



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 09:15 AM UTC

PDB ID : 8WJR / pdb_00008wjr
EMDB ID : EMD-37590
Title : Cryo-EM structure of the MS ring (C34) within the flagellar motor-hook complex in the CW state
Authors : Tan, J.X.; Zhang, L.; Zhou, Y.; Zhu, Y.Q.
Deposited on : 2023-09-26
Resolution : 2.90 Å(reported)
Based on initial model : .

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

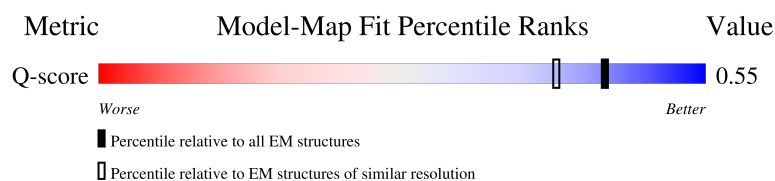
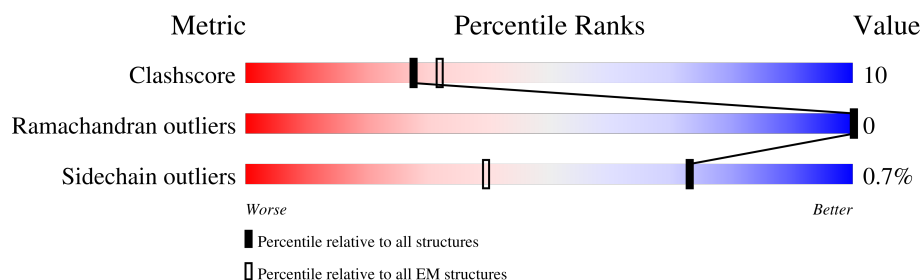
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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.



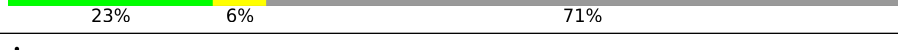
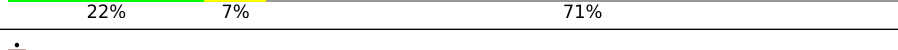
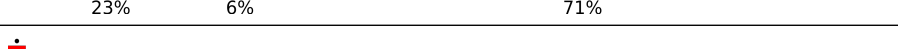
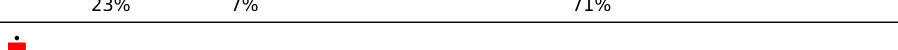
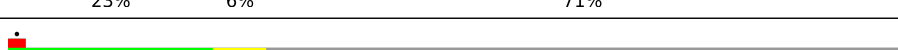
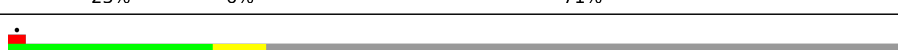
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13054 (2.40 - 3.40)

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	
1	F	560	
1	G	560	
1	H	560	
1	I	560	
1	J	560	
1	K	560	
1	L	560	
1	M	560	
1	N	560	
1	O	560	
1	P	560	
1	Q	560	
1	R	560	
1	S	560	
1	T	560	
1	U	560	
1	V	560	
1	W	560	
1	X	560	
1	Y	560	
1	Z	560	
1	a	560	
1	b	560	
1	c	560	

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Mol	Chain	Length	Quality of chain
1	d	560	23%6%71%
1	e	560	22%7%71%
1	f	560	23%6%71%
1	g	560	23%6%71%
1	h	560	23%6%71%

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 43350 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	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	B	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	C	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	D	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	E	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	F	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	G	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	H	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	I	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	J	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	K	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	L	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	M	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	N	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	O	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	P	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	Q	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		

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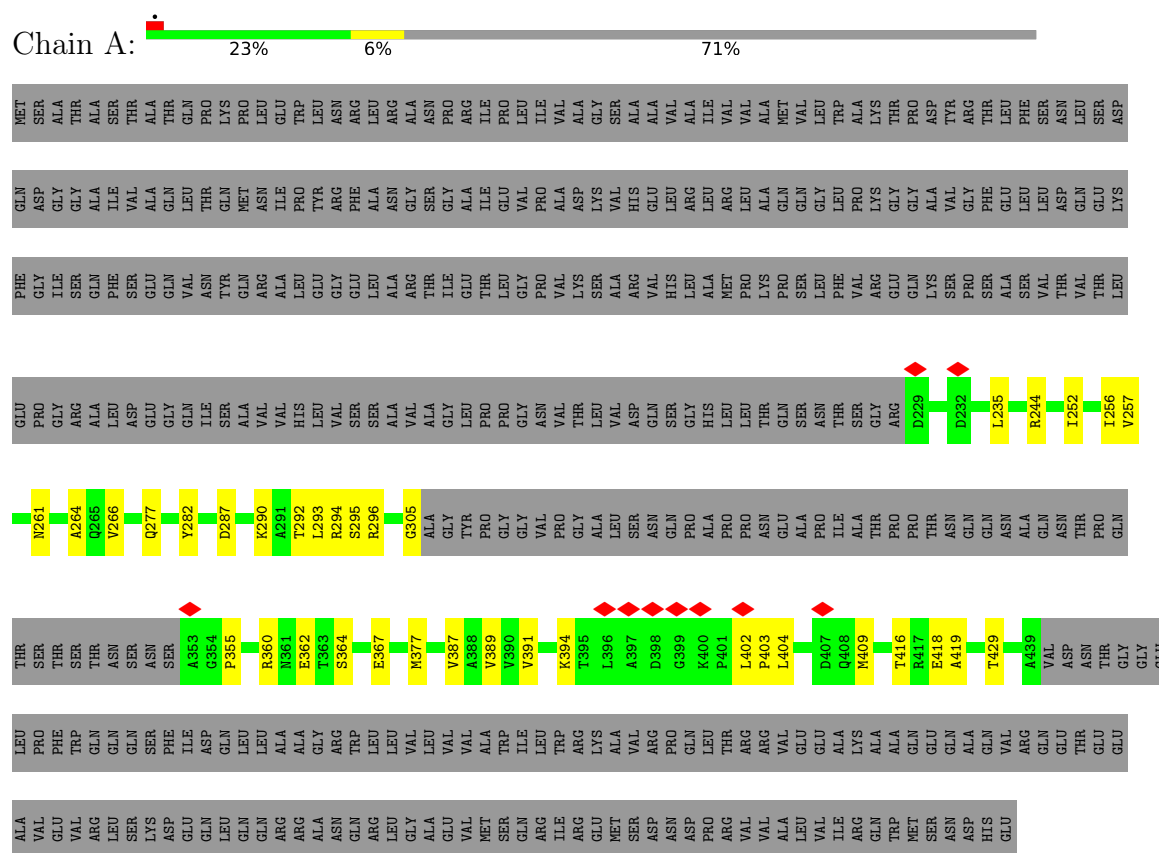
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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	164	Total 1275	C 776	N 237	O 259	S 3	0	0
1	S	164	Total 1275	C 776	N 237	O 259	S 3	0	0
1	T	164	Total 1275	C 776	N 237	O 259	S 3	0	0
1	U	164	Total 1275	C 776	N 237	O 259	S 3	0	0
1	V	164	Total 1275	C 776	N 237	O 259	S 3	0	0
1	W	164	Total 1275	C 776	N 237	O 259	S 3	0	0
1	X	164	Total 1275	C 776	N 237	O 259	S 3	0	0
1	Y	164	Total 1275	C 776	N 237	O 259	S 3	0	0
1	Z	164	Total 1275	C 776	N 237	O 259	S 3	0	0
1	a	164	Total 1275	C 776	N 237	O 259	S 3	0	0
1	b	164	Total 1275	C 776	N 237	O 259	S 3	0	0
1	c	164	Total 1275	C 776	N 237	O 259	S 3	0	0
1	d	164	Total 1275	C 776	N 237	O 259	S 3	0	0
1	e	164	Total 1275	C 776	N 237	O 259	S 3	0	0
1	f	164	Total 1275	C 776	N 237	O 259	S 3	0	0
1	g	164	Total 1275	C 776	N 237	O 259	S 3	0	0
1	h	164	Total 1275	C 776	N 237	O 259	S 3	0	0

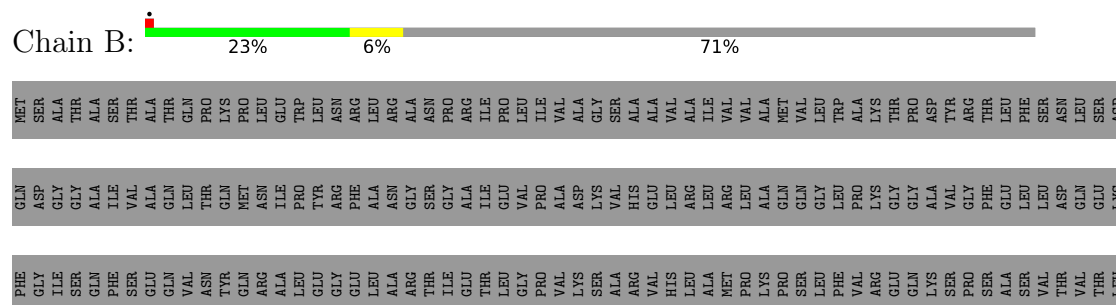
3 Residue-property plots

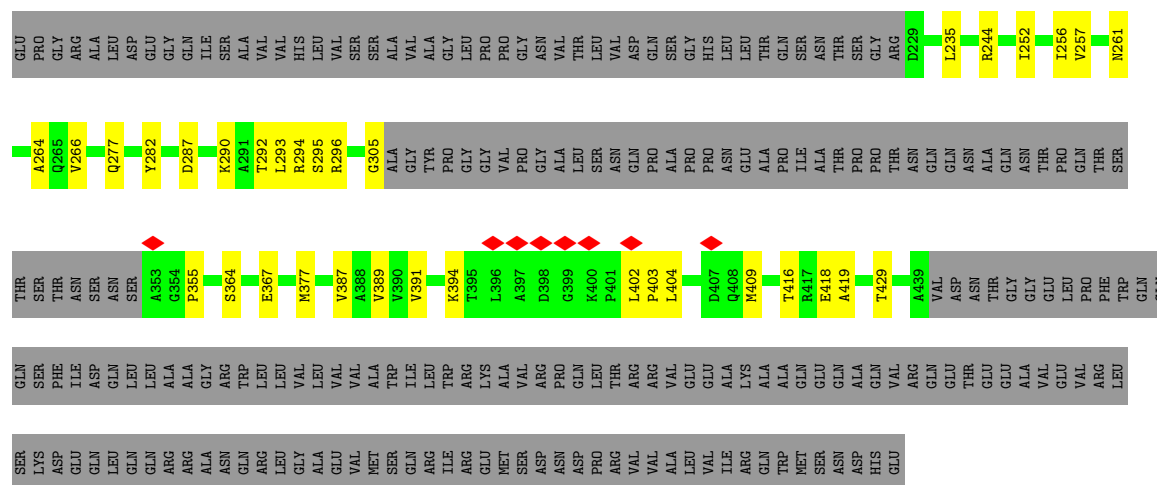
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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

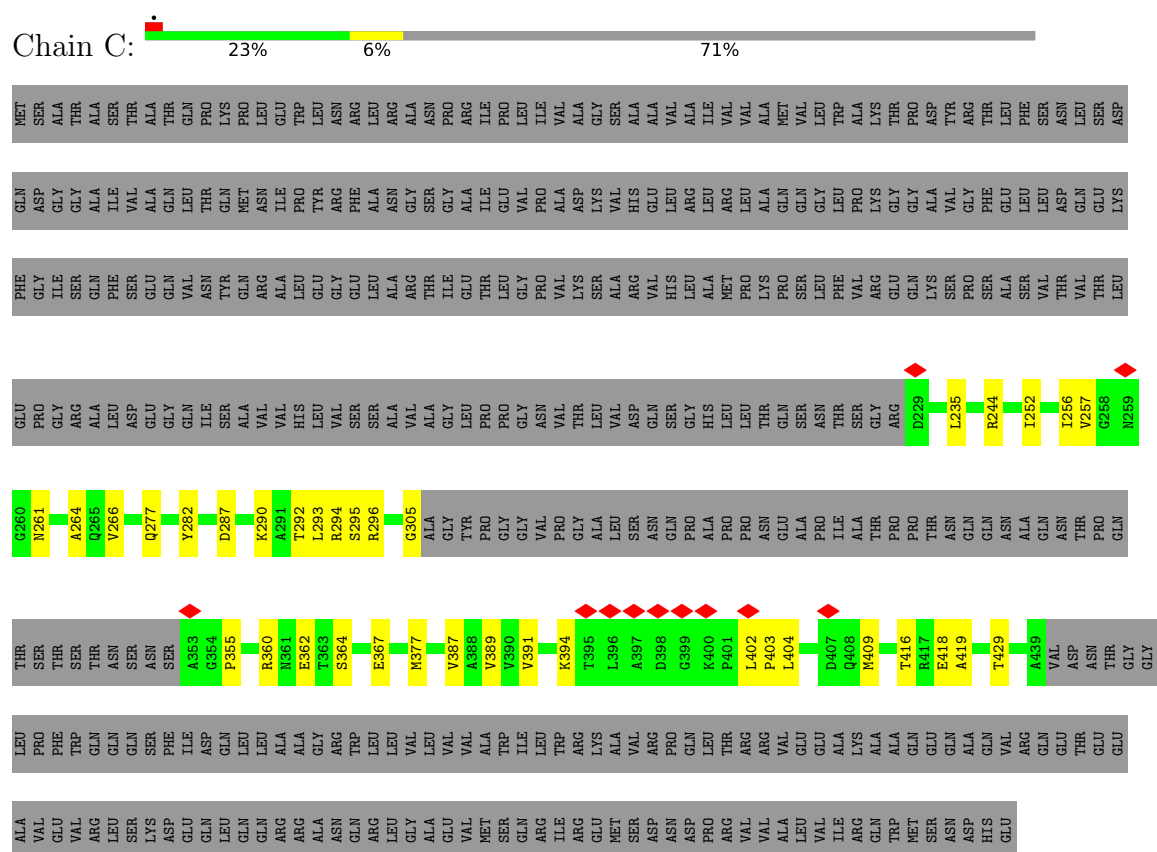


• Molecule 1: Flagellar M-ring protein

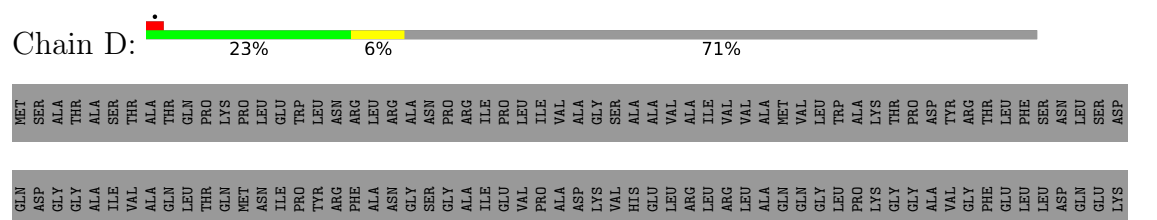


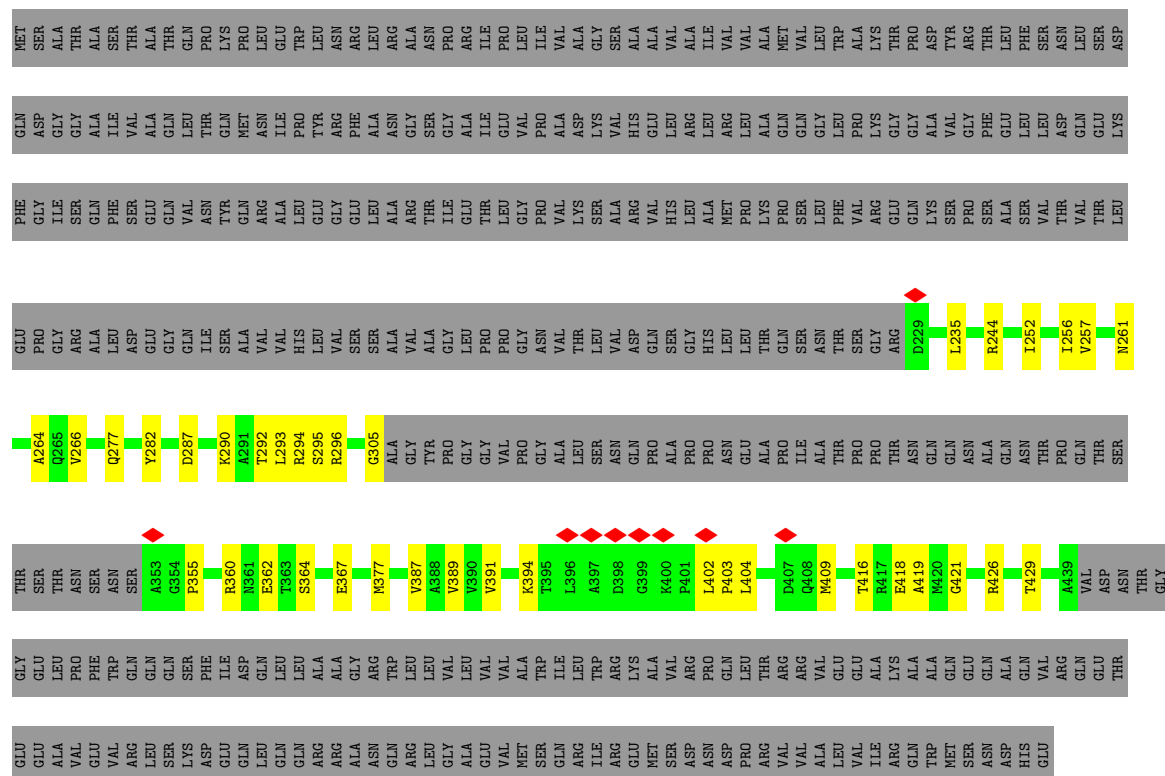


• Molecule 1: Flagellar M-ring protein

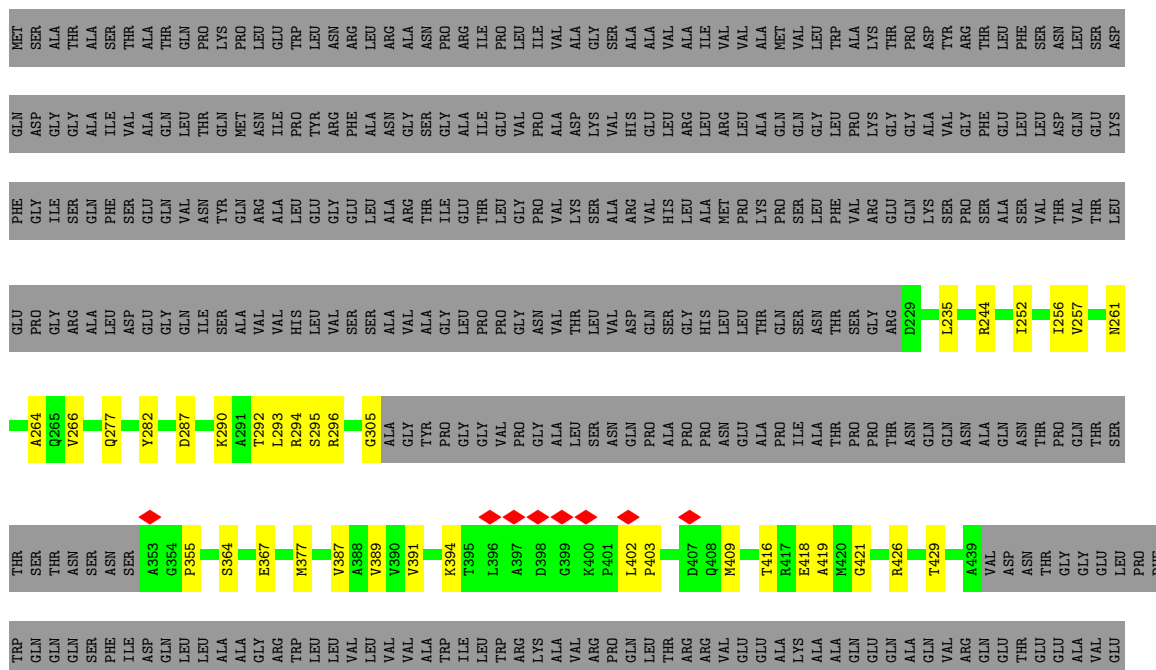


• Molecule 1: Flagellar M-ring protein





Chain J: 23% 6% 71%



[illegible]

- 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	ALA	ILE	VAL	VAL	VAL	MET	VAL	LEU	TRP	ALA	ALA	LYS	THR	PRO	ASP	TYP	ARG	THR	LEU	PHE	SER	ASN	LEU	SER	ASD
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[illegible]

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THR
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GLU	PRO	GLY	ARG	ALA	LEU	ASP	GLU	GLY	GLN	ILE	SER	SER	ALA	VAL	VAL	LEU	VAL	SER	SER	ALA	VAL	GLY	LEU	PRO	PRO	PRO	GLY	ASN	ASN	VAL	THR	THR	LEU	VAL	ASP	ASP	GLN	SER	SER	GLY	HIS	LEU	LEU	THR	THR	GLN	SER	ASN	THR	SER	SER	GLY	ARG	D229	L235	R244	L252	L256	V257
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	A264		Q265		V266			Q277			Y282		D287			K290		Z291		L293		R294		S295		R296			G305		ALA		GLY		TYR		PRO		GLY		VAL		PRO		GLY		ALA		LEU		SER		ASN		GLN		PRO		ALA		PRO		PRO		THR		THR		PRO		THR		ASW		GLM		GLN		ALA		ALA		GLN		ASW		THR		PRO		GLN		THR		THR		FER
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[illegible]

GLU PRO PRO 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 VAL GLU GLU ALA ALA LYS GLN GLN ALA ALA GLN VAL ARG GLN GLU THR THR

GLU
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MET
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GLU
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VAL
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GLN
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ASP
HIS

- Molecule 1: Flagellar M-ring protein



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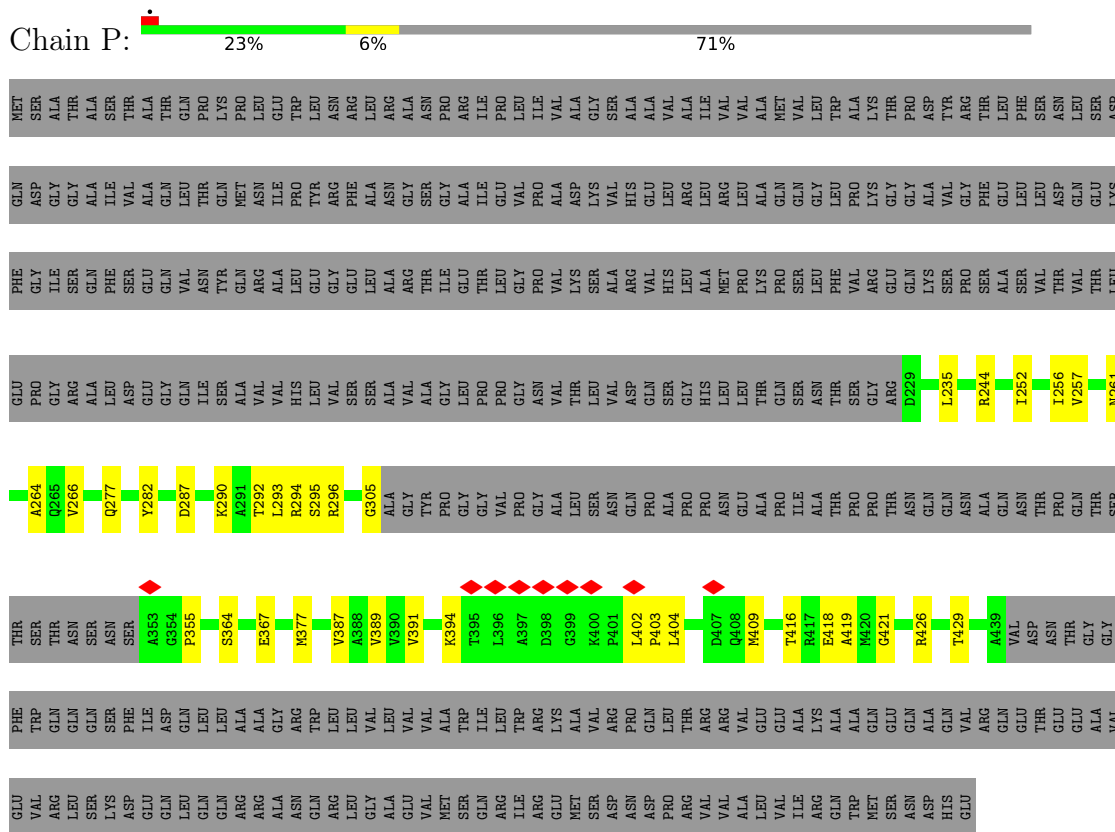
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PHE GLY ILE SER PHE SER GLU VAL TYR GLN ARG ALA LEU GLY GLU THR ILE GLU THR LEU GLY VAL LYS SER ALA ARG VAL HIS LEU ALA MET PRO LYS PRO SER LEU PHE VAL ARG GLN LYS SER PRO ARG ALA SER THR THR LEU

GLU	PRO	GLY	ARG	ALA	LEU	ASP	GLU	GLN	ILE	SER	ALA	VAL	HIS	LEU	VAL	SER	ALA	VAL	ALA	GLY	LEU	PRO	PRO	GLY	ASN	VAL	THR	LEU	VAL	ASP	GLN	SER	GLY	HIS	LEU	LEU	THR	GLN	SER	ASN	THR	SER	GLY	ARG	D229	D232	L235	R244	I252	I256
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Category	Value
N261	100
A264	100
Q265	100
V266	100
Q277	100
Y282	100
D287	100
K290	100
A291	100
T292	100
L293	100
R294	100
S295	100
R296	100
G305	100
ALA	100
GLY	100
TYR	100
PRO	100
GLY	100
GLY	100
VAL	100
PRO	100
GLY	100
ALA	100
ALA	100
LEU	100
SER	100
ASN	100
GLN	100
PRO	100
PRO	100
ALA	100
ALA	100
ILE	100
ALA	100
THR	100
PRO	100
PRO	100
THR	100
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GLN	100
ASN	100
THR	100
PRO	100
GLN	100

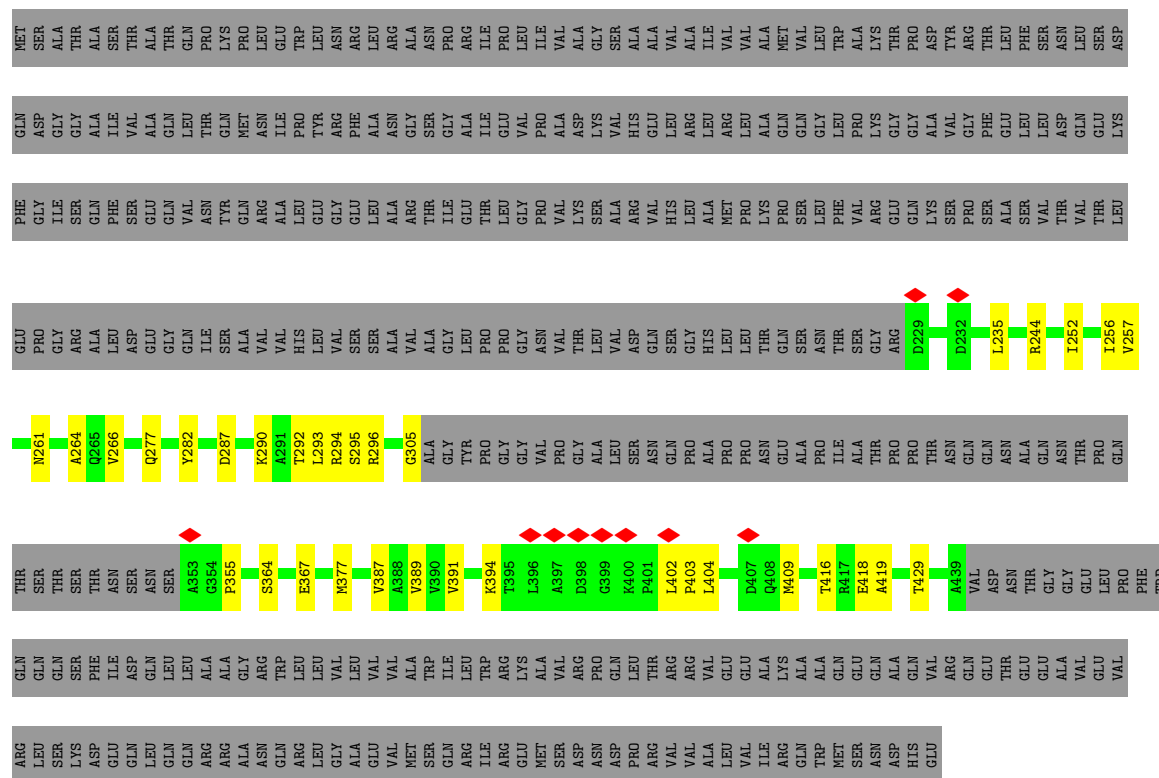
- Molecule 1: Flagellar M-ring protein



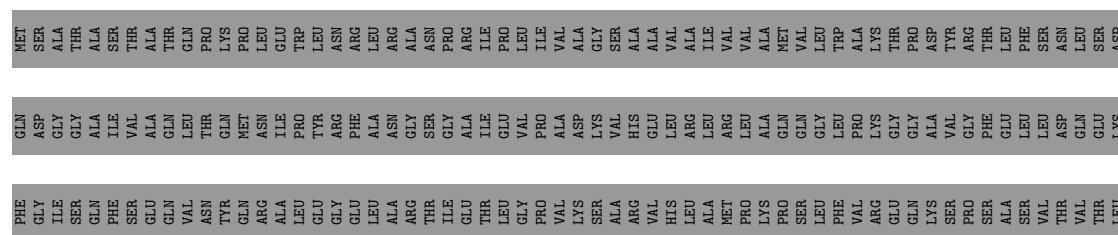
- Molecule 1: Flagellar M-ring protein



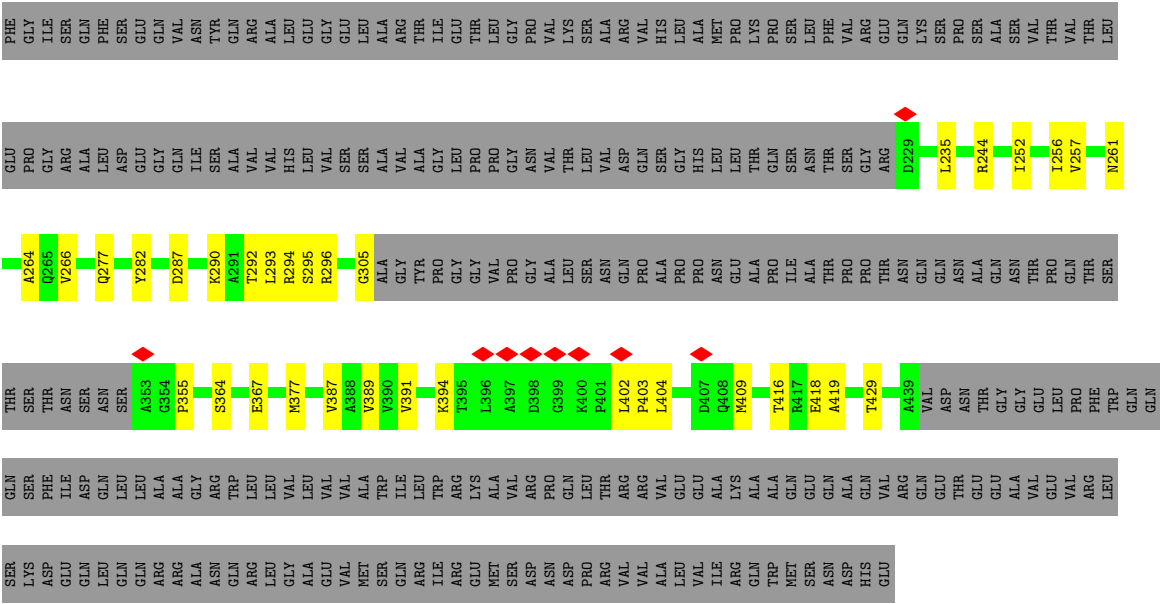
- Molecule 1: Flagellar M-ring protein



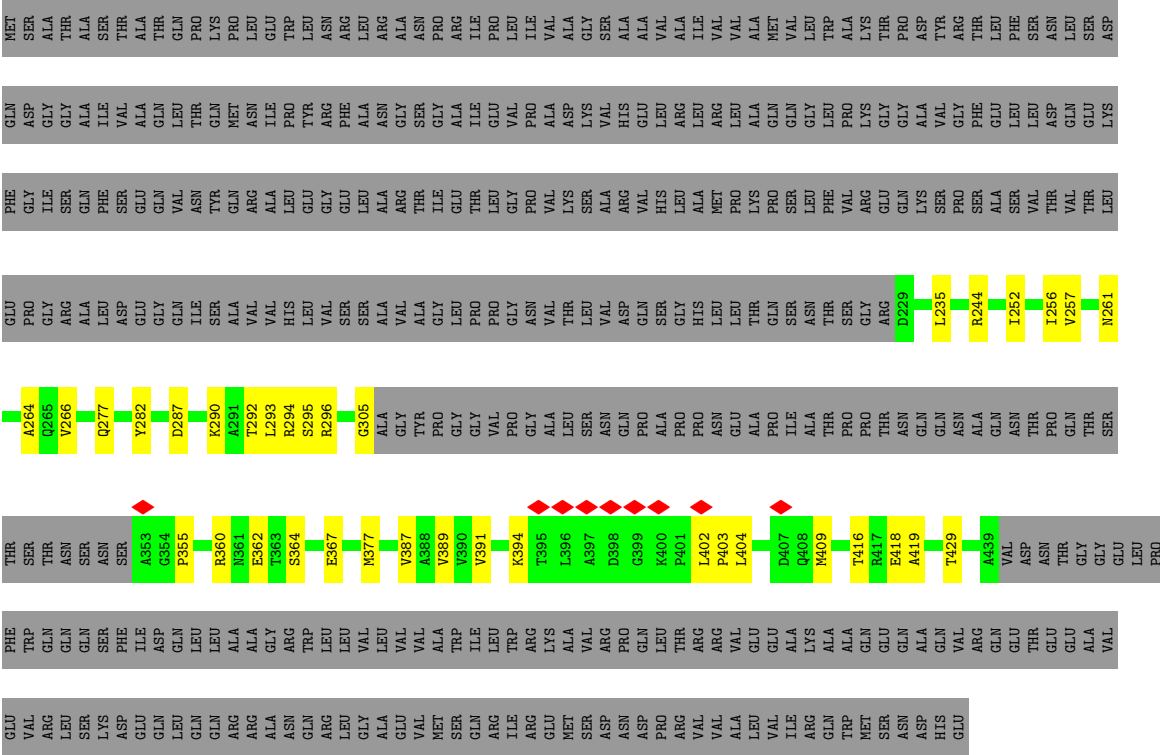
- Molecule 1: Flagellar M-ring protein



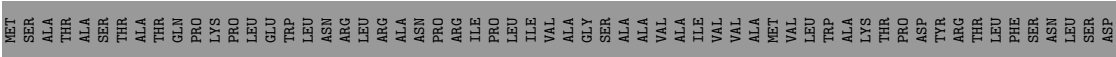




● Molecule 1: Flagellar M-ring protein

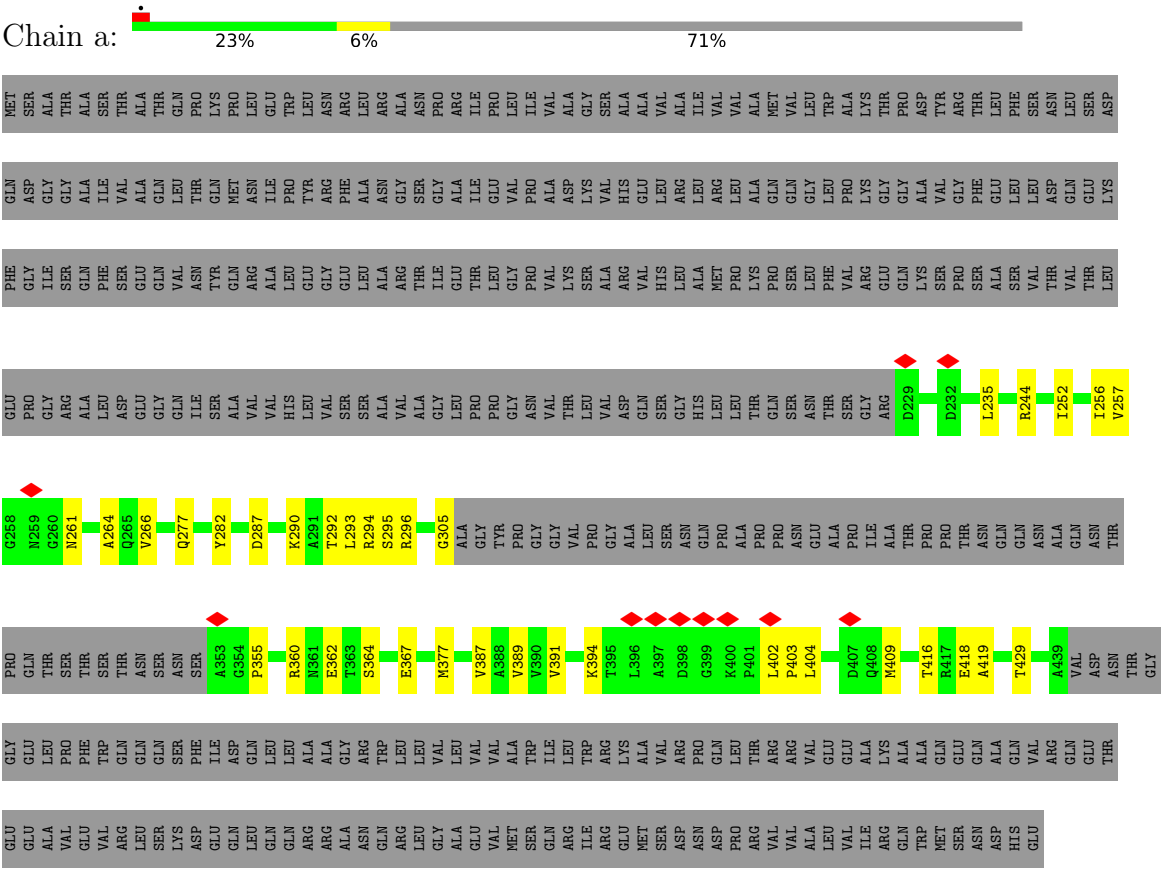


● Molecule 1: Flagellar M-ring protein

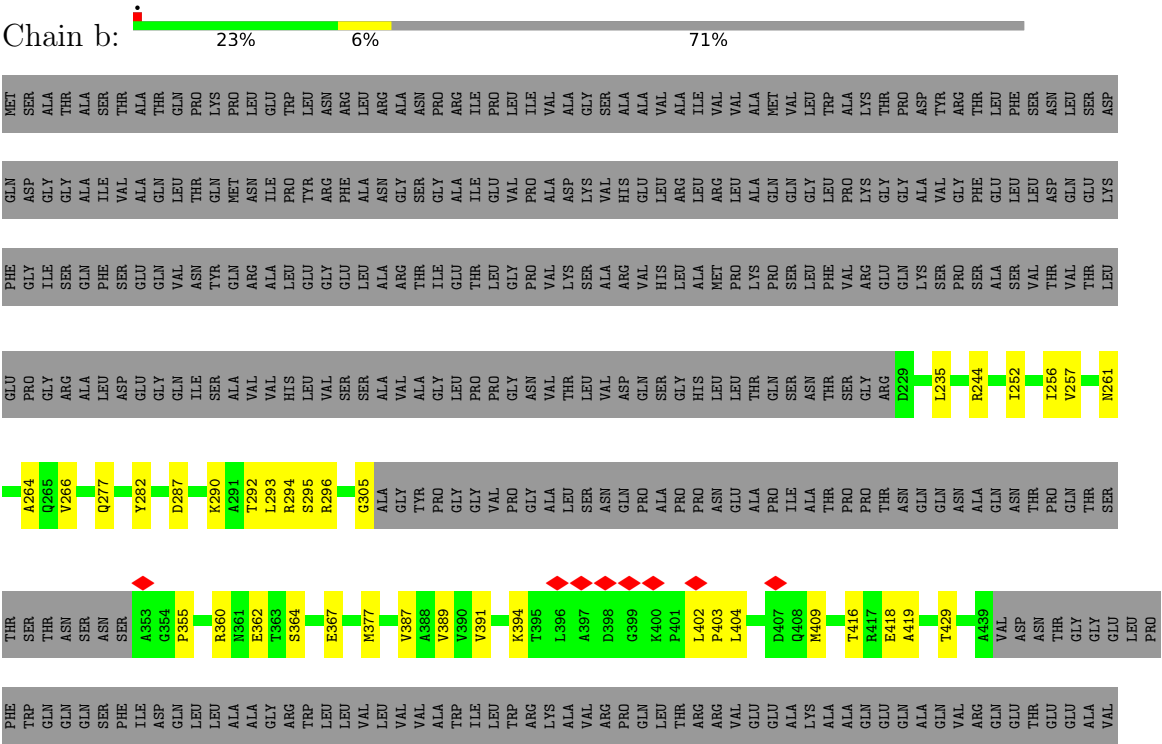




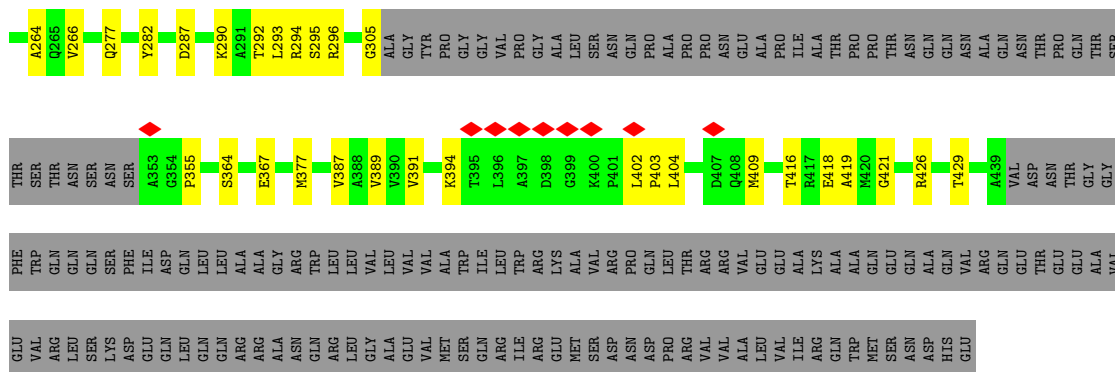
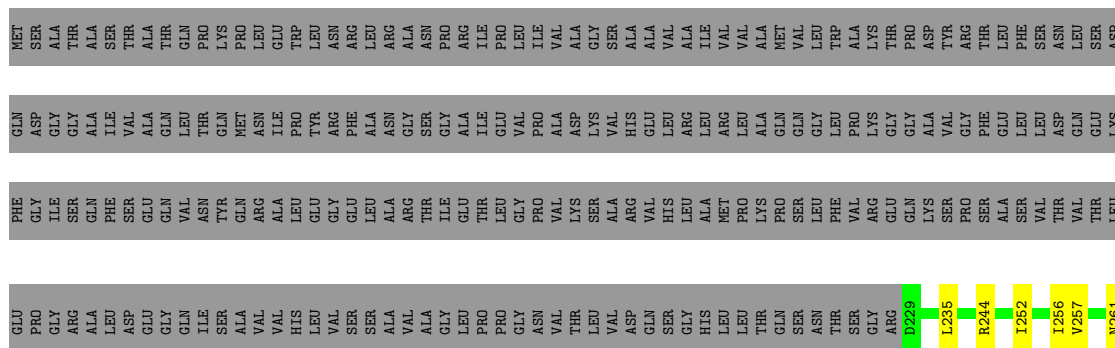
• Molecule 1: Flagellar M-ring protein



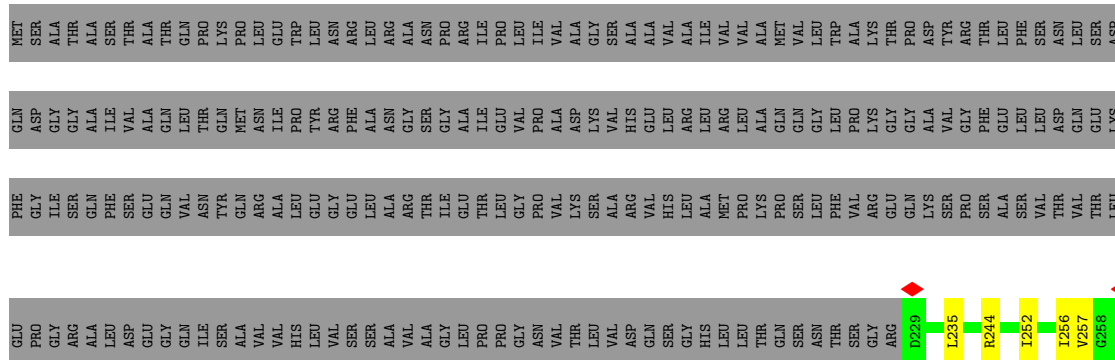
• Molecule 1: Flagellar M-ring protein

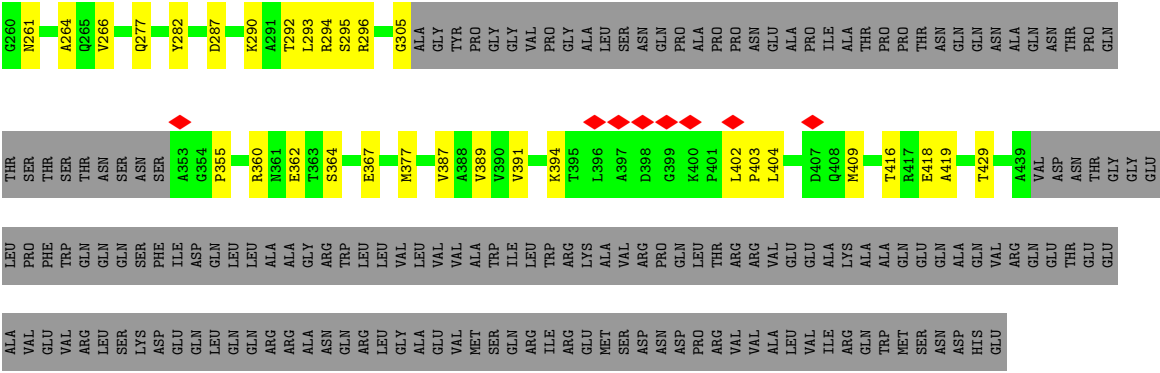


- Molecule 1: Flagellar M-ring protein



- Molecule 1: Flagellar M-ring protein





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C34	Depositor
Number of particles used	24190	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	105000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	3.464	Depositor
Minimum map value	-2.520	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.082	Depositor
Recommended contour level	0.35	Depositor
Map size (Å)	614.4, 614.4, 614.4	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2, 1.2, 1.2	Depositor

5 Model quality

5.1 Standard geometry

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	0.22	0/1289	0.44	1/1741 (0.1%)
1	B	0.22	0/1289	0.44	1/1741 (0.1%)
1	C	0.22	0/1289	0.44	1/1741 (0.1%)
1	D	0.22	0/1289	0.44	1/1741 (0.1%)
1	E	0.22	0/1289	0.44	1/1741 (0.1%)
1	F	0.22	0/1289	0.44	1/1741 (0.1%)
1	G	0.22	0/1289	0.44	1/1741 (0.1%)
1	H	0.22	0/1289	0.44	1/1741 (0.1%)
1	I	0.22	0/1289	0.44	1/1741 (0.1%)
1	J	0.22	0/1289	0.44	1/1741 (0.1%)
1	K	0.22	0/1289	0.44	1/1741 (0.1%)
1	L	0.22	0/1289	0.44	1/1741 (0.1%)
1	M	0.22	0/1289	0.44	1/1741 (0.1%)
1	N	0.22	0/1289	0.44	1/1741 (0.1%)
1	O	0.22	0/1289	0.44	1/1741 (0.1%)
1	P	0.22	0/1289	0.44	1/1741 (0.1%)
1	Q	0.22	0/1289	0.44	1/1741 (0.1%)
1	R	0.22	0/1289	0.44	1/1741 (0.1%)
1	S	0.22	0/1289	0.44	1/1741 (0.1%)
1	T	0.22	0/1289	0.44	1/1741 (0.1%)
1	U	0.22	0/1289	0.44	1/1741 (0.1%)
1	V	0.22	0/1289	0.44	1/1741 (0.1%)
1	W	0.22	0/1289	0.44	1/1741 (0.1%)
1	X	0.22	0/1289	0.44	1/1741 (0.1%)
1	Y	0.22	0/1289	0.44	1/1741 (0.1%)
1	Z	0.22	0/1289	0.44	1/1741 (0.1%)
1	a	0.22	0/1289	0.44	1/1741 (0.1%)
1	b	0.22	0/1289	0.44	1/1741 (0.1%)
1	c	0.22	0/1289	0.44	1/1741 (0.1%)
1	d	0.22	0/1289	0.44	1/1741 (0.1%)
1	e	0.22	0/1289	0.44	1/1741 (0.1%)
1	f	0.22	0/1289	0.44	1/1741 (0.1%)
1	g	0.22	0/1289	0.44	1/1741 (0.1%)
1	h	0.22	0/1289	0.44	1/1741 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.22	0/43826	0.44	34/59194 (0.1%)

There are no bond length outliers.

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	261	ASN	N-CA-C	-5.39	106.55	113.02
1	h	261	ASN	N-CA-C	-5.39	106.55	113.02
1	g	261	ASN	N-CA-C	-5.38	106.56	113.02
1	E	261	ASN	N-CA-C	-5.38	106.56	113.02
1	K	261	ASN	N-CA-C	-5.38	106.57	113.02

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	1275	0	1254	29	0
1	B	1275	0	1254	28	0
1	C	1275	0	1254	29	0
1	D	1275	0	1254	30	0
1	E	1275	0	1254	28	0
1	F	1275	0	1254	29	0
1	G	1275	0	1254	30	0
1	H	1275	0	1254	29	0
1	I	1275	0	1254	30	0
1	J	1275	0	1254	31	0
1	K	1275	0	1254	29	0
1	L	1275	0	1254	30	0
1	M	1275	0	1254	30	0
1	N	1275	0	1254	30	0
1	O	1275	0	1254	30	0
1	P	1275	0	1254	32	0
1	Q	1275	0	1254	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	R	1275	0	1254	29	0
1	S	1275	0	1254	31	0
1	T	1275	0	1254	30	0
1	U	1275	0	1254	30	0
1	V	1275	0	1254	32	0
1	W	1275	0	1254	30	0
1	X	1275	0	1254	29	0
1	Y	1275	0	1254	31	0
1	Z	1275	0	1254	29	0
1	a	1275	0	1254	31	0
1	b	1275	0	1254	31	0
1	c	1275	0	1254	29	0
1	d	1275	0	1254	29	0
1	e	1275	0	1254	32	0
1	f	1275	0	1254	31	0
1	g	1275	0	1254	30	0
1	h	1275	0	1254	30	0
All	All	43350	0	42636	832	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 10.

The worst 5 of 832 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:W:391:VAL:HG21	1:W:409:MET:HE1	1.78	0.66
1:X:391:VAL:HG21	1:X:409:MET:HE1	1.78	0.66
1:Y:391:VAL:HG21	1:Y:409:MET:HE1	1.78	0.66
1:Z:391:VAL:HG21	1:Z:409:MET:HE1	1.78	0.66
1:a:391:VAL:HG21	1:a:409:MET:HE1	1.78	0.66

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	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	B	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	C	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	D	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	E	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	F	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	G	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	H	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	I	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	J	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	K	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	L	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	M	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	N	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	O	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	P	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	Q	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	R	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	S	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	T	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	U	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	V	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	W	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	X	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	Y	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	Z	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	a	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	b	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	c	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	d	160/560 (29%)	158 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	e	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	f	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	g	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	h	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
All	All	5440/19040 (29%)	5372 (99%)	68 (1%)	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%)	140 (99%)	1 (1%)	76	92
1	B	141/467 (30%)	140 (99%)	1 (1%)	76	92
1	C	141/467 (30%)	140 (99%)	1 (1%)	76	92
1	D	141/467 (30%)	140 (99%)	1 (1%)	76	92
1	E	141/467 (30%)	140 (99%)	1 (1%)	76	92
1	F	141/467 (30%)	140 (99%)	1 (1%)	76	92
1	G	141/467 (30%)	140 (99%)	1 (1%)	76	92
1	H	141/467 (30%)	140 (99%)	1 (1%)	76	92
1	I	141/467 (30%)	140 (99%)	1 (1%)	76	92
1	J	141/467 (30%)	140 (99%)	1 (1%)	76	92
1	K	141/467 (30%)	140 (99%)	1 (1%)	76	92
1	L	141/467 (30%)	140 (99%)	1 (1%)	76	92
1	M	141/467 (30%)	140 (99%)	1 (1%)	76	92
1	N	141/467 (30%)	140 (99%)	1 (1%)	76	92
1	O	141/467 (30%)	140 (99%)	1 (1%)	76	92
1	P	141/467 (30%)	140 (99%)	1 (1%)	76	92
1	Q	141/467 (30%)	140 (99%)	1 (1%)	76	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	R	141/467 (30%)	140 (99%)	1 (1%)	76	92
1	S	141/467 (30%)	140 (99%)	1 (1%)	76	92
1	T	141/467 (30%)	140 (99%)	1 (1%)	76	92
1	U	141/467 (30%)	140 (99%)	1 (1%)	76	92
1	V	141/467 (30%)	140 (99%)	1 (1%)	76	92
1	W	141/467 (30%)	140 (99%)	1 (1%)	76	92
1	X	141/467 (30%)	140 (99%)	1 (1%)	76	92
1	Y	141/467 (30%)	140 (99%)	1 (1%)	76	92
1	Z	141/467 (30%)	140 (99%)	1 (1%)	76	92
1	a	141/467 (30%)	140 (99%)	1 (1%)	76	92
1	b	141/467 (30%)	140 (99%)	1 (1%)	76	92
1	c	141/467 (30%)	140 (99%)	1 (1%)	76	92
1	d	141/467 (30%)	140 (99%)	1 (1%)	76	92
1	e	141/467 (30%)	140 (99%)	1 (1%)	76	92
1	f	141/467 (30%)	140 (99%)	1 (1%)	76	92
1	g	141/467 (30%)	140 (99%)	1 (1%)	76	92
1	h	141/467 (30%)	140 (99%)	1 (1%)	76	92
All	All	4794/15878 (30%)	4760 (99%)	34 (1%)	73	92

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	c	295	SER
1	d	295	SER
1	g	295	SER
1	M	295	SER
1	L	295	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 213 such sidechains are listed below:

Mol	Chain	Res	Type
1	S	434	ASN
1	W	378	ASN
1	f	303	GLN
1	T	281	HIS

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Mol	Chain	Res	Type
1	U	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.

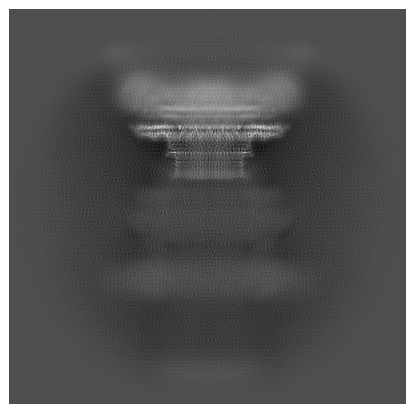
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37590. These allow visual inspection of the internal detail of the map and identification of artifacts.

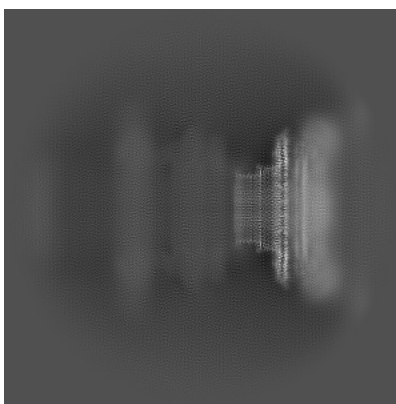
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

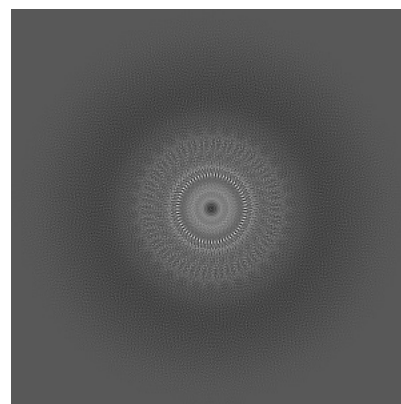
6.1.1 Primary map



X

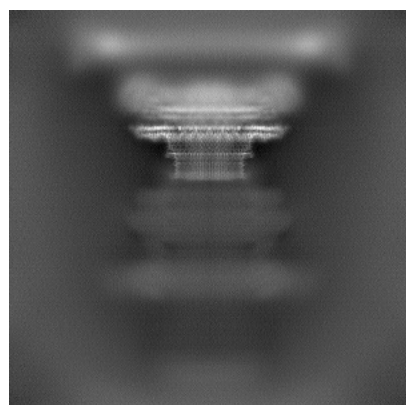


Y

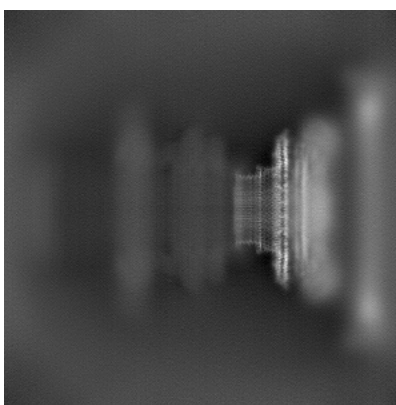


Z

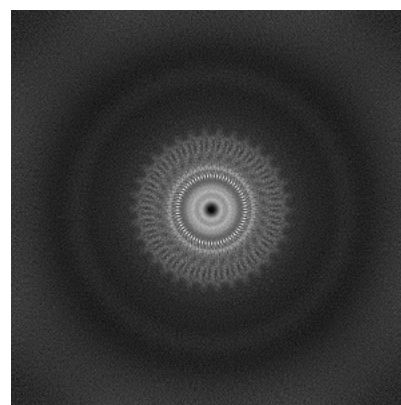
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices [i](#)

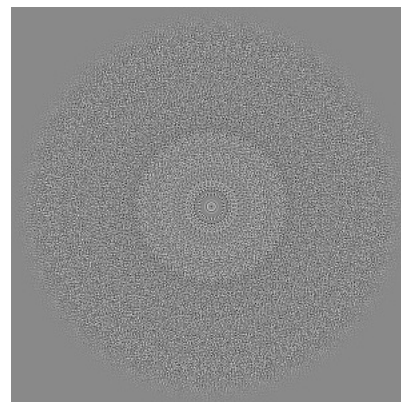
6.2.1 Primary map



X Index: 256

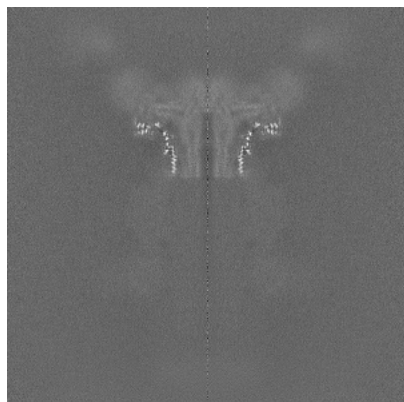


Y Index: 256

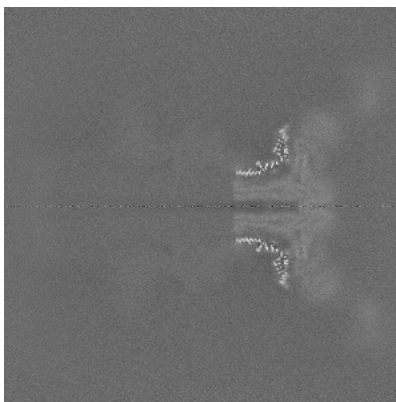


Z Index: 256

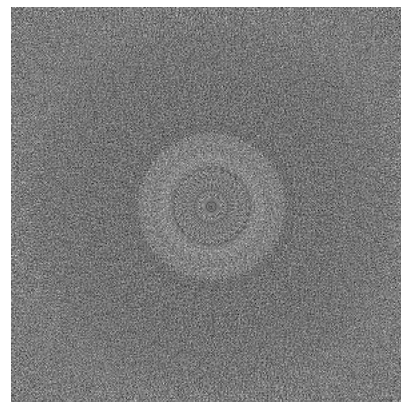
6.2.2 Raw map



X Index: 256



Y Index: 256

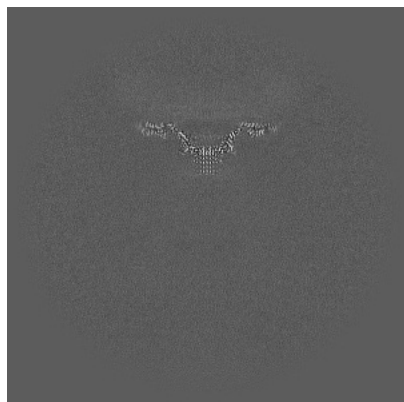


Z Index: 256

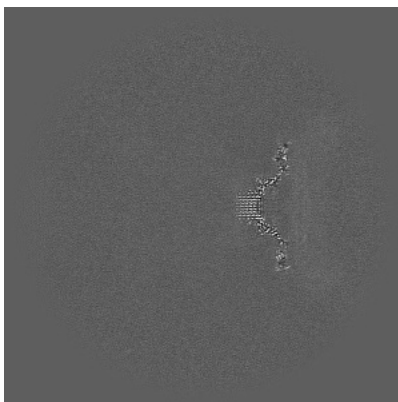
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

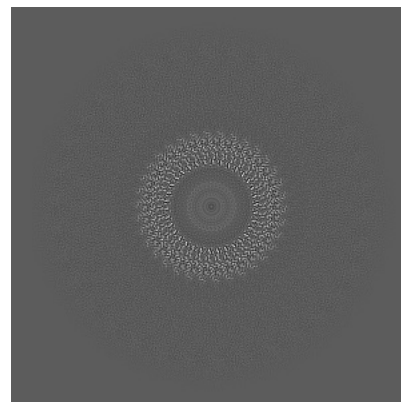
6.3.1 Primary map



X Index: 212



Y Index: 214

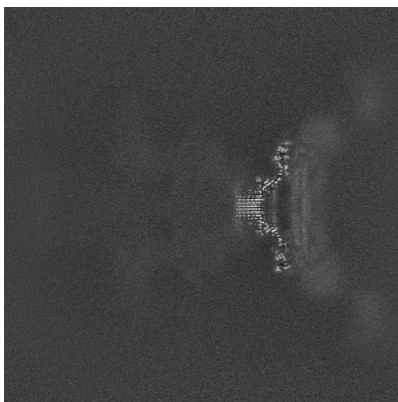


Z Index: 352

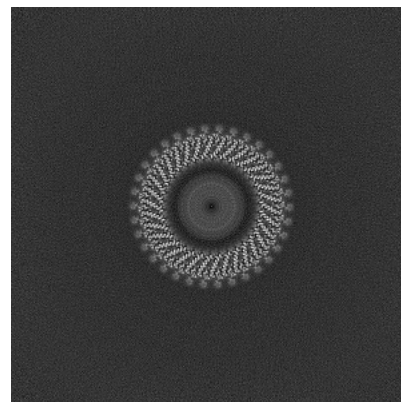
6.3.2 Raw map



X Index: 213



Y Index: 213

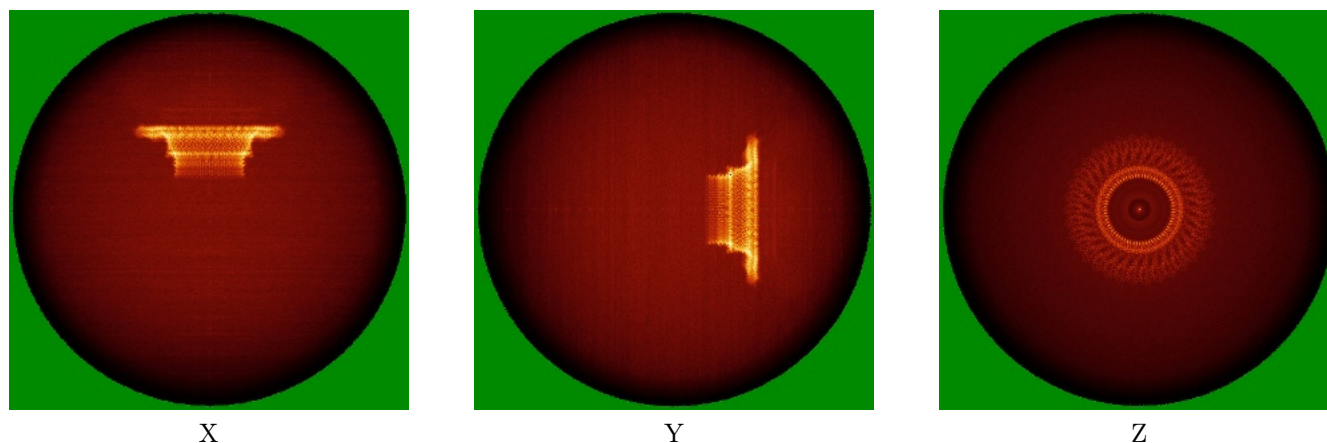


Z Index: 360

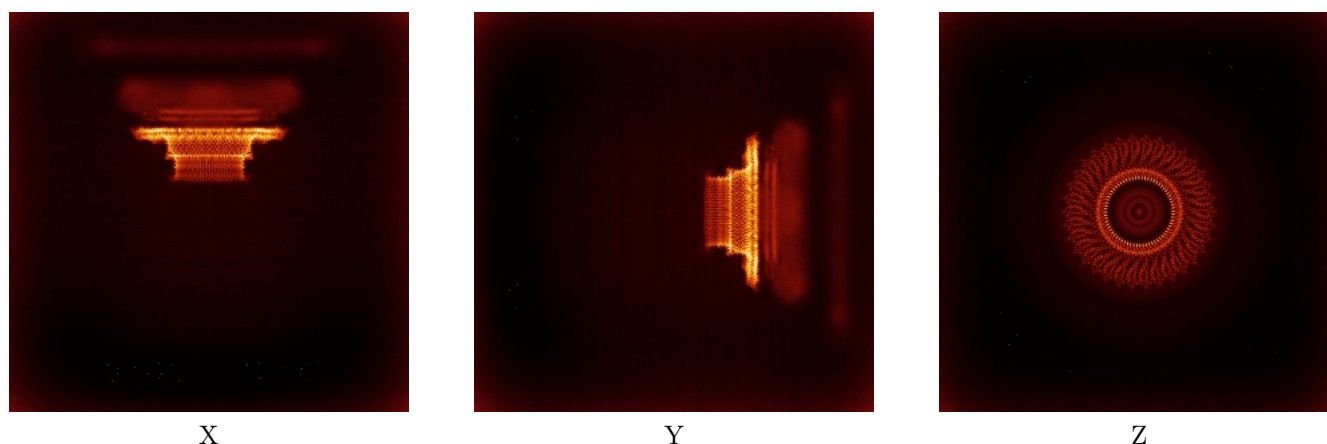
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

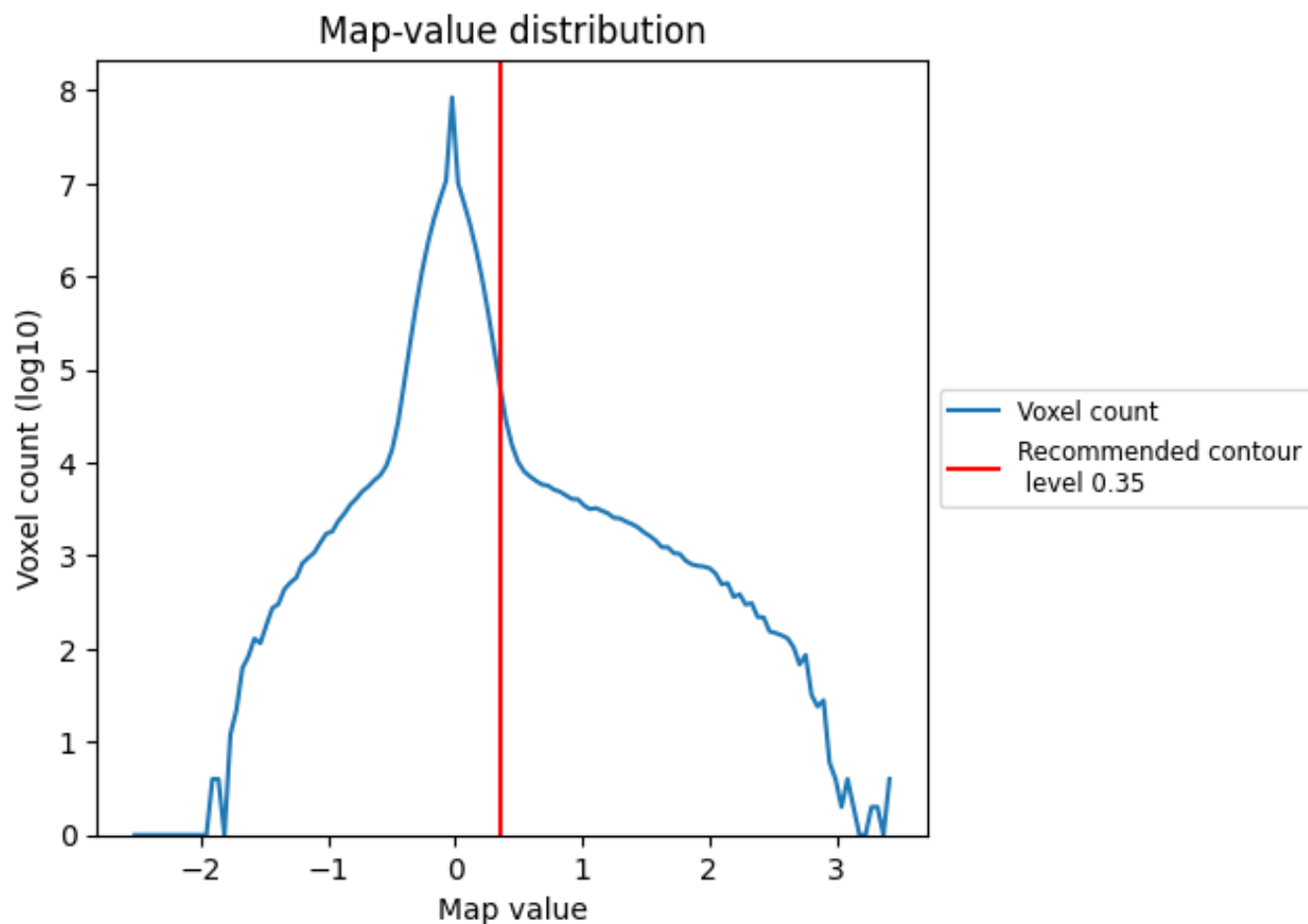
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

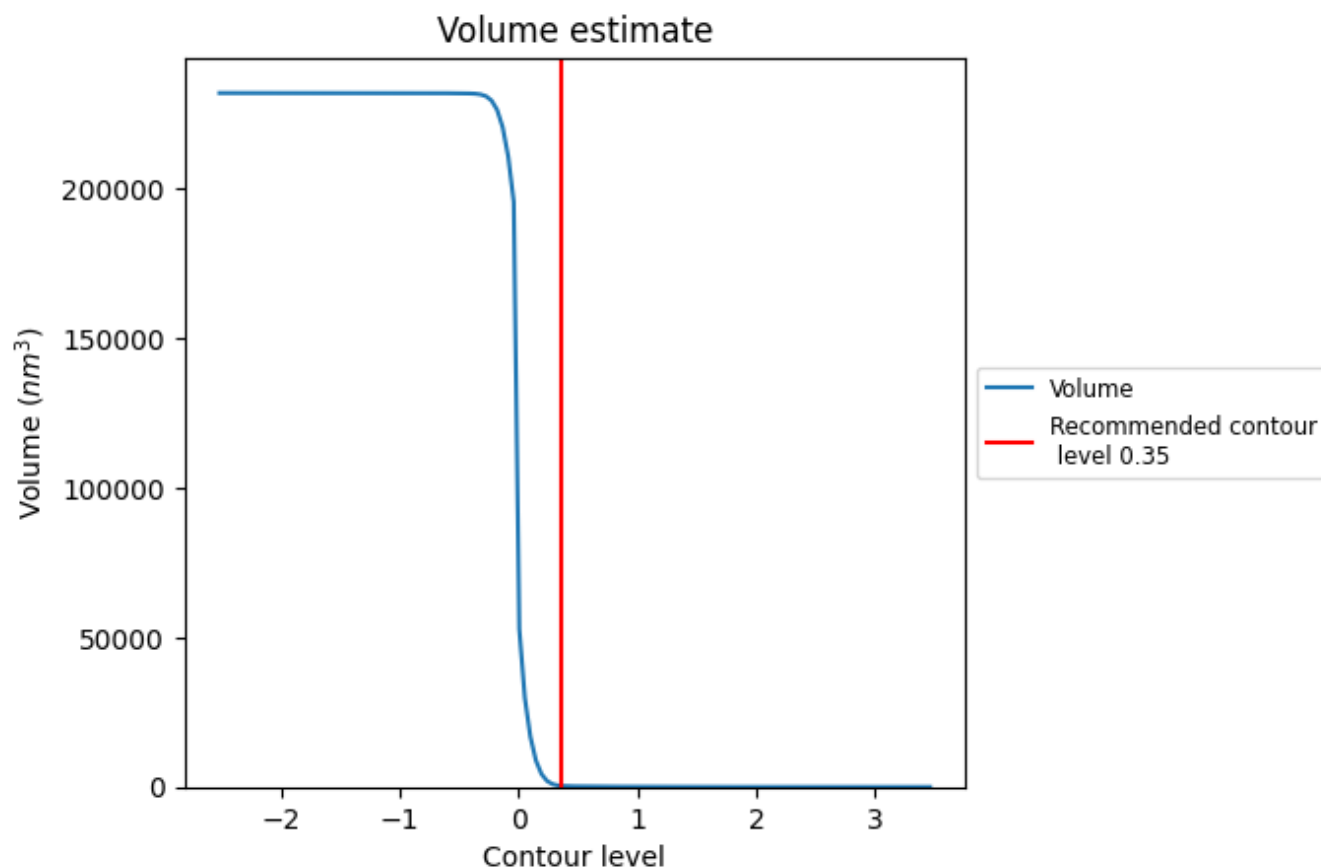
This section contains the results of statistical analysis of the map.

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.

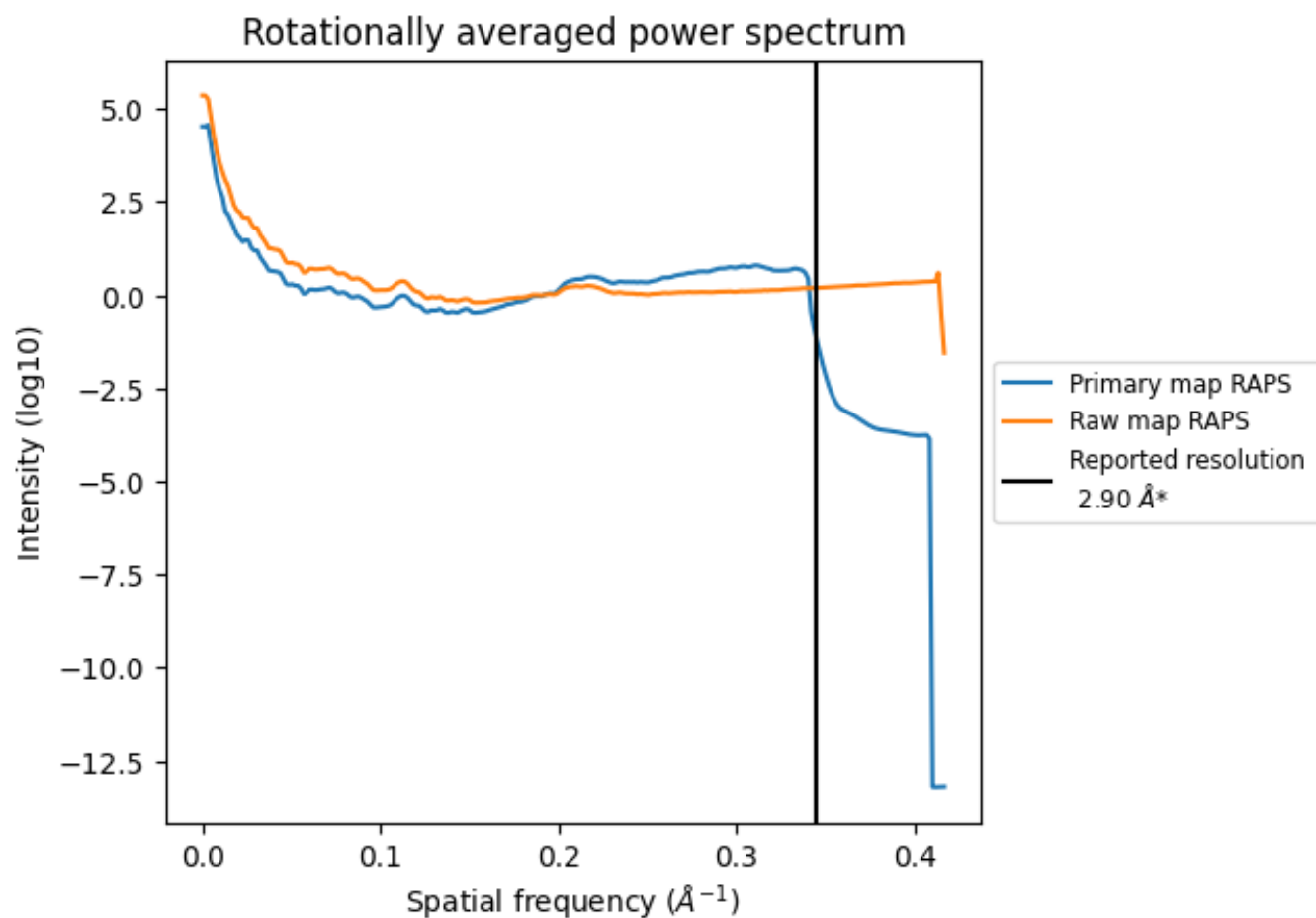
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 418 nm^3 ; this corresponds to an approximate mass of 378 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 ⓘ

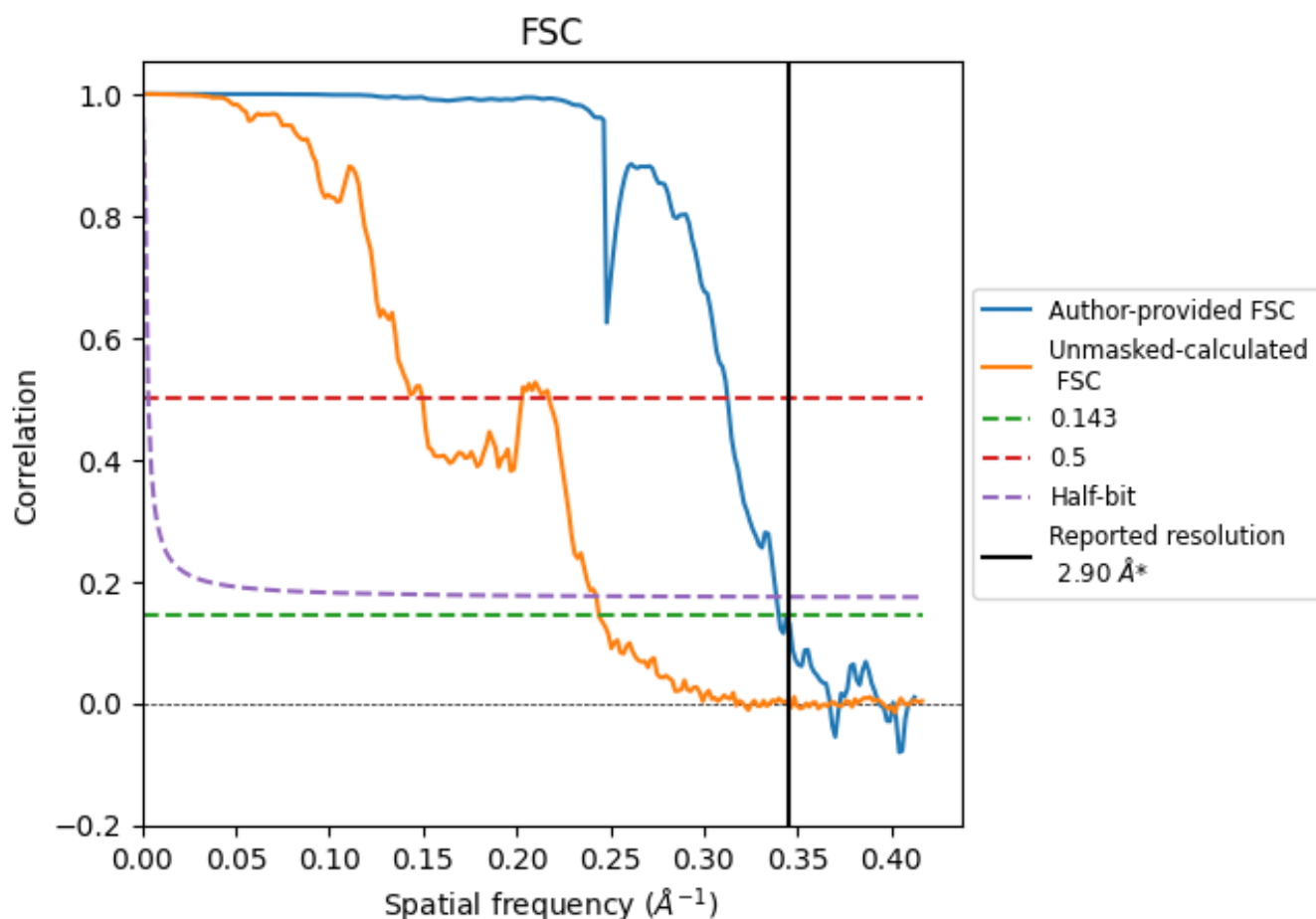


*Reported resolution corresponds to spatial frequency of 0.345 $\text{\AA}^{-1}$

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 $0.345 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

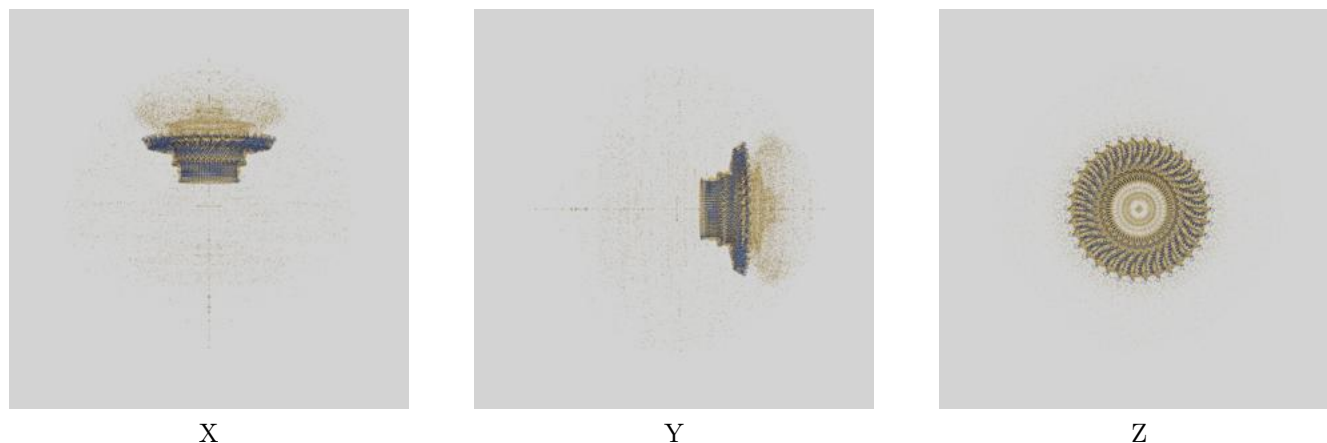
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.94	3.20	2.95
Unmasked-calculated*	4.10	6.68	4.12

*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 4.10 differs from the reported value 2.9 by more than 10 %

9 Map-model fit [i](#)

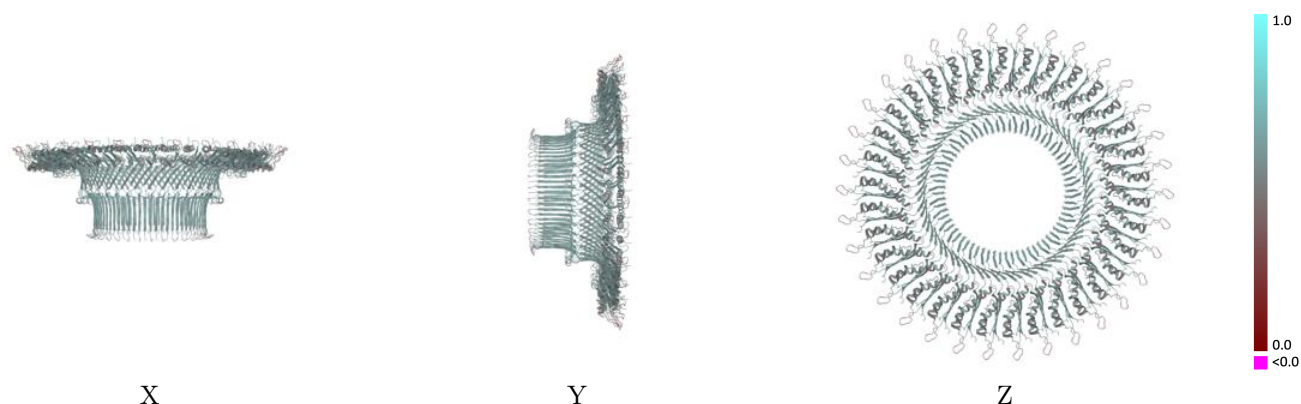
This section contains information regarding the fit between EMDB map EMD-37590 and PDB model 8WJR. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



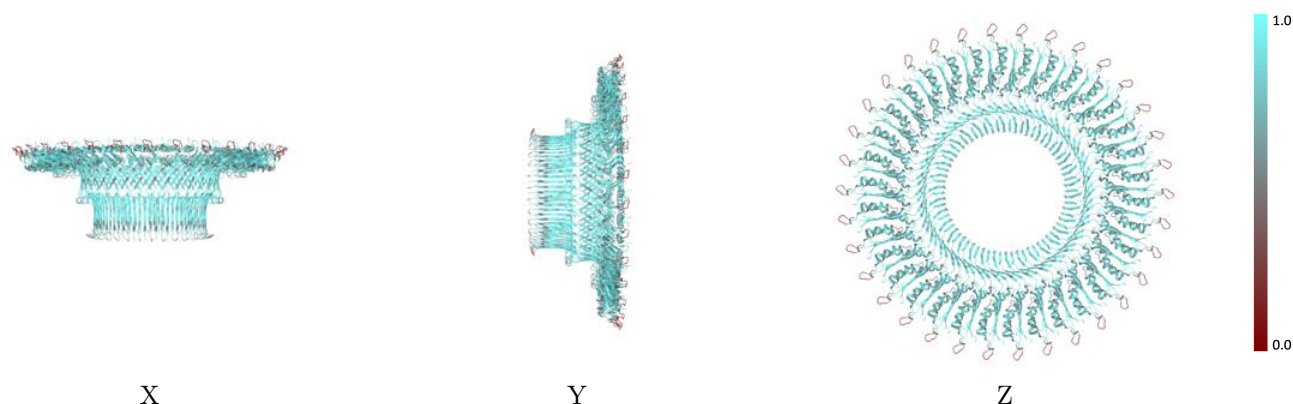
The images above show the 3D surface view of the map at the recommended contour level 0.35 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



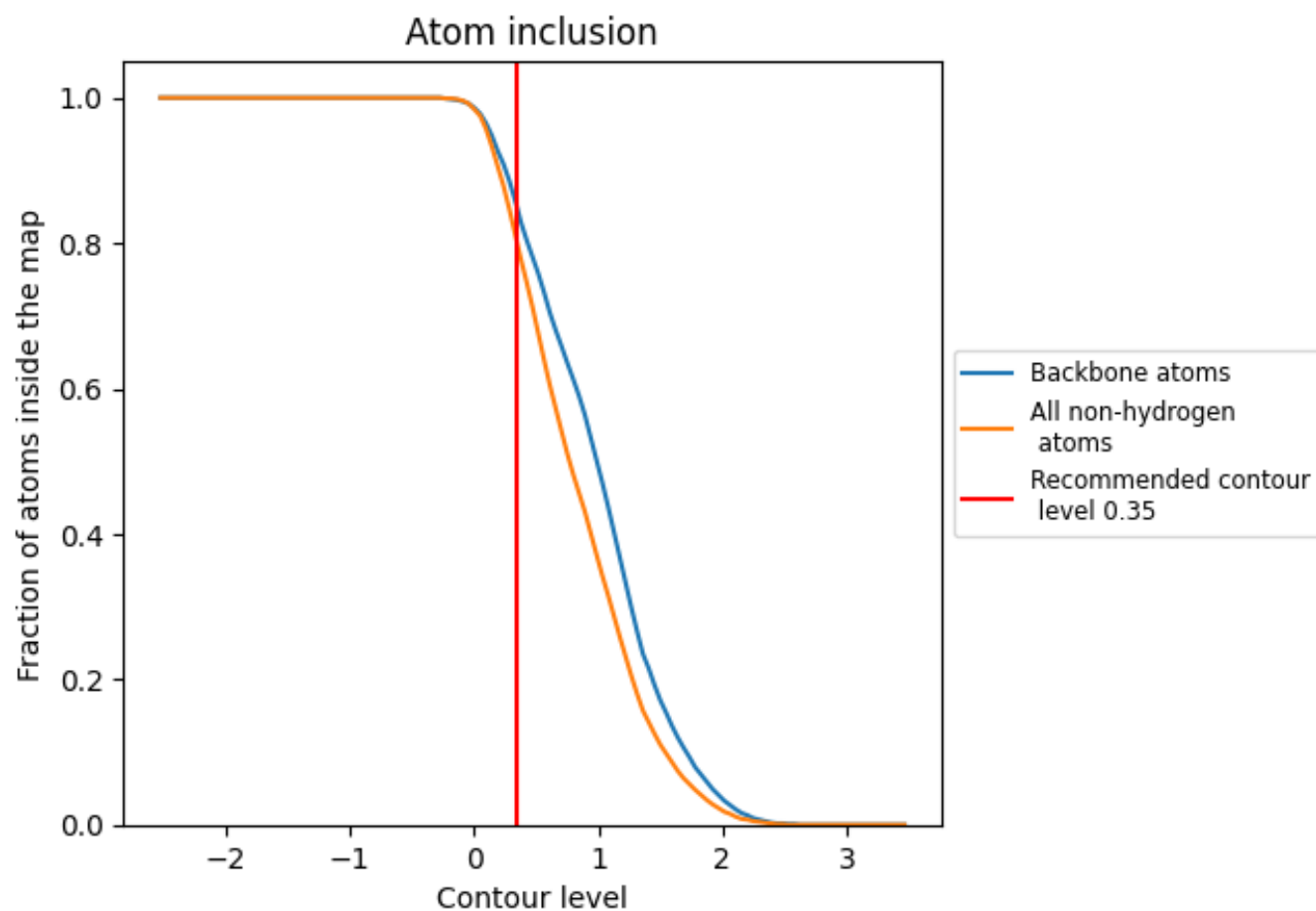
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.35).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 80% 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 (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7990	 0.5500
A	 0.7990	 0.5480
B	 0.8050	 0.5490
C	 0.7920	 0.5510
D	 0.8000	 0.5490
E	 0.8000	 0.5510
F	 0.8000	 0.5520
G	 0.8020	 0.5510
H	 0.7960	 0.5530
I	 0.8040	 0.5500
J	 0.7960	 0.5510
K	 0.8040	 0.5490
L	 0.7880	 0.5500
M	 0.8110	 0.5530
N	 0.7940	 0.5480
O	 0.7930	 0.5500
P	 0.7960	 0.5510
Q	 0.7980	 0.5500
R	 0.7990	 0.5490
S	 0.8050	 0.5490
T	 0.7920	 0.5510
U	 0.8000	 0.5480
V	 0.8000	 0.5500
W	 0.8000	 0.5490
X	 0.8020	 0.5480
Y	 0.7960	 0.5510
Z	 0.8040	 0.5490
a	 0.7960	 0.5510
b	 0.8040	 0.5490
c	 0.7880	 0.5510
d	 0.8110	 0.5540
e	 0.7940	 0.5470
f	 0.7930	 0.5490
g	 0.7960	 0.5490
h	 0.7980	 0.5490

