



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 06:42 AM UTC

PDB ID : 9E01 / pdb_00009e01
EMDB ID : EMD-47345
Title : Cryo-EM structure of a TatBC-MdoD complex from Escherichia coli
Authors : Deme, J.C.; Bryant, O.J.; Berks, B.C.; Lea, S.M.
Deposited on : 2024-10-17
Resolution : 2.40 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:

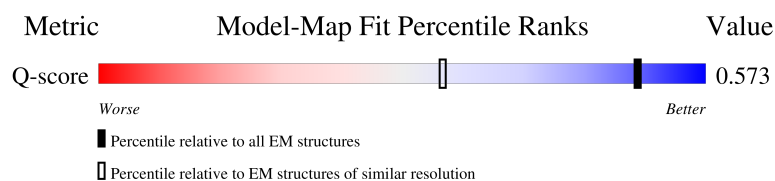
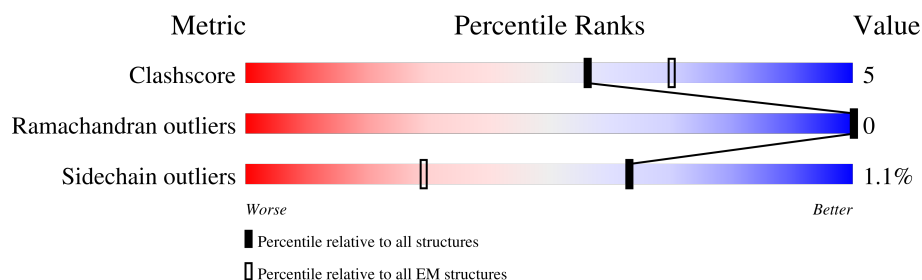
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.40 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.




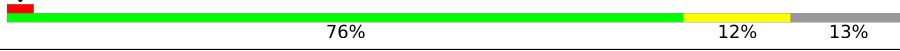
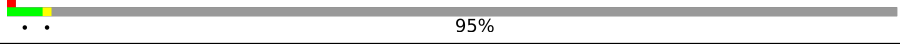
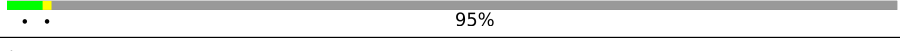
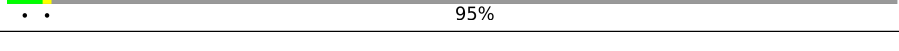
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5628 (1.90 - 2.90)

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	B	171	
1	D	171	
1	F	171	
2	A	266	

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Mol	Chain	Length	Quality of chain
2	C	266	 <div>74%13%13%</div>
2	E	266	 <div>76%12%13%</div>
3	G	552	 <div>95%</div>
3	H	552	 <div>95%</div>
3	I	552	 <div>95%</div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7638 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 Sec-independent protein translocase protein TatB.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	64	Total	C	N	O	S	0	0
			504	331	83	89	1		
1	D	64	Total	C	N	O	S	0	0
			504	331	83	89	1		
1	F	64	Total	C	N	O	S	0	0
			504	331	83	89	1		

- Molecule 2 is a protein called Sec-independent protein translocase protein TatC.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	232	Total	C	N	O	S	2	0
			1845	1252	279	302	12		
2	C	232	Total	C	N	O	S	2	0
			1845	1252	279	302	12		
2	E	232	Total	C	N	O	S	2	0
			1845	1252	279	302	12		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	259	ARG	-	expression tag	UNP C3SK12
A	260	SER	-	expression tag	UNP C3SK12
A	261	HIS	-	expression tag	UNP C3SK12
A	262	HIS	-	expression tag	UNP C3SK12
A	263	HIS	-	expression tag	UNP C3SK12
A	264	HIS	-	expression tag	UNP C3SK12
A	265	HIS	-	expression tag	UNP C3SK12
A	266	HIS	-	expression tag	UNP C3SK12
C	259	ARG	-	expression tag	UNP C3SK12
C	260	SER	-	expression tag	UNP C3SK12
C	261	HIS	-	expression tag	UNP C3SK12
C	262	HIS	-	expression tag	UNP C3SK12
C	263	HIS	-	expression tag	UNP C3SK12

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Chain	Residue	Modelled	Actual	Comment	Reference
C	264	HIS	-	expression tag	UNP C3SK12
C	265	HIS	-	expression tag	UNP C3SK12
C	266	HIS	-	expression tag	UNP C3SK12
E	259	ARG	-	expression tag	UNP C3SK12
E	260	SER	-	expression tag	UNP C3SK12
E	261	HIS	-	expression tag	UNP C3SK12
E	262	HIS	-	expression tag	UNP C3SK12
E	263	HIS	-	expression tag	UNP C3SK12
E	264	HIS	-	expression tag	UNP C3SK12
E	265	HIS	-	expression tag	UNP C3SK12
E	266	HIS	-	expression tag	UNP C3SK12

- Molecule 3 is a protein called Glucans biosynthesis protein D.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	27	Total 196	C 121	N 37	O 34	S 4	0	0
3	H	27	Total 196	C 121	N 37	O 34	S 4	0	0
3	I	27	Total 196	C 121	N 37	O 34	S 4	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	0	SER	-	expression tag	UNP A0A138L4Y6
H	0	SER	-	expression tag	UNP A0A138L4Y6
I	0	SER	-	expression tag	UNP A0A138L4Y6

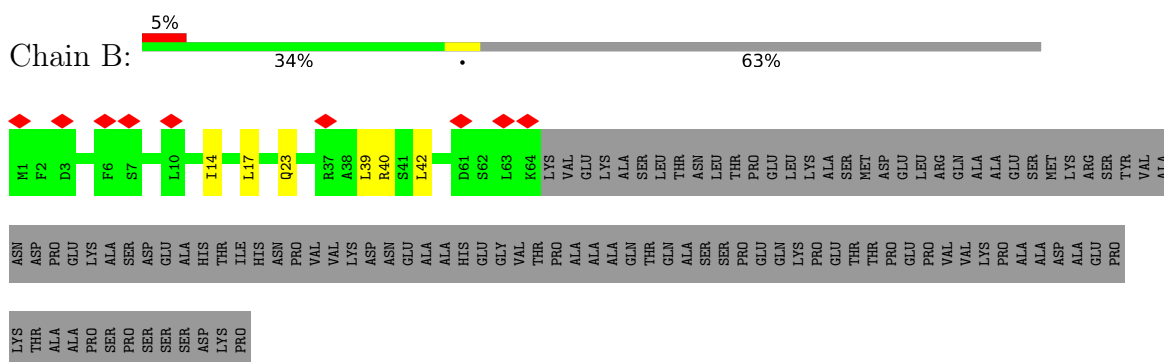
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total 1	O 1	0
4	C	1	Total 1	O 1	0
4	E	1	Total 1	O 1	0

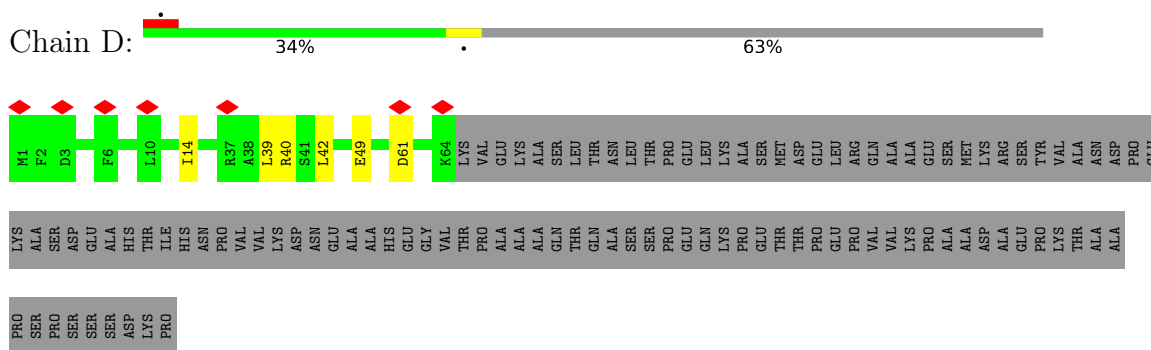
3 Residue-property plots [i](#)

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.

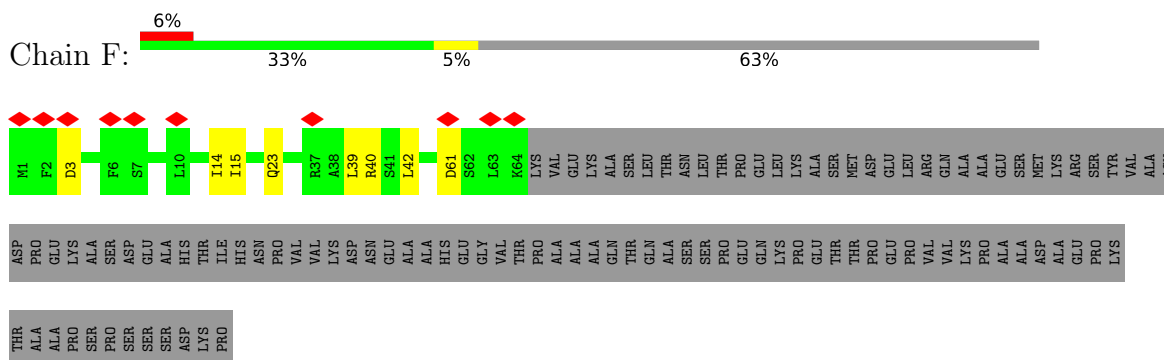
- Molecule 1: Sec-independent protein translocase protein TatB



- Molecule 1: Sec-independent protein translocase protein TatB



- Molecule 1: Sec-independent protein translocase protein TatB



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Category	Value	Color	Category	Value	Color
NET	100	Grey	D211	100	Green
SER	100	Grey	V212	100	Green
VAL	100	Grey	F213	100	Green
GLU	100	Grey	S214	100	Green
D5	100	Red	L217	100	Green
L20	100	Orange	L218	100	Green
D40	100	Yellow	P221	100	Green
Q52	100	Yellow	M222	100	Green
D63	100	Yellow	Y223	100	Green
V64	100	Yellow	C224	100	Green
A65	100	Yellow	L225	100	Green
S66	100	Yellow	I228	100	Green
P67	100	Green	F232	100	Green
F68	100	Green	S233	100	Green
F69	100	Green	R234	100	Green
L74	100	Green	F235	100	Green
M77	100	Green	Y236	100	Green
V86	100	Green	VAL	100	Grey
Q90	100	Green	GLY	100	Grey
H102	100	Green	LYS	100	Grey
ASN	100	Green	GLY	100	Grey
E103	100	Green	ARG	100	Grey
R104	100	Green	ASN	100	Grey
R105	100	Green	ASN	100	Grey
L117	100	Green	ASP	100	Grey
V129	100	Green	ALA	100	Grey
G135	100	Green	GLU	100	Grey
V158	100	Green	ALA	100	Grey
M159	100	Green	GLU	100	Grey
F162	100	Green	SER	100	Grey
F165	100	Green	GLU	100	Grey
V173	100	Green	LYS	100	Grey
L177	100	Green	THR	100	Grey
M180	100	Green	GLU	100	Grey
M181	100	Green	ARG	100	Grey
P186	100	Green	SER	100	Grey
R190	100	Green	HIS	100	Grey
G204	100	Green	HIS	100	Grey
T208	100	Green	HIS	100	Grey
			HIS	100	Grey

Amino Acid	Value (approx.)
MET	0
SER	10
VAL	10
GLU	10
D5	20
T6	20
L20	20
D40	20
T50	20
M59	20
D63	20
V64	20
A65	20
S66	20
F69	20
T70	20
P71	20
L88	20
H102	20
E103	20
R104	30
R105	30
L106	30
V107	30
V108	30
P109	30
T140	30
V158	30
M181	30
P186	30
F201	30
G204	30
L207	40
T208	40
P210	40
F213	40
L217	40
L218	40
P221	40
W222	40

[illegible]

[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1201445	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 ($e^-/\text{\AA}^2$)	52.1	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.965	Depositor
Minimum map value	-0.043	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	354.816, 354.816, 354.816	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.693, 0.693, 0.693	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	B	0.07	0/511	0.15	0/692
1	D	0.07	0/511	0.14	0/692
1	F	0.08	0/511	0.16	0/692
2	A	0.10	0/1906	0.23	0/2606
2	C	0.11	0/1906	0.25	0/2606
2	E	0.10	0/1906	0.24	0/2606
3	G	0.08	0/197	0.21	0/259
3	H	0.09	0/197	0.24	0/259
3	I	0.09	0/197	0.22	0/259
All	All	0.10	0/7842	0.22	0/10671

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	B	504	0	541	5	0
1	D	504	0	541	5	0
1	F	504	0	541	9	0
2	A	1845	0	1927	15	0
2	C	1845	0	1927	22	0
2	E	1845	0	1927	23	0
3	G	196	0	206	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	196	0	206	5	0
3	I	196	0	206	6	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
All	All	7638	0	8022	77	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 5.

The worst 5 of 77 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)
2:A:63:ASP:HB2	2:A:66:SER:HB2	1.67	0.77
2:C:63:ASP:HB2	2:C:66:SER:HB2	1.68	0.76
2:E:63:ASP:HB2	2:E:66:SER:HB2	1.70	0.72
2:E:225:LEU:HD13	2:E:228:ILE:HD12	1.76	0.67
2:C:74:LEU:HA	2:C:77:MET:HE2	1.79	0.65

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	B	62/171 (36%)	62 (100%)	0	0	100	100
1	D	62/171 (36%)	62 (100%)	0	0	100	100
1	F	62/171 (36%)	62 (100%)	0	0	100	100
2	A	232/266 (87%)	230 (99%)	2 (1%)	0	100	100
2	C	232/266 (87%)	229 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	232/266 (87%)	229 (99%)	3 (1%)	0	100	100
3	G	25/552 (4%)	25 (100%)	0	0	100	100
3	H	25/552 (4%)	25 (100%)	0	0	100	100
3	I	25/552 (4%)	25 (100%)	0	0	100	100
All	All	957/2967 (32%)	949 (99%)	8 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	56/144 (39%)	55 (98%)	1 (2%)	51	73
1	D	56/144 (39%)	55 (98%)	1 (2%)	51	73
1	F	56/144 (39%)	56 (100%)	0	100	100
2	A	205/233 (88%)	203 (99%)	2 (1%)	68	84
2	C	205/233 (88%)	202 (98%)	3 (2%)	57	77
2	E	205/233 (88%)	203 (99%)	2 (1%)	68	84
3	G	20/463 (4%)	20 (100%)	0	100	100
3	H	20/463 (4%)	20 (100%)	0	100	100
3	I	20/463 (4%)	20 (100%)	0	100	100
All	All	843/2520 (34%)	834 (99%)	9 (1%)	63	82

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	158	VAL
1	D	39	LEU
2	C	20	LEU
2	C	64	VAL
2	C	158	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	52	GLN
2	A	102	HIS
2	C	102	HIS
2	E	102	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

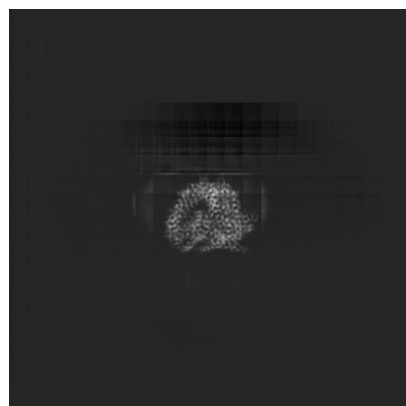
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47345. These allow visual inspection of the internal detail of the map and identification of artifacts.

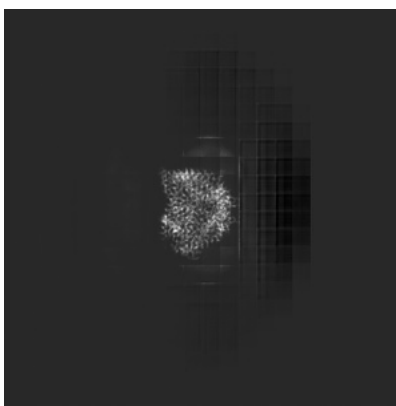
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

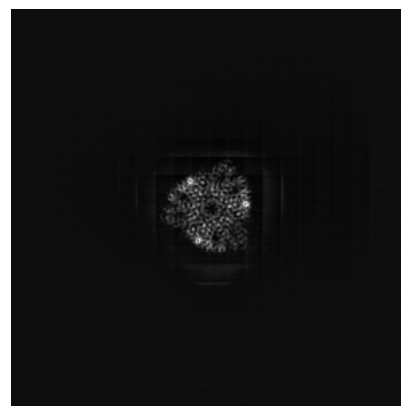
6.1.1 Primary map



X

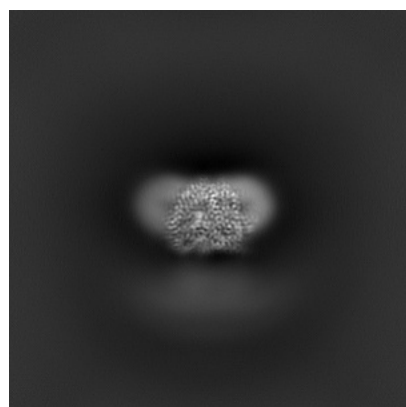


Y

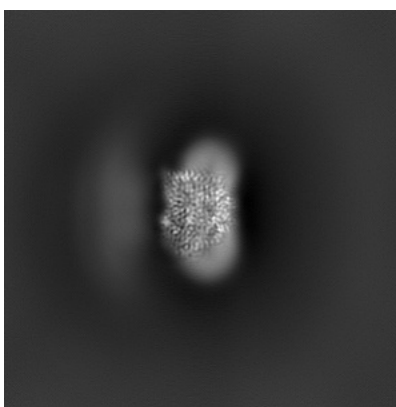


Z

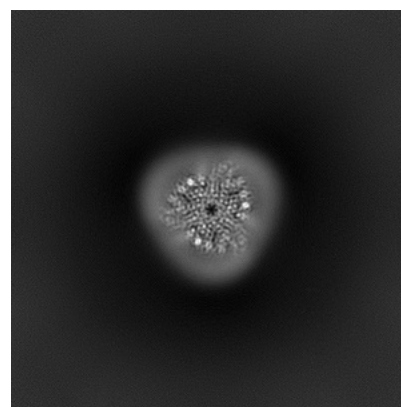
6.1.2 Raw map



X



Y

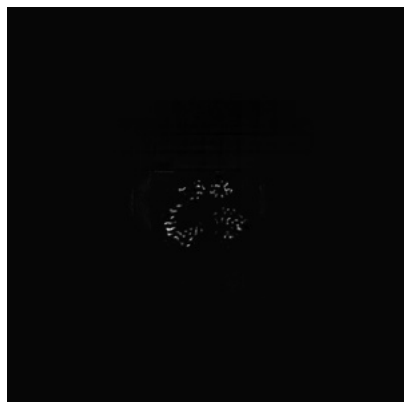


Z

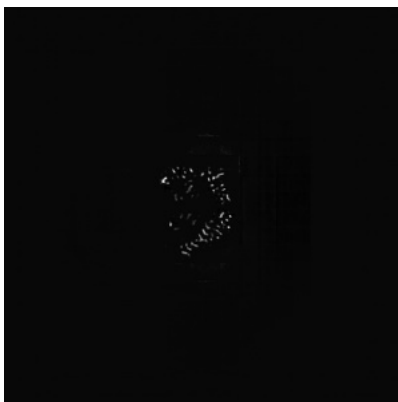
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

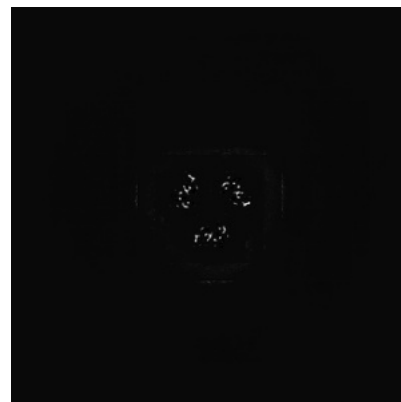
6.2.1 Primary map



X Index: 256

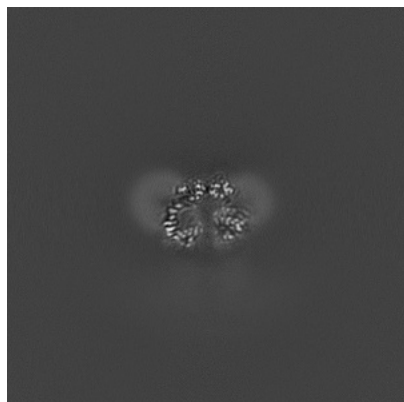


Y Index: 256

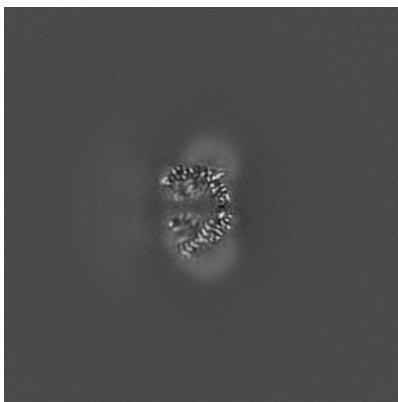


Z Index: 256

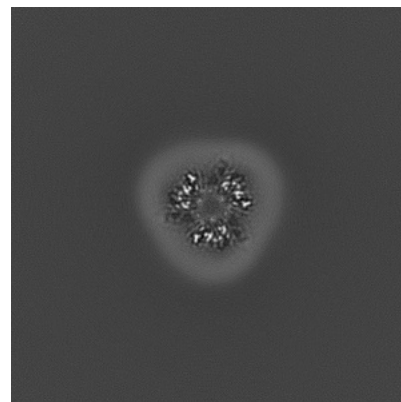
6.2.2 Raw map



X Index: 256



Y Index: 256

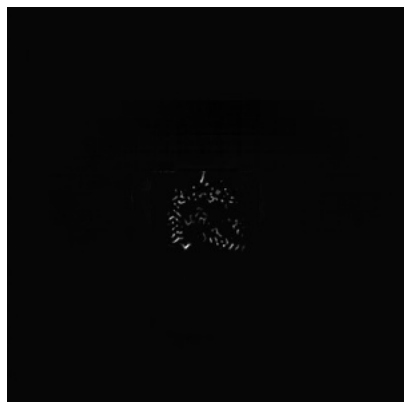


Z Index: 256

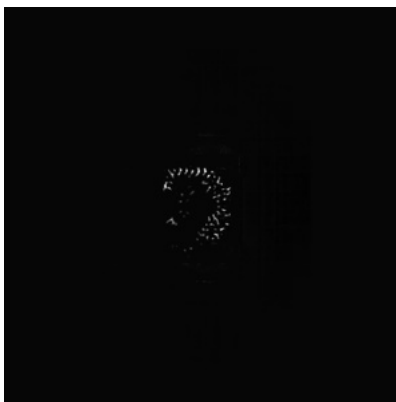
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

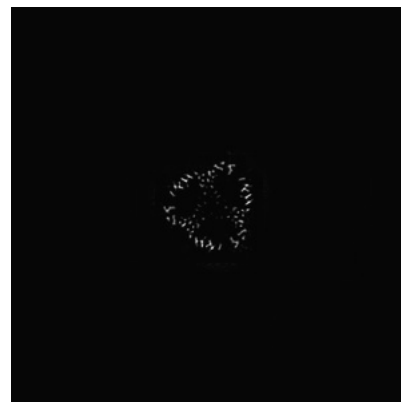
6.3.1 Primary map



X Index: 239

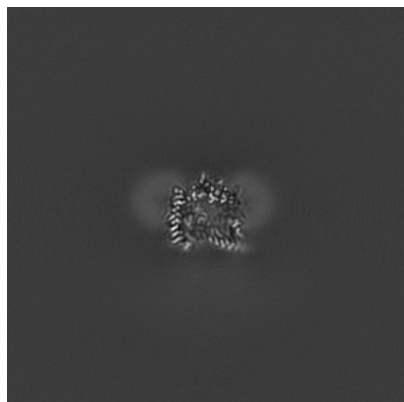


Y Index: 260

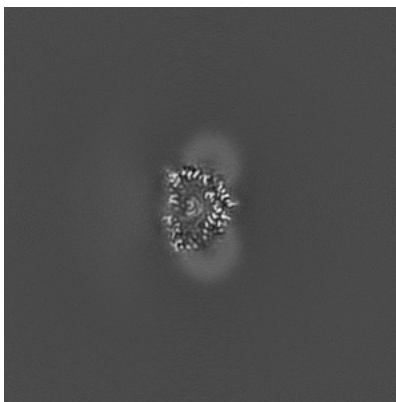


Z Index: 234

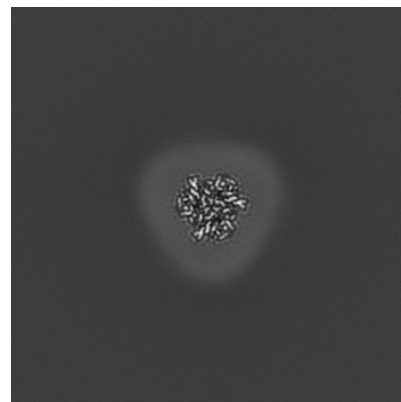
6.3.2 Raw map



X Index: 240



Y Index: 274

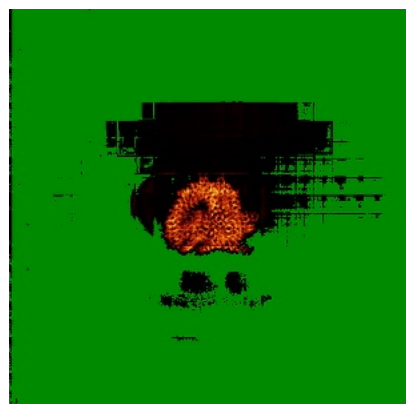


Z Index: 275

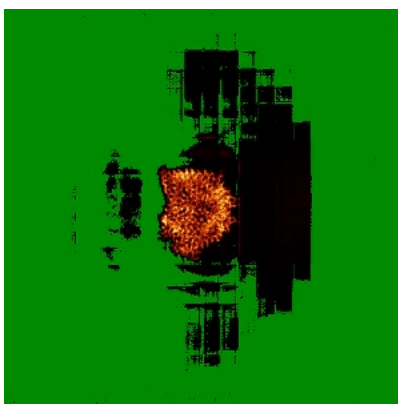
The images above show the largest variance slices of the map in three orthogonal directions.

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

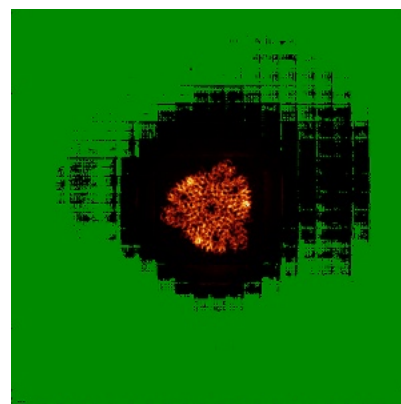
6.4.1 Primary map



X

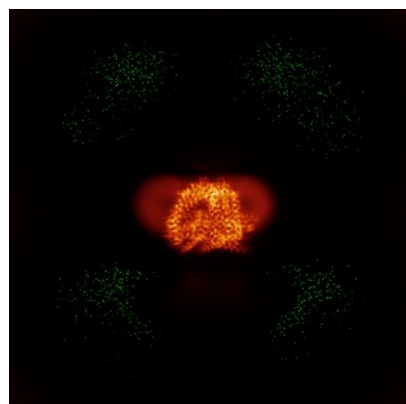


Y

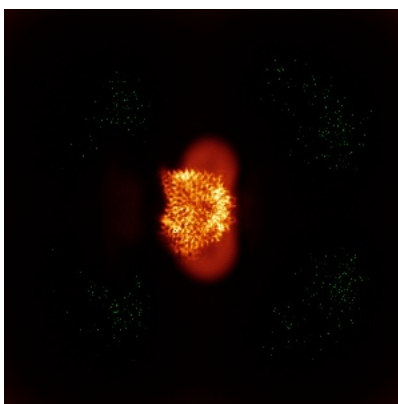


Z

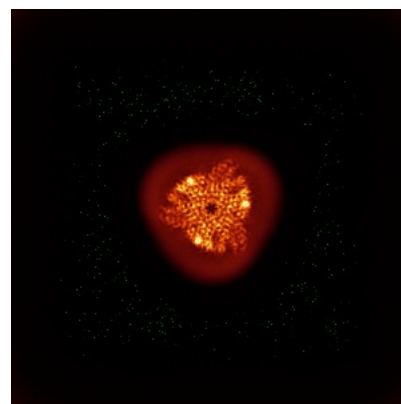
6.4.2 Raw map



X



Y

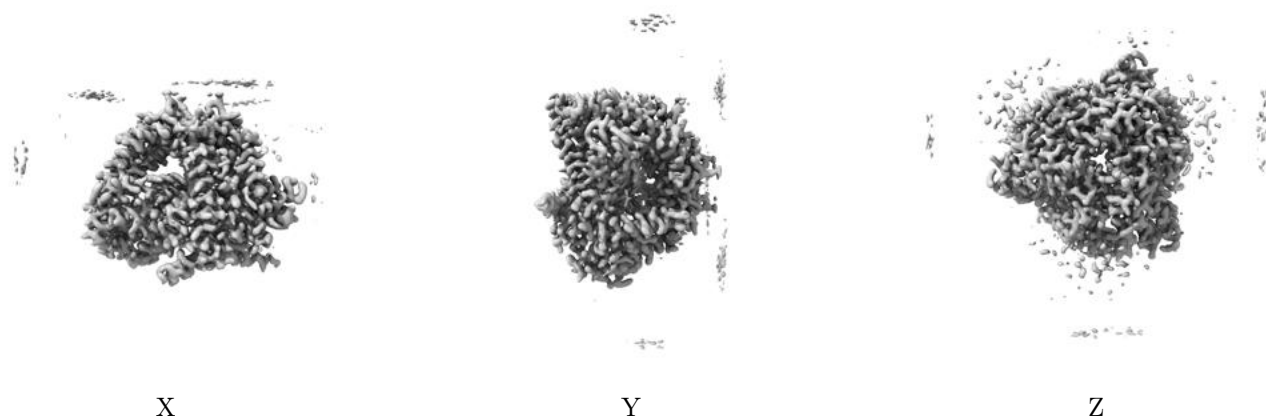


Z

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

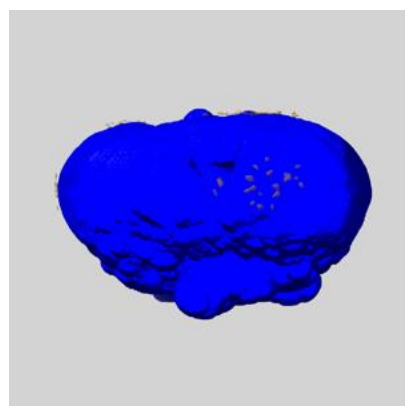
6.6 Mask visualisation [i](#)

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

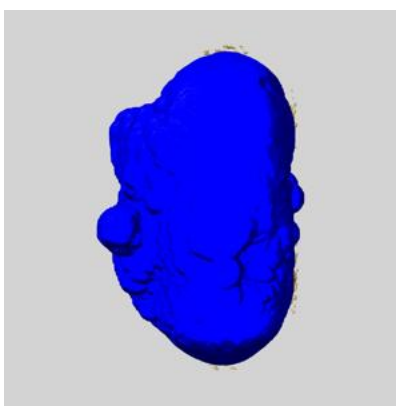
A mask typically either:

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

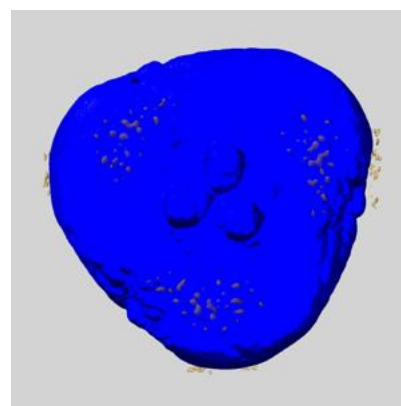
6.6.1 emd_47345_msk_1.map [i](#)



X



Y

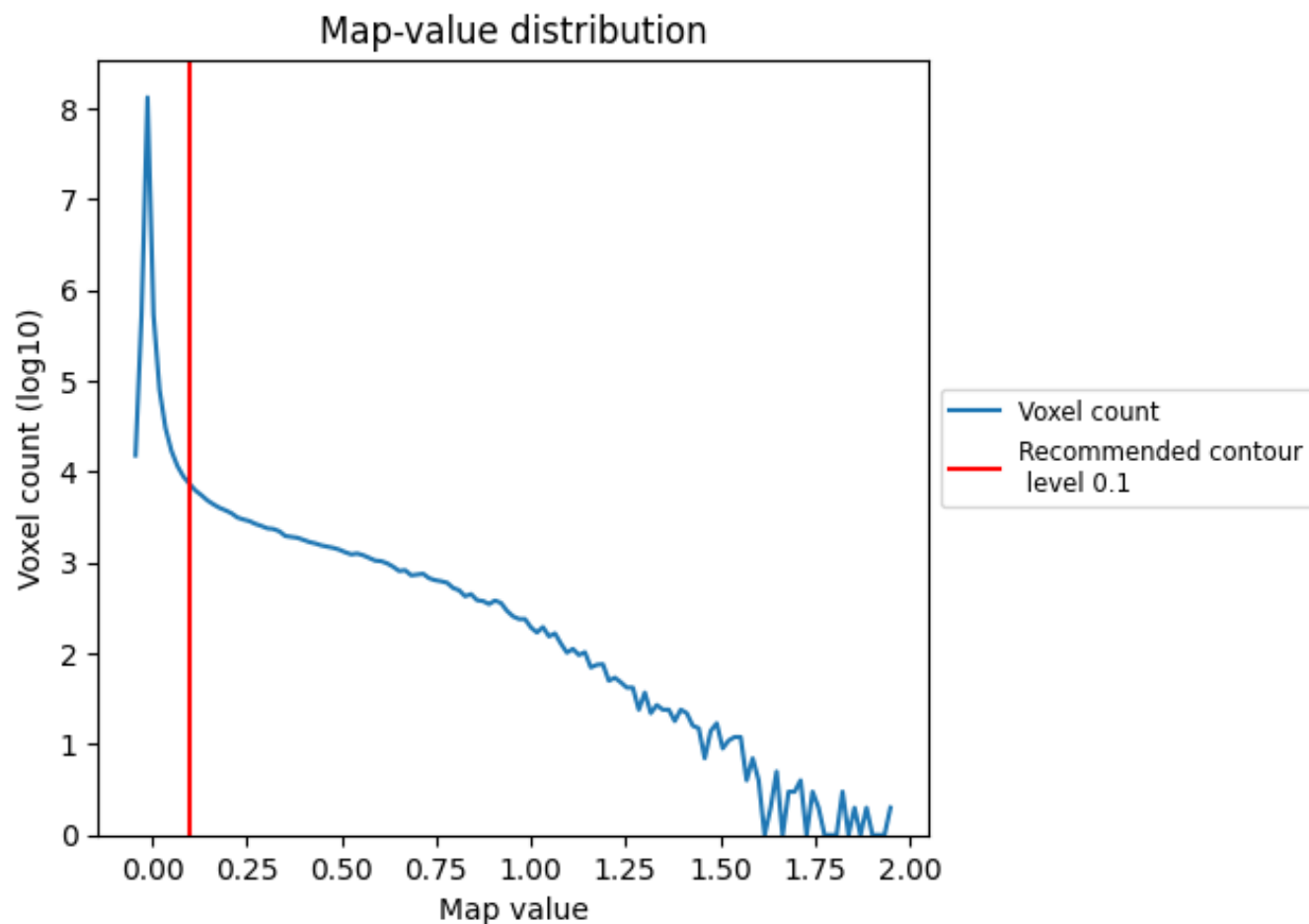


Z

7 Map analysis [i](#)

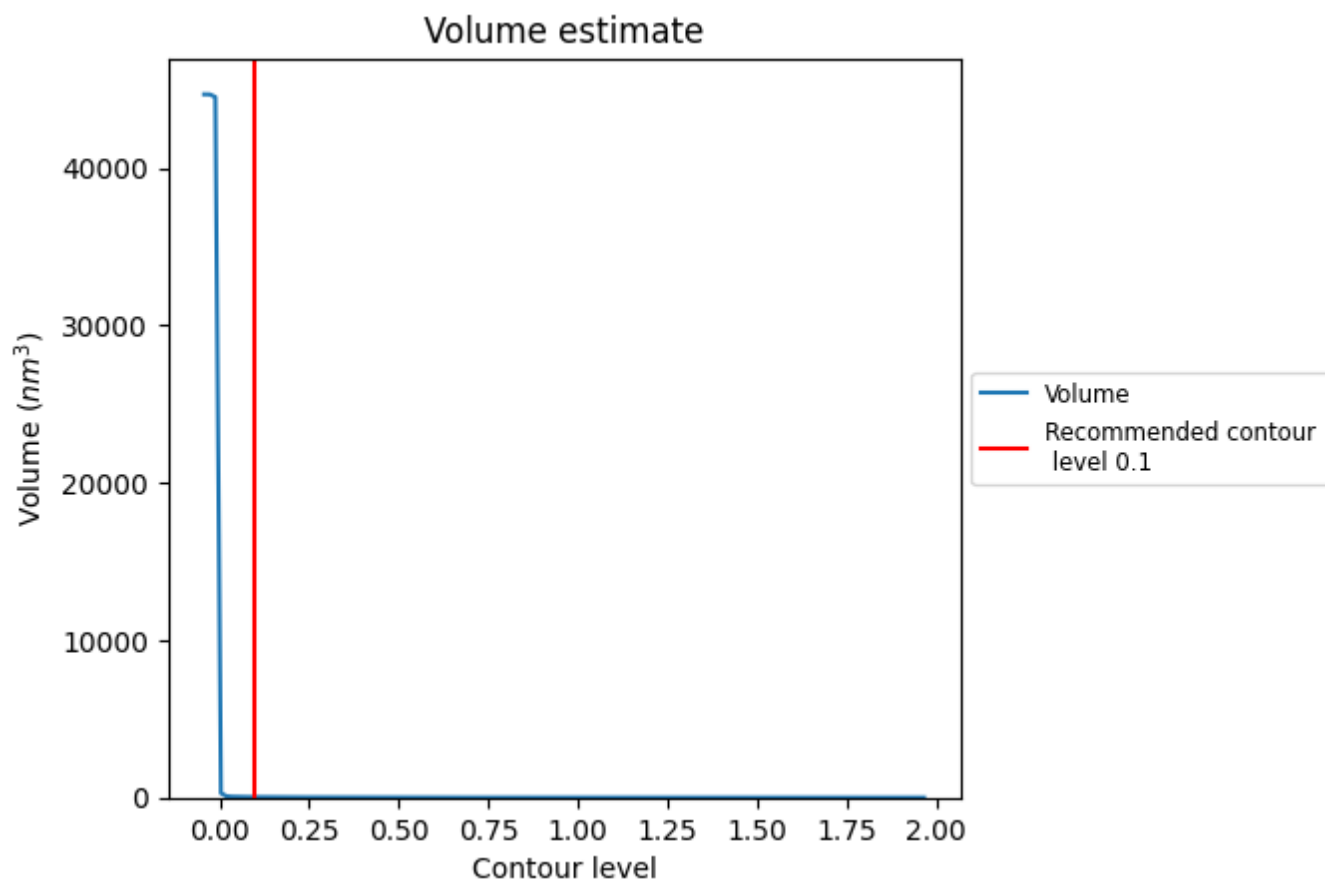
This section contains the results of statistical analysis of the map.

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.

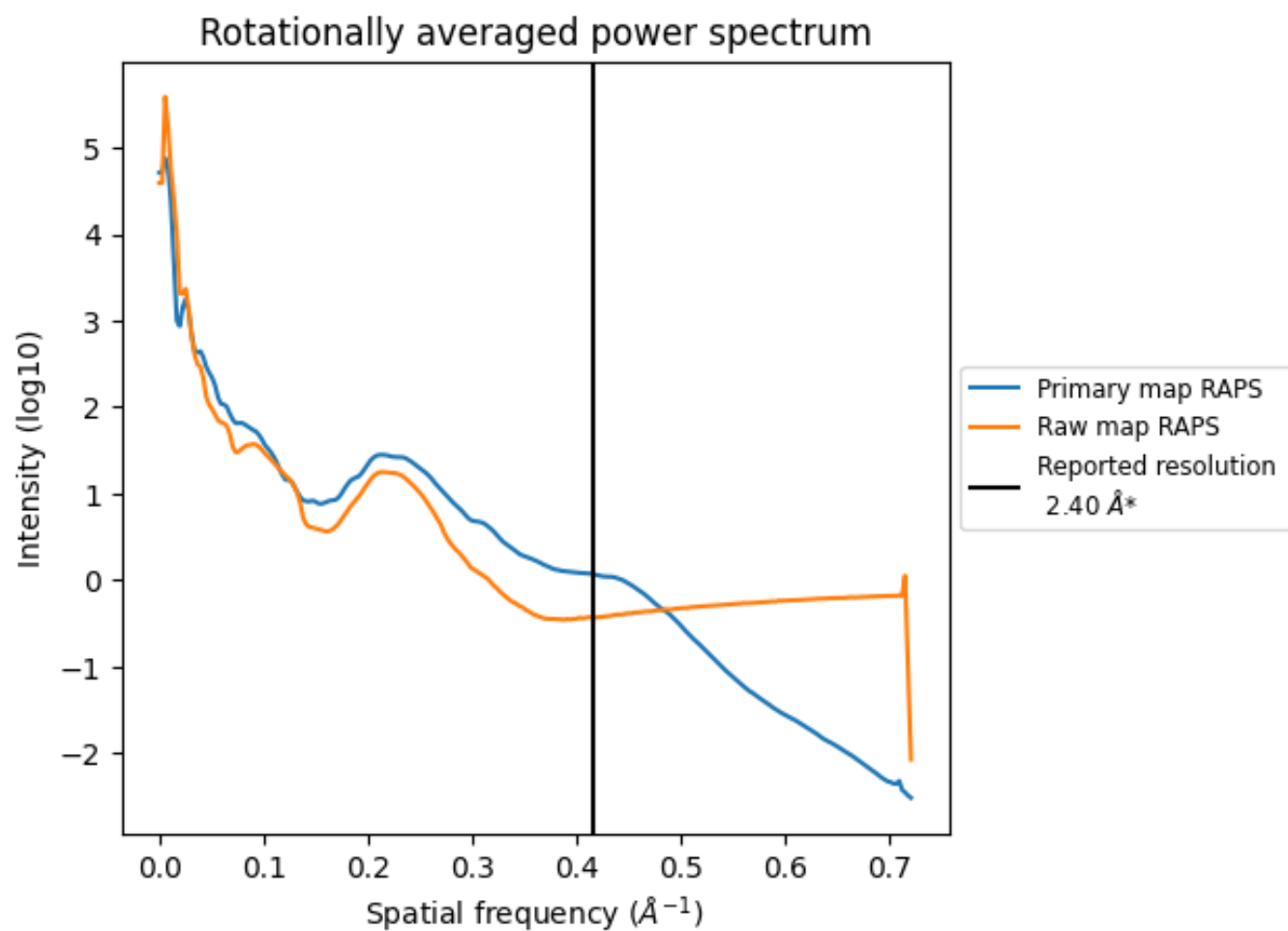
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 33 nm^3 ; this corresponds to an approximate mass of 30 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 ⓘ

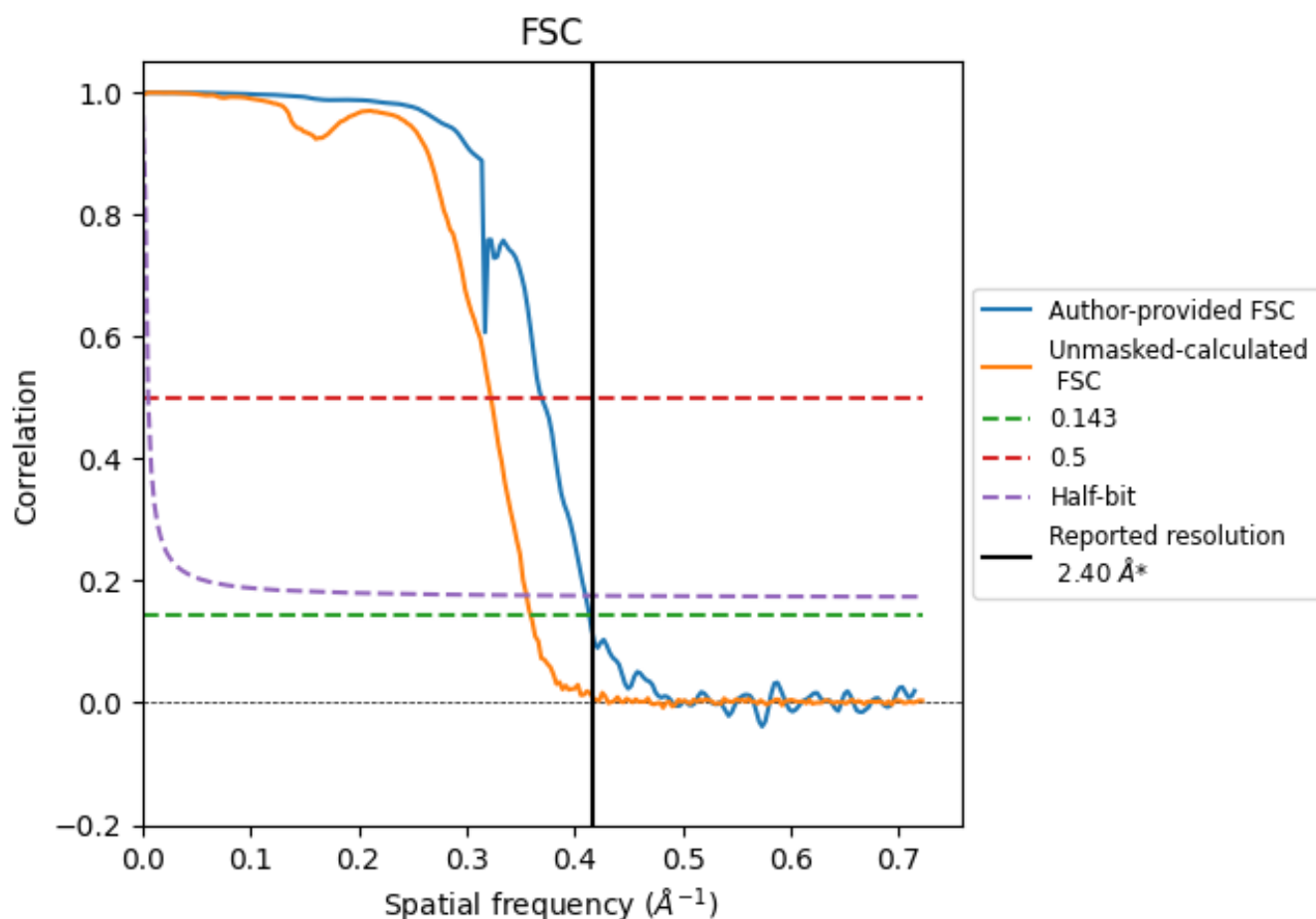


*Reported resolution corresponds to spatial frequency of 0.417 \AA^{-1}

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 0.417 \AA^{-1}

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.40	-	-
Author-provided FSC curve	2.42	2.71	2.44
Unmasked-calculated*	2.78	3.10	2.81

*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 2.78 differs from the reported value 2.4 by more than 10 %

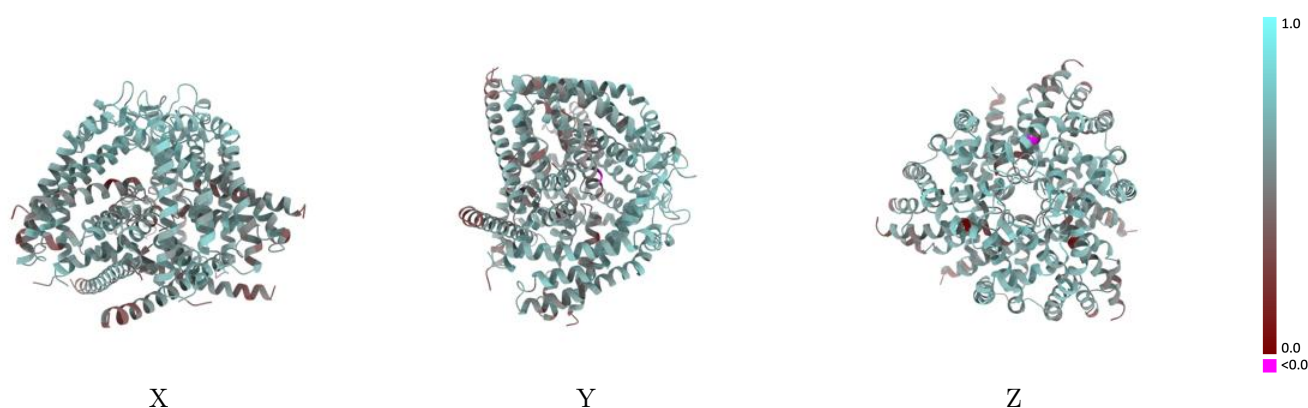
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-47345 and PDB model 9E01. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)

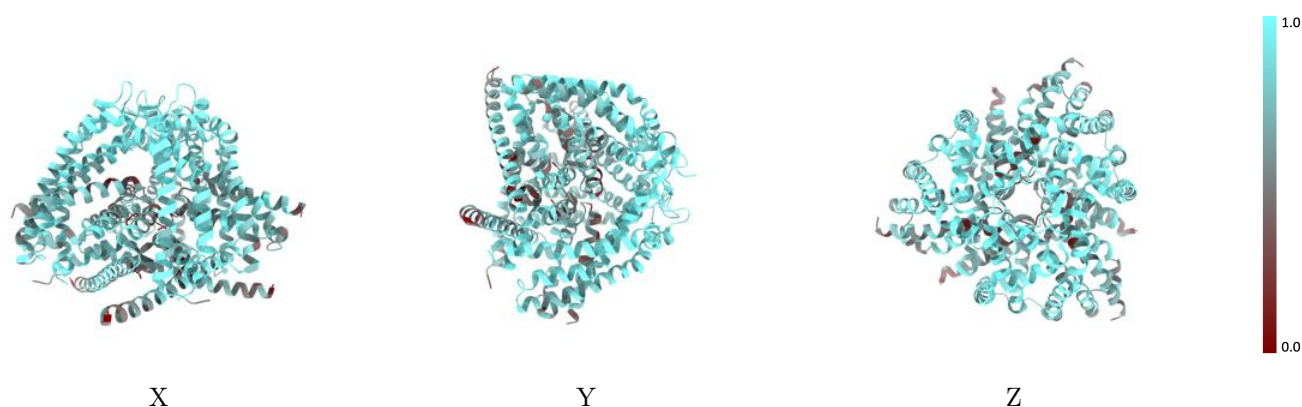
This section was not generated.

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



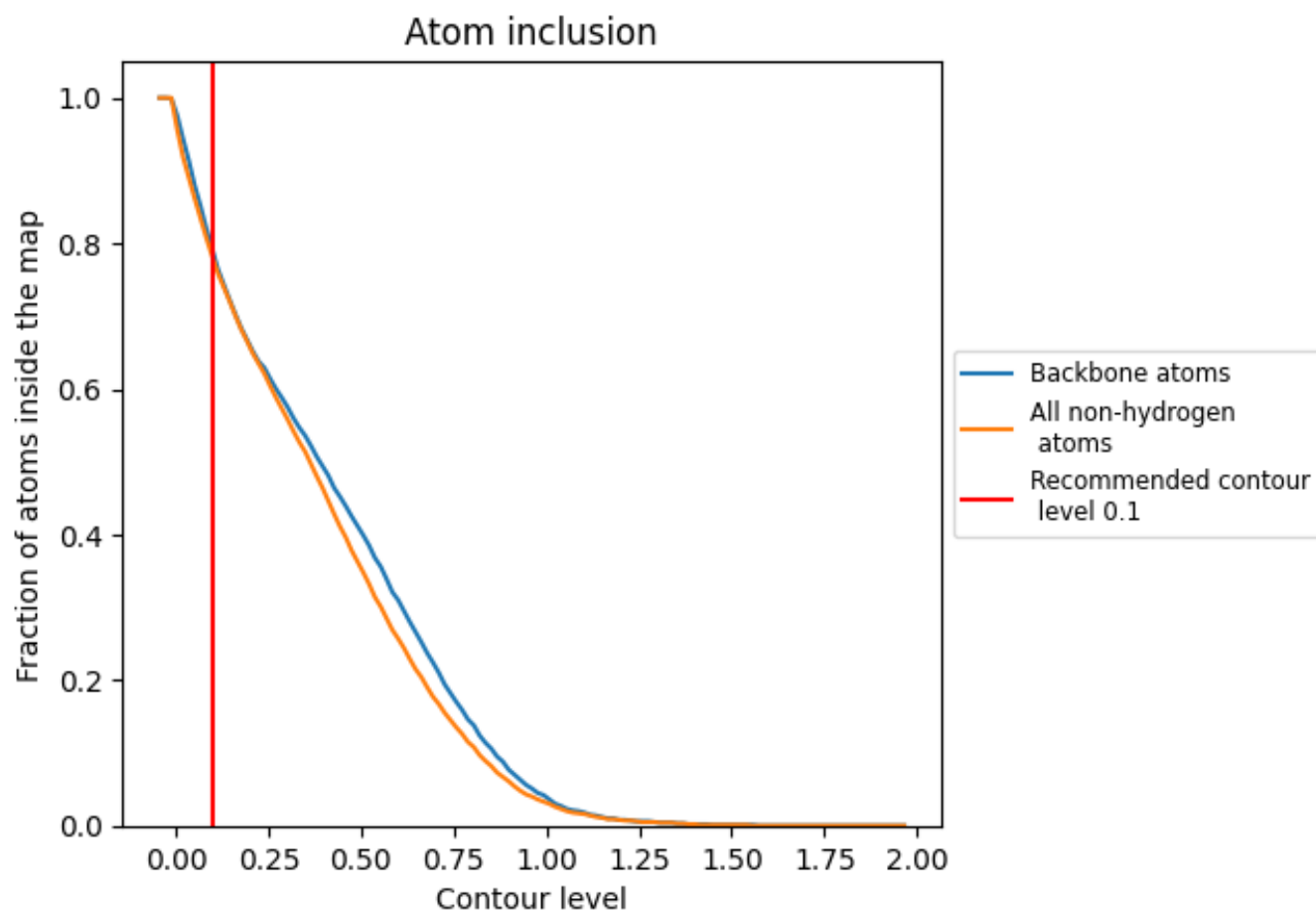
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 78% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7800	<div></div> 0.5730
A	<div></div> 0.8260	<div></div> 0.5900
B	<div></div> 0.6660	<div></div> 0.5190
C	<div></div> 0.8240	<div></div> 0.5900
D	<div></div> 0.6740	<div></div> 0.5140
E	<div></div> 0.8230	<div></div> 0.5890
F	<div></div> 0.6420	<div></div> 0.5060
G	<div></div> 0.7110	<div></div> 0.5790
H	<div></div> 0.7740	<div></div> 0.5850
I	<div></div> 0.7320	<div></div> 0.5730

1.0

0.0

<0.0