



Full wwPDB EM Validation Report ⓘ

Feb 24, 2024 – 06:21 PM EST

PDB ID : 7LJR
EMDB ID : EMD-23400
Title : SARS-CoV-2 Spike Protein Trimer bound to DH1043 fab
Authors : Gobeil, S.; Acharya, P.
Deposited on : 2021-01-30
Resolution : 3.66 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.dev70
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

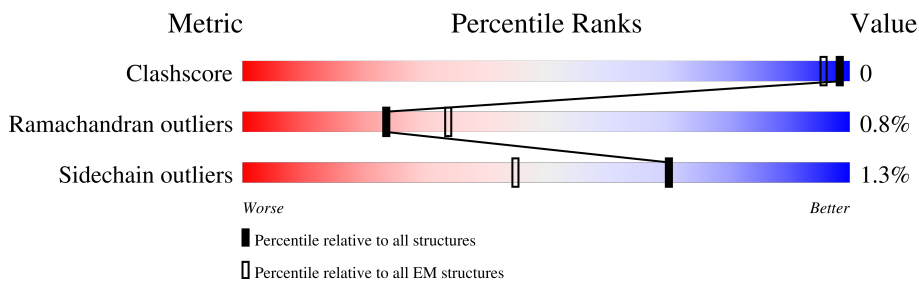
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.66 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	1288	
1	B	1288	
1	C	1288	
2	S	472	
3	T	233	

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 26291 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	1002	7823	4996	1300	1492	35	0	0
1	B	972	7597	4855	1262	1447	33	0	0
1	C	972	7604	4861	1262	1448	33	0	0

There are 255 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	682	GLY	ARG	conflict	UNP P0DTC2
A	683	SER	ARG	conflict	UNP P0DTC2
A	685	SER	ARG	conflict	UNP P0DTC2
A	986	PRO	LYS	conflict	UNP P0DTC2
A	987	PRO	VAL	conflict	UNP P0DTC2
A	1209	GLY	-	expression tag	UNP P0DTC2
A	1210	SER	-	expression tag	UNP P0DTC2
A	1211	GLY	-	expression tag	UNP P0DTC2
A	1212	TYR	-	expression tag	UNP P0DTC2
A	1213	ILE	-	expression tag	UNP P0DTC2
A	1214	PRO	-	expression tag	UNP P0DTC2
A	1215	GLU	-	expression tag	UNP P0DTC2
A	1216	ALA	-	expression tag	UNP P0DTC2
A	1217	PRO	-	expression tag	UNP P0DTC2
A	1218	ARG	-	expression tag	UNP P0DTC2
A	1219	ASP	-	expression tag	UNP P0DTC2
A	1220	GLY	-	expression tag	UNP P0DTC2
A	1221	GLN	-	expression tag	UNP P0DTC2
A	1222	ALA	-	expression tag	UNP P0DTC2
A	1223	TYR	-	expression tag	UNP P0DTC2
A	1224	VAL	-	expression tag	UNP P0DTC2
A	1225	ARG	-	expression tag	UNP P0DTC2
A	1226	LYS	-	expression tag	UNP P0DTC2
A	1227	ASP	-	expression tag	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	1228	GLY	-	expression tag	UNP P0DTC2
A	1229	GLU	-	expression tag	UNP P0DTC2
A	1230	TRP	-	expression tag	UNP P0DTC2
A	1231	VAL	-	expression tag	UNP P0DTC2
A	1232	LEU	-	expression tag	UNP P0DTC2
A	1233	LEU	-	expression tag	UNP P0DTC2
A	1234	SER	-	expression tag	UNP P0DTC2
A	1235	THR	-	expression tag	UNP P0DTC2
A	1236	PHE	-	expression tag	UNP P0DTC2
A	1237	LEU	-	expression tag	UNP P0DTC2
A	1238	GLY	-	expression tag	UNP P0DTC2
A	1239	ARG	-	expression tag	UNP P0DTC2
A	1240	SER	-	expression tag	UNP P0DTC2
A	1241	LEU	-	expression tag	UNP P0DTC2
A	1242	GLU	-	expression tag	UNP P0DTC2
A	1243	VAL	-	expression tag	UNP P0DTC2
A	1244	LEU	-	expression tag	UNP P0DTC2
A	1245	PHE	-	expression tag	UNP P0DTC2
A	1246	GLN	-	expression tag	UNP P0DTC2
A	1247	GLY	-	expression tag	UNP P0DTC2
A	1248	PRO	-	expression tag	UNP P0DTC2
A	1249	GLY	-	expression tag	UNP P0DTC2
A	1250	HIS	-	expression tag	UNP P0DTC2
A	1251	HIS	-	expression tag	UNP P0DTC2
A	1252	HIS	-	expression tag	UNP P0DTC2
A	1253	HIS	-	expression tag	UNP P0DTC2
A	1254	HIS	-	expression tag	UNP P0DTC2
A	1255	HIS	-	expression tag	UNP P0DTC2
A	1256	HIS	-	expression tag	UNP P0DTC2
A	1257	HIS	-	expression tag	UNP P0DTC2
A	1258	SER	-	expression tag	UNP P0DTC2
A	1259	ALA	-	expression tag	UNP P0DTC2
A	1260	TRP	-	expression tag	UNP P0DTC2
A	1261	SER	-	expression tag	UNP P0DTC2
A	1262	HIS	-	expression tag	UNP P0DTC2
A	1263	PRO	-	expression tag	UNP P0DTC2
A	1264	GLN	-	expression tag	UNP P0DTC2
A	1265	PHE	-	expression tag	UNP P0DTC2
A	1266	GLU	-	expression tag	UNP P0DTC2
A	1267	LYS	-	expression tag	UNP P0DTC2
A	1268	GLY	-	expression tag	UNP P0DTC2
A	1269	GLY	-	expression tag	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	1270	GLY	-	expression tag	UNP P0DTC2
A	1271	SER	-	expression tag	UNP P0DTC2
A	1272	GLY	-	expression tag	UNP P0DTC2
A	1273	GLY	-	expression tag	UNP P0DTC2
A	1274	GLY	-	expression tag	UNP P0DTC2
A	1275	GLY	-	expression tag	UNP P0DTC2
A	1276	SER	-	expression tag	UNP P0DTC2
A	1277	GLY	-	expression tag	UNP P0DTC2
A	1278	GLY	-	expression tag	UNP P0DTC2
A	1279	SER	-	expression tag	UNP P0DTC2
A	1280	ALA	-	expression tag	UNP P0DTC2
A	1281	TRP	-	expression tag	UNP P0DTC2
A	1282	SER	-	expression tag	UNP P0DTC2
A	1283	HIS	-	expression tag	UNP P0DTC2
A	1284	PRO	-	expression tag	UNP P0DTC2
A	1285	GLN	-	expression tag	UNP P0DTC2
A	1286	PHE	-	expression tag	UNP P0DTC2
A	1287	GLU	-	expression tag	UNP P0DTC2
A	1288	LYS	-	expression tag	UNP P0DTC2
B	682	GLY	ARG	conflict	UNP P0DTC2
B	683	SER	ARG	conflict	UNP P0DTC2
B	685	SER	ARG	conflict	UNP P0DTC2
B	986	PRO	LYS	conflict	UNP P0DTC2
B	987	PRO	VAL	conflict	UNP P0DTC2
B	1209	GLY	-	expression tag	UNP P0DTC2
B	1210	SER	-	expression tag	UNP P0DTC2
B	1211	GLY	-	expression tag	UNP P0DTC2
B	1212	TYR	-	expression tag	UNP P0DTC2
B	1213	ILE	-	expression tag	UNP P0DTC2
B	1214	PRO	-	expression tag	UNP P0DTC2
B	1215	GLU	-	expression tag	UNP P0DTC2
B	1216	ALA	-	expression tag	UNP P0DTC2
B	1217	PRO	-	expression tag	UNP P0DTC2
B	1218	ARG	-	expression tag	UNP P0DTC2
B	1219	ASP	-	expression tag	UNP P0DTC2
B	1220	GLY	-	expression tag	UNP P0DTC2
B	1221	GLN	-	expression tag	UNP P0DTC2
B	1222	ALA	-	expression tag	UNP P0DTC2
B	1223	TYR	-	expression tag	UNP P0DTC2
B	1224	VAL	-	expression tag	UNP P0DTC2
B	1225	ARG	-	expression tag	UNP P0DTC2
B	1226	LYS	-	expression tag	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	1227	ASP	-	expression tag	UNP P0DTC2
B	1228	GLY	-	expression tag	UNP P0DTC2
B	1229	GLU	-	expression tag	UNP P0DTC2
B	1230	TRP	-	expression tag	UNP P0DTC2
B	1231	VAL	-	expression tag	UNP P0DTC2
B	1232	LEU	-	expression tag	UNP P0DTC2
B	1233	LEU	-	expression tag	UNP P0DTC2
B	1234	SER	-	expression tag	UNP P0DTC2
B	1235	THR	-	expression tag	UNP P0DTC2
B	1236	PHE	-	expression tag	UNP P0DTC2
B	1237	LEU	-	expression tag	UNP P0DTC2
B	1238	GLY	-	expression tag	UNP P0DTC2
B	1239	ARG	-	expression tag	UNP P0DTC2
B	1240	SER	-	expression tag	UNP P0DTC2
B	1241	LEU	-	expression tag	UNP P0DTC2
B	1242	GLU	-	expression tag	UNP P0DTC2
B	1243	VAL	-	expression tag	UNP P0DTC2
B	1244	LEU	-	expression tag	UNP P0DTC2
B	1245	PHE	-	expression tag	UNP P0DTC2
B	1246	GLN	-	expression tag	UNP P0DTC2
B	1247	GLY	-	expression tag	UNP P0DTC2
B	1248	PRO	-	expression tag	UNP P0DTC2
B	1249	GLY	-	expression tag	UNP P0DTC2
B	1250	HIS	-	expression tag	UNP P0DTC2
B	1251	HIS	-	expression tag	UNP P0DTC2
B	1252	HIS	-	expression tag	UNP P0DTC2
B	1253	HIS	-	expression tag	UNP P0DTC2
B	1254	HIS	-	expression tag	UNP P0DTC2
B	1255	HIS	-	expression tag	UNP P0DTC2
B	1256	HIS	-	expression tag	UNP P0DTC2
B	1257	HIS	-	expression tag	UNP P0DTC2
B	1258	SER	-	expression tag	UNP P0DTC2
B	1259	ALA	-	expression tag	UNP P0DTC2
B	1260	TRP	-	expression tag	UNP P0DTC2
B	1261	SER	-	expression tag	UNP P0DTC2
B	1262	HIS	-	expression tag	UNP P0DTC2
B	1263	PRO	-	expression tag	UNP P0DTC2
B	1264	GLN	-	expression tag	UNP P0DTC2
B	1265	PHE	-	expression tag	UNP P0DTC2
B	1266	GLU	-	expression tag	UNP P0DTC2
B	1267	LYS	-	expression tag	UNP P0DTC2
B	1268	GLY	-	expression tag	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	1269	GLY	-	expression tag	UNP P0DTC2
B	1270	GLY	-	expression tag	UNP P0DTC2
B	1271	SER	-	expression tag	UNP P0DTC2
B	1272	GLY	-	expression tag	UNP P0DTC2
B	1273	GLY	-	expression tag	UNP P0DTC2
B	1274	GLY	-	expression tag	UNP P0DTC2
B	1275	GLY	-	expression tag	UNP P0DTC2
B	1276	SER	-	expression tag	UNP P0DTC2
B	1277	GLY	-	expression tag	UNP P0DTC2
B	1278	GLY	-	expression tag	UNP P0DTC2
B	1279	SER	-	expression tag	UNP P0DTC2
B	1280	ALA	-	expression tag	UNP P0DTC2
B	1281	TRP	-	expression tag	UNP P0DTC2
B	1282	SER	-	expression tag	UNP P0DTC2
B	1283	HIS	-	expression tag	UNP P0DTC2
B	1284	PRO	-	expression tag	UNP P0DTC2
B	1285	GLN	-	expression tag	UNP P0DTC2
B	1286	PHE	-	expression tag	UNP P0DTC2
B	1287	GLU	-	expression tag	UNP P0DTC2
B	1288	LYS	-	expression tag	UNP P0DTC2
C	682	GLY	ARG	conflict	UNP P0DTC2
C	683	SER	ARG	conflict	UNP P0DTC2
C	685	SER	ARG	conflict	UNP P0DTC2
C	986	PRO	LYS	conflict	UNP P0DTC2
C	987	PRO	VAL	conflict	UNP P0DTC2
C	1209	GLY	-	expression tag	UNP P0DTC2
C	1210	SER	-	expression tag	UNP P0DTC2
C	1211	GLY	-	expression tag	UNP P0DTC2
C	1212	TYR	-	expression tag	UNP P0DTC2
C	1213	ILE	-	expression tag	UNP P0DTC2
C	1214	PRO	-	expression tag	UNP P0DTC2
C	1215	GLU	-	expression tag	UNP P0DTC2
C	1216	ALA	-	expression tag	UNP P0DTC2
C	1217	PRO	-	expression tag	UNP P0DTC2
C	1218	ARG	-	expression tag	UNP P0DTC2
C	1219	ASP	-	expression tag	UNP P0DTC2
C	1220	GLY	-	expression tag	UNP P0DTC2
C	1221	GLN	-	expression tag	UNP P0DTC2
C	1222	ALA	-	expression tag	UNP P0DTC2
C	1223	TYR	-	expression tag	UNP P0DTC2
C	1224	VAL	-	expression tag	UNP P0DTC2
C	1225	ARG	-	expression tag	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	1226	LYS	-	expression tag	UNP P0DTC2
C	1227	ASP	-	expression tag	UNP P0DTC2
C	1228	GLY	-	expression tag	UNP P0DTC2
C	1229	GLU	-	expression tag	UNP P0DTC2
C	1230	TRP	-	expression tag	UNP P0DTC2
C	1231	VAL	-	expression tag	UNP P0DTC2
C	1232	LEU	-	expression tag	UNP P0DTC2
C	1233	LEU	-	expression tag	UNP P0DTC2
C	1234	SER	-	expression tag	UNP P0DTC2
C	1235	THR	-	expression tag	UNP P0DTC2
C	1236	PHE	-	expression tag	UNP P0DTC2
C	1237	LEU	-	expression tag	UNP P0DTC2
C	1238	GLY	-	expression tag	UNP P0DTC2
C	1239	ARG	-	expression tag	UNP P0DTC2
C	1240	SER	-	expression tag	UNP P0DTC2
C	1241	LEU	-	expression tag	UNP P0DTC2
C	1242	GLU	-	expression tag	UNP P0DTC2
C	1243	VAL	-	expression tag	UNP P0DTC2
C	1244	LEU	-	expression tag	UNP P0DTC2
C	1245	PHE	-	expression tag	UNP P0DTC2
C	1246	GLN	-	expression tag	UNP P0DTC2
C	1247	GLY	-	expression tag	UNP P0DTC2
C	1248	PRO	-	expression tag	UNP P0DTC2
C	1249	GLY	-	expression tag	UNP P0DTC2
C	1250	HIS	-	expression tag	UNP P0DTC2
C	1251	HIS	-	expression tag	UNP P0DTC2
C	1252	HIS	-	expression tag	UNP P0DTC2
C	1253	HIS	-	expression tag	UNP P0DTC2
C	1254	HIS	-	expression tag	UNP P0DTC2
C	1255	HIS	-	expression tag	UNP P0DTC2
C	1256	HIS	-	expression tag	UNP P0DTC2
C	1257	HIS	-	expression tag	UNP P0DTC2
C	1258	SER	-	expression tag	UNP P0DTC2
C	1259	ALA	-	expression tag	UNP P0DTC2
C	1260	TRP	-	expression tag	UNP P0DTC2
C	1261	SER	-	expression tag	UNP P0DTC2
C	1262	HIS	-	expression tag	UNP P0DTC2
C	1263	PRO	-	expression tag	UNP P0DTC2
C	1264	GLN	-	expression tag	UNP P0DTC2
C	1265	PHE	-	expression tag	UNP P0DTC2
C	1266	GLU	-	expression tag	UNP P0DTC2
C	1267	LYS	-	expression tag	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	1268	GLY	-	expression tag	UNP P0DTC2
C	1269	GLY	-	expression tag	UNP P0DTC2
C	1270	GLY	-	expression tag	UNP P0DTC2
C	1271	SER	-	expression tag	UNP P0DTC2
C	1272	GLY	-	expression tag	UNP P0DTC2
C	1273	GLY	-	expression tag	UNP P0DTC2
C	1274	GLY	-	expression tag	UNP P0DTC2
C	1275	GLY	-	expression tag	UNP P0DTC2
C	1276	SER	-	expression tag	UNP P0DTC2
C	1277	GLY	-	expression tag	UNP P0DTC2
C	1278	GLY	-	expression tag	UNP P0DTC2
C	1279	SER	-	expression tag	UNP P0DTC2
C	1280	ALA	-	expression tag	UNP P0DTC2
C	1281	TRP	-	expression tag	UNP P0DTC2
C	1282	SER	-	expression tag	UNP P0DTC2
C	1283	HIS	-	expression tag	UNP P0DTC2
C	1284	PRO	-	expression tag	UNP P0DTC2
C	1285	GLN	-	expression tag	UNP P0DTC2
C	1286	PHE	-	expression tag	UNP P0DTC2
C	1287	GLU	-	expression tag	UNP P0DTC2
C	1288	LYS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called Fab DH1043 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	S	226	1694	1076	280	331	7	0	0

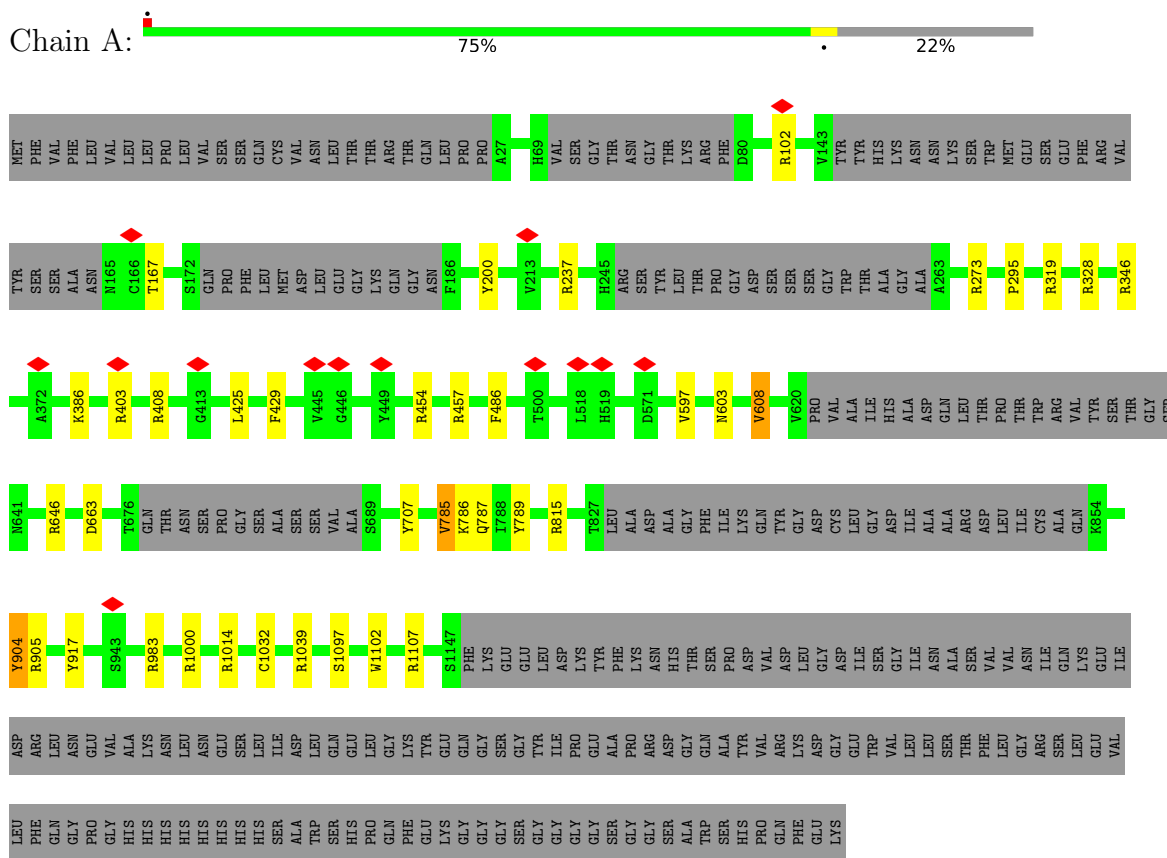
- Molecule 3 is a protein called Fab DH1043 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	T	206	1573	979	272	318	4	0	0

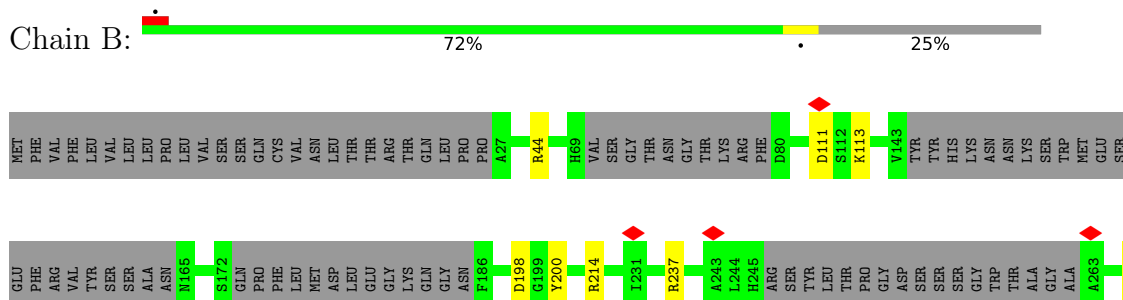
3 Residue-property plots

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



- 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	133814	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 ($e^-/\text{\AA}^2$)	66.77	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.915	Depositor
Minimum map value	-0.842	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.046	Depositor
Recommended contour level	0.25	Depositor
Map size (\AA)	370.3, 370.3, 370.3	wwPDB
Map dimensions	350, 350, 350	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\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	0.65	0/7999	0.95	23/10885 (0.2%)
1	B	0.66	0/7764	0.97	23/10561 (0.2%)
1	C	0.66	0/7772	0.97	19/10572 (0.2%)
2	S	0.71	0/1736	1.01	3/2362 (0.1%)
3	T	0.70	0/1606	1.00	7/2177 (0.3%)
All	All	0.66	0/26877	0.97	75/36557 (0.2%)

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	3
1	B	0	6
1	C	0	1
2	S	0	2
All	All	0	12

There are no bond length outliers.

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	328	ARG	NE-CZ-NH1	8.15	124.38	120.30
1	B	1107	ARG	NE-CZ-NH1	8.04	124.32	120.30
2	S	117	ARG	NE-CZ-NH1	7.95	124.28	120.30
1	C	423	TYR	CB-CG-CD2	-7.93	116.24	121.00
1	C	328	ARG	NE-CZ-NH1	7.63	124.12	120.30
1	A	457	ARG	NE-CZ-NH1	7.45	124.03	120.30
1	A	273	ARG	NE-CZ-NH1	7.41	124.01	120.30
1	C	1014	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	B	237	ARG	NE-CZ-NH1	7.17	123.89	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	454	ARG	NE-CZ-NH1	7.13	123.87	120.30
1	A	319	ARG	NE-CZ-NH1	7.11	123.85	120.30
1	C	273	ARG	NE-CZ-NH1	7.08	123.84	120.30
3	T	65	ARG	NE-CZ-NH2	6.98	123.79	120.30
1	B	357	ARG	NE-CZ-NH1	6.87	123.74	120.30
1	A	1014	ARG	NE-CZ-NH1	6.87	123.74	120.30
1	C	904	TYR	CB-CG-CD2	-6.87	116.88	121.00
1	A	328	ARG	NE-CZ-NH1	6.83	123.72	120.30
3	T	27	PRO	CA-N-CD	-6.77	102.02	111.50
1	B	273	ARG	NE-CZ-NH1	6.63	123.61	120.30
1	C	815	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	B	760	CYS	CA-CB-SG	-6.37	102.53	114.00
1	A	403	ARG	NE-CZ-NH2	6.33	123.47	120.30
1	B	1039	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	A	983	ARG	NE-CZ-NH1	6.29	123.45	120.30
1	A	237	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	A	408	ARG	NE-CZ-NH2	6.09	123.35	120.30
1	A	457	ARG	NE-CZ-NH2	-6.07	117.27	120.30
1	C	346	ARG	NE-CZ-NH1	5.95	123.27	120.30
1	B	200	TYR	CB-CG-CD2	-5.93	117.44	121.00
1	A	200	TYR	CB-CG-CD2	-5.91	117.45	121.00
1	A	905	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	B	1019	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	C	423	TYR	CB-CG-CD1	5.77	124.46	121.00
1	B	495	TYR	CB-CG-CD2	-5.68	117.59	121.00
1	A	608	VAL	CG1-CB-CG2	-5.66	101.85	110.90
1	A	1039	ARG	NE-CZ-NH2	-5.65	117.48	120.30
3	T	81	ARG	NE-CZ-NH2	5.62	123.11	120.30
1	A	904	TYR	CB-CG-CD2	-5.61	117.63	121.00
1	C	1019	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	C	1039	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	A	454	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	C	1000	ARG	NE-CZ-NH1	5.57	123.09	120.30
1	B	214	ARG	NE-CZ-NH1	5.55	123.07	120.30
1	B	1014	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	A	646	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	B	44	ARG	NE-CZ-NH1	5.51	123.06	120.30
3	T	97	ARG	NE-CZ-NH2	5.48	123.04	120.30
1	C	567	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	A	815	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	C	237	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	C	403	ARG	NE-CZ-NH1	5.41	123.01	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	319	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	B	995	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	B	403	ARG	NE-CZ-NH1	5.35	122.98	120.30
1	A	1000	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	A	785	VAL	CG1-CB-CG2	-5.34	102.36	110.90
1	B	515	PHE	CB-CG-CD1	-5.33	117.07	120.80
1	C	319	ARG	NE-CZ-NH1	5.32	122.96	120.30
3	T	127	ARG	NE-CZ-NH1	5.25	122.93	120.30
1	C	227	VAL	CG1-CB-CG2	-5.24	102.52	110.90
1	C	995	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	B	1039	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	B	408	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	B	351	TYR	CB-CG-CD1	-5.19	117.89	121.00
1	C	34	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	C	102	ARG	NE-CZ-NH1	5.15	122.87	120.30
1	B	1107	ARG	CD-NE-CZ	5.15	130.81	123.60
3	T	115	ARG	NE-CZ-NH2	5.13	122.86	120.30
2	S	131	TYR	CB-CG-CD2	-5.11	117.93	121.00
1	A	1039	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	B	515	PHE	CB-CG-CD2	5.09	124.36	120.80
3	T	230	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	A	1107	ARG	NE-CZ-NH1	5.05	122.82	120.30
1	A	346	ARG	NE-CZ-NH1	5.03	122.81	120.30
2	S	129	PHE	CB-CG-CD2	-5.00	117.30	120.80

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	707	TYR	Sidechain
1	A	789	TYR	Sidechain
1	A	917	TYR	Sidechain
1	B	113	LYS	Peptide
1	B	421	TYR	Sidechain
1	B	707	TYR	Sidechain
1	B	789	TYR	Sidechain
1	B	904	TYR	Sidechain
1	B	917	TYR	Sidechain
1	C	707	TYR	Sidechain
2	S	121	TYR	Sidechain
2	S	122	TYR	Sidechain

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	7823	0	7666	7	0
1	B	7597	0	7447	3	0
1	C	7604	0	7454	3	0
2	S	1694	0	1666	0	0
3	T	1573	0	1533	0	0
All	All	26291	0	25766	12	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 (12) 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:520:ALA:HB1	1:B:521:PRO:HD2	1.81	0.62
1:A:785:VAL:HG12	1:A:787:GLN:H	1.79	0.47
1:A:295:PRO:HB2	1:A:608:VAL:HG11	1.98	0.46
1:A:904:TYR:OH	1:C:1094:VAL:HG13	2.16	0.45
1:C:391:CYS:H	1:C:517:LEU:HD11	1.82	0.45
1:A:1097:SER:HB2	1:A:1102:TRP:CD2	2.54	0.43
1:A:425:LEU:HD22	1:A:429:PHE:CD1	2.54	0.42
1:A:102:ARG:CZ	1:A:102:ARG:HA	2.50	0.42
1:C:786:LYS:H	1:C:786:LYS:HD3	1.84	0.41
1:B:903:ALA:CB	1:B:917:TYR:CZ	3.04	0.41
1:A:597:VAL:HG13	1:A:608:VAL:CG1	2.51	0.40
1:B:343:ASN:HD21	1:B:441:LEU:HD22	1.86	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	986/1288 (77%)	898 (91%)	86 (9%)	2 (0%)	47	78
1	B	948/1288 (74%)	858 (90%)	82 (9%)	8 (1%)	19	56
1	C	948/1288 (74%)	847 (89%)	94 (10%)	7 (1%)	22	59
2	S	224/472 (48%)	202 (90%)	18 (8%)	4 (2%)	8	41
3	T	204/233 (88%)	175 (86%)	23 (11%)	6 (3%)	4	32
All	All	3310/4569 (72%)	2980 (90%)	303 (9%)	27 (1%)	24	56

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	111	ASP
1	B	339	GLY
1	B	518	LEU
1	C	138	ASP
1	C	356	LYS
3	T	49	SER
1	C	358	ILE
2	S	103	SER
3	T	112	SER
1	B	360	ASN
1	C	187	LYS
2	S	110	THR
2	S	126	GLY
3	T	45	SER
3	T	140	SER
1	A	603	ASN
1	A	663	ASP
1	B	375	SER
1	B	514	SER
1	C	614	ASP
3	T	89	THR
3	T	93	LEU
1	B	376	THR
1	C	136	CYS
2	S	190	SER
1	C	381	GLY
1	B	1057	PRO

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	876/1113 (79%)	871 (99%)	5 (1%)	86	93
1	B	851/1113 (76%)	839 (99%)	12 (1%)	67	82
1	C	852/1113 (76%)	834 (98%)	18 (2%)	53	73
2	S	188/414 (45%)	185 (98%)	3 (2%)	62	79
3	T	177/201 (88%)	176 (99%)	1 (1%)	86	93
All	All	2944/3954 (74%)	2905 (99%)	39 (1%)	70	82

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	167	THR
1	A	386	LYS
1	A	486	PHE
1	A	786	LYS
1	A	1032	CYS
1	B	198	ASP
1	B	351	TYR
1	B	355	ARG
1	B	377	PHE
1	B	396	TYR
1	B	436	TRP
1	B	497	PHE
1	B	515	PHE
1	B	544	ASN
1	B	547	THR
1	B	553	THR
1	B	817	PHE
1	C	52	GLN
1	C	88	ASP
1	C	108	THR
1	C	122	ASN
1	C	286	THR
1	C	294	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	400	PHE
1	C	423	TYR
1	C	493	GLN
1	C	517	LEU
1	C	581	THR
1	C	786	LYS
1	C	907	ASN
1	C	912	THR
1	C	983	ARG
1	C	1106	GLN
1	C	1127	ASP
1	C	1135	ASN
2	S	122	TYR
2	S	129	PHE
2	S	167	LEU
3	T	115	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	655	HIS
1	B	134	GLN
1	B	655	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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.

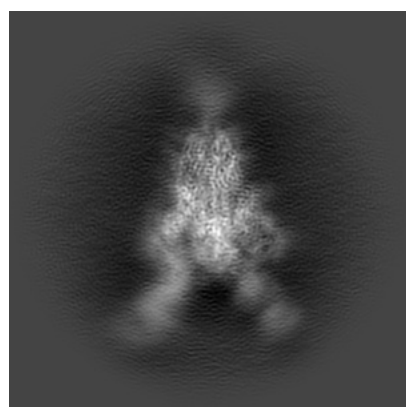
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23400. These allow visual inspection of the internal detail of the map and identification of artifacts.

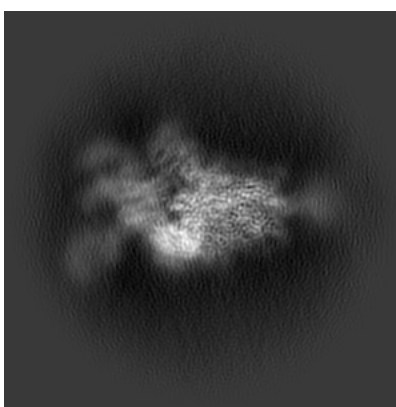
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

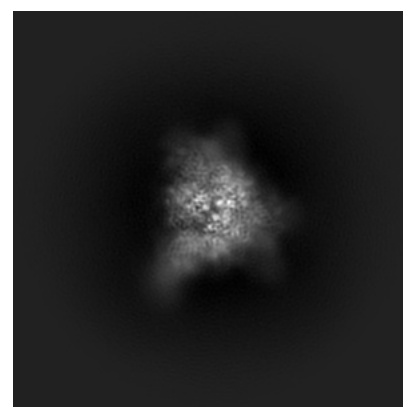
6.1.1 Primary map



X



Y

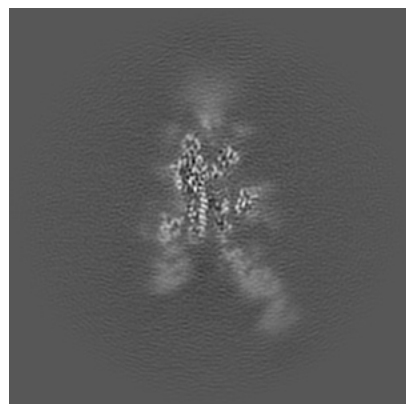


Z

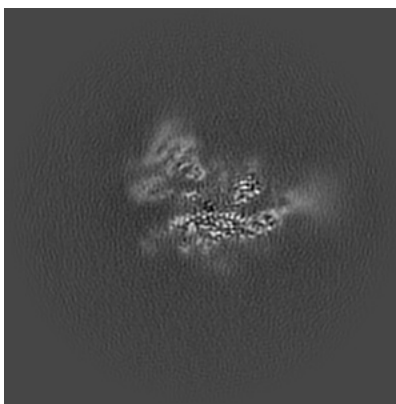
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

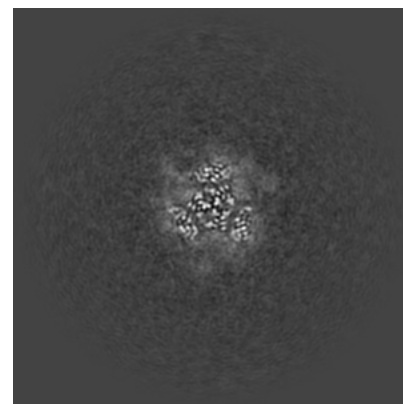
6.2.1 Primary map



X Index: 175



Y Index: 175

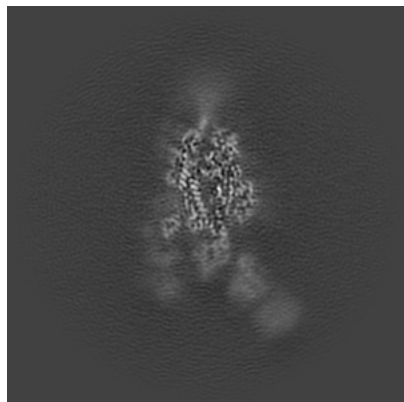


Z Index: 175

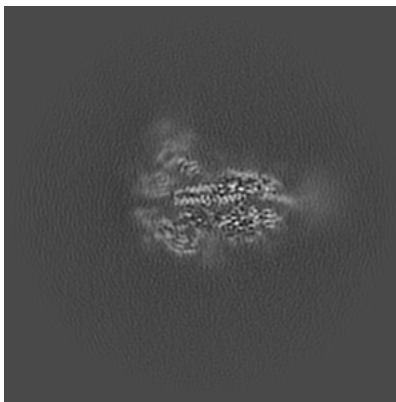
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

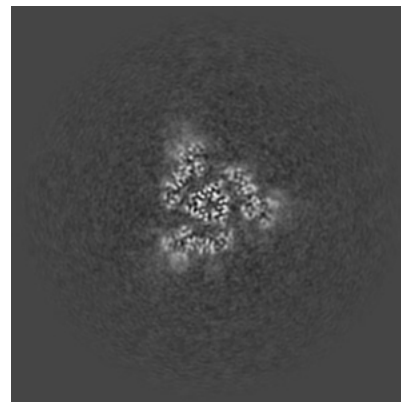
6.3.1 Primary map



X Index: 185



Y Index: 182

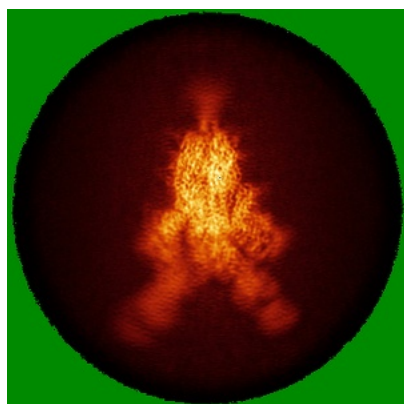


Z Index: 159

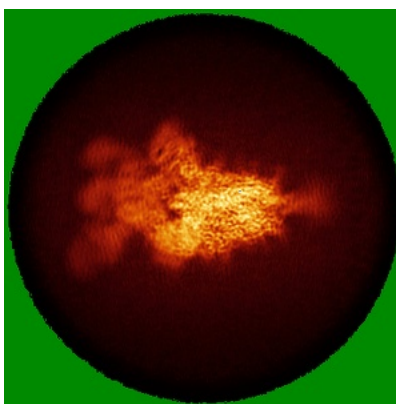
The images above show the largest variance slices of the map in three orthogonal directions.

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

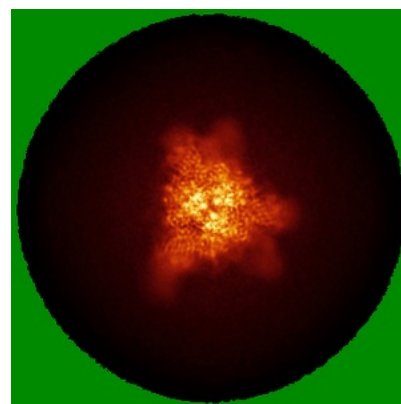
6.4.1 Primary map



X



Y

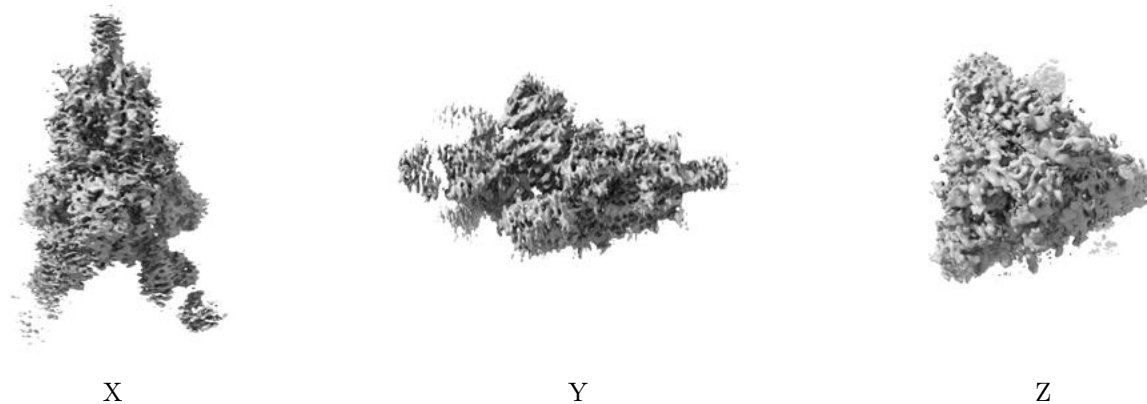


Z

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

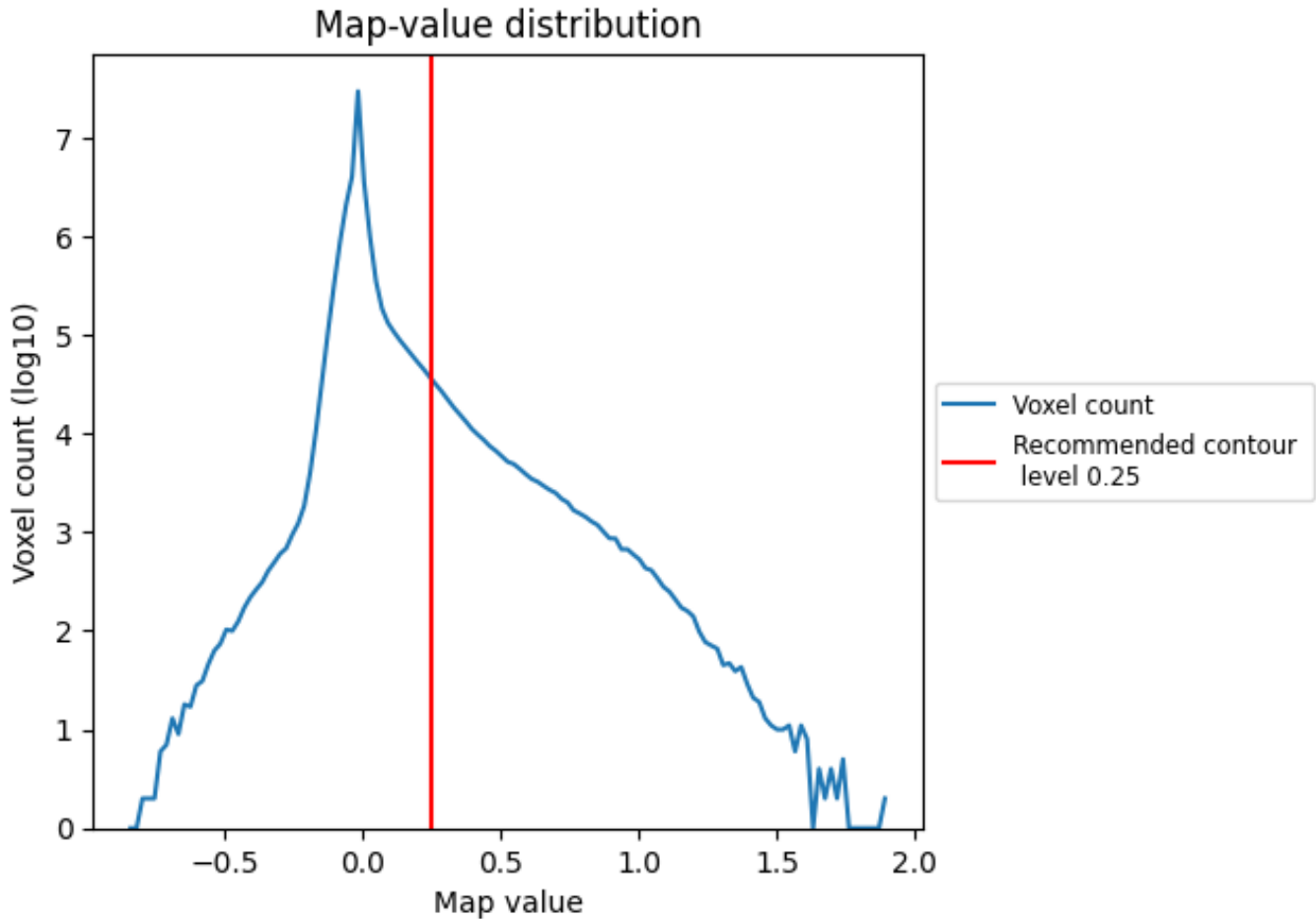
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

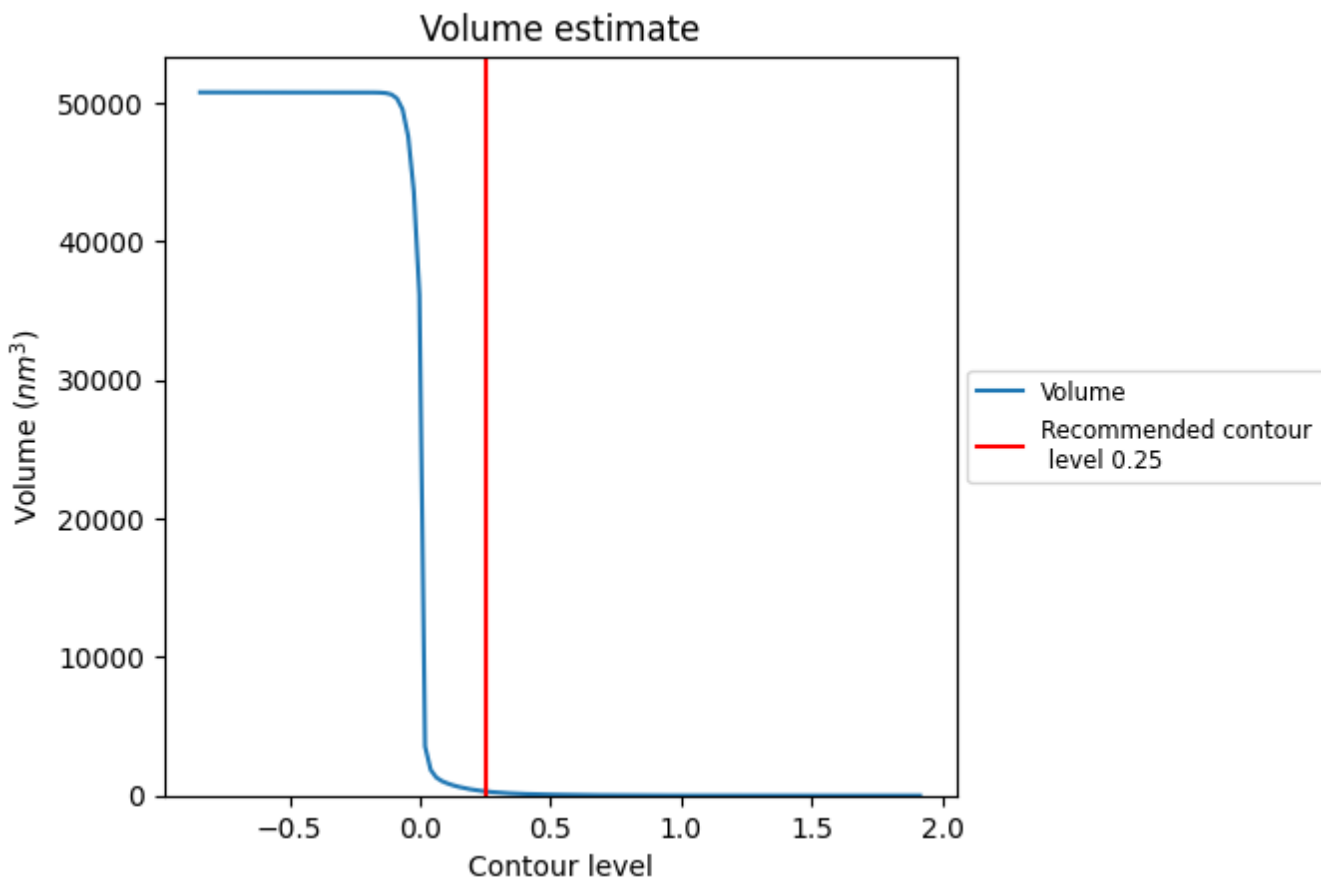
This section contains the results of statistical analysis of the map.

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.

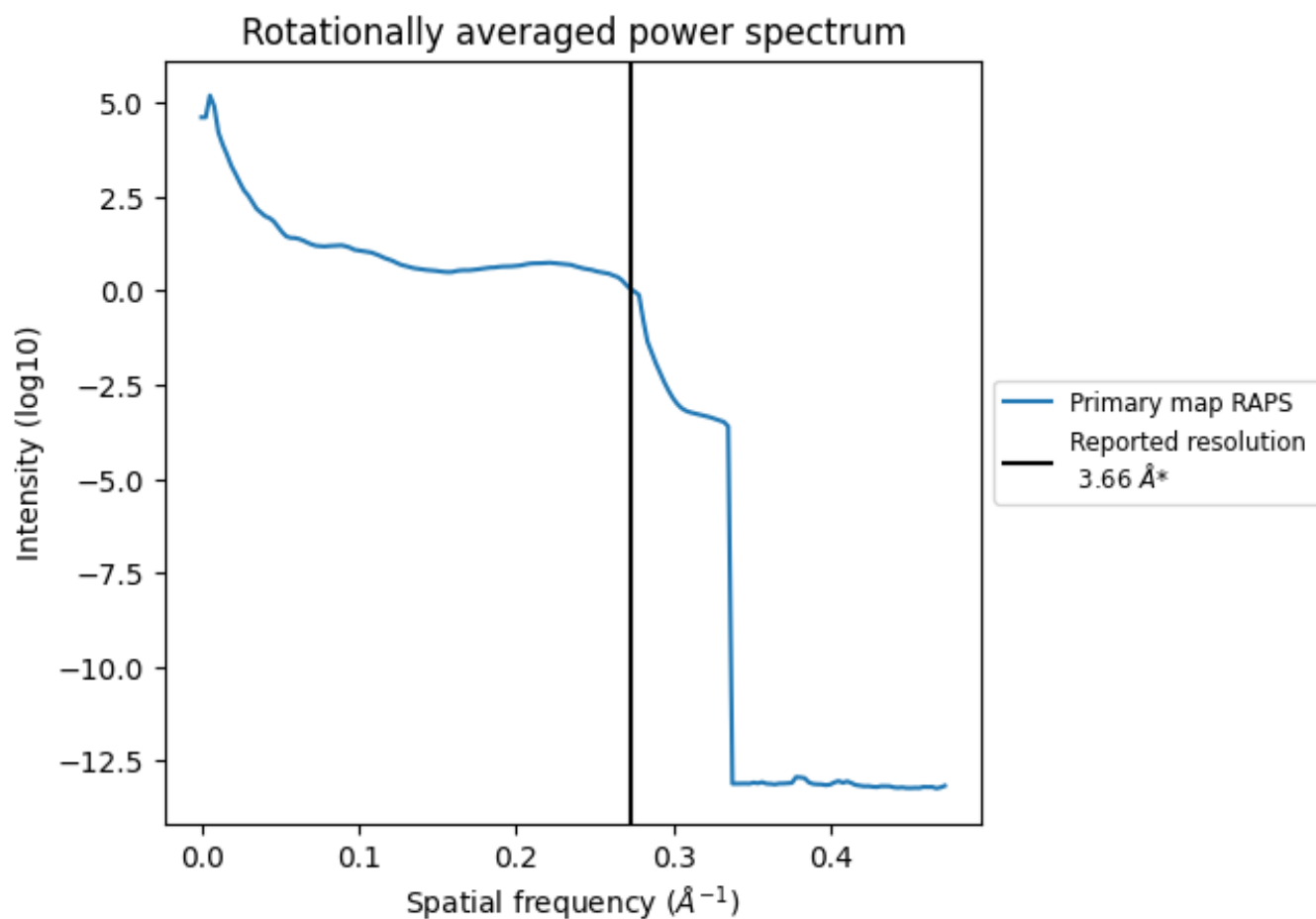
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 303 nm³; this corresponds to an approximate mass of 273 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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.273 Å⁻¹

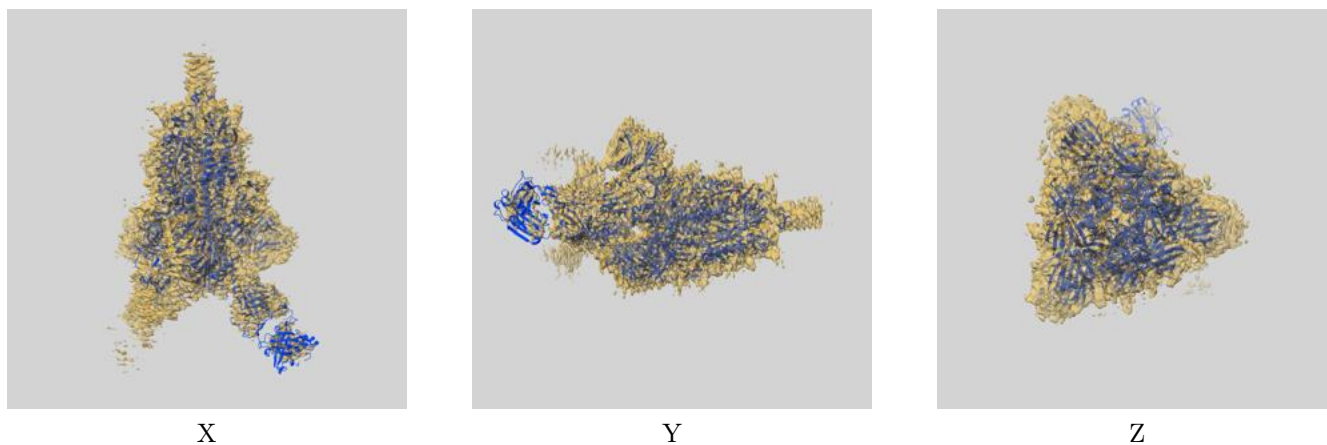
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

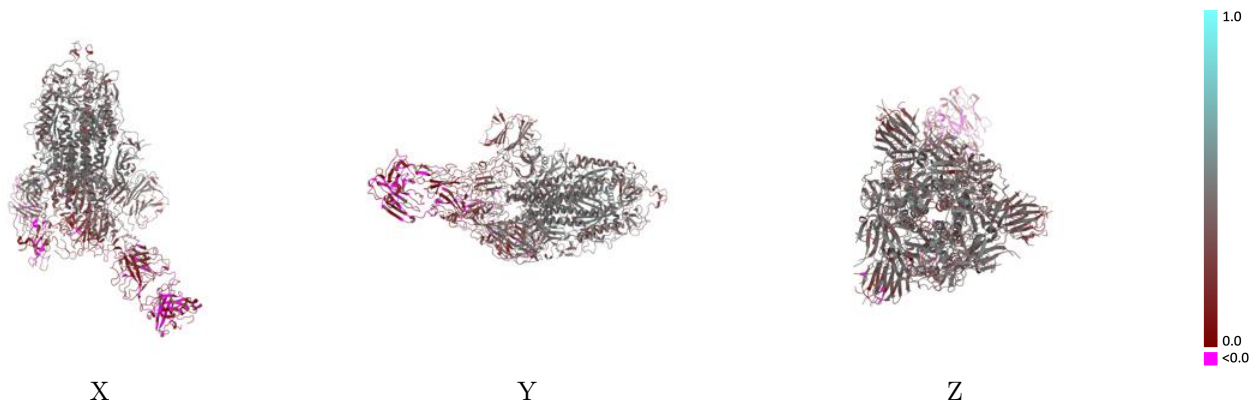
This section contains information regarding the fit between EMDB map EMD-23400 and PDB model 7LJR. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay [i](#)



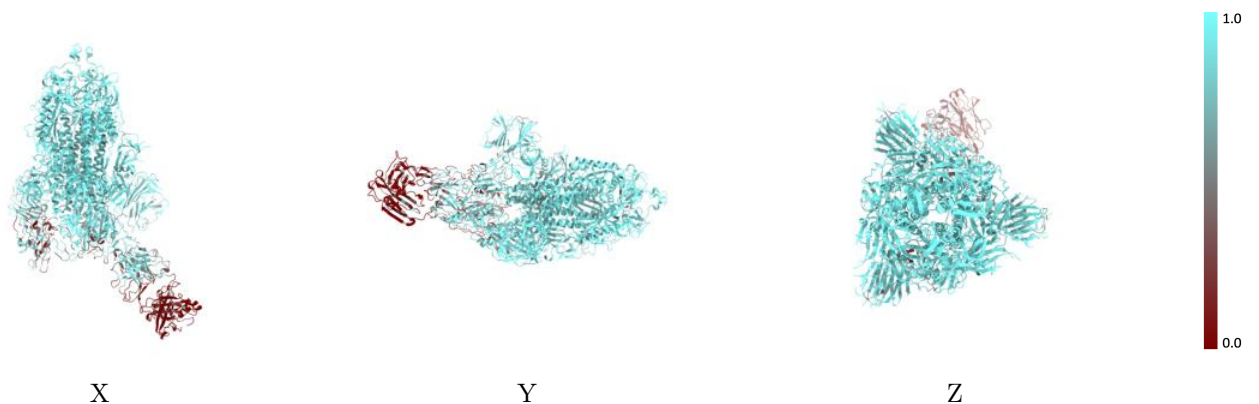
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



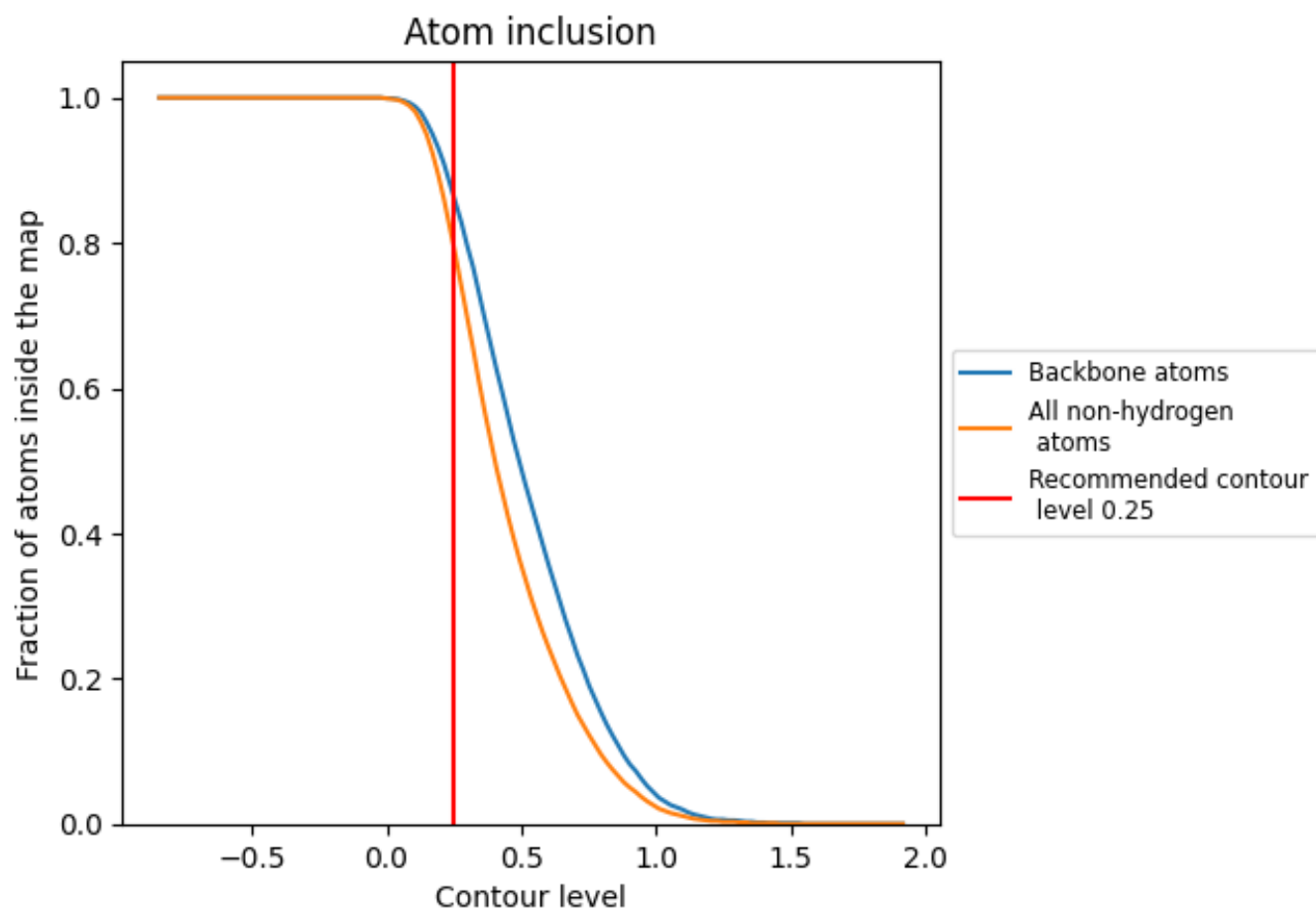
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.25).













9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 79% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7930	 0.3500
A	 0.8830	 0.3920
B	 0.8720	 0.3860
C	 0.8200	 0.3620
S	 0.3950	 0.1420
T	 0.2610	 0.1320

