



Full wwPDB EM Validation Report ⓘ

Jul 13, 2026 – 03:37 pm BST

PDB ID : 9HXJ / pdb_00009hxj
EMDB ID : EMD-52479
Title : Bacterial antiviral defense protein Ec3ApeA from Escherichia coli strain KK-NP016
Authors : Sasnauskas, G.; Juozapaitis, J.; Puteikiene, R.; Tamulaitiene, G.
Deposited on : 2025-01-08
Resolution : 3.00 Å(reported)
Based on initial model : .

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

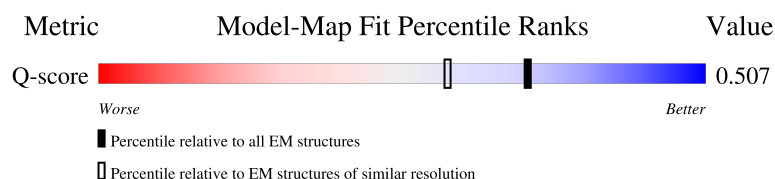
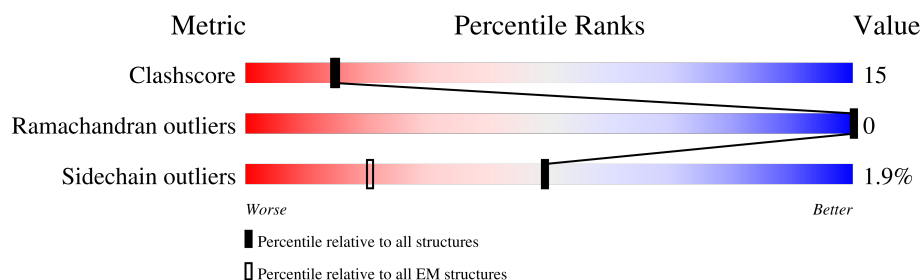
EMDB validation analysis : 0.0.1.dev133
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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.



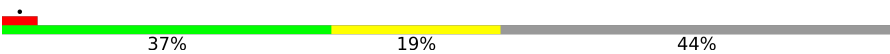
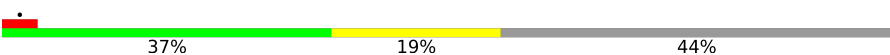
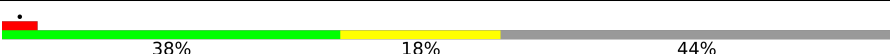
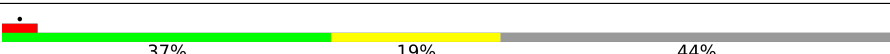
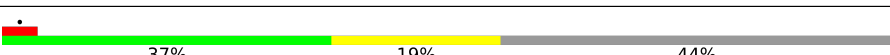
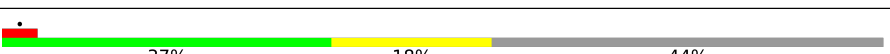
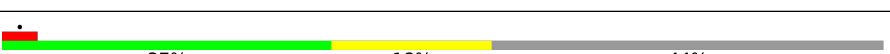
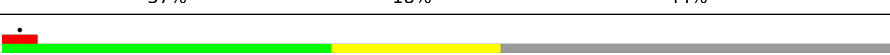
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14081 (2.50 - 3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1029	
1	B	1029	
1	C	1029	
1	D	1029	

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Mol	Chain	Length	Quality of chain
1	E	1029	
1	F	1029	
1	G	1029	
1	H	1029	
1	I	1029	
1	J	1029	
1	K	1029	
1	L	1029	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 53808 atoms, of which 0 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 Maltose/maltodextrin-binding periplasmic protein,Bacterial antiviral defense protein Ec3ApeA from Escherichia coli strain KK-NP016.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	575	Total	C	N	O	S	0	0
			4483	2911	762	797	13		
1	B	575	Total	C	N	O	S	0	0
			4483	2911	762	797	13		
1	C	575	Total	C	N	O	S	0	0
			4483	2911	762	797	13		
1	D	575	Total	C	N	O	S	0	0
			4483	2911	762	797	13		
1	E	575	Total	C	N	O	S	0	0
			4483	2911	762	797	13		
1	F	575	Total	C	N	O	S	0	0
			4483	2911	762	797	13		
1	G	575	Total	C	N	O	S	0	0
			4483	2911	762	797	13		
1	H	575	Total	C	N	O	S	0	0
			4483	2911	762	797	13		
1	I	575	Total	C	N	O	S	0	0
			4483	2911	762	797	13		
1	J	575	Total	C	N	O	S	0	0
			4483	2911	762	797	13		
1	K	575	Total	C	N	O	S	0	0
			4483	2911	762	797	13		
1	L	575	Total	C	N	O	S	0	0
			4483	2911	762	797	13		

There are 1044 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-444	MET	-	initiating methionine	UNP P0AEX9
A	-443	GLY	-	expression tag	UNP P0AEX9
A	-442	GLY	-	expression tag	UNP P0AEX9
A	-441	SER	-	expression tag	UNP P0AEX9
A	-440	ALA	-	expression tag	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-439	TRP	-	expression tag	UNP P0AEX9
A	-438	SER	-	expression tag	UNP P0AEX9
A	-437	HIS	-	expression tag	UNP P0AEX9
A	-436	PRO	-	expression tag	UNP P0AEX9
A	-435	GLN	-	expression tag	UNP P0AEX9
A	-434	PHE	-	expression tag	UNP P0AEX9
A	-433	GLU	-	expression tag	UNP P0AEX9
A	-432	LYS	-	expression tag	UNP P0AEX9
A	-431	GLY	-	expression tag	UNP P0AEX9
A	-430	GLY	-	expression tag	UNP P0AEX9
A	-429	GLY	-	expression tag	UNP P0AEX9
A	-428	SER	-	expression tag	UNP P0AEX9
A	-427	GLY	-	expression tag	UNP P0AEX9
A	-426	GLY	-	expression tag	UNP P0AEX9
A	-425	GLY	-	expression tag	UNP P0AEX9
A	-424	SER	-	expression tag	UNP P0AEX9
A	-423	GLY	-	expression tag	UNP P0AEX9
A	-422	GLY	-	expression tag	UNP P0AEX9
A	-421	SER	-	expression tag	UNP P0AEX9
A	-420	ALA	-	expression tag	UNP P0AEX9
A	-419	TRP	-	expression tag	UNP P0AEX9
A	-418	SER	-	expression tag	UNP P0AEX9
A	-417	HIS	-	expression tag	UNP P0AEX9
A	-416	PRO	-	expression tag	UNP P0AEX9
A	-415	GLN	-	expression tag	UNP P0AEX9
A	-414	PHE	-	expression tag	UNP P0AEX9
A	-413	GLU	-	expression tag	UNP P0AEX9
A	-412	LYS	-	expression tag	UNP P0AEX9
A	-411	GLY	-	expression tag	UNP P0AEX9
A	-410	SER	-	expression tag	UNP P0AEX9
A	-409	MET	-	expression tag	UNP P0AEX9
A	-408	GLY	-	expression tag	UNP P0AEX9
A	-407	GLY	-	expression tag	UNP P0AEX9
A	-406	SER	-	expression tag	UNP P0AEX9
A	-405	HIS	-	expression tag	UNP P0AEX9
A	-404	HIS	-	expression tag	UNP P0AEX9
A	-403	HIS	-	expression tag	UNP P0AEX9
A	-402	HIS	-	expression tag	UNP P0AEX9
A	-401	HIS	-	expression tag	UNP P0AEX9
A	-400	HIS	-	expression tag	UNP P0AEX9
A	-399	HIS	-	expression tag	UNP P0AEX9
A	-398	HIS	-	expression tag	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-397	HIS	-	expression tag	UNP P0AEX9
A	-396	HIS	-	expression tag	UNP P0AEX9
A	-395	GLY	-	expression tag	UNP P0AEX9
A	-394	MET	-	expression tag	UNP P0AEX9
A	-393	ALA	-	expression tag	UNP P0AEX9
A	-392	SER	-	expression tag	UNP P0AEX9
A	-391	MET	-	expression tag	UNP P0AEX9
A	-24	ASN	-	linker	UNP P0AEX9
A	-23	SER	-	linker	UNP P0AEX9
A	-22	SER	-	linker	UNP P0AEX9
A	-21	SER	-	linker	UNP P0AEX9
A	-20	ASN	-	linker	UNP P0AEX9
A	-19	ASN	-	linker	UNP P0AEX9
A	-18	ASN	-	linker	UNP P0AEX9
A	-17	ASN	-	linker	UNP P0AEX9
A	-16	ASN	-	linker	UNP P0AEX9
A	-15	ASN	-	linker	UNP P0AEX9
A	-14	ASN	-	linker	UNP P0AEX9
A	-13	ASN	-	linker	UNP P0AEX9
A	-12	ASN	-	linker	UNP P0AEX9
A	-11	ASN	-	linker	UNP P0AEX9
A	-10	LEU	-	linker	UNP P0AEX9
A	-9	GLY	-	linker	UNP P0AEX9
A	-8	ILE	-	linker	UNP P0AEX9
A	-7	GLU	-	linker	UNP P0AEX9
A	-6	GLU	-	linker	UNP P0AEX9
A	-5	ASN	-	linker	UNP P0AEX9
A	-4	LEU	-	linker	UNP P0AEX9
A	-3	TYR	-	linker	UNP P0AEX9
A	-2	PHE	-	linker	UNP P0AEX9
A	-1	GLN	-	linker	UNP P0AEX9
A	0	SER	-	linker	UNP P0AEX9
A	1	MET	-	linker	UNP P0AEX9
A	2	LYS	-	linker	UNP P0AEX9
A	3	PHE	-	linker	UNP P0AEX9
A	4	ARG	-	linker	UNP P0AEX9
A	5	SER	-	linker	UNP P0AEX9
A	6	LEU	-	linker	UNP P0AEX9
A	7	TYR	-	linker	UNP P0AEX9
A	8	LYS	-	linker	UNP P0AEX9
B	-444	MET	-	initiating methionine	UNP P0AEX9
B	-443	GLY	-	expression tag	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-442	GLY	-	expression tag	UNP P0AEX9
B	-441	SER	-	expression tag	UNP P0AEX9
B	-440	ALA	-	expression tag	UNP P0AEX9
B	-439	TRP	-	expression tag	UNP P0AEX9
B	-438	SER	-	expression tag	UNP P0AEX9
B	-437	HIS	-	expression tag	UNP P0AEX9
B	-436	PRO	-	expression tag	UNP P0AEX9
B	-435	GLN	-	expression tag	UNP P0AEX9
B	-434	PHE	-	expression tag	UNP P0AEX9
B	-433	GLU	-	expression tag	UNP P0AEX9
B	-432	LYS	-	expression tag	UNP P0AEX9
B	-431	GLY	-	expression tag	UNP P0AEX9
B	-430	GLY	-	expression tag	UNP P0AEX9
B	-429	GLY	-	expression tag	UNP P0AEX9
B	-428	SER	-	expression tag	UNP P0AEX9
B	-427	GLY	-	expression tag	UNP P0AEX9
B	-426	GLY	-	expression tag	UNP P0AEX9
B	-425	GLY	-	expression tag	UNP P0AEX9
B	-424	SER	-	expression tag	UNP P0AEX9
B	-423	GLY	-	expression tag	UNP P0AEX9
B	-422	GLY	-	expression tag	UNP P0AEX9
B	-421	SER	-	expression tag	UNP P0AEX9
B	-420	ALA	-	expression tag	UNP P0AEX9
B	-419	TRP	-	expression tag	UNP P0AEX9
B	-418	SER	-	expression tag	UNP P0AEX9
B	-417	HIS	-	expression tag	UNP P0AEX9
B	-416	PRO	-	expression tag	UNP P0AEX9
B	-415	GLN	-	expression tag	UNP P0AEX9
B	-414	PHE	-	expression tag	UNP P0AEX9
B	-413	GLU	-	expression tag	UNP P0AEX9
B	-412	LYS	-	expression tag	UNP P0AEX9
B	-411	GLY	-	expression tag	UNP P0AEX9
B	-410	SER	-	expression tag	UNP P0AEX9
B	-409	MET	-	expression tag	UNP P0AEX9
B	-408	GLY	-	expression tag	UNP P0AEX9
B	-407	GLY	-	expression tag	UNP P0AEX9
B	-406	SER	-	expression tag	UNP P0AEX9
B	-405	HIS	-	expression tag	UNP P0AEX9
B	-404	HIS	-	expression tag	UNP P0AEX9
B	-403	HIS	-	expression tag	UNP P0AEX9
B	-402	HIS	-	expression tag	UNP P0AEX9
B	-401	HIS	-	expression tag	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-400	HIS	-	expression tag	UNP P0AEX9
B	-399	HIS	-	expression tag	UNP P0AEX9
B	-398	HIS	-	expression tag	UNP P0AEX9
B	-397	HIS	-	expression tag	UNP P0AEX9
B	-396	HIS	-	expression tag	UNP P0AEX9
B	-395	GLY	-	expression tag	UNP P0AEX9
B	-394	MET	-	expression tag	UNP P0AEX9
B	-393	ALA	-	expression tag	UNP P0AEX9
B	-392	SER	-	expression tag	UNP P0AEX9
B	-391	MET	-	expression tag	UNP P0AEX9
B	-24	ASN	-	linker	UNP P0AEX9
B	-23	SER	-	linker	UNP P0AEX9
B	-22	SER	-	linker	UNP P0AEX9
B	-21	SER	-	linker	UNP P0AEX9
B	-20	ASN	-	linker	UNP P0AEX9
B	-19	ASN	-	linker	UNP P0AEX9
B	-18	ASN	-	linker	UNP P0AEX9
B	-17	ASN	-	linker	UNP P0AEX9
B	-16	ASN	-	linker	UNP P0AEX9
B	-15	ASN	-	linker	UNP P0AEX9
B	-14	ASN	-	linker	UNP P0AEX9
B	-13	ASN	-	linker	UNP P0AEX9
B	-12	ASN	-	linker	UNP P0AEX9
B	-11	ASN	-	linker	UNP P0AEX9
B	-10	LEU	-	linker	UNP P0AEX9
B	-9	GLY	-	linker	UNP P0AEX9
B	-8	ILE	-	linker	UNP P0AEX9
B	-7	GLU	-	linker	UNP P0AEX9
B	-6	GLU	-	linker	UNP P0AEX9
B	-5	ASN	-	linker	UNP P0AEX9
B	-4	LEU	-	linker	UNP P0AEX9
B	-3	TYR	-	linker	UNP P0AEX9
B	-2	PHE	-	linker	UNP P0AEX9
B	-1	GLN	-	linker	UNP P0AEX9
B	0	SER	-	linker	UNP P0AEX9
B	1	MET	-	linker	UNP P0AEX9
B	2	LYS	-	linker	UNP P0AEX9
B	3	PHE	-	linker	UNP P0AEX9
B	4	ARG	-	linker	UNP P0AEX9
B	5	SER	-	linker	UNP P0AEX9
B	6	LEU	-	linker	UNP P0AEX9
B	7	TYR	-	linker	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	8	LYS	-	linker	UNP P0AEX9
C	-444	MET	-	initiating methionine	UNP P0AEX9
C	-443	GLY	-	expression tag	UNP P0AEX9
C	-442	GLY	-	expression tag	UNP P0AEX9
C	-441	SER	-	expression tag	UNP P0AEX9
C	-440	ALA	-	expression tag	UNP P0AEX9
C	-439	TRP	-	expression tag	UNP P0AEX9
C	-438	SER	-	expression tag	UNP P0AEX9
C	-437	HIS	-	expression tag	UNP P0AEX9
C	-436	PRO	-	expression tag	UNP P0AEX9
C	-435	GLN	-	expression tag	UNP P0AEX9
C	-434	PHE	-	expression tag	UNP P0AEX9
C	-433	GLU	-	expression tag	UNP P0AEX9
C	-432	LYS	-	expression tag	UNP P0AEX9
C	-431	GLY	-	expression tag	UNP P0AEX9
C	-430	GLY	-	expression tag	UNP P0AEX9
C	-429	GLY	-	expression tag	UNP P0AEX9
C	-428	SER	-	expression tag	UNP P0AEX9
C	-427	GLY	-	expression tag	UNP P0AEX9
C	-426	GLY	-	expression tag	UNP P0AEX9
C	-425	GLY	-	expression tag	UNP P0AEX9
C	-424	SER	-	expression tag	UNP P0AEX9
C	-423	GLY	-	expression tag	UNP P0AEX9
C	-422	GLY	-	expression tag	UNP P0AEX9
C	-421	SER	-	expression tag	UNP P0AEX9
C	-420	ALA	-	expression tag	UNP P0AEX9
C	-419	TRP	-	expression tag	UNP P0AEX9
C	-418	SER	-	expression tag	UNP P0AEX9
C	-417	HIS	-	expression tag	UNP P0AEX9
C	-416	PRO	-	expression tag	UNP P0AEX9
C	-415	GLN	-	expression tag	UNP P0AEX9
C	-414	PHE	-	expression tag	UNP P0AEX9
C	-413	GLU	-	expression tag	UNP P0AEX9
C	-412	LYS	-	expression tag	UNP P0AEX9
C	-411	GLY	-	expression tag	UNP P0AEX9
C	-410	SER	-	expression tag	UNP P0AEX9
C	-409	MET	-	expression tag	UNP P0AEX9
C	-408	GLY	-	expression tag	UNP P0AEX9
C	-407	GLY	-	expression tag	UNP P0AEX9
C	-406	SER	-	expression tag	UNP P0AEX9
C	-405	HIS	-	expression tag	UNP P0AEX9
C	-404	HIS	-	expression tag	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-403	HIS	-	expression tag	UNP P0AEX9
C	-402	HIS	-	expression tag	UNP P0AEX9
C	-401	HIS	-	expression tag	UNP P0AEX9
C	-400	HIS	-	expression tag	UNP P0AEX9
C	-399	HIS	-	expression tag	UNP P0AEX9
C	-398	HIS	-	expression tag	UNP P0AEX9
C	-397	HIS	-	expression tag	UNP P0AEX9
C	-396	HIS	-	expression tag	UNP P0AEX9
C	-395	GLY	-	expression tag	UNP P0AEX9
C	-394	MET	-	expression tag	UNP P0AEX9
C	-393	ALA	-	expression tag	UNP P0AEX9
C	-392	SER	-	expression tag	UNP P0AEX9
C	-391	MET	-	expression tag	UNP P0AEX9
C	-24	ASN	-	linker	UNP P0AEX9
C	-23	SER	-	linker	UNP P0AEX9
C	-22	SER	-	linker	UNP P0AEX9
C	-21	SER	-	linker	UNP P0AEX9
C	-20	ASN	-	linker	UNP P0AEX9
C	-19	ASN	-	linker	UNP P0AEX9
C	-18	ASN	-	linker	UNP P0AEX9
C	-17	ASN	-	linker	UNP P0AEX9
C	-16	ASN	-	linker	UNP P0AEX9
C	-15	ASN	-	linker	UNP P0AEX9
C	-14	ASN	-	linker	UNP P0AEX9
C	-13	ASN	-	linker	UNP P0AEX9
C	-12	ASN	-	linker	UNP P0AEX9
C	-11	ASN	-	linker	UNP P0AEX9
C	-10	LEU	-	linker	UNP P0AEX9
C	-9	GLY	-	linker	UNP P0AEX9
C	-8	ILE	-	linker	UNP P0AEX9
C	-7	GLU	-	linker	UNP P0AEX9
C	-6	GLU	-	linker	UNP P0AEX9
C	-5	ASN	-	linker	UNP P0AEX9
C	-4	LEU	-	linker	UNP P0AEX9
C	-3	TYR	-	linker	UNP P0AEX9
C	-2	PHE	-	linker	UNP P0AEX9
C	-1	GLN	-	linker	UNP P0AEX9
C	0	SER	-	linker	UNP P0AEX9
C	1	MET	-	linker	UNP P0AEX9
C	2	LYS	-	linker	UNP P0AEX9
C	3	PHE	-	linker	UNP P0AEX9
C	4	ARG	-	linker	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	5	SER	-	linker	UNP P0AEX9
C	6	LEU	-	linker	UNP P0AEX9
C	7	TYR	-	linker	UNP P0AEX9
C	8	LYS	-	linker	UNP P0AEX9
D	-444	MET	-	initiating methionine	UNP P0AEX9
D	-443	GLY	-	expression tag	UNP P0AEX9
D	-442	GLY	-	expression tag	UNP P0AEX9
D	-441	SER	-	expression tag	UNP P0AEX9
D	-440	ALA	-	expression tag	UNP P0AEX9
D	-439	TRP	-	expression tag	UNP P0AEX9
D	-438	SER	-	expression tag	UNP P0AEX9
D	-437	HIS	-	expression tag	UNP P0AEX9
D	-436	PRO	-	expression tag	UNP P0AEX9
D	-435	GLN	-	expression tag	UNP P0AEX9
D	-434	PHE	-	expression tag	UNP P0AEX9
D	-433	GLU	-	expression tag	UNP P0AEX9
D	-432	LYS	-	expression tag	UNP P0AEX9
D	-431	GLY	-	expression tag	UNP P0AEX9
D	-430	GLY	-	expression tag	UNP P0AEX9
D	-429	GLY	-	expression tag	UNP P0AEX9
D	-428	SER	-	expression tag	UNP P0AEX9
D	-427	GLY	-	expression tag	UNP P0AEX9
D	-426	GLY	-	expression tag	UNP P0AEX9
D	-425	GLY	-	expression tag	UNP P0AEX9
D	-424	SER	-	expression tag	UNP P0AEX9
D	-423	GLY	-	expression tag	UNP P0AEX9
D	-422	GLY	-	expression tag	UNP P0AEX9
D	-421	SER	-	expression tag	UNP P0AEX9
D	-420	ALA	-	expression tag	UNP P0AEX9
D	-419	TRP	-	expression tag	UNP P0AEX9
D	-418	SER	-	expression tag	UNP P0AEX9
D	-417	HIS	-	expression tag	UNP P0AEX9
D	-416	PRO	-	expression tag	UNP P0AEX9
D	-415	GLN	-	expression tag	UNP P0AEX9
D	-414	PHE	-	expression tag	UNP P0AEX9
D	-413	GLU	-	expression tag	UNP P0AEX9
D	-412	LYS	-	expression tag	UNP P0AEX9
D	-411	GLY	-	expression tag	UNP P0AEX9
D	-410	SER	-	expression tag	UNP P0AEX9
D	-409	MET	-	expression tag	UNP P0AEX9
D	-408	GLY	-	expression tag	UNP P0AEX9
D	-407	GLY	-	expression tag	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-406	SER	-	expression tag	UNP P0AEX9
D	-405	HIS	-	expression tag	UNP P0AEX9
D	-404	HIS	-	expression tag	UNP P0AEX9
D	-403	HIS	-	expression tag	UNP P0AEX9
D	-402	HIS	-	expression tag	UNP P0AEX9
D	-401	HIS	-	expression tag	UNP P0AEX9
D	-400	HIS	-	expression tag	UNP P0AEX9
D	-399	HIS	-	expression tag	UNP P0AEX9
D	-398	HIS	-	expression tag	UNP P0AEX9
D	-397	HIS	-	expression tag	UNP P0AEX9
D	-396	HIS	-	expression tag	UNP P0AEX9
D	-395	GLY	-	expression tag	UNP P0AEX9
D	-394	MET	-	expression tag	UNP P0AEX9
D	-393	ALA	-	expression tag	UNP P0AEX9
D	-392	SER	-	expression tag	UNP P0AEX9
D	-391	MET	-	expression tag	UNP P0AEX9
D	-24	ASN	-	linker	UNP P0AEX9
D	-23	SER	-	linker	UNP P0AEX9
D	-22	SER	-	linker	UNP P0AEX9
D	-21	SER	-	linker	UNP P0AEX9
D	-20	ASN	-	linker	UNP P0AEX9
D	-19	ASN	-	linker	UNP P0AEX9
D	-18	ASN	-	linker	UNP P0AEX9
D	-17	ASN	-	linker	UNP P0AEX9
D	-16	ASN	-	linker	UNP P0AEX9
D	-15	ASN	-	linker	UNP P0AEX9
D	-14	ASN	-	linker	UNP P0AEX9
D	-13	ASN	-	linker	UNP P0AEX9
D	-12	ASN	-	linker	UNP P0AEX9
D	-11	ASN	-	linker	UNP P0AEX9
D	-10	LEU	-	linker	UNP P0AEX9
D	-9	GLY	-	linker	UNP P0AEX9
D	-8	ILE	-	linker	UNP P0AEX9
D	-7	GLU	-	linker	UNP P0AEX9
D	-6	GLU	-	linker	UNP P0AEX9
D	-5	ASN	-	linker	UNP P0AEX9
D	-4	LEU	-	linker	UNP P0AEX9
D	-3	TYR	-	linker	UNP P0AEX9
D	-2	PHE	-	linker	UNP P0AEX9
D	-1	GLN	-	linker	UNP P0AEX9
D	0	SER	-	linker	UNP P0AEX9
D	1	MET	-	linker	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
D	2	LYS	-	linker	UNP P0AEX9
D	3	PHE	-	linker	UNP P0AEX9
D	4	ARG	-	linker	UNP P0AEX9
D	5	SER	-	linker	UNP P0AEX9
D	6	LEU	-	linker	UNP P0AEX9
D	7	TYR	-	linker	UNP P0AEX9
D	8	LYS	-	linker	UNP P0AEX9
E	-444	MET	-	initiating methionine	UNP P0AEX9
E	-443	GLY	-	expression tag	UNP P0AEX9
E	-442	GLY	-	expression tag	UNP P0AEX9
E	-441	SER	-	expression tag	UNP P0AEX9
E	-440	ALA	-	expression tag	UNP P0AEX9
E	-439	TRP	-	expression tag	UNP P0AEX9
E	-438	SER	-	expression tag	UNP P0AEX9
E	-437	HIS	-	expression tag	UNP P0AEX9
E	-436	PRO	-	expression tag	UNP P0AEX9
E	-435	GLN	-	expression tag	UNP P0AEX9
E	-434	PHE	-	expression tag	UNP P0AEX9
E	-433	GLU	-	expression tag	UNP P0AEX9
E	-432	LYS	-	expression tag	UNP P0AEX9
E	-431	GLY	-	expression tag	UNP P0AEX9
E	-430	GLY	-	expression tag	UNP P0AEX9
E	-429	GLY	-	expression tag	UNP P0AEX9
E	-428	SER	-	expression tag	UNP P0AEX9
E	-427	GLY	-	expression tag	UNP P0AEX9
E	-426	GLY	-	expression tag	UNP P0AEX9
E	-425	GLY	-	expression tag	UNP P0AEX9
E	-424	SER	-	expression tag	UNP P0AEX9
E	-423	GLY	-	expression tag	UNP P0AEX9
E	-422	GLY	-	expression tag	UNP P0AEX9
E	-421	SER	-	expression tag	UNP P0AEX9
E	-420	ALA	-	expression tag	UNP P0AEX9
E	-419	TRP	-	expression tag	UNP P0AEX9
E	-418	SER	-	expression tag	UNP P0AEX9
E	-417	HIS	-	expression tag	UNP P0AEX9
E	-416	PRO	-	expression tag	UNP P0AEX9
E	-415	GLN	-	expression tag	UNP P0AEX9
E	-414	PHE	-	expression tag	UNP P0AEX9
E	-413	GLU	-	expression tag	UNP P0AEX9
E	-412	LYS	-	expression tag	UNP P0AEX9
E	-411	GLY	-	expression tag	UNP P0AEX9
E	-410	SER	-	expression tag	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-409	MET	-	expression tag	UNP P0AEX9
E	-408	GLY	-	expression tag	UNP P0AEX9
E	-407	GLY	-	expression tag	UNP P0AEX9
E	-406	SER	-	expression tag	UNP P0AEX9
E	-405	HIS	-	expression tag	UNP P0AEX9
E	-404	HIS	-	expression tag	UNP P0AEX9
E	-403	HIS	-	expression tag	UNP P0AEX9
E	-402	HIS	-	expression tag	UNP P0AEX9
E	-401	HIS	-	expression tag	UNP P0AEX9
E	-400	HIS	-	expression tag	UNP P0AEX9
E	-399	HIS	-	expression tag	UNP P0AEX9
E	-398	HIS	-	expression tag	UNP P0AEX9
E	-397	HIS	-	expression tag	UNP P0AEX9
E	-396	HIS	-	expression tag	UNP P0AEX9
E	-395	GLY	-	expression tag	UNP P0AEX9
E	-394	MET	-	expression tag	UNP P0AEX9
E	-393	ALA	-	expression tag	UNP P0AEX9
E	-392	SER	-	expression tag	UNP P0AEX9
E	-391	MET	-	expression tag	UNP P0AEX9
E	-24	ASN	-	linker	UNP P0AEX9
E	-23	SER	-	linker	UNP P0AEX9
E	-22	SER	-	linker	UNP P0AEX9
E	-21	SER	-	linker	UNP P0AEX9
E	-20	ASN	-	linker	UNP P0AEX9
E	-19	ASN	-	linker	UNP P0AEX9
E	-18	ASN	-	linker	UNP P0AEX9
E	-17	ASN	-	linker	UNP P0AEX9
E	-16	ASN	-	linker	UNP P0AEX9
E	-15	ASN	-	linker	UNP P0AEX9
E	-14	ASN	-	linker	UNP P0AEX9
E	-13	ASN	-	linker	UNP P0AEX9
E	-12	ASN	-	linker	UNP P0AEX9
E	-11	ASN	-	linker	UNP P0AEX9
E	-10	LEU	-	linker	UNP P0AEX9
E	-9	GLY	-	linker	UNP P0AEX9
E	-8	ILE	-	linker	UNP P0AEX9
E	-7	GLU	-	linker	UNP P0AEX9
E	-6	GLU	-	linker	UNP P0AEX9
E	-5	ASN	-	linker	UNP P0AEX9
E	-4	LEU	-	linker	UNP P0AEX9
E	-3	TYR	-	linker	UNP P0AEX9
E	-2	PHE	-	linker	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	GLN	-	linker	UNP P0AEX9
E	0	SER	-	linker	UNP P0AEX9
E	1	MET	-	linker	UNP P0AEX9
E	2	LYS	-	linker	UNP P0AEX9
E	3	PHE	-	linker	UNP P0AEX9
E	4	ARG	-	linker	UNP P0AEX9
E	5	SER	-	linker	UNP P0AEX9
E	6	LEU	-	linker	UNP P0AEX9
E	7	TYR	-	linker	UNP P0AEX9
E	8	LYS	-	linker	UNP P0AEX9
F	-444	MET	-	initiating methionine	UNP P0AEX9
F	-443	GLY	-	expression tag	UNP P0AEX9
F	-442	GLY	-	expression tag	UNP P0AEX9
F	-441	SER	-	expression tag	UNP P0AEX9
F	-440	ALA	-	expression tag	UNP P0AEX9
F	-439	TRP	-	expression tag	UNP P0AEX9
F	-438	SER	-	expression tag	UNP P0AEX9
F	-437	HIS	-	expression tag	UNP P0AEX9
F	-436	PRO	-	expression tag	UNP P0AEX9
F	-435	GLN	-	expression tag	UNP P0AEX9
F	-434	PHE	-	expression tag	UNP P0AEX9
F	-433	GLU	-	expression tag	UNP P0AEX9
F	-432	LYS	-	expression tag	UNP P0AEX9
F	-431	GLY	-	expression tag	UNP P0AEX9
F	-430	GLY	-	expression tag	UNP P0AEX9
F	-429	GLY	-	expression tag	UNP P0AEX9
F	-428	SER	-	expression tag	UNP P0AEX9
F	-427	GLY	-	expression tag	UNP P0AEX9
F	-426	GLY	-	expression tag	UNP P0AEX9
F	-425	GLY	-	expression tag	UNP P0AEX9
F	-424	SER	-	expression tag	UNP P0AEX9
F	-423	GLY	-	expression tag	UNP P0AEX9
F	-422	GLY	-	expression tag	UNP P0AEX9
F	-421	SER	-	expression tag	UNP P0AEX9
F	-420	ALA	-	expression tag	UNP P0AEX9
F	-419	TRP	-	expression tag	UNP P0AEX9
F	-418	SER	-	expression tag	UNP P0AEX9
F	-417	HIS	-	expression tag	UNP P0AEX9
F	-416	PRO	-	expression tag	UNP P0AEX9
F	-415	GLN	-	expression tag	UNP P0AEX9
F	-414	PHE	-	expression tag	UNP P0AEX9
F	-413	GLU	-	expression tag	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-412	LYS	-	expression tag	UNP P0AEX9
F	-411	GLY	-	expression tag	UNP P0AEX9
F	-410	SER	-	expression tag	UNP P0AEX9
F	-409	MET	-	expression tag	UNP P0AEX9
F	-408	GLY	-	expression tag	UNP P0AEX9
F	-407	GLY	-	expression tag	UNP P0AEX9
F	-406	SER	-	expression tag	UNP P0AEX9
F	-405	HIS	-	expression tag	UNP P0AEX9
F	-404	HIS	-	expression tag	UNP P0AEX9
F	-403	HIS	-	expression tag	UNP P0AEX9
F	-402	HIS	-	expression tag	UNP P0AEX9
F	-401	HIS	-	expression tag	UNP P0AEX9
F	-400	HIS	-	expression tag	UNP P0AEX9
F	-399	HIS	-	expression tag	UNP P0AEX9
F	-398	HIS	-	expression tag	UNP P0AEX9
F	-397	HIS	-	expression tag	UNP P0AEX9
F	-396	HIS	-	expression tag	UNP P0AEX9
F	-395	GLY	-	expression tag	UNP P0AEX9
F	-394	MET	-	expression tag	UNP P0AEX9
F	-393	ALA	-	expression tag	UNP P0AEX9
F	-392	SER	-	expression tag	UNP P0AEX9
F	-391	MET	-	expression tag	UNP P0AEX9
F	-24	ASN	-	linker	UNP P0AEX9
F	-23	SER	-	linker	UNP P0AEX9
F	-22	SER	-	linker	UNP P0AEX9
F	-21	SER	-	linker	UNP P0AEX9
F	-20	ASN	-	linker	UNP P0AEX9
F	-19	ASN	-	linker	UNP P0AEX9
F	-18	ASN	-	linker	UNP P0AEX9
F	-17	ASN	-	linker	UNP P0AEX9
F	-16	ASN	-	linker	UNP P0AEX9
F	-15	ASN	-	linker	UNP P0AEX9
F	-14	ASN	-	linker	UNP P0AEX9
F	-13	ASN	-	linker	UNP P0AEX9
F	-12	ASN	-	linker	UNP P0AEX9
F	-11	ASN	-	linker	UNP P0AEX9
F	-10	LEU	-	linker	UNP P0AEX9
F	-9	GLY	-	linker	UNP P0AEX9
F	-8	ILE	-	linker	UNP P0AEX9
F	-7	GLU	-	linker	UNP P0AEX9
F	-6	GLU	-	linker	UNP P0AEX9
F	-5	ASN	-	linker	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-4	LEU	-	linker	UNP P0AEX9
F	-3	TYR	-	linker	UNP P0AEX9
F	-2	PHE	-	linker	UNP P0AEX9
F	-1	GLN	-	linker	UNP P0AEX9
F	0	SER	-	linker	UNP P0AEX9
F	1	MET	-	linker	UNP P0AEX9
F	2	LYS	-	linker	UNP P0AEX9
F	3	PHE	-	linker	UNP P0AEX9
F	4	ARG	-	linker	UNP P0AEX9
F	5	SER	-	linker	UNP P0AEX9
F	6	LEU	-	linker	UNP P0AEX9
F	7	TYR	-	linker	UNP P0AEX9
F	8	LYS	-	linker	UNP P0AEX9
G	-444	MET	-	initiating methionine	UNP P0AEX9
G	-443	GLY	-	expression tag	UNP P0AEX9
G	-442	GLY	-	expression tag	UNP P0AEX9
G	-441	SER	-	expression tag	UNP P0AEX9
G	-440	ALA	-	expression tag	UNP P0AEX9
G	-439	TRP	-	expression tag	UNP P0AEX9
G	-438	SER	-	expression tag	UNP P0AEX9
G	-437	HIS	-	expression tag	UNP P0AEX9
G	-436	PRO	-	expression tag	UNP P0AEX9
G	-435	GLN	-	expression tag	UNP P0AEX9
G	-434	PHE	-	expression tag	UNP P0AEX9
G	-433	GLU	-	expression tag	UNP P0AEX9
G	-432	LYS	-	expression tag	UNP P0AEX9
G	-431	GLY	-	expression tag	UNP P0AEX9
G	-430	GLY	-	expression tag	UNP P0AEX9
G	-429	GLY	-	expression tag	UNP P0AEX9
G	-428	SER	-	expression tag	UNP P0AEX9
G	-427	GLY	-	expression tag	UNP P0AEX9
G	-426	GLY	-	expression tag	UNP P0AEX9
G	-425	GLY	-	expression tag	UNP P0AEX9
G	-424	SER	-	expression tag	UNP P0AEX9
G	-423	GLY	-	expression tag	UNP P0AEX9
G	-422	GLY	-	expression tag	UNP P0AEX9
G	-421	SER	-	expression tag	UNP P0AEX9
G	-420	ALA	-	expression tag	UNP P0AEX9
G	-419	TRP	-	expression tag	UNP P0AEX9
G	-418	SER	-	expression tag	UNP P0AEX9
G	-417	HIS	-	expression tag	UNP P0AEX9
G	-416	PRO	-	expression tag	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-415	GLN	-	expression tag	UNP P0AEX9
G	-414	PHE	-	expression tag	UNP P0AEX9
G	-413	GLU	-	expression tag	UNP P0AEX9
G	-412	LYS	-	expression tag	UNP P0AEX9
G	-411	GLY	-	expression tag	UNP P0AEX9
G	-410	SER	-	expression tag	UNP P0AEX9
G	-409	MET	-	expression tag	UNP P0AEX9
G	-408	GLY	-	expression tag	UNP P0AEX9
G	-407	GLY	-	expression tag	UNP P0AEX9
G	-406	SER	-	expression tag	UNP P0AEX9
G	-405	HIS	-	expression tag	UNP P0AEX9
G	-404	HIS	-	expression tag	UNP P0AEX9
G	-403	HIS	-	expression tag	UNP P0AEX9
G	-402	HIS	-	expression tag	UNP P0AEX9
G	-401	HIS	-	expression tag	UNP P0AEX9
G	-400	HIS	-	expression tag	UNP P0AEX9
G	-399	HIS	-	expression tag	UNP P0AEX9
G	-398	HIS	-	expression tag	UNP P0AEX9
G	-397	HIS	-	expression tag	UNP P0AEX9
G	-396	HIS	-	expression tag	UNP P0AEX9
G	-395	GLY	-	expression tag	UNP P0AEX9
G	-394	MET	-	expression tag	UNP P0AEX9
G	-393	ALA	-	expression tag	UNP P0AEX9
G	-392	SER	-	expression tag	UNP P0AEX9
G	-391	MET	-	expression tag	UNP P0AEX9
G	-24	ASN	-	linker	UNP P0AEX9
G	-23	SER	-	linker	UNP P0AEX9
G	-22	SER	-	linker	UNP P0AEX9
G	-21	SER	-	linker	UNP P0AEX9
G	-20	ASN	-	linker	UNP P0AEX9
G	-19	ASN	-	linker	UNP P0AEX9
G	-18	ASN	-	linker	UNP P0AEX9
G	-17	ASN	-	linker	UNP P0AEX9
G	-16	ASN	-	linker	UNP P0AEX9
G	-15	ASN	-	linker	UNP P0AEX9
G	-14	ASN	-	linker	UNP P0AEX9
G	-13	ASN	-	linker	UNP P0AEX9
G	-12	ASN	-	linker	UNP P0AEX9
G	-11	ASN	-	linker	UNP P0AEX9
G	-10	LEU	-	linker	UNP P0AEX9
G	-9	GLY	-	linker	UNP P0AEX9
G	-8	ILE	-	linker	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-7	GLU	-	linker	UNP P0AEX9
G	-6	GLU	-	linker	UNP P0AEX9
G	-5	ASN	-	linker	UNP P0AEX9
G	-4	LEU	-	linker	UNP P0AEX9
G	-3	TYR	-	linker	UNP P0AEX9
G	-2	PHE	-	linker	UNP P0AEX9
G	-1	GLN	-	linker	UNP P0AEX9
G	0	SER	-	linker	UNP P0AEX9
G	1	MET	-	linker	UNP P0AEX9
G	2	LYS	-	linker	UNP P0AEX9
G	3	PHE	-	linker	UNP P0AEX9
G	4	ARG	-	linker	UNP P0AEX9
G	5	SER	-	linker	UNP P0AEX9
G	6	LEU	-	linker	UNP P0AEX9
G	7	TYR	-	linker	UNP P0AEX9
G	8	LYS	-	linker	UNP P0AEX9
H	-444	MET	-	initiating methionine	UNP P0AEX9
H	-443	GLY	-	expression tag	UNP P0AEX9
H	-442	GLY	-	expression tag	UNP P0AEX9
H	-441	SER	-	expression tag	UNP P0AEX9
H	-440	ALA	-	expression tag	UNP P0AEX9
H	-439	TRP	-	expression tag	UNP P0AEX9
H	-438	SER	-	expression tag	UNP P0AEX9
H	-437	HIS	-	expression tag	UNP P0AEX9
H	-436	PRO	-	expression tag	UNP P0AEX9
H	-435	GLN	-	expression tag	UNP P0AEX9
H	-434	PHE	-	expression tag	UNP P0AEX9
H	-433	GLU	-	expression tag	UNP P0AEX9
H	-432	LYS	-	expression tag	UNP P0AEX9
H	-431	GLY	-	expression tag	UNP P0AEX9
H	-430	GLY	-	expression tag	UNP P0AEX9
H	-429	GLY	-	expression tag	UNP P0AEX9
H	-428	SER	-	expression tag	UNP P0AEX9
H	-427	GLY	-	expression tag	UNP P0AEX9
H	-426	GLY	-	expression tag	UNP P0AEX9
H	-425	GLY	-	expression tag	UNP P0AEX9
H	-424	SER	-	expression tag	UNP P0AEX9
H	-423	GLY	-	expression tag	UNP P0AEX9
H	-422	GLY	-	expression tag	UNP P0AEX9
H	-421	SER	-	expression tag	UNP P0AEX9
H	-420	ALA	-	expression tag	UNP P0AEX9
H	-419	TRP	-	expression tag	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-418	SER	-	expression tag	UNP P0AEX9
H	-417	HIS	-	expression tag	UNP P0AEX9
H	-416	PRO	-	expression tag	UNP P0AEX9
H	-415	GLN	-	expression tag	UNP P0AEX9
H	-414	PHE	-	expression tag	UNP P0AEX9
H	-413	GLU	-	expression tag	UNP P0AEX9
H	-412	LYS	-	expression tag	UNP P0AEX9
H	-411	GLY	-	expression tag	UNP P0AEX9
H	-410	SER	-	expression tag	UNP P0AEX9
H	-409	MET	-	expression tag	UNP P0AEX9
H	-408	GLY	-	expression tag	UNP P0AEX9
H	-407	GLY	-	expression tag	UNP P0AEX9
H	-406	SER	-	expression tag	UNP P0AEX9
H	-405	HIS	-	expression tag	UNP P0AEX9
H	-404	HIS	-	expression tag	UNP P0AEX9
H	-403	HIS	-	expression tag	UNP P0AEX9
H	-402	HIS	-	expression tag	UNP P0AEX9
H	-401	HIS	-	expression tag	UNP P0AEX9
H	-400	HIS	-	expression tag	UNP P0AEX9
H	-399	HIS	-	expression tag	UNP P0AEX9
H	-398	HIS	-	expression tag	UNP P0AEX9
H	-397	HIS	-	expression tag	UNP P0AEX9
H	-396	HIS	-	expression tag	UNP P0AEX9
H	-395	GLY	-	expression tag	UNP P0AEX9
H	-394	MET	-	expression tag	UNP P0AEX9
H	-393	ALA	-	expression tag	UNP P0AEX9
H	-392	SER	-	expression tag	UNP P0AEX9
H	-391	MET	-	expression tag	UNP P0AEX9
H	-24	ASN	-	linker	UNP P0AEX9
H	-23	SER	-	linker	UNP P0AEX9
H	-22	SER	-	linker	UNP P0AEX9
H	-21	SER	-	linker	UNP P0AEX9
H	-20	ASN	-	linker	UNP P0AEX9
H	-19	ASN	-	linker	UNP P0AEX9
H	-18	ASN	-	linker	UNP P0AEX9
H	-17	ASN	-	linker	UNP P0AEX9
H	-16	ASN	-	linker	UNP P0AEX9
H	-15	ASN	-	linker	UNP P0AEX9
H	-14	ASN	-	linker	UNP P0AEX9
H	-13	ASN	-	linker	UNP P0AEX9
H	-12	ASN	-	linker	UNP P0AEX9
H	-11	ASN	-	linker	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-10	LEU	-	linker	UNP P0AEX9
H	-9	GLY	-	linker	UNP P0AEX9
H	-8	ILE	-	linker	UNP P0AEX9
H	-7	GLU	-	linker	UNP P0AEX9
H	-6	GLU	-	linker	UNP P0AEX9
H	-5	ASN	-	linker	UNP P0AEX9
H	-4	LEU	-	linker	UNP P0AEX9
H	-3	TYR	-	linker	UNP P0AEX9
H	-2	PHE	-	linker	UNP P0AEX9
H	-1	GLN	-	linker	UNP P0AEX9
H	0	SER	-	linker	UNP P0AEX9
H	1	MET	-	linker	UNP P0AEX9
H	2	LYS	-	linker	UNP P0AEX9
H	3	PHE	-	linker	UNP P0AEX9
H	4	ARG	-	linker	UNP P0AEX9
H	5	SER	-	linker	UNP P0AEX9
H	6	LEU	-	linker	UNP P0AEX9
H	7	TYR	-	linker	UNP P0AEX9
H	8	LYS	-	linker	UNP P0AEX9
I	-444	MET	-	initiating methionine	UNP P0AEX9
I	-443	GLY	-	expression tag	UNP P0AEX9
I	-442	GLY	-	expression tag	UNP P0AEX9
I	-441	SER	-	expression tag	UNP P0AEX9
I	-440	ALA	-	expression tag	UNP P0AEX9
I	-439	TRP	-	expression tag	UNP P0AEX9
I	-438	SER	-	expression tag	UNP P0AEX9
I	-437	HIS	-	expression tag	UNP P0AEX9
I	-436	PRO	-	expression tag	UNP P0AEX9
I	-435	GLN	-	expression tag	UNP P0AEX9
I	-434	PHE	-	expression tag	UNP P0AEX9
I	-433	GLU	-	expression tag	UNP P0AEX9
I	-432	LYS	-	expression tag	UNP P0AEX9
I	-431	GLY	-	expression tag	UNP P0AEX9
I	-430	GLY	-	expression tag	UNP P0AEX9
I	-429	GLY	-	expression tag	UNP P0AEX9
I	-428	SER	-	expression tag	UNP P0AEX9
I	-427	GLY	-	expression tag	UNP P0AEX9
I	-426	GLY	-	expression tag	UNP P0AEX9
I	-425	GLY	-	expression tag	UNP P0AEX9
I	-424	SER	-	expression tag	UNP P0AEX9
I	-423	GLY	-	expression tag	UNP P0AEX9
I	-422	GLY	-	expression tag	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-421	SER	-	expression tag	UNP P0AEX9
I	-420	ALA	-	expression tag	UNP P0AEX9
I	-419	TRP	-	expression tag	UNP P0AEX9
I	-418	SER	-	expression tag	UNP P0AEX9
I	-417	HIS	-	expression tag	UNP P0AEX9
I	-416	PRO	-	expression tag	UNP P0AEX9
I	-415	GLN	-	expression tag	UNP P0AEX9
I	-414	PHE	-	expression tag	UNP P0AEX9
I	-413	GLU	-	expression tag	UNP P0AEX9
I	-412	LYS	-	expression tag	UNP P0AEX9
I	-411	GLY	-	expression tag	UNP P0AEX9
I	-410	SER	-	expression tag	UNP P0AEX9
I	-409	MET	-	expression tag	UNP P0AEX9
I	-408	GLY	-	expression tag	UNP P0AEX9
I	-407	GLY	-	expression tag	UNP P0AEX9
I	-406	SER	-	expression tag	UNP P0AEX9
I	-405	HIS	-	expression tag	UNP P0AEX9
I	-404	HIS	-	expression tag	UNP P0AEX9
I	-403	HIS	-	expression tag	UNP P0AEX9
I	-402	HIS	-	expression tag	UNP P0AEX9
I	-401	HIS	-	expression tag	UNP P0AEX9
I	-400	HIS	-	expression tag	UNP P0AEX9
I	-399	HIS	-	expression tag	UNP P0AEX9
I	-398	HIS	-	expression tag	UNP P0AEX9
I	-397	HIS	-	expression tag	UNP P0AEX9
I	-396	HIS	-	expression tag	UNP P0AEX9
I	-395	GLY	-	expression tag	UNP P0AEX9
I	-394	MET	-	expression tag	UNP P0AEX9
I	-393	ALA	-	expression tag	UNP P0AEX9
I	-392	SER	-	expression tag	UNP P0AEX9
I	-391	MET	-	expression tag	UNP P0AEX9
I	-24	ASN	-	linker	UNP P0AEX9
I	-23	SER	-	linker	UNP P0AEX9
I	-22	SER	-	linker	UNP P0AEX9
I	-21	SER	-	linker	UNP P0AEX9
I	-20	ASN	-	linker	UNP P0AEX9
I	-19	ASN	-	linker	UNP P0AEX9
I	-18	ASN	-	linker	UNP P0AEX9
I	-17	ASN	-	linker	UNP P0AEX9
I	-16	ASN	-	linker	UNP P0AEX9
I	-15	ASN	-	linker	UNP P0AEX9
I	-14	ASN	-	linker	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-13	ASN	-	linker	UNP P0AEX9
I	-12	ASN	-	linker	UNP P0AEX9
I	-11	ASN	-	linker	UNP P0AEX9
I	-10	LEU	-	linker	UNP P0AEX9
I	-9	GLY	-	linker	UNP P0AEX9
I	-8	ILE	-	linker	UNP P0AEX9
I	-7	GLU	-	linker	UNP P0AEX9
I	-6	GLU	-	linker	UNP P0AEX9
I	-5	ASN	-	linker	UNP P0AEX9
I	-4	LEU	-	linker	UNP P0AEX9
I	-3	TYR	-	linker	UNP P0AEX9
I	-2	PHE	-	linker	UNP P0AEX9
I	-1	GLN	-	linker	UNP P0AEX9
I	0	SER	-	linker	UNP P0AEX9
I	1	MET	-	linker	UNP P0AEX9
I	2	LYS	-	linker	UNP P0AEX9
I	3	PHE	-	linker	UNP P0AEX9
I	4	ARG	-	linker	UNP P0AEX9
I	5	SER	-	linker	UNP P0AEX9
I	6	LEU	-	linker	UNP P0AEX9
I	7	TYR	-	linker	UNP P0AEX9
I	8	LYS	-	linker	UNP P0AEX9
J	-444	MET	-	initiating methionine	UNP P0AEX9
J	-443	GLY	-	expression tag	UNP P0AEX9
J	-442	GLY	-	expression tag	UNP P0AEX9
J	-441	SER	-	expression tag	UNP P0AEX9
J	-440	ALA	-	expression tag	UNP P0AEX9
J	-439	TRP	-	expression tag	UNP P0AEX9
J	-438	SER	-	expression tag	UNP P0AEX9
J	-437	HIS	-	expression tag	UNP P0AEX9
J	-436	PRO	-	expression tag	UNP P0AEX9
J	-435	GLN	-	expression tag	UNP P0AEX9
J	-434	PHE	-	expression tag	UNP P0AEX9
J	-433	GLU	-	expression tag	UNP P0AEX9
J	-432	LYS	-	expression tag	UNP P0AEX9
J	-431	GLY	-	expression tag	UNP P0AEX9
J	-430	GLY	-	expression tag	UNP P0AEX9
J	-429	GLY	-	expression tag	UNP P0AEX9
J	-428	SER	-	expression tag	UNP P0AEX9
J	-427	GLY	-	expression tag	UNP P0AEX9
J	-426	GLY	-	expression tag	UNP P0AEX9
J	-425	GLY	-	expression tag	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
J	-424	SER	-	expression tag	UNP P0AEX9
J	-423	GLY	-	expression tag	UNP P0AEX9
J	-422	GLY	-	expression tag	UNP P0AEX9
J	-421	SER	-	expression tag	UNP P0AEX9
J	-420	ALA	-	expression tag	UNP P0AEX9
J	-419	TRP	-	expression tag	UNP P0AEX9
J	-418	SER	-	expression tag	UNP P0AEX9
J	-417	HIS	-	expression tag	UNP P0AEX9
J	-416	PRO	-	expression tag	UNP P0AEX9
J	-415	GLN	-	expression tag	UNP P0AEX9
J	-414	PHE	-	expression tag	UNP P0AEX9
J	-413	GLU	-	expression tag	UNP P0AEX9
J	-412	LYS	-	expression tag	UNP P0AEX9
J	-411	GLY	-	expression tag	UNP P0AEX9
J	-410	SER	-	expression tag	UNP P0AEX9
J	-409	MET	-	expression tag	UNP P0AEX9
J	-408	GLY	-	expression tag	UNP P0AEX9
J	-407	GLY	-	expression tag	UNP P0AEX9
J	-406	SER	-	expression tag	UNP P0AEX9
J	-405	HIS	-	expression tag	UNP P0AEX9
J	-404	HIS	-	expression tag	UNP P0AEX9
J	-403	HIS	-	expression tag	UNP P0AEX9
J	-402	HIS	-	expression tag	UNP P0AEX9
J	-401	HIS	-	expression tag	UNP P0AEX9
J	-400	HIS	-	expression tag	UNP P0AEX9
J	-399	HIS	-	expression tag	UNP P0AEX9
J	-398	HIS	-	expression tag	UNP P0AEX9
J	-397	HIS	-	expression tag	UNP P0AEX9
J	-396	HIS	-	expression tag	UNP P0AEX9
J	-395	GLY	-	expression tag	UNP P0AEX9
J	-394	MET	-	expression tag	UNP P0AEX9
J	-393	ALA	-	expression tag	UNP P0AEX9
J	-392	SER	-	expression tag	UNP P0AEX9
J	-391	MET	-	expression tag	UNP P0AEX9
J	-24	ASN	-	linker	UNP P0AEX9
J	-23	SER	-	linker	UNP P0AEX9
J	-22	SER	-	linker	UNP P0AEX9
J	-21	SER	-	linker	UNP P0AEX9
J	-20	ASN	-	linker	UNP P0AEX9
J	-19	ASN	-	linker	UNP P0AEX9
J	-18	ASN	-	linker	UNP P0AEX9
J	-17	ASN	-	linker	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
J	-16	ASN	-	linker	UNP P0AEX9
J	-15	ASN	-	linker	UNP P0AEX9
J	-14	ASN	-	linker	UNP P0AEX9
J	-13	ASN	-	linker	UNP P0AEX9
J	-12	ASN	-	linker	UNP P0AEX9
J	-11	ASN	-	linker	UNP P0AEX9
J	-10	LEU	-	linker	UNP P0AEX9
J	-9	GLY	-	linker	UNP P0AEX9
J	-8	ILE	-	linker	UNP P0AEX9
J	-7	GLU	-	linker	UNP P0AEX9
J	-6	GLU	-	linker	UNP P0AEX9
J	-5	ASN	-	linker	UNP P0AEX9
J	-4	LEU	-	linker	UNP P0AEX9
J	-3	TYR	-	linker	UNP P0AEX9
J	-2	PHE	-	linker	UNP P0AEX9
J	-1	GLN	-	linker	UNP P0AEX9
J	0	SER	-	linker	UNP P0AEX9
J	1	MET	-	linker	UNP P0AEX9
J	2	LYS	-	linker	UNP P0AEX9
J	3	PHE	-	linker	UNP P0AEX9
J	4	ARG	-	linker	UNP P0AEX9
J	5	SER	-	linker	UNP P0AEX9
J	6	LEU	-	linker	UNP P0AEX9
J	7	TYR	-	linker	UNP P0AEX9
J	8	LYS	-	linker	UNP P0AEX9
K	-444	MET	-	initiating methionine	UNP P0AEX9
K	-443	GLY	-	expression tag	UNP P0AEX9
K	-442	GLY	-	expression tag	UNP P0AEX9
K	-441	SER	-	expression tag	UNP P0AEX9
K	-440	ALA	-	expression tag	UNP P0AEX9
K	-439	TRP	-	expression tag	UNP P0AEX9
K	-438	SER	-	expression tag	UNP P0AEX9
K	-437	HIS	-	expression tag	UNP P0AEX9
K	-436	PRO	-	expression tag	UNP P0AEX9
K	-435	GLN	-	expression tag	UNP P0AEX9
K	-434	PHE	-	expression tag	UNP P0AEX9
K	-433	GLU	-	expression tag	UNP P0AEX9
K	-432	LYS	-	expression tag	UNP P0AEX9
K	-431	GLY	-	expression tag	UNP P0AEX9
K	-430	GLY	-	expression tag	UNP P0AEX9
K	-429	GLY	-	expression tag	UNP P0AEX9
K	-428	SER	-	expression tag	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
K	-427	GLY	-	expression tag	UNP P0AEX9
K	-426	GLY	-	expression tag	UNP P0AEX9
K	-425	GLY	-	expression tag	UNP P0AEX9
K	-424	SER	-	expression tag	UNP P0AEX9
K	-423	GLY	-	expression tag	UNP P0AEX9
K	-422	GLY	-	expression tag	UNP P0AEX9
K	-421	SER	-	expression tag	UNP P0AEX9
K	-420	ALA	-	expression tag	UNP P0AEX9
K	-419	TRP	-	expression tag	UNP P0AEX9
K	-418	SER	-	expression tag	UNP P0AEX9
K	-417	HIS	-	expression tag	UNP P0AEX9
K	-416	PRO	-	expression tag	UNP P0AEX9
K	-415	GLN	-	expression tag	UNP P0AEX9
K	-414	PHE	-	expression tag	UNP P0AEX9
K	-413	GLU	-	expression tag	UNP P0AEX9
K	-412	LYS	-	expression tag	UNP P0AEX9
K	-411	GLY	-	expression tag	UNP P0AEX9
K	-410	SER	-	expression tag	UNP P0AEX9
K	-409	MET	-	expression tag	UNP P0AEX9
K	-408	GLY	-	expression tag	UNP P0AEX9
K	-407	GLY	-	expression tag	UNP P0AEX9
K	-406	SER	-	expression tag	UNP P0AEX9
K	-405	HIS	-	expression tag	UNP P0AEX9
K	-404	HIS	-	expression tag	UNP P0AEX9
K	-403	HIS	-	expression tag	UNP P0AEX9
K	-402	HIS	-	expression tag	UNP P0AEX9
K	-401	HIS	-	expression tag	UNP P0AEX9
K	-400	HIS	-	expression tag	UNP P0AEX9
K	-399	HIS	-	expression tag	UNP P0AEX9
K	-398	HIS	-	expression tag	UNP P0AEX9
K	-397	HIS	-	expression tag	UNP P0AEX9
K	-396	HIS	-	expression tag	UNP P0AEX9
K	-395	GLY	-	expression tag	UNP P0AEX9
K	-394	MET	-	expression tag	UNP P0AEX9
K	-393	ALA	-	expression tag	UNP P0AEX9
K	-392	SER	-	expression tag	UNP P0AEX9
K	-391	MET	-	expression tag	UNP P0AEX9
K	-24	ASN	-	linker	UNP P0AEX9
K	-23	SER	-	linker	UNP P0AEX9
K	-22	SER	-	linker	UNP P0AEX9
K	-21	SER	-	linker	UNP P0AEX9
K	-20	ASN	-	linker	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
K	-19	ASN	-	linker	UNP P0AEX9
K	-18	ASN	-	linker	UNP P0AEX9
K	-17	ASN	-	linker	UNP P0AEX9
K	-16	ASN	-	linker	UNP P0AEX9
K	-15	ASN	-	linker	UNP P0AEX9
K	-14	ASN	-	linker	UNP P0AEX9
K	-13	ASN	-	linker	UNP P0AEX9
K	-12	ASN	-	linker	UNP P0AEX9
K	-11	ASN	-	linker	UNP P0AEX9
K	-10	LEU	-	linker	UNP P0AEX9
K	-9	GLY	-	linker	UNP P0AEX9
K	-8	ILE	-	linker	UNP P0AEX9
K	-7	GLU	-	linker	UNP P0AEX9
K	-6	GLU	-	linker	UNP P0AEX9
K	-5	ASN	-	linker	UNP P0AEX9
K	-4	LEU	-	linker	UNP P0AEX9
K	-3	TYR	-	linker	UNP P0AEX9
K	-2	PHE	-	linker	UNP P0AEX9
K	-1	GLN	-	linker	UNP P0AEX9
K	0	SER	-	linker	UNP P0AEX9
K	1	MET	-	linker	UNP P0AEX9
K	2	LYS	-	linker	UNP P0AEX9
K	3	PHE	-	linker	UNP P0AEX9
K	4	ARG	-	linker	UNP P0AEX9
K	5	SER	-	linker	UNP P0AEX9
K	6	LEU	-	linker	UNP P0AEX9
K	7	TYR	-	linker	UNP P0AEX9
K	8	LYS	-	linker	UNP P0AEX9
L	-444	MET	-	initiating methionine	UNP P0AEX9
L	-443	GLY	-	expression tag	UNP P0AEX9
L	-442	GLY	-	expression tag	UNP P0AEX9
L	-441	SER	-	expression tag	UNP P0AEX9
L	-440	ALA	-	expression tag	UNP P0AEX9
L	-439	TRP	-	expression tag	UNP P0AEX9
L	-438	SER	-	expression tag	UNP P0AEX9
L	-437	HIS	-	expression tag	UNP P0AEX9
L	-436	PRO	-	expression tag	UNP P0AEX9
L	-435	GLN	-	expression tag	UNP P0AEX9
L	-434	PHE	-	expression tag	UNP P0AEX9
L	-433	GLU	-	expression tag	UNP P0AEX9
L	-432	LYS	-	expression tag	UNP P0AEX9
L	-431	GLY	-	expression tag	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
L	-430	GLY	-	expression tag	UNP P0AEX9
L	-429	GLY	-	expression tag	UNP P0AEX9
L	-428	SER	-	expression tag	UNP P0AEX9
L	-427	GLY	-	expression tag	UNP P0AEX9
L	-426	GLY	-	expression tag	UNP P0AEX9
L	-425	GLY	-	expression tag	UNP P0AEX9
L	-424	SER	-	expression tag	UNP P0AEX9
L	-423	GLY	-	expression tag	UNP P0AEX9
L	-422	GLY	-	expression tag	UNP P0AEX9
L	-421	SER	-	expression tag	UNP P0AEX9
L	-420	ALA	-	expression tag	UNP P0AEX9
L	-419	TRP	-	expression tag	UNP P0AEX9
L	-418	SER	-	expression tag	UNP P0AEX9
L	-417	HIS	-	expression tag	UNP P0AEX9
L	-416	PRO	-	expression tag	UNP P0AEX9
L	-415	GLN	-	expression tag	UNP P0AEX9
L	-414	PHE	-	expression tag	UNP P0AEX9
L	-413	GLU	-	expression tag	UNP P0AEX9
L	-412	LYS	-	expression tag	UNP P0AEX9
L	-411	GLY	-	expression tag	UNP P0AEX9
L	-410	SER	-	expression tag	UNP P0AEX9
L	-409	MET	-	expression tag	UNP P0AEX9
L	-408	GLY	-	expression tag	UNP P0AEX9
L	-407	GLY	-	expression tag	UNP P0AEX9
L	-406	SER	-	expression tag	UNP P0AEX9
L	-405	HIS	-	expression tag	UNP P0AEX9
L	-404	HIS	-	expression tag	UNP P0AEX9
L	-403	HIS	-	expression tag	UNP P0AEX9
L	-402	HIS	-	expression tag	UNP P0AEX9
L	-401	HIS	-	expression tag	UNP P0AEX9
L	-400	HIS	-	expression tag	UNP P0AEX9
L	-399	HIS	-	expression tag	UNP P0AEX9
L	-398	HIS	-	expression tag	UNP P0AEX9
L	-397	HIS	-	expression tag	UNP P0AEX9
L	-396	HIS	-	expression tag	UNP P0AEX9
L	-395	GLY	-	expression tag	UNP P0AEX9
L	-394	MET	-	expression tag	UNP P0AEX9
L	-393	ALA	-	expression tag	UNP P0AEX9
L	-392	SER	-	expression tag	UNP P0AEX9
L	-391	MET	-	expression tag	UNP P0AEX9
L	-24	ASN	-	linker	UNP P0AEX9
L	-23	SER	-	linker	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
L	-22	SER	-	linker	UNP P0AEX9
L	-21	SER	-	linker	UNP P0AEX9
L	-20	ASN	-	linker	UNP P0AEX9
L	-19	ASN	-	linker	UNP P0AEX9
L	-18	ASN	-	linker	UNP P0AEX9
L	-17	ASN	-	linker	UNP P0AEX9
L	-16	ASN	-	linker	UNP P0AEX9
L	-15	ASN	-	linker	UNP P0AEX9
L	-14	ASN	-	linker	UNP P0AEX9
L	-13	ASN	-	linker	UNP P0AEX9
L	-12	ASN	-	linker	UNP P0AEX9
L	-11	ASN	-	linker	UNP P0AEX9
L	-10	LEU	-	linker	UNP P0AEX9
L	-9	GLY	-	linker	UNP P0AEX9
L	-8	ILE	-	linker	UNP P0AEX9
L	-7	GLU	-	linker	UNP P0AEX9
L	-6	GLU	-	linker	UNP P0AEX9
L	-5	ASN	-	linker	UNP P0AEX9
L	-4	LEU	-	linker	UNP P0AEX9
L	-3	TYR	-	linker	UNP P0AEX9
L	-2	PHE	-	linker	UNP P0AEX9
L	-1	GLN	-	linker	UNP P0AEX9
L	0	SER	-	linker	UNP P0AEX9
L	1	MET	-	linker	UNP P0AEX9
L	2	LYS	-	linker	UNP P0AEX9
L	3	PHE	-	linker	UNP P0AEX9
L	4	ARG	-	linker	UNP P0AEX9
L	5	SER	-	linker	UNP P0AEX9
L	6	LEU	-	linker	UNP P0AEX9
L	7	TYR	-	linker	UNP P0AEX9
L	8	LYS	-	linker	UNP P0AEX9

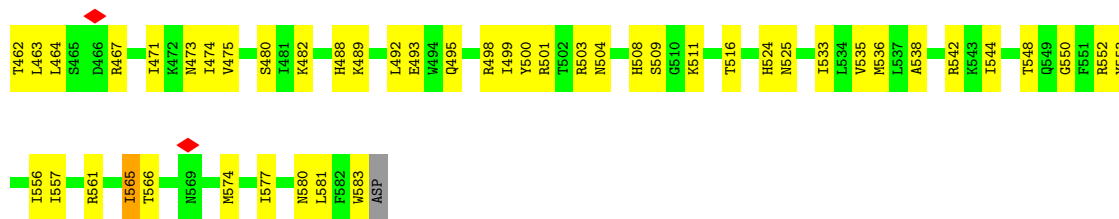
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
2	A	1	Total Zn 1 1	0
2	B	1	Total Zn 1 1	0
2	C	1	Total Zn 1 1	0
2	D	1	Total Zn 1 1	0

Continued on next page...

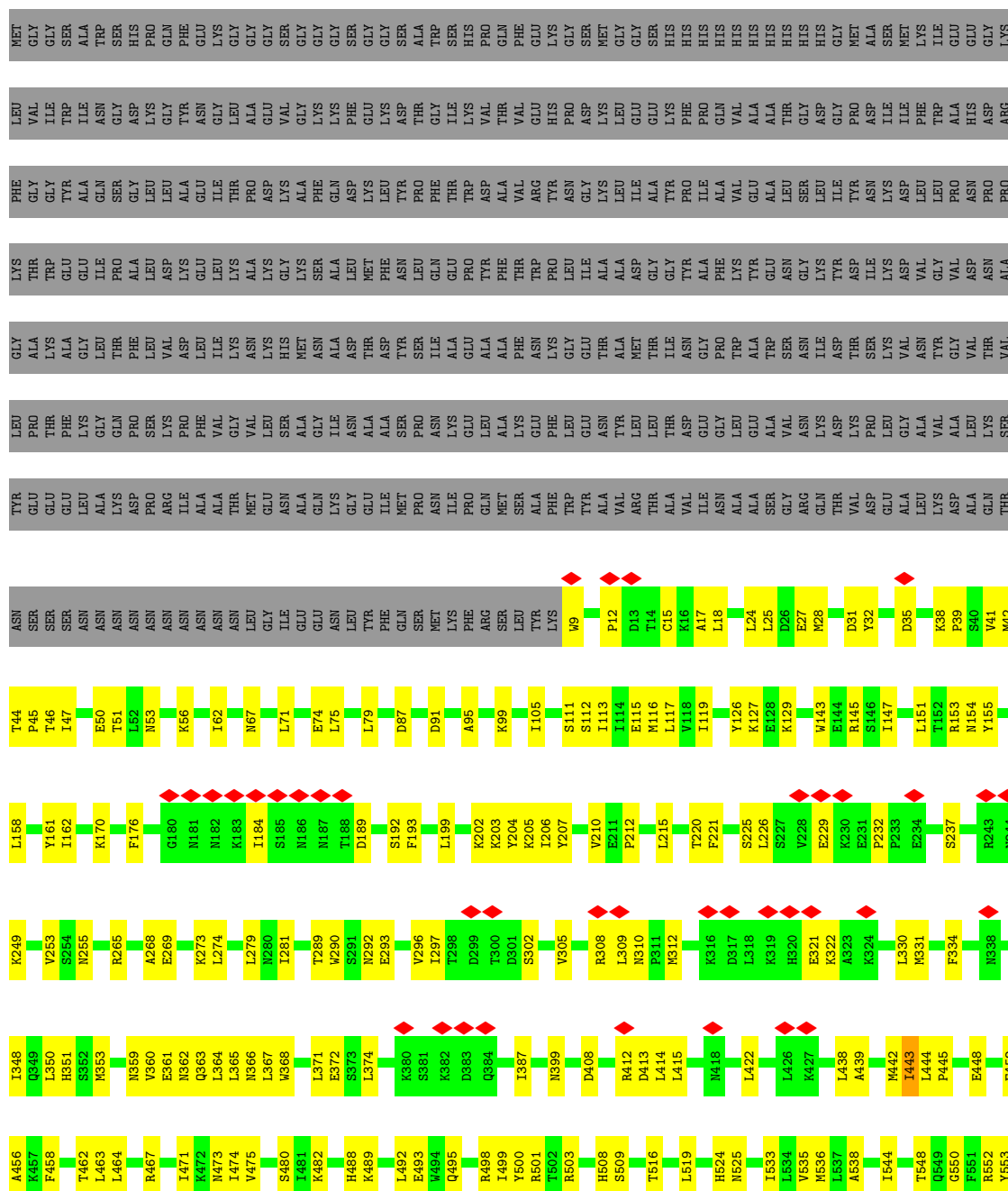
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
2	E	1	Total 1	Zn 1	0
2	F	1	Total 1	Zn 1	0
2	G	1	Total 1	Zn 1	0
2	H	1	Total 1	Zn 1	0
2	I	1	Total 1	Zn 1	0
2	J	1	Total 1	Zn 1	0
2	K	1	Total 1	Zn 1	0
2	L	1	Total 1	Zn 1	0



- Molecule 1: Maltose/maltodextrin-binding periplasmic protein, Bacterial antiviral defense protein Ec3ApeA from Escherichia coli strain KK-NP016

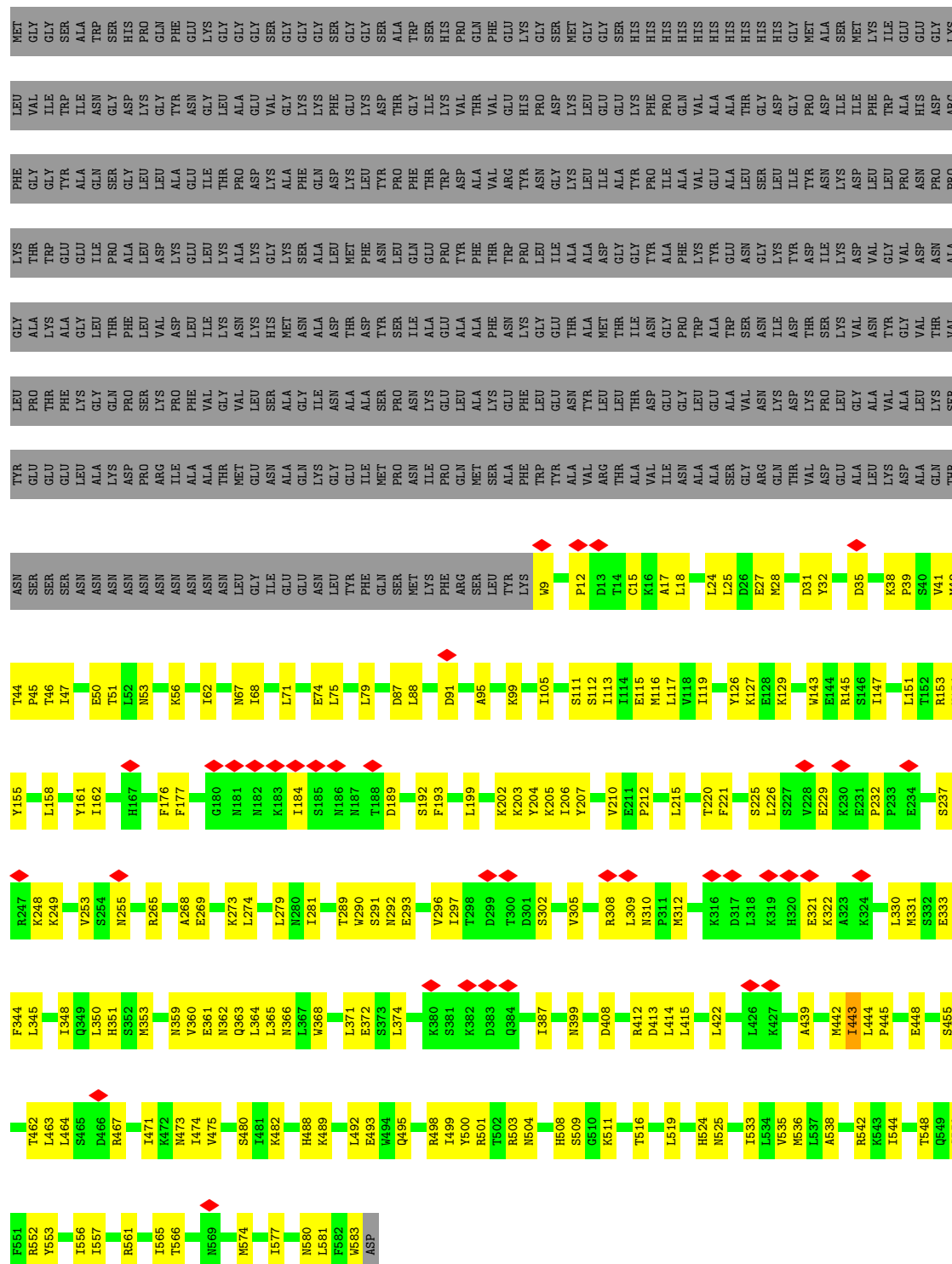
Chain C: 37% 19% 44%



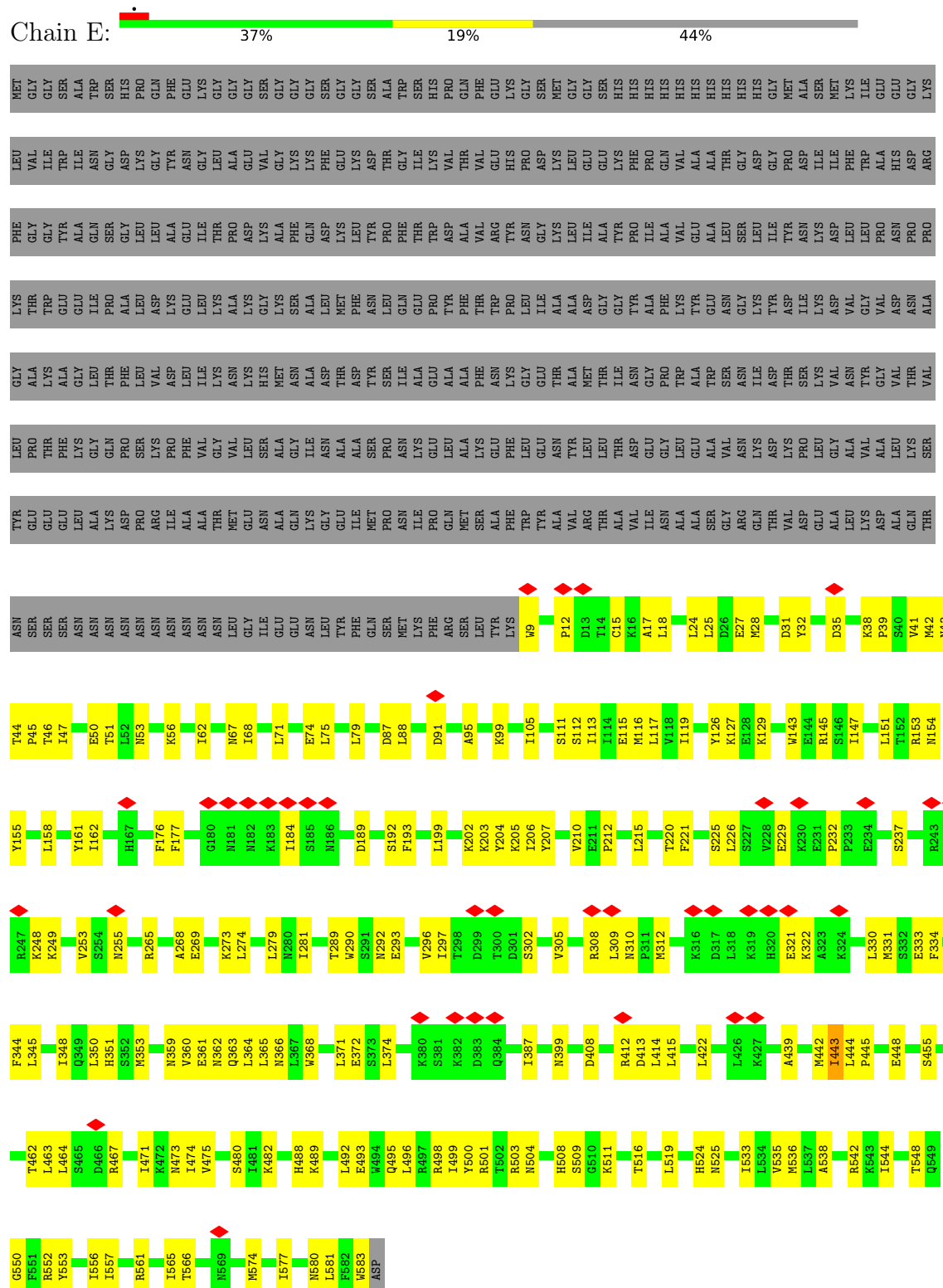


- Molecule 1: Maltose/maltodextrin-binding periplasmic protein, Bacterial antiviral defense protein Ec3ApeA from Escherichia coli strain KK-NP016

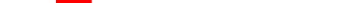
Chain D: 37% 19% 44%

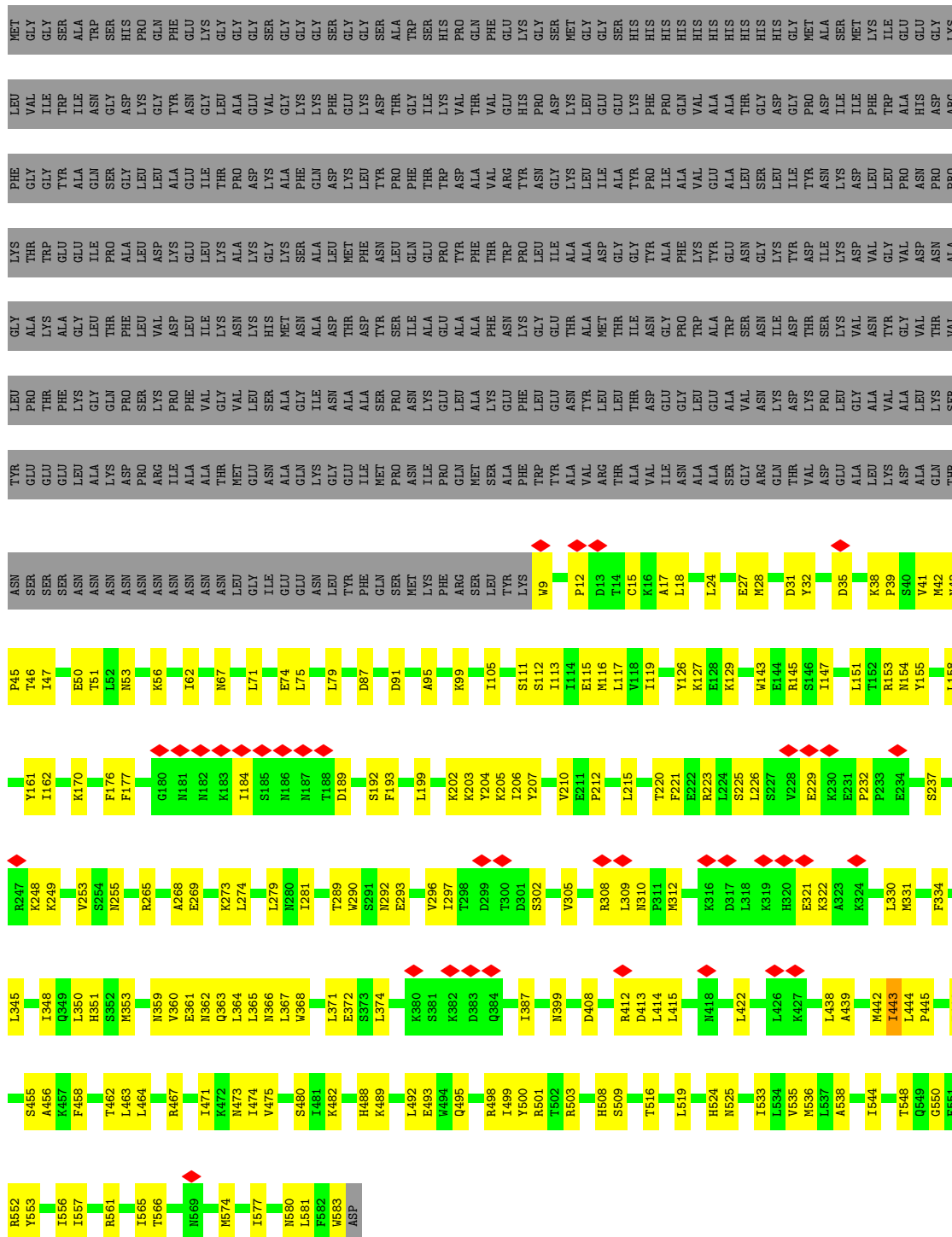


- Molecule 1: Maltose/maltodextrin-binding periplasmic protein,Bacterial antiviral defense protein Ec3ApeA from Escherichia coli strain KK-NP016

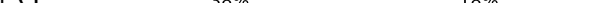


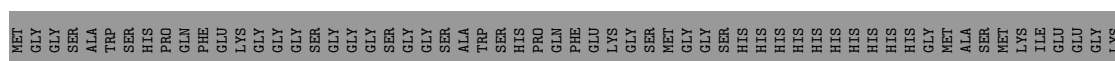
- Molecule 1: Maltose/maltodextrin-binding periplasmic protein,Bacterial antiviral defense protein Ec3ApeA from Escherichia coli strain KK-NP016

Chain F:  37% 19% 44%



- Molecule 1: Maltose/maltodextrin-binding periplasmic protein, Bacterial antiviral defense protein Ec3ApeA from *Escherichia coli* strain KK-NP016

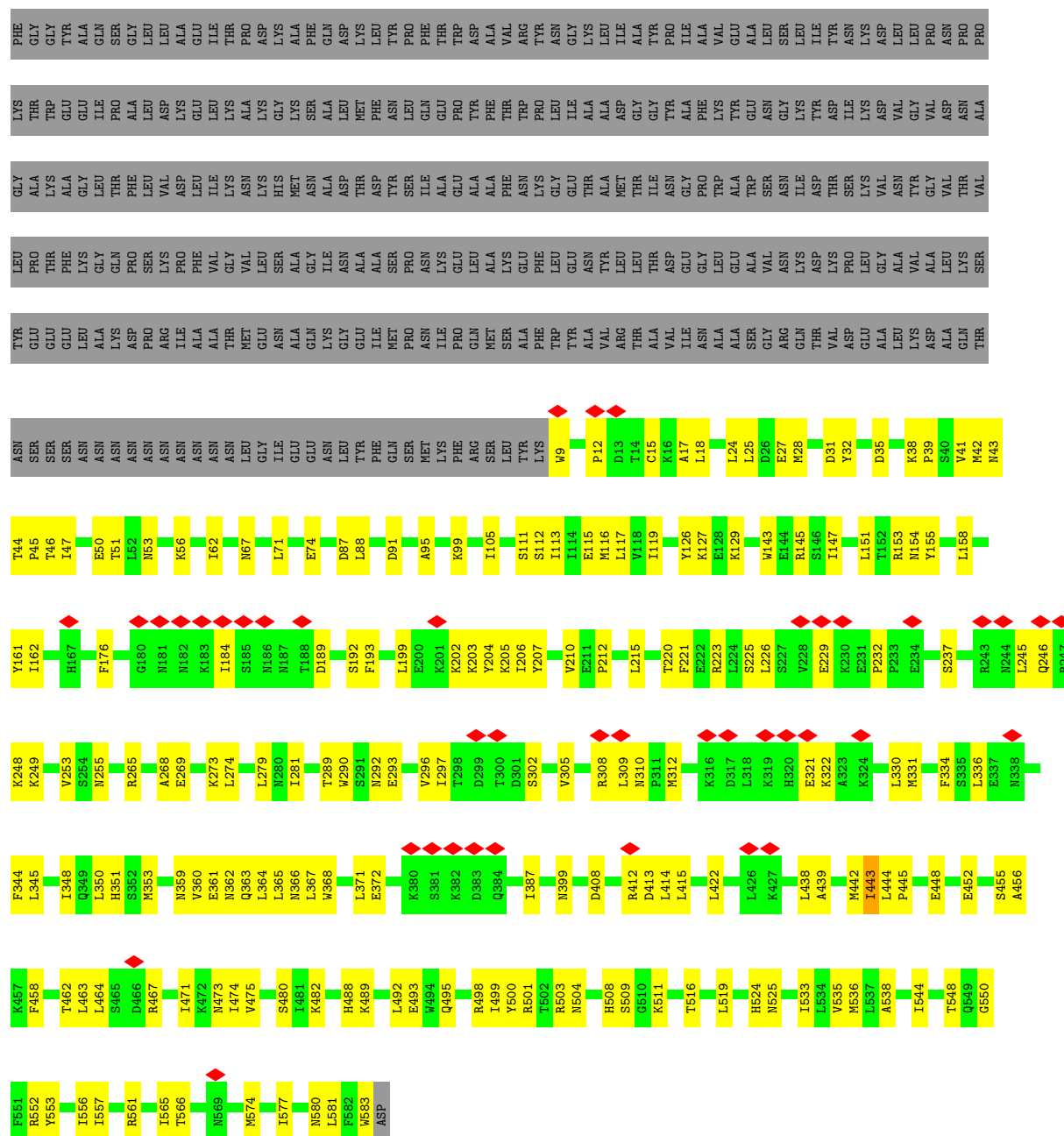
Chain G:  38% 18% 44%





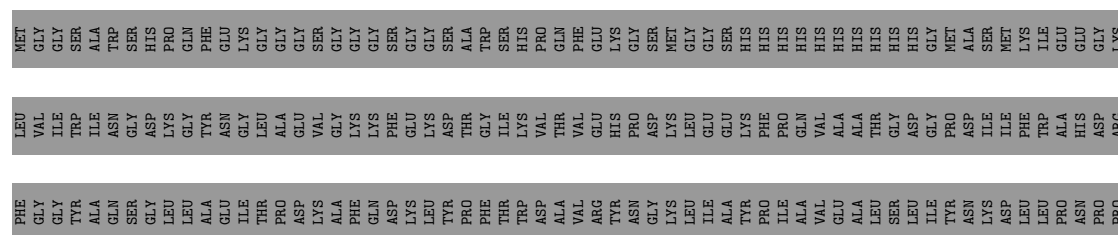
Frequency	Percentage
Daily	37%
Weekly	19%
Monthly	44%



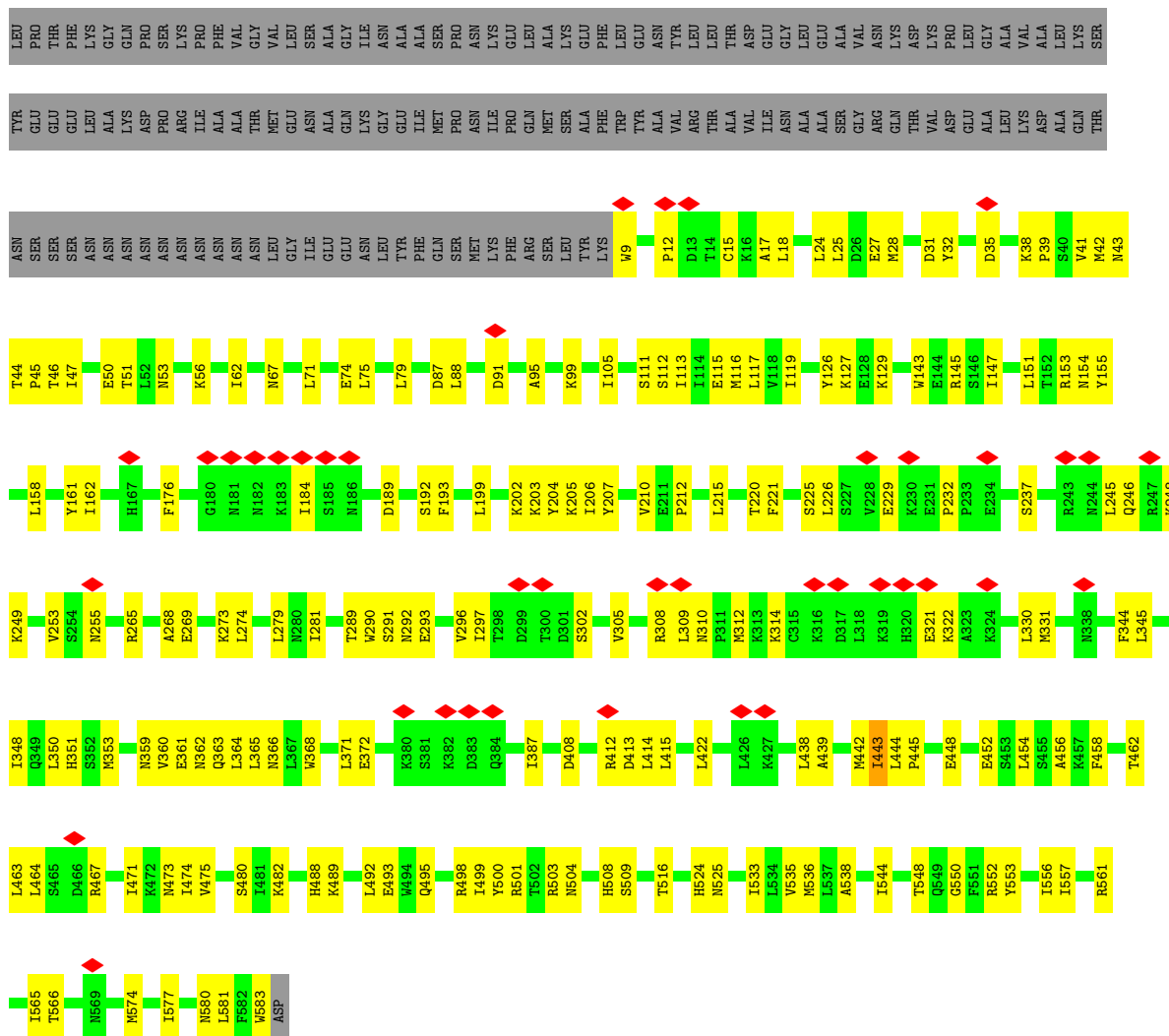


- Molecule 1: Maltose/maltodextrin-binding periplasmic protein, Bacterial antiviral defense protein Ec3ApeA from Escherichia coli strain KK-NP016

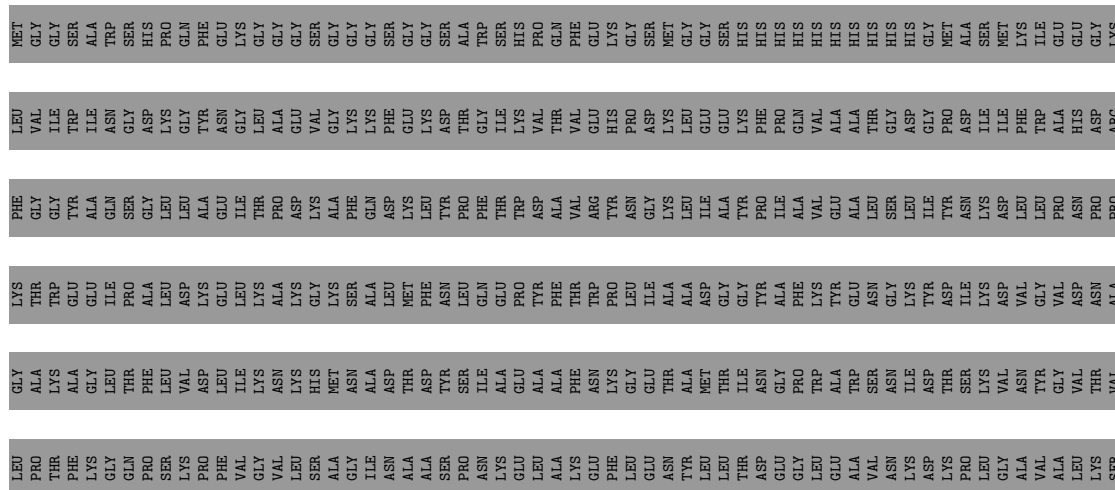
Chain I: 37% 19% 44%







- Molecule 1: Maltose/maltodextrin-binding periplasmic protein, Bacterial antiviral defense protein Ec3ApeA from *Escherichia coli* strain KK-NP016



R552	Y553	Y556	Y557	R561	T565	T566	R569	M574	I577	N580	L581	F582	F583	ASP	R247	K248	K249	L345	I348	G349	L350	H351	S352	M353	N359	V360	E361	N362	Q363	L364	L365	N366	L367	W368	E372	S373	L374	K380	S381	K382	D383	Q384	L387	D408	R412	D413	L414	M418	L422	L426	K427	L438	A439	M442	I443	L444	P445	E448	E452	S453	L454	S455	A456	F344
R457	F458	T462	L463	L464	R467	L471	K472	M473	L474	V475	S480	I481	K482	H488	K489	L492	E493	W494	Q495	R496	L499	Y500	R501	T502	R503	N504	H508	S509	G510	K511	T516	H524	N525	T533	L534	V535	M536	L537	A538	R542	K543	I544	T548	Q549	G550	F551																		
R247	K248	K249	L345	I348	G349	L350	H351	S352	M353	N359	V360	E361	N362	Q363	L364	L365	N366	L367	W368	E372	S373	L374	K380	S381	K382	D383	Q384	L387	D408	R412	D413	L414	M418	L422	L426	K427	L438	A439	M442	I443	L444	P445	E448	E452	S453	L454	S455	A456	F344															
R247	K248	K249	L345	I348	G349	L350	H351	S352	M353	N359	V360	E361	N362	Q363	L364	L365	N366	L367	W368	E372	S373	L374	K380	S381	K382	D383	Q384	L387	D408	R412	D413	L414	M418	L422	L426	K427	L438	A439	M442	I443	L444	P445	E448	E452	S453	L454	S455	A456	F344															
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R247	K248	K249	L345	I348	G349	L350	H351	S352	M353	N359	V360	E361	N362	Q363	L364	L365	N366	L367	W368	E372	S373	L374	K380	S381	K382	D383	Q384	L387	D408	R412	D413	L414	M418	L422	L426	K427	L438	A439	M442	I443	L444	P445	E448	E452	S453	L454	S455	A456	F344															
R247	K248	K249	L345	I348	G349	L350	H351	S352	M353	N359	V360	E361	N362	Q363	L364	L365	N366	L367	W368	E372	S373	L374	K380	S381	K382	D383	Q384	L387	D408	R412	D413	L414	M418	L422	L426	K427	L438	A439	M442	I443	L444	P445	E448	E452	S453	L454	S455	A456	F344															
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R247	K248	K249	L345	I348	G349	L350	H351	S352	M353	N359	V360	E361	N362	Q363	L364	L365	N366	L367	W368	E372	S373	L374	K380	S381	K382	D383	Q384	L387	D408	R412	D413	L414	M418	L422	L426	K427	L438	A439	M442	I443	L444	P445	E448	E452	S453	L454	S455	A456	F344															
R247	K248	K249	L345	I348	G349	L350	H351	S352																																																								

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D6	Depositor
Number of particles used	60670	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	92000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	34.546	Depositor
Minimum map value	-22.719	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	5	Depositor
Map size (Å)	369.6, 369.6, 369.6	wwPDB
Map dimensions	336, 336, 336	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	A	0.25	0/4582	0.48	0/6227
1	B	0.25	0/4582	0.48	0/6227
1	C	0.25	0/4582	0.48	0/6227
1	D	0.25	0/4582	0.48	0/6227
1	E	0.25	0/4582	0.48	0/6227
1	F	0.25	0/4582	0.48	0/6227
1	G	0.25	0/4582	0.48	0/6227
1	H	0.25	0/4582	0.48	0/6227
1	I	0.25	0/4582	0.48	0/6227
1	J	0.25	0/4582	0.48	0/6227
1	K	0.25	0/4582	0.48	0/6227
1	L	0.25	0/4582	0.48	0/6227
All	All	0.25	0/54984	0.48	0/74724

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 [i](#)

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	A	4483	0	4415	146	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	4483	0	4415	141	0
1	C	4483	0	4415	143	0
1	D	4483	0	4415	145	0
1	E	4483	0	4415	144	0
1	F	4483	0	4415	141	0
1	G	4483	0	4415	140	0
1	H	4483	0	4415	144	0
1	I	4483	0	4415	143	0
1	J	4483	0	4415	140	0
1	K	4483	0	4415	140	0
1	L	4483	0	4415	142	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
All	All	53808	0	52980	1617	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 15.

All (1617) 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:I:87:ASP:HB3	1:I:129:LYS:HE2	1.57	0.87
1:L:87:ASP:HB3	1:L:129:LYS:HE2	1.57	0.86
1:C:87:ASP:HB3	1:C:129:LYS:HE2	1.57	0.86
1:F:87:ASP:HB3	1:F:129:LYS:HE2	1.57	0.86
1:D:87:ASP:HB3	1:D:129:LYS:HE2	1.57	0.86
1:E:87:ASP:HB3	1:E:129:LYS:HE2	1.57	0.86
1:J:87:ASP:HB3	1:J:129:LYS:HE2	1.57	0.86
1:K:87:ASP:HB3	1:K:129:LYS:HE2	1.57	0.86
1:G:87:ASP:HB3	1:G:129:LYS:HE2	1.57	0.85
1:B:87:ASP:HB3	1:B:129:LYS:HE2	1.57	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:ASP:HB3	1:A:129:LYS:HE2	1.57	0.84
1:H:87:ASP:HB3	1:H:129:LYS:HE2	1.57	0.84
1:E:18:LEU:HD22	1:E:184:ILE:HG21	1.66	0.78
1:D:18:LEU:HD22	1:D:184:ILE:HG21	1.66	0.78
1:H:18:LEU:HD22	1:H:184:ILE:HG21	1.66	0.77
1:A:18:LEU:HD22	1:A:184:ILE:HG21	1.66	0.77
1:B:18:LEU:HD22	1:B:184:ILE:HG21	1.66	0.77
1:G:18:LEU:HD22	1:G:184:ILE:HG21	1.66	0.77
1:J:18:LEU:HD22	1:J:184:ILE:HG21	1.66	0.77
1:K:18:LEU:HD22	1:K:184:ILE:HG21	1.66	0.77
1:I:18:LEU:HD22	1:I:184:ILE:HG21	1.66	0.77
1:L:18:LEU:HD22	1:L:184:ILE:HG21	1.66	0.76
1:C:18:LEU:HD22	1:C:184:ILE:HG21	1.66	0.76
1:F:18:LEU:HD22	1:F:184:ILE:HG21	1.66	0.76
1:F:414:LEU:HB3	1:F:422:LEU:HD22	1.68	0.75
1:A:414:LEU:HB3	1:A:422:LEU:HD22	1.68	0.75
1:L:414:LEU:HB3	1:L:422:LEU:HD22	1.68	0.75
1:B:414:LEU:HB3	1:B:422:LEU:HD22	1.68	0.75
1:C:414:LEU:HB3	1:C:422:LEU:HD22	1.68	0.75
1:E:414:LEU:HB3	1:E:422:LEU:HD22	1.68	0.75
1:G:414:LEU:HB3	1:G:422:LEU:HD22	1.68	0.75
1:H:414:LEU:HB3	1:H:422:LEU:HD22	1.68	0.75
1:I:414:LEU:HB3	1:I:422:LEU:HD22	1.68	0.75
1:K:414:LEU:HB3	1:K:422:LEU:HD22	1.68	0.75
1:D:414:LEU:HB3	1:D:422:LEU:HD22	1.68	0.75
1:J:414:LEU:HB3	1:J:422:LEU:HD22	1.68	0.75
1:C:44:THR:OG1	1:C:45:PRO:HD3	1.88	0.74
1:F:44:THR:OG1	1:F:45:PRO:HD3	1.88	0.74
1:G:44:THR:OG1	1:G:45:PRO:HD3	1.88	0.74
1:B:44:THR:OG1	1:B:45:PRO:HD3	1.88	0.74
1:K:44:THR:OG1	1:K:45:PRO:HD3	1.88	0.74
1:J:44:THR:OG1	1:J:45:PRO:HD3	1.88	0.73
1:L:44:THR:OG1	1:L:45:PRO:HD3	1.88	0.73
1:D:44:THR:OG1	1:D:45:PRO:HD3	1.88	0.73
1:E:44:THR:OG1	1:E:45:PRO:HD3	1.88	0.73
1:I:44:THR:OG1	1:I:45:PRO:HD3	1.88	0.73
1:A:44:THR:OG1	1:A:45:PRO:HD3	1.88	0.72
1:H:44:THR:OG1	1:H:45:PRO:HD3	1.88	0.72
1:C:274:LEU:HD21	1:D:345:LEU:HD22	1.71	0.71
1:I:27:GLU:OE2	1:I:467:ARG:NH2	2.23	0.71
1:J:27:GLU:OE2	1:J:467:ARG:NH2	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:345:LEU:HD22	1:D:274:LEU:HD21	1.72	0.71
1:K:27:GLU:OE2	1:K:467:ARG:NH2	2.23	0.71
1:L:27:GLU:OE2	1:L:467:ARG:NH2	2.23	0.71
1:B:27:GLU:OE2	1:B:467:ARG:NH2	2.23	0.71
1:G:27:GLU:OE2	1:G:467:ARG:NH2	2.23	0.71
1:I:274:LEU:HD21	1:J:345:LEU:HD22	1.73	0.71
1:I:345:LEU:HD22	1:J:274:LEU:HD21	1.74	0.70
1:K:345:LEU:HD22	1:L:274:LEU:HD21	1.74	0.70
1:D:27:GLU:OE2	1:D:467:ARG:NH2	2.23	0.70
1:E:27:GLU:OE2	1:E:467:ARG:NH2	2.23	0.70
1:E:345:LEU:HD22	1:F:274:LEU:HD21	1.73	0.70
1:C:27:GLU:OE2	1:C:467:ARG:NH2	2.23	0.70
1:A:27:GLU:OE2	1:A:467:ARG:NH2	2.23	0.70
1:E:274:LEU:HD21	1:F:345:LEU:HD22	1.74	0.70
1:F:27:GLU:OE2	1:F:467:ARG:NH2	2.23	0.70
1:K:274:LEU:HD21	1:L:345:LEU:HD22	1.74	0.70
1:C:413:ASP:OD2	1:C:467:ARG:NH1	2.25	0.69
1:D:413:ASP:OD2	1:D:467:ARG:NH1	2.25	0.69
1:F:413:ASP:OD2	1:F:467:ARG:NH1	2.25	0.69
1:H:27:GLU:OE2	1:H:467:ARG:NH2	2.23	0.69
1:E:413:ASP:OD2	1:E:467:ARG:NH1	2.25	0.69
1:J:413:ASP:OD2	1:J:467:ARG:NH1	2.25	0.69
1:K:413:ASP:OD2	1:K:467:ARG:NH1	2.25	0.69
1:B:413:ASP:OD2	1:B:467:ARG:NH1	2.25	0.69
1:G:274:LEU:HD21	1:H:345:LEU:HD22	1.75	0.69
1:G:413:ASP:OD2	1:G:467:ARG:NH1	2.25	0.69
1:H:413:ASP:OD2	1:H:467:ARG:NH1	2.25	0.69
1:A:345:LEU:HD22	1:B:274:LEU:HD21	1.75	0.69
1:A:413:ASP:OD2	1:A:467:ARG:NH1	2.25	0.69
1:G:345:LEU:HD22	1:H:274:LEU:HD21	1.74	0.69
1:A:274:LEU:HD21	1:B:345:LEU:HD22	1.75	0.69
1:L:413:ASP:OD2	1:L:467:ARG:NH1	2.25	0.68
1:I:413:ASP:OD2	1:I:467:ARG:NH1	2.25	0.68
1:C:31:ASP:OD1	1:C:32:TYR:CD1	2.47	0.68
1:F:31:ASP:OD1	1:F:32:TYR:CD1	2.47	0.68
1:A:31:ASP:OD1	1:A:32:TYR:CD1	2.47	0.68
1:B:28:MET:HE1	1:B:153:ARG:HA	1.76	0.68
1:G:28:MET:HE1	1:G:153:ARG:HA	1.76	0.68
1:K:31:ASP:OD1	1:K:32:TYR:CD1	2.47	0.68
1:L:31:ASP:OD1	1:L:32:TYR:CD1	2.47	0.68
1:D:31:ASP:OD1	1:D:32:TYR:CD1	2.47	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:87:ASP:CB	1:G:129:LYS:HE2	2.24	0.68
1:H:31:ASP:OD1	1:H:32:TYR:CD1	2.47	0.68
1:I:31:ASP:OD1	1:I:32:TYR:CD1	2.47	0.68
1:J:28:MET:HE1	1:J:153:ARG:HA	1.76	0.68
1:K:28:MET:HE1	1:K:153:ARG:HA	1.76	0.68
1:E:31:ASP:OD1	1:E:32:TYR:CD1	2.47	0.67
1:J:31:ASP:OD1	1:J:32:TYR:CD1	2.47	0.67
1:A:205:LYS:HE2	1:A:207:TYR:OH	1.95	0.67
1:B:87:ASP:CB	1:B:129:LYS:HE2	2.24	0.67
1:L:28:MET:HE1	1:L:153:ARG:HA	1.76	0.67
1:H:205:LYS:HE2	1:H:207:TYR:OH	1.95	0.67
1:F:205:LYS:HE2	1:F:207:TYR:OH	1.95	0.67
1:C:205:LYS:HE2	1:C:207:TYR:OH	1.95	0.67
1:G:31:ASP:OD1	1:G:32:TYR:CD1	2.47	0.67
1:I:28:MET:HE1	1:I:153:ARG:HA	1.77	0.67
1:B:31:ASP:OD1	1:B:32:TYR:CD1	2.47	0.67
1:D:28:MET:HE1	1:D:153:ARG:HA	1.76	0.67
1:D:41:VAL:HG21	1:D:495:GLN:HE22	1.60	0.67
1:E:41:VAL:HG21	1:E:495:GLN:HE22	1.60	0.67
1:J:205:LYS:HE2	1:J:207:TYR:OH	1.95	0.67
1:K:205:LYS:HE2	1:K:207:TYR:OH	1.95	0.67
1:E:28:MET:HE1	1:E:153:ARG:HA	1.77	0.67
1:L:87:ASP:CB	1:L:129:LYS:HE2	2.24	0.67
1:B:41:VAL:HG21	1:B:495:GLN:HE22	1.60	0.67
1:I:87:ASP:CB	1:I:129:LYS:HE2	2.24	0.67
1:G:41:VAL:HG21	1:G:495:GLN:HE22	1.60	0.67
1:A:28:MET:HE1	1:A:153:ARG:HA	1.76	0.66
1:F:87:ASP:CB	1:F:129:LYS:HE2	2.24	0.66
1:H:28:MET:HE1	1:H:153:ARG:HA	1.76	0.66
1:J:87:ASP:CB	1:J:129:LYS:HE2	2.24	0.66
1:K:366:ASN:ND2	1:L:353:MET:SD	2.65	0.66
1:C:87:ASP:CB	1:C:129:LYS:HE2	2.24	0.66
1:I:353:MET:SD	1:J:366:ASN:ND2	2.65	0.66
1:K:87:ASP:CB	1:K:129:LYS:HE2	2.24	0.66
1:I:366:ASN:ND2	1:J:353:MET:SD	2.65	0.66
1:C:41:VAL:HG21	1:C:495:GLN:HE22	1.60	0.66
1:F:41:VAL:HG21	1:F:495:GLN:HE22	1.60	0.66
1:G:366:ASN:ND2	1:H:353:MET:SD	2.66	0.66
1:B:359:ASN:HB3	1:B:362:ASN:HB2	1.78	0.66
1:C:28:MET:HE1	1:C:153:ARG:HA	1.76	0.66
1:H:359:ASN:HB3	1:H:362:ASN:HB2	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:205:LYS:HE2	1:I:207:TYR:OH	1.95	0.66
1:L:205:LYS:HE2	1:L:207:TYR:OH	1.95	0.66
1:A:359:ASN:HB3	1:A:362:ASN:HB2	1.78	0.66
1:C:353:MET:SD	1:D:366:ASN:ND2	2.64	0.66
1:G:359:ASN:HB3	1:G:362:ASN:HB2	1.78	0.66
1:H:87:ASP:CB	1:H:129:LYS:HE2	2.24	0.66
1:A:87:ASP:CB	1:A:129:LYS:HE2	2.24	0.66
1:E:205:LYS:HE2	1:E:207:TYR:OH	1.95	0.66
1:F:28:MET:HE1	1:F:153:ARG:HA	1.77	0.66
1:G:205:LYS:HE2	1:G:207:TYR:OH	1.95	0.66
1:I:41:VAL:HG21	1:I:495:GLN:HE22	1.60	0.66
1:K:359:ASN:HB3	1:K:362:ASN:HB2	1.78	0.66
1:B:205:LYS:HE2	1:B:207:TYR:OH	1.95	0.66
1:C:359:ASN:HB3	1:C:362:ASN:HB2	1.78	0.66
1:D:87:ASP:CB	1:D:129:LYS:HE2	2.24	0.66
1:D:359:ASN:HB3	1:D:362:ASN:HB2	1.78	0.66
1:E:359:ASN:HB3	1:E:362:ASN:HB2	1.78	0.66
1:J:359:ASN:HB3	1:J:362:ASN:HB2	1.78	0.66
1:L:41:VAL:HG21	1:L:495:GLN:HE22	1.60	0.66
1:L:359:ASN:HB3	1:L:362:ASN:HB2	1.78	0.66
1:D:205:LYS:HE2	1:D:207:TYR:OH	1.95	0.65
1:F:359:ASN:HB3	1:F:362:ASN:HB2	1.78	0.65
1:I:359:ASN:HB3	1:I:362:ASN:HB2	1.78	0.65
1:E:87:ASP:CB	1:E:129:LYS:HE2	2.24	0.65
1:A:353:MET:SD	1:B:366:ASN:ND2	2.66	0.65
1:J:41:VAL:HG21	1:J:495:GLN:HE22	1.60	0.65
1:K:353:MET:SD	1:L:366:ASN:ND2	2.65	0.65
1:K:41:VAL:HG21	1:K:495:GLN:HE22	1.60	0.65
1:E:366:ASN:ND2	1:F:353:MET:SD	2.65	0.65
1:A:43:ASN:HD21	1:A:158:LEU:HB2	1.62	0.65
1:H:43:ASN:HD21	1:H:158:LEU:HB2	1.62	0.65
1:A:41:VAL:HG21	1:A:495:GLN:HE22	1.60	0.65
1:J:43:ASN:HD21	1:J:158:LEU:HB2	1.62	0.65
1:K:43:ASN:HD21	1:K:158:LEU:HB2	1.62	0.65
1:F:43:ASN:HD21	1:F:158:LEU:HB2	1.62	0.64
1:H:41:VAL:HG21	1:H:495:GLN:HE22	1.60	0.64
1:C:43:ASN:HD21	1:C:158:LEU:HB2	1.62	0.64
1:C:366:ASN:ND2	1:D:353:MET:SD	2.64	0.64
1:C:212:PRO:HA	1:C:215:LEU:HD23	1.81	0.63
1:I:43:ASN:HD21	1:I:158:LEU:HB2	1.62	0.63
1:L:43:ASN:HD21	1:L:158:LEU:HB2	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:212:PRO:HA	1:F:215:LEU:HD23	1.81	0.63
1:D:212:PRO:HA	1:D:215:LEU:HD23	1.81	0.63
1:E:212:PRO:HA	1:E:215:LEU:HD23	1.81	0.63
1:E:43:ASN:HD21	1:E:158:LEU:HB2	1.62	0.63
1:A:212:PRO:HA	1:A:215:LEU:HD23	1.81	0.63
1:D:43:ASN:HD21	1:D:158:LEU:HB2	1.62	0.63
1:E:353:MET:SD	1:F:366:ASN:ND2	2.65	0.63
1:H:212:PRO:HA	1:H:215:LEU:HD23	1.81	0.63
1:J:212:PRO:HA	1:J:215:LEU:HD23	1.81	0.62
1:K:212:PRO:HA	1:K:215:LEU:HD23	1.81	0.62
1:H:206:ILE:HG12	1:H:296:VAL:HG13	1.82	0.62
1:A:206:ILE:HG12	1:A:296:VAL:HG13	1.82	0.62
1:F:206:ILE:HG12	1:F:296:VAL:HG13	1.82	0.62
1:C:206:ILE:HG12	1:C:296:VAL:HG13	1.82	0.62
1:B:212:PRO:HA	1:B:215:LEU:HD23	1.81	0.62
1:G:212:PRO:HA	1:G:215:LEU:HD23	1.81	0.62
1:I:212:PRO:HA	1:I:215:LEU:HD23	1.81	0.62
1:L:212:PRO:HA	1:L:215:LEU:HD23	1.81	0.62
1:G:43:ASN:HD21	1:G:158:LEU:HB2	1.62	0.62
1:K:206:ILE:HG12	1:K:296:VAL:HG13	1.82	0.62
1:D:206:ILE:HG12	1:D:296:VAL:HG13	1.82	0.62
1:E:206:ILE:HG12	1:E:296:VAL:HG13	1.82	0.62
1:J:206:ILE:HG12	1:J:296:VAL:HG13	1.82	0.62
1:B:43:ASN:HD21	1:B:158:LEU:HB2	1.62	0.61
1:I:111:SER:O	1:I:115:GLU:HG3	2.01	0.61
1:J:62:ILE:HG23	1:J:508:HIS:HB2	1.82	0.61
1:K:62:ILE:HG23	1:K:508:HIS:HB2	1.82	0.61
1:L:111:SER:O	1:L:115:GLU:HG3	2.01	0.61
1:B:111:SER:O	1:B:115:GLU:HG3	2.01	0.61
1:I:206:ILE:HG12	1:I:296:VAL:HG13	1.82	0.61
1:L:206:ILE:HG12	1:L:296:VAL:HG13	1.82	0.61
1:B:206:ILE:HG12	1:B:296:VAL:HG13	1.82	0.61
1:D:111:SER:O	1:D:115:GLU:HG3	2.01	0.61
1:E:111:SER:O	1:E:115:GLU:HG3	2.01	0.61
1:G:206:ILE:HG12	1:G:296:VAL:HG13	1.82	0.61
1:G:111:SER:O	1:G:115:GLU:HG3	2.01	0.61
1:I:62:ILE:HG23	1:I:508:HIS:HB2	1.82	0.61
1:B:62:ILE:HG23	1:B:508:HIS:HB2	1.82	0.61
1:D:62:ILE:HG23	1:D:508:HIS:HB2	1.82	0.61
1:C:62:ILE:HG23	1:C:508:HIS:HB2	1.82	0.61
1:C:111:SER:O	1:C:115:GLU:HG3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:62:ILE:HG23	1:E:508:HIS:HB2	1.82	0.61
1:G:62:ILE:HG23	1:G:508:HIS:HB2	1.82	0.61
1:J:111:SER:O	1:J:115:GLU:HG3	2.01	0.61
1:K:111:SER:O	1:K:115:GLU:HG3	2.01	0.61
1:L:62:ILE:HG23	1:L:508:HIS:HB2	1.82	0.61
1:F:62:ILE:HG23	1:F:508:HIS:HB2	1.82	0.60
1:F:111:SER:O	1:F:115:GLU:HG3	2.01	0.60
1:A:111:SER:O	1:A:115:GLU:HG3	2.01	0.60
1:H:62:ILE:HG23	1:H:508:HIS:HB2	1.82	0.60
1:A:62:ILE:HG23	1:A:508:HIS:HB2	1.82	0.60
1:A:91:ASP:OD1	1:A:91:ASP:N	2.35	0.60
1:B:310:ASN:HB2	1:B:363:GLN:HE22	1.67	0.60
1:E:310:ASN:HB2	1:E:363:GLN:HE22	1.66	0.60
1:G:310:ASN:HB2	1:G:363:GLN:HE22	1.67	0.60
1:H:111:SER:O	1:H:115:GLU:HG3	2.01	0.60
1:J:310:ASN:HB2	1:J:363:GLN:HE22	1.67	0.60
1:B:91:ASP:N	1:B:91:ASP:OD1	2.35	0.60
1:D:310:ASN:HB2	1:D:363:GLN:HE22	1.67	0.60
1:G:91:ASP:N	1:G:91:ASP:OD1	2.35	0.60
1:J:91:ASP:OD1	1:J:91:ASP:N	2.35	0.60
1:K:91:ASP:OD1	1:K:91:ASP:N	2.35	0.60
1:K:310:ASN:HB2	1:K:363:GLN:HE22	1.67	0.60
1:A:310:ASN:HB2	1:A:363:GLN:HE22	1.67	0.60
1:D:473:ASN:O	1:D:480:SER:OG	2.20	0.60
1:E:473:ASN:O	1:E:480:SER:OG	2.20	0.60
1:H:310:ASN:HB2	1:H:363:GLN:HE22	1.67	0.60
1:I:310:ASN:HB2	1:I:363:GLN:HE22	1.67	0.60
1:D:91:ASP:N	1:D:91:ASP:OD1	2.35	0.60
1:I:91:ASP:OD1	1:I:91:ASP:N	2.35	0.60
1:L:91:ASP:OD1	1:L:91:ASP:N	2.35	0.60
1:E:91:ASP:OD1	1:E:91:ASP:N	2.35	0.60
1:K:473:ASN:O	1:K:480:SER:OG	2.20	0.60
1:L:310:ASN:HB2	1:L:363:GLN:HE22	1.67	0.60
1:A:445:PRO:O	1:A:448:GLU:HB2	2.02	0.59
1:H:445:PRO:O	1:H:448:GLU:HB2	2.02	0.59
1:H:473:ASN:O	1:H:480:SER:OG	2.20	0.59
1:I:445:PRO:O	1:I:448:GLU:HB2	2.02	0.59
1:J:473:ASN:O	1:J:480:SER:OG	2.20	0.59
1:K:445:PRO:O	1:K:448:GLU:HB2	2.02	0.59
1:L:445:PRO:O	1:L:448:GLU:HB2	2.02	0.59
1:A:473:ASN:O	1:A:480:SER:OG	2.20	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:445:PRO:O	1:J:448:GLU:HB2	2.02	0.59
1:G:473:ASN:O	1:G:480:SER:OG	2.20	0.59
1:A:544:ILE:HG21	1:A:550:GLY:HA2	1.85	0.59
1:C:310:ASN:HB2	1:C:363:GLN:HE22	1.66	0.59
1:I:544:ILE:HG21	1:I:550:GLY:HA2	1.85	0.59
1:J:544:ILE:HG21	1:J:550:GLY:HA2	1.85	0.59
1:L:544:ILE:HG21	1:L:550:GLY:HA2	1.85	0.59
1:A:366:ASN:ND2	1:B:353:MET:SD	2.66	0.59
1:B:544:ILE:HG21	1:B:550:GLY:HA2	1.85	0.59
1:F:310:ASN:HB2	1:F:363:GLN:HE22	1.67	0.59
1:F:445:PRO:O	1:F:448:GLU:HB2	2.02	0.59
1:G:445:PRO:O	1:G:448:GLU:HB2	2.02	0.59
1:H:544:ILE:HG21	1:H:550:GLY:HA2	1.85	0.59
1:K:544:ILE:HG21	1:K:550:GLY:HA2	1.85	0.59
1:B:445:PRO:O	1:B:448:GLU:HB2	2.02	0.59
1:B:473:ASN:O	1:B:480:SER:OG	2.20	0.59
1:C:445:PRO:O	1:C:448:GLU:HB2	2.02	0.59
1:G:544:ILE:HG21	1:G:550:GLY:HA2	1.85	0.59
1:F:544:ILE:HG21	1:F:550:GLY:HA2	1.85	0.59
1:C:473:ASN:O	1:C:480:SER:OG	2.20	0.59
1:C:544:ILE:HG21	1:C:550:GLY:HA2	1.85	0.59
1:D:544:ILE:HG21	1:D:550:GLY:HA2	1.85	0.58
1:G:353:MET:SD	1:H:366:ASN:ND2	2.66	0.58
1:E:544:ILE:HG21	1:E:550:GLY:HA2	1.85	0.58
1:F:473:ASN:O	1:F:480:SER:OG	2.20	0.58
1:F:91:ASP:OD1	1:F:91:ASP:N	2.35	0.58
1:E:365:LEU:HD12	1:F:350:LEU:HD21	1.85	0.58
1:G:74:GLU:OE1	1:G:498:ARG:NH2	2.32	0.58
1:A:350:LEU:HD21	1:B:365:LEU:HD12	1.86	0.58
1:D:445:PRO:O	1:D:448:GLU:HB2	2.02	0.58
1:F:47:ILE:O	1:F:51:THR:OG1	2.20	0.58
1:G:365:LEU:HD12	1:H:350:LEU:HD21	1.86	0.58
1:B:74:GLU:OE1	1:B:498:ARG:NH2	2.32	0.58
1:C:47:ILE:O	1:C:51:THR:OG1	2.20	0.58
1:E:445:PRO:O	1:E:448:GLU:HB2	2.02	0.58
1:C:350:LEU:HD21	1:D:365:LEU:HD12	1.86	0.58
1:D:74:GLU:OE1	1:D:498:ARG:NH2	2.32	0.57
1:E:74:GLU:OE1	1:E:498:ARG:NH2	2.32	0.57
1:J:47:ILE:O	1:J:51:THR:OG1	2.20	0.57
1:A:365:LEU:HD12	1:B:350:LEU:HD21	1.86	0.57
1:C:345:LEU:HD22	1:D:274:LEU:CD2	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:47:ILE:O	1:K:51:THR:OG1	2.20	0.57
1:K:105:ILE:HD11	1:K:113:ILE:HD12	1.87	0.57
1:K:350:LEU:HD21	1:L:365:LEU:HD12	1.86	0.57
1:I:473:ASN:O	1:I:480:SER:OG	2.20	0.57
1:J:105:ILE:HD11	1:J:113:ILE:HD12	1.87	0.57
1:I:365:LEU:HD12	1:J:350:LEU:HD21	1.86	0.57
1:K:365:LEU:HD12	1:L:350:LEU:HD21	1.85	0.57
1:E:350:LEU:HD21	1:F:365:LEU:HD12	1.85	0.56
1:L:473:ASN:O	1:L:480:SER:OG	2.20	0.56
1:B:47:ILE:O	1:B:51:THR:OG1	2.20	0.56
1:C:274:LEU:CD2	1:D:345:LEU:HD22	2.34	0.56
1:E:253:VAL:HG21	1:E:268:ALA:HB1	1.87	0.56
1:A:105:ILE:HD11	1:A:113:ILE:HD12	1.87	0.56
1:D:253:VAL:HG21	1:D:268:ALA:HB1	1.87	0.56
1:G:350:LEU:HD21	1:H:365:LEU:HD12	1.86	0.56
1:H:105:ILE:HD11	1:H:113:ILE:HD12	1.87	0.56
1:I:350:LEU:HD21	1:J:365:LEU:HD12	1.86	0.56
1:G:253:VAL:HG21	1:G:268:ALA:HB1	1.87	0.56
1:J:533:ILE:HG23	1:J:583:TRP:HE1	1.71	0.56
1:K:533:ILE:HG23	1:K:583:TRP:HE1	1.71	0.56
1:B:253:VAL:HG21	1:B:268:ALA:HB1	1.87	0.56
1:C:365:LEU:HD12	1:D:350:LEU:HD21	1.86	0.56
1:I:74:GLU:OE1	1:I:498:ARG:NH2	2.32	0.56
1:L:74:GLU:OE1	1:L:498:ARG:NH2	2.32	0.56
1:F:330:LEU:HB2	1:F:535:VAL:HG13	1.88	0.56
1:H:533:ILE:HG23	1:H:583:TRP:HE1	1.71	0.56
1:A:533:ILE:HG23	1:A:583:TRP:HE1	1.71	0.56
1:C:330:LEU:HB2	1:C:535:VAL:HG13	1.88	0.56
1:I:274:LEU:CD2	1:J:345:LEU:HD22	2.36	0.55
1:L:253:VAL:HG21	1:L:268:ALA:HB1	1.87	0.55
1:C:368:TRP:CD1	1:C:503:ARG:HD2	2.41	0.55
1:F:368:TRP:CD1	1:F:503:ARG:HD2	2.41	0.55
1:I:105:ILE:HD11	1:I:113:ILE:HD12	1.87	0.55
1:J:368:TRP:CD1	1:J:503:ARG:HD2	2.41	0.55
1:L:533:ILE:HG23	1:L:583:TRP:HE1	1.71	0.55
1:C:253:VAL:HG21	1:C:268:ALA:HB1	1.87	0.55
1:I:533:ILE:HG23	1:I:583:TRP:HE1	1.71	0.55
1:K:368:TRP:CD1	1:K:503:ARG:HD2	2.41	0.55
1:L:368:TRP:CD1	1:L:503:ARG:HD2	2.41	0.55
1:A:226:LEU:HD22	1:A:253:VAL:HG22	1.88	0.55
1:C:226:LEU:HD22	1:C:253:VAL:HG22	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:368:TRP:CD1	1:D:503:ARG:HD2	2.41	0.55
1:E:274:LEU:CD2	1:F:345:LEU:HD22	2.37	0.55
1:F:253:VAL:HG21	1:F:268:ALA:HB1	1.87	0.55
1:I:253:VAL:HG21	1:I:268:ALA:HB1	1.87	0.55
1:L:105:ILE:HD11	1:L:113:ILE:HD12	1.87	0.55
1:B:533:ILE:HG23	1:B:583:TRP:HE1	1.71	0.55
1:D:533:ILE:HG23	1:D:583:TRP:HE1	1.71	0.55
1:G:533:ILE:HG23	1:G:583:TRP:HE1	1.71	0.55
1:H:226:LEU:HD22	1:H:253:VAL:HG22	1.88	0.55
1:I:226:LEU:HD22	1:I:253:VAL:HG22	1.88	0.55
1:I:345:LEU:HD22	1:J:274:LEU:CD2	2.37	0.55
1:I:368:TRP:CD1	1:I:503:ARG:HD2	2.41	0.55
1:L:226:LEU:HD22	1:L:253:VAL:HG22	1.88	0.55
1:C:548:THR:O	1:C:552:ARG:HG3	2.07	0.55
1:E:533:ILE:HG23	1:E:583:TRP:HE1	1.71	0.55
1:F:533:ILE:HG23	1:F:583:TRP:HE1	1.71	0.55
1:F:548:THR:O	1:F:552:ARG:HG3	2.07	0.55
1:H:253:VAL:HG21	1:H:268:ALA:HB1	1.87	0.55
1:K:345:LEU:HD22	1:L:274:LEU:CD2	2.37	0.55
1:A:253:VAL:HG21	1:A:268:ALA:HB1	1.87	0.55
1:B:105:ILE:HD11	1:B:113:ILE:HD12	1.87	0.55
1:C:297:ILE:HG23	1:C:302:SER:HB3	1.89	0.55
1:C:533:ILE:HG23	1:C:583:TRP:HE1	1.71	0.55
1:E:105:ILE:HD11	1:E:113:ILE:HD12	1.87	0.55
1:E:368:TRP:CD1	1:E:503:ARG:HD2	2.41	0.55
1:F:226:LEU:HD22	1:F:253:VAL:HG22	1.88	0.55
1:H:548:THR:O	1:H:552:ARG:HG3	2.07	0.55
1:I:548:THR:O	1:I:552:ARG:HG3	2.07	0.55
1:J:548:THR:O	1:J:552:ARG:HG3	2.07	0.55
1:K:548:THR:O	1:K:552:ARG:HG3	2.07	0.55
1:D:105:ILE:HD11	1:D:113:ILE:HD12	1.87	0.55
1:F:297:ILE:HG23	1:F:302:SER:HB3	1.89	0.55
1:F:321:GLU:OE1	1:F:321:GLU:N	2.29	0.55
1:G:226:LEU:HD22	1:G:253:VAL:HG22	1.88	0.55
1:A:368:TRP:CD1	1:A:503:ARG:HD2	2.41	0.55
1:A:548:THR:O	1:A:552:ARG:HG3	2.07	0.55
1:B:226:LEU:HD22	1:B:253:VAL:HG22	1.88	0.55
1:D:548:THR:O	1:D:552:ARG:HG3	2.07	0.55
1:G:105:ILE:HD11	1:G:113:ILE:HD12	1.87	0.55
1:H:368:TRP:CD1	1:H:503:ARG:HD2	2.41	0.55
1:L:548:THR:O	1:L:552:ARG:HG3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:548:THR:O	1:E:552:ARG:HG3	2.07	0.55
1:A:330:LEU:HB2	1:A:535:VAL:HG13	1.88	0.54
1:B:368:TRP:CD1	1:B:503:ARG:HD2	2.41	0.54
1:D:297:ILE:HG23	1:D:302:SER:HB3	1.89	0.54
1:E:297:ILE:HG23	1:E:302:SER:HB3	1.89	0.54
1:E:345:LEU:HD22	1:F:274:LEU:CD2	2.36	0.54
1:H:91:ASP:OD1	1:H:91:ASP:N	2.35	0.54
1:K:274:LEU:CD2	1:L:345:LEU:HD22	2.37	0.54
1:H:330:LEU:HB2	1:H:535:VAL:HG13	1.88	0.54
1:C:74:GLU:OE1	1:C:498:ARG:NH2	2.32	0.54
1:C:321:GLU:OE1	1:C:321:GLU:N	2.29	0.54
1:F:74:GLU:OE1	1:F:498:ARG:NH2	2.32	0.54
1:G:368:TRP:CD1	1:G:503:ARG:HD2	2.41	0.54
1:J:253:VAL:HG21	1:J:268:ALA:HB1	1.87	0.54
1:C:105:ILE:HD11	1:C:113:ILE:HD12	1.87	0.54
1:D:321:GLU:OE1	1:D:321:GLU:N	2.29	0.54
1:E:189:ASP:O	1:E:192:SER:OG	2.25	0.54
1:I:330:LEU:HB2	1:I:535:VAL:HG13	1.88	0.54
1:I:364:LEU:HD11	1:I:499:ILE:HG23	1.90	0.54
1:J:226:LEU:HD22	1:J:253:VAL:HG22	1.88	0.54
1:A:297:ILE:HG23	1:A:302:SER:HB3	1.89	0.54
1:B:330:LEU:HB2	1:B:535:VAL:HG13	1.88	0.54
1:C:364:LEU:HD11	1:C:499:ILE:HG23	1.90	0.54
1:D:189:ASP:O	1:D:192:SER:OG	2.25	0.54
1:D:330:LEU:HB2	1:D:535:VAL:HG13	1.88	0.54
1:G:330:LEU:HB2	1:G:535:VAL:HG13	1.88	0.54
1:I:281:ILE:HD11	1:J:348:ILE:HG22	1.90	0.54
1:K:226:LEU:HD22	1:K:253:VAL:HG22	1.88	0.54
1:K:253:VAL:HG21	1:K:268:ALA:HB1	1.87	0.54
1:K:439:ALA:O	1:K:443:ILE:HD12	2.08	0.54
1:L:330:LEU:HB2	1:L:535:VAL:HG13	1.88	0.54
1:B:439:ALA:O	1:B:443:ILE:HD12	2.08	0.54
1:E:321:GLU:OE1	1:E:321:GLU:N	2.29	0.54
1:E:330:LEU:HB2	1:E:535:VAL:HG13	1.88	0.54
1:F:105:ILE:HD11	1:F:113:ILE:HD12	1.87	0.54
1:J:439:ALA:O	1:J:443:ILE:HD12	2.08	0.54
1:L:364:LEU:HD11	1:L:499:ILE:HG23	1.90	0.54
1:D:439:ALA:O	1:D:443:ILE:HD12	2.08	0.54
1:E:226:LEU:HD22	1:E:253:VAL:HG22	1.88	0.54
1:F:364:LEU:HD11	1:F:499:ILE:HG23	1.90	0.54
1:G:274:LEU:CD2	1:H:345:LEU:HD22	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:281:ILE:HD11	1:H:348:ILE:HG22	1.90	0.54
1:G:348:ILE:HG22	1:H:281:ILE:HD11	1.90	0.54
1:G:439:ALA:O	1:G:443:ILE:HD12	2.08	0.54
1:H:297:ILE:HG23	1:H:302:SER:HB3	1.89	0.54
1:I:348:ILE:HG22	1:J:281:ILE:HD11	1.90	0.54
1:A:345:LEU:HD22	1:B:274:LEU:CD2	2.38	0.54
1:D:364:LEU:HD11	1:D:499:ILE:HG23	1.90	0.54
1:C:281:ILE:HD11	1:D:348:ILE:HG22	1.90	0.54
1:D:226:LEU:HD22	1:D:253:VAL:HG22	1.88	0.54
1:E:348:ILE:O	1:E:351:HIS:HB3	2.08	0.54
1:E:364:LEU:HD11	1:E:499:ILE:HG23	1.90	0.54
1:E:439:ALA:O	1:E:443:ILE:HD12	2.08	0.54
1:J:330:LEU:HB2	1:J:535:VAL:HG13	1.88	0.54
1:K:330:LEU:HB2	1:K:535:VAL:HG13	1.88	0.54
1:A:348:ILE:HG22	1:B:281:ILE:HD11	1.90	0.53
1:C:348:ILE:O	1:C:351:HIS:HB3	2.08	0.53
1:D:348:ILE:O	1:D:351:HIS:HB3	2.08	0.53
1:E:127:LYS:HG3	1:E:155:TYR:HE1	1.73	0.53
1:F:348:ILE:O	1:F:351:HIS:HB3	2.08	0.53
1:G:345:LEU:HD22	1:H:274:LEU:CD2	2.37	0.53
1:A:281:ILE:HD11	1:B:348:ILE:HG22	1.91	0.53
1:C:439:ALA:O	1:C:443:ILE:HD12	2.08	0.53
1:G:47:ILE:O	1:G:51:THR:OG1	2.20	0.53
1:G:548:THR:O	1:G:552:ARG:HG3	2.07	0.53
1:J:364:LEU:HD11	1:J:499:ILE:HG23	1.90	0.53
1:K:364:LEU:HD11	1:K:499:ILE:HG23	1.90	0.53
1:B:348:ILE:O	1:B:351:HIS:HB3	2.08	0.53
1:C:220:THR:HG22	1:D:331:MET:SD	2.48	0.53
1:C:348:ILE:HG22	1:D:281:ILE:HD11	1.90	0.53
1:D:127:LYS:HG3	1:D:155:TYR:HE1	1.73	0.53
1:F:439:ALA:O	1:F:443:ILE:HD12	2.08	0.53
1:I:308:ARG:NH1	1:I:309:LEU:O	2.41	0.53
1:J:297:ILE:HG23	1:J:302:SER:HB3	1.89	0.53
1:K:348:ILE:HG22	1:L:281:ILE:HD11	1.91	0.53
1:B:548:THR:O	1:B:552:ARG:HG3	2.07	0.53
1:I:297:ILE:HG23	1:I:302:SER:HB3	1.89	0.53
1:K:281:ILE:HD11	1:L:348:ILE:HG22	1.90	0.53
1:L:297:ILE:HG23	1:L:302:SER:HB3	1.89	0.53
1:L:308:ARG:NH1	1:L:309:LEU:O	2.41	0.53
1:C:91:ASP:OD1	1:C:91:ASP:N	2.35	0.53
1:C:308:ARG:NH1	1:C:309:LEU:O	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:308:ARG:NH1	1:F:309:LEU:O	2.41	0.53
1:G:348:ILE:O	1:G:351:HIS:HB3	2.08	0.53
1:H:189:ASP:O	1:H:192:SER:OG	2.25	0.53
1:J:308:ARG:NH1	1:J:309:LEU:O	2.41	0.53
1:J:348:ILE:O	1:J:351:HIS:HB3	2.08	0.53
1:K:297:ILE:HG23	1:K:302:SER:HB3	1.89	0.53
1:E:245:LEU:O	1:E:248:LYS:HG2	2.09	0.53
1:E:348:ILE:HG22	1:F:281:ILE:HD11	1.91	0.53
1:J:189:ASP:O	1:J:192:SER:OG	2.25	0.53
1:K:308:ARG:NH1	1:K:309:LEU:O	2.41	0.53
1:L:348:ILE:O	1:L:351:HIS:HB3	2.08	0.53
1:A:189:ASP:O	1:A:192:SER:OG	2.25	0.53
1:A:274:LEU:CD2	1:B:345:LEU:HD22	2.37	0.53
1:B:308:ARG:NH1	1:B:309:LEU:O	2.41	0.53
1:G:308:ARG:NH1	1:G:309:LEU:O	2.41	0.53
1:I:348:ILE:O	1:I:351:HIS:HB3	2.08	0.53
1:K:74:GLU:OE1	1:K:498:ARG:NH2	2.32	0.53
1:K:348:ILE:O	1:K:351:HIS:HB3	2.08	0.53
1:A:42:MET:HB3	1:A:47:ILE:HG13	1.91	0.53
1:D:245:LEU:O	1:D:248:LYS:HG2	2.09	0.53
1:E:281:ILE:HD11	1:F:348:ILE:HG22	1.91	0.53
1:H:42:MET:HB3	1:H:47:ILE:HG13	1.91	0.53
1:H:47:ILE:O	1:H:51:THR:OG1	2.20	0.53
1:J:74:GLU:OE1	1:J:498:ARG:NH2	2.32	0.53
1:K:189:ASP:O	1:K:192:SER:OG	2.25	0.53
1:A:43:ASN:N	1:A:46:THR:OG1	2.42	0.53
1:B:43:ASN:N	1:B:46:THR:OG1	2.42	0.53
1:G:364:LEU:HD11	1:G:499:ILE:HG23	1.90	0.53
1:B:127:LYS:HG3	1:B:155:TYR:HE1	1.73	0.53
1:B:245:LEU:O	1:B:248:LYS:HG2	2.09	0.53
1:F:42:MET:HB3	1:F:47:ILE:HG13	1.91	0.53
1:G:43:ASN:N	1:G:46:THR:OG1	2.42	0.53
1:H:43:ASN:N	1:H:46:THR:OG1	2.42	0.53
1:H:439:ALA:O	1:H:443:ILE:HD12	2.08	0.53
1:I:127:LYS:HG3	1:I:155:TYR:HE1	1.73	0.53
1:C:331:MET:SD	1:D:220:THR:HG22	2.49	0.52
1:G:127:LYS:HG3	1:G:155:TYR:HE1	1.73	0.52
1:G:245:LEU:O	1:G:248:LYS:HG2	2.09	0.52
1:A:47:ILE:O	1:A:51:THR:OG1	2.20	0.52
1:A:127:LYS:HG3	1:A:155:TYR:HE1	1.73	0.52
1:A:364:LEU:HD11	1:A:499:ILE:HG23	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:439:ALA:O	1:A:443:ILE:HD12	2.08	0.52
1:B:297:ILE:HG23	1:B:302:SER:HB3	1.89	0.52
1:B:364:LEU:HD11	1:B:499:ILE:HG23	1.90	0.52
1:C:42:MET:HB3	1:C:47:ILE:HG13	1.91	0.52
1:C:43:ASN:N	1:C:46:THR:OG1	2.42	0.52
1:H:127:LYS:HG3	1:H:155:TYR:HE1	1.73	0.52
1:I:245:LEU:O	1:I:248:LYS:HG2	2.09	0.52
1:I:439:ALA:O	1:I:443:ILE:HD12	2.08	0.52
1:K:42:MET:HB3	1:K:47:ILE:HG13	1.91	0.52
1:K:43:ASN:N	1:K:46:THR:OG1	2.42	0.52
1:L:127:LYS:HG3	1:L:155:TYR:HE1	1.73	0.52
1:L:439:ALA:O	1:L:443:ILE:HD12	2.08	0.52
1:D:43:ASN:N	1:D:46:THR:OG1	2.42	0.52
1:F:127:LYS:HG3	1:F:155:TYR:HE1	1.73	0.52
1:G:297:ILE:HG23	1:G:302:SER:HB3	1.89	0.52
1:H:145:ARG:NH2	1:H:462:THR:HB	2.25	0.52
1:H:348:ILE:O	1:H:351:HIS:HB3	2.08	0.52
1:J:43:ASN:N	1:J:46:THR:OG1	2.42	0.52
1:J:127:LYS:HG3	1:J:155:TYR:HE1	1.73	0.52
1:L:245:LEU:O	1:L:248:LYS:HG2	2.09	0.52
1:A:145:ARG:NH2	1:A:462:THR:HB	2.25	0.52
1:C:127:LYS:HG3	1:C:155:TYR:HE1	1.73	0.52
1:D:47:ILE:O	1:D:51:THR:OG1	2.20	0.52
1:F:43:ASN:N	1:F:46:THR:OG1	2.42	0.52
1:J:42:MET:HB3	1:J:47:ILE:HG13	1.91	0.52
1:A:74:GLU:OE1	1:A:498:ARG:NH2	2.32	0.52
1:A:348:ILE:O	1:A:351:HIS:HB3	2.08	0.52
1:E:308:ARG:NH1	1:E:309:LEU:O	2.41	0.52
1:G:74:GLU:CD	1:G:498:ARG:HH22	2.16	0.52
1:H:364:LEU:HD11	1:H:499:ILE:HG23	1.90	0.52
1:L:43:ASN:N	1:L:46:THR:OG1	2.42	0.52
1:A:308:ARG:NH1	1:A:309:LEU:O	2.41	0.52
1:B:145:ARG:NH2	1:B:462:THR:HB	2.25	0.52
1:D:308:ARG:NH1	1:D:309:LEU:O	2.41	0.52
1:E:43:ASN:N	1:E:46:THR:OG1	2.42	0.52
1:E:145:ARG:NH2	1:E:462:THR:HB	2.25	0.52
1:G:145:ARG:NH2	1:G:462:THR:HB	2.25	0.52
1:H:74:GLU:OE1	1:H:498:ARG:NH2	2.32	0.52
1:K:127:LYS:HG3	1:K:155:TYR:HE1	1.73	0.52
1:J:321:GLU:OE1	1:J:321:GLU:N	2.29	0.52
1:A:408:ASP:O	1:A:412:ARG:HG3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:GLU:CD	1:B:498:ARG:HH22	2.17	0.52
1:C:189:ASP:O	1:C:192:SER:OG	2.25	0.52
1:E:47:ILE:O	1:E:51:THR:OG1	2.20	0.52
1:E:74:GLU:CD	1:E:498:ARG:HH22	2.16	0.52
1:F:189:ASP:O	1:F:192:SER:OG	2.25	0.52
1:F:408:ASP:O	1:F:412:ARG:HG3	2.10	0.52
1:H:308:ARG:NH1	1:H:309:LEU:O	2.41	0.52
1:H:408:ASP:O	1:H:412:ARG:HG3	2.10	0.52
1:I:43:ASN:N	1:I:46:THR:OG1	2.42	0.52
1:C:74:GLU:CD	1:C:498:ARG:HH22	2.16	0.52
1:C:408:ASP:O	1:C:412:ARG:HG3	2.10	0.52
1:L:145:ARG:NH2	1:L:462:THR:HB	2.25	0.52
1:B:321:GLU:OE1	1:B:321:GLU:N	2.29	0.52
1:D:74:GLU:CD	1:D:498:ARG:HH22	2.16	0.52
1:D:145:ARG:NH2	1:D:462:THR:HB	2.25	0.52
1:F:145:ARG:NH2	1:F:462:THR:HB	2.25	0.52
1:F:245:LEU:O	1:F:248:LYS:HG2	2.09	0.52
1:I:145:ARG:NH2	1:I:462:THR:HB	2.25	0.52
1:D:42:MET:HB3	1:D:47:ILE:HG13	1.91	0.51
1:F:74:GLU:CD	1:F:498:ARG:HH22	2.16	0.51
1:L:47:ILE:O	1:L:51:THR:OG1	2.20	0.51
1:A:17:ALA:HA	1:A:143:TRP:CZ3	2.46	0.51
1:C:145:ARG:NH2	1:C:462:THR:HB	2.25	0.51
1:C:245:LEU:O	1:C:248:LYS:HG2	2.09	0.51
1:D:87:ASP:HB3	1:D:129:LYS:CE	2.37	0.51
1:E:42:MET:HB3	1:E:47:ILE:HG13	1.91	0.51
1:E:87:ASP:HB3	1:E:129:LYS:CE	2.37	0.51
1:H:17:ALA:HA	1:H:143:TRP:CZ3	2.46	0.51
1:I:408:ASP:O	1:I:412:ARG:HG3	2.10	0.51
1:K:145:ARG:NH2	1:K:462:THR:HB	2.25	0.51
1:K:321:GLU:OE1	1:K:321:GLU:N	2.29	0.51
1:L:42:MET:HB3	1:L:47:ILE:HG13	1.91	0.51
1:B:42:MET:HB3	1:B:47:ILE:HG13	1.91	0.51
1:J:145:ARG:NH2	1:J:462:THR:HB	2.25	0.51
1:J:210:VAL:HG12	1:J:290:TRP:HB3	1.92	0.51
1:J:245:LEU:O	1:J:248:LYS:HG2	2.09	0.51
1:K:17:ALA:HA	1:K:143:TRP:CZ3	2.46	0.51
1:L:408:ASP:O	1:L:412:ARG:HG3	2.10	0.51
1:A:245:LEU:O	1:A:248:LYS:HG2	2.09	0.51
1:B:368:TRP:O	1:B:372:GLU:HG3	2.10	0.51
1:I:47:ILE:O	1:I:51:THR:OG1	2.20	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:17:ALA:HA	1:J:143:TRP:CZ3	2.46	0.51
1:K:210:VAL:HG12	1:K:290:TRP:HB3	1.92	0.51
1:L:321:GLU:OE1	1:L:321:GLU:N	2.29	0.51
1:E:210:VAL:HG12	1:E:290:TRP:HB3	1.92	0.51
1:F:368:TRP:O	1:F:372:GLU:HG3	2.10	0.51
1:G:42:MET:HB3	1:G:47:ILE:HG13	1.91	0.51
1:G:321:GLU:OE1	1:G:321:GLU:N	2.29	0.51
1:G:368:TRP:O	1:G:372:GLU:HG3	2.11	0.51
1:G:408:ASP:O	1:G:412:ARG:HG3	2.10	0.51
1:H:245:LEU:O	1:H:248:LYS:HG2	2.09	0.51
1:I:42:MET:HB3	1:I:47:ILE:HG13	1.91	0.51
1:I:189:ASP:O	1:I:192:SER:OG	2.25	0.51
1:K:245:LEU:O	1:K:248:LYS:HG2	2.09	0.51
1:L:189:ASP:O	1:L:192:SER:OG	2.25	0.51
1:B:408:ASP:O	1:B:412:ARG:HG3	2.10	0.51
1:C:368:TRP:O	1:C:372:GLU:HG3	2.11	0.51
1:D:210:VAL:HG12	1:D:290:TRP:HB3	1.92	0.51
1:H:368:TRP:O	1:H:372:GLU:HG3	2.10	0.51
1:I:74:GLU:CD	1:I:498:ARG:HH22	2.16	0.51
1:J:408:ASP:O	1:J:412:ARG:HG3	2.10	0.51
1:A:368:TRP:O	1:A:372:GLU:HG3	2.10	0.51
1:A:444:LEU:HD23	1:A:445:PRO:HD2	1.93	0.51
1:D:28:MET:HE2	1:D:39:PRO:HG3	1.93	0.51
1:E:28:MET:HE2	1:E:39:PRO:HG3	1.93	0.51
1:E:368:TRP:O	1:E:372:GLU:HG3	2.10	0.51
1:F:444:LEU:HD23	1:F:445:PRO:HD2	1.93	0.51
1:H:444:LEU:HD23	1:H:445:PRO:HD2	1.93	0.51
1:A:74:GLU:CD	1:A:498:ARG:HH22	2.16	0.51
1:C:17:ALA:HA	1:C:143:TRP:CZ3	2.46	0.51
1:C:444:LEU:HD23	1:C:445:PRO:HD2	1.93	0.51
1:D:368:TRP:O	1:D:372:GLU:HG3	2.10	0.51
1:F:17:ALA:HA	1:F:143:TRP:CZ3	2.46	0.51
1:G:87:ASP:HB3	1:G:129:LYS:CE	2.37	0.51
1:B:28:MET:HE2	1:B:39:PRO:HG3	1.93	0.51
1:B:87:ASP:HB3	1:B:129:LYS:CE	2.37	0.51
1:F:210:VAL:HG12	1:F:290:TRP:HB3	1.92	0.51
1:G:28:MET:HE2	1:G:39:PRO:HG3	1.93	0.51
1:I:321:GLU:OE1	1:I:321:GLU:N	2.29	0.51
1:I:331:MET:SD	1:J:220:THR:HG22	2.51	0.51
1:J:462:THR:OG1	1:J:463:LEU:N	2.44	0.51
1:K:408:ASP:O	1:K:412:ARG:HG3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:462:THR:OG1	1:K:463:LEU:N	2.44	0.51
1:L:74:GLU:CD	1:L:498:ARG:HH22	2.16	0.51
1:L:462:THR:OG1	1:L:463:LEU:N	2.44	0.51
1:C:210:VAL:HG12	1:C:290:TRP:HB3	1.92	0.51
1:D:482:LYS:HB2	1:D:566:THR:HB	1.93	0.51
1:E:331:MET:SD	1:F:220:THR:HG22	2.51	0.51
1:E:408:ASP:O	1:E:412:ARG:HG3	2.10	0.51
1:I:17:ALA:HA	1:I:143:TRP:CZ3	2.46	0.51
1:I:462:THR:OG1	1:I:463:LEU:N	2.44	0.51
1:L:17:ALA:HA	1:L:143:TRP:CZ3	2.46	0.51
1:A:462:THR:OG1	1:A:463:LEU:N	2.44	0.50
1:C:482:LYS:HB2	1:C:566:THR:HB	1.93	0.50
1:E:482:LYS:HB2	1:E:566:THR:HB	1.93	0.50
1:G:482:LYS:HB2	1:G:566:THR:HB	1.93	0.50
1:H:74:GLU:CD	1:H:498:ARG:HH22	2.17	0.50
1:H:321:GLU:OE1	1:H:321:GLU:N	2.29	0.50
1:H:462:THR:OG1	1:H:463:LEU:N	2.44	0.50
1:H:482:LYS:HB2	1:H:566:THR:HB	1.93	0.50
1:A:482:LYS:HB2	1:A:566:THR:HB	1.93	0.50
1:B:482:LYS:HB2	1:B:566:THR:HB	1.94	0.50
1:D:408:ASP:O	1:D:412:ARG:HG3	2.10	0.50
1:E:444:LEU:HD23	1:E:445:PRO:HD2	1.93	0.50
1:J:28:MET:HE2	1:J:39:PRO:HG3	1.93	0.50
1:G:331:MET:SD	1:H:220:THR:HG22	2.52	0.50
1:I:220:THR:HG22	1:J:331:MET:SD	2.51	0.50
1:L:482:LYS:HB2	1:L:566:THR:HB	1.93	0.50
1:F:482:LYS:HB2	1:F:566:THR:HB	1.93	0.50
1:I:210:VAL:HG12	1:I:290:TRP:HB3	1.92	0.50
1:I:482:LYS:HB2	1:I:566:THR:HB	1.94	0.50
1:J:482:LYS:HB2	1:J:566:THR:HB	1.93	0.50
1:K:28:MET:HE2	1:K:39:PRO:HG3	1.93	0.50
1:K:482:LYS:HB2	1:K:566:THR:HB	1.93	0.50
1:C:28:MET:HE2	1:C:39:PRO:HG3	1.93	0.50
1:D:444:LEU:HD23	1:D:445:PRO:HD2	1.93	0.50
1:G:210:VAL:HG12	1:G:290:TRP:HB3	1.92	0.50
1:L:210:VAL:HG12	1:L:290:TRP:HB3	1.92	0.50
1:A:321:GLU:OE1	1:A:321:GLU:N	2.29	0.50
1:B:210:VAL:HG12	1:B:290:TRP:HB3	1.92	0.50
1:B:444:LEU:HD23	1:B:445:PRO:HD2	1.93	0.50
1:D:462:THR:OG1	1:D:463:LEU:N	2.44	0.50
1:G:220:THR:HG22	1:H:331:MET:SD	2.52	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:444:LEU:HD23	1:G:445:PRO:HD2	1.93	0.50
1:H:42:MET:HE1	1:H:50:GLU:HB3	1.94	0.50
1:K:87:ASP:HB3	1:K:129:LYS:CE	2.37	0.50
1:A:42:MET:HE1	1:A:50:GLU:HB3	1.94	0.50
1:F:28:MET:HE2	1:F:39:PRO:HG3	1.93	0.50
1:I:368:TRP:O	1:I:372:GLU:HG3	2.11	0.50
1:I:444:LEU:HD23	1:I:445:PRO:HD2	1.93	0.50
1:J:368:TRP:O	1:J:372:GLU:HG3	2.10	0.50
1:J:471:ILE:O	1:J:475:VAL:HG22	2.12	0.50
1:K:368:TRP:O	1:K:372:GLU:HG3	2.11	0.50
1:K:471:ILE:O	1:K:475:VAL:HG22	2.12	0.50
1:L:444:LEU:HD23	1:L:445:PRO:HD2	1.93	0.50
1:B:462:THR:OG1	1:B:463:LEU:N	2.44	0.50
1:E:462:THR:OG1	1:E:463:LEU:N	2.44	0.50
1:H:28:MET:HE2	1:H:39:PRO:HG3	1.93	0.50
1:L:368:TRP:O	1:L:372:GLU:HG3	2.10	0.50
1:I:28:MET:HE2	1:I:39:PRO:HG3	1.93	0.50
1:I:471:ILE:O	1:I:475:VAL:HG22	2.12	0.50
1:J:87:ASP:HB3	1:J:129:LYS:CE	2.37	0.50
1:K:220:THR:HG22	1:L:331:MET:SD	2.52	0.50
1:A:28:MET:HE2	1:A:39:PRO:HG3	1.93	0.49
1:D:17:ALA:HA	1:D:143:TRP:CZ3	2.46	0.49
1:G:462:THR:OG1	1:G:463:LEU:N	2.44	0.49
1:K:74:GLU:CD	1:K:498:ARG:HH22	2.16	0.49
1:A:331:MET:SD	1:B:220:THR:HG22	2.52	0.49
1:B:42:MET:HE1	1:B:50:GLU:HB3	1.94	0.49
1:E:17:ALA:HA	1:E:143:TRP:CZ3	2.46	0.49
1:E:220:THR:HG22	1:F:331:MET:SD	2.51	0.49
1:G:42:MET:HE1	1:G:50:GLU:HB3	1.94	0.49
1:L:28:MET:HE2	1:L:39:PRO:HG3	1.93	0.49
1:B:189:ASP:O	1:B:192:SER:OG	2.25	0.49
1:F:42:MET:HE1	1:F:50:GLU:HB3	1.94	0.49
1:G:189:ASP:O	1:G:192:SER:OG	2.25	0.49
1:L:471:ILE:O	1:L:475:VAL:HG22	2.12	0.49
1:C:471:ILE:O	1:C:475:VAL:HG22	2.12	0.49
1:F:471:ILE:O	1:F:475:VAL:HG22	2.12	0.49
1:J:74:GLU:CD	1:J:498:ARG:HH22	2.16	0.49
1:A:210:VAL:HG12	1:A:290:TRP:HB3	1.92	0.49
1:C:42:MET:HE1	1:C:50:GLU:HB3	1.94	0.49
1:C:67:ASN:OD1	1:C:501:ARG:NH1	2.46	0.49
1:E:42:MET:HE1	1:E:50:GLU:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:471:ILE:O	1:E:475:VAL:HG22	2.12	0.49
1:F:67:ASN:OD1	1:F:501:ARG:NH1	2.46	0.49
1:G:17:ALA:HA	1:G:143:TRP:CZ3	2.46	0.49
1:A:220:THR:HG22	1:B:331:MET:SD	2.53	0.49
1:B:17:ALA:HA	1:B:143:TRP:CZ3	2.46	0.49
1:D:471:ILE:O	1:D:475:VAL:HG22	2.12	0.49
1:H:210:VAL:HG12	1:H:290:TRP:HB3	1.92	0.49
1:J:444:LEU:HD23	1:J:445:PRO:HD2	1.93	0.49
1:K:331:MET:SD	1:L:220:THR:HG22	2.52	0.49
1:D:42:MET:HE1	1:D:50:GLU:HB3	1.94	0.49
1:K:444:LEU:HD23	1:K:445:PRO:HD2	1.93	0.49
1:B:471:ILE:O	1:B:475:VAL:HG22	2.12	0.49
1:C:462:THR:OG1	1:C:463:LEU:N	2.44	0.49
1:F:462:THR:OG1	1:F:463:LEU:N	2.44	0.49
1:H:471:ILE:O	1:H:475:VAL:HG22	2.12	0.49
1:I:67:ASN:OD1	1:I:501:ARG:NH1	2.46	0.49
1:K:42:MET:HE1	1:K:50:GLU:HB3	1.94	0.49
1:A:471:ILE:O	1:A:475:VAL:HG22	2.12	0.49
1:G:471:ILE:O	1:G:475:VAL:HG22	2.12	0.48
1:J:42:MET:HE1	1:J:50:GLU:HB3	1.94	0.48
1:L:67:ASN:OD1	1:L:501:ARG:NH1	2.46	0.48
1:G:232:PRO:HB2	1:G:237:SER:HA	1.95	0.48
1:I:35:ASP:OD2	1:I:525:ASN:ND2	2.47	0.48
1:L:35:ASP:OD2	1:L:525:ASN:ND2	2.47	0.48
1:B:232:PRO:HB2	1:B:237:SER:HA	1.95	0.48
1:D:232:PRO:HB2	1:D:237:SER:HA	1.95	0.48
1:L:232:PRO:HB2	1:L:237:SER:HA	1.95	0.48
1:I:232:PRO:HB2	1:I:237:SER:HA	1.95	0.48
1:L:42:MET:HE1	1:L:50:GLU:HB3	1.94	0.48
1:B:221:PHE:HB3	1:B:226:LEU:O	2.14	0.48
1:E:232:PRO:HB2	1:E:237:SER:HA	1.95	0.48
1:I:42:MET:HE1	1:I:50:GLU:HB3	1.94	0.48
1:B:87:ASP:CB	1:B:129:LYS:CE	2.92	0.48
1:C:232:PRO:HB2	1:C:237:SER:HA	1.95	0.48
1:G:87:ASP:CB	1:G:129:LYS:CE	2.92	0.48
1:G:221:PHE:HB3	1:G:226:LEU:O	2.14	0.48
1:D:35:ASP:OD2	1:D:525:ASN:ND2	2.47	0.48
1:E:87:ASP:CB	1:E:129:LYS:CE	2.92	0.48
1:F:232:PRO:HB2	1:F:237:SER:HA	1.95	0.48
1:C:221:PHE:HB3	1:C:226:LEU:O	2.14	0.48
1:D:87:ASP:CB	1:D:129:LYS:CE	2.92	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:35:ASP:OD2	1:E:525:ASN:ND2	2.47	0.48
1:E:67:ASN:OD1	1:E:501:ARG:NH1	2.46	0.48
1:H:221:PHE:HB3	1:H:226:LEU:O	2.14	0.48
1:H:536:MET:SD	1:H:583:TRP:NE1	2.87	0.48
1:A:489:LYS:NZ	1:A:493:GLU:OE2	2.47	0.48
1:A:536:MET:SD	1:A:583:TRP:NE1	2.87	0.48
1:I:221:PHE:HB3	1:I:226:LEU:O	2.14	0.48
1:J:536:MET:SD	1:J:583:TRP:NE1	2.87	0.48
1:L:221:PHE:HB3	1:L:226:LEU:O	2.14	0.48
1:A:221:PHE:HB3	1:A:226:LEU:O	2.14	0.47
1:B:489:LYS:NZ	1:B:493:GLU:OE2	2.47	0.47
1:D:536:MET:SD	1:D:583:TRP:NE1	2.87	0.47
1:E:536:MET:SD	1:E:583:TRP:NE1	2.87	0.47
1:F:221:PHE:HB3	1:F:226:LEU:O	2.14	0.47
1:G:489:LYS:NZ	1:G:493:GLU:OE2	2.47	0.47
1:H:489:LYS:NZ	1:H:493:GLU:OE2	2.47	0.47
1:K:536:MET:SD	1:K:583:TRP:NE1	2.87	0.47
1:A:67:ASN:OD1	1:A:501:ARG:NH1	2.46	0.47
1:D:67:ASN:OD1	1:D:501:ARG:NH1	2.46	0.47
1:J:221:PHE:HB3	1:J:226:LEU:O	2.14	0.47
1:K:221:PHE:HB3	1:K:226:LEU:O	2.14	0.47
1:A:35:ASP:OD2	1:A:525:ASN:ND2	2.47	0.47
1:B:536:MET:SD	1:B:583:TRP:NE1	2.87	0.47
1:C:536:MET:SD	1:C:583:TRP:NE1	2.87	0.47
1:E:176:PHE:CD2	1:E:193:PHE:HB2	2.50	0.47
1:F:536:MET:SD	1:F:583:TRP:NE1	2.87	0.47
1:G:536:MET:SD	1:G:583:TRP:NE1	2.87	0.47
1:H:35:ASP:OD2	1:H:525:ASN:ND2	2.47	0.47
1:C:87:ASP:CB	1:C:129:LYS:CE	2.92	0.47
1:D:176:PHE:CD2	1:D:193:PHE:HB2	2.50	0.47
1:D:293:GLU:HA	1:D:305:VAL:O	2.15	0.47
1:E:38:LYS:HB3	1:E:38:LYS:HE2	1.76	0.47
1:E:293:GLU:HA	1:E:305:VAL:O	2.15	0.47
1:H:67:ASN:OD1	1:H:501:ARG:NH1	2.46	0.47
1:J:31:ASP:CG	1:J:32:TYR:CD1	2.93	0.47
1:J:489:LYS:NZ	1:J:493:GLU:OE2	2.47	0.47
1:L:127:LYS:HD3	1:L:199:LEU:HD21	1.97	0.47
1:L:176:PHE:CD2	1:L:193:PHE:HB2	2.50	0.47
1:A:232:PRO:HB2	1:A:237:SER:HA	1.95	0.47
1:H:232:PRO:HB2	1:H:237:SER:HA	1.95	0.47
1:I:31:ASP:CG	1:I:32:TYR:CD1	2.93	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:127:LYS:HD3	1:I:199:LEU:HD21	1.97	0.47
1:I:176:PHE:CD2	1:I:193:PHE:HB2	2.50	0.47
1:K:31:ASP:CG	1:K:32:TYR:CD1	2.93	0.47
1:F:87:ASP:CB	1:F:129:LYS:CE	2.92	0.47
1:I:536:MET:SD	1:I:583:TRP:NE1	2.87	0.47
1:J:293:GLU:HA	1:J:305:VAL:O	2.15	0.47
1:K:489:LYS:NZ	1:K:493:GLU:OE2	2.47	0.47
1:L:31:ASP:CG	1:L:32:TYR:CD1	2.93	0.47
1:B:127:LYS:HD3	1:B:199:LEU:HD21	1.97	0.47
1:B:293:GLU:HA	1:B:305:VAL:O	2.15	0.47
1:D:127:LYS:HD3	1:D:199:LEU:HD21	1.97	0.47
1:D:489:LYS:NZ	1:D:493:GLU:OE2	2.47	0.47
1:D:577:ILE:O	1:D:581:LEU:HB2	2.15	0.47
1:E:127:LYS:HD3	1:E:199:LEU:HD21	1.97	0.47
1:E:577:ILE:O	1:E:581:LEU:HB2	2.15	0.47
1:F:489:LYS:NZ	1:F:493:GLU:OE2	2.47	0.47
1:G:127:LYS:HD3	1:G:199:LEU:HD21	1.97	0.47
1:G:293:GLU:HA	1:G:305:VAL:O	2.15	0.47
1:H:293:GLU:HA	1:H:305:VAL:O	2.15	0.47
1:I:293:GLU:HA	1:I:305:VAL:O	2.15	0.47
1:I:489:LYS:NZ	1:I:493:GLU:OE2	2.47	0.47
1:J:176:PHE:CD2	1:J:193:PHE:HB2	2.50	0.47
1:J:322:LYS:HE3	1:J:322:LYS:HB2	1.66	0.47
1:J:577:ILE:O	1:J:581:LEU:HB2	2.15	0.47
1:K:176:PHE:CD2	1:K:193:PHE:HB2	2.50	0.47
1:K:293:GLU:HA	1:K:305:VAL:O	2.15	0.47
1:K:322:LYS:HE3	1:K:322:LYS:HB2	1.66	0.47
1:K:577:ILE:O	1:K:581:LEU:HB2	2.15	0.47
1:L:536:MET:SD	1:L:583:TRP:NE1	2.87	0.47
1:A:112:SER:O	1:A:116:MET:HG3	2.15	0.47
1:B:577:ILE:O	1:B:581:LEU:HB2	2.15	0.47
1:C:489:LYS:NZ	1:C:493:GLU:OE2	2.47	0.47
1:E:489:LYS:NZ	1:E:493:GLU:OE2	2.47	0.47
1:G:176:PHE:CD2	1:G:193:PHE:HB2	2.50	0.47
1:H:31:ASP:CG	1:H:32:TYR:CD1	2.93	0.47
1:H:112:SER:O	1:H:116:MET:HG3	2.15	0.47
1:I:87:ASP:HB3	1:I:129:LYS:CE	2.37	0.47
1:J:35:ASP:OD2	1:J:525:ASN:ND2	2.47	0.47
1:J:232:PRO:HB2	1:J:237:SER:HA	1.95	0.47
1:L:293:GLU:HA	1:L:305:VAL:O	2.15	0.47
1:A:31:ASP:CG	1:A:32:TYR:CD1	2.93	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:GLU:HA	1:A:305:VAL:O	2.15	0.47
1:B:176:PHE:CD2	1:B:193:PHE:HB2	2.50	0.47
1:D:221:PHE:HB3	1:D:226:LEU:O	2.14	0.47
1:K:35:ASP:OD2	1:K:525:ASN:ND2	2.47	0.47
1:K:127:LYS:HD3	1:K:199:LEU:HD21	1.97	0.47
1:K:232:PRO:HB2	1:K:237:SER:HA	1.95	0.47
1:L:489:LYS:NZ	1:L:493:GLU:OE2	2.47	0.47
1:B:31:ASP:CG	1:B:32:TYR:CD1	2.93	0.47
1:B:35:ASP:OD2	1:B:525:ASN:ND2	2.47	0.47
1:D:38:LYS:HE2	1:D:38:LYS:HB3	1.76	0.47
1:G:31:ASP:CG	1:G:32:TYR:CD1	2.93	0.47
1:G:577:ILE:O	1:G:581:LEU:HB2	2.15	0.47
1:J:127:LYS:HD3	1:J:199:LEU:HD21	1.97	0.47
1:E:221:PHE:HB3	1:E:226:LEU:O	2.14	0.46
1:G:112:SER:O	1:G:116:MET:HG3	2.15	0.46
1:L:87:ASP:HB3	1:L:129:LYS:CE	2.37	0.46
1:L:577:ILE:O	1:L:581:LEU:HB2	2.15	0.46
1:B:112:SER:O	1:B:116:MET:HG3	2.15	0.46
1:I:577:ILE:O	1:I:581:LEU:HB2	2.15	0.46
1:B:249:LYS:HE2	1:B:249:LYS:HB3	1.75	0.46
1:C:577:ILE:O	1:C:581:LEU:HB2	2.15	0.46
1:G:35:ASP:OD2	1:G:525:ASN:ND2	2.47	0.46
1:H:577:ILE:O	1:H:581:LEU:HB2	2.15	0.46
1:I:112:SER:O	1:I:116:MET:HG3	2.15	0.46
1:L:112:SER:O	1:L:116:MET:HG3	2.15	0.46
1:A:577:ILE:O	1:A:581:LEU:HB2	2.15	0.46
1:C:293:GLU:HA	1:C:305:VAL:O	2.15	0.46
1:F:322:LYS:HE3	1:F:322:LYS:HB2	1.66	0.46
1:F:413:ASP:HB3	1:F:464:LEU:HD21	1.98	0.46
1:F:577:ILE:O	1:F:581:LEU:HB2	2.15	0.46
1:H:361:GLU:HG3	1:H:516:THR:HG21	1.98	0.46
1:J:112:SER:O	1:J:116:MET:HG3	2.15	0.46
1:A:127:LYS:HD3	1:A:199:LEU:HD21	1.97	0.46
1:A:176:PHE:CD2	1:A:193:PHE:HB2	2.50	0.46
1:A:361:GLU:HG3	1:A:516:THR:HG21	1.98	0.46
1:C:112:SER:O	1:C:116:MET:HG3	2.15	0.46
1:C:127:LYS:HD3	1:C:199:LEU:HD21	1.97	0.46
1:C:176:PHE:CD2	1:C:193:PHE:HB2	2.50	0.46
1:C:361:GLU:HG3	1:C:516:THR:HG21	1.98	0.46
1:C:413:ASP:HB3	1:C:464:LEU:HD21	1.98	0.46
1:D:322:LYS:HE3	1:D:322:LYS:HB2	1.66	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:31:ASP:CG	1:E:32:TYR:CD1	2.93	0.46
1:E:112:SER:O	1:E:116:MET:HG3	2.15	0.46
1:F:112:SER:O	1:F:116:MET:HG3	2.15	0.46
1:F:176:PHE:CD2	1:F:193:PHE:HB2	2.50	0.46
1:F:361:GLU:HG3	1:F:516:THR:HG21	1.98	0.46
1:H:127:LYS:HD3	1:H:199:LEU:HD21	1.97	0.46
1:H:249:LYS:HB3	1:H:249:LYS:HE2	1.75	0.46
1:K:112:SER:O	1:K:116:MET:HG3	2.15	0.46
1:A:360:VAL:HG12	1:A:516:THR:HG22	1.98	0.46
1:B:25:LEU:HD23	1:B:25:LEU:HA	1.81	0.46
1:D:112:SER:O	1:D:116:MET:HG3	2.15	0.46
1:D:413:ASP:HB3	1:D:464:LEU:HD21	1.98	0.46
1:E:126:TYR:HD2	1:E:158:LEU:HD22	1.80	0.46
1:E:203:LYS:HE2	1:E:255:ASN:HA	1.98	0.46
1:E:413:ASP:HB3	1:E:464:LEU:HD21	1.98	0.46
1:F:127:LYS:HD3	1:F:199:LEU:HD21	1.97	0.46
1:F:293:GLU:HA	1:F:305:VAL:O	2.15	0.46
1:H:360:VAL:HG12	1:H:516:THR:HG22	1.98	0.46
1:J:126:TYR:HD2	1:J:158:LEU:HD22	1.80	0.46
1:K:126:TYR:HD2	1:K:158:LEU:HD22	1.80	0.46
1:L:511:LYS:HB2	1:L:511:LYS:HE3	1.53	0.46
1:A:95:ALA:HB1	1:C:556:ILE:HG22	1.97	0.46
1:D:126:TYR:HD2	1:D:158:LEU:HD22	1.80	0.46
1:D:203:LYS:HE2	1:D:255:ASN:HA	1.98	0.46
1:E:322:LYS:HE3	1:E:322:LYS:HB2	1.66	0.46
1:H:176:PHE:CD2	1:H:193:PHE:HB2	2.50	0.46
1:H:511:LYS:HE3	1:H:511:LYS:HB2	1.53	0.46
1:I:361:GLU:HG3	1:I:516:THR:HG21	1.98	0.46
1:J:67:ASN:OD1	1:J:501:ARG:NH1	2.46	0.46
1:K:67:ASN:OD1	1:K:501:ARG:NH1	2.46	0.46
1:K:361:GLU:HG3	1:K:516:THR:HG21	1.98	0.46
1:A:87:ASP:CB	1:A:129:LYS:CE	2.92	0.46
1:B:361:GLU:HG3	1:B:516:THR:HG21	1.98	0.46
1:C:322:LYS:HE3	1:C:322:LYS:HB2	1.66	0.46
1:D:31:ASP:CG	1:D:32:TYR:CD1	2.93	0.46
1:D:344:PHE:O	1:D:348:ILE:HG23	2.16	0.46
1:G:361:GLU:HG3	1:G:516:THR:HG21	1.98	0.46
1:H:126:TYR:HD2	1:H:158:LEU:HD22	1.80	0.46
1:J:344:PHE:O	1:J:348:ILE:HG23	2.16	0.46
1:J:361:GLU:HG3	1:J:516:THR:HG21	1.98	0.46
1:K:344:PHE:O	1:K:348:ILE:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:360:VAL:HG12	1:K:516:THR:HG22	1.98	0.46
1:A:50:GLU:OE2	1:A:501:ARG:NH2	2.49	0.46
1:A:265:ARG:NH2	1:A:292:ASN:O	2.49	0.46
1:C:360:VAL:HG12	1:C:516:THR:HG22	1.98	0.46
1:D:361:GLU:HG3	1:D:516:THR:HG21	1.98	0.46
1:E:361:GLU:HG3	1:E:516:THR:HG21	1.98	0.46
1:F:31:ASP:CG	1:F:32:TYR:CD1	2.93	0.46
1:F:360:VAL:HG12	1:F:516:THR:HG22	1.98	0.46
1:G:203:LYS:HE2	1:G:255:ASN:HA	1.98	0.46
1:H:87:ASP:CB	1:H:129:LYS:CE	2.92	0.46
1:H:265:ARG:NH2	1:H:292:ASN:O	2.49	0.46
1:H:344:PHE:O	1:H:348:ILE:HG23	2.16	0.46
1:A:126:TYR:HD2	1:A:158:LEU:HD22	1.80	0.46
1:A:344:PHE:O	1:A:348:ILE:HG23	2.16	0.46
1:C:31:ASP:CG	1:C:32:TYR:CD1	2.93	0.46
1:E:344:PHE:O	1:E:348:ILE:HG23	2.16	0.46
1:G:249:LYS:HB3	1:G:249:LYS:HE2	1.75	0.46
1:H:413:ASP:HB3	1:H:464:LEU:HD21	1.98	0.46
1:I:203:LYS:HE2	1:I:255:ASN:HA	1.98	0.46
1:J:360:VAL:HG12	1:J:516:THR:HG22	1.98	0.46
1:J:438:LEU:HD12	1:J:438:LEU:HA	1.84	0.46
1:L:126:TYR:HD2	1:L:158:LEU:HD22	1.80	0.46
1:L:203:LYS:HE2	1:L:255:ASN:HA	1.98	0.46
1:L:361:GLU:HG3	1:L:516:THR:HG21	1.98	0.46
1:A:249:LYS:HB3	1:A:249:LYS:HE2	1.75	0.45
1:A:413:ASP:HB3	1:A:464:LEU:HD21	1.98	0.45
1:B:203:LYS:HE2	1:B:255:ASN:HA	1.98	0.45
1:F:35:ASP:OD2	1:F:525:ASN:ND2	2.47	0.45
1:F:203:LYS:HE2	1:F:255:ASN:HA	1.98	0.45
1:G:344:PHE:O	1:G:348:ILE:HG23	2.16	0.45
1:H:50:GLU:OE2	1:H:501:ARG:NH2	2.49	0.45
1:B:344:PHE:O	1:B:348:ILE:HG23	2.16	0.45
1:B:413:ASP:HB3	1:B:464:LEU:HD21	1.98	0.45
1:C:126:TYR:HD2	1:C:158:LEU:HD22	1.80	0.45
1:C:203:LYS:HE2	1:C:255:ASN:HA	1.98	0.45
1:C:439:ALA:HA	1:C:442:MET:HE2	1.99	0.45
1:D:24:LEU:O	1:D:28:MET:HG3	2.17	0.45
1:D:360:VAL:HG12	1:D:516:THR:HG22	1.98	0.45
1:E:24:LEU:O	1:E:28:MET:HG3	2.17	0.45
1:E:360:VAL:HG12	1:E:516:THR:HG22	1.98	0.45
1:F:439:ALA:HA	1:F:442:MET:HE2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:126:TYR:HD2	1:G:158:LEU:HD22	1.80	0.45
1:G:413:ASP:HB3	1:G:464:LEU:HD21	1.98	0.45
1:I:25:LEU:HD23	1:I:25:LEU:HA	1.81	0.45
1:I:126:TYR:HD2	1:I:158:LEU:HD22	1.80	0.45
1:K:438:LEU:HD12	1:K:438:LEU:HA	1.84	0.45
1:L:360:VAL:HG12	1:L:516:THR:HG22	1.98	0.45
1:C:35:ASP:OD2	1:C:525:ASN:ND2	2.47	0.45
1:C:51:THR:HA	1:C:71:LEU:HD13	1.99	0.45
1:D:75:LEU:O	1:D:79:LEU:N	2.45	0.45
1:F:51:THR:HA	1:F:71:LEU:HD13	1.99	0.45
1:F:265:ARG:NH2	1:F:292:ASN:O	2.49	0.45
1:F:452:GLU:O	1:F:456:ALA:N	2.48	0.45
1:H:367:LEU:HD23	1:H:367:LEU:HA	1.77	0.45
1:I:511:LYS:HB2	1:I:511:LYS:HE3	1.53	0.45
1:A:439:ALA:HA	1:A:442:MET:HE2	1.99	0.45
1:B:126:TYR:HD2	1:B:158:LEU:HD22	1.80	0.45
1:C:265:ARG:NH2	1:C:292:ASN:O	2.49	0.45
1:C:452:GLU:O	1:C:456:ALA:N	2.48	0.45
1:D:439:ALA:HA	1:D:442:MET:HE2	1.99	0.45
1:E:75:LEU:O	1:E:79:LEU:N	2.45	0.45
1:F:126:TYR:HD2	1:F:158:LEU:HD22	1.80	0.45
1:G:67:ASN:OD1	1:G:501:ARG:NH1	2.46	0.45
1:H:24:LEU:O	1:H:28:MET:HG3	2.16	0.45
1:I:360:VAL:HG12	1:I:516:THR:HG22	1.98	0.45
1:B:360:VAL:HG12	1:B:516:THR:HG22	1.98	0.45
1:E:439:ALA:HA	1:E:442:MET:HE2	1.99	0.45
1:G:360:VAL:HG12	1:G:516:THR:HG22	1.98	0.45
1:G:439:ALA:HA	1:G:442:MET:HE2	1.99	0.45
1:H:439:ALA:HA	1:H:442:MET:HE2	1.99	0.45
1:I:24:LEU:O	1:I:28:MET:HG3	2.17	0.45
1:K:87:ASP:CB	1:K:129:LYS:CE	2.92	0.45
1:L:24:LEU:O	1:L:28:MET:HG3	2.17	0.45
1:L:25:LEU:HD23	1:L:25:LEU:HA	1.81	0.45
1:A:24:LEU:O	1:A:28:MET:HG3	2.17	0.45
1:B:439:ALA:HA	1:B:442:MET:HE2	1.99	0.45
1:I:50:GLU:OE2	1:I:501:ARG:NH2	2.49	0.45
1:I:344:PHE:O	1:I:348:ILE:HG23	2.16	0.45
1:J:24:LEU:O	1:J:28:MET:HG3	2.17	0.45
1:K:24:LEU:O	1:K:28:MET:HG3	2.17	0.45
1:L:50:GLU:OE2	1:L:501:ARG:NH2	2.49	0.45
1:L:265:ARG:NH2	1:L:292:ASN:O	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:MET:HG2	1:A:524:HIS:HB2	1.99	0.45
1:G:158:LEU:O	1:G:162:ILE:HG23	2.17	0.45
1:H:312:MET:HG2	1:H:524:HIS:HB2	1.99	0.45
1:I:158:LEU:O	1:I:162:ILE:HG23	2.17	0.45
1:I:265:ARG:NH2	1:I:292:ASN:O	2.49	0.45
1:J:87:ASP:CB	1:J:129:LYS:CE	2.92	0.45
1:J:265:ARG:NH2	1:J:292:ASN:O	2.49	0.45
1:K:265:ARG:NH2	1:K:292:ASN:O	2.49	0.45
1:B:62:ILE:HD13	1:B:509:SER:HB2	1.99	0.45
1:B:67:ASN:OD1	1:B:501:ARG:NH1	2.46	0.45
1:C:538:ALA:HB2	1:C:544:ILE:HG13	1.99	0.45
1:E:158:LEU:O	1:E:162:ILE:HG23	2.17	0.45
1:G:62:ILE:HD13	1:G:509:SER:HB2	1.99	0.45
1:G:265:ARG:NH2	1:G:292:ASN:O	2.49	0.45
1:L:158:LEU:O	1:L:162:ILE:HG23	2.17	0.45
1:L:344:PHE:O	1:L:348:ILE:HG23	2.16	0.45
1:A:538:ALA:HB2	1:A:544:ILE:HG13	1.99	0.45
1:B:158:LEU:O	1:B:162:ILE:HG23	2.17	0.45
1:B:265:ARG:NH2	1:B:292:ASN:O	2.49	0.45
1:B:511:LYS:HB2	1:B:511:LYS:HE3	1.53	0.45
1:D:158:LEU:O	1:D:162:ILE:HG23	2.17	0.45
1:F:556:ILE:HG22	1:H:95:ALA:HB1	1.98	0.45
1:I:413:ASP:HB3	1:I:464:LEU:HD21	1.98	0.45
1:I:439:ALA:HA	1:I:442:MET:HE2	1.99	0.45
1:J:203:LYS:HE2	1:J:255:ASN:HA	1.98	0.45
1:K:158:LEU:O	1:K:162:ILE:HG23	2.17	0.45
1:K:312:MET:HG2	1:K:524:HIS:HB2	1.99	0.45
1:L:439:ALA:HA	1:L:442:MET:HE2	1.99	0.45
1:A:367:LEU:HD23	1:A:367:LEU:HA	1.77	0.45
1:B:75:LEU:O	1:B:79:LEU:N	2.45	0.45
1:E:249:LYS:HB3	1:E:249:LYS:HE2	1.75	0.45
1:F:538:ALA:HB2	1:F:544:ILE:HG13	1.99	0.45
1:H:538:ALA:HB2	1:H:544:ILE:HG13	1.99	0.45
1:I:87:ASP:CB	1:I:129:LYS:CE	2.92	0.45
1:J:158:LEU:O	1:J:162:ILE:HG23	2.17	0.45
1:J:439:ALA:HA	1:J:442:MET:HE2	1.99	0.45
1:K:203:LYS:HE2	1:K:255:ASN:HA	1.98	0.45
1:K:413:ASP:HB3	1:K:464:LEU:HD21	1.98	0.45
1:K:439:ALA:HA	1:K:442:MET:HE2	1.99	0.45
1:L:87:ASP:CB	1:L:129:LYS:CE	2.92	0.45
1:L:413:ASP:HB3	1:L:464:LEU:HD21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:MET:HE2	1:A:442:MET:HB2	1.84	0.44
1:C:312:MET:HG2	1:C:524:HIS:HB2	1.99	0.44
1:D:265:ARG:NH2	1:D:292:ASN:O	2.49	0.44
1:E:265:ARG:NH2	1:E:292:ASN:O	2.49	0.44
1:F:344:PHE:O	1:F:348:ILE:HG23	2.16	0.44
1:G:511:LYS:HB2	1:G:511:LYS:HE3	1.53	0.44
1:I:269:GLU:O	1:I:273:LYS:HG3	2.17	0.44
1:J:312:MET:HG2	1:J:524:HIS:HB2	1.99	0.44
1:L:269:GLU:O	1:L:273:LYS:HG3	2.17	0.44
1:A:51:THR:HA	1:A:71:LEU:HD13	1.98	0.44
1:D:51:THR:HA	1:D:71:LEU:HD13	1.99	0.44
1:E:51:THR:HA	1:E:71:LEU:HD13	1.98	0.44
1:F:312:MET:HG2	1:F:524:HIS:HB2	1.99	0.44
1:G:75:LEU:O	1:G:79:LEU:N	2.45	0.44
1:J:413:ASP:HB3	1:J:464:LEU:HD21	1.98	0.44
1:A:158:LEU:O	1:A:162:ILE:HG23	2.17	0.44
1:A:203:LYS:HE2	1:A:255:ASN:HA	1.98	0.44
1:A:511:LYS:HE3	1:A:511:LYS:HB2	1.53	0.44
1:C:344:PHE:O	1:C:348:ILE:HG23	2.16	0.44
1:G:24:LEU:O	1:G:28:MET:HG3	2.17	0.44
1:G:43:ASN:ND2	1:G:154:ASN:O	2.51	0.44
1:H:51:THR:HA	1:H:71:LEU:HD13	1.98	0.44
1:H:158:LEU:O	1:H:162:ILE:HG23	2.17	0.44
1:I:503:ARG:NH1	1:I:504:ASN:OD1	2.49	0.44
1:J:538:ALA:HB2	1:J:544:ILE:HG13	1.99	0.44
1:L:503:ARG:NH1	1:L:504:ASN:OD1	2.49	0.44
1:B:24:LEU:O	1:B:28:MET:HG3	2.16	0.44
1:B:43:ASN:ND2	1:B:154:ASN:O	2.51	0.44
1:H:62:ILE:HD13	1:H:509:SER:HB2	1.99	0.44
1:H:203:LYS:HE2	1:H:255:ASN:HA	1.98	0.44
1:K:46:THR:HG22	1:K:161:TYR:CD2	2.53	0.44
1:K:51:THR:HA	1:K:71:LEU:HD13	1.98	0.44
1:K:269:GLU:O	1:K:273:LYS:HG3	2.17	0.44
1:K:538:ALA:HB2	1:K:544:ILE:HG13	1.99	0.44
1:L:62:ILE:HD13	1:L:509:SER:HB2	1.99	0.44
1:A:62:ILE:HD13	1:A:509:SER:HB2	1.99	0.44
1:A:269:GLU:O	1:A:273:LYS:HG3	2.17	0.44
1:B:207:TYR:HE1	1:B:229:GLU:HG3	1.82	0.44
1:C:24:LEU:O	1:C:28:MET:HG3	2.17	0.44
1:G:207:TYR:HE1	1:G:229:GLU:HG3	1.82	0.44
1:I:51:THR:HA	1:I:71:LEU:HD13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:46:THR:HG22	1:J:161:TYR:CD2	2.53	0.44
1:J:51:THR:HA	1:J:71:LEU:HD13	1.99	0.44
1:J:269:GLU:O	1:J:273:LYS:HG3	2.17	0.44
1:L:51:THR:HA	1:L:71:LEU:HD13	1.99	0.44
1:G:51:THR:HA	1:G:71:LEU:HD13	1.98	0.44
1:H:269:GLU:O	1:H:273:LYS:HG3	2.17	0.44
1:I:62:ILE:HD13	1:I:509:SER:HB2	1.99	0.44
1:I:309:LEU:HD12	1:I:309:LEU:HA	1.88	0.44
1:J:99:LYS:HB3	1:J:99:LYS:HE3	1.83	0.44
1:K:25:LEU:HD23	1:K:25:LEU:HA	1.81	0.44
1:K:452:GLU:O	1:K:456:ALA:N	2.48	0.44
1:B:46:THR:HG22	1:B:161:TYR:CD2	2.53	0.44
1:D:46:THR:HG22	1:D:161:TYR:CD2	2.53	0.44
1:D:51:THR:HG23	1:D:71:LEU:HB3	2.00	0.44
1:D:62:ILE:HD13	1:D:509:SER:HB2	1.99	0.44
1:D:249:LYS:HB3	1:D:249:LYS:HE2	1.75	0.44
1:E:51:THR:HG23	1:E:71:LEU:HB3	2.00	0.44
1:E:62:ILE:HD13	1:E:509:SER:HB2	1.99	0.44
1:F:24:LEU:O	1:F:28:MET:HG3	2.17	0.44
1:H:87:ASP:HB3	1:H:129:LYS:CE	2.37	0.44
1:H:452:GLU:O	1:H:456:ALA:N	2.48	0.44
1:J:62:ILE:HD13	1:J:509:SER:HB2	1.99	0.44
1:K:207:TYR:HE1	1:K:229:GLU:HG3	1.82	0.44
1:K:553:TYR:O	1:K:557:ILE:HG12	2.18	0.44
1:B:51:THR:HA	1:B:71:LEU:HD13	1.98	0.44
1:B:322:LYS:HB2	1:B:322:LYS:HE3	1.66	0.44
1:B:367:LEU:HD23	1:B:367:LEU:HA	1.77	0.44
1:E:50:GLU:OE2	1:E:501:ARG:NH2	2.49	0.44
1:G:46:THR:HG22	1:G:161:TYR:CD2	2.53	0.44
1:J:207:TYR:HE1	1:J:229:GLU:HG3	1.82	0.44
1:J:553:TYR:O	1:J:557:ILE:HG12	2.18	0.44
1:K:62:ILE:HD13	1:K:509:SER:HB2	1.99	0.44
1:K:99:LYS:HB3	1:K:99:LYS:HE3	1.83	0.44
1:L:374:LEU:HD23	1:L:374:LEU:HA	1.84	0.44
1:A:87:ASP:HB3	1:A:129:LYS:CE	2.37	0.44
1:A:452:GLU:O	1:A:456:ALA:N	2.48	0.44
1:C:553:TYR:O	1:C:557:ILE:HG12	2.18	0.44
1:D:43:ASN:ND2	1:D:154:ASN:O	2.51	0.44
1:D:50:GLU:OE2	1:D:501:ARG:NH2	2.49	0.44
1:D:538:ALA:HB2	1:D:544:ILE:HG13	1.99	0.44
1:E:43:ASN:ND2	1:E:154:ASN:O	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:46:THR:HG22	1:E:161:TYR:CD2	2.53	0.44
1:F:51:THR:HG23	1:F:71:LEU:HB3	2.00	0.44
1:F:553:TYR:O	1:F:557:ILE:HG12	2.18	0.44
1:G:322:LYS:HB2	1:G:322:LYS:HE3	1.66	0.44
1:C:207:TYR:HE1	1:C:229:GLU:HG3	1.82	0.43
1:D:207:TYR:HE1	1:D:229:GLU:HG3	1.82	0.43
1:E:207:TYR:HE1	1:E:229:GLU:HG3	1.82	0.43
1:G:503:ARG:NH1	1:G:504:ASN:OD1	2.49	0.43
1:I:99:LYS:HE3	1:I:99:LYS:HB3	1.83	0.43
1:A:553:TYR:O	1:A:557:ILE:HG12	2.18	0.43
1:B:28:MET:HE2	1:B:28:MET:HB3	1.85	0.43
1:B:503:ARG:NH1	1:B:504:ASN:OD1	2.49	0.43
1:C:46:THR:HG22	1:C:161:TYR:CD2	2.53	0.43
1:C:51:THR:HG23	1:C:71:LEU:HB3	2.00	0.43
1:C:95:ALA:HB1	1:E:556:ILE:HG22	2.00	0.43
1:D:269:GLU:O	1:D:273:LYS:HG3	2.17	0.43
1:E:269:GLU:O	1:E:273:LYS:HG3	2.17	0.43
1:E:538:ALA:HB2	1:E:544:ILE:HG13	1.99	0.43
1:F:46:THR:HG22	1:F:161:TYR:CD2	2.53	0.43
1:F:207:TYR:HE1	1:F:229:GLU:HG3	1.82	0.43
1:G:538:ALA:HB2	1:G:544:ILE:HG13	1.99	0.43
1:H:553:TYR:O	1:H:557:ILE:HG12	2.18	0.43
1:I:207:TYR:HE1	1:I:229:GLU:HG3	1.82	0.43
1:I:538:ALA:HB2	1:I:544:ILE:HG13	1.99	0.43
1:J:51:THR:HG23	1:J:71:LEU:HB3	2.00	0.43
1:K:51:THR:HG23	1:K:71:LEU:HB3	2.00	0.43
1:L:207:TYR:HE1	1:L:229:GLU:HG3	1.82	0.43
1:L:309:LEU:HD12	1:L:309:LEU:HA	1.88	0.43
1:L:538:ALA:HB2	1:L:544:ILE:HG13	1.99	0.43
1:B:538:ALA:HB2	1:B:544:ILE:HG13	1.99	0.43
1:G:28:MET:HE2	1:G:28:MET:HB3	1.85	0.43
1:G:312:MET:HG2	1:G:524:HIS:HB2	1.99	0.43
1:J:25:LEU:HA	1:J:25:LEU:HD23	1.81	0.43
1:J:503:ARG:NH1	1:J:504:ASN:OD1	2.49	0.43
1:K:88:LEU:HD23	1:K:88:LEU:HA	1.85	0.43
1:A:330:LEU:HG	1:A:331:MET:HE2	2.01	0.43
1:B:312:MET:HG2	1:B:524:HIS:HB2	1.99	0.43
1:C:158:LEU:O	1:C:162:ILE:HG23	2.17	0.43
1:C:330:LEU:HG	1:C:331:MET:HE2	2.01	0.43
1:C:519:LEU:HD23	1:C:519:LEU:HA	1.83	0.43
1:E:312:MET:HG2	1:E:524:HIS:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:158:LEU:O	1:F:162:ILE:HG23	2.17	0.43
1:F:269:GLU:O	1:F:273:LYS:HG3	2.17	0.43
1:G:367:LEU:HD23	1:G:367:LEU:HA	1.77	0.43
1:H:46:THR:HG22	1:H:161:TYR:CD2	2.53	0.43
1:I:310:ASN:OD1	1:I:310:ASN:N	2.52	0.43
1:K:309:LEU:HD12	1:K:309:LEU:HA	1.88	0.43
1:K:503:ARG:NH1	1:K:504:ASN:OD1	2.49	0.43
1:L:99:LYS:HE3	1:L:99:LYS:HB3	1.83	0.43
1:A:46:THR:HG22	1:A:161:TYR:CD2	2.53	0.43
1:C:127:LYS:HZ3	1:C:127:LYS:HG2	1.61	0.43
1:C:269:GLU:O	1:C:273:LYS:HG3	2.17	0.43
1:D:25:LEU:HD23	1:D:25:LEU:HA	1.81	0.43
1:E:553:TYR:O	1:E:557:ILE:HG12	2.18	0.43
1:F:330:LEU:HG	1:F:331:MET:HE2	2.01	0.43
1:H:207:TYR:HE1	1:H:229:GLU:HG3	1.82	0.43
1:H:330:LEU:HG	1:H:331:MET:HE2	2.01	0.43
1:I:43:ASN:ND2	1:I:154:ASN:O	2.51	0.43
1:I:312:MET:HG2	1:I:524:HIS:HB2	1.99	0.43
1:I:374:LEU:HD23	1:I:374:LEU:HA	1.85	0.43
1:I:553:TYR:O	1:I:557:ILE:HG12	2.18	0.43
1:J:488:HIS:O	1:J:492:LEU:HB2	2.19	0.43
1:K:488:HIS:O	1:K:492:LEU:HB2	2.19	0.43
1:L:177:PHE:HD1	1:L:177:PHE:HA	1.72	0.43
1:L:310:ASN:OD1	1:L:310:ASN:N	2.52	0.43
1:L:312:MET:HG2	1:L:524:HIS:HB2	1.99	0.43
1:L:488:HIS:O	1:L:492:LEU:HB2	2.19	0.43
1:A:51:THR:HG23	1:A:71:LEU:HB3	2.00	0.43
1:D:68:ILE:HD13	1:D:68:ILE:HA	1.93	0.43
1:D:312:MET:HG2	1:D:524:HIS:HB2	1.99	0.43
1:F:519:LEU:HD23	1:F:519:LEU:HA	1.83	0.43
1:H:51:THR:HG23	1:H:71:LEU:HB3	2.00	0.43
1:I:488:HIS:O	1:I:492:LEU:HB2	2.19	0.43
1:J:330:LEU:HG	1:J:331:MET:HE2	2.01	0.43
1:J:452:GLU:O	1:J:456:ALA:N	2.48	0.43
1:J:556:ILE:HG22	1:L:95:ALA:HB1	1.99	0.43
1:L:43:ASN:ND2	1:L:154:ASN:O	2.51	0.43
1:L:553:TYR:O	1:L:557:ILE:HG12	2.18	0.43
1:A:207:TYR:HE1	1:A:229:GLU:HG3	1.82	0.43
1:B:269:GLU:O	1:B:273:LYS:HG3	2.17	0.43
1:C:50:GLU:OE2	1:C:501:ARG:NH2	2.49	0.43
1:D:553:TYR:O	1:D:557:ILE:HG12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:245:LEU:HD12	1:G:245:LEU:HA	1.87	0.43
1:G:269:GLU:O	1:G:273:LYS:HG3	2.17	0.43
1:I:204:TYR:HD2	1:I:296:VAL:HG12	1.84	0.43
1:K:330:LEU:HG	1:K:331:MET:HE2	2.01	0.43
1:L:46:THR:HG22	1:L:161:TYR:CD2	2.53	0.43
1:D:556:ILE:HG22	1:F:95:ALA:HB1	2.00	0.43
1:I:46:THR:HG22	1:I:161:TYR:CD2	2.53	0.43
1:I:75:LEU:O	1:I:79:LEU:N	2.45	0.43
1:I:177:PHE:HD1	1:I:177:PHE:HA	1.72	0.43
1:I:291:SER:OG	1:I:293:GLU:O	2.36	0.43
1:I:322:LYS:HE3	1:I:322:LYS:HB2	1.66	0.43
1:J:309:LEU:HD12	1:J:309:LEU:HA	1.88	0.43
1:L:291:SER:OG	1:L:293:GLU:O	2.36	0.43
1:L:452:GLU:O	1:L:456:ALA:N	2.48	0.43
1:A:336:LEU:HD12	1:A:336:LEU:HA	1.93	0.43
1:D:561:ARG:HG2	1:D:580:ASN:HA	2.01	0.43
1:E:330:LEU:HG	1:E:331:MET:HE2	2.01	0.43
1:F:50:GLU:OE2	1:F:501:ARG:NH2	2.49	0.43
1:F:62:ILE:HD13	1:F:509:SER:HB2	1.99	0.43
1:F:75:LEU:O	1:F:79:LEU:N	2.45	0.43
1:F:367:LEU:HD23	1:F:367:LEU:HA	1.77	0.43
1:H:309:LEU:HD12	1:H:309:LEU:HA	1.88	0.43
1:J:88:LEU:HD23	1:J:88:LEU:HA	1.85	0.43
1:L:75:LEU:O	1:L:79:LEU:N	2.45	0.43
1:L:127:LYS:HZ2	1:L:127:LYS:HG2	1.61	0.43
1:L:204:TYR:HD2	1:L:296:VAL:HG12	1.84	0.43
1:L:322:LYS:HE3	1:L:322:LYS:HB2	1.66	0.43
1:L:438:LEU:HD12	1:L:438:LEU:HA	1.84	0.43
1:C:62:ILE:HD13	1:C:509:SER:HB2	1.99	0.43
1:C:75:LEU:O	1:C:79:LEU:N	2.46	0.43
1:D:442:MET:HE2	1:D:442:MET:HB2	1.83	0.43
1:F:371:LEU:HD12	1:F:371:LEU:HA	1.91	0.43
1:H:99:LYS:HB3	1:H:99:LYS:HE3	1.83	0.43
1:I:28:MET:HE2	1:I:28:MET:HB3	1.85	0.43
1:I:51:THR:HG23	1:I:71:LEU:HB3	2.00	0.43
1:I:452:GLU:O	1:I:456:ALA:N	2.48	0.43
1:L:561:ARG:HG2	1:L:580:ASN:HA	2.01	0.43
1:D:330:LEU:HG	1:D:331:MET:HE2	2.01	0.42
1:E:99:LYS:HE3	1:E:99:LYS:HB3	1.83	0.42
1:E:561:ARG:HG2	1:E:580:ASN:HA	2.01	0.42
1:F:99:LYS:HB3	1:F:99:LYS:HE3	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:95:ALA:HB1	1:I:556:ILE:HG22	1.99	0.42
1:G:561:ARG:HG2	1:G:580:ASN:HA	2.01	0.42
1:H:147:ILE:O	1:H:151:LEU:HG	2.19	0.42
1:H:556:ILE:HG22	1:J:95:ALA:HB1	2.00	0.42
1:A:147:ILE:O	1:A:151:LEU:HG	2.19	0.42
1:A:310:ASN:OD1	1:A:310:ASN:N	2.52	0.42
1:B:51:THR:HG23	1:B:71:LEU:HB3	2.00	0.42
1:B:245:LEU:HD12	1:B:245:LEU:HA	1.87	0.42
1:B:488:HIS:O	1:B:492:LEU:HB2	2.19	0.42
1:C:99:LYS:HB3	1:C:99:LYS:HE3	1.83	0.42
1:C:147:ILE:O	1:C:151:LEU:HG	2.19	0.42
1:C:371:LEU:HD12	1:C:371:LEU:HA	1.91	0.42
1:E:68:ILE:HD13	1:E:68:ILE:HA	1.93	0.42
1:F:147:ILE:O	1:F:151:LEU:HG	2.19	0.42
1:G:488:HIS:O	1:G:492:LEU:HB2	2.19	0.42
1:H:488:HIS:O	1:H:492:LEU:HB2	2.19	0.42
1:I:371:LEU:HD12	1:I:371:LEU:HA	1.91	0.42
1:I:438:LEU:HD12	1:I:438:LEU:HA	1.84	0.42
1:I:561:ARG:HG2	1:I:580:ASN:HA	2.01	0.42
1:J:204:TYR:HD2	1:J:296:VAL:HG12	1.84	0.42
1:K:50:GLU:OE2	1:K:501:ARG:NH2	2.49	0.42
1:K:561:ARG:HG2	1:K:580:ASN:HA	2.01	0.42
1:L:28:MET:HE2	1:L:28:MET:HB3	1.86	0.42
1:A:31:ASP:OD1	1:A:32:TYR:N	2.53	0.42
1:A:488:HIS:O	1:A:492:LEU:HB2	2.19	0.42
1:A:519:LEU:HD23	1:A:519:LEU:HA	1.83	0.42
1:B:561:ARG:HG2	1:B:580:ASN:HA	2.01	0.42
1:C:53:ASN:HA	1:C:56:LYS:HD3	2.01	0.42
1:C:561:ARG:HG2	1:C:580:ASN:HA	2.01	0.42
1:E:442:MET:HE2	1:E:442:MET:HB2	1.83	0.42
1:F:53:ASN:HA	1:F:56:LYS:HD3	2.01	0.42
1:G:51:THR:HG23	1:G:71:LEU:HB3	2.00	0.42
1:H:31:ASP:OD1	1:H:32:TYR:N	2.53	0.42
1:H:310:ASN:OD1	1:H:310:ASN:N	2.52	0.42
1:H:322:LYS:HE3	1:H:322:LYS:HB2	1.66	0.42
1:H:336:LEU:HD12	1:H:336:LEU:HA	1.93	0.42
1:I:31:ASP:OD1	1:I:32:TYR:N	2.53	0.42
1:K:204:TYR:HD2	1:K:296:VAL:HG12	1.84	0.42
1:L:51:THR:HG23	1:L:71:LEU:HB3	2.00	0.42
1:A:43:ASN:ND2	1:A:154:ASN:O	2.51	0.42
1:D:99:LYS:HE3	1:D:99:LYS:HB3	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:442:MET:HE2	1:F:442:MET:HB2	1.83	0.42
1:F:561:ARG:HG2	1:F:580:ASN:HA	2.01	0.42
1:G:553:TYR:O	1:G:557:ILE:HG12	2.18	0.42
1:I:95:ALA:HB1	1:K:556:ILE:HG22	2.00	0.42
1:J:561:ARG:HG2	1:J:580:ASN:HA	2.01	0.42
1:L:12:PRO:HA	1:L:15:CYS:HB2	2.01	0.42
1:L:31:ASP:OD1	1:L:32:TYR:N	2.53	0.42
1:A:99:LYS:HB3	1:A:99:LYS:HE3	1.83	0.42
1:A:438:LEU:HA	1:A:438:LEU:HD12	1.84	0.42
1:B:553:TYR:O	1:B:557:ILE:HG12	2.18	0.42
1:D:374:LEU:HD23	1:D:374:LEU:HA	1.85	0.42
1:E:95:ALA:HB1	1:G:556:ILE:HG22	2.00	0.42
1:I:12:PRO:HA	1:I:15:CYS:HB2	2.01	0.42
1:I:330:LEU:HG	1:I:331:MET:HE2	2.01	0.42
1:J:31:ASP:OD1	1:J:32:TYR:N	2.53	0.42
1:J:50:GLU:OE2	1:J:501:ARG:NH2	2.49	0.42
1:K:31:ASP:OD1	1:K:32:TYR:N	2.53	0.42
1:L:38:LYS:HB3	1:L:38:LYS:HE2	1.76	0.42
1:L:249:LYS:HB3	1:L:249:LYS:HE2	1.75	0.42
1:L:330:LEU:HG	1:L:331:MET:HE2	2.01	0.42
1:A:314:LYS:HB3	1:A:314:LYS:HE2	1.87	0.42
1:A:322:LYS:HE3	1:A:322:LYS:HB2	1.66	0.42
1:B:95:ALA:HB1	1:L:556:ILE:HG22	2.00	0.42
1:B:330:LEU:HG	1:B:331:MET:HE2	2.01	0.42
1:C:367:LEU:HD23	1:C:367:LEU:HA	1.77	0.42
1:D:53:ASN:HA	1:D:56:LYS:HD3	2.01	0.42
1:D:488:HIS:O	1:D:492:LEU:HB2	2.19	0.42
1:E:147:ILE:O	1:E:151:LEU:HG	2.19	0.42
1:F:204:TYR:HD2	1:F:296:VAL:HG12	1.84	0.42
1:H:43:ASN:ND2	1:H:154:ASN:O	2.51	0.42
1:H:221:PHE:CG	1:H:226:LEU:HB2	2.55	0.42
1:A:221:PHE:CG	1:A:226:LEU:HB2	2.55	0.42
1:A:561:ARG:HG2	1:A:580:ASN:HA	2.01	0.42
1:B:291:SER:OG	1:B:293:GLU:O	2.36	0.42
1:C:12:PRO:HA	1:C:15:CYS:HB2	2.01	0.42
1:C:31:ASP:OD1	1:C:32:TYR:N	2.53	0.42
1:E:53:ASN:HA	1:E:56:LYS:HD3	2.01	0.42
1:F:12:PRO:HA	1:F:15:CYS:HB2	2.01	0.42
1:F:31:ASP:OD1	1:F:32:TYR:N	2.53	0.42
1:G:330:LEU:HG	1:G:331:MET:HE2	2.01	0.42
1:H:519:LEU:HD23	1:H:519:LEU:HA	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:147:ILE:O	1:J:151:LEU:HG	2.19	0.42
1:A:556:ILE:HG22	1:K:95:ALA:HB1	2.00	0.42
1:B:31:ASP:OD1	1:B:32:TYR:N	2.53	0.42
1:B:147:ILE:O	1:B:151:LEU:HG	2.19	0.42
1:B:556:ILE:HG22	1:D:95:ALA:HB1	2.00	0.42
1:C:221:PHE:CG	1:C:226:LEU:HB2	2.55	0.42
1:C:310:ASN:N	1:C:310:ASN:OD1	2.52	0.42
1:C:488:HIS:O	1:C:492:LEU:HB2	2.19	0.42
1:D:147:ILE:O	1:D:151:LEU:HG	2.19	0.42
1:D:310:ASN:OD1	1:D:310:ASN:N	2.52	0.42
1:E:25:LEU:HD23	1:E:25:LEU:HA	1.81	0.42
1:E:221:PHE:CG	1:E:226:LEU:HB2	2.55	0.42
1:E:310:ASN:N	1:E:310:ASN:OD1	2.52	0.42
1:E:488:HIS:O	1:E:492:LEU:HB2	2.19	0.42
1:F:488:HIS:O	1:F:492:LEU:HB2	2.19	0.42
1:G:12:PRO:HA	1:G:15:CYS:HB2	2.01	0.42
1:G:291:SER:OG	1:G:293:GLU:O	2.36	0.42
1:H:561:ARG:HG2	1:H:580:ASN:HA	2.01	0.42
1:J:221:PHE:CG	1:J:226:LEU:HB2	2.55	0.42
1:J:291:SER:OG	1:J:293:GLU:O	2.36	0.42
1:K:221:PHE:CG	1:K:226:LEU:HB2	2.55	0.42
1:K:291:SER:OG	1:K:293:GLU:O	2.36	0.42
1:A:215:LEU:HD21	1:A:249:LYS:HB2	2.02	0.42
1:B:374:LEU:HD23	1:B:374:LEU:HA	1.85	0.42
1:C:204:TYR:HD2	1:C:296:VAL:HG12	1.84	0.42
1:C:442:MET:HE2	1:C:442:MET:HB2	1.83	0.42
1:E:115:GLU:O	1:E:119:ILE:HG13	2.20	0.42
1:F:221:PHE:CG	1:F:226:LEU:HB2	2.55	0.42
1:F:310:ASN:N	1:F:310:ASN:OD1	2.52	0.42
1:G:31:ASP:OD1	1:G:32:TYR:N	2.53	0.42
1:G:147:ILE:O	1:G:151:LEU:HG	2.19	0.42
1:G:204:TYR:HD2	1:G:296:VAL:HG12	1.84	0.42
1:G:297:ILE:HG12	1:G:302:SER:HB2	2.02	0.42
1:J:12:PRO:HA	1:J:15:CYS:HB2	2.01	0.42
1:J:442:MET:HE2	1:J:442:MET:HB2	1.83	0.42
1:K:12:PRO:HA	1:K:15:CYS:HB2	2.01	0.42
1:K:147:ILE:O	1:K:151:LEU:HG	2.19	0.42
1:B:12:PRO:HA	1:B:15:CYS:HB2	2.01	0.42
1:B:204:TYR:HD2	1:B:296:VAL:HG12	1.84	0.42
1:B:297:ILE:HG12	1:B:302:SER:HB2	2.02	0.42
1:B:452:GLU:O	1:B:456:ALA:N	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:115:GLU:O	1:D:119:ILE:HG13	2.20	0.42
1:D:221:PHE:CG	1:D:226:LEU:HB2	2.55	0.42
1:H:215:LEU:HD21	1:H:249:LYS:HB2	2.02	0.42
1:H:438:LEU:HD12	1:H:438:LEU:HA	1.84	0.42
1:J:215:LEU:HD21	1:J:249:LYS:HB2	2.02	0.42
1:K:215:LEU:HD21	1:K:249:LYS:HB2	2.02	0.42
1:K:245:LEU:HD12	1:K:245:LEU:HA	1.87	0.42
1:A:53:ASN:HA	1:A:56:LYS:HD3	2.01	0.41
1:A:221:PHE:O	1:A:225:SER:N	2.53	0.41
1:C:38:LYS:HE2	1:C:38:LYS:HB3	1.76	0.41
1:H:53:ASN:HA	1:H:56:LYS:HD3	2.01	0.41
1:K:442:MET:HE2	1:K:442:MET:HB2	1.84	0.41
1:D:204:TYR:HD2	1:D:296:VAL:HG12	1.84	0.41
1:E:374:LEU:HD23	1:E:374:LEU:HA	1.85	0.41
1:G:374:LEU:HD23	1:G:374:LEU:HA	1.85	0.41
1:H:221:PHE:O	1:H:225:SER:N	2.54	0.41
1:I:249:LYS:HB3	1:I:249:LYS:HE2	1.75	0.41
1:J:371:LEU:HD12	1:J:371:LEU:HA	1.91	0.41
1:K:371:LEU:HD12	1:K:371:LEU:HA	1.91	0.41
1:L:147:ILE:O	1:L:151:LEU:HG	2.19	0.41
1:L:297:ILE:HG12	1:L:302:SER:HB2	2.02	0.41
1:B:53:ASN:HA	1:B:56:LYS:HD3	2.01	0.41
1:B:115:GLU:O	1:B:119:ILE:HG13	2.20	0.41
1:B:310:ASN:OD1	1:B:310:ASN:N	2.52	0.41
1:C:215:LEU:HD21	1:C:249:LYS:HB2	2.02	0.41
1:E:204:TYR:HD2	1:E:296:VAL:HG12	1.84	0.41
1:F:215:LEU:HD21	1:F:249:LYS:HB2	2.02	0.41
1:G:217:ALA:O	1:G:220:THR:OG1	2.36	0.41
1:I:147:ILE:O	1:I:151:LEU:HG	2.19	0.41
1:A:12:PRO:HA	1:A:15:CYS:HB2	2.01	0.41
1:B:177:PHE:HD1	1:B:177:PHE:HA	1.71	0.41
1:C:87:ASP:HB3	1:C:129:LYS:CE	2.37	0.41
1:D:215:LEU:HD21	1:D:249:LYS:HB2	2.02	0.41
1:E:215:LEU:HD21	1:E:249:LYS:HB2	2.02	0.41
1:E:503:ARG:NH1	1:E:504:ASN:OD1	2.49	0.41
1:F:43:ASN:ND2	1:F:154:ASN:O	2.51	0.41
1:F:87:ASP:HB3	1:F:129:LYS:CE	2.37	0.41
1:G:53:ASN:HA	1:G:56:LYS:HD3	2.01	0.41
1:G:115:GLU:O	1:G:119:ILE:HG13	2.20	0.41
1:G:221:PHE:CG	1:G:226:LEU:HB2	2.55	0.41
1:G:452:GLU:O	1:G:456:ALA:N	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:38:LYS:HB3	1:I:38:LYS:HE2	1.75	0.41
1:I:297:ILE:HG12	1:I:302:SER:HB2	2.02	0.41
1:J:245:LEU:HD12	1:J:245:LEU:HA	1.87	0.41
1:K:38:LYS:HE2	1:K:38:LYS:HB3	1.75	0.41
1:B:217:ALA:O	1:B:220:THR:OG1	2.36	0.41
1:B:221:PHE:CG	1:B:226:LEU:HB2	2.55	0.41
1:C:348:ILE:CG2	1:D:281:ILE:HD11	2.50	0.41
1:D:297:ILE:HG12	1:D:302:SER:HB2	2.02	0.41
1:D:371:LEU:HD12	1:D:371:LEU:HA	1.91	0.41
1:D:503:ARG:NH1	1:D:504:ASN:OD1	2.49	0.41
1:E:31:ASP:OD1	1:E:32:TYR:N	2.53	0.41
1:G:281:ILE:HD11	1:H:348:ILE:CG2	2.50	0.41
1:G:387:ILE:HB	1:G:500:TYR:CD2	2.56	0.41
1:H:12:PRO:HA	1:H:15:CYS:HB2	2.01	0.41
1:I:115:GLU:O	1:I:119:ILE:HG13	2.20	0.41
1:J:43:ASN:ND2	1:J:154:ASN:O	2.51	0.41
1:K:310:ASN:OD1	1:K:310:ASN:N	2.52	0.41
1:L:115:GLU:O	1:L:119:ILE:HG13	2.20	0.41
1:A:115:GLU:O	1:A:119:ILE:HG13	2.20	0.41
1:B:387:ILE:HB	1:B:500:TYR:CD2	2.56	0.41
1:C:43:ASN:ND2	1:C:154:ASN:O	2.51	0.41
1:D:31:ASP:OD1	1:D:32:TYR:N	2.53	0.41
1:D:334:PHE:CZ	1:D:345:LEU:HD21	2.56	0.41
1:F:221:PHE:O	1:F:225:SER:N	2.53	0.41
1:F:374:LEU:HD23	1:F:374:LEU:HA	1.85	0.41
1:H:115:GLU:O	1:H:119:ILE:HG13	2.20	0.41
1:H:204:TYR:HD2	1:H:296:VAL:HG12	1.84	0.41
1:I:53:ASN:HA	1:I:56:LYS:HD3	2.01	0.41
1:I:202:LYS:HB2	1:I:204:TYR:CE1	2.56	0.41
1:L:53:ASN:HA	1:L:56:LYS:HD3	2.01	0.41
1:L:202:LYS:HB2	1:L:204:TYR:CE1	2.56	0.41
1:L:221:PHE:CG	1:L:226:LEU:HB2	2.55	0.41
1:A:28:MET:HE2	1:A:28:MET:HB3	1.85	0.41
1:A:204:TYR:HD2	1:A:296:VAL:HG12	1.84	0.41
1:A:223:ARG:HA	1:A:223:ARG:HD2	1.95	0.41
1:C:334:PHE:CZ	1:C:345:LEU:HD21	2.56	0.41
1:D:177:PHE:HD1	1:D:177:PHE:HA	1.71	0.41
1:D:511:LYS:HB2	1:D:511:LYS:HE3	1.53	0.41
1:E:245:LEU:HD12	1:E:245:LEU:HA	1.87	0.41
1:E:297:ILE:HG12	1:E:302:SER:HB2	2.02	0.41
1:E:334:PHE:CZ	1:E:345:LEU:HD21	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:334:PHE:CZ	1:F:345:LEU:HD21	2.56	0.41
1:G:202:LYS:HB2	1:G:204:TYR:CE1	2.56	0.41
1:H:202:LYS:HB2	1:H:204:TYR:CE1	2.56	0.41
1:H:503:ARG:NH1	1:H:504:ASN:OD1	2.49	0.41
1:I:221:PHE:CG	1:I:226:LEU:HB2	2.55	0.41
1:J:454:LEU:HG	1:J:458:PHE:CZ	2.56	0.41
1:A:25:LEU:HD23	1:A:25:LEU:HA	1.81	0.41
1:A:202:LYS:HB2	1:A:204:TYR:CE1	2.56	0.41
1:A:503:ARG:NH1	1:A:504:ASN:OD1	2.49	0.41
1:B:202:LYS:HB2	1:B:204:TYR:CE1	2.56	0.41
1:C:115:GLU:O	1:C:119:ILE:HG13	2.20	0.41
1:C:221:PHE:O	1:C:225:SER:N	2.54	0.41
1:C:281:ILE:HD11	1:D:348:ILE:CG2	2.51	0.41
1:D:12:PRO:HA	1:D:15:CYS:HB2	2.01	0.41
1:E:12:PRO:HA	1:E:15:CYS:HB2	2.01	0.41
1:E:371:LEU:HD12	1:E:371:LEU:HA	1.91	0.41
1:F:38:LYS:HE2	1:F:38:LYS:HB3	1.76	0.41
1:F:438:LEU:HD12	1:F:438:LEU:HA	1.84	0.41
1:G:177:PHE:HD1	1:G:177:PHE:HA	1.71	0.41
1:G:310:ASN:OD1	1:G:310:ASN:N	2.52	0.41
1:J:310:ASN:OD1	1:J:310:ASN:N	2.52	0.41
1:K:43:ASN:ND2	1:K:154:ASN:O	2.51	0.41
1:A:38:LYS:HE2	1:A:38:LYS:HB3	1.76	0.41
1:A:334:PHE:CZ	1:A:345:LEU:HD21	2.56	0.41
1:A:455:SER:HA	1:A:458:PHE:CD2	2.56	0.41
1:B:413:ASP:HB3	1:B:464:LEU:CD2	2.51	0.41
1:C:309:LEU:HD12	1:C:309:LEU:HA	1.88	0.41
1:C:399:ASN:HD21	1:C:489:LYS:HB2	1.86	0.41
1:C:455:SER:HA	1:C:458:PHE:CD2	2.56	0.41
1:D:245:LEU:HD12	1:D:245:LEU:HA	1.87	0.41
1:E:88:LEU:HD23	1:E:88:LEU:HA	1.85	0.41
1:E:511:LYS:HB2	1:E:511:LYS:HE3	1.53	0.41
1:F:115:GLU:O	1:F:119:ILE:HG13	2.20	0.41
1:F:297:ILE:HG12	1:F:302:SER:HB2	2.02	0.41
1:F:455:SER:HA	1:F:458:PHE:CD2	2.56	0.41
1:G:50:GLU:OE2	1:G:501:ARG:NH2	2.49	0.41
1:G:413:ASP:HB3	1:G:464:LEU:CD2	2.51	0.41
1:G:561:ARG:O	1:G:565:ILE:HB	2.21	0.41
1:H:25:LEU:HD23	1:H:25:LEU:HA	1.81	0.41
1:H:223:ARG:HA	1:H:223:ARG:HD2	1.95	0.41
1:H:334:PHE:CZ	1:H:345:LEU:HD21	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:455:SER:HA	1:H:458:PHE:CD2	2.56	0.41
1:I:215:LEU:HD21	1:I:249:LYS:HB2	2.02	0.41
1:I:221:PHE:O	1:I:225:SER:N	2.54	0.41
1:I:413:ASP:HB3	1:I:464:LEU:CD2	2.51	0.41
1:J:53:ASN:HA	1:J:56:LYS:HD3	2.01	0.41
1:J:206:ILE:HD12	1:J:268:ALA:HB2	2.03	0.41
1:J:387:ILE:HB	1:J:500:TYR:CD2	2.56	0.41
1:K:53:ASN:HA	1:K:56:LYS:HD3	2.01	0.41
1:K:206:ILE:HD12	1:K:268:ALA:HB2	2.03	0.41
1:K:454:LEU:HG	1:K:458:PHE:CZ	2.56	0.41
1:L:215:LEU:HD21	1:L:249:LYS:HB2	2.02	0.41
1:L:221:PHE:O	1:L:225:SER:N	2.54	0.41
1:L:413:ASP:HB3	1:L:464:LEU:CD2	2.51	0.41
1:A:88:LEU:HD23	1:A:88:LEU:HA	1.85	0.41
1:A:206:ILE:HD12	1:A:268:ALA:HB2	2.03	0.41
1:A:387:ILE:HB	1:A:500:TYR:CD2	2.56	0.41
1:B:215:LEU:HD21	1:B:249:LYS:HB2	2.02	0.41
1:C:297:ILE:HG12	1:C:302:SER:HB2	2.02	0.41
1:C:413:ASP:HB3	1:C:464:LEU:CD2	2.51	0.41
1:D:28:MET:HE2	1:D:28:MET:HB3	1.85	0.41
1:D:455:SER:HA	1:D:458:PHE:CD2	2.56	0.41
1:F:399:ASN:HD21	1:F:489:LYS:HB2	1.86	0.41
1:F:413:ASP:HB3	1:F:464:LEU:CD2	2.51	0.41
1:G:221:PHE:O	1:G:225:SER:N	2.53	0.41
1:G:334:PHE:CZ	1:G:345:LEU:HD21	2.56	0.41
1:H:28:MET:HE2	1:H:28:MET:HB3	1.85	0.41
1:H:206:ILE:HD12	1:H:268:ALA:HB2	2.03	0.41
1:H:387:ILE:HB	1:H:500:TYR:CD2	2.56	0.41
1:I:88:LEU:HD23	1:I:88:LEU:HA	1.85	0.41
1:I:561:ARG:O	1:I:565:ILE:HB	2.21	0.41
1:J:38:LYS:HE2	1:J:38:LYS:HB3	1.76	0.41
1:J:44:THR:HG1	1:J:45:PRO:HD3	1.84	0.41
1:K:221:PHE:O	1:K:225:SER:N	2.53	0.41
1:K:387:ILE:HB	1:K:500:TYR:CD2	2.56	0.41
1:L:561:ARG:O	1:L:565:ILE:HB	2.21	0.41
1:A:348:ILE:CG2	1:B:281:ILE:HD11	2.51	0.40
1:A:399:ASN:HD21	1:A:489:LYS:HB2	1.86	0.40
1:A:413:ASP:HB3	1:A:464:LEU:CD2	2.51	0.40
1:B:206:ILE:HD12	1:B:268:ALA:HB2	2.03	0.40
1:B:333:GLU:HB3	1:B:542:ARG:HD2	2.04	0.40
1:C:170:LYS:HB2	1:C:170:LYS:HE2	1.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:220:THR:HA	1:D:331:MET:HG3	2.02	0.40
1:C:374:LEU:HD23	1:C:374:LEU:HA	1.85	0.40
1:C:387:ILE:HB	1:C:500:TYR:CD2	2.56	0.40
1:C:438:LEU:HD12	1:C:438:LEU:HA	1.84	0.40
1:D:221:PHE:O	1:D:225:SER:N	2.53	0.40
1:E:177:PHE:HD1	1:E:177:PHE:HA	1.71	0.40
1:E:202:LYS:HB2	1:E:204:TYR:CE1	2.56	0.40
1:E:221:PHE:O	1:E:225:SER:N	2.54	0.40
1:E:281:ILE:HD11	1:F:348:ILE:CG2	2.51	0.40
1:E:399:ASN:HD21	1:E:489:LYS:HB2	1.86	0.40
1:E:455:SER:HA	1:E:458:PHE:CD2	2.56	0.40
1:F:387:ILE:HB	1:F:500:TYR:CD2	2.56	0.40
1:G:215:LEU:HD21	1:G:249:LYS:HB2	2.02	0.40
1:G:333:GLU:HB3	1:G:542:ARG:HD2	2.04	0.40
1:H:38:LYS:HE2	1:H:38:LYS:HB3	1.76	0.40
1:H:399:ASN:HD21	1:H:489:LYS:HB2	1.86	0.40
1:J:221:PHE:O	1:J:225:SER:N	2.54	0.40
1:J:297:ILE:HG12	1:J:302:SER:HB2	2.02	0.40
1:J:314:LYS:HB3	1:J:314:LYS:HE2	1.87	0.40
1:K:44:THR:HG1	1:K:45:PRO:HD3	1.84	0.40
1:L:68:ILE:HD13	1:L:68:ILE:HA	1.94	0.40
1:L:217:ALA:O	1:L:220:THR:OG1	2.36	0.40
1:B:50:GLU:OE2	1:B:501:ARG:NH2	2.49	0.40
1:B:99:LYS:HB3	1:B:99:LYS:HE3	1.83	0.40
1:B:221:PHE:O	1:B:225:SER:N	2.54	0.40
1:B:334:PHE:CZ	1:B:345:LEU:HD21	2.56	0.40
1:B:561:ARG:O	1:B:565:ILE:HB	2.21	0.40
1:E:28:MET:HE2	1:E:28:MET:HB3	1.86	0.40
1:E:387:ILE:HB	1:E:500:TYR:CD2	2.56	0.40
1:F:202:LYS:HB2	1:F:204:TYR:CE1	2.56	0.40
1:F:415:LEU:HD23	1:F:422:LEU:HD23	2.04	0.40
1:G:206:ILE:HD12	1:G:268:ALA:HB2	2.03	0.40
1:H:371:LEU:HD12	1:H:371:LEU:HA	1.91	0.40
1:H:413:ASP:HB3	1:H:464:LEU:CD2	2.51	0.40
1:I:217:ALA:O	1:I:220:THR:OG1	2.36	0.40
1:J:413:ASP:HB3	1:J:464:LEU:CD2	2.51	0.40
1:K:28:MET:HE2	1:K:28:MET:HB3	1.86	0.40
1:K:413:ASP:HB3	1:K:464:LEU:CD2	2.51	0.40
1:C:415:LEU:HD23	1:C:422:LEU:HD23	2.04	0.40
1:D:88:LEU:HD23	1:D:88:LEU:HA	1.85	0.40
1:D:202:LYS:HB2	1:D:204:TYR:CE1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:399:ASN:HD21	1:D:489:LYS:HB2	1.86	0.40
1:E:333:GLU:HB3	1:E:542:ARG:HD2	2.04	0.40
1:F:170:LYS:HB2	1:F:170:LYS:HE2	1.91	0.40
1:H:88:LEU:HD23	1:H:88:LEU:HA	1.85	0.40
1:H:297:ILE:HG12	1:H:302:SER:HB2	2.02	0.40
1:I:127:LYS:HZ3	1:I:127:LYS:HG2	1.60	0.40
1:J:115:GLU:O	1:J:119:ILE:HG13	2.20	0.40
1:J:202:LYS:HB2	1:J:204:TYR:CE1	2.56	0.40
1:K:75:LEU:O	1:K:79:LEU:N	2.45	0.40
1:K:297:ILE:HG12	1:K:302:SER:HB2	2.02	0.40
1:L:333:GLU:HB3	1:L:542:ARG:HD2	2.03	0.40
1:A:127:LYS:HZ3	1:A:127:LYS:HG2	1.60	0.40
1:A:297:ILE:HG12	1:A:302:SER:HB2	2.02	0.40
1:A:371:LEU:HD12	1:A:371:LEU:HA	1.91	0.40
1:A:415:LEU:HD23	1:A:422:LEU:HD23	2.04	0.40
1:B:38:LYS:HB3	1:B:38:LYS:HE2	1.75	0.40
1:C:56:LYS:HB2	1:C:56:LYS:HE2	1.96	0.40
1:C:202:LYS:HB2	1:C:204:TYR:CE1	2.56	0.40
1:D:333:GLU:HB3	1:D:542:ARG:HD2	2.04	0.40
1:D:387:ILE:HB	1:D:500:TYR:CD2	2.56	0.40
1:D:415:LEU:HD23	1:D:422:LEU:HD23	2.04	0.40
1:E:415:LEU:HD23	1:E:422:LEU:HD23	2.04	0.40
1:E:496:LEU:HD23	1:E:496:LEU:HA	1.93	0.40
1:E:519:LEU:HD23	1:E:519:LEU:HA	1.83	0.40
1:F:177:PHE:HD1	1:F:177:PHE:HA	1.71	0.40
1:G:348:ILE:CG2	1:H:281:ILE:HD11	2.51	0.40
1:I:206:ILE:HD12	1:I:268:ALA:HB2	2.03	0.40
1:I:223:ARG:HA	1:I:223:ARG:HD2	1.95	0.40
1:I:333:GLU:HB3	1:I:542:ARG:HD2	2.04	0.40
1:J:28:MET:HE2	1:J:28:MET:HB3	1.86	0.40
1:J:75:LEU:O	1:J:79:LEU:N	2.45	0.40
1:K:115:GLU:O	1:K:119:ILE:HG13	2.20	0.40
1:K:202:LYS:HB2	1:K:204:TYR:CE1	2.56	0.40
1:L:206:ILE:HD12	1:L:268:ALA:HB2	2.03	0.40
1:L:454:LEU:HG	1:L:458:PHE:CZ	2.56	0.40
1:A:75:LEU:O	1:A:79:LEU:N	2.45	0.40
1:C:25:LEU:HD23	1:C:25:LEU:HA	1.81	0.40
1:D:291:SER:OG	1:D:293:GLU:O	2.36	0.40
1:D:519:LEU:HD23	1:D:519:LEU:HA	1.83	0.40
1:E:348:ILE:CG2	1:F:281:ILE:HD11	2.52	0.40
1:F:223:ARG:HA	1:F:223:ARG:HD2	1.95	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:309:LEU:HD12	1:F:309:LEU:HA	1.88	0.40
1:G:99:LYS:HB3	1:G:99:LYS:HE3	1.83	0.40
1:H:415:LEU:HD23	1:H:422:LEU:HD23	2.04	0.40
1:I:454:LEU:HG	1:I:458:PHE:CZ	2.56	0.40
1:J:455:SER:HA	1:J:458:PHE:CD2	2.56	0.40
1:K:314:LYS:HB3	1:K:314:LYS:HE2	1.87	0.40
1:K:415:LEU:HD23	1:K:422:LEU:HD23	2.04	0.40
1:L:387:ILE:HB	1:L:500:TYR:CD2	2.56	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	A	573/1029 (56%)	564 (98%)	9 (2%)	0	100	100
1	B	573/1029 (56%)	564 (98%)	9 (2%)	0	100	100
1	C	573/1029 (56%)	564 (98%)	9 (2%)	0	100	100
1	D	573/1029 (56%)	564 (98%)	9 (2%)	0	100	100
1	E	573/1029 (56%)	564 (98%)	9 (2%)	0	100	100
1	F	573/1029 (56%)	564 (98%)	9 (2%)	0	100	100
1	G	573/1029 (56%)	564 (98%)	9 (2%)	0	100	100
1	H	573/1029 (56%)	564 (98%)	9 (2%)	0	100	100
1	I	573/1029 (56%)	564 (98%)	9 (2%)	0	100	100
1	J	573/1029 (56%)	564 (98%)	9 (2%)	0	100	100
1	K	573/1029 (56%)	564 (98%)	9 (2%)	0	100	100
1	L	573/1029 (56%)	564 (98%)	9 (2%)	0	100	100
All	All	6876/12348 (56%)	6768 (98%)	108 (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	A	470/901 (52%)	461 (98%)	9 (2%)	50	76
1	B	470/901 (52%)	461 (98%)	9 (2%)	50	76
1	C	470/901 (52%)	461 (98%)	9 (2%)	50	76
1	D	470/901 (52%)	461 (98%)	9 (2%)	50	76
1	E	470/901 (52%)	461 (98%)	9 (2%)	50	76
1	F	470/901 (52%)	461 (98%)	9 (2%)	50	76
1	G	470/901 (52%)	461 (98%)	9 (2%)	50	76
1	H	470/901 (52%)	461 (98%)	9 (2%)	50	76
1	I	470/901 (52%)	461 (98%)	9 (2%)	50	76
1	J	470/901 (52%)	461 (98%)	9 (2%)	50	76
1	K	470/901 (52%)	461 (98%)	9 (2%)	50	76
1	L	470/901 (52%)	461 (98%)	9 (2%)	50	76
All	All	5640/10812 (52%)	5532 (98%)	108 (2%)	49	76

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	TRP
1	A	117	LEU
1	A	246	GLN
1	A	279	LEU
1	A	289	THR
1	A	443	ILE
1	A	474	ILE
1	A	565	ILE
1	A	574	MET
1	B	9	TRP
1	B	117	LEU

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Mol	Chain	Res	Type
1	B	246	GLN
1	B	279	LEU
1	B	289	THR
1	B	443	ILE
1	B	474	ILE
1	B	565	ILE
1	B	574	MET
1	C	9	TRP
1	C	117	LEU
1	C	246	GLN
1	C	279	LEU
1	C	289	THR
1	C	443	ILE
1	C	474	ILE
1	C	565	ILE
1	C	574	MET
1	D	9	TRP
1	D	117	LEU
1	D	246	GLN
1	D	279	LEU
1	D	289	THR
1	D	443	ILE
1	D	474	ILE
1	D	565	ILE
1	D	574	MET
1	E	9	TRP
1	E	117	LEU
1	E	246	GLN
1	E	279	LEU
1	E	289	THR
1	E	443	ILE
1	E	474	ILE
1	E	565	ILE
1	E	574	MET
1	F	9	TRP
1	F	117	LEU
1	F	246	GLN
1	F	279	LEU
1	F	289	THR
1	F	443	ILE
1	F	474	ILE
1	F	565	ILE

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Mol	Chain	Res	Type
1	F	574	MET
1	G	9	TRP
1	G	117	LEU
1	G	246	GLN
1	G	279	LEU
1	G	289	THR
1	G	443	ILE
1	G	474	ILE
1	G	565	ILE
1	G	574	MET
1	H	9	TRP
1	H	117	LEU
1	H	246	GLN
1	H	279	LEU
1	H	289	THR
1	H	443	ILE
1	H	474	ILE
1	H	565	ILE
1	H	574	MET
1	I	9	TRP
1	I	117	LEU
1	I	246	GLN
1	I	279	LEU
1	I	289	THR
1	I	443	ILE
1	I	474	ILE
1	I	565	ILE
1	I	574	MET
1	J	9	TRP
1	J	117	LEU
1	J	246	GLN
1	J	279	LEU
1	J	289	THR
1	J	443	ILE
1	J	474	ILE
1	J	565	ILE
1	J	574	MET
1	K	9	TRP
1	K	117	LEU
1	K	246	GLN
1	K	279	LEU
1	K	289	THR

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Mol	Chain	Res	Type
1	K	443	ILE
1	K	474	ILE
1	K	565	ILE
1	K	574	MET
1	L	9	TRP
1	L	117	LEU
1	L	246	GLN
1	L	279	LEU
1	L	289	THR
1	L	443	ILE
1	L	474	ILE
1	L	565	ILE
1	L	574	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	ASN
1	A	167	HIS
1	A	495	GLN
1	B	78	ASN
1	B	167	HIS
1	B	495	GLN
1	B	580	ASN
1	C	78	ASN
1	C	167	HIS
1	C	495	GLN
1	C	580	ASN
1	D	78	ASN
1	D	495	GLN
1	E	78	ASN
1	E	495	GLN
1	F	78	ASN
1	F	167	HIS
1	F	495	GLN
1	F	580	ASN
1	G	78	ASN
1	G	167	HIS
1	G	495	GLN
1	G	580	ASN
1	H	78	ASN
1	H	167	HIS

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Mol	Chain	Res	Type
1	H	495	GLN
1	I	78	ASN
1	I	167	HIS
1	I	495	GLN
1	I	580	ASN
1	J	78	ASN
1	J	167	HIS
1	J	495	GLN
1	K	78	ASN
1	K	167	HIS
1	K	495	GLN
1	L	78	ASN
1	L	167	HIS
1	L	495	GLN
1	L	580	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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](#)

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

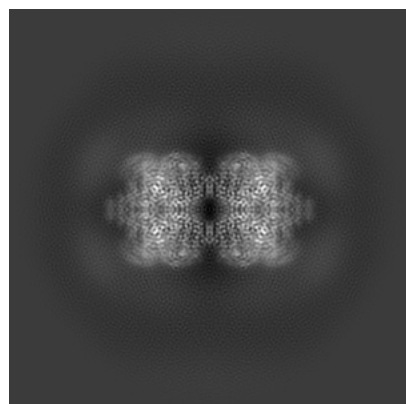
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52479. These allow visual inspection of the internal detail of the map and identification of artifacts.

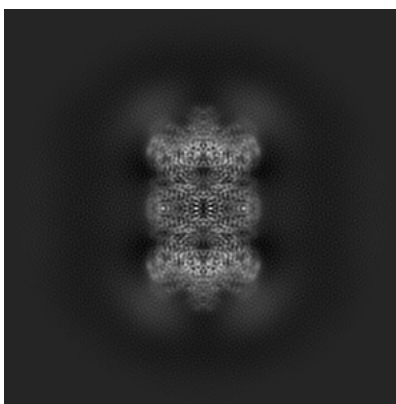
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

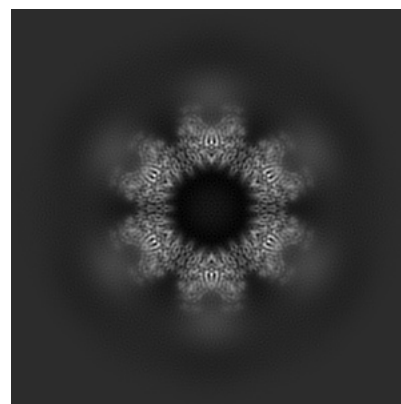
6.1.1 Primary map



X

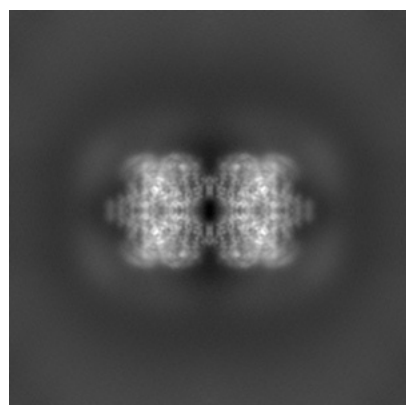


Y

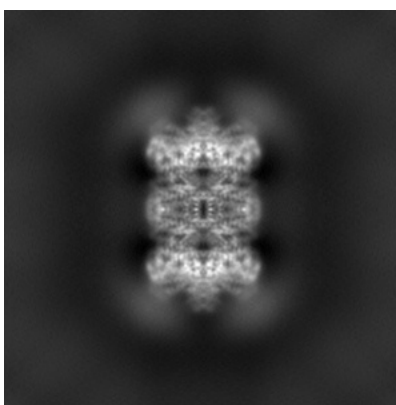


Z

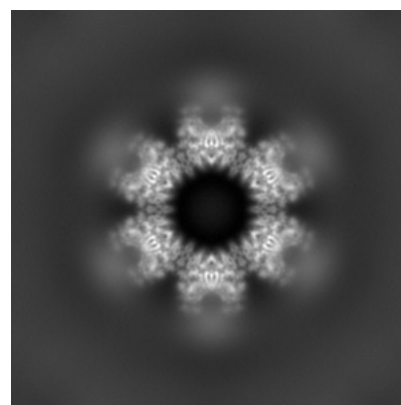
6.1.2 Raw map



X



Y

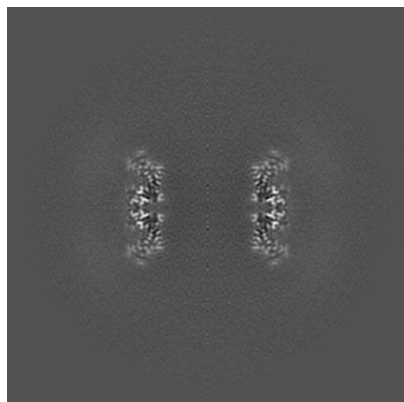


Z

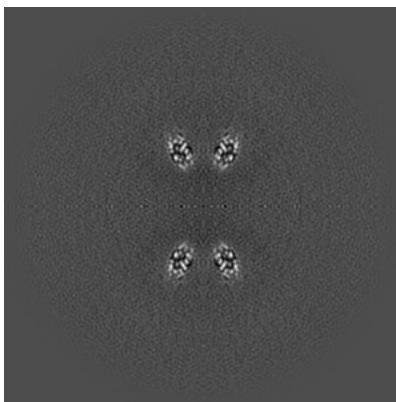
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

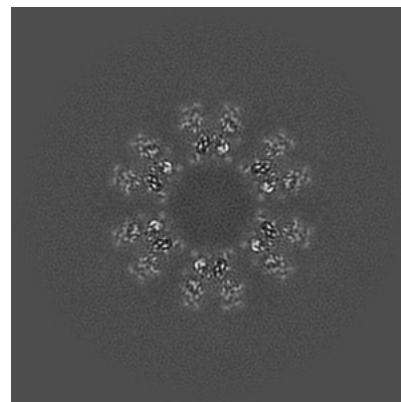
6.2.1 Primary map



X Index: 168

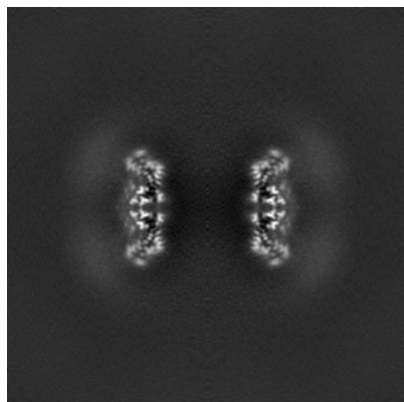


Y Index: 168

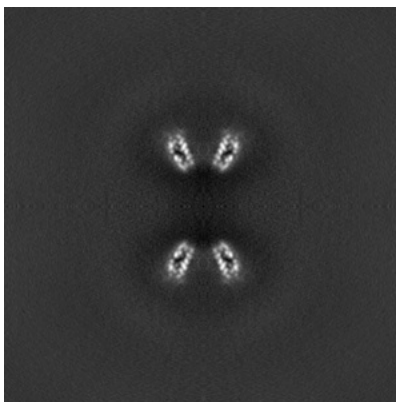


Z Index: 168

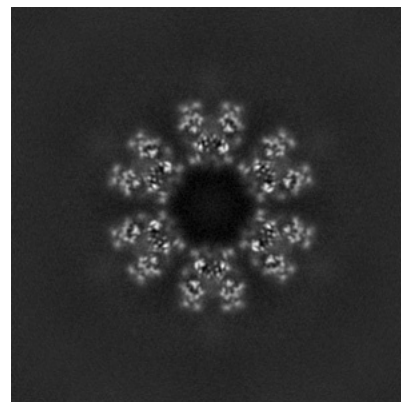
6.2.2 Raw map



X Index: 168



Y Index: 168

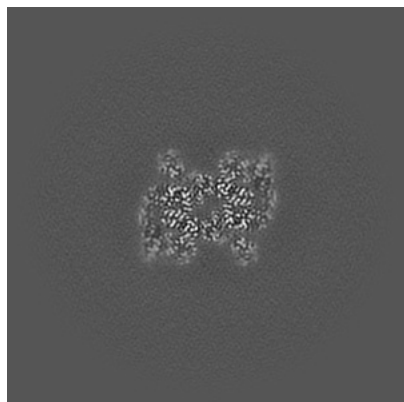


Z Index: 168

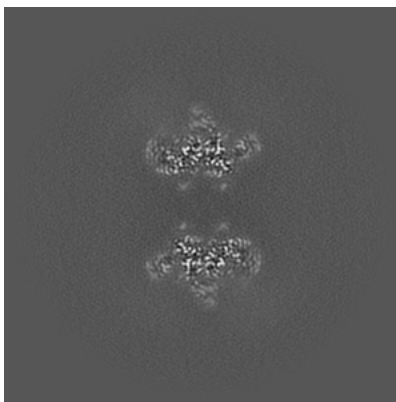
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

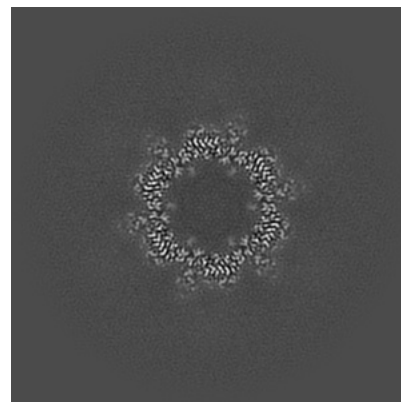
6.3.1 Primary map



X Index: 213

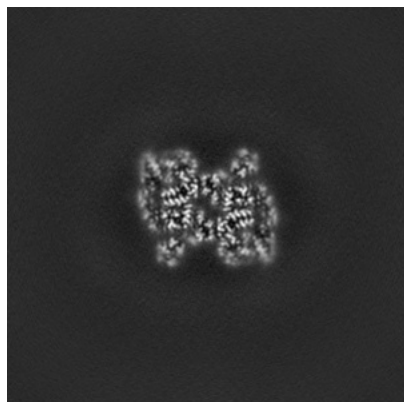


Y Index: 196

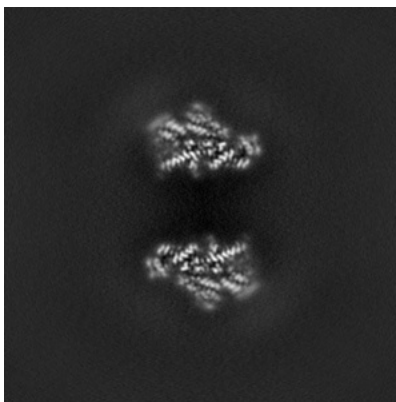


Z Index: 152

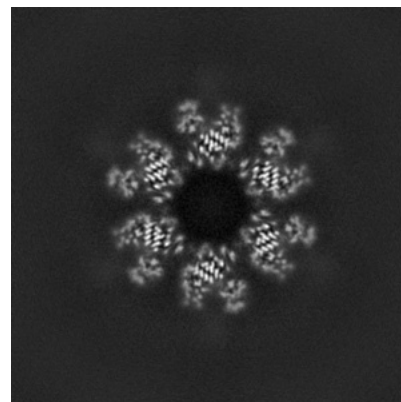
6.3.2 Raw map



X Index: 123



Y Index: 187

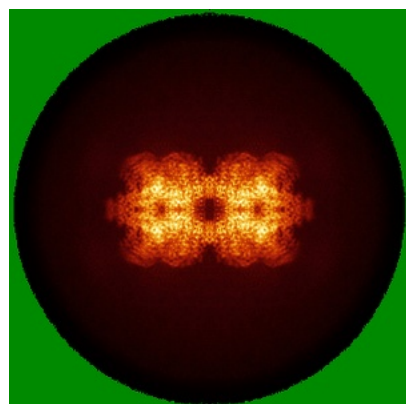


Z Index: 173

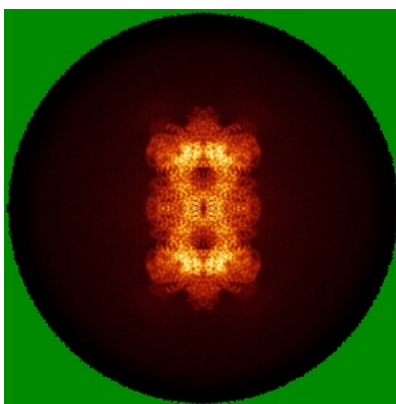
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

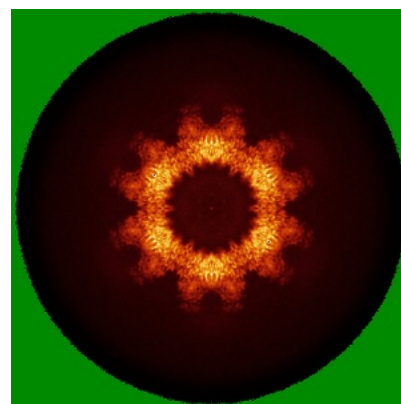
6.4.1 Primary map



X

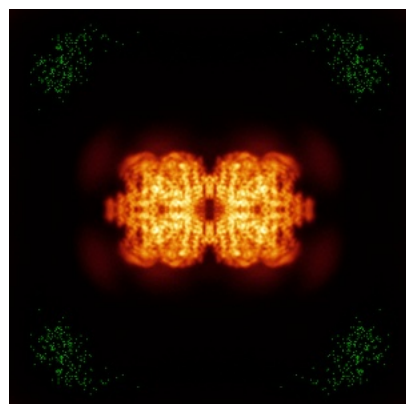


Y

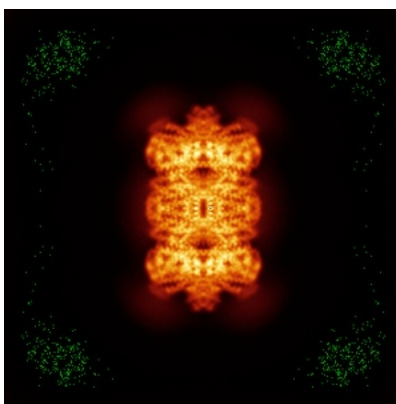


Z

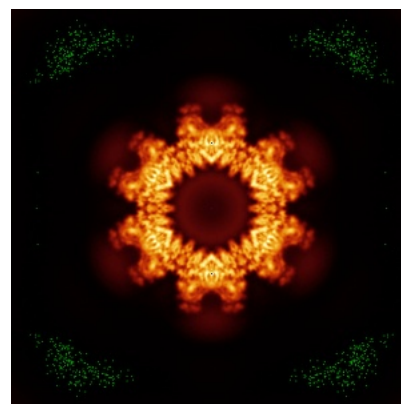
6.4.2 Raw map



X



Y

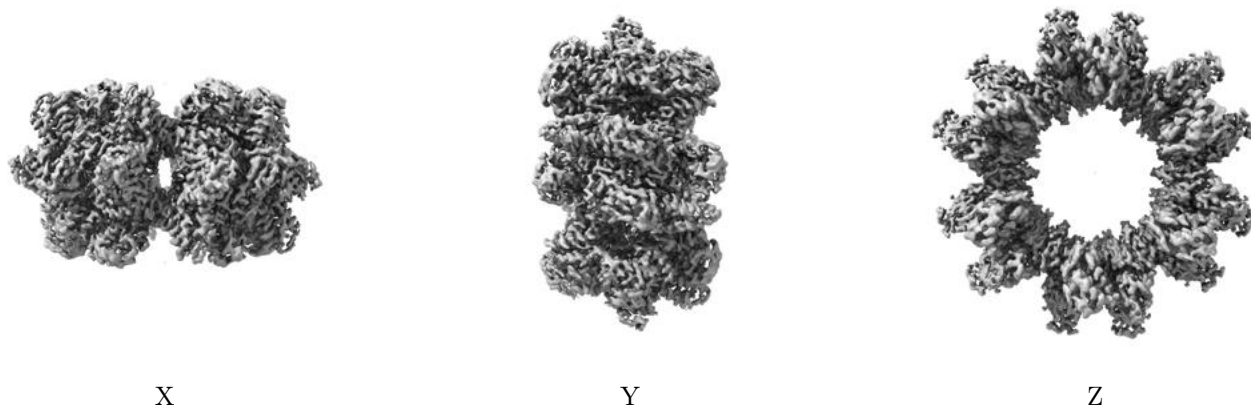


Z

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

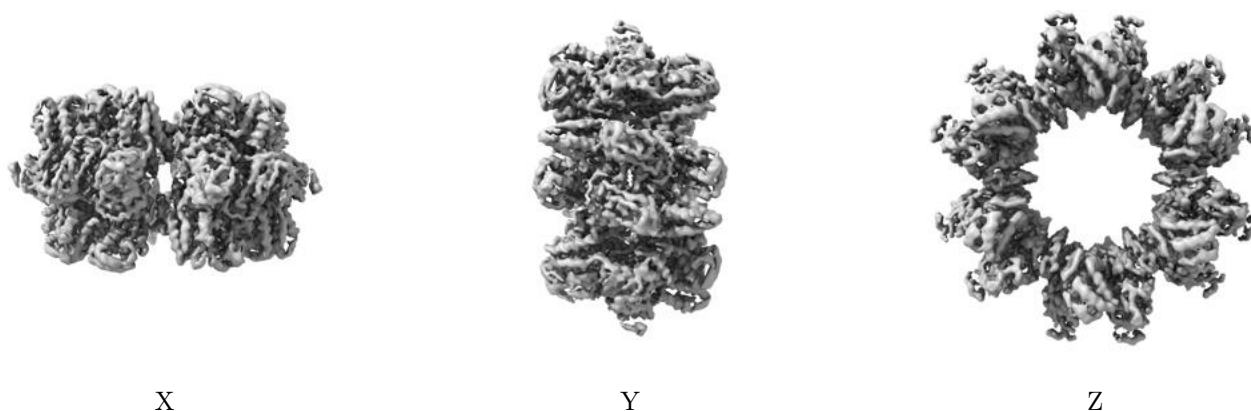
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 5.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

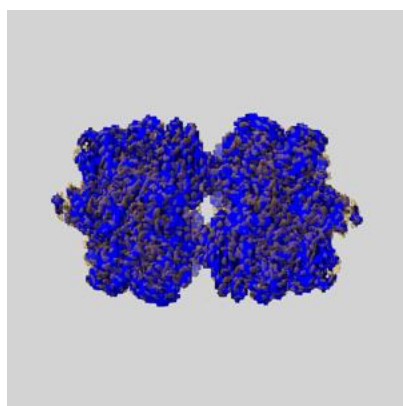
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

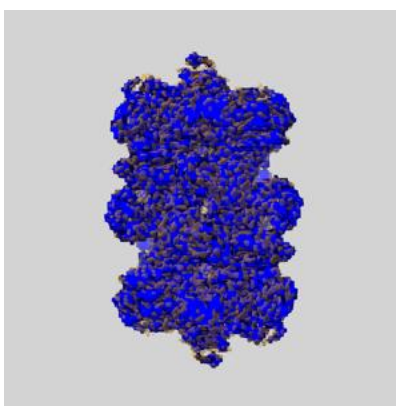
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

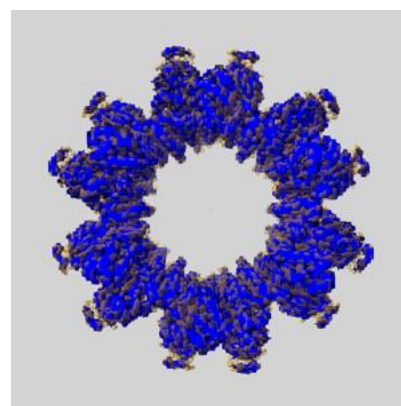
6.6.1 emd_52479_msk_1.map [i](#)



X



Y

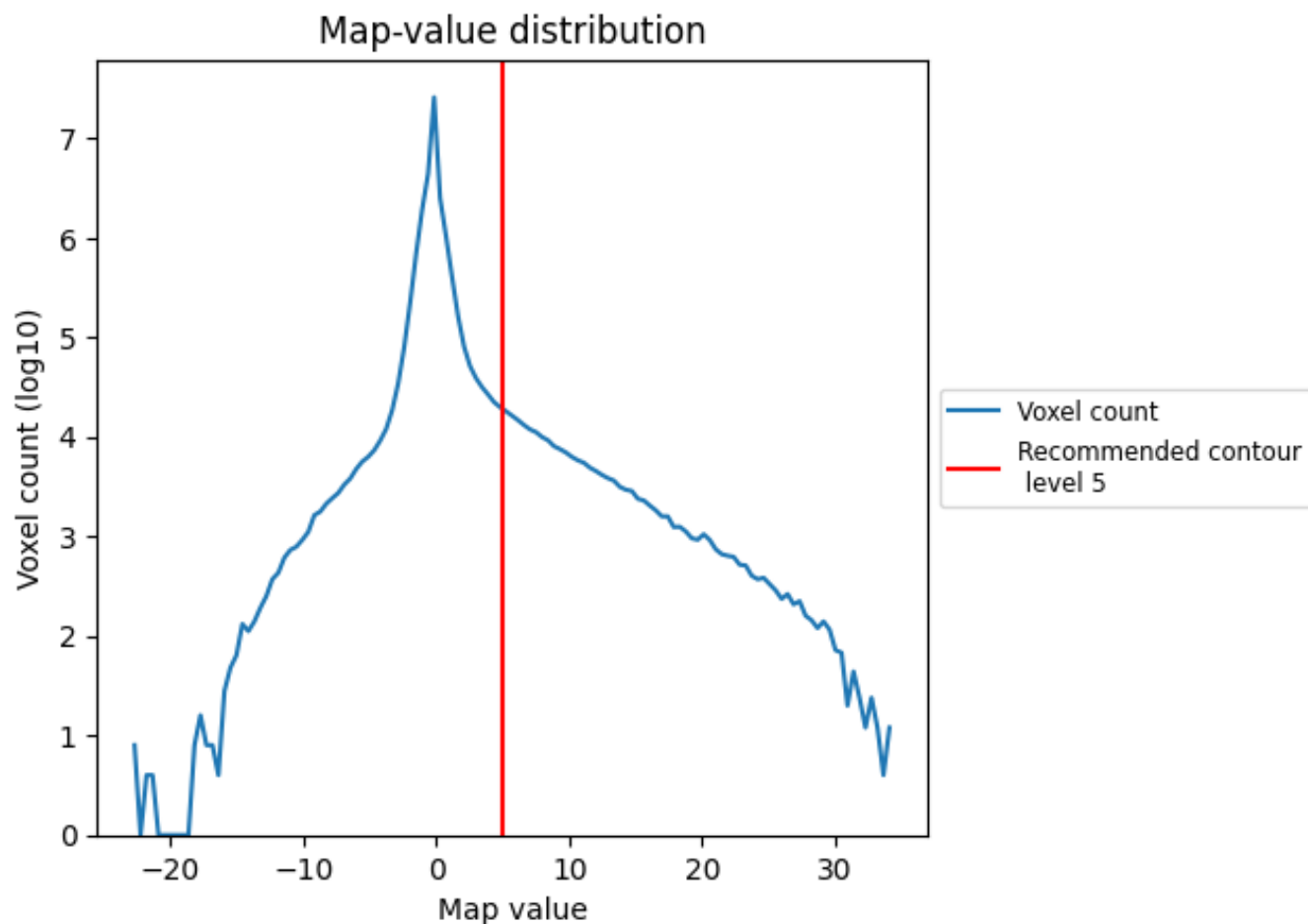


Z

7 Map analysis [i](#)

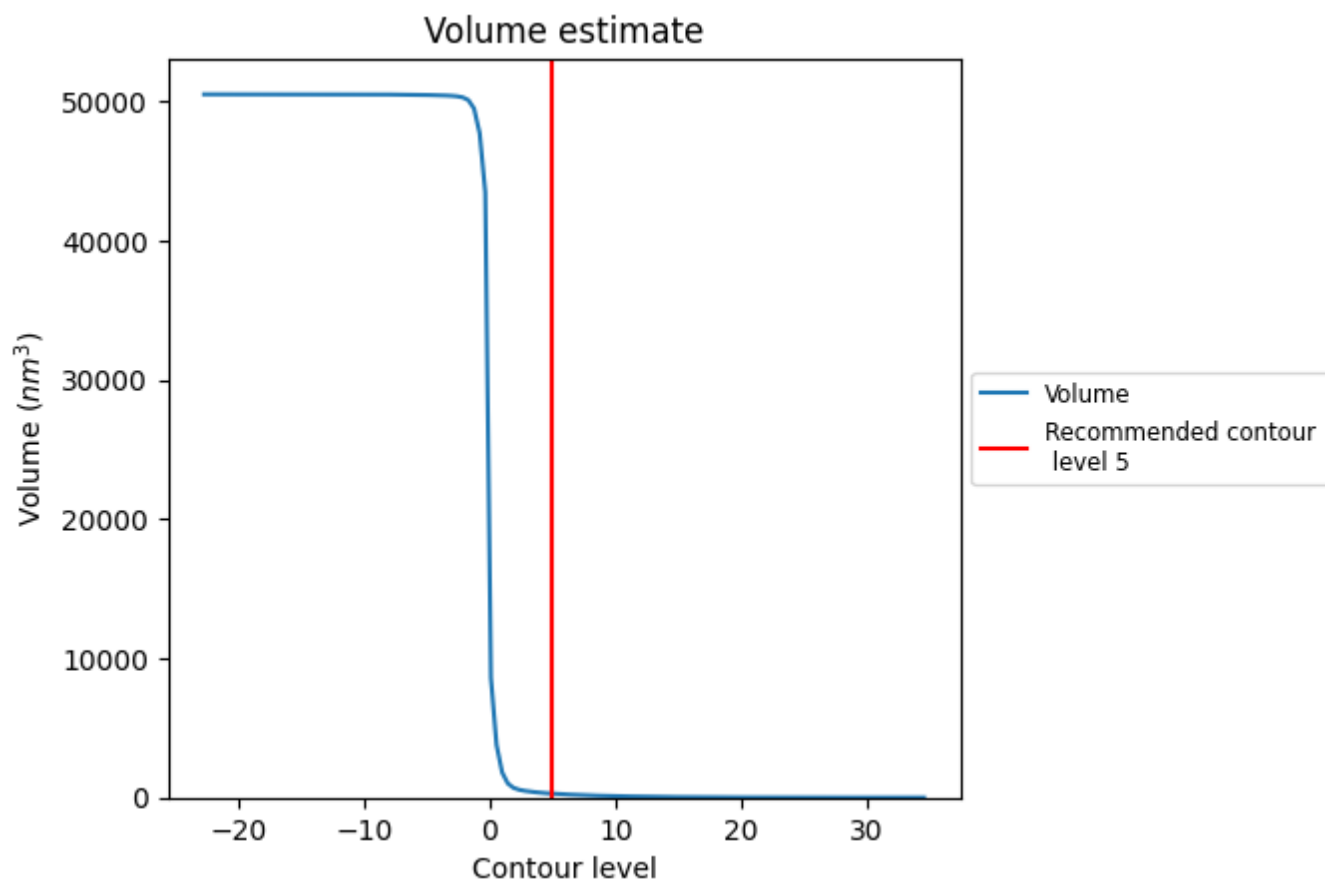
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

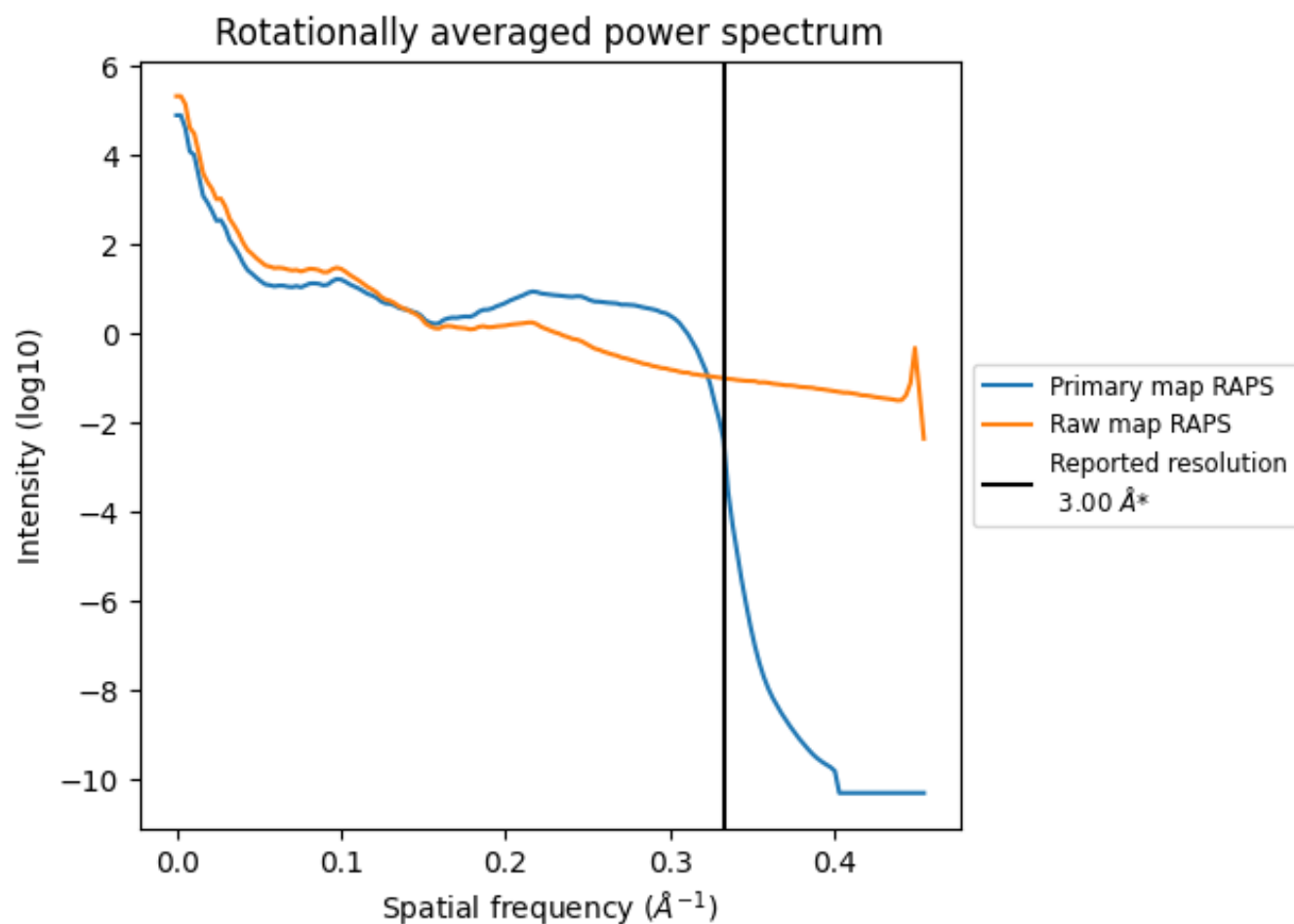
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 282 nm³; this corresponds to an approximate mass of 255 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

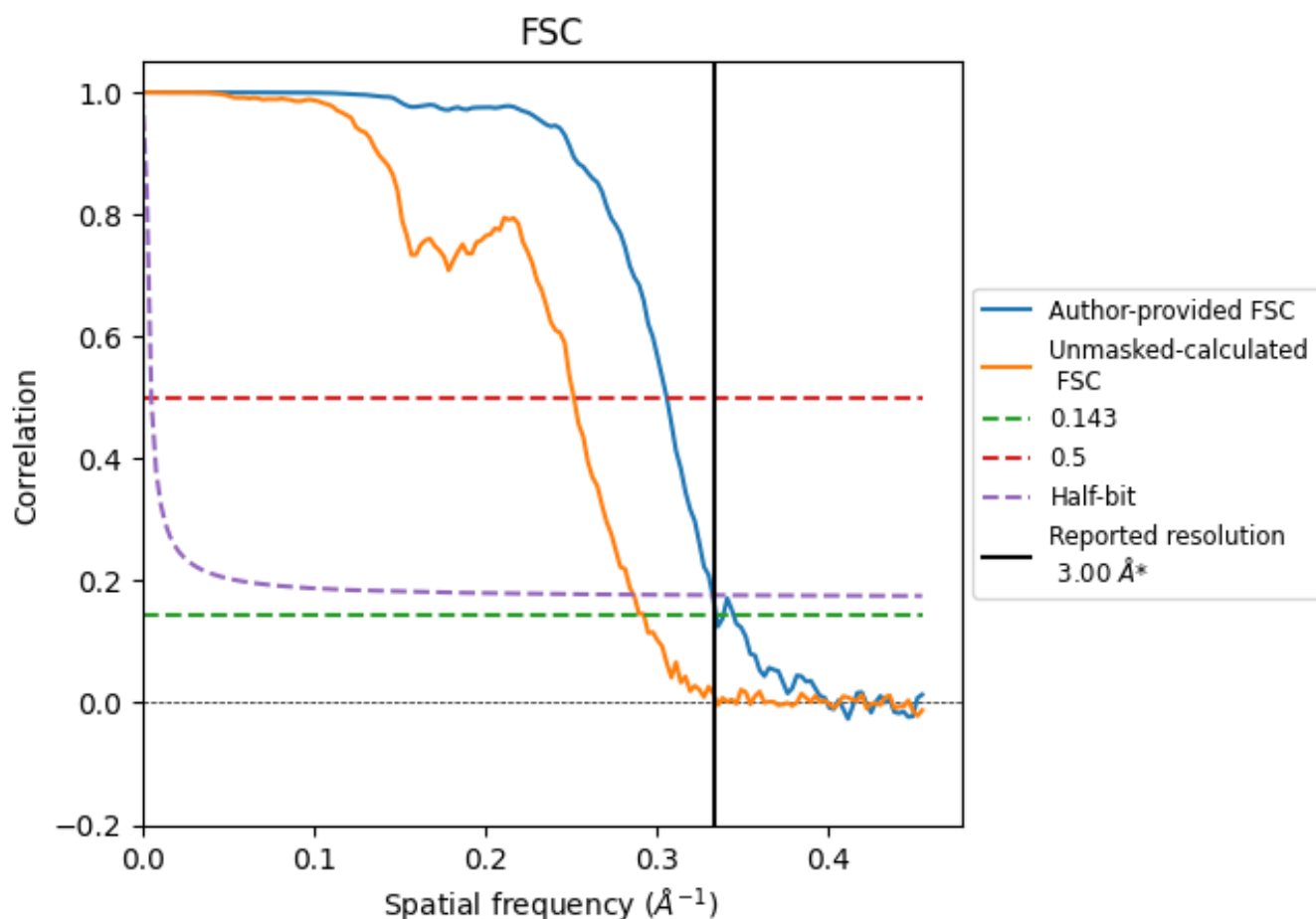


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.333 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

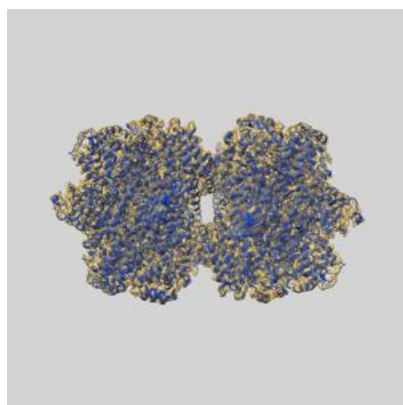
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	2.99	3.27	3.01
Unmasked-calculated*	3.42	3.97	3.49

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.42 differs from the reported value 3.0 by more than 10 %

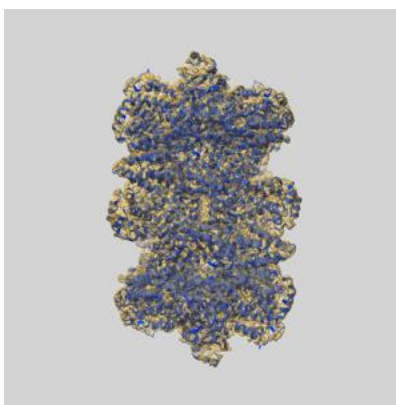
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-52479 and PDB model 9HXJ. Per-residue inclusion information can be found in [section 3](#) on [page 31](#).

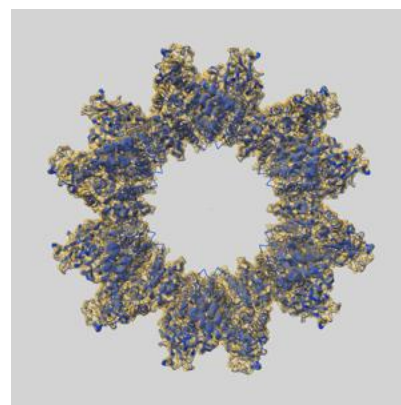
9.1 Map-model overlay [i](#)



X



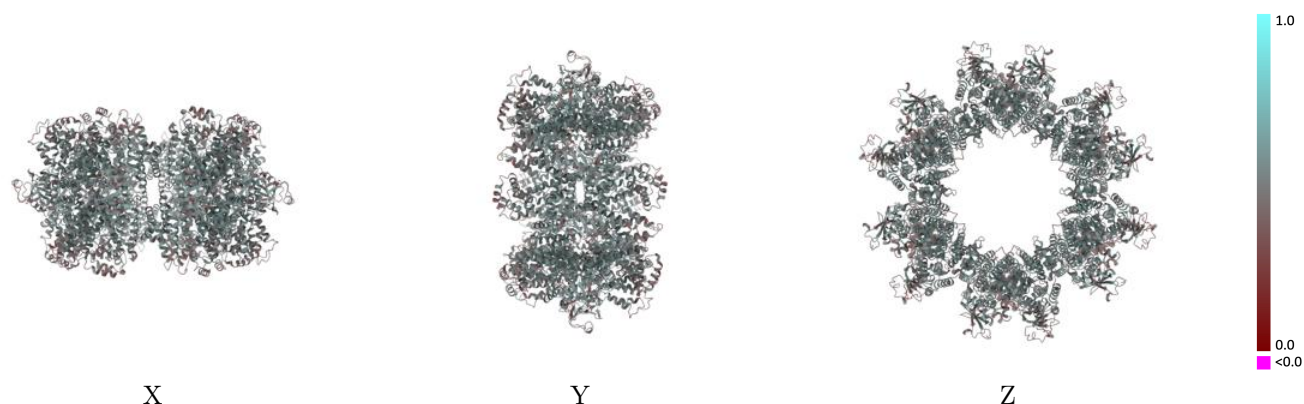
Y



Z

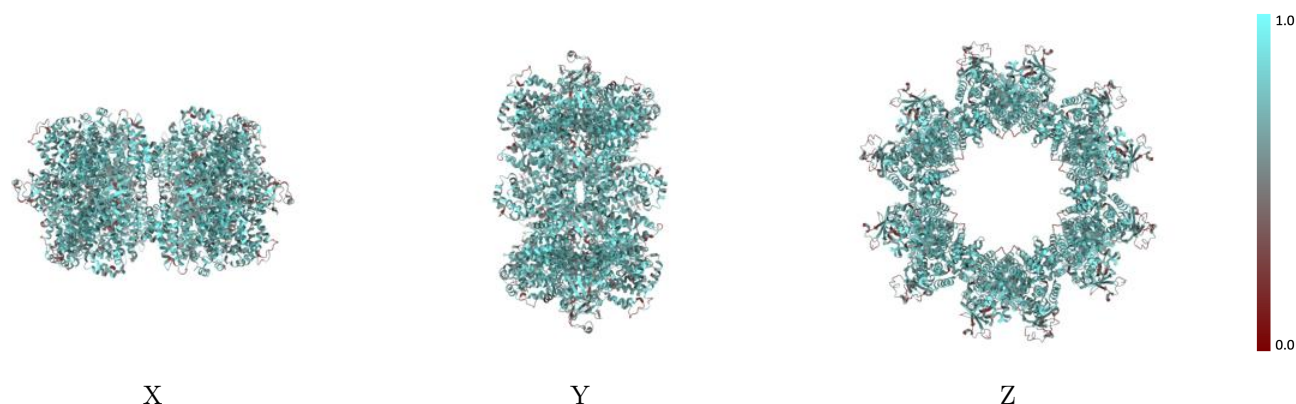
The images above show the 3D surface view of the map at the recommended contour level 5.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



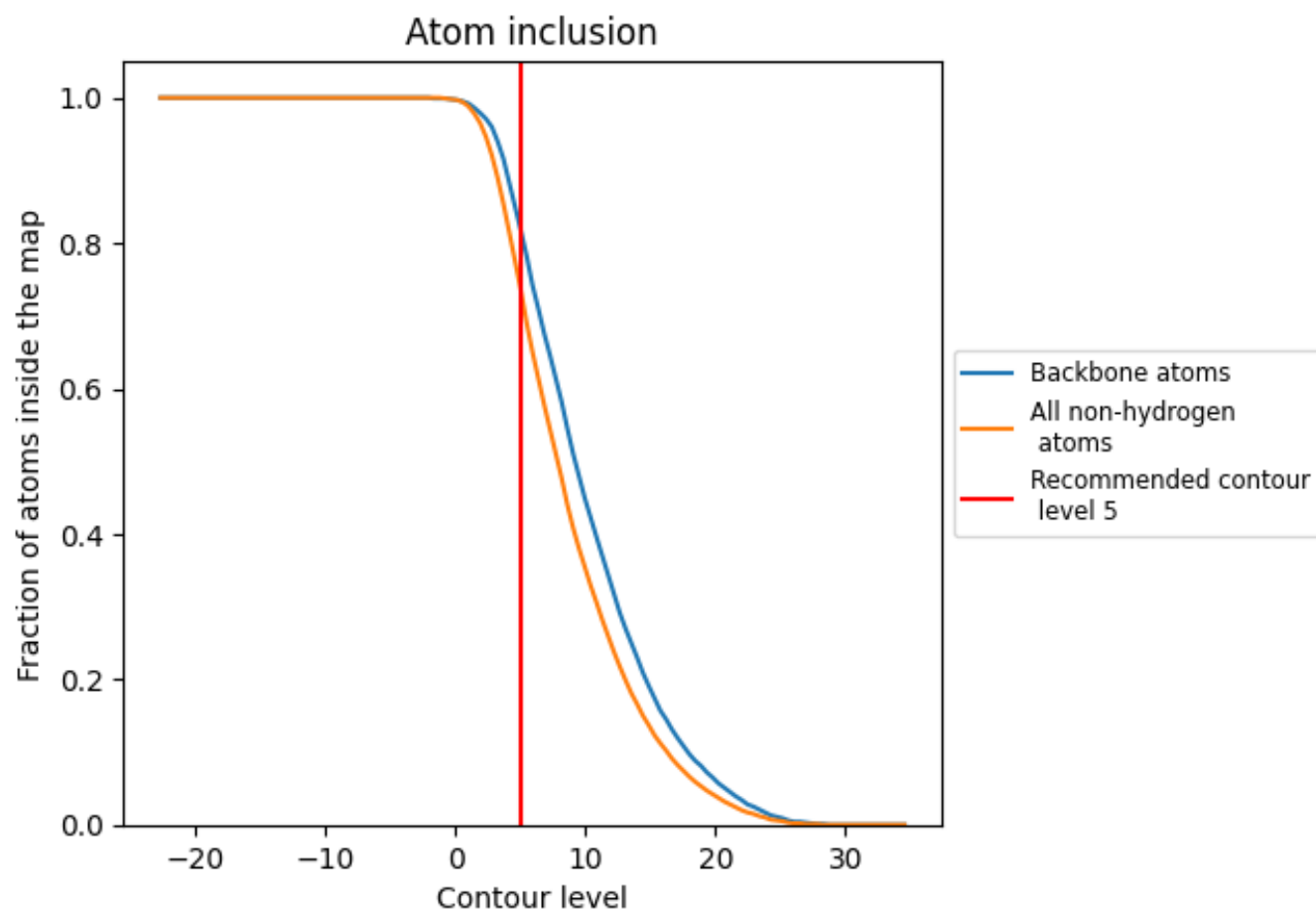
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 74% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7360	0.5070
A	0.7350	0.5070
B	0.7340	0.5060
C	0.7380	0.5080
D	0.7380	0.5060
E	0.7370	0.5070
F	0.7370	0.5080
G	0.7360	0.5080
H	0.7350	0.5070
I	0.7370	0.5080
J	0.7370	0.5070
K	0.7360	0.5060
L	0.7370	0.5070

