



Full wwPDB EM Validation Report ⓘ

Mar 23, 2026 – 05:55 PM UTC

PDB ID : 7D84 / pdb_00007d84
EMDB ID : EMD-30612
Title : 34-fold symmetry Salmonella S ring formed by full-length FliF
Authors : Kawamoto, A.; Miyata, T.; Makino, F.; Kinoshita, M.; Minamino, T.; Imada, K.; Kato, T.; Namba, K.
Deposited on : 2020-10-07
Resolution : 3.70 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:

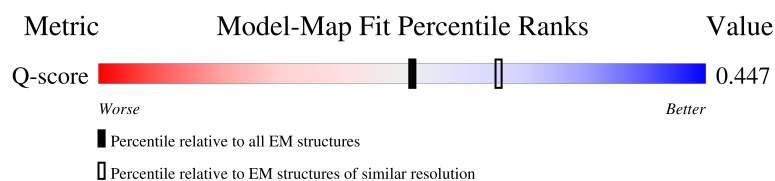
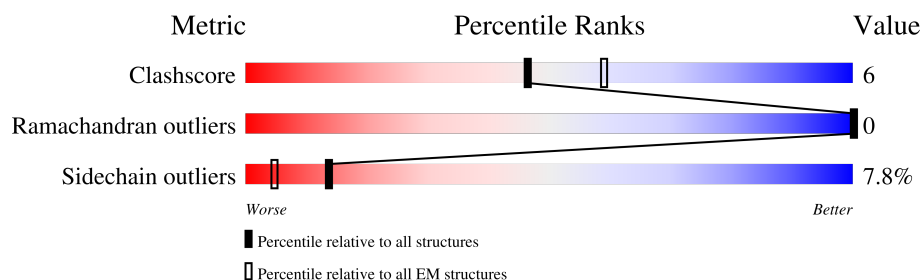
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.70 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.



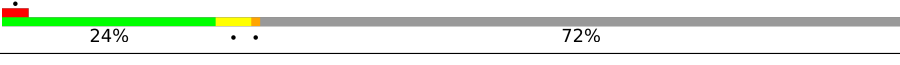
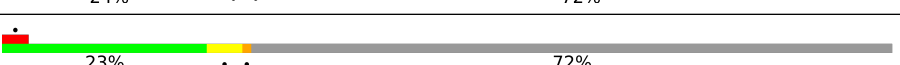
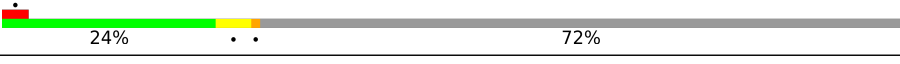
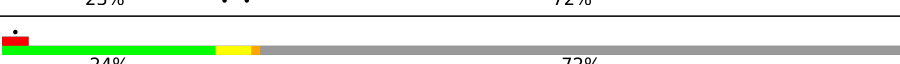
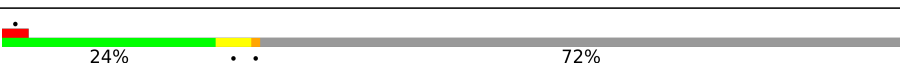
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11569 (3.20 - 4.20)

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

Mol	Chain	Length	Quality of chain
1	A	560	
1	B	560	
1	C	560	
1	D	560	

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Mol	Chain	Length	Quality of chain
1	E	560	 23% 72%
1	F	560	 24% 72%
1	G	560	 23% 72%
1	H	560	 23% 72%
1	I	560	 24% 72%
1	J	560	 23% 72%
1	K	560	 24% 72%
1	L	560	 23% 72%
1	M	560	 23% 72%
1	N	560	 23% 72%
1	O	560	 24% 72%
1	P	560	 24% 72%
1	Q	560	 24% 72%
1	R	560	 23% 72%
1	S	560	 23% 72%
1	T	560	 23% 72%
1	U	560	 24% 72%
1	V	560	 24% 72%
1	W	560	 24% 72%
1	X	560	 24% 72%
1	Y	560	 23% 72%
1	Z	560	 24% 72%
1	a	560	 24% 72%
1	b	560	 23% 72%
1	c	560	 24% 72%

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Mol	Chain	Length	Quality of chain
1	d	560	 23% 72%
1	e	560	 23% 72%
1	f	560	 23% 72%
1	g	560	 23% 72%
1	h	560	 24% 72%

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 42704 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.

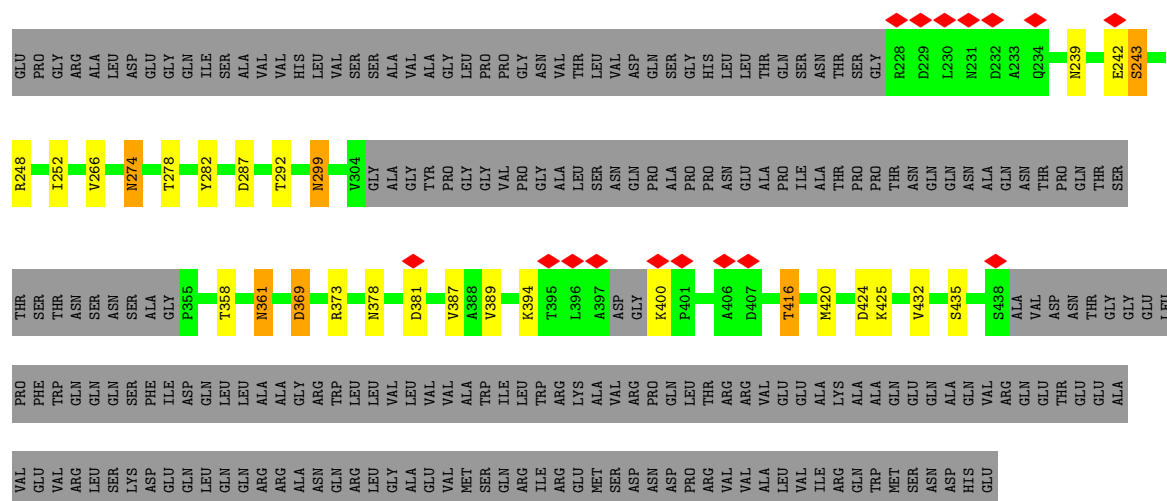
- Molecule 1 is a protein called Flagellar M-ring protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	159	Total	C	N	O	S	0	0
			1256	766	235	252	3		
1	B	159	Total	C	N	O	S	0	0
			1256	766	235	252	3		
1	C	159	Total	C	N	O	S	0	0
			1256	766	235	252	3		
1	D	159	Total	C	N	O	S	0	0
			1256	766	235	252	3		
1	E	159	Total	C	N	O	S	0	0
			1256	766	235	252	3		
1	F	159	Total	C	N	O	S	0	0
			1256	766	235	252	3		
1	G	159	Total	C	N	O	S	0	0
			1256	766	235	252	3		
1	H	159	Total	C	N	O	S	0	0
			1256	766	235	252	3		
1	I	159	Total	C	N	O	S	0	0
			1256	766	235	252	3		
1	J	159	Total	C	N	O	S	0	0
			1256	766	235	252	3		
1	K	159	Total	C	N	O	S	0	0
			1256	766	235	252	3		
1	L	159	Total	C	N	O	S	0	0
			1256	766	235	252	3		
1	M	159	Total	C	N	O	S	0	0
			1256	766	235	252	3		
1	N	159	Total	C	N	O	S	0	0
			1256	766	235	252	3		
1	O	159	Total	C	N	O	S	0	0
			1256	766	235	252	3		
1	P	159	Total	C	N	O	S	0	0
			1256	766	235	252	3		
1	Q	159	Total	C	N	O	S	0	0
			1256	766	235	252	3		

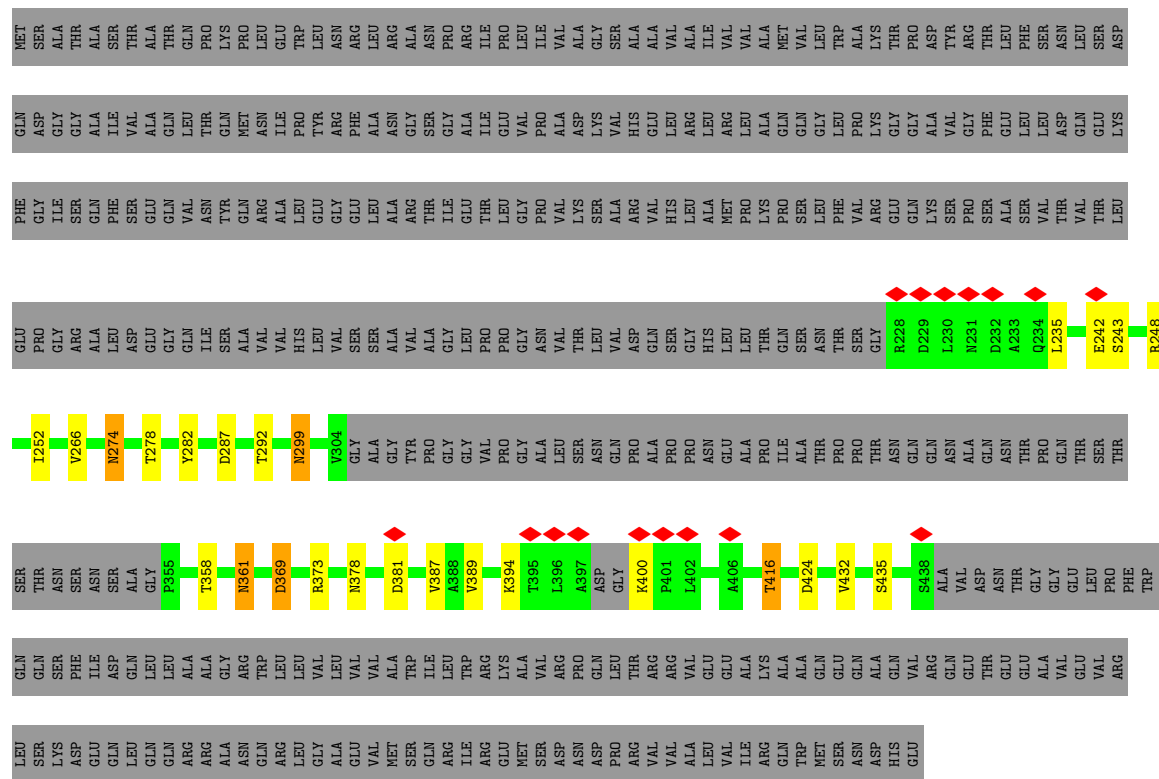
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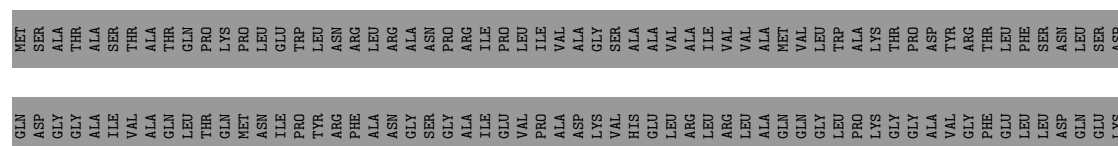
Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	159	Total	C	N	O	S	0	0
			1256	766	235	252	3		
1	S	159	Total	C	N	O	S	0	0
			1256	766	235	252	3		
1	T	159	Total	C	N	O	S	0	0
			1256	766	235	252	3		
1	U	159	Total	C	N	O	S	0	0
			1256	766	235	252	3		
1	V	159	Total	C	N	O	S	0	0
			1256	766	235	252	3		
1	W	159	Total	C	N	O	S	0	0
			1256	766	235	252	3		
1	X	159	Total	C	N	O	S	0	0
			1256	766	235	252	3		
1	Y	159	Total	C	N	O	S	0	0
			1256	766	235	252	3		
1	Z	159	Total	C	N	O	S	0	0
			1256	766	235	252	3		
1	a	159	Total	C	N	O	S	0	0
			1256	766	235	252	3		
1	b	159	Total	C	N	O	S	0	0
			1256	766	235	252	3		
1	c	159	Total	C	N	O	S	0	0
			1256	766	235	252	3		
1	d	159	Total	C	N	O	S	0	0
			1256	766	235	252	3		
1	e	159	Total	C	N	O	S	0	0
			1256	766	235	252	3		
1	f	159	Total	C	N	O	S	0	0
			1256	766	235	252	3		
1	g	159	Total	C	N	O	S	0	0
			1256	766	235	252	3		
1	h	159	Total	C	N	O	S	0	0
			1256	766	235	252	3		



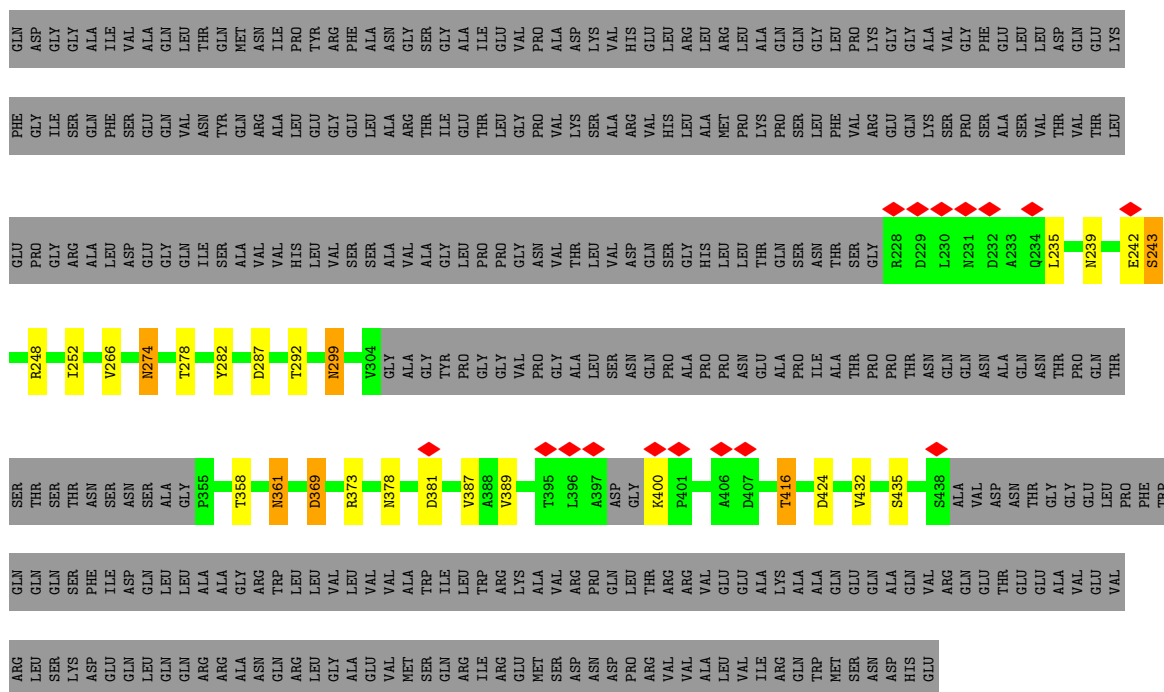
• Molecule 1: Flagellar M-ring protein



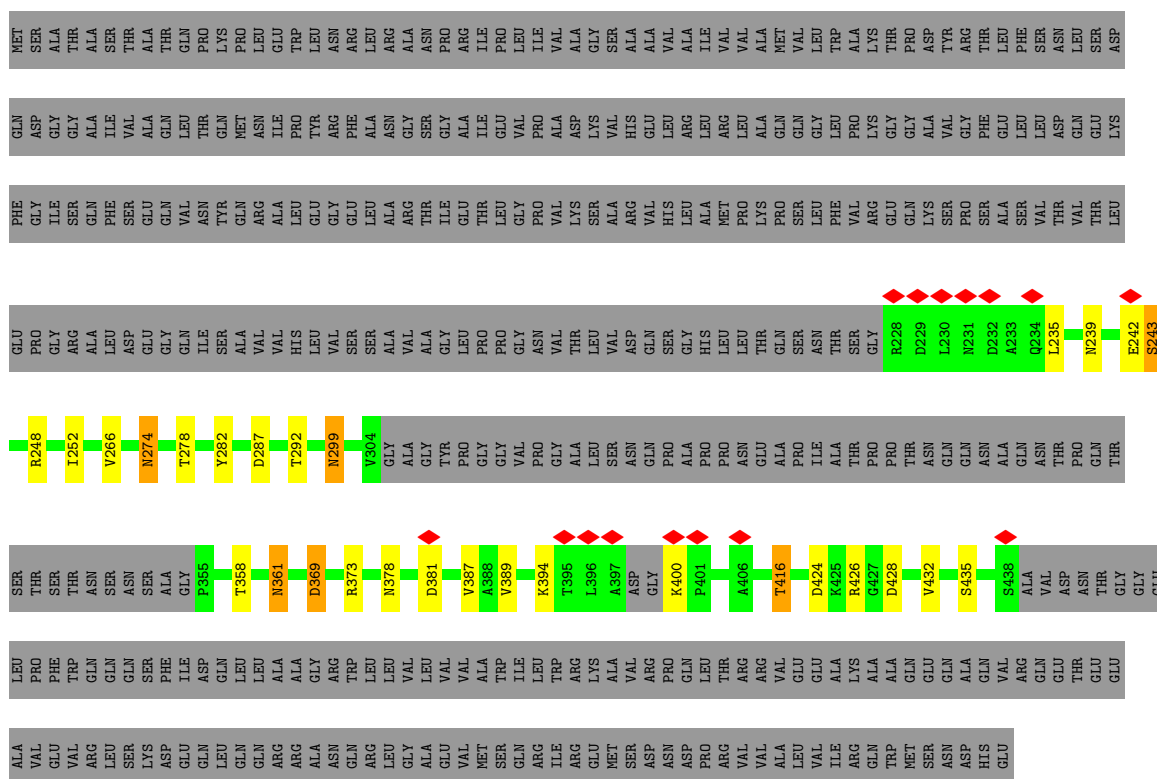
• Molecule 1: Flagellar M-ring protein





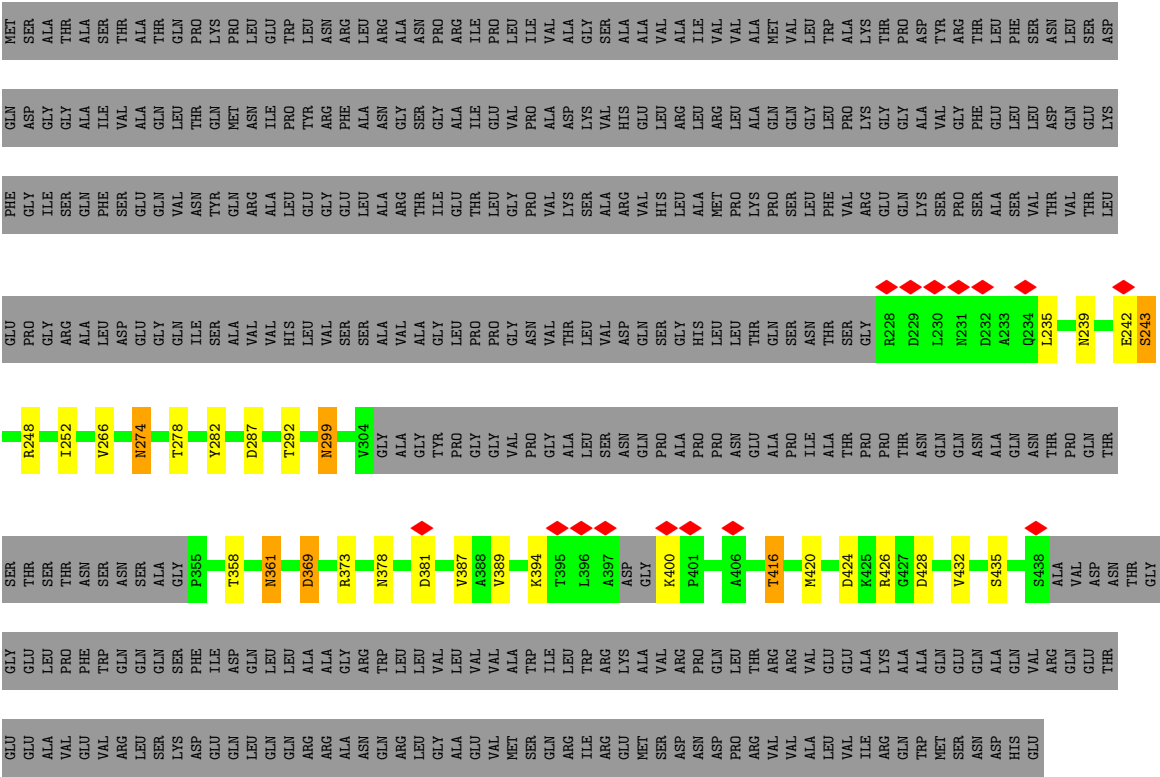


- Molecule 1: Flagellar M-ring protein

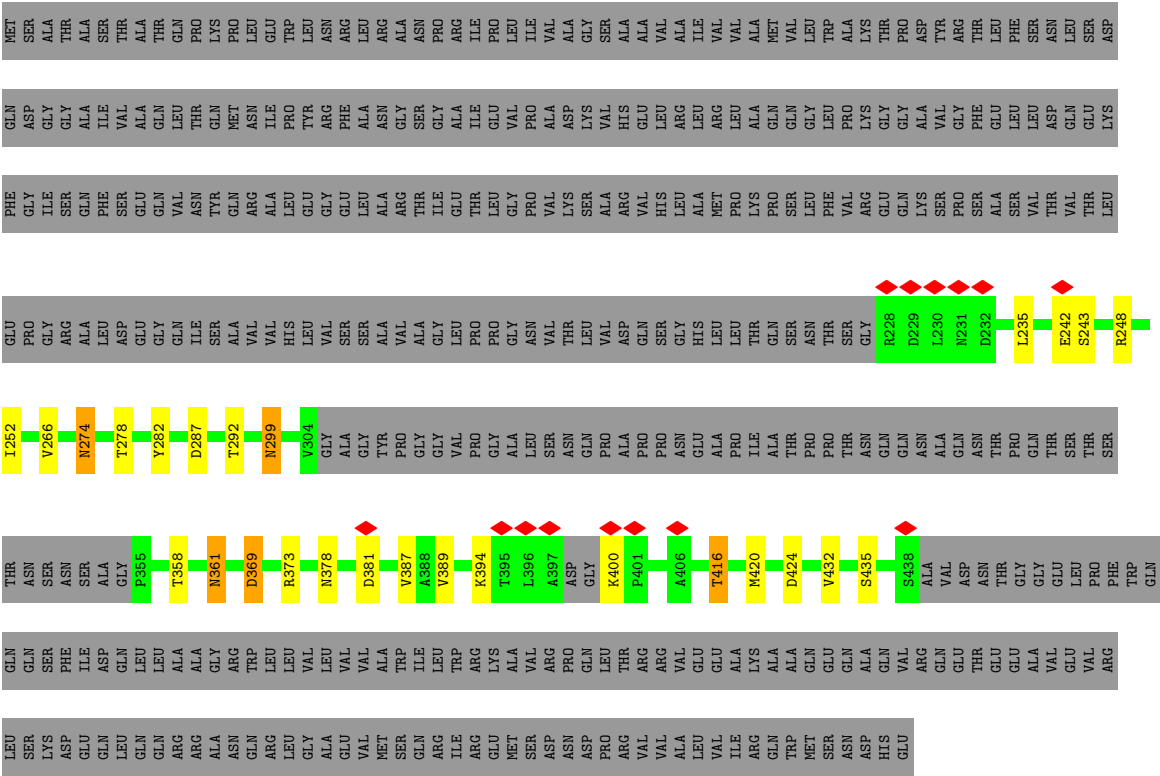


- Molecule 1: Flagellar M-ring protein

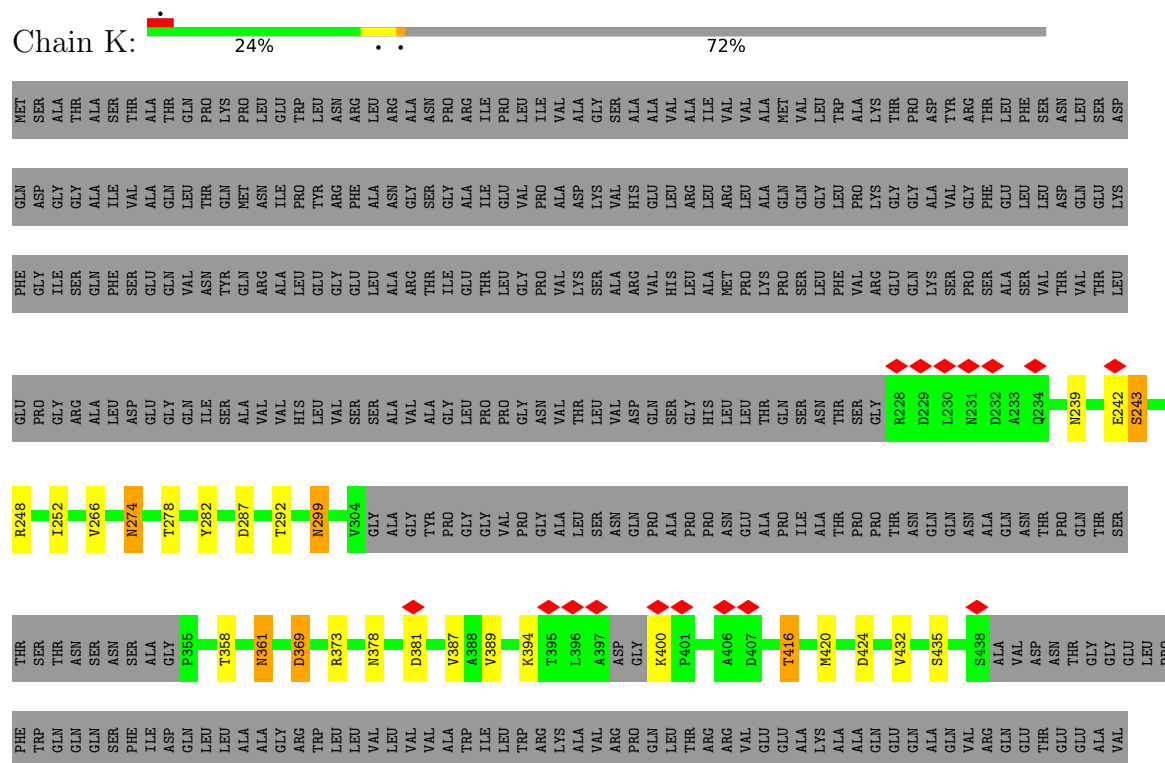




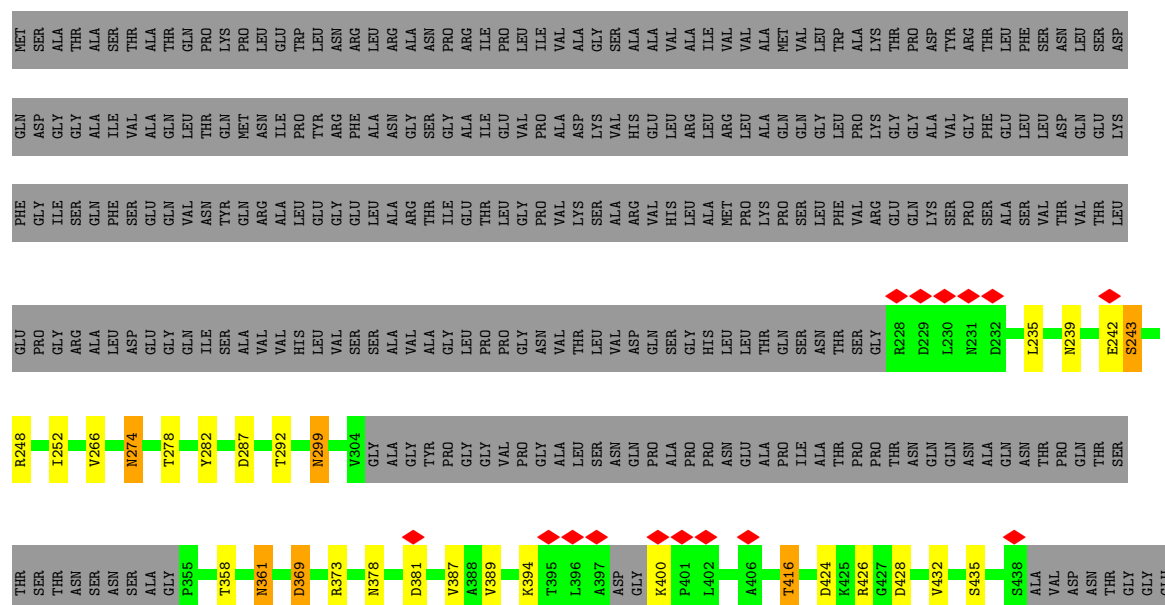
• Molecule 1: Flagellar M-ring protein

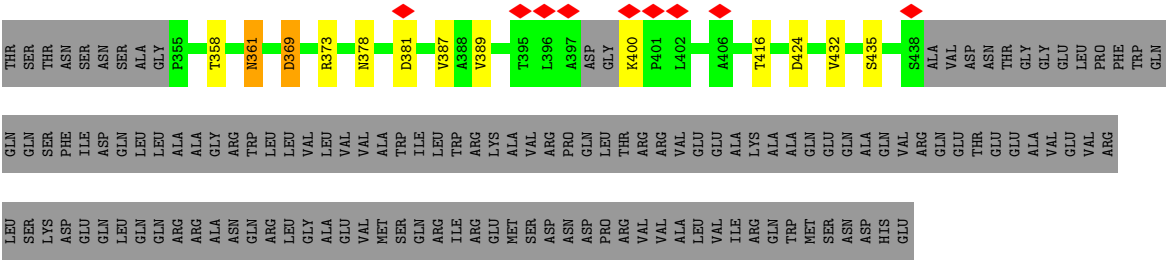


• Molecule 1: Flagellar M-ring protein

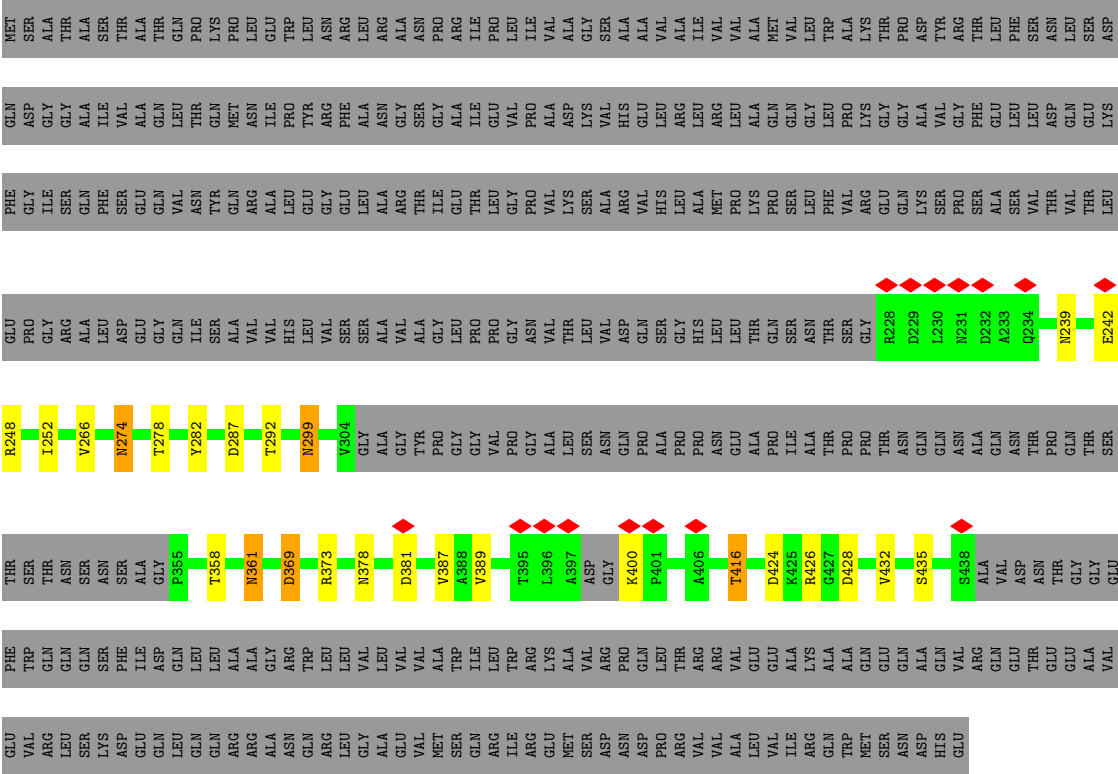


Chain L: 23% .. 72%

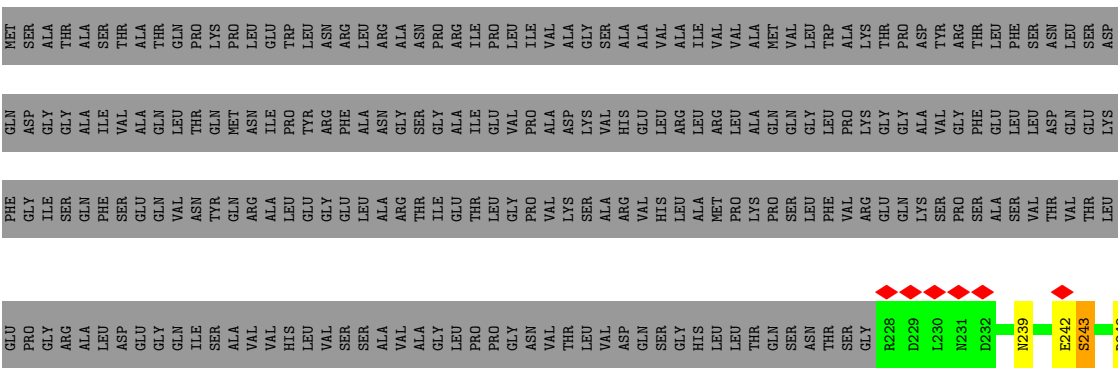




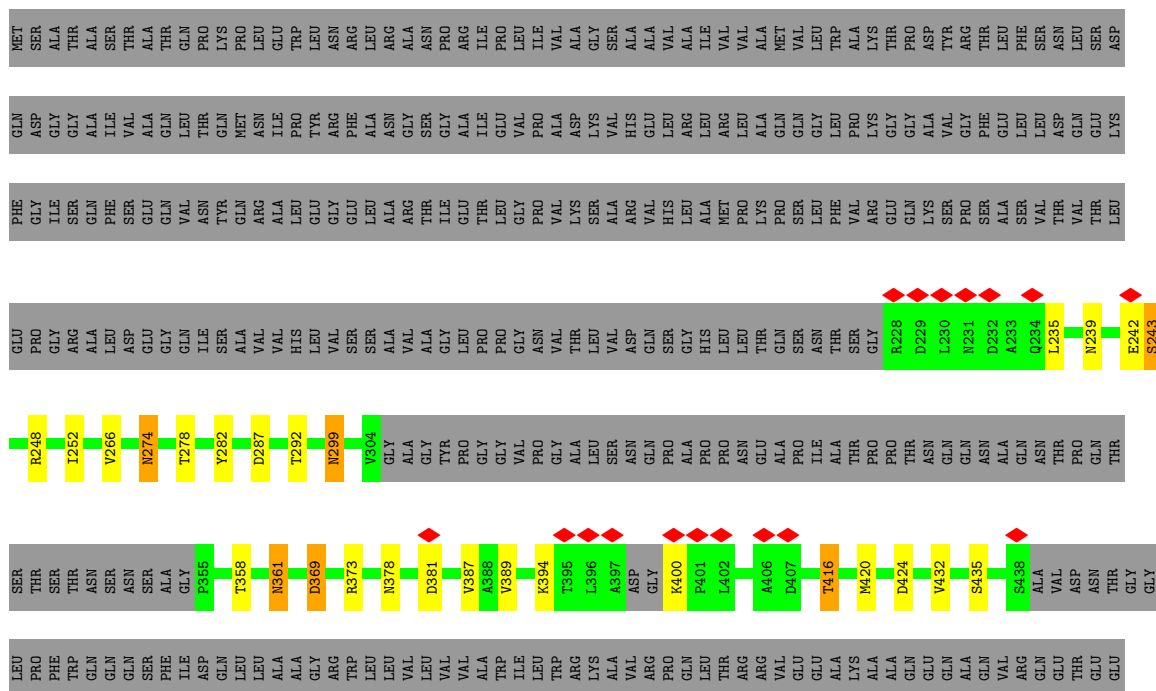
• Molecule 1: Flagellar M-ring protein



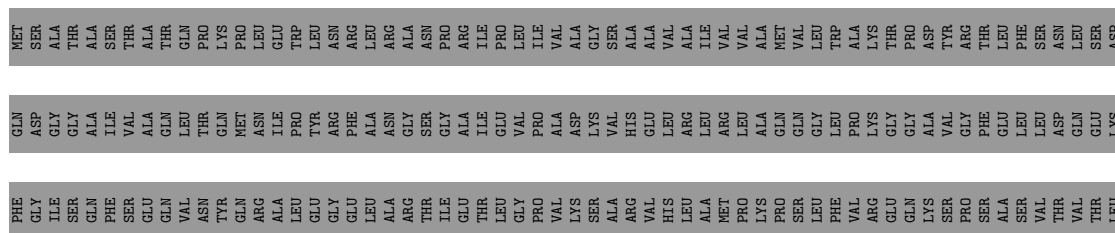
• Molecule 1: Flagellar M-ring protein

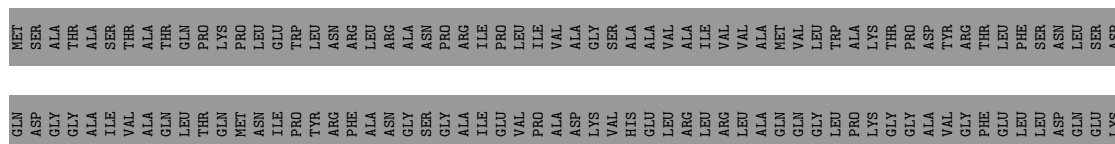


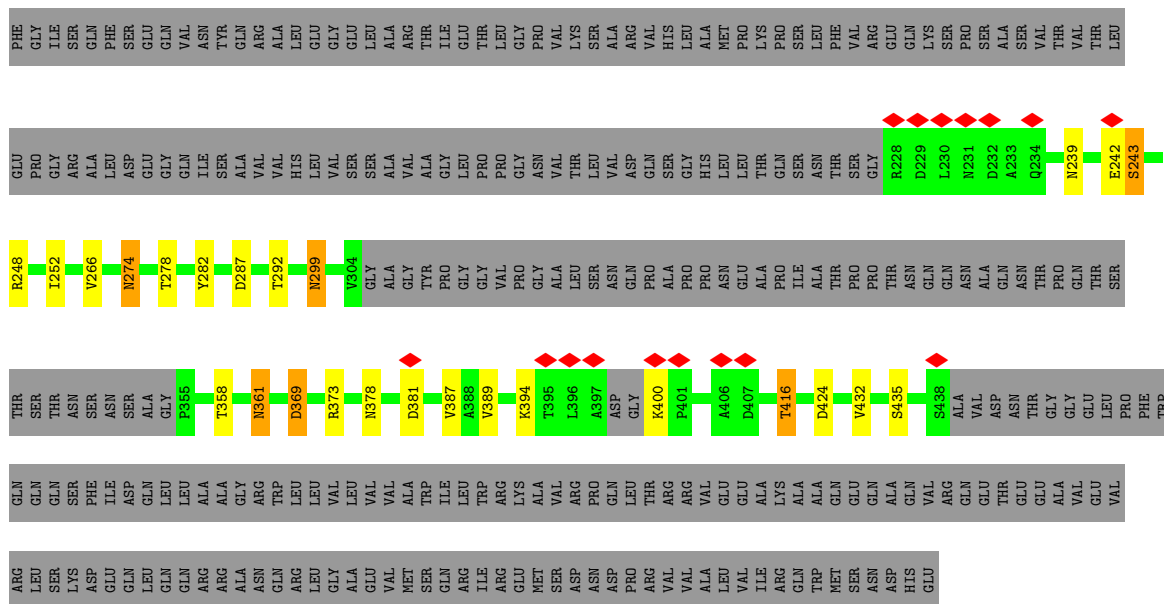
- Molecule 1: Flagellar M-ring protein



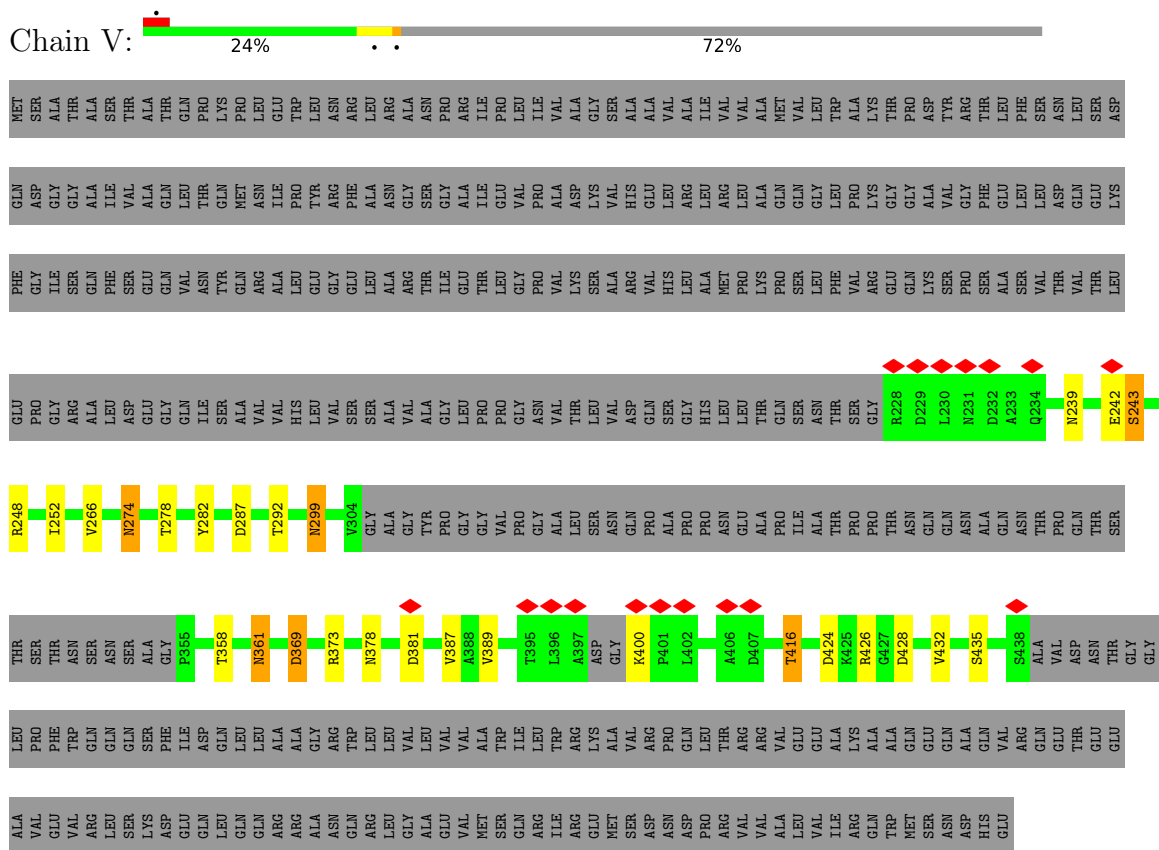
- Molecule 1: Flagellar M-ring protein



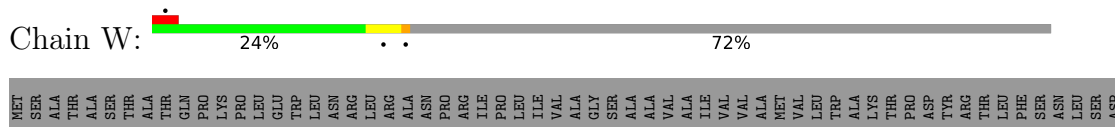


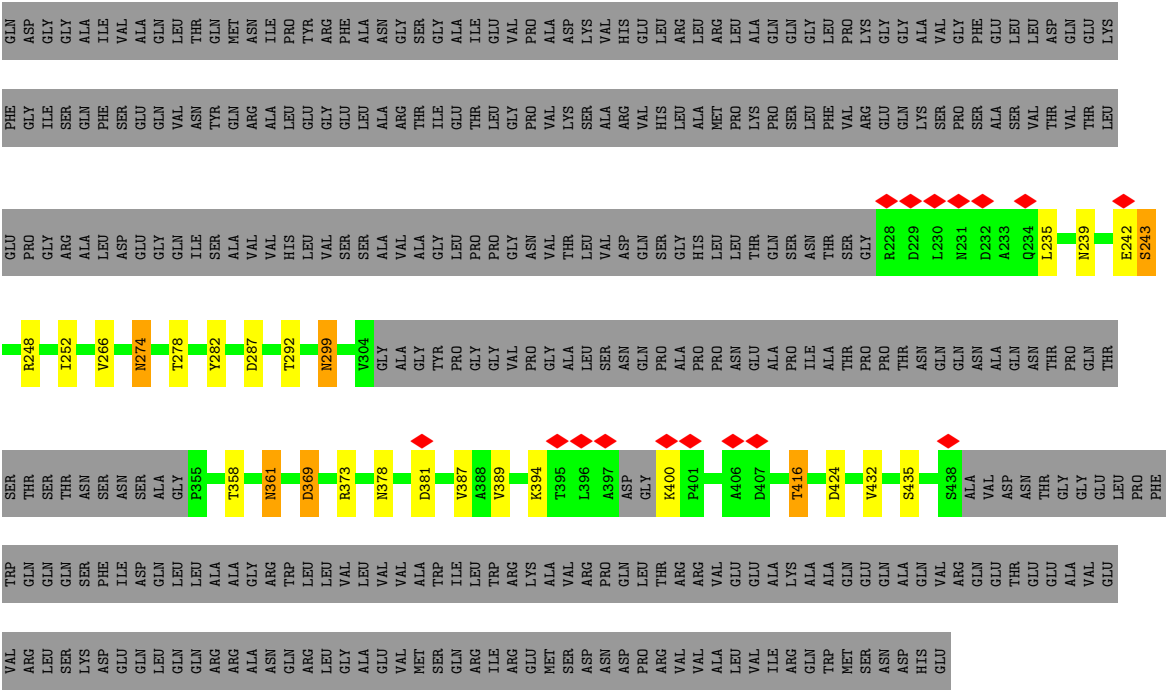


- Molecule 1: Flagellar M-ring protein

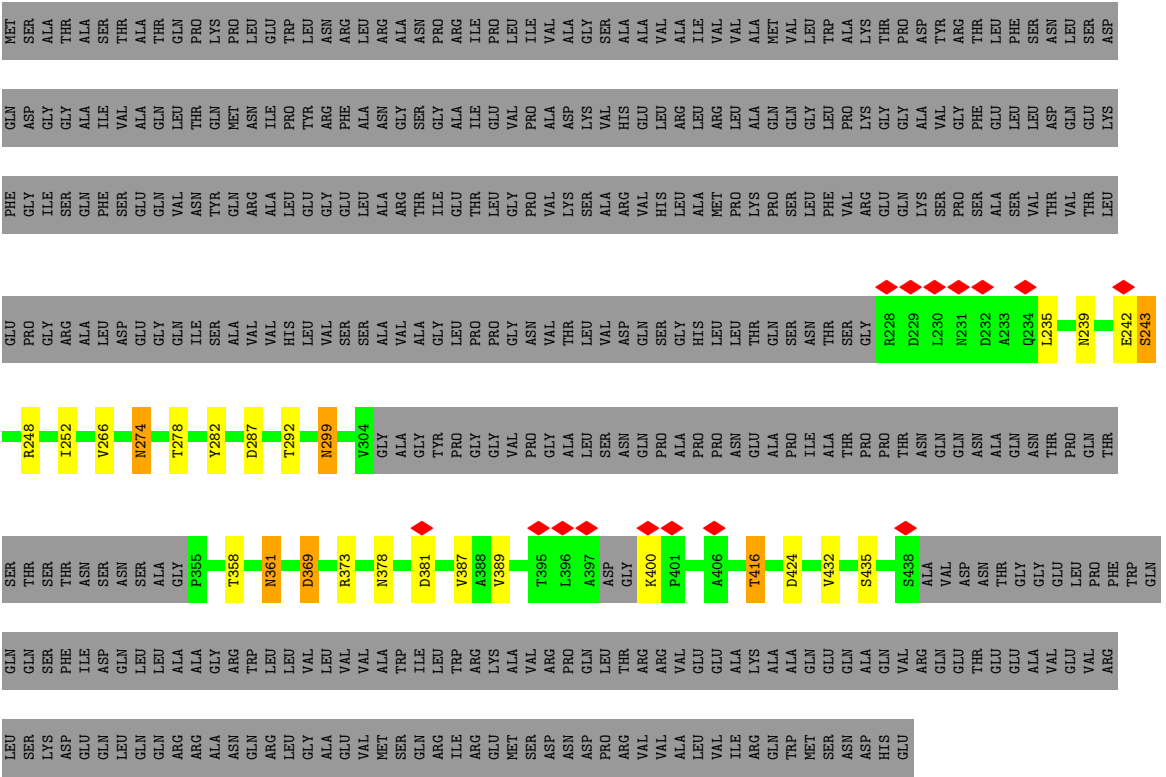


- Molecule 1: Flagellar M-ring protein



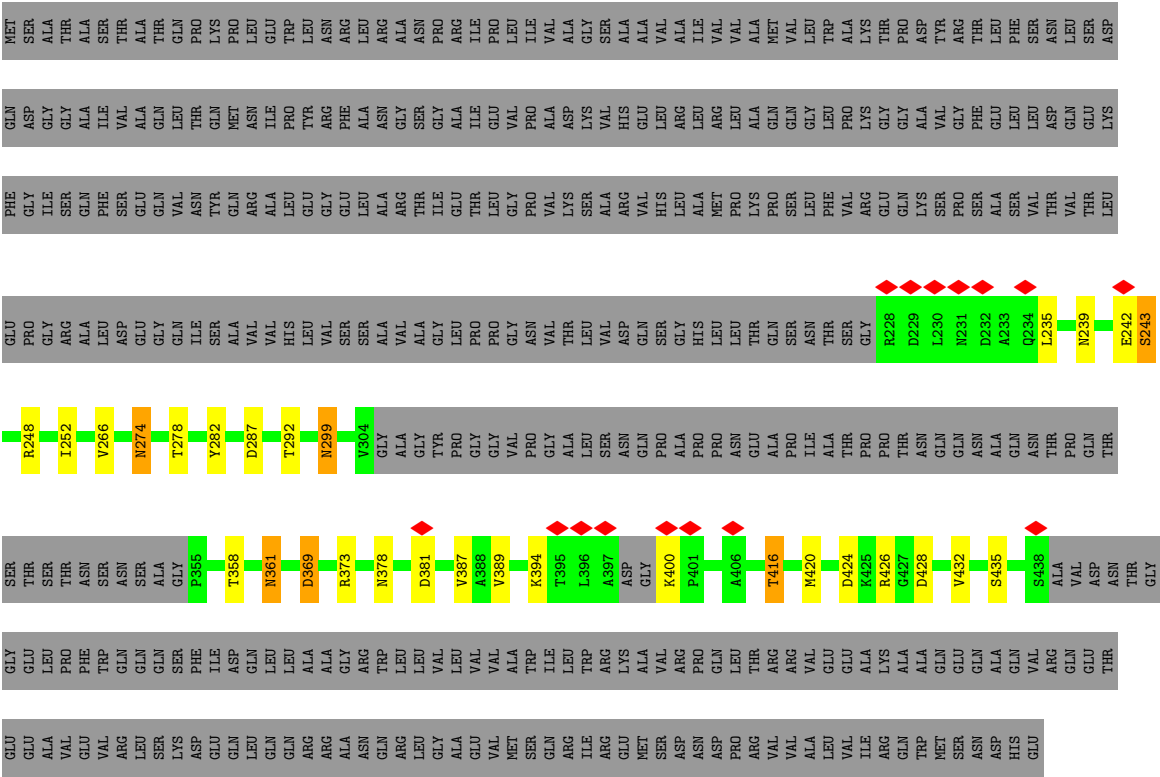


● Molecule 1: Flagellar M-ring protein

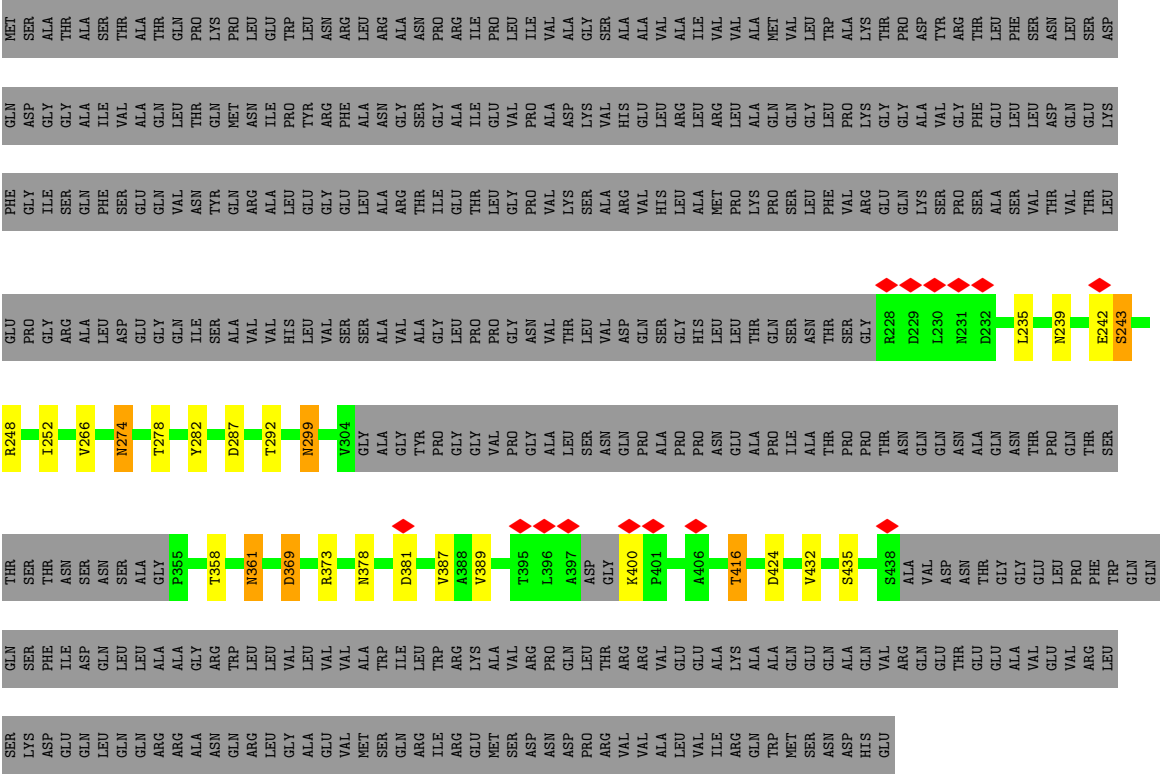


● Molecule 1: Flagellar M-ring protein





• Molecule 1: Flagellar M-ring protein



• Molecule 1: Flagellar M-ring protein



[illegible]

- Molecule 1: Flagellar M-ring protein

[illegible]

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

PHE
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GLJ	PRO	GLY	ARG	ALA	LEU	ASP	GLU	GLY	GLN	ILE	SER	ALA	VAL	VAL	HIS	LEU	HIS	VAL	SER	SER	ALA	VAL	ALA	ALA	GLY	LEU	PRO	PRO	GLY	ASN	VAL	THR	LEU	VAL	ASP	GLN	SER	SER	GLY	HIS	GLY	LEU	LEU	THR	GLN	SER	ASN	THR	SER	SER	GLY	R298	R229	L290	N231	D232	A233	Q234	L235	N236	E242	S243
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THR	THR	ASN	ASN	ALA	GLY	P355	T358	N351	D369	R373	N378	D381	P387	A388	P389	T395	L396	A397	ASP	GLY	K400	P401	L402	A406	D407	T416	D424	K425	R426	G427	D428	V432	S435	S438	ALA	VAL	ASP	ASN	THR	GLY	TYR
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[illegible]

GLU
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ARG
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ASN
GLN
ARG
LEU
GLY
ALA
GLU
VAL
MET
SER
GLN
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ARG
GLU
MET
SER
ASP
ASN
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ASP
HIS

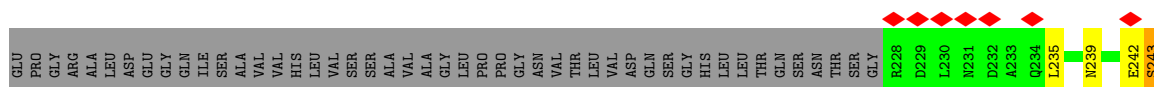
- Molecule 1: Flagellar M-ring protein

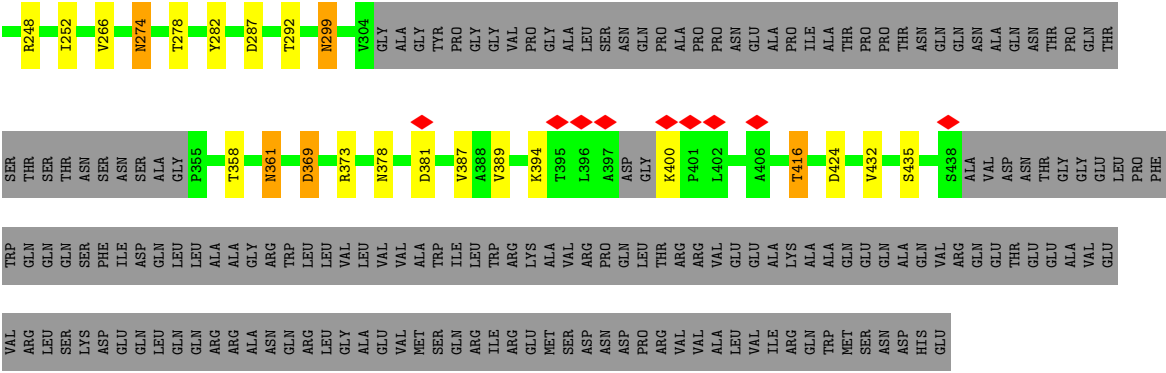
[illegible]

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

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

[illegible][illegible]





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C34	Depositor
Number of particles used	38889	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	90	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	4.229	Depositor
Minimum map value	-2.469	Depositor
Average map value	-0.004	Depositor
Map value standard deviation	0.093	Depositor
Recommended contour level	0.749	Depositor
Map size ($\text{\AA}$)	462.24002, 462.24002, 462.24002	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.07, 1.07, 1.07	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	A	0.41	0/1269	0.53	0/1711
1	B	0.41	0/1269	0.53	0/1711
1	C	0.41	0/1269	0.53	0/1711
1	D	0.41	0/1269	0.53	0/1711
1	E	0.41	0/1269	0.53	0/1711
1	F	0.41	0/1269	0.53	0/1711
1	G	0.41	0/1269	0.53	0/1711
1	H	0.41	0/1269	0.53	0/1711
1	I	0.41	0/1269	0.53	0/1711
1	J	0.41	0/1269	0.53	0/1711
1	K	0.41	0/1269	0.53	0/1711
1	L	0.41	0/1269	0.53	0/1711
1	M	0.41	0/1269	0.53	0/1711
1	N	0.41	0/1269	0.53	0/1711
1	O	0.41	0/1269	0.53	0/1711
1	P	0.41	0/1269	0.53	0/1711
1	Q	0.41	0/1269	0.53	0/1711
1	R	0.41	0/1269	0.53	0/1711
1	S	0.41	0/1269	0.53	0/1711
1	T	0.41	0/1269	0.53	0/1711
1	U	0.41	0/1269	0.53	0/1711
1	V	0.41	0/1269	0.53	0/1711
1	W	0.41	0/1269	0.53	0/1711
1	X	0.41	0/1269	0.53	0/1711
1	Y	0.41	0/1269	0.53	0/1711
1	Z	0.41	0/1269	0.53	0/1711
1	a	0.41	0/1269	0.53	0/1711
1	b	0.41	0/1269	0.53	0/1711
1	c	0.41	0/1269	0.53	0/1711
1	d	0.41	0/1269	0.53	0/1711
1	e	0.41	0/1269	0.53	0/1711
1	f	0.41	0/1269	0.53	0/1711
1	g	0.41	0/1269	0.53	0/1711
1	h	0.41	0/1269	0.53	0/1711

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.41	0/43146	0.53	0/58174

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1256	0	1244	19	0
1	B	1256	0	1244	18	0
1	C	1256	0	1244	16	0
1	D	1256	0	1244	18	0
1	E	1256	0	1244	19	0
1	F	1256	0	1244	16	0
1	G	1256	0	1244	18	0
1	H	1256	0	1244	19	0
1	I	1256	0	1244	17	0
1	J	1256	0	1244	18	0
1	K	1256	0	1244	17	0
1	L	1256	0	1244	19	0
1	M	1256	0	1244	18	0
1	N	1256	0	1244	19	0
1	O	1256	0	1244	16	0
1	P	1256	0	1244	16	0
1	Q	1256	0	1244	17	0
1	R	1256	0	1244	18	0
1	S	1256	0	1244	17	0
1	T	1256	0	1244	17	0
1	U	1256	0	1244	16	0
1	V	1256	0	1244	16	0
1	W	1256	0	1244	17	0
1	X	1256	0	1244	16	0
1	Y	1256	0	1244	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Z	1256	0	1244	16	0
1	a	1256	0	1244	16	0
1	b	1256	0	1244	19	0
1	c	1256	0	1244	15	0
1	d	1256	0	1244	18	0
1	e	1256	0	1244	17	0
1	f	1256	0	1244	17	0
1	g	1256	0	1244	18	0
1	h	1256	0	1244	17	0
All	All	42704	0	42296	520	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 6.

All (520) 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:D:369:ASP:OD1	1:D:369:ASP:N	2.27	0.68
1:C:369:ASP:N	1:C:369:ASP:OD1	2.27	0.67
1:K:369:ASP:OD1	1:K:369:ASP:N	2.27	0.67
1:L:369:ASP:N	1:L:369:ASP:OD1	2.27	0.67
1:E:369:ASP:N	1:E:369:ASP:OD1	2.27	0.67
1:M:369:ASP:OD1	1:M:369:ASP:N	2.27	0.67
1:B:369:ASP:OD1	1:B:369:ASP:N	2.27	0.67
1:J:369:ASP:N	1:J:369:ASP:OD1	2.27	0.67
1:F:369:ASP:OD1	1:F:369:ASP:N	2.27	0.67
1:N:369:ASP:OD1	1:N:369:ASP:N	2.27	0.67
1:A:369:ASP:OD1	1:A:369:ASP:N	2.27	0.67
1:I:369:ASP:OD1	1:I:369:ASP:N	2.27	0.67
1:G:369:ASP:OD1	1:G:369:ASP:N	2.27	0.67
1:O:369:ASP:N	1:O:369:ASP:OD1	2.27	0.67
1:H:369:ASP:N	1:H:369:ASP:OD1	2.27	0.66
1:h:369:ASP:OD1	1:h:369:ASP:N	2.27	0.66
1:P:369:ASP:OD1	1:P:369:ASP:N	2.27	0.66
1:g:369:ASP:N	1:g:369:ASP:OD1	2.27	0.66
1:Q:369:ASP:N	1:Q:369:ASP:OD1	2.27	0.66
1:U:369:ASP:OD1	1:U:369:ASP:N	2.27	0.65
1:a:369:ASP:OD1	1:a:369:ASP:N	2.27	0.65
1:b:369:ASP:N	1:b:369:ASP:OD1	2.27	0.65
1:c:369:ASP:OD1	1:c:369:ASP:N	2.27	0.65
1:d:369:ASP:OD1	1:d:369:ASP:N	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:369:ASP:OD1	1:S:369:ASP:N	2.27	0.65
1:T:369:ASP:N	1:T:369:ASP:OD1	2.27	0.65
1:V:369:ASP:N	1:V:369:ASP:OD1	2.27	0.65
1:W:369:ASP:OD1	1:W:369:ASP:N	2.27	0.65
1:X:369:ASP:OD1	1:X:369:ASP:N	2.27	0.65
1:Y:369:ASP:N	1:Y:369:ASP:OD1	2.27	0.65
1:Z:369:ASP:OD1	1:Z:369:ASP:N	2.27	0.65
1:e:369:ASP:N	1:e:369:ASP:OD1	2.27	0.65
1:f:369:ASP:OD1	1:f:369:ASP:N	2.27	0.65
1:R:369:ASP:OD1	1:R:369:ASP:N	2.27	0.65
1:B:274:ASN:OD1	1:B:274:ASN:N	2.31	0.65
1:E:274:ASN:OD1	1:E:274:ASN:N	2.30	0.65
1:T:274:ASN:OD1	1:T:274:ASN:N	2.30	0.65
1:H:274:ASN:OD1	1:H:274:ASN:N	2.31	0.64
1:K:274:ASN:N	1:K:274:ASN:OD1	2.31	0.64
1:W:274:ASN:N	1:W:274:ASN:OD1	2.31	0.64
1:g:274:ASN:OD1	1:g:274:ASN:N	2.31	0.64
1:R:274:ASN:N	1:R:274:ASN:OD1	2.31	0.64
1:O:274:ASN:OD1	1:O:274:ASN:N	2.30	0.64
1:U:274:ASN:N	1:U:274:ASN:OD1	2.31	0.64
1:b:274:ASN:OD1	1:b:274:ASN:N	2.31	0.64
1:e:274:ASN:OD1	1:e:274:ASN:N	2.31	0.64
1:Z:274:ASN:N	1:Z:274:ASN:OD1	2.31	0.64
1:h:274:ASN:N	1:h:274:ASN:OD1	2.30	0.64
1:L:274:ASN:OD1	1:L:274:ASN:N	2.31	0.64
1:C:274:ASN:OD1	1:C:274:ASN:N	2.31	0.64
1:F:274:ASN:N	1:F:274:ASN:OD1	2.31	0.64
1:I:274:ASN:N	1:I:274:ASN:OD1	2.31	0.64
1:X:274:ASN:OD1	1:X:274:ASN:N	2.31	0.63
1:c:274:ASN:N	1:c:274:ASN:OD1	2.31	0.63
1:S:274:ASN:OD1	1:S:274:ASN:N	2.31	0.62
1:f:274:ASN:N	1:f:274:ASN:OD1	2.31	0.62
1:P:274:ASN:N	1:P:274:ASN:OD1	2.31	0.62
1:a:274:ASN:N	1:a:274:ASN:OD1	2.31	0.62
1:V:274:ASN:OD1	1:V:274:ASN:N	2.31	0.62
1:A:274:ASN:N	1:A:274:ASN:OD1	2.31	0.62
1:M:274:ASN:OD1	1:M:274:ASN:N	2.31	0.62
1:D:274:ASN:N	1:D:274:ASN:OD1	2.31	0.61
1:J:274:ASN:OD1	1:J:274:ASN:N	2.31	0.61
1:G:274:ASN:OD1	1:G:274:ASN:N	2.31	0.61
1:d:274:ASN:OD1	1:d:274:ASN:N	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:266:VAL:HG22	1:e:387:VAL:HG22	1.83	0.61
1:Y:274:ASN:OD1	1:Y:274:ASN:N	2.31	0.61
1:Z:266:VAL:HG22	1:Z:387:VAL:HG22	1.83	0.61
1:a:266:VAL:HG22	1:a:387:VAL:HG22	1.83	0.61
1:d:266:VAL:HG22	1:d:387:VAL:HG22	1.83	0.61
1:f:266:VAL:HG22	1:f:387:VAL:HG22	1.83	0.61
1:B:266:VAL:HG22	1:B:387:VAL:HG22	1.83	0.60
1:U:266:VAL:HG22	1:U:387:VAL:HG22	1.83	0.60
1:V:266:VAL:HG22	1:V:387:VAL:HG22	1.83	0.60
1:Y:266:VAL:HG22	1:Y:387:VAL:HG22	1.83	0.60
1:C:266:VAL:HG22	1:C:387:VAL:HG22	1.83	0.60
1:A:266:VAL:HG22	1:A:387:VAL:HG22	1.83	0.60
1:N:274:ASN:OD1	1:N:274:ASN:N	2.31	0.60
1:T:266:VAL:HG22	1:T:387:VAL:HG22	1.83	0.60
1:b:266:VAL:HG22	1:b:387:VAL:HG22	1.83	0.60
1:W:266:VAL:HG22	1:W:387:VAL:HG22	1.83	0.60
1:g:266:VAL:HG22	1:g:387:VAL:HG22	1.83	0.60
1:H:266:VAL:HG22	1:H:387:VAL:HG22	1.83	0.59
1:O:266:VAL:HG22	1:O:387:VAL:HG22	1.83	0.59
1:Q:274:ASN:OD1	1:Q:274:ASN:N	2.30	0.59
1:c:266:VAL:HG22	1:c:387:VAL:HG22	1.83	0.59
1:D:266:VAL:HG22	1:D:387:VAL:HG22	1.83	0.59
1:P:266:VAL:HG22	1:P:387:VAL:HG22	1.83	0.59
1:I:266:VAL:HG22	1:I:387:VAL:HG22	1.83	0.59
1:h:266:VAL:HG22	1:h:387:VAL:HG22	1.83	0.59
1:G:266:VAL:HG22	1:G:387:VAL:HG22	1.83	0.59
1:N:266:VAL:HG22	1:N:387:VAL:HG22	1.83	0.59
1:X:266:VAL:HG22	1:X:387:VAL:HG22	1.83	0.59
1:L:266:VAL:HG22	1:L:387:VAL:HG22	1.83	0.59
1:S:266:VAL:HG22	1:S:387:VAL:HG22	1.83	0.59
1:Q:266:VAL:HG22	1:Q:387:VAL:HG22	1.83	0.59
1:J:266:VAL:HG22	1:J:387:VAL:HG22	1.83	0.59
1:K:266:VAL:HG22	1:K:387:VAL:HG22	1.83	0.59
1:F:266:VAL:HG22	1:F:387:VAL:HG22	1.83	0.58
1:M:266:VAL:HG22	1:M:387:VAL:HG22	1.83	0.58
1:E:266:VAL:HG22	1:E:387:VAL:HG22	1.83	0.58
1:R:266:VAL:HG22	1:R:387:VAL:HG22	1.83	0.58
1:M:424:ASP:OD1	1:M:424:ASP:N	2.38	0.57
1:O:424:ASP:OD1	1:O:424:ASP:N	2.38	0.57
1:g:424:ASP:OD1	1:g:424:ASP:N	2.38	0.57
1:A:424:ASP:OD1	1:A:424:ASP:N	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:424:ASP:OD1	1:K:424:ASP:N	2.38	0.57
1:C:424:ASP:OD1	1:C:424:ASP:N	2.38	0.56
1:I:424:ASP:N	1:I:424:ASP:OD1	2.38	0.56
1:E:424:ASP:OD1	1:E:424:ASP:N	2.38	0.56
1:G:424:ASP:N	1:G:424:ASP:OD1	2.38	0.56
1:L:424:ASP:OD1	1:L:424:ASP:N	2.38	0.56
1:d:424:ASP:N	1:d:424:ASP:OD1	2.38	0.56
1:f:424:ASP:N	1:f:424:ASP:OD1	2.38	0.56
1:h:424:ASP:OD1	1:h:424:ASP:N	2.38	0.56
1:B:424:ASP:N	1:B:424:ASP:OD1	2.38	0.56
1:D:424:ASP:N	1:D:424:ASP:OD1	2.38	0.55
1:J:424:ASP:OD1	1:J:424:ASP:N	2.38	0.55
1:F:424:ASP:OD1	1:F:424:ASP:N	2.38	0.55
1:H:424:ASP:OD1	1:H:424:ASP:N	2.38	0.55
1:N:424:ASP:N	1:N:424:ASP:OD1	2.38	0.55
1:P:424:ASP:N	1:P:424:ASP:OD1	2.38	0.54
1:O:248:ARG:NH2	1:P:242:GLU:OE1	2.40	0.54
1:E:248:ARG:NH2	1:F:242:GLU:OE1	2.41	0.54
1:Y:424:ASP:OD1	1:Y:424:ASP:N	2.38	0.54
1:R:424:ASP:OD1	1:R:424:ASP:N	2.38	0.54
1:A:248:ARG:NH2	1:B:242:GLU:OE1	2.42	0.53
1:B:248:ARG:NH2	1:C:242:GLU:OE1	2.42	0.53
1:A:242:GLU:OE1	1:h:248:ARG:NH2	2.42	0.53
1:a:424:ASP:N	1:a:424:ASP:OD1	2.38	0.53
1:c:248:ARG:NH2	1:d:242:GLU:OE1	2.42	0.53
1:d:248:ARG:NH2	1:e:242:GLU:OE1	2.42	0.53
1:e:248:ARG:NH2	1:f:242:GLU:OE1	2.42	0.53
1:g:248:ARG:NH2	1:h:242:GLU:OE1	2.42	0.53
1:C:248:ARG:NH2	1:D:242:GLU:OE1	2.42	0.53
1:a:248:ARG:NH2	1:b:242:GLU:OE1	2.42	0.53
1:f:248:ARG:NH2	1:g:242:GLU:OE1	2.42	0.53
1:b:248:ARG:NH2	1:c:242:GLU:OE1	2.42	0.53
1:F:248:ARG:NH2	1:G:242:GLU:OE1	2.42	0.53
1:T:424:ASP:OD1	1:T:424:ASP:N	2.38	0.53
1:Y:248:ARG:NH2	1:Z:242:GLU:OE1	2.42	0.53
1:Z:248:ARG:NH2	1:a:242:GLU:OE1	2.42	0.53
1:G:248:ARG:NH2	1:H:242:GLU:OE1	2.42	0.53
1:H:248:ARG:NH2	1:I:242:GLU:OE1	2.42	0.53
1:X:424:ASP:N	1:X:424:ASP:OD1	2.38	0.53
1:D:248:ARG:NH2	1:E:242:GLU:OE1	2.42	0.53
1:X:248:ARG:NH2	1:Y:242:GLU:OE1	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:248:ARG:NH2	1:J:242:GLU:OE1	2.42	0.52
1:J:248:ARG:NH2	1:K:242:GLU:OE1	2.42	0.52
1:W:248:ARG:NH2	1:X:242:GLU:OE1	2.42	0.52
1:V:248:ARG:NH2	1:W:242:GLU:OE1	2.42	0.52
1:c:424:ASP:OD1	1:c:424:ASP:N	2.38	0.52
1:K:248:ARG:NH2	1:L:242:GLU:OE1	2.42	0.52
1:L:248:ARG:NH2	1:M:242:GLU:OE1	2.42	0.52
1:U:248:ARG:NH2	1:V:242:GLU:OE1	2.42	0.52
1:M:248:ARG:NH2	1:N:242:GLU:OE1	2.42	0.52
1:P:248:ARG:NH2	1:Q:242:GLU:OE1	2.42	0.52
1:Q:248:ARG:NH2	1:R:242:GLU:OE1	2.42	0.52
1:R:248:ARG:NH2	1:S:242:GLU:OE1	2.42	0.52
1:T:248:ARG:NH2	1:U:242:GLU:OE1	2.42	0.51
1:V:424:ASP:OD1	1:V:424:ASP:N	2.38	0.51
1:N:248:ARG:NH2	1:O:242:GLU:OE1	2.42	0.51
1:e:424:ASP:OD1	1:e:424:ASP:N	2.38	0.51
1:Q:299:ASN:OD1	1:Q:299:ASN:N	2.44	0.51
1:R:299:ASN:OD1	1:R:299:ASN:N	2.44	0.51
1:S:299:ASN:N	1:S:299:ASN:OD1	2.44	0.51
1:d:299:ASN:N	1:d:299:ASN:OD1	2.44	0.51
1:e:299:ASN:OD1	1:e:299:ASN:N	2.44	0.51
1:f:299:ASN:N	1:f:299:ASN:OD1	2.44	0.51
1:H:299:ASN:OD1	1:H:299:ASN:N	2.44	0.51
1:S:248:ARG:NH2	1:T:242:GLU:OE1	2.43	0.51
1:T:299:ASN:OD1	1:T:299:ASN:N	2.44	0.51
1:c:299:ASN:OD1	1:c:299:ASN:N	2.44	0.51
1:F:299:ASN:N	1:F:299:ASN:OD1	2.44	0.51
1:G:299:ASN:OD1	1:G:299:ASN:N	2.44	0.51
1:P:299:ASN:N	1:P:299:ASN:OD1	2.44	0.51
1:g:299:ASN:OD1	1:g:299:ASN:N	2.44	0.51
1:h:299:ASN:OD1	1:h:299:ASN:N	2.44	0.51
1:b:299:ASN:OD1	1:b:299:ASN:N	2.44	0.51
1:O:299:ASN:OD1	1:O:299:ASN:N	2.44	0.51
1:U:299:ASN:N	1:U:299:ASN:OD1	2.44	0.51
1:a:299:ASN:N	1:a:299:ASN:OD1	2.44	0.51
1:A:299:ASN:OD1	1:A:299:ASN:N	2.44	0.50
1:E:299:ASN:OD1	1:E:299:ASN:N	2.44	0.50
1:Z:299:ASN:N	1:Z:299:ASN:OD1	2.44	0.50
1:D:299:ASN:N	1:D:299:ASN:OD1	2.44	0.50
1:B:299:ASN:OD1	1:B:299:ASN:N	2.44	0.50
1:N:299:ASN:N	1:N:299:ASN:OD1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:299:ASN:OD1	1:V:299:ASN:N	2.44	0.50
1:Y:299:ASN:OD1	1:Y:299:ASN:N	2.44	0.50
1:P:389:VAL:HG21	1:P:416:THR:HG21	1.94	0.50
1:R:389:VAL:HG21	1:R:416:THR:HG21	1.94	0.50
1:T:389:VAL:HG21	1:T:416:THR:HG21	1.94	0.50
1:V:389:VAL:HG21	1:V:416:THR:HG21	1.94	0.50
1:W:299:ASN:OD1	1:W:299:ASN:N	2.44	0.50
1:X:299:ASN:N	1:X:299:ASN:OD1	2.44	0.50
1:C:299:ASN:OD1	1:C:299:ASN:N	2.44	0.50
1:M:299:ASN:OD1	1:M:299:ASN:N	2.44	0.50
1:N:389:VAL:HG21	1:N:416:THR:HG21	1.94	0.50
1:S:389:VAL:HG21	1:S:416:THR:HG21	1.94	0.50
1:X:389:VAL:HG21	1:X:416:THR:HG21	1.94	0.50
1:O:389:VAL:HG21	1:O:416:THR:HG21	1.94	0.49
1:Q:389:VAL:HG21	1:Q:416:THR:HG21	1.94	0.49
1:U:389:VAL:HG21	1:U:416:THR:HG21	1.94	0.49
1:Z:389:VAL:HG21	1:Z:416:THR:HG21	1.94	0.49
1:L:389:VAL:HG21	1:L:416:THR:HG21	1.94	0.49
1:W:389:VAL:HG21	1:W:416:THR:HG21	1.94	0.49
1:B:389:VAL:HG21	1:B:416:THR:HG21	1.94	0.49
1:L:299:ASN:OD1	1:L:299:ASN:N	2.44	0.49
1:M:389:VAL:HG21	1:M:416:THR:HG21	1.94	0.49
1:Y:389:VAL:HG21	1:Y:416:THR:HG21	1.94	0.49
1:Q:424:ASP:OD1	1:Q:424:ASP:N	2.38	0.49
1:A:389:VAL:HG21	1:A:416:THR:HG21	1.94	0.49
1:J:389:VAL:HG21	1:J:416:THR:HG21	1.94	0.49
1:a:389:VAL:HG21	1:a:416:THR:HG21	1.94	0.49
1:b:389:VAL:HG21	1:b:416:THR:HG21	1.94	0.49
1:K:389:VAL:HG21	1:K:416:THR:HG21	1.94	0.49
1:C:389:VAL:HG21	1:C:416:THR:HG21	1.94	0.49
1:e:389:VAL:HG21	1:e:416:THR:HG21	1.94	0.49
1:G:389:VAL:HG21	1:G:416:THR:HG21	1.94	0.48
1:F:389:VAL:HG21	1:F:416:THR:HG21	1.94	0.48
1:c:389:VAL:HG21	1:c:416:THR:HG21	1.94	0.48
1:H:389:VAL:HG21	1:H:416:THR:HG21	1.94	0.48
1:Z:424:ASP:N	1:Z:424:ASP:OD1	2.38	0.48
1:d:389:VAL:HG21	1:d:416:THR:HG21	1.94	0.48
1:f:389:VAL:HG21	1:f:416:THR:HG21	1.94	0.48
1:I:389:VAL:HG21	1:I:416:THR:HG21	1.94	0.48
1:K:299:ASN:N	1:K:299:ASN:OD1	2.44	0.48
1:h:389:VAL:HG21	1:h:416:THR:HG21	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:389:VAL:HG21	1:D:416:THR:HG21	1.94	0.48
1:E:389:VAL:HG21	1:E:416:THR:HG21	1.94	0.48
1:g:389:VAL:HG21	1:g:416:THR:HG21	1.94	0.48
1:S:424:ASP:N	1:S:424:ASP:OD1	2.38	0.48
1:J:299:ASN:OD1	1:J:299:ASN:N	2.44	0.48
1:I:299:ASN:N	1:I:299:ASN:OD1	2.44	0.47
1:b:424:ASP:OD1	1:b:424:ASP:N	2.38	0.47
1:U:424:ASP:N	1:U:424:ASP:OD1	2.38	0.46
1:X:239:ASN:O	1:X:243:SER:OG	2.34	0.46
1:A:235:LEU:HD23	1:A:235:LEU:HA	1.82	0.46
1:K:361:ASN:OD1	1:K:361:ASN:N	2.49	0.46
1:L:361:ASN:N	1:L:361:ASN:OD1	2.49	0.46
1:W:239:ASN:O	1:W:243:SER:OG	2.34	0.46
1:N:420:MET:HE2	1:N:420:MET:HB3	1.83	0.46
1:W:424:ASP:OD1	1:W:424:ASP:N	2.38	0.46
1:F:235:LEU:HD23	1:F:235:LEU:HA	1.82	0.46
1:Y:235:LEU:HD23	1:Y:235:LEU:HA	1.82	0.46
1:S:389:VAL:HB	1:S:432:VAL:HG22	1.98	0.45
1:U:389:VAL:HB	1:U:432:VAL:HG22	1.98	0.45
1:X:389:VAL:HB	1:X:432:VAL:HG22	1.98	0.45
1:P:389:VAL:HB	1:P:432:VAL:HG22	1.98	0.45
1:W:361:ASN:OD1	1:W:361:ASN:N	2.49	0.45
1:a:239:ASN:O	1:a:243:SER:OG	2.34	0.45
1:B:239:ASN:O	1:B:243:SER:OG	2.34	0.45
1:H:420:MET:HE2	1:H:420:MET:HB3	1.83	0.45
1:R:239:ASN:O	1:R:243:SER:OG	2.34	0.45
1:V:389:VAL:HB	1:V:432:VAL:HG22	1.98	0.45
1:X:361:ASN:N	1:X:361:ASN:OD1	2.49	0.45
1:a:389:VAL:HB	1:a:432:VAL:HG22	1.98	0.45
1:J:235:LEU:HD23	1:J:235:LEU:HA	1.82	0.45
1:J:239:ASN:O	1:J:243:SER:OG	2.34	0.45
1:e:361:ASN:OD1	1:e:361:ASN:N	2.49	0.45
1:H:239:ASN:O	1:H:243:SER:OG	2.34	0.45
1:Y:361:ASN:OD1	1:Y:361:ASN:N	2.49	0.45
1:Z:361:ASN:N	1:Z:361:ASN:OD1	2.49	0.45
1:c:361:ASN:OD1	1:c:361:ASN:N	2.49	0.45
1:d:361:ASN:N	1:d:361:ASN:OD1	2.49	0.45
1:e:239:ASN:O	1:e:243:SER:OG	2.34	0.45
1:h:235:LEU:HD23	1:h:235:LEU:HA	1.82	0.45
1:M:239:ASN:O	1:M:243:SER:OG	2.34	0.45
1:S:235:LEU:HD23	1:S:235:LEU:HA	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:361:ASN:OD1	1:a:361:ASN:N	2.49	0.45
1:b:361:ASN:N	1:b:361:ASN:OD1	2.49	0.45
1:M:389:VAL:HB	1:M:432:VAL:HG22	1.98	0.45
1:R:389:VAL:HB	1:R:432:VAL:HG22	1.98	0.45
1:V:239:ASN:O	1:V:243:SER:OG	2.34	0.45
1:Z:389:VAL:HB	1:Z:432:VAL:HG22	1.98	0.45
1:N:389:VAL:HB	1:N:432:VAL:HG22	1.98	0.45
1:Q:389:VAL:HB	1:Q:432:VAL:HG22	1.98	0.45
1:c:389:VAL:HB	1:c:432:VAL:HG22	1.98	0.45
1:d:389:VAL:HB	1:d:432:VAL:HG22	1.98	0.45
1:G:239:ASN:O	1:G:243:SER:OG	2.34	0.45
1:G:426:ARG:NH2	1:G:428:ASP:OD2	2.44	0.45
1:W:389:VAL:HB	1:W:432:VAL:HG22	1.98	0.45
1:g:235:LEU:HD23	1:g:235:LEU:HA	1.82	0.45
1:J:426:ARG:NH2	1:J:428:ASP:OD2	2.44	0.44
1:K:389:VAL:HB	1:K:432:VAL:HG22	1.98	0.44
1:Y:389:VAL:HB	1:Y:432:VAL:HG22	1.98	0.44
1:g:420:MET:HE2	1:g:420:MET:HB3	1.83	0.44
1:D:361:ASN:OD1	1:D:361:ASN:N	2.49	0.44
1:E:420:MET:HE2	1:E:420:MET:HB3	1.83	0.44
1:Q:420:MET:HE2	1:Q:420:MET:HB3	1.83	0.44
1:f:389:VAL:HB	1:f:432:VAL:HG22	1.98	0.44
1:A:239:ASN:O	1:A:243:SER:OG	2.34	0.44
1:D:389:VAL:HB	1:D:432:VAL:HG22	1.98	0.44
1:F:389:VAL:HB	1:F:432:VAL:HG22	1.98	0.44
1:E:389:VAL:HB	1:E:432:VAL:HG22	1.98	0.44
1:J:389:VAL:HB	1:J:432:VAL:HG22	1.98	0.44
1:N:235:LEU:HD23	1:N:235:LEU:HA	1.82	0.44
1:Q:239:ASN:O	1:Q:243:SER:OG	2.34	0.44
1:Z:239:ASN:O	1:Z:243:SER:OG	2.34	0.44
1:f:361:ASN:OD1	1:f:361:ASN:N	2.49	0.44
1:C:389:VAL:HB	1:C:432:VAL:HG22	1.98	0.44
1:E:361:ASN:OD1	1:E:361:ASN:N	2.49	0.44
1:G:389:VAL:HB	1:G:432:VAL:HG22	1.98	0.44
1:T:389:VAL:HB	1:T:432:VAL:HG22	1.98	0.44
1:V:361:ASN:OD1	1:V:361:ASN:N	2.49	0.44
1:g:278:THR:HA	1:g:373:ARG:O	2.18	0.44
1:g:389:VAL:HB	1:g:432:VAL:HG22	1.98	0.44
1:A:389:VAL:HB	1:A:432:VAL:HG22	1.98	0.44
1:B:389:VAL:HB	1:B:432:VAL:HG22	1.98	0.44
1:B:420:MET:HE2	1:B:420:MET:HB3	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:426:ARG:NH2	1:D:428:ASP:OD2	2.44	0.44
1:H:389:VAL:HB	1:H:432:VAL:HG22	1.98	0.44
1:L:239:ASN:O	1:L:243:SER:OG	2.34	0.44
1:N:292:THR:HG21	1:O:282:TYR:HB3	1.99	0.44
1:E:235:LEU:HD23	1:E:235:LEU:HA	1.82	0.44
1:M:278:THR:HA	1:M:373:ARG:O	2.18	0.44
1:N:278:THR:HA	1:N:373:ARG:O	2.18	0.44
1:O:389:VAL:HB	1:O:432:VAL:HG22	1.98	0.44
1:g:361:ASN:OD1	1:g:361:ASN:N	2.49	0.44
1:F:239:ASN:O	1:F:243:SER:OG	2.34	0.44
1:F:278:THR:HA	1:F:373:ARG:O	2.18	0.44
1:M:426:ARG:NH2	1:M:428:ASP:OD2	2.44	0.44
1:h:278:THR:HA	1:h:373:ARG:O	2.18	0.44
1:E:278:THR:HA	1:E:373:ARG:O	2.18	0.44
1:F:361:ASN:OD1	1:F:361:ASN:N	2.49	0.44
1:G:278:THR:HA	1:G:373:ARG:O	2.18	0.44
1:I:389:VAL:HB	1:I:432:VAL:HG22	1.98	0.44
1:L:278:THR:HA	1:L:373:ARG:O	2.18	0.44
1:T:278:THR:HA	1:T:373:ARG:O	2.18	0.44
1:U:361:ASN:OD1	1:U:361:ASN:N	2.49	0.44
1:X:235:LEU:HD23	1:X:235:LEU:HA	1.82	0.44
1:Y:420:MET:HE2	1:Y:420:MET:HB3	1.83	0.44
1:b:389:VAL:HB	1:b:432:VAL:HG22	1.98	0.44
1:d:239:ASN:O	1:d:243:SER:OG	2.34	0.44
1:f:235:LEU:HD23	1:f:235:LEU:HA	1.82	0.44
1:f:278:THR:HA	1:f:373:ARG:O	2.18	0.44
1:h:389:VAL:HB	1:h:432:VAL:HG22	1.98	0.44
1:A:278:THR:HA	1:A:373:ARG:O	2.18	0.43
1:O:278:THR:HA	1:O:373:ARG:O	2.18	0.43
1:S:278:THR:HA	1:S:373:ARG:O	2.18	0.43
1:U:278:THR:HA	1:U:373:ARG:O	2.18	0.43
1:Z:278:THR:HA	1:Z:373:ARG:O	2.18	0.43
1:a:278:THR:HA	1:a:373:ARG:O	2.18	0.43
1:H:278:THR:HA	1:H:373:ARG:O	2.18	0.43
1:P:278:THR:HA	1:P:373:ARG:O	2.18	0.43
1:Z:292:THR:HG21	1:a:282:TYR:HB3	2.00	0.43
1:b:278:THR:HA	1:b:373:ARG:O	2.18	0.43
1:c:278:THR:HA	1:c:373:ARG:O	2.18	0.43
1:d:278:THR:HA	1:d:373:ARG:O	2.18	0.43
1:e:278:THR:HA	1:e:373:ARG:O	2.18	0.43
1:h:361:ASN:OD1	1:h:361:ASN:N	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:361:ASN:OD1	1:T:361:ASN:N	2.49	0.43
1:a:292:THR:HG21	1:b:282:TYR:HB3	2.01	0.43
1:b:292:THR:HG21	1:c:282:TYR:HB3	2.01	0.43
1:b:426:ARG:NH2	1:b:428:ASP:OD2	2.44	0.43
1:d:292:THR:HG21	1:e:282:TYR:HB3	2.00	0.43
1:B:278:THR:HA	1:B:373:ARG:O	2.18	0.43
1:C:278:THR:HA	1:C:373:ARG:O	2.18	0.43
1:Y:292:THR:HG21	1:Z:282:TYR:HB3	2.00	0.43
1:c:292:THR:HG21	1:d:282:TYR:HB3	2.01	0.43
1:A:361:ASN:OD1	1:A:361:ASN:N	2.49	0.43
1:D:278:THR:HA	1:D:373:ARG:O	2.18	0.43
1:G:361:ASN:N	1:G:361:ASN:OD1	2.49	0.43
1:I:278:THR:HA	1:I:373:ARG:O	2.18	0.43
1:K:278:THR:HA	1:K:373:ARG:O	2.18	0.43
1:Q:278:THR:HA	1:Q:373:ARG:O	2.18	0.43
1:R:278:THR:HA	1:R:373:ARG:O	2.18	0.43
1:U:239:ASN:O	1:U:243:SER:OG	2.34	0.43
1:V:278:THR:HA	1:V:373:ARG:O	2.18	0.43
1:W:278:THR:HA	1:W:373:ARG:O	2.18	0.43
1:W:292:THR:HG21	1:X:282:TYR:HB3	2.00	0.43
1:X:292:THR:HG21	1:Y:282:TYR:HB3	2.00	0.43
1:e:292:THR:HG21	1:f:282:TYR:HB3	2.00	0.43
1:f:292:THR:HG21	1:g:282:TYR:HB3	2.00	0.43
1:D:292:THR:HG21	1:E:282:TYR:HB3	2.00	0.43
1:J:278:THR:HA	1:J:373:ARG:O	2.18	0.43
1:Y:278:THR:HA	1:Y:373:ARG:O	2.18	0.43
1:L:389:VAL:HB	1:L:432:VAL:HG22	1.98	0.43
1:P:426:ARG:NH2	1:P:428:ASP:OD2	2.44	0.43
1:S:361:ASN:OD1	1:S:361:ASN:N	2.49	0.43
1:V:292:THR:HG21	1:W:282:TYR:HB3	2.00	0.43
1:X:278:THR:HA	1:X:373:ARG:O	2.18	0.43
1:e:389:VAL:HB	1:e:432:VAL:HG22	1.98	0.43
1:g:292:THR:HG21	1:h:282:TYR:HB3	2.00	0.43
1:A:282:TYR:HB3	1:h:292:THR:HG21	2.01	0.43
1:K:239:ASN:O	1:K:243:SER:OG	2.34	0.43
1:N:394:LYS:H	1:N:394:LYS:HG2	1.73	0.43
1:T:292:THR:HG21	1:U:282:TYR:HB3	2.00	0.43
1:B:361:ASN:OD1	1:B:361:ASN:N	2.49	0.43
1:I:235:LEU:HD23	1:I:235:LEU:HA	1.82	0.43
1:U:292:THR:HG21	1:V:282:TYR:HB3	2.01	0.43
1:h:239:ASN:O	1:h:243:SER:OG	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:THR:HG21	1:B:282:TYR:HB3	2.01	0.43
1:P:239:ASN:O	1:P:243:SER:OG	2.34	0.43
1:A:426:ARG:NH2	1:A:428:ASP:OD2	2.44	0.42
1:E:239:ASN:O	1:E:243:SER:OG	2.34	0.42
1:H:361:ASN:OD1	1:H:361:ASN:N	2.49	0.42
1:R:361:ASN:OD1	1:R:361:ASN:N	2.49	0.42
1:Y:426:ARG:NH2	1:Y:428:ASP:OD2	2.44	0.42
1:e:235:LEU:HD23	1:e:235:LEU:HA	1.82	0.42
1:g:394:LYS:H	1:g:394:LYS:HG2	1.73	0.42
1:B:292:THR:HG21	1:C:282:TYR:HB3	2.01	0.42
1:C:361:ASN:OD1	1:C:361:ASN:N	2.49	0.42
1:D:235:LEU:HD23	1:D:235:LEU:HA	1.82	0.42
1:I:292:THR:HG21	1:J:282:TYR:HB3	2.00	0.42
1:Y:239:ASN:O	1:Y:243:SER:OG	2.34	0.42
1:C:292:THR:HG21	1:D:282:TYR:HB3	2.00	0.42
1:R:235:LEU:HD23	1:R:235:LEU:HA	1.82	0.42
1:S:292:THR:HG21	1:T:282:TYR:HB3	2.01	0.42
1:S:426:ARG:NH2	1:S:428:ASP:OD2	2.44	0.42
1:L:292:THR:HG21	1:M:282:TYR:HB3	2.01	0.42
1:M:394:LYS:H	1:M:394:LYS:HG2	1.73	0.42
1:R:292:THR:HG21	1:S:282:TYR:HB3	2.01	0.42
1:V:426:ARG:NH2	1:V:428:ASP:OD2	2.44	0.42
1:I:361:ASN:N	1:I:361:ASN:OD1	2.49	0.42
1:f:394:LYS:H	1:f:394:LYS:HG2	1.73	0.42
1:Q:292:THR:HG21	1:R:282:TYR:HB3	2.01	0.42
1:Q:361:ASN:OD1	1:Q:361:ASN:N	2.49	0.42
1:Q:378:ASN:ND2	1:Q:381:ASP:OD1	2.53	0.42
1:F:292:THR:HG21	1:G:282:TYR:HB3	2.00	0.42
1:H:378:ASN:ND2	1:H:381:ASP:OD1	2.53	0.42
1:I:378:ASN:ND2	1:I:381:ASP:OD1	2.53	0.42
1:K:292:THR:HG21	1:L:282:TYR:HB3	2.01	0.42
1:R:378:ASN:ND2	1:R:381:ASP:OD1	2.53	0.42
1:G:378:ASN:ND2	1:G:381:ASP:OD1	2.53	0.42
1:J:378:ASN:ND2	1:J:381:ASP:OD1	2.53	0.42
1:L:394:LYS:H	1:L:394:LYS:HG2	1.73	0.42
1:P:292:THR:HG21	1:Q:282:TYR:HB3	2.00	0.42
1:P:378:ASN:ND2	1:P:381:ASP:OD1	2.53	0.42
1:S:378:ASN:ND2	1:S:381:ASP:OD1	2.53	0.42
1:T:420:MET:HE2	1:T:420:MET:HB3	1.83	0.42
1:Z:378:ASN:ND2	1:Z:381:ASP:OD1	2.53	0.42
1:a:378:ASN:ND2	1:a:381:ASP:OD1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:235:LEU:HA	1:b:235:LEU:HD23	1.82	0.42
1:b:378:ASN:ND2	1:b:381:ASP:OD1	2.53	0.42
1:Y:378:ASN:ND2	1:Y:381:ASP:OD1	2.53	0.42
1:b:394:LYS:H	1:b:394:LYS:HG2	1.73	0.42
1:A:394:LYS:H	1:A:394:LYS:HG2	1.73	0.41
1:F:378:ASN:ND2	1:F:381:ASP:OD1	2.53	0.41
1:G:292:THR:HG21	1:H:282:TYR:HB3	2.00	0.41
1:K:378:ASN:ND2	1:K:381:ASP:OD1	2.53	0.41
1:P:361:ASN:OD1	1:P:361:ASN:N	2.49	0.41
1:T:378:ASN:ND2	1:T:381:ASP:OD1	2.53	0.41
1:c:239:ASN:O	1:c:243:SER:OG	2.34	0.41
1:c:378:ASN:ND2	1:c:381:ASP:OD1	2.53	0.41
1:h:378:ASN:ND2	1:h:381:ASP:OD1	2.53	0.41
1:A:378:ASN:ND2	1:A:381:ASP:OD1	2.53	0.41
1:H:292:THR:HG21	1:I:282:TYR:HB3	2.01	0.41
1:O:378:ASN:ND2	1:O:381:ASP:OD1	2.53	0.41
1:U:378:ASN:ND2	1:U:381:ASP:OD1	2.53	0.41
1:g:378:ASN:ND2	1:g:381:ASP:OD1	2.53	0.41
1:B:378:ASN:ND2	1:B:381:ASP:OD1	2.53	0.41
1:J:361:ASN:OD1	1:J:361:ASN:N	2.49	0.41
1:M:292:THR:HG21	1:N:282:TYR:HB3	2.00	0.41
1:T:426:ARG:NH2	1:T:428:ASP:OD2	2.44	0.41
1:X:378:ASN:ND2	1:X:381:ASP:OD1	2.53	0.41
1:d:378:ASN:ND2	1:d:381:ASP:OD1	2.53	0.41
1:f:378:ASN:ND2	1:f:381:ASP:OD1	2.53	0.41
1:E:378:ASN:ND2	1:E:381:ASP:OD1	2.53	0.41
1:J:292:THR:HG21	1:K:282:TYR:HB3	2.01	0.41
1:K:394:LYS:H	1:K:394:LYS:HG2	1.73	0.41
1:O:361:ASN:OD1	1:O:361:ASN:N	2.49	0.41
1:V:378:ASN:ND2	1:V:381:ASP:OD1	2.53	0.41
1:W:235:LEU:HD23	1:W:235:LEU:HA	1.82	0.41
1:W:378:ASN:ND2	1:W:381:ASP:OD1	2.53	0.41
1:d:235:LEU:HD23	1:d:235:LEU:HA	1.82	0.41
1:C:378:ASN:ND2	1:C:381:ASP:OD1	2.53	0.41
1:L:378:ASN:ND2	1:L:381:ASP:OD1	2.53	0.41
1:N:378:ASN:ND2	1:N:381:ASP:OD1	2.53	0.41
1:T:239:ASN:O	1:T:243:SER:OG	2.34	0.41
1:A:425:LYS:HE3	1:A:425:LYS:HB2	1.93	0.41
1:D:378:ASN:ND2	1:D:381:ASP:OD1	2.53	0.41
1:G:235:LEU:HA	1:G:235:LEU:HD23	1.82	0.41
1:M:235:LEU:HD23	1:M:235:LEU:HA	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:361:ASN:N	1:N:361:ASN:OD1	2.49	0.41
1:R:420:MET:HE2	1:R:420:MET:HB3	1.83	0.41
1:U:394:LYS:H	1:U:394:LYS:HG2	1.73	0.41
1:b:420:MET:HE2	1:b:420:MET:HB3	1.83	0.41
1:e:378:ASN:ND2	1:e:381:ASP:OD1	2.53	0.41
1:M:361:ASN:OD1	1:M:361:ASN:N	2.49	0.41
1:S:394:LYS:H	1:S:394:LYS:HG2	1.73	0.41
1:b:239:ASN:O	1:b:243:SER:OG	2.34	0.41
1:f:426:ARG:NH2	1:f:428:ASP:OD2	2.44	0.41
1:h:394:LYS:H	1:h:394:LYS:HG2	1.73	0.41
1:D:239:ASN:O	1:D:243:SER:OG	2.34	0.41
1:J:394:LYS:H	1:J:394:LYS:HG2	1.73	0.41
1:W:394:LYS:H	1:W:394:LYS:HG2	1.73	0.41
1:a:235:LEU:HA	1:a:235:LEU:HD23	1.82	0.41
1:d:394:LYS:H	1:d:394:LYS:HG2	1.73	0.41
1:d:420:MET:HB3	1:d:420:MET:HE2	1.83	0.41
1:C:235:LEU:HD23	1:C:235:LEU:HA	1.82	0.41
1:C:394:LYS:H	1:C:394:LYS:HG2	1.73	0.41
1:M:378:ASN:ND2	1:M:381:ASP:OD1	2.53	0.41
1:N:239:ASN:O	1:N:243:SER:OG	2.34	0.41
1:O:239:ASN:O	1:O:243:SER:OG	2.34	0.41
1:g:239:ASN:O	1:g:243:SER:OG	2.34	0.41
1:E:292:THR:HG21	1:F:282:TYR:HB3	2.02	0.41
1:I:394:LYS:H	1:I:394:LYS:HG2	1.73	0.40
1:L:235:LEU:HA	1:L:235:LEU:HD23	1.82	0.40
1:B:394:LYS:H	1:B:394:LYS:HG2	1.73	0.40
1:E:394:LYS:H	1:E:394:LYS:HG2	1.73	0.40
1:H:426:ARG:NH2	1:H:428:ASP:OD2	2.44	0.40
1:L:420:MET:HE2	1:L:420:MET:HB3	1.83	0.40
1:N:367:GLU:HG2	1:O:282:TYR:CE1	2.56	0.40
1:R:394:LYS:H	1:R:394:LYS:HG2	1.73	0.40
1:e:426:ARG:NH2	1:e:428:ASP:OD2	2.44	0.40
1:B:425:LYS:HE3	1:B:425:LYS:HB2	1.93	0.40
1:O:292:THR:HG21	1:P:282:TYR:HB3	2.02	0.40
1:Y:394:LYS:H	1:Y:394:LYS:HG2	1.73	0.40
1:Z:235:LEU:HA	1:Z:235:LEU:HD23	1.82	0.40
1:E:294:ARG:HE	1:E:294:ARG:HB2	1.76	0.40
1:G:394:LYS:H	1:G:394:LYS:HG2	1.73	0.40
1:H:235:LEU:HD23	1:H:235:LEU:HA	1.82	0.40
1:H:394:LYS:H	1:H:394:LYS:HG2	1.73	0.40
1:I:420:MET:HE2	1:I:420:MET:HB3	1.83	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:420:MET:HE2	1:K:420:MET:HB3	1.83	0.40
1:Q:394:LYS:H	1:Q:394:LYS:HG2	1.73	0.40
1:D:294:ARG:HE	1:D:294:ARG:HB2	1.76	0.40
1:L:426:ARG:NH2	1:L:428:ASP:OD2	2.44	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	153/560 (27%)	150 (98%)	3 (2%)	0	100	100
1	B	153/560 (27%)	150 (98%)	3 (2%)	0	100	100
1	C	153/560 (27%)	150 (98%)	3 (2%)	0	100	100
1	D	153/560 (27%)	150 (98%)	3 (2%)	0	100	100
1	E	153/560 (27%)	149 (97%)	4 (3%)	0	100	100
1	F	153/560 (27%)	150 (98%)	3 (2%)	0	100	100
1	G	153/560 (27%)	150 (98%)	3 (2%)	0	100	100
1	H	153/560 (27%)	150 (98%)	3 (2%)	0	100	100
1	I	153/560 (27%)	150 (98%)	3 (2%)	0	100	100
1	J	153/560 (27%)	149 (97%)	4 (3%)	0	100	100
1	K	153/560 (27%)	150 (98%)	3 (2%)	0	100	100
1	L	153/560 (27%)	150 (98%)	3 (2%)	0	100	100
1	M	153/560 (27%)	149 (97%)	4 (3%)	0	100	100
1	N	153/560 (27%)	149 (97%)	4 (3%)	0	100	100
1	O	153/560 (27%)	150 (98%)	3 (2%)	0	100	100
1	P	153/560 (27%)	150 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Q	153/560 (27%)	149 (97%)	4 (3%)	0	100	100
1	R	153/560 (27%)	150 (98%)	3 (2%)	0	100	100
1	S	153/560 (27%)	150 (98%)	3 (2%)	0	100	100
1	T	153/560 (27%)	150 (98%)	3 (2%)	0	100	100
1	U	153/560 (27%)	150 (98%)	3 (2%)	0	100	100
1	V	153/560 (27%)	150 (98%)	3 (2%)	0	100	100
1	W	153/560 (27%)	150 (98%)	3 (2%)	0	100	100
1	X	153/560 (27%)	150 (98%)	3 (2%)	0	100	100
1	Y	153/560 (27%)	150 (98%)	3 (2%)	0	100	100
1	Z	153/560 (27%)	150 (98%)	3 (2%)	0	100	100
1	a	153/560 (27%)	149 (97%)	4 (3%)	0	100	100
1	b	153/560 (27%)	150 (98%)	3 (2%)	0	100	100
1	c	153/560 (27%)	150 (98%)	3 (2%)	0	100	100
1	d	153/560 (27%)	149 (97%)	4 (3%)	0	100	100
1	e	153/560 (27%)	149 (97%)	4 (3%)	0	100	100
1	f	153/560 (27%)	150 (98%)	3 (2%)	0	100	100
1	g	153/560 (27%)	150 (98%)	3 (2%)	0	100	100
1	h	153/560 (27%)	149 (97%)	4 (3%)	0	100	100
All	All	5202/19040 (27%)	5091 (98%)	111 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	141/467 (30%)	130 (92%)	11 (8%)	11	37
1	B	141/467 (30%)	130 (92%)	11 (8%)	11	37
1	C	141/467 (30%)	130 (92%)	11 (8%)	11	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	141/467 (30%)	130 (92%)	11 (8%)	11	37
1	E	141/467 (30%)	130 (92%)	11 (8%)	11	37
1	F	141/467 (30%)	130 (92%)	11 (8%)	11	37
1	G	141/467 (30%)	130 (92%)	11 (8%)	11	37
1	H	141/467 (30%)	130 (92%)	11 (8%)	11	37
1	I	141/467 (30%)	130 (92%)	11 (8%)	11	37
1	J	141/467 (30%)	130 (92%)	11 (8%)	11	37
1	K	141/467 (30%)	130 (92%)	11 (8%)	11	37
1	L	141/467 (30%)	130 (92%)	11 (8%)	11	37
1	M	141/467 (30%)	130 (92%)	11 (8%)	11	37
1	N	141/467 (30%)	130 (92%)	11 (8%)	11	37
1	O	141/467 (30%)	131 (93%)	10 (7%)	13	40
1	P	141/467 (30%)	130 (92%)	11 (8%)	11	37
1	Q	141/467 (30%)	130 (92%)	11 (8%)	11	37
1	R	141/467 (30%)	130 (92%)	11 (8%)	11	37
1	S	141/467 (30%)	130 (92%)	11 (8%)	11	37
1	T	141/467 (30%)	130 (92%)	11 (8%)	11	37
1	U	141/467 (30%)	130 (92%)	11 (8%)	11	37
1	V	141/467 (30%)	130 (92%)	11 (8%)	11	37
1	W	141/467 (30%)	130 (92%)	11 (8%)	11	37
1	X	141/467 (30%)	130 (92%)	11 (8%)	11	37
1	Y	141/467 (30%)	130 (92%)	11 (8%)	11	37
1	Z	141/467 (30%)	130 (92%)	11 (8%)	11	37
1	a	141/467 (30%)	130 (92%)	11 (8%)	11	37
1	b	141/467 (30%)	130 (92%)	11 (8%)	11	37
1	c	141/467 (30%)	130 (92%)	11 (8%)	11	37
1	d	141/467 (30%)	130 (92%)	11 (8%)	11	37
1	e	141/467 (30%)	130 (92%)	11 (8%)	11	37
1	f	141/467 (30%)	130 (92%)	11 (8%)	11	37
1	g	141/467 (30%)	130 (92%)	11 (8%)	11	37
1	h	141/467 (30%)	130 (92%)	11 (8%)	11	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	4794/15878 (30%)	4421 (92%)	373 (8%)	14	37

All (373) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	243	SER
1	A	252	ILE
1	A	274	ASN
1	A	287	ASP
1	A	299	ASN
1	A	358	THR
1	A	361	ASN
1	A	369	ASP
1	A	400	LYS
1	A	416	THR
1	A	435	SER
1	B	243	SER
1	B	252	ILE
1	B	274	ASN
1	B	287	ASP
1	B	299	ASN
1	B	358	THR
1	B	361	ASN
1	B	369	ASP
1	B	400	LYS
1	B	416	THR
1	B	435	SER
1	C	243	SER
1	C	252	ILE
1	C	274	ASN
1	C	287	ASP
1	C	299	ASN
1	C	358	THR
1	C	361	ASN
1	C	369	ASP
1	C	400	LYS
1	C	416	THR
1	C	435	SER
1	D	243	SER
1	D	252	ILE
1	D	274	ASN
1	D	287	ASP

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Mol	Chain	Res	Type
1	D	299	ASN
1	D	358	THR
1	D	361	ASN
1	D	369	ASP
1	D	400	LYS
1	D	416	THR
1	D	435	SER
1	E	243	SER
1	E	252	ILE
1	E	274	ASN
1	E	287	ASP
1	E	299	ASN
1	E	358	THR
1	E	361	ASN
1	E	369	ASP
1	E	400	LYS
1	E	416	THR
1	E	435	SER
1	F	243	SER
1	F	252	ILE
1	F	274	ASN
1	F	287	ASP
1	F	299	ASN
1	F	358	THR
1	F	361	ASN
1	F	369	ASP
1	F	400	LYS
1	F	416	THR
1	F	435	SER
1	G	243	SER
1	G	252	ILE
1	G	274	ASN
1	G	287	ASP
1	G	299	ASN
1	G	358	THR
1	G	361	ASN
1	G	369	ASP
1	G	400	LYS
1	G	416	THR
1	G	435	SER
1	H	243	SER
1	H	252	ILE

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Mol	Chain	Res	Type
1	H	274	ASN
1	H	287	ASP
1	H	299	ASN
1	H	358	THR
1	H	361	ASN
1	H	369	ASP
1	H	400	LYS
1	H	416	THR
1	H	435	SER
1	I	243	SER
1	I	252	ILE
1	I	274	ASN
1	I	287	ASP
1	I	299	ASN
1	I	358	THR
1	I	361	ASN
1	I	369	ASP
1	I	400	LYS
1	I	416	THR
1	I	435	SER
1	J	243	SER
1	J	252	ILE
1	J	274	ASN
1	J	287	ASP
1	J	299	ASN
1	J	358	THR
1	J	361	ASN
1	J	369	ASP
1	J	400	LYS
1	J	416	THR
1	J	435	SER
1	K	243	SER
1	K	252	ILE
1	K	274	ASN
1	K	287	ASP
1	K	299	ASN
1	K	358	THR
1	K	361	ASN
1	K	369	ASP
1	K	400	LYS
1	K	416	THR
1	K	435	SER

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Mol	Chain	Res	Type
1	L	243	SER
1	L	252	ILE
1	L	274	ASN
1	L	287	ASP
1	L	299	ASN
1	L	358	THR
1	L	361	ASN
1	L	369	ASP
1	L	400	LYS
1	L	416	THR
1	L	435	SER
1	M	243	SER
1	M	252	ILE
1	M	274	ASN
1	M	287	ASP
1	M	299	ASN
1	M	358	THR
1	M	361	ASN
1	M	369	ASP
1	M	400	LYS
1	M	416	THR
1	M	435	SER
1	N	243	SER
1	N	252	ILE
1	N	274	ASN
1	N	287	ASP
1	N	299	ASN
1	N	358	THR
1	N	361	ASN
1	N	369	ASP
1	N	400	LYS
1	N	416	THR
1	N	435	SER
1	O	243	SER
1	O	252	ILE
1	O	274	ASN
1	O	287	ASP
1	O	299	ASN
1	O	358	THR
1	O	361	ASN
1	O	369	ASP
1	O	400	LYS

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Mol	Chain	Res	Type
1	O	435	SER
1	P	243	SER
1	P	252	ILE
1	P	274	ASN
1	P	287	ASP
1	P	299	ASN
1	P	358	THR
1	P	361	ASN
1	P	369	ASP
1	P	400	LYS
1	P	416	THR
1	P	435	SER
1	Q	243	SER
1	Q	252	ILE
1	Q	274	ASN
1	Q	287	ASP
1	Q	299	ASN
1	Q	358	THR
1	Q	361	ASN
1	Q	369	ASP
1	Q	400	LYS
1	Q	416	THR
1	Q	435	SER
1	R	243	SER
1	R	252	ILE
1	R	274	ASN
1	R	287	ASP
1	R	299	ASN
1	R	358	THR
1	R	361	ASN
1	R	369	ASP
1	R	400	LYS
1	R	416	THR
1	R	435	SER
1	S	243	SER
1	S	252	ILE
1	S	274	ASN
1	S	287	ASP
1	S	299	ASN
1	S	358	THR
1	S	361	ASN
1	S	369	ASP

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Mol	Chain	Res	Type
1	S	400	LYS
1	S	416	THR
1	S	435	SER
1	T	243	SER
1	T	252	ILE
1	T	274	ASN
1	T	287	ASP
1	T	299	ASN
1	T	358	THR
1	T	361	ASN
1	T	369	ASP
1	T	400	LYS
1	T	416	THR
1	T	435	SER
1	U	243	SER
1	U	252	ILE
1	U	274	ASN
1	U	287	ASP
1	U	299	ASN
1	U	358	THR
1	U	361	ASN
1	U	369	ASP
1	U	400	LYS
1	U	416	THR
1	U	435	SER
1	V	243	SER
1	V	252	ILE
1	V	274	ASN
1	V	287	ASP
1	V	299	ASN
1	V	358	THR
1	V	361	ASN
1	V	369	ASP
1	V	400	LYS
1	V	416	THR
1	V	435	SER
1	W	243	SER
1	W	252	ILE
1	W	274	ASN
1	W	287	ASP
1	W	299	ASN
1	W	358	THR

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Mol	Chain	Res	Type
1	W	361	ASN
1	W	369	ASP
1	W	400	LYS
1	W	416	THR
1	W	435	SER
1	X	243	SER
1	X	252	ILE
1	X	274	ASN
1	X	287	ASP
1	X	299	ASN
1	X	358	THR
1	X	361	ASN
1	X	369	ASP
1	X	400	LYS
1	X	416	THR
1	X	435	SER
1	Y	243	SER
1	Y	252	ILE
1	Y	274	ASN
1	Y	287	ASP
1	Y	299	ASN
1	Y	358	THR
1	Y	361	ASN
1	Y	369	ASP
1	Y	400	LYS
1	Y	416	THR
1	Y	435	SER
1	Z	243	SER
1	Z	252	ILE
1	Z	274	ASN
1	Z	287	ASP
1	Z	299	ASN
1	Z	358	THR
1	Z	361	ASN
1	Z	369	ASP
1	Z	400	LYS
1	Z	416	THR
1	Z	435	SER
1	a	243	SER
1	a	252	ILE
1	a	274	ASN
1	a	287	ASP

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Mol	Chain	Res	Type
1	a	299	ASN
1	a	358	THR
1	a	361	ASN
1	a	369	ASP
1	a	400	LYS
1	a	416	THR
1	a	435	SER
1	b	243	SER
1	b	252	ILE
1	b	274	ASN
1	b	287	ASP
1	b	299	ASN
1	b	358	THR
1	b	361	ASN
1	b	369	ASP
1	b	400	LYS
1	b	416	THR
1	b	435	SER
1	c	243	SER
1	c	252	ILE
1	c	274	ASN
1	c	287	ASP
1	c	299	ASN
1	c	358	THR
1	c	361	ASN
1	c	369	ASP
1	c	400	LYS
1	c	416	THR
1	c	435	SER
1	d	243	SER
1	d	252	ILE
1	d	274	ASN
1	d	287	ASP
1	d	299	ASN
1	d	358	THR
1	d	361	ASN
1	d	369	ASP
1	d	400	LYS
1	d	416	THR
1	d	435	SER
1	e	243	SER
1	e	252	ILE

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Mol	Chain	Res	Type
1	e	274	ASN
1	e	287	ASP
1	e	299	ASN
1	e	358	THR
1	e	361	ASN
1	e	369	ASP
1	e	400	LYS
1	e	416	THR
1	e	435	SER
1	f	243	SER
1	f	252	ILE
1	f	274	ASN
1	f	287	ASP
1	f	299	ASN
1	f	358	THR
1	f	361	ASN
1	f	369	ASP
1	f	400	LYS
1	f	416	THR
1	f	435	SER
1	g	243	SER
1	g	252	ILE
1	g	274	ASN
1	g	287	ASP
1	g	299	ASN
1	g	358	THR
1	g	361	ASN
1	g	369	ASP
1	g	400	LYS
1	g	416	THR
1	g	435	SER
1	h	243	SER
1	h	252	ILE
1	h	274	ASN
1	h	287	ASP
1	h	299	ASN
1	h	358	THR
1	h	361	ASN
1	h	369	ASP
1	h	400	LYS
1	h	416	THR
1	h	435	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	434	ASN
1	B	434	ASN
1	C	434	ASN
1	D	434	ASN
1	E	434	ASN
1	F	359	GLN
1	F	434	ASN
1	G	434	ASN
1	H	434	ASN
1	I	359	GLN
1	J	434	ASN
1	K	434	ASN
1	L	434	ASN
1	M	434	ASN
1	N	359	GLN
1	N	434	ASN
1	O	434	ASN
1	P	359	GLN
1	P	434	ASN
1	Q	359	GLN
1	R	434	ASN
1	S	359	GLN
1	S	434	ASN
1	T	434	ASN
1	U	359	GLN
1	U	434	ASN
1	V	434	ASN
1	W	359	GLN
1	W	434	ASN
1	X	359	GLN
1	X	434	ASN
1	Y	359	GLN
1	Y	434	ASN
1	Z	359	GLN
1	Z	434	ASN
1	a	359	GLN
1	a	434	ASN
1	b	259	ASN
1	b	359	GLN
1	b	434	ASN
1	c	434	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	d	434	ASN
1	e	434	ASN
1	f	359	GLN
1	f	434	ASN
1	g	434	ASN
1	h	359	GLN
1	h	434	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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.

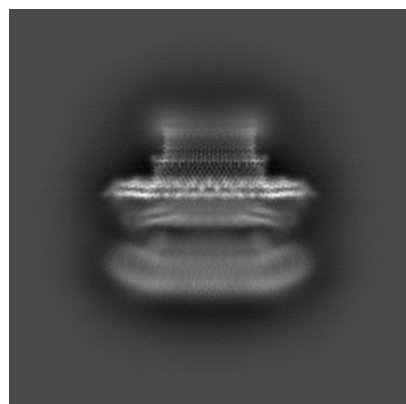
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30612. These allow visual inspection of the internal detail of the map and identification of artifacts.

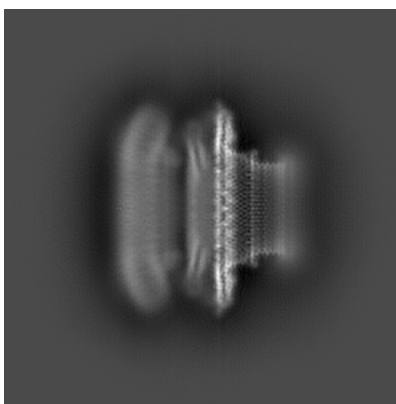
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

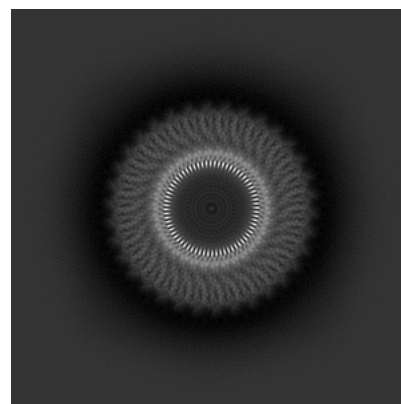
6.1.1 Primary map



X

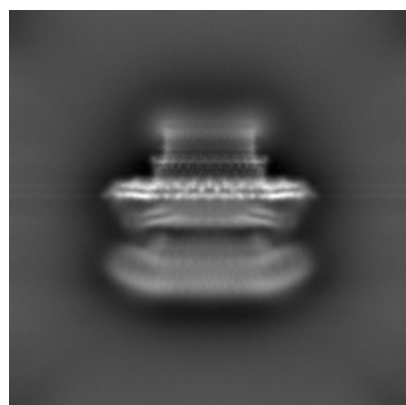


Y

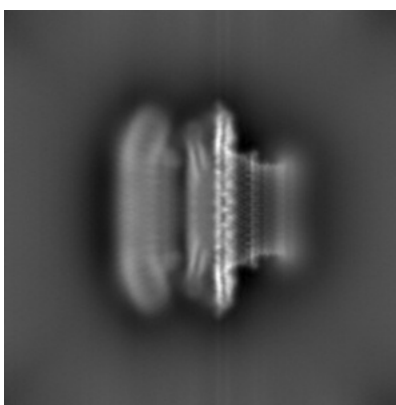


Z

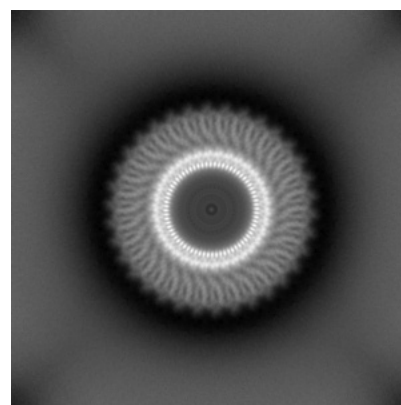
6.1.2 Raw map



X



Y

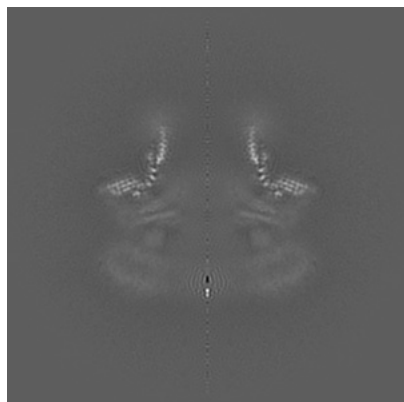


Z

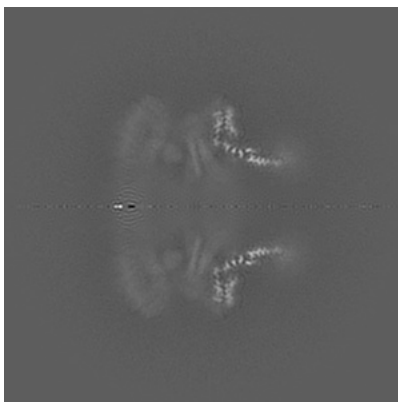
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

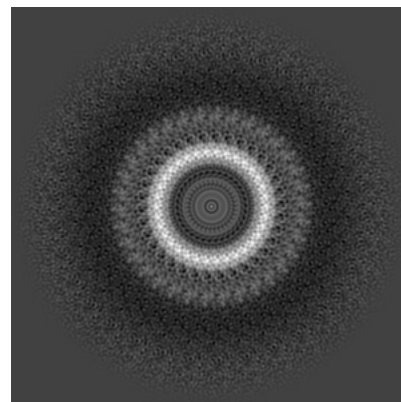
6.2.1 Primary map



X Index: 216

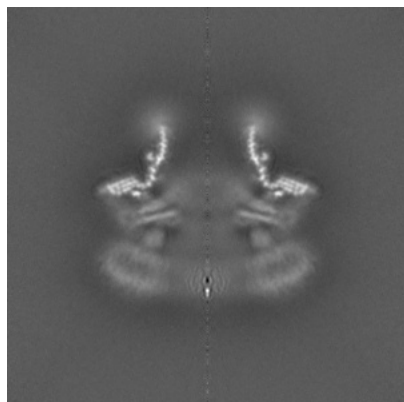


Y Index: 216

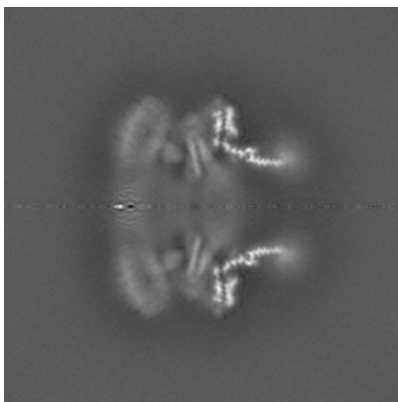


Z Index: 216

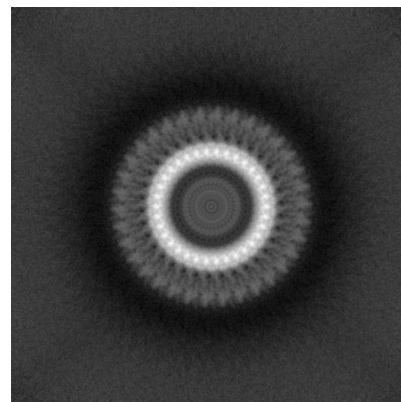
6.2.2 Raw map



X Index: 216



Y Index: 216

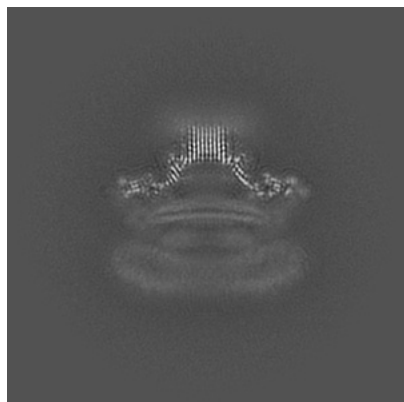


Z Index: 216

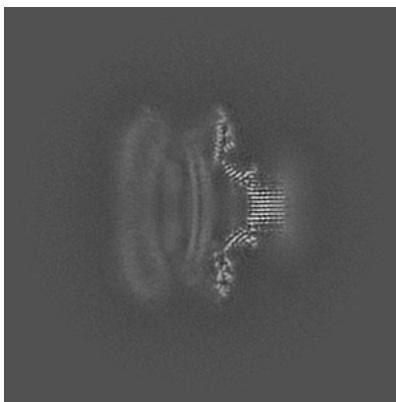
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

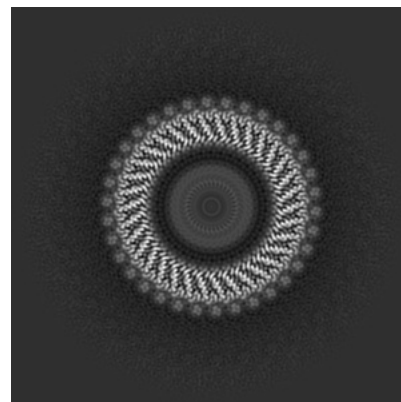
6.3.1 Primary map



X Index: 169

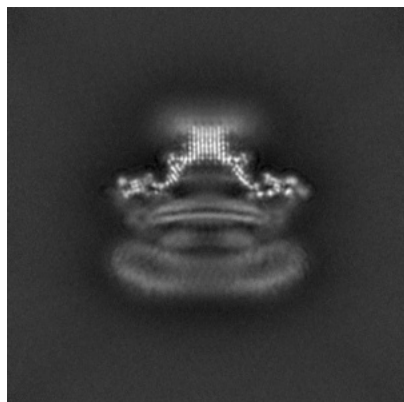


Y Index: 168

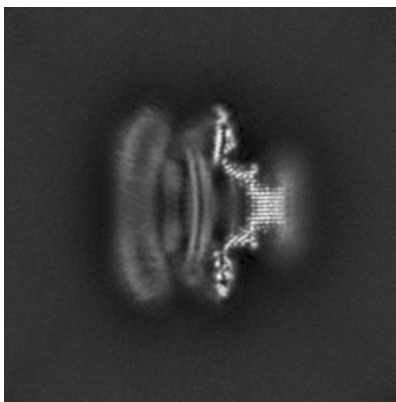


Z Index: 231

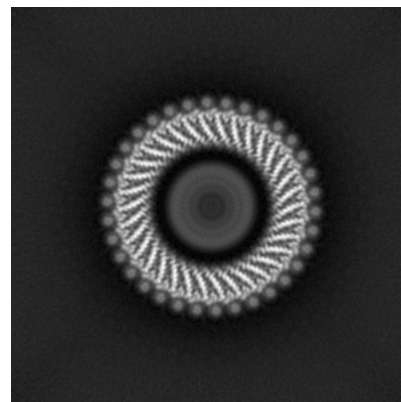
6.3.2 Raw map



X Index: 169



Y Index: 169

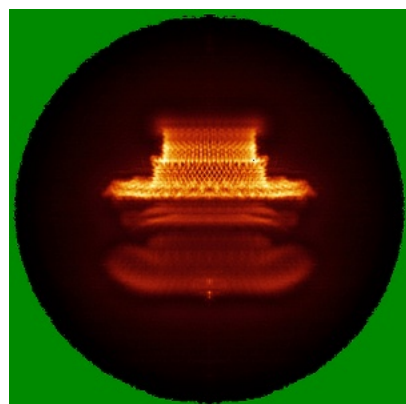


Z Index: 231

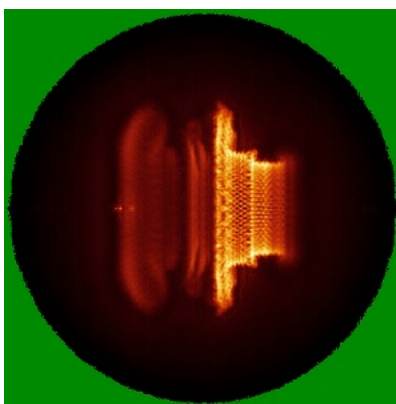
The images above show the largest variance slices of the map in three orthogonal directions.

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

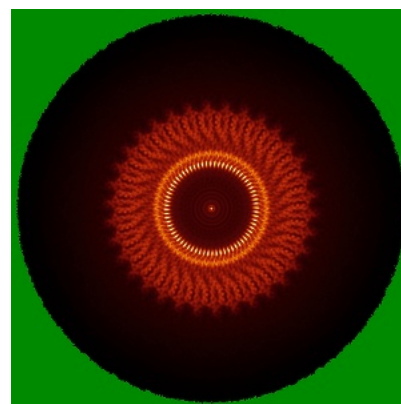
6.4.1 Primary map



X

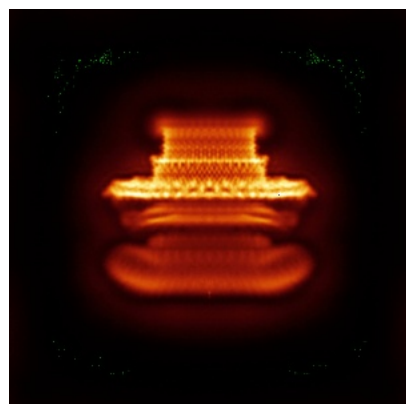


Y

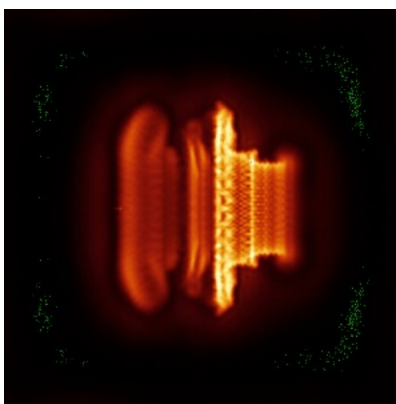


Z

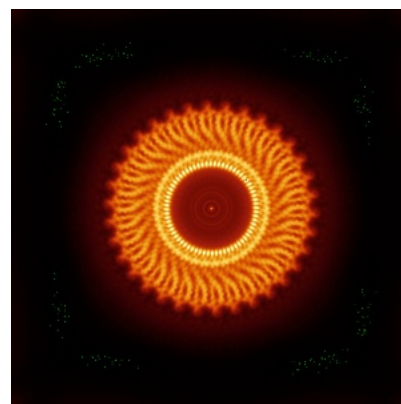
6.4.2 Raw map



X



Y

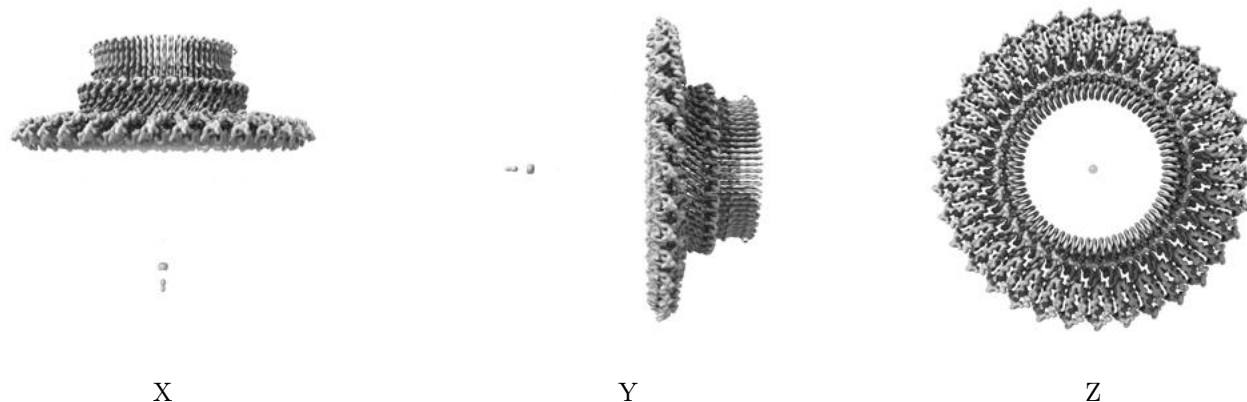


Z

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.

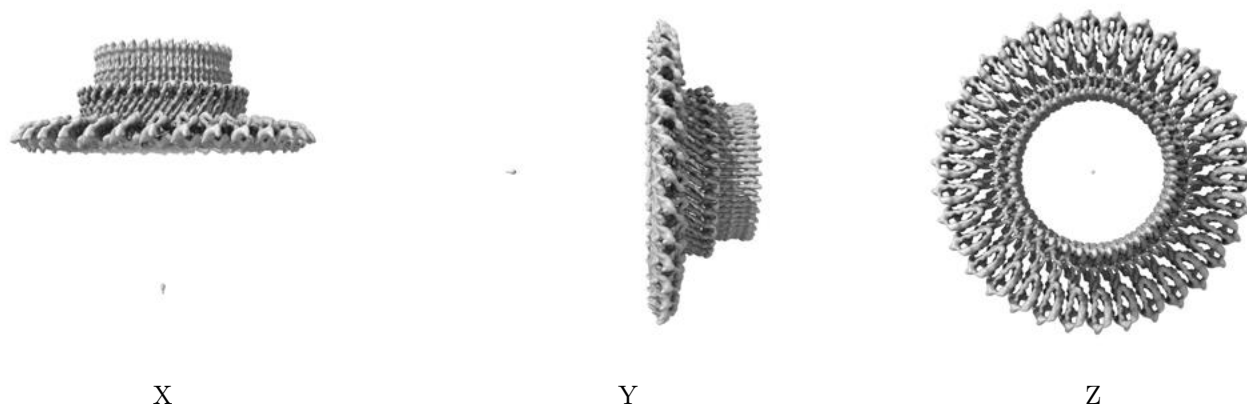
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.749. 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.

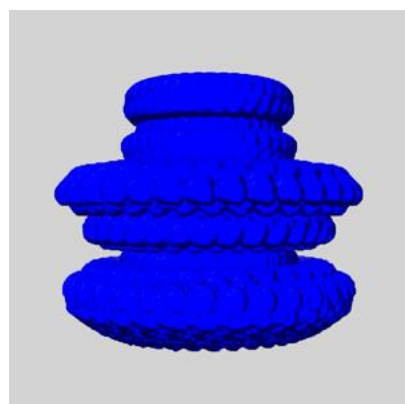
6.6 Mask visualisation [i](#)

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

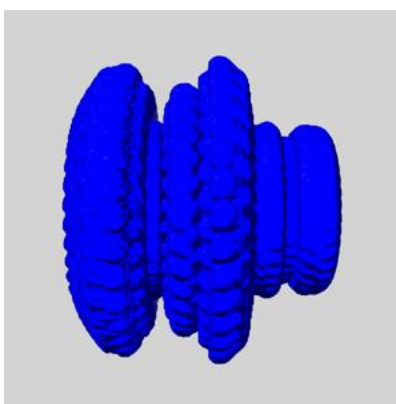
A mask typically either:

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

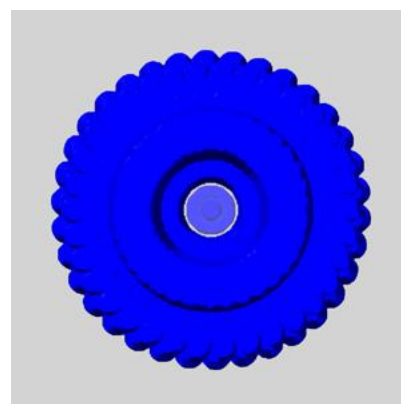
6.6.1 emd_30612_msk_1.map [i](#)



X



Y

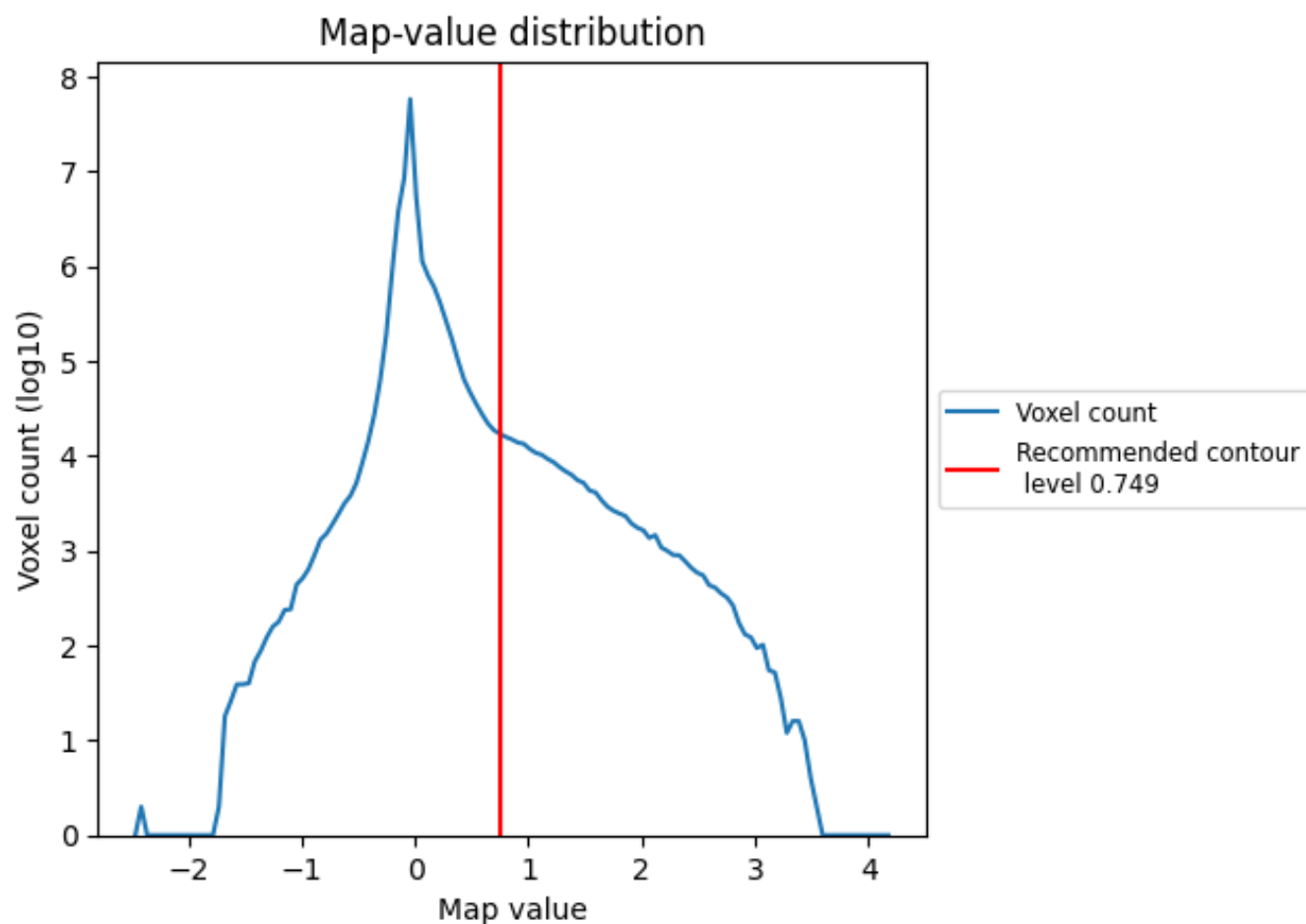


Z

7 Map analysis [i](#)

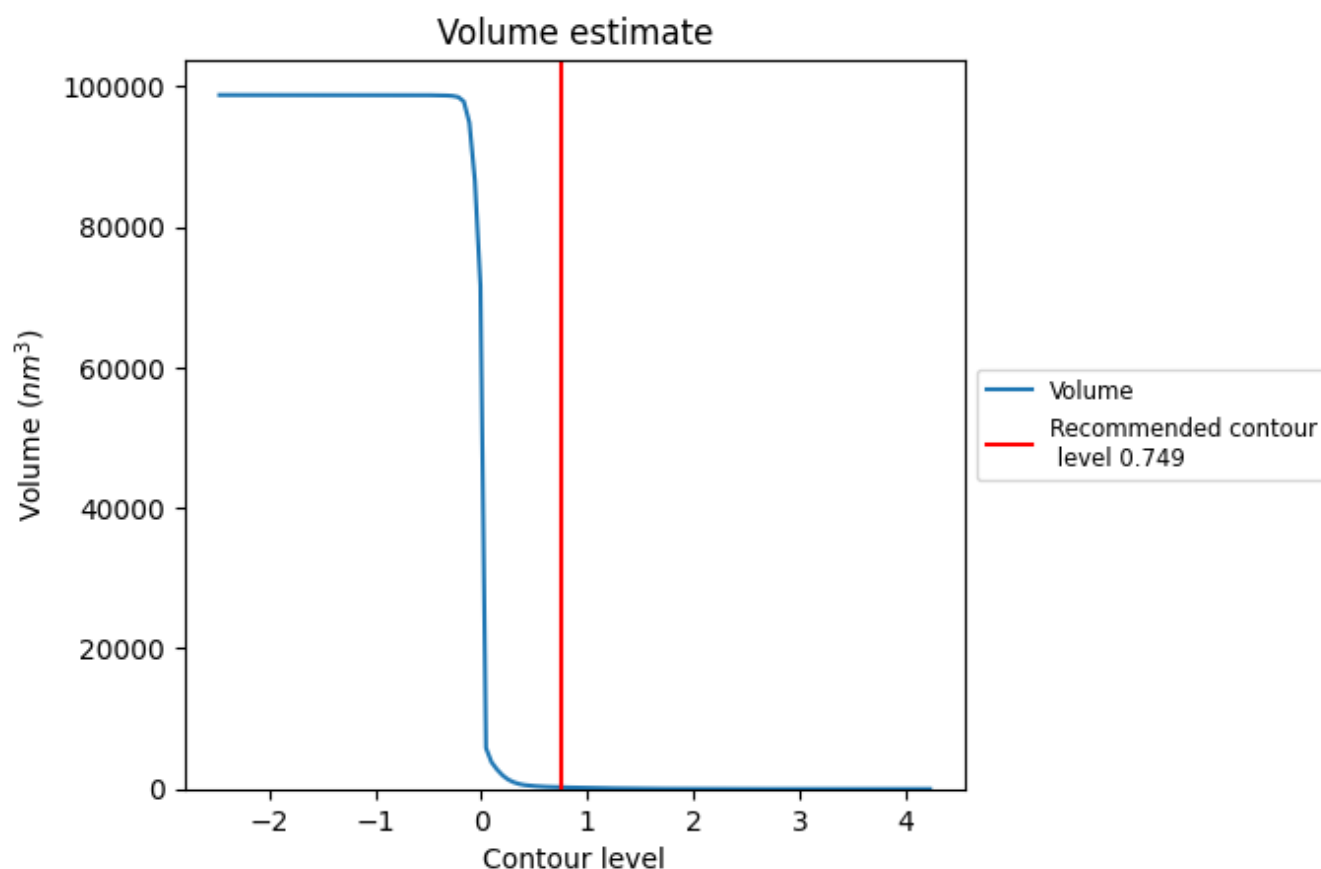
This section contains the results of statistical analysis of the map.

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.

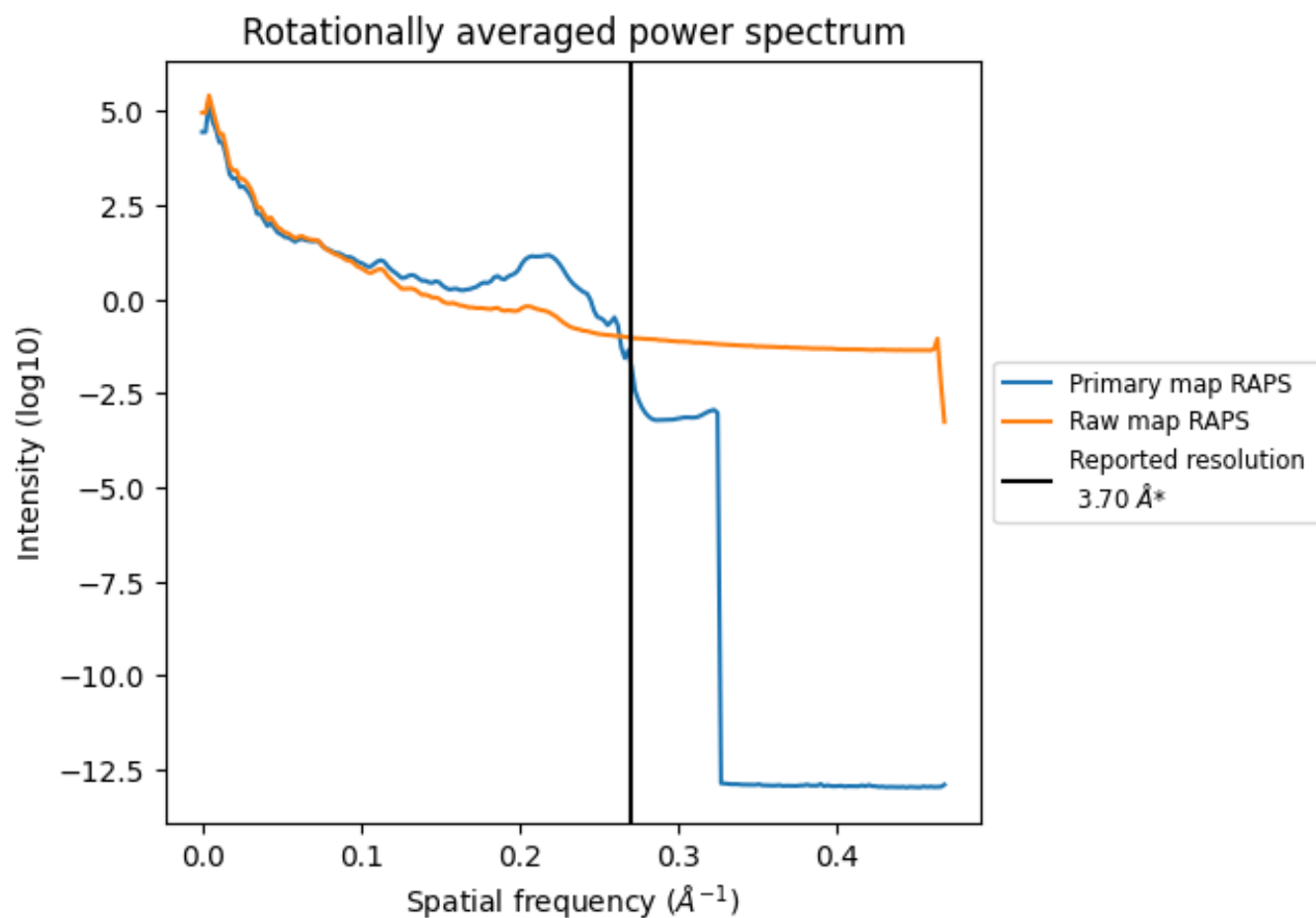
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 241 nm³; this corresponds to an approximate mass of 218 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 ⓘ

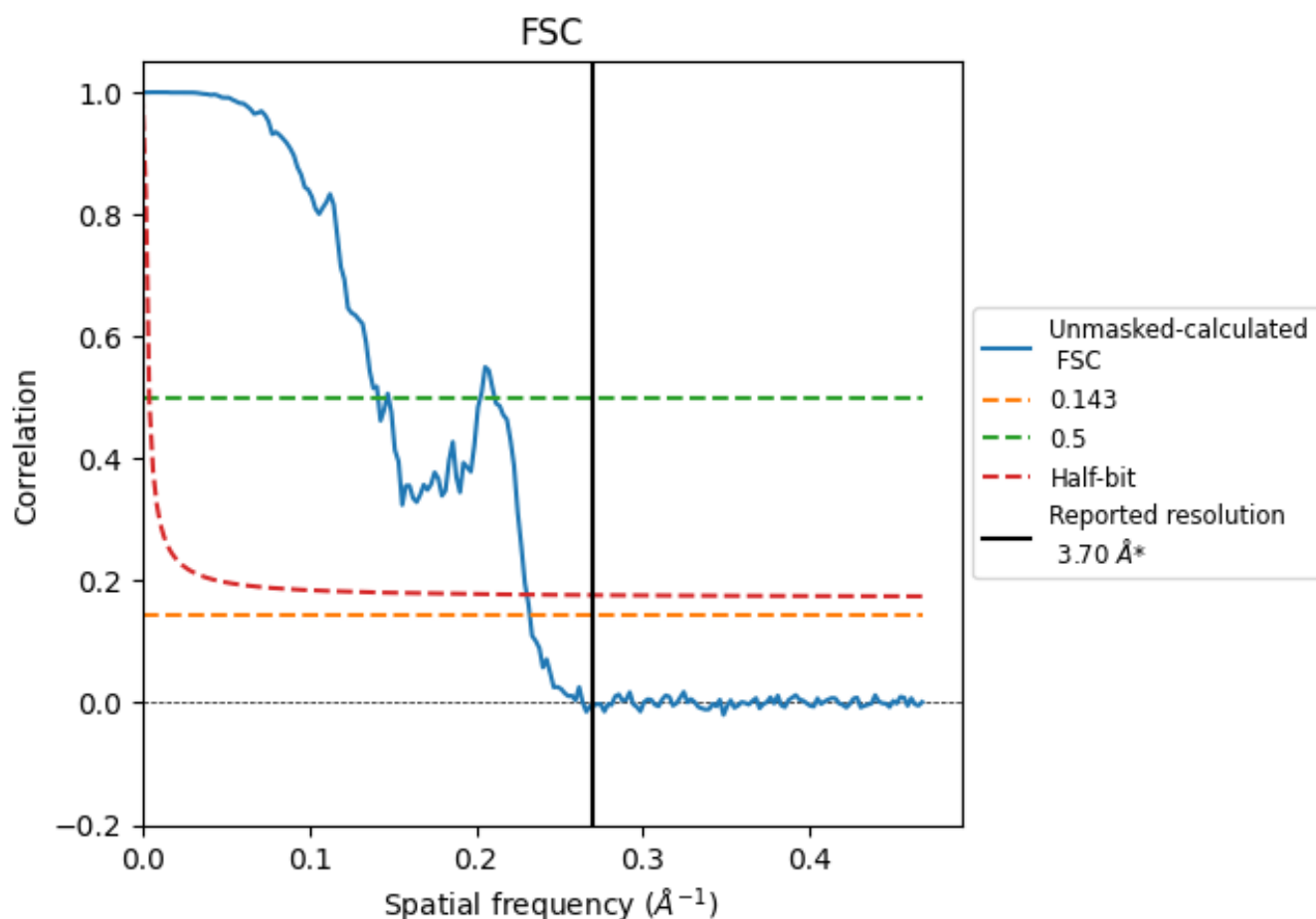


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

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 $0.270 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

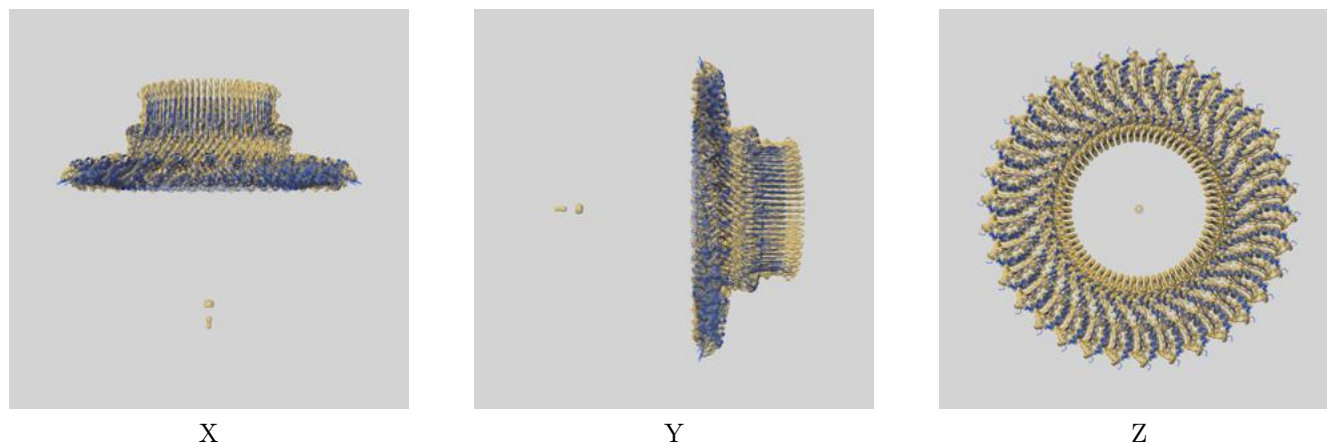
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.31	7.08	4.34

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.31 differs from the reported value 3.7 by more than 10 %

9 Map-model fit [i](#)

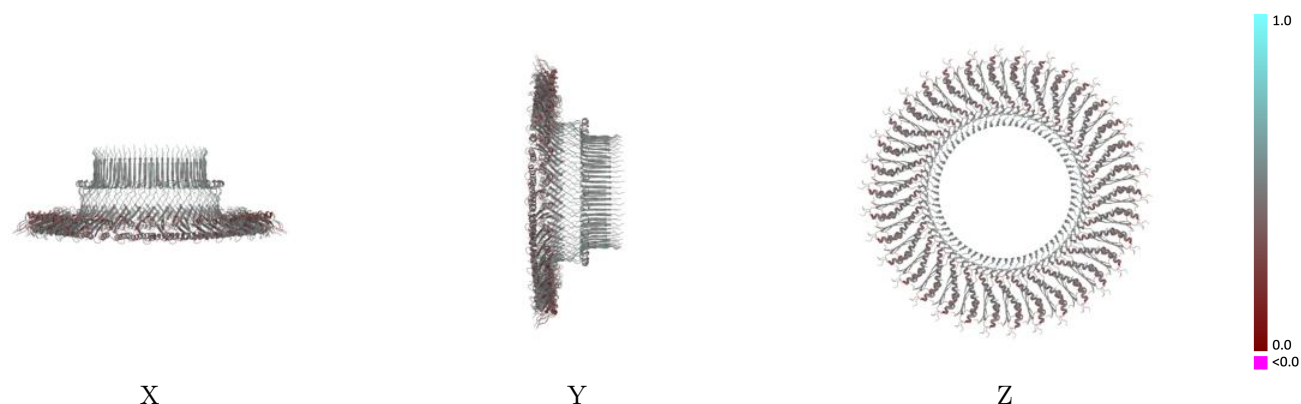
This section contains information regarding the fit between EMDB map EMD-30612 and PDB model 7D84. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



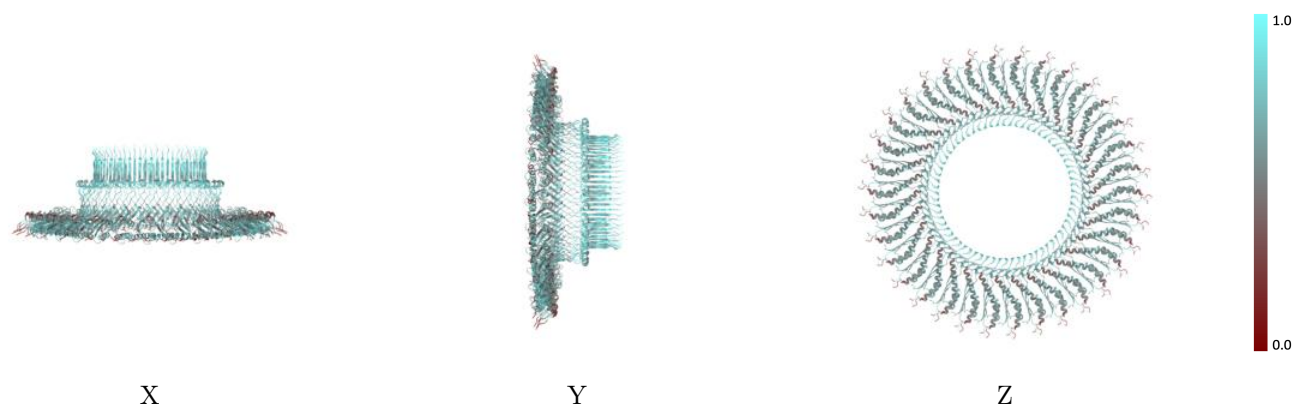
The images above show the 3D surface view of the map at the recommended contour level 0.749 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



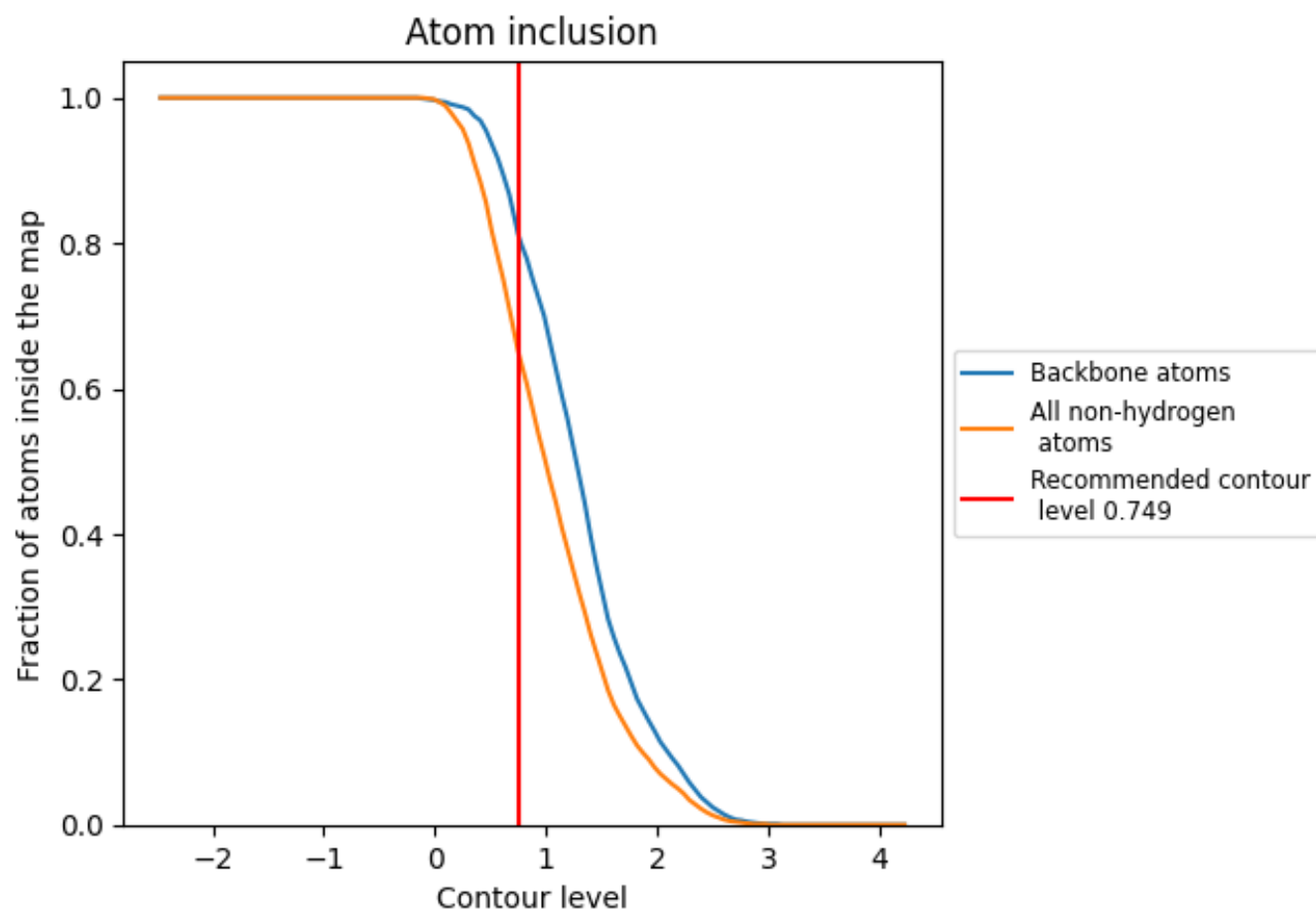
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.749).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 65% 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 (0.749) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6520	 0.4470
A	 0.6540	 0.4460
B	 0.6500	 0.4460
C	 0.6510	 0.4470
D	 0.6530	 0.4470
E	 0.6500	 0.4460
F	 0.6550	 0.4480
G	 0.6550	 0.4490
H	 0.6460	 0.4490
I	 0.6510	 0.4490
J	 0.6510	 0.4490
K	 0.6540	 0.4500
L	 0.6520	 0.4500
M	 0.6550	 0.4490
N	 0.6490	 0.4480
O	 0.6580	 0.4460
P	 0.6510	 0.4490
Q	 0.6510	 0.4480
R	 0.6520	 0.4490
S	 0.6500	 0.4480
T	 0.6480	 0.4480
U	 0.6530	 0.4480
V	 0.6510	 0.4460
W	 0.6540	 0.4460
X	 0.6550	 0.4460
Y	 0.6450	 0.4460
Z	 0.6520	 0.4460
a	 0.6510	 0.4460
b	 0.6540	 0.4450
c	 0.6520	 0.4450
d	 0.6550	 0.4440
e	 0.6490	 0.4450
f	 0.6540	 0.4460
g	 0.6510	 0.4460
h	 0.6500	 0.4450

