



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 04:26 AM UTC

PDB ID : 8HQZ / pdb_00008hqz
EMDB ID : EMD-34955
Title : Baseplate of DT57C bacteriophage in the full state
Authors : Ayala, R.; Moiseenko, A.V.; Chen, T.H.; Kulikov, E.E.; Golomidova, A.K.;
Orekhov, P.S.; Street, M.A.; Sokolova, O.S.; Letarov, A.V.; Wolf, M.
Deposited on : 2022-12-14
Resolution : 3.80 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

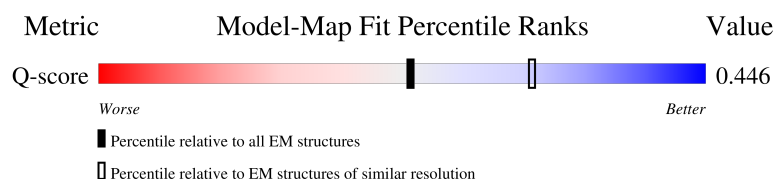
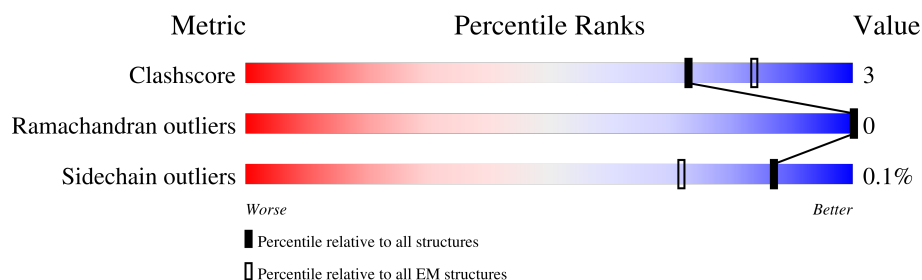
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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	10198 (3.30 - 4.30)

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	949	 90% 8% .
2	H	204	 95% 5%
2	I	204	 94% 6%
3	L	300	 92% 7% .

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Mol	Chain	Length	Quality of chain
4	Q	140	86% 14%
4	R	140	90% 9%
4	S	140	92% 7%
4	T	140	89% 9%
5	d	1076	96%
5	e	1076	96%
5	f	1076	96%
6	k	1227	97%
7	p	468	16% 93% 6%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 22127 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 Baseplate hub protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	930	Total	C	N	O	S	0	0
			7438	4707	1259	1462	10		

- Molecule 2 is a protein called Distal tail protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	204	Total	C	N	O	S	0	0
			1600	1023	266	308	3		
2	I	204	Total	C	N	O	S	0	0
			1600	1023	266	308	3		

- Molecule 3 is a protein called Minor tail protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	296	Total	C	N	O	S	0	0
			2400	1533	395	464	8		

- Molecule 4 is a protein called L-shaped tail fiber assembly.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	Q	139	Total	C	N	O	S	0	0
			1069	669	175	221	4		
4	R	139	Total	C	N	O	S	0	0
			1069	669	175	221	4		
4	S	139	Total	C	N	O	S	0	0
			1069	669	175	221	4		
4	T	137	Total	C	N	O	S	0	0
			1056	662	173	217	4		

- Molecule 5 is a protein called L-shaped tail fiber assembly.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	d	46	Total	C	N	O	0	0
			338	213	53	72		
5	e	47	Total	C	N	O	0	0
			343	216	54	73		
5	f	47	Total	C	N	O	0	0
			336	209	53	74		

- Molecule 6 is a protein called Tape measure protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	k	36	Total	C	N	O	0	0
			257	155	47	55		

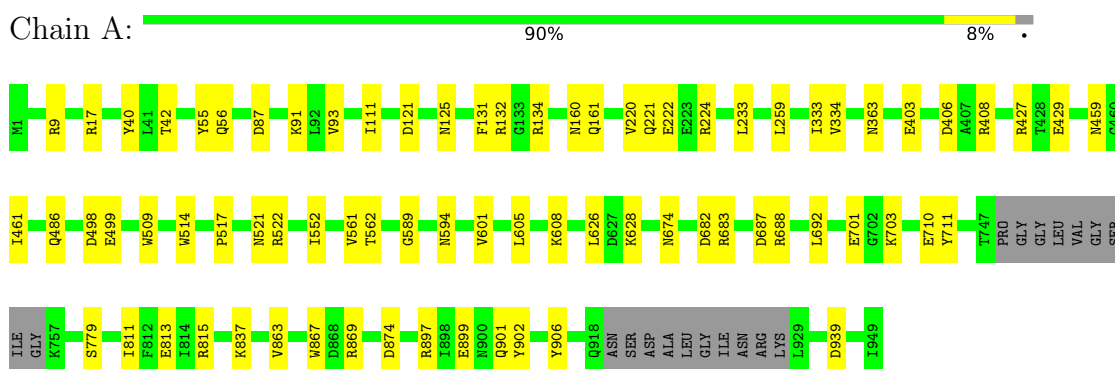
- Molecule 7 is a protein called Tail tube protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	p	466	Total	C	N	O	S	0	0
			3552	2222	577	744	9		

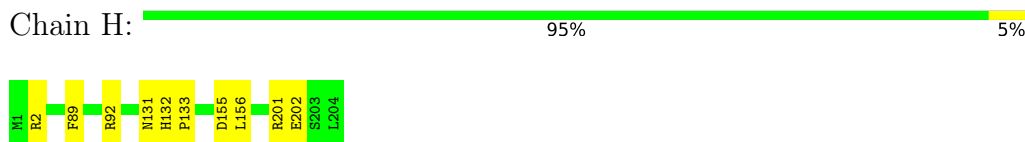
3 Residue-property plots [i](#)

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.

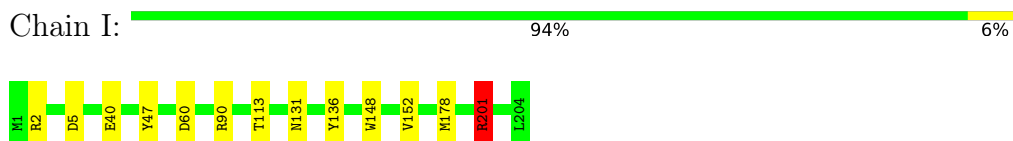
- Molecule 1: Baseplate hub protein



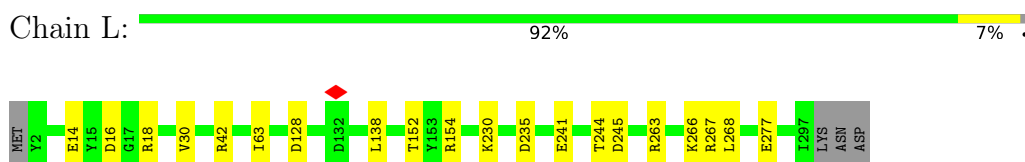
- Molecule 2: Distal tail protein



- Molecule 2: Distal tail protein

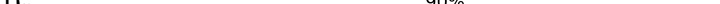


- Molecule 3: Minor tail protein



- Molecule 4: L-shaped tail fiber assembly

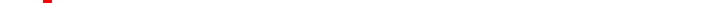
MET
S2
K15
Y32
P33
N40
Y44
S45
L46
T49
I50
V82
T86
R96
I111
L112
M113
T114
R115
M128
D136
T139
Q140

- Chain R:  90% 9%

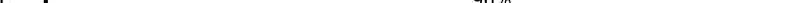
MET
 S2
 T3
 K15
 V16
 P17
 D26
 V27
 V82
 V85
 G89
 K98
 E129
 I134
 G137
 Q140

- Chain S: 92% 7%

The diagram shows a sequence of residues: MET, S2, V16, P17, Q23, V27, Q73, R102, L112, I118, G119, S120, E121, V122, and Q140. The residues are represented by colored blocks: MET is grey, S2 is green, V16 and P17 are yellow, Q23 is green, V27 is yellow, Q73 is green, R102 is yellow, L112 is green, I118 and G119 are yellow, S120 is green and marked with a red diamond, E121 is yellow, V122 is green, and Q140 is yellow.

- Chain T:  89% 9% .

MET		E4		E14 K15		M22	Q23	F24	N25	V39	T42	I111	R115	G119	S120	E129	G137	Q140
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- Chain d:  96%

MET	ALA	LEU	LYS	THR	K6	T18	T19	K27	S95	S51	ALA	GLY	SER	ALA	ALA	ALA	LYS	GLY	SER	GLU	ILE	ALA	ALA	LYS	GLU	SER	GLU	LEU	ASN	ALA	LYS	ASP	SER	GLU	ASN	GLU	ALA	ALA	ILE	SER	GLY	ALA	GLU	SER	GLU	GLN	ALA	ALA	SER
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ALA ALA
GLU GLU
SER SER
GLY GLY
ARG ARG
GLN GLN
ALA ALA
LEU LEU
SER SER
LYS LYS
GLY GLY
SER SER
ASP ASP
ASN ASN
SER SER
ALA ALA
SER SER
GLY GLY
PHE PHE
ARG ARG
ASP ASP
SER SER
ALA ALA
GLU GLU
LEU LEU
ALA ALA
ALA ALA
GLN GLN
SER SER
ARG ARG
LEU LEU
LEU LEU
ALA ALA
ALA ALA
ALA ALA
GLN GLN
GLN GLN
ALA ALA
LYS LYS
THR THR
ALA ALA
ALA ALA
GLN GLN
THR THR
ALA ALA

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

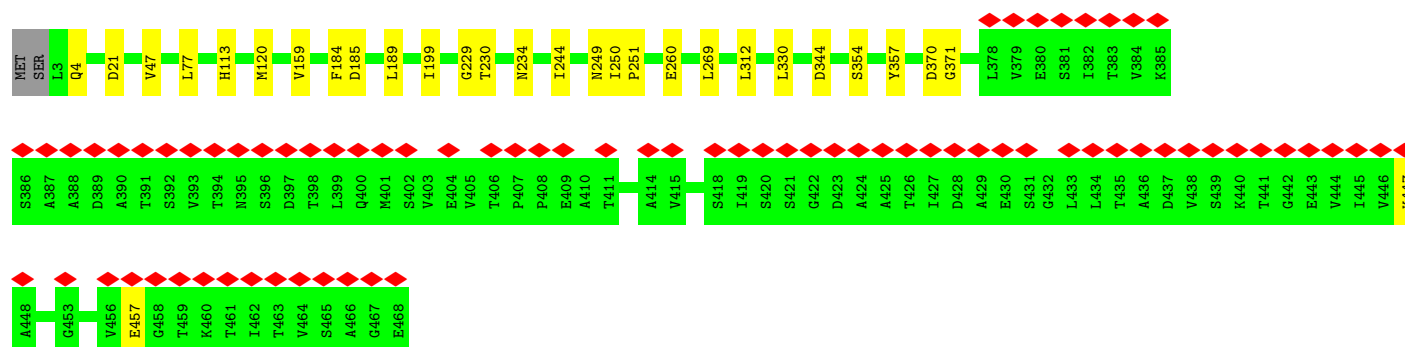
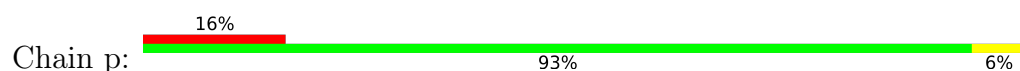
- Molecule 5: L-shaped tail fiber assembly

Chain f: 96%

[illegible]

[illegible]

- Molecule 7: Tail tube protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	42697	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 ($e^-/\text{\AA}^2$)	67	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	29.178	Depositor
Minimum map value	-11.233	Depositor
Average map value	0.001	Depositor
Map value standard deviation	1.012	Depositor
Recommended contour level	4	Depositor
Map size (Å)	560.0, 560.0, 560.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4, 1.4, 1.4	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	0.40	0/7597	0.54	0/10315
2	H	0.43	0/1638	0.49	0/2229
2	I	0.45	0/1638	0.52	0/2229
3	L	0.43	0/2455	0.54	0/3334
4	Q	0.37	0/1084	0.57	0/1469
4	R	0.38	0/1084	0.51	0/1469
4	S	0.39	0/1084	0.51	0/1469
4	T	0.35	0/1071	0.54	0/1451
5	d	0.38	0/340	0.51	0/464
5	e	0.29	0/345	0.50	0/471
5	f	0.35	0/338	0.60	0/462
6	k	0.39	0/258	0.60	0/346
7	p	0.38	0/3613	0.52	0/4931
All	All	0.40	0/22545	0.53	0/30639

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	I	0	2
3	L	0	1
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	522	ARG	Sidechain
2	I	201	ARG	Sidechain
2	I	90	ARG	Sidechain
3	L	42	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7438	0	7221	49	0
2	H	1600	0	1579	6	0
2	I	1600	0	1579	9	0
3	L	2400	0	2324	13	0
4	Q	1069	0	1054	11	0
4	R	1069	0	1054	9	0
4	S	1069	0	1054	8	0
4	T	1056	0	1042	9	0
5	d	338	0	351	4	0
5	e	343	0	356	6	0
5	f	336	0	340	8	0
6	k	257	0	247	2	0
7	p	3552	0	3459	21	0
All	All	22127	0	21660	144	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 3.

All (144) 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:A:589:GLY:O	1:A:628:LYS:NZ	2.31	0.64
4:Q:115:ARG:NH1	5:f:36:ILE:O	2.33	0.62
1:A:682:ASP:OD1	1:A:683:ARG:N	2.35	0.60
1:A:687:ASP:OD1	1:A:688:ARG:NE	2.26	0.60
4:T:14:GLU:OE1	4:T:137:GLY:N	2.26	0.60
1:A:562:THR:O	1:A:674:ASN:ND2	2.31	0.59
1:A:486:GLN:NE2	1:A:561:VAL:O	2.31	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:p:229:GLY:O	7:p:230:THR:HG23	2.03	0.58
3:L:263:ARG:HH11	3:L:263:ARG:HG2	1.70	0.57
3:L:267:ARG:NH2	3:L:277:GLU:OE1	2.36	0.56
1:A:403:GLU:OE1	1:A:408:ARG:NH2	2.29	0.56
1:A:220:VAL:HG12	1:A:222:GLU:H	1.70	0.56
7:p:234:ASN:OD1	7:p:260:GLU:HB2	2.06	0.56
1:A:869:ARG:NH1	1:A:874:ASP:OD1	2.38	0.55
7:p:370:ASP:OD1	7:p:371:GLY:N	2.39	0.55
4:T:22:MET:HB3	5:e:12:ILE:HD11	1.90	0.54
1:A:9:ARG:HH11	1:A:9:ARG:HG2	1.72	0.54
3:L:241:GLU:O	3:L:266:LYS:NZ	2.41	0.53
4:T:23:GLN:O	5:e:12:ILE:HD12	2.08	0.53
1:A:93:VAL:HG12	1:A:93:VAL:O	2.10	0.52
1:A:701:GLU:OE1	1:A:703:LYS:N	2.37	0.52
6:k:176:ASN:OD1	6:k:177:SER:N	2.42	0.52
4:Q:15:LYS:HE3	4:Q:139:THR:O	2.09	0.52
1:A:40:TYR:HB3	1:A:55:TYR:CD1	2.46	0.51
2:H:2:ARG:HG2	2:H:2:ARG:HH11	1.75	0.51
1:A:867:TRP:CE2	1:A:902:TYR:HA	2.46	0.51
2:I:2:ARG:NH2	2:I:5:ASP:OD2	2.40	0.51
1:A:17:ARG:NE	2:I:40:GLU:OE2	2.38	0.51
1:A:459:ASN:OD1	1:A:461:ILE:N	2.41	0.51
1:A:514:TRP:CD2	1:A:521:ASN:HB3	2.46	0.50
5:d:27:LYS:N	5:e:27:LYS:O	2.41	0.50
1:A:514:TRP:CG	1:A:521:ASN:HB3	2.46	0.50
4:R:98:LYS:NZ	7:p:344:ASP:OD1	2.38	0.50
1:A:498:ASP:OD1	1:A:499:GLU:N	2.45	0.50
4:R:15:LYS:HE2	4:R:137:GLY:O	2.12	0.50
1:A:552:ILE:HG22	1:A:561:VAL:HG22	1.94	0.49
4:Q:113:MET:SD	4:Q:114:THR:N	2.86	0.49
1:A:333:ILE:HG23	1:A:334:VAL:HG23	1.93	0.49
5:f:39:ILE:HG22	5:f:40:THR:N	2.27	0.49
1:A:710:GLU:O	1:A:711:TYR:CD1	2.66	0.48
4:T:25:MET:N	4:T:25:MET:SD	2.86	0.48
1:A:333:ILE:HG23	1:A:334:VAL:N	2.28	0.48
1:A:131:PHE:CG	1:A:132:ARG:N	2.81	0.48
5:e:8:ILE:CG2	5:e:9:VAL:N	2.77	0.48
1:A:514:TRP:CD2	1:A:521:ASN:CB	2.96	0.48
2:I:136:TYR:HB3	2:I:152:VAL:CG2	2.44	0.48
1:A:42:THR:HG22	1:A:56:GLN:O	2.13	0.47
7:p:21:ASP:C	7:p:21:ASP:OD1	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:901:GLN:CD	1:A:902:TYR:H	2.22	0.47
2:H:201:ARG:NH1	2:H:202:GLU:O	2.41	0.47
4:T:42:THR:O	4:T:115:ARG:NH1	2.43	0.47
7:p:250:ILE:HG23	7:p:251:PRO:HD2	1.95	0.47
5:d:18:THR:OG1	5:d:19:THR:N	2.47	0.47
7:p:244:ILE:N	7:p:249:ASN:OD1	2.40	0.47
7:p:113:HIS:NE2	7:p:120:MET:HE3	2.30	0.47
5:f:17:ASP:OD1	5:f:17:ASP:C	2.58	0.47
7:p:77:LEU:HB3	7:p:199:ILE:HD11	1.97	0.47
1:A:233:LEU:HD12	1:A:601:VAL:HG23	1.96	0.46
7:p:47:VAL:O	7:p:47:VAL:HG13	2.16	0.46
3:L:14:GLU:OE1	3:L:154:ARG:NE	2.48	0.46
4:Q:82:VAL:O	4:Q:86:THR:HG23	2.15	0.46
4:Q:96:ARG:NH2	4:Q:136:ASP:OD2	2.47	0.46
1:A:509:TRP:CH2	1:A:517:PRO:HD3	2.49	0.46
1:A:813:GLU:OE2	1:A:815:ARG:NE	2.40	0.46
1:A:692:LEU:HD12	1:A:711:TYR:CE2	2.51	0.46
1:A:406:ASP:OD1	1:A:406:ASP:C	2.59	0.45
4:R:82:VAL:HA	4:R:85:VAL:HG12	1.98	0.45
1:A:863:VAL:HG22	1:A:906:TYR:HB3	1.98	0.45
1:A:897:ARG:NE	1:A:899:GLU:OE2	2.46	0.45
6:k:176:ASN:OD1	6:k:176:ASN:C	2.59	0.45
4:S:122:VAL:O	4:S:122:VAL:HG13	2.15	0.45
1:A:837:LYS:NZ	1:A:939:ASP:OD2	2.38	0.45
2:I:113:THR:HG21	2:I:148:TRP:CE2	2.52	0.45
4:R:89:GLY:HA2	4:R:134:ILE:HD13	1.99	0.45
1:A:605:LEU:O	1:A:608:LYS:HG2	2.18	0.44
4:R:16:VAL:HG13	4:R:17:PRO:HD2	1.99	0.44
7:p:354:SER:HB3	7:p:357:TYR:CD1	2.53	0.44
4:T:15:LYS:HE2	4:T:140:GLN:HG3	1.99	0.44
1:A:259:LEU:HD12	1:A:259:LEU:N	2.33	0.44
4:R:26:ASP:OD1	4:R:27:VAL:N	2.51	0.44
1:A:869:ARG:NH2	1:A:874:ASP:OD1	2.49	0.44
4:T:25:MET:C	4:T:39:VAL:HG23	2.43	0.44
7:p:4:GLN:N	7:p:4:GLN:OE1	2.49	0.44
4:S:118:ILE:O	4:S:119:GLY:C	2.59	0.44
5:f:19:THR:O	5:f:20:THR:C	2.60	0.44
1:A:221:GLN:OE1	1:A:224:ARG:HD3	2.18	0.43
3:L:268:LEU:C	3:L:268:LEU:HD23	2.43	0.43
1:A:111:ILE:O	1:A:111:ILE:HG23	2.17	0.43
1:A:220:VAL:HG23	1:A:429:GLU:OE1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:897:ARG:NH2	1:A:899:GLU:OE2	2.49	0.43
7:p:159:VAL:O	7:p:159:VAL:HG13	2.18	0.43
4:Q:111:ILE:HD11	4:Q:128:MET:HB3	2.00	0.43
4:Q:40:ASN:OD1	4:Q:40:ASN:C	2.62	0.43
7:p:229:GLY:O	7:p:230:THR:CG2	2.65	0.43
2:H:89:PHE:HB2	2:H:92:ARG:NH2	2.33	0.43
4:T:111:ILE:O	4:T:111:ILE:HG23	2.18	0.43
4:Q:49:THR:HG22	4:Q:50:ILE:N	2.34	0.43
7:p:312:LEU:C	7:p:312:LEU:HD23	2.44	0.42
4:T:23:GLN:O	4:T:25:MET:HE1	2.19	0.42
2:H:155:ASP:OD1	2:H:156:LEU:N	2.50	0.42
5:f:39:ILE:HG22	5:f:40:THR:H	1.85	0.42
2:I:47:TYR:CE2	2:I:201:ARG:NH2	2.87	0.42
3:L:138:LEU:C	3:L:138:LEU:HD23	2.44	0.42
3:L:235:ASP:OD1	3:L:235:ASP:C	2.62	0.42
1:A:87:ASP:OD2	1:A:91:LYS:NZ	2.41	0.42
3:L:128:ASP:OD1	3:L:128:ASP:C	2.63	0.42
5:f:24:LYS:HG2	5:f:26:PRO:CD	2.49	0.42
1:A:134:ARG:HE	1:A:161:GLN:CD	2.28	0.42
1:A:363:ASN:O	1:A:427:ARG:NH2	2.53	0.42
4:Q:45:SER:C	4:Q:46:LEU:HD12	2.45	0.42
3:L:152:THR:HG23	4:R:3:THR:CG2	2.50	0.42
5:d:35:SER:OG	5:f:38:SER:HB3	2.19	0.42
5:e:8:ILE:HG22	5:e:9:VAL:N	2.34	0.42
7:p:77:LEU:HB3	7:p:199:ILE:CG1	2.50	0.42
3:L:244:THR:HG22	3:L:245:ASP:N	2.34	0.42
1:A:779:SER:HB3	1:A:811:ILE:HG12	2.01	0.42
2:H:131:ASN:C	2:H:131:ASN:OD1	2.62	0.41
2:I:47:TYR:CD2	2:I:201:ARG:CZ	3.03	0.41
7:p:269:LEU:HD12	7:p:330:LEU:HB3	2.01	0.41
4:S:16:VAL:HG13	4:S:17:PRO:HD2	2.02	0.41
1:A:160:ASN:OD1	1:A:160:ASN:C	2.62	0.41
2:I:131:ASN:OD1	2:I:131:ASN:C	2.63	0.41
4:S:23:GLN:NE2	4:S:73:GLN:O	2.50	0.41
2:H:132:HIS:CG	2:H:133:PRO:HD2	2.56	0.41
4:S:27:VAL:O	5:d:6:LYS:NZ	2.46	0.41
1:A:121:ASP:O	1:A:125:ASN:N	2.54	0.41
3:L:30:VAL:HG22	3:L:63:ILE:CD1	2.50	0.41
3:L:230:LYS:NZ	3:L:235:ASP:OD1	2.46	0.41
7:p:354:SER:CB	7:p:357:TYR:CD1	3.04	0.41
1:A:333:ILE:CG2	1:A:334:VAL:N	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:178:MET:SD	2:I:201:ARG:HD2	2.61	0.41
4:R:129:GLU:OE1	4:S:102:ARG:NH1	2.54	0.41
4:S:112:LEU:HD12	4:S:112:LEU:O	2.21	0.41
4:S:112:LEU:HD12	4:S:112:LEU:C	2.46	0.41
2:I:60:ASP:OD1	2:I:60:ASP:N	2.53	0.40
4:R:16:VAL:CG1	4:R:17:PRO:HD2	2.51	0.40
5:e:45:THR:HA	5:e:48:VAL:HG22	2.03	0.40
3:L:16:ASP:OD2	3:L:18:ARG:NH1	2.42	0.40
1:A:594:ASN:ND2	1:A:626:LEU:O	2.50	0.40
7:p:447:LYS:NZ	7:p:457:GLU:OE1	2.42	0.40
4:Q:32:TYR:HA	4:Q:33:PRO:C	2.47	0.40
4:Q:44:TYR:CE1	5:f:36:ILE:HD11	2.57	0.40
7:p:184:PHE:CD1	7:p:189:LEU:HD12	2.56	0.40
7:p:185:ASP:OD1	7:p:185:ASP:C	2.64	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	924/949 (97%)	891 (96%)	33 (4%)	0	100	100
2	H	202/204 (99%)	196 (97%)	6 (3%)	0	100	100
2	I	202/204 (99%)	195 (96%)	7 (4%)	0	100	100
3	L	294/300 (98%)	281 (96%)	13 (4%)	0	100	100
4	Q	137/140 (98%)	131 (96%)	6 (4%)	0	100	100
4	R	137/140 (98%)	134 (98%)	3 (2%)	0	100	100
4	S	137/140 (98%)	132 (96%)	5 (4%)	0	100	100
4	T	135/140 (96%)	132 (98%)	3 (2%)	0	100	100
5	d	44/1076 (4%)	42 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	e	45/1076 (4%)	43 (96%)	2 (4%)	0	100	100
5	f	45/1076 (4%)	39 (87%)	6 (13%)	0	100	100
6	k	34/1227 (3%)	34 (100%)	0	0	100	100
7	p	464/468 (99%)	446 (96%)	18 (4%)	0	100	100
All	All	2800/7140 (39%)	2696 (96%)	104 (4%)	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	819/832 (98%)	819 (100%)	0	100	100
2	H	179/179 (100%)	179 (100%)	0	100	100
2	I	179/179 (100%)	178 (99%)	1 (1%)	78	79
3	L	270/274 (98%)	270 (100%)	0	100	100
4	Q	120/121 (99%)	120 (100%)	0	100	100
4	R	120/121 (99%)	120 (100%)	0	100	100
4	S	120/121 (99%)	120 (100%)	0	100	100
4	T	118/121 (98%)	117 (99%)	1 (1%)	73	76
5	d	39/825 (5%)	39 (100%)	0	100	100
5	e	39/825 (5%)	39 (100%)	0	100	100
5	f	38/825 (5%)	38 (100%)	0	100	100
6	k	26/967 (3%)	26 (100%)	0	100	100
7	p	398/400 (100%)	398 (100%)	0	100	100
All	All	2465/5790 (43%)	2463 (100%)	2 (0%)	87	89

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	I	201	ARG
4	T	129	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	A	51	ASN
1	A	157	ASN
1	A	200	GLN
1	A	446	HIS
1	A	481	GLN
1	A	597	GLN
1	A	631	GLN
1	A	639	ASN
1	A	721	GLN
1	A	789	GLN
1	A	800	GLN
2	H	51	ASN
2	H	108	ASN
2	H	151	ASN
2	H	169	ASN
2	I	25	ASN
2	I	51	ASN
3	L	190	GLN
3	L	209	ASN
3	L	219	ASN
4	R	103	GLN
6	k	152	ASN
7	p	20	HIS
7	p	135	HIS
7	p	158	ASN

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 [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.

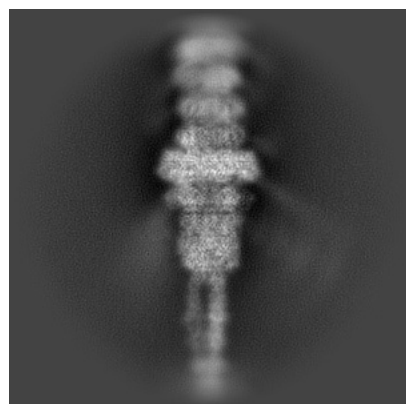
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34955. These allow visual inspection of the internal detail of the map and identification of artifacts.

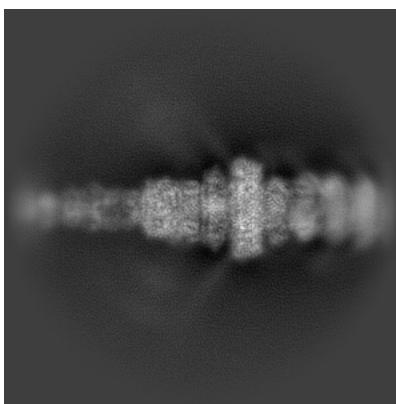
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

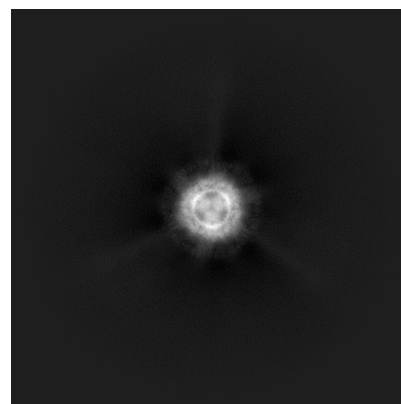
6.1.1 Primary map



X

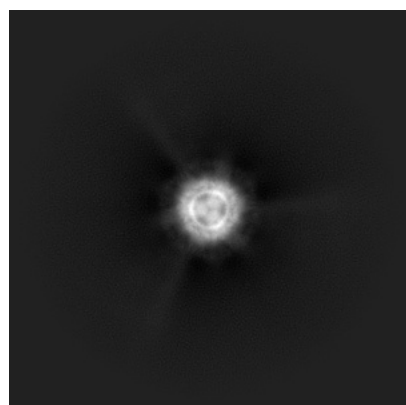


Y

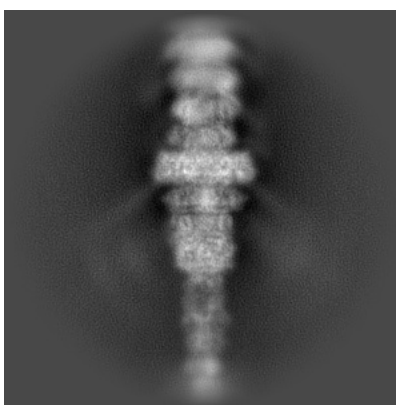


Z

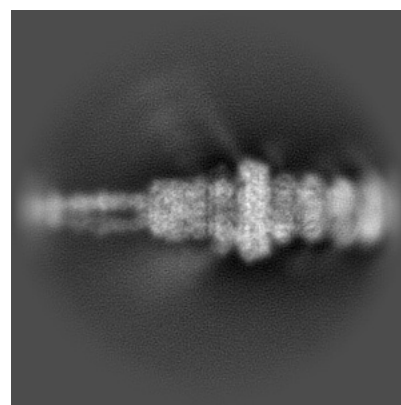
6.1.2 Raw map



X



Y

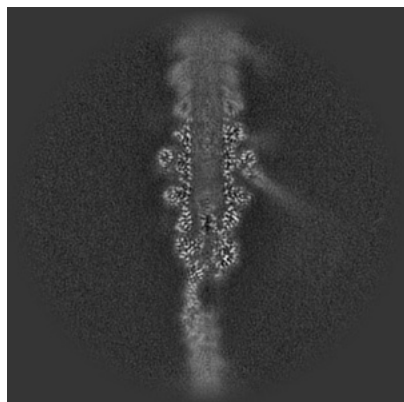


Z

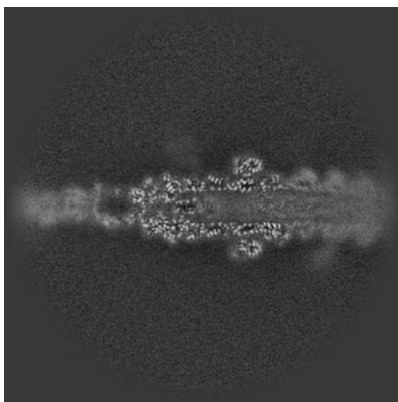
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

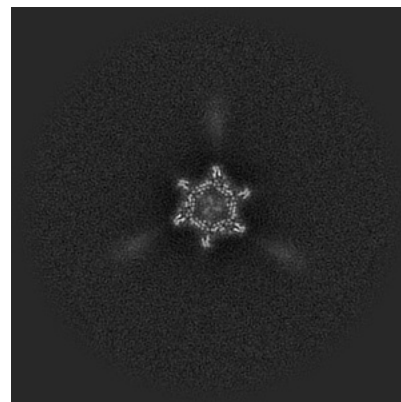
6.2.1 Primary map



X Index: 200

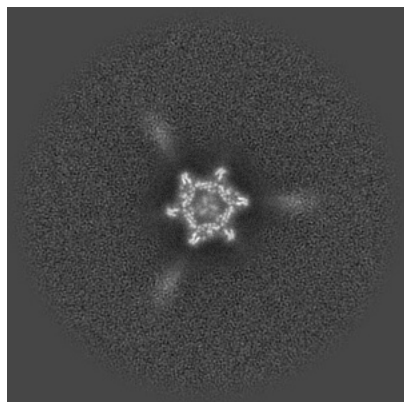


Y Index: 200

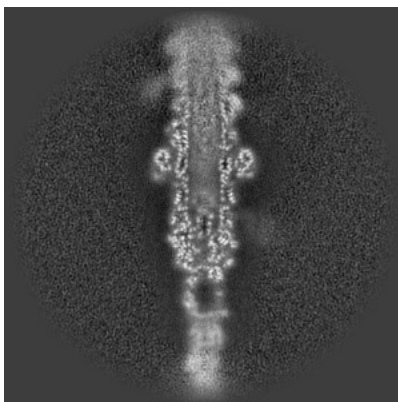


Z Index: 200

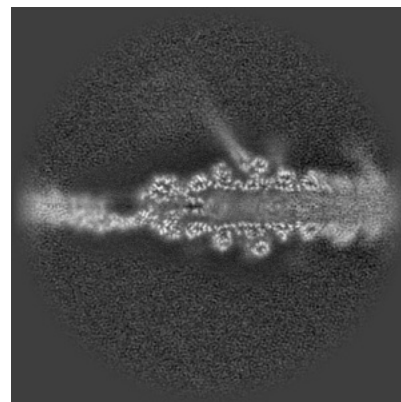
6.2.2 Raw map



X Index: 200



Y Index: 200

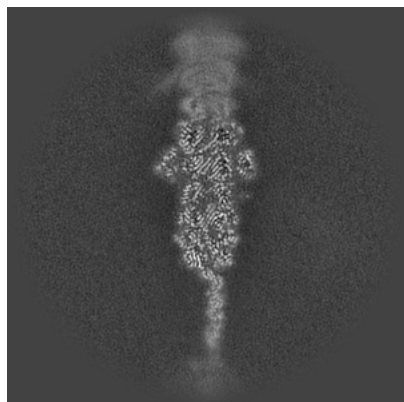


Z Index: 200

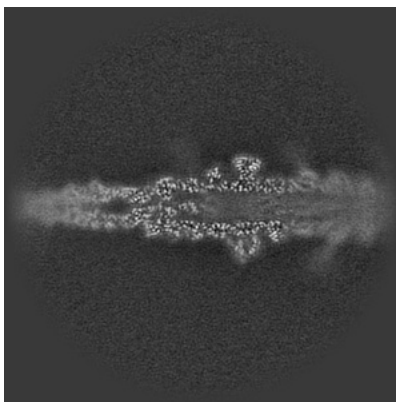
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

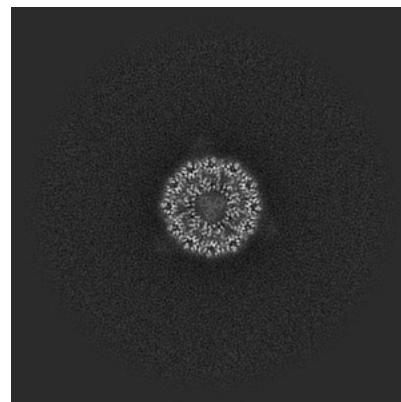
6.3.1 Primary map



X Index: 216

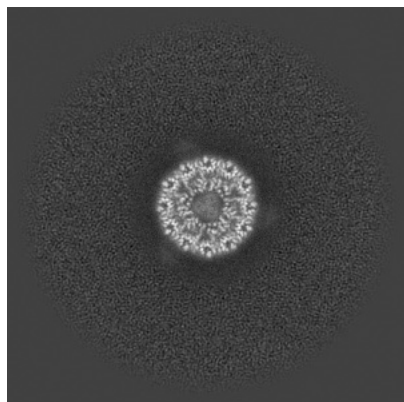


Y Index: 206

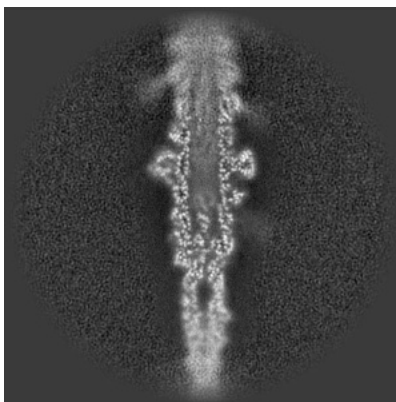


Z Index: 249

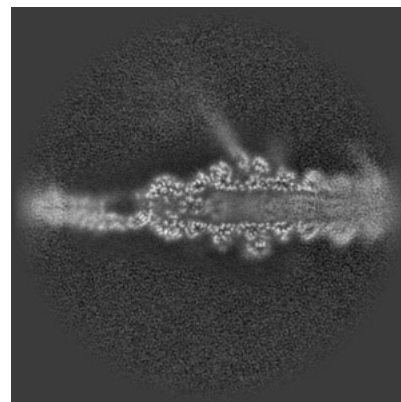
6.3.2 Raw map



X Index: 249



Y Index: 206

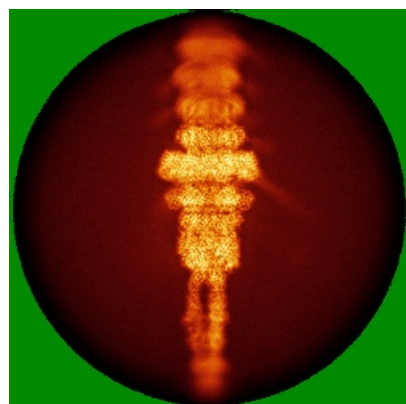


Z Index: 202

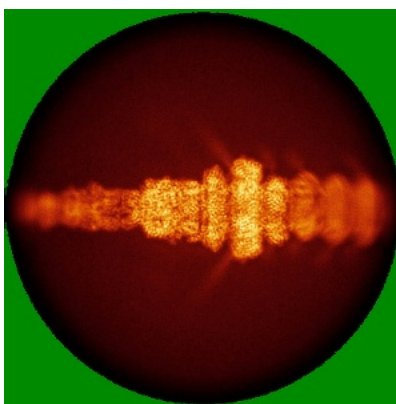
The images above show the largest variance slices of the map in three orthogonal directions.

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

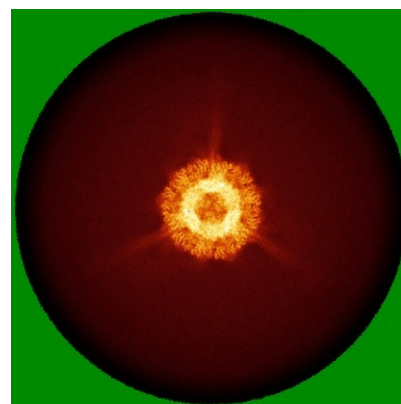
6.4.1 Primary map



X

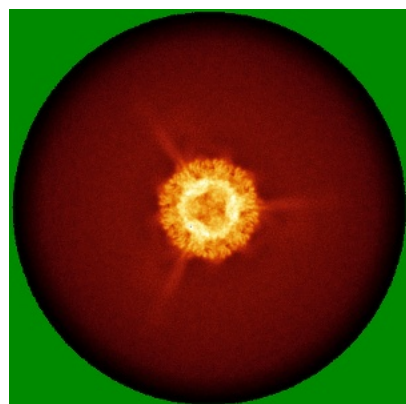


Y

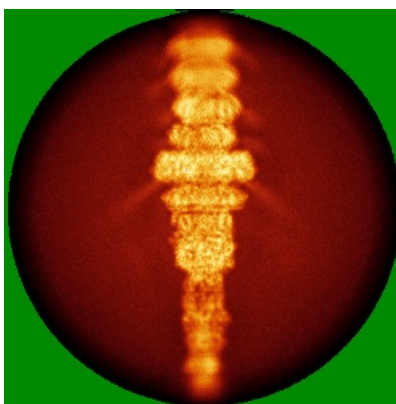


Z

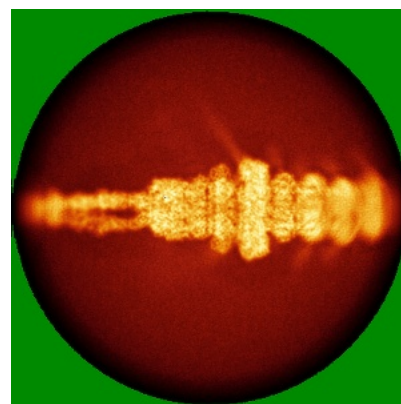
6.4.2 Raw map



X



Y

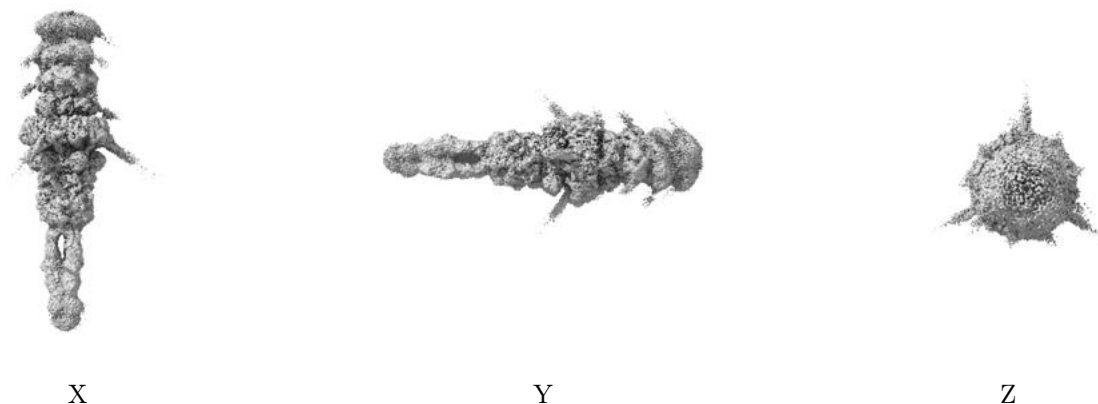


Z

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 4.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.6 Mask visualisation [i](#)

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

A mask typically either:

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

6.6.1 emd_34955_msk_1.map [i](#)



X



Y

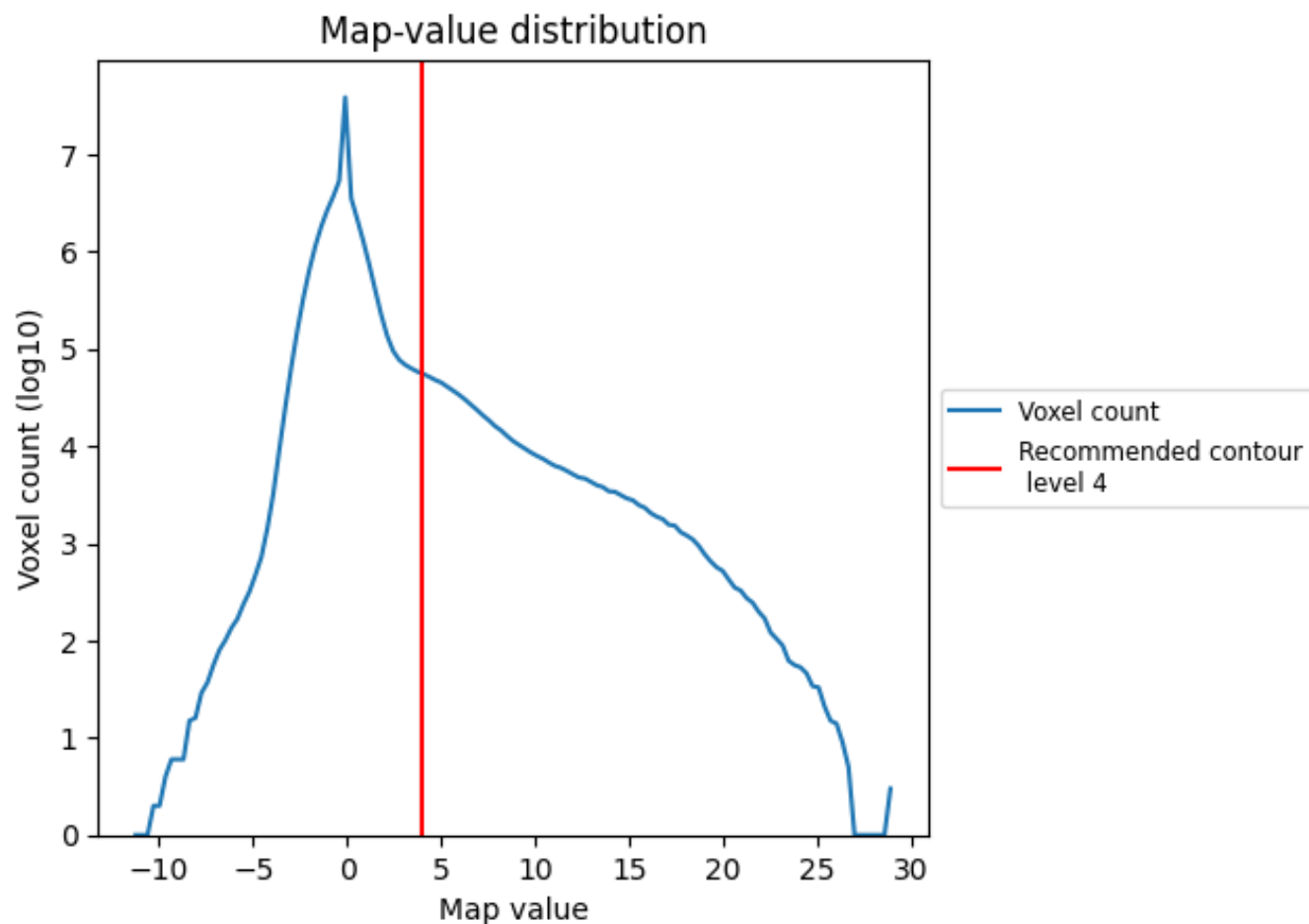


Z

7 Map analysis [i](#)

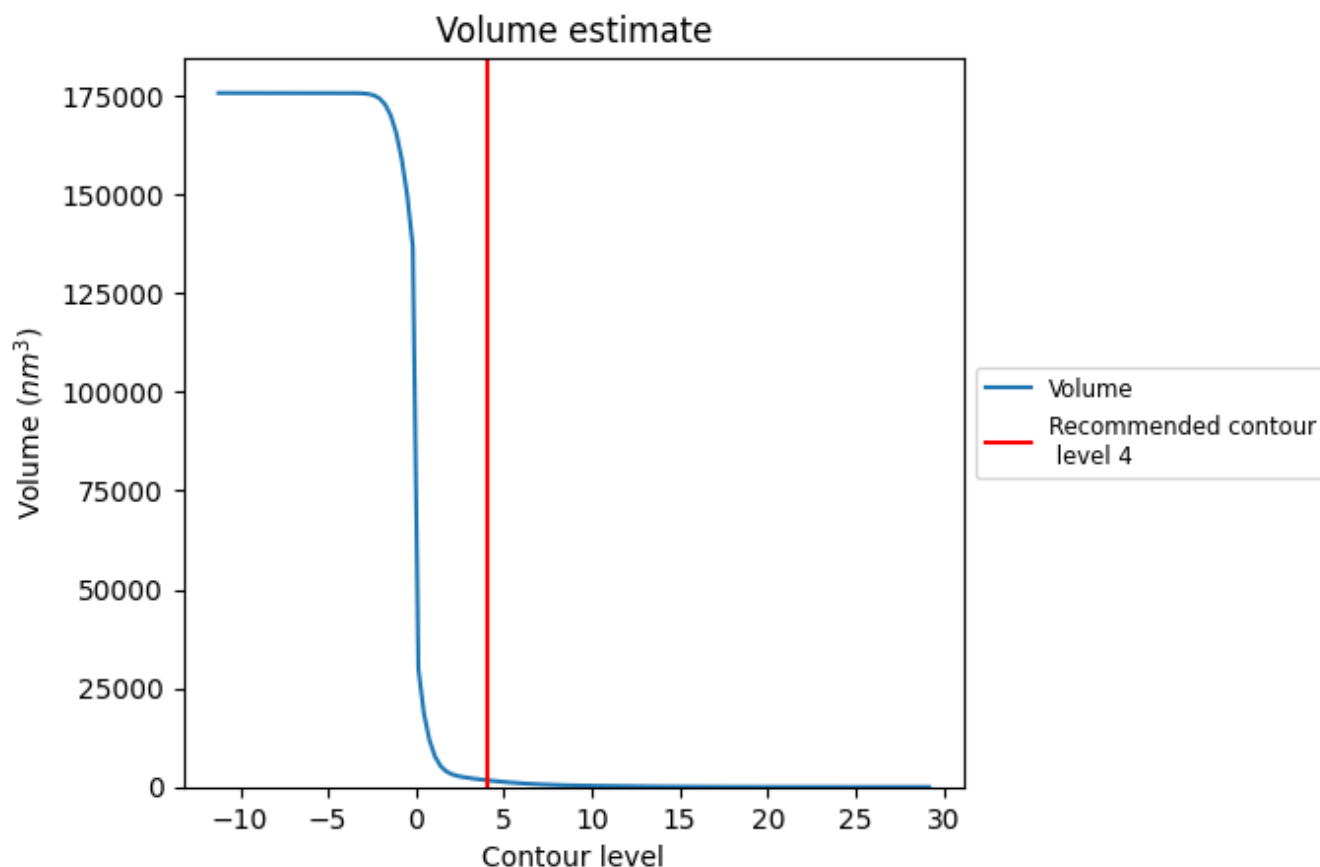
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

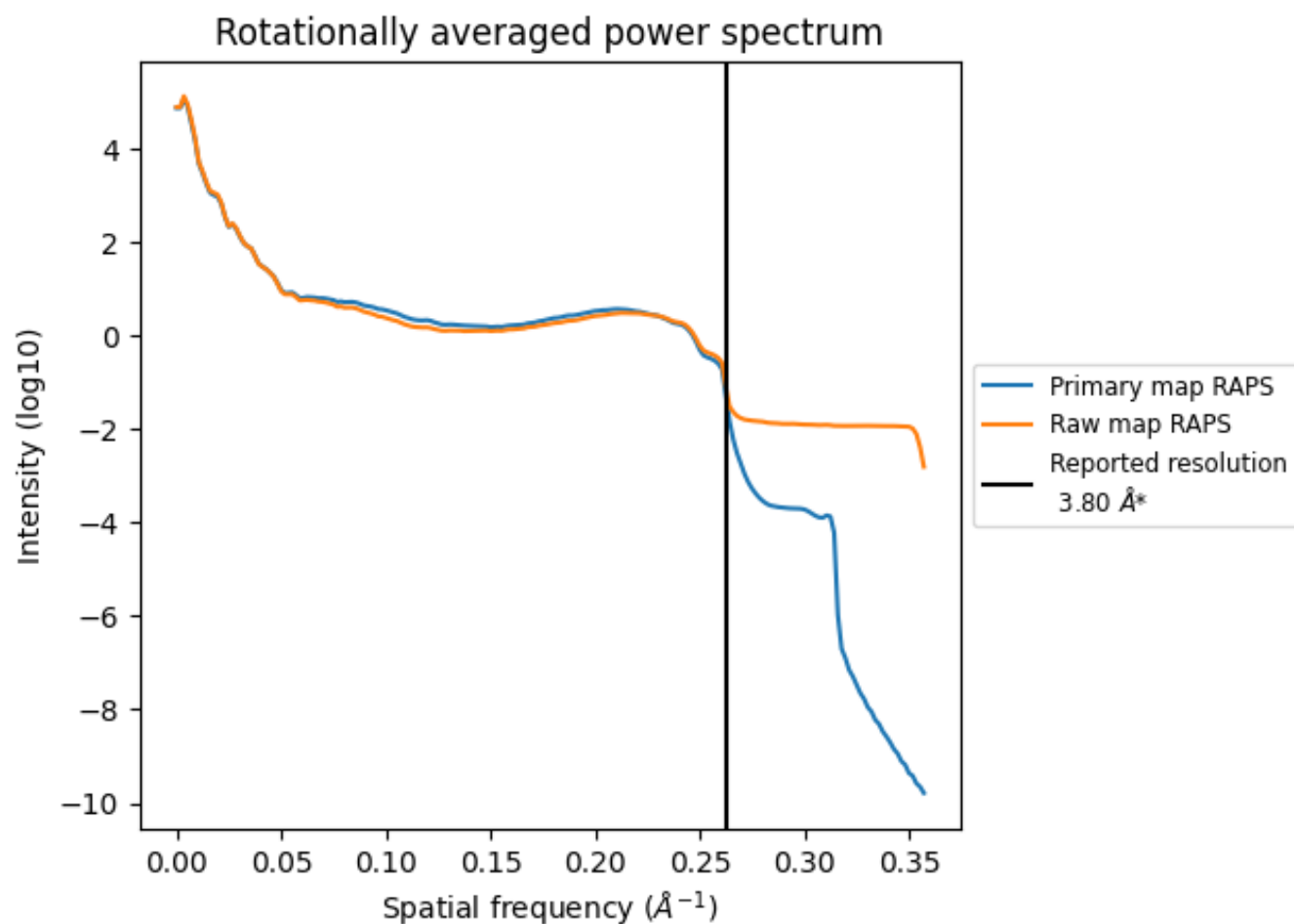
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1719 nm³; this corresponds to an approximate mass of 1552 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 ⓘ

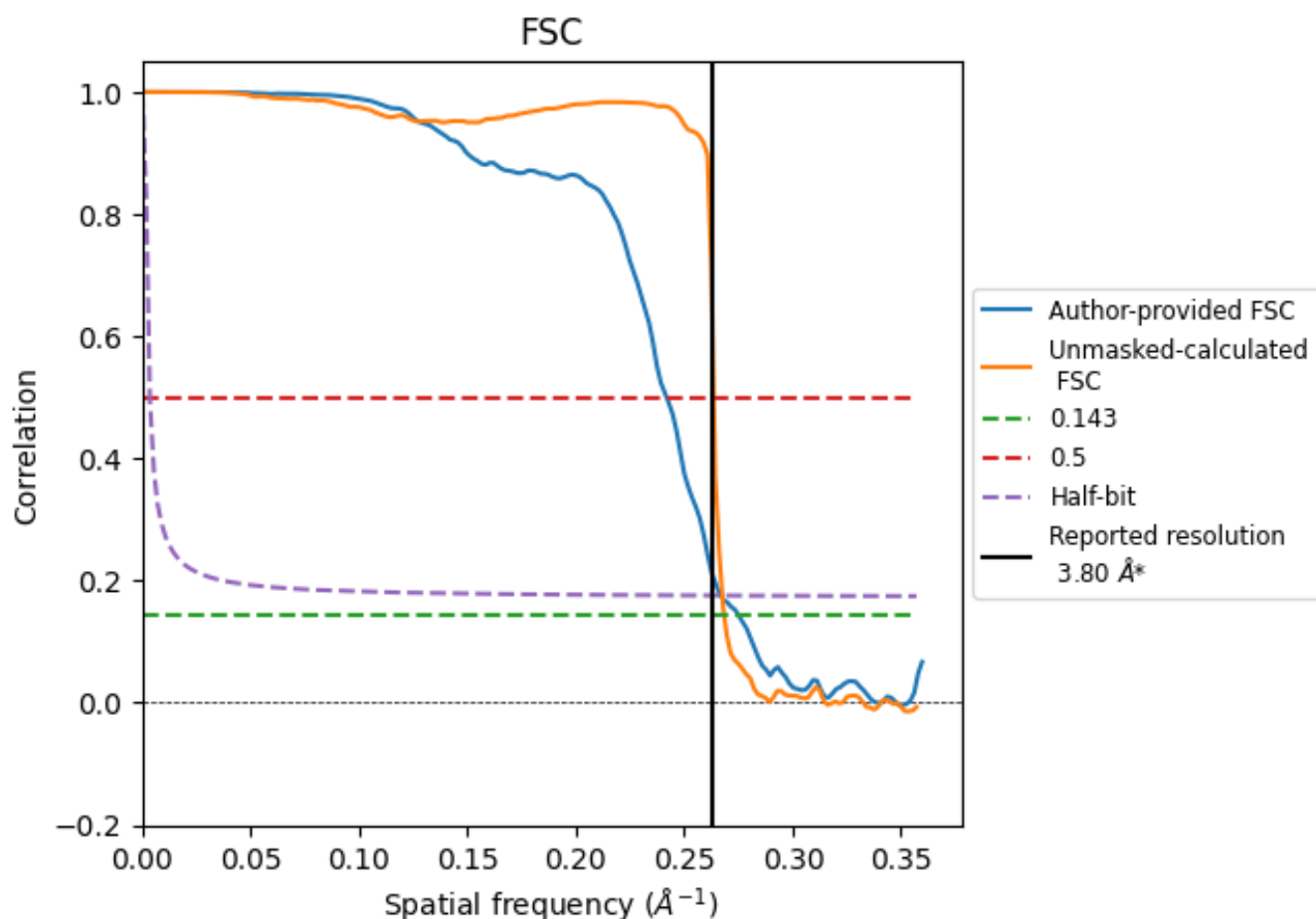


*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.263 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.64	4.14	3.75
Unmasked-calculated*	3.73	3.79	3.74

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-34955 and PDB model 8HQZ. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlays

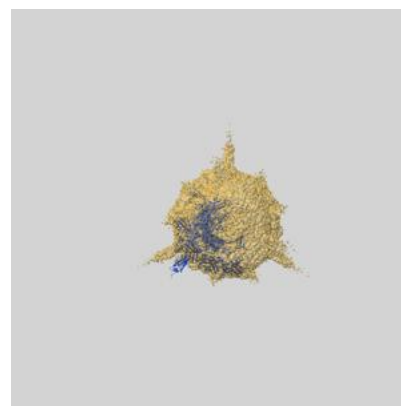
9.1.1 Map-model overlay [i](#)



X

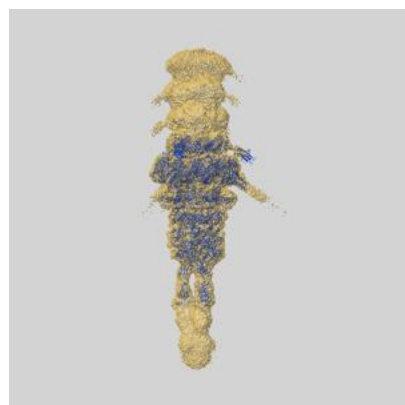


Y



Z

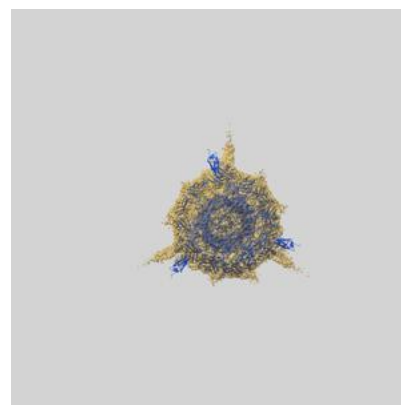
9.1.2 Map-model assembly overlay [i](#)



X



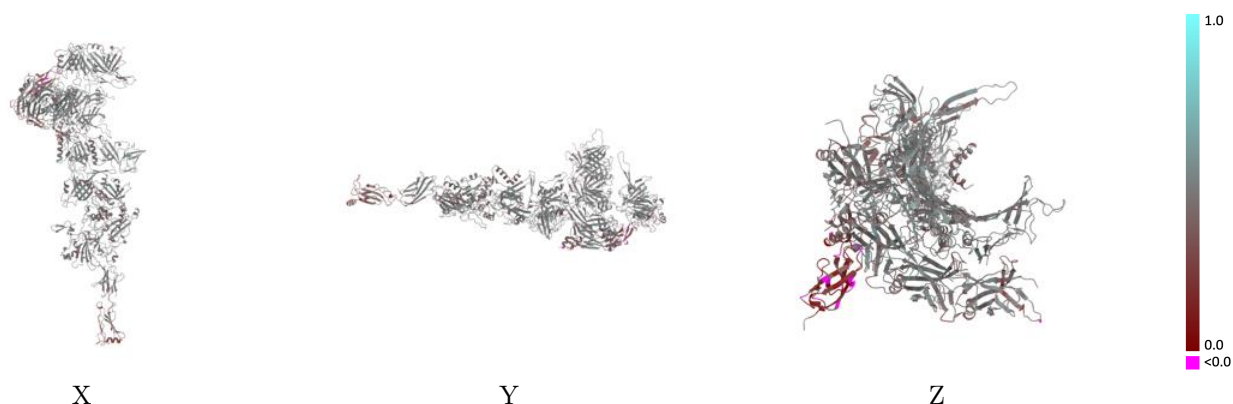
Y



Z

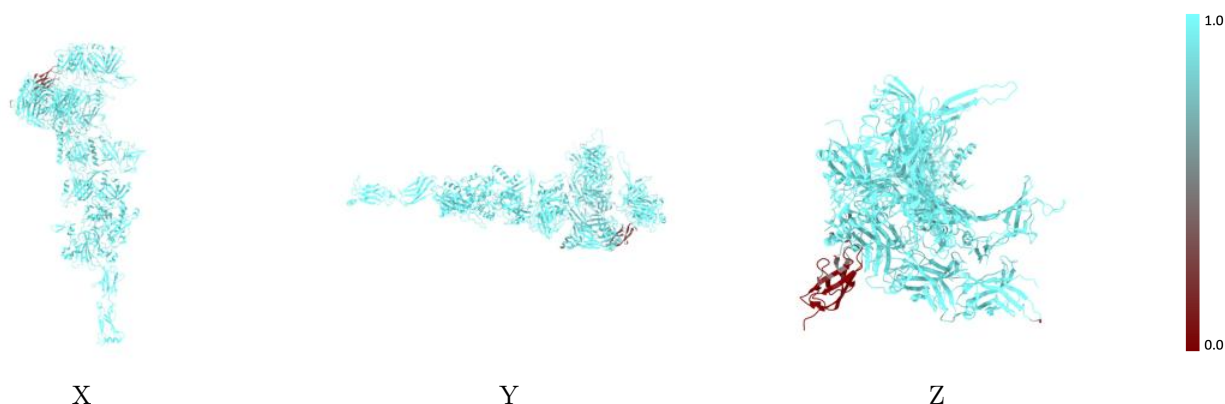
The images above show the 3D surface view of the map at the recommended contour level 4.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



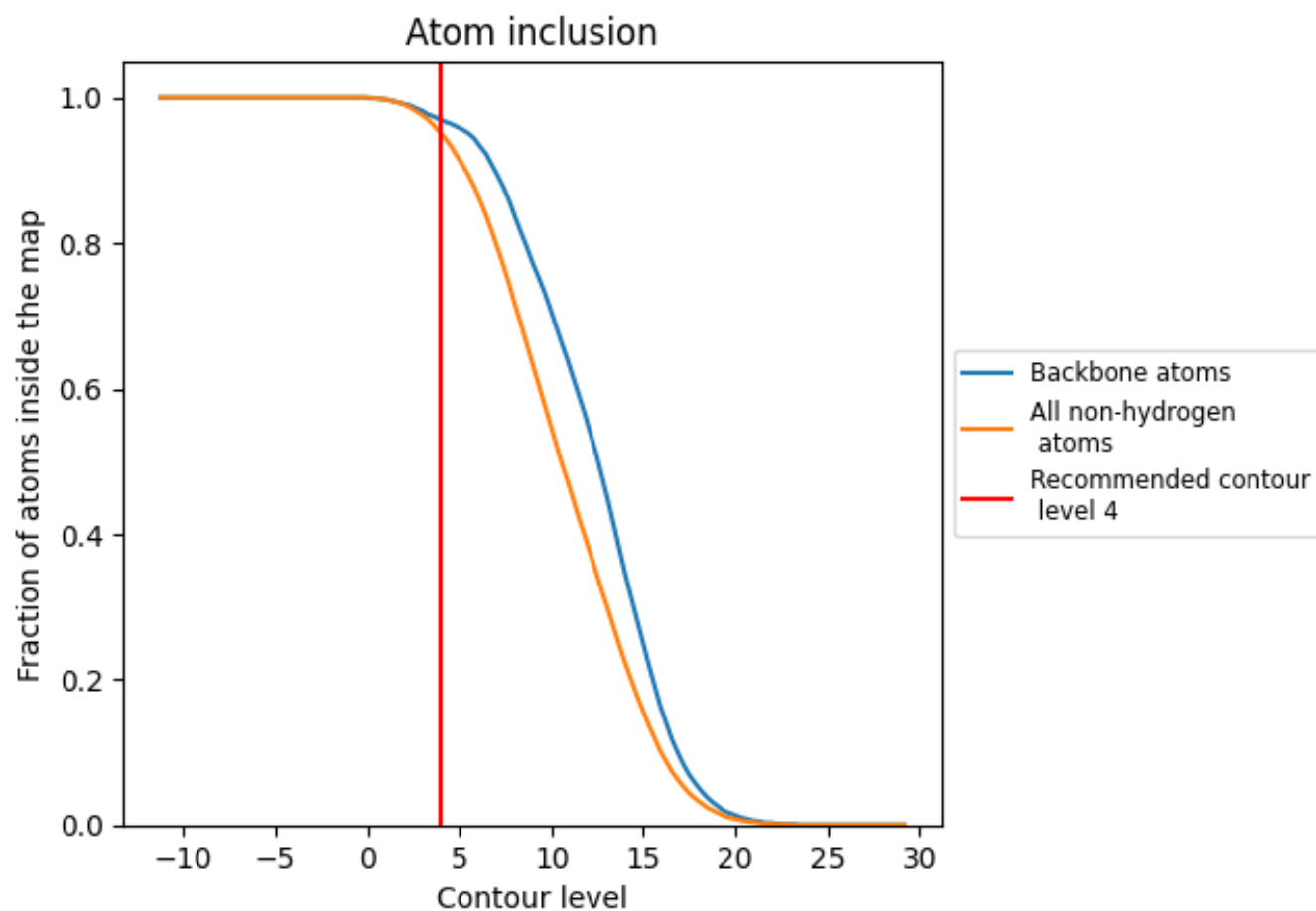
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 95% 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 (4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9510	 0.4460
A	 0.9880	 0.4480
H	 0.9770	 0.4710
I	 0.9760	 0.4730
L	 0.9560	 0.4760
Q	 0.9750	 0.4440
R	 0.9780	 0.4550
S	 0.9650	 0.4430
T	 0.9670	 0.4290
d	 0.9730	 0.4360
e	 0.9530	 0.4060
f	 0.9760	 0.4130
k	 0.9490	 0.4010
p	 0.8210	 0.4120

