



wwPDB EM Validation Summary Report ⓘ

Mar 6, 2026 – 07:50 AM UTC

PDB ID : 7L7K / pdb_0000717k
EMDB ID : EMD-23215
Title : Cryo-EM structure of protein encoded by vaccine candidate BNT162b2
Authors : Lees, J.A.; Han, S.
Deposited on : 2020-12-28
Resolution : 3.29 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:

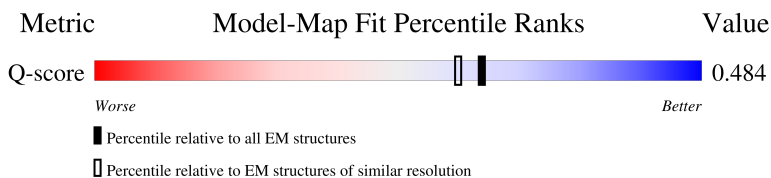
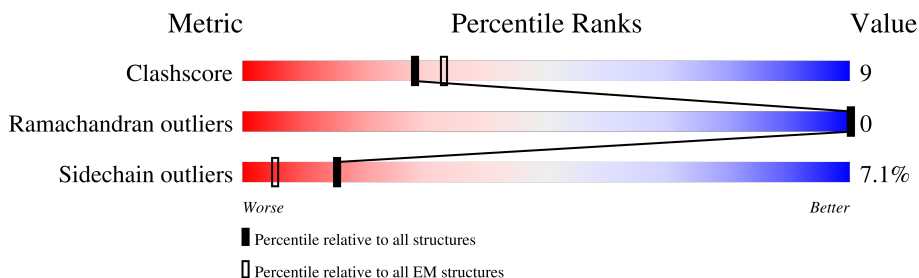
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.29 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	14466 (2.79 - 3.79)

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	
1	B	1273	
1	C	1273	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 22124 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	B	973	Total	C	N	O	S	0	0
			7370	4708	1225	1403	34		
1	C	973	Total	C	N	O	S	0	0
			7384	4720	1225	1405	34		
1	A	973	Total	C	N	O	S	0	0
			7370	4708	1225	1403	34		

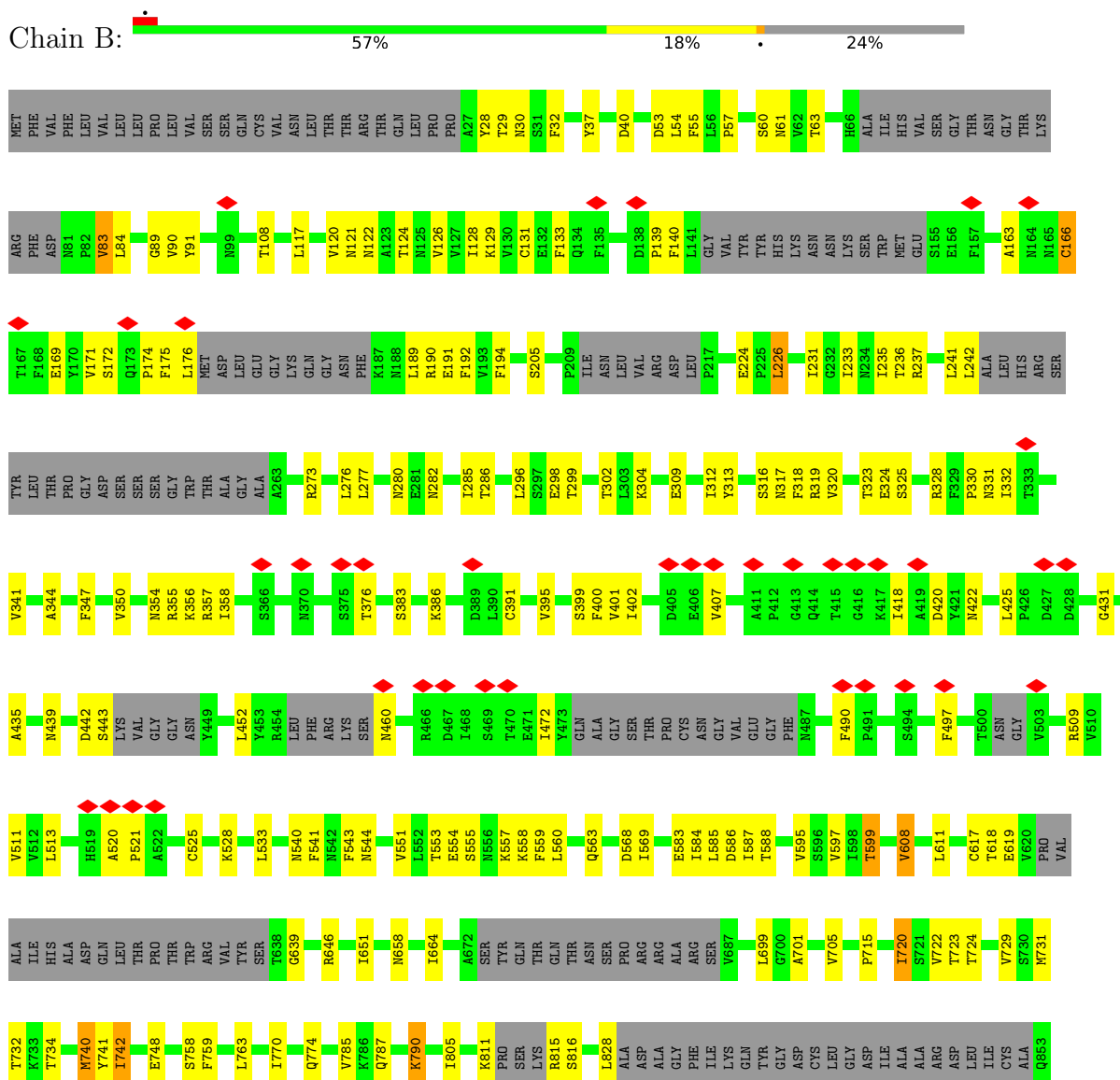
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	986	PRO	LYS	conflict	UNP P0DTC2
B	987	PRO	VAL	conflict	UNP P0DTC2
C	986	PRO	LYS	conflict	UNP P0DTC2
C	987	PRO	VAL	conflict	UNP P0DTC2
A	986	PRO	LYS	conflict	UNP P0DTC2
A	987	PRO	VAL	conflict	UNP P0DTC2

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: Spike glycoprotein



HIS TYR THR	LYS	TRP	LEU	GLU	1997
	PRO	ASP	LYS	LEU	
HIS TYR THR	TYR	TRP	TYR	TYR	L1001
	ILE	PHE	PHE	PHE	Q1005
HIS TYR THR	TRP	TRP	LYS	LYS	T1006
	GLY	GLY	ASN	ASN	Y1007
HIS TYR THR	PHE	PHE	THR	THR	Q1011
	ILE	SER	SER	SER	R1014
HIS TYR THR	ALA	ALA	PRO	PRO	G1035
	GLY	GLY	ASP	ASP	Q1038
HIS TYR THR	LEU	LEU	VAL	VAL	R1039
	ILE	ALA	ALA	LEU	V1040
HIS TYR THR	VAL	VAL	ASP	ASP	K1045
	MET	MET	ILE	ILE	H1048
HIS TYR THR	VAL	THR	SER	GLY	L1049
	THR	ILE	GLY	ILE	H1050
HIS TYR THR	MET	MET	ASN	ASN	S1051
	LEU	LEU	ALA	ALA	F1052
HIS TYR THR	CYS	CYS	SER	SER	Q1054
	VAL	VAL	VAL	VAL	H1058
HIS TYR THR	THR	THR	ASN	ASN	V1065
	SER	SER	ILE	ILE	Q1071
HIS TYR THR	CYS	CYS	GLN	GLN	E1072
	SYS	SYS	LYS	LYS	K1086
HIS TYR THR	CYS	CYS	GLU	GLU	G1093
	SER	SER	VAL	VAL	V1104
HIS TYR THR	CYS	CYS	ALA	ALA	T1105
	GLY	GLY	LYS	LYS	I1115
HIS TYR THR	SER	SER	ASN	ASN	V1122
	ASP	ASP	LEU	LEU	M1125
HIS TYR THR	GLU	GLU	ILE	ILE	V1128
	ASP	ASP	ASP	ASP	V1129
HIS TYR THR	SER	SER	GLN	GLN	I1132
	GLU	GLU	LEU	LEU	D1146
HIS TYR THR	PRO	PRO	GLY	GLY	SER
	VAL	VAL	LYS	LYS	PHE
HIS TYR THR	LEU	LEU	TYR	TYR	LYS
	GLY	GLY	GLN	GLN	THR

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	58295	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 ($e^-/\text{\AA}^2$)	50.22	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.002	Depositor
Minimum map value	-0.001	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.000	Depositor
Recommended contour level	0.0003	Depositor
Map size (Å)	378.0, 378.0, 378.0	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.84, 0.84, 0.84	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	0.16	0/7527	0.36	0/10258
1	B	0.16	0/7527	0.37	0/10258
1	C	0.15	0/7540	0.36	0/10279
All	All	0.16	0/22594	0.36	0/30795

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	A	7370	0	7024	155	0
1	B	7370	0	7024	139	0
1	C	7384	0	7061	143	0
All	All	22124	0	21109	410	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 9.

The worst 5 of 410 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:C:103:GLY:HA3	1:C:119:ILE:O	1.53	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:391:CYS:HA	1:B:525:CYS:HB3	1.53	0.91
1:C:105:ILE:HG12	1:C:241:LEU:HD11	1.58	0.85
1:C:391:CYS:HA	1:C:525:CYS:HB3	1.59	0.85
1:A:347:PHE:HD2	1:A:509:ARG:HD3	1.48	0.78

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	945/1273 (74%)	897 (95%)	48 (5%)	0	100	100
1	B	945/1273 (74%)	890 (94%)	55 (6%)	0	100	100
1	C	945/1273 (74%)	895 (95%)	50 (5%)	0	100	100
All	All	2835/3819 (74%)	2682 (95%)	153 (5%)	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	A	792/1112 (71%)	734 (93%)	58 (7%)	13	39
1	B	792/1112 (71%)	737 (93%)	55 (7%)	14	41
1	C	796/1112 (72%)	741 (93%)	55 (7%)	14	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2380/3336 (71%)	2212 (93%)	168 (7%)	15 40

5 of 168 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	166	CYS
1	A	734	THR
1	A	302	THR
1	A	553	THR
1	A	801	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 53 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	751	ASN
1	C	1002	GLN
1	A	901	GLN
1	C	755	GLN
1	C	965	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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

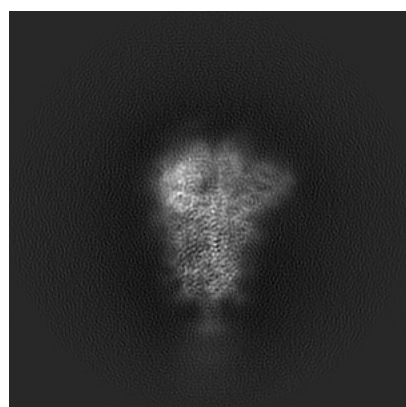
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23215. These allow visual inspection of the internal detail of the map and identification of artifacts.

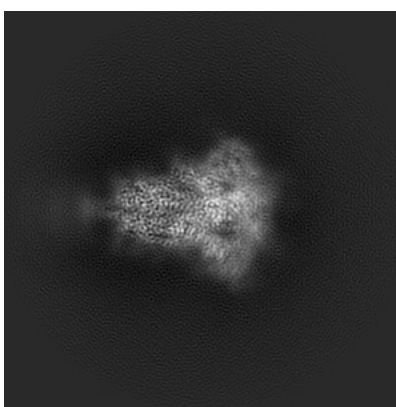
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

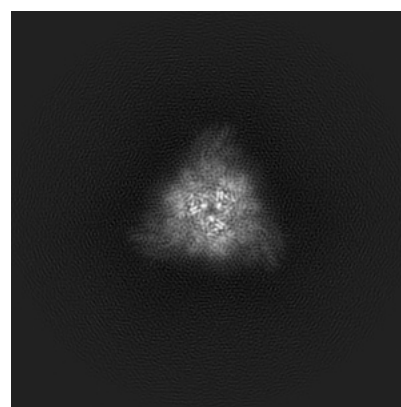
6.1.1 Primary map



X



Y

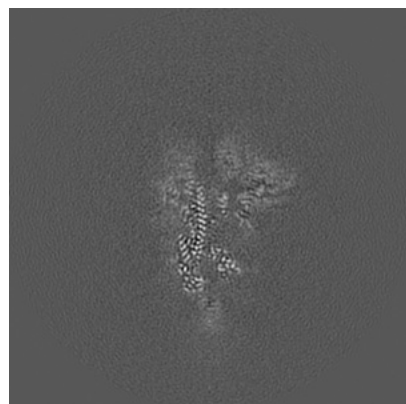


Z

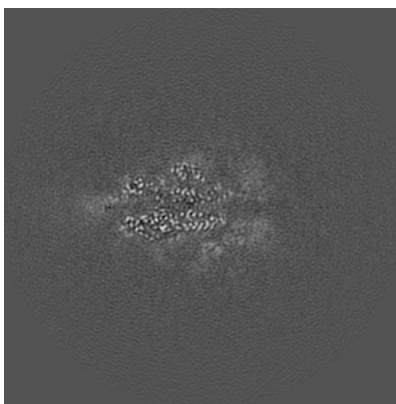
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

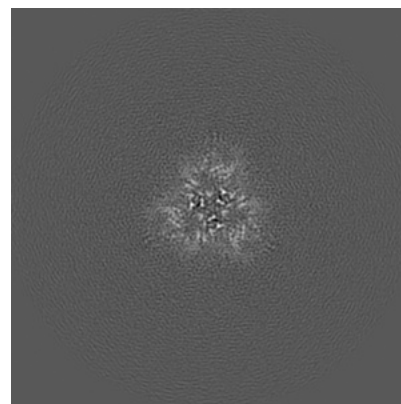
6.2.1 Primary map



X Index: 225



Y Index: 225

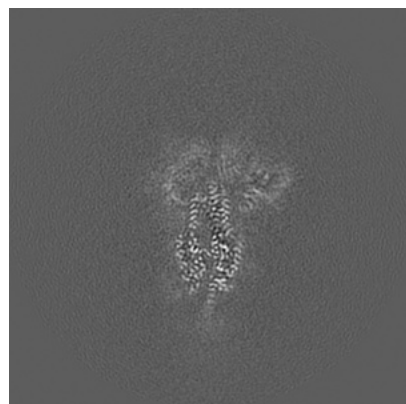


Z Index: 225

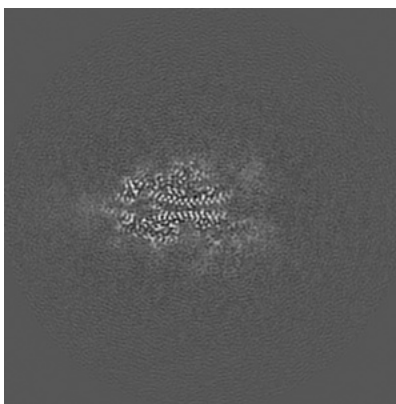
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

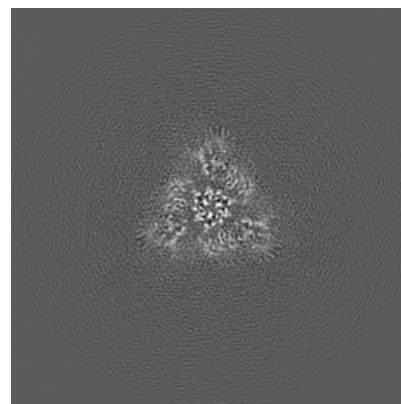
6.3.1 Primary map



X Index: 236



Y Index: 230

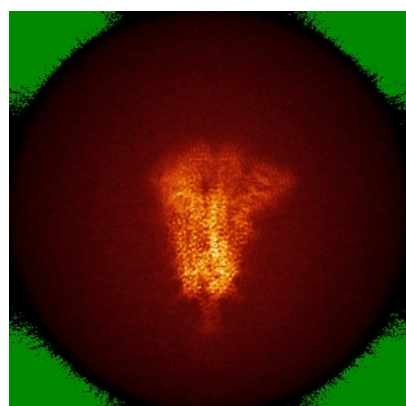


Z Index: 235

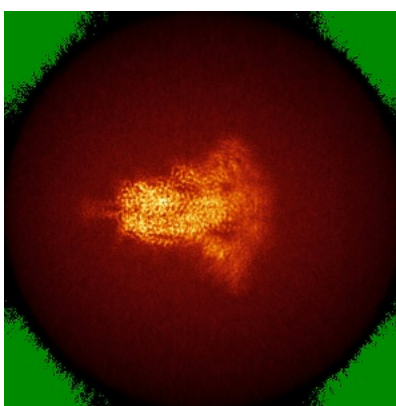
The images above show the largest variance slices of the map in three orthogonal directions.

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

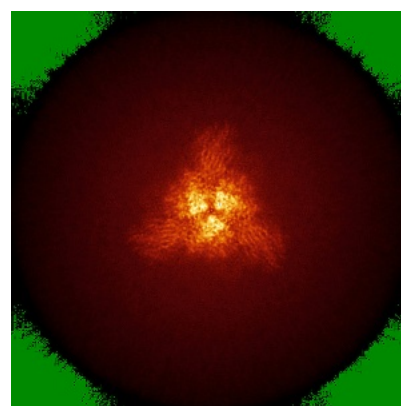
6.4.1 Primary map



X



Y

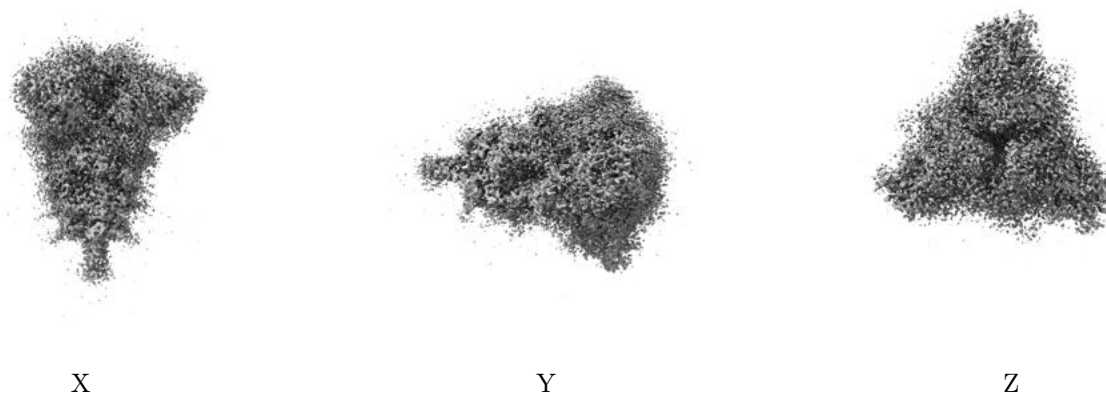


Z

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 0.0003. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

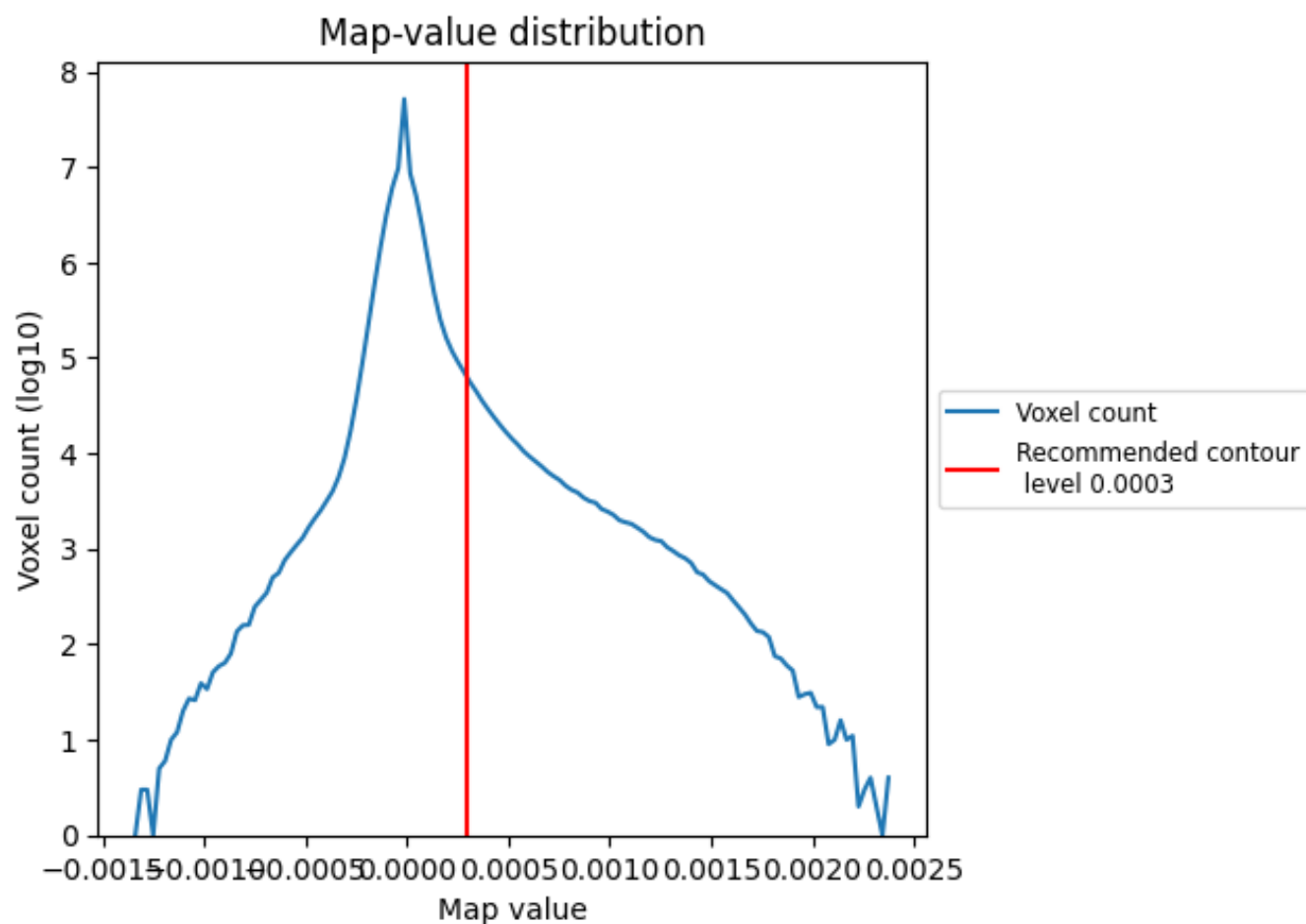
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

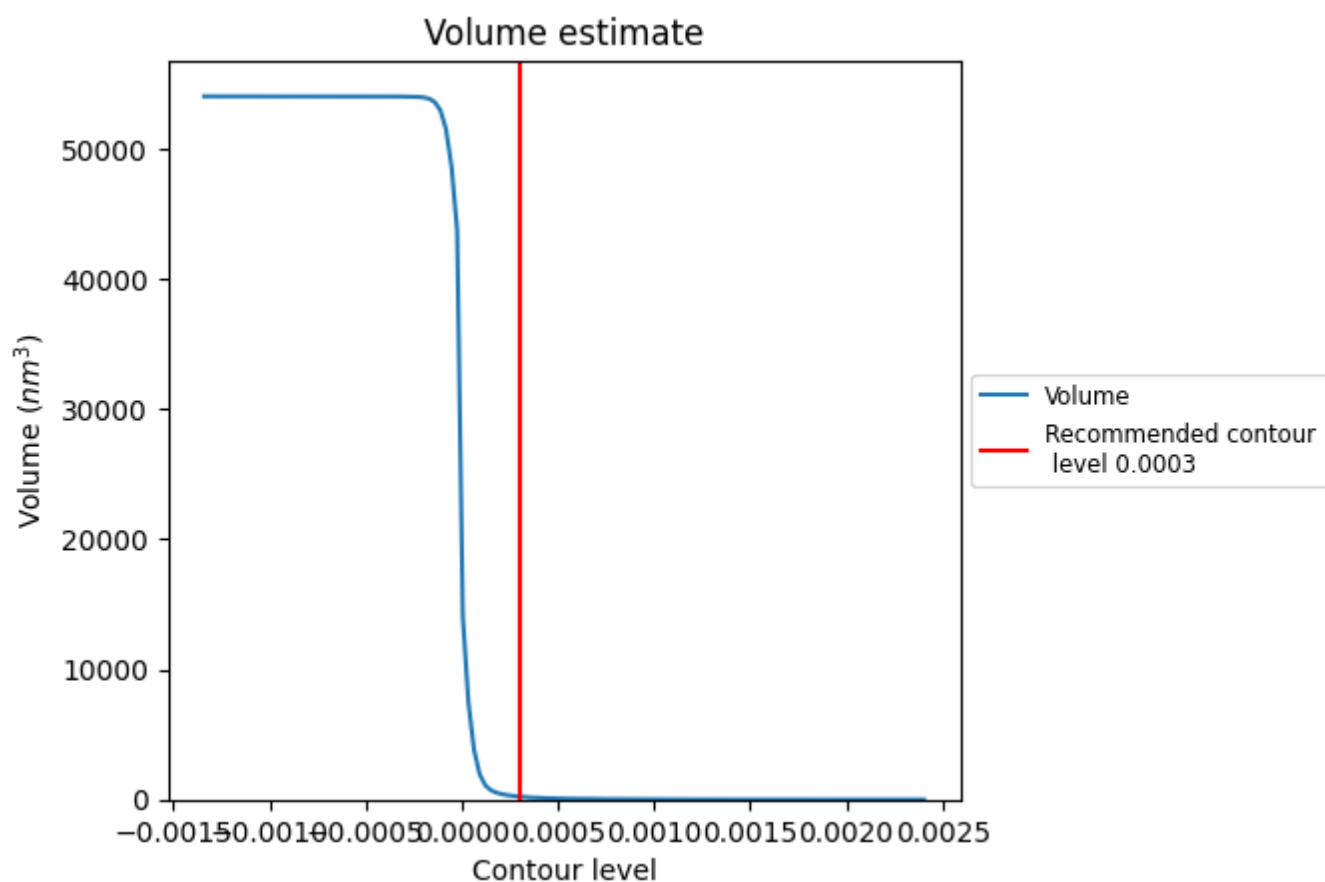
This section contains the results of statistical analysis of the map.

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.

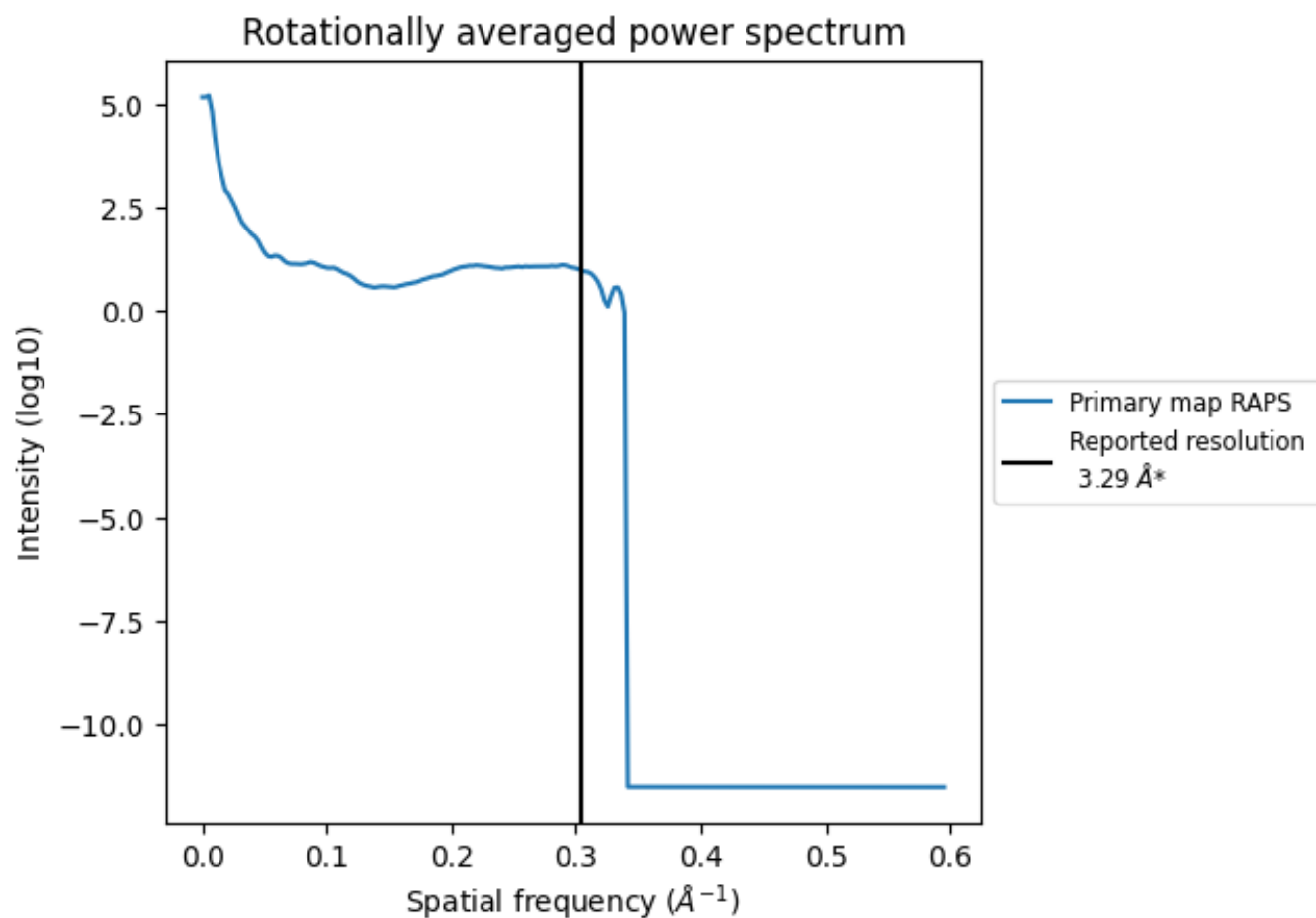
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 226 nm^3 ; this corresponds to an approximate mass of 204 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 0.304 Å⁻¹

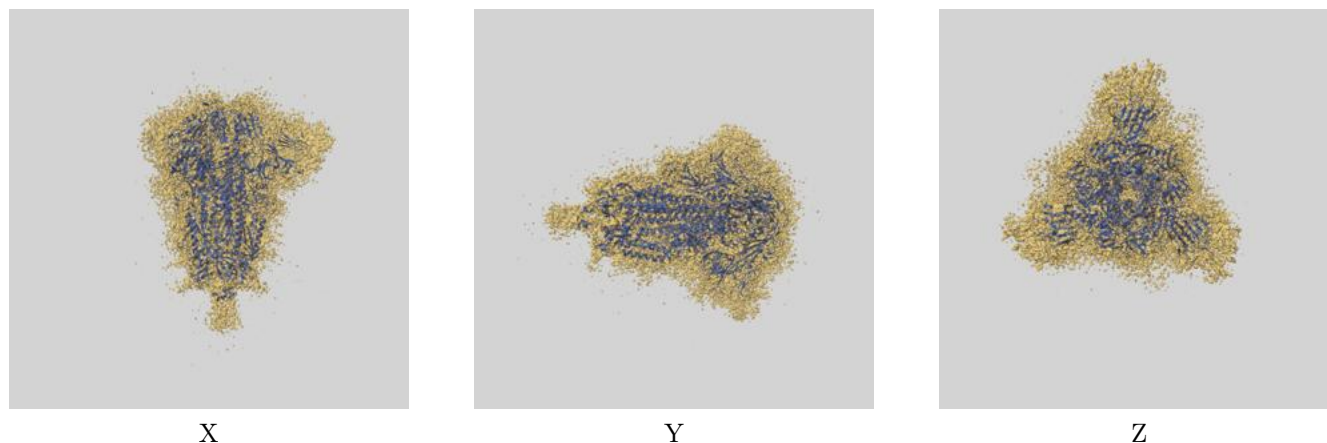
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

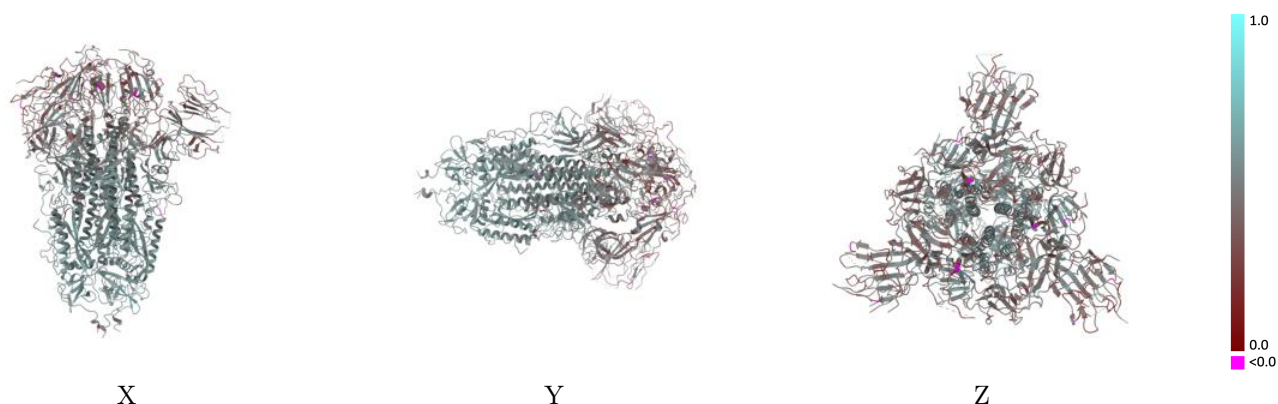
This section contains information regarding the fit between EMDB map EMD-23215 and PDB model 7L7K. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



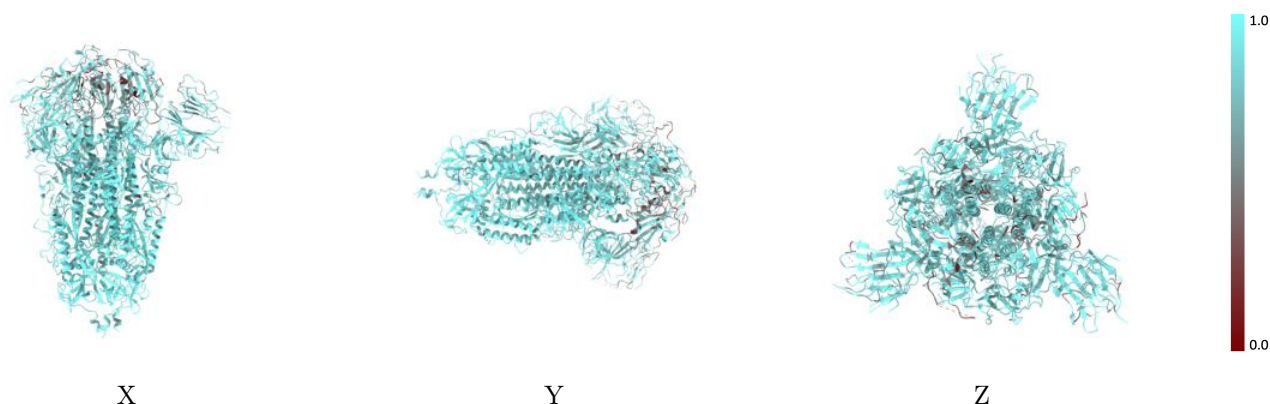
The images above show the 3D surface view of the map at the recommended contour level 0.0003 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



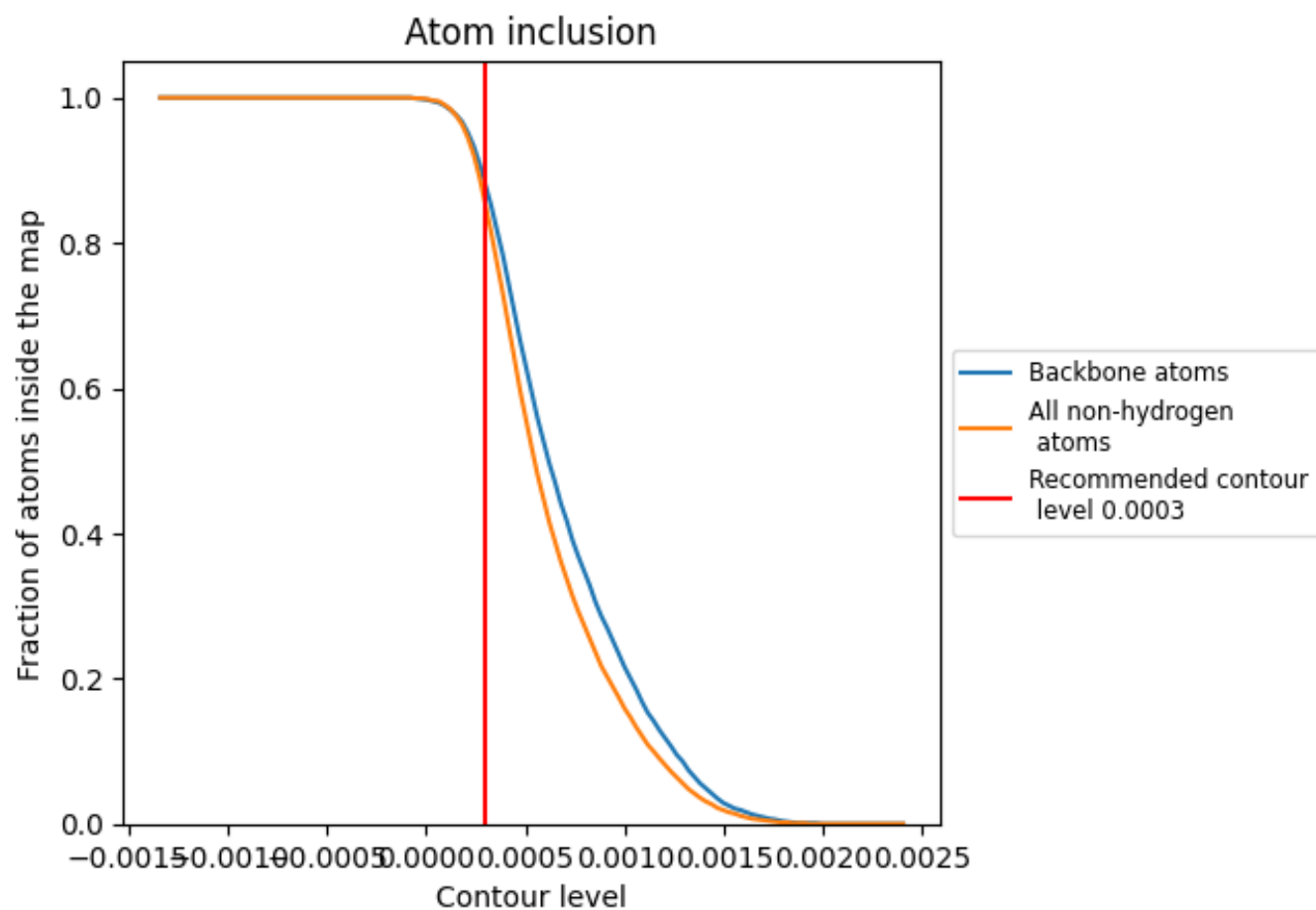
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0003).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 85% 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 (0.0003) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8510	0.4840
A	0.8520	0.4850
B	0.8490	0.4820
C	0.8530	0.4850

