



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 10:20 AM UTC

PDB ID : 5XLR / pdb_00005xlr
EMDB ID : EMD-6732
Title : Structure of SARS-CoV spike glycoprotein
Authors : Gui, M.; Song, W.; Xiang, Y.; Wang, X.
Deposited on : 2017-05-11
Resolution : 3.80 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

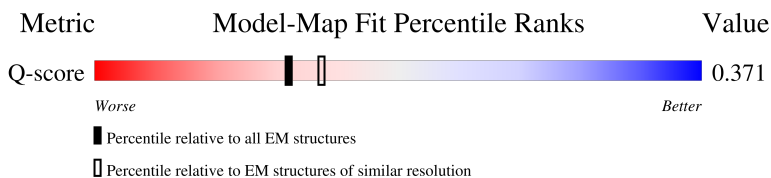
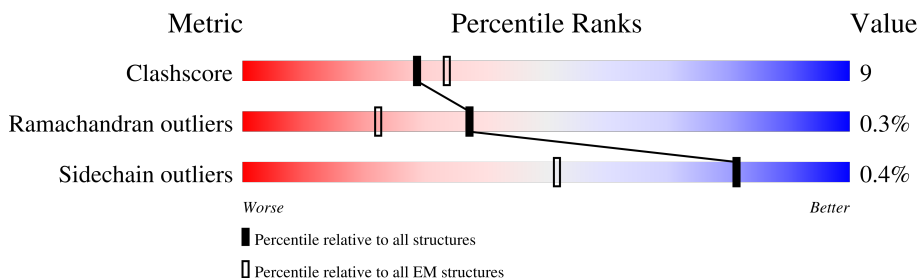
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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	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	10198 (3.30 - 4.30)

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	1203	25% 66% 19% 15%
1	B	1203	26% 66% 18% 15%
1	C	1203	25% 66% 18% 15%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 23901 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	1022	Total	C	N	O	S	0	0
			7967	5093	1318	1512	44		
1	B	1022	Total	C	N	O	S	0	0
			7967	5093	1318	1512	44		
1	C	1022	Total	C	N	O	S	0	0
			7967	5093	1318	1512	44		

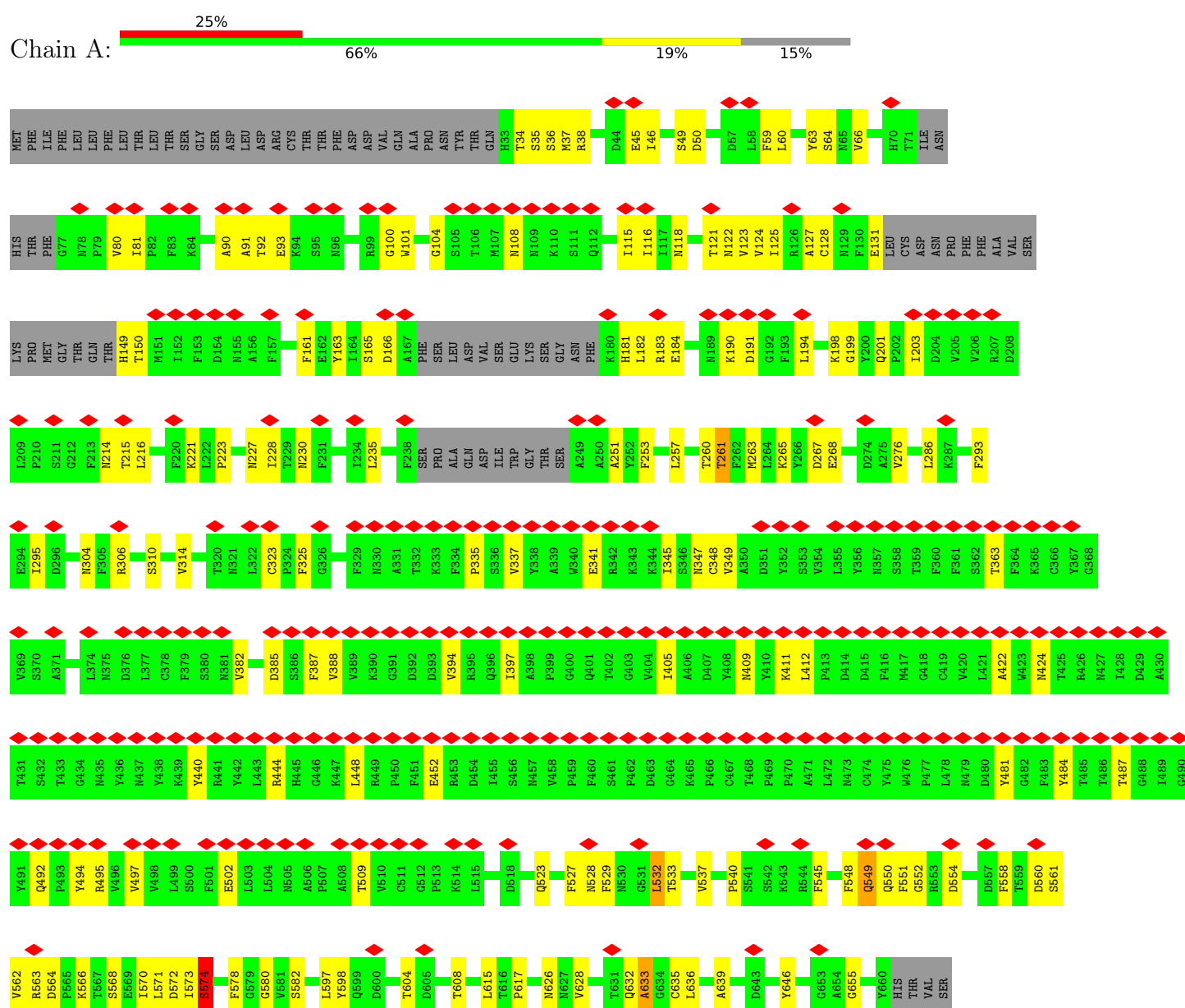
There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	667	ALA	ARG	engineered mutation	UNP P59594
A	1197	SER	-	expression tag	UNP P59594
A	1198	HIS	-	expression tag	UNP P59594
A	1199	PRO	-	expression tag	UNP P59594
A	1200	GLN	-	expression tag	UNP P59594
A	1201	PHE	-	expression tag	UNP P59594
A	1202	GLU	-	expression tag	UNP P59594
A	1203	LYS	-	expression tag	UNP P59594
B	667	ALA	ARG	engineered mutation	UNP P59594
B	1197	SER	-	expression tag	UNP P59594
B	1198	HIS	-	expression tag	UNP P59594
B	1199	PRO	-	expression tag	UNP P59594
B	1200	GLN	-	expression tag	UNP P59594
B	1201	PHE	-	expression tag	UNP P59594
B	1202	GLU	-	expression tag	UNP P59594
B	1203	LYS	-	expression tag	UNP P59594
C	667	ALA	ARG	engineered mutation	UNP P59594
C	1197	SER	-	expression tag	UNP P59594
C	1198	HIS	-	expression tag	UNP P59594
C	1199	PRO	-	expression tag	UNP P59594
C	1200	GLN	-	expression tag	UNP P59594
C	1201	PHE	-	expression tag	UNP P59594
C	1202	GLU	-	expression tag	UNP P59594
C	1203	LYS	-	expression tag	UNP P59594

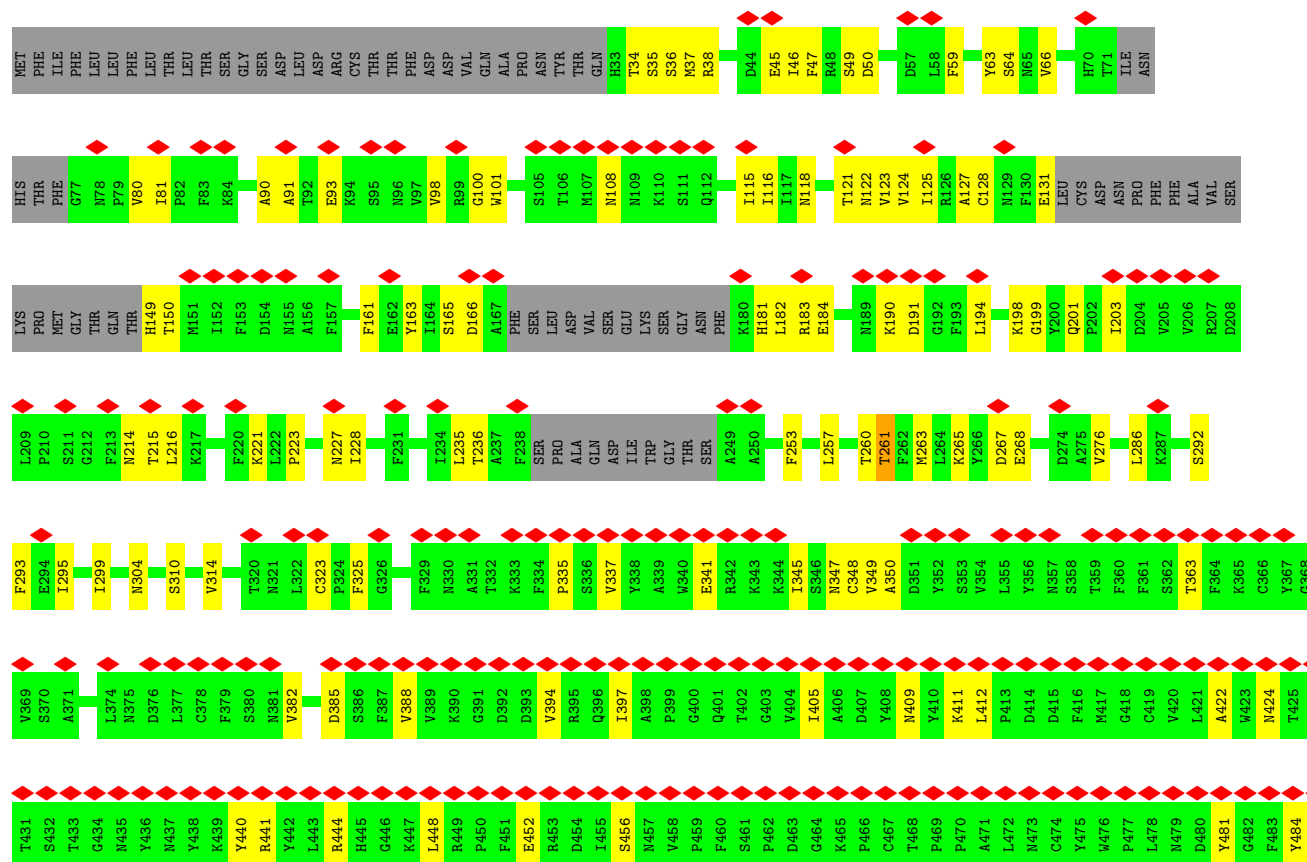
3 Residue-property plots

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







LYS	GLU	ILE	ASP	ARG	LEU	ASN	GLU	VAL	ALA	LYS	ASN	LEU	ILE	ASP	LEU	GLN	GLU	TYR	GLU	GLN	TYR	ILE	TRP	PRO	TRP	LEU	ASP	LYS	PRO	GLN	PHE	GLU	GLU	LYS																			
T1098	T1099	D1100	F1103	G1106	D1109	V1110	V1111	T1112	G1113	T1114	M1117	Y1120	ASP	PRO	LEU	GLN	PRO	GLU	LEU	ASP	SER	PHE	LYS	GLU	GLU	LEU	ASP	LYS	TYR	PHE	LYS	ASN	HIS	THR	SER	PRO	ASP	VAL	ASP	LEU	GLY	ILE	ASN	ALA	SER	VAL	ASN	ILE	GLN				
L927	D932	A954	L959	N960	D967	K968	V969	E970	Q987	Y988	Y989	V990	L1031	V1043	F1044	Y1049	Q1053	F1057	T1058	T1059	I1063	C1064	H1065	E1066	G1067	Y1070	R1073	E1074	G1075	V1076	F1077	V1078	F1079	I1080	S1083	T1086	T1087	Q1088	R1089	N1090	F1091	F1092	I1097										
A811	D812	A813	G814	F815	M816	K817	Q818	Y819	G820	E821	C822	L823	GLY	ASP	ASN	ALA	ARG	ASP	LEU	I832	C833	A834	F837	N838	G839	P844	A866	G867	W868	T869	F870	G871	A872	G873	A874	A875	L876	Q877	I878	P879	M882	N896	Y899	Q904	Q917	T921	T922	T923					
D564	P565	K566	T567	S568	E569	I570	L571	D572	I573	S574	F578	G579	G580	V581	S582	V583	I584	L597	Y598	Q599	D600	D605	L615	T616	P617	N626	T631	Q632	A633	G634	C635	A639	D643	Y646	D649	I650	G653	A654	G655	I656	C657	Y660	HIS	THR	VAL	SER	LEU						
Y491	Q492	P493	Y494	R495	V496	V497	V498	L499	E502	L503	L504	N505	A506	P507	A508	T509	V510	C511	G512	P513	K514	L515	D518	Q523	F527	N528	F529	N530	G531	L532	T533	P540	S541	S542	K543	R544	F545	Q546	P547	F548	Q549	Q550	F551	G552	R553	D554	D557	F558	T559	D560	S561	V562	R563

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	42135	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)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.303	Depositor
Minimum map value	-0.142	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	380.16, 380.16, 380.16	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.32, 1.32, 1.32	Depositor

5 Model quality

5.1 Standard geometry

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	0.37	0/8151	0.72	5/11085 (0.0%)
1	B	0.37	0/8151	0.72	5/11085 (0.0%)
1	C	0.37	0/8151	0.72	5/11085 (0.0%)
All	All	0.37	0/24453	0.72	15/33255 (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
1	B	0	8
1	C	0	8
All	All	0	24

There are no bond length outliers.

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	227	ASN	N-CA-C	5.86	115.58	107.73
1	B	227	ASN	N-CA-C	5.86	115.58	107.73
1	C	227	ASN	N-CA-C	5.85	115.56	107.73
1	A	566	LYS	CA-C-N	5.37	130.94	122.78
1	A	566	LYS	C-N-CA	5.37	130.94	122.78

There are no chirality outliers.

5 of 24 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	261	THR	Peptide
1	A	502	GLU	Mainchain,Peptide

Continued on next page...

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Mol	Chain	Res	Type	Group
1	A	548	PHE	Peptide
1	A	573	ILE	Peptide
1	A	574	SER	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	7967	0	7762	192	0
1	B	7967	0	7762	172	0
1	C	7967	0	7762	177	0
All	All	23901	0	23286	444	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 444 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:194:LEU:O	1:A:223:PRO:HA	1.72	0.88
1:B:194:LEU:O	1:B:223:PRO:HA	1.72	0.88
1:C:194:LEU:O	1:C:223:PRO:HA	1.72	0.87
1:A:122:ASN:HA	1:A:166:ASP:O	1.74	0.87
1:B:34:THR:O	1:B:66:VAL:HB	1.75	0.87

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	1008/1203 (84%)	859 (85%)	146 (14%)	3 (0%)	36	67
1	B	1008/1203 (84%)	858 (85%)	147 (15%)	3 (0%)	36	67
1	C	1008/1203 (84%)	858 (85%)	147 (15%)	3 (0%)	36	67
All	All	3024/3609 (84%)	2575 (85%)	440 (15%)	9 (0%)	37	67

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	549	GLN
1	B	549	GLN
1	C	549	GLN
1	A	1092	PHE
1	B	1092	PHE

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	881/1047 (84%)	878 (100%)	3 (0%)	86	84
1	B	881/1047 (84%)	877 (100%)	4 (0%)	81	81
1	C	881/1047 (84%)	878 (100%)	3 (0%)	86	84
All	All	2643/3141 (84%)	2633 (100%)	10 (0%)	81	83

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	216	LEU
1	C	323	CYS
1	C	532	LEU
1	B	216	LEU
1	B	257	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40

such sidechains are listed below:

Mol	Chain	Res	Type
1	C	149	HIS
1	C	769	GLN
1	C	201	GLN
1	C	523	GLN
1	C	904	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.

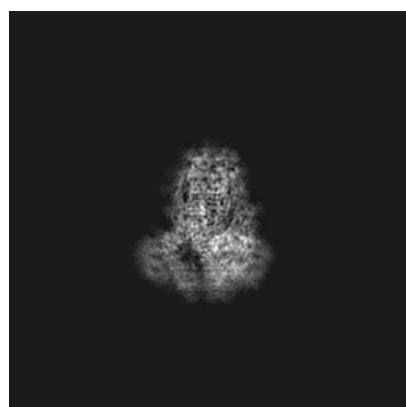
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6732. These allow visual inspection of the internal detail of the map and identification of artifacts.

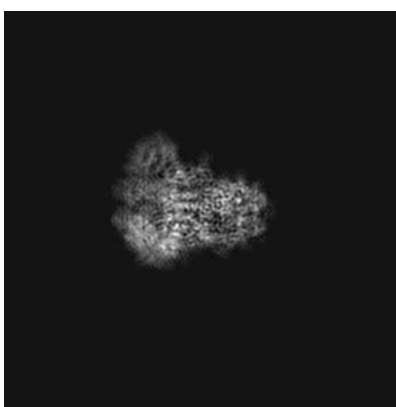
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

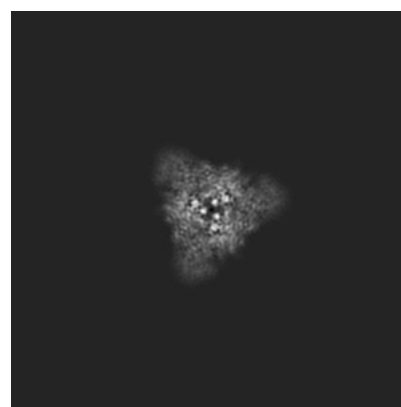
6.1.1 Primary map



X



Y

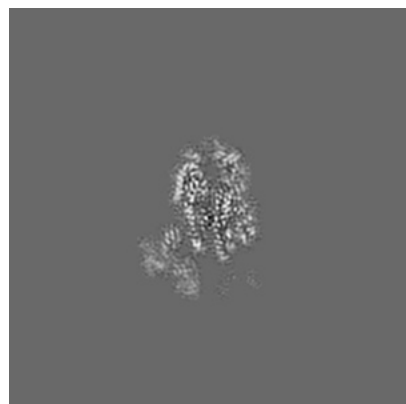


Z

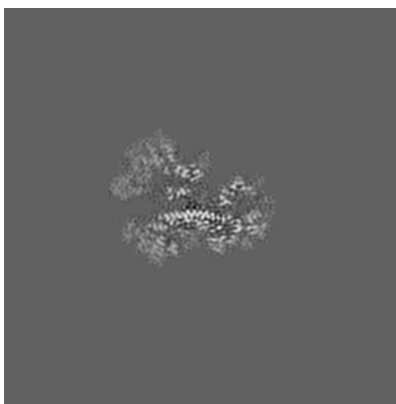
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

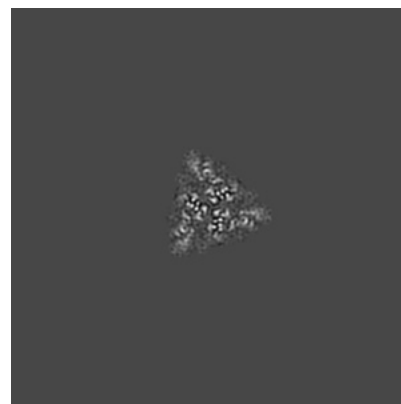
6.2.1 Primary map



X Index: 144



Y Index: 144



Z Index: 144

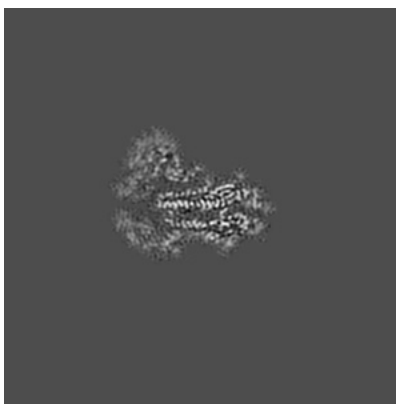
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

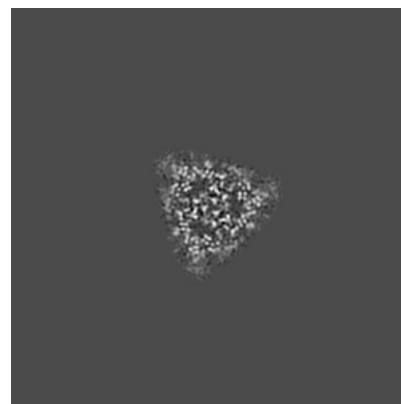
6.3.1 Primary map



X Index: 146



Y Index: 150

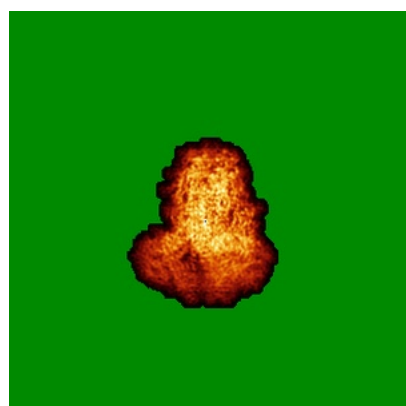


Z Index: 124

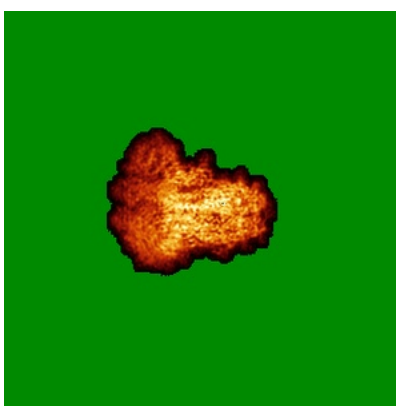
The images above show the largest variance slices of the map in three orthogonal directions.

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

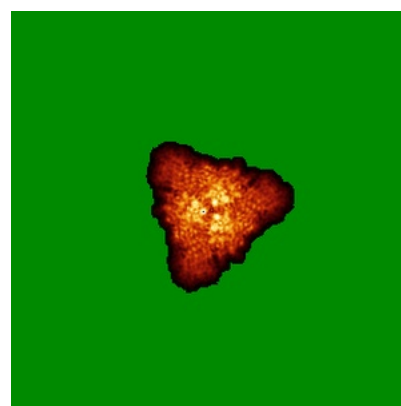
6.4.1 Primary map



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

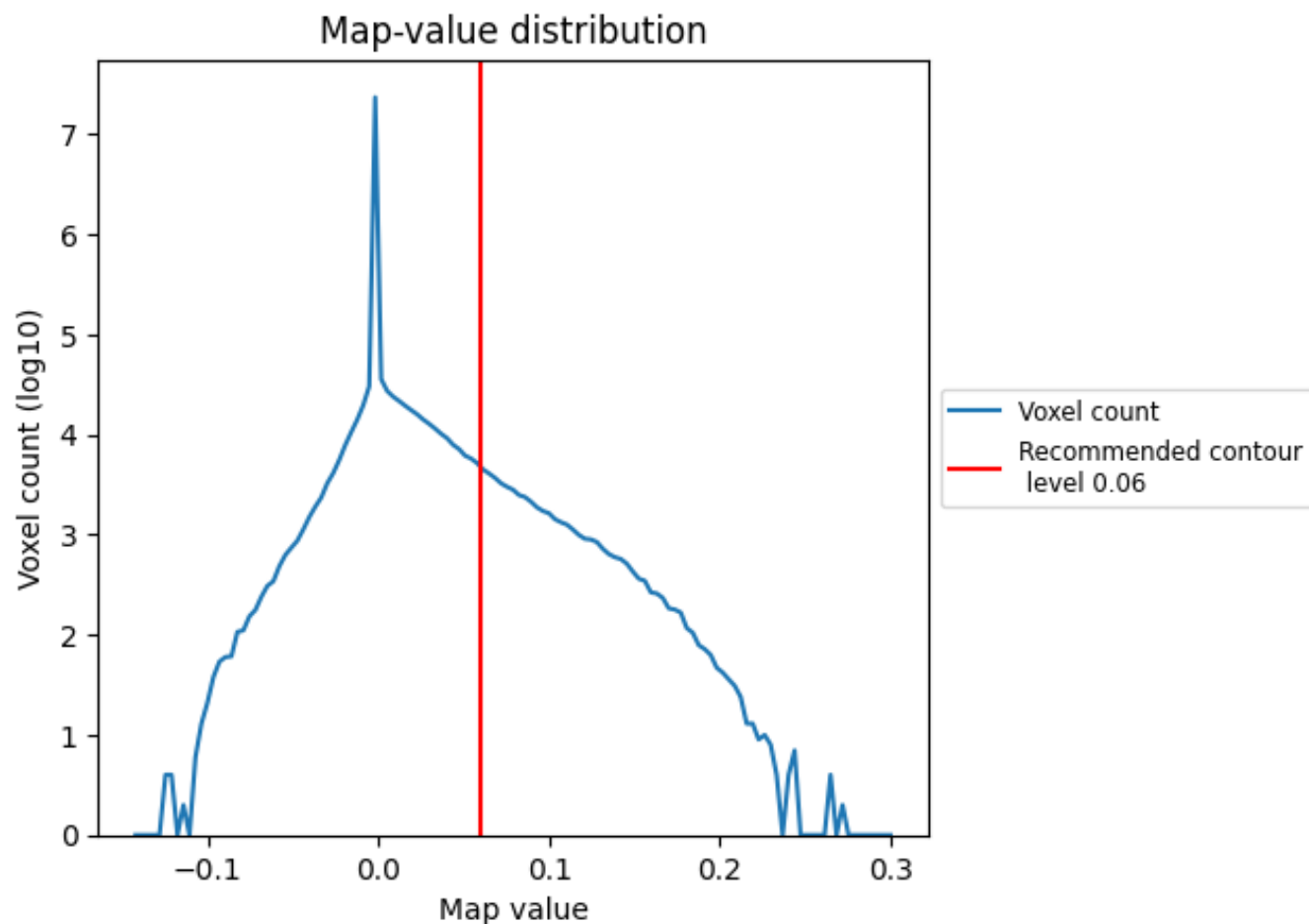
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

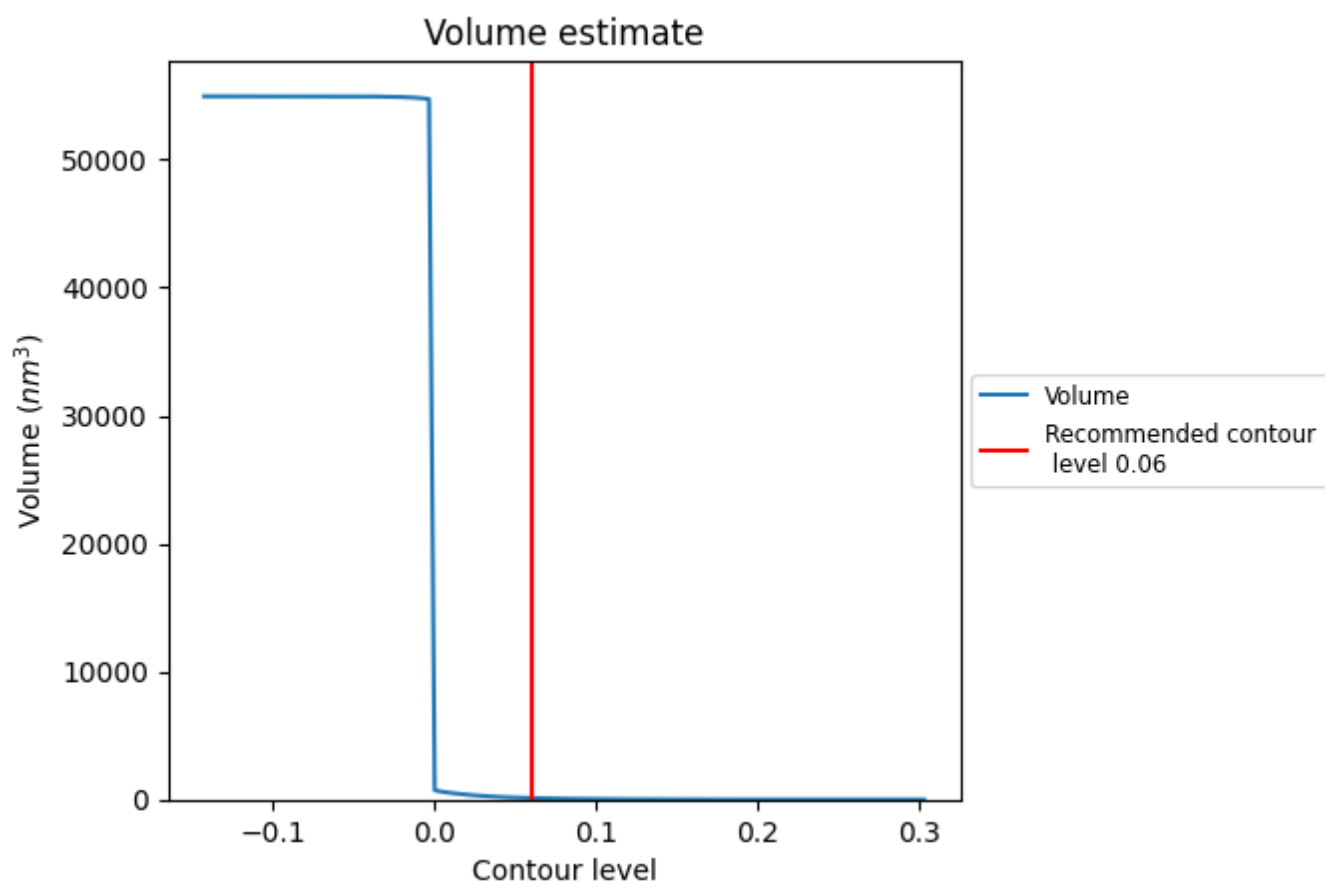
This section contains the results of statistical analysis of the map.

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.

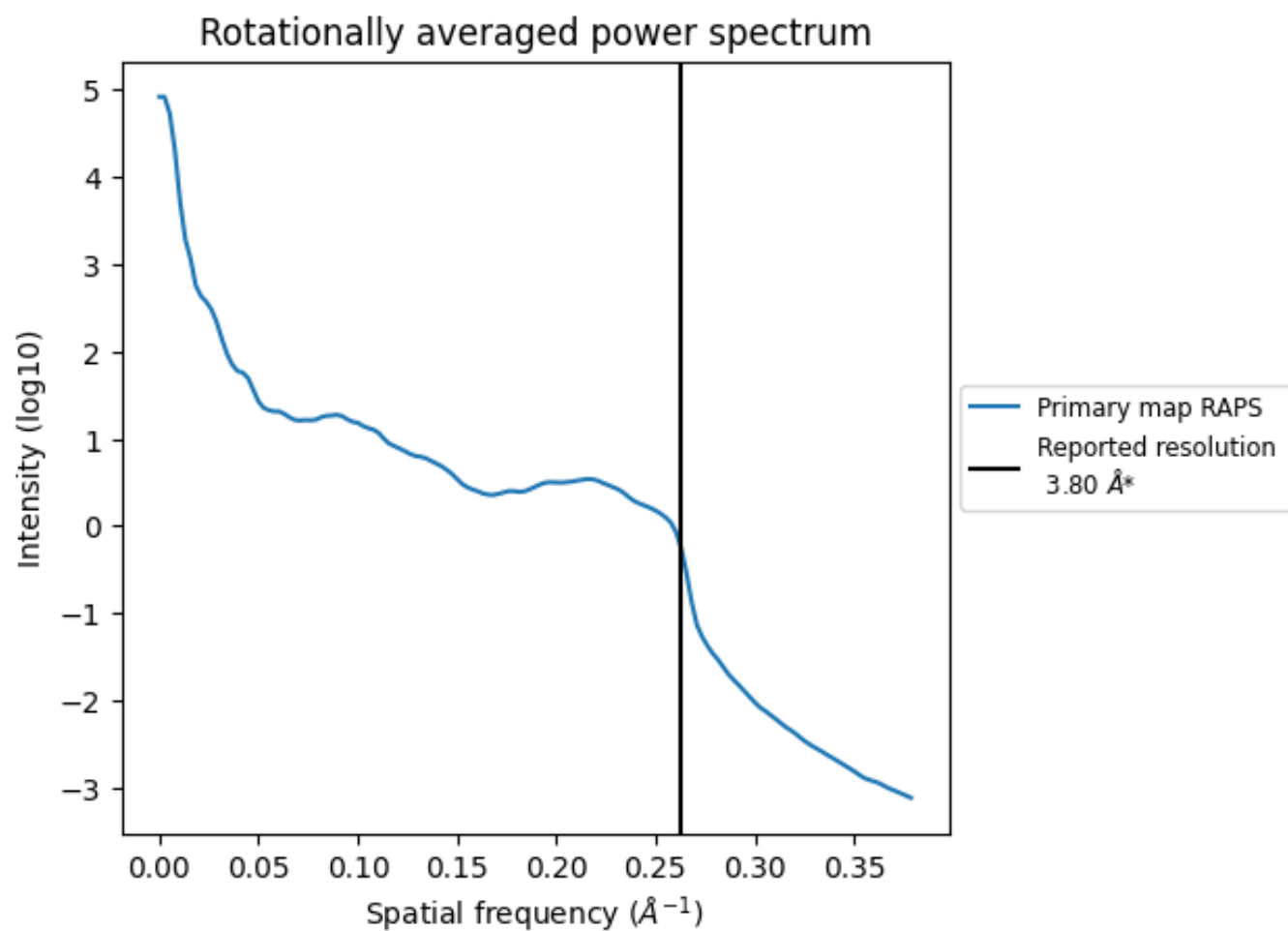
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 116 nm^3 ; this corresponds to an approximate mass of 105 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 0.263 Å⁻¹

8 Fourier-Shell correlation

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

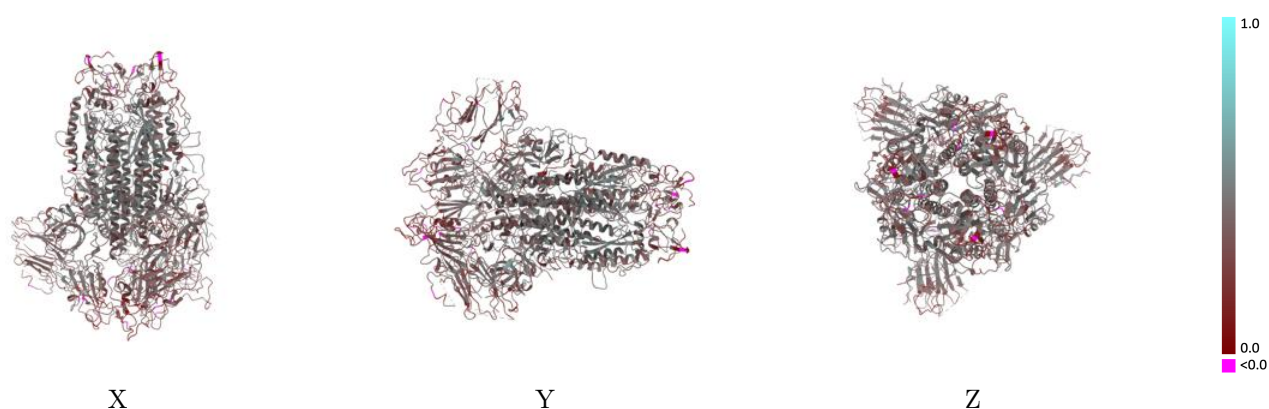
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-6732 and PDB model 5XLR. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlay [i](#)

This section was not generated.

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

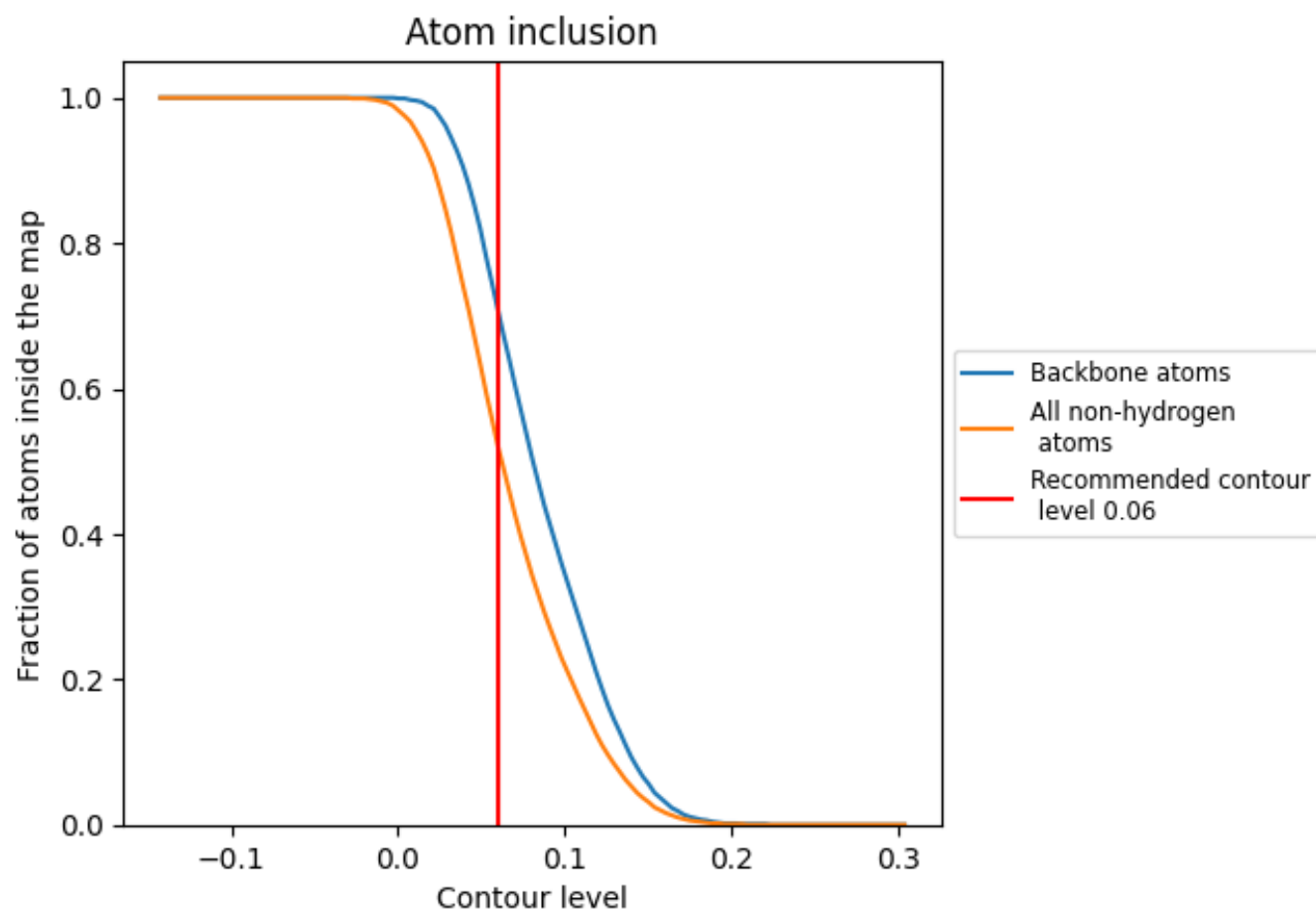


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 52% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5190	0.3710
A	0.5190	0.3700
B	0.5190	0.3710
C	0.5190	0.3740

