



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 05:32 PM UTC

PDB ID : 7FG7 / pdb_00007fg7
EMDB ID : EMD-31578
Title : Cryo-EM structure of S protein trimer of SARS-CoV2
Authors : Song, C.; Murata, K.; Katayama, K.
Deposited on : 2021-07-26
Resolution : 6.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

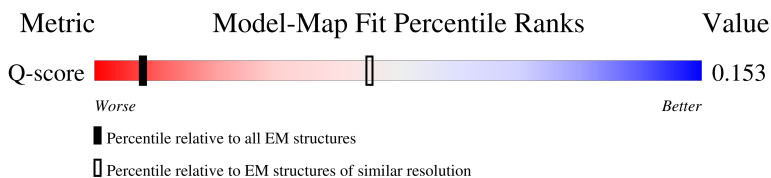
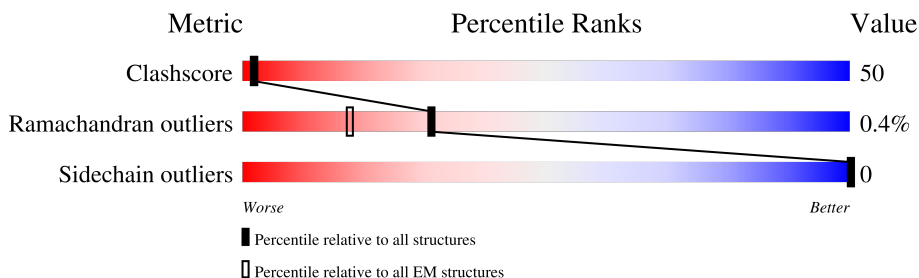
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.90 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	479 (6.40 - 7.40)

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	1273	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 8690 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.

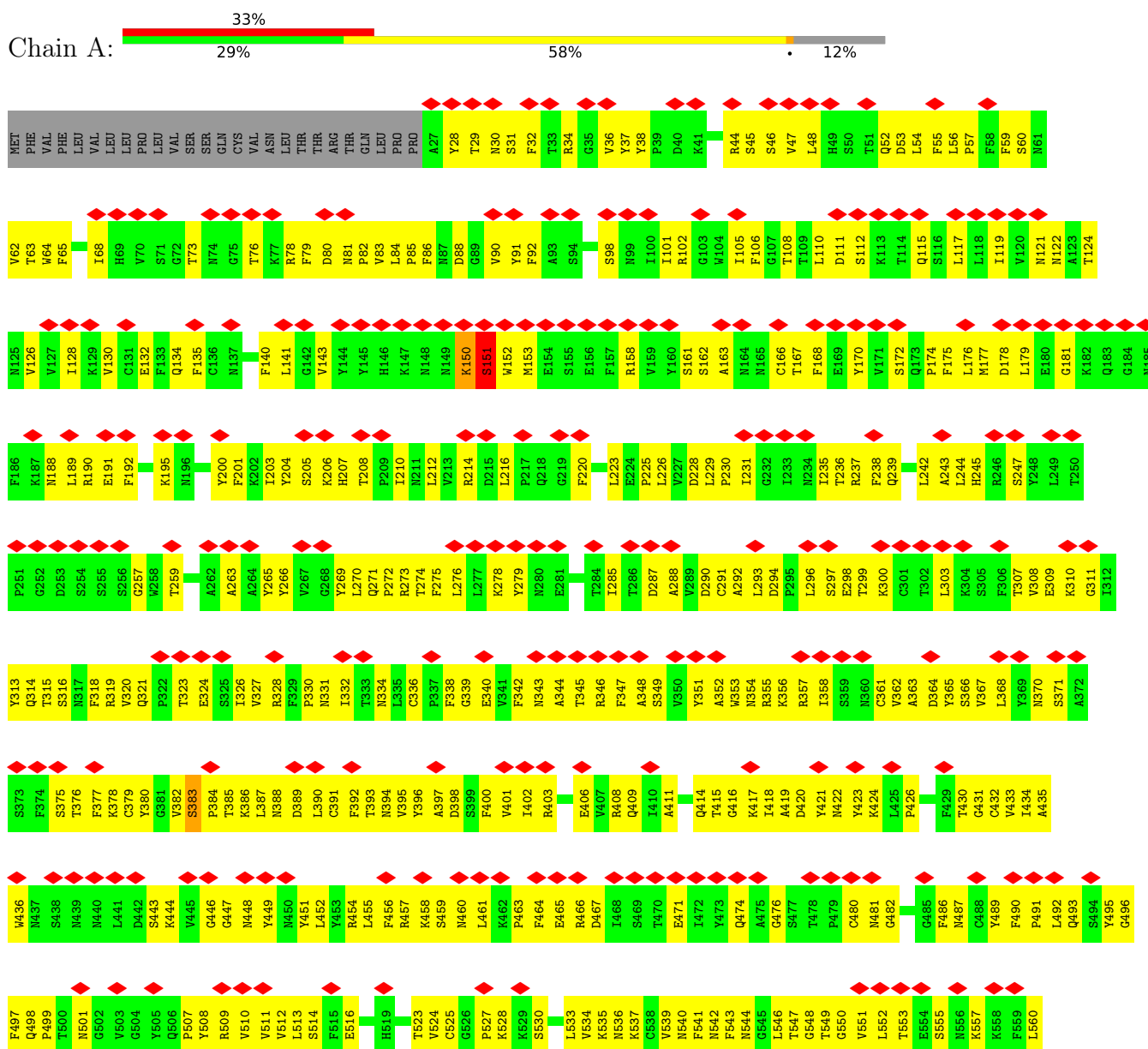
- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1114	8690	5534	1460	1657	39	0	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: Spike glycoprotein



GLY	CYS	ASN	LEU	C1126	H1064	L1001	D936	T874	K814	L754	V687	A526	P561
CYS	CYS	ASN	LEU	D1127	V1065	Q1002	S937	S875	R815	Q755	A688	D827	Q561
SER	SER	GLU	VAL	V1128	T1066	L1004	L938	A876	S816	T756	S889	Q828	Q564
CYS	CYS	ALA	VAL	V1129	T1067	Q1005	S939	L877	F817	G757	Q590	L829	F565
GLY	GLY	LYS	ASN	I1130	V1068	T1006	T941	L878	I818	S758	S691	T630	G566
SER	SER	ASN	LEU	P1069	F1069	Y1007	Q941	G880	D820	F759	I692	P631	R567
CYS	CYS	LEU	LEU	V1132	A1070	V1008	D950	T881	L821	C760	I693	T632	D569
CYS	CYS	ASN	ASN	V1133	A1071	T1009	V951	T882	L822	T761	A694	M634	I569
LYS	LYS	GLU	GLN	Q1010	Q1071	Q1010	V952	T883	F823	Q762	G995	V635	A570
PHE	PHE	SER	SER	H1134	E1072	Q1011	G946	T884	N824	L763	T696	Y636	D571
ASP	ASP	LEU	LEU	N1135	K1073	L1012	K947	S884	K825	L764	M697	Y636	D571
GLY	GLY	ILE	ILE	T1136		L1013	L948	G885	V626	R765	S698	T637	T572
ASP	ASP	ASP	ASP	V1137	T1077	R1014	D950	N886	T627	A766	L699	L767	T572
LEU	LEU	LEU	LEU	Y1138	A1078	A1015	V951	T887	L828	T768	V705	T638	T573
GLN	GLN	GLN	GLN	P1079	Q1071	E1017	V952	F888	A829	Q769	A706	G639	D574
GLU	GLU	GLU	GLU	A1080	E1072	I1018	N953	G889	D830	I770	T707	S640	A575
PRO	PRO	PRO	PRO	I1140	K1073	R1019	Q954	A890	A831	A771	S708	N641	V576
VAL	VAL	VAL	VAL			A1020	N955	G891	G832	D775	S708	V642	R577
LEU	LEU	LEU	LEU			S1021	Q957	A892	F833	Q774	N709	F643	D578
LYS	LYS	LYS	LYS			L1024	A958	A893	I834	D775	N710	Q644	P579
GLY	GLY	GLY	GLY			L1025	N960	L894	K835	D776	S711	T645	Q580
GLN	GLN	GLN	GLN			A1026	N961	Q895	Q836	N777	I712	R646	T581
ILE	ILE	ILE	ILE			T1027	T961	I896	Y837	T778	A713	C649	L582
LYS	LYS	LYS	LYS			P1028	L962	P897	G838	Q779	I714	L850	E583
TRP	TRP	TRP	TRP			M1029	V963	F898	D839	E780	P715	I584	I584
TRP	TRP	TRP	TRP			E1030	K964	A899	C940	T716	T716	A585	L585
LEU	LEU	LEU	LEU			C1032	Q965	N900	C940	N717	T718	A585	D586
ASP	ASP	ASP	ASP			V1033	L966	Q901	L841	F782	T719	H655	T588
LYS	LYS	LYS	LYS			L1034	F970	N902	G842	Q784	I720	V656	P589
TYR	TYR	TYR	TYR			G1035	I973	A903	D843	Q785		N657	C590
PHE	PHE	PHE	PHE			Q1036	S974	Y904	I844	Q786	E725	N658	S591
LYS	LYS	LYS	LYS			S1037	S975	R905	A845	Q787	I726	N659	F592
ALA	ALA	ALA	ALA			K1038	V976	F906	A846	I788	I726	Y660	V595
SER	SER	SER	SER			R1039	L977	N907	R847	Y789	L727	E661	S596
PRO	PRO	PRO	PRO			V1040	N978	I909	D848	P792	P728	C662	V597
ASP	ASP	ASP	ASP			P1041	N979	G910	L849	F793	V729	D663	I598
VAL	VAL	VAL	VAL			F1042	I980	V911	I850	I794	M731	I664	I598
LEU	LEU	LEU	LEU			C1043	R983	T912	C951	K795	T732	I666	T599
GLY	GLY	GLY	GLY			Y1047	L984	Q913	A852	D796	T734	G667	P600
ASP	ASP	ASP	ASP			H1048	D965	L916	Q854	F797	S735	A668	G801
ILE	ILE	ILE	ILE			L1049	K986	Y917	F955	Q798	V736	G669	T602
SER	SER	SER	SER			M1050	V987	E918	G857	G799	C737	I670	N603
LYS	LYS	LYS	LYS			S1051	E988	N919	L858	F800	T739	C671	T604
ASN	ASN	ASN	ASN			F1052	A989	Q920	T859	N801	M740	A672	Q607
MET	MET	MET	MET			P1053	E990	K921	V860	F802	T741	S673	V608
THR	THR	THR	THR			Q1054	V991	L922	L861	Q804	I742	Y674	A609
VAL	VAL	VAL	VAL			S1055	Q992	L923	P862	I805	C743	Q675	V610
ASN	ASN	ASN	ASN			A1056	I993	A924	P863	L806	G744	T676	L611
ILE	ILE	ILE	ILE			P1057	I994	F927	L864	P807	D745	Q677	L612
CYS	CYS	CYS	CYS			H1058	R995	N928	L865	D808	T746	T678	Q613
SER	SER	SER	SER			L1059	L996	S929	T866	P809	T747	N679	Q613
GLN	GLN	GLN	GLN			V1060	I997	S929	T867	S810	T747	S880	D614
LEU	LEU	LEU	LEU			F1061	T998	A930	E868	P812	E748	P681	V615
ILE	ILE	ILE	ILE			L1062	G999	T931	N869	K311	C749	R682	N616
ASP	ASP	ASP	ASP			L1063	R1000	G932	I870	S750	S750	R683	V620
ARG	ARG	ARG	ARG					K933	A871	N751	L752	R685	P621
								I934	Q872	L752	L753	S886	V622
								Q935	Y873				A623
													I624
													H625

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	14235	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	JEOL 2200FS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	1578.3	Depositor
Maximum defocus (nm)	4967.2	Depositor
Magnification	45065	Depositor
Image detector	DIRECT ELECTRON DE-20 (5k x 3k)	Depositor
Maximum map value	0.213	Depositor
Minimum map value	-0.145	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.02	Depositor
Map size ($\text{\AA}$)	363.52, 363.52, 363.52	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.42, 1.42, 1.42	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	A	0.43	2/8893 (0.0%)	0.69	2/12105 (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	8

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	590	CYS	C-N	11.58	1.49	1.33
1	A	274	THR	C-N	10.68	1.48	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1049	LEU	CA-C-N	5.37	130.97	121.80
1	A	1049	LEU	C-N-CA	5.37	130.97	121.80

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	151	SER	Peptide
1	A	383	SER	Peptide
1	A	590	CYS	Peptide
1	A	837	TYR	Peptide
1	A	845	ALA	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8690	0	8483	865	0
All	All	8690	0	8483	865	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 50.

The worst 5 of 865 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:866:THR:HG22	1:A:869:MET:HE3	1.36	1.02
1:A:620:VAL:HG11	1:A:623:ALA:HB2	1.44	1.00
1:A:781:VAL:HG12	1:A:1026:ALA:HB2	1.48	0.96
1:A:1010:GLN:HB3	1:A:1014:ARG:HH12	1.30	0.94
1:A:448:ASN:HB3	1:A:497:PHE:HB3	1.51	0.93

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	1112/1273 (87%)	927 (83%)	180 (16%)	5 (0%)	30 67

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	838	GLY
1	A	839	ASP
1	A	150	LYS
1	A	151	SER
1	A	836	GLN

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	965/1112 (87%)	965 (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 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1058	HIS
1	A	1010	GLN
1	A	655	HIS
1	A	644	GLN
1	A	955	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

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-31578. These allow visual inspection of the internal detail of the map and identification of artifacts.

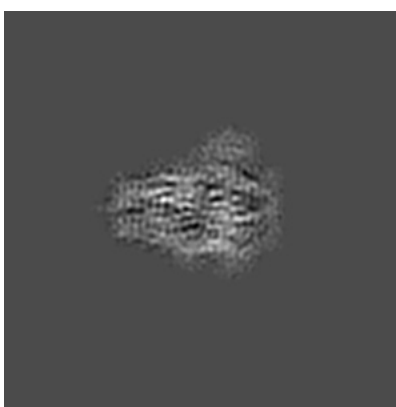
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

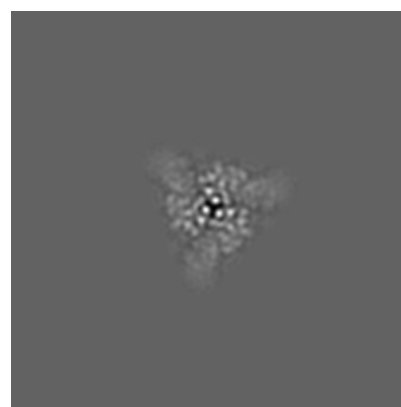
6.1.1 Primary map



X



Y



Z

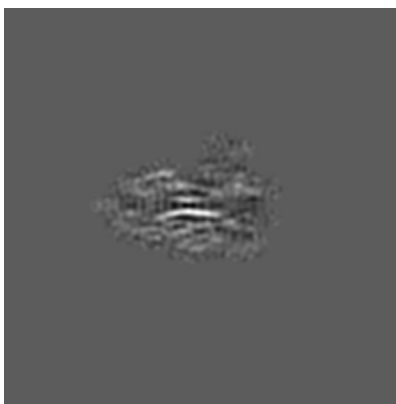
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 128



Y Index: 128



Z Index: 128

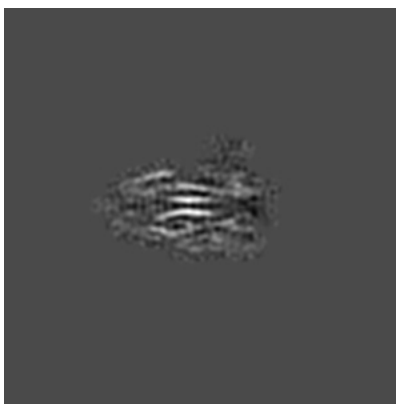
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 133



Y Index: 127

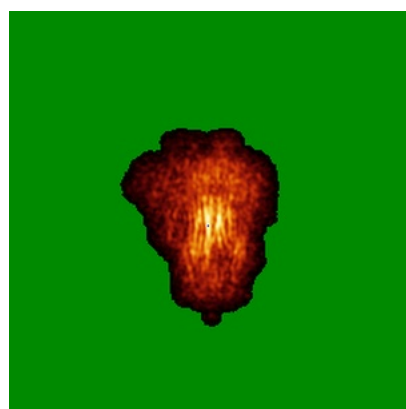


Z Index: 124

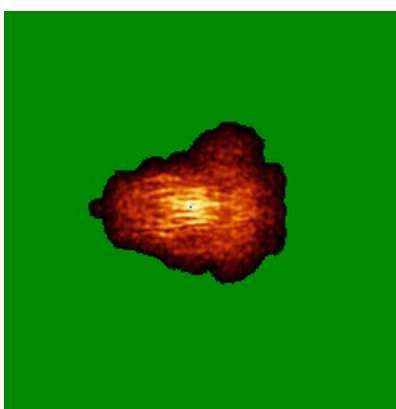
The images above show the largest variance slices of the map in three orthogonal directions.

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

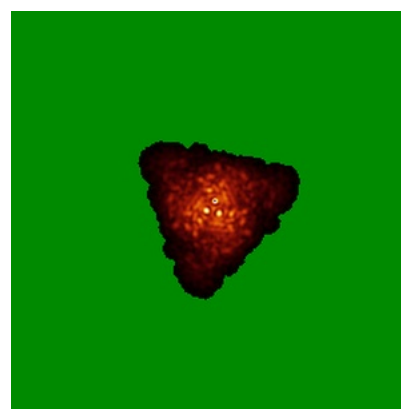
6.4.1 Primary map



X



Y

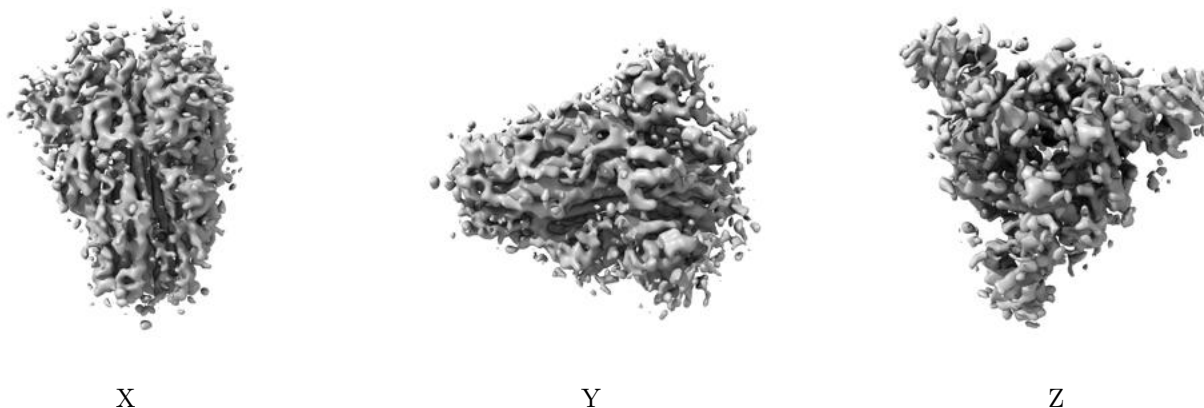


Z

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 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

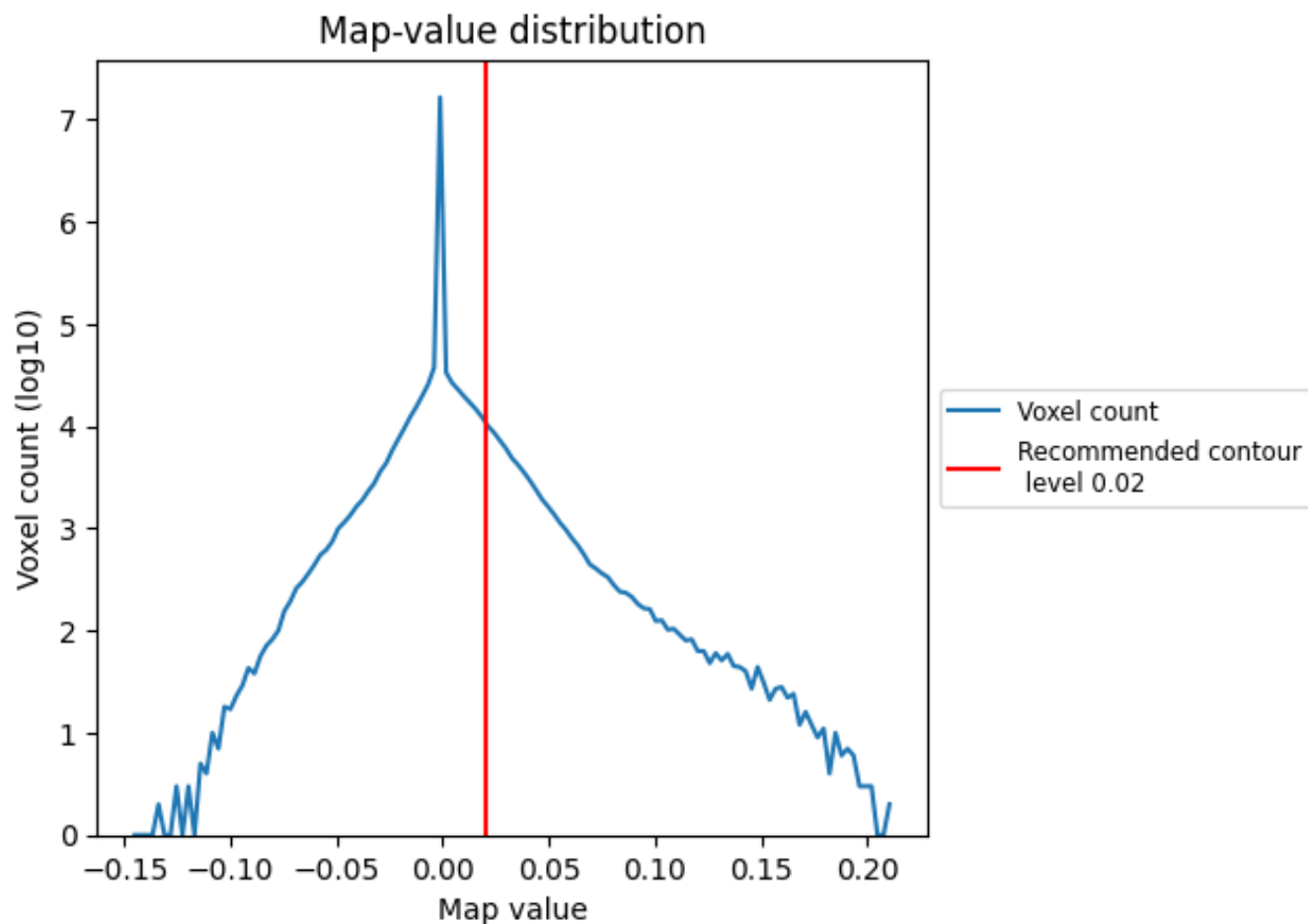
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

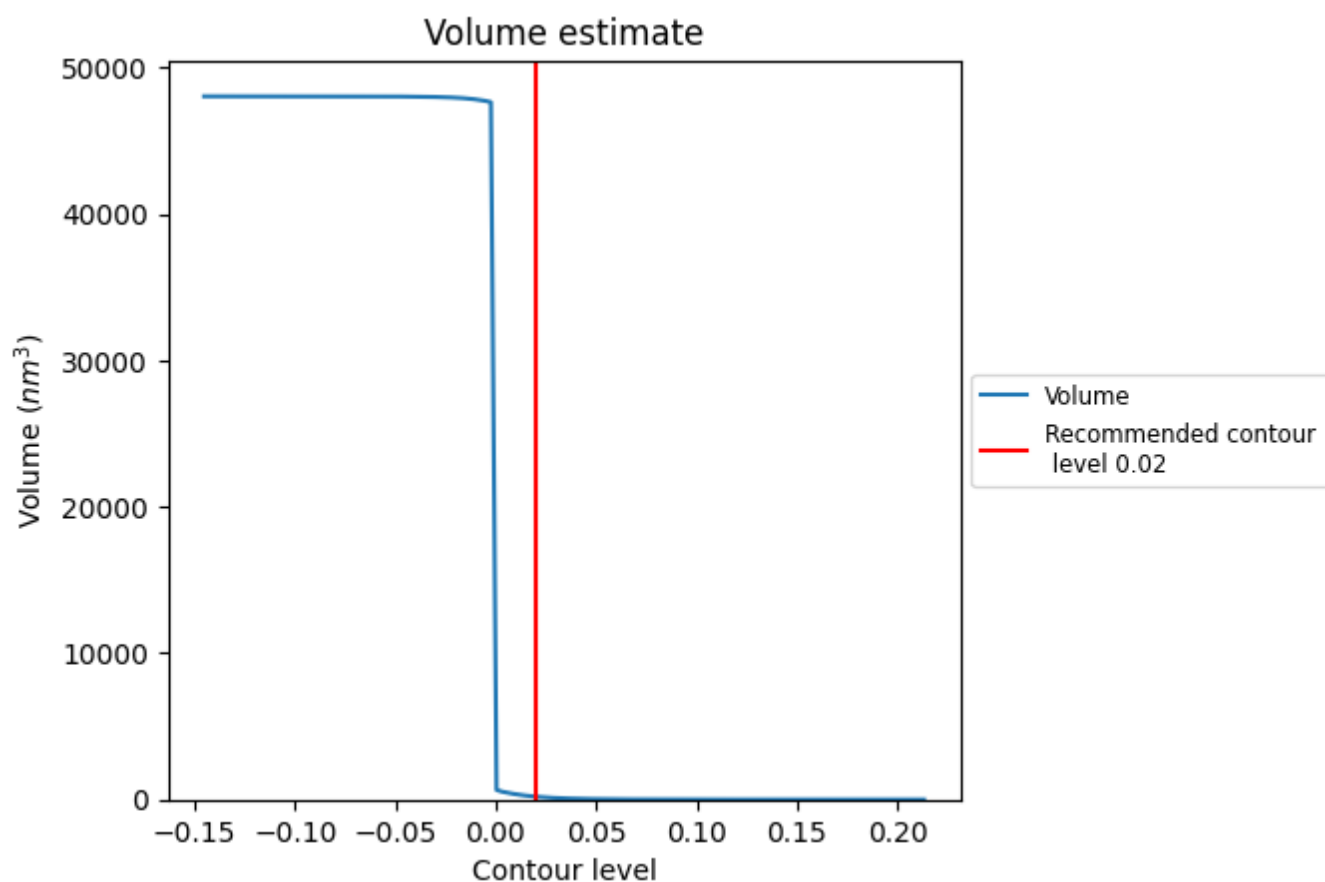
This section contains the results of statistical analysis of the map.

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.

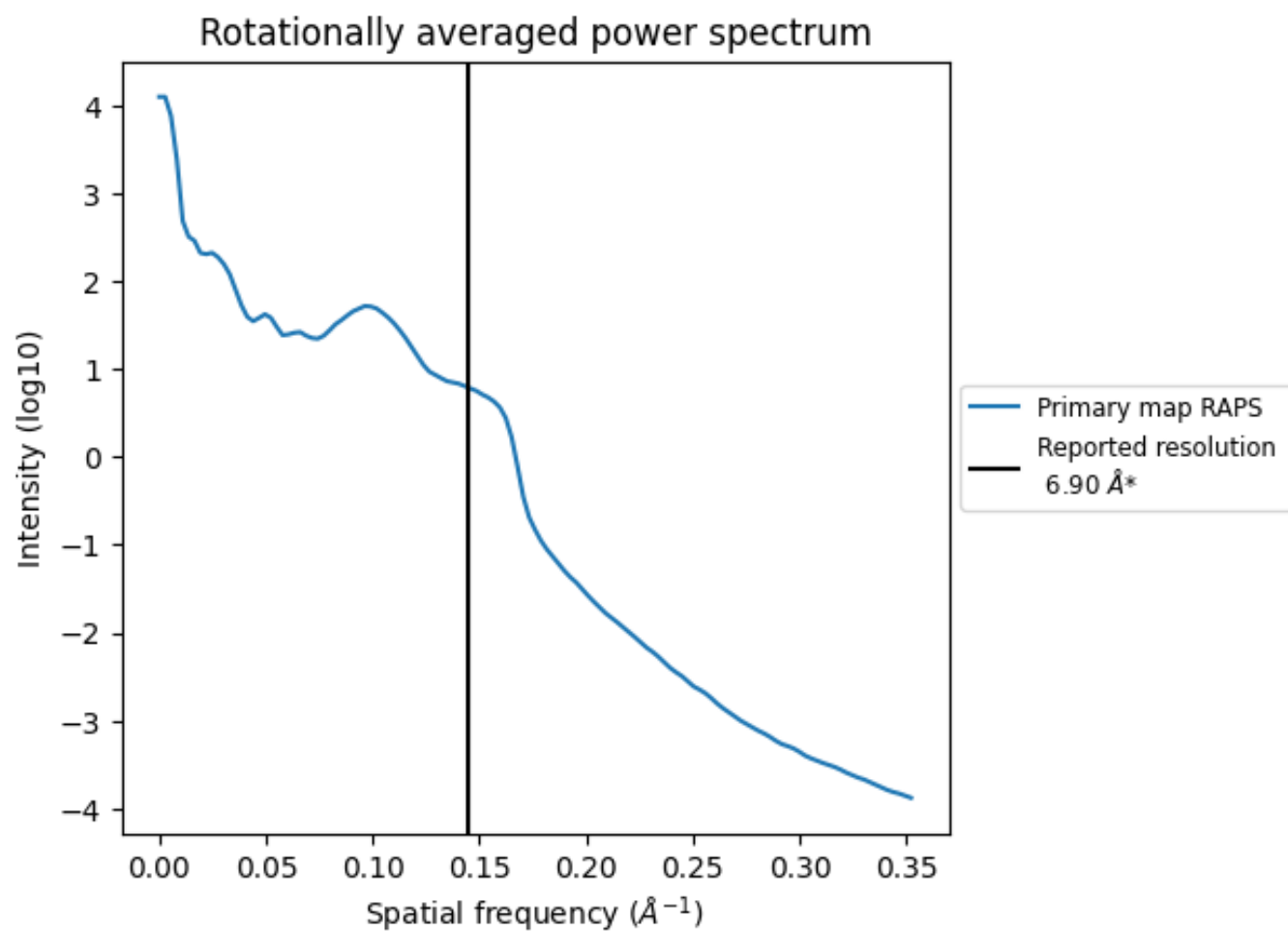
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 197 nm³; this corresponds to an approximate mass of 178 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 ⓘ

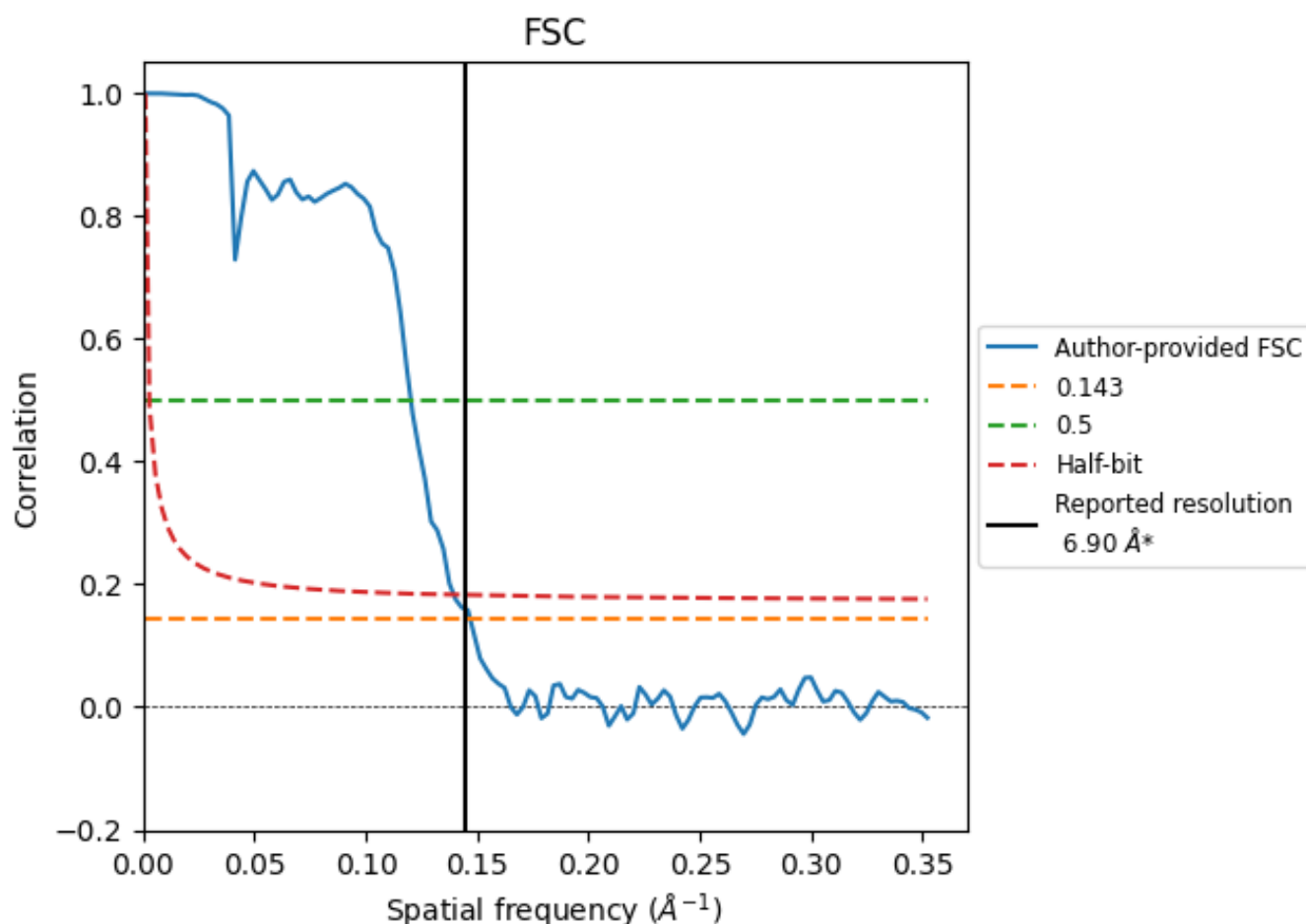


*Reported resolution corresponds to spatial frequency of 0.145 $\text{\AA}^{-1}$

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 0.145 Å⁻¹

8.2 Resolution estimates [i](#)

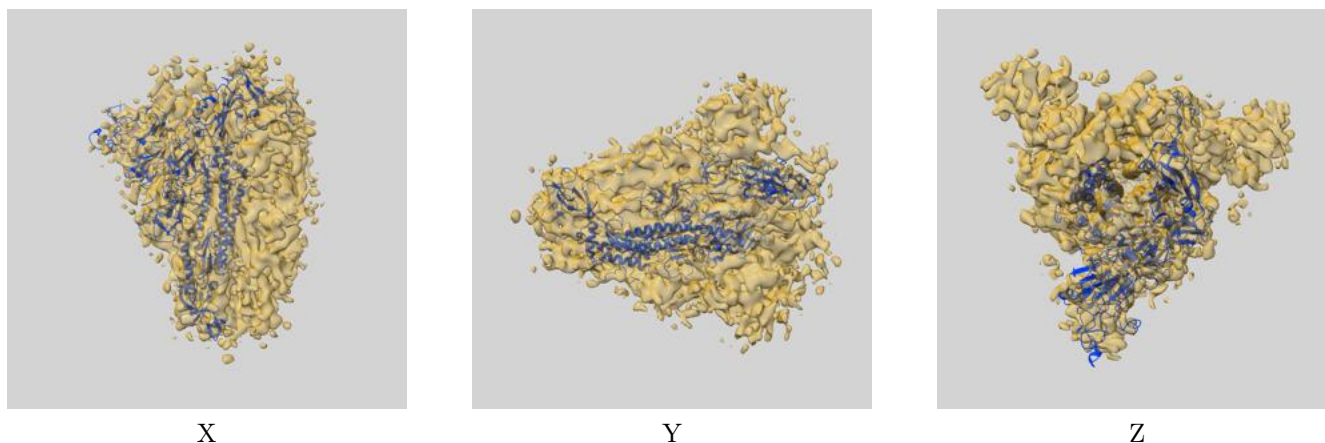
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.90	-	-
Author-provided FSC curve	6.81	8.32	7.17
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

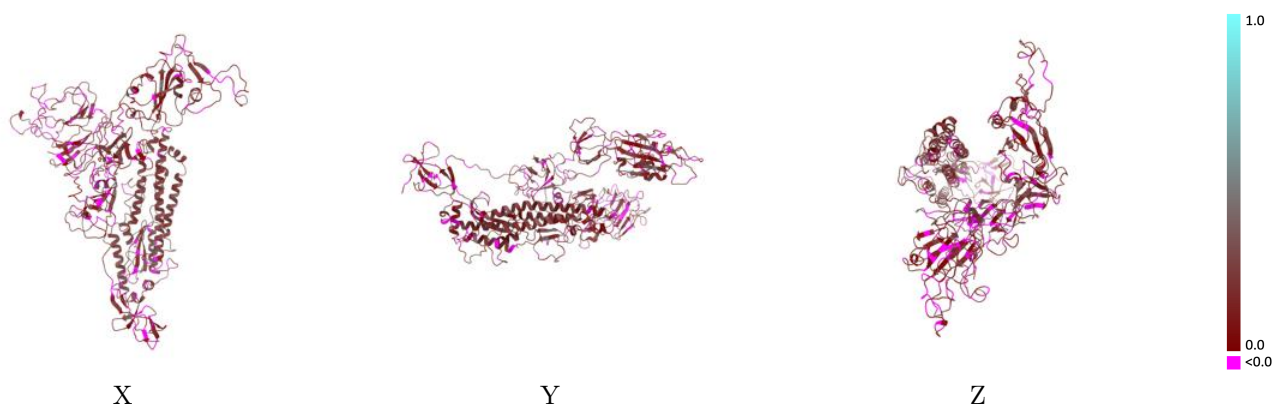
This section contains information regarding the fit between EMDB map EMD-31578 and PDB model 7FG7. Per-residue inclusion information can be found in section [3](#) on page [4](#).

9.1 Map-model overlay [i](#)



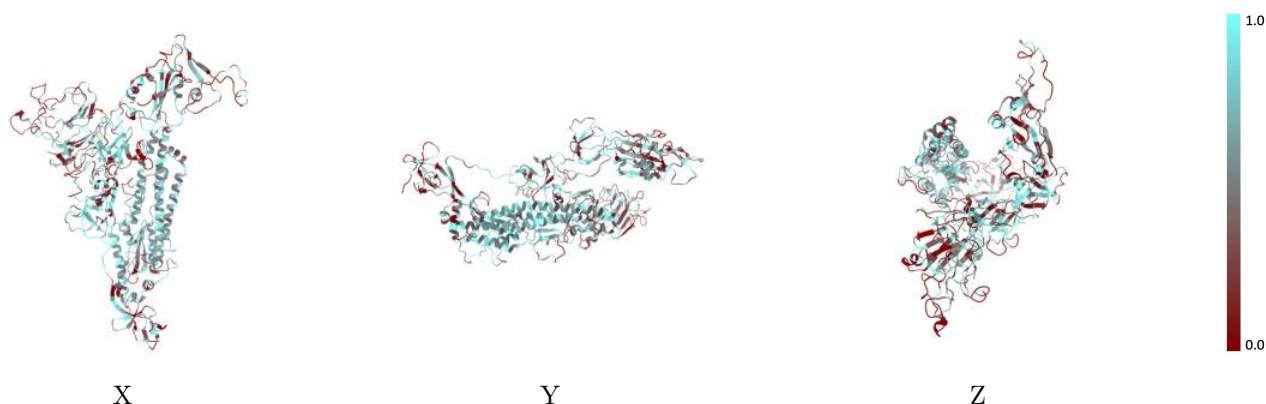
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



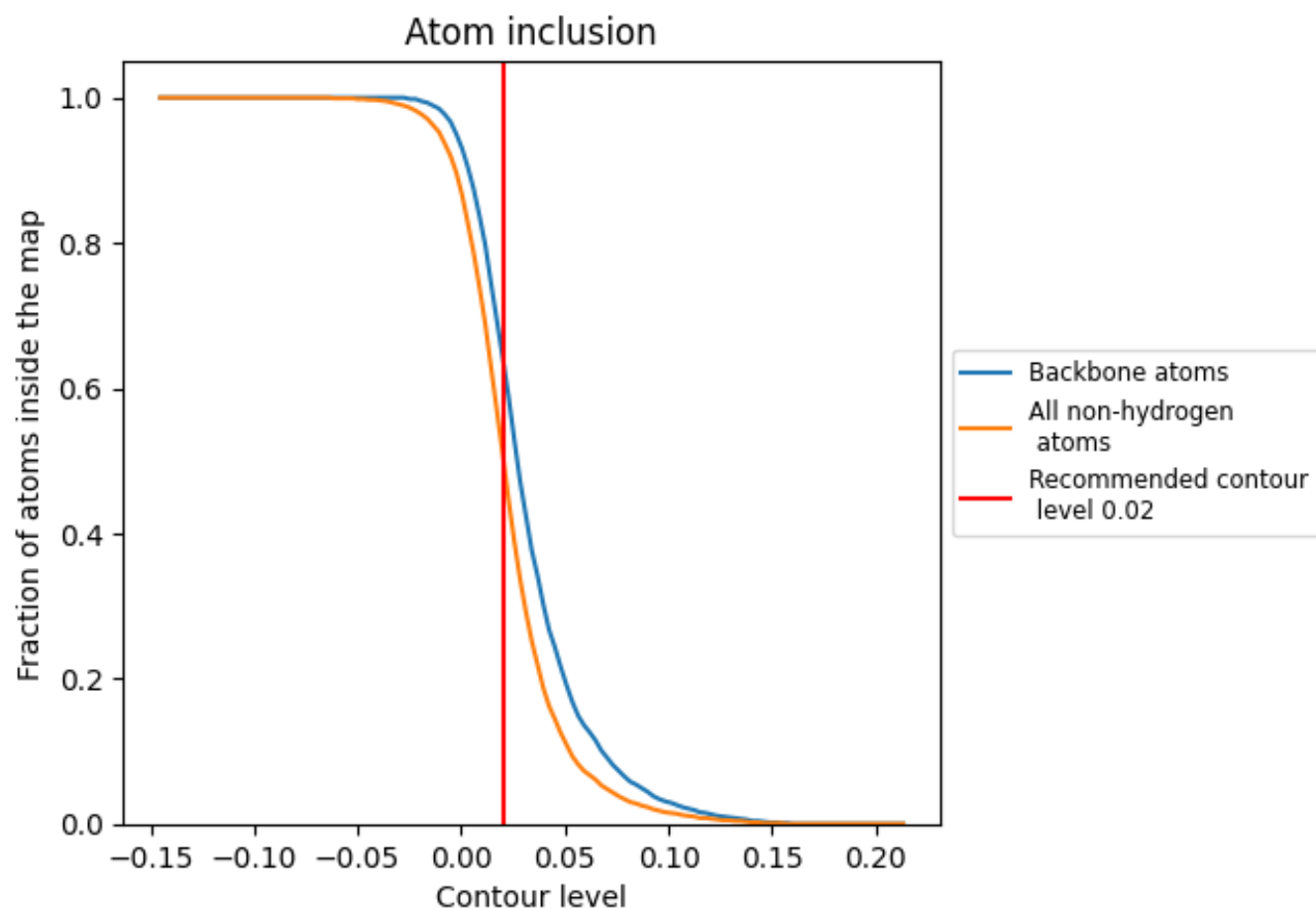
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 64% of all backbone atoms, 51% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5100	0.1530
A	0.5100	0.1530

