



wwPDB EM Validation Summary Report ⓘ

May 18, 2025 – 01:06 PM EDT

PDB ID : 9O11 / pdb_00009o11
EMDB ID : EMD-49994
Title : Kv2.1 with voltage sensor in the up conformation under low potassium
Authors : Mandala, V.S.; MacKinnon, R.
Deposited on : 2025-04-03
Resolution : 3.30 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

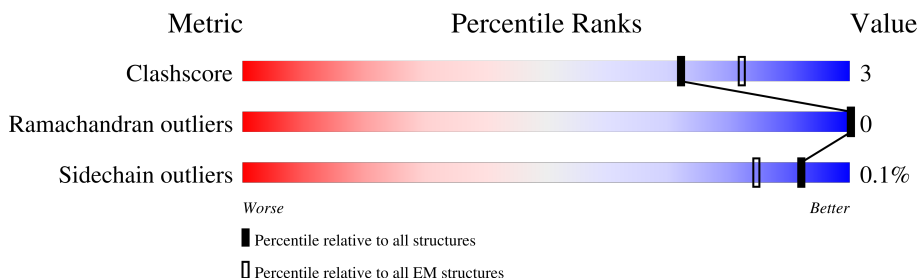
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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	858	
1	B	858	
1	C	858	
1	D	858	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 17136 atoms, of which 8772 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 Potassium voltage-gated channel subfamily B member 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	261	Total	C	H	N	O	S	0	0
			4284	1380	2193	339	361	11		
1	B	261	Total	C	H	N	O	S	0	0
			4284	1380	2193	339	361	11		
1	C	261	Total	C	H	N	O	S	0	0
			4284	1380	2193	339	361	11		
1	D	261	Total	C	H	N	O	S	0	0
			4284	1380	2193	339	361	11		

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

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	47718	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.281	Depositor
Minimum map value	-0.153	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	213.984, 213.984, 213.984	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.743, 0.743, 0.743	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	0.16	0/2137	0.28	0/2893
1	B	0.15	0/2137	0.27	0/2893
1	C	0.15	0/2137	0.28	0/2893
1	D	0.15	0/2137	0.27	0/2893
All	All	0.15	0/8548	0.28	0/11572

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	2091	2193	2192	17	0
1	B	2091	2193	2192	12	0
1	C	2091	2193	2192	14	0
1	D	2091	2193	2192	15	0
All	All	8364	8772	8768	54	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 54 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:C:353:GLU:OE2	1:C:387:THR:OG1	2.02	0.77
1:A:294:ARG:NH1	1:A:297:GLN:OE1	2.19	0.75
1:A:239:TRP:NE1	1:A:243:GLU:OE2	2.19	0.75
1:C:275:VAL:HG11	1:C:299:PHE:CD2	2.21	0.74
1:C:266:ASP:OD2	1:C:312:ARG:NH2	2.22	0.72

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	259/858 (30%)	254 (98%)	5 (2%)	0	100	100
1	B	259/858 (30%)	254 (98%)	5 (2%)	0	100	100
1	C	259/858 (30%)	253 (98%)	6 (2%)	0	100	100
1	D	259/858 (30%)	254 (98%)	5 (2%)	0	100	100
All	All	1036/3432 (30%)	1015 (98%)	21 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	232/753 (31%)	232 (100%)	0	100	100
1	B	232/753 (31%)	232 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	232/753 (31%)	231 (100%)	1 (0%)	89	93
1	D	232/753 (31%)	232 (100%)	0	100	100
All	All	928/3012 (31%)	927 (100%)	1 (0%)	92	96

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	331	LEU

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	D	226	ASN
1	D	283	ASN
1	D	313	HIS
1	D	291	ASN
1	D	209	ASN

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 ⓘ

There are no chain breaks in this entry.

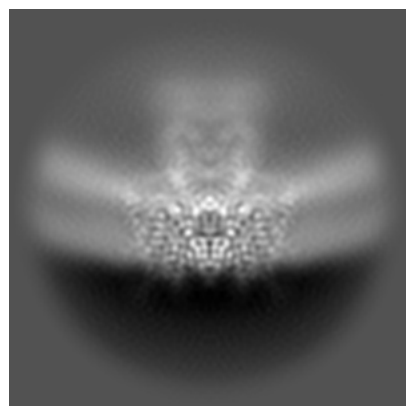
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49994. These allow visual inspection of the internal detail of the map and identification of artifacts.

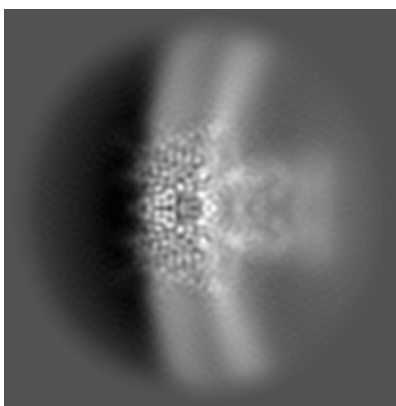
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

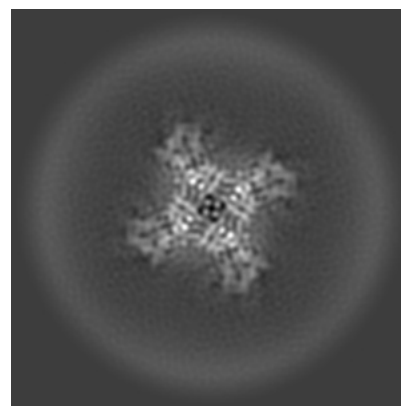
6.1.1 Primary map



X

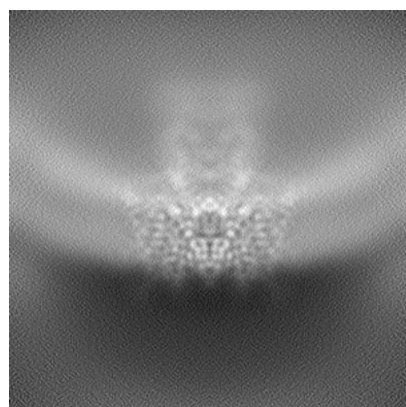


Y

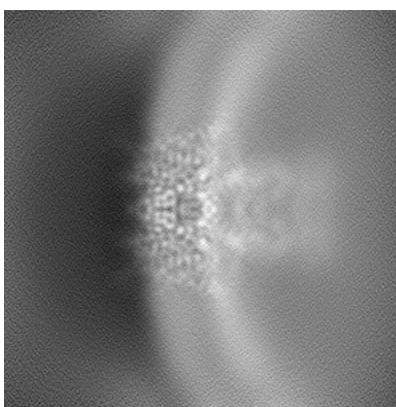


Z

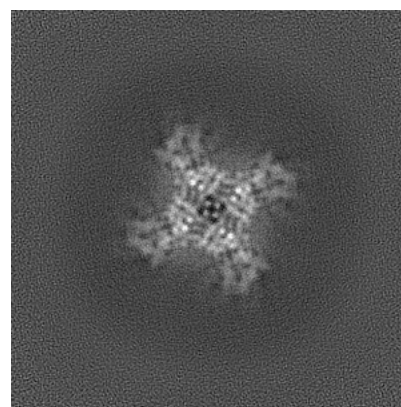
6.1.2 Raw map



X



Y

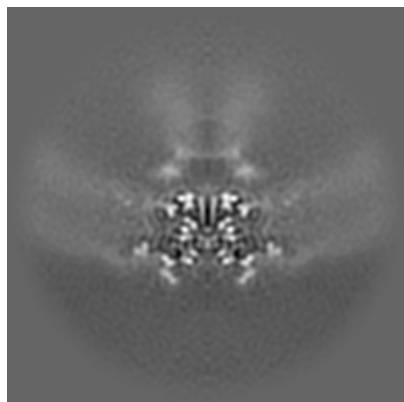


Z

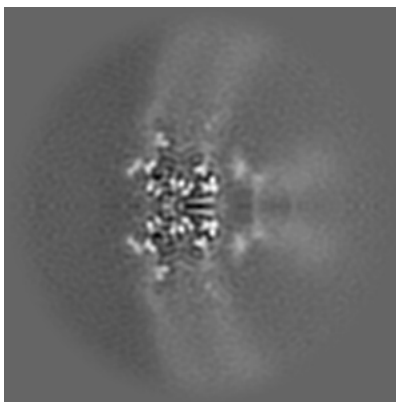
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

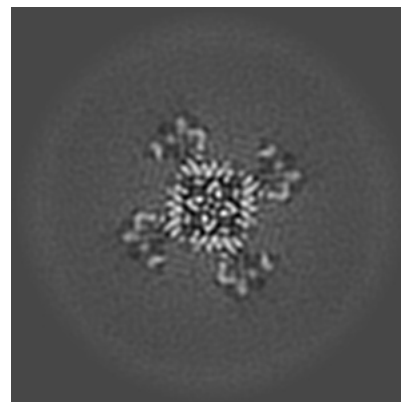
6.2.1 Primary map



X Index: 144

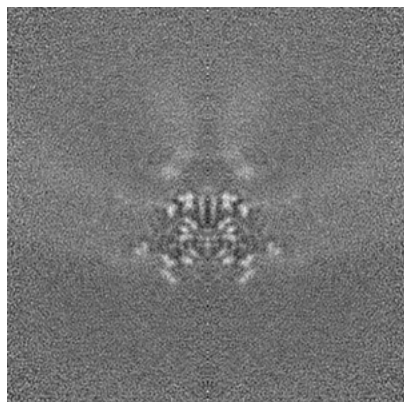


Y Index: 144

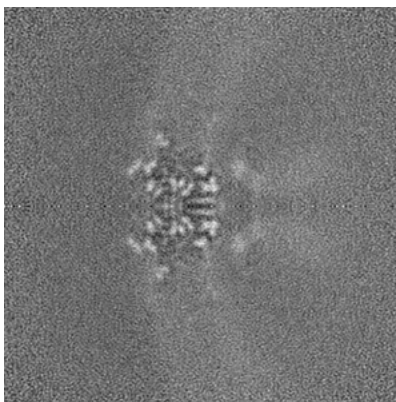


Z Index: 144

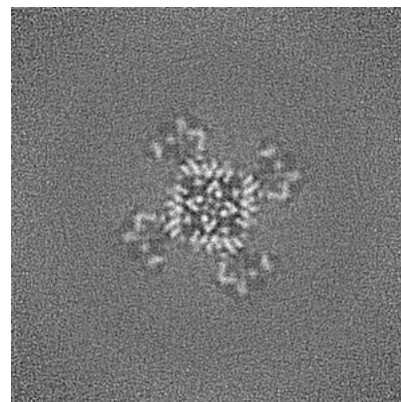
6.2.2 Raw map



X Index: 144



Y Index: 144

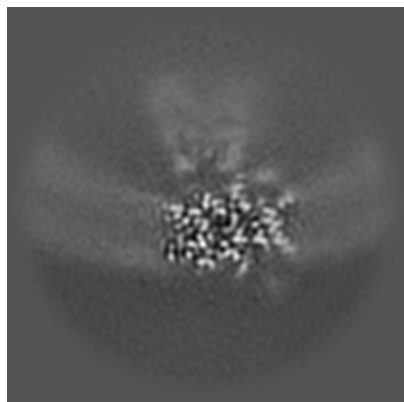


Z Index: 144

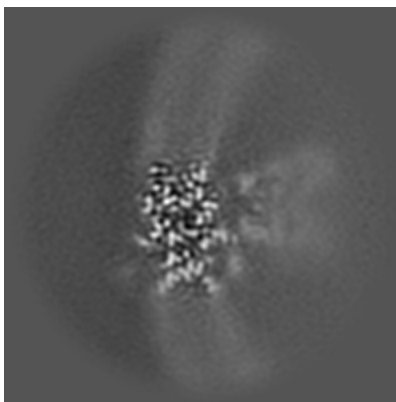
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

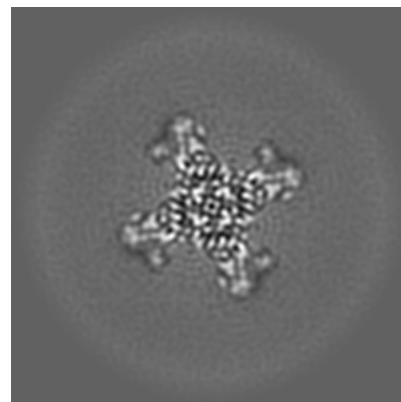
6.3.1 Primary map



X Index: 132

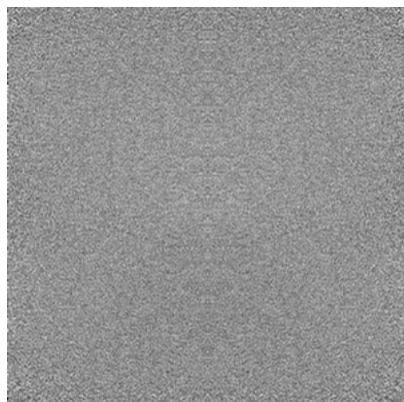


Y Index: 132

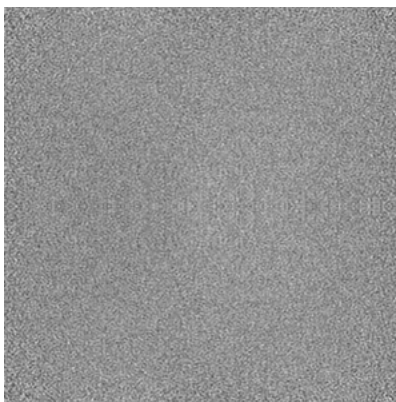


Z Index: 141

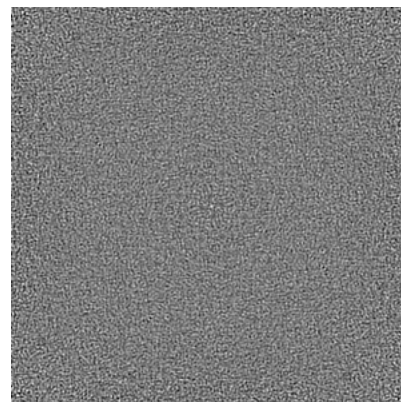
6.3.2 Raw map



X Index: 0



Y Index: 0

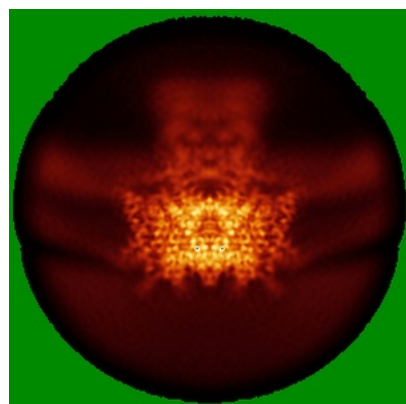


Z Index: 0

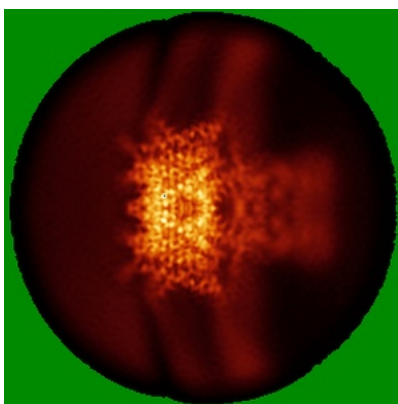
The images above show the largest variance slices of the map in three orthogonal directions.

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

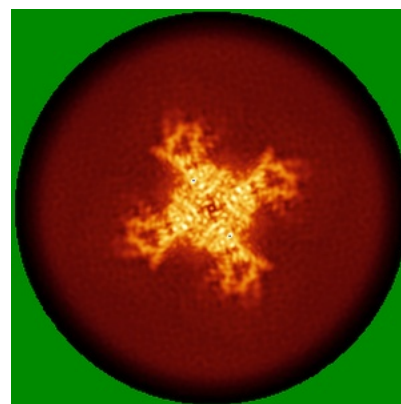
6.4.1 Primary map



X

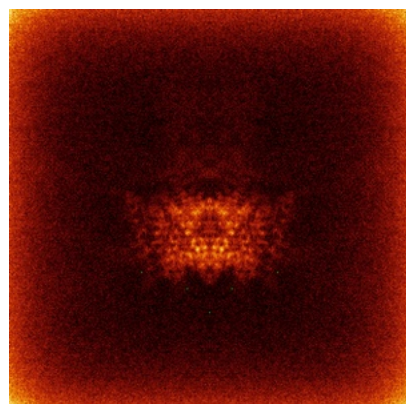


Y

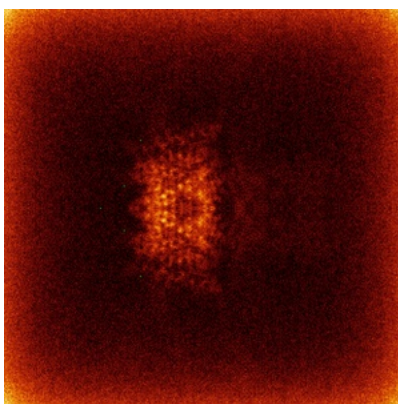


Z

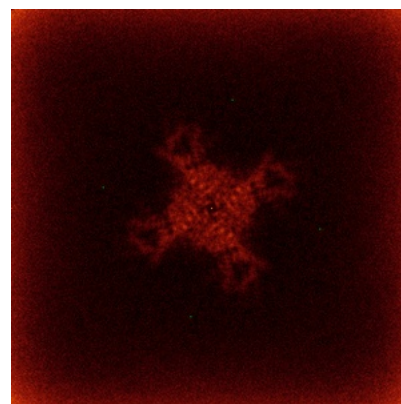
6.4.2 Raw map



X



Y

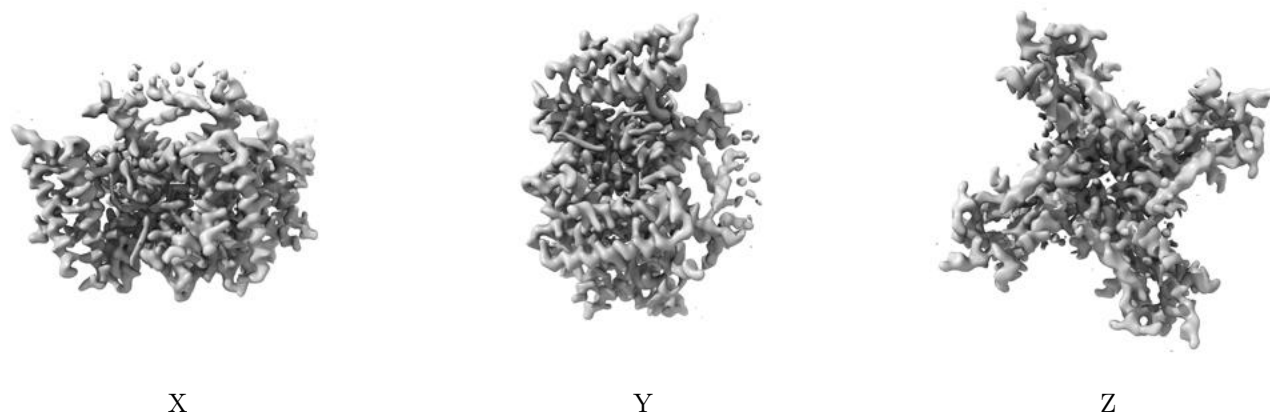


Z

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.

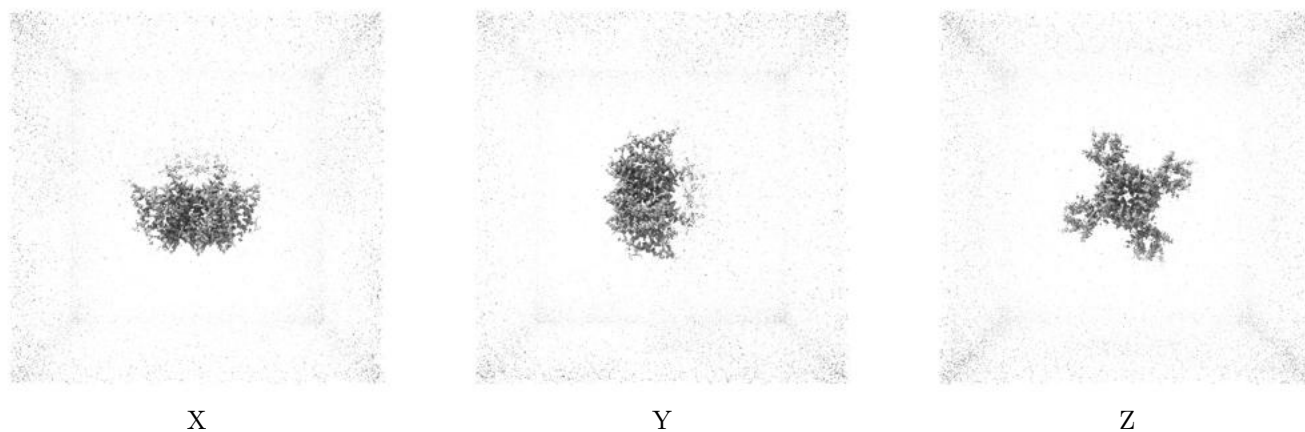
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.08. 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.

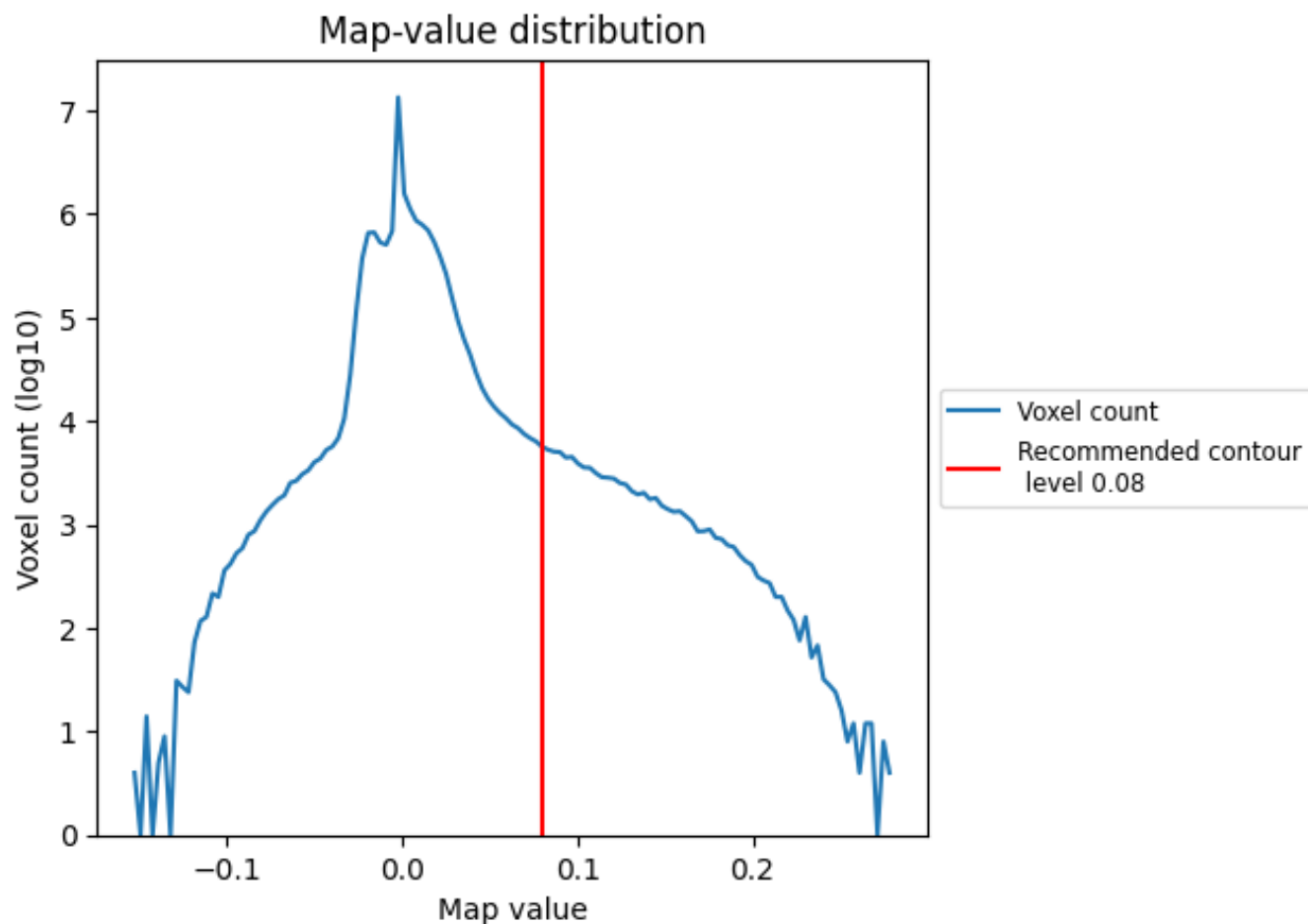
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

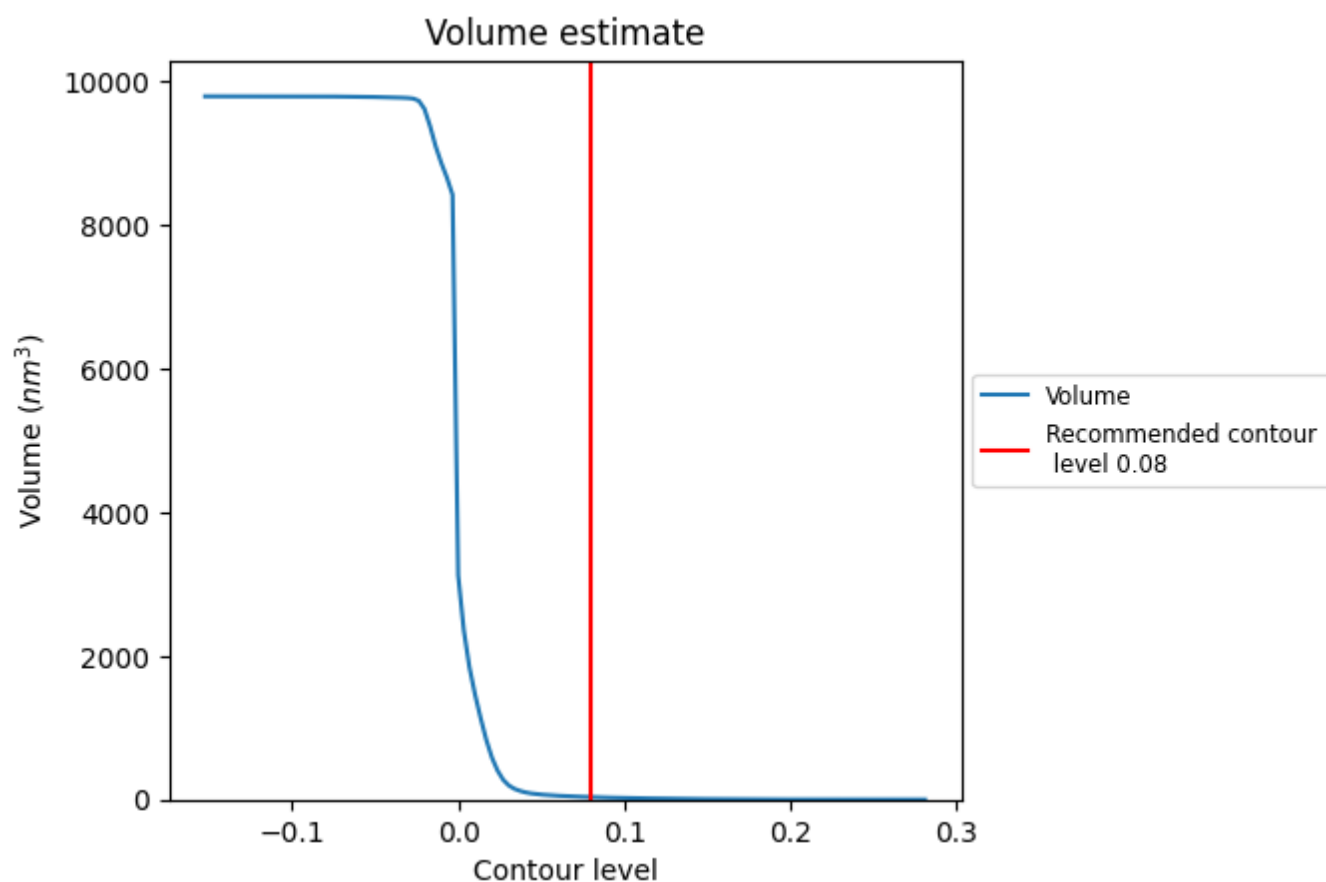
This section contains the results of statistical analysis of the map.

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.

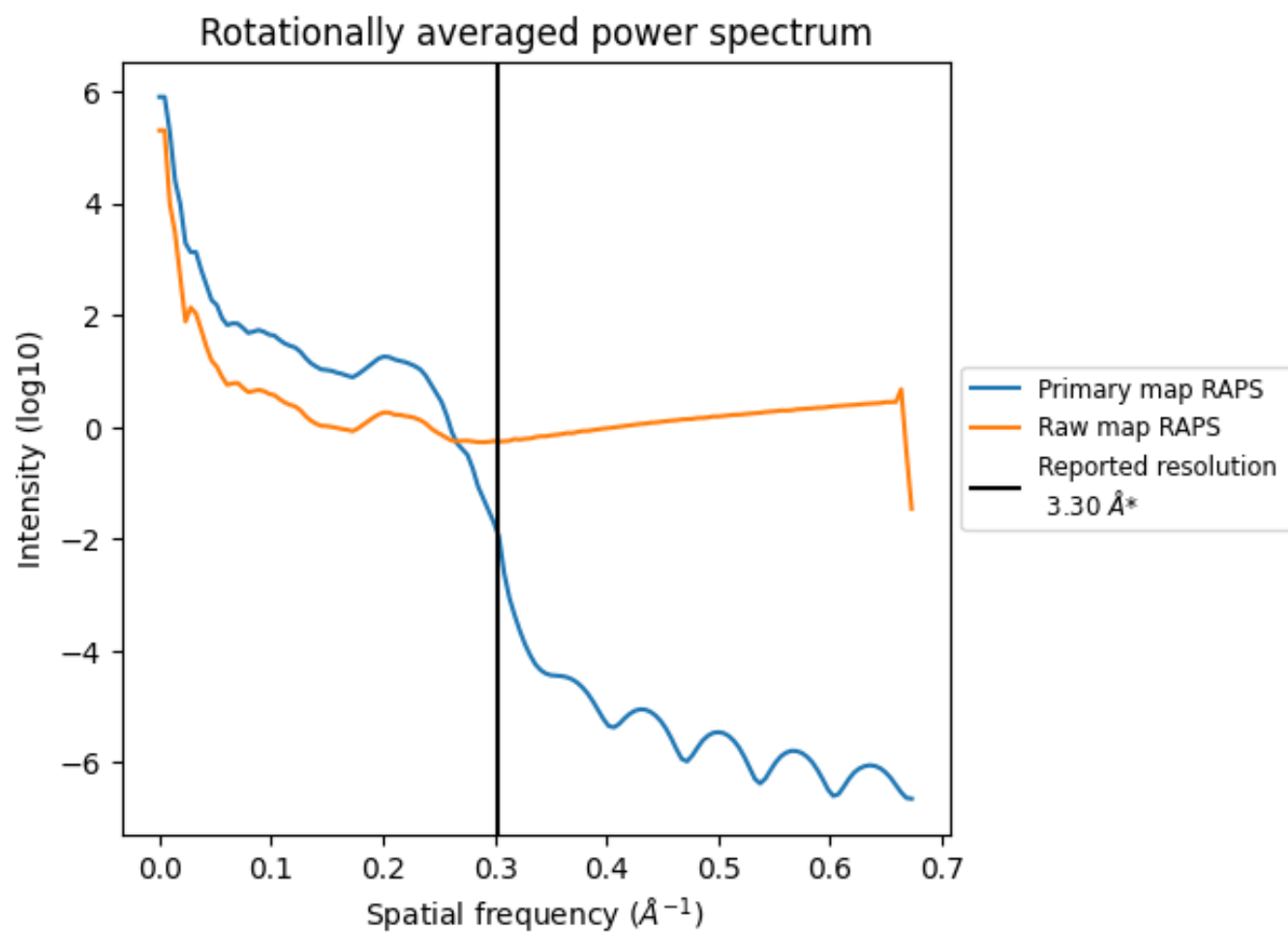
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 34 nm³; this corresponds to an approximate mass of 31 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 ⓘ

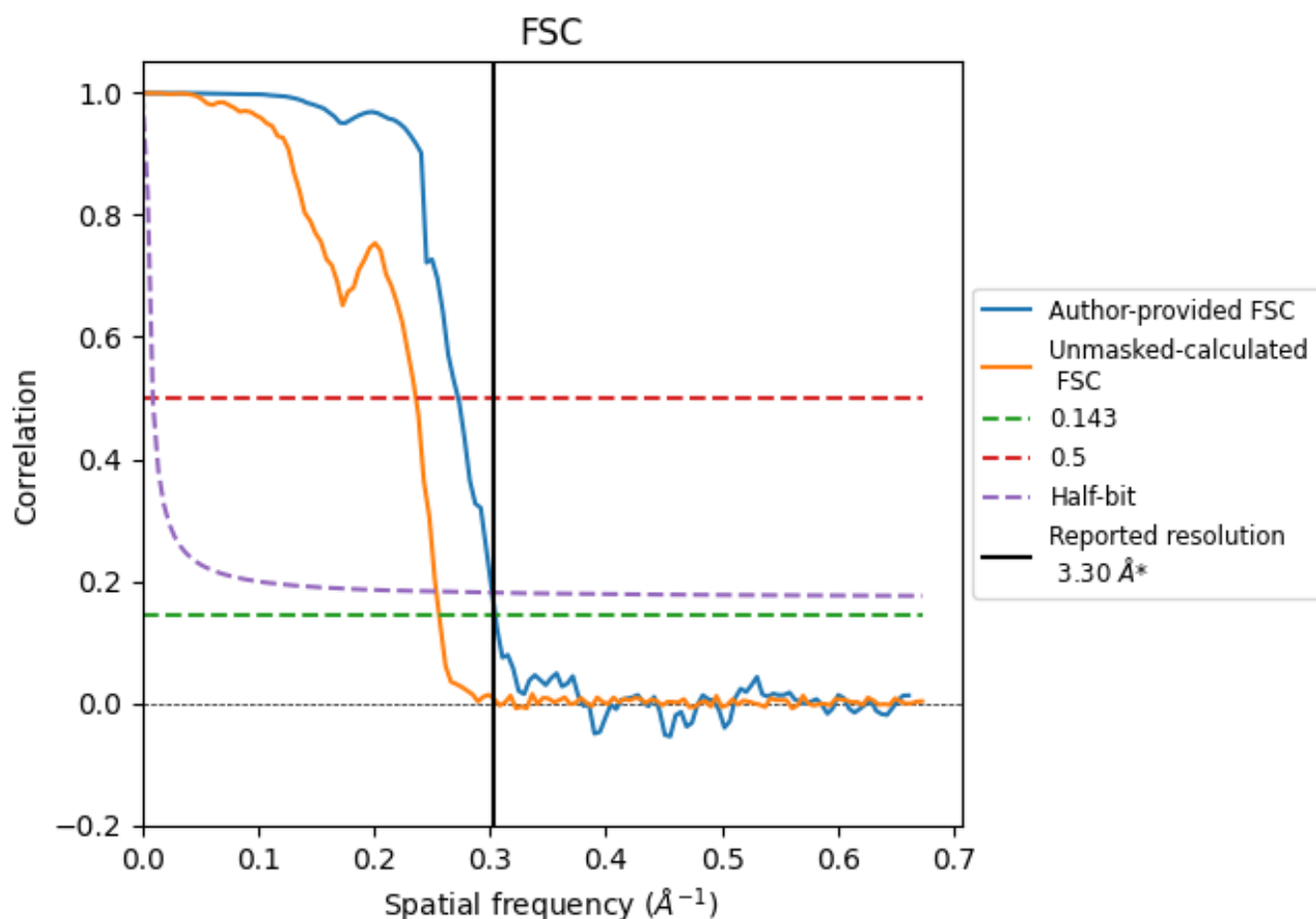


*Reported resolution corresponds to spatial frequency of 0.303 \AA^{-1}

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 0.303 Å⁻¹

8.2 Resolution estimates [i](#)

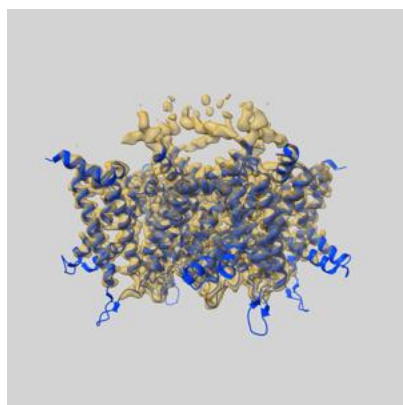
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.28	3.67	3.31
Unmasked-calculated*	3.90	4.24	3.94

*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 3.90 differs from the reported value 3.3 by more than 10 %

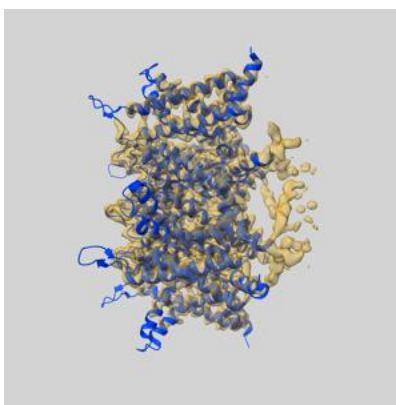
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-49994 and PDB model 9O11. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

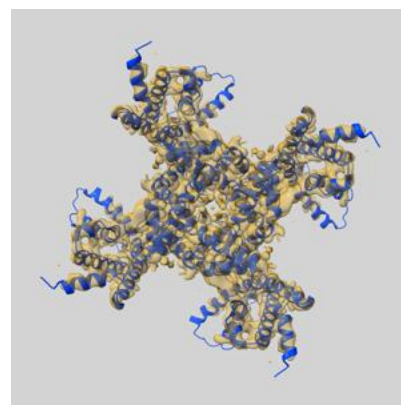
9.1 Map-model overlay [i](#)



X



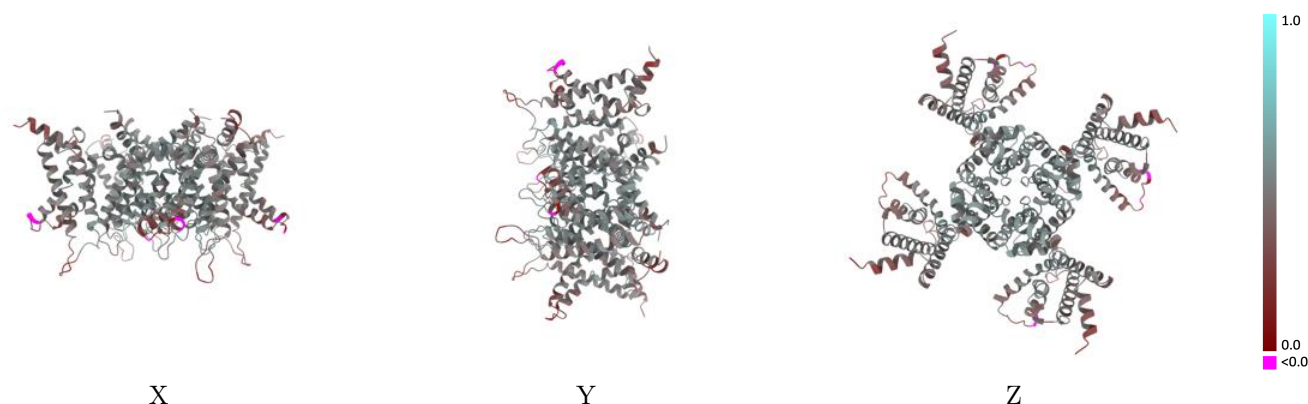
Y



Z

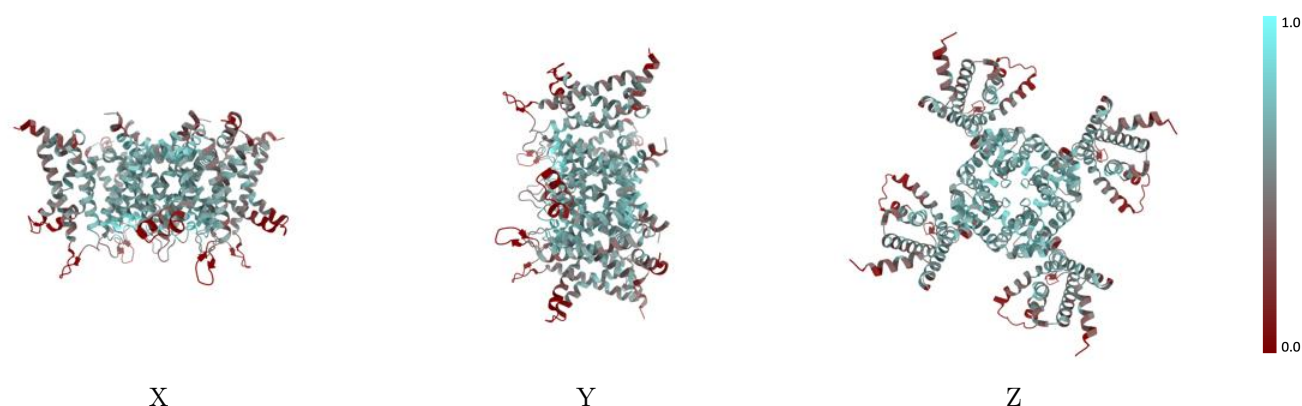
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



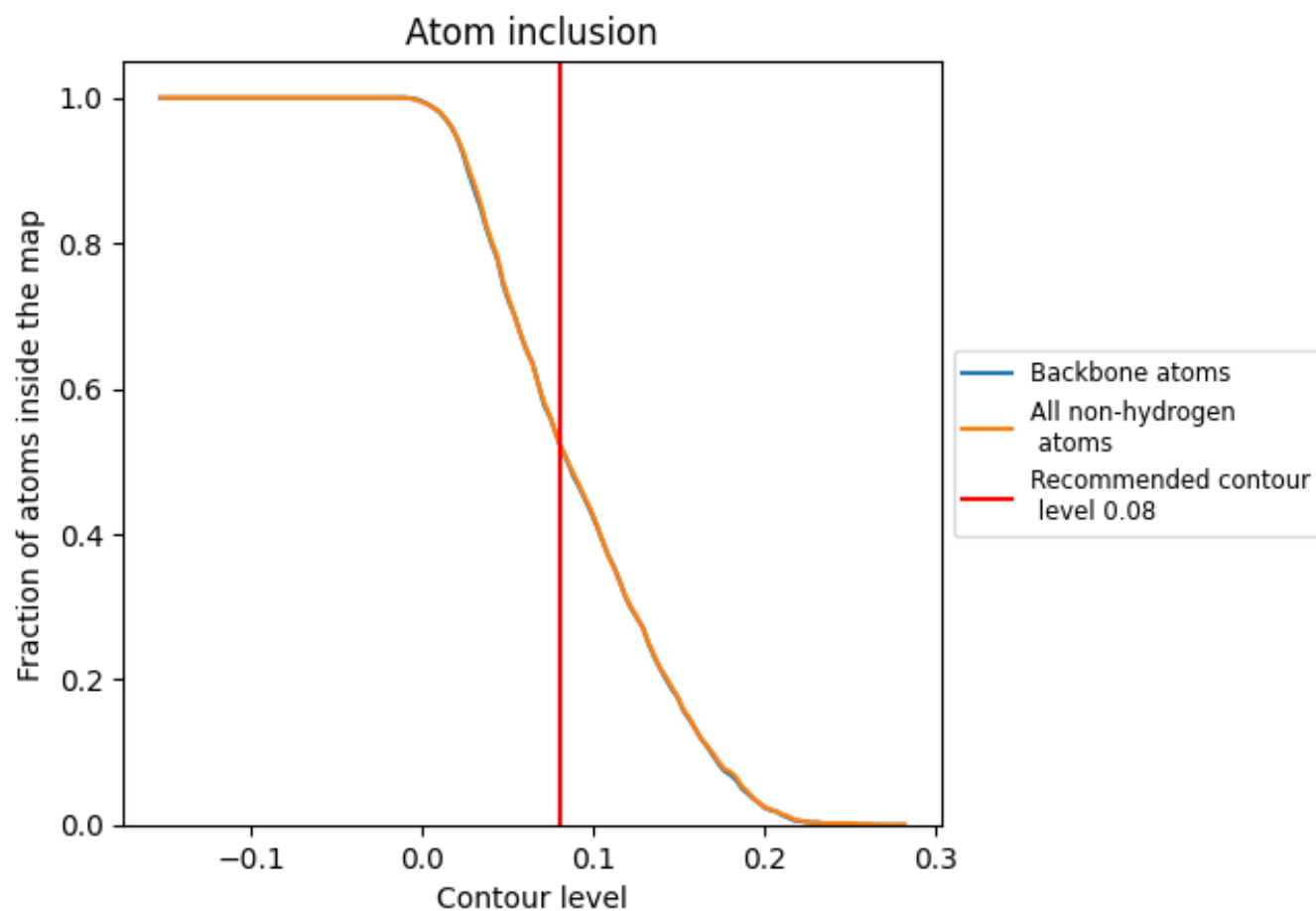
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.08).

9.4 Atom inclusion [i](#)



At the recommended contour level, 52% of all backbone atoms, 52% 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.5250	<div></div> 0.4560
A	<div></div> 0.5350	<div></div> 0.4570
B	<div></div> 0.5350	<div></div> 0.4560
C	<div></div> 0.5330	<div></div> 0.4530
D	<div></div> 0.5320	<div></div> 0.4570

