



Full wwPDB EM Validation Report ⓘ

Aug 7, 2025 – 07:15 am BST

PDB ID : 9HZQ / pdb_00009hzq
EMDB ID : EMD-52530
Title : 280 A SynPspA H1-5 rod after incubation with EPL
Authors : Hudina, E.; Junglas, B.; Sachse, C.
Deposited on : 2025-01-14
Resolution : 3.95 Å(reported)

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

We welcome your comments at 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:

EMDB validation analysis : 0.0.1.dev126
MolProbity : 4-5-2 with Phenix2.0rc1
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

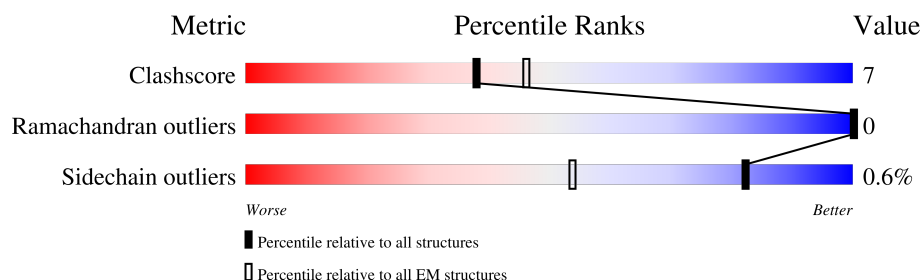
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.95 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.









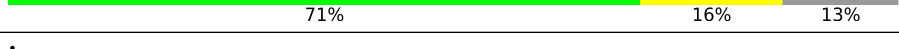
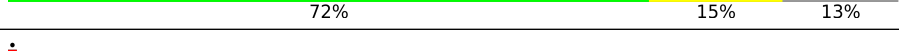
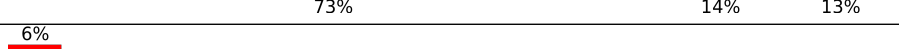
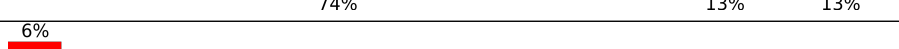
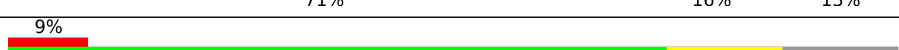

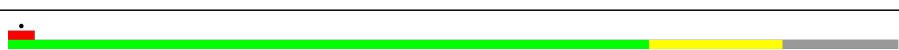

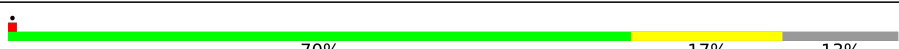





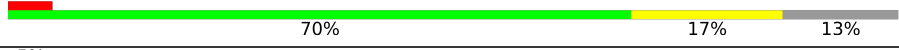
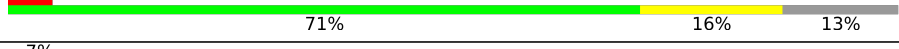



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 ≥ 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	223	
1	1	223	
1	2	223	
1	3	223	
1	4	223	
1	5	223	
1	6	223	
1	7	223	







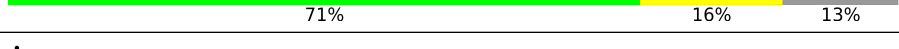
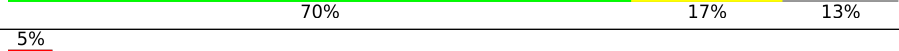
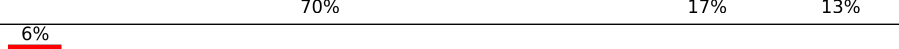
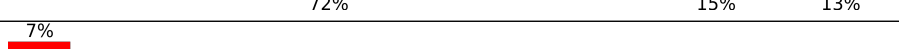
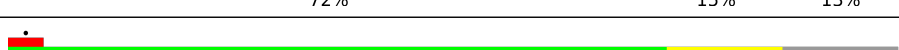

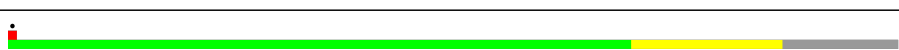

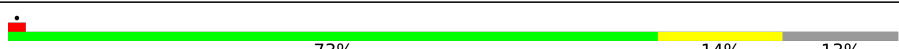





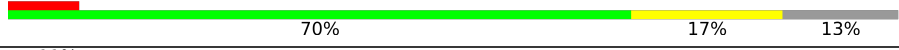
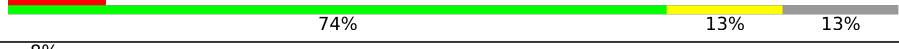



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Mol	Chain	Length	Quality of chain
1	A	223	
1	B	223	
1	C	223	
1	D	223	
1	E	223	
1	F	223	
1	G	223	
1	H	223	
1	I	223	
1	J	223	
1	K	223	
1	L	223	
1	M	223	
1	N	223	
1	O	223	
1	P	223	
1	Q	223	
1	R	223	
1	S	223	
1	T	223	
1	U	223	
1	V	223	
1	W	223	
1	X	223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

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Mol	Chain	Length	Quality of chain
1	Z	223	
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	

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Mol	Chain	Length	Quality of chain
1	y	223	<div><div></div><div></div><div></div></div> <div>71%16%13%</div>
1	z	223	<div><div></div><div></div><div></div></div> <div>70%17%13%</div>

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		

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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

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Mol	Chain	Residues	Atoms						AltConf	Trace
1	e	194	Total 3149	C 968	H 1590	N 286	O 303	S 2	0	0
1	f	194	Total 3149	C 968	H 1590	N 286	O 303	S 2	0	0
1	g	194	Total 3149	C 968	H 1590	N 286	O 303	S 2	0	0
1	h	194	Total 3149	C 968	H 1590	N 286	O 303	S 2	0	0
1	i	194	Total 3149	C 968	H 1590	N 286	O 303	S 2	0	0
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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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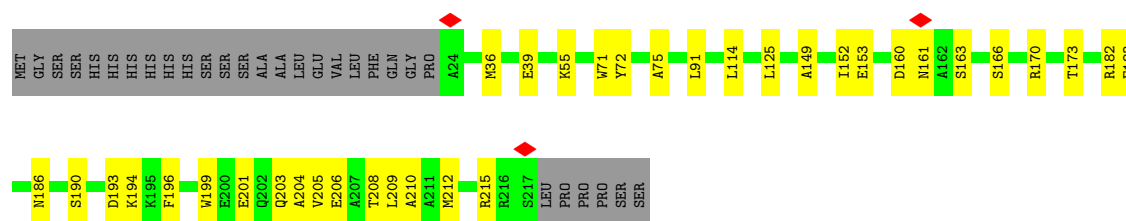
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Chain	Residue	Modelled	Actual	Comment	Reference
w	9	HIS	-	expression tag	UNP P74717
w	10	HIS	-	expression tag	UNP P74717
w	11	SER	-	expression tag	UNP P74717
w	12	SER	-	expression tag	UNP P74717
w	13	SER	-	expression tag	UNP P74717
w	14	ALA	-	expression 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

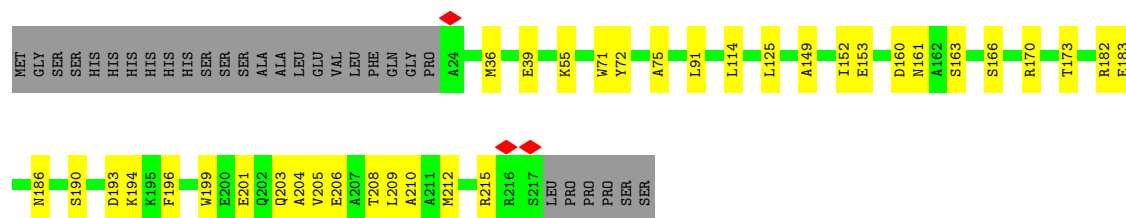
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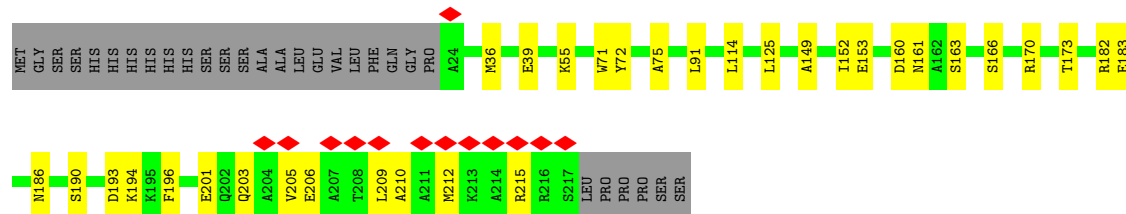
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y	5	HIS	-	expression tag	UNP P74717
y	6	HIS	-	expression tag	UNP P74717
y	7	HIS	-	expression tag	UNP P74717
y	8	HIS	-	expression tag	UNP P74717
y	9	HIS	-	expression tag	UNP P74717
y	10	HIS	-	expression tag	UNP P74717
y	11	SER	-	expression tag	UNP P74717
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



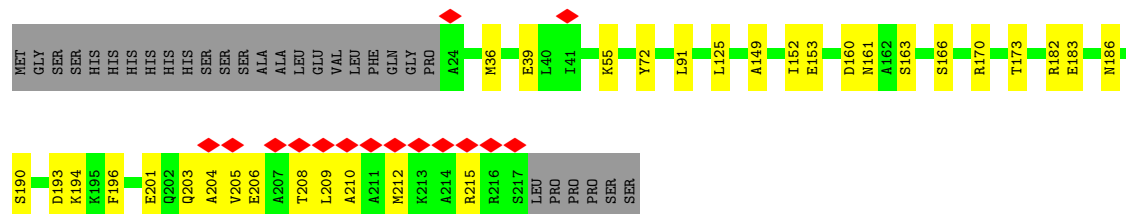
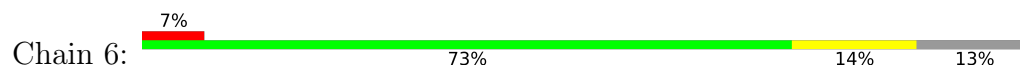
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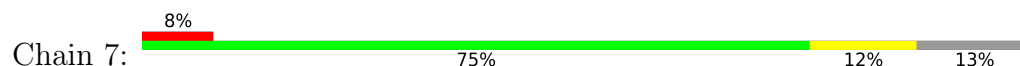
- Molecule 1: Chloroplast membrane-associated 30 kD protein



- Molecule 1: Chloroplast membrane-associated 30 kD protein



- Molecule 1: Chloroplast membrane-associated 30 kD protein



The chart displays the distribution of 199 amino acids across 199 categories. The categories are labeled on the left and right. The bars are color-coded: red for 'A24', yellow for 'K36', 'E39', 'K55', 'Y72', 'L91', 'L125', 'A149', 'I152', 'E153', 'D160', 'N161', 'A162', 'S163', 'S166', 'R170', 'T173', 'R182', 'E183', 'N186', and 'S190'. A red diamond marker is placed above the 'A24' bar, and a red diamond marker is placed below the 'S217' bar.

- Chain F:  73% 14% 13%

The chart displays the amino acid composition of two protein sequences, S190 and S217. The y-axis lists 36 amino acids, with some labeled as A24, M36, E39, K65, Y72, L91, L114, L125, A149, I152, E153, D160, N161, A162, S163, S166, R170, T173, R182, E183, and N186. The x-axis represents the relative frequency or count of each amino acid, with a central vertical line at 100. Bars are color-coded: green for 'High' (above 100), yellow for 'Normal' (around 100), and grey for 'Low' (below 100). Red diamonds indicate significant differences between the two sequences. The chart shows that S190 is generally enriched in green (High) and yellow (Normal) amino acids, while S217 is generally enriched in grey (Low) amino acids. Notable differences are marked with red diamonds at positions A24, M36, E39, K65, Y72, L91, L114, L125, A149, I152, E153, D160, N161, A162, S163, S166, R170, T173, R182, E183, and N186.

- Chain G:  71% 16% 13%

Diagram illustrating a sequence of amino acids and their corresponding codons, with a large grey rectangle highlighting the top row of amino acids.

Amino Acid Sequence (Top Row):

- MET
- GLY
- SER
- SER
- HIS
- HIS
- HIS
- HIS
- HIS
- SER
- SER
- SER
- ALA
- ALA
- LEU
- LEU
- VAL
- LEU
- PHE
- GLN
- GLY
- PRO
- A24
- K36
- E39
- K55
- Y72
- L91
- L114
- L125
- A149
- I152
- E153
- D160
- N161
- A162
- S163
- S166
- R170
- T173
- L176
- A180
- S181
- S192

Codon Sequence (Bottom Row):

- E183
- N186
- S190
- D193
- K194
- K195
- F196
- W199
- E200
- E201
- Q202
- Q203
- A204
- V205
- E206
- A207
- T208
- L209
- A210
- A211
- M212
- R215
- R216
- S217
- LEU
- PRO
- PRO
- PRO
- SER

- Chain H:  72% 15% 13%

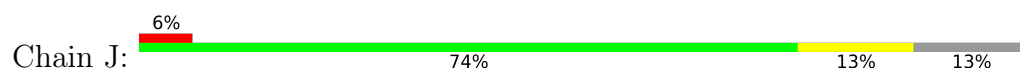
Category	Item	Value	Color
Top 18 Items	MET	100	Grey
	GLY	95	Green
	SER	90	Green
	K194	85	Green
	HIS	80	Green
	HIS	75	Green
	HIS	70	Green
	HIS	65	Green
	HIS	60	Green
	SER	55	Green
	SER	50	Green
	SER	45	Green
	ALA	40	Green
	ALA	35	Green
	LEU	30	Green
	GLU	25	Green
	VAL	20	Green
	Bottom 18 Items	LEU	15
PHE		10	Green
GLN		5	Green
GLY		0	Green
PRO		-5	Red
A24		-10	Red
K36		-15	Yellow
E39		-20	Yellow
K65		-25	Yellow
Y72		-30	Yellow
L91		-35	Yellow
L114		-40	Yellow
L125		-45	Yellow
A149		-50	Yellow
I152		-55	Yellow
E153		-60	Yellow
D160		-65	Yellow
N161		-70	Yellow
A162	-75	Yellow	
S163	-80	Yellow	
S166	-85	Yellow	
R170	-90	Yellow	
T173	-95	Yellow	
R182	-100	Yellow	
E183	-105	Yellow	
N186	-110	Yellow	
Bottom 12 Items	S190	-115	Yellow
	D193	-120	Yellow
	K195	-125	Yellow
	F196	-130	Yellow
	W199	-135	Yellow
	E200	-140	Yellow
	E201	-145	Yellow
	Q202	-150	Yellow
	Q203	-155	Yellow
	A204	-160	Yellow
	V205	-165	Yellow
	A206	-170	Yellow
A207	-175	Yellow	
T208	-180	Yellow	
L209	-185	Yellow	
A210	-190	Yellow	
A211	-195	Yellow	
M212	-200	Yellow	
R215	-205	Yellow	
E216	-210	Yellow	
S217	-215	Yellow	
LEU	-220	Yellow	
PRO	-225	Yellow	
PRO	-230	Yellow	
PRO	-235	Yellow	
SER	-240	Yellow	
SER	-245	Yellow	

- Chain I: 73% 14% 13%

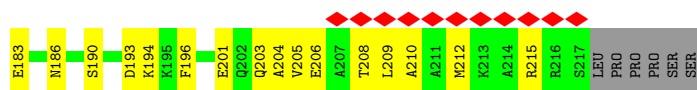
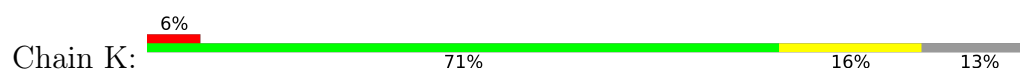
MET	GLY	SER	SER	HIS	HIS	HIS	HIS	HIS	HIS	SER	SER	ALA	ALA	LEU	GLU	VAL	LEU	PHE	GLN	GLY	PRO	A24	M36	E39	K55	Y72	L91	L125	A149	I152	E153	D160	M161	A162	S163	S166	R170	T173	R182	E183	M186	S190
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------



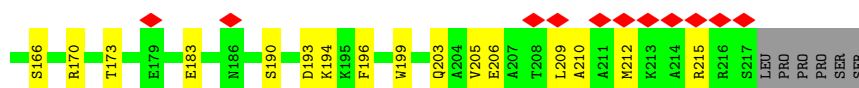
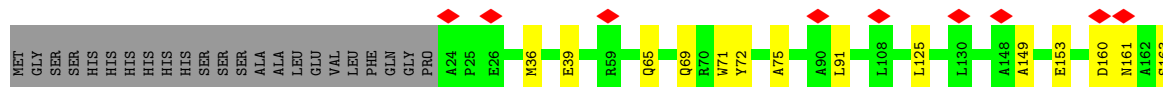
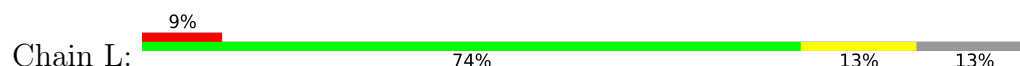
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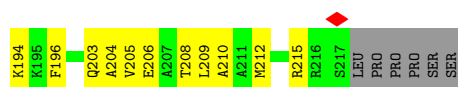
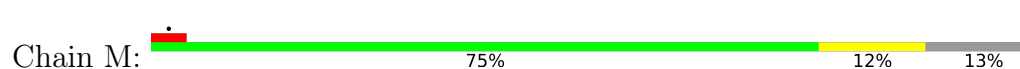
- Molecule 1: Chloroplast membrane-associated 30 kD protein



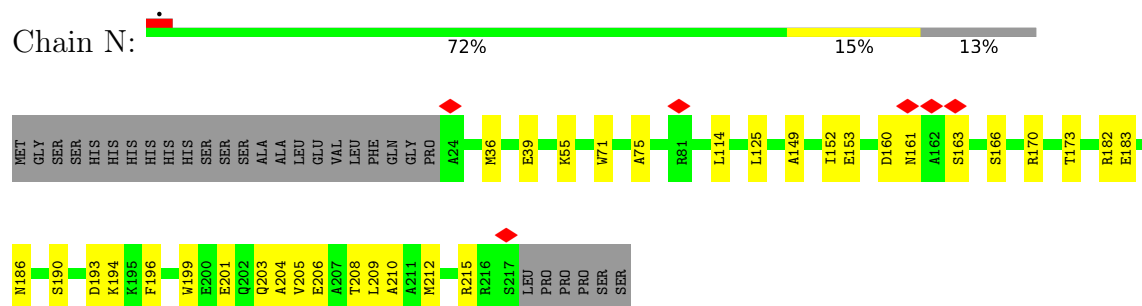
- Molecule 1: Chloroplast membrane-associated 30 kD protein



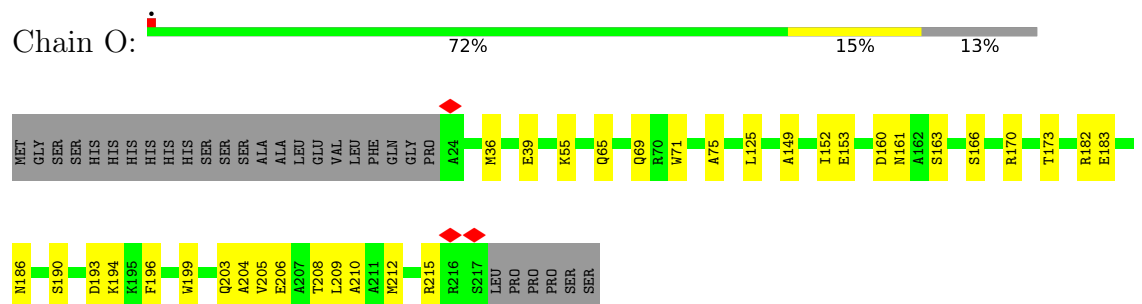
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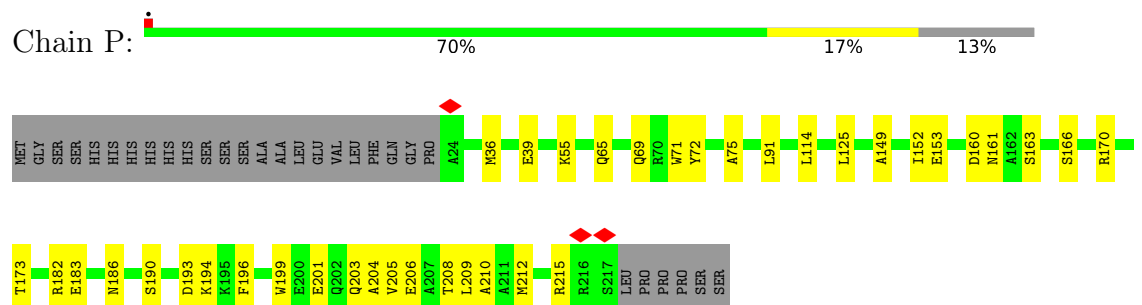
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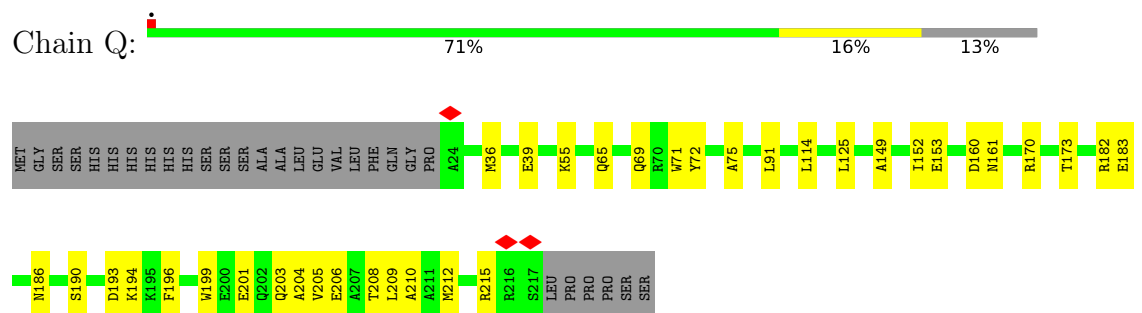
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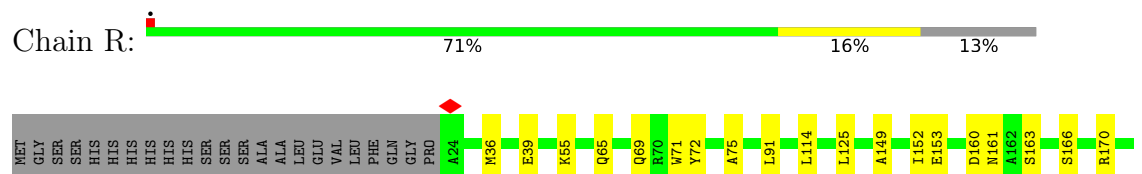
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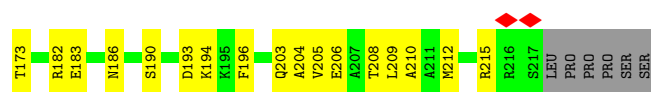


- Molecule 1: Chloroplast membrane-associated 30 kD protein



- Molecule 1: Chloroplast membrane-associated 30 kD protein

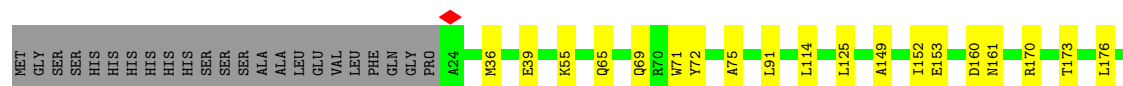




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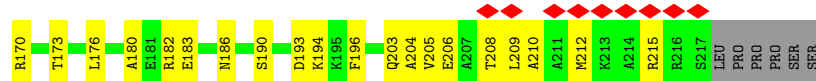
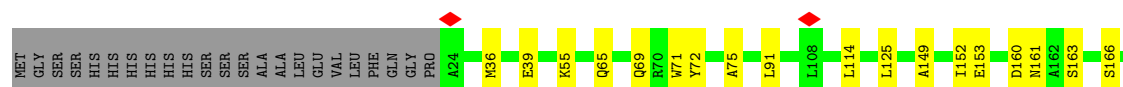
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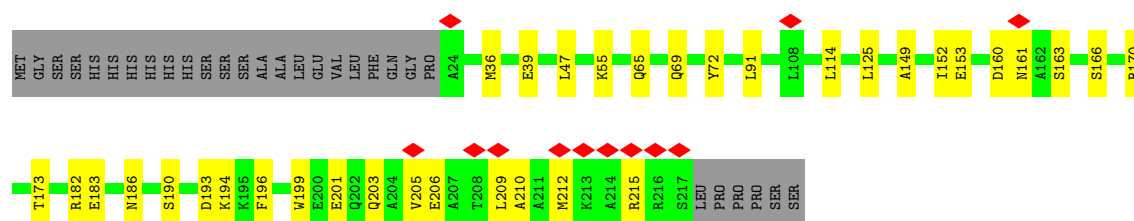
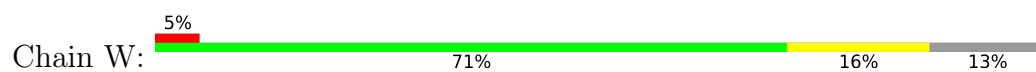
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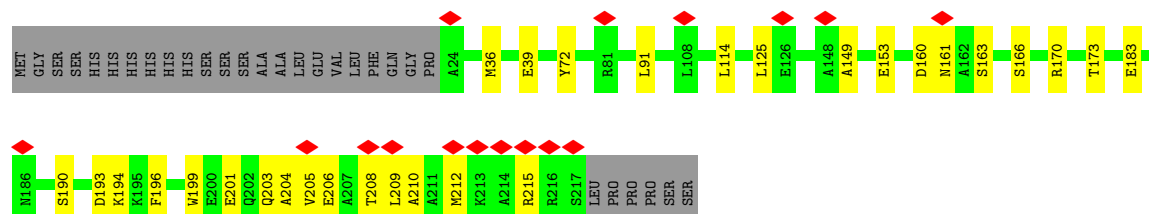
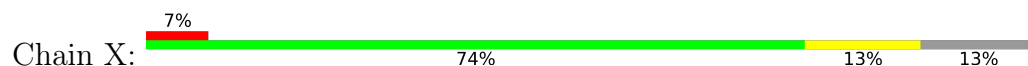
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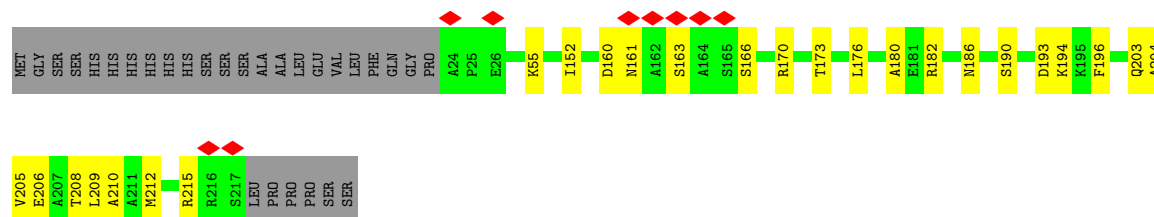
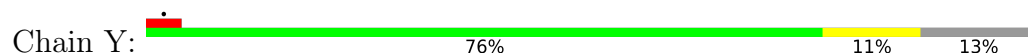
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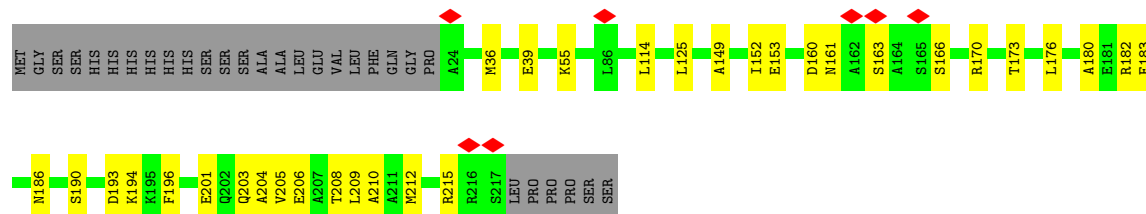
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- Molecule 1: Chloroplast membrane-associated 30 kD protein



- Molecule 1: Chloroplast membrane-associated 30 kD protein



- Molecule 1: Chloroplast membrane-associated 30 kD protein





- Molecule 1: Chloroplast membrane-associated 30 kD protein



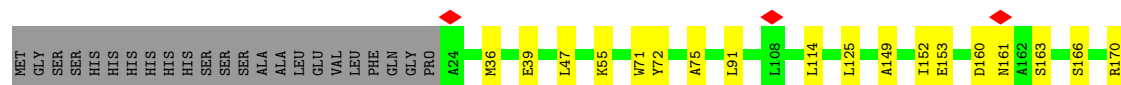
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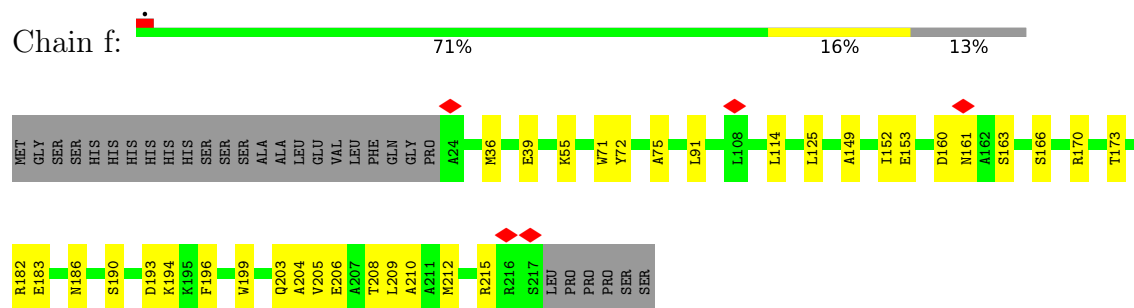
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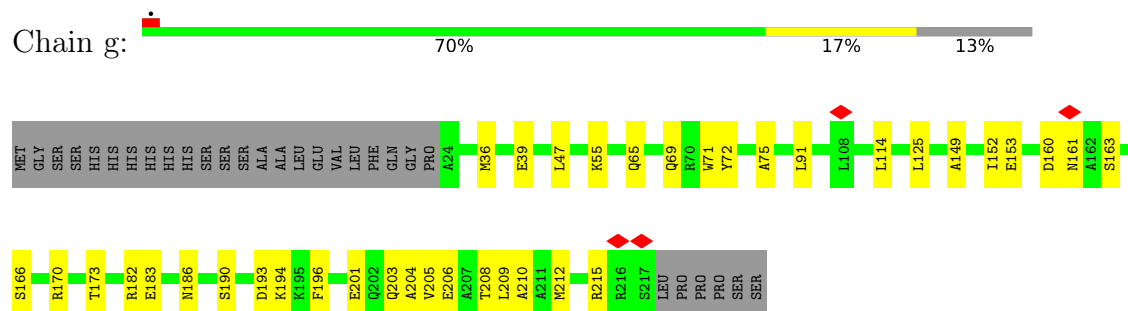
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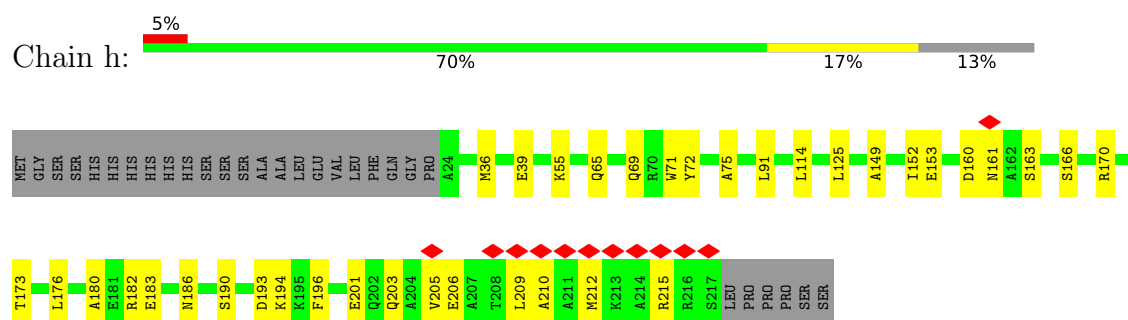
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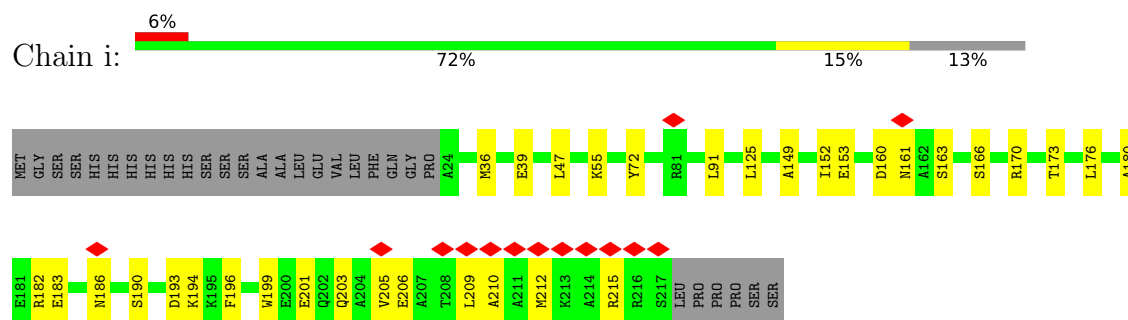
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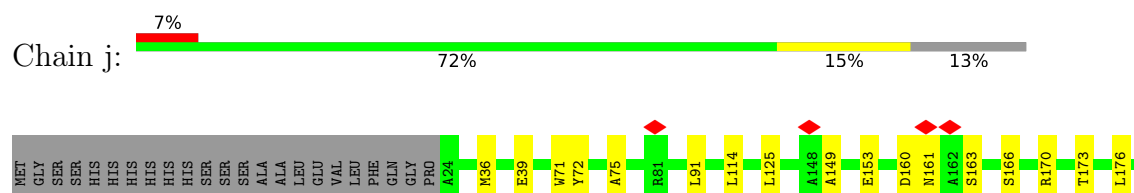
- Molecule 1: Chloroplast membrane-associated 30 kD protein



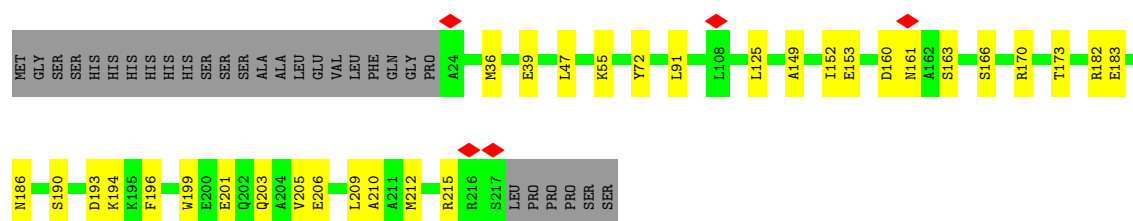
- Molecule 1: Chloroplast membrane-associated 30 kD protein




- Molecule 1: Chloroplast membrane-associated 30 kD protein

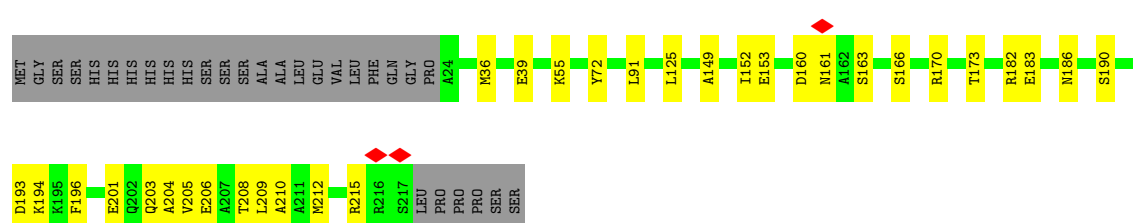


Chain o: 



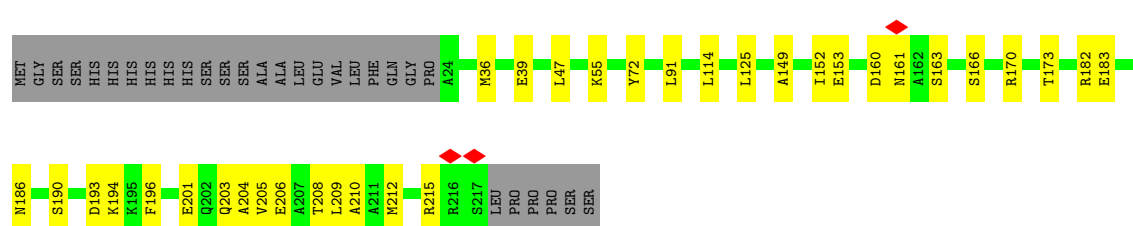
- Molecule 1: Chloroplast membrane-associated 30 kD protein

Chain p: 



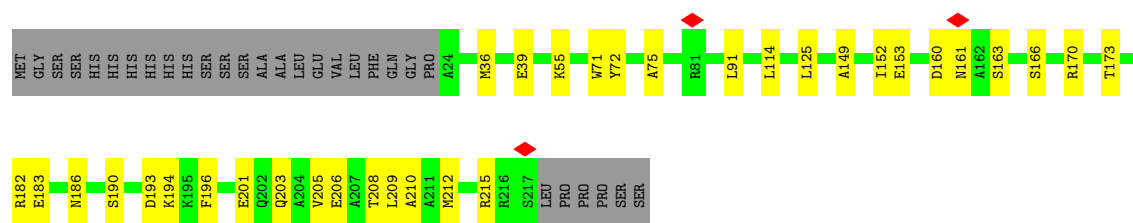
- Molecule 1: Chloroplast membrane-associated 30 kD protein

Chain q: 



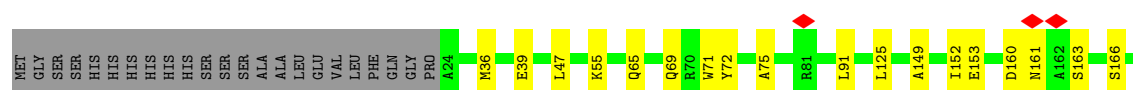
- Molecule 1: Chloroplast membrane-associated 30 kD protein

Chain r: 



- Molecule 1: Chloroplast membrane-associated 30 kD protein

Chain s: 

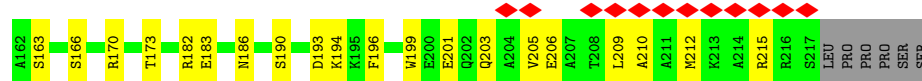
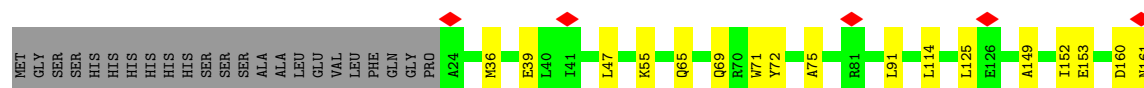




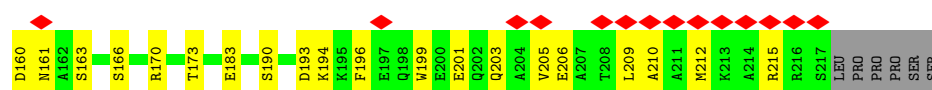
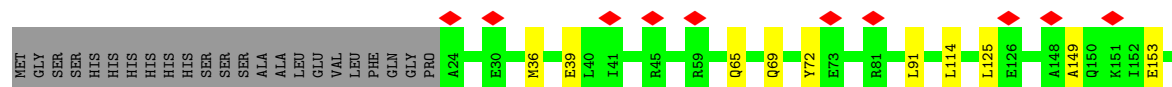
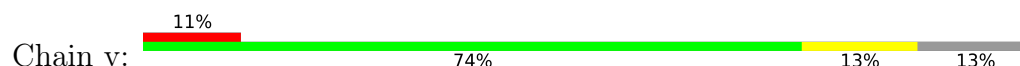
- Molecule 1: Chloroplast membrane-associated 30 kD protein



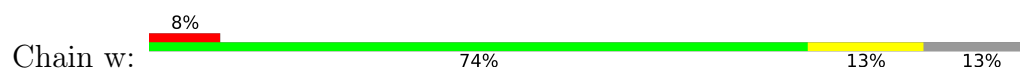
- Molecule 1: Chloroplast membrane-associated 30 kD protein



- Molecule 1: Chloroplast membrane-associated 30 kD protein

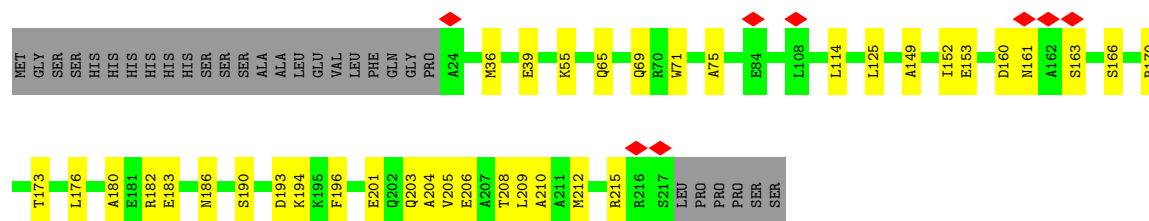


- Molecule 1: Chloroplast membrane-associated 30 kD protein



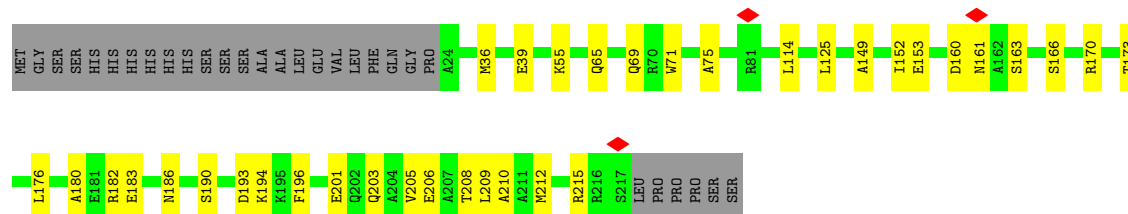
- Molecule 1: Chloroplast membrane-associated 30 kD protein

Chain x: 



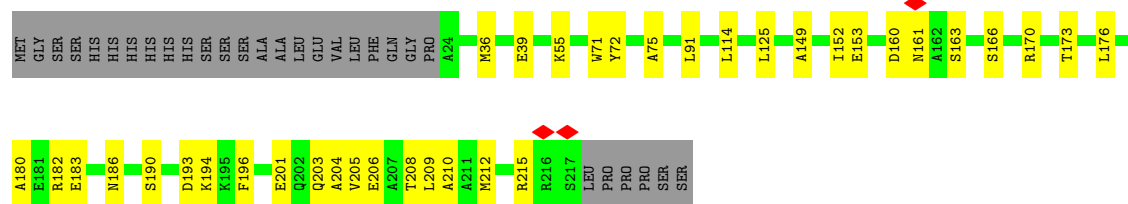
- Molecule 1: Chloroplast membrane-associated 30 kD protein

Chain y: 



- Molecule 1: Chloroplast membrane-associated 30 kD protein

Chain z: 



4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=21.9°, rise=9.03 Å, axial sym=C5	Depositor
Number of segments used	636672	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 ($e^-/\text{Å}^2$)	44	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.544	Depositor
Minimum map value	-0.219	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	544.0, 544.0, 544.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.36, 1.36, 1.36	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.10	0/1575	0.26	0/2114
1	1	0.10	0/1575	0.26	0/2114
1	2	0.10	0/1575	0.26	0/2114
1	3	0.10	0/1575	0.26	0/2114
1	4	0.10	0/1575	0.26	0/2114
1	5	0.10	0/1575	0.26	0/2114
1	6	0.10	0/1575	0.26	0/2114
1	7	0.10	0/1575	0.26	0/2114
1	A	0.10	0/1575	0.26	0/2114
1	B	0.10	0/1575	0.26	0/2114
1	C	0.10	0/1575	0.26	0/2114
1	D	0.10	0/1575	0.26	0/2114
1	E	0.10	0/1575	0.26	0/2114
1	F	0.10	0/1575	0.26	0/2114
1	G	0.10	0/1575	0.26	0/2114
1	H	0.10	0/1575	0.26	0/2114
1	I	0.10	0/1575	0.26	0/2114
1	J	0.10	0/1575	0.26	0/2114
1	K	0.10	0/1575	0.26	0/2114
1	L	0.10	0/1575	0.26	0/2114
1	M	0.10	0/1575	0.26	0/2114
1	N	0.10	0/1575	0.26	0/2114
1	O	0.10	0/1575	0.26	0/2114
1	P	0.10	0/1575	0.26	0/2114
1	Q	0.10	0/1575	0.26	0/2114
1	R	0.10	0/1575	0.26	0/2114
1	S	0.10	0/1575	0.26	0/2114
1	T	0.10	0/1575	0.26	0/2114
1	U	0.10	0/1575	0.26	0/2114
1	V	0.10	0/1575	0.26	0/2114
1	W	0.10	0/1575	0.26	0/2114
1	X	0.10	0/1575	0.26	0/2114
1	Y	0.10	0/1575	0.26	0/2114
1	Z	0.10	0/1575	0.26	0/2114

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	a	0.10	0/1575	0.26	0/2114
1	b	0.10	0/1575	0.26	0/2114
1	c	0.10	0/1575	0.26	0/2114
1	d	0.10	0/1575	0.26	0/2114
1	e	0.10	0/1575	0.26	0/2114
1	f	0.10	0/1575	0.26	0/2114
1	g	0.10	0/1575	0.26	0/2114
1	h	0.10	0/1575	0.26	0/2114
1	i	0.10	0/1575	0.26	0/2114
1	j	0.10	0/1575	0.26	0/2114
1	k	0.10	0/1575	0.26	0/2114
1	l	0.10	0/1575	0.26	0/2114
1	m	0.10	0/1575	0.26	0/2114
1	n	0.10	0/1575	0.26	0/2114
1	o	0.10	0/1575	0.26	0/2114
1	p	0.10	0/1575	0.26	0/2114
1	q	0.10	0/1575	0.26	0/2114
1	r	0.10	0/1575	0.26	0/2114
1	s	0.10	0/1575	0.26	0/2114
1	t	0.10	0/1575	0.26	0/2114
1	u	0.10	0/1575	0.26	0/2114
1	v	0.10	0/1575	0.26	0/2114
1	w	0.10	0/1575	0.26	0/2114
1	x	0.10	0/1575	0.26	0/2114
1	y	0.10	0/1575	0.26	0/2114
1	z	0.10	0/1575	0.26	0/2114
All	All	0.10	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	35	0
1	1	1559	1590	1589	36	0
1	2	1559	1590	1589	36	0
1	3	1559	1590	1589	35	0
1	4	1559	1590	1589	35	0
1	5	1559	1590	1589	29	0
1	6	1559	1590	1589	28	0
1	7	1559	1590	1589	20	0
1	A	1559	1590	1589	24	0
1	B	1559	1590	1589	32	0
1	C	1559	1590	1589	31	0
1	D	1559	1590	1589	33	0
1	E	1559	1590	1589	32	0
1	F	1559	1590	1589	32	0
1	G	1559	1590	1589	35	0
1	H	1559	1590	1589	34	0
1	I	1559	1590	1589	32	0
1	J	1559	1590	1589	26	0
1	K	1559	1590	1589	30	0
1	L	1559	1590	1589	23	0
1	M	1559	1590	1589	23	0
1	N	1559	1590	1589	31	0
1	O	1559	1590	1589	30	0
1	P	1559	1590	1589	35	0
1	Q	1559	1590	1589	35	0
1	R	1559	1590	1589	34	0
1	S	1559	1590	1589	36	0
1	T	1559	1590	1589	35	0
1	U	1559	1590	1589	37	0
1	V	1559	1590	1589	31	0
1	W	1559	1590	1589	31	0
1	X	1559	1590	1589	24	0
1	Y	1559	1590	1589	22	0
1	Z	1559	1590	1589	30	0
1	a	1559	1590	1589	31	0
1	b	1559	1590	1589	33	0
1	c	1559	1590	1589	35	0
1	d	1559	1590	1589	33	0
1	e	1559	1590	1589	36	0
1	f	1559	1590	1589	34	0
1	g	1559	1590	1589	36	0
1	h	1559	1590	1589	30	0
1	i	1559	1590	1589	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	j	1559	1590	1589	26	0
1	k	1559	1590	1589	25	0
1	l	1559	1590	1589	31	0
1	m	1559	1590	1589	32	0
1	n	1559	1590	1589	33	0
1	o	1559	1590	1589	32	0
1	p	1559	1590	1589	32	0
1	q	1559	1590	1589	34	0
1	r	1559	1590	1589	32	0
1	s	1559	1590	1589	35	0
1	t	1559	1590	1589	29	0
1	u	1559	1590	1589	31	0
1	v	1559	1590	1589	24	0
1	w	1559	1590	1589	25	0
1	x	1559	1590	1589	32	0
1	y	1559	1590	1589	31	0
1	z	1559	1590	1589	35	0
All	All	93540	95400	95340	1362	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 7.

All (1362) 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)
1:1:160:ASP:OD1	1:1:161:ASN:ND2	2.12	0.83
1:M:160:ASP:OD1	1:M:161:ASN:ND2	2.12	0.83
1:0:160:ASP:OD1	1:0:161:ASN:ND2	2.12	0.83
1:2:160:ASP:OD1	1:2:161:ASN:ND2	2.12	0.83
1:L:160:ASP:OD1	1:L:161:ASN:ND2	2.12	0.83
1:N:160:ASP:OD1	1:N:161:ASN:ND2	2.12	0.83
1:k:160:ASP:OD1	1:k:161:ASN:ND2	2.12	0.83
1:d:160:ASP:OD1	1:d:161:ASN:ND2	2.12	0.82
1:e:160:ASP:OD1	1:e:161:ASN:ND2	2.12	0.82
1:i:160:ASP:OD1	1:i:161:ASN:ND2	2.12	0.82
1:3:160:ASP:OD1	1:3:161:ASN:ND2	2.12	0.82
1:K:160:ASP:OD1	1:K:161:ASN:ND2	2.12	0.82
1:R:160:ASP:OD1	1:R:161:ASN:ND2	2.12	0.82
1:S:160:ASP:OD1	1:S:161:ASN:ND2	2.12	0.82
1:j:160:ASP:OD1	1:j:161:ASN:ND2	2.12	0.82
1:w:160:ASP:OD1	1:w:161:ASN:ND2	2.12	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:z:160:ASP:OD1	1:z:161:ASN:ND2	2.12	0.82
1:7:160:ASP:OD1	1:7:161:ASN:ND2	2.12	0.82
1:c:160:ASP:OD1	1:c:161:ASN:ND2	2.12	0.82
1:h:160:ASP:OD1	1:h:161:ASN:ND2	2.12	0.82
1:v:160:ASP:OD1	1:v:161:ASN:ND2	2.12	0.82
1:l:160:ASP:OD1	1:l:161:ASN:ND2	2.12	0.82
1:u:160:ASP:OD1	1:u:161:ASN:ND2	2.12	0.82
1:O:160:ASP:OD1	1:O:161:ASN:ND2	2.12	0.82
1:Q:160:ASP:OD1	1:Q:161:ASN:ND2	2.12	0.82
1:4:160:ASP:OD1	1:4:161:ASN:ND2	2.12	0.82
1:T:160:ASP:OD1	1:T:161:ASN:ND2	2.12	0.82
1:W:160:ASP:OD1	1:W:161:ASN:ND2	2.12	0.82
1:X:160:ASP:OD1	1:X:161:ASN:ND2	2.12	0.82
1:f:160:ASP:OD1	1:f:161:ASN:ND2	2.12	0.82
1:6:160:ASP:OD1	1:6:161:ASN:ND2	2.12	0.82
1:x:160:ASP:OD1	1:x:161:ASN:ND2	2.12	0.82
1:F:160:ASP:OD1	1:F:161:ASN:ND2	2.12	0.82
1:G:160:ASP:OD1	1:G:161:ASN:ND2	2.12	0.82
1:J:160:ASP:OD1	1:J:161:ASN:ND2	2.12	0.82
1:g:160:ASP:OD1	1:g:161:ASN:ND2	2.12	0.82
1:t:160:ASP:OD1	1:t:161:ASN:ND2	2.12	0.82
1:y:160:ASP:OD1	1:y:161:ASN:ND2	2.12	0.82
1:Y:160:ASP:OD1	1:Y:161:ASN:ND2	2.12	0.82
1:H:160:ASP:OD1	1:H:161:ASN:ND2	2.12	0.82
1:V:160:ASP:OD1	1:V:161:ASN:ND2	2.12	0.82
1:Z:160:ASP:OD1	1:Z:161:ASN:ND2	2.12	0.82
1:b:160:ASP:OD1	1:b:161:ASN:ND2	2.12	0.82
1:o:160:ASP:OD1	1:o:161:ASN:ND2	2.12	0.82
1:p:160:ASP:OD1	1:p:161:ASN:ND2	2.12	0.82
1:A:160:ASP:OD1	1:A:161:ASN:ND2	2.12	0.81
1:C:160:ASP:OD1	1:C:161:ASN:ND2	2.12	0.81
1:E:160:ASP:OD1	1:E:161:ASN:ND2	2.12	0.81
1:m:160:ASP:OD1	1:m:161:ASN:ND2	2.12	0.81
1:P:160:ASP:OD1	1:P:161:ASN:ND2	2.12	0.81
1:s:160:ASP:OD1	1:s:161:ASN:ND2	2.12	0.81
1:5:160:ASP:OD1	1:5:161:ASN:ND2	2.12	0.81
1:D:160:ASP:OD1	1:D:161:ASN:ND2	2.12	0.81
1:U:160:ASP:OD1	1:U:161:ASN:ND2	2.12	0.81
1:q:160:ASP:OD1	1:q:161:ASN:ND2	2.12	0.81
1:B:160:ASP:OD1	1:B:161:ASN:ND2	2.12	0.81
1:I:160:ASP:OD1	1:I:161:ASN:ND2	2.12	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:160:ASP:OD1	1:a:161:ASN:ND2	2.12	0.81
1:n:160:ASP:OD1	1:n:161:ASN:ND2	2.12	0.81
1:r:160:ASP:OD1	1:r:161:ASN:ND2	2.12	0.81
1:5:203:GLN:N	1:5:203:GLN:OE1	2.16	0.79
1:l:203:GLN:OE1	1:l:203:GLN:N	2.16	0.79
1:v:203:GLN:OE1	1:v:203:GLN:N	2.16	0.79
1:H:203:GLN:OE1	1:H:203:GLN:N	2.16	0.79
1:N:203:GLN:N	1:N:203:GLN:OE1	2.16	0.79
1:R:203:GLN:N	1:R:203:GLN:OE1	2.16	0.79
1:b:203:GLN:N	1:b:203:GLN:OE1	2.16	0.79
1:c:203:GLN:N	1:c:203:GLN:OE1	2.16	0.79
1:L:203:GLN:N	1:L:203:GLN:OE1	2.16	0.79
1:S:203:GLN:N	1:S:203:GLN:OE1	2.16	0.79
1:V:203:GLN:OE1	1:V:203:GLN:N	2.16	0.79
1:m:203:GLN:N	1:m:203:GLN:OE1	2.16	0.79
1:4:203:GLN:OE1	1:4:203:GLN:N	2.16	0.79
1:D:203:GLN:N	1:D:203:GLN:OE1	2.16	0.79
1:G:203:GLN:N	1:G:203:GLN:OE1	2.16	0.79
1:I:203:GLN:N	1:I:203:GLN:OE1	2.16	0.79
1:f:203:GLN:N	1:f:203:GLN:OE1	2.16	0.79
1:6:203:GLN:N	1:6:203:GLN:OE1	2.16	0.79
1:Q:203:GLN:N	1:Q:203:GLN:OE1	2.16	0.79
1:W:203:GLN:N	1:W:203:GLN:OE1	2.16	0.79
1:M:203:GLN:N	1:M:203:GLN:OE1	2.16	0.79
1:1:203:GLN:N	1:1:203:GLN:OE1	2.16	0.79
1:2:203:GLN:OE1	1:2:203:GLN:N	2.16	0.79
1:a:203:GLN:N	1:a:203:GLN:OE1	2.16	0.79
1:p:203:GLN:N	1:p:203:GLN:OE1	2.16	0.79
1:w:203:GLN:N	1:w:203:GLN:OE1	2.16	0.79
1:A:203:GLN:N	1:A:203:GLN:OE1	2.16	0.79
1:i:203:GLN:N	1:i:203:GLN:OE1	2.16	0.79
1:k:203:GLN:N	1:k:203:GLN:OE1	2.16	0.79
1:s:203:GLN:N	1:s:203:GLN:OE1	2.16	0.79
1:y:203:GLN:OE1	1:y:203:GLN:N	2.16	0.79
1:E:203:GLN:OE1	1:E:203:GLN:N	2.16	0.78
1:T:203:GLN:OE1	1:T:203:GLN:N	2.16	0.78
1:u:203:GLN:N	1:u:203:GLN:OE1	2.16	0.78
1:O:203:GLN:OE1	1:O:203:GLN:N	2.16	0.78
1:Y:203:GLN:OE1	1:Y:203:GLN:N	2.16	0.78
1:o:203:GLN:OE1	1:o:203:GLN:N	2.16	0.78
1:d:203:GLN:N	1:d:203:GLN:OE1	2.16	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:g:203:GLN:N	1:g:203:GLN:OE1	2.16	0.78
1:J:203:GLN:OE1	1:J:203:GLN:N	2.16	0.78
1:e:203:GLN:OE1	1:e:203:GLN:N	2.16	0.78
1:z:203:GLN:N	1:z:203:GLN:OE1	2.16	0.78
1:C:203:GLN:OE1	1:C:203:GLN:N	2.16	0.78
1:K:203:GLN:N	1:K:203:GLN:OE1	2.16	0.78
1:P:203:GLN:N	1:P:203:GLN:OE1	2.16	0.78
1:U:203:GLN:N	1:U:203:GLN:OE1	2.16	0.78
1:j:203:GLN:OE1	1:j:203:GLN:N	2.16	0.78
1:7:203:GLN:N	1:7:203:GLN:OE1	2.16	0.78
1:F:203:GLN:N	1:F:203:GLN:OE1	2.16	0.78
1:r:203:GLN:N	1:r:203:GLN:OE1	2.16	0.78
1:Z:203:GLN:N	1:Z:203:GLN:OE1	2.16	0.78
1:S:186:ASN:ND2	1:T:153:GLU:OE2	2.17	0.78
1:T:186:ASN:ND2	1:U:153:GLU:OE2	2.17	0.78
1:n:203:GLN:N	1:n:203:GLN:OE1	2.16	0.78
1:B:203:GLN:N	1:B:203:GLN:OE1	2.16	0.78
1:e:186:ASN:ND2	1:f:153:GLU:OE2	2.17	0.78
1:f:186:ASN:ND2	1:g:153:GLU:OE2	2.17	0.78
1:t:203:GLN:OE1	1:t:203:GLN:N	2.16	0.78
1:R:186:ASN:ND2	1:S:153:GLU:OE2	2.17	0.77
1:d:186:ASN:ND2	1:e:153:GLU:OE2	2.17	0.77
1:w:186:ASN:ND2	1:x:153:GLU:OE2	2.17	0.77
1:3:203:GLN:N	1:3:203:GLN:OE1	2.16	0.77
1:g:186:ASN:ND2	1:h:153:GLU:OE2	2.17	0.77
1:X:203:GLN:N	1:X:203:GLN:OE1	2.16	0.77
1:h:203:GLN:N	1:h:203:GLN:OE1	2.16	0.77
1:k:186:ASN:ND2	1:l:153:GLU:OE2	2.17	0.77
1:q:203:GLN:OE1	1:q:203:GLN:N	2.16	0.77
1:x:203:GLN:N	1:x:203:GLN:OE1	2.16	0.77
1:K:186:ASN:ND2	1:L:153:GLU:OE2	2.17	0.77
1:Q:186:ASN:ND2	1:R:153:GLU:OE2	2.17	0.77
1:S:152:ILE:HG23	1:T:39:GLU:OE1	1.85	0.77
1:U:186:ASN:ND2	1:V:153:GLU:OE2	2.17	0.77
1:a:152:ILE:HG23	1:b:39:GLU:OE1	1.85	0.77
1:l:152:ILE:HG23	1:m:39:GLU:OE1	1.85	0.77
1:x:186:ASN:ND2	1:y:153:GLU:OE2	2.17	0.77
1:K:152:ILE:HG23	1:L:39:GLU:OE1	1.85	0.77
1:c:186:ASN:ND2	1:d:153:GLU:OE2	2.17	0.77
1:h:152:ILE:HG23	1:i:39:GLU:OE1	1.85	0.77
1:0:152:ILE:HG23	1:1:39:GLU:OE1	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:203:GLN:N	1:O:203:GLN:OE1	2.16	0.77
1:C:152:ILE:HG23	1:D:39:GLU:OE1	1.85	0.77
1:M:186:ASN:ND2	1:N:153:GLU:OE2	2.17	0.77
1:N:186:ASN:ND2	1:O:153:GLU:OE2	2.17	0.77
1:d:152:ILE:HG23	1:e:39:GLU:OE1	1.85	0.77
1:s:152:ILE:HG23	1:t:39:GLU:OE1	1.85	0.77
1:O:39:GLU:OE1	1:z:152:ILE:HG23	1.85	0.77
1:A:186:ASN:ND2	1:B:153:GLU:OE2	2.17	0.77
1:J:186:ASN:ND2	1:K:153:GLU:OE2	2.17	0.77
1:h:186:ASN:ND2	1:i:153:GLU:OE2	2.17	0.77
1:l:186:ASN:ND2	1:m:153:GLU:OE2	2.17	0.77
1:p:152:ILE:HG23	1:q:39:GLU:OE1	1.85	0.77
1:p:186:ASN:ND2	1:q:153:GLU:OE2	2.17	0.77
1:u:186:ASN:ND2	1:v:153:GLU:OE2	2.17	0.77
1:w:152:ILE:HG23	1:x:39:GLU:OE1	1.85	0.77
1:2:152:ILE:HG23	1:3:39:GLU:OE1	1.85	0.77
1:A:152:ILE:HG23	1:B:39:GLU:OE1	1.85	0.77
1:T:152:ILE:HG23	1:U:39:GLU:OE1	1.85	0.77
1:V:152:ILE:HG23	1:W:39:GLU:OE1	1.85	0.77
1:V:186:ASN:ND2	1:W:153:GLU:OE2	2.17	0.77
1:W:152:ILE:HG23	1:X:39:GLU:OE1	1.85	0.77
1:g:152:ILE:HG23	1:h:39:GLU:OE1	1.85	0.77
1:o:152:ILE:HG23	1:p:39:GLU:OE1	1.85	0.77
1:q:186:ASN:ND2	1:r:153:GLU:OE2	2.17	0.77
1:1:186:ASN:ND2	1:2:153:GLU:OE2	2.17	0.77
1:2:186:ASN:ND2	1:3:153:GLU:OE2	2.17	0.77
1:3:186:ASN:ND2	1:4:153:GLU:OE2	2.17	0.77
1:5:152:ILE:HG23	1:6:39:GLU:OE1	1.85	0.77
1:H:152:ILE:HG23	1:I:39:GLU:OE1	1.85	0.77
1:I:152:ILE:HG23	1:J:39:GLU:OE1	1.85	0.77
1:O:186:ASN:ND2	1:P:153:GLU:OE2	2.17	0.77
1:P:152:ILE:HG23	1:Q:39:GLU:OE1	1.85	0.77
1:b:186:ASN:ND2	1:c:153:GLU:OE2	2.17	0.77
1:r:152:ILE:HG23	1:s:39:GLU:OE1	1.85	0.77
1:t:186:ASN:ND2	1:u:153:GLU:OE2	2.17	0.77
1:x:152:ILE:HG23	1:y:39:GLU:OE1	1.85	0.77
1:F:152:ILE:HG23	1:G:39:GLU:OE1	1.85	0.77
1:H:186:ASN:ND2	1:I:153:GLU:OE2	2.17	0.77
1:N:152:ILE:HG23	1:O:39:GLU:OE1	1.85	0.77
1:P:186:ASN:ND2	1:Q:153:GLU:OE2	2.17	0.77
1:e:152:ILE:HG23	1:f:39:GLU:OE1	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:o:186:ASN:ND2	1:p:153:GLU:OE2	2.17	0.77
1:r:186:ASN:ND2	1:s:153:GLU:OE2	2.17	0.77
1:s:186:ASN:ND2	1:t:153:GLU:OE2	2.17	0.77
1:u:152:ILE:HG23	1:v:39:GLU:OE1	1.85	0.77
1:y:186:ASN:ND2	1:z:153:GLU:OE2	2.17	0.77
1:4:186:ASN:ND2	1:5:153:GLU:OE2	2.17	0.76
1:B:186:ASN:ND2	1:C:153:GLU:OE2	2.17	0.76
1:E:186:ASN:ND2	1:F:153:GLU:OE2	2.17	0.76
1:I:186:ASN:ND2	1:J:153:GLU:OE2	2.17	0.76
1:Q:152:ILE:HG23	1:R:39:GLU:OE1	1.85	0.76
1:b:152:ILE:HG23	1:c:39:GLU:OE1	1.85	0.76
1:0:186:ASN:ND2	1:1:153:GLU:OE2	2.17	0.76
1:3:152:ILE:HG23	1:4:39:GLU:OE1	1.85	0.76
1:D:152:ILE:HG23	1:E:39:GLU:OE1	1.85	0.76
1:D:186:ASN:ND2	1:E:153:GLU:OE2	2.17	0.76
1:F:186:ASN:ND2	1:G:153:GLU:OE2	2.17	0.76
1:G:186:ASN:ND2	1:H:153:GLU:OE2	2.17	0.76
1:Y:152:ILE:HG23	1:Z:39:GLU:OE1	1.85	0.76
1:i:186:ASN:ND2	1:j:153:GLU:OE2	2.17	0.76
1:m:152:ILE:HG23	1:n:39:GLU:OE1	1.85	0.76
1:6:186:ASN:ND2	1:7:153:GLU:OE2	2.17	0.76
1:W:186:ASN:ND2	1:X:153:GLU:OE2	2.17	0.76
1:f:152:ILE:HG23	1:g:39:GLU:OE1	1.85	0.76
1:k:152:ILE:HG23	1:l:39:GLU:OE1	1.85	0.76
1:m:186:ASN:ND2	1:n:153:GLU:OE2	2.17	0.76
1:5:186:ASN:ND2	1:6:153:GLU:OE2	2.17	0.76
1:a:186:ASN:ND2	1:b:153:GLU:OE2	2.17	0.76
1:C:186:ASN:ND2	1:D:153:GLU:OE2	2.17	0.76
1:n:152:ILE:HG23	1:o:39:GLU:OE1	1.85	0.76
1:n:186:ASN:ND2	1:o:153:GLU:OE2	2.17	0.76
1:t:152:ILE:HG23	1:u:39:GLU:OE1	1.85	0.76
1:0:153:GLU:OE2	1:z:186:ASN:ND2	2.17	0.76
1:M:152:ILE:HG23	1:N:39:GLU:OE1	1.85	0.76
1:O:152:ILE:HG23	1:P:39:GLU:OE1	1.85	0.76
1:c:152:ILE:HG23	1:d:39:GLU:OE1	1.85	0.76
1:1:152:ILE:HG23	1:2:39:GLU:OE1	1.85	0.76
1:4:152:ILE:HG23	1:5:39:GLU:OE1	1.85	0.76
1:E:152:ILE:HG23	1:F:39:GLU:OE1	1.85	0.76
1:R:152:ILE:HG23	1:S:39:GLU:OE1	1.85	0.76
1:Y:186:ASN:ND2	1:Z:153:GLU:OE2	2.17	0.76
1:Z:152:ILE:HG23	1:a:39:GLU:OE1	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:i:152:ILE:HG23	1:j:39:GLU:OE1	1.85	0.76
1:G:152:ILE:HG23	1:H:39:GLU:OE1	1.85	0.76
1:Z:186:ASN:ND2	1:a:153:GLU:OE2	2.17	0.76
1:J:152:ILE:HG23	1:K:39:GLU:OE1	1.85	0.76
1:B:152:ILE:HG23	1:C:39:GLU:OE1	1.85	0.75
1:6:152:ILE:HG23	1:7:39:GLU:OE1	1.85	0.75
1:q:152:ILE:HG23	1:r:39:GLU:OE1	1.85	0.75
1:U:152:ILE:HG23	1:V:39:GLU:OE1	1.85	0.75
1:y:152:ILE:HG23	1:z:39:GLU:OE1	1.85	0.75
1:O:170:ARG:O	1:O:173:THR:OG1	2.08	0.72
1:N:170:ARG:O	1:N:173:THR:OG1	2.08	0.71
1:A:170:ARG:O	1:A:173:THR:OG1	2.08	0.71
1:C:170:ARG:O	1:C:173:THR:OG1	2.08	0.71
1:K:170:ARG:O	1:K:173:THR:OG1	2.08	0.71
1:e:170:ARG:O	1:e:173:THR:OG1	2.08	0.71
1:2:170:ARG:O	1:2:173:THR:OG1	2.08	0.71
1:F:170:ARG:O	1:F:173:THR:OG1	2.08	0.71
1:Y:170:ARG:O	1:Y:173:THR:OG1	2.08	0.71
1:n:170:ARG:O	1:n:173:THR:OG1	2.08	0.71
1:u:170:ARG:O	1:u:173:THR:OG1	2.08	0.71
1:5:170:ARG:O	1:5:173:THR:OG1	2.08	0.71
1:d:170:ARG:O	1:d:173:THR:OG1	2.08	0.71
1:h:170:ARG:O	1:h:173:THR:OG1	2.08	0.71
1:k:170:ARG:O	1:k:173:THR:OG1	2.08	0.71
1:R:170:ARG:O	1:R:173:THR:OG1	2.08	0.71
1:q:170:ARG:O	1:q:173:THR:OG1	2.08	0.71
1:J:170:ARG:O	1:J:173:THR:OG1	2.08	0.71
1:W:170:ARG:O	1:W:173:THR:OG1	2.08	0.71
1:X:170:ARG:O	1:X:173:THR:OG1	2.08	0.71
1:j:170:ARG:O	1:j:173:THR:OG1	2.08	0.71
1:r:170:ARG:O	1:r:173:THR:OG1	2.08	0.71
1:g:170:ARG:O	1:g:173:THR:OG1	2.08	0.70
1:z:170:ARG:O	1:z:173:THR:OG1	2.08	0.70
1:U:170:ARG:O	1:U:173:THR:OG1	2.08	0.70
1:p:170:ARG:O	1:p:173:THR:OG1	2.08	0.70
1:I:170:ARG:O	1:I:173:THR:OG1	2.08	0.70
1:V:170:ARG:O	1:V:173:THR:OG1	2.08	0.70
1:b:170:ARG:O	1:b:173:THR:OG1	2.08	0.70
1:c:170:ARG:O	1:c:173:THR:OG1	2.08	0.70
1:x:170:ARG:O	1:x:173:THR:OG1	2.08	0.70
1:M:170:ARG:O	1:M:173:THR:OG1	2.08	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:170:ARG:O	1:Q:173:THR:OG1	2.08	0.70
1:y:170:ARG:O	1:y:173:THR:OG1	2.08	0.70
1:f:170:ARG:O	1:f:173:THR:OG1	2.08	0.70
1:w:170:ARG:O	1:w:173:THR:OG1	2.08	0.70
1:E:170:ARG:O	1:E:173:THR:OG1	2.08	0.69
1:P:170:ARG:O	1:P:173:THR:OG1	2.08	0.69
1:a:170:ARG:O	1:a:173:THR:OG1	2.08	0.69
1:6:170:ARG:O	1:6:173:THR:OG1	2.08	0.69
1:B:170:ARG:O	1:B:173:THR:OG1	2.08	0.69
1:1:170:ARG:O	1:1:173:THR:OG1	2.08	0.69
1:H:170:ARG:O	1:H:173:THR:OG1	2.08	0.69
1:S:170:ARG:O	1:S:173:THR:OG1	2.08	0.69
1:4:170:ARG:O	1:4:173:THR:OG1	2.08	0.69
1:T:170:ARG:O	1:T:173:THR:OG1	2.08	0.69
1:l:170:ARG:O	1:l:173:THR:OG1	2.08	0.69
1:7:170:ARG:O	1:7:173:THR:OG1	2.08	0.69
1:L:170:ARG:O	1:L:173:THR:OG1	2.08	0.69
1:t:170:ARG:O	1:t:173:THR:OG1	2.08	0.69
1:o:170:ARG:O	1:o:173:THR:OG1	2.08	0.68
1:v:170:ARG:O	1:v:173:THR:OG1	2.08	0.68
1:i:170:ARG:O	1:i:173:THR:OG1	2.08	0.68
1:m:170:ARG:O	1:m:173:THR:OG1	2.08	0.68
1:s:170:ARG:O	1:s:173:THR:OG1	2.08	0.68
1:G:170:ARG:O	1:G:173:THR:OG1	2.08	0.67
1:o:183:GLU:OE2	1:z:55:LYS:NZ	2.28	0.67
1:O:183:GLU:OE2	1:Z:55:LYS:NZ	2.28	0.67
1:P:183:GLU:OE2	1:a:55:LYS:NZ	2.28	0.67
1:W:183:GLU:OE2	1:h:55:LYS:NZ	2.28	0.67
1:Z:170:ARG:O	1:Z:173:THR:OG1	2.08	0.67
1:n:183:GLU:OE2	1:y:55:LYS:NZ	2.28	0.67
1:I:183:GLU:OE2	1:T:55:LYS:NZ	2.28	0.67
1:J:183:GLU:OE2	1:U:55:LYS:NZ	2.28	0.67
1:V:183:GLU:OE2	1:g:55:LYS:NZ	2.28	0.67
1:b:183:GLU:OE2	1:m:55:LYS:NZ	2.28	0.67
1:4:183:GLU:OE2	1:H:55:LYS:NZ	2.28	0.67
1:N:183:GLU:OE2	1:Y:55:LYS:NZ	2.28	0.67
1:U:183:GLU:OE2	1:f:55:LYS:NZ	2.28	0.67
1:a:183:GLU:OE2	1:l:55:LYS:NZ	2.28	0.67
1:0:55:LYS:NZ	1:p:183:GLU:OE2	2.28	0.67
1:3:183:GLU:OE2	1:G:55:LYS:NZ	2.28	0.67
1:5:183:GLU:OE2	1:I:55:LYS:NZ	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:183:GLU:OE2	1:S:55:LYS:NZ	2.28	0.67
1:Q:183:GLU:OE2	1:b:55:LYS:NZ	2.28	0.67
1:X:183:GLU:OE2	1:i:55:LYS:NZ	2.28	0.67
1:c:183:GLU:OE2	1:n:55:LYS:NZ	2.28	0.67
1:h:183:GLU:OE2	1:s:55:LYS:NZ	2.28	0.67
1:m:183:GLU:OE2	1:x:55:LYS:NZ	2.28	0.67
1:2:183:GLU:OE2	1:F:55:LYS:NZ	2.28	0.67
1:K:183:GLU:OE2	1:V:55:LYS:NZ	2.28	0.67
1:Z:183:GLU:OE2	1:k:55:LYS:NZ	2.28	0.67
1:i:183:GLU:OE2	1:t:55:LYS:NZ	2.28	0.67
1:j:183:GLU:OE2	1:u:55:LYS:NZ	2.28	0.67
1:6:183:GLU:OE2	1:J:55:LYS:NZ	2.28	0.67
1:T:183:GLU:OE2	1:e:55:LYS:NZ	2.28	0.67
1:g:183:GLU:OE2	1:r:55:LYS:NZ	2.28	0.67
1:0:183:GLU:OE2	1:D:55:LYS:NZ	2.28	0.67
1:1:183:GLU:OE2	1:E:55:LYS:NZ	2.28	0.67
1:G:183:GLU:OE2	1:R:55:LYS:NZ	2.28	0.67
1:d:183:GLU:OE2	1:o:55:LYS:NZ	2.28	0.67
1:1:55:LYS:NZ	1:q:183:GLU:OE2	2.28	0.66
1:B:183:GLU:OE2	1:M:55:LYS:NZ	2.28	0.66
1:3:55:LYS:NZ	1:s:183:GLU:OE2	2.28	0.66
1:6:55:LYS:NZ	1:v:183:GLU:OE2	2.28	0.66
1:C:55:LYS:NZ	1:z:183:GLU:OE2	2.28	0.66
1:D:170:ARG:O	1:D:173:THR:OG1	2.08	0.66
1:L:183:GLU:OE2	1:W:55:LYS:NZ	2.28	0.66
1:l:183:GLU:OE2	1:w:55:LYS:NZ	2.28	0.66
1:B:55:LYS:NZ	1:y:183:GLU:OE2	2.28	0.66
1:C:183:GLU:OE2	1:N:55:LYS:NZ	2.28	0.66
1:R:183:GLU:OE2	1:c:55:LYS:NZ	2.28	0.66
1:S:183:GLU:OE2	1:d:55:LYS:NZ	2.28	0.66
1:f:183:GLU:OE2	1:q:55:LYS:NZ	2.28	0.66
1:2:55:LYS:NZ	1:r:183:GLU:OE2	2.28	0.66
1:D:183:GLU:OE2	1:O:55:LYS:NZ	2.28	0.66
1:F:183:GLU:OE2	1:Q:55:LYS:NZ	2.28	0.66
1:e:183:GLU:OE2	1:p:55:LYS:NZ	2.28	0.66
1:7:183:GLU:OE2	1:K:55:LYS:NZ	2.28	0.66
1:A:55:LYS:NZ	1:x:183:GLU:OE2	2.28	0.66
1:E:183:GLU:OE2	1:P:55:LYS:NZ	2.28	0.66
1:5:55:LYS:NZ	1:u:183:GLU:OE2	2.28	0.66
1:3:170:ARG:O	1:3:173:THR:OG1	2.08	0.66
1:4:55:LYS:NZ	1:t:183:GLU:OE2	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:170:ARG:O	1:0:173:THR:OG1	2.08	0.65
1:C:209:LEU:HD12	1:C:212:MET:HB2	1.81	0.63
1:2:209:LEU:HD12	1:2:212:MET:HB2	1.81	0.63
1:u:209:LEU:HD12	1:u:212:MET:HB2	1.81	0.63
1:0:209:LEU:HD12	1:0:212:MET:HB2	1.81	0.63
1:h:209:LEU:HD12	1:h:212:MET:HB2	1.81	0.63
1:j:209:LEU:HD12	1:j:212:MET:HB2	1.81	0.63
1:r:209:LEU:HD12	1:r:212:MET:HB2	1.81	0.63
1:N:209:LEU:HD12	1:N:212:MET:HB2	1.81	0.62
1:s:209:LEU:HD12	1:s:212:MET:HB2	1.81	0.62
1:z:209:LEU:HD12	1:z:212:MET:HB2	1.81	0.62
1:M:209:LEU:HD12	1:M:212:MET:HB2	1.81	0.62
1:p:209:LEU:HD12	1:p:212:MET:HB2	1.81	0.62
1:A:209:LEU:HD12	1:A:212:MET:HB2	1.81	0.62
1:F:209:LEU:HD12	1:F:212:MET:HB2	1.81	0.62
1:E:209:LEU:HD12	1:E:212:MET:HB2	1.81	0.62
1:c:163:SER:O	1:c:166:SER:OG	2.16	0.62
1:4:209:LEU:HD12	1:4:212:MET:HB2	1.81	0.62
1:5:209:LEU:HD12	1:5:212:MET:HB2	1.81	0.62
1:x:209:LEU:HD12	1:x:212:MET:HB2	1.81	0.62
1:3:209:LEU:HD12	1:3:212:MET:HB2	1.81	0.62
1:B:209:LEU:HD12	1:B:212:MET:HB2	1.81	0.62
1:D:209:LEU:HD12	1:D:212:MET:HB2	1.81	0.62
1:v:209:LEU:HD12	1:v:212:MET:HB2	1.81	0.62
1:1:209:LEU:HD12	1:1:212:MET:HB2	1.81	0.62
1:J:209:LEU:HD12	1:J:212:MET:HB2	1.81	0.62
1:K:209:LEU:HD12	1:K:212:MET:HB2	1.81	0.62
1:P:209:LEU:HD12	1:P:212:MET:HB2	1.81	0.62
1:W:209:LEU:HD12	1:W:212:MET:HB2	1.81	0.62
1:g:209:LEU:HD12	1:g:212:MET:HB2	1.81	0.62
1:L:209:LEU:HD12	1:L:212:MET:HB2	1.81	0.61
1:o:209:LEU:HD12	1:o:212:MET:HB2	1.81	0.61
1:t:209:LEU:HD12	1:t:212:MET:HB2	1.81	0.61
1:R:209:LEU:HD12	1:R:212:MET:HB2	1.81	0.61
1:S:209:LEU:HD12	1:S:212:MET:HB2	1.81	0.61
1:T:209:LEU:HD12	1:T:212:MET:HB2	1.81	0.61
1:X:209:LEU:HD12	1:X:212:MET:HB2	1.81	0.61
1:b:209:LEU:HD12	1:b:212:MET:HB2	1.81	0.61
1:w:209:LEU:HD12	1:w:212:MET:HB2	1.81	0.61
1:c:209:LEU:HD12	1:c:212:MET:HB2	1.81	0.61
1:i:209:LEU:HD12	1:i:212:MET:HB2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:209:LEU:HD12	1:I:212:MET:HB2	1.81	0.61
1:U:209:LEU:HD12	1:U:212:MET:HB2	1.81	0.61
1:Y:209:LEU:HD12	1:Y:212:MET:HB2	1.81	0.61
1:a:209:LEU:HD12	1:a:212:MET:HB2	1.81	0.61
1:e:209:LEU:HD12	1:e:212:MET:HB2	1.81	0.61
1:d:209:LEU:HD12	1:d:212:MET:HB2	1.81	0.61
1:k:209:LEU:HD12	1:k:212:MET:HB2	1.81	0.61
1:l:209:LEU:HD12	1:l:212:MET:HB2	1.81	0.61
1:q:209:LEU:HD12	1:q:212:MET:HB2	1.81	0.61
1:7:209:LEU:HD12	1:7:212:MET:HB2	1.81	0.61
1:H:209:LEU:HD12	1:H:212:MET:HB2	1.81	0.61
1:Z:209:LEU:HD12	1:Z:212:MET:HB2	1.81	0.61
1:Q:209:LEU:HD12	1:Q:212:MET:HB2	1.81	0.61
1:m:209:LEU:HD12	1:m:212:MET:HB2	1.81	0.61
1:V:209:LEU:HD12	1:V:212:MET:HB2	1.81	0.61
1:f:209:LEU:HD12	1:f:212:MET:HB2	1.81	0.61
1:y:209:LEU:HD12	1:y:212:MET:HB2	1.81	0.61
1:6:209:LEU:HD12	1:6:212:MET:HB2	1.81	0.60
1:n:209:LEU:HD12	1:n:212:MET:HB2	1.81	0.60
1:G:209:LEU:HD12	1:G:212:MET:HB2	1.81	0.60
1:O:209:LEU:HD12	1:O:212:MET:HB2	1.81	0.60
1:V:163:SER:O	1:V:166:SER:OG	2.16	0.59
1:X:163:SER:O	1:X:166:SER:OG	2.16	0.59
1:F:163:SER:O	1:F:166:SER:OG	2.16	0.58
1:l:163:SER:O	1:l:166:SER:OG	2.16	0.58
1:1:190:SER:N	1:1:193:ASP:OD2	2.37	0.58
1:H:190:SER:N	1:H:193:ASP:OD2	2.37	0.58
1:Z:190:SER:N	1:Z:193:ASP:OD2	2.37	0.58
1:f:163:SER:O	1:f:166:SER:OG	2.16	0.58
1:5:190:SER:N	1:5:193:ASP:OD2	2.37	0.58
1:E:190:SER:N	1:E:193:ASP:OD2	2.37	0.58
1:j:190:SER:N	1:j:193:ASP:OD2	2.37	0.58
1:r:190:SER:N	1:r:193:ASP:OD2	2.37	0.58
1:u:190:SER:N	1:u:193:ASP:OD2	2.37	0.58
1:4:190:SER:N	1:4:193:ASP:OD2	2.37	0.58
1:B:190:SER:N	1:B:193:ASP:OD2	2.37	0.58
1:L:190:SER:N	1:L:193:ASP:OD2	2.37	0.58
1:O:190:SER:N	1:O:193:ASP:OD2	2.37	0.58
1:P:190:SER:N	1:P:193:ASP:OD2	2.37	0.58
1:R:190:SER:N	1:R:193:ASP:OD2	2.37	0.58
1:V:190:SER:N	1:V:193:ASP:OD2	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:d:190:SER:N	1:d:193:ASP:OD2	2.37	0.58
1:n:190:SER:N	1:n:193:ASP:OD2	2.37	0.58
1:f:190:SER:N	1:f:193:ASP:OD2	2.37	0.58
1:x:190:SER:N	1:x:193:ASP:OD2	2.37	0.58
1:7:190:SER:N	1:7:193:ASP:OD2	2.37	0.58
1:A:190:SER:N	1:A:193:ASP:OD2	2.37	0.58
1:D:190:SER:N	1:D:193:ASP:OD2	2.37	0.58
1:T:190:SER:N	1:T:193:ASP:OD2	2.37	0.58
1:p:190:SER:N	1:p:193:ASP:OD2	2.37	0.58
1:t:190:SER:N	1:t:193:ASP:OD2	2.37	0.58
1:2:190:SER:N	1:2:193:ASP:OD2	2.37	0.58
1:l:190:SER:N	1:l:193:ASP:OD2	2.37	0.58
1:K:190:SER:N	1:K:193:ASP:OD2	2.37	0.58
1:M:190:SER:N	1:M:193:ASP:OD2	2.37	0.58
1:X:190:SER:N	1:X:193:ASP:OD2	2.37	0.58
1:Y:190:SER:N	1:Y:193:ASP:OD2	2.37	0.58
1:h:190:SER:N	1:h:193:ASP:OD2	2.37	0.58
1:k:190:SER:N	1:k:193:ASP:OD2	2.37	0.58
1:y:190:SER:N	1:y:193:ASP:OD2	2.37	0.58
1:z:190:SER:N	1:z:193:ASP:OD2	2.37	0.58
1:4:206:GLU:O	1:4:210:ALA:N	2.38	0.57
1:I:190:SER:N	1:I:193:ASP:OD2	2.37	0.57
1:S:190:SER:N	1:S:193:ASP:OD2	2.37	0.57
1:q:190:SER:N	1:q:193:ASP:OD2	2.37	0.57
1:G:190:SER:N	1:G:193:ASP:OD2	2.37	0.57
1:G:206:GLU:O	1:G:210:ALA:N	2.38	0.57
1:N:190:SER:N	1:N:193:ASP:OD2	2.37	0.57
1:U:190:SER:N	1:U:193:ASP:OD2	2.37	0.57
1:a:190:SER:N	1:a:193:ASP:OD2	2.37	0.57
1:b:190:SER:N	1:b:193:ASP:OD2	2.37	0.57
1:c:190:SER:N	1:c:193:ASP:OD2	2.37	0.57
1:m:190:SER:N	1:m:193:ASP:OD2	2.37	0.57
1:o:190:SER:N	1:o:193:ASP:OD2	2.37	0.57
1:u:206:GLU:O	1:u:210:ALA:N	2.38	0.57
1:v:190:SER:N	1:v:193:ASP:OD2	2.37	0.57
1:3:190:SER:N	1:3:193:ASP:OD2	2.37	0.57
1:F:190:SER:N	1:F:193:ASP:OD2	2.37	0.57
1:H:206:GLU:O	1:H:210:ALA:N	2.38	0.57
1:J:190:SER:N	1:J:193:ASP:OD2	2.37	0.57
1:M:206:GLU:O	1:M:210:ALA:N	2.38	0.57
1:Q:206:GLU:O	1:Q:210:ALA:N	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:g:190:SER:N	1:g:193:ASP:OD2	2.37	0.57
1:0:190:SER:N	1:0:193:ASP:OD2	2.37	0.57
1:3:206:GLU:O	1:3:210:ALA:N	2.38	0.57
1:5:206:GLU:O	1:5:210:ALA:N	2.38	0.57
1:C:206:GLU:O	1:C:210:ALA:N	2.38	0.57
1:W:190:SER:N	1:W:193:ASP:OD2	2.37	0.57
1:a:206:GLU:O	1:a:210:ALA:N	2.38	0.57
1:e:190:SER:N	1:e:193:ASP:OD2	2.37	0.57
1:i:190:SER:N	1:i:193:ASP:OD2	2.37	0.57
1:t:206:GLU:O	1:t:210:ALA:N	2.38	0.57
1:v:206:GLU:O	1:v:210:ALA:N	2.38	0.57
1:w:190:SER:N	1:w:193:ASP:OD2	2.37	0.57
1:0:206:GLU:O	1:0:210:ALA:N	2.38	0.57
1:B:206:GLU:O	1:B:210:ALA:N	2.38	0.57
1:F:206:GLU:O	1:F:210:ALA:N	2.38	0.57
1:P:206:GLU:O	1:P:210:ALA:N	2.38	0.57
1:R:206:GLU:O	1:R:210:ALA:N	2.38	0.57
1:j:206:GLU:O	1:j:210:ALA:N	2.38	0.57
1:s:190:SER:N	1:s:193:ASP:OD2	2.37	0.57
1:6:190:SER:N	1:6:193:ASP:OD2	2.37	0.57
1:Z:206:GLU:O	1:Z:210:ALA:N	2.38	0.57
1:t:163:SER:O	1:t:166:SER:OG	2.16	0.57
1:C:190:SER:N	1:C:193:ASP:OD2	2.37	0.57
1:N:163:SER:O	1:N:166:SER:OG	2.16	0.57
1:N:206:GLU:O	1:N:210:ALA:N	2.38	0.57
1:Q:190:SER:N	1:Q:193:ASP:OD2	2.37	0.57
1:q:206:GLU:O	1:q:210:ALA:N	2.38	0.57
1:K:206:GLU:O	1:K:210:ALA:N	2.38	0.57
1:k:206:GLU:O	1:k:210:ALA:N	2.38	0.57
1:z:206:GLU:O	1:z:210:ALA:N	2.38	0.57
1:D:206:GLU:O	1:D:210:ALA:N	2.38	0.57
1:1:206:GLU:O	1:1:210:ALA:N	2.38	0.56
1:6:206:GLU:O	1:6:210:ALA:N	2.38	0.56
1:p:163:SER:O	1:p:166:SER:OG	2.16	0.56
1:2:206:GLU:O	1:2:210:ALA:N	2.38	0.56
1:7:206:GLU:O	1:7:210:ALA:N	2.38	0.56
1:b:206:GLU:O	1:b:210:ALA:N	2.38	0.56
1:r:206:GLU:O	1:r:210:ALA:N	2.38	0.56
1:E:206:GLU:O	1:E:210:ALA:N	2.38	0.56
1:I:206:GLU:O	1:I:210:ALA:N	2.38	0.56
1:J:206:GLU:O	1:J:210:ALA:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:206:GLU:O	1:T:210:ALA:N	2.38	0.56
1:U:206:GLU:O	1:U:210:ALA:N	2.38	0.56
1:X:206:GLU:O	1:X:210:ALA:N	2.38	0.56
1:d:206:GLU:O	1:d:210:ALA:N	2.38	0.56
1:g:206:GLU:O	1:g:210:ALA:N	2.38	0.56
1:h:206:GLU:O	1:h:210:ALA:N	2.38	0.56
1:D:163:SER:O	1:D:166:SER:OG	2.16	0.56
1:L:206:GLU:O	1:L:210:ALA:N	2.38	0.56
1:O:206:GLU:O	1:O:210:ALA:N	2.38	0.56
1:n:206:GLU:O	1:n:210:ALA:N	2.38	0.56
1:s:206:GLU:O	1:s:210:ALA:N	2.38	0.56
1:x:206:GLU:O	1:x:210:ALA:N	2.38	0.56
1:w:206:GLU:O	1:w:210:ALA:N	2.38	0.56
1:A:206:GLU:O	1:A:210:ALA:N	2.38	0.56
1:V:206:GLU:O	1:V:210:ALA:N	2.38	0.56
1:W:206:GLU:O	1:W:210:ALA:N	2.38	0.56
1:Y:206:GLU:O	1:Y:210:ALA:N	2.38	0.56
1:e:206:GLU:O	1:e:210:ALA:N	2.38	0.56
1:p:206:GLU:O	1:p:210:ALA:N	2.38	0.56
1:f:206:GLU:O	1:f:210:ALA:N	2.38	0.56
1:m:206:GLU:O	1:m:210:ALA:N	2.38	0.56
1:S:206:GLU:O	1:S:210:ALA:N	2.38	0.56
1:l:206:GLU:O	1:l:210:ALA:N	2.38	0.56
1:i:206:GLU:O	1:i:210:ALA:N	2.38	0.55
1:o:206:GLU:O	1:o:210:ALA:N	2.38	0.55
1:j:163:SER:O	1:j:166:SER:OG	2.16	0.55
1:c:206:GLU:O	1:c:210:ALA:N	2.38	0.55
1:y:206:GLU:O	1:y:210:ALA:N	2.38	0.55
1:k:163:SER:O	1:k:166:SER:OG	2.16	0.55
1:6:163:SER:O	1:6:166:SER:OG	2.16	0.55
1:S:163:SER:O	1:S:166:SER:OG	2.16	0.55
1:1:163:SER:O	1:1:166:SER:OG	2.16	0.55
1:R:212:MET:HE3	1:U:91:LEU:HD21	1.89	0.55
1:1:212:MET:HE3	1:4:91:LEU:HD21	1.89	0.55
1:A:212:MET:HE3	1:D:91:LEU:HD21	1.89	0.55
1:G:212:MET:HE3	1:J:91:LEU:HD21	1.89	0.55
1:I:212:MET:HE3	1:L:91:LEU:HD21	1.89	0.55
1:N:212:MET:HE3	1:Q:91:LEU:HD21	1.89	0.55
1:2:91:LEU:HD21	1:z:212:MET:HE3	1.89	0.54
1:3:212:MET:HE3	1:6:91:LEU:HD21	1.89	0.54
1:C:212:MET:HE3	1:F:91:LEU:HD21	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:212:MET:HE3	1:H:91:LEU:HD21	1.89	0.54
1:P:212:MET:HE3	1:S:91:LEU:HD21	1.90	0.54
1:Y:212:MET:HE3	1:b:91:LEU:HD21	1.90	0.54
1:a:163:SER:O	1:a:166:SER:OG	2.16	0.54
1:r:212:MET:HE3	1:u:91:LEU:HD21	1.89	0.54
1:s:212:MET:HE3	1:v:91:LEU:HD21	1.90	0.54
1:0:212:MET:HE3	1:3:91:LEU:HD21	1.89	0.54
1:1:91:LEU:HD21	1:y:212:MET:HE3	1.89	0.54
1:B:212:MET:HE3	1:E:91:LEU:HD21	1.90	0.54
1:q:212:MET:HE3	1:t:91:LEU:HD21	1.90	0.54
1:2:212:MET:HE3	1:5:91:LEU:HD21	1.89	0.54
1:H:212:MET:HE3	1:K:91:LEU:HD21	1.89	0.54
1:M:212:MET:HE3	1:P:91:LEU:HD21	1.89	0.54
1:Q:212:MET:HE3	1:T:91:LEU:HD21	1.89	0.54
1:a:212:MET:HE3	1:d:91:LEU:HD21	1.90	0.54
1:g:212:MET:HE3	1:j:91:LEU:HD21	1.89	0.54
1:F:212:MET:HE3	1:I:91:LEU:HD21	1.89	0.54
1:Z:212:MET:HE3	1:c:91:LEU:HD21	1.90	0.54
1:z:163:SER:O	1:z:166:SER:OG	2.16	0.54
1:0:91:LEU:HD21	1:x:212:MET:HE3	1.89	0.54
1:4:212:MET:HE3	1:7:91:LEU:HD21	1.89	0.54
1:D:212:MET:HE3	1:G:91:LEU:HD21	1.89	0.54
1:c:212:MET:HE3	1:f:91:LEU:HD21	1.89	0.54
1:l:212:MET:HE3	1:o:91:LEU:HD21	1.89	0.54
1:p:212:MET:HE3	1:s:91:LEU:HD21	1.90	0.54
1:O:212:MET:HE3	1:R:91:LEU:HD21	1.90	0.54
1:S:212:MET:HE3	1:V:91:LEU:HD21	1.90	0.54
1:T:212:MET:HE3	1:W:91:LEU:HD21	1.90	0.54
1:U:212:MET:HE3	1:X:91:LEU:HD21	1.89	0.54
1:b:212:MET:HE3	1:e:91:LEU:HD21	1.90	0.54
1:e:212:MET:HE3	1:h:91:LEU:HD21	1.89	0.54
1:f:212:MET:HE3	1:i:91:LEU:HD21	1.89	0.54
1:k:212:MET:HE3	1:n:91:LEU:HD21	1.89	0.54
1:n:212:MET:HE3	1:q:91:LEU:HD21	1.89	0.54
1:o:212:MET:HE3	1:r:91:LEU:HD21	1.90	0.54
1:r:163:SER:O	1:r:166:SER:OG	2.16	0.54
1:w:212:MET:HE3	1:z:91:LEU:HD21	1.89	0.54
1:d:212:MET:HE3	1:g:91:LEU:HD21	1.89	0.54
1:g:163:SER:O	1:g:166:SER:OG	2.16	0.54
1:u:182:ARG:NH2	1:v:149:ALA:O	2.41	0.54
1:G:182:ARG:NH2	1:H:149:ALA:O	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:182:ARG:NH2	1:I:149:ALA:O	2.41	0.54
1:I:182:ARG:NH2	1:J:149:ALA:O	2.41	0.54
1:J:182:ARG:NH2	1:K:149:ALA:O	2.41	0.54
1:O:204:ALA:O	1:O:208:THR:OG1	2.26	0.54
1:U:163:SER:O	1:U:166:SER:OG	2.16	0.54
1:m:212:MET:HE3	1:p:91:LEU:HD21	1.90	0.54
1:t:182:ARG:NH2	1:u:149:ALA:O	2.41	0.54
1:E:182:ARG:NH2	1:F:149:ALA:O	2.41	0.54
1:F:182:ARG:NH2	1:G:149:ALA:O	2.41	0.54
1:K:182:ARG:NH2	1:L:149:ALA:O	2.41	0.54
1:s:182:ARG:NH2	1:t:149:ALA:O	2.41	0.54
1:D:182:ARG:NH2	1:E:149:ALA:O	2.41	0.53
1:a:182:ARG:NH2	1:b:149:ALA:O	2.41	0.53
1:C:182:ARG:NH2	1:D:149:ALA:O	2.41	0.53
1:G:204:ALA:O	1:G:208:THR:OG1	2.26	0.53
1:Z:182:ARG:NH2	1:a:149:ALA:O	2.41	0.53
1:b:182:ARG:NH2	1:c:149:ALA:O	2.41	0.53
1:c:182:ARG:NH2	1:d:149:ALA:O	2.41	0.53
1:3:204:ALA:O	1:3:208:THR:OG1	2.26	0.53
1:B:182:ARG:NH2	1:C:149:ALA:O	2.41	0.53
1:Y:182:ARG:NH2	1:Z:149:ALA:O	2.41	0.53
1:b:204:ALA:O	1:b:208:THR:OG1	2.26	0.53
1:A:182:ARG:NH2	1:B:149:ALA:O	2.41	0.53
1:G:163:SER:O	1:G:166:SER:OG	2.16	0.53
1:T:204:ALA:O	1:T:208:THR:OG1	2.26	0.53
1:d:182:ARG:NH2	1:e:149:ALA:O	2.41	0.53
1:e:204:ALA:O	1:e:208:THR:OG1	2.26	0.53
1:m:204:ALA:O	1:m:208:THR:OG1	2.26	0.53
1:P:204:ALA:O	1:P:208:THR:OG1	2.26	0.53
1:R:204:ALA:O	1:R:208:THR:OG1	2.26	0.53
1:c:204:ALA:O	1:c:208:THR:OG1	2.26	0.53
1:Q:204:ALA:O	1:Q:208:THR:OG1	2.26	0.53
1:e:182:ARG:NH2	1:f:149:ALA:O	2.41	0.53
1:W:163:SER:O	1:W:166:SER:OG	2.16	0.53
1:Z:204:ALA:O	1:Z:208:THR:OG1	2.26	0.53
1:d:163:SER:O	1:d:166:SER:OG	2.16	0.53
1:4:163:SER:O	1:4:166:SER:OG	2.16	0.52
1:Y:204:ALA:O	1:Y:208:THR:OG1	2.26	0.52
1:f:182:ARG:NH2	1:g:149:ALA:O	2.41	0.52
1:x:204:ALA:O	1:x:208:THR:OG1	2.26	0.52
1:B:163:SER:O	1:B:166:SER:OG	2.16	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:204:ALA:O	1:4:208:THR:OG1	2.26	0.52
1:D:204:ALA:O	1:D:208:THR:OG1	2.26	0.52
1:g:182:ARG:NH2	1:h:149:ALA:O	2.41	0.52
1:h:182:ARG:NH2	1:i:149:ALA:O	2.41	0.52
1:i:182:ARG:NH2	1:j:149:ALA:O	2.41	0.52
1:0:212:MET:HE1	1:3:72:TYR:CD1	2.45	0.52
1:1:212:MET:HE1	1:4:72:TYR:CD1	2.45	0.52
1:2:212:MET:HE1	1:5:72:TYR:CD1	2.45	0.52
1:6:182:ARG:NH2	1:7:149:ALA:O	2.41	0.52
1:e:163:SER:O	1:e:166:SER:OG	2.16	0.52
1:w:182:ARG:NH2	1:x:149:ALA:O	2.41	0.52
1:o:212:MET:HE1	1:r:72:TYR:CD1	2.45	0.52
1:p:212:MET:HE1	1:s:72:TYR:CD1	2.45	0.52
1:y:182:ARG:NH2	1:z:149:ALA:O	2.41	0.52
1:2:72:TYR:CD1	1:z:212:MET:HE1	2.45	0.52
1:3:212:MET:HE1	1:6:72:TYR:CD1	2.45	0.52
1:4:182:ARG:NH2	1:5:149:ALA:O	2.41	0.52
1:5:182:ARG:NH2	1:6:149:ALA:O	2.41	0.52
1:S:204:ALA:O	1:S:208:THR:OG1	2.26	0.52
1:n:212:MET:HE1	1:q:72:TYR:CD1	2.45	0.52
1:u:163:SER:O	1:u:166:SER:OG	2.16	0.52
1:x:182:ARG:NH2	1:y:149:ALA:O	2.41	0.52
1:1:72:TYR:CD1	1:y:212:MET:HE1	2.45	0.52
1:2:182:ARG:NH2	1:3:149:ALA:O	2.41	0.52
1:3:182:ARG:NH2	1:4:149:ALA:O	2.41	0.52
1:B:212:MET:HE1	1:E:72:TYR:CD1	2.45	0.52
1:M:212:MET:HE1	1:P:72:TYR:CD1	2.45	0.52
1:Y:163:SER:O	1:Y:166:SER:OG	2.16	0.52
1:1:182:ARG:NH2	1:2:149:ALA:O	2.41	0.51
1:H:163:SER:O	1:H:166:SER:OG	2.16	0.51
1:q:212:MET:HE1	1:t:72:TYR:CD1	2.45	0.51
1:0:72:TYR:CD1	1:x:212:MET:HE1	2.45	0.51
1:0:149:ALA:O	1:z:182:ARG:NH2	2.41	0.51
1:I:212:MET:HE1	1:L:72:TYR:CD1	2.45	0.51
1:g:212:MET:HE1	1:j:72:TYR:CD1	2.45	0.51
1:r:212:MET:HE1	1:u:72:TYR:CD1	2.45	0.51
1:0:182:ARG:NH2	1:1:149:ALA:O	2.41	0.51
1:4:212:MET:HE1	1:7:72:TYR:CD1	2.45	0.51
1:Q:212:MET:HE1	1:T:72:TYR:CD1	2.45	0.51
1:S:212:MET:HE1	1:V:72:TYR:CD1	2.45	0.51
1:Y:212:MET:HE1	1:b:72:TYR:CD1	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:204:ALA:O	1:a:208:THR:OG1	2.26	0.51
1:a:212:MET:HE1	1:d:72:TYR:CD1	2.45	0.51
1:m:212:MET:HE1	1:p:72:TYR:CD1	2.45	0.51
1:U:212:MET:HE1	1:X:72:TYR:CD1	2.45	0.51
1:m:163:SER:O	1:m:166:SER:OG	2.16	0.51
1:N:212:MET:HE1	1:Q:72:TYR:CD1	2.45	0.51
1:S:182:ARG:NH2	1:T:149:ALA:O	2.41	0.51
1:T:182:ARG:NH2	1:U:149:ALA:O	2.41	0.51
1:d:204:ALA:O	1:d:208:THR:OG1	2.26	0.51
1:k:212:MET:HE1	1:n:72:TYR:CD1	2.45	0.51
1:l:204:ALA:O	1:l:208:THR:OG1	2.26	0.51
1:G:212:MET:HE1	1:J:72:TYR:CD1	2.45	0.51
1:Q:182:ARG:NH2	1:R:149:ALA:O	2.41	0.51
1:R:182:ARG:NH2	1:S:149:ALA:O	2.41	0.51
1:c:212:MET:HE1	1:f:72:TYR:CD1	2.45	0.51
1:w:212:MET:HE1	1:z:72:TYR:CD1	2.45	0.51
1:D:212:MET:HE1	1:G:72:TYR:CD1	2.45	0.51
1:E:204:ALA:O	1:E:208:THR:OG1	2.26	0.51
1:O:212:MET:HE1	1:R:72:TYR:CD1	2.45	0.51
1:P:182:ARG:NH2	1:Q:149:ALA:O	2.41	0.51
1:q:182:ARG:NH2	1:r:149:ALA:O	2.41	0.51
1:s:204:ALA:O	1:s:208:THR:OG1	2.26	0.51
1:C:212:MET:HE1	1:F:72:TYR:CD1	2.45	0.51
1:U:182:ARG:NH2	1:V:149:ALA:O	2.41	0.51
1:l:212:MET:HE1	1:o:72:TYR:CD1	2.45	0.51
1:o:163:SER:O	1:o:166:SER:OG	2.16	0.51
1:s:212:MET:HE1	1:v:72:TYR:CD1	2.45	0.51
1:A:212:MET:HE1	1:D:72:TYR:CD1	2.45	0.51
1:E:163:SER:O	1:E:166:SER:OG	2.16	0.51
1:E:212:MET:HE1	1:H:72:TYR:CD1	2.45	0.51
1:N:182:ARG:NH2	1:O:149:ALA:O	2.41	0.51
1:O:182:ARG:NH2	1:P:149:ALA:O	2.41	0.51
1:r:182:ARG:NH2	1:s:149:ALA:O	2.41	0.51
1:M:182:ARG:NH2	1:N:149:ALA:O	2.41	0.51
1:T:212:MET:HE1	1:W:72:TYR:CD1	2.45	0.51
1:f:212:MET:HE1	1:i:72:TYR:CD1	2.45	0.51
1:p:182:ARG:NH2	1:q:149:ALA:O	2.41	0.51
1:R:212:MET:HE1	1:U:72:TYR:CD1	2.45	0.50
1:S:215:ARG:O	1:S:215:ARG:NE	2.44	0.50
1:W:182:ARG:NH2	1:X:149:ALA:O	2.41	0.50
1:d:212:MET:HE1	1:g:72:TYR:CD1	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:212:MET:HE1	1:K:72:TYR:CD1	2.45	0.50
1:T:215:ARG:O	1:T:215:ARG:NE	2.44	0.50
1:V:182:ARG:NH2	1:W:149:ALA:O	2.41	0.50
1:b:212:MET:HE1	1:e:72:TYR:CD1	2.45	0.50
1:k:215:ARG:O	1:k:215:ARG:NE	2.44	0.50
1:R:215:ARG:O	1:R:215:ARG:NE	2.44	0.50
1:U:215:ARG:O	1:U:215:ARG:NE	2.44	0.50
1:Z:212:MET:HE1	1:c:72:TYR:CD1	2.45	0.50
1:e:212:MET:HE1	1:h:72:TYR:CD1	2.45	0.50
1:F:212:MET:HE1	1:I:72:TYR:CD1	2.45	0.50
1:P:212:MET:HE1	1:S:72:TYR:CD1	2.45	0.50
1:l:215:ARG:NE	1:l:215:ARG:O	2.44	0.50
1:o:182:ARG:NH2	1:p:149:ALA:O	2.41	0.50
1:Q:215:ARG:NE	1:Q:215:ARG:O	2.44	0.50
1:V:215:ARG:NE	1:V:215:ARG:O	2.44	0.50
1:h:163:SER:O	1:h:166:SER:OG	2.16	0.50
1:I:215:ARG:O	1:I:215:ARG:NE	2.44	0.50
1:k:182:ARG:NH2	1:l:149:ALA:O	2.41	0.50
1:m:215:ARG:O	1:m:215:ARG:NE	2.44	0.50
1:J:215:ARG:O	1:J:215:ARG:NE	2.44	0.50
1:M:204:ALA:O	1:M:208:THR:OG1	2.26	0.50
1:l:182:ARG:NH2	1:m:149:ALA:O	2.41	0.50
1:7:215:ARG:O	1:7:215:ARG:NE	2.44	0.50
1:H:215:ARG:O	1:H:215:ARG:NE	2.44	0.50
1:J:163:SER:O	1:J:166:SER:OG	2.16	0.50
1:G:215:ARG:O	1:G:215:ARG:NE	2.44	0.49
1:K:215:ARG:O	1:K:215:ARG:NE	2.44	0.49
1:w:215:ARG:O	1:w:215:ARG:NE	2.44	0.49
1:P:215:ARG:O	1:P:215:ARG:NE	2.44	0.49
1:W:215:ARG:O	1:W:215:ARG:NE	2.44	0.49
1:n:215:ARG:O	1:n:215:ARG:NE	2.44	0.49
1:w:204:ALA:O	1:w:208:THR:OG1	2.26	0.49
1:Z:215:ARG:O	1:Z:215:ARG:NE	2.44	0.49
1:d:215:ARG:O	1:d:215:ARG:NE	2.44	0.49
1:e:215:ARG:O	1:e:215:ARG:NE	2.44	0.49
1:m:182:ARG:NH2	1:n:149:ALA:O	2.41	0.49
1:0:204:ALA:O	1:0:208:THR:OG1	2.26	0.49
1:2:163:SER:O	1:2:166:SER:OG	2.16	0.49
1:L:215:ARG:NE	1:L:215:ARG:O	2.44	0.49
1:Y:215:ARG:O	1:Y:215:ARG:NE	2.44	0.49
1:a:215:ARG:O	1:a:215:ARG:NE	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:n:182:ARG:NH2	1:o:149:ALA:O	2.41	0.49
1:6:215:ARG:NE	1:6:215:ARG:O	2.44	0.49
1:F:215:ARG:O	1:F:215:ARG:NE	2.44	0.49
1:w:163:SER:O	1:w:166:SER:OG	2.16	0.49
1:x:215:ARG:NE	1:x:215:ARG:O	2.44	0.49
1:0:215:ARG:O	1:0:215:ARG:NE	2.44	0.49
1:b:215:ARG:NE	1:b:215:ARG:O	2.44	0.49
1:f:215:ARG:O	1:f:215:ARG:NE	2.44	0.49
1:1:215:ARG:NE	1:1:215:ARG:O	2.44	0.49
1:X:215:ARG:NE	1:X:215:ARG:O	2.44	0.49
1:f:204:ALA:O	1:f:208:THR:OG1	2.26	0.49
1:v:215:ARG:O	1:v:215:ARG:NE	2.44	0.49
1:2:215:ARG:O	1:2:215:ARG:NE	2.44	0.49
1:E:215:ARG:NE	1:E:215:ARG:O	2.44	0.49
1:O:215:ARG:O	1:O:215:ARG:NE	2.44	0.49
1:g:215:ARG:NE	1:g:215:ARG:O	2.44	0.49
1:c:215:ARG:O	1:c:215:ARG:NE	2.44	0.49
1:o:215:ARG:O	1:o:215:ARG:NE	2.44	0.49
1:y:215:ARG:O	1:y:215:ARG:NE	2.44	0.49
1:7:163:SER:O	1:7:166:SER:OG	2.16	0.48
1:3:215:ARG:O	1:3:215:ARG:NE	2.44	0.48
1:5:215:ARG:O	1:5:215:ARG:NE	2.44	0.48
1:b:163:SER:O	1:b:166:SER:OG	2.16	0.48
1:g:204:ALA:O	1:g:208:THR:OG1	2.26	0.48
1:Z:163:SER:O	1:Z:166:SER:OG	2.16	0.48
1:h:215:ARG:O	1:h:215:ARG:NE	2.44	0.48
1:D:215:ARG:O	1:D:215:ARG:NE	2.44	0.48
1:N:204:ALA:O	1:N:208:THR:OG1	2.26	0.48
1:I:193:ASP:OD1	1:I:194:LYS:N	2.47	0.48
1:Z:193:ASP:OD1	1:Z:194:LYS:N	2.47	0.48
1:u:215:ARG:NE	1:u:215:ARG:O	2.44	0.48
1:z:215:ARG:O	1:z:215:ARG:NE	2.44	0.48
1:5:193:ASP:OD1	1:5:194:LYS:N	2.47	0.48
1:6:193:ASP:OD1	1:6:194:LYS:N	2.47	0.48
1:H:193:ASP:OD1	1:H:194:LYS:N	2.47	0.48
1:M:163:SER:O	1:M:166:SER:OG	2.16	0.48
1:Y:193:ASP:OD1	1:Y:194:LYS:N	2.47	0.48
1:i:215:ARG:NE	1:i:215:ARG:O	2.44	0.48
1:G:193:ASP:OD1	1:G:194:LYS:N	2.47	0.48
1:O:193:ASP:OD1	1:O:194:LYS:N	2.47	0.48
1:P:193:ASP:OD1	1:P:194:LYS:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:193:ASP:OD1	1:S:194:LYS:N	2.47	0.48
1:A:193:ASP:OD1	1:A:194:LYS:N	2.47	0.48
1:F:193:ASP:OD1	1:F:194:LYS:N	2.47	0.48
1:N:215:ARG:O	1:N:215:ARG:NE	2.44	0.48
1:g:193:ASP:OD1	1:g:194:LYS:N	2.47	0.48
1:p:215:ARG:O	1:p:215:ARG:NE	2.44	0.48
1:r:193:ASP:OD1	1:r:194:LYS:N	2.47	0.48
1:x:193:ASP:OD1	1:x:194:LYS:N	2.47	0.48
1:y:193:ASP:OD1	1:y:194:LYS:N	2.47	0.48
1:z:193:ASP:OD1	1:z:194:LYS:N	2.47	0.48
1:4:215:ARG:O	1:4:215:ARG:NE	2.44	0.48
1:h:193:ASP:OD1	1:h:194:LYS:N	2.47	0.48
1:i:193:ASP:OD1	1:i:194:LYS:N	2.47	0.48
1:j:215:ARG:O	1:j:215:ARG:NE	2.44	0.48
1:k:193:ASP:OD1	1:k:194:LYS:N	2.47	0.48
1:v:193:ASP:OD1	1:v:194:LYS:N	2.47	0.48
1:0:193:ASP:OD1	1:0:194:LYS:N	2.47	0.48
1:C:215:ARG:O	1:C:215:ARG:NE	2.44	0.48
1:R:193:ASP:OD1	1:R:194:LYS:N	2.47	0.48
1:X:193:ASP:OD1	1:X:194:LYS:N	2.47	0.48
1:q:193:ASP:OD1	1:q:194:LYS:N	2.47	0.48
1:s:163:SER:O	1:s:166:SER:OG	2.16	0.48
1:t:215:ARG:O	1:t:215:ARG:NE	2.44	0.48
1:B:215:ARG:NE	1:B:215:ARG:O	2.44	0.47
1:E:193:ASP:OD1	1:E:194:LYS:N	2.47	0.47
1:J:193:ASP:OD1	1:J:194:LYS:N	2.47	0.47
1:M:215:ARG:O	1:M:215:ARG:NE	2.44	0.47
1:T:193:ASP:OD1	1:T:194:LYS:N	2.47	0.47
1:W:193:ASP:OD1	1:W:194:LYS:N	2.47	0.47
1:i:163:SER:O	1:i:166:SER:OG	2.16	0.47
1:j:193:ASP:OD1	1:j:194:LYS:N	2.47	0.47
1:n:193:ASP:OD1	1:n:194:LYS:N	2.47	0.47
1:A:215:ARG:O	1:A:215:ARG:NE	2.44	0.47
1:Q:193:ASP:OD1	1:Q:194:LYS:N	2.47	0.47
1:a:193:ASP:OD1	1:a:194:LYS:N	2.47	0.47
1:c:193:ASP:OD1	1:c:194:LYS:N	2.47	0.47
1:l:193:ASP:OD1	1:l:194:LYS:N	2.47	0.47
1:K:193:ASP:OD1	1:K:194:LYS:N	2.47	0.47
1:l:193:ASP:OD1	1:l:194:LYS:N	2.47	0.47
1:o:193:ASP:OD1	1:o:194:LYS:N	2.47	0.47
1:w:193:ASP:OD1	1:w:194:LYS:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:y:163:SER:O	1:y:166:SER:OG	2.16	0.47
1:1:204:ALA:O	1:1:208:THR:OG1	2.26	0.47
1:U:193:ASP:OD1	1:U:194:LYS:N	2.47	0.47
1:V:193:ASP:OD1	1:V:194:LYS:N	2.47	0.47
1:f:193:ASP:OD1	1:f:194:LYS:N	2.47	0.47
1:4:193:ASP:OD1	1:4:194:LYS:N	2.47	0.47
1:7:193:ASP:OD1	1:7:194:LYS:N	2.47	0.47
1:A:204:ALA:O	1:A:208:THR:OG1	2.26	0.47
1:L:193:ASP:OD1	1:L:194:LYS:N	2.47	0.47
1:R:163:SER:O	1:R:166:SER:OG	2.16	0.47
1:p:193:ASP:OD1	1:p:194:LYS:N	2.47	0.47
1:s:193:ASP:OD1	1:s:194:LYS:N	2.47	0.47
1:s:215:ARG:NE	1:s:215:ARG:O	2.44	0.47
1:3:193:ASP:OD1	1:3:194:LYS:N	2.47	0.47
1:B:193:ASP:OD1	1:B:194:LYS:N	2.47	0.47
1:N:193:ASP:OD1	1:N:194:LYS:N	2.47	0.47
1:q:215:ARG:NE	1:q:215:ARG:O	2.44	0.47
1:2:193:ASP:OD1	1:2:194:LYS:N	2.47	0.47
1:C:193:ASP:OD1	1:C:194:LYS:N	2.47	0.47
1:D:193:ASP:OD1	1:D:194:LYS:N	2.47	0.47
1:b:193:ASP:OD1	1:b:194:LYS:N	2.47	0.47
1:d:193:ASP:OD1	1:d:194:LYS:N	2.47	0.47
1:m:193:ASP:OD1	1:m:194:LYS:N	2.47	0.47
1:r:215:ARG:O	1:r:215:ARG:NE	2.44	0.47
1:u:193:ASP:OD1	1:u:194:LYS:N	2.47	0.47
1:L:163:SER:O	1:L:166:SER:OG	2.16	0.47
1:H:204:ALA:O	1:H:208:THR:OG1	2.26	0.47
1:e:193:ASP:OD1	1:e:194:LYS:N	2.47	0.47
1:C:163:SER:O	1:C:166:SER:OG	2.16	0.47
1:M:193:ASP:OD1	1:M:194:LYS:N	2.47	0.46
1:k:204:ALA:O	1:k:208:THR:OG1	2.26	0.46
1:t:193:ASP:OD1	1:t:194:LYS:N	2.47	0.46
1:6:204:ALA:O	1:6:208:THR:OG1	2.26	0.46
1:n:204:ALA:O	1:n:208:THR:OG1	2.26	0.46
1:B:204:ALA:O	1:B:208:THR:OG1	2.26	0.46
1:5:163:SER:O	1:5:166:SER:OG	2.16	0.45
1:V:71:TRP:O	1:V:75:ALA:N	2.44	0.45
1:z:204:ALA:O	1:z:208:THR:OG1	2.26	0.45
1:7:71:TRP:O	1:7:75:ALA:N	2.44	0.45
1:3:163:SER:O	1:3:166:SER:OG	2.16	0.45
1:h:71:TRP:O	1:h:75:ALA:N	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:204:ALA:O	1:2:208:THR:OG1	2.26	0.45
1:n:71:TRP:O	1:n:75:ALA:N	2.44	0.45
1:p:204:ALA:O	1:p:208:THR:OG1	2.26	0.45
1:v:163:SER:O	1:v:166:SER:OG	2.16	0.45
1:U:71:TRP:O	1:U:75:ALA:N	2.44	0.45
1:z:71:TRP:O	1:z:75:ALA:N	2.44	0.45
1:K:204:ALA:O	1:K:208:THR:OG1	2.26	0.45
1:0:163:SER:O	1:0:166:SER:OG	2.16	0.44
1:1:212:MET:HE1	1:4:72:TYR:HD1	1.83	0.44
1:r:212:MET:HE1	1:u:72:TYR:HD1	1.83	0.44
1:3:212:MET:HE1	1:6:72:TYR:HD1	1.82	0.44
1:D:212:MET:HE1	1:G:72:TYR:HD1	1.83	0.44
1:f:212:MET:HE1	1:i:72:TYR:HD1	1.83	0.44
1:B:212:MET:HE1	1:E:72:TYR:HD1	1.83	0.44
1:S:71:TRP:O	1:S:75:ALA:N	2.44	0.44
1:T:71:TRP:O	1:T:75:ALA:N	2.44	0.44
1:p:212:MET:HE1	1:s:72:TYR:HD1	1.83	0.44
1:2:72:TYR:HD1	1:z:212:MET:HE1	1.83	0.44
1:C:204:ALA:O	1:C:208:THR:OG1	2.26	0.44
1:G:176:LEU:O	1:G:180:ALA:N	2.45	0.44
1:R:71:TRP:O	1:R:75:ALA:N	2.44	0.44
1:n:212:MET:HE1	1:q:72:TYR:HD1	1.83	0.44
1:5:71:TRP:O	1:5:75:ALA:N	2.44	0.44
1:h:176:LEU:O	1:h:180:ALA:N	2.45	0.44
1:0:72:TYR:HD1	1:x:212:MET:HE1	1.83	0.44
1:A:163:SER:O	1:A:166:SER:OG	2.16	0.44
1:N:212:MET:HE1	1:Q:72:TYR:HD1	1.83	0.44
1:T:212:MET:HE1	1:W:72:TYR:HD1	1.83	0.44
1:d:212:MET:HE1	1:g:72:TYR:HD1	1.83	0.44
1:m:71:TRP:O	1:m:75:ALA:N	2.44	0.44
1:w:212:MET:HE1	1:z:72:TYR:HD1	1.83	0.44
1:F:212:MET:HE1	1:I:72:TYR:HD1	1.83	0.44
1:O:163:SER:O	1:O:166:SER:OG	2.16	0.44
1:c:176:LEU:O	1:c:180:ALA:N	2.45	0.44
1:P:163:SER:O	1:P:166:SER:OG	2.16	0.44
1:Q:71:TRP:O	1:Q:75:ALA:N	2.44	0.44
1:g:212:MET:HE1	1:j:72:TYR:HD1	1.83	0.44
1:m:212:MET:HE1	1:p:72:TYR:HD1	1.83	0.44
1:H:212:MET:HE1	1:K:72:TYR:HD1	1.83	0.44
1:i:176:LEU:O	1:i:180:ALA:N	2.45	0.44
1:R:212:MET:HE1	1:U:72:TYR:HD1	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:176:LEU:O	1:b:180:ALA:N	2.45	0.43
1:b:212:MET:HE1	1:e:72:TYR:HD1	1.83	0.43
1:l:212:MET:HE1	1:o:72:TYR:HD1	1.83	0.43
1:o:212:MET:HE1	1:r:72:TYR:HD1	1.83	0.43
1:q:204:ALA:O	1:q:208:THR:OG1	2.26	0.43
1:l:72:TYR:HD1	1:y:212:MET:HE1	1.83	0.43
1:A:212:MET:HE1	1:D:72:TYR:HD1	1.83	0.43
1:P:212:MET:HE1	1:S:72:TYR:HD1	1.83	0.43
1:g:71:TRP:O	1:g:75:ALA:N	2.44	0.43
1:l:71:TRP:O	1:l:75:ALA:N	2.44	0.43
1:C:212:MET:HE1	1:F:72:TYR:HD1	1.83	0.43
1:2:212:MET:HE1	1:5:72:TYR:HD1	1.83	0.43
1:K:163:SER:O	1:K:166:SER:OG	2.16	0.43
1:Z:212:MET:HE1	1:c:72:TYR:HD1	1.83	0.43
1:a:176:LEU:O	1:a:180:ALA:N	2.45	0.43
1:s:71:TRP:O	1:s:75:ALA:N	2.44	0.43
1:k:71:TRP:O	1:k:75:ALA:N	2.44	0.43
1:v:65:GLN:O	1:v:69:GLN:N	2.43	0.43
1:C:65:GLN:O	1:C:69:GLN:N	2.43	0.43
1:P:71:TRP:O	1:P:75:ALA:N	2.44	0.43
1:X:204:ALA:O	1:X:208:THR:OG1	2.26	0.43
1:j:176:LEU:O	1:j:180:ALA:N	2.45	0.43
1:Z:176:LEU:O	1:Z:180:ALA:N	2.45	0.43
1:y:71:TRP:O	1:y:75:ALA:N	2.44	0.43
1:F:152:ILE:CD1	1:G:125:LEU:HD13	2.49	0.43
1:c:212:MET:HE1	1:f:72:TYR:HD1	1.83	0.43
1:p:152:ILE:CD1	1:q:125:LEU:HD13	2.49	0.43
1:s:152:ILE:CD1	1:t:125:LEU:HD13	2.49	0.43
1:w:176:LEU:O	1:w:180:ALA:N	2.45	0.43
1:x:176:LEU:O	1:x:180:ALA:N	2.45	0.43
1:y:65:GLN:O	1:y:69:GLN:N	2.43	0.43
1:0:125:LEU:HD13	1:z:152:ILE:CD1	2.49	0.43
1:0:152:ILE:CD1	1:1:125:LEU:HD13	2.49	0.43
1:3:152:ILE:CD1	1:4:125:LEU:HD13	2.49	0.43
1:C:71:TRP:O	1:C:75:ALA:N	2.44	0.43
1:C:152:ILE:CD1	1:D:125:LEU:HD13	2.49	0.43
1:P:152:ILE:CD1	1:Q:125:LEU:HD13	2.49	0.43
1:W:152:ILE:CD1	1:X:125:LEU:HD13	2.49	0.43
1:Y:176:LEU:O	1:Y:180:ALA:N	2.45	0.43
1:i:152:ILE:CD1	1:j:125:LEU:HD13	2.49	0.43
1:l:152:ILE:CD1	1:m:125:LEU:HD13	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:x:163:SER:O	1:x:166:SER:OG	2.16	0.43
1:4:71:TRP:O	1:4:75:ALA:N	2.44	0.43
1:K:152:ILE:CD1	1:L:125:LEU:HD13	2.49	0.43
1:M:152:ILE:CD1	1:N:125:LEU:HD13	2.49	0.43
1:e:152:ILE:CD1	1:f:125:LEU:HD13	2.49	0.43
1:j:204:ALA:O	1:j:208:THR:OG1	2.26	0.43
1:n:152:ILE:CD1	1:o:125:LEU:HD13	2.49	0.43
1:u:65:GLN:O	1:u:69:GLN:N	2.43	0.43
1:x:152:ILE:CD1	1:y:125:LEU:HD13	2.49	0.43
1:y:176:LEU:O	1:y:180:ALA:N	2.45	0.43
1:6:152:ILE:CD1	1:7:125:LEU:HD13	2.49	0.42
1:R:152:ILE:CD1	1:S:125:LEU:HD13	2.49	0.42
1:U:152:ILE:CD1	1:V:125:LEU:HD13	2.49	0.42
1:b:152:ILE:CD1	1:c:125:LEU:HD13	2.49	0.42
1:d:152:ILE:CD1	1:e:125:LEU:HD13	2.49	0.42
1:f:152:ILE:CD1	1:g:125:LEU:HD13	2.49	0.42
1:h:152:ILE:CD1	1:i:125:LEU:HD13	2.49	0.42
1:s:212:MET:HE1	1:v:72:TYR:HD1	1.83	0.42
1:w:152:ILE:CD1	1:x:125:LEU:HD13	2.49	0.42
1:2:152:ILE:CD1	1:3:125:LEU:HD13	2.49	0.42
1:H:152:ILE:CD1	1:I:125:LEU:HD13	2.49	0.42
1:N:152:ILE:CD1	1:O:125:LEU:HD13	2.49	0.42
1:W:65:GLN:O	1:W:69:GLN:N	2.43	0.42
1:Y:152:ILE:CD1	1:Z:125:LEU:HD13	2.49	0.42
1:q:152:ILE:CD1	1:r:125:LEU:HD13	2.49	0.42
1:A:152:ILE:CD1	1:B:125:LEU:HD13	2.49	0.42
1:D:152:ILE:CD1	1:E:125:LEU:HD13	2.49	0.42
1:O:152:ILE:CD1	1:P:125:LEU:HD13	2.49	0.42
1:Z:152:ILE:CD1	1:a:125:LEU:HD13	2.49	0.42
1:g:152:ILE:CD1	1:h:125:LEU:HD13	2.49	0.42
1:k:212:MET:HE1	1:n:72:TYR:HD1	1.83	0.42
1:m:152:ILE:CD1	1:n:125:LEU:HD13	2.49	0.42
1:o:152:ILE:CD1	1:p:125:LEU:HD13	2.49	0.42
1:t:152:ILE:CD1	1:u:125:LEU:HD13	2.49	0.42
1:5:152:ILE:CD1	1:6:125:LEU:HD13	2.49	0.42
1:B:152:ILE:CD1	1:C:125:LEU:HD13	2.49	0.42
1:u:152:ILE:CD1	1:v:125:LEU:HD13	2.49	0.42
1:z:176:LEU:O	1:z:180:ALA:N	2.45	0.42
1:4:152:ILE:CD1	1:5:125:LEU:HD13	2.49	0.42
1:4:212:MET:HE1	1:7:72:TYR:HD1	1.83	0.42
1:D:208:THR:HG21	1:G:91:LEU:HD12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:152:ILE:CD1	1:J:125:LEU:HD13	2.49	0.42
1:N:208:THR:HG21	1:Q:91:LEU:HD12	2.02	0.42
1:T:152:ILE:CD1	1:U:125:LEU:HD13	2.49	0.42
1:h:65:GLN:O	1:h:69:GLN:N	2.44	0.42
1:k:152:ILE:CD1	1:l:125:LEU:HD13	2.49	0.42
1:O:208:THR:HG21	1:3:91:LEU:HD12	2.02	0.42
1:3:208:THR:HG21	1:6:91:LEU:HD12	2.02	0.42
1:4:152:ILE:HG22	1:5:36:MET:HG3	2.02	0.42
1:4:208:THR:HG21	1:7:91:LEU:HD12	2.02	0.42
1:E:152:ILE:HG22	1:F:36:MET:HG3	2.02	0.42
1:E:152:ILE:CD1	1:F:125:LEU:HD13	2.49	0.42
1:I:163:SER:O	1:I:166:SER:OG	2.16	0.42
1:M:152:ILE:HG22	1:N:36:MET:HG3	2.02	0.42
1:V:152:ILE:CD1	1:W:125:LEU:HD13	2.49	0.42
1:r:152:ILE:CD1	1:s:125:LEU:HD13	2.49	0.42
1:r:152:ILE:HG22	1:s:36:MET:HG3	2.02	0.42
1:O:212:MET:HE1	1:3:72:TYR:HD1	1.82	0.42
1:1:208:THR:HG21	1:4:91:LEU:HD12	2.02	0.42
1:2:152:ILE:HG22	1:3:36:MET:HG3	2.02	0.42
1:B:65:GLN:O	1:B:69:GLN:N	2.43	0.42
1:G:152:ILE:CD1	1:H:125:LEU:HD13	2.49	0.42
1:G:208:THR:HG21	1:J:91:LEU:HD12	2.02	0.42
1:H:152:ILE:HG22	1:I:36:MET:HG3	2.02	0.42
1:P:152:ILE:HG22	1:Q:36:MET:HG3	2.02	0.42
1:S:152:ILE:CD1	1:T:125:LEU:HD13	2.49	0.42
1:f:71:TRP:O	1:f:75:ALA:N	2.44	0.42
1:y:152:ILE:CD1	1:z:125:LEU:HD13	2.49	0.42
1:O:36:MET:HG3	1:z:152:ILE:HG22	2.02	0.42
1:1:152:ILE:CD1	1:2:125:LEU:HD13	2.49	0.42
1:A:208:THR:HG21	1:D:91:LEU:HD12	2.02	0.42
1:C:152:ILE:HG22	1:D:36:MET:HG3	2.02	0.42
1:O:208:THR:HG21	1:R:91:LEU:HD12	2.02	0.42
1:Q:152:ILE:CD1	1:R:125:LEU:HD13	2.49	0.42
1:Y:208:THR:HG21	1:b:91:LEU:HD12	2.02	0.42
1:Y:212:MET:HE1	1:b:72:TYR:HD1	1.83	0.42
1:m:65:GLN:O	1:m:69:GLN:N	2.44	0.42
1:q:208:THR:HG21	1:t:91:LEU:HD12	2.02	0.42
1:q:212:MET:HE1	1:t:72:TYR:HD1	1.83	0.42
1:t:65:GLN:O	1:t:69:GLN:N	2.43	0.42
1:u:152:ILE:HG22	1:v:36:MET:HG3	2.02	0.42
1:O:176:LEU:O	1:O:180:ALA:N	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:ILE:HG22	1:C:36:MET:HG3	2.02	0.42
1:C:208:THR:HG21	1:F:91:LEU:HD12	2.02	0.42
1:J:152:ILE:CD1	1:K:125:LEU:HD13	2.49	0.42
1:O:71:TRP:O	1:O:75:ALA:N	2.44	0.42
1:c:152:ILE:CD1	1:d:125:LEU:HD13	2.49	0.42
1:E:212:MET:HE1	1:H:72:TYR:HD1	1.83	0.42
1:Z:152:ILE:HG22	1:a:36:MET:HG3	2.02	0.42
1:a:152:ILE:CD1	1:b:125:LEU:HD13	2.49	0.42
1:1:152:ILE:HG22	1:2:36:MET:HG3	2.02	0.41
1:5:152:ILE:HG22	1:6:36:MET:HG3	2.02	0.41
1:F:152:ILE:HG22	1:G:36:MET:HG3	2.02	0.41
1:F:208:THR:HG21	1:I:91:LEU:HD12	2.02	0.41
1:Q:208:THR:HG21	1:T:91:LEU:HD12	2.02	0.41
1:Q:212:MET:HE1	1:T:72:TYR:HD1	1.83	0.41
1:a:152:ILE:HG22	1:b:36:MET:HG3	2.02	0.41
1:q:163:SER:O	1:q:166:SER:OG	2.16	0.41
1:s:208:THR:HG21	1:v:91:LEU:HD12	2.02	0.41
1:t:152:ILE:HG22	1:u:36:MET:HG3	2.02	0.41
1:N:152:ILE:HG22	1:O:36:MET:HG3	2.02	0.41
1:O:152:ILE:HG22	1:P:36:MET:HG3	2.02	0.41
1:S:152:ILE:HG22	1:T:36:MET:HG3	2.02	0.41
1:g:152:ILE:HG22	1:h:36:MET:HG3	2.02	0.41
1:l:65:GLN:O	1:l:69:GLN:N	2.43	0.41
1:E:208:THR:HG21	1:H:91:LEU:HD12	2.02	0.41
1:G:152:ILE:HG22	1:H:36:MET:HG3	2.02	0.41
1:G:205:VAL:HG13	1:G:206:GLU:N	2.36	0.41
1:G:212:MET:HE1	1:J:72:TYR:HD1	1.83	0.41
1:K:152:ILE:HG22	1:L:36:MET:HG3	2.02	0.41
1:R:152:ILE:HG22	1:S:36:MET:HG3	2.02	0.41
1:V:65:GLN:O	1:V:69:GLN:N	2.43	0.41
1:n:163:SER:O	1:n:166:SER:OG	2.16	0.41
1:o:152:ILE:HG22	1:p:36:MET:HG3	2.02	0.41
1:r:71:TRP:O	1:r:75:ALA:N	2.44	0.41
1:x:65:GLN:O	1:x:69:GLN:N	2.43	0.41
1:H:205:VAL:HG13	1:H:206:GLU:N	2.36	0.41
1:Y:205:VAL:HG13	1:Y:206:GLU:N	2.36	0.41
1:b:65:GLN:O	1:b:69:GLN:N	2.43	0.41
1:d:152:ILE:HG22	1:e:36:MET:HG3	2.02	0.41
1:e:212:MET:HE1	1:h:72:TYR:HD1	1.83	0.41
1:h:152:ILE:HG22	1:i:36:MET:HG3	2.02	0.41
1:k:65:GLN:O	1:k:69:GLN:N	2.43	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:w:152:ILE:HG22	1:x:36:MET:HG3	2.02	0.41
1:0:91:LEU:HD12	1:x:208:THR:HG21	2.02	0.41
1:1:91:LEU:HD12	1:y:208:THR:HG21	2.02	0.41
1:2:205:VAL:HG13	1:2:206:GLU:N	2.36	0.41
1:6:152:ILE:HG22	1:7:36:MET:HG3	2.02	0.41
1:H:208:THR:HG21	1:K:91:LEU:HD12	2.02	0.41
1:I:205:VAL:HG13	1:I:206:GLU:N	2.36	0.41
1:M:212:MET:HE1	1:P:72:TYR:HD1	1.83	0.41
1:O:212:MET:HE1	1:R:72:TYR:HD1	1.83	0.41
1:R:208:THR:HG21	1:U:91:LEU:HD12	2.02	0.41
1:S:212:MET:HE1	1:V:72:TYR:HD1	1.83	0.41
1:V:152:ILE:HG22	1:W:36:MET:HG3	2.02	0.41
1:W:201:GLU:O	1:W:205:VAL:HG12	2.21	0.41
1:Z:205:VAL:HG13	1:Z:206:GLU:N	2.36	0.41
1:k:152:ILE:HG22	1:l:36:MET:HG3	2.02	0.41
1:p:205:VAL:HG13	1:p:206:GLU:N	2.36	0.41
1:q:205:VAL:HG13	1:q:206:GLU:N	2.36	0.41
1:s:152:ILE:HG22	1:t:36:MET:HG3	2.02	0.41
1:x:71:TRP:O	1:x:75:ALA:N	2.44	0.41
1:0:152:ILE:HG22	1:1:36:MET:HG3	2.02	0.41
1:0:205:VAL:HG13	1:0:206:GLU:N	2.36	0.41
1:1:176:LEU:O	1:1:180:ALA:N	2.45	0.41
1:1:205:VAL:HG13	1:1:206:GLU:N	2.36	0.41
1:B:208:THR:HG21	1:E:91:LEU:HD12	2.02	0.41
1:F:205:VAL:HG13	1:F:206:GLU:N	2.36	0.41
1:M:208:THR:HG21	1:P:91:LEU:HD12	2.02	0.41
1:V:205:VAL:HG13	1:V:206:GLU:N	2.36	0.41
1:g:201:GLU:O	1:g:205:VAL:HG12	2.21	0.41
1:i:152:ILE:HG22	1:j:36:MET:HG3	2.02	0.41
1:p:208:THR:HG21	1:s:91:LEU:HD12	2.02	0.41
1:r:205:VAL:HG13	1:r:206:GLU:N	2.36	0.41
1:r:208:THR:HG21	1:u:91:LEU:HD12	2.02	0.41
1:y:152:ILE:HG22	1:z:36:MET:HG3	2.02	0.41
1:2:71:TRP:O	1:2:75:ALA:N	2.44	0.41
1:3:71:TRP:O	1:3:75:ALA:N	2.44	0.41
1:3:205:VAL:HG13	1:3:206:GLU:N	2.36	0.41
1:4:205:VAL:HG13	1:4:206:GLU:N	2.36	0.41
1:B:201:GLU:O	1:B:205:VAL:HG12	2.21	0.41
1:I:152:ILE:HG22	1:J:36:MET:HG3	2.02	0.41
1:I:212:MET:HE1	1:L:72:TYR:HD1	1.83	0.41
1:L:205:VAL:HG13	1:L:206:GLU:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:205:VAL:HG13	1:S:206:GLU:N	2.36	0.41
1:U:212:MET:HE1	1:X:72:TYR:HD1	1.83	0.41
1:X:205:VAL:HG13	1:X:206:GLU:N	2.36	0.41
1:d:205:VAL:HG13	1:d:206:GLU:N	2.36	0.41
1:e:201:GLU:O	1:e:205:VAL:HG12	2.21	0.41
1:f:208:THR:HG21	1:i:91:LEU:HD12	2.02	0.41
1:g:208:THR:HG21	1:j:91:LEU:HD12	2.02	0.41
1:i:201:GLU:O	1:i:205:VAL:HG12	2.21	0.41
1:l:152:ILE:HG22	1:m:36:MET:HG3	2.02	0.41
1:n:205:VAL:HG13	1:n:206:GLU:N	2.36	0.41
1:o:205:VAL:HG13	1:o:206:GLU:N	2.36	0.41
1:q:152:ILE:HG22	1:r:36:MET:HG3	2.02	0.41
1:q:201:GLU:O	1:q:205:VAL:HG12	2.21	0.41
1:3:199:TRP:O	1:3:203:GLN:OE1	2.39	0.41
1:A:152:ILE:HG22	1:B:36:MET:HG3	2.02	0.41
1:D:201:GLU:O	1:D:205:VAL:HG12	2.21	0.41
1:J:152:ILE:HG22	1:K:36:MET:HG3	2.02	0.41
1:J:205:VAL:HG13	1:J:206:GLU:N	2.36	0.41
1:L:71:TRP:O	1:L:75:ALA:N	2.44	0.41
1:M:205:VAL:HG13	1:M:206:GLU:N	2.36	0.41
1:U:201:GLU:O	1:U:205:VAL:HG12	2.21	0.41
1:V:204:ALA:O	1:V:208:THR:OG1	2.26	0.41
1:k:205:VAL:HG13	1:k:206:GLU:N	2.36	0.41
1:o:201:GLU:O	1:o:205:VAL:HG12	2.21	0.41
1:p:152:ILE:HG22	1:q:36:MET:HG3	2.02	0.41
1:s:65:GLN:O	1:s:69:GLN:N	2.43	0.41
1:v:199:TRP:O	1:v:203:GLN:OE1	2.39	0.41
1:1:71:TRP:O	1:1:75:ALA:N	2.44	0.41
1:1:201:GLU:O	1:1:205:VAL:HG12	2.21	0.41
1:2:91:LEU:HD12	1:z:208:THR:HG21	2.02	0.41
1:2:199:TRP:O	1:2:203:GLN:OE1	2.39	0.41
1:2:208:THR:HG21	1:5:91:LEU:HD12	2.02	0.41
1:3:152:ILE:HG22	1:4:36:MET:HG3	2.02	0.41
1:4:114:LEU:HD12	1:4:114:LEU:N	2.36	0.41
1:A:205:VAL:HG13	1:A:206:GLU:N	2.36	0.41
1:B:71:TRP:O	1:B:75:ALA:N	2.44	0.41
1:I:201:GLU:O	1:I:205:VAL:HG12	2.21	0.41
1:K:201:GLU:O	1:K:205:VAL:HG12	2.21	0.41
1:K:205:VAL:HG13	1:K:206:GLU:N	2.36	0.41
1:L:65:GLN:O	1:L:69:GLN:N	2.43	0.41
1:M:71:TRP:O	1:M:75:ALA:N	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:201:GLU:O	1:N:205:VAL:HG12	2.21	0.41
1:O:199:TRP:O	1:O:203:GLN:OE1	2.39	0.41
1:P:199:TRP:O	1:P:203:GLN:OE1	2.39	0.41
1:Q:114:LEU:HD12	1:Q:114:LEU:N	2.36	0.41
1:Q:152:ILE:HG22	1:R:36:MET:HG3	2.02	0.41
1:T:176:LEU:O	1:T:180:ALA:N	2.45	0.41
1:T:205:VAL:HG13	1:T:206:GLU:N	2.36	0.41
1:U:176:LEU:O	1:U:180:ALA:N	2.45	0.41
1:U:208:THR:HG21	1:X:91:LEU:HD12	2.02	0.41
1:W:114:LEU:N	1:W:114:LEU:HD12	2.36	0.41
1:W:152:ILE:HG22	1:X:36:MET:HG3	2.02	0.41
1:W:205:VAL:HG13	1:W:206:GLU:N	2.36	0.41
1:Y:152:ILE:HG22	1:Z:36:MET:HG3	2.02	0.41
1:Z:208:THR:HG21	1:c:91:LEU:HD12	2.02	0.41
1:a:205:VAL:HG13	1:a:206:GLU:N	2.36	0.41
1:b:208:THR:HG21	1:e:91:LEU:HD12	2.02	0.41
1:c:152:ILE:HG22	1:d:36:MET:HG3	2.02	0.41
1:c:201:GLU:O	1:c:205:VAL:HG12	2.21	0.41
1:c:205:VAL:HG13	1:c:206:GLU:N	2.36	0.41
1:e:71:TRP:O	1:e:75:ALA:N	2.44	0.41
1:f:205:VAL:HG13	1:f:206:GLU:N	2.36	0.41
1:g:65:GLN:O	1:g:69:GLN:N	2.43	0.41
1:g:205:VAL:HG13	1:g:206:GLU:N	2.36	0.41
1:j:205:VAL:HG13	1:j:206:GLU:N	2.36	0.41
1:k:208:THR:HG21	1:n:91:LEU:HD12	2.02	0.41
1:l:208:THR:HG21	1:o:91:LEU:HD12	2.02	0.41
1:m:30:GLU:OE2	1:m:136:LYS:NZ	2.53	0.41
1:m:201:GLU:O	1:m:205:VAL:HG12	2.21	0.41
1:n:152:ILE:HG22	1:o:36:MET:HG3	2.02	0.41
1:s:201:GLU:O	1:s:205:VAL:HG12	2.21	0.41
1:s:205:VAL:HG13	1:s:206:GLU:N	2.36	0.41
1:u:114:LEU:HD12	1:u:114:LEU:N	2.36	0.41
1:u:201:GLU:O	1:u:205:VAL:HG12	2.21	0.41
1:w:201:GLU:O	1:w:205:VAL:HG12	2.21	0.41
1:x:205:VAL:HG13	1:x:206:GLU:N	2.36	0.41
1:y:201:GLU:O	1:y:205:VAL:HG12	2.21	0.41
1:z:201:GLU:O	1:z:205:VAL:HG12	2.21	0.41
1:z:205:VAL:HG13	1:z:206:GLU:N	2.36	0.41
1:0:114:LEU:N	1:0:114:LEU:HD12	2.36	0.41
1:0:201:GLU:O	1:0:205:VAL:HG12	2.21	0.41
1:3:201:GLU:O	1:3:205:VAL:HG12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:199:TRP:O	1:4:203:GLN:OE1	2.39	0.41
1:5:205:VAL:HG13	1:5:206:GLU:N	2.36	0.41
1:A:65:GLN:O	1:A:69:GLN:N	2.43	0.41
1:C:114:LEU:HD12	1:C:114:LEU:N	2.36	0.41
1:C:199:TRP:O	1:C:203:GLN:OE1	2.39	0.41
1:D:152:ILE:HG22	1:E:36:MET:HG3	2.02	0.41
1:E:205:VAL:HG13	1:E:206:GLU:N	2.36	0.41
1:G:114:LEU:HD12	1:G:114:LEU:N	2.36	0.41
1:M:114:LEU:HD12	1:M:114:LEU:N	2.36	0.41
1:N:199:TRP:O	1:N:203:GLN:OE1	2.39	0.41
1:N:205:VAL:HG13	1:N:206:GLU:N	2.36	0.41
1:P:201:GLU:O	1:P:205:VAL:HG12	2.21	0.41
1:U:65:GLN:O	1:U:69:GLN:N	2.43	0.41
1:U:114:LEU:N	1:U:114:LEU:HD12	2.36	0.41
1:X:114:LEU:HD12	1:X:114:LEU:N	2.36	0.41
1:a:114:LEU:HD12	1:a:114:LEU:N	2.36	0.41
1:a:201:GLU:O	1:a:205:VAL:HG12	2.21	0.41
1:c:208:THR:HG21	1:f:91:LEU:HD12	2.02	0.41
1:l:205:VAL:HG13	1:l:206:GLU:N	2.36	0.41
1:m:205:VAL:HG13	1:m:206:GLU:N	2.36	0.41
1:m:208:THR:HG21	1:p:91:LEU:HD12	2.02	0.41
1:r:201:GLU:O	1:r:205:VAL:HG12	2.21	0.41
1:u:199:TRP:O	1:u:203:GLN:OE1	2.39	0.41
1:x:201:GLU:O	1:x:205:VAL:HG12	2.21	0.41
1:1:199:TRP:O	1:1:203:GLN:OE1	2.39	0.40
1:2:201:GLU:O	1:2:205:VAL:HG12	2.21	0.40
1:5:114:LEU:HD12	1:5:114:LEU:N	2.36	0.40
1:5:201:GLU:O	1:5:205:VAL:HG12	2.21	0.40
1:A:201:GLU:O	1:A:205:VAL:HG12	2.21	0.40
1:D:199:TRP:O	1:D:203:GLN:OE1	2.39	0.40
1:F:201:GLU:O	1:F:205:VAL:HG12	2.21	0.40
1:H:114:LEU:HD12	1:H:114:LEU:N	2.36	0.40
1:I:208:THR:HG21	1:L:91:LEU:HD12	2.02	0.40
1:N:71:TRP:O	1:N:75:ALA:N	2.44	0.40
1:P:65:GLN:O	1:P:69:GLN:N	2.43	0.40
1:R:205:VAL:HG13	1:R:206:GLU:N	2.36	0.40
1:T:114:LEU:N	1:T:114:LEU:HD12	2.36	0.40
1:U:152:ILE:HG22	1:V:36:MET:HG3	2.02	0.40
1:V:114:LEU:N	1:V:114:LEU:HD12	2.37	0.40
1:V:176:LEU:O	1:V:180:ALA:N	2.45	0.40
1:X:201:GLU:O	1:X:205:VAL:HG12	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:114:LEU:N	1:c:114:LEU:HD12	2.36	0.40
1:d:114:LEU:N	1:d:114:LEU:HD12	2.36	0.40
1:e:208:THR:HG21	1:h:91:LEU:HD12	2.02	0.40
1:n:208:THR:HG21	1:q:91:LEU:HD12	2.02	0.40
1:p:201:GLU:O	1:p:205:VAL:HG12	2.21	0.40
1:t:201:GLU:O	1:t:205:VAL:HG12	2.21	0.40
1:x:152:ILE:HG22	1:y:36:MET:HG3	2.02	0.40
1:2:176:LEU:O	1:2:180:ALA:N	2.45	0.40
1:3:114:LEU:HD12	1:3:114:LEU:N	2.36	0.40
1:4:201:GLU:O	1:4:205:VAL:HG12	2.21	0.40
1:6:201:GLU:O	1:6:205:VAL:HG12	2.21	0.40
1:B:114:LEU:HD12	1:B:114:LEU:N	2.37	0.40
1:B:199:TRP:O	1:B:203:GLN:OE1	2.39	0.40
1:D:205:VAL:HG13	1:D:206:GLU:N	2.36	0.40
1:G:199:TRP:O	1:G:203:GLN:OE1	2.39	0.40
1:H:199:TRP:O	1:H:203:GLN:OE1	2.39	0.40
1:K:71:TRP:O	1:K:75:ALA:N	2.44	0.40
1:K:114:LEU:HD12	1:K:114:LEU:N	2.36	0.40
1:O:65:GLN:O	1:O:69:GLN:N	2.43	0.40
1:P:208:THR:HG21	1:S:91:LEU:HD12	2.02	0.40
1:Q:65:GLN:O	1:Q:69:GLN:N	2.43	0.40
1:Q:201:GLU:O	1:Q:205:VAL:HG12	2.21	0.40
1:R:114:LEU:HD12	1:R:114:LEU:N	2.36	0.40
1:S:201:GLU:O	1:S:205:VAL:HG12	2.21	0.40
1:U:199:TRP:O	1:U:203:GLN:OE1	2.39	0.40
1:U:205:VAL:HG13	1:U:206:GLU:N	2.36	0.40
1:b:114:LEU:N	1:b:114:LEU:HD12	2.36	0.40
1:d:208:THR:HG21	1:g:91:LEU:HD12	2.02	0.40
1:e:47:LEU:HD23	1:e:47:LEU:C	2.47	0.40
1:e:114:LEU:N	1:e:114:LEU:HD12	2.36	0.40
1:e:152:ILE:HG22	1:f:36:MET:HG3	2.02	0.40
1:f:114:LEU:N	1:f:114:LEU:HD12	2.36	0.40
1:f:152:ILE:HG22	1:g:36:MET:HG3	2.02	0.40
1:g:114:LEU:N	1:g:114:LEU:HD12	2.36	0.40
1:j:71:TRP:O	1:j:75:ALA:N	2.44	0.40
1:j:199:TRP:O	1:j:203:GLN:OE1	2.39	0.40
1:k:201:GLU:O	1:k:205:VAL:HG12	2.21	0.40
1:n:199:TRP:O	1:n:203:GLN:OE1	2.39	0.40
1:q:114:LEU:HD12	1:q:114:LEU:N	2.36	0.40
1:t:114:LEU:HD12	1:t:114:LEU:N	2.36	0.40
1:v:114:LEU:HD12	1:v:114:LEU:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:x:114:LEU:N	1:x:114:LEU:HD12	2.36	0.40
1:y:114:LEU:N	1:y:114:LEU:HD12	2.36	0.40
1:y:205:VAL:HG13	1:y:206:GLU:N	2.36	0.40
1:6:205:VAL:HG13	1:6:206:GLU:N	2.36	0.40
1:A:114:LEU:N	1:A:114:LEU:HD12	2.36	0.40
1:B:205:VAL:HG13	1:B:206:GLU:N	2.36	0.40
1:E:201:GLU:O	1:E:205:VAL:HG12	2.21	0.40
1:F:114:LEU:HD12	1:F:114:LEU:N	2.36	0.40
1:L:199:TRP:O	1:L:203:GLN:OE1	2.39	0.40
1:Q:199:TRP:O	1:Q:203:GLN:OE1	2.39	0.40
1:S:176:LEU:O	1:S:180:ALA:N	2.45	0.40
1:S:208:THR:HG21	1:V:91:LEU:HD12	2.02	0.40
1:T:152:ILE:HG22	1:U:36:MET:HG3	2.02	0.40
1:T:208:THR:HG21	1:W:91:LEU:HD12	2.02	0.40
1:U:47:LEU:HD23	1:U:47:LEU:C	2.47	0.40
1:W:199:TRP:O	1:W:203:GLN:OE1	2.39	0.40
1:Z:114:LEU:HD12	1:Z:114:LEU:N	2.36	0.40
1:Z:201:GLU:O	1:Z:205:VAL:HG12	2.21	0.40
1:a:208:THR:HG21	1:d:91:LEU:HD12	2.02	0.40
1:a:212:MET:HE1	1:d:72:TYR:HD1	1.83	0.40
1:b:205:VAL:HG13	1:b:206:GLU:N	2.36	0.40
1:e:199:TRP:O	1:e:203:GLN:OE1	2.39	0.40
1:f:199:TRP:O	1:f:203:GLN:OE1	2.39	0.40
1:g:47:LEU:HD23	1:g:47:LEU:C	2.47	0.40
1:i:47:LEU:HD23	1:i:47:LEU:C	2.47	0.40
1:j:114:LEU:HD12	1:j:114:LEU:N	2.36	0.40
1:j:201:GLU:O	1:j:205:VAL:HG12	2.21	0.40
1:k:114:LEU:HD12	1:k:114:LEU:N	2.36	0.40
1:m:47:LEU:HD23	1:m:47:LEU:C	2.47	0.40
1:m:199:TRP:O	1:m:203:GLN:OE1	2.39	0.40
1:n:201:GLU:O	1:n:205:VAL:HG12	2.21	0.40
1:w:114:LEU:N	1:w:114:LEU:HD12	2.36	0.40
1:w:199:TRP:O	1:w:203:GLN:OE1	2.39	0.40
1:w:208:THR:HG21	1:z:91:LEU:HD12	2.02	0.40
1:z:114:LEU:HD12	1:z:114:LEU:N	2.36	0.40
1:C:201:GLU:O	1:C:205:VAL:HG12	2.21	0.40
1:H:201:GLU:O	1:H:205:VAL:HG12	2.21	0.40
1:I:199:TRP:O	1:I:203:GLN:OE1	2.39	0.40
1:N:114:LEU:HD12	1:N:114:LEU:N	2.36	0.40
1:P:114:LEU:HD12	1:P:114:LEU:N	2.36	0.40
1:Q:205:VAL:HG13	1:Q:206:GLU:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:65:GLN:O	1:R:69:GLN:N	2.44	0.40
1:S:114:LEU:N	1:S:114:LEU:HD12	2.36	0.40
1:T:65:GLN:O	1:T:69:GLN:N	2.43	0.40
1:W:47:LEU:HD23	1:W:47:LEU:C	2.47	0.40
1:a:65:GLN:O	1:a:69:GLN:N	2.44	0.40
1:c:199:TRP:O	1:c:203:GLN:OE1	2.39	0.40
1:d:199:TRP:O	1:d:203:GLN:OE1	2.39	0.40
1:h:114:LEU:N	1:h:114:LEU:HD12	2.36	0.40
1:i:199:TRP:O	1:i:203:GLN:OE1	2.39	0.40
1:i:205:VAL:HG13	1:i:206:GLU:N	2.36	0.40
1:l:199:TRP:O	1:l:203:GLN:OE1	2.39	0.40
1:o:47:LEU:HD23	1:o:47:LEU:C	2.47	0.40
1:s:47:LEU:HD23	1:s:47:LEU:C	2.47	0.40
1:t:205:VAL:HG13	1:t:206:GLU:N	2.36	0.40
1:u:47:LEU:HD23	1:u:47:LEU:C	2.47	0.40
1:v:205:VAL:HG13	1:v:206:GLU:N	2.36	0.40
1:w:47:LEU:HD23	1:w:47:LEU:C	2.47	0.40
1:0:47:LEU:HD23	1:0:47:LEU:C	2.47	0.40
1:1:114:LEU:HD12	1:1:114:LEU:N	2.36	0.40
1:2:47:LEU:HD23	1:2:47:LEU:C	2.47	0.40
1:G:201:GLU:O	1:G:205:VAL:HG12	2.21	0.40
1:O:205:VAL:HG13	1:O:206:GLU:N	2.36	0.40
1:S:65:GLN:O	1:S:69:GLN:N	2.44	0.40
1:T:199:TRP:O	1:T:203:GLN:OE1	2.39	0.40
1:X:199:TRP:O	1:X:203:GLN:OE1	2.39	0.40
1:c:47:LEU:HD23	1:c:47:LEU:C	2.47	0.40
1:e:205:VAL:HG13	1:e:206:GLU:N	2.36	0.40
1:h:201:GLU:O	1:h:205:VAL:HG12	2.21	0.40
1:l:201:GLU:O	1:l:205:VAL:HG12	2.21	0.40
1:o:199:TRP:O	1:o:203:GLN:OE1	2.39	0.40
1:q:47:LEU:HD23	1:q:47:LEU:C	2.47	0.40
1:r:114:LEU:HD12	1:r:114:LEU:N	2.36	0.40
1:u:71:TRP:O	1:u:75:ALA:N	2.44	0.40
1:v:201:GLU:O	1:v:205:VAL:HG12	2.21	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%)	188 (98%)	4 (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%)	188 (98%)	4 (2%)	0	100	100
1	4	192/223 (86%)	188 (98%)	4 (2%)	0	100	100
1	5	192/223 (86%)	188 (98%)	4 (2%)	0	100	100
1	6	192/223 (86%)	188 (98%)	4 (2%)	0	100	100
1	7	192/223 (86%)	188 (98%)	4 (2%)	0	100	100
1	A	192/223 (86%)	188 (98%)	4 (2%)	0	100	100
1	B	192/223 (86%)	188 (98%)	4 (2%)	0	100	100
1	C	192/223 (86%)	188 (98%)	4 (2%)	0	100	100
1	D	192/223 (86%)	188 (98%)	4 (2%)	0	100	100
1	E	192/223 (86%)	188 (98%)	4 (2%)	0	100	100
1	F	192/223 (86%)	188 (98%)	4 (2%)	0	100	100
1	G	192/223 (86%)	188 (98%)	4 (2%)	0	100	100
1	H	192/223 (86%)	188 (98%)	4 (2%)	0	100	100
1	I	192/223 (86%)	188 (98%)	4 (2%)	0	100	100
1	J	192/223 (86%)	188 (98%)	4 (2%)	0	100	100
1	K	192/223 (86%)	188 (98%)	4 (2%)	0	100	100
1	L	192/223 (86%)	188 (98%)	4 (2%)	0	100	100
1	M	192/223 (86%)	188 (98%)	4 (2%)	0	100	100
1	N	192/223 (86%)	188 (98%)	4 (2%)	0	100	100
1	O	192/223 (86%)	188 (98%)	4 (2%)	0	100	100
1	P	192/223 (86%)	188 (98%)	4 (2%)	0	100	100
1	Q	192/223 (86%)	188 (98%)	4 (2%)	0	100	100

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	w	192/223 (86%)	188 (98%)	4 (2%)	0	100	100
1	x	192/223 (86%)	188 (98%)	4 (2%)	0	100	100
1	y	192/223 (86%)	188 (98%)	4 (2%)	0	100	100
1	z	192/223 (86%)	188 (98%)	4 (2%)	0	100	100
All	All	11520/13380 (86%)	11280 (98%)	240 (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%)	84	88
1	1	161/186 (87%)	160 (99%)	1 (1%)	84	88
1	2	161/186 (87%)	160 (99%)	1 (1%)	84	88
1	3	161/186 (87%)	160 (99%)	1 (1%)	84	88
1	4	161/186 (87%)	160 (99%)	1 (1%)	84	88
1	5	161/186 (87%)	160 (99%)	1 (1%)	84	88
1	6	161/186 (87%)	160 (99%)	1 (1%)	84	88
1	7	161/186 (87%)	160 (99%)	1 (1%)	84	88
1	A	161/186 (87%)	160 (99%)	1 (1%)	84	88
1	B	161/186 (87%)	160 (99%)	1 (1%)	84	88
1	C	161/186 (87%)	160 (99%)	1 (1%)	84	88
1	D	161/186 (87%)	160 (99%)	1 (1%)	84	88
1	E	161/186 (87%)	160 (99%)	1 (1%)	84	88
1	F	161/186 (87%)	160 (99%)	1 (1%)	84	88
1	G	161/186 (87%)	160 (99%)	1 (1%)	84	88
1	H	161/186 (87%)	160 (99%)	1 (1%)	84	88
1	I	161/186 (87%)	160 (99%)	1 (1%)	84	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	161/186 (87%)	160 (99%)	1 (1%)	84	88
1	K	161/186 (87%)	160 (99%)	1 (1%)	84	88
1	L	161/186 (87%)	160 (99%)	1 (1%)	84	88
1	M	161/186 (87%)	160 (99%)	1 (1%)	84	88
1	N	161/186 (87%)	160 (99%)	1 (1%)	84	88
1	O	161/186 (87%)	160 (99%)	1 (1%)	84	88
1	P	161/186 (87%)	160 (99%)	1 (1%)	84	88
1	Q	161/186 (87%)	160 (99%)	1 (1%)	84	88
1	R	161/186 (87%)	160 (99%)	1 (1%)	84	88
1	S	161/186 (87%)	160 (99%)	1 (1%)	84	88
1	T	161/186 (87%)	160 (99%)	1 (1%)	84	88
1	U	161/186 (87%)	160 (99%)	1 (1%)	84	88
1	V	161/186 (87%)	160 (99%)	1 (1%)	84	88
1	W	161/186 (87%)	160 (99%)	1 (1%)	84	88
1	X	161/186 (87%)	160 (99%)	1 (1%)	84	88
1	Y	161/186 (87%)	160 (99%)	1 (1%)	84	88
1	Z	161/186 (87%)	160 (99%)	1 (1%)	84	88
1	a	161/186 (87%)	160 (99%)	1 (1%)	84	88
1	b	161/186 (87%)	160 (99%)	1 (1%)	84	88
1	c	161/186 (87%)	160 (99%)	1 (1%)	84	88
1	d	161/186 (87%)	160 (99%)	1 (1%)	84	88
1	e	161/186 (87%)	160 (99%)	1 (1%)	84	88
1	f	161/186 (87%)	160 (99%)	1 (1%)	84	88
1	g	161/186 (87%)	160 (99%)	1 (1%)	84	88
1	h	161/186 (87%)	160 (99%)	1 (1%)	84	88
1	i	161/186 (87%)	160 (99%)	1 (1%)	84	88
1	j	161/186 (87%)	160 (99%)	1 (1%)	84	88
1	k	161/186 (87%)	160 (99%)	1 (1%)	84	88
1	l	161/186 (87%)	160 (99%)	1 (1%)	84	88
1	m	161/186 (87%)	160 (99%)	1 (1%)	84	88
1	n	161/186 (87%)	160 (99%)	1 (1%)	84	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	o	161/186 (87%)	160 (99%)	1 (1%)	84	88
1	p	161/186 (87%)	160 (99%)	1 (1%)	84	88
1	q	161/186 (87%)	160 (99%)	1 (1%)	84	88
1	r	161/186 (87%)	160 (99%)	1 (1%)	84	88
1	s	161/186 (87%)	160 (99%)	1 (1%)	84	88
1	t	161/186 (87%)	160 (99%)	1 (1%)	84	88
1	u	161/186 (87%)	160 (99%)	1 (1%)	84	88
1	v	161/186 (87%)	160 (99%)	1 (1%)	84	88
1	w	161/186 (87%)	160 (99%)	1 (1%)	84	88
1	x	161/186 (87%)	160 (99%)	1 (1%)	84	88
1	y	161/186 (87%)	160 (99%)	1 (1%)	84	88
1	z	161/186 (87%)	160 (99%)	1 (1%)	84	88
All	All	9660/11160 (87%)	9600 (99%)	60 (1%)	82	88

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	196	PHE
1	1	196	PHE
1	2	196	PHE
1	3	196	PHE
1	4	196	PHE
1	5	196	PHE
1	6	196	PHE
1	7	196	PHE
1	A	196	PHE
1	B	196	PHE
1	C	196	PHE
1	D	196	PHE
1	E	196	PHE
1	F	196	PHE
1	G	196	PHE
1	H	196	PHE
1	I	196	PHE
1	J	196	PHE
1	K	196	PHE
1	L	196	PHE
1	M	196	PHE

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Mol	Chain	Res	Type
1	N	196	PHE
1	O	196	PHE
1	P	196	PHE
1	Q	196	PHE
1	R	196	PHE
1	S	196	PHE
1	T	196	PHE
1	U	196	PHE
1	V	196	PHE
1	W	196	PHE
1	X	196	PHE
1	Y	196	PHE
1	Z	196	PHE
1	a	196	PHE
1	b	196	PHE
1	c	196	PHE
1	d	196	PHE
1	e	196	PHE
1	f	196	PHE
1	g	196	PHE
1	h	196	PHE
1	i	196	PHE
1	j	196	PHE
1	k	196	PHE
1	l	196	PHE
1	m	196	PHE
1	n	196	PHE
1	o	196	PHE
1	p	196	PHE
1	q	196	PHE
1	r	196	PHE
1	s	196	PHE
1	t	196	PHE
1	u	196	PHE
1	v	196	PHE
1	w	196	PHE
1	x	196	PHE
1	y	196	PHE
1	z	196	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	83	ASN
1	1	83	ASN
1	2	83	ASN
1	3	83	ASN
1	3	111	GLN
1	4	83	ASN
1	5	83	ASN
1	6	83	ASN
1	7	83	ASN
1	A	83	ASN
1	B	83	ASN
1	C	83	ASN
1	D	83	ASN
1	E	83	ASN
1	F	83	ASN
1	G	83	ASN
1	H	83	ASN
1	H	111	GLN
1	I	83	ASN
1	J	83	ASN
1	K	83	ASN
1	L	83	ASN
1	M	83	ASN
1	N	83	ASN
1	O	83	ASN
1	O	111	GLN
1	P	83	ASN
1	Q	83	ASN
1	R	83	ASN
1	S	83	ASN
1	T	83	ASN
1	U	83	ASN
1	V	83	ASN
1	W	83	ASN
1	X	83	ASN
1	Y	83	ASN
1	Z	83	ASN
1	a	83	ASN
1	b	83	ASN
1	c	83	ASN
1	c	111	GLN
1	d	83	ASN
1	e	83	ASN

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Mol	Chain	Res	Type
1	f	83	ASN
1	g	83	ASN
1	g	111	GLN
1	h	83	ASN
1	i	83	ASN
1	j	83	ASN
1	j	111	GLN
1	k	83	ASN
1	l	83	ASN
1	m	83	ASN
1	n	83	ASN
1	n	111	GLN
1	o	83	ASN
1	o	111	GLN
1	p	83	ASN
1	p	111	GLN
1	q	83	ASN
1	q	111	GLN
1	r	83	ASN
1	s	83	ASN
1	t	83	ASN
1	u	83	ASN
1	v	83	ASN
1	w	83	ASN
1	x	83	ASN
1	y	83	ASN
1	z	83	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 ⓘ

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.

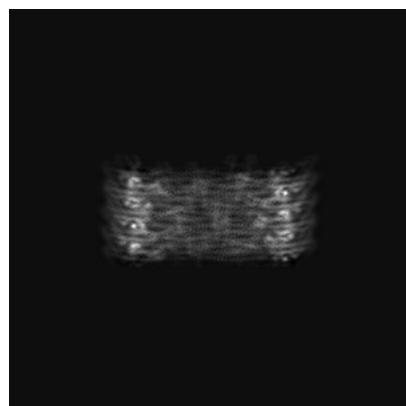
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52530. These allow visual inspection of the internal detail of the map and identification of artifacts.

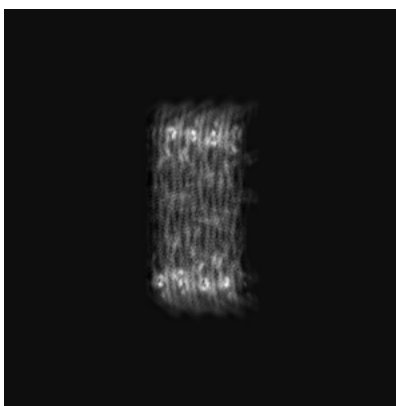
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

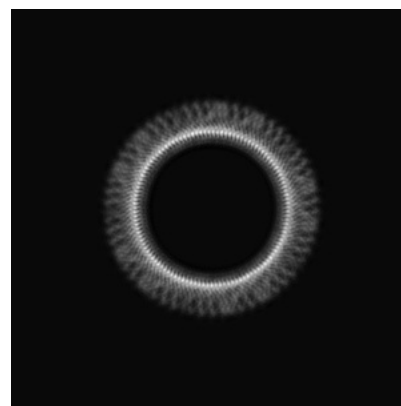
6.1.1 Primary map



X

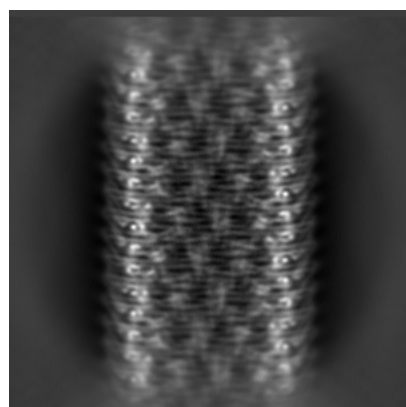


Y

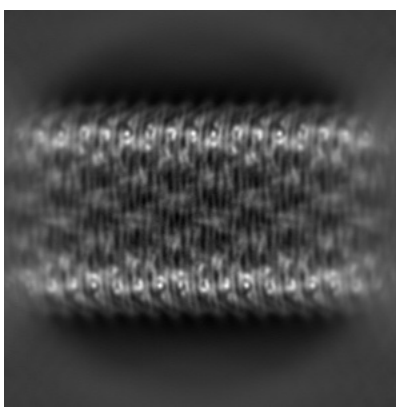


Z

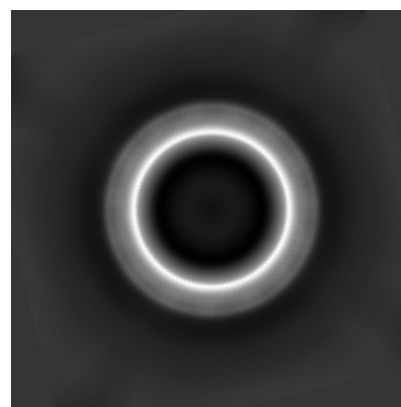
6.1.2 Raw map



X



Y

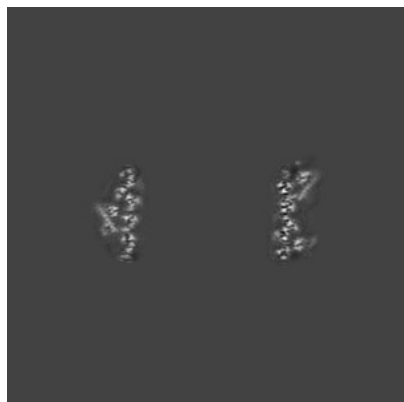


Z

The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

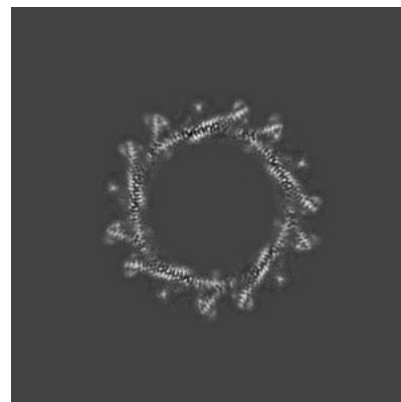
6.2.1 Primary map



X Index: 200

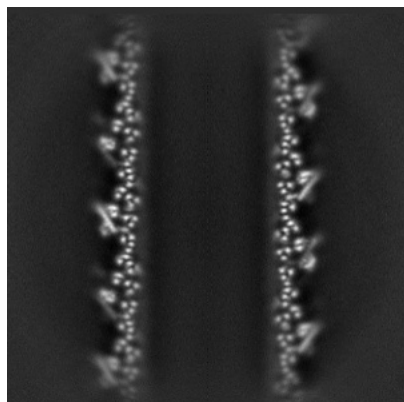


Y Index: 200

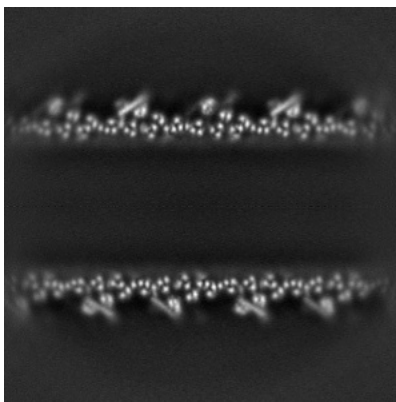


Z Index: 200

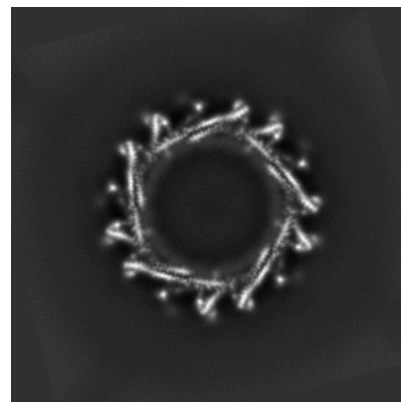
6.2.2 Raw map



X Index: 200



Y Index: 200

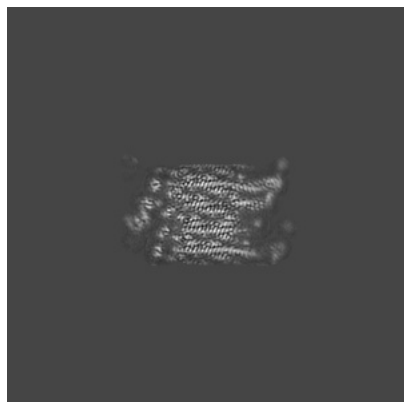


Z Index: 200

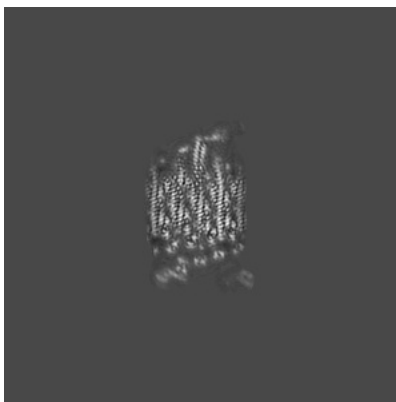
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

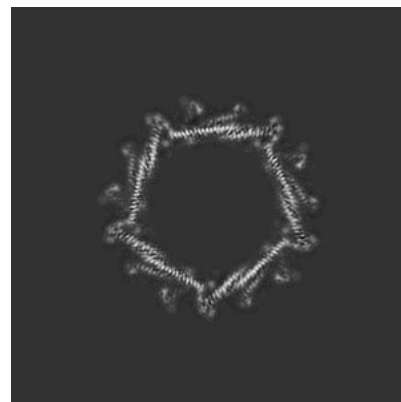
6.3.1 Primary map



X Index: 124

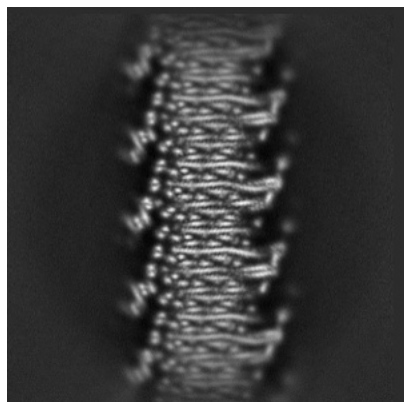


Y Index: 276

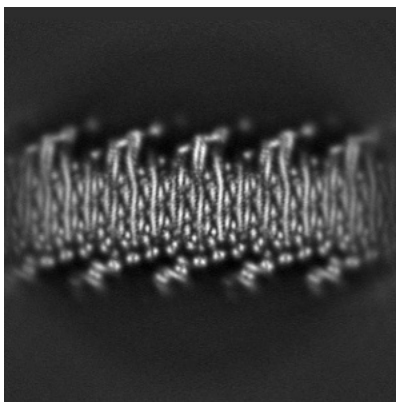


Z Index: 196

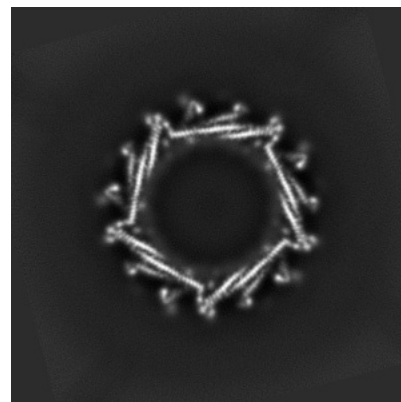
6.3.2 Raw map



X Index: 124



Y Index: 276

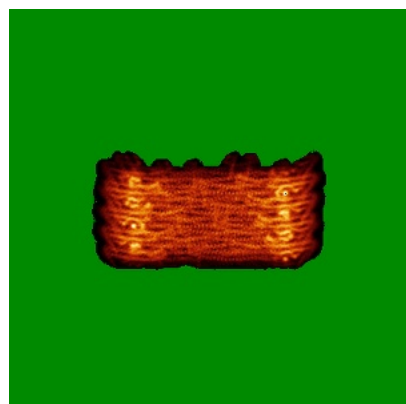


Z Index: 196

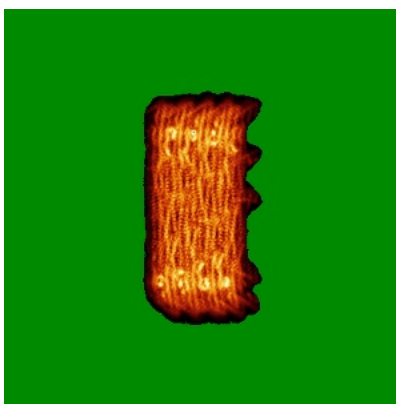
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

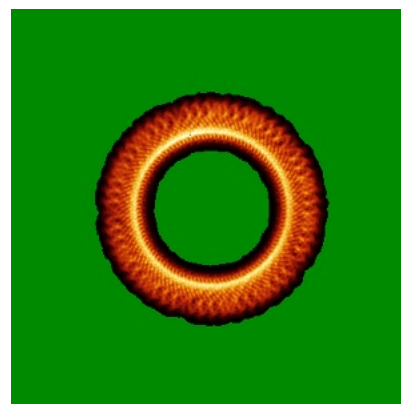
6.4.1 Primary map



X

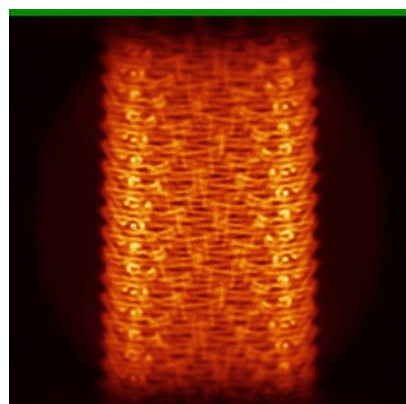


Y

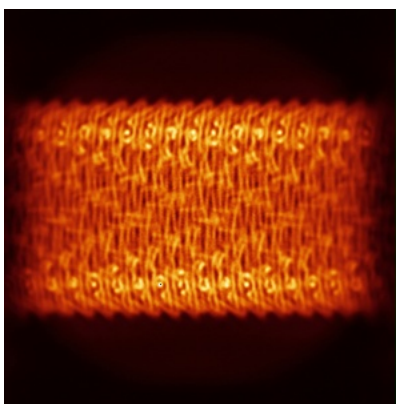


Z

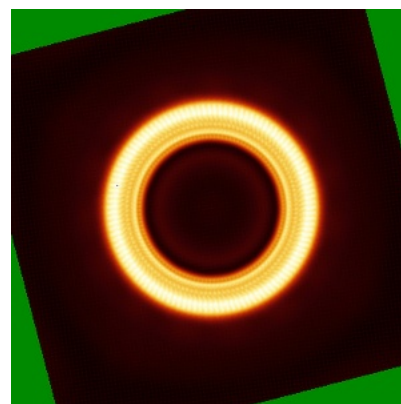
6.4.2 Raw map



X



Y

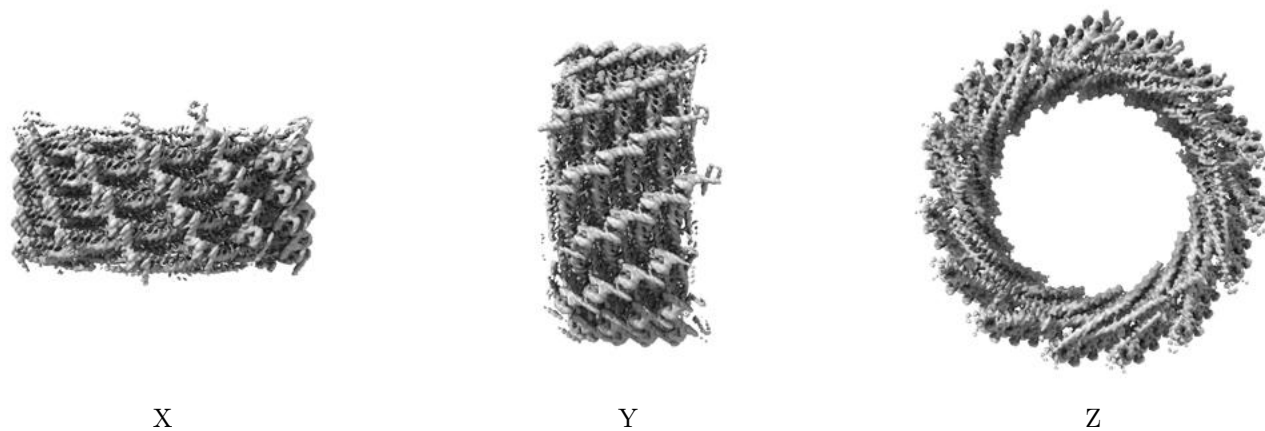


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

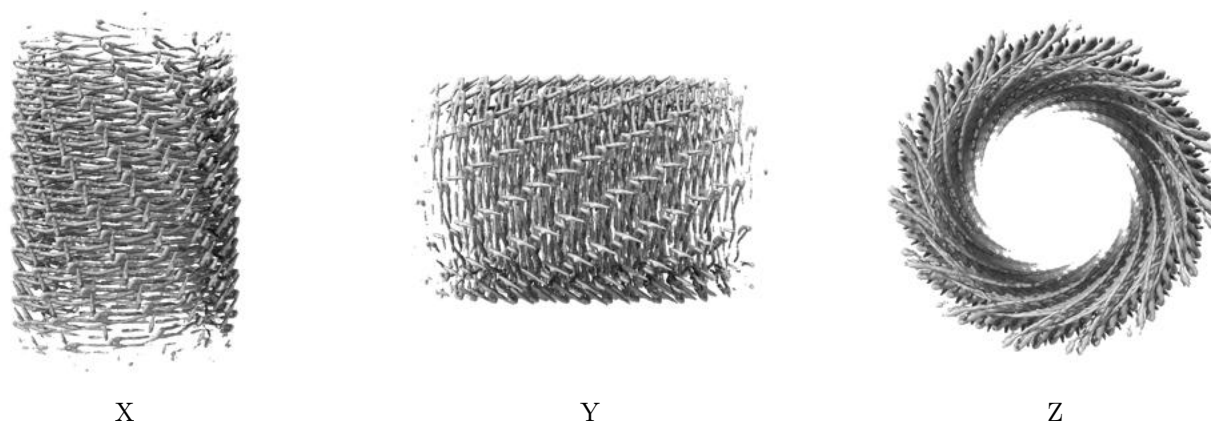
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

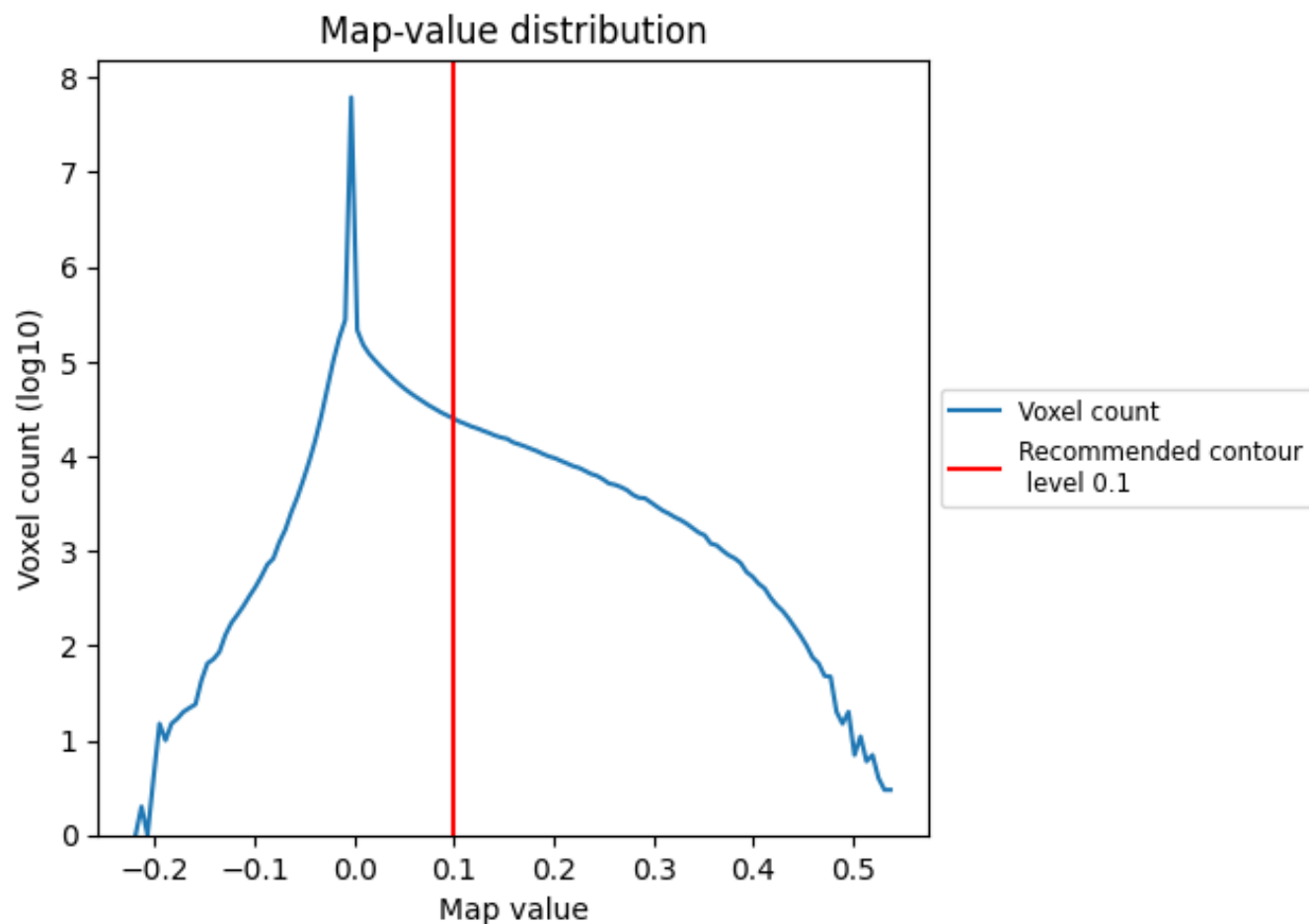
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

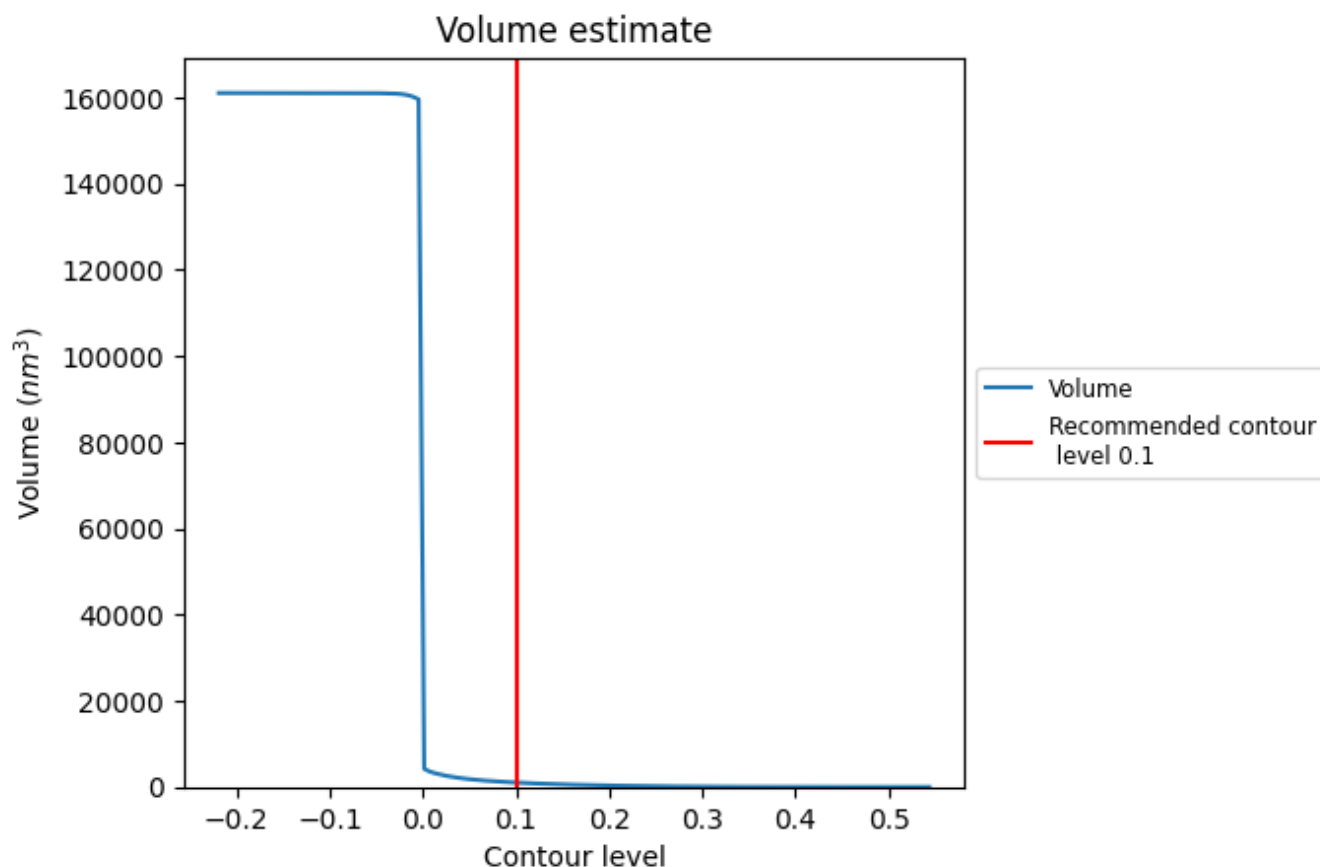
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

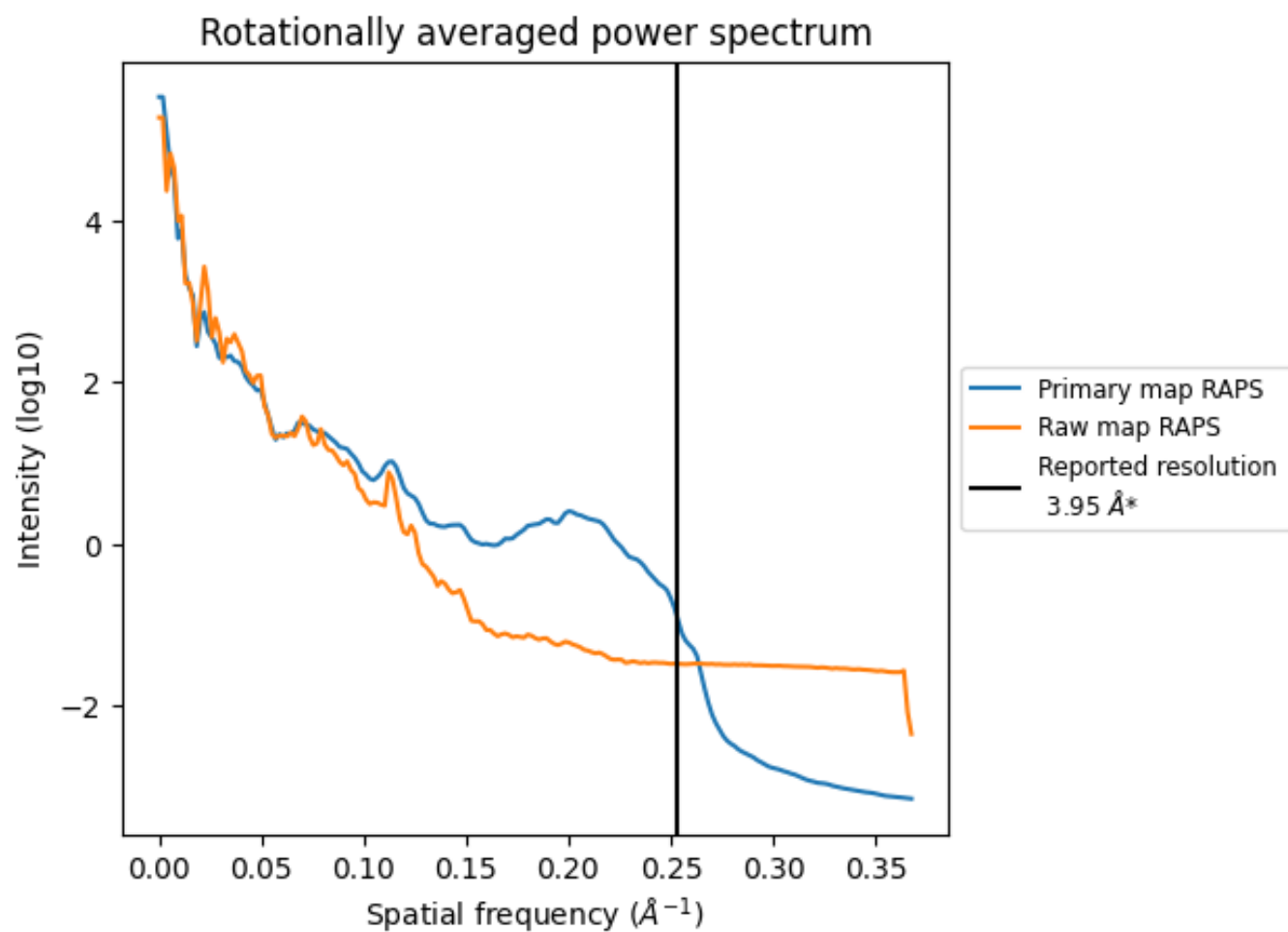
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1022 nm^3 ; this corresponds to an approximate mass of 923 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

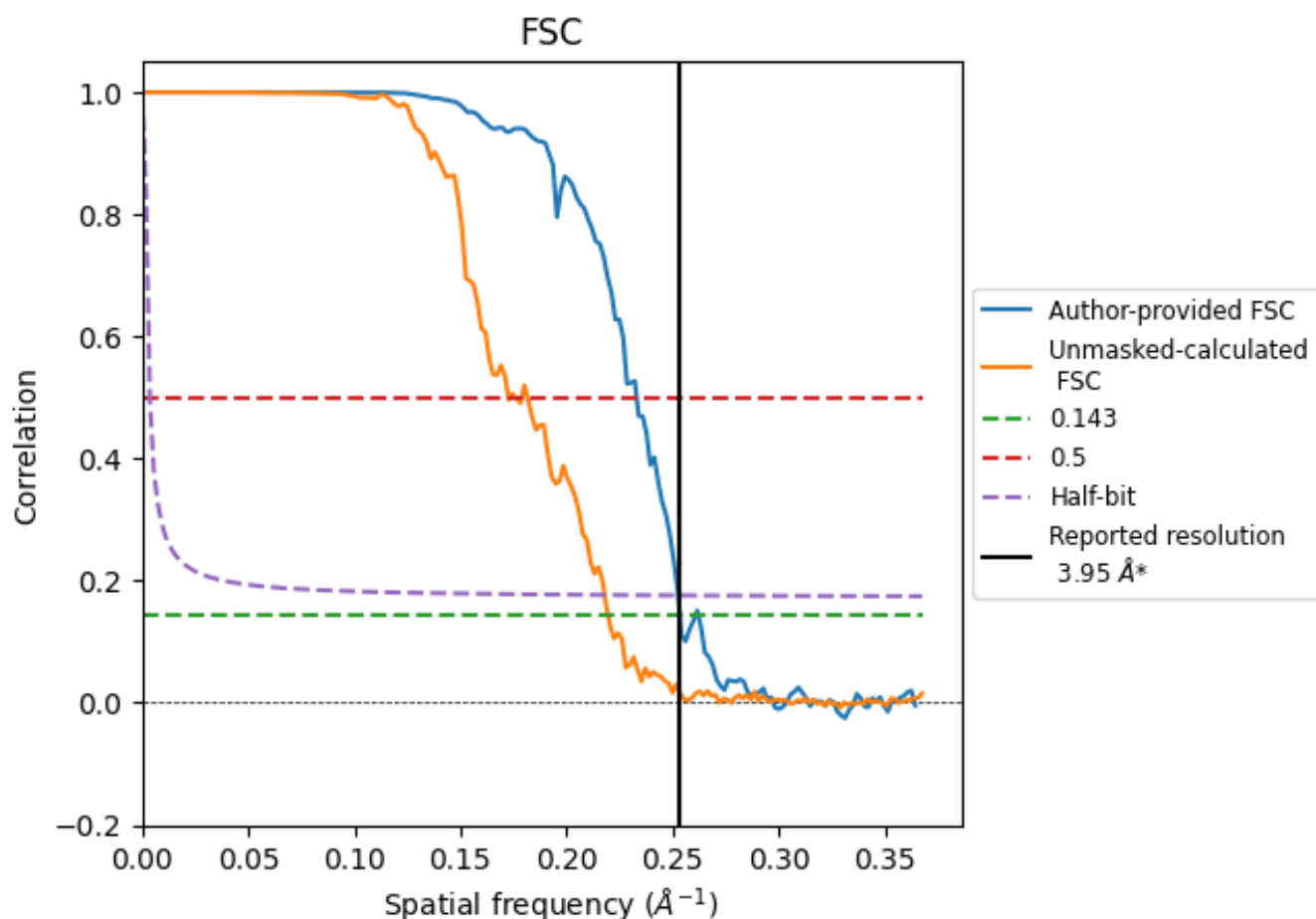


*Reported resolution corresponds to spatial frequency of 0.253 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.253 \AA^{-1}

8.2 Resolution estimates [i](#)

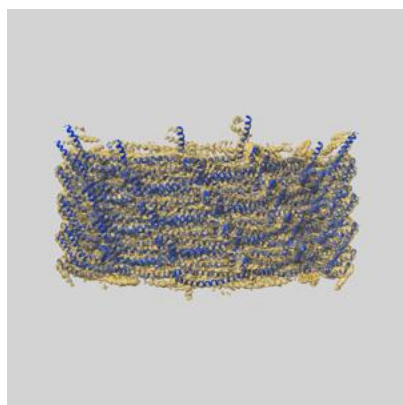
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.95	-	-
Author-provided FSC curve	3.95	4.29	3.96
Unmasked-calculated*	4.55	5.79	4.59

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.55 differs from the reported value 3.95 by more than 10 %

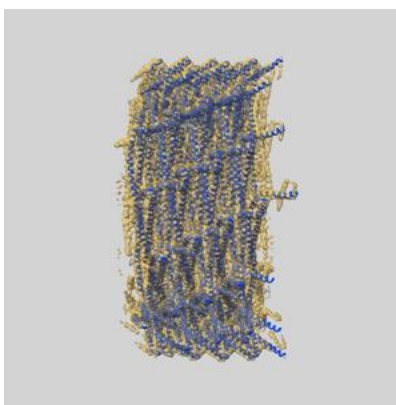
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-52530 and PDB model 9HZQ. Per-residue inclusion information can be found in section 3 on page 42.

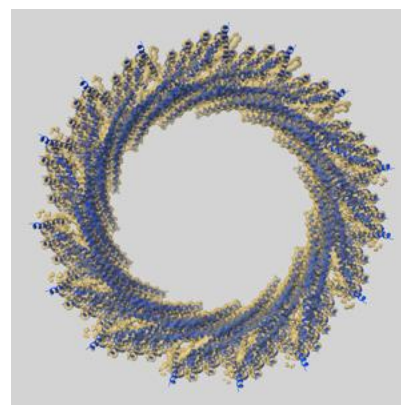
9.1 Map-model overlay [i](#)



X



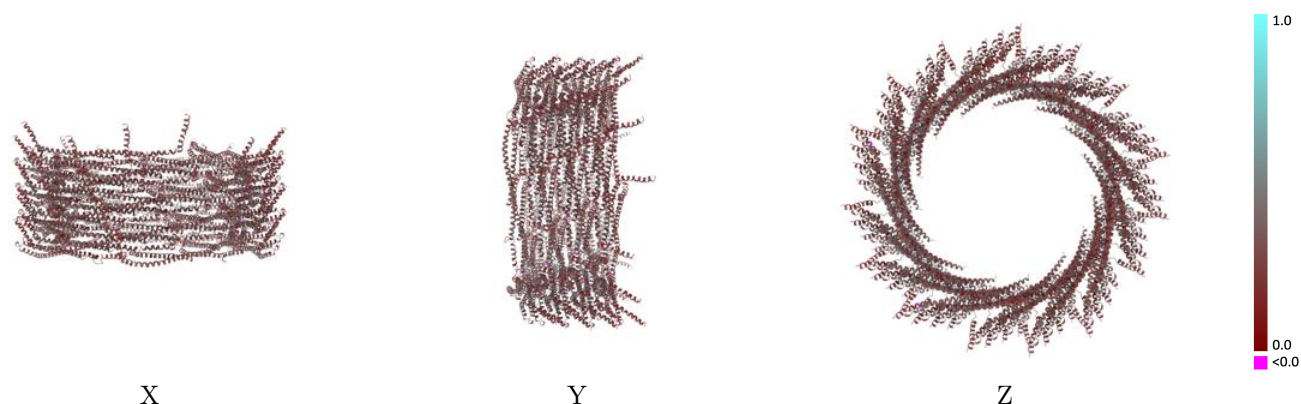
Y



Z

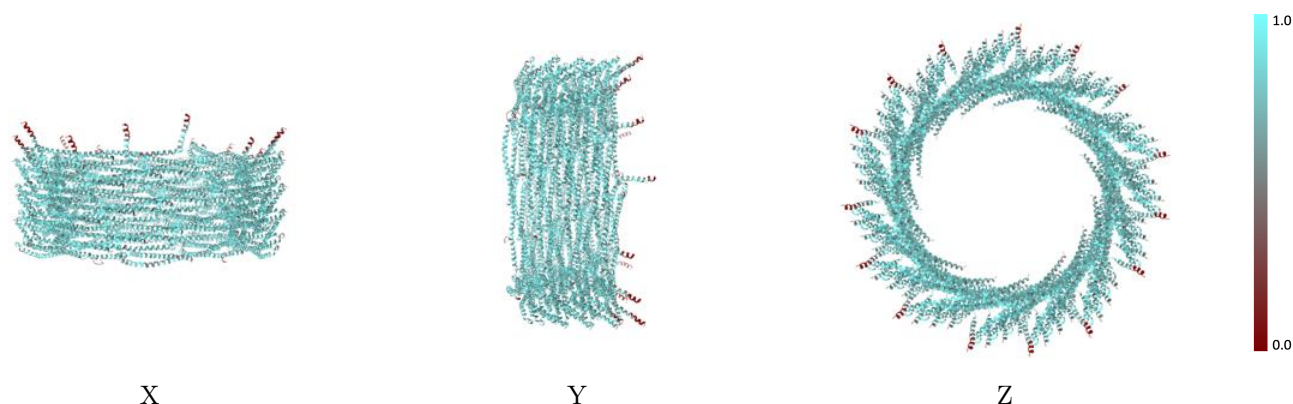
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



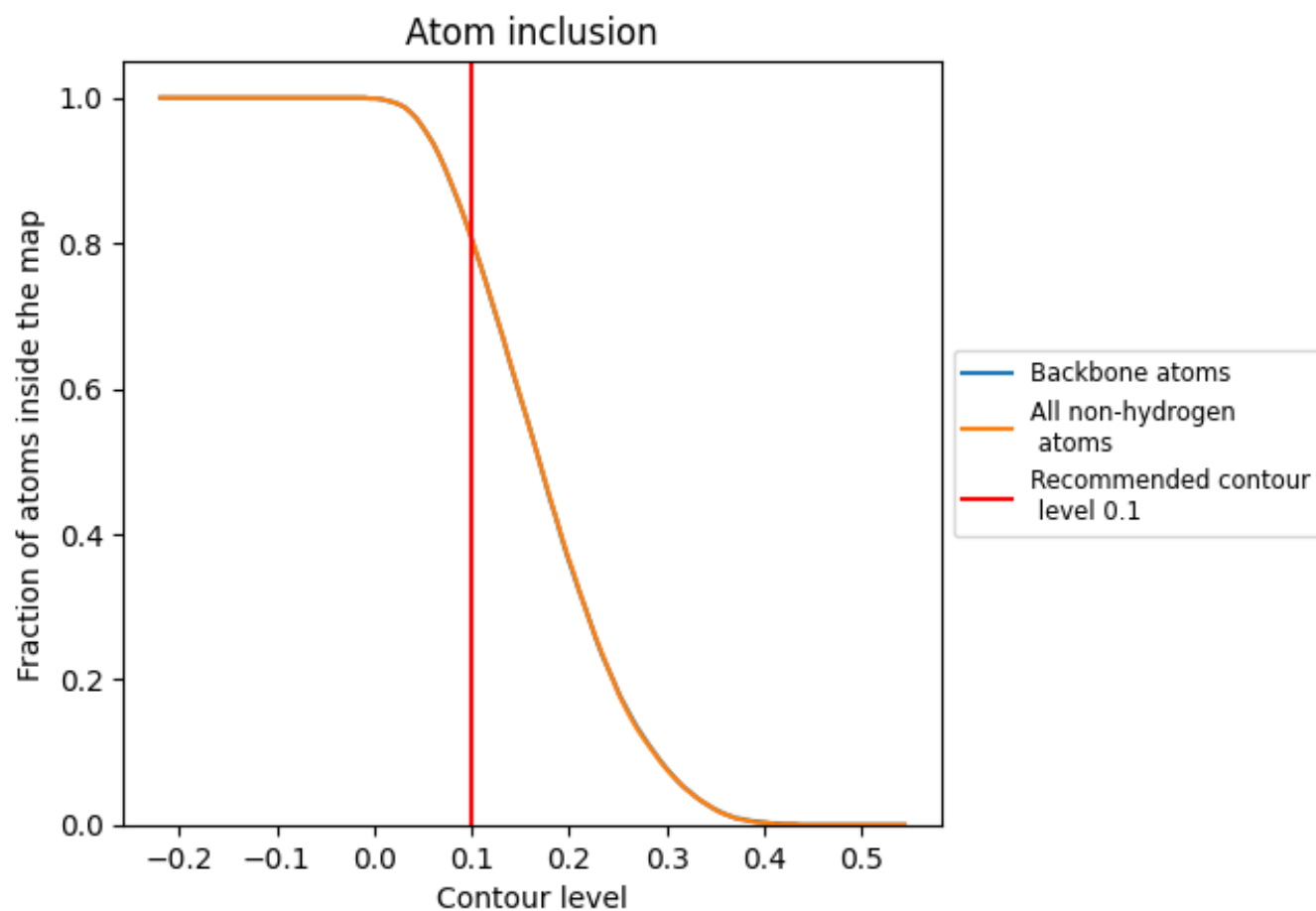
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 81% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ





















































The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8060	 0.3130
0	 0.8370	 0.3080
1	 0.8320	 0.3080
2	 0.8370	 0.3170
3	 0.8430	 0.3250
4	 0.8430	 0.3280
5	 0.8120	 0.3270
6	 0.8050	 0.3210
7	 0.7470	 0.3100
A	 0.7720	 0.3150
B	 0.8170	 0.3120
C	 0.8260	 0.3190
D	 0.8510	 0.3260
E	 0.8520	 0.3350
F	 0.8560	 0.3380
G	 0.8640	 0.3350
H	 0.8580	 0.3270
I	 0.8510	 0.3160
J	 0.8060	 0.3070
K	 0.7780	 0.3010
L	 0.7210	 0.2960
M	 0.7650	 0.3360
N	 0.8260	 0.3420
O	 0.8450	 0.3410
P	 0.8690	 0.3390
Q	 0.8660	 0.3270
R	 0.8540	 0.3160
S	 0.8510	 0.3070
T	 0.8400	 0.3030
U	 0.8320	 0.3040
V	 0.7900	 0.3060
W	 0.7810	 0.3040
X	 0.7470	 0.2940
Y	 0.7920	 0.3350
Z	 0.8320	 0.3240



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Chain	Atom inclusion	Q-score
a	 0.8470	 0.3120
b	 0.8450	 0.3050
c	 0.8440	 0.3040
d	 0.8430	 0.3080
e	 0.8410	 0.3100
f	 0.8380	 0.3090
g	 0.8370	 0.3030
h	 0.7990	 0.3020
i	 0.7690	 0.2900
j	 0.7260	 0.2840
k	 0.7600	 0.2990
l	 0.8000	 0.3010
m	 0.8240	 0.3090
n	 0.8430	 0.3140
o	 0.8420	 0.3130
p	 0.8540	 0.3110
q	 0.8370	 0.3110
r	 0.8250	 0.3010
s	 0.8220	 0.2970
t	 0.7850	 0.3000
u	 0.7740	 0.3080
v	 0.7320	 0.3090
w	 0.7600	 0.3110
x	 0.8210	 0.3150
y	 0.8400	 0.3160
z	 0.8350	 0.3140