wwPDB EM Validation Summary Report (i)

Feb 27, 2023 – 01:49 PM EST

PDB ID	:	8DTF
EMDB ID	:	EMD-27696
Title	:	Cryo-EM structure of the full length Arabidopsis SPY with complete TPRs
Authors	:	Kumar, S.; Zhou, Y.; Dillard, L.; Borgnia, M.J.; Bartesaghi, A.; Zhou, P.
Deposited on	:	2022-07-25
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 (i) 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 (i)) were used in the production of this report:

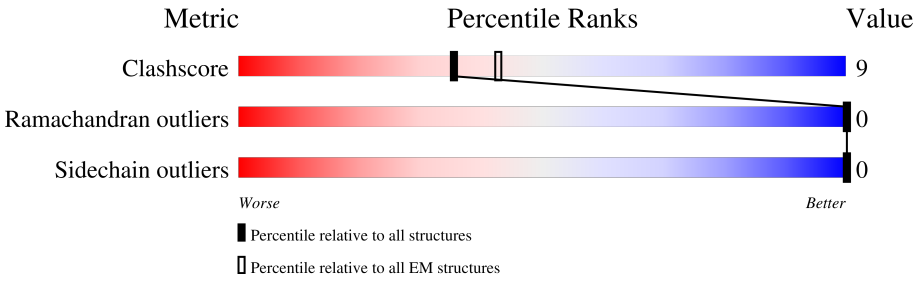
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

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
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 <=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	946	69% 16% 15%
1	B	946	69% 16% 15%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 12414 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 Probable UDP-N-acetylglucosamine--peptide N-acetylglucosaminyltransferase SPINDLY.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	803	Total	C	N	O	S	0	0
			6203	3951	1035	1169	48		
1	B	803	Total	C	N	O	S	0	0
			6211	3956	1036	1171	48		

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	915	GLY	-	expression tag	UNP Q96301
A	916	GLY	-	expression tag	UNP Q96301
A	917	SER	-	expression tag	UNP Q96301
A	918	GLU	-	expression tag	UNP Q96301
A	919	ASN	-	expression tag	UNP Q96301
A	920	LEU	-	expression tag	UNP Q96301
A	921	TYR	-	expression tag	UNP Q96301
A	922	PHE	-	expression tag	UNP Q96301
A	923	GLN	-	expression tag	UNP Q96301
A	924	GLY	-	expression tag	UNP Q96301
A	925	GLY	-	expression tag	UNP Q96301
A	926	SER	-	expression tag	UNP Q96301
A	927	HIS	-	expression tag	UNP Q96301
A	928	HIS	-	expression tag	UNP Q96301
A	929	HIS	-	expression tag	UNP Q96301
A	930	HIS	-	expression tag	UNP Q96301
A	931	HIS	-	expression tag	UNP Q96301
A	932	HIS	-	expression tag	UNP Q96301
A	933	HIS	-	expression tag	UNP Q96301
A	934	HIS	-	expression tag	UNP Q96301
A	935	HIS	-	expression tag	UNP Q96301
A	936	HIS	-	expression tag	UNP Q96301
A	937	GLY	-	expression tag	UNP Q96301
A	938	GLY	-	expression tag	UNP Q96301
A	939	TRP	-	expression tag	UNP Q96301

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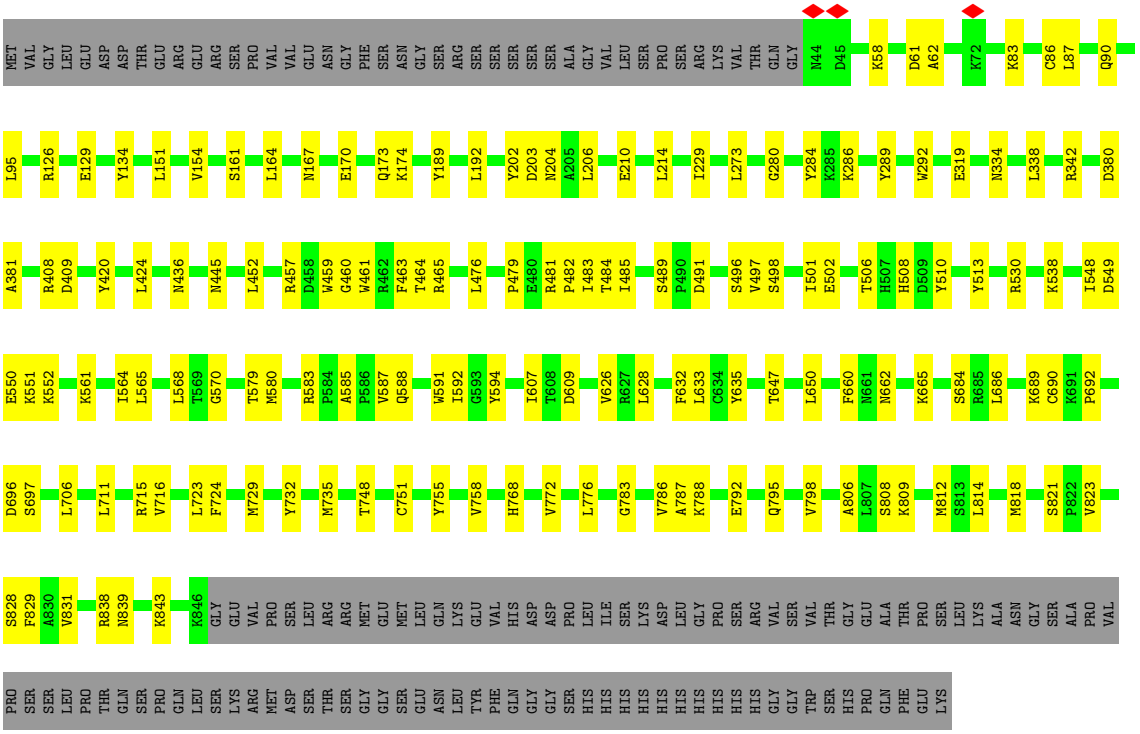
Chain	Residue	Modelled	Actual	Comment	Reference
A	940	SER	-	expression tag	UNP Q96301
A	941	HIS	-	expression tag	UNP Q96301
A	942	PRO	-	expression tag	UNP Q96301
A	943	GLN	-	expression tag	UNP Q96301
A	944	PHE	-	expression tag	UNP Q96301
A	945	GLU	-	expression tag	UNP Q96301
A	946	LYS	-	expression tag	UNP Q96301
B	915	GLY	-	expression tag	UNP Q96301
B	916	GLY	-	expression tag	UNP Q96301
B	917	SER	-	expression tag	UNP Q96301
B	918	GLU	-	expression tag	UNP Q96301
B	919	ASN	-	expression tag	UNP Q96301
B	920	LEU	-	expression tag	UNP Q96301
B	921	TYR	-	expression tag	UNP Q96301
B	922	PHE	-	expression tag	UNP Q96301
B	923	GLN	-	expression tag	UNP Q96301
B	924	GLY	-	expression tag	UNP Q96301
B	925	GLY	-	expression tag	UNP Q96301
B	926	SER	-	expression tag	UNP Q96301
B	927	HIS	-	expression tag	UNP Q96301
B	928	HIS	-	expression tag	UNP Q96301
B	929	HIS	-	expression tag	UNP Q96301
B	930	HIS	-	expression tag	UNP Q96301
B	931	HIS	-	expression tag	UNP Q96301
B	932	HIS	-	expression tag	UNP Q96301
B	933	HIS	-	expression tag	UNP Q96301
B	934	HIS	-	expression tag	UNP Q96301
B	935	HIS	-	expression tag	UNP Q96301
B	936	HIS	-	expression tag	UNP Q96301
B	937	GLY	-	expression tag	UNP Q96301
B	938	GLY	-	expression tag	UNP Q96301
B	939	TRP	-	expression tag	UNP Q96301
B	940	SER	-	expression tag	UNP Q96301
B	941	HIS	-	expression tag	UNP Q96301
B	942	PRO	-	expression tag	UNP Q96301
B	943	GLN	-	expression tag	UNP Q96301
B	944	PHE	-	expression tag	UNP Q96301
B	945	GLU	-	expression tag	UNP Q96301
B	946	LYS	-	expression tag	UNP Q96301

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.

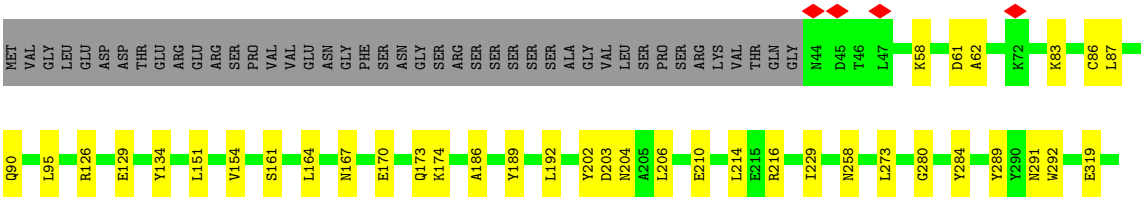
• Molecule 1: Probable UDP-N-acetylglucosamine--peptide N-acetylglucosaminyltransferase SPINDLY

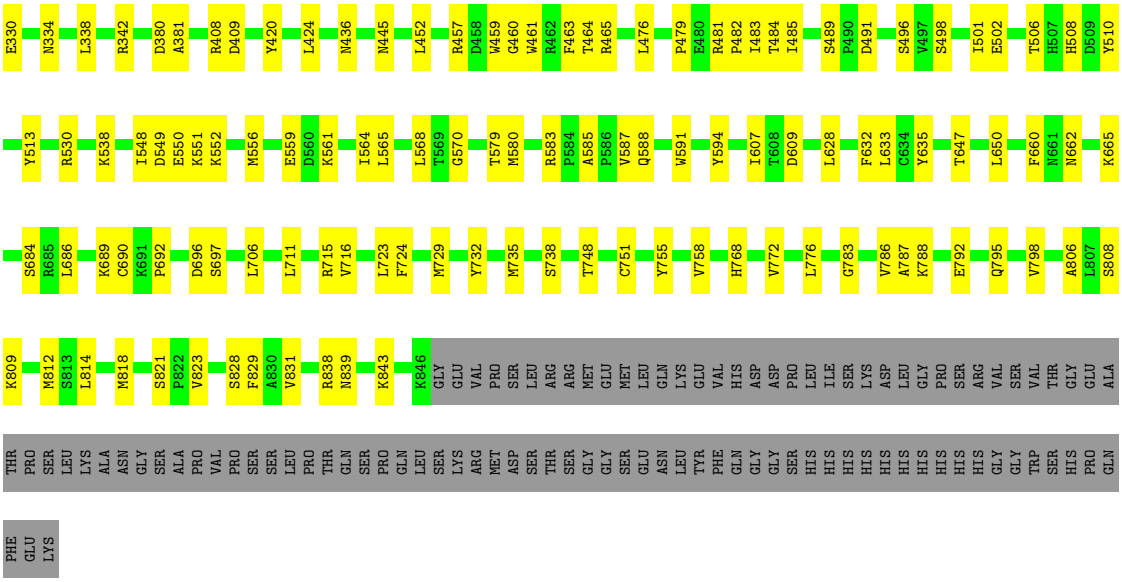
Chain A:



• Molecule 1: Probable UDP-N-acetylglucosamine--peptide N-acetylglucosaminyltransferase SPINDLY

Chain B:




E330 N334 L338 R342 D380 A381 R408 D409 Y420 L424 N436 N445 L452 R457 D458 W459 G460 W461 R462 F463 T464 R465 L476 P479 E480 R481 P482 I483 T484 I485 S489 P490 D491 S496 V497 S498 I501 E502 T506 H507 H508 D509 Y510
Y513 R530 K538 I548 D549 E550 K551 K552 M556 E559 D560 K561 I564 L565 L568 T569 G570 T579 M580 R583 P584 A585 P586 V587 Q588 W591 Y594 I607 T608 D609 L628 F632 L633 C634 Y635 T647 L650 F660 N661 N662 K665
S684 R685 L686 K689 C690 K691 P692 D696 S697 L706 L711 R715 V716 L723 F724 M729 Y732 M735 S738 T748 C751 Y755 V758 H768 V772 L776 G783 V786 A787 K788 E792 Q795 V798 A806 L807 S808
K809 M812 S813 L814 M818 S821 P822 V823 S828 F829 A830 V831 R838 N839 K843 K846 GLY GLU VAL PRO SER LEU ARG ARG MET GLU MET LEU GLN LYS GLU VAL HIS ASP ASP PRO LEU ILE SER LYS ASP LEU GLY PRO SER ARG VAL SER VAL THR GLY GLU ALA
THR PRO SER LEU LYS ALA ASN GLY SER ALA PRO VAL PRO SER SER LEU PRO THR GLN SER PRO GLN LEU SER LYS ARG MET ASP SER THR SER GLY GLY SER GLU ASN LEU TYR PHE GLN GLY GLY SER HIS HIS HIS HIS HIS HIS HIS HIS HIS HIS GLY GLY TRP SER HIS PRO GLN
PHE GLU LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	91837	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	55	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	54900	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	61.923	Depositor
Minimum map value	-32.947	Depositor
Average map value	0.001	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	4.0	Depositor
Map size (Å)	337.91998, 337.91998, 337.91998	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.87999994, 0.87999994, 0.87999994	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.26	0/6345	0.52	0/8638
1	B	0.26	0/6353	0.52	0/8647
All	All	0.26	0/12698	0.52	0/17285

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

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	6203	0	6018	104	0
1	B	6211	0	6033	110	0
All	All	12414	0	12051	210	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 210 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:B:87:LEU:HD23	1:B:95:LEU:HB2	1.83	0.59
1:A:87:LEU:HD23	1:A:95:LEU:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:GLU:HA	1:A:173:GLN:OE1	2.04	0.58
1:B:170:GLU:HA	1:B:173:GLN:OE1	2.04	0.58
1:A:506:THR:O	1:A:538:LYS:NZ	2.37	0.57

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	801/946 (85%)	765 (96%)	36 (4%)	0	100	100
1	B	801/946 (85%)	767 (96%)	34 (4%)	0	100	100
All	All	1602/1892 (85%)	1532 (96%)	70 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	652/800 (82%)	652 (100%)	0	100	100
1	B	654/800 (82%)	654 (100%)	0	100	100
All	All	1306/1600 (82%)	1306 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	HIS
1	B	80	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 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)

There are no chain breaks in this entry.

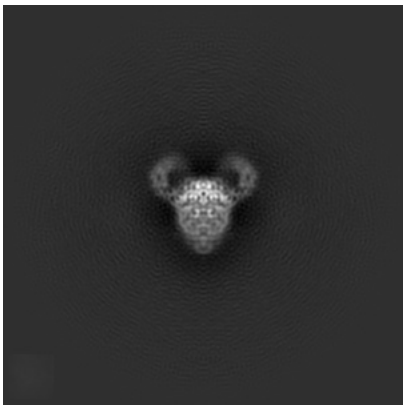
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-27696. These allow visual inspection of the internal detail of the map and identification of artifacts.

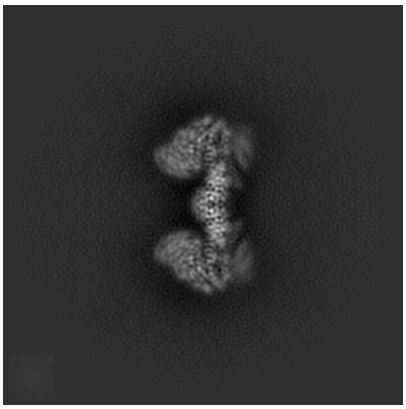
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

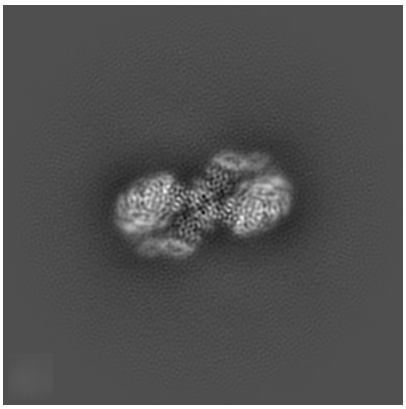
6.1.1 Primary map



X

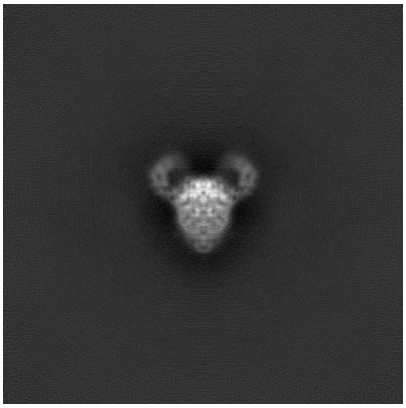


Y

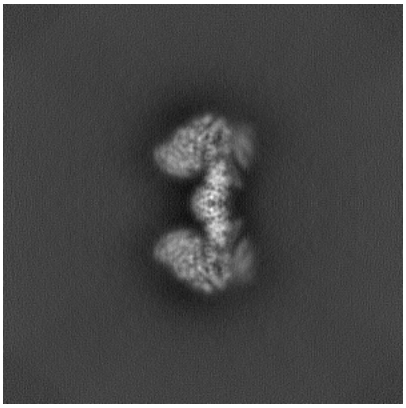


Z

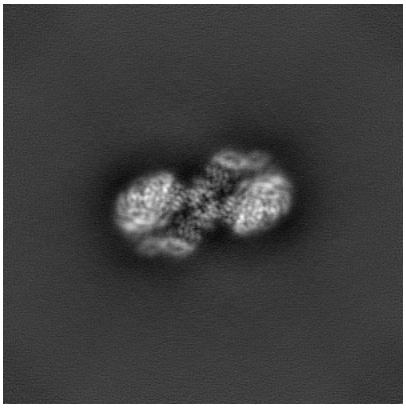
6.1.2 Raw map



X



Y

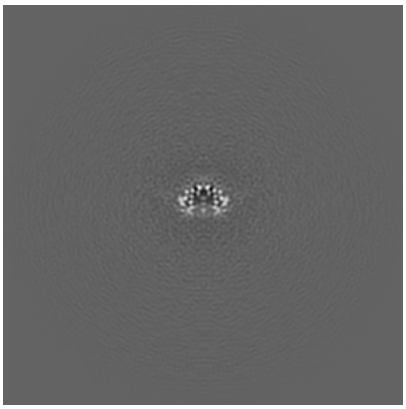


Z

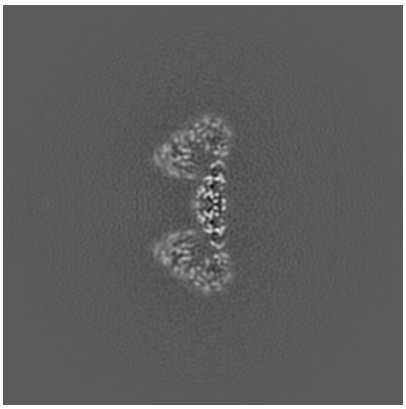
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

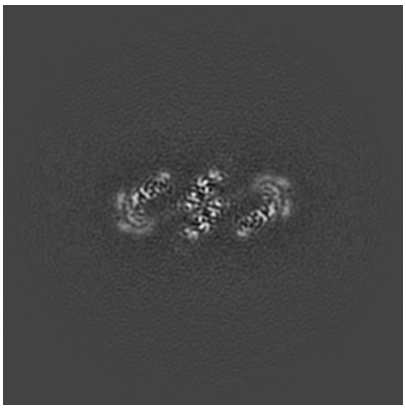
6.2.1 Primary map



X Index: 192

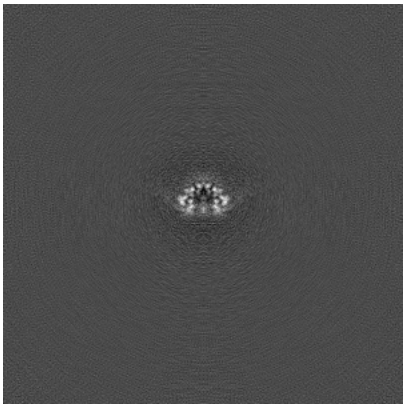


Y Index: 192

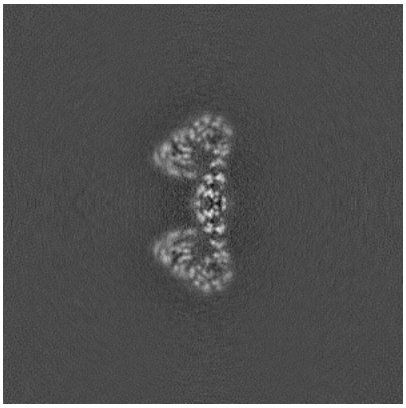


Z Index: 192

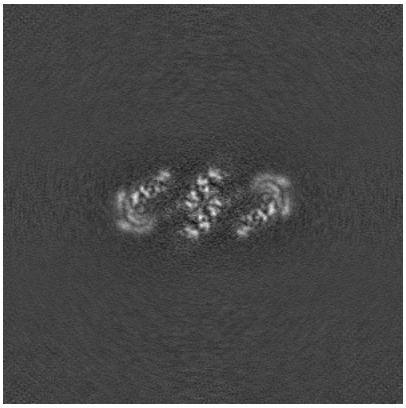
6.2.2 Raw map



X Index: 192



Y Index: 192

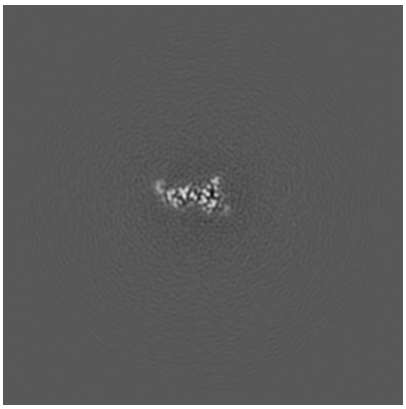


Z Index: 192

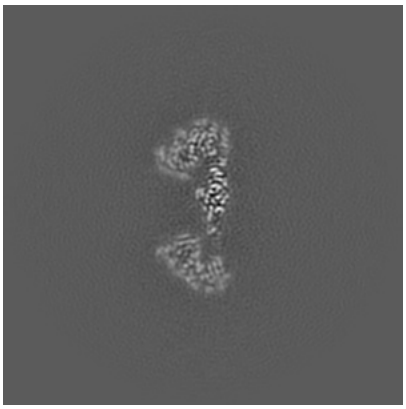
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

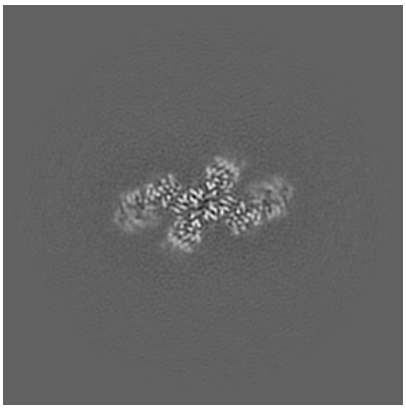
6.3.1 Primary map



X Index: 182

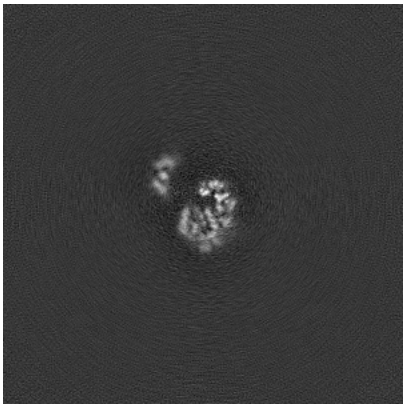


Y Index: 185

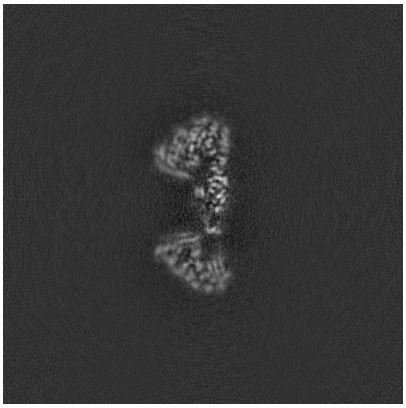


Z Index: 201

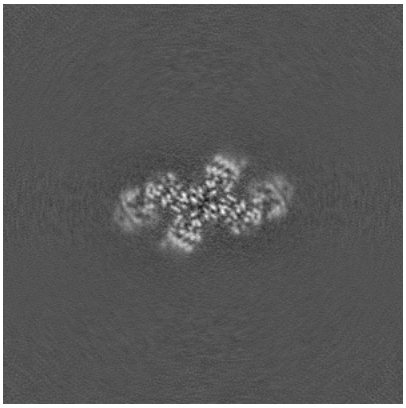
6.3.2 Raw map



X Index: 154



Y Index: 186



Z Index: 202

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 4.0. 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.

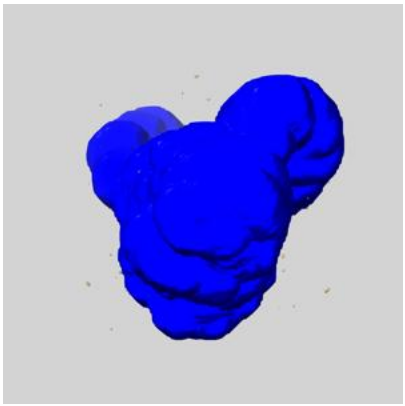
6.5 Mask visualisation

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

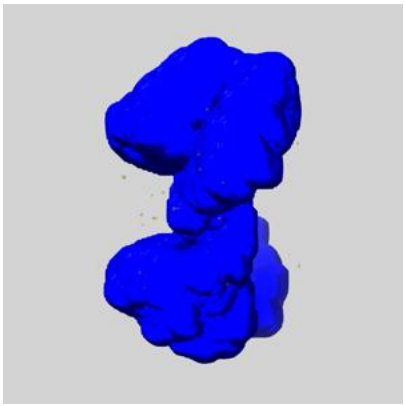
A mask typically either:

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

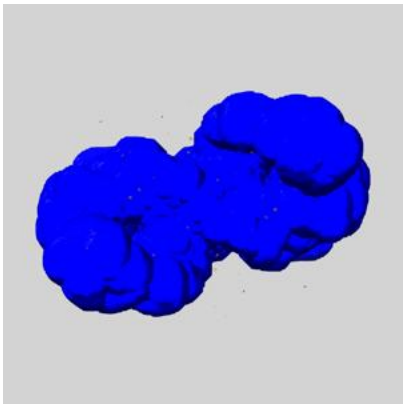
6.5.1 emd_27696_msk_1.map



X



Y

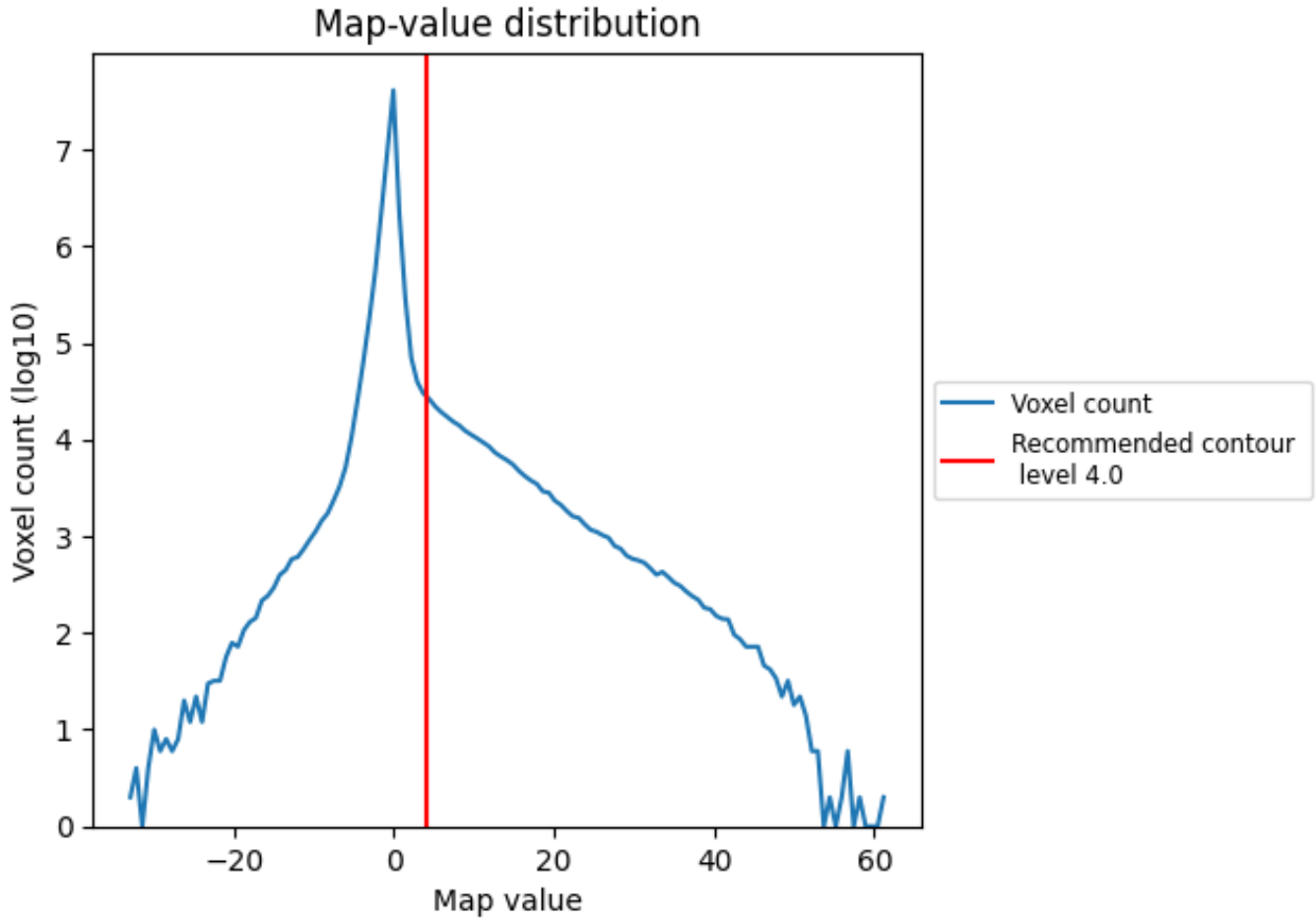


Z

7 Map analysis

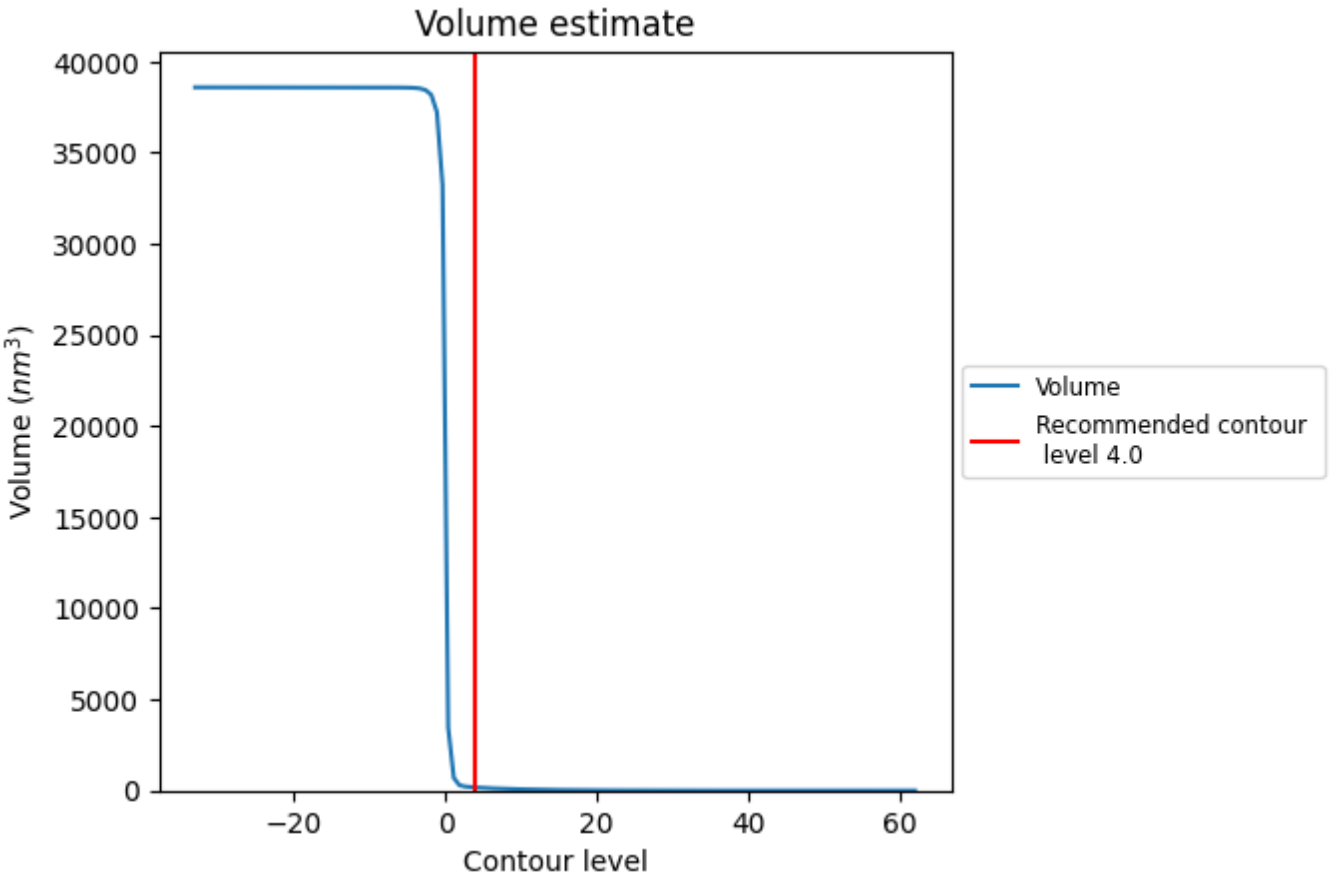
This section contains the results of statistical analysis of the map.

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.

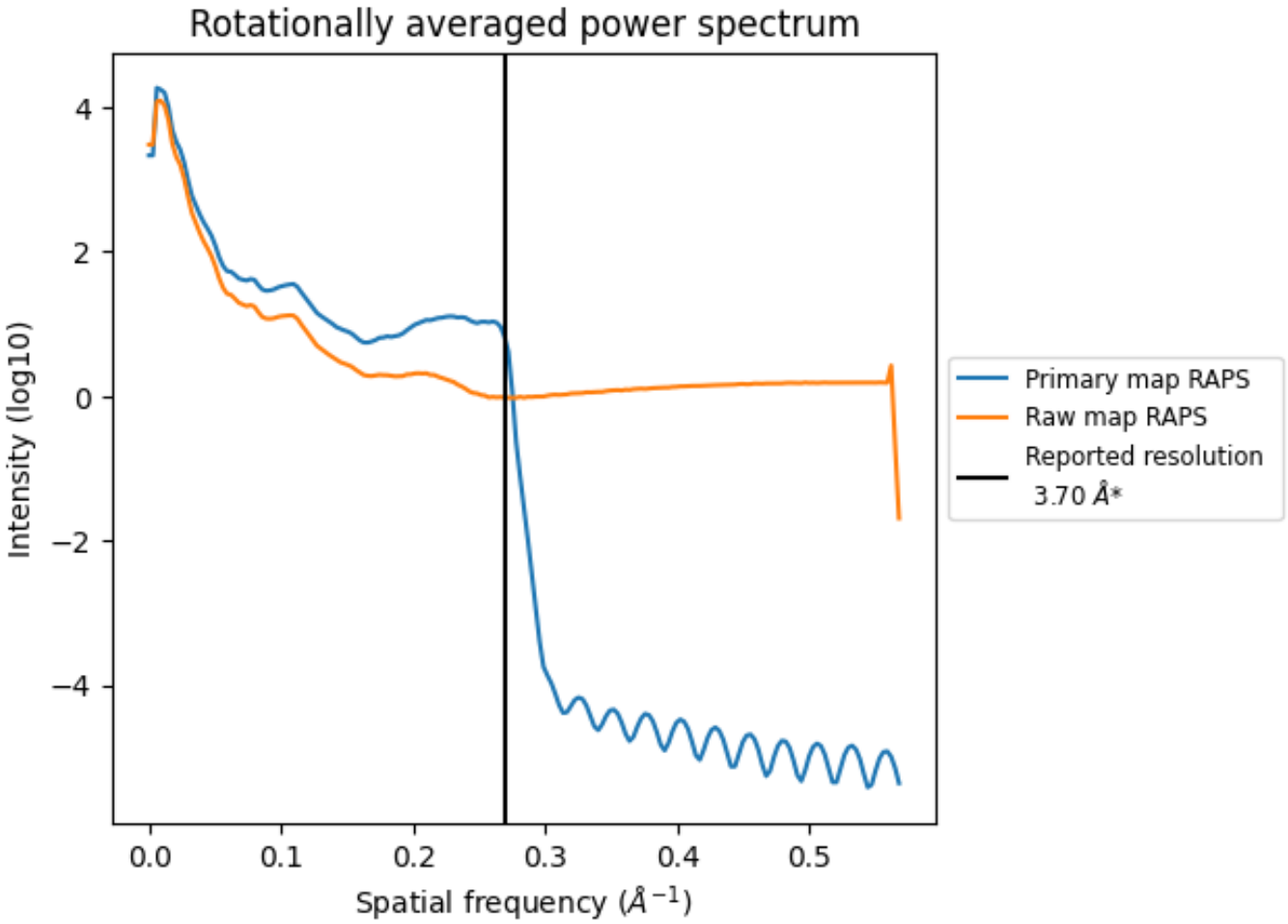
7.2 Volume estimate (i)



The volume at the recommended contour level is 172 nm^3; this corresponds to an approximate mass of 155 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)

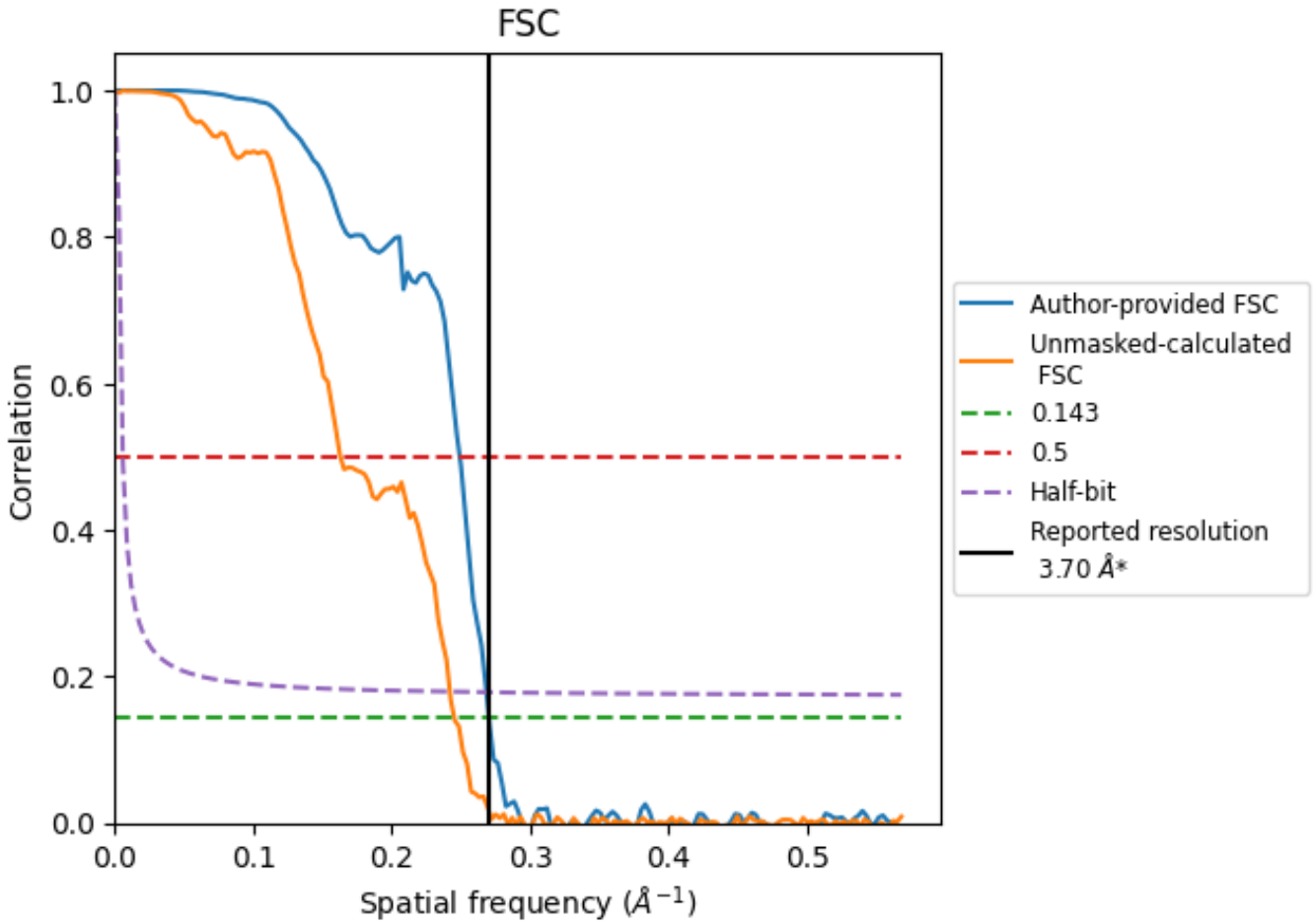


*Reported resolution corresponds to spatial frequency of 0.270 Å^{-1}

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)

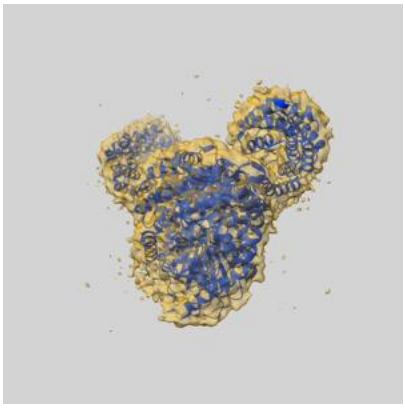
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.70	4.01	3.72
Unmasked-calculated*	4.08	6.14	4.13

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

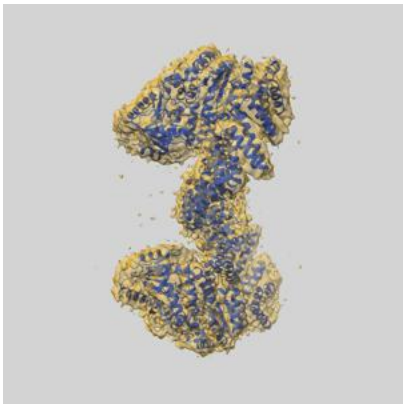
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-27696 and PDB model 8DTF. Per-residue inclusion information can be found in section 3 on page 5.

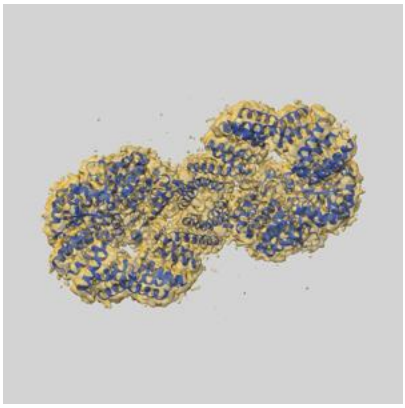
9.1 Map-model overlay



X



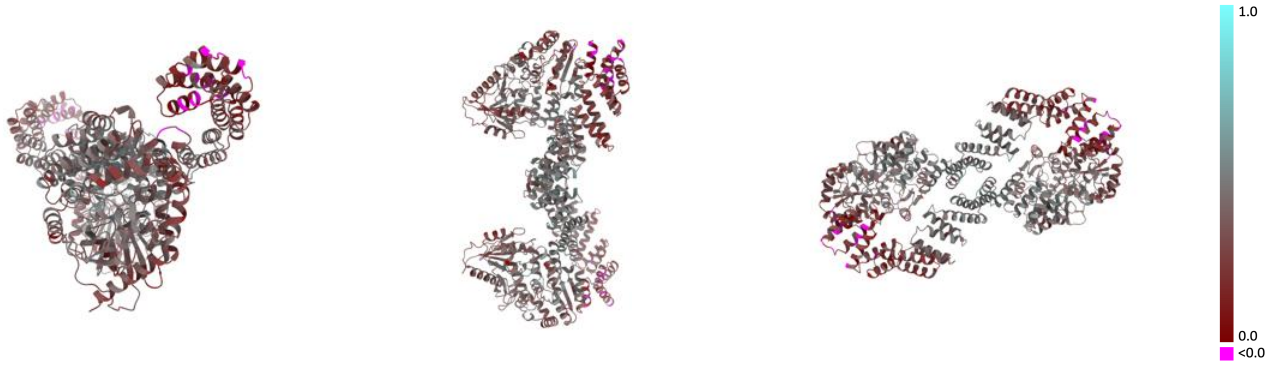
Y



Z

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

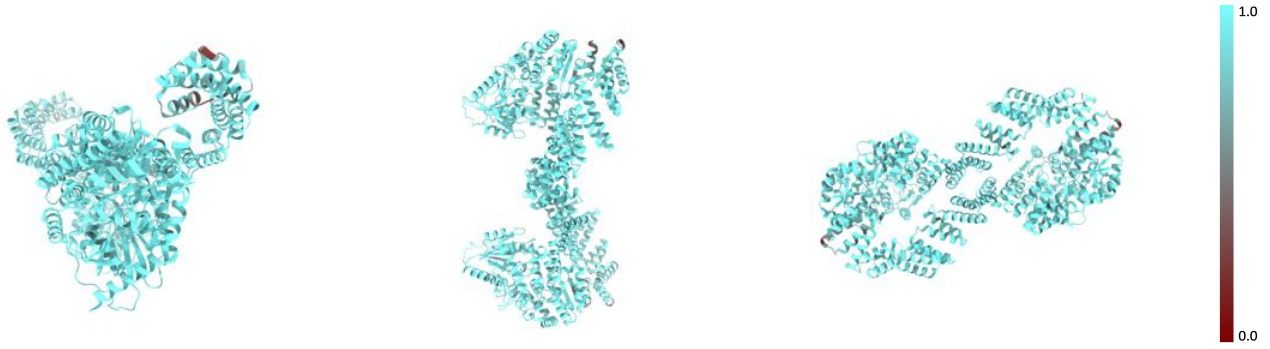
9.2 Q-score mapped to coordinate model (i)



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.

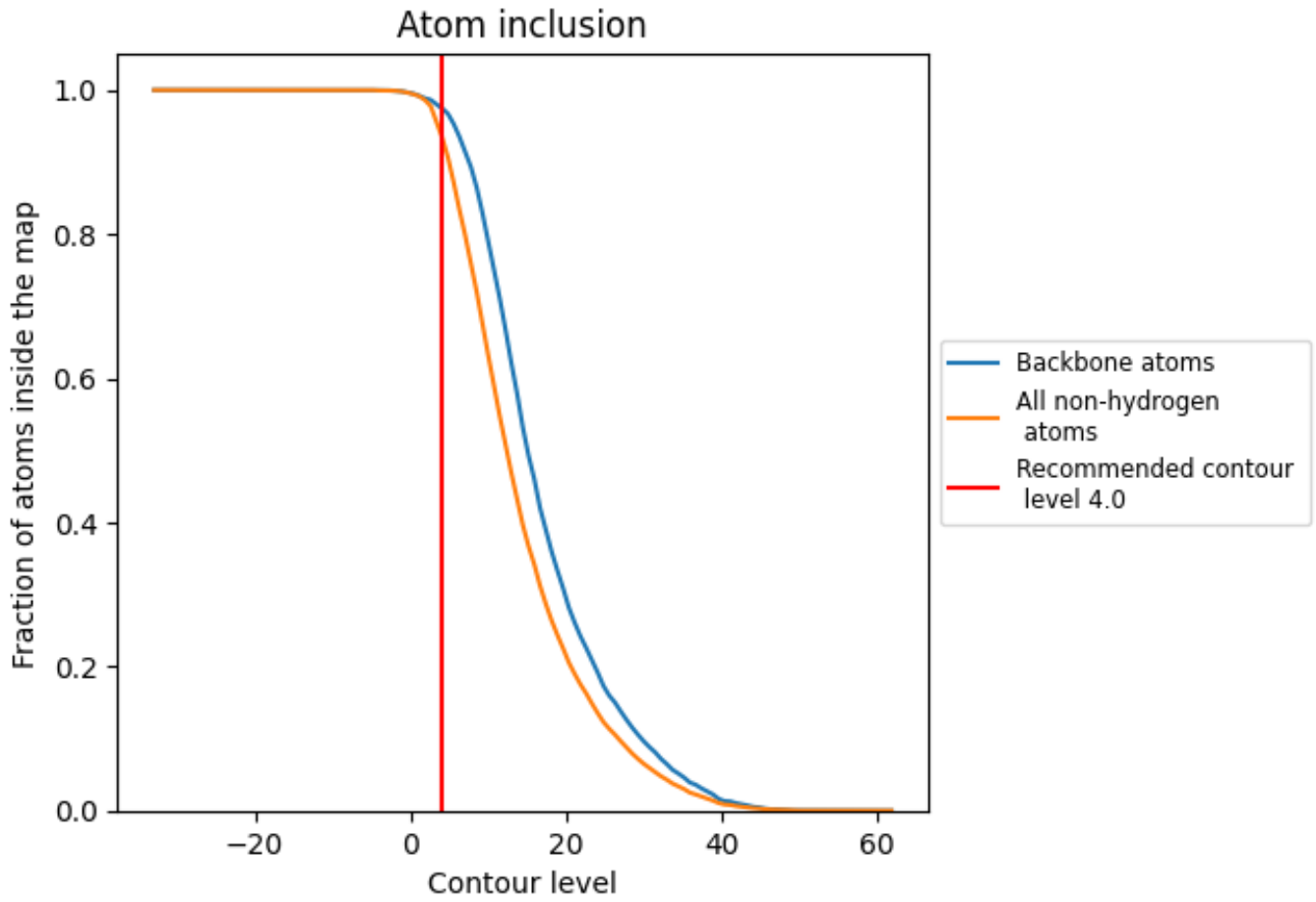
9.3 Atom inclusion mapped to coordinate model (i)



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 (4.0).

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 (4.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9363	0.3630
A	0.9366	0.3630
B	0.9361	0.3620