



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 06:48 AM UTC

PDB ID : 8TA3 / pdb_00008ta3
EMDB ID : EMD-41127
Title : Cryo-EM structure of the human CLC-2 chloride channel transmembrane domain Apo state with resolved N-terminal hairpin
Authors : Xu, M.; Neelands, T.; Powers, A.S.; Liu, Y.; Miller, S.; Pintilie, G.; Du Bois, J.; Dror, R.O.; Chiu, W.; Maduke, M.
Deposited on : 2023-06-26
Resolution : 2.46 Å (reported)
Based on initial model : .

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.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

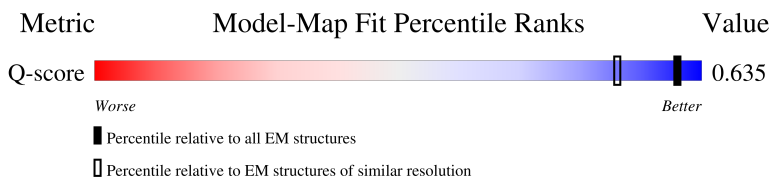
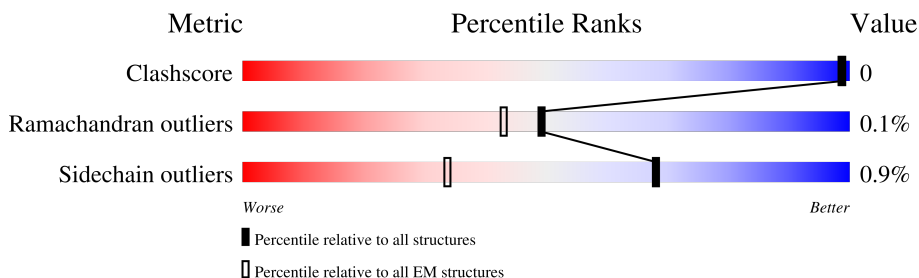
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.46 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	6014 (1.96 - 2.96)

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	869	
1	B	869	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14837 atoms, of which 7545 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 Chloride channel protein 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	470	Total	C	H	N	O	S	0	0
			7406	2409	3768	596	610	23		
1	B	472	Total	C	H	N	O	S	0	0
			7429	2416	3777	598	615	23		

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	668	SER	THR	variant	UNP P51788
A	?	-	THR	deletion	UNP P51788
A	?	-	HIS	deletion	UNP P51788
A	?	-	THR	deletion	UNP P51788
A	?	-	ILE	deletion	UNP P51788
A	?	-	PHE	deletion	UNP P51788
A	?	-	SER	deletion	UNP P51788
A	?	-	LEU	deletion	UNP P51788
A	?	-	LEU	deletion	UNP P51788
A	?	-	GLY	deletion	UNP P51788
A	?	-	VAL	deletion	UNP P51788
A	?	-	ASP	deletion	UNP P51788
A	?	-	HIS	deletion	UNP P51788
A	?	-	ALA	deletion	UNP P51788
A	?	-	TYR	deletion	UNP P51788
A	?	-	VAL	deletion	UNP P51788
A	?	-	THR	deletion	UNP P51788
A	?	-	SER	deletion	UNP P51788
A	?	-	ILE	deletion	UNP P51788
A	?	-	GLY	deletion	UNP P51788
A	?	-	ARG	deletion	UNP P51788
A	?	-	LEU	deletion	UNP P51788
A	?	-	ILE	deletion	UNP P51788
A	?	-	GLY	deletion	UNP P51788
A	?	-	ILE	deletion	UNP P51788
A	?	-	VAL	deletion	UNP P51788

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	THR	deletion	UNP P51788
A	?	-	LEU	deletion	UNP P51788
A	?	-	LYS	deletion	UNP P51788
A	?	-	GLU	deletion	UNP P51788
B	668	SER	THR	variant	UNP P51788
B	?	-	THR	deletion	UNP P51788
B	?	-	HIS	deletion	UNP P51788
B	?	-	THR	deletion	UNP P51788
B	?	-	ILE	deletion	UNP P51788
B	?	-	PHE	deletion	UNP P51788
B	?	-	SER	deletion	UNP P51788
B	?	-	LEU	deletion	UNP P51788
B	?	-	LEU	deletion	UNP P51788
B	?	-	GLY	deletion	UNP P51788
B	?	-	VAL	deletion	UNP P51788
B	?	-	ASP	deletion	UNP P51788
B	?	-	HIS	deletion	UNP P51788
B	?	-	ALA	deletion	UNP P51788
B	?	-	TYR	deletion	UNP P51788
B	?	-	VAL	deletion	UNP P51788
B	?	-	THR	deletion	UNP P51788
B	?	-	SER	deletion	UNP P51788
B	?	-	ILE	deletion	UNP P51788
B	?	-	GLY	deletion	UNP P51788
B	?	-	ARG	deletion	UNP P51788
B	?	-	LEU	deletion	UNP P51788
B	?	-	ILE	deletion	UNP P51788
B	?	-	GLY	deletion	UNP P51788
B	?	-	ILE	deletion	UNP P51788
B	?	-	VAL	deletion	UNP P51788
B	?	-	THR	deletion	UNP P51788
B	?	-	LEU	deletion	UNP P51788
B	?	-	LYS	deletion	UNP P51788
B	?	-	GLU	deletion	UNP P51788

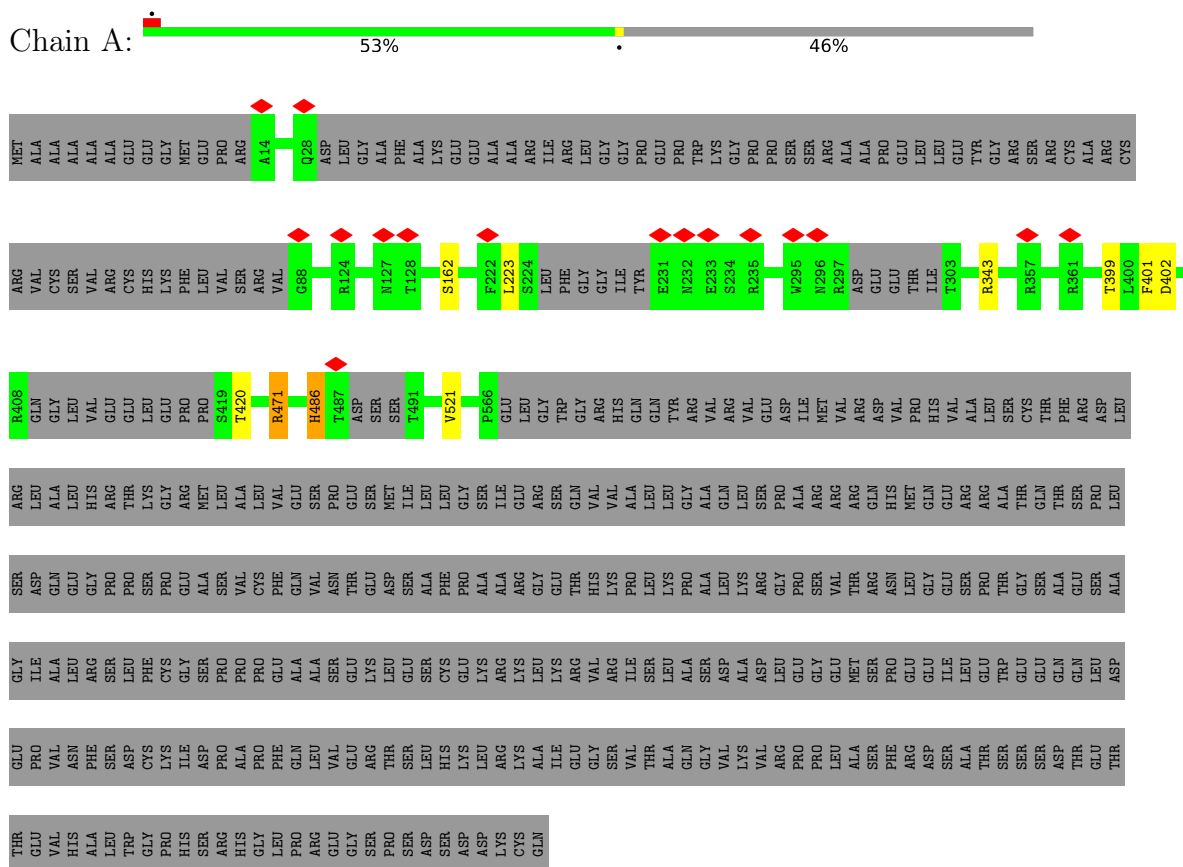
- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	AltConf
2	A	1	Total Cl 1 1	0
2	B	1	Total Cl 1 1	0

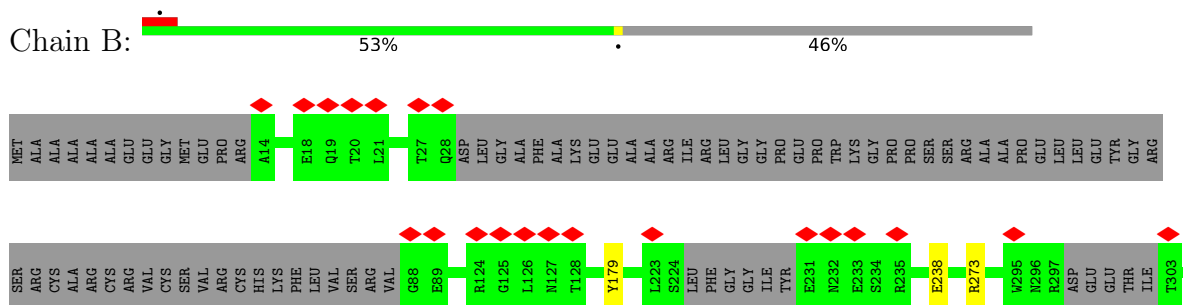
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Chloride channel protein 2



• Molecule 1: Chloride channel protein 2



R343	K353	T354	I355	N356	R357	M360	R361	K362	F401	D402	R408	G419	P426	R427	R428	A429	R471	H486	T487	D488	SER	S490	T491	V521	P566	GLU	LEU	GLY	TRP	GLY	ARG	HIS	GLN	GLN	TYR	ARG	VAL	ARG	VAL	GLU				
ASP	ILE	MET	VAL	ARG	ASP	VAL	PRO	HIS	THR	PHE	ARG	ASP	LEU	LEU	VAL	GLU	PRO	GLU	SER	MET	ILE	LEU	GLY	ILE	GLU	ARG	SER	GLN	VAL	VAL	ALA	LEU	GLY	ALA	GLN	GLN	TYR	ARG	VAL	ARG	VAL	GLU		
PRO	ALA	ARG	ARG	GLN	HIS	VAL	MET	PRO	GLN	THR	ALA	SER	GLN	SER	ASP	VAL	ASN	THR	GLU	ASP	SER	ILE	LEU	PHE	GLY	GLU	THR	HIS	VAL	LYS	PRO	LEU	LYS	PRO	ALA	ALA	GLN	GLN	TYR	ARG	VAL	ARG	VAL	GLU
GLY	PRO	SER	THR	VAL	ASN	GLY	LEU	GLY	SER	ALA	THR	CYS	GLN	THR	GLY	GLY	ASN	THR	GLU	ASP	SER	ILE	LEU	PHE	GLY	GLU	THR	HIS	VAL	LYS	PRO	LEU	LYS	PRO	ALA	ALA	GLN	GLN	TYR	ARG	VAL	ARG	VAL	GLU
LEU	GLU	GLY	MET	SER	PRO	ILE	GLU	GLY	GLU	ALA	ASP	GLY	ILE	PRO	GLU	ALA	SER	PRO	LYS	LEU	SER	CYS	GLY	LYS	LYS	LEU	ARG	GLY	VAL	ARG	ILE	SER	LEU	ALA	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
ARG	PRO	PRO	LEU	ALA	SER	THR	GLU	SER	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	2415222	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)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	8.553	Depositor
Minimum map value	-7.290	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.198	Depositor
Recommended contour level	0.8	Depositor
Map size (Å)	242.176, 242.176, 242.176	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.946, 0.946, 0.946	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: CL

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	0.80	0/3727	1.39	5/5067 (0.1%)
1	B	0.80	1/3741 (0.0%)	1.37	7/5086 (0.1%)
All	All	0.80	1/7468 (0.0%)	1.38	12/10153 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	426	PRO	CA-C	5.17	1.54	1.51

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	471	ARG	NE-CZ-NH2	8.13	126.52	119.20
1	A	471	ARG	NE-CZ-NH2	7.96	126.37	119.20
1	B	402	ASP	CA-CB-CG	6.37	118.97	112.60
1	B	426	PRO	N-CA-CB	6.04	106.58	103.19
1	B	401	PHE	CA-CB-CG	5.84	119.64	113.80
1	A	471	ARG	NE-CZ-NH1	-5.84	115.66	121.50
1	A	401	PHE	CA-CB-CG	5.64	119.44	113.80
1	A	471	ARG	CD-NE-CZ	5.62	132.27	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	343	ARG	NE-CZ-NH2	5.50	124.15	119.20
1	A	402	ASP	CA-CB-CG	5.47	118.07	112.60
1	B	273	ARG	NE-CZ-NH2	5.13	123.81	119.20
1	B	471	ARG	CD-NE-CZ	5.07	131.50	124.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	343	ARG	Sidechain
1	B	179	TYR	Sidechain

5.2 Too-close contacts ⓘ

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	3638	3768	3762	2	0
1	B	3652	3777	3771	0	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
All	All	7292	7545	7533	2	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 0.

All (2) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:THR:HG22	1:A:420:THR:HA	1.95	0.48
1:A:486:HIS:H	1:A:486:HIS:CD2	2.37	0.42

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	458/869 (53%)	443 (97%)	14 (3%)	1 (0%)	43	54
1	B	460/869 (53%)	451 (98%)	9 (2%)	0	100	100
All	All	918/1738 (53%)	894 (97%)	23 (2%)	1 (0%)	49	61

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	162	SER

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	381/716 (53%)	377 (99%)	4 (1%)	68	77
1	B	383/716 (54%)	380 (99%)	3 (1%)	73	83
All	All	764/1432 (53%)	757 (99%)	7 (1%)	68	81

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	223	LEU
1	A	471	ARG
1	A	486	HIS
1	A	521	VAL
1	B	238	GLU

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Mol	Chain	Res	Type
1	B	486	HIS
1	B	521	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	133	GLN
1	A	319	GLN
1	A	342	ASN
1	A	356	ASN
1	A	542	ASN
1	B	356	ASN
1	B	422	GLN
1	B	425	ASN
1	B	542	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](#)

Of 2 ligands modelled in this entry, 2 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

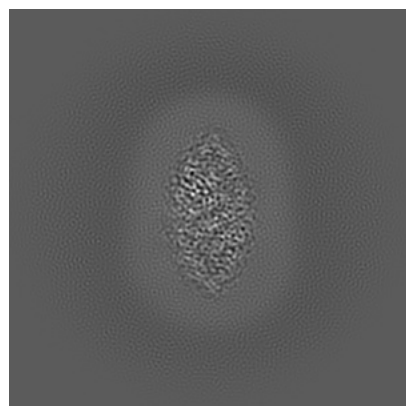
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41127. These allow visual inspection of the internal detail of the map and identification of artifacts.

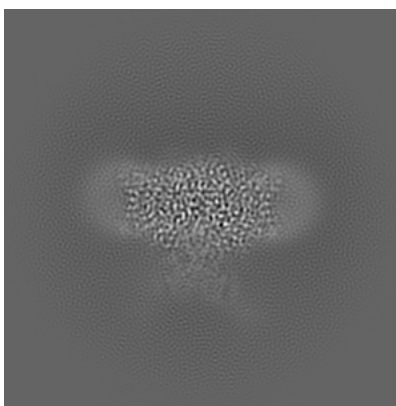
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

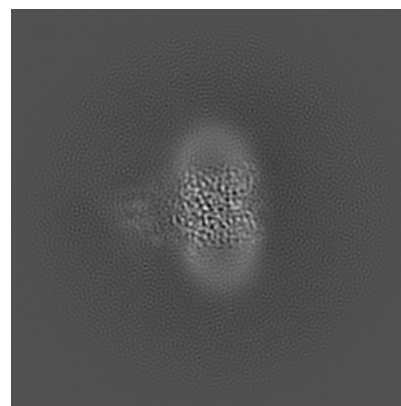
6.1.1 Primary map



X

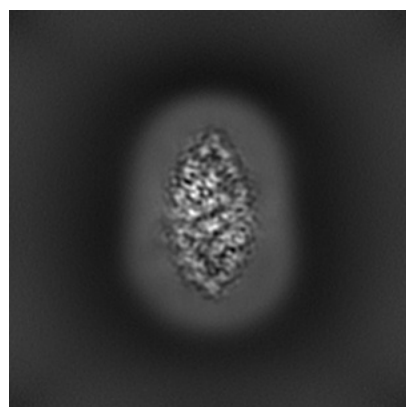


Y

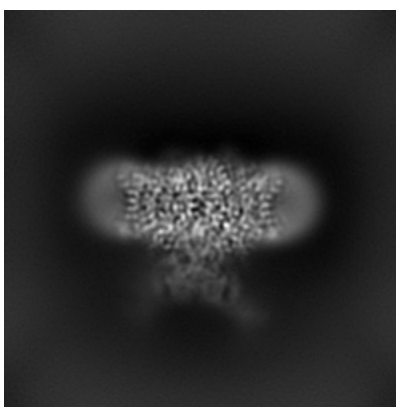


Z

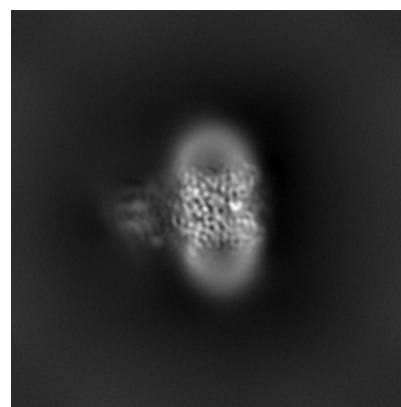
6.1.2 Raw map



X



Y

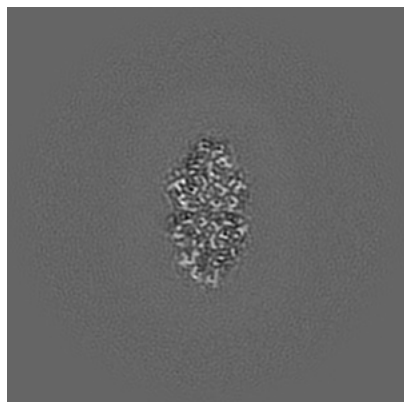


Z

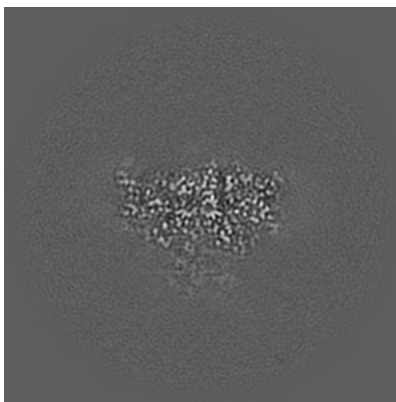
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

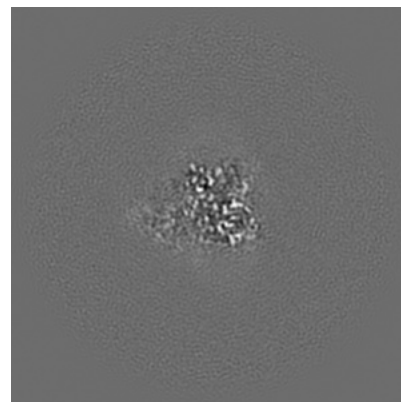
6.2.1 Primary map



X Index: 128

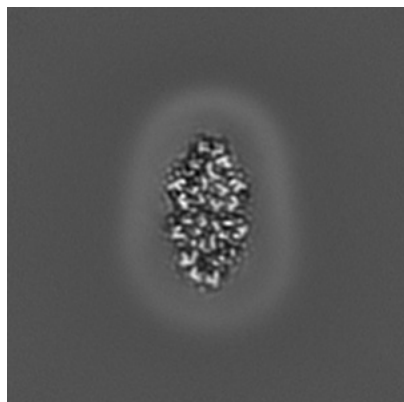


Y Index: 128

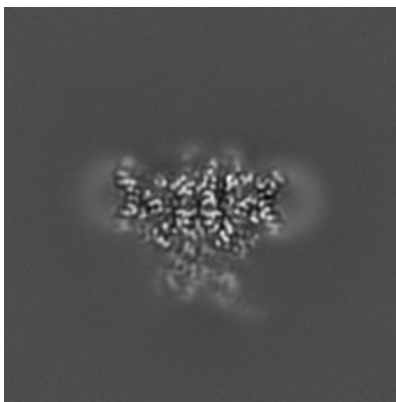


Z Index: 128

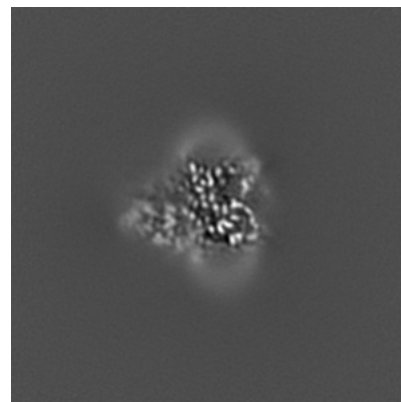
6.2.2 Raw map



X Index: 128



Y Index: 128

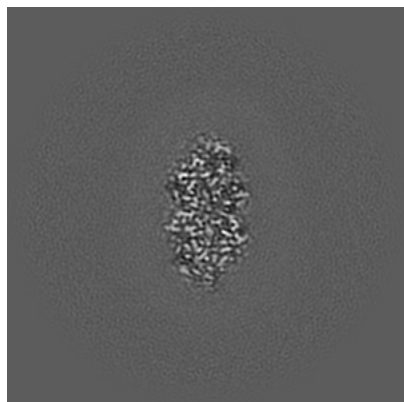


Z Index: 128

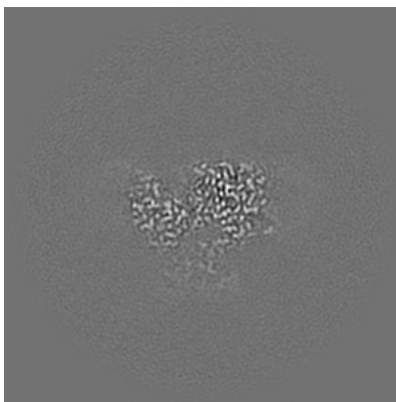
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

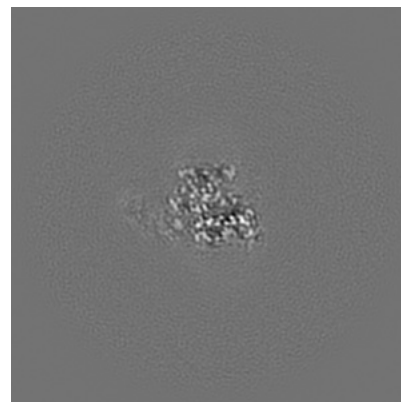
6.3.1 Primary map



X Index: 125

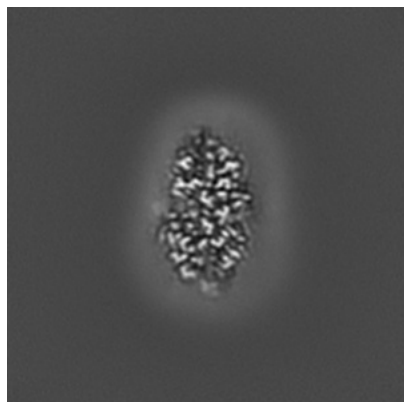


Y Index: 119

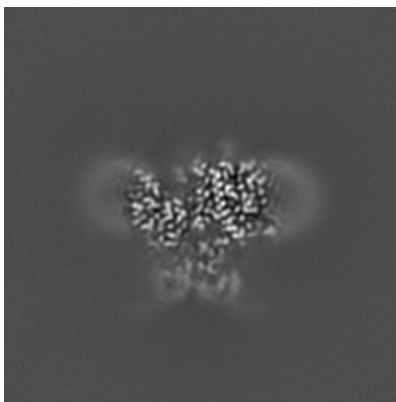


Z Index: 137

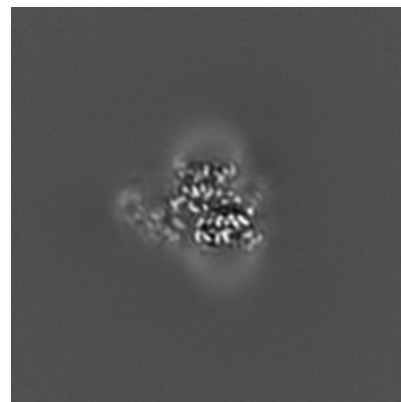
6.3.2 Raw map



X Index: 118



Y Index: 119

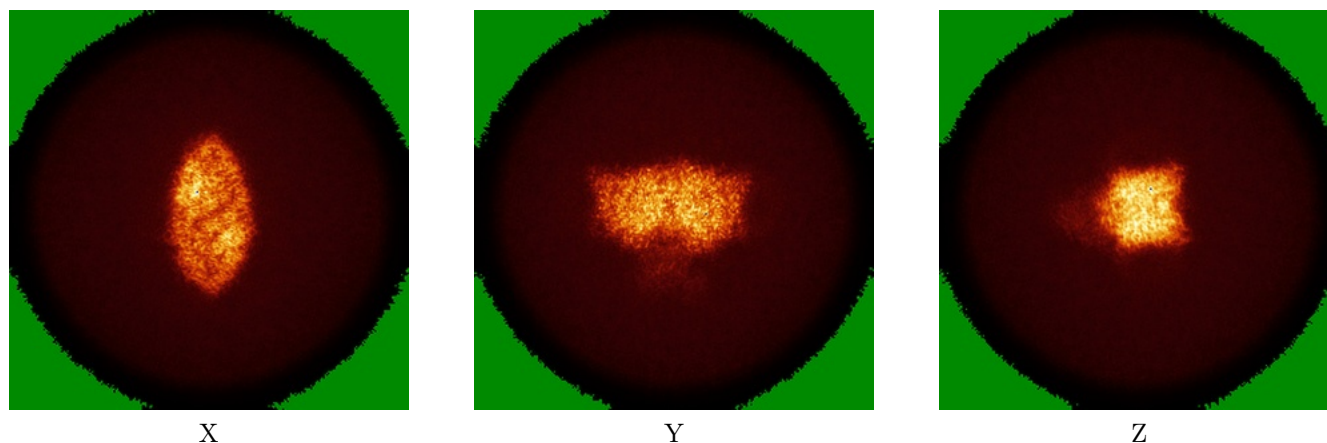


Z Index: 136

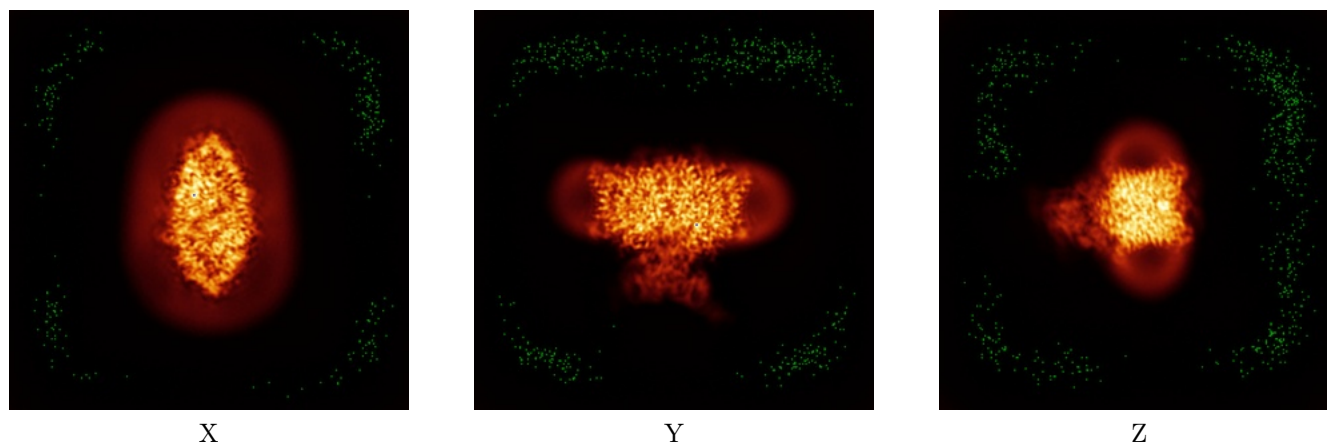
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

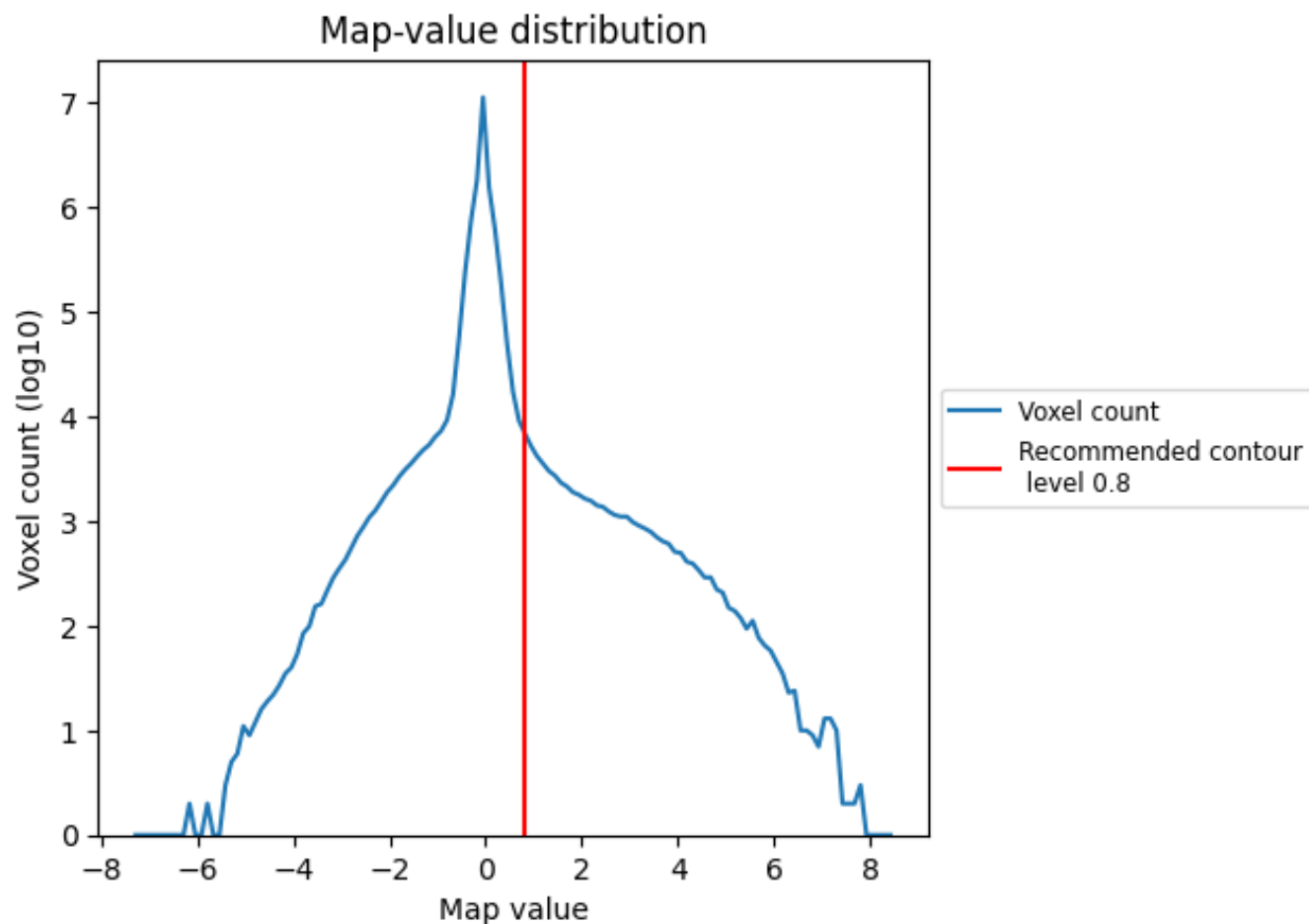
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

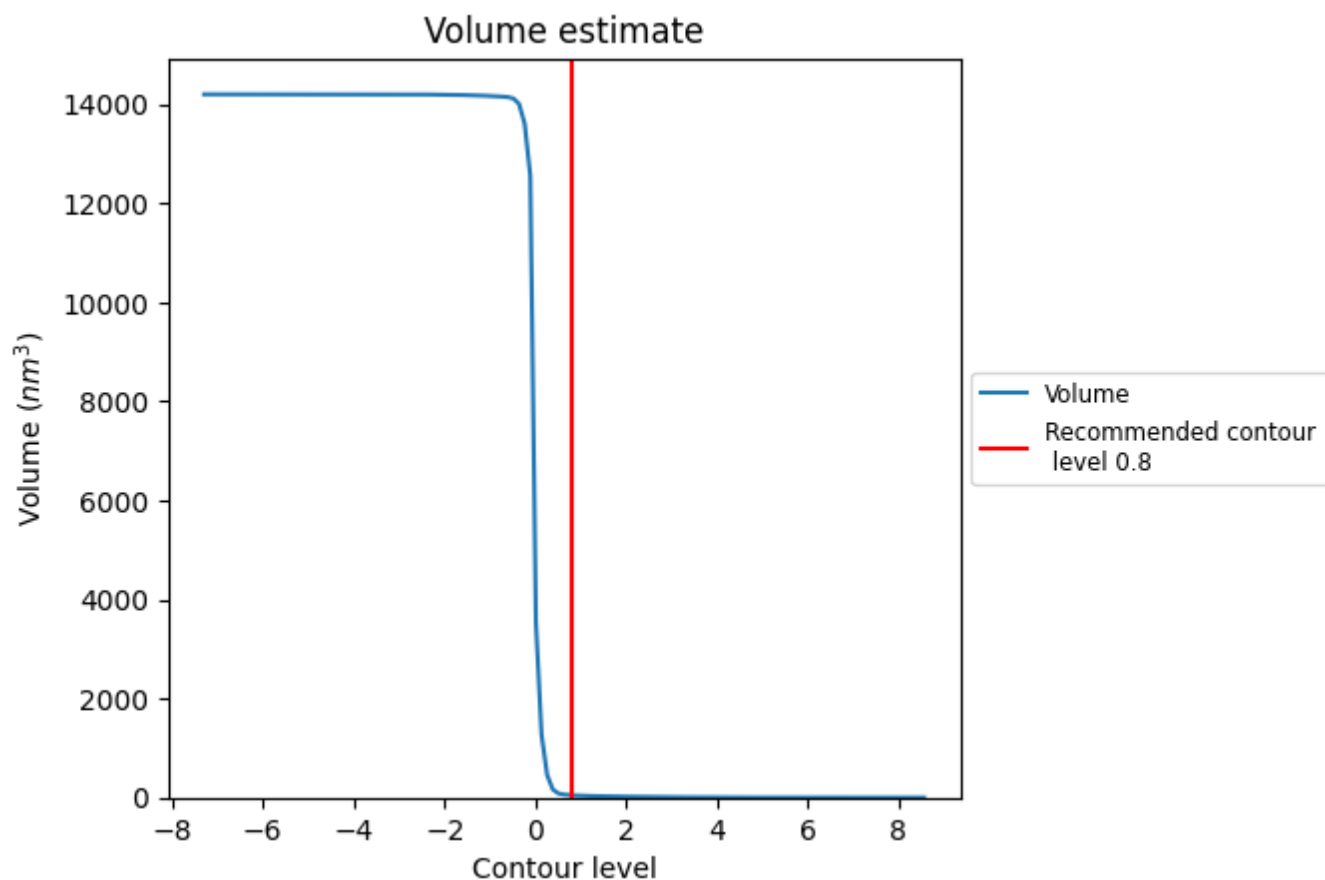
This section contains the results of statistical analysis of the map.

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.

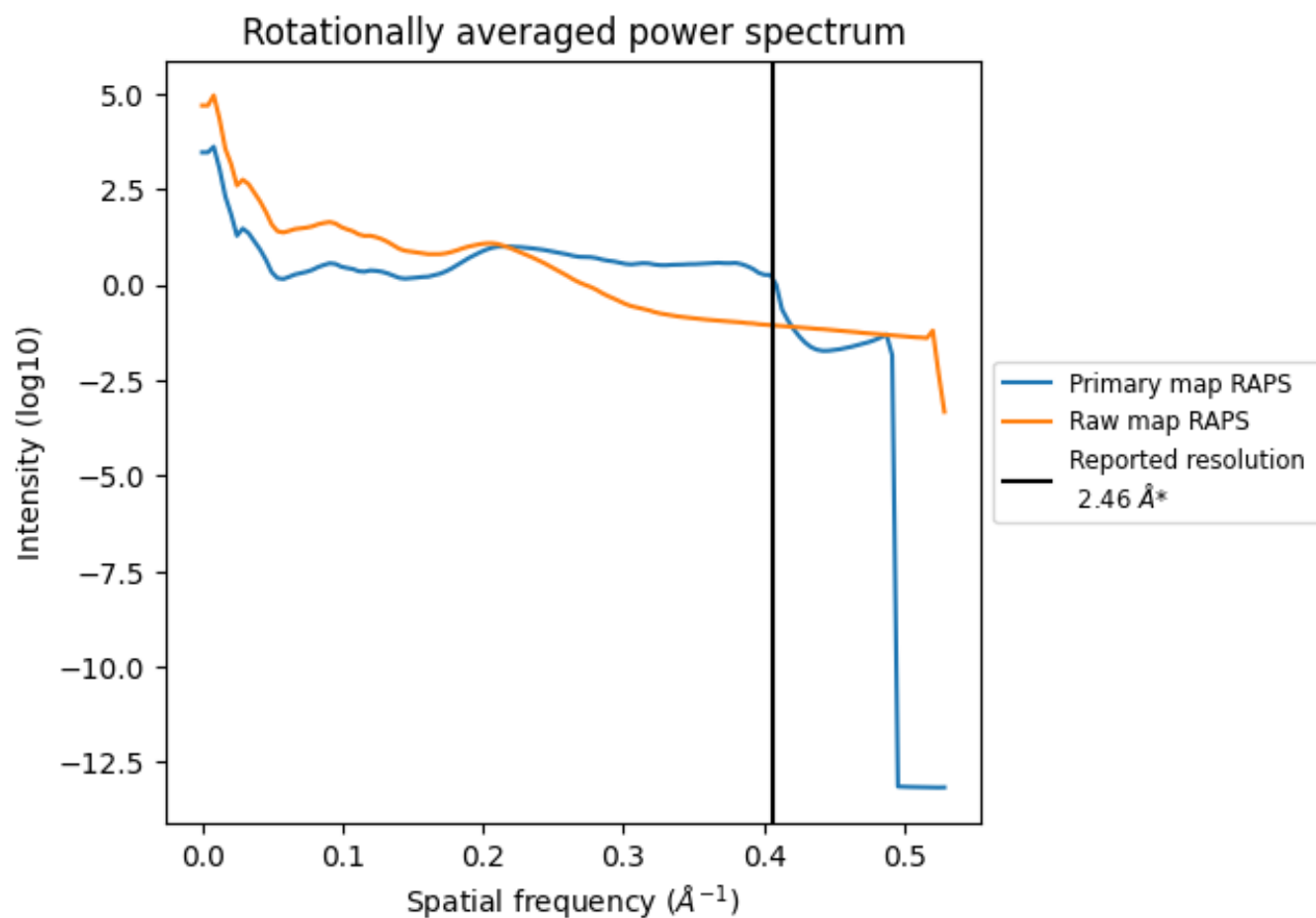
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 47 nm^3 ; this corresponds to an approximate mass of 42 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 ⓘ

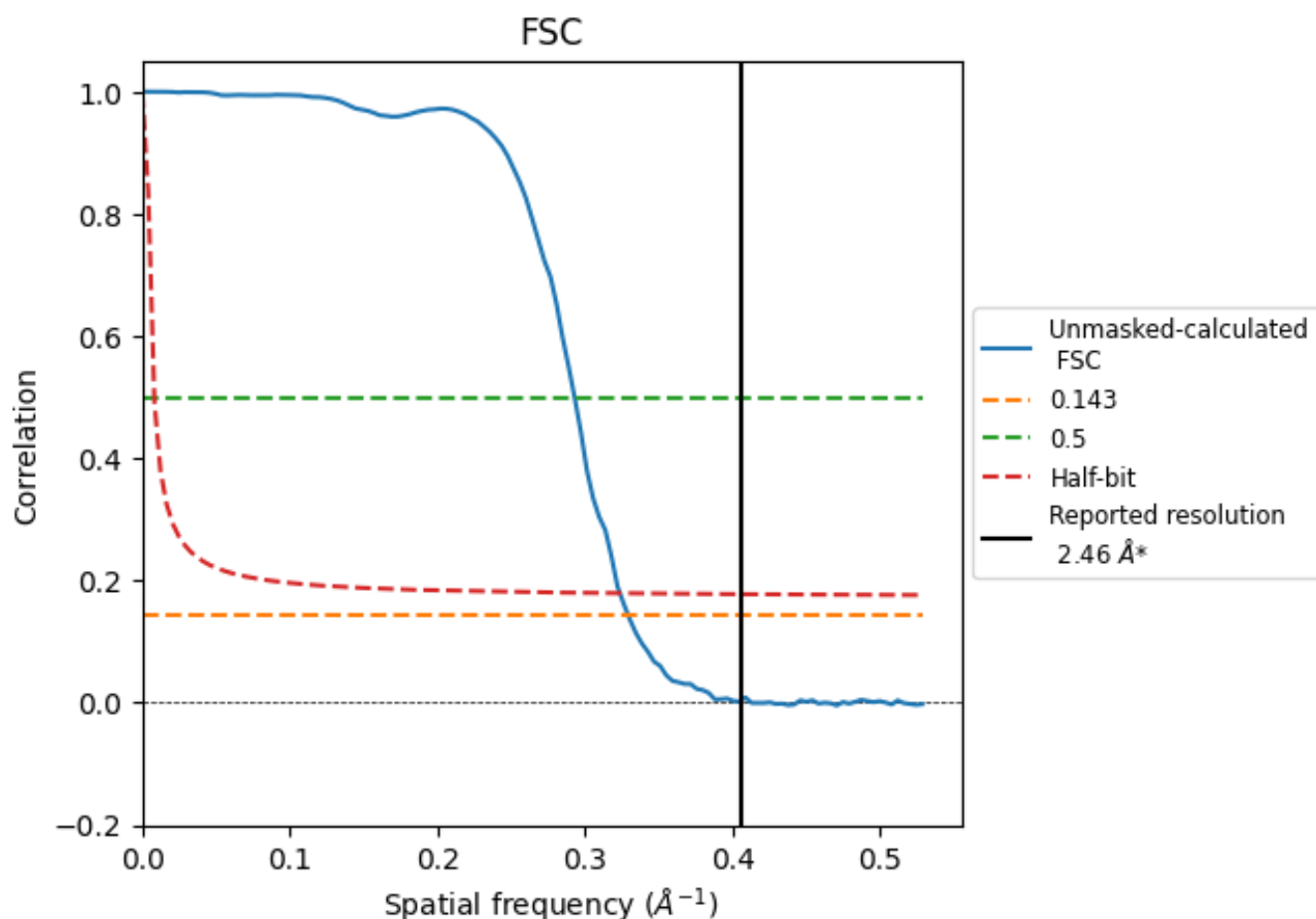


*Reported resolution corresponds to spatial frequency of 0.407 $\text{\AA}^{-1}$

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 $0.407 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

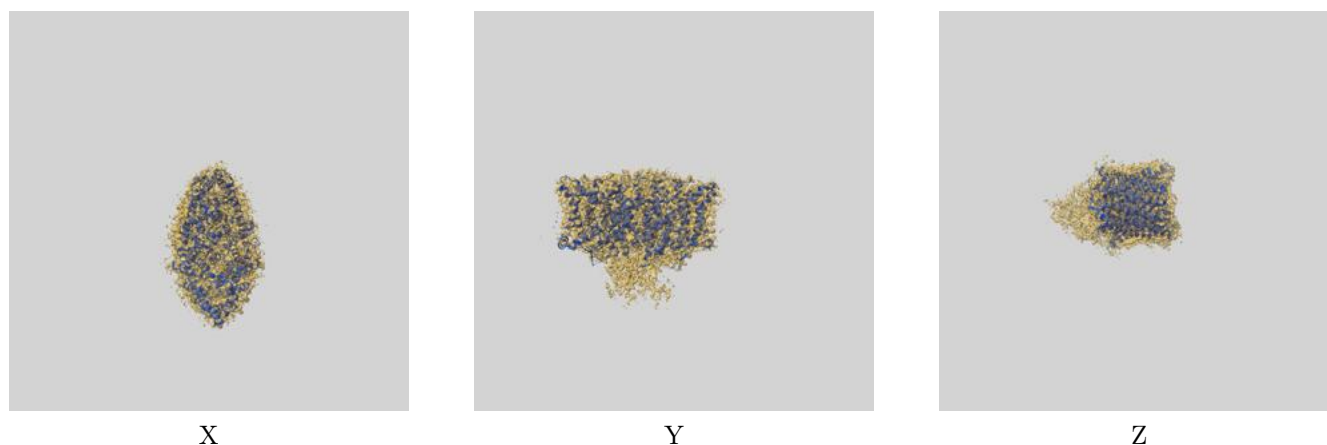
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.46	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.04	3.41	3.09

*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 3.04 differs from the reported value 2.46 by more than 10 %

9 Map-model fit [i](#)

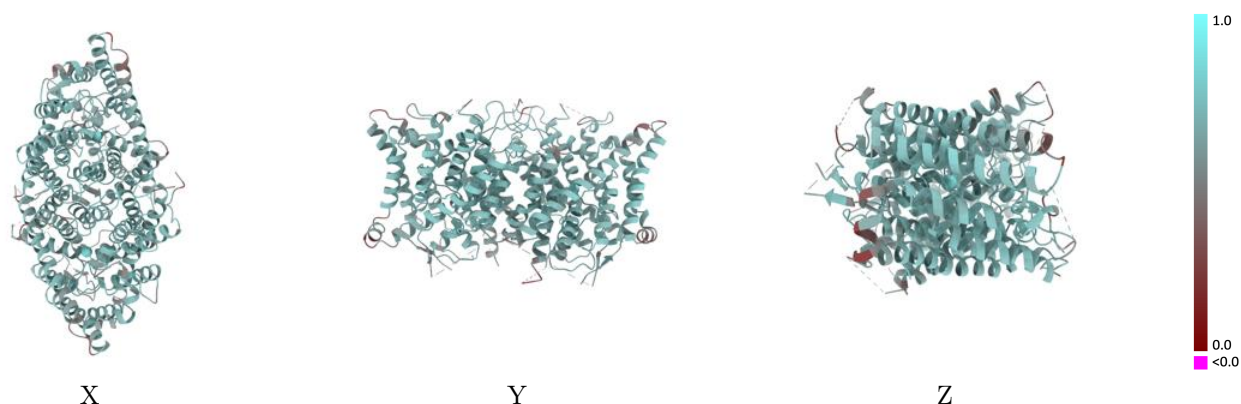
This section contains information regarding the fit between EMDB map EMD-41127 and PDB model 8TA3. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



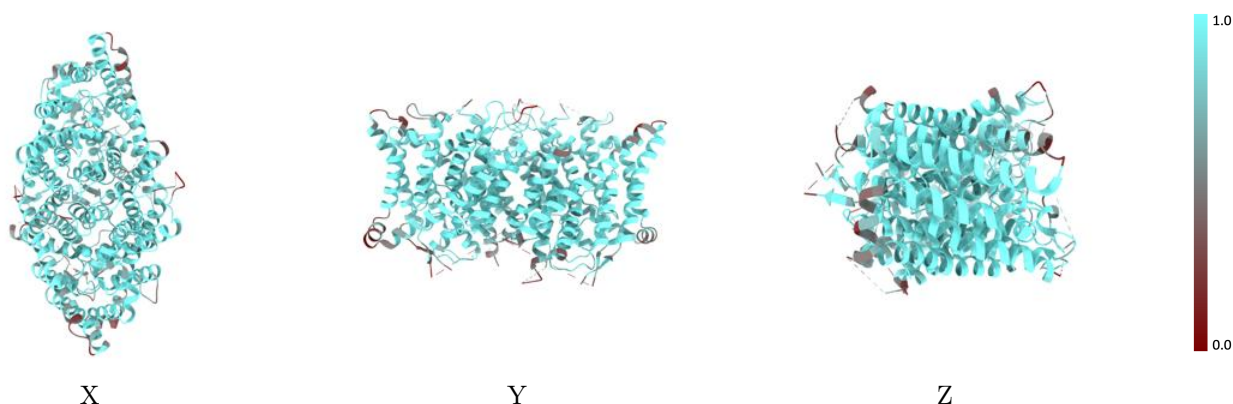
The images above show the 3D surface view of the map at the recommended contour level 0.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



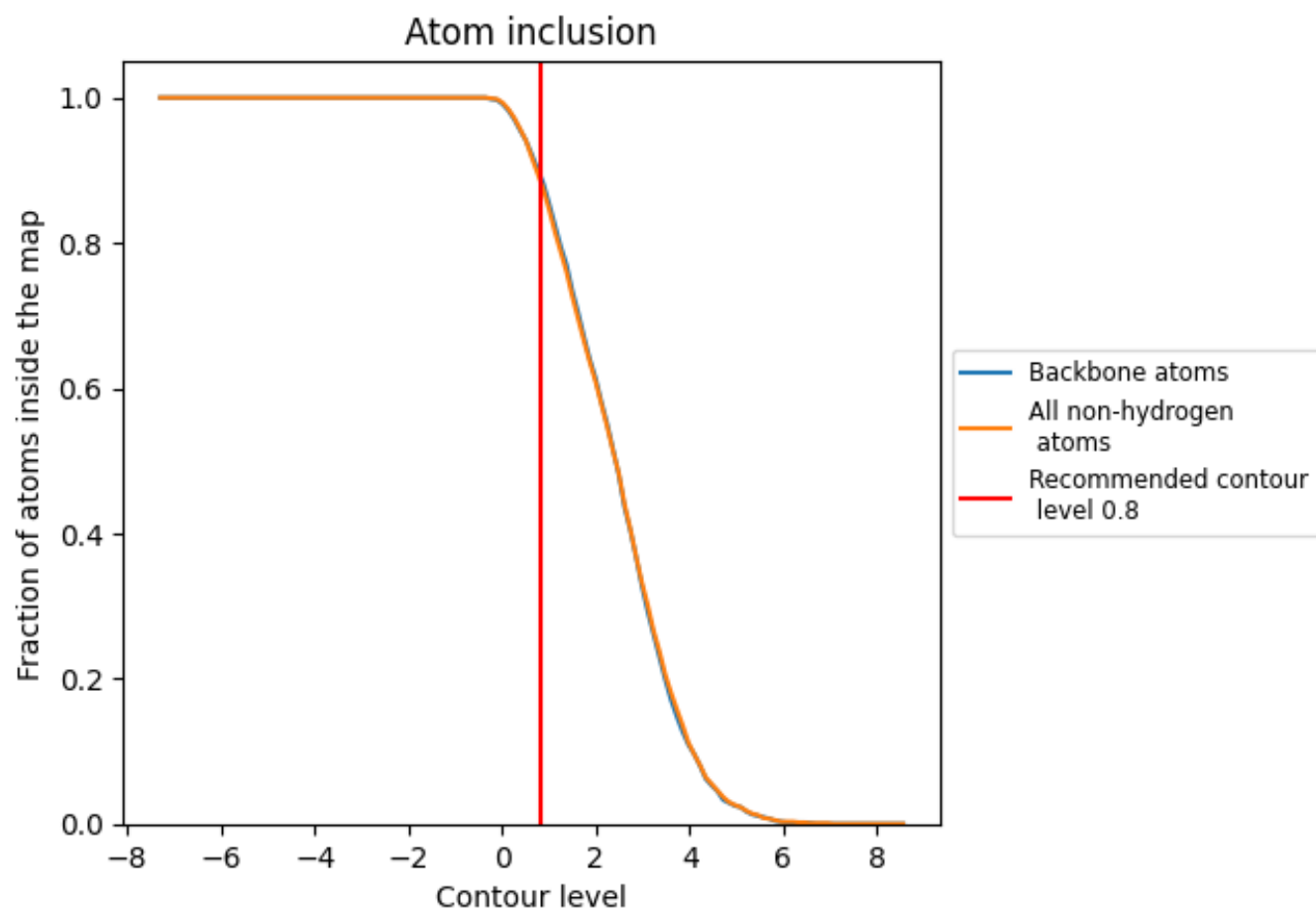
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.8).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 89% 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 (0.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8880	0.6350
A	0.9070	0.6400
B	0.8710	0.6300

