



wwPDB EM Validation Summary Report ⓘ

May 20, 2024 – 10:19 AM JST

PDB ID : 8XCG
EMDB ID : EMD-38242
Title : Tail tip complex of bacteriophage lambda in the open state
Authors : Ge, X.F.; Wang, J.W.
Deposited on : 2023-12-09
Resolution : 3.46 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:

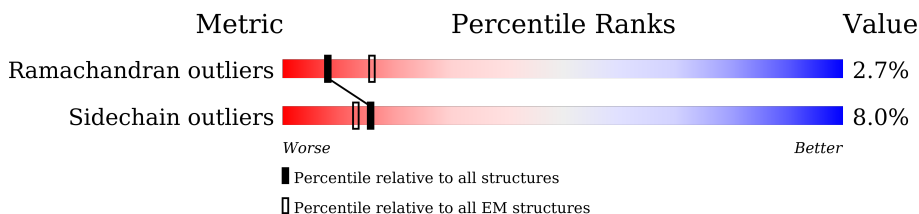
EMDB validation analysis : 0.0.1.dev92
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.46 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	154571	4023
Sidechain outliers	154315	3826

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	E	109	33% (Upper red bar), 94% (Green), 6% (Yellow)
1	K	109	28% (Upper red bar), 94% (Green), 6% (Yellow)
1	M	109	22% (Upper red bar), 96% (Green), . (Yellow)
1	Y	109	35% (Upper red bar), 97% (Green), . (Yellow)
1	e	109	26% (Upper red bar), 93% (Green), 7% (Yellow)
1	m	109	18% (Upper red bar), 94% (Green), 6% (Yellow)
2	F	1132	. (Upper red bar), 45% (Green), 6% (Yellow), 48% (Grey)
2	J	1132	7% (Upper red bar), 47% (Green), 5% (Yellow), 47% (Grey)
2	Z	1132	6% (Upper red bar), 49% (Green), . (Yellow), 47% (Grey)

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Mol	Chain	Length	Quality of chain
3	I	223	<p>6% 21% 75%</p>
3	P	223	<p>7% 22% 74%</p>
3	h	223	<p>7% 21% 74%</p>
4	L	232	<p>6% 91% 8%</p>
4	N	232	<p>5% 91% 9%</p>
4	f	232	<p>6% 90% 9%</p>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 25941 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 Tail tip protein M.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	E	109	884	569	154	157	4	0	0
1	K	109	884	569	154	157	4	0	0
1	M	109	884	569	154	157	4	0	0
1	Y	109	884	569	154	157	4	0	0
1	e	109	884	569	154	157	4	0	0
1	m	109	884	569	154	157	4	0	0

- Molecule 2 is a protein called Tip attachment protein J.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	F	594	4627	2884	815	909	19	0	0
2	J	598	4657	2903	819	916	19	0	0
2	Z	597	4650	2899	818	914	19	0	0

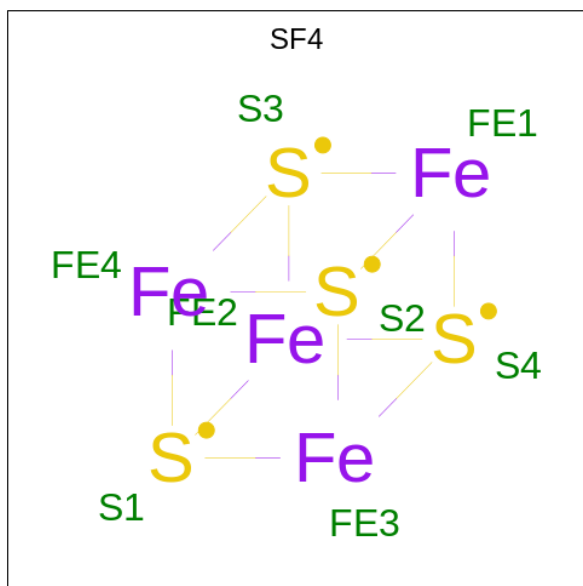
- Molecule 3 is a protein called Tail tip assembly protein I.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	I	56	412	251	71	88	2	0	0
3	P	59	436	266	75	93	2	0	0
3	h	58	428	260	74	92	2	0	0

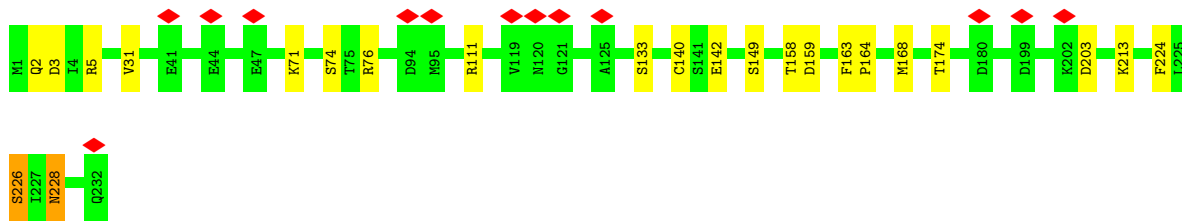
- Molecule 4 is a protein called Tail tip protein L.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	L	232	Total 1801	C 1117	N 309	O 362	S 13	0	0
4	N	232	Total 1801	C 1117	N 309	O 362	S 13	0	0
4	f	232	Total 1801	C 1117	N 309	O 362	S 13	0	0

- Molecule 5 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
5	L	1	Total 8	Fe 4	S 4	0
5	N	1	Total 8	Fe 4	S 4	0
5	f	1	Total 8	Fe 4	S 4	0



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	358235	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.933	Depositor
Minimum map value	-1.412	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.067	Depositor
Recommended contour level	0.4	Depositor
Map size (\AA)	343.74402, 343.74402, 343.74402	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.0742, 1.0742, 1.0742	Depositor

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: SF4

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	E	0.71	0/909	0.81	0/1231
1	K	0.71	0/909	0.79	0/1231
1	M	0.69	0/909	0.80	0/1231
1	Y	0.70	0/909	0.77	0/1231
1	e	0.70	0/909	0.78	0/1231
1	m	0.69	0/909	0.83	0/1231
2	F	0.77	1/4722 (0.0%)	1.05	5/6430 (0.1%)
2	J	0.74	0/4753	0.97	4/6473 (0.1%)
2	Z	0.70	0/4746	0.89	1/6462 (0.0%)
3	I	0.83	0/415	1.08	0/561
3	P	0.86	0/439	1.05	0/594
3	h	0.76	0/431	0.94	0/583
4	L	0.74	0/1836	0.96	3/2487 (0.1%)
4	N	0.74	0/1836	0.95	3/2487 (0.1%)
4	f	0.70	0/1836	0.84	0/2487
All	All	0.73	1/26468 (0.0%)	0.93	16/35950 (0.0%)

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
2	F	0	5
2	J	0	3
2	Z	0	2
3	I	0	2
3	P	0	1
4	L	0	1
4	f	0	3
All	All	0	17

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	31	SER	CA-CB	-6.42	1.43	1.52

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	177	PHE	CB-CA-C	-11.60	87.21	110.40
4	L	166	ARG	NE-CZ-NH1	9.62	125.11	120.30
2	F	348	CYS	CB-CA-C	-7.38	95.63	110.40
4	N	163	PHE	N-CA-CB	6.87	122.97	110.60
4	L	166	ARG	NE-CZ-NH2	-6.54	117.03	120.30

There are no chirality outliers.

5 of 17 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	F	174	PRO	Peptide
2	F	175	ARG	Peptide
2	F	176	PRO	Peptide
2	F	31	SER	Peptide
2	F	348	CYS	Peptide

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	E	107/109 (98%)	87 (81%)	19 (18%)	1 (1%)	17 54
1	K	107/109 (98%)	90 (84%)	16 (15%)	1 (1%)	17 54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	M	107/109 (98%)	88 (82%)	17 (16%)	2 (2%)	8	38
1	Y	107/109 (98%)	91 (85%)	15 (14%)	1 (1%)	17	54
1	e	107/109 (98%)	94 (88%)	12 (11%)	1 (1%)	17	54
1	m	107/109 (98%)	94 (88%)	12 (11%)	1 (1%)	17	54
2	F	592/1132 (52%)	489 (83%)	81 (14%)	22 (4%)	3	25
2	J	596/1132 (53%)	495 (83%)	87 (15%)	14 (2%)	6	34
2	Z	595/1132 (53%)	501 (84%)	80 (13%)	14 (2%)	6	34
3	I	54/223 (24%)	39 (72%)	12 (22%)	3 (6%)	2	15
3	P	57/223 (26%)	37 (65%)	12 (21%)	8 (14%)	0	3
3	h	56/223 (25%)	43 (77%)	8 (14%)	5 (9%)	1	7
4	L	230/232 (99%)	202 (88%)	23 (10%)	5 (2%)	6	35
4	N	230/232 (99%)	198 (86%)	26 (11%)	6 (3%)	5	32
4	f	230/232 (99%)	200 (87%)	25 (11%)	5 (2%)	6	35
All	All	3282/5415 (61%)	2748 (84%)	445 (14%)	89 (3%)	8	31

5 of 89 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	159	THR
2	F	213	PRO
2	F	231	GLN
2	F	294	ALA
2	F	326	ASN

5.3.2 Protein sidechains [i](#)

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	E	96/96 (100%)	90 (94%)	6 (6%)	18	50
1	K	96/96 (100%)	90 (94%)	6 (6%)	18	50
1	M	96/96 (100%)	94 (98%)	2 (2%)	53	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	Y	96/96 (100%)	94 (98%)	2 (2%)	53 78
1	e	96/96 (100%)	89 (93%)	7 (7%)	14 45
1	m	96/96 (100%)	91 (95%)	5 (5%)	23 55
2	F	514/958 (54%)	457 (89%)	57 (11%)	6 26
2	J	517/958 (54%)	471 (91%)	46 (9%)	9 36
2	Z	516/958 (54%)	483 (94%)	33 (6%)	17 49
3	I	46/162 (28%)	40 (87%)	6 (13%)	4 20
3	P	49/162 (30%)	46 (94%)	3 (6%)	18 51
3	h	48/162 (30%)	39 (81%)	9 (19%)	1 7
4	L	198/198 (100%)	183 (92%)	15 (8%)	13 42
4	N	198/198 (100%)	184 (93%)	14 (7%)	14 46
4	f	198/198 (100%)	181 (91%)	17 (9%)	10 37
All	All	2860/4530 (63%)	2632 (92%)	228 (8%)	16 40

5 of 228 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	1	MET
3	h	214	ASP
4	N	133	SER
3	h	197	ARG
4	f	31	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
3	P	185	GLN
4	f	6	GLN
1	m	65	HIS
4	f	232	GLN
2	Z	270	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	SF4	f	301	4	0,12,12	-	-	-		
5	SF4	N	301	4	0,12,12	-	-	-		
5	SF4	L	301	4	0,12,12	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	SF4	f	301	4	-	-	0/6/5/5
5	SF4	N	301	4	-	-	0/6/5/5
5	SF4	L	301	4	-	-	0/6/5/5

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 [i](#)

There are no chain breaks in this entry.

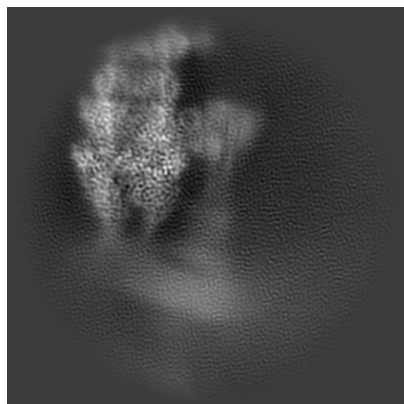
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38242. These allow visual inspection of the internal detail of the map and identification of artifacts.

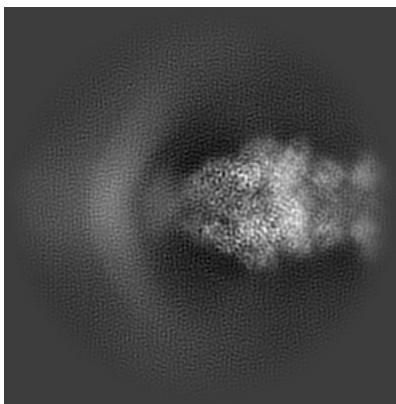
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

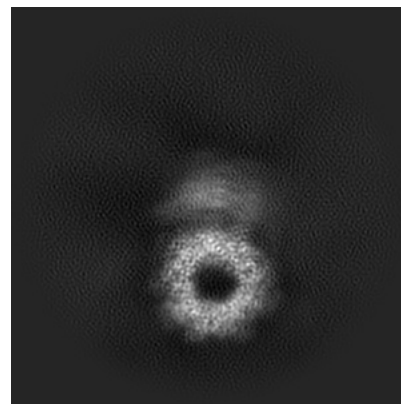
6.1.1 Primary map



X

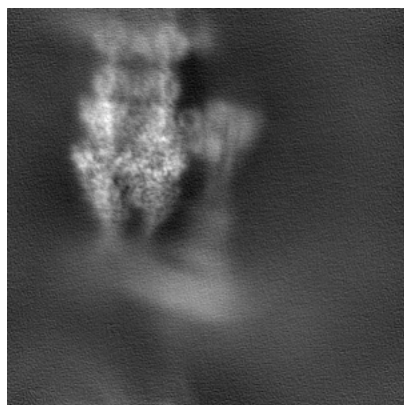


Y

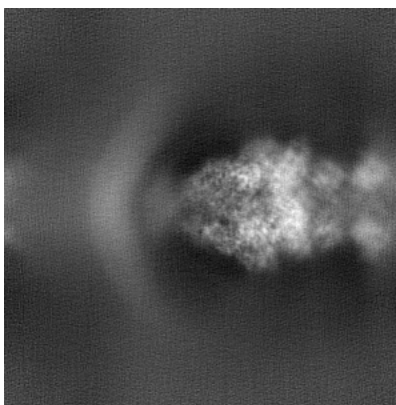


Z

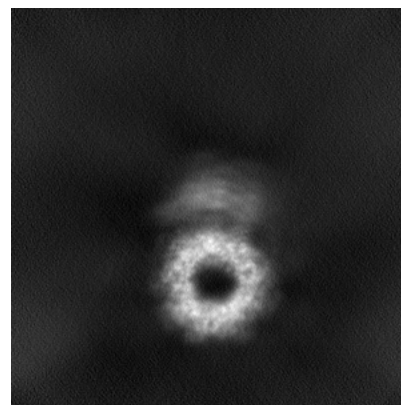
6.1.2 Raw map



X



Y

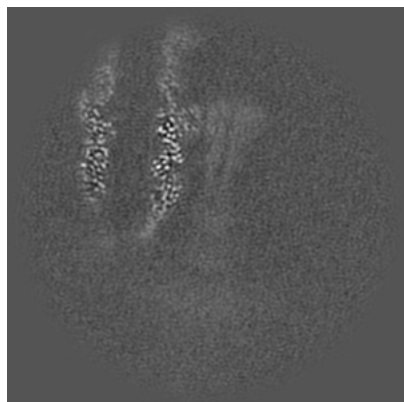


Z

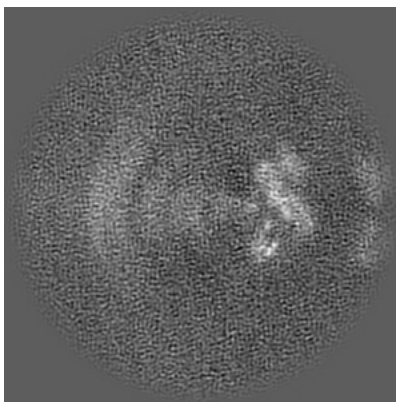
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

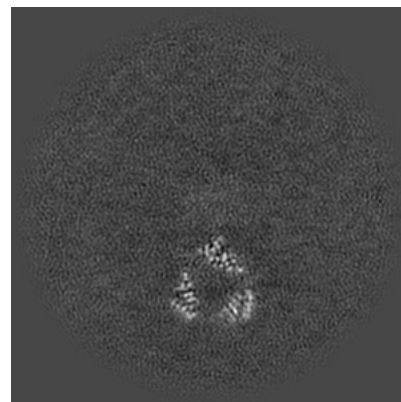
6.2.1 Primary map



X Index: 160

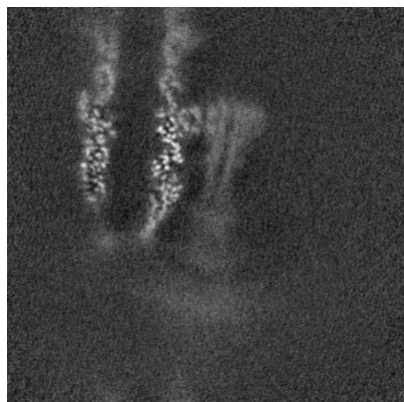


Y Index: 160

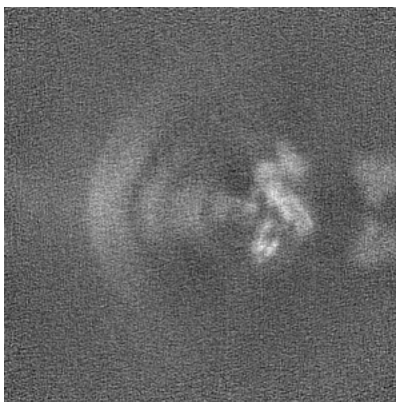


Z Index: 160

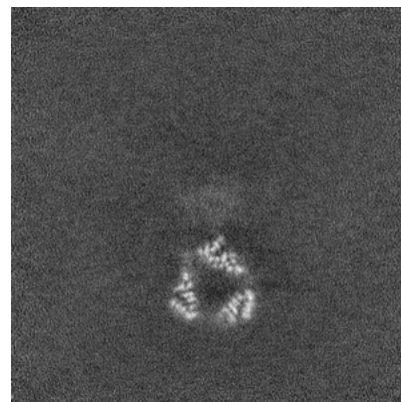
6.2.2 Raw map



X Index: 160



Y Index: 160

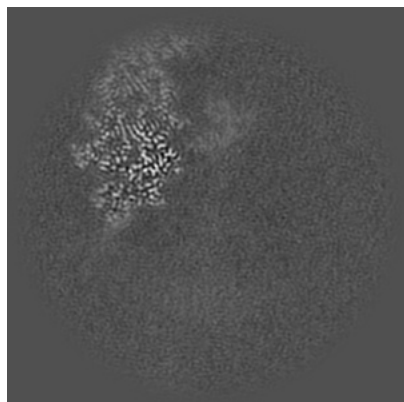


Z Index: 160

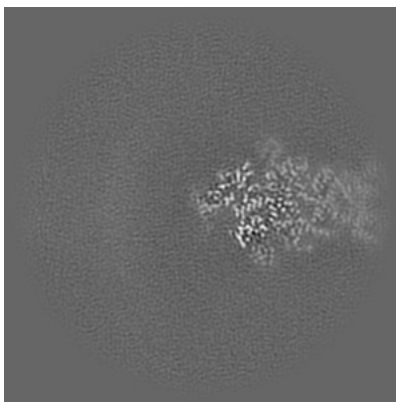
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

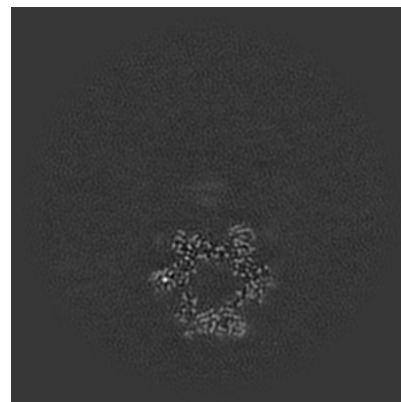
6.3.1 Primary map



X Index: 141

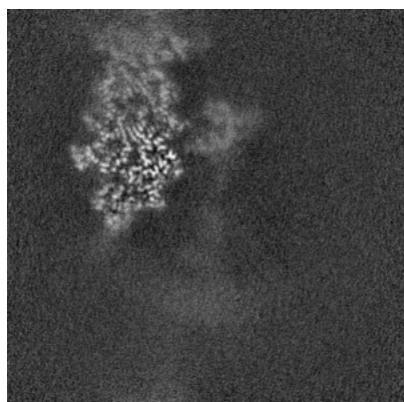


Y Index: 126

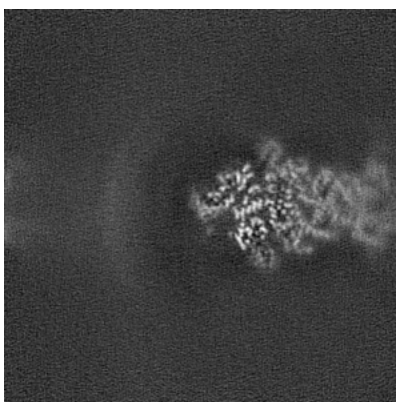


Z Index: 193

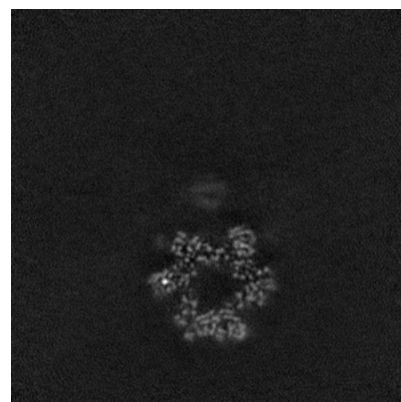
6.3.2 Raw map



X Index: 141



Y Index: 126

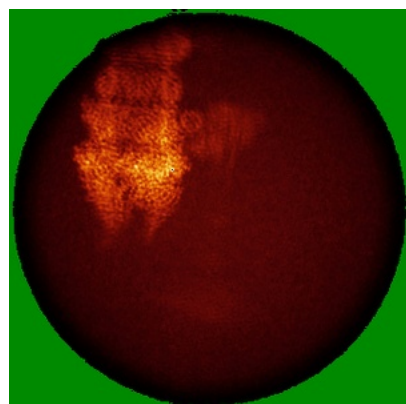


Z Index: 193

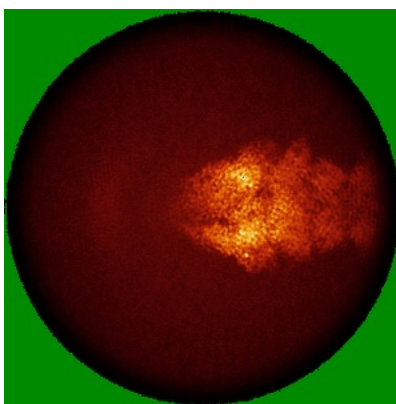
The images above show the largest variance slices of the map in three orthogonal directions.

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

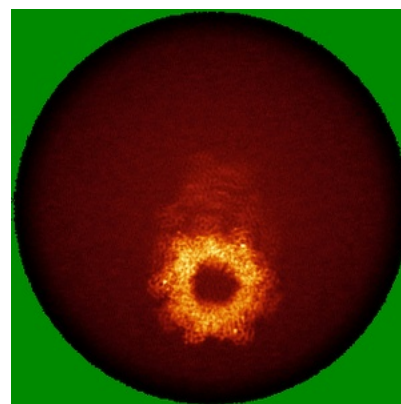
6.4.1 Primary map



X

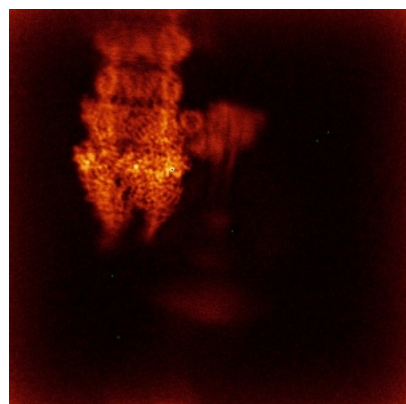


Y

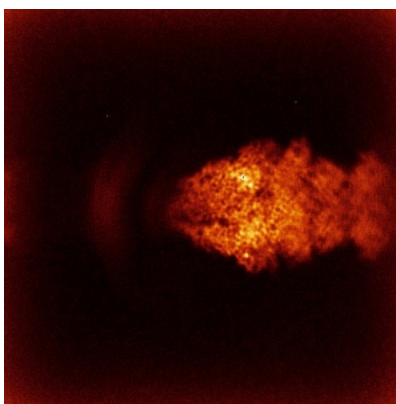


Z

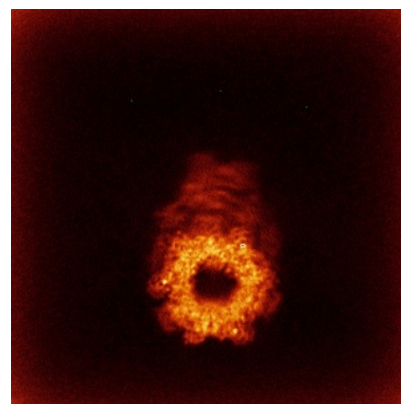
6.4.2 Raw map



X



Y

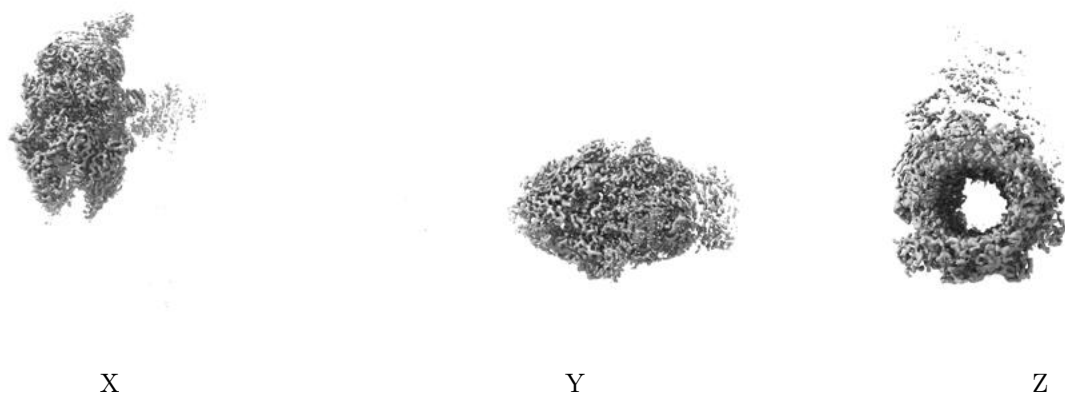


Z

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.

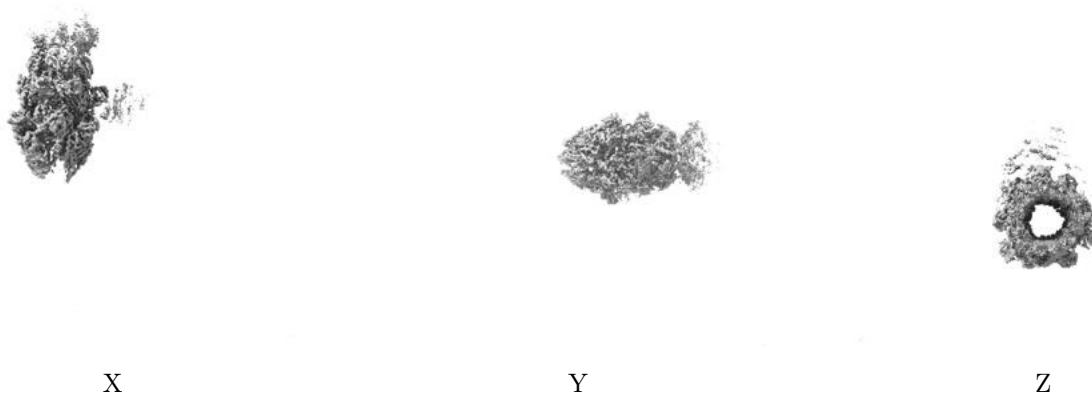
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.4. 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.

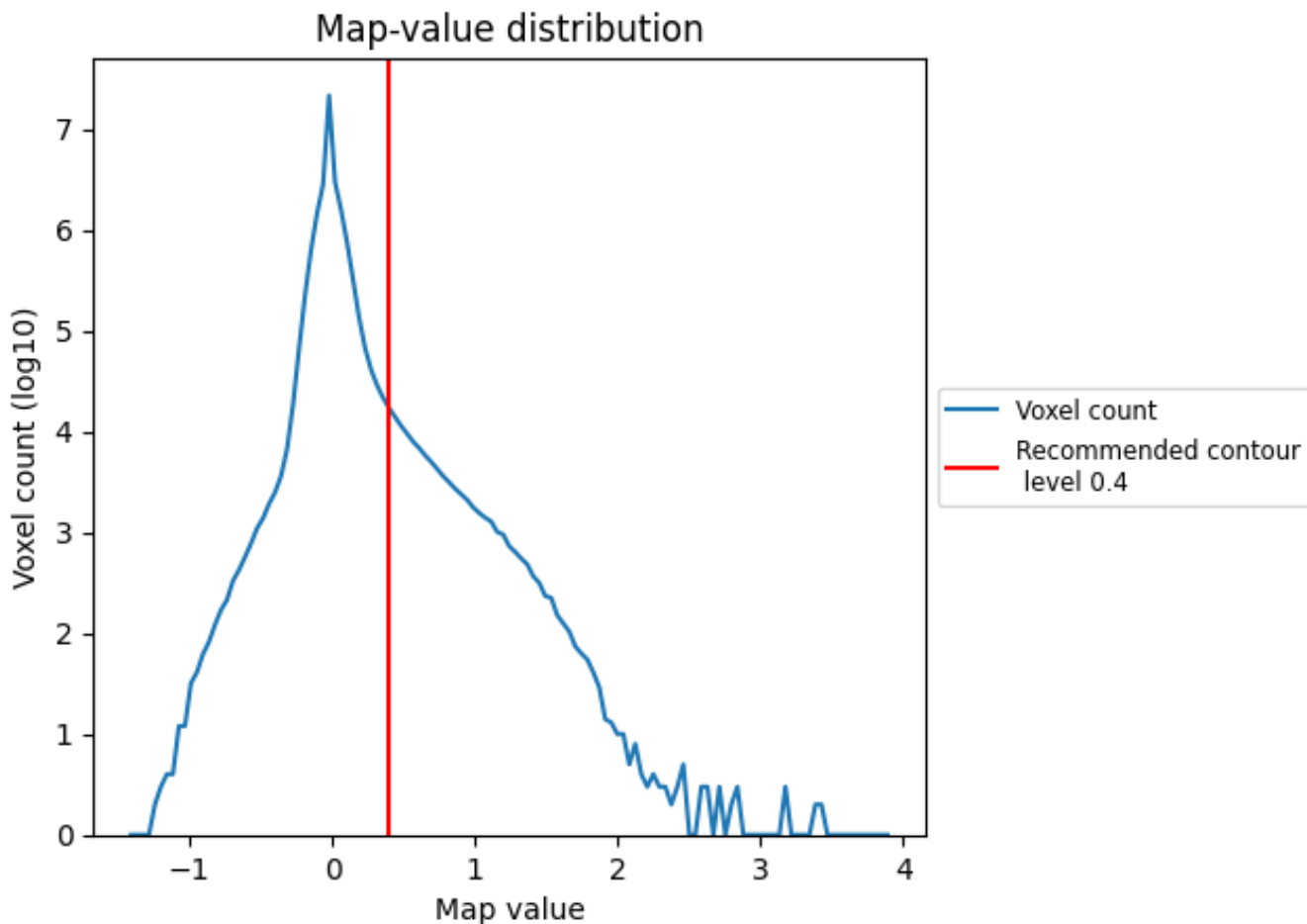
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

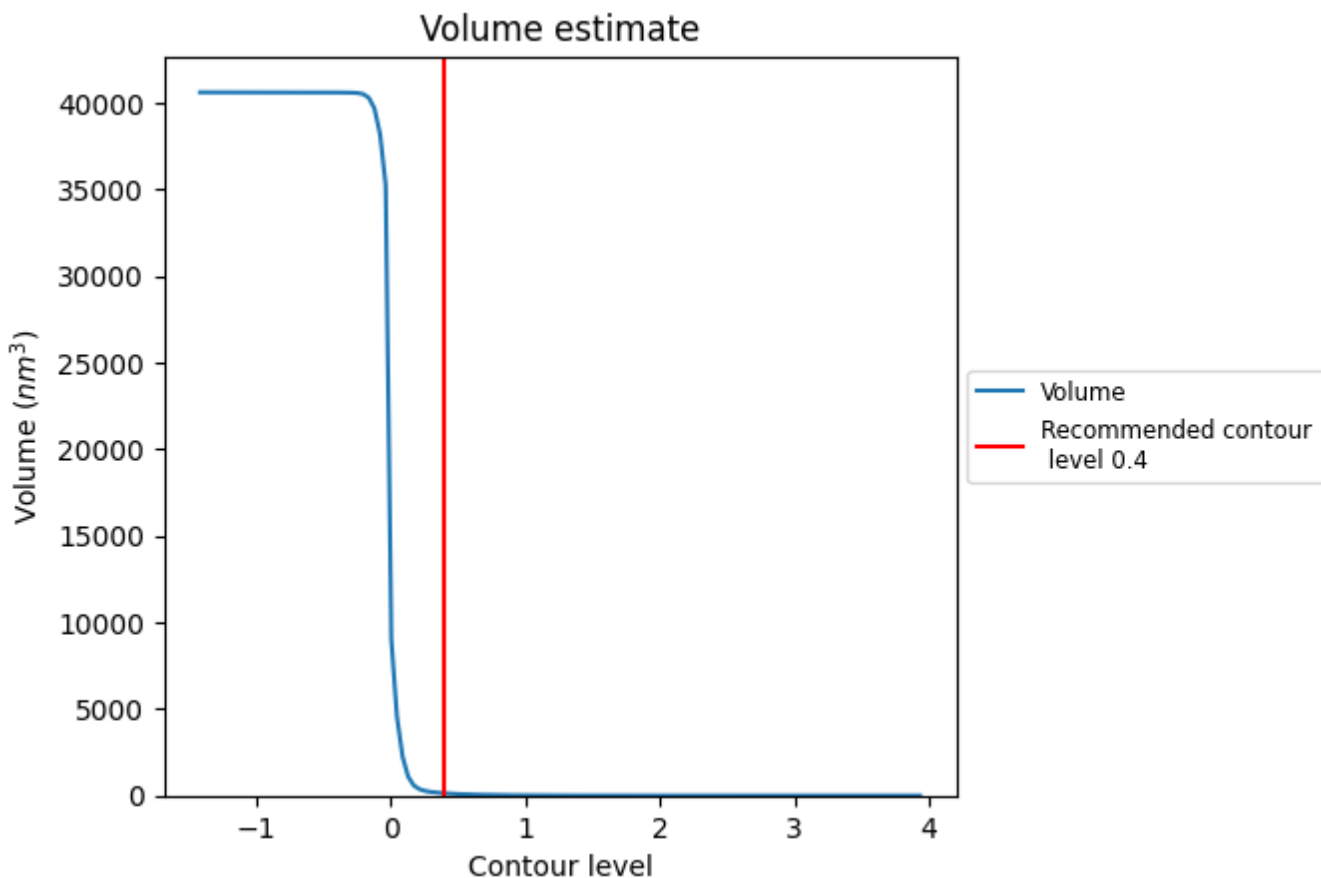
This section contains the results of statistical analysis of the map.

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.

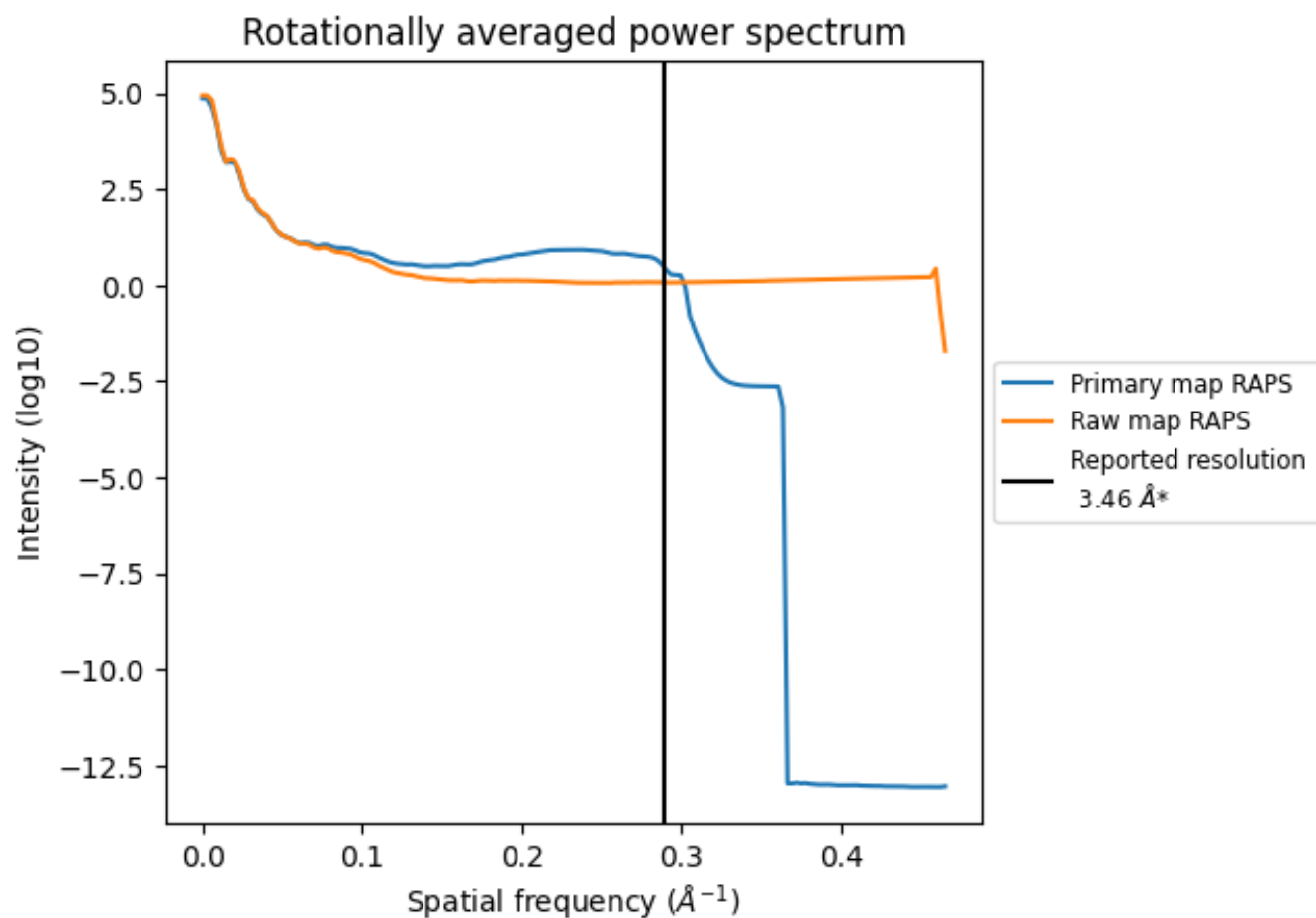
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 133 nm^3 ; this corresponds to an approximate mass of 120 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 [i](#)

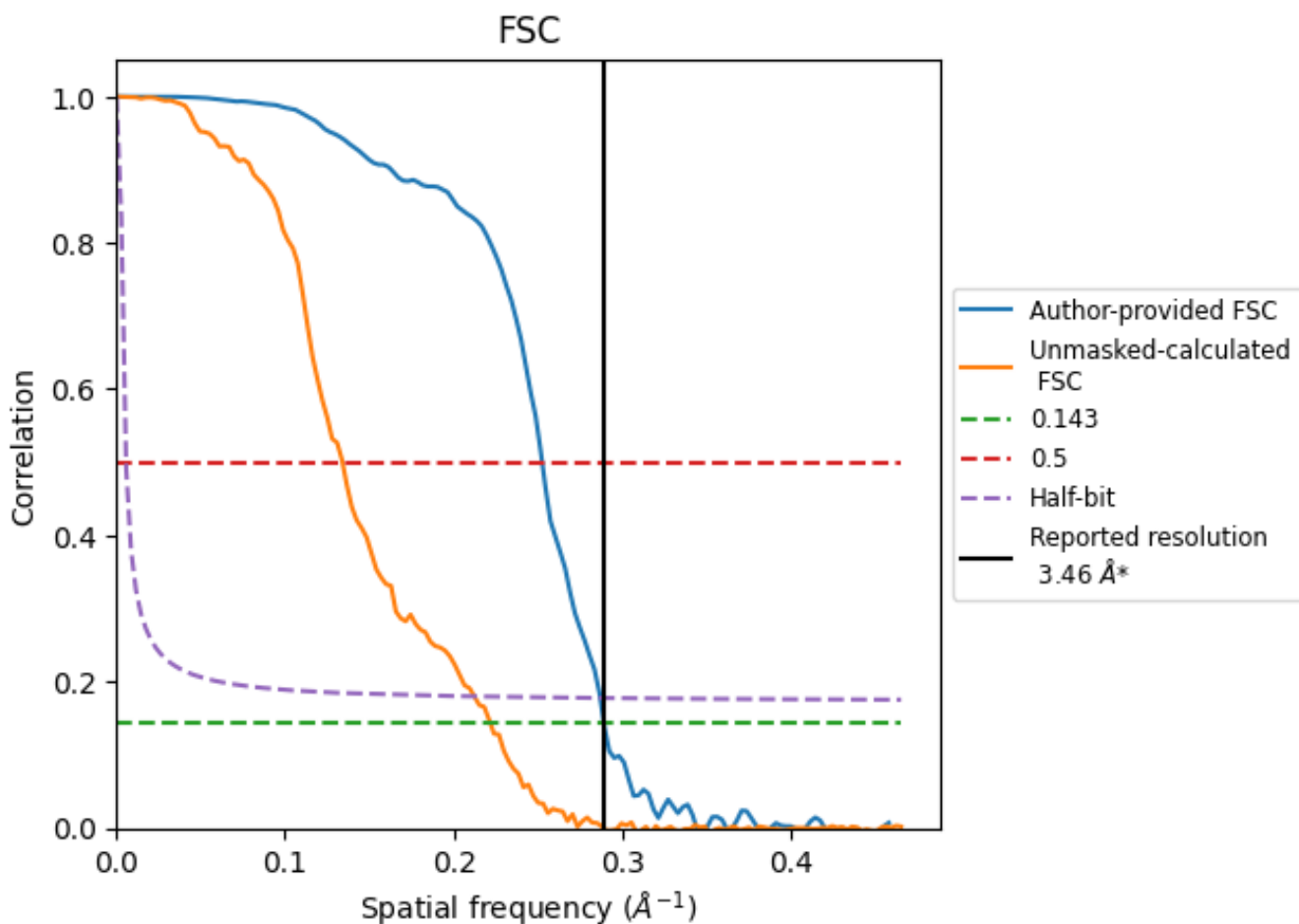


*Reported resolution corresponds to spatial frequency of 0.289 Å⁻¹

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 0.289 Å⁻¹

8.2 Resolution estimates [i](#)

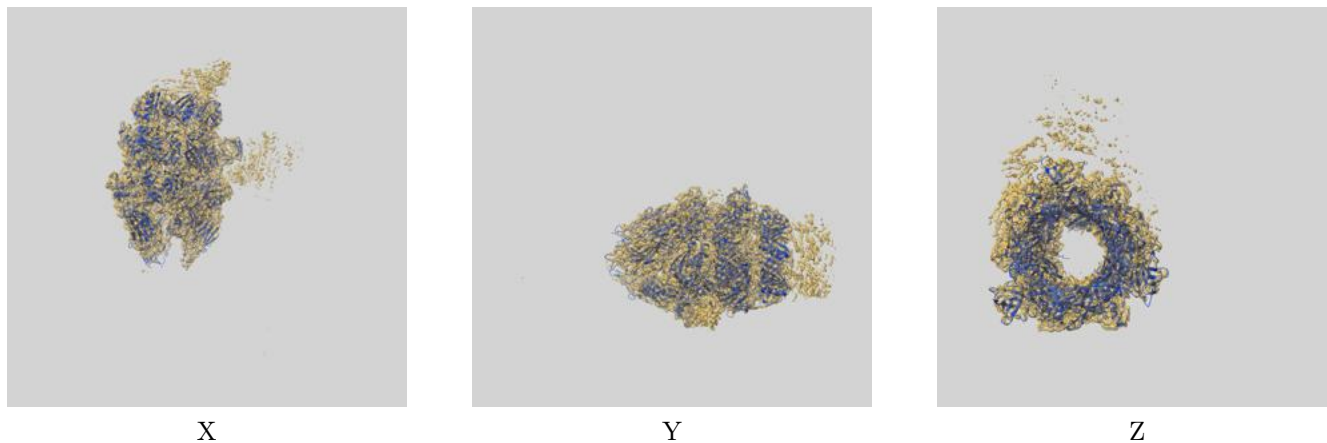
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.46	-	-
Author-provided FSC curve	3.46	3.96	3.48
Unmasked-calculated*	4.51	7.46	4.71

*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 4.51 differs from the reported value 3.46 by more than 10 %

9 Map-model fit [i](#)

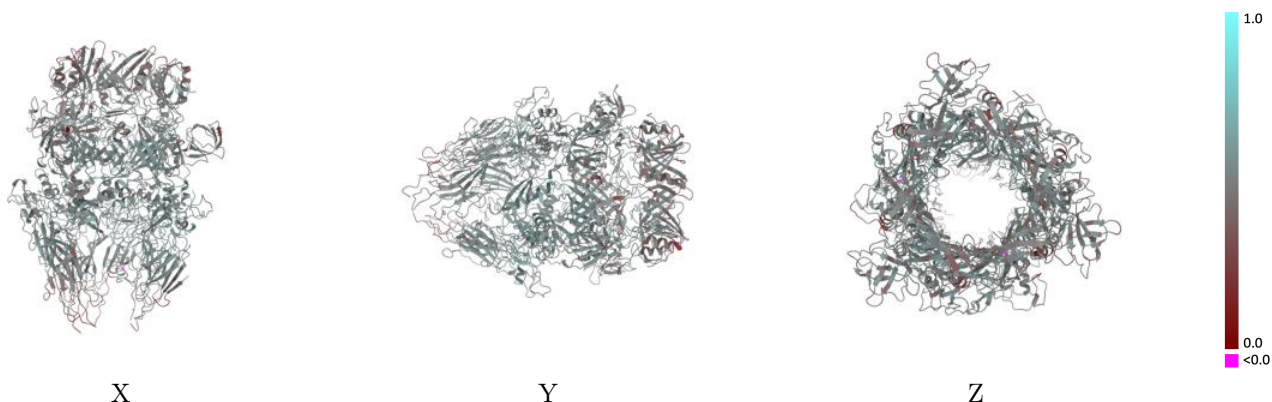
This section contains information regarding the fit between EMDB map EMD-38242 and PDB model 8XCG. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



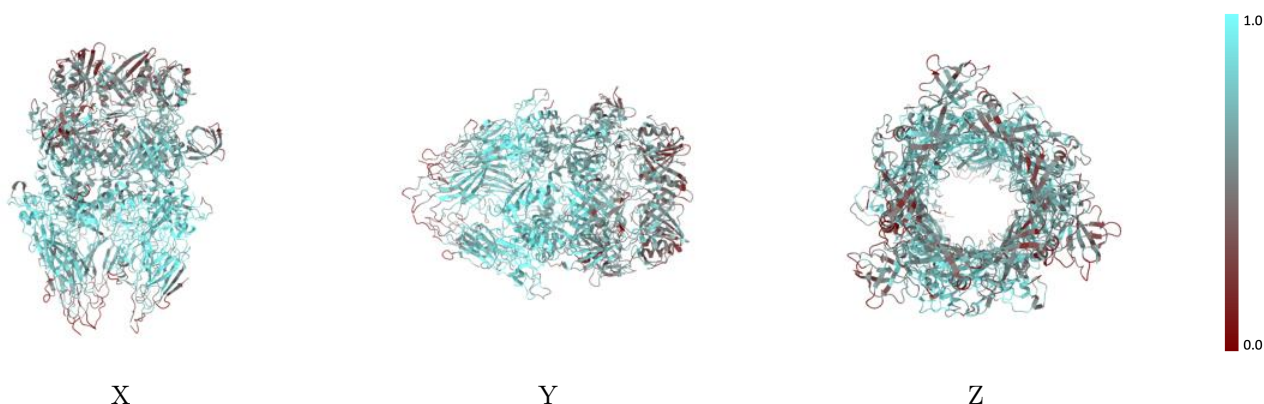
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



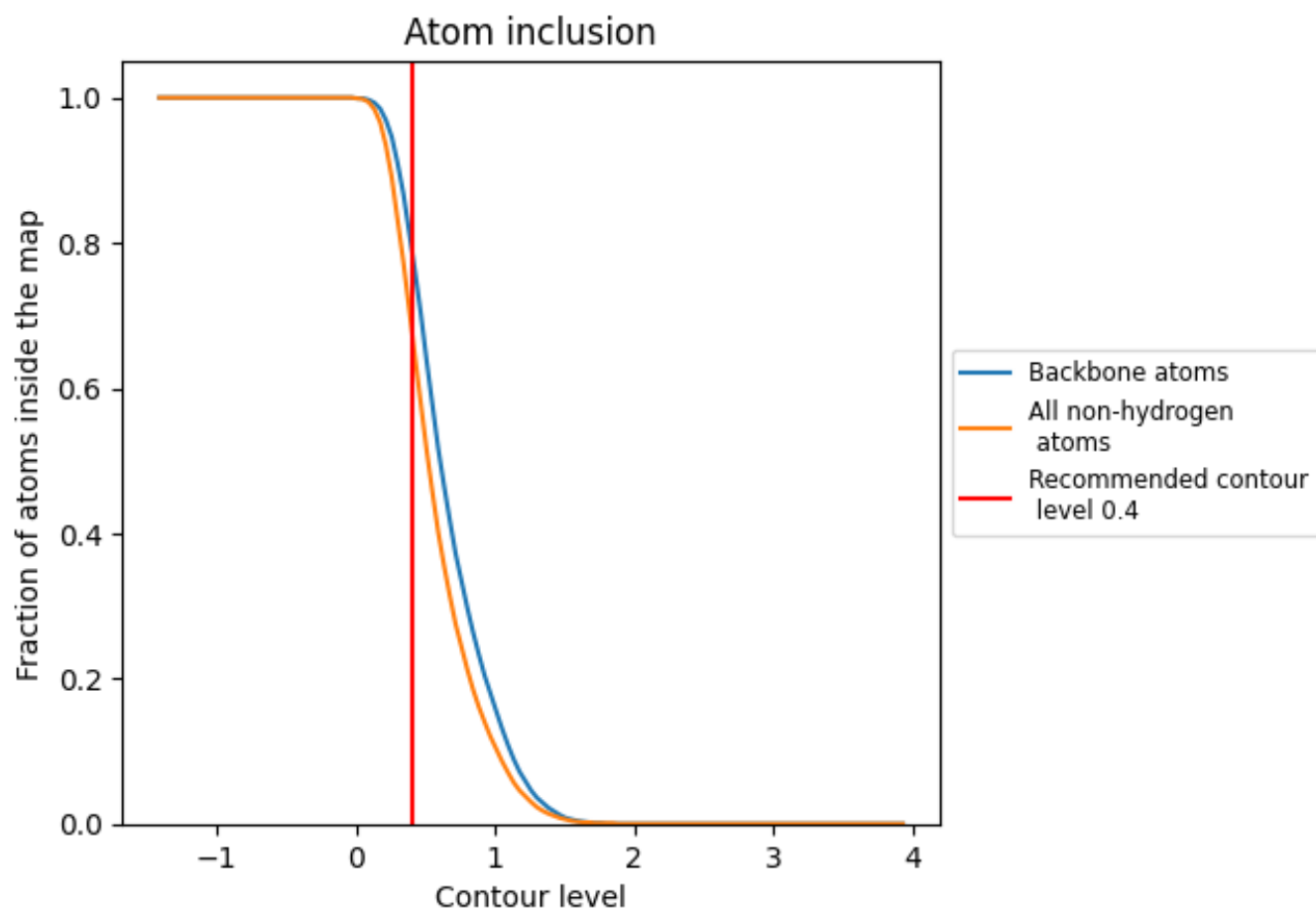
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.4).

































9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 68% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6820	 0.5000
E	 0.5090	 0.4760
F	 0.7700	 0.5160
I	 0.6750	 0.4860
J	 0.6920	 0.5020
K	 0.5150	 0.4620
L	 0.7260	 0.5140
M	 0.5450	 0.4740
N	 0.7200	 0.5200
P	 0.6650	 0.4990
Y	 0.4960	 0.4590
Z	 0.7060	 0.5010
e	 0.5170	 0.4720
f	 0.7440	 0.5130
h	 0.6400	 0.4780
m	 0.5860	 0.4830

