



wwPDB EM Validation Summary Report ⓘ

Mar 23, 2026 – 05:54 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 wwPDB EM Validation Summary 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:

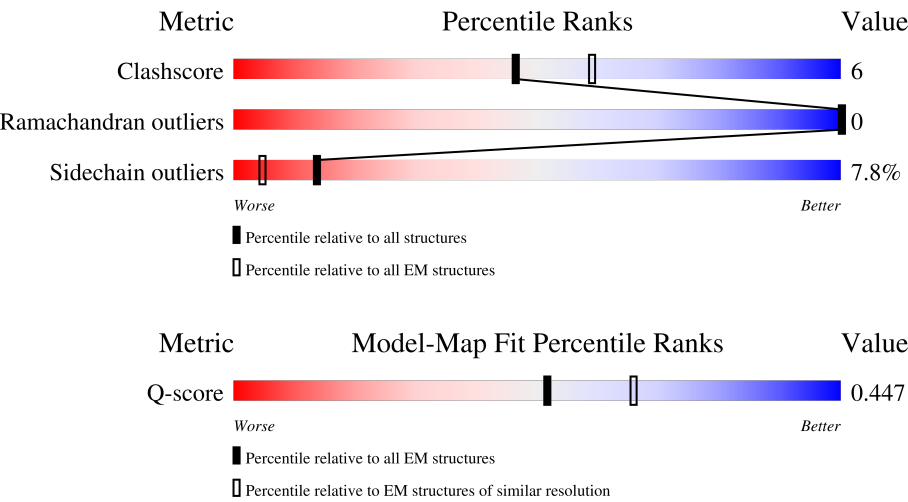
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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.



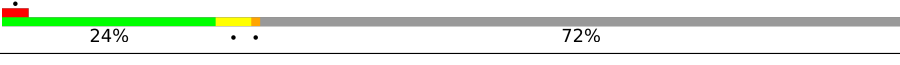
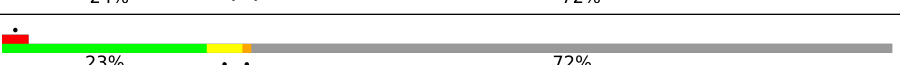
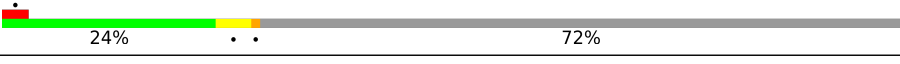
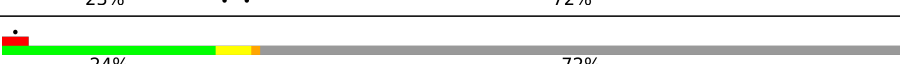
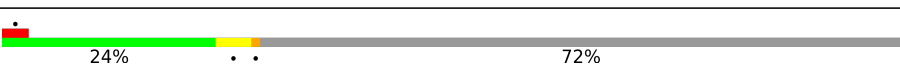
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11569 (3.20 - 4.20)

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	
1	e	560	
1	f	560	
1	g	560	
1	h	560	

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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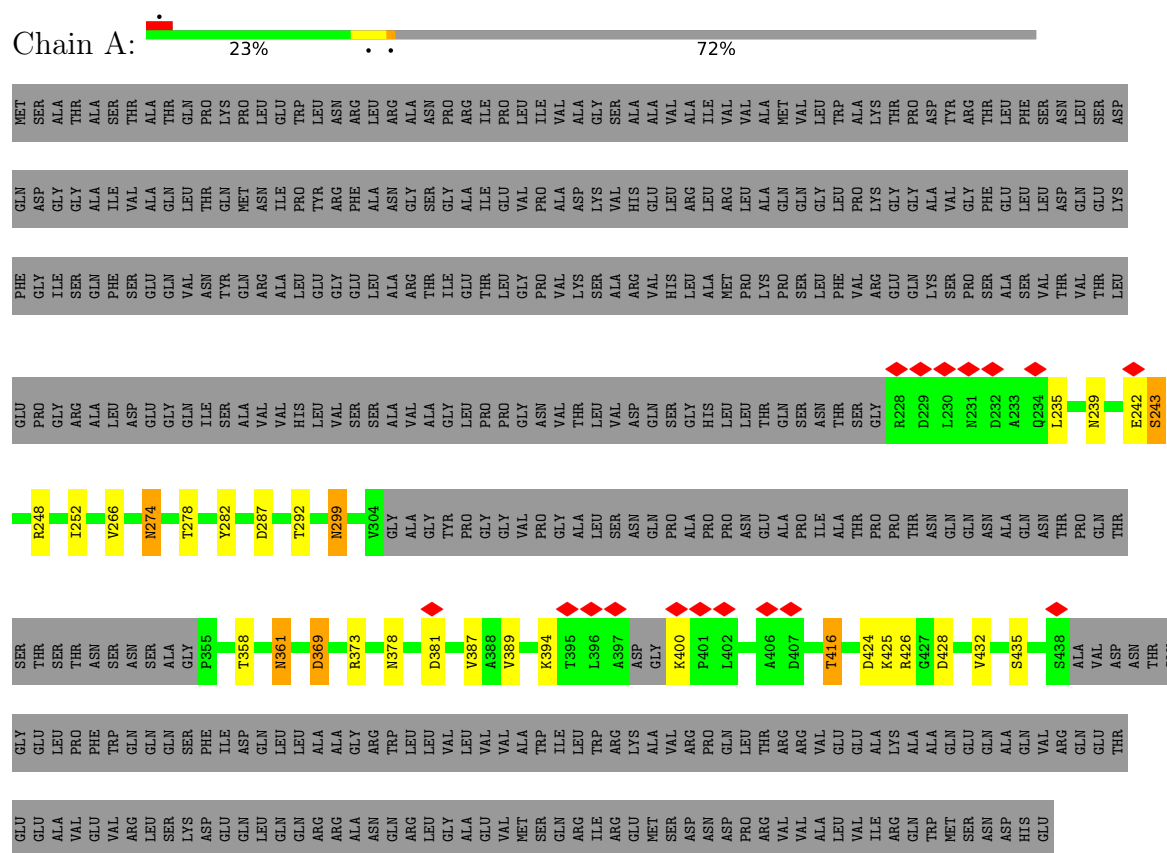
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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	159	Total	C	N	O	S	0	0
			1256	766	235	252	3		
1	S	159	Total	C	N	O	S	0	0
			1256	766	235	252	3		
1	T	159	Total	C	N	O	S	0	0
			1256	766	235	252	3		
1	U	159	Total	C	N	O	S	0	0
			1256	766	235	252	3		
1	V	159	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		

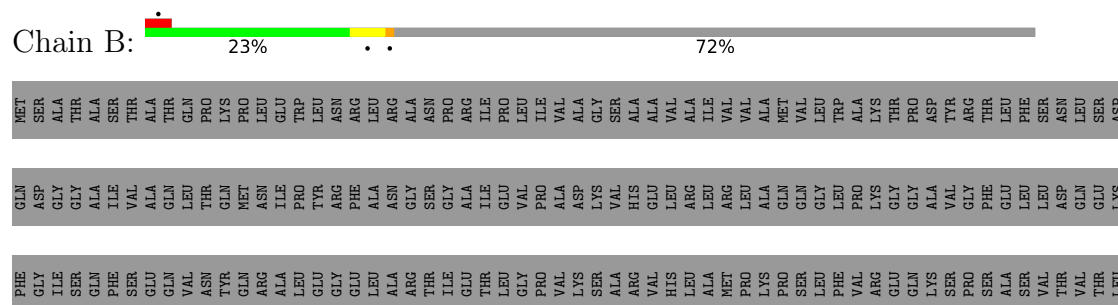
3 Residue-property plots

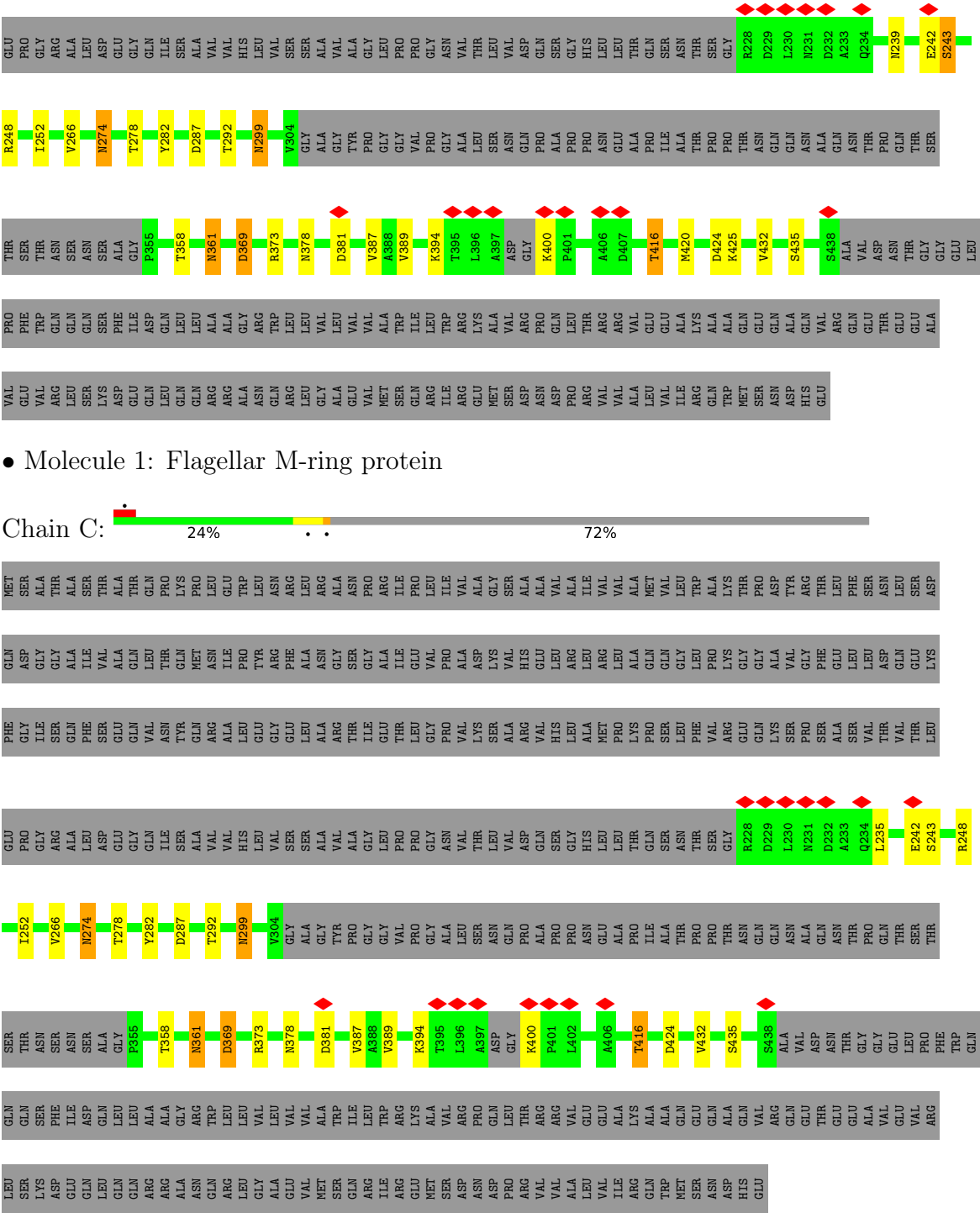
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Flagellar M-ring protein

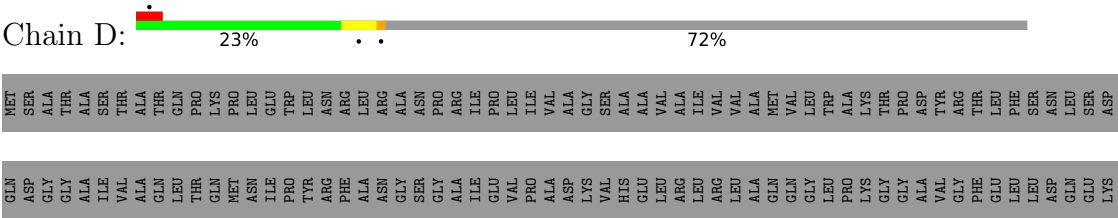


• Molecule 1: Flagellar M-ring protein

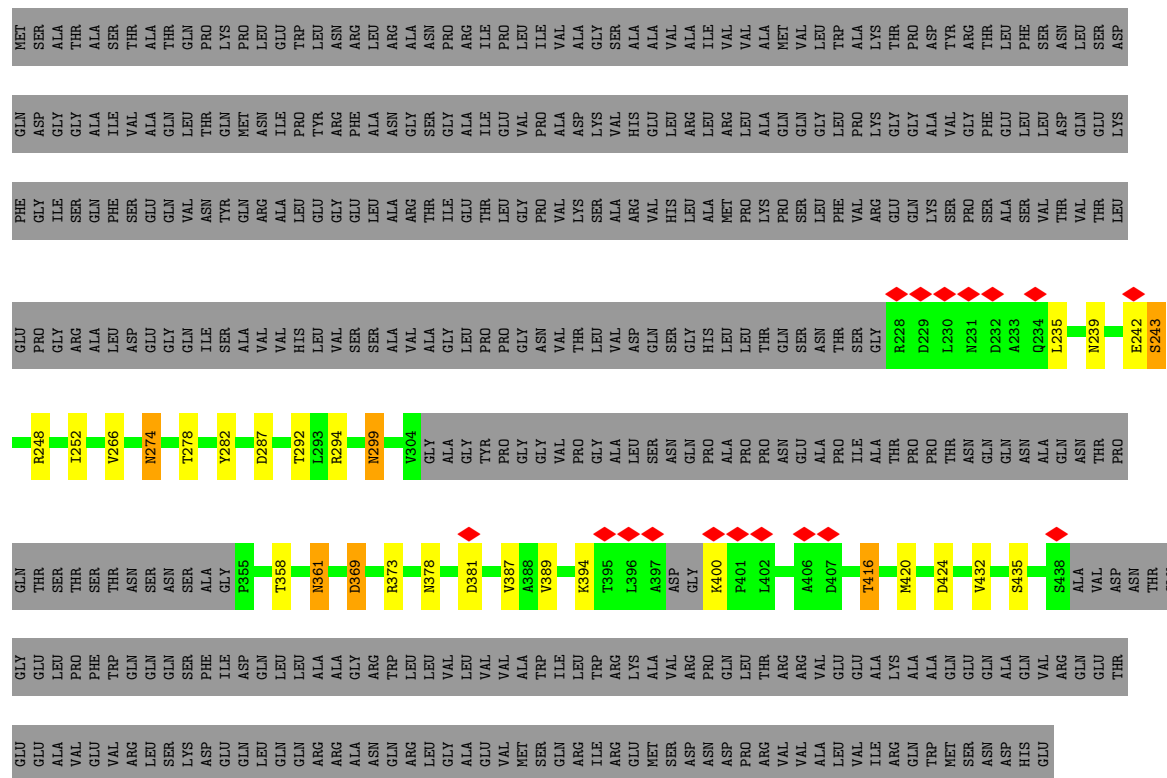




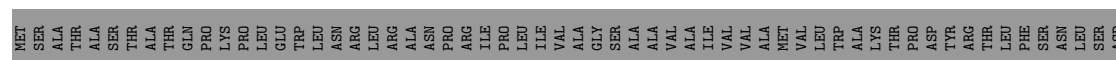
• Molecule 1: Flagellar M-ring protein

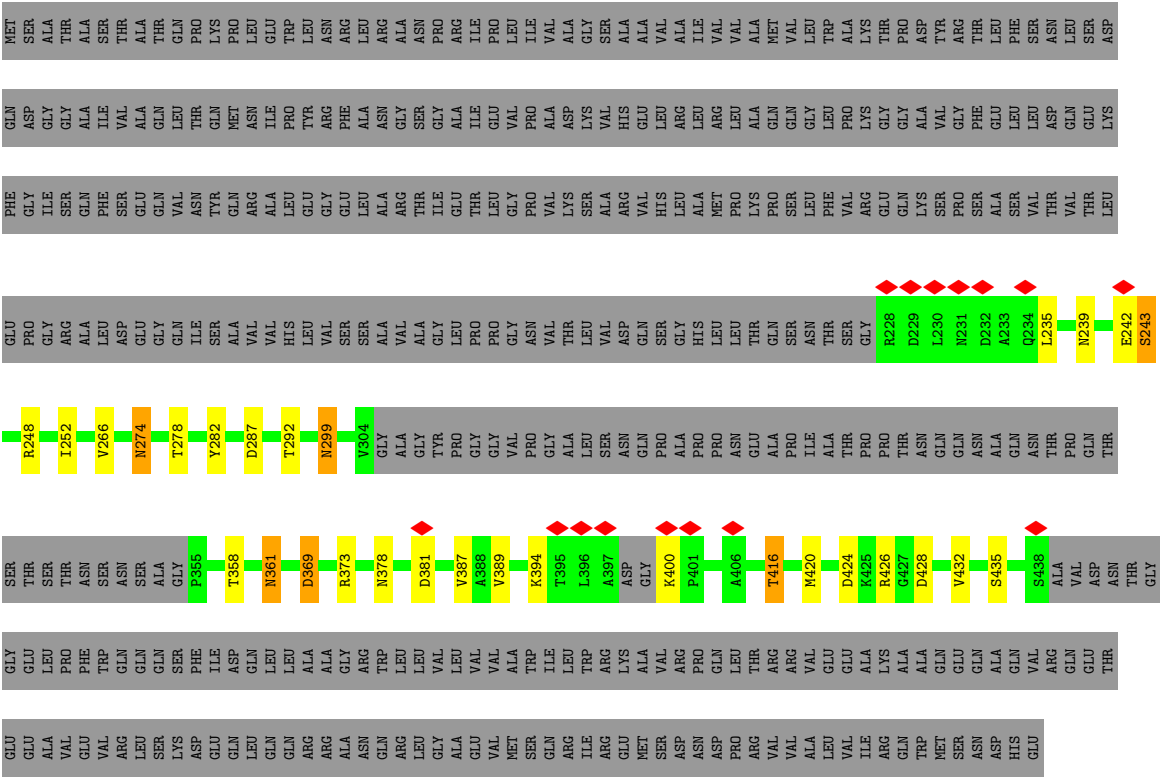


- Molecule 1: Flagellar M-ring protein

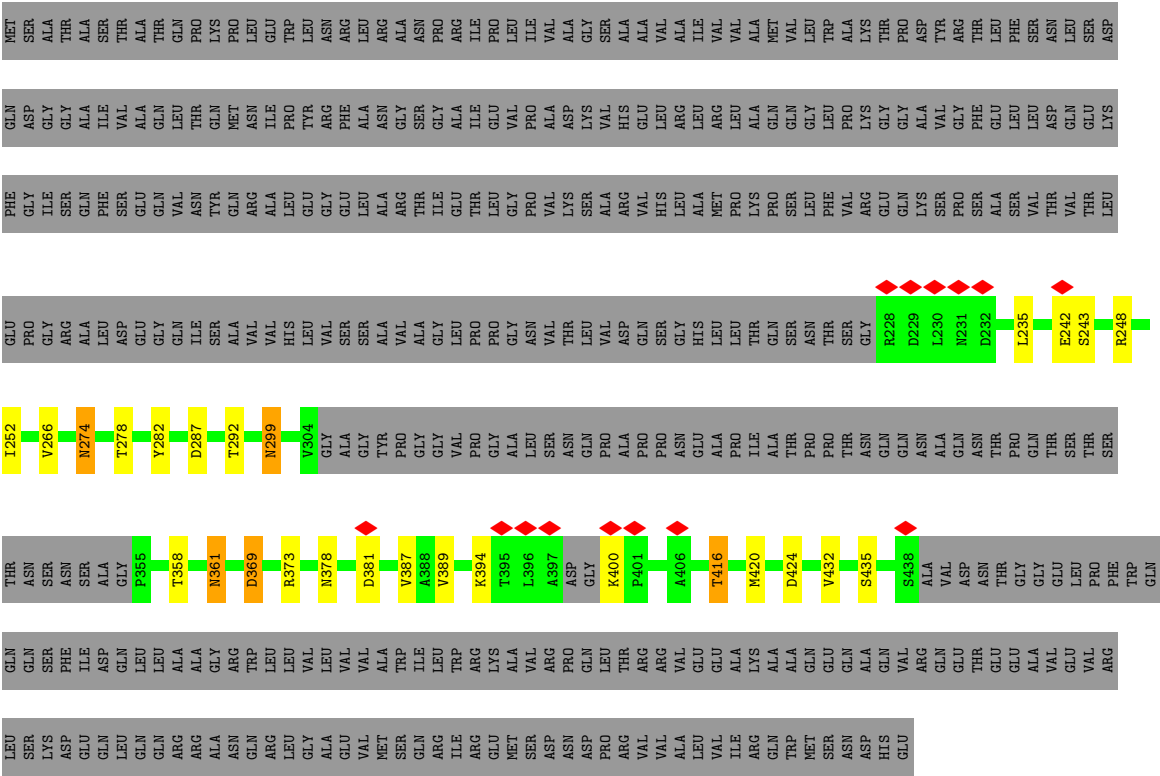


- Molecule 1: Flagellar M-ring protein





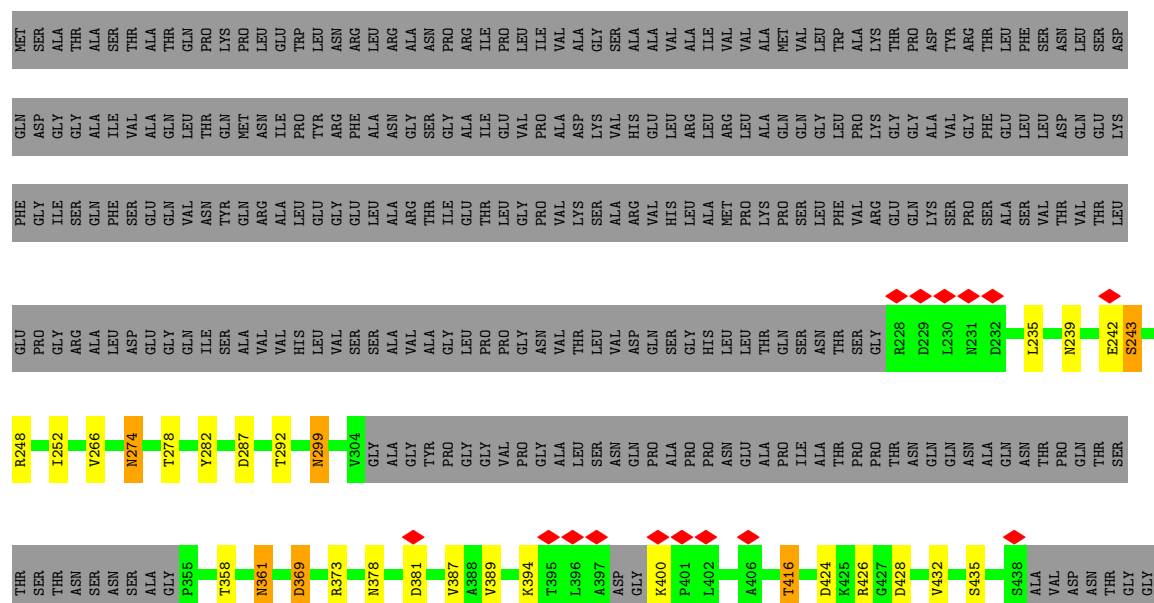
• Molecule 1: Flagellar M-ring protein

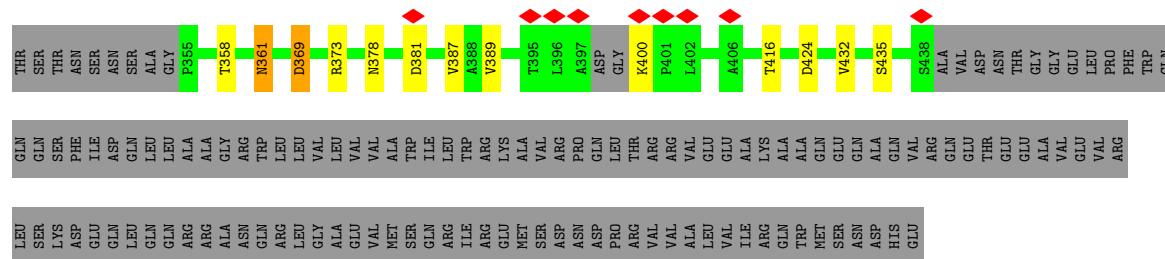


• Molecule 1: Flagellar M-ring protein

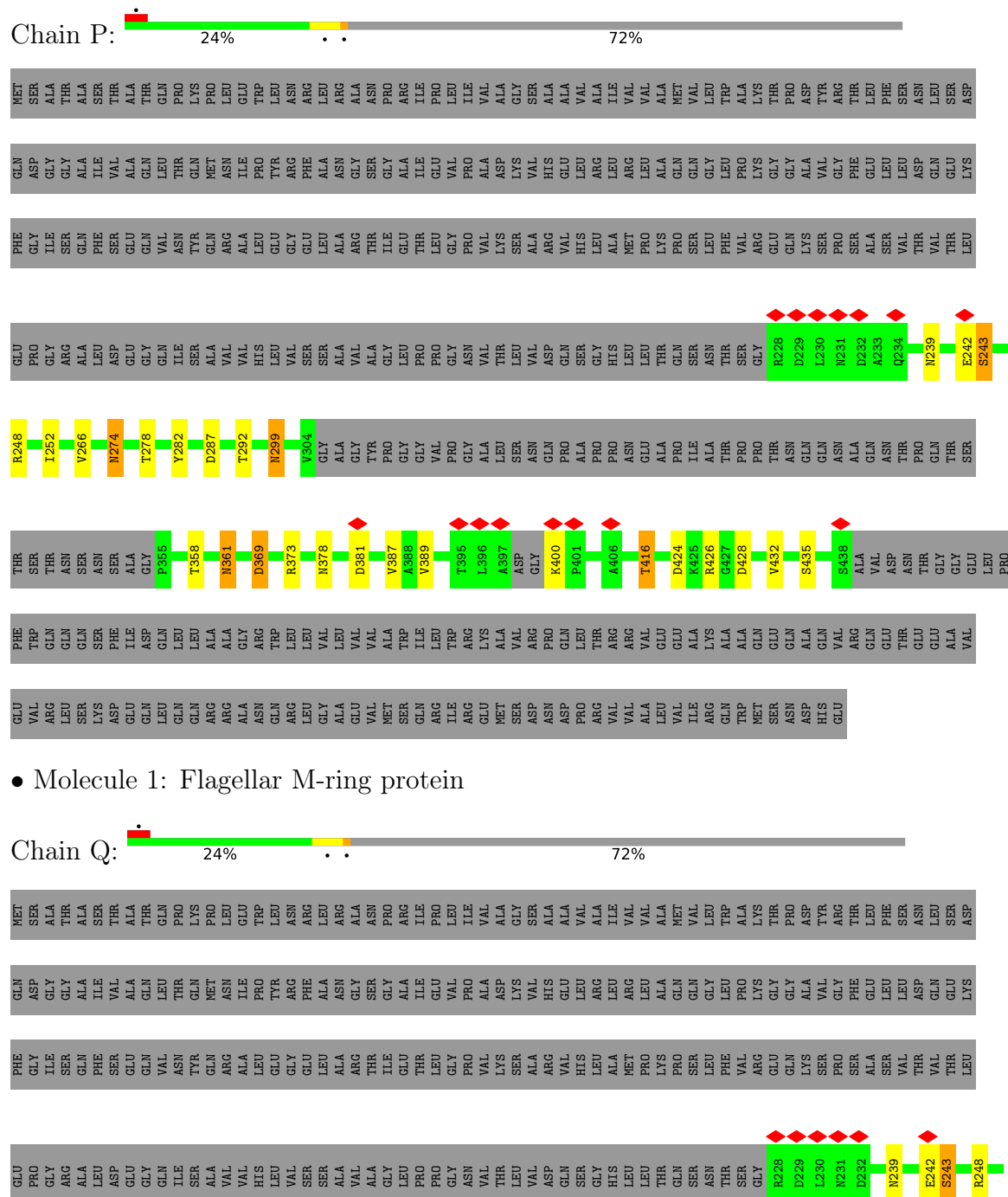


Chain L: 23% 72%

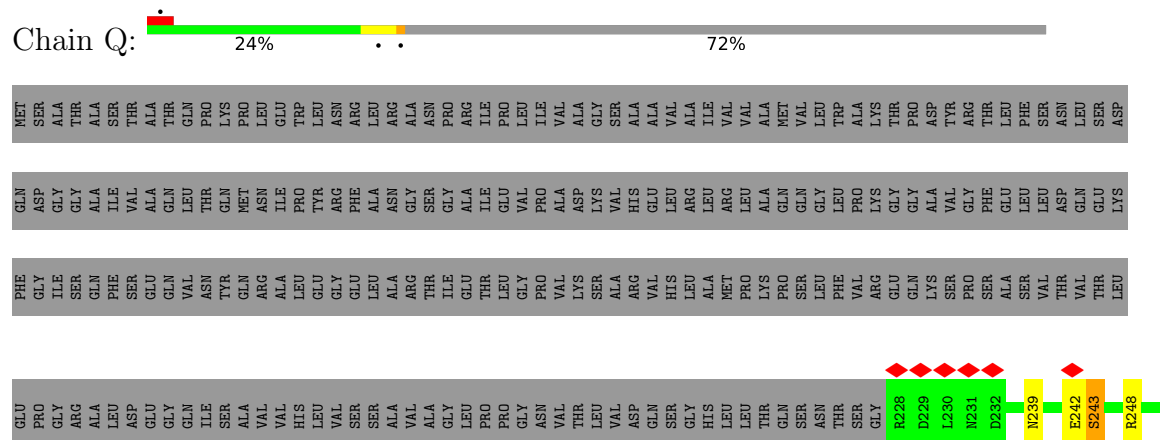


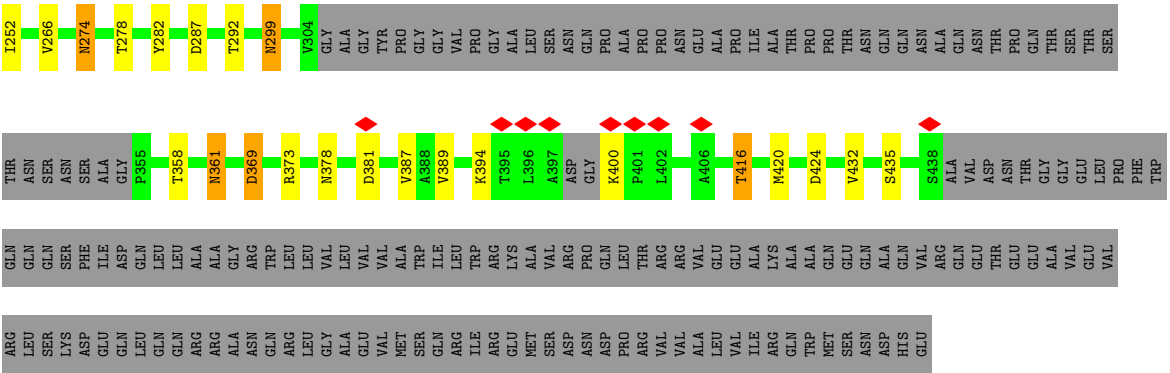


Molecule 1: Flagellar M-ring protein

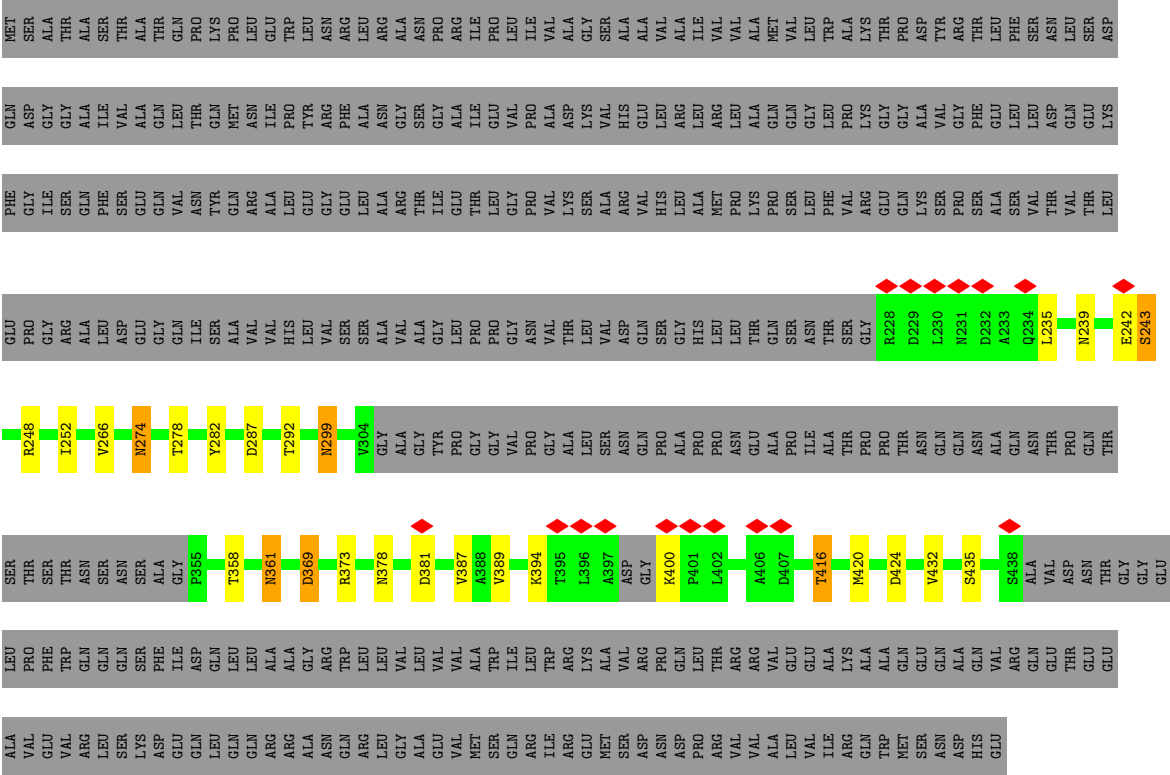


Molecule 1: Flagellar M-ring protein

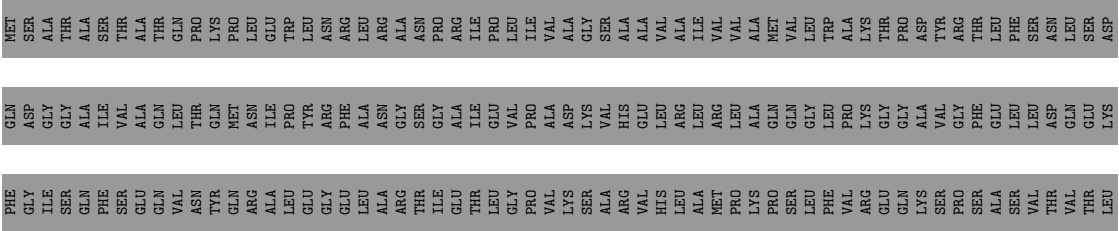


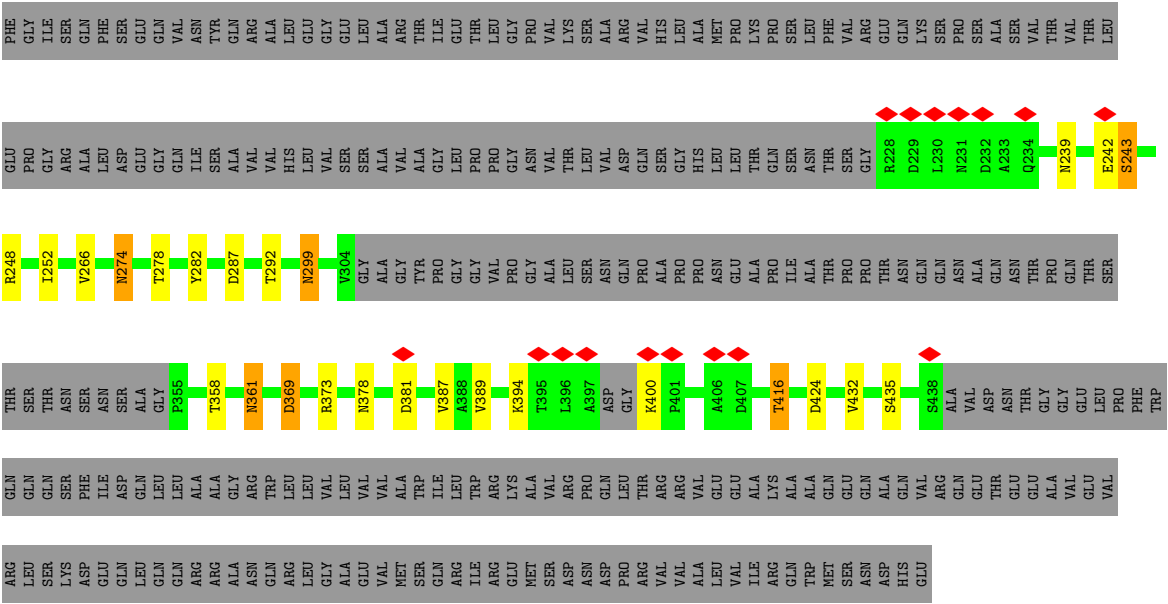


• Molecule 1: Flagellar M-ring protein

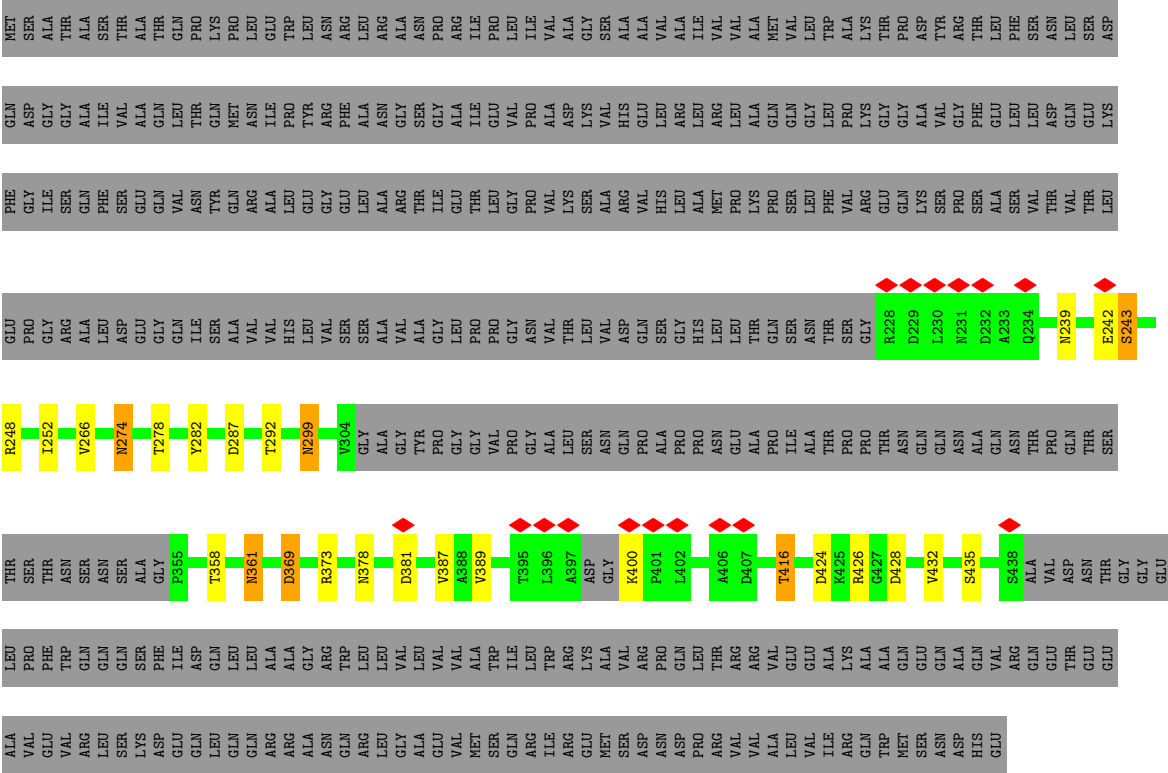


• Molecule 1: Flagellar M-ring protein



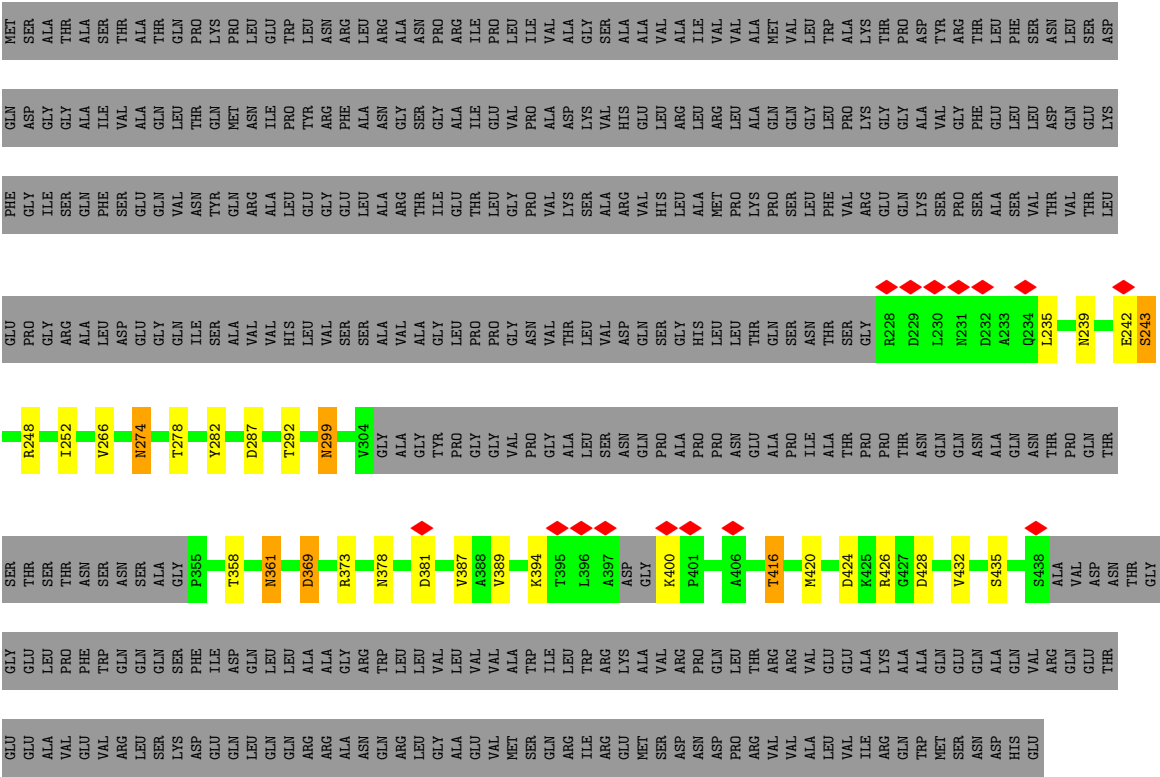


• Molecule 1: Flagellar M-ring protein



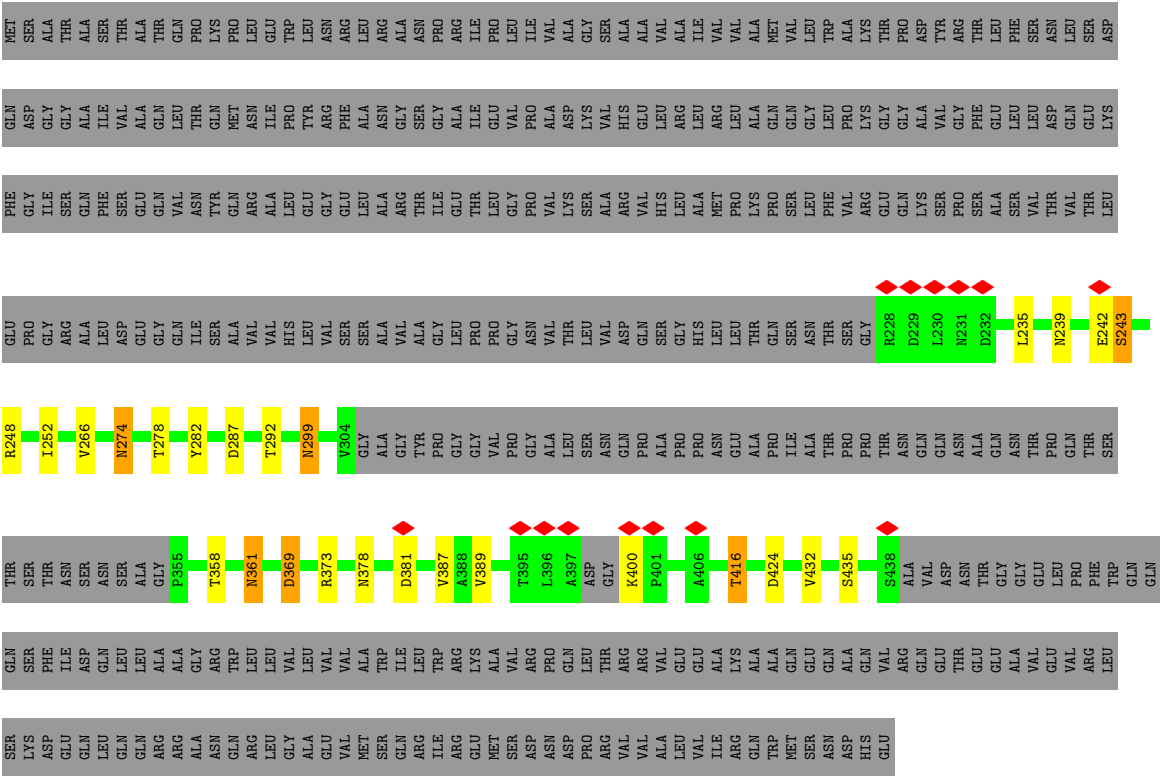
• Molecule 1: Flagellar M-ring protein



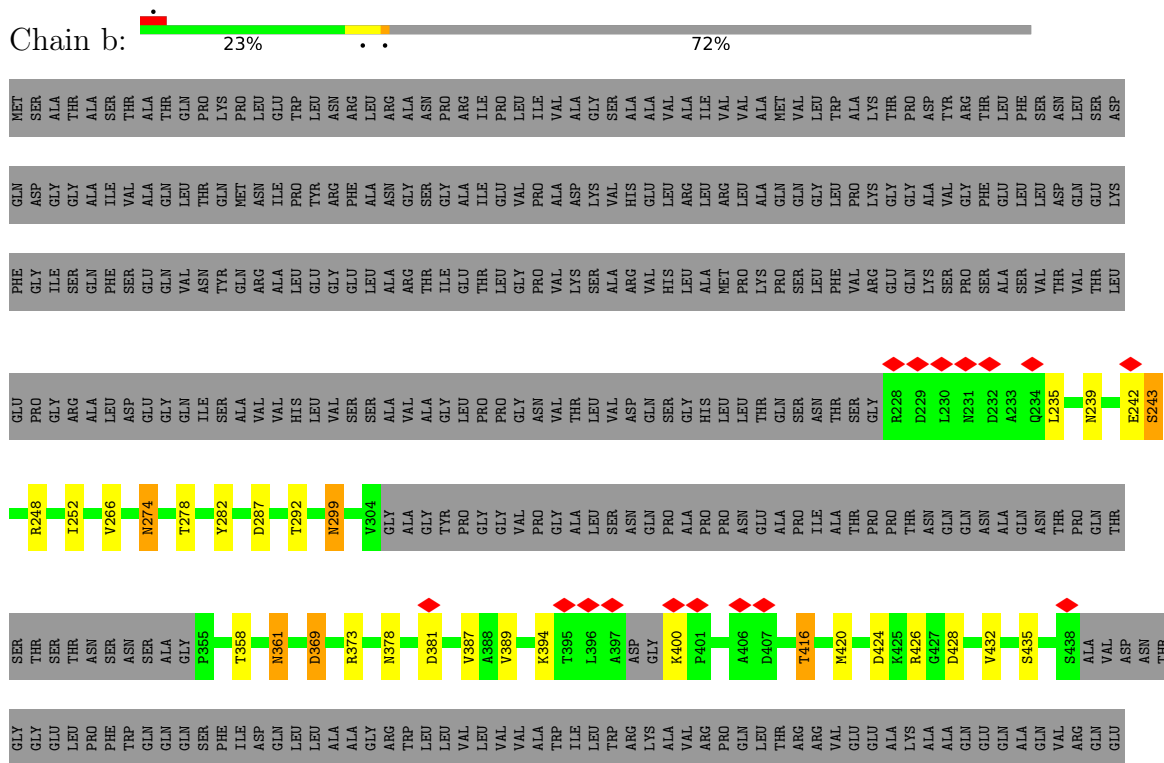


• Molecule 1: Flagellar M-ring protein

Chain Z: 24% 72%



• Molecule 1: Flagellar M-ring protein



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

- Molecule 1: Flagellar M-ring protein



MET	SER	ALA	THR	ALA	SER	THR	ALA	GLN	PRO	LYS	PRO	LEU	GLU	TRP	LEU	ASN	ARG	ARG	ARG	ASN	PRO	ARG	ILE	PRO	LEU	LEU	VAL	ALA	GLY	SER	ALA	ALA	VAL	VAL	ALA	ILE	VAL	VAL	VAL	MET	VAL	VAL	LEU	TRP	ALA	LYS	THR	PRO	ASP	TYS	ARG	THR	LEU	PHE	SER	ASN	LEU	SER	SER	ASP
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[illegible]

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

	GLU	PRO	GLY	ARG	ALA	LEU	ASP	GLU	GLN	ILE	SER	ALA	VAL	VAL	HIS	HEU	VAL	SER	SER	ALA	VAL	ALA	ALA	GLY	LEU	PRO	PRO	GLY	ASN	THR	VAL	THR	LEU	VAL	ASP	GLN	SER	GLY	HIS	GLY	LEU	LEU	LEU	THR	GLN	SER	ASN	THR	SER	SER	GLY	R228	D229	L230	N231	D232	D233	Z234	L235	N236	E242	E243
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R248
I252
V266
Y274
T278
Y282
D287
T292
N299
V304
GLY
ALA
GLY
TYR
PRO
GLY
GLY
VAL
PRO
PRO
GLY
ALA
LEU
SER
SER
ASN
GLN
PRO
ALA
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PRO
GLU
GLU
ALA
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ALA
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PRO
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ASN
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PRO
PRO
GLN
THR
THR
GLN

SER	THR	SER	THR	ASN	SER	ASN	SER	GLY	P355	T358	N361	D369	R373	N378	D381	V387	A388	V389	T395	L396	A397	ASP	GLY	K400	P401	L402	A406	D407	T416	D424	K425	G426	G427	D428	V432	S435	S438	ALA	VAL	ASP	ASN	THR	GLY
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GLU PRO LEU PHE TRP GLN GLN SER PHE ASP GLN LEU LEU ALA ALA GLY ARG TRP LEU LEU VAL VAL VAL ALA ALA LYS ARG ARG VAL VAL ARG PRO GLN LEU LEU THR ARG ARG VAL GLU GLU ALA ALA LYS GLN GLN ALA ALA GLN VAL ARG GLN GLU THR THR

GLU	ALA	VAL	GLU	VAL	ARG	LEU	SER	LYS	ASP	GLN	GLU	LEU	GLN	GLN	ARG	ARG	ALA	ASN	GLN	ARG	GLY	ALA	ALA	GLU	VAL	VAL	NET	SER	GLN	ARG	ILE	ARG	GLU	NET	SER	ASP	ASN	ASP	PRO	ARG	VAL	VAL	ALA	LEU	VAL	ILE	ARG	GLN	TRP	NET	SER	ASN	ASP	HIS
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- Molecule 1: Flagellar M-ring protein

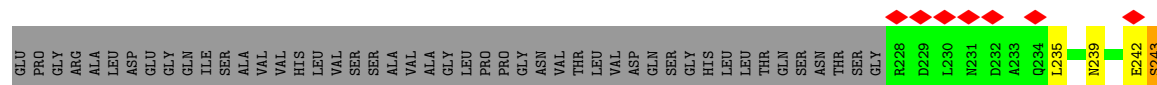


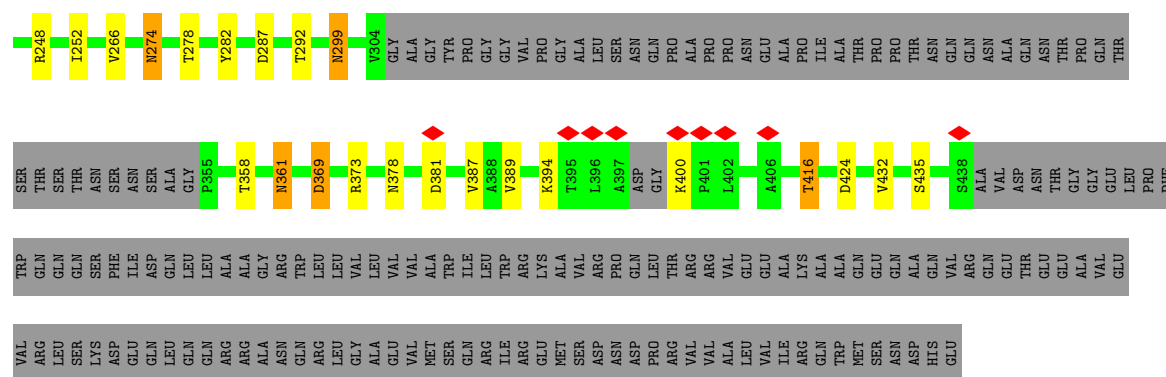
MET	SER	ALA	ALA	ALA	ALA	SER	THR	THR	ALA	GLN	PRO	LYS	PRO	LEU	GLU	TRP	LEU	ASN	ARG	ARG	LEU	ALA	ARG	ALA	ASN	PRO	ARG	ILE	ILE	ILE	VAL	GLY	GLY	SER	ALA	ALA	ALA	VAL	VAL	VAL	VAL	VAL	VAL	MET	VAL	VAL	LEU	LEU	TRP	ALA	ALA	ALA	LYS	THR	PRO	ASP	TYP	ARG	THR	LEU	PHE	SER	ASN	ASN	LEU	LEU	SER	SER
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GLN ASP GLY GLY ALA 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 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 (Å)	462.24002, 462.24002, 462.24002	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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.

The worst 5 of 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

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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

5 of 373 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	V	252	ILE
1	a	252	ILE
1	V	400	LYS
1	X	400	LYS
1	b	299	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 48 such sidechains are listed below:

Mol	Chain	Res	Type
1	W	434	ASN
1	a	359	GLN
1	X	359	GLN
1	Y	434	ASN
1	b	259	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.

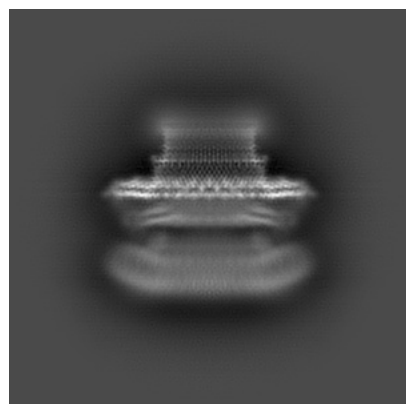
6 Map visualisation [i](#)

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.

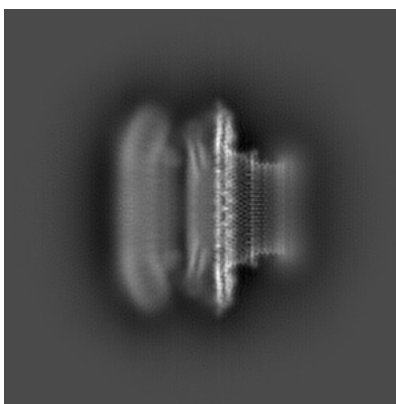
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

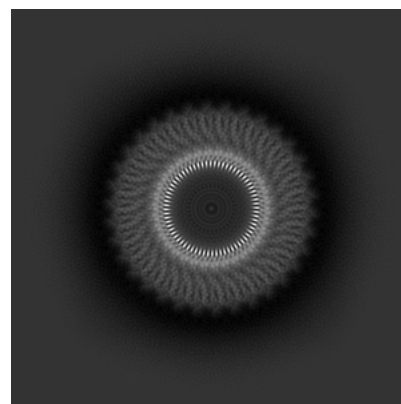
6.1.1 Primary map



X

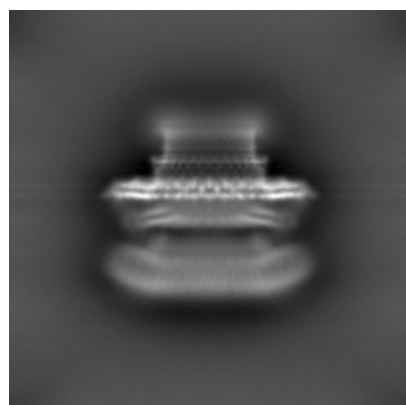


Y

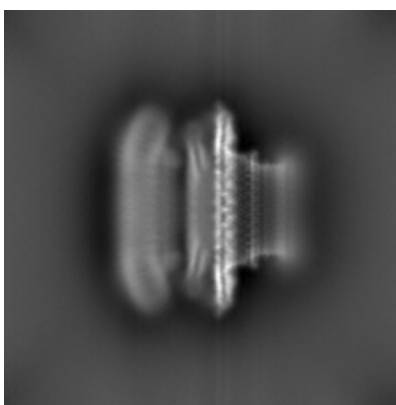


Z

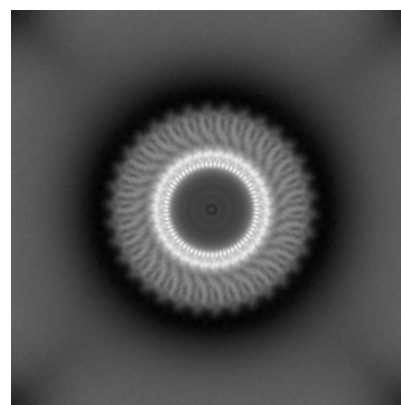
6.1.2 Raw map



X



Y

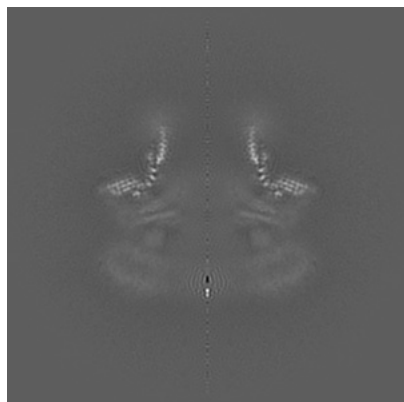


Z

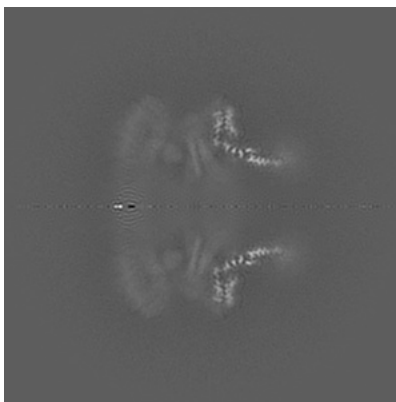
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

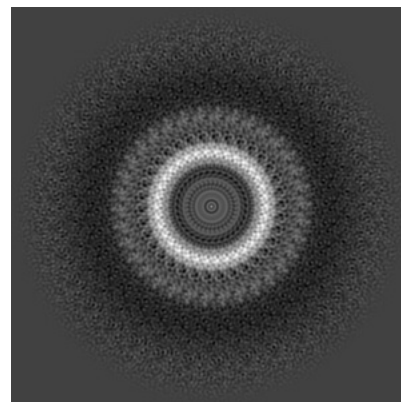
6.2.1 Primary map



X Index: 216

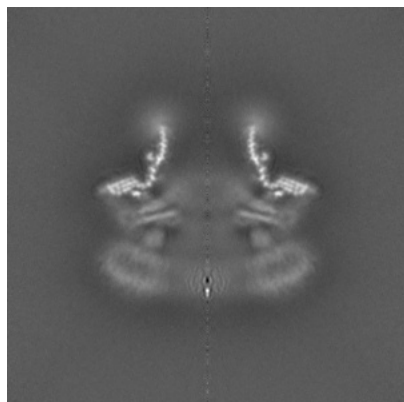


Y Index: 216

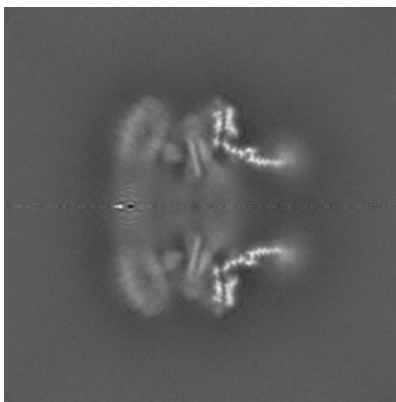


Z Index: 216

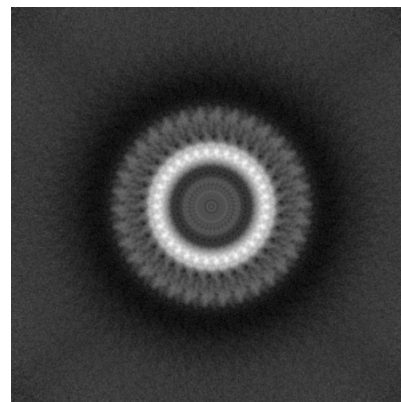
6.2.2 Raw map



X Index: 216



Y Index: 216

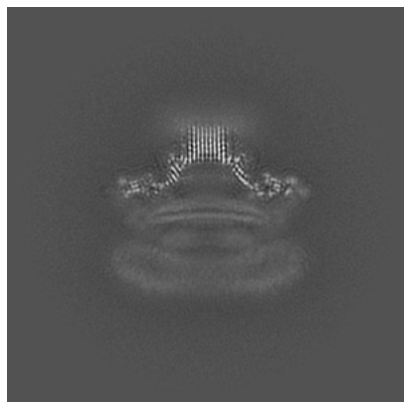


Z Index: 216

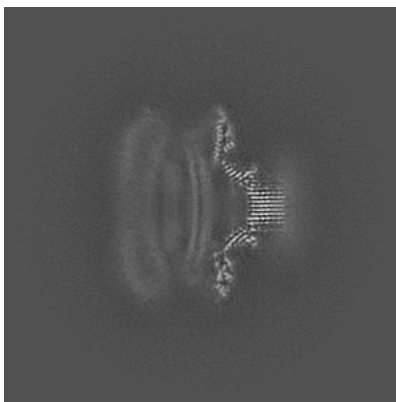
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

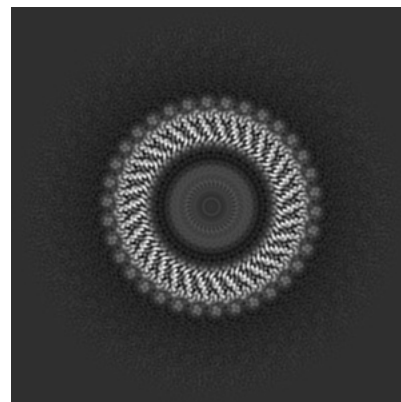
6.3.1 Primary map



X Index: 169

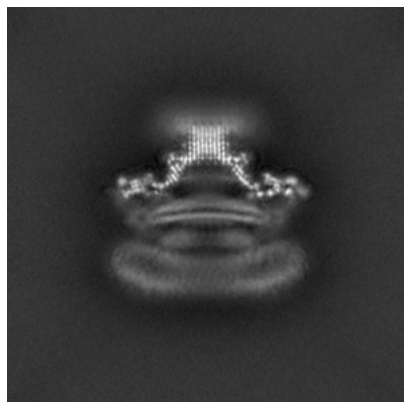


Y Index: 168

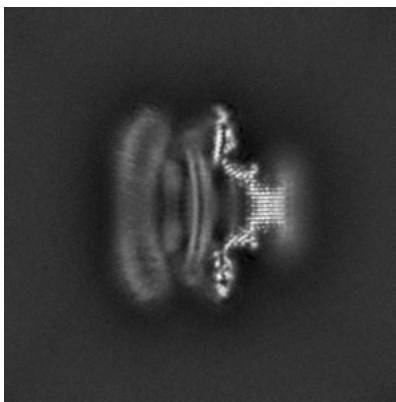


Z Index: 231

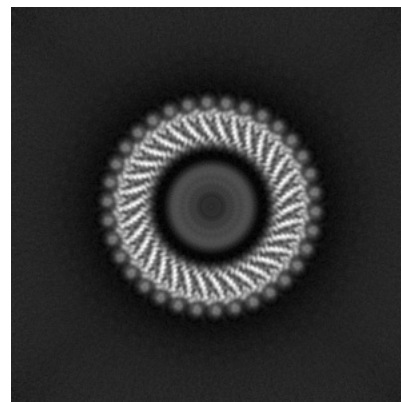
6.3.2 Raw map



X Index: 169



Y Index: 169

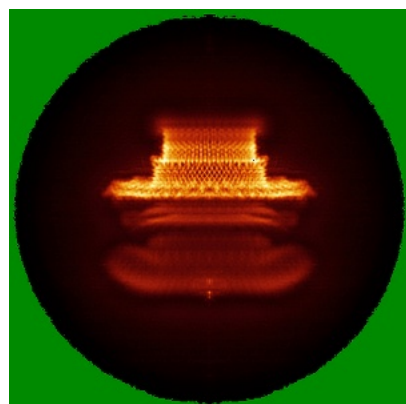


Z Index: 231

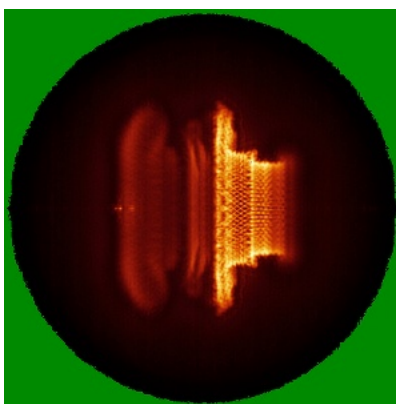
The images above show the largest variance slices of the map in three orthogonal directions.

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

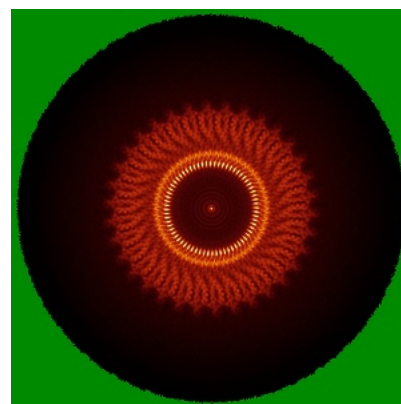
6.4.1 Primary map



X

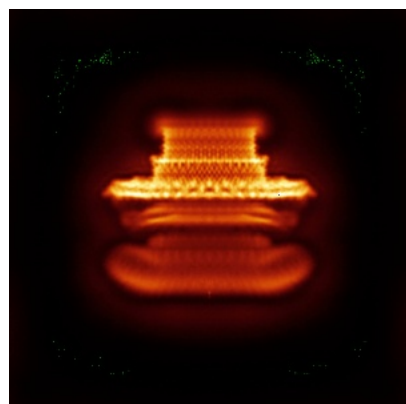


Y

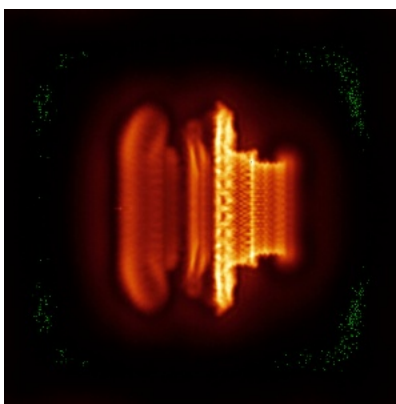


Z

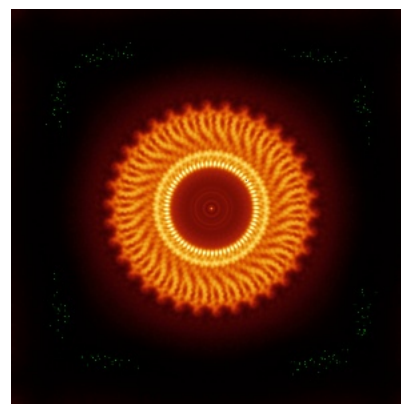
6.4.2 Raw map



X



Y

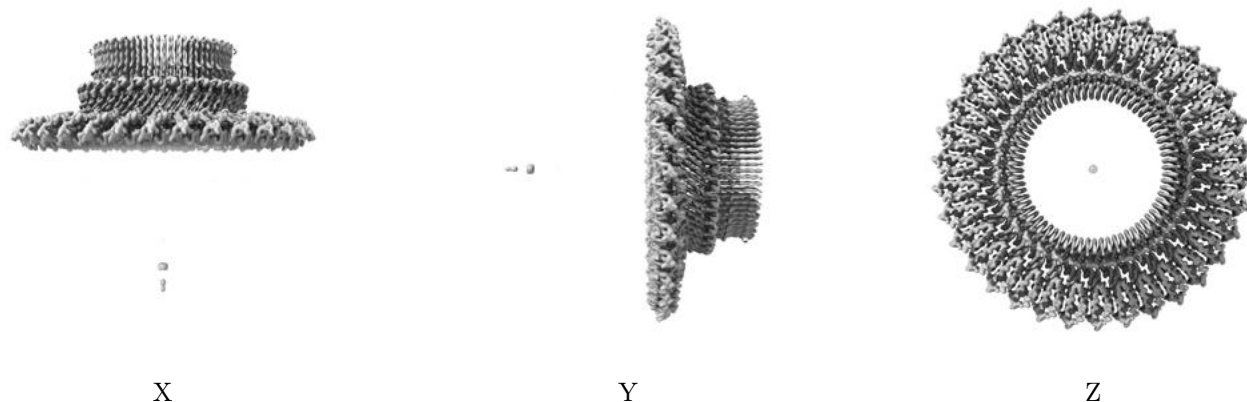


Z

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.

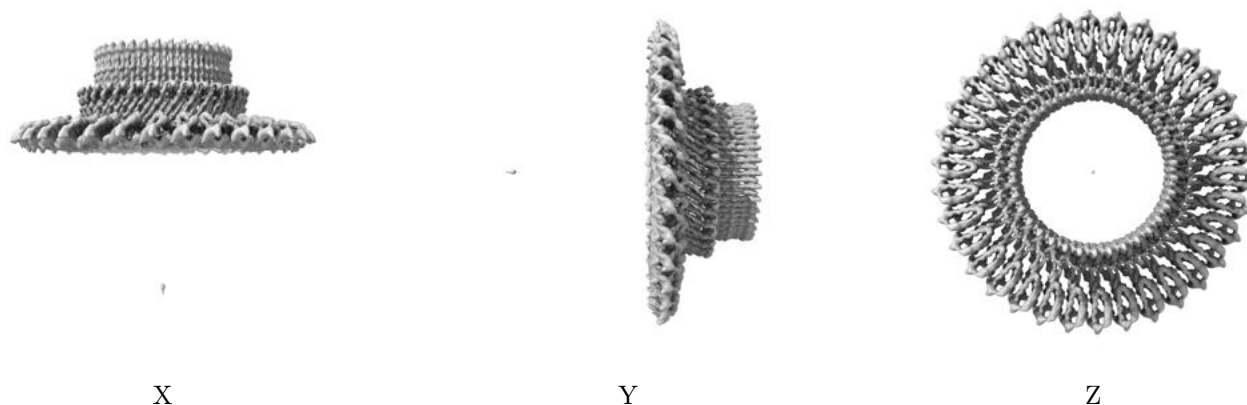
6.5 Orthogonal surface views [i](#)

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.

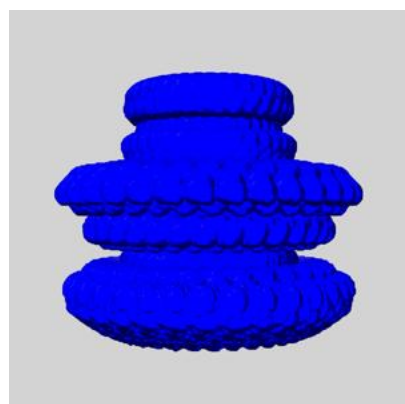
6.6 Mask visualisation [i](#)

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

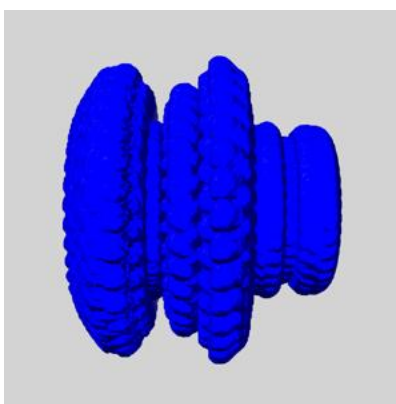
A mask typically either:

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

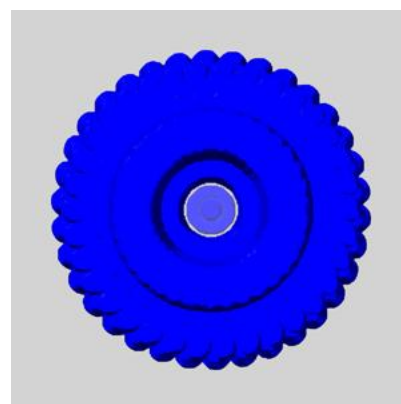
6.6.1 emd_30612_msk_1.map [i](#)



X



Y

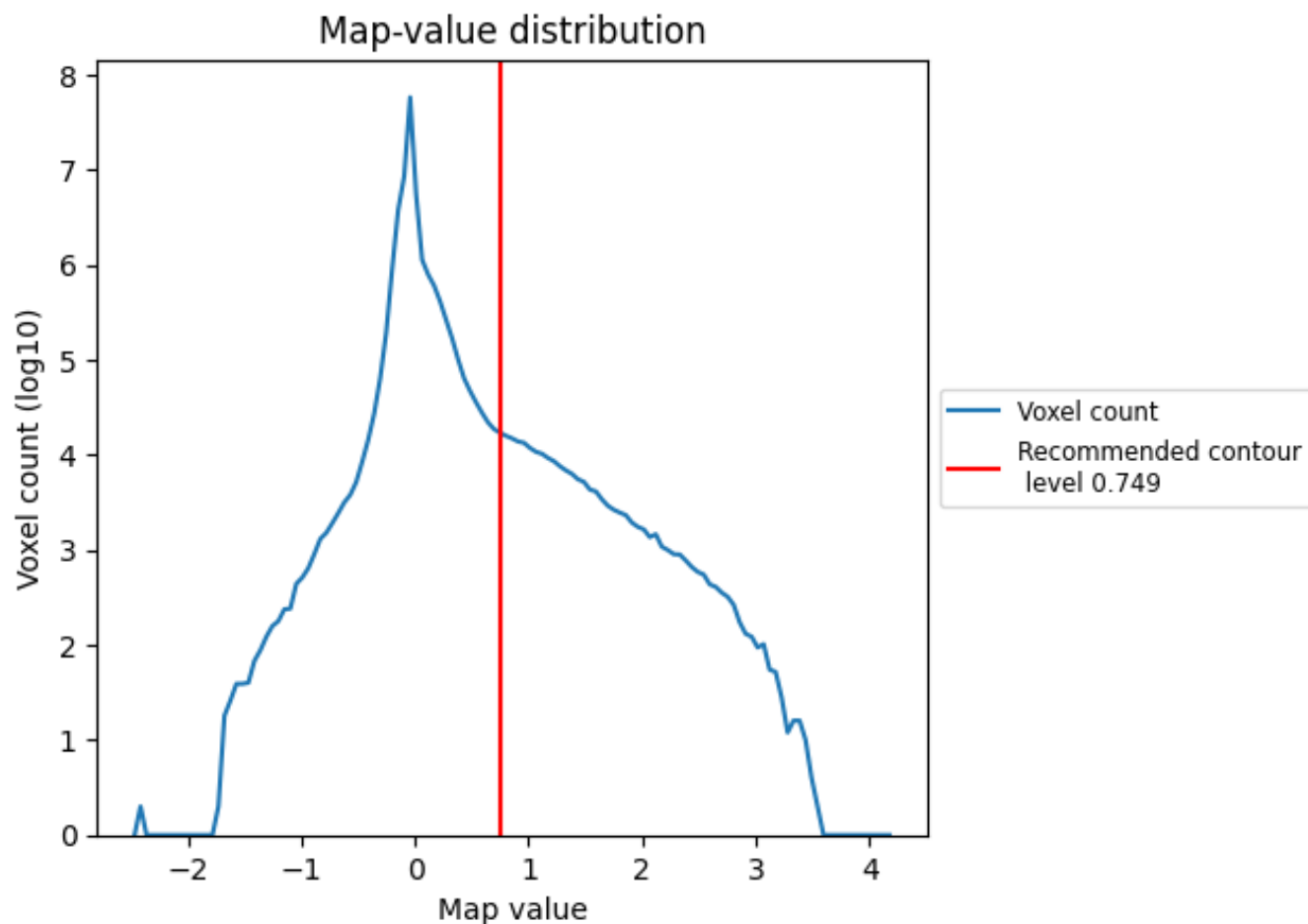


Z

7 Map analysis [i](#)

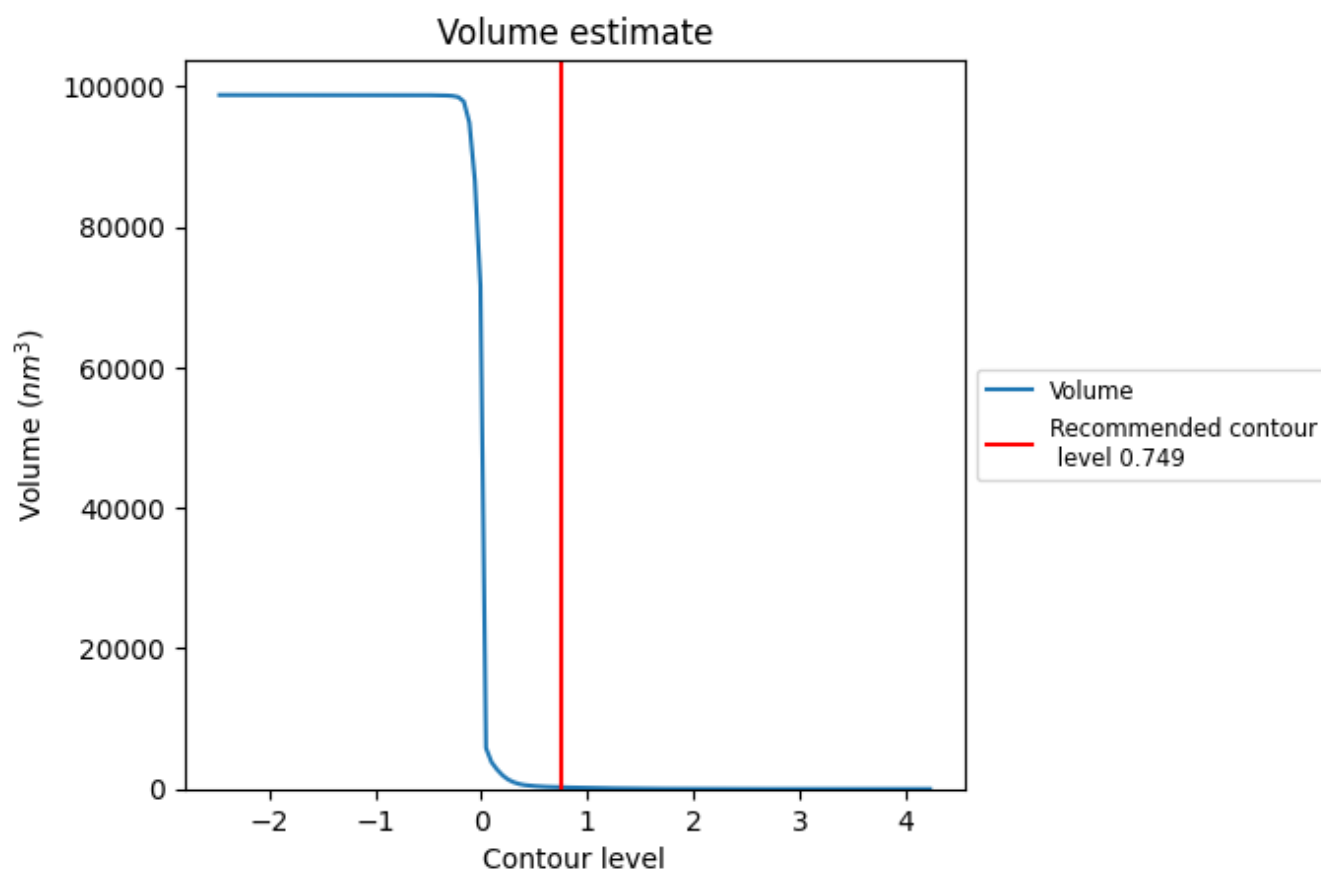
This section contains the results of statistical analysis of the map.

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.

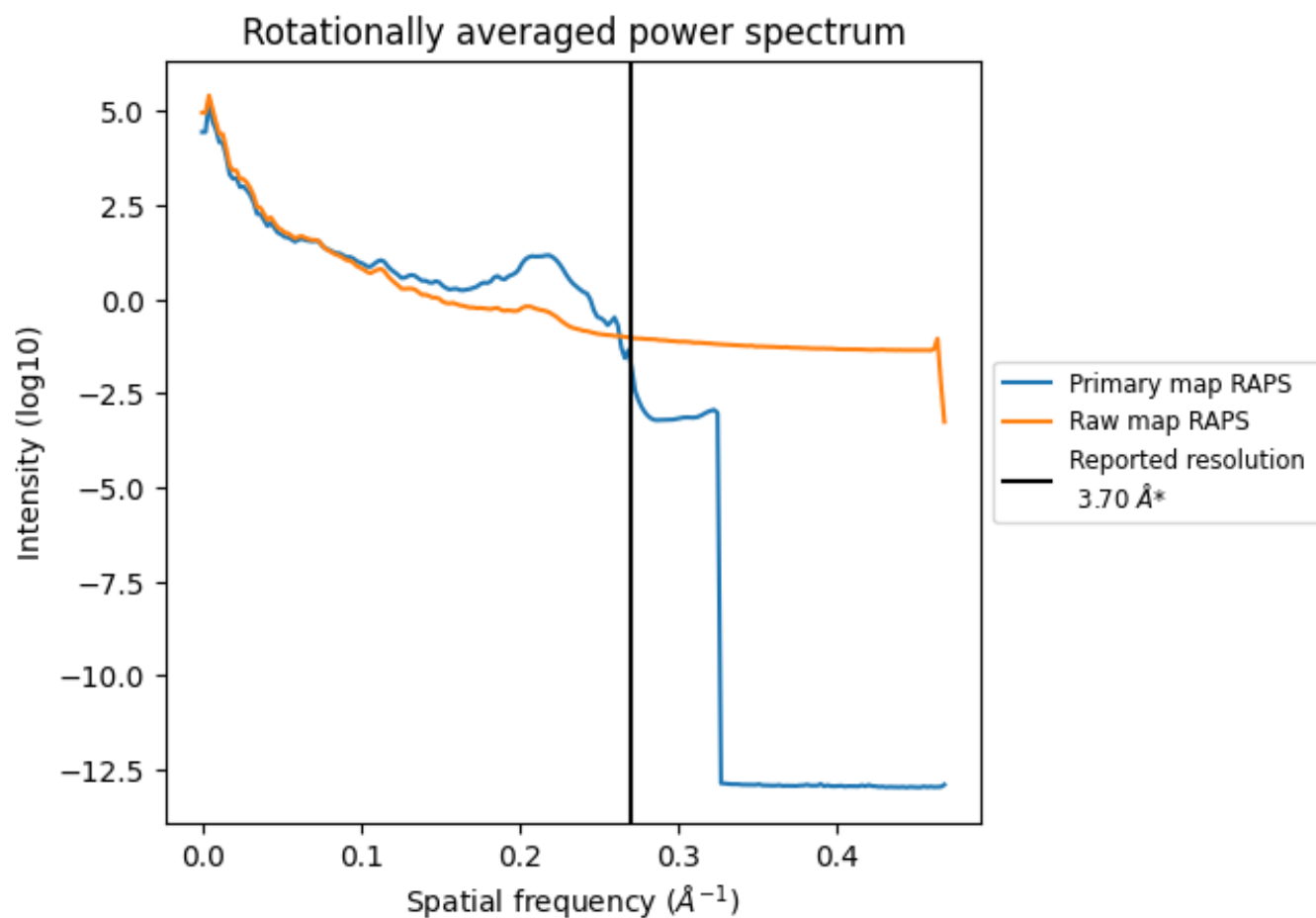
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 241 nm^3 ; 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 ⓘ

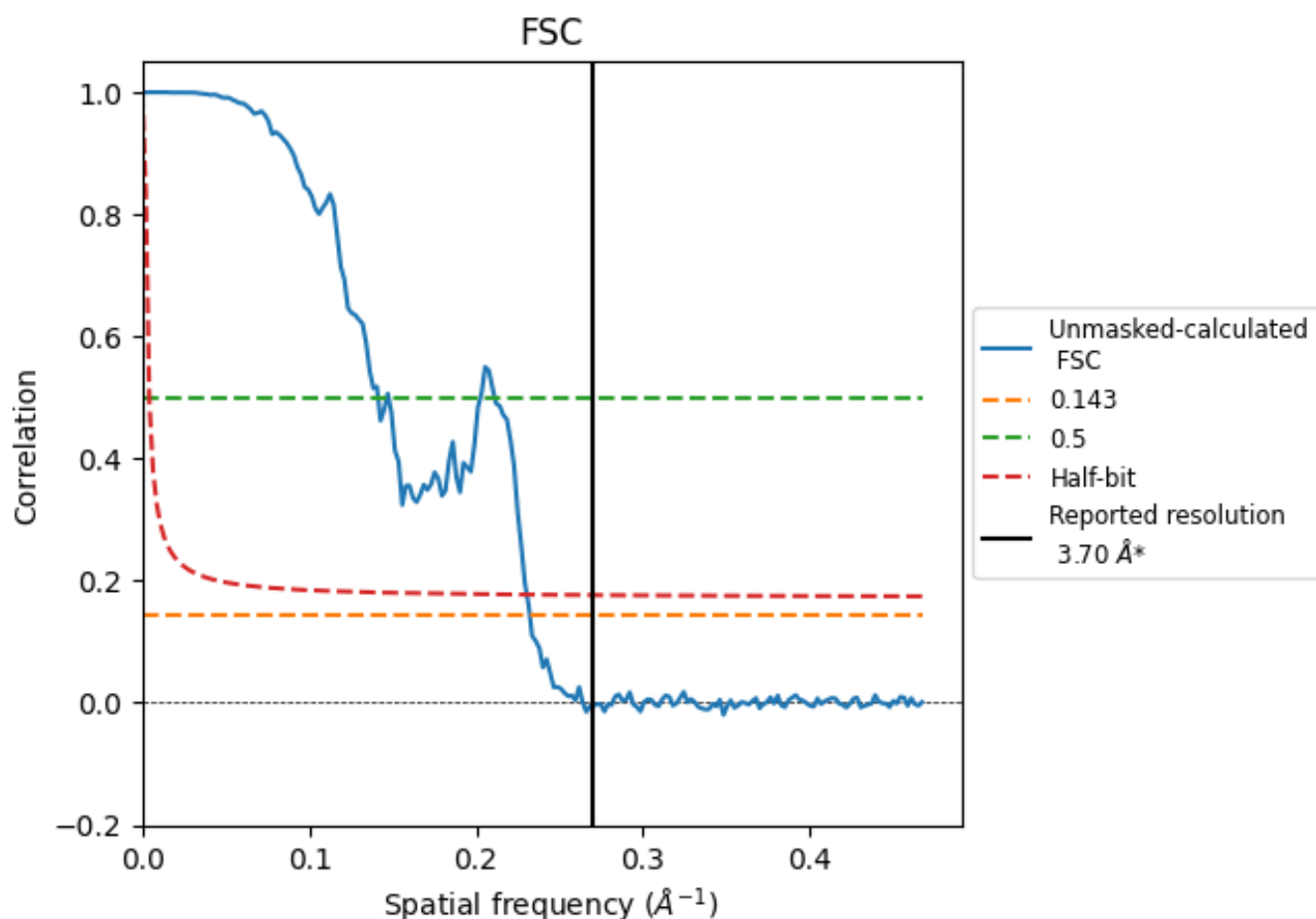


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

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 Å⁻¹

8.2 Resolution estimates [i](#)

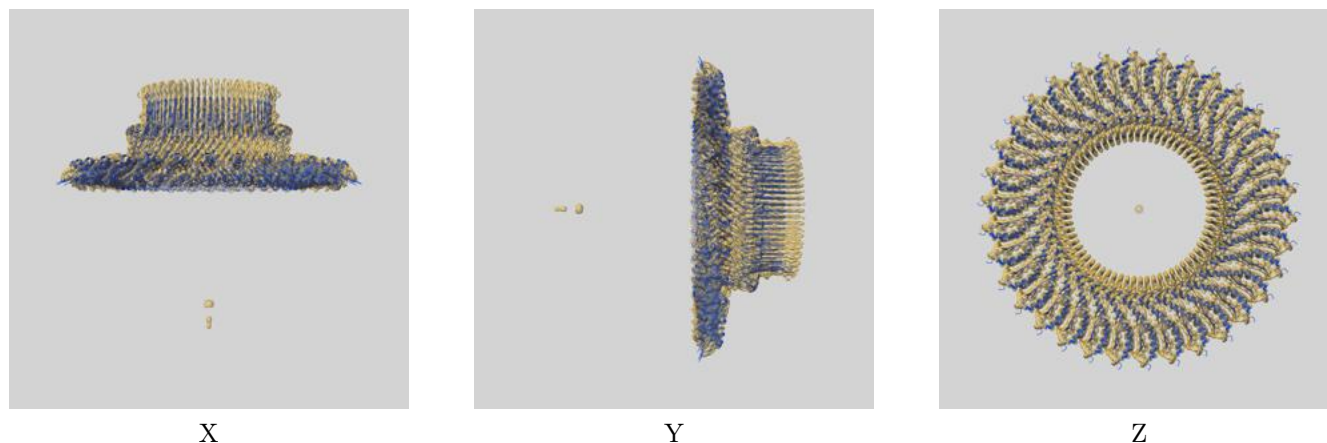
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.31	7.08	4.34

*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](#)

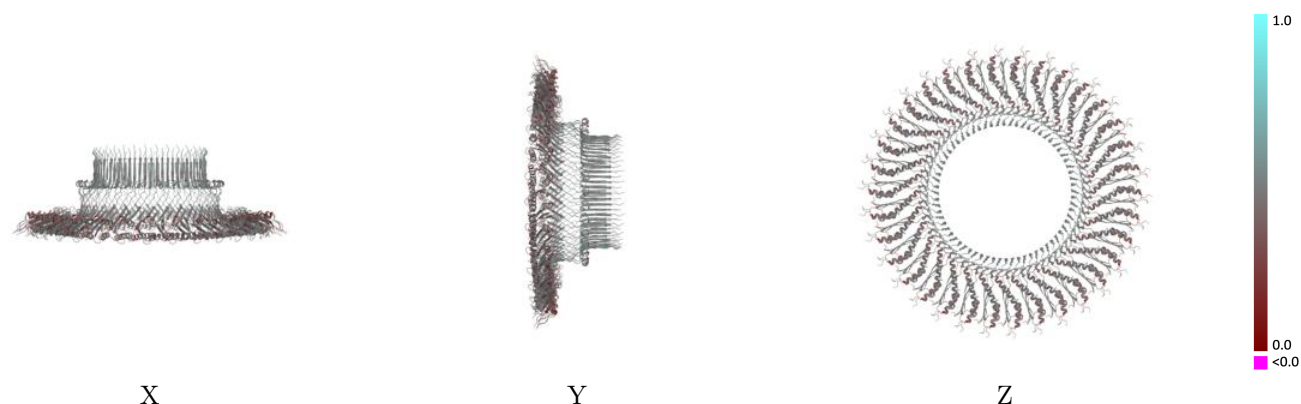
This section contains information regarding the fit between EMDB map EMD-30612 and PDB model 7D84. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



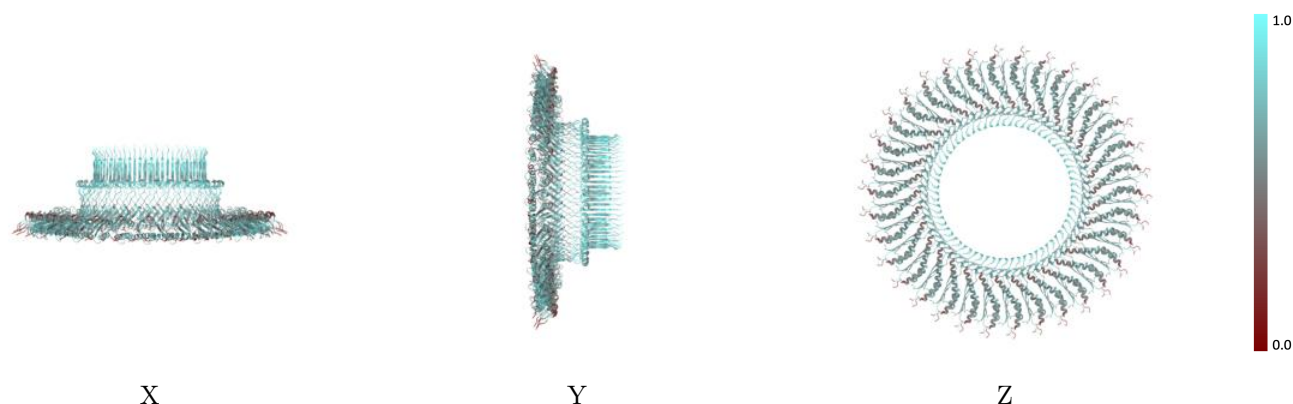
The images above show the 3D surface view of the map at the recommended contour level 0.749 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



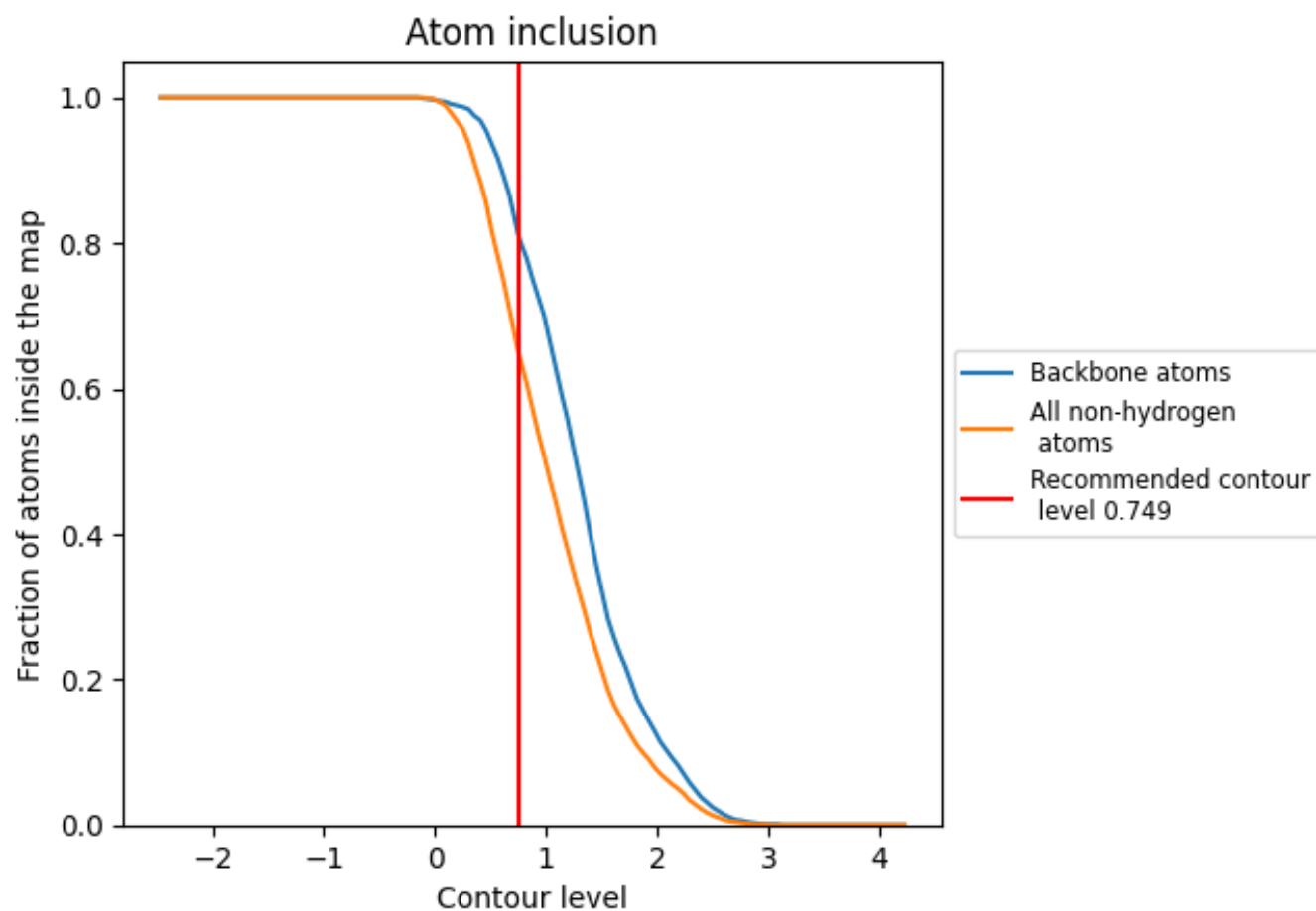
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

