:212:MET:HE2	1:K:216:ARG:HH21	1.87	0.40
1:N:34:GLY:O	1:N:38:LEU:HD23	2.22	0.40
1:O:154:GLU:OE1	1:O:154:GLU:N	2.46	0.40
1:R:170:ARG:O	1:R:173:THR:OG1	2.26	0.40
1:S:190:SER:O	1:S:194:LYS:HB3	2.21	0.40
1:S:212:MET:HE2	1:S:216:ARG:HH21	1.87	0.40
1:Y:194:LYS:O	1:Y:194:LYS:HD3	2.21	0.40
1:Y:212:MET:HE2	1:Y:216:ARG:HH21	1.87	0.40
1:Z:194:LYS:O	1:Z:194:LYS:HD3	2.21	0.40
1:r:190:SER:O	1:r:194:LYS:HB3	2.22	0.40
1:r:212:MET:HE2	1:r:216:ARG:HH21	1.87	0.40
1:t:202:GLN:O	1:t:206:GLU:N	2.54	0.40
1:t:212:MET:HE2	1:t:216:ARG:HH21	1.87	0.40
1:v:34:GLY:O	1:v:38:LEU:HD23	2.22	0.40
1:w:212:MET:HE2	1:w:216:ARG:HH21	1.87	0.40
1:y:212:MET:HE2	1:y:216:ARG:HH21	1.87	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	192/223 (86%)	189 (98%)	3 (2%)	0	100	100
1	1	192/223 (86%)	188 (98%)	4 (2%)	0	100	100
1	2	192/223 (86%)	188 (98%)	4 (2%)	0	100	100
1	3	192/223 (86%)	189 (98%)	3 (2%)	0	100	100
1	4	192/223 (86%)	189 (98%)	3 (2%)	0	100	100
1	5	192/223 (86%)	189 (98%)	3 (2%)	0	100	100
1	6	192/223 (86%)	189 (98%)	3 (2%)	0	100	100
1	7	192/223 (86%)	189 (98%)	3 (2%)	0	100	100
1	A	192/223 (86%)	189 (98%)	3 (2%)	0	100	100
1	B	192/223 (86%)	189 (98%)	3 (2%)	0	100	100
1	C	192/223 (86%)	189 (98%)	3 (2%)	0	100	100
1	D	192/223 (86%)	189 (98%)	3 (2%)	0	100	100
1	E	192/223 (86%)	189 (98%)	3 (2%)	0	100	100
1	F	192/223 (86%)	189 (98%)	3 (2%)	0	100	100
1	G	192/223 (86%)	188 (98%)	4 (2%)	0	100	100
1	H	192/223 (86%)	189 (98%)	3 (2%)	0	100	100
1	I	192/223 (86%)	189 (98%)	3 (2%)	0	100	100
1	J	192/223 (86%)	189 (98%)	3 (2%)	0	100	100
1	K	192/223 (86%)	189 (98%)	3 (2%)	0	100	100
1	L	192/223 (86%)	188 (98%)	4 (2%)	0	100	100
1	M	192/223 (86%)	189 (98%)	3 (2%)	0	100	100
1	N	192/223 (86%)	189 (98%)	3 (2%)	0	100	100
1	O	192/223 (86%)	189 (98%)	3 (2%)	0	100	100
1	P	192/223 (86%)	189 (98%)	3 (2%)	0	100	100
1	Q	192/223 (86%)	189 (98%)	3 (2%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	R	192/223 (86%)	189 (98%)	3 (2%)	0	100	100
1	S	192/223 (86%)	189 (98%)	3 (2%)	0	100	100
1	T	192/223 (86%)	189 (98%)	3 (2%)	0	100	100
1	U	192/223 (86%)	189 (98%)	3 (2%)	0	100	100
1	V	192/223 (86%)	189 (98%)	3 (2%)	0	100	100
1	W	192/223 (86%)	189 (98%)	3 (2%)	0	100	100
1	X	192/223 (86%)	189 (98%)	3 (2%)	0	100	100
1	Y	192/223 (86%)	189 (98%)	3 (2%)	0	100	100
1	Z	192/223 (86%)	189 (98%)	3 (2%)	0	100	100
1	a	192/223 (86%)	189 (98%)	3 (2%)	0	100	100
1	b	192/223 (86%)	189 (98%)	3 (2%)	0	100	100
1	c	192/223 (86%)	189 (98%)	3 (2%)	0	100	100
1	d	192/223 (86%)	189 (98%)	3 (2%)	0	100	100
1	e	192/223 (86%)	189 (98%)	3 (2%)	0	100	100
1	f	192/223 (86%)	189 (98%)	3 (2%)	0	100	100
1	g	192/223 (86%)	189 (98%)	3 (2%)	0	100	100
1	h	192/223 (86%)	189 (98%)	3 (2%)	0	100	100
1	i	192/223 (86%)	189 (98%)	3 (2%)	0	100	100
1	j	192/223 (86%)	189 (98%)	3 (2%)	0	100	100
1	k	192/223 (86%)	188 (98%)	4 (2%)	0	100	100
1	l	192/223 (86%)	189 (98%)	3 (2%)	0	100	100
1	m	192/223 (86%)	189 (98%)	3 (2%)	0	100	100
1	n	192/223 (86%)	189 (98%)	3 (2%)	0	100	100
1	o	192/223 (86%)	189 (98%)	3 (2%)	0	100	100
1	p	192/223 (86%)	189 (98%)	3 (2%)	0	100	100
1	q	192/223 (86%)	189 (98%)	3 (2%)	0	100	100
1	r	192/223 (86%)	189 (98%)	3 (2%)	0	100	100
1	s	192/223 (86%)	189 (98%)	3 (2%)	0	100	100
1	t	192/223 (86%)	188 (98%)	4 (2%)	0	100	100
1	u	192/223 (86%)	189 (98%)	3 (2%)	0	100	100
1	v	192/223 (86%)	189 (98%)	3 (2%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	w	192/223 (86%)	189 (98%)	3 (2%)	0	100	100
1	x	192/223 (86%)	189 (98%)	3 (2%)	0	100	100
1	y	192/223 (86%)	189 (98%)	3 (2%)	0	100	100
1	z	192/223 (86%)	189 (98%)	3 (2%)	0	100	100
All	All	11520/13380 (86%)	11334 (98%)	186 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	161/186 (87%)	160 (99%)	1 (1%)	78	79
1	1	161/186 (87%)	161 (100%)	0	100	100
1	2	161/186 (87%)	160 (99%)	1 (1%)	78	79
1	3	161/186 (87%)	160 (99%)	1 (1%)	78	79
1	4	161/186 (87%)	160 (99%)	1 (1%)	78	79
1	5	161/186 (87%)	160 (99%)	1 (1%)	78	79
1	6	161/186 (87%)	161 (100%)	0	100	100
1	7	161/186 (87%)	160 (99%)	1 (1%)	78	79
1	A	161/186 (87%)	160 (99%)	1 (1%)	78	79
1	B	161/186 (87%)	160 (99%)	1 (1%)	78	79
1	C	161/186 (87%)	160 (99%)	1 (1%)	78	79
1	D	161/186 (87%)	160 (99%)	1 (1%)	78	79
1	E	161/186 (87%)	160 (99%)	1 (1%)	78	79
1	F	161/186 (87%)	160 (99%)	1 (1%)	78	79
1	G	161/186 (87%)	160 (99%)	1 (1%)	78	79
1	H	161/186 (87%)	160 (99%)	1 (1%)	78	79
1	I	161/186 (87%)	160 (99%)	1 (1%)	78	79

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	161/186 (87%)	160 (99%)	1 (1%)	78	79
1	K	161/186 (87%)	161 (100%)	0	100	100
1	L	161/186 (87%)	161 (100%)	0	100	100
1	M	161/186 (87%)	160 (99%)	1 (1%)	78	79
1	N	161/186 (87%)	161 (100%)	0	100	100
1	O	161/186 (87%)	160 (99%)	1 (1%)	78	79
1	P	161/186 (87%)	161 (100%)	0	100	100
1	Q	161/186 (87%)	160 (99%)	1 (1%)	78	79
1	R	161/186 (87%)	161 (100%)	0	100	100
1	S	161/186 (87%)	161 (100%)	0	100	100
1	T	161/186 (87%)	161 (100%)	0	100	100
1	U	161/186 (87%)	161 (100%)	0	100	100
1	V	161/186 (87%)	161 (100%)	0	100	100
1	W	161/186 (87%)	160 (99%)	1 (1%)	78	79
1	X	161/186 (87%)	160 (99%)	1 (1%)	78	79
1	Y	161/186 (87%)	160 (99%)	1 (1%)	78	79
1	Z	161/186 (87%)	160 (99%)	1 (1%)	78	79
1	a	161/186 (87%)	160 (99%)	1 (1%)	78	79
1	b	161/186 (87%)	160 (99%)	1 (1%)	78	79
1	c	161/186 (87%)	161 (100%)	0	100	100
1	d	161/186 (87%)	160 (99%)	1 (1%)	78	79
1	e	161/186 (87%)	160 (99%)	1 (1%)	78	79
1	f	161/186 (87%)	160 (99%)	1 (1%)	78	79
1	g	161/186 (87%)	160 (99%)	1 (1%)	78	79
1	h	161/186 (87%)	161 (100%)	0	100	100
1	i	161/186 (87%)	160 (99%)	1 (1%)	78	79
1	j	161/186 (87%)	160 (99%)	1 (1%)	78	79
1	k	161/186 (87%)	160 (99%)	1 (1%)	78	79
1	l	161/186 (87%)	161 (100%)	0	100	100
1	m	161/186 (87%)	160 (99%)	1 (1%)	78	79
1	n	161/186 (87%)	160 (99%)	1 (1%)	78	79

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	o	161/186 (87%)	161 (100%)	0	100	100
1	p	161/186 (87%)	161 (100%)	0	100	100
1	q	161/186 (87%)	161 (100%)	0	100	100
1	r	161/186 (87%)	161 (100%)	0	100	100
1	s	161/186 (87%)	160 (99%)	1 (1%)	78	79
1	t	161/186 (87%)	161 (100%)	0	100	100
1	u	161/186 (87%)	160 (99%)	1 (1%)	78	79
1	v	161/186 (87%)	161 (100%)	0	100	100
1	w	161/186 (87%)	160 (99%)	1 (1%)	78	79
1	x	161/186 (87%)	161 (100%)	0	100	100
1	y	161/186 (87%)	160 (99%)	1 (1%)	78	79
1	z	161/186 (87%)	161 (100%)	0	100	100
All	All	9660/11160 (87%)	9622 (100%)	38 (0%)	81	83

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	209	LEU
1	2	209	LEU
1	3	209	LEU
1	4	209	LEU
1	5	209	LEU
1	7	209	LEU
1	A	209	LEU
1	B	209	LEU
1	C	209	LEU
1	D	209	LEU
1	E	209	LEU
1	F	209	LEU
1	G	209	LEU
1	H	209	LEU
1	I	209	LEU
1	J	209	LEU
1	M	209	LEU
1	O	209	LEU
1	Q	209	LEU
1	W	209	LEU
1	X	209	LEU

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	Y	209	LEU
1	Z	209	LEU
1	a	209	LEU
1	b	209	LEU
1	d	209	LEU
1	e	209	LEU
1	f	209	LEU
1	g	209	LEU
1	i	209	LEU
1	j	209	LEU
1	k	209	LEU
1	m	209	LEU
1	n	209	LEU
1	s	209	LEU
1	u	209	LEU
1	w	209	LEU
1	y	209	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	O	137	ASN
1	H	137	ASN
1	K	137	ASN
1	R	137	ASN
1	Y	137	ASN
1	b	137	ASN
1	f	137	ASN
1	j	137	ASN
1	k	137	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.