



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 02:51 PM UTC

PDB ID : 8FEZ / pdb_00008fez
EMDB ID : EMD-29035
Title : Prefusion-stabilized SARS-CoV-2 spike protein
Authors : Gonzalez, K.J.; Mousa, J.J.; Strauch, E.M.
Deposited on : 2022-12-07
Resolution : 3.72 Å(reported)

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

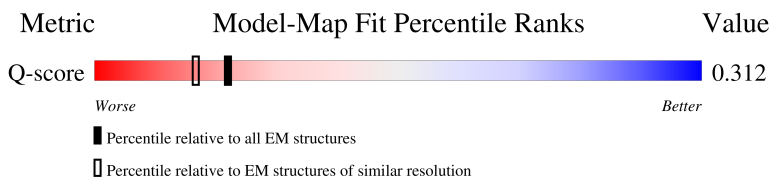
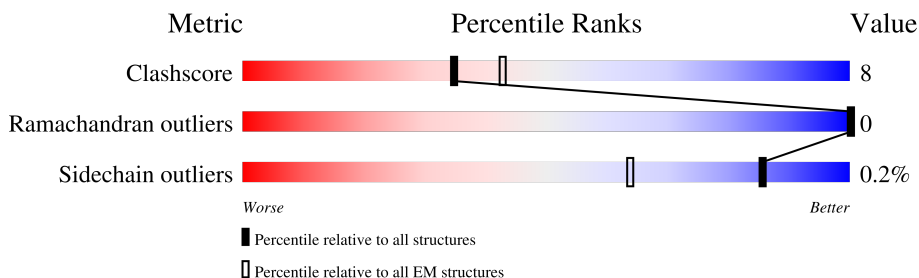
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.72 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	10474 (3.22 - 4.22)

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	1243	 65% 11% 23%
1	B	1243	 67% 6% 26%
1	C	1243	 68% 10% 22%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 17515 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	955	Total	C	N	O	S	0	0
			5931	3732	1057	1116	26		
1	B	916	Total	C	N	O	S	0	0
			5621	3562	1002	1030	27		
1	C	972	Total	C	N	O	S	0	0
			5963	3762	1068	1109	24		

There are 147 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	682	GLY	ARG	conflict	UNP P0DTC2
A	683	SER	ARG	conflict	UNP P0DTC2
A	685	SER	ARG	conflict	UNP P0DTC2
A	856	LEU	ASN	engineered mutation	UNP P0DTC2
A	899	GLN	ALA	engineered mutation	UNP P0DTC2
A	916	PHE	LEU	engineered mutation	UNP P0DTC2
A	917	TRP	TYR	engineered mutation	UNP P0DTC2
A	941	ASP	THR	engineered mutation	UNP P0DTC2
A	956	LEU	ALA	engineered mutation	UNP P0DTC2
A	964	GLU	LYS	engineered mutation	UNP P0DTC2
A	985	ASN	ASP	engineered mutation	UNP P0DTC2
A	986	PRO	LYS	conflict	UNP P0DTC2
A	987	PRO	VAL	conflict	UNP P0DTC2
A	1143	GLN	PRO	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

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1219	ASP	-	expression tag	UNP P0DTC2
A	1220	GLY	-	expression tag	UNP P0DTC2
A	1221	GLN	-	expression tag	UNP P0DTC2
A	1222	ALA	-	expression tag	UNP P0DTC2
A	1223	TYR	-	expression tag	UNP P0DTC2
A	1224	VAL	-	expression tag	UNP P0DTC2
A	1225	ARG	-	expression tag	UNP P0DTC2
A	1226	LYS	-	expression tag	UNP P0DTC2
A	1227	ASP	-	expression tag	UNP P0DTC2
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	HIS	-	expression tag	UNP P0DTC2
A	1239	HIS	-	expression tag	UNP P0DTC2
A	1240	HIS	-	expression tag	UNP P0DTC2
A	1241	HIS	-	expression tag	UNP P0DTC2
A	1242	HIS	-	expression tag	UNP P0DTC2
A	1243	HIS	-	expression tag	UNP P0DTC2
B	682	GLY	ARG	conflict	UNP P0DTC2
B	683	SER	ARG	conflict	UNP P0DTC2
B	685	SER	ARG	conflict	UNP P0DTC2
B	856	LEU	ASN	engineered mutation	UNP P0DTC2
B	899	GLN	ALA	engineered mutation	UNP P0DTC2
B	916	PHE	LEU	engineered mutation	UNP P0DTC2
B	917	TRP	TYR	engineered mutation	UNP P0DTC2
B	941	ASP	THR	engineered mutation	UNP P0DTC2
B	956	LEU	ALA	engineered mutation	UNP P0DTC2
B	964	GLU	LYS	engineered mutation	UNP P0DTC2
B	985	ASN	ASP	engineered mutation	UNP P0DTC2
B	986	PRO	LYS	conflict	UNP P0DTC2
B	987	PRO	VAL	conflict	UNP P0DTC2
B	1143	GLN	PRO	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

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1212	TYR	-	expression tag	UNP P0DTC2
B	1213	ILE	-	expression tag	UNP P0DTC2
B	1214	PRO	-	expression tag	UNP P0DTC2
B	1215	GLU	-	expression tag	UNP P0DTC2
B	1216	ALA	-	expression tag	UNP P0DTC2
B	1217	PRO	-	expression tag	UNP P0DTC2
B	1218	ARG	-	expression tag	UNP P0DTC2
B	1219	ASP	-	expression tag	UNP P0DTC2
B	1220	GLY	-	expression tag	UNP P0DTC2
B	1221	GLN	-	expression tag	UNP P0DTC2
B	1222	ALA	-	expression tag	UNP P0DTC2
B	1223	TYR	-	expression tag	UNP P0DTC2
B	1224	VAL	-	expression tag	UNP P0DTC2
B	1225	ARG	-	expression tag	UNP P0DTC2
B	1226	LYS	-	expression tag	UNP P0DTC2
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	HIS	-	expression tag	UNP P0DTC2
B	1239	HIS	-	expression tag	UNP P0DTC2
B	1240	HIS	-	expression tag	UNP P0DTC2
B	1241	HIS	-	expression tag	UNP P0DTC2
B	1242	HIS	-	expression tag	UNP P0DTC2
B	1243	HIS	-	expression tag	UNP P0DTC2
C	682	GLY	ARG	conflict	UNP P0DTC2
C	683	SER	ARG	conflict	UNP P0DTC2
C	685	SER	ARG	conflict	UNP P0DTC2
C	856	LEU	ASN	engineered mutation	UNP P0DTC2
C	899	GLN	ALA	engineered mutation	UNP P0DTC2
C	916	PHE	LEU	engineered mutation	UNP P0DTC2
C	917	TRP	TYR	engineered mutation	UNP P0DTC2
C	941	ASP	THR	engineered mutation	UNP P0DTC2
C	956	LEU	ALA	engineered mutation	UNP P0DTC2
C	964	GLU	LYS	engineered mutation	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	985	ASN	ASP	engineered mutation	UNP P0DTC2
C	986	PRO	LYS	conflict	UNP P0DTC2
C	987	PRO	VAL	conflict	UNP P0DTC2
C	1143	GLN	PRO	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
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	HIS	-	expression tag	UNP P0DTC2
C	1239	HIS	-	expression tag	UNP P0DTC2
C	1240	HIS	-	expression tag	UNP P0DTC2
C	1241	HIS	-	expression tag	UNP P0DTC2
C	1242	HIS	-	expression tag	UNP P0DTC2
C	1243	HIS	-	expression tag	UNP P0DTC2

ASP	LYS	TYR	PHE	LYS	ASN	HIS	THR	SER	PRO	ASP	VAL	ASP	GLY	ASP	ILE	SER	GLY	ILE	ASN	VAL	VAL	ASN	ILE	GLN	LYS	GLU	ASP	ARG	ASP	LEU	ASN	GLU	VAL	ALA	LYS	ASN	ASN	LEU	ILE	ASN	ASN	GLU	GLY	LYS	TYR	GLU	GLN	GLY	GLY	TYR																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
ILE	PRO	GLU	ALA	PRO	ARG	ASP	GLY	GLN	ALA	TYR	VAL	ARG	LYS	ASP	GLY	TRP	VAL	LEU	LEU	SER	THR	PHE	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS

• Molecule 1: Spike glycoprotein

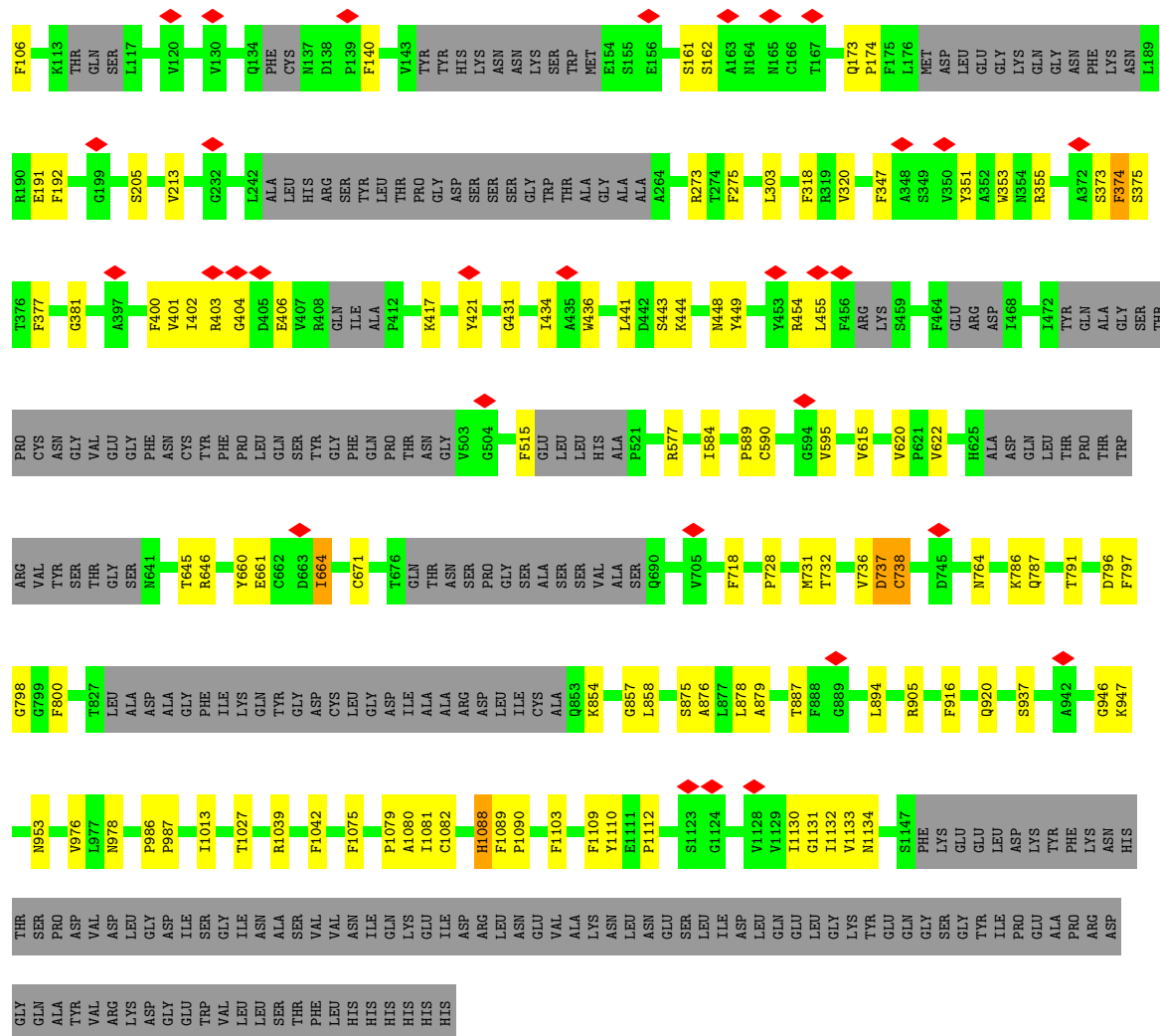
Chain B:  67% 6% 26%

PRO	ARG	GLY	GLN	ALA	TYR	VAL	ARG	LYS	ASP	GLY	GLU	TRP	VAL	LEU	ASN	ALA	SER	THR	PHE	HIS	HIS	HIS	HIS	HIS	HIS	ALA	GLU	TYR	ASP	LYS	GLY	PHE	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
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• Molecule 1: Spike glycoprotein

Chain C:  68% 10% 22%

MET	PHE	VAL	PHE	LEU	VAL	LEU	LEU	PRO	VAL	SER	SER	GLN	CYS	VAL	ASN	THR	THR	ARG	GLN	THR	LEU	P25	P26	T29	Y37	H49	S50	F55	V62	T63	W64	I68	H69	VAL	SER	GLY	THR	ASN	GLY	THR	K77	A93	K97	S98	N99	I100	W104	I105
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	87514	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	58.24	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.797	Depositor
Minimum map value	-0.025	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.034	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	262.144, 262.144, 262.144	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.024, 1.024, 1.024	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.12	5/6029 (0.1%)	1.29	39/8284 (0.5%)
1	B	1.08	2/5727 (0.0%)	1.22	24/7866 (0.3%)
1	C	1.13	5/6083 (0.1%)	1.26	33/8359 (0.4%)
All	All	1.11	12/17839 (0.1%)	1.26	96/24509 (0.4%)

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	1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	434	ILE	CA-CB	-6.08	1.46	1.54
1	A	116	SER	CA-CB	-5.61	1.45	1.53
1	C	97	LYS	CA-C	-5.57	1.45	1.52
1	A	1048	HIS	CA-C	-5.53	1.44	1.52
1	A	550	GLY	CA-C	-5.53	1.45	1.52
1	A	190	ARG	CA-C	-5.47	1.45	1.52
1	C	1088	HIS	CA-C	-5.40	1.50	1.53
1	C	764	ASN	C-O	-5.37	1.17	1.24
1	B	513	LEU	CA-C	-5.32	1.46	1.52
1	A	953	ASN	CA-C	-5.07	1.46	1.52
1	B	760	CYS	CA-C	-5.03	1.45	1.52
1	C	436	TRP	CA-CB	-5.00	1.46	1.53

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1088	HIS	N-CA-C	12.59	119.11	108.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	410	ILE	N-CA-C	-11.49	98.30	110.36
1	A	99	ASN	N-CA-C	-9.85	102.05	114.56
1	B	1122	VAL	N-CA-C	9.01	120.73	112.17
1	C	374	PHE	N-CA-C	-8.95	97.62	110.24
1	B	799	GLY	N-CA-C	-8.29	101.26	111.45
1	A	1142	GLN	N-CA-C	-8.17	102.06	110.97
1	A	404	GLY	N-CA-C	7.46	121.49	111.72
1	A	900	MET	N-CA-C	-7.33	103.31	111.82
1	B	761	THR	N-CA-C	-7.28	103.28	111.07
1	C	737	ASP	N-CA-C	-7.27	95.35	108.58
1	C	417	LYS	N-CA-C	-7.25	103.37	111.28
1	A	512	VAL	N-CA-C	7.24	118.55	108.12
1	C	786	LYS	CB-CA-C	-7.24	108.23	116.63
1	C	875	SER	N-CA-C	-7.20	103.37	111.07
1	A	585	LEU	N-CA-C	7.17	120.64	109.52
1	C	796	ASP	N-CA-C	-7.17	103.40	111.07
1	A	218	GLN	N-CA-C	-6.79	98.15	108.67
1	A	1099	GLY	N-CA-C	-6.78	106.62	114.69
1	A	588	THR	CA-C-N	6.75	126.78	119.90
1	A	588	THR	C-N-CA	6.75	126.78	119.90
1	A	102	ARG	N-CA-C	-6.60	103.80	112.24
1	A	502	GLY	N-CA-C	-6.59	107.08	114.40
1	B	428	ASP	N-CA-C	-6.58	101.53	110.68
1	B	335	LEU	N-CA-C	-6.58	100.30	110.10
1	A	618	THR	N-CA-C	-6.57	105.89	114.04
1	C	937	SER	N-CA-C	-6.56	104.31	112.90
1	C	402	ILE	N-CA-C	6.49	117.64	108.17
1	C	622	VAL	N-CA-C	6.48	116.62	110.53
1	A	554	GLU	N-CA-C	6.47	118.48	110.91
1	C	879	ALA	N-CA-C	-6.43	104.28	111.28
1	A	879	ALA	N-CA-C	-6.37	101.52	110.50
1	A	656	VAL	N-CA-C	6.35	117.27	108.89
1	C	347	PHE	N-CA-C	-6.23	105.99	113.97
1	A	197	ILE	N-CA-C	6.21	117.23	111.45
1	C	620	VAL	CA-C-N	6.17	126.53	119.92
1	C	620	VAL	C-N-CA	6.17	126.53	119.92
1	A	342	PHE	N-CA-C	-6.08	104.72	111.71
1	A	550	GLY	N-CA-C	6.03	120.26	112.54
1	B	700	GLY	N-CA-C	-6.01	105.11	112.68
1	A	407	VAL	N-CA-C	-5.99	104.93	113.07
1	A	920	GLN	N-CA-C	-5.91	102.16	110.50
1	C	375	SER	N-CA-C	5.89	118.80	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	213	VAL	N-CA-C	5.87	117.16	108.65
1	A	411	ALA	N-CA-C	5.85	122.73	109.81
1	A	226	LEU	CA-C-N	-5.83	117.01	122.66
1	A	226	LEU	C-N-CA	-5.83	117.01	122.66
1	A	352	ALA	N-CA-C	5.83	117.54	107.93
1	B	134	GLN	N-CA-C	-5.82	101.43	110.10
1	B	973	ILE	N-CA-C	5.81	117.25	110.62
1	C	100	ILE	N-CA-C	5.78	117.00	108.45
1	B	87	ASN	CB-CA-C	-5.70	109.99	116.54
1	B	602	THR	CA-C-N	5.64	127.84	120.28
1	B	602	THR	C-N-CA	5.64	127.84	120.28
1	C	615	VAL	N-CA-C	5.62	116.40	108.36
1	A	620	VAL	CA-C-N	5.57	125.76	120.31
1	A	620	VAL	C-N-CA	5.57	125.76	120.31
1	B	610	VAL	N-CA-C	5.54	115.87	108.11
1	B	973	ILE	CB-CA-C	-5.53	104.80	112.04
1	C	140	PHE	N-CA-C	5.52	117.19	108.96
1	C	1132	ILE	N-CA-C	5.52	116.34	107.73
1	B	660	TYR	CB-CA-C	-5.51	110.20	116.54
1	B	136	CYS	N-CA-C	-5.50	101.71	109.96
1	C	403	ARG	N-CA-C	-5.48	106.96	113.97
1	B	1074	ASN	N-CA-C	5.44	118.02	108.56
1	B	737	ASP	CA-C-N	5.43	127.82	120.38
1	B	737	ASP	C-N-CA	5.43	127.82	120.38
1	C	661	GLU	N-CA-C	-5.40	102.05	110.10
1	A	812	PRO	N-CA-C	-5.40	103.66	111.22
1	A	922	LEU	N-CA-C	-5.39	106.76	113.55
1	A	1049	LEU	N-CA-C	-5.38	107.26	113.88
1	B	125	ASN	N-CA-C	5.36	117.16	108.26
1	C	664	ILE	CB-CA-C	-5.36	105.99	111.08
1	C	404	GLY	N-CA-C	-5.34	103.56	111.03
1	B	589	PRO	N-CA-C	-5.30	102.86	111.03
1	B	361	CYS	CA-C-N	-5.30	115.75	122.43
1	B	361	CYS	C-N-CA	-5.30	115.75	122.43
1	C	1027	THR	N-CA-C	-5.26	105.55	111.28
1	A	588	THR	N-CA-C	5.24	118.17	108.94
1	B	862	PRO	CA-C-N	5.24	125.14	119.85
1	B	862	PRO	C-N-CA	5.24	125.14	119.85
1	C	905	ARG	N-CA-C	-5.20	105.69	111.36
1	C	406	GLU	CB-CA-C	-5.15	110.62	116.54
1	A	985	ASN	CA-C-N	-5.15	115.08	120.38
1	A	985	ASN	C-N-CA	-5.15	115.08	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	993	ILE	N-CA-C	-5.15	105.69	110.53
1	A	857	GLY	N-CA-C	-5.13	108.25	114.92
1	C	660	TYR	N-CA-C	5.06	116.94	108.99
1	C	791	THR	CA-C-N	5.03	123.28	119.66
1	C	791	THR	C-N-CA	5.03	123.28	119.66
1	A	942	ALA	N-CA-C	-5.03	106.44	112.58
1	A	406	GLU	N-CA-C	5.03	117.32	107.57
1	A	586	ASP	CB-CA-C	-5.03	102.57	111.22
1	C	1088	HIS	N-CA-CB	-5.03	102.00	110.49
1	C	1079	PRO	N-CA-C	5.02	121.05	114.27
1	C	441	LEU	N-CA-CB	-5.01	104.34	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	612	TYR	Sidechain

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	5931	0	4279	104	0
1	B	5621	0	3892	58	0
1	C	5963	0	4077	85	0
All	All	17515	0	12248	239	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.

All (239) 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:C:1103:PHE:CD1	1:C:1112:PRO:HB3	1.39	1.57
1:A:195:LYS:NZ	1:A:203:ILE:CB	1.69	1.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:LEU:CD1	1:A:492:LEU:HA	1.60	1.28
1:A:825:LYS:O	1:A:826:VAL:HG12	1.34	1.22
1:B:392:PHE:O	1:B:524:VAL:HG22	1.42	1.16
1:C:1103:PHE:CD1	1:C:1112:PRO:CB	2.35	1.08
1:A:455:LEU:HD11	1:A:492:LEU:HA	1.15	1.08
1:A:501:ASN:HB3	1:A:503:VAL:HG22	1.38	1.05
1:C:29:THR:HG22	1:C:64:TRP:HD1	1.18	1.04
1:B:359:SER:HA	1:B:524:VAL:HG12	1.42	1.00
1:C:29:THR:HG22	1:C:64:TRP:CD1	1.98	0.97
1:A:455:LEU:HD12	1:A:492:LEU:HA	1.47	0.95
1:A:550:GLY:HA2	1:A:589:PRO:HA	1.48	0.95
1:B:307:THR:HA	1:B:602:THR:HG21	1.49	0.94
1:C:1103:PHE:CE1	1:C:1112:PRO:HB3	2.04	0.92
1:A:195:LYS:HZ1	1:A:203:ILE:CB	1.81	0.92
1:B:524:VAL:HG23	1:B:524:VAL:O	1.69	0.89
1:C:797:PHE:CB	1:C:800:PHE:HB2	2.02	0.89
1:C:1103:PHE:HD1	1:C:1112:PRO:HB3	1.24	0.89
1:A:455:LEU:HD11	1:A:492:LEU:CA	2.04	0.86
1:A:825:LYS:O	1:A:826:VAL:CG1	2.22	0.84
1:A:455:LEU:CD1	1:A:492:LEU:CA	2.53	0.83
1:B:392:PHE:C	1:B:524:VAL:HG22	2.04	0.82
1:C:29:THR:CG2	1:C:64:TRP:HD1	1.94	0.81
1:A:612:TYR:CE2	1:A:650:LEU:CB	2.66	0.79
1:C:728:PRO:HD3	1:C:947:LYS:HG3	1.62	0.79
1:A:612:TYR:HE2	1:A:650:LEU:CB	1.96	0.79
1:A:501:ASN:CB	1:A:503:VAL:HG22	2.13	0.78
1:C:26:PRO:HG2	1:C:64:TRP:CZ2	2.22	0.74
1:A:896:ILE:HG22	1:A:898:PHE:H	1.50	0.74
1:C:1103:PHE:CZ	1:C:1110:TYR:OH	2.42	0.72
1:A:1047:TYR:HD2	1:A:1067:TYR:HD2	1.36	0.71
1:A:501:ASN:OD1	1:A:502:GLY:N	2.24	0.70
1:C:1103:PHE:HZ	1:C:1110:TYR:HH	1.34	0.69
1:A:455:LEU:HD12	1:A:492:LEU:CA	2.22	0.69
1:B:985:ASN:OD1	1:B:987:PRO:HG2	1.93	0.69
1:B:574:ASP:OD1	1:B:574:ASP:O	2.11	0.68
1:A:550:GLY:CA	1:A:589:PRO:HA	2.21	0.66
1:A:195:LYS:HD3	1:A:203:ILE:HA	1.78	0.66
1:B:524:VAL:O	1:B:524:VAL:CG2	2.42	0.66
1:B:1053:PRO:HB3	1:B:1062:PHE:CE1	2.31	0.66
1:B:335:LEU:HA	1:B:362:VAL:HB	1.79	0.65
1:A:905:ARG:HB3	1:A:1049:LEU:HB2	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:55:PHE:HB2	1:C:275:PHE:CE1	2.33	0.63
1:A:978:ASN:OD1	1:A:978:ASN:N	2.31	0.63
1:C:448:ASN:OD1	1:C:449:TYR:N	2.32	0.63
1:A:501:ASN:HB3	1:A:503:VAL:CG2	2.24	0.62
1:C:1103:PHE:CE1	1:C:1110:TYR:OH	2.49	0.62
1:A:195:LYS:HD3	1:A:202:LYS:O	1.99	0.62
1:B:1098:ASN:H	1:B:1101:HIS:H	1.48	0.62
1:B:902:MET:HB3	1:B:916:PHE:CE2	2.34	0.61
1:C:1080:ALA:O	1:C:1133:VAL:N	2.33	0.61
1:C:320:VAL:HB	1:C:590:CYS:SG	2.40	0.61
1:A:116:SER:N	1:A:130:VAL:O	2.33	0.61
1:A:314:GLN:HE22	1:A:595:VAL:H	1.48	0.61
1:B:307:THR:HA	1:B:602:THR:CG2	2.29	0.60
1:B:392:PHE:HB2	1:B:524:VAL:CG2	2.31	0.60
1:A:550:GLY:HA2	1:A:589:PRO:CA	2.29	0.60
1:C:1039:ARG:HG2	1:C:1042:PHE:HB2	1.84	0.60
1:A:195:LYS:CD	1:A:202:LYS:O	2.50	0.60
1:A:896:ILE:HG21	1:A:901:GLN:HB2	1.84	0.59
1:A:541:PHE:HA	1:A:547:THR:HA	1.85	0.59
1:A:663:ASP:O	1:A:664:ILE:C	2.45	0.59
1:A:547:THR:HG23	1:B:978:ASN:CG	2.28	0.58
1:B:392:PHE:HB2	1:B:524:VAL:HG21	1.86	0.58
1:B:431:GLY:HA3	1:B:513:LEU:O	2.03	0.57
1:A:1078:ALA:O	1:A:1095:PHE:HB2	2.04	0.56
1:A:94:SER:OG	1:A:264:ALA:O	2.21	0.56
1:A:321:GLN:HG2	1:A:623:ALA:HB1	1.87	0.56
1:A:1047:TYR:HE2	1:A:1069:PRO:HD3	1.70	0.56
1:A:1047:TYR:CE2	1:A:1069:PRO:HD3	2.41	0.55
1:A:1009:THR:O	1:A:1013:ILE:HG23	2.06	0.55
1:B:359:SER:CA	1:B:524:VAL:HG12	2.28	0.55
1:B:618:THR:O	1:B:621:PRO:HD2	2.06	0.54
1:A:411:ALA:HA	1:A:414:GLN:HB2	1.89	0.54
1:B:392:PHE:H	1:B:524:VAL:HG23	1.72	0.54
1:C:1103:PHE:HE1	1:C:1110:TYR:HH	1.50	0.54
1:C:68:ILE:HG22	1:C:69:HIS:N	2.23	0.54
1:C:1075:PHE:CE2	1:C:1110:TYR:CZ	2.96	0.54
1:C:37:TYR:CE2	1:C:55:PHE:CD1	2.96	0.54
1:C:1103:PHE:CE1	1:C:1112:PRO:CB	2.82	0.54
1:C:1103:PHE:HZ	1:C:1110:TYR:OH	1.85	0.54
1:C:1109:PHE:CG	1:C:1110:TYR:N	2.76	0.54
1:C:26:PRO:HG2	1:C:64:TRP:CH2	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:ARG:NH1	1:A:503:VAL:HA	2.22	0.54
1:B:570:ALA:HB2	1:C:854:LYS:HB2	1.90	0.54
1:A:1047:TYR:HD2	1:A:1067:TYR:CD2	2.21	0.53
1:C:1039:ARG:CG	1:C:1042:PHE:HB2	2.38	0.53
1:A:1086:LYS:HA	1:A:1125:ASN:HA	1.89	0.53
1:C:29:THR:CG2	1:C:64:TRP:CD1	2.79	0.53
1:C:373:SER:O	1:C:374:PHE:C	2.50	0.53
1:C:448:ASN:OD1	1:C:448:ASN:C	2.51	0.53
1:C:577:ARG:HA	1:C:584:ILE:HA	1.91	0.53
1:B:1138:TYR:OH	1:B:1140:PRO:HB3	2.09	0.52
1:B:700:GLY:HA3	1:C:787:GLN:HA	1.92	0.52
1:A:327:VAL:CG2	1:A:528:LYS:HG3	2.40	0.52
1:C:26:PRO:CG	1:C:64:TRP:CZ2	2.91	0.51
1:A:711:SER:O	1:B:897:PRO:HG3	2.10	0.51
1:B:539:VAL:HG12	1:B:540:ASN:N	2.26	0.51
1:C:161:SER:O	1:C:162:SER:C	2.53	0.51
1:B:1078:ALA:CB	1:B:1131:GLY:O	2.59	0.50
1:A:380:TYR:CE2	1:A:412:PRO:HG2	2.46	0.50
1:B:125:ASN:HA	1:B:174:PRO:HD3	1.92	0.50
1:B:376:THR:HG23	1:B:436:TRP:HA	1.93	0.50
1:A:501:ASN:CG	1:A:503:VAL:HG22	2.37	0.50
1:C:192:PHE:CE2	1:C:205:SER:HB2	2.46	0.50
1:C:645:THR:OG1	1:C:646:ARG:N	2.45	0.50
1:A:886:TRP:C	1:A:893:ALA:HB2	2.36	0.50
1:B:437:ASN:O	1:B:438:SER:C	2.55	0.50
1:B:1053:PRO:HB3	1:B:1062:PHE:CD1	2.46	0.50
1:C:1088:HIS:CG	1:C:1089:PHE:N	2.79	0.50
1:C:318:PHE:HB2	1:C:595:VAL:CG2	2.42	0.49
1:C:93:ALA:HA	1:C:191:GLU:HA	1.95	0.49
1:A:1110:TYR:O	1:A:1111:GLU:C	2.56	0.49
1:B:319:ARG:HB2	1:B:321:GLN:HE22	1.78	0.49
1:B:438:SER:O	1:B:439:ASN:C	2.55	0.49
1:C:49:HIS:CG	1:C:50:SER:N	2.80	0.49
1:A:663:ASP:H	1:A:671:CYS:HB3	1.78	0.49
1:C:916:PHE:O	1:C:920:GLN:N	2.45	0.49
1:A:1139:ASP:OD2	1:A:1142:GLN:N	2.46	0.49
1:A:320:VAL:O	1:A:590:CYS:SG	2.70	0.48
1:A:1012:LEU:HG	1:C:1013:ILE:HG21	1.95	0.48
1:A:195:LYS:NZ	1:A:203:ILE:CA	2.67	0.48
1:C:986:PRO:HB2	1:C:987:PRO:HD3	1.96	0.48
1:A:392:PHE:CD1	1:A:516:GLU:O	2.65	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:ALA:CA	1:A:414:GLN:HB2	2.44	0.48
1:B:590:CYS:O	1:B:591:SER:C	2.57	0.48
1:A:555:SER:HA	1:A:585:LEU:HB3	1.94	0.48
1:C:431:GLY:HA2	1:C:515:PHE:CD2	2.49	0.47
1:C:1081:ILE:O	1:C:1088:HIS:HB3	2.13	0.47
1:A:409:GLN:O	1:A:410:ILE:C	2.54	0.47
1:C:431:GLY:HA2	1:C:515:PHE:CE2	2.49	0.47
1:C:736:VAL:HG12	1:C:858:LEU:HA	1.97	0.47
1:C:976:VAL:HG12	1:C:978:ASN:H	1.80	0.47
1:C:454:ARG:O	1:C:455:LEU:C	2.57	0.46
1:A:611:LEU:HB3	1:A:648:GLY:HA3	1.97	0.46
1:C:443:SER:O	1:C:444:LYS:C	2.54	0.46
1:C:953:ASN:C	1:C:953:ASN:OD1	2.57	0.46
1:B:1077:THR:OG1	1:B:1078:ALA:N	2.48	0.46
1:C:1103:PHE:CE1	1:C:1112:PRO:CG	2.99	0.46
1:A:656:VAL:HG12	1:A:658:ASN:H	1.79	0.46
1:A:455:LEU:CD1	1:A:491:PRO:O	2.63	0.46
1:C:731:MET:O	1:C:732:THR:C	2.58	0.46
1:B:28:TYR:CD1	1:B:63:THR:HA	2.50	0.46
1:A:893:ALA:O	1:A:894:LEU:C	2.57	0.46
1:B:109:THR:HG21	1:B:113:LYS:HB2	1.98	0.46
1:C:318:PHE:HB2	1:C:595:VAL:HG22	1.98	0.46
1:C:887:THR:HG21	1:C:894:LEU:HB2	1.98	0.46
1:B:336:CYS:HB3	1:B:361:CYS:HB2	1.57	0.45
1:C:99:ASN:O	1:C:100:ILE:HG13	2.16	0.45
1:A:32:PHE:O	1:A:33:THR:C	2.60	0.45
1:B:799:GLY:O	1:B:800:PHE:C	2.58	0.45
1:C:718:PHE:CD1	1:C:718:PHE:C	2.94	0.45
1:C:1130:ILE:CG2	1:C:1131:GLY:N	2.79	0.45
1:A:234:ASN:OD1	1:A:234:ASN:N	2.50	0.45
1:A:615:VAL:HG22	1:A:617:CYS:H	1.81	0.45
1:A:801:ASN:ND2	1:A:804:GLN:OE1	2.49	0.45
1:B:436:TRP:O	1:B:437:ASN:C	2.59	0.45
1:B:760:CYS:O	1:B:761:THR:C	2.58	0.45
1:A:405:ASP:CG	1:A:503:VAL:HG11	2.42	0.45
1:A:455:LEU:HD12	1:A:492:LEU:CB	2.46	0.45
1:A:1043:CYS:HB2	1:A:1048:HIS:CG	2.52	0.45
1:A:341:VAL:O	1:A:342:PHE:C	2.59	0.44
1:C:68:ILE:CG2	1:C:69:HIS:N	2.80	0.44
1:A:398:ASP:OD2	1:A:512:VAL:N	2.50	0.44
1:A:405:ASP:OD1	1:A:405:ASP:O	2.34	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:938:LEU:O	1:A:942:ALA:N	2.45	0.44
1:C:104:TRP:HB2	1:C:106:PHE:CZ	2.52	0.44
1:A:790:LYS:O	1:A:791:THR:C	2.61	0.44
1:A:195:LYS:HD2	1:A:202:LYS:O	2.17	0.44
1:B:713:ALA:HB2	1:B:1074:ASN:HB3	1.98	0.44
1:A:1101:HIS:O	1:A:1102:TRP:C	2.58	0.44
1:B:330:PRO:O	1:B:331:ASN:C	2.61	0.44
1:C:351:TYR:CE2	1:C:421:TYR:O	2.70	0.44
1:C:1103:PHE:HE1	1:C:1110:TYR:CZ	2.36	0.44
1:C:381:GLY:H	1:C:431:GLY:H	1.65	0.44
1:A:405:ASP:HB2	1:A:503:VAL:HB	2.00	0.43
1:A:1116:THR:O	1:A:1117:THR:C	2.61	0.43
1:A:897:PRO:O	1:A:898:PHE:HB3	2.18	0.43
1:C:737:ASP:N	1:C:857:GLY:O	2.51	0.43
1:C:946:GLY:O	1:C:947:LYS:C	2.62	0.43
1:A:485:GLY:O	1:A:486:PHE:C	2.61	0.43
1:A:501:ASN:C	1:A:503:VAL:N	2.75	0.43
1:B:738:CYS:O	1:B:739:THR:C	2.59	0.43
1:C:353:TRP:CD1	1:C:355:ARG:HB2	2.54	0.43
1:B:197:ILE:HG22	1:B:200:TYR:O	2.19	0.42
1:A:986:PRO:N	1:A:987:PRO:HD2	2.34	0.42
1:B:319:ARG:HG2	1:B:592:PHE:CD1	2.54	0.42
1:C:273:ARG:HB2	1:C:275:PHE:HE1	1.83	0.42
1:A:295:PRO:HD3	1:A:628:GLN:HG2	2.01	0.42
1:A:933:LYS:O	1:A:937:SER:OG	2.31	0.42
1:C:736:VAL:O	1:C:738:CYS:N	2.52	0.42
1:B:308:VAL:H	1:B:602:THR:CG2	2.32	0.42
1:C:876:ALA:C	1:C:878:LEU:H	2.28	0.42
1:A:941:ASP:O	1:A:942:ALA:HB3	2.20	0.42
1:C:736:VAL:C	1:C:738:CYS:N	2.78	0.42
1:C:1082:CYS:H	1:C:1134:ASN:HA	1.84	0.42
1:B:377:PHE:O	1:B:432:CYS:SG	2.78	0.42
1:C:55:PHE:HB2	1:C:275:PHE:CZ	2.55	0.42
1:A:309:GLU:OE2	1:A:309:GLU:N	2.52	0.42
1:A:411:ALA:CB	1:A:414:GLN:CB	2.97	0.42
1:A:501:ASN:C	1:A:503:VAL:H	2.28	0.42
1:C:173:GLN:N	1:C:174:PRO:CD	2.83	0.42
1:A:490:PHE:N	1:A:491:PRO:CD	2.83	0.41
1:A:886:TRP:HB2	1:A:890:ALA:HB3	2.01	0.41
1:A:1039:ARG:HB2	1:A:1042:PHE:HB3	2.01	0.41
1:C:664:ILE:O	1:C:671:CYS:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:SER:OG	1:A:95:THR:N	2.50	0.41
1:C:29:THR:N	1:C:62:VAL:O	2.54	0.41
1:C:1133:VAL:O	1:C:1134:ASN:CG	2.63	0.41
1:A:58:PHE:N	1:A:58:PHE:CD1	2.84	0.41
1:A:111:ASP:O	1:A:112:SER:C	2.63	0.41
1:B:907:ASN:HA	1:B:911:VAL:O	2.20	0.41
1:C:374:PHE:O	1:C:377:PHE:CE1	2.73	0.41
1:B:985:ASN:CG	1:B:987:PRO:HG2	2.43	0.41
1:B:695:TYR:CD1	1:B:695:TYR:N	2.88	0.41
1:C:400:PHE:CG	1:C:401:VAL:N	2.89	0.41
1:A:327:VAL:HG21	1:A:528:LYS:HG3	2.02	0.41
1:A:407:VAL:C	1:A:409:GLN:N	2.77	0.41
1:A:808:ASP:N	1:A:809:PRO:CD	2.84	0.41
1:B:308:VAL:H	1:B:602:THR:HG22	1.86	0.41
1:B:539:VAL:CG1	1:B:540:ASN:N	2.84	0.41
1:C:303:LEU:O	1:C:303:LEU:CG	2.69	0.41
1:C:373:SER:C	1:C:374:PHE:O	2.62	0.41
1:C:1089:PHE:O	1:C:1090:PRO:C	2.61	0.41
1:A:566:GLY:HA2	1:B:43:PHE:H	1.85	0.41
1:A:855:PHE:HB3	1:C:589:PRO:HG2	2.03	0.41
1:A:711:SER:O	1:B:897:PRO:HD3	2.20	0.40
1:B:620:VAL:N	1:B:621:PRO:CD	2.84	0.40
1:C:797:PHE:O	1:C:798:GLY:C	2.64	0.40
1:A:354:ASN:O	1:A:397:ALA:HA	2.22	0.40
1:B:986:PRO:N	1:B:987:PRO:HD2	2.36	0.40
1:B:43:PHE:CD1	1:B:43:PHE:C	2.98	0.40
1:A:201:PHE:O	1:A:228:ASP:HA	2.21	0.40
1:A:490:PHE:N	1:A:491:PRO:HD2	2.36	0.40
1:A:294:ASP:HA	1:A:628:GLN:HG2	2.04	0.40
1:A:336:CYS:SG	1:A:338:PHE:HB3	2.61	0.40
1:B:376:THR:HA	1:B:435:ALA:C	2.47	0.40
1:C:1103:PHE:HE1	1:C:1110:TYR:OH	2.01	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	919/1243 (74%)	851 (93%)	68 (7%)	0	100	100
1	B	880/1243 (71%)	861 (98%)	19 (2%)	0	100	100
1	C	942/1243 (76%)	903 (96%)	39 (4%)	0	100	100
All	All	2741/3729 (74%)	2615 (95%)	126 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	336/1084 (31%)	335 (100%)	1 (0%)	86	83
1	B	281/1084 (26%)	281 (100%)	0	100	100
1	C	301/1084 (28%)	300 (100%)	1 (0%)	86	83
All	All	918/3252 (28%)	916 (100%)	2 (0%)	85	86

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	797	PHE
1	C	738	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	314	GLN
1	A	321	GLN
1	A	343	ASN
1	A	801	ASN

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Mol	Chain	Res	Type
1	C	641	ASN
1	C	717	ASN
1	C	1064	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.

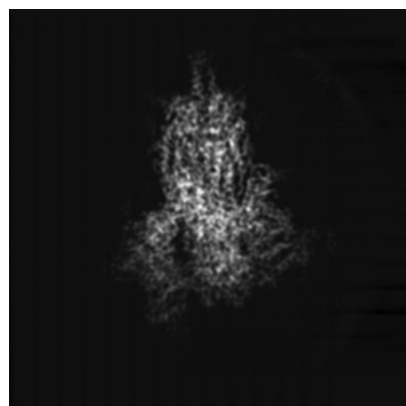
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29035. These allow visual inspection of the internal detail of the map and identification of artifacts.

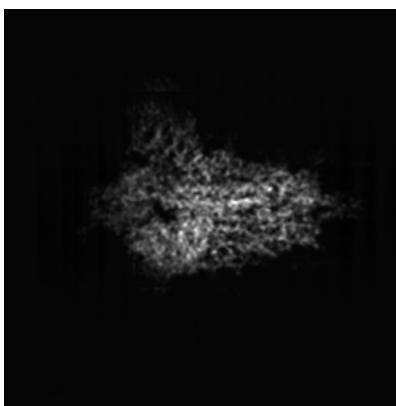
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

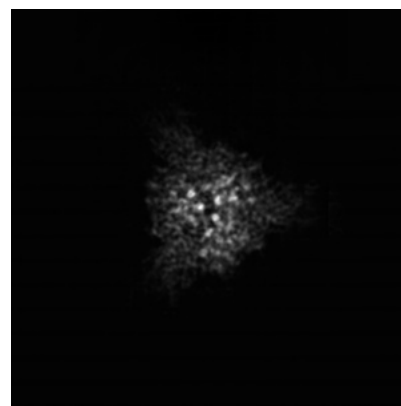
6.1.1 Primary map



X

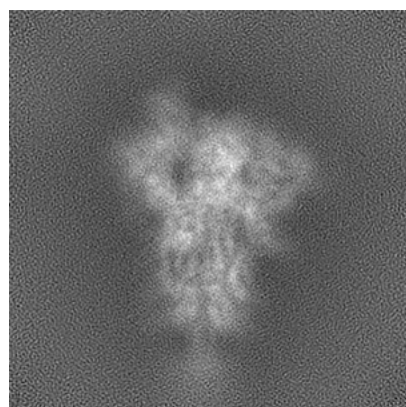


Y

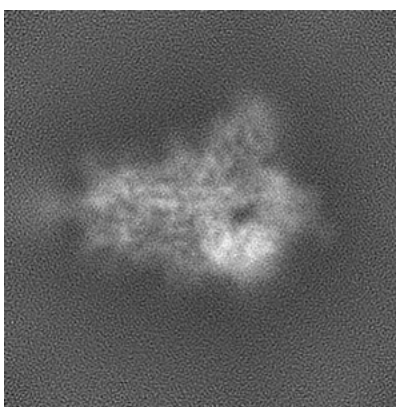


Z

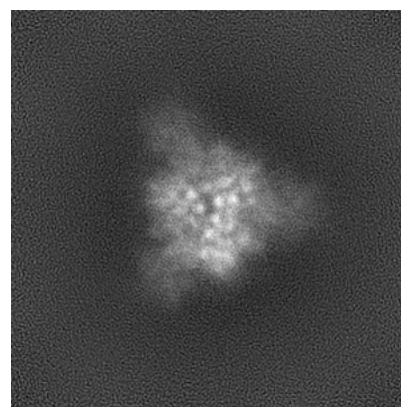
6.1.2 Raw map



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: 128

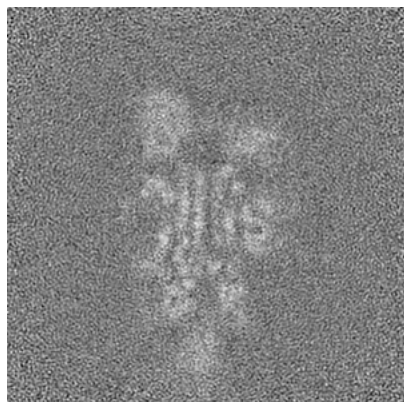


Y Index: 128



Z Index: 128

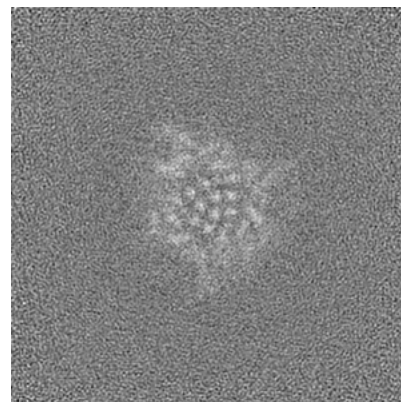
6.2.2 Raw map



X Index: 128



Y Index: 128



Z Index: 128

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: 132

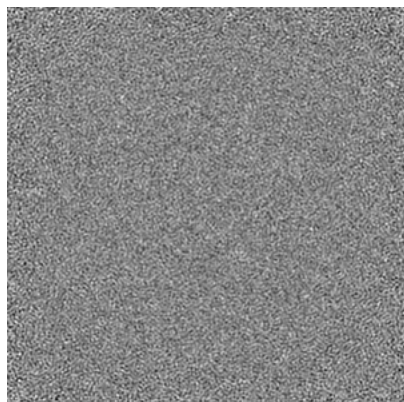


Y Index: 133

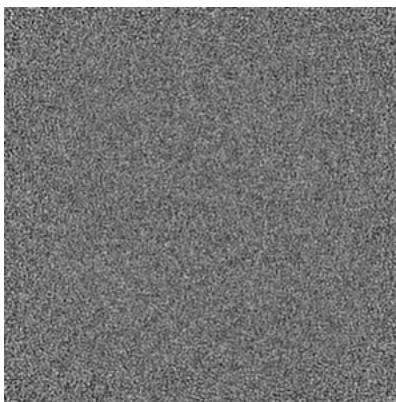


Z Index: 123

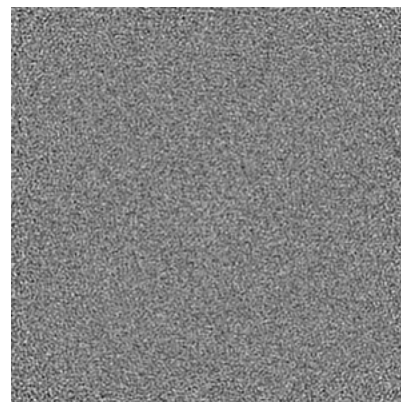
6.3.2 Raw map



X Index: 0



Y Index: 0

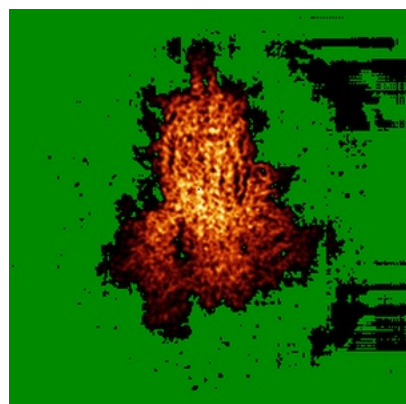


Z Index: 0

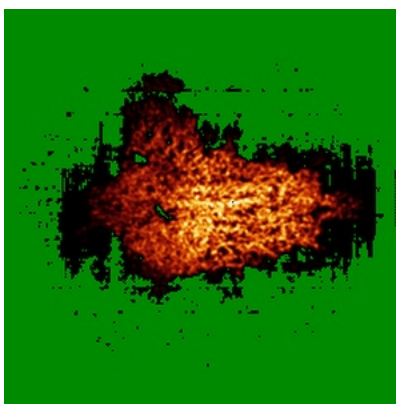
The images above show the largest variance slices of the map in three orthogonal directions.

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

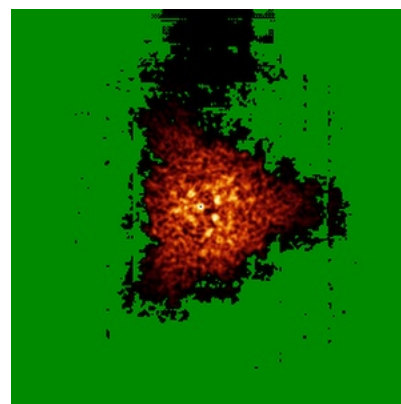
6.4.1 Primary map



X

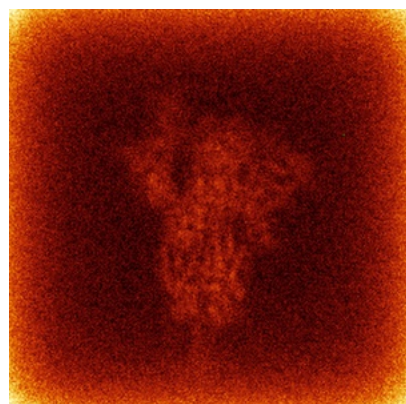


Y

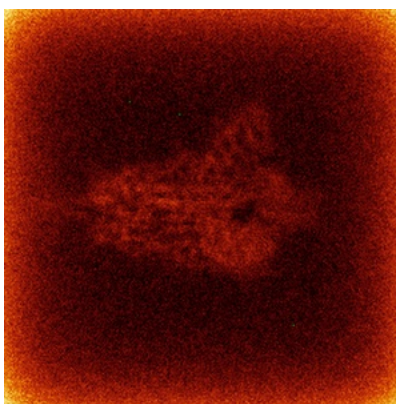


Z

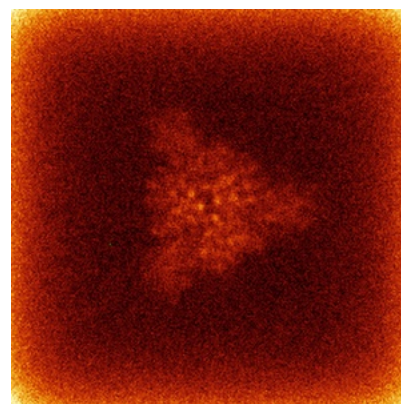
6.4.2 Raw map



X



Y



Z

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

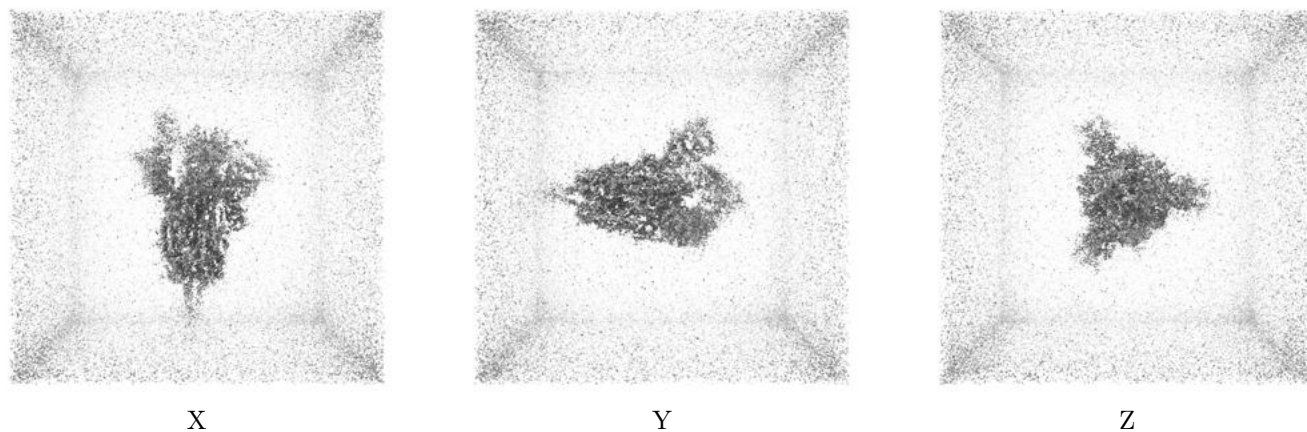
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

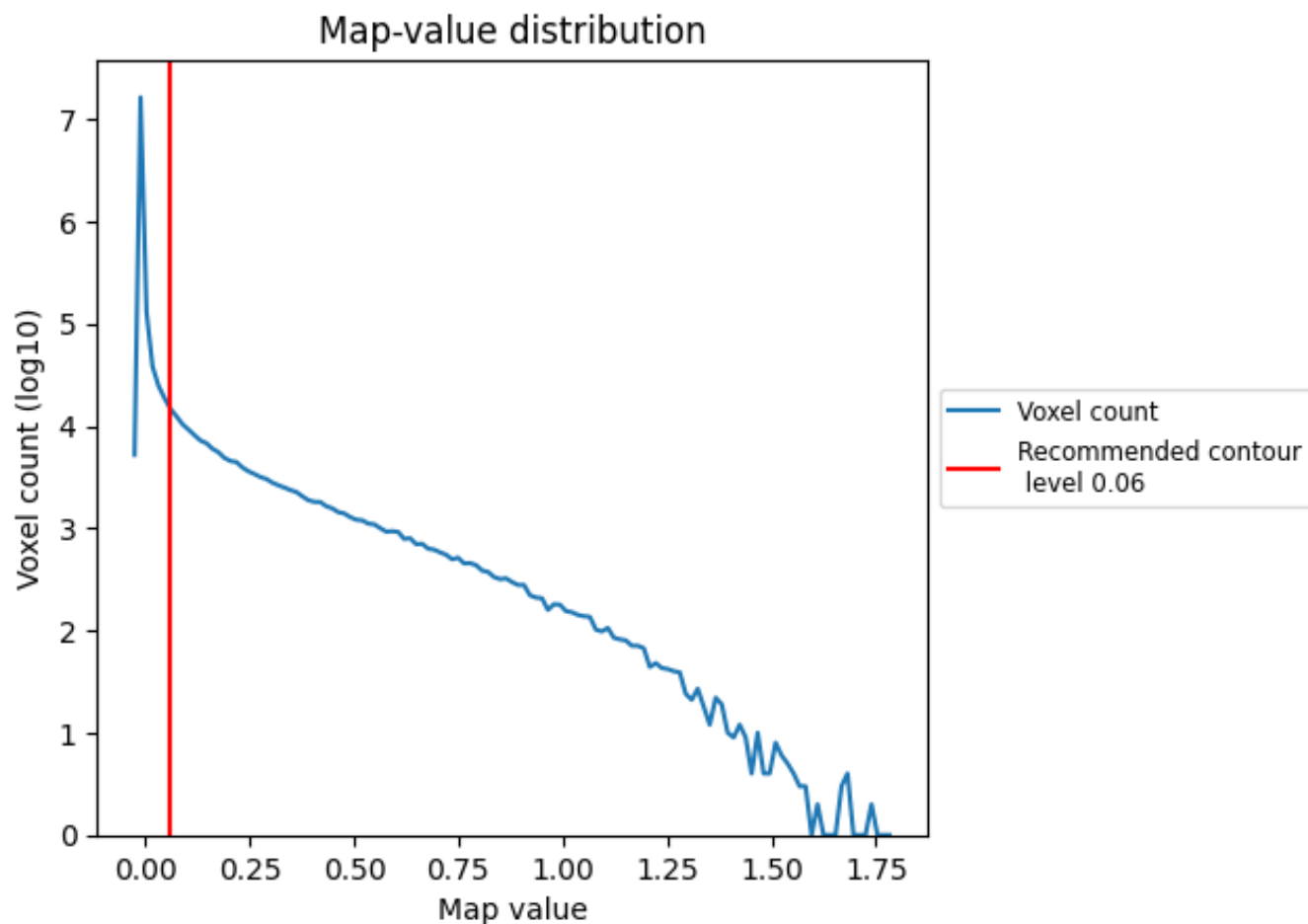
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

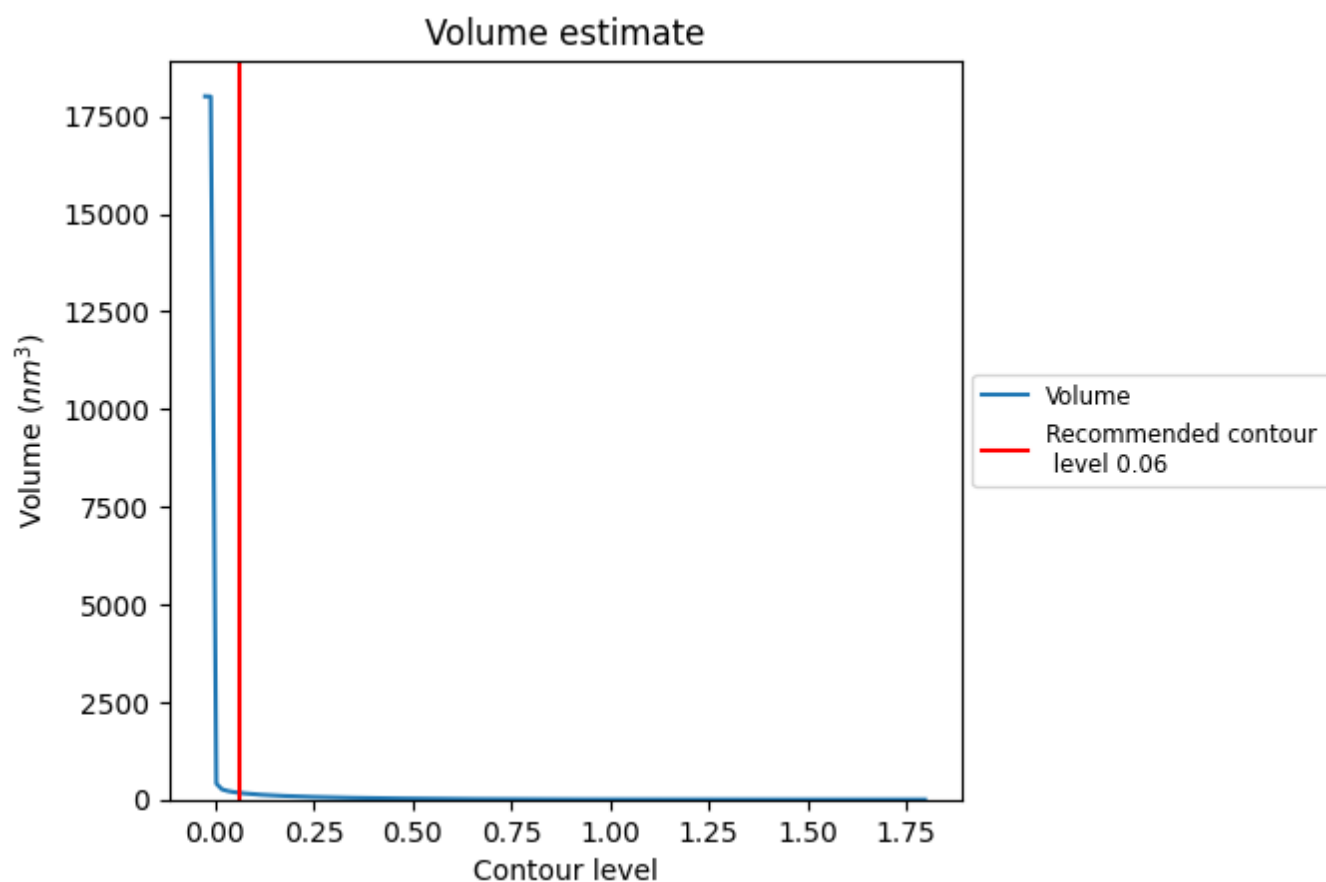
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

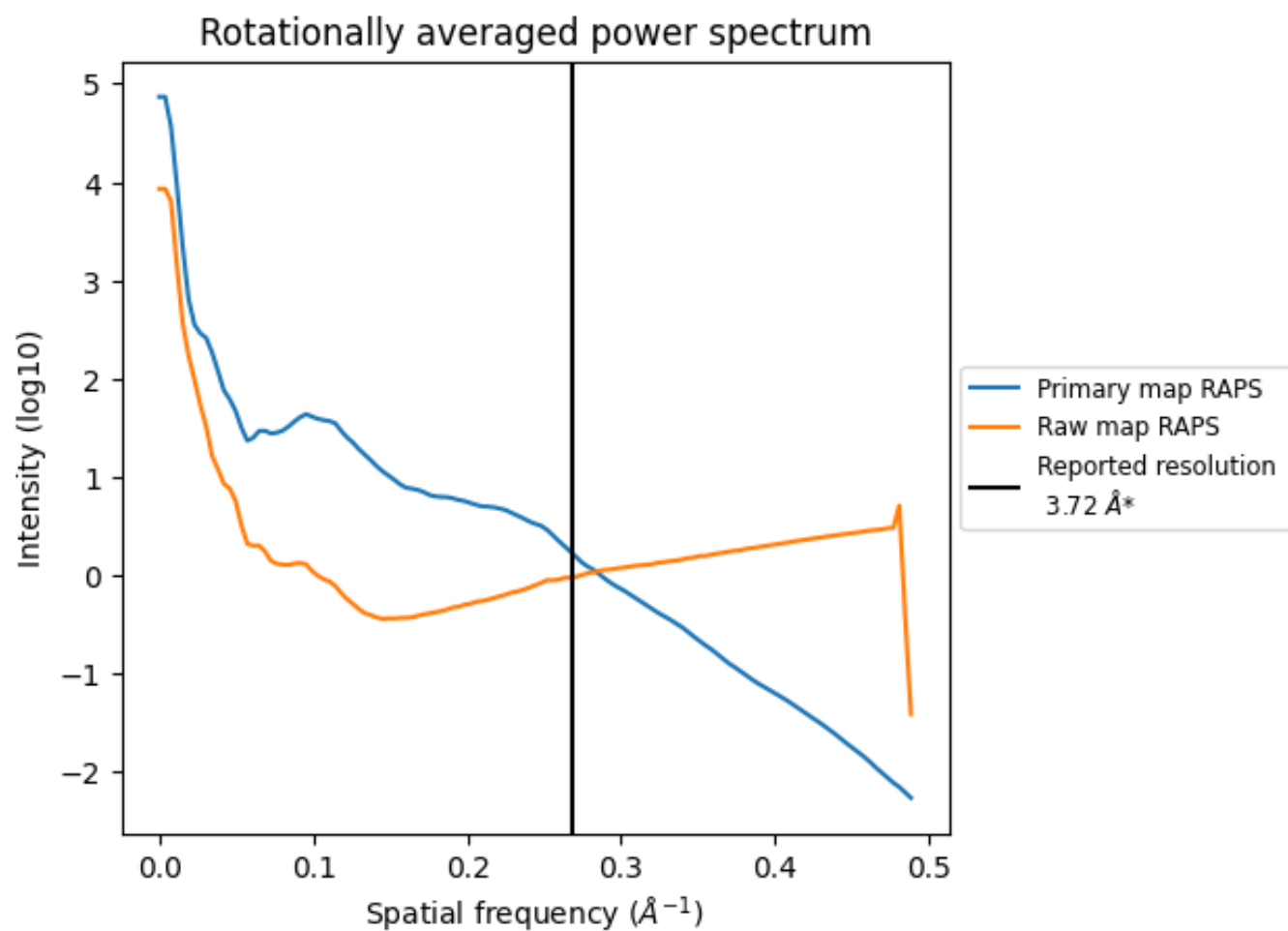
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 174 nm^3 ; this corresponds to an approximate mass of 157 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 ⓘ

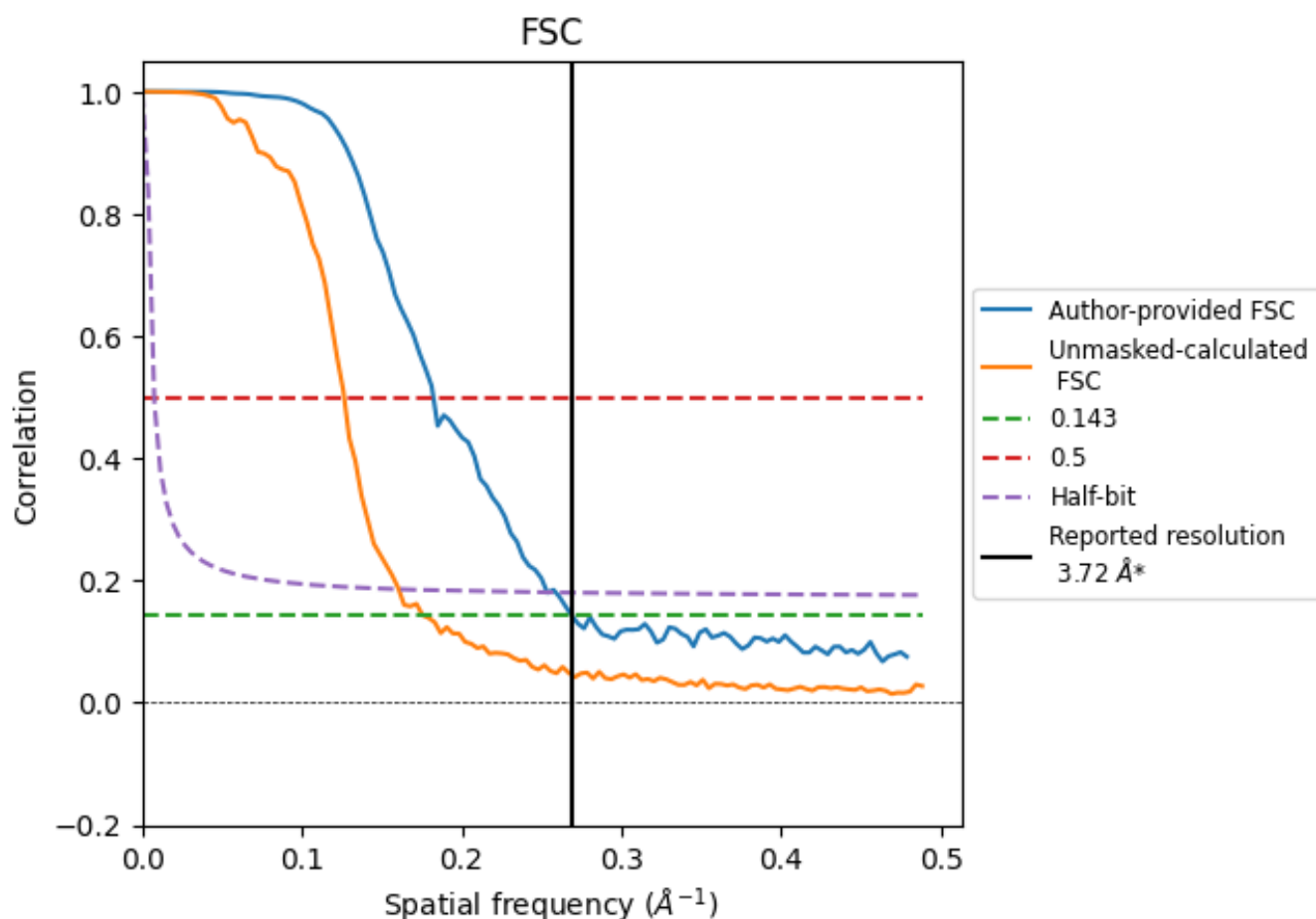


*Reported resolution corresponds to spatial frequency of $0.269 \text{ \AA}^{-1}$

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 0.269 Å⁻¹

8.2 Resolution estimates [i](#)

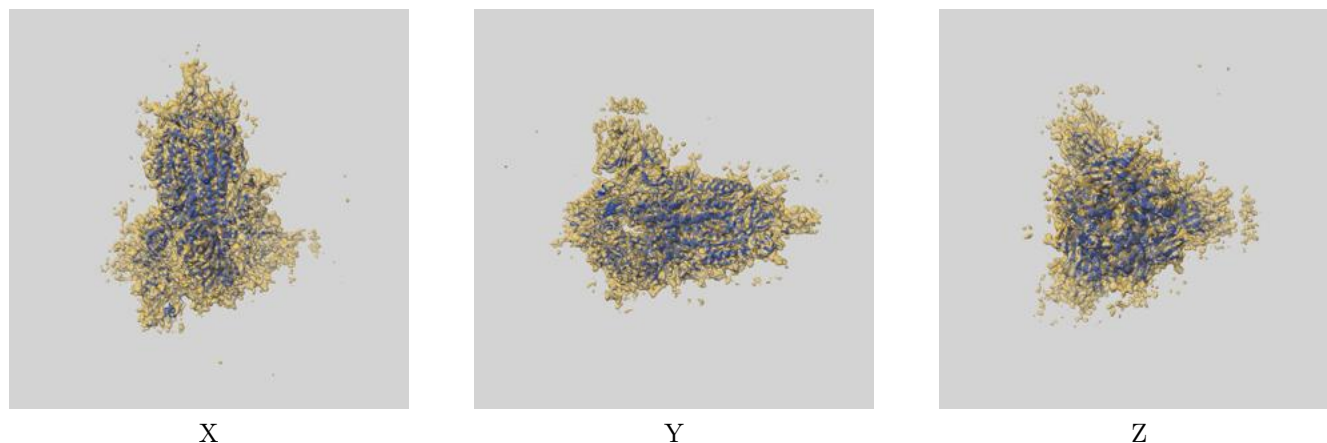
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.72	-	-
Author-provided FSC curve	3.72	5.49	3.94
Unmasked-calculated*	5.70	7.91	6.23

*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 5.70 differs from the reported value 3.72 by more than 10 %

9 Map-model fit [i](#)

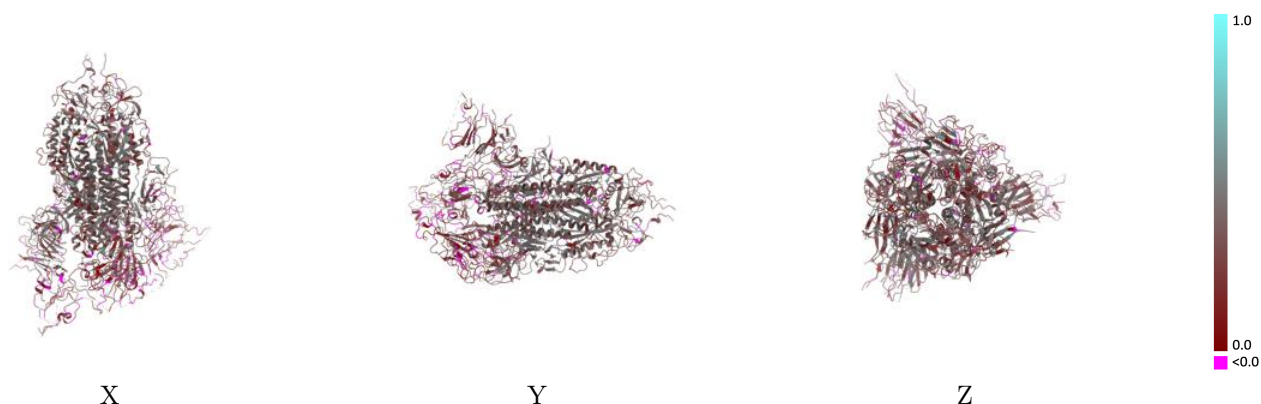
This section contains information regarding the fit between EMDB map EMD-29035 and PDB model 8FEZ. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



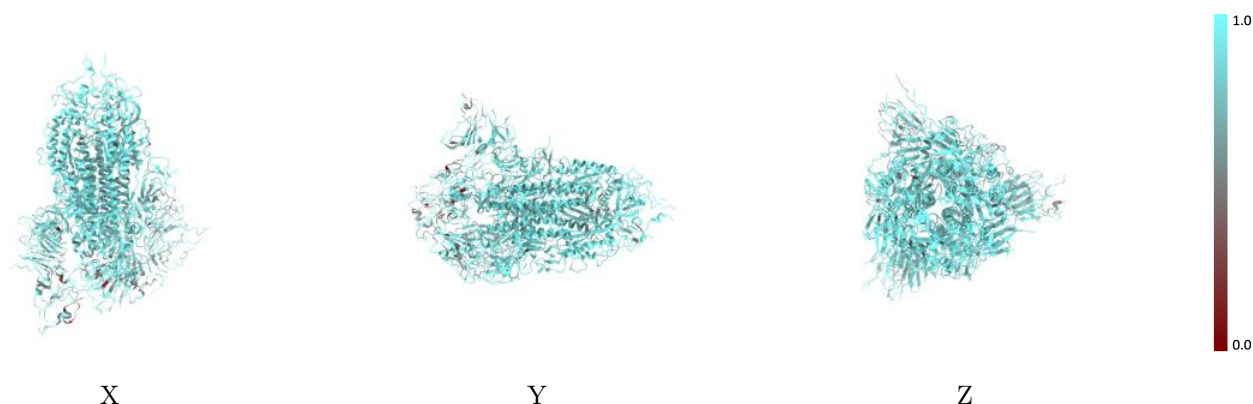
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



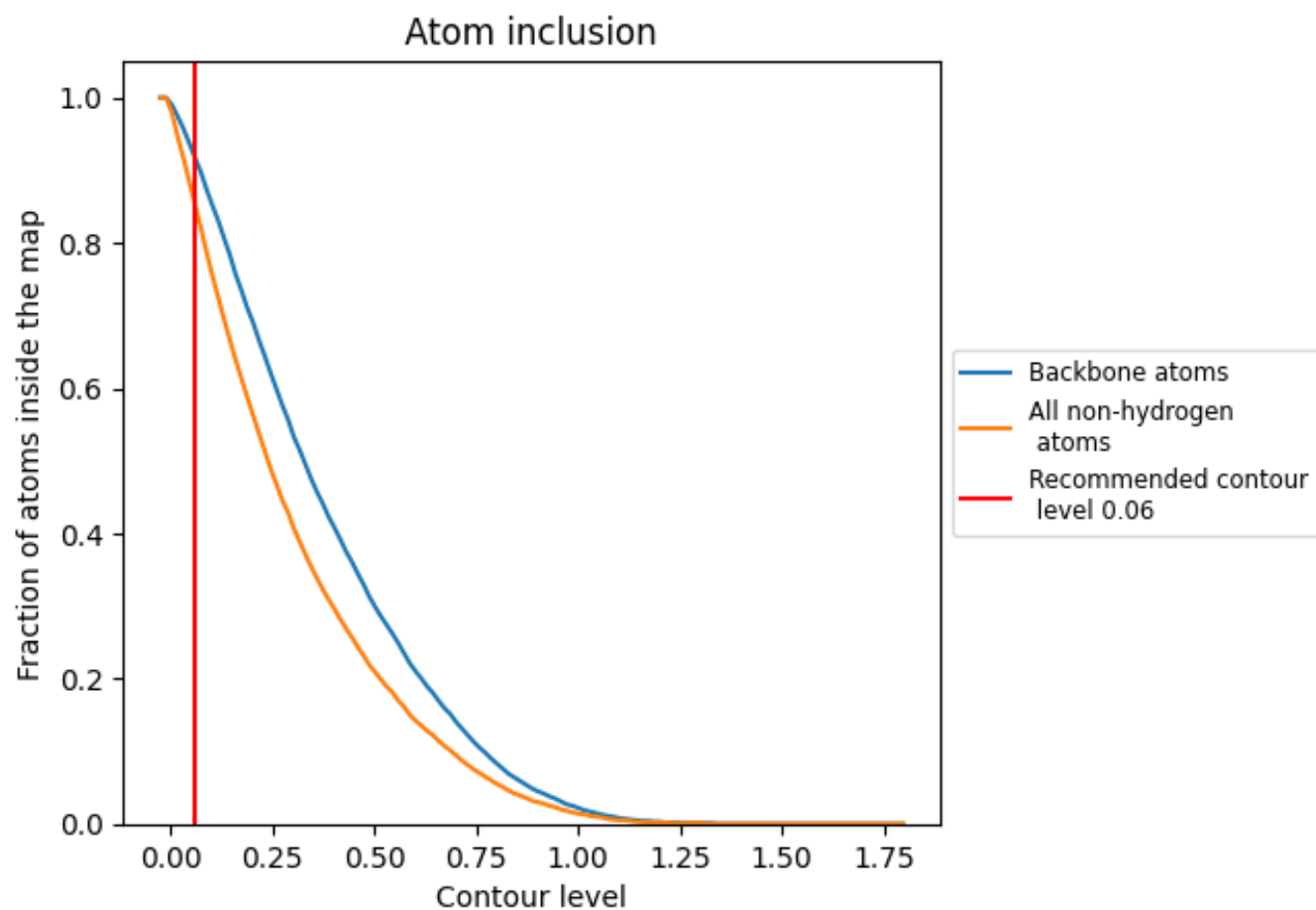
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.06).

9.4 Atom inclusion ⓘ



At the recommended contour level, 92% of all backbone atoms, 85% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8530	0.3120
A	0.8330	0.2990
B	0.8570	0.3200
C	0.8690	0.3170

