



Full wwPDB EM Validation Report ⓘ

Mar 18, 2025 – 08:37 PM JST

PDB ID : 8WJR
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 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.dev117
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41.4

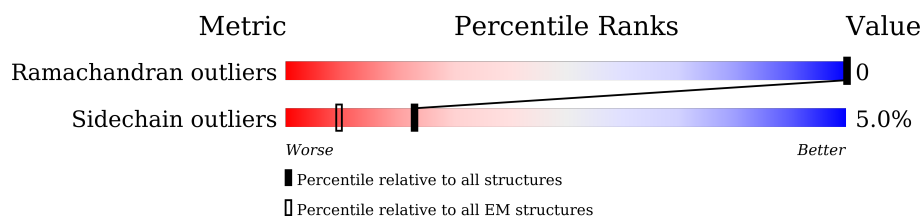
1 Overall quality at a glance

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.








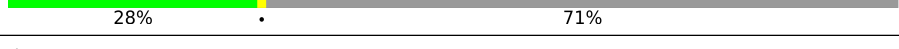

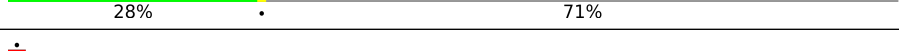
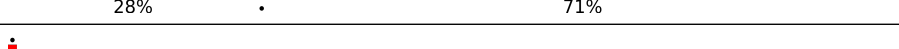
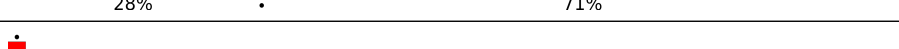















Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	 28% 71%
1	B	560	 28% 71%
1	C	560	 28% 71%
1	D	560	 28% 71%
1	E	560	 28% 71%
1	F	560	 28% 71%
1	G	560	 28% 71%
1	H	560	 28% 71%
1	I	560	 28% 71%

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Mol	Chain	Length	Quality of chain
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	
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 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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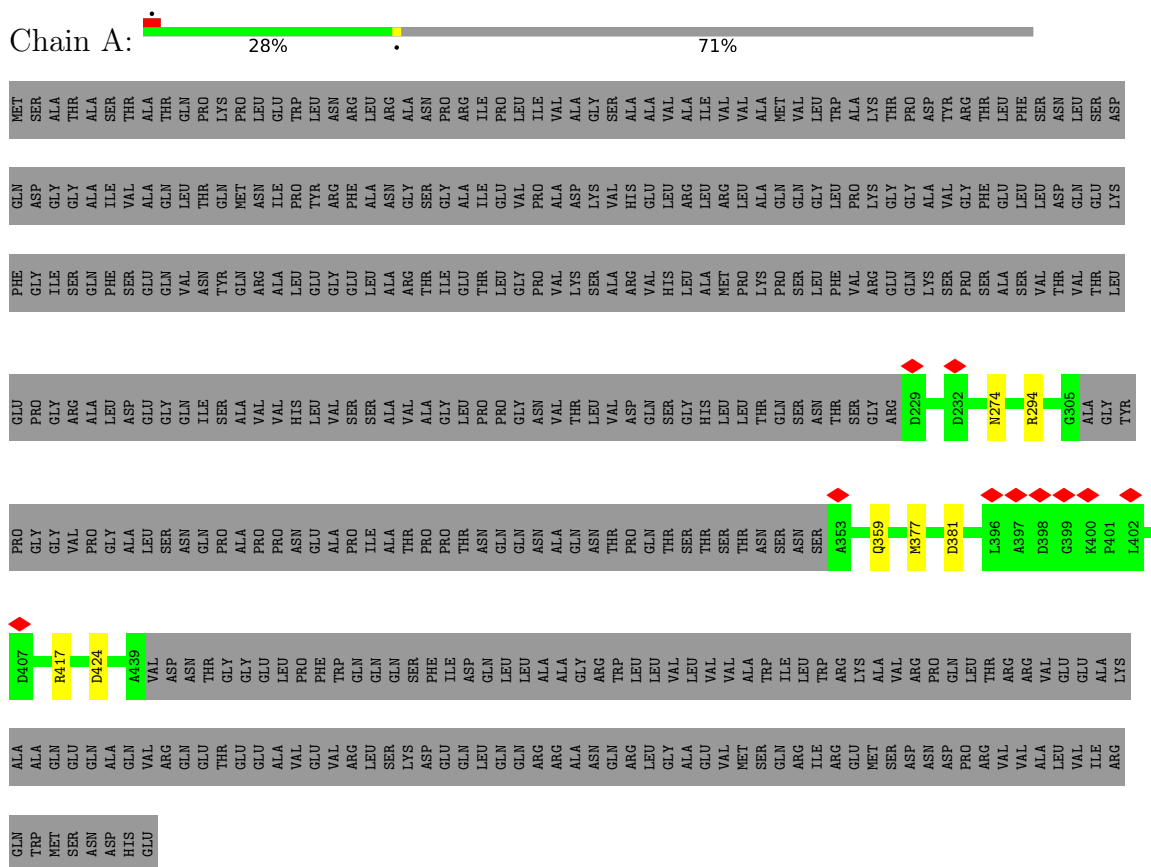
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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	164	Total 1275	C 776	N 237	O 259	S 3	0	0
1	S	164	Total 1275	C 776	N 237	O 259	S 3	0	0
1	T	164	Total 1275	C 776	N 237	O 259	S 3	0	0
1	U	164	Total 1275	C 776	N 237	O 259	S 3	0	0
1	V	164	Total 1275	C 776	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

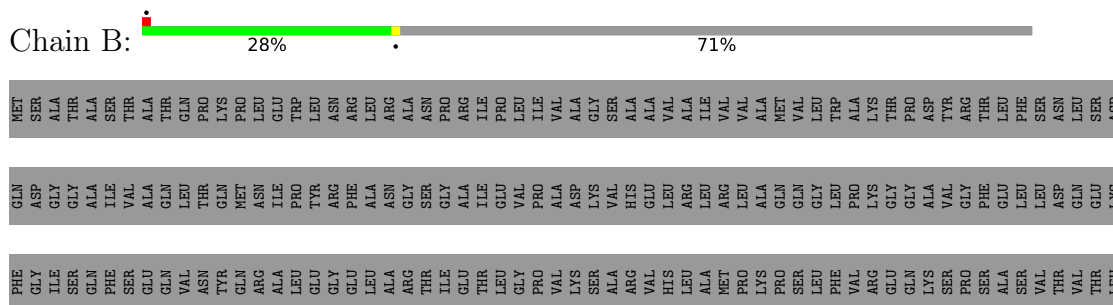
3 Residue-property plots

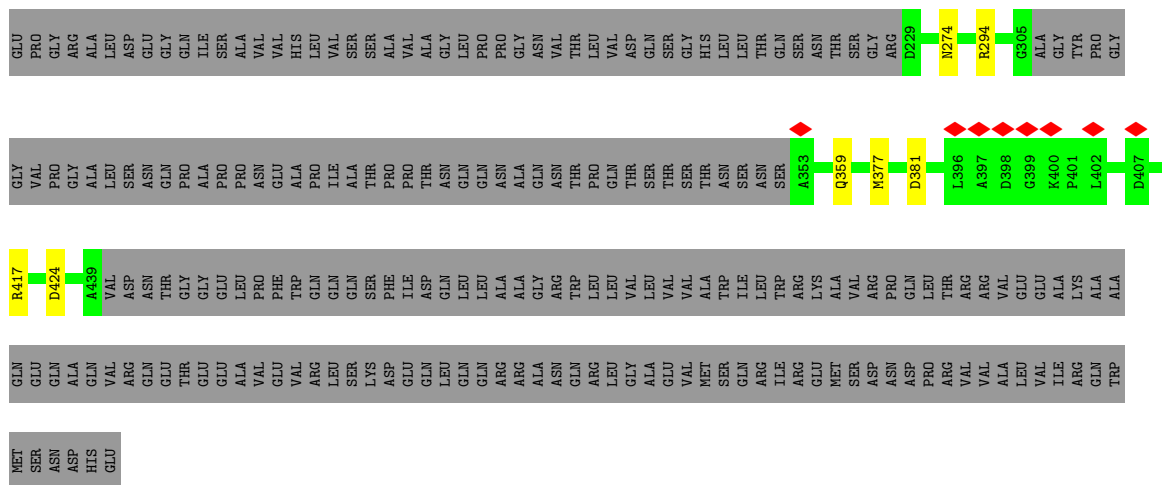
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

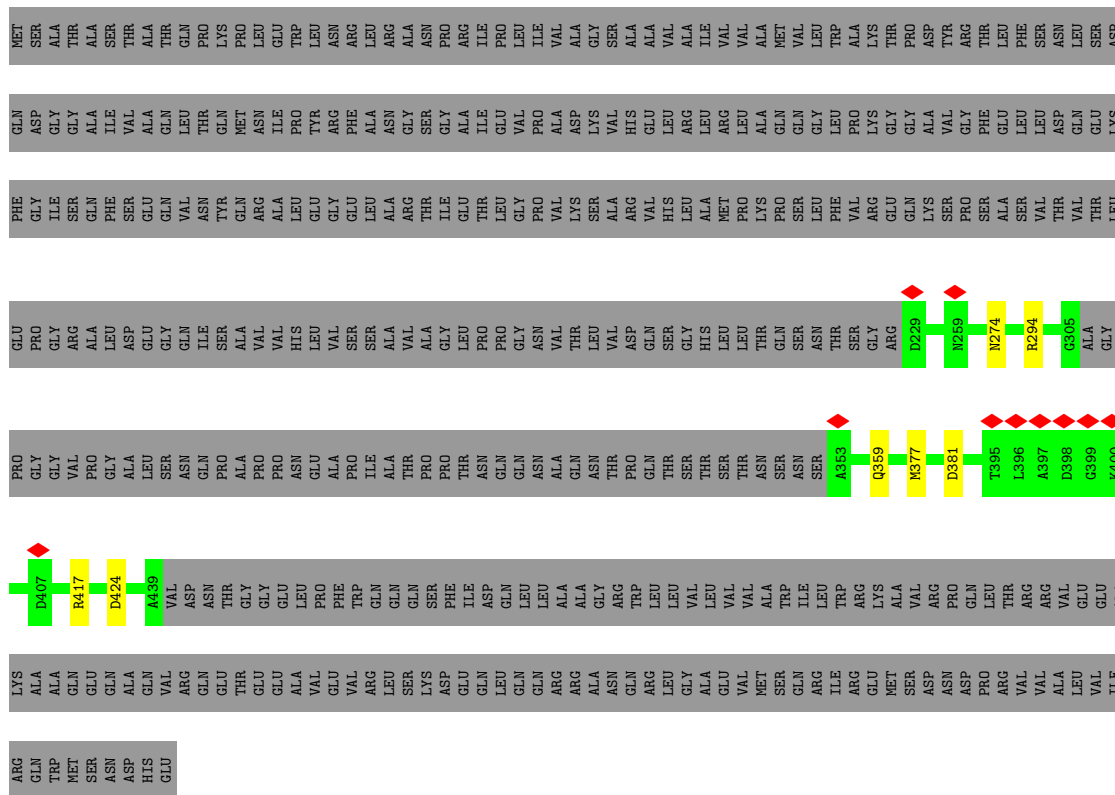


• Molecule 1: Flagellar M-ring protein

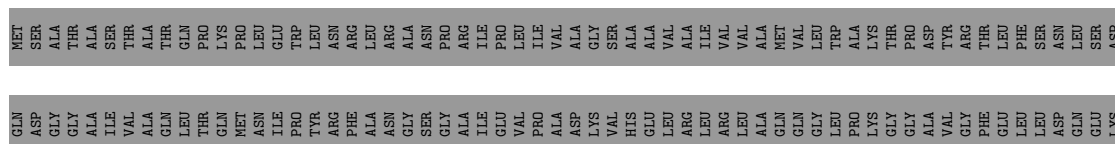




- Molecule 1: Flagellar M-ring protein

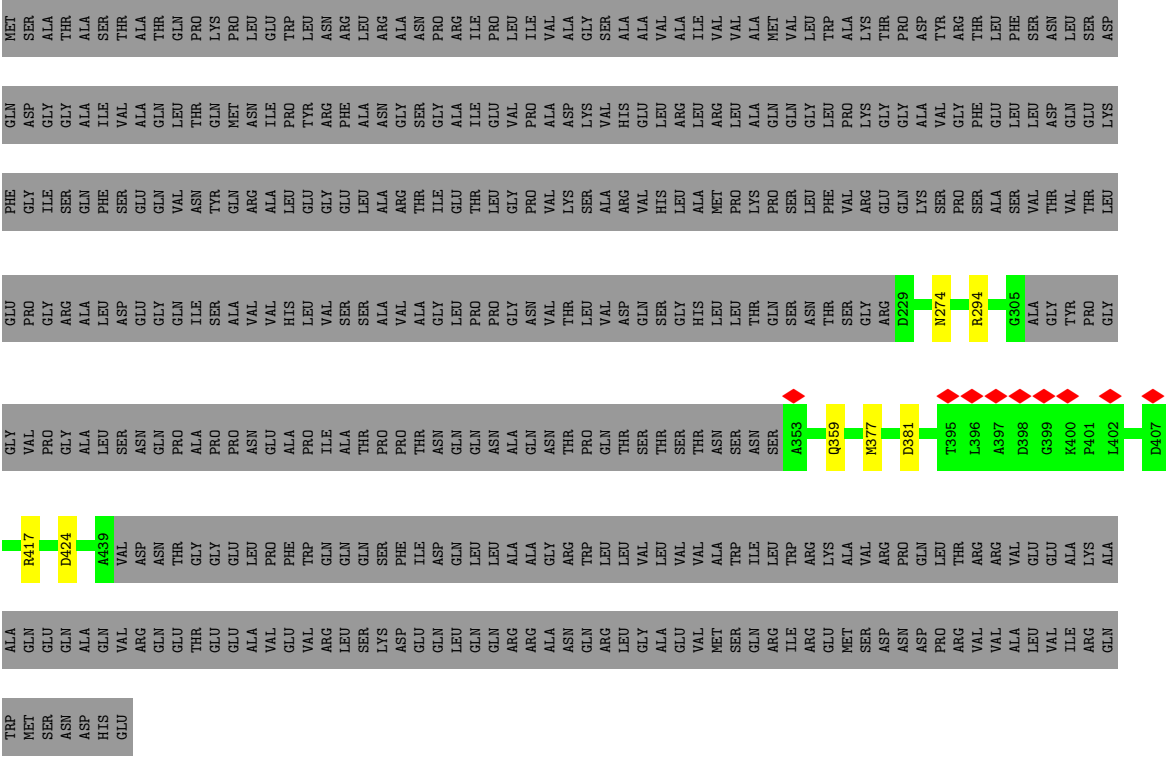


- Molecule 1: Flagellar M-ring protein

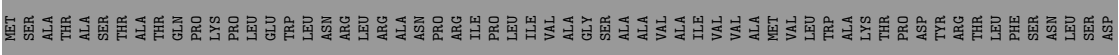


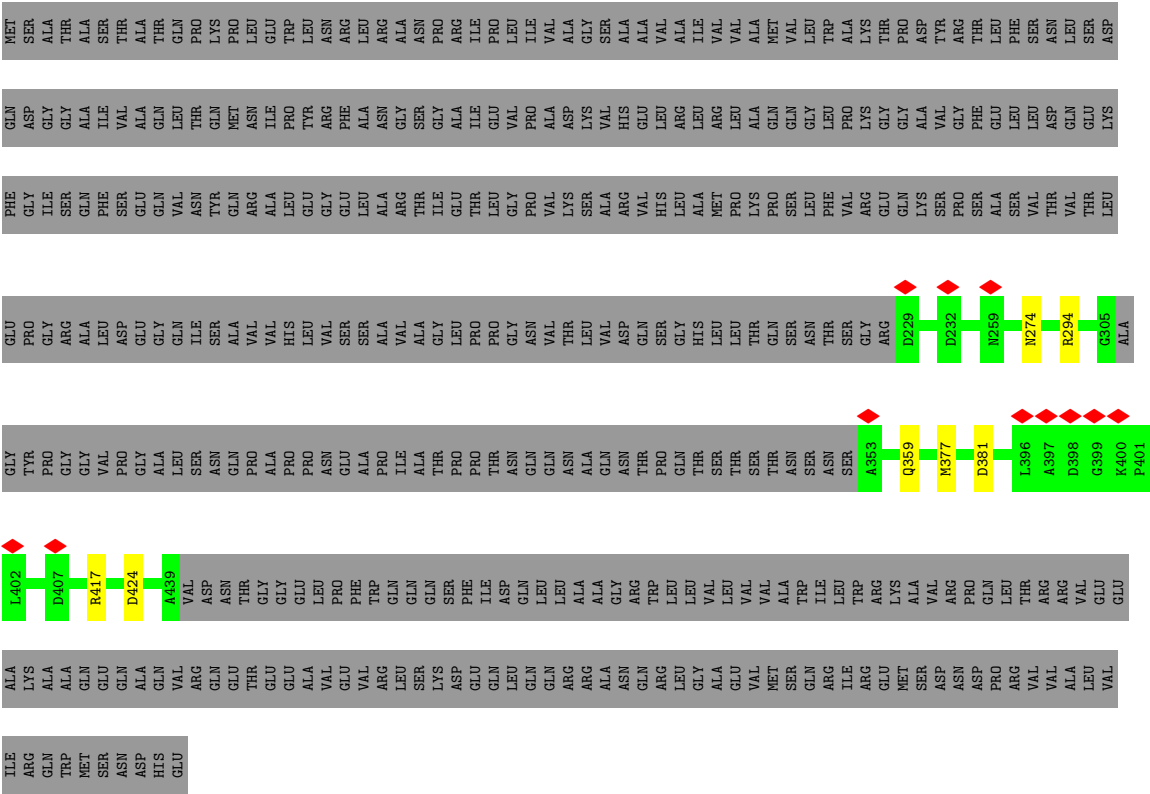


• Molecule 1: Flagellar M-ring protein

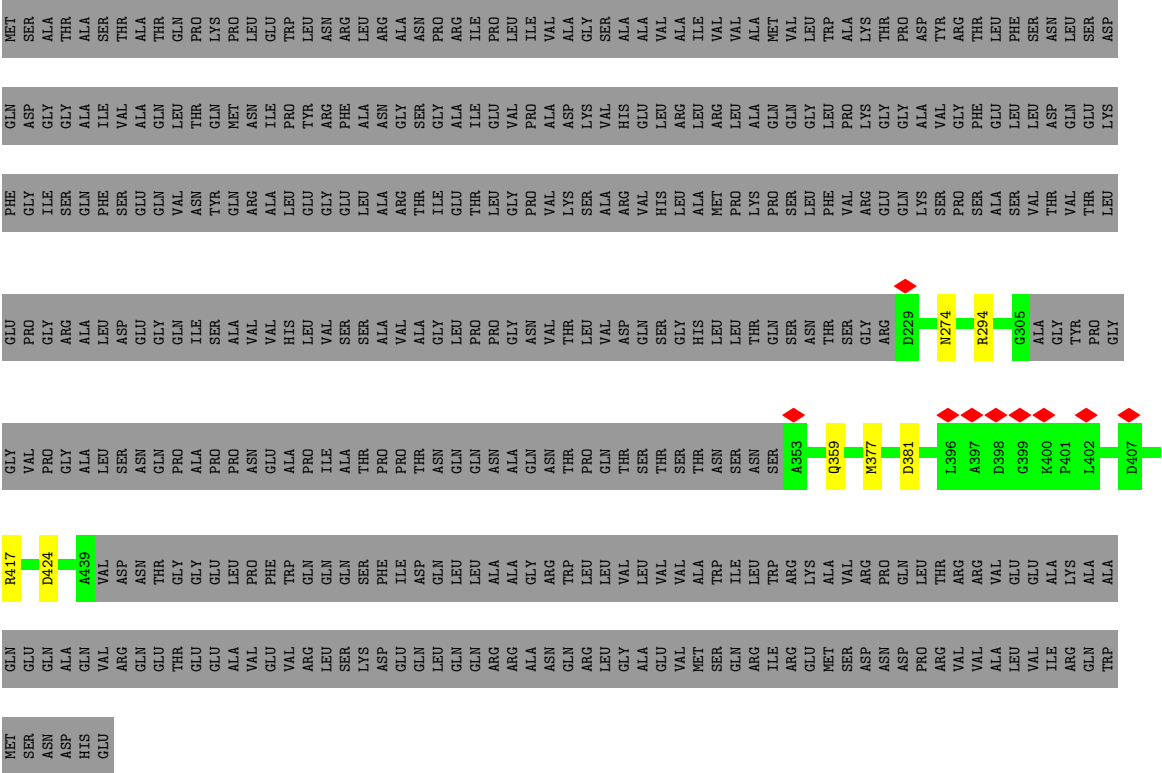


• Molecule 1: Flagellar M-ring protein





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

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

GLU	PRO	GLY	ARG	ALA	LEU	ASP	GLU	GLY	GLN	ILE	SER	ALA	VAL	VAL	HIS	LEU	VAL	SER	SER	ALA	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	N274	R294	G305	ALA	GLY	TYR	PRO
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GLY	VAL	PRO	GLY	ALA	LEU	SER	ASN	GLN	PRO	ALA	PRO	PRO	ASN	GLU	ALA	ALA	PRO	ILE	ALA	THR	PRO	PRO	THR	ASN	GLN	GLN	ASN	ALA	GLN	ASN	THR	PRO	GLN	THR	SER	THR	SER	THR	ASN	SER	ASN	SER	A363		D381	L396	A397	D398	G399	K400	P401	L402	D407
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[illegible][illegible]

MET
SER
ASN
ASP
HIS
GLU

- Molecule 1: Flagellar M-ring protein



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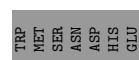
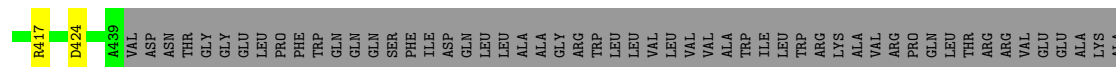
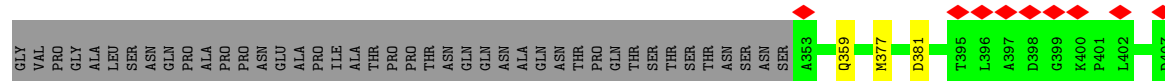
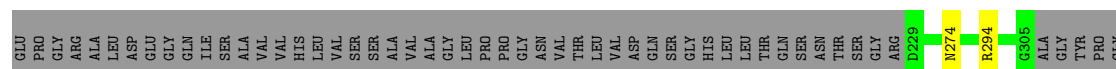
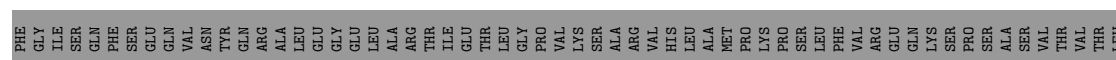
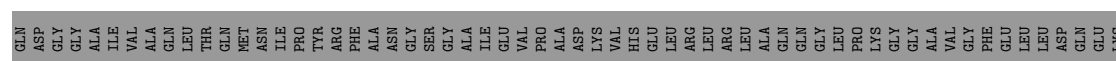
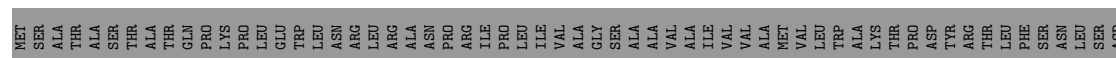
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PHE GLY ILE SER GLN PHE SER GLU GLN VAL TYR GLN ARG ALA LEU GLU GLY GLU LEU LEU THR LEU GLY GLY VAL LYS SER SER ARG ARG HIS LEU LEU MET MET PRO PRO PRO SER PHE VAL VAL ARG ARG GLU GLN LYS SER SER PRO PRO SER ALA ALA THR THR VAL VAL THR THR LEU

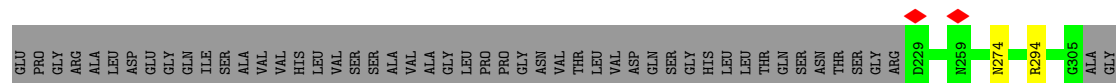
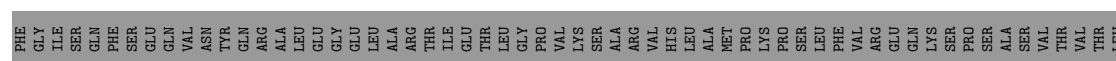
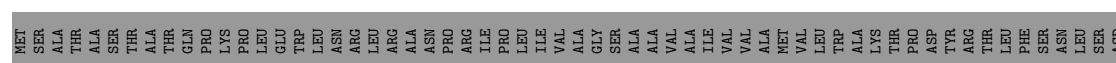
GLU PRO GLY ARG ALA LEU ASP GLU GLY GLN ILE SER ALA VAL VAL HIS LEU VAL SER SER ALA VAL VAL ALA GLY LEU PRO PRO GLY ASN VAL THR THR LEU ASP ASP GLN SER GLY HIS LEU LEU THR GLN SER ASN THR SER GLY ARG

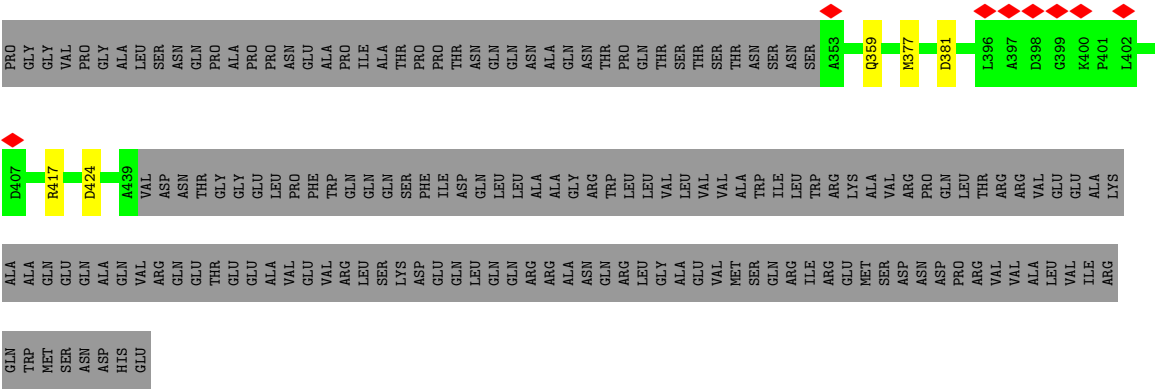
[illegible]

- Molecule 1: Flagellar M-ring protein

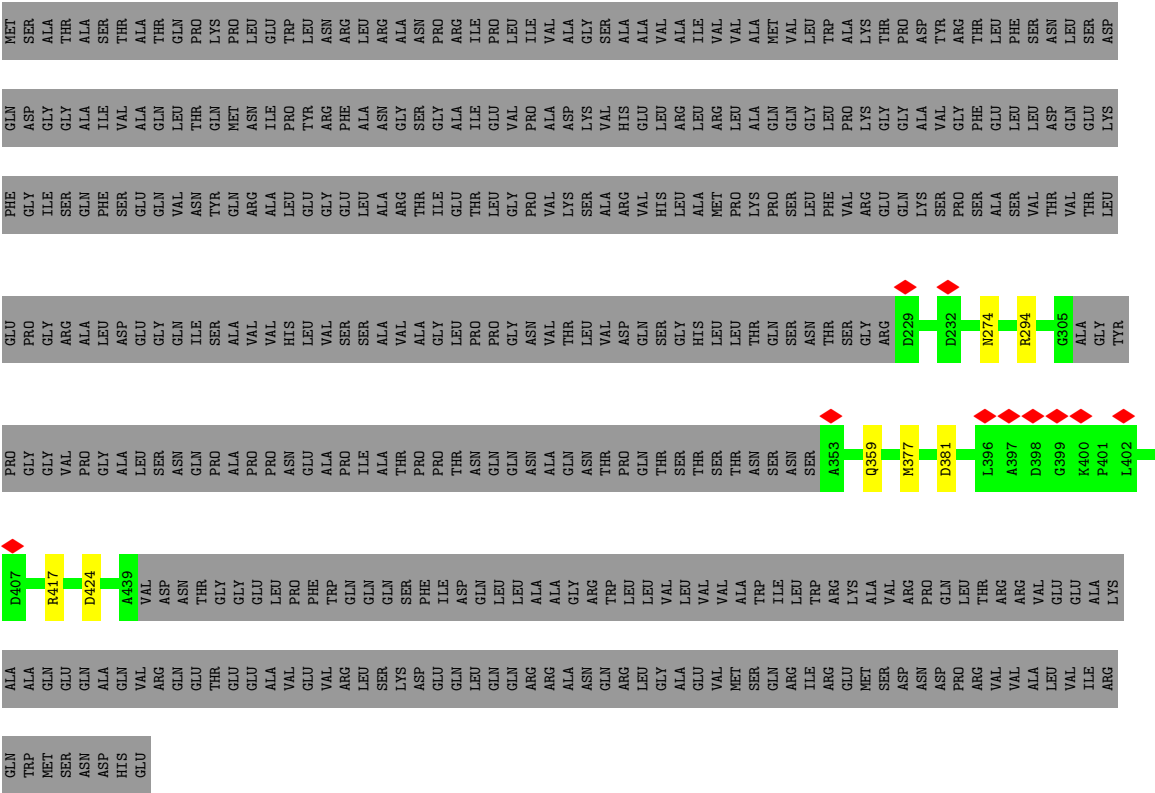


- Molecule 1: Flagellar M-ring protein

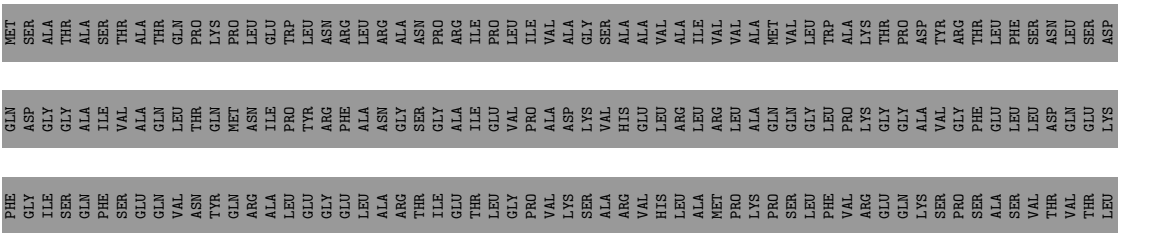




• Molecule 1: Flagellar M-ring protein

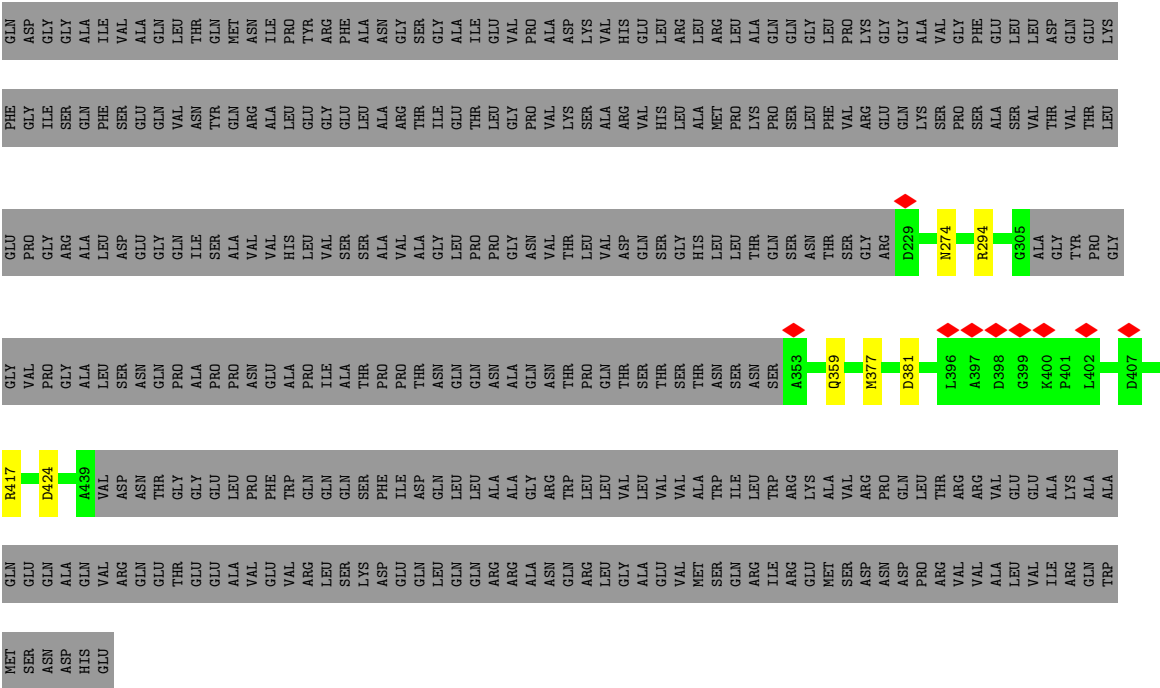


• Molecule 1: Flagellar M-ring protein

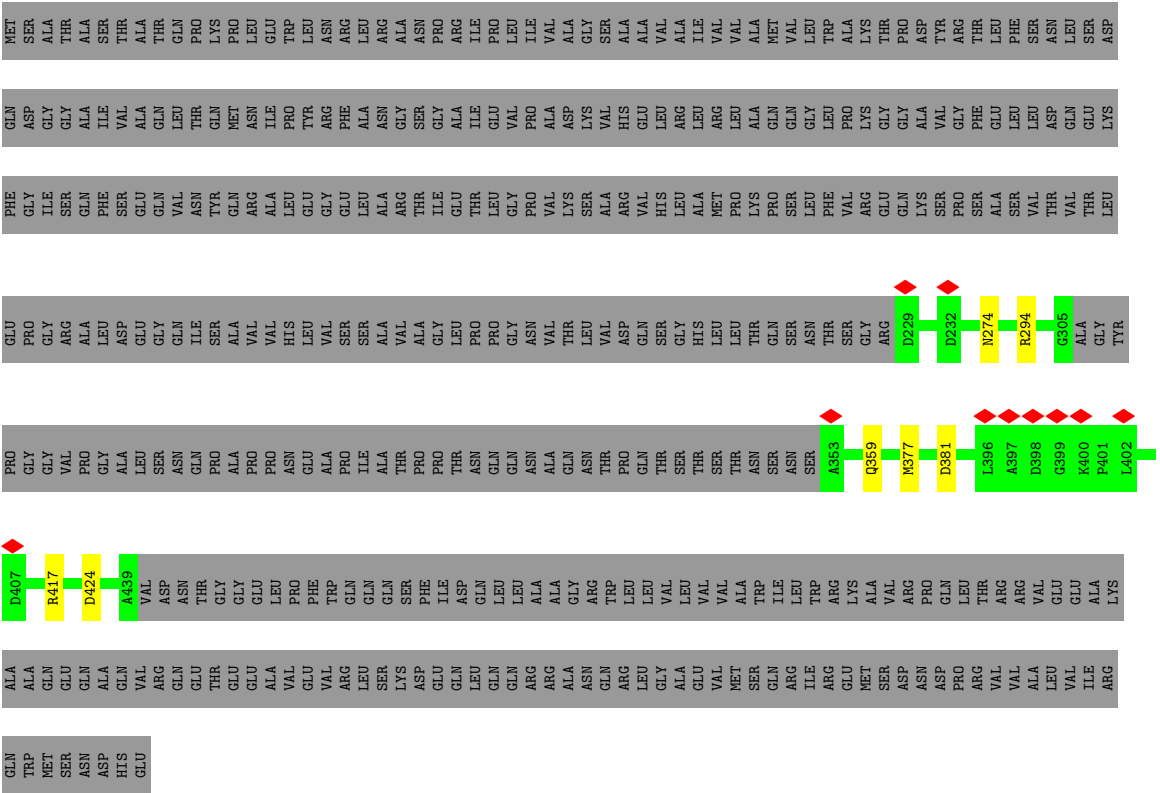








● Molecule 1: Flagellar M-ring protein



● Molecule 1: Flagellar M-ring protein



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

● Molecule 1: Flagellar M-ring protein

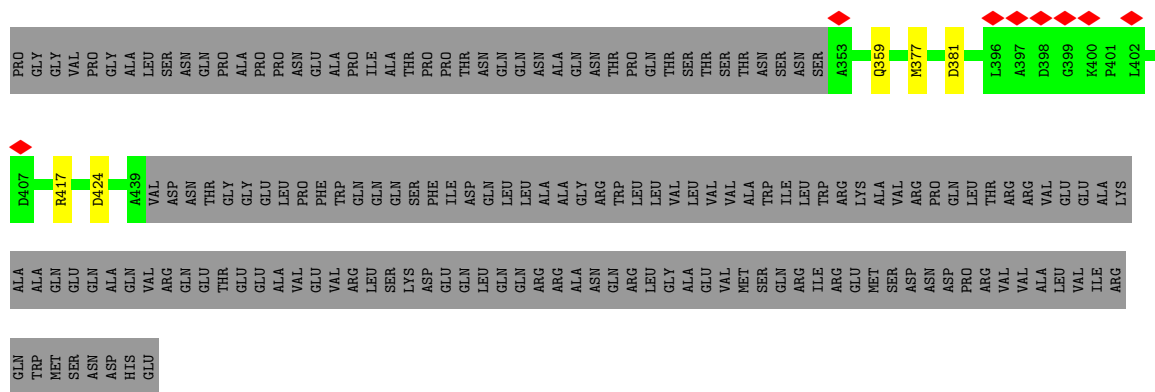


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● Molecule 1: Flagellar M-ring protein



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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 [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	0.26	0/1289	0.53	0/1741
1	B	0.26	0/1289	0.53	0/1741
1	C	0.26	0/1289	0.53	0/1741
1	D	0.26	0/1289	0.53	0/1741
1	E	0.26	0/1289	0.53	0/1741
1	F	0.26	0/1289	0.53	0/1741
1	G	0.26	0/1289	0.53	0/1741
1	H	0.26	0/1289	0.53	0/1741
1	I	0.26	0/1289	0.53	0/1741
1	J	0.26	0/1289	0.53	0/1741
1	K	0.26	0/1289	0.53	0/1741
1	L	0.26	0/1289	0.53	0/1741
1	M	0.26	0/1289	0.53	0/1741
1	N	0.26	0/1289	0.53	0/1741
1	O	0.26	0/1289	0.53	0/1741
1	P	0.26	0/1289	0.53	0/1741
1	Q	0.26	0/1289	0.53	0/1741
1	R	0.26	0/1289	0.53	0/1741
1	S	0.26	0/1289	0.53	0/1741
1	T	0.26	0/1289	0.53	0/1741
1	U	0.26	0/1289	0.53	0/1741
1	V	0.26	0/1289	0.53	0/1741
1	W	0.26	0/1289	0.53	0/1741
1	X	0.26	0/1289	0.53	0/1741
1	Y	0.26	0/1289	0.53	0/1741
1	Z	0.26	0/1289	0.53	0/1741
1	a	0.26	0/1289	0.53	0/1741
1	b	0.26	0/1289	0.53	0/1741
1	c	0.26	0/1289	0.53	0/1741
1	d	0.26	0/1289	0.53	0/1741
1	e	0.26	0/1289	0.53	0/1741
1	f	0.26	0/1289	0.53	0/1741
1	g	0.26	0/1289	0.53	0/1741
1	h	0.26	0/1289	0.53	0/1741

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.26	0/43826	0.53	0/59194

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](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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%)	134 (95%)	7 (5%)	20	52
1	B	141/467 (30%)	134 (95%)	7 (5%)	20	52
1	C	141/467 (30%)	134 (95%)	7 (5%)	20	52
1	D	141/467 (30%)	134 (95%)	7 (5%)	20	52
1	E	141/467 (30%)	134 (95%)	7 (5%)	20	52
1	F	141/467 (30%)	134 (95%)	7 (5%)	20	52
1	G	141/467 (30%)	134 (95%)	7 (5%)	20	52
1	H	141/467 (30%)	134 (95%)	7 (5%)	20	52
1	I	141/467 (30%)	134 (95%)	7 (5%)	20	52
1	J	141/467 (30%)	134 (95%)	7 (5%)	20	52
1	K	141/467 (30%)	134 (95%)	7 (5%)	20	52
1	L	141/467 (30%)	134 (95%)	7 (5%)	20	52
1	M	141/467 (30%)	134 (95%)	7 (5%)	20	52
1	N	141/467 (30%)	134 (95%)	7 (5%)	20	52
1	O	141/467 (30%)	134 (95%)	7 (5%)	20	52
1	P	141/467 (30%)	134 (95%)	7 (5%)	20	52
1	Q	141/467 (30%)	134 (95%)	7 (5%)	20	52
1	R	141/467 (30%)	134 (95%)	7 (5%)	20	52
1	S	141/467 (30%)	134 (95%)	7 (5%)	20	52
1	T	141/467 (30%)	134 (95%)	7 (5%)	20	52
1	U	141/467 (30%)	134 (95%)	7 (5%)	20	52
1	V	141/467 (30%)	134 (95%)	7 (5%)	20	52
1	W	141/467 (30%)	134 (95%)	7 (5%)	20	52
1	X	141/467 (30%)	134 (95%)	7 (5%)	20	52
1	Y	141/467 (30%)	134 (95%)	7 (5%)	20	52
1	Z	141/467 (30%)	134 (95%)	7 (5%)	20	52
1	a	141/467 (30%)	134 (95%)	7 (5%)	20	52
1	b	141/467 (30%)	134 (95%)	7 (5%)	20	52
1	c	141/467 (30%)	134 (95%)	7 (5%)	20	52
1	d	141/467 (30%)	134 (95%)	7 (5%)	20	52
1	e	141/467 (30%)	134 (95%)	7 (5%)	20	52
1	f	141/467 (30%)	134 (95%)	7 (5%)	20	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	g	141/467 (30%)	134 (95%)	7 (5%)	20	52
1	h	141/467 (30%)	134 (95%)	7 (5%)	20	52
All	All	4794/15878 (30%)	4556 (95%)	238 (5%)	23	52

All (238) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	274	ASN
1	A	294	ARG
1	A	359	GLN
1	A	377	MET
1	A	381	ASP
1	A	417	ARG
1	A	424	ASP
1	B	274	ASN
1	B	294	ARG
1	B	359	GLN
1	B	377	MET
1	B	381	ASP
1	B	417	ARG
1	B	424	ASP
1	C	274	ASN
1	C	294	ARG
1	C	359	GLN
1	C	377	MET
1	C	381	ASP
1	C	417	ARG
1	C	424	ASP
1	D	274	ASN
1	D	294	ARG
1	D	359	GLN
1	D	377	MET
1	D	381	ASP
1	D	417	ARG
1	D	424	ASP
1	E	274	ASN
1	E	294	ARG
1	E	359	GLN
1	E	377	MET
1	E	381	ASP
1	E	417	ARG

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Mol	Chain	Res	Type
1	E	424	ASP
1	F	274	ASN
1	F	294	ARG
1	F	359	GLN
1	F	377	MET
1	F	381	ASP
1	F	417	ARG
1	F	424	ASP
1	G	274	ASN
1	G	294	ARG
1	G	359	GLN
1	G	377	MET
1	G	381	ASP
1	G	417	ARG
1	G	424	ASP
1	H	274	ASN
1	H	294	ARG
1	H	359	GLN
1	H	377	MET
1	H	381	ASP
1	H	417	ARG
1	H	424	ASP
1	I	274	ASN
1	I	294	ARG
1	I	359	GLN
1	I	377	MET
1	I	381	ASP
1	I	417	ARG
1	I	424	ASP
1	J	274	ASN
1	J	294	ARG
1	J	359	GLN
1	J	377	MET
1	J	381	ASP
1	J	417	ARG
1	J	424	ASP
1	K	274	ASN
1	K	294	ARG
1	K	359	GLN
1	K	377	MET
1	K	381	ASP
1	K	417	ARG

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Mol	Chain	Res	Type
1	K	424	ASP
1	L	274	ASN
1	L	294	ARG
1	L	359	GLN
1	L	377	MET
1	L	381	ASP
1	L	417	ARG
1	L	424	ASP
1	M	274	ASN
1	M	294	ARG
1	M	359	GLN
1	M	377	MET
1	M	381	ASP
1	M	417	ARG
1	M	424	ASP
1	N	274	ASN
1	N	294	ARG
1	N	359	GLN
1	N	377	MET
1	N	381	ASP
1	N	417	ARG
1	N	424	ASP
1	O	274	ASN
1	O	294	ARG
1	O	359	GLN
1	O	377	MET
1	O	381	ASP
1	O	417	ARG
1	O	424	ASP
1	P	274	ASN
1	P	294	ARG
1	P	359	GLN
1	P	377	MET
1	P	381	ASP
1	P	417	ARG
1	P	424	ASP
1	Q	274	ASN
1	Q	294	ARG
1	Q	359	GLN
1	Q	377	MET
1	Q	381	ASP
1	Q	417	ARG

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Mol	Chain	Res	Type
1	Q	424	ASP
1	R	274	ASN
1	R	294	ARG
1	R	359	GLN
1	R	377	MET
1	R	381	ASP
1	R	417	ARG
1	R	424	ASP
1	S	274	ASN
1	S	294	ARG
1	S	359	GLN
1	S	377	MET
1	S	381	ASP
1	S	417	ARG
1	S	424	ASP
1	T	274	ASN
1	T	294	ARG
1	T	359	GLN
1	T	377	MET
1	T	381	ASP
1	T	417	ARG
1	T	424	ASP
1	U	274	ASN
1	U	294	ARG
1	U	359	GLN
1	U	377	MET
1	U	381	ASP
1	U	417	ARG
1	U	424	ASP
1	V	274	ASN
1	V	294	ARG
1	V	359	GLN
1	V	377	MET
1	V	381	ASP
1	V	417	ARG
1	V	424	ASP
1	W	274	ASN
1	W	294	ARG
1	W	359	GLN
1	W	377	MET
1	W	381	ASP
1	W	417	ARG

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Mol	Chain	Res	Type
1	W	424	ASP
1	X	274	ASN
1	X	294	ARG
1	X	359	GLN
1	X	377	MET
1	X	381	ASP
1	X	417	ARG
1	X	424	ASP
1	Y	274	ASN
1	Y	294	ARG
1	Y	359	GLN
1	Y	377	MET
1	Y	381	ASP
1	Y	417	ARG
1	Y	424	ASP
1	Z	274	ASN
1	Z	294	ARG
1	Z	359	GLN
1	Z	377	MET
1	Z	381	ASP
1	Z	417	ARG
1	Z	424	ASP
1	a	274	ASN
1	a	294	ARG
1	a	359	GLN
1	a	377	MET
1	a	381	ASP
1	a	417	ARG
1	a	424	ASP
1	b	274	ASN
1	b	294	ARG
1	b	359	GLN
1	b	377	MET
1	b	381	ASP
1	b	417	ARG
1	b	424	ASP
1	c	274	ASN
1	c	294	ARG
1	c	359	GLN
1	c	377	MET
1	c	381	ASP
1	c	417	ARG

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Mol	Chain	Res	Type
1	c	424	ASP
1	d	274	ASN
1	d	294	ARG
1	d	359	GLN
1	d	377	MET
1	d	381	ASP
1	d	417	ARG
1	d	424	ASP
1	e	274	ASN
1	e	294	ARG
1	e	359	GLN
1	e	377	MET
1	e	381	ASP
1	e	417	ARG
1	e	424	ASP
1	f	274	ASN
1	f	294	ARG
1	f	359	GLN
1	f	377	MET
1	f	381	ASP
1	f	417	ARG
1	f	424	ASP
1	g	274	ASN
1	g	294	ARG
1	g	359	GLN
1	g	377	MET
1	g	381	ASP
1	g	417	ARG
1	g	424	ASP
1	h	274	ASN
1	h	294	ARG
1	h	359	GLN
1	h	377	MET
1	h	381	ASP
1	h	417	ARG
1	h	424	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	303	GLN
1	A	374	HIS

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Mol	Chain	Res	Type
1	B	303	GLN
1	B	374	HIS
1	C	303	GLN
1	C	374	HIS
1	D	303	GLN
1	D	374	HIS
1	E	303	GLN
1	E	374	HIS
1	F	303	GLN
1	F	374	HIS
1	G	303	GLN
1	G	374	HIS
1	H	303	GLN
1	H	374	HIS
1	I	303	GLN
1	I	374	HIS
1	J	303	GLN
1	J	374	HIS
1	K	303	GLN
1	K	374	HIS
1	L	303	GLN
1	L	374	HIS
1	M	303	GLN
1	M	374	HIS
1	N	303	GLN
1	N	374	HIS
1	O	303	GLN
1	O	374	HIS
1	P	303	GLN
1	P	374	HIS
1	Q	303	GLN
1	Q	374	HIS
1	R	303	GLN
1	R	374	HIS
1	S	303	GLN
1	S	374	HIS
1	T	303	GLN
1	T	374	HIS
1	U	303	GLN
1	U	374	HIS
1	V	303	GLN
1	V	374	HIS

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Mol	Chain	Res	Type
1	W	303	GLN
1	W	374	HIS
1	X	303	GLN
1	X	374	HIS
1	Y	303	GLN
1	Y	374	HIS
1	Z	303	GLN
1	Z	374	HIS
1	Z	434	ASN
1	a	303	GLN
1	a	374	HIS
1	b	303	GLN
1	b	374	HIS
1	c	303	GLN
1	c	374	HIS
1	c	434	ASN
1	d	303	GLN
1	d	374	HIS
1	e	303	GLN
1	e	374	HIS
1	f	303	GLN
1	f	374	HIS
1	g	303	GLN
1	g	374	HIS
1	h	303	GLN
1	h	374	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

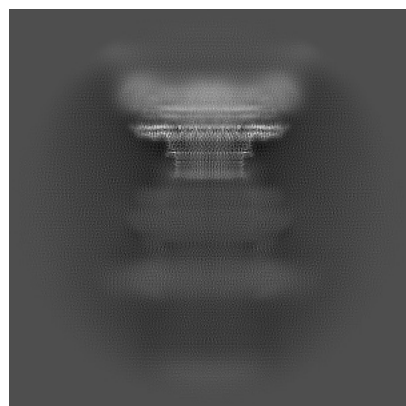
6 Map visualisation [i](#)

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.

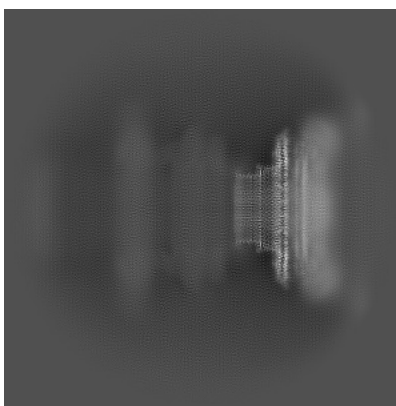
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

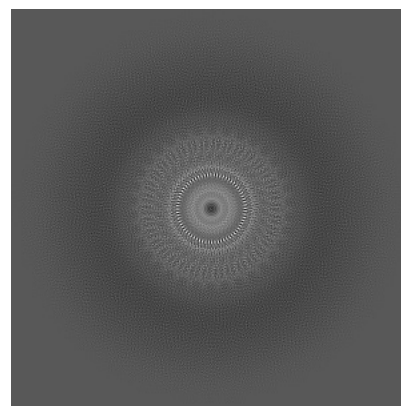
6.1.1 Primary map



X

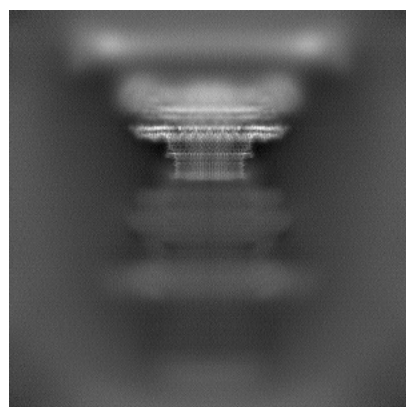


Y

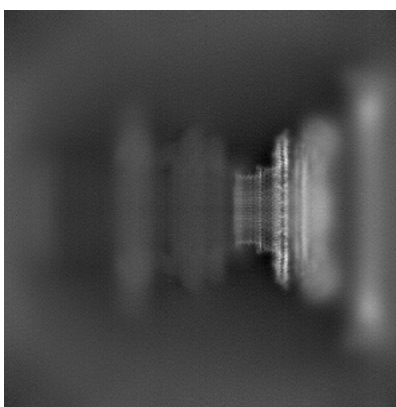


Z

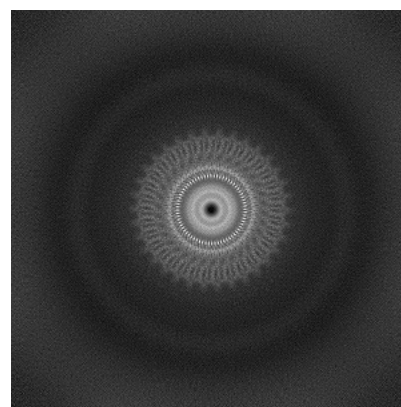
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices [i](#)

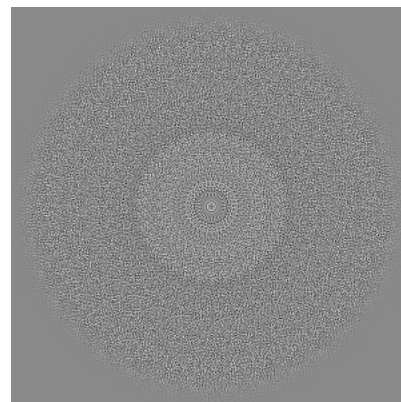
6.2.1 Primary map



X Index: 256

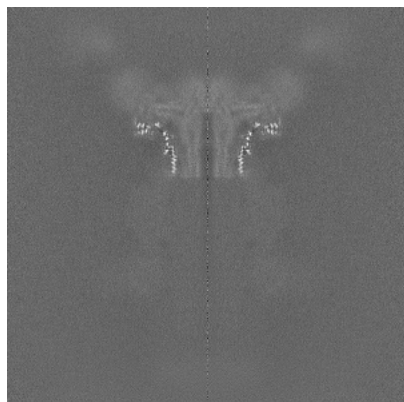


Y Index: 256

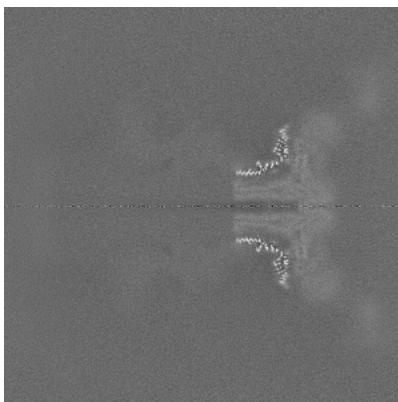


Z Index: 256

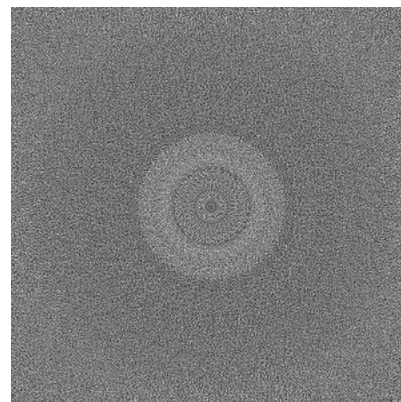
6.2.2 Raw map



X Index: 256



Y Index: 256

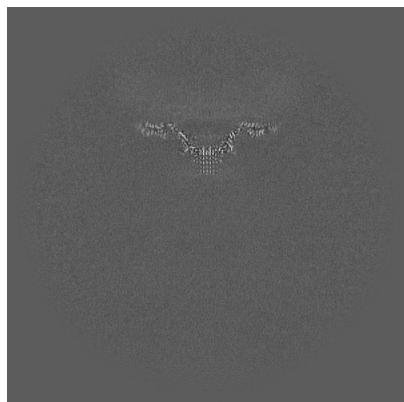


Z Index: 256

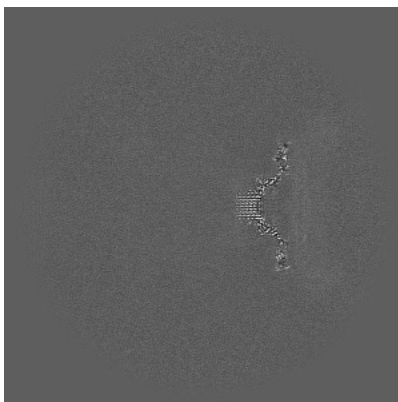
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

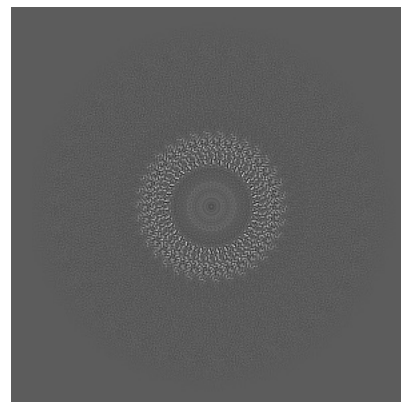
6.3.1 Primary map



X Index: 212



Y Index: 214

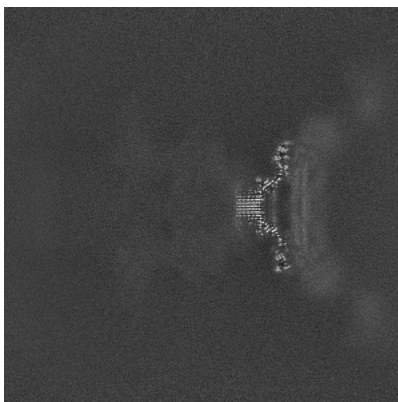


Z Index: 352

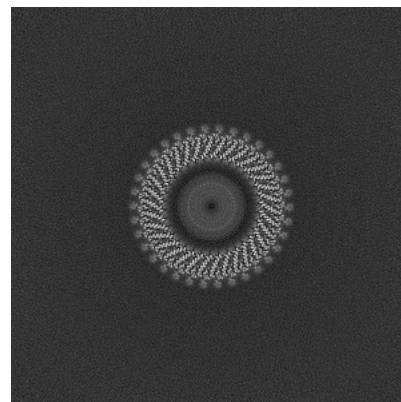
6.3.2 Raw map



X Index: 213



Y Index: 213

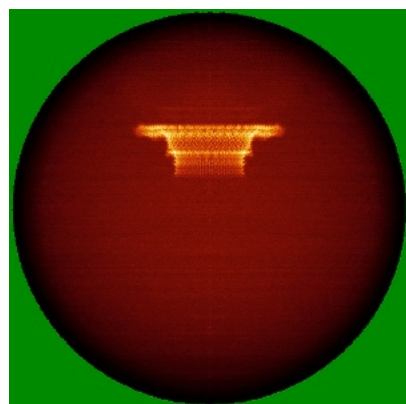


Z Index: 360

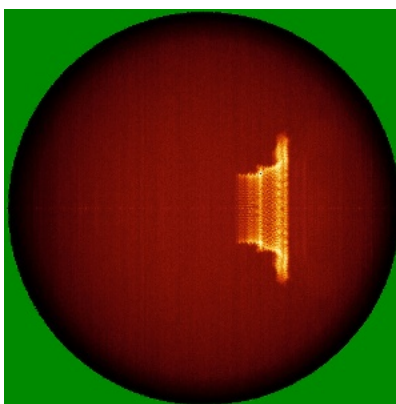
The images above show the largest variance slices of the map in three orthogonal directions.

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

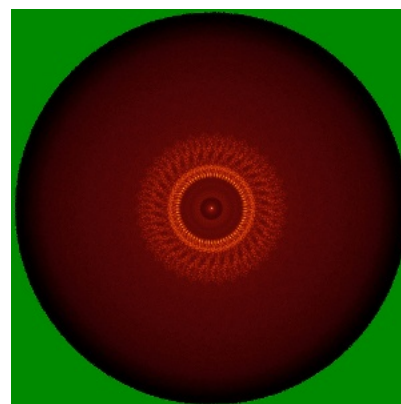
6.4.1 Primary map



X

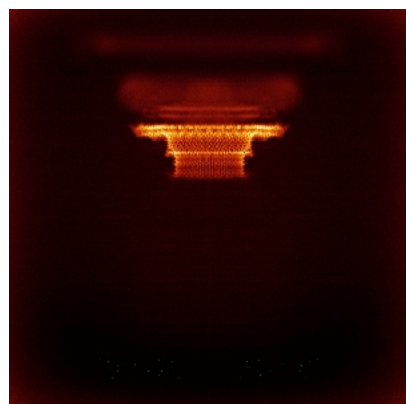


Y

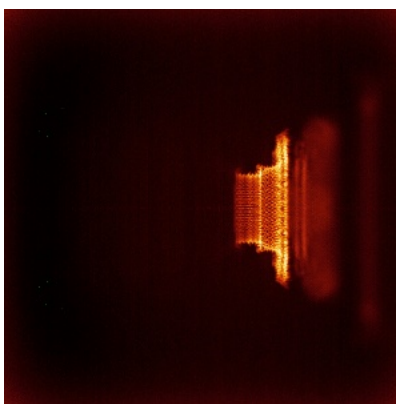


Z

6.4.2 Raw map



X



Y

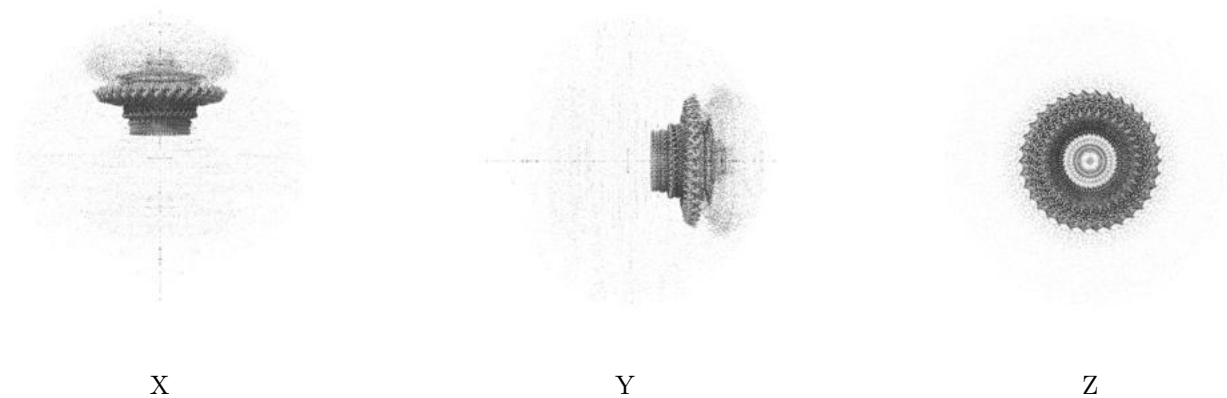


Z

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.

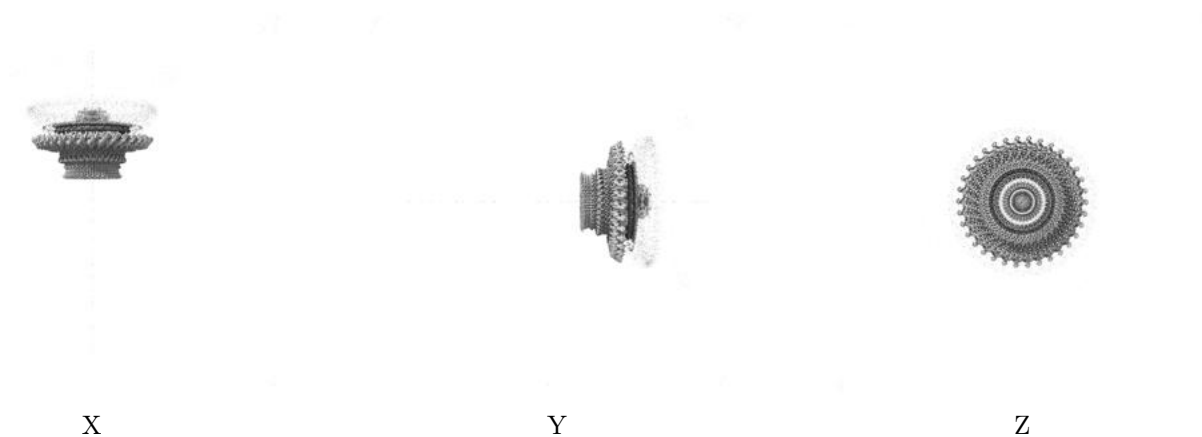
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.35. 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.

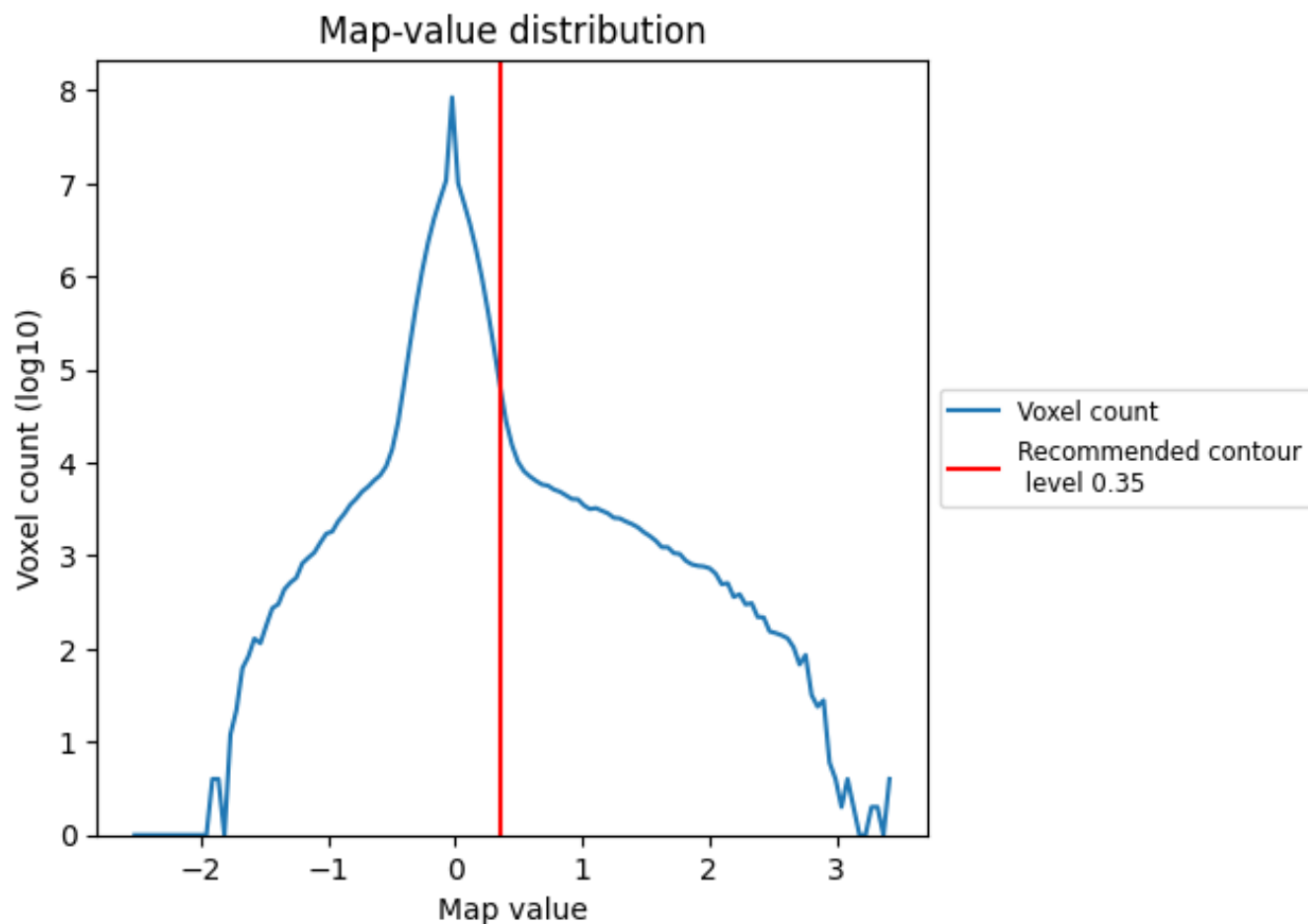
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

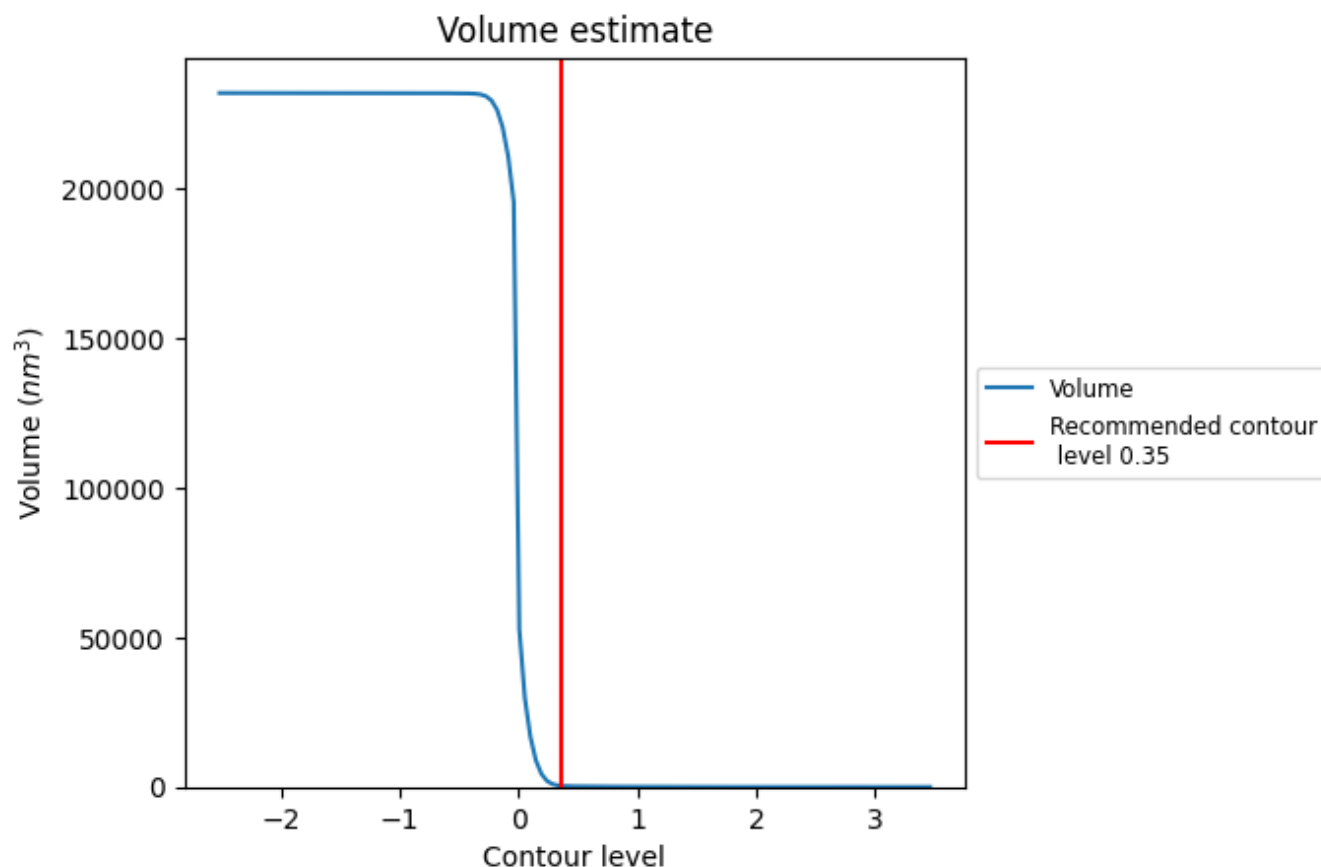
This section contains the results of statistical analysis of the map.

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.

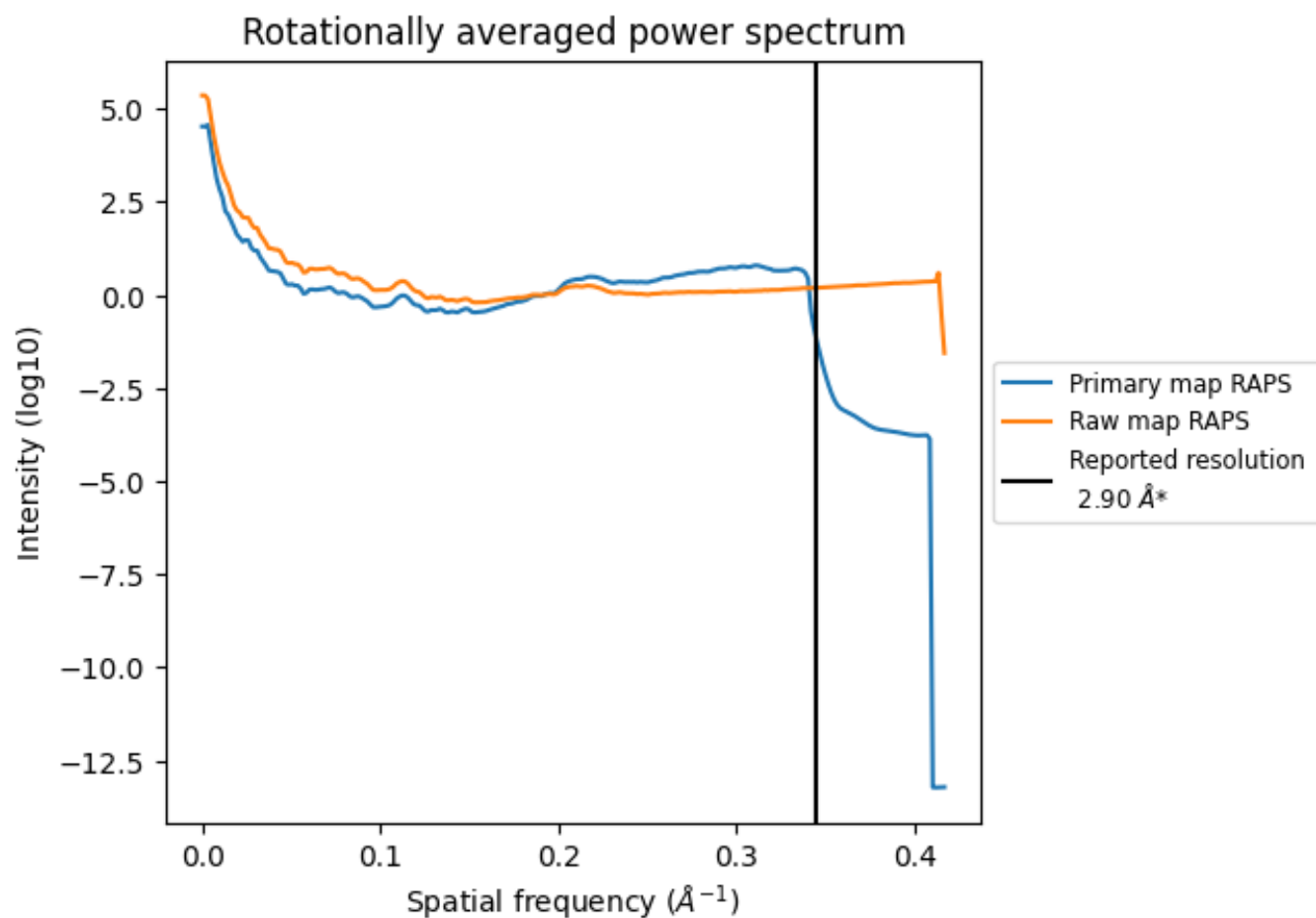
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 418 nm³; 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 ⓘ

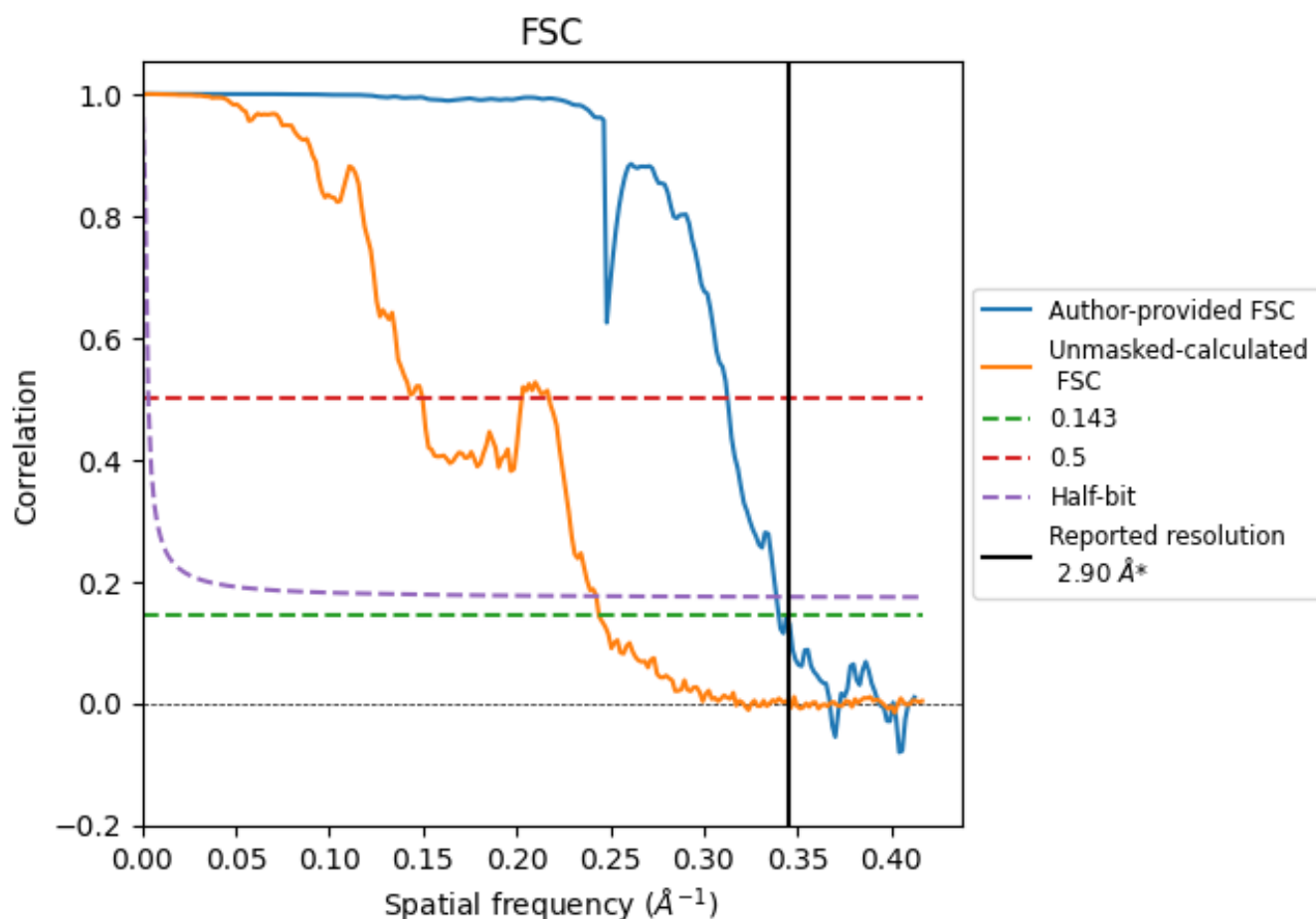


*Reported resolution corresponds to spatial frequency of 0.345 \AA^{-1}

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 \AA^{-1}

8.2 Resolution estimates [i](#)

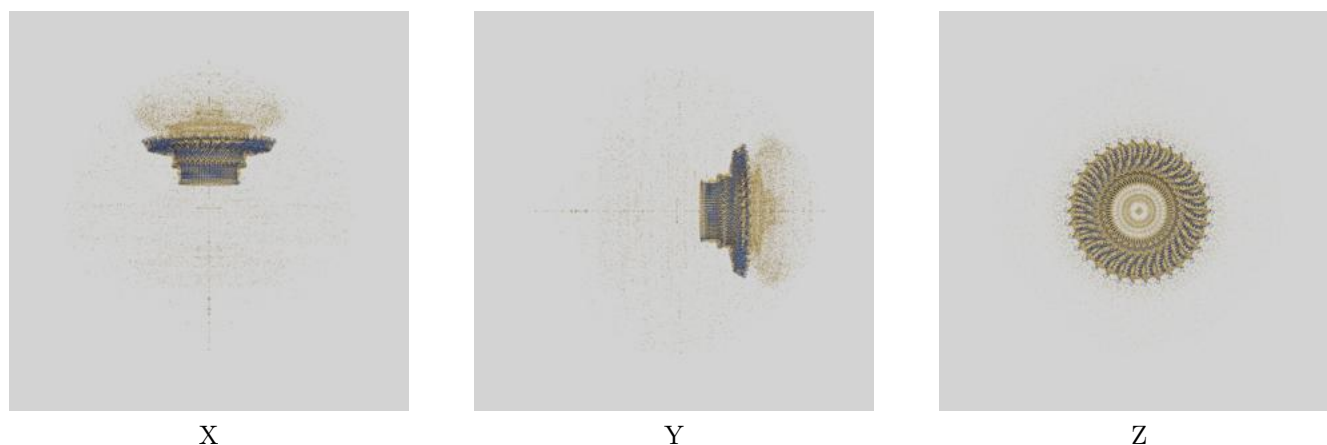
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.94	3.20	2.95
Unmasked-calculated*	4.10	6.68	4.12

*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](#)

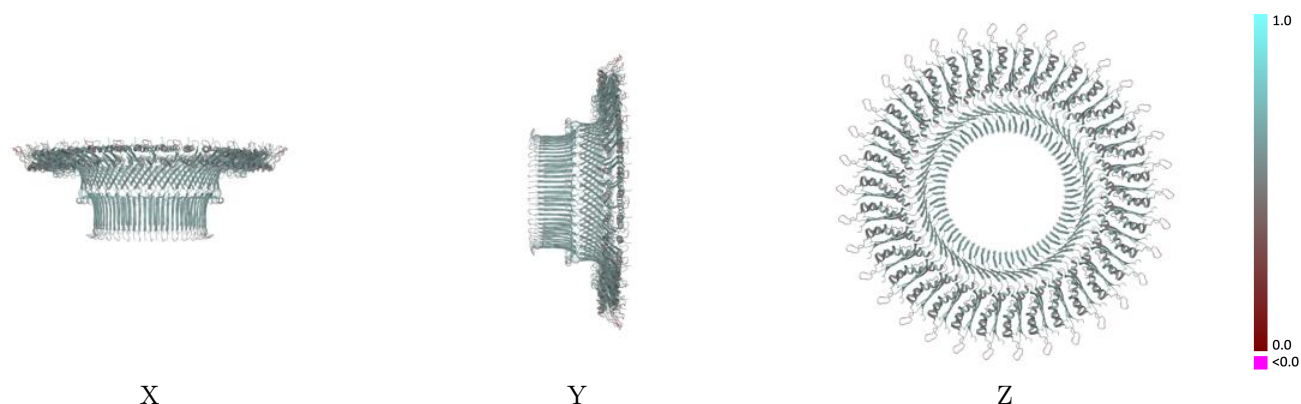
This section contains information regarding the fit between EMDB map EMD-37590 and PDB model 8WJR. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



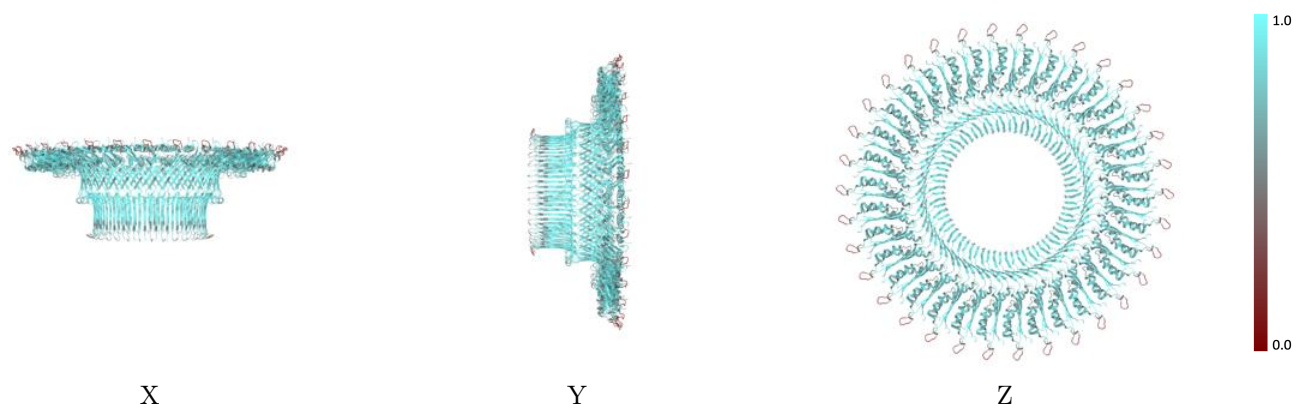
The images above show the 3D surface view of the map at the recommended contour level 0.35 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



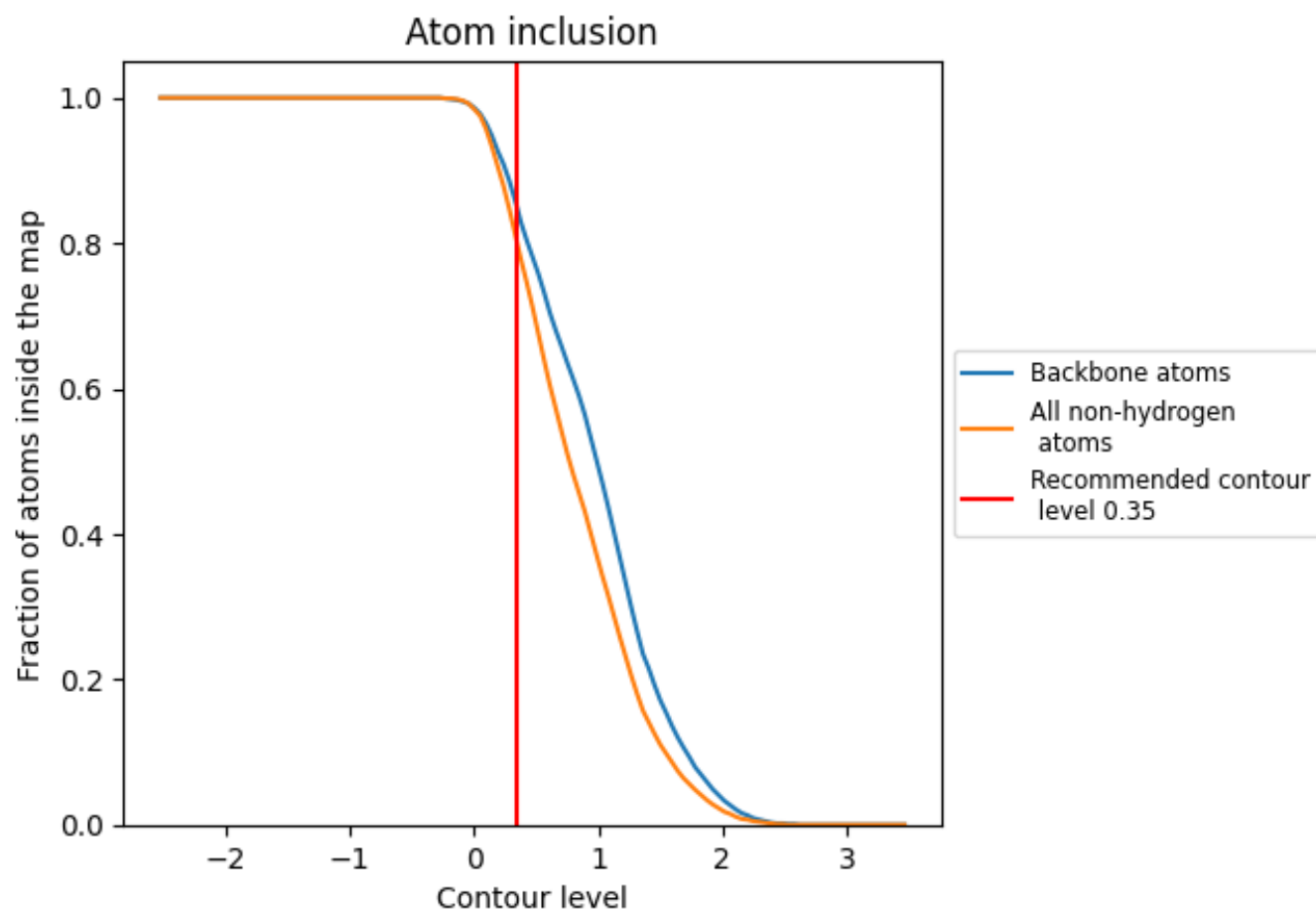
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

