



wwPDB EM Validation Summary Report ⓘ

Mar 24, 2026 – 10:30 AM UTC

PDB ID : 8E3I / pdb_00008e3i
EMDB ID : EMD-27866
Title : CRYO-EM STRUCTURE OF the human MPSF IN COMPLEX WITH THE AUUAAA poly(A) signal
Authors : Gutierrez, P.A.; Wei, J.; Sun, Y.; Tong, L.
Deposited on : 2022-08-17
Resolution : 2.53 Å(reported)
Based on initial model : 6DNH

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:

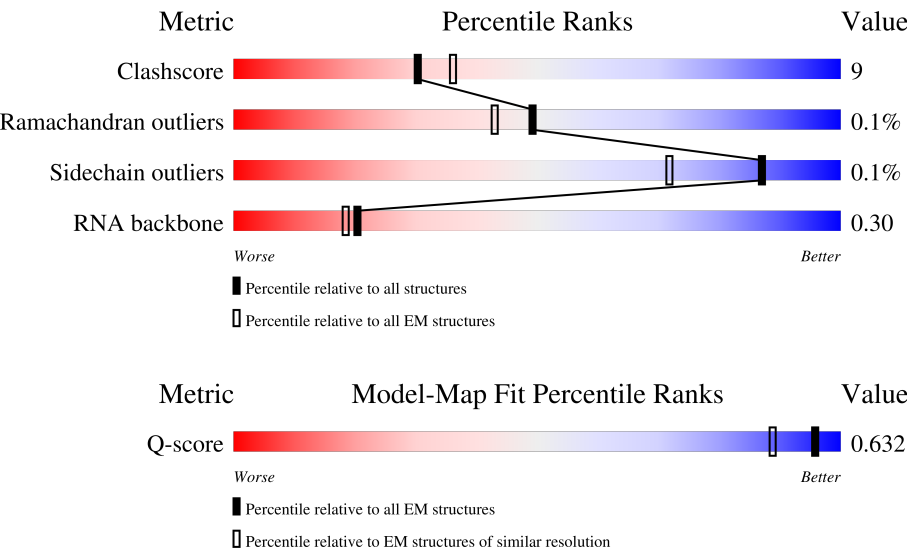
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.53 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	-
RNA backbone	8273	3508	-
Q-score	-	25397	7309 (2.03 - 3.03)

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	1443	
2	C	245	
3	E	11	

Continued on next page...

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Mol	Chain	Length	Quality of chain
4	B	572	 49% 16% 34%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13431 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 Cleavage and polyadenylation specificity factor subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1178	Total	C	N	O	S	0	0
			9344	6008	1601	1680	55		

- Molecule 2 is a protein called Cleavage and polyadenylation specificity factor subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	117	Total	C	N	O	S	0	0
			917	587	151	165	14		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	0	GLY	-	expression tag	UNP O95639

- Molecule 3 is a RNA chain called RNA (5'-R(P*CP*AP*UP*UP*AP*AP*AP*CP*AP*AP*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	7	Total	C	N	O	P	0	0
			132	58	24	43	7		

- Molecule 4 is a protein called pre-mRNA 3' end processing protein WDR33.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	376	Total	C	N	O	S	0	0
			3035	1916	557	542	20		

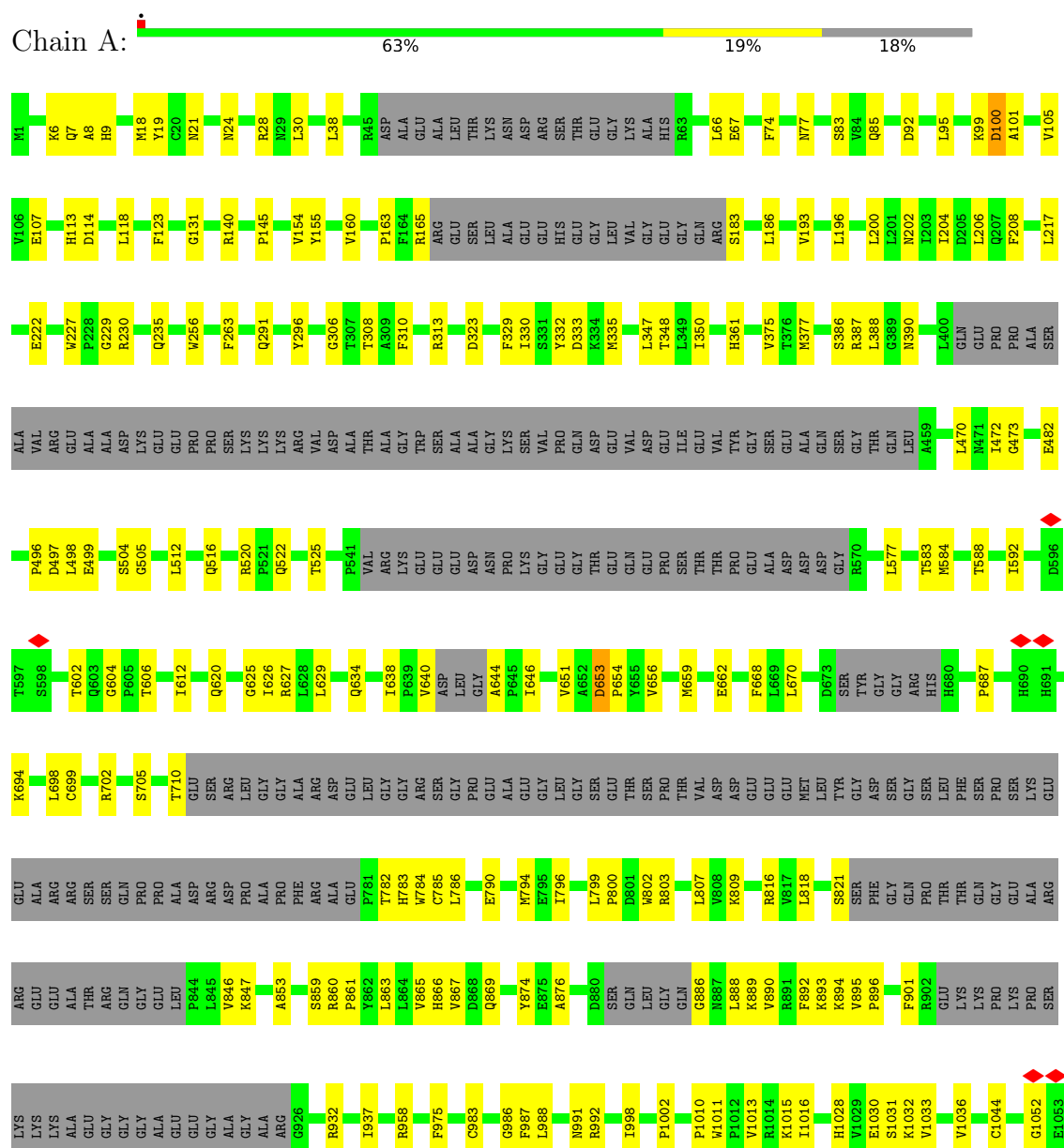
- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

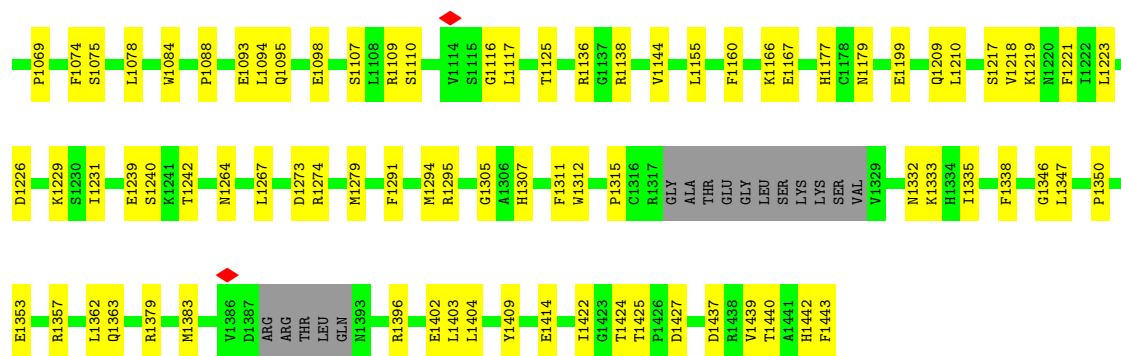
Mol	Chain	Residues	Atoms		AltConf
5	C	3	Total	Zn	0
			3	3	

3 Residue-property plots

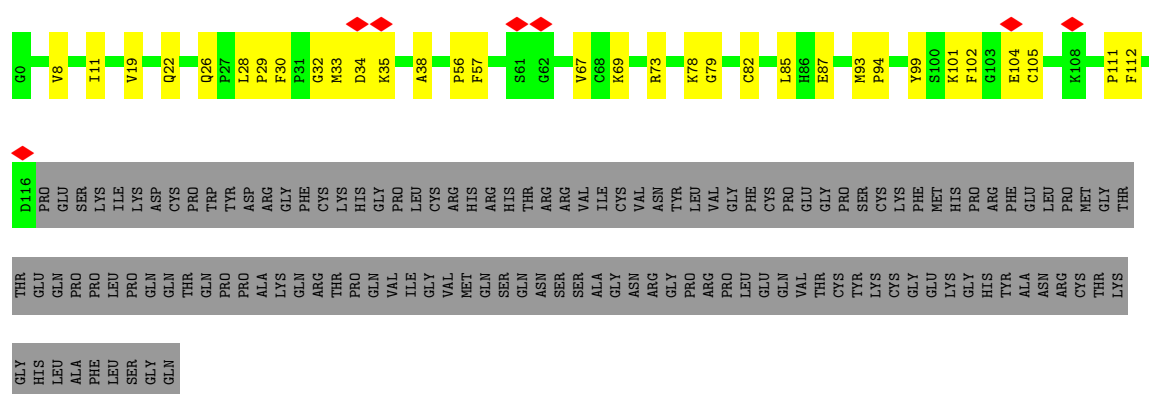
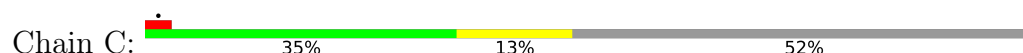
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Cleavage and polyadenylation specificity factor subunit 1

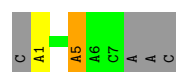




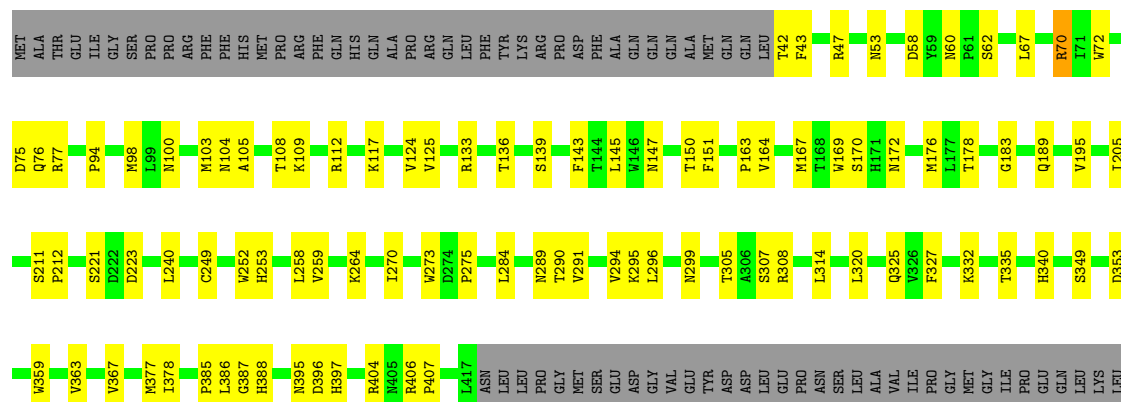
• Molecule 2: Cleavage and polyadenylation specificity factor subunit 4



• Molecule 3: RNA (5'-R(P*CP*AP*UP*UP*AP*AP*AP*CP*AP*AP*C)-3')



• Molecule 4: pre-mRNA 3' end processing protein WDR33



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

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	858038	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 ($e^-/\text{\AA}^2$)	58	Depositor
Minimum defocus (nm)	-1000	Depositor
Maximum defocus (nm)	-2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.816	Depositor
Minimum map value	-2.883	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.176	Depositor
Recommended contour level	0.451	Depositor
Map size (Å)	212.48, 212.48, 212.48	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	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: ZN

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	0.18	0/9560	0.35	0/12977
2	C	0.13	0/941	0.33	0/1261
3	E	0.10	0/147	0.14	0/227
4	B	0.18	0/3120	0.35	0/4224
All	All	0.17	0/13768	0.35	0/18689

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9344	0	9399	167	0
2	C	917	0	883	23	0
3	E	132	0	64	3	0
4	B	3035	0	2949	65	0
5	C	3	0	0	0	0
All	All	13431	0	13295	240	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 9.

The worst 5 of 240 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:113:HIS:HB3	1:A:893:LYS:HD2	1.60	0.83
4:B:67:LEU:HA	4:B:70:ARG:HD3	1.64	0.80
1:A:653:ASP:HB3	1:A:654:PRO:HD2	1.64	0.79
4:B:270:ILE:HD11	4:B:291:VAL:HG11	1.64	0.77
1:A:193:VAL:HA	1:A:196:LEU:HD13	1.69	0.75

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	1152/1443 (80%)	1090 (95%)	60 (5%)	2 (0%)	43	62
2	C	115/245 (47%)	106 (92%)	9 (8%)	0	100	100
4	B	374/572 (65%)	356 (95%)	18 (5%)	0	100	100
All	All	1641/2260 (73%)	1552 (95%)	87 (5%)	2 (0%)	49	67

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	653	ASP
1	A	100	ASP

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	A	1031/1235 (84%)	1031 (100%)	0	100	100
2	C	99/211 (47%)	99 (100%)	0	100	100
4	B	326/501 (65%)	325 (100%)	1 (0%)	86	94
All	All	1456/1947 (75%)	1455 (100%)	1 (0%)	87	95

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	B	70	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1266	GLN
4	B	158	GLN
4	B	319	ASN
4	B	194	ASN
1	A	887	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	E	5/11 (45%)	1 (20%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	E	5	A

There are no RNA pucker outliers to report.

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](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

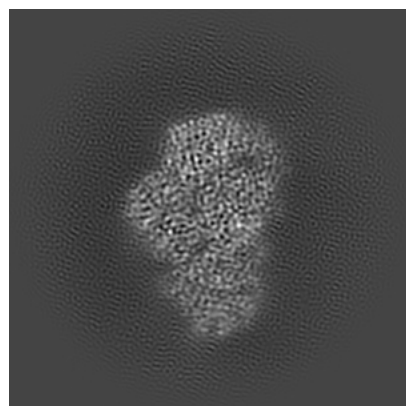
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27866. These allow visual inspection of the internal detail of the map and identification of artifacts.

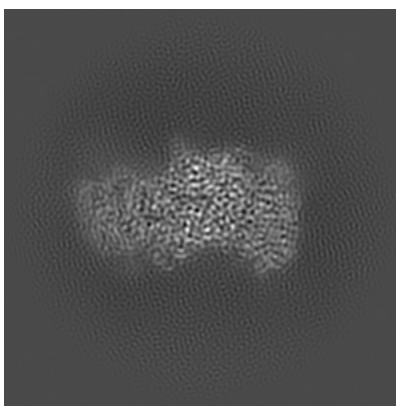
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

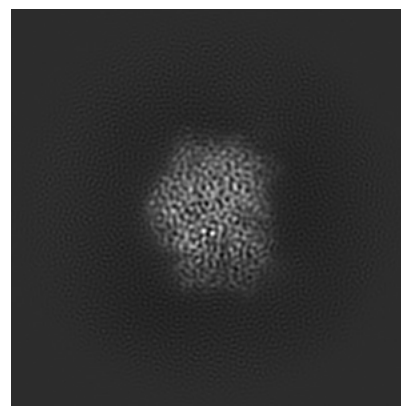
6.1.1 Primary map



X

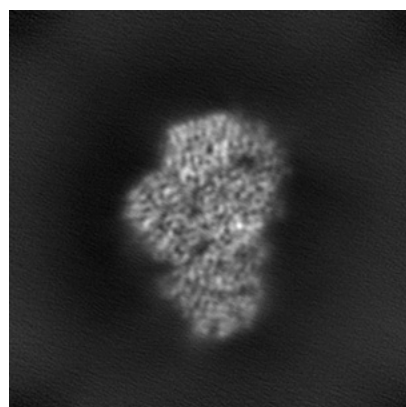


Y

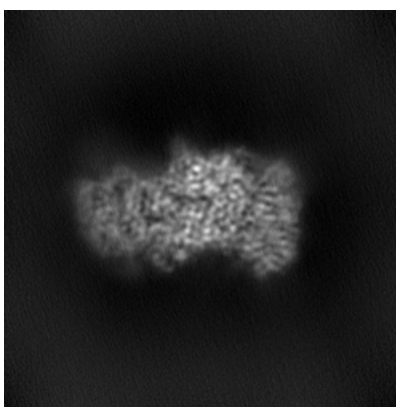


Z

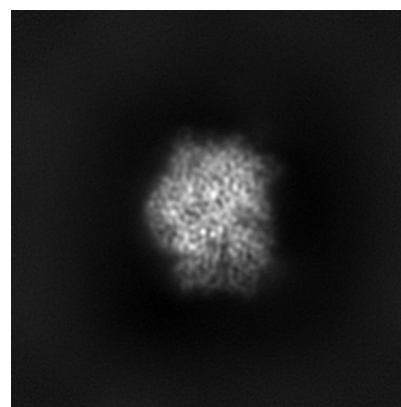
6.1.2 Raw map



X



Y

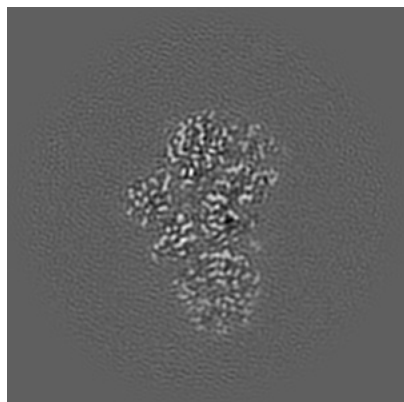


Z

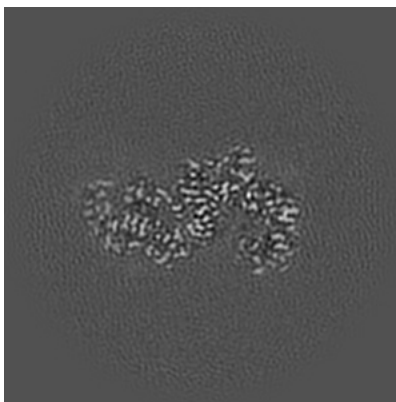
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

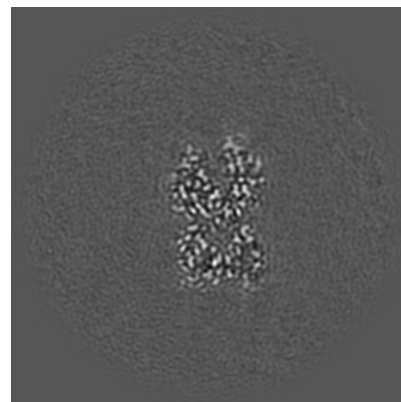
6.2.1 Primary map



X Index: 128

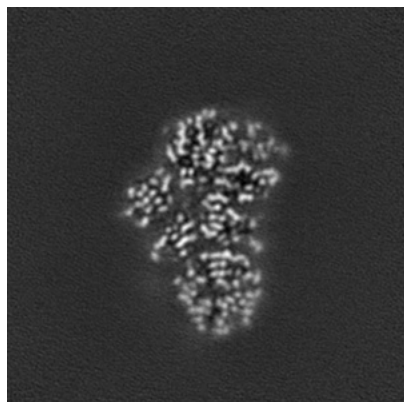


Y Index: 128

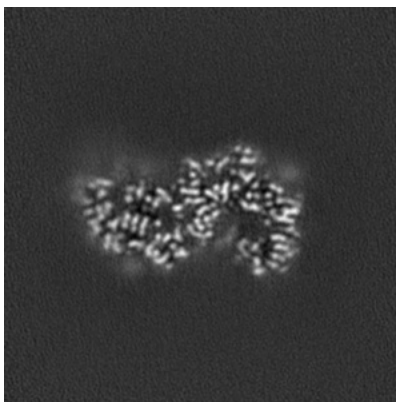


Z Index: 128

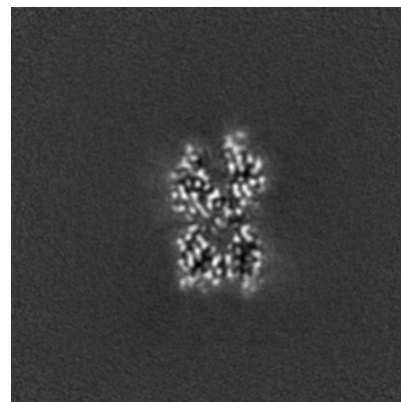
6.2.2 Raw map



X Index: 128



Y Index: 128

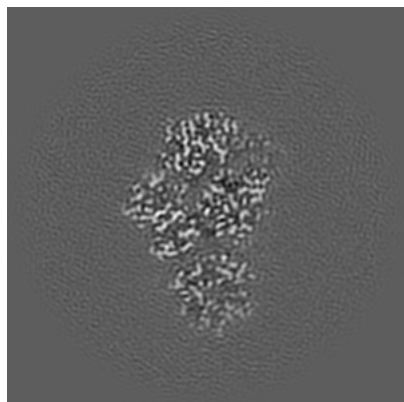


Z Index: 128

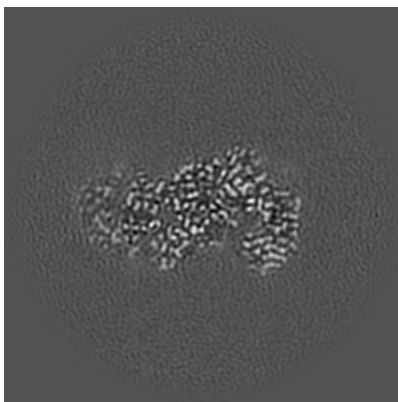
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

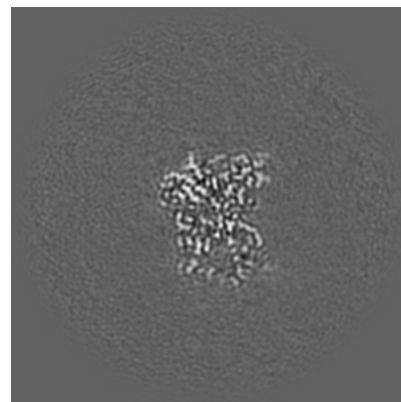
6.3.1 Primary map



X Index: 124

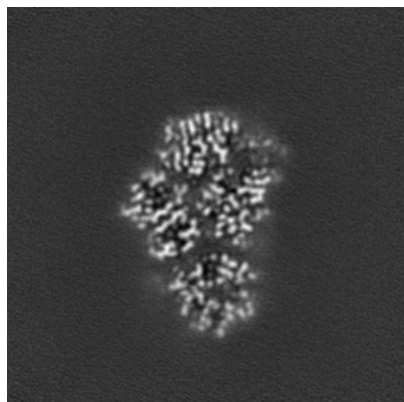


Y Index: 132

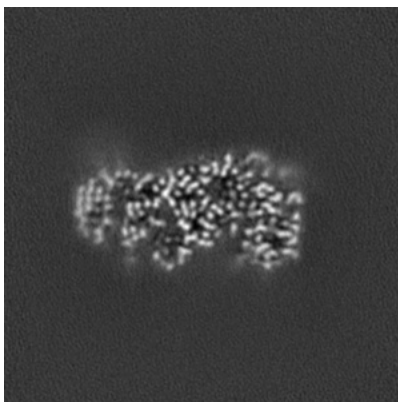


Z Index: 117

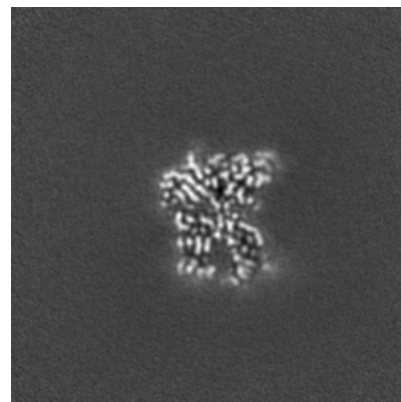
6.3.2 Raw map



X Index: 124



Y Index: 136

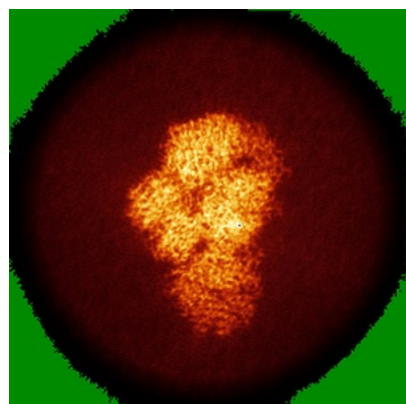


Z Index: 117

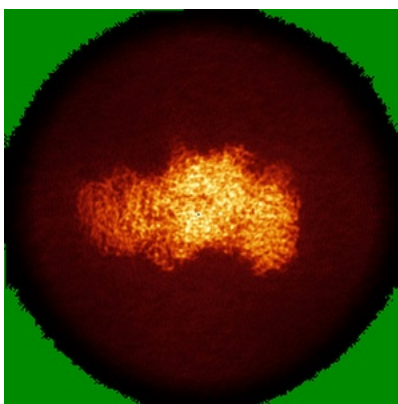
The images above show the largest variance slices of the map in three orthogonal directions.

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

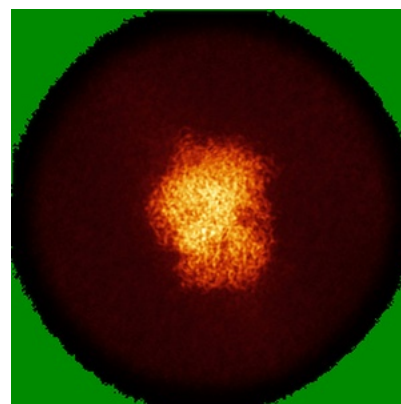
6.4.1 Primary map



X

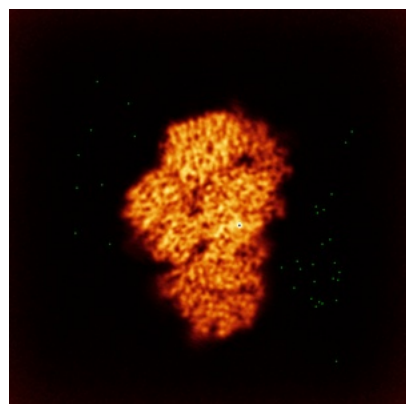


Y

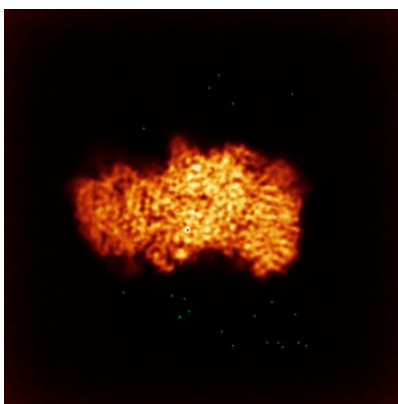


Z

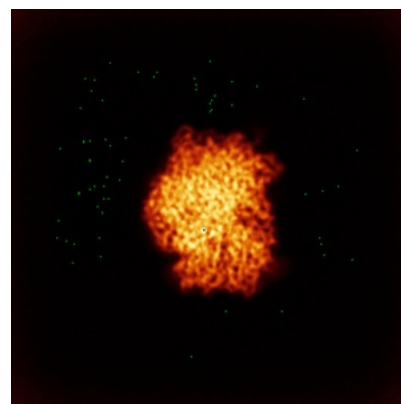
6.4.2 Raw map



X



Y

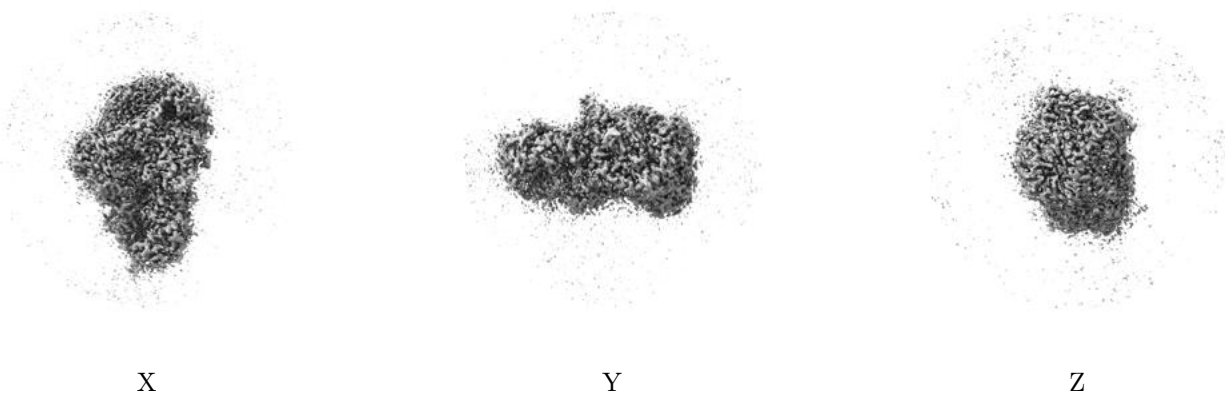


Z

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.

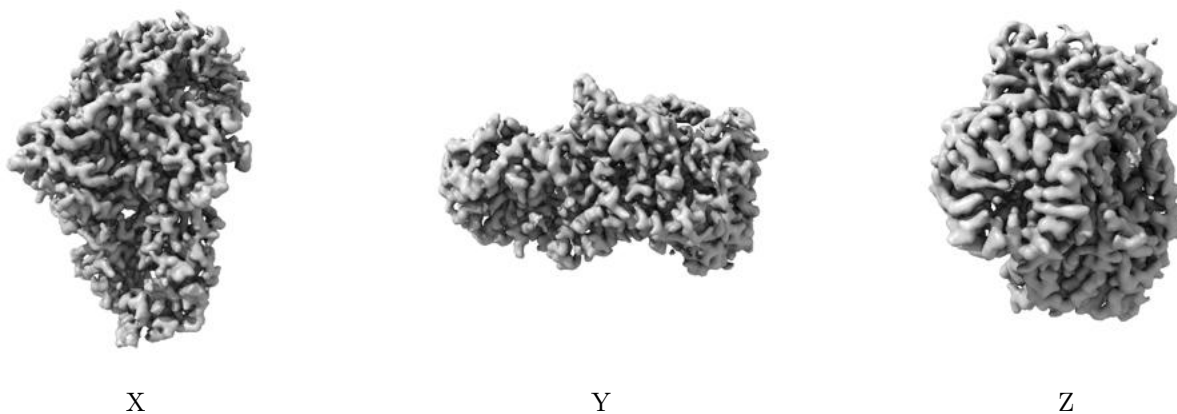
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.451. 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.

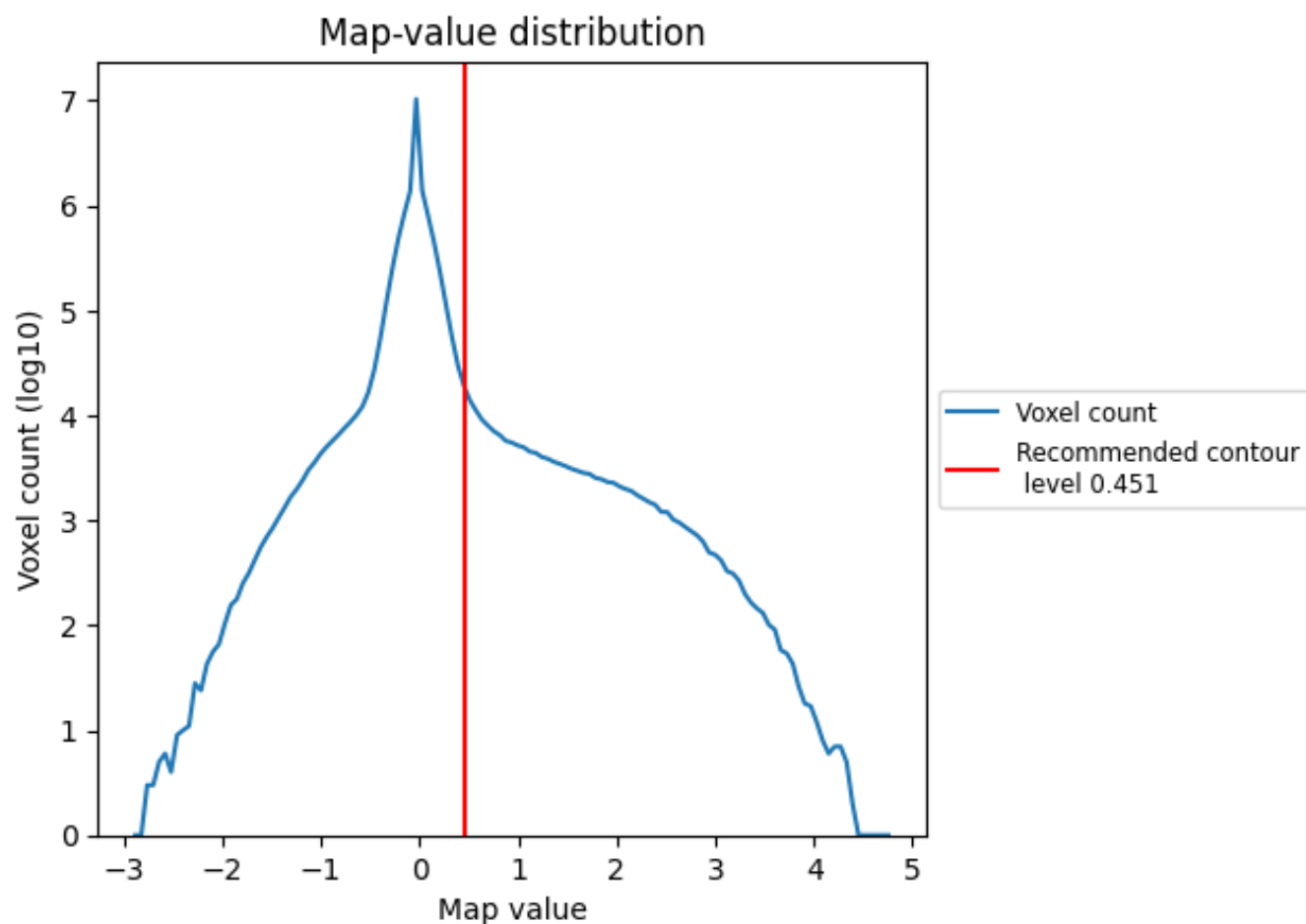
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

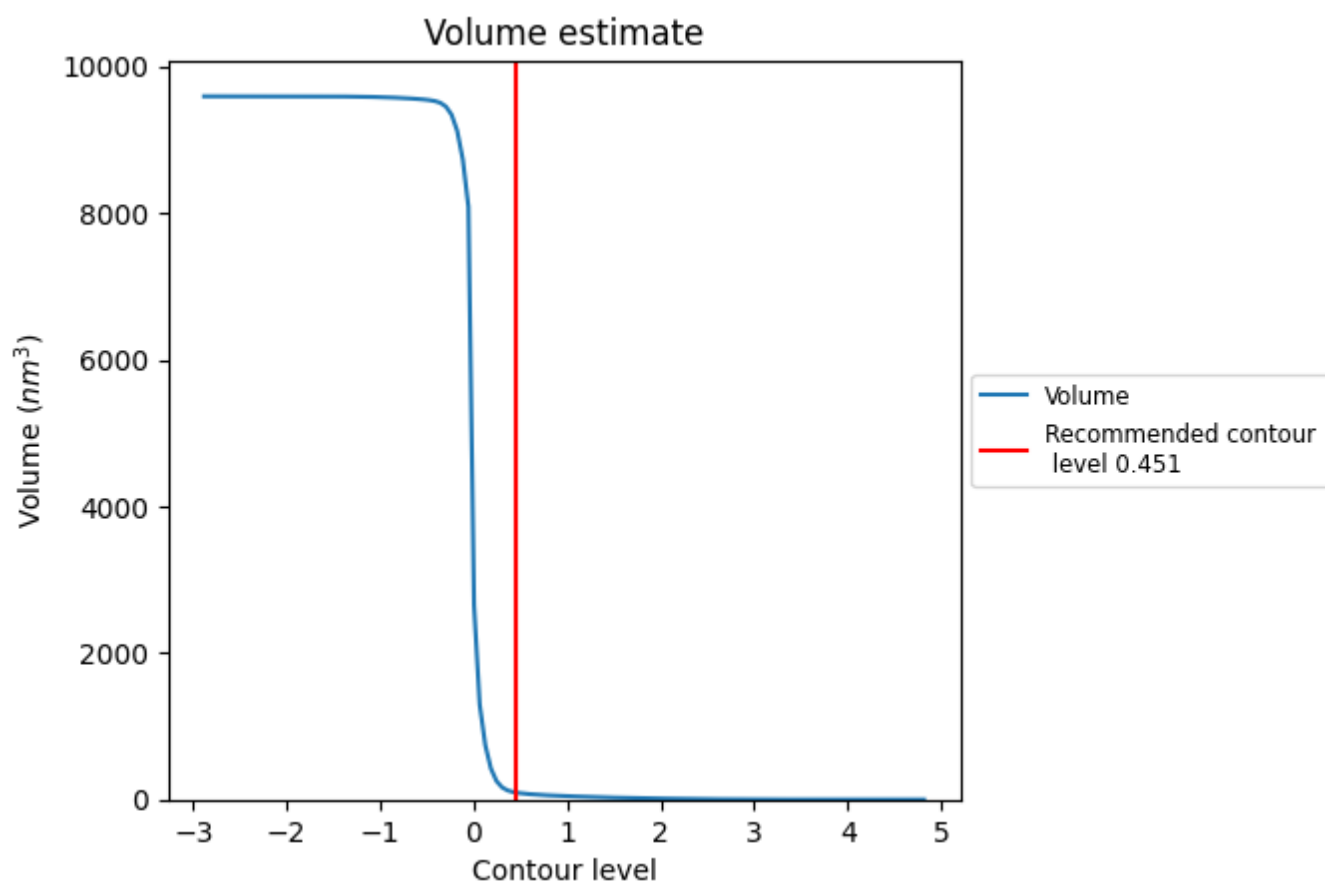
This section contains the results of statistical analysis of the map.

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.

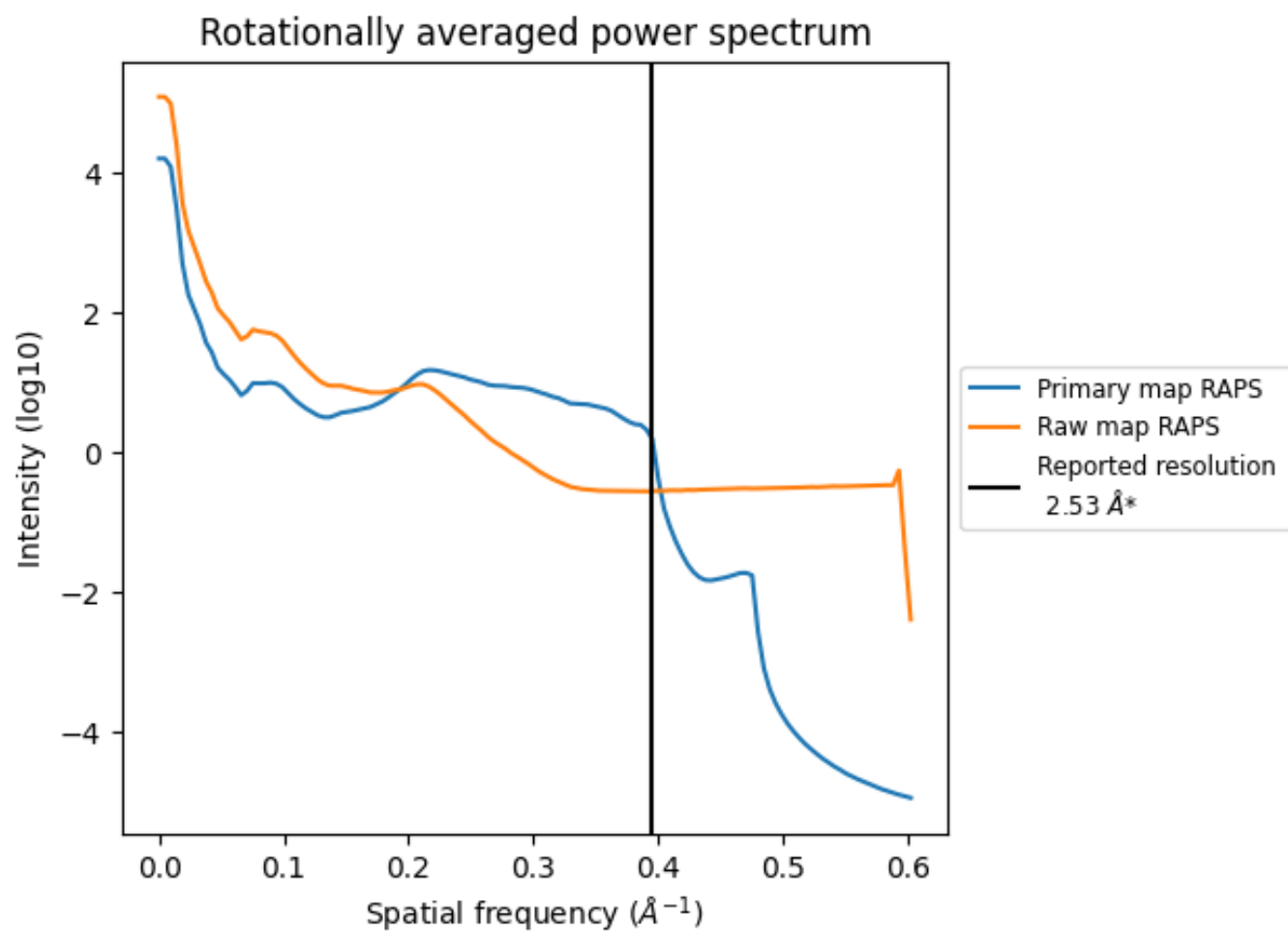
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 96 nm³; this corresponds to an approximate mass of 87 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 ⓘ

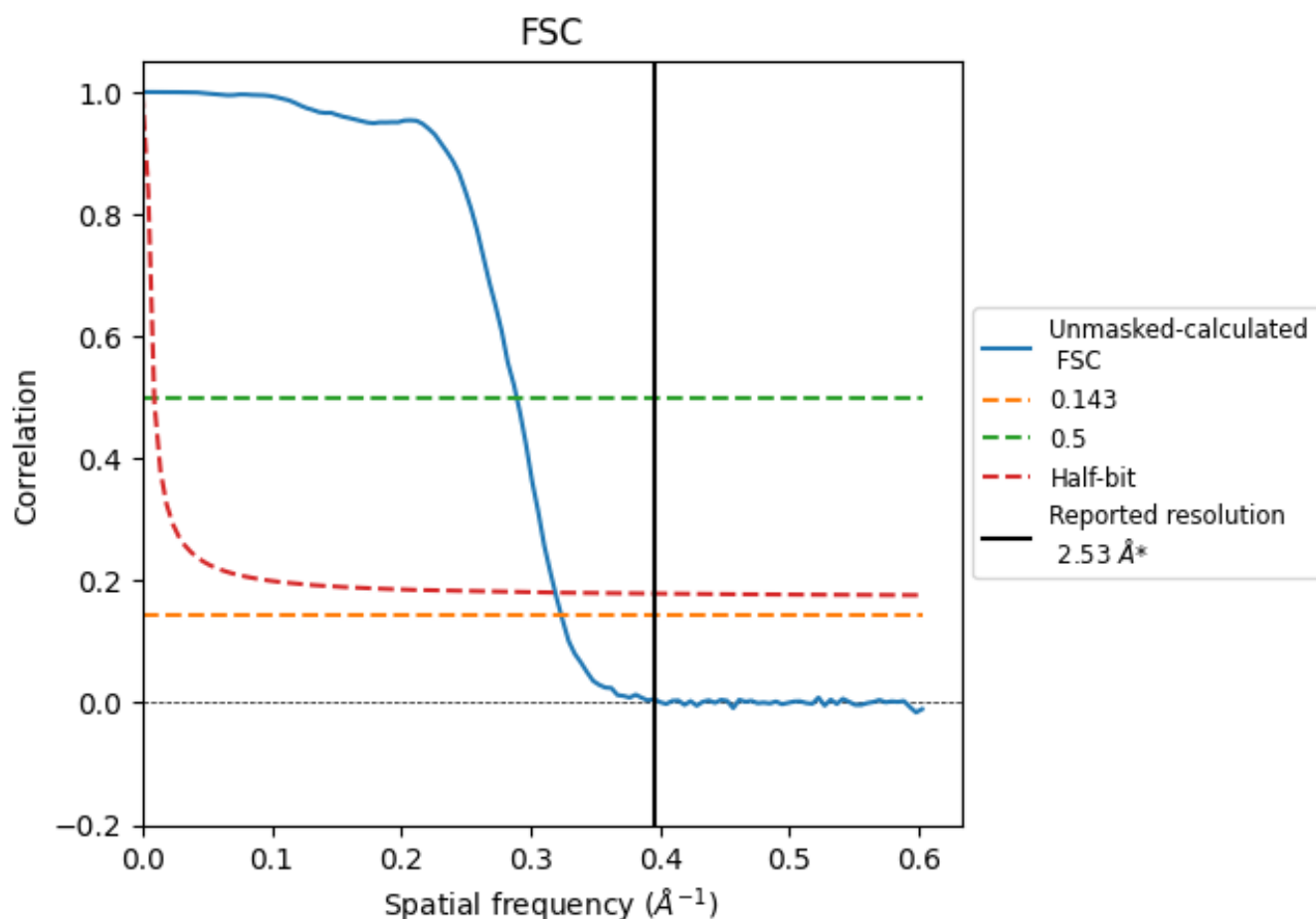


*Reported resolution corresponds to spatial frequency of $0.395 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.395 Å⁻¹

8.2 Resolution estimates [i](#)

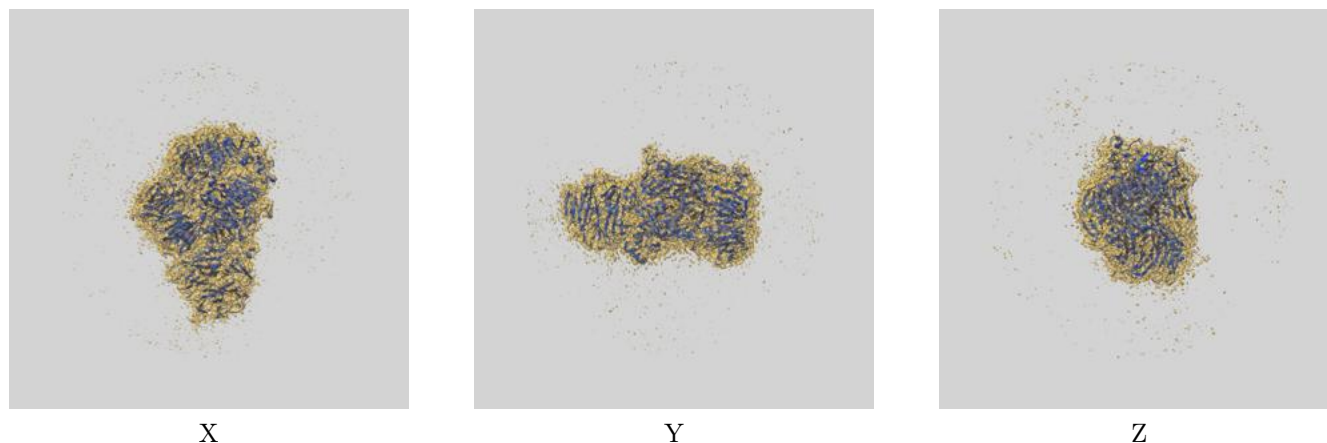
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.53	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.09	3.46	3.13

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.09 differs from the reported value 2.53 by more than 10 %

9 Map-model fit [i](#)

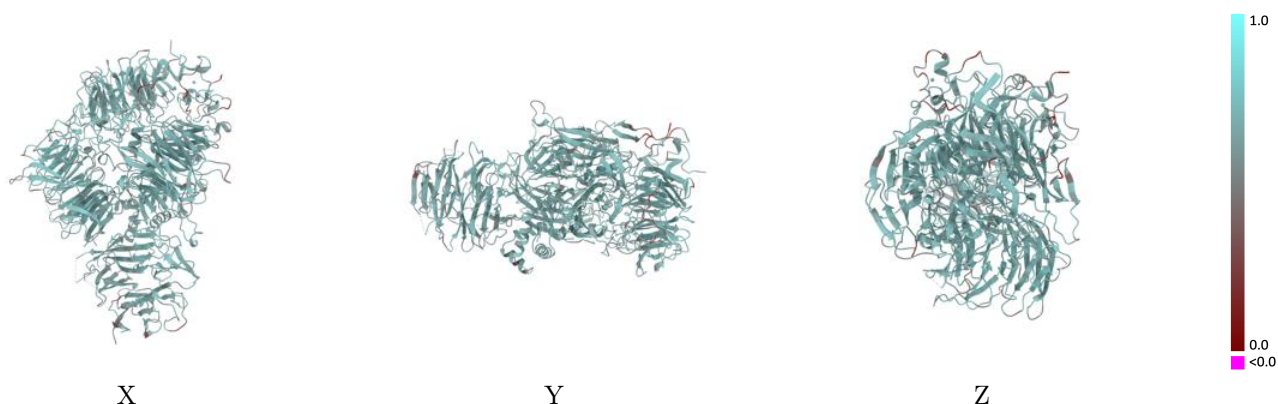
This section contains information regarding the fit between EMDB map EMD-27866 and PDB model 8E3I. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

9.1 Map-model overlay [i](#)



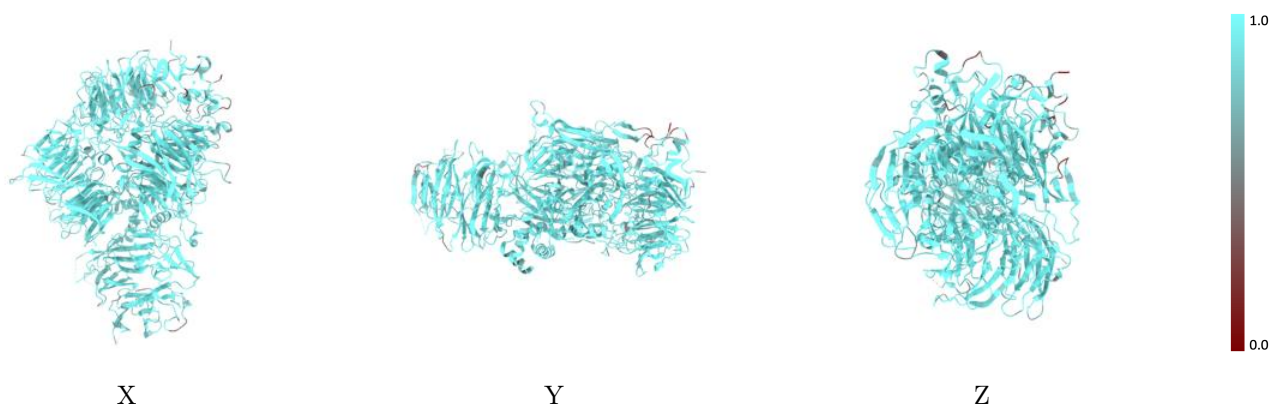
The images above show the 3D surface view of the map at the recommended contour level 0.451 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



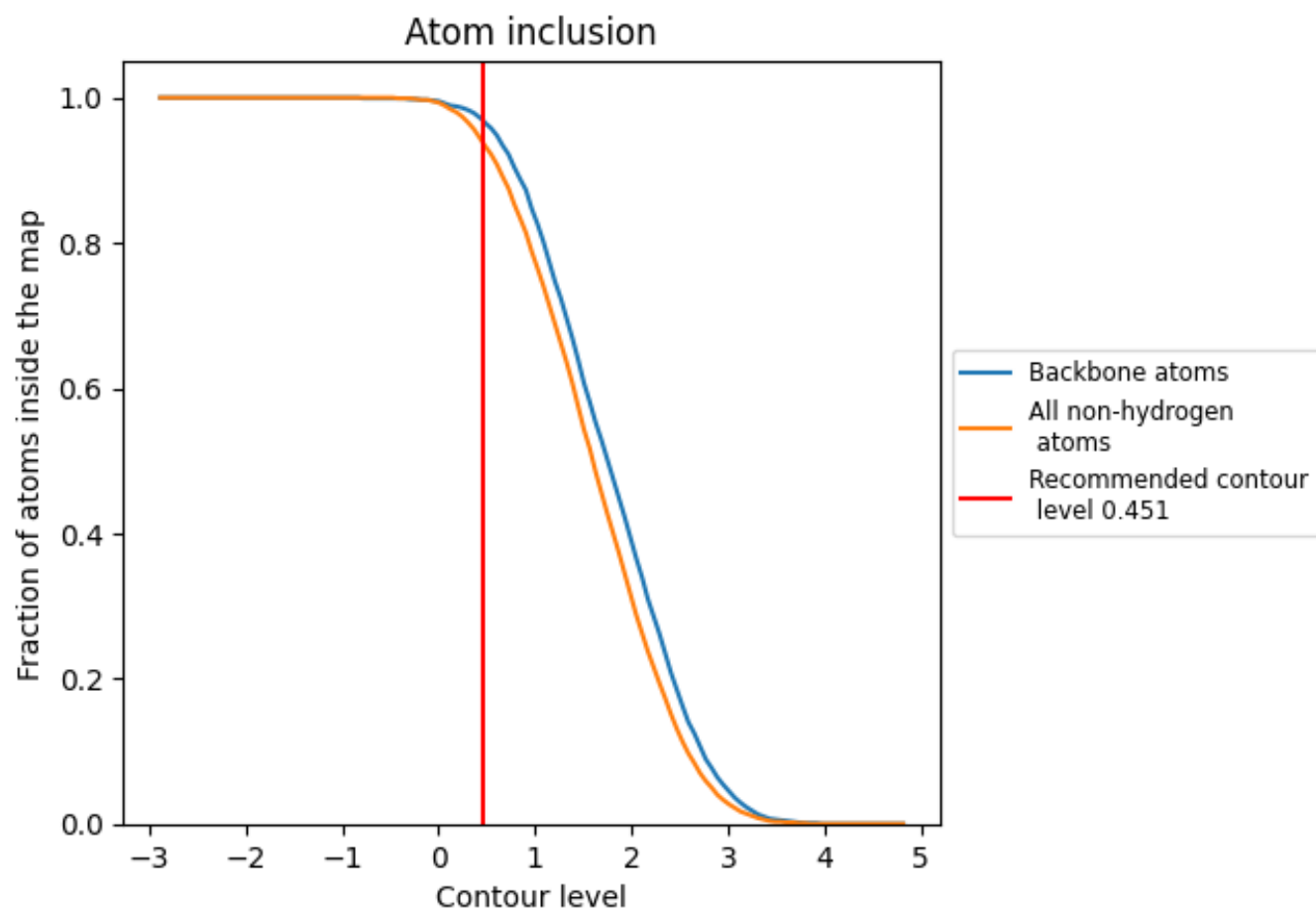
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.451).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 94% 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 (0.451) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9400	0.6320
A	0.9450	0.6340
B	0.9590	0.6460
C	0.8290	0.5600
E	1.0000	0.6570

