wwPDB EM Validation Summary Report

Nov 20, 2022 – 03:35 PM JST

PDB ID	:	7BZY
EMDB ID	:	EMD-30263
Title	:	Hsp21-DXPS
Authors	:	Lau, W.C.Y.
Deposited on	:	2020-04-29
Resolution	:	3.70 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:

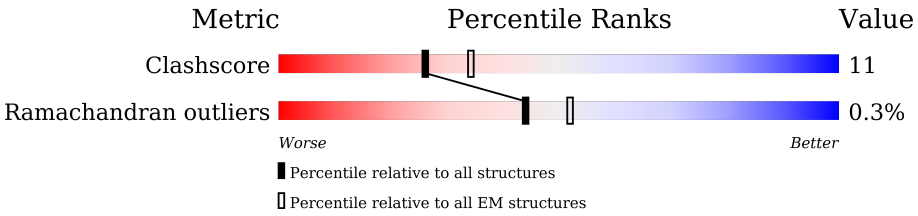
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 3.70 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023

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 <=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	11	691	
1	13	691	
2	12	207	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6169 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 1-deoxy-D-xylulose-5-phosphate synthase, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	11	584	Total 2857	C 1691	N 584	O 582	0	0
1	13	584	Total 2857	C 1691	N 584	O 582	0	0

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
11	41	MET	-	expression tag	UNP Q38854
11	42	ALA	-	expression tag	UNP Q38854
11	43	ASP	-	expression tag	UNP Q38854
11	44	LEU	-	expression tag	UNP Q38854
11	45	ASN	-	expression tag	UNP Q38854
11	46	TRP	-	expression tag	UNP Q38854
11	47	ILE	-	expression tag	UNP Q38854
11	48	SER	-	expression tag	UNP Q38854
11	49	ALA	-	expression tag	UNP Q38854
11	50	GLY	-	expression tag	UNP Q38854
11	51	HIS	-	expression tag	UNP Q38854
11	52	ALA	-	expression tag	UNP Q38854
11	53	ILE	-	expression tag	UNP Q38854
11	54	ALA	-	expression tag	UNP Q38854
11	55	ASP	-	expression tag	UNP Q38854
11	56	VAL	-	expression tag	UNP Q38854
11	57	GLY	-	expression tag	UNP Q38854
11	58	THR	-	expression tag	UNP Q38854
11	718	HIS	-	expression tag	UNP Q38854
11	719	HIS	-	expression tag	UNP Q38854
11	720	HIS	-	expression tag	UNP Q38854
11	721	HIS	-	expression tag	UNP Q38854
11	722	HIS	-	expression tag	UNP Q38854
11	723	HIS	-	expression tag	UNP Q38854
11	724	ASP	-	expression tag	UNP Q38854
11	725	TYR	-	expression tag	UNP Q38854

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Chain	Residue	Modelled	Actual	Comment	Reference
11	726	LYS	-	expression tag	UNP Q38854
11	727	ASP	-	expression tag	UNP Q38854
11	728	ASP	-	expression tag	UNP Q38854
11	729	ASP	-	expression tag	UNP Q38854
11	730	ASP	-	expression tag	UNP Q38854
11	731	LYS	-	expression tag	UNP Q38854
13	41	MET	-	expression tag	UNP Q38854
13	42	ALA	-	expression tag	UNP Q38854
13	43	ASP	-	expression tag	UNP Q38854
13	44	LEU	-	expression tag	UNP Q38854
13	45	ASN	-	expression tag	UNP Q38854
13	46	TRP	-	expression tag	UNP Q38854
13	47	ILE	-	expression tag	UNP Q38854
13	48	SER	-	expression tag	UNP Q38854
13	49	ALA	-	expression tag	UNP Q38854
13	50	GLY	-	expression tag	UNP Q38854
13	51	HIS	-	expression tag	UNP Q38854
13	52	ALA	-	expression tag	UNP Q38854
13	53	ILE	-	expression tag	UNP Q38854
13	54	ALA	-	expression tag	UNP Q38854
13	55	ASP	-	expression tag	UNP Q38854
13	56	VAL	-	expression tag	UNP Q38854
13	57	GLY	-	expression tag	UNP Q38854
13	58	THR	-	expression tag	UNP Q38854
13	718	HIS	-	expression tag	UNP Q38854
13	719	HIS	-	expression tag	UNP Q38854
13	720	HIS	-	expression tag	UNP Q38854
13	721	HIS	-	expression tag	UNP Q38854
13	722	HIS	-	expression tag	UNP Q38854
13	723	HIS	-	expression tag	UNP Q38854
13	724	ASP	-	expression tag	UNP Q38854
13	725	TYR	-	expression tag	UNP Q38854
13	726	LYS	-	expression tag	UNP Q38854
13	727	ASP	-	expression tag	UNP Q38854
13	728	ASP	-	expression tag	UNP Q38854
13	729	ASP	-	expression tag	UNP Q38854
13	730	ASP	-	expression tag	UNP Q38854
13	731	LYS	-	expression tag	UNP Q38854

- Molecule 2 is a protein called Heat shock protein 21, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	12	92	Total	C	N	O	0	0
			455	271	92	92		

There are 23 discrepancies between the modelled and reference sequences:

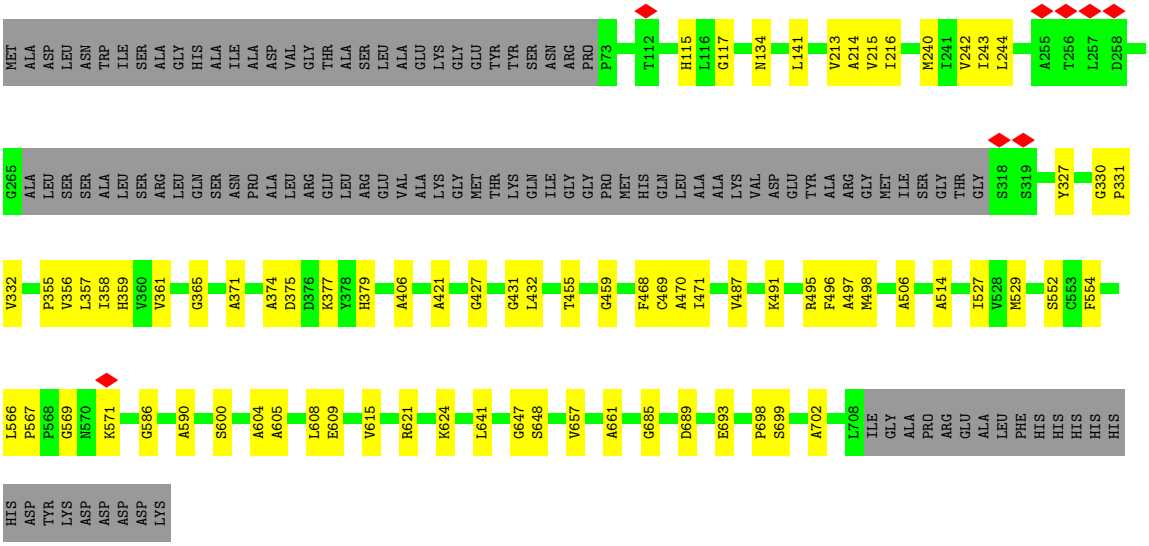
Chain	Residue	Modelled	Actual	Comment	Reference
12	21	MET	-	expression tag	UNP P31170
12	22	GLY	-	expression tag	UNP P31170
12	23	SER	-	expression tag	UNP P31170
12	24	SER	-	expression tag	UNP P31170
12	25	HIS	-	expression tag	UNP P31170
12	26	HIS	-	expression tag	UNP P31170
12	27	HIS	-	expression tag	UNP P31170
12	28	HIS	-	expression tag	UNP P31170
12	29	HIS	-	expression tag	UNP P31170
12	30	HIS	-	expression tag	UNP P31170
12	31	SER	-	expression tag	UNP P31170
12	32	GLN	-	expression tag	UNP P31170
12	33	ASP	-	expression tag	UNP P31170
12	34	PRO	-	expression tag	UNP P31170
12	35	ASN	-	expression tag	UNP P31170
12	36	SER	-	expression tag	UNP P31170
12	37	GLU	-	expression tag	UNP P31170
12	38	ASN	-	expression tag	UNP P31170
12	39	LEU	-	expression tag	UNP P31170
12	40	TYR	-	expression tag	UNP P31170
12	41	PHE	-	expression tag	UNP P31170
12	42	GLN	-	expression tag	UNP P31170
12	43	SER	-	expression tag	UNP P31170

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.

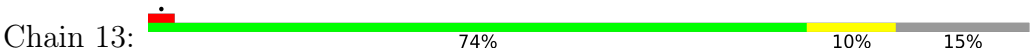
• Molecule 1: 1-deoxy-D-xylulose-5-phosphate synthase, chloroplastic

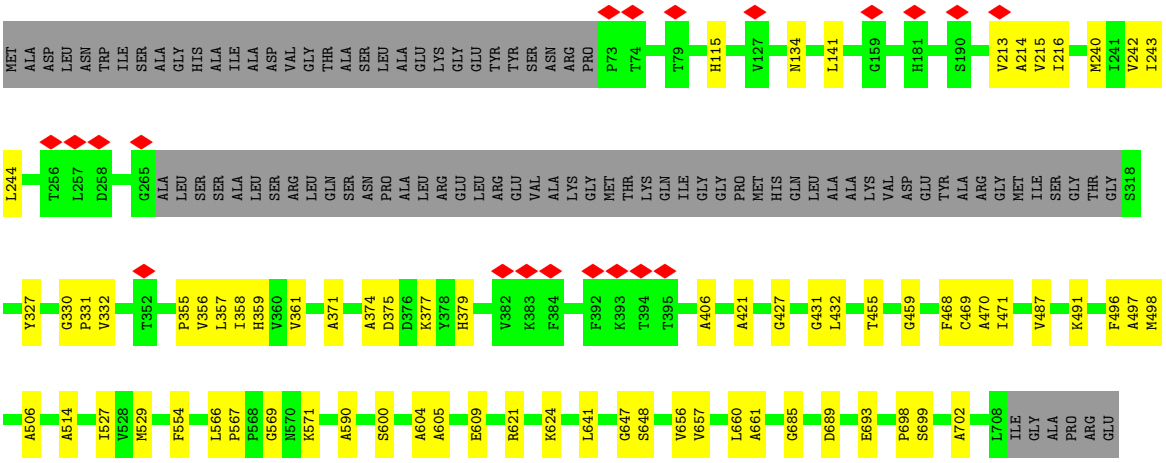
Chain 11:



• Molecule 1: 1-deoxy-D-xylulose-5-phosphate synthase, chloroplastic

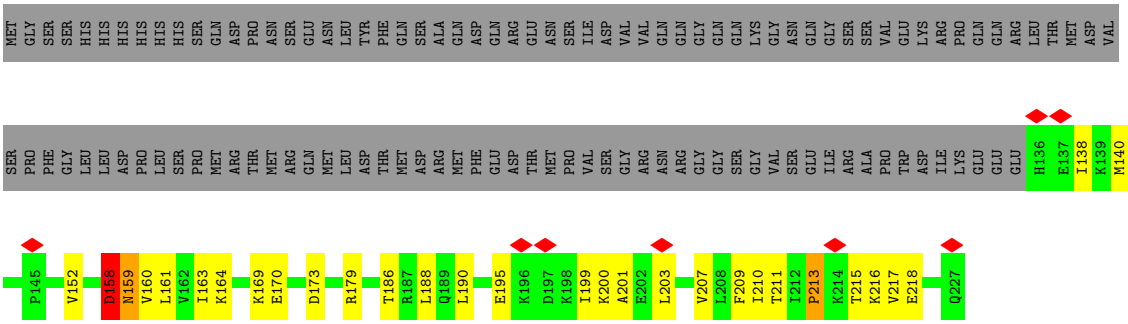
Chain 13:





• Molecule 2: Heat shock protein 21, chloroplastic

Chain 12:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	162426	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 ($e^-/Å^2$)	45	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.096	Depositor
Minimum map value	-0.045	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.007	Depositor
Map size (Å)	197.76, 197.76, 197.76	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.03, 1.03, 1.03	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	11	0.34	1/2855 (0.0%)	0.51	0/3958
1	13	0.33	1/2855 (0.0%)	0.51	0/3958
2	12	0.31	0/454	0.70	0/631
All	All	0.33	2/6164 (0.0%)	0.52	0/8547

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	12	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	11	134	ASN	C-N	-6.76	1.18	1.34
1	13	134	ASN	C-N	-6.75	1.18	1.34

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	12	158	ASP	Peptide
2	12	213	PRO	Peptide
2	12	215	THR	Peptide
2	12	216	LYS	Peptide

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	11	2857	0	1362	45	0
1	13	2857	0	1362	42	0
2	12	455	0	188	15	0
All	All	6169	0	2912	102	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 11.

The worst 5 of 102 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)
2:12:163:ILE:O	2:12:186:THR:CB	2.32	0.77
1:13:214:ALA:O	1:13:243:ILE:N	2.18	0.77
1:11:214:ALA:O	1:11:243:ILE:N	2.18	0.75
1:11:327:TYR:O	1:11:357:LEU:N	2.18	0.73
1:13:327:TYR:O	1:13:357:LEU:N	2.18	0.73

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	11	580/691 (84%)	498 (86%)	82 (14%)	0	100 100
1	13	580/691 (84%)	498 (86%)	82 (14%)	0	100 100
2	12	90/207 (44%)	62 (69%)	24 (27%)	4 (4%)	2 24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1250/1589 (79%)	1058 (85%)	188 (15%)	4 (0%)	44 74

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	12	159	ASN
2	12	158	ASP
2	12	217	VAL
2	12	218	GLU

5.3.2 Protein sidechains (i)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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)

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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	11	1
1	13	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	11	134:ASN	C	135:THR	N	1.18
1	13	134:ASN	C	135:THR	N	1.18

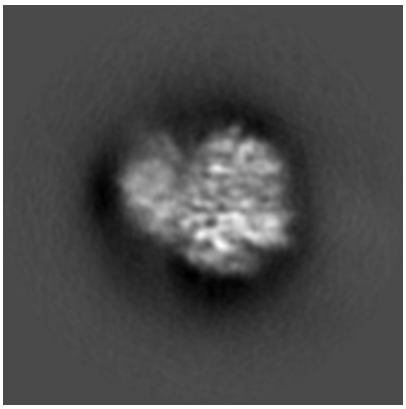
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-30263. These allow visual inspection of the internal detail of the map and identification of artifacts.

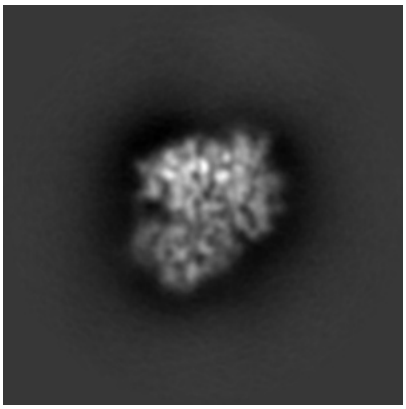
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

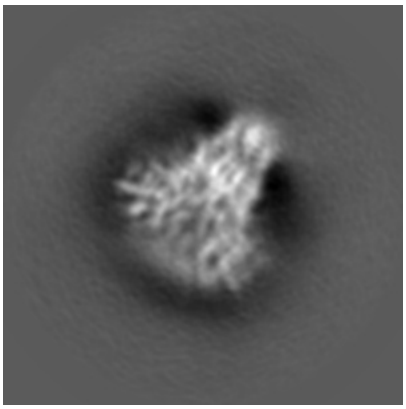
6.1.1 Primary map



X

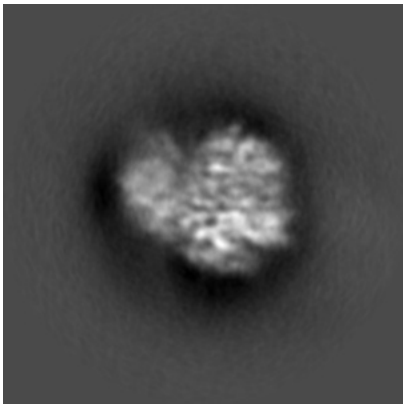


Y



Z

6.1.2 Raw map



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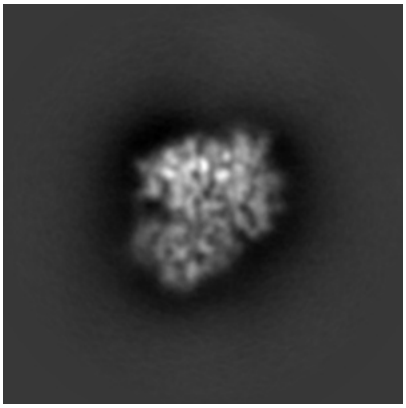
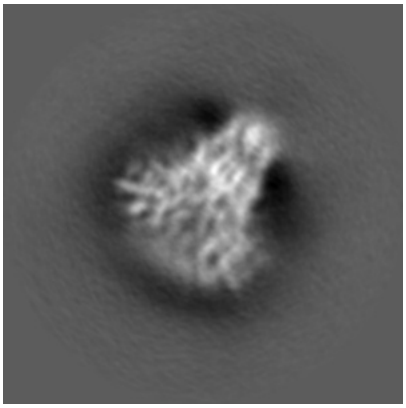


Y

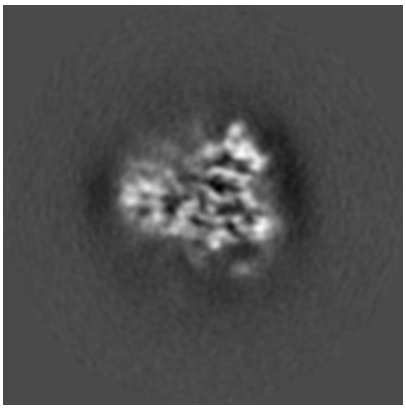


Z

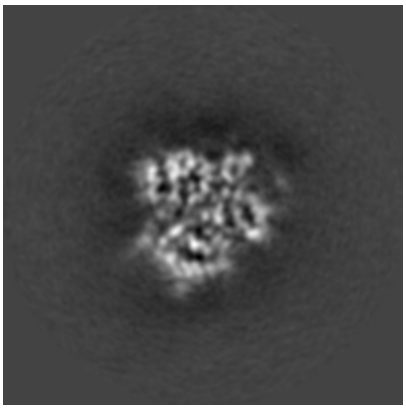
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

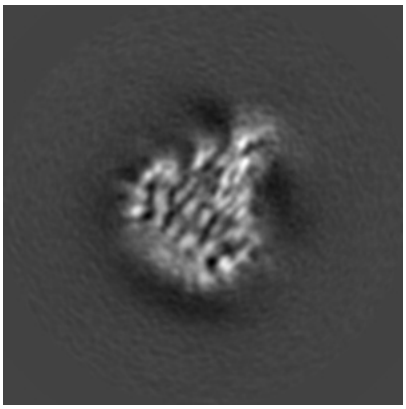
6.2.1 Primary map



X Index: 96

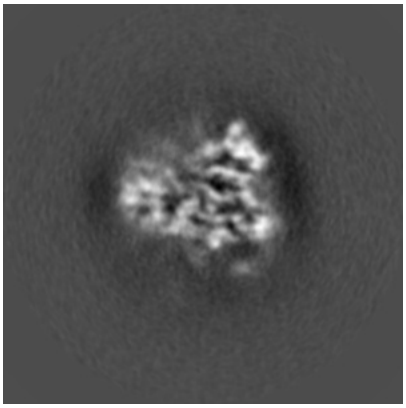


Y Index: 96

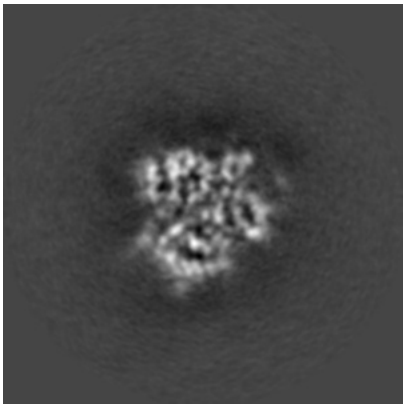


Z Index: 96

6.2.2 Raw map



X Index: 96



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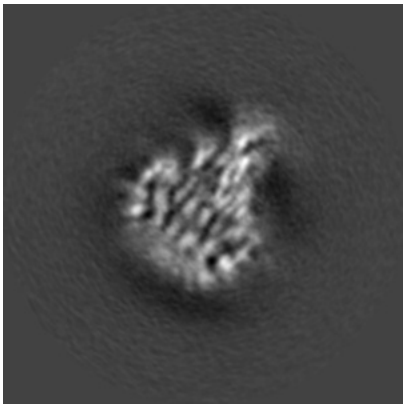
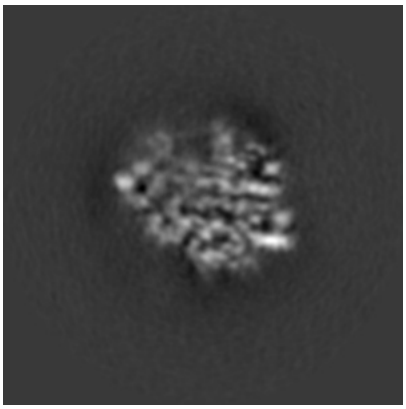


Z Index: 96

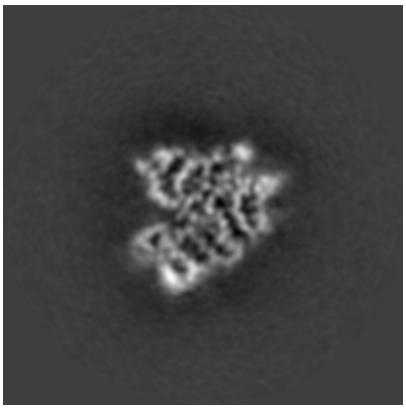
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 110



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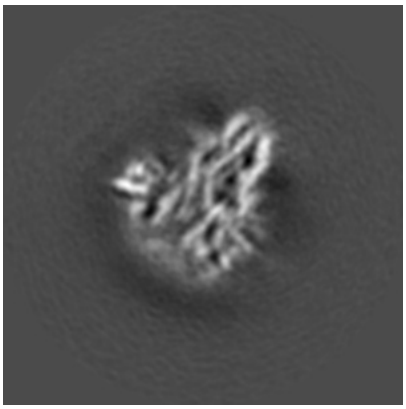
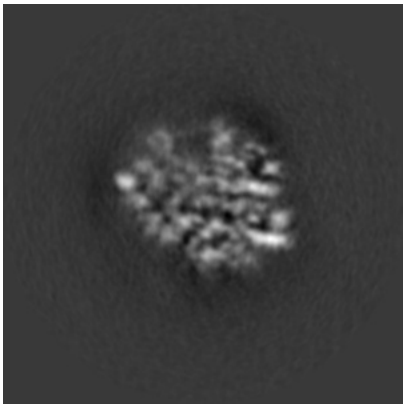
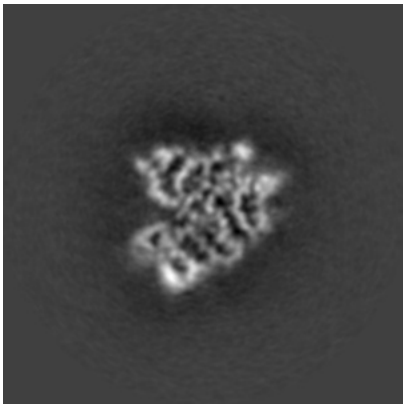


Z Index: 90

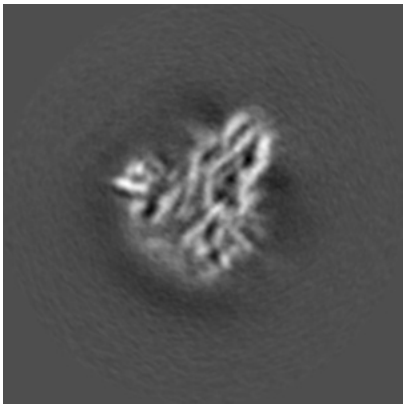
6.3.2 Raw map



X Index: 109



Y Index: 103

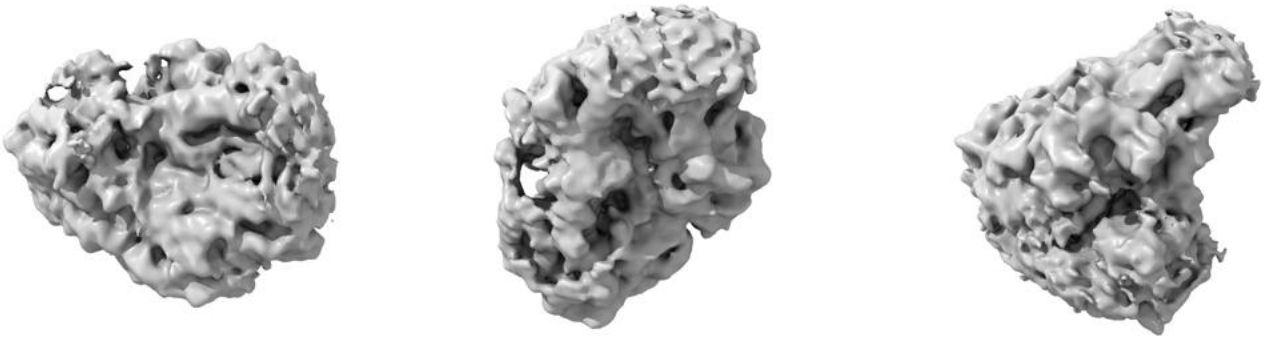


Z Index: 90

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

6.4 Orthogonal surface views (i)

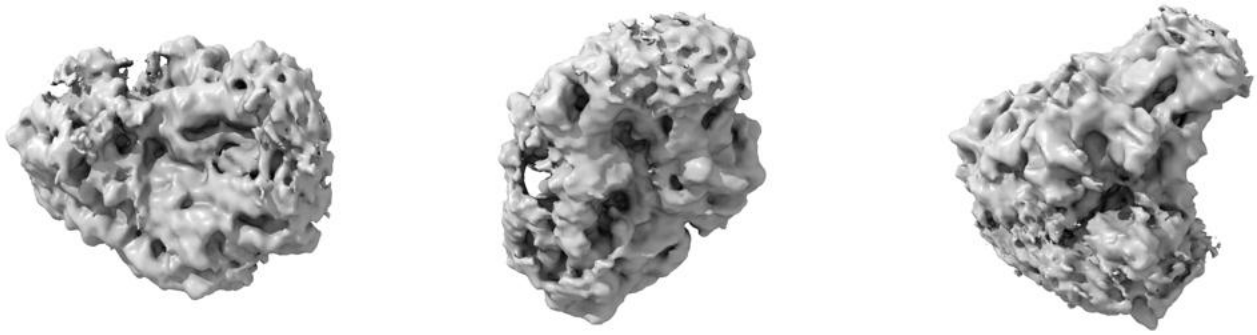
6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.007. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



X Y Z

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.

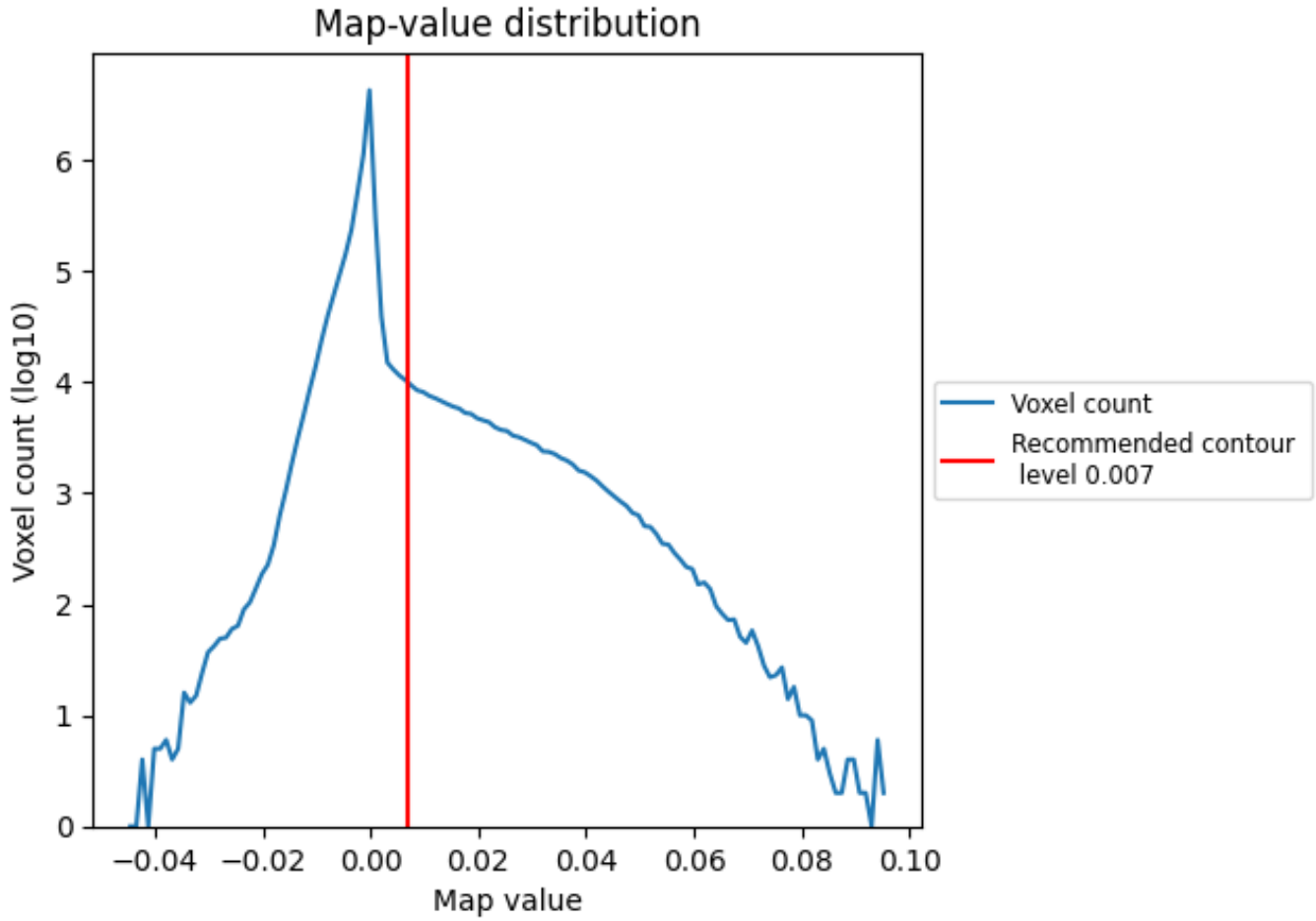
6.5 Mask visualisation (i)

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

7 Map analysis

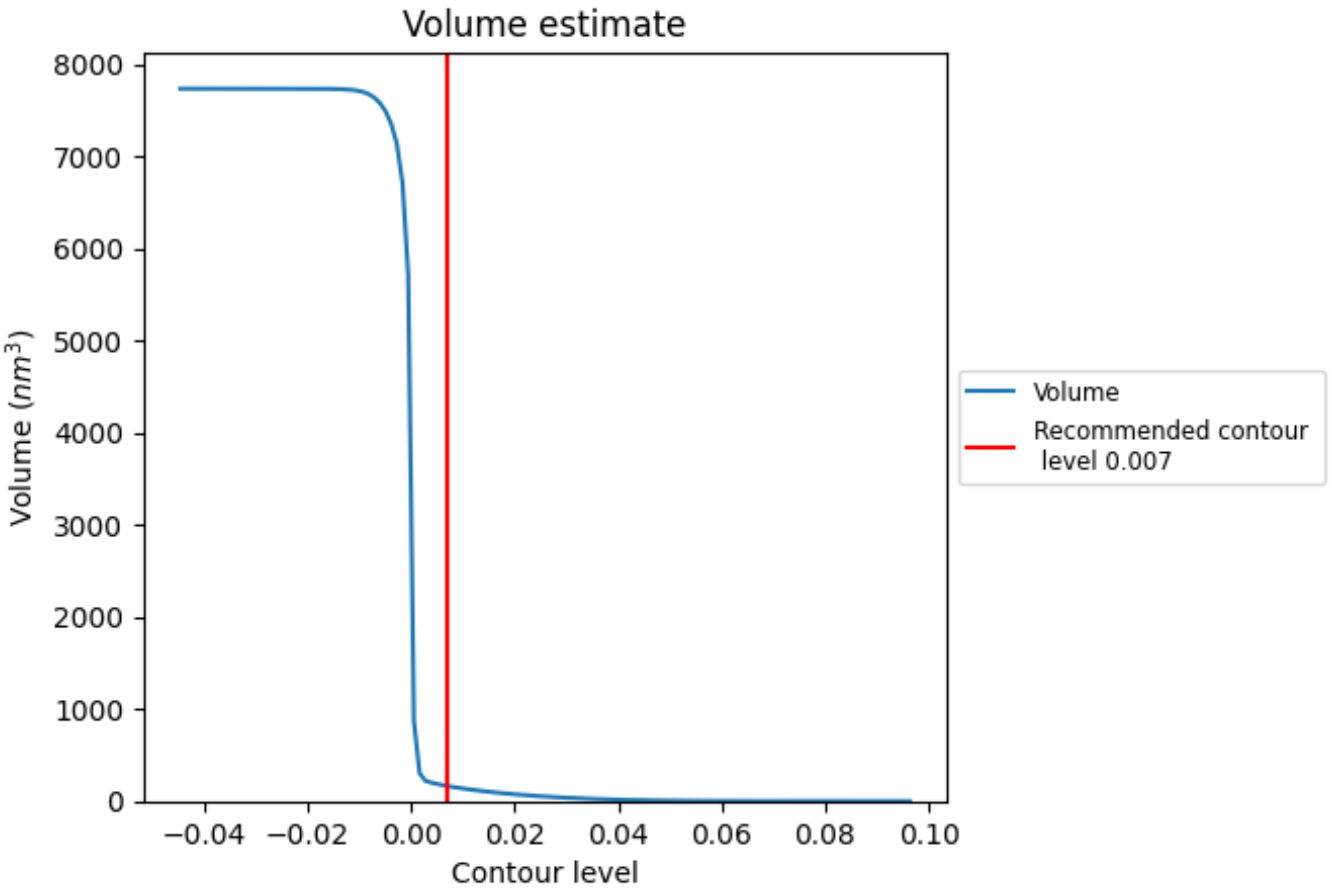
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

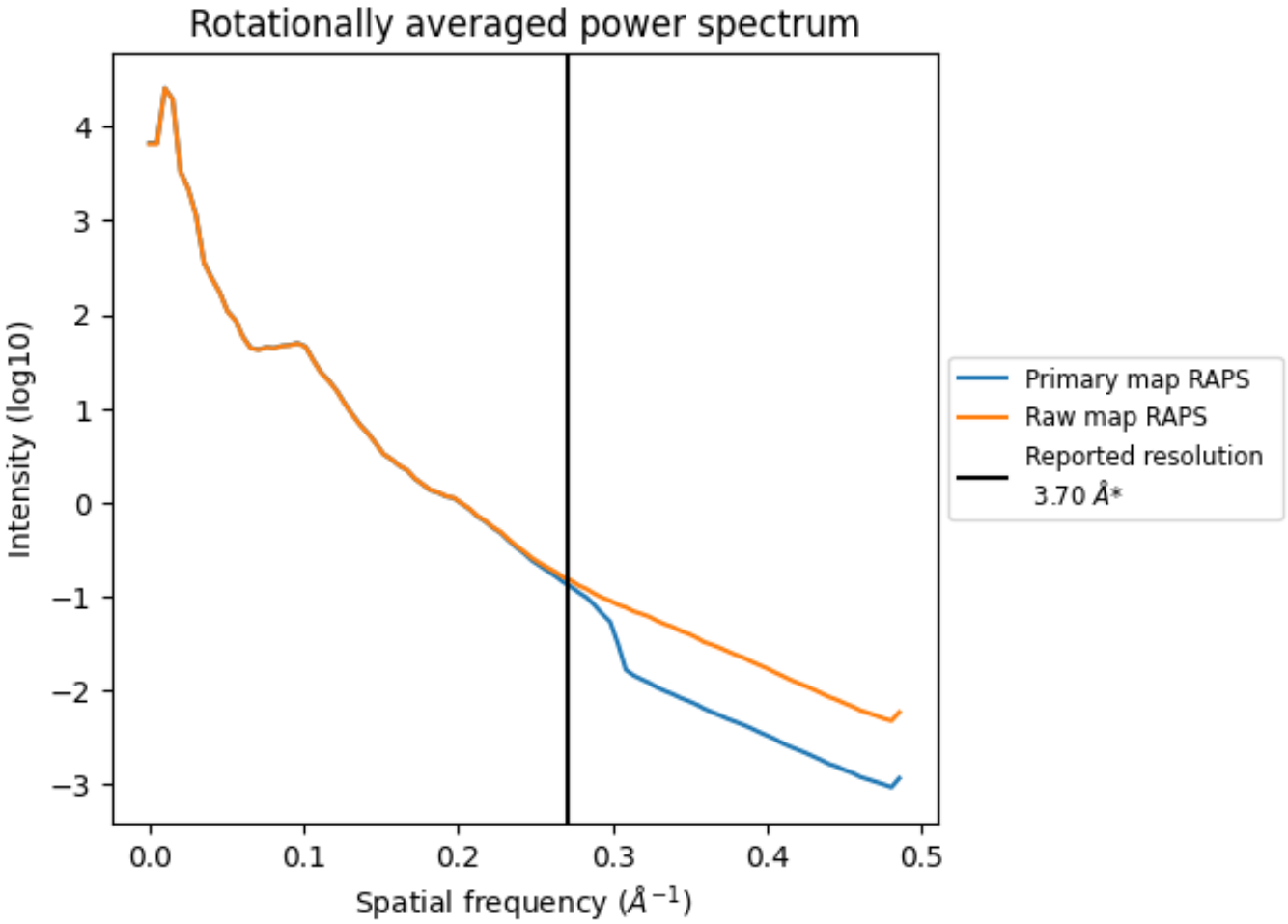
7.2 Volume estimate (i)



The volume at the recommended contour level is 164 nm^3; this corresponds to an approximate mass of 149 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)

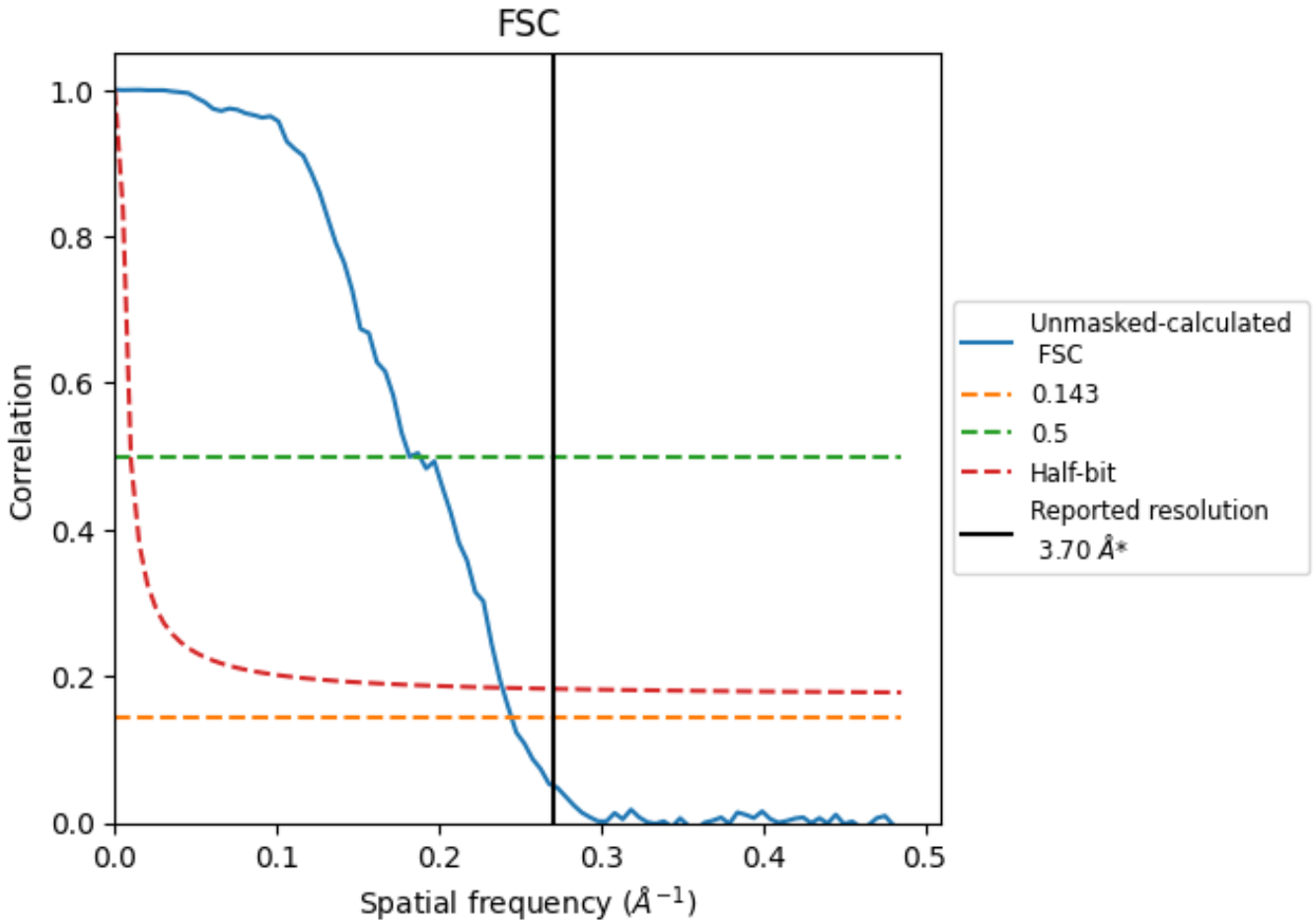


*Reported resolution corresponds to spatial frequency of 0.270 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.270 Å^{-1}

8.2 Resolution estimates (i)

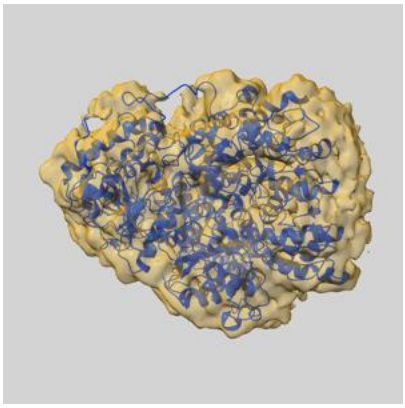
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.08	5.50	4.18

*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 4.08 differs from the reported value 3.7 by more than 10 %

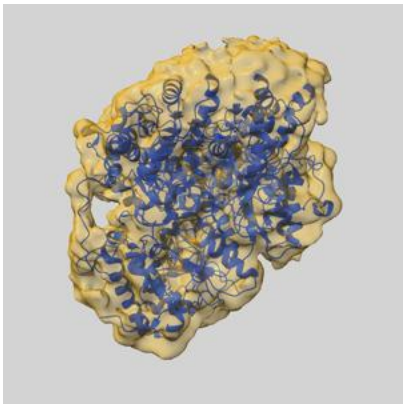
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-30263 and PDB model 7BZY. Per-residue inclusion information can be found in section 3 on page 6.

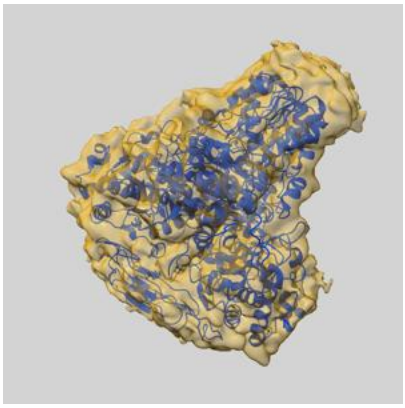
9.1 Map-model overlay



X



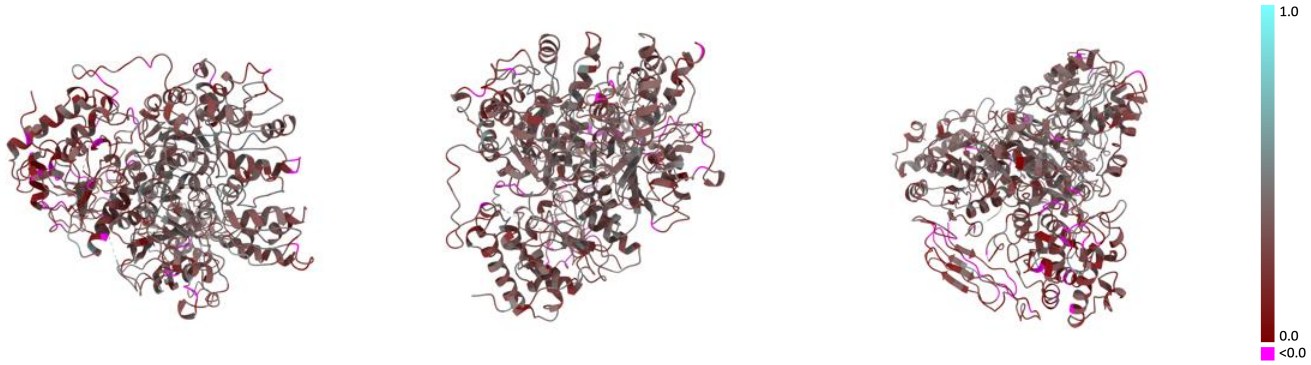
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.007 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.

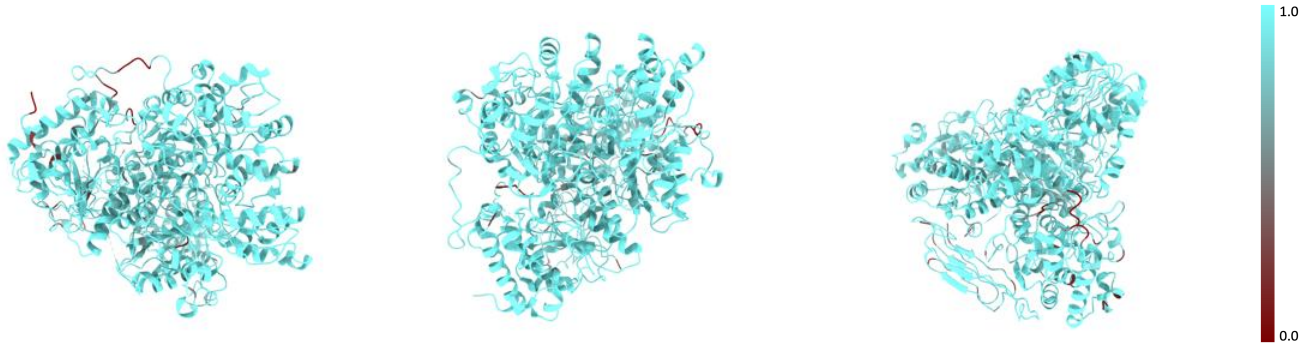
9.2 Q-score mapped to coordinate model



X Y Z

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

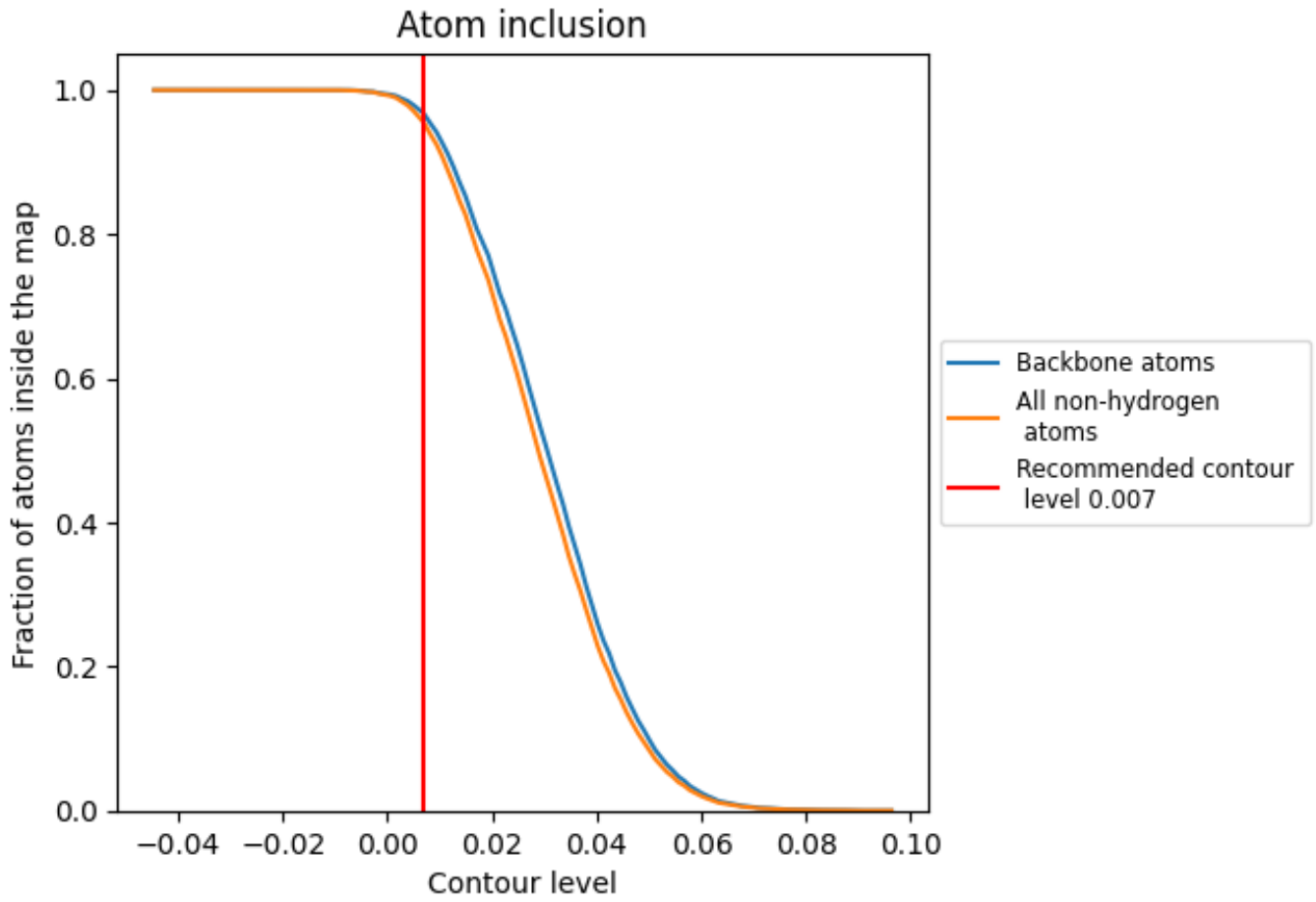
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.007).

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 (i)

The table lists the average atom inclusion at the recommended contour level (0.007) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9543	0.3050
11	0.9706	0.3390
12	0.9011	0.1310
13	0.9464	0.2980