



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 05:55 PM UTC

PDB ID : 8WRM / pdb_00008wrn
EMDB ID : EMD-37781
Title : XBB.1.5 spike protein in complex with ACE2
Authors : Feng, L.L.; Feng, L.L.
Deposited on : 2023-10-15
Resolution : 4.34 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

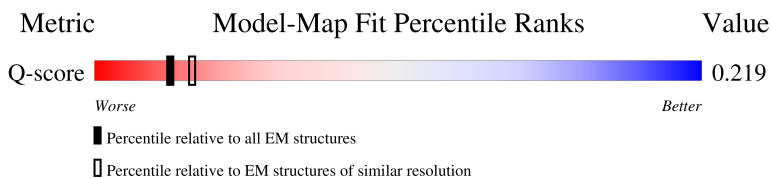
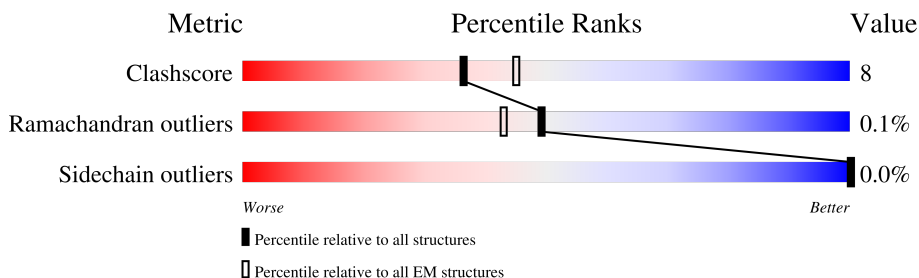
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.34 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	3836 (3.84 - 4.84)

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	C	1221	 8% 68% 20% 13%
1	F	1221	 8% 70% 17% 13%
1	G	1221	 30% 71% 16% 13%
2	D	594	 30% 82% 18%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 29931 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	F	1066	Total	C	N	O	S	0	0
			8360	5346	1396	1579	39		
1	G	1066	Total	C	N	O	S	0	0
			8359	5344	1396	1580	39		
1	C	1067	Total	C	N	O	S	0	0
			8367	5350	1397	1581	39		

There are 372 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	19	ILE	THR	variant	UNP P0DTC2
F	26	GLN	PRO	conflict	UNP P0DTC2
F	27	SER	ALA	conflict	UNP P0DTC2
F	83	ALA	VAL	variant	UNP P0DTC2
F	142	ASP	GLY	variant	UNP P0DTC2
F	146	GLN	HIS	variant	UNP P0DTC2
F	183	GLU	GLN	variant	UNP P0DTC2
F	213	GLU	VAL	variant	UNP P0DTC2
F	252	VAL	GLY	variant	UNP P0DTC2
F	339	HIS	GLY	variant	UNP P0DTC2
F	346	THR	ARG	variant	UNP P0DTC2
F	368	ILE	LEU	variant	UNP P0DTC2
F	371	PHE	SER	variant	UNP P0DTC2
F	373	PRO	SER	variant	UNP P0DTC2
F	375	PHE	SER	variant	UNP P0DTC2
F	376	ALA	THR	variant	UNP P0DTC2
F	405	ASN	ASP	variant	UNP P0DTC2
F	408	SER	ARG	variant	UNP P0DTC2
F	417	ASN	LYS	variant	UNP P0DTC2
F	440	LYS	ASN	variant	UNP P0DTC2
F	445	PRO	VAL	variant	UNP P0DTC2
F	446	SER	GLY	variant	UNP P0DTC2
F	460	LYS	ASN	variant	UNP P0DTC2
F	477	ASN	SER	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
F	478	LYS	THR	variant	UNP P0DTC2
F	484	ALA	GLU	variant	UNP P0DTC2
F	486	PRO	PHE	variant	UNP P0DTC2
F	490	SER	PHE	variant	UNP P0DTC2
F	498	ARG	GLN	variant	UNP P0DTC2
F	501	TYR	ASN	variant	UNP P0DTC2
F	505	HIS	TYR	variant	UNP P0DTC2
F	614	GLY	ASP	variant	UNP P0DTC2
F	655	TYR	HIS	variant	UNP P0DTC2
F	764	LYS	ASN	variant	UNP P0DTC2
F	796	TYR	ASP	variant	UNP P0DTC2
F	817	PRO	PHE	conflict	UNP P0DTC2
F	892	PRO	ALA	conflict	UNP P0DTC2
F	899	PRO	ALA	conflict	UNP P0DTC2
F	942	PRO	ALA	conflict	UNP P0DTC2
F	954	HIS	GLN	variant	UNP P0DTC2
F	969	LYS	ASN	variant	UNP P0DTC2
F	986	PRO	LYS	variant	UNP P0DTC2
F	987	PRO	VAL	variant	UNP P0DTC2
F	1141	GLY	-	expression tag	UNP P0DTC2
F	1142	GLY	-	expression tag	UNP P0DTC2
F	1143	SER	-	expression tag	UNP P0DTC2
F	1144	GLY	-	expression tag	UNP P0DTC2
F	1145	GLY	-	expression tag	UNP P0DTC2
F	1146	SER	-	expression tag	UNP P0DTC2
F	1147	TYR	-	expression tag	UNP P0DTC2
F	1148	ILE	-	expression tag	UNP P0DTC2
F	1149	PRO	-	expression tag	UNP P0DTC2
F	1150	GLU	-	expression tag	UNP P0DTC2
F	1151	ALA	-	expression tag	UNP P0DTC2
F	1152	PRO	-	expression tag	UNP P0DTC2
F	1153	ARG	-	expression tag	UNP P0DTC2
F	1154	ASP	-	expression tag	UNP P0DTC2
F	1155	GLY	-	expression tag	UNP P0DTC2
F	1156	GLN	-	expression tag	UNP P0DTC2
F	1157	ALA	-	expression tag	UNP P0DTC2
F	1158	TYR	-	expression tag	UNP P0DTC2
F	1159	VAL	-	expression tag	UNP P0DTC2
F	1160	ARG	-	expression tag	UNP P0DTC2
F	1161	LYS	-	expression tag	UNP P0DTC2
F	1162	ASP	-	expression tag	UNP P0DTC2
F	1163	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
F	1164	GLU	-	expression tag	UNP P0DTC2
F	1165	TRP	-	expression tag	UNP P0DTC2
F	1166	VAL	-	expression tag	UNP P0DTC2
F	1167	LEU	-	expression tag	UNP P0DTC2
F	1168	LEU	-	expression tag	UNP P0DTC2
F	1169	SER	-	expression tag	UNP P0DTC2
F	1170	THR	-	expression tag	UNP P0DTC2
F	1171	PHE	-	expression tag	UNP P0DTC2
F	1172	LEU	-	expression tag	UNP P0DTC2
F	1173	GLY	-	expression tag	UNP P0DTC2
F	1174	ARG	-	expression tag	UNP P0DTC2
F	1175	SER	-	expression tag	UNP P0DTC2
F	1176	LEU	-	expression tag	UNP P0DTC2
F	1177	GLU	-	expression tag	UNP P0DTC2
F	1178	VAL	-	expression tag	UNP P0DTC2
F	1179	LEU	-	expression tag	UNP P0DTC2
F	1180	PHE	-	expression tag	UNP P0DTC2
F	1181	GLN	-	expression tag	UNP P0DTC2
F	1182	GLY	-	expression tag	UNP P0DTC2
F	1183	PRO	-	expression tag	UNP P0DTC2
F	1184	GLY	-	expression tag	UNP P0DTC2
F	1185	TRP	-	expression tag	UNP P0DTC2
F	1186	SER	-	expression tag	UNP P0DTC2
F	1187	HIS	-	expression tag	UNP P0DTC2
F	1188	PRO	-	expression tag	UNP P0DTC2
F	1189	GLN	-	expression tag	UNP P0DTC2
F	1190	PHE	-	expression tag	UNP P0DTC2
F	1191	GLU	-	expression tag	UNP P0DTC2
F	1192	LYS	-	expression tag	UNP P0DTC2
F	1193	GLY	-	expression tag	UNP P0DTC2
F	1194	GLY	-	expression tag	UNP P0DTC2
F	1195	GLY	-	expression tag	UNP P0DTC2
F	1196	SER	-	expression tag	UNP P0DTC2
F	1197	GLY	-	expression tag	UNP P0DTC2
F	1198	GLY	-	expression tag	UNP P0DTC2
F	1199	GLY	-	expression tag	UNP P0DTC2
F	1200	SER	-	expression tag	UNP P0DTC2
F	1201	GLY	-	expression tag	UNP P0DTC2
F	1202	GLY	-	expression tag	UNP P0DTC2
F	1203	SER	-	expression tag	UNP P0DTC2
F	1204	SER	-	expression tag	UNP P0DTC2
F	1205	ALA	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
F	1206	TRP	-	expression tag	UNP P0DTC2
F	1207	SER	-	expression tag	UNP P0DTC2
F	1208	HIS	-	expression tag	UNP P0DTC2
F	1209	PRO	-	expression tag	UNP P0DTC2
F	1210	GLN	-	expression tag	UNP P0DTC2
F	1211	PHE	-	expression tag	UNP P0DTC2
F	1212	GLU	-	expression tag	UNP P0DTC2
F	1213	LYS	-	expression tag	UNP P0DTC2
F	1214	HIS	-	expression tag	UNP P0DTC2
F	1215	HIS	-	expression tag	UNP P0DTC2
F	1216	HIS	-	expression tag	UNP P0DTC2
F	1217	HIS	-	expression tag	UNP P0DTC2
F	1218	HIS	-	expression tag	UNP P0DTC2
F	1219	HIS	-	expression tag	UNP P0DTC2
F	1220	HIS	-	expression tag	UNP P0DTC2
F	1221	HIS	-	expression tag	UNP P0DTC2
G	19	ILE	THR	variant	UNP P0DTC2
G	26	GLN	PRO	conflict	UNP P0DTC2
G	27	SER	ALA	conflict	UNP P0DTC2
G	83	ALA	VAL	variant	UNP P0DTC2
G	142	ASP	GLY	variant	UNP P0DTC2
G	146	GLN	HIS	variant	UNP P0DTC2
G	183	GLU	GLN	variant	UNP P0DTC2
G	213	GLU	VAL	variant	UNP P0DTC2
G	252	VAL	GLY	variant	UNP P0DTC2
G	339	HIS	GLY	variant	UNP P0DTC2
G	346	THR	ARG	variant	UNP P0DTC2
G	368	ILE	LEU	variant	UNP P0DTC2
G	371	PHE	SER	variant	UNP P0DTC2
G	373	PRO	SER	variant	UNP P0DTC2
G	375	PHE	SER	variant	UNP P0DTC2
G	376	ALA	THR	variant	UNP P0DTC2
G	405	ASN	ASP	variant	UNP P0DTC2
G	408	SER	ARG	variant	UNP P0DTC2
G	417	ASN	LYS	variant	UNP P0DTC2
G	440	LYS	ASN	variant	UNP P0DTC2
G	445	PRO	VAL	variant	UNP P0DTC2
G	446	SER	GLY	variant	UNP P0DTC2
G	460	LYS	ASN	variant	UNP P0DTC2
G	477	ASN	SER	variant	UNP P0DTC2
G	478	LYS	THR	variant	UNP P0DTC2
G	484	ALA	GLU	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
G	486	PRO	PHE	variant	UNP P0DTC2
G	490	SER	PHE	variant	UNP P0DTC2
G	498	ARG	GLN	variant	UNP P0DTC2
G	501	TYR	ASN	variant	UNP P0DTC2
G	505	HIS	TYR	variant	UNP P0DTC2
G	614	GLY	ASP	variant	UNP P0DTC2
G	655	TYR	HIS	variant	UNP P0DTC2
G	764	LYS	ASN	variant	UNP P0DTC2
G	796	TYR	ASP	variant	UNP P0DTC2
G	817	PRO	PHE	conflict	UNP P0DTC2
G	892	PRO	ALA	conflict	UNP P0DTC2
G	899	PRO	ALA	conflict	UNP P0DTC2
G	942	PRO	ALA	conflict	UNP P0DTC2
G	954	HIS	GLN	variant	UNP P0DTC2
G	969	LYS	ASN	variant	UNP P0DTC2
G	986	PRO	LYS	variant	UNP P0DTC2
G	987	PRO	VAL	variant	UNP P0DTC2
G	1141	GLY	-	expression tag	UNP P0DTC2
G	1142	GLY	-	expression tag	UNP P0DTC2
G	1143	SER	-	expression tag	UNP P0DTC2
G	1144	GLY	-	expression tag	UNP P0DTC2
G	1145	GLY	-	expression tag	UNP P0DTC2
G	1146	SER	-	expression tag	UNP P0DTC2
G	1147	TYR	-	expression tag	UNP P0DTC2
G	1148	ILE	-	expression tag	UNP P0DTC2
G	1149	PRO	-	expression tag	UNP P0DTC2
G	1150	GLU	-	expression tag	UNP P0DTC2
G	1151	ALA	-	expression tag	UNP P0DTC2
G	1152	PRO	-	expression tag	UNP P0DTC2
G	1153	ARG	-	expression tag	UNP P0DTC2
G	1154	ASP	-	expression tag	UNP P0DTC2
G	1155	GLY	-	expression tag	UNP P0DTC2
G	1156	GLN	-	expression tag	UNP P0DTC2
G	1157	ALA	-	expression tag	UNP P0DTC2
G	1158	TYR	-	expression tag	UNP P0DTC2
G	1159	VAL	-	expression tag	UNP P0DTC2
G	1160	ARG	-	expression tag	UNP P0DTC2
G	1161	LYS	-	expression tag	UNP P0DTC2
G	1162	ASP	-	expression tag	UNP P0DTC2
G	1163	GLY	-	expression tag	UNP P0DTC2
G	1164	GLU	-	expression tag	UNP P0DTC2
G	1165	TRP	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
G	1166	VAL	-	expression tag	UNP P0DTC2
G	1167	LEU	-	expression tag	UNP P0DTC2
G	1168	LEU	-	expression tag	UNP P0DTC2
G	1169	SER	-	expression tag	UNP P0DTC2
G	1170	THR	-	expression tag	UNP P0DTC2
G	1171	PHE	-	expression tag	UNP P0DTC2
G	1172	LEU	-	expression tag	UNP P0DTC2
G	1173	GLY	-	expression tag	UNP P0DTC2
G	1174	ARG	-	expression tag	UNP P0DTC2
G	1175	SER	-	expression tag	UNP P0DTC2
G	1176	LEU	-	expression tag	UNP P0DTC2
G	1177	GLU	-	expression tag	UNP P0DTC2
G	1178	VAL	-	expression tag	UNP P0DTC2
G	1179	LEU	-	expression tag	UNP P0DTC2
G	1180	PHE	-	expression tag	UNP P0DTC2
G	1181	GLN	-	expression tag	UNP P0DTC2
G	1182	GLY	-	expression tag	UNP P0DTC2
G	1183	PRO	-	expression tag	UNP P0DTC2
G	1184	GLY	-	expression tag	UNP P0DTC2
G	1185	TRP	-	expression tag	UNP P0DTC2
G	1186	SER	-	expression tag	UNP P0DTC2
G	1187	HIS	-	expression tag	UNP P0DTC2
G	1188	PRO	-	expression tag	UNP P0DTC2
G	1189	GLN	-	expression tag	UNP P0DTC2
G	1190	PHE	-	expression tag	UNP P0DTC2
G	1191	GLU	-	expression tag	UNP P0DTC2
G	1192	LYS	-	expression tag	UNP P0DTC2
G	1193	GLY	-	expression tag	UNP P0DTC2
G	1194	GLY	-	expression tag	UNP P0DTC2
G	1195	GLY	-	expression tag	UNP P0DTC2
G	1196	SER	-	expression tag	UNP P0DTC2
G	1197	GLY	-	expression tag	UNP P0DTC2
G	1198	GLY	-	expression tag	UNP P0DTC2
G	1199	GLY	-	expression tag	UNP P0DTC2
G	1200	SER	-	expression tag	UNP P0DTC2
G	1201	GLY	-	expression tag	UNP P0DTC2
G	1202	GLY	-	expression tag	UNP P0DTC2
G	1203	SER	-	expression tag	UNP P0DTC2
G	1204	SER	-	expression tag	UNP P0DTC2
G	1205	ALA	-	expression tag	UNP P0DTC2
G	1206	TRP	-	expression tag	UNP P0DTC2
G	1207	SER	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
G	1208	HIS	-	expression tag	UNP P0DTC2
G	1209	PRO	-	expression tag	UNP P0DTC2
G	1210	GLN	-	expression tag	UNP P0DTC2
G	1211	PHE	-	expression tag	UNP P0DTC2
G	1212	GLU	-	expression tag	UNP P0DTC2
G	1213	LYS	-	expression tag	UNP P0DTC2
G	1214	HIS	-	expression tag	UNP P0DTC2
G	1215	HIS	-	expression tag	UNP P0DTC2
G	1216	HIS	-	expression tag	UNP P0DTC2
G	1217	HIS	-	expression tag	UNP P0DTC2
G	1218	HIS	-	expression tag	UNP P0DTC2
G	1219	HIS	-	expression tag	UNP P0DTC2
G	1220	HIS	-	expression tag	UNP P0DTC2
G	1221	HIS	-	expression tag	UNP P0DTC2
C	19	ILE	THR	variant	UNP P0DTC2
C	26	GLN	PRO	conflict	UNP P0DTC2
C	27	SER	ALA	conflict	UNP P0DTC2
C	83	ALA	VAL	variant	UNP P0DTC2
C	142	ASP	GLY	variant	UNP P0DTC2
C	146	GLN	HIS	variant	UNP P0DTC2
C	183	GLU	GLN	variant	UNP P0DTC2
C	213	GLU	VAL	variant	UNP P0DTC2
C	252	VAL	GLY	variant	UNP P0DTC2
C	339	HIS	GLY	variant	UNP P0DTC2
C	346	THR	ARG	variant	UNP P0DTC2
C	368	ILE	LEU	variant	UNP P0DTC2
C	371	PHE	SER	variant	UNP P0DTC2
C	373	PRO	SER	variant	UNP P0DTC2
C	375	PHE	SER	variant	UNP P0DTC2
C	376	ALA	THR	variant	UNP P0DTC2
C	405	ASN	ASP	variant	UNP P0DTC2
C	408	SER	ARG	variant	UNP P0DTC2
C	417	ASN	LYS	variant	UNP P0DTC2
C	440	LYS	ASN	variant	UNP P0DTC2
C	445	PRO	VAL	variant	UNP P0DTC2
C	446	SER	GLY	variant	UNP P0DTC2
C	460	LYS	ASN	variant	UNP P0DTC2
C	477	ASN	SER	variant	UNP P0DTC2
C	478	LYS	THR	variant	UNP P0DTC2
C	484	ALA	GLU	variant	UNP P0DTC2
C	486	PRO	PHE	variant	UNP P0DTC2
C	490	SER	PHE	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	498	ARG	GLN	variant	UNP P0DTC2
C	501	TYR	ASN	variant	UNP P0DTC2
C	505	HIS	TYR	variant	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	655	TYR	HIS	variant	UNP P0DTC2
C	764	LYS	ASN	variant	UNP P0DTC2
C	796	TYR	ASP	variant	UNP P0DTC2
C	817	PRO	PHE	conflict	UNP P0DTC2
C	892	PRO	ALA	conflict	UNP P0DTC2
C	899	PRO	ALA	conflict	UNP P0DTC2
C	942	PRO	ALA	conflict	UNP P0DTC2
C	954	HIS	GLN	variant	UNP P0DTC2
C	969	LYS	ASN	variant	UNP P0DTC2
C	986	PRO	LYS	variant	UNP P0DTC2
C	987	PRO	VAL	variant	UNP P0DTC2
C	1141	GLY	-	expression tag	UNP P0DTC2
C	1142	GLY	-	expression tag	UNP P0DTC2
C	1143	SER	-	expression tag	UNP P0DTC2
C	1144	GLY	-	expression tag	UNP P0DTC2
C	1145	GLY	-	expression tag	UNP P0DTC2
C	1146	SER	-	expression tag	UNP P0DTC2
C	1147	TYR	-	expression tag	UNP P0DTC2
C	1148	ILE	-	expression tag	UNP P0DTC2
C	1149	PRO	-	expression tag	UNP P0DTC2
C	1150	GLU	-	expression tag	UNP P0DTC2
C	1151	ALA	-	expression tag	UNP P0DTC2
C	1152	PRO	-	expression tag	UNP P0DTC2
C	1153	ARG	-	expression tag	UNP P0DTC2
C	1154	ASP	-	expression tag	UNP P0DTC2
C	1155	GLY	-	expression tag	UNP P0DTC2
C	1156	GLN	-	expression tag	UNP P0DTC2
C	1157	ALA	-	expression tag	UNP P0DTC2
C	1158	TYR	-	expression tag	UNP P0DTC2
C	1159	VAL	-	expression tag	UNP P0DTC2
C	1160	ARG	-	expression tag	UNP P0DTC2
C	1161	LYS	-	expression tag	UNP P0DTC2
C	1162	ASP	-	expression tag	UNP P0DTC2
C	1163	GLY	-	expression tag	UNP P0DTC2
C	1164	GLU	-	expression tag	UNP P0DTC2
C	1165	TRP	-	expression tag	UNP P0DTC2
C	1166	VAL	-	expression tag	UNP P0DTC2
C	1167	LEU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1168	LEU	-	expression tag	UNP P0DTC2
C	1169	SER	-	expression tag	UNP P0DTC2
C	1170	THR	-	expression tag	UNP P0DTC2
C	1171	PHE	-	expression tag	UNP P0DTC2
C	1172	LEU	-	expression tag	UNP P0DTC2
C	1173	GLY	-	expression tag	UNP P0DTC2
C	1174	ARG	-	expression tag	UNP P0DTC2
C	1175	SER	-	expression tag	UNP P0DTC2
C	1176	LEU	-	expression tag	UNP P0DTC2
C	1177	GLU	-	expression tag	UNP P0DTC2
C	1178	VAL	-	expression tag	UNP P0DTC2
C	1179	LEU	-	expression tag	UNP P0DTC2
C	1180	PHE	-	expression tag	UNP P0DTC2
C	1181	GLN	-	expression tag	UNP P0DTC2
C	1182	GLY	-	expression tag	UNP P0DTC2
C	1183	PRO	-	expression tag	UNP P0DTC2
C	1184	GLY	-	expression tag	UNP P0DTC2
C	1185	TRP	-	expression tag	UNP P0DTC2
C	1186	SER	-	expression tag	UNP P0DTC2
C	1187	HIS	-	expression tag	UNP P0DTC2
C	1188	PRO	-	expression tag	UNP P0DTC2
C	1189	GLN	-	expression tag	UNP P0DTC2
C	1190	PHE	-	expression tag	UNP P0DTC2
C	1191	GLU	-	expression tag	UNP P0DTC2
C	1192	LYS	-	expression tag	UNP P0DTC2
C	1193	GLY	-	expression tag	UNP P0DTC2
C	1194	GLY	-	expression tag	UNP P0DTC2
C	1195	GLY	-	expression tag	UNP P0DTC2
C	1196	SER	-	expression tag	UNP P0DTC2
C	1197	GLY	-	expression tag	UNP P0DTC2
C	1198	GLY	-	expression tag	UNP P0DTC2
C	1199	GLY	-	expression tag	UNP P0DTC2
C	1200	SER	-	expression tag	UNP P0DTC2
C	1201	GLY	-	expression tag	UNP P0DTC2
C	1202	GLY	-	expression tag	UNP P0DTC2
C	1203	SER	-	expression tag	UNP P0DTC2
C	1204	SER	-	expression tag	UNP P0DTC2
C	1205	ALA	-	expression tag	UNP P0DTC2
C	1206	TRP	-	expression tag	UNP P0DTC2
C	1207	SER	-	expression tag	UNP P0DTC2
C	1208	HIS	-	expression tag	UNP P0DTC2
C	1209	PRO	-	expression tag	UNP P0DTC2

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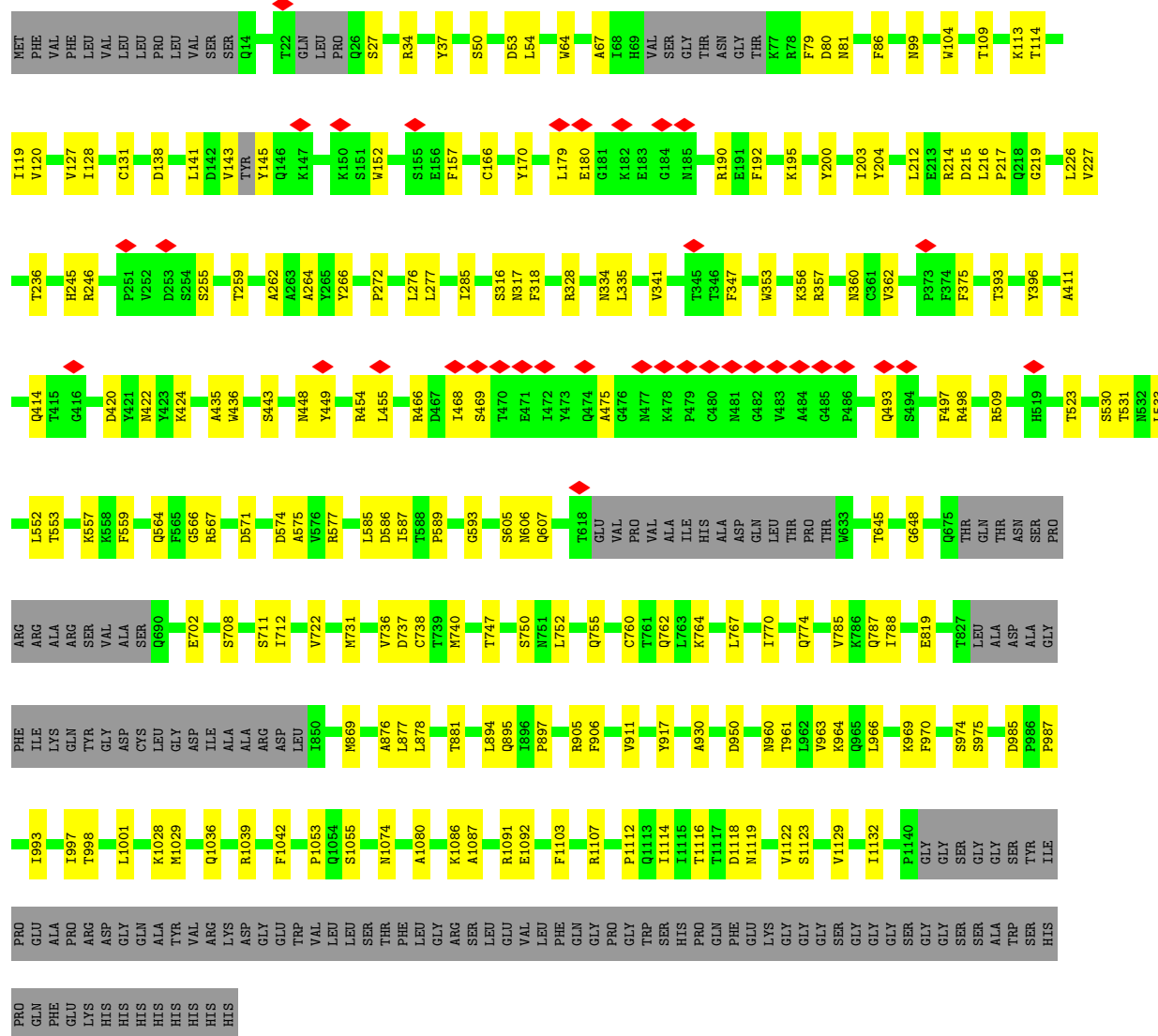
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	1210	GLN	-	expression tag	UNP P0DTC2
C	1211	PHE	-	expression tag	UNP P0DTC2
C	1212	GLU	-	expression tag	UNP P0DTC2
C	1213	LYS	-	expression tag	UNP P0DTC2
C	1214	HIS	-	expression tag	UNP P0DTC2
C	1215	HIS	-	expression tag	UNP P0DTC2
C	1216	HIS	-	expression tag	UNP P0DTC2
C	1217	HIS	-	expression tag	UNP P0DTC2
C	1218	HIS	-	expression tag	UNP P0DTC2
C	1219	HIS	-	expression tag	UNP P0DTC2
C	1220	HIS	-	expression tag	UNP P0DTC2
C	1221	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called Processed angiotensin-converting enzyme 2.

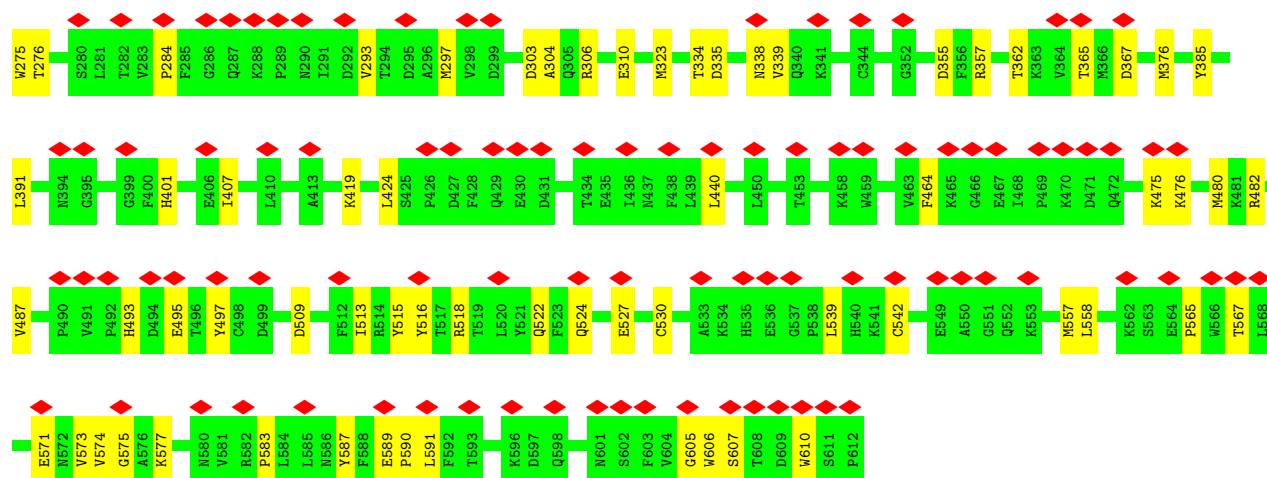
Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	594	Total	C	N	O	S	0	0
			4845	3099	803	914	29		

- 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	136454	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	52	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	1.138	Depositor
Minimum map value	-0.420	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.043	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	374.4, 374.4, 374.4	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	C	0.19	0/8568	0.53	3/11658 (0.0%)
1	F	0.18	0/8561	0.49	1/11648 (0.0%)
1	G	0.18	0/8560	0.49	0/11647
2	D	0.20	0/4981	0.52	0/6767
All	All	0.19	0/30670	0.51	4/41720 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	559	PHE	CB-CA-C	-6.44	108.12	115.79
1	C	909	ILE	N-CA-C	-6.26	106.41	112.29
1	C	773	GLU	N-CA-CB	5.47	119.32	110.40
1	C	986	PRO	N-CA-C	5.33	117.21	110.70

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	C	8367	0	8181	151	0
1	F	8360	0	8174	134	0
1	G	8359	0	8168	125	0
2	D	4845	0	4625	62	0
All	All	29931	0	29148	452	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 8.

The worst 5 of 452 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:F:431:GLY:HA3	1:F:513:LEU:O	1.69	0.93
1:C:431:GLY:HA3	1:C:513:LEU:O	1.73	0.88
1:C:81:ASN:HB3	1:C:138:ASP:HB3	1.71	0.72
1:F:1052:PHE:HB2	1:F:1063:LEU:HB2	1.72	0.72
1:G:80:ASP:H	1:G:262:ALA:HB2	1.55	0.71

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	C	1053/1221 (86%)	947 (90%)	106 (10%)	0	100	100
1	F	1052/1221 (86%)	959 (91%)	92 (9%)	1 (0%)	48	83
1	G	1052/1221 (86%)	960 (91%)	91 (9%)	1 (0%)	48	83
2	D	592/594 (100%)	565 (95%)	26 (4%)	1 (0%)	43	77
All	All	3749/4257 (88%)	3431 (92%)	315 (8%)	3 (0%)	49	83

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	303	ASP
1	F	248	TYR
1	G	443	SER

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	C	935/1056 (88%)	935 (100%)	0	100	100
1	F	934/1056 (88%)	934 (100%)	0	100	100
1	G	934/1056 (88%)	933 (100%)	1 (0%)	88	88
2	D	525/525 (100%)	525 (100%)	0	100	100
All	All	3328/3693 (90%)	3327 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	895	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	774	GLN
2	D	287	GLN
1	G	1108	ASN
1	C	1101	HIS
1	G	1048	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

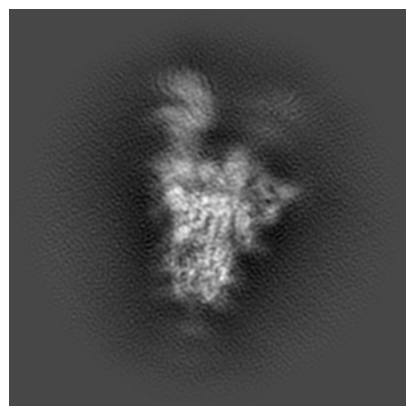
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37781. These allow visual inspection of the internal detail of the map and identification of artifacts.

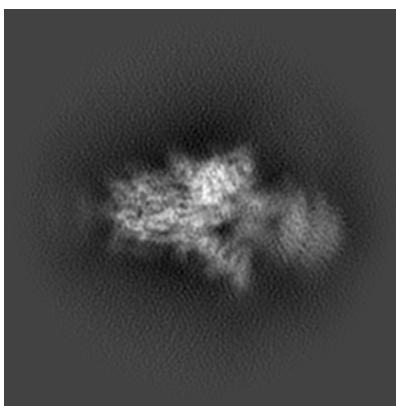
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

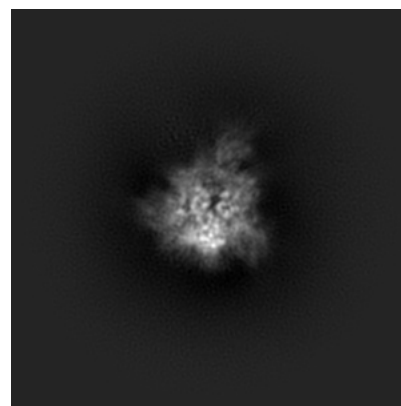
6.1.1 Primary map



X

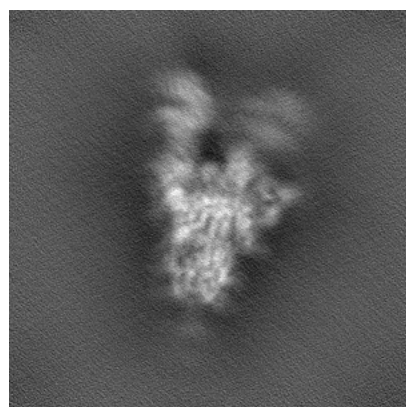


Y

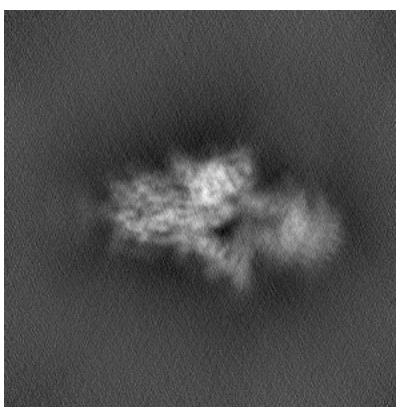


Z

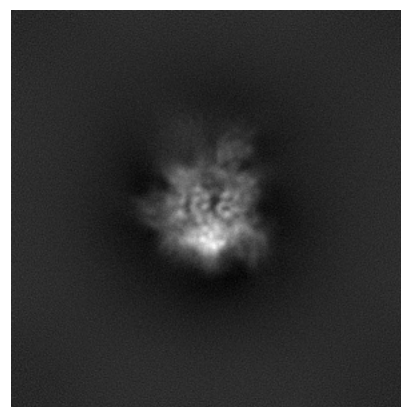
6.1.2 Raw map



X



Y

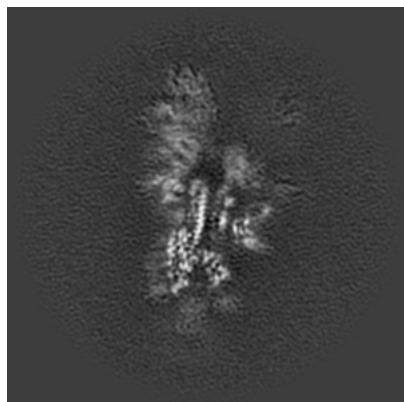


Z

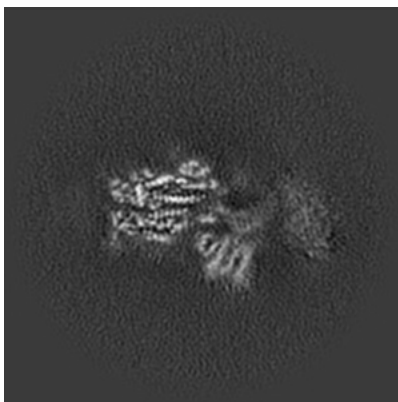
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

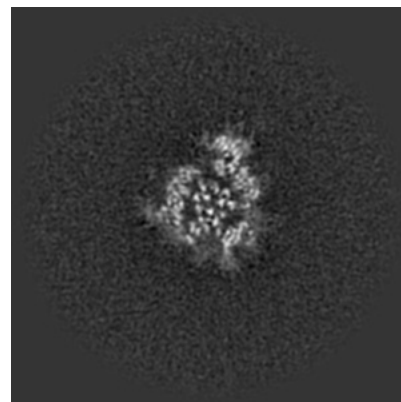
6.2.1 Primary map



X Index: 180

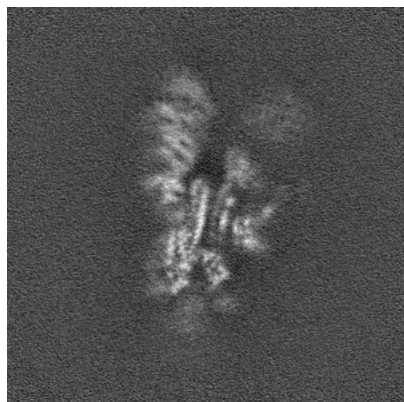


Y Index: 180

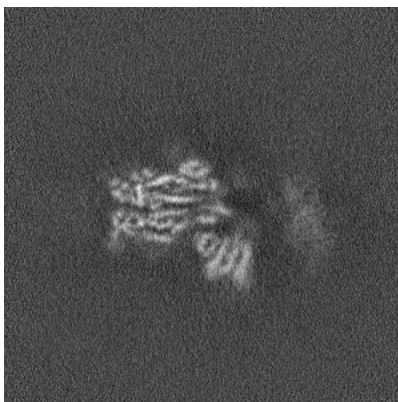


Z Index: 180

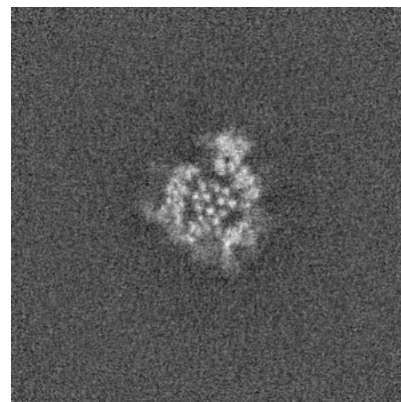
6.2.2 Raw map



X Index: 180



Y Index: 180

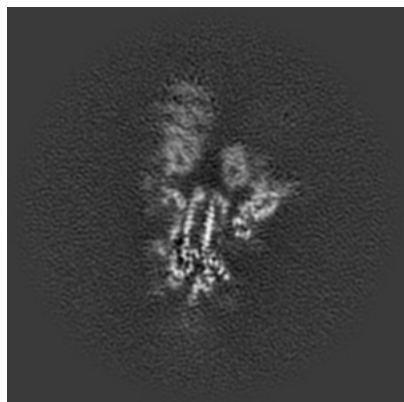


Z Index: 180

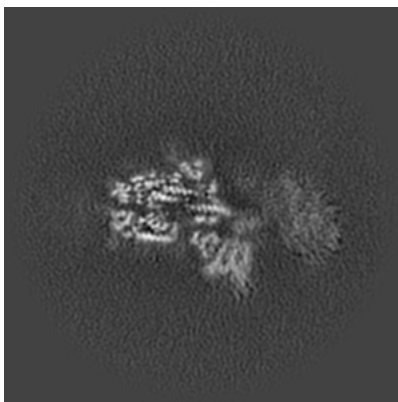
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

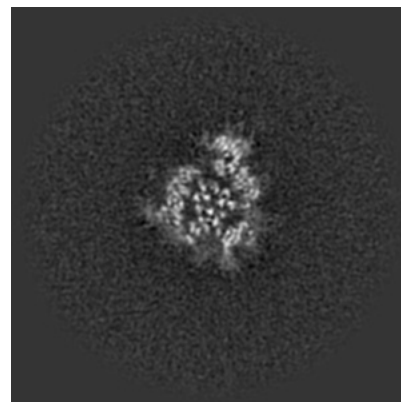
6.3.1 Primary map



X Index: 186

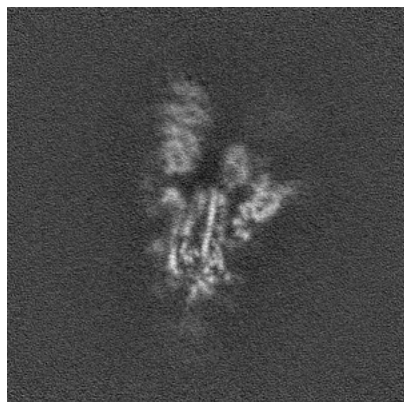


Y Index: 177



Z Index: 180

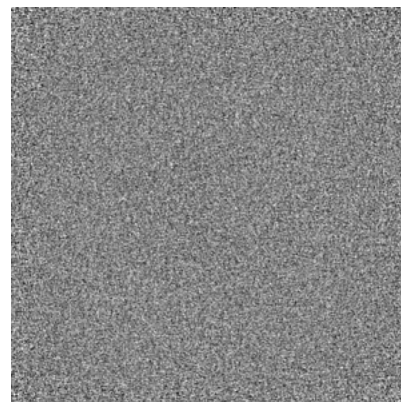
6.3.2 Raw map



X Index: 188



Y Index: 152

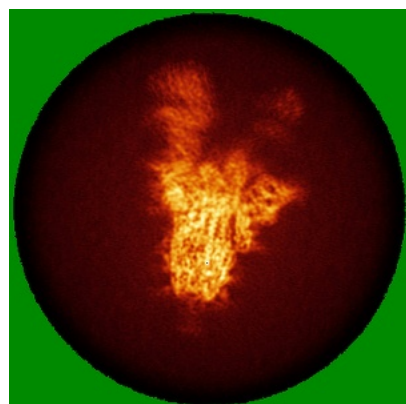


Z Index: 359

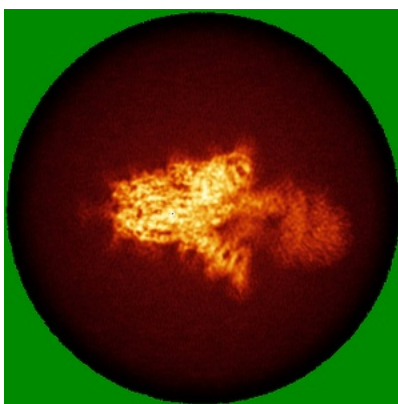
The images above show the largest variance slices of the map in three orthogonal directions.

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

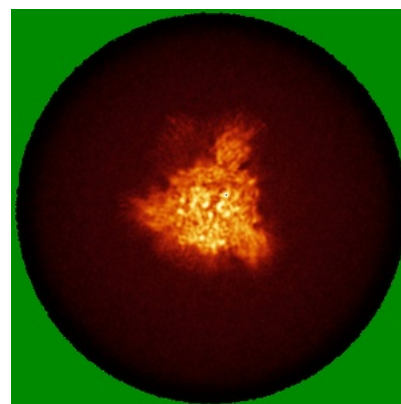
6.4.1 Primary map



X

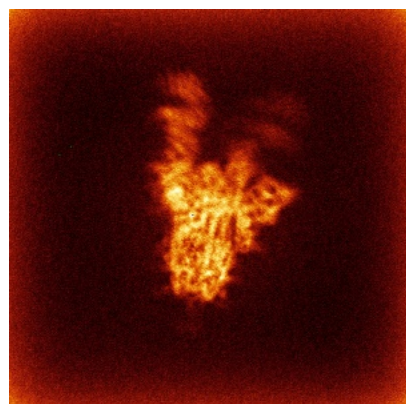


Y

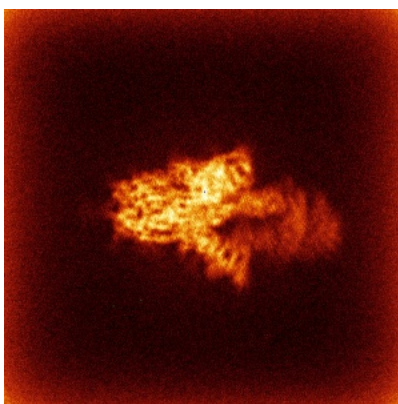


Z

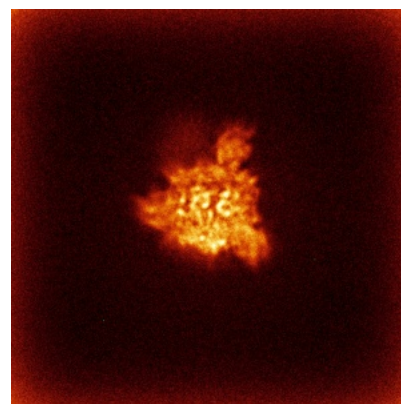
6.4.2 Raw map



X



Y

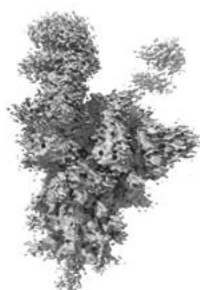


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



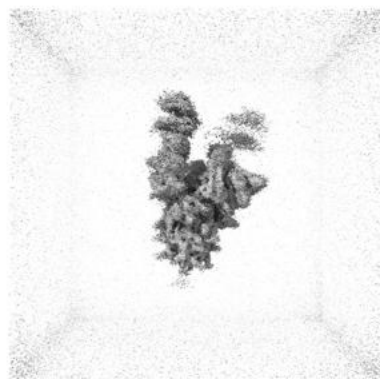
Y



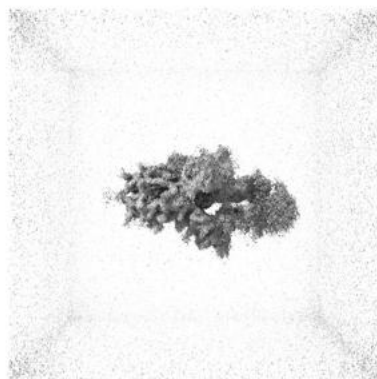
Z

The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

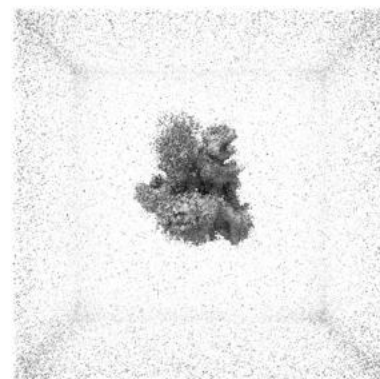
6.5.2 Raw map



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.

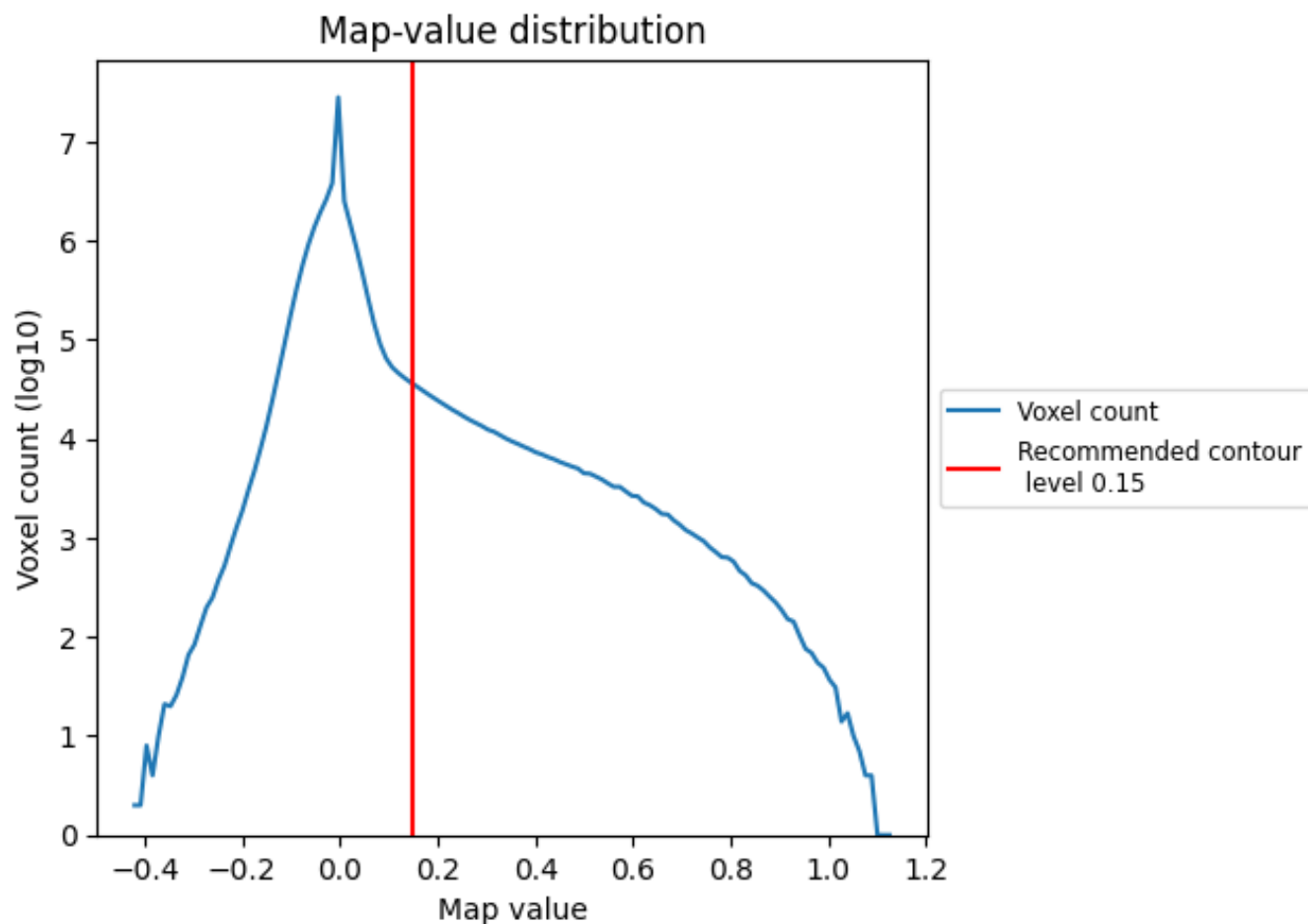
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

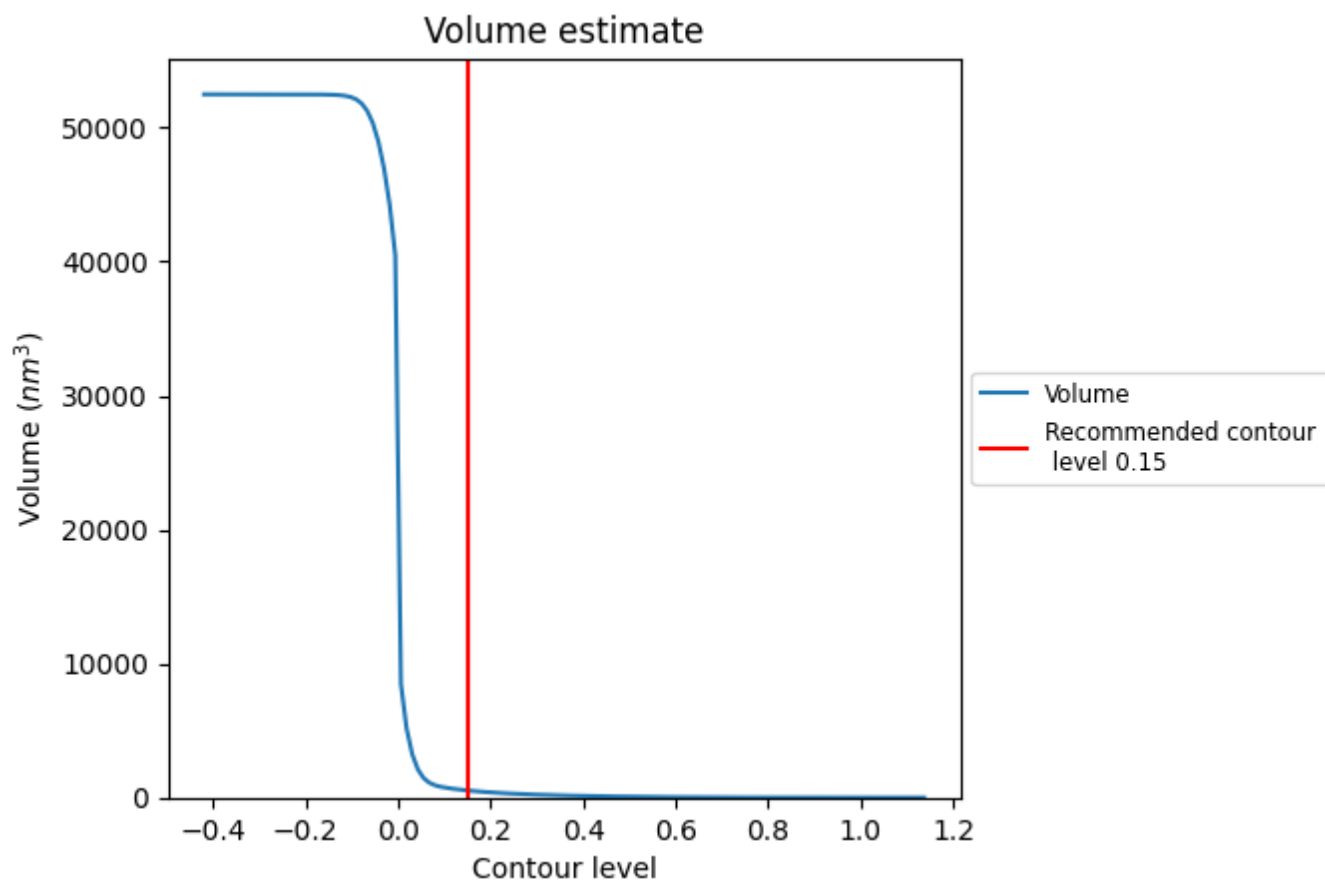
This section contains the results of statistical analysis of the map.

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.

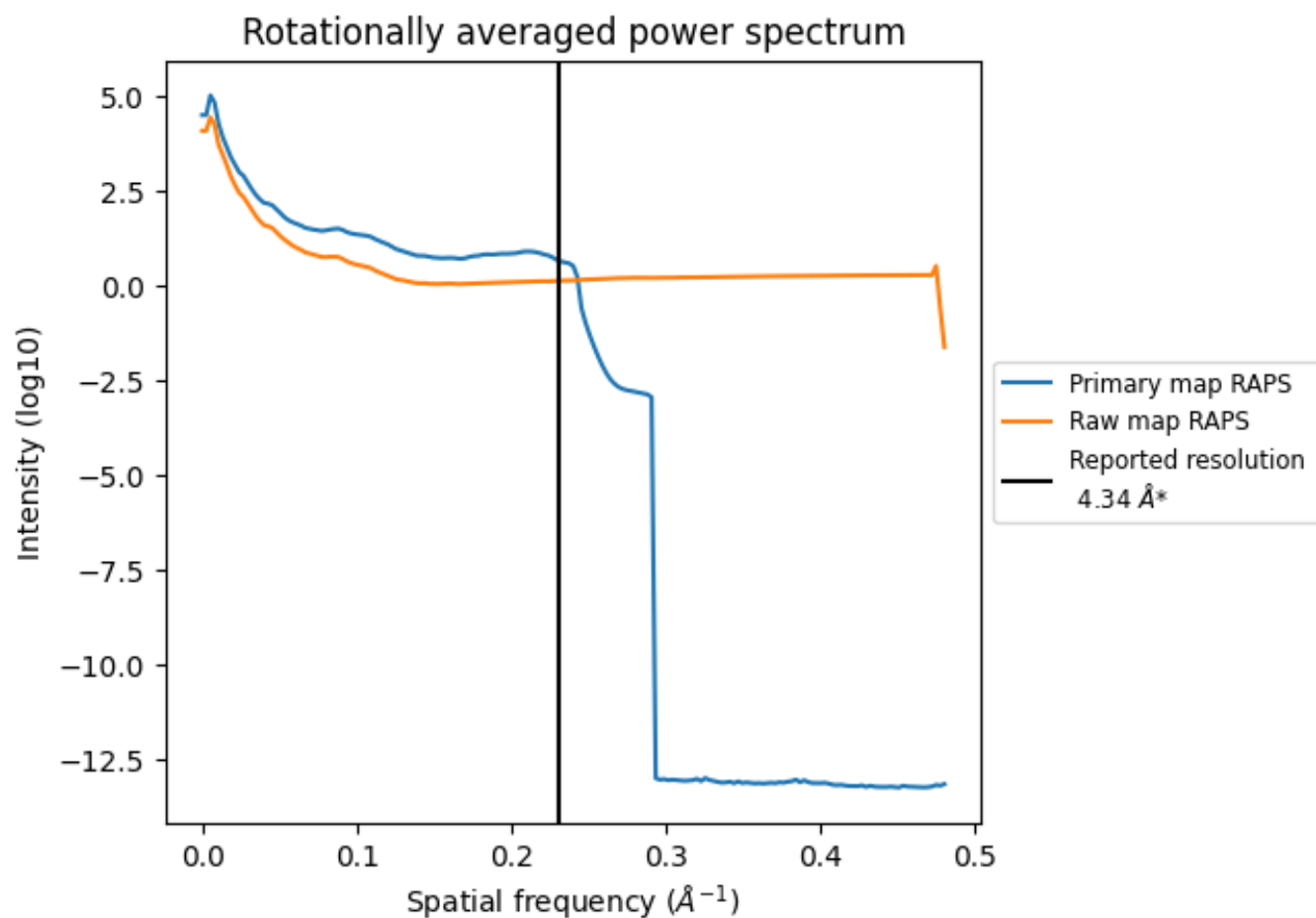
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 529 nm³; this corresponds to an approximate mass of 478 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 ⓘ

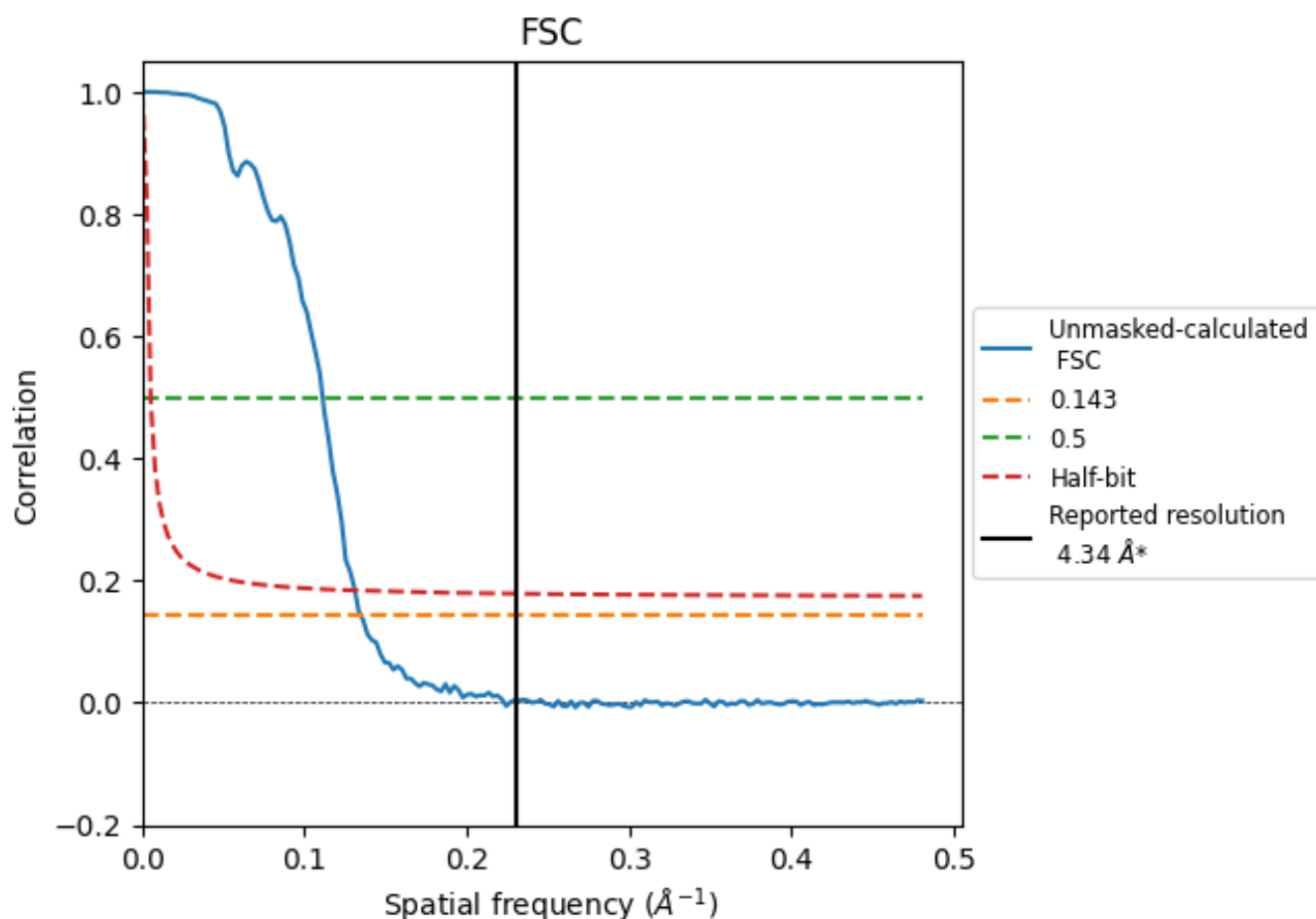


*Reported resolution corresponds to spatial frequency of 0.230 $\text{\AA}^{-1}$

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 0.230 Å⁻¹

8.2 Resolution estimates [i](#)

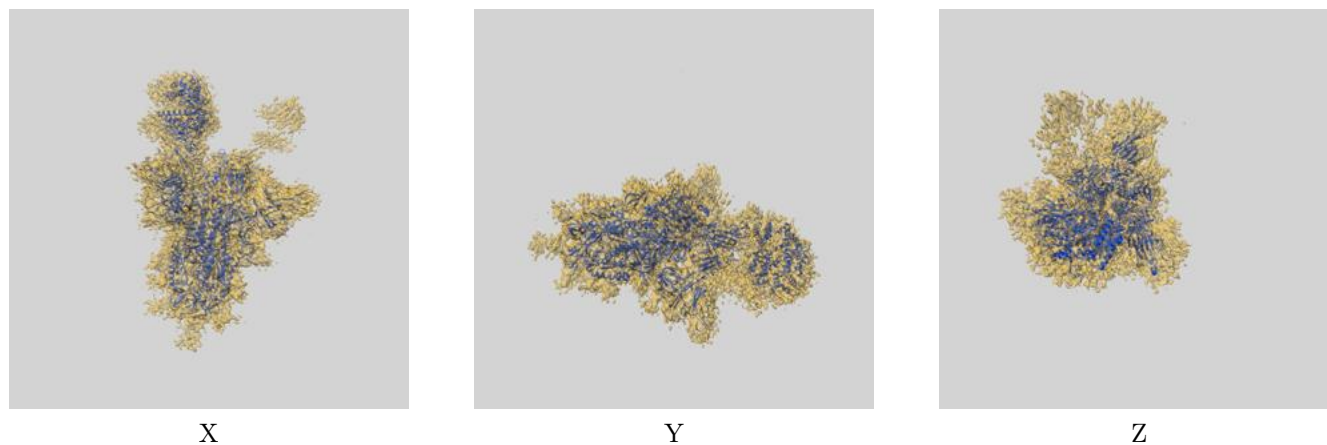
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.34	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.42	8.99	7.63

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.42 differs from the reported value 4.34 by more than 10 %

9 Map-model fit [i](#)

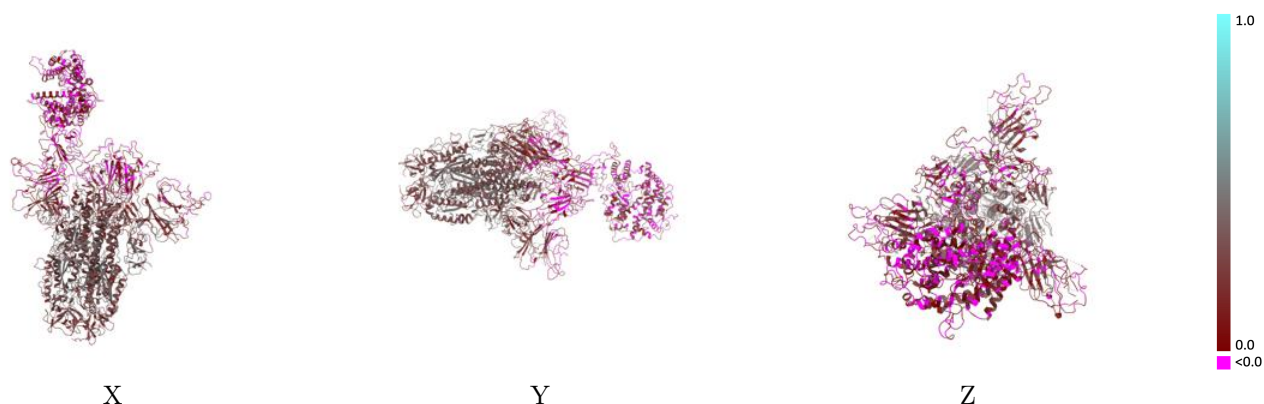
This section contains information regarding the fit between EMDB map EMD-37781 and PDB model 8WRM. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay [i](#)



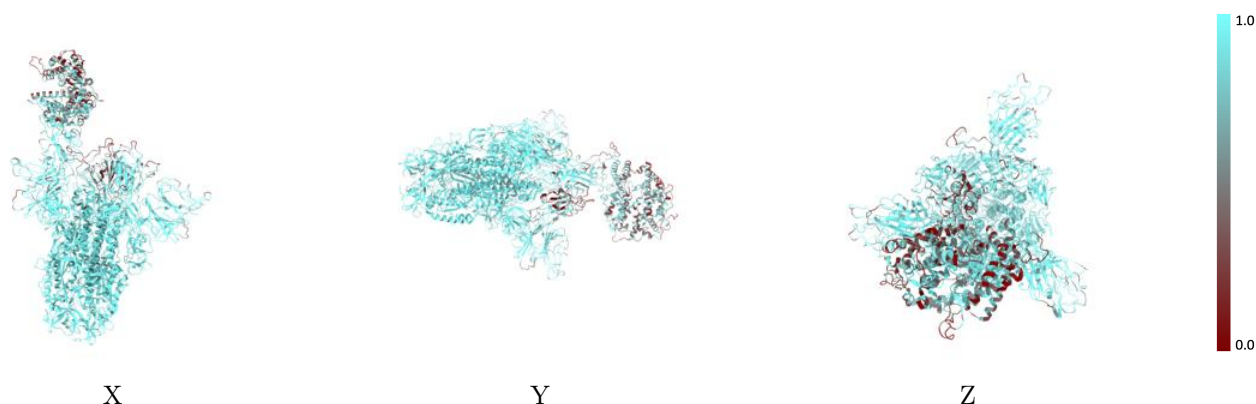
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



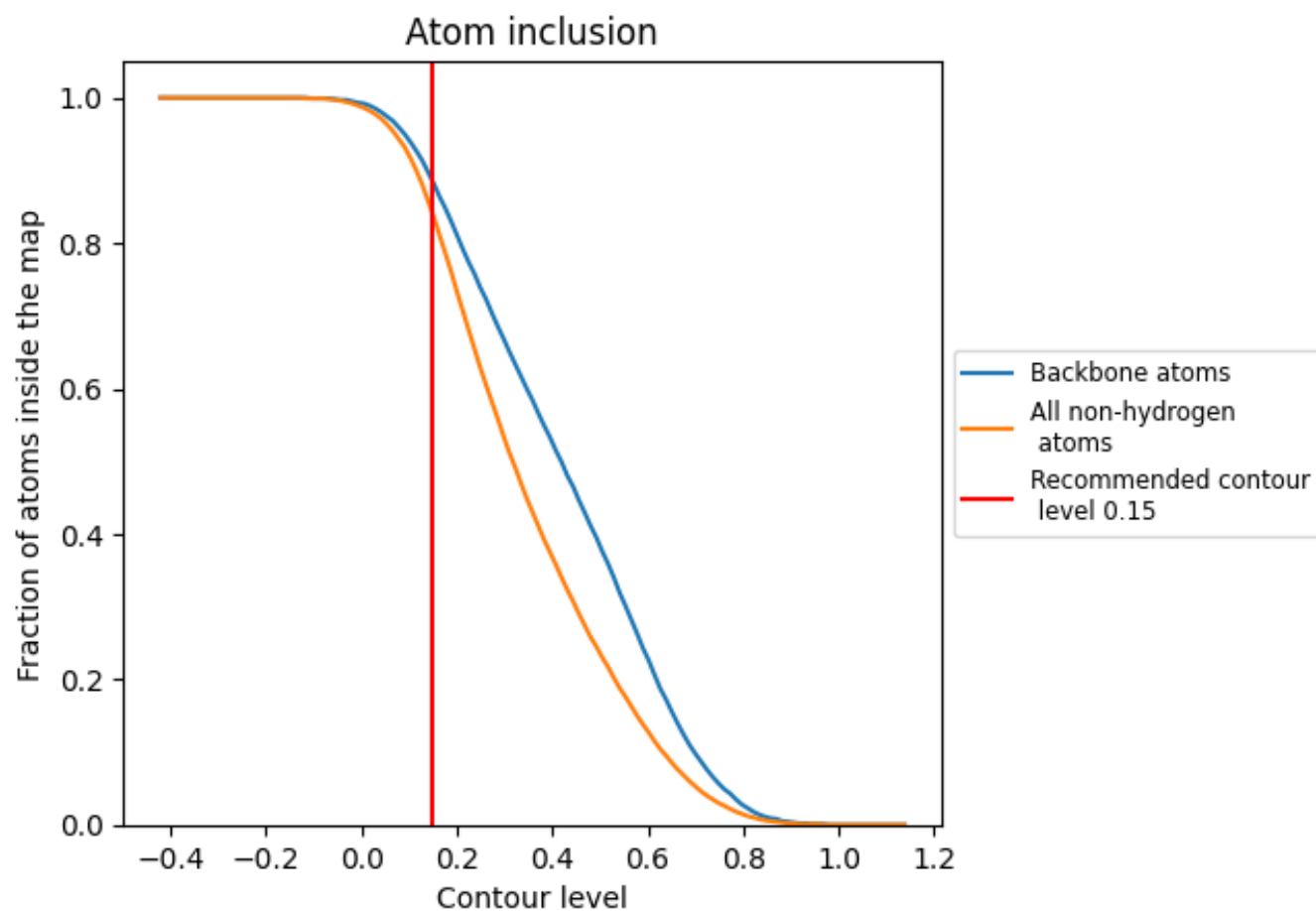
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 84% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8390	0.2190
C	0.9070	0.2540
D	0.5840	0.0670
F	0.8520	0.2500
G	0.9060	0.2420

