wwPDB EM Validation Summary Report

Oct 19, 2026 – 02:55 PM JST

PDB ID	:	9XCO / pdb_00009xco
EMDB ID	:	EMD-66738
Title	:	Cryo-EM structure of HalT (C23A mutant), a peptidase-domain containing ABC Transporter, in an apo state
Authors	:	Gan, B.K.; Luo, M.
Deposited on	:	2025-10-26
Resolution	:	3.77 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:

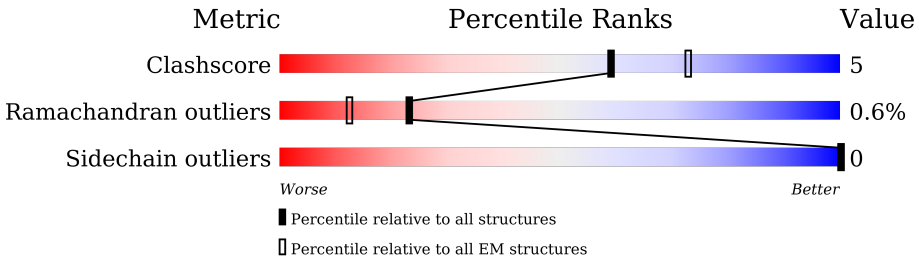
EMDB validation analysis	:	0.0.1.dev133
MolProbity	:	4-5-2 with Phenix2.2
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

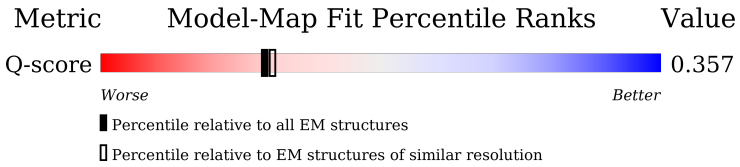
1 Overall quality at a glance

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

The reported resolution of this entry is 3.77 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	10146 (3.27 - 4.27)

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 <=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	724	27% 85% 13%
1	B	724	28% 85% 12%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 11239 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 Lantibiotic mersacidin transporter system.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	709	Total	C	N	O	S	0	0
			5628	3644	952	1005	27		
1	B	709	Total	C	N	O	S	0	0
			5611	3632	952	1000	27		

There are 2 discrepancies between the modelled and reference sequences:

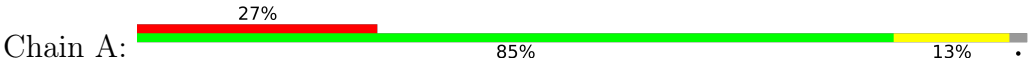
Chain	Residue	Modelled	Actual	Comment	Reference
A	23	ALA	CYS	engineered mutation	UNP Q9KFM8
B	23	ALA	CYS	engineered mutation	UNP Q9KFM8

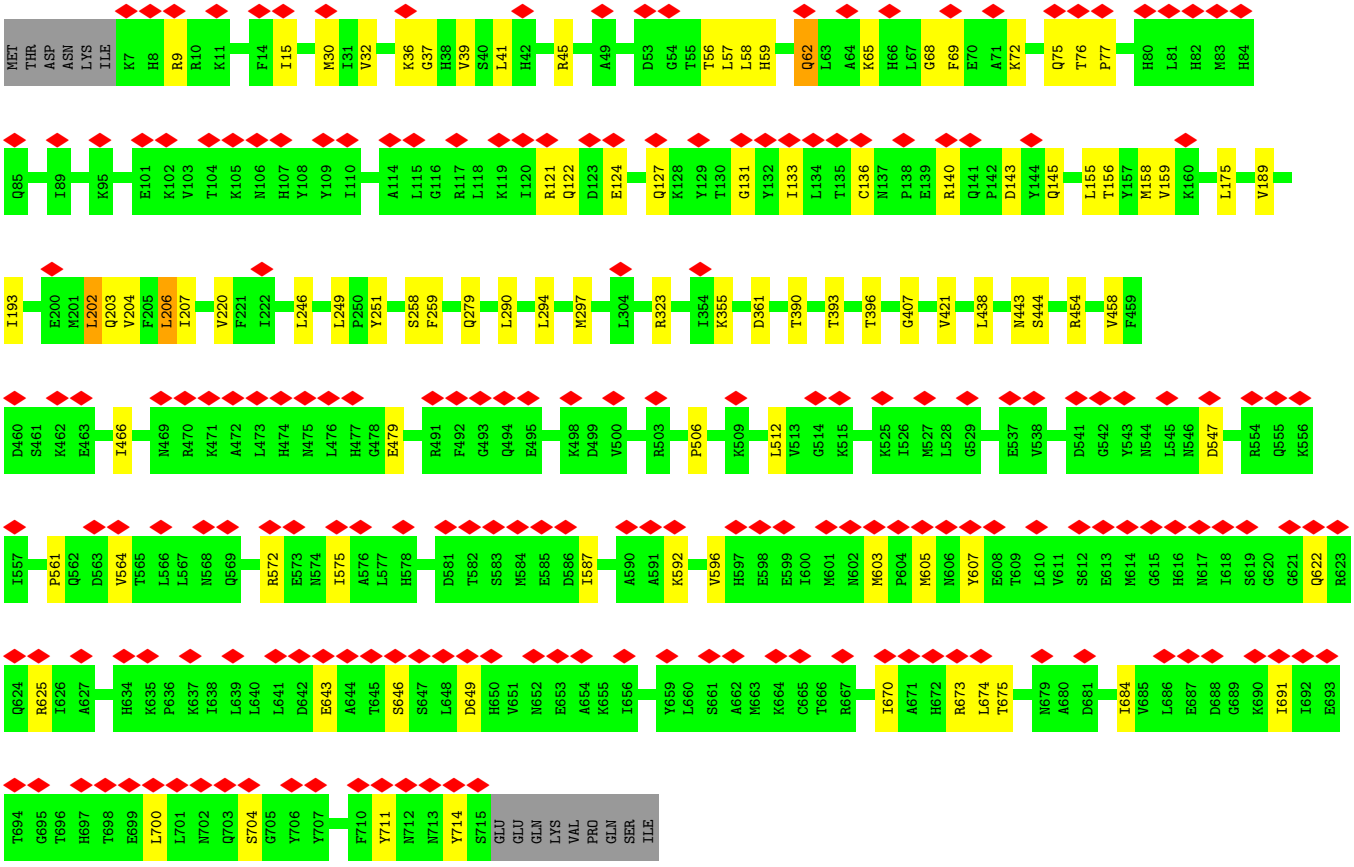
3 Residue-property plots (i)

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: Lantibiotic mersacidin transporter system

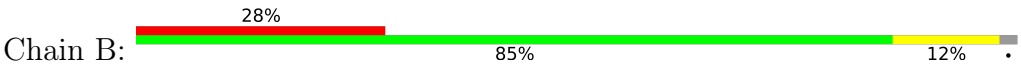
Chain A:

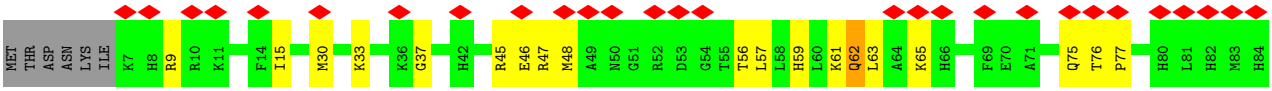


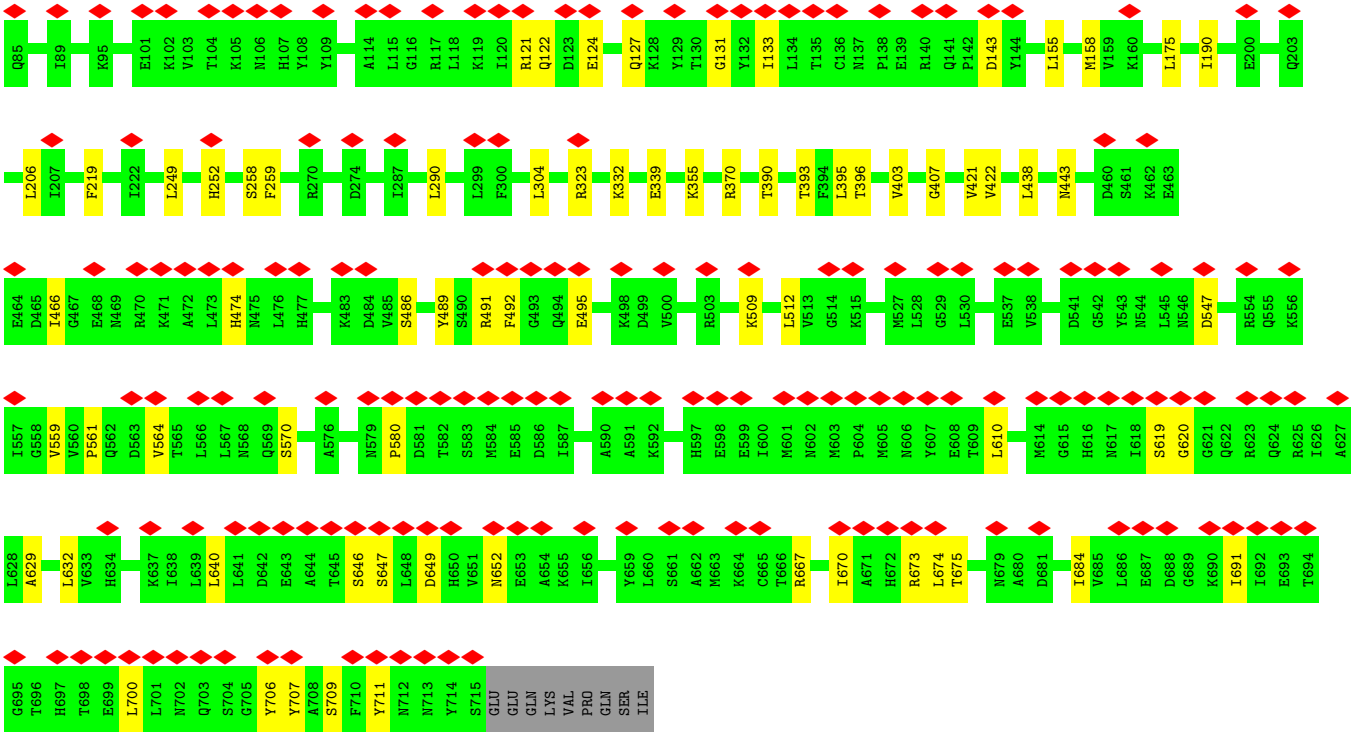


• Molecule 1: Lantibiotic mersacidin transporter system

Chain B:






Q85 I89 K95 E101 K102 V103 T104 K105 N106 H107 Y108 Y109 A114 L115 G116 R117 L118 K119 I120 R121 Q122 D123 E124 Q127 K128 Y129 T130 G131 Y132 I133 L134 T135 C136 N137 P138 E139 R140 Q141 P142 D143 Y144 L155 M158 V159 K160 L175 I190 E200 Q203
L206 I207 F219 T222 L249 H252 S258 F259 R270 D274 I287 L290 L299 F300 L304 R323 K332 E339 K355 R370 T390 T393 F394 L395 T396 V403 G407 V421 V422 L438 N443 D460 S461 K462 E463
E464 D465 I466 G467 E468 N469 R470 K471 A472 L473 H474 N475 L476 H477 K483 D484 V485 S486 Y489 S490 R491 F492 G493 Q494 E495 K498 D499 V500 R503 K509 L512 V513 G514 K515 M527 L528 G529 L530 E537 V538 D541 G542 Y543 N544 L545 N546 D547 R554 Q555 K556
I557 G558 V559 V560 P561 Q562 D563 V564 T565 L566 L567 N568 Q569 S570 A576 N579 P580 D581 T582 S583 M584 E585 D586 I587 A590 A591 K592 H597 E598 E599 I600 M601 N602 M603 P604 M605 N606 Y607 E608 T609 L610 M614 G615 H616 N617 I618 S619 G620 G621 Q622 R623 Q624 R625 I626 A627
L628 A629 L632 V633 H634 K637 I638 L639 L640 L641 D642 E643 A644 T645 S646 S647 L648 D649 H650 V651 N652 E653 A654 K655 I656 Y659 L660 S661 A662 M663 K664 C665 T666 R667 I670 A671 H672 R673 L674 T675 N679 A680 D681 I684 V685 L686 E687 D688 G689 K690 I691 I692 E693 T694
G695 T696 H697 T698 E699 L700 L701 N702 Q703 S704 G705 Y706 Y707 A708 S709 F710 Y711 N712 N713 Y714 S715 GLU GLU GLN LYS VAL PRO GLN SER ILE

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	51230	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 ($e^-/Å^2$)	47	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.618	Depositor
Minimum map value	-1.447	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.064	Depositor
Recommended contour level	0.499	Depositor
Map size (Å)	282.88, 282.88, 282.88	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.105, 1.105, 1.105	Depositor

5 Model quality

5.1 Standard geometry

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	0.25	0/5742	0.66	4/7776 (0.1%)
1	B	0.25	0/5724	0.65	1/7751 (0.0%)
All	All	0.25	0/11466	0.65	5/15527 (0.0%)

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

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	603	MET	CA-CB-CG	6.55	127.20	114.10
1	A	62	GLN	N-CA-CB	6.12	119.73	110.30
1	B	62	GLN	N-CA-CB	5.44	119.26	110.40
1	A	45	ARG	CA-C-N	5.18	131.43	121.54
1	A	45	ARG	C-N-CA	5.18	131.43	121.54

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	605	MET	Peptide

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	5628	0	5739	56	0
1	B	5611	0	5697	52	0
All	All	11239	0	11436	105	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 5.

The worst 5 of 105 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:57:LEU:HD12	1:B:133:ILE:HG21	1.80	0.63
1:A:56:THR:H	1:A:59:HIS:HD2	1.48	0.60
1:A:57:LEU:HD12	1:A:133:ILE:HG21	1.85	0.58
1:A:75:GLN:HG3	1:A:76:THR:HG23	1.84	0.58
1:B:75:GLN:HG3	1:B:76:THR:HG23	1.84	0.58

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	707/724 (98%)	646 (91%)	57 (8%)	4 (1%)	21	53
1	B	707/724 (98%)	634 (90%)	69 (10%)	4 (1%)	21	53
All	All	1414/1448 (98%)	1280 (90%)	126 (9%)	8 (1%)	23	53

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	203	GLN
1	A	206	LEU
1	B	580	PRO
1	A	202	LEU
1	B	206	LEU

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	609/640 (95%)	609 (100%)	0	100	100
1	B	601/640 (94%)	601 (100%)	0	100	100
All	All	1210/1280 (94%)	1210 (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 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	20	GLN
1	B	248	ASN
1	B	409	HIS
1	B	75	GLN
1	A	440	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

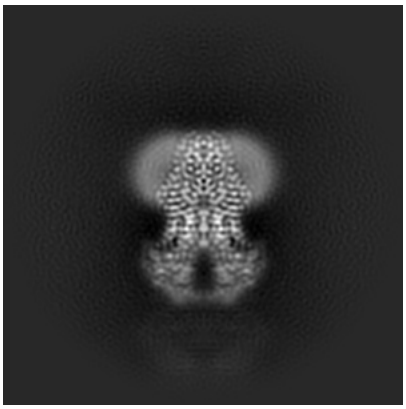
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-66738. These allow visual inspection of the internal detail of the map and identification of artifacts.

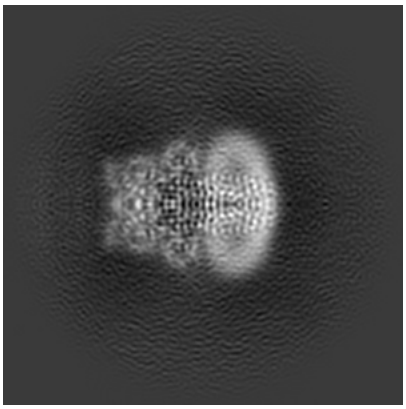
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

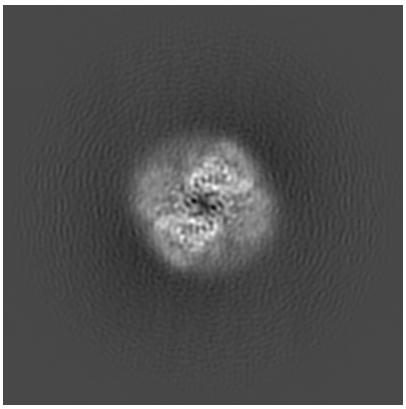
6.1.1 Primary map



X

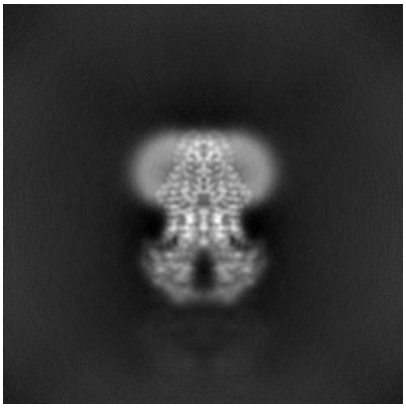


Y

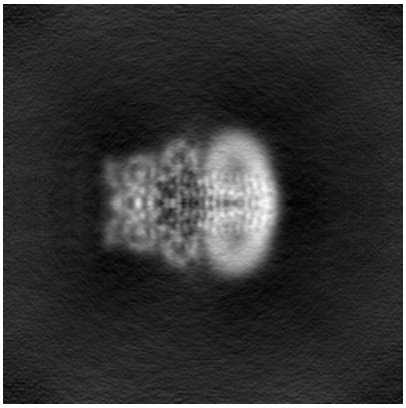


Z

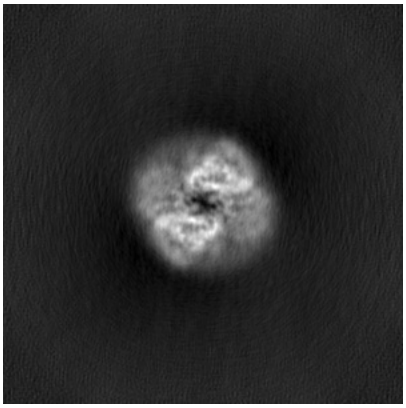
6.1.2 Raw map



X



Y

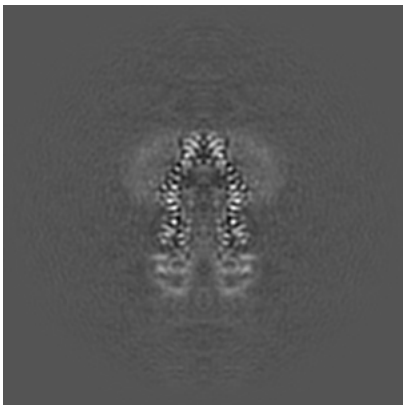


Z

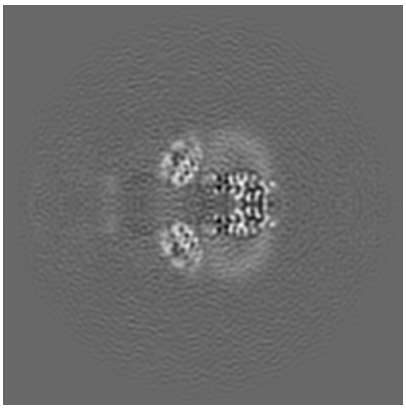
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

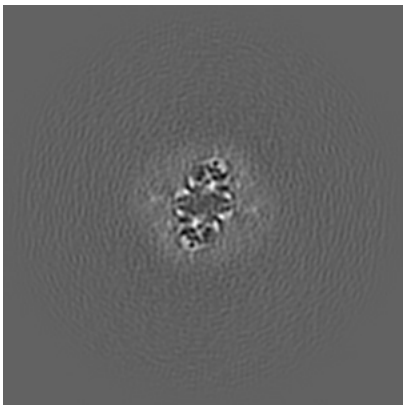
6.2.1 Primary map



X Index: 128

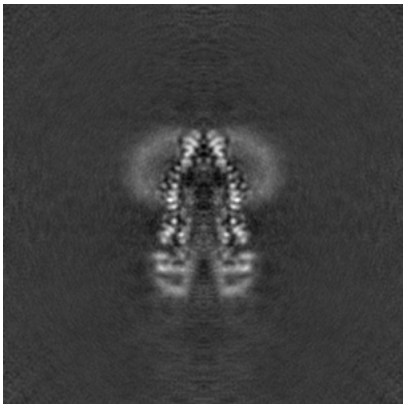


Y Index: 128

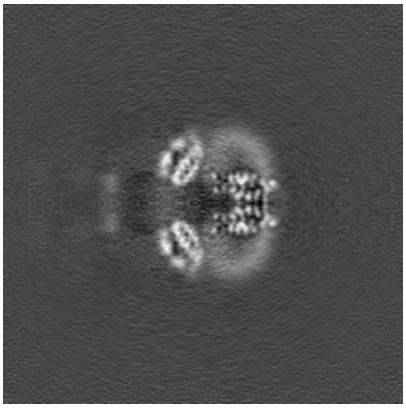


Z Index: 128

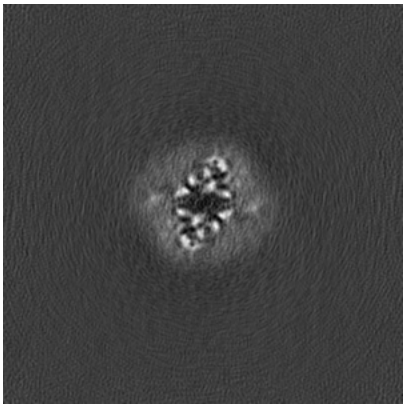
6.2.2 Raw map



X Index: 128



Y Index: 128

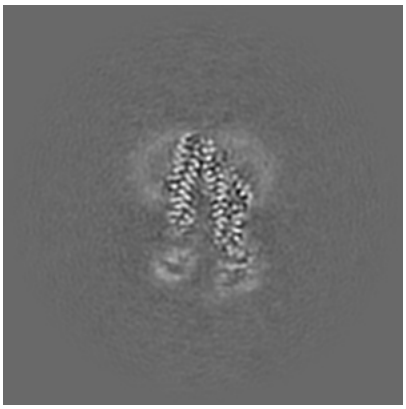


Z Index: 128

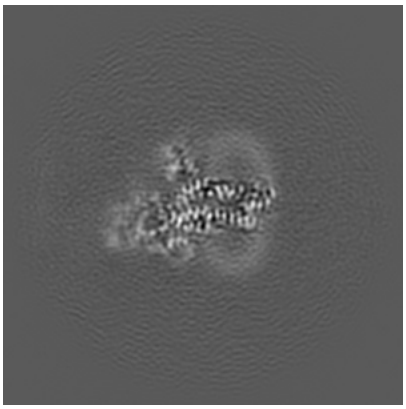
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

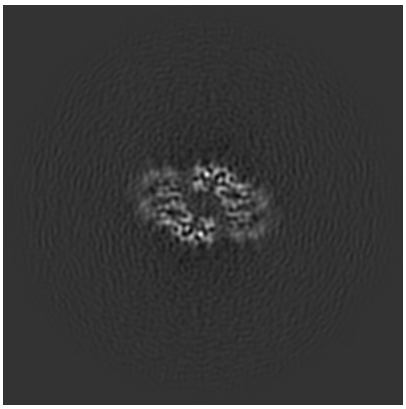
6.3.1 Primary map



X Index: 135

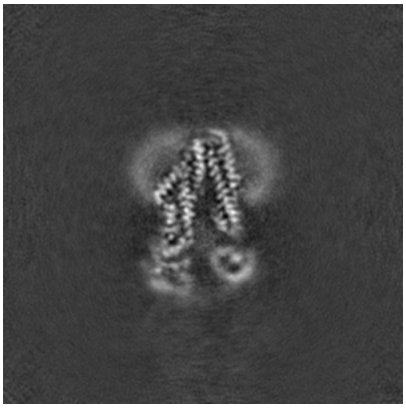


Y Index: 118

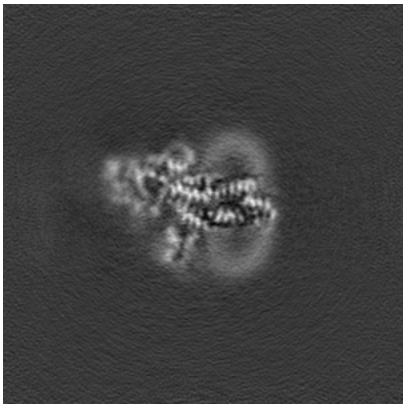


Z Index: 112

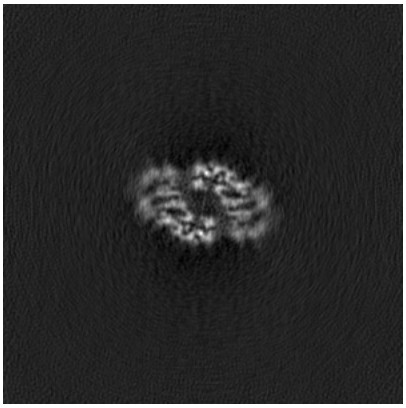
6.3.2 Raw map



X Index: 122



Y Index: 138

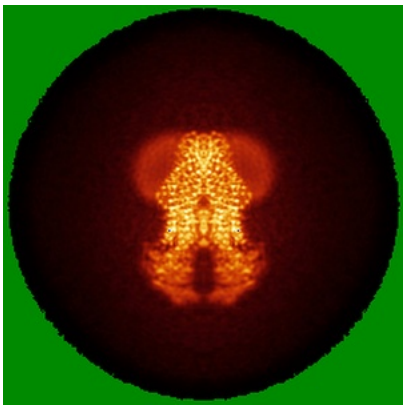


Z Index: 112

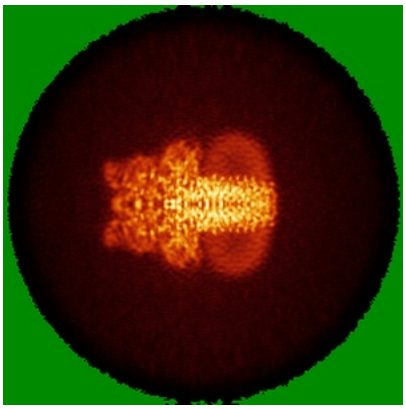
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

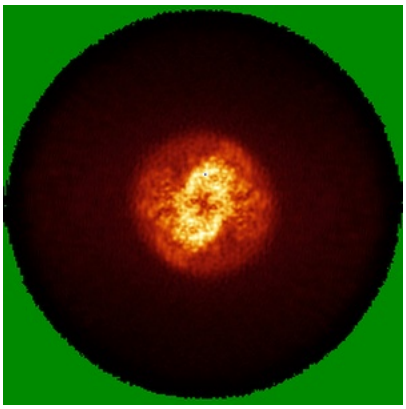
6.4.1 Primary map



X

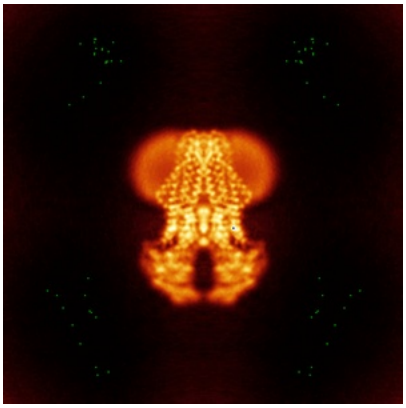


Y

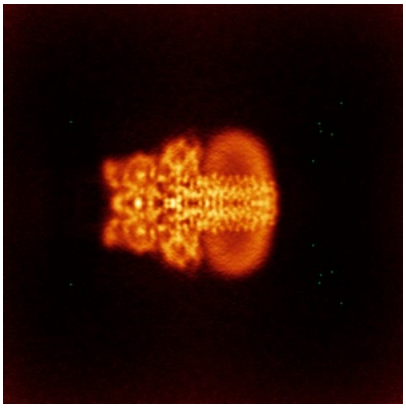


Z

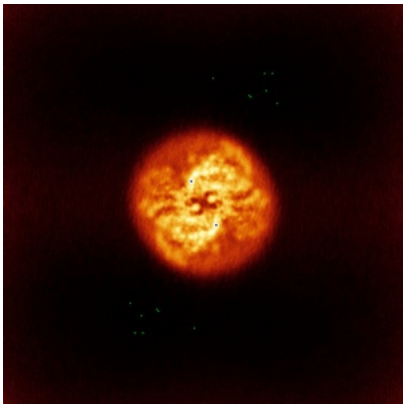
6.4.2 Raw map



X



Y

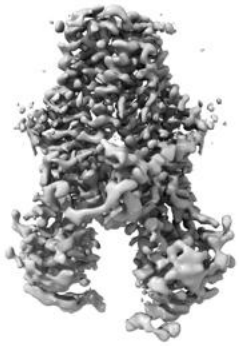


Z

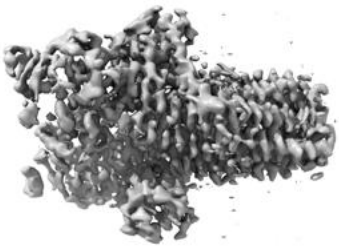
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

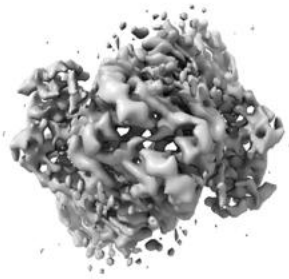
6.5.1 Primary map



X



Y



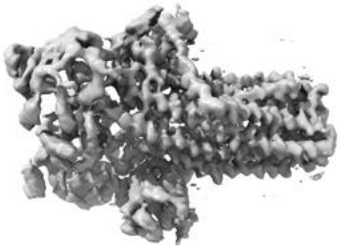
Z

The images above show the 3D surface view of the map at the recommended contour level 0.499. 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.

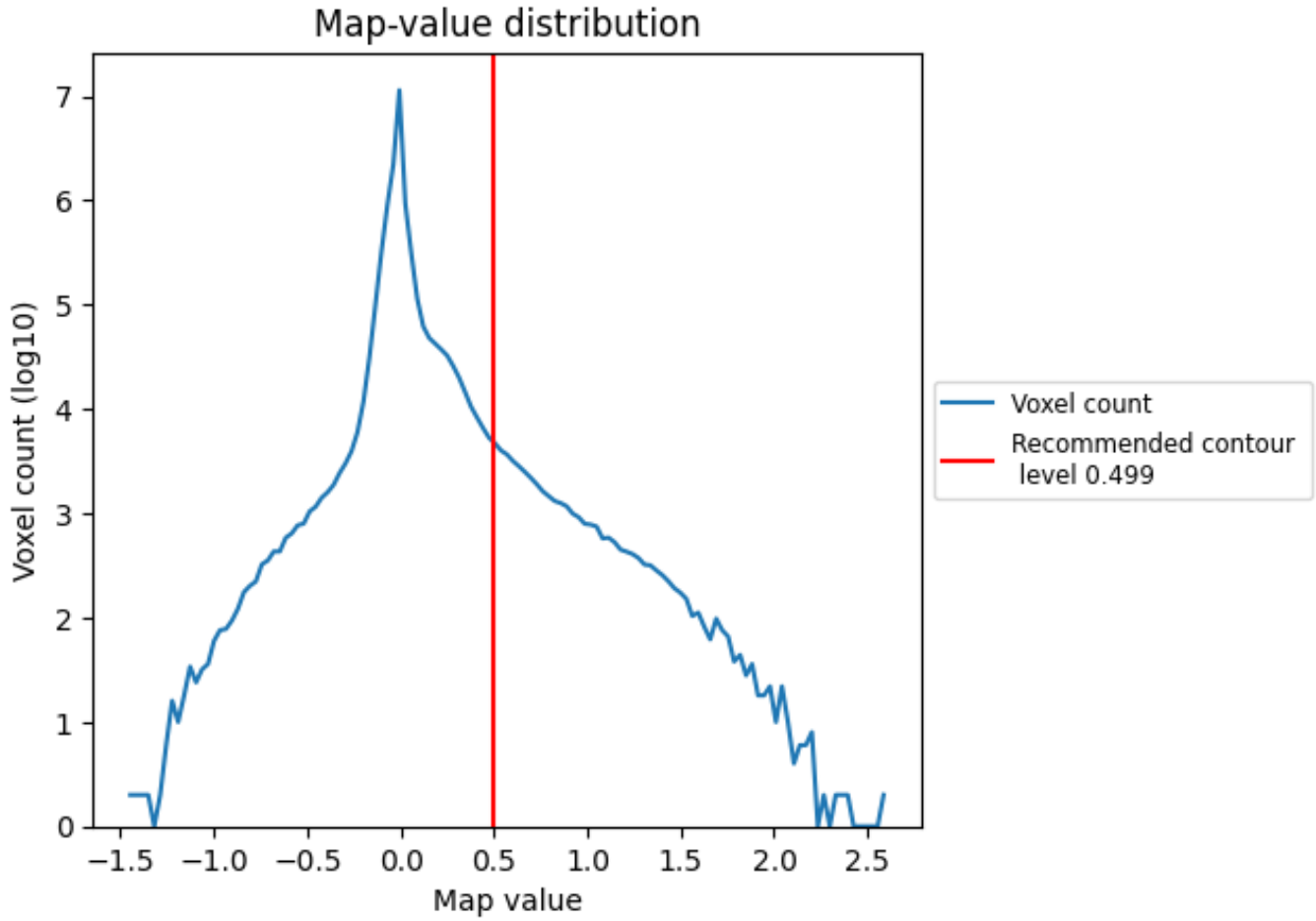
6.6 Mask visualisation (i)

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

7 Map analysis

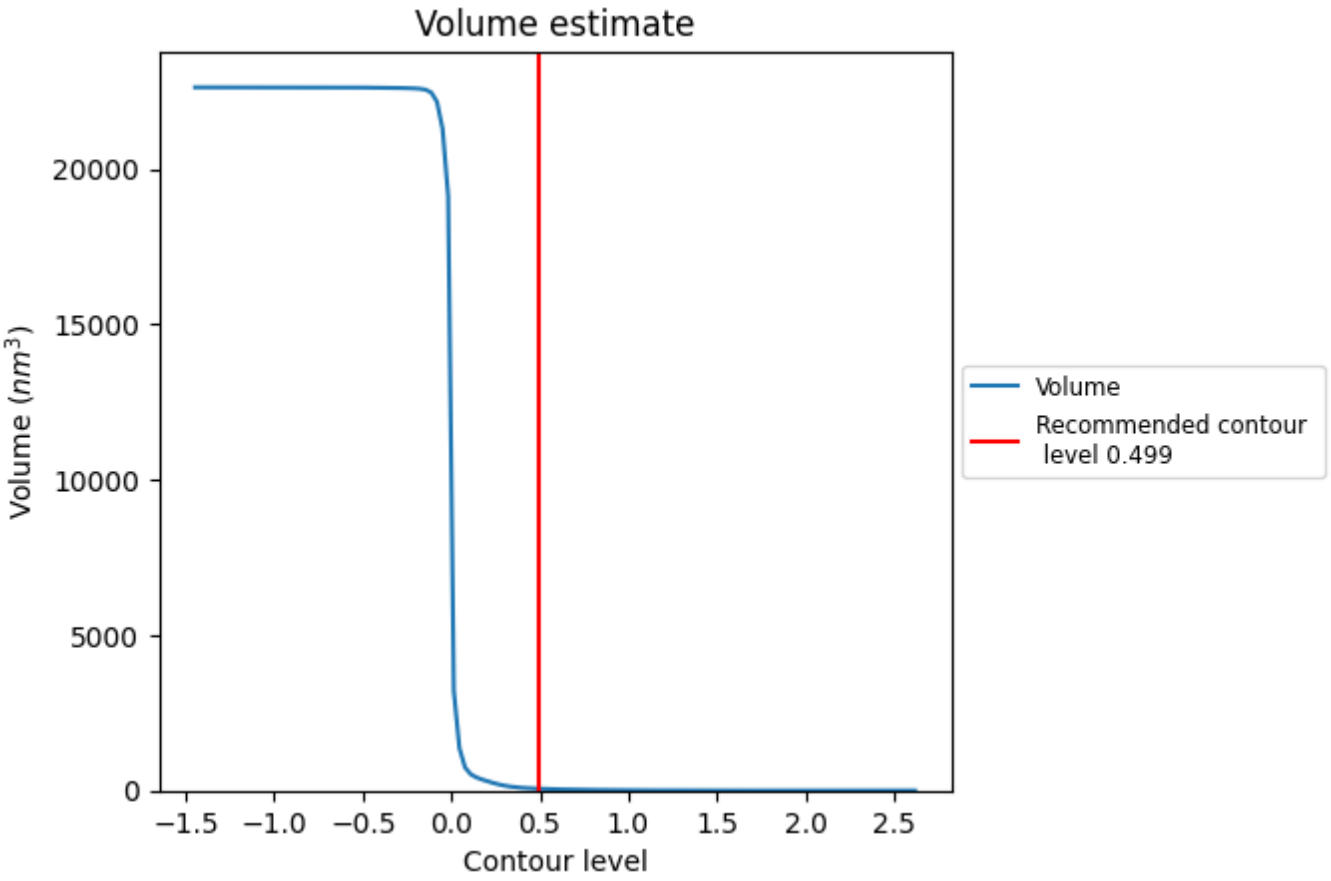
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

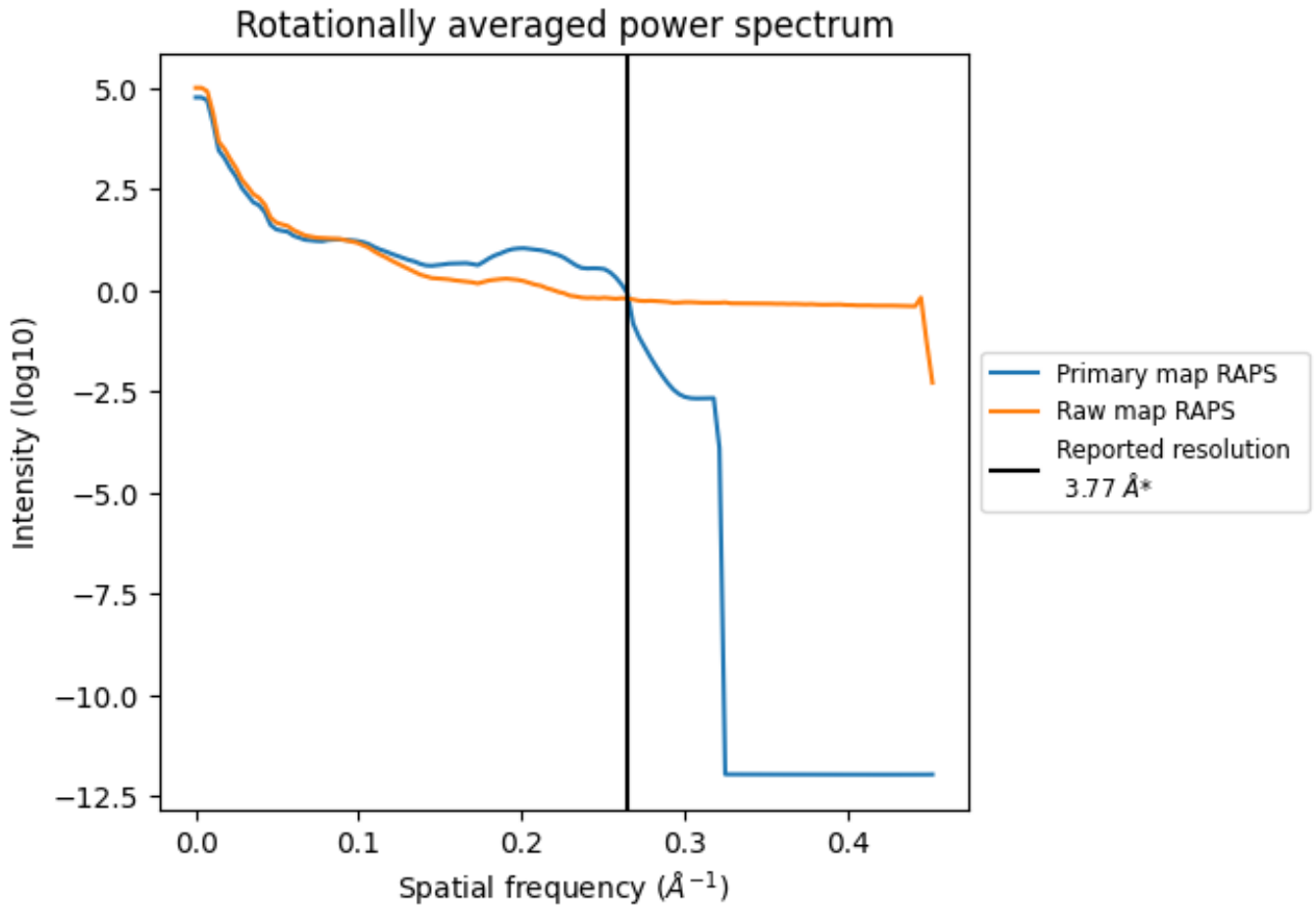
7.2 Volume estimate (i)



The volume at the recommended contour level is 59 nm^3; this corresponds to an approximate mass of 53 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 (i)

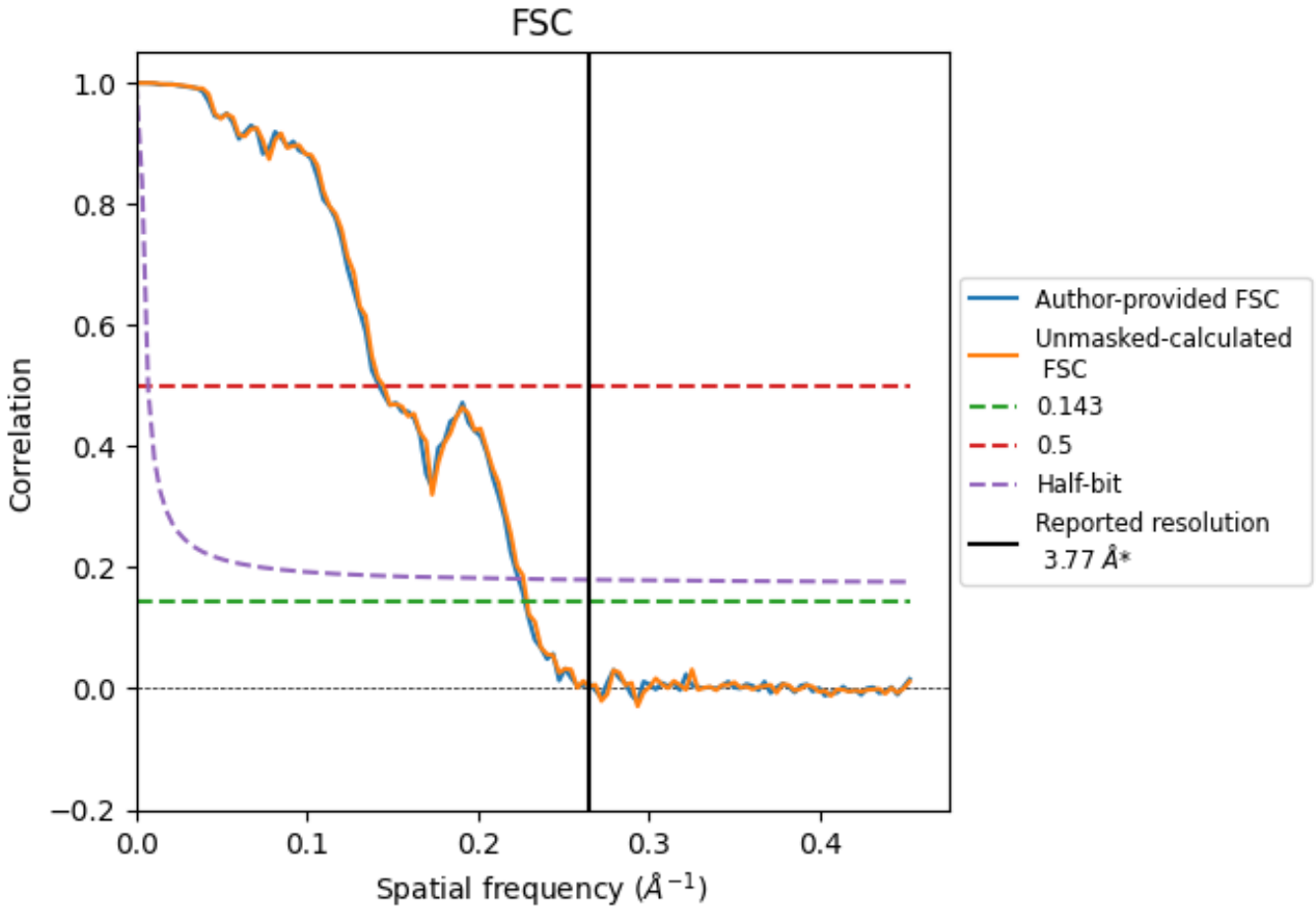


*Reported resolution corresponds to spatial frequency of 0.265 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.265 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.77	-	-
Author-provided FSC curve	4.40	7.03	4.47
Unmasked-calculated*	4.37	6.91	4.41

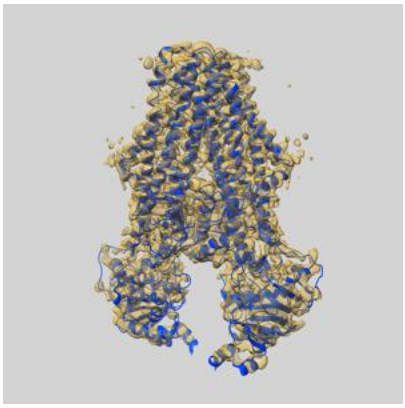
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 4.40 differs from the reported value 3.77 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.37 differs from the reported value 3.77 by more than 10 %

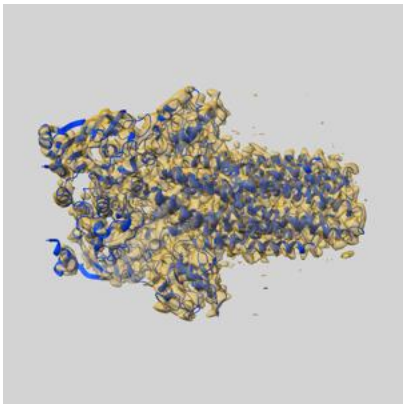
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-66738 and PDB model 9XCO. Per-residue inclusion information can be found in section 3 on page 4.

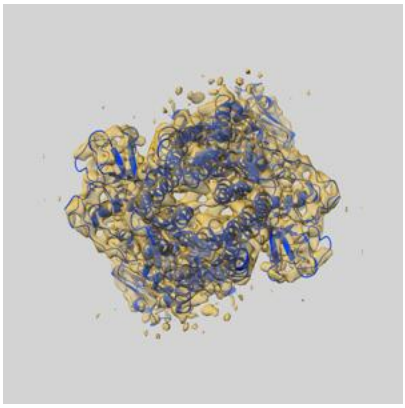
9.1 Map-model overlay



X



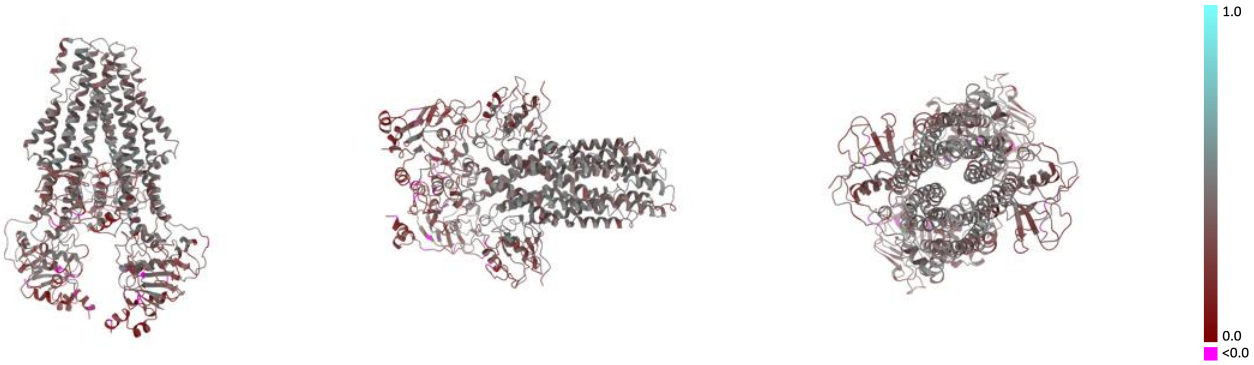
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.499 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.

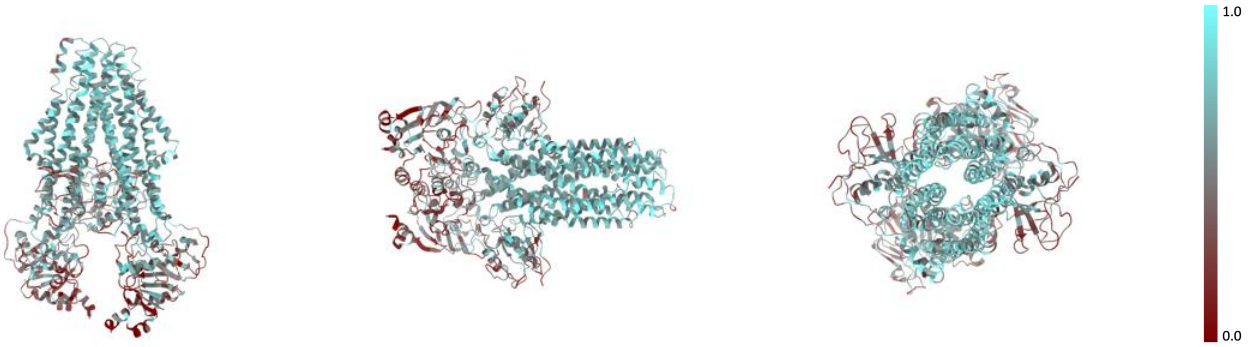
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

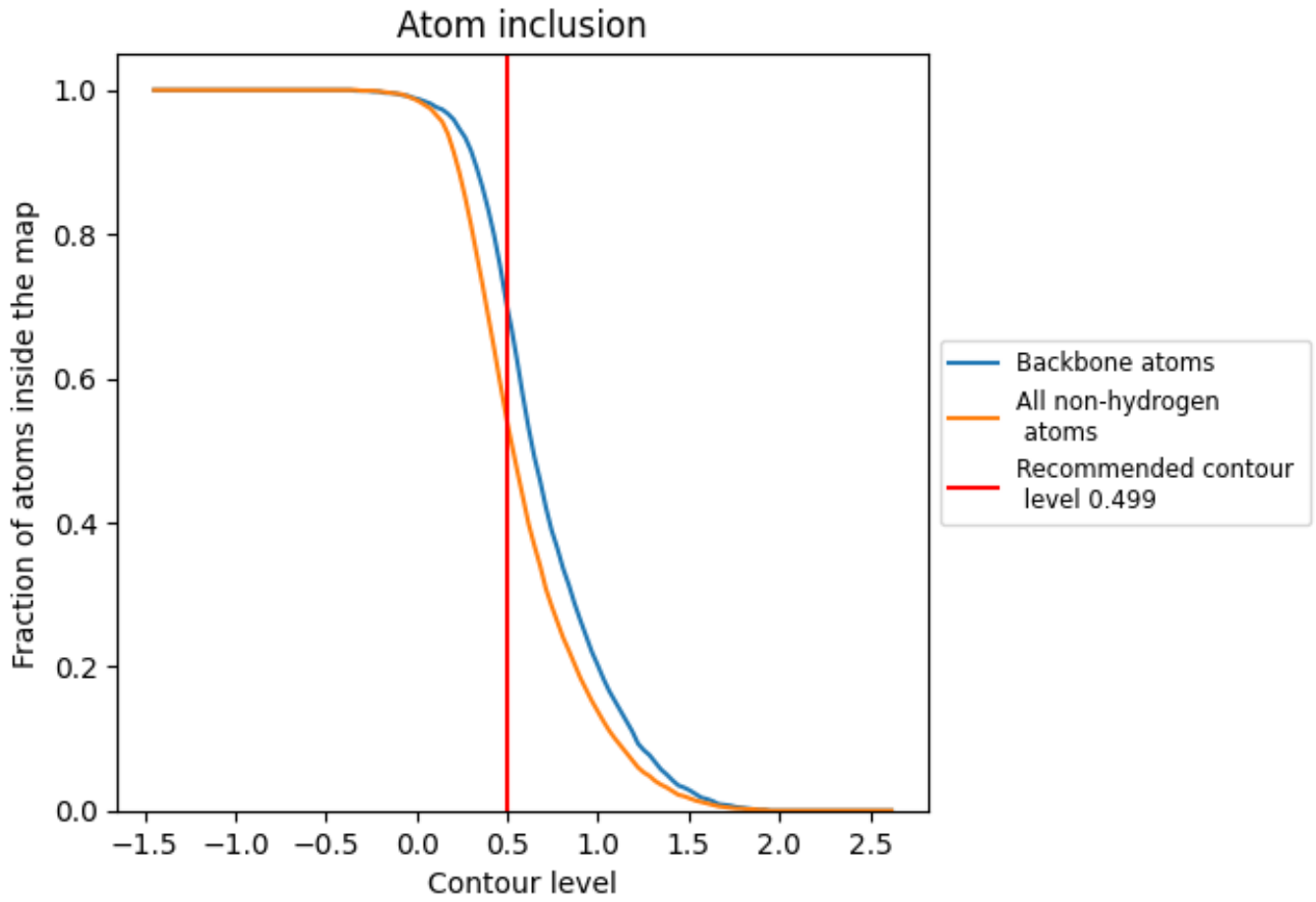
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.499).

9.4 Atom inclusion (i)



At the recommended contour level, 70% of all backbone atoms, 54% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.499) and Q-score for the entire model and for each chain.



Chain	Atom inclusion	Q-score
All	0.5400	0.3570
A	0.5400	0.3560
B	0.5410	0.3580