



Full wwPDB EM Validation Report ⓘ

Aug 7, 2025 – 07:12 am BST

PDB ID : 9HZU / pdb_00009hzu
EMDB ID : EMD-52534
Title : 235 A SynPspA rod after incubation with EPL
Authors : Hudina, E.; Junglas, B.; Sachse, C.
Deposited on : 2025-01-14
Resolution : 6.20 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

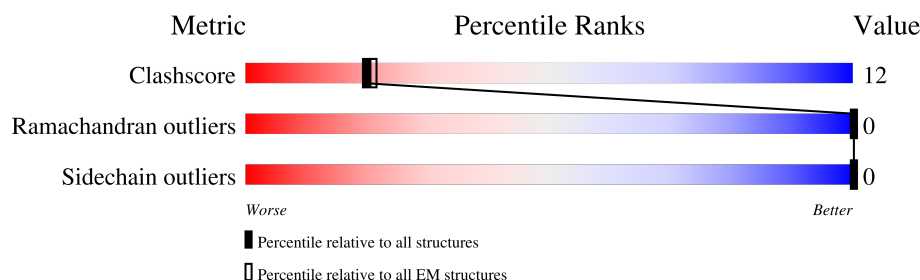
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.20 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.
















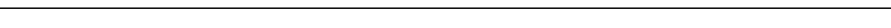











Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	0	246	54% 26% 20%
1	1	246	53% 26% 20%
1	2	246	53% 27% 20%
1	3	246	54% 26% 20%
1	4	246	56% 24% 20%
1	5	246	55% 25% 20%
1	6	246	54% 26% 20%
1	7	246	57% 23% 20%
1	A	246	57% 23% 20%


























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Mol	Chain	Length	Quality of chain
1	B	246	
1	C	246	
1	D	246	
1	E	246	
1	F	246	
1	G	246	
1	H	246	
1	I	246	
1	J	246	
1	K	246	
1	L	246	
1	M	246	
1	N	246	
1	O	246	
1	P	246	
1	Q	246	
1	R	246	
1	S	246	
1	T	246	
1	U	246	
1	V	246	
1	W	246	
1	X	246	
1	Y	246	
1	Z	246	


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Mol	Chain	Length	Quality of chain
1	a	246	
1	b	246	
1	c	246	
1	d	246	
1	e	246	
1	f	246	
1	g	246	
1	h	246	
1	i	246	
1	j	246	
1	k	246	
1	l	246	
1	m	246	
1	n	246	
1	o	246	
1	p	246	
1	q	246	
1	r	246	
1	s	246	
1	t	246	
1	u	246	
1	v	246	
1	w	246	
1	x	246	
1	y	246	

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Mol	Chain	Length	Quality of chain
1	z	246	 55% 25% 20%

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 190860 atoms, of which 96240 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	196	Total	C	H	N	O	S	0	0
			3181	978	1604	289	308	2		
1	1	196	Total	C	H	N	O	S	0	0
			3181	978	1604	289	308	2		
1	2	196	Total	C	H	N	O	S	0	0
			3181	978	1604	289	308	2		
1	3	196	Total	C	H	N	O	S	0	0
			3181	978	1604	289	308	2		
1	4	196	Total	C	H	N	O	S	0	0
			3181	978	1604	289	308	2		
1	5	196	Total	C	H	N	O	S	0	0
			3181	978	1604	289	308	2		
1	6	196	Total	C	H	N	O	S	0	0
			3181	978	1604	289	308	2		
1	7	196	Total	C	H	N	O	S	0	0
			3181	978	1604	289	308	2		
1	A	196	Total	C	H	N	O	S	0	0
			3181	978	1604	289	308	2		
1	B	196	Total	C	H	N	O	S	0	0
			3181	978	1604	289	308	2		
1	C	196	Total	C	H	N	O	S	0	0
			3181	978	1604	289	308	2		
1	D	196	Total	C	H	N	O	S	0	0
			3181	978	1604	289	308	2		
1	E	196	Total	C	H	N	O	S	0	0
			3181	978	1604	289	308	2		
1	F	196	Total	C	H	N	O	S	0	0
			3181	978	1604	289	308	2		
1	G	196	Total	C	H	N	O	S	0	0
			3181	978	1604	289	308	2		
1	H	196	Total	C	H	N	O	S	0	0
			3181	978	1604	289	308	2		
1	I	196	Total	C	H	N	O	S	0	0
			3181	978	1604	289	308	2		

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Mol	Chain	Residues	Atoms						AltConf	Trace
1	J	196	Total 3181	C 978	H 1604	N 289	O 308	S 2	0	0
1	K	196	Total 3181	C 978	H 1604	N 289	O 308	S 2	0	0
1	L	196	Total 3181	C 978	H 1604	N 289	O 308	S 2	0	0
1	M	196	Total 3181	C 978	H 1604	N 289	O 308	S 2	0	0
1	N	196	Total 3181	C 978	H 1604	N 289	O 308	S 2	0	0
1	O	196	Total 3181	C 978	H 1604	N 289	O 308	S 2	0	0
1	P	196	Total 3181	C 978	H 1604	N 289	O 308	S 2	0	0
1	Q	196	Total 3181	C 978	H 1604	N 289	O 308	S 2	0	0
1	R	196	Total 3181	C 978	H 1604	N 289	O 308	S 2	0	0
1	S	196	Total 3181	C 978	H 1604	N 289	O 308	S 2	0	0
1	T	196	Total 3181	C 978	H 1604	N 289	O 308	S 2	0	0
1	U	196	Total 3181	C 978	H 1604	N 289	O 308	S 2	0	0
1	V	196	Total 3181	C 978	H 1604	N 289	O 308	S 2	0	0
1	W	196	Total 3181	C 978	H 1604	N 289	O 308	S 2	0	0
1	X	196	Total 3181	C 978	H 1604	N 289	O 308	S 2	0	0
1	Y	196	Total 3181	C 978	H 1604	N 289	O 308	S 2	0	0
1	Z	196	Total 3181	C 978	H 1604	N 289	O 308	S 2	0	0
1	a	196	Total 3181	C 978	H 1604	N 289	O 308	S 2	0	0
1	b	196	Total 3181	C 978	H 1604	N 289	O 308	S 2	0	0
1	c	196	Total 3181	C 978	H 1604	N 289	O 308	S 2	0	0
1	d	196	Total 3181	C 978	H 1604	N 289	O 308	S 2	0	0

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Mol	Chain	Residues	Atoms						AltConf	Trace
1	e	196	Total 3181	C 978	H 1604	N 289	O 308	S 2	0	0
1	f	196	Total 3181	C 978	H 1604	N 289	O 308	S 2	0	0
1	g	196	Total 3181	C 978	H 1604	N 289	O 308	S 2	0	0
1	h	196	Total 3181	C 978	H 1604	N 289	O 308	S 2	0	0
1	i	196	Total 3181	C 978	H 1604	N 289	O 308	S 2	0	0
1	j	196	Total 3181	C 978	H 1604	N 289	O 308	S 2	0	0
1	k	196	Total 3181	C 978	H 1604	N 289	O 308	S 2	0	0
1	l	196	Total 3181	C 978	H 1604	N 289	O 308	S 2	0	0
1	m	196	Total 3181	C 978	H 1604	N 289	O 308	S 2	0	0
1	n	196	Total 3181	C 978	H 1604	N 289	O 308	S 2	0	0
1	o	196	Total 3181	C 978	H 1604	N 289	O 308	S 2	0	0
1	p	196	Total 3181	C 978	H 1604	N 289	O 308	S 2	0	0
1	q	196	Total 3181	C 978	H 1604	N 289	O 308	S 2	0	0
1	r	196	Total 3181	C 978	H 1604	N 289	O 308	S 2	0	0
1	s	196	Total 3181	C 978	H 1604	N 289	O 308	S 2	0	0
1	t	196	Total 3181	C 978	H 1604	N 289	O 308	S 2	0	0
1	u	196	Total 3181	C 978	H 1604	N 289	O 308	S 2	0	0
1	v	196	Total 3181	C 978	H 1604	N 289	O 308	S 2	0	0
1	w	196	Total 3181	C 978	H 1604	N 289	O 308	S 2	0	0
1	x	196	Total 3181	C 978	H 1604	N 289	O 308	S 2	0	0
1	y	196	Total 3181	C 978	H 1604	N 289	O 308	S 2	0	0

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Mol	Chain	Residues	Atoms						AltConf	Trace
1	z	196	Total	C	H	N	O	S	0	0
			3181	978	1604	289	308	2		

There are 1380 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

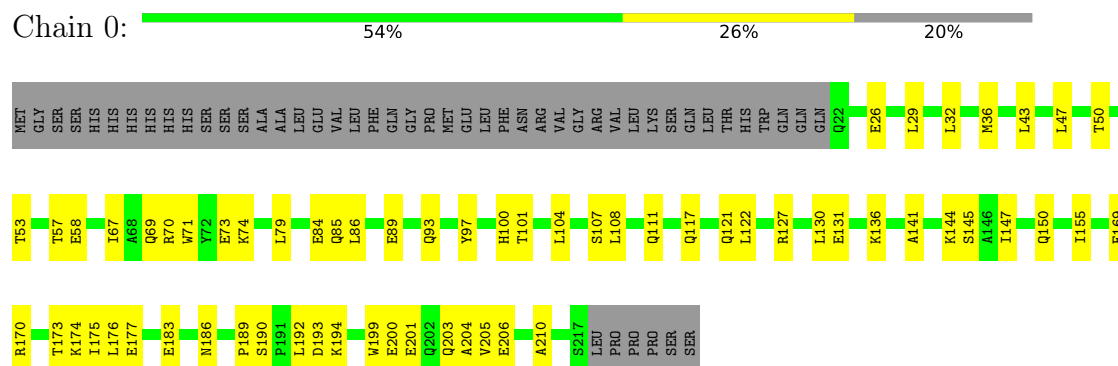
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Chain	Residue	Modelled	Actual	Comment	Reference
y	-18	HIS	-	expression tag	UNP P74717
y	-17	HIS	-	expression tag	UNP P74717
y	-16	HIS	-	expression tag	UNP P74717
y	-15	HIS	-	expression tag	UNP P74717
y	-14	HIS	-	expression tag	UNP P74717
y	-13	HIS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

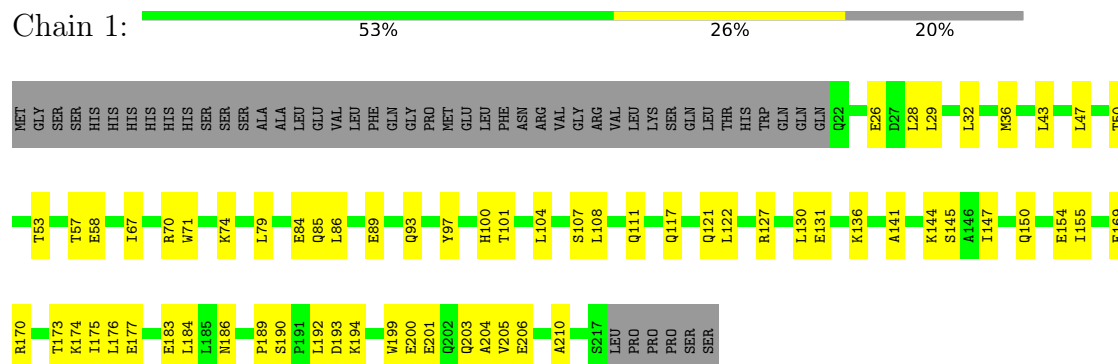
3 Residue-property plots

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

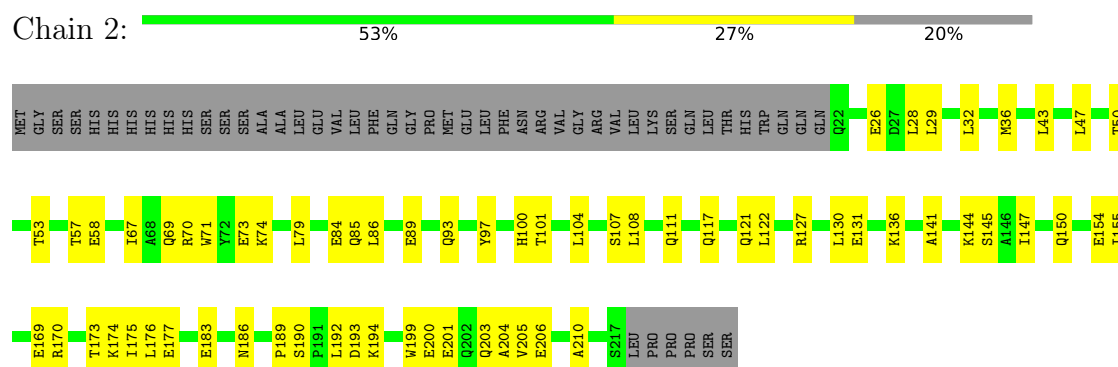
- Molecule 1: Chloroplast membrane-associated 30 kD protein



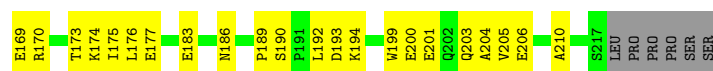
- Molecule 1: Chloroplast membrane-associated 30 kD protein



- Molecule 1: Chloroplast membrane-associated 30 kD protein

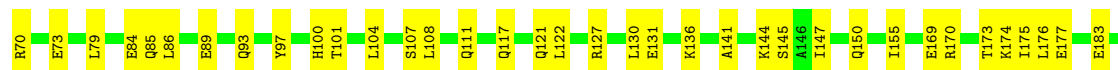
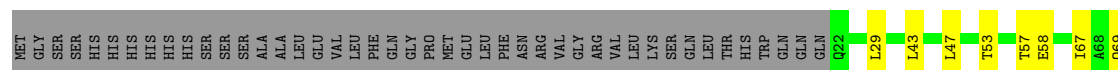


- [illegible]



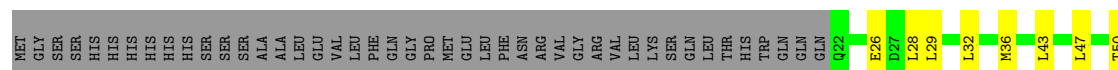
- Molecule 1: Chloroplast membrane-associated 30 kD protein

Chain 7: 57% 23% 20%



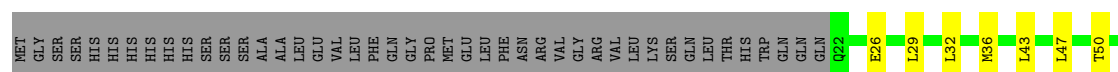
- Molecule 1: Chloroplast membrane-associated 30 kD protein

Chain A: 57% 23% 20%



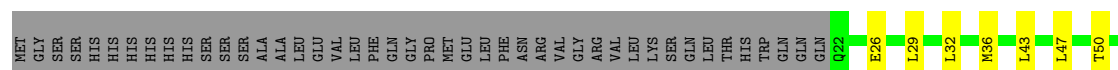
- Molecule 1: Chloroplast membrane-associated 30 kD protein

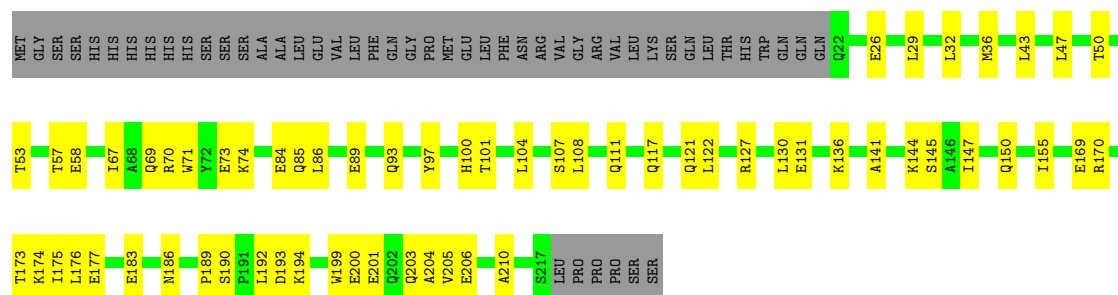
Chain B: 54% 25% 20%



- Molecule 1: Chloroplast membrane-associated 30 kD protein

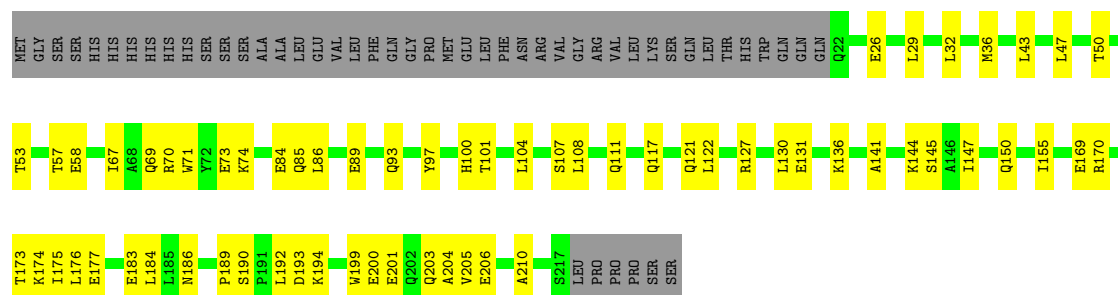
Chain C: 54% 25% 20%





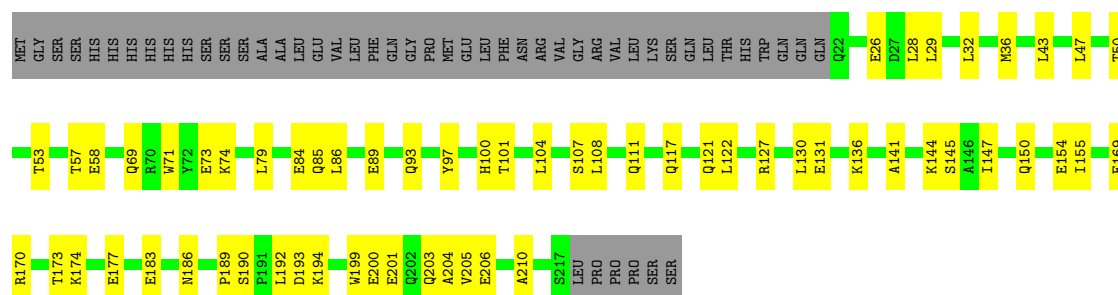
- Molecule 1: Chloroplast membrane-associated 30 kD protein

Chain H: 54% 26% 20%



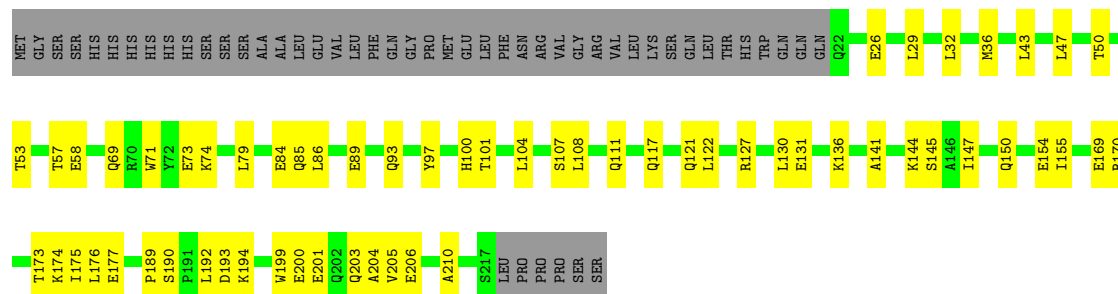
- Molecule 1: Chloroplast membrane-associated 30 kD protein

Chain I: 54% 25% 20%

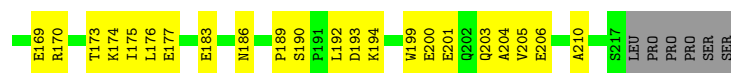


- Molecule 1: Chloroplast membrane-associated 30 kD protein

Chain J: 55% 25% 20%

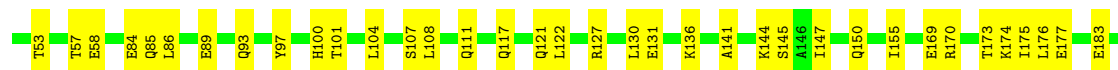
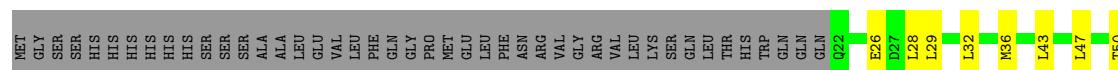


- Molecule 1: Chloroplast membrane-associated 30 kD protein



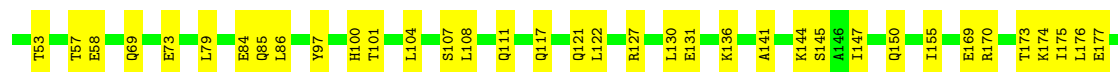
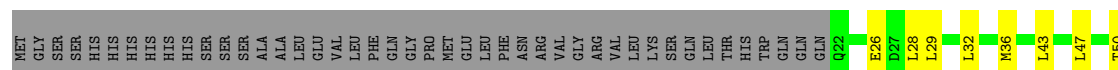
- Molecule 1: Chloroplast membrane-associated 30 kD protein

Chain O: 56% 24% 20%



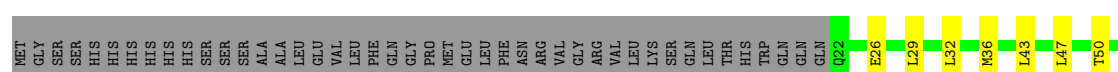
- Molecule 1: Chloroplast membrane-associated 30 kD protein

Chain P: 57% 23% 20%



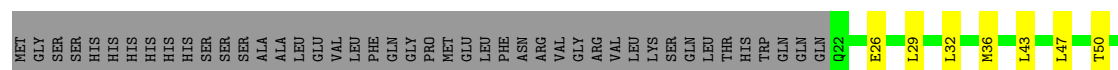
- Molecule 1: Chloroplast membrane-associated 30 kD protein

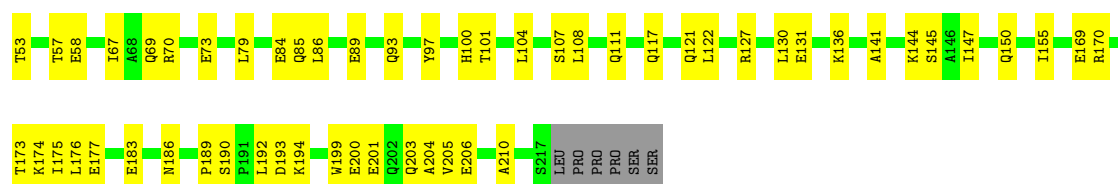
Chain Q: 55% 24% 20%



- Molecule 1: Chloroplast membrane-associated 30 kD protein

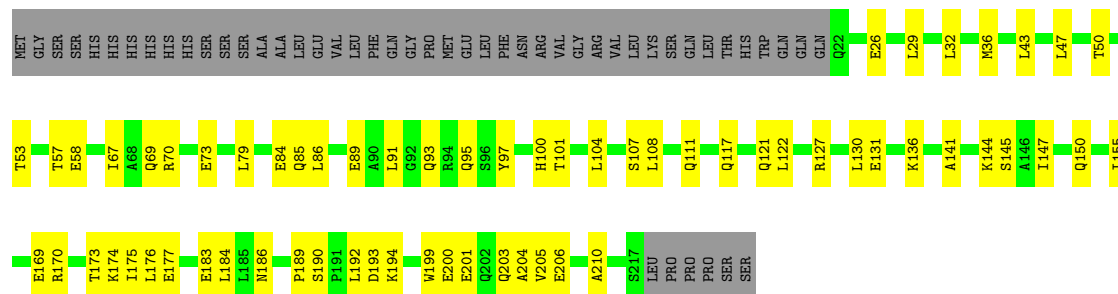
Chain R: 54% 25% 20%





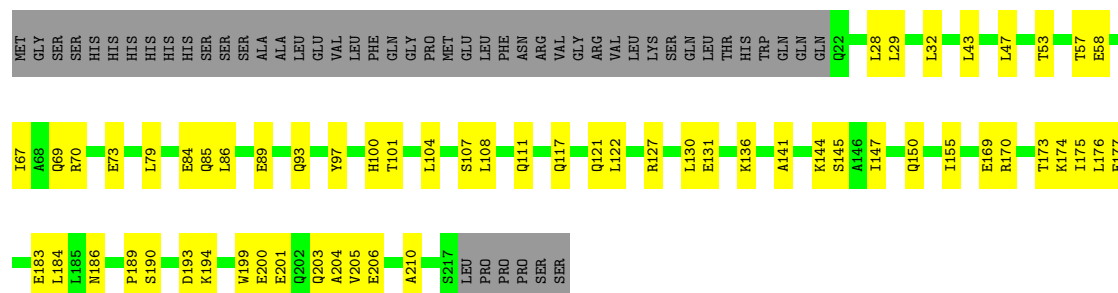
- Molecule 1: Chloroplast membrane-associated 30 kD protein

Chain S: 53% 26% 20%



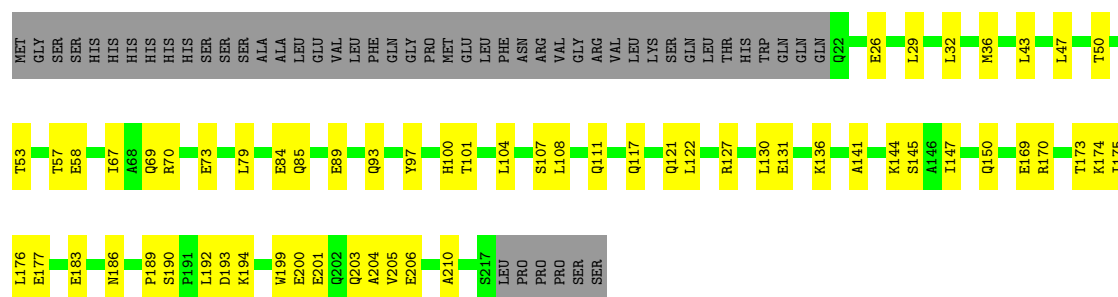
- Molecule 1: Chloroplast membrane-associated 30 kD protein

Chain T: 55% 24% 20%



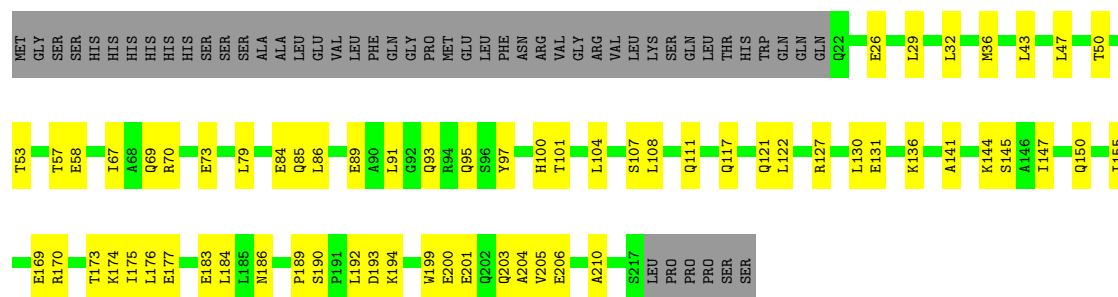
- Molecule 1: Chloroplast membrane-associated 30 kD protein

Chain U: 55% 24% 20%



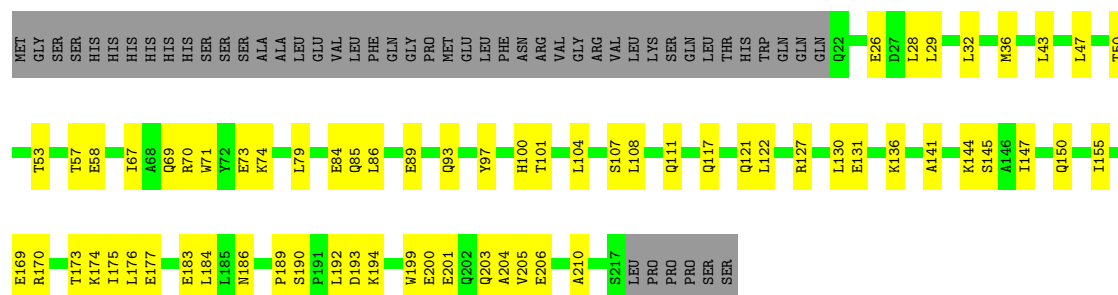
- Molecule 1: Chloroplast membrane-associated 30 kD protein

Chain V: 53% 26% 20%



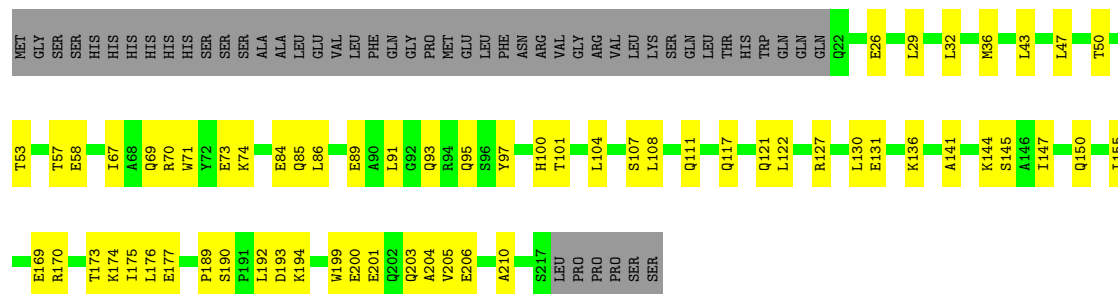
- Molecule 1: Chloroplast membrane-associated 30 kD protein

Chain W: 53% 27% 20%



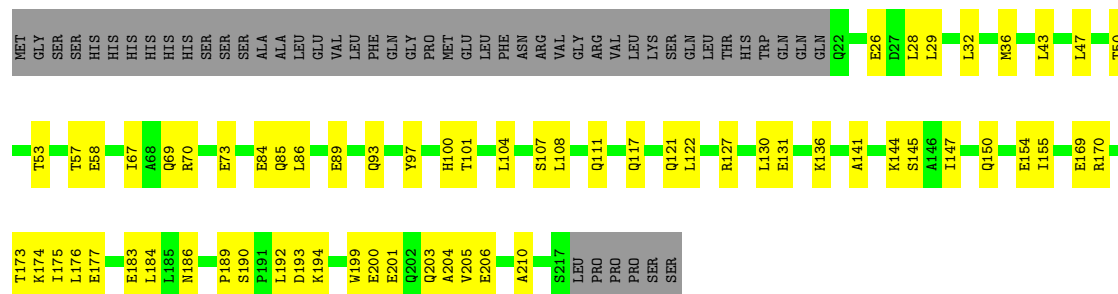
- Molecule 1: Chloroplast membrane-associated 30 kD protein

Chain X: 54% 26% 20%

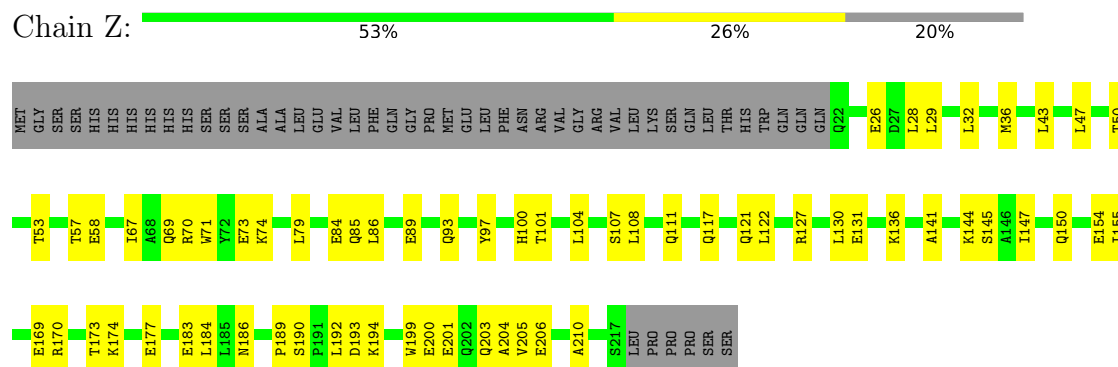


- Molecule 1: Chloroplast membrane-associated 30 kD protein

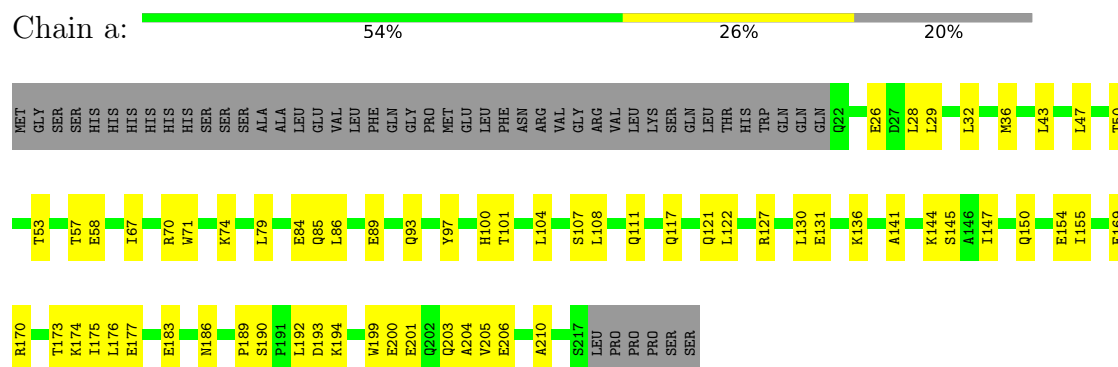
Chain Y: 54% 26% 20%



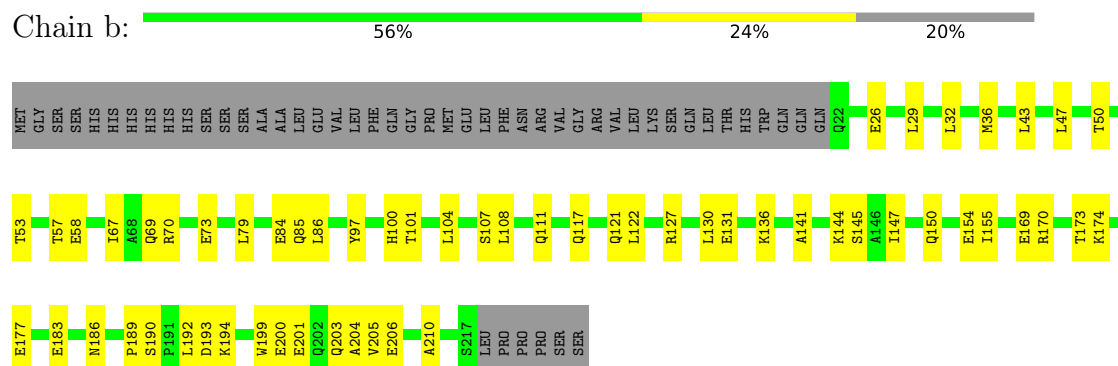
- Molecule 1: Chloroplast membrane-associated 30 kD protein



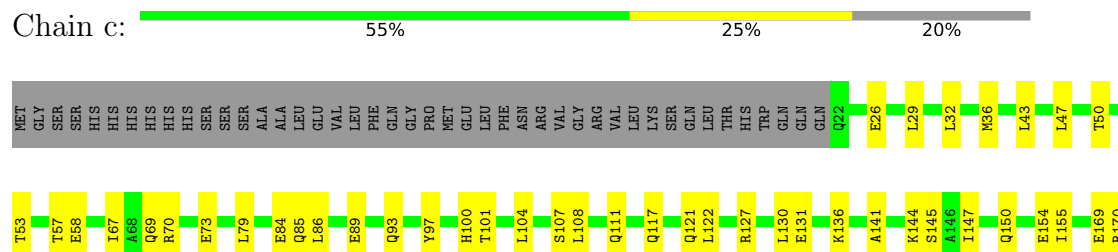
- Molecule 1: Chloroplast membrane-associated 30 kD protein



- Molecule 1: Chloroplast membrane-associated 30 kD protein.

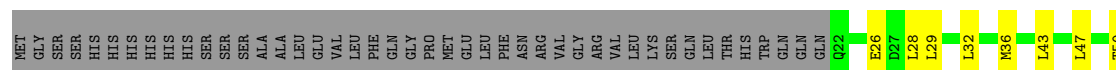


- Molecule 1: Chloroplast membrane-associated 30 kD protein.

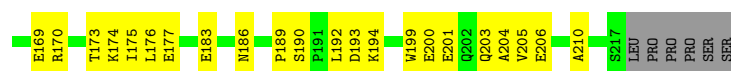
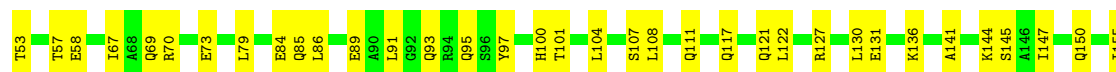
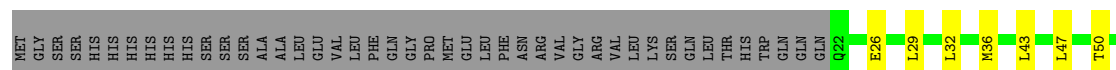




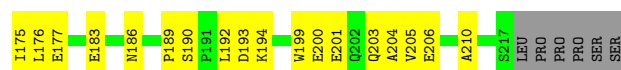
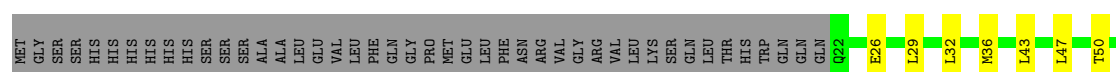
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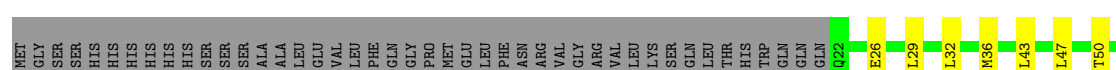
- Molecule 1: Chloroplast membrane-associated 30 kD protein

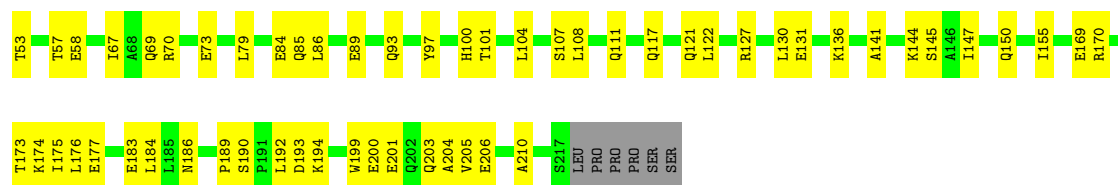


- Molecule 1: Chloroplast membrane-associated 30 kD protein

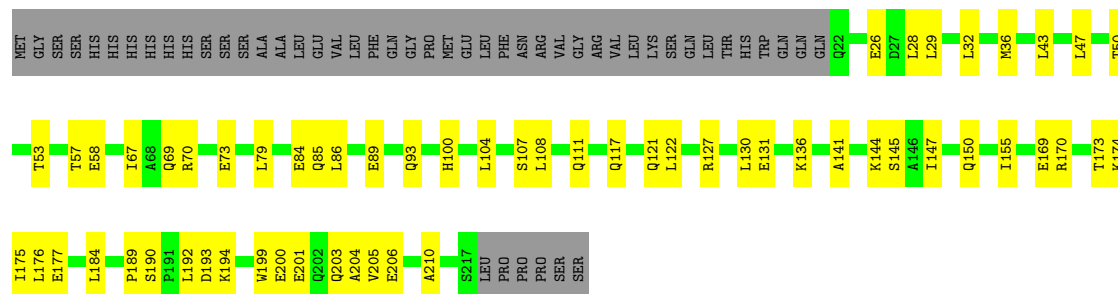


- Molecule 1: Chloroplast membrane-associated 30 kD protein

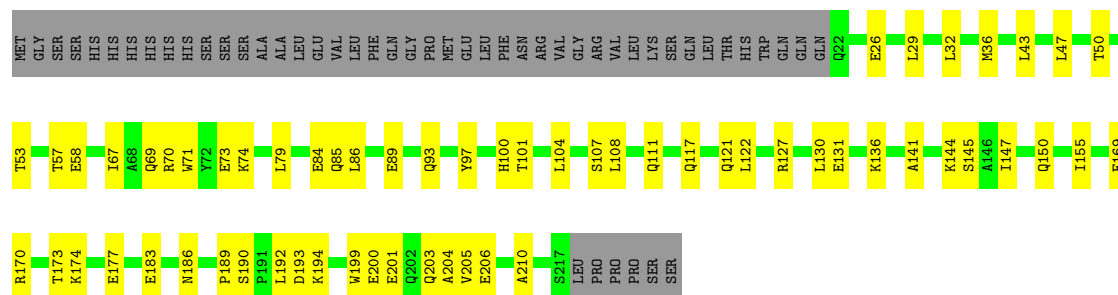




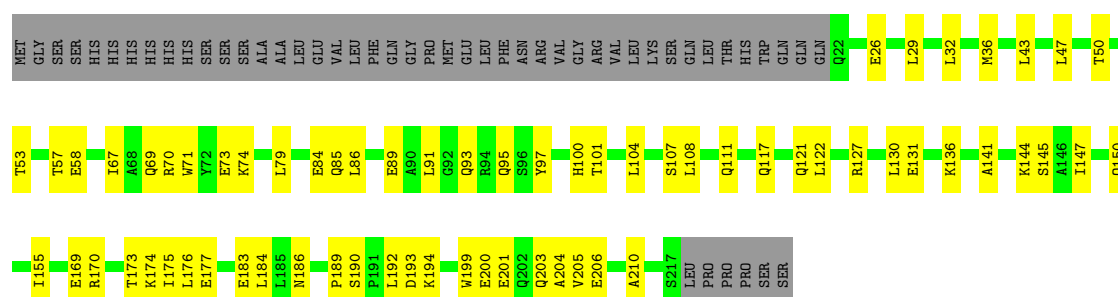
- Molecule 1: Chloroplast membrane-associated 30 kD protein



- Molecule 1: Chloroplast membrane-associated 30 kD protein

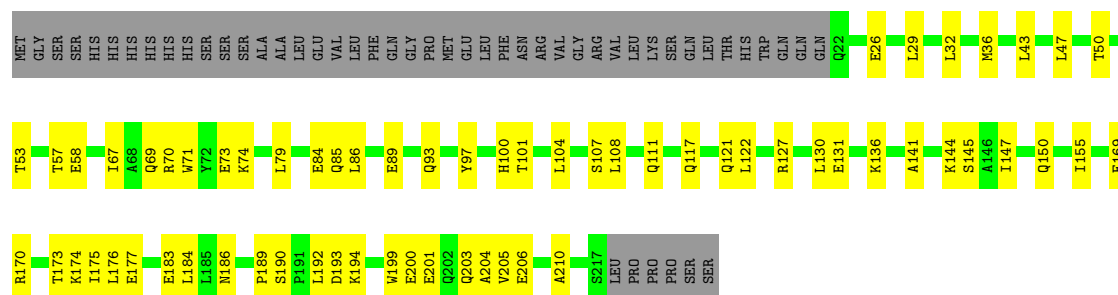


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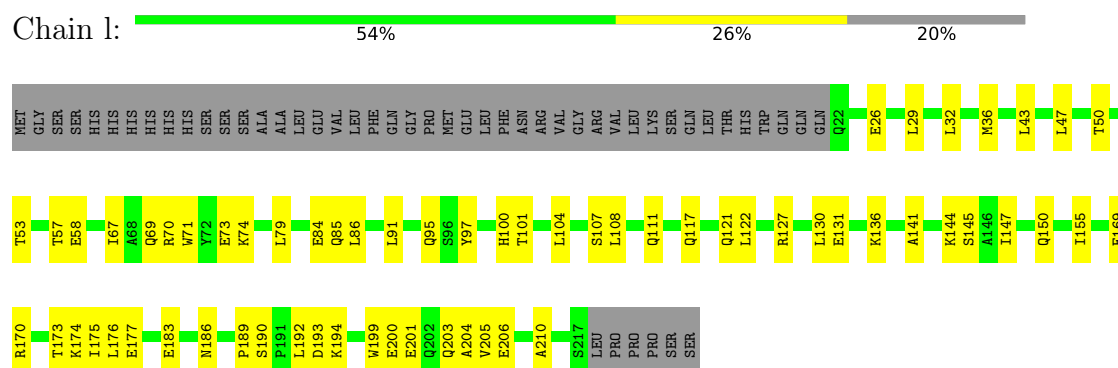


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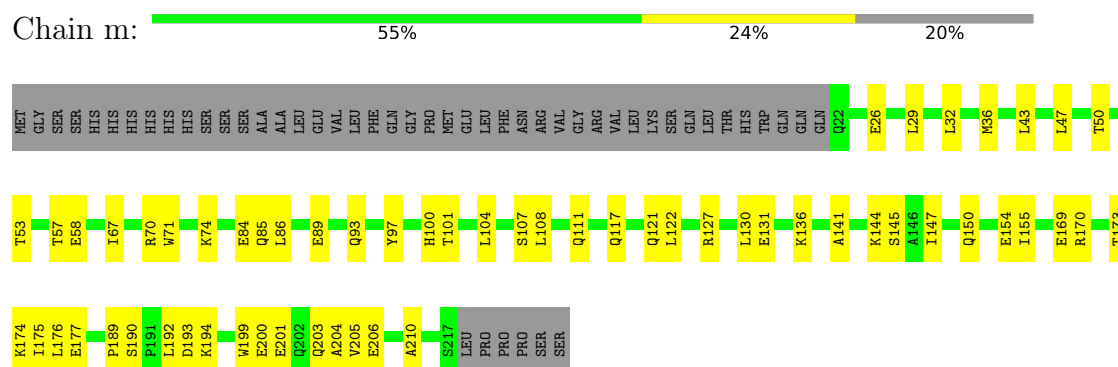




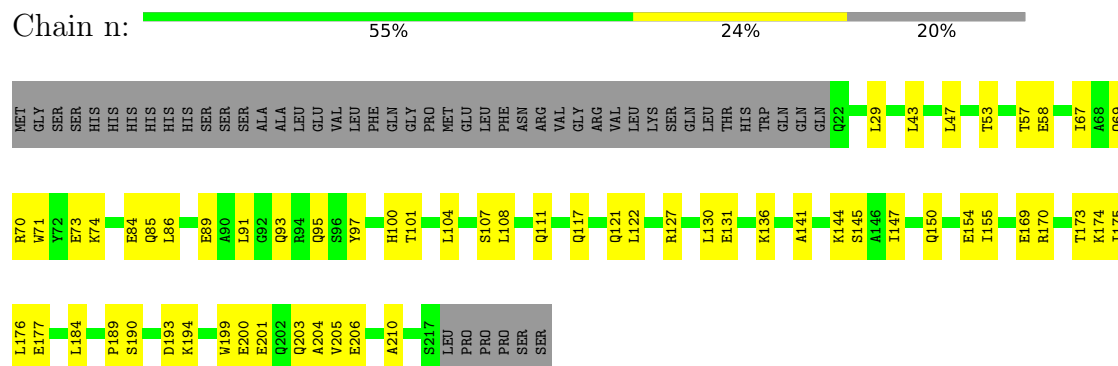
- Molecule 1: Chloroplast membrane-associated 30 kD protein



- Molecule 1: Chloroplast membrane-associated 30 kD protein



- Molecule 1: Chloroplast membrane-associated 30 kD protein



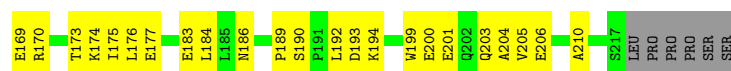
- Molecule 1: Chloroplast membrane-associated 30 kD protein

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P191	Q69	HIS
L192	R70	HIS
D193	W1	HIS
K194	Y72	SER
W199	E73	SER
E200	K74	SER
E201	L79	ALA
Q202	E84	ALA
Q203	Q85	LEU
A204	L91	VAL
V205	Q95	LEU
E206	S86	PHE
A210	Y97	GLN
S217	H100	GLY
LEU	T101	PRO
PRO	L104	LEU
PRO	S107	ASN
PRO	L108	ARG
SER	Q111	VAL
SER	Q117	ARG
	Q121	LYS
	L122	SER
	R127	GLN
	L130	LEU
	E131	THR
	K136	HIS
	K144	TRP
	I147	GLN
	Q150	GLN
	E169	GLN
	R170	GLN
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		L32
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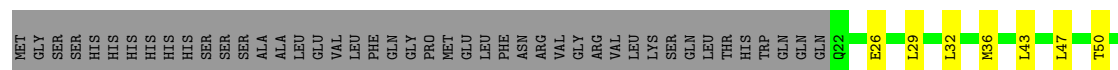
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| P189 | T67 | HIS |
| S190 | | HIS |
| P191 | R70 | HIS |
| L192 | W71 | HIS |
| D193 | | HIS |
| K194 | K74 | SER |
| | | SER |
| W199 | E84 | SER |
| E200 | Q85 | ALA |
| E201 | L86 | ALA |
| Q202 | | LEU |
| Q203 | E89 | GLU |
| A204 | | VAL |
| V205 | Q93 | LEU |
| E206 | | PHE |
| | Y97 | GLN |
| A210 | | GLY |
| | | PRO |
| S217 | H100 | PRO |
| LEU | T101 | MET |
| PRO | | GLU |
| PRO | L104 | LEU |
| PRO | | PHE |
| PRO | S107 | ASN |
| SER | L108 | ARG |
| SER | | VAL |
| SER | Q111 | GLY |
| | | ARG |
| | Q117 | VAL |
| | | LEU |
| | Q121 | LYS |
| | L122 | SER |
| | | GLN |
| | R127 | LEU |
| | | THR |
| | L130 | HIS |
| | E131 | TRP |
| | | GLN |
| | K136 | GLN |
| | | GLN |
| | A141 | Q22 |
| | | |
| | K144 | E26 |
| | S145 | |
| | A146 | L29 |
| | I147 | |
| | | L32 |
| | Q150 | |
| | | K36 |
| | E154 | |
| | I155 | L43 |
| | | |
| | E169 | L47 |
| | R170 | |
| | | T50 |
| | T172 | |

- | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| ET54 | ET57 | ET69 | ET73 | ET84 | ET89 | ET90 | ET91 | ET92 | ET93 | ET94 | ET95 | ET96 | ET97 | ET100 | ET101 | ET104 | ET107 | ET108 | ET111 | ET117 | ET121 | ET122 | ET127 | ET130 | ET131 | ET136 | ET141 | ET144 | ET145 | ET147 | ET150 | | | | | | | | | | | | |
| I155 | E58 | R170 | T173 | K174 | I175 | L176 | E177 | L184 | P189 | S190 | F191 | L192 | D193 | K194 | W199 | E200 | Q202 | Q203 | A204 | V205 | E206 | A210 | S217 | L1E1 | P1PRO | P1PRO | P1PRO | S1SER | S1SER | L43 | L47 | T50 | | | | | | | | | | | |
| HIS | HIS | HIS | HIS | HIS | HIS | SER | SER | ALA | ALA | LEU | GLU | VAL | LEU | PHE | GLN | GLY | PRO | MET | GLU | PHE | ASN | ARG | VAL | GLY | VAL | LEU | LYS | SER | GLN | THR | HIS | TRP | GLN | GLN | GLN | Q22 | E26 | L29 | L32 | K36 | L43 | L47 | T50 |

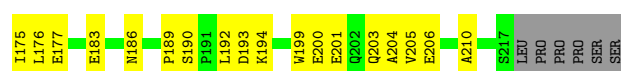
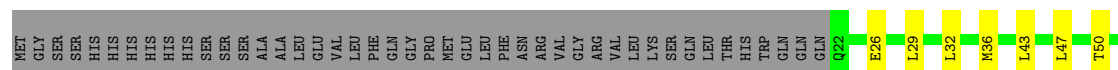
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| T63 | T57 | E58 | I67 | A68 | Q69 | R70 | W71 | Y72 | E73 | K74 | L79 | E84 | Q85 | L86 | E89 | Q93 | Y97 | H100 | T101 | L104 | S107 | L108 | Q111 | Q117 | Q121 | L122 | R127 | L130 | E131 | K136 | A141 | K144 | S145 | A146 | L147 | Q150 | E154 | I155 | | | | | | | | |
| MET | GLY | SER | SER | HIS | HIS | HIS | HIS | SER | SER | SER | ALA | ALA | LEU | GLU | VAL | LEU | PHE | GLN | GLY | PRO | MET | GLU | PHE | ASN | ARG | VAL | LEU | LYS | SER | GLN | GLN | LEU | THR | HIS | TRP | GLN | GLN | GLN | Q22 | E26 | L29 | L32 | M36 | L43 | L47 | T50 |



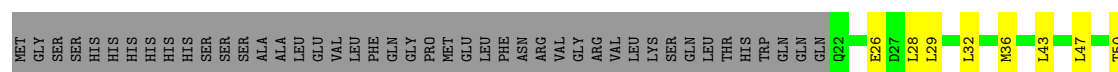
- Molecule 1: Chloroplast membrane-associated 30 kD protein



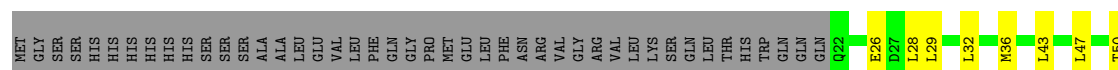
- Molecule 1: Chloroplast membrane-associated 30 kD protein

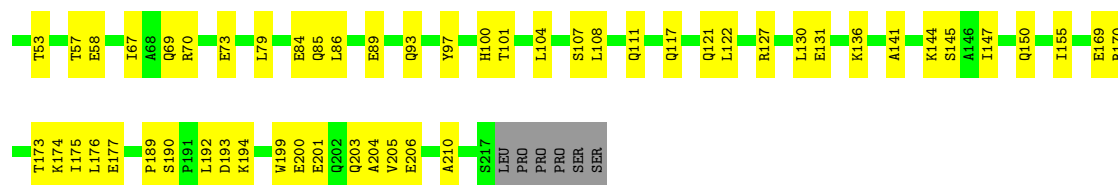


- Molecule 1: Chloroplast membrane-associated 30 kD protein



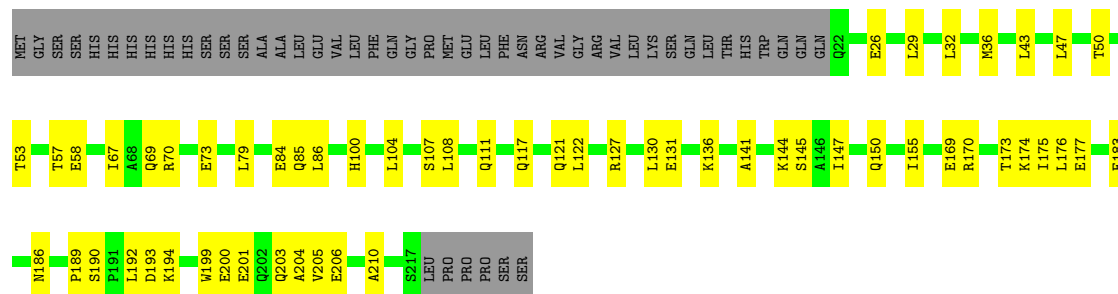
- Molecule 1: Chloroplast membrane-associated 30 kD protein





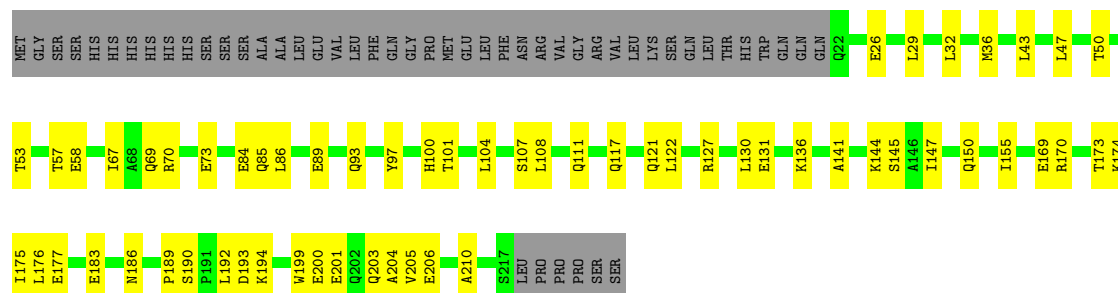
- Molecule 1: Chloroplast membrane-associated 30 kD protein

Chain w:



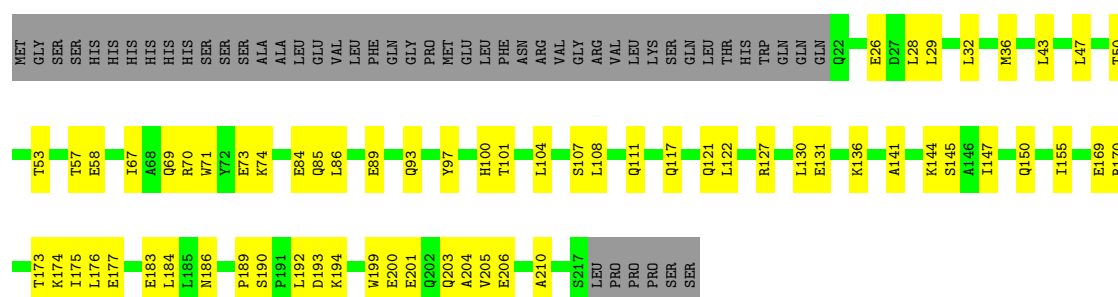
- Molecule 1: Chloroplast membrane-associated 30 kD protein

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=28.2°, rise=7.01 Å, axial sym=C3	Depositor
Number of segments used	52698	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

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	0.14	0/1593	0.27	0/2138
1	1	0.14	0/1593	0.27	0/2138
1	2	0.14	0/1593	0.27	0/2138
1	3	0.14	0/1593	0.27	0/2138
1	4	0.14	0/1593	0.27	0/2138
1	5	0.14	0/1593	0.27	0/2138
1	6	0.14	0/1593	0.27	0/2138
1	7	0.14	0/1593	0.27	0/2138
1	A	0.14	0/1593	0.27	0/2138
1	B	0.14	0/1593	0.27	0/2138
1	C	0.14	0/1593	0.27	0/2138
1	D	0.14	0/1593	0.27	0/2138
1	E	0.14	0/1593	0.27	0/2138
1	F	0.14	0/1593	0.27	0/2138
1	G	0.14	0/1593	0.27	0/2138
1	H	0.14	0/1593	0.27	0/2138
1	I	0.14	0/1593	0.27	0/2138
1	J	0.14	0/1593	0.27	0/2138
1	K	0.14	0/1593	0.27	0/2138
1	L	0.14	0/1593	0.27	0/2138
1	M	0.14	0/1593	0.27	0/2138
1	N	0.14	0/1593	0.27	0/2138
1	O	0.14	0/1593	0.27	0/2138
1	P	0.14	0/1593	0.27	0/2138
1	Q	0.14	0/1593	0.27	0/2138
1	R	0.14	0/1593	0.27	0/2138
1	S	0.14	0/1593	0.27	0/2138
1	T	0.14	0/1593	0.27	0/2138
1	U	0.14	0/1593	0.27	0/2138
1	V	0.14	0/1593	0.27	0/2138
1	W	0.14	0/1593	0.27	0/2138
1	X	0.14	0/1593	0.27	0/2138
1	Y	0.14	0/1593	0.27	0/2138
1	Z	0.14	0/1593	0.27	0/2138

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	a	0.14	0/1593	0.27	0/2138
1	b	0.14	0/1593	0.27	0/2138
1	c	0.14	0/1593	0.27	0/2138
1	d	0.14	0/1593	0.27	0/2138
1	e	0.14	0/1593	0.27	0/2138
1	f	0.14	0/1593	0.27	0/2138
1	g	0.14	0/1593	0.27	0/2138
1	h	0.14	0/1593	0.27	0/2138
1	i	0.14	0/1593	0.27	0/2138
1	j	0.14	0/1593	0.27	0/2138
1	k	0.14	0/1593	0.27	0/2138
1	l	0.14	0/1593	0.27	0/2138
1	m	0.14	0/1593	0.27	0/2138
1	n	0.14	0/1593	0.27	0/2138
1	o	0.14	0/1593	0.27	0/2138
1	p	0.14	0/1593	0.27	0/2138
1	q	0.14	0/1593	0.27	0/2138
1	r	0.14	0/1593	0.27	0/2138
1	s	0.14	0/1593	0.27	0/2138
1	t	0.14	0/1593	0.27	0/2138
1	u	0.14	0/1593	0.27	0/2138
1	v	0.14	0/1593	0.27	0/2138
1	w	0.14	0/1593	0.27	0/2138
1	x	0.14	0/1593	0.27	0/2138
1	y	0.14	0/1593	0.27	0/2138
1	z	0.14	0/1593	0.27	0/2138
All	All	0.14	0/95580	0.27	0/128280

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	1577	1604	1603	46	0
1	1	1577	1604	1603	47	0
1	2	1577	1604	1603	47	0
1	3	1577	1604	1603	45	0
1	4	1577	1604	1603	42	0
1	5	1577	1604	1603	44	0
1	6	1577	1604	1603	45	0
1	7	1577	1604	1603	38	0
1	A	1577	1604	1603	38	0
1	B	1577	1604	1603	44	0
1	C	1577	1604	1603	44	0
1	D	1577	1604	1603	44	0
1	E	1577	1604	1603	48	0
1	F	1577	1604	1603	45	0
1	G	1577	1604	1603	45	0
1	H	1577	1604	1603	46	0
1	I	1577	1604	1603	45	0
1	J	1577	1604	1603	44	0
1	K	1577	1604	1603	45	0
1	L	1577	1604	1603	46	0
1	M	1577	1604	1603	43	0
1	N	1577	1604	1603	45	0
1	O	1577	1604	1603	42	0
1	P	1577	1604	1603	43	0
1	Q	1577	1604	1603	44	0
1	R	1577	1604	1603	45	0
1	S	1577	1604	1603	47	0
1	T	1577	1604	1603	41	0
1	U	1577	1604	1603	39	0
1	V	1577	1604	1603	47	0
1	W	1577	1604	1603	48	0
1	X	1577	1604	1603	44	0
1	Y	1577	1604	1603	46	0
1	Z	1577	1604	1603	47	0
1	a	1577	1604	1603	46	0
1	b	1577	1604	1603	43	0
1	c	1577	1604	1603	44	0
1	d	1577	1604	1603	42	0
1	e	1577	1604	1603	46	0
1	f	1577	1604	1603	44	0
1	g	1577	1604	1603	46	0
1	h	1577	1604	1603	45	0
1	i	1577	1604	1603	45	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	j	1577	1604	1603	48	0
1	k	1577	1604	1603	47	0
1	l	1577	1604	1603	45	0
1	m	1577	1604	1603	43	0
1	n	1577	1604	1603	40	0
1	o	1577	1604	1603	39	0
1	p	1577	1604	1603	43	0
1	q	1577	1604	1603	47	0
1	r	1577	1604	1603	47	0
1	s	1577	1604	1603	42	0
1	t	1577	1604	1603	43	0
1	u	1577	1604	1603	45	0
1	v	1577	1604	1603	45	0
1	w	1577	1604	1603	43	0
1	x	1577	1604	1603	44	0
1	y	1577	1604	1603	47	0
1	z	1577	1604	1603	45	0
All	All	94620	96240	96180	2321	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 12.

All (2321) 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:g:107:SER:OG	1:g:111:GLN:OE1	2.10	0.70
1:D:107:SER:OG	1:D:111:GLN:OE1	2.10	0.70
1:F:107:SER:OG	1:F:111:GLN:OE1	2.10	0.70
1:O:107:SER:OG	1:O:111:GLN:OE1	2.10	0.70
1:T:107:SER:OG	1:T:111:GLN:OE1	2.10	0.70
1:W:107:SER:OG	1:W:111:GLN:OE1	2.10	0.70
1:t:107:SER:OG	1:t:111:GLN:OE1	2.10	0.70
1:y:107:SER:OG	1:y:111:GLN:OE1	2.10	0.70
1:z:107:SER:OG	1:z:111:GLN:OE1	2.10	0.70
1:N:107:SER:OG	1:N:111:GLN:OE1	2.10	0.70
1:S:107:SER:OG	1:S:111:GLN:OE1	2.10	0.70
1:f:107:SER:OG	1:f:111:GLN:OE1	2.10	0.70
1:G:26:GLU:OE2	1:H:170:ARG:NH2	2.26	0.69
1:V:107:SER:OG	1:V:111:GLN:OE1	2.10	0.69
1:X:107:SER:OG	1:X:111:GLN:OE1	2.10	0.69
1:0:107:SER:OG	1:0:111:GLN:OE1	2.10	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:200:GLU:O	1:E:204:ALA:N	2.26	0.69
1:K:170:ARG:O	1:K:173:THR:OG1	2.10	0.69
1:N:200:GLU:O	1:N:204:ALA:N	2.26	0.69
1:R:170:ARG:O	1:R:173:THR:OG1	2.10	0.69
1:i:26:GLU:OE2	1:j:170:ARG:NH2	2.26	0.69
1:j:26:GLU:OE2	1:k:170:ARG:NH2	2.26	0.69
1:n:170:ARG:O	1:n:173:THR:OG1	2.10	0.69
1:q:170:ARG:O	1:q:173:THR:OG1	2.10	0.69
1:v:26:GLU:OE2	1:w:170:ARG:NH2	2.26	0.69
1:x:170:ARG:O	1:x:173:THR:OG1	2.10	0.69
1:F:26:GLU:OE2	1:G:170:ARG:NH2	2.26	0.69
1:L:170:ARG:O	1:L:173:THR:OG1	2.10	0.69
1:P:26:GLU:OE2	1:Q:170:ARG:NH2	2.26	0.69
1:Q:26:GLU:OE2	1:R:170:ARG:NH2	2.26	0.69
1:Q:170:ARG:O	1:Q:173:THR:OG1	2.10	0.69
1:S:170:ARG:O	1:S:173:THR:OG1	2.10	0.69
1:U:170:ARG:O	1:U:173:THR:OG1	2.10	0.69
1:V:170:ARG:O	1:V:173:THR:OG1	2.10	0.69
1:g:200:GLU:O	1:g:204:ALA:N	2.26	0.69
1:h:200:GLU:O	1:h:204:ALA:N	2.25	0.69
1:p:170:ARG:O	1:p:173:THR:OG1	2.10	0.69
1:s:107:SER:OG	1:s:111:GLN:OE1	2.10	0.69
1:s:200:GLU:O	1:s:204:ALA:N	2.26	0.69
1:7:107:SER:OG	1:7:111:GLN:OE1	2.10	0.69
1:D:200:GLU:O	1:D:204:ALA:N	2.26	0.69
1:H:26:GLU:OE2	1:I:170:ARG:NH2	2.26	0.69
1:M:200:GLU:O	1:M:204:ALA:N	2.25	0.69
1:h:26:GLU:OE2	1:i:170:ARG:NH2	2.25	0.69
1:m:170:ARG:O	1:m:173:THR:OG1	2.10	0.69
1:u:26:GLU:OE2	1:v:170:ARG:NH2	2.26	0.69
1:x:107:SER:OG	1:x:111:GLN:OE1	2.10	0.69
1:C:107:SER:OG	1:C:111:GLN:OE1	2.10	0.69
1:D:170:ARG:O	1:D:173:THR:OG1	2.10	0.69
1:Y:107:SER:OG	1:Y:111:GLN:OE1	2.10	0.69
1:w:26:GLU:OE2	1:x:170:ARG:NH2	2.26	0.69
1:y:170:ARG:O	1:y:173:THR:OG1	2.10	0.69
1:C:170:ARG:O	1:C:173:THR:OG1	2.10	0.69
1:E:26:GLU:OE2	1:F:170:ARG:NH2	2.26	0.69
1:J:170:ARG:O	1:J:173:THR:OG1	2.10	0.69
1:P:170:ARG:O	1:P:173:THR:OG1	2.10	0.69
1:R:26:GLU:OE2	1:S:170:ARG:NH2	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:f:170:ARG:O	1:f:173:THR:OG1	2.10	0.69
1:f:200:GLU:O	1:f:204:ALA:N	2.26	0.69
1:g:170:ARG:O	1:g:173:THR:OG1	2.10	0.69
1:7:170:ARG:O	1:7:173:THR:OG1	2.10	0.69
1:C:200:GLU:O	1:C:204:ALA:N	2.25	0.69
1:E:170:ARG:O	1:E:173:THR:OG1	2.10	0.69
1:M:107:SER:OG	1:M:111:GLN:OE1	2.10	0.69
1:T:170:ARG:O	1:T:173:THR:OG1	2.10	0.69
1:U:26:GLU:OE2	1:V:170:ARG:NH2	2.26	0.69
1:W:170:ARG:O	1:W:173:THR:OG1	2.10	0.69
1:Y:26:GLU:OE2	1:Z:170:ARG:NH2	2.26	0.69
1:g:26:GLU:OE2	1:h:170:ARG:NH2	2.26	0.69
1:0:26:GLU:OE2	1:1:170:ARG:NH2	2.26	0.69
1:1:26:GLU:OE2	1:2:170:ARG:NH2	2.26	0.69
1:1:107:SER:OG	1:1:111:GLN:OE1	2.10	0.69
1:7:200:GLU:O	1:7:204:ALA:N	2.25	0.69
1:O:26:GLU:OE2	1:P:170:ARG:NH2	2.26	0.69
1:a:200:GLU:O	1:a:204:ALA:N	2.26	0.69
1:e:170:ARG:O	1:e:173:THR:OG1	2.10	0.69
1:h:170:ARG:O	1:h:173:THR:OG1	2.10	0.69
1:k:26:GLU:OE2	1:l:170:ARG:NH2	2.26	0.69
1:o:170:ARG:O	1:o:173:THR:OG1	2.10	0.69
1:r:200:GLU:O	1:r:204:ALA:N	2.25	0.69
1:x:26:GLU:OE2	1:y:170:ARG:NH2	2.26	0.69
1:5:26:GLU:OE2	1:6:170:ARG:NH2	2.25	0.69
1:6:26:GLU:OE2	1:7:170:ARG:NH2	2.26	0.69
1:6:170:ARG:O	1:6:173:THR:OG1	2.10	0.69
1:B:170:ARG:O	1:B:173:THR:OG1	2.10	0.69
1:D:26:GLU:OE2	1:E:170:ARG:NH2	2.25	0.69
1:F:170:ARG:O	1:F:173:THR:OG1	2.10	0.69
1:R:107:SER:OG	1:R:111:GLN:OE1	2.10	0.69
1:S:26:GLU:OE2	1:T:170:ARG:NH2	2.26	0.69
1:T:200:GLU:O	1:T:204:ALA:N	2.26	0.69
1:W:200:GLU:O	1:W:204:ALA:N	2.26	0.69
1:X:26:GLU:OE2	1:Y:170:ARG:NH2	2.26	0.69
1:Z:107:SER:OG	1:Z:111:GLN:OE1	2.10	0.69
1:d:26:GLU:OE2	1:e:170:ARG:NH2	2.26	0.69
1:e:107:SER:OG	1:e:111:GLN:OE1	2.10	0.69
1:e:200:GLU:O	1:e:204:ALA:N	2.26	0.69
1:l:170:ARG:O	1:l:173:THR:OG1	2.10	0.69
1:y:200:GLU:O	1:y:204:ALA:N	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:z:170:ARG:O	1:z:173:THR:OG1	2.10	0.69
1:2:107:SER:OG	1:2:111:GLN:OE1	2.10	0.69
1:A:26:GLU:OE2	1:B:170:ARG:NH2	2.26	0.69
1:B:26:GLU:OE2	1:C:170:ARG:NH2	2.26	0.69
1:M:170:ARG:O	1:M:173:THR:OG1	2.10	0.69
1:U:107:SER:OG	1:U:111:GLN:OE1	2.10	0.69
1:V:26:GLU:OE2	1:W:170:ARG:NH2	2.26	0.69
1:d:107:SER:OG	1:d:111:GLN:OE1	2.10	0.69
1:r:107:SER:OG	1:r:111:GLN:OE1	2.10	0.69
1:z:200:GLU:O	1:z:204:ALA:N	2.26	0.69
1:2:200:GLU:O	1:2:204:ALA:N	2.26	0.68
1:S:200:GLU:O	1:S:204:ALA:N	2.25	0.68
1:V:200:GLU:O	1:V:204:ALA:N	2.25	0.68
1:Z:26:GLU:OE2	1:a:170:ARG:NH2	2.25	0.68
1:b:107:SER:OG	1:b:111:GLN:OE1	2.10	0.68
1:d:170:ARG:O	1:d:173:THR:OG1	2.10	0.68
1:t:26:GLU:OE2	1:u:170:ARG:NH2	2.26	0.68
1:0:170:ARG:NH2	1:z:26:GLU:OE2	2.26	0.68
1:4:170:ARG:O	1:4:173:THR:OG1	2.10	0.68
1:5:170:ARG:O	1:5:173:THR:OG1	2.10	0.68
1:A:170:ARG:O	1:A:173:THR:OG1	2.10	0.68
1:B:200:GLU:O	1:B:204:ALA:N	2.26	0.68
1:I:26:GLU:OE2	1:J:170:ARG:NH2	2.26	0.68
1:L:107:SER:OG	1:L:111:GLN:OE1	2.10	0.68
1:a:107:SER:OG	1:a:111:GLN:OE1	2.10	0.68
1:c:26:GLU:OE2	1:d:170:ARG:NH2	2.26	0.68
1:c:170:ARG:O	1:c:173:THR:OG1	2.10	0.68
1:l:200:GLU:O	1:l:204:ALA:N	2.26	0.68
1:o:200:GLU:O	1:o:204:ALA:N	2.26	0.68
1:y:26:GLU:OE2	1:z:170:ARG:NH2	2.25	0.68
1:6:200:GLU:O	1:6:204:ALA:N	2.26	0.68
1:X:170:ARG:O	1:X:173:THR:OG1	2.10	0.68
1:e:26:GLU:OE2	1:f:170:ARG:NH2	2.26	0.68
1:i:170:ARG:O	1:i:173:THR:OG1	2.10	0.68
1:6:107:SER:OG	1:6:111:GLN:OE1	2.10	0.68
1:I:200:GLU:O	1:I:204:ALA:N	2.25	0.68
1:L:26:GLU:OE2	1:M:170:ARG:NH2	2.26	0.68
1:L:200:GLU:O	1:L:204:ALA:N	2.26	0.68
1:b:170:ARG:O	1:b:173:THR:OG1	2.10	0.68
1:f:26:GLU:OE2	1:g:170:ARG:NH2	2.26	0.68
1:q:26:GLU:OE2	1:r:170:ARG:NH2	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:x:200:GLU:O	1:x:204:ALA:N	2.26	0.68
1:I:170:ARG:O	1:I:173:THR:OG1	2.10	0.68
1:K:26:GLU:OE2	1:L:170:ARG:NH2	2.26	0.68
1:W:26:GLU:OE2	1:X:170:ARG:NH2	2.26	0.68
1:n:107:SER:OG	1:n:111:GLN:OE1	2.10	0.68
1:2:26:GLU:OE2	1:3:170:ARG:NH2	2.25	0.68
1:4:26:GLU:OE2	1:5:170:ARG:NH2	2.26	0.68
1:B:107:SER:OG	1:B:111:GLN:OE1	2.10	0.68
1:C:26:GLU:OE2	1:D:170:ARG:NH2	2.26	0.68
1:d:200:GLU:O	1:d:204:ALA:N	2.25	0.68
1:q:107:SER:OG	1:q:111:GLN:OE1	2.10	0.68
1:w:107:SER:OG	1:w:111:GLN:OE1	2.10	0.68
1:3:170:ARG:O	1:3:173:THR:OG1	2.10	0.68
1:G:170:ARG:O	1:G:173:THR:OG1	2.10	0.68
1:K:107:SER:OG	1:K:111:GLN:OE1	2.10	0.68
1:Z:200:GLU:O	1:Z:204:ALA:N	2.26	0.68
1:k:200:GLU:O	1:k:204:ALA:N	2.25	0.68
1:r:26:GLU:OE2	1:s:170:ARG:NH2	2.26	0.68
1:0:170:ARG:O	1:0:173:THR:OG1	2.10	0.68
1:J:107:SER:OG	1:J:111:GLN:OE1	2.10	0.68
1:U:200:GLU:O	1:U:204:ALA:N	2.25	0.68
1:l:107:SER:OG	1:l:111:GLN:OE1	2.10	0.68
1:m:26:GLU:OE2	1:n:170:ARG:NH2	2.26	0.68
1:m:107:SER:OG	1:m:111:GLN:OE1	2.10	0.68
1:p:26:GLU:OE2	1:q:170:ARG:NH2	2.26	0.68
1:I:107:SER:OG	1:I:111:GLN:OE1	2.10	0.68
1:N:26:GLU:OE2	1:O:170:ARG:NH2	2.26	0.68
1:R:200:GLU:O	1:R:204:ALA:N	2.25	0.68
1:k:107:SER:OG	1:k:111:GLN:OE1	2.10	0.68
1:l:26:GLU:OE2	1:m:170:ARG:NH2	2.26	0.68
1:o:107:SER:OG	1:o:111:GLN:OE1	2.10	0.68
1:p:107:SER:OG	1:p:111:GLN:OE1	2.10	0.68
1:A:200:GLU:O	1:A:204:ALA:N	2.26	0.68
1:M:26:GLU:OE2	1:N:170:ARG:NH2	2.26	0.68
1:a:170:ARG:O	1:a:173:THR:OG1	2.10	0.68
1:o:26:GLU:OE2	1:p:170:ARG:NH2	2.26	0.68
1:q:200:GLU:O	1:q:204:ALA:N	2.25	0.68
1:5:200:GLU:O	1:5:204:ALA:N	2.26	0.67
1:H:107:SER:OG	1:H:111:GLN:OE1	2.10	0.67
1:H:200:GLU:O	1:H:204:ALA:N	2.25	0.67
1:J:200:GLU:O	1:J:204:ALA:N	2.26	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:n:200:GLU:O	1:n:204:ALA:N	2.25	0.67
1:J:26:GLU:OE2	1:K:170:ARG:NH2	2.26	0.67
1:Q:107:SER:OG	1:Q:111:GLN:OE1	2.10	0.67
1:b:26:GLU:OE2	1:c:170:ARG:NH2	2.26	0.67
1:a:26:GLU:OE2	1:b:170:ARG:NH2	2.26	0.67
1:j:107:SER:OG	1:j:111:GLN:OE1	2.10	0.67
1:j:170:ARG:O	1:j:173:THR:OG1	2.10	0.67
1:k:170:ARG:O	1:k:173:THR:OG1	2.10	0.67
1:s:26:GLU:OE2	1:t:170:ARG:NH2	2.26	0.67
1:1:200:GLU:O	1:1:204:ALA:N	2.25	0.67
1:Y:170:ARG:O	1:Y:173:THR:OG1	2.10	0.67
1:j:200:GLU:O	1:j:204:ALA:N	2.25	0.67
1:p:200:GLU:O	1:p:204:ALA:N	2.26	0.67
1:w:200:GLU:O	1:w:204:ALA:N	2.26	0.67
1:2:170:ARG:O	1:2:173:THR:OG1	2.10	0.67
1:m:200:GLU:O	1:m:204:ALA:N	2.26	0.67
1:G:200:GLU:O	1:G:204:ALA:N	2.26	0.67
1:c:200:GLU:O	1:c:204:ALA:N	2.26	0.67
1:5:107:SER:OG	1:5:111:GLN:OE1	2.10	0.67
1:K:200:GLU:O	1:K:204:ALA:N	2.26	0.67
1:A:107:SER:OG	1:A:111:GLN:OE1	2.10	0.67
1:G:107:SER:OG	1:G:111:GLN:OE1	2.10	0.67
1:H:170:ARG:O	1:H:173:THR:OG1	2.10	0.67
1:Q:200:GLU:O	1:Q:204:ALA:N	2.25	0.67
1:1:170:ARG:O	1:1:173:THR:OG1	2.10	0.66
1:3:26:GLU:OE2	1:4:170:ARG:NH2	2.26	0.66
1:Z:170:ARG:O	1:Z:173:THR:OG1	2.10	0.66
1:r:170:ARG:O	1:r:173:THR:OG1	2.10	0.66
1:u:170:ARG:O	1:u:173:THR:OG1	2.10	0.66
1:s:170:ARG:O	1:s:173:THR:OG1	2.10	0.66
1:v:107:SER:OG	1:v:111:GLN:OE1	2.10	0.66
1:N:170:ARG:O	1:N:173:THR:OG1	2.10	0.66
1:O:170:ARG:O	1:O:173:THR:OG1	2.10	0.66
1:Y:200:GLU:O	1:Y:204:ALA:N	2.26	0.66
1:i:107:SER:OG	1:i:111:GLN:OE1	2.10	0.66
1:t:170:ARG:O	1:t:173:THR:OG1	2.10	0.66
1:v:170:ARG:O	1:v:173:THR:OG1	2.10	0.66
1:v:200:GLU:O	1:v:204:ALA:N	2.26	0.66
1:3:107:SER:OG	1:3:111:GLN:OE1	2.10	0.66
1:4:200:GLU:O	1:4:204:ALA:N	2.26	0.66
1:c:107:SER:OG	1:c:111:GLN:OE1	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:200:GLU:O	1:0:204:ALA:N	2.26	0.66
1:X:200:GLU:O	1:X:204:ALA:N	2.26	0.66
1:P:200:GLU:O	1:P:204:ALA:N	2.25	0.66
1:4:107:SER:OG	1:4:111:GLN:OE1	2.10	0.65
1:6:29:LEU:HD21	1:6:136:LYS:HG3	1.79	0.65
1:B:29:LEU:HD21	1:B:136:LYS:HG3	1.79	0.65
1:M:29:LEU:HD21	1:M:136:LYS:HG3	1.79	0.65
1:P:107:SER:OG	1:P:111:GLN:OE1	2.10	0.65
1:b:29:LEU:HD21	1:b:136:LYS:HG3	1.79	0.65
1:m:29:LEU:HD21	1:m:136:LYS:HG3	1.79	0.65
1:p:29:LEU:HD21	1:p:136:LYS:HG3	1.79	0.65
1:1:29:LEU:HD21	1:1:136:LYS:HG3	1.79	0.65
1:2:29:LEU:HD21	1:2:136:LYS:HG3	1.79	0.65
1:5:29:LEU:HD21	1:5:136:LYS:HG3	1.79	0.65
1:A:29:LEU:HD21	1:A:136:LYS:HG3	1.79	0.65
1:J:29:LEU:HD21	1:J:136:LYS:HG3	1.79	0.65
1:L:29:LEU:HD21	1:L:136:LYS:HG3	1.79	0.65
1:N:29:LEU:HD21	1:N:136:LYS:HG3	1.79	0.65
1:a:29:LEU:HD21	1:a:136:LYS:HG3	1.79	0.65
1:f:29:LEU:HD21	1:f:136:LYS:HG3	1.79	0.65
1:i:200:GLU:O	1:i:204:ALA:N	2.25	0.65
1:n:29:LEU:HD21	1:n:136:LYS:HG3	1.79	0.65
1:q:29:LEU:HD21	1:q:136:LYS:HG3	1.79	0.65
1:u:29:LEU:HD21	1:u:136:LYS:HG3	1.79	0.65
1:I:29:LEU:HD21	1:I:136:LYS:HG3	1.79	0.65
1:O:29:LEU:HD21	1:O:136:LYS:HG3	1.79	0.65
1:t:29:LEU:HD21	1:t:136:LYS:HG3	1.79	0.65
1:w:170:ARG:O	1:w:173:THR:OG1	2.10	0.65
1:4:29:LEU:HD21	1:4:136:LYS:HG3	1.79	0.65
1:7:29:LEU:HD21	1:7:136:LYS:HG3	1.79	0.65
1:C:29:LEU:HD21	1:C:136:LYS:HG3	1.79	0.65
1:Y:29:LEU:HD21	1:Y:136:LYS:HG3	1.79	0.65
1:c:29:LEU:HD21	1:c:136:LYS:HG3	1.79	0.65
1:d:29:LEU:HD21	1:d:136:LYS:HG3	1.79	0.65
1:e:29:LEU:HD21	1:e:136:LYS:HG3	1.79	0.65
1:u:200:GLU:O	1:u:204:ALA:N	2.26	0.65
1:K:29:LEU:HD21	1:K:136:LYS:HG3	1.79	0.65
1:P:29:LEU:HD21	1:P:136:LYS:HG3	1.79	0.65
1:Q:29:LEU:HD21	1:Q:136:LYS:HG3	1.79	0.65
1:X:29:LEU:HD21	1:X:136:LYS:HG3	1.79	0.65
1:Z:29:LEU:HD21	1:Z:136:LYS:HG3	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:200:GLU:O	1:b:204:ALA:N	2.26	0.65
1:o:29:LEU:HD21	1:o:136:LYS:HG3	1.79	0.65
1:s:29:LEU:HD21	1:s:136:LYS:HG3	1.79	0.65
1:D:29:LEU:HD21	1:D:136:LYS:HG3	1.79	0.65
1:k:29:LEU:HD21	1:k:136:LYS:HG3	1.79	0.65
1:l:29:LEU:HD21	1:l:136:LYS:HG3	1.79	0.65
1:r:29:LEU:HD21	1:r:136:LYS:HG3	1.79	0.65
1:v:29:LEU:HD21	1:v:136:LYS:HG3	1.79	0.65
1:0:29:LEU:HD21	1:0:136:LYS:HG3	1.79	0.65
1:E:29:LEU:HD21	1:E:136:LYS:HG3	1.79	0.65
1:z:29:LEU:HD21	1:z:136:LYS:HG3	1.79	0.65
1:3:29:LEU:HD21	1:3:136:LYS:HG3	1.79	0.65
1:G:29:LEU:HD21	1:G:136:LYS:HG3	1.79	0.65
1:S:29:LEU:HD21	1:S:136:LYS:HG3	1.79	0.65
1:g:29:LEU:HD21	1:g:136:LYS:HG3	1.79	0.65
1:h:29:LEU:HD21	1:h:136:LYS:HG3	1.79	0.65
1:j:29:LEU:HD21	1:j:136:LYS:HG3	1.79	0.65
1:w:29:LEU:HD21	1:w:136:LYS:HG3	1.79	0.65
1:V:29:LEU:HD21	1:V:136:LYS:HG3	1.79	0.65
1:F:29:LEU:HD21	1:F:136:LYS:HG3	1.79	0.64
1:O:200:GLU:O	1:O:204:ALA:N	2.26	0.64
1:x:29:LEU:HD21	1:x:136:LYS:HG3	1.79	0.64
1:y:29:LEU:HD21	1:y:136:LYS:HG3	1.79	0.64
1:F:200:GLU:O	1:F:204:ALA:N	2.26	0.64
1:U:29:LEU:HD21	1:U:136:LYS:HG3	1.79	0.64
1:h:107:SER:OG	1:h:111:GLN:OE1	2.10	0.64
1:u:107:SER:OG	1:u:111:GLN:OE1	2.10	0.64
1:H:29:LEU:HD21	1:H:136:LYS:HG3	1.79	0.64
1:R:29:LEU:HD21	1:R:136:LYS:HG3	1.79	0.64
1:i:29:LEU:HD21	1:i:136:LYS:HG3	1.79	0.64
1:T:29:LEU:HD21	1:T:136:LYS:HG3	1.79	0.64
1:W:29:LEU:HD21	1:W:136:LYS:HG3	1.79	0.64
1:t:200:GLU:O	1:t:204:ALA:N	2.26	0.64
1:3:200:GLU:O	1:3:204:ALA:N	2.25	0.64
1:N:147:ILE:O	1:N:150:GLN:NE2	2.31	0.64
1:s:147:ILE:O	1:s:150:GLN:NE2	2.32	0.64
1:M:147:ILE:O	1:M:150:GLN:NE2	2.32	0.63
1:r:147:ILE:O	1:r:150:GLN:NE2	2.32	0.63
1:t:147:ILE:O	1:t:150:GLN:NE2	2.31	0.63
1:C:147:ILE:O	1:C:150:GLN:NE2	2.31	0.63
1:L:147:ILE:O	1:L:150:GLN:NE2	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:147:ILE:O	1:O:150:GLN:NE2	2.31	0.63
1:1:84:GLU:OE2	1:1:85:GLN:NE2	2.32	0.63
1:2:147:ILE:O	1:2:150:GLN:NE2	2.31	0.63
1:D:147:ILE:O	1:D:150:GLN:NE2	2.31	0.63
1:E:107:SER:OG	1:E:111:GLN:OE1	2.10	0.63
1:I:84:GLU:OE2	1:I:85:GLN:NE2	2.32	0.63
1:X:84:GLU:OE2	1:X:85:GLN:NE2	2.32	0.63
1:e:84:GLU:OE2	1:e:85:GLN:NE2	2.32	0.63
1:f:147:ILE:O	1:f:150:GLN:NE2	2.31	0.63
1:j:84:GLU:OE2	1:j:85:GLN:NE2	2.32	0.63
1:t:84:GLU:OE2	1:t:85:GLN:NE2	2.32	0.63
1:u:147:ILE:O	1:u:150:GLN:NE2	2.31	0.63
1:3:147:ILE:O	1:3:150:GLN:NE2	2.31	0.63
1:5:84:GLU:OE2	1:5:85:GLN:NE2	2.32	0.63
1:7:147:ILE:O	1:7:150:GLN:NE2	2.32	0.63
1:A:84:GLU:OE2	1:A:85:GLN:NE2	2.32	0.63
1:C:84:GLU:OE2	1:C:85:GLN:NE2	2.32	0.63
1:a:147:ILE:O	1:a:150:GLN:NE2	2.31	0.63
1:m:84:GLU:OE2	1:m:85:GLN:NE2	2.32	0.63
1:q:147:ILE:O	1:q:150:GLN:NE2	2.31	0.63
1:v:84:GLU:OE2	1:v:85:GLN:NE2	2.32	0.63
1:7:84:GLU:OE2	1:7:85:GLN:NE2	2.32	0.63
1:B:147:ILE:O	1:B:150:GLN:NE2	2.31	0.63
1:P:84:GLU:OE2	1:P:85:GLN:NE2	2.32	0.63
1:Z:147:ILE:O	1:Z:150:GLN:NE2	2.31	0.63
1:e:147:ILE:O	1:e:150:GLN:NE2	2.31	0.63
1:g:84:GLU:OE2	1:g:85:GLN:NE2	2.32	0.63
1:n:147:ILE:O	1:n:150:GLN:NE2	2.32	0.63
1:p:84:GLU:OE2	1:p:85:GLN:NE2	2.32	0.63
1:O:84:GLU:OE2	1:O:85:GLN:NE2	2.32	0.63
1:g:147:ILE:O	1:g:150:GLN:NE2	2.31	0.63
1:y:84:GLU:OE2	1:y:85:GLN:NE2	2.32	0.63
1:1:147:ILE:O	1:1:150:GLN:NE2	2.31	0.63
1:6:147:ILE:O	1:6:150:GLN:NE2	2.32	0.63
1:M:84:GLU:OE2	1:M:85:GLN:NE2	2.32	0.63
1:P:147:ILE:O	1:P:150:GLN:NE2	2.31	0.63
1:Q:84:GLU:OE1	1:Q:84:GLU:N	2.32	0.63
1:a:84:GLU:OE2	1:a:85:GLN:NE2	2.32	0.63
1:b:147:ILE:O	1:b:150:GLN:NE2	2.31	0.63
1:c:84:GLU:OE2	1:c:85:GLN:NE2	2.32	0.63
1:i:84:GLU:N	1:i:84:GLU:OE1	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:v:84:GLU:N	1:v:84:GLU:OE1	2.32	0.63
1:2:84:GLU:OE2	1:2:85:GLN:NE2	2.32	0.63
1:J:84:GLU:OE2	1:J:85:GLN:NE2	2.32	0.63
1:N:84:GLU:OE2	1:N:85:GLN:NE2	2.32	0.63
1:R:84:GLU:OE2	1:R:85:GLN:NE2	2.32	0.63
1:w:84:GLU:OE1	1:w:84:GLU:N	2.32	0.63
1:D:84:GLU:OE2	1:D:85:GLN:NE2	2.32	0.62
1:G:84:GLU:OE1	1:G:84:GLU:N	2.32	0.62
1:H:84:GLU:OE2	1:H:85:GLN:NE2	2.32	0.62
1:K:147:ILE:O	1:K:150:GLN:NE2	2.31	0.62
1:U:84:GLU:OE2	1:U:85:GLN:NE2	2.32	0.62
1:W:84:GLU:OE2	1:W:85:GLN:NE2	2.32	0.62
1:Y:84:GLU:OE2	1:Y:85:GLN:NE2	2.32	0.62
1:d:147:ILE:O	1:d:150:GLN:NE2	2.31	0.62
1:r:84:GLU:OE2	1:r:85:GLN:NE2	2.32	0.62
1:0:84:GLU:OE2	1:0:85:GLN:NE2	2.32	0.62
1:4:147:ILE:O	1:4:150:GLN:NE2	2.32	0.62
1:F:84:GLU:OE2	1:F:85:GLN:NE2	2.32	0.62
1:T:84:GLU:OE2	1:T:85:GLN:NE2	2.32	0.62
1:a:84:GLU:N	1:a:84:GLU:OE1	2.32	0.62
1:d:84:GLU:OE2	1:d:85:GLN:NE2	2.32	0.62
1:k:84:GLU:OE2	1:k:85:GLN:NE2	2.32	0.62
1:6:84:GLU:OE2	1:6:85:GLN:NE2	2.32	0.62
1:A:147:ILE:O	1:A:150:GLN:NE2	2.31	0.62
1:E:84:GLU:OE2	1:E:85:GLN:NE2	2.32	0.62
1:E:147:ILE:O	1:E:150:GLN:NE2	2.32	0.62
1:R:84:GLU:OE1	1:R:84:GLU:N	2.32	0.62
1:U:84:GLU:OE1	1:U:84:GLU:N	2.32	0.62
1:Y:147:ILE:O	1:Y:150:GLN:NE2	2.31	0.62
1:b:84:GLU:OE2	1:b:85:GLN:NE2	2.32	0.62
1:f:84:GLU:OE2	1:f:85:GLN:NE2	2.32	0.62
1:u:84:GLU:OE2	1:u:85:GLN:NE2	2.32	0.62
1:2:84:GLU:OE1	1:2:84:GLU:N	2.32	0.62
1:3:84:GLU:N	1:3:84:GLU:OE1	2.32	0.62
1:3:84:GLU:OE2	1:3:85:GLN:NE2	2.32	0.62
1:5:147:ILE:O	1:5:150:GLN:NE2	2.31	0.62
1:J:84:GLU:OE1	1:J:84:GLU:N	2.32	0.62
1:L:84:GLU:OE2	1:L:85:GLN:NE2	2.32	0.62
1:U:147:ILE:O	1:U:150:GLN:NE2	2.31	0.62
1:V:147:ILE:O	1:V:150:GLN:NE2	2.31	0.62
1:c:147:ILE:O	1:c:150:GLN:NE2	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:i:84:GLU:OE2	1:i:85:GLN:NE2	2.32	0.62
1:j:84:GLU:OE1	1:j:84:GLU:N	2.32	0.62
1:l:84:GLU:OE2	1:l:85:GLN:NE2	2.32	0.62
1:n:84:GLU:OE2	1:n:85:GLN:NE2	2.32	0.62
1:o:84:GLU:OE2	1:o:85:GLN:NE2	2.32	0.62
1:r:84:GLU:OE1	1:r:84:GLU:N	2.32	0.62
1:x:147:ILE:O	1:x:150:GLN:NE2	2.31	0.62
1:z:84:GLU:OE2	1:z:85:GLN:NE2	2.32	0.62
1:B:84:GLU:OE2	1:B:85:GLN:NE2	2.32	0.62
1:L:84:GLU:OE1	1:L:84:GLU:N	2.32	0.62
1:Q:84:GLU:OE2	1:Q:85:GLN:NE2	2.32	0.62
1:R:147:ILE:O	1:R:150:GLN:NE2	2.31	0.62
1:S:147:ILE:O	1:S:150:GLN:NE2	2.31	0.62
1:k:147:ILE:O	1:k:150:GLN:NE2	2.31	0.62
1:p:84:GLU:OE1	1:p:84:GLU:N	2.32	0.62
1:q:84:GLU:OE2	1:q:85:GLN:NE2	2.32	0.62
1:H:147:ILE:O	1:H:150:GLN:NE2	2.32	0.62
1:I:147:ILE:O	1:I:150:GLN:NE2	2.31	0.62
1:M:84:GLU:OE1	1:M:84:GLU:N	2.32	0.62
1:Z:84:GLU:OE2	1:Z:85:GLN:NE2	2.32	0.62
1:m:84:GLU:OE1	1:m:84:GLU:N	2.32	0.62
1:p:147:ILE:O	1:p:150:GLN:NE2	2.31	0.62
1:s:84:GLU:OE2	1:s:85:GLN:NE2	2.32	0.62
1:v:147:ILE:O	1:v:150:GLN:NE2	2.31	0.62
1:w:84:GLU:OE2	1:w:85:GLN:NE2	2.32	0.62
1:x:84:GLU:OE2	1:x:85:GLN:NE2	2.32	0.62
1:G:147:ILE:O	1:G:150:GLN:NE2	2.31	0.62
1:l:84:GLU:OE1	1:l:84:GLU:N	2.32	0.62
1:l:147:ILE:O	1:l:150:GLN:NE2	2.31	0.62
1:m:147:ILE:O	1:m:150:GLN:NE2	2.31	0.62
1:o:84:GLU:OE1	1:o:84:GLU:N	2.32	0.62
1:o:147:ILE:O	1:o:150:GLN:NE2	2.31	0.62
1:w:147:ILE:O	1:w:150:GLN:NE2	2.31	0.62
1:x:84:GLU:OE1	1:x:84:GLU:N	2.32	0.62
1:y:147:ILE:O	1:y:150:GLN:NE2	2.31	0.62
1:z:147:ILE:O	1:z:150:GLN:NE2	2.31	0.62
1:G:84:GLU:OE2	1:G:85:GLN:NE2	2.32	0.62
1:K:84:GLU:OE2	1:K:85:GLN:NE2	2.32	0.62
1:T:147:ILE:O	1:T:150:GLN:NE2	2.32	0.62
1:W:147:ILE:O	1:W:150:GLN:NE2	2.32	0.62
1:X:147:ILE:O	1:X:150:GLN:NE2	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:h:147:ILE:O	1:h:150:GLN:NE2	2.31	0.62
1:i:147:ILE:O	1:i:150:GLN:NE2	2.31	0.62
1:j:147:ILE:O	1:j:150:GLN:NE2	2.31	0.62
1:4:84:GLU:OE2	1:4:85:GLN:NE2	2.32	0.62
1:5:84:GLU:OE1	1:5:84:GLU:N	2.32	0.62
1:H:84:GLU:OE1	1:H:84:GLU:N	2.32	0.62
1:0:84:GLU:N	1:0:84:GLU:OE1	2.32	0.62
1:0:147:ILE:O	1:0:150:GLN:NE2	2.31	0.62
1:A:84:GLU:OE1	1:A:84:GLU:N	2.32	0.62
1:B:84:GLU:OE1	1:B:84:GLU:N	2.32	0.62
1:F:147:ILE:O	1:F:150:GLN:NE2	2.32	0.62
1:S:84:GLU:OE2	1:S:85:GLN:NE2	2.32	0.62
1:b:84:GLU:OE1	1:b:84:GLU:N	2.32	0.62
1:c:84:GLU:OE1	1:c:84:GLU:N	2.32	0.62
1:3:100:HIS:CE1	1:3:104:LEU:HD11	2.35	0.61
1:6:84:GLU:N	1:6:84:GLU:OE1	2.32	0.61
1:C:84:GLU:N	1:C:84:GLU:OE1	2.32	0.61
1:J:147:ILE:O	1:J:150:GLN:NE2	2.31	0.61
1:M:100:HIS:CE1	1:M:104:LEU:HD11	2.35	0.61
1:V:84:GLU:OE2	1:V:85:GLN:NE2	2.32	0.61
1:Y:84:GLU:N	1:Y:84:GLU:OE1	2.32	0.61
1:e:84:GLU:OE1	1:e:84:GLU:N	2.32	0.61
1:h:100:HIS:CE1	1:h:104:LEU:HD11	2.35	0.61
1:n:84:GLU:N	1:n:84:GLU:OE1	2.32	0.61
1:y:100:HIS:CE1	1:y:104:LEU:HD11	2.35	0.61
1:7:84:GLU:OE1	1:7:84:GLU:N	2.32	0.61
1:G:100:HIS:CE1	1:G:104:LEU:HD11	2.35	0.61
1:K:84:GLU:N	1:K:84:GLU:OE1	2.32	0.61
1:V:84:GLU:N	1:V:84:GLU:OE1	2.32	0.61
1:Z:84:GLU:OE1	1:Z:84:GLU:N	2.32	0.61
1:c:100:HIS:CE1	1:c:104:LEU:HD11	2.35	0.61
1:h:84:GLU:OE2	1:h:85:GLN:NE2	2.32	0.61
1:q:84:GLU:N	1:q:84:GLU:OE1	2.32	0.61
1:L:100:HIS:CE1	1:L:104:LEU:HD11	2.35	0.61
1:S:84:GLU:N	1:S:84:GLU:OE1	2.32	0.61
1:d:84:GLU:OE1	1:d:84:GLU:N	2.32	0.61
1:x:100:HIS:CE1	1:x:104:LEU:HD11	2.36	0.61
1:D:100:HIS:CE1	1:D:104:LEU:HD11	2.35	0.61
1:Q:100:HIS:CE1	1:Q:104:LEU:HD11	2.35	0.61
1:Q:147:ILE:O	1:Q:150:GLN:NE2	2.31	0.61
1:d:100:HIS:CE1	1:d:104:LEU:HD11	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:f:84:GLU:N	1:f:84:GLU:OE1	2.32	0.61
1:k:84:GLU:OE1	1:k:84:GLU:N	2.32	0.61
1:s:84:GLU:OE1	1:s:84:GLU:N	2.32	0.61
1:t:100:HIS:CE1	1:t:104:LEU:HD11	2.35	0.61
1:4:84:GLU:OE1	1:4:84:GLU:N	2.32	0.61
1:4:100:HIS:CE1	1:4:104:LEU:HD11	2.35	0.61
1:H:100:HIS:CE1	1:H:104:LEU:HD11	2.35	0.61
1:I:84:GLU:OE1	1:I:84:GLU:N	2.32	0.61
1:O:100:HIS:CE1	1:O:104:LEU:HD11	2.35	0.61
1:f:100:HIS:CE1	1:f:104:LEU:HD11	2.35	0.61
1:g:100:HIS:CE1	1:g:104:LEU:HD11	2.35	0.61
1:m:100:HIS:CE1	1:m:104:LEU:HD11	2.35	0.61
1:7:100:HIS:CE1	1:7:104:LEU:HD11	2.35	0.61
1:C:100:HIS:CE1	1:C:104:LEU:HD11	2.35	0.61
1:N:100:HIS:CE1	1:N:104:LEU:HD11	2.35	0.61
1:U:100:HIS:CE1	1:U:104:LEU:HD11	2.35	0.61
1:X:84:GLU:OE1	1:X:84:GLU:N	2.32	0.61
1:n:100:HIS:CE1	1:n:104:LEU:HD11	2.35	0.61
1:p:100:HIS:CE1	1:p:104:LEU:HD11	2.35	0.61
1:u:100:HIS:CE1	1:u:104:LEU:HD11	2.35	0.61
1:l:84:GLU:OE1	1:l:84:GLU:N	2.32	0.61
1:l:100:HIS:CE1	1:l:104:LEU:HD11	2.35	0.61
1:2:100:HIS:CE1	1:2:104:LEU:HD11	2.35	0.61
1:R:100:HIS:CE1	1:R:104:LEU:HD11	2.35	0.61
1:X:100:HIS:CE1	1:X:104:LEU:HD11	2.35	0.61
1:Z:100:HIS:CE1	1:Z:104:LEU:HD11	2.35	0.61
1:i:100:HIS:CE1	1:i:104:LEU:HD11	2.35	0.61
1:q:100:HIS:CE1	1:q:104:LEU:HD11	2.35	0.61
1:t:84:GLU:N	1:t:84:GLU:OE1	2.32	0.61
1:E:100:HIS:CE1	1:E:104:LEU:HD11	2.35	0.61
1:O:84:GLU:OE1	1:O:84:GLU:N	2.32	0.61
1:Y:100:HIS:CE1	1:Y:104:LEU:HD11	2.35	0.61
1:k:100:HIS:CE1	1:k:104:LEU:HD11	2.35	0.61
1:D:84:GLU:OE1	1:D:84:GLU:N	2.32	0.61
1:F:100:HIS:CE1	1:F:104:LEU:HD11	2.35	0.61
1:I:100:HIS:CE1	1:I:104:LEU:HD11	2.35	0.61
1:P:100:HIS:CE1	1:P:104:LEU:HD11	2.35	0.61
1:T:100:HIS:CE1	1:T:104:LEU:HD11	2.35	0.61
1:e:100:HIS:CE1	1:e:104:LEU:HD11	2.35	0.61
1:l:100:HIS:CE1	1:l:104:LEU:HD11	2.35	0.61
1:o:100:HIS:CE1	1:o:104:LEU:HD11	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:y:84:GLU:N	1:y:84:GLU:OE1	2.32	0.61
1:z:100:HIS:CE1	1:z:104:LEU:HD11	2.35	0.61
1:6:100:HIS:CE1	1:6:104:LEU:HD11	2.35	0.61
1:S:100:HIS:CE1	1:S:104:LEU:HD11	2.35	0.61
1:W:100:HIS:CE1	1:W:104:LEU:HD11	2.35	0.61
1:b:100:HIS:CE1	1:b:104:LEU:HD11	2.35	0.61
1:s:100:HIS:CE1	1:s:104:LEU:HD11	2.35	0.61
1:B:100:HIS:CE1	1:B:104:LEU:HD11	2.35	0.60
1:N:84:GLU:N	1:N:84:GLU:OE1	2.32	0.60
1:K:100:HIS:CE1	1:K:104:LEU:HD11	2.35	0.60
1:V:100:HIS:CE1	1:V:104:LEU:HD11	2.35	0.60
1:j:100:HIS:CE1	1:j:104:LEU:HD11	2.35	0.60
1:u:193:ASP:OD1	1:u:194:LYS:N	2.34	0.60
1:w:100:HIS:CE1	1:w:104:LEU:HD11	2.35	0.60
1:0:100:HIS:CE1	1:0:104:LEU:HD11	2.35	0.60
1:f:193:ASP:OD1	1:f:194:LYS:N	2.35	0.60
1:t:193:ASP:OD1	1:t:194:LYS:N	2.35	0.60
1:5:100:HIS:CE1	1:5:104:LEU:HD11	2.35	0.60
1:5:193:ASP:OD1	1:5:194:LYS:N	2.35	0.60
1:A:100:HIS:CE1	1:A:104:LEU:HD11	2.35	0.60
1:A:193:ASP:OD1	1:A:194:LYS:N	2.35	0.60
1:r:100:HIS:CE1	1:r:104:LEU:HD11	2.35	0.60
1:u:84:GLU:OE1	1:u:84:GLU:N	2.32	0.60
1:I:193:ASP:OD1	1:I:194:LYS:N	2.35	0.60
1:a:100:HIS:CE1	1:a:104:LEU:HD11	2.35	0.60
1:e:193:ASP:OD1	1:e:194:LYS:N	2.35	0.60
1:g:84:GLU:OE1	1:g:84:GLU:N	2.32	0.60
1:v:100:HIS:CE1	1:v:104:LEU:HD11	2.35	0.60
1:z:84:GLU:OE1	1:z:84:GLU:N	2.32	0.60
1:1:193:ASP:OD1	1:1:194:LYS:N	2.34	0.60
1:6:193:ASP:OD1	1:6:194:LYS:N	2.35	0.60
1:T:84:GLU:OE1	1:T:84:GLU:N	2.32	0.60
1:W:84:GLU:OE1	1:W:84:GLU:N	2.32	0.60
1:X:193:ASP:OD1	1:X:194:LYS:N	2.35	0.60
1:g:193:ASP:OD1	1:g:194:LYS:N	2.35	0.60
1:B:193:ASP:OD1	1:B:194:LYS:N	2.35	0.60
1:j:193:ASP:OD1	1:j:194:LYS:N	2.35	0.60
1:s:193:ASP:OD1	1:s:194:LYS:N	2.35	0.60
1:O:193:ASP:OD1	1:O:194:LYS:N	2.35	0.60
1:Q:193:ASP:OD1	1:Q:194:LYS:N	2.35	0.60
1:d:193:ASP:OD1	1:d:194:LYS:N	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:m:193:ASP:OD1	1:m:194:LYS:N	2.35	0.60
1:p:193:ASP:OD1	1:p:194:LYS:N	2.35	0.60
1:v:193:ASP:OD1	1:v:194:LYS:N	2.35	0.60
1:0:193:ASP:OD1	1:0:194:LYS:N	2.34	0.60
1:4:193:ASP:OD1	1:4:194:LYS:N	2.35	0.60
1:7:193:ASP:OD1	1:7:194:LYS:N	2.34	0.60
1:M:193:ASP:OD1	1:M:194:LYS:N	2.35	0.60
1:N:193:ASP:OD1	1:N:194:LYS:N	2.35	0.60
1:U:193:ASP:OD1	1:U:194:LYS:N	2.35	0.60
1:H:193:ASP:OD1	1:H:194:LYS:N	2.35	0.60
1:J:100:HIS:CE1	1:J:104:LEU:HD11	2.35	0.60
1:R:193:ASP:OD1	1:R:194:LYS:N	2.35	0.60
1:Y:193:ASP:OD1	1:Y:194:LYS:N	2.35	0.60
1:k:193:ASP:OD1	1:k:194:LYS:N	2.35	0.60
1:C:193:ASP:OD1	1:C:194:LYS:N	2.35	0.59
1:L:193:ASP:OD1	1:L:194:LYS:N	2.35	0.59
1:P:193:ASP:OD1	1:P:194:LYS:N	2.35	0.59
1:a:193:ASP:OD1	1:a:194:LYS:N	2.34	0.59
1:y:193:ASP:OD1	1:y:194:LYS:N	2.35	0.59
1:z:193:ASP:OD1	1:z:194:LYS:N	2.35	0.59
1:E:84:GLU:OE1	1:E:84:GLU:N	2.32	0.59
1:G:193:ASP:OD1	1:G:194:LYS:N	2.35	0.59
1:J:193:ASP:OD1	1:J:194:LYS:N	2.35	0.59
1:c:193:ASP:OD1	1:c:194:LYS:N	2.35	0.59
1:h:84:GLU:OE1	1:h:84:GLU:N	2.32	0.59
1:o:193:ASP:OD1	1:o:194:LYS:N	2.35	0.59
1:E:193:ASP:OD1	1:E:194:LYS:N	2.35	0.59
1:F:193:ASP:OD1	1:F:194:LYS:N	2.35	0.59
1:S:193:ASP:OD1	1:S:194:LYS:N	2.35	0.59
1:T:193:ASP:OD1	1:T:194:LYS:N	2.35	0.59
1:l:193:ASP:OD1	1:l:194:LYS:N	2.34	0.59
1:2:193:ASP:OD1	1:2:194:LYS:N	2.35	0.59
1:D:193:ASP:OD1	1:D:194:LYS:N	2.35	0.59
1:W:193:ASP:OD1	1:W:194:LYS:N	2.35	0.59
1:Z:193:ASP:OD1	1:Z:194:LYS:N	2.35	0.59
1:h:193:ASP:OD1	1:h:194:LYS:N	2.35	0.59
1:F:84:GLU:N	1:F:84:GLU:OE1	2.32	0.59
1:P:84:GLU:OE1	1:P:84:GLU:N	2.32	0.59
1:V:193:ASP:OD1	1:V:194:LYS:N	2.35	0.59
1:b:193:ASP:OD1	1:b:194:LYS:N	2.35	0.59
1:E:199:TRP:O	1:E:203:GLN:N	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:193:ASP:OD1	1:K:194:LYS:N	2.35	0.59
1:e:199:TRP:O	1:e:203:GLN:N	2.34	0.59
1:r:193:ASP:OD1	1:r:194:LYS:N	2.34	0.59
1:w:193:ASP:OD1	1:w:194:LYS:N	2.35	0.59
1:3:193:ASP:OD1	1:3:194:LYS:N	2.35	0.59
1:x:193:ASP:OD1	1:x:194:LYS:N	2.35	0.59
1:n:193:ASP:OD1	1:n:194:LYS:N	2.35	0.59
1:q:193:ASP:OD1	1:q:194:LYS:N	2.35	0.59
1:t:199:TRP:O	1:t:203:GLN:N	2.34	0.59
1:v:199:TRP:O	1:v:203:GLN:N	2.34	0.59
1:5:199:TRP:O	1:5:203:GLN:N	2.34	0.59
1:A:199:TRP:O	1:A:203:GLN:N	2.34	0.59
1:M:199:TRP:O	1:M:203:GLN:N	2.34	0.59
1:n:199:TRP:O	1:n:203:GLN:N	2.34	0.59
1:q:199:TRP:O	1:q:203:GLN:N	2.34	0.59
1:S:199:TRP:O	1:S:203:GLN:N	2.34	0.58
1:V:199:TRP:O	1:V:203:GLN:N	2.34	0.58
1:b:199:TRP:O	1:b:203:GLN:N	2.34	0.58
1:i:193:ASP:OD1	1:i:194:LYS:N	2.35	0.58
1:7:199:TRP:O	1:7:203:GLN:N	2.34	0.58
1:C:199:TRP:O	1:C:203:GLN:N	2.34	0.58
1:Q:199:TRP:O	1:Q:203:GLN:N	2.34	0.58
1:h:199:TRP:O	1:h:203:GLN:N	2.34	0.58
1:O:199:TRP:O	1:O:203:GLN:N	2.34	0.57
1:f:199:TRP:O	1:f:203:GLN:N	2.34	0.57
1:Z:206:GLU:O	1:Z:210:ALA:N	2.37	0.57
1:d:199:TRP:O	1:d:203:GLN:N	2.34	0.57
1:l:206:GLU:O	1:l:210:ALA:N	2.37	0.57
1:o:206:GLU:O	1:o:210:ALA:N	2.37	0.57
1:0:206:GLU:O	1:0:210:ALA:N	2.37	0.57
1:P:206:GLU:O	1:P:210:ALA:N	2.37	0.57
1:K:206:GLU:O	1:K:210:ALA:N	2.37	0.57
1:w:199:TRP:O	1:w:203:GLN:N	2.34	0.57
1:O:206:GLU:O	1:O:210:ALA:N	2.37	0.57
1:H:206:GLU:O	1:H:210:ALA:N	2.37	0.56
1:3:206:GLU:O	1:3:210:ALA:N	2.37	0.56
1:P:47:LEU:HD22	1:P:122:LEU:HD22	1.88	0.56
1:X:199:TRP:O	1:X:203:GLN:N	2.34	0.56
1:j:199:TRP:O	1:j:203:GLN:N	2.34	0.56
1:s:199:TRP:O	1:s:203:GLN:N	2.34	0.56
1:1:36:MET:HE2	1:2:155:ILE:HG21	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:7:47:LEU:HD22	1:7:122:LEU:HD22	1.88	0.56
1:C:47:LEU:HD22	1:C:122:LEU:HD22	1.88	0.56
1:E:47:LEU:HD22	1:E:122:LEU:HD22	1.88	0.56
1:I:199:TRP:O	1:I:203:GLN:N	2.34	0.56
1:J:36:MET:HE2	1:K:155:ILE:HG21	1.88	0.56
1:K:36:MET:HE2	1:L:155:ILE:HG21	1.88	0.56
1:N:206:GLU:O	1:N:210:ALA:N	2.37	0.56
1:U:47:LEU:HD22	1:U:122:LEU:HD22	1.88	0.56
1:a:36:MET:HE2	1:b:155:ILE:HG21	1.88	0.56
1:b:36:MET:HE2	1:c:155:ILE:HG21	1.88	0.56
1:g:47:LEU:HD22	1:g:122:LEU:HD22	1.88	0.56
1:i:47:LEU:HD22	1:i:122:LEU:HD22	1.88	0.56
1:w:47:LEU:HD22	1:w:122:LEU:HD22	1.88	0.56
1:y:199:TRP:O	1:y:203:GLN:N	2.34	0.56
1:0:36:MET:HE2	1:1:155:ILE:HG21	1.88	0.56
1:4:199:TRP:O	1:4:203:GLN:N	2.34	0.56
1:L:36:MET:HE2	1:M:155:ILE:HG21	1.88	0.56
1:R:47:LEU:HD22	1:R:122:LEU:HD22	1.88	0.56
1:c:36:MET:HE2	1:d:155:ILE:HG21	1.88	0.56
1:f:47:LEU:HD22	1:f:122:LEU:HD22	1.88	0.56
1:s:36:MET:HE2	1:t:155:ILE:HG21	1.88	0.56
1:v:47:LEU:HD22	1:v:122:LEU:HD22	1.88	0.56
1:1:199:TRP:O	1:1:203:GLN:N	2.34	0.56
1:B:47:LEU:HD22	1:B:122:LEU:HD22	1.88	0.56
1:F:47:LEU:HD22	1:F:122:LEU:HD22	1.88	0.56
1:N:47:LEU:HD22	1:N:122:LEU:HD22	1.88	0.56
1:S:47:LEU:HD22	1:S:122:LEU:HD22	1.88	0.56
1:T:206:GLU:O	1:T:210:ALA:N	2.37	0.56
1:V:47:LEU:HD22	1:V:122:LEU:HD22	1.88	0.56
1:W:206:GLU:O	1:W:210:ALA:N	2.37	0.56
1:d:47:LEU:HD22	1:d:122:LEU:HD22	1.88	0.56
1:h:47:LEU:HD22	1:h:122:LEU:HD22	1.88	0.56
1:r:206:GLU:O	1:r:210:ALA:N	2.37	0.56
1:u:47:LEU:HD22	1:u:122:LEU:HD22	1.88	0.56
1:2:36:MET:HE2	1:3:155:ILE:HG21	1.88	0.56
1:6:47:LEU:HD22	1:6:122:LEU:HD22	1.88	0.56
1:G:47:LEU:HD22	1:G:122:LEU:HD22	1.88	0.56
1:L:199:TRP:O	1:L:203:GLN:N	2.34	0.56
1:Q:47:LEU:HD22	1:Q:122:LEU:HD22	1.88	0.56
1:W:47:LEU:HD22	1:W:122:LEU:HD22	1.88	0.56
1:e:47:LEU:HD22	1:e:122:LEU:HD22	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:m:199:TRP:O	1:m:203:GLN:N	2.34	0.56
1:r:36:MET:HE2	1:s:155:ILE:HG21	1.88	0.56
1:t:47:LEU:HD22	1:t:122:LEU:HD22	1.88	0.56
1:u:199:TRP:O	1:u:203:GLN:N	2.34	0.56
1:y:47:LEU:HD22	1:y:122:LEU:HD22	1.88	0.56
1:5:47:LEU:HD22	1:5:122:LEU:HD22	1.88	0.56
1:I:36:MET:HE2	1:J:155:ILE:HG21	1.88	0.56
1:a:199:TRP:O	1:a:203:GLN:N	2.34	0.56
1:k:36:MET:HE2	1:l:155:ILE:HG21	1.88	0.56
1:p:199:TRP:O	1:p:203:GLN:N	2.34	0.56
1:t:36:MET:HE2	1:u:155:ILE:HG21	1.88	0.56
1:x:47:LEU:HD22	1:x:122:LEU:HD22	1.88	0.56
1:0:155:ILE:HG21	1:z:36:MET:HE2	1.88	0.56
1:A:47:LEU:HD22	1:A:122:LEU:HD22	1.88	0.56
1:D:47:LEU:HD22	1:D:122:LEU:HD22	1.88	0.56
1:T:47:LEU:HD22	1:T:122:LEU:HD22	1.88	0.56
1:j:36:MET:HE2	1:k:155:ILE:HG21	1.88	0.56
1:F:199:TRP:O	1:F:203:GLN:N	2.34	0.56
1:J:206:GLU:O	1:J:210:ALA:N	2.37	0.56
1:O:47:LEU:HD22	1:O:122:LEU:HD22	1.88	0.56
1:Y:206:GLU:O	1:Y:210:ALA:N	2.37	0.56
1:Z:36:MET:HE2	1:a:155:ILE:HG21	1.88	0.56
1:c:206:GLU:O	1:c:210:ALA:N	2.37	0.56
1:d:36:MET:HE2	1:e:155:ILE:HG21	1.88	0.56
1:k:206:GLU:O	1:k:210:ALA:N	2.37	0.56
1:s:47:LEU:HD22	1:s:122:LEU:HD22	1.88	0.56
1:M:36:MET:HE2	1:N:155:ILE:HG21	1.88	0.56
1:l:36:MET:HE2	1:m:155:ILE:HG21	1.88	0.56
1:o:36:MET:HE2	1:p:155:ILE:HG21	1.88	0.56
1:z:47:LEU:HD22	1:z:122:LEU:HD22	1.88	0.56
1:2:206:GLU:O	1:2:210:ALA:N	2.37	0.55
1:A:36:MET:HE2	1:B:155:ILE:HG21	1.88	0.55
1:D:199:TRP:O	1:D:203:GLN:N	2.34	0.55
1:H:47:LEU:HD22	1:H:122:LEU:HD22	1.88	0.55
1:X:47:LEU:HD22	1:X:122:LEU:HD22	1.88	0.55
1:j:47:LEU:HD22	1:j:122:LEU:HD22	1.88	0.55
1:k:47:LEU:HD22	1:k:122:LEU:HD22	1.88	0.55
1:q:36:MET:HE2	1:r:155:ILE:HG21	1.88	0.55
1:0:47:LEU:HD22	1:0:122:LEU:HD22	1.88	0.55
1:4:47:LEU:HD22	1:4:122:LEU:HD22	1.88	0.55
1:5:36:MET:HE2	1:6:155:ILE:HG21	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:206:GLU:O	1:E:210:ALA:N	2.37	0.55
1:M:47:LEU:HD22	1:M:122:LEU:HD22	1.88	0.55
1:i:206:GLU:O	1:i:210:ALA:N	2.37	0.55
1:r:47:LEU:HD22	1:r:122:LEU:HD22	1.88	0.55
1:u:36:MET:HE2	1:v:155:ILE:HG21	1.88	0.55
1:y:36:MET:HE2	1:z:155:ILE:HG21	1.88	0.55
1:z:206:GLU:O	1:z:210:ALA:N	2.37	0.55
1:3:36:MET:HE2	1:4:155:ILE:HG21	1.88	0.55
1:6:36:MET:HE2	1:7:155:ILE:HG21	1.88	0.55
1:B:36:MET:HE2	1:C:155:ILE:HG21	1.88	0.55
1:D:206:GLU:O	1:D:210:ALA:N	2.37	0.55
1:F:206:GLU:O	1:F:210:ALA:N	2.37	0.55
1:H:36:MET:HE2	1:I:155:ILE:HG21	1.88	0.55
1:I:47:LEU:HD22	1:I:122:LEU:HD22	1.88	0.55
1:b:47:LEU:HD22	1:b:122:LEU:HD22	1.88	0.55
1:i:36:MET:HE2	1:j:155:ILE:HG21	1.88	0.55
1:L:47:LEU:HD22	1:L:122:LEU:HD22	1.88	0.55
1:c:47:LEU:HD22	1:c:122:LEU:HD22	1.88	0.55
1:n:206:GLU:O	1:n:210:ALA:N	2.37	0.55
1:3:47:LEU:HD22	1:3:122:LEU:HD22	1.88	0.55
1:7:206:GLU:O	1:7:210:ALA:N	2.37	0.55
1:C:206:GLU:O	1:C:210:ALA:N	2.37	0.55
1:e:36:MET:HE2	1:f:155:ILE:HG21	1.88	0.55
1:q:206:GLU:O	1:q:210:ALA:N	2.37	0.55
1:2:47:LEU:HD22	1:2:122:LEU:HD22	1.88	0.55
1:4:36:MET:HE2	1:5:155:ILE:HG21	1.88	0.55
1:6:199:TRP:O	1:6:203:GLN:N	2.34	0.55
1:J:47:LEU:HD22	1:J:122:LEU:HD22	1.88	0.55
1:Y:47:LEU:HD22	1:Y:122:LEU:HD22	1.88	0.55
1:Z:47:LEU:HD22	1:Z:122:LEU:HD22	1.88	0.55
1:p:47:LEU:HD22	1:p:122:LEU:HD22	1.88	0.55
1:1:47:LEU:HD22	1:1:122:LEU:HD22	1.88	0.55
1:B:199:TRP:O	1:B:203:GLN:N	2.34	0.55
1:C:36:MET:HE2	1:D:155:ILE:HG21	1.88	0.55
1:K:47:LEU:HD22	1:K:122:LEU:HD22	1.88	0.55
1:X:36:MET:HE2	1:Y:155:ILE:HG21	1.88	0.55
1:Y:36:MET:HE2	1:Z:155:ILE:HG21	1.88	0.55
1:b:206:GLU:O	1:b:210:ALA:N	2.37	0.55
1:m:47:LEU:HD22	1:m:122:LEU:HD22	1.88	0.55
1:n:47:LEU:HD22	1:n:122:LEU:HD22	1.88	0.55
1:x:36:MET:HE2	1:y:155:ILE:HG21	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:199:TRP:O	1:R:203:GLN:N	2.34	0.55
1:W:36:MET:HE2	1:X:155:ILE:HG21	1.88	0.55
1:h:36:MET:HE2	1:i:155:ILE:HG21	1.88	0.55
1:m:36:MET:HE2	1:n:155:ILE:HG21	1.88	0.55
1:o:47:LEU:HD22	1:o:122:LEU:HD22	1.88	0.55
1:p:36:MET:HE2	1:q:155:ILE:HG21	1.88	0.55
1:v:36:MET:HE2	1:w:155:ILE:HG21	1.88	0.55
1:6:206:GLU:O	1:6:210:ALA:N	2.37	0.55
1:B:206:GLU:O	1:B:210:ALA:N	2.37	0.55
1:G:36:MET:HE2	1:H:155:ILE:HG21	1.88	0.55
1:G:206:GLU:O	1:G:210:ALA:N	2.37	0.55
1:N:36:MET:HE2	1:O:155:ILE:HG21	1.88	0.55
1:U:199:TRP:O	1:U:203:GLN:N	2.34	0.55
1:a:47:LEU:HD22	1:a:122:LEU:HD22	1.88	0.55
1:w:36:MET:HE2	1:x:155:ILE:HG21	1.88	0.55
1:R:206:GLU:O	1:R:210:ALA:N	2.37	0.55
1:U:206:GLU:O	1:U:210:ALA:N	2.37	0.55
1:f:36:MET:HE2	1:g:155:ILE:HG21	1.88	0.55
1:g:36:MET:HE2	1:h:155:ILE:HG21	1.88	0.55
1:l:47:LEU:HD22	1:l:122:LEU:HD22	1.88	0.55
1:q:47:LEU:HD22	1:q:122:LEU:HD22	1.88	0.55
1:x:206:GLU:O	1:x:210:ALA:N	2.37	0.55
1:D:36:MET:HE2	1:E:155:ILE:HG21	1.88	0.54
1:M:206:GLU:O	1:M:210:ALA:N	2.37	0.54
1:S:36:MET:HE2	1:T:155:ILE:HG21	1.88	0.54
1:V:36:MET:HE2	1:W:155:ILE:HG21	1.88	0.54
1:4:206:GLU:O	1:4:210:ALA:N	2.37	0.54
1:5:206:GLU:O	1:5:210:ALA:N	2.37	0.54
1:A:206:GLU:O	1:A:210:ALA:N	2.37	0.54
1:F:36:MET:HE2	1:G:155:ILE:HG21	1.88	0.54
1:E:36:MET:HE2	1:F:155:ILE:HG21	1.88	0.54
1:O:36:MET:HE2	1:P:155:ILE:HG21	1.88	0.54
1:P:199:TRP:O	1:P:203:GLN:N	2.34	0.54
1:N:199:TRP:O	1:N:203:GLN:N	2.34	0.54
1:g:206:GLU:O	1:g:210:ALA:N	2.37	0.54
1:t:206:GLU:O	1:t:210:ALA:N	2.37	0.54
1:R:36:MET:HE2	1:S:155:ILE:HG21	1.88	0.54
1:S:206:GLU:O	1:S:210:ALA:N	2.37	0.54
1:U:36:MET:HE2	1:V:155:ILE:HG21	1.88	0.54
1:V:206:GLU:O	1:V:210:ALA:N	2.37	0.54
1:Y:199:TRP:O	1:Y:203:GLN:N	2.34	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:206:GLU:O	1:e:210:ALA:N	2.37	0.54
1:P:36:MET:HE2	1:Q:155:ILE:HG21	1.88	0.54
1:Q:36:MET:HE2	1:R:155:ILE:HG21	1.88	0.54
1:k:199:TRP:O	1:k:203:GLN:N	2.34	0.54
1:I:206:GLU:O	1:I:210:ALA:N	2.37	0.53
1:Z:199:TRP:O	1:Z:203:GLN:N	2.34	0.53
1:g:199:TRP:O	1:g:203:GLN:N	2.34	0.53
1:0:199:TRP:O	1:0:203:GLN:N	2.34	0.53
1:1:190:SER:N	1:1:193:ASP:OD2	2.42	0.53
1:1:206:GLU:O	1:1:210:ALA:N	2.37	0.53
1:X:206:GLU:O	1:X:210:ALA:N	2.37	0.53
1:Z:190:SER:N	1:Z:193:ASP:OD2	2.42	0.53
1:m:206:GLU:O	1:m:210:ALA:N	2.37	0.53
1:v:206:GLU:O	1:v:210:ALA:N	2.37	0.53
1:2:190:SER:N	1:2:193:ASP:OD2	2.42	0.53
1:3:190:SER:N	1:3:193:ASP:OD2	2.42	0.53
1:4:190:SER:N	1:4:193:ASP:OD2	2.42	0.53
1:A:190:SER:N	1:A:193:ASP:OD2	2.42	0.53
1:H:199:TRP:O	1:H:203:GLN:N	2.34	0.53
1:J:117:GLN:O	1:J:121:GLN:N	2.41	0.53
1:P:190:SER:N	1:P:193:ASP:OD2	2.42	0.53
1:Y:190:SER:N	1:Y:193:ASP:OD2	2.42	0.53
1:a:190:SER:N	1:a:193:ASP:OD2	2.42	0.53
1:d:190:SER:N	1:d:193:ASP:OD2	2.42	0.53
1:p:206:GLU:O	1:p:210:ALA:N	2.37	0.53
1:0:190:SER:N	1:0:193:ASP:OD2	2.42	0.53
1:2:117:GLN:O	1:2:121:GLN:N	2.41	0.53
1:5:190:SER:N	1:5:193:ASP:OD2	2.42	0.53
1:B:190:SER:N	1:B:193:ASP:OD2	2.42	0.53
1:L:117:GLN:O	1:L:121:GLN:N	2.41	0.53
1:Q:190:SER:N	1:Q:193:ASP:OD2	2.42	0.53
1:b:190:SER:N	1:b:193:ASP:OD2	2.42	0.53
1:c:190:SER:N	1:c:193:ASP:OD2	2.42	0.53
1:u:190:SER:N	1:u:193:ASP:OD2	2.42	0.53
1:v:190:SER:N	1:v:193:ASP:OD2	2.42	0.53
1:6:190:SER:N	1:6:193:ASP:OD2	2.42	0.53
1:H:190:SER:N	1:H:193:ASP:OD2	2.42	0.53
1:J:199:TRP:O	1:J:203:GLN:N	2.34	0.53
1:O:190:SER:N	1:O:193:ASP:OD2	2.42	0.53
1:Y:117:GLN:O	1:Y:121:GLN:N	2.41	0.53
1:c:199:TRP:O	1:c:203:GLN:N	2.34	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:j:190:SER:N	1:j:193:ASP:OD2	2.42	0.53
1:j:206:GLU:O	1:j:210:ALA:N	2.37	0.53
1:l:199:TRP:O	1:l:203:GLN:N	2.34	0.53
1:o:199:TRP:O	1:o:203:GLN:N	2.34	0.53
1:w:206:GLU:O	1:w:210:ALA:N	2.37	0.53
1:G:190:SER:N	1:G:193:ASP:OD2	2.42	0.53
1:K:199:TRP:O	1:K:203:GLN:N	2.34	0.53
1:T:199:TRP:O	1:T:203:GLN:N	2.34	0.53
1:X:190:SER:N	1:X:193:ASP:OD2	2.42	0.53
1:e:190:SER:N	1:e:193:ASP:OD2	2.42	0.53
1:i:190:SER:N	1:i:193:ASP:OD2	2.42	0.53
1:k:190:SER:N	1:k:193:ASP:OD2	2.42	0.53
1:n:117:GLN:O	1:n:121:GLN:N	2.41	0.53
1:t:190:SER:N	1:t:193:ASP:OD2	2.42	0.53
1:w:190:SER:N	1:w:193:ASP:OD2	2.42	0.53
1:2:199:TRP:O	1:2:203:GLN:N	2.34	0.53
1:4:117:GLN:O	1:4:121:GLN:N	2.41	0.53
1:C:190:SER:N	1:C:193:ASP:OD2	2.42	0.53
1:F:190:SER:N	1:F:193:ASP:OD2	2.42	0.53
1:I:190:SER:N	1:I:193:ASP:OD2	2.42	0.53
1:W:199:TRP:O	1:W:203:GLN:N	2.34	0.53
1:a:206:GLU:O	1:a:210:ALA:N	2.37	0.53
1:h:206:GLU:O	1:h:210:ALA:N	2.37	0.53
1:k:117:GLN:O	1:k:121:GLN:N	2.41	0.53
1:q:117:GLN:O	1:q:121:GLN:N	2.41	0.53
1:7:190:SER:N	1:7:193:ASP:OD2	2.42	0.53
1:N:190:SER:N	1:N:193:ASP:OD2	2.42	0.53
1:R:190:SER:N	1:R:193:ASP:OD2	2.42	0.53
1:U:190:SER:N	1:U:193:ASP:OD2	2.42	0.53
1:h:190:SER:N	1:h:193:ASP:OD2	2.42	0.53
1:o:190:SER:N	1:o:193:ASP:OD2	2.42	0.53
1:Q:206:GLU:O	1:Q:210:ALA:N	2.37	0.53
1:i:199:TRP:O	1:i:203:GLN:N	2.34	0.53
1:l:190:SER:N	1:l:193:ASP:OD2	2.42	0.53
1:r:199:TRP:O	1:r:203:GLN:N	2.34	0.53
1:z:190:SER:N	1:z:193:ASP:OD2	2.42	0.53
1:z:199:TRP:O	1:z:203:GLN:N	2.34	0.53
1:L:206:GLU:O	1:L:210:ALA:N	2.37	0.52
1:l:117:GLN:O	1:l:121:GLN:N	2.40	0.52
1:s:190:SER:N	1:s:193:ASP:OD2	2.42	0.52
1:u:206:GLU:O	1:u:210:ALA:N	2.37	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:117:GLN:O	1:0:121:GLN:N	2.41	0.52
1:J:190:SER:N	1:J:193:ASP:OD2	2.42	0.52
1:M:190:SER:N	1:M:193:ASP:OD2	2.42	0.52
1:c:117:GLN:O	1:c:121:GLN:N	2.41	0.52
1:y:206:GLU:O	1:y:210:ALA:N	2.37	0.52
1:1:130:LEU:HD12	1:1:131:GLU:N	2.25	0.52
1:2:130:LEU:HD12	1:2:131:GLU:N	2.25	0.52
1:D:130:LEU:HD12	1:D:131:GLU:N	2.25	0.52
1:E:190:SER:N	1:E:193:ASP:OD2	2.42	0.52
1:Z:130:LEU:HD12	1:Z:131:GLU:N	2.25	0.52
1:d:206:GLU:O	1:d:210:ALA:N	2.37	0.52
1:f:190:SER:N	1:f:193:ASP:OD2	2.42	0.52
1:h:130:LEU:HD12	1:h:131:GLU:N	2.25	0.52
1:o:117:GLN:O	1:o:121:GLN:N	2.41	0.52
1:x:190:SER:N	1:x:193:ASP:OD2	2.42	0.52
1:3:199:TRP:O	1:3:203:GLN:N	2.34	0.52
1:7:130:LEU:HD12	1:7:131:GLU:N	2.25	0.52
1:C:130:LEU:HD12	1:C:131:GLU:N	2.25	0.52
1:Q:130:LEU:HD12	1:Q:131:GLU:N	2.25	0.52
1:T:130:LEU:HD12	1:T:131:GLU:N	2.25	0.52
1:T:190:SER:N	1:T:193:ASP:OD2	2.42	0.52
1:W:130:LEU:HD12	1:W:131:GLU:N	2.25	0.52
1:W:190:SER:N	1:W:193:ASP:OD2	2.42	0.52
1:Z:117:GLN:O	1:Z:121:GLN:N	2.41	0.52
1:b:117:GLN:O	1:b:121:GLN:N	2.41	0.52
1:f:130:LEU:HD12	1:f:131:GLU:N	2.25	0.52
1:k:130:LEU:HD12	1:k:131:GLU:N	2.25	0.52
1:p:190:SER:N	1:p:193:ASP:OD2	2.42	0.52
1:s:206:GLU:O	1:s:210:ALA:N	2.37	0.52
1:v:130:LEU:HD12	1:v:131:GLU:N	2.25	0.52
1:z:117:GLN:O	1:z:121:GLN:N	2.40	0.52
1:E:130:LEU:HD12	1:E:131:GLU:N	2.25	0.52
1:H:117:GLN:O	1:H:121:GLN:N	2.41	0.52
1:I:130:LEU:HD12	1:I:131:GLU:N	2.25	0.52
1:P:130:LEU:HD12	1:P:131:GLU:N	2.25	0.52
1:S:190:SER:N	1:S:193:ASP:OD2	2.42	0.52
1:V:190:SER:N	1:V:193:ASP:OD2	2.42	0.52
1:Y:130:LEU:HD12	1:Y:131:GLU:N	2.25	0.52
1:g:130:LEU:HD12	1:g:131:GLU:N	2.25	0.52
1:g:190:SER:N	1:g:193:ASP:OD2	2.42	0.52
1:m:190:SER:N	1:m:193:ASP:OD2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:s:117:GLN:O	1:s:121:GLN:N	2.41	0.52
1:y:130:LEU:HD12	1:y:131:GLU:N	2.25	0.52
1:F:130:LEU:HD12	1:F:131:GLU:N	2.25	0.52
1:H:130:LEU:HD12	1:H:131:GLU:N	2.25	0.52
1:N:117:GLN:O	1:N:121:GLN:N	2.40	0.52
1:a:130:LEU:HD12	1:a:131:GLU:N	2.25	0.52
1:q:130:LEU:HD12	1:q:131:GLU:N	2.25	0.52
1:6:130:LEU:HD12	1:6:131:GLU:N	2.25	0.52
1:B:130:LEU:HD12	1:B:131:GLU:N	2.25	0.52
1:D:190:SER:N	1:D:193:ASP:OD2	2.42	0.52
1:K:190:SER:N	1:K:193:ASP:OD2	2.42	0.52
1:L:130:LEU:HD12	1:L:131:GLU:N	2.25	0.52
1:d:130:LEU:HD12	1:d:131:GLU:N	2.25	0.52
1:e:130:LEU:HD12	1:e:131:GLU:N	2.25	0.52
1:n:130:LEU:HD12	1:n:131:GLU:N	2.25	0.52
1:0:130:LEU:HD12	1:0:131:GLU:N	2.25	0.52
1:3:130:LEU:HD12	1:3:131:GLU:N	2.25	0.52
1:G:199:TRP:O	1:G:203:GLN:N	2.34	0.52
1:K:130:LEU:HD12	1:K:131:GLU:N	2.25	0.52
1:N:130:LEU:HD12	1:N:131:GLU:N	2.25	0.52
1:S:130:LEU:HD12	1:S:131:GLU:N	2.25	0.52
1:V:130:LEU:HD12	1:V:131:GLU:N	2.25	0.52
1:r:130:LEU:HD12	1:r:131:GLU:N	2.25	0.52
1:s:130:LEU:HD12	1:s:131:GLU:N	2.25	0.52
1:w:130:LEU:HD12	1:w:131:GLU:N	2.25	0.52
1:x:199:TRP:O	1:x:203:GLN:N	2.34	0.52
1:5:130:LEU:HD12	1:5:131:GLU:N	2.25	0.52
1:A:130:LEU:HD12	1:A:131:GLU:N	2.25	0.52
1:K:117:GLN:O	1:K:121:GLN:N	2.41	0.52
1:M:130:LEU:HD12	1:M:131:GLU:N	2.25	0.52
1:n:190:SER:N	1:n:193:ASP:OD2	2.42	0.52
1:o:130:LEU:HD12	1:o:131:GLU:N	2.25	0.52
1:q:190:SER:N	1:q:193:ASP:OD2	2.42	0.52
1:u:130:LEU:HD12	1:u:131:GLU:N	2.25	0.52
1:y:190:SER:N	1:y:193:ASP:OD2	2.42	0.52
1:z:130:LEU:HD12	1:z:131:GLU:N	2.25	0.52
1:K:43:LEU:HD23	1:K:47:LEU:HD13	1.92	0.52
1:T:117:GLN:O	1:T:121:GLN:N	2.41	0.52
1:W:117:GLN:O	1:W:121:GLN:N	2.41	0.52
1:X:130:LEU:HD12	1:X:131:GLU:N	2.25	0.52
1:f:206:GLU:O	1:f:210:ALA:N	2.37	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:i:130:LEU:HD12	1:i:131:GLU:N	2.25	0.52
1:l:130:LEU:HD12	1:l:131:GLU:N	2.25	0.52
1:m:43:LEU:HD23	1:m:47:LEU:HD13	1.92	0.52
1:0:43:LEU:HD23	1:0:47:LEU:HD13	1.92	0.51
1:2:43:LEU:HD23	1:2:47:LEU:HD13	1.93	0.51
1:4:43:LEU:HD23	1:4:47:LEU:HD13	1.92	0.51
1:L:190:SER:N	1:L:193:ASP:OD2	2.42	0.51
1:M:117:GLN:O	1:M:121:GLN:N	2.41	0.51
1:j:130:LEU:HD12	1:j:131:GLU:N	2.25	0.51
1:p:43:LEU:HD23	1:p:47:LEU:HD13	1.93	0.51
1:t:130:LEU:HD12	1:t:131:GLU:N	2.25	0.51
1:G:117:GLN:O	1:G:121:GLN:N	2.41	0.51
1:G:130:LEU:HD12	1:G:131:GLU:N	2.25	0.51
1:I:43:LEU:HD23	1:I:47:LEU:HD13	1.93	0.51
1:J:43:LEU:HD23	1:J:47:LEU:HD13	1.93	0.51
1:M:43:LEU:HD23	1:M:47:LEU:HD13	1.93	0.51
1:Y:43:LEU:HD23	1:Y:47:LEU:HD13	1.93	0.51
1:Z:43:LEU:HD23	1:Z:47:LEU:HD13	1.93	0.51
1:a:43:LEU:HD23	1:a:47:LEU:HD13	1.93	0.51
1:b:43:LEU:HD23	1:b:47:LEU:HD13	1.93	0.51
1:b:130:LEU:HD12	1:b:131:GLU:N	2.25	0.51
1:c:130:LEU:HD12	1:c:131:GLU:N	2.25	0.51
1:d:117:GLN:O	1:d:121:GLN:N	2.41	0.51
1:p:130:LEU:HD12	1:p:131:GLU:N	2.25	0.51
1:r:43:LEU:HD23	1:r:47:LEU:HD13	1.93	0.51
1:r:190:SER:N	1:r:193:ASP:OD2	2.42	0.51
1:6:117:GLN:O	1:6:121:GLN:N	2.41	0.51
1:B:117:GLN:O	1:B:121:GLN:N	2.41	0.51
1:L:43:LEU:HD23	1:L:47:LEU:HD13	1.93	0.51
1:O:130:LEU:HD12	1:O:131:GLU:N	2.25	0.51
1:R:130:LEU:HD12	1:R:131:GLU:N	2.25	0.51
1:k:43:LEU:HD23	1:k:47:LEU:HD13	1.93	0.51
1:l:43:LEU:HD23	1:l:47:LEU:HD13	1.93	0.51
1:m:130:LEU:HD12	1:m:131:GLU:N	2.25	0.51
1:o:43:LEU:HD23	1:o:47:LEU:HD13	1.93	0.51
1:x:130:LEU:HD12	1:x:131:GLU:N	2.25	0.51
1:3:43:LEU:HD23	1:3:47:LEU:HD13	1.93	0.51
1:U:130:LEU:HD12	1:U:131:GLU:N	2.25	0.51
1:X:43:LEU:HD23	1:X:47:LEU:HD13	1.92	0.51
1:4:130:LEU:HD12	1:4:131:GLU:N	2.25	0.51
1:J:130:LEU:HD12	1:J:131:GLU:N	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:43:LEU:HD23	1:N:47:LEU:HD13	1.93	0.51
1:c:43:LEU:HD23	1:c:47:LEU:HD13	1.93	0.51
1:i:117:GLN:O	1:i:121:GLN:N	2.40	0.51
1:n:43:LEU:HD23	1:n:47:LEU:HD13	1.93	0.51
1:q:43:LEU:HD23	1:q:47:LEU:HD13	1.93	0.51
1:3:117:GLN:O	1:3:121:GLN:N	2.41	0.51
1:5:43:LEU:HD23	1:5:47:LEU:HD13	1.93	0.51
1:6:43:LEU:HD23	1:6:47:LEU:HD13	1.92	0.51
1:A:43:LEU:HD23	1:A:47:LEU:HD13	1.93	0.51
1:T:43:LEU:HD23	1:T:47:LEU:HD13	1.92	0.51
1:d:43:LEU:HD23	1:d:47:LEU:HD13	1.93	0.51
1:s:43:LEU:HD23	1:s:47:LEU:HD13	1.93	0.51
1:t:43:LEU:HD23	1:t:47:LEU:HD13	1.93	0.51
1:1:43:LEU:HD23	1:1:47:LEU:HD13	1.93	0.51
1:B:43:LEU:HD23	1:B:47:LEU:HD13	1.93	0.51
1:W:43:LEU:HD23	1:W:47:LEU:HD13	1.93	0.51
1:z:43:LEU:HD23	1:z:47:LEU:HD13	1.92	0.51
1:H:43:LEU:HD23	1:H:47:LEU:HD13	1.93	0.51
1:j:43:LEU:HD23	1:j:47:LEU:HD13	1.93	0.51
1:G:43:LEU:HD23	1:G:47:LEU:HD13	1.93	0.51
1:e:117:GLN:O	1:e:121:GLN:N	2.40	0.51
1:t:117:GLN:O	1:t:121:GLN:N	2.41	0.51
1:5:117:GLN:O	1:5:121:GLN:N	2.41	0.51
1:I:117:GLN:O	1:I:121:GLN:N	2.41	0.51
1:O:43:LEU:HD23	1:O:47:LEU:HD13	1.93	0.51
1:O:117:GLN:O	1:O:121:GLN:N	2.41	0.51
1:S:117:GLN:O	1:S:121:GLN:N	2.41	0.51
1:V:117:GLN:O	1:V:121:GLN:N	2.41	0.51
1:X:117:GLN:O	1:X:121:GLN:N	2.41	0.51
1:i:43:LEU:HD23	1:i:47:LEU:HD13	1.92	0.51
1:j:117:GLN:O	1:j:121:GLN:N	2.41	0.51
1:u:117:GLN:O	1:u:121:GLN:N	2.41	0.51
1:y:43:LEU:HD23	1:y:47:LEU:HD13	1.93	0.51
1:A:117:GLN:O	1:A:121:GLN:N	2.41	0.50
1:x:117:GLN:O	1:x:121:GLN:N	2.41	0.50
1:7:43:LEU:HD23	1:7:47:LEU:HD13	1.93	0.50
1:C:43:LEU:HD23	1:C:47:LEU:HD13	1.92	0.50
1:P:43:LEU:HD23	1:P:47:LEU:HD13	1.93	0.50
1:e:43:LEU:HD23	1:e:47:LEU:HD13	1.93	0.50
1:g:117:GLN:O	1:g:121:GLN:N	2.41	0.50
1:1:117:GLN:O	1:1:121:GLN:N	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:f:43:LEU:HD23	1:f:47:LEU:HD13	1.93	0.50
1:h:32:LEU:HD13	1:i:155:ILE:HD11	1.94	0.50
1:h:43:LEU:HD23	1:h:47:LEU:HD13	1.93	0.50
1:u:43:LEU:HD23	1:u:47:LEU:HD13	1.92	0.50
1:v:43:LEU:HD23	1:v:47:LEU:HD13	1.93	0.50
1:y:117:GLN:O	1:y:121:GLN:N	2.41	0.50
1:E:117:GLN:O	1:E:121:GLN:N	2.41	0.50
1:R:89:GLU:O	1:R:93:GLN:N	2.38	0.50
1:S:43:LEU:HD23	1:S:47:LEU:HD13	1.93	0.50
1:U:43:LEU:HD23	1:U:47:LEU:HD13	1.93	0.50
1:V:89:GLU:O	1:V:93:GLN:N	2.38	0.50
1:f:117:GLN:O	1:f:121:GLN:N	2.41	0.50
1:w:43:LEU:HD23	1:w:47:LEU:HD13	1.92	0.50
1:x:89:GLU:O	1:x:93:GLN:N	2.38	0.50
1:A:89:GLU:O	1:A:93:GLN:N	2.38	0.50
1:E:43:LEU:HD23	1:E:47:LEU:HD13	1.93	0.50
1:F:32:LEU:HD13	1:G:155:ILE:HD11	1.94	0.50
1:F:43:LEU:HD23	1:F:47:LEU:HD13	1.93	0.50
1:Q:117:GLN:O	1:Q:121:GLN:N	2.41	0.50
1:R:32:LEU:HD13	1:S:155:ILE:HD11	1.94	0.50
1:R:43:LEU:HD23	1:R:47:LEU:HD13	1.93	0.50
1:U:32:LEU:HD13	1:V:155:ILE:HD11	1.94	0.50
1:V:43:LEU:HD23	1:V:47:LEU:HD13	1.93	0.50
1:h:117:GLN:O	1:h:121:GLN:N	2.41	0.50
1:x:32:LEU:HD13	1:y:155:ILE:HD11	1.94	0.50
1:x:43:LEU:HD23	1:x:47:LEU:HD13	1.93	0.50
1:7:117:GLN:O	1:7:121:GLN:N	2.41	0.50
1:C:117:GLN:O	1:C:121:GLN:N	2.41	0.50
1:D:43:LEU:HD23	1:D:47:LEU:HD13	1.93	0.50
1:G:32:LEU:HD13	1:H:155:ILE:HD11	1.94	0.50
1:S:89:GLU:O	1:S:93:GLN:N	2.38	0.50
1:r:117:GLN:O	1:r:121:GLN:N	2.41	0.50
1:y:89:GLU:O	1:y:93:GLN:N	2.38	0.50
1:5:89:GLU:O	1:5:93:GLN:N	2.38	0.50
1:D:32:LEU:HD13	1:E:155:ILE:HD11	1.94	0.50
1:K:57:THR:OG1	1:K:108:LEU:HD21	2.12	0.50
1:P:117:GLN:O	1:P:121:GLN:N	2.41	0.50
1:Q:43:LEU:HD23	1:Q:47:LEU:HD13	1.93	0.50
1:S:32:LEU:HD13	1:T:155:ILE:HD11	1.94	0.50
1:V:32:LEU:HD13	1:W:155:ILE:HD11	1.94	0.50
1:W:32:LEU:HD13	1:X:155:ILE:HD11	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:89:GLU:O	1:W:93:GLN:N	2.38	0.50
1:h:57:THR:OG1	1:h:108:LEU:HD21	2.12	0.50
1:j:32:LEU:HD13	1:k:155:ILE:HD11	1.94	0.50
1:l:57:THR:OG1	1:l:108:LEU:HD21	2.12	0.50
1:m:57:THR:OG1	1:m:108:LEU:HD21	2.12	0.50
1:v:32:LEU:HD13	1:w:155:ILE:HD11	1.94	0.50
1:E:32:LEU:HD13	1:F:155:ILE:HD11	1.94	0.50
1:E:57:THR:OG1	1:E:108:LEU:HD21	2.12	0.50
1:F:117:GLN:O	1:F:121:GLN:N	2.41	0.50
1:H:57:THR:OG1	1:H:108:LEU:HD21	2.12	0.50
1:g:43:LEU:HD23	1:g:47:LEU:HD13	1.93	0.50
1:i:32:LEU:HD13	1:j:155:ILE:HD11	1.94	0.50
1:m:117:GLN:O	1:m:121:GLN:N	2.41	0.50
1:n:57:THR:OG1	1:n:108:LEU:HD21	2.12	0.50
1:o:57:THR:OG1	1:o:108:LEU:HD21	2.12	0.50
1:q:57:THR:OG1	1:q:108:LEU:HD21	2.12	0.50
1:w:32:LEU:HD13	1:x:155:ILE:HD11	1.94	0.50
1:y:32:LEU:HD13	1:z:155:ILE:HD11	1.94	0.50
1:0:57:THR:OG1	1:0:108:LEU:HD21	2.12	0.49
1:0:155:ILE:HD11	1:z:32:LEU:HD13	1.94	0.49
1:D:117:GLN:O	1:D:121:GLN:N	2.41	0.49
1:F:57:THR:OG1	1:F:108:LEU:HD21	2.12	0.49
1:Q:32:LEU:HD13	1:R:155:ILE:HD11	1.94	0.49
1:T:89:GLU:O	1:T:93:GLN:N	2.38	0.49
1:W:57:THR:OG1	1:W:108:LEU:HD21	2.12	0.49
1:Z:57:THR:OG1	1:Z:108:LEU:HD21	2.12	0.49
1:g:57:THR:OG1	1:g:108:LEU:HD21	2.12	0.49
1:j:57:THR:OG1	1:j:108:LEU:HD21	2.12	0.49
1:p:57:THR:OG1	1:p:108:LEU:HD21	2.12	0.49
1:w:117:GLN:O	1:w:121:GLN:N	2.41	0.49
1:y:57:THR:OG1	1:y:108:LEU:HD21	2.12	0.49
1:3:32:LEU:HD13	1:4:155:ILE:HD11	1.94	0.49
1:A:57:THR:OG1	1:A:108:LEU:HD21	2.12	0.49
1:L:57:THR:OG1	1:L:108:LEU:HD21	2.12	0.49
1:P:57:THR:OG1	1:P:108:LEU:HD21	2.12	0.49
1:R:57:THR:OG1	1:R:108:LEU:HD21	2.12	0.49
1:T:57:THR:OG1	1:T:108:LEU:HD21	2.12	0.49
1:X:57:THR:OG1	1:X:108:LEU:HD21	2.12	0.49
1:b:32:LEU:HD13	1:c:155:ILE:HD11	1.94	0.49
1:c:57:THR:OG1	1:c:108:LEU:HD21	2.12	0.49
1:f:32:LEU:HD13	1:g:155:ILE:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:g:32:LEU:HD13	1:h:155:ILE:HD11	1.94	0.49
1:p:117:GLN:O	1:p:121:GLN:N	2.41	0.49
1:2:57:THR:OG1	1:2:108:LEU:HD21	2.12	0.49
1:4:57:THR:OG1	1:4:108:LEU:HD21	2.12	0.49
1:5:57:THR:OG1	1:5:108:LEU:HD21	2.12	0.49
1:H:32:LEU:HD13	1:I:155:ILE:HD11	1.94	0.49
1:J:57:THR:OG1	1:J:108:LEU:HD21	2.12	0.49
1:U:57:THR:OG1	1:U:108:LEU:HD21	2.12	0.49
1:Y:57:THR:OG1	1:Y:108:LEU:HD21	2.12	0.49
1:i:57:THR:OG1	1:i:108:LEU:HD21	2.12	0.49
1:u:57:THR:OG1	1:u:108:LEU:HD21	2.12	0.49
1:v:57:THR:OG1	1:v:108:LEU:HD21	2.12	0.49
1:v:117:GLN:O	1:v:121:GLN:N	2.41	0.49
1:z:57:THR:OG1	1:z:108:LEU:HD21	2.12	0.49
1:4:32:LEU:HD13	1:5:155:ILE:HD11	1.94	0.49
1:P:32:LEU:HD13	1:Q:155:ILE:HD11	1.94	0.49
1:R:117:GLN:O	1:R:121:GLN:N	2.41	0.49
1:U:117:GLN:O	1:U:121:GLN:N	2.41	0.49
1:X:32:LEU:HD13	1:Y:155:ILE:HD11	1.94	0.49
1:b:57:THR:OG1	1:b:108:LEU:HD21	2.12	0.49
1:d:57:THR:OG1	1:d:108:LEU:HD21	2.12	0.49
1:z:89:GLU:O	1:z:93:GLN:N	2.38	0.49
1:1:57:THR:OG1	1:1:108:LEU:HD21	2.12	0.49
1:O:57:THR:OG1	1:O:108:LEU:HD21	2.12	0.49
1:Q:57:THR:OG1	1:Q:108:LEU:HD21	2.12	0.49
1:r:57:THR:OG1	1:r:108:LEU:HD21	2.12	0.49
1:0:32:LEU:HD13	1:1:155:ILE:HD11	1.94	0.49
1:C:32:LEU:HD13	1:D:155:ILE:HD11	1.94	0.49
1:D:57:THR:OG1	1:D:108:LEU:HD21	2.12	0.49
1:G:57:THR:OG1	1:G:108:LEU:HD21	2.12	0.49
1:N:32:LEU:HD13	1:O:155:ILE:HD11	1.94	0.49
1:a:32:LEU:HD13	1:b:155:ILE:HD11	1.94	0.49
1:s:32:LEU:HD13	1:t:155:ILE:HD11	1.94	0.49
1:B:57:THR:OG1	1:B:108:LEU:HD21	2.12	0.49
1:I:32:LEU:HD13	1:J:155:ILE:HD11	1.94	0.49
1:S:57:THR:OG1	1:S:108:LEU:HD21	2.12	0.49
1:d:89:GLU:O	1:d:93:GLN:N	2.38	0.49
1:6:57:THR:OG1	1:6:108:LEU:HD21	2.12	0.49
1:I:57:THR:OG1	1:I:108:LEU:HD21	2.12	0.49
1:V:57:THR:OG1	1:V:108:LEU:HD21	2.12	0.49
1:X:89:GLU:O	1:X:93:GLN:N	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:32:LEU:HD13	1:Z:155:ILE:HD11	1.94	0.49
1:k:32:LEU:HD13	1:l:155:ILE:HD11	1.94	0.49
1:m:32:LEU:HD13	1:n:155:ILE:HD11	1.94	0.49
1:o:32:LEU:HD13	1:p:155:ILE:HD11	1.94	0.49
1:q:89:GLU:O	1:q:93:GLN:N	2.38	0.49
1:t:57:THR:OG1	1:t:108:LEU:HD21	2.12	0.49
1:w:57:THR:OG1	1:w:108:LEU:HD21	2.12	0.49
1:x:57:THR:OG1	1:x:108:LEU:HD21	2.12	0.49
1:2:32:LEU:HD13	1:3:155:ILE:HD11	1.94	0.49
1:3:57:THR:OG1	1:3:108:LEU:HD21	2.12	0.49
1:K:32:LEU:HD13	1:L:155:ILE:HD11	1.94	0.49
1:M:32:LEU:HD13	1:N:155:ILE:HD11	1.94	0.49
1:O:32:LEU:HD13	1:P:155:ILE:HD11	1.94	0.49
1:e:32:LEU:HD13	1:f:155:ILE:HD11	1.94	0.49
1:l:32:LEU:HD13	1:m:155:ILE:HD11	1.94	0.49
1:p:32:LEU:HD13	1:q:155:ILE:HD11	1.94	0.49
1:t:32:LEU:HD13	1:u:155:ILE:HD11	1.94	0.49
1:J:32:LEU:HD13	1:K:155:ILE:HD11	1.94	0.49
1:c:32:LEU:HD13	1:d:155:ILE:HD11	1.94	0.49
1:k:57:THR:OG1	1:k:108:LEU:HD21	2.12	0.49
1:n:89:GLU:O	1:n:93:GLN:N	2.38	0.49
1:u:32:LEU:HD13	1:v:155:ILE:HD11	1.94	0.49
1:B:32:LEU:HD13	1:C:155:ILE:HD11	1.94	0.48
1:M:57:THR:OG1	1:M:108:LEU:HD21	2.12	0.48
1:a:117:GLN:O	1:a:121:GLN:N	2.41	0.48
1:f:57:THR:OG1	1:f:108:LEU:HD21	2.12	0.48
1:1:32:LEU:HD13	1:2:155:ILE:HD11	1.94	0.48
1:6:32:LEU:HD13	1:7:155:ILE:HD11	1.94	0.48
1:N:57:THR:OG1	1:N:108:LEU:HD21	2.12	0.48
1:P:97:TYR:O	1:P:101:THR:N	2.38	0.48
1:e:57:THR:OG1	1:e:108:LEU:HD21	2.12	0.48
1:r:32:LEU:HD13	1:s:155:ILE:HD11	1.94	0.48
1:A:32:LEU:HD13	1:B:155:ILE:HD11	1.94	0.48
1:d:32:LEU:HD13	1:e:155:ILE:HD11	1.94	0.48
1:q:32:LEU:HD13	1:r:155:ILE:HD11	1.94	0.48
1:7:57:THR:OG1	1:7:108:LEU:HD21	2.12	0.48
1:C:57:THR:OG1	1:C:108:LEU:HD21	2.12	0.48
1:V:97:TYR:O	1:V:101:THR:N	2.38	0.48
1:a:57:THR:OG1	1:a:108:LEU:HD21	2.12	0.48
1:0:89:GLU:O	1:0:93:GLN:N	2.38	0.48
1:5:32:LEU:HD13	1:6:155:ILE:HD11	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:GLU:O	1:B:93:GLN:N	2.38	0.48
1:S:97:TYR:O	1:S:101:THR:N	2.38	0.48
1:Z:32:LEU:HD13	1:a:155:ILE:HD11	1.94	0.48
1:s:57:THR:OG1	1:s:108:LEU:HD21	2.12	0.48
1:6:89:GLU:O	1:6:93:GLN:N	2.38	0.48
1:x:169:GLU:OE1	1:x:169:GLU:N	2.46	0.48
1:L:32:LEU:HD13	1:M:155:ILE:HD11	1.94	0.48
1:e:97:TYR:O	1:e:101:THR:N	2.38	0.48
1:r:169:GLU:OE1	1:r:169:GLU:N	2.46	0.48
1:B:69:GLN:O	1:B:73:GLU:N	2.38	0.47
1:L:89:GLU:O	1:L:93:GLN:N	2.38	0.47
1:Y:89:GLU:O	1:Y:93:GLN:N	2.38	0.47
1:u:69:GLN:O	1:u:73:GLU:N	2.38	0.47
1:z:169:GLU:OE1	1:z:169:GLU:N	2.46	0.47
1:1:201:GLU:O	1:1:205:VAL:HG22	2.15	0.47
1:3:201:GLU:O	1:3:205:VAL:HG22	2.15	0.47
1:6:69:GLN:O	1:6:73:GLU:N	2.38	0.47
1:A:53:THR:O	1:A:57:THR:HG23	2.15	0.47
1:G:97:TYR:O	1:G:101:THR:N	2.38	0.47
1:G:201:GLU:O	1:G:205:VAL:HG22	2.15	0.47
1:c:169:GLU:OE1	1:c:169:GLU:N	2.46	0.47
1:n:144:LYS:HA	1:n:147:ILE:HG22	1.97	0.47
1:q:144:LYS:HA	1:q:147:ILE:HG22	1.97	0.47
1:x:201:GLU:O	1:x:205:VAL:HG22	2.15	0.47
1:5:53:THR:O	1:5:57:THR:HG23	2.15	0.47
1:I:169:GLU:OE1	1:I:169:GLU:N	2.46	0.47
1:I:201:GLU:O	1:I:205:VAL:HG22	2.15	0.47
1:K:144:LYS:HA	1:K:147:ILE:HG22	1.97	0.47
1:R:201:GLU:O	1:R:205:VAL:HG22	2.15	0.47
1:a:201:GLU:O	1:a:205:VAL:HG22	2.15	0.47
1:b:201:GLU:O	1:b:205:VAL:HG22	2.15	0.47
1:c:53:THR:O	1:c:57:THR:HG23	2.15	0.47
1:c:144:LYS:HA	1:c:147:ILE:HG22	1.96	0.47
1:f:69:GLN:O	1:f:73:GLU:N	2.38	0.47
1:i:169:GLU:OE1	1:i:169:GLU:N	2.46	0.47
1:m:201:GLU:O	1:m:205:VAL:HG22	2.15	0.47
1:o:201:GLU:O	1:o:205:VAL:HG22	2.15	0.47
1:z:201:GLU:O	1:z:205:VAL:HG22	2.15	0.47
1:2:89:GLU:O	1:2:93:GLN:N	2.38	0.47
1:2:201:GLU:O	1:2:205:VAL:HG22	2.15	0.47
1:4:53:THR:O	1:4:57:THR:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:7:201:GLU:O	1:7:205:VAL:HG22	2.15	0.47
1:C:201:GLU:O	1:C:205:VAL:HG22	2.15	0.47
1:D:201:GLU:O	1:D:205:VAL:HG22	2.15	0.47
1:G:53:THR:O	1:G:57:THR:HG23	2.15	0.47
1:L:144:LYS:HA	1:L:147:ILE:HG22	1.97	0.47
1:N:69:GLN:O	1:N:73:GLU:N	2.38	0.47
1:S:201:GLU:O	1:S:205:VAL:HG22	2.15	0.47
1:U:97:TYR:O	1:U:101:THR:N	2.38	0.47
1:U:201:GLU:O	1:U:205:VAL:HG22	2.15	0.47
1:V:201:GLU:O	1:V:205:VAL:HG22	2.15	0.47
1:b:53:THR:O	1:b:57:THR:HG23	2.15	0.47
1:c:69:GLN:O	1:c:73:GLU:N	2.38	0.47
1:d:53:THR:O	1:d:57:THR:HG23	2.15	0.47
1:g:53:THR:O	1:g:57:THR:HG23	2.15	0.47
1:g:169:GLU:OE1	1:g:169:GLU:N	2.46	0.47
1:j:53:THR:O	1:j:57:THR:HG23	2.15	0.47
1:k:201:GLU:O	1:k:205:VAL:HG22	2.15	0.47
1:l:201:GLU:O	1:l:205:VAL:HG22	2.15	0.47
1:m:144:LYS:HA	1:m:147:ILE:HG22	1.97	0.47
1:p:144:LYS:HA	1:p:147:ILE:HG22	1.97	0.47
1:p:201:GLU:O	1:p:205:VAL:HG22	2.15	0.47
1:v:169:GLU:OE1	1:v:169:GLU:N	2.46	0.47
1:0:53:THR:O	1:0:57:THR:HG23	2.15	0.47
1:1:53:THR:O	1:1:57:THR:HG23	2.15	0.47
1:2:53:THR:O	1:2:57:THR:HG23	2.15	0.47
1:3:53:THR:O	1:3:57:THR:HG23	2.15	0.47
1:4:144:LYS:HA	1:4:147:ILE:HG22	1.97	0.47
1:5:144:LYS:HA	1:5:147:ILE:HG22	1.97	0.47
1:6:53:THR:O	1:6:57:THR:HG23	2.15	0.47
1:A:144:LYS:HA	1:A:147:ILE:HG22	1.97	0.47
1:B:53:THR:O	1:B:57:THR:HG23	2.15	0.47
1:D:53:THR:O	1:D:57:THR:HG23	2.15	0.47
1:E:53:THR:O	1:E:57:THR:HG23	2.15	0.47
1:E:69:GLN:O	1:E:73:GLU:N	2.38	0.47
1:E:201:GLU:O	1:E:205:VAL:HG22	2.15	0.47
1:F:53:THR:O	1:F:57:THR:HG23	2.15	0.47
1:H:53:THR:O	1:H:57:THR:HG23	2.15	0.47
1:H:69:GLN:O	1:H:73:GLU:N	2.38	0.47
1:H:201:GLU:O	1:H:205:VAL:HG22	2.15	0.47
1:J:201:GLU:O	1:J:205:VAL:HG22	2.15	0.47
1:N:97:TYR:O	1:N:101:THR:N	2.38	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:201:GLU:O	1:N:205:VAL:HG22	2.15	0.47
1:P:53:THR:O	1:P:57:THR:HG23	2.15	0.47
1:P:169:GLU:OE1	1:P:169:GLU:N	2.46	0.47
1:Q:69:GLN:O	1:Q:73:GLU:N	2.38	0.47
1:R:97:TYR:O	1:R:101:THR:N	2.38	0.47
1:V:53:THR:O	1:V:57:THR:HG23	2.15	0.47
1:W:201:GLU:O	1:W:205:VAL:HG22	2.15	0.47
1:X:201:GLU:O	1:X:205:VAL:HG22	2.15	0.47
1:Y:53:THR:O	1:Y:57:THR:HG23	2.15	0.47
1:Y:201:GLU:O	1:Y:205:VAL:HG22	2.15	0.47
1:Z:53:THR:O	1:Z:57:THR:HG23	2.15	0.47
1:a:53:THR:O	1:a:57:THR:HG23	2.15	0.47
1:e:89:GLU:O	1:e:93:GLN:N	2.38	0.47
1:f:201:GLU:O	1:f:205:VAL:HG22	2.15	0.47
1:g:97:TYR:O	1:g:101:THR:N	2.38	0.47
1:g:201:GLU:O	1:g:205:VAL:HG22	2.15	0.47
1:h:201:GLU:O	1:h:205:VAL:HG22	2.15	0.47
1:i:53:THR:O	1:i:57:THR:HG23	2.15	0.47
1:i:201:GLU:O	1:i:205:VAL:HG22	2.15	0.47
1:o:69:GLN:O	1:o:73:GLU:N	2.38	0.47
1:r:69:GLN:O	1:r:73:GLU:N	2.38	0.47
1:s:201:GLU:O	1:s:205:VAL:HG22	2.15	0.47
1:u:53:THR:O	1:u:57:THR:HG23	2.15	0.47
1:v:53:THR:O	1:v:57:THR:HG23	2.15	0.47
1:w:201:GLU:O	1:w:205:VAL:HG22	2.15	0.47
1:x:69:GLN:O	1:x:73:GLU:N	2.38	0.47
1:y:201:GLU:O	1:y:205:VAL:HG22	2.15	0.47
1:1:144:LYS:HA	1:1:147:ILE:HG22	1.97	0.47
1:1:169:GLU:OE1	1:1:169:GLU:N	2.46	0.47
1:4:201:GLU:O	1:4:205:VAL:HG22	2.15	0.47
1:O:53:THR:O	1:O:57:THR:HG23	2.15	0.47
1:Q:53:THR:O	1:Q:57:THR:HG23	2.15	0.47
1:S:53:THR:O	1:S:57:THR:HG23	2.15	0.47
1:W:69:GLN:O	1:W:73:GLU:N	2.38	0.47
1:Y:144:LYS:HA	1:Y:147:ILE:HG22	1.97	0.47
1:Z:69:GLN:O	1:Z:73:GLU:N	2.38	0.47
1:Z:144:LYS:HA	1:Z:147:ILE:HG22	1.97	0.47
1:Z:201:GLU:O	1:Z:205:VAL:HG22	2.15	0.47
1:k:53:THR:O	1:k:57:THR:HG23	2.15	0.47
1:m:169:GLU:OE1	1:m:169:GLU:N	2.46	0.47
1:t:201:GLU:O	1:t:205:VAL:HG22	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:y:53:THR:O	1:y:57:THR:HG23	2.15	0.47
1:0:69:GLN:O	1:0:73:GLU:N	2.38	0.47
1:0:144:LYS:HA	1:0:147:ILE:HG22	1.97	0.47
1:1:127:ARG:HA	1:1:130:LEU:HD21	1.97	0.47
1:3:127:ARG:HA	1:3:130:LEU:HD21	1.97	0.47
1:J:144:LYS:HA	1:J:147:ILE:HG22	1.97	0.47
1:M:201:GLU:O	1:M:205:VAL:HG22	2.15	0.47
1:N:169:GLU:OE1	1:N:169:GLU:N	2.46	0.47
1:Q:201:GLU:O	1:Q:205:VAL:HG22	2.15	0.47
1:T:201:GLU:O	1:T:205:VAL:HG22	2.15	0.47
1:X:53:THR:O	1:X:57:THR:HG23	2.15	0.47
1:a:127:ARG:HA	1:a:130:LEU:HD21	1.97	0.47
1:b:144:LYS:HA	1:b:147:ILE:HG22	1.97	0.47
1:e:201:GLU:O	1:e:205:VAL:HG22	2.15	0.47
1:f:53:THR:O	1:f:57:THR:HG23	2.15	0.47
1:h:53:THR:O	1:h:57:THR:HG23	2.15	0.47
1:i:69:GLN:O	1:i:73:GLU:N	2.38	0.47
1:j:201:GLU:O	1:j:205:VAL:HG22	2.15	0.47
1:m:127:ARG:HA	1:m:130:LEU:HD21	1.97	0.47
1:p:127:ARG:HA	1:p:130:LEU:HD21	1.97	0.47
1:p:169:GLU:OE1	1:p:169:GLU:N	2.46	0.47
1:r:144:LYS:HA	1:r:147:ILE:HG22	1.97	0.47
1:v:97:TYR:O	1:v:101:THR:N	2.38	0.47
1:x:53:THR:O	1:x:57:THR:HG23	2.15	0.47
1:3:69:GLN:O	1:3:73:GLU:N	2.38	0.47
1:F:97:TYR:O	1:F:101:THR:N	2.38	0.47
1:I:53:THR:O	1:I:57:THR:HG23	2.15	0.47
1:K:69:GLN:O	1:K:73:GLU:N	2.38	0.47
1:K:127:ARG:HA	1:K:130:LEU:HD21	1.97	0.47
1:K:201:GLU:O	1:K:205:VAL:HG22	2.15	0.47
1:L:201:GLU:O	1:L:205:VAL:HG22	2.15	0.47
1:R:169:GLU:OE1	1:R:169:GLU:N	2.46	0.47
1:T:53:THR:O	1:T:57:THR:HG23	2.15	0.47
1:T:69:GLN:O	1:T:73:GLU:N	2.38	0.47
1:Z:89:GLU:O	1:Z:93:GLN:N	2.38	0.47
1:e:53:THR:O	1:e:57:THR:HG23	2.15	0.47
1:k:127:ARG:HA	1:k:130:LEU:HD21	1.97	0.47
1:l:69:GLN:O	1:l:73:GLU:N	2.38	0.47
1:r:127:ARG:HA	1:r:130:LEU:HD21	1.97	0.47
1:t:53:THR:O	1:t:57:THR:HG23	2.15	0.47
1:w:53:THR:O	1:w:57:THR:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:6:201:GLU:O	1:6:205:VAL:HG22	2.15	0.46
1:I:127:ARG:HA	1:I:130:LEU:HD21	1.97	0.46
1:L:127:ARG:HA	1:L:130:LEU:HD21	1.97	0.46
1:O:201:GLU:O	1:O:205:VAL:HG22	2.15	0.46
1:U:169:GLU:OE1	1:U:169:GLU:N	2.46	0.46
1:W:53:THR:O	1:W:57:THR:HG23	2.15	0.46
1:X:144:LYS:HA	1:X:147:ILE:HG22	1.97	0.46
1:Y:127:ARG:HA	1:Y:130:LEU:HD21	1.97	0.46
1:Z:127:ARG:HA	1:Z:130:LEU:HD21	1.97	0.46
1:a:169:GLU:OE1	1:a:169:GLU:N	2.46	0.46
1:d:144:LYS:HA	1:d:147:ILE:HG22	1.97	0.46
1:k:169:GLU:OE1	1:k:169:GLU:N	2.46	0.46
1:l:127:ARG:HA	1:l:130:LEU:HD21	1.97	0.46
1:r:201:GLU:O	1:r:205:VAL:HG22	2.15	0.46
1:t:97:TYR:O	1:t:101:THR:N	2.38	0.46
1:z:53:THR:O	1:z:57:THR:HG23	2.15	0.46
1:4:127:ARG:HA	1:4:130:LEU:HD21	1.97	0.46
1:C:89:GLU:O	1:C:93:GLN:N	2.38	0.46
1:J:127:ARG:HA	1:J:130:LEU:HD21	1.97	0.46
1:R:53:THR:O	1:R:57:THR:HG23	2.15	0.46
1:T:169:GLU:OE1	1:T:169:GLU:N	2.46	0.46
1:U:53:THR:O	1:U:57:THR:HG23	2.15	0.46
1:Z:169:GLU:OE1	1:Z:169:GLU:N	2.46	0.46
1:b:127:ARG:HA	1:b:130:LEU:HD21	1.97	0.46
1:c:127:ARG:HA	1:c:130:LEU:HD21	1.97	0.46
1:o:53:THR:O	1:o:57:THR:HG23	2.15	0.46
1:o:127:ARG:HA	1:o:130:LEU:HD21	1.97	0.46
1:r:89:GLU:O	1:r:93:GLN:N	2.38	0.46
1:z:127:ARG:HA	1:z:130:LEU:HD21	1.97	0.46
1:2:127:ARG:HA	1:2:130:LEU:HD21	1.97	0.46
1:2:144:LYS:HA	1:2:147:ILE:HG22	1.97	0.46
1:3:144:LYS:HA	1:3:147:ILE:HG22	1.97	0.46
1:5:127:ARG:HA	1:5:130:LEU:HD21	1.97	0.46
1:B:201:GLU:O	1:B:205:VAL:HG22	2.15	0.46
1:C:53:THR:O	1:C:57:THR:HG23	2.15	0.46
1:H:97:TYR:O	1:H:101:THR:N	2.38	0.46
1:M:127:ARG:HA	1:M:130:LEU:HD21	1.97	0.46
1:M:144:LYS:HA	1:M:147:ILE:HG22	1.96	0.46
1:N:53:THR:O	1:N:57:THR:HG23	2.15	0.46
1:U:144:LYS:HA	1:U:147:ILE:HG22	1.97	0.46
1:W:169:GLU:OE1	1:W:169:GLU:N	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:127:ARG:HA	1:X:130:LEU:HD21	1.97	0.46
1:c:201:GLU:O	1:c:205:VAL:HG22	2.15	0.46
1:l:53:THR:O	1:l:57:THR:HG23	2.15	0.46
1:q:127:ARG:HA	1:q:130:LEU:HD21	1.97	0.46
1:u:201:GLU:O	1:u:205:VAL:HG22	2.15	0.46
1:w:144:LYS:HA	1:w:147:ILE:HG22	1.97	0.46
1:0:127:ARG:HA	1:0:130:LEU:HD21	1.97	0.46
1:1:89:GLU:O	1:1:93:GLN:N	2.38	0.46
1:7:53:THR:O	1:7:57:THR:HG23	2.15	0.46
1:7:89:GLU:O	1:7:93:GLN:N	2.38	0.46
1:A:127:ARG:HA	1:A:130:LEU:HD21	1.97	0.46
1:B:144:LYS:HA	1:B:147:ILE:HG22	1.96	0.46
1:E:144:LYS:HA	1:E:147:ILE:HG22	1.97	0.46
1:H:127:ARG:HA	1:H:130:LEU:HD21	1.97	0.46
1:N:127:ARG:HA	1:N:130:LEU:HD21	1.97	0.46
1:R:144:LYS:HA	1:R:147:ILE:HG22	1.97	0.46
1:g:144:LYS:HA	1:g:147:ILE:HG22	1.97	0.46
1:j:127:ARG:HA	1:j:130:LEU:HD21	1.97	0.46
1:l:144:LYS:HA	1:l:147:ILE:HG22	1.97	0.46
1:n:127:ARG:HA	1:n:130:LEU:HD21	1.97	0.46
1:6:144:LYS:HA	1:6:147:ILE:HG22	1.97	0.46
1:6:169:GLU:OE1	1:6:169:GLU:N	2.46	0.46
1:D:169:GLU:OE1	1:D:169:GLU:N	2.46	0.46
1:G:127:ARG:HA	1:G:130:LEU:HD21	1.97	0.46
1:J:53:THR:O	1:J:57:THR:HG23	2.15	0.46
1:e:169:GLU:OE1	1:e:169:GLU:N	2.46	0.46
1:h:144:LYS:HA	1:h:147:ILE:HG22	1.97	0.46
1:o:144:LYS:HA	1:o:147:ILE:HG22	1.97	0.46
1:s:127:ARG:HA	1:s:130:LEU:HD21	1.97	0.46
1:z:97:TYR:O	1:z:101:THR:N	2.38	0.46
1:B:169:GLU:OE1	1:B:169:GLU:N	2.46	0.46
1:C:97:TYR:O	1:C:101:THR:N	2.38	0.46
1:L:169:GLU:OE1	1:L:169:GLU:N	2.46	0.46
1:O:144:LYS:HA	1:O:147:ILE:HG22	1.97	0.46
1:Q:144:LYS:HA	1:Q:147:ILE:HG22	1.97	0.46
1:T:127:ARG:HA	1:T:130:LEU:HD21	1.97	0.46
1:V:144:LYS:HA	1:V:147:ILE:HG22	1.97	0.46
1:s:53:THR:O	1:s:57:THR:HG23	2.15	0.46
1:v:201:GLU:O	1:v:205:VAL:HG22	2.15	0.46
1:6:127:ARG:HA	1:6:130:LEU:HD21	1.97	0.46
1:B:127:ARG:HA	1:B:130:LEU:HD21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:144:LYS:HA	1:S:147:ILE:HG22	1.97	0.46
1:W:127:ARG:HA	1:W:130:LEU:HD21	1.97	0.46
1:d:127:ARG:HA	1:d:130:LEU:HD21	1.97	0.46
1:m:53:THR:O	1:m:57:THR:HG23	2.15	0.46
1:p:53:THR:O	1:p:57:THR:HG23	2.15	0.46
1:t:127:ARG:HA	1:t:130:LEU:HD21	1.97	0.46
1:t:144:LYS:HA	1:t:147:ILE:HG22	1.97	0.46
1:t:169:GLU:OE1	1:t:169:GLU:N	2.46	0.46
1:x:144:LYS:HA	1:x:147:ILE:HG22	1.97	0.46
1:y:127:ARG:HA	1:y:130:LEU:HD21	1.97	0.46
1:y:144:LYS:HA	1:y:147:ILE:HG22	1.97	0.46
1:5:201:GLU:O	1:5:205:VAL:HG22	2.15	0.46
1:7:97:TYR:O	1:7:101:THR:N	2.38	0.46
1:A:201:GLU:O	1:A:205:VAL:HG22	2.15	0.46
1:C:144:LYS:HA	1:C:147:ILE:HG22	1.96	0.46
1:D:144:LYS:HA	1:D:147:ILE:HG22	1.97	0.46
1:F:144:LYS:HA	1:F:147:ILE:HG22	1.97	0.46
1:F:169:GLU:OE1	1:F:169:GLU:N	2.46	0.46
1:F:201:GLU:O	1:F:205:VAL:HG22	2.15	0.46
1:G:144:LYS:HA	1:G:147:ILE:HG22	1.97	0.46
1:M:53:THR:O	1:M:57:THR:HG23	2.15	0.46
1:N:144:LYS:HA	1:N:147:ILE:HG22	1.96	0.46
1:P:144:LYS:HA	1:P:147:ILE:HG22	1.97	0.46
1:S:127:ARG:HA	1:S:130:LEU:HD21	1.97	0.46
1:V:127:ARG:HA	1:V:130:LEU:HD21	1.97	0.46
1:d:201:GLU:O	1:d:205:VAL:HG22	2.15	0.46
1:f:144:LYS:HA	1:f:147:ILE:HG22	1.97	0.46
1:i:144:LYS:HA	1:i:147:ILE:HG22	1.97	0.46
1:n:201:GLU:O	1:n:205:VAL:HG22	2.15	0.46
1:q:201:GLU:O	1:q:205:VAL:HG22	2.15	0.46
1:u:144:LYS:HA	1:u:147:ILE:HG22	1.97	0.46
1:v:144:LYS:HA	1:v:147:ILE:HG22	1.96	0.46
1:z:144:LYS:HA	1:z:147:ILE:HG22	1.97	0.46
1:H:144:LYS:HA	1:H:147:ILE:HG22	1.97	0.46
1:P:201:GLU:O	1:P:205:VAL:HG22	2.15	0.46
1:c:97:TYR:O	1:c:101:THR:N	2.38	0.46
1:j:144:LYS:HA	1:j:147:ILE:HG22	1.97	0.46
1:q:53:THR:O	1:q:57:THR:HG23	2.15	0.46
1:y:97:TYR:O	1:y:101:THR:N	2.38	0.46
1:0:201:GLU:O	1:0:205:VAL:HG22	2.15	0.46
1:7:144:LYS:HA	1:7:147:ILE:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:53:THR:O	1:K:57:THR:HG23	2.15	0.46
1:L:53:THR:O	1:L:57:THR:HG23	2.15	0.46
1:O:127:ARG:HA	1:O:130:LEU:HD21	1.97	0.46
1:T:144:LYS:HA	1:T:147:ILE:HG22	1.96	0.46
1:e:127:ARG:HA	1:e:130:LEU:HD21	1.97	0.46
1:f:89:GLU:O	1:f:93:GLN:N	2.38	0.46
1:n:169:GLU:OE1	1:n:169:GLU:N	2.46	0.46
1:r:53:THR:O	1:r:57:THR:HG23	2.15	0.46
1:u:127:ARG:HA	1:u:130:LEU:HD21	1.97	0.46
1:F:127:ARG:HA	1:F:130:LEU:HD21	1.97	0.45
1:W:144:LYS:HA	1:W:147:ILE:HG22	1.97	0.45
1:a:144:LYS:HA	1:a:147:ILE:HG22	1.97	0.45
1:i:127:ARG:HA	1:i:130:LEU:HD21	1.97	0.45
1:n:53:THR:O	1:n:57:THR:HG23	2.15	0.45
1:q:169:GLU:OE1	1:q:169:GLU:N	2.46	0.45
1:w:169:GLU:OE1	1:w:169:GLU:N	2.46	0.45
1:4:169:GLU:OE1	1:4:169:GLU:N	2.46	0.45
1:C:127:ARG:HA	1:C:130:LEU:HD21	1.97	0.45
1:R:127:ARG:HA	1:R:130:LEU:HD21	1.97	0.45
1:U:127:ARG:HA	1:U:130:LEU:HD21	1.97	0.45
1:e:144:LYS:HA	1:e:147:ILE:HG22	1.97	0.45
1:h:127:ARG:HA	1:h:130:LEU:HD21	1.97	0.45
1:k:144:LYS:HA	1:k:147:ILE:HG22	1.97	0.45
1:5:97:TYR:O	1:5:101:THR:N	2.38	0.45
1:7:127:ARG:HA	1:7:130:LEU:HD21	1.97	0.45
1:A:97:TYR:O	1:A:101:THR:N	2.38	0.45
1:f:127:ARG:HA	1:f:130:LEU:HD21	1.97	0.45
1:g:127:ARG:HA	1:g:130:LEU:HD21	1.97	0.45
1:s:144:LYS:HA	1:s:147:ILE:HG22	1.97	0.45
1:v:127:ARG:HA	1:v:130:LEU:HD21	1.97	0.45
1:0:97:TYR:O	1:0:101:THR:N	2.38	0.45
1:E:127:ARG:HA	1:E:130:LEU:HD21	1.97	0.45
1:I:144:LYS:HA	1:I:147:ILE:HG22	1.97	0.45
1:P:127:ARG:HA	1:P:130:LEU:HD21	1.97	0.45
1:Q:127:ARG:HA	1:Q:130:LEU:HD21	1.97	0.45
1:u:169:GLU:OE1	1:u:169:GLU:N	2.46	0.45
1:x:127:ARG:HA	1:x:130:LEU:HD21	1.97	0.45
1:y:69:GLN:O	1:y:73:GLU:N	2.38	0.45
1:D:89:GLU:O	1:D:93:GLN:N	2.38	0.45
1:E:89:GLU:O	1:E:93:GLN:N	2.38	0.45
1:K:169:GLU:OE1	1:K:169:GLU:N	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:w:127:ARG:HA	1:w:130:LEU:HD21	1.97	0.45
1:4:97:TYR:O	1:4:101:THR:N	2.38	0.45
1:F:69:GLN:O	1:F:73:GLU:N	2.38	0.45
1:H:89:GLU:O	1:H:93:GLN:N	2.38	0.45
1:H:169:GLU:OE1	1:H:169:GLU:N	2.46	0.45
1:X:69:GLN:O	1:X:73:GLU:N	2.38	0.45
1:j:69:GLN:O	1:j:73:GLU:N	2.38	0.45
1:M:89:GLU:O	1:M:93:GLN:N	2.38	0.45
1:O:97:TYR:O	1:O:101:THR:N	2.38	0.45
1:Y:169:GLU:OE1	1:Y:169:GLU:N	2.46	0.45
1:h:169:GLU:OE1	1:h:169:GLU:N	2.46	0.45
1:D:127:ARG:HA	1:D:130:LEU:HD21	1.97	0.45
1:e:69:GLN:O	1:e:73:GLU:N	2.38	0.45
1:k:97:TYR:O	1:k:101:THR:N	2.38	0.45
1:y:169:GLU:OE1	1:y:169:GLU:N	2.46	0.45
1:I:69:GLN:O	1:I:73:GLU:N	2.38	0.45
1:S:169:GLU:OE1	1:S:169:GLU:N	2.46	0.45
1:U:69:GLN:O	1:U:73:GLU:N	2.38	0.45
1:j:97:TYR:O	1:j:101:THR:N	2.38	0.45
1:r:97:TYR:O	1:r:101:THR:N	2.38	0.45
1:C:86:LEU:HD22	1:V:192:LEU:HD13	2.00	0.44
1:D:86:LEU:HD22	1:W:192:LEU:HD13	2.00	0.44
1:J:86:LEU:HD22	1:c:192:LEU:HD13	2.00	0.44
1:V:169:GLU:OE1	1:V:169:GLU:N	2.46	0.44
1:e:86:LEU:HD22	1:x:192:LEU:HD13	2.00	0.44
1:g:89:GLU:O	1:g:93:GLN:N	2.38	0.44
1:s:169:GLU:OE1	1:s:169:GLU:N	2.46	0.44
1:v:89:GLU:O	1:v:93:GLN:N	2.38	0.44
1:6:86:LEU:HD22	1:R:192:LEU:HD13	2.00	0.44
1:7:86:LEU:HD22	1:S:192:LEU:HD13	2.00	0.44
1:B:86:LEU:HD22	1:U:192:LEU:HD13	2.00	0.44
1:G:169:GLU:OE1	1:G:169:GLU:N	2.46	0.44
1:G:192:LEU:HD13	1:v:86:LEU:HD22	2.00	0.44
1:I:97:TYR:O	1:I:101:THR:N	2.38	0.44
1:J:169:GLU:OE1	1:J:169:GLU:N	2.46	0.44
1:K:86:LEU:HD22	1:d:192:LEU:HD13	2.00	0.44
1:P:86:LEU:HD22	1:i:192:LEU:HD13	2.00	0.44
1:a:86:LEU:HD22	1:t:192:LEU:HD13	2.00	0.44
1:b:169:GLU:OE1	1:b:169:GLU:N	2.46	0.44
1:j:89:GLU:O	1:j:93:GLN:N	2.38	0.44
1:0:86:LEU:HD22	1:L:192:LEU:HD13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:86:LEU:HD22	1:M:192:LEU:HD13	2.00	0.44
1:2:86:LEU:HD22	1:N:192:LEU:HD13	2.00	0.44
1:3:86:LEU:HD22	1:O:192:LEU:HD13	2.00	0.44
1:5:192:LEU:HD13	1:m:86:LEU:HD22	2.00	0.44
1:A:192:LEU:HD13	1:p:86:LEU:HD22	2.00	0.44
1:F:192:LEU:HD13	1:u:86:LEU:HD22	2.00	0.44
1:L:86:LEU:HD22	1:e:192:LEU:HD13	2.00	0.44
1:O:86:LEU:HD22	1:h:192:LEU:HD13	2.00	0.44
1:Q:86:LEU:HD22	1:j:192:LEU:HD13	2.00	0.44
1:R:69:GLN:O	1:R:73:GLU:N	2.38	0.44
1:Z:86:LEU:HD22	1:s:192:LEU:HD13	2.00	0.44
1:d:86:LEU:HD22	1:w:192:LEU:HD13	2.00	0.44
1:f:86:LEU:HD22	1:y:192:LEU:HD13	2.00	0.44
1:f:169:GLU:OE1	1:f:169:GLU:N	2.46	0.44
1:0:141:ALA:CB	1:z:50:THR:HG22	2.48	0.44
1:2:169:GLU:OE1	1:2:169:GLU:N	2.46	0.44
1:4:86:LEU:HD22	1:P:192:LEU:HD13	2.00	0.44
1:4:192:LEU:HD13	1:l:86:LEU:HD22	2.00	0.44
1:5:86:LEU:HD22	1:Q:192:LEU:HD13	2.00	0.44
1:6:192:LEU:HD13	1:n:86:LEU:HD22	2.00	0.44
1:B:192:LEU:HD13	1:q:86:LEU:HD22	2.00	0.44
1:C:192:LEU:HD13	1:r:86:LEU:HD22	2.00	0.44
1:E:86:LEU:HD22	1:X:192:LEU:HD13	2.00	0.44
1:E:192:LEU:HD13	1:t:86:LEU:HD22	2.00	0.44
1:I:86:LEU:HD22	1:b:192:LEU:HD13	2.00	0.44
1:M:86:LEU:HD22	1:f:192:LEU:HD13	2.00	0.44
1:U:50:THR:HG22	1:V:141:ALA:CB	2.48	0.44
1:Y:86:LEU:HD22	1:r:192:LEU:HD13	2.00	0.44
1:c:86:LEU:HD22	1:v:192:LEU:HD13	2.00	0.44
1:g:86:LEU:HD22	1:z:192:LEU:HD13	2.00	0.44
1:l:97:TYR:O	1:l:101:THR:N	2.38	0.44
1:o:97:TYR:O	1:o:101:THR:N	2.38	0.44
1:0:50:THR:HG22	1:1:141:ALA:CB	2.48	0.44
1:3:192:LEU:HD13	1:k:86:LEU:HD22	2.00	0.44
1:D:192:LEU:HD13	1:s:86:LEU:HD22	2.00	0.44
1:H:192:LEU:HD13	1:w:86:LEU:HD22	2.00	0.44
1:J:50:THR:HG22	1:K:141:ALA:CB	2.48	0.44
1:L:97:TYR:O	1:L:101:THR:N	2.38	0.44
1:M:97:TYR:O	1:M:101:THR:N	2.38	0.44
1:N:86:LEU:HD22	1:g:192:LEU:HD13	2.00	0.44
1:Q:50:THR:HG22	1:R:141:ALA:CB	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:50:THR:HG22	1:S:141:ALA:CB	2.48	0.44
1:R:86:LEU:HD22	1:k:192:LEU:HD13	2.00	0.44
1:b:86:LEU:HD22	1:u:192:LEU:HD13	2.00	0.44
1:h:50:THR:HG22	1:i:141:ALA:CB	2.48	0.44
1:i:50:THR:HG22	1:j:141:ALA:CB	2.48	0.44
1:j:50:THR:HG22	1:k:141:ALA:CB	2.48	0.44
1:O:192:LEU:HD13	1:h:86:LEU:HD22	2.00	0.44
1:1:50:THR:HG22	1:2:141:ALA:CB	2.48	0.44
1:6:56:SER:OG	1:6:60:GLN:OE1	2.17	0.44
1:C:50:THR:HG22	1:D:141:ALA:CB	2.48	0.44
1:D:50:THR:HG22	1:E:141:ALA:CB	2.48	0.44
1:E:97:TYR:O	1:E:101:THR:N	2.38	0.44
1:G:50:THR:HG22	1:H:141:ALA:CB	2.48	0.44
1:I:50:THR:HG22	1:J:141:ALA:CB	2.48	0.44
1:I:192:LEU:HD13	1:x:86:LEU:HD22	2.00	0.44
1:P:50:THR:HG22	1:Q:141:ALA:CB	2.48	0.44
1:S:86:LEU:HD22	1:l:192:LEU:HD13	2.00	0.44
1:V:50:THR:HG22	1:W:141:ALA:CB	2.48	0.44
1:X:86:LEU:HD22	1:q:192:LEU:HD13	2.00	0.44
1:h:89:GLU:O	1:h:93:GLN:N	2.38	0.44
1:6:50:THR:HG22	1:7:141:ALA:CB	2.48	0.44
1:B:50:THR:HG22	1:C:141:ALA:CB	2.48	0.44
1:F:50:THR:HG22	1:G:141:ALA:CB	2.48	0.44
1:J:192:LEU:HD13	1:y:86:LEU:HD22	2.00	0.44
1:K:50:THR:HG22	1:L:141:ALA:CB	2.48	0.44
1:S:50:THR:HG22	1:T:141:ALA:CB	2.48	0.44
1:g:50:THR:HG22	1:h:141:ALA:CB	2.48	0.44
1:s:89:GLU:O	1:s:93:GLN:N	2.38	0.44
1:y:50:THR:HG22	1:z:141:ALA:CB	2.48	0.44
1:F:86:LEU:HD22	1:Y:192:LEU:HD13	2.00	0.44
1:F:89:GLU:O	1:F:93:GLN:N	2.38	0.44
1:H:86:LEU:HD22	1:a:192:LEU:HD13	2.00	0.44
1:K:192:LEU:HD13	1:z:86:LEU:HD22	2.00	0.44
1:O:50:THR:HG22	1:P:141:ALA:CB	2.48	0.44
1:V:86:LEU:HD22	1:o:192:LEU:HD13	2.00	0.44
1:Y:97:TYR:O	1:Y:101:THR:N	2.38	0.44
1:d:97:TYR:O	1:d:101:THR:N	2.38	0.44
1:k:50:THR:HG22	1:l:141:ALA:CB	2.48	0.44
1:1:192:LEU:HD13	1:i:86:LEU:HD22	2.00	0.44
1:2:50:THR:HG22	1:3:141:ALA:CB	2.48	0.44
1:2:192:LEU:HD13	1:j:86:LEU:HD22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:97:TYR:O	1:3:101:THR:N	2.38	0.44
1:5:50:THR:HG22	1:6:141:ALA:CB	2.48	0.44
1:H:50:THR:HG22	1:I:141:ALA:CB	2.48	0.44
1:Q:97:TYR:O	1:Q:101:THR:N	2.38	0.44
1:T:86:LEU:HD22	1:m:192:LEU:HD13	2.00	0.44
1:d:169:GLU:OE1	1:d:169:GLU:N	2.46	0.44
1:g:69:GLN:O	1:g:73:GLU:N	2.38	0.44
1:x:97:TYR:O	1:x:101:THR:N	2.38	0.44
1:1:97:TYR:O	1:1:101:THR:N	2.38	0.43
1:3:50:THR:HG22	1:4:141:ALA:CB	2.48	0.43
1:E:50:THR:HG22	1:F:141:ALA:CB	2.48	0.43
1:G:86:LEU:HD22	1:Z:192:LEU:HD13	2.00	0.43
1:L:50:THR:HG22	1:M:141:ALA:CB	2.48	0.43
1:M:50:THR:HG22	1:N:141:ALA:CB	2.48	0.43
1:N:50:THR:HG22	1:O:141:ALA:CB	2.48	0.43
1:W:86:LEU:HD22	1:p:192:LEU:HD13	2.00	0.43
1:X:50:THR:HG22	1:Y:141:ALA:CB	2.48	0.43
1:Y:50:THR:HG22	1:Z:141:ALA:CB	2.48	0.43
1:Z:50:THR:HG22	1:a:141:ALA:CB	2.48	0.43
1:w:50:THR:HG22	1:x:141:ALA:CB	2.48	0.43
1:4:50:THR:HG22	1:5:141:ALA:CB	2.48	0.43
1:A:50:THR:HG22	1:B:141:ALA:CB	2.48	0.43
1:H:174:LYS:O	1:H:177:GLU:HG2	2.19	0.43
1:N:89:GLU:O	1:N:93:GLN:N	2.38	0.43
1:N:121:GLN:OE1	1:O:145:SER:OG	2.37	0.43
1:Q:169:GLU:OE1	1:Q:169:GLU:N	2.46	0.43
1:T:174:LYS:O	1:T:177:GLU:HG2	2.19	0.43
1:W:174:LYS:O	1:W:177:GLU:HG2	2.19	0.43
1:X:97:TYR:O	1:X:101:THR:N	2.38	0.43
1:Z:97:TYR:O	1:Z:101:THR:N	2.38	0.43
1:u:174:LYS:O	1:u:177:GLU:HG2	2.19	0.43
1:v:50:THR:HG22	1:w:141:ALA:CB	2.48	0.43
1:x:50:THR:HG22	1:y:141:ALA:CB	2.48	0.43
1:3:169:GLU:OE1	1:3:169:GLU:N	2.46	0.43
1:6:121:GLN:OE1	1:7:145:SER:OG	2.37	0.43
1:6:174:LYS:O	1:6:177:GLU:HG2	2.19	0.43
1:B:121:GLN:OE1	1:C:145:SER:OG	2.37	0.43
1:B:174:LYS:O	1:B:177:GLU:HG2	2.19	0.43
1:E:174:LYS:O	1:E:177:GLU:HG2	2.19	0.43
1:K:97:TYR:O	1:K:101:THR:N	2.38	0.43
1:W:50:THR:HG22	1:X:141:ALA:CB	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:50:THR:HG22	1:b:141:ALA:CB	2.48	0.43
1:a:97:TYR:O	1:a:101:THR:N	2.38	0.43
1:c:121:GLN:OE1	1:d:145:SER:OG	2.37	0.43
1:f:50:THR:HG22	1:g:141:ALA:CB	2.48	0.43
1:f:174:LYS:O	1:f:177:GLU:HG2	2.19	0.43
1:i:89:GLU:O	1:i:93:GLN:N	2.38	0.43
1:i:174:LYS:O	1:i:177:GLU:HG2	2.19	0.43
1:u:50:THR:HG22	1:v:141:ALA:CB	2.48	0.43
1:u:121:GLN:OE1	1:v:145:SER:OG	2.37	0.43
1:0:169:GLU:OE1	1:0:169:GLU:N	2.46	0.43
1:0:174:LYS:O	1:0:177:GLU:HG2	2.19	0.43
1:Q:174:LYS:O	1:Q:177:GLU:HG2	2.19	0.43
1:f:121:GLN:OE1	1:g:145:SER:OG	2.37	0.43
1:l:50:THR:HG22	1:m:141:ALA:CB	2.48	0.43
1:m:97:TYR:O	1:m:101:THR:N	2.38	0.43
1:o:50:THR:HG22	1:p:141:ALA:CB	2.48	0.43
1:t:50:THR:HG22	1:u:141:ALA:CB	2.48	0.43
1:x:174:LYS:O	1:x:177:GLU:HG2	2.19	0.43
1:3:121:GLN:OE1	1:4:145:SER:OG	2.37	0.43
1:G:89:GLU:O	1:G:93:GLN:N	2.38	0.43
1:M:169:GLU:OE1	1:M:169:GLU:N	2.46	0.43
1:N:174:LYS:O	1:N:177:GLU:HG2	2.19	0.43
1:Q:121:GLN:OE1	1:R:145:SER:OG	2.37	0.43
1:b:97:TYR:O	1:b:101:THR:N	2.38	0.43
1:e:50:THR:HG22	1:f:141:ALA:CB	2.48	0.43
1:f:97:TYR:O	1:f:101:THR:N	2.38	0.43
1:h:174:LYS:O	1:h:177:GLU:HG2	2.19	0.43
1:i:97:TYR:O	1:i:101:THR:N	2.38	0.43
1:j:169:GLU:OE1	1:j:169:GLU:N	2.46	0.43
1:p:97:TYR:O	1:p:101:THR:N	2.38	0.43
1:r:121:GLN:OE1	1:s:145:SER:OG	2.37	0.43
1:t:69:GLN:O	1:t:73:GLU:N	2.38	0.43
1:t:89:GLU:O	1:t:93:GLN:N	2.38	0.43
1:K:89:GLU:O	1:K:93:GLN:N	2.38	0.43
1:Y:174:LYS:O	1:Y:177:GLU:HG2	2.19	0.43
1:b:50:THR:HG22	1:c:141:ALA:CB	2.48	0.43
1:k:174:LYS:O	1:k:177:GLU:HG2	2.19	0.43
1:m:50:THR:HG22	1:n:141:ALA:CB	2.48	0.43
1:o:174:LYS:O	1:o:177:GLU:HG2	2.19	0.43
1:p:50:THR:HG22	1:q:141:ALA:CB	2.48	0.43
1:s:50:THR:HG22	1:t:141:ALA:CB	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:w:174:LYS:O	1:w:177:GLU:HG2	2.19	0.43
1:D:174:LYS:O	1:D:177:GLU:HG2	2.19	0.43
1:E:121:GLN:OE1	1:F:145:SER:OG	2.37	0.43
1:J:174:LYS:O	1:J:177:GLU:HG2	2.19	0.43
1:P:174:LYS:O	1:P:177:GLU:HG2	2.19	0.43
1:S:174:LYS:O	1:S:177:GLU:HG2	2.19	0.43
1:V:174:LYS:O	1:V:177:GLU:HG2	2.19	0.43
1:c:50:THR:HG22	1:d:141:ALA:CB	2.48	0.43
1:d:50:THR:HG22	1:e:141:ALA:CB	2.48	0.43
1:l:174:LYS:O	1:l:177:GLU:HG2	2.19	0.43
1:z:174:LYS:O	1:z:177:GLU:HG2	2.19	0.43
1:2:174:LYS:O	1:2:177:GLU:HG2	2.19	0.43
1:A:121:GLN:OE1	1:B:145:SER:OG	2.37	0.43
1:D:121:GLN:OE1	1:E:145:SER:OG	2.37	0.43
1:G:174:LYS:O	1:G:177:GLU:HG2	2.19	0.43
1:P:121:GLN:OE1	1:Q:145:SER:OG	2.37	0.43
1:e:121:GLN:OE1	1:f:145:SER:OG	2.37	0.43
1:e:174:LYS:O	1:e:177:GLU:HG2	2.19	0.43
1:r:50:THR:HG22	1:s:141:ALA:CB	2.48	0.43
1:t:121:GLN:OE1	1:u:145:SER:OG	2.37	0.43
1:0:58:GLU:HA	1:0:108:LEU:HD11	2.01	0.43
1:4:174:LYS:O	1:4:177:GLU:HG2	2.19	0.43
1:I:58:GLU:HA	1:I:108:LEU:HD11	2.01	0.43
1:J:97:TYR:O	1:J:101:THR:N	2.38	0.43
1:K:121:GLN:OE1	1:L:145:SER:OG	2.37	0.43
1:L:174:LYS:O	1:L:177:GLU:HG2	2.19	0.43
1:O:169:GLU:OE1	1:O:169:GLU:N	2.46	0.43
1:k:58:GLU:HA	1:k:108:LEU:HD11	2.01	0.43
1:q:50:THR:HG22	1:r:141:ALA:CB	2.48	0.43
1:s:174:LYS:O	1:s:177:GLU:HG2	2.19	0.43
1:v:69:GLN:O	1:v:73:GLU:N	2.38	0.43
1:1:58:GLU:HA	1:1:108:LEU:HD11	2.01	0.43
1:3:174:LYS:O	1:3:177:GLU:HG2	2.19	0.43
1:4:121:GLN:OE1	1:5:145:SER:OG	2.37	0.43
1:5:121:GLN:OE1	1:6:145:SER:OG	2.37	0.43
1:H:58:GLU:HA	1:H:108:LEU:HD11	2.01	0.43
1:M:121:GLN:OE1	1:N:145:SER:OG	2.37	0.43
1:O:121:GLN:OE1	1:P:145:SER:OG	2.37	0.43
1:O:174:LYS:O	1:O:177:GLU:HG2	2.19	0.43
1:X:58:GLU:HA	1:X:108:LEU:HD11	2.01	0.43
1:Y:58:GLU:HA	1:Y:108:LEU:HD11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:121:GLN:OE1	1:c:145:SER:OG	2.37	0.43
1:c:174:LYS:O	1:c:177:GLU:HG2	2.19	0.43
1:d:121:GLN:OE1	1:e:145:SER:OG	2.37	0.43
1:d:174:LYS:O	1:d:177:GLU:HG2	2.19	0.43
1:l:58:GLU:HA	1:l:108:LEU:HD11	2.01	0.43
1:s:121:GLN:OE1	1:t:145:SER:OG	2.37	0.43
1:x:121:GLN:OE1	1:y:145:SER:OG	2.37	0.43
1:z:58:GLU:HA	1:z:108:LEU:HD11	2.01	0.43
1:C:121:GLN:OE1	1:D:145:SER:OG	2.37	0.42
1:E:169:GLU:OE1	1:E:169:GLU:N	2.46	0.42
1:J:58:GLU:HA	1:J:108:LEU:HD11	2.01	0.42
1:L:121:GLN:OE1	1:M:145:SER:OG	2.37	0.42
1:O:89:GLU:O	1:O:93:GLN:N	2.38	0.42
1:T:58:GLU:HA	1:T:108:LEU:HD11	2.01	0.42
1:W:58:GLU:HA	1:W:108:LEU:HD11	2.01	0.42
1:j:58:GLU:HA	1:j:108:LEU:HD11	2.01	0.42
1:j:174:LYS:O	1:j:177:GLU:HG2	2.19	0.42
1:o:58:GLU:HA	1:o:108:LEU:HD11	2.01	0.42
1:q:97:TYR:O	1:q:101:THR:N	2.38	0.42
1:s:97:TYR:O	1:s:101:THR:N	2.38	0.42
1:w:121:GLN:OE1	1:x:145:SER:OG	2.37	0.42
1:2:58:GLU:HA	1:2:108:LEU:HD11	2.01	0.42
1:2:97:TYR:O	1:2:101:THR:N	2.38	0.42
1:7:174:LYS:O	1:7:177:GLU:HG2	2.19	0.42
1:C:174:LYS:O	1:C:177:GLU:HG2	2.19	0.42
1:F:174:LYS:O	1:F:177:GLU:HG2	2.19	0.42
1:G:58:GLU:HA	1:G:108:LEU:HD11	2.01	0.42
1:X:174:LYS:O	1:X:177:GLU:HG2	2.19	0.42
1:Z:58:GLU:HA	1:Z:108:LEU:HD11	2.01	0.42
1:Z:174:LYS:O	1:Z:177:GLU:HG2	2.19	0.42
1:a:174:LYS:O	1:a:177:GLU:HG2	2.19	0.42
1:m:58:GLU:HA	1:m:108:LEU:HD11	2.01	0.42
1:n:97:TYR:O	1:n:101:THR:N	2.38	0.42
1:n:174:LYS:O	1:n:177:GLU:HG2	2.19	0.42
1:p:58:GLU:HA	1:p:108:LEU:HD11	2.01	0.42
1:q:121:GLN:OE1	1:r:145:SER:OG	2.37	0.42
1:q:174:LYS:O	1:q:177:GLU:HG2	2.19	0.42
1:t:174:LYS:O	1:t:177:GLU:HG2	2.19	0.42
1:v:121:GLN:OE1	1:w:145:SER:OG	2.37	0.42
1:v:174:LYS:O	1:v:177:GLU:HG2	2.19	0.42
1:y:174:LYS:O	1:y:177:GLU:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:GLN:O	1:A:73:GLU:N	2.38	0.42
1:K:58:GLU:HA	1:K:108:LEU:HD11	2.01	0.42
1:R:174:LYS:O	1:R:177:GLU:HG2	2.19	0.42
1:U:174:LYS:O	1:U:177:GLU:HG2	2.19	0.42
1:W:97:TYR:O	1:W:101:THR:N	2.38	0.42
1:Z:121:GLN:OE1	1:a:145:SER:OG	2.37	0.42
1:a:121:GLN:OE1	1:b:145:SER:OG	2.37	0.42
1:g:174:LYS:O	1:g:177:GLU:HG2	2.19	0.42
1:h:121:GLN:OE1	1:i:145:SER:OG	2.37	0.42
1:i:58:GLU:HA	1:i:108:LEU:HD11	2.01	0.42
1:p:89:GLU:O	1:p:93:GLN:N	2.38	0.42
1:r:174:LYS:O	1:r:177:GLU:HG2	2.19	0.42
1:u:97:TYR:O	1:u:101:THR:N	2.38	0.42
1:y:58:GLU:HA	1:y:108:LEU:HD11	2.01	0.42
1:l:174:LYS:O	1:l:177:GLU:HG2	2.19	0.42
1:A:174:LYS:O	1:A:177:GLU:HG2	2.19	0.42
1:D:69:GLN:O	1:D:73:GLU:N	2.38	0.42
1:P:69:GLN:O	1:P:73:GLU:N	2.38	0.42
1:S:58:GLU:HA	1:S:108:LEU:HD11	2.01	0.42
1:T:97:TYR:O	1:T:101:THR:N	2.38	0.42
1:V:58:GLU:HA	1:V:108:LEU:HD11	2.01	0.42
1:a:58:GLU:HA	1:a:108:LEU:HD11	2.01	0.42
1:a:89:GLU:O	1:a:93:GLN:N	2.38	0.42
1:g:121:GLN:OE1	1:h:145:SER:OG	2.37	0.42
1:n:58:GLU:HA	1:n:108:LEU:HD11	2.01	0.42
1:p:174:LYS:O	1:p:177:GLU:HG2	2.19	0.42
1:3:58:GLU:HA	1:3:108:LEU:HD11	2.01	0.42
1:5:174:LYS:O	1:5:177:GLU:HG2	2.19	0.42
1:K:174:LYS:O	1:K:177:GLU:HG2	2.19	0.42
1:b:174:LYS:O	1:b:177:GLU:HG2	2.19	0.42
1:i:121:GLN:OE1	1:j:145:SER:OG	2.37	0.42
1:m:89:GLU:O	1:m:93:GLN:N	2.38	0.42
1:m:174:LYS:O	1:m:177:GLU:HG2	2.19	0.42
1:o:121:GLN:OE1	1:p:145:SER:OG	2.37	0.42
1:q:58:GLU:HA	1:q:108:LEU:HD11	2.01	0.42
1:u:89:GLU:O	1:u:93:GLN:N	2.38	0.42
1:x:58:GLU:HA	1:x:108:LEU:HD11	2.01	0.42
1:2:121:GLN:OE1	1:3:145:SER:OG	2.37	0.42
1:5:69:GLN:O	1:5:73:GLU:N	2.38	0.42
1:F:58:GLU:HA	1:F:108:LEU:HD11	2.01	0.42
1:L:58:GLU:HA	1:L:108:LEU:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:121:GLN:OE1	1:S:145:SER:OG	2.37	0.42
1:U:121:GLN:OE1	1:V:145:SER:OG	2.37	0.42
1:V:121:GLN:OE1	1:W:145:SER:OG	2.37	0.42
1:W:121:GLN:OE1	1:X:145:SER:OG	2.37	0.42
1:h:58:GLU:HA	1:h:108:LEU:HD11	2.01	0.42
1:l:121:GLN:OE1	1:m:145:SER:OG	2.37	0.42
1:m:121:GLN:OE1	1:n:145:SER:OG	2.37	0.42
1:w:69:GLN:O	1:w:73:GLU:N	2.38	0.42
1:0:121:GLN:OE1	1:1:145:SER:OG	2.37	0.42
1:D:189:PRO:HA	1:D:193:ASP:OD2	2.20	0.42
1:E:189:PRO:HA	1:E:193:ASP:OD2	2.20	0.42
1:H:121:GLN:OE1	1:I:145:SER:OG	2.37	0.42
1:I:174:LYS:O	1:I:177:GLU:HG2	2.19	0.42
1:P:189:PRO:HA	1:P:193:ASP:OD2	2.20	0.42
1:R:58:GLU:HA	1:R:108:LEU:HD11	2.01	0.42
1:S:121:GLN:OE1	1:T:145:SER:OG	2.37	0.42
1:U:58:GLU:HA	1:U:108:LEU:HD11	2.01	0.42
1:a:150:GLN:O	1:a:154:GLU:N	2.44	0.42
1:g:189:PRO:HA	1:g:193:ASP:OD2	2.20	0.42
1:h:189:PRO:HA	1:h:193:ASP:OD2	2.20	0.42
1:k:121:GLN:OE1	1:l:145:SER:OG	2.37	0.42
1:p:121:GLN:OE1	1:q:145:SER:OG	2.37	0.42
1:u:189:PRO:HA	1:u:193:ASP:OD2	2.20	0.42
1:0:145:SER:OG	1:z:121:GLN:OE1	2.37	0.42
1:4:58:GLU:HA	1:4:108:LEU:HD11	2.01	0.42
1:E:58:GLU:HA	1:E:108:LEU:HD11	2.01	0.42
1:M:69:GLN:O	1:M:73:GLU:N	2.38	0.42
1:M:174:LYS:O	1:M:177:GLU:HG2	2.19	0.42
1:S:189:PRO:HA	1:S:193:ASP:OD2	2.20	0.42
1:V:69:GLN:O	1:V:73:GLU:N	2.38	0.42
1:V:189:PRO:HA	1:V:193:ASP:OD2	2.20	0.42
1:X:121:GLN:OE1	1:Y:145:SER:OG	2.37	0.42
1:b:58:GLU:HA	1:b:108:LEU:HD11	2.01	0.42
1:e:189:PRO:HA	1:e:193:ASP:OD2	2.20	0.42
1:j:121:GLN:OE1	1:k:145:SER:OG	2.37	0.42
1:w:189:PRO:HA	1:w:193:ASP:OD2	2.20	0.42
1:5:189:PRO:HA	1:5:193:ASP:OD2	2.20	0.42
1:7:169:GLU:OE1	1:7:169:GLU:N	2.46	0.42
1:A:189:PRO:HA	1:A:193:ASP:OD2	2.20	0.42
1:G:69:GLN:O	1:G:73:GLU:N	2.38	0.42
1:I:121:GLN:OE1	1:J:145:SER:OG	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:58:GLU:HA	1:M:108:LEU:HD11	2.01	0.42
1:O:189:PRO:HA	1:O:193:ASP:OD2	2.20	0.42
1:Y:121:GLN:OE1	1:Z:145:SER:OG	2.37	0.42
1:b:69:GLN:O	1:b:73:GLU:N	2.38	0.42
1:m:150:GLN:O	1:m:154:GLU:N	2.44	0.42
1:p:150:GLN:O	1:p:154:GLU:N	2.44	0.42
1:q:69:GLN:O	1:q:73:GLU:N	2.38	0.42
1:r:58:GLU:HA	1:r:108:LEU:HD11	2.01	0.42
1:w:58:GLU:HA	1:w:108:LEU:HD11	2.01	0.42
1:y:189:PRO:HA	1:y:193:ASP:OD2	2.20	0.42
1:1:121:GLN:OE1	1:2:145:SER:OG	2.37	0.42
1:5:169:GLU:OE1	1:5:169:GLU:N	2.46	0.42
1:F:121:GLN:OE1	1:G:145:SER:OG	2.37	0.42
1:G:121:GLN:OE1	1:H:145:SER:OG	2.37	0.42
1:J:121:GLN:OE1	1:K:145:SER:OG	2.37	0.42
1:L:150:GLN:O	1:L:154:GLU:N	2.44	0.42
1:Q:58:GLU:HA	1:Q:108:LEU:HD11	2.01	0.42
1:Q:89:GLU:O	1:Q:93:GLN:N	2.38	0.42
1:S:69:GLN:O	1:S:73:GLU:N	2.38	0.42
1:S:141:ALA:O	1:S:145:SER:N	2.52	0.42
1:V:141:ALA:O	1:V:145:SER:N	2.52	0.42
1:Y:69:GLN:O	1:Y:73:GLU:N	2.38	0.42
1:c:58:GLU:HA	1:c:108:LEU:HD11	2.01	0.42
1:c:189:PRO:HA	1:c:193:ASP:OD2	2.20	0.42
1:d:189:PRO:HA	1:d:193:ASP:OD2	2.20	0.42
1:g:58:GLU:HA	1:g:108:LEU:HD11	2.01	0.42
1:h:69:GLN:O	1:h:73:GLU:N	2.38	0.42
1:h:141:ALA:O	1:h:145:SER:N	2.52	0.42
1:t:189:PRO:HA	1:t:193:ASP:OD2	2.20	0.42
1:x:189:PRO:HA	1:x:193:ASP:OD2	2.20	0.42
1:y:121:GLN:OE1	1:z:145:SER:OG	2.37	0.42
1:z:69:GLN:O	1:z:73:GLU:N	2.38	0.42
1:2:69:GLN:O	1:2:73:GLU:N	2.38	0.41
1:5:58:GLU:HA	1:5:108:LEU:HD11	2.01	0.41
1:A:58:GLU:HA	1:A:108:LEU:HD11	2.01	0.41
1:C:69:GLN:O	1:C:73:GLU:N	2.38	0.41
1:C:169:GLU:OE1	1:C:169:GLU:N	2.46	0.41
1:D:58:GLU:HA	1:D:108:LEU:HD11	2.01	0.41
1:E:141:ALA:O	1:E:145:SER:N	2.52	0.41
1:J:69:GLN:O	1:J:73:GLU:N	2.38	0.41
1:T:189:PRO:HA	1:T:193:ASP:OD2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:189:PRO:HA	1:W:193:ASP:OD2	2.20	0.41
1:f:58:GLU:HA	1:f:108:LEU:HD11	2.01	0.41
1:s:58:GLU:HA	1:s:108:LEU:HD11	2.01	0.41
1:v:58:GLU:HA	1:v:108:LEU:HD11	2.01	0.41
1:v:189:PRO:HA	1:v:193:ASP:OD2	2.20	0.41
1:w:141:ALA:O	1:w:145:SER:N	2.52	0.41
1:x:141:ALA:O	1:x:145:SER:N	2.52	0.41
1:2:150:GLN:O	1:2:154:GLU:N	2.44	0.41
1:6:58:GLU:HA	1:6:108:LEU:HD11	2.01	0.41
1:7:58:GLU:HA	1:7:108:LEU:HD11	2.01	0.41
1:A:169:GLU:OE1	1:A:169:GLU:N	2.46	0.41
1:C:58:GLU:HA	1:C:108:LEU:HD11	2.01	0.41
1:G:141:ALA:O	1:G:145:SER:N	2.52	0.41
1:G:189:PRO:HA	1:G:193:ASP:OD2	2.20	0.41
1:H:189:PRO:HA	1:H:193:ASP:OD2	2.20	0.41
1:N:58:GLU:HA	1:N:108:LEU:HD11	2.01	0.41
1:P:58:GLU:HA	1:P:108:LEU:HD11	2.01	0.41
1:d:58:GLU:HA	1:d:108:LEU:HD11	2.01	0.41
1:e:58:GLU:HA	1:e:108:LEU:HD11	2.01	0.41
1:i:141:ALA:O	1:i:145:SER:N	2.52	0.41
1:k:69:GLN:O	1:k:73:GLU:N	2.38	0.41
1:n:69:GLN:O	1:n:73:GLU:N	2.38	0.41
1:t:58:GLU:HA	1:t:108:LEU:HD11	2.01	0.41
1:u:58:GLU:HA	1:u:108:LEU:HD11	2.01	0.41
1:3:150:GLN:O	1:3:154:GLU:N	2.44	0.41
1:6:189:PRO:HA	1:6:193:ASP:OD2	2.20	0.41
1:B:58:GLU:HA	1:B:108:LEU:HD11	2.01	0.41
1:B:97:TYR:O	1:B:101:THR:N	2.38	0.41
1:B:189:PRO:HA	1:B:193:ASP:OD2	2.20	0.41
1:F:189:PRO:HA	1:F:193:ASP:OD2	2.20	0.41
1:O:58:GLU:HA	1:O:108:LEU:HD11	2.01	0.41
1:Q:141:ALA:O	1:Q:145:SER:N	2.52	0.41
1:f:189:PRO:HA	1:f:193:ASP:OD2	2.20	0.41
1:j:189:PRO:HA	1:j:193:ASP:OD2	2.20	0.41
1:k:189:PRO:HA	1:k:193:ASP:OD2	2.20	0.41
1:l:169:GLU:OE1	1:l:169:GLU:N	2.46	0.41
1:7:69:GLN:O	1:7:73:GLU:N	2.38	0.41
1:J:89:GLU:O	1:J:93:GLN:N	2.38	0.41
1:K:150:GLN:O	1:K:154:GLU:N	2.44	0.41
1:L:189:PRO:HA	1:L:193:ASP:OD2	2.20	0.41
1:Q:189:PRO:HA	1:Q:193:ASP:OD2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:189:PRO:HA	1:R:193:ASP:OD2	2.20	0.41
1:U:189:PRO:HA	1:U:193:ASP:OD2	2.20	0.41
1:r:189:PRO:HA	1:r:193:ASP:OD2	2.20	0.41
1:z:189:PRO:HA	1:z:193:ASP:OD2	2.20	0.41
1:4:67:ILE:HG13	1:4:70:ARG:NH2	2.36	0.41
1:4:189:PRO:HA	1:4:193:ASP:OD2	2.20	0.41
1:6:97:TYR:O	1:6:101:THR:N	2.38	0.41
1:7:189:PRO:HA	1:7:193:ASP:OD2	2.20	0.41
1:D:141:ALA:O	1:D:145:SER:N	2.52	0.41
1:H:183:GLU:HA	1:H:186:ASN:HB3	2.03	0.41
1:I:189:PRO:HA	1:I:193:ASP:OD2	2.20	0.41
1:M:189:PRO:HA	1:M:193:ASP:OD2	2.20	0.41
1:T:67:ILE:HG13	1:T:70:ARG:NH2	2.36	0.41
1:T:141:ALA:O	1:T:145:SER:N	2.52	0.41
1:W:67:ILE:HG13	1:W:70:ARG:NH2	2.36	0.41
1:W:141:ALA:O	1:W:145:SER:N	2.52	0.41
1:Z:189:PRO:HA	1:Z:193:ASP:OD2	2.20	0.41
1:n:150:GLN:O	1:n:154:GLU:N	2.44	0.41
1:n:189:PRO:HA	1:n:193:ASP:OD2	2.20	0.41
1:o:169:GLU:OE1	1:o:169:GLU:N	2.46	0.41
1:q:150:GLN:O	1:q:154:GLU:N	2.44	0.41
1:t:67:ILE:HG13	1:t:70:ARG:NH2	2.36	0.41
1:u:67:ILE:HG13	1:u:70:ARG:NH2	2.36	0.41
1:1:150:GLN:O	1:1:154:GLU:N	2.44	0.41
1:3:67:ILE:HG13	1:3:70:ARG:NH2	2.36	0.41
1:7:183:GLU:HA	1:7:186:ASN:HB3	2.03	0.41
1:C:183:GLU:HA	1:C:186:ASN:HB3	2.03	0.41
1:C:189:PRO:HA	1:C:193:ASP:OD2	2.20	0.41
1:E:91:LEU:O	1:E:95:GLN:NE2	2.53	0.41
1:F:67:ILE:HG13	1:F:70:ARG:NH2	2.36	0.41
1:G:67:ILE:HG13	1:G:70:ARG:NH2	2.36	0.41
1:J:150:GLN:O	1:J:154:GLU:N	2.44	0.41
1:R:183:GLU:HA	1:R:186:ASN:HB3	2.03	0.41
1:S:183:GLU:HA	1:S:186:ASN:HB3	2.03	0.41
1:U:183:GLU:HA	1:U:186:ASN:HB3	2.03	0.41
1:X:169:GLU:OE1	1:X:169:GLU:N	2.46	0.41
1:f:183:GLU:HA	1:f:186:ASN:HB3	2.03	0.41
1:j:183:GLU:HA	1:j:186:ASN:HB3	2.03	0.41
1:k:67:ILE:HG13	1:k:70:ARG:NH2	2.36	0.41
1:k:183:GLU:HA	1:k:186:ASN:HB3	2.03	0.41
1:n:67:ILE:HG13	1:n:70:ARG:NH2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:r:67:ILE:HG13	1:r:70:ARG:NH2	2.36	0.41
1:s:67:ILE:HG13	1:s:70:ARG:NH2	2.36	0.41
1:v:67:ILE:HG13	1:v:70:ARG:NH2	2.36	0.41
1:v:175:ILE:HG13	1:v:176:LEU:N	2.36	0.41
1:x:175:ILE:HG13	1:x:176:LEU:N	2.36	0.41
1:x:183:GLU:HA	1:x:186:ASN:HB3	2.03	0.41
1:z:141:ALA:O	1:z:145:SER:N	2.52	0.41
1:0:175:ILE:HG13	1:0:176:LEU:N	2.36	0.41
1:1:189:PRO:HA	1:1:193:ASP:OD2	2.20	0.41
1:2:67:ILE:HG13	1:2:70:ARG:NH2	2.36	0.41
1:4:150:GLN:O	1:4:154:GLU:N	2.44	0.41
1:5:67:ILE:HG13	1:5:70:ARG:NH2	2.36	0.41
1:D:183:GLU:HA	1:D:186:ASN:HB3	2.03	0.41
1:I:183:GLU:HA	1:I:186:ASN:HB3	2.03	0.41
1:J:175:ILE:HG13	1:J:176:LEU:N	2.36	0.41
1:N:189:PRO:HA	1:N:193:ASP:OD2	2.20	0.41
1:S:175:ILE:HG13	1:S:176:LEU:N	2.36	0.41
1:T:175:ILE:HG13	1:T:176:LEU:N	2.36	0.41
1:V:67:ILE:HG13	1:V:70:ARG:NH2	2.36	0.41
1:V:175:ILE:HG13	1:V:176:LEU:N	2.36	0.41
1:W:175:ILE:HG13	1:W:176:LEU:N	2.36	0.41
1:X:67:ILE:HG13	1:X:70:ARG:NH2	2.36	0.41
1:Y:175:ILE:HG13	1:Y:176:LEU:N	2.36	0.41
1:f:141:ALA:O	1:f:145:SER:N	2.52	0.41
1:k:89:GLU:O	1:k:93:GLN:N	2.38	0.41
1:o:67:ILE:HG13	1:o:70:ARG:NH2	2.36	0.41
1:q:67:ILE:HG13	1:q:70:ARG:NH2	2.36	0.41
1:q:189:PRO:HA	1:q:193:ASP:OD2	2.20	0.41
1:r:150:GLN:O	1:r:154:GLU:N	2.44	0.41
1:t:183:GLU:HA	1:t:186:ASN:HB3	2.03	0.41
1:y:175:ILE:HG13	1:y:176:LEU:N	2.36	0.41
1:z:175:ILE:HG13	1:z:176:LEU:N	2.36	0.41
1:A:67:ILE:HG13	1:A:70:ARG:NH2	2.36	0.41
1:C:67:ILE:HG13	1:C:70:ARG:NH2	2.36	0.41
1:E:67:ILE:HG13	1:E:70:ARG:NH2	2.36	0.41
1:N:183:GLU:HA	1:N:186:ASN:HB3	2.03	0.41
1:P:175:ILE:HG13	1:P:176:LEU:N	2.36	0.41
1:R:175:ILE:HG13	1:R:176:LEU:N	2.36	0.41
1:S:67:ILE:HG13	1:S:70:ARG:NH2	2.36	0.41
1:U:79:LEU:C	1:U:79:LEU:HD23	2.46	0.41
1:U:175:ILE:HG13	1:U:176:LEU:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:183:GLU:HA	1:V:186:ASN:HB3	2.03	0.41
1:e:175:ILE:HG13	1:e:176:LEU:N	2.36	0.41
1:e:183:GLU:HA	1:e:186:ASN:HB3	2.03	0.41
1:i:189:PRO:HA	1:i:193:ASP:OD2	2.20	0.41
1:j:67:ILE:HG13	1:j:70:ARG:NH2	2.36	0.41
1:l:67:ILE:HG13	1:l:70:ARG:NH2	2.36	0.41
1:m:67:ILE:HG13	1:m:70:ARG:NH2	2.36	0.41
1:n:91:LEU:O	1:n:95:GLN:NE2	2.53	0.41
1:p:67:ILE:HG13	1:p:70:ARG:NH2	2.36	0.41
1:q:91:LEU:O	1:q:95:GLN:NE2	2.53	0.41
1:w:67:ILE:HG13	1:w:70:ARG:NH2	2.36	0.41
1:y:183:GLU:HA	1:y:186:ASN:HB3	2.03	0.41
1:0:79:LEU:C	1:0:79:LEU:HD23	2.46	0.41
1:1:67:ILE:HG13	1:1:70:ARG:NH2	2.36	0.41
1:2:175:ILE:HG13	1:2:176:LEU:N	2.36	0.41
1:2:183:GLU:HA	1:2:186:ASN:HB3	2.03	0.41
1:2:189:PRO:HA	1:2:193:ASP:OD2	2.20	0.41
1:4:91:LEU:O	1:4:95:GLN:NE2	2.53	0.41
1:6:67:ILE:HG13	1:6:70:ARG:NH2	2.36	0.41
1:6:79:LEU:HD23	1:6:79:LEU:C	2.46	0.41
1:7:67:ILE:HG13	1:7:70:ARG:NH2	2.36	0.41
1:7:175:ILE:HG13	1:7:176:LEU:N	2.36	0.41
1:B:67:ILE:HG13	1:B:70:ARG:NH2	2.36	0.41
1:B:79:LEU:HD23	1:B:79:LEU:C	2.46	0.41
1:C:175:ILE:HG13	1:C:176:LEU:N	2.36	0.41
1:D:67:ILE:HG13	1:D:70:ARG:NH2	2.36	0.41
1:D:79:LEU:C	1:D:79:LEU:HD23	2.46	0.41
1:E:175:ILE:HG13	1:E:176:LEU:N	2.36	0.41
1:F:141:ALA:O	1:F:145:SER:N	2.52	0.41
1:G:183:GLU:HA	1:G:186:ASN:HB3	2.03	0.41
1:H:67:ILE:HG13	1:H:70:ARG:NH2	2.36	0.41
1:H:175:ILE:HG13	1:H:176:LEU:N	2.36	0.41
1:J:79:LEU:C	1:J:79:LEU:HD23	2.46	0.41
1:K:79:LEU:C	1:K:79:LEU:HD23	2.46	0.41
1:L:175:ILE:HG13	1:L:176:LEU:N	2.36	0.41
1:M:79:LEU:HD23	1:M:79:LEU:C	2.46	0.41
1:M:183:GLU:HA	1:M:186:ASN:HB3	2.03	0.41
1:N:91:LEU:O	1:N:95:GLN:NE2	2.53	0.41
1:N:175:ILE:HG13	1:N:176:LEU:N	2.36	0.41
1:O:183:GLU:HA	1:O:186:ASN:HB3	2.03	0.41
1:P:79:LEU:HD23	1:P:79:LEU:C	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:141:ALA:O	1:P:145:SER:N	2.52	0.41
1:R:79:LEU:C	1:R:79:LEU:HD23	2.46	0.41
1:S:79:LEU:C	1:S:79:LEU:HD23	2.46	0.41
1:S:91:LEU:O	1:S:95:GLN:NE2	2.53	0.41
1:U:141:ALA:O	1:U:145:SER:N	2.52	0.41
1:V:79:LEU:C	1:V:79:LEU:HD23	2.46	0.41
1:V:91:LEU:O	1:V:95:GLN:NE2	2.53	0.41
1:X:91:LEU:O	1:X:95:GLN:NE2	2.53	0.41
1:X:175:ILE:HG13	1:X:176:LEU:N	2.36	0.41
1:Y:67:ILE:HG13	1:Y:70:ARG:NH2	2.36	0.41
1:Y:189:PRO:HA	1:Y:193:ASP:OD2	2.20	0.41
1:Z:150:GLN:O	1:Z:154:GLU:N	2.44	0.41
1:Z:183:GLU:HA	1:Z:186:ASN:HB3	2.03	0.41
1:a:175:ILE:HG13	1:a:176:LEU:N	2.36	0.41
1:b:189:PRO:HA	1:b:193:ASP:OD2	2.20	0.41
1:c:89:GLU:O	1:c:93:GLN:N	2.38	0.41
1:c:175:ILE:HG13	1:c:176:LEU:N	2.36	0.41
1:d:79:LEU:HD23	1:d:79:LEU:C	2.46	0.41
1:e:67:ILE:HG13	1:e:70:ARG:NH2	2.36	0.41
1:e:79:LEU:HD23	1:e:79:LEU:C	2.46	0.41
1:e:91:LEU:O	1:e:95:GLN:NE2	2.53	0.41
1:g:175:ILE:HG13	1:g:176:LEU:N	2.36	0.41
1:g:183:GLU:HA	1:g:186:ASN:HB3	2.03	0.41
1:j:175:ILE:HG13	1:j:176:LEU:N	2.36	0.41
1:m:175:ILE:HG13	1:m:176:LEU:N	2.36	0.41
1:p:175:ILE:HG13	1:p:176:LEU:N	2.36	0.41
1:r:79:LEU:C	1:r:79:LEU:HD23	2.46	0.41
1:s:79:LEU:HD23	1:s:79:LEU:C	2.46	0.41
1:s:183:GLU:HA	1:s:186:ASN:HB3	2.03	0.41
1:t:175:ILE:HG13	1:t:176:LEU:N	2.36	0.41
1:v:79:LEU:HD23	1:v:79:LEU:C	2.46	0.41
1:w:175:ILE:HG13	1:w:176:LEU:N	2.36	0.41
1:w:183:GLU:HA	1:w:186:ASN:HB3	2.03	0.41
1:x:67:ILE:HG13	1:x:70:ARG:NH2	2.36	0.41
1:0:67:ILE:HG13	1:0:70:ARG:NH2	2.36	0.41
1:1:79:LEU:C	1:1:79:LEU:HD23	2.46	0.41
1:1:183:GLU:HA	1:1:186:ASN:HB3	2.03	0.41
1:5:79:LEU:HD23	1:5:79:LEU:C	2.46	0.41
1:6:175:ILE:HG13	1:6:176:LEU:N	2.36	0.41
1:H:141:ALA:O	1:H:145:SER:N	2.52	0.41
1:K:189:PRO:HA	1:K:193:ASP:OD2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:79:LEU:HD23	1:Q:79:LEU:C	2.46	0.41
1:T:183:GLU:HA	1:T:186:ASN:HB3	2.03	0.41
1:X:189:PRO:HA	1:X:193:ASP:OD2	2.20	0.41
1:a:79:LEU:HD23	1:a:79:LEU:C	2.46	0.41
1:a:183:GLU:HA	1:a:186:ASN:HB3	2.03	0.41
1:a:189:PRO:HA	1:a:193:ASP:OD2	2.20	0.41
1:b:79:LEU:C	1:b:79:LEU:HD23	2.46	0.41
1:b:150:GLN:O	1:b:154:GLU:N	2.44	0.41
1:d:67:ILE:HG13	1:d:70:ARG:NH2	2.36	0.41
1:f:67:ILE:HG13	1:f:70:ARG:NH2	2.36	0.41
1:i:183:GLU:HA	1:i:186:ASN:HB3	2.03	0.41
1:l:175:ILE:HG13	1:l:176:LEU:N	2.36	0.41
1:l:183:GLU:HA	1:l:186:ASN:HB3	2.03	0.41
1:l:189:PRO:HA	1:l:193:ASP:OD2	2.20	0.41
1:o:175:ILE:HG13	1:o:176:LEU:N	2.36	0.41
1:o:189:PRO:HA	1:o:193:ASP:OD2	2.20	0.41
1:p:189:PRO:HA	1:p:193:ASP:OD2	2.20	0.41
1:s:189:PRO:HA	1:s:193:ASP:OD2	2.20	0.41
1:2:79:LEU:HD23	1:2:79:LEU:C	2.46	0.40
1:3:89:GLU:O	1:3:93:GLN:N	2.38	0.40
1:3:183:GLU:HA	1:3:186:ASN:HB3	2.03	0.40
1:6:183:GLU:HA	1:6:186:ASN:HB3	2.03	0.40
1:A:79:LEU:HD23	1:A:79:LEU:C	2.46	0.40
1:B:175:ILE:HG13	1:B:176:LEU:N	2.36	0.40
1:B:183:GLU:HA	1:B:186:ASN:HB3	2.03	0.40
1:E:79:LEU:HD23	1:E:79:LEU:C	2.46	0.40
1:L:67:ILE:HG13	1:L:70:ARG:NH2	2.36	0.40
1:L:79:LEU:C	1:L:79:LEU:HD23	2.46	0.40
1:L:184:LEU:C	1:L:184:LEU:HD23	2.47	0.40
1:Q:175:ILE:HG13	1:Q:176:LEU:N	2.36	0.40
1:Q:183:GLU:HA	1:Q:186:ASN:HB3	2.03	0.40
1:R:141:ALA:O	1:R:145:SER:N	2.52	0.40
1:W:183:GLU:HA	1:W:186:ASN:HB3	2.03	0.40
1:Y:183:GLU:HA	1:Y:186:ASN:HB3	2.03	0.40
1:f:175:ILE:HG13	1:f:176:LEU:N	2.36	0.40
1:g:67:ILE:HG13	1:g:70:ARG:NH2	2.36	0.40
1:i:79:LEU:C	1:i:79:LEU:HD23	2.46	0.40
1:j:79:LEU:C	1:j:79:LEU:HD23	2.46	0.40
1:n:184:LEU:HD23	1:n:184:LEU:C	2.47	0.40
1:o:183:GLU:HA	1:o:186:ASN:HB3	2.03	0.40
1:r:175:ILE:HG13	1:r:176:LEU:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:u:183:GLU:HA	1:u:186:ASN:HB3	2.03	0.40
1:y:141:ALA:O	1:y:145:SER:N	2.52	0.40
1:1:184:LEU:HD23	1:1:184:LEU:C	2.47	0.40
1:4:175:ILE:HG13	1:4:176:LEU:N	2.36	0.40
1:7:79:LEU:HD23	1:7:79:LEU:C	2.46	0.40
1:D:175:ILE:HG13	1:D:176:LEU:N	2.36	0.40
1:E:183:GLU:HA	1:E:186:ASN:HB3	2.03	0.40
1:E:184:LEU:HD23	1:E:184:LEU:C	2.47	0.40
1:I:79:LEU:HD23	1:I:79:LEU:C	2.46	0.40
1:M:67:ILE:HG13	1:M:70:ARG:NH2	2.36	0.40
1:P:28:LEU:O	1:P:32:LEU:HG	2.22	0.40
1:R:67:ILE:HG13	1:R:70:ARG:NH2	2.36	0.40
1:T:28:LEU:O	1:T:32:LEU:HG	2.22	0.40
1:U:67:ILE:HG13	1:U:70:ARG:NH2	2.36	0.40
1:Y:150:GLN:O	1:Y:154:GLU:N	2.44	0.40
1:h:28:LEU:O	1:h:32:LEU:HG	2.22	0.40
1:h:79:LEU:HD23	1:h:79:LEU:C	2.46	0.40
1:h:175:ILE:HG13	1:h:176:LEU:N	2.36	0.40
1:k:141:ALA:O	1:k:145:SER:N	2.52	0.40
1:m:189:PRO:HA	1:m:193:ASP:OD2	2.20	0.40
1:r:183:GLU:HA	1:r:186:ASN:HB3	2.03	0.40
1:u:79:LEU:HD23	1:u:79:LEU:C	2.46	0.40
1:u:141:ALA:O	1:u:145:SER:N	2.52	0.40
1:y:67:ILE:HG13	1:y:70:ARG:NH2	2.36	0.40
1:y:184:LEU:HD23	1:y:184:LEU:C	2.47	0.40
1:z:79:LEU:C	1:z:79:LEU:HD23	2.46	0.40
1:0:189:PRO:HA	1:0:193:ASP:OD2	2.20	0.40
1:1:175:ILE:HG13	1:1:176:LEU:N	2.36	0.40
1:3:79:LEU:HD23	1:3:79:LEU:C	2.46	0.40
1:C:79:LEU:HD23	1:C:79:LEU:C	2.46	0.40
1:E:28:LEU:O	1:E:32:LEU:HG	2.22	0.40
1:G:71:TRP:HA	1:G:74:LYS:HE3	2.04	0.40
1:H:71:TRP:HA	1:H:74:LYS:HE3	2.04	0.40
1:H:184:LEU:HD23	1:H:184:LEU:C	2.47	0.40
1:J:189:PRO:HA	1:J:193:ASP:OD2	2.20	0.40
1:K:67:ILE:HG13	1:K:70:ARG:NH2	2.36	0.40
1:K:184:LEU:HD23	1:K:184:LEU:C	2.47	0.40
1:T:184:LEU:HD23	1:T:184:LEU:C	2.47	0.40
1:U:89:GLU:O	1:U:93:GLN:N	2.38	0.40
1:W:28:LEU:O	1:W:32:LEU:HG	2.22	0.40
1:W:71:TRP:HA	1:W:74:LYS:HE3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:184:LEU:HD23	1:Y:184:LEU:C	2.47	0.40
1:Z:79:LEU:HD23	1:Z:79:LEU:C	2.46	0.40
1:b:183:GLU:HA	1:b:186:ASN:HB3	2.03	0.40
1:c:67:ILE:HG13	1:c:70:ARG:NH2	2.36	0.40
1:g:141:ALA:O	1:g:145:SER:N	2.52	0.40
1:g:184:LEU:C	1:g:184:LEU:HD23	2.47	0.40
1:i:67:ILE:HG13	1:i:70:ARG:NH2	2.36	0.40
1:j:71:TRP:HA	1:j:74:LYS:HE3	2.04	0.40
1:k:79:LEU:C	1:k:79:LEU:HD23	2.46	0.40
1:k:175:ILE:HG13	1:k:176:LEU:N	2.36	0.40
1:m:71:TRP:HA	1:m:74:LYS:HE3	2.04	0.40
1:o:91:LEU:O	1:o:95:GLN:NE2	2.53	0.40
1:q:71:TRP:HA	1:q:74:LYS:HE3	2.04	0.40
1:q:184:LEU:C	1:q:184:LEU:HD23	2.47	0.40
1:u:28:LEU:O	1:u:32:LEU:HG	2.22	0.40
1:0:71:TRP:HA	1:0:74:LYS:HE3	2.04	0.40
1:0:183:GLU:HA	1:0:186:ASN:HB3	2.03	0.40
1:1:28:LEU:O	1:1:32:LEU:HG	2.22	0.40
1:2:28:LEU:O	1:2:32:LEU:HG	2.22	0.40
1:2:71:TRP:HA	1:2:74:LYS:HE3	2.04	0.40
1:5:28:LEU:O	1:5:32:LEU:HG	2.22	0.40
1:A:28:LEU:O	1:A:32:LEU:HG	2.22	0.40
1:A:175:ILE:HG13	1:A:176:LEU:N	2.36	0.40
1:F:28:LEU:O	1:F:32:LEU:HG	2.22	0.40
1:G:175:ILE:HG13	1:G:176:LEU:N	2.36	0.40
1:I:71:TRP:HA	1:I:74:LYS:HE3	2.04	0.40
1:J:71:TRP:HA	1:J:74:LYS:HE3	2.04	0.40
1:K:71:TRP:HA	1:K:74:LYS:HE3	2.04	0.40
1:L:71:TRP:HA	1:L:74:LYS:HE3	2.04	0.40
1:N:79:LEU:HD23	1:N:79:LEU:C	2.46	0.40
1:V:184:LEU:HD23	1:V:184:LEU:C	2.47	0.40
1:W:79:LEU:C	1:W:79:LEU:HD23	2.46	0.40
1:W:184:LEU:HD23	1:W:184:LEU:C	2.47	0.40
1:X:71:TRP:HA	1:X:74:LYS:HE3	2.04	0.40
1:Z:28:LEU:O	1:Z:32:LEU:HG	2.22	0.40
1:Z:67:ILE:HG13	1:Z:70:ARG:NH2	2.36	0.40
1:a:71:TRP:HA	1:a:74:LYS:HE3	2.04	0.40
1:b:67:ILE:HG13	1:b:70:ARG:NH2	2.36	0.40
1:c:150:GLN:O	1:c:154:GLU:N	2.44	0.40
1:h:184:LEU:HD23	1:h:184:LEU:C	2.47	0.40
1:j:141:ALA:O	1:j:145:SER:N	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:k:184:LEU:HD23	1:k:184:LEU:C	2.47	0.40
1:l:71:TRP:HA	1:l:74:LYS:HE3	2.04	0.40
1:l:79:LEU:HD23	1:l:79:LEU:C	2.46	0.40
1:o:71:TRP:HA	1:o:74:LYS:HE3	2.04	0.40
1:p:71:TRP:HA	1:p:74:LYS:HE3	2.04	0.40
1:r:71:TRP:HA	1:r:74:LYS:HE3	2.04	0.40
1:r:184:LEU:C	1:r:184:LEU:HD23	2.47	0.40
1:v:28:LEU:O	1:v:32:LEU:HG	2.22	0.40
1:y:71:TRP:HA	1:y:74:LYS:HE3	2.04	0.40
1:z:28:LEU:O	1:z:32:LEU:HG	2.22	0.40
1:0:141:ALA:O	1:0:145:SER:N	2.52	0.40
1:1:71:TRP:HA	1:1:74:LYS:HE3	2.04	0.40
1:3:71:TRP:HA	1:3:74:LYS:HE3	2.04	0.40
1:3:175:ILE:HG13	1:3:176:LEU:N	2.36	0.40
1:5:175:ILE:HG13	1:5:176:LEU:N	2.36	0.40
1:F:71:TRP:HA	1:F:74:LYS:HE3	2.04	0.40
1:F:79:LEU:HD23	1:F:79:LEU:C	2.46	0.40
1:I:28:LEU:O	1:I:32:LEU:HG	2.22	0.40
1:I:89:GLU:O	1:I:93:GLN:N	2.38	0.40
1:I:150:GLN:O	1:I:154:GLU:N	2.44	0.40
1:L:183:GLU:HA	1:L:186:ASN:HB3	2.03	0.40
1:N:67:ILE:HG13	1:N:70:ARG:NH2	2.36	0.40
1:O:28:LEU:O	1:O:32:LEU:HG	2.22	0.40
1:O:175:ILE:HG13	1:O:176:LEU:N	2.36	0.40
1:S:184:LEU:HD23	1:S:184:LEU:C	2.47	0.40
1:T:79:LEU:C	1:T:79:LEU:HD23	2.46	0.40
1:Y:28:LEU:O	1:Y:32:LEU:HG	2.22	0.40
1:Z:71:TRP:HA	1:Z:74:LYS:HE3	2.04	0.40
1:Z:184:LEU:HD23	1:Z:184:LEU:C	2.47	0.40
1:a:28:LEU:O	1:a:32:LEU:HG	2.22	0.40
1:a:67:ILE:HG13	1:a:70:ARG:NH2	2.36	0.40
1:c:79:LEU:HD23	1:c:79:LEU:C	2.46	0.40
1:d:28:LEU:O	1:d:32:LEU:HG	2.22	0.40
1:e:141:ALA:O	1:e:145:SER:N	2.52	0.40
1:g:79:LEU:HD23	1:g:79:LEU:C	2.46	0.40
1:h:67:ILE:HG13	1:h:70:ARG:NH2	2.36	0.40
1:i:71:TRP:HA	1:i:74:LYS:HE3	2.04	0.40
1:j:91:LEU:O	1:j:95:GLN:NE2	2.53	0.40
1:j:184:LEU:HD23	1:j:184:LEU:C	2.47	0.40
1:k:71:TRP:HA	1:k:74:LYS:HE3	2.04	0.40
1:l:91:LEU:O	1:l:95:GLN:NE2	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:n:71:TRP:HA	1:n:74:LYS:HE3	2.04	0.40
1:n:175:ILE:HG13	1:n:176:LEU:N	2.36	0.40
1:o:79:LEU:HD23	1:o:79:LEU:C	2.46	0.40
1:q:79:LEU:HD23	1:q:79:LEU:C	2.46	0.40
1:q:175:ILE:HG13	1:q:176:LEU:N	2.36	0.40
1:v:141:ALA:O	1:v:145:SER:N	2.52	0.40
1:w:79:LEU:HD23	1:w:79:LEU:C	2.46	0.40
1:y:28:LEU:O	1:y:32:LEU:HG	2.22	0.40
1:z:71:TRP:HA	1:z:74:LYS:HE3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	194/246 (79%)	191 (98%)	3 (2%)	0	100	100
1	1	194/246 (79%)	191 (98%)	3 (2%)	0	100	100
1	2	194/246 (79%)	191 (98%)	3 (2%)	0	100	100
1	3	194/246 (79%)	191 (98%)	3 (2%)	0	100	100
1	4	194/246 (79%)	191 (98%)	3 (2%)	0	100	100
1	5	194/246 (79%)	191 (98%)	3 (2%)	0	100	100
1	6	194/246 (79%)	191 (98%)	3 (2%)	0	100	100
1	7	194/246 (79%)	191 (98%)	3 (2%)	0	100	100
1	A	194/246 (79%)	191 (98%)	3 (2%)	0	100	100
1	B	194/246 (79%)	191 (98%)	3 (2%)	0	100	100
1	C	194/246 (79%)	191 (98%)	3 (2%)	0	100	100
1	D	194/246 (79%)	191 (98%)	3 (2%)	0	100	100
1	E	194/246 (79%)	191 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	194/246 (79%)	191 (98%)	3 (2%)	0	100	100
1	G	194/246 (79%)	191 (98%)	3 (2%)	0	100	100
1	H	194/246 (79%)	191 (98%)	3 (2%)	0	100	100
1	I	194/246 (79%)	191 (98%)	3 (2%)	0	100	100
1	J	194/246 (79%)	191 (98%)	3 (2%)	0	100	100
1	K	194/246 (79%)	191 (98%)	3 (2%)	0	100	100
1	L	194/246 (79%)	191 (98%)	3 (2%)	0	100	100
1	M	194/246 (79%)	191 (98%)	3 (2%)	0	100	100
1	N	194/246 (79%)	191 (98%)	3 (2%)	0	100	100
1	O	194/246 (79%)	191 (98%)	3 (2%)	0	100	100
1	P	194/246 (79%)	191 (98%)	3 (2%)	0	100	100
1	Q	194/246 (79%)	191 (98%)	3 (2%)	0	100	100
1	R	194/246 (79%)	191 (98%)	3 (2%)	0	100	100
1	S	194/246 (79%)	191 (98%)	3 (2%)	0	100	100
1	T	194/246 (79%)	191 (98%)	3 (2%)	0	100	100
1	U	194/246 (79%)	191 (98%)	3 (2%)	0	100	100
1	V	194/246 (79%)	191 (98%)	3 (2%)	0	100	100
1	W	194/246 (79%)	191 (98%)	3 (2%)	0	100	100
1	X	194/246 (79%)	191 (98%)	3 (2%)	0	100	100
1	Y	194/246 (79%)	191 (98%)	3 (2%)	0	100	100
1	Z	194/246 (79%)	191 (98%)	3 (2%)	0	100	100
1	a	194/246 (79%)	191 (98%)	3 (2%)	0	100	100
1	b	194/246 (79%)	191 (98%)	3 (2%)	0	100	100
1	c	194/246 (79%)	191 (98%)	3 (2%)	0	100	100
1	d	194/246 (79%)	191 (98%)	3 (2%)	0	100	100
1	e	194/246 (79%)	191 (98%)	3 (2%)	0	100	100
1	f	194/246 (79%)	191 (98%)	3 (2%)	0	100	100
1	g	194/246 (79%)	191 (98%)	3 (2%)	0	100	100
1	h	194/246 (79%)	191 (98%)	3 (2%)	0	100	100
1	i	194/246 (79%)	191 (98%)	3 (2%)	0	100	100
1	j	194/246 (79%)	191 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	k	194/246 (79%)	191 (98%)	3 (2%)	0	100	100
1	l	194/246 (79%)	191 (98%)	3 (2%)	0	100	100
1	m	194/246 (79%)	191 (98%)	3 (2%)	0	100	100
1	n	194/246 (79%)	191 (98%)	3 (2%)	0	100	100
1	o	194/246 (79%)	191 (98%)	3 (2%)	0	100	100
1	p	194/246 (79%)	191 (98%)	3 (2%)	0	100	100
1	q	194/246 (79%)	191 (98%)	3 (2%)	0	100	100
1	r	194/246 (79%)	191 (98%)	3 (2%)	0	100	100
1	s	194/246 (79%)	191 (98%)	3 (2%)	0	100	100
1	t	194/246 (79%)	191 (98%)	3 (2%)	0	100	100
1	u	194/246 (79%)	191 (98%)	3 (2%)	0	100	100
1	v	194/246 (79%)	191 (98%)	3 (2%)	0	100	100
1	w	194/246 (79%)	191 (98%)	3 (2%)	0	100	100
1	x	194/246 (79%)	191 (98%)	3 (2%)	0	100	100
1	y	194/246 (79%)	191 (98%)	3 (2%)	0	100	100
1	z	194/246 (79%)	191 (98%)	3 (2%)	0	100	100
All	All	11640/14760 (79%)	11460 (98%)	180 (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	163/208 (78%)	163 (100%)	0	100	100
1	1	163/208 (78%)	163 (100%)	0	100	100
1	2	163/208 (78%)	163 (100%)	0	100	100
1	3	163/208 (78%)	163 (100%)	0	100	100
1	4	163/208 (78%)	163 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	5	163/208 (78%)	163 (100%)	0	100	100
1	6	163/208 (78%)	163 (100%)	0	100	100
1	7	163/208 (78%)	163 (100%)	0	100	100
1	A	163/208 (78%)	163 (100%)	0	100	100
1	B	163/208 (78%)	163 (100%)	0	100	100
1	C	163/208 (78%)	163 (100%)	0	100	100
1	D	163/208 (78%)	163 (100%)	0	100	100
1	E	163/208 (78%)	163 (100%)	0	100	100
1	F	163/208 (78%)	163 (100%)	0	100	100
1	G	163/208 (78%)	163 (100%)	0	100	100
1	H	163/208 (78%)	163 (100%)	0	100	100
1	I	163/208 (78%)	163 (100%)	0	100	100
1	J	163/208 (78%)	163 (100%)	0	100	100
1	K	163/208 (78%)	163 (100%)	0	100	100
1	L	163/208 (78%)	163 (100%)	0	100	100
1	M	163/208 (78%)	163 (100%)	0	100	100
1	N	163/208 (78%)	163 (100%)	0	100	100
1	O	163/208 (78%)	163 (100%)	0	100	100
1	P	163/208 (78%)	163 (100%)	0	100	100
1	Q	163/208 (78%)	163 (100%)	0	100	100
1	R	163/208 (78%)	163 (100%)	0	100	100
1	S	163/208 (78%)	163 (100%)	0	100	100
1	T	163/208 (78%)	163 (100%)	0	100	100
1	U	163/208 (78%)	163 (100%)	0	100	100
1	V	163/208 (78%)	163 (100%)	0	100	100
1	W	163/208 (78%)	163 (100%)	0	100	100
1	X	163/208 (78%)	163 (100%)	0	100	100
1	Y	163/208 (78%)	163 (100%)	0	100	100
1	Z	163/208 (78%)	163 (100%)	0	100	100
1	a	163/208 (78%)	163 (100%)	0	100	100
1	b	163/208 (78%)	163 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	c	163/208 (78%)	163 (100%)	0	100	100
1	d	163/208 (78%)	163 (100%)	0	100	100
1	e	163/208 (78%)	163 (100%)	0	100	100
1	f	163/208 (78%)	163 (100%)	0	100	100
1	g	163/208 (78%)	163 (100%)	0	100	100
1	h	163/208 (78%)	163 (100%)	0	100	100
1	i	163/208 (78%)	163 (100%)	0	100	100
1	j	163/208 (78%)	163 (100%)	0	100	100
1	k	163/208 (78%)	163 (100%)	0	100	100
1	l	163/208 (78%)	163 (100%)	0	100	100
1	m	163/208 (78%)	163 (100%)	0	100	100
1	n	163/208 (78%)	163 (100%)	0	100	100
1	o	163/208 (78%)	163 (100%)	0	100	100
1	p	163/208 (78%)	163 (100%)	0	100	100
1	q	163/208 (78%)	163 (100%)	0	100	100
1	r	163/208 (78%)	163 (100%)	0	100	100
1	s	163/208 (78%)	163 (100%)	0	100	100
1	t	163/208 (78%)	163 (100%)	0	100	100
1	u	163/208 (78%)	163 (100%)	0	100	100
1	v	163/208 (78%)	163 (100%)	0	100	100
1	w	163/208 (78%)	163 (100%)	0	100	100
1	x	163/208 (78%)	163 (100%)	0	100	100
1	y	163/208 (78%)	163 (100%)	0	100	100
1	z	163/208 (78%)	163 (100%)	0	100	100
All	All	9780/12480 (78%)	9780 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (245) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	76	GLN
1	0	135	GLN

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Mol	Chain	Res	Type
1	0	203	GLN
1	1	76	GLN
1	1	100	HIS
1	1	135	GLN
1	1	203	GLN
1	2	76	GLN
1	2	100	HIS
1	2	135	GLN
1	2	203	GLN
1	3	76	GLN
1	3	100	HIS
1	3	135	GLN
1	3	203	GLN
1	4	76	GLN
1	4	100	HIS
1	4	135	GLN
1	4	203	GLN
1	5	76	GLN
1	5	100	HIS
1	5	135	GLN
1	5	203	GLN
1	6	76	GLN
1	6	100	HIS
1	6	203	GLN
1	7	65	GLN
1	7	76	GLN
1	7	100	HIS
1	7	135	GLN
1	7	203	GLN
1	A	76	GLN
1	A	100	HIS
1	A	135	GLN
1	A	203	GLN
1	B	76	GLN
1	B	100	HIS
1	B	203	GLN
1	C	65	GLN
1	C	76	GLN
1	C	100	HIS
1	C	135	GLN
1	C	203	GLN
1	D	65	GLN

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Mol	Chain	Res	Type
1	D	76	GLN
1	D	100	HIS
1	D	135	GLN
1	D	203	GLN
1	E	76	GLN
1	E	100	HIS
1	E	135	GLN
1	E	203	GLN
1	F	65	GLN
1	F	76	GLN
1	F	100	HIS
1	F	135	GLN
1	F	203	GLN
1	G	65	GLN
1	G	76	GLN
1	G	100	HIS
1	G	135	GLN
1	G	203	GLN
1	H	65	GLN
1	H	76	GLN
1	H	100	HIS
1	H	135	GLN
1	H	203	GLN
1	I	76	GLN
1	I	100	HIS
1	I	135	GLN
1	I	203	GLN
1	J	76	GLN
1	J	100	HIS
1	J	135	GLN
1	J	203	GLN
1	K	76	GLN
1	K	100	HIS
1	K	135	GLN
1	K	203	GLN
1	L	76	GLN
1	L	100	HIS
1	L	135	GLN
1	L	203	GLN
1	M	76	GLN
1	M	100	HIS
1	M	135	GLN

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Mol	Chain	Res	Type
1	M	203	GLN
1	N	76	GLN
1	N	100	HIS
1	N	135	GLN
1	N	203	GLN
1	O	65	GLN
1	O	76	GLN
1	O	100	HIS
1	O	135	GLN
1	O	203	GLN
1	P	76	GLN
1	P	100	HIS
1	P	135	GLN
1	P	203	GLN
1	Q	76	GLN
1	Q	100	HIS
1	Q	135	GLN
1	Q	203	GLN
1	R	76	GLN
1	R	100	HIS
1	R	135	GLN
1	R	203	GLN
1	S	76	GLN
1	S	100	HIS
1	S	135	GLN
1	S	203	GLN
1	T	76	GLN
1	T	100	HIS
1	T	135	GLN
1	T	203	GLN
1	U	76	GLN
1	U	100	HIS
1	U	135	GLN
1	U	203	GLN
1	V	76	GLN
1	V	100	HIS
1	V	135	GLN
1	V	203	GLN
1	W	76	GLN
1	W	100	HIS
1	W	135	GLN
1	W	203	GLN

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Mol	Chain	Res	Type
1	X	76	GLN
1	X	135	GLN
1	X	203	GLN
1	Y	76	GLN
1	Y	100	HIS
1	Y	135	GLN
1	Y	203	GLN
1	Z	76	GLN
1	Z	100	HIS
1	Z	203	GLN
1	a	76	GLN
1	a	100	HIS
1	a	135	GLN
1	a	203	GLN
1	b	65	GLN
1	b	76	GLN
1	b	100	HIS
1	b	135	GLN
1	b	203	GLN
1	c	76	GLN
1	c	100	HIS
1	c	135	GLN
1	c	203	GLN
1	d	76	GLN
1	d	100	HIS
1	d	135	GLN
1	d	203	GLN
1	e	76	GLN
1	e	100	HIS
1	e	135	GLN
1	e	203	GLN
1	f	76	GLN
1	f	100	HIS
1	f	135	GLN
1	f	203	GLN
1	g	76	GLN
1	g	100	HIS
1	g	135	GLN
1	g	203	GLN
1	h	76	GLN
1	h	100	HIS
1	h	135	GLN

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Mol	Chain	Res	Type
1	h	203	GLN
1	i	65	GLN
1	i	76	GLN
1	i	100	HIS
1	i	135	GLN
1	i	203	GLN
1	j	65	GLN
1	j	76	GLN
1	j	100	HIS
1	j	135	GLN
1	j	203	GLN
1	k	65	GLN
1	k	76	GLN
1	k	135	GLN
1	k	203	GLN
1	l	76	GLN
1	l	100	HIS
1	l	135	GLN
1	l	203	GLN
1	m	65	GLN
1	m	76	GLN
1	m	100	HIS
1	m	135	GLN
1	m	203	GLN
1	n	76	GLN
1	n	100	HIS
1	n	135	GLN
1	n	203	GLN
1	o	76	GLN
1	o	100	HIS
1	o	135	GLN
1	o	203	GLN
1	p	76	GLN
1	p	100	HIS
1	p	135	GLN
1	p	203	GLN
1	q	76	GLN
1	q	100	HIS
1	q	135	GLN
1	q	203	GLN
1	r	76	GLN
1	r	100	HIS

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Mol	Chain	Res	Type
1	r	203	GLN
1	s	76	GLN
1	s	100	HIS
1	s	135	GLN
1	s	203	GLN
1	t	76	GLN
1	t	100	HIS
1	t	203	GLN
1	u	76	GLN
1	u	100	HIS
1	u	135	GLN
1	u	203	GLN
1	v	65	GLN
1	v	76	GLN
1	v	100	HIS
1	v	135	GLN
1	v	203	GLN
1	w	76	GLN
1	w	100	HIS
1	w	135	GLN
1	w	203	GLN
1	x	76	GLN
1	x	100	HIS
1	x	135	GLN
1	x	203	GLN
1	y	76	GLN
1	y	100	HIS
1	y	135	GLN
1	y	203	GLN
1	z	76	GLN
1	z	100	HIS
1	z	135	GLN
1	z	203	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.