



Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 10:45 PM UTC

PDB ID : 9GDY / pdb_00009gdy
EMDB ID : EMD-51280
Title : SARS-CoV-2 Spike protein Beta Variant at 37C structural flexibility / heterogeneity analyses
Authors : Herreros, D.; Mata, C.P.; Noddings, C.; Irene, D.; Agard, D.A.; Tsai, M.-D.; Sorzano, C.O.S.; Carazo, J.M.
Deposited on : 2024-08-06
Resolution : 2.80 Å(reported)
Based on initial models : 7VX1, 7WEV

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 : **FAILED**
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

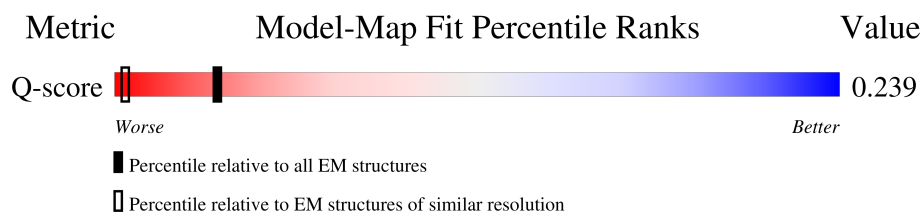
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 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	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Q-score	25397	11806 (2.30 - 3.30)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 509160 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 Spike glycoprotein,Fibritin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1-A	1079	Total	C	N	O	S	0	0
			8454	5399	1410	1606	39		
1	2-A	1079	Total	C	N	O	S	0	0
			8454	5399	1410	1606	39		
1	3-A	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		
1	4-A	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		
1	5-A	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		
1	6-A	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		
1	7-A	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		
1	8-A	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		
1	9-A	1079	Total	C	N	O	S	0	0
			8454	5399	1410	1606	39		
1	10-A	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		
1	11-A	1079	Total	C	N	O	S	0	0
			8454	5399	1410	1606	39		
1	12-A	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		
1	13-A	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		
1	14-A	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		
1	15-A	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		
1	16-A	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		
1	17-A	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	18-A	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		
1	19-A	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		
1	20-A	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		
1	1-B	1079	Total	C	N	O	S	0	0
			8454	5399	1410	1606	39		
1	2-B	1079	Total	C	N	O	S	0	0
			8454	5399	1410	1606	39		
1	3-B	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		
1	4-B	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		
1	5-B	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		
1	6-B	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		
1	7-B	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		
1	8-B	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		
1	9-B	1079	Total	C	N	O	S	0	0
			8454	5399	1410	1606	39		
1	10-B	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		
1	11-B	1079	Total	C	N	O	S	0	0
			8454	5399	1410	1606	39		
1	12-B	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		
1	13-B	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		
1	14-B	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		
1	15-B	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		
1	16-B	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		
1	17-B	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		
1	18-B	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	19-B	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		
1	20-B	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		
1	1-C	1079	Total	C	N	O	S	0	0
			8454	5399	1410	1606	39		
1	2-C	1079	Total	C	N	O	S	0	0
			8454	5399	1410	1606	39		
1	3-C	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		
1	4-C	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		
1	5-C	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		
1	6-C	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		
1	7-C	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		
1	8-C	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		
1	9-C	1079	Total	C	N	O	S	0	0
			8454	5399	1410	1606	39		
1	10-C	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		
1	11-C	1079	Total	C	N	O	S	0	0
			8454	5399	1410	1606	39		
1	12-C	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		
1	13-C	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		
1	14-C	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		
1	15-C	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		
1	16-C	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		
1	17-C	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		
1	18-C	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		
1	19-C	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	20-C	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		

There are 87 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	PHE	LEU	variant	UNP P0DTC2
A	80	ALA	ASP	variant	UNP P0DTC2
A	215	GLY	ASP	variant	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	ALA	deletion	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	246	ILE	ARG	conflict	UNP P0DTC2
A	417	ASN	LYS	variant	UNP P0DTC2
A	484	LYS	GLU	variant	UNP P0DTC2
A	501	TYR	ASN	variant	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2
A	682	GLY	ARG	engineered mutation	UNP P0DTC2
A	683	SER	ARG	engineered mutation	UNP P0DTC2
A	685	SER	ARG	engineered mutation	UNP P0DTC2
A	701	VAL	ALA	variant	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
A	1209	GLY	-	linker	UNP P0DTC2
A	1210	SER	-	linker	UNP P0DTC2
A	1232	LEU	PHE	engineered mutation	UNP P10104
A	1238	GLY	-	expression tag	UNP P10104
A	1239	ARG	-	expression tag	UNP P10104
A	1240	SER	-	expression tag	UNP P10104
A	1241	LEU	-	expression tag	UNP P10104
A	1242	GLU	-	expression tag	UNP P10104
A	1243	VAL	-	expression tag	UNP P10104
A	1244	LEU	-	expression tag	UNP P10104
A	1245	PHE	-	expression tag	UNP P10104
A	1246	GLN	-	expression tag	UNP P10104
B	18	PHE	LEU	variant	UNP P0DTC2
B	80	ALA	ASP	variant	UNP P0DTC2
B	215	GLY	ASP	variant	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2
B	?	-	ALA	deletion	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2
B	246	ILE	ARG	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	417	ASN	LYS	variant	UNP P0DTC2
B	484	LYS	GLU	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2
B	682	GLY	ARG	engineered mutation	UNP P0DTC2
B	683	SER	ARG	engineered mutation	UNP P0DTC2
B	685	SER	ARG	engineered mutation	UNP P0DTC2
B	701	VAL	ALA	variant	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	1209	GLY	-	linker	UNP P0DTC2
B	1210	SER	-	linker	UNP P0DTC2
B	1232	LEU	PHE	engineered mutation	UNP P10104
B	1238	GLY	-	expression tag	UNP P10104
B	1239	ARG	-	expression tag	UNP P10104
B	1240	SER	-	expression tag	UNP P10104
B	1241	LEU	-	expression tag	UNP P10104
B	1242	GLU	-	expression tag	UNP P10104
B	1243	VAL	-	expression tag	UNP P10104
B	1244	LEU	-	expression tag	UNP P10104
B	1245	PHE	-	expression tag	UNP P10104
B	1246	GLN	-	expression tag	UNP P10104
C	18	PHE	LEU	variant	UNP P0DTC2
C	80	ALA	ASP	variant	UNP P0DTC2
C	215	GLY	ASP	variant	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	?	-	ALA	deletion	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	246	ILE	ARG	conflict	UNP P0DTC2
C	417	ASN	LYS	variant	UNP P0DTC2
C	484	LYS	GLU	variant	UNP P0DTC2
C	501	TYR	ASN	variant	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	682	GLY	ARG	engineered mutation	UNP P0DTC2
C	683	SER	ARG	engineered mutation	UNP P0DTC2
C	685	SER	ARG	engineered mutation	UNP P0DTC2
C	701	VAL	ALA	variant	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	1209	GLY	-	linker	UNP P0DTC2
C	1210	SER	-	linker	UNP P0DTC2
C	1232	LEU	PHE	engineered mutation	UNP P10104

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1238	GLY	-	expression tag	UNP P10104
C	1239	ARG	-	expression tag	UNP P10104
C	1240	SER	-	expression tag	UNP P10104
C	1241	LEU	-	expression tag	UNP P10104
C	1242	GLU	-	expression tag	UNP P10104
C	1243	VAL	-	expression tag	UNP P10104
C	1244	LEU	-	expression tag	UNP P10104
C	1245	PHE	-	expression tag	UNP P10104
C	1246	GLN	-	expression tag	UNP P10104

MolProbity failed to run properly - this section is therefore empty.

3 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	309062	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.384	Depositor
Minimum map value	-0.335	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.057	Depositor
Recommended contour level	0.15	Depositor
Map size ($\text{\AA}$)	313.6, 313.6, 313.6	wwPDB
Map dimensions	224, 224, 224	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.4, 1.4, 1.4	Depositor

4 Model quality [i](#)

4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

There are no ligands in this entry.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	1-C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	320:VAL	C	321:GLN	N	1.70

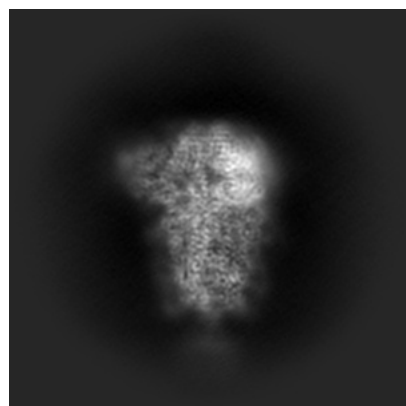
5 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51280. These allow visual inspection of the internal detail of the map and identification of artifacts.

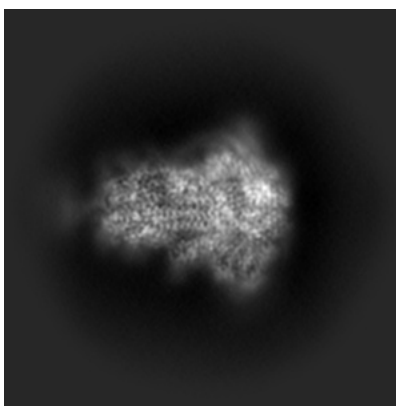
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

5.1 Orthogonal projections [i](#)

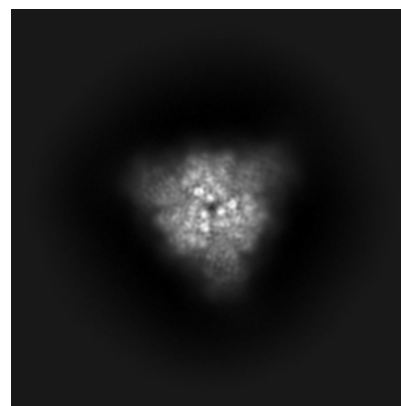
5.1.1 Primary map



X

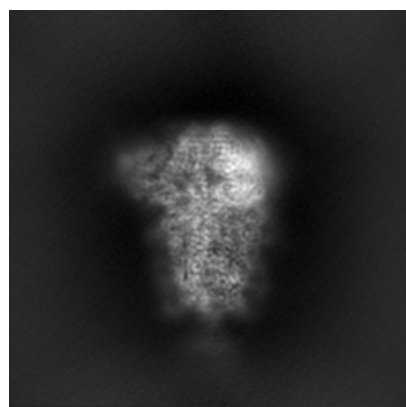


Y

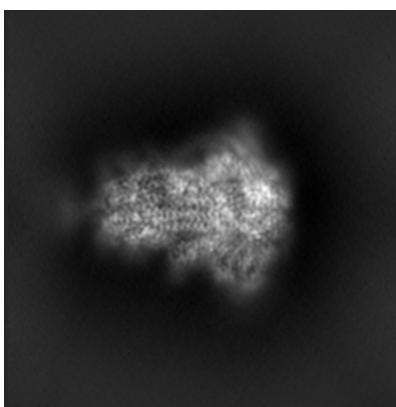


Z

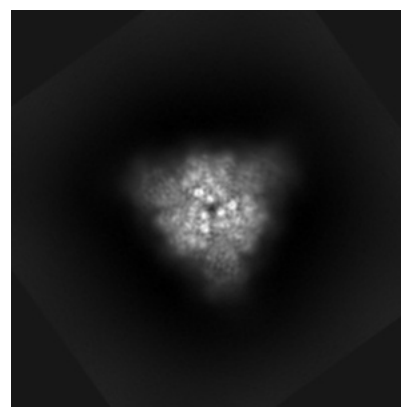
5.1.2 Raw map



X



Y

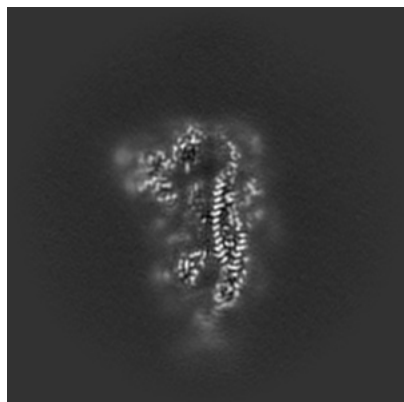


Z

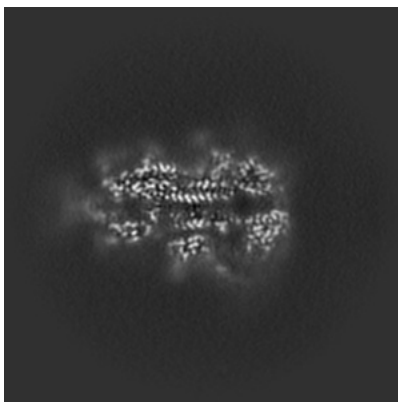
The images above show the map projected in three orthogonal directions.

5.2 Central slices [i](#)

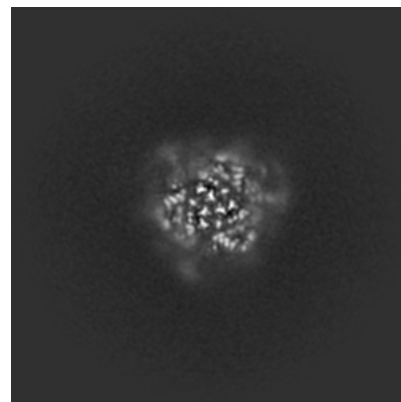
5.2.1 Primary map



X Index: 112

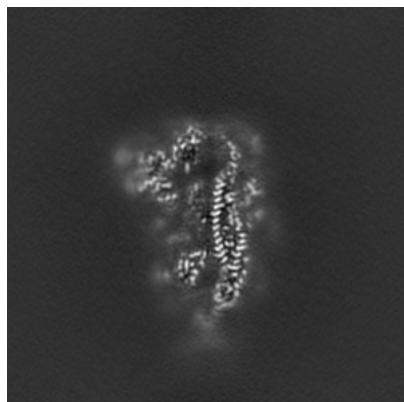


Y Index: 112

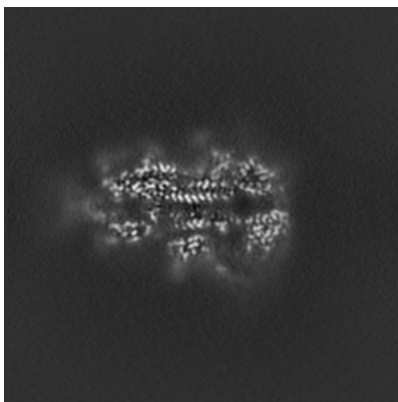


Z Index: 112

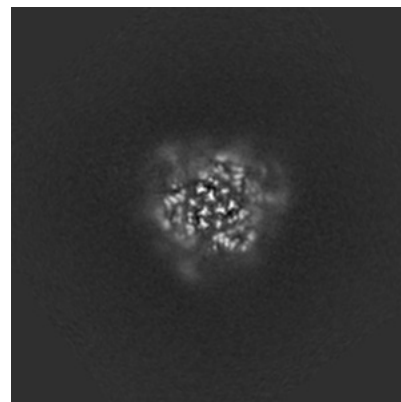
5.2.2 Raw map



X Index: 112



Y Index: 112

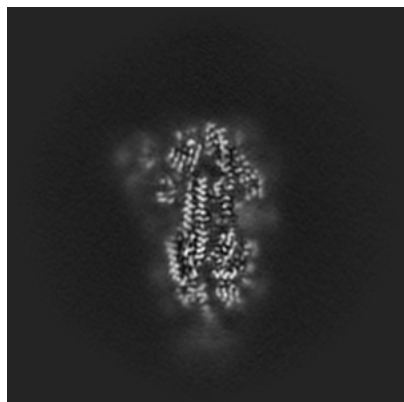


Z Index: 112

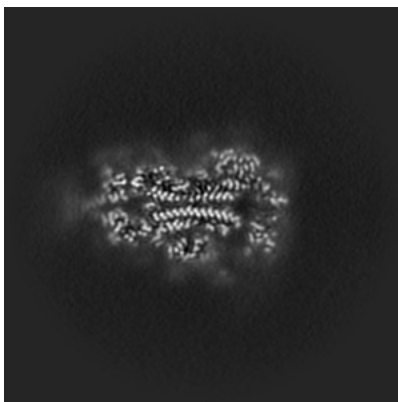
The images above show central slices of the map in three orthogonal directions.

5.3 Largest variance slices [i](#)

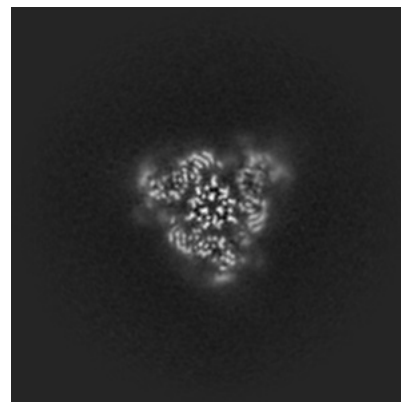
5.3.1 Primary map



X Index: 107

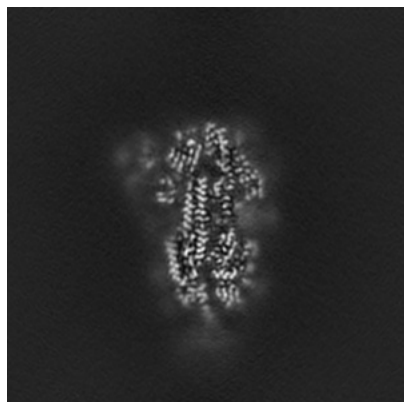


Y Index: 109

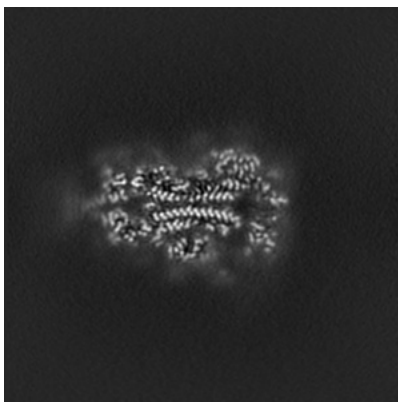


Z Index: 119

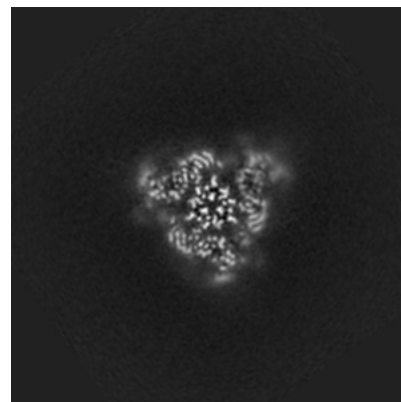
5.3.2 Raw map



X Index: 107



Y Index: 109

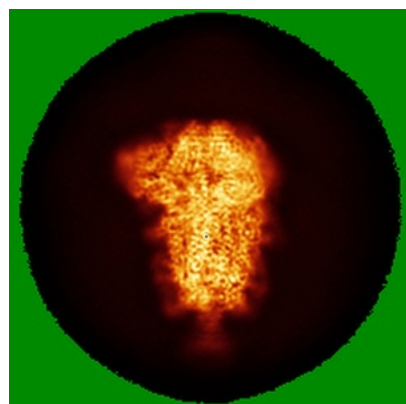


Z Index: 119

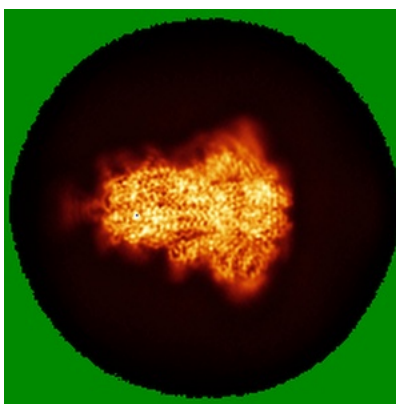
The images above show the largest variance slices of the map in three orthogonal directions.

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

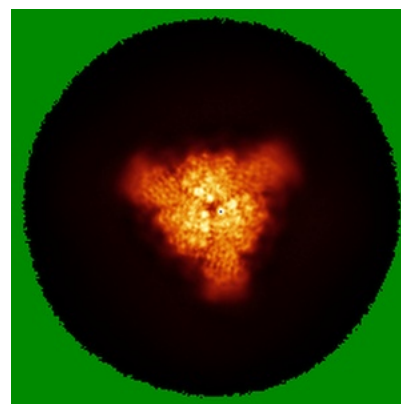
5.4.1 Primary map



X

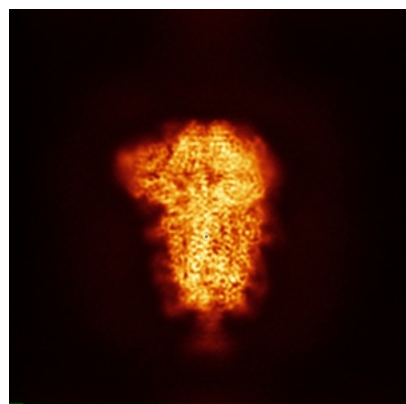


Y

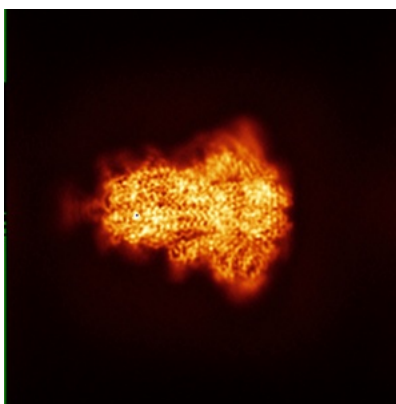


Z

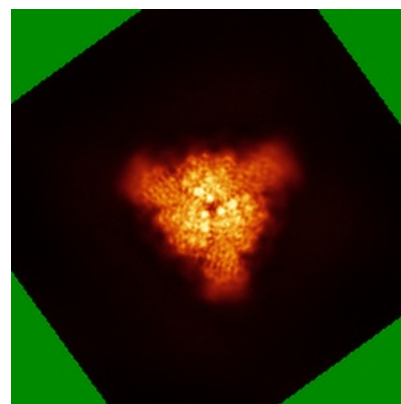
5.4.2 Raw map



X



Y

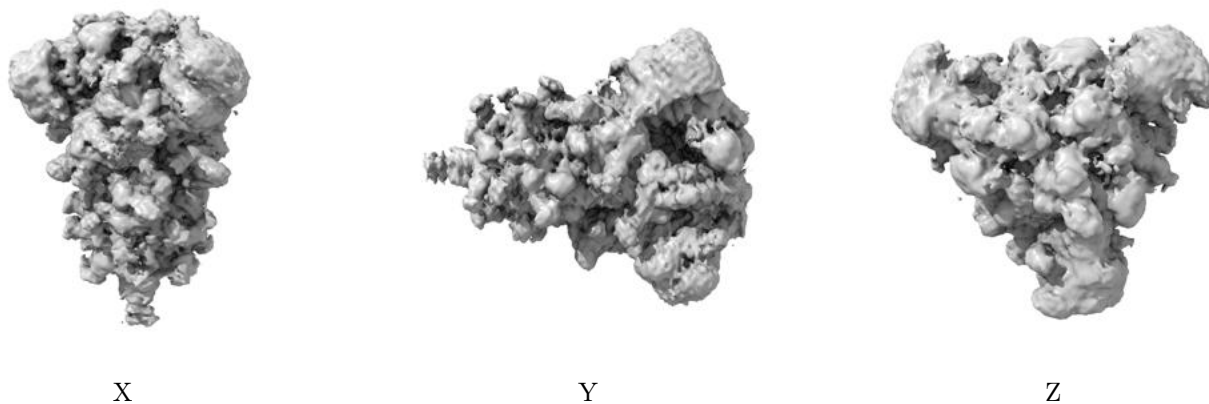


Z

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.

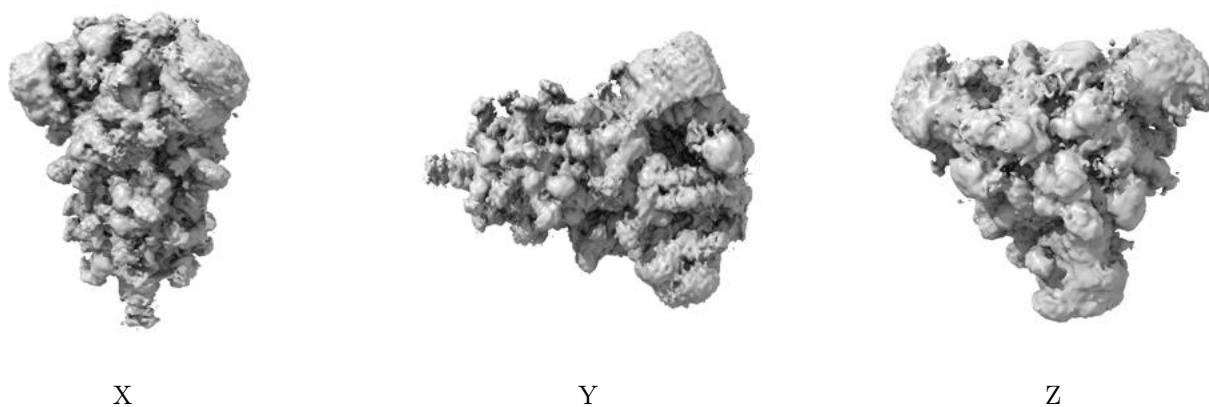
5.5 Orthogonal surface views [i](#)

5.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

5.5.2 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.

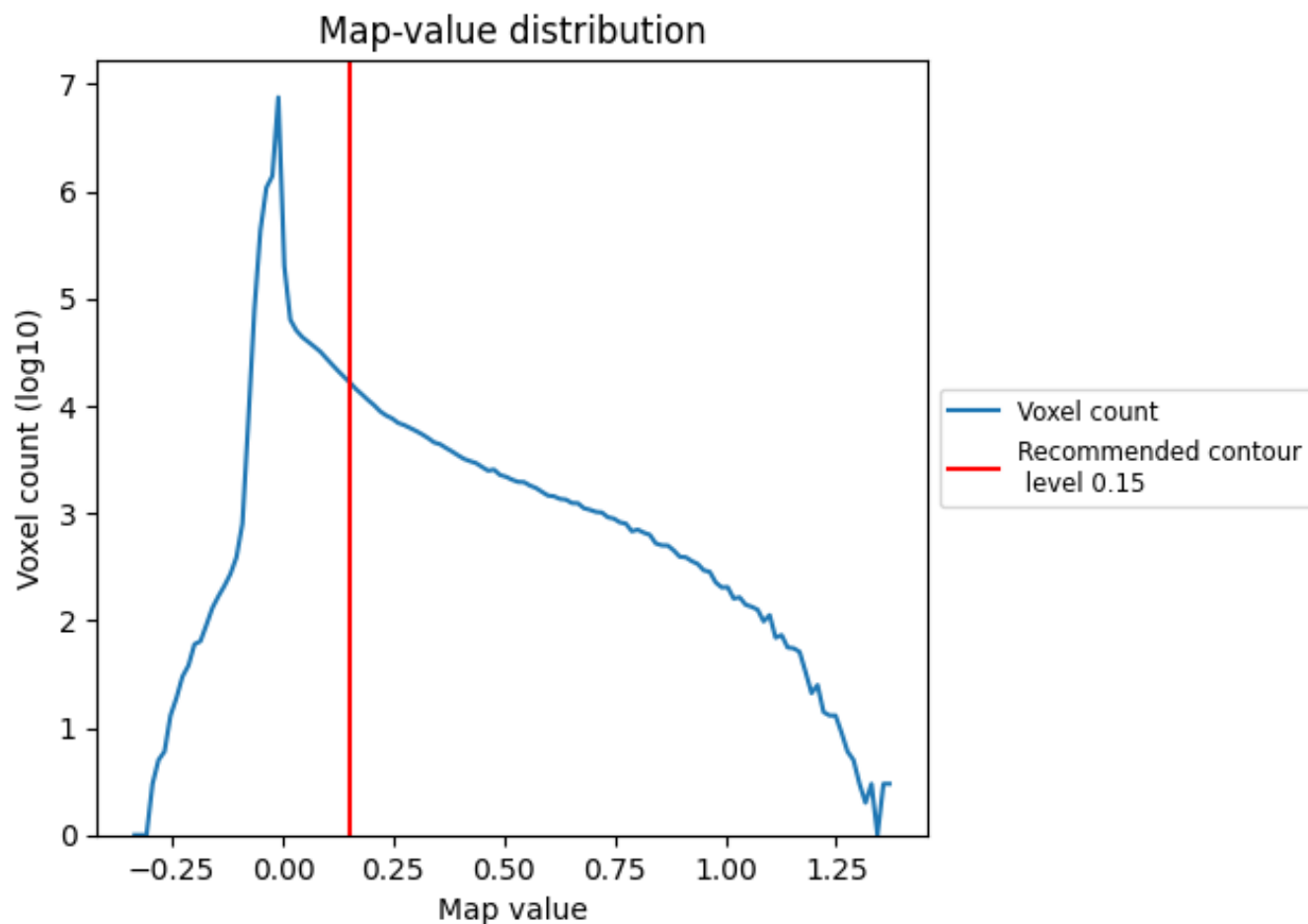
5.6 Mask visualisation [i](#)

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

6 Map analysis [i](#)

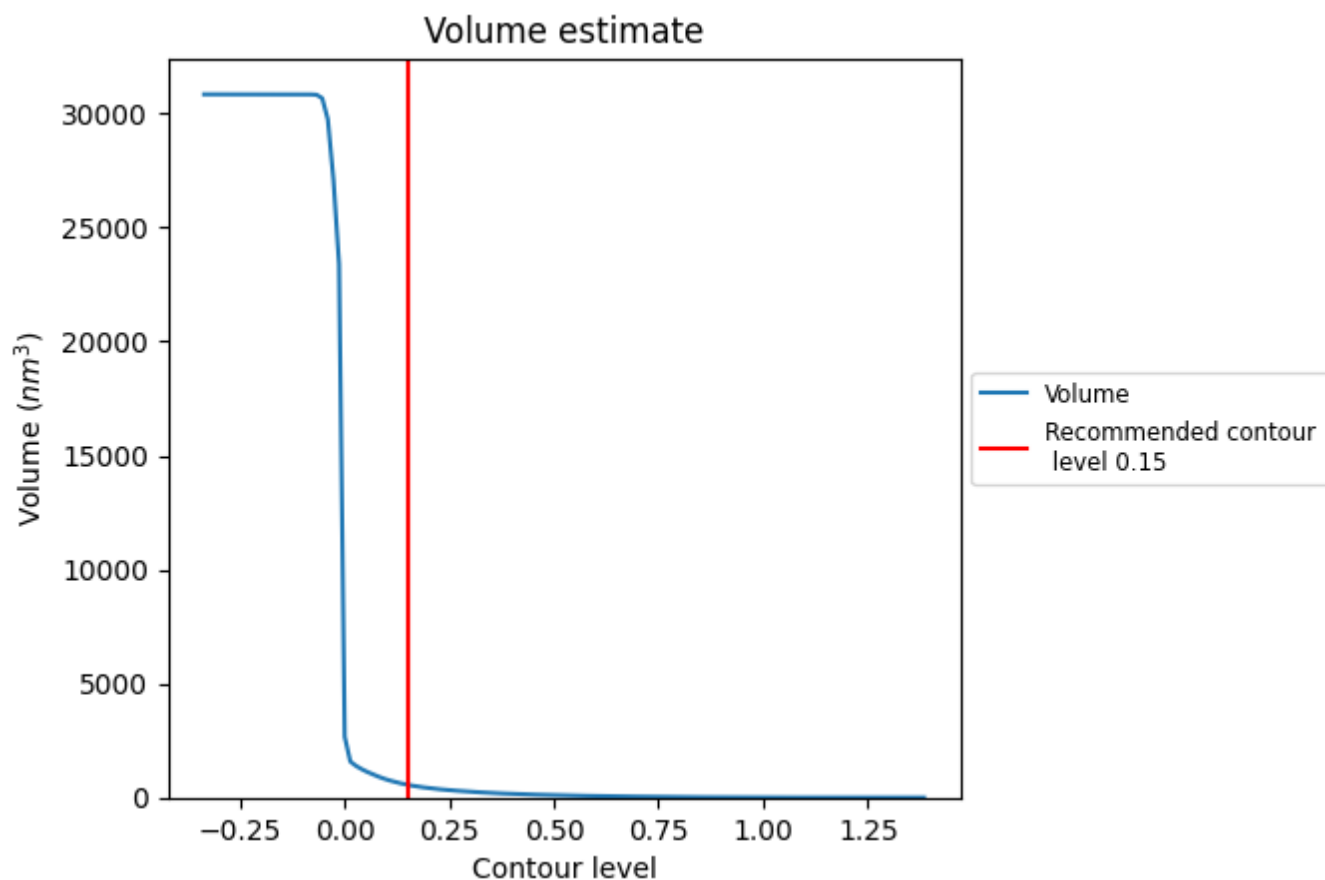
This section contains the results of statistical analysis of the map.

6.1 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.

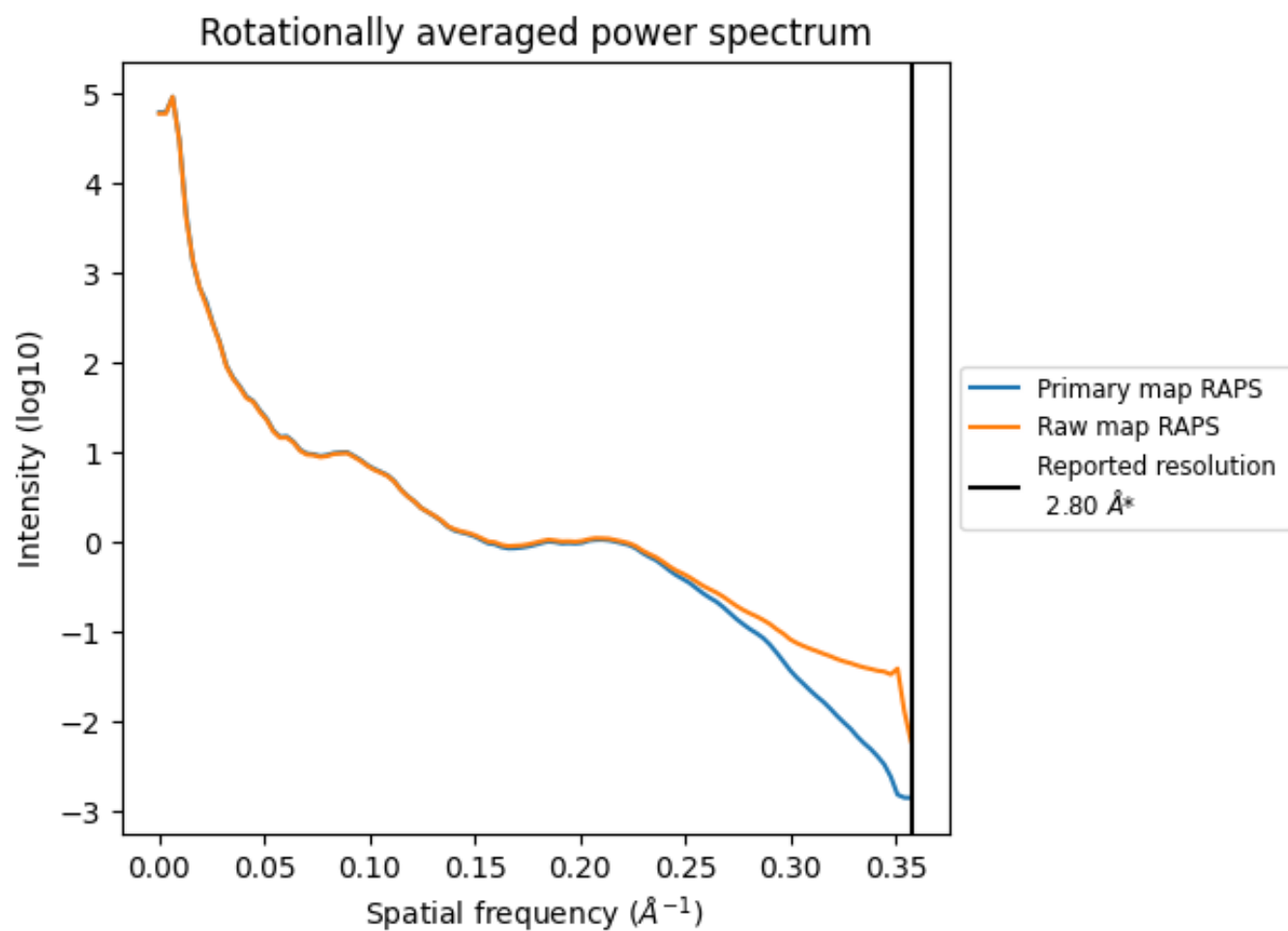
6.2 Volume estimate [i](#)



The volume at the recommended contour level is 564 nm^3 ; this corresponds to an approximate mass of 510 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.

6.3 Rotationally averaged power spectrum ⓘ

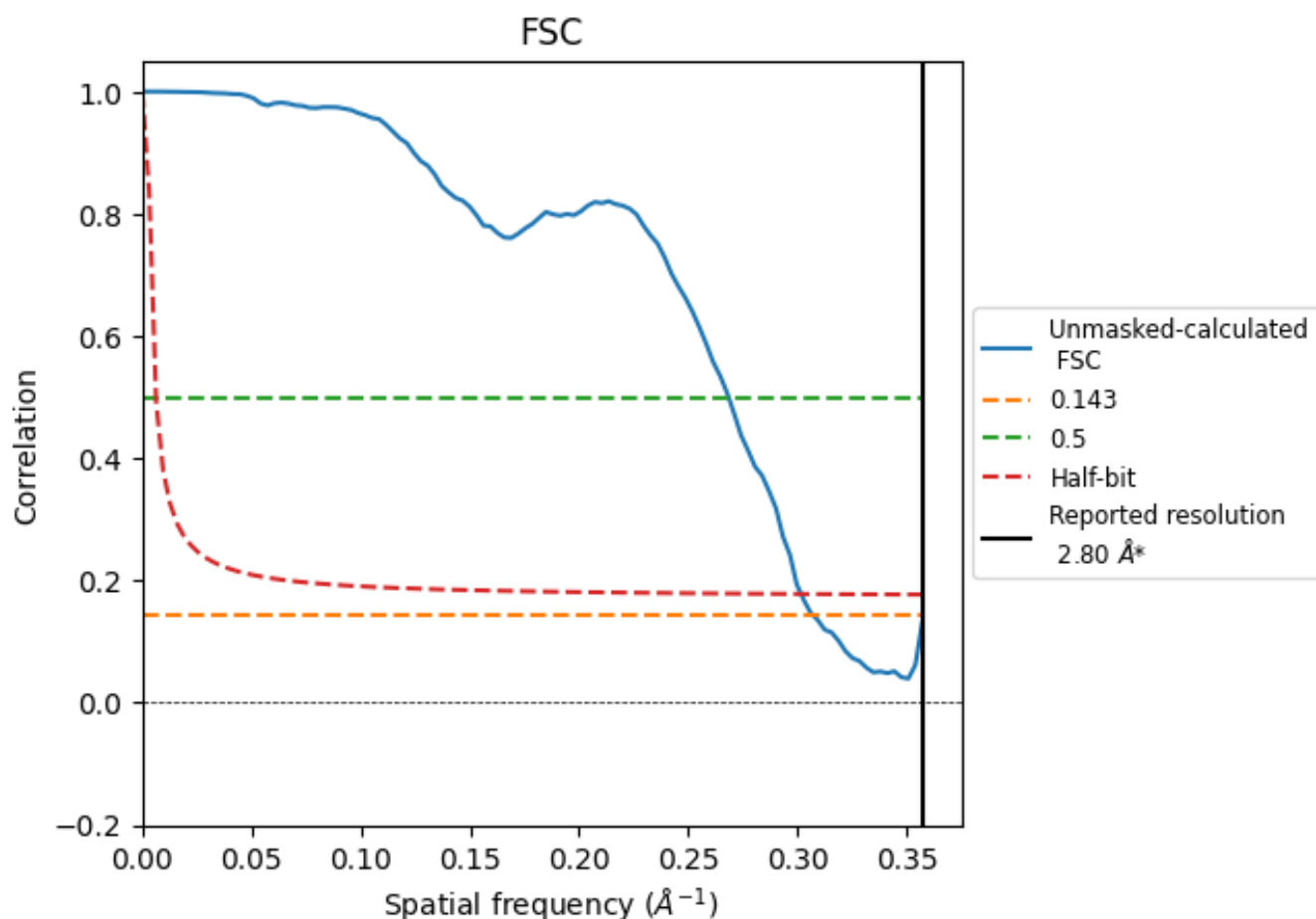


*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

7 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.

7.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.357 \text{ \AA}^{-1}$

7.2 Resolution estimates [i](#)

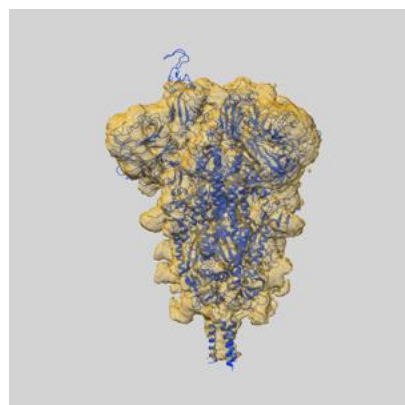
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.26	3.73	3.31

*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 3.26 differs from the reported value 2.8 by more than 10 %

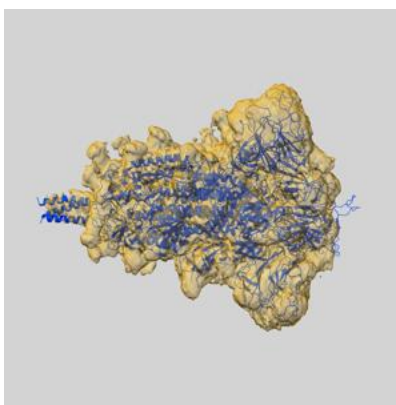
8 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-51280 and PDB model 9GDY. Per-residue inclusion information can be found in section ?? on page ??.

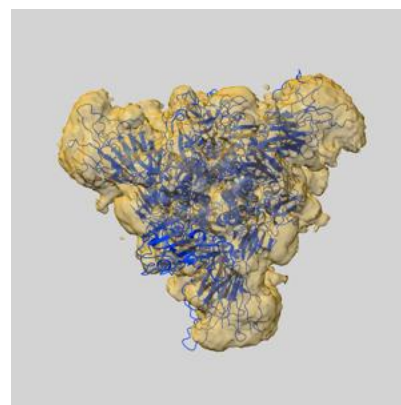
8.1 Map-model overlay [i](#)



X



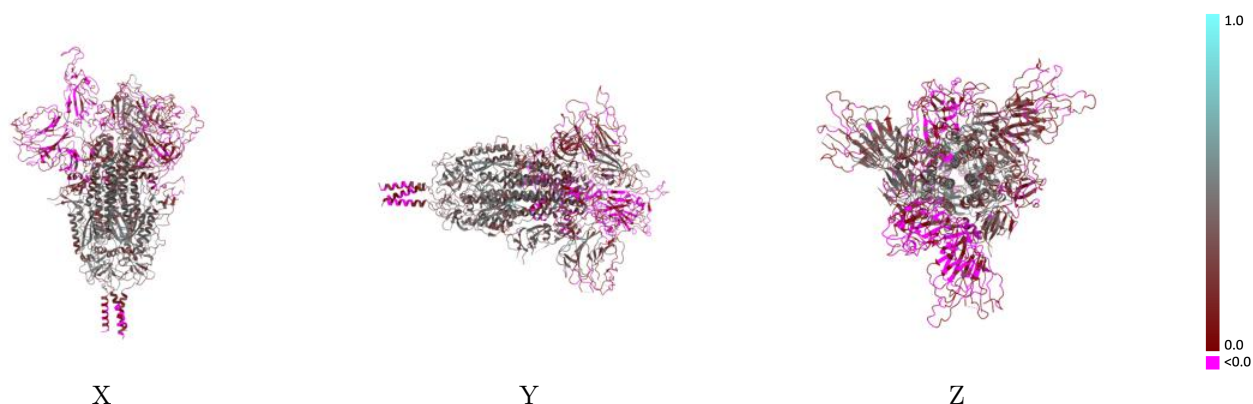
Y



Z

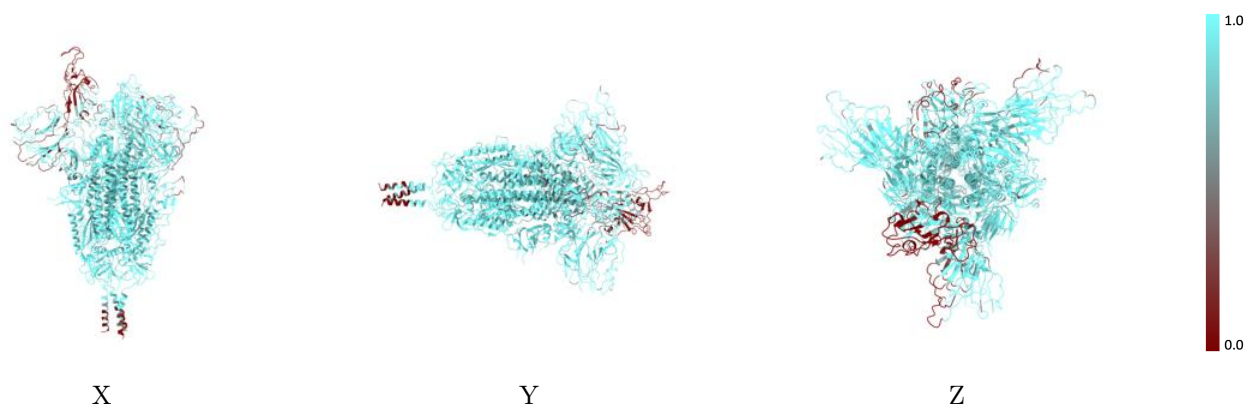
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



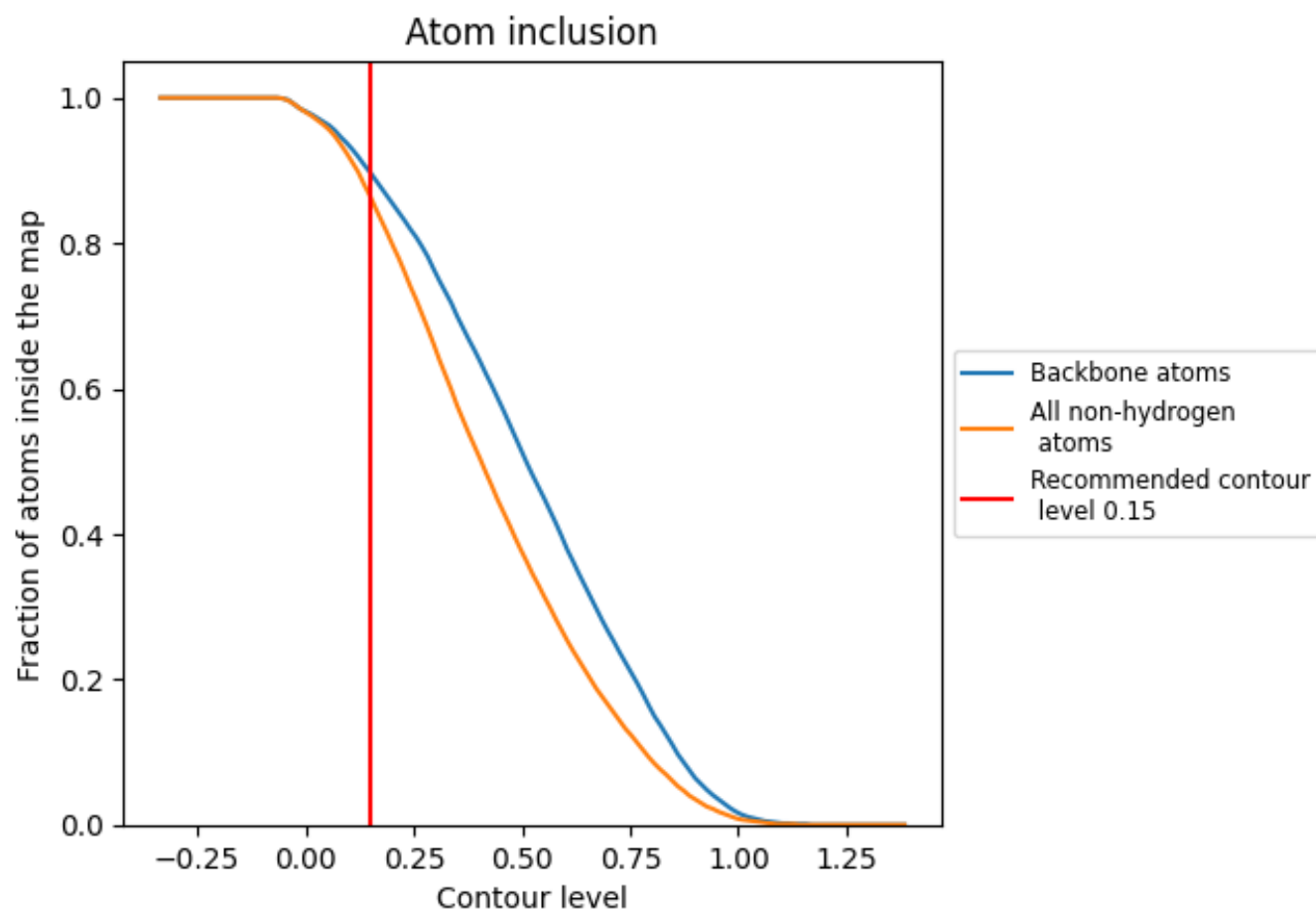
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

8.3 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 (0.15).

8.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 86% of all non-hydrogen atoms, are inside the map.

8.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8640	0.2390
A	0.8260	0.2590
B	0.8900	0.2410
C	0.8750	0.2170

