



Full wwPDB EM Validation Report ⓘ

Aug 23, 2026 – 07:53 pm BST

PDB ID : 28NO / pdb_000028no
EMDB ID : EMD-56657
Title : CTX/MthK complex
Authors : Qoraj, D.; Sprink, T.; Lange, A.
Deposited on : 2026-02-10
Resolution : 4.10 Å(reported)

This is a Full wwPDB EM Validation 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.dev133
Mogul : 1.8.4, CSD as541be (2020)
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) : 2.50

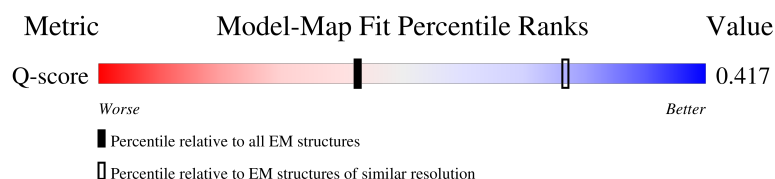
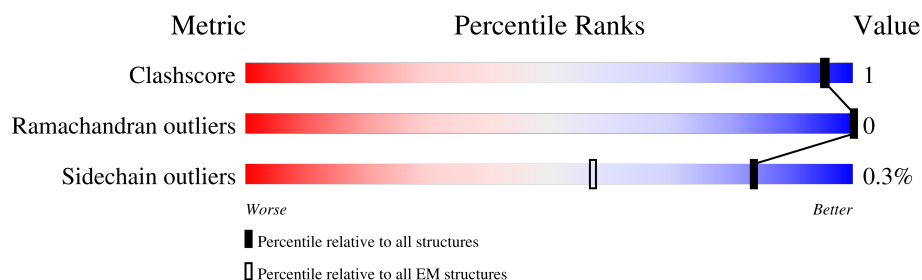
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	6458 (3.60 - 4.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	E	37	24% 97%
2	A	344	25% 74%
2	B	344	25% 74%
2	C	344	25% 74%

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Mol	Chain	Length	Quality of chain
2	D	344	25% 74%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6225 atoms, of which 3141 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 channel toxin alpha-KTx 1.1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	E	37	Total	C	H	N	O	S	0	0
			576	176	281	57	55	7		

- Molecule 2 is a protein called Calcium-gated potassium channel MthK.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	A	89	Total	C	H	N	O	S	0	0
			1412	467	715	105	122	3		
2	B	89	Total	C	H	N	O	S	0	0
			1412	467	715	105	122	3		
2	C	89	Total	C	H	N	O	S	0	0
			1412	467	715	105	122	3		
2	D	89	Total	C	H	N	O	S	0	0
			1412	467	715	105	122	3		

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	337	LEU	-	expression tag	UNP O27564
A	338	GLU	-	expression tag	UNP O27564
A	339	GLU	-	expression tag	UNP O27564
A	340	ASN	-	expression tag	UNP O27564
A	341	LEU	-	expression tag	UNP O27564
A	342	TYR	-	expression tag	UNP O27564
A	343	PHE	-	expression tag	UNP O27564
A	344	GLN	-	expression tag	UNP O27564
B	337	LEU	-	expression tag	UNP O27564
B	338	GLU	-	expression tag	UNP O27564
B	339	GLU	-	expression tag	UNP O27564
B	340	ASN	-	expression tag	UNP O27564
B	341	LEU	-	expression tag	UNP O27564
B	342	TYR	-	expression tag	UNP O27564
B	343	PHE	-	expression tag	UNP O27564

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Chain	Residue	Modelled	Actual	Comment	Reference
B	344	GLN	-	expression tag	UNP O27564
C	337	LEU	-	expression tag	UNP O27564
C	338	GLU	-	expression tag	UNP O27564
C	339	GLU	-	expression tag	UNP O27564
C	340	ASN	-	expression tag	UNP O27564
C	341	LEU	-	expression tag	UNP O27564
C	342	TYR	-	expression tag	UNP O27564
C	343	PHE	-	expression tag	UNP O27564
C	344	GLN	-	expression tag	UNP O27564
D	337	LEU	-	expression tag	UNP O27564
D	338	GLU	-	expression tag	UNP O27564
D	339	GLU	-	expression tag	UNP O27564
D	340	ASN	-	expression tag	UNP O27564
D	341	LEU	-	expression tag	UNP O27564
D	342	TYR	-	expression tag	UNP O27564
D	343	PHE	-	expression tag	UNP O27564
D	344	GLN	-	expression tag	UNP O27564

- Molecule 3 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
3	A	1	Total K 1 1	0

ASP	ILE	LEU	GLY	ILE	GLY	PRO	GLU	GLU	ILE	GLU	ARG	LEU	LYS	ASN	TYR	ILE	SER	ALA	LEU	GLU	GLU	ASN	LEU	TYR	PHE	GLN
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- Molecule 2: Calcium-gated potassium channel MthK



MET	VAL	VAL	LEU	LEU	VAL	VAL	ILE	ILE	GLU	ILE	ILE	ARG	ARG	LYS	HIS	LEU	PRO	PRO	ARG	VAL	LEU	LEU	LYS	VAL	PRO	PRO	A20	T21	W52	V55	E96	G108	GLU	ILE	ASP	VAL	ALA	LYS	SER	SER	ARG	HIS	ARG	VAL	VAL	ILE	CYS	GLY	TRP	SER	GLU	GLU	THR	LEU	LEU	CYS	ARG	LEU	GLU	GLY	ARG	GLY	SER	GLU
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PHE VAL LEU LEU ALA GLU ASP GLU ASN ASN PHE VAL VAL HIS VAL GLY ASP ASP LEU GLU LYS LYS VAL ARG ARG SER SER GLY ASN ASN THR ARG ARG VAL VAL ASP ASP LEU GLU LYS LYS ALA ALA ASN VAL ARG GLY GLY ALA ALA ARG VAL ILE VAL ASP ASP GLU THR THR ILE HIS CYS ILE LEU LEU GLY LEU ILE PRC

LYS ILE ASP ASP SER SER ARG ARG ILE ILE ILE ALA ALA GLU GLU ALA GLU GLU TYR ARG ARG ARG ARG MET MET ALA GLY ASP ASP GLN GLN VAL VAL ILE ILE SER SER GLY GLY ARG ARG ILE ILE ASP ASP ASP GLY TYR GLU ALA ALA LEU LEU PHE PHE VAL VAL GLN ASP VAL VAL LEU LEU GLU GLU

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

- Molecule 2: Calcium-gated potassium channel MthK



MET	VAL	LEU	VAL	VAL	ILE	GLU	GLU	ILE	ILE	ARG	LYS	HIS	LEU	PRO	ARG	VAL	LEU	LYS	VAL	PRG	A20	L24	W52	V55	E92	E96	G108	LEU	ILE	ASP	ALA	ALA	VAL	LYS	SER	ARG	HIS	VAL	VAL	VAL	ILE	CYS	GLY	TRP	SER	SER	THR	LEU	GLU	CYS	ARG	GLU	LEU	ARG
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SER	GLU	VAL	PHE	VAL	LEU	ALA	GLU	ASP	ASN	VAL	ARG	LYS	LYS	VAL	LEU	ARG	SER	GLY	ALA	ASN	PHE	VAL	HIS	GLY	ASP	PRO	THR	ARG	VAL	SER	ASP	LEU	GLY	LYS	ALA	ASN	VAL	VAL	ARG	ALA	ARG	VAL	ILE	ILE	VAL	ASP	LEU	GLU	SER	ASP	SER	GLU	THR	ILE	HIS	CYS	ILE	LEU
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GLY ILE ARG ARG LYS ILE ASP GLU SER VAL ARG ARG ILE ILE ALA GLU ALA ALA ARG TYR GLU ASN MET MET GLY GLN LEU ARG ASP GLN VAL ILE ILE SER PRO PHE VAL ILE ILE GLY GLY LEU LEU MET SER ARG ARG ILE ASP ASP GLY TYR GLU GLU MET PHE VAL GLN ASP ASP VAL LEU

[illegible]

ILE ILE LEU GLY ILE GLY LYS PRO GLU GLU ILE GLU ARG LEU LYS ASN TYR ILE SER ALA LEU LEU GLU GLU ASN LEU TYR PHE GLN

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	92302	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 ($e^-/\text{\AA}^2$)	60.76	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.045	Depositor
Minimum map value	-0.033	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0058	Depositor
Map size (Å)	272.0, 272.0, 272.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85, 0.85, 0.85	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: PCA, 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	E	0.10	0/292	0.44	0/389
2	A	0.16	0/714	0.42	0/974
2	B	0.16	0/714	0.40	0/974
2	C	0.16	0/714	0.41	0/974
2	D	0.16	0/714	0.41	0/974
All	All	0.15	0/3148	0.41	0/4285

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	E	295	281	282	0	0
2	A	697	715	714	1	0
2	B	697	715	714	3	0
2	C	697	715	714	1	0
2	D	697	715	714	1	0
3	A	1	0	0	0	0
All	All	3084	3141	3138	6	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 1.

All (6) 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)
2:B:52:TRP:HA	2:B:55:VAL:HG22	1.93	0.51
2:B:69:THR:HG23	2:B:70:PRO:HD2	1.96	0.47
2:D:52:TRP:HA	2:D:55:VAL:HG22	1.97	0.45
2:C:52:TRP:HA	2:C:55:VAL:HG22	2.01	0.43
2:B:69:THR:CG2	2:B:70:PRO:HD2	2.50	0.42
2:A:52:TRP:HA	2:A:55:VAL:HG22	2.02	0.41

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	E	35/37 (95%)	30 (86%)	5 (14%)	0	100	100
2	A	87/344 (25%)	85 (98%)	2 (2%)	0	100	100
2	B	87/344 (25%)	87 (100%)	0	0	100	100
2	C	87/344 (25%)	84 (97%)	3 (3%)	0	100	100
2	D	87/344 (25%)	83 (95%)	4 (5%)	0	100	100
All	All	383/1413 (27%)	369 (96%)	14 (4%)	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	E	35/35 (100%)	35 (100%)	0	100	100
2	A	74/296 (25%)	74 (100%)	0	100	100
2	B	74/296 (25%)	74 (100%)	0	100	100
2	C	74/296 (25%)	74 (100%)	0	100	100
2	D	74/296 (25%)	73 (99%)	1 (1%)	59	71
All	All	331/1219 (27%)	330 (100%)	1 (0%)	84	85

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

Mol	Chain	Res	Type
2	D	92	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	21	HIS
2	C	39	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	PCA	E	1	1	7,8,9	0.81	0	9,10,12	1.71	1 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PCA	E	1	1	-	0/0/11/13	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	E	1	PCA	O-C-CA	-4.12	113.98	124.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

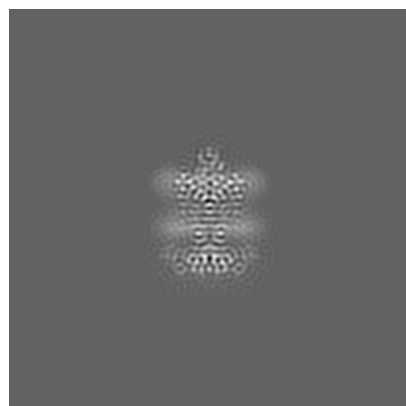
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-56657. These allow visual inspection of the internal detail of the map and identification of artifacts.

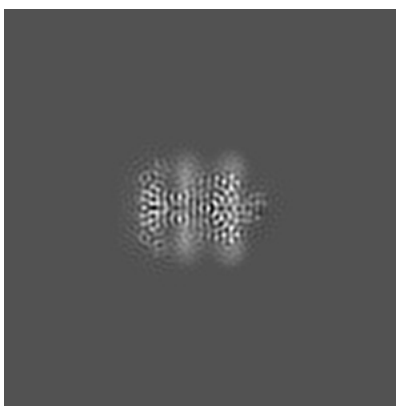
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

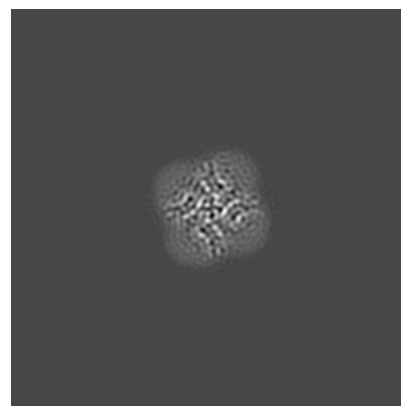
6.1.1 Primary map



X

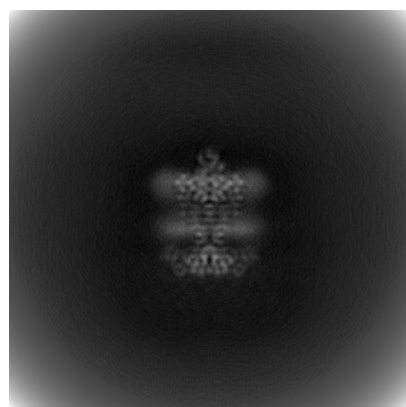


Y

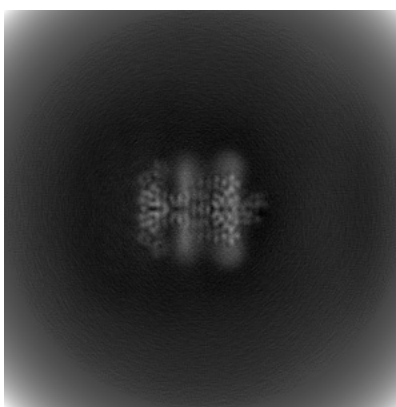


Z

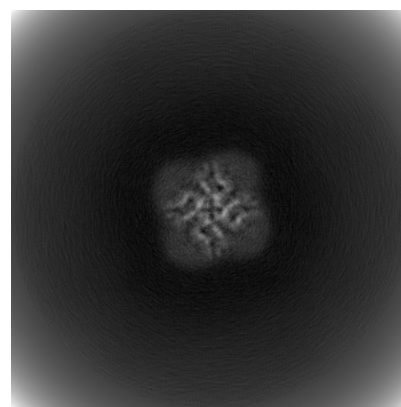
6.1.2 Raw map



X



Y

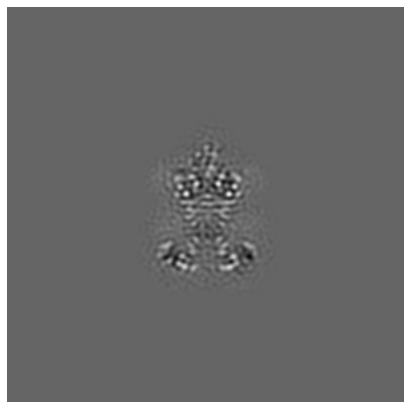


Z

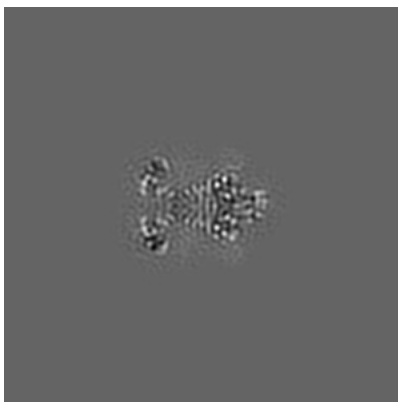
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 160

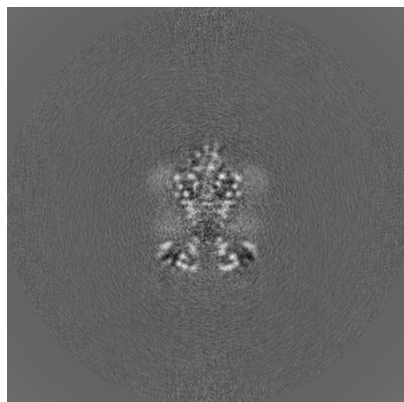


Y Index: 160

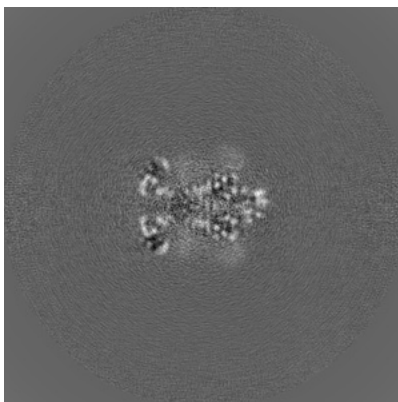


Z Index: 160

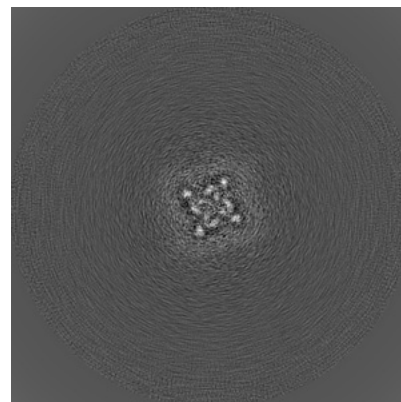
6.2.2 Raw map



X Index: 160



Y Index: 160



Z Index: 160

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: 164

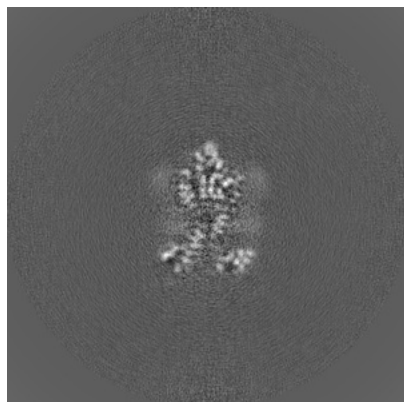


Y Index: 164

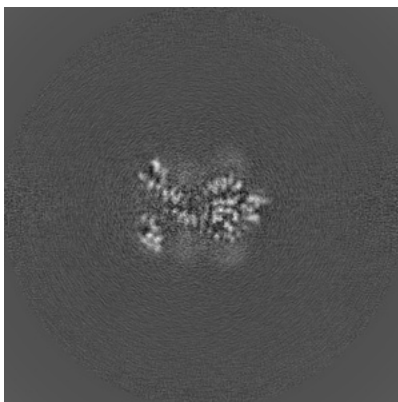


Z Index: 181

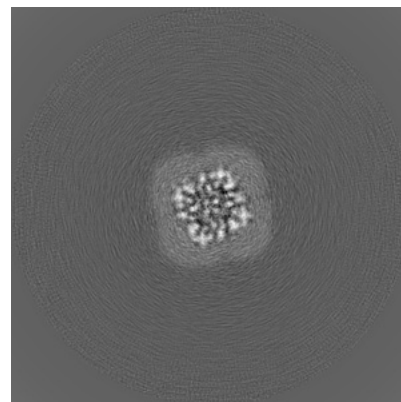
6.3.2 Raw map



X Index: 164



Y Index: 164

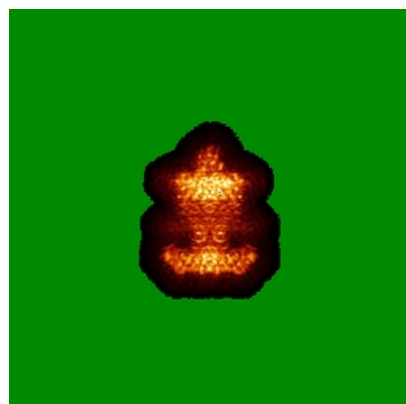


Z Index: 182

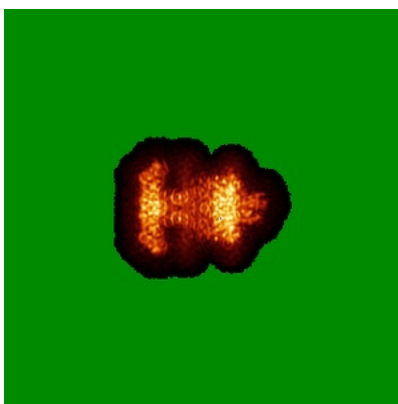
The images above show the largest variance slices of the map in three orthogonal directions.

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

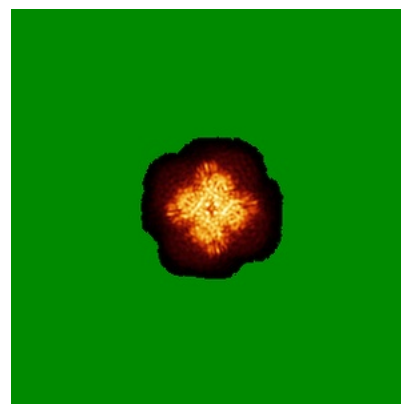
6.4.1 Primary map



X

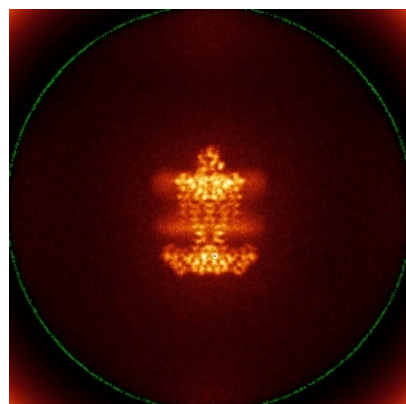


Y

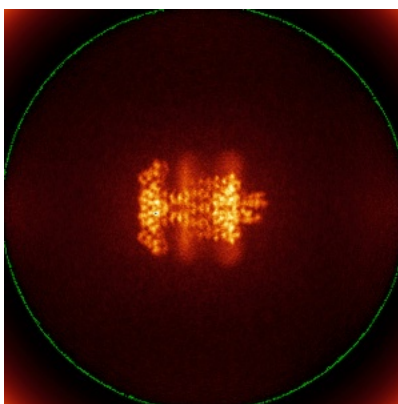


Z

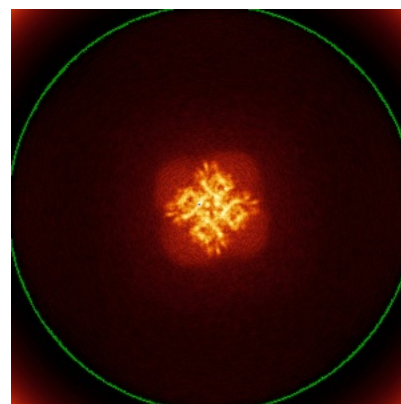
6.4.2 Raw map



X



Y

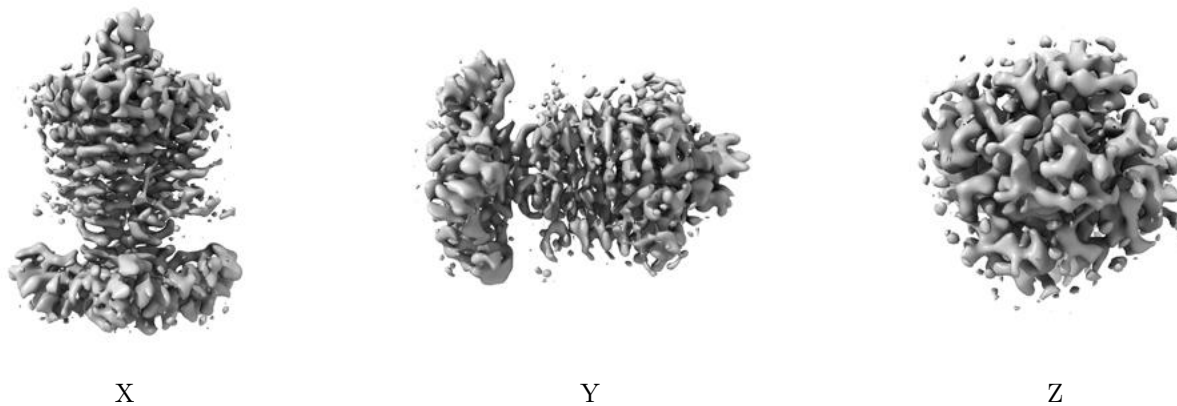


Z

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 0.0058. 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.

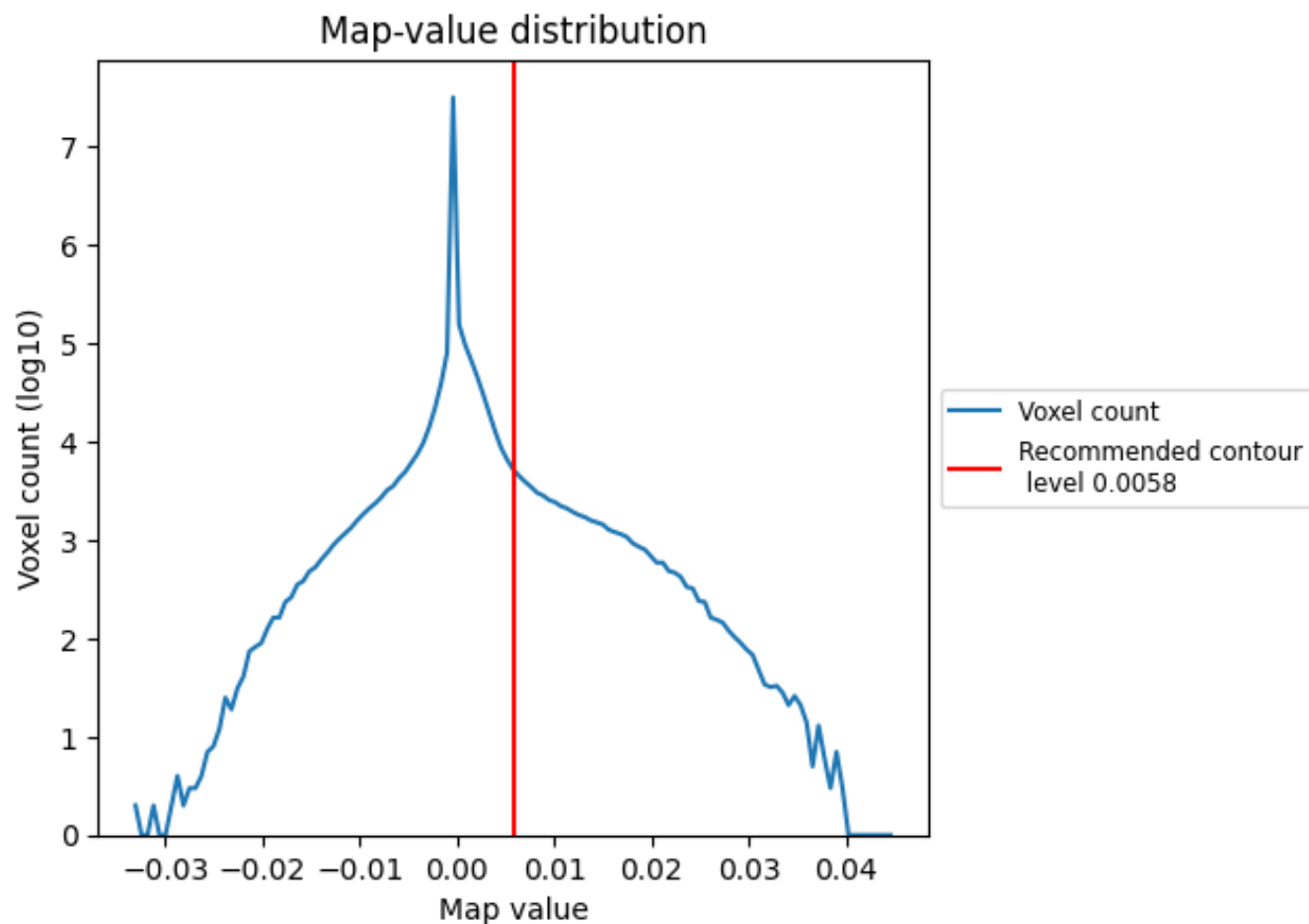
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

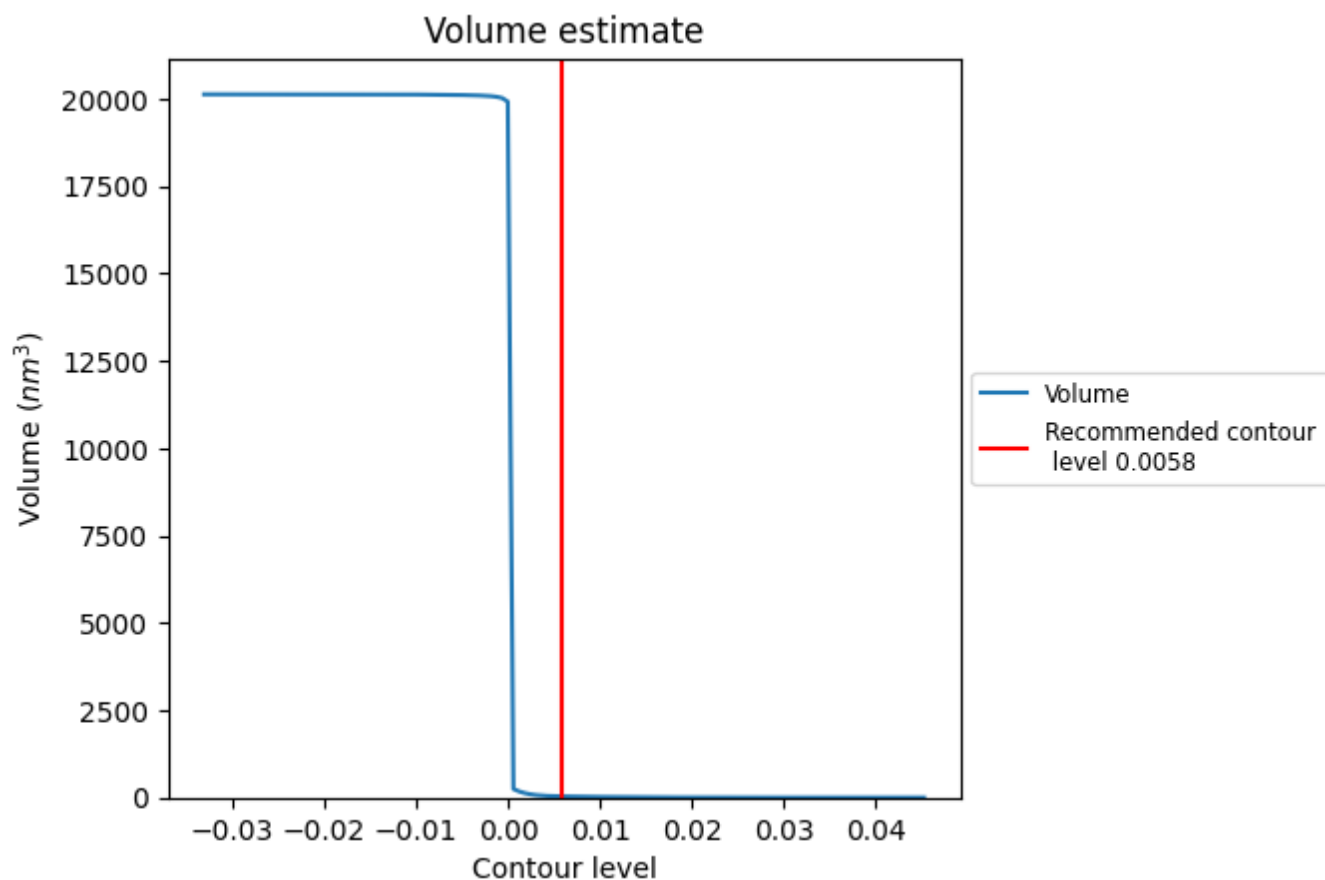
This section contains the results of statistical analysis of the map.

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.

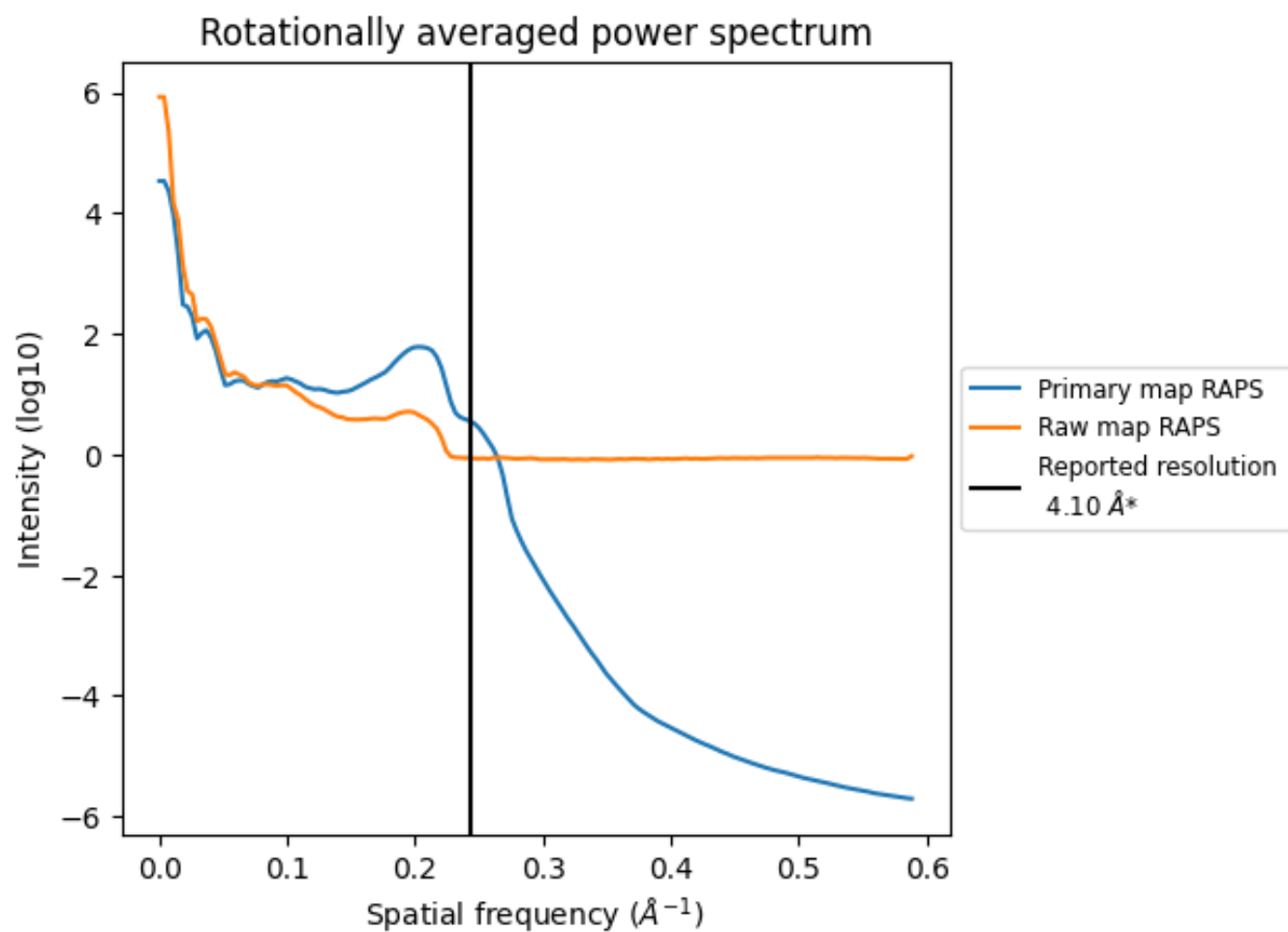
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 34 nm^3 ; 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 ⓘ

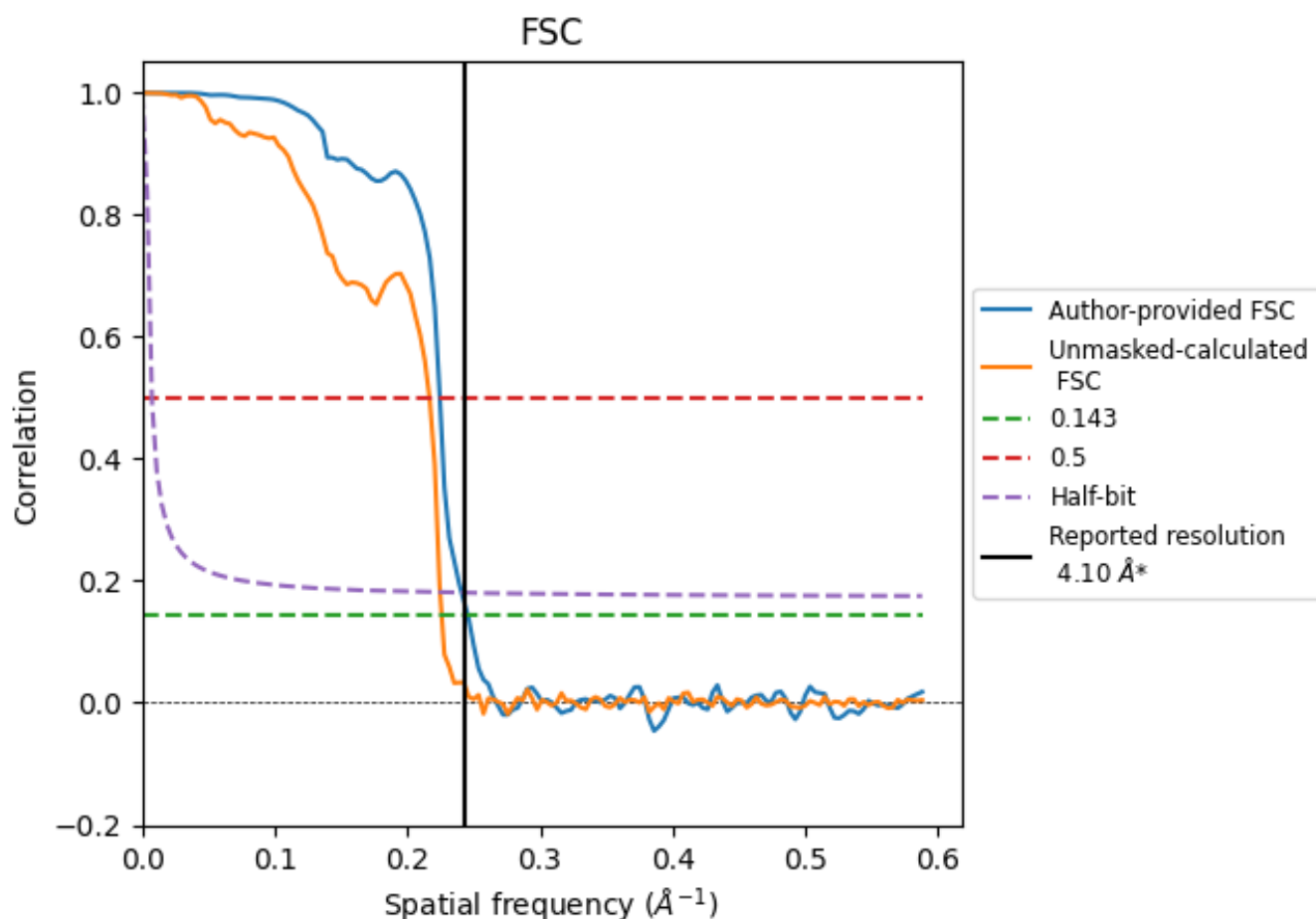


*Reported resolution corresponds to spatial frequency of $0.244 \text{ \AA}^{-1}$

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 $0.244 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

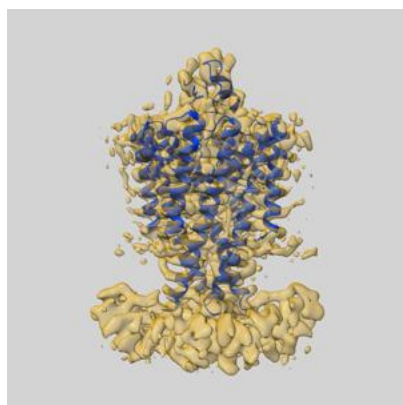
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	4.07	4.46	4.15
Unmasked-calculated*	4.43	4.61	4.45

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

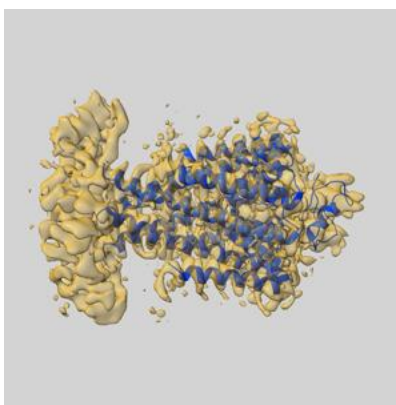
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-56657 and PDB model 28NO. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

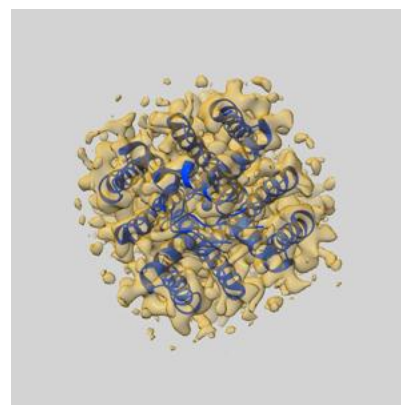
9.1 Map-model overlay [i](#)



X



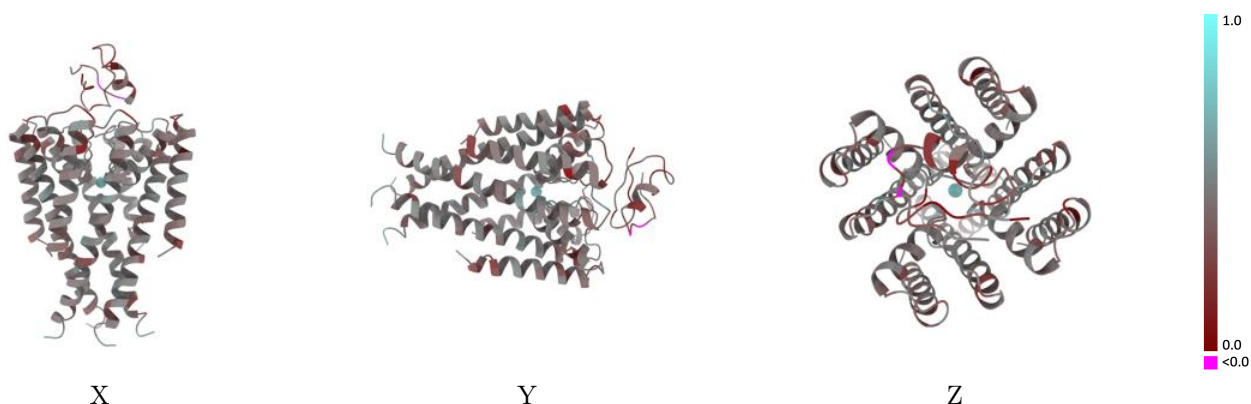
Y



Z

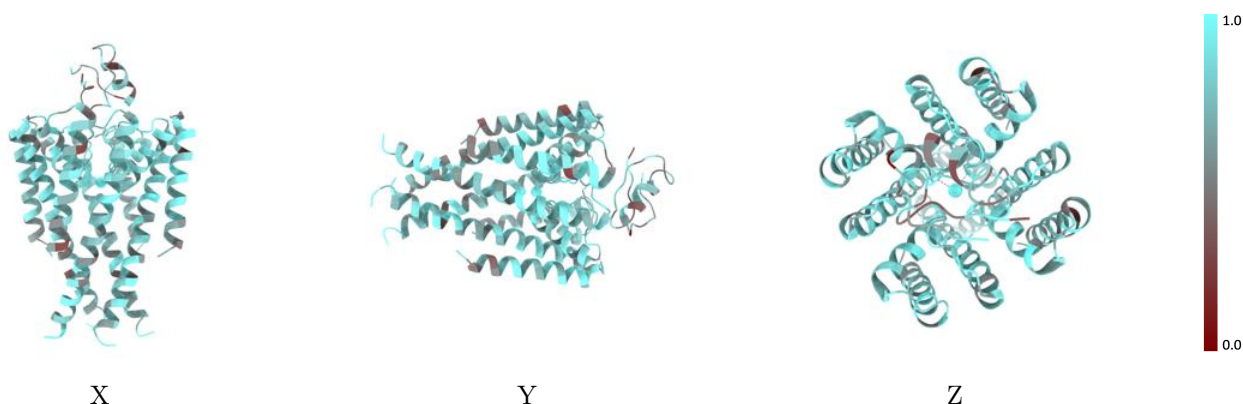
The images above show the 3D surface view of the map at the recommended contour level 0.0058 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



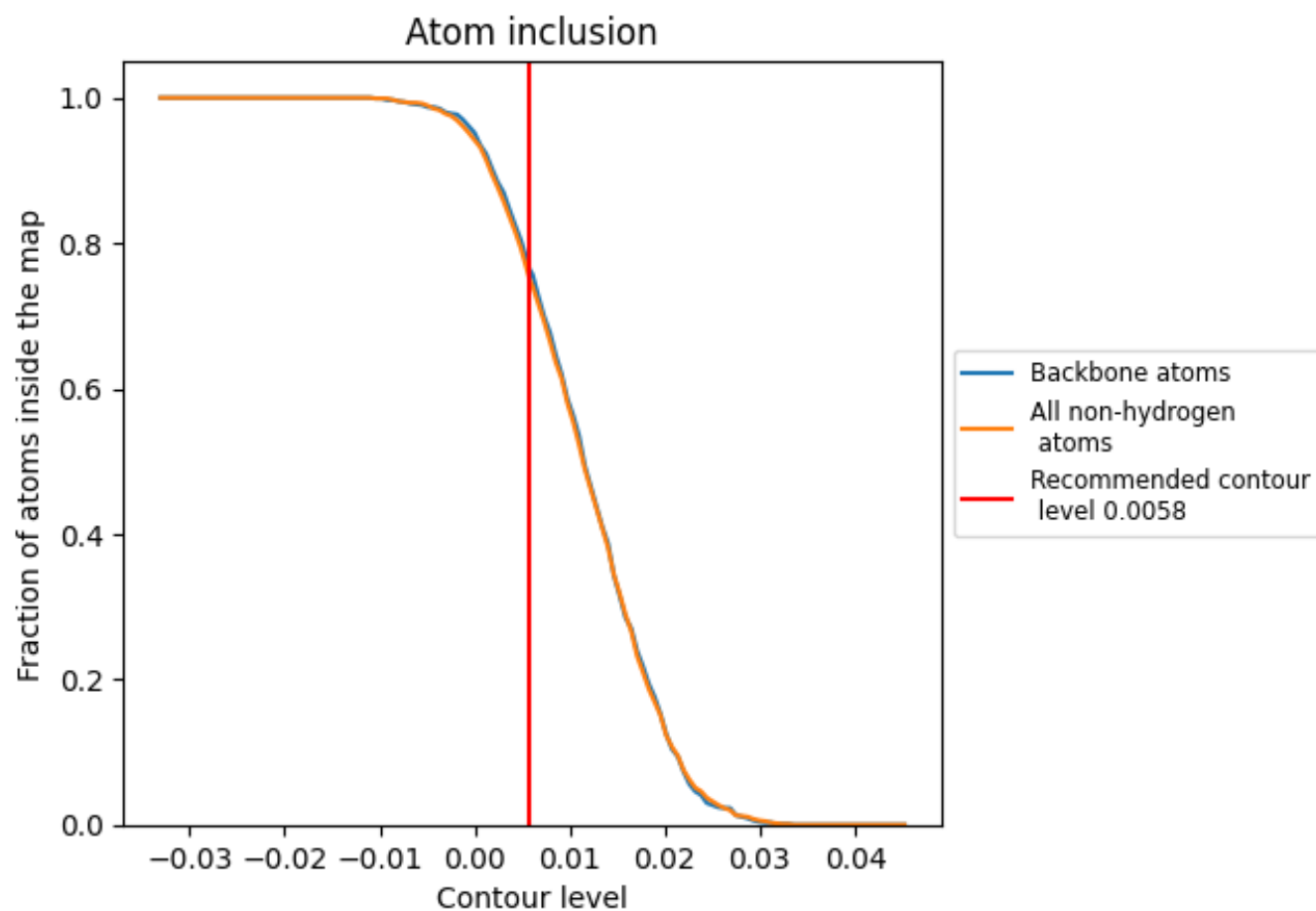
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0058).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 75% 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 (0.0058) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7490	0.4170
A	0.7870	0.4290
B	0.7600	0.4320
C	0.7700	0.4290
D	0.7780	0.4330
E	0.5990	0.2910

