



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 01:55 AM UTC

PDB ID : 7TLC / pdb_00007tlc
EMDB ID : EMD-25987
Title : Down-state locked, S2 stabilized rS2d-HexaPro SARS-CoV-2 spike ectodomain
in the RBD-down conformation, State 1
Authors : Henderson, R.; Acharya, P.
Deposited on : 2022-01-18
Resolution : 2.83 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

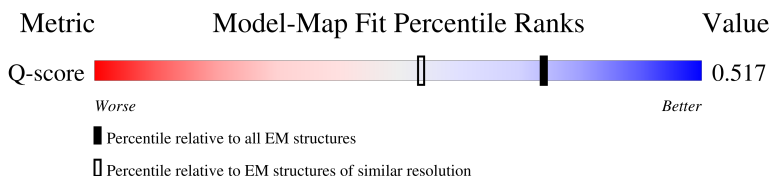
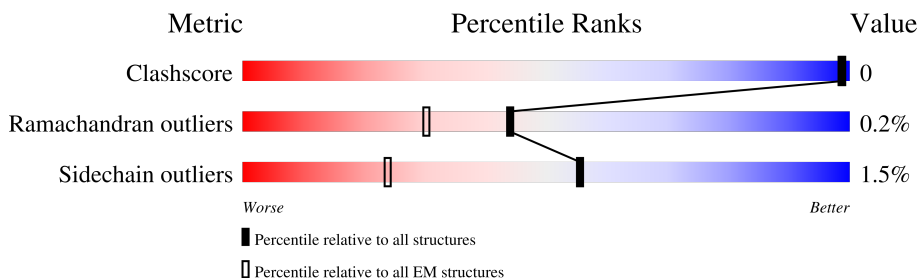
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.83 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	11847 (2.33 - 3.33)

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	1208	11% 78% 20%
1	B	1208	13% 80% 18%
1	C	1208	16% 79% 19%

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 23058 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
1	A	972	Total	C	N	O	S	0	0
			7604	4862	1262	1445	35		
1	B	992	Total	C	N	O	S	0	0
			7759	4961	1289	1474	35		
1	C	984	Total	C	N	O	S	0	0
			7695	4921	1276	1463	35		

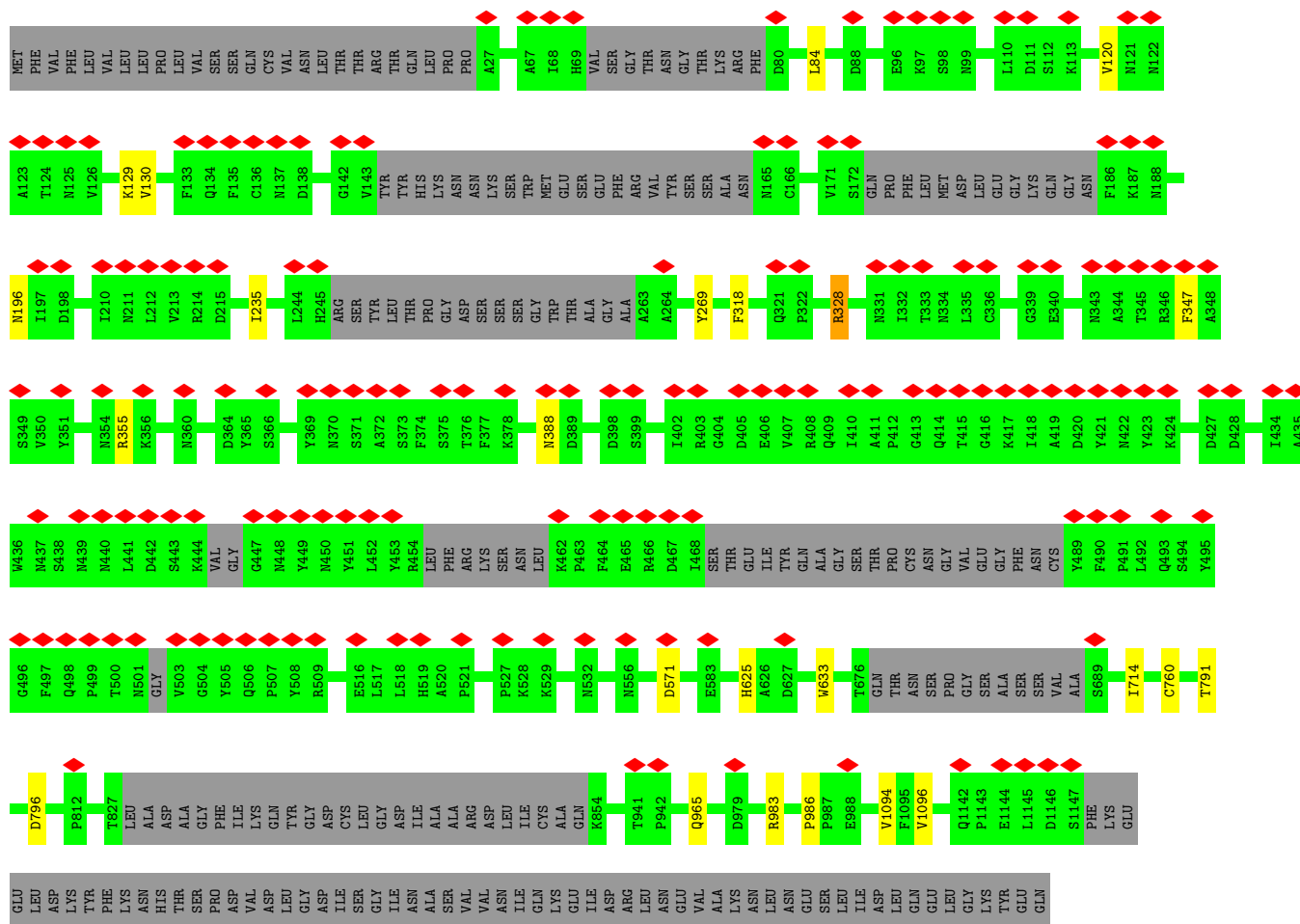
There are 33 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	383	CYS	SER	conflict	UNP P0DTC2
A	682	GLY	ARG	conflict	UNP P0DTC2
A	683	SER	ARG	conflict	UNP P0DTC2
A	685	SER	ARG	conflict	UNP P0DTC2
A	817	PRO	PHE	conflict	UNP P0DTC2
A	892	PRO	ALA	conflict	UNP P0DTC2
A	899	PRO	ALA	conflict	UNP P0DTC2
A	942	PRO	ALA	conflict	UNP P0DTC2
A	985	CYS	ASP	conflict	UNP P0DTC2
A	986	PRO	LYS	conflict	UNP P0DTC2
A	987	PRO	VAL	conflict	UNP P0DTC2
B	383	CYS	SER	conflict	UNP P0DTC2
B	682	GLY	ARG	conflict	UNP P0DTC2
B	683	SER	ARG	conflict	UNP P0DTC2
B	685	SER	ARG	conflict	UNP P0DTC2
B	817	PRO	PHE	conflict	UNP P0DTC2
B	892	PRO	ALA	conflict	UNP P0DTC2
B	899	PRO	ALA	conflict	UNP P0DTC2
B	942	PRO	ALA	conflict	UNP P0DTC2
B	985	CYS	ASP	conflict	UNP P0DTC2
B	986	PRO	LYS	conflict	UNP P0DTC2
B	987	PRO	VAL	conflict	UNP P0DTC2
C	383	CYS	SER	conflict	UNP P0DTC2
C	682	GLY	ARG	conflict	UNP P0DTC2

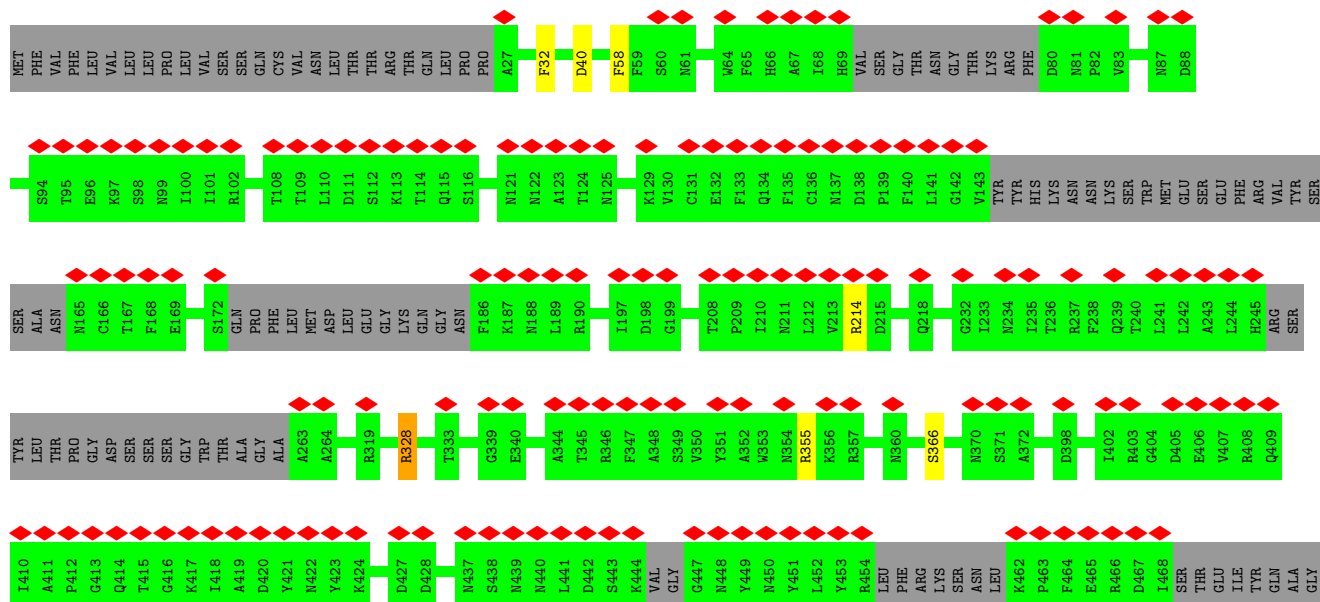
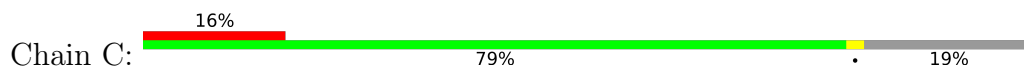
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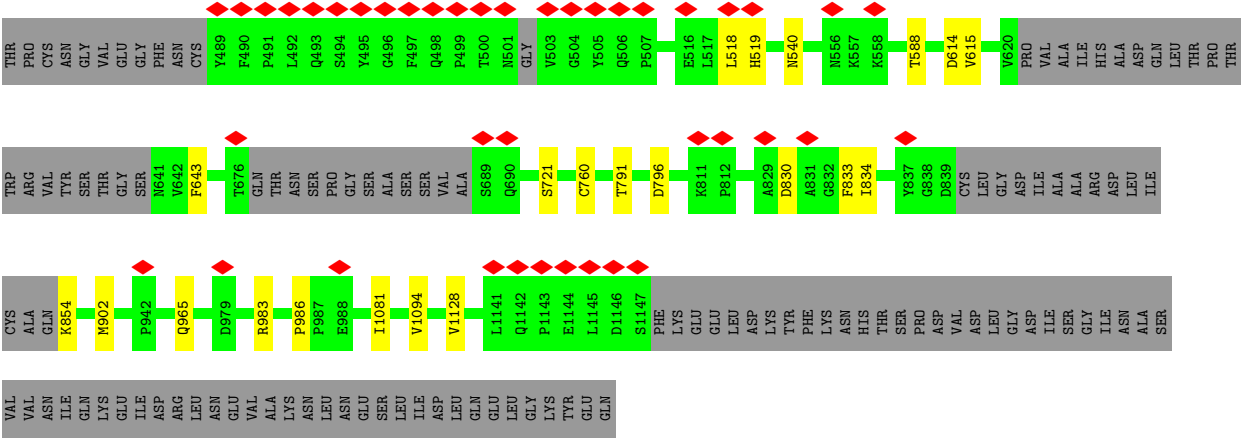
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Chain	Residue	Modelled	Actual	Comment	Reference
C	683	SER	ARG	conflict	UNP P0DTC2
C	685	SER	ARG	conflict	UNP P0DTC2
C	817	PRO	PHE	conflict	UNP P0DTC2
C	892	PRO	ALA	conflict	UNP P0DTC2
C	899	PRO	ALA	conflict	UNP P0DTC2
C	942	PRO	ALA	conflict	UNP P0DTC2
C	985	CYS	ASP	conflict	UNP P0DTC2
C	986	PRO	LYS	conflict	UNP P0DTC2
C	987	PRO	VAL	conflict	UNP P0DTC2



• Molecule 1: Spike glycoprotein





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	394297	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	45.522	Depositor
Minimum map value	-30.976	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	4.24	Depositor
Map size ($\text{\AA}$)	317.4, 317.4, 317.4	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.058, 1.058, 1.058	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	0.74	0/7775	1.29	6/10580 (0.1%)
1	B	0.74	0/7937	1.29	5/10807 (0.0%)
1	C	0.74	0/7868	1.30	8/10705 (0.1%)
All	All	0.74	0/23580	1.29	19/32092 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	4
1	C	0	4
All	All	0	13

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	986	PRO	N-CA-C	6.78	118.97	110.70
1	B	986	PRO	N-CA-C	6.27	118.35	110.70
1	B	796	ASP	CA-CB-CG	5.97	118.57	112.60
1	A	1084	ASP	CA-CB-CG	5.53	118.13	112.60
1	C	986	PRO	N-CA-C	5.48	117.39	110.70
1	C	518	LEU	N-CA-C	5.46	117.38	110.33
1	A	796	ASP	CA-CB-CG	5.45	118.05	112.60
1	A	965	GLN	OE1-CD-NE2	-5.35	117.25	122.60
1	C	58	PHE	CA-CB-CG	5.34	119.14	113.80
1	C	965	GLN	OE1-CD-NE2	-5.32	117.28	122.60
1	C	796	ASP	CA-CB-CG	5.31	117.91	112.60
1	B	965	GLN	OE1-CD-NE2	-5.30	117.30	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	643	PHE	CA-CB-CG	5.26	119.06	113.80
1	A	643	PHE	CA-CB-CG	5.10	118.90	113.80
1	C	40	ASP	CA-CB-CG	5.06	117.66	112.60
1	C	519	HIS	CB-CG-CD2	-5.05	124.63	131.20
1	B	625	HIS	CB-CG-CD2	-5.03	124.66	131.20
1	A	559	PHE	CA-CB-CG	5.03	118.83	113.80
1	B	347	PHE	CA-CB-CG	5.01	118.81	113.80

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	269	TYR	Sidechain
1	A	279	TYR	Sidechain
1	A	328	ARG	Sidechain
1	A	355	ARG	Sidechain
1	A	983	ARG	Sidechain
1	B	269	TYR	Sidechain
1	B	328	ARG	Sidechain
1	B	355	ARG	Sidechain
1	B	983	ARG	Sidechain
1	C	214	ARG	Peptide
1	C	328	ARG	Sidechain
1	C	355	ARG	Sidechain
1	C	983	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7604	0	7433	1	0
1	B	7759	0	7583	2	0
1	C	7695	0	7518	0	0
All	All	23058	0	22534	3	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 0.

All (3) 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:196:ASN:HD21	1:B:235:ILE:HD12	1.78	0.49
1:B:714:ILE:HD12	1:B:1096:VAL:HG11	2.02	0.41
1:A:714:ILE:HD12	1:A:1096:VAL:HG11	2.03	0.40

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	948/1208 (78%)	896 (94%)	48 (5%)	4 (0%)	30	48
1	B	970/1208 (80%)	921 (95%)	48 (5%)	1 (0%)	48	69
1	C	960/1208 (80%)	902 (94%)	56 (6%)	2 (0%)	43	62
All	All	2878/3624 (79%)	2719 (94%)	152 (5%)	7 (0%)	44	62

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	614	ASP
1	B	318	PHE
1	C	32	PHE
1	A	419	ALA
1	A	291	CYS
1	C	614	ASP
1	A	571	ASP

5.3.2 Protein sidechains ⓘ

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	855/1056 (81%)	842 (98%)	13 (2%)	57	77
1	B	872/1056 (83%)	861 (99%)	11 (1%)	61	79
1	C	863/1056 (82%)	847 (98%)	16 (2%)	50	73
All	All	2590/3168 (82%)	2550 (98%)	40 (2%)	55	77

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	130	VAL
1	A	227	VAL
1	A	366	SER
1	A	388	ASN
1	A	519	HIS
1	A	546	LEU
1	A	603	ASN
1	A	615	VAL
1	A	619	GLU
1	A	760	CYS
1	A	791	THR
1	A	948	LEU
1	A	1094	VAL
1	B	84	LEU
1	B	120	VAL
1	B	129	LYS
1	B	130	VAL
1	B	328	ARG
1	B	388	ASN
1	B	571	ASP
1	B	633	TRP
1	B	760	CYS
1	B	791	THR
1	B	1094	VAL
1	C	328	ARG
1	C	366	SER

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Mol	Chain	Res	Type
1	C	540	ASN
1	C	588	THR
1	C	615	VAL
1	C	721	SER
1	C	760	CYS
1	C	791	THR
1	C	830	ASP
1	C	833	PHE
1	C	834	ILE
1	C	854	LYS
1	C	902	MET
1	C	1081	ILE
1	C	1094	VAL
1	C	1128	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	245	HIS
1	A	314	GLN
1	A	343	ASN
1	A	360	ASN
1	A	437	ASN
1	A	493	GLN
1	A	506	GLN
1	A	606	ASN
1	A	613	GLN
1	A	901	GLN
1	A	969	ASN
1	B	196	ASN
1	B	437	ASN
1	B	450	ASN
1	B	628	GLN
1	B	779	GLN
1	B	901	GLN
1	B	957	GLN
1	B	969	ASN
1	B	1010	GLN
1	B	1048	HIS
1	B	1125	ASN
1	C	188	ASN
1	C	314	GLN

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Mol	Chain	Res	Type
1	C	536	ASN
1	C	606	ASN
1	C	613	GLN
1	C	641	ASN
1	C	764	ASN
1	C	804	GLN
1	C	901	GLN
1	C	935	GLN
1	C	954	GLN

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.

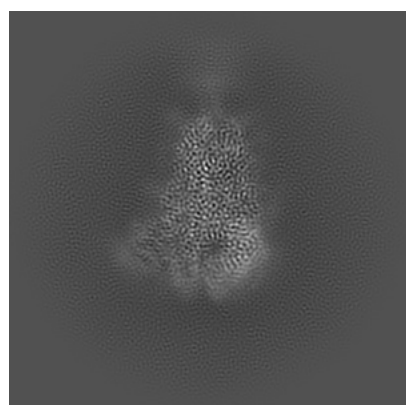
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25987. These allow visual inspection of the internal detail of the map and identification of artifacts.

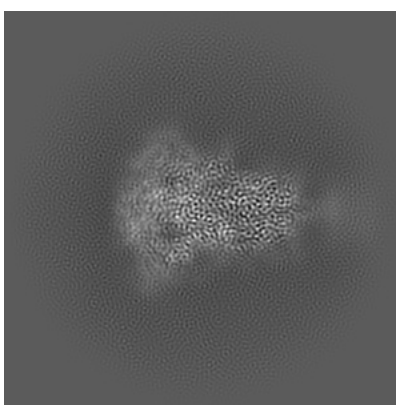
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

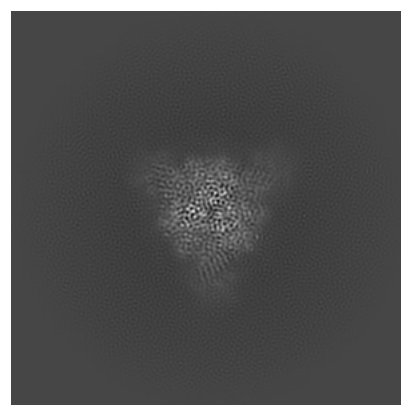
6.1.1 Primary map



X



Y

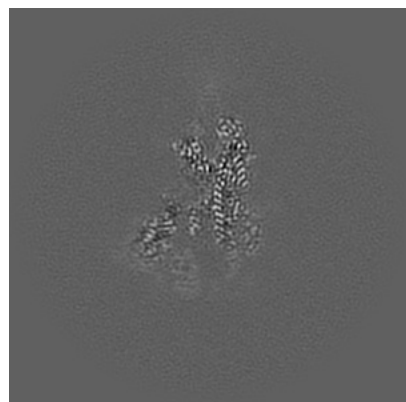


Z

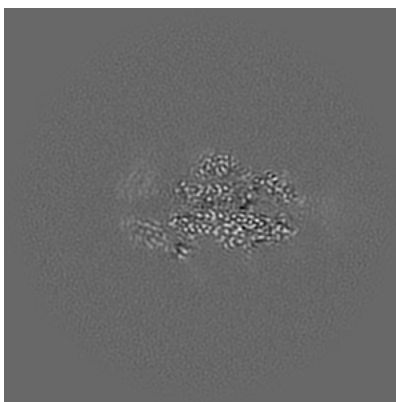
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

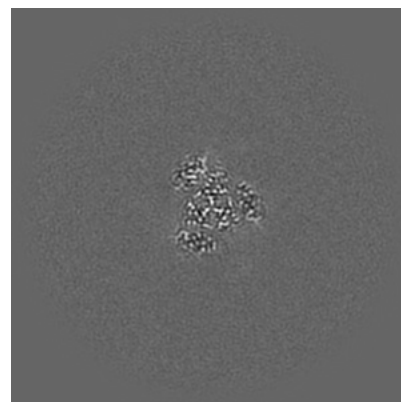
6.2.1 Primary map



X Index: 150



Y Index: 150

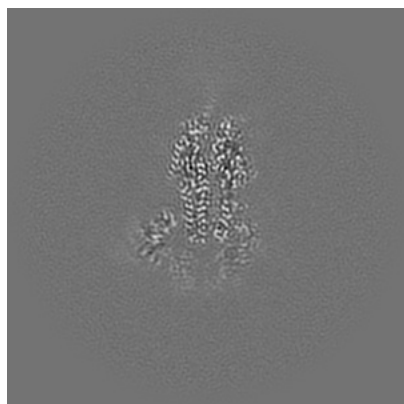


Z Index: 150

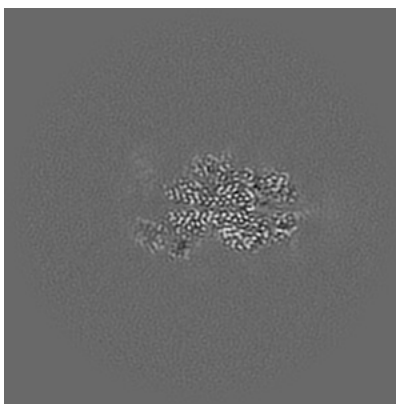
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

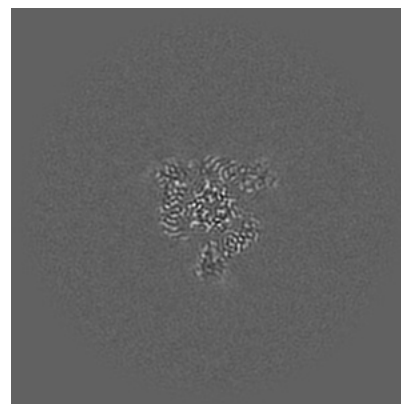
6.3.1 Primary map



X Index: 157



Y Index: 146

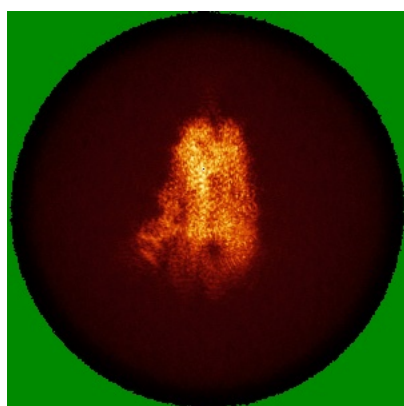


Z Index: 135

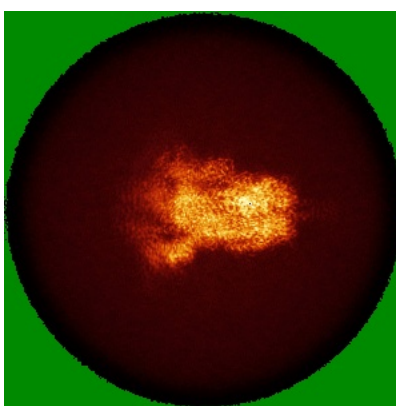
The images above show the largest variance slices of the map in three orthogonal directions.

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

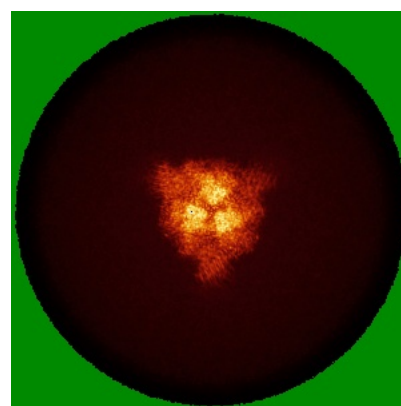
6.4.1 Primary map



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

This section was not generated.

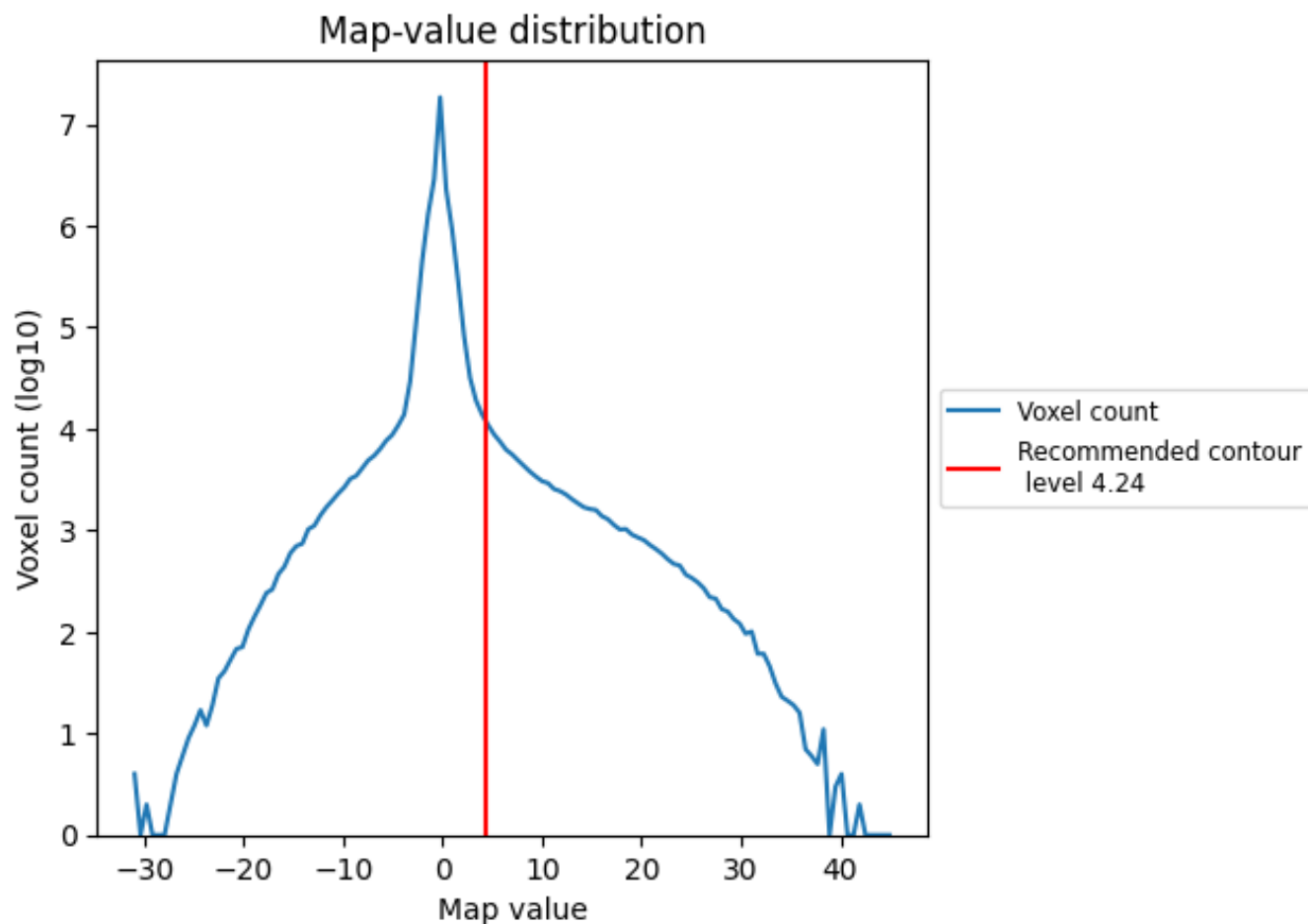
6.6 Mask visualisation

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

7 Map analysis [i](#)

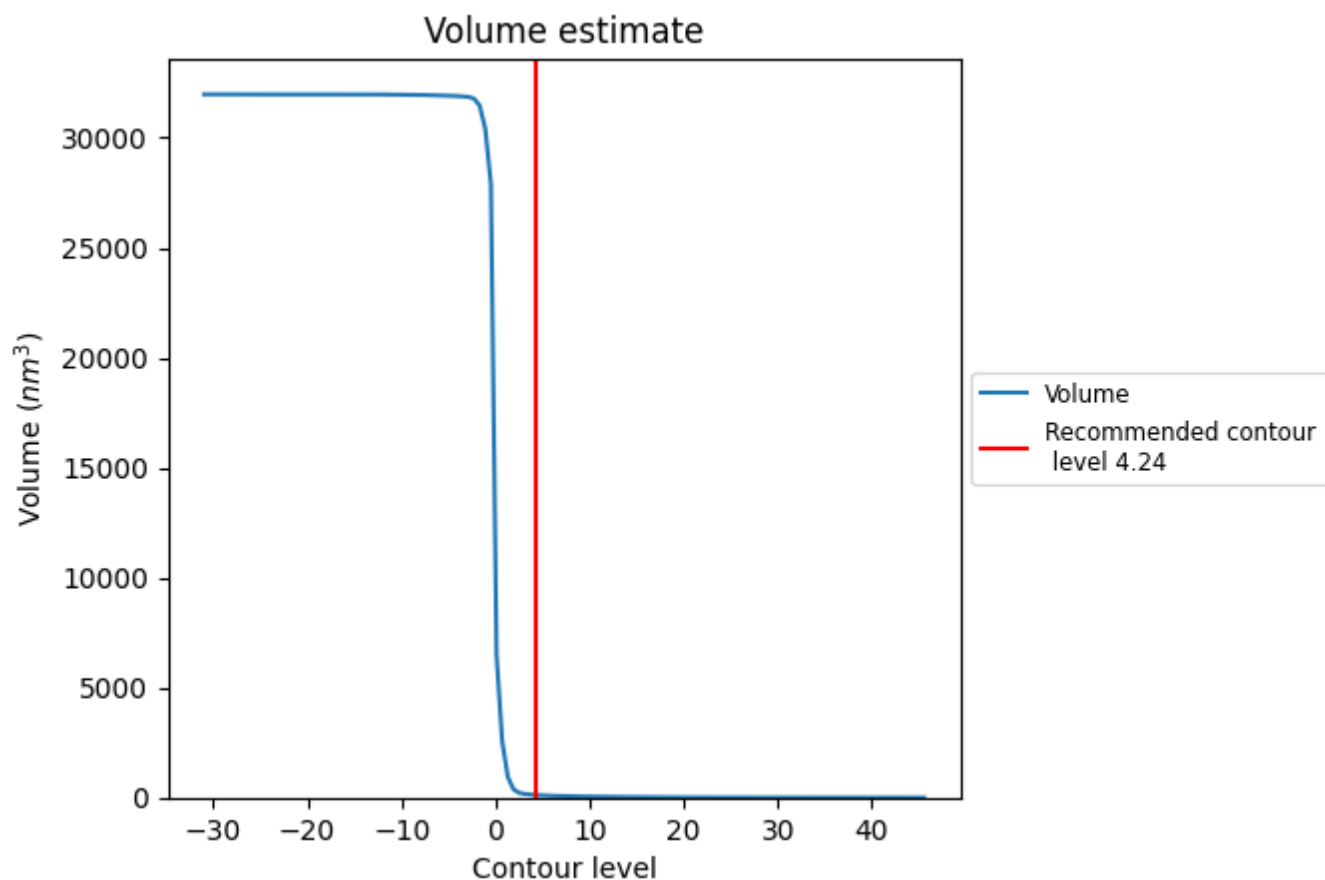
This section contains the results of statistical analysis of the map.

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.

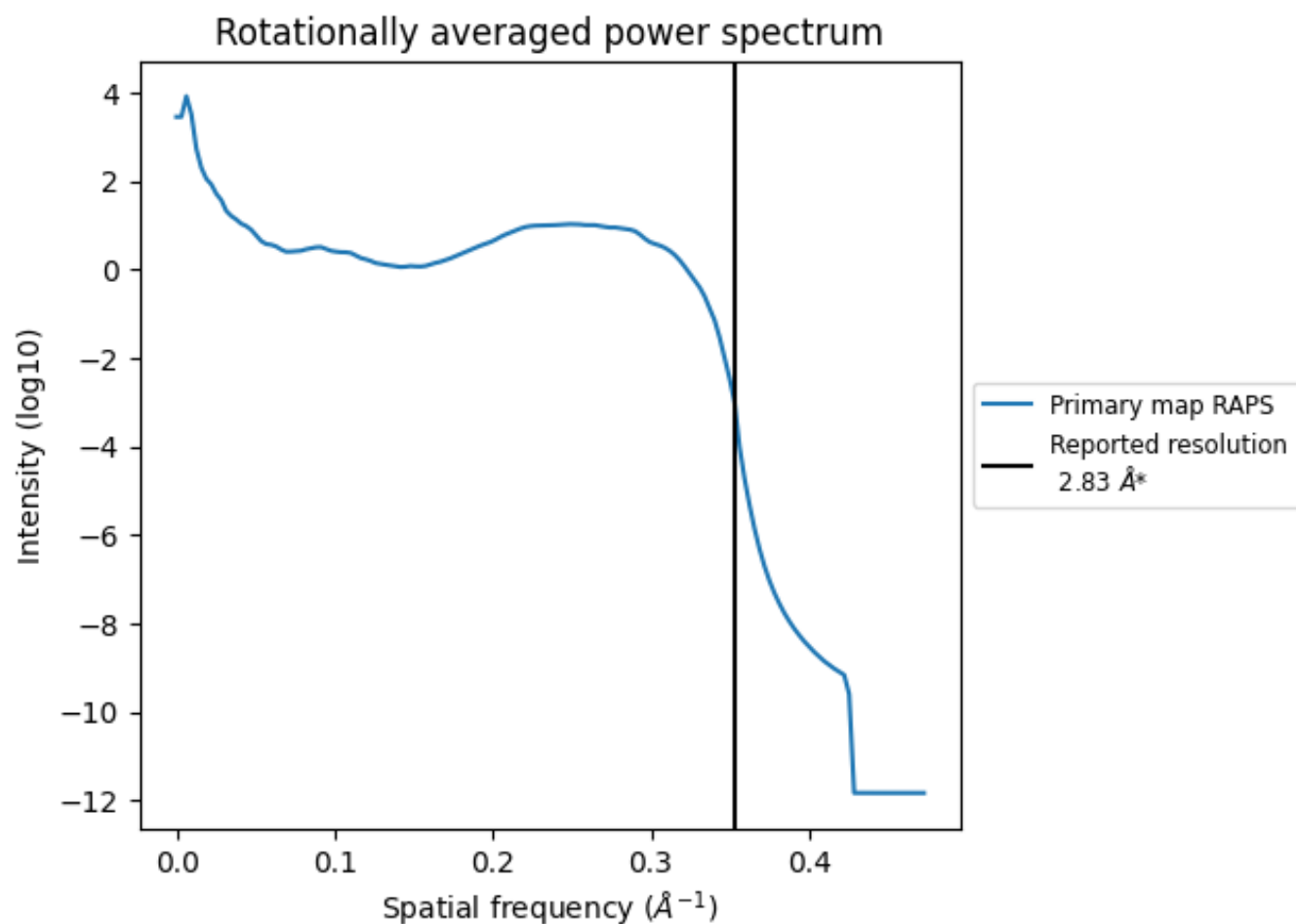
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 118 nm³; this corresponds to an approximate mass of 106 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 0.353 $\text{\AA}^{-1}$

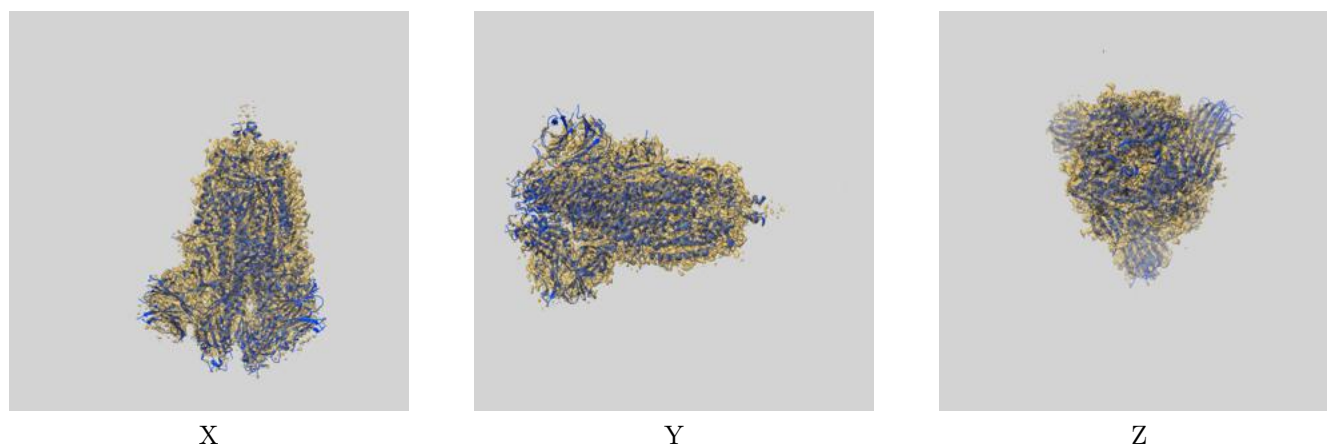
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

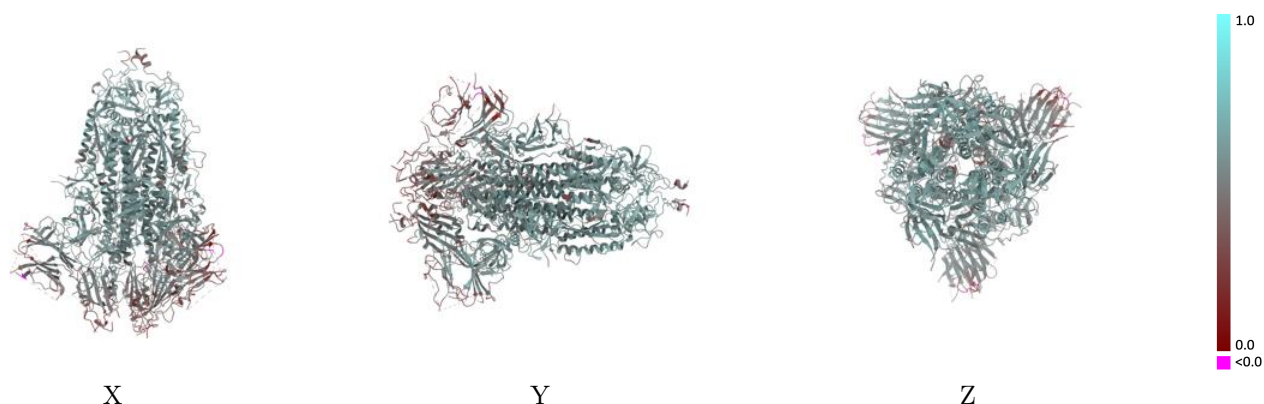
This section contains information regarding the fit between EMDB map EMD-25987 and PDB model 7TLC. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



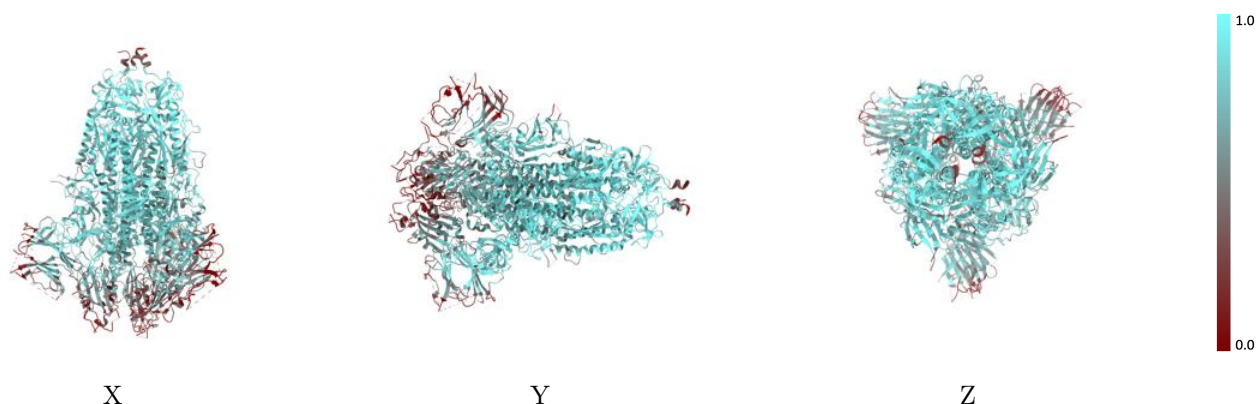
The images above show the 3D surface view of the map at the recommended contour level 4.24 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



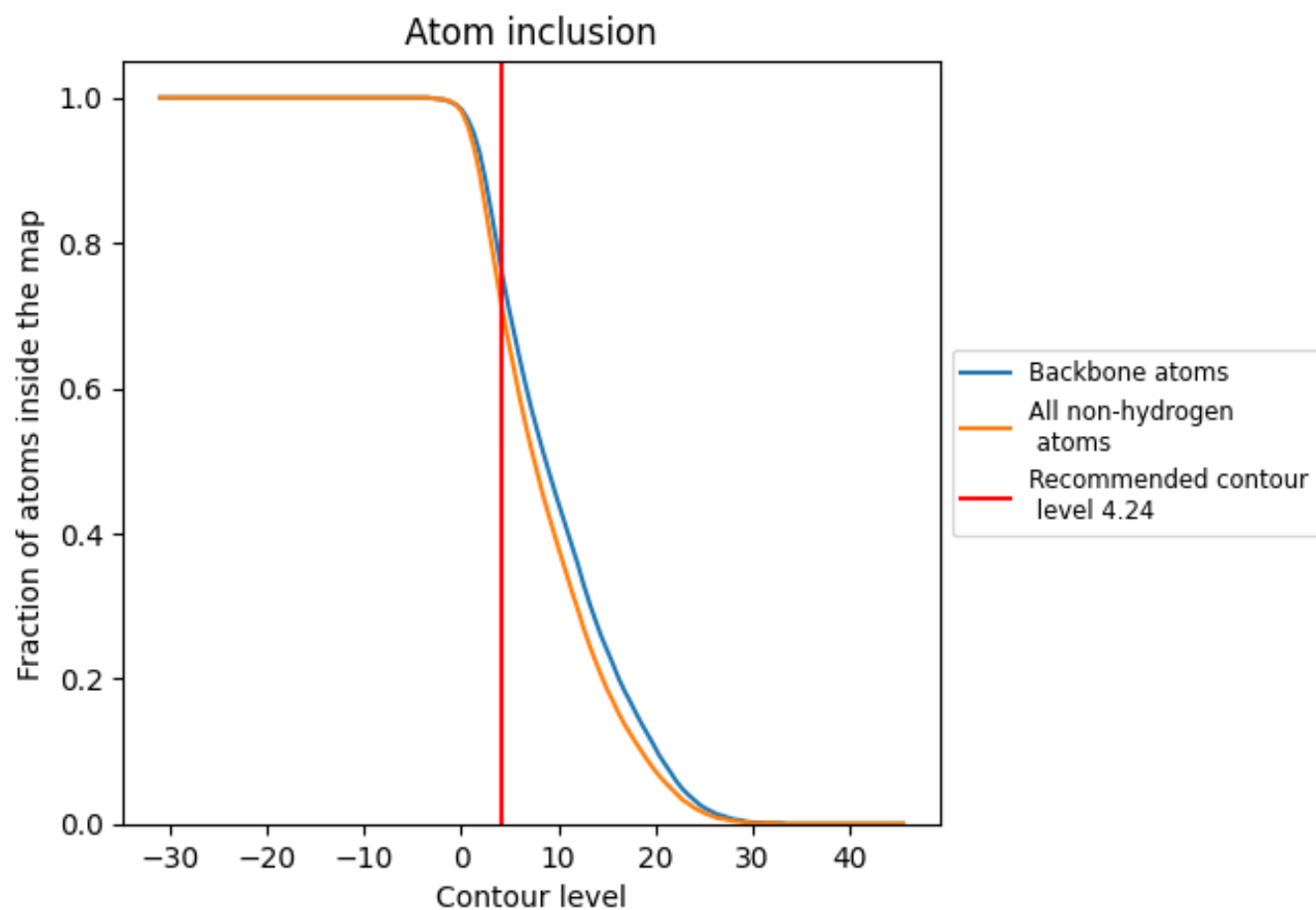
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4.24).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 71% 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 (4.24) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7070	0.5170
A	0.7250	0.5230
B	0.7210	0.5210
C	0.6760	0.5060

