



# Full wwPDB EM Validation Report (i)

Nov 20, 2022 – 12:28 AM EST

PDB ID : 7M0J  
EMDB ID : EMD-23612  
Title : SARS-CoV-2 u1S2q All Down RBD State Spike Protein Trimer - asymmetric refinement  
Authors : Henderson, R.; Acharya, P.  
Deposited on : 2021-03-11  
Resolution : 3.52 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](mailto: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 (i) 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 \(i\)](#)) were used in the production of this report:

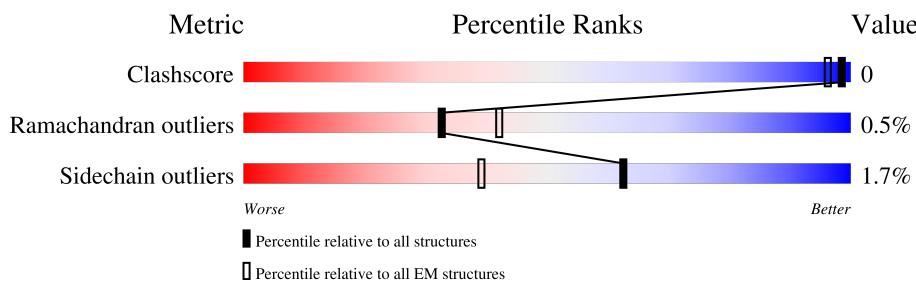
EMDB validation analysis : 0.0.1.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

# 1 Overall quality at a glance

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

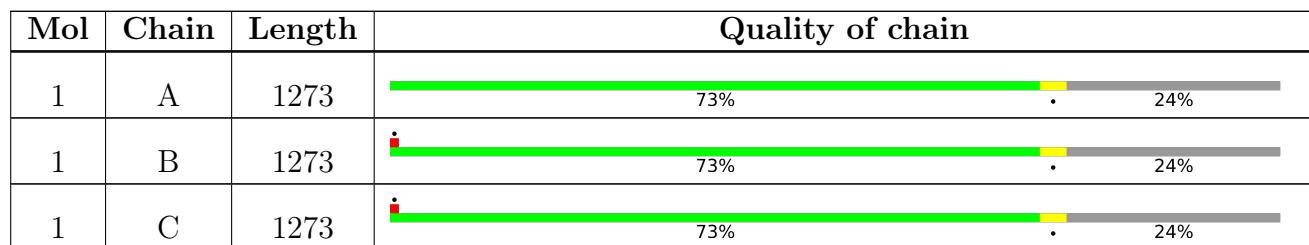
The reported resolution of this entry is 3.52 Å.

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 <=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.



## 2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 22827 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	972	Total	C	N	O	S	0	0
			7609	4868	1261	1447	33		
1	B	972	Total	C	N	O	S	0	0
			7609	4868	1261	1447	33		
1	C	972	Total	C	N	O	S	0	0
			7609	4868	1261	1447	33		

There are 267 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	570	LEU	ALA	engineered mutation	UNP P0DTC2
A	572	ILE	THR	engineered mutation	UNP P0DTC2
A	682	GLY	ARG	engineered mutation	UNP P0DTC2
A	683	SER	ARG	engineered mutation	UNP P0DTC2
A	685	SER	ARG	engineered mutation	UNP P0DTC2
A	855	TYR	PHE	engineered mutation	UNP P0DTC2
A	856	ILE	ASN	engineered mutation	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	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

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
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
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

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
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
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	570	LEU	ALA	engineered mutation	UNP P0DTC2
B	572	ILE	THR	engineered mutation	UNP P0DTC2
B	682	GLY	ARG	engineered mutation	UNP P0DTC2
B	683	SER	ARG	engineered mutation	UNP P0DTC2
B	685	SER	ARG	engineered mutation	UNP P0DTC2
B	855	TYR	PHE	engineered mutation	UNP P0DTC2
B	856	ILE	ASN	engineered mutation	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	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

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
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
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

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
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
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	570	LEU	ALA	engineered mutation	UNP P0DTC2
C	572	ILE	THR	engineered mutation	UNP P0DTC2
C	682	GLY	ARG	engineered mutation	UNP P0DTC2
C	683	SER	ARG	engineered mutation	UNP P0DTC2
C	685	SER	ARG	engineered mutation	UNP P0DTC2
C	855	TYR	PHE	engineered mutation	UNP P0DTC2
C	856	ILE	ASN	engineered mutation	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	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

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
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
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

*Continued on next page...*

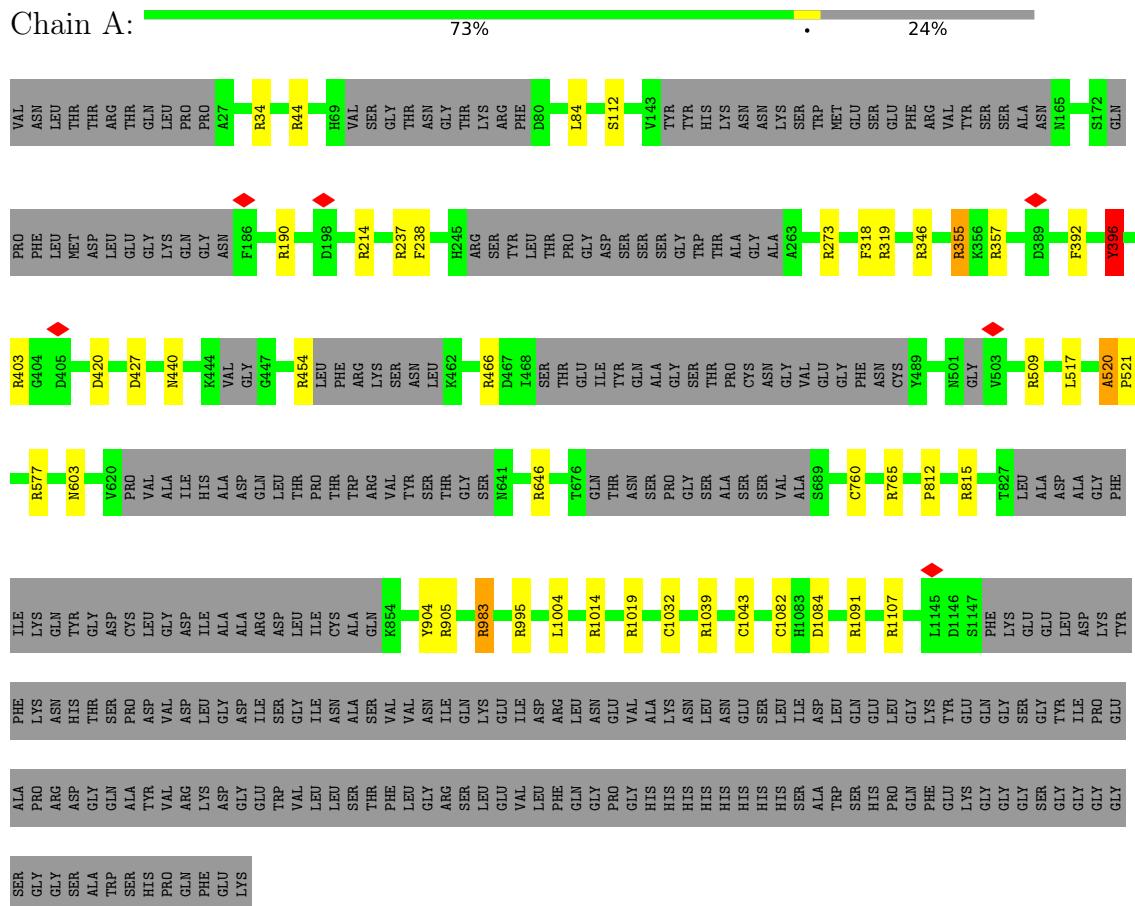
*Continued from previous page...*

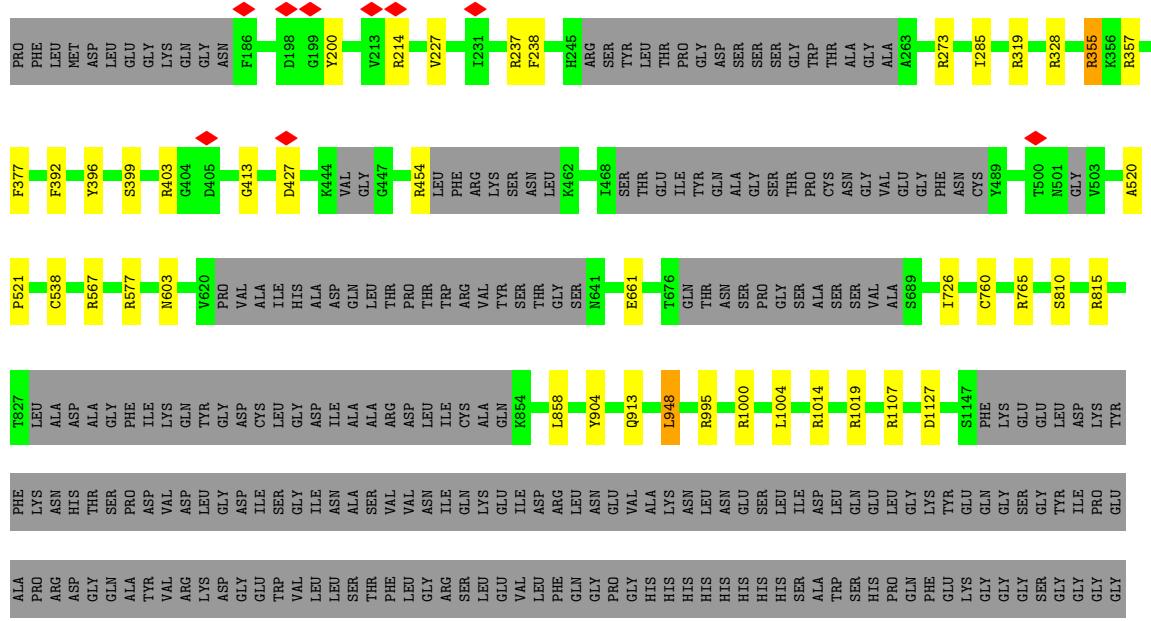
Chain	Residue	Modelled	Actual	Comment	Reference
C	1256	HIS	-	expression tag	UNP P0DTC2
C	1257	HIS	-	expression tag	UNP P0DTC2
C	1258	SER	-	expression tag	UNP P0DTC2
C	1259	ALA	-	expression tag	UNP P0DTC2
C	1260	TRP	-	expression tag	UNP P0DTC2
C	1261	SER	-	expression tag	UNP P0DTC2
C	1262	HIS	-	expression 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
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

### 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.

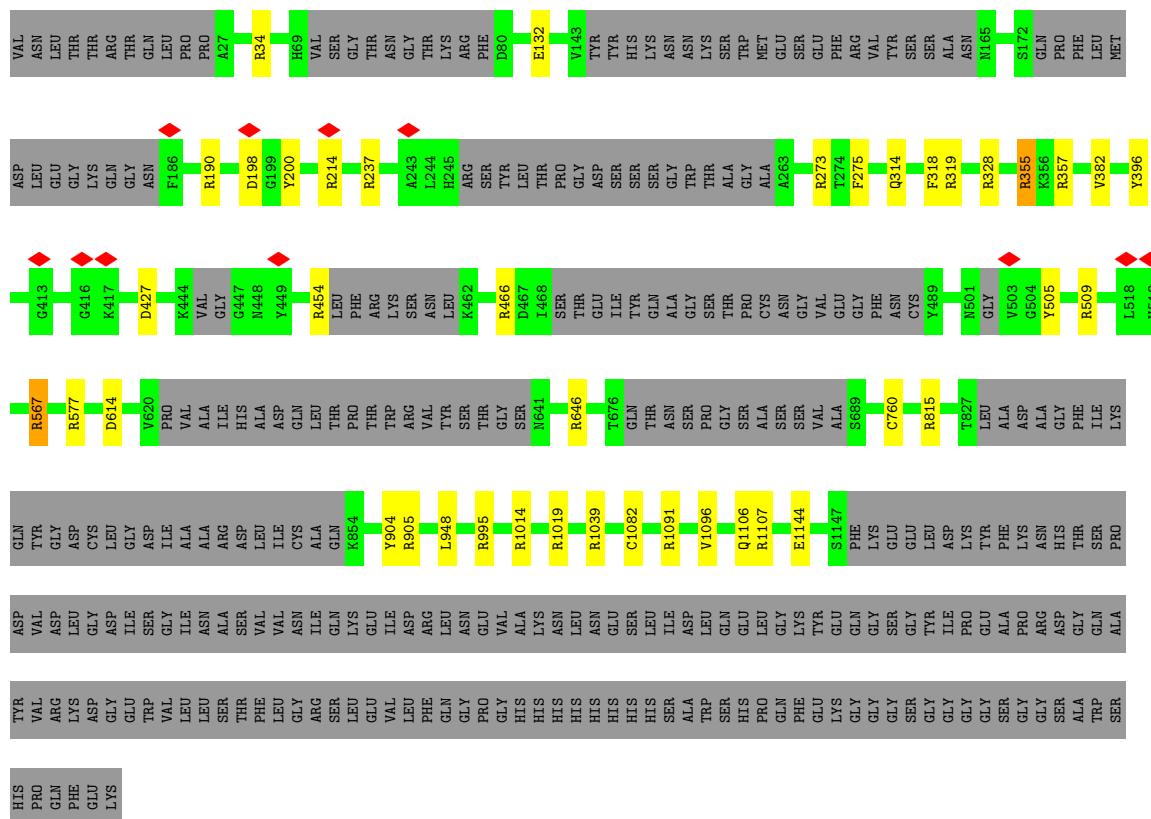
- Molecule 1: Spike glycoprotein





- Molecule 1: Spike glycoprotein

Chain C:



## 4 Experimental information i

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	139267	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	66.82	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	2.166	Depositor
Minimum map value	-1.161	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.060	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	317.4, 317.4, 317.4	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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	0/7777	1.00	29/10579 (0.3%)
1	B	0.65	0/7777	0.99	21/10579 (0.2%)
1	C	0.65	0/7777	1.00	25/10579 (0.2%)
All	All	0.65	0/23331	1.00	75/31737 (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	2
1	B	0	2
1	C	0	2
All	All	0	6

There are no bond length outliers.

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	C	1014	ARG	NE-CZ-NH1	9.27	124.94	120.30
1	A	273	ARG	NE-CZ-NH1	9.20	124.90	120.30
1	A	403	ARG	NE-CZ-NH1	8.46	124.53	120.30
1	A	1014	ARG	NE-CZ-NH1	8.40	124.50	120.30
1	C	509	ARG	NE-CZ-NH1	8.18	124.39	120.30
1	B	34	ARG	NE-CZ-NH1	8.03	124.32	120.30
1	B	1014	ARG	NE-CZ-NH1	7.61	124.10	120.30
1	C	1019	ARG	NE-CZ-NH1	7.57	124.08	120.30
1	B	328	ARG	NE-CZ-NH1	7.52	124.06	120.30
1	B	577	ARG	NE-CZ-NH1	7.35	123.97	120.30
1	C	567	ARG	NE-CZ-NH1	7.33	123.96	120.30
1	A	1107	ARG	NE-CZ-NH1	7.33	123.96	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1107	ARG	NE-CZ-NH1	7.19	123.89	120.30
1	C	319	ARG	NE-CZ-NH1	7.13	123.87	120.30
1	A	237	ARG	NE-CZ-NH1	7.11	123.86	120.30
1	A	577	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	C	466	ARG	NE-CZ-NH1	6.95	123.78	120.30
1	C	646	ARG	NE-CZ-NH1	6.95	123.78	120.30
1	B	1019	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	A	1091	ARG	NE-CZ-NH1	6.75	123.67	120.30
1	B	815	ARG	NE-CZ-NH1	6.73	123.66	120.30
1	C	273	ARG	NE-CZ-NH1	6.67	123.64	120.30
1	C	1107	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	A	1019	ARG	NE-CZ-NH1	6.61	123.60	120.30
1	C	577	ARG	NE-CZ-NH1	6.55	123.57	120.30
1	A	904	TYR	CB-CG-CD2	-6.47	117.12	121.00
1	C	355	ARG	NE-CZ-NH1	6.45	123.53	120.30
1	C	995	ARG	NE-CZ-NH1	6.45	123.52	120.30
1	C	815	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	A	454	ARG	NE-CZ-NH1	6.43	123.52	120.30
1	C	454	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	A	355	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	C	357	ARG	NE-CZ-NH1	6.35	123.47	120.30
1	B	995	ARG	NE-CZ-NH1	6.33	123.47	120.30
1	C	237	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	B	765	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	C	214	ARG	NE-CZ-NH1	6.23	123.42	120.30
1	C	904	TYR	CB-CG-CD2	-6.22	117.27	121.00
1	C	34	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	C	1039	ARG	NE-CZ-NH1	6.17	123.39	120.30
1	B	904	TYR	CB-CG-CD2	-6.14	117.32	121.00
1	A	646	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	A	319	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	A	1039	ARG	NE-CZ-NH1	6.03	123.32	120.30
1	B	319	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	A	765	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	B	355	ARG	NE-CZ-NH1	5.95	123.28	120.30
1	C	1091	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	B	214	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	C	905	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	A	466	ARG	NE-CZ-NH1	5.77	123.19	120.30
1	B	237	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	A	1039	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	B	567	ARG	NE-CZ-NH1	5.68	123.14	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	905	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	A	44	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	A	357	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	B	102	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	C	190	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	B	1000	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	A	34	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	A	214	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	A	995	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	A	815	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	C	1039	ARG	NE-CZ-NH2	-5.37	117.62	120.30
1	B	357	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	A	983	ARG	NE-CZ-NH1	5.31	122.96	120.30
1	A	509	ARG	NE-CZ-NH1	5.29	122.95	120.30
1	B	403	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	A	190	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	C	328	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	B	273	ARG	NE-CZ-NH1	5.13	122.87	120.30
1	A	396	TYR	CB-CG-CD2	-5.13	117.92	121.00
1	A	346	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	B	454	ARG	NE-CZ-NH1	5.10	122.85	120.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	355	ARG	Sidechain
1	A	983	ARG	Sidechain
1	B	200	TYR	Sidechain
1	B	355	ARG	Sidechain
1	C	355	ARG	Sidechain
1	C	567	ARG	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	7609	0	7445	2	0
1	B	7609	0	7445	4	0
1	C	7609	0	7445	0	0
All	All	22827	0	22335	6	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 (6) 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:38:TYR:CZ	1:B:285:ILE:HG22	2.44	0.52
1:A:520:ALA:HB1	1:A:521:PRO:CD	2.40	0.51
1:B:520:ALA:HB1	1:B:521:PRO:CD	2.47	0.45
1:B:726:ILE:HG22	1:B:948:LEU:HD13	1.99	0.45
1:B:520:ALA:HB1	1:B:521:PRO:HD2	2.01	0.42
1:A:520:ALA:HB1	1:A:521:PRO:HD2	2.03	0.41

There are no symmetry-related clashes.

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	948/1273 (74%)	876 (92%)	68 (7%)	4 (0%)	34 71
1	B	948/1273 (74%)	869 (92%)	75 (8%)	4 (0%)	34 71
1	C	948/1273 (74%)	876 (92%)	67 (7%)	5 (0%)	29 67
All	All	2844/3819 (74%)	2621 (92%)	210 (7%)	13 (0%)	32 67

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	396	TYR
1	A	396	TYR
1	A	112	SER
1	A	812	PRO
1	C	198	ASP
1	C	505	TYR
1	B	413	GLY
1	B	913	GLN
1	C	396	TYR
1	C	132	GLU
1	B	132	GLU
1	C	614	ASP
1	A	520	ALA

### 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	853/1099 (78%)	837 (98%)	16 (2%)	57 80
1	B	853/1099 (78%)	838 (98%)	15 (2%)	59 81
1	C	853/1099 (78%)	841 (99%)	12 (1%)	67 85
All	All	2559/3297 (78%)	2516 (98%)	43 (2%)	62 82

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	LEU
1	A	238	PHE
1	A	318	PHE
1	A	392	PHE
1	A	396	TYR
1	A	420	ASP
1	A	427	ASP
1	A	440	ASN
1	A	517	LEU
1	A	603	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	760	CYS
1	A	1004	LEU
1	A	1032	CYS
1	A	1043	CYS
1	A	1082	CYS
1	A	1084	ASP
1	B	227	VAL
1	B	238	PHE
1	B	377	PHE
1	B	392	PHE
1	B	399	SER
1	B	427	ASP
1	B	538	CYS
1	B	603	ASN
1	B	661	GLU
1	B	760	CYS
1	B	810	SER
1	B	858	LEU
1	B	948	LEU
1	B	1004	LEU
1	B	1127	ASP
1	C	200	TYR
1	C	275	PHE
1	C	314	GLN
1	C	318	PHE
1	C	382	VAL
1	C	427	ASP
1	C	760	CYS
1	C	948	LEU
1	C	1082	CYS
1	C	1096	VAL
1	C	1106	GLN
1	C	1144	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	87	ASN

### 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 [\(i\)](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

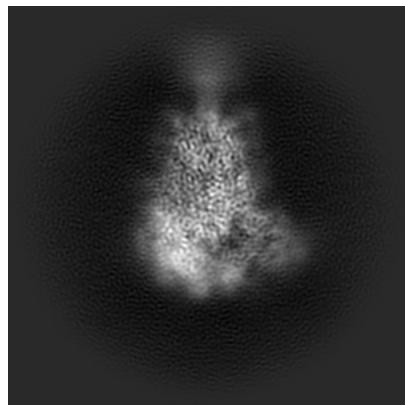
## 6 Map visualisation i

This section contains visualisations of the EMDB entry EMD-23612. These allow visual inspection of the internal detail of the map and identification of artifacts.

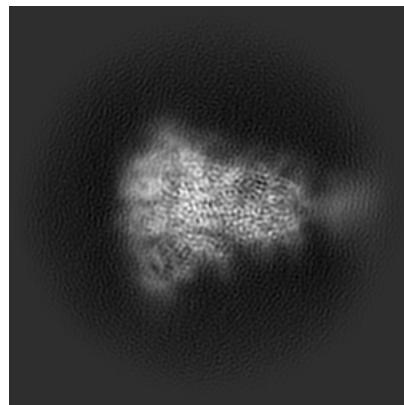
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections i

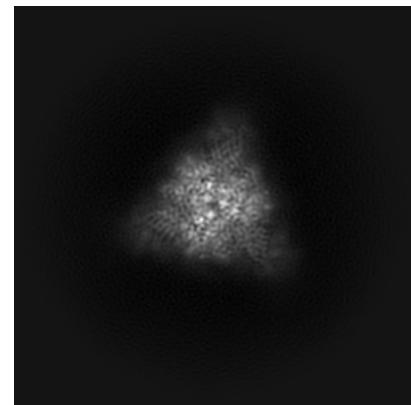
#### 6.1.1 Primary map



X



Y

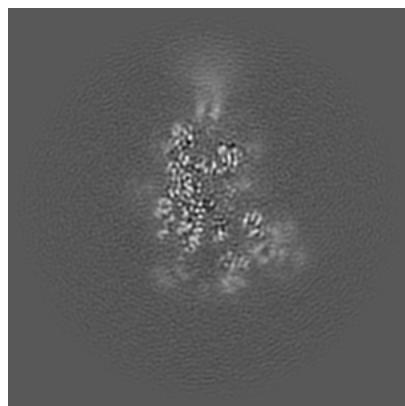


Z

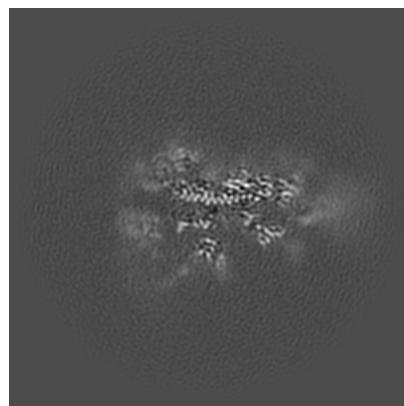
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices i

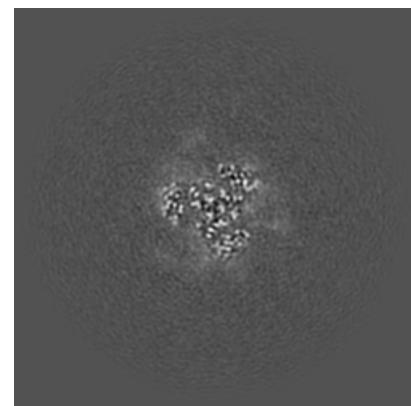
#### 6.2.1 Primary map



X Index: 150



Y Index: 150

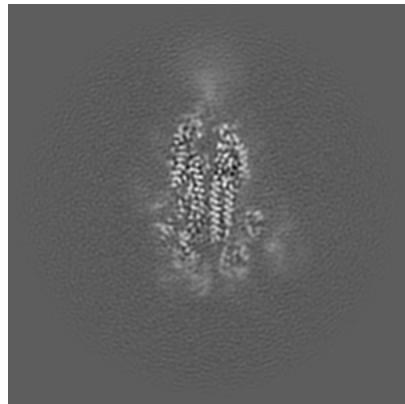


Z Index: 150

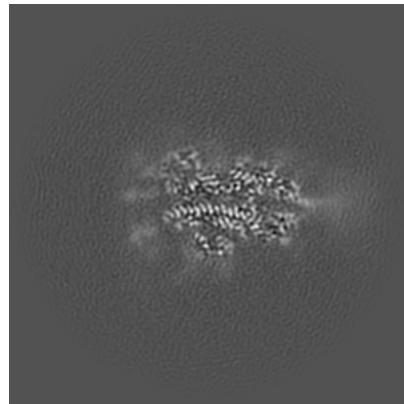
The images above show central slices of the map in three orthogonal directions.

### 6.3 Largest variance slices [\(i\)](#)

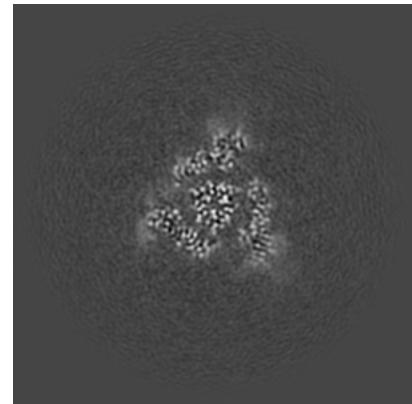
#### 6.3.1 Primary map



X Index: 145



Y Index: 156

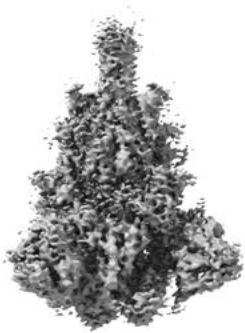


Z Index: 133

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

### 6.4 Orthogonal surface views [\(i\)](#)

#### 6.4.1 Primary map



X



Y



Z

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.

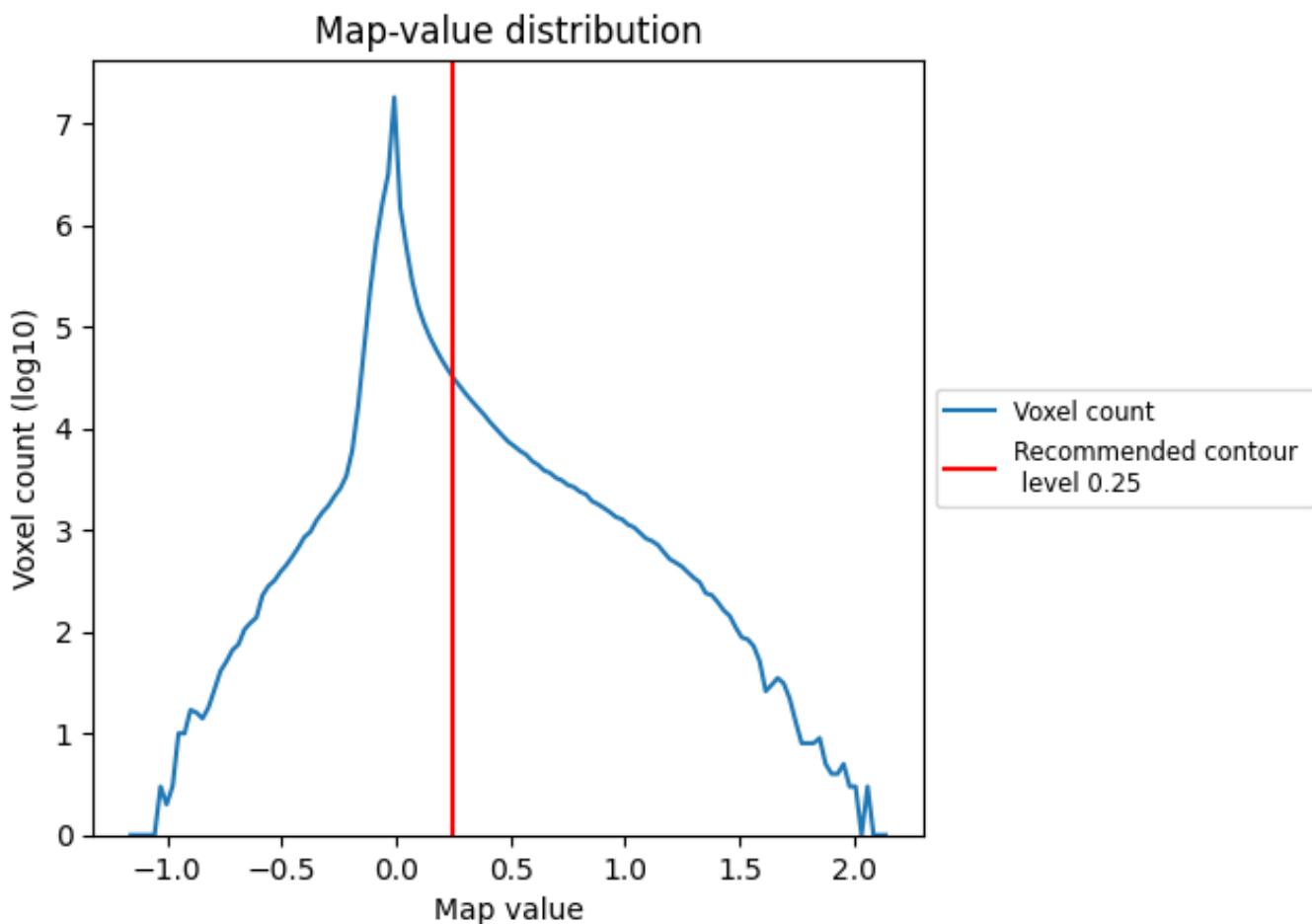
## 6.5 Mask visualisation

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

## 7 Map analysis (i)

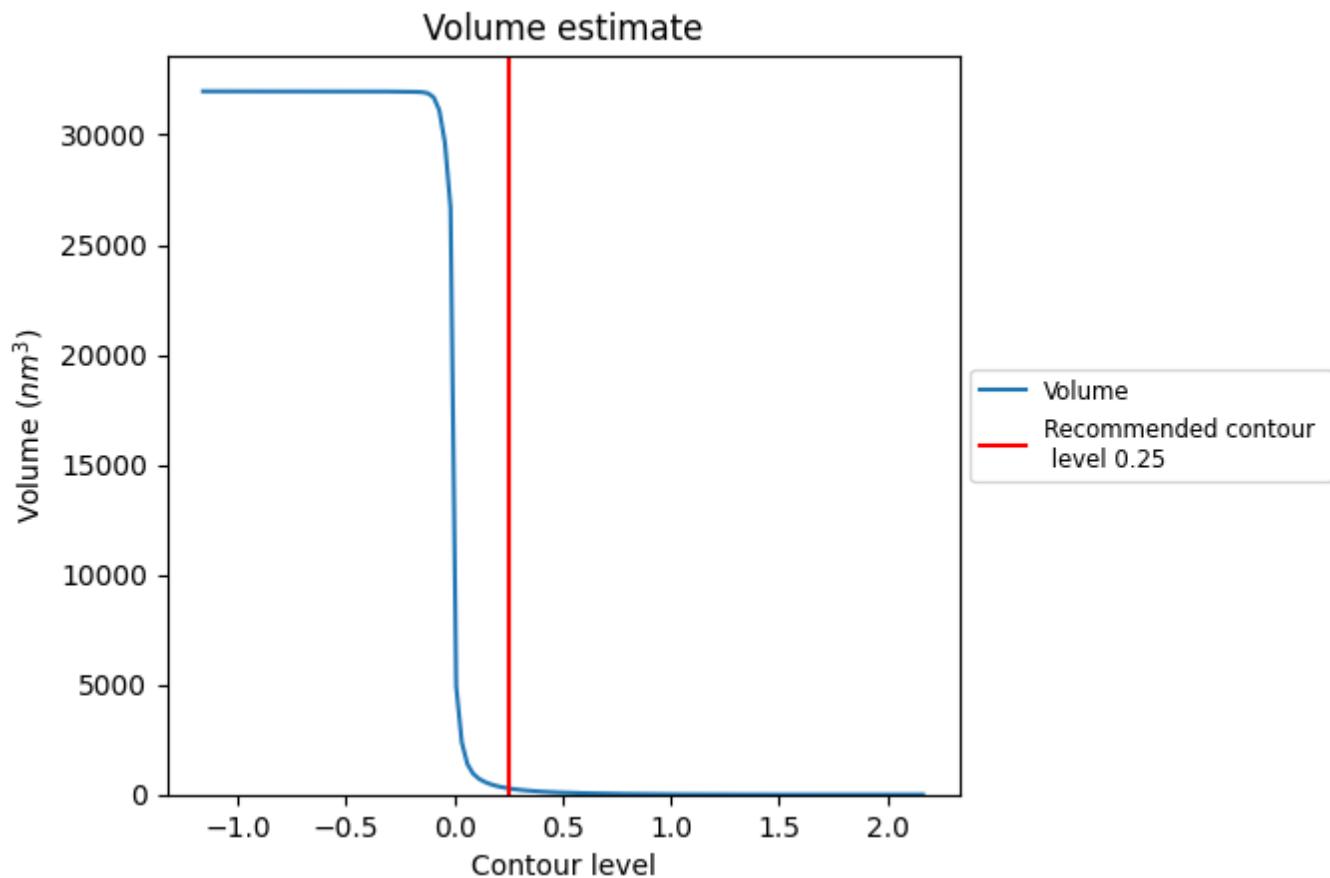
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

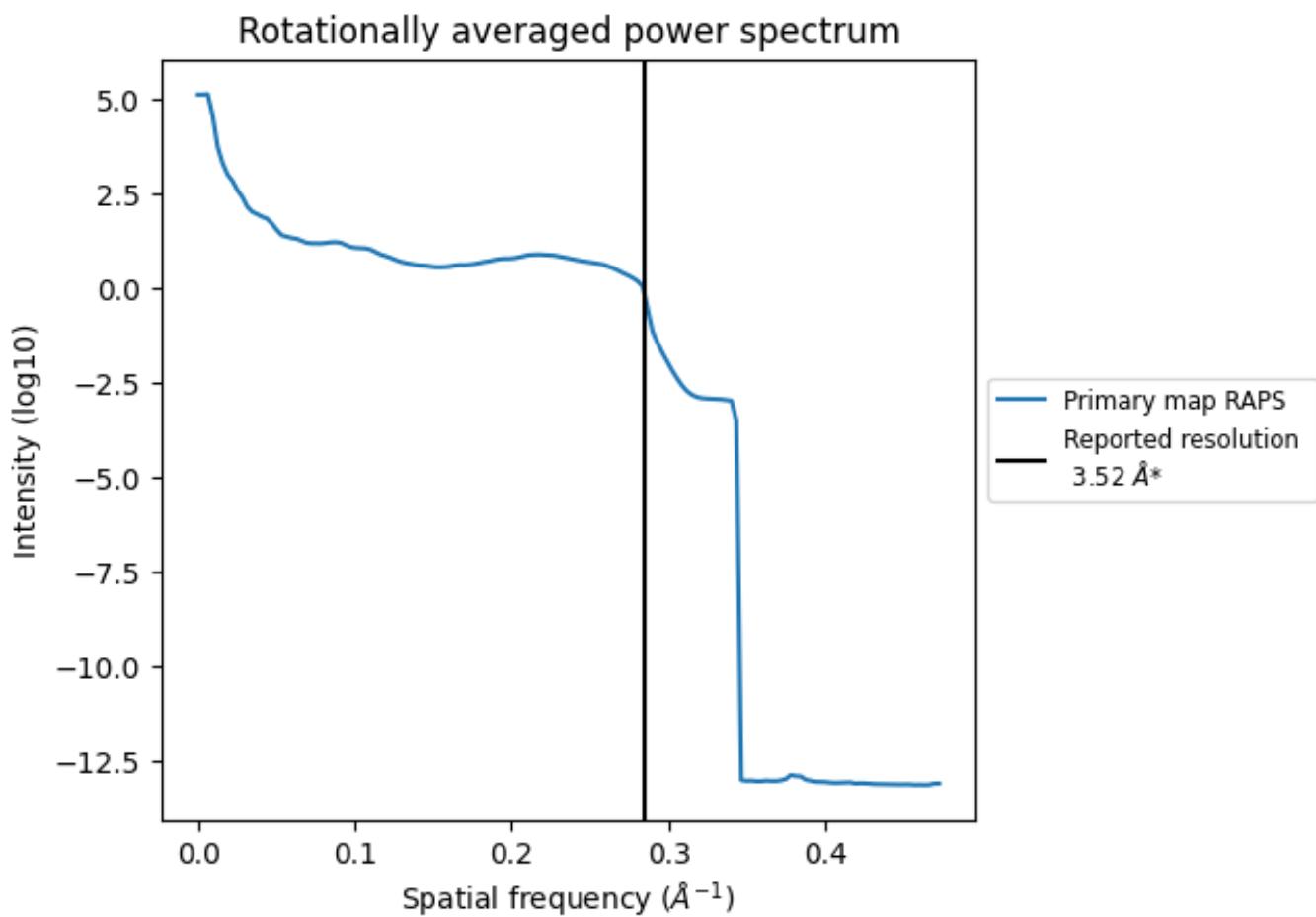
## 7.2 Volume estimate (i)



The volume at the recommended contour level is 283 nm<sup>3</sup>; this corresponds to an approximate mass of 256 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  $0.284 \text{ \AA}^{-1}$

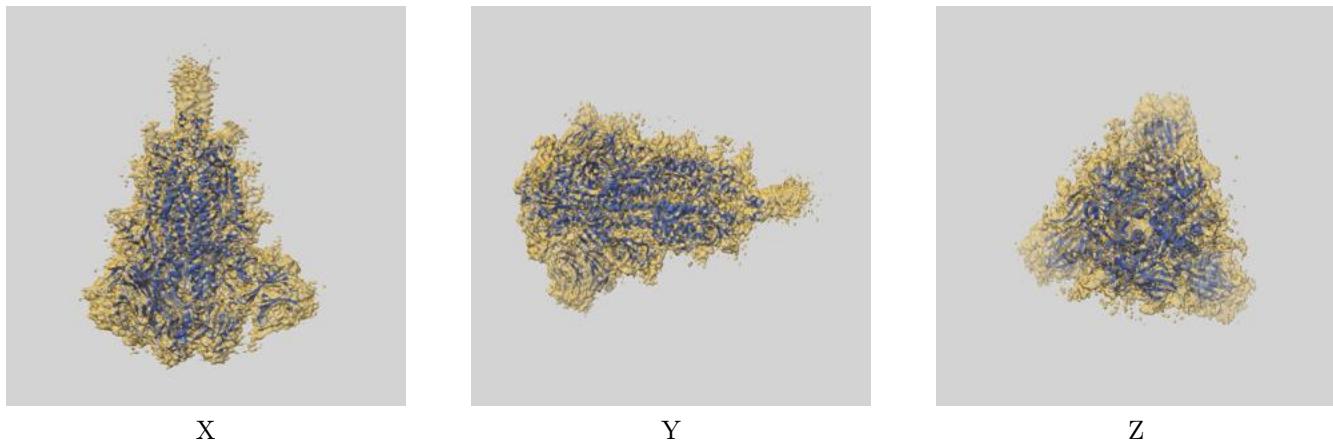
## 8 Fourier-Shell correlation

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

## 9 Map-model fit [\(i\)](#)

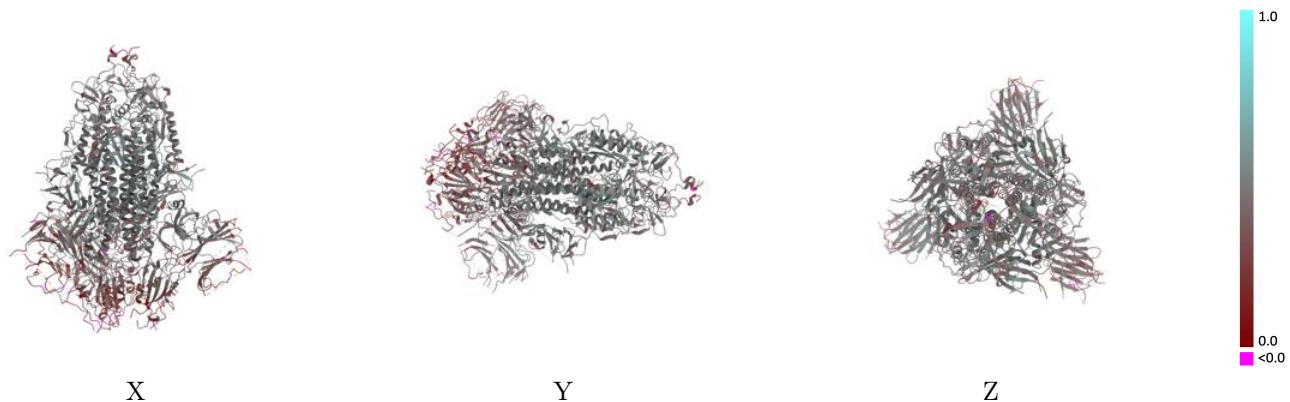
This section contains information regarding the fit between EMDB map EMD-23612 and PDB model 7M0J. Per-residue inclusion information can be found in section 3 on page 10.

### 9.1 Map-model overlay [\(i\)](#)



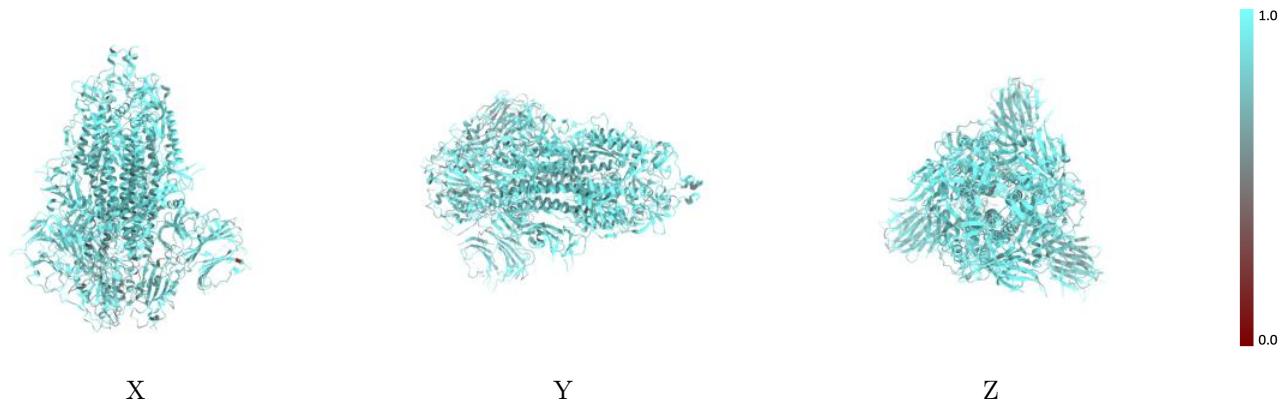
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



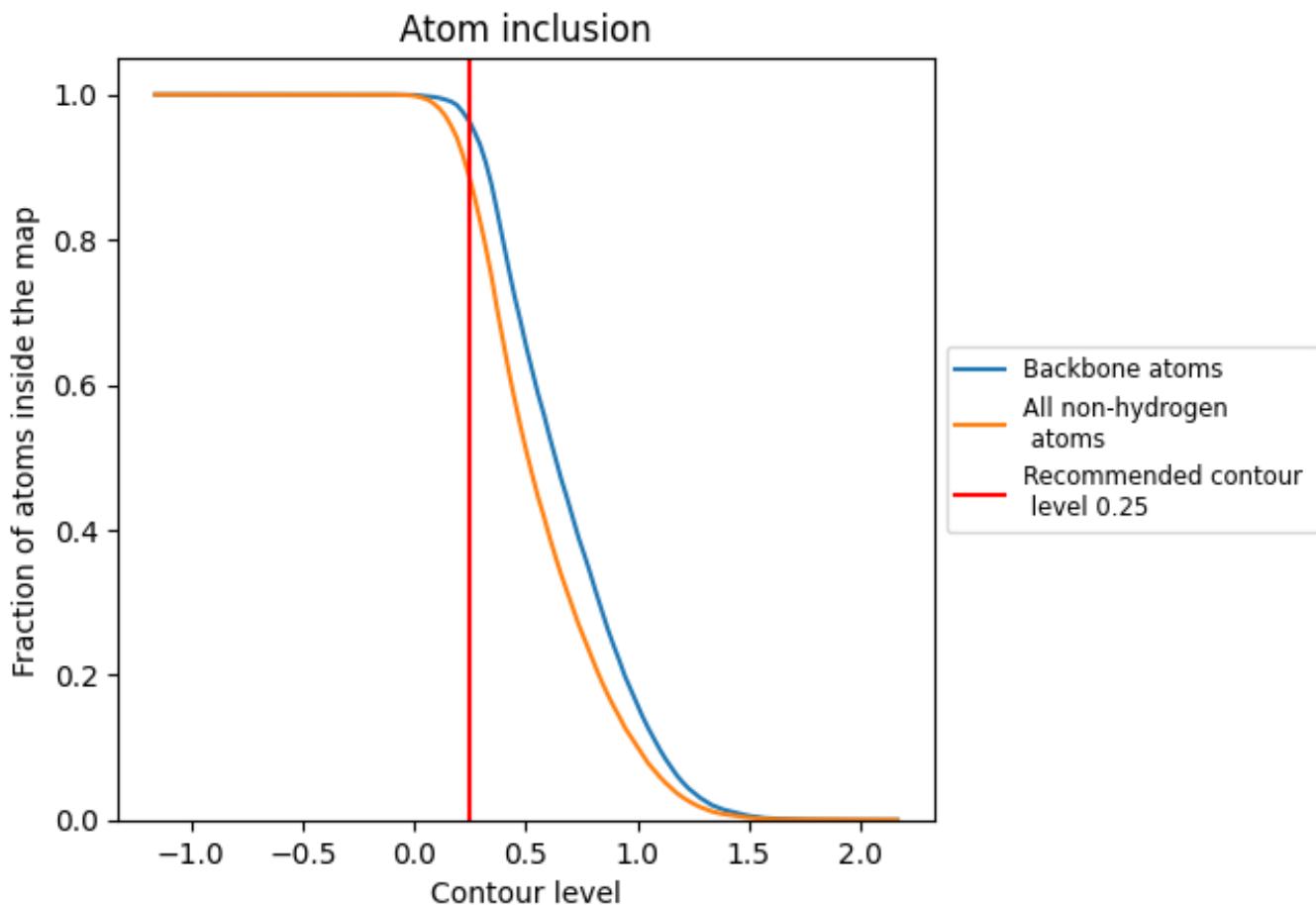
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 96% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary [\(i\)](#)

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	0.8826	0.4170
A	0.8821	0.4140
B	0.8865	0.4220
C	0.8792	0.4160

