



wwPDB EM Validation Summary Report ⓘ

Jun 26, 2024 – 08:22 PM JST

PDB ID : 7YIG
EMDB ID : EMD-33858
Title : Human KCNH5 pre-open state 2
Authors : Zhang, M.F.
Deposited on : 2022-07-16
Resolution : 3.60 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.dev92
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

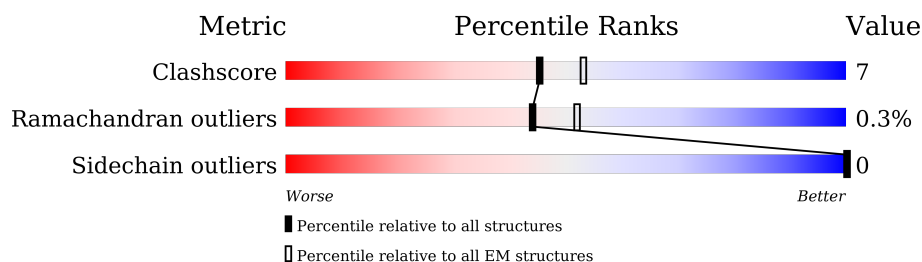
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	988	 10% 55% 11% 33%
1	B	988	 10% 55% 12% 33%
1	C	988	 10% 55% 12% 33%
1	D	988	 10% 55% 12% 33%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 21320 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 Potassium voltage-gated channel subfamily H member 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	660	Total	C	N	O	S	0	0
			5328	3449	886	961	32		
1	B	660	Total	C	N	O	S	0	0
			5328	3449	886	961	32		
1	C	660	Total	C	N	O	S	0	0
			5328	3449	886	961	32		
1	D	660	Total	C	N	O	S	0	0
			5328	3449	886	961	32		

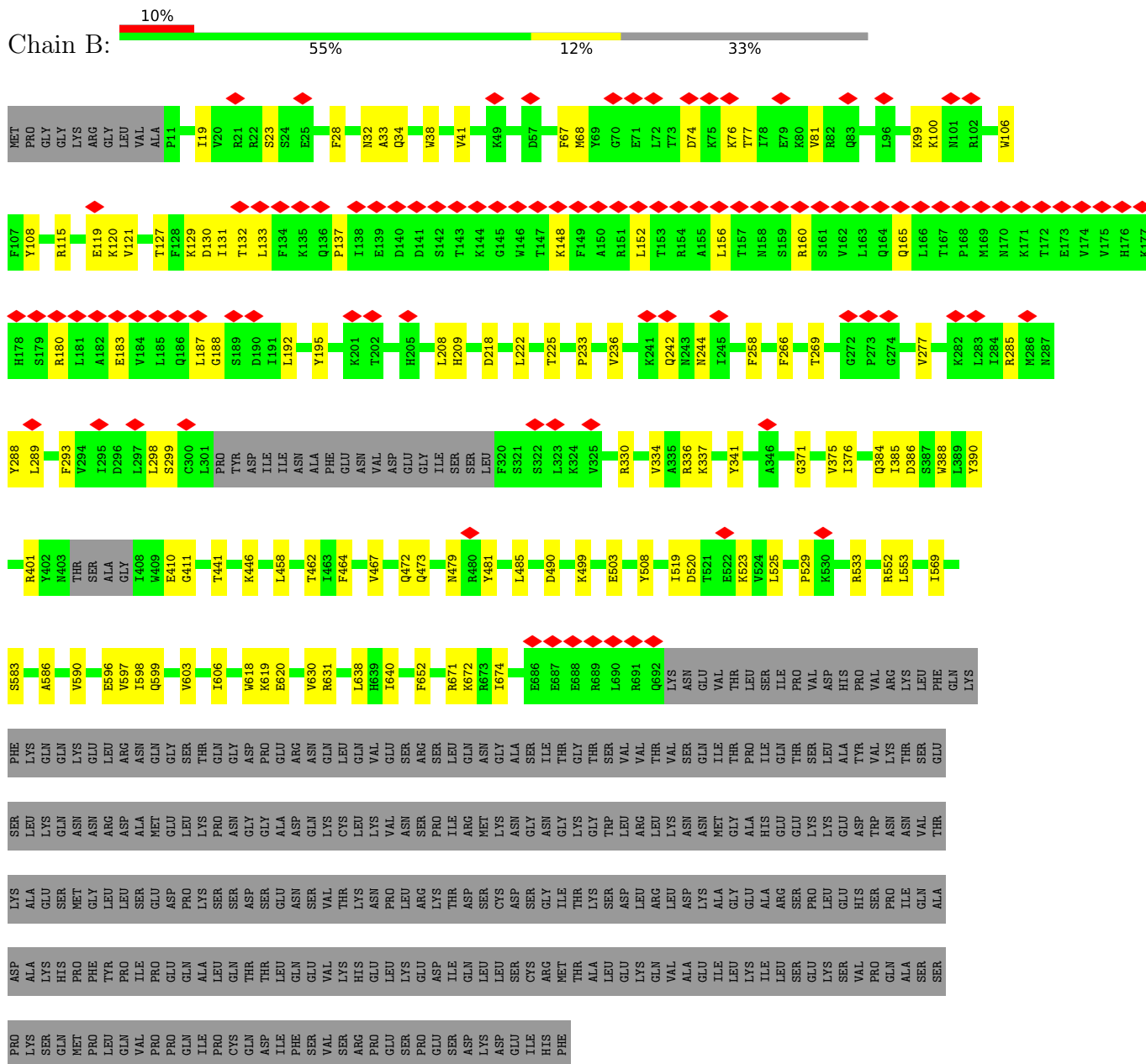
- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
2	A	4	Total	K	0
			4	4	

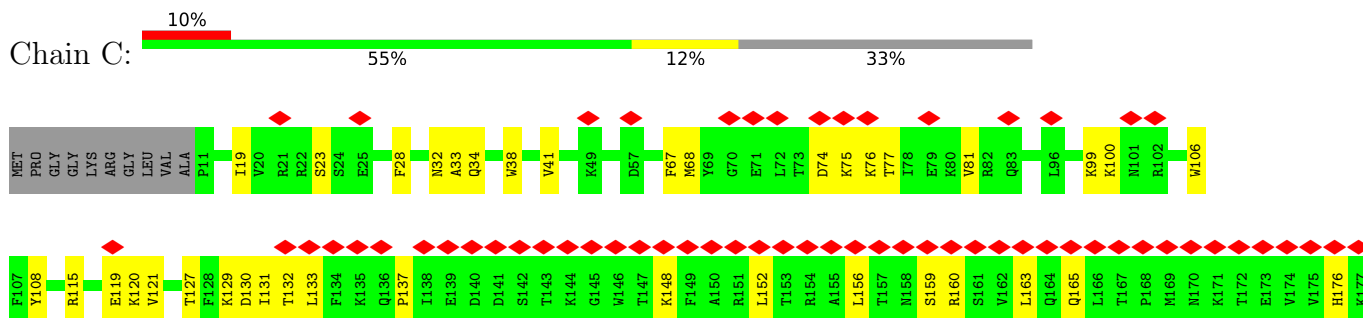
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	O	0
			1	1	
3	B	1	Total	O	0
			1	1	
3	C	1	Total	O	0
			1	1	
3	D	1	Total	O	0
			1	1	

Chain B:



Chain C:



SER	ALA	THR	GLU	LYS	IS69
	ASP	LYS	SER	PHE	
PRO	ALA	ALA	LEU	LYS	SS83
LYS	LYS	GLU	GLN	GLN	
SER	HIS	SER	ASN	LYS	AS86
GLN	PRO	MET	ASN		
MET	PRO	GLY	ASN	GLU	VS90
PRO	PHE	LEU	ASN	LEU	
LEU	TYR	LEU	ARG	ARG	ES96
GLN	PRO	LEU	ASP	ARG	VS97
VAL	ILE	SER	ALA	ASN	IS98
PRO	PRO	GLU	MET	GLN	QS99
PRO	GLN	ASP	GLU	GLY	
GLM	GLU	PRO	LEU	SER	
ILE	ALA	LYS	LYS	THR	V603
PRO	LEU	SER	PRO	GLN	
CYS	GLN	SER	ASN	GLY	IG06
GLN	THR	ASP	GLY	ASP	
ASP	THR	SER	GLY	PRO	W618
ILE	LEU	GLU	ALA	GLU	K619
PHE	GLN	ASN	ASP	ARG	ES20
SER	GLU	SER	GLN	ASN	
VAL	VAL	VAL	LYS	GLN	V630
SER	LYS	THR	CYS	LEU	R631
ARG	HIS	LYS	LEU	GLN	
PRO	GLU	ASN	LYS	VAL	L638
GLU	LEU	PRO	VAL	GLU	H639
SER	LYS	LEU	ASN	SER	IG40
PRO	GLU	ARG	SER	ARG	
GLU	ASP	LYS	PRO	LYS	F652
SER	ILE	THR	ILE	LEU	
ASP	GLN	ASP	ARG	GLN	R671
LYS	LEU	SER	MET	ASN	
ASP	LEU	CYS	LYS	GLY	IG74
GLU	SER	ASP	ASN	ALA	
ILE	CYS	SER	GLY	SER	ES86
HIS	ARG	GLY	ASN	ILE	
PHE	MET	ILE	GLY	THR	ES87
	THR	THR	LYS	GLY	ES88
	ALA	LYS	GLY	THR	R689
	LEU	SER	TRP	SER	L690
	GLU	ASP	LEU	VAL	R691
	LYS	LEU	ARG	VAL	Q692
	GLN	ARG	LEU	THR	LYS
	VAL	LEU	LYS	VAL	
	ALA	ASP	ASN	SER	GLU
	GLU	LYS	ASN	GLN	GLU
	ILE	ALA	MET	ILE	VAL
	ILE	GLY	GLY	THR	THR
	LYS	GLU	ALA	PRO	LEU
	ILE	ALA	HIS	ILE	SER
	LEU	ARG	GLU	GLN	ILE
	SER	SER	GLU	THR	PRO
	SER	PRO	LYS	SER	VAL
	GLU	PRO	LYS	LEU	ASP
	VAL	GLU	ASP	ALA	HIS
	PRO	HIS	TRP	TYR	PRO
	PRO	SER	TRP	VAL	ARG
	GLN	PRO	ASN	LYS	VAL
	ALA	ILE	ASN	THR	LYS
	SER	GLN	VAL	SER	LEU
					PHE

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	97894	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.367	Depositor
Minimum map value	-1.708	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.043	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	339.59998, 339.59998, 339.59998	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8489999, 0.8489999, 0.8489999	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: K

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	0.26	0/5451	0.48	0/7396
1	B	0.26	0/5451	0.48	0/7396
1	C	0.26	0/5451	0.48	0/7396
1	D	0.26	0/5451	0.48	0/7396
All	All	0.26	0/21804	0.48	0/29584

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	5328	0	5364	78	0
1	B	5328	0	5364	79	0
1	C	5328	0	5364	82	0
1	D	5328	0	5364	79	0
2	A	4	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
All	All	21320	0	21456	288	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 7.

The worst 5 of 288 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:188:GLY:HA2	1:B:192:LEU:HD12	1.64	0.80
1:C:188:GLY:HA2	1:C:192:LEU:HD12	1.64	0.79
1:A:188:GLY:HA2	1:A:192:LEU:HD12	1.64	0.79
1:D:188:GLY:HA2	1:D:192:LEU:HD12	1.64	0.77
1:D:225:THR:HG22	1:D:330:ARG:HG2	1.68	0.76

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	654/988 (66%)	601 (92%)	51 (8%)	2 (0%)	41	75
1	B	654/988 (66%)	601 (92%)	51 (8%)	2 (0%)	41	75
1	C	654/988 (66%)	601 (92%)	51 (8%)	2 (0%)	41	75
1	D	654/988 (66%)	601 (92%)	51 (8%)	2 (0%)	41	75
All	All	2616/3952 (66%)	2404 (92%)	204 (8%)	8 (0%)	44	75

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	VAL
1	A	244	ASN
1	B	121	VAL
1	B	244	ASN
1	C	121	VAL

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	595/888 (67%)	595 (100%)	0	100	100
1	B	595/888 (67%)	595 (100%)	0	100	100
1	C	595/888 (67%)	595 (100%)	0	100	100
1	D	595/888 (67%)	595 (100%)	0	100	100
All	All	2380/3552 (67%)	2380 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	473	GLN
1	C	479	ASN
1	D	479	ASN
1	D	165	GLN
1	B	165	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 monosaccharides in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 are monoatomic - 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

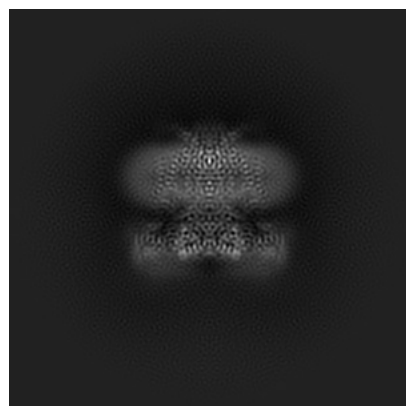
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33858. These allow visual inspection of the internal detail of the map and identification of artifacts.

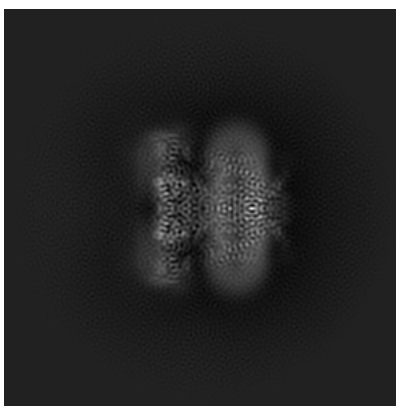
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

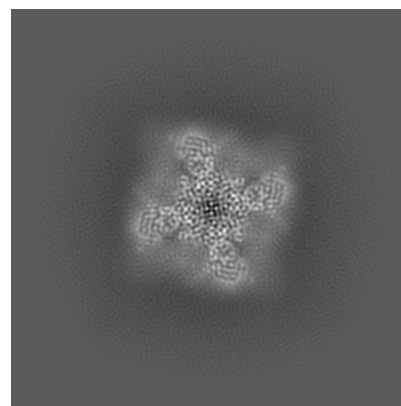
6.1.1 Primary map



X

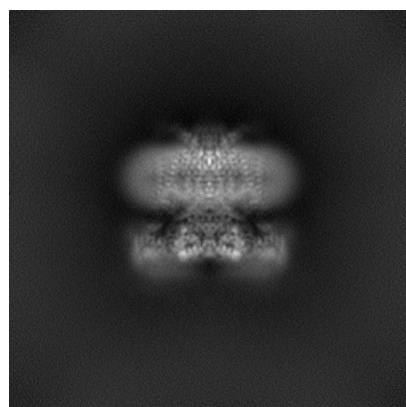


Y

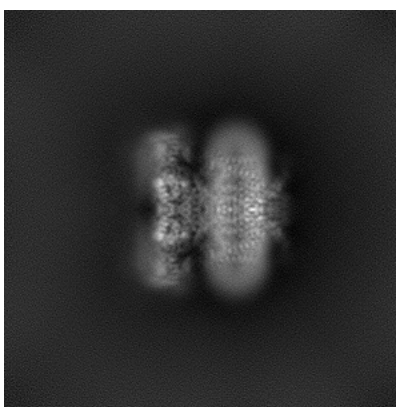


Z

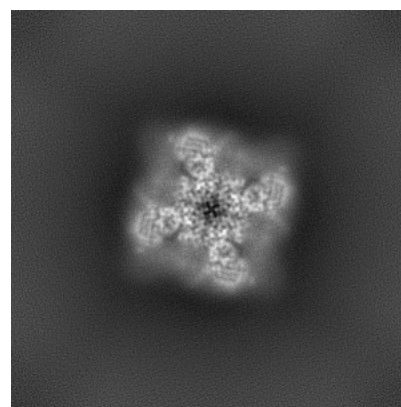
6.1.2 Raw map



X



Y

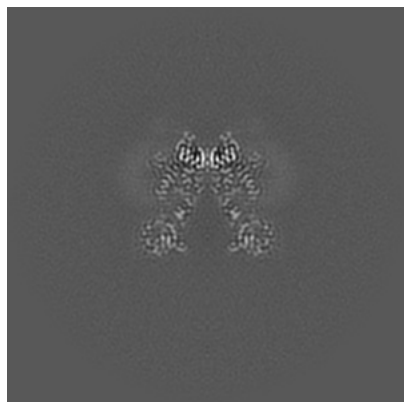


Z

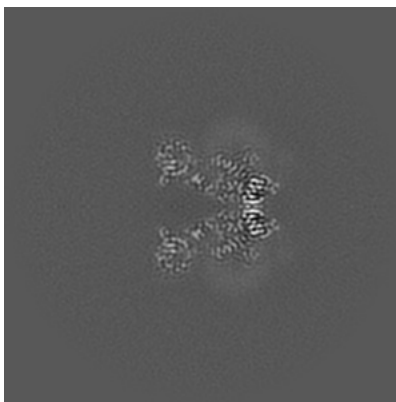
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

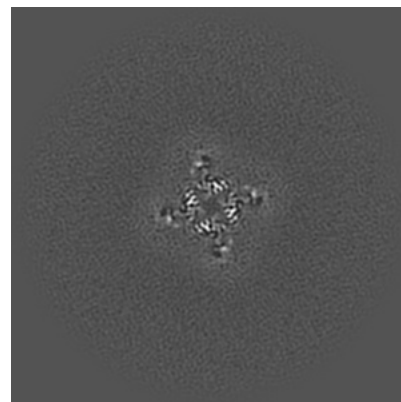
6.2.1 Primary map



X Index: 200

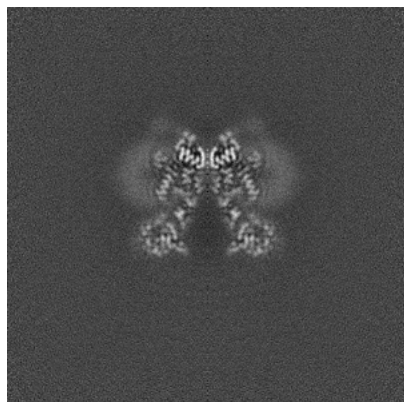


Y Index: 200

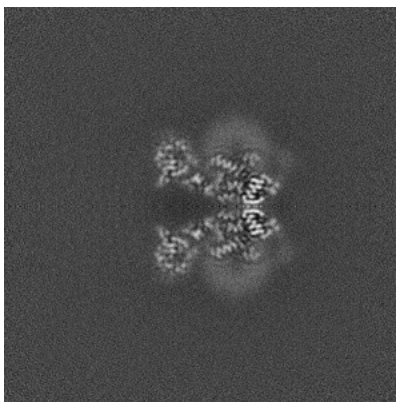


Z Index: 200

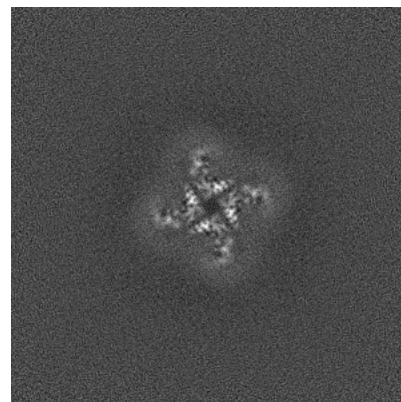
6.2.2 Raw map



X Index: 200



Y Index: 200

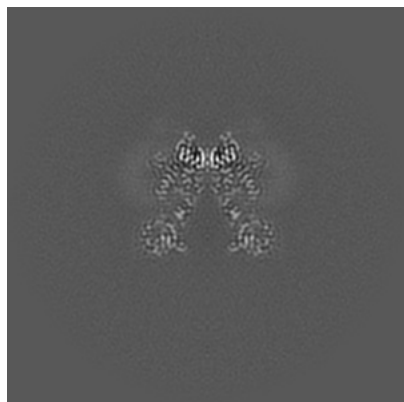


Z Index: 200

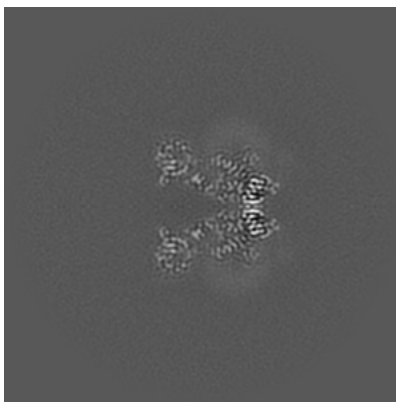
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

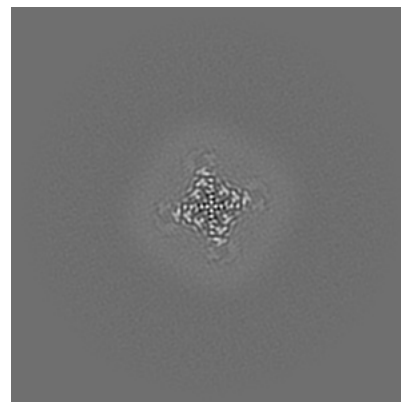
6.3.1 Primary map



X Index: 200

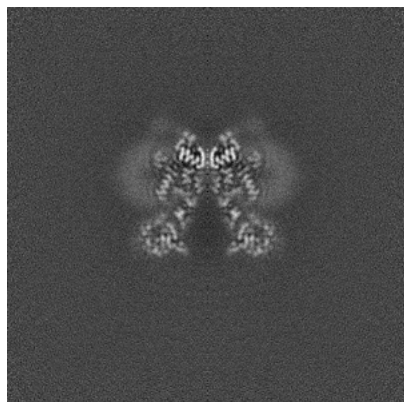


Y Index: 200

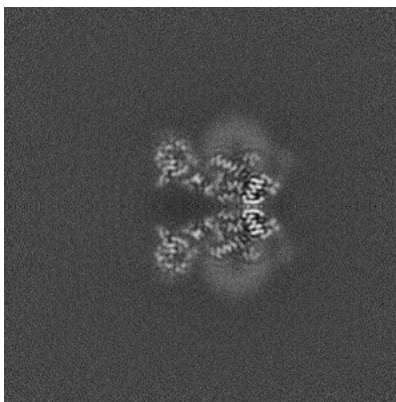


Z Index: 248

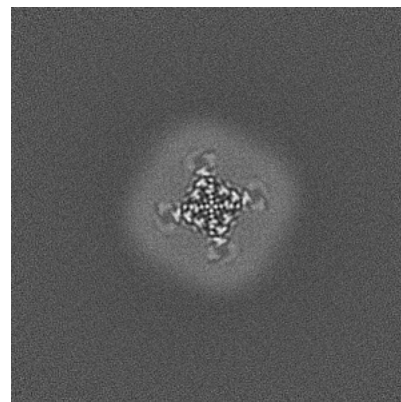
6.3.2 Raw map



X Index: 200



Y Index: 200

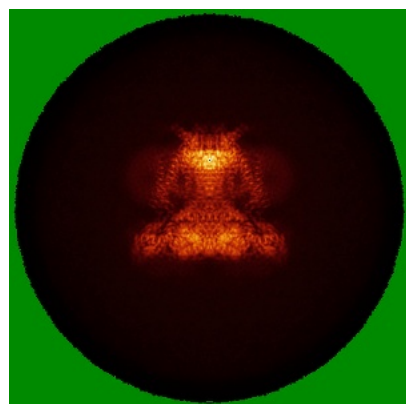


Z Index: 248

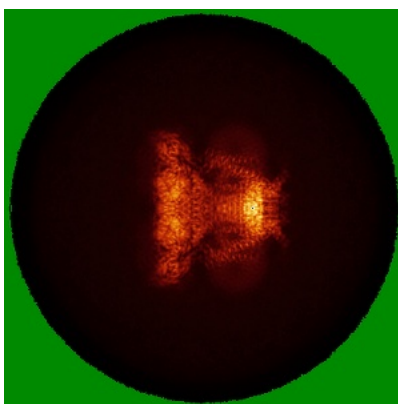
The images above show the largest variance slices of the map in three orthogonal directions.

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

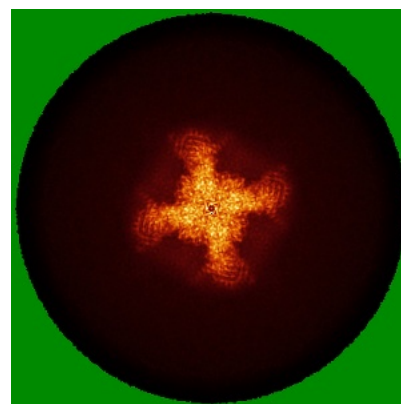
6.4.1 Primary map



X

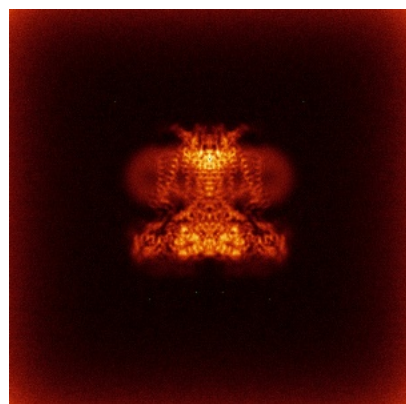


Y

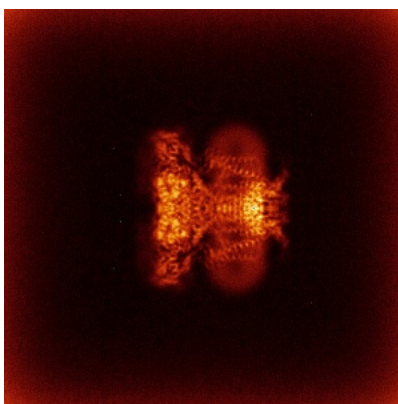


Z

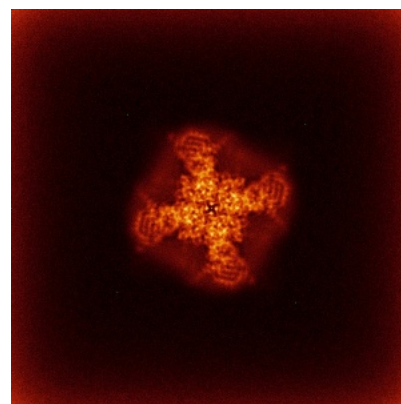
6.4.2 Raw map



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.

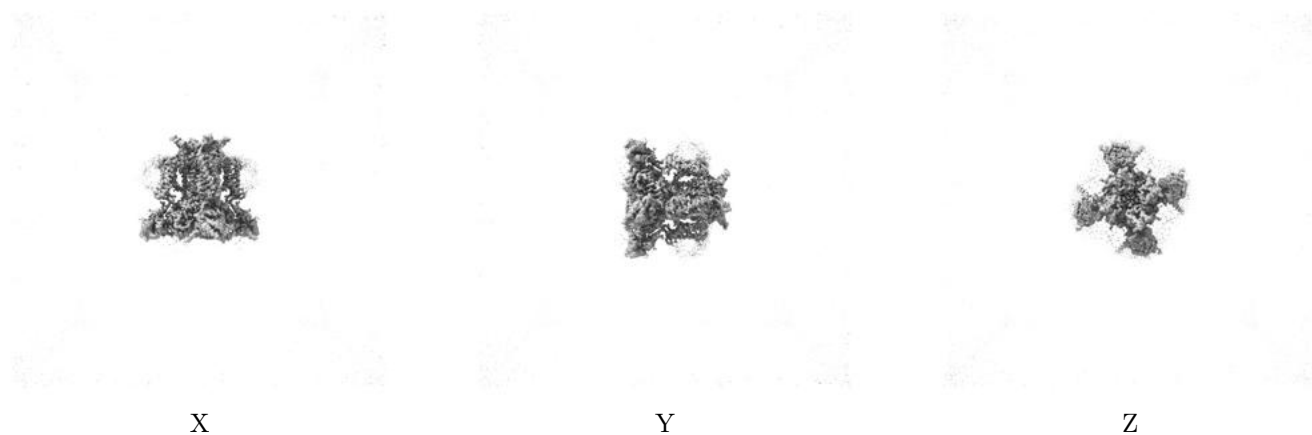
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.25. 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.

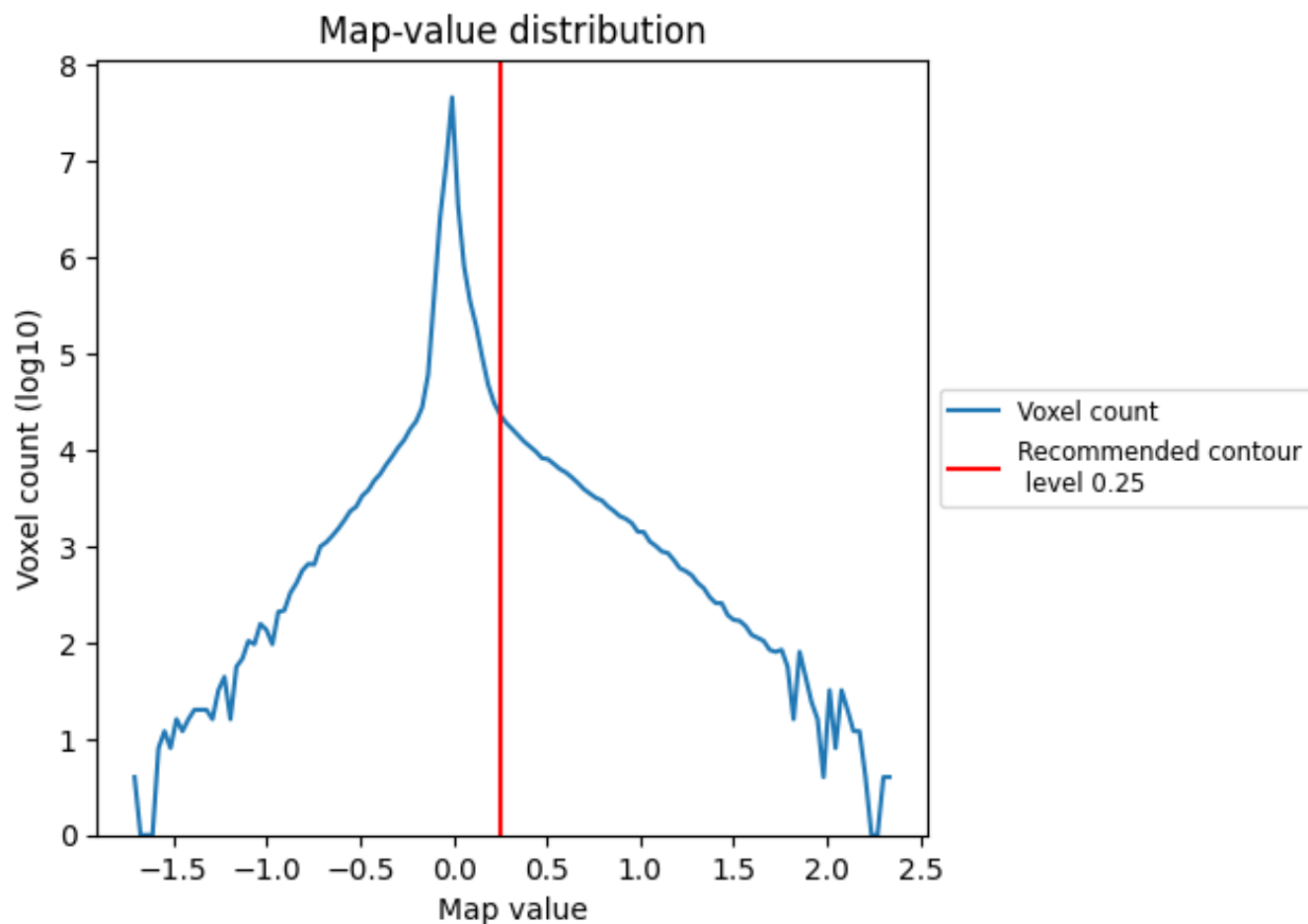
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

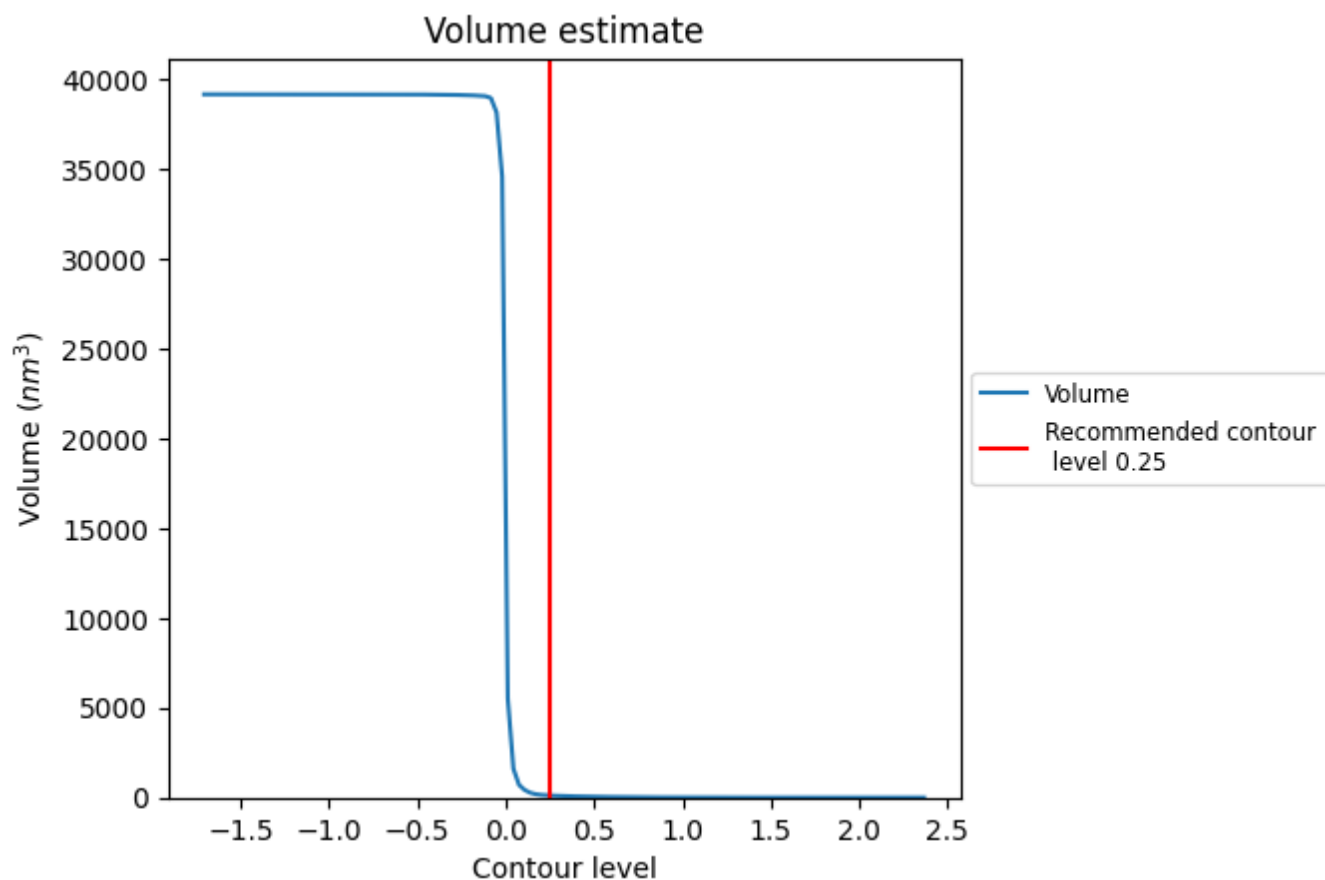
This section contains the results of statistical analysis of the map.

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.

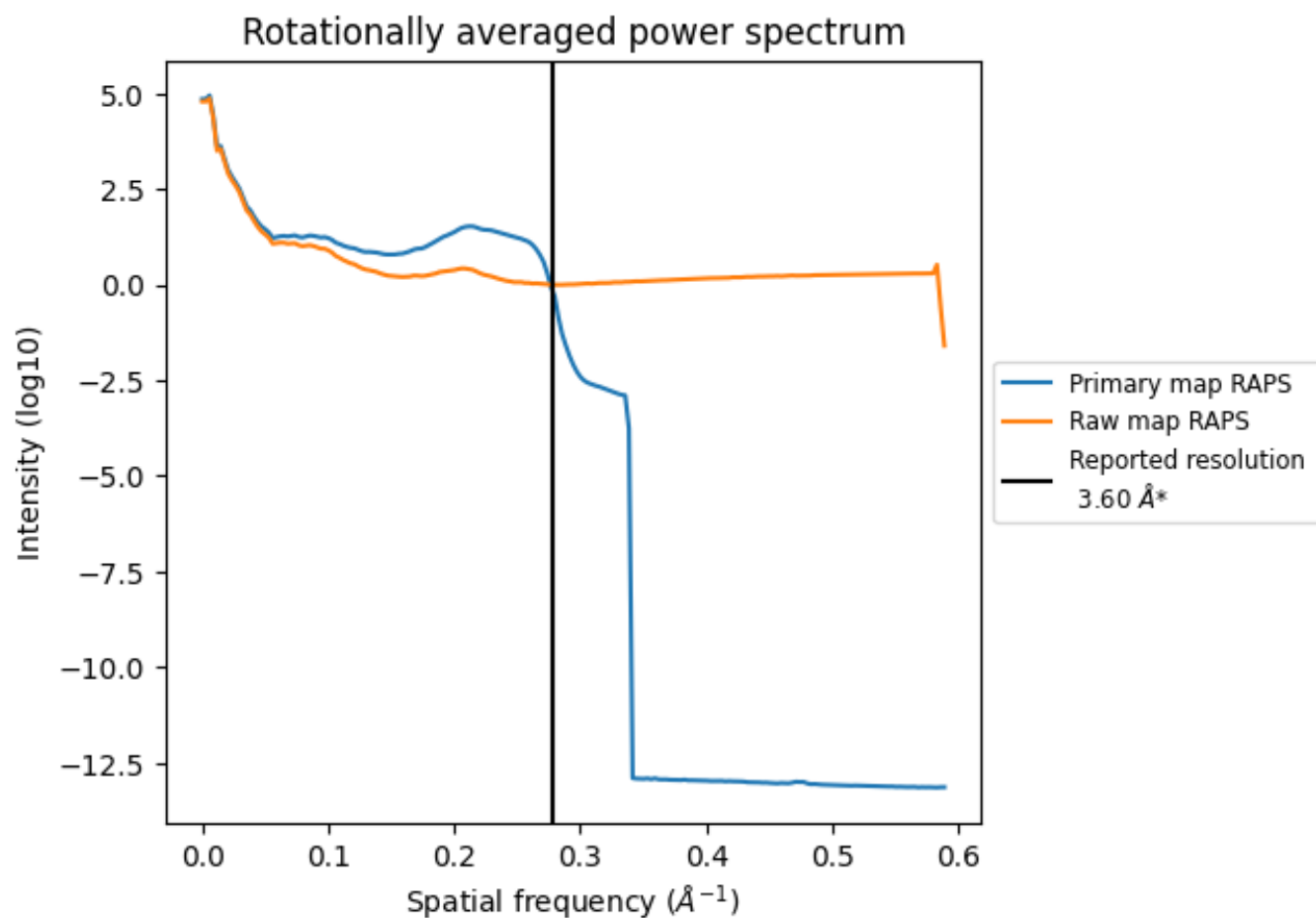
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 115 nm³; this corresponds to an approximate mass of 104 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 ⓘ

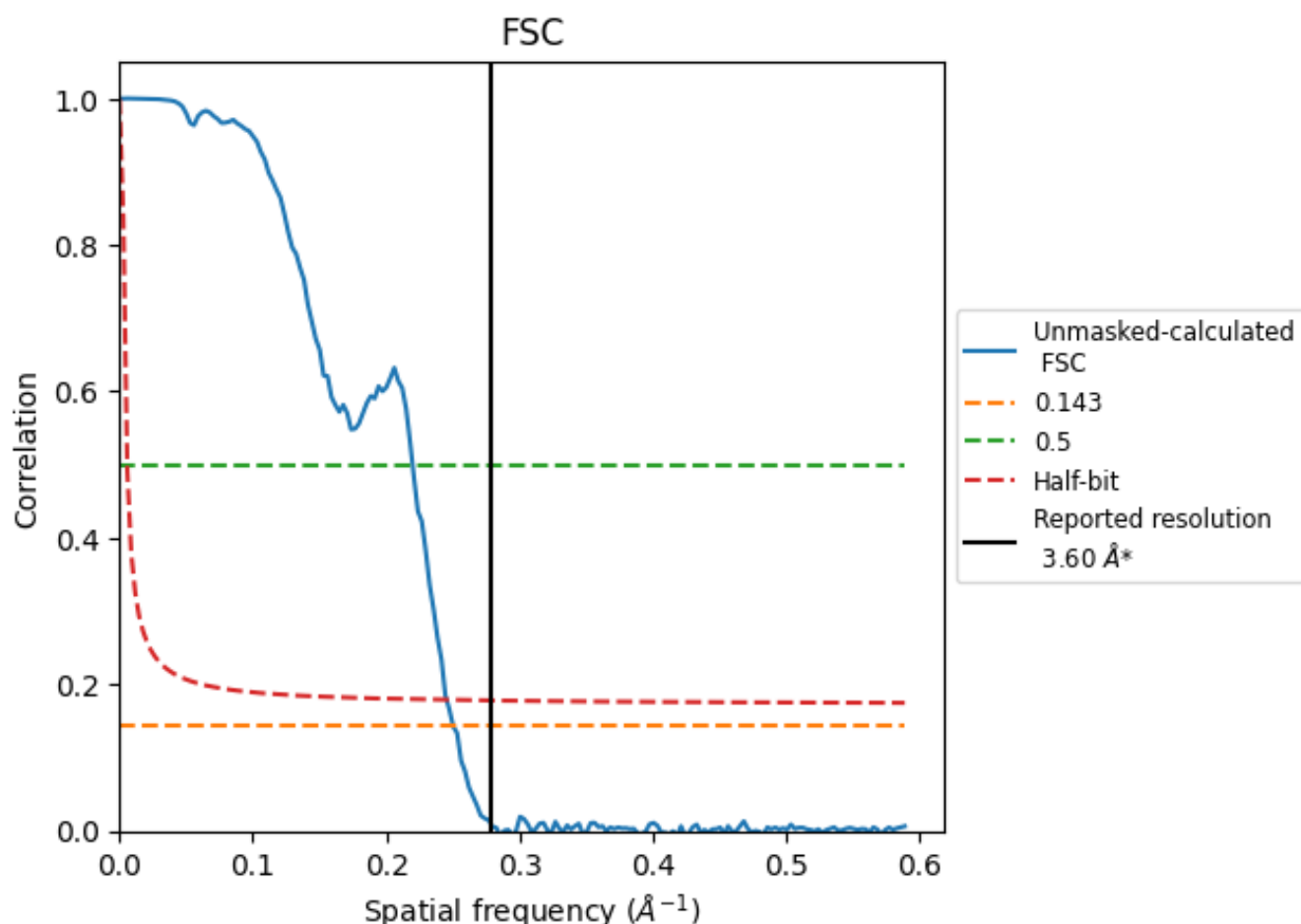


*Reported resolution corresponds to spatial frequency of 0.278 \AA^{-1}

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 0.278 Å⁻¹

8.2 Resolution estimates [i](#)

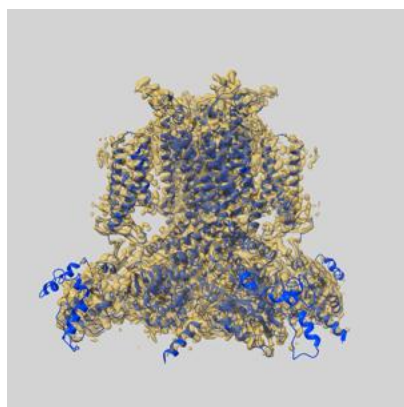
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.00	4.55	4.07

*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 4.00 differs from the reported value 3.6 by more than 10 %

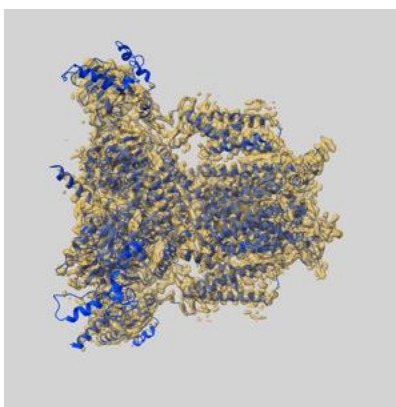
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-33858 and PDB model 7YIG. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

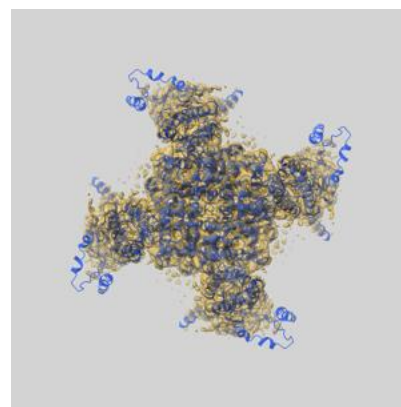
9.1 Map-model overlay [i](#)



X



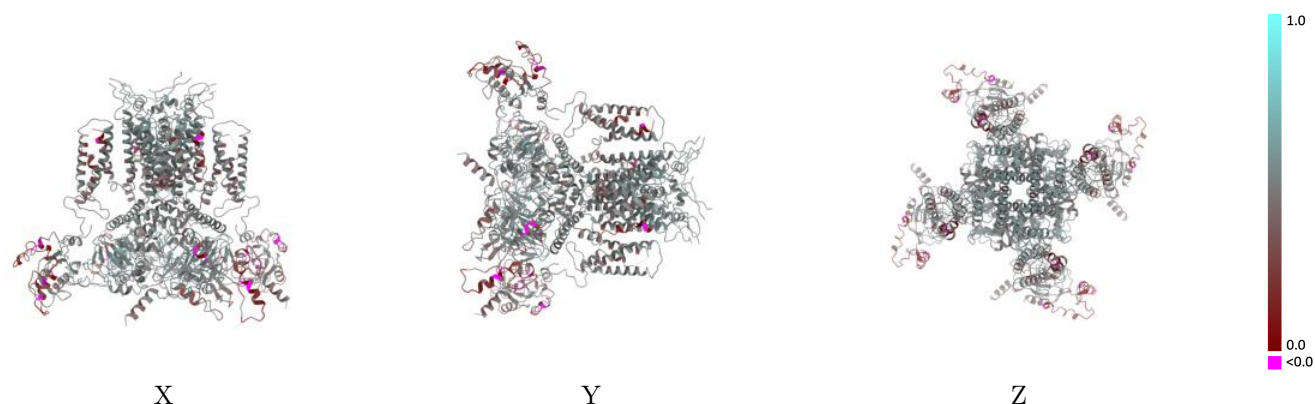
Y



Z

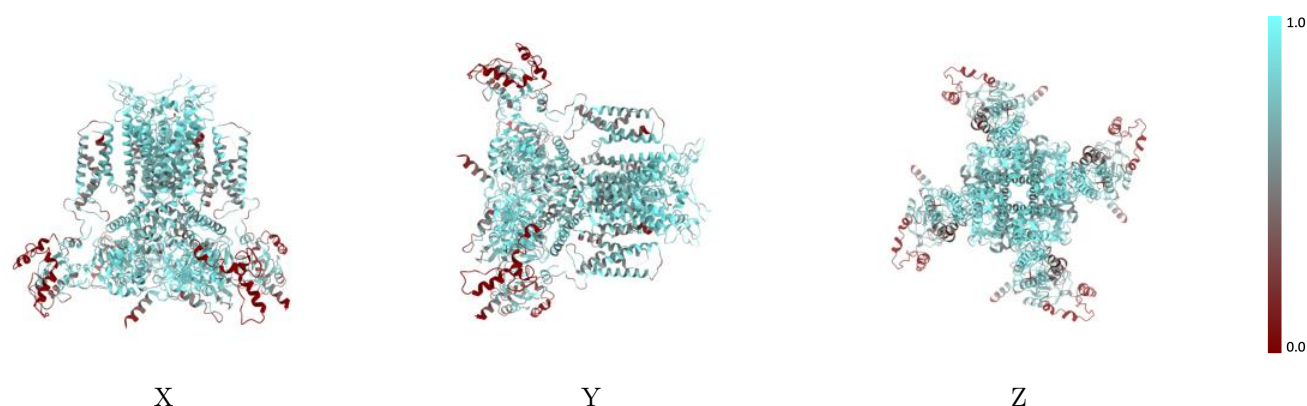
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



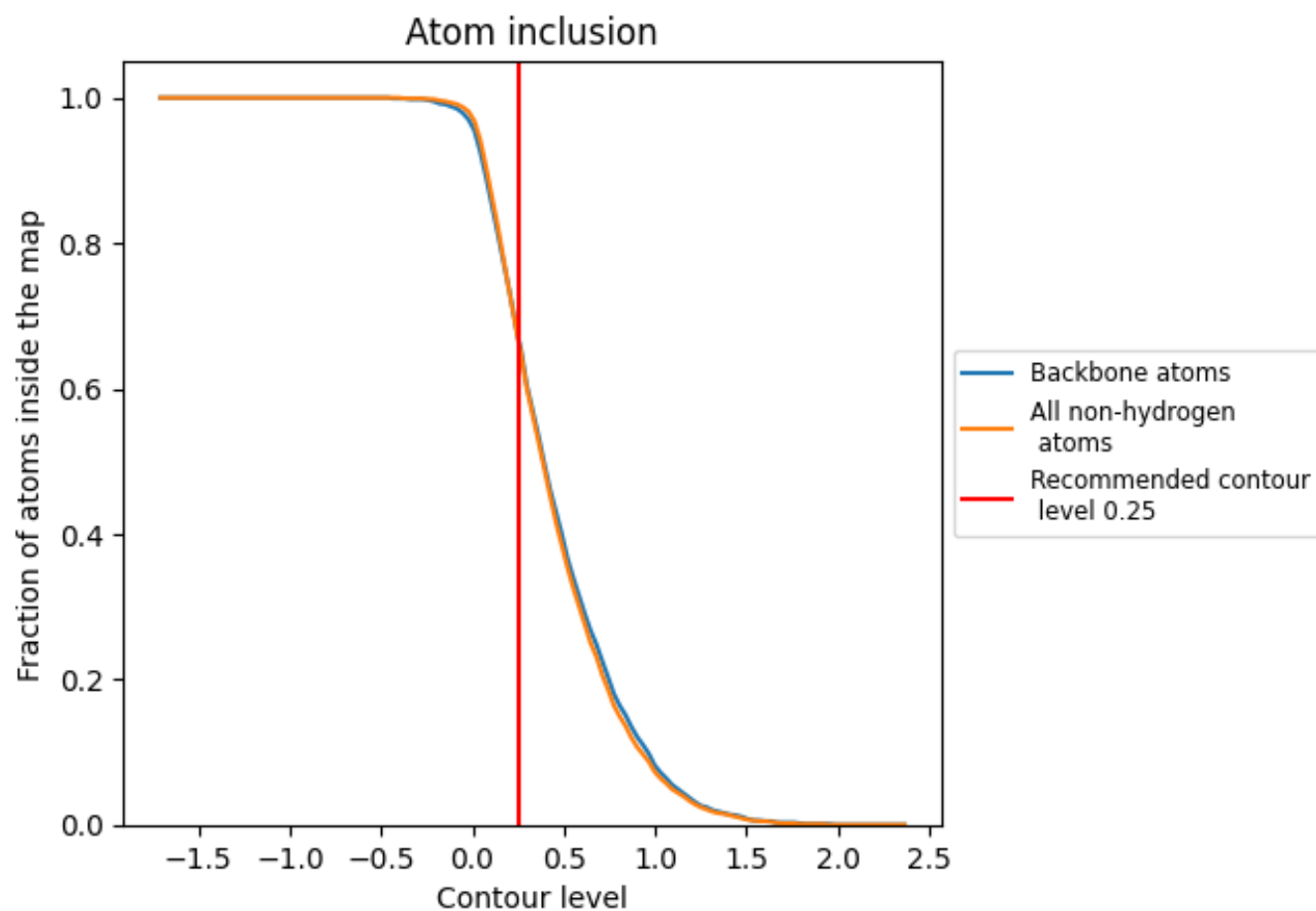
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.25).

9.4 Atom inclusion [i](#)



At the recommended contour level, 67% of all backbone atoms, 67% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6680	<div></div> 0.4610
A	<div></div> 0.6740	<div></div> 0.4620
B	<div></div> 0.6740	<div></div> 0.4600
C	<div></div> 0.6740	<div></div> 0.4610
D	<div></div> 0.6740	<div></div> 0.4610

