



wwPDB EM Validation Summary Report ⓘ

Mar 20, 2026 – 02:04 AM UTC

PDB ID : 8CUZ / pdb_00008cuz
EMDB ID : EMD-27003
Title : KS-AT domains of mycobacterial Pks13 with inward 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 : 3.00 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

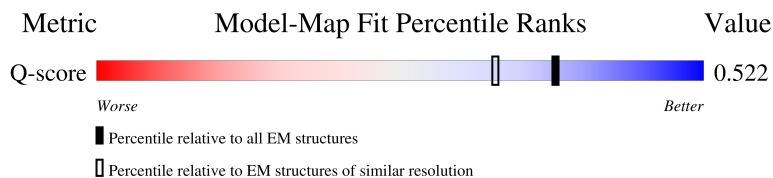
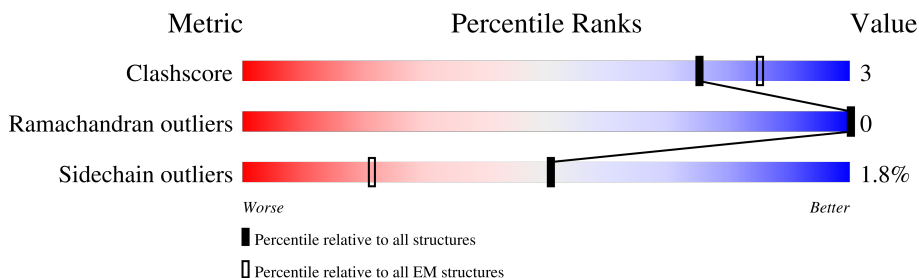
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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	14081 (2.50 - 3.50)

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	

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

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	123116	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	0.054	Depositor
Minimum map value	-0.014	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0126	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

5.1 Standard geometry

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	0.06	0/7162	0.24	2/9719 (0.0%)
1	B	0.06	0/7162	0.24	2/9719 (0.0%)
All	All	0.06	0/14324	0.24	4/19438 (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.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	718	LYS	CD-CE-NZ	8.49	139.06	111.90
1	B	718	LYS	CD-CE-NZ	8.48	139.05	111.90
1	A	835	PHE	O-C-N	-6.56	115.37	123.44
1	B	835	PHE	O-C-N	-6.53	115.41	123.44

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	835	PHE	Mainchain
1	B	835	PHE	Mainchain

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	7021	6858	6900	43	0
1	B	7021	6853	6900	44	0
2	A	19	34	0	0	0
2	B	19	34	0	0	0
All	All	14080	13779	13800	86	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 86 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:864:VAL:O	1:A:963:SER:OG	1.98	0.80
1:B:864:VAL:O	1:B:963:SER:OG	1.99	0.80
1:B:325:ASP:N	1:B:325:ASP:OD1	2.21	0.73
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

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	919/1816 (51%)	888 (97%)	31 (3%)	0	100	100
1	B	919/1816 (51%)	887 (96%)	32 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1838/3632 (51%)	1775 (97%)	63 (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%)	710 (98%)	13 (2%)	51	77
1	B	723/1414 (51%)	710 (98%)	13 (2%)	51	77
All	All	1446/2828 (51%)	1420 (98%)	26 (2%)	51	77

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	325	ASP
1	B	608	GLU
1	B	861	ASP
1	B	510	PHE
1	B	609	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	276	GLN
1	B	403	HIS
1	B	1032	HIS
1	B	777	GLN
1	A	1032	HIS

5.3.3 RNA ⓘ

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.

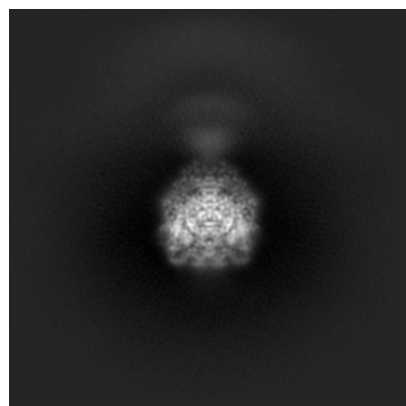
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27003. These allow visual inspection of the internal detail of the map and identification of artifacts.

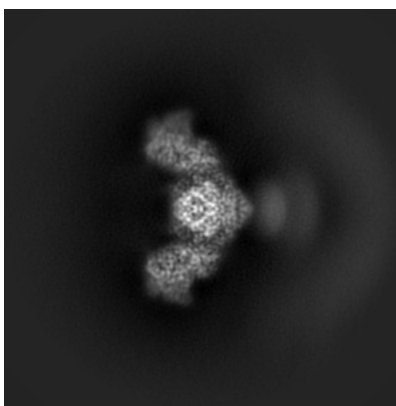
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

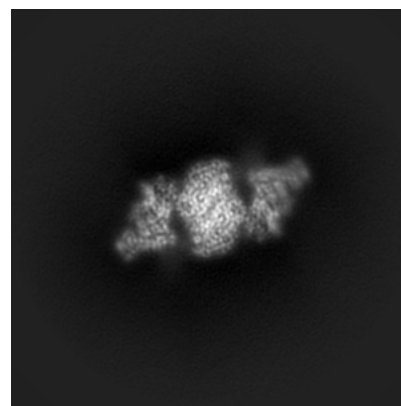
6.1.1 Primary map



X

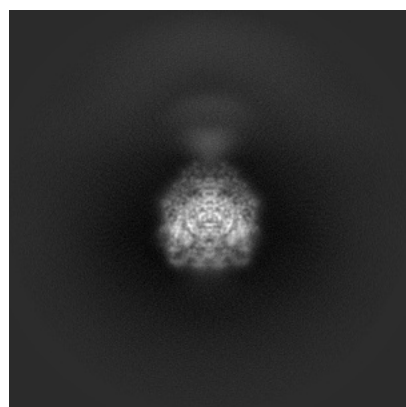


Y

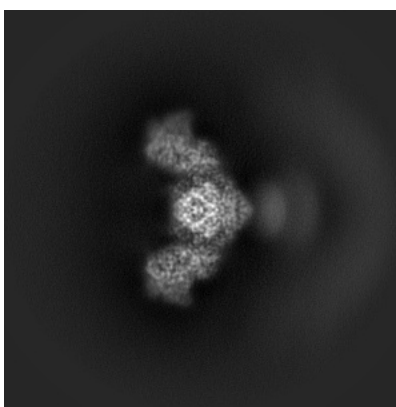


Z

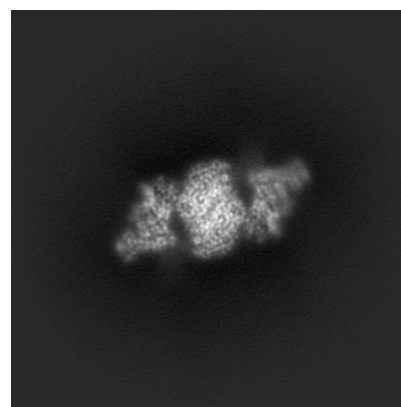
6.1.2 Raw map



X



Y

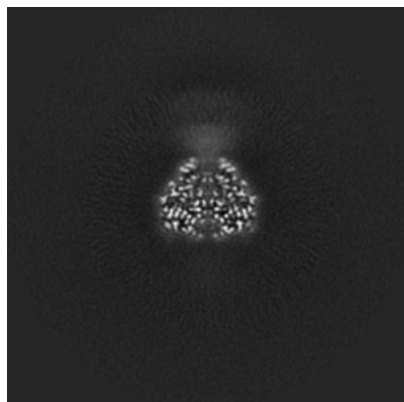


Z

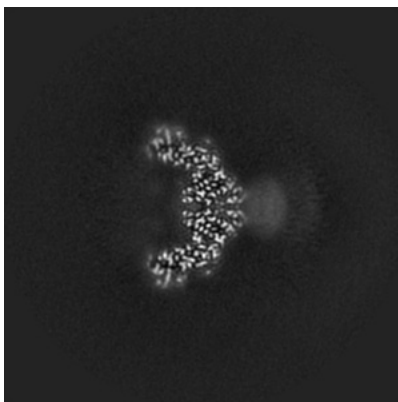
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

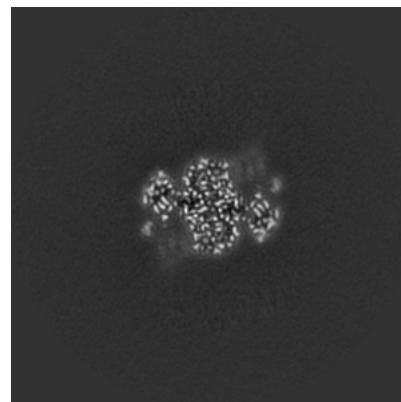
6.2.1 Primary map



X Index: 193

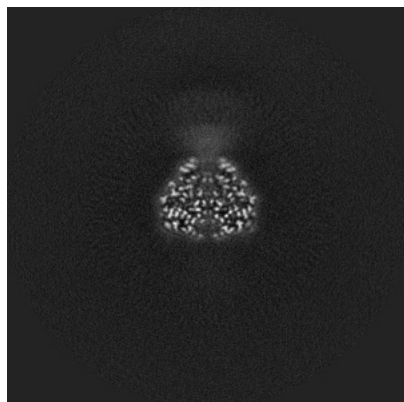


Y Index: 193

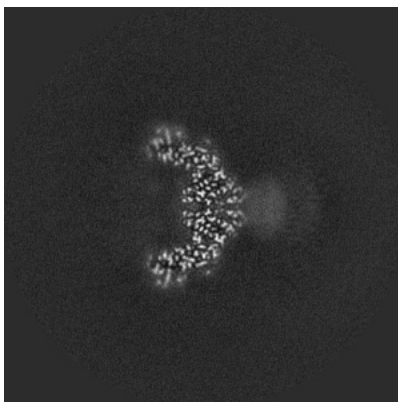


Z Index: 193

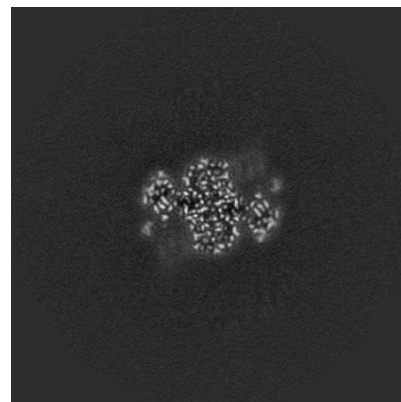
6.2.2 Raw map



X Index: 193



Y Index: 193

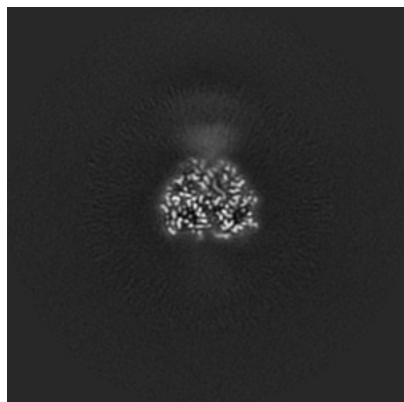


Z Index: 193

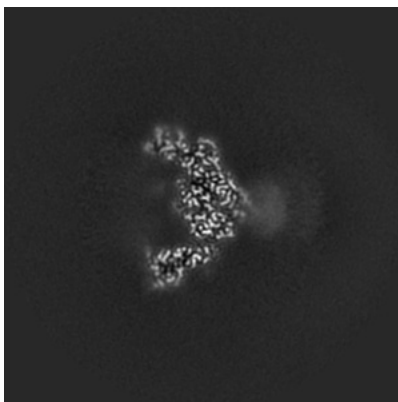
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

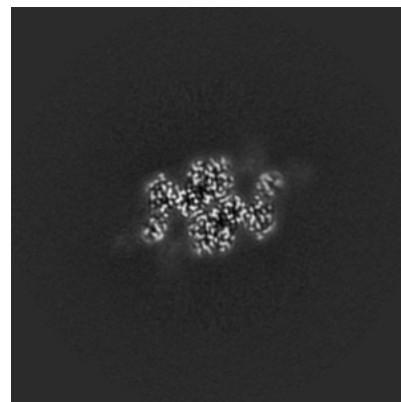
6.3.1 Primary map



X Index: 197

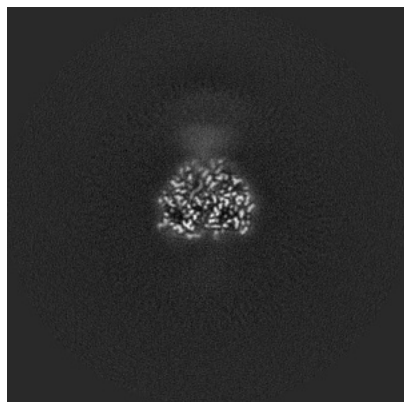


Y Index: 189

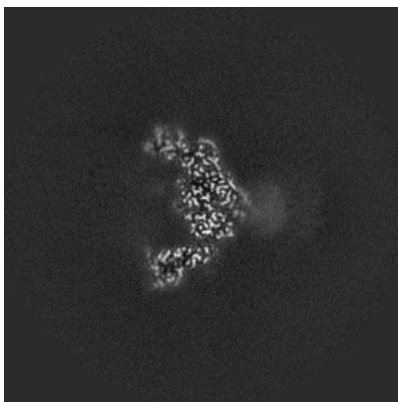


Z Index: 185

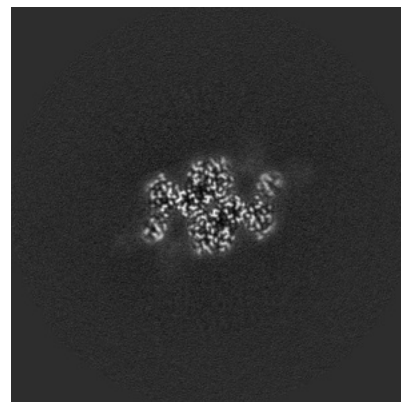
6.3.2 Raw map



X Index: 188



Y Index: 189

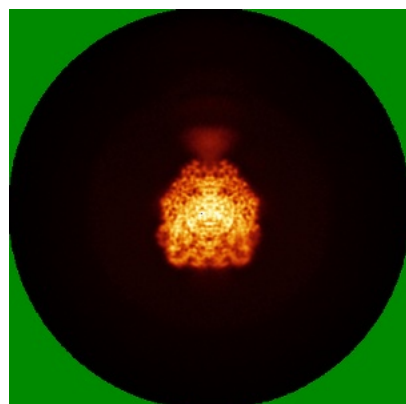


Z Index: 185

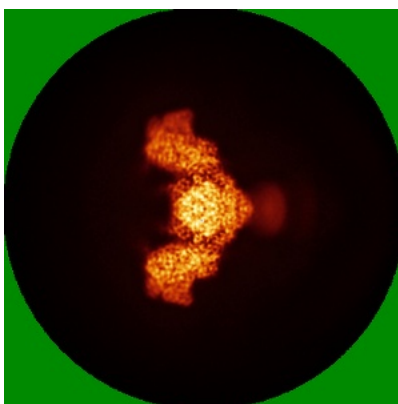
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X

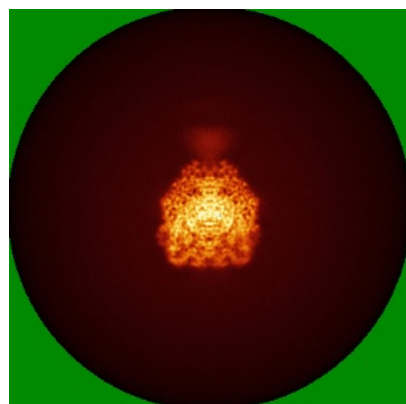


Y

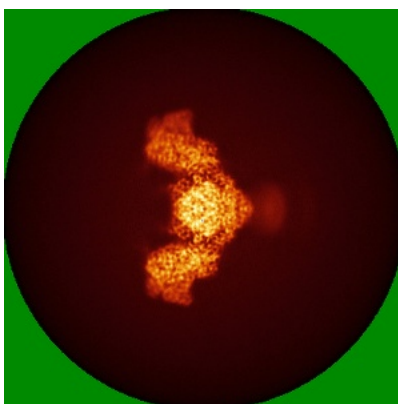


Z

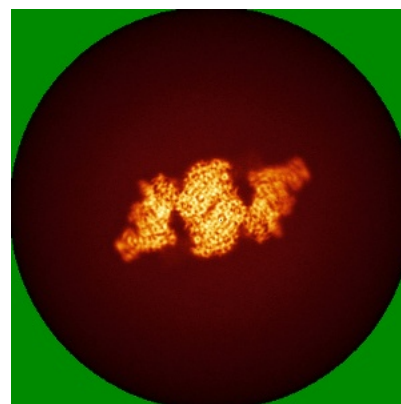
6.4.2 Raw map



X



Y

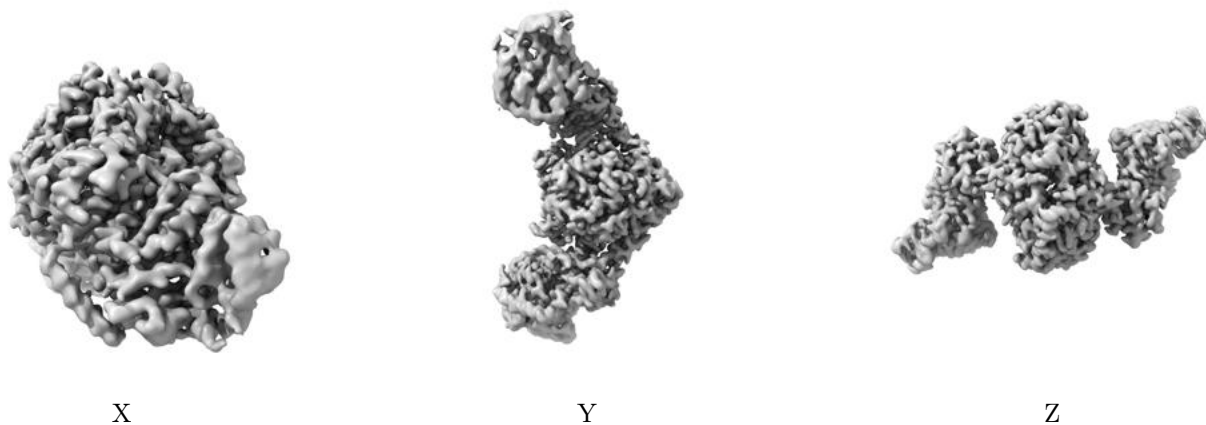


Z

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.

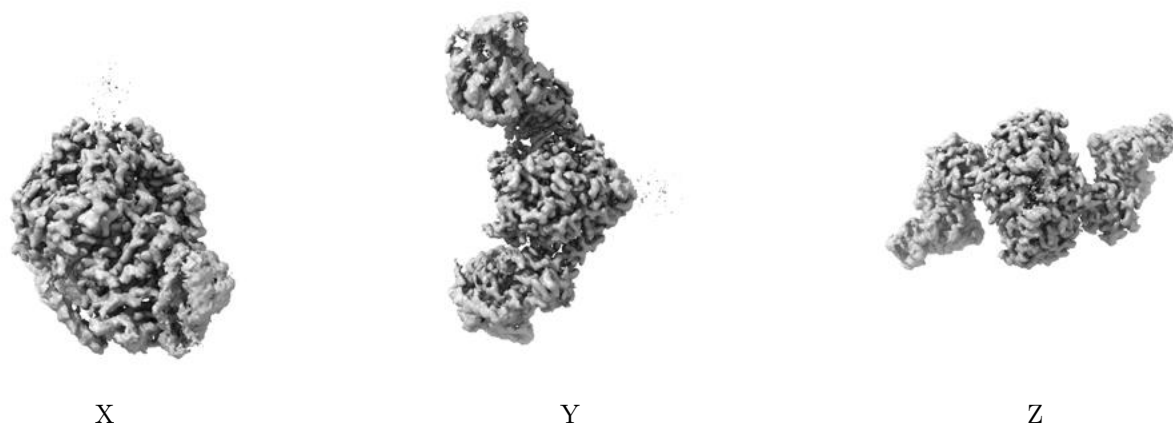
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0126. 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.

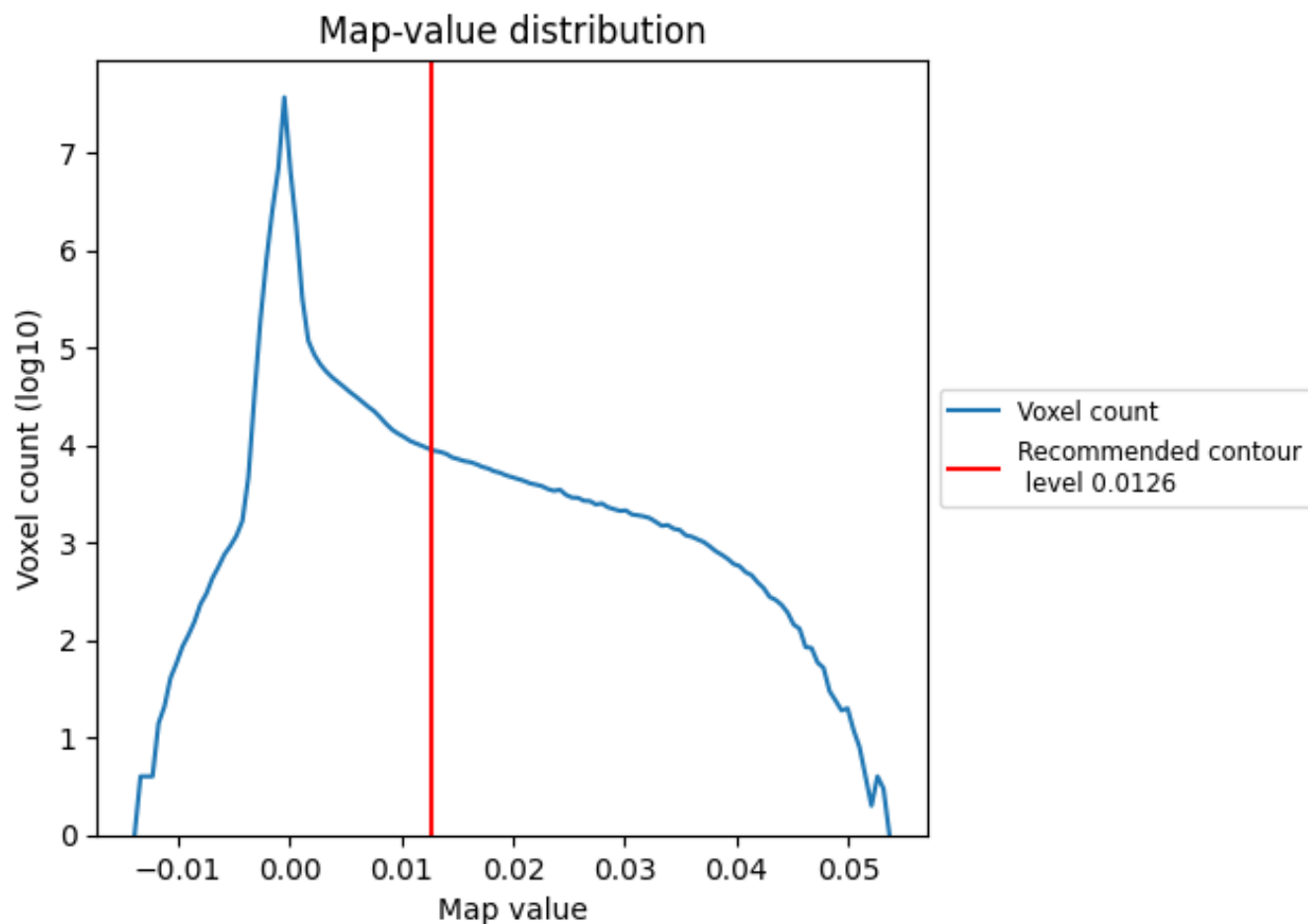
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

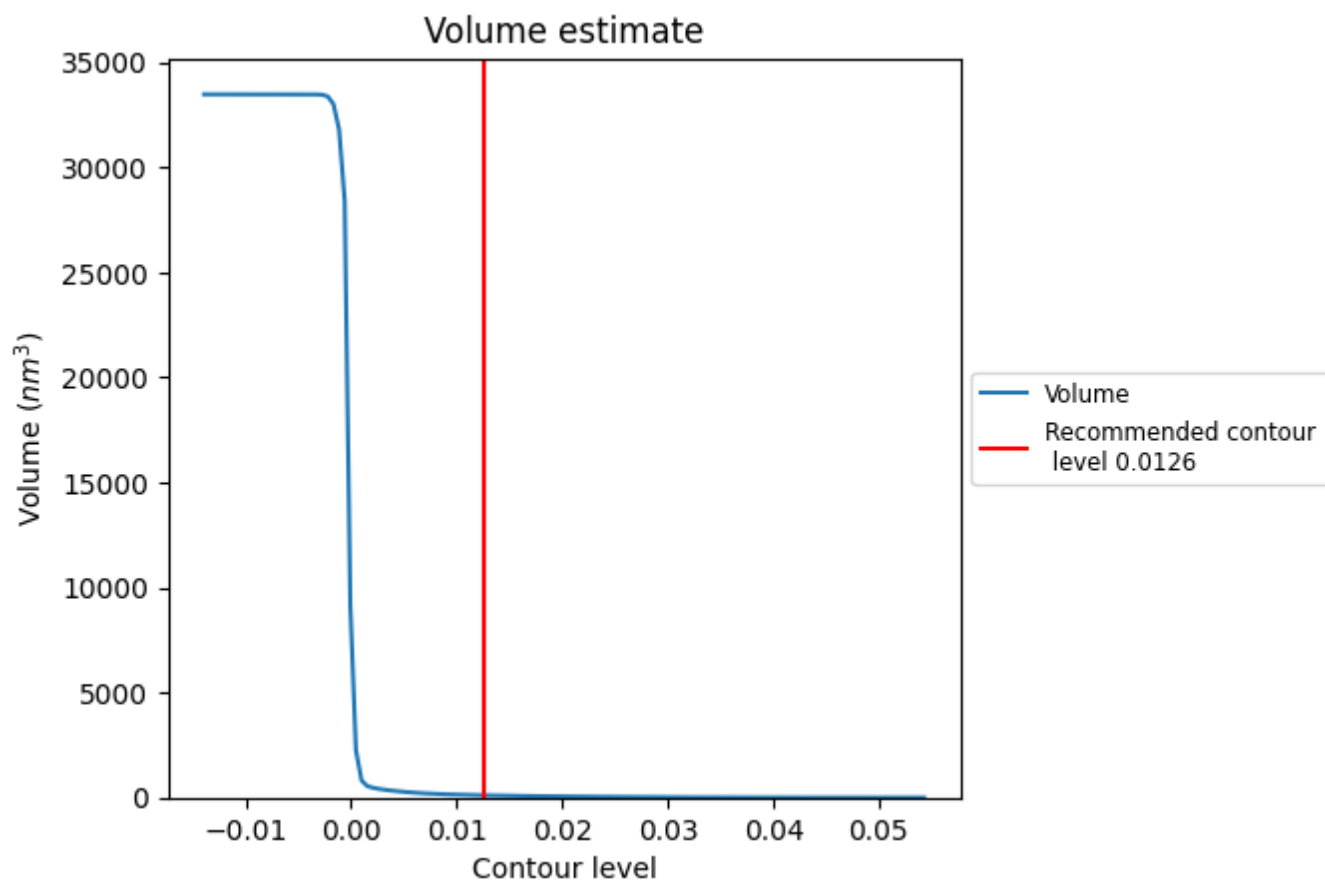
This section contains the results of statistical analysis of the map.

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.

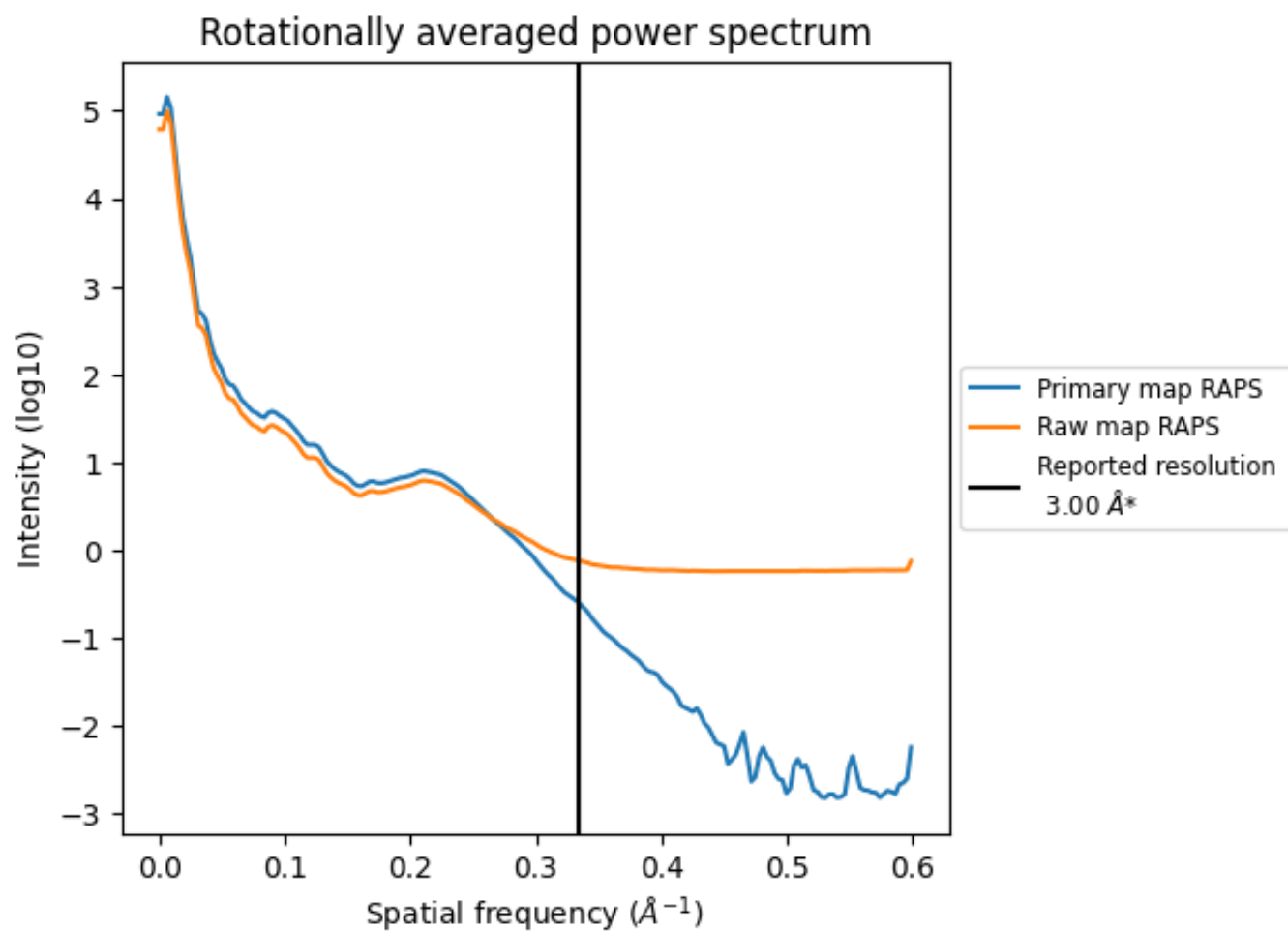
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 107 nm³; this corresponds to an approximate mass of 97 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 ⓘ

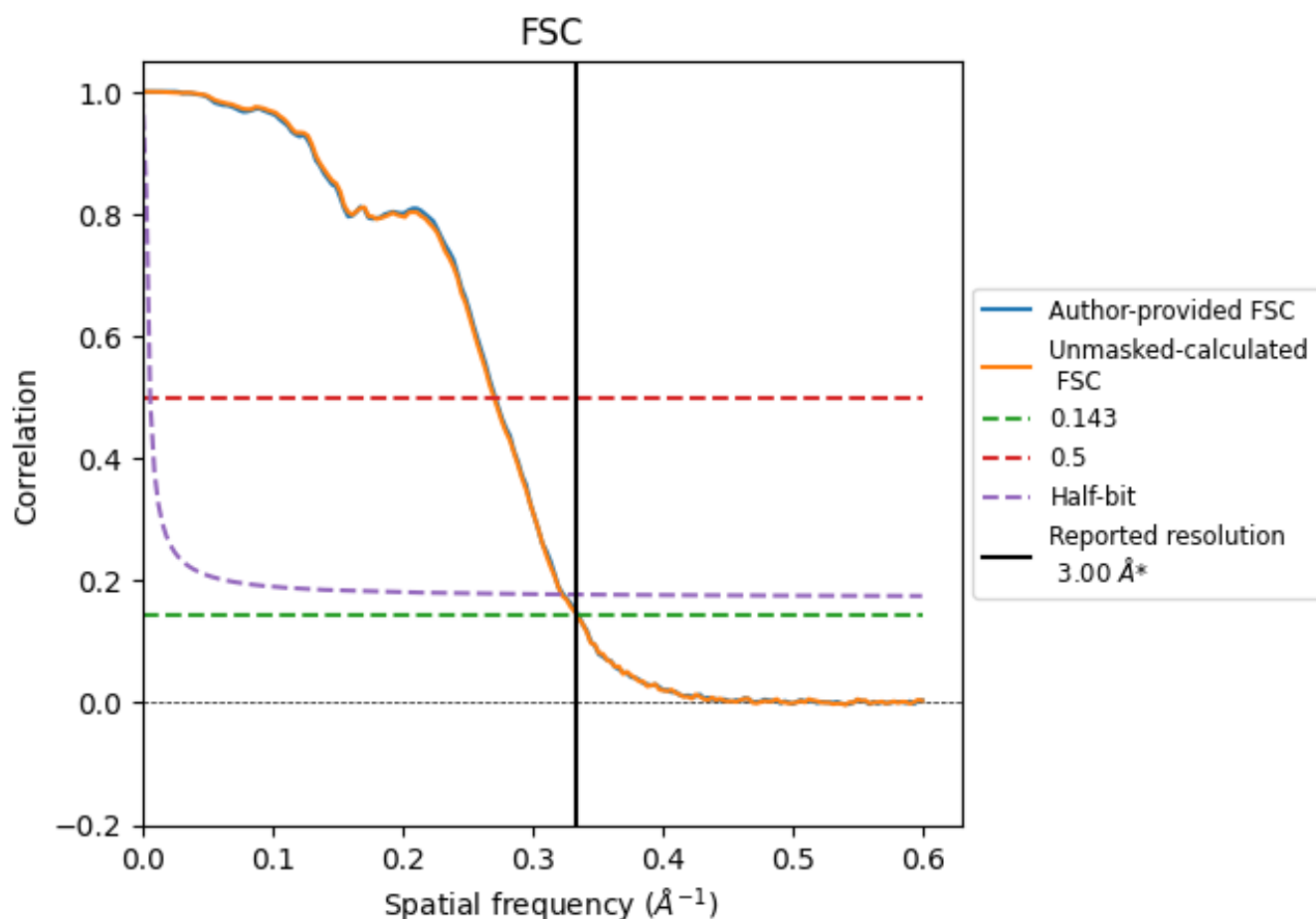


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

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 0.333 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	2.99	3.69	3.09
Unmasked-calculated*	3.00	3.70	3.10

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

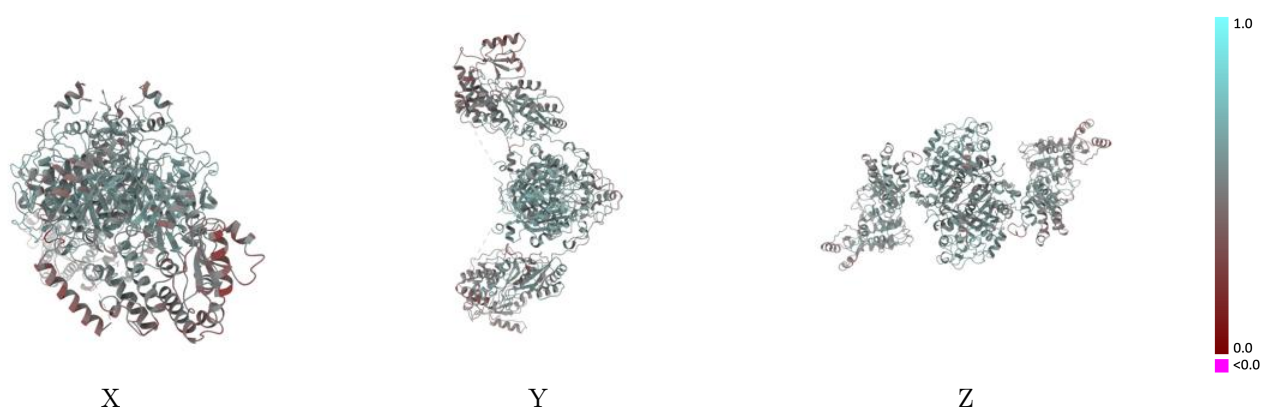
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-27003 and PDB model 8CUZ. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlay [i](#)

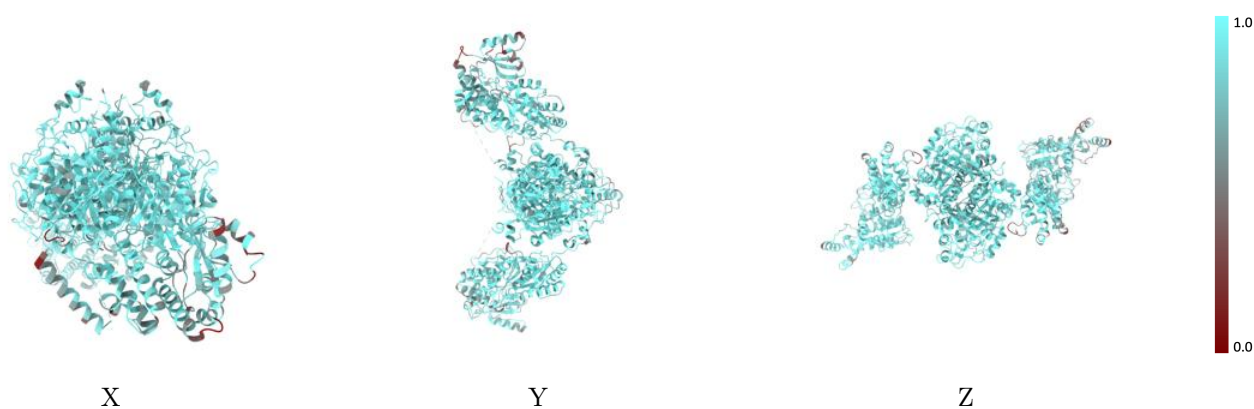
This section was not generated.

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



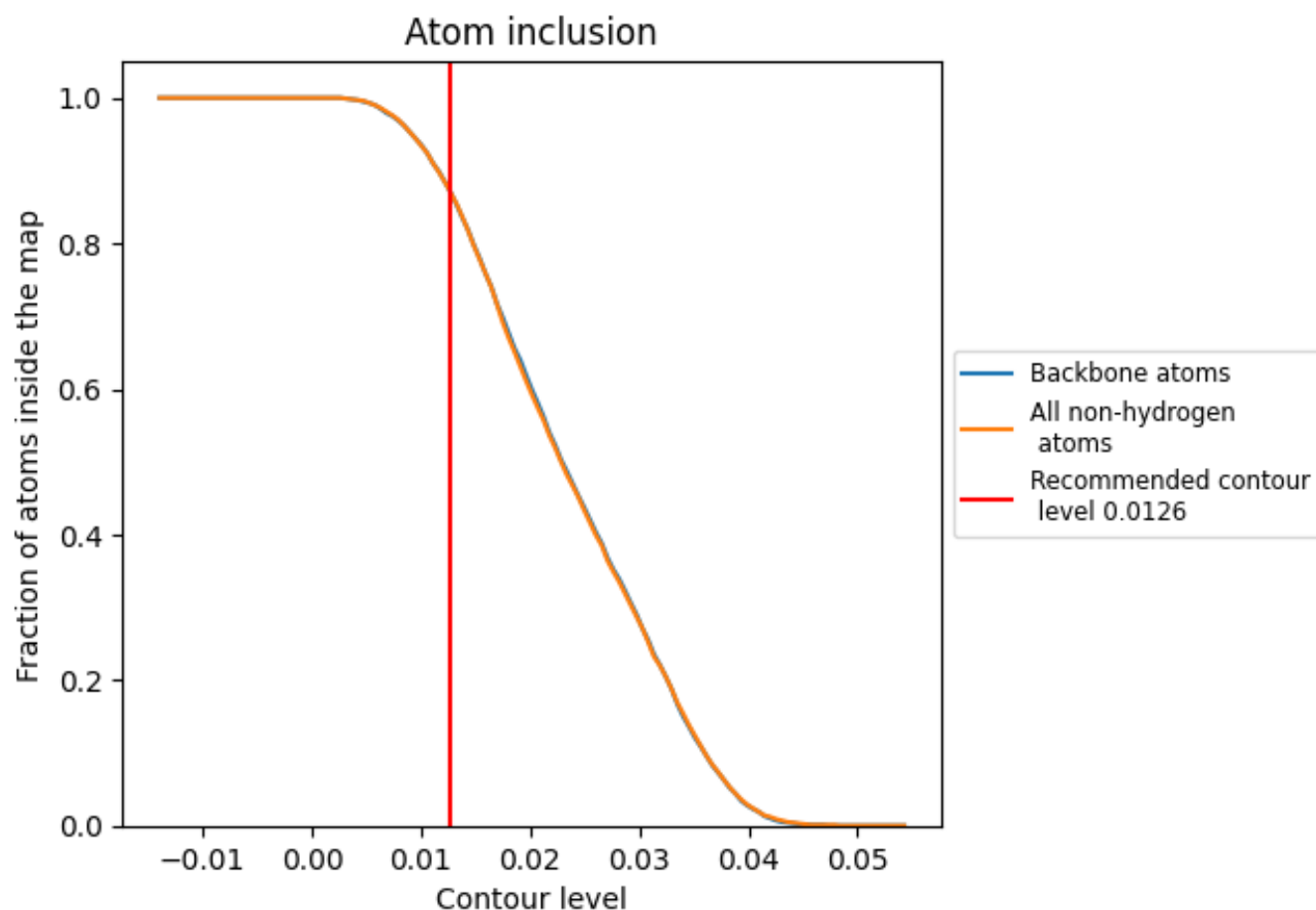
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0126).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 87% 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 (0.0126) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8740	0.5220
A	0.8960	0.5280
B	0.8600	0.5150

