



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 01:20 PM UTC

PDB ID : 8CV0 / pdb_00008cv0
EMDB ID : EMD-27004
Title : KS-AT domains of mycobacterial Pks13 with outward AT conformation
Authors : Kim, S.K.; Dickinson, M.S.; Finer-Moore, J.S.; Rosenberg, O.S.; Stroud, R.M.
Deposited on : 2022-05-17
Resolution : 3.10 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

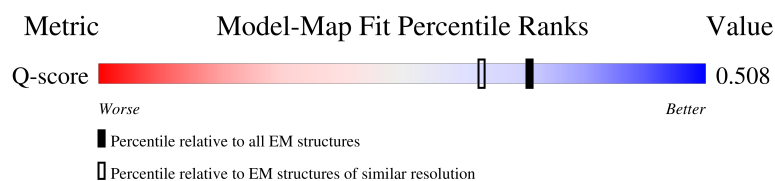
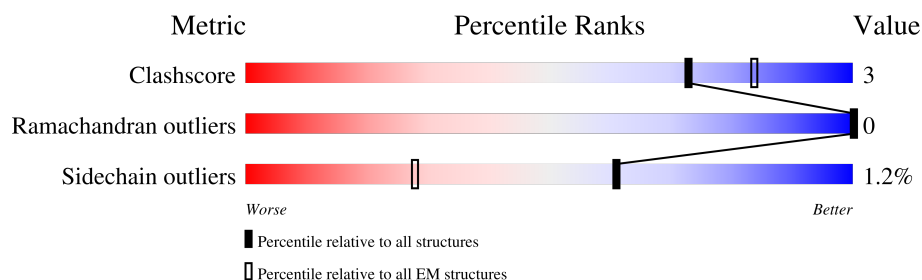
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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	14724 (2.60 - 3.60)

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	1816	
1	B	1816	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 27859 atoms, of which 13779 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	925	Total	C	H	N	O	S	0	0
			13879	4409	6858	1240	1352	20		
1	B	925	Total	C	H	N	O	S	0	0
			13874	4409	6853	1240	1352	20		

- Molecule 2 is UNKNOWN LIGAND (CCD ID: UNL) (formula:) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	H	O	0
			53	18	34	1	
2	B	1	Total	C	H	O	0
			53	18	34	1	

[illegible]

- Molecule 1: Polyketide synthase PKS13



Q881	V882	D883	A884	I885	A886	A887	R888	A889	E890	S891	E892	G893	K894	A896	R897	K898	F899	Q900	T901	K902	G903	A904	S905	Q909	M910	L913	L914	G915	E916	L917	E920	L921	Q922	G923	I924	E925	L929	T930	Y933	E939	G940				
A760	T761	C762	E763	Y764	T766	E801	H825	G828	E829	G830	E831	A832	M833	L834	F835	G836	E837	Y838	I839	R840	L841	M842	A843	L844	T847	S848	A849	D850	E851	I852	K853	T854	V855	F856	S857	D858	Y859	F860	D861	L862	E863	V864			
E596	A599	E600	E601	L602	E603	A604	K605	E606	A607	E608	E609	P610	T611	K612	Q613	L614	V615	E642	S646	S647	L648	K686	V705	L706	A707	G708	Q712	H713	R714	K715	L720	N724	E725	D735	G743	Y744	S745	I746	E589	E748	L751				
A233	G240	I245	F253	C267	S270	A280	L281	R282	A283	G284	V294	L297	Y298	T299	D316	G317	R318	D325	T343	A358	D365	G366	R367	E401	L434	V437	S446	L141	D142	E143	I146	Q185	E190	E194	D229	S230	P231	G232	L233	A234					
THR	VAL	ASN	GLU	MET	ARG	GLU	TRP	ARG	ASN	TRP	VAL	ASN	THR	GLY	GLN	SER	ALA	ASP	ALA	ILE	ASP	GLU	SER	THR	PRO	MET	VAL	LEU	GLY	LEU	GLY	MET	ALA	SER	ASP	ILE	GLU	LEU	THR	GLY	VAL	THR	ALA	THR	VAL



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	92662	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 ($e^-/\text{\AA}^2$)	45.8	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.051	Depositor
Minimum map value	-0.013	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0162	Depositor
Map size (Å)	322.31, 322.31, 322.31	wwPDB
Map dimensions	386, 386, 386	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.835, 0.835, 0.835	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: UNL

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	0.07	0/7162	0.28	3/9719 (0.0%)
1	B	0.07	0/7162	0.28	3/9719 (0.0%)
All	All	0.07	0/14324	0.28	6/19438 (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	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	835	PHE	O-C-N	-6.51	115.44	123.44
1	A	835	PHE	O-C-N	-6.41	115.56	123.44
1	A	646	SER	CA-C-N	5.37	129.20	120.60
1	A	646	SER	C-N-CA	5.37	129.20	120.60
1	B	646	SER	CA-C-N	5.37	129.19	120.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	835	PHE	Mainchain

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Mol	Chain	Res	Type	Group
1	B	835	PHE	Mainchain

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	7021	6858	6900	46	0
1	B	7021	6853	6900	48	0
2	A	19	34	0	0	0
2	B	19	34	0	0	0
All	All	14080	13779	13800	92	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 3.

The worst 5 of 92 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:864:VAL:O	1:B:963:SER:OG	2.00	0.77
1:A:864:VAL:O	1:A:963:SER:OG	2.00	0.76
1:A:365:ASP:OD1	1:A:514:ASN:ND2	2.22	0.73
1:B:365:ASP:OD1	1:B:514:ASN:ND2	2.22	0.72
1:A:608:GLU:N	1:A:608:GLU:OE1	2.25	0.70

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	919/1816 (51%)	888 (97%)	31 (3%)	0	100	100
1	B	919/1816 (51%)	888 (97%)	31 (3%)	0	100	100
All	All	1838/3632 (51%)	1776 (97%)	62 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	723/1414 (51%)	714 (99%)	9 (1%)	63	78
1	B	723/1414 (51%)	714 (99%)	9 (1%)	63	78
All	All	1446/2828 (51%)	1428 (99%)	18 (1%)	61	78

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	835	PHE
1	B	895	PHE
1	B	861	ASP
1	A	895	PHE
1	B	825	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	777	GLN
1	B	276	GLN
1	B	403	HIS
1	A	276	GLN
1	A	184	GLN

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](#)

Of 2 ligands modelled in this entry, 2 are unknown - 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.

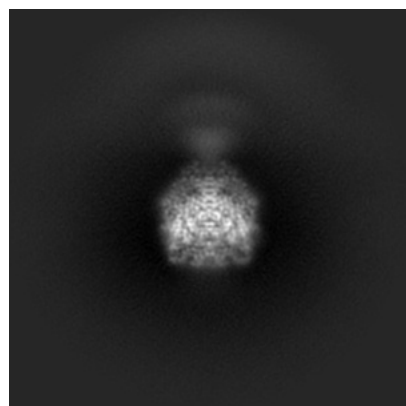
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27004. These allow visual inspection of the internal detail of the map and identification of artifacts.

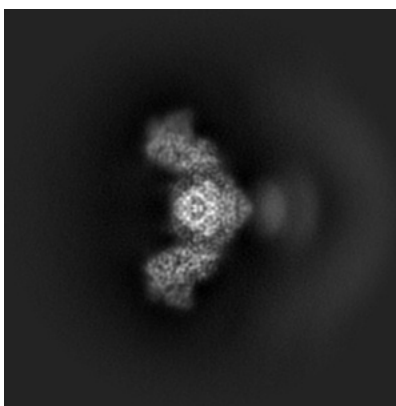
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

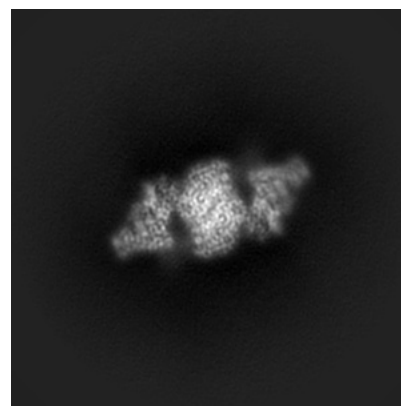
6.1.1 Primary map



X

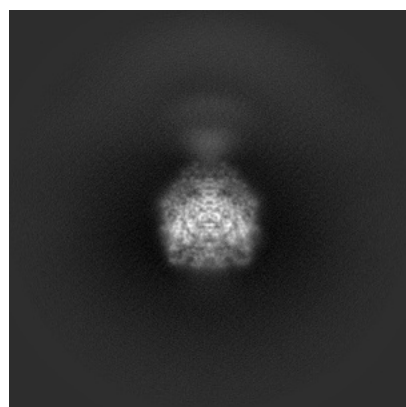


Y

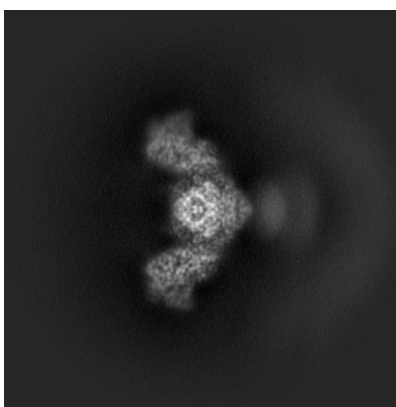


Z

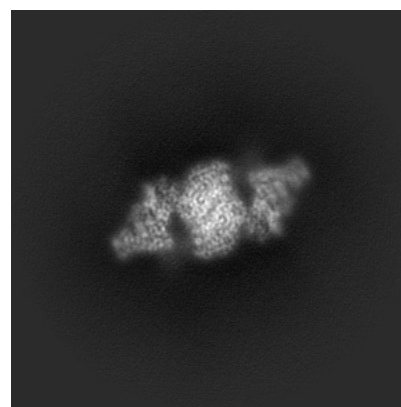
6.1.2 Raw map



X



Y

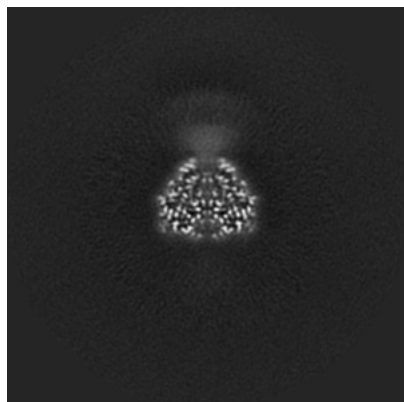


Z

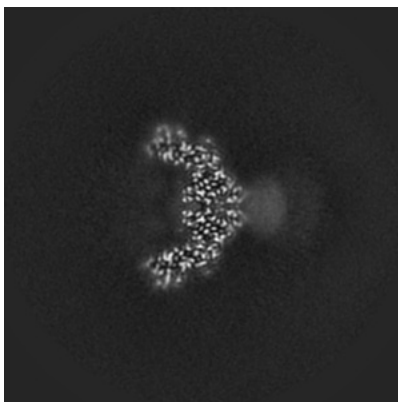
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

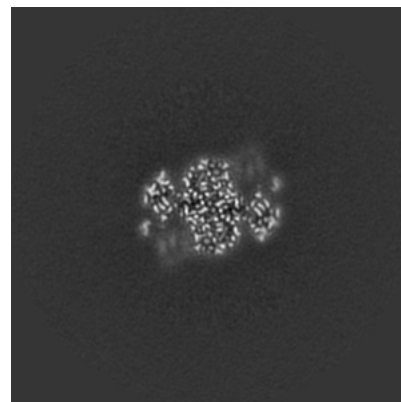
6.2.1 Primary map



X Index: 193

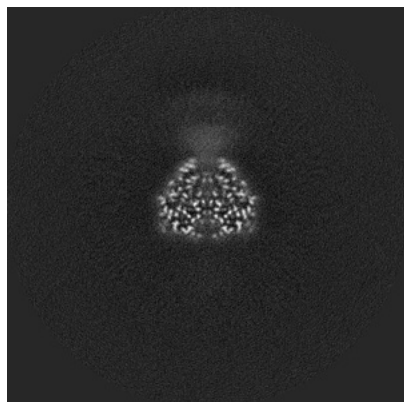


Y Index: 193

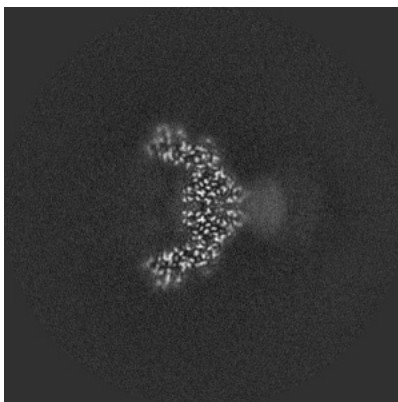


Z Index: 193

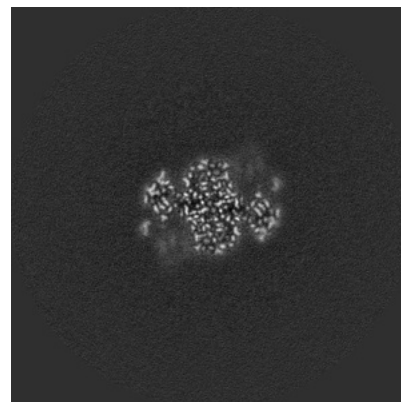
6.2.2 Raw map



X Index: 193



Y Index: 193

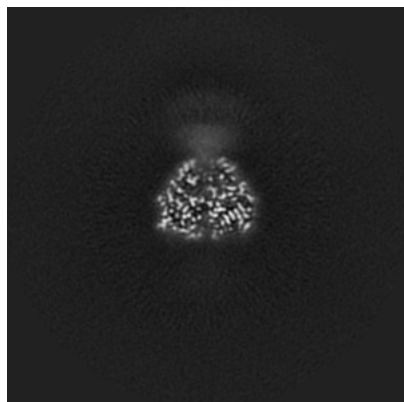


Z Index: 193

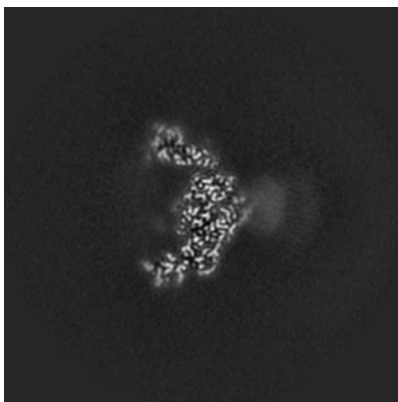
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

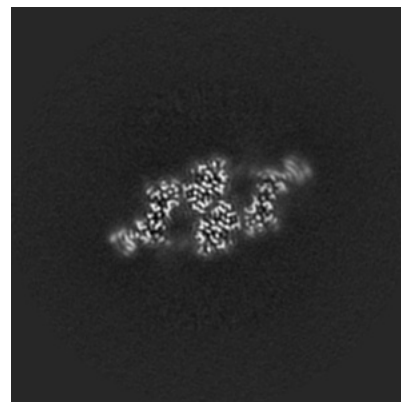
6.3.1 Primary map



X Index: 191

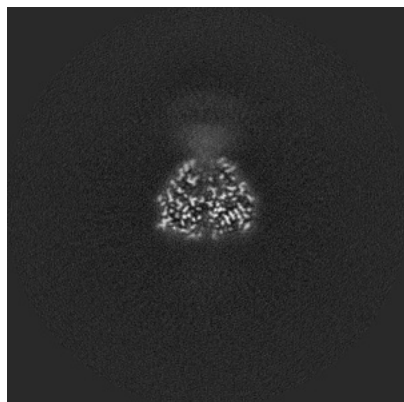


Y Index: 197

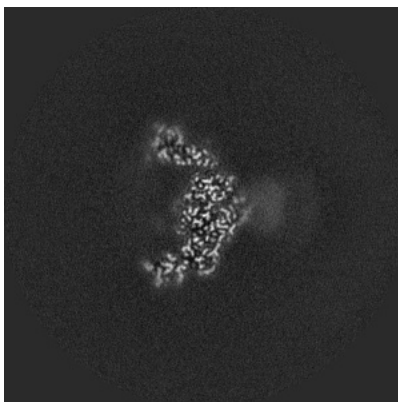


Z Index: 178

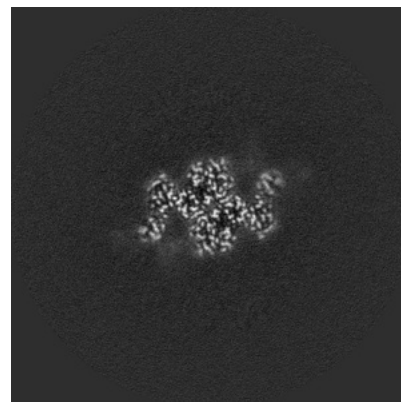
6.3.2 Raw map



X Index: 191



Y Index: 197

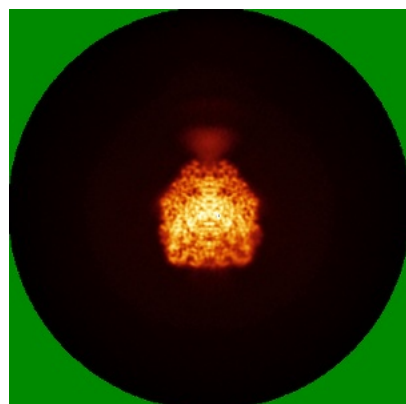


Z Index: 185

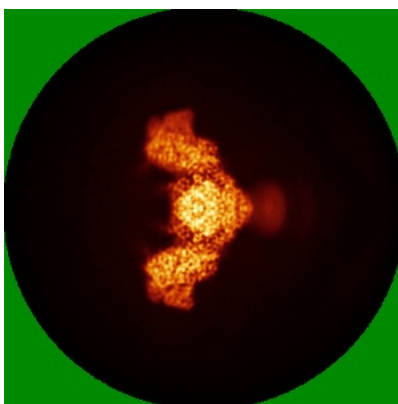
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X

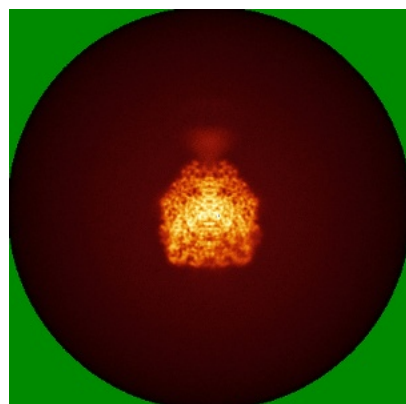


Y

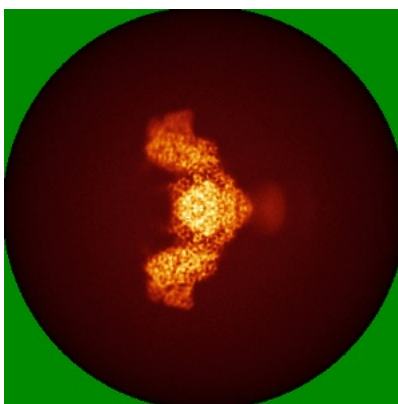


Z

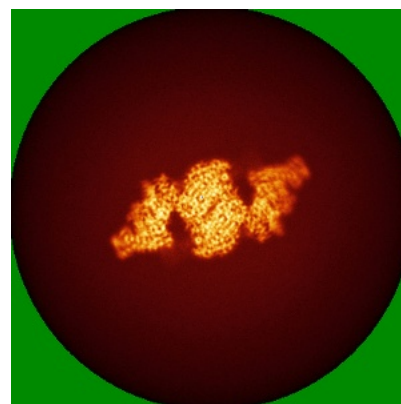
6.4.2 Raw map



X



Y

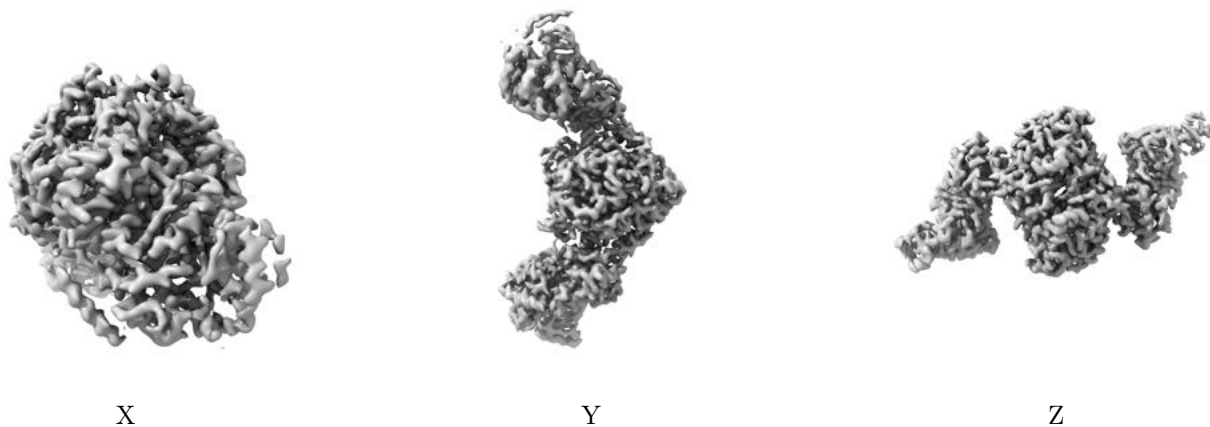


Z

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.

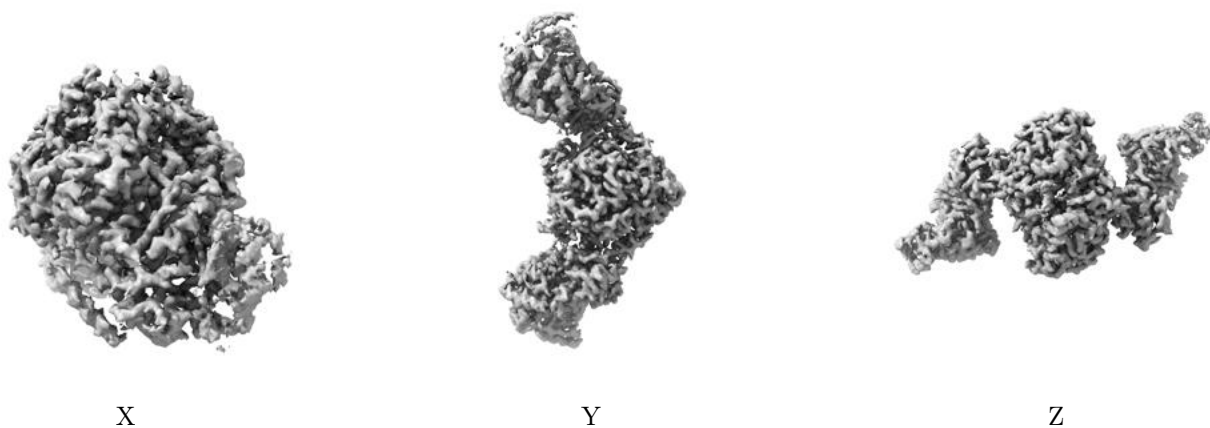
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0162. 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.

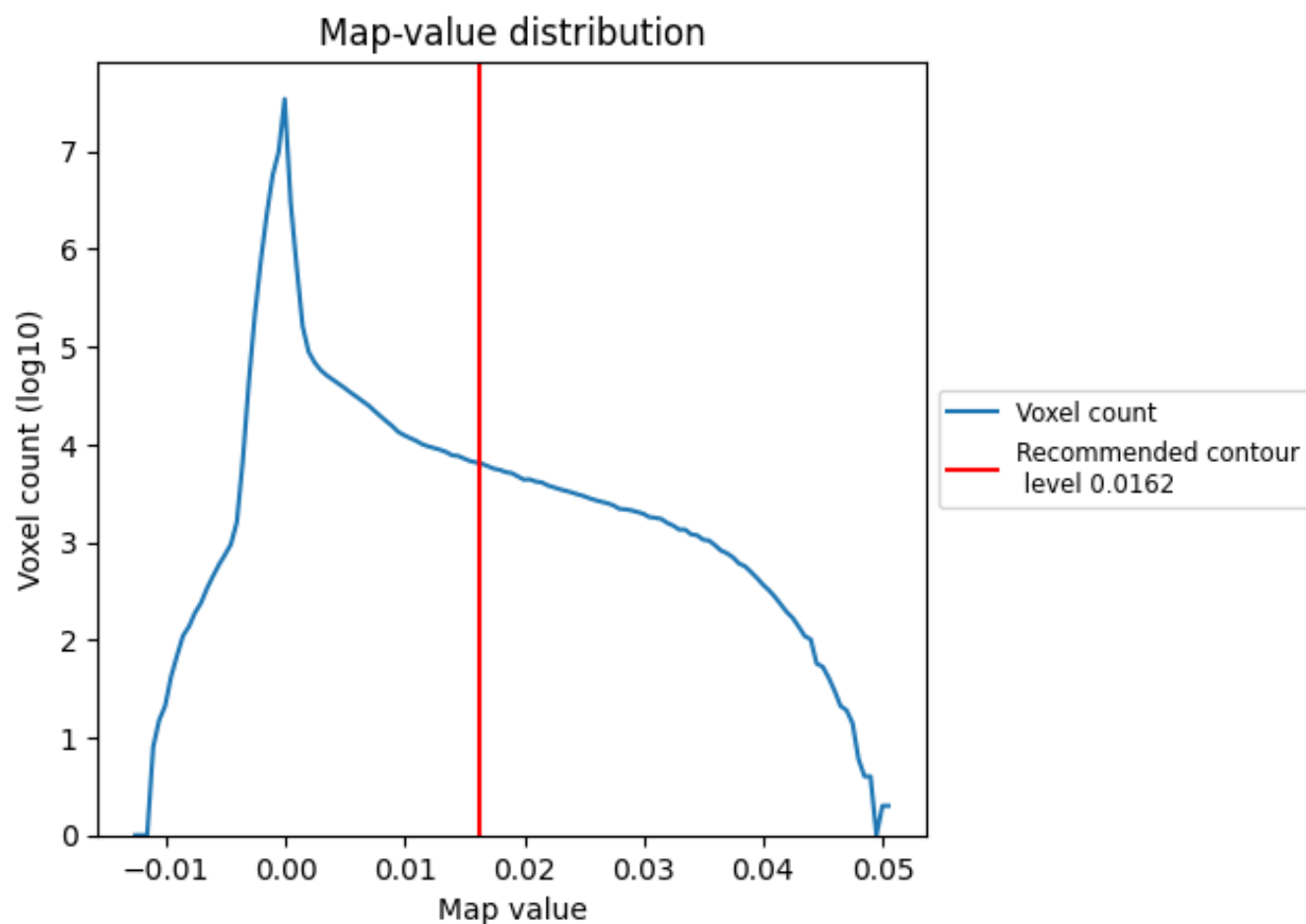
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

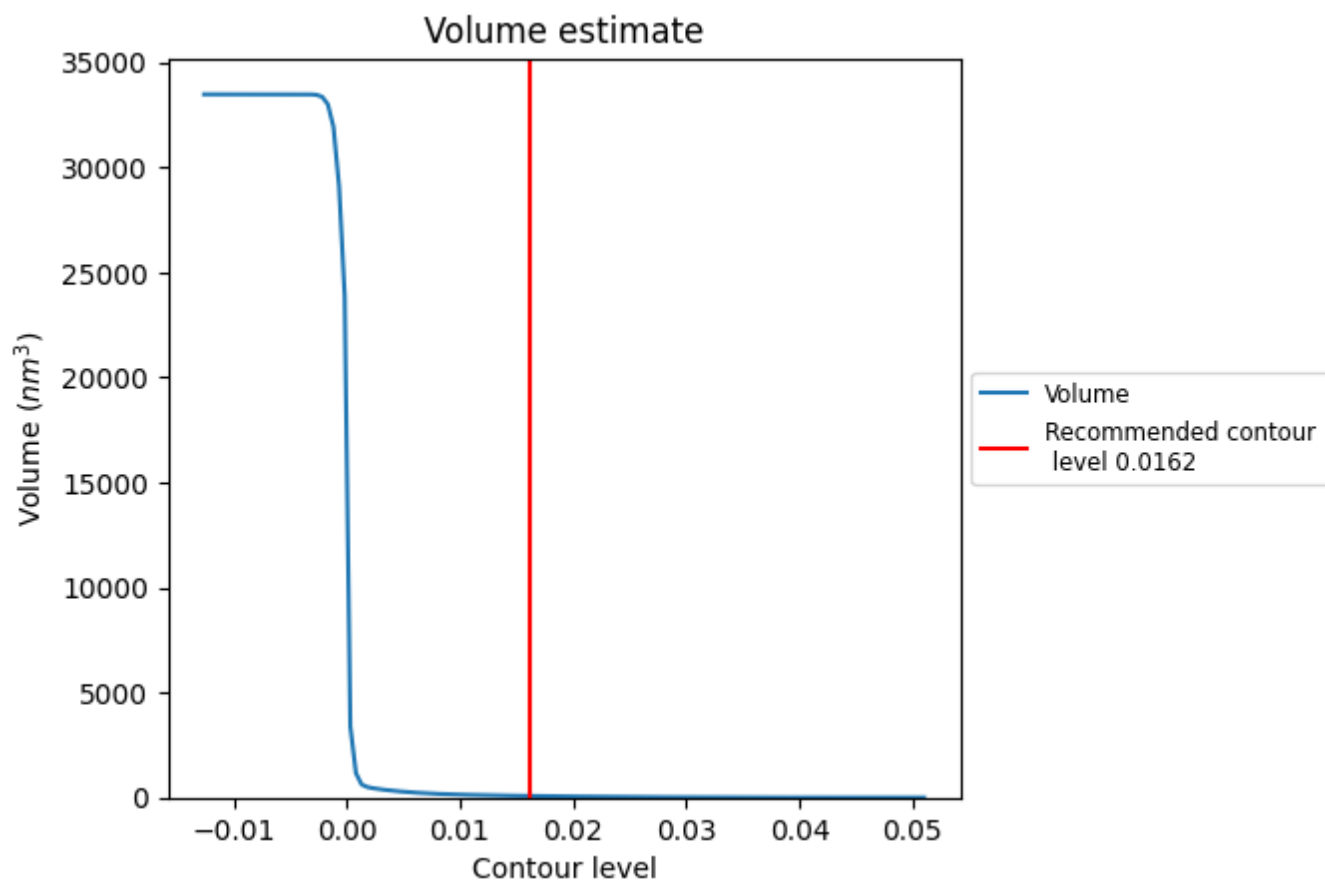
This section contains the results of statistical analysis of the map.

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.

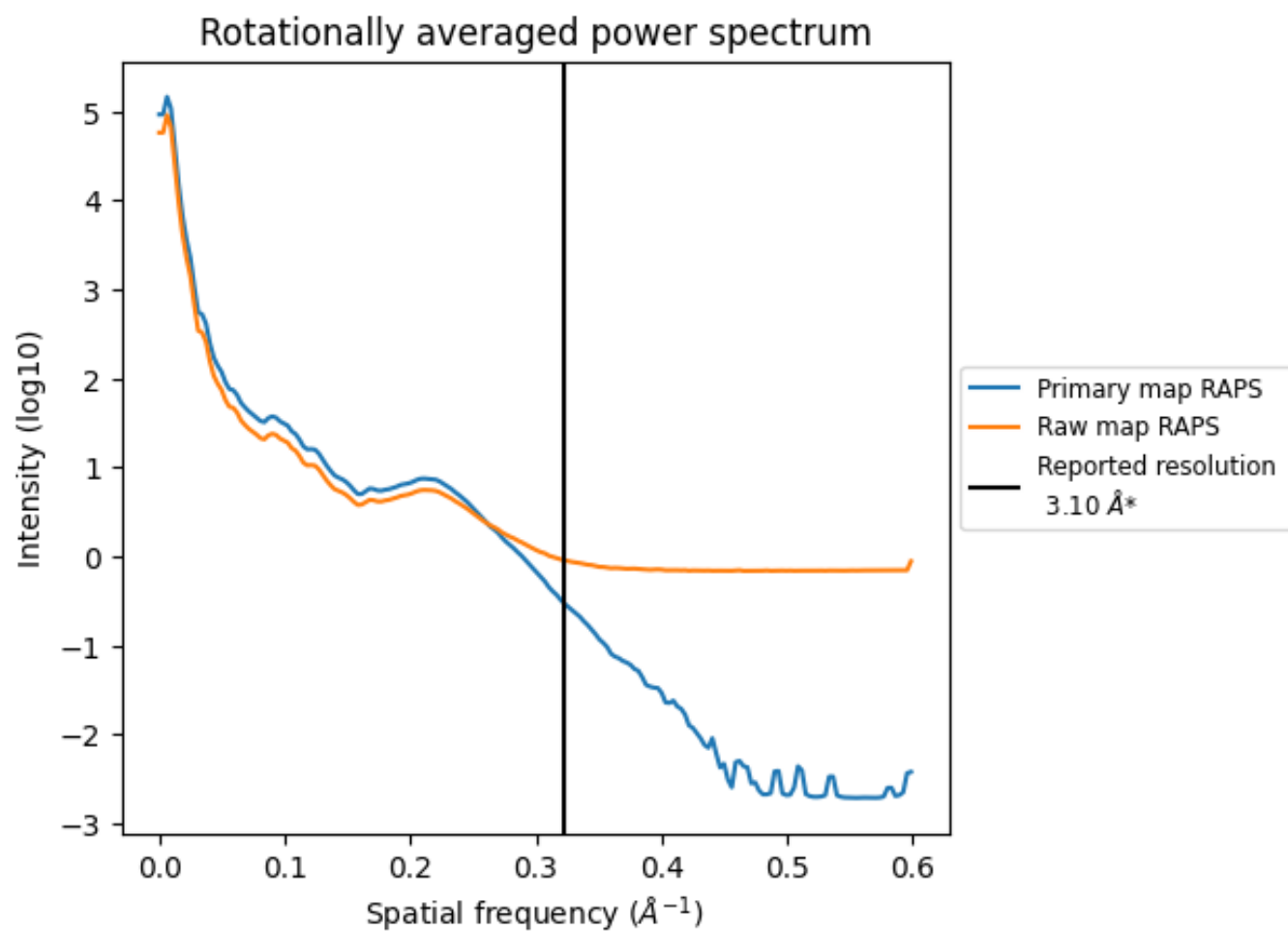
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 75 nm³; this corresponds to an approximate mass of 67 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 ⓘ

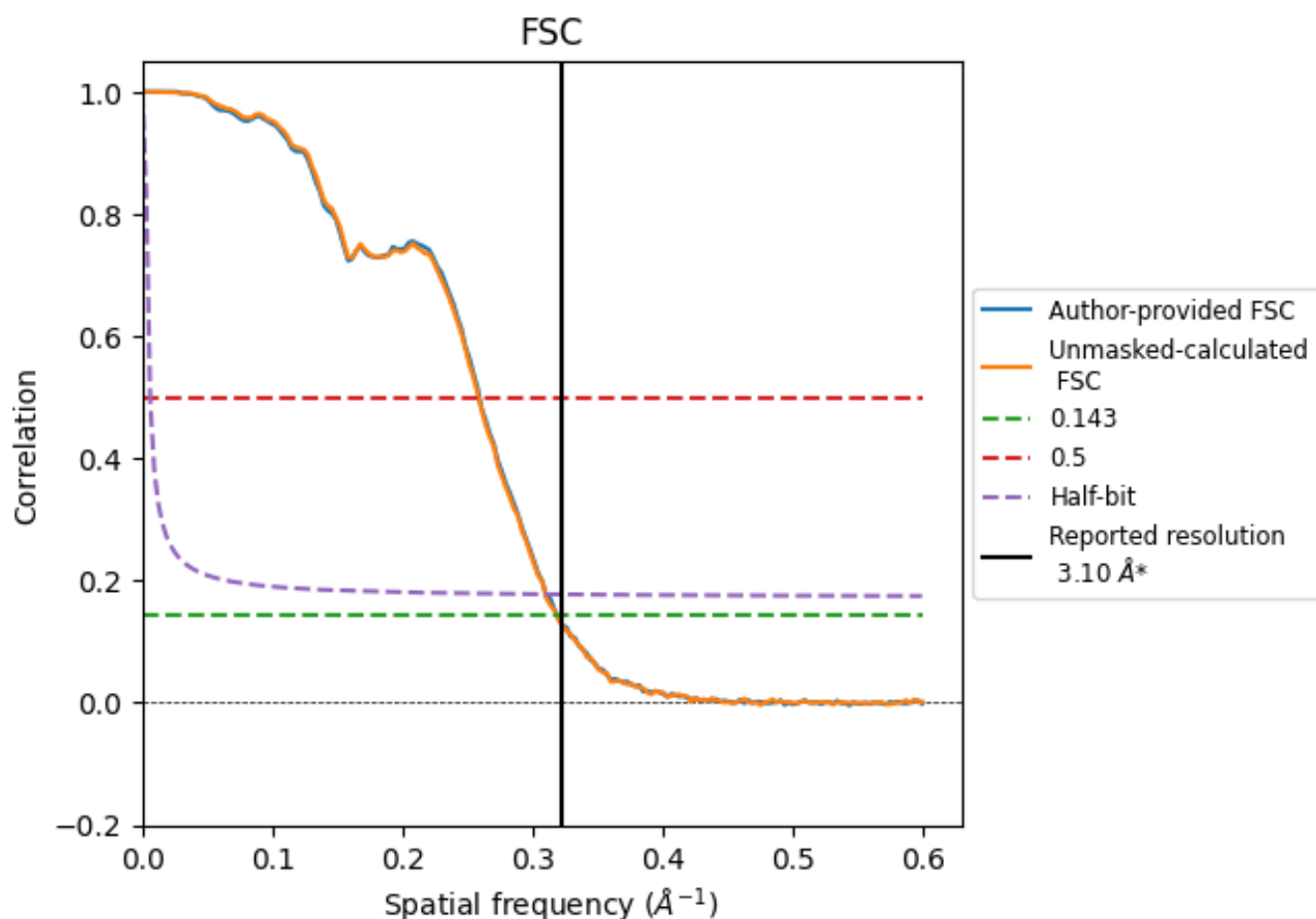


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

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 0.323 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

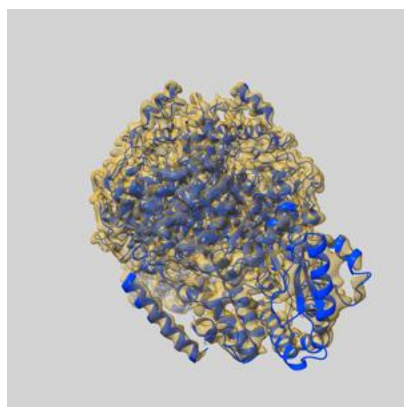
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.14	3.86	3.23
Unmasked-calculated*	3.14	3.87	3.23

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

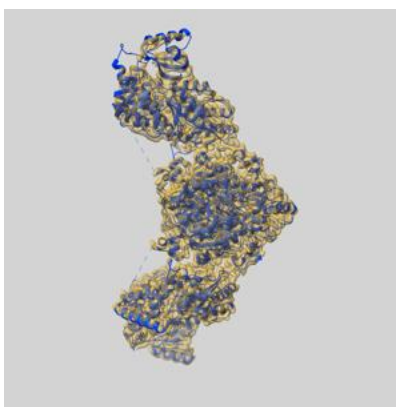
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-27004 and PDB model 8CV0. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

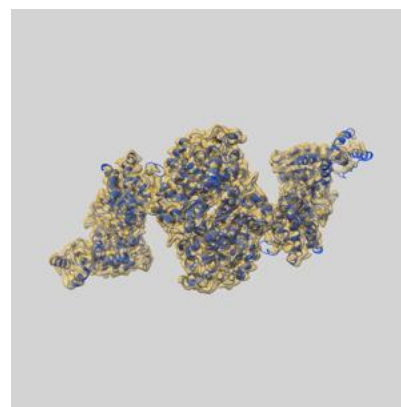
9.1 Map-model overlay [i](#)



X



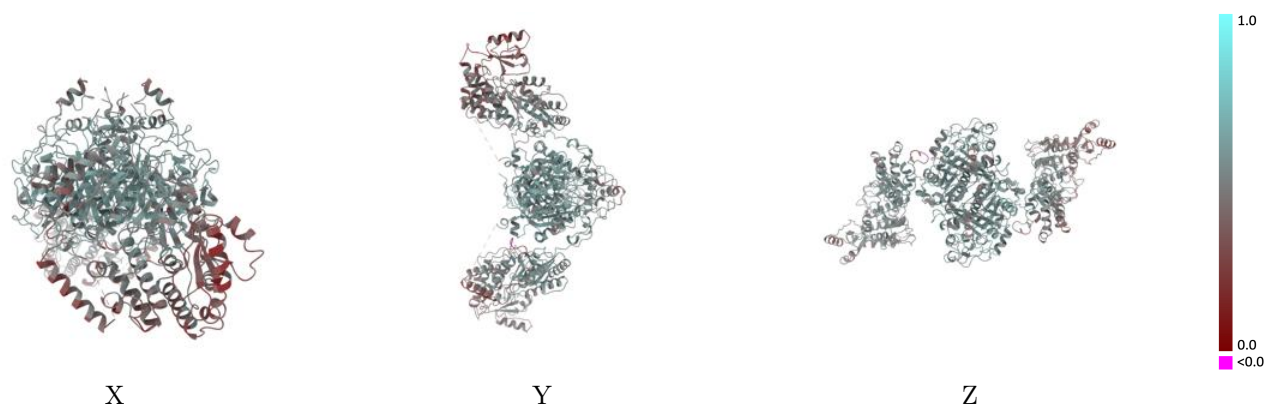
Y



Z

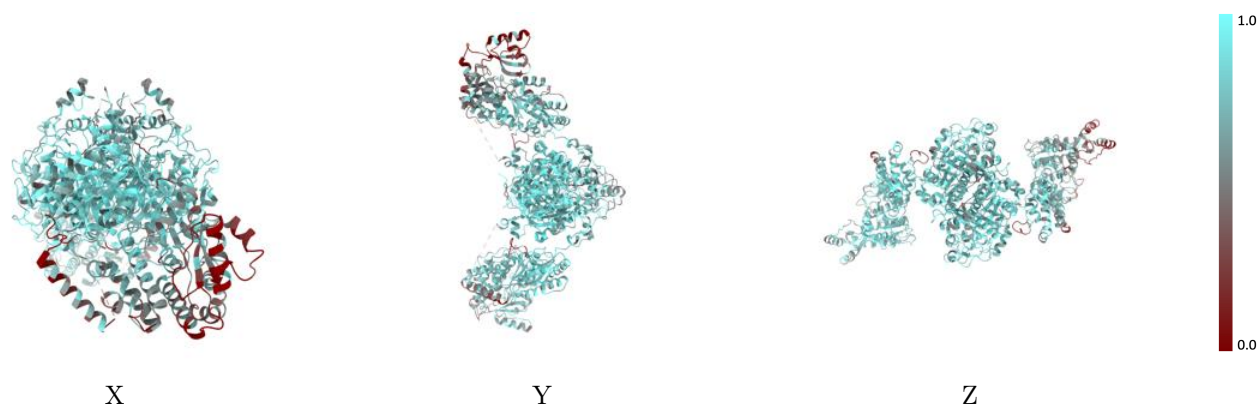
The images above show the 3D surface view of the map at the recommended contour level 0.0162 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



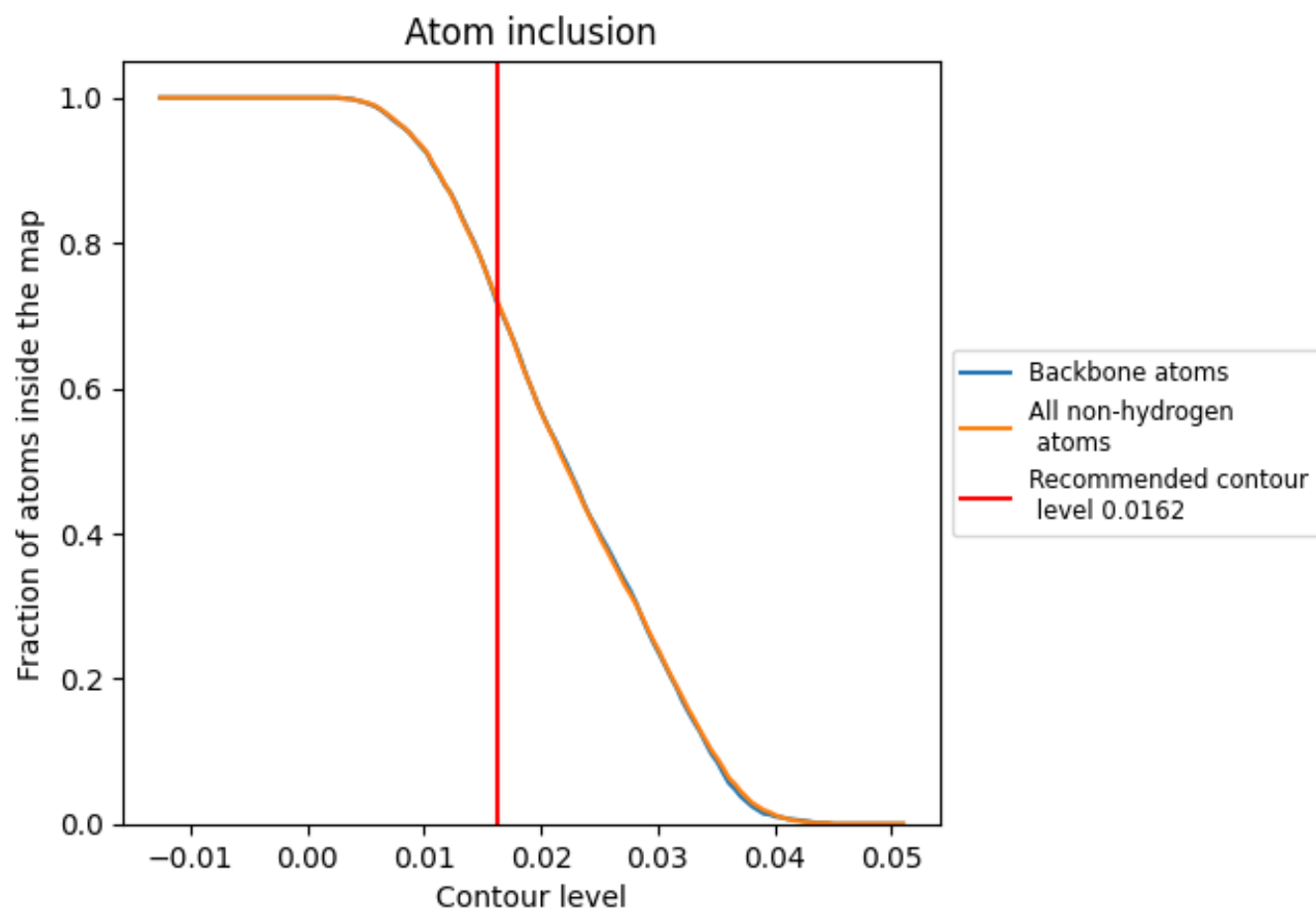
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0162).

9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 72% 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 (0.0162) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7230	0.5080
A	0.7780	0.5190
B	0.6890	0.4970

