



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 12:52 PM UTC

PDB ID : 8Z4G / pdb_00008z4g
EMDB ID : EMD-39763
Title : Structure of the S-ring region of the Vibrio flagellar MS-ring protein FliF with 35-fold symmetry applied
Authors : Takekawa, N.; Nishikino, T.; Kishikawa, J.; Hirose, M.; Kato, T.; Imada, K.; Homma, M.
Deposited on : 2024-04-17
Resolution : 3.23 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
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) : 2.49

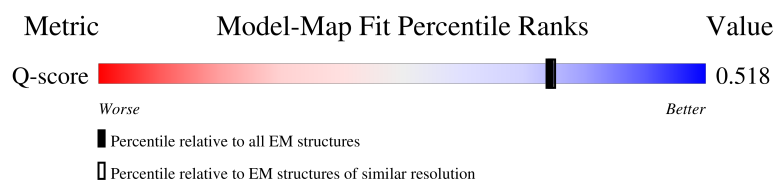
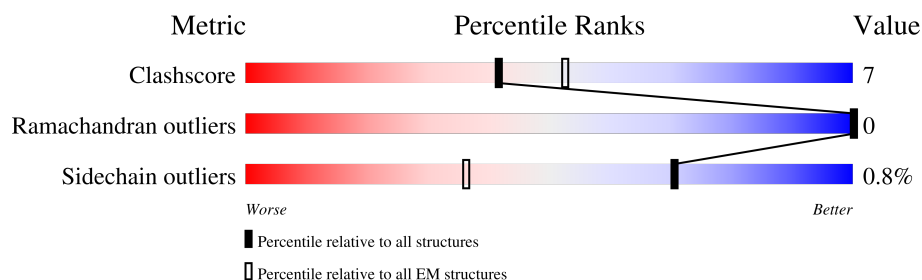
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.23 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.



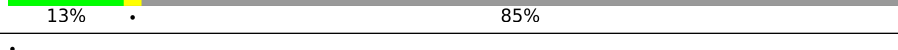
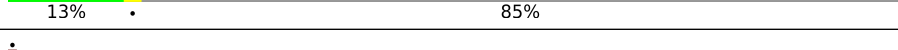
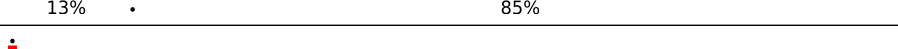
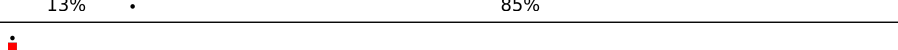
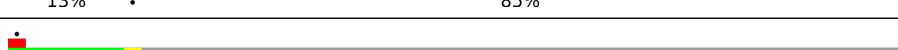
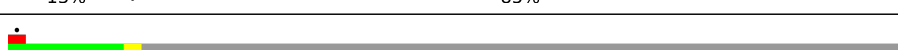
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14612 (2.73 - 3.73)

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.

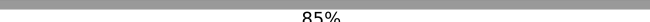
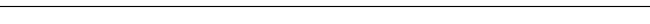
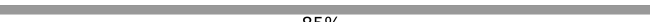
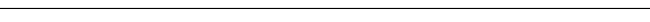
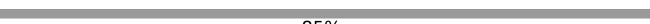
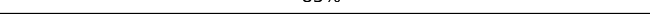
Mol	Chain	Length	Quality of chain
1	1	945	
1	2	945	
1	3	945	
1	4	945	

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Mol	Chain	Length	Quality of chain
1	5	945	 13% 85%
1	6	945	 13% 85%
1	7	945	 13% 85%
1	8	945	 13% 85%
1	9	945	 13% 85%
1	A	945	 13% 85%
1	B	945	 13% 85%
1	C	945	 13% 85%
1	D	945	 13% 85%
1	E	945	 13% 85%
1	F	945	 13% 85%
1	G	945	 13% 85%
1	H	945	 13% 85%
1	I	945	 13% 85%
1	J	945	 13% 85%
1	K	945	 13% 85%
1	L	945	 13% 85%
1	M	945	 13% 85%
1	N	945	 13% 85%
1	O	945	 13% 85%
1	P	945	 13% 85%
1	Q	945	 13% 85%
1	R	945	 13% 85%
1	S	945	 13% 85%
1	T	945	 13% 85%

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Mol	Chain	Length	Quality of chain
1	U	945	
1	V	945	
1	W	945	
1	X	945	
1	Y	945	
1	Z	945	

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 40565 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 Flagellar M-ring protein,Flagellar motor switch protein FliG.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	146	Total	C	N	O	S	0	0
			1159	713	210	234	2		
1	2	146	Total	C	N	O	S	0	0
			1159	713	210	234	2		
1	3	146	Total	C	N	O	S	0	0
			1159	713	210	234	2		
1	4	146	Total	C	N	O	S	0	0
			1159	713	210	234	2		
1	5	146	Total	C	N	O	S	0	0
			1159	713	210	234	2		
1	6	146	Total	C	N	O	S	0	0
			1159	713	210	234	2		
1	7	146	Total	C	N	O	S	0	0
			1159	713	210	234	2		
1	8	146	Total	C	N	O	S	0	0
			1159	713	210	234	2		
1	9	146	Total	C	N	O	S	0	0
			1159	713	210	234	2		
1	A	146	Total	C	N	O	S	0	0
			1159	713	210	234	2		
1	B	146	Total	C	N	O	S	0	0
			1159	713	210	234	2		
1	C	146	Total	C	N	O	S	0	0
			1159	713	210	234	2		
1	D	146	Total	C	N	O	S	0	0
			1159	713	210	234	2		
1	E	146	Total	C	N	O	S	0	0
			1159	713	210	234	2		
1	F	146	Total	C	N	O	S	0	0
			1159	713	210	234	2		
1	G	146	Total	C	N	O	S	0	0
			1159	713	210	234	2		
1	H	146	Total	C	N	O	S	0	0
			1159	713	210	234	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	I	146	Total	C	N	O	S	0	0
			1159	713	210	234	2		
1	J	146	Total	C	N	O	S	0	0
			1159	713	210	234	2		
1	K	146	Total	C	N	O	S	0	0
			1159	713	210	234	2		
1	L	146	Total	C	N	O	S	0	0
			1159	713	210	234	2		
1	M	146	Total	C	N	O	S	0	0
			1159	713	210	234	2		
1	N	146	Total	C	N	O	S	0	0
			1159	713	210	234	2		
1	O	146	Total	C	N	O	S	0	0
			1159	713	210	234	2		
1	P	146	Total	C	N	O	S	0	0
			1159	713	210	234	2		
1	Q	146	Total	C	N	O	S	0	0
			1159	713	210	234	2		
1	R	146	Total	C	N	O	S	0	0
			1159	713	210	234	2		
1	S	146	Total	C	N	O	S	0	0
			1159	713	210	234	2		
1	T	146	Total	C	N	O	S	0	0
			1159	713	210	234	2		
1	U	146	Total	C	N	O	S	0	0
			1159	713	210	234	2		
1	V	146	Total	C	N	O	S	0	0
			1159	713	210	234	2		
1	W	146	Total	C	N	O	S	0	0
			1159	713	210	234	2		
1	X	146	Total	C	N	O	S	0	0
			1159	713	210	234	2		
1	Y	146	Total	C	N	O	S	0	0
			1159	713	210	234	2		
1	Z	146	Total	C	N	O	S	0	0
			1159	713	210	234	2		

There are 595 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	-15	MET	-	initiating methionine	UNP Q75N27
1	-14	ASN	-	expression tag	UNP Q75N27
1	-13	HIS	-	expression tag	UNP Q75N27

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Chain	Residue	Modelled	Actual	Comment	Reference
1	-12	LYS	-	expression tag	UNP Q75N27
1	-11	VAL	-	expression tag	UNP Q75N27
1	-10	HIS	-	expression tag	UNP Q75N27
1	-9	HIS	-	expression tag	UNP Q75N27
1	-8	HIS	-	expression tag	UNP Q75N27
1	-7	HIS	-	expression tag	UNP Q75N27
1	-6	HIS	-	expression tag	UNP Q75N27
1	-5	HIS	-	expression tag	UNP Q75N27
1	-4	ILE	-	expression tag	UNP Q75N27
1	-3	GLU	-	expression tag	UNP Q75N27
1	-2	GLY	-	expression tag	UNP Q75N27
1	-1	ARG	-	expression tag	UNP Q75N27
1	0	HIS	-	expression tag	UNP Q75N27
1	792	SER	GLY	engineered mutation	UNP A0A0T7EAG0
2	-15	MET	-	initiating methionine	UNP Q75N27
2	-14	ASN	-	expression tag	UNP Q75N27
2	-13	HIS	-	expression tag	UNP Q75N27
2	-12	LYS	-	expression tag	UNP Q75N27
2	-11	VAL	-	expression tag	UNP Q75N27
2	-10	HIS	-	expression tag	UNP Q75N27
2	-9	HIS	-	expression tag	UNP Q75N27
2	-8	HIS	-	expression tag	UNP Q75N27
2	-7	HIS	-	expression tag	UNP Q75N27
2	-6	HIS	-	expression tag	UNP Q75N27
2	-5	HIS	-	expression tag	UNP Q75N27
2	-4	ILE	-	expression tag	UNP Q75N27
2	-3	GLU	-	expression tag	UNP Q75N27
2	-2	GLY	-	expression tag	UNP Q75N27
2	-1	ARG	-	expression tag	UNP Q75N27
2	0	HIS	-	expression tag	UNP Q75N27
2	792	SER	GLY	engineered mutation	UNP A0A0T7EAG0
3	-15	MET	-	initiating methionine	UNP Q75N27
3	-14	ASN	-	expression tag	UNP Q75N27
3	-13	HIS	-	expression tag	UNP Q75N27
3	-12	LYS	-	expression tag	UNP Q75N27
3	-11	VAL	-	expression tag	UNP Q75N27
3	-10	HIS	-	expression tag	UNP Q75N27
3	-9	HIS	-	expression tag	UNP Q75N27
3	-8	HIS	-	expression tag	UNP Q75N27
3	-7	HIS	-	expression tag	UNP Q75N27
3	-6	HIS	-	expression tag	UNP Q75N27
3	-5	HIS	-	expression tag	UNP Q75N27

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Chain	Residue	Modelled	Actual	Comment	Reference
3	-4	ILE	-	expression tag	UNP Q75N27
3	-3	GLU	-	expression tag	UNP Q75N27
3	-2	GLY	-	expression tag	UNP Q75N27
3	-1	ARG	-	expression tag	UNP Q75N27
3	0	HIS	-	expression tag	UNP Q75N27
3	792	SER	GLY	engineered mutation	UNP A0A0T7EAG0
4	-15	MET	-	initiating methionine	UNP Q75N27
4	-14	ASN	-	expression tag	UNP Q75N27
4	-13	HIS	-	expression tag	UNP Q75N27
4	-12	LYS	-	expression tag	UNP Q75N27
4	-11	VAL	-	expression tag	UNP Q75N27
4	-10	HIS	-	expression tag	UNP Q75N27
4	-9	HIS	-	expression tag	UNP Q75N27
4	-8	HIS	-	expression tag	UNP Q75N27
4	-7	HIS	-	expression tag	UNP Q75N27
4	-6	HIS	-	expression tag	UNP Q75N27
4	-5	HIS	-	expression tag	UNP Q75N27
4	-4	ILE	-	expression tag	UNP Q75N27
4	-3	GLU	-	expression tag	UNP Q75N27
4	-2	GLY	-	expression tag	UNP Q75N27
4	-1	ARG	-	expression tag	UNP Q75N27
4	0	HIS	-	expression tag	UNP Q75N27
4	792	SER	GLY	engineered mutation	UNP A0A0T7EAG0
5	-15	MET	-	initiating methionine	UNP Q75N27
5	-14	ASN	-	expression tag	UNP Q75N27
5	-13	HIS	-	expression tag	UNP Q75N27
5	-12	LYS	-	expression tag	UNP Q75N27
5	-11	VAL	-	expression tag	UNP Q75N27
5	-10	HIS	-	expression tag	UNP Q75N27
5	-9	HIS	-	expression tag	UNP Q75N27
5	-8	HIS	-	expression tag	UNP Q75N27
5	-7	HIS	-	expression tag	UNP Q75N27
5	-6	HIS	-	expression tag	UNP Q75N27
5	-5	HIS	-	expression tag	UNP Q75N27
5	-4	ILE	-	expression tag	UNP Q75N27
5	-3	GLU	-	expression tag	UNP Q75N27
5	-2	GLY	-	expression tag	UNP Q75N27
5	-1	ARG	-	expression tag	UNP Q75N27
5	0	HIS	-	expression tag	UNP Q75N27
5	792	SER	GLY	engineered mutation	UNP A0A0T7EAG0
6	-15	MET	-	initiating methionine	UNP Q75N27
6	-14	ASN	-	expression tag	UNP Q75N27

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Chain	Residue	Modelled	Actual	Comment	Reference
6	-13	HIS	-	expression tag	UNP Q75N27
6	-12	LYS	-	expression tag	UNP Q75N27
6	-11	VAL	-	expression tag	UNP Q75N27
6	-10	HIS	-	expression tag	UNP Q75N27
6	-9	HIS	-	expression tag	UNP Q75N27
6	-8	HIS	-	expression tag	UNP Q75N27
6	-7	HIS	-	expression tag	UNP Q75N27
6	-6	HIS	-	expression tag	UNP Q75N27
6	-5	HIS	-	expression tag	UNP Q75N27
6	-4	ILE	-	expression tag	UNP Q75N27
6	-3	GLU	-	expression tag	UNP Q75N27
6	-2	GLY	-	expression tag	UNP Q75N27
6	-1	ARG	-	expression tag	UNP Q75N27
6	0	HIS	-	expression tag	UNP Q75N27
6	792	SER	GLY	engineered mutation	UNP A0A0T7EAG0
7	-15	MET	-	initiating methionine	UNP Q75N27
7	-14	ASN	-	expression tag	UNP Q75N27
7	-13	HIS	-	expression tag	UNP Q75N27
7	-12	LYS	-	expression tag	UNP Q75N27
7	-11	VAL	-	expression tag	UNP Q75N27
7	-10	HIS	-	expression tag	UNP Q75N27
7	-9	HIS	-	expression tag	UNP Q75N27
7	-8	HIS	-	expression tag	UNP Q75N27
7	-7	HIS	-	expression tag	UNP Q75N27
7	-6	HIS	-	expression tag	UNP Q75N27
7	-5	HIS	-	expression tag	UNP Q75N27
7	-4	ILE	-	expression tag	UNP Q75N27
7	-3	GLU	-	expression tag	UNP Q75N27
7	-2	GLY	-	expression tag	UNP Q75N27
7	-1	ARG	-	expression tag	UNP Q75N27
7	0	HIS	-	expression tag	UNP Q75N27
7	792	SER	GLY	engineered mutation	UNP A0A0T7EAG0
8	-15	MET	-	initiating methionine	UNP Q75N27
8	-14	ASN	-	expression tag	UNP Q75N27
8	-13	HIS	-	expression tag	UNP Q75N27
8	-12	LYS	-	expression tag	UNP Q75N27
8	-11	VAL	-	expression tag	UNP Q75N27
8	-10	HIS	-	expression tag	UNP Q75N27
8	-9	HIS	-	expression tag	UNP Q75N27
8	-8	HIS	-	expression tag	UNP Q75N27
8	-7	HIS	-	expression tag	UNP Q75N27
8	-6	HIS	-	expression tag	UNP Q75N27

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Chain	Residue	Modelled	Actual	Comment	Reference
8	-5	HIS	-	expression tag	UNP Q75N27
8	-4	ILE	-	expression tag	UNP Q75N27
8	-3	GLU	-	expression tag	UNP Q75N27
8	-2	GLY	-	expression tag	UNP Q75N27
8	-1	ARG	-	expression tag	UNP Q75N27
8	0	HIS	-	expression tag	UNP Q75N27
8	792	SER	GLY	engineered mutation	UNP A0A0T7EAG0
9	-15	MET	-	initiating methionine	UNP Q75N27
9	-14	ASN	-	expression tag	UNP Q75N27
9	-13	HIS	-	expression tag	UNP Q75N27
9	-12	LYS	-	expression tag	UNP Q75N27
9	-11	VAL	-	expression tag	UNP Q75N27
9	-10	HIS	-	expression tag	UNP Q75N27
9	-9	HIS	-	expression tag	UNP Q75N27
9	-8	HIS	-	expression tag	UNP Q75N27
9	-7	HIS	-	expression tag	UNP Q75N27
9	-6	HIS	-	expression tag	UNP Q75N27
9	-5	HIS	-	expression tag	UNP Q75N27
9	-4	ILE	-	expression tag	UNP Q75N27
9	-3	GLU	-	expression tag	UNP Q75N27
9	-2	GLY	-	expression tag	UNP Q75N27
9	-1	ARG	-	expression tag	UNP Q75N27
9	0	HIS	-	expression tag	UNP Q75N27
9	792	SER	GLY	engineered mutation	UNP A0A0T7EAG0
A	-15	MET	-	initiating methionine	UNP Q75N27
A	-14	ASN	-	expression tag	UNP Q75N27
A	-13	HIS	-	expression tag	UNP Q75N27
A	-12	LYS	-	expression tag	UNP Q75N27
A	-11	VAL	-	expression tag	UNP Q75N27
A	-10	HIS	-	expression tag	UNP Q75N27
A	-9	HIS	-	expression tag	UNP Q75N27
A	-8	HIS	-	expression tag	UNP Q75N27
A	-7	HIS	-	expression tag	UNP Q75N27
A	-6	HIS	-	expression tag	UNP Q75N27
A	-5	HIS	-	expression tag	UNP Q75N27
A	-4	ILE	-	expression tag	UNP Q75N27
A	-3	GLU	-	expression tag	UNP Q75N27
A	-2	GLY	-	expression tag	UNP Q75N27
A	-1	ARG	-	expression tag	UNP Q75N27
A	0	HIS	-	expression tag	UNP Q75N27
A	792	SER	GLY	engineered mutation	UNP A0A0T7EAG0
B	-15	MET	-	initiating methionine	UNP Q75N27

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	ASN	-	expression tag	UNP Q75N27
B	-13	HIS	-	expression tag	UNP Q75N27
B	-12	LYS	-	expression tag	UNP Q75N27
B	-11	VAL	-	expression tag	UNP Q75N27
B	-10	HIS	-	expression tag	UNP Q75N27
B	-9	HIS	-	expression tag	UNP Q75N27
B	-8	HIS	-	expression tag	UNP Q75N27
B	-7	HIS	-	expression tag	UNP Q75N27
B	-6	HIS	-	expression tag	UNP Q75N27
B	-5	HIS	-	expression tag	UNP Q75N27
B	-4	ILE	-	expression tag	UNP Q75N27
B	-3	GLU	-	expression tag	UNP Q75N27
B	-2	GLY	-	expression tag	UNP Q75N27
B	-1	ARG	-	expression tag	UNP Q75N27
B	0	HIS	-	expression tag	UNP Q75N27
B	792	SER	GLY	engineered mutation	UNP A0A0T7EAG0
C	-15	MET	-	initiating methionine	UNP Q75N27
C	-14	ASN	-	expression tag	UNP Q75N27
C	-13	HIS	-	expression tag	UNP Q75N27
C	-12	LYS	-	expression tag	UNP Q75N27
C	-11	VAL	-	expression tag	UNP Q75N27
C	-10	HIS	-	expression tag	UNP Q75N27
C	-9	HIS	-	expression tag	UNP Q75N27
C	-8	HIS	-	expression tag	UNP Q75N27
C	-7	HIS	-	expression tag	UNP Q75N27
C	-6	HIS	-	expression tag	UNP Q75N27
C	-5	HIS	-	expression tag	UNP Q75N27
C	-4	ILE	-	expression tag	UNP Q75N27
C	-3	GLU	-	expression tag	UNP Q75N27
C	-2	GLY	-	expression tag	UNP Q75N27
C	-1	ARG	-	expression tag	UNP Q75N27
C	0	HIS	-	expression tag	UNP Q75N27
C	792	SER	GLY	engineered mutation	UNP A0A0T7EAG0
D	-15	MET	-	initiating methionine	UNP Q75N27
D	-14	ASN	-	expression tag	UNP Q75N27
D	-13	HIS	-	expression tag	UNP Q75N27
D	-12	LYS	-	expression tag	UNP Q75N27
D	-11	VAL	-	expression tag	UNP Q75N27
D	-10	HIS	-	expression tag	UNP Q75N27
D	-9	HIS	-	expression tag	UNP Q75N27
D	-8	HIS	-	expression tag	UNP Q75N27
D	-7	HIS	-	expression tag	UNP Q75N27

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-6	HIS	-	expression tag	UNP Q75N27
D	-5	HIS	-	expression tag	UNP Q75N27
D	-4	ILE	-	expression tag	UNP Q75N27
D	-3	GLU	-	expression tag	UNP Q75N27
D	-2	GLY	-	expression tag	UNP Q75N27
D	-1	ARG	-	expression tag	UNP Q75N27
D	0	HIS	-	expression tag	UNP Q75N27
D	792	SER	GLY	engineered mutation	UNP A0A0T7EAG0
E	-15	MET	-	initiating methionine	UNP Q75N27
E	-14	ASN	-	expression tag	UNP Q75N27
E	-13	HIS	-	expression tag	UNP Q75N27
E	-12	LYS	-	expression tag	UNP Q75N27
E	-11	VAL	-	expression tag	UNP Q75N27
E	-10	HIS	-	expression tag	UNP Q75N27
E	-9	HIS	-	expression tag	UNP Q75N27
E	-8	HIS	-	expression tag	UNP Q75N27
E	-7	HIS	-	expression tag	UNP Q75N27
E	-6	HIS	-	expression tag	UNP Q75N27
E	-5	HIS	-	expression tag	UNP Q75N27
E	-4	ILE	-	expression tag	UNP Q75N27
E	-3	GLU	-	expression tag	UNP Q75N27
E	-2	GLY	-	expression tag	UNP Q75N27
E	-1	ARG	-	expression tag	UNP Q75N27
E	0	HIS	-	expression tag	UNP Q75N27
E	792	SER	GLY	engineered mutation	UNP A0A0T7EAG0
F	-15	MET	-	initiating methionine	UNP Q75N27
F	-14	ASN	-	expression tag	UNP Q75N27
F	-13	HIS	-	expression tag	UNP Q75N27
F	-12	LYS	-	expression tag	UNP Q75N27
F	-11	VAL	-	expression tag	UNP Q75N27
F	-10	HIS	-	expression tag	UNP Q75N27
F	-9	HIS	-	expression tag	UNP Q75N27
F	-8	HIS	-	expression tag	UNP Q75N27
F	-7	HIS	-	expression tag	UNP Q75N27
F	-6	HIS	-	expression tag	UNP Q75N27
F	-5	HIS	-	expression tag	UNP Q75N27
F	-4	ILE	-	expression tag	UNP Q75N27
F	-3	GLU	-	expression tag	UNP Q75N27
F	-2	GLY	-	expression tag	UNP Q75N27
F	-1	ARG	-	expression tag	UNP Q75N27
F	0	HIS	-	expression tag	UNP Q75N27
F	792	SER	GLY	engineered mutation	UNP A0A0T7EAG0

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-15	MET	-	initiating methionine	UNP Q75N27
G	-14	ASN	-	expression tag	UNP Q75N27
G	-13	HIS	-	expression tag	UNP Q75N27
G	-12	LYS	-	expression tag	UNP Q75N27
G	-11	VAL	-	expression tag	UNP Q75N27
G	-10	HIS	-	expression tag	UNP Q75N27
G	-9	HIS	-	expression tag	UNP Q75N27
G	-8	HIS	-	expression tag	UNP Q75N27
G	-7	HIS	-	expression tag	UNP Q75N27
G	-6	HIS	-	expression tag	UNP Q75N27
G	-5	HIS	-	expression tag	UNP Q75N27
G	-4	ILE	-	expression tag	UNP Q75N27
G	-3	GLU	-	expression tag	UNP Q75N27
G	-2	GLY	-	expression tag	UNP Q75N27
G	-1	ARG	-	expression tag	UNP Q75N27
G	0	HIS	-	expression tag	UNP Q75N27
G	792	SER	GLY	engineered mutation	UNP A0A0T7EAG0
H	-15	MET	-	initiating methionine	UNP Q75N27
H	-14	ASN	-	expression tag	UNP Q75N27
H	-13	HIS	-	expression tag	UNP Q75N27
H	-12	LYS	-	expression tag	UNP Q75N27
H	-11	VAL	-	expression tag	UNP Q75N27
H	-10	HIS	-	expression tag	UNP Q75N27
H	-9	HIS	-	expression tag	UNP Q75N27
H	-8	HIS	-	expression tag	UNP Q75N27
H	-7	HIS	-	expression tag	UNP Q75N27
H	-6	HIS	-	expression tag	UNP Q75N27
H	-5	HIS	-	expression tag	UNP Q75N27
H	-4	ILE	-	expression tag	UNP Q75N27
H	-3	GLU	-	expression tag	UNP Q75N27
H	-2	GLY	-	expression tag	UNP Q75N27
H	-1	ARG	-	expression tag	UNP Q75N27
H	0	HIS	-	expression tag	UNP Q75N27
H	792	SER	GLY	engineered mutation	UNP A0A0T7EAG0
I	-15	MET	-	initiating methionine	UNP Q75N27
I	-14	ASN	-	expression tag	UNP Q75N27
I	-13	HIS	-	expression tag	UNP Q75N27
I	-12	LYS	-	expression tag	UNP Q75N27
I	-11	VAL	-	expression tag	UNP Q75N27
I	-10	HIS	-	expression tag	UNP Q75N27
I	-9	HIS	-	expression tag	UNP Q75N27
I	-8	HIS	-	expression tag	UNP Q75N27

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-7	HIS	-	expression tag	UNP Q75N27
I	-6	HIS	-	expression tag	UNP Q75N27
I	-5	HIS	-	expression tag	UNP Q75N27
I	-4	ILE	-	expression tag	UNP Q75N27
I	-3	GLU	-	expression tag	UNP Q75N27
I	-2	GLY	-	expression tag	UNP Q75N27
I	-1	ARG	-	expression tag	UNP Q75N27
I	0	HIS	-	expression tag	UNP Q75N27
I	792	SER	GLY	engineered mutation	UNP A0A0T7EAG0
J	-15	MET	-	initiating methionine	UNP Q75N27
J	-14	ASN	-	expression tag	UNP Q75N27
J	-13	HIS	-	expression tag	UNP Q75N27
J	-12	LYS	-	expression tag	UNP Q75N27
J	-11	VAL	-	expression tag	UNP Q75N27
J	-10	HIS	-	expression tag	UNP Q75N27
J	-9	HIS	-	expression tag	UNP Q75N27
J	-8	HIS	-	expression tag	UNP Q75N27
J	-7	HIS	-	expression tag	UNP Q75N27
J	-6	HIS	-	expression tag	UNP Q75N27
J	-5	HIS	-	expression tag	UNP Q75N27
J	-4	ILE	-	expression tag	UNP Q75N27
J	-3	GLU	-	expression tag	UNP Q75N27
J	-2	GLY	-	expression tag	UNP Q75N27
J	-1	ARG	-	expression tag	UNP Q75N27
J	0	HIS	-	expression tag	UNP Q75N27
J	792	SER	GLY	engineered mutation	UNP A0A0T7EAG0
K	-15	MET	-	initiating methionine	UNP Q75N27
K	-14	ASN	-	expression tag	UNP Q75N27
K	-13	HIS	-	expression tag	UNP Q75N27
K	-12	LYS	-	expression tag	UNP Q75N27
K	-11	VAL	-	expression tag	UNP Q75N27
K	-10	HIS	-	expression tag	UNP Q75N27
K	-9	HIS	-	expression tag	UNP Q75N27
K	-8	HIS	-	expression tag	UNP Q75N27
K	-7	HIS	-	expression tag	UNP Q75N27
K	-6	HIS	-	expression tag	UNP Q75N27
K	-5	HIS	-	expression tag	UNP Q75N27
K	-4	ILE	-	expression tag	UNP Q75N27
K	-3	GLU	-	expression tag	UNP Q75N27
K	-2	GLY	-	expression tag	UNP Q75N27
K	-1	ARG	-	expression tag	UNP Q75N27
K	0	HIS	-	expression tag	UNP Q75N27

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Chain	Residue	Modelled	Actual	Comment	Reference
K	792	SER	GLY	engineered mutation	UNP A0A0T7EAG0
L	-15	MET	-	initiating methionine	UNP Q75N27
L	-14	ASN	-	expression tag	UNP Q75N27
L	-13	HIS	-	expression tag	UNP Q75N27
L	-12	LYS	-	expression tag	UNP Q75N27
L	-11	VAL	-	expression tag	UNP Q75N27
L	-10	HIS	-	expression tag	UNP Q75N27
L	-9	HIS	-	expression tag	UNP Q75N27
L	-8	HIS	-	expression tag	UNP Q75N27
L	-7	HIS	-	expression tag	UNP Q75N27
L	-6	HIS	-	expression tag	UNP Q75N27
L	-5	HIS	-	expression tag	UNP Q75N27
L	-4	ILE	-	expression tag	UNP Q75N27
L	-3	GLU	-	expression tag	UNP Q75N27
L	-2	GLY	-	expression tag	UNP Q75N27
L	-1	ARG	-	expression tag	UNP Q75N27
L	0	HIS	-	expression tag	UNP Q75N27
L	792	SER	GLY	engineered mutation	UNP A0A0T7EAG0
M	-15	MET	-	initiating methionine	UNP Q75N27
M	-14	ASN	-	expression tag	UNP Q75N27
M	-13	HIS	-	expression tag	UNP Q75N27
M	-12	LYS	-	expression tag	UNP Q75N27
M	-11	VAL	-	expression tag	UNP Q75N27
M	-10	HIS	-	expression tag	UNP Q75N27
M	-9	HIS	-	expression tag	UNP Q75N27
M	-8	HIS	-	expression tag	UNP Q75N27
M	-7	HIS	-	expression tag	UNP Q75N27
M	-6	HIS	-	expression tag	UNP Q75N27
M	-5	HIS	-	expression tag	UNP Q75N27
M	-4	ILE	-	expression tag	UNP Q75N27
M	-3	GLU	-	expression tag	UNP Q75N27
M	-2	GLY	-	expression tag	UNP Q75N27
M	-1	ARG	-	expression tag	UNP Q75N27
M	0	HIS	-	expression tag	UNP Q75N27
M	792	SER	GLY	engineered mutation	UNP A0A0T7EAG0
N	-15	MET	-	initiating methionine	UNP Q75N27
N	-14	ASN	-	expression tag	UNP Q75N27
N	-13	HIS	-	expression tag	UNP Q75N27
N	-12	LYS	-	expression tag	UNP Q75N27
N	-11	VAL	-	expression tag	UNP Q75N27
N	-10	HIS	-	expression tag	UNP Q75N27
N	-9	HIS	-	expression tag	UNP Q75N27

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Chain	Residue	Modelled	Actual	Comment	Reference
N	-8	HIS	-	expression tag	UNP Q75N27
N	-7	HIS	-	expression tag	UNP Q75N27
N	-6	HIS	-	expression tag	UNP Q75N27
N	-5	HIS	-	expression tag	UNP Q75N27
N	-4	ILE	-	expression tag	UNP Q75N27
N	-3	GLU	-	expression tag	UNP Q75N27
N	-2	GLY	-	expression tag	UNP Q75N27
N	-1	ARG	-	expression tag	UNP Q75N27
N	0	HIS	-	expression tag	UNP Q75N27
N	792	SER	GLY	engineered mutation	UNP A0A0T7EAG0
O	-15	MET	-	initiating methionine	UNP Q75N27
O	-14	ASN	-	expression tag	UNP Q75N27
O	-13	HIS	-	expression tag	UNP Q75N27
O	-12	LYS	-	expression tag	UNP Q75N27
O	-11	VAL	-	expression tag	UNP Q75N27
O	-10	HIS	-	expression tag	UNP Q75N27
O	-9	HIS	-	expression tag	UNP Q75N27
O	-8	HIS	-	expression tag	UNP Q75N27
O	-7	HIS	-	expression tag	UNP Q75N27
O	-6	HIS	-	expression tag	UNP Q75N27
O	-5	HIS	-	expression tag	UNP Q75N27
O	-4	ILE	-	expression tag	UNP Q75N27
O	-3	GLU	-	expression tag	UNP Q75N27
O	-2	GLY	-	expression tag	UNP Q75N27
O	-1	ARG	-	expression tag	UNP Q75N27
O	0	HIS	-	expression tag	UNP Q75N27
O	792	SER	GLY	engineered mutation	UNP A0A0T7EAG0
P	-15	MET	-	initiating methionine	UNP Q75N27
P	-14	ASN	-	expression tag	UNP Q75N27
P	-13	HIS	-	expression tag	UNP Q75N27
P	-12	LYS	-	expression tag	UNP Q75N27
P	-11	VAL	-	expression tag	UNP Q75N27
P	-10	HIS	-	expression tag	UNP Q75N27
P	-9	HIS	-	expression tag	UNP Q75N27
P	-8	HIS	-	expression tag	UNP Q75N27
P	-7	HIS	-	expression tag	UNP Q75N27
P	-6	HIS	-	expression tag	UNP Q75N27
P	-5	HIS	-	expression tag	UNP Q75N27
P	-4	ILE	-	expression tag	UNP Q75N27
P	-3	GLU	-	expression tag	UNP Q75N27
P	-2	GLY	-	expression tag	UNP Q75N27
P	-1	ARG	-	expression tag	UNP Q75N27

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Chain	Residue	Modelled	Actual	Comment	Reference
P	0	HIS	-	expression tag	UNP Q75N27
P	792	SER	GLY	engineered mutation	UNP A0A0T7EAG0
Q	-15	MET	-	initiating methionine	UNP Q75N27
Q	-14	ASN	-	expression tag	UNP Q75N27
Q	-13	HIS	-	expression tag	UNP Q75N27
Q	-12	LYS	-	expression tag	UNP Q75N27
Q	-11	VAL	-	expression tag	UNP Q75N27
Q	-10	HIS	-	expression tag	UNP Q75N27
Q	-9	HIS	-	expression tag	UNP Q75N27
Q	-8	HIS	-	expression tag	UNP Q75N27
Q	-7	HIS	-	expression tag	UNP Q75N27
Q	-6	HIS	-	expression tag	UNP Q75N27
Q	-5	HIS	-	expression tag	UNP Q75N27
Q	-4	ILE	-	expression tag	UNP Q75N27
Q	-3	GLU	-	expression tag	UNP Q75N27
Q	-2	GLY	-	expression tag	UNP Q75N27
Q	-1	ARG	-	expression tag	UNP Q75N27
Q	0	HIS	-	expression tag	UNP Q75N27
Q	792	SER	GLY	engineered mutation	UNP A0A0T7EAG0
R	-15	MET	-	initiating methionine	UNP Q75N27
R	-14	ASN	-	expression tag	UNP Q75N27
R	-13	HIS	-	expression tag	UNP Q75N27
R	-12	LYS	-	expression tag	UNP Q75N27
R	-11	VAL	-	expression tag	UNP Q75N27
R	-10	HIS	-	expression tag	UNP Q75N27
R	-9	HIS	-	expression tag	UNP Q75N27
R	-8	HIS	-	expression tag	UNP Q75N27
R	-7	HIS	-	expression tag	UNP Q75N27
R	-6	HIS	-	expression tag	UNP Q75N27
R	-5	HIS	-	expression tag	UNP Q75N27
R	-4	ILE	-	expression tag	UNP Q75N27
R	-3	GLU	-	expression tag	UNP Q75N27
R	-2	GLY	-	expression tag	UNP Q75N27
R	-1	ARG	-	expression tag	UNP Q75N27
R	0	HIS	-	expression tag	UNP Q75N27
R	792	SER	GLY	engineered mutation	UNP A0A0T7EAG0
S	-15	MET	-	initiating methionine	UNP Q75N27
S	-14	ASN	-	expression tag	UNP Q75N27
S	-13	HIS	-	expression tag	UNP Q75N27
S	-12	LYS	-	expression tag	UNP Q75N27
S	-11	VAL	-	expression tag	UNP Q75N27
S	-10	HIS	-	expression tag	UNP Q75N27

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Chain	Residue	Modelled	Actual	Comment	Reference
S	-9	HIS	-	expression tag	UNP Q75N27
S	-8	HIS	-	expression tag	UNP Q75N27
S	-7	HIS	-	expression tag	UNP Q75N27
S	-6	HIS	-	expression tag	UNP Q75N27
S	-5	HIS	-	expression tag	UNP Q75N27
S	-4	ILE	-	expression tag	UNP Q75N27
S	-3	GLU	-	expression tag	UNP Q75N27
S	-2	GLY	-	expression tag	UNP Q75N27
S	-1	ARG	-	expression tag	UNP Q75N27
S	0	HIS	-	expression tag	UNP Q75N27
S	792	SER	GLY	engineered mutation	UNP A0A0T7EAG0
T	-15	MET	-	initiating methionine	UNP Q75N27
T	-14	ASN	-	expression tag	UNP Q75N27
T	-13	HIS	-	expression tag	UNP Q75N27
T	-12	LYS	-	expression tag	UNP Q75N27
T	-11	VAL	-	expression tag	UNP Q75N27
T	-10	HIS	-	expression tag	UNP Q75N27
T	-9	HIS	-	expression tag	UNP Q75N27
T	-8	HIS	-	expression tag	UNP Q75N27
T	-7	HIS	-	expression tag	UNP Q75N27
T	-6	HIS	-	expression tag	UNP Q75N27
T	-5	HIS	-	expression tag	UNP Q75N27
T	-4	ILE	-	expression tag	UNP Q75N27
T	-3	GLU	-	expression tag	UNP Q75N27
T	-2	GLY	-	expression tag	UNP Q75N27
T	-1	ARG	-	expression tag	UNP Q75N27
T	0	HIS	-	expression tag	UNP Q75N27
T	792	SER	GLY	engineered mutation	UNP A0A0T7EAG0
U	-15	MET	-	initiating methionine	UNP Q75N27
U	-14	ASN	-	expression tag	UNP Q75N27
U	-13	HIS	-	expression tag	UNP Q75N27
U	-12	LYS	-	expression tag	UNP Q75N27
U	-11	VAL	-	expression tag	UNP Q75N27
U	-10	HIS	-	expression tag	UNP Q75N27
U	-9	HIS	-	expression tag	UNP Q75N27
U	-8	HIS	-	expression tag	UNP Q75N27
U	-7	HIS	-	expression tag	UNP Q75N27
U	-6	HIS	-	expression tag	UNP Q75N27
U	-5	HIS	-	expression tag	UNP Q75N27
U	-4	ILE	-	expression tag	UNP Q75N27
U	-3	GLU	-	expression tag	UNP Q75N27
U	-2	GLY	-	expression tag	UNP Q75N27

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Chain	Residue	Modelled	Actual	Comment	Reference
U	-1	ARG	-	expression tag	UNP Q75N27
U	0	HIS	-	expression tag	UNP Q75N27
U	792	SER	GLY	engineered mutation	UNP A0A0T7EAG0
V	-15	MET	-	initiating methionine	UNP Q75N27
V	-14	ASN	-	expression tag	UNP Q75N27
V	-13	HIS	-	expression tag	UNP Q75N27
V	-12	LYS	-	expression tag	UNP Q75N27
V	-11	VAL	-	expression tag	UNP Q75N27
V	-10	HIS	-	expression tag	UNP Q75N27
V	-9	HIS	-	expression tag	UNP Q75N27
V	-8	HIS	-	expression tag	UNP Q75N27
V	-7	HIS	-	expression tag	UNP Q75N27
V	-6	HIS	-	expression tag	UNP Q75N27
V	-5	HIS	-	expression tag	UNP Q75N27
V	-4	ILE	-	expression tag	UNP Q75N27
V	-3	GLU	-	expression tag	UNP Q75N27
V	-2	GLY	-	expression tag	UNP Q75N27
V	-1	ARG	-	expression tag	UNP Q75N27
V	0	HIS	-	expression tag	UNP Q75N27
V	792	SER	GLY	engineered mutation	UNP A0A0T7EAG0
W	-15	MET	-	initiating methionine	UNP Q75N27
W	-14	ASN	-	expression tag	UNP Q75N27
W	-13	HIS	-	expression tag	UNP Q75N27
W	-12	LYS	-	expression tag	UNP Q75N27
W	-11	VAL	-	expression tag	UNP Q75N27
W	-10	HIS	-	expression tag	UNP Q75N27
W	-9	HIS	-	expression tag	UNP Q75N27
W	-8	HIS	-	expression tag	UNP Q75N27
W	-7	HIS	-	expression tag	UNP Q75N27
W	-6	HIS	-	expression tag	UNP Q75N27
W	-5	HIS	-	expression tag	UNP Q75N27
W	-4	ILE	-	expression tag	UNP Q75N27
W	-3	GLU	-	expression tag	UNP Q75N27
W	-2	GLY	-	expression tag	UNP Q75N27
W	-1	ARG	-	expression tag	UNP Q75N27
W	0	HIS	-	expression tag	UNP Q75N27
W	792	SER	GLY	engineered mutation	UNP A0A0T7EAG0
X	-15	MET	-	initiating methionine	UNP Q75N27
X	-14	ASN	-	expression tag	UNP Q75N27
X	-13	HIS	-	expression tag	UNP Q75N27
X	-12	LYS	-	expression tag	UNP Q75N27
X	-11	VAL	-	expression tag	UNP Q75N27

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Chain	Residue	Modelled	Actual	Comment	Reference
X	-10	HIS	-	expression tag	UNP Q75N27
X	-9	HIS	-	expression tag	UNP Q75N27
X	-8	HIS	-	expression tag	UNP Q75N27
X	-7	HIS	-	expression tag	UNP Q75N27
X	-6	HIS	-	expression tag	UNP Q75N27
X	-5	HIS	-	expression tag	UNP Q75N27
X	-4	ILE	-	expression tag	UNP Q75N27
X	-3	GLU	-	expression tag	UNP Q75N27
X	-2	GLY	-	expression tag	UNP Q75N27
X	-1	ARG	-	expression tag	UNP Q75N27
X	0	HIS	-	expression tag	UNP Q75N27
X	792	SER	GLY	engineered mutation	UNP A0A0T7EAG0
Y	-15	MET	-	initiating methionine	UNP Q75N27
Y	-14	ASN	-	expression tag	UNP Q75N27
Y	-13	HIS	-	expression tag	UNP Q75N27
Y	-12	LYS	-	expression tag	UNP Q75N27
Y	-11	VAL	-	expression tag	UNP Q75N27
Y	-10	HIS	-	expression tag	UNP Q75N27
Y	-9	HIS	-	expression tag	UNP Q75N27
Y	-8	HIS	-	expression tag	UNP Q75N27
Y	-7	HIS	-	expression tag	UNP Q75N27
Y	-6	HIS	-	expression tag	UNP Q75N27
Y	-5	HIS	-	expression tag	UNP Q75N27
Y	-4	ILE	-	expression tag	UNP Q75N27
Y	-3	GLU	-	expression tag	UNP Q75N27
Y	-2	GLY	-	expression tag	UNP Q75N27
Y	-1	ARG	-	expression tag	UNP Q75N27
Y	0	HIS	-	expression tag	UNP Q75N27
Y	792	SER	GLY	engineered mutation	UNP A0A0T7EAG0
Z	-15	MET	-	initiating methionine	UNP Q75N27
Z	-14	ASN	-	expression tag	UNP Q75N27
Z	-13	HIS	-	expression tag	UNP Q75N27
Z	-12	LYS	-	expression tag	UNP Q75N27
Z	-11	VAL	-	expression tag	UNP Q75N27
Z	-10	HIS	-	expression tag	UNP Q75N27
Z	-9	HIS	-	expression tag	UNP Q75N27
Z	-8	HIS	-	expression tag	UNP Q75N27
Z	-7	HIS	-	expression tag	UNP Q75N27
Z	-6	HIS	-	expression tag	UNP Q75N27
Z	-5	HIS	-	expression tag	UNP Q75N27
Z	-4	ILE	-	expression tag	UNP Q75N27
Z	-3	GLU	-	expression tag	UNP Q75N27

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Chain	Residue	Modelled	Actual	Comment	Reference
Z	-2	GLY	-	expression tag	UNP Q75N27
Z	-1	ARG	-	expression tag	UNP Q75N27
Z	0	HIS	-	expression tag	UNP Q75N27
Z	792	SER	GLY	engineered mutation	UNP A0A0T7EAG0

GLY
GLY
ALA
ASP
GLU
PHE
LEU

Chain 2: 13% 85%

GLY	ALA	ASP	ASP	SER	LEU	ARG	GLU	LYS	PHE	LYS	ASN	MET	SER	LYS	ARG	ALA	ALA	GLU	MET	MET	ARG	ASP	ILE	LEU	GLU	ALA	ALA	ALA	ALA	LYS	GLU	ILE	LEU	ALA	ALA	ILE	ALA	ARG	ARG	MET	ALA	ALA	ASP	ALA	ALA	GLY	LEU	LEU	MET	LEU	LEU	SER
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[illegible]

- Molecule 1: Flagellar M-ring protein, Flagellar motor switch protein FliG

Chain 8: 13% 85%

[illegible]

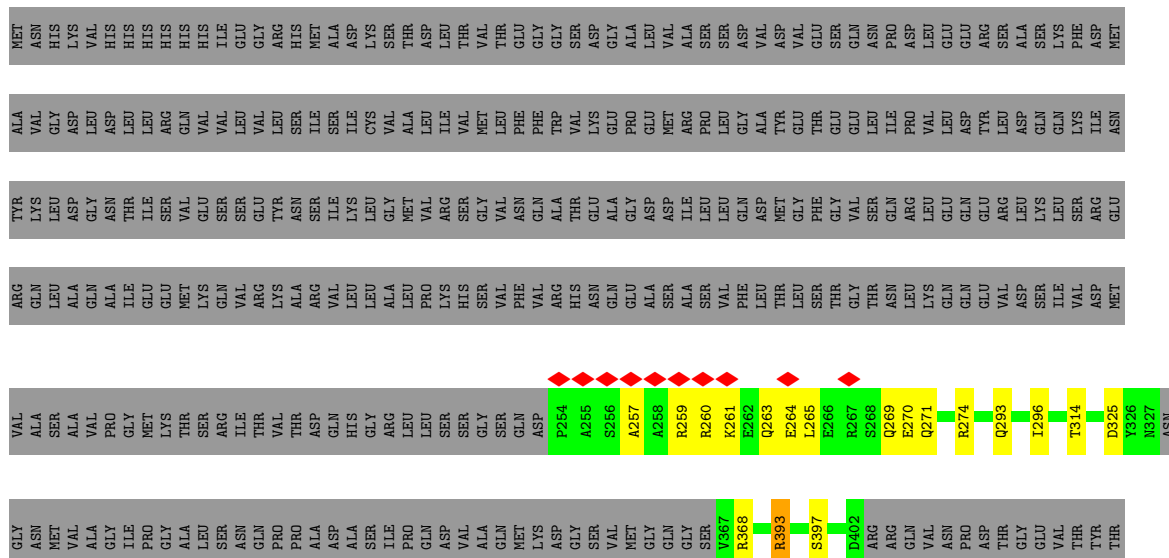
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- Molecule 1: Flagellar M-ring protein,Flagellar motor switch protein FliG



GLU	LEU	LEU	MET	LEU	SER	GLY	ALA	ILE	GLU	ILE	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
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- Molecule 1: Flagellar M-ring protein,Flagellar motor switch protein FliG

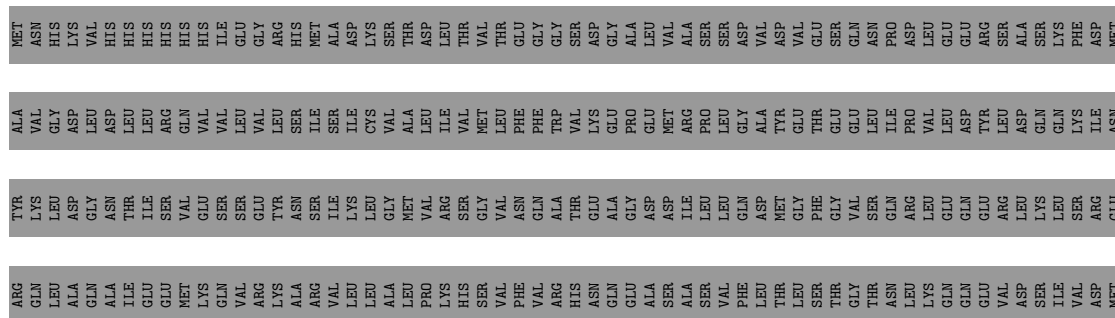


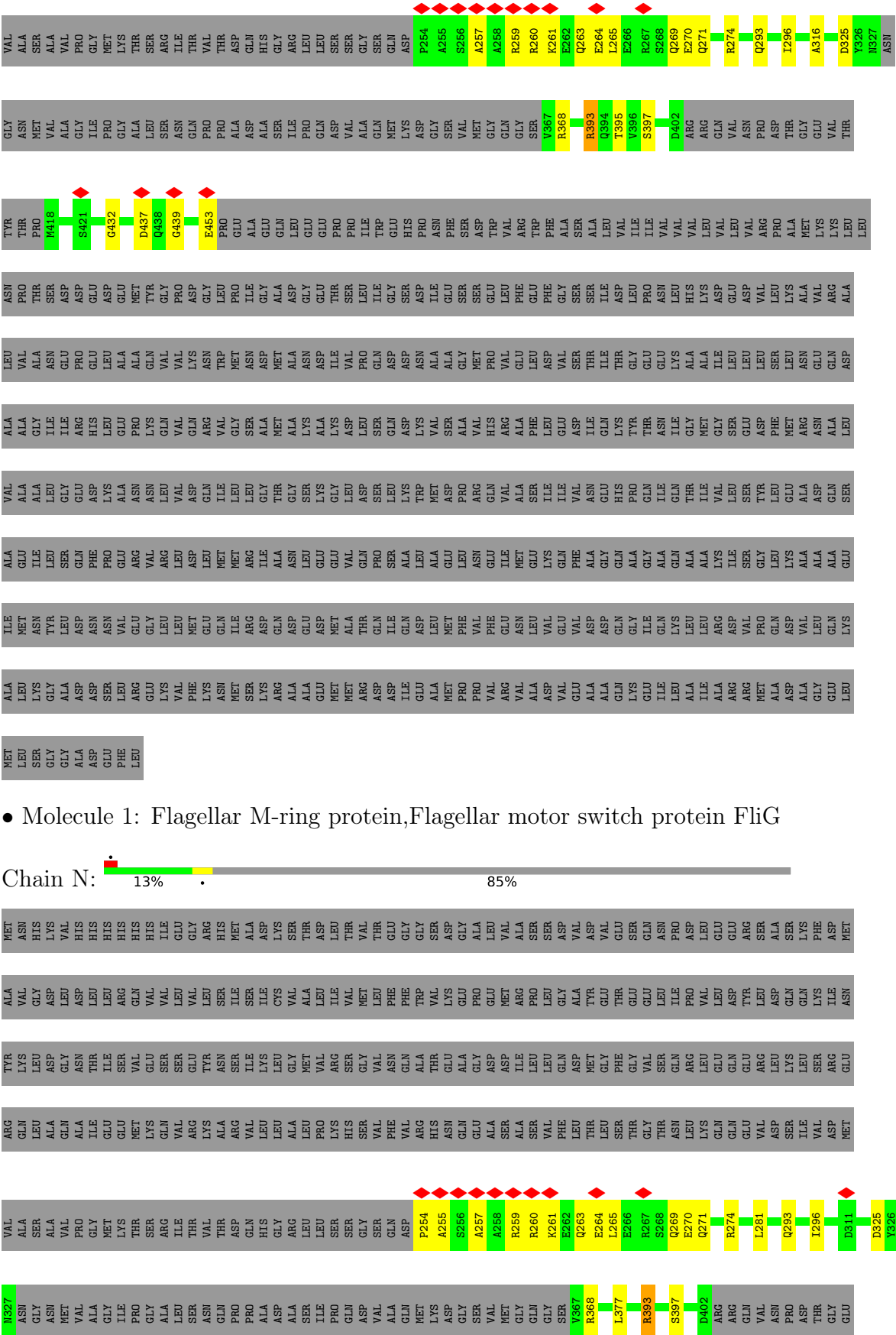




- Molecule 1: Flagellar M-ring protein, Flagellar motor switch protein FliG







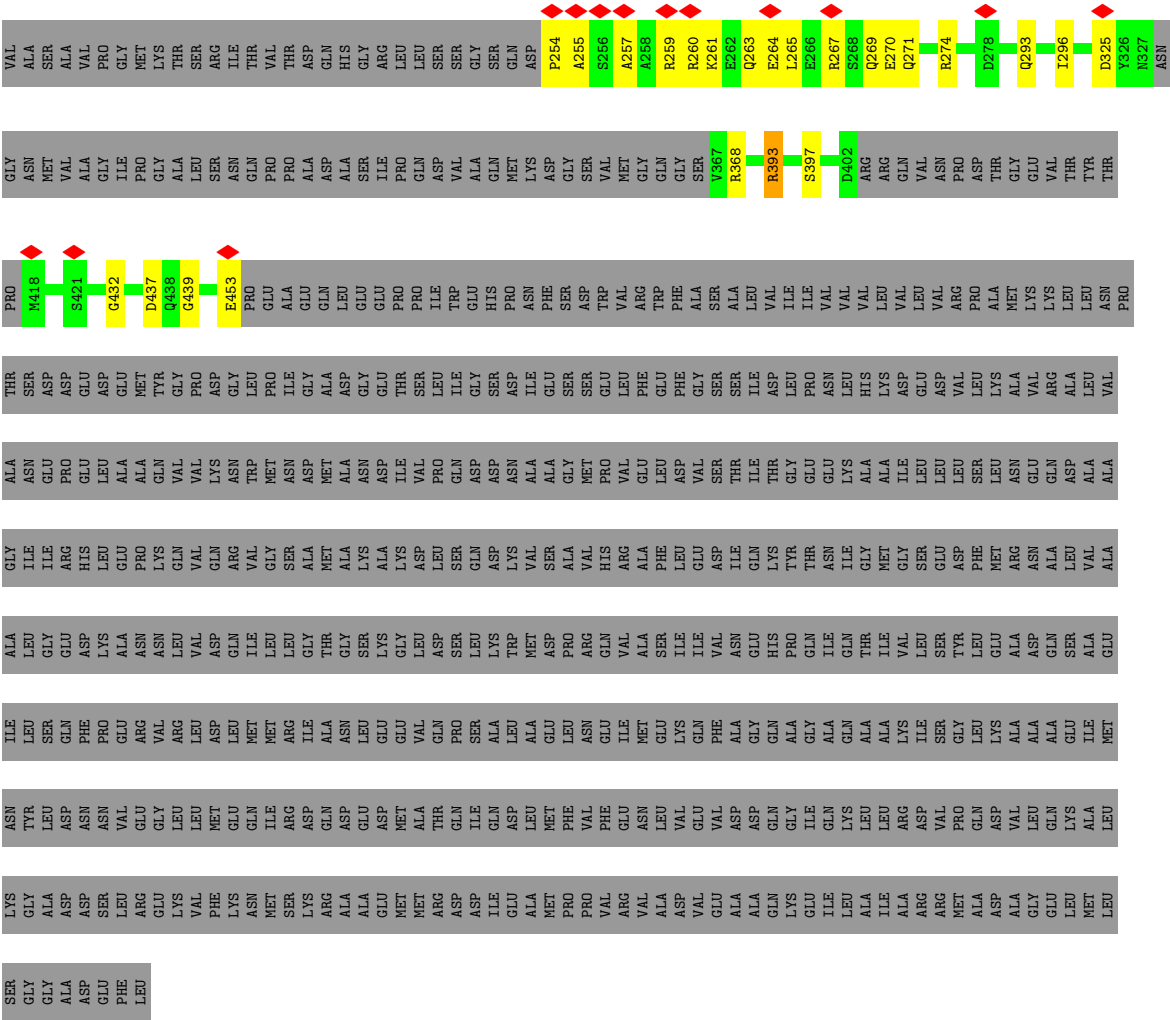
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MET	ALA	ILE	ALA	VAL	ALA	VAL
LEU	LEU	MET	GLU	ALA	ALA	ALA
SER	LYS	ASN	ILE	ALA	GLY	ASN
GLY	GLY	TYR	LEU	LEU	ILE	GLU
ALA	ALA	LEU	SER	GLY	ARG	GLU
ASP	ASP	ASP	GLN	GLU	ASP	GLU
ASP	ASN	ASN	PHE	ASP	HIS	PRO
SER	SER	ASN	PRO	LEU	LEU	GLU
GLU	LEU	VAL	GLU	ALA	GLU	ALA
PHE	ARG	GLU	ARG	ASN	PRO	ALA
LEU	GLU	GLY	VAL	ASN	LYS	GLN
	LYS	LEU	ARG	LEU	GLN	VAL
		LEU	LEU	VAL	VAL	LYS
	PHE	MET	ASP	ASP	GLN	VAL
	LYS	GLU	LEU	GLN	ARG	LYS
	ASN	GLN	MET	ILE	VAL	TRP
	MET	ILE	MET	LEU	GLY	WET
	SER	ARG	ARG	LEU	SER	ASN
	LYS	ASP	ILE	GLY	ALA	ASP
	ARG	GLN	ALA	THR	MET	MET
	ALA	ALA	ASN	GLY	ALA	ALA
	ALA	GLU	LEU	SER	LYS	ASN
	GLU	ASP	GLU	LYS	ALA	ASP
	MET	MET	GLU	GLY	LYS	ILE
	MET	ALA	VAL	LEU	ASP	VAL
	ARG	THR	GLN	ASP	LEU	PRO
	ASP	PRO	PRO	SER	GLN	ASN
	ASP	ILE	SER	LEU	GLN	ASP
	ILE	GLN	ALA	LYS	ASP	ASP
	GLU	ASP	LEU	TRP	LYS	ASN
	ALA	LEU	ALA	MET	VAL	ALA
	MET	MET	GLU	ASP	SER	ALA
	PRO	PHE	LEU	PRO	ALA	GLY
	PRO	VAL	ASN	ARG	VAL	MET
	VAL	PHE	GLU	GLN	HIS	PRO
	ARG	GLU	ILE	VAL	ARG	VAL
	VAL	ASN	MET	ALA	GLU	GLU
	ASP	VAL	GLU	ILE	PHE	LEU
	VAL	GLU	LYS	ILE	LEU	ASP
	VAL	GLU	GLN	ILE	GLU	VAL
	GLU	VAL	PHE	VAL	ASP	SER
	ALA	ASP	ALA	ASN	ILE	THR
	ALA	ASP	GLY	GLU	GLN	ILE
	GLN	GLN	GLN	HIS	LYS	THR
	LYS	GLY	ALA	PRO	TYR	GLY
	GLU	ILE	GLY	GLN	THR	GLU
	ILE	GLN	ALA	ILE	ASN	GLU
	LEU	LYS	GLN	GLN	ILE	LYS
	ALA	LEU	ALA	THR	GLY	ALA
	ILE	LEU	ALA	ILE	MET	ALA
	ALA	ARG	LYS	VAL	GLY	ILE
	ARG	ASP	ILE	LEU	SER	LEU
	ARG	VAL	SER	SER	GLU	LEU
	MET	PRO	GLY	TYR	ASP	LEU
	ALA	GLN	LEU	LEU	PHE	SER
	ASP	ASP	LYS	GLU	MET	ASN
	ALA	VAL	ALA	ALA	ARG	ASN
	GLY	LEU	ALA	GLN	GLU	GLN

- Molecule 1: Flagellar M-ring protein, Flagellar motor switch protein FliG

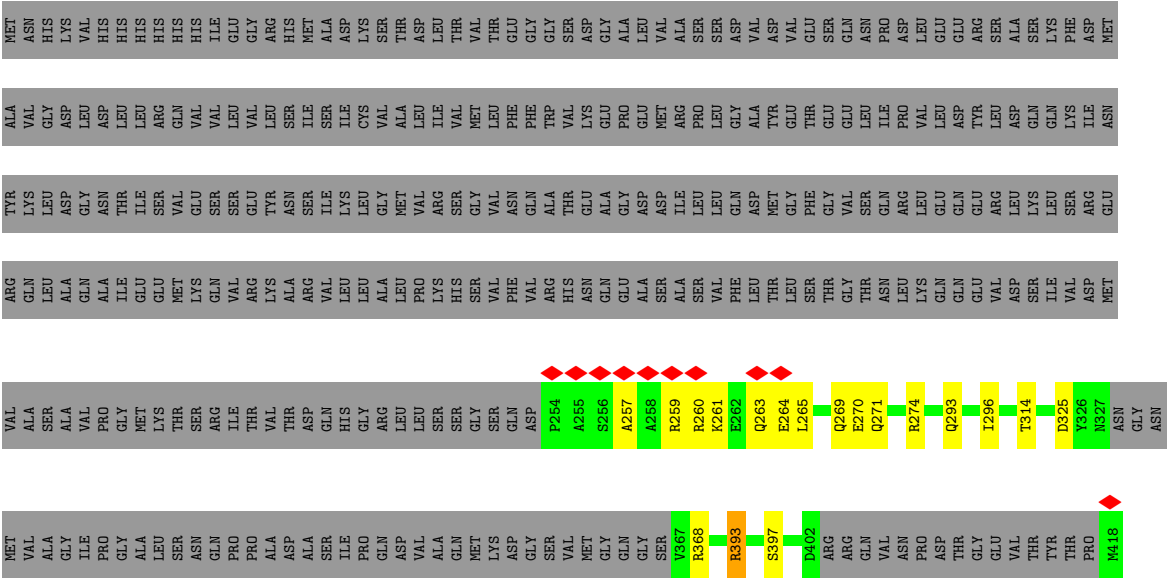
[illegible]





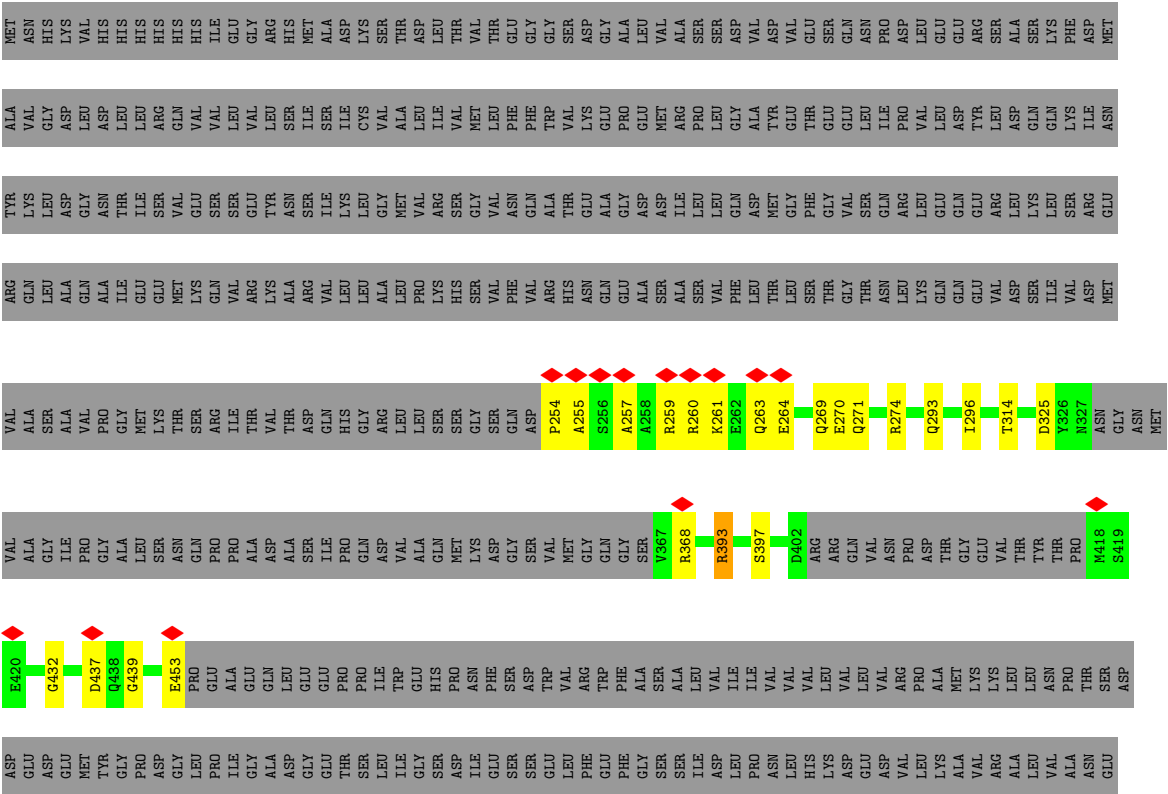


● Molecule 1: Flagellar M-ring protein,Flagellar motor switch protein FliG





● Molecule 1: Flagellar M-ring protein,Flagellar motor switch protein FliG



[illegible]

- Molecule 1: Flagellar M-ring protein, Flagellar motor switch protein FliG

Chain X: 13% 85%

[illegible]

[illegible]

- Molecule 1: Flagellar M-ring protein, Flagellar motor switch protein FliG



5419	GLY	ASN	ASN	GLN	VAL	ARG	TTR	ALA	MET
E420	ASN	MET	LEU	GLN	ALA	LEU	LEU	GLY	ASN
G432	ALA	VAL	ALA	GLN	VAL	ALA	GLY	LEU	LYS
D437	GLY	PRO	GLY	ILE	PRO	ALA	ASN	ASP	HIS
Q438	PRO	PRO	MET	GLY	LYS	GLU	ILE	LEU	HIS
Q439	ALA	ALA	THR	THR	THR	MET	SER	ARG	HIS
A452	LEU	LEU	SER	SER	SER	LYS	GLU	VAL	HIS
E453	SER	SER	ARG	ILE	ARG	VAL	SER	VAL	ILE
PRO	ASN	ASN	ILE	THR	THR	VAL	SER	LEU	GLU
ALA	GLN	PRO	THR	VAL	VAL	LYS	TTR	VAL	GLY
GLU	PRO	PRO	THR	THR	ALA	ALA	ASN	SER	ARG
GLN	ALA	ALA	ASP	GLN	GLN	VAL	ILE	ILE	MET
LEU	ALA	SER	ALA	HIS	GLY	LEU	LYS	ILE	ALA
GLU	ILE	ILE	ILE	ARG	ALA	LEU	GLY	CYS	ASP
PRO	PRO	PRO	PRO	LEU	LEU	LEU	MET	VAL	LYS
PRO	GLN	GLN	LEU	LEU	PRO	PRO	VAL	ALA	THR
ILE	ASP	ASP	SER	SER	LYS	HIS	ARG	LEU	ASP
TRP	VAL	VAL	SER	SER	ILE	PRO	THR	LEU	LEU
GLU	GLU	GLU	GLY	GLY	GLN	VAL	GLY	VAL	THR
HIS	ALA	ALA	ALA	SER	SER	VAL	GLY	MET	VAL
PRO	GLN	GLN	SER	VAL	VAL	PHE	ASN	PHE	GLY
ASN	MET	LYS	ASP	GLN	ASP	VAL	GLN	TRP	GLY
PHE	ASN	ASP	GLY	ASP	P254	ARG	ALA	VAL	GLY
SER	SER	GLY	SER	ASN	A255	HIS	THR	VAL	SER
ASP	ASP	SER	VAL	ASN	A256	ASN	GLY	LYS	ASP
TRP	VAL	VAL	VAL	GLN	S256	GLN	ALA	GLY	GLY
VAL	MET	MET	MET	ILE	A257	GLU	GLY	PRO	ALA
ARG	GLY	GLY	GLY	GLN	A258	ALA	ASP	GLU	LEU
TRP	GLN	GLN	GLN	GLN	ALA	SER	ASP	MET	VAL
PHE	GLY	GLY	GLY	ALA	R259	ALA	ILE	ARG	ALA
ALA	GLY	GLY	ALA	SER	R260	VAL	LEU	PRO	SER
SER	SER	SER	VAL	VAL	R261	SER	SER	LEU	SER
ALA	ALA	GLY	PHE	PHE	A262	LEU	GLN	GLY	ASP
LEU	LEU	GLY	GLY	LEU	Q263	LEU	MET	ALA	VAL
VAL	VAL	ILE	ILE	ILE	Q264	THR	THR	TYR	ASP
ILE	ILE	R393	R393	R393	E264	LEU	PHE	GLY	VAL
ILE	ILE	ILE	ILE	ILE	L265	SER	THR	THR	GLU
VAL	VAL	GLY	GLY	GLY	E266	SER	GLY	GLU	ASN
VAL	ARG	ARG	ARG	ARG	R267	THR	VAL	LEU	PRO
VAL	GLN	GLN	GLN	GLN	S268	GLY	VAL	GLU	ASN
VAL	VAL	VAL	VAL	VAL	Q269	THR	SER	ILE	ASN
VAL	ASN	ASN	ASN	ASN	E270	ASN	GLN	PRO	PRO
VAL	PRO	PRO	PRO	PRO	Q271	LYS	GLN	VAL	ASP
ARG	ASP	ASP	THR	THR	R274	GLN	GLY	TYR	ARG
PRO	THR	THR	GLY	GLY	Q293	VAL	ARG	LEU	SER
ALA	ALA	GLY	GLY	GLY	Q293	VAL	ARG	LEU	ALA
MET	VAL	VAL	VAL	VAL	I296	ASP	LYS	GLN	SER
LYS	THR	THR	THR	THR	I296	ILE	LEU	GLN	ALA
LEU	THR	THR	THR	THR	A316	VAL	SER	LYS	PHE
LEU	PRO	PRO	PRO	PRO	A316	VAL	ARG	GLN	LYS
ASN	ASN	ASN	ASN	ASN	D325	ASP	THR	ILE	PHE
						MET	GLY	ASN	MET

[illegible]

GLY
GLY
ALA
ASP
GLU
PHE
LEU

- Molecule 1: Flagellar M-ring protein, Flagellar motor switch protein FliG



ARG GLN LEU LEU ALA ALA ALA ILE GLU GLU MET MET LYS LYS GLN VAL VAL LEU LEU LEU LEU PRO LYS HIS SER SER PHE VAL ARG HIS ASN GLN GLU ALA ALA SER SER ALA ALA SER VAL VAL PHE THR THR ASN LEU LEU SER SER THR GLY THR THR ASN LEU LEU GLN GLN GLN VAL VAL ASP SER ILE VAL ASP MET

VAL	ALA	SER	ALA	VAL	PRO	GLY	MET	LYS	THR	SER	ARG	ILE	THR	VAL	THR	ASP	GLN	SER	SER	SER	SER	GLN	ASP	P254	A255	S256	A257	R259	R260	K261	E262	Q263	E264	L265	L266	R267	S268	Q269	E270	Q271	R274	V280	Q293	L296	T314	P315	A316
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D325	I326	I327	ASN	GLY	ASN	ASN	MET	VAL	ALA	ALA	ILE	PRO	GLY	ALA	LEU	SER	ASN	GLN	PRO	PRO	ASP	ALA	ALA	VAL	ASP	GLY	SER	VAL	GLY	GLN	GLY	SER	D402	ARG	ARG	GLN	VAL	ASN	PRO	ASP
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[illegible]

MET LYS LYS LEU LEU ASN PRO THR SER ASP ASP GLY GLY MET TYR GLY PRO ASP GLY LEU PRO ILE GLY ASP PHE GLU PHE GLY SER SER GLU PHO LEU LEU HIS LYS ASP ASP VAL LEU

[illegible]

LEU ASN GLU GLN ASP ALA ALA GLY ILE ILE ARG HIS LEU LEU GLU PRO LYS GLN VAL GLN ARG ARG LYS GLY SER SER ALA MET ALA ALA ALA LYS LYS ASP LEU LEU GLN ASP ASP LYS VAL SER SER ALA VAL VAL ARG ALA PHE LEU GLU ASP ASP ILE GLN LYS TYR THR ASN ASN ILE GLY MET GLY SER GLU ASP ASP

NET	ARG	ASN	ALA	LEU	VAL	ALA	ALA	GLY	GLU	ASP	LYS	ASN	ASN	ASN	VAL	ASP	GLN	LEU	LEU	LYS	GLY	LEU	THR	GLY	SER	SER	LEU	LYS	TRP	GLN	VAL	ALA	SER	LEU	ILE	VAL	ASN	GLU	HIS	PRO	GLN	ILE	GLN	THR	ILE	VAL	LEU	SER	TYR	LEU
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GLU ALA ASP GLN SER ALA GLU ILE LEU LEU GLN PHE PRO GLU ARG VAL ARG LEU ASP LEU MET MET ARG ILE ALA ASN LEU GLU GLU VAL GLN PRO SER ALA ALA LEU GLU ASN GLN LYS GLN PHE GLY GLN ALA ALA ALA ALA ALA LYS ILE ILE GLY LEU

LYS ALA ALA ALA ALA GLU ILE MET ASN ASN VAL VAL GLY GLY LEU LEU MET MET GLU GLU GLN ILE ILE ARG ARG ASP ASP GLN GLN LEU LEU MET PHE PHE VAL VAL VAL VAL ASP ASP GLN GLN ILE ILE LEU LEU MET PHE PHE VAL VAL VAL VAL ASP ASP GLN GLN LYS LYS LEU LEU LEU ARG ASP ASP VAL VAL PRO TRP

ASP	VAL	LEU	GLN	LYS	ALA	LEU	LYS	GLY	ALA	ALA	ASP	ASP	SER	LEU	ARG	GLU	LYS	VAL	PHE	LYS	ASN	MET	SER	LYS	ARG	ALA	ALA	GLU	MET	MET	ASP	ASP	ILE	VAL	VAL	ARG	VAL	VAL	ALA	ASP	VAL	GLN	LYS	GLU	ILE	LEU	ALA	ILE	ALA	ARG	ARG	MET	ALA
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ASP
ALA
GLY
GLU
LEU
MET
LEU
SER
GLY
GLY
ALA
ASP
GLU
PHE
LEU

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C35	Depositor
Number of particles used	184915	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	49.7	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1700	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	1.682	Depositor
Minimum map value	-0.966	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.037	Depositor
Recommended contour level	0.45	Depositor
Map size ($\text{\AA}$)	684.0, 684.0, 684.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.14, 1.14, 1.14	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1	0.19	0/1170	0.36	0/1573
1	2	0.19	0/1170	0.36	0/1573
1	3	0.19	0/1170	0.36	0/1573
1	4	0.19	0/1170	0.36	0/1573
1	5	0.19	0/1170	0.36	0/1573
1	6	0.19	0/1170	0.36	0/1573
1	7	0.19	0/1170	0.36	0/1573
1	8	0.19	0/1170	0.36	0/1573
1	9	0.19	0/1170	0.36	0/1573
1	A	0.19	0/1170	0.36	0/1573
1	B	0.19	0/1170	0.36	0/1573
1	C	0.19	0/1170	0.36	0/1573
1	D	0.19	0/1170	0.36	0/1573
1	E	0.19	0/1170	0.36	0/1573
1	F	0.19	0/1170	0.36	0/1573
1	G	0.19	0/1170	0.36	0/1573
1	H	0.19	0/1170	0.36	0/1573
1	I	0.19	0/1170	0.36	0/1573
1	J	0.19	0/1170	0.36	0/1573
1	K	0.19	0/1170	0.36	0/1573
1	L	0.19	0/1170	0.36	0/1573
1	M	0.19	0/1170	0.36	0/1573
1	N	0.19	0/1170	0.36	0/1573
1	O	0.19	0/1170	0.36	0/1573
1	P	0.19	0/1170	0.36	0/1573
1	Q	0.19	0/1170	0.36	0/1573
1	R	0.19	0/1170	0.36	0/1573
1	S	0.19	0/1170	0.36	0/1573
1	T	0.19	0/1170	0.36	0/1573
1	U	0.19	0/1170	0.36	0/1573
1	V	0.19	0/1170	0.36	0/1573
1	W	0.19	0/1170	0.36	0/1573
1	X	0.19	0/1170	0.36	0/1573
1	Y	0.19	0/1170	0.36	0/1573

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	Z	0.19	0/1170	0.36	0/1573
All	All	0.19	0/40950	0.36	0/55055

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1	0	1
1	2	0	1
1	3	0	1
1	4	0	1
1	5	0	1
1	6	0	1
1	7	0	1
1	8	0	1
1	9	0	1
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	1
1	H	0	1
1	I	0	1
1	J	0	1
1	K	0	1
1	L	0	1
1	M	0	1
1	N	0	1
1	O	0	1
1	P	0	1
1	Q	0	1
1	R	0	1
1	S	0	1
1	T	0	1
1	U	0	1
1	V	0	1
1	W	0	1
1	X	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	Y	0	1
1	Z	0	1
All	All	0	35

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (35) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	393	ARG	Sidechain
1	2	393	ARG	Sidechain
1	3	393	ARG	Sidechain
1	4	393	ARG	Sidechain
1	5	393	ARG	Sidechain
1	6	393	ARG	Sidechain
1	7	393	ARG	Sidechain
1	8	393	ARG	Sidechain
1	9	393	ARG	Sidechain
1	A	393	ARG	Sidechain
1	B	393	ARG	Sidechain
1	C	393	ARG	Sidechain
1	D	393	ARG	Sidechain
1	E	393	ARG	Sidechain
1	F	393	ARG	Sidechain
1	G	393	ARG	Sidechain
1	H	393	ARG	Sidechain
1	I	393	ARG	Sidechain
1	J	393	ARG	Sidechain
1	K	393	ARG	Sidechain
1	L	393	ARG	Sidechain
1	M	393	ARG	Sidechain
1	N	393	ARG	Sidechain
1	O	393	ARG	Sidechain
1	P	393	ARG	Sidechain
1	Q	393	ARG	Sidechain
1	R	393	ARG	Sidechain
1	S	393	ARG	Sidechain
1	T	393	ARG	Sidechain
1	U	393	ARG	Sidechain
1	V	393	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	W	393	ARG	Sidechain
1	X	393	ARG	Sidechain
1	Y	393	ARG	Sidechain
1	Z	393	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1159	0	1149	22	0
1	2	1159	0	1149	16	0
1	3	1159	0	1149	18	0
1	4	1159	0	1149	21	0
1	5	1159	0	1149	20	0
1	6	1159	0	1149	21	0
1	7	1159	0	1149	23	0
1	8	1159	0	1149	20	0
1	9	1159	0	1149	20	0
1	A	1159	0	1149	20	0
1	B	1159	0	1149	19	0
1	C	1159	0	1149	20	0
1	D	1159	0	1149	20	0
1	E	1159	0	1149	19	0
1	F	1159	0	1149	20	0
1	G	1159	0	1149	18	0
1	H	1159	0	1149	18	0
1	I	1159	0	1149	20	0
1	J	1159	0	1149	22	0
1	K	1159	0	1149	20	0
1	L	1159	0	1149	19	0
1	M	1159	0	1149	19	0
1	N	1159	0	1149	21	0
1	O	1159	0	1149	20	0
1	P	1159	0	1149	20	0
1	Q	1159	0	1149	20	0
1	R	1159	0	1149	20	0
1	S	1159	0	1149	19	0
1	T	1159	0	1149	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	U	1159	0	1149	19	0
1	V	1159	0	1149	18	0
1	W	1159	0	1149	18	0
1	X	1159	0	1149	18	0
1	Y	1159	0	1149	18	0
1	Z	1159	0	1149	25	0
All	All	40565	0	40215	545	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (545) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:263:GLN:NE2	1:Z:269:GLN:HE21	1.71	0.87
1:2:269:GLN:HE21	1:3:263:GLN:NE2	1.72	0.87
1:L:269:GLN:HE21	1:M:263:GLN:NE2	1.73	0.86
1:5:269:GLN:HE21	1:6:263:GLN:NE2	1.74	0.85
1:K:269:GLN:HE21	1:L:263:GLN:NE2	1.76	0.83
1:I:269:GLN:HE21	1:J:263:GLN:NE2	1.78	0.82
1:6:269:GLN:HE21	1:7:263:GLN:NE2	1.78	0.81
1:Y:269:GLN:HE21	1:Z:263:GLN:NE2	1.80	0.80
1:7:269:GLN:HE21	1:8:263:GLN:NE2	1.79	0.79
1:J:269:GLN:HE21	1:K:263:GLN:NE2	1.80	0.79
1:E:269:GLN:HE21	1:F:263:GLN:NE2	1.80	0.79
1:N:269:GLN:HE21	1:O:263:GLN:NE2	1.82	0.78
1:G:269:GLN:HE21	1:H:263:GLN:NE2	1.82	0.78
1:M:269:GLN:HE21	1:N:263:GLN:NE2	1.81	0.78
1:X:269:GLN:HE21	1:Y:263:GLN:NE2	1.83	0.76
1:4:269:GLN:HE21	1:5:263:GLN:NE2	1.82	0.76
1:B:269:GLN:HE21	1:C:263:GLN:NE2	1.83	0.75
1:P:269:GLN:HE21	1:Q:263:GLN:NE2	1.86	0.74
1:W:269:GLN:HE21	1:X:263:GLN:NE2	1.86	0.74
1:H:269:GLN:HE21	1:I:263:GLN:NE2	1.87	0.73
1:1:269:GLN:HE21	1:2:263:GLN:NE2	1.87	0.72
1:3:269:GLN:HE21	1:4:263:GLN:NE2	1.87	0.72
1:F:269:GLN:HE21	1:G:263:GLN:NE2	1.88	0.71
1:O:269:GLN:HE21	1:P:263:GLN:NE2	1.88	0.71
1:Q:269:GLN:HE21	1:R:263:GLN:NE2	1.91	0.69
1:S:269:GLN:HE21	1:T:263:GLN:NE2	1.92	0.67
1:1:259:ARG:HG2	1:Z:265:LEU:HD11	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:269:GLN:HE21	1:V:263:GLN:NE2	1.93	0.67
1:V:269:GLN:HE21	1:W:263:GLN:NE2	1.93	0.67
1:A:269:GLN:HE21	1:B:263:GLN:NE2	1.92	0.67
1:C:269:GLN:HE21	1:D:263:GLN:NE2	1.93	0.66
1:8:269:GLN:HE21	1:9:263:GLN:NE2	1.93	0.66
1:1:263:GLN:HE21	1:Z:269:GLN:HE21	1.44	0.66
1:2:269:GLN:HE21	1:3:263:GLN:HE21	1.44	0.66
1:9:269:GLN:HE21	1:A:263:GLN:NE2	1.94	0.65
1:R:269:GLN:HE21	1:S:263:GLN:NE2	1.95	0.65
1:D:269:GLN:HE21	1:E:263:GLN:NE2	1.95	0.65
1:L:269:GLN:HE21	1:M:263:GLN:HE21	1.44	0.63
1:3:437:ASP:OD2	1:3:439:GLY:N	2.28	0.63
1:2:437:ASP:OD2	1:2:439:GLY:N	2.28	0.63
1:5:269:GLN:HE21	1:6:263:GLN:HE21	1.47	0.63
1:6:437:ASP:OD2	1:6:439:GLY:N	2.28	0.62
1:Y:437:ASP:OD2	1:Y:439:GLY:N	2.28	0.62
1:7:437:ASP:OD2	1:7:439:GLY:N	2.28	0.62
1:Z:437:ASP:OD2	1:Z:439:GLY:N	2.28	0.62
1:X:437:ASP:OD2	1:X:439:GLY:N	2.28	0.62
1:5:437:ASP:OD2	1:5:439:GLY:N	2.28	0.62
1:T:269:GLN:HE21	1:U:263:GLN:NE2	1.97	0.62
1:1:437:ASP:OD2	1:1:439:GLY:N	2.28	0.62
1:9:437:ASP:OD2	1:9:439:GLY:N	2.28	0.61
1:A:437:ASP:OD2	1:A:439:GLY:N	2.28	0.61
1:8:437:ASP:OD2	1:8:439:GLY:N	2.28	0.61
1:W:437:ASP:OD2	1:W:439:GLY:N	2.28	0.61
1:4:437:ASP:OD2	1:4:439:GLY:N	2.28	0.61
1:U:437:ASP:OD2	1:U:439:GLY:N	2.28	0.61
1:V:437:ASP:OD2	1:V:439:GLY:N	2.28	0.61
1:B:437:ASP:OD2	1:B:439:GLY:N	2.28	0.61
1:K:269:GLN:HE21	1:L:263:GLN:HE21	1.49	0.61
1:T:437:ASP:OD2	1:T:439:GLY:N	2.28	0.61
1:J:265:LEU:HD11	1:K:259:ARG:HG2	1.84	0.60
1:N:437:ASP:OD2	1:N:439:GLY:N	2.28	0.60
1:C:437:ASP:OD2	1:C:439:GLY:N	2.28	0.60
1:S:437:ASP:OD2	1:S:439:GLY:N	2.28	0.59
1:J:269:GLN:HE21	1:K:263:GLN:HE21	1.49	0.59
1:D:437:ASP:OD2	1:D:439:GLY:N	2.28	0.59
1:E:437:ASP:OD2	1:E:439:GLY:N	2.28	0.59
1:L:265:LEU:HD11	1:M:259:ARG:HG2	1.85	0.59
1:Q:437:ASP:OD2	1:Q:439:GLY:N	2.28	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:437:ASP:OD2	1:R:439:GLY:N	2.28	0.59
1:F:437:ASP:OD2	1:F:439:GLY:N	2.28	0.59
1:P:437:ASP:OD2	1:P:439:GLY:N	2.28	0.59
1:G:437:ASP:OD2	1:G:439:GLY:N	2.28	0.58
1:O:437:ASP:OD2	1:O:439:GLY:N	2.28	0.58
1:6:269:GLN:HE21	1:7:263:GLN:HE21	1.52	0.57
1:K:437:ASP:OD2	1:K:439:GLY:N	2.28	0.57
1:J:437:ASP:OD2	1:J:439:GLY:N	2.28	0.57
1:L:437:ASP:OD2	1:L:439:GLY:N	2.28	0.57
1:M:269:GLN:HE21	1:N:263:GLN:HE21	1.52	0.57
1:H:437:ASP:OD2	1:H:439:GLY:N	2.28	0.57
1:I:437:ASP:OD2	1:I:439:GLY:N	2.28	0.57
1:M:437:ASP:OD2	1:M:439:GLY:N	2.28	0.57
1:4:265:LEU:HD11	1:5:259:ARG:HG2	1.85	0.56
1:X:269:GLN:HE21	1:Y:263:GLN:HE21	1.54	0.56
1:M:265:LEU:HD11	1:N:259:ARG:HG2	1.88	0.56
1:G:270:GLU:HG2	1:G:296:ILE:HD12	1.88	0.56
1:L:270:GLU:HG2	1:L:296:ILE:HD12	1.88	0.56
1:Q:270:GLU:HG2	1:Q:296:ILE:HD12	1.88	0.56
1:B:270:GLU:HG2	1:B:296:ILE:HD12	1.88	0.55
1:O:270:GLU:HG2	1:O:296:ILE:HD12	1.88	0.55
1:J:270:GLU:HG2	1:J:296:ILE:HD12	1.88	0.55
1:T:270:GLU:HG2	1:T:296:ILE:HD12	1.89	0.55
1:8:270:GLU:HG2	1:8:296:ILE:HD12	1.88	0.55
1:D:270:GLU:HG2	1:D:296:ILE:HD12	1.88	0.55
1:E:270:GLU:HG2	1:E:296:ILE:HD12	1.89	0.55
1:P:265:LEU:HD11	1:Q:259:ARG:HG2	1.88	0.55
1:X:265:LEU:HD11	1:Y:259:ARG:HG2	1.87	0.55
1:2:265:LEU:HD11	1:3:259:ARG:HG2	1.87	0.55
1:I:270:GLU:HG2	1:I:296:ILE:HD12	1.88	0.55
1:N:269:GLN:HE21	1:O:263:GLN:HE21	1.55	0.55
1:N:270:GLU:HG2	1:N:296:ILE:HD12	1.88	0.55
1:W:270:GLU:HG2	1:W:296:ILE:HD12	1.88	0.55
1:R:270:GLU:HG2	1:R:296:ILE:HD12	1.89	0.55
1:7:265:LEU:HD11	1:8:259:ARG:HG2	1.88	0.55
1:V:270:GLU:HG2	1:V:296:ILE:HD12	1.88	0.55
1:5:270:GLU:HG2	1:5:296:ILE:HD12	1.89	0.55
1:7:269:GLN:HE21	1:8:263:GLN:HE21	1.52	0.55
1:A:270:GLU:HG2	1:A:296:ILE:HD12	1.88	0.55
1:S:270:GLU:HG2	1:S:296:ILE:HD12	1.88	0.55
1:Y:270:GLU:HG2	1:Y:296:ILE:HD12	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:270:GLU:HG2	1:2:296:ILE:HD12	1.89	0.55
1:H:270:GLU:HG2	1:H:296:ILE:HD12	1.88	0.55
1:M:270:GLU:HG2	1:M:296:ILE:HD12	1.89	0.55
1:Z:270:GLU:HG2	1:Z:296:ILE:HD12	1.88	0.55
1:6:270:GLU:HG2	1:6:296:ILE:HD12	1.88	0.55
1:I:269:GLN:HE21	1:J:263:GLN:HE21	1.55	0.55
1:9:270:GLU:HG2	1:9:296:ILE:HD12	1.89	0.54
1:G:269:GLN:HE21	1:H:263:GLN:HE21	1.55	0.54
1:3:270:GLU:HG2	1:3:296:ILE:HD12	1.89	0.54
1:F:270:GLU:HG2	1:F:296:ILE:HD12	1.88	0.54
1:U:270:GLU:HG2	1:U:296:ILE:HD12	1.88	0.54
1:C:270:GLU:HG2	1:C:296:ILE:HD12	1.89	0.54
1:K:265:LEU:HD11	1:L:259:ARG:HG2	1.89	0.54
1:K:270:GLU:HG2	1:K:296:ILE:HD12	1.88	0.54
1:5:265:LEU:HD11	1:6:259:ARG:HG2	1.88	0.54
1:P:270:GLU:HG2	1:P:296:ILE:HD12	1.88	0.54
1:7:270:GLU:HG2	1:7:296:ILE:HD12	1.89	0.54
1:7:432:GLY:HA3	1:8:397:SER:HB3	1.88	0.54
1:4:269:GLN:HE21	1:5:263:GLN:HE21	1.53	0.54
1:4:270:GLU:HG2	1:4:296:ILE:HD12	1.88	0.54
1:E:269:GLN:HE21	1:F:263:GLN:HE21	1.55	0.53
1:1:270:GLU:HG2	1:1:296:ILE:HD12	1.88	0.53
1:X:270:GLU:HG2	1:X:296:ILE:HD12	1.89	0.53
1:G:265:LEU:HD11	1:H:259:ARG:HG2	1.91	0.53
1:X:257:ALA:O	1:X:261:LYS:HG2	2.10	0.52
1:Y:269:GLN:HE21	1:Z:263:GLN:HE21	1.56	0.52
1:E:257:ALA:O	1:E:261:LYS:HG2	2.10	0.52
1:O:257:ALA:O	1:O:261:LYS:HG2	2.10	0.52
1:W:257:ALA:O	1:W:261:LYS:HG2	2.10	0.52
1:Y:257:ALA:O	1:Y:261:LYS:HG2	2.10	0.52
1:S:257:ALA:O	1:S:261:LYS:HG2	2.10	0.52
1:D:257:ALA:O	1:D:261:LYS:HG2	2.10	0.52
1:F:257:ALA:O	1:F:261:LYS:HG2	2.10	0.52
1:L:257:ALA:O	1:L:261:LYS:HG2	2.10	0.52
1:N:257:ALA:O	1:N:261:LYS:HG2	2.10	0.52
1:P:257:ALA:O	1:P:261:LYS:HG2	2.10	0.52
1:K:257:ALA:O	1:K:261:LYS:HG2	2.10	0.52
1:M:257:ALA:O	1:M:261:LYS:HG2	2.10	0.52
1:R:265:LEU:HD11	1:S:259:ARG:HG2	1.92	0.52
1:6:257:ALA:O	1:6:261:LYS:HG2	2.10	0.52
1:V:257:ALA:O	1:V:261:LYS:HG2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:257:ALA:O	1:5:261:LYS:HG2	2.10	0.52
1:7:257:ALA:O	1:7:261:LYS:HG2	2.10	0.52
1:A:265:LEU:HD11	1:B:259:ARG:HG2	1.92	0.52
1:G:257:ALA:O	1:G:261:LYS:HG2	2.10	0.52
1:H:257:ALA:O	1:H:261:LYS:HG2	2.10	0.52
1:Q:432:GLY:HA3	1:R:397:SER:HB3	1.92	0.52
1:Z:257:ALA:O	1:Z:261:LYS:HG2	2.10	0.52
1:C:257:ALA:O	1:C:261:LYS:HG2	2.10	0.51
1:R:257:ALA:O	1:R:261:LYS:HG2	2.10	0.51
1:1:257:ALA:O	1:1:261:LYS:HG2	2.10	0.51
1:4:257:ALA:O	1:4:261:LYS:HG2	2.10	0.51
1:I:257:ALA:O	1:I:261:LYS:HG2	2.10	0.51
1:Q:257:ALA:O	1:Q:261:LYS:HG2	2.10	0.51
1:T:257:ALA:O	1:T:261:LYS:HG2	2.10	0.51
1:U:257:ALA:O	1:U:261:LYS:HG2	2.10	0.51
1:1:395:THR:OG1	1:Z:432:GLY:O	2.28	0.51
1:8:257:ALA:O	1:8:261:LYS:HG2	2.10	0.51
1:3:274:ARG:NH1	1:3:293:GLN:OE1	2.44	0.51
1:N:265:LEU:HD11	1:O:259:ARG:HG2	1.93	0.51
1:V:274:ARG:NH1	1:V:293:GLN:OE1	2.44	0.51
1:4:274:ARG:NH1	1:4:293:GLN:OE1	2.44	0.51
1:B:257:ALA:O	1:B:261:LYS:HG2	2.10	0.51
1:A:432:GLY:HA3	1:B:397:SER:HB3	1.92	0.51
1:J:257:ALA:O	1:J:261:LYS:HG2	2.10	0.51
1:P:269:GLN:HE21	1:Q:263:GLN:HE21	1.58	0.51
1:3:257:ALA:O	1:3:261:LYS:HG2	2.10	0.51
1:N:274:ARG:NH1	1:N:293:GLN:OE1	2.44	0.51
1:W:274:ARG:NH1	1:W:293:GLN:OE1	2.44	0.51
1:5:274:ARG:NH1	1:5:293:GLN:OE1	2.44	0.51
1:6:265:LEU:HD11	1:7:259:ARG:HG2	1.91	0.51
1:O:274:ARG:NH1	1:O:293:GLN:OE1	2.44	0.51
1:O:265:LEU:HD11	1:P:259:ARG:HG2	1.93	0.51
1:3:265:LEU:HD11	1:4:259:ARG:HG2	1.93	0.50
1:9:257:ALA:O	1:9:261:LYS:HG2	2.10	0.50
1:A:257:ALA:O	1:A:261:LYS:HG2	2.10	0.50
1:2:257:ALA:O	1:2:261:LYS:HG2	2.10	0.50
1:B:269:GLN:HE21	1:C:263:GLN:HE21	1.59	0.50
1:P:274:ARG:NH1	1:P:293:GLN:OE1	2.44	0.50
1:X:274:ARG:NH1	1:X:293:GLN:OE1	2.44	0.50
1:6:274:ARG:NH1	1:6:293:GLN:OE1	2.44	0.50
1:T:432:GLY:HA3	1:U:397:SER:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:274:ARG:NH1	1:Q:293:GLN:OE1	2.44	0.50
1:D:274:ARG:NH1	1:D:293:GLN:OE1	2.44	0.50
1:Y:274:ARG:NH1	1:Y:293:GLN:OE1	2.44	0.50
1:7:274:ARG:NH1	1:7:293:GLN:OE1	2.44	0.50
1:C:432:GLY:HA3	1:D:397:SER:HB3	1.94	0.50
1:E:274:ARG:NH1	1:E:293:GLN:OE1	2.44	0.50
1:V:432:GLY:HA3	1:W:397:SER:HB3	1.94	0.49
1:F:274:ARG:NH1	1:F:293:GLN:OE1	2.44	0.49
1:B:432:GLY:HA3	1:C:397:SER:HB3	1.93	0.49
1:R:274:ARG:NH1	1:R:293:GLN:OE1	2.44	0.49
1:I:274:ARG:NH1	1:I:293:GLN:OE1	2.44	0.49
1:G:274:ARG:NH1	1:G:293:GLN:OE1	2.44	0.49
1:Z:274:ARG:NH1	1:Z:293:GLN:OE1	2.44	0.49
1:D:432:GLY:HA3	1:E:397:SER:HB3	1.94	0.49
1:J:274:ARG:NH1	1:J:293:GLN:OE1	2.44	0.49
1:O:269:GLN:HE21	1:P:263:GLN:HE21	1.60	0.49
1:H:274:ARG:NH1	1:H:293:GLN:OE1	2.44	0.49
1:8:274:ARG:NH1	1:8:293:GLN:OE1	2.44	0.49
1:9:274:ARG:NH1	1:9:293:GLN:OE1	2.44	0.48
1:S:274:ARG:NH1	1:S:293:GLN:OE1	2.44	0.48
1:A:274:ARG:NH1	1:A:293:GLN:OE1	2.44	0.48
1:W:432:GLY:HA3	1:X:397:SER:HB3	1.95	0.48
1:1:274:ARG:NH1	1:1:293:GLN:OE1	2.44	0.48
1:F:432:GLY:HA3	1:G:397:SER:HB3	1.95	0.48
1:3:269:GLN:HE21	1:4:263:GLN:HE21	1.59	0.48
1:K:274:ARG:NH1	1:K:293:GLN:OE1	2.44	0.48
1:B:274:ARG:NH1	1:B:293:GLN:OE1	2.44	0.48
1:1:269:GLN:HE21	1:2:263:GLN:HE21	1.60	0.48
1:I:432:GLY:HA3	1:J:397:SER:HB3	1.95	0.47
1:Q:265:LEU:HD11	1:R:259:ARG:HG2	1.97	0.47
1:S:265:LEU:HD11	1:T:259:ARG:HG2	1.97	0.47
1:T:274:ARG:NH1	1:T:293:GLN:OE1	2.44	0.47
1:2:274:ARG:NH1	1:2:293:GLN:OE1	2.44	0.47
1:U:265:LEU:HD11	1:V:259:ARG:HG2	1.97	0.47
1:H:269:GLN:HE21	1:I:263:GLN:HE21	1.62	0.47
1:L:274:ARG:NH1	1:L:293:GLN:OE1	2.44	0.47
1:F:269:GLN:HE21	1:G:263:GLN:HE21	1.62	0.47
1:Q:269:GLN:HE21	1:R:263:GLN:HE21	1.63	0.47
1:8:432:GLY:HA3	1:9:397:SER:HB3	1.96	0.47
1:C:274:ARG:NH1	1:C:293:GLN:OE1	2.44	0.47
1:S:432:GLY:HA3	1:T:397:SER:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:432:GLY:HA3	1:Q:397:SER:HB3	1.97	0.46
1:6:316:ALA:HB1	1:7:377:LEU:HD13	1.97	0.46
1:9:265:LEU:HD11	1:A:259:ARG:HG2	1.98	0.46
1:1:293:GLN:HG3	1:Z:280:VAL:HG23	1.97	0.46
1:9:432:GLY:HA3	1:A:397:SER:HB3	1.98	0.46
1:M:453:GLU:O	1:M:453:GLU:HG2	2.16	0.46
1:U:274:ARG:NH1	1:U:293:GLN:OE1	2.44	0.46
1:J:453:GLU:O	1:J:453:GLU:HG2	2.16	0.46
1:K:453:GLU:O	1:K:453:GLU:HG2	2.16	0.46
1:L:453:GLU:O	1:L:453:GLU:HG2	2.16	0.46
1:N:453:GLU:O	1:N:453:GLU:HG2	2.16	0.46
1:I:453:GLU:O	1:I:453:GLU:HG2	2.16	0.46
1:O:453:GLU:O	1:O:453:GLU:HG2	2.16	0.46
1:P:453:GLU:O	1:P:453:GLU:HG2	2.16	0.46
1:M:274:ARG:NH1	1:M:293:GLN:OE1	2.44	0.46
1:1:397:SER:HB3	1:Z:432:GLY:HA3	1.98	0.46
1:H:453:GLU:O	1:H:453:GLU:HG2	2.16	0.46
1:O:432:GLY:HA3	1:P:397:SER:HB3	1.97	0.46
1:Q:453:GLU:O	1:Q:453:GLU:HG2	2.16	0.46
1:4:432:GLY:O	1:5:395:THR:OG1	2.29	0.46
1:G:453:GLU:O	1:G:453:GLU:HG2	2.16	0.46
1:Y:432:GLY:HA3	1:Z:397:SER:HB3	1.98	0.46
1:F:453:GLU:O	1:F:453:GLU:HG2	2.16	0.46
1:R:453:GLU:O	1:R:453:GLU:HG2	2.16	0.46
1:5:453:GLU:O	1:5:453:GLU:HG2	2.16	0.45
1:9:314:THR:O	1:9:314:THR:OG1	2.33	0.45
1:E:453:GLU:O	1:E:453:GLU:HG2	2.16	0.45
1:N:432:GLY:HA3	1:O:397:SER:HB3	1.98	0.45
1:S:453:GLU:O	1:S:453:GLU:HG2	2.16	0.45
1:3:453:GLU:O	1:3:453:GLU:HG2	2.16	0.45
1:4:453:GLU:O	1:4:453:GLU:HG2	2.16	0.45
1:6:453:GLU:O	1:6:453:GLU:HG2	2.16	0.45
1:7:453:GLU:O	1:7:453:GLU:HG2	2.16	0.45
1:8:453:GLU:O	1:8:453:GLU:HG2	2.16	0.45
1:B:453:GLU:O	1:B:453:GLU:HG2	2.16	0.45
1:D:453:GLU:O	1:D:453:GLU:HG2	2.16	0.45
1:9:453:GLU:O	1:9:453:GLU:HG2	2.16	0.45
1:T:453:GLU:O	1:T:453:GLU:HG2	2.16	0.45
1:U:453:GLU:O	1:U:453:GLU:HG2	2.16	0.45
1:W:314:THR:O	1:W:314:THR:OG1	2.33	0.45
1:1:453:GLU:O	1:1:453:GLU:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:453:GLU:O	1:2:453:GLU:HG2	2.16	0.45
1:A:453:GLU:O	1:A:453:GLU:HG2	2.16	0.45
1:C:453:GLU:O	1:C:453:GLU:HG2	2.16	0.45
1:S:269:GLN:HE21	1:T:263:GLN:HE21	1.64	0.45
1:F:265:LEU:HD11	1:G:259:ARG:HG2	1.99	0.45
1:L:432:GLY:O	1:M:395:THR:OG1	2.34	0.45
1:Z:453:GLU:O	1:Z:453:GLU:HG2	2.16	0.45
1:8:265:LEU:HD11	1:9:259:ARG:HG2	1.99	0.45
1:E:265:LEU:HD11	1:F:259:ARG:HG2	1.99	0.45
1:V:453:GLU:O	1:V:453:GLU:HG2	2.16	0.45
1:E:432:GLY:HA3	1:F:397:SER:HB3	1.98	0.45
1:G:432:GLY:HA3	1:H:397:SER:HB3	1.99	0.45
1:W:453:GLU:O	1:W:453:GLU:HG2	2.16	0.45
1:5:271:GLN:OE1	1:5:271:GLN:HA	2.17	0.45
1:N:271:GLN:OE1	1:N:271:GLN:HA	2.17	0.45
1:P:271:GLN:OE1	1:P:271:GLN:HA	2.17	0.45
1:R:271:GLN:OE1	1:R:271:GLN:HA	2.17	0.45
1:X:453:GLU:O	1:X:453:GLU:HG2	2.16	0.45
1:7:271:GLN:OE1	1:7:271:GLN:HA	2.17	0.45
1:C:271:GLN:OE1	1:C:271:GLN:HA	2.17	0.45
1:Y:453:GLU:O	1:Y:453:GLU:HG2	2.16	0.45
1:1:271:GLN:OE1	1:1:271:GLN:HA	2.17	0.44
1:3:271:GLN:OE1	1:3:271:GLN:HA	2.17	0.44
1:8:314:THR:O	1:8:314:THR:OG1	2.33	0.44
1:9:271:GLN:HA	1:9:271:GLN:OE1	2.17	0.44
1:E:271:GLN:HA	1:E:271:GLN:OE1	2.17	0.44
1:L:271:GLN:HA	1:L:271:GLN:OE1	2.17	0.44
1:T:271:GLN:HA	1:T:271:GLN:OE1	2.17	0.44
1:A:271:GLN:OE1	1:A:271:GLN:HA	2.17	0.44
1:B:271:GLN:OE1	1:B:271:GLN:HA	2.17	0.44
1:G:271:GLN:HA	1:G:271:GLN:OE1	2.17	0.44
1:H:271:GLN:OE1	1:H:271:GLN:HA	2.17	0.44
1:I:265:LEU:HD11	1:J:259:ARG:HG2	1.99	0.44
1:J:271:GLN:HA	1:J:271:GLN:OE1	2.17	0.44
1:Y:271:GLN:HA	1:Y:271:GLN:OE1	2.17	0.44
1:V:271:GLN:HA	1:V:271:GLN:OE1	2.17	0.44
1:D:271:GLN:OE1	1:D:271:GLN:HA	2.17	0.44
1:F:271:GLN:OE1	1:F:271:GLN:HA	2.17	0.44
1:U:269:GLN:HE21	1:V:263:GLN:HE21	1.65	0.44
1:W:271:GLN:OE1	1:W:271:GLN:HA	2.17	0.44
1:6:432:GLY:HA3	1:7:397:SER:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:8:271:GLN:OE1	1:8:271:GLN:HA	2.17	0.44
1:F:314:THR:O	1:F:314:THR:OG1	2.33	0.44
1:Q:260:ARG:O	1:Q:264:GLU:HG2	2.18	0.44
1:W:260:ARG:O	1:W:264:GLU:HG2	2.18	0.44
1:1:293:GLN:CB	1:Z:433:THR:HG23	2.48	0.44
1:I:271:GLN:OE1	1:I:271:GLN:HA	2.17	0.44
1:S:260:ARG:O	1:S:264:GLU:HG2	2.18	0.44
1:U:260:ARG:O	1:U:264:GLU:HG2	2.18	0.44
1:6:271:GLN:HA	1:6:271:GLN:OE1	2.17	0.44
1:A:260:ARG:O	1:A:264:GLU:HG2	2.18	0.44
1:C:260:ARG:O	1:C:264:GLU:HG2	2.18	0.44
1:E:260:ARG:O	1:E:264:GLU:HG2	2.18	0.44
1:H:260:ARG:O	1:H:264:GLU:HG2	2.18	0.44
1:I:260:ARG:O	1:I:264:GLU:HG2	2.18	0.44
1:M:260:ARG:O	1:M:264:GLU:HG2	2.18	0.44
1:N:260:ARG:O	1:N:264:GLU:HG2	2.18	0.44
1:O:260:ARG:O	1:O:264:GLU:HG2	2.18	0.44
1:U:271:GLN:OE1	1:U:271:GLN:HA	2.17	0.44
1:V:314:THR:O	1:V:314:THR:OG1	2.33	0.44
1:X:271:GLN:HA	1:X:271:GLN:OE1	2.17	0.44
1:Y:260:ARG:O	1:Y:264:GLU:HG2	2.18	0.44
1:6:260:ARG:O	1:6:264:GLU:HG2	2.18	0.44
1:8:260:ARG:O	1:8:264:GLU:HG2	2.18	0.44
1:G:260:ARG:O	1:G:264:GLU:HG2	2.18	0.44
1:J:260:ARG:O	1:J:264:GLU:HG2	2.18	0.44
1:K:260:ARG:O	1:K:264:GLU:HG2	2.18	0.44
1:L:260:ARG:O	1:L:264:GLU:HG2	2.18	0.44
1:1:260:ARG:O	1:1:264:GLU:HG2	2.18	0.43
1:2:260:ARG:O	1:2:264:GLU:HG2	2.18	0.43
1:F:260:ARG:O	1:F:264:GLU:HG2	2.18	0.43
1:P:260:ARG:O	1:P:264:GLU:HG2	2.18	0.43
1:S:271:GLN:OE1	1:S:271:GLN:HA	2.17	0.43
1:4:260:ARG:O	1:4:264:GLU:HG2	2.18	0.43
1:4:271:GLN:HA	1:4:271:GLN:OE1	2.17	0.43
1:K:271:GLN:OE1	1:K:271:GLN:HA	2.17	0.43
1:9:260:ARG:O	1:9:264:GLU:HG2	2.18	0.43
1:R:260:ARG:O	1:R:264:GLU:HG2	2.18	0.43
1:T:260:ARG:O	1:T:264:GLU:HG2	2.18	0.43
1:V:260:ARG:O	1:V:264:GLU:HG2	2.18	0.43
1:X:260:ARG:O	1:X:264:GLU:HG2	2.18	0.43
1:Z:260:ARG:O	1:Z:264:GLU:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:271:GLN:OE1	1:Z:271:GLN:HA	2.17	0.43
1:D:260:ARG:O	1:D:264:GLU:HG2	2.18	0.43
1:L:432:GLY:HA3	1:M:397:SER:HB3	2.00	0.43
1:Q:271:GLN:HA	1:Q:271:GLN:OE1	2.17	0.43
1:R:269:GLN:HE21	1:S:263:GLN:HE21	1.66	0.43
1:U:432:GLY:HA3	1:V:397:SER:HB3	1.99	0.43
1:2:271:GLN:OE1	1:2:271:GLN:HA	2.17	0.43
1:3:260:ARG:O	1:3:264:GLU:HG2	2.18	0.43
1:B:260:ARG:O	1:B:264:GLU:HG2	2.18	0.43
1:7:314:THR:O	1:7:314:THR:OG1	2.33	0.43
1:M:271:GLN:OE1	1:M:271:GLN:HA	2.17	0.43
1:N:254:PRO:HB2	1:N:255:ALA:H	1.67	0.43
1:O:271:GLN:HA	1:O:271:GLN:OE1	2.17	0.43
1:E:314:THR:O	1:E:314:THR:OG1	2.33	0.43
1:5:260:ARG:O	1:5:264:GLU:HG2	2.18	0.43
1:A:269:GLN:HE21	1:B:263:GLN:HE21	1.65	0.43
1:7:260:ARG:O	1:7:264:GLU:HG2	2.18	0.43
1:D:325:ASP:HB3	1:D:368:ARG:HB2	2.01	0.43
1:I:316:ALA:HB1	1:J:377:LEU:HD13	2.01	0.43
1:U:325:ASP:HB3	1:U:368:ARG:HB2	2.01	0.43
1:3:432:GLY:HA3	1:4:397:SER:HB3	2.00	0.42
1:A:325:ASP:HB3	1:A:368:ARG:HB2	2.01	0.42
1:B:265:LEU:HD11	1:C:259:ARG:HG2	2.02	0.42
1:C:325:ASP:HB3	1:C:368:ARG:HB2	2.01	0.42
1:P:325:ASP:HB3	1:P:368:ARG:HB2	2.01	0.42
1:R:432:GLY:HA3	1:S:397:SER:HB3	1.99	0.42
1:S:325:ASP:HB3	1:S:368:ARG:HB2	2.01	0.42
1:W:254:PRO:HB2	1:W:255:ALA:H	1.66	0.42
1:W:325:ASP:HB3	1:W:368:ARG:HB2	2.01	0.42
1:6:325:ASP:HB3	1:6:368:ARG:HB2	2.01	0.42
1:8:325:ASP:HB3	1:8:368:ARG:HB2	2.02	0.42
1:F:325:ASP:HB3	1:F:368:ARG:HB2	2.01	0.42
1:R:325:ASP:HB3	1:R:368:ARG:HB2	2.01	0.42
1:2:325:ASP:HB3	1:2:368:ARG:HB2	2.01	0.42
1:8:269:GLN:HE21	1:9:263:GLN:HE21	1.66	0.42
1:9:325:ASP:HB3	1:9:368:ARG:HB2	2.01	0.42
1:B:325:ASP:HB3	1:B:368:ARG:HB2	2.01	0.42
1:E:257:ALA:HA	1:E:260:ARG:HG2	2.02	0.42
1:I:325:ASP:HB3	1:I:368:ARG:HB2	2.01	0.42
1:M:325:ASP:HB3	1:M:368:ARG:HB2	2.01	0.42
1:N:325:ASP:HB3	1:N:368:ARG:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:325:ASP:HB3	1:Q:368:ARG:HB2	2.01	0.42
1:Y:325:ASP:HB3	1:Y:368:ARG:HB2	2.01	0.42
1:1:325:ASP:HB3	1:1:368:ARG:HB2	2.01	0.42
1:1:377:LEU:HD13	1:Z:316:ALA:HB1	2.01	0.42
1:4:316:ALA:HB1	1:5:377:LEU:HD13	2.01	0.42
1:9:257:ALA:HA	1:9:260:ARG:HG2	2.02	0.42
1:B:257:ALA:HA	1:B:260:ARG:HG2	2.02	0.42
1:C:257:ALA:HA	1:C:260:ARG:HG2	2.02	0.42
1:K:281:LEU:HD23	1:K:281:LEU:HA	1.91	0.42
1:K:325:ASP:HB3	1:K:368:ARG:HB2	2.01	0.42
1:T:325:ASP:HB3	1:T:368:ARG:HB2	2.02	0.42
1:X:325:ASP:HB3	1:X:368:ARG:HB2	2.01	0.42
1:4:325:ASP:HB3	1:4:368:ARG:HB2	2.01	0.42
1:5:325:ASP:HB3	1:5:368:ARG:HB2	2.01	0.42
1:6:257:ALA:HA	1:6:260:ARG:HG2	2.02	0.42
1:8:257:ALA:HA	1:8:260:ARG:HG2	2.02	0.42
1:D:265:LEU:HD11	1:E:259:ARG:HG2	2.02	0.42
1:G:325:ASP:HB3	1:G:368:ARG:HB2	2.02	0.42
1:H:257:ALA:HA	1:H:260:ARG:HG2	2.02	0.42
1:H:325:ASP:HB3	1:H:368:ARG:HB2	2.01	0.42
1:L:325:ASP:HB3	1:L:368:ARG:HB2	2.01	0.42
1:O:432:GLY:O	1:P:395:THR:OG1	2.35	0.42
1:7:325:ASP:HB3	1:7:368:ARG:HB2	2.01	0.42
1:C:265:LEU:HD11	1:D:259:ARG:HG2	2.02	0.42
1:D:257:ALA:HA	1:D:260:ARG:HG2	2.02	0.42
1:E:325:ASP:HB3	1:E:368:ARG:HB2	2.01	0.42
1:F:257:ALA:HA	1:F:260:ARG:HG2	2.02	0.42
1:F:281:LEU:HD23	1:F:281:LEU:HA	1.91	0.42
1:V:325:ASP:HB3	1:V:368:ARG:HB2	2.02	0.42
1:Z:325:ASP:HB3	1:Z:368:ARG:HB2	2.02	0.42
1:3:325:ASP:HB3	1:3:368:ARG:HB2	2.02	0.42
1:7:257:ALA:HA	1:7:260:ARG:HG2	2.02	0.42
1:A:257:ALA:HA	1:A:260:ARG:HG2	2.02	0.42
1:G:257:ALA:HA	1:G:260:ARG:HG2	2.02	0.42
1:I:257:ALA:HA	1:I:260:ARG:HG2	2.02	0.42
1:J:254:PRO:HB2	1:J:255:ALA:H	1.67	0.42
1:J:325:ASP:HB3	1:J:368:ARG:HB2	2.01	0.42
1:O:325:ASP:HB3	1:O:368:ARG:HB2	2.01	0.42
1:T:281:LEU:HD23	1:T:281:LEU:HA	1.91	0.42
1:Z:314:THR:O	1:Z:314:THR:OG1	2.33	0.42
1:5:257:ALA:HA	1:5:260:ARG:HG2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:257:ALA:HA	1:J:260:ARG:HG2	2.02	0.42
1:K:257:ALA:HA	1:K:260:ARG:HG2	2.02	0.42
1:6:314:THR:O	1:6:314:THR:OG1	2.33	0.42
1:I:254:PRO:HB2	1:I:255:ALA:H	1.67	0.42
1:D:314:THR:O	1:D:314:THR:OG1	2.33	0.42
1:R:254:PRO:HB2	1:R:255:ALA:H	1.67	0.42
1:T:265:LEU:HD11	1:U:259:ARG:HG2	2.02	0.42
1:U:254:PRO:HB2	1:U:255:ALA:H	1.66	0.42
1:2:257:ALA:HA	1:2:260:ARG:HG2	2.02	0.41
1:3:257:ALA:HA	1:3:260:ARG:HG2	2.02	0.41
1:4:257:ALA:HA	1:4:260:ARG:HG2	2.02	0.41
1:L:257:ALA:HA	1:L:260:ARG:HG2	2.02	0.41
1:N:257:ALA:HA	1:N:260:ARG:HG2	2.02	0.41
1:9:269:GLN:HE21	1:A:263:GLN:HE21	1.67	0.41
1:A:281:LEU:HD23	1:A:281:LEU:HA	1.91	0.41
1:M:257:ALA:HA	1:M:260:ARG:HG2	2.02	0.41
1:N:281:LEU:HD23	1:N:281:LEU:HA	1.91	0.41
1:Y:316:ALA:HB1	1:Z:377:LEU:HD13	2.01	0.41
1:Z:257:ALA:HA	1:Z:260:ARG:HG2	2.02	0.41
1:7:281:LEU:HD23	1:7:281:LEU:HA	1.91	0.41
1:P:314:THR:O	1:P:314:THR:OG1	2.33	0.41
1:5:432:GLY:HA3	1:6:397:SER:HB3	2.01	0.41
1:M:316:ALA:HB1	1:N:377:LEU:HD13	2.03	0.41
1:O:254:PRO:HB2	1:O:255:ALA:H	1.66	0.41
1:Q:281:LEU:HD23	1:Q:281:LEU:HA	1.91	0.41
1:1:257:ALA:HA	1:1:260:ARG:HG2	2.02	0.41
1:4:281:LEU:HD23	1:4:281:LEU:HA	1.91	0.41
1:K:254:PRO:HB2	1:K:255:ALA:H	1.67	0.41
1:O:257:ALA:HA	1:O:260:ARG:HG2	2.02	0.41
1:P:257:ALA:HA	1:P:260:ARG:HG2	2.02	0.41
1:X:254:PRO:HB2	1:X:255:ALA:H	1.67	0.41
1:Y:257:ALA:HA	1:Y:260:ARG:HG2	2.02	0.41
1:Y:437:ASP:OD2	1:Y:437:ASP:C	2.64	0.41
1:Z:254:PRO:HB2	1:Z:255:ALA:H	1.67	0.41
1:Z:437:ASP:OD2	1:Z:437:ASP:C	2.64	0.41
1:J:432:GLY:HA3	1:K:397:SER:HB3	2.03	0.41
1:Q:257:ALA:HA	1:Q:260:ARG:HG2	2.02	0.41
1:V:257:ALA:HA	1:V:260:ARG:HG2	2.02	0.41
1:W:257:ALA:HA	1:W:260:ARG:HG2	2.02	0.41
1:X:437:ASP:OD2	1:X:437:ASP:C	2.64	0.41
1:1:437:ASP:OD2	1:1:437:ASP:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:6:432:GLY:O	1:7:395:THR:OG1	2.35	0.41
1:T:257:ALA:HA	1:T:260:ARG:HG2	2.02	0.41
1:W:437:ASP:OD2	1:W:437:ASP:C	2.64	0.41
1:2:437:ASP:OD2	1:2:437:ASP:C	2.64	0.41
1:H:265:LEU:HD11	1:I:259:ARG:HG2	2.03	0.41
1:J:432:GLY:O	1:K:395:THR:OG1	2.36	0.41
1:M:432:GLY:HA3	1:N:397:SER:HB3	2.03	0.41
1:P:437:ASP:OD2	1:P:437:ASP:C	2.64	0.41
1:Q:437:ASP:OD2	1:Q:437:ASP:C	2.64	0.41
1:R:257:ALA:HA	1:R:260:ARG:HG2	2.02	0.41
1:S:257:ALA:HA	1:S:260:ARG:HG2	2.02	0.41
1:U:257:ALA:HA	1:U:260:ARG:HG2	2.02	0.41
1:X:257:ALA:HA	1:X:260:ARG:HG2	2.02	0.41
1:C:269:GLN:HE21	1:D:263:GLN:HE21	1.69	0.41
1:O:437:ASP:OD2	1:O:437:ASP:C	2.64	0.41
1:R:437:ASP:OD2	1:R:437:ASP:C	2.64	0.41
1:S:437:ASP:OD2	1:S:437:ASP:C	2.64	0.41
1:V:437:ASP:OD2	1:V:437:ASP:C	2.64	0.41
1:Y:265:LEU:HD11	1:Z:259:ARG:HG2	2.02	0.41
1:5:314:THR:O	1:5:314:THR:OG1	2.33	0.40
1:F:453:GLU:N	1:F:453:GLU:OE1	2.55	0.40
1:G:453:GLU:N	1:G:453:GLU:OE1	2.55	0.40
1:H:254:PRO:HB2	1:H:255:ALA:H	1.66	0.40
1:T:437:ASP:OD2	1:T:437:ASP:C	2.64	0.40
1:W:269:GLN:HE21	1:X:263:GLN:HE21	1.63	0.40
1:B:453:GLU:N	1:B:453:GLU:OE1	2.55	0.40
1:C:453:GLU:N	1:C:453:GLU:OE1	2.55	0.40
1:D:453:GLU:N	1:D:453:GLU:OE1	2.55	0.40
1:E:453:GLU:N	1:E:453:GLU:OE1	2.55	0.40
1:H:453:GLU:N	1:H:453:GLU:OE1	2.55	0.40
1:I:453:GLU:N	1:I:453:GLU:OE1	2.55	0.40
1:J:453:GLU:N	1:J:453:GLU:OE1	2.55	0.40
1:1:254:PRO:HB2	1:1:255:ALA:H	1.67	0.40
1:2:263:GLN:O	1:2:267:ARG:HG3	2.22	0.40
1:3:437:ASP:OD2	1:3:437:ASP:C	2.64	0.40
1:7:437:ASP:OD2	1:7:437:ASP:C	2.64	0.40
1:9:453:GLU:N	1:9:453:GLU:OE1	2.55	0.40
1:A:453:GLU:N	1:A:453:GLU:OE1	2.55	0.40
1:L:314:THR:O	1:L:314:THR:OG1	2.33	0.40
1:Q:263:GLN:O	1:Q:267:ARG:HG3	2.22	0.40
1:1:263:GLN:O	1:1:267:ARG:HG3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:263:GLN:O	1:3:267:ARG:HG3	2.22	0.40
1:8:453:GLU:N	1:8:453:GLU:OE1	2.55	0.40
1:A:430:LEU:HA	1:A:430:LEU:HD23	1.86	0.40
1:B:437:ASP:OD2	1:B:437:ASP:C	2.64	0.40
1:C:314:THR:O	1:C:314:THR:OG1	2.33	0.40
1:C:437:ASP:OD2	1:C:437:ASP:C	2.64	0.40
1:D:281:LEU:HD23	1:D:281:LEU:HA	1.91	0.40
1:D:437:ASP:OD2	1:D:437:ASP:C	2.64	0.40
1:K:453:GLU:N	1:K:453:GLU:OE1	2.55	0.40
1:L:453:GLU:N	1:L:453:GLU:OE1	2.55	0.40
1:N:437:ASP:OD2	1:N:437:ASP:C	2.64	0.40
1:R:263:GLN:O	1:R:267:ARG:HG3	2.22	0.40
1:S:263:GLN:O	1:S:267:ARG:HG3	2.22	0.40
1:U:437:ASP:OD2	1:U:437:ASP:C	2.64	0.40
1:V:265:LEU:HD11	1:W:259:ARG:HG2	2.03	0.40
1:4:263:GLN:O	1:4:267:ARG:HG3	2.22	0.40
1:4:432:GLY:HA3	1:5:397:SER:HB3	2.04	0.40
1:6:437:ASP:OD2	1:6:437:ASP:C	2.64	0.40
1:7:453:GLU:N	1:7:453:GLU:OE1	2.55	0.40
1:8:437:ASP:OD2	1:8:437:ASP:C	2.64	0.40
1:9:437:ASP:OD2	1:9:437:ASP:C	2.64	0.40
1:E:437:ASP:OD2	1:E:437:ASP:C	2.64	0.40
1:I:281:LEU:HD23	1:I:281:LEU:HA	1.91	0.40
1:J:263:GLN:O	1:J:267:ARG:HG3	2.22	0.40
1:U:263:GLN:O	1:U:267:ARG:HG3	2.22	0.40
1:X:263:GLN:O	1:X:267:ARG:HG3	2.22	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	1	140/945 (15%)	139 (99%)	1 (1%)	0	100	100
1	2	140/945 (15%)	139 (99%)	1 (1%)	0	100	100
1	3	140/945 (15%)	139 (99%)	1 (1%)	0	100	100
1	4	140/945 (15%)	140 (100%)	0	0	100	100
1	5	140/945 (15%)	140 (100%)	0	0	100	100
1	6	140/945 (15%)	139 (99%)	1 (1%)	0	100	100
1	7	140/945 (15%)	140 (100%)	0	0	100	100
1	8	140/945 (15%)	140 (100%)	0	0	100	100
1	9	140/945 (15%)	140 (100%)	0	0	100	100
1	A	140/945 (15%)	139 (99%)	1 (1%)	0	100	100
1	B	140/945 (15%)	139 (99%)	1 (1%)	0	100	100
1	C	140/945 (15%)	139 (99%)	1 (1%)	0	100	100
1	D	140/945 (15%)	139 (99%)	1 (1%)	0	100	100
1	E	140/945 (15%)	140 (100%)	0	0	100	100
1	F	140/945 (15%)	140 (100%)	0	0	100	100
1	G	140/945 (15%)	139 (99%)	1 (1%)	0	100	100
1	H	140/945 (15%)	139 (99%)	1 (1%)	0	100	100
1	I	140/945 (15%)	139 (99%)	1 (1%)	0	100	100
1	J	140/945 (15%)	140 (100%)	0	0	100	100
1	K	140/945 (15%)	139 (99%)	1 (1%)	0	100	100
1	L	140/945 (15%)	139 (99%)	1 (1%)	0	100	100
1	M	140/945 (15%)	140 (100%)	0	0	100	100
1	N	140/945 (15%)	139 (99%)	1 (1%)	0	100	100
1	O	140/945 (15%)	139 (99%)	1 (1%)	0	100	100
1	P	140/945 (15%)	140 (100%)	0	0	100	100
1	Q	140/945 (15%)	140 (100%)	0	0	100	100
1	R	140/945 (15%)	139 (99%)	1 (1%)	0	100	100
1	S	140/945 (15%)	140 (100%)	0	0	100	100
1	T	140/945 (15%)	139 (99%)	1 (1%)	0	100	100
1	U	140/945 (15%)	139 (99%)	1 (1%)	0	100	100
1	V	140/945 (15%)	139 (99%)	1 (1%)	0	100	100
1	W	140/945 (15%)	139 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	X	140/945 (15%)	140 (100%)	0	0	100	100
1	Y	140/945 (15%)	139 (99%)	1 (1%)	0	100	100
1	Z	140/945 (15%)	139 (99%)	1 (1%)	0	100	100
All	All	4900/33075 (15%)	4878 (100%)	22 (0%)	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	1	127/802 (16%)	126 (99%)	1 (1%)	73	80
1	2	127/802 (16%)	126 (99%)	1 (1%)	73	80
1	3	127/802 (16%)	126 (99%)	1 (1%)	73	80
1	4	127/802 (16%)	126 (99%)	1 (1%)	73	80
1	5	127/802 (16%)	126 (99%)	1 (1%)	73	80
1	6	127/802 (16%)	126 (99%)	1 (1%)	73	80
1	7	127/802 (16%)	126 (99%)	1 (1%)	73	80
1	8	127/802 (16%)	126 (99%)	1 (1%)	73	80
1	9	127/802 (16%)	126 (99%)	1 (1%)	73	80
1	A	127/802 (16%)	126 (99%)	1 (1%)	73	80
1	B	127/802 (16%)	126 (99%)	1 (1%)	73	80
1	C	127/802 (16%)	126 (99%)	1 (1%)	73	80
1	D	127/802 (16%)	126 (99%)	1 (1%)	73	80
1	E	127/802 (16%)	126 (99%)	1 (1%)	73	80
1	F	127/802 (16%)	126 (99%)	1 (1%)	73	80
1	G	127/802 (16%)	126 (99%)	1 (1%)	73	80
1	H	127/802 (16%)	126 (99%)	1 (1%)	73	80
1	I	127/802 (16%)	126 (99%)	1 (1%)	73	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	127/802 (16%)	126 (99%)	1 (1%)	73	80
1	K	127/802 (16%)	126 (99%)	1 (1%)	73	80
1	L	127/802 (16%)	126 (99%)	1 (1%)	73	80
1	M	127/802 (16%)	126 (99%)	1 (1%)	73	80
1	N	127/802 (16%)	126 (99%)	1 (1%)	73	80
1	O	127/802 (16%)	126 (99%)	1 (1%)	73	80
1	P	127/802 (16%)	126 (99%)	1 (1%)	73	80
1	Q	127/802 (16%)	126 (99%)	1 (1%)	73	80
1	R	127/802 (16%)	126 (99%)	1 (1%)	73	80
1	S	127/802 (16%)	126 (99%)	1 (1%)	73	80
1	T	127/802 (16%)	126 (99%)	1 (1%)	73	80
1	U	127/802 (16%)	126 (99%)	1 (1%)	73	80
1	V	127/802 (16%)	126 (99%)	1 (1%)	73	80
1	W	127/802 (16%)	126 (99%)	1 (1%)	73	80
1	X	127/802 (16%)	126 (99%)	1 (1%)	73	80
1	Y	127/802 (16%)	126 (99%)	1 (1%)	73	80
1	Z	127/802 (16%)	126 (99%)	1 (1%)	73	80
All	All	4445/28070 (16%)	4410 (99%)	35 (1%)	70	80

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	393	ARG
1	2	393	ARG
1	3	393	ARG
1	4	393	ARG
1	5	393	ARG
1	6	393	ARG
1	7	393	ARG
1	8	393	ARG
1	9	393	ARG
1	A	393	ARG
1	B	393	ARG
1	C	393	ARG
1	D	393	ARG
1	E	393	ARG

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Mol	Chain	Res	Type
1	F	393	ARG
1	G	393	ARG
1	H	393	ARG
1	I	393	ARG
1	J	393	ARG
1	K	393	ARG
1	L	393	ARG
1	M	393	ARG
1	N	393	ARG
1	O	393	ARG
1	P	393	ARG
1	Q	393	ARG
1	R	393	ARG
1	S	393	ARG
1	T	393	ARG
1	U	393	ARG
1	V	393	ARG
1	W	393	ARG
1	X	393	ARG
1	Y	393	ARG
1	Z	393	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (140) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	263	GLN
1	1	327	ASN
1	1	383	HIS
1	1	394	GLN
1	2	263	GLN
1	2	327	ASN
1	2	383	HIS
1	2	394	GLN
1	3	263	GLN
1	3	327	ASN
1	3	383	HIS
1	3	394	GLN
1	4	263	GLN
1	4	327	ASN
1	4	383	HIS
1	4	394	GLN
1	5	263	GLN

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Mol	Chain	Res	Type
1	5	327	ASN
1	5	383	HIS
1	5	394	GLN
1	6	263	GLN
1	6	327	ASN
1	6	383	HIS
1	6	394	GLN
1	7	263	GLN
1	7	327	ASN
1	7	383	HIS
1	7	394	GLN
1	8	263	GLN
1	8	327	ASN
1	8	383	HIS
1	8	394	GLN
1	9	263	GLN
1	9	327	ASN
1	9	383	HIS
1	9	394	GLN
1	A	263	GLN
1	A	327	ASN
1	A	383	HIS
1	A	394	GLN
1	B	263	GLN
1	B	327	ASN
1	B	383	HIS
1	B	394	GLN
1	C	263	GLN
1	C	327	ASN
1	C	383	HIS
1	C	394	GLN
1	D	263	GLN
1	D	327	ASN
1	D	383	HIS
1	D	394	GLN
1	E	263	GLN
1	E	327	ASN
1	E	383	HIS
1	E	394	GLN
1	F	263	GLN
1	F	327	ASN
1	F	383	HIS

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Mol	Chain	Res	Type
1	F	394	GLN
1	G	263	GLN
1	G	327	ASN
1	G	383	HIS
1	G	394	GLN
1	H	263	GLN
1	H	327	ASN
1	H	383	HIS
1	H	394	GLN
1	I	263	GLN
1	I	327	ASN
1	I	383	HIS
1	I	394	GLN
1	J	263	GLN
1	J	327	ASN
1	J	383	HIS
1	J	394	GLN
1	K	263	GLN
1	K	327	ASN
1	K	383	HIS
1	K	394	GLN
1	L	263	GLN
1	L	327	ASN
1	L	383	HIS
1	L	394	GLN
1	M	263	GLN
1	M	327	ASN
1	M	383	HIS
1	M	394	GLN
1	N	263	GLN
1	N	327	ASN
1	N	383	HIS
1	N	394	GLN
1	O	263	GLN
1	O	327	ASN
1	O	383	HIS
1	O	394	GLN
1	P	263	GLN
1	P	327	ASN
1	P	383	HIS
1	P	394	GLN
1	Q	263	GLN

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Mol	Chain	Res	Type
1	Q	327	ASN
1	Q	383	HIS
1	Q	394	GLN
1	R	263	GLN
1	R	327	ASN
1	R	383	HIS
1	R	394	GLN
1	S	263	GLN
1	S	327	ASN
1	S	383	HIS
1	S	394	GLN
1	T	263	GLN
1	T	327	ASN
1	T	383	HIS
1	T	394	GLN
1	U	263	GLN
1	U	327	ASN
1	U	383	HIS
1	U	394	GLN
1	V	263	GLN
1	V	327	ASN
1	V	383	HIS
1	V	394	GLN
1	W	263	GLN
1	W	327	ASN
1	W	383	HIS
1	W	394	GLN
1	X	263	GLN
1	X	327	ASN
1	X	383	HIS
1	X	394	GLN
1	Y	263	GLN
1	Y	327	ASN
1	Y	383	HIS
1	Y	394	GLN
1	Z	263	GLN
1	Z	327	ASN
1	Z	383	HIS
1	Z	394	GLN

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

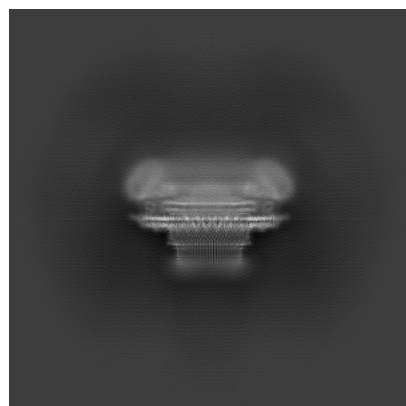
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39763. These allow visual inspection of the internal detail of the map and identification of artifacts.

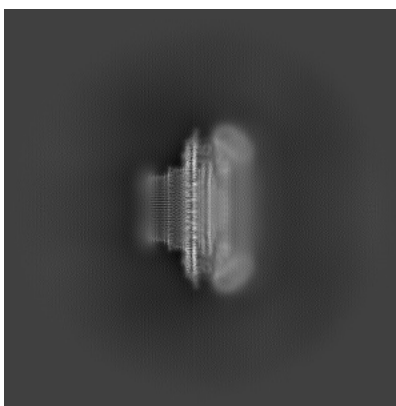
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

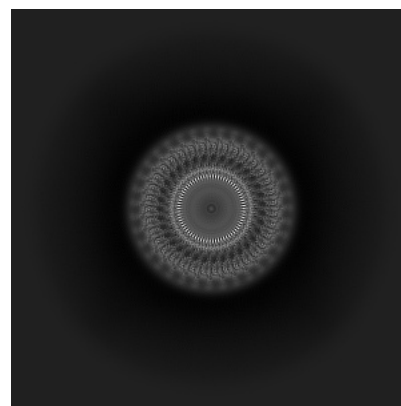
6.1.1 Primary map



X

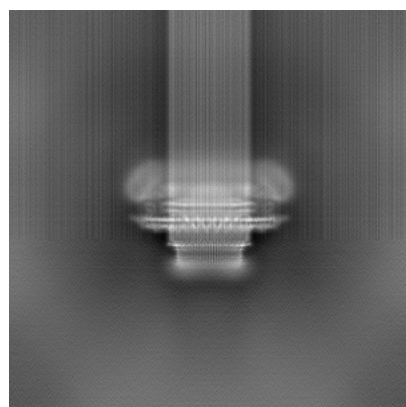


Y

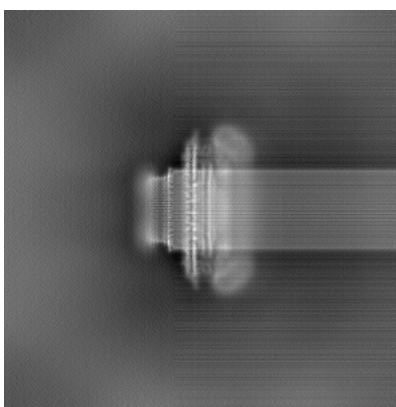


Z

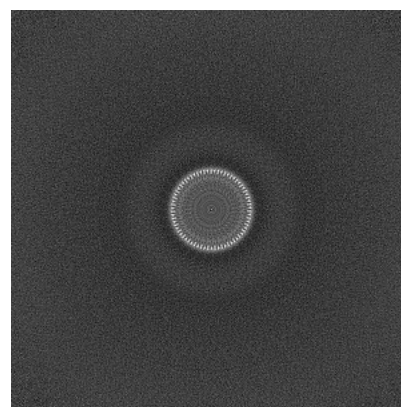
6.1.2 Raw map



X



Y

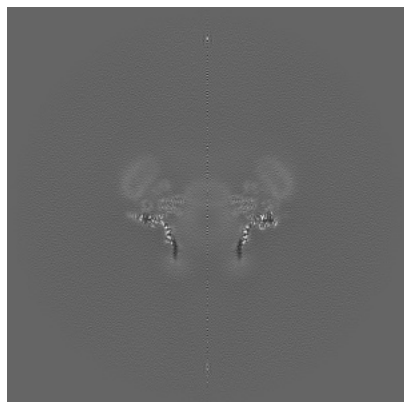


Z

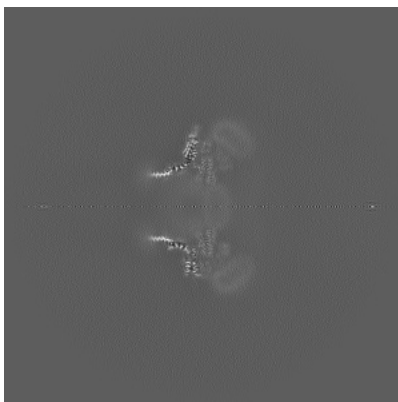
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

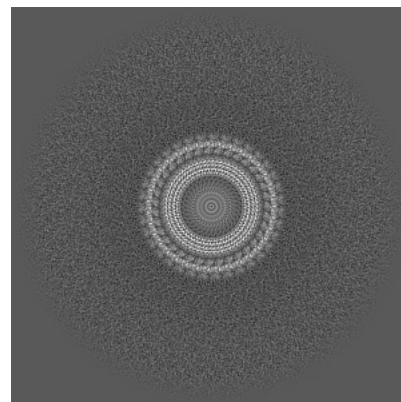
6.2.1 Primary map



X Index: 300

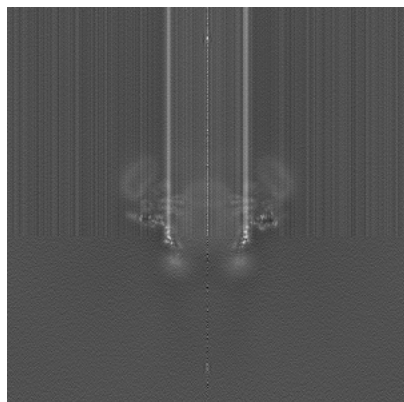


Y Index: 300

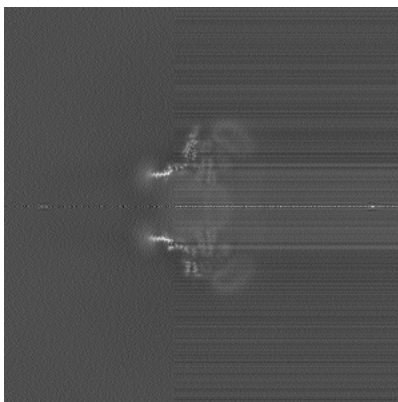


Z Index: 300

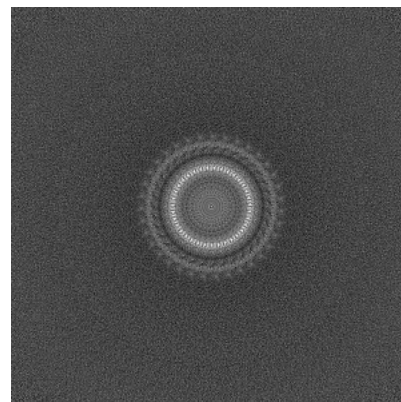
6.2.2 Raw map



X Index: 300



Y Index: 300



Z Index: 300

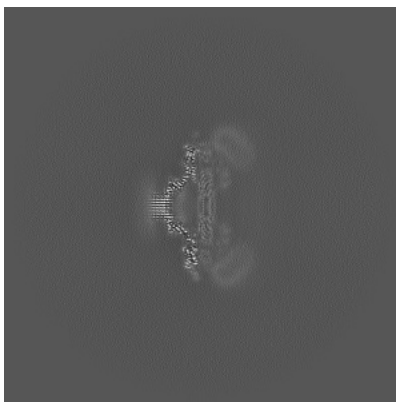
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

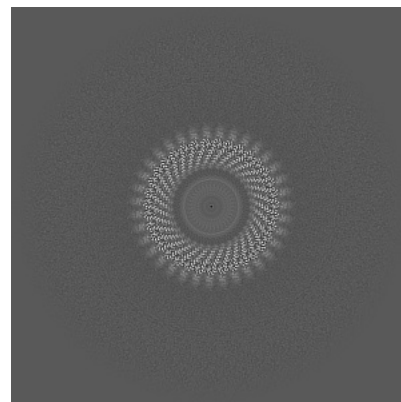
6.3.1 Primary map



X Index: 349

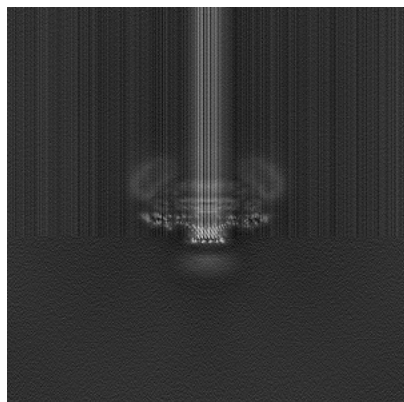


Y Index: 348

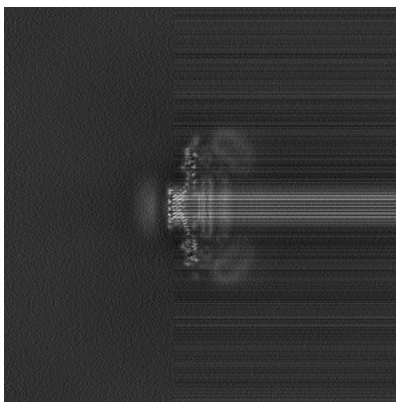


Z Index: 285

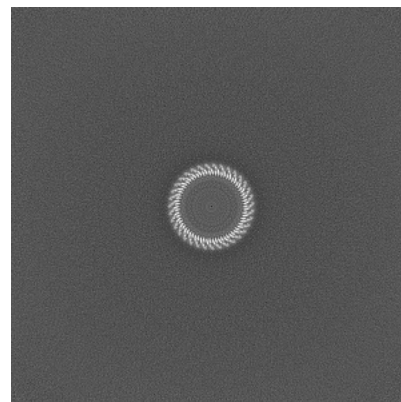
6.3.2 Raw map



X Index: 242



Y Index: 243

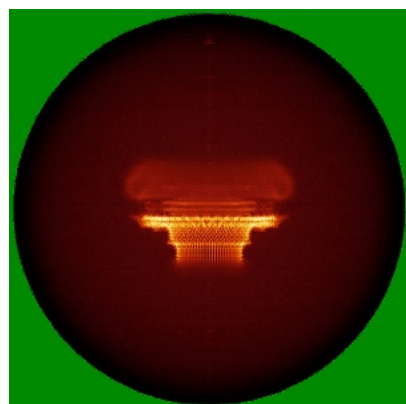


Z Index: 247

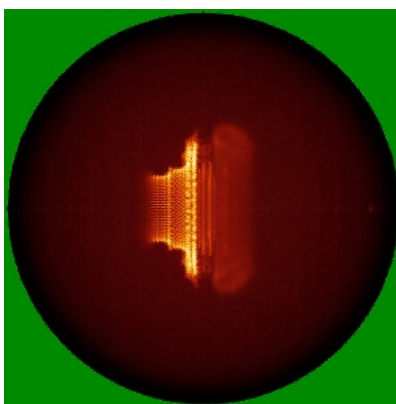
The images above show the largest variance slices of the map in three orthogonal directions.

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

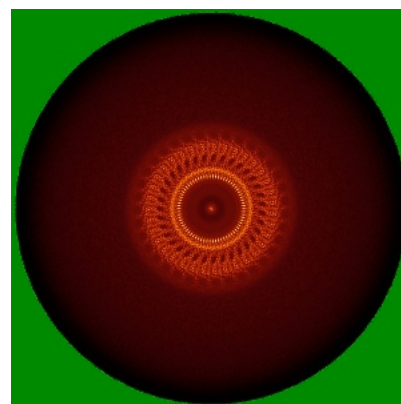
6.4.1 Primary map



X

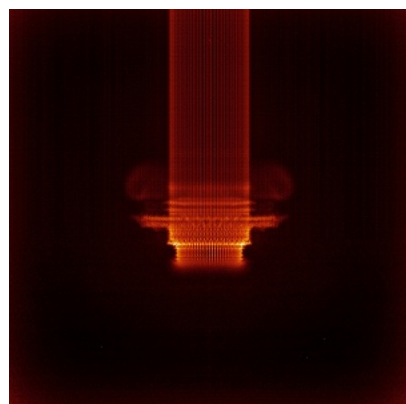


Y

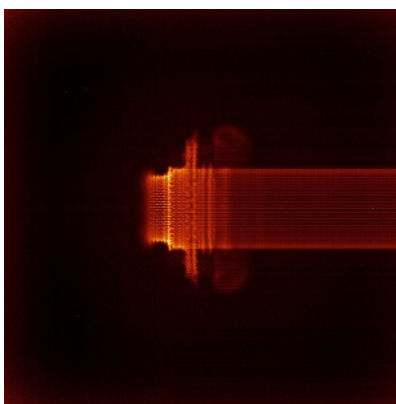


Z

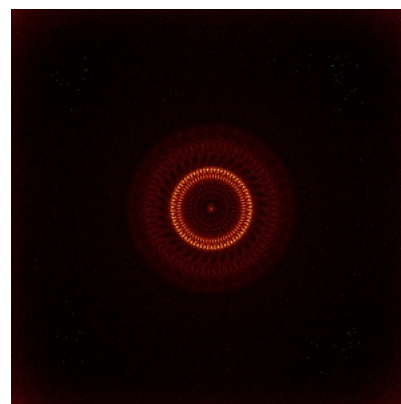
6.4.2 Raw map



X



Y

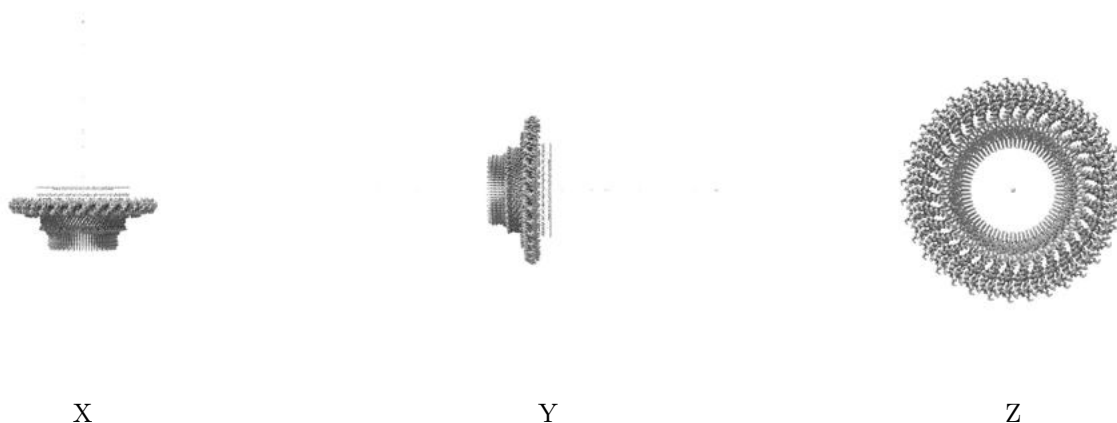


Z

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

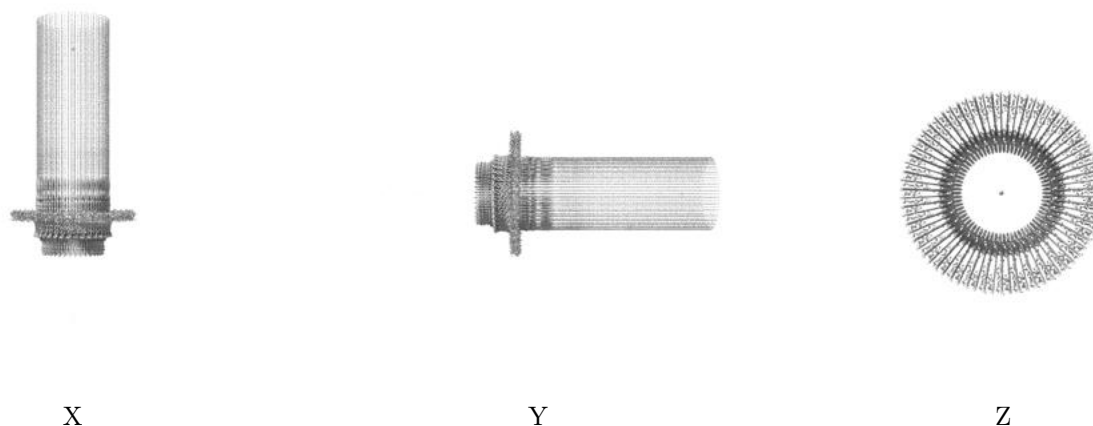
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.45. 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.

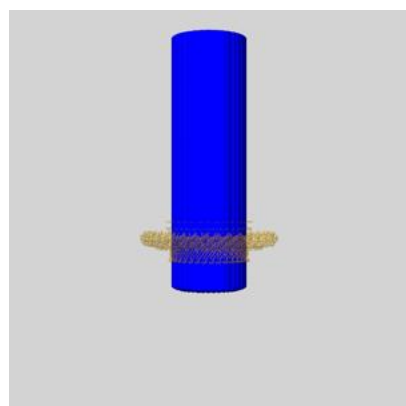
6.6 Mask visualisation [i](#)

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

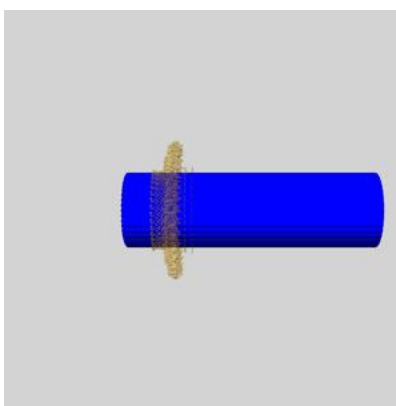
A mask typically either:

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

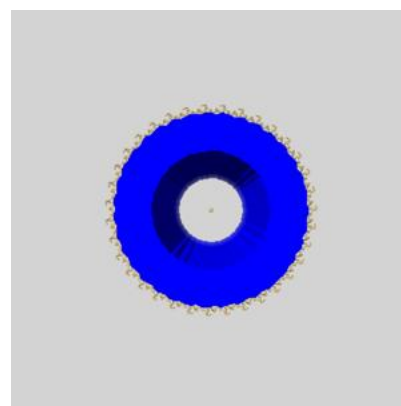
6.6.1 emd_39763_msk_1.map [i](#)



X



Y

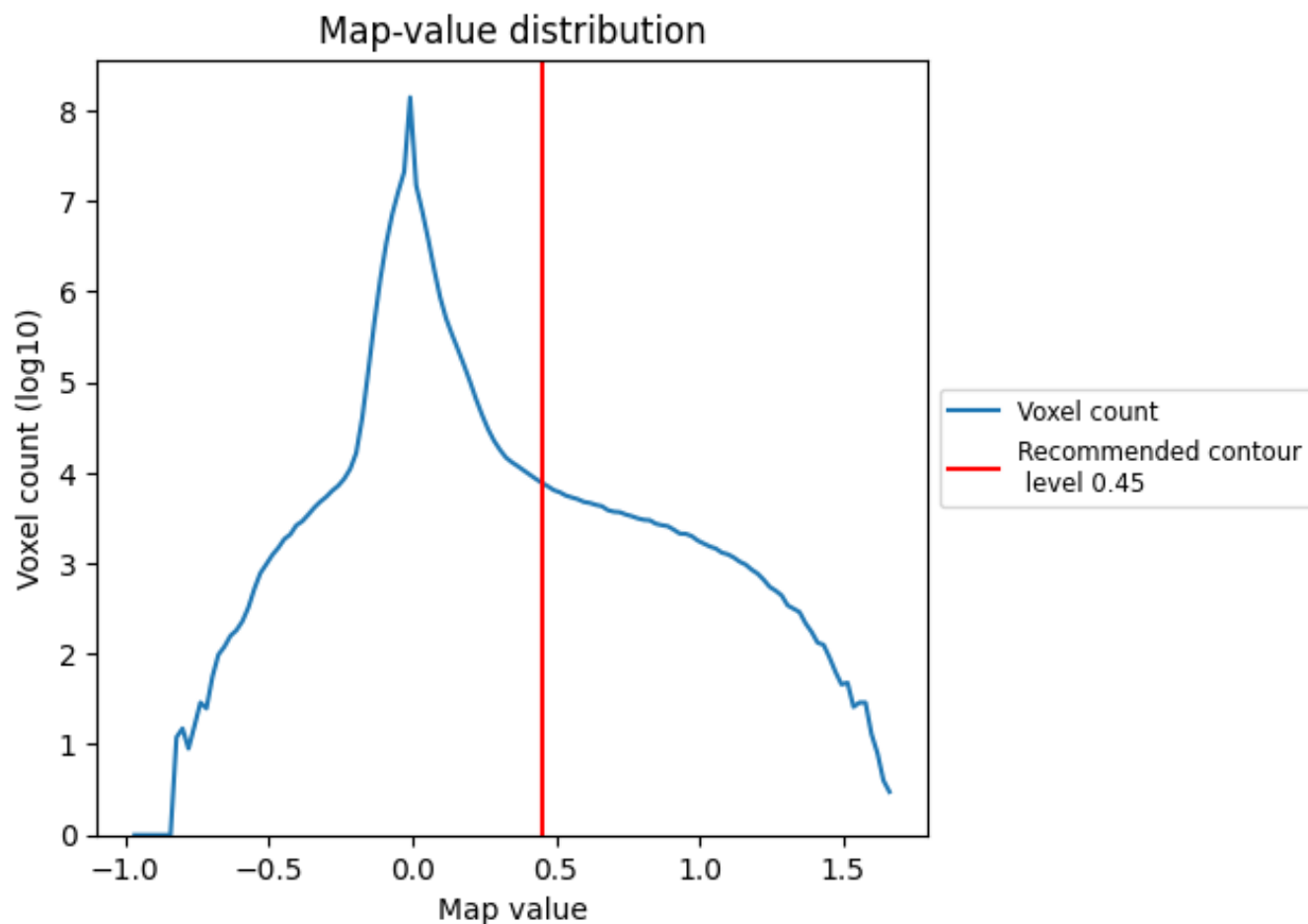


Z

7 Map analysis [i](#)

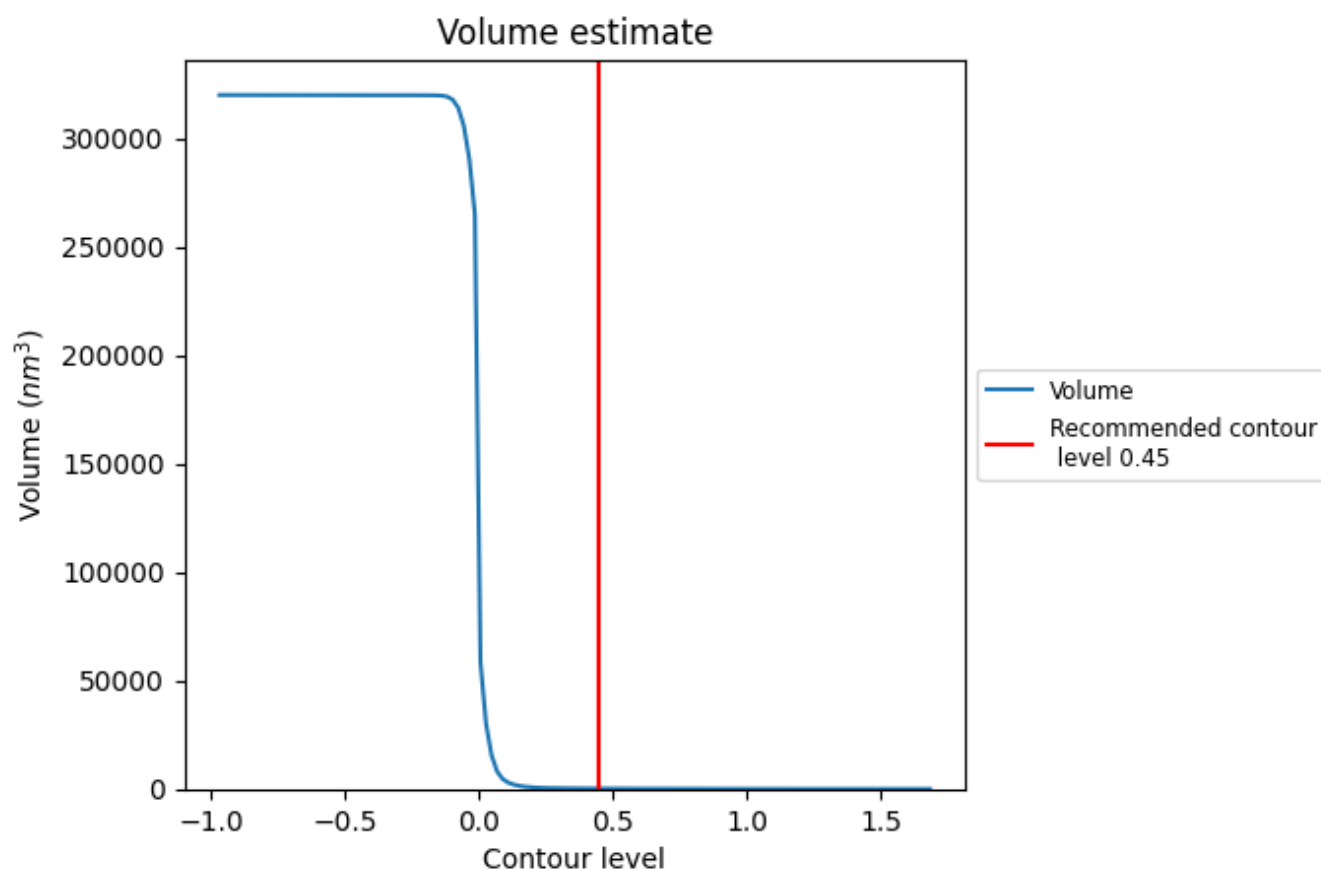
This section contains the results of statistical analysis of the map.

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.

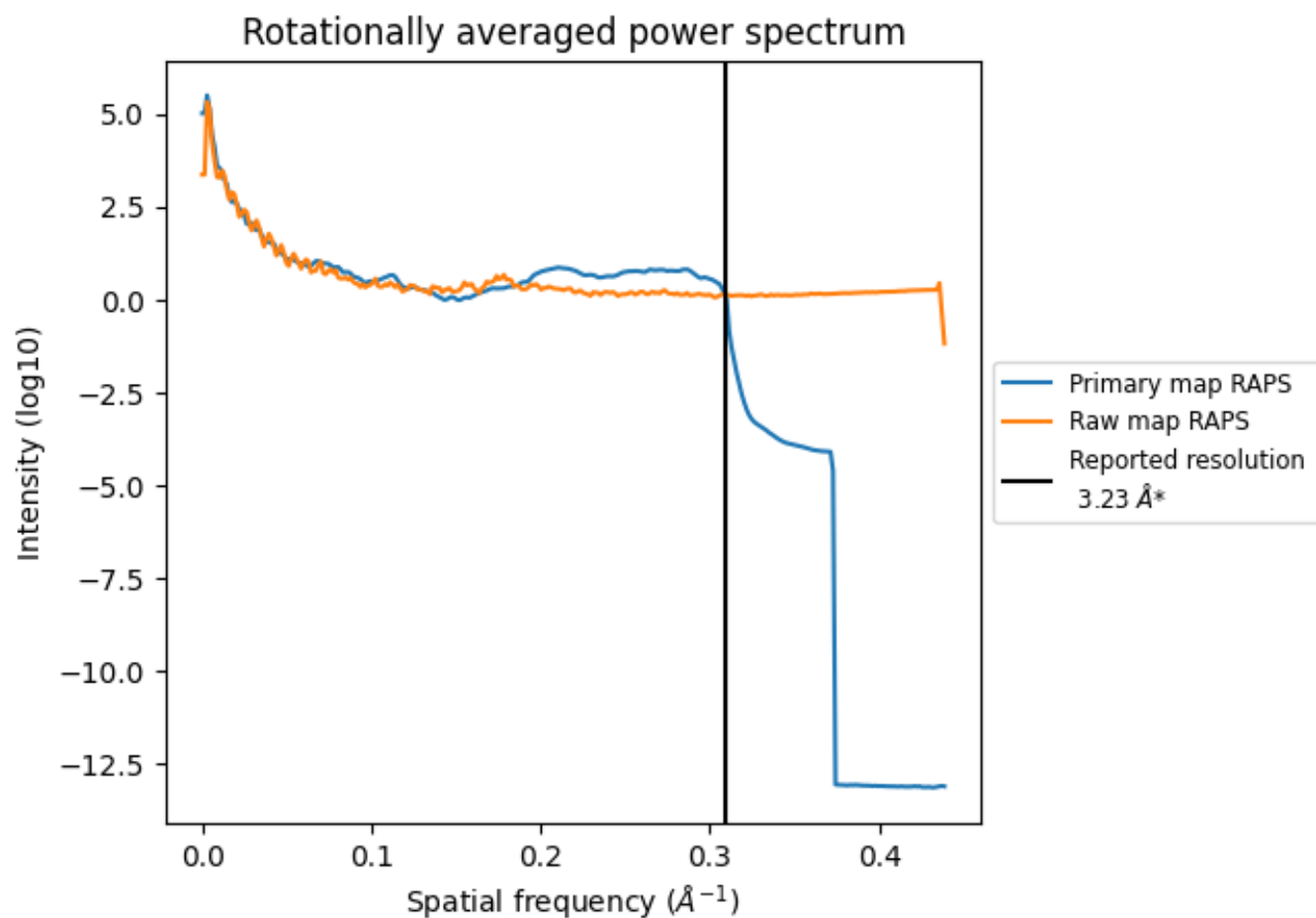
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 183 nm^3 ; this corresponds to an approximate mass of 165 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 ⓘ

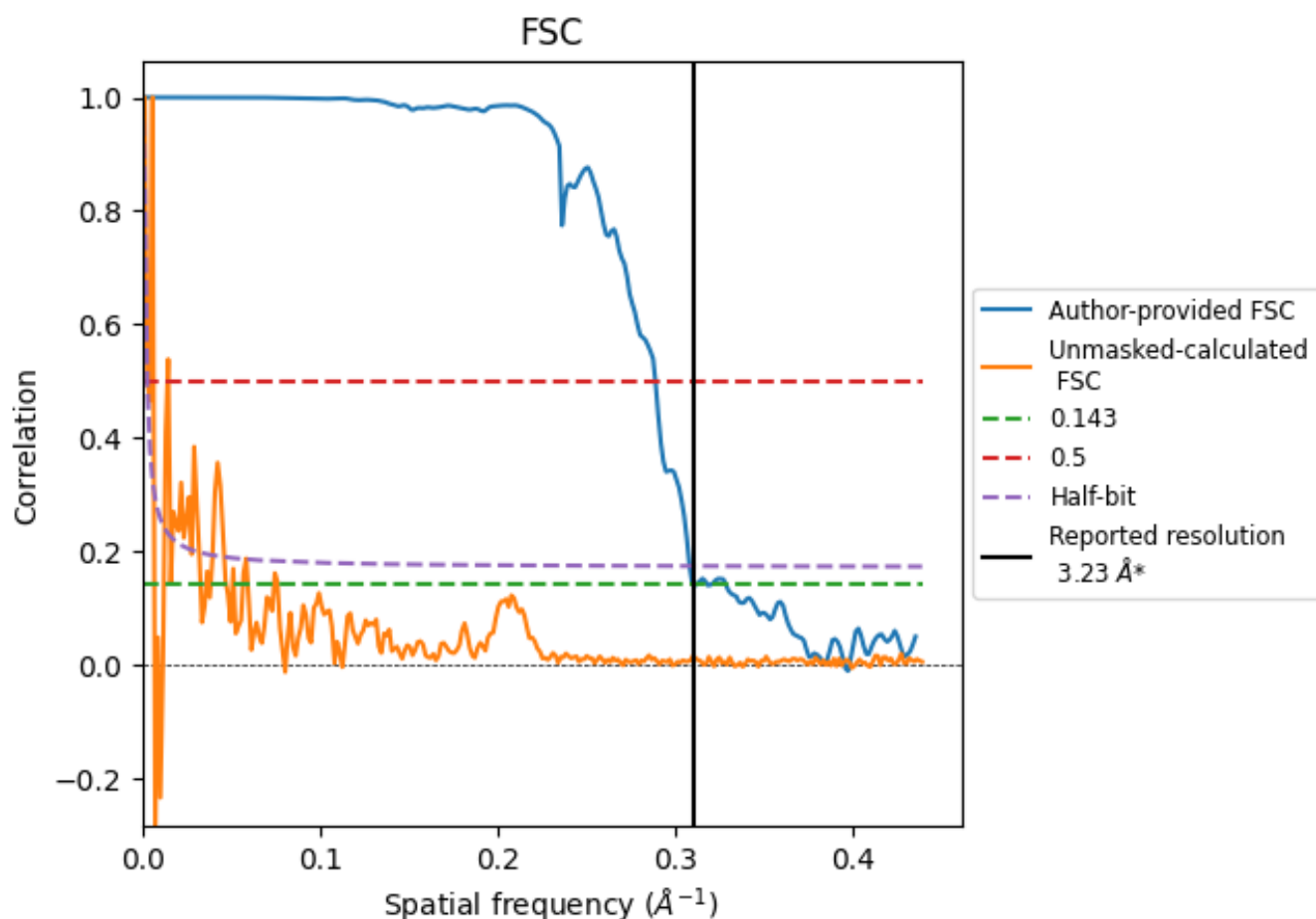


*Reported resolution corresponds to spatial frequency of 0.310 Å⁻¹

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 $0.310 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

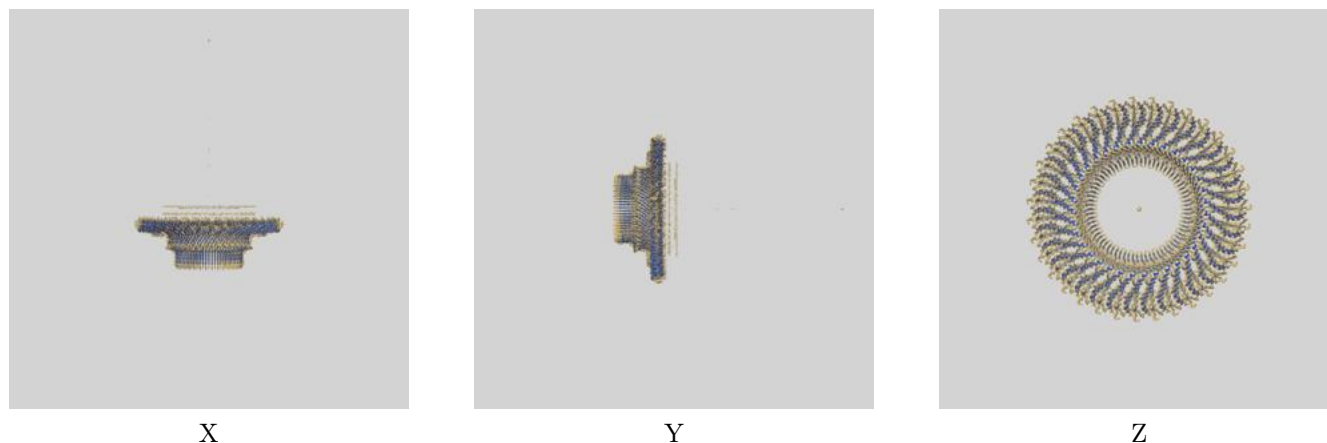
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.23	-	-
Author-provided FSC curve	3.23	3.46	3.25
Unmasked-calculated*	147.06	344.83	151.52

*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 147.06 differs from the reported value 3.23 by more than 10 %

9 Map-model fit [i](#)

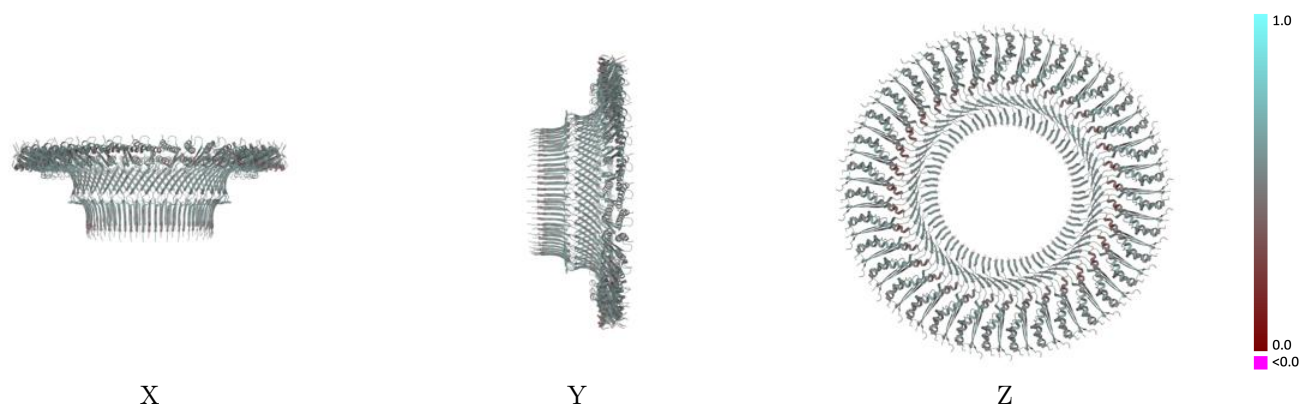
This section contains information regarding the fit between EMDB map EMD-39763 and PDB model 8Z4G. Per-residue inclusion information can be found in section [3](#) on page [22](#).

9.1 Map-model overlay [i](#)



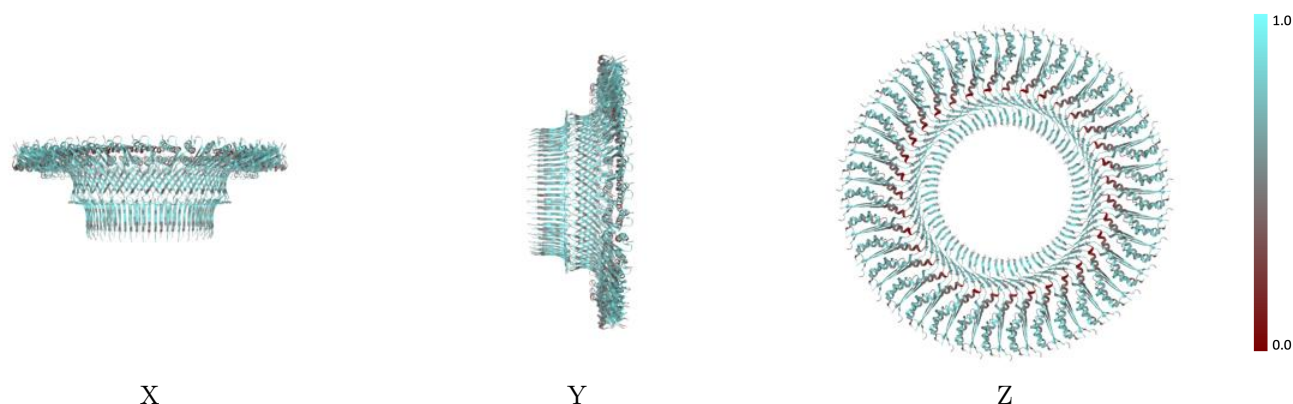
The images above show the 3D surface view of the map at the recommended contour level 0.45 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



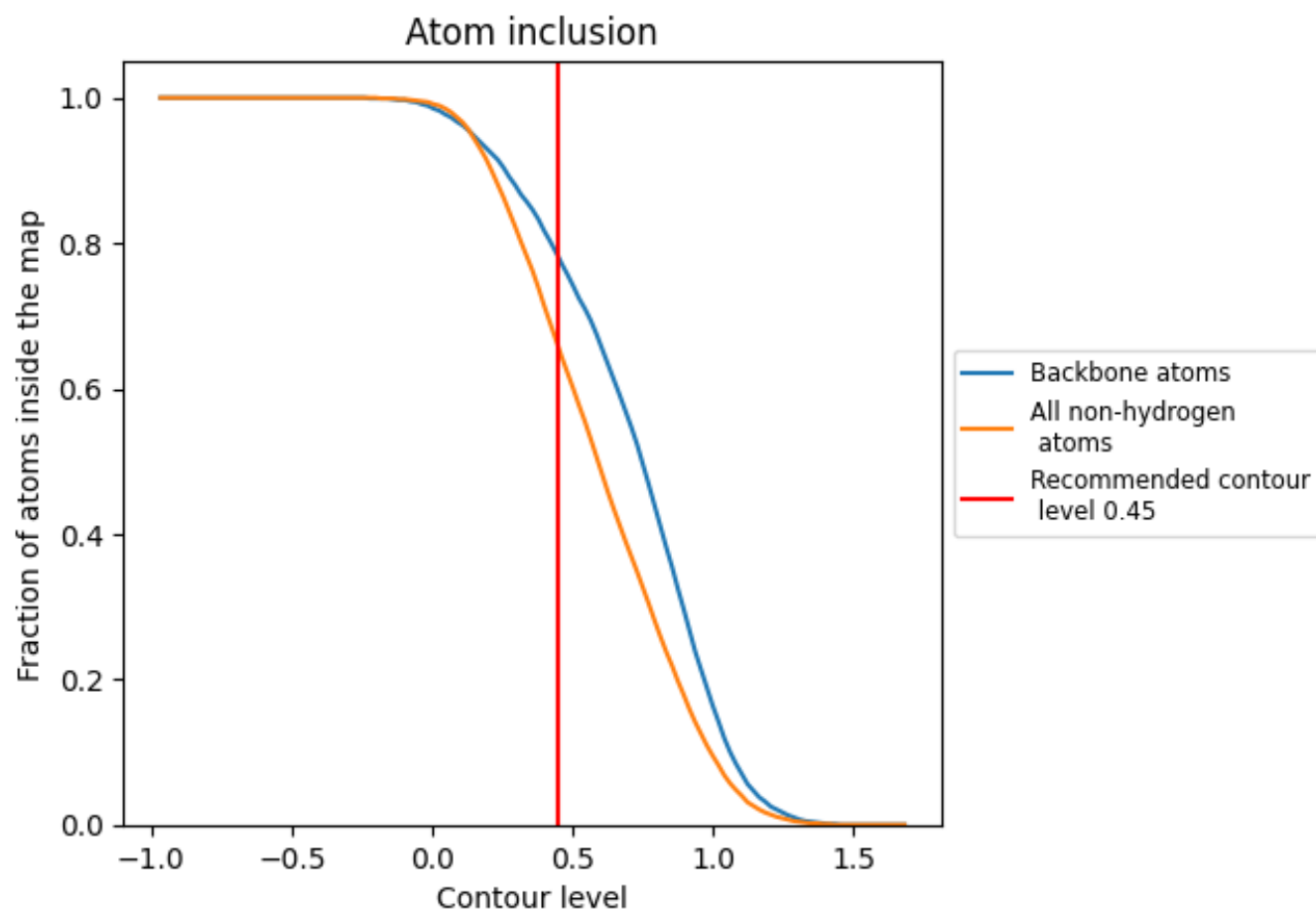
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.45).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 66% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.45) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6570	 0.5180
1	 0.6580	 0.5320
2	 0.6520	 0.5130
3	 0.6470	 0.5120
4	 0.6510	 0.5130
5	 0.6500	 0.5190
6	 0.6540	 0.5120
7	 0.6530	 0.5120
8	 0.6510	 0.5140
9	 0.6620	 0.5170
A	 0.6670	 0.5240
B	 0.6680	 0.5220
C	 0.6660	 0.5280
D	 0.6650	 0.5290
E	 0.6550	 0.5260
F	 0.6620	 0.5260
G	 0.6640	 0.5220
H	 0.6540	 0.5260
I	 0.6510	 0.5160
J	 0.6470	 0.5140
K	 0.6490	 0.5190
L	 0.6490	 0.5150
M	 0.6550	 0.5130
N	 0.6550	 0.5140
O	 0.6480	 0.5110
P	 0.6560	 0.5110
Q	 0.6620	 0.5100
R	 0.6610	 0.5110
S	 0.6610	 0.5140
T	 0.6560	 0.5180
U	 0.6700	 0.5190
V	 0.6650	 0.5200
W	 0.6660	 0.5180
X	 0.6560	 0.5170
Y	 0.6580	 0.5190
Z	 0.6540	 0.5170

