



wwPDB EM Validation Summary Report ⓘ

Jun 9, 2025 – 12:49 PM EDT

PDB ID : 9CKZ / pdb_00009ckz
EMDB ID : EMD-45656
Title : Cryo-EM structure of human XPR1 in apo state
Authors : Wang, Z.; Wu, H.
Deposited on : 2024-07-10
Resolution : 3.45 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.dev118
MolProbity : 4-5-2 with Phenix2.0rc1
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

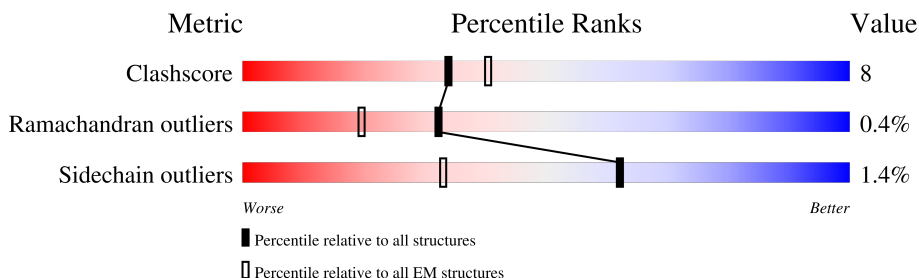
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.45 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	724	
1	B	724	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 9475 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 Solute carrier family 53 member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	591	Total	C	N	O	S	0	0
			4925	3247	807	850	21		
1	B	546	Total	C	N	O	S	0	0
			4550	3009	744	778	19		

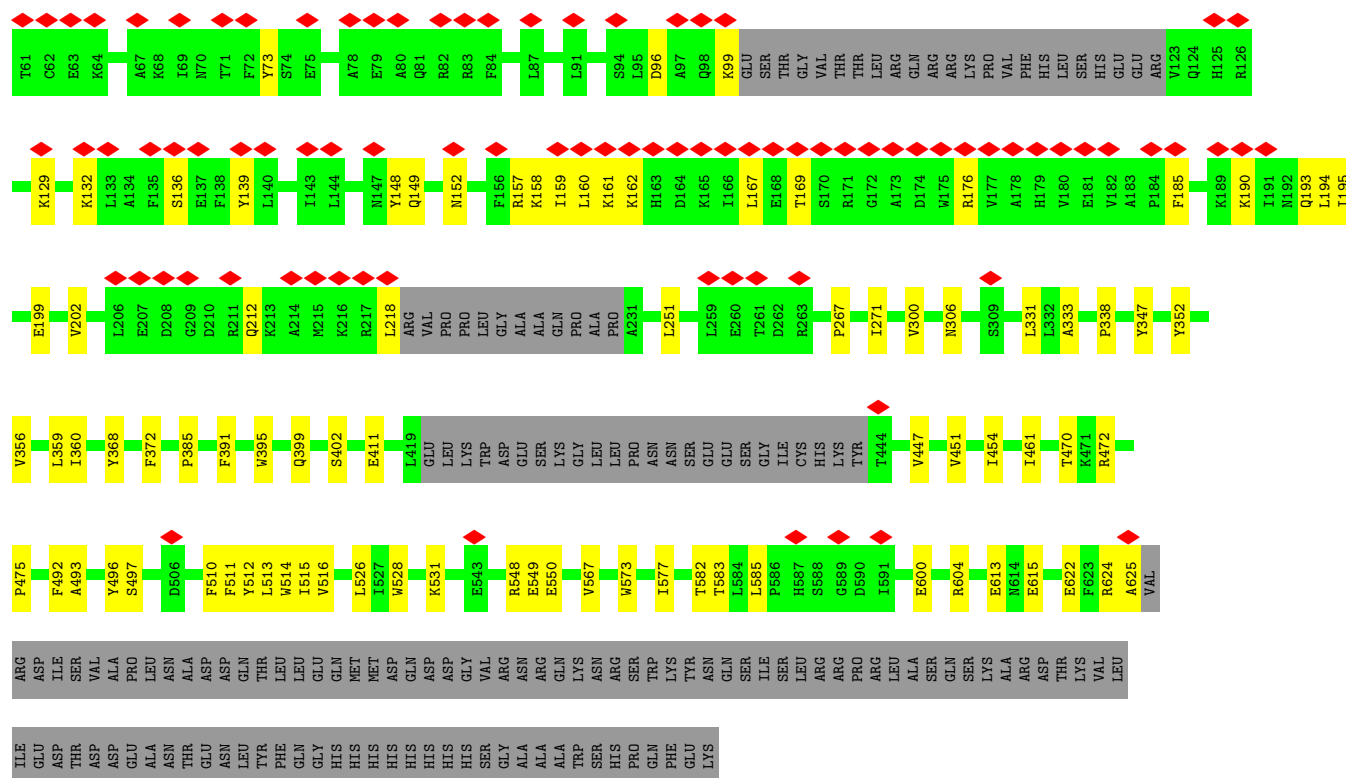
There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	697	GLU	-	expression tag	UNP Q9UBH6
A	698	ASN	-	expression tag	UNP Q9UBH6
A	699	LEU	-	expression tag	UNP Q9UBH6
A	700	TYR	-	expression tag	UNP Q9UBH6
A	701	PHE	-	expression tag	UNP Q9UBH6
A	702	GLN	-	expression tag	UNP Q9UBH6
A	703	GLY	-	expression tag	UNP Q9UBH6
A	704	HIS	-	expression tag	UNP Q9UBH6
A	705	HIS	-	expression tag	UNP Q9UBH6
A	706	HIS	-	expression tag	UNP Q9UBH6
A	707	HIS	-	expression tag	UNP Q9UBH6
A	708	HIS	-	expression tag	UNP Q9UBH6
A	709	HIS	-	expression tag	UNP Q9UBH6
A	710	HIS	-	expression tag	UNP Q9UBH6
A	711	HIS	-	expression tag	UNP Q9UBH6
A	712	SER	-	expression tag	UNP Q9UBH6
A	713	GLY	-	expression tag	UNP Q9UBH6
A	714	ALA	-	expression tag	UNP Q9UBH6
A	715	ALA	-	expression tag	UNP Q9UBH6
A	716	ALA	-	expression tag	UNP Q9UBH6
A	717	TRP	-	expression tag	UNP Q9UBH6
A	718	SER	-	expression tag	UNP Q9UBH6
A	719	HIS	-	expression tag	UNP Q9UBH6
A	720	PRO	-	expression tag	UNP Q9UBH6
A	721	GLN	-	expression tag	UNP Q9UBH6
A	722	PHE	-	expression tag	UNP Q9UBH6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	723	GLU	-	expression tag	UNP Q9UBH6
A	724	LYS	-	expression tag	UNP Q9UBH6
B	697	GLU	-	expression tag	UNP Q9UBH6
B	698	ASN	-	expression tag	UNP Q9UBH6
B	699	LEU	-	expression tag	UNP Q9UBH6
B	700	TYR	-	expression tag	UNP Q9UBH6
B	701	PHE	-	expression tag	UNP Q9UBH6
B	702	GLN	-	expression tag	UNP Q9UBH6
B	703	GLY	-	expression tag	UNP Q9UBH6
B	704	HIS	-	expression tag	UNP Q9UBH6
B	705	HIS	-	expression tag	UNP Q9UBH6
B	706	HIS	-	expression tag	UNP Q9UBH6
B	707	HIS	-	expression tag	UNP Q9UBH6
B	708	HIS	-	expression tag	UNP Q9UBH6
B	709	HIS	-	expression tag	UNP Q9UBH6
B	710	HIS	-	expression tag	UNP Q9UBH6
B	711	HIS	-	expression tag	UNP Q9UBH6
B	712	SER	-	expression tag	UNP Q9UBH6
B	713	GLY	-	expression tag	UNP Q9UBH6
B	714	ALA	-	expression tag	UNP Q9UBH6
B	715	ALA	-	expression tag	UNP Q9UBH6
B	716	ALA	-	expression tag	UNP Q9UBH6
B	717	TRP	-	expression tag	UNP Q9UBH6
B	718	SER	-	expression tag	UNP Q9UBH6
B	719	HIS	-	expression tag	UNP Q9UBH6
B	720	PRO	-	expression tag	UNP Q9UBH6
B	721	GLN	-	expression tag	UNP Q9UBH6
B	722	PHE	-	expression tag	UNP Q9UBH6
B	723	GLU	-	expression tag	UNP Q9UBH6
B	724	LYS	-	expression tag	UNP Q9UBH6



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	230861	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	3.785	Depositor
Minimum map value	-2.328	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.050	Depositor
Recommended contour level	0.219	Depositor
Map size (Å)	299.52002, 299.52002, 299.52002	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8320001, 0.8320001, 0.8320001	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	0.40	1/5061 (0.0%)	0.64	9/6858 (0.1%)
1	B	0.24	0/4677	0.40	0/6336
All	All	0.33	1/9738 (0.0%)	0.54	9/13194 (0.1%)

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	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	204	ASN	C-N	14.44	1.55	1.33

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	204	ASN	CA-C-N	-12.16	99.15	121.41
1	A	204	ASN	C-N-CA	-12.16	99.15	121.41
1	A	207	GLU	O-C-N	12.09	138.39	122.19
1	A	207	GLU	CA-C-N	-10.93	106.44	122.07
1	A	207	GLU	C-N-CA	-10.93	106.44	122.07

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	204	ASN	Mainchain
1	A	258	LYS	Mainchain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	A	442	LYS	Peptide
1	A	627	ARG	Sidechain

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	4925	0	4900	92	0
1	B	4550	0	4537	60	0
All	All	9475	0	9437	151	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 151 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:13:PRO:O	1:A:17:LYS:HB2	1.68	0.92
1:A:202:VAL:HG13	1:A:206:LEU:HD12	1.51	0.92
1:A:263:ARG:O	1:A:263:ARG:CZ	2.19	0.90
1:A:263:ARG:NH1	1:A:265:ILE:HA	1.88	0.89
1:A:263:ARG:HH12	1:A:265:ILE:HA	1.44	0.82

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	583/724 (80%)	550 (94%)	29 (5%)	4 (1%)	19	53
1	B	538/724 (74%)	516 (96%)	22 (4%)	0	100	100
All	All	1121/1448 (77%)	1066 (95%)	51 (4%)	4 (0%)	32	64

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	180	VAL
1	A	259	LEU
1	A	264	SER
1	A	634	LEU

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	527/644 (82%)	514 (98%)	13 (2%)	42	69
1	B	486/644 (76%)	485 (100%)	1 (0%)	92	96
All	All	1013/1288 (79%)	999 (99%)	14 (1%)	62	79

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	620	CYS
1	A	624	ARG
1	B	300	VAL
1	A	628	ASP
1	A	648	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	288	ASN
1	B	399	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	544	ASN
1	A	544	ASN
1	A	576	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](#)

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.

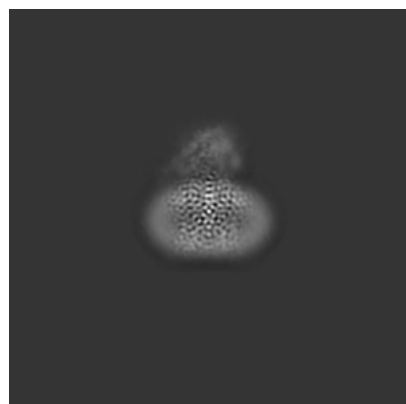
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45656. These allow visual inspection of the internal detail of the map and identification of artifacts.

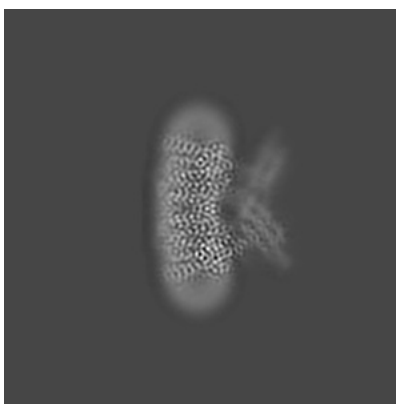
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

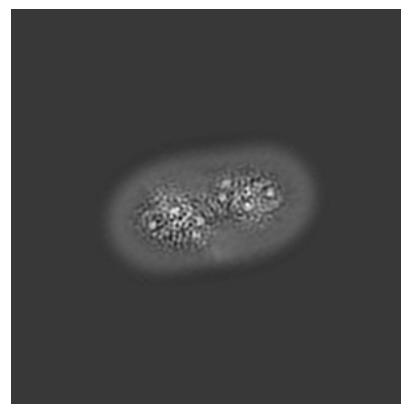
6.1.1 Primary map



X

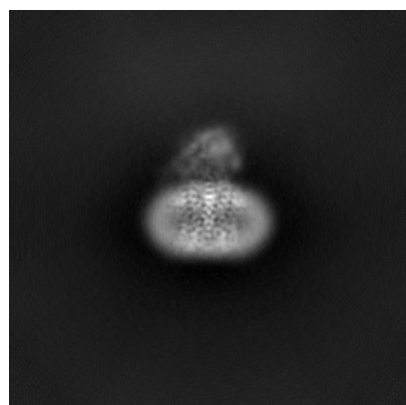


Y



Z

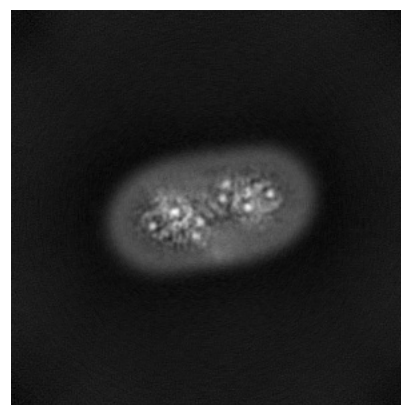
6.1.2 Raw map



X



Y

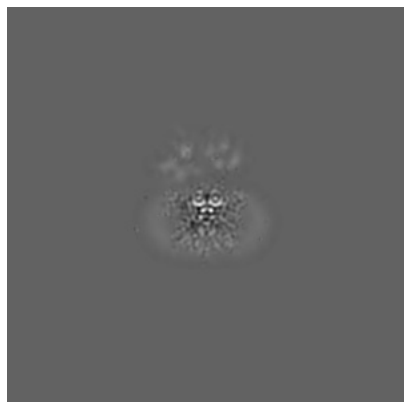


Z

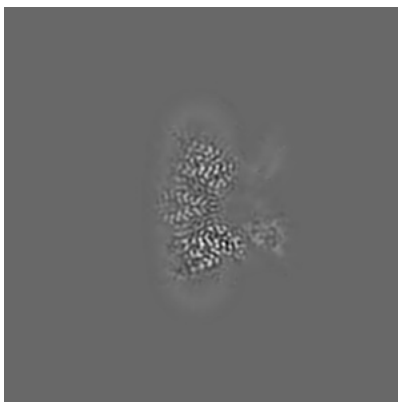
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

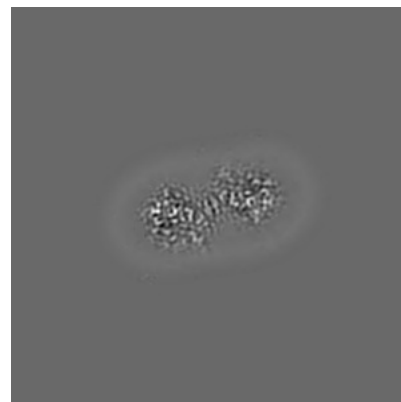
6.2.1 Primary map



X Index: 180

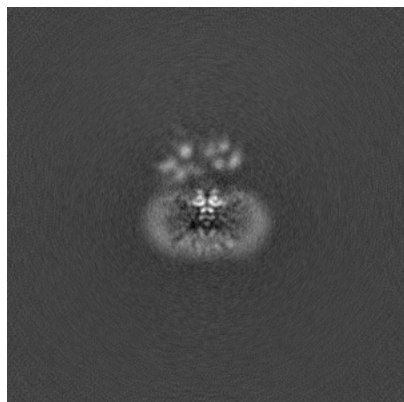


Y Index: 180

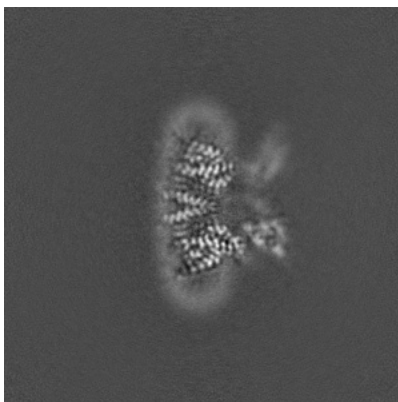


Z Index: 180

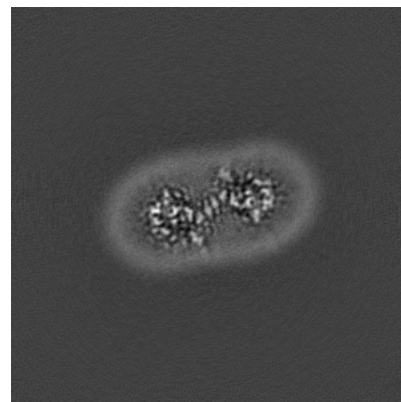
6.2.2 Raw map



X Index: 180



Y Index: 180

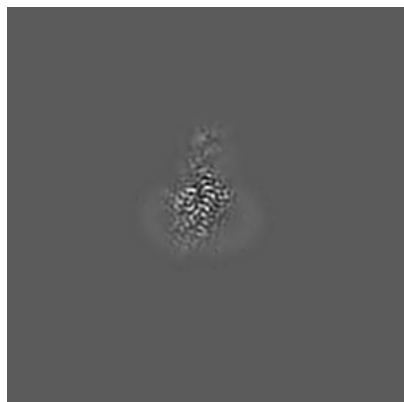


Z Index: 180

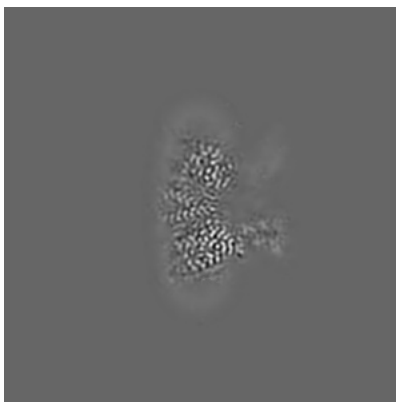
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

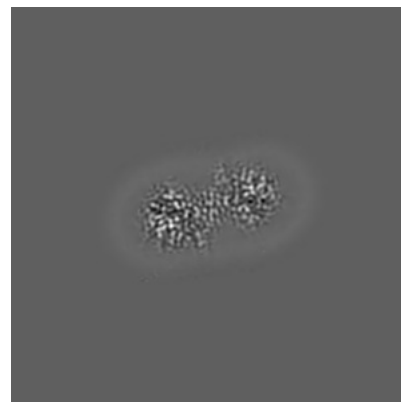
6.3.1 Primary map



X Index: 146

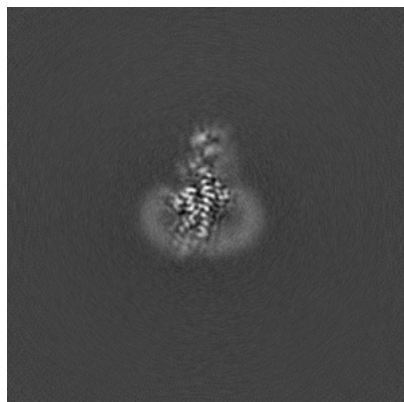


Y Index: 178

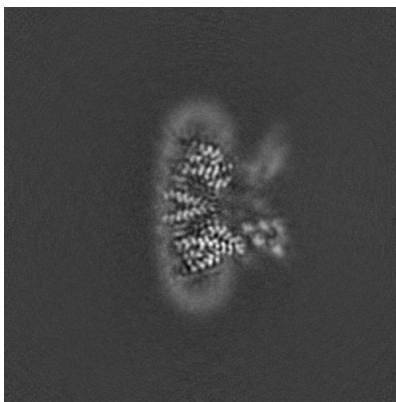


Z Index: 183

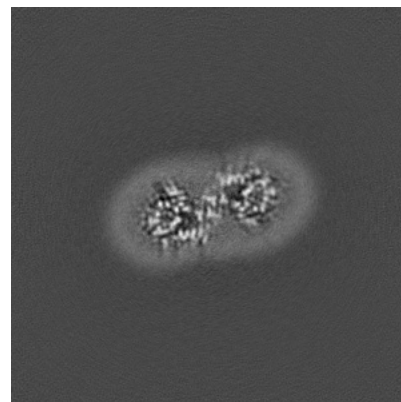
6.3.2 Raw map



X Index: 146



Y Index: 179

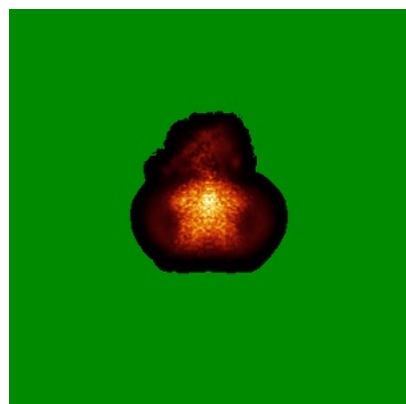


Z Index: 188

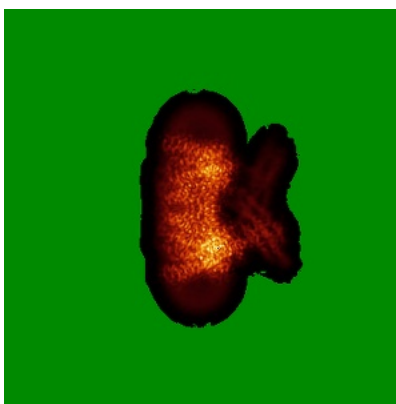
The images above show the largest variance slices of the map in three orthogonal directions.

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

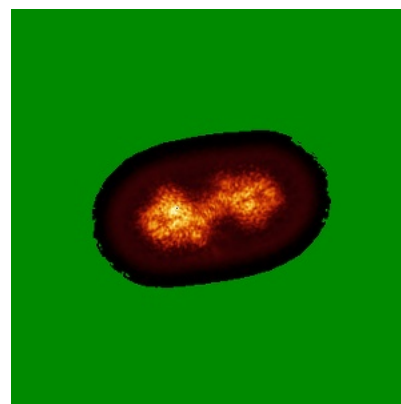
6.4.1 Primary map



X

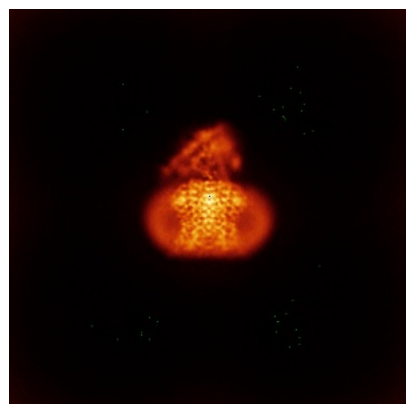


Y

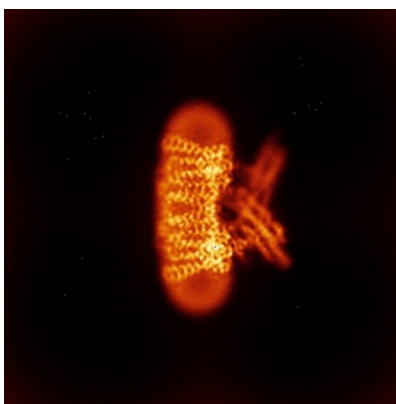


Z

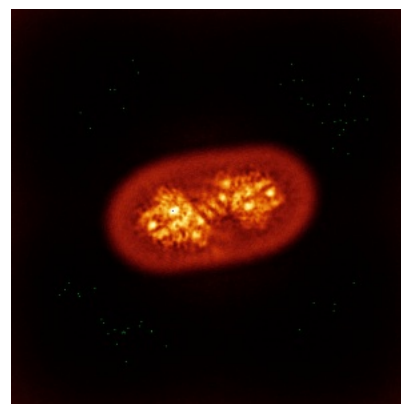
6.4.2 Raw map



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 0.219. 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.

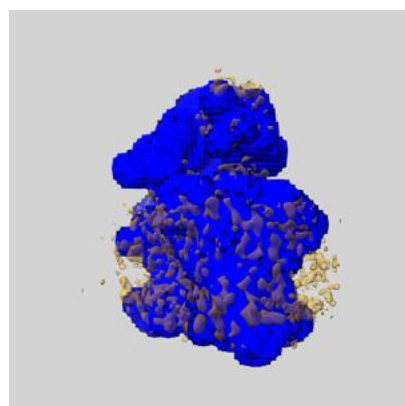
6.6 Mask visualisation [i](#)

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

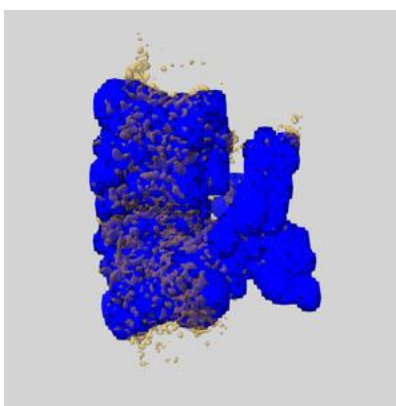
A mask typically either:

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

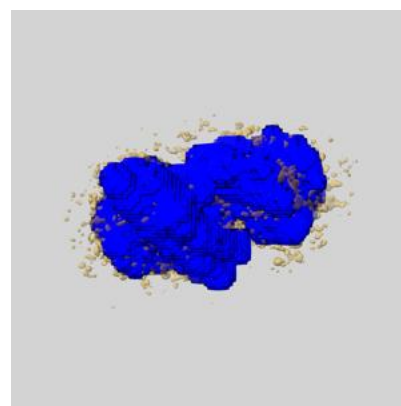
6.6.1 emd_45656_msk_1.map [i](#)



X



Y

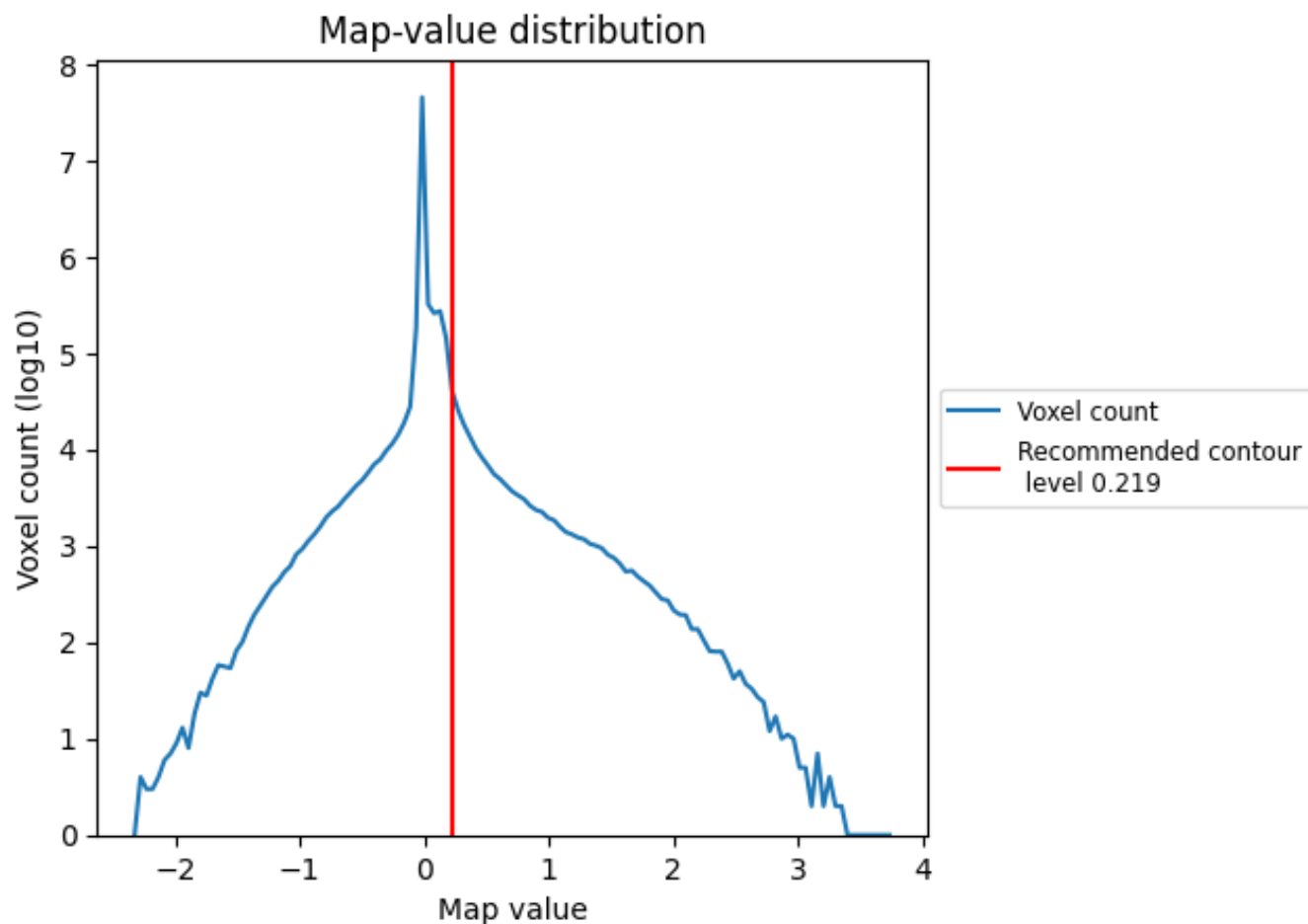


Z

7 Map analysis [i](#)

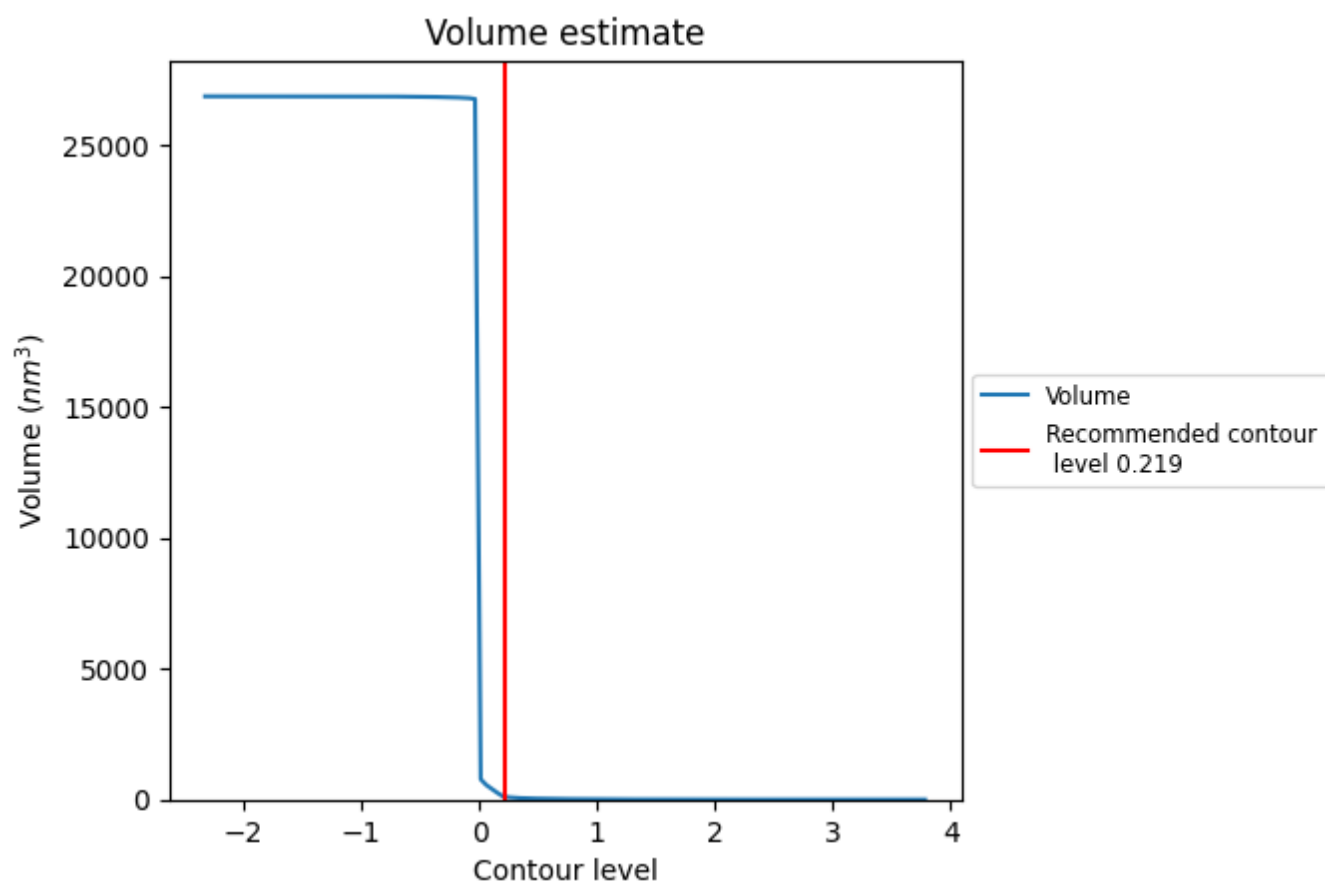
This section contains the results of statistical analysis of the map.

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.

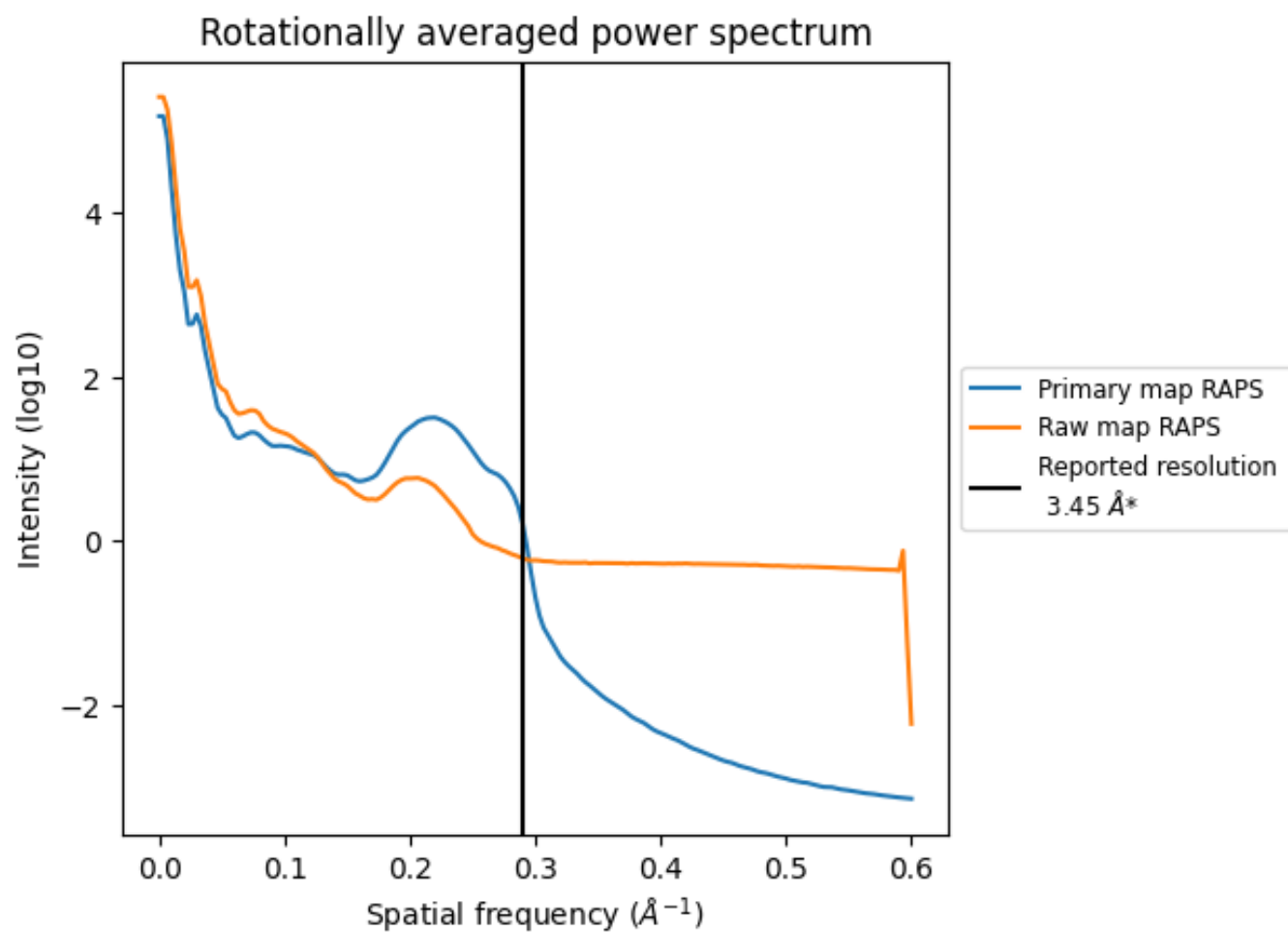
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 108 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 ⓘ

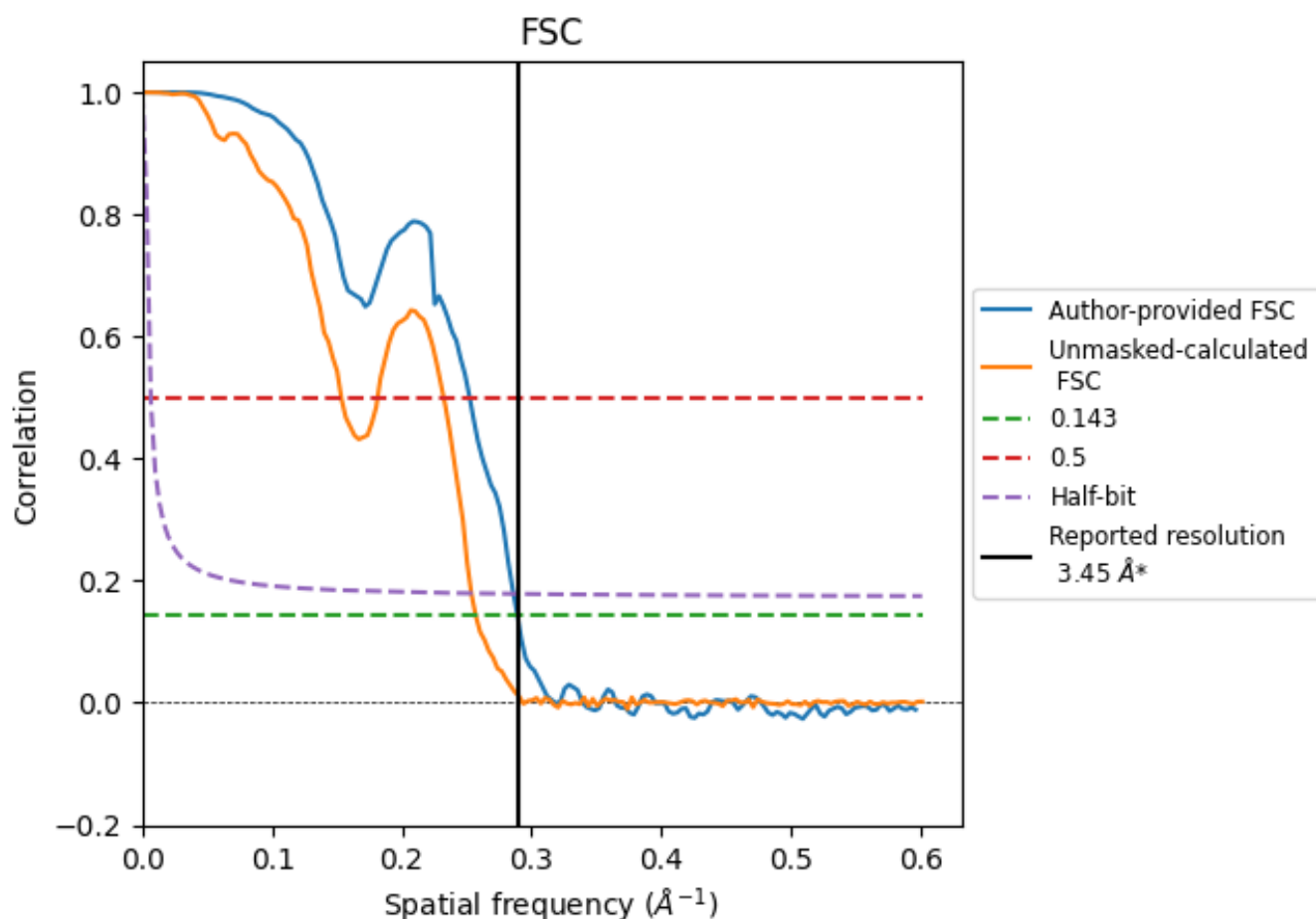


*Reported resolution corresponds to spatial frequency of 0.290 \AA^{-1}

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 0.290 \AA^{-1}

8.2 Resolution estimates [i](#)

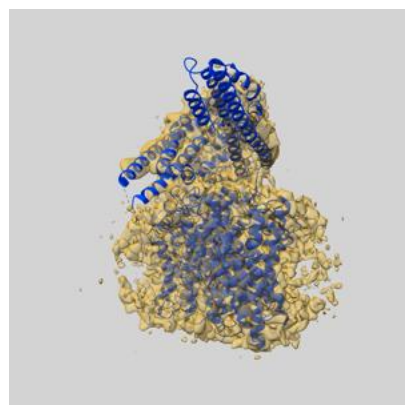
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.45	-	-
Author-provided FSC curve	3.46	3.96	3.50
Unmasked-calculated*	3.89	6.52	3.94

*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 3.89 differs from the reported value 3.45 by more than 10 %

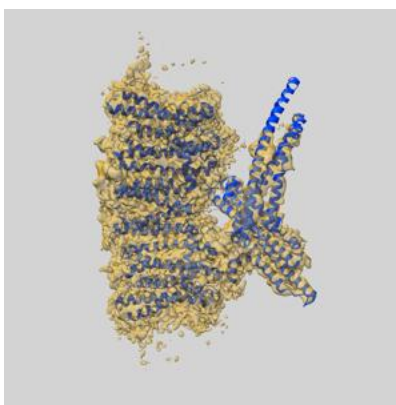
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-45656 and PDB model 9CKZ. Per-residue inclusion information can be found in section [3](#) on page [5](#).

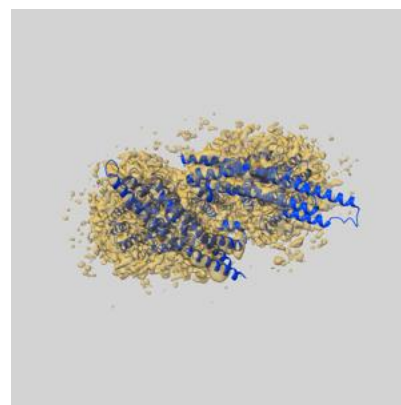
9.1 Map-model overlay [i](#)



X



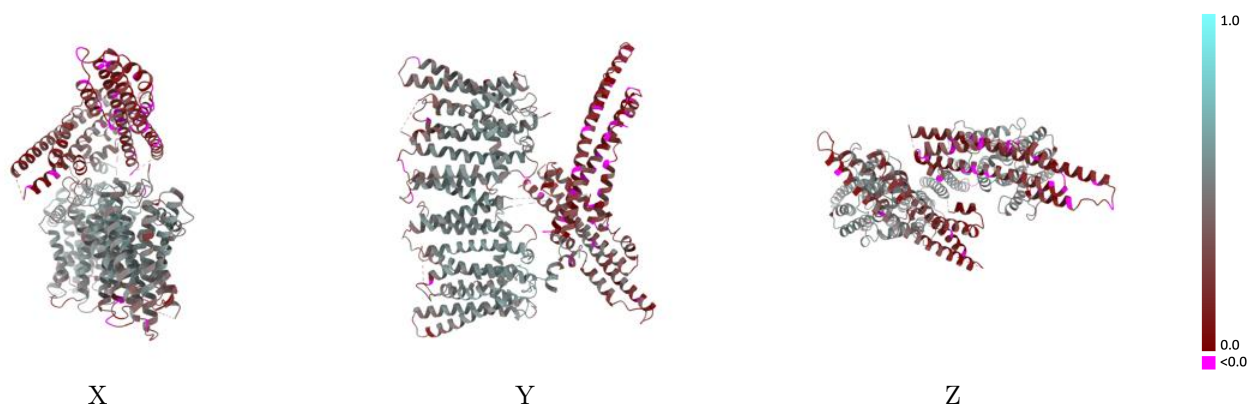
Y



Z

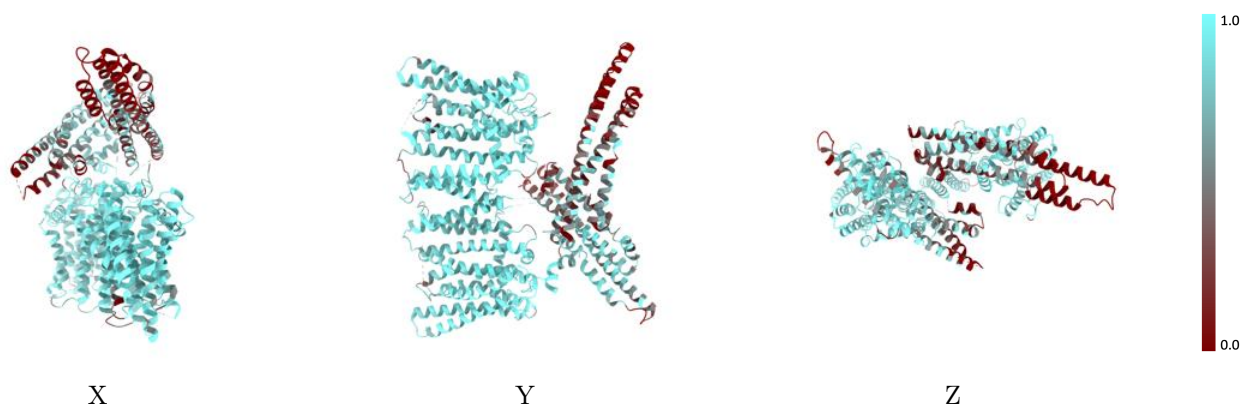
The images above show the 3D surface view of the map at the recommended contour level 0.219 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



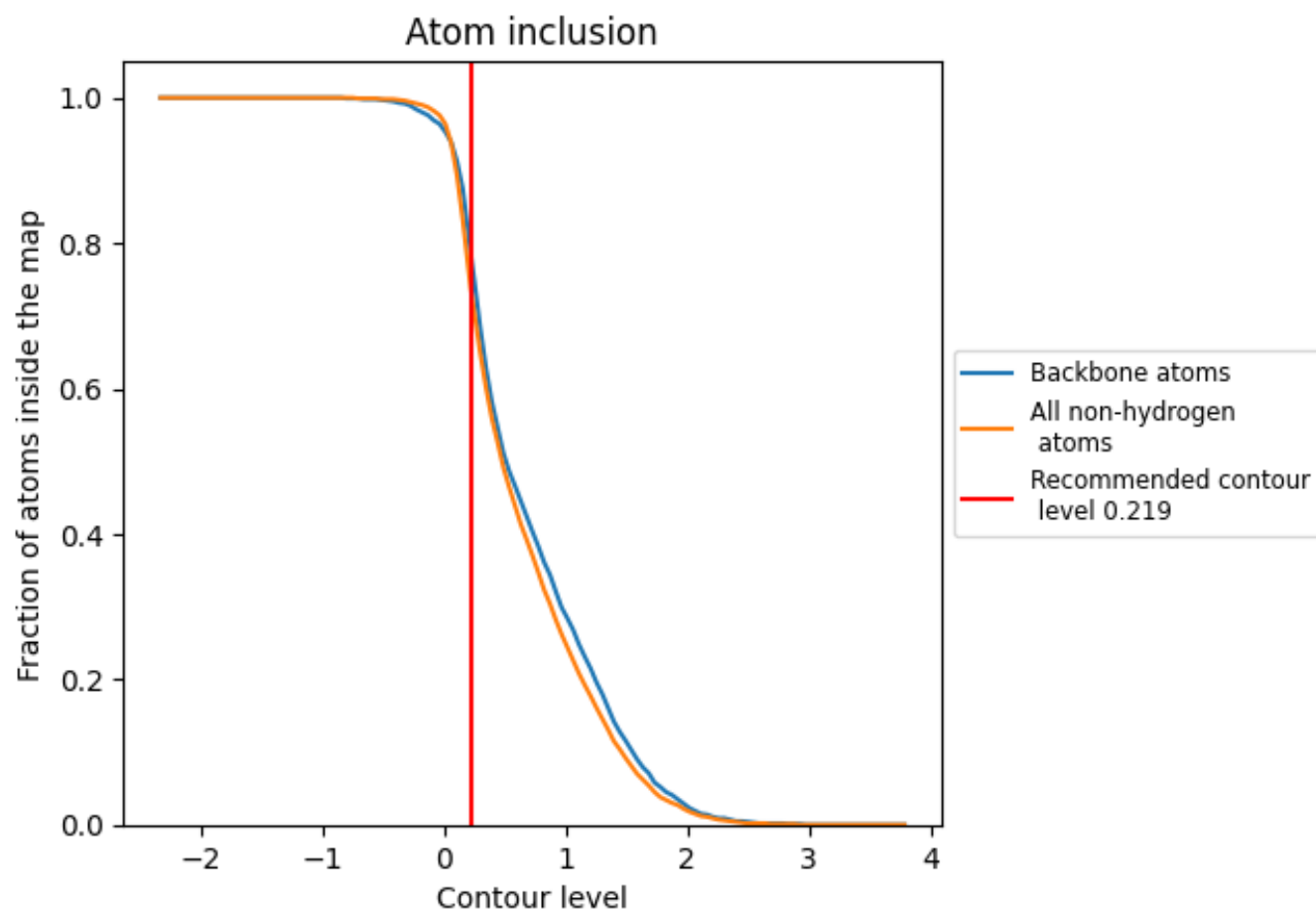
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.219).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 74% 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 (0.219) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7390	<div></div> 0.3890
A	<div></div> 0.7910	<div></div> 0.4160
B	<div></div> 0.6830	<div></div> 0.3600

