



wwPDB EM Validation Summary Report ⓘ

Aug 4, 2026 – 02:33 PM JST

PDB ID : 9XI8 / pdb_00009xi8
EMDB ID : EMD-66900
Title : Sarbecovirus GX2013 Spike S1 in complex with C092 Fab
Authors : Niu, C.; Liu, B.; Gao, X.; Li, Z.; He, J.; Xiong, X.
Deposited on : 2025-11-02
Resolution : 3.45 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 Phenix2.0
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

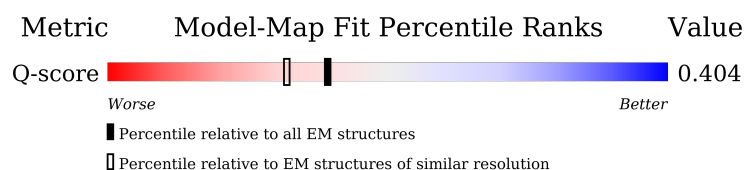
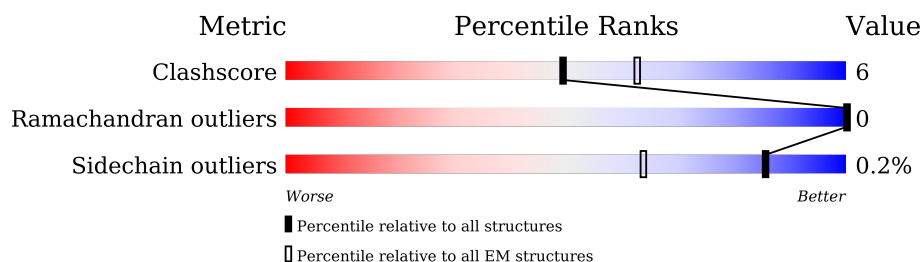
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.45 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	13836 (2.95 - 3.95)

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	H	228	21% 83% 14% .
2	L	217	16% 85% 13% .
3	A	1256	13% 86%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4622 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 Heavy chain of C092 Fab.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	H	222	Total	C	N	O	S	2	0
			1645	1035	275	326	9		

- Molecule 2 is a protein called Light chain of C092 Fab.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	213	Total	C	N	O	S	0	0
			1570	978	263	325	4		

- Molecule 3 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	177	Total	C	N	O	S	0	0
			1407	899	231	271	6		

There are 79 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1178	GLY	-	expression tag	UNP A0A0U1WHJ8
A	1179	SER	-	expression tag	UNP A0A0U1WHJ8
A	1180	GLY	-	expression tag	UNP A0A0U1WHJ8
A	1181	TYR	-	expression tag	UNP A0A0U1WHJ8
A	1182	ILE	-	expression tag	UNP A0A0U1WHJ8
A	1183	PRO	-	expression tag	UNP A0A0U1WHJ8
A	1184	GLU	-	expression tag	UNP A0A0U1WHJ8
A	1185	ALA	-	expression tag	UNP A0A0U1WHJ8
A	1186	PRO	-	expression tag	UNP A0A0U1WHJ8
A	1187	ARG	-	expression tag	UNP A0A0U1WHJ8
A	1188	ASP	-	expression tag	UNP A0A0U1WHJ8
A	1189	GLY	-	expression tag	UNP A0A0U1WHJ8
A	1190	GLN	-	expression tag	UNP A0A0U1WHJ8
A	1191	ALA	-	expression tag	UNP A0A0U1WHJ8
A	1192	TYR	-	expression tag	UNP A0A0U1WHJ8

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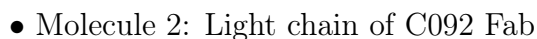
Chain	Residue	Modelled	Actual	Comment	Reference
A	1193	VAL	-	expression tag	UNP A0A0U1WHJ8
A	1194	ARG	-	expression tag	UNP A0A0U1WHJ8
A	1195	LYS	-	expression tag	UNP A0A0U1WHJ8
A	1196	ASP	-	expression tag	UNP A0A0U1WHJ8
A	1197	GLY	-	expression tag	UNP A0A0U1WHJ8
A	1198	GLU	-	expression tag	UNP A0A0U1WHJ8
A	1199	TRP	-	expression tag	UNP A0A0U1WHJ8
A	1200	VAL	-	expression tag	UNP A0A0U1WHJ8
A	1201	LEU	-	expression tag	UNP A0A0U1WHJ8
A	1202	LEU	-	expression tag	UNP A0A0U1WHJ8
A	1203	SER	-	expression tag	UNP A0A0U1WHJ8
A	1204	THR	-	expression tag	UNP A0A0U1WHJ8
A	1205	PHE	-	expression tag	UNP A0A0U1WHJ8
A	1206	LEU	-	expression tag	UNP A0A0U1WHJ8
A	1207	LEU	-	expression tag	UNP A0A0U1WHJ8
A	1208	GLU	-	expression tag	UNP A0A0U1WHJ8
A	1209	VAL	-	expression tag	UNP A0A0U1WHJ8
A	1210	LEU	-	expression tag	UNP A0A0U1WHJ8
A	1211	PHE	-	expression tag	UNP A0A0U1WHJ8
A	1212	GLN	-	expression tag	UNP A0A0U1WHJ8
A	1213	GLY	-	expression tag	UNP A0A0U1WHJ8
A	1214	PRO	-	expression tag	UNP A0A0U1WHJ8
A	1215	GLY	-	expression tag	UNP A0A0U1WHJ8
A	1216	HIS	-	expression tag	UNP A0A0U1WHJ8
A	1217	HIS	-	expression tag	UNP A0A0U1WHJ8
A	1218	HIS	-	expression tag	UNP A0A0U1WHJ8
A	1219	HIS	-	expression tag	UNP A0A0U1WHJ8
A	1220	HIS	-	expression tag	UNP A0A0U1WHJ8
A	1221	HIS	-	expression tag	UNP A0A0U1WHJ8
A	1222	HIS	-	expression tag	UNP A0A0U1WHJ8
A	1223	HIS	-	expression tag	UNP A0A0U1WHJ8
A	1224	SER	-	expression tag	UNP A0A0U1WHJ8
A	1225	ALA	-	expression tag	UNP A0A0U1WHJ8
A	1226	TRP	-	expression tag	UNP A0A0U1WHJ8
A	1227	SER	-	expression tag	UNP A0A0U1WHJ8
A	1228	HIS	-	expression tag	UNP A0A0U1WHJ8
A	1229	PRO	-	expression tag	UNP A0A0U1WHJ8
A	1230	GLN	-	expression tag	UNP A0A0U1WHJ8
A	1231	PHE	-	expression tag	UNP A0A0U1WHJ8
A	1232	GLU	-	expression tag	UNP A0A0U1WHJ8
A	1233	LYS	-	expression tag	UNP A0A0U1WHJ8
A	1234	GLY	-	expression tag	UNP A0A0U1WHJ8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1235	GLY	-	expression tag	UNP A0A0U1WHJ8
A	1236	GLY	-	expression tag	UNP A0A0U1WHJ8
A	1237	SER	-	expression tag	UNP A0A0U1WHJ8
A	1238	GLY	-	expression tag	UNP A0A0U1WHJ8
A	1239	GLY	-	expression tag	UNP A0A0U1WHJ8
A	1240	GLY	-	expression tag	UNP A0A0U1WHJ8
A	1241	GLY	-	expression tag	UNP A0A0U1WHJ8
A	1242	SER	-	expression tag	UNP A0A0U1WHJ8
A	1243	GLY	-	expression tag	UNP A0A0U1WHJ8
A	1244	GLY	-	expression tag	UNP A0A0U1WHJ8
A	1245	SER	-	expression tag	UNP A0A0U1WHJ8
A	1246	ALA	-	expression tag	UNP A0A0U1WHJ8
A	1247	TRP	-	expression tag	UNP A0A0U1WHJ8
A	1248	SER	-	expression tag	UNP A0A0U1WHJ8
A	1249	HIS	-	expression tag	UNP A0A0U1WHJ8
A	1250	PRO	-	expression tag	UNP A0A0U1WHJ8
A	1251	GLN	-	expression tag	UNP A0A0U1WHJ8
A	1252	PHE	-	expression tag	UNP A0A0U1WHJ8
A	1253	GLU	-	expression tag	UNP A0A0U1WHJ8
A	1254	LYS	-	expression tag	UNP A0A0U1WHJ8
A	1255	SER	-	expression tag	UNP A0A0U1WHJ8
A	1256	ALA	-	expression tag	UNP A0A0U1WHJ8

- Molecule 1: Heavy chain of C092 Fab





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	385893	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.780	Depositor
Minimum map value	-1.897	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.051	Depositor
Recommended contour level	0.22	Depositor
Map size ($\text{\AA}$)	253.44, 253.44, 253.44	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.32, 1.32, 1.32	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	H	0.22	0/1691	0.37	0/2301
2	L	0.21	0/1608	0.40	0/2201
3	A	0.28	0/1445	0.39	0/1973
All	All	0.24	0/4744	0.39	0/6475

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	H	1645	0	1614	25	0
2	L	1570	0	1504	18	0
3	A	1407	0	1344	16	0
All	All	4622	0	4462	52	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 6.

The worst 5 of 52 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)
3:A:382:CYS:HA	3:A:498:CYS:HB3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:152:ALA:HB3	2:L:199:GLN:HE22	1.60	0.66
1:H:54:ILE:HG23	1:H:55:LEU:HG	1.76	0.66
1:H:52:ILE:HD13	1:H:55:LEU:HD12	1.78	0.65
1:H:55:LEU:HD13	3:A:438:TYR:CE1	2.36	0.60

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	H	222/228 (97%)	219 (99%)	3 (1%)	0	100	100
2	L	211/217 (97%)	201 (95%)	10 (5%)	0	100	100
3	A	175/1256 (14%)	171 (98%)	4 (2%)	0	100	100
All	All	608/1701 (36%)	591 (97%)	17 (3%)	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	H	186/191 (97%)	185 (100%)	1 (0%)	81	81
2	L	177/183 (97%)	177 (100%)	0	100	100
3	A	157/1084 (14%)	157 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	520/1458 (36%)	519 (100%)	1 (0%)	85	84

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

Mol	Chain	Res	Type
1	H	54	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	31	ASN
1	H	166	ASN
2	L	175	ASN
2	L	189	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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.

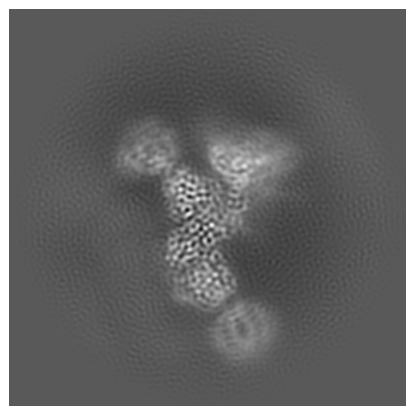
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-66900. These allow visual inspection of the internal detail of the map and identification of artifacts.

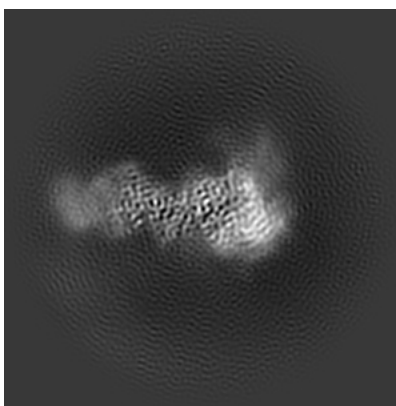
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

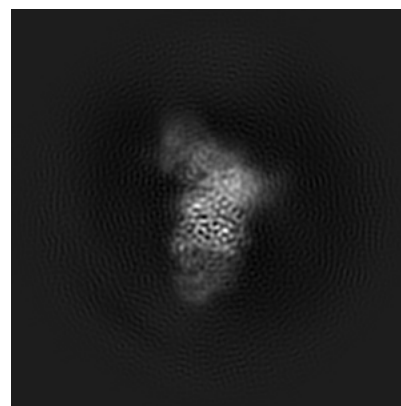
6.1.1 Primary map



X

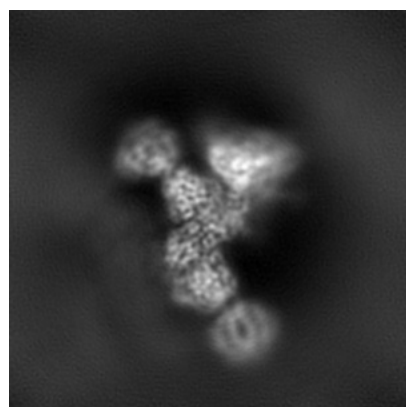


Y

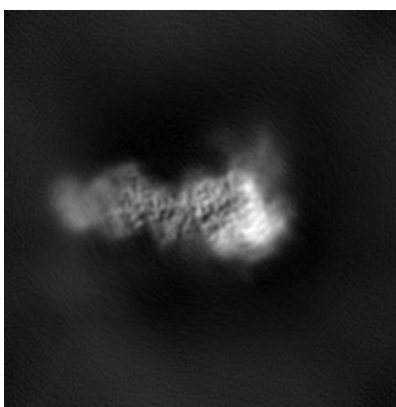


Z

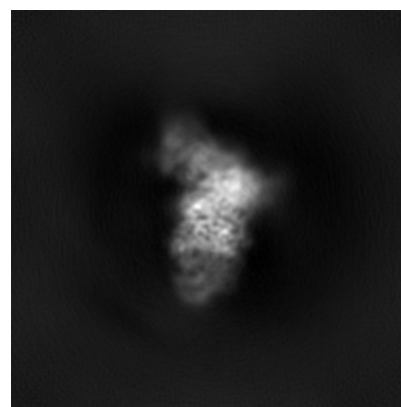
6.1.2 Raw map



X



Y

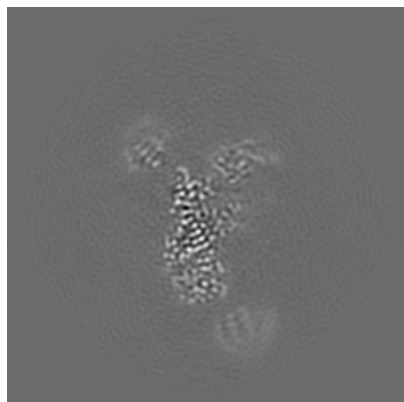


Z

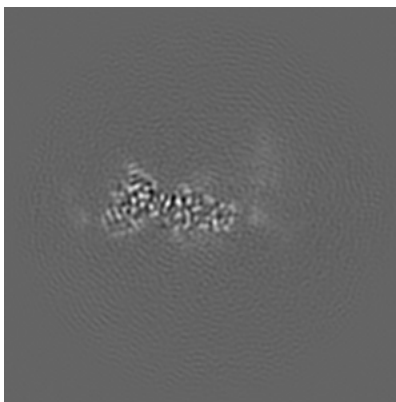
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

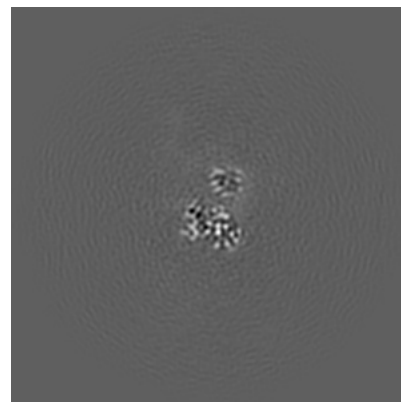
6.2.1 Primary map



X Index: 96

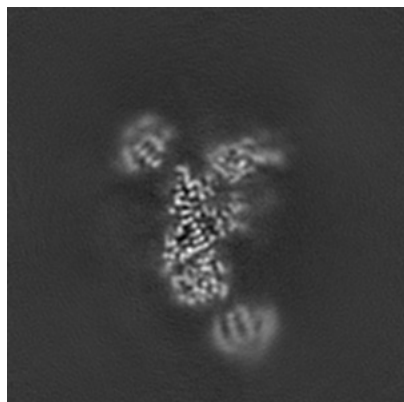


Y Index: 96

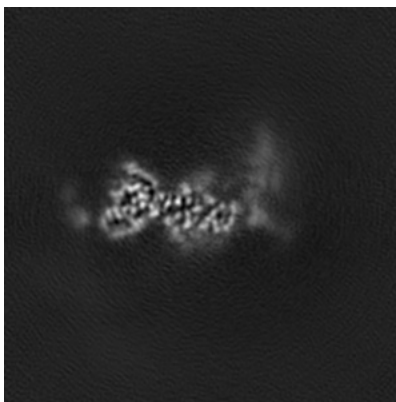


Z Index: 96

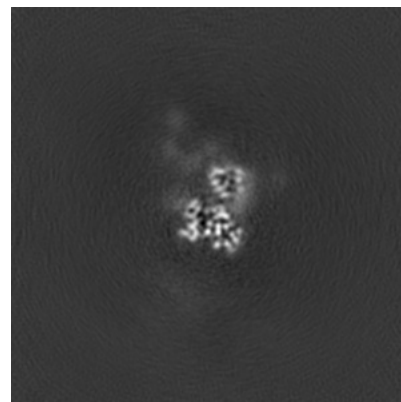
6.2.2 Raw map



X Index: 96



Y Index: 96

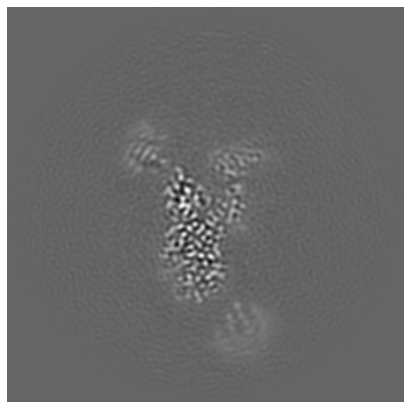


Z Index: 96

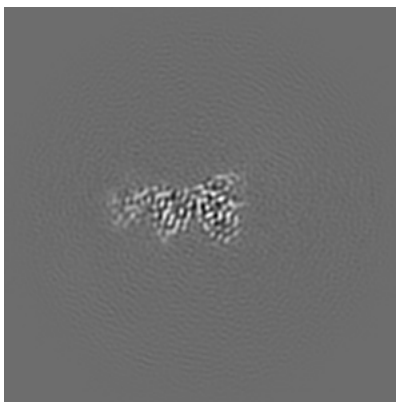
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

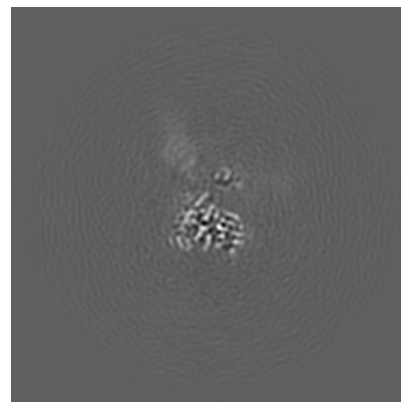
6.3.1 Primary map



X Index: 99

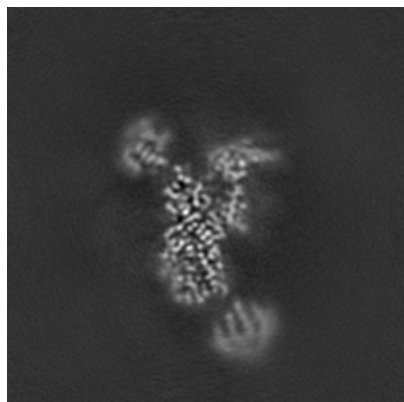


Y Index: 86

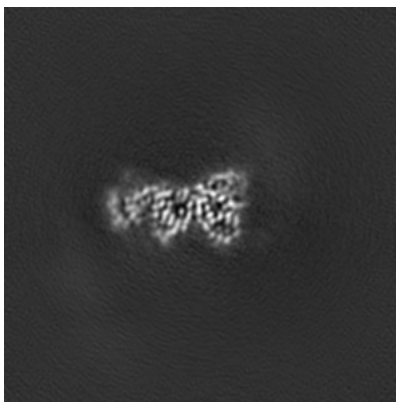


Z Index: 104

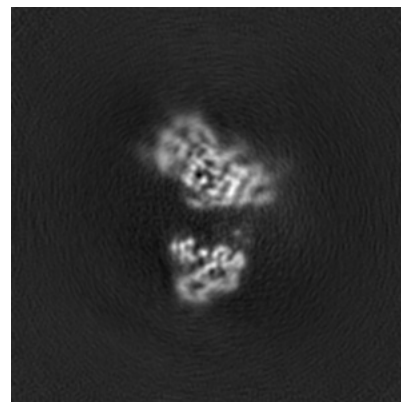
6.3.2 Raw map



X Index: 98



Y Index: 86

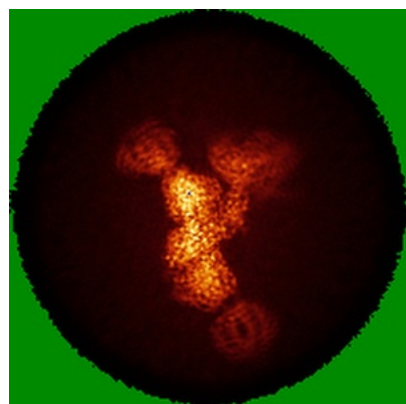


Z Index: 118

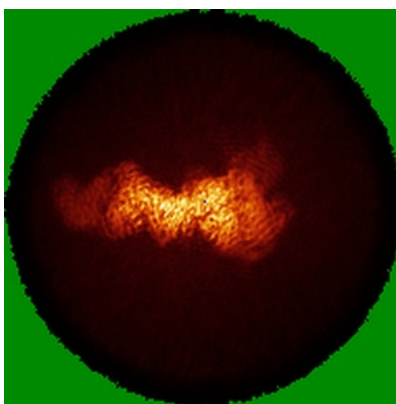
The images above show the largest variance slices of the map in three orthogonal directions.

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

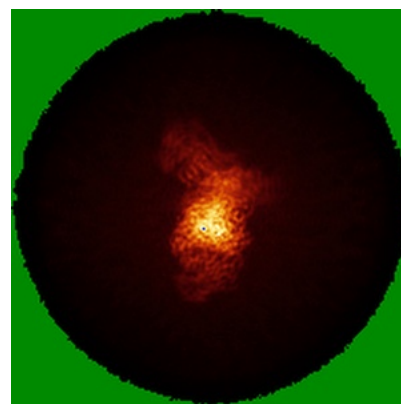
6.4.1 Primary map



X

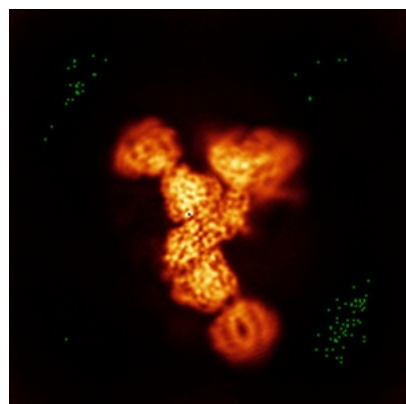


Y

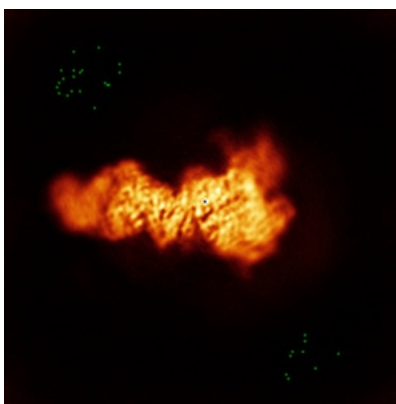


Z

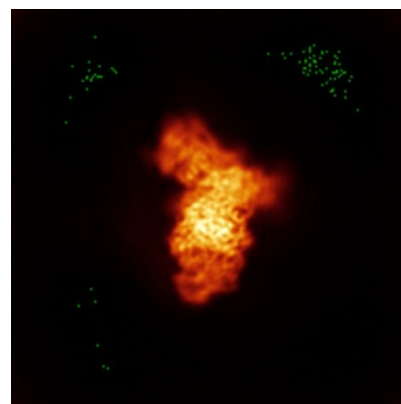
6.4.2 Raw map



X



Y

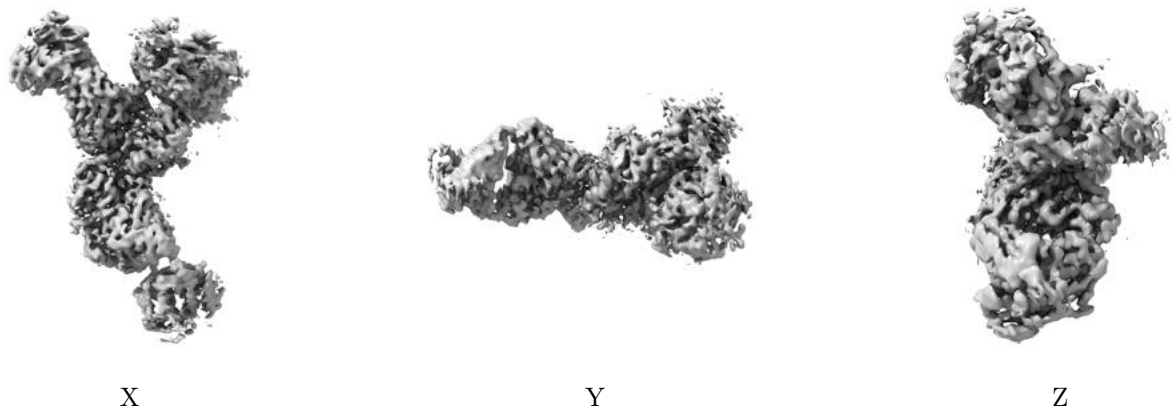


Z

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 0.22. 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.

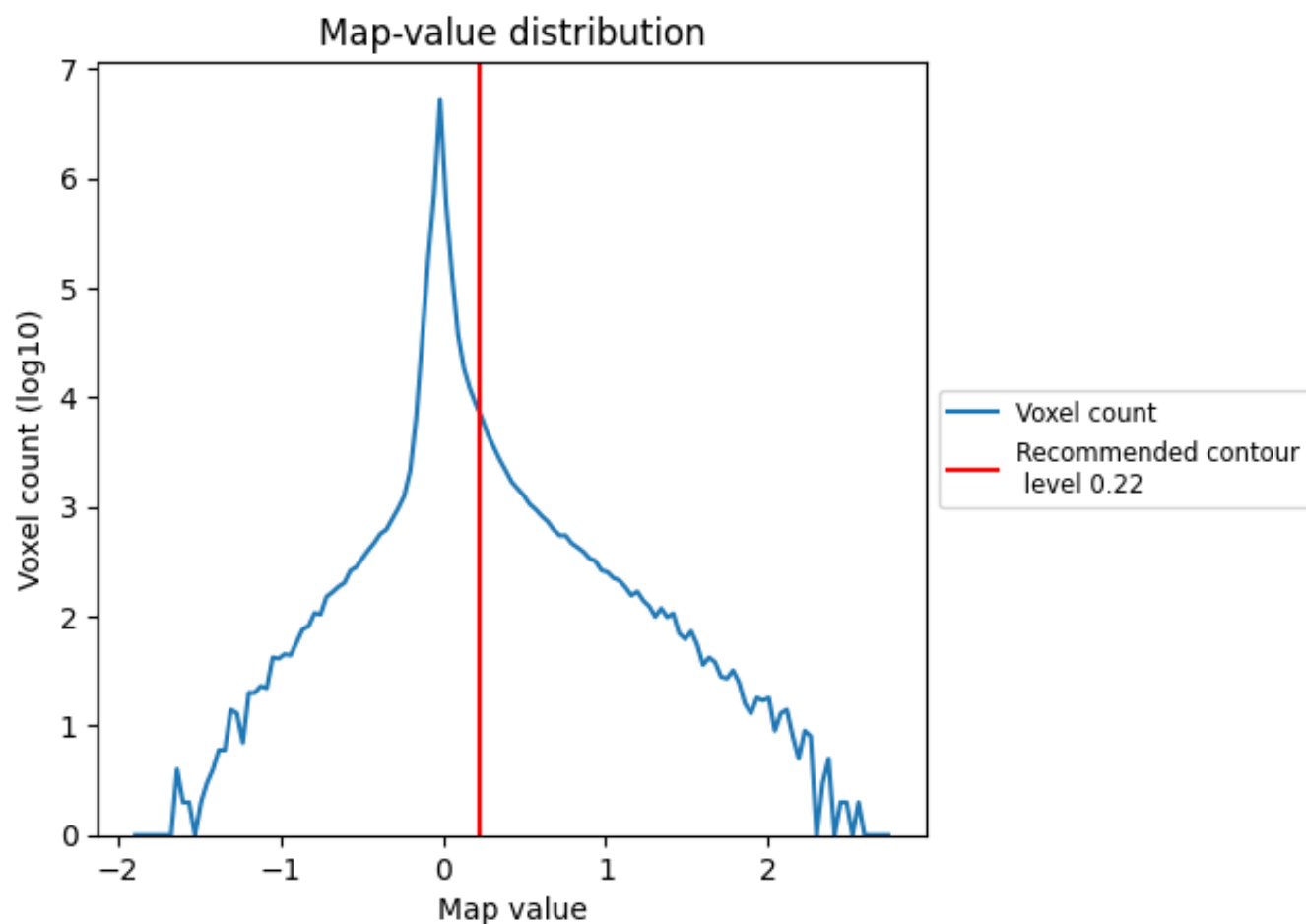
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

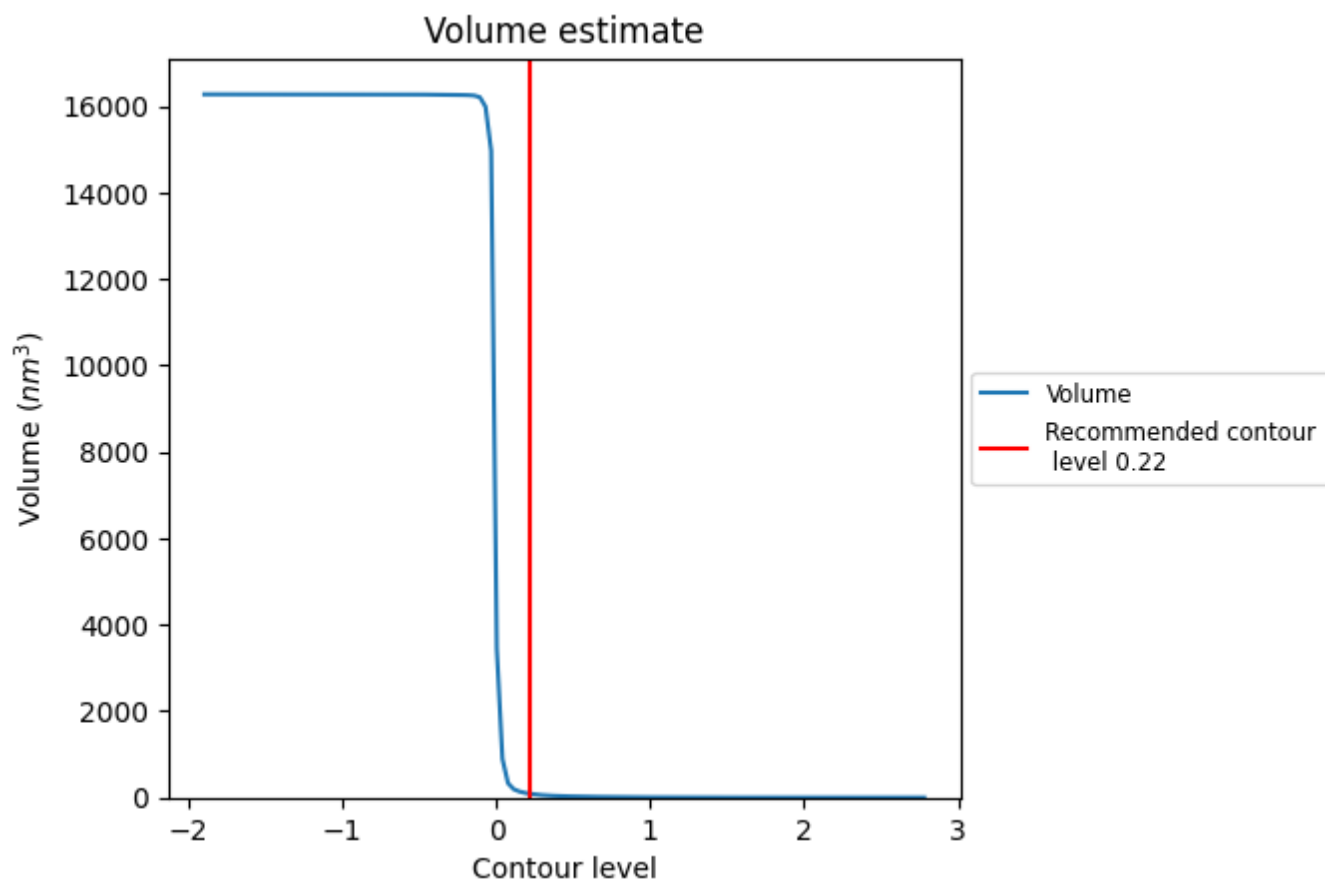
This section contains the results of statistical analysis of the map.

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.

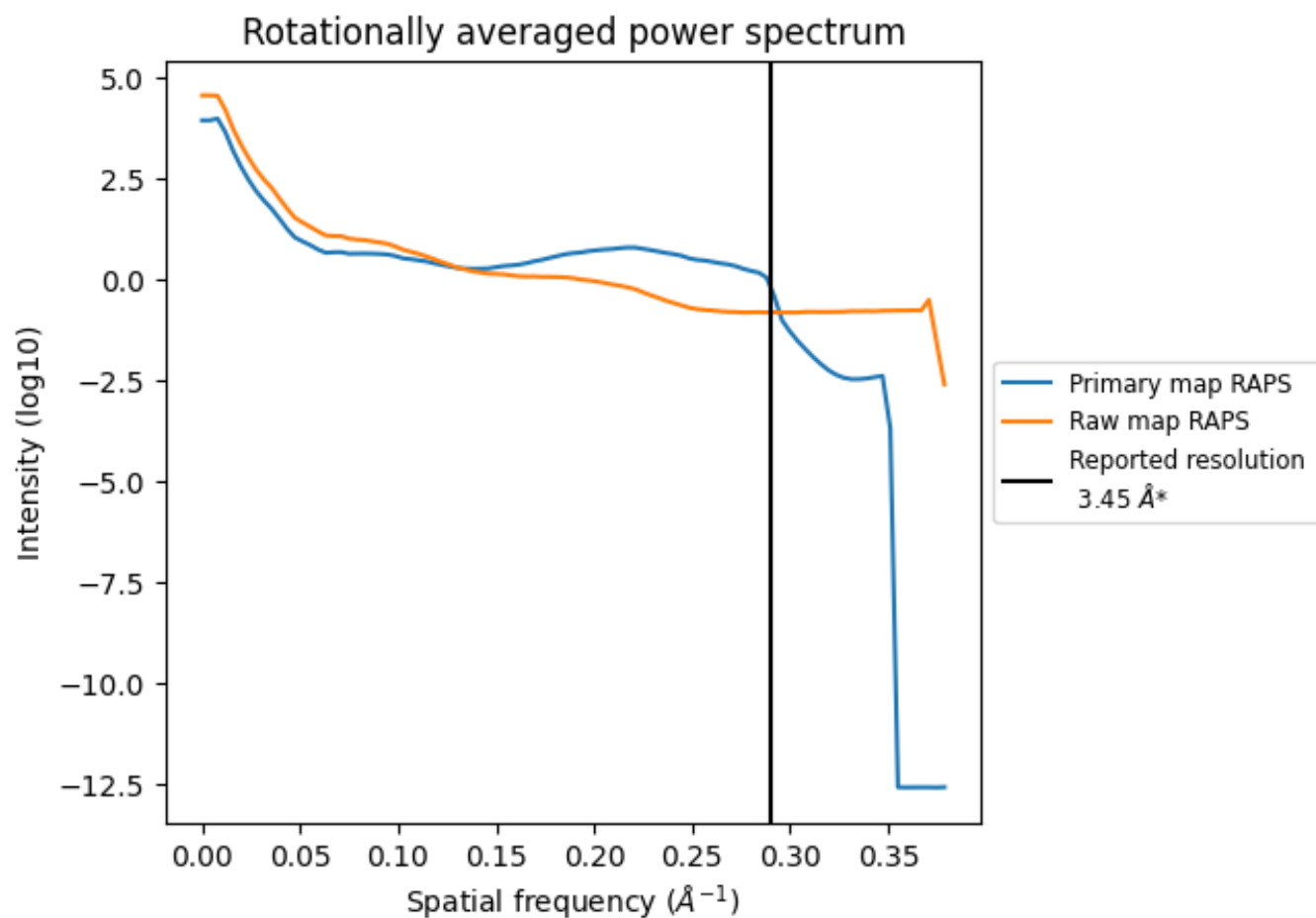
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 87 nm³; this corresponds to an approximate mass of 79 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 ⓘ

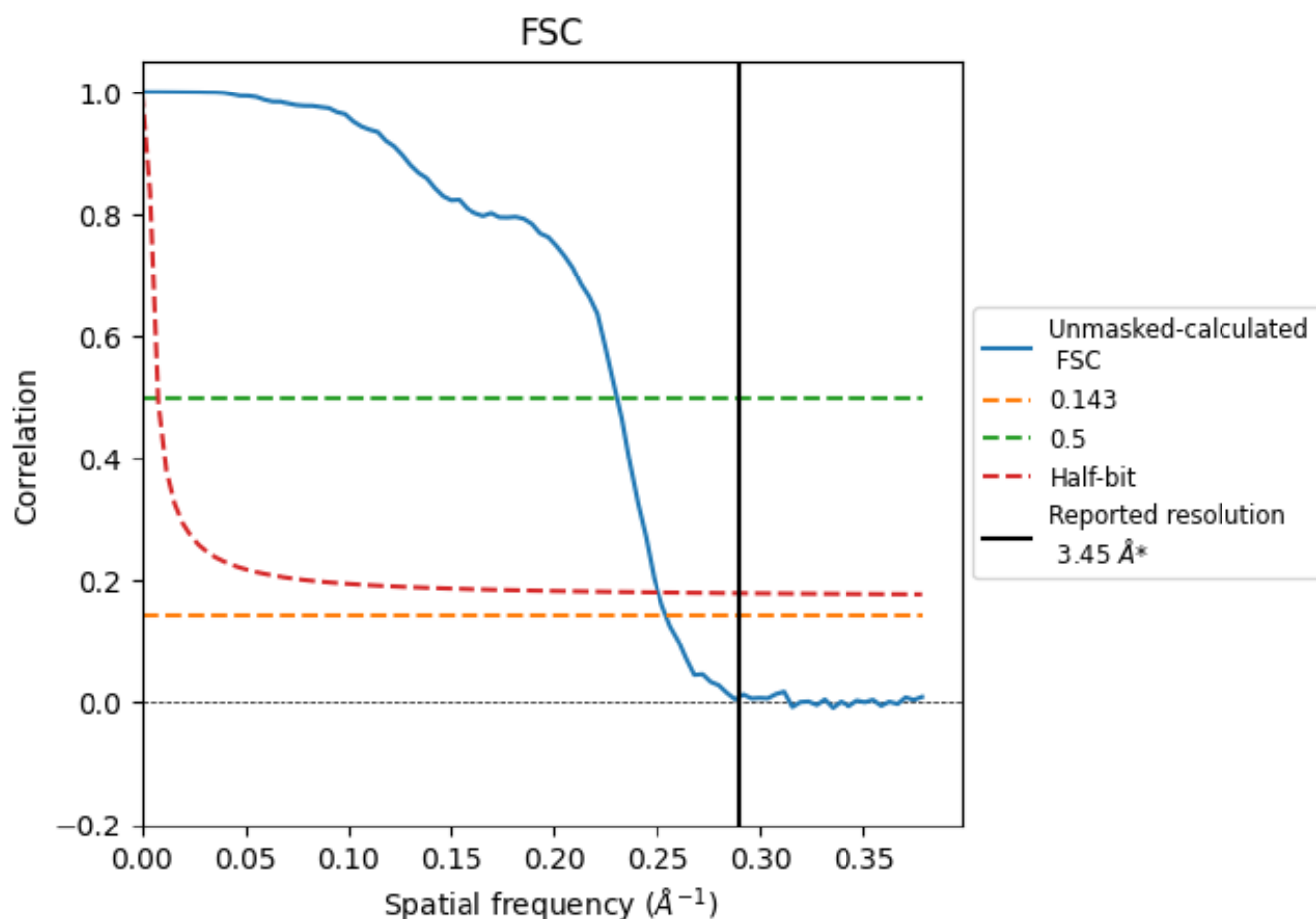


*Reported resolution corresponds to spatial frequency of 0.290 $\text{\AA}^{-1}$

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 0.290 Å⁻¹

8.2 Resolution estimates [i](#)

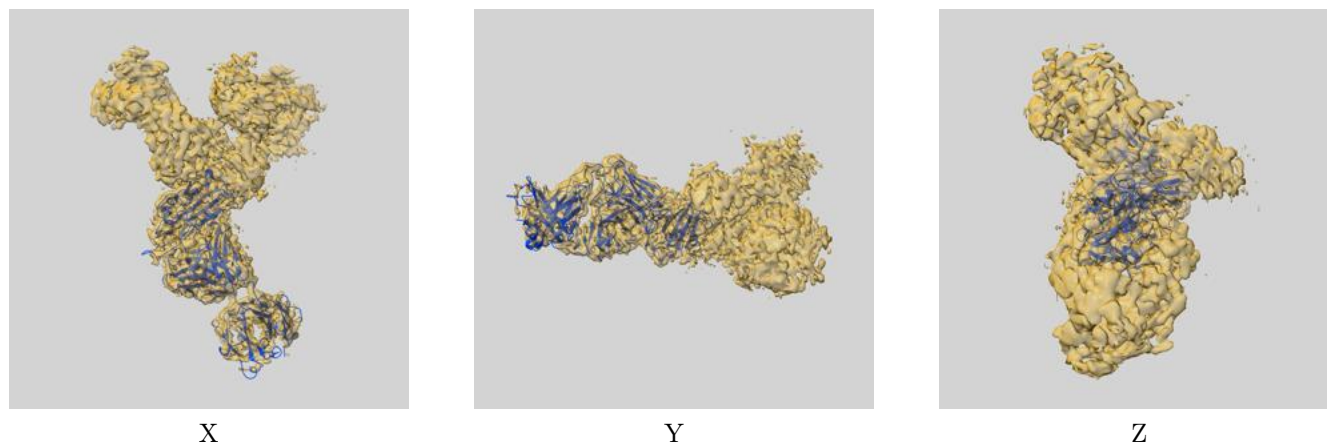
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.45	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.93	4.34	3.99

*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 3.93 differs from the reported value 3.45 by more than 10 %

9 Map-model fit [i](#)

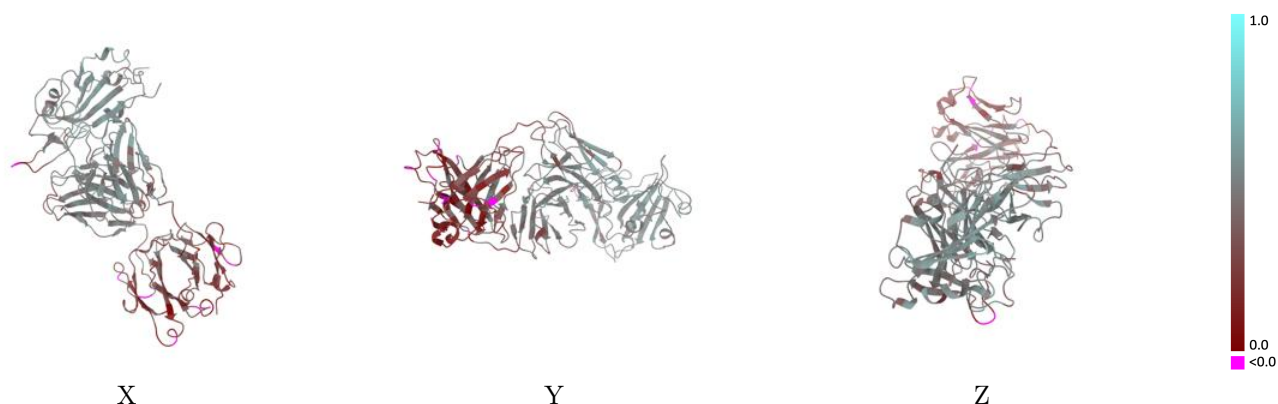
This section contains information regarding the fit between EMDB map EMD-66900 and PDB model 9XI8. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



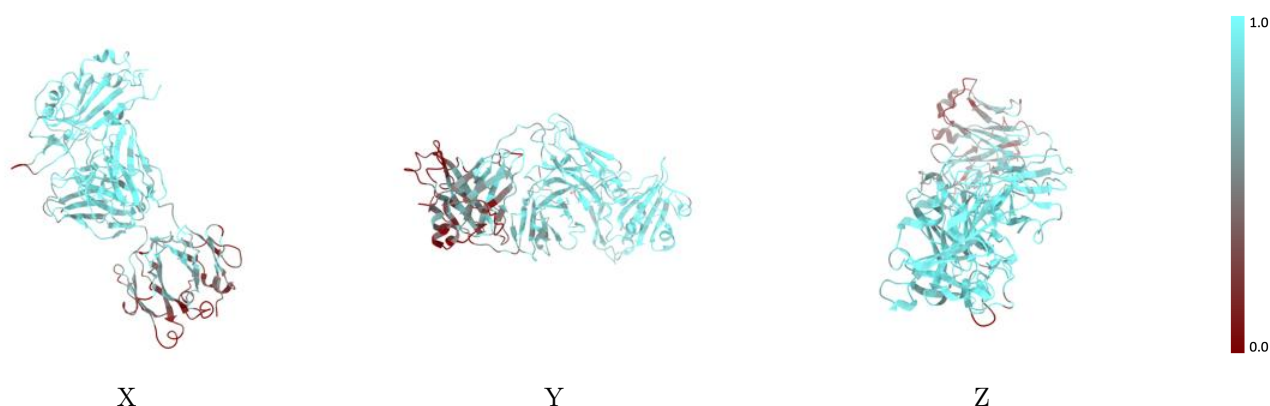
The images above show the 3D surface view of the map at the recommended contour level 0.22 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



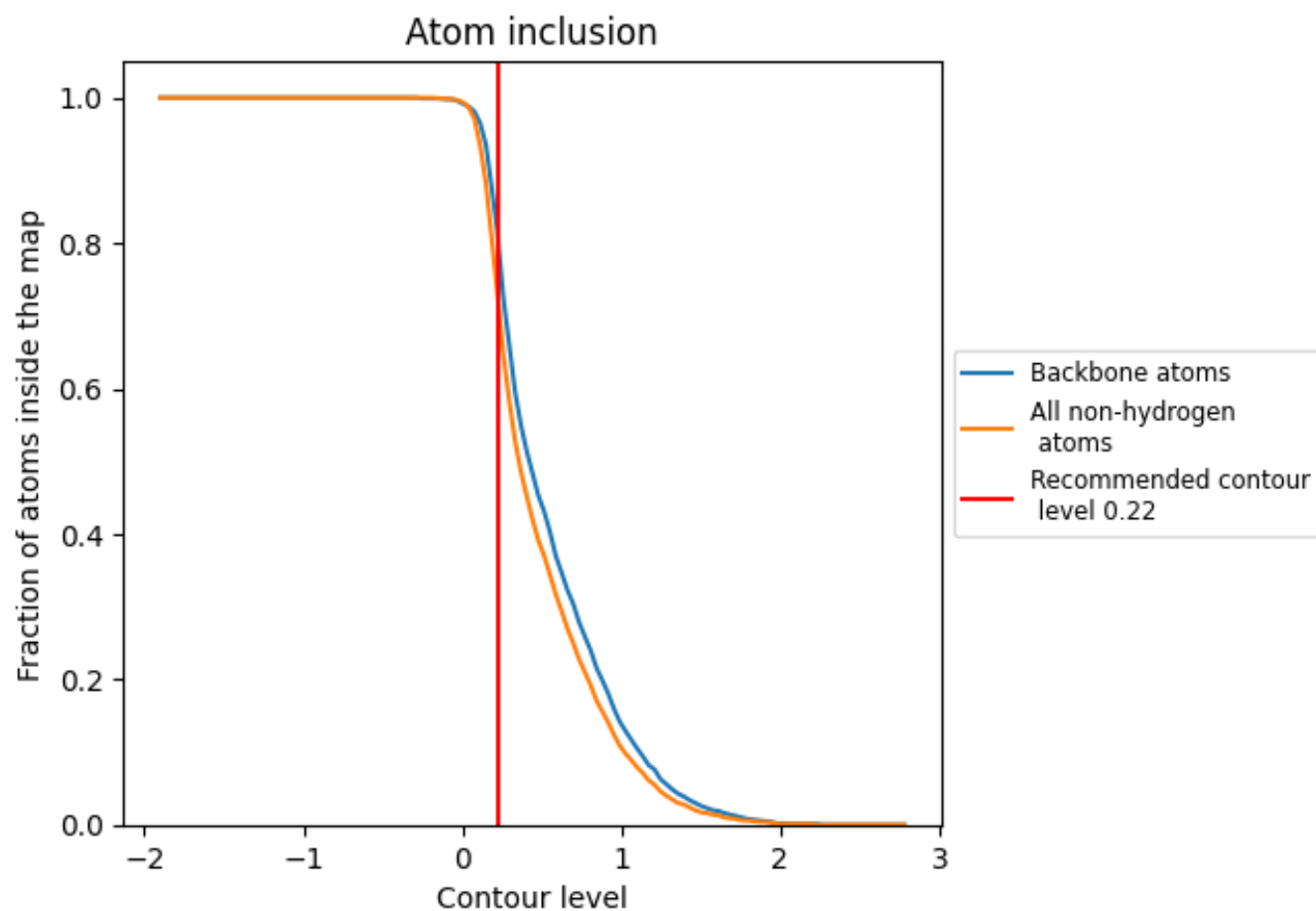
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.22).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 73% 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 (0.22) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7330	0.4040
A	0.8640	0.4790
H	0.6610	0.3700
L	0.6920	0.3720

