



wwPDB EM Validation Summary Report ⓘ

Nov 21, 2022 – 10:19 AM EST

PDB ID : 8DYA
EMDB ID : EMD-27779
Title : Structure of the SARS-CoV-2 spike glycoprotein S2 subunit
Authors : Park, Y.J.; Seattle Structural Genomics Center for Infectious Disease (SSG-CID); Veesler, D.
Deposited on : 2022-08-03
Resolution : 3.67 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

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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.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
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

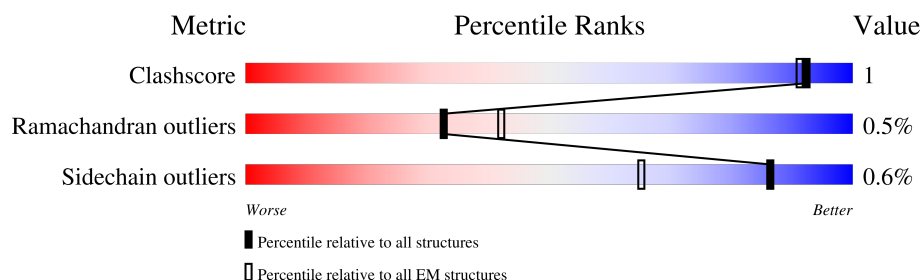
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.67 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	624	 60% 38%
1	B	624	 60% 38%
1	C	624	 59% 38%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7896 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	388	Total	C	N	O	S	0	0
			2548	1630	450	456	12		
1	B	388	Total	C	N	O	S	0	0
			2548	1630	450	456	12		
1	C	388	Total	C	N	O	S	0	0
			2548	1630	450	456	12		

There are 327 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	654	MET	-	initiating methionine	UNP A0A8B6RDW3
A	655	GLY	-	expression tag	UNP A0A8B6RDW3
A	656	ILE	-	expression tag	UNP A0A8B6RDW3
A	657	LEU	-	expression tag	UNP A0A8B6RDW3
A	658	PRO	-	expression tag	UNP A0A8B6RDW3
A	659	SER	-	expression tag	UNP A0A8B6RDW3
A	660	PRO	-	expression tag	UNP A0A8B6RDW3
A	661	GLY	-	expression tag	UNP A0A8B6RDW3
A	662	MET	-	expression tag	UNP A0A8B6RDW3
A	663	PRO	-	expression tag	UNP A0A8B6RDW3
A	664	ALA	-	expression tag	UNP A0A8B6RDW3
A	665	LEU	-	expression tag	UNP A0A8B6RDW3
A	666	LEU	-	expression tag	UNP A0A8B6RDW3
A	667	SER	-	expression tag	UNP A0A8B6RDW3
A	668	LEU	-	expression tag	UNP A0A8B6RDW3
A	669	VAL	-	expression tag	UNP A0A8B6RDW3
A	670	SER	-	expression tag	UNP A0A8B6RDW3
A	671	LEU	-	expression tag	UNP A0A8B6RDW3
A	672	LEU	-	expression tag	UNP A0A8B6RDW3
A	673	SER	-	expression tag	UNP A0A8B6RDW3
A	674	VAL	-	expression tag	UNP A0A8B6RDW3
A	675	LEU	-	expression tag	UNP A0A8B6RDW3
A	676	LEU	-	expression tag	UNP A0A8B6RDW3
A	677	MET	-	expression tag	UNP A0A8B6RDW3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	678	GLY	-	expression tag	UNP A0A8B6RDW3
A	679	CYS	-	expression tag	UNP A0A8B6RDW3
A	680	VAL	-	expression tag	UNP A0A8B6RDW3
A	681	ALA	-	expression tag	UNP A0A8B6RDW3
A	682	GLU	-	expression tag	UNP A0A8B6RDW3
A	683	THR	-	expression tag	UNP A0A8B6RDW3
A	684	GLY	-	expression tag	UNP A0A8B6RDW3
A	685	THR	-	expression tag	UNP A0A8B6RDW3
A	707	CYS	TYR	engineered mutation	UNP A0A8B6RDW3
A	883	CYS	THR	engineered mutation	UNP A0A8B6RDW3
A	892	PRO	ALA	engineered mutation	UNP A0A8B6RDW3
A	899	PRO	ALA	engineered mutation	UNP A0A8B6RDW3
A	942	PRO	ALA	engineered mutation	UNP A0A8B6RDW3
A	970	CYS	PHE	engineered mutation	UNP A0A8B6RDW3
A	987	PRO	VAL	engineered mutation	UNP A0A8B6RDW3
A	999	CYS	GLY	engineered mutation	UNP A0A8B6RDW3
A	1209	GLY	-	expression tag	UNP A0A8B6RDW3
A	1210	SER	-	expression tag	UNP A0A8B6RDW3
A	1211	GLY	-	expression tag	UNP A0A8B6RDW3
A	1212	TYR	-	expression tag	UNP A0A8B6RDW3
A	1213	ILE	-	expression tag	UNP A0A8B6RDW3
A	1214	PRO	-	expression tag	UNP A0A8B6RDW3
A	1215	GLU	-	expression tag	UNP A0A8B6RDW3
A	1216	ALA	-	expression tag	UNP A0A8B6RDW3
A	1217	PRO	-	expression tag	UNP A0A8B6RDW3
A	1218	ARG	-	expression tag	UNP A0A8B6RDW3
A	1219	ASP	-	expression tag	UNP A0A8B6RDW3
A	1220	GLY	-	expression tag	UNP A0A8B6RDW3
A	1221	GLN	-	expression tag	UNP A0A8B6RDW3
A	1222	ALA	-	expression tag	UNP A0A8B6RDW3
A	1223	TYR	-	expression tag	UNP A0A8B6RDW3
A	1224	VAL	-	expression tag	UNP A0A8B6RDW3
A	1225	ARG	-	expression tag	UNP A0A8B6RDW3
A	1226	LYS	-	expression tag	UNP A0A8B6RDW3
A	1227	ASP	-	expression tag	UNP A0A8B6RDW3
A	1228	GLY	-	expression tag	UNP A0A8B6RDW3
A	1229	GLU	-	expression tag	UNP A0A8B6RDW3
A	1230	TRP	-	expression tag	UNP A0A8B6RDW3
A	1231	VAL	-	expression tag	UNP A0A8B6RDW3
A	1232	LEU	-	expression tag	UNP A0A8B6RDW3
A	1233	LEU	-	expression tag	UNP A0A8B6RDW3
A	1234	SER	-	expression tag	UNP A0A8B6RDW3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1235	THR	-	expression tag	UNP A0A8B6RDW3
A	1236	PHE	-	expression tag	UNP A0A8B6RDW3
A	1237	LEU	-	expression tag	UNP A0A8B6RDW3
A	1238	GLY	-	expression tag	UNP A0A8B6RDW3
A	1239	ARG	-	expression tag	UNP A0A8B6RDW3
A	1240	SER	-	expression tag	UNP A0A8B6RDW3
A	1241	LEU	-	expression tag	UNP A0A8B6RDW3
A	1242	GLU	-	expression tag	UNP A0A8B6RDW3
A	1243	VAL	-	expression tag	UNP A0A8B6RDW3
A	1244	LEU	-	expression tag	UNP A0A8B6RDW3
A	1245	PHE	-	expression tag	UNP A0A8B6RDW3
A	1246	GLN	-	expression tag	UNP A0A8B6RDW3
A	1247	GLY	-	expression tag	UNP A0A8B6RDW3
A	1248	PRO	-	expression tag	UNP A0A8B6RDW3
A	1249	GLY	-	expression tag	UNP A0A8B6RDW3
A	1250	SER	-	expression tag	UNP A0A8B6RDW3
A	1251	GLY	-	expression tag	UNP A0A8B6RDW3
A	1252	GLY	-	expression tag	UNP A0A8B6RDW3
A	1253	LEU	-	expression tag	UNP A0A8B6RDW3
A	1254	ASN	-	expression tag	UNP A0A8B6RDW3
A	1255	ASP	-	expression tag	UNP A0A8B6RDW3
A	1256	ILE	-	expression tag	UNP A0A8B6RDW3
A	1257	PHE	-	expression tag	UNP A0A8B6RDW3
A	1258	GLU	-	expression tag	UNP A0A8B6RDW3
A	1259	ALA	-	expression tag	UNP A0A8B6RDW3
A	1260	GLN	-	expression tag	UNP A0A8B6RDW3
A	1261	LYS	-	expression tag	UNP A0A8B6RDW3
A	1262	ILE	-	expression tag	UNP A0A8B6RDW3
A	1263	GLU	-	expression tag	UNP A0A8B6RDW3
A	1264	TRP	-	expression tag	UNP A0A8B6RDW3
A	1265	HIS	-	expression tag	UNP A0A8B6RDW3
A	1266	GLU	-	expression tag	UNP A0A8B6RDW3
A	1267	GLY	-	expression tag	UNP A0A8B6RDW3
A	1268	SER	-	expression tag	UNP A0A8B6RDW3
A	1269	GLY	-	expression tag	UNP A0A8B6RDW3
A	1270	HIS	-	expression tag	UNP A0A8B6RDW3
A	1271	HIS	-	expression tag	UNP A0A8B6RDW3
A	1272	HIS	-	expression tag	UNP A0A8B6RDW3
A	1273	HIS	-	expression tag	UNP A0A8B6RDW3
A	1274	HIS	-	expression tag	UNP A0A8B6RDW3
A	1275	HIS	-	expression tag	UNP A0A8B6RDW3
A	1276	HIS	-	expression tag	UNP A0A8B6RDW3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1277	HIS	-	expression tag	UNP A0A8B6RDW3
B	654	MET	-	initiating methionine	UNP A0A8B6RDW3
B	655	GLY	-	expression tag	UNP A0A8B6RDW3
B	656	ILE	-	expression tag	UNP A0A8B6RDW3
B	657	LEU	-	expression tag	UNP A0A8B6RDW3
B	658	PRO	-	expression tag	UNP A0A8B6RDW3
B	659	SER	-	expression tag	UNP A0A8B6RDW3
B	660	PRO	-	expression tag	UNP A0A8B6RDW3
B	661	GLY	-	expression tag	UNP A0A8B6RDW3
B	662	MET	-	expression tag	UNP A0A8B6RDW3
B	663	PRO	-	expression tag	UNP A0A8B6RDW3
B	664	ALA	-	expression tag	UNP A0A8B6RDW3
B	665	LEU	-	expression tag	UNP A0A8B6RDW3
B	666	LEU	-	expression tag	UNP A0A8B6RDW3
B	667	SER	-	expression tag	UNP A0A8B6RDW3
B	668	LEU	-	expression tag	UNP A0A8B6RDW3
B	669	VAL	-	expression tag	UNP A0A8B6RDW3
B	670	SER	-	expression tag	UNP A0A8B6RDW3
B	671	LEU	-	expression tag	UNP A0A8B6RDW3
B	672	LEU	-	expression tag	UNP A0A8B6RDW3
B	673	SER	-	expression tag	UNP A0A8B6RDW3
B	674	VAL	-	expression tag	UNP A0A8B6RDW3
B	675	LEU	-	expression tag	UNP A0A8B6RDW3
B	676	LEU	-	expression tag	UNP A0A8B6RDW3
B	677	MET	-	expression tag	UNP A0A8B6RDW3
B	678	GLY	-	expression tag	UNP A0A8B6RDW3
B	679	CYS	-	expression tag	UNP A0A8B6RDW3
B	680	VAL	-	expression tag	UNP A0A8B6RDW3
B	681	ALA	-	expression tag	UNP A0A8B6RDW3
B	682	GLU	-	expression tag	UNP A0A8B6RDW3
B	683	THR	-	expression tag	UNP A0A8B6RDW3
B	684	GLY	-	expression tag	UNP A0A8B6RDW3
B	685	THR	-	expression tag	UNP A0A8B6RDW3
B	707	CYS	TYR	engineered mutation	UNP A0A8B6RDW3
B	883	CYS	THR	engineered mutation	UNP A0A8B6RDW3
B	892	PRO	ALA	engineered mutation	UNP A0A8B6RDW3
B	899	PRO	ALA	engineered mutation	UNP A0A8B6RDW3
B	942	PRO	ALA	engineered mutation	UNP A0A8B6RDW3
B	970	CYS	PHE	engineered mutation	UNP A0A8B6RDW3
B	987	PRO	VAL	engineered mutation	UNP A0A8B6RDW3
B	999	CYS	GLY	engineered mutation	UNP A0A8B6RDW3
B	1209	GLY	-	expression tag	UNP A0A8B6RDW3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1210	SER	-	expression tag	UNP A0A8B6RDW3
B	1211	GLY	-	expression tag	UNP A0A8B6RDW3
B	1212	TYR	-	expression tag	UNP A0A8B6RDW3
B	1213	ILE	-	expression tag	UNP A0A8B6RDW3
B	1214	PRO	-	expression tag	UNP A0A8B6RDW3
B	1215	GLU	-	expression tag	UNP A0A8B6RDW3
B	1216	ALA	-	expression tag	UNP A0A8B6RDW3
B	1217	PRO	-	expression tag	UNP A0A8B6RDW3
B	1218	ARG	-	expression tag	UNP A0A8B6RDW3
B	1219	ASP	-	expression tag	UNP A0A8B6RDW3
B	1220	GLY	-	expression tag	UNP A0A8B6RDW3
B	1221	GLN	-	expression tag	UNP A0A8B6RDW3
B	1222	ALA	-	expression tag	UNP A0A8B6RDW3
B	1223	TYR	-	expression tag	UNP A0A8B6RDW3
B	1224	VAL	-	expression tag	UNP A0A8B6RDW3
B	1225	ARG	-	expression tag	UNP A0A8B6RDW3
B	1226	LYS	-	expression tag	UNP A0A8B6RDW3
B	1227	ASP	-	expression tag	UNP A0A8B6RDW3
B	1228	GLY	-	expression tag	UNP A0A8B6RDW3
B	1229	GLU	-	expression tag	UNP A0A8B6RDW3
B	1230	TRP	-	expression tag	UNP A0A8B6RDW3
B	1231	VAL	-	expression tag	UNP A0A8B6RDW3
B	1232	LEU	-	expression tag	UNP A0A8B6RDW3
B	1233	LEU	-	expression tag	UNP A0A8B6RDW3
B	1234	SER	-	expression tag	UNP A0A8B6RDW3
B	1235	THR	-	expression tag	UNP A0A8B6RDW3
B	1236	PHE	-	expression tag	UNP A0A8B6RDW3
B	1237	LEU	-	expression tag	UNP A0A8B6RDW3
B	1238	GLY	-	expression tag	UNP A0A8B6RDW3
B	1239	ARG	-	expression tag	UNP A0A8B6RDW3
B	1240	SER	-	expression tag	UNP A0A8B6RDW3
B	1241	LEU	-	expression tag	UNP A0A8B6RDW3
B	1242	GLU	-	expression tag	UNP A0A8B6RDW3
B	1243	VAL	-	expression tag	UNP A0A8B6RDW3
B	1244	LEU	-	expression tag	UNP A0A8B6RDW3
B	1245	PHE	-	expression tag	UNP A0A8B6RDW3
B	1246	GLN	-	expression tag	UNP A0A8B6RDW3
B	1247	GLY	-	expression tag	UNP A0A8B6RDW3
B	1248	PRO	-	expression tag	UNP A0A8B6RDW3
B	1249	GLY	-	expression tag	UNP A0A8B6RDW3
B	1250	SER	-	expression tag	UNP A0A8B6RDW3
B	1251	GLY	-	expression tag	UNP A0A8B6RDW3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1252	GLY	-	expression tag	UNP A0A8B6RDW3
B	1253	LEU	-	expression tag	UNP A0A8B6RDW3
B	1254	ASN	-	expression tag	UNP A0A8B6RDW3
B	1255	ASP	-	expression tag	UNP A0A8B6RDW3
B	1256	ILE	-	expression tag	UNP A0A8B6RDW3
B	1257	PHE	-	expression tag	UNP A0A8B6RDW3
B	1258	GLU	-	expression tag	UNP A0A8B6RDW3
B	1259	ALA	-	expression tag	UNP A0A8B6RDW3
B	1260	GLN	-	expression tag	UNP A0A8B6RDW3
B	1261	LYS	-	expression tag	UNP A0A8B6RDW3
B	1262	ILE	-	expression tag	UNP A0A8B6RDW3
B	1263	GLU	-	expression tag	UNP A0A8B6RDW3
B	1264	TRP	-	expression tag	UNP A0A8B6RDW3
B	1265	HIS	-	expression tag	UNP A0A8B6RDW3
B	1266	GLU	-	expression tag	UNP A0A8B6RDW3
B	1267	GLY	-	expression tag	UNP A0A8B6RDW3
B	1268	SER	-	expression tag	UNP A0A8B6RDW3
B	1269	GLY	-	expression tag	UNP A0A8B6RDW3
B	1270	HIS	-	expression tag	UNP A0A8B6RDW3
B	1271	HIS	-	expression tag	UNP A0A8B6RDW3
B	1272	HIS	-	expression tag	UNP A0A8B6RDW3
B	1273	HIS	-	expression tag	UNP A0A8B6RDW3
B	1274	HIS	-	expression tag	UNP A0A8B6RDW3
B	1275	HIS	-	expression tag	UNP A0A8B6RDW3
B	1276	HIS	-	expression tag	UNP A0A8B6RDW3
B	1277	HIS	-	expression tag	UNP A0A8B6RDW3
C	654	MET	-	initiating methionine	UNP A0A8B6RDW3
C	655	GLY	-	expression tag	UNP A0A8B6RDW3
C	656	ILE	-	expression tag	UNP A0A8B6RDW3
C	657	LEU	-	expression tag	UNP A0A8B6RDW3
C	658	PRO	-	expression tag	UNP A0A8B6RDW3
C	659	SER	-	expression tag	UNP A0A8B6RDW3
C	660	PRO	-	expression tag	UNP A0A8B6RDW3
C	661	GLY	-	expression tag	UNP A0A8B6RDW3
C	662	MET	-	expression tag	UNP A0A8B6RDW3
C	663	PRO	-	expression tag	UNP A0A8B6RDW3
C	664	ALA	-	expression tag	UNP A0A8B6RDW3
C	665	LEU	-	expression tag	UNP A0A8B6RDW3
C	666	LEU	-	expression tag	UNP A0A8B6RDW3
C	667	SER	-	expression tag	UNP A0A8B6RDW3
C	668	LEU	-	expression tag	UNP A0A8B6RDW3
C	669	VAL	-	expression tag	UNP A0A8B6RDW3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	670	SER	-	expression tag	UNP A0A8B6RDW3
C	671	LEU	-	expression tag	UNP A0A8B6RDW3
C	672	LEU	-	expression tag	UNP A0A8B6RDW3
C	673	SER	-	expression tag	UNP A0A8B6RDW3
C	674	VAL	-	expression tag	UNP A0A8B6RDW3
C	675	LEU	-	expression tag	UNP A0A8B6RDW3
C	676	LEU	-	expression tag	UNP A0A8B6RDW3
C	677	MET	-	expression tag	UNP A0A8B6RDW3
C	678	GLY	-	expression tag	UNP A0A8B6RDW3
C	679	CYS	-	expression tag	UNP A0A8B6RDW3
C	680	VAL	-	expression tag	UNP A0A8B6RDW3
C	681	ALA	-	expression tag	UNP A0A8B6RDW3
C	682	GLU	-	expression tag	UNP A0A8B6RDW3
C	683	THR	-	expression tag	UNP A0A8B6RDW3
C	684	GLY	-	expression tag	UNP A0A8B6RDW3
C	685	THR	-	expression tag	UNP A0A8B6RDW3
C	707	CYS	TYR	engineered mutation	UNP A0A8B6RDW3
C	883	CYS	THR	engineered mutation	UNP A0A8B6RDW3
C	892	PRO	ALA	engineered mutation	UNP A0A8B6RDW3
C	899	PRO	ALA	engineered mutation	UNP A0A8B6RDW3
C	942	PRO	ALA	engineered mutation	UNP A0A8B6RDW3
C	970	CYS	PHE	engineered mutation	UNP A0A8B6RDW3
C	987	PRO	VAL	engineered mutation	UNP A0A8B6RDW3
C	999	CYS	GLY	engineered mutation	UNP A0A8B6RDW3
C	1209	GLY	-	expression tag	UNP A0A8B6RDW3
C	1210	SER	-	expression tag	UNP A0A8B6RDW3
C	1211	GLY	-	expression tag	UNP A0A8B6RDW3
C	1212	TYR	-	expression tag	UNP A0A8B6RDW3
C	1213	ILE	-	expression tag	UNP A0A8B6RDW3
C	1214	PRO	-	expression tag	UNP A0A8B6RDW3
C	1215	GLU	-	expression tag	UNP A0A8B6RDW3
C	1216	ALA	-	expression tag	UNP A0A8B6RDW3
C	1217	PRO	-	expression tag	UNP A0A8B6RDW3
C	1218	ARG	-	expression tag	UNP A0A8B6RDW3
C	1219	ASP	-	expression tag	UNP A0A8B6RDW3
C	1220	GLY	-	expression tag	UNP A0A8B6RDW3
C	1221	GLN	-	expression tag	UNP A0A8B6RDW3
C	1222	ALA	-	expression tag	UNP A0A8B6RDW3
C	1223	TYR	-	expression tag	UNP A0A8B6RDW3
C	1224	VAL	-	expression tag	UNP A0A8B6RDW3
C	1225	ARG	-	expression tag	UNP A0A8B6RDW3
C	1226	LYS	-	expression tag	UNP A0A8B6RDW3

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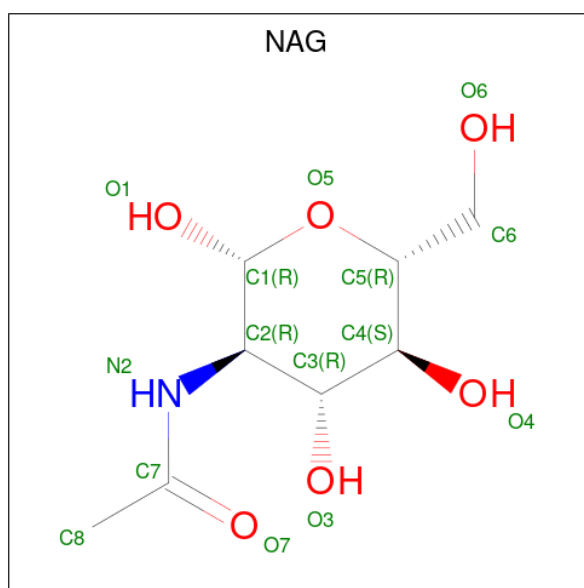
Chain	Residue	Modelled	Actual	Comment	Reference
C	1227	ASP	-	expression tag	UNP A0A8B6RDW3
C	1228	GLY	-	expression tag	UNP A0A8B6RDW3
C	1229	GLU	-	expression tag	UNP A0A8B6RDW3
C	1230	TRP	-	expression tag	UNP A0A8B6RDW3
C	1231	VAL	-	expression tag	UNP A0A8B6RDW3
C	1232	LEU	-	expression tag	UNP A0A8B6RDW3
C	1233	LEU	-	expression tag	UNP A0A8B6RDW3
C	1234	SER	-	expression tag	UNP A0A8B6RDW3
C	1235	THR	-	expression tag	UNP A0A8B6RDW3
C	1236	PHE	-	expression tag	UNP A0A8B6RDW3
C	1237	LEU	-	expression tag	UNP A0A8B6RDW3
C	1238	GLY	-	expression tag	UNP A0A8B6RDW3
C	1239	ARG	-	expression tag	UNP A0A8B6RDW3
C	1240	SER	-	expression tag	UNP A0A8B6RDW3
C	1241	LEU	-	expression tag	UNP A0A8B6RDW3
C	1242	GLU	-	expression tag	UNP A0A8B6RDW3
C	1243	VAL	-	expression tag	UNP A0A8B6RDW3
C	1244	LEU	-	expression tag	UNP A0A8B6RDW3
C	1245	PHE	-	expression tag	UNP A0A8B6RDW3
C	1246	GLN	-	expression tag	UNP A0A8B6RDW3
C	1247	GLY	-	expression tag	UNP A0A8B6RDW3
C	1248	PRO	-	expression tag	UNP A0A8B6RDW3
C	1249	GLY	-	expression tag	UNP A0A8B6RDW3
C	1250	SER	-	expression tag	UNP A0A8B6RDW3
C	1251	GLY	-	expression tag	UNP A0A8B6RDW3
C	1252	GLY	-	expression tag	UNP A0A8B6RDW3
C	1253	LEU	-	expression tag	UNP A0A8B6RDW3
C	1254	ASN	-	expression tag	UNP A0A8B6RDW3
C	1255	ASP	-	expression tag	UNP A0A8B6RDW3
C	1256	ILE	-	expression tag	UNP A0A8B6RDW3
C	1257	PHE	-	expression tag	UNP A0A8B6RDW3
C	1258	GLU	-	expression tag	UNP A0A8B6RDW3
C	1259	ALA	-	expression tag	UNP A0A8B6RDW3
C	1260	GLN	-	expression tag	UNP A0A8B6RDW3
C	1261	LYS	-	expression tag	UNP A0A8B6RDW3
C	1262	ILE	-	expression tag	UNP A0A8B6RDW3
C	1263	GLU	-	expression tag	UNP A0A8B6RDW3
C	1264	TRP	-	expression tag	UNP A0A8B6RDW3
C	1265	HIS	-	expression tag	UNP A0A8B6RDW3
C	1266	GLU	-	expression tag	UNP A0A8B6RDW3
C	1267	GLY	-	expression tag	UNP A0A8B6RDW3
C	1268	SER	-	expression tag	UNP A0A8B6RDW3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1269	GLY	-	expression tag	UNP A0A8B6RDW3
C	1270	HIS	-	expression tag	UNP A0A8B6RDW3
C	1271	HIS	-	expression tag	UNP A0A8B6RDW3
C	1272	HIS	-	expression tag	UNP A0A8B6RDW3
C	1273	HIS	-	expression tag	UNP A0A8B6RDW3
C	1274	HIS	-	expression tag	UNP A0A8B6RDW3
C	1275	HIS	-	expression tag	UNP A0A8B6RDW3
C	1276	HIS	-	expression tag	UNP A0A8B6RDW3
C	1277	HIS	-	expression tag	UNP A0A8B6RDW3

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



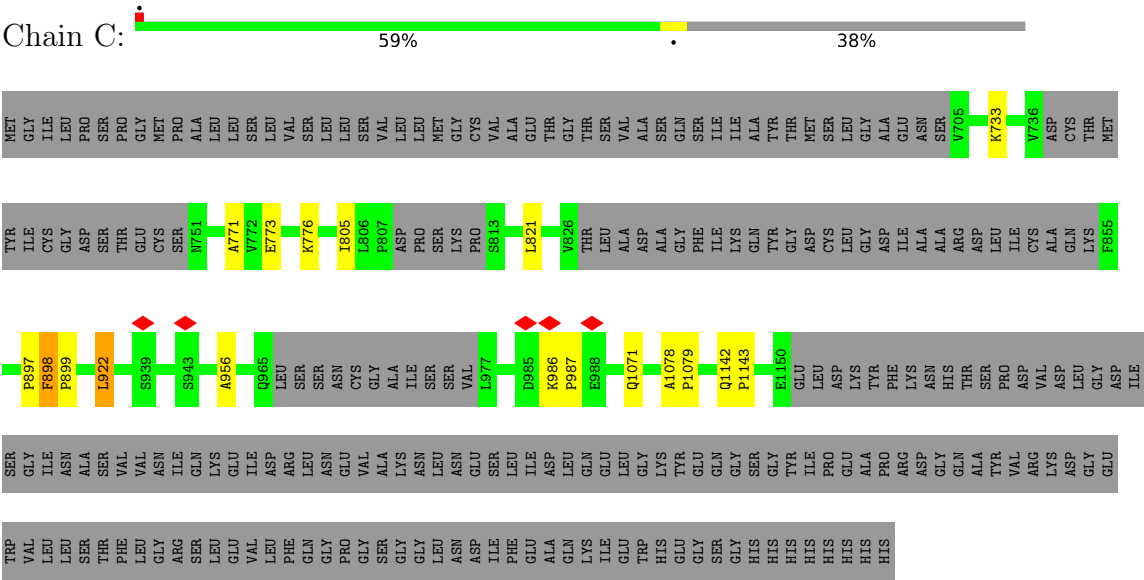
Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			84	48	6	30	
2	A	1	Total	C	N	O	0
			84	48	6	30	
2	A	1	Total	C	N	O	0
			84	48	6	30	
2	A	1	Total	C	N	O	0
			84	48	6	30	
2	A	1	Total	C	N	O	0
			84	48	6	30	

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Mol	Chain	Residues	Atoms				AltConf
2	B	1	Total	C	N	O	0
			84	48	6	30	
2	B	1	Total	C	N	O	0
			84	48	6	30	
2	B	1	Total	C	N	O	0
			84	48	6	30	
2	B	1	Total	C	N	O	0
			84	48	6	30	
2	B	1	Total	C	N	O	0
			84	48	6	30	
2	C	1	Total	C	N	O	0
			84	48	6	30	
2	C	1	Total	C	N	O	0
			84	48	6	30	
2	C	1	Total	C	N	O	0
			84	48	6	30	
2	C	1	Total	C	N	O	0
			84	48	6	30	
2	C	1	Total	C	N	O	0
			84	48	6	30	
2	C	1	Total	C	N	O	0
			84	48	6	30	

● 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	137737	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	5.461	Depositor
Minimum map value	-4.255	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.082	Depositor
Recommended contour level	0.25	Depositor
Map size (\AA)	304.0, 304.0, 304.0	wwPDB
Map dimensions	304, 304, 304	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.0, 1.0, 1.0	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

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	0.48	0/2601	0.61	4/3578 (0.1%)
1	B	0.48	0/2601	0.61	4/3578 (0.1%)
1	C	0.48	0/2601	0.61	4/3578 (0.1%)
All	All	0.48	0/7803	0.61	12/10734 (0.1%)

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	922	LEU	CD1-CG-CD2	7.15	131.95	110.50
1	A	922	LEU	CD1-CG-CD2	7.14	131.92	110.50
1	C	922	LEU	CD1-CG-CD2	7.12	131.85	110.50
1	A	821	LEU	CD1-CG-CD2	6.63	130.40	110.50
1	B	821	LEU	CD1-CG-CD2	6.63	130.40	110.50

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	2548	0	2030	6	0
1	B	2548	0	2030	6	0
1	C	2548	0	2030	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	84	0	78	1	0
2	B	84	0	78	1	0
2	C	84	0	78	1	0
All	All	7896	0	6324	20	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 1.

The worst 5 of 20 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:733:LYS:HD2	1:A:771:ALA:HB1	1.84	0.59
1:B:733:LYS:HD2	1:B:771:ALA:HB1	1.84	0.58
1:C:733:LYS:HD2	1:C:771:ALA:HB1	1.84	0.58
1:C:773:GLU:O	1:C:776:LYS:HB3	2.07	0.56
1:B:773:GLU:O	1:B:776:LYS:HB3	2.06	0.55

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	378/624 (61%)	362 (96%)	14 (4%)	2 (0%)	29	66
1	B	378/624 (61%)	361 (96%)	15 (4%)	2 (0%)	29	66
1	C	378/624 (61%)	361 (96%)	15 (4%)	2 (0%)	29	66
All	All	1134/1872 (61%)	1084 (96%)	44 (4%)	6 (0%)	32	66

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	898	PHE
1	B	898	PHE
1	C	898	PHE
1	A	897	PRO
1	B	897	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	179/534 (34%)	178 (99%)	1 (1%)	86	93
1	B	179/534 (34%)	178 (99%)	1 (1%)	86	93
1	C	179/534 (34%)	178 (99%)	1 (1%)	86	93
All	All	537/1602 (34%)	534 (99%)	3 (1%)	86	93

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	922	LEU
1	B	922	LEU
1	C	922	LEU

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	804	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

18 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	NAG	B	1304	1	14,14,15	1.18	1 (7%)	17,19,21	1.12	1 (5%)
2	NAG	C	1302	1	14,14,15	1.13	1 (7%)	17,19,21	0.94	1 (5%)
2	NAG	A	1301	1	14,14,15	1.15	1 (7%)	17,19,21	1.01	1 (5%)
2	NAG	A	1304	1	14,14,15	1.17	1 (7%)	17,19,21	1.12	1 (5%)
2	NAG	B	1303	1	14,14,15	1.09	2 (14%)	17,19,21	1.01	1 (5%)
2	NAG	A	1305	1	14,14,15	1.17	1 (7%)	17,19,21	0.97	1 (5%)
2	NAG	A	1302	1	14,14,15	1.14	1 (7%)	17,19,21	0.95	1 (5%)
2	NAG	A	1303	1	14,14,15	1.09	2 (14%)	17,19,21	1.01	1 (5%)
2	NAG	A	1306	-	14,14,15	0.41	0	17,19,21	1.17	2 (11%)
2	NAG	B	1301	1	14,14,15	1.14	1 (7%)	17,19,21	1.01	1 (5%)
2	NAG	C	1301	1	14,14,15	1.14	1 (7%)	17,19,21	1.01	1 (5%)
2	NAG	B	1305	1	14,14,15	1.16	1 (7%)	17,19,21	0.97	1 (5%)
2	NAG	C	1306	-	14,14,15	0.41	0	17,19,21	1.17	1 (5%)
2	NAG	B	1302	1	14,14,15	1.14	1 (7%)	17,19,21	0.95	1 (5%)
2	NAG	C	1303	1	14,14,15	1.08	1 (7%)	17,19,21	1.02	1 (5%)
2	NAG	C	1304	1	14,14,15	1.17	1 (7%)	17,19,21	1.12	1 (5%)
2	NAG	C	1305	1	14,14,15	1.17	1 (7%)	17,19,21	0.97	1 (5%)
2	NAG	B	1306	-	14,14,15	0.41	0	17,19,21	1.16	2 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	1304	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1302	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1301	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1304	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1303	1	-	1/6/23/26	0/1/1/1
2	NAG	A	1305	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1302	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1303	1	-	1/6/23/26	0/1/1/1
2	NAG	A	1306	-	-	0/6/23/26	0/1/1/1
2	NAG	B	1301	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1301	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1305	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1306	-	-	0/6/23/26	0/1/1/1
2	NAG	B	1302	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1303	1	-	1/6/23/26	0/1/1/1
2	NAG	C	1304	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1305	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1306	-	-	0/6/23/26	0/1/1/1

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1302	NAG	C1-C2	3.52	1.57	1.52
2	A	1302	NAG	C1-C2	3.50	1.57	1.52
2	B	1304	NAG	C1-C2	3.47	1.57	1.52
2	C	1302	NAG	C1-C2	3.45	1.57	1.52
2	A	1304	NAG	C1-C2	3.43	1.57	1.52

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1304	NAG	C8-C7-N2	2.67	120.62	116.10
2	B	1304	NAG	C8-C7-N2	2.66	120.61	116.10
2	C	1304	NAG	C8-C7-N2	2.66	120.61	116.10
2	A	1301	NAG	C8-C7-N2	2.43	120.22	116.10
2	C	1301	NAG	C8-C7-N2	2.41	120.18	116.10

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1303	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	A	1303	NAG	C4-C5-C6-O6
2	B	1303	NAG	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1306	NAG	1	0
2	C	1306	NAG	1	0
2	B	1306	NAG	1	0

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.

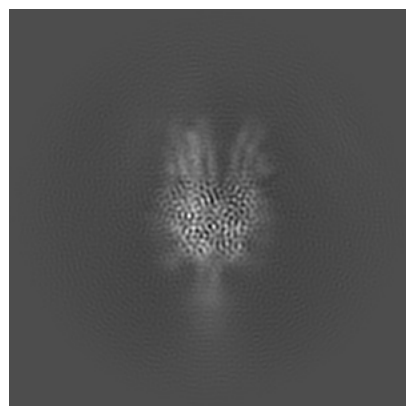
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27779. These allow visual inspection of the internal detail of the map and identification of artifacts.

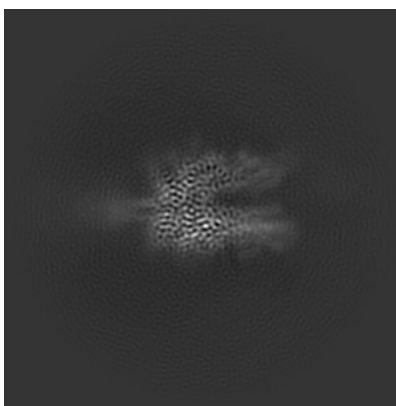
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

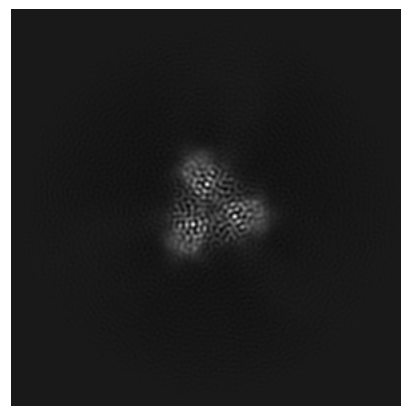
6.1.1 Primary map



X

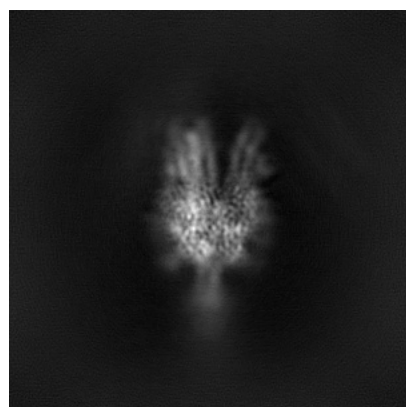


Y

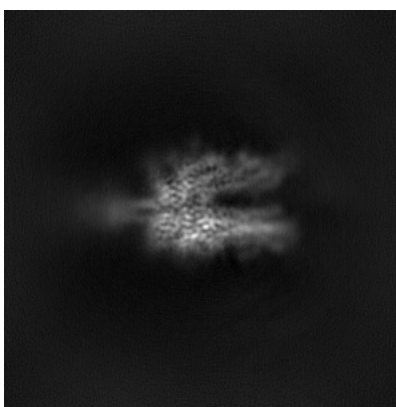


Z

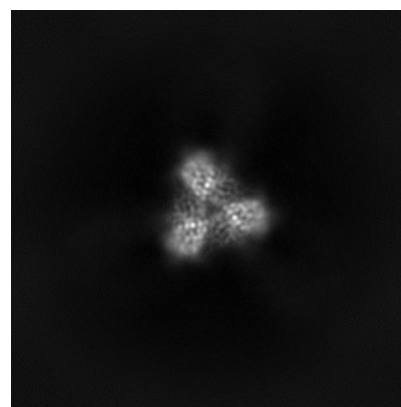
6.1.2 Raw map



X



Y

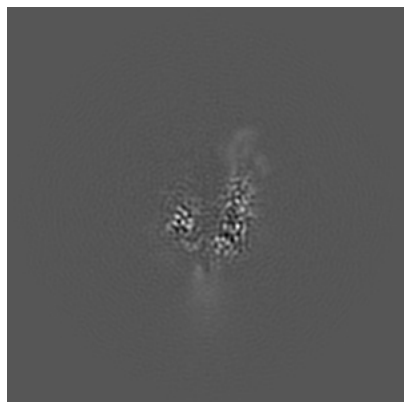


Z

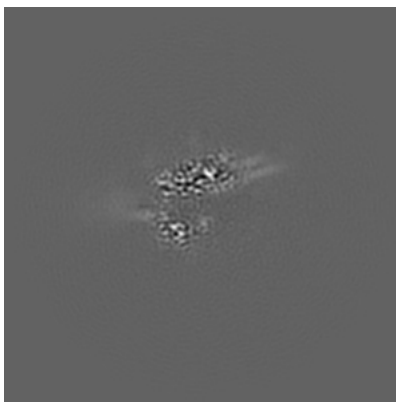
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

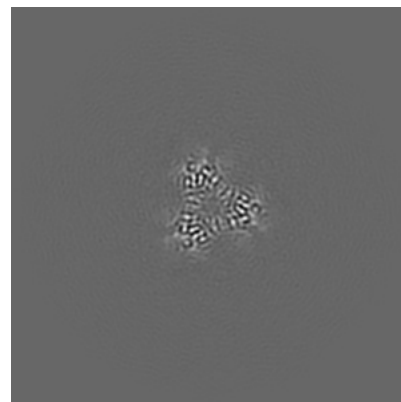
6.2.1 Primary map



X Index: 152

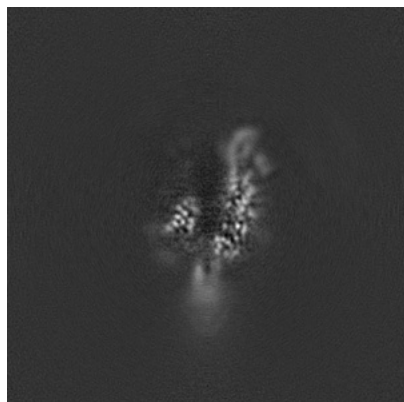


Y Index: 152

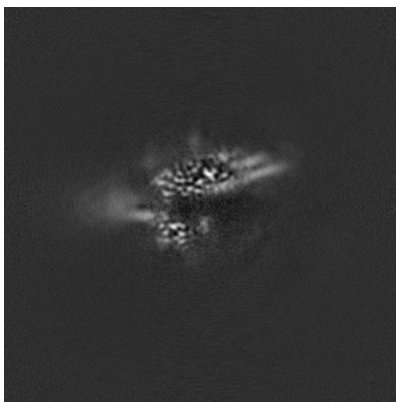


Z Index: 152

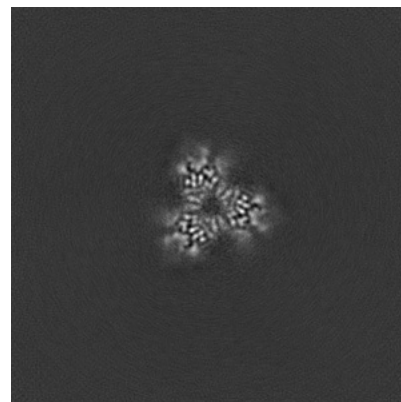
6.2.2 Raw map



X Index: 152



Y Index: 152

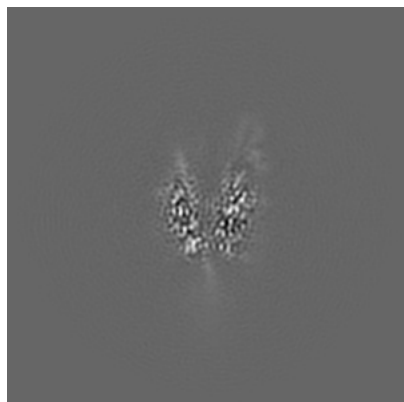


Z Index: 152

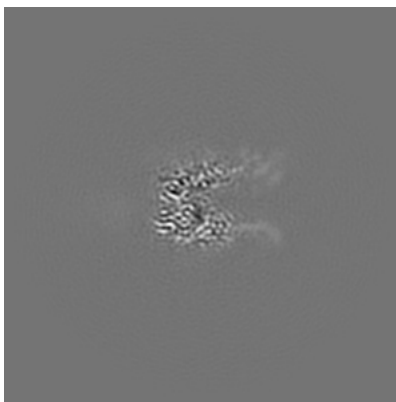
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

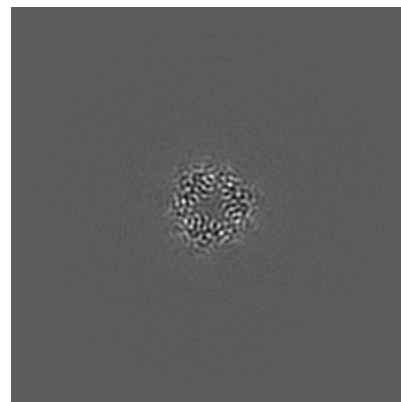
6.3.1 Primary map



X Index: 143

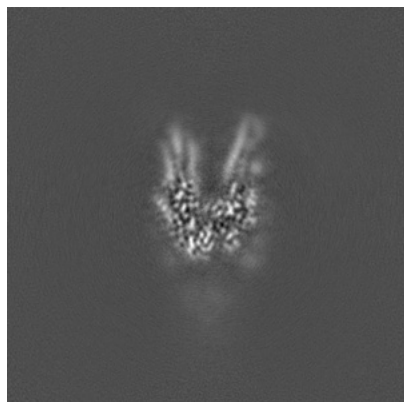


Y Index: 139

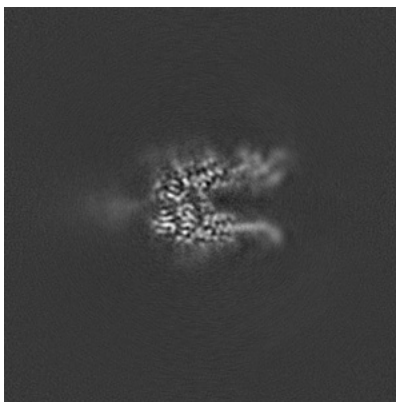


Z Index: 137

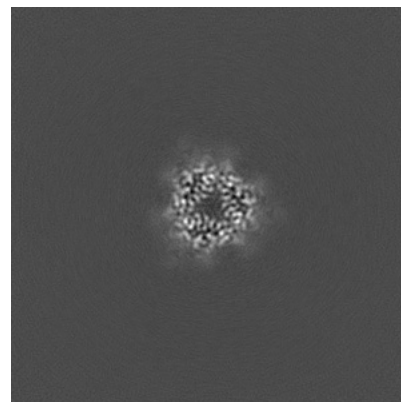
6.3.2 Raw map



X Index: 138



Y Index: 140



Z Index: 137

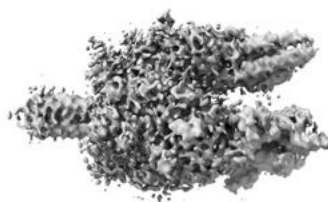
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

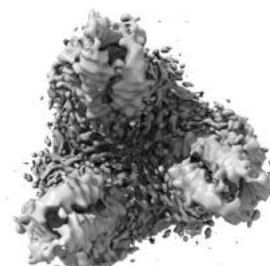
6.4.1 Primary map



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.

6.4.2 Raw map



X



Y



Z

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.

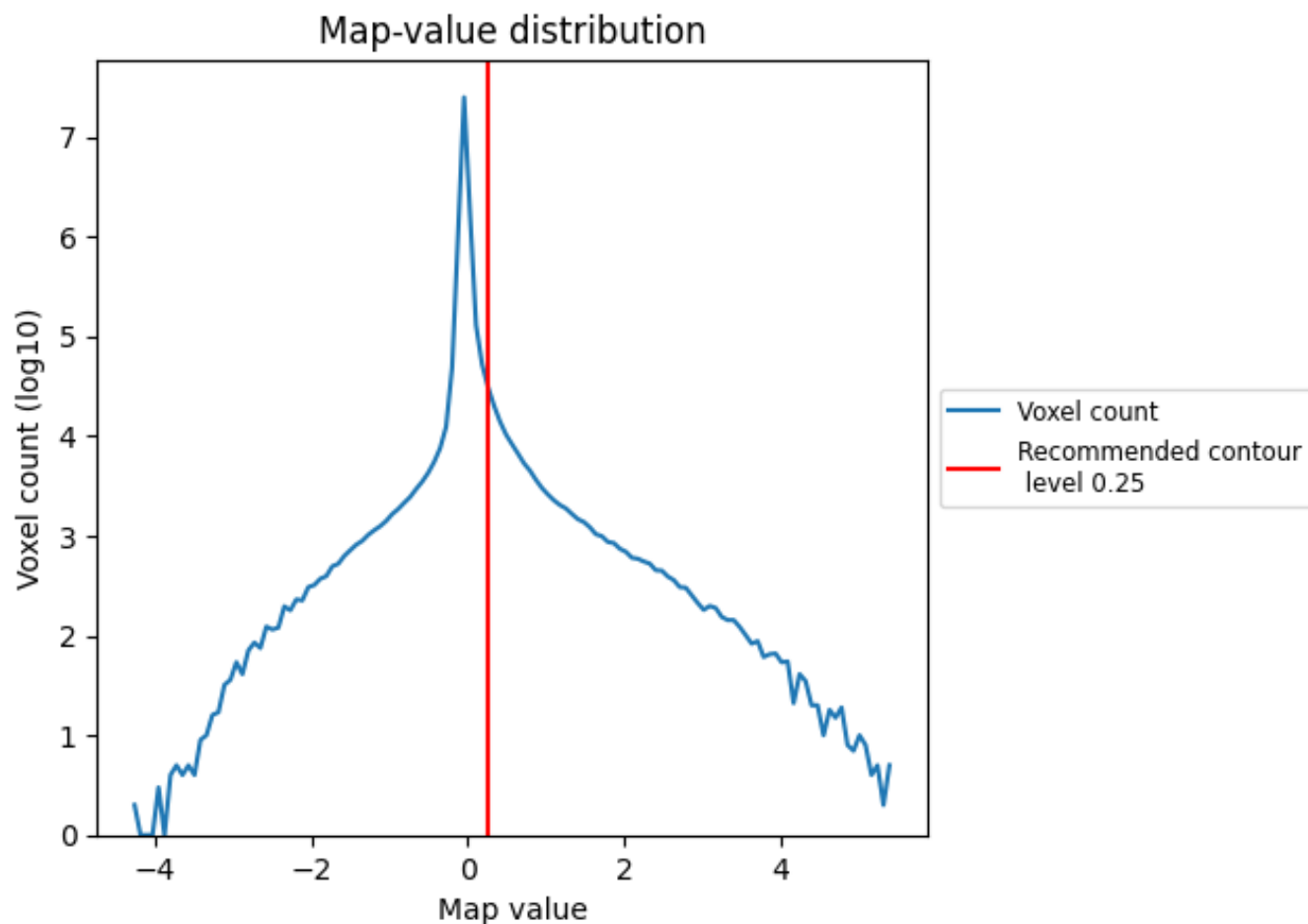
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

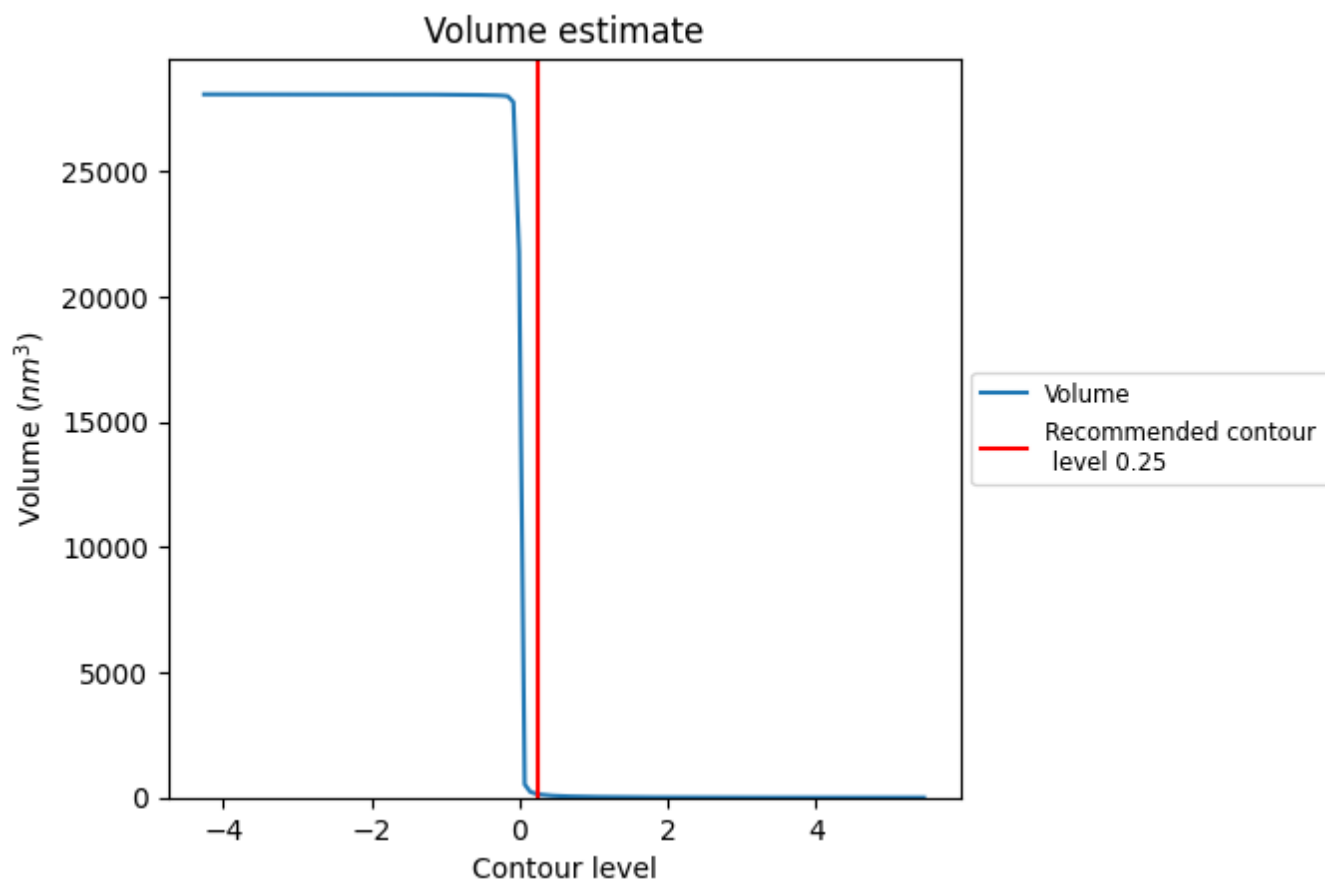
This section contains the results of statistical analysis of the map.

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.

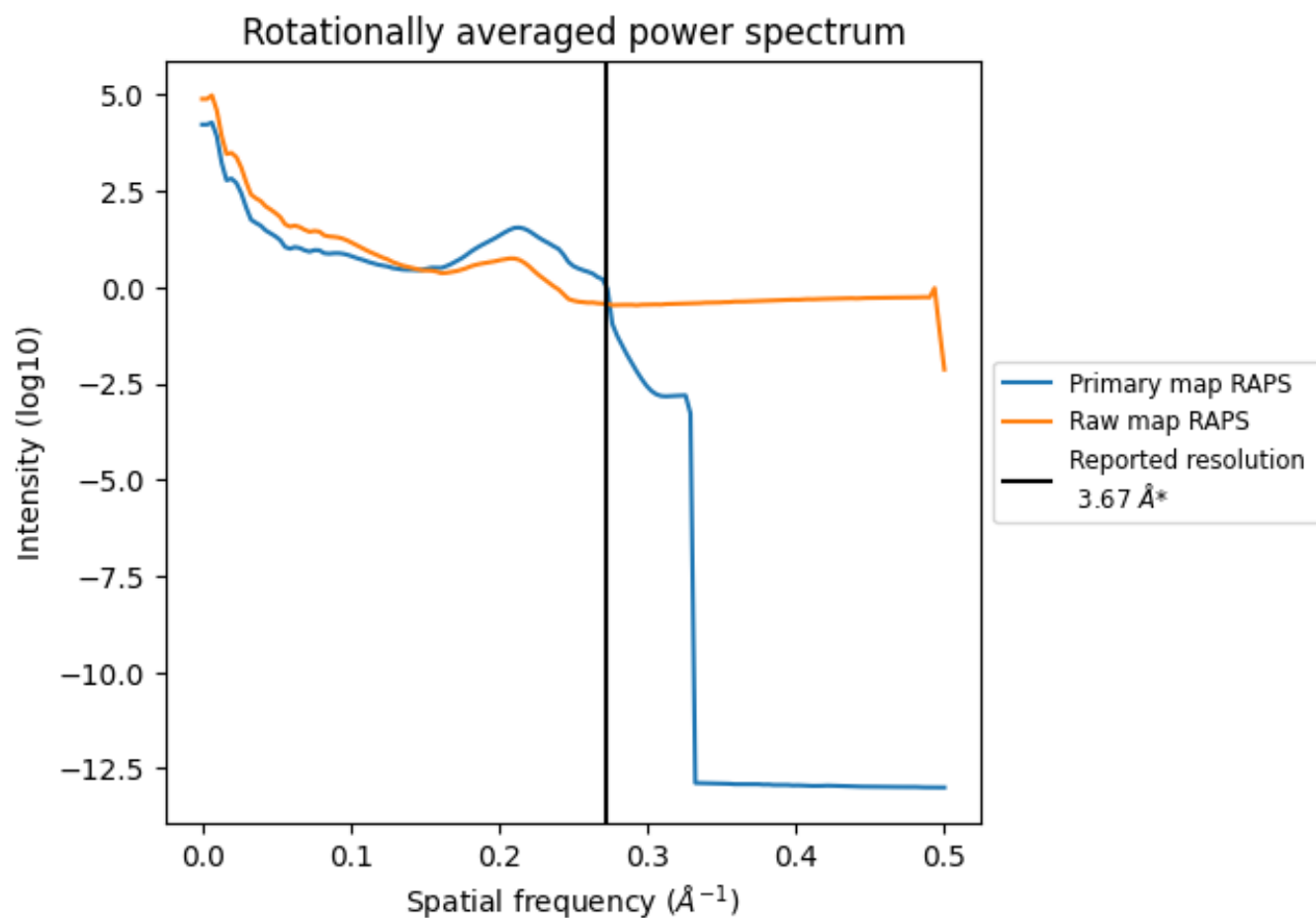
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 140 nm^3 ; this corresponds to an approximate mass of 127 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 ⓘ

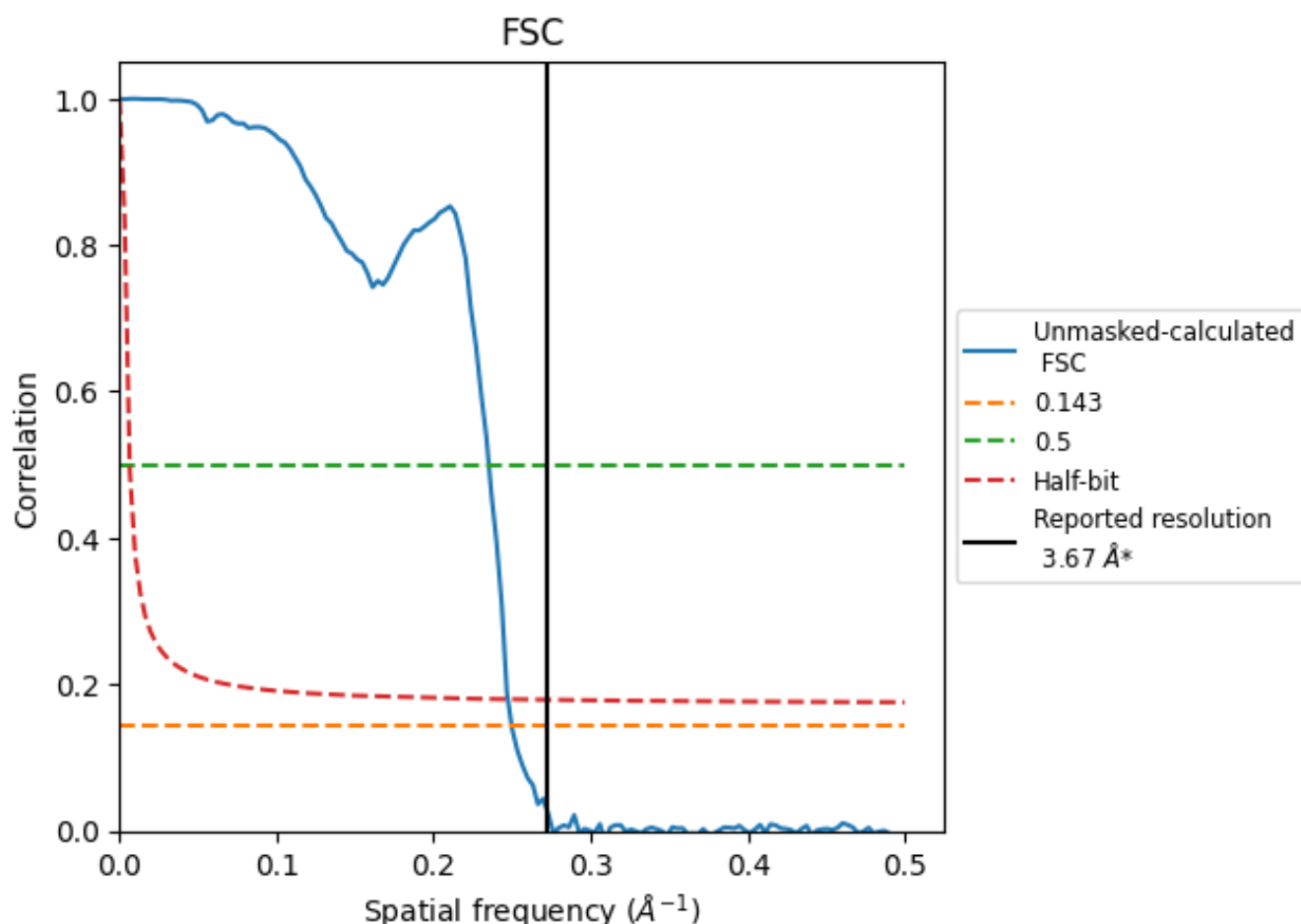


*Reported resolution corresponds to spatial frequency of 0.272 Å⁻¹

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 0.272 \AA^{-1}

8.2 Resolution estimates [i](#)

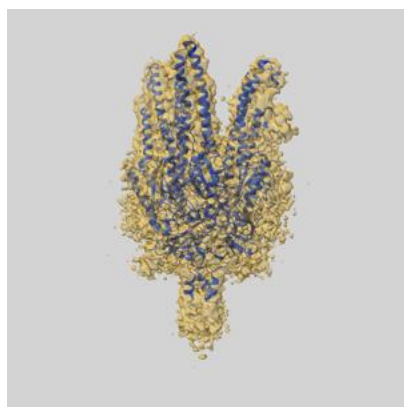
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.67	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.00	4.25	4.04

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

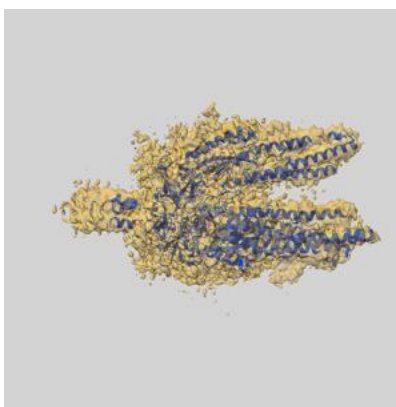
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-27779 and PDB model 8DYA. Per-residue inclusion information can be found in section 3 on page 13.

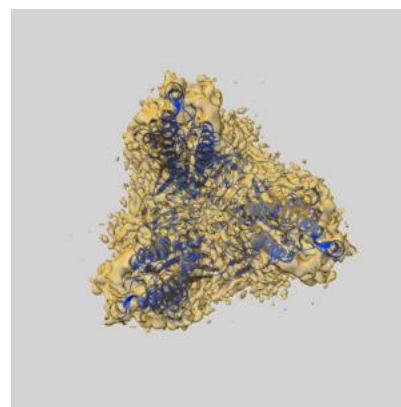
9.1 Map-model overlay [i](#)



X



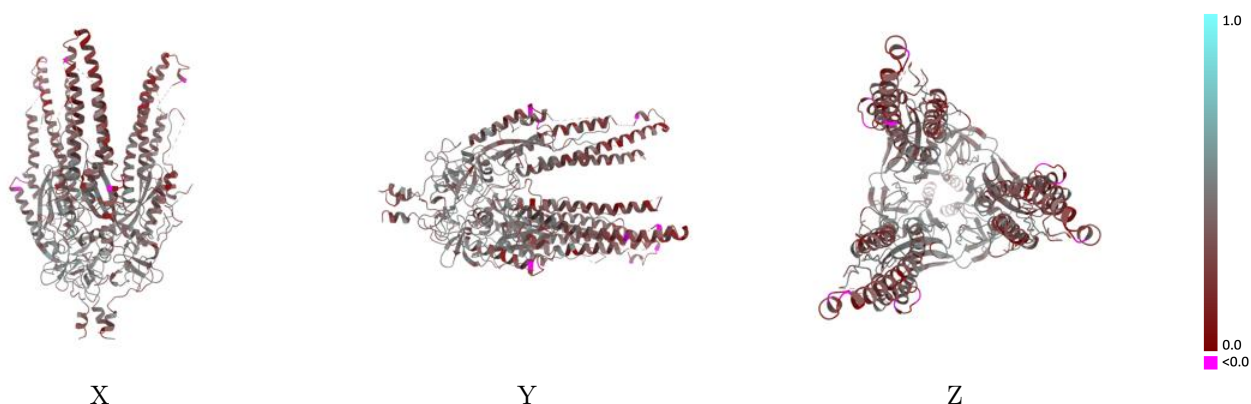
Y



Z

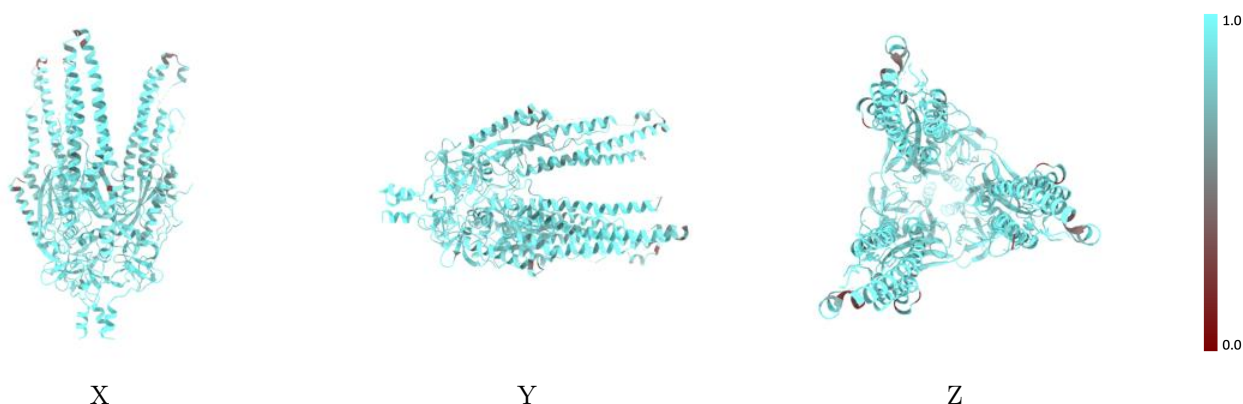
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



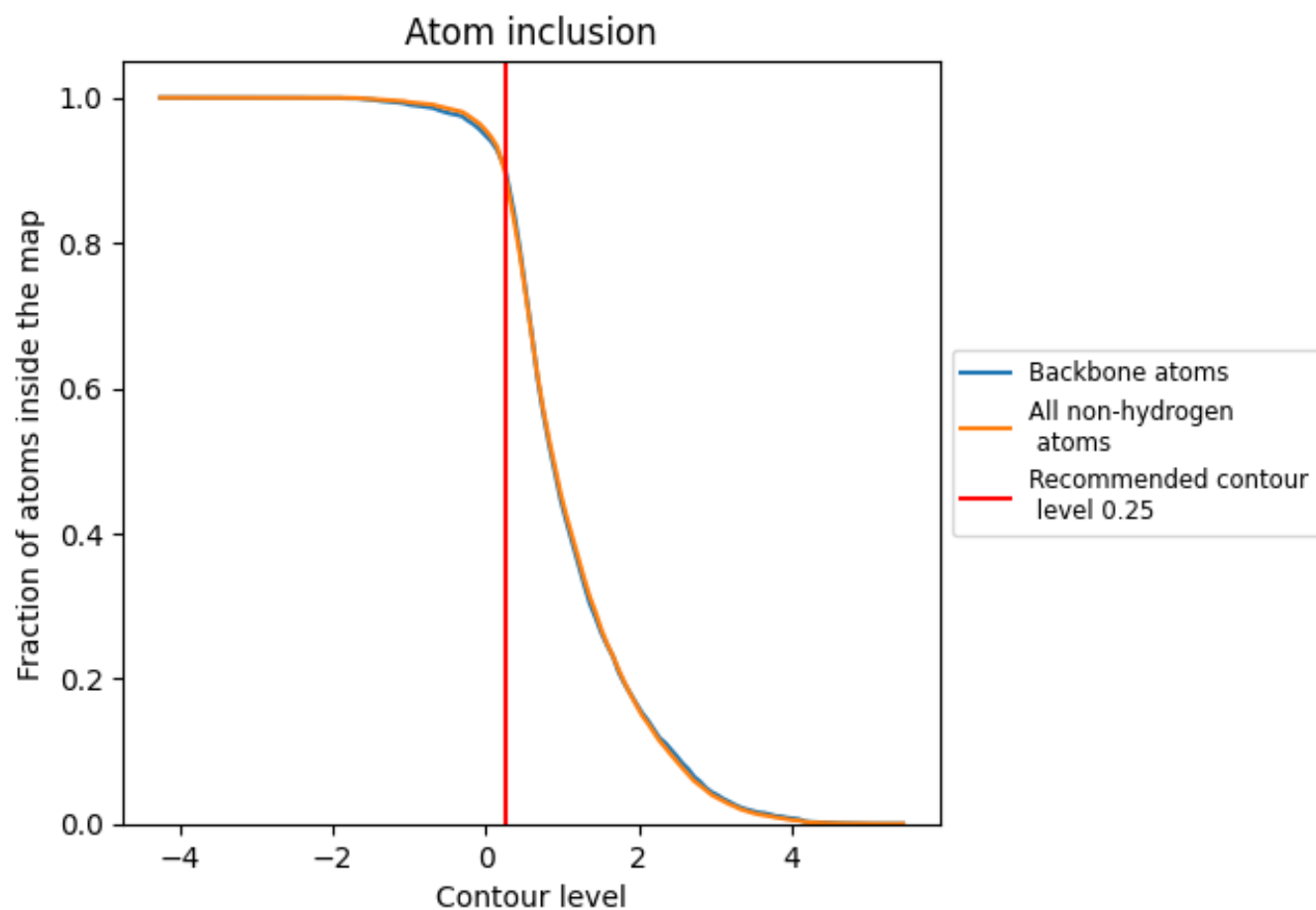
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 90% of all backbone atoms, 90% 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	<div></div> 0.8995	<div></div> 0.3820
A	<div></div> 0.9134	<div></div> 0.4050
B	<div></div> 0.8939	<div></div> 0.3730
C	<div></div> 0.8912	<div></div> 0.3680

