



wwPDB EM Validation Summary Report ⓘ

Jul 13, 2026 – 08:26 PM JST

PDB ID : 9V96 / pdb_00009v96
EMDB ID : EMD-64862
Title : Cryo-EM structure of the inner core of ArlA2 filament of *Haloarcula marismortui*
Authors : Meshcheryakov, V.A.; Hyun, J.; Syutkin, A.S.; Pyatibratov, M.G.; Wolf, M.
Deposited on : 2025-05-30
Resolution : 3.14 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.dev133
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) : 2.50

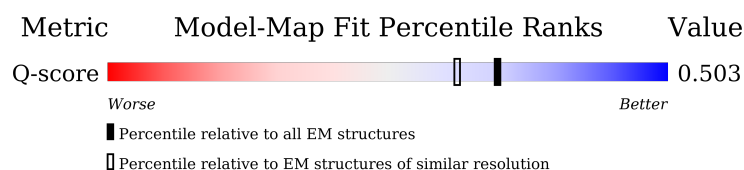
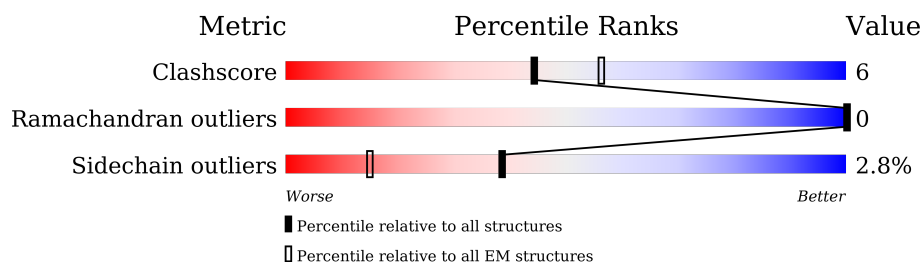
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.14 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	14483 (2.64 - 3.64)

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	463	
1	B	463	
1	C	463	
1	D	463	

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Mol	Chain	Length	Quality of chain
1	E	463	
1	G	463	
1	H	463	
1	I	463	
1	J	463	
1	K	463	
1	L	463	
1	M	463	
1	N	463	
1	O	463	
1	P	463	
1	R	463	
1	S	463	
1	T	463	
1	U	463	
1	V	463	
1	W	463	
1	X	463	
1	Y	463	
1	Z	463	
1	a	463	
1	b	463	
1	d	463	
1	e	463	
1	f	463	

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Mol	Chain	Length	Quality of chain
1	g	463	
1	i	463	
1	j	463	
1	k	463	
1	l	463	
1	m	463	
1	n	463	
1	o	463	
1	p	463	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 48061 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 Flagellin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	176	Total	C	N	O	S	0	0
			1264	775	204	281	4		
1	C	176	Total	C	N	O	S	0	0
			1264	775	204	281	4		
1	D	176	Total	C	N	O	S	0	0
			1264	775	204	281	4		
1	E	176	Total	C	N	O	S	0	0
			1264	775	204	281	4		
1	G	176	Total	C	N	O	S	0	0
			1264	775	204	281	4		
1	H	176	Total	C	N	O	S	0	0
			1264	775	204	281	4		
1	I	176	Total	C	N	O	S	0	0
			1264	775	204	281	4		
1	J	176	Total	C	N	O	S	0	0
			1264	775	204	281	4		
1	K	176	Total	C	N	O	S	0	0
			1264	775	204	281	4		
1	L	176	Total	C	N	O	S	0	0
			1264	775	204	281	4		
1	M	176	Total	C	N	O	S	0	0
			1264	775	204	281	4		
1	N	176	Total	C	N	O	S	0	0
			1264	775	204	281	4		
1	O	176	Total	C	N	O	S	0	0
			1264	775	204	281	4		
1	P	176	Total	C	N	O	S	0	0
			1264	775	204	281	4		
1	R	176	Total	C	N	O	S	0	0
			1264	775	204	281	4		
1	S	176	Total	C	N	O	S	0	0
			1264	775	204	281	4		
1	T	176	Total	C	N	O	S	0	0
			1264	775	204	281	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	U	176	Total 1264	C 775	N 204	O 281	S 4	0	0
1	V	176	Total 1264	C 775	N 204	O 281	S 4	0	0
1	W	176	Total 1264	C 775	N 204	O 281	S 4	0	0
1	X	176	Total 1264	C 775	N 204	O 281	S 4	0	0
1	Y	176	Total 1264	C 775	N 204	O 281	S 4	0	0
1	Z	176	Total 1264	C 775	N 204	O 281	S 4	0	0
1	a	176	Total 1264	C 775	N 204	O 281	S 4	0	0
1	b	176	Total 1264	C 775	N 204	O 281	S 4	0	0
1	d	176	Total 1264	C 775	N 204	O 281	S 4	0	0
1	e	176	Total 1264	C 775	N 204	O 281	S 4	0	0
1	f	176	Total 1264	C 775	N 204	O 281	S 4	0	0
1	g	176	Total 1264	C 775	N 204	O 281	S 4	0	0
1	i	175	Total 1255	C 770	N 202	O 279	S 4	0	0
1	j	176	Total 1264	C 775	N 204	O 281	S 4	0	0
1	k	176	Total 1264	C 775	N 204	O 281	S 4	0	0
1	l	176	Total 1264	C 775	N 204	O 281	S 4	0	0
1	m	176	Total 1264	C 775	N 204	O 281	S 4	0	0
1	n	176	Total 1264	C 775	N 204	O 281	S 4	0	0
1	o	176	Total 1264	C 775	N 204	O 281	S 4	0	0
1	p	176	Total 1264	C 775	N 204	O 281	S 4	0	0
1	B	176	Total 1264	C 775	N 204	O 281	S 4	0	0

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total 1	Na 1	0
2	C	1	Total 1	Na 1	0
2	D	1	Total 1	Na 1	0
2	E	1	Total 1	Na 1	0
2	G	1	Total 1	Na 1	0
2	H	1	Total 1	Na 1	0
2	I	1	Total 1	Na 1	0
2	J	1	Total 1	Na 1	0
2	K	1	Total 1	Na 1	0
2	L	1	Total 1	Na 1	0
2	M	1	Total 1	Na 1	0
2	N	1	Total 1	Na 1	0
2	O	1	Total 1	Na 1	0
2	P	1	Total 1	Na 1	0
2	R	1	Total 1	Na 1	0
2	S	1	Total 1	Na 1	0
2	T	1	Total 1	Na 1	0
2	U	1	Total 1	Na 1	0
2	V	1	Total 1	Na 1	0
2	W	1	Total 1	Na 1	0
2	X	1	Total 1	Na 1	0

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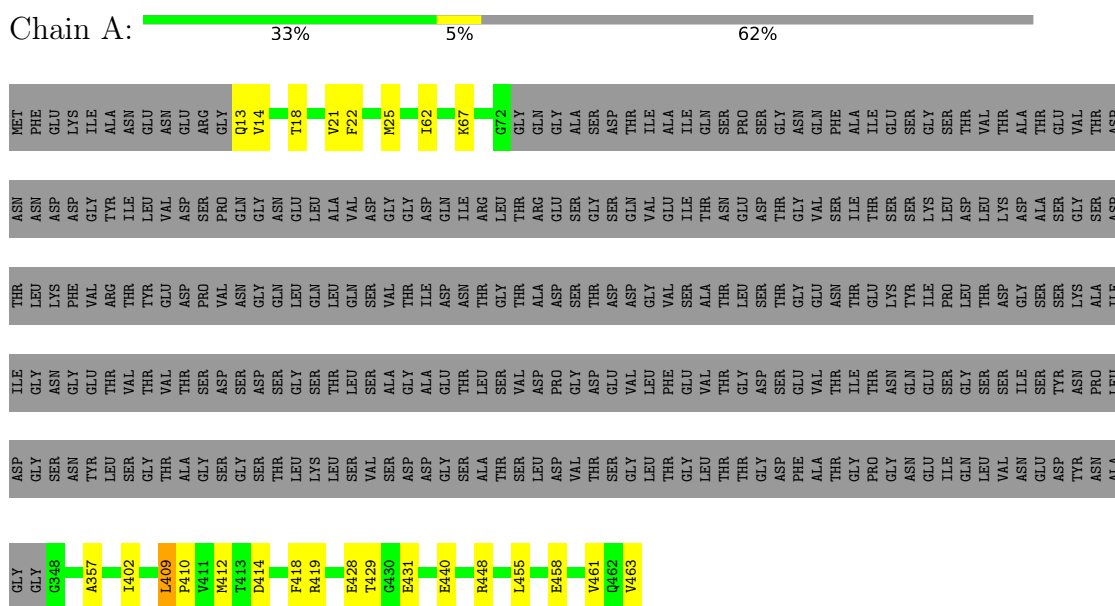
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Mol	Chain	Residues	Atoms		AltConf
2	Y	1	Total 1	Na 1	0
2	Z	1	Total 1	Na 1	0
2	a	1	Total 1	Na 1	0
2	b	1	Total 1	Na 1	0
2	d	1	Total 1	Na 1	0
2	e	1	Total 1	Na 1	0
2	f	1	Total 1	Na 1	0
2	g	1	Total 1	Na 1	0
2	i	1	Total 1	Na 1	0
2	j	1	Total 1	Na 1	0
2	k	1	Total 1	Na 1	0
2	l	1	Total 1	Na 1	0
2	m	1	Total 1	Na 1	0
2	n	1	Total 1	Na 1	0
2	o	1	Total 1	Na 1	0
2	p	1	Total 1	Na 1	0
2	B	1	Total 1	Na 1	0

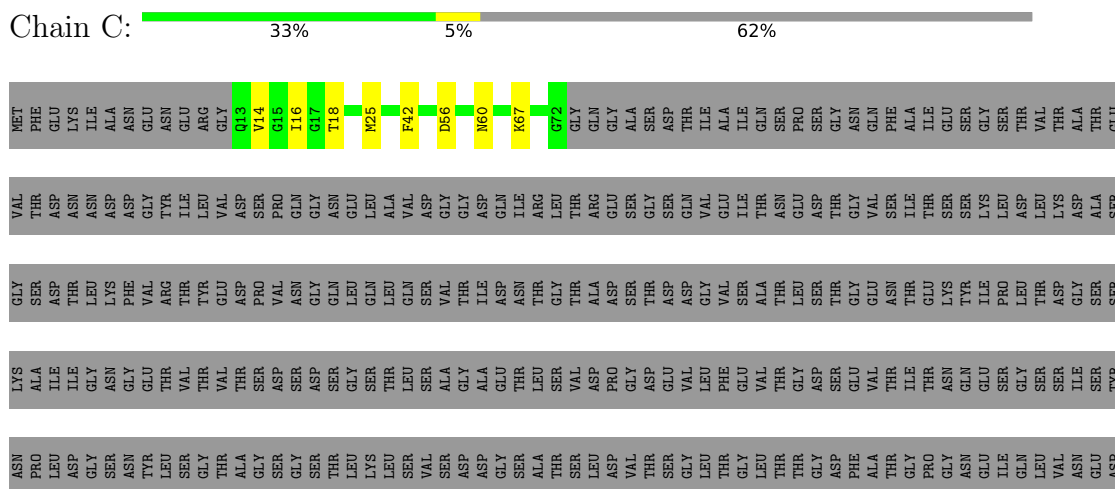
3 Residue-property plots [i](#)

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.

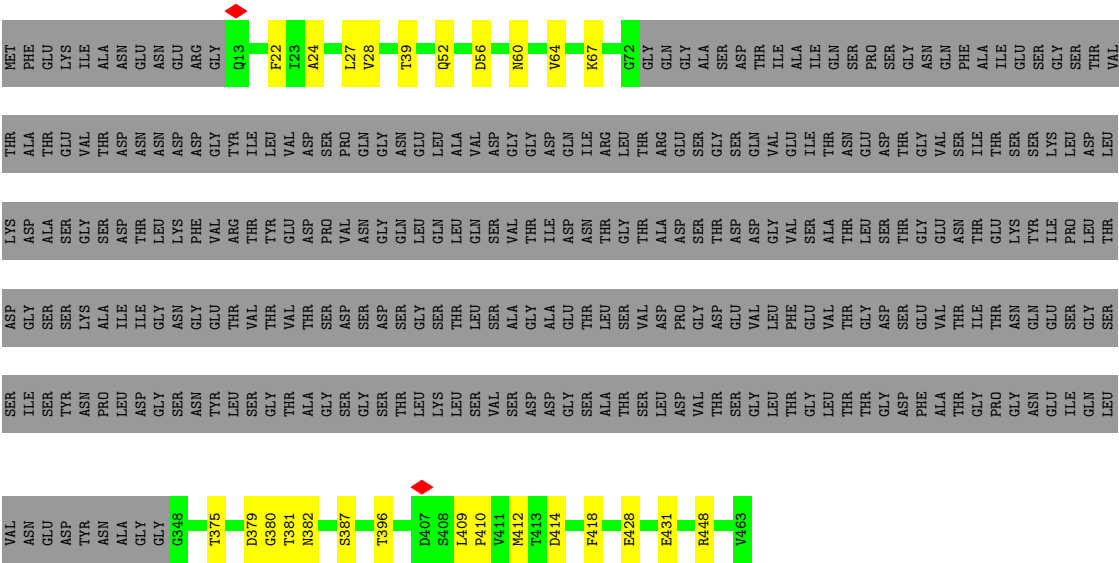
• Molecule 1: Flagellin



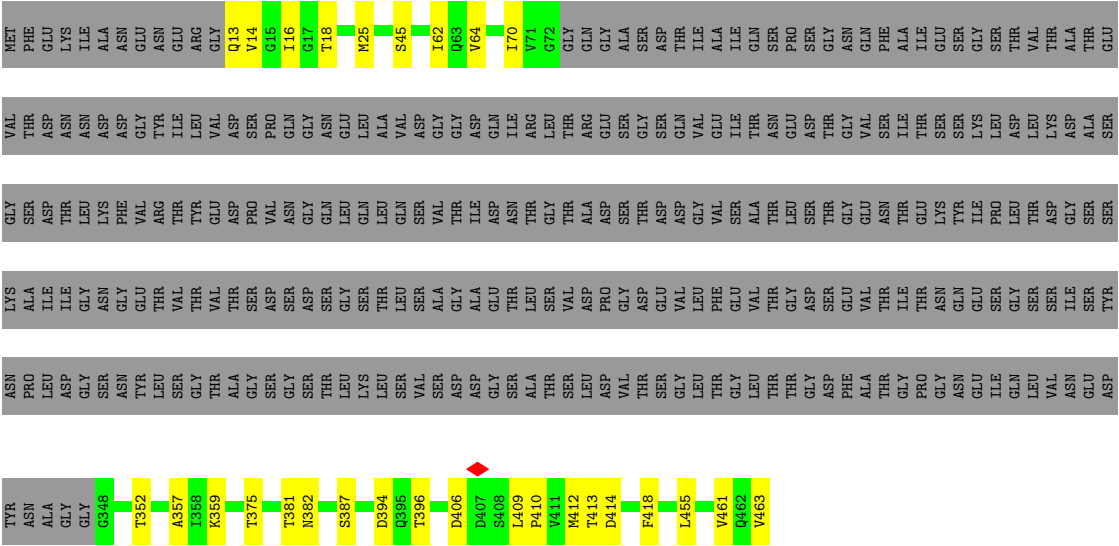
• Molecule 1: Flagellin



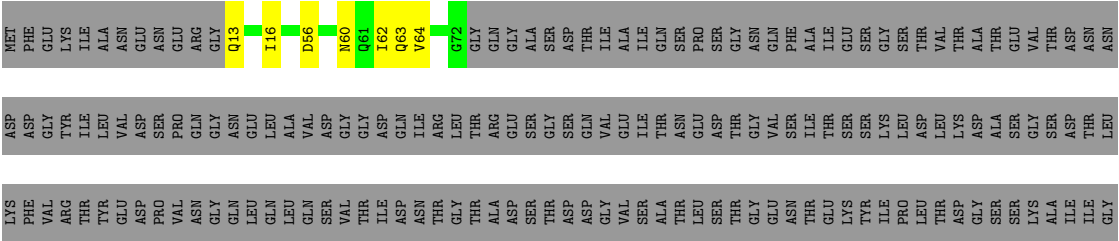




● Molecule 1: Flagellin



● Molecule 1: Flagellin





62%

ASP	Tyr	ASN	ALA	GLY	GLY
G348					
T352					
E370					
T375					
T381					
N382					
T392					
Q395					
D407					
S408					
L409					
P410					
D414					
M433					
E440					
A443					
L455					
E458					
V461					
Q462					
V463					

- Molecule 1: Flagellin

62%

AS	ASN
G349	TUR
V350	LEU
G351	SER
T352	GLY
D379	THR
S387	ALA
D388	GLY
D389	SER
T392	THR
E393	LEU
D394	LYS
Q395	LEU
Q403	SER
D407	VAL
S408	SER
L409	ASP
P410	GLY
V411	SER
R417	ALA
L427	THR
E428	SER
T439	THR
E440	GLY
A443	LEU
R448	THR
L455	THR
V461	GLY
Q462	ASP
V463	PHE
	ALA
	THR
	GLY
	PRO
	GLY
	ASN
	GLU
	IIE
	GLN
	LEU
	VAL
	ASN
	GLU
	THR
	ASP
	ASN
	GLY
	C349

- Molecule 1: Flagellin

62%

ASP	GLY	TYR	ILE	LEU	VAL	ASP	SER	PRO	GLN	GLY	ASN	GLU	LEU	ALA	VAL	ASP	GLY	GLY	ASP	GLN	ILE	GLU	THR	THR	GLU	ASP	THR	THR	GLY	VAL	SER	SER	ILE	THR	SER	LYS	LEU	ASP	LEU	LYS	ASP	ALA	SER	SER	GLY	SER	ASP	THR	LEU	LYS
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ILE	SER	TYR	ASP	PRO	ILE	LEU	ASP	GLY	SER	ASN	TYR	LEU	SER	GLY	THR	ALA	GLY	SER	GLY	VAL	SER	ASP	GLY	SER	ALA	THR	SER	GLY	THR	GLY	THR	GLY	ASP	PHE	ALA	THR	THR	GLY	ASN	ILE	GLN	LEU	VAL	SER
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ASN	GLU	ASP	TYR	ASN	ALA	GLY	G348	T352	K359	T366	E370	L409	P410	S415	T438	S66	K67	V68	G72	GLY	GLN	GLY	SER	ALA	THR	SER	GLY	THR	GLY	THR	GLY	ASP	PHE	ALA	THR	THR	GLY	ASN	ILE	GLN	LEU	VAL	SER
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● Molecule 1: Flagellin



MET	PHE	GLU	LYS	ILE	ALA	ASN	GLU	GLY	Q13	I16	F22	M25	L36	S415	T438	S66	K67	V68	G72	GLY	GLN	GLY	SER	ALA	THR	SER	GLY	THR	GLY	THR	GLY	ASP	PHE	ALA	THR	THR	GLY	ASN	ILE	GLN	LEU	VAL	SER
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ASP	ASN	ASN	ASP	ASP	GLY	TYR	ILE	VAL	SER	PRO	GLN	GLY	ASN	GLN	LEU	LEU	ALA	VAL	ASP	GLY	THR	THR	ALA	ASP	SER	GLY	THR	GLY	SER	ASP	GLN	VAL	THR	THR	GLY	VAL	GLY	ASN	ILE	GLN	LEU	VAL	SER
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ASP	THR	LEU	LYS	PHE	VAL	ARG	THR	THR	GLU	ASP	PRO	VAL	ASN	GLN	LEU	LEU	GLN	VAL	SER	ASP	GLY	THR	THR	ALA	ASP	SER	THR	THR	GLY	THR	GLY	THR	THR	GLY	THR	THR	GLY	ASN	ILE	GLN	LEU	VAL	SER
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ILE	ILE	GLY	ASN	GLY	THR	VAL	THR	THR	SER	ASP	SER	ASP	GLY	THR	LEU	THR	LEU	ALA	VAL	SER	ASP	GLY	THR	THR	ALA	ASP	SER	THR	THR	GLY	THR	THR	THR	GLY	THR	THR	GLY	ASN	ILE	GLN	LEU	VAL	SER
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LEU	ASP	SER	SER	TYR	LEU	SER	GLY	THR	THR	ALA	GLY	SER	GLY	THR	LEU	LYS	LEU	SER	VAL	SER	THR	THR	ALA	SER	ASP	VAL	THR	THR	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
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ALA	GLY	G348	K359	D364	T374	D379	G380	N382	D394	D406	L409	P410	V411	M412	T413	E428	E431	L435	E436	V437	S441	T444	R448	I449	P452	E458	V463
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● Molecule 1: Flagellin



MET	PHE	GLU	LYS	ILE	ALA	ASN	GLU	GLY	Q13	V14	G15	I16	L19	F22	T39	D56	M60	V64	A65	S66	G72	GLY	GLN	GLY	GLY	ALA	SER	ASP	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
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THR	GLU	VAL	THR	ASP	ASN	ASN	ASP	GLY	ILE	VAL	ASP	PRO	GLN	GLY	ASN	GLU	GLY	GLY	GLN	ILE	ARG	LEU	THR	ALA	ASP	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
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ALA	SER	GLY	SER	ASP	THR	THR	LYS	GLY	THR	THR	GLU	ASP	VAL	GLY	ASN	GLN	GLY	GLY	ILE	THR	THR	GLY	THR	ALA	ASP	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
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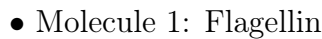
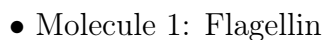
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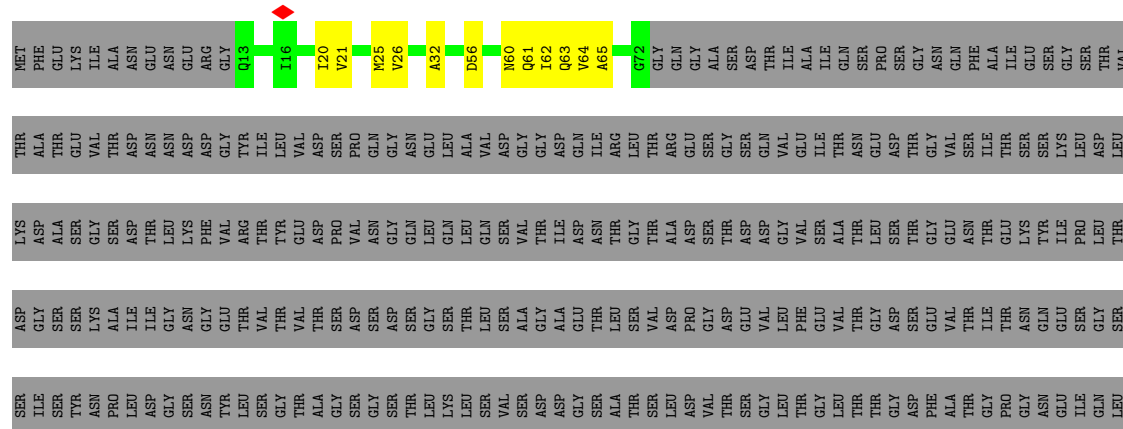
SER	THR	ASN	PRO	LEU	ASP	GLY	SER	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
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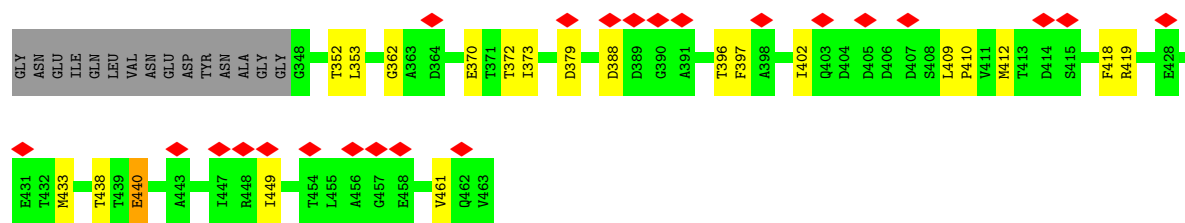
GLU	ASP	TYR	ASN	ALA	GLY	G348	K359	D364	E369	E370	T381	E400	S401	I402	D405	D406	L409	P410	R419	E428	T438	T439	E440	I447	P452	V463
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● Molecule 1: Flagellin

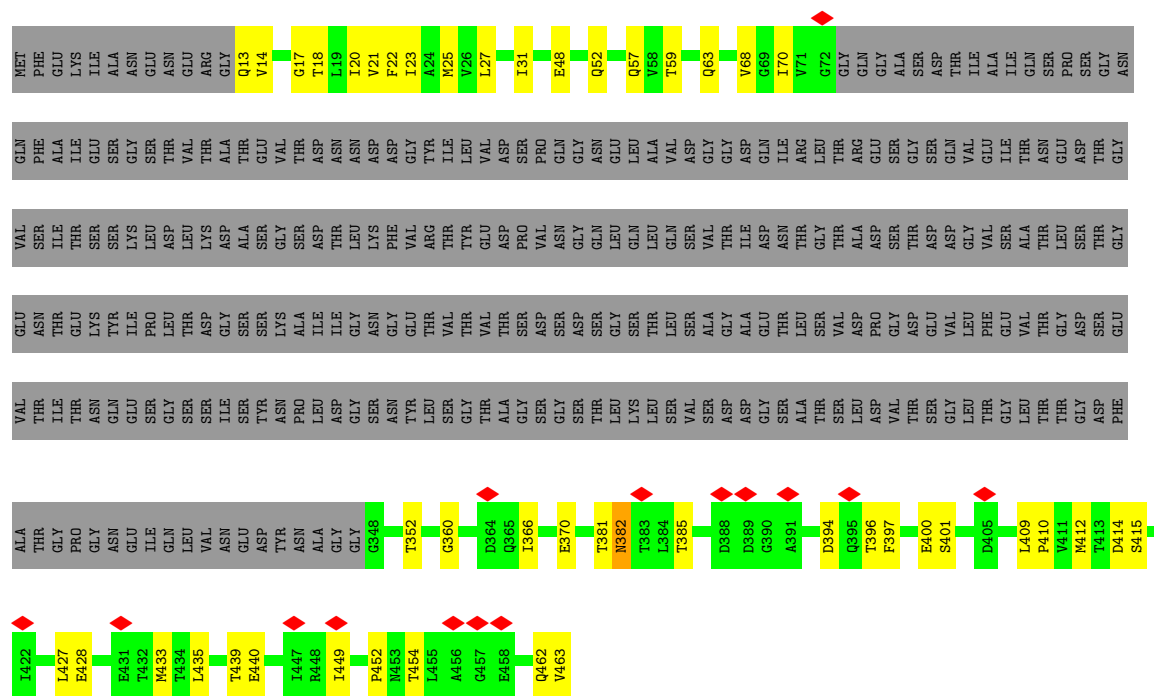




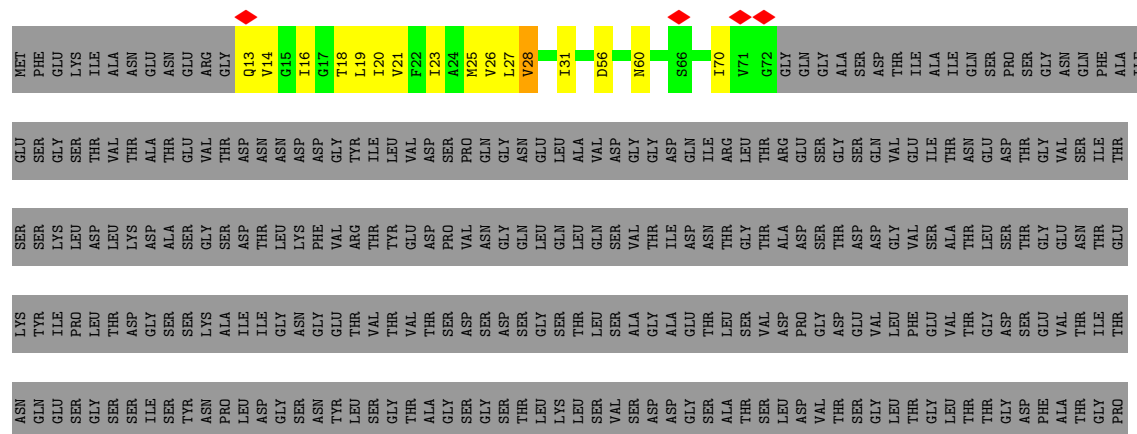


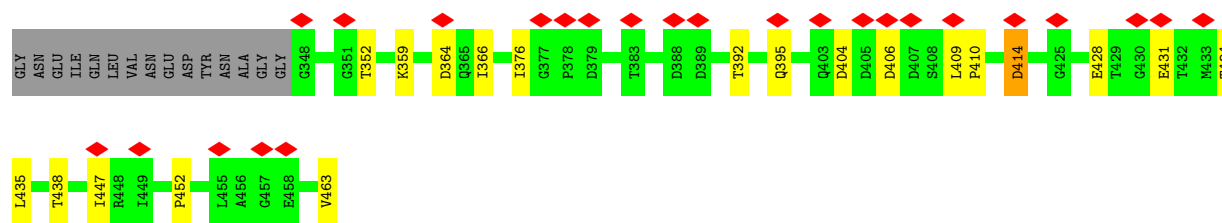


• Molecule 1: Flagellin

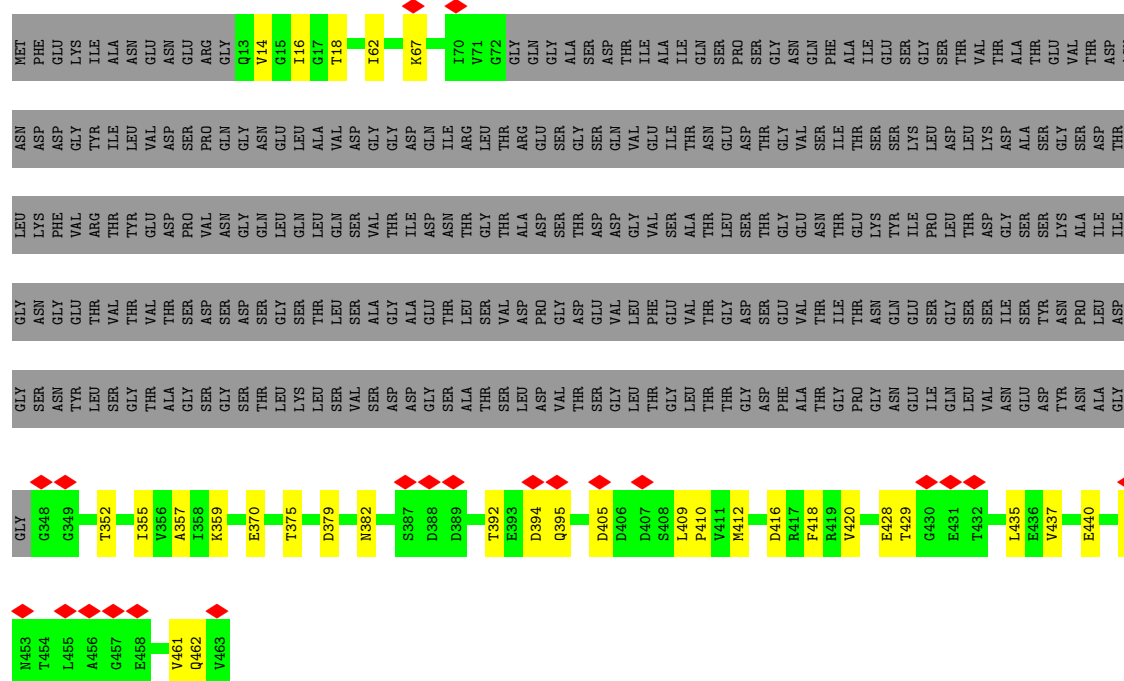


• Molecule 1: Flagellin

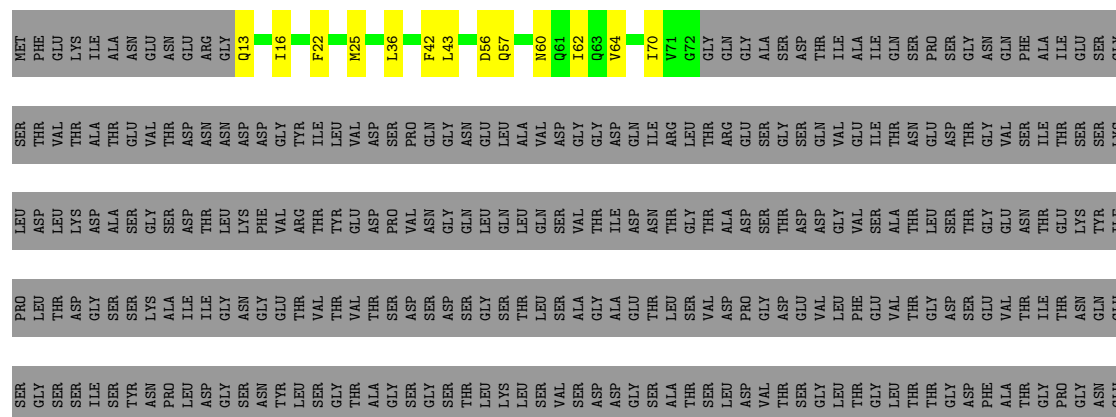


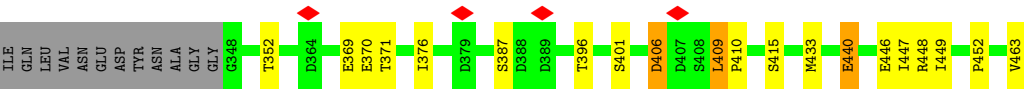


• Molecule 1: Flagellin

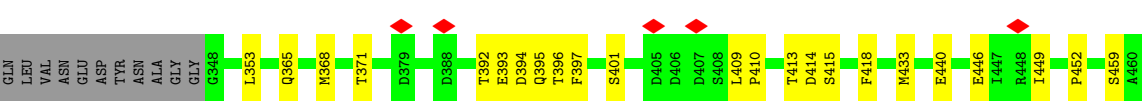
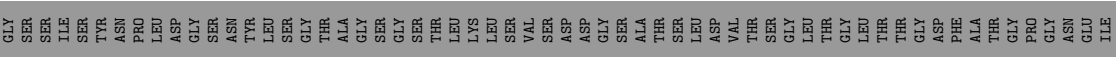
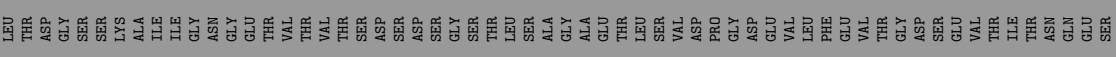
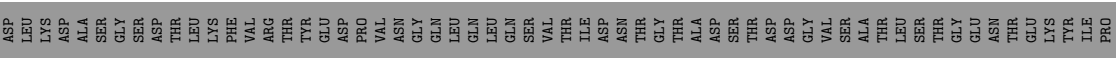
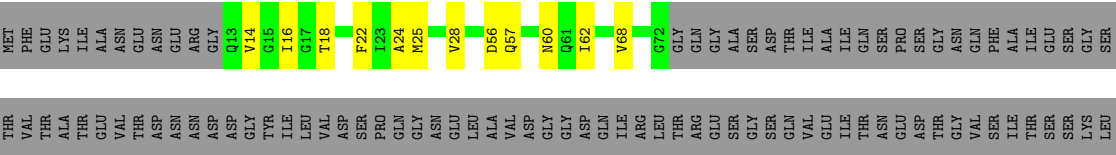


• Molecule 1: Flagellin

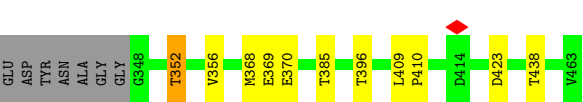
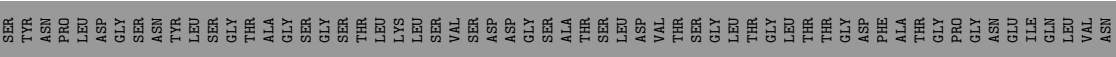
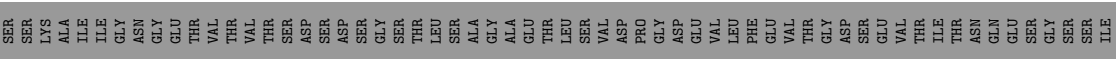
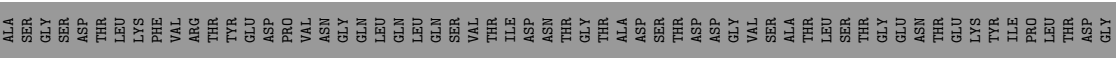
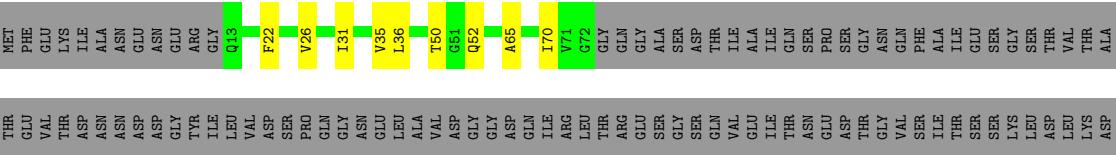




• Molecule 1: Flagellin

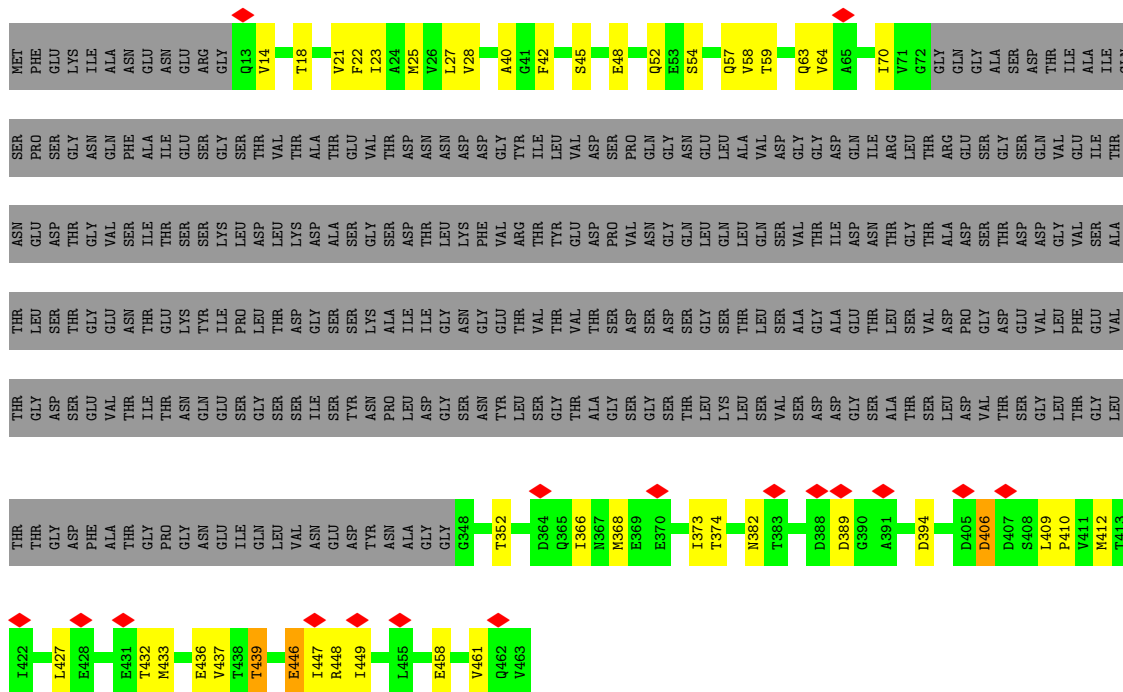


• Molecule 1: Flagellin



• Molecule 1: Flagellin





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	309194	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	2.801	Depositor
Minimum map value	-1.719	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.088	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	433.19998, 433.19998, 433.19998	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.083, 1.083, 1.083	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section:
NA

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	0.12	0/1271	0.33	0/1733
1	B	0.13	0/1271	0.36	0/1733
1	C	0.13	0/1271	0.36	0/1733
1	D	0.11	0/1271	0.30	0/1733
1	E	0.11	0/1271	0.30	0/1733
1	G	0.12	0/1271	0.30	0/1733
1	H	0.12	0/1271	0.29	0/1733
1	I	0.11	0/1271	0.31	0/1733
1	J	0.12	0/1271	0.29	0/1733
1	K	0.11	0/1271	0.29	0/1733
1	L	0.11	0/1271	0.29	0/1733
1	M	0.11	0/1271	0.31	0/1733
1	N	0.12	0/1271	0.33	0/1733
1	O	0.11	0/1271	0.30	0/1733
1	P	0.11	0/1271	0.29	0/1733
1	R	0.10	0/1271	0.29	0/1733
1	S	0.12	0/1271	0.32	0/1733
1	T	0.11	0/1271	0.34	0/1733
1	U	0.12	0/1271	0.32	0/1733
1	V	0.12	0/1271	0.30	0/1733
1	W	0.12	0/1271	0.31	0/1733
1	X	0.13	0/1271	0.35	0/1733
1	Y	0.11	0/1271	0.32	0/1733
1	Z	0.13	0/1271	0.34	0/1733
1	a	0.10	0/1271	0.28	0/1733
1	b	0.13	0/1271	0.34	0/1733
1	d	0.13	0/1271	0.35	0/1733
1	e	0.12	0/1271	0.33	0/1733
1	f	0.12	0/1271	0.36	0/1733
1	g	0.12	0/1271	0.36	0/1733
1	i	0.15	0/1262	0.42	0/1721
1	j	0.13	0/1271	0.36	0/1733

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	k	0.11	0/1271	0.33	0/1733
1	l	0.12	0/1271	0.33	0/1733
1	m	0.12	0/1271	0.30	0/1733
1	n	0.12	0/1271	0.33	0/1733
1	o	0.12	0/1271	0.35	0/1733
1	p	0.11	0/1271	0.31	0/1733
All	All	0.12	0/48289	0.32	0/65842

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	1264	0	1241	15	0
1	B	1264	0	1240	30	0
1	C	1264	0	1241	19	0
1	D	1264	0	1242	18	0
1	E	1264	0	1241	14	0
1	G	1264	0	1241	14	0
1	H	1264	0	1241	17	0
1	I	1264	0	1241	19	0
1	J	1264	0	1241	12	0
1	K	1264	0	1241	19	0
1	L	1264	0	1241	16	0
1	M	1264	0	1241	16	0
1	N	1264	0	1240	16	0
1	O	1264	0	1241	9	0
1	P	1264	0	1240	21	0
1	R	1264	0	1241	21	0
1	S	1264	0	1241	17	0
1	T	1264	0	1241	20	0
1	U	1264	0	1240	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	V	1264	0	1241	16	0
1	W	1264	0	1241	21	0
1	X	1264	0	1240	19	0
1	Y	1264	0	1240	22	0
1	Z	1264	0	1241	13	0
1	a	1264	0	1241	13	0
1	b	1264	0	1240	17	0
1	d	1264	0	1241	22	0
1	e	1264	0	1241	23	0
1	f	1264	0	1240	20	0
1	g	1264	0	1240	22	0
1	i	1255	0	1232	21	0
1	j	1264	0	1241	31	0
1	k	1264	0	1241	26	0
1	l	1264	0	1241	19	0
1	m	1264	0	1241	21	0
1	n	1264	0	1242	25	0
1	o	1264	0	1241	15	0
1	p	1264	0	1241	12	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
2	M	1	0	0	0	0
2	N	1	0	0	0	0
2	O	1	0	0	0	0
2	P	1	0	0	0	0
2	R	1	0	0	0	0
2	S	1	0	0	0	0
2	T	1	0	0	0	0
2	U	1	0	0	0	0
2	V	1	0	0	0	0
2	W	1	0	0	0	0
2	X	1	0	0	0	0
2	Y	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Z	1	0	0	0	0
2	a	1	0	0	0	0
2	b	1	0	0	0	0
2	d	1	0	0	0	0
2	e	1	0	0	0	0
2	f	1	0	0	0	0
2	g	1	0	0	0	0
2	i	1	0	0	0	0
2	j	1	0	0	0	0
2	k	1	0	0	0	0
2	l	1	0	0	0	0
2	m	1	0	0	0	0
2	n	1	0	0	0	0
2	o	1	0	0	0	0
2	p	1	0	0	0	0
All	All	48061	0	47142	613	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 613 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:Y:14:VAL:HB	1:k:21:VAL:HG11	1.65	0.79
1:B:373:ILE:HG12	1:B:437:VAL:HG22	1.64	0.79
1:j:63:GLN:OE1	1:m:57:GLN:NE2	2.18	0.77
1:B:382:ASN:ND2	1:B:394:ASP:OD2	2.18	0.76
1:P:68:VAL:HG21	1:U:381:THR:HG21	1.71	0.72

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	172/463 (37%)	160 (93%)	12 (7%)	0	100	100
1	B	172/463 (37%)	166 (96%)	6 (4%)	0	100	100
1	C	172/463 (37%)	164 (95%)	8 (5%)	0	100	100
1	D	172/463 (37%)	162 (94%)	10 (6%)	0	100	100
1	E	172/463 (37%)	165 (96%)	7 (4%)	0	100	100
1	G	172/463 (37%)	162 (94%)	10 (6%)	0	100	100
1	H	172/463 (37%)	160 (93%)	12 (7%)	0	100	100
1	I	172/463 (37%)	164 (95%)	8 (5%)	0	100	100
1	J	172/463 (37%)	160 (93%)	12 (7%)	0	100	100
1	K	172/463 (37%)	162 (94%)	10 (6%)	0	100	100
1	L	172/463 (37%)	160 (93%)	12 (7%)	0	100	100
1	M	172/463 (37%)	162 (94%)	10 (6%)	0	100	100
1	N	172/463 (37%)	159 (92%)	13 (8%)	0	100	100
1	O	172/463 (37%)	163 (95%)	9 (5%)	0	100	100
1	P	172/463 (37%)	164 (95%)	8 (5%)	0	100	100
1	R	172/463 (37%)	164 (95%)	8 (5%)	0	100	100
1	S	172/463 (37%)	162 (94%)	10 (6%)	0	100	100
1	T	172/463 (37%)	162 (94%)	10 (6%)	0	100	100
1	U	172/463 (37%)	163 (95%)	9 (5%)	0	100	100
1	V	172/463 (37%)	160 (93%)	12 (7%)	0	100	100
1	W	172/463 (37%)	162 (94%)	10 (6%)	0	100	100
1	X	172/463 (37%)	160 (93%)	12 (7%)	0	100	100
1	Y	172/463 (37%)	160 (93%)	12 (7%)	0	100	100
1	Z	172/463 (37%)	164 (95%)	8 (5%)	0	100	100
1	a	172/463 (37%)	164 (95%)	8 (5%)	0	100	100
1	b	172/463 (37%)	158 (92%)	14 (8%)	0	100	100
1	d	172/463 (37%)	161 (94%)	11 (6%)	0	100	100
1	e	172/463 (37%)	165 (96%)	7 (4%)	0	100	100
1	f	172/463 (37%)	167 (97%)	5 (3%)	0	100	100
1	g	172/463 (37%)	166 (96%)	6 (4%)	0	100	100
1	i	171/463 (37%)	164 (96%)	7 (4%)	0	100	100
1	j	172/463 (37%)	166 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	k	172/463 (37%)	163 (95%)	9 (5%)	0	100	100
1	l	172/463 (37%)	161 (94%)	11 (6%)	0	100	100
1	m	172/463 (37%)	162 (94%)	10 (6%)	0	100	100
1	n	172/463 (37%)	163 (95%)	9 (5%)	0	100	100
1	o	172/463 (37%)	162 (94%)	10 (6%)	0	100	100
1	p	172/463 (37%)	161 (94%)	11 (6%)	0	100	100
All	All	6535/17594 (37%)	6173 (94%)	362 (6%)	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	142/377 (38%)	141 (99%)	1 (1%)	76	79
1	B	142/377 (38%)	136 (96%)	6 (4%)	26	54
1	C	142/377 (38%)	141 (99%)	1 (1%)	76	79
1	D	142/377 (38%)	135 (95%)	7 (5%)	22	49
1	E	142/377 (38%)	137 (96%)	5 (4%)	32	58
1	G	142/377 (38%)	138 (97%)	4 (3%)	38	62
1	H	142/377 (38%)	139 (98%)	3 (2%)	47	67
1	I	142/377 (38%)	138 (97%)	4 (3%)	38	62
1	J	142/377 (38%)	138 (97%)	4 (3%)	38	62
1	K	142/377 (38%)	141 (99%)	1 (1%)	76	79
1	L	142/377 (38%)	138 (97%)	4 (3%)	38	62
1	M	142/377 (38%)	138 (97%)	4 (3%)	38	62
1	N	142/377 (38%)	139 (98%)	3 (2%)	47	67
1	O	142/377 (38%)	140 (99%)	2 (1%)	59	72
1	P	142/377 (38%)	137 (96%)	5 (4%)	32	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	R	142/377 (38%)	139 (98%)	3 (2%)	47	67
1	S	142/377 (38%)	137 (96%)	5 (4%)	32	58
1	T	142/377 (38%)	139 (98%)	3 (2%)	47	67
1	U	142/377 (38%)	141 (99%)	1 (1%)	76	79
1	V	142/377 (38%)	141 (99%)	1 (1%)	76	79
1	W	142/377 (38%)	138 (97%)	4 (3%)	38	62
1	X	142/377 (38%)	138 (97%)	4 (3%)	38	62
1	Y	142/377 (38%)	137 (96%)	5 (4%)	32	58
1	Z	142/377 (38%)	138 (97%)	4 (3%)	38	62
1	a	142/377 (38%)	137 (96%)	5 (4%)	32	58
1	b	142/377 (38%)	141 (99%)	1 (1%)	76	79
1	d	142/377 (38%)	137 (96%)	5 (4%)	32	58
1	e	142/377 (38%)	139 (98%)	3 (2%)	47	67
1	f	142/377 (38%)	137 (96%)	5 (4%)	32	58
1	g	142/377 (38%)	132 (93%)	10 (7%)	14	37
1	i	141/377 (37%)	136 (96%)	5 (4%)	32	58
1	j	142/377 (38%)	134 (94%)	8 (6%)	19	45
1	k	142/377 (38%)	138 (97%)	4 (3%)	38	62
1	l	142/377 (38%)	137 (96%)	5 (4%)	32	58
1	m	142/377 (38%)	136 (96%)	6 (4%)	26	54
1	n	142/377 (38%)	138 (97%)	4 (3%)	38	62
1	o	142/377 (38%)	140 (99%)	2 (1%)	59	72
1	p	142/377 (38%)	138 (97%)	4 (3%)	38	62
All	All	5395/14326 (38%)	5244 (97%)	151 (3%)	38	62

5 of 151 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	j	394	ASP
1	p	409	LEU
1	j	454	THR
1	m	369	GLU
1	B	461	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 46 such sidechains are listed below:

Mol	Chain	Res	Type
1	d	38	ASN
1	j	63	GLN
1	e	13	GLN
1	g	365	GLN
1	k	13	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 38 ligands modelled in this entry, 38 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

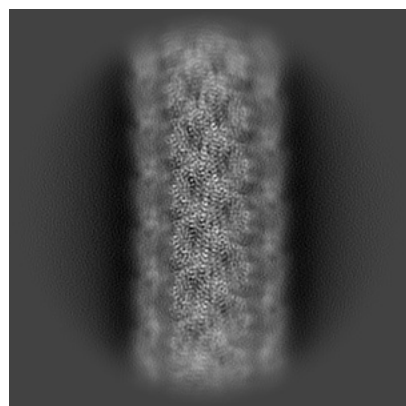
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-64862. These allow visual inspection of the internal detail of the map and identification of artifacts.

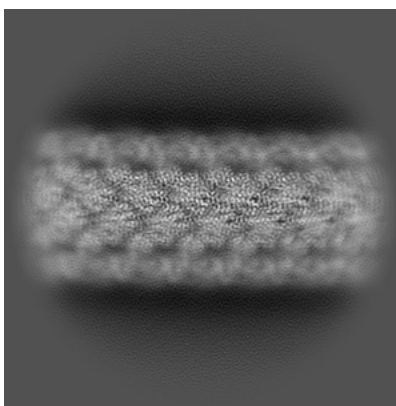
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

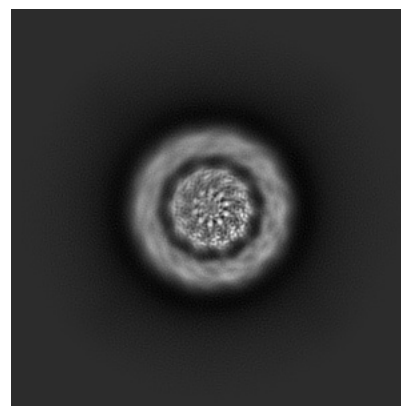
6.1.1 Primary map



X

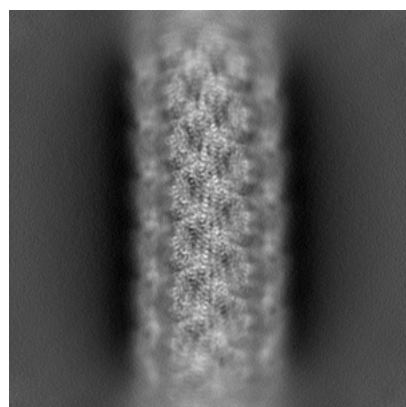


Y

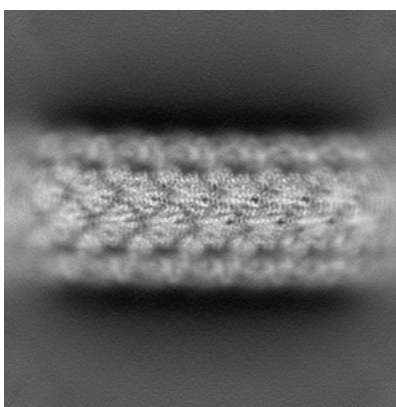


Z

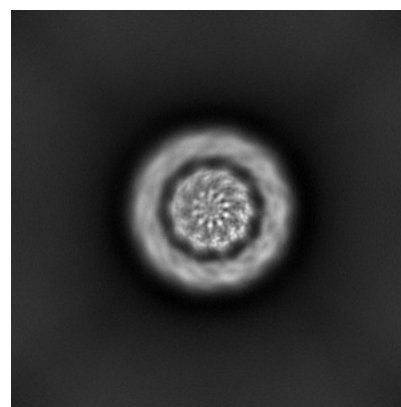
6.1.2 Raw map



X



Y

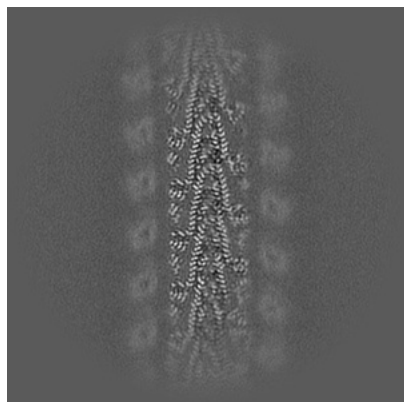


Z

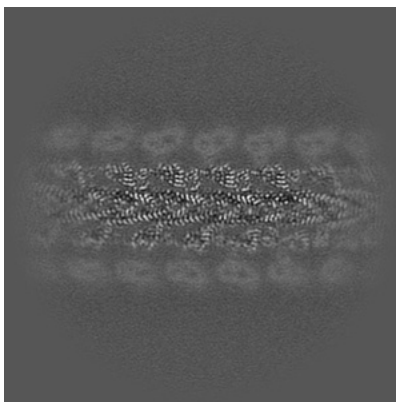
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

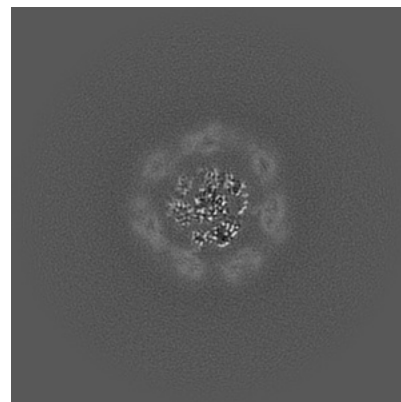
6.2.1 Primary map



X Index: 200

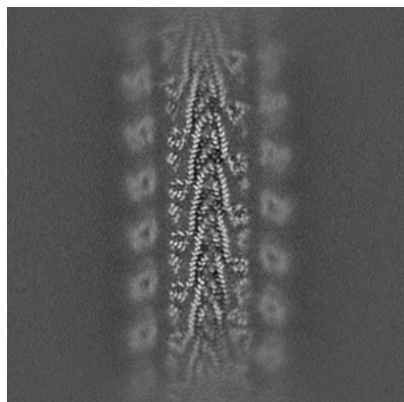


Y Index: 200

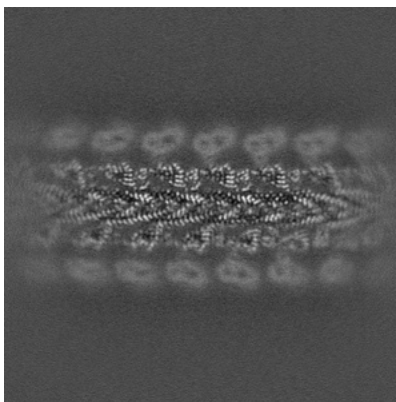


Z Index: 200

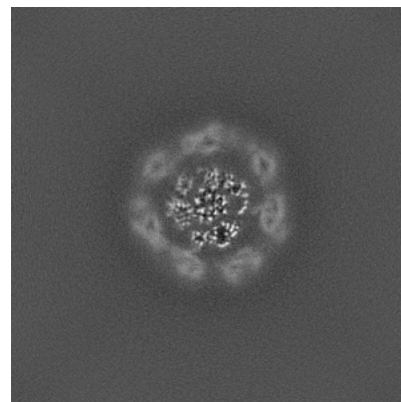
6.2.2 Raw map



X Index: 200



Y Index: 200

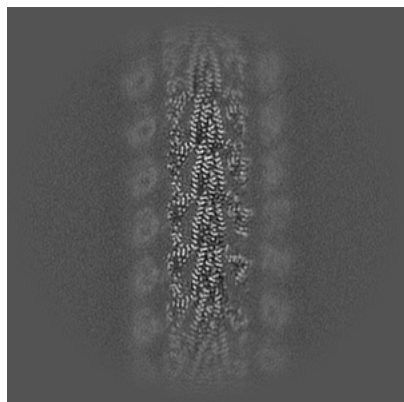


Z Index: 200

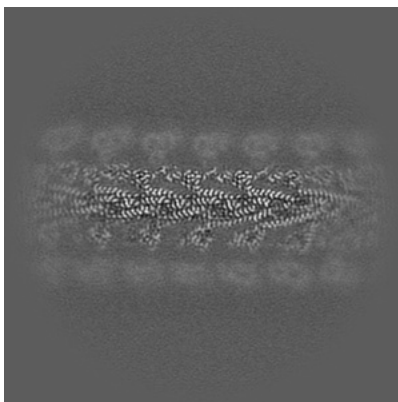
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

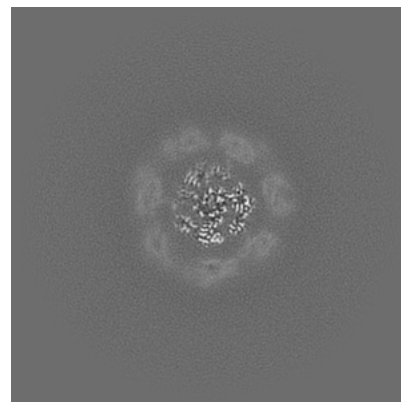
6.3.1 Primary map



X Index: 207

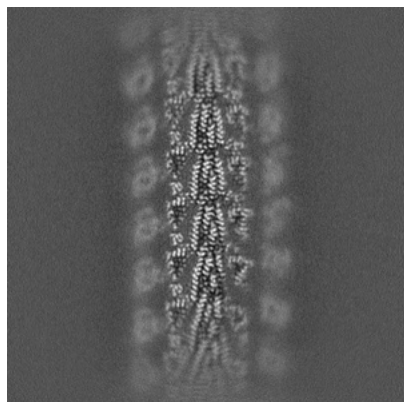


Y Index: 194

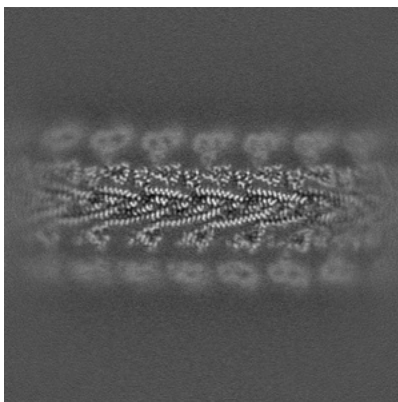


Z Index: 172

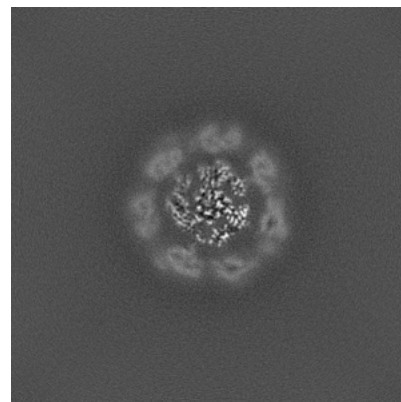
6.3.2 Raw map



X Index: 208



Y Index: 196

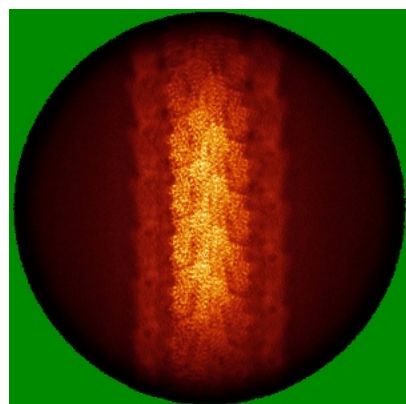


Z Index: 193

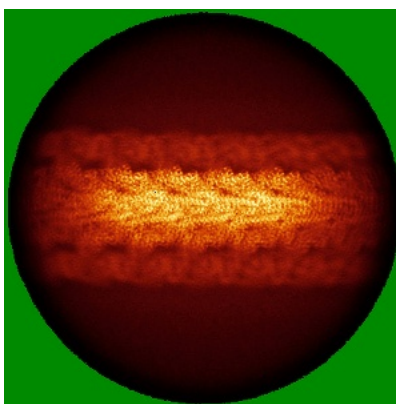
The images above show the largest variance slices of the map in three orthogonal directions.

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

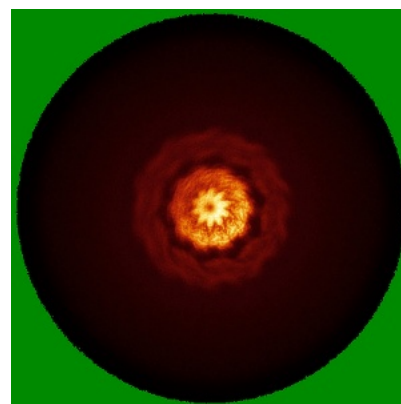
6.4.1 Primary map



X

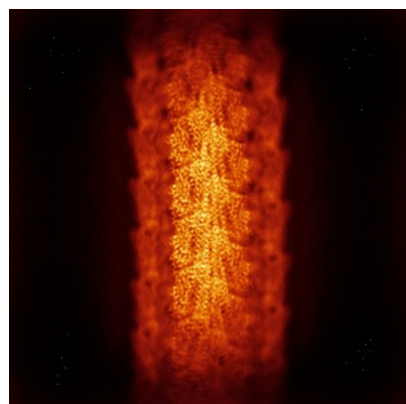


Y

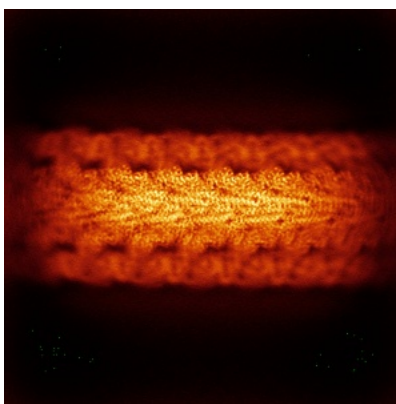


Z

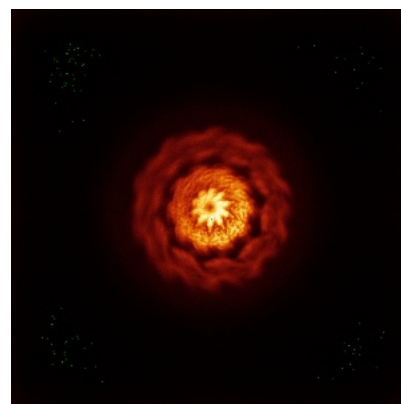
6.4.2 Raw map



X



Y

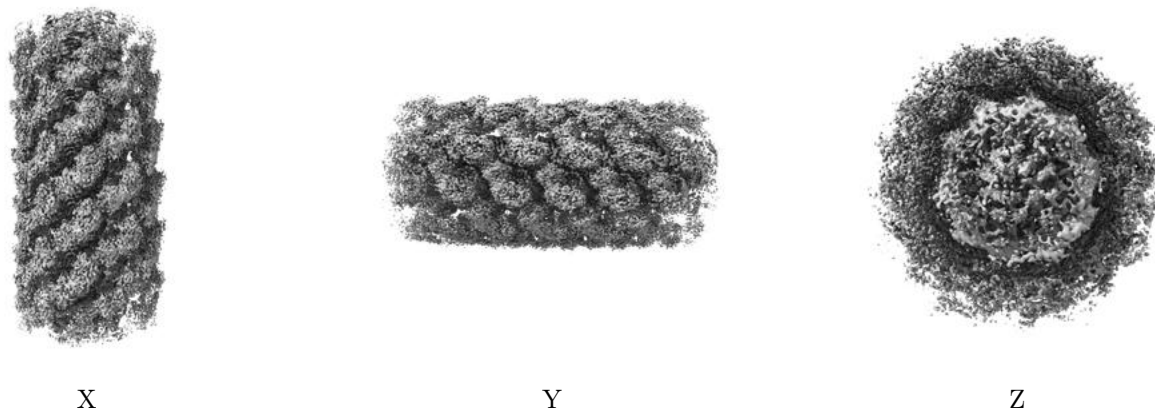


Z

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.

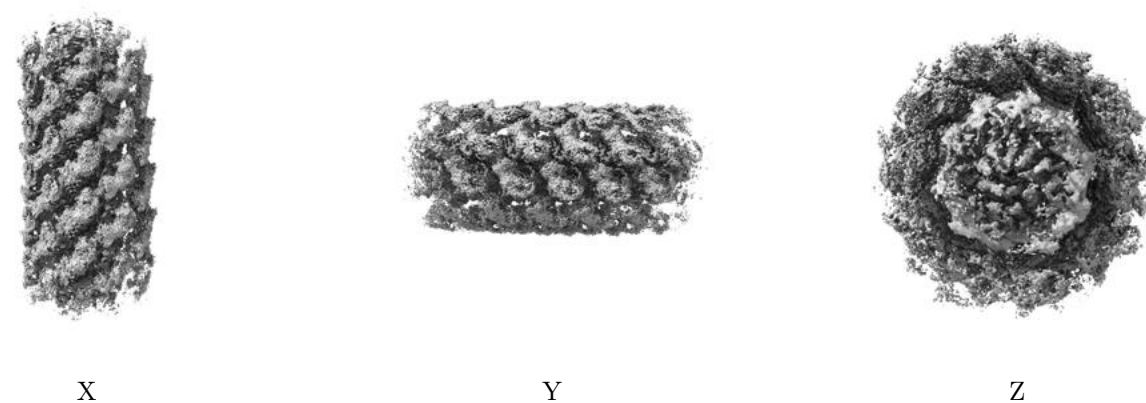
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.3. 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.

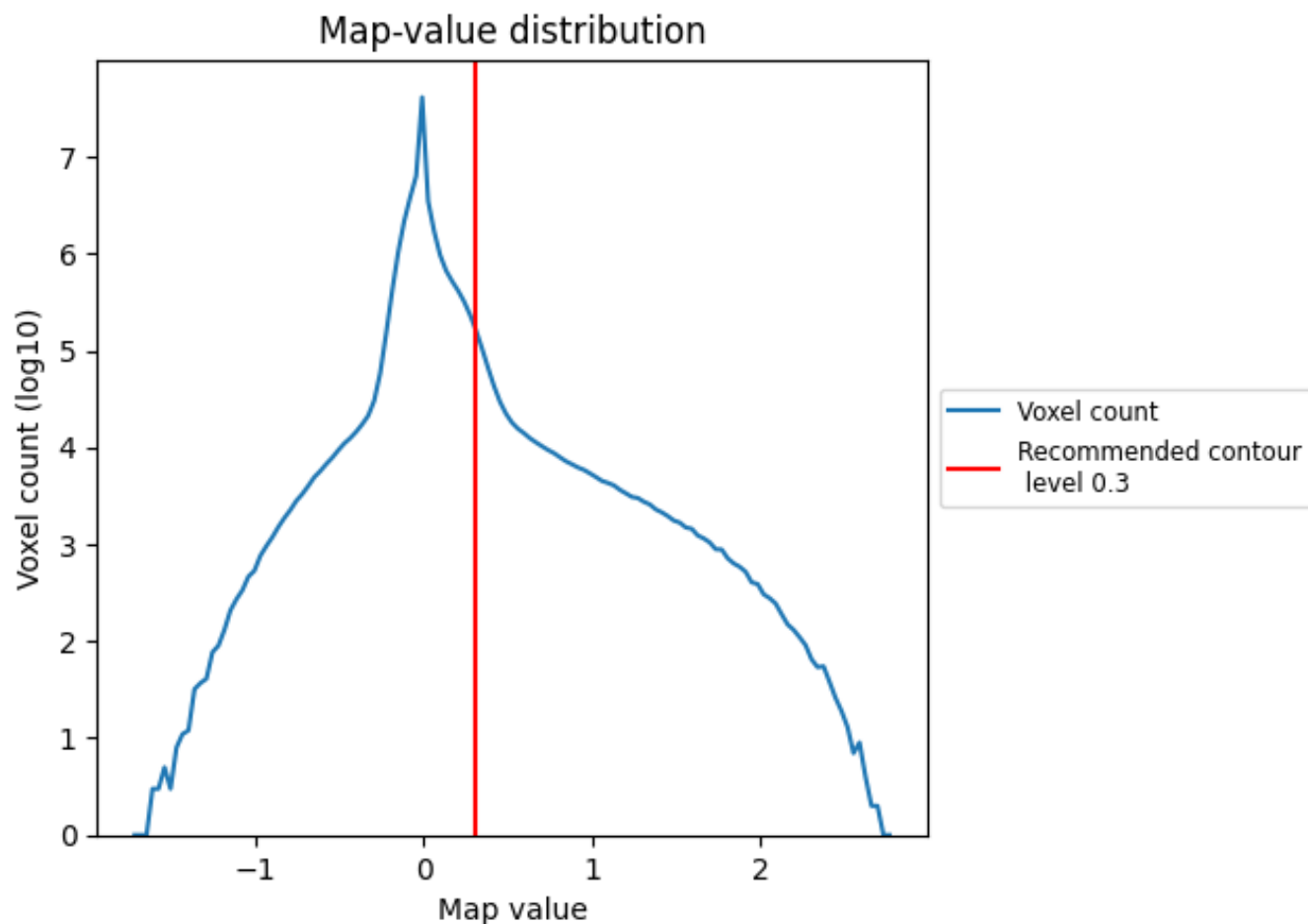
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

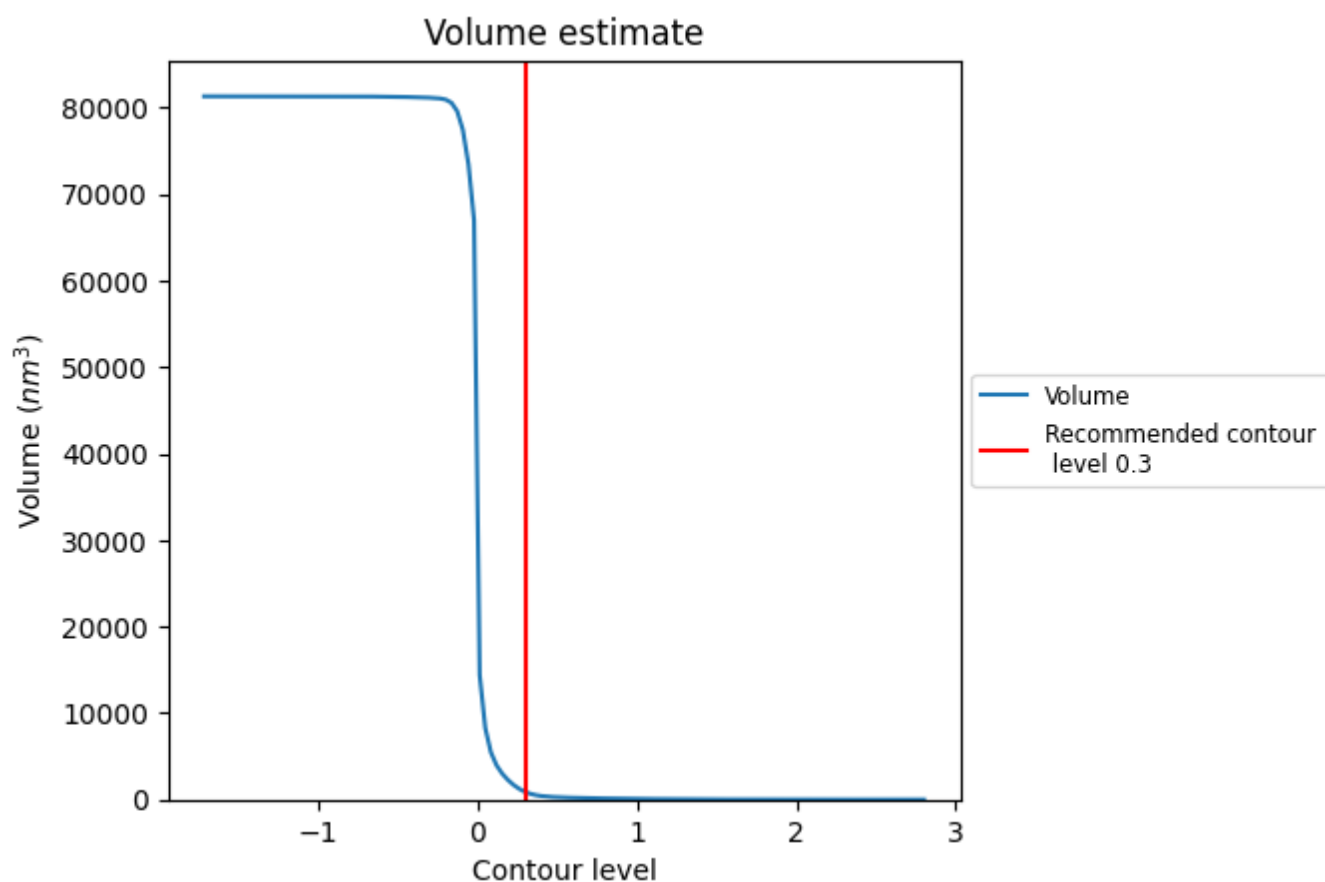
This section contains the results of statistical analysis of the map.

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.

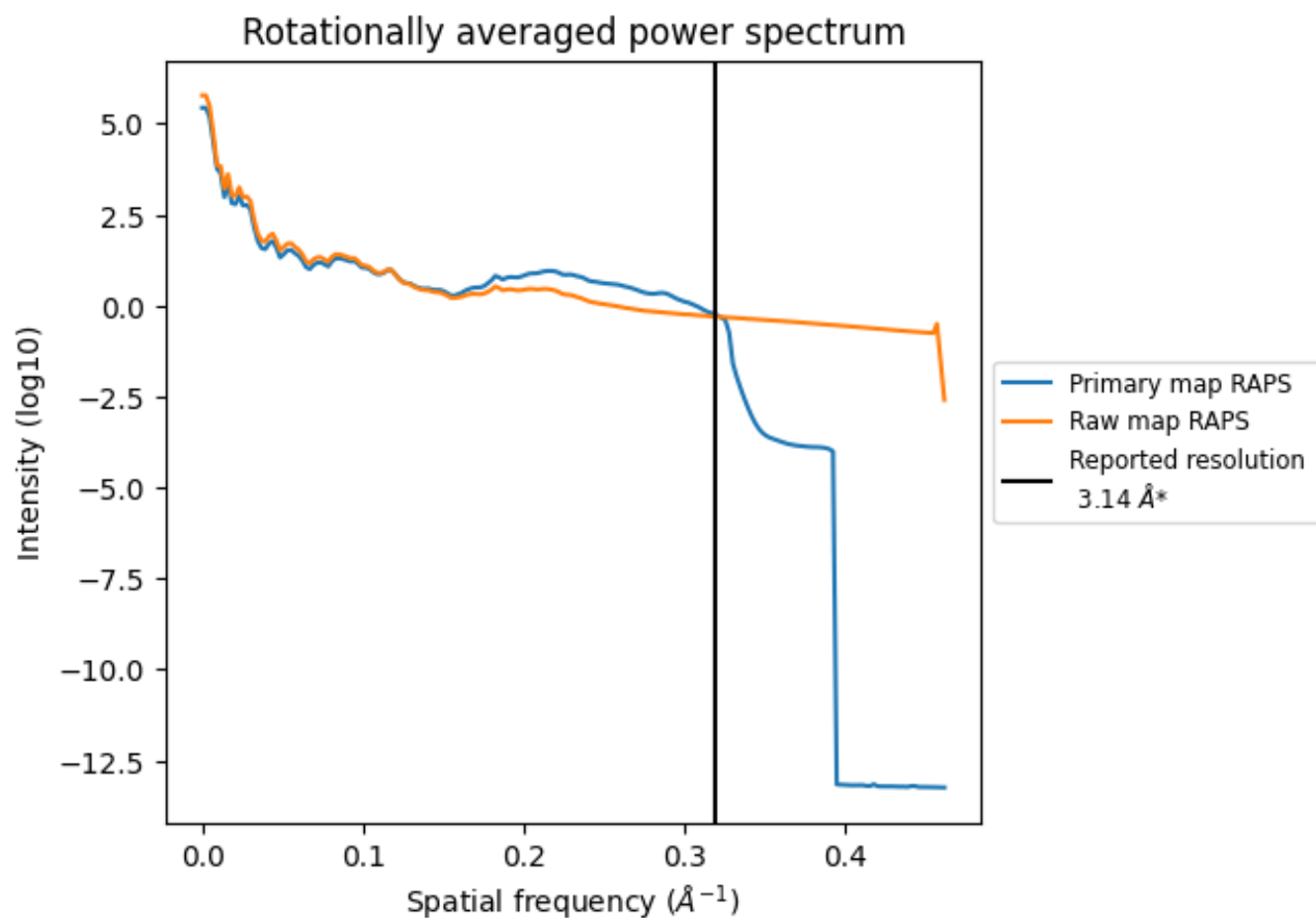
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 869 nm³; this corresponds to an approximate mass of 785 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 ⓘ

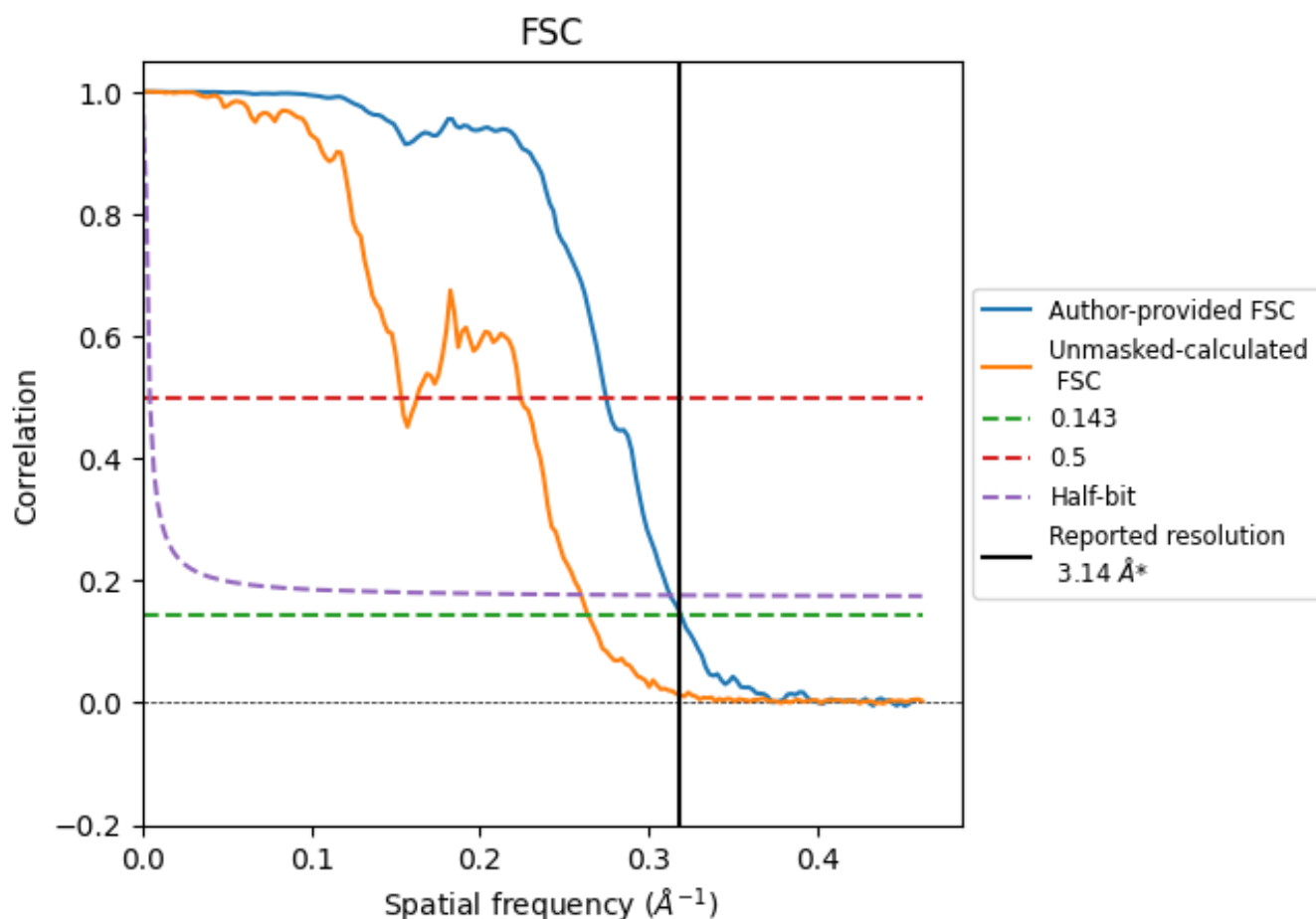


*Reported resolution corresponds to spatial frequency of $0.318 \text{ \AA}^{-1}$

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 0.318 Å⁻¹

8.2 Resolution estimates [i](#)

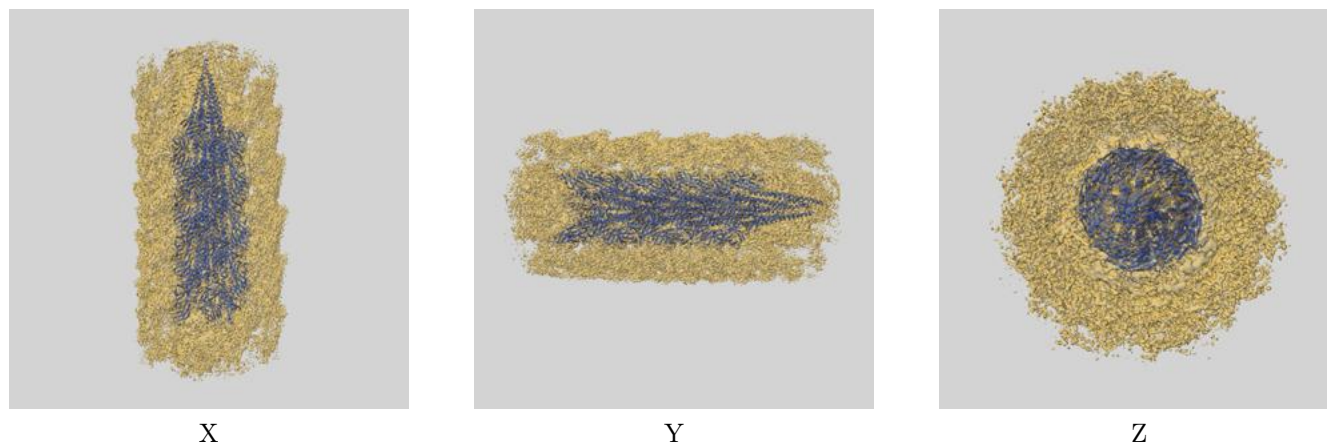
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.14	-	-
Author-provided FSC curve	3.14	3.64	3.20
Unmasked-calculated*	3.79	6.52	3.85

*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 3.79 differs from the reported value 3.14 by more than 10 %

9 Map-model fit [i](#)

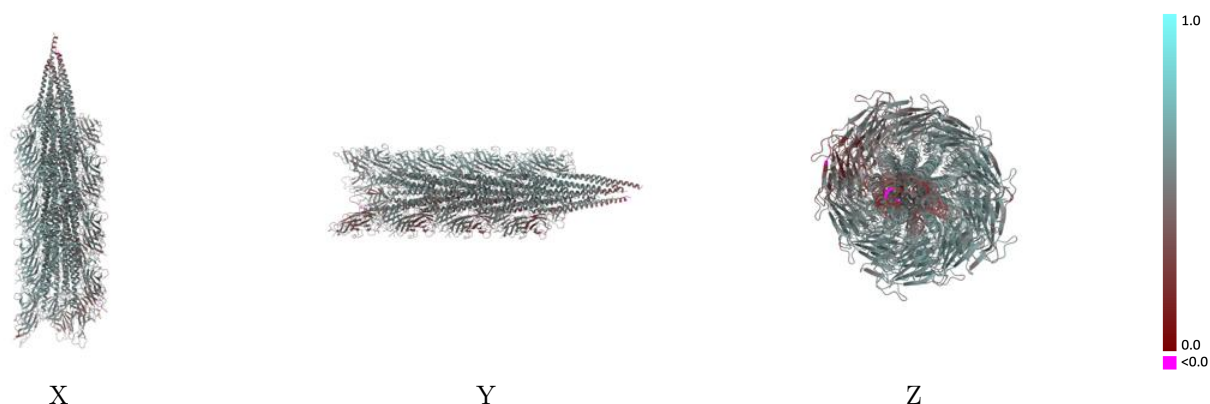
This section contains information regarding the fit between EMDB map EMD-64862 and PDB model 9V96. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

9.1 Map-model overlay [i](#)



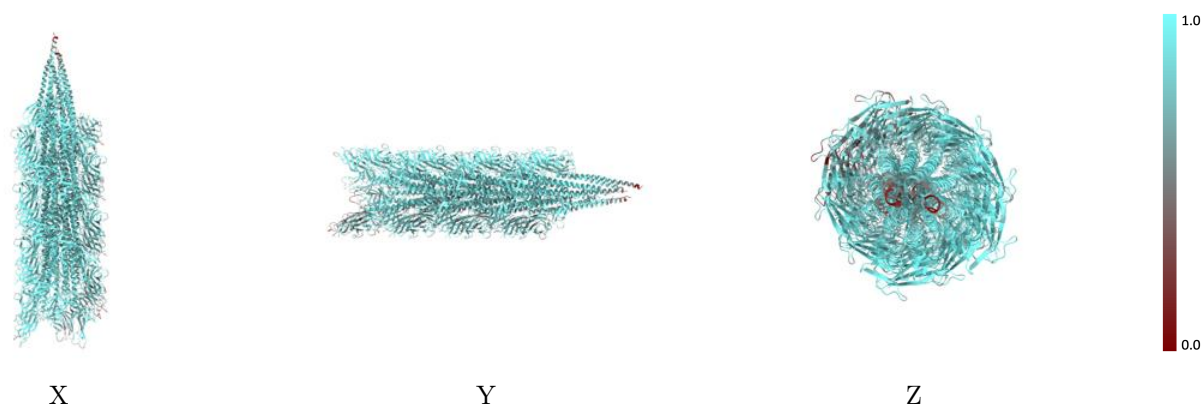
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



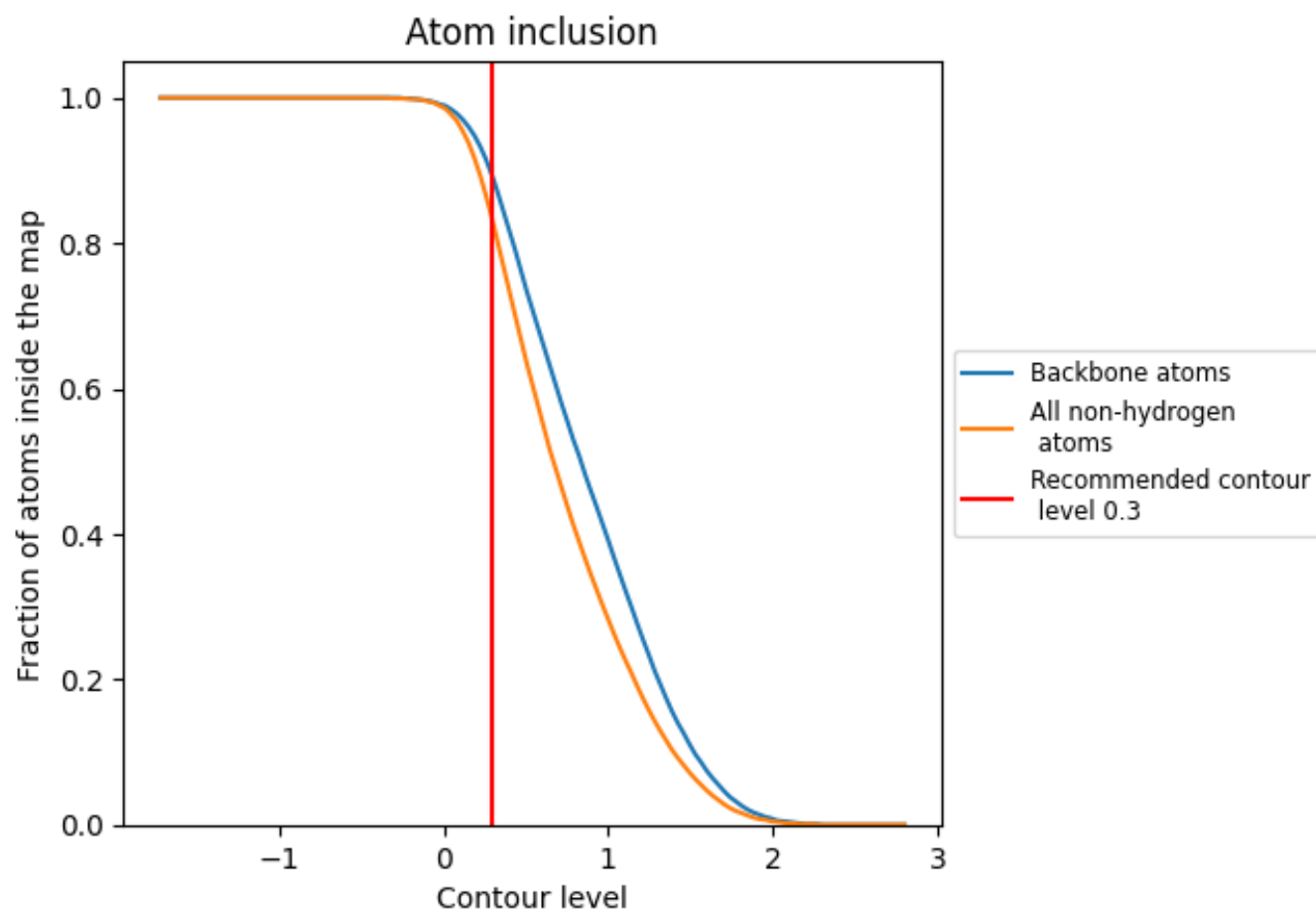
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 83% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8290	 0.5030
A	 0.9130	 0.5580
B	 0.6960	 0.3820
C	 0.8770	 0.5410
D	 0.8780	 0.5430
E	 0.8470	 0.5320
G	 0.8630	 0.5230
H	 0.9050	 0.5550
I	 0.8650	 0.5340
J	 0.9010	 0.5530
K	 0.9190	 0.5600
L	 0.9080	 0.5620
M	 0.8210	 0.5020
N	 0.9050	 0.5560
O	 0.9160	 0.5650
P	 0.8880	 0.5470
R	 0.8550	 0.5220
S	 0.9090	 0.5550
T	 0.9010	 0.5530
U	 0.8900	 0.5340
V	 0.8770	 0.5350
W	 0.8950	 0.5370
X	 0.8810	 0.5300
Y	 0.8120	 0.4940
Z	 0.8360	 0.5050
a	 0.8480	 0.4990
b	 0.8150	 0.4900
d	 0.7060	 0.4500
e	 0.7520	 0.4610
f	 0.7570	 0.4530
g	 0.6860	 0.4070
i	 0.6600	 0.3750
j	 0.6950	 0.3810
k	 0.6470	 0.3940
l	 0.7000	 0.4500



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Chain	Atom inclusion	Q-score
m	 0.8130	 0.4910
n	 0.8260	 0.4970
o	 0.8190	 0.4920
p	 0.8250	 0.5010