



wwPDB EM Validation Summary Report ⓘ

Mar 20, 2026 – 06:38 AM UTC

PDB ID : 9CAS / pdb_00009cas
EMDB ID : EMD-45402
Title : Bat SARS-like Coronavirus RsSHC014 Spike Protein
Authors : Acreman, C.M.; McLellan, J.S.
Deposited on : 2024-06-17
Resolution : 3.10 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

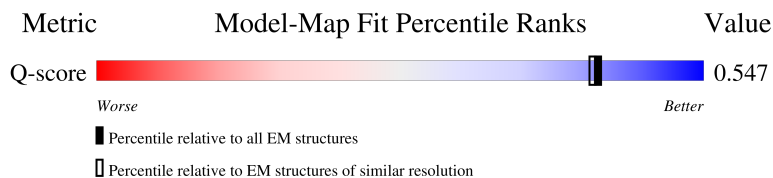
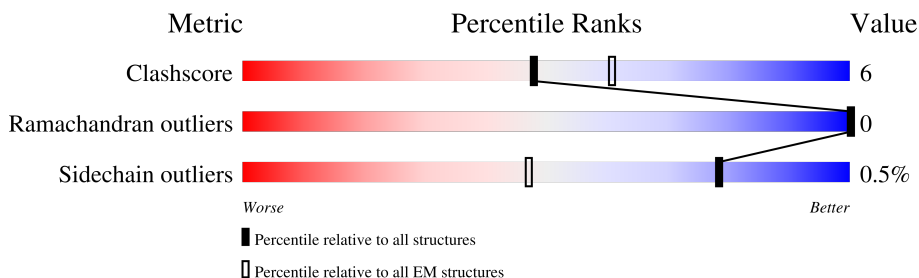
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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	14724 (2.60 - 3.60)

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	1271	 66% 11% 23%
1	B	1271	 67% 10% 23%
1	C	1271	 66% 10% 23%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 45023 atoms, of which 22251 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	975	Total	C	H	N	O	S	0	0
			15009	4847	7419	1270	1433	40		
1	B	974	Total	C	H	N	O	S	0	0
			14999	4845	7413	1269	1432	40		
1	C	976	Total	C	H	N	O	S	0	0
			15015	4850	7419	1271	1435	40		

There are 240 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1192	GLY	-	expression tag	UNP U5WLK5
A	1193	SER	-	expression tag	UNP U5WLK5
A	1194	GLY	-	expression tag	UNP U5WLK5
A	1195	TYR	-	expression tag	UNP U5WLK5
A	1196	ILE	-	expression tag	UNP U5WLK5
A	1197	PRO	-	expression tag	UNP U5WLK5
A	1198	GLU	-	expression tag	UNP U5WLK5
A	1199	ALA	-	expression tag	UNP U5WLK5
A	1200	PRO	-	expression tag	UNP U5WLK5
A	1201	ARG	-	expression tag	UNP U5WLK5
A	1202	ASP	-	expression tag	UNP U5WLK5
A	1203	GLY	-	expression tag	UNP U5WLK5
A	1204	GLN	-	expression tag	UNP U5WLK5
A	1205	ALA	-	expression tag	UNP U5WLK5
A	1206	TYR	-	expression tag	UNP U5WLK5
A	1207	VAL	-	expression tag	UNP U5WLK5
A	1208	ARG	-	expression tag	UNP U5WLK5
A	1209	LYS	-	expression tag	UNP U5WLK5
A	1210	ASP	-	expression tag	UNP U5WLK5
A	1211	GLY	-	expression tag	UNP U5WLK5
A	1212	GLU	-	expression tag	UNP U5WLK5
A	1213	TRP	-	expression tag	UNP U5WLK5
A	1214	VAL	-	expression tag	UNP U5WLK5
A	1215	LEU	-	expression tag	UNP U5WLK5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1216	LEU	-	expression tag	UNP U5WLK5
A	1217	SER	-	expression tag	UNP U5WLK5
A	1218	THR	-	expression tag	UNP U5WLK5
A	1219	PHE	-	expression tag	UNP U5WLK5
A	1220	LEU	-	expression tag	UNP U5WLK5
A	1221	GLY	-	expression tag	UNP U5WLK5
A	1222	ARG	-	expression tag	UNP U5WLK5
A	1223	SER	-	expression tag	UNP U5WLK5
A	1224	LEU	-	expression tag	UNP U5WLK5
A	1225	GLU	-	expression tag	UNP U5WLK5
A	1226	VAL	-	expression tag	UNP U5WLK5
A	1227	LEU	-	expression tag	UNP U5WLK5
A	1228	PHE	-	expression tag	UNP U5WLK5
A	1229	GLN	-	expression tag	UNP U5WLK5
A	1230	GLY	-	expression tag	UNP U5WLK5
A	1231	PRO	-	expression tag	UNP U5WLK5
A	1232	GLY	-	expression tag	UNP U5WLK5
A	1233	HIS	-	expression tag	UNP U5WLK5
A	1234	HIS	-	expression tag	UNP U5WLK5
A	1235	HIS	-	expression tag	UNP U5WLK5
A	1236	HIS	-	expression tag	UNP U5WLK5
A	1237	HIS	-	expression tag	UNP U5WLK5
A	1238	HIS	-	expression tag	UNP U5WLK5
A	1239	HIS	-	expression tag	UNP U5WLK5
A	1240	HIS	-	expression tag	UNP U5WLK5
A	1241	SER	-	expression tag	UNP U5WLK5
A	1242	ALA	-	expression tag	UNP U5WLK5
A	1243	TRP	-	expression tag	UNP U5WLK5
A	1244	SER	-	expression tag	UNP U5WLK5
A	1245	HIS	-	expression tag	UNP U5WLK5
A	1246	PRO	-	expression tag	UNP U5WLK5
A	1247	GLN	-	expression tag	UNP U5WLK5
A	1248	PHE	-	expression tag	UNP U5WLK5
A	1249	GLU	-	expression tag	UNP U5WLK5
A	1250	LYS	-	expression tag	UNP U5WLK5
A	1251	GLY	-	expression tag	UNP U5WLK5
A	1252	GLY	-	expression tag	UNP U5WLK5
A	1253	GLY	-	expression tag	UNP U5WLK5
A	1254	SER	-	expression tag	UNP U5WLK5
A	1255	GLY	-	expression tag	UNP U5WLK5
A	1256	GLY	-	expression tag	UNP U5WLK5
A	1257	GLY	-	expression tag	UNP U5WLK5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1258	GLY	-	expression tag	UNP U5WLK5
A	1259	SER	-	expression tag	UNP U5WLK5
A	1260	GLY	-	expression tag	UNP U5WLK5
A	1261	GLY	-	expression tag	UNP U5WLK5
A	1262	SER	-	expression tag	UNP U5WLK5
A	1263	ALA	-	expression tag	UNP U5WLK5
A	1264	TRP	-	expression tag	UNP U5WLK5
A	1265	SER	-	expression tag	UNP U5WLK5
A	1266	HIS	-	expression tag	UNP U5WLK5
A	1267	PRO	-	expression tag	UNP U5WLK5
A	1268	GLN	-	expression tag	UNP U5WLK5
A	1269	PHE	-	expression tag	UNP U5WLK5
A	1270	GLU	-	expression tag	UNP U5WLK5
A	1271	LYS	-	expression tag	UNP U5WLK5
B	1192	GLY	-	expression tag	UNP U5WLK5
B	1193	SER	-	expression tag	UNP U5WLK5
B	1194	GLY	-	expression tag	UNP U5WLK5
B	1195	TYR	-	expression tag	UNP U5WLK5
B	1196	ILE	-	expression tag	UNP U5WLK5
B	1197	PRO	-	expression tag	UNP U5WLK5
B	1198	GLU	-	expression tag	UNP U5WLK5
B	1199	ALA	-	expression tag	UNP U5WLK5
B	1200	PRO	-	expression tag	UNP U5WLK5
B	1201	ARG	-	expression tag	UNP U5WLK5
B	1202	ASP	-	expression tag	UNP U5WLK5
B	1203	GLY	-	expression tag	UNP U5WLK5
B	1204	GLN	-	expression tag	UNP U5WLK5
B	1205	ALA	-	expression tag	UNP U5WLK5
B	1206	TYR	-	expression tag	UNP U5WLK5
B	1207	VAL	-	expression tag	UNP U5WLK5
B	1208	ARG	-	expression tag	UNP U5WLK5
B	1209	LYS	-	expression tag	UNP U5WLK5
B	1210	ASP	-	expression tag	UNP U5WLK5
B	1211	GLY	-	expression tag	UNP U5WLK5
B	1212	GLU	-	expression tag	UNP U5WLK5
B	1213	TRP	-	expression tag	UNP U5WLK5
B	1214	VAL	-	expression tag	UNP U5WLK5
B	1215	LEU	-	expression tag	UNP U5WLK5
B	1216	LEU	-	expression tag	UNP U5WLK5
B	1217	SER	-	expression tag	UNP U5WLK5
B	1218	THR	-	expression tag	UNP U5WLK5
B	1219	PHE	-	expression tag	UNP U5WLK5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1220	LEU	-	expression tag	UNP U5WLK5
B	1221	GLY	-	expression tag	UNP U5WLK5
B	1222	ARG	-	expression tag	UNP U5WLK5
B	1223	SER	-	expression tag	UNP U5WLK5
B	1224	LEU	-	expression tag	UNP U5WLK5
B	1225	GLU	-	expression tag	UNP U5WLK5
B	1226	VAL	-	expression tag	UNP U5WLK5
B	1227	LEU	-	expression tag	UNP U5WLK5
B	1228	PHE	-	expression tag	UNP U5WLK5
B	1229	GLN	-	expression tag	UNP U5WLK5
B	1230	GLY	-	expression tag	UNP U5WLK5
B	1231	PRO	-	expression tag	UNP U5WLK5
B	1232	GLY	-	expression tag	UNP U5WLK5
B	1233	HIS	-	expression tag	UNP U5WLK5
B	1234	HIS	-	expression tag	UNP U5WLK5
B	1235	HIS	-	expression tag	UNP U5WLK5
B	1236	HIS	-	expression tag	UNP U5WLK5
B	1237	HIS	-	expression tag	UNP U5WLK5
B	1238	HIS	-	expression tag	UNP U5WLK5
B	1239	HIS	-	expression tag	UNP U5WLK5
B	1240	HIS	-	expression tag	UNP U5WLK5
B	1241	SER	-	expression tag	UNP U5WLK5
B	1242	ALA	-	expression tag	UNP U5WLK5
B	1243	TRP	-	expression tag	UNP U5WLK5
B	1244	SER	-	expression tag	UNP U5WLK5
B	1245	HIS	-	expression tag	UNP U5WLK5
B	1246	PRO	-	expression tag	UNP U5WLK5
B	1247	GLN	-	expression tag	UNP U5WLK5
B	1248	PHE	-	expression tag	UNP U5WLK5
B	1249	GLU	-	expression tag	UNP U5WLK5
B	1250	LYS	-	expression tag	UNP U5WLK5
B	1251	GLY	-	expression tag	UNP U5WLK5
B	1252	GLY	-	expression tag	UNP U5WLK5
B	1253	GLY	-	expression tag	UNP U5WLK5
B	1254	SER	-	expression tag	UNP U5WLK5
B	1255	GLY	-	expression tag	UNP U5WLK5
B	1256	GLY	-	expression tag	UNP U5WLK5
B	1257	GLY	-	expression tag	UNP U5WLK5
B	1258	GLY	-	expression tag	UNP U5WLK5
B	1259	SER	-	expression tag	UNP U5WLK5
B	1260	GLY	-	expression tag	UNP U5WLK5
B	1261	GLY	-	expression tag	UNP U5WLK5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1262	SER	-	expression tag	UNP U5WLK5
B	1263	ALA	-	expression tag	UNP U5WLK5
B	1264	TRP	-	expression tag	UNP U5WLK5
B	1265	SER	-	expression tag	UNP U5WLK5
B	1266	HIS	-	expression tag	UNP U5WLK5
B	1267	PRO	-	expression tag	UNP U5WLK5
B	1268	GLN	-	expression tag	UNP U5WLK5
B	1269	PHE	-	expression tag	UNP U5WLK5
B	1270	GLU	-	expression tag	UNP U5WLK5
B	1271	LYS	-	expression tag	UNP U5WLK5
C	1192	GLY	-	expression tag	UNP U5WLK5
C	1193	SER	-	expression tag	UNP U5WLK5
C	1194	GLY	-	expression tag	UNP U5WLK5
C	1195	TYR	-	expression tag	UNP U5WLK5
C	1196	ILE	-	expression tag	UNP U5WLK5
C	1197	PRO	-	expression tag	UNP U5WLK5
C	1198	GLU	-	expression tag	UNP U5WLK5
C	1199	ALA	-	expression tag	UNP U5WLK5
C	1200	PRO	-	expression tag	UNP U5WLK5
C	1201	ARG	-	expression tag	UNP U5WLK5
C	1202	ASP	-	expression tag	UNP U5WLK5
C	1203	GLY	-	expression tag	UNP U5WLK5
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C	1211	GLY	-	expression tag	UNP U5WLK5
C	1212	GLU	-	expression tag	UNP U5WLK5
C	1213	TRP	-	expression tag	UNP U5WLK5
C	1214	VAL	-	expression tag	UNP U5WLK5
C	1215	LEU	-	expression tag	UNP U5WLK5
C	1216	LEU	-	expression tag	UNP U5WLK5
C	1217	SER	-	expression tag	UNP U5WLK5
C	1218	THR	-	expression tag	UNP U5WLK5
C	1219	PHE	-	expression tag	UNP U5WLK5
C	1220	LEU	-	expression tag	UNP U5WLK5
C	1221	GLY	-	expression tag	UNP U5WLK5
C	1222	ARG	-	expression tag	UNP U5WLK5
C	1223	SER	-	expression tag	UNP U5WLK5

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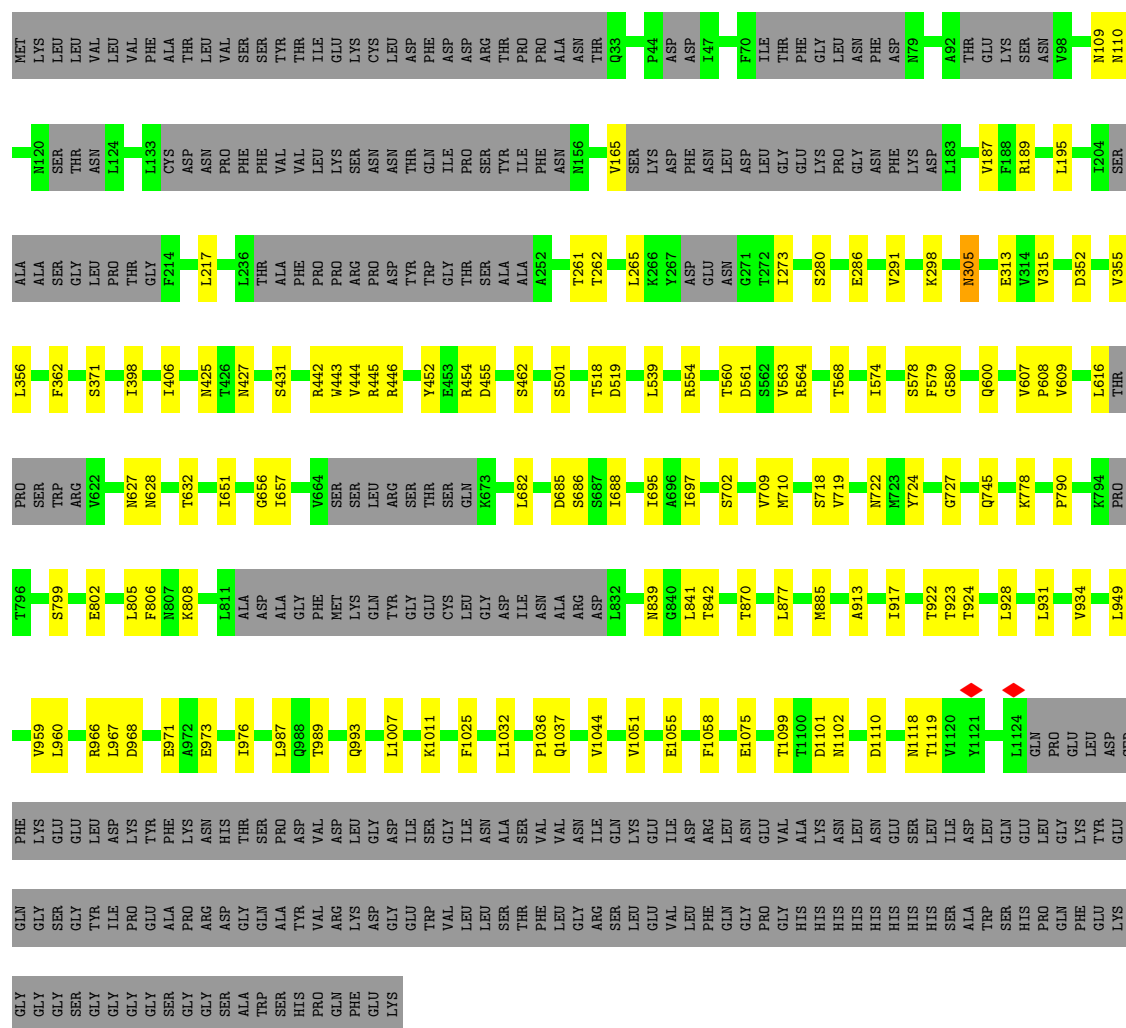
Chain	Residue	Modelled	Actual	Comment	Reference
C	1224	LEU	-	expression tag	UNP U5WLK5
C	1225	GLU	-	expression tag	UNP U5WLK5
C	1226	VAL	-	expression tag	UNP U5WLK5
C	1227	LEU	-	expression tag	UNP U5WLK5
C	1228	PHE	-	expression tag	UNP U5WLK5
C	1229	GLN	-	expression tag	UNP U5WLK5
C	1230	GLY	-	expression tag	UNP U5WLK5
C	1231	PRO	-	expression tag	UNP U5WLK5
C	1232	GLY	-	expression tag	UNP U5WLK5
C	1233	HIS	-	expression tag	UNP U5WLK5
C	1234	HIS	-	expression tag	UNP U5WLK5
C	1235	HIS	-	expression tag	UNP U5WLK5
C	1236	HIS	-	expression tag	UNP U5WLK5
C	1237	HIS	-	expression tag	UNP U5WLK5
C	1238	HIS	-	expression tag	UNP U5WLK5
C	1239	HIS	-	expression tag	UNP U5WLK5
C	1240	HIS	-	expression tag	UNP U5WLK5
C	1241	SER	-	expression tag	UNP U5WLK5
C	1242	ALA	-	expression tag	UNP U5WLK5
C	1243	TRP	-	expression tag	UNP U5WLK5
C	1244	SER	-	expression tag	UNP U5WLK5
C	1245	HIS	-	expression tag	UNP U5WLK5
C	1246	PRO	-	expression tag	UNP U5WLK5
C	1247	GLN	-	expression tag	UNP U5WLK5
C	1248	PHE	-	expression tag	UNP U5WLK5
C	1249	GLU	-	expression tag	UNP U5WLK5
C	1250	LYS	-	expression tag	UNP U5WLK5
C	1251	GLY	-	expression tag	UNP U5WLK5
C	1252	GLY	-	expression tag	UNP U5WLK5
C	1253	GLY	-	expression tag	UNP U5WLK5
C	1254	SER	-	expression tag	UNP U5WLK5
C	1255	GLY	-	expression tag	UNP U5WLK5
C	1256	GLY	-	expression tag	UNP U5WLK5
C	1257	GLY	-	expression tag	UNP U5WLK5
C	1258	GLY	-	expression tag	UNP U5WLK5
C	1259	SER	-	expression tag	UNP U5WLK5
C	1260	GLY	-	expression tag	UNP U5WLK5
C	1261	GLY	-	expression tag	UNP U5WLK5
C	1262	SER	-	expression tag	UNP U5WLK5
C	1263	ALA	-	expression tag	UNP U5WLK5
C	1264	TRP	-	expression tag	UNP U5WLK5
C	1265	SER	-	expression tag	UNP U5WLK5

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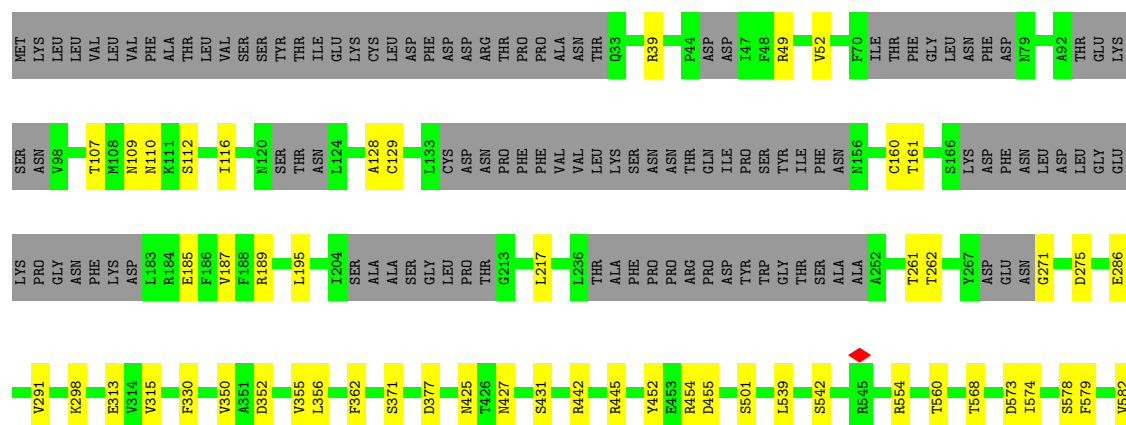
Chain	Residue	Modelled	Actual	Comment	Reference
C	1266	HIS	-	expression tag	UNP U5WLK5
C	1267	PRO	-	expression tag	UNP U5WLK5
C	1268	GLN	-	expression tag	UNP U5WLK5
C	1269	PHE	-	expression tag	UNP U5WLK5
C	1270	GLU	-	expression tag	UNP U5WLK5
C	1271	LYS	-	expression tag	UNP U5WLK5

Chain B:  67% 10% 23%



● Molecule 1: Spike glycoprotein

Chain C:  66% 10% 23%



HIS	ASN	Q918	K778	Y599
HIS	GLU	E919	K778	Q600
HIS	SER	T922	I788	V607
HIS	LEU	T923	L789	P608
SER	ILE	T924	P790	V609
ALA	ASP	L928	K794	L616
TRP	LEU	L931	PRO	THR
SER	GLN	V934	T796	PRO
HIS	LEU	V934	S799	SER
SER	GLY	L949	F800	TRP
GLN	PHE	V959	I801	ARG
GLY	LYS	L967	E802	V622
GLY	GLU	D968	K808	N627
GLY	GLY	E971	V809	Q631
GLY	TYR	A972	T810	T632
GLY	PHE	E973	L811	G635
GLY	PRO	I976	ALA	I651
GLY	ASN	T980	ASP	I657
SER	HIS	L987	GLY	H662
ALA	THR	Q988	GLY	T663
GLY	SER	T989	CYS	V664
TRP	GLY	V990	LEU	SER
VAL	ASP	K1011	LEU	SER
ARG	ASP	F1025	GLY	ARG
GLN	LYS	L1032	ILE	THR
PHE	GLY	P1036	ALA	SER
GLU	ASP	Q1037	ARG	GLN
GLY	ILE	V1044	ASP	K673
TRP	SER	V1051	N839	V676
VAL	GLY	E1055	G840	D685
VAL	ILE	F1058	L841	I688
LEU	ILE	T1059	T842	I697
LEU	ASN	T1060	L847	S702
SER	ALA	E1075	M852	V709
THR	SER	F1078	L877	S718
PHE	VAL	T1099	Q878	V719
LEU	ASN	T1100	I879	Y724
GLY	GLU	D1101	M885	Q745
GLY	VAL		A913	L750
GLY	ALA		I917	
GLY	LYS			
GLY	LEU			

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	76442	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.458	Depositor
Minimum map value	-1.044	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.18	Depositor
Map size (Å)	481.28, 481.28, 481.28	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.94, 0.94, 0.94	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	0.19	0/7753	0.35	0/10532
1	B	0.19	0/7749	0.35	0/10527
1	C	0.18	0/7759	0.33	0/10540
All	All	0.19	0/23261	0.34	0/31599

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

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	7590	7419	7426	99	0
1	B	7586	7413	7423	90	0
1	C	7596	7419	7431	99	0
All	All	22772	22251	22280	264	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 6.

The worst 5 of 264 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:70:PHE:O	1:A:252:ALA:N	2.07	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:THR:HG1	1:A:112:SER:HG	1.16	0.85
1:A:427:ASN:O	1:A:431:SER:OG	1.95	0.83
1:C:427:ASN:O	1:C:431:SER:OG	1.97	0.82
1:B:427:ASN:O	1:B:431:SER:OG	1.98	0.80

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	947/1271 (74%)	907 (96%)	40 (4%)	0	100	100
1	B	946/1271 (74%)	911 (96%)	35 (4%)	0	100	100
1	C	948/1271 (75%)	909 (96%)	39 (4%)	0	100	100
All	All	2841/3813 (74%)	2727 (96%)	114 (4%)	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	846/1099 (77%)	840 (99%)	6 (1%)	76	82
1	B	846/1099 (77%)	842 (100%)	4 (0%)	81	85
1	C	847/1099 (77%)	845 (100%)	2 (0%)	87	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2539/3297 (77%)	2527 (100%)	12 (0%)	78 85

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	600	GLN
1	B	808	LYS
1	C	922	THR
1	B	922	THR
1	A	920	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	458	ASN
1	C	745	GLN
1	C	1037	GLN
1	C	884	GLN
1	C	734	ASN

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.

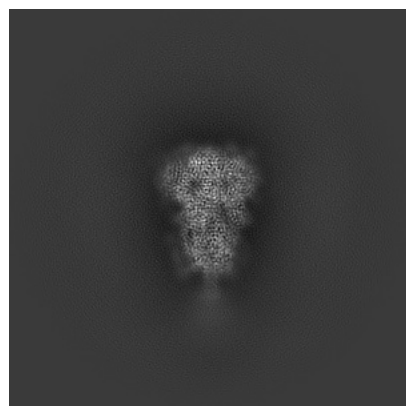
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45402. These allow visual inspection of the internal detail of the map and identification of artifacts.

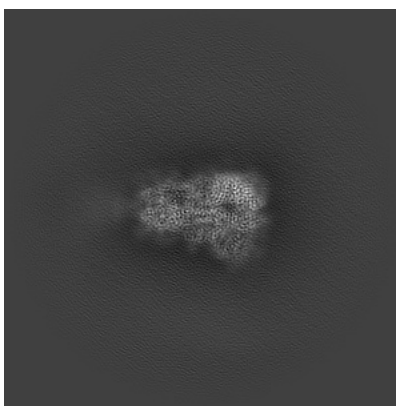
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

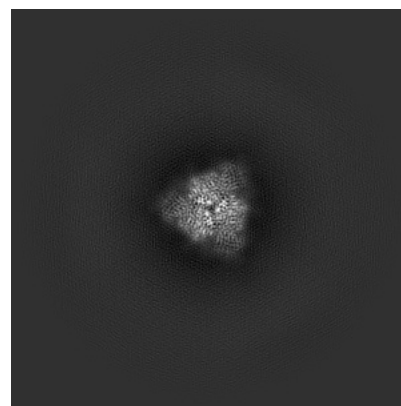
6.1.1 Primary map



X

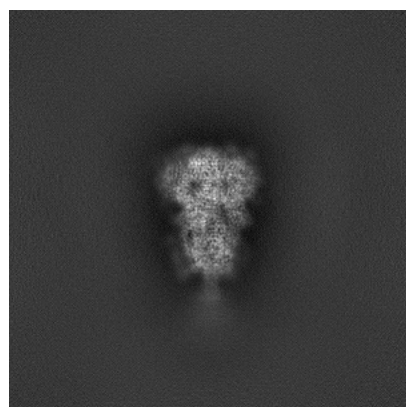


Y

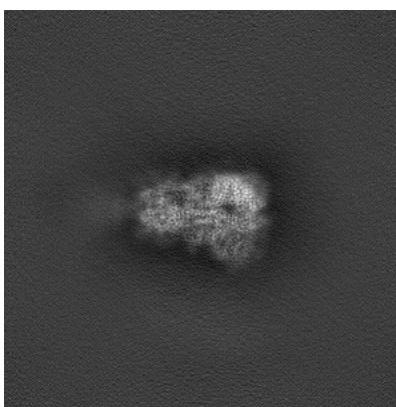


Z

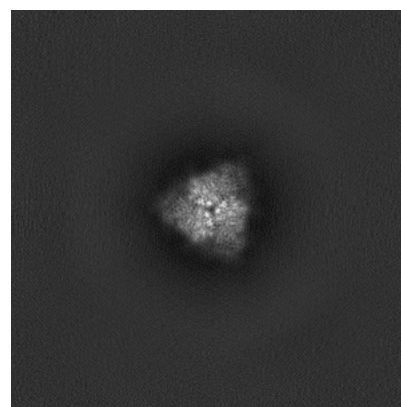
6.1.2 Raw map



X



Y

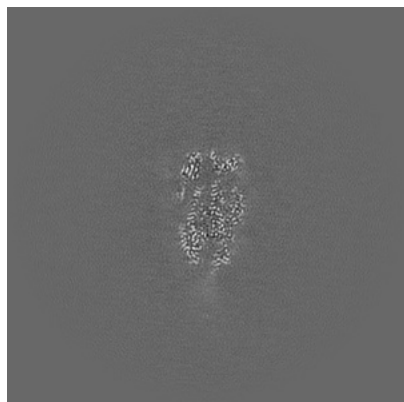


Z

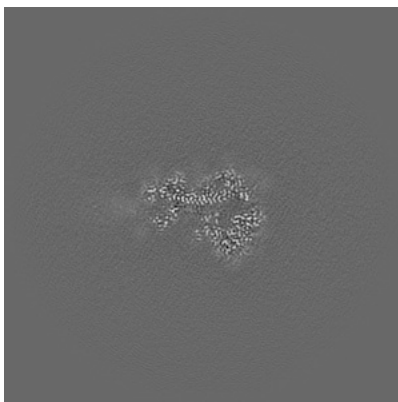
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

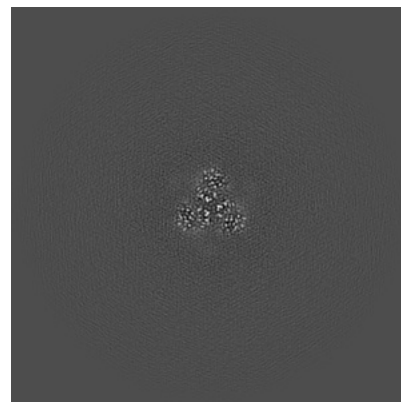
6.2.1 Primary map



X Index: 256

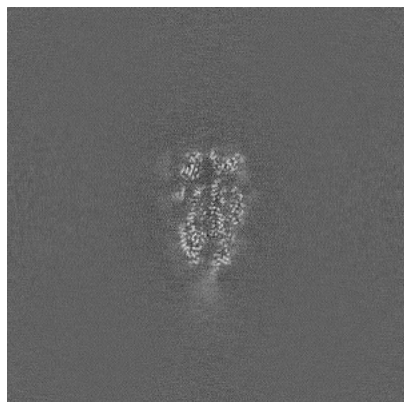


Y Index: 256

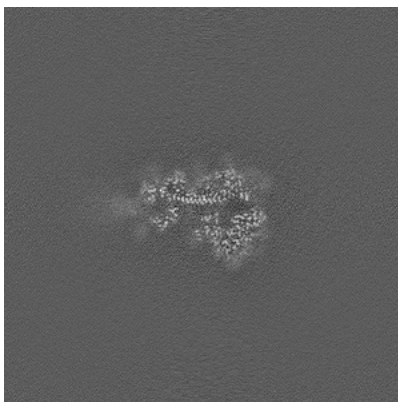


Z Index: 256

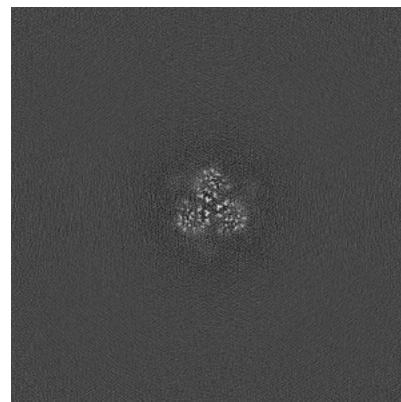
6.2.2 Raw map



X Index: 256



Y Index: 256

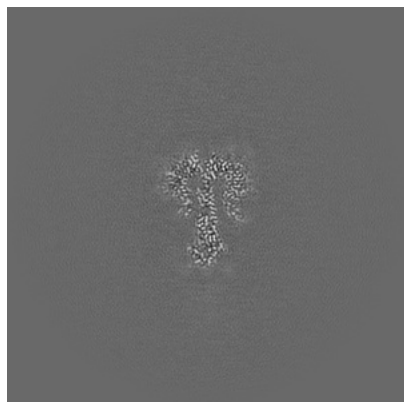


Z Index: 256

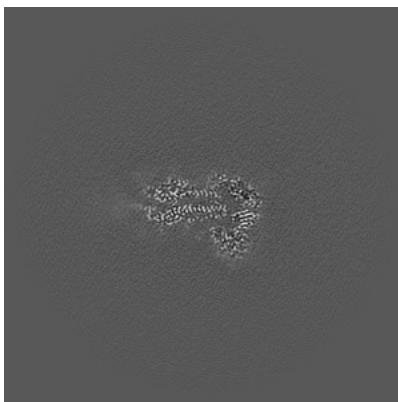
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

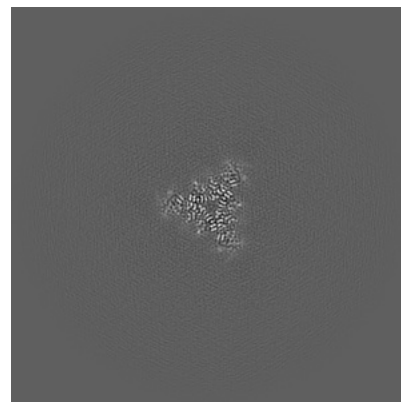
6.3.1 Primary map



X Index: 272

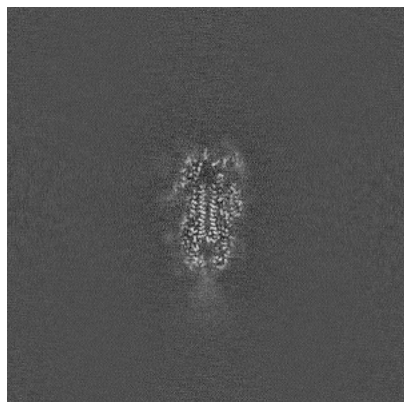


Y Index: 264

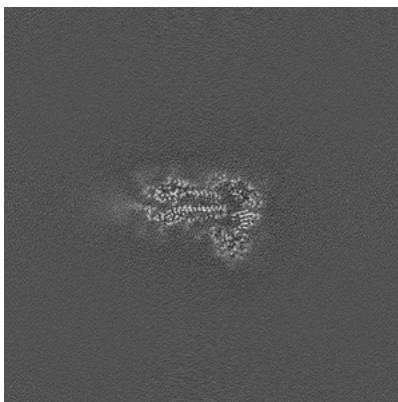


Z Index: 305

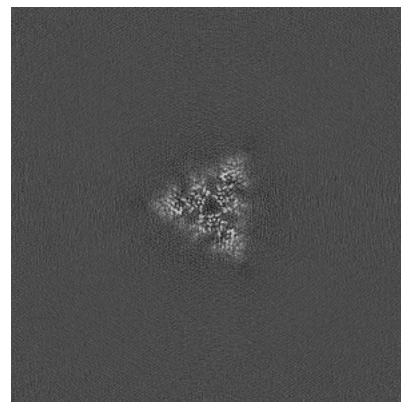
6.3.2 Raw map



X Index: 251



Y Index: 264

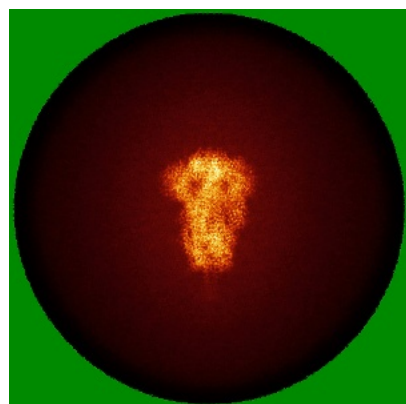


Z Index: 296

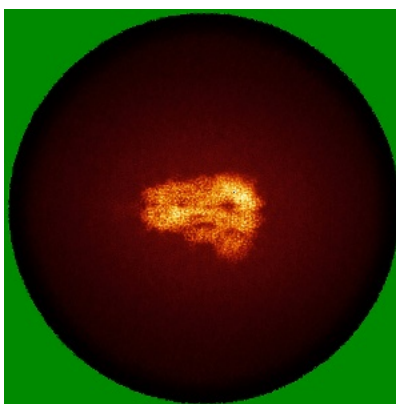
The images above show the largest variance slices of the map in three orthogonal directions.

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

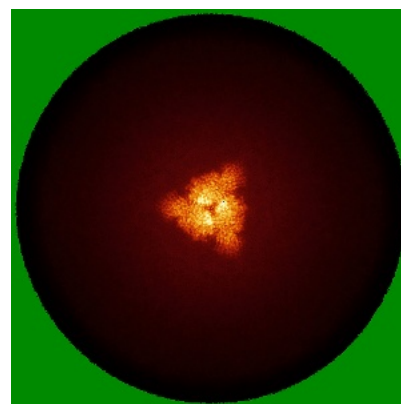
6.4.1 Primary map



X

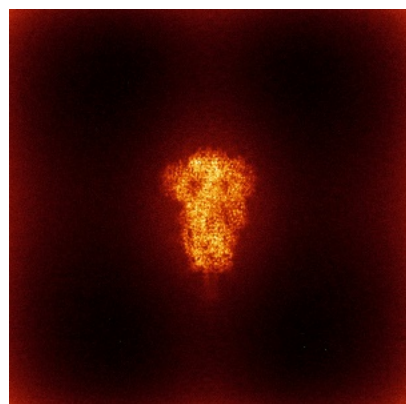


Y

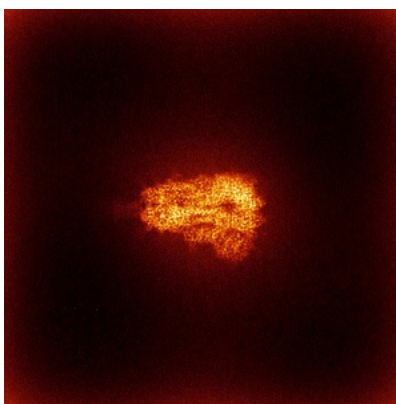


Z

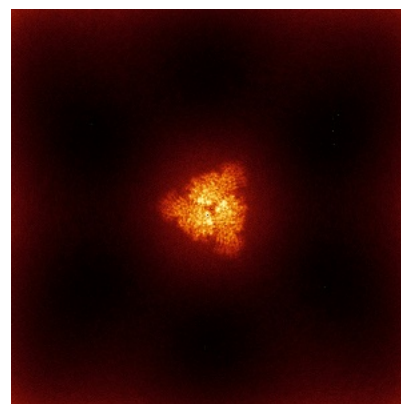
6.4.2 Raw map



X



Y

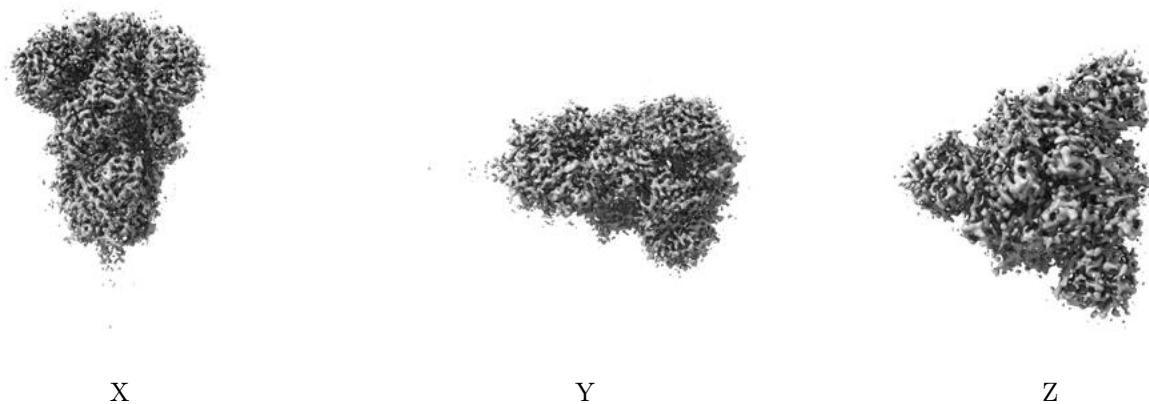


Z

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.

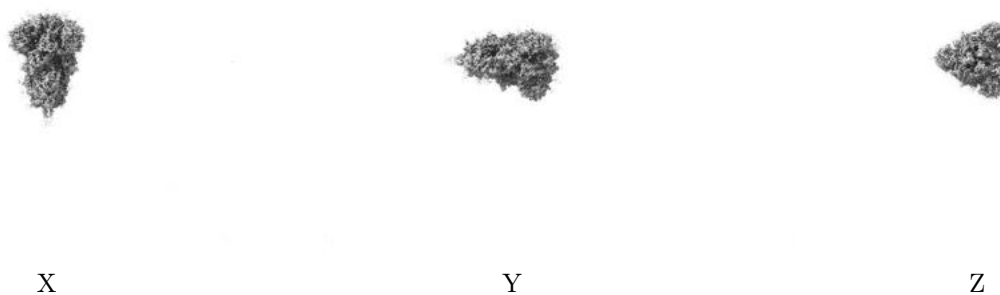
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.18. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 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.

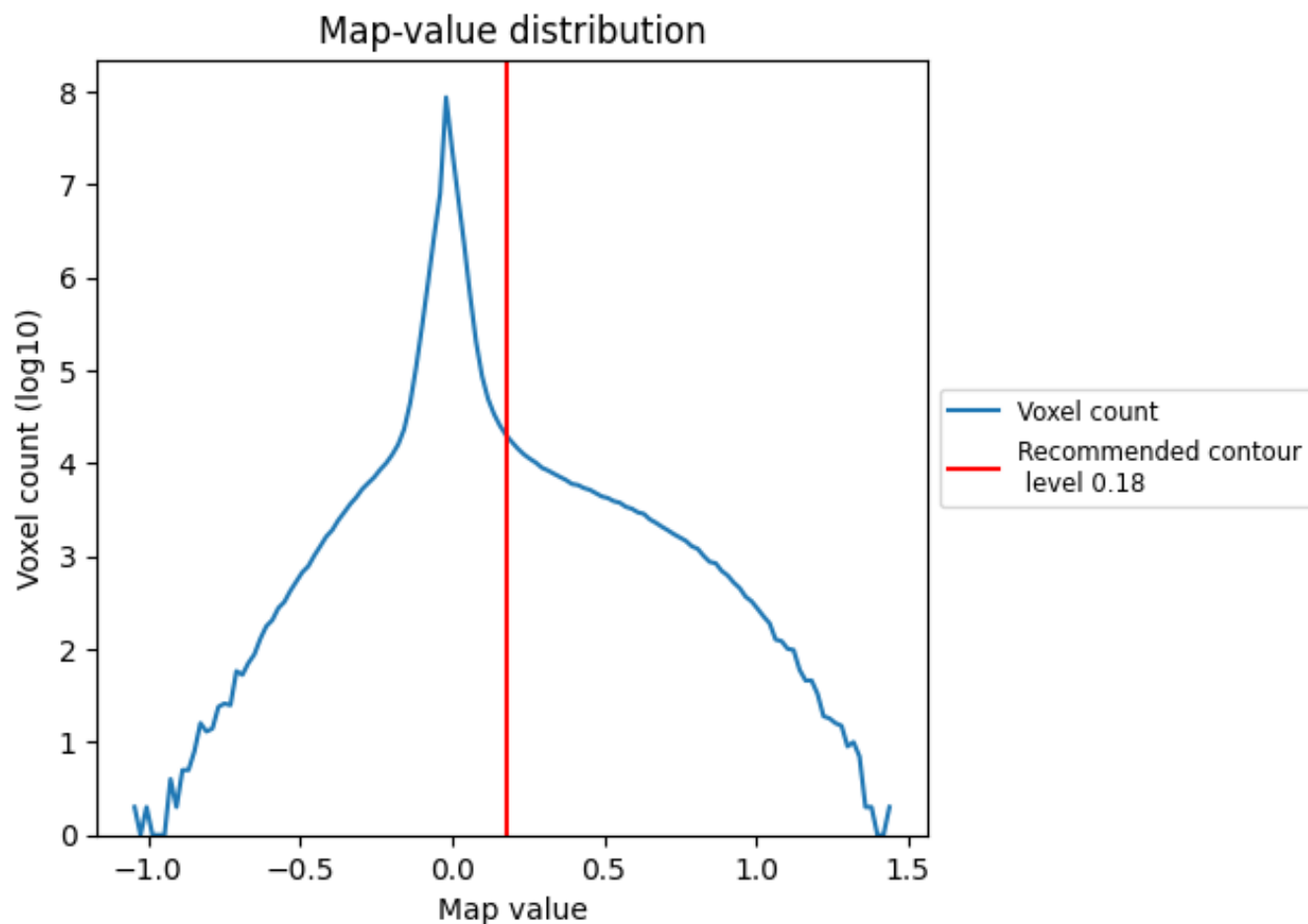
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

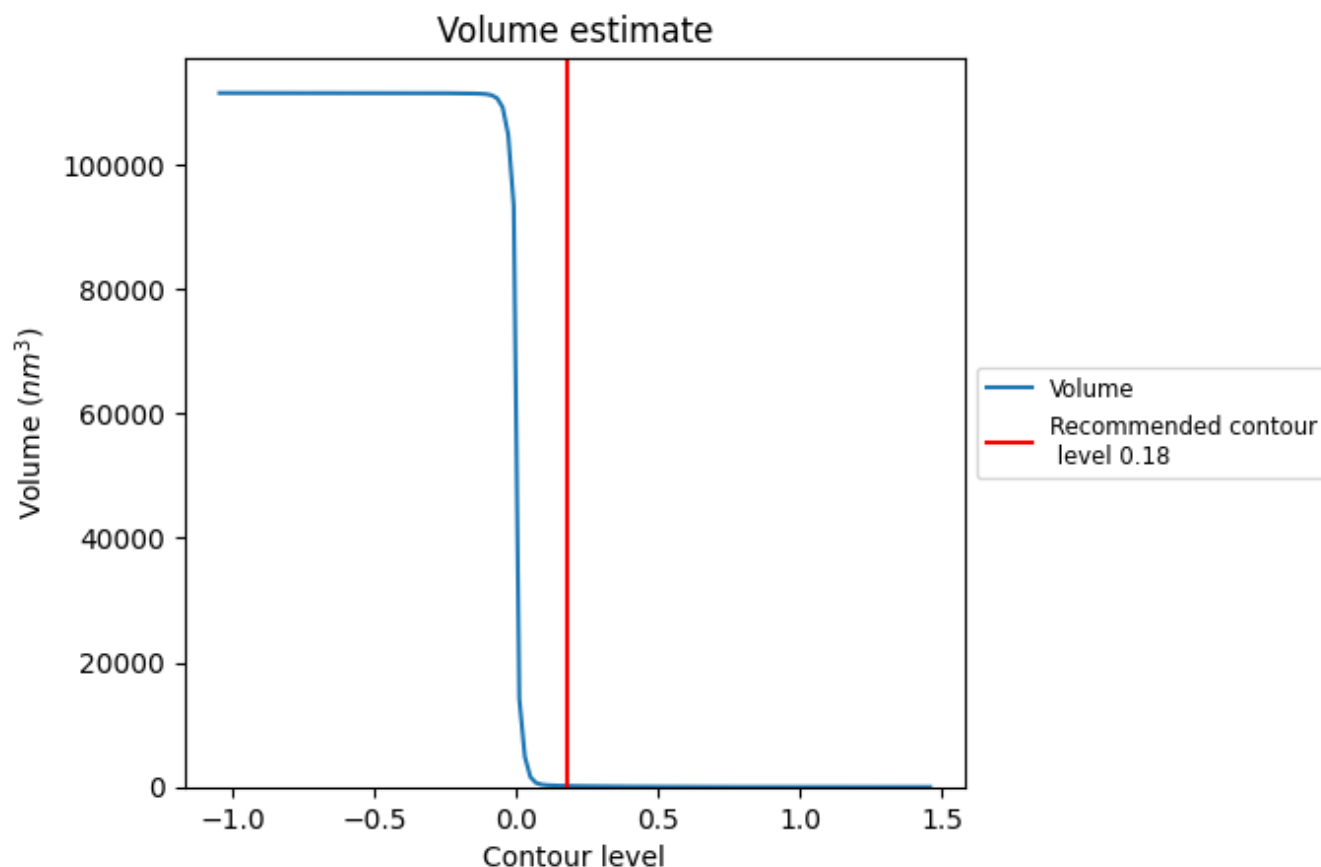
This section contains the results of statistical analysis of the map.

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.

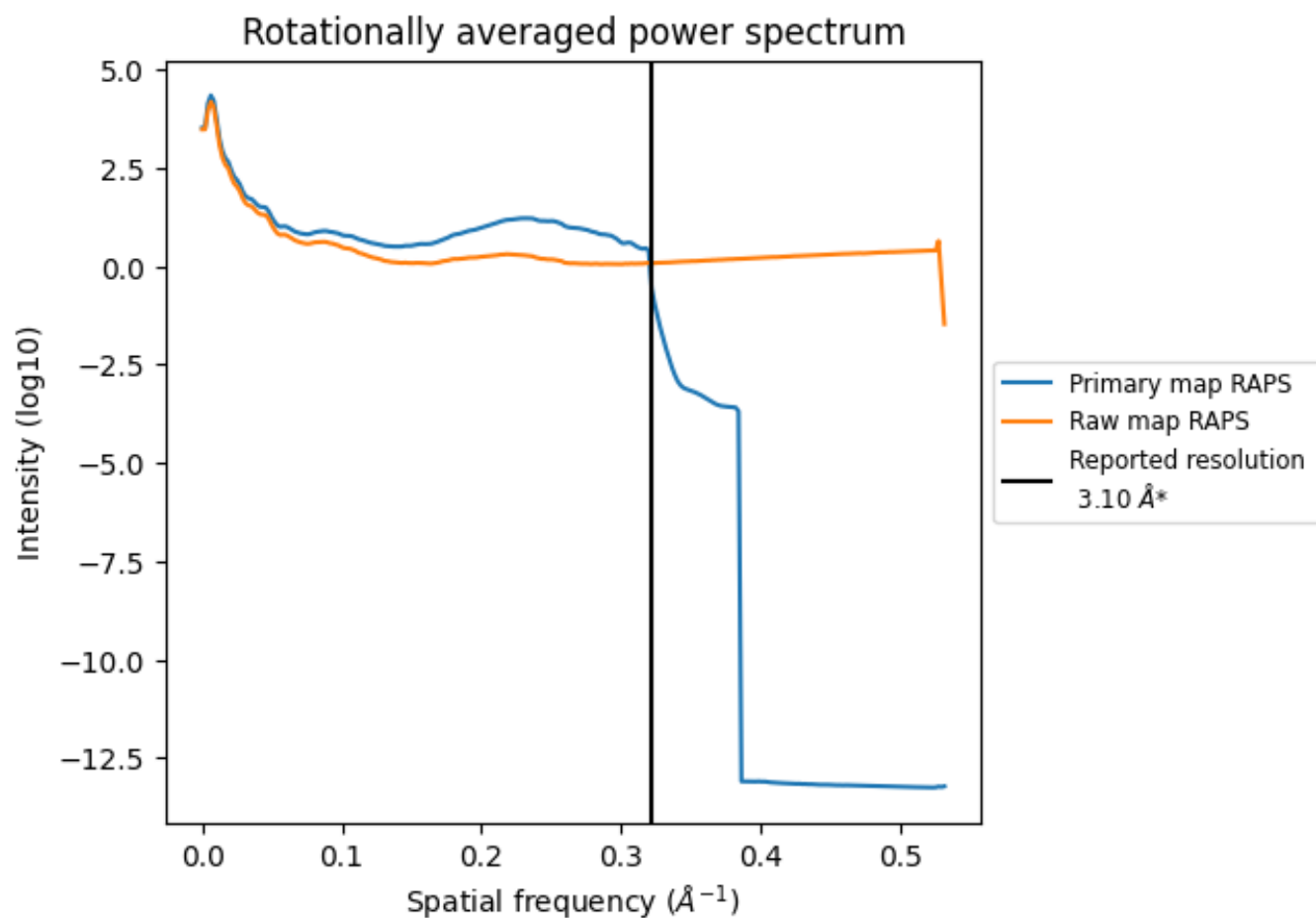
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 167 nm³; this corresponds to an approximate mass of 151 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 ⓘ

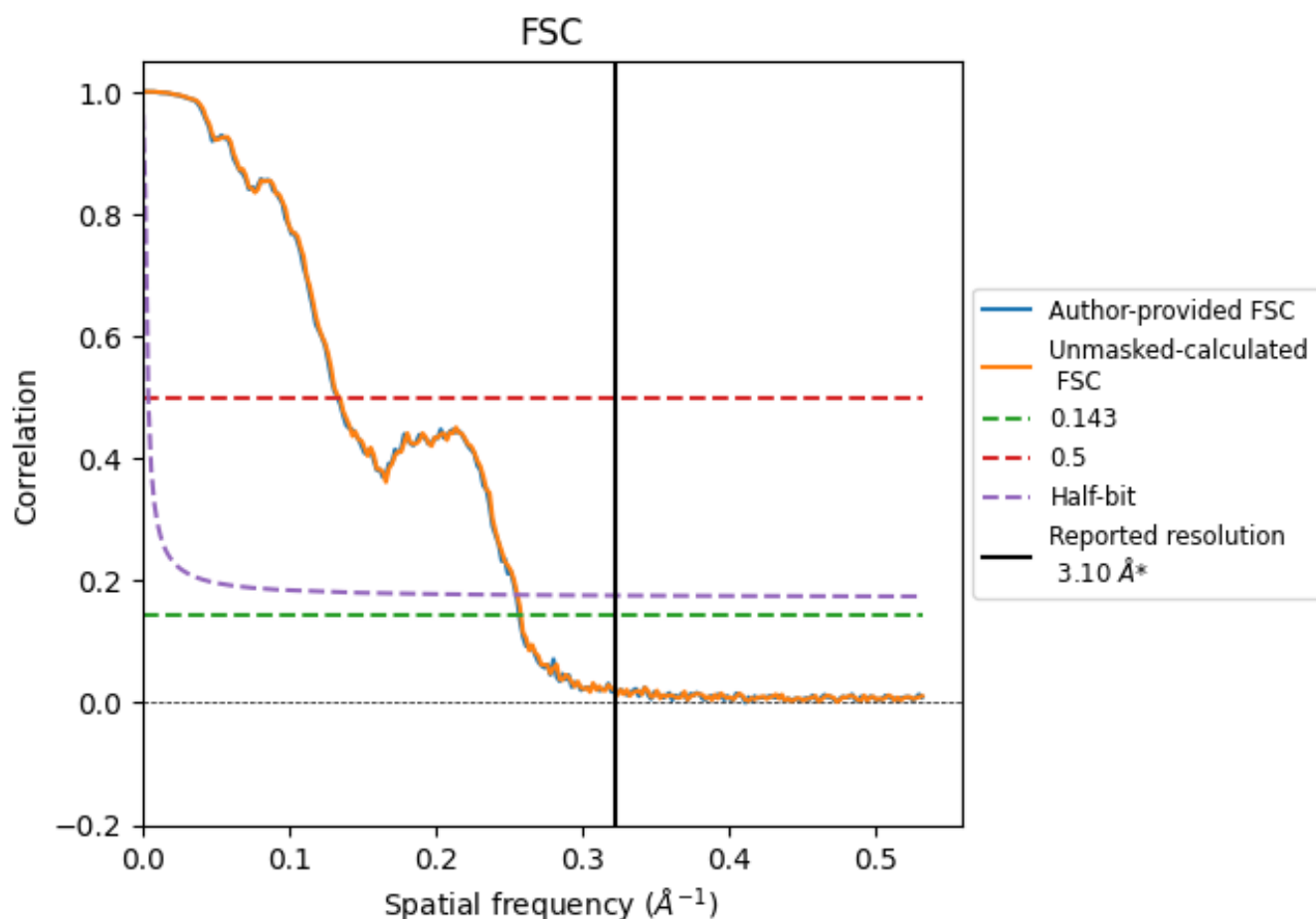


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

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 $0.323 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.89	7.51	3.92
Unmasked-calculated*	3.87	7.45	3.91

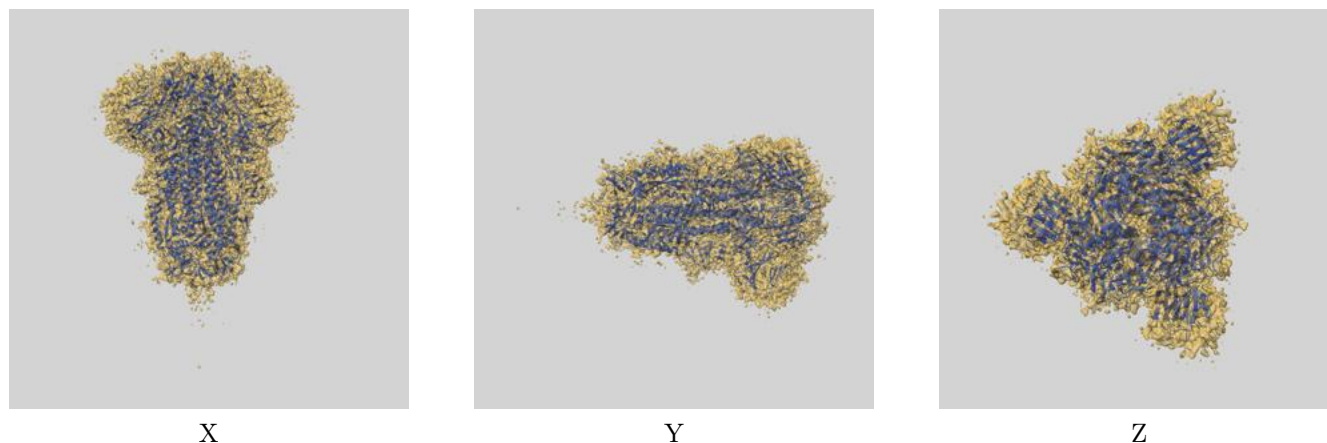
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 3.89 differs from the reported value 3.1 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.87 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-45402 and PDB model 9CAS. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

9.1 Map-model overlay [i](#)



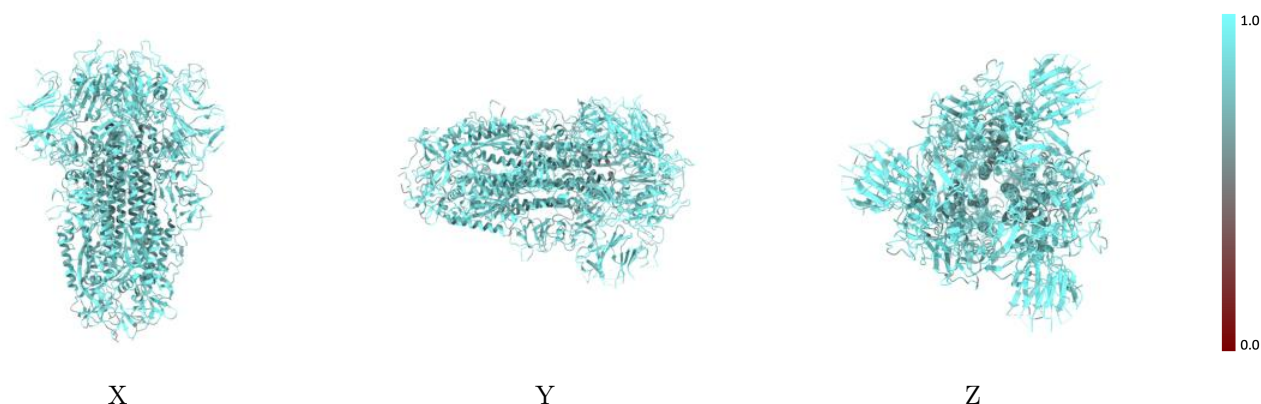
The images above show the 3D surface view of the map at the recommended contour level 0.18 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



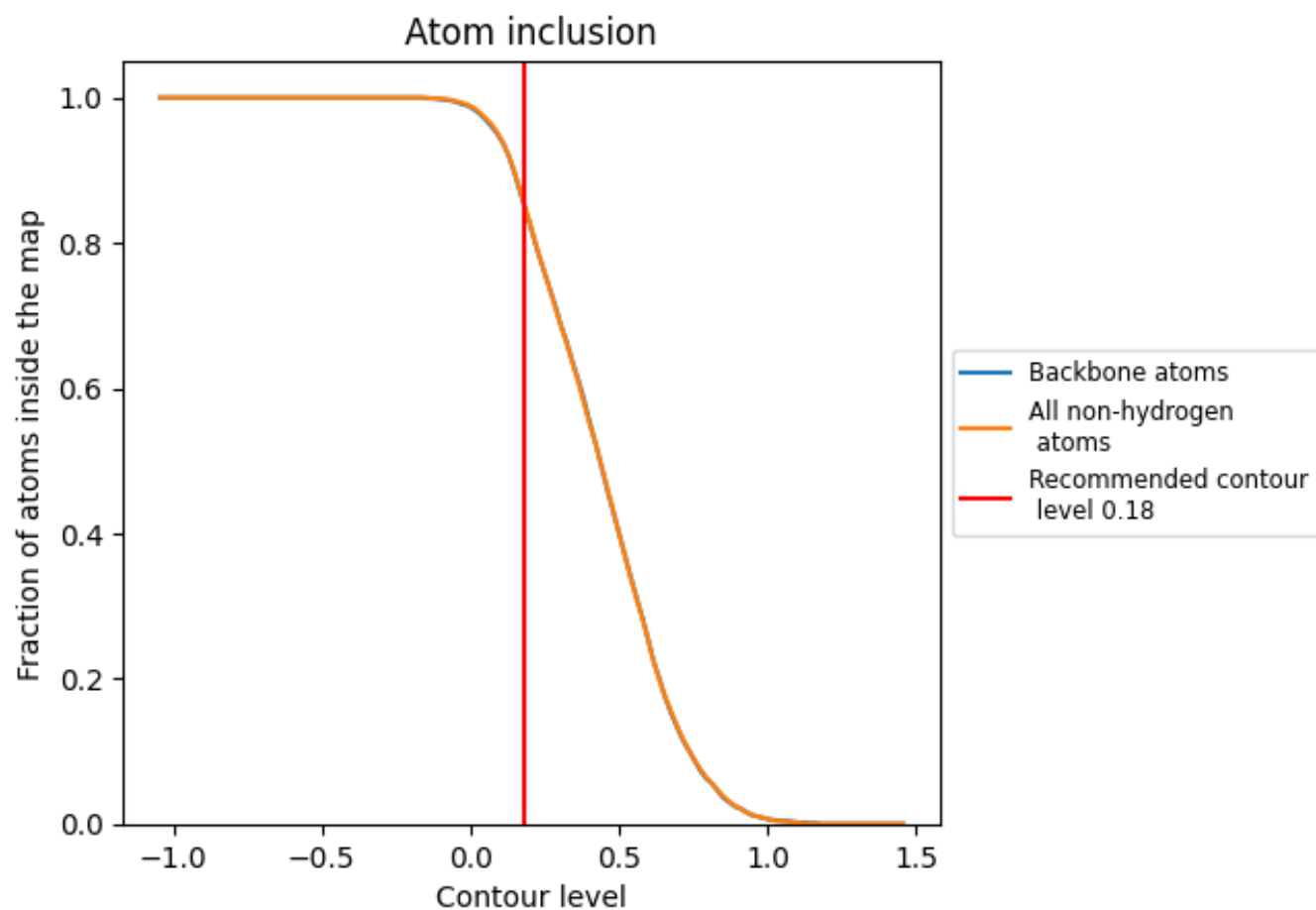
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.18).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 86% 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 (0.18) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8560	0.5470
A	0.8610	0.5470
B	0.8600	0.5470
C	0.8600	0.5470

