



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 12:22 PM UTC

PDB ID : 9F48 / pdb_00009f48
EMDB ID : EMD-50185
Title : KS + AT di-domain of polyketide synthase 13 in Mycobacterium tuberculosis
Authors : Johnston, H.E.; Futterer, K.
Deposited on : 2024-04-26
Resolution : 3.40 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

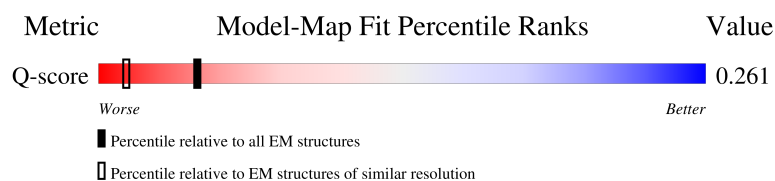
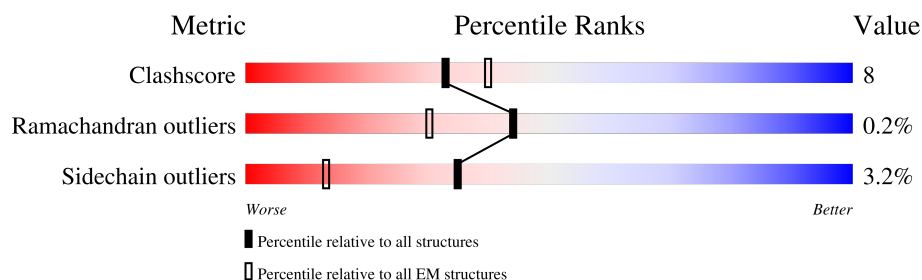
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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	14717 (2.90 - 3.90)

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	A	1733	 42% 11% 47%
1	B	1733	 43% 10% 47%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 13803 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.

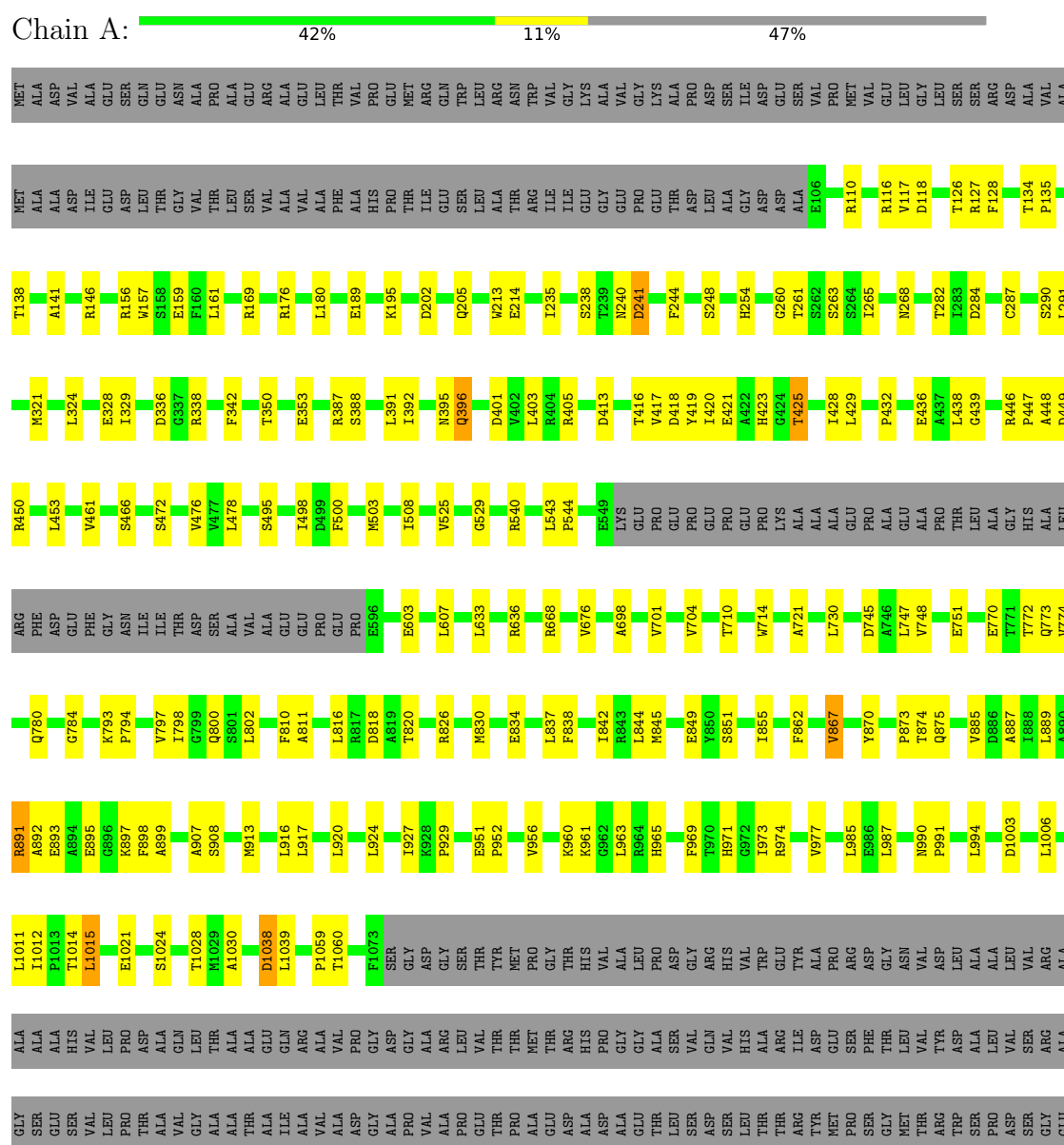
- Molecule 1 is a protein called Polyketide synthase Pks13.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	922	Total	C	N	O	S	0	0
			6900	4350	1215	1315	20		
1	B	923	Total	C	N	O	S	0	0
			6903	4351	1216	1316	20		

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: Polyketide synthase Pks13



[illegible]

- Molecule 1: Polyketide synthase Pks13

Chain B: 43% 10% 47%

PHE	Q780	K897	Q780	V476	S290	F164	THR	MET
	Q781	K901	G784	P487	L291	R165	ALA	
	Q782	F902	E785	M490	V298	ASP	ALA	
	Q783	H909	L786	THR	R302	GLU	ALA	
	Q784	T910	K793	ASP	N303	ASP	GLU	
	Q785	M913	A796	SER	E305	LEU	GLN	
	Q786	D914	P915	VAL	G304	THR	GLY	
	Q787	L916	S801	ALA	S495	ALA	ASN	
	Q788	L917	E804	GLU	M503	VAL	ALA	
	Q789	P929	S807	PRO	R504	PRO	PRO	
MET	F810	L936	F810	P511	L317	F186	THR	MET
	F811	H941	S815	T512	I318	D187	LEU	
	F812	H942	R817	L522	I319	S188	SER	
	F813	R944	D818	E523	T323	F190	ALA	
	F814	L945	P946	M534	I329	A198	ALA	
	F815	P952	S825	R540	L333	I201	ALA	
	F816	L953	R826	E541	D336	D202	HIS	
	F817	K960	M830	D546	G337	P203	PRO	
	F818	L963	G833	K550	R338	R206	THR	
	F819	R964	L837	GLU	A344	M207	GLU	
THR	T970	T970	F838	R540	E210	E210	LEU	MET
	T971	L973	T842	E541	L211	L211	ARG	
	T972	V977	M845	D546	E214	E214	ARG	
	T973	L985	Y850	A698	S352	R227	ILE	
	T974	M995	R856	A698	E353	G228	GLY	
	T975	D1008	E857	ALA	M357	Y234	VAL	
	T976	M1025	F859	ALA	V376	Y234	GLY	
	T977	L1030	L865	ALA	R387	I235	PRO	
	T978	Q1031	Y870	ALA	S388	S238	LEU	
	T979	Y1032	T874	ALA	LYS	T239	ASP	
SER	S1033	Y1033	Q875	ALA	A398	N240	SER	MET
	S1034	V1034	Q876	ALA	V402	D241	GLY	
	S1035	L1039	T877	ALA	I412	Y242	ASP	
	S1040	F1062	P881	GLU	L245	L245	ALA	
	S1041	F1073	P882	LEU	I413	S263	VAL	
	S1042	SER	E884	THR	R415	S864	PRO	
	S1043	ALA	N895	LEU	T416	I265	VAL	
	S1044	ALA	ALA	ALA	E421	A267	GLU	
	S1045	ALA	ALA	ALA	R446	H277	GLY	
	S1046	ALA	ALA	ALA	HIS	R127	SER	



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	168566	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	16.5	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.115	Depositor
Minimum map value	-0.059	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.000747	Depositor
Map size ($\text{\AA}$)	392.40002, 392.40002, 392.40002	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.09, 1.09, 1.09	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	A	0.17	0/7048	0.43	0/9593
1	B	0.17	0/7051	0.45	6/9597 (0.1%)
All	All	0.17	0/14099	0.44	6/19190 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
All	All	0	3

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	329	ILE	N-CA-C	-6.49	107.54	113.71
1	B	946	ILE	CA-C-N	6.15	129.22	120.49
1	B	946	ILE	C-N-CA	6.15	129.22	120.49
1	B	909	HIS	CA-C-N	-5.39	115.11	121.90
1	B	909	HIS	C-N-CA	-5.39	115.11	121.90

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	328	GLU	Peptide
1	A	449	ASP	Peptide
1	B	201	ILE	Peptide

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	6900	0	6750	119	0
1	B	6903	0	6745	114	0
All	All	13803	0	13495	228	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 8.

The worst 5 of 228 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:892:ALA:HB1	1:A:897:LYS:HB2	1.66	0.77
1:B:127:ARG:HG2	1:B:180:LEU:HD21	1.67	0.77
1:B:202:ASP:HB3	1:B:203:PRO:HA	1.69	0.73
1:B:336:ASP:N	1:B:336:ASP:OD1	2.24	0.71
1:B:317:LEU:HG	1:B:353:GLU:HB3	1.72	0.70

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	918/1733 (53%)	837 (91%)	80 (9%)	1 (0%)	48 78
1	B	919/1733 (53%)	852 (93%)	64 (7%)	3 (0%)	36 65
All	All	1837/3466 (53%)	1689 (92%)	144 (8%)	4 (0%)	44 71

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	159	GLU
1	B	286	ALA
1	B	202	ASP
1	A	329	ILE

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	A	698/1358 (51%)	672 (96%)	26 (4%)	30	55
1	B	697/1358 (51%)	679 (97%)	18 (3%)	40	61
All	All	1395/2716 (51%)	1351 (97%)	44 (3%)	35	58

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	241	ASP
1	B	512	THR
1	B	323	THR
1	B	412	ILE
1	B	732	LEU

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	B	490	ASN
1	B	670	HIS
1	B	1037	HIS
1	B	682	HIS
1	A	1007	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.

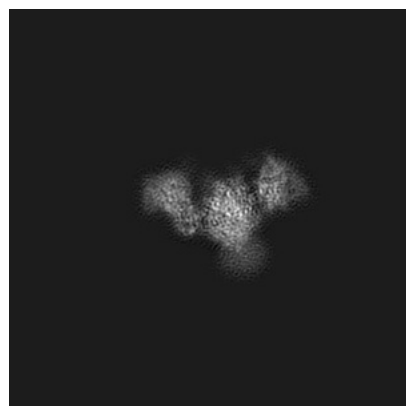
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50185. These allow visual inspection of the internal detail of the map and identification of artifacts.

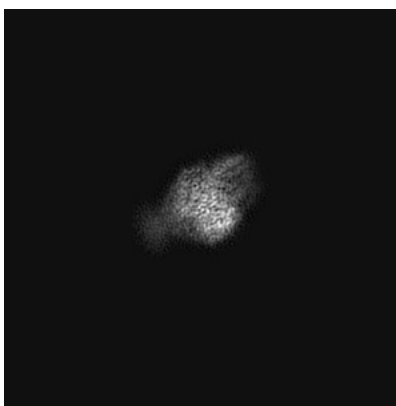
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

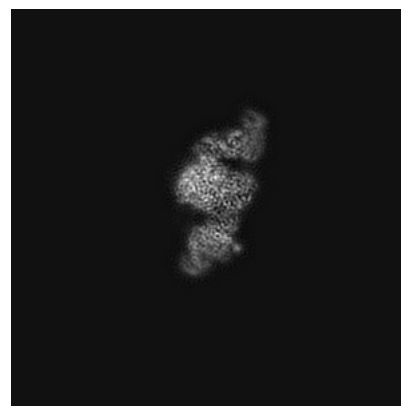
6.1.1 Primary map



X

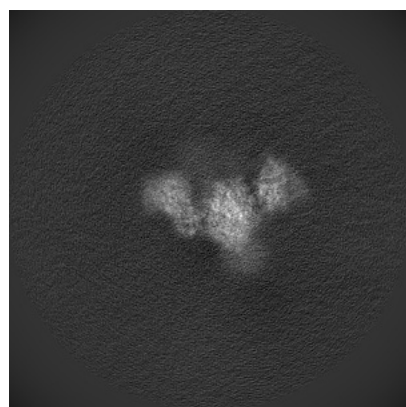


Y

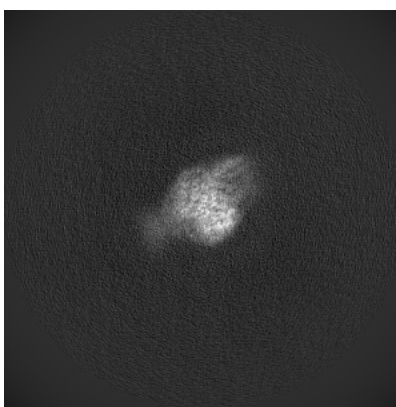


Z

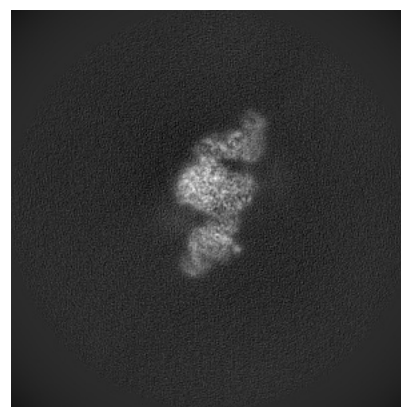
6.1.2 Raw map



X



Y

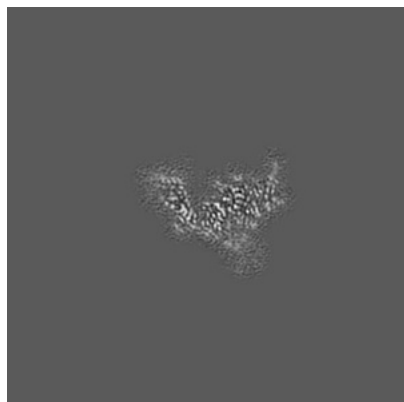


Z

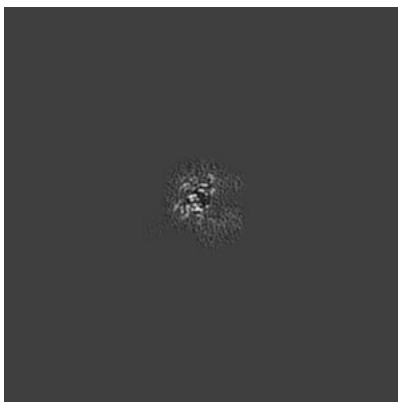
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

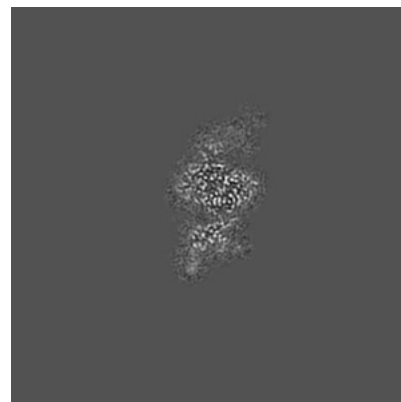
6.2.1 Primary map



X Index: 180

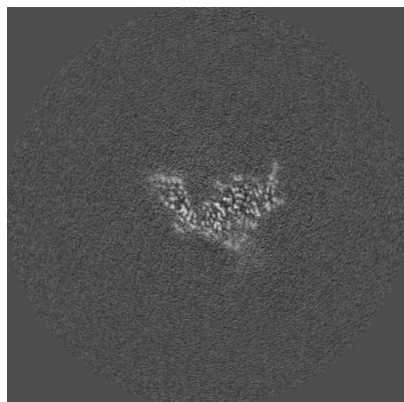


Y Index: 180

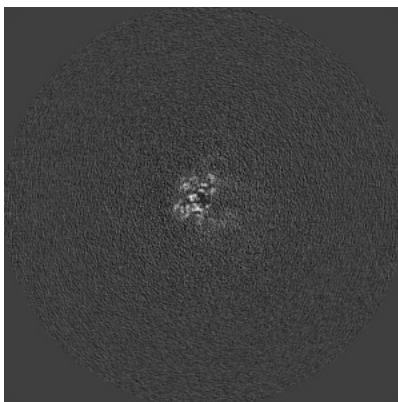


Z Index: 180

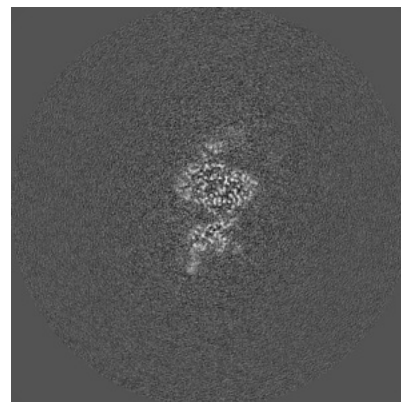
6.2.2 Raw map



X Index: 180



Y Index: 180



Z Index: 180

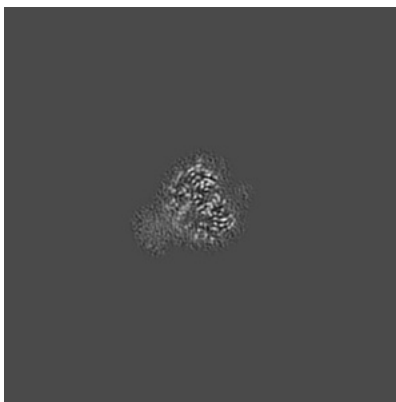
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

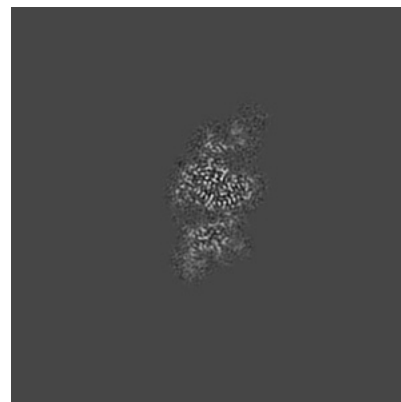
6.3.1 Primary map



X Index: 176

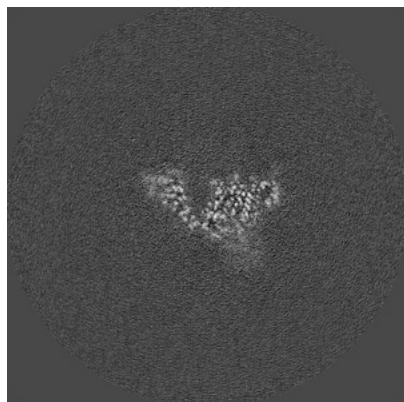


Y Index: 199

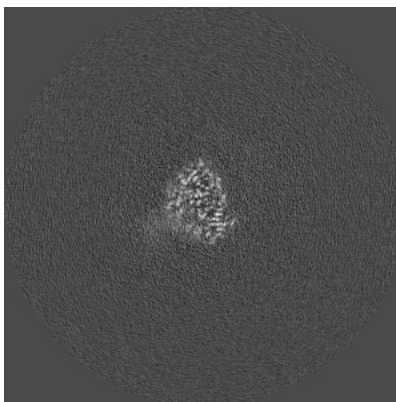


Z Index: 182

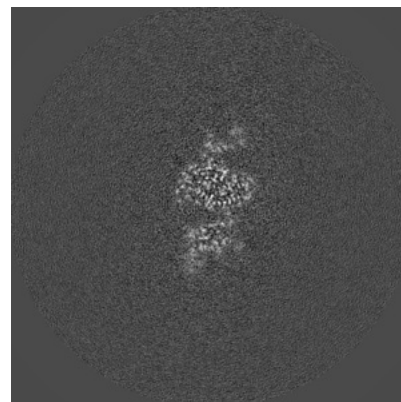
6.3.2 Raw map



X Index: 176



Y Index: 197

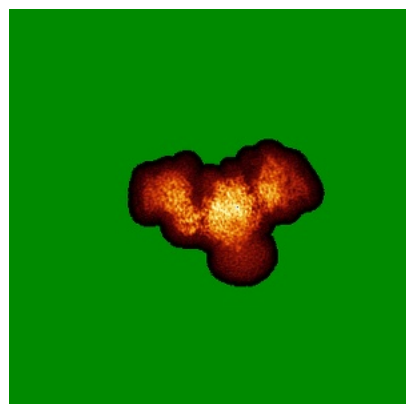


Z Index: 182

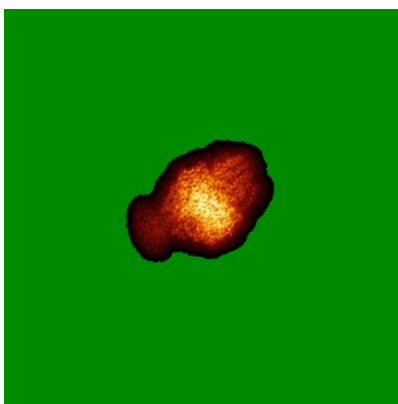
The images above show the largest variance slices of the map in three orthogonal directions.

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

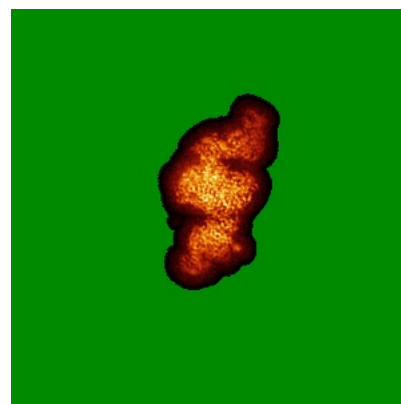
6.4.1 Primary map



X

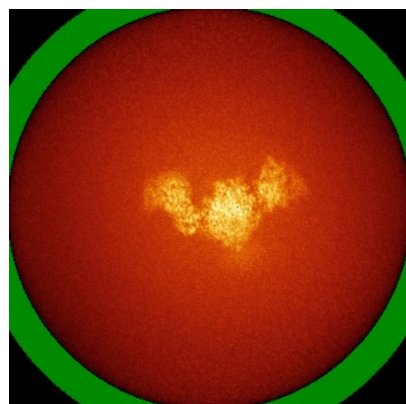


Y

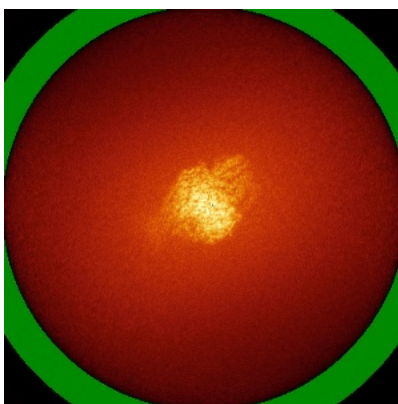


Z

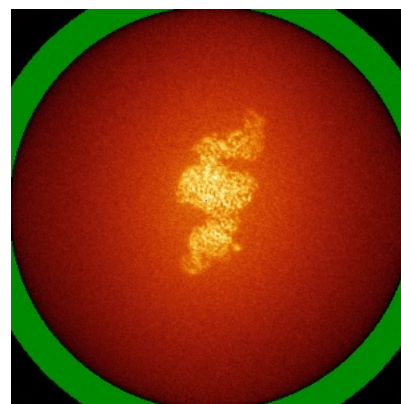
6.4.2 Raw map



X



Y

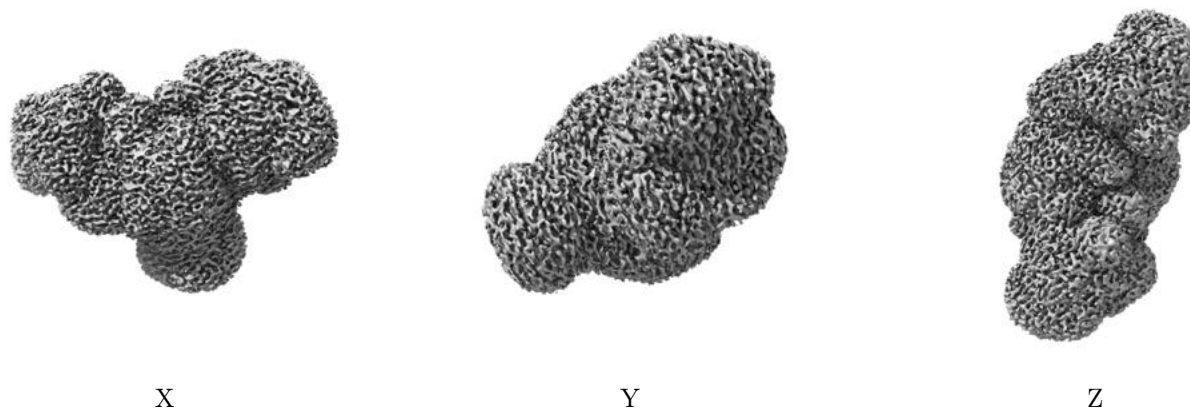


Z

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.

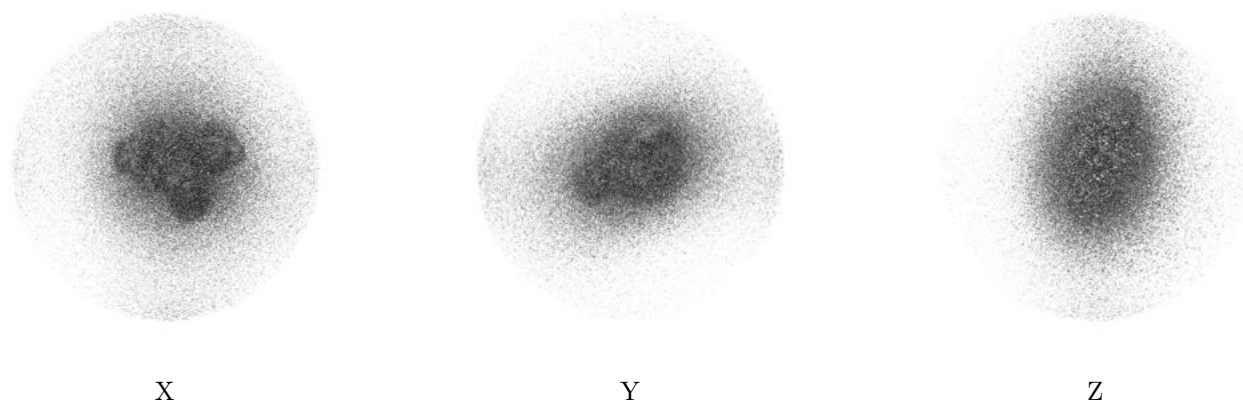
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.000747. 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.

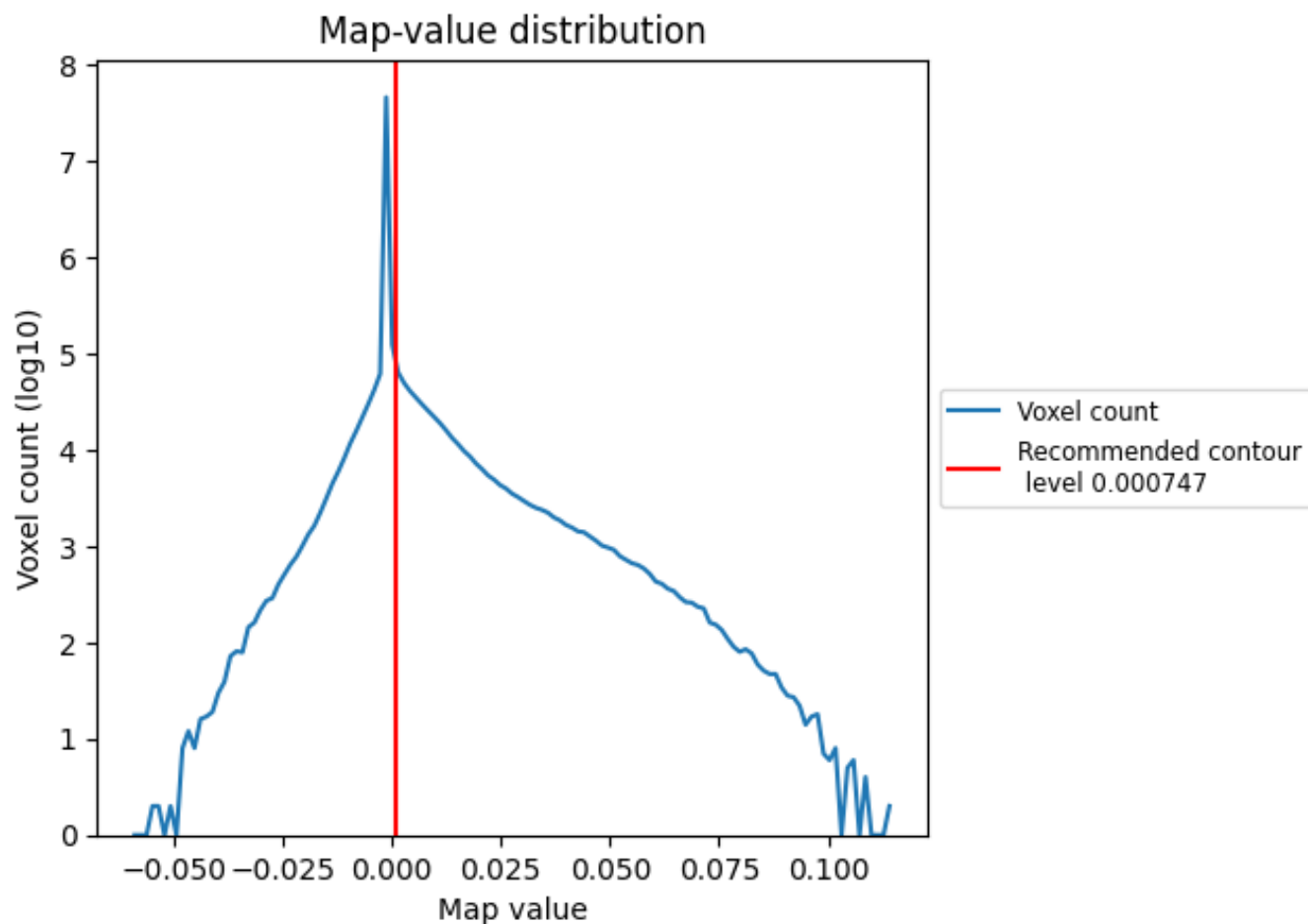
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

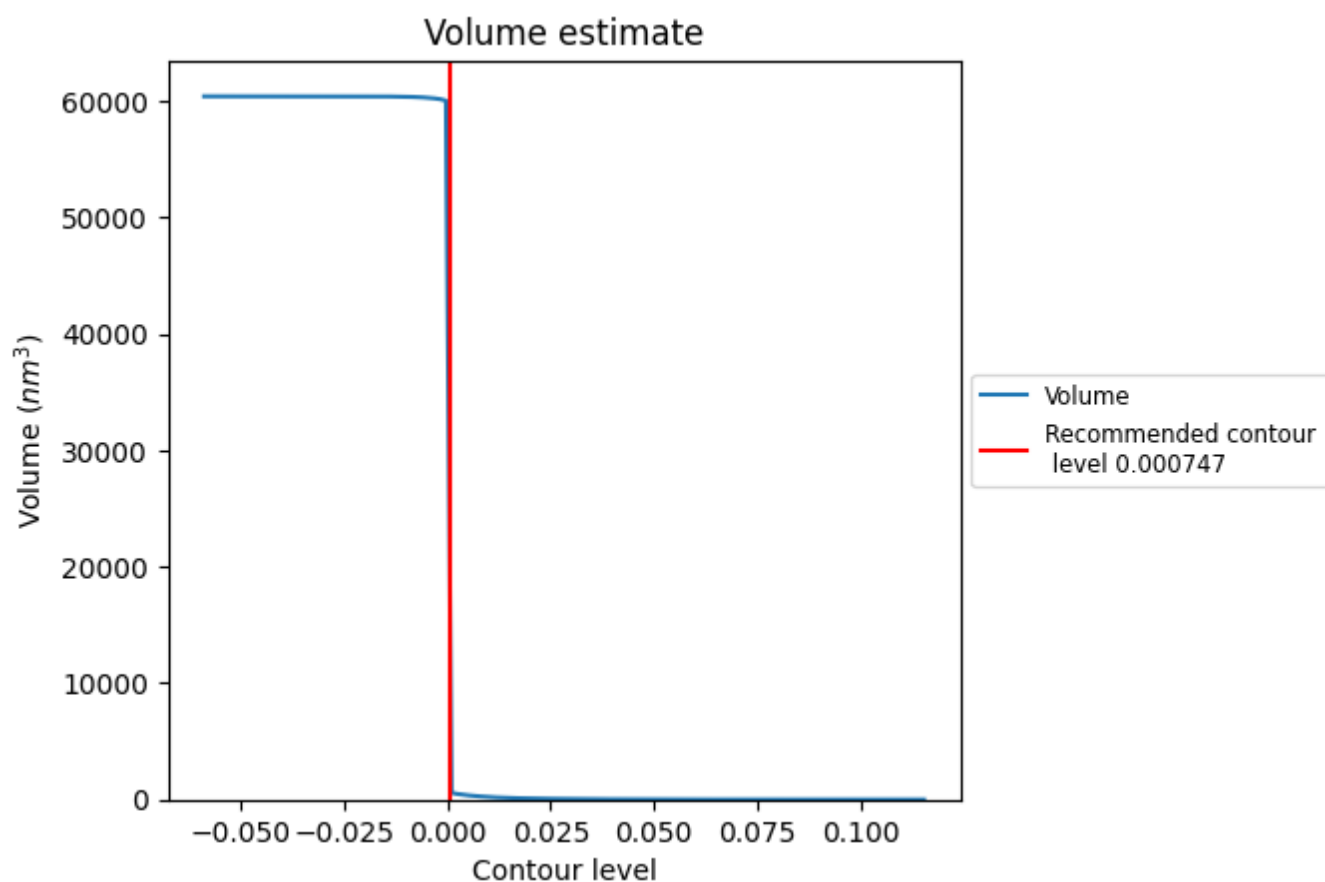
This section contains the results of statistical analysis of the map.

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.

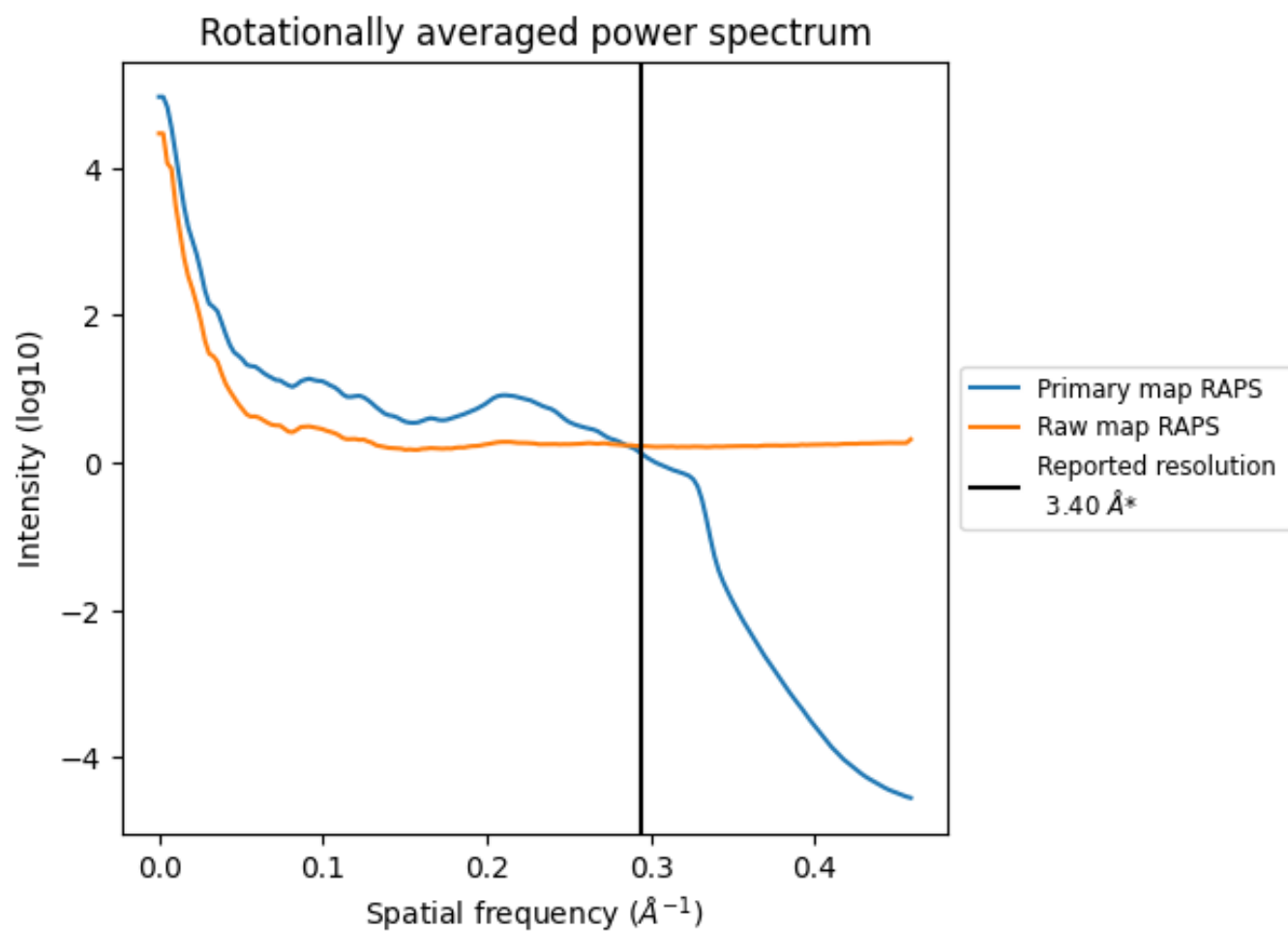
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 11355 nm³; this corresponds to an approximate mass of 10257 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 ⓘ

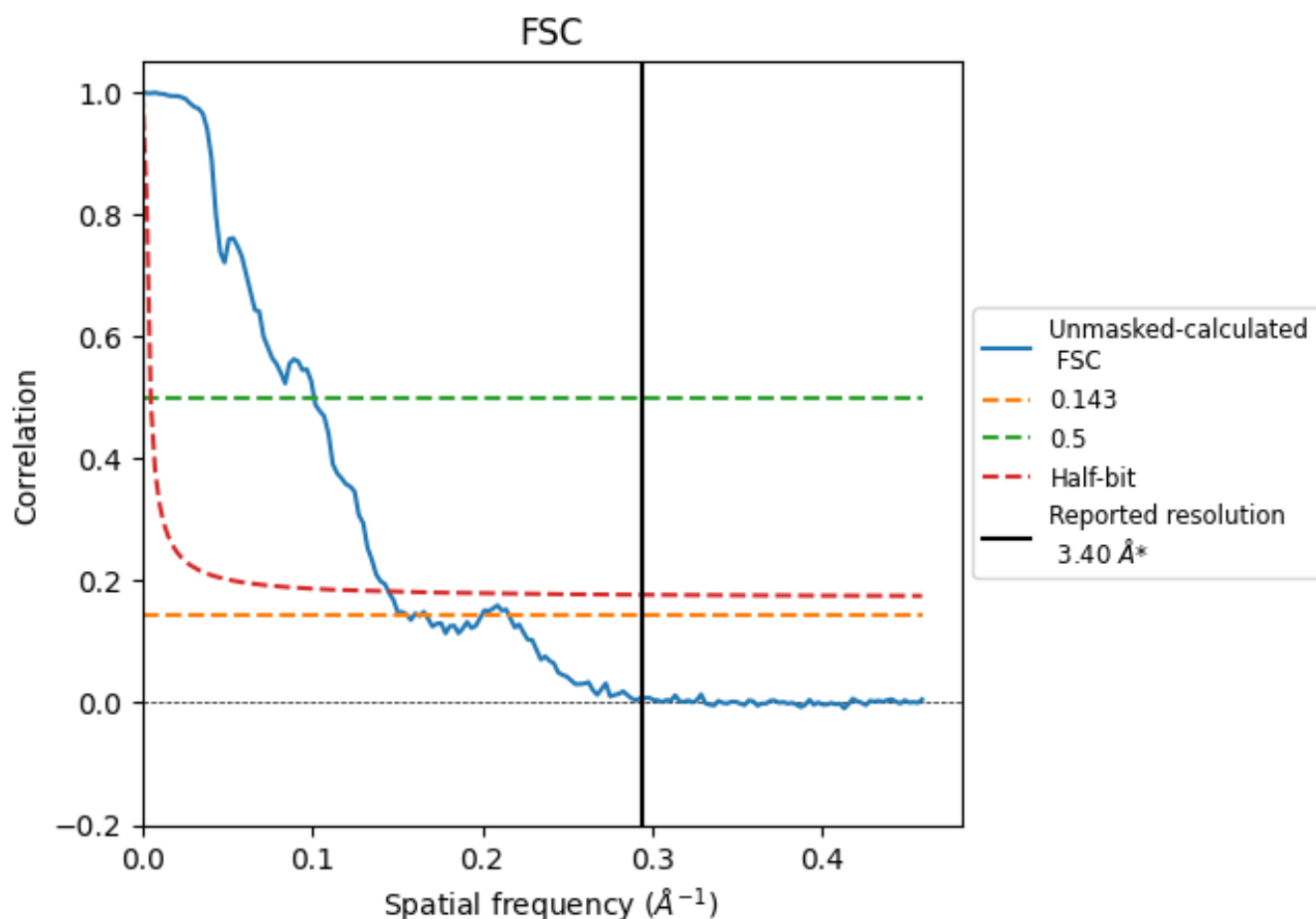


*Reported resolution corresponds to spatial frequency of 0.294 $\text{\AA}^{-1}$

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 0.294 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

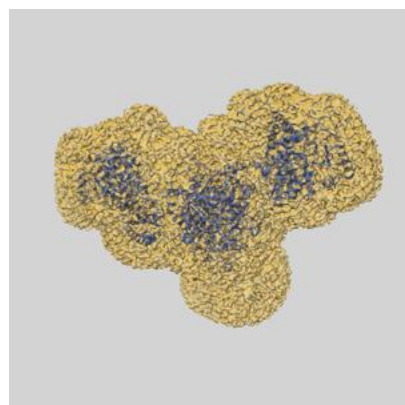
Resolution estimate (Å)	Estimation criterion (FSC cut-off)			
	0.143	0.5	Half-bit	Other
Reported by author	-	-	-	3.40
Author-provided FSC curve	-	-	-	-
Unmasked-calculated*	6.42	9.89	6.91	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

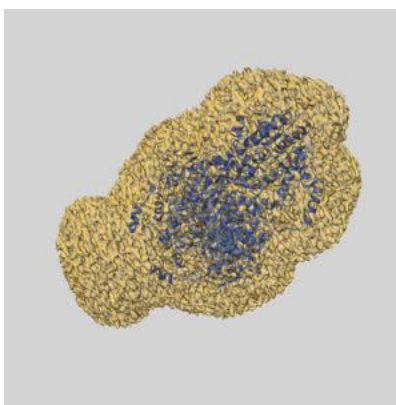
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-50185 and PDB model 9F48. Per-residue inclusion information can be found in section [3](#) on page [4](#).

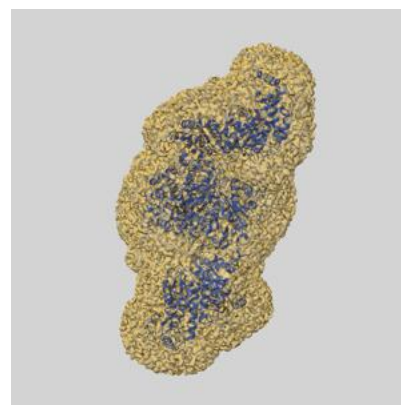
9.1 Map-model overlay [i](#)



X



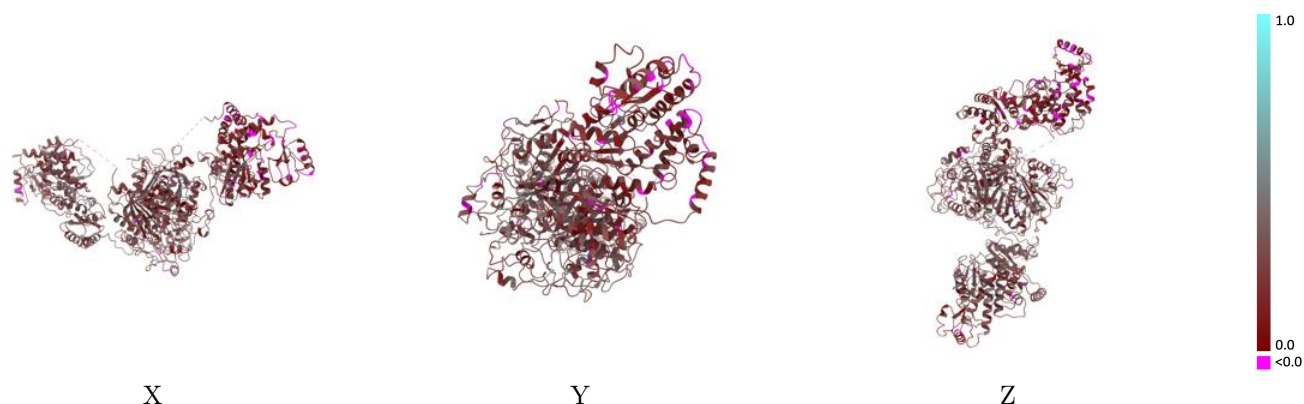
Y



Z

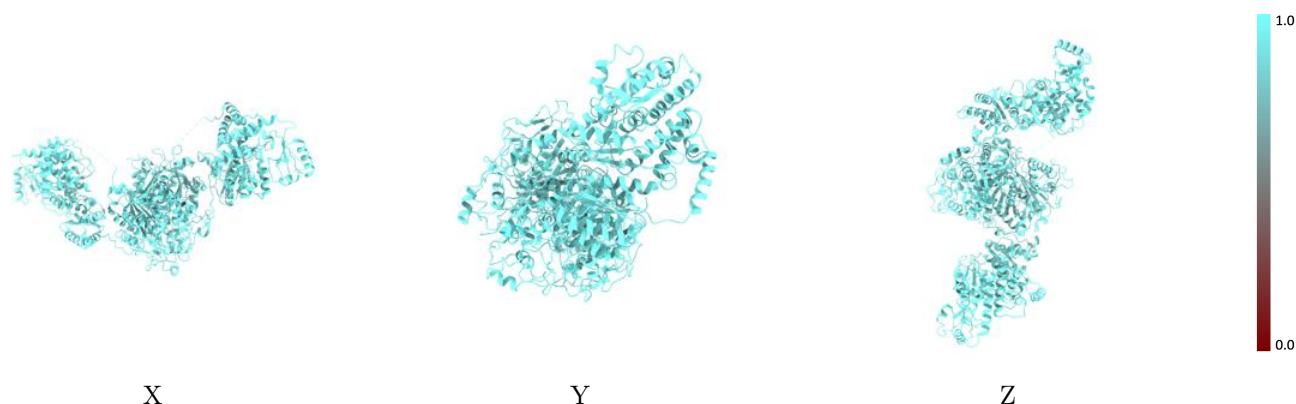
The images above show the 3D surface view of the map at the recommended contour level 0.000747 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



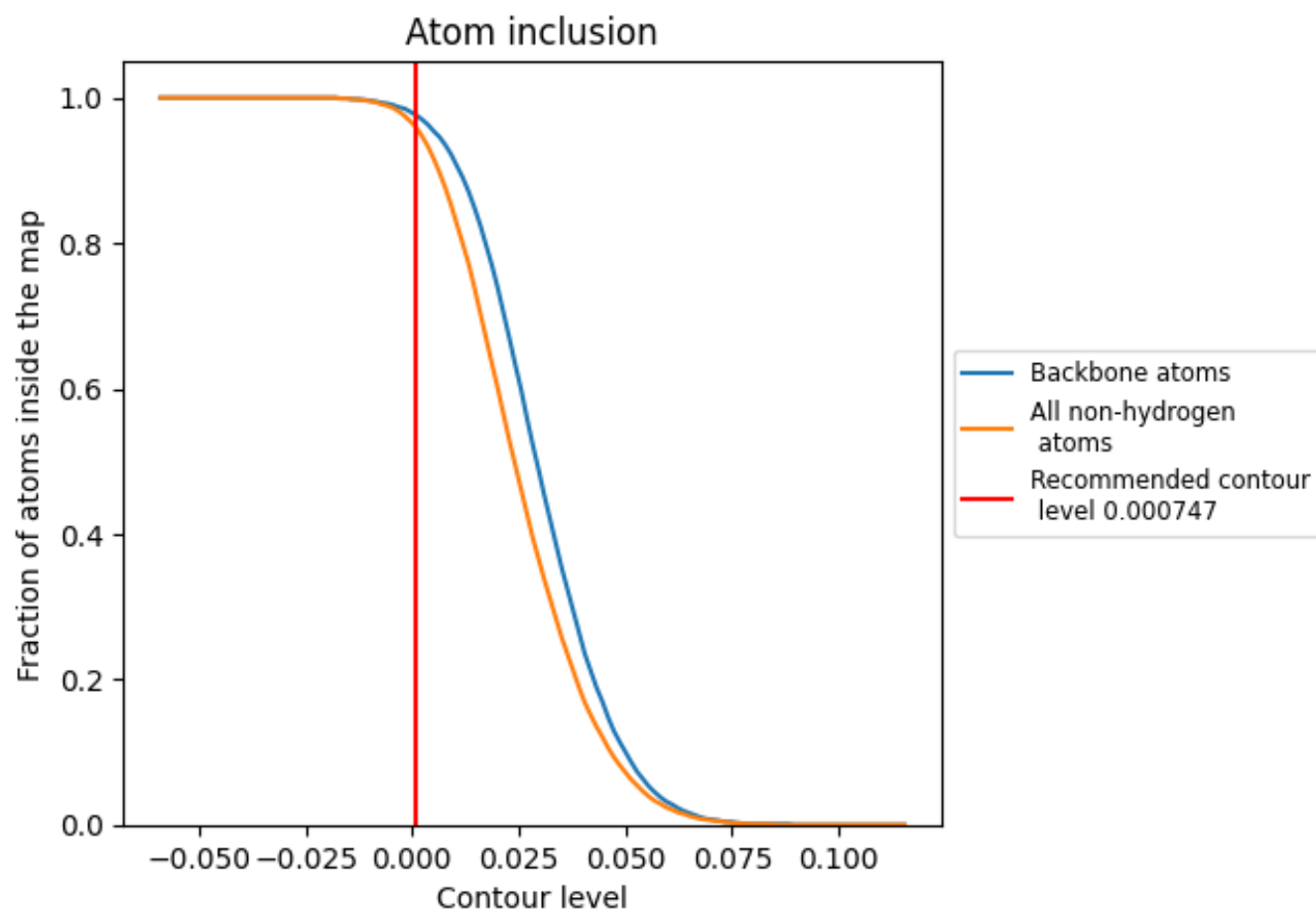
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.000747).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 96% 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 (0.000747) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9610	0.2610
A	0.9560	0.2370
B	0.9660	0.2850

