



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 12:15 PM UTC

PDB ID : 8Q8P / pdb_00008q8p
EMDB ID : EMD-18256
Title : Cryo-EM structure of the magnesium channel CtMrs2 in the closed state
Authors : Gourdon, P.; Li, P.
Deposited on : 2023-08-18
Resolution : 2.68 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

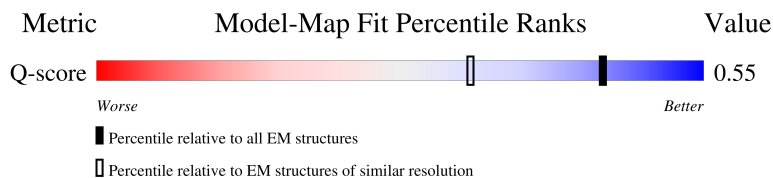
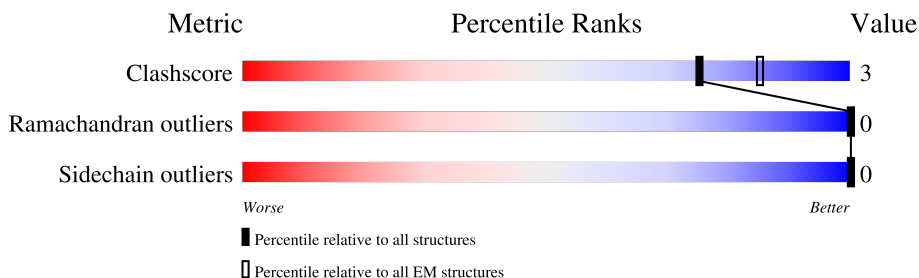
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.68 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	9255 (2.18 - 3.18)

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	425	
1	B	425	
1	C	425	
1	D	425	

Continued on next page...

Mol	Chain	Length	Quality of chain
1	E	425	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12579 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 Magnesium channel Mrs2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	317	Total	C	N	O	S	0	0
			2511	1596	425	480	10		
1	B	317	Total	C	N	O	S	0	0
			2511	1596	425	480	10		
1	C	317	Total	C	N	O	S	0	0
			2511	1596	425	480	10		
1	D	317	Total	C	N	O	S	0	0
			2511	1596	425	480	10		
1	E	317	Total	C	N	O	S	0	0
			2511	1596	425	480	10		

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
2	A	8	Total	Mg	0
			8	8	
2	B	3	Total	Mg	0
			3	3	
2	C	5	Total	Mg	0
			5	5	
2	D	4	Total	Mg	0
			4	4	
2	E	4	Total	Mg	0
			4	4	

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

● Molecule 1: Magnesium channel Mrs2



SER	GLY	ARG	THR	TRP	ARG	GLU	LEU	PHE	GLY	SER	PRO	SER	ASN	ARG	GLU	LYS	GLN	SER	LEU	ARG	GLU	LYS	ALA	LYS	ILE	MET	LYS	ASN	LYS	GLU	GLU	GLU	GLU	ILE	SER	HIS	MET	ALA	LYS	ARG	LYS	GLN	LYS	THR	ALA	SER	ALA	GLY	ALA	LYS	ILE	PHE	GLN	ARG	TRP	PRO	LEU	ASN	LYS	THR	SER	LYS	ALA	ALA	LEU	LEU	ASP	P166	P211	N223	H226	V236
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M254	K264	G267	G268	A269	L272	P273	Y274	R277	E280	M284	E289	V301	I304	L305	D310	E315	R318	L321	D349	D362	D368	T401	T404	R413	N414	R482	VAL	LYS	MET	ASN	GLY	ALA	GLY	PHE	THR	ARG	HIS	ASN
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HIS	TRP	PHE	ARG	THR	ASP	SER	THR	ASP	VAL	LEU	PHE	LEU	GLY	SER	PRO	SER	ASN	ARG	GLU	SER	ARG	LEU	ARG	LYS	ILE	LYS	ASN	MET	MET	LYS	SER	HIS	ALA	LYS	GLN	LYS	THR	ALA	ALA	LYS	LYS	TRP	PRO	LEU	ASN	LYS	LEU
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● Molecule 1: Magnesium channel Mrs2



SER	GLY	ARG	LEU	THR	TRP	ARG	GLU	LEU	PHE	LEU	GLY	SER	GLY	ALA	LYS	GLN	SER	GLU	GLU	ALA	MET	LYS	ILE	GLU	GLU	ILE	MET	LYS	ASN	MET	LYS	LEU	GLN	GLU	ASP	SER	GLY	ALA	ILE	PHE	GLN	ARG	TRP	PRO	LEU	SER	THR	SER	LYS	ALA	ALA	LEU	LEU	ASP	P166	T171	V182	P211	N223
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L224	L225	H226	V236	M254	K264	A269	L272	P273	Y274	R277	E280	M284	E289	V301	I304	L305	D310	E315	R318	L321	D349	D362	D368	T401	T404	R413	N414	R482	VAL	LYS	MET	ASN	GLY	ALA	GLY	PHE	THR
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ARG	HIS	ASN	HIS	TRP	PHE	ARG	ASP	ASP	THR	SER	VAL	LEU	LEU	ASP	PRO	SER	ASN	ARG	GLU	ARG	ARG	LYS	ILE	ASN	MET	MET	LYS	LYS	SER	HIS	ALA	GLN	LYS	THR	ALA	ALA	ALA	LYS	LYS	TRP	PRO	LEU	ASN	LYS	LEU
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	222578	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	6.043	Depositor
Minimum map value	-3.520	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.100	Depositor
Recommended contour level	0.45	Depositor
Map size (Å)	344.68, 344.68, 344.68	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8617, 0.8617, 0.8617	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: MG

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	0.10	0/2546	0.23	0/3439
1	B	0.10	0/2546	0.23	0/3439
1	C	0.10	0/2546	0.23	0/3439
1	D	0.10	0/2546	0.23	0/3439
1	E	0.10	0/2546	0.23	0/3439
All	All	0.10	0/12730	0.23	0/17195

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	2511	0	2568	17	0
1	B	2511	0	2568	17	0
1	C	2511	0	2568	17	0
1	D	2511	0	2568	17	0
1	E	2511	0	2568	17	0
2	A	8	0	0	0	0
2	B	3	0	0	0	0
2	C	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	4	0	0	0	0
2	E	4	0	0	0	0
All	All	12579	0	12840	79	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 79 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:E:280:GLU:HG2	1:E:284:MET:HE2	1.78	0.66
1:D:280:GLU:HG2	1:D:284:MET:HE2	1.77	0.66
1:A:280:GLU:HG2	1:A:284:MET:HE2	1.78	0.66
1:C:280:GLU:HG2	1:C:284:MET:HE2	1.78	0.66
1:B:280:GLU:HG2	1:B:284:MET:HE2	1.78	0.65

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	315/425 (74%)	311 (99%)	4 (1%)	0	100	100
1	B	315/425 (74%)	311 (99%)	4 (1%)	0	100	100
1	C	315/425 (74%)	311 (99%)	4 (1%)	0	100	100
1	D	315/425 (74%)	311 (99%)	4 (1%)	0	100	100
1	E	315/425 (74%)	311 (99%)	4 (1%)	0	100	100
All	All	1575/2125 (74%)	1555 (99%)	20 (1%)	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	278/370 (75%)	278 (100%)	0	100	100
1	B	278/370 (75%)	278 (100%)	0	100	100
1	C	278/370 (75%)	278 (100%)	0	100	100
1	D	278/370 (75%)	278 (100%)	0	100	100
1	E	278/370 (75%)	278 (100%)	0	100	100
All	All	1390/1850 (75%)	1390 (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 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	176	ASN
1	E	393	ASN
1	E	223	ASN
1	C	178	ASN
1	D	223	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

Of 24 ligands modelled in this entry, 24 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.

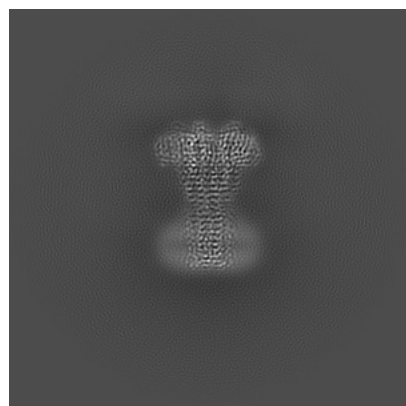
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18256. These allow visual inspection of the internal detail of the map and identification of artifacts.

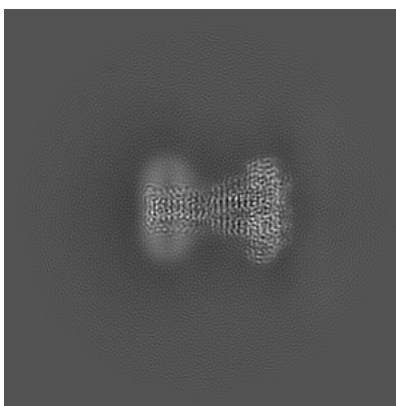
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

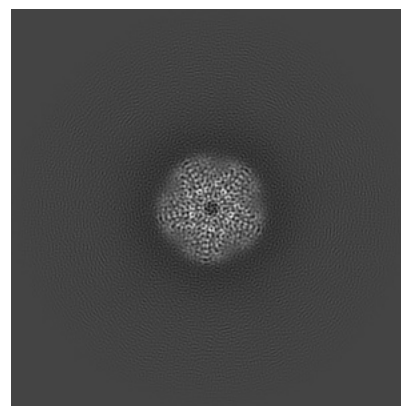
6.1.1 Primary map



X

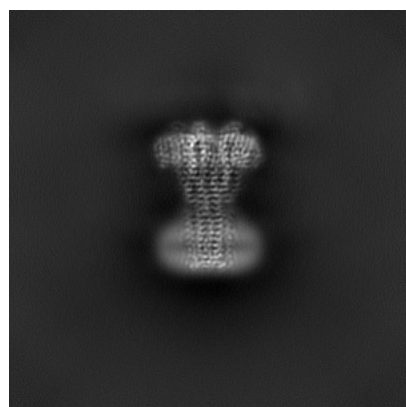


Y

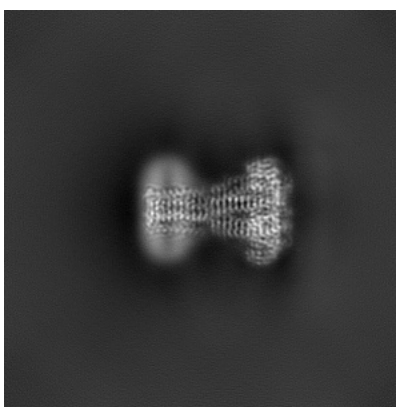


Z

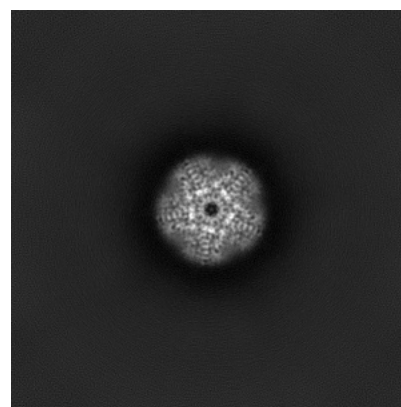
6.1.2 Raw map



X



Y



Z

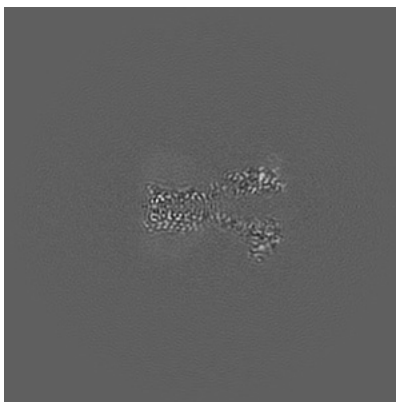
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

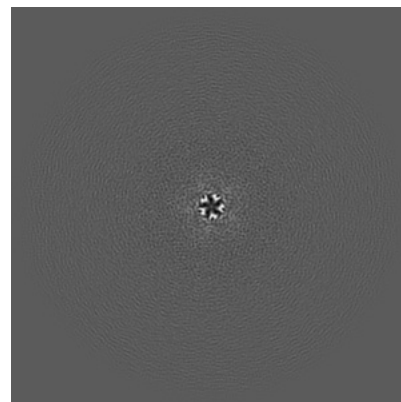
6.2.1 Primary map



X Index: 200

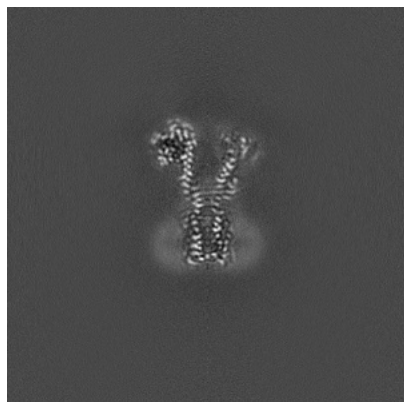


Y Index: 200

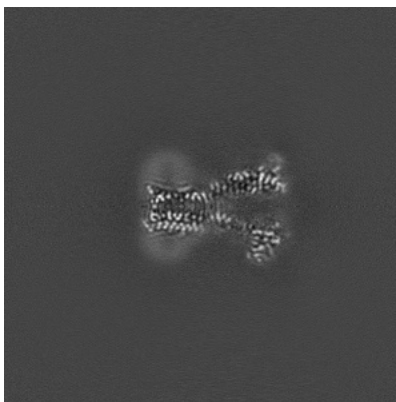


Z Index: 200

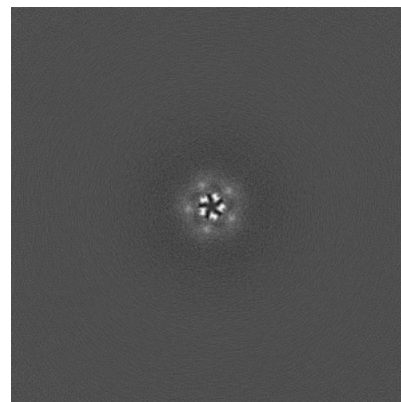
6.2.2 Raw map



X Index: 200



Y Index: 200

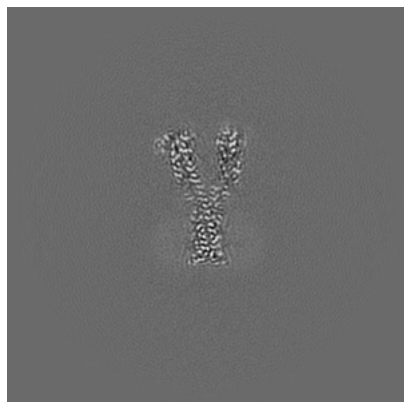


Z Index: 200

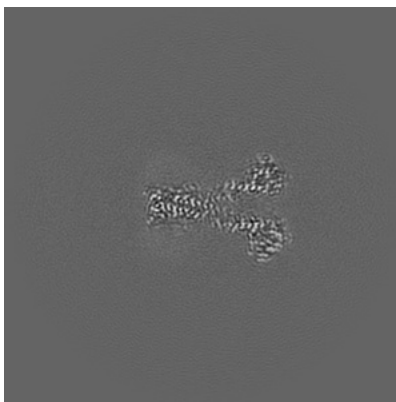
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

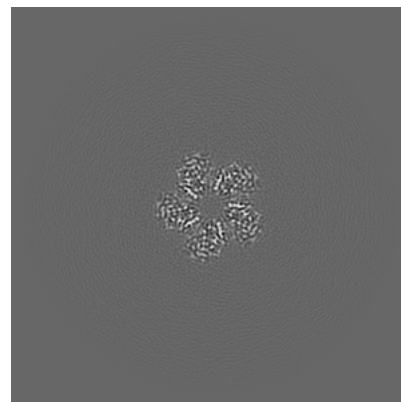
6.3.1 Primary map



X Index: 208

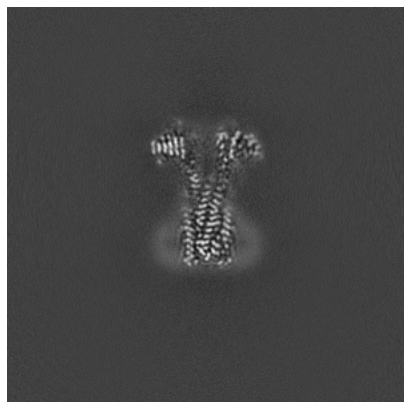


Y Index: 192

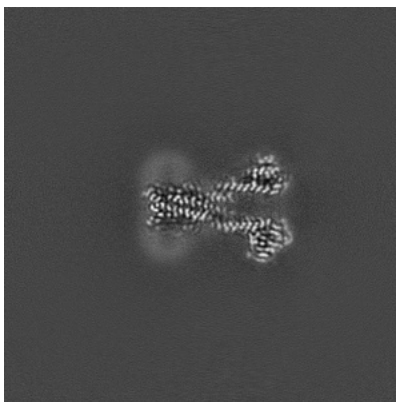


Z Index: 256

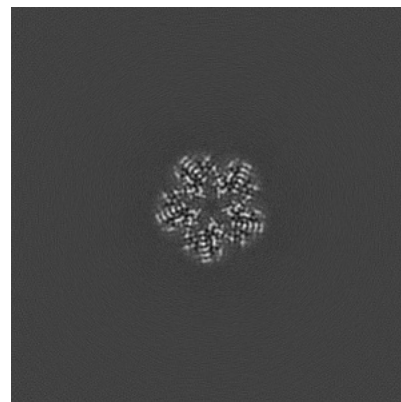
6.3.2 Raw map



X Index: 192



Y Index: 193

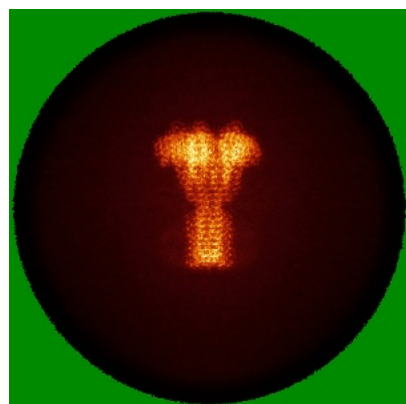


Z Index: 263

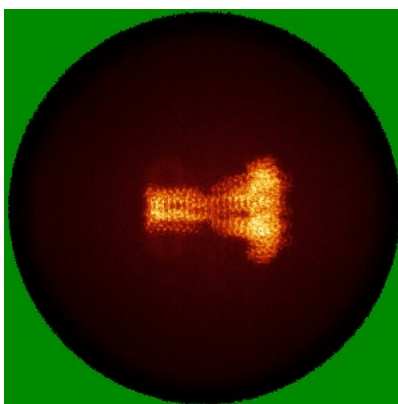
The images above show the largest variance slices of the map in three orthogonal directions.

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

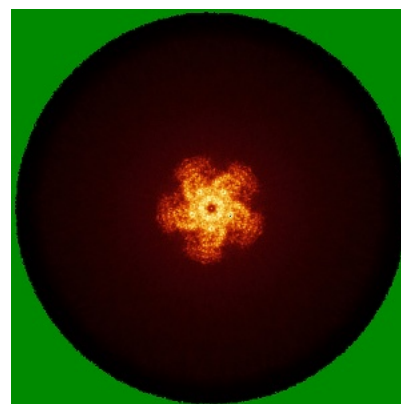
6.4.1 Primary map



X

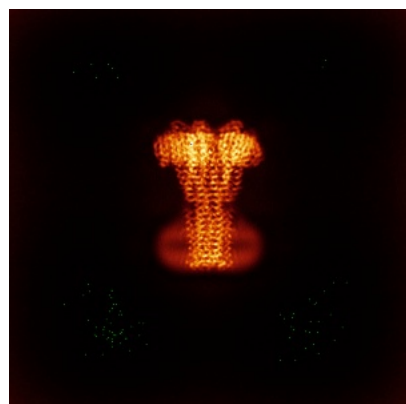


Y

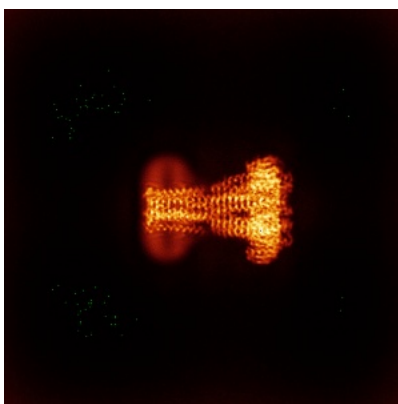


Z

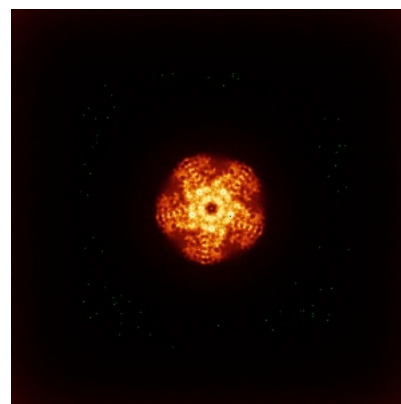
6.4.2 Raw map



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](#)

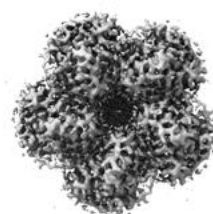
6.5.1 Primary map



X



Y



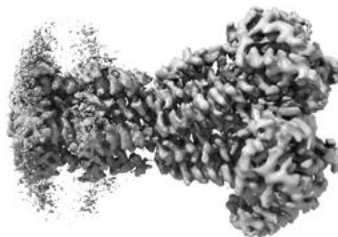
Z

The images above show the 3D surface view of the map at the recommended contour level 0.45. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

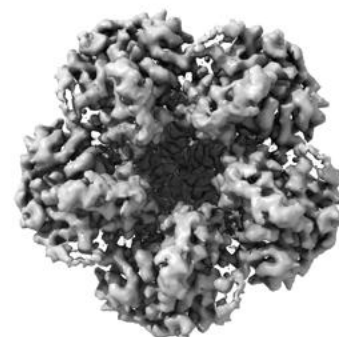
6.5.2 Raw map



X



Y



Z

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.

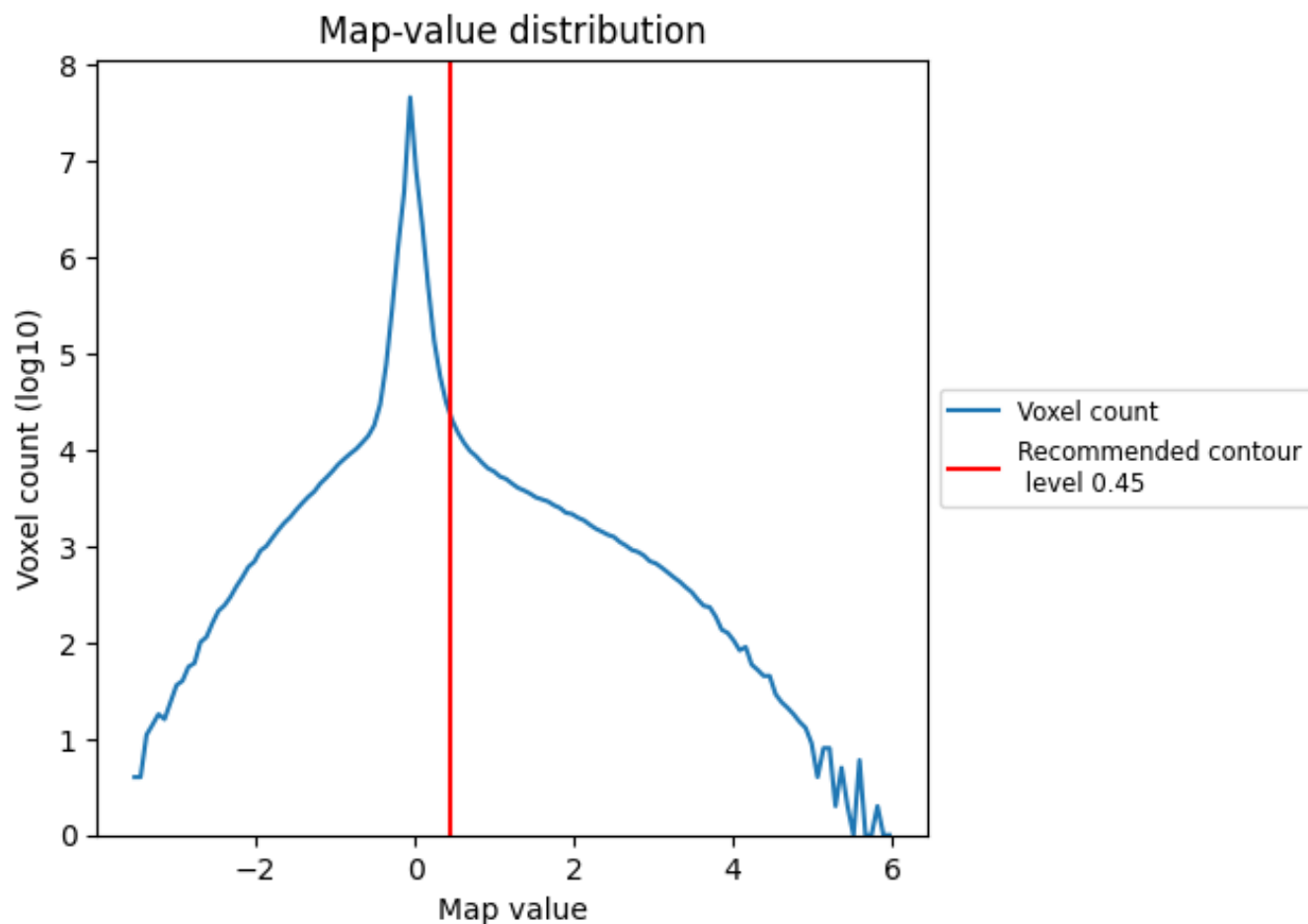
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

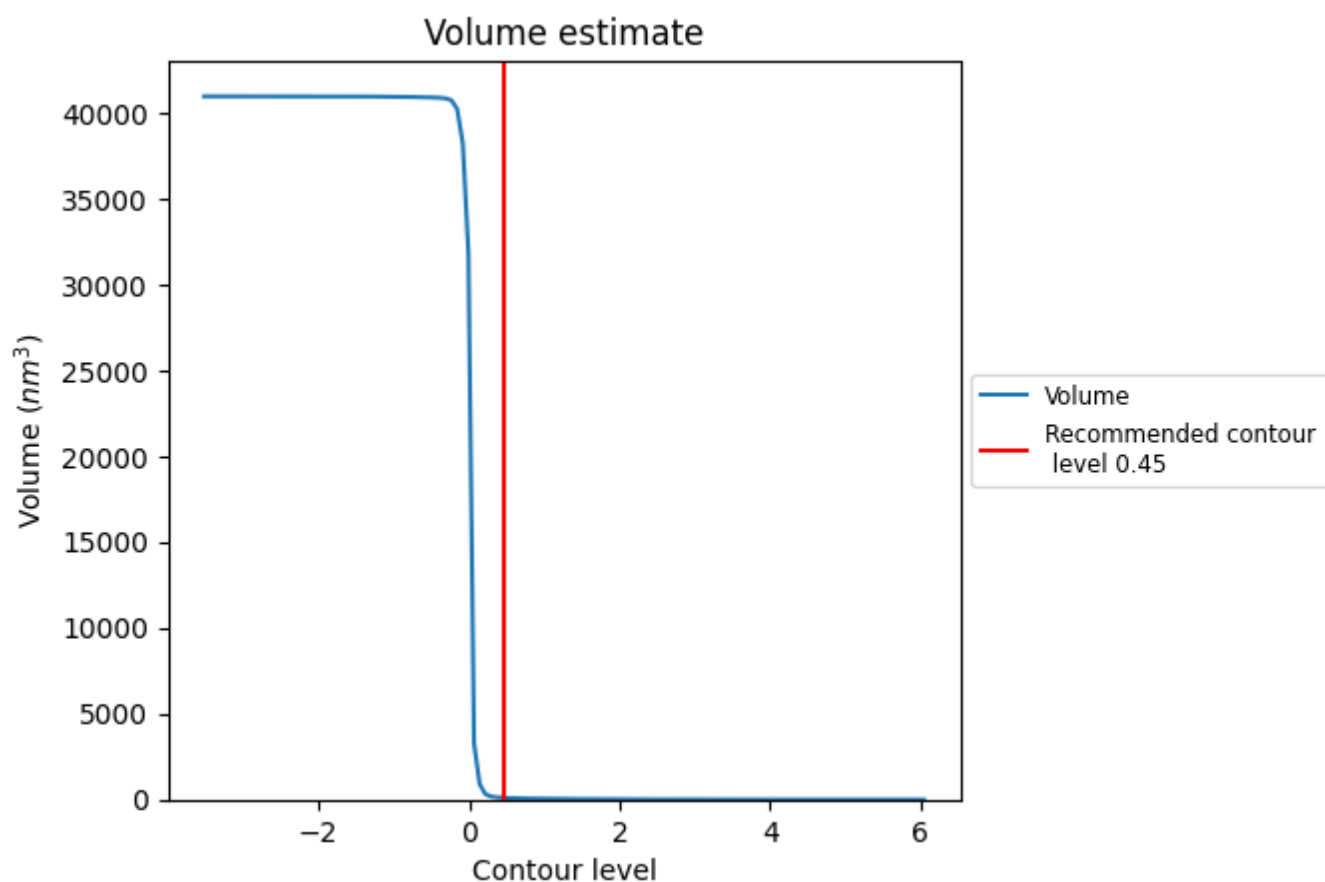
This section contains the results of statistical analysis of the map.

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.

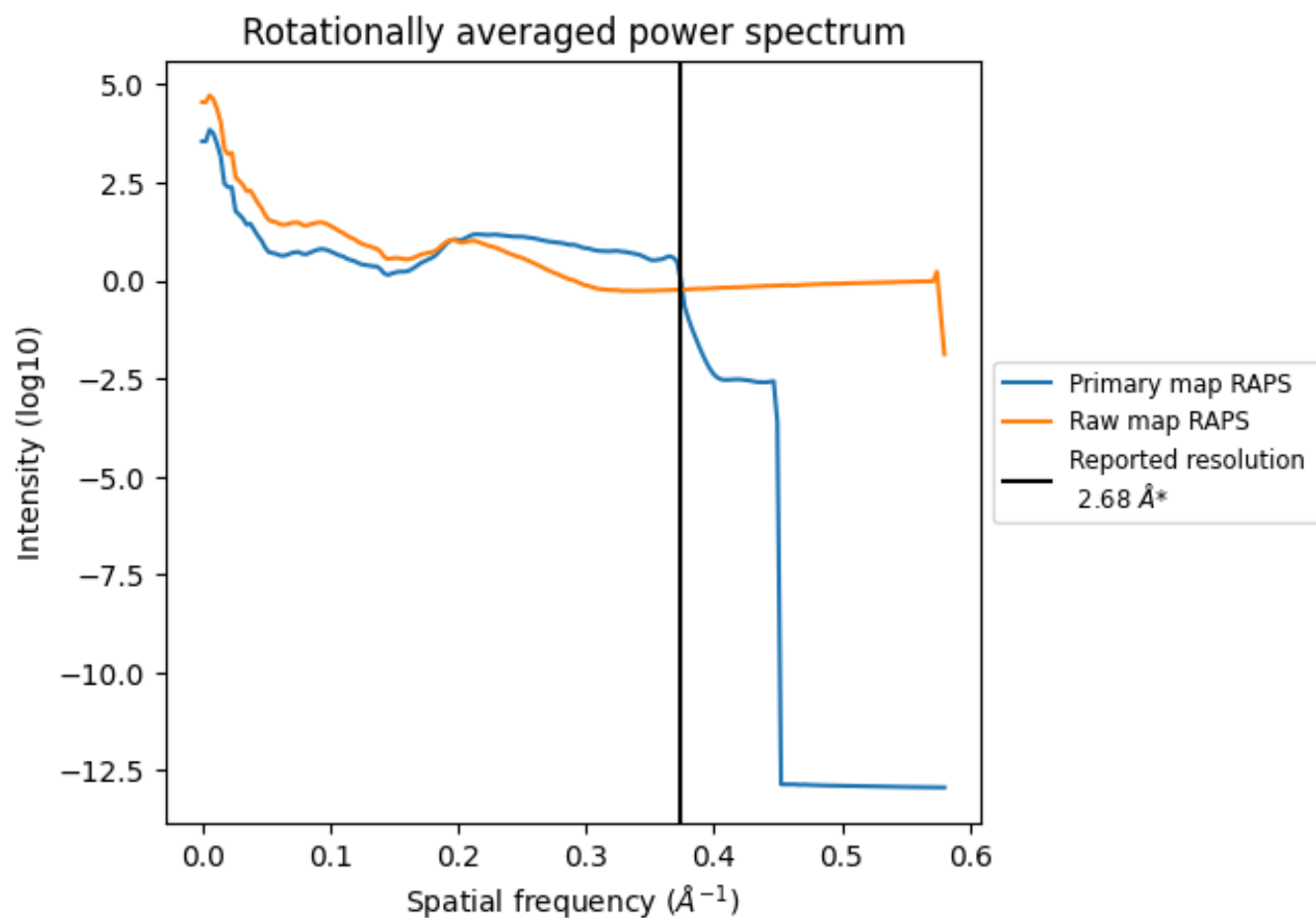
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 103 nm^3 ; this corresponds to an approximate mass of 93 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 ⓘ

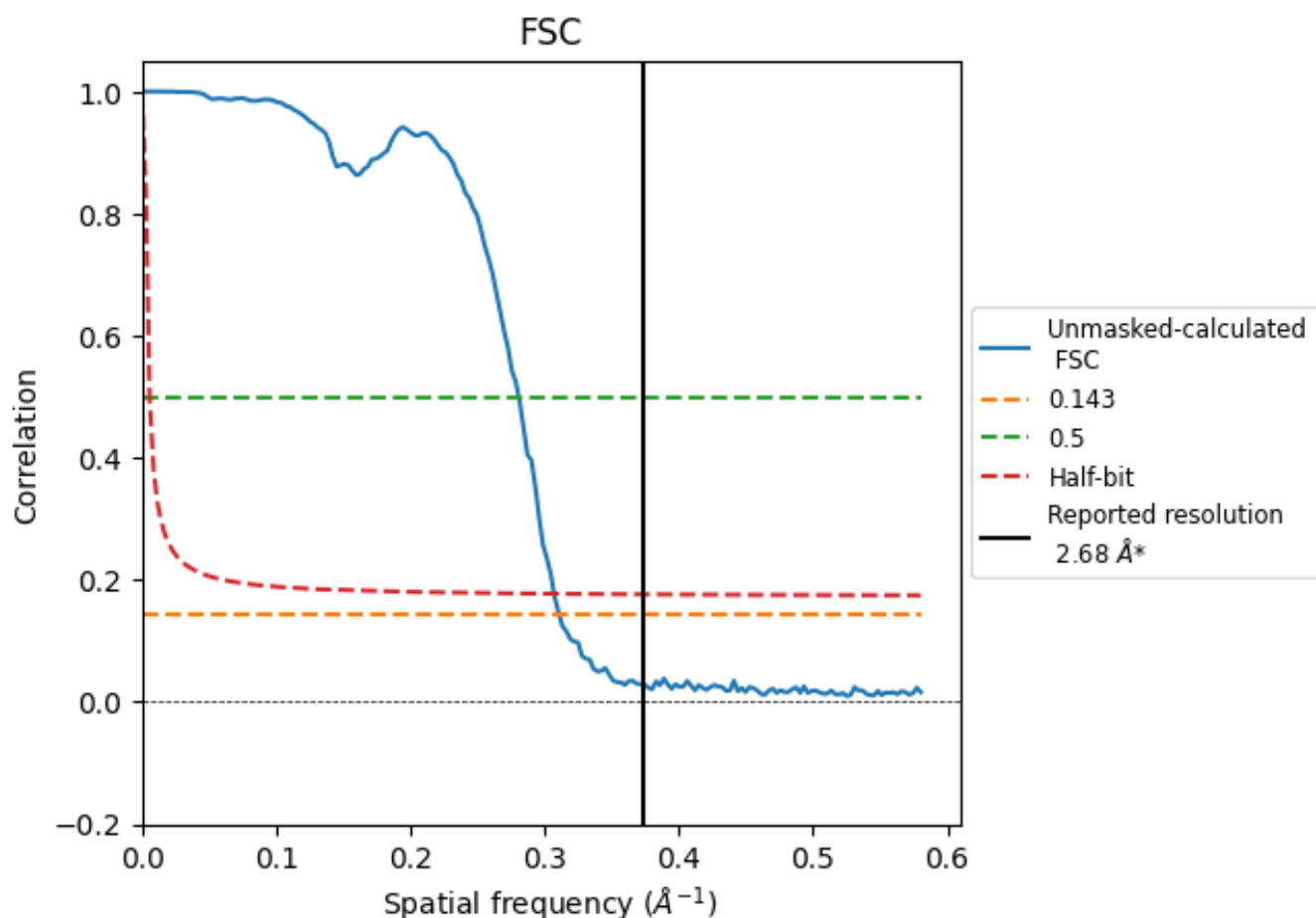


*Reported resolution corresponds to spatial frequency of 0.373 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.373 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.68	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.22	3.56	3.26

*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 3.22 differs from the reported value 2.68 by more than 10 %

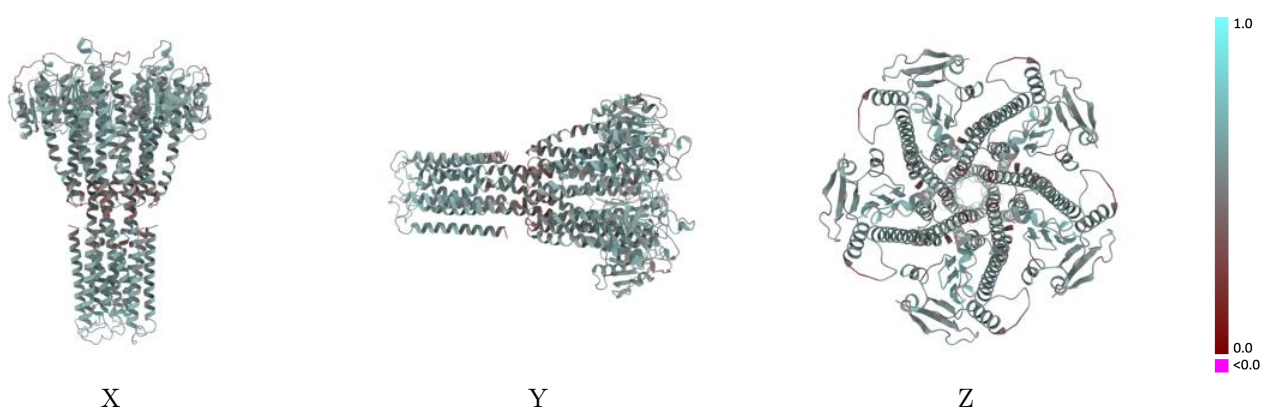
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-18256 and PDB model 8Q8P. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)

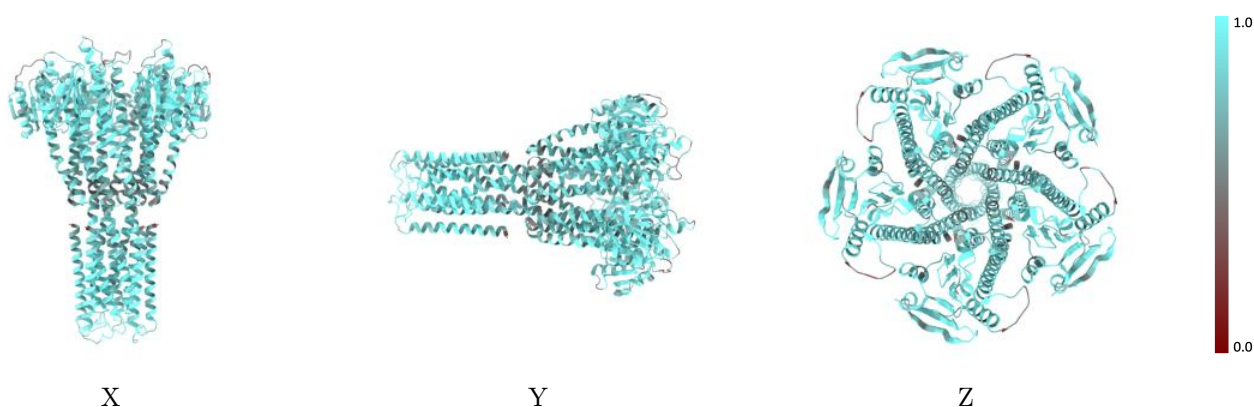
This section was not generated.

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



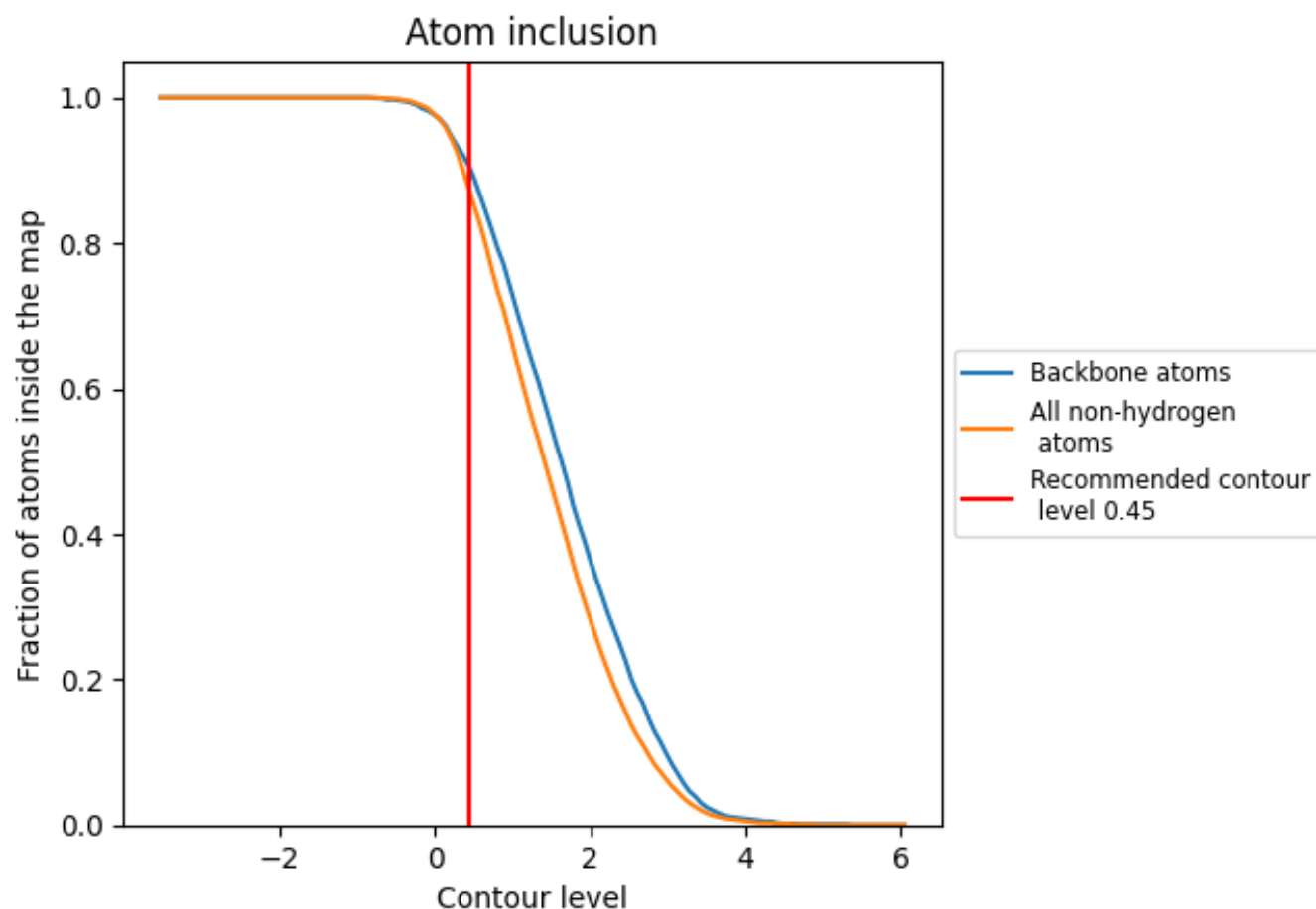
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.45).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 87% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.45) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8720	0.5500
A	0.8730	0.5490
B	0.8710	0.5490
C	0.8700	0.5510
D	0.8730	0.5520
E	0.8730	0.5490

