



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 11:30 AM UTC

PDB ID : 7TF4 / pdb_00007tf4
EMDB ID : EMD-25861
Title : Cryo-EM structure of SARS-CoV-2 Kappa (B.1.617.1) spike protein (focused refinement of RBD)
Authors : Zhu, X.; Saville, J.W.; Mannar, D.; Srivastava, S.S.; Berezuk, A.M.; Demers, J.P.; Zhou, S.; Tuttle, K.S.; Subramaniam, S.
Deposited on : 2022-01-06
Resolution : 3.01 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
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

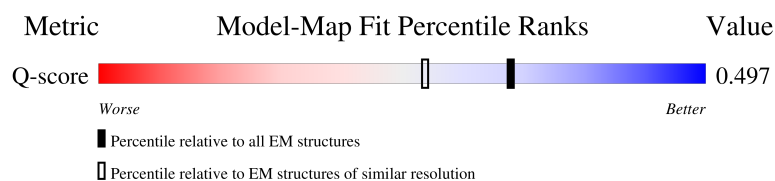
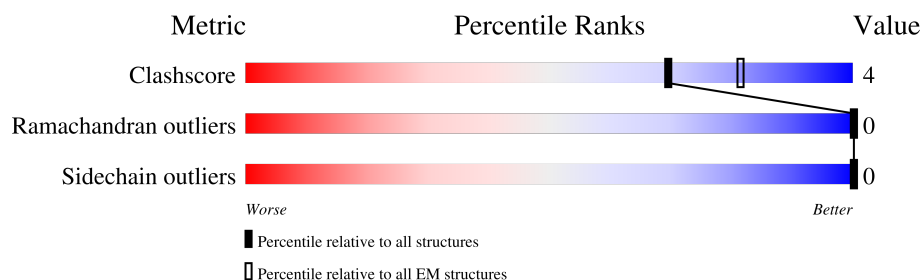
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.01 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	13882 (2.51 - 3.51)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1288	
1	B	1288	
1	C	1288	
1	D	1288	

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Mol	Chain	Length	Quality of chain
1	E	1288	 19% 79%
1	F	1288	 19% 79%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12792 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	268	Total	C	N	O	S	0	0
			2104	1345	354	396	9		
1	B	268	Total	C	N	O	S	0	0
			2104	1345	354	396	9		
1	C	268	Total	C	N	O	S	0	0
			2104	1345	354	396	9		
1	D	268	Total	C	N	O	S	0	0
			2104	1345	354	396	9		
1	E	268	Total	C	N	O	S	0	0
			2104	1345	354	396	9		
1	F	268	Total	C	N	O	S	0	0
			2104	1345	354	396	9		

There are 570 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	154	LYS	GLU	variant	UNP P0DTC2
A	452	ARG	LEU	variant	UNP P0DTC2
A	484	GLN	GLU	variant	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2
A	681	ARG	PRO	variant	UNP P0DTC2
A	682	GLY	ARG	variant	UNP P0DTC2
A	683	SER	ARG	variant	UNP P0DTC2
A	685	SER	ARG	variant	UNP P0DTC2
A	817	PRO	PHE	variant	UNP P0DTC2
A	892	PRO	ALA	variant	UNP P0DTC2
A	899	PRO	ALA	variant	UNP P0DTC2
A	942	PRO	ALA	variant	UNP P0DTC2
A	986	PRO	LYS	variant	UNP P0DTC2
A	987	PRO	VAL	variant	UNP P0DTC2
A	1071	HIS	GLN	variant	UNP P0DTC2
A	1209	GLY	-	expression tag	UNP P0DTC2
A	1210	SER	-	expression tag	UNP P0DTC2
A	1211	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1212	TYR	-	expression tag	UNP P0DTC2
A	1213	ILE	-	expression tag	UNP P0DTC2
A	1214	PRO	-	expression tag	UNP P0DTC2
A	1215	GLU	-	expression tag	UNP P0DTC2
A	1216	ALA	-	expression tag	UNP P0DTC2
A	1217	PRO	-	expression tag	UNP P0DTC2
A	1218	ARG	-	expression tag	UNP P0DTC2
A	1219	ASP	-	expression tag	UNP P0DTC2
A	1220	GLY	-	expression tag	UNP P0DTC2
A	1221	GLN	-	expression tag	UNP P0DTC2
A	1222	ALA	-	expression tag	UNP P0DTC2
A	1223	TYR	-	expression tag	UNP P0DTC2
A	1224	VAL	-	expression tag	UNP P0DTC2
A	1225	ARG	-	expression tag	UNP P0DTC2
A	1226	LYS	-	expression tag	UNP P0DTC2
A	1227	ASP	-	expression tag	UNP P0DTC2
A	1228	GLY	-	expression tag	UNP P0DTC2
A	1229	GLU	-	expression tag	UNP P0DTC2
A	1230	TRP	-	expression tag	UNP P0DTC2
A	1231	VAL	-	expression tag	UNP P0DTC2
A	1232	LEU	-	expression tag	UNP P0DTC2
A	1233	LEU	-	expression tag	UNP P0DTC2
A	1234	SER	-	expression tag	UNP P0DTC2
A	1235	THR	-	expression tag	UNP P0DTC2
A	1236	PHE	-	expression tag	UNP P0DTC2
A	1237	LEU	-	expression tag	UNP P0DTC2
A	1238	GLY	-	expression tag	UNP P0DTC2
A	1239	ARG	-	expression tag	UNP P0DTC2
A	1240	SER	-	expression tag	UNP P0DTC2
A	1241	LEU	-	expression tag	UNP P0DTC2
A	1242	GLU	-	expression tag	UNP P0DTC2
A	1243	VAL	-	expression tag	UNP P0DTC2
A	1244	LEU	-	expression tag	UNP P0DTC2
A	1245	PHE	-	expression tag	UNP P0DTC2
A	1246	GLN	-	expression tag	UNP P0DTC2
A	1247	GLY	-	expression tag	UNP P0DTC2
A	1248	PRO	-	expression tag	UNP P0DTC2
A	1249	GLY	-	expression tag	UNP P0DTC2
A	1250	HIS	-	expression tag	UNP P0DTC2
A	1251	HIS	-	expression tag	UNP P0DTC2
A	1252	HIS	-	expression tag	UNP P0DTC2
A	1253	HIS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1254	HIS	-	expression tag	UNP P0DTC2
A	1255	HIS	-	expression tag	UNP P0DTC2
A	1256	HIS	-	expression tag	UNP P0DTC2
A	1257	HIS	-	expression tag	UNP P0DTC2
A	1258	SER	-	expression tag	UNP P0DTC2
A	1259	ALA	-	expression tag	UNP P0DTC2
A	1260	TRP	-	expression tag	UNP P0DTC2
A	1261	SER	-	expression tag	UNP P0DTC2
A	1262	HIS	-	expression tag	UNP P0DTC2
A	1263	PRO	-	expression tag	UNP P0DTC2
A	1264	GLN	-	expression tag	UNP P0DTC2
A	1265	PHE	-	expression tag	UNP P0DTC2
A	1266	GLU	-	expression tag	UNP P0DTC2
A	1267	LYS	-	expression tag	UNP P0DTC2
A	1268	GLY	-	expression tag	UNP P0DTC2
A	1269	GLY	-	expression tag	UNP P0DTC2
A	1270	GLY	-	expression tag	UNP P0DTC2
A	1271	SER	-	expression tag	UNP P0DTC2
A	1272	GLY	-	expression tag	UNP P0DTC2
A	1273	GLY	-	expression tag	UNP P0DTC2
A	1274	GLY	-	expression tag	UNP P0DTC2
A	1275	GLY	-	expression tag	UNP P0DTC2
A	1276	SER	-	expression tag	UNP P0DTC2
A	1277	GLY	-	expression tag	UNP P0DTC2
A	1278	GLY	-	expression tag	UNP P0DTC2
A	1279	SER	-	expression tag	UNP P0DTC2
A	1280	ALA	-	expression tag	UNP P0DTC2
A	1281	TRP	-	expression tag	UNP P0DTC2
A	1282	SER	-	expression tag	UNP P0DTC2
A	1283	HIS	-	expression tag	UNP P0DTC2
A	1284	PRO	-	expression tag	UNP P0DTC2
A	1285	GLN	-	expression tag	UNP P0DTC2
A	1286	PHE	-	expression tag	UNP P0DTC2
A	1287	GLU	-	expression tag	UNP P0DTC2
A	1288	LYS	-	expression tag	UNP P0DTC2
B	154	LYS	GLU	variant	UNP P0DTC2
B	452	ARG	LEU	variant	UNP P0DTC2
B	484	GLN	GLU	variant	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2
B	681	ARG	PRO	variant	UNP P0DTC2
B	682	GLY	ARG	variant	UNP P0DTC2
B	683	SER	ARG	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	685	SER	ARG	variant	UNP P0DTC2
B	817	PRO	PHE	variant	UNP P0DTC2
B	892	PRO	ALA	variant	UNP P0DTC2
B	899	PRO	ALA	variant	UNP P0DTC2
B	942	PRO	ALA	variant	UNP P0DTC2
B	986	PRO	LYS	variant	UNP P0DTC2
B	987	PRO	VAL	variant	UNP P0DTC2
B	1071	HIS	GLN	variant	UNP P0DTC2
B	1209	GLY	-	expression tag	UNP P0DTC2
B	1210	SER	-	expression tag	UNP P0DTC2
B	1211	GLY	-	expression tag	UNP P0DTC2
B	1212	TYR	-	expression tag	UNP P0DTC2
B	1213	ILE	-	expression tag	UNP P0DTC2
B	1214	PRO	-	expression tag	UNP P0DTC2
B	1215	GLU	-	expression tag	UNP P0DTC2
B	1216	ALA	-	expression tag	UNP P0DTC2
B	1217	PRO	-	expression tag	UNP P0DTC2
B	1218	ARG	-	expression tag	UNP P0DTC2
B	1219	ASP	-	expression tag	UNP P0DTC2
B	1220	GLY	-	expression tag	UNP P0DTC2
B	1221	GLN	-	expression tag	UNP P0DTC2
B	1222	ALA	-	expression tag	UNP P0DTC2
B	1223	TYR	-	expression tag	UNP P0DTC2
B	1224	VAL	-	expression tag	UNP P0DTC2
B	1225	ARG	-	expression tag	UNP P0DTC2
B	1226	LYS	-	expression tag	UNP P0DTC2
B	1227	ASP	-	expression tag	UNP P0DTC2
B	1228	GLY	-	expression tag	UNP P0DTC2
B	1229	GLU	-	expression tag	UNP P0DTC2
B	1230	TRP	-	expression tag	UNP P0DTC2
B	1231	VAL	-	expression tag	UNP P0DTC2
B	1232	LEU	-	expression tag	UNP P0DTC2
B	1233	LEU	-	expression tag	UNP P0DTC2
B	1234	SER	-	expression tag	UNP P0DTC2
B	1235	THR	-	expression tag	UNP P0DTC2
B	1236	PHE	-	expression tag	UNP P0DTC2
B	1237	LEU	-	expression tag	UNP P0DTC2
B	1238	GLY	-	expression tag	UNP P0DTC2
B	1239	ARG	-	expression tag	UNP P0DTC2
B	1240	SER	-	expression tag	UNP P0DTC2
B	1241	LEU	-	expression tag	UNP P0DTC2
B	1242	GLU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1243	VAL	-	expression tag	UNP P0DTC2
B	1244	LEU	-	expression tag	UNP P0DTC2
B	1245	PHE	-	expression tag	UNP P0DTC2
B	1246	GLN	-	expression tag	UNP P0DTC2
B	1247	GLY	-	expression tag	UNP P0DTC2
B	1248	PRO	-	expression tag	UNP P0DTC2
B	1249	GLY	-	expression tag	UNP P0DTC2
B	1250	HIS	-	expression tag	UNP P0DTC2
B	1251	HIS	-	expression tag	UNP P0DTC2
B	1252	HIS	-	expression tag	UNP P0DTC2
B	1253	HIS	-	expression tag	UNP P0DTC2
B	1254	HIS	-	expression tag	UNP P0DTC2
B	1255	HIS	-	expression tag	UNP P0DTC2
B	1256	HIS	-	expression tag	UNP P0DTC2
B	1257	HIS	-	expression tag	UNP P0DTC2
B	1258	SER	-	expression tag	UNP P0DTC2
B	1259	ALA	-	expression tag	UNP P0DTC2
B	1260	TRP	-	expression tag	UNP P0DTC2
B	1261	SER	-	expression tag	UNP P0DTC2
B	1262	HIS	-	expression tag	UNP P0DTC2
B	1263	PRO	-	expression tag	UNP P0DTC2
B	1264	GLN	-	expression tag	UNP P0DTC2
B	1265	PHE	-	expression tag	UNP P0DTC2
B	1266	GLU	-	expression tag	UNP P0DTC2
B	1267	LYS	-	expression tag	UNP P0DTC2
B	1268	GLY	-	expression tag	UNP P0DTC2
B	1269	GLY	-	expression tag	UNP P0DTC2
B	1270	GLY	-	expression tag	UNP P0DTC2
B	1271	SER	-	expression tag	UNP P0DTC2
B	1272	GLY	-	expression tag	UNP P0DTC2
B	1273	GLY	-	expression tag	UNP P0DTC2
B	1274	GLY	-	expression tag	UNP P0DTC2
B	1275	GLY	-	expression tag	UNP P0DTC2
B	1276	SER	-	expression tag	UNP P0DTC2
B	1277	GLY	-	expression tag	UNP P0DTC2
B	1278	GLY	-	expression tag	UNP P0DTC2
B	1279	SER	-	expression tag	UNP P0DTC2
B	1280	ALA	-	expression tag	UNP P0DTC2
B	1281	TRP	-	expression tag	UNP P0DTC2
B	1282	SER	-	expression tag	UNP P0DTC2
B	1283	HIS	-	expression tag	UNP P0DTC2
B	1284	PRO	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1285	GLN	-	expression tag	UNP P0DTC2
B	1286	PHE	-	expression tag	UNP P0DTC2
B	1287	GLU	-	expression tag	UNP P0DTC2
B	1288	LYS	-	expression tag	UNP P0DTC2
C	154	LYS	GLU	variant	UNP P0DTC2
C	452	ARG	LEU	variant	UNP P0DTC2
C	484	GLN	GLU	variant	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	681	ARG	PRO	variant	UNP P0DTC2
C	682	GLY	ARG	variant	UNP P0DTC2
C	683	SER	ARG	variant	UNP P0DTC2
C	685	SER	ARG	variant	UNP P0DTC2
C	817	PRO	PHE	variant	UNP P0DTC2
C	892	PRO	ALA	variant	UNP P0DTC2
C	899	PRO	ALA	variant	UNP P0DTC2
C	942	PRO	ALA	variant	UNP P0DTC2
C	986	PRO	LYS	variant	UNP P0DTC2
C	987	PRO	VAL	variant	UNP P0DTC2
C	1071	HIS	GLN	variant	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

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1232	LEU	-	expression tag	UNP P0DTC2
C	1233	LEU	-	expression tag	UNP P0DTC2
C	1234	SER	-	expression tag	UNP P0DTC2
C	1235	THR	-	expression tag	UNP P0DTC2
C	1236	PHE	-	expression tag	UNP P0DTC2
C	1237	LEU	-	expression tag	UNP P0DTC2
C	1238	GLY	-	expression tag	UNP P0DTC2
C	1239	ARG	-	expression tag	UNP P0DTC2
C	1240	SER	-	expression tag	UNP P0DTC2
C	1241	LEU	-	expression tag	UNP P0DTC2
C	1242	GLU	-	expression tag	UNP P0DTC2
C	1243	VAL	-	expression tag	UNP P0DTC2
C	1244	LEU	-	expression tag	UNP P0DTC2
C	1245	PHE	-	expression tag	UNP P0DTC2
C	1246	GLN	-	expression tag	UNP P0DTC2
C	1247	GLY	-	expression tag	UNP P0DTC2
C	1248	PRO	-	expression tag	UNP P0DTC2
C	1249	GLY	-	expression tag	UNP P0DTC2
C	1250	HIS	-	expression tag	UNP P0DTC2
C	1251	HIS	-	expression tag	UNP P0DTC2
C	1252	HIS	-	expression tag	UNP P0DTC2
C	1253	HIS	-	expression tag	UNP P0DTC2
C	1254	HIS	-	expression tag	UNP P0DTC2
C	1255	HIS	-	expression tag	UNP P0DTC2
C	1256	HIS	-	expression tag	UNP P0DTC2
C	1257	HIS	-	expression tag	UNP P0DTC2
C	1258	SER	-	expression tag	UNP P0DTC2
C	1259	ALA	-	expression tag	UNP P0DTC2
C	1260	TRP	-	expression tag	UNP P0DTC2
C	1261	SER	-	expression tag	UNP P0DTC2
C	1262	HIS	-	expression tag	UNP P0DTC2
C	1263	PRO	-	expression tag	UNP P0DTC2
C	1264	GLN	-	expression tag	UNP P0DTC2
C	1265	PHE	-	expression tag	UNP P0DTC2
C	1266	GLU	-	expression tag	UNP P0DTC2
C	1267	LYS	-	expression tag	UNP P0DTC2
C	1268	GLY	-	expression tag	UNP P0DTC2
C	1269	GLY	-	expression tag	UNP P0DTC2
C	1270	GLY	-	expression tag	UNP P0DTC2
C	1271	SER	-	expression tag	UNP P0DTC2
C	1272	GLY	-	expression tag	UNP P0DTC2
C	1273	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1274	GLY	-	expression tag	UNP P0DTC2
C	1275	GLY	-	expression tag	UNP P0DTC2
C	1276	SER	-	expression tag	UNP P0DTC2
C	1277	GLY	-	expression tag	UNP P0DTC2
C	1278	GLY	-	expression tag	UNP P0DTC2
C	1279	SER	-	expression tag	UNP P0DTC2
C	1280	ALA	-	expression tag	UNP P0DTC2
C	1281	TRP	-	expression tag	UNP P0DTC2
C	1282	SER	-	expression tag	UNP P0DTC2
C	1283	HIS	-	expression tag	UNP P0DTC2
C	1284	PRO	-	expression tag	UNP P0DTC2
C	1285	GLN	-	expression tag	UNP P0DTC2
C	1286	PHE	-	expression tag	UNP P0DTC2
C	1287	GLU	-	expression tag	UNP P0DTC2
C	1288	LYS	-	expression tag	UNP P0DTC2
D	154	LYS	GLU	variant	UNP P0DTC2
D	452	ARG	LEU	variant	UNP P0DTC2
D	484	GLN	GLU	variant	UNP P0DTC2
D	614	GLY	ASP	variant	UNP P0DTC2
D	681	ARG	PRO	variant	UNP P0DTC2
D	682	GLY	ARG	variant	UNP P0DTC2
D	683	SER	ARG	variant	UNP P0DTC2
D	685	SER	ARG	variant	UNP P0DTC2
D	817	PRO	PHE	variant	UNP P0DTC2
D	892	PRO	ALA	variant	UNP P0DTC2
D	899	PRO	ALA	variant	UNP P0DTC2
D	942	PRO	ALA	variant	UNP P0DTC2
D	986	PRO	LYS	variant	UNP P0DTC2
D	987	PRO	VAL	variant	UNP P0DTC2
D	1071	HIS	GLN	variant	UNP P0DTC2
D	1209	GLY	-	expression tag	UNP P0DTC2
D	1210	SER	-	expression tag	UNP P0DTC2
D	1211	GLY	-	expression tag	UNP P0DTC2
D	1212	TYR	-	expression tag	UNP P0DTC2
D	1213	ILE	-	expression tag	UNP P0DTC2
D	1214	PRO	-	expression tag	UNP P0DTC2
D	1215	GLU	-	expression tag	UNP P0DTC2
D	1216	ALA	-	expression tag	UNP P0DTC2
D	1217	PRO	-	expression tag	UNP P0DTC2
D	1218	ARG	-	expression tag	UNP P0DTC2
D	1219	ASP	-	expression tag	UNP P0DTC2
D	1220	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1221	GLN	-	expression tag	UNP P0DTC2
D	1222	ALA	-	expression tag	UNP P0DTC2
D	1223	TYR	-	expression tag	UNP P0DTC2
D	1224	VAL	-	expression tag	UNP P0DTC2
D	1225	ARG	-	expression tag	UNP P0DTC2
D	1226	LYS	-	expression tag	UNP P0DTC2
D	1227	ASP	-	expression tag	UNP P0DTC2
D	1228	GLY	-	expression tag	UNP P0DTC2
D	1229	GLU	-	expression tag	UNP P0DTC2
D	1230	TRP	-	expression tag	UNP P0DTC2
D	1231	VAL	-	expression tag	UNP P0DTC2
D	1232	LEU	-	expression tag	UNP P0DTC2
D	1233	LEU	-	expression tag	UNP P0DTC2
D	1234	SER	-	expression tag	UNP P0DTC2
D	1235	THR	-	expression tag	UNP P0DTC2
D	1236	PHE	-	expression tag	UNP P0DTC2
D	1237	LEU	-	expression tag	UNP P0DTC2
D	1238	GLY	-	expression tag	UNP P0DTC2
D	1239	ARG	-	expression tag	UNP P0DTC2
D	1240	SER	-	expression tag	UNP P0DTC2
D	1241	LEU	-	expression tag	UNP P0DTC2
D	1242	GLU	-	expression tag	UNP P0DTC2
D	1243	VAL	-	expression tag	UNP P0DTC2
D	1244	LEU	-	expression tag	UNP P0DTC2
D	1245	PHE	-	expression tag	UNP P0DTC2
D	1246	GLN	-	expression tag	UNP P0DTC2
D	1247	GLY	-	expression tag	UNP P0DTC2
D	1248	PRO	-	expression tag	UNP P0DTC2
D	1249	GLY	-	expression tag	UNP P0DTC2
D	1250	HIS	-	expression tag	UNP P0DTC2
D	1251	HIS	-	expression tag	UNP P0DTC2
D	1252	HIS	-	expression tag	UNP P0DTC2
D	1253	HIS	-	expression tag	UNP P0DTC2
D	1254	HIS	-	expression tag	UNP P0DTC2
D	1255	HIS	-	expression tag	UNP P0DTC2
D	1256	HIS	-	expression tag	UNP P0DTC2
D	1257	HIS	-	expression tag	UNP P0DTC2
D	1258	SER	-	expression tag	UNP P0DTC2
D	1259	ALA	-	expression tag	UNP P0DTC2
D	1260	TRP	-	expression tag	UNP P0DTC2
D	1261	SER	-	expression tag	UNP P0DTC2
D	1262	HIS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1263	PRO	-	expression tag	UNP P0DTC2
D	1264	GLN	-	expression tag	UNP P0DTC2
D	1265	PHE	-	expression tag	UNP P0DTC2
D	1266	GLU	-	expression tag	UNP P0DTC2
D	1267	LYS	-	expression tag	UNP P0DTC2
D	1268	GLY	-	expression tag	UNP P0DTC2
D	1269	GLY	-	expression tag	UNP P0DTC2
D	1270	GLY	-	expression tag	UNP P0DTC2
D	1271	SER	-	expression tag	UNP P0DTC2
D	1272	GLY	-	expression tag	UNP P0DTC2
D	1273	GLY	-	expression tag	UNP P0DTC2
D	1274	GLY	-	expression tag	UNP P0DTC2
D	1275	GLY	-	expression tag	UNP P0DTC2
D	1276	SER	-	expression tag	UNP P0DTC2
D	1277	GLY	-	expression tag	UNP P0DTC2
D	1278	GLY	-	expression tag	UNP P0DTC2
D	1279	SER	-	expression tag	UNP P0DTC2
D	1280	ALA	-	expression tag	UNP P0DTC2
D	1281	TRP	-	expression tag	UNP P0DTC2
D	1282	SER	-	expression tag	UNP P0DTC2
D	1283	HIS	-	expression tag	UNP P0DTC2
D	1284	PRO	-	expression tag	UNP P0DTC2
D	1285	GLN	-	expression tag	UNP P0DTC2
D	1286	PHE	-	expression tag	UNP P0DTC2
D	1287	GLU	-	expression tag	UNP P0DTC2
D	1288	LYS	-	expression tag	UNP P0DTC2
E	154	LYS	GLU	variant	UNP P0DTC2
E	452	ARG	LEU	variant	UNP P0DTC2
E	484	GLN	GLU	variant	UNP P0DTC2
E	614	GLY	ASP	variant	UNP P0DTC2
E	681	ARG	PRO	variant	UNP P0DTC2
E	682	GLY	ARG	variant	UNP P0DTC2
E	683	SER	ARG	variant	UNP P0DTC2
E	685	SER	ARG	variant	UNP P0DTC2
E	817	PRO	PHE	variant	UNP P0DTC2
E	892	PRO	ALA	variant	UNP P0DTC2
E	899	PRO	ALA	variant	UNP P0DTC2
E	942	PRO	ALA	variant	UNP P0DTC2
E	986	PRO	LYS	variant	UNP P0DTC2
E	987	PRO	VAL	variant	UNP P0DTC2
E	1071	HIS	GLN	variant	UNP P0DTC2
E	1209	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
E	1210	SER	-	expression tag	UNP P0DTC2
E	1211	GLY	-	expression tag	UNP P0DTC2
E	1212	TYR	-	expression tag	UNP P0DTC2
E	1213	ILE	-	expression tag	UNP P0DTC2
E	1214	PRO	-	expression tag	UNP P0DTC2
E	1215	GLU	-	expression tag	UNP P0DTC2
E	1216	ALA	-	expression tag	UNP P0DTC2
E	1217	PRO	-	expression tag	UNP P0DTC2
E	1218	ARG	-	expression tag	UNP P0DTC2
E	1219	ASP	-	expression tag	UNP P0DTC2
E	1220	GLY	-	expression tag	UNP P0DTC2
E	1221	GLN	-	expression tag	UNP P0DTC2
E	1222	ALA	-	expression tag	UNP P0DTC2
E	1223	TYR	-	expression tag	UNP P0DTC2
E	1224	VAL	-	expression tag	UNP P0DTC2
E	1225	ARG	-	expression tag	UNP P0DTC2
E	1226	LYS	-	expression tag	UNP P0DTC2
E	1227	ASP	-	expression tag	UNP P0DTC2
E	1228	GLY	-	expression tag	UNP P0DTC2
E	1229	GLU	-	expression tag	UNP P0DTC2
E	1230	TRP	-	expression tag	UNP P0DTC2
E	1231	VAL	-	expression tag	UNP P0DTC2
E	1232	LEU	-	expression tag	UNP P0DTC2
E	1233	LEU	-	expression tag	UNP P0DTC2
E	1234	SER	-	expression tag	UNP P0DTC2
E	1235	THR	-	expression tag	UNP P0DTC2
E	1236	PHE	-	expression tag	UNP P0DTC2
E	1237	LEU	-	expression tag	UNP P0DTC2
E	1238	GLY	-	expression tag	UNP P0DTC2
E	1239	ARG	-	expression tag	UNP P0DTC2
E	1240	SER	-	expression tag	UNP P0DTC2
E	1241	LEU	-	expression tag	UNP P0DTC2
E	1242	GLU	-	expression tag	UNP P0DTC2
E	1243	VAL	-	expression tag	UNP P0DTC2
E	1244	LEU	-	expression tag	UNP P0DTC2
E	1245	PHE	-	expression tag	UNP P0DTC2
E	1246	GLN	-	expression tag	UNP P0DTC2
E	1247	GLY	-	expression tag	UNP P0DTC2
E	1248	PRO	-	expression tag	UNP P0DTC2
E	1249	GLY	-	expression tag	UNP P0DTC2
E	1250	HIS	-	expression tag	UNP P0DTC2
E	1251	HIS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
E	1252	HIS	-	expression tag	UNP P0DTC2
E	1253	HIS	-	expression tag	UNP P0DTC2
E	1254	HIS	-	expression tag	UNP P0DTC2
E	1255	HIS	-	expression tag	UNP P0DTC2
E	1256	HIS	-	expression tag	UNP P0DTC2
E	1257	HIS	-	expression tag	UNP P0DTC2
E	1258	SER	-	expression tag	UNP P0DTC2
E	1259	ALA	-	expression tag	UNP P0DTC2
E	1260	TRP	-	expression tag	UNP P0DTC2
E	1261	SER	-	expression tag	UNP P0DTC2
E	1262	HIS	-	expression tag	UNP P0DTC2
E	1263	PRO	-	expression tag	UNP P0DTC2
E	1264	GLN	-	expression tag	UNP P0DTC2
E	1265	PHE	-	expression tag	UNP P0DTC2
E	1266	GLU	-	expression tag	UNP P0DTC2
E	1267	LYS	-	expression tag	UNP P0DTC2
E	1268	GLY	-	expression tag	UNP P0DTC2
E	1269	GLY	-	expression tag	UNP P0DTC2
E	1270	GLY	-	expression tag	UNP P0DTC2
E	1271	SER	-	expression tag	UNP P0DTC2
E	1272	GLY	-	expression tag	UNP P0DTC2
E	1273	GLY	-	expression tag	UNP P0DTC2
E	1274	GLY	-	expression tag	UNP P0DTC2
E	1275	GLY	-	expression tag	UNP P0DTC2
E	1276	SER	-	expression tag	UNP P0DTC2
E	1277	GLY	-	expression tag	UNP P0DTC2
E	1278	GLY	-	expression tag	UNP P0DTC2
E	1279	SER	-	expression tag	UNP P0DTC2
E	1280	ALA	-	expression tag	UNP P0DTC2
E	1281	TRP	-	expression tag	UNP P0DTC2
E	1282	SER	-	expression tag	UNP P0DTC2
E	1283	HIS	-	expression tag	UNP P0DTC2
E	1284	PRO	-	expression tag	UNP P0DTC2
E	1285	GLN	-	expression tag	UNP P0DTC2
E	1286	PHE	-	expression tag	UNP P0DTC2
E	1287	GLU	-	expression tag	UNP P0DTC2
E	1288	LYS	-	expression tag	UNP P0DTC2
F	154	LYS	GLU	variant	UNP P0DTC2
F	452	ARG	LEU	variant	UNP P0DTC2
F	484	GLN	GLU	variant	UNP P0DTC2
F	614	GLY	ASP	variant	UNP P0DTC2
F	681	ARG	PRO	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
F	682	GLY	ARG	variant	UNP P0DTC2
F	683	SER	ARG	variant	UNP P0DTC2
F	685	SER	ARG	variant	UNP P0DTC2
F	817	PRO	PHE	variant	UNP P0DTC2
F	892	PRO	ALA	variant	UNP P0DTC2
F	899	PRO	ALA	variant	UNP P0DTC2
F	942	PRO	ALA	variant	UNP P0DTC2
F	986	PRO	LYS	variant	UNP P0DTC2
F	987	PRO	VAL	variant	UNP P0DTC2
F	1071	HIS	GLN	variant	UNP P0DTC2
F	1209	GLY	-	expression tag	UNP P0DTC2
F	1210	SER	-	expression tag	UNP P0DTC2
F	1211	GLY	-	expression tag	UNP P0DTC2
F	1212	TYR	-	expression tag	UNP P0DTC2
F	1213	ILE	-	expression tag	UNP P0DTC2
F	1214	PRO	-	expression tag	UNP P0DTC2
F	1215	GLU	-	expression tag	UNP P0DTC2
F	1216	ALA	-	expression tag	UNP P0DTC2
F	1217	PRO	-	expression tag	UNP P0DTC2
F	1218	ARG	-	expression tag	UNP P0DTC2
F	1219	ASP	-	expression tag	UNP P0DTC2
F	1220	GLY	-	expression tag	UNP P0DTC2
F	1221	GLN	-	expression tag	UNP P0DTC2
F	1222	ALA	-	expression tag	UNP P0DTC2
F	1223	TYR	-	expression tag	UNP P0DTC2
F	1224	VAL	-	expression tag	UNP P0DTC2
F	1225	ARG	-	expression tag	UNP P0DTC2
F	1226	LYS	-	expression tag	UNP P0DTC2
F	1227	ASP	-	expression tag	UNP P0DTC2
F	1228	GLY	-	expression tag	UNP P0DTC2
F	1229	GLU	-	expression tag	UNP P0DTC2
F	1230	TRP	-	expression tag	UNP P0DTC2
F	1231	VAL	-	expression tag	UNP P0DTC2
F	1232	LEU	-	expression tag	UNP P0DTC2
F	1233	LEU	-	expression tag	UNP P0DTC2
F	1234	SER	-	expression tag	UNP P0DTC2
F	1235	THR	-	expression tag	UNP P0DTC2
F	1236	PHE	-	expression tag	UNP P0DTC2
F	1237	LEU	-	expression tag	UNP P0DTC2
F	1238	GLY	-	expression tag	UNP P0DTC2
F	1239	ARG	-	expression tag	UNP P0DTC2
F	1240	SER	-	expression tag	UNP P0DTC2

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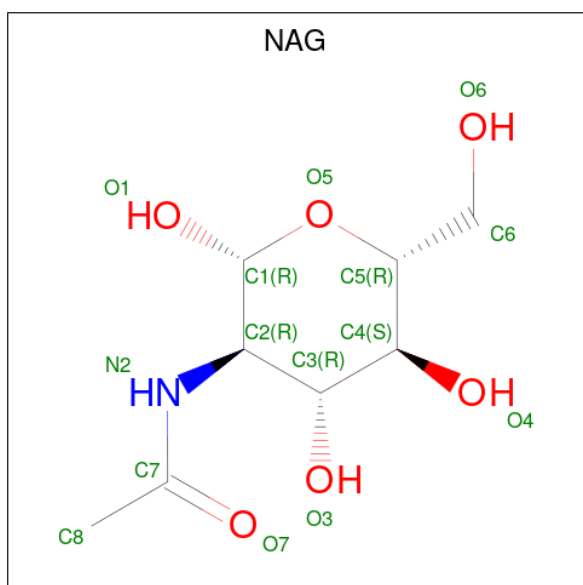
Chain	Residue	Modelled	Actual	Comment	Reference
F	1241	LEU	-	expression tag	UNP P0DTC2
F	1242	GLU	-	expression tag	UNP P0DTC2
F	1243	VAL	-	expression tag	UNP P0DTC2
F	1244	LEU	-	expression tag	UNP P0DTC2
F	1245	PHE	-	expression tag	UNP P0DTC2
F	1246	GLN	-	expression tag	UNP P0DTC2
F	1247	GLY	-	expression tag	UNP P0DTC2
F	1248	PRO	-	expression tag	UNP P0DTC2
F	1249	GLY	-	expression tag	UNP P0DTC2
F	1250	HIS	-	expression tag	UNP P0DTC2
F	1251	HIS	-	expression tag	UNP P0DTC2
F	1252	HIS	-	expression tag	UNP P0DTC2
F	1253	HIS	-	expression tag	UNP P0DTC2
F	1254	HIS	-	expression tag	UNP P0DTC2
F	1255	HIS	-	expression tag	UNP P0DTC2
F	1256	HIS	-	expression tag	UNP P0DTC2
F	1257	HIS	-	expression tag	UNP P0DTC2
F	1258	SER	-	expression tag	UNP P0DTC2
F	1259	ALA	-	expression tag	UNP P0DTC2
F	1260	TRP	-	expression tag	UNP P0DTC2
F	1261	SER	-	expression tag	UNP P0DTC2
F	1262	HIS	-	expression tag	UNP P0DTC2
F	1263	PRO	-	expression tag	UNP P0DTC2
F	1264	GLN	-	expression tag	UNP P0DTC2
F	1265	PHE	-	expression tag	UNP P0DTC2
F	1266	GLU	-	expression tag	UNP P0DTC2
F	1267	LYS	-	expression tag	UNP P0DTC2
F	1268	GLY	-	expression tag	UNP P0DTC2
F	1269	GLY	-	expression tag	UNP P0DTC2
F	1270	GLY	-	expression tag	UNP P0DTC2
F	1271	SER	-	expression tag	UNP P0DTC2
F	1272	GLY	-	expression tag	UNP P0DTC2
F	1273	GLY	-	expression tag	UNP P0DTC2
F	1274	GLY	-	expression tag	UNP P0DTC2
F	1275	GLY	-	expression tag	UNP P0DTC2
F	1276	SER	-	expression tag	UNP P0DTC2
F	1277	GLY	-	expression tag	UNP P0DTC2
F	1278	GLY	-	expression tag	UNP P0DTC2
F	1279	SER	-	expression tag	UNP P0DTC2
F	1280	ALA	-	expression tag	UNP P0DTC2
F	1281	TRP	-	expression tag	UNP P0DTC2
F	1282	SER	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
F	1283	HIS	-	expression tag	UNP P0DTC2
F	1284	PRO	-	expression tag	UNP P0DTC2
F	1285	GLN	-	expression tag	UNP P0DTC2
F	1286	PHE	-	expression tag	UNP P0DTC2
F	1287	GLU	-	expression tag	UNP P0DTC2
F	1288	LYS	-	expression tag	UNP P0DTC2

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



Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	D	1	Total	C	N	O	0
			14	8	1	5	
2	D	1	Total	C	N	O	0
			14	8	1	5	

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Mol	Chain	Residues	Atoms				AltConf
2	E	1	Total	C	N	O	0
			14	8	1	5	
2	E	1	Total	C	N	O	0
			14	8	1	5	
2	F	1	Total	C	N	O	0
			14	8	1	5	
2	F	1	Total	C	N	O	0
			14	8	1	5	

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

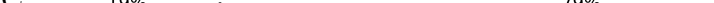
- Molecule 1: Spike glycoprotein

Chain B: 19% 79%

	GLN	PRO	LEU	ILE	THR	V810	CYS	LEU	GLY	ASN	ASN	MET
	TYR	SER	LEU	ILE	TRP	V811	THR	LEU	LYS	ASN	PHE	VAL
	THR	ARG	LEU	ALA	ARG	V811	THR	LEU	ALA	ALA	THR	THR
	SER	ARG	GLN	TYR	VAL	A520	SER	HIS	GLY	THR	PHE	TRP
	ALA	SER	TYR	THR	TYR	A520	SER	HIS	ASN	ASN	PHE	LEU
	LEU	PRO	GLY	MET	SER	V624	THR	ARG	PHE	VAL	HIS	VAL
	LEU	ILE	SER	SER	THR	K528	THR	SER	LYS	VAL	ALA	LEU
	ALA	GLU	PHE	LEU	GLY	K528	VAL	TYR	ASN	ILE	ILE	LEU
	GLY	ASP	CYS	GLY	SER	L533	GLU	THR	LEU	LYS	HIS	PRO
	THR	LEU	GLN	ALA	ASN	L533	LYS	THR	ARG	VAL	VAL	LEU
	ILE	LEU	GLN	GLU	VAL	F643	GLY	PRO	GLY	CYS	SER	VAL
	THR	PHE	LEU	ASN	PHE	F643	ILE	GLY	PHE	GLY	SER	VAL
	SER	ASN	ASN	SER	GLN	L546	TYR	ASP	VAL	PHE	THR	SER
	GLY	LYS	ARG	VAL	THR	L546	GLN	SER	PHE	GLN	ASN	GLN
	TRP	VAL	ALA	ALA	ARG	L585	THR	SER	LYS	PHE	CYS	CYS
	THR	THR	THR	TYR	ALA	L585	ASN	SER	ASN	THR	VAL	THR
	PHE	LEU	LEU	SER	GLY	F689	ASN	GLY	ILE	LYS	ASN	ASN
	GLY	ALA	GLY	ASN	CYS	F689	PHE	TPP	ASP	ASP	ARG	LEU
	ALA	ASP	ILE	ASN	LEU	CYS	ARG	THR	THR	PRO	PHE	THR
	GLY	ALA	ALA	SER	ILE	SER	VAL	ALA	TYR	ASP	THR	THR
	PRO	GLY	VAL	ILE	GLY	PHE	ARG	GLY	PHE	LEU	ASN	ARG
	ALA	PHE	ALA	ALA	ALA	GLY	P322	ALA	LYS	GLY	PRO	THR
	LEU	ILE	GLN	GLU	HIS	GLY	P322	ALA	ILE	VAL	VAL	GLN
	ASN	LYS	ASP	PRO	GLU	VAL	N354	ALA	TYR	TVR	LEU	LEU
	GLN	GLN	LYS	THR	VAL	SER	N354	TTR	SER	TTR	PRO	PRO
	ILE	GLN	LYS	THR	VAL	SER	T368	ALA	LYS	HIS	PHE	PRO
	PRO	GLY	ASN	PHE	ASN	VAL	T368	VAL	ASN	TYR	ASN	ASN
	PHE	THR	THR	THR	ASN	ILE	Y365	GLY	THR	LYS	ASN	ALA
	PRO	ASP	GLN	THR	THR	PRO	Y365	THR	THR	ASN	GLY	TYR
	MET	ASN	GLU	ILE	TYR	THR	PRO	TVR	ARG	ASN	GLY	THR
	GLN	LEU	VAL	SER	GLU	GLY	S373	LEU	ILE	LYS	VAL	ASN
	MET	GLY	PHE	VAL	CYS	THR	S373	GLN	ASN	SER	THR	ASN
	ALA	ASP	ALA	THR	THR	ASN	P384	PRO	LEU	TRP	PHE	SER
	ALA	ILE	ALA	GLU	ILE	THR	P384	ARG	VAL	ALA	THR	ARG
	ARG	ALA	VAL	GLU	PRO	SER	L387	THR	ARG	LYS	SER	THR
	PHE	ALA	LYS	ILE	ILE	ASN	L387	PHE	ASP	THR	GLY	GLY
	ASN	ARG	GLN	LEU	GLY	GLN	T393	LEU	LEU	GLU	GLU	TYR
	ASP	ASP	ILE	PRO	ALA	VAL	N394	LEU	PRO	PHE	LYS	TTR
	LEU	LEU	TYR	VAL	GLY	ALA	V395	LYS	GLN	ARG	SER	TYR
	PHE	ILE	LYS	SER	ILE	VAL	V395	TVR	ASN	VAL	ASN	PRO
	GLY	CYS	THR	MET	CYS	LEU	D396	PHE	PHE	ASN	ILE	ASP
	ALA	ALA	PRO	ALA	ALA	TYR	D396	GLU	SER	SER	LYS	LYS
	GLN	GLN	PRO	LYS	SER	GLN	V401	ASN	ALA	SER	ARG	VAL
	LYS	ILE	ILE	THR	TYR	GLY	V401	ASN	GLY	THR	PHE	THR
	ASN	PHE	LYS	SER	GLN	VAL	T418	THR	GLU	ALA	GLY	ARG
	VAL	ASN	ASP	VAL	THR	ASN	T418	ILE	PRO	ASN	ILE	SER
	LEU	GLY	PHE	ASP	GLN	CYS	N422	THR	LEU	CYS	PHE	SER
	GLU	GLY	GLY	CYS	THR	THR	N422	ASP	VAL	THR	GLY	VAL
	ASN	LEU	GLY	THR	ASN	GLU	S438	ALA	ASP	PHE	THR	LEU
	THR	VAL	PHE	MET	SER	VAL	S438	VAL	LEU	THR	THR	HIS
	VAL	LEU	ASN	TYR	ARG	PRO	D442	ASP	PRO	TYR	THR	LEU
	LYS	PRO	PHE	ILE	GLY	VAL	D442	CYS	PRO	VAL	ASP	THR
	ILE	PRO	SER	CYS	SER	ALA	Y453	ALA	GLY	SER	GLN	ASN
	GLY	GLY	GLN	GLY	ALA	ILE	Y453	LEU	ILE	SER	LYS	LYS
	ASN	LEU	ILE	ASP	SER	HIS	L455	ASP	ASN	PRO	THR	LEU
	PRO	THR	LEU	SER	SER	ALA	L455	PRO	ASN	GLN	THR	PHE
	GLN	THR	VAL	VAL	VAL	ASP	F497	LEU	THR	ILE	GLN	THR
	ALA	GLU	ALA	ALA	ALA	GLN	F497	SER	ARG	THR	LEU	THR
	SER	GLU	PRO	GLU	SER	THR	P507	GLU	PHE	MET	ASP	PRO
	ALA	MET	ASP	CYS	SER	LEU	P507	LEU	THR	GLY	LEU	LEU
	ILE	ILE	THR	SER	GLN	THR	Y508	THR	GLN	ILE	THR	PHE
	ALA	ALA	TYR	ASN	SER	PRO	Y508	THR	THR	VAL	VAL	VAL

[illegible]

- Molecule 1: Spike glycoprotein

Chain C:  19% : 79%

THR	THR	LEU	THR	ALA	ASN	S555	CYS	LEU	GLY	ASN	ASN	MET
PRO	PRO	LEU	ILE	GLU	VAL	G566	THR	LEU	LYS	ASN	PHE	THR
ALA	ALA	ASN	SER	ASN	PHE	G566	THR	ALA	GLN	ASN	THR	VAL
GLY	GLY	LYS	ARG	VAL	GLN	A575	SER	HIS	ASN	THR	PHE	THR
THR	THR	VAL	ALA	THR	ALA	D586	PHE	ARG	PHE	VAL	HIS	VAL
PRO	PRO	THR	LEU	THR	ALA	D586	THR	SER	LYS	VAL	ALA	LEU
GLN	GLN	ALA	ILE	SER	GLY	P589	VAL	TYR	ASN	ILE	ILE	PRO
ASN	ASN	ALA	ILE	SER	CYS	P589	GLU	LEU	ARG	VAL	HIS	PRO
VAL	VAL	ALA	VAL	ILE	ILE	CYS	LYS	THR	THR	VAL	VAL	VAL
ASN	ASN	PHE	VAL	ALA	ALA	SER	GLY	PRO	PHE	CYS	SER	VAL
GLN	GLN	ILE	GLU	ILE	GLY	PHE	ILE	GLY	GLY	GLY	GLY	SER
PRO	PRO	ALA	GLU	ALA	ALA	GLY	TYR	ASP	VAL	PHE	THR	SER
ALA	ALA	THR	THR	THR	THR	GLY	THR	THR	THR	THR	THR	THR
LEU	LEU	THR	THR	THR	THR	THR	ARG	THR	GLY	ASN	ASN	THR
ASN	ASN	CYS	GLU	ILE	TYR	PRO	THR	VAL	TYR	PHE	ASN	THR
THR	THR	LEU	VAL	SER	GLU	GLY	GLN	ALA	PHE	GLY	GLY	ARG
VAL	VAL	ASP	PHE	VAL	CYS	THR	P322	ALA	ILE	VAL	VAL	GLN
ALA	ALA	ASP	ALA	THR	ASP	ASN	C336	ALA	ILE	VAL	VAL	ASN
GLN	GLN	ILE	GLN	THR	ILE	THR	C336	THR	TYR	TYR	LEU	LEU
ARG	ARG	ALA	VAL	GLU	PRO	SER	C336	ALA	SER	PRO	PRO	PRO
LEU	LEU	ALA	LYS	ILE	ILE	ASN	W353	THR	HIS	PHE	PHE	ASN
ASN	ASN	ARG	GLN	LEU	GLY	GLN	W353	VAL	LYS	ASN	ASN	ALA
GLY	GLY	ASP	ILE	PRO	ALA	VAL	1358	GLY	THR	ASN	GLY	THR
ASN	ASN	LEU	TYR	VAL	GLY	ALA	3359	TYR	PRO	ASN	GLY	THR
PHE	PHE	ILE	LYS	SER	ILE	VAL	N360	LEU	ILE	LYS	VAL	ASN
GLY	GLY	CYS	THR	MET	CYS	LEU	C361	GLN	ASN	SER	TYR	SER
ALA	ALA	THR	THR	THR	ALA	TYR	V395	PRO	VAL	THR	ALA	THR
THR	THR	LYS	ILE	THR	TYR	GLY	V395	THR	ARG	LYS	SER	THR
VAL	VAL	PHE	ASP	SER	GLN	VAL	V401	PHE	ASP	SER	THR	GLY
LEU	LEU	ASN	VAL	VAL	THR	ASN	V401	LEU	LEU	GLU	GLU	VAL
TYR	TYR	GLY	PHE	ASP	GLN	CYS	T418	LEU	PRO	PHE	LYS	TYR
ASN	ASN	LEU	GLY	THR	GLN	THR	T418	LEU	GLN	SER	ASN	THR
ASP	ASP	THR	GLY	CYS	ASN	GLY	N422	TYR	GLY	VAL	ASN	PRO
ILE	ILE	VAL	PHE	MET	SER	THR	N422	ASN	PHE	TYR	ILE	ASN
LYS	LYS	LEU	ASN	THR	ARG	PRO	G431	GLU	SER	SER	ILE	LYS
LEU	LEU	PRO	PHE	ILE	GLY	VAL	G431	ASN	ALA	SER	ARG	VAL
ARG	ARG	PRO	ILE	CYS	SER	ALA	N439	GLY	LEU	PHE	GLY	VAL
LEU	LEU	LEU	GLN	GLY	ALA	ILE	N439	THR	GLU	ASN	TRP	ARG
ASP	ASP	LEU	ILE	ASP	SER	HIS	K444	ILE	PRO	ASN	ILE	SER
PRO	PRO	THR	THR	SER	SER	ALA	K444	THR	LEU	CYS	PHE	SER
PRO	PRO	ASP	THR	THR	VAL	ASP	R466	ASP	VAL	THR	GLY	VAL
GLU	GLU	MET	ASP	GLU	ALA	GLN	R466	ALA	ASP	THR	THR	LEU
ALA	ALA	THR	PRO	CYS	SER	LEU	Q493	VAL	LEU	PHE	THR	THR
GLU	GLU	ILE	ILE	SER	GLN	THR	Q493	ASP	LEU	THR	THR	HIS
VAL	VAL	ALA	LYS	ASN	SER	PRO	F497	CYS	ILE	VAL	ASP	SER
GLN	GLN	GLY	PRO	LEU	ILE	THR	F497	ALA	GLY	SER	SER	GLN
ILE	ILE	TYR	SER	LEU	ILE	THR	P507	LEU	ILE	GLN	LYS	ASP
ASP	ASP	THR	LYS	LEU	ALA	ARG	Y508	ASP	ASN	PRO	THR	LEU
ARG	ARG	SER	ANG	GLN	TYR	VAL	Y508	PRO	ILE	PHE	GLN	PHE
LEU	LEU	ALA	SER	THR	THR	THR	R509	LEU	THR	LEU	SER	THR
ILE	ILE	SER	PRO	GLY	MET	SER	L513	SER	ARG	MET	LEU	PRO
THR	THR	LEU	ILE	SER	THR	THR	L513	GLU	PHE	ASP	LEU	PRO
SER	SER	GLY	ASP	PHE	LEU	GLY	T523	THR	GLN	LEU	ILE	PHE
ARG	ARG	THR	ASN	THR	THR	SER	T523	LYS	THR	GLU	VAL	SER

[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	116459	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.705	Depositor
Minimum map value	-0.793	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.136	Depositor
Map size (Å)	520.0, 520.0, 520.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3, 1.3, 1.3	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.23	0/2158	0.52	0/2936
1	B	0.20	0/2158	0.49	0/2936
1	C	0.22	0/2158	0.50	0/2936
1	D	0.21	0/2158	0.47	0/2936
1	E	0.22	0/2158	0.48	0/2936
1	F	0.22	0/2158	0.58	4/2936 (0.1%)
All	All	0.21	0/12948	0.51	4/17616 (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	410	ILE	N-CA-C	-8.20	104.61	111.91
1	F	391	CYS	CA-CB-SG	5.68	127.46	114.40
1	F	515	PHE	CA-C-N	-5.24	114.85	122.65
1	F	515	PHE	C-N-CA	-5.24	114.85	122.65

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2104	0	2021	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2104	0	2021	18	0
1	C	2104	0	2021	13	0
1	D	2104	0	2021	22	0
1	E	2104	0	2021	14	0
1	F	2104	0	2021	15	0
2	A	28	0	26	1	0
2	B	28	0	26	0	0
2	C	28	0	26	0	0
2	D	28	0	26	1	0
2	E	28	0	26	0	0
2	F	28	0	26	0	0
All	All	12792	0	12282	91	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 4.

All (91) 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:D:339:GLY:O	1:D:343:ASN:HB2	1.98	0.62
1:F:577:ARG:HB2	1:F:584:ILE:HG13	1.81	0.60
1:E:411:ALA:HB3	1:E:414:GLN:HG3	1.83	0.60
1:C:353:TRP:O	1:C:466:ARG:NH1	2.36	0.59
1:B:358:ILE:HB	1:B:395:VAL:HB	1.84	0.59
1:F:577:ARG:HA	1:F:584:ILE:HA	1.84	0.57
1:D:358:ILE:HB	1:D:395:VAL:HB	1.87	0.57
1:F:383:SER:HB3	1:F:386:LYS:HB2	1.86	0.56
1:B:365:TYR:HD2	1:B:387:LEU:HB3	1.71	0.56
1:D:442:ASP:O	1:D:448:ASN:ND2	2.37	0.56
1:A:401:VAL:HG22	1:A:509:ARG:HG2	1.88	0.56
1:B:418:ILE:HA	1:B:422:ASN:HB2	1.88	0.55
1:B:398:ASP:O	1:B:511:VAL:HA	2.08	0.54
1:A:418:ILE:HA	1:A:422:ASN:HB2	1.90	0.53
1:F:328:ARG:NH1	1:F:531:THR:O	2.41	0.53
1:A:329:PHE:O	1:A:580:GLN:NE2	2.41	0.53
1:F:403:ARG:NH1	1:F:405:ASP:OD2	2.41	0.53
1:C:439:ASN:ND2	1:F:437:ASN:OD1	2.42	0.53
1:B:543:PHE:O	1:B:546:LEU:HB2	2.10	0.52
1:E:327:VAL:HG11	1:E:528:LYS:HD2	1.91	0.52
1:F:577:ARG:HD2	1:F:582:LEU:HD22	1.91	0.52
1:D:328:ARG:NH2	1:D:578:ASP:OD2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:329:PHE:O	1:E:580:GLN:NE2	2.42	0.51
1:F:354:ASN:O	1:F:398:ASP:HA	2.10	0.51
1:A:358:ILE:HB	1:A:395:VAL:HB	1.92	0.51
1:C:444:LYS:HG3	1:F:372:ALA:HB1	1.94	0.50
1:D:411:ALA:HB3	1:D:414:GLN:HG3	1.93	0.50
1:A:357:ARG:HG3	1:A:396:TYR:HE1	1.77	0.50
1:C:497:PHE:CG	1:C:507:PRO:HG3	2.47	0.50
1:D:335:LEU:HD23	1:D:362:VAL:HG13	1.95	0.49
1:C:401:VAL:HG22	1:C:509:ARG:HG2	1.95	0.48
1:C:555:SER:HB3	1:C:586:ASP:HB2	1.95	0.48
1:A:354:ASN:O	1:A:398:ASP:HA	2.14	0.47
1:A:326:ILE:HD11	1:A:533:LEU:HA	1.95	0.47
1:E:521:PRO:HG3	1:E:564:GLN:HG3	1.97	0.47
1:C:358:ILE:HB	1:C:395:VAL:HB	1.96	0.47
1:B:395:VAL:HG23	1:B:524:VAL:HG11	1.97	0.47
1:E:401:VAL:HG22	1:E:509:ARG:HG2	1.97	0.47
1:B:533:LEU:HD21	1:B:585:LEU:HD11	1.97	0.46
1:B:393:THR:HG21	1:B:520:ALA:HB3	1.98	0.46
1:C:360:ASN:H	1:C:523:THR:HB	1.81	0.46
1:B:497:PHE:CG	1:B:507:PRO:HG3	2.51	0.45
1:D:567:ARG:NH1	1:D:573:THR:OG1	2.49	0.45
1:B:528:LYS:HE3	1:B:528:LYS:HB2	1.82	0.45
1:E:418:ILE:HA	1:E:422:ASN:HB2	1.99	0.45
1:E:376:THR:HB	1:E:435:ALA:HB3	2.00	0.44
1:F:325:SER:HA	1:F:540:ASN:O	2.18	0.44
1:D:578:ASP:OD2	1:D:581:THR:OG1	2.28	0.44
1:A:566:GLY:N	1:A:575:ALA:O	2.50	0.44
1:D:360:ASN:H	1:D:523:THR:HB	1.83	0.44
1:F:393:THR:O	1:F:523:THR:OG1	2.33	0.44
1:B:401:VAL:HG22	1:B:509:ARG:HG2	1.98	0.43
1:B:438:SER:OG	1:B:442:ASP:OD2	2.35	0.43
1:D:362:VAL:HA	1:D:525:CYS:O	2.18	0.43
1:A:372:ALA:HB1	1:E:444:LYS:HB2	1.99	0.43
1:A:342:PHE:HB2	2:A:1302:NAG:H82	2.01	0.43
1:C:336:CYS:HB3	1:C:361:CYS:HB3	1.91	0.43
1:F:395:VAL:HG22	1:F:515:PHE:HD2	1.84	0.43
1:B:354:ASN:O	1:B:398:ASP:HA	2.19	0.42
1:D:401:VAL:HG22	1:D:509:ARG:HG2	2.01	0.42
1:D:434:ILE:O	1:D:510:VAL:HA	2.18	0.42
1:C:418:ILE:HA	1:C:422:ASN:HB2	2.01	0.42
1:F:376:THR:HG23	1:F:378:LYS:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:495:TYR:O	1:E:505:TYR:OH	2.31	0.42
1:C:431:GLY:HA3	1:C:513:LEU:O	2.20	0.42
1:D:418:ILE:HA	1:D:422:ASN:HB2	2.01	0.42
1:B:533:LEU:HD12	1:B:533:LEU:HA	1.91	0.42
1:D:388:ASN:HB3	1:D:527:PRO:HD2	2.02	0.42
1:D:357:ARG:HH11	1:D:394:ASN:HD21	1.68	0.42
1:D:366:SER:H	1:D:388:ASN:HD21	1.68	0.42
1:E:393:THR:OG1	1:E:516:GLU:O	2.29	0.42
1:E:497:PHE:CG	1:E:507:PRO:HG3	2.55	0.41
1:A:565:PHE:HA	1:A:576:VAL:HA	2.02	0.41
1:D:393:THR:HA	1:D:522:ALA:HA	2.02	0.41
1:B:384:PRO:HA	1:B:387:LEU:HG	2.01	0.41
1:A:376:THR:HB	1:A:435:ALA:HB3	2.02	0.41
1:C:566:GLY:N	1:C:575:ALA:O	2.51	0.41
1:A:454:ARG:NH2	1:A:467:ASP:O	2.53	0.41
1:B:373:SER:HA	1:D:445:VAL:HG11	2.02	0.41
1:E:393:THR:HA	1:E:522:ALA:HA	2.03	0.41
1:A:403:ARG:HG3	1:A:406:GLU:HG3	2.01	0.41
1:D:497:PHE:CG	1:D:507:PRO:HG3	2.56	0.41
1:D:342:PHE:HB2	2:D:1302:NAG:H82	2.03	0.41
1:E:412:PRO:HG3	1:E:429:PHE:HB3	2.03	0.41
1:B:438:SER:OG	1:B:438:SER:O	2.38	0.40
1:D:457:ARG:NE	1:D:467:ASP:OD2	2.43	0.40
1:B:453:TYR:HE2	1:B:455:LEU:HD13	1.86	0.40
1:D:398:ASP:OD2	1:D:423:TYR:OH	2.32	0.40
1:C:493:GLN:OE1	1:E:493:GLN:NE2	2.42	0.40
1:F:410:ILE:HD12	1:F:410:ILE:HG23	1.89	0.40
1:F:418:ILE:HA	1:F:422:ASN:HB2	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	266/1288 (21%)	256 (96%)	10 (4%)	0	100	100
1	B	266/1288 (21%)	262 (98%)	4 (2%)	0	100	100
1	C	266/1288 (21%)	258 (97%)	8 (3%)	0	100	100
1	D	266/1288 (21%)	260 (98%)	6 (2%)	0	100	100
1	E	266/1288 (21%)	257 (97%)	9 (3%)	0	100	100
1	F	266/1288 (21%)	258 (97%)	8 (3%)	0	100	100
All	All	1596/7728 (21%)	1551 (97%)	45 (3%)	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	231/1115 (21%)	231 (100%)	0	100	100
1	B	231/1115 (21%)	231 (100%)	0	100	100
1	C	231/1115 (21%)	231 (100%)	0	100	100
1	D	231/1115 (21%)	231 (100%)	0	100	100
1	E	231/1115 (21%)	231 (100%)	0	100	100
1	F	231/1115 (21%)	231 (100%)	0	100	100
All	All	1386/6690 (21%)	1386 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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	360	ASN
1	A	542	ASN
1	B	370	ASN
1	C	484	GLN
1	D	484	GLN

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Mol	Chain	Res	Type
1	E	394	ASN
1	F	484	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

12 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	D	1302	1	14,14,15	0.32	0	17,19,21	0.54	0
2	NAG	F	1301	1	14,14,15	0.93	2 (14%)	17,19,21	0.68	1 (5%)
2	NAG	A	1302	1	14,14,15	0.37	0	17,19,21	0.58	0
2	NAG	E	1302	1	14,14,15	0.34	0	17,19,21	0.57	0
2	NAG	D	1301	1	14,14,15	0.44	0	17,19,21	0.47	0
2	NAG	F	1302	1	14,14,15	0.37	0	17,19,21	0.56	0
2	NAG	A	1301	1	14,14,15	0.29	0	17,19,21	0.45	0
2	NAG	B	1302	1	14,14,15	0.46	0	17,19,21	0.62	1 (5%)
2	NAG	C	1302	1	14,14,15	0.35	0	17,19,21	0.54	0
2	NAG	C	1301	1	14,14,15	0.42	0	17,19,21	0.45	0
2	NAG	E	1301	1	14,14,15	0.33	0	17,19,21	0.45	0
2	NAG	B	1301	1	14,14,15	0.32	0	17,19,21	0.43	0

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	D	1302	1	-	2/6/23/26	0/1/1/1
2	NAG	F	1301	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1302	1	-	2/6/23/26	0/1/1/1
2	NAG	E	1302	1	-	2/6/23/26	0/1/1/1
2	NAG	D	1301	1	-	0/6/23/26	0/1/1/1
2	NAG	F	1302	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1301	1	-	1/6/23/26	0/1/1/1
2	NAG	B	1302	1	-	1/6/23/26	0/1/1/1
2	NAG	C	1302	1	-	2/6/23/26	0/1/1/1
2	NAG	C	1301	1	-	0/6/23/26	0/1/1/1
2	NAG	E	1301	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1301	1	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1301	NAG	O5-C1	2.75	1.48	1.43
2	F	1301	NAG	C1-C2	2.03	1.55	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1301	NAG	C1-O5-C5	2.44	115.46	112.19
2	B	1302	NAG	C1-O5-C5	2.14	115.05	112.19

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1302	NAG	C4-C5-C6-O6
2	F	1301	NAG	O5-C5-C6-O6
2	D	1302	NAG	O5-C5-C6-O6
2	A	1302	NAG	O5-C5-C6-O6
2	C	1302	NAG	O5-C5-C6-O6
2	F	1302	NAG	O5-C5-C6-O6
2	C	1302	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	E	1302	NAG	O5-C5-C6-O6
2	F	1301	NAG	C4-C5-C6-O6
2	B	1302	NAG	O5-C5-C6-O6
2	E	1302	NAG	C4-C5-C6-O6
2	A	1302	NAG	C4-C5-C6-O6
2	F	1302	NAG	C4-C5-C6-O6
2	A	1301	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1302	NAG	1	0
2	A	1302	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.

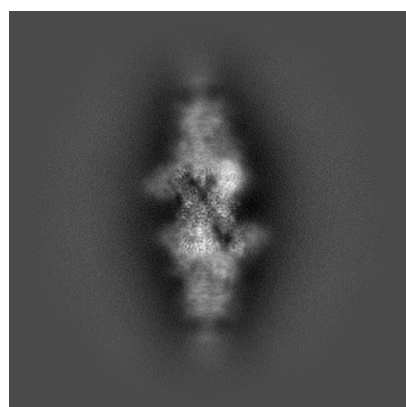
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25861. These allow visual inspection of the internal detail of the map and identification of artifacts.

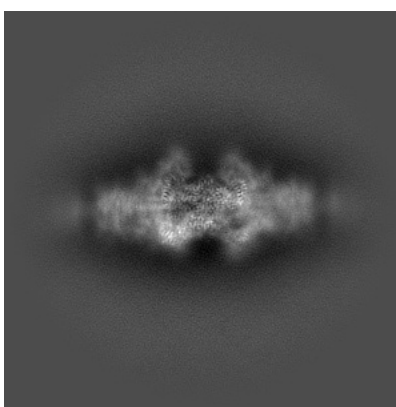
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

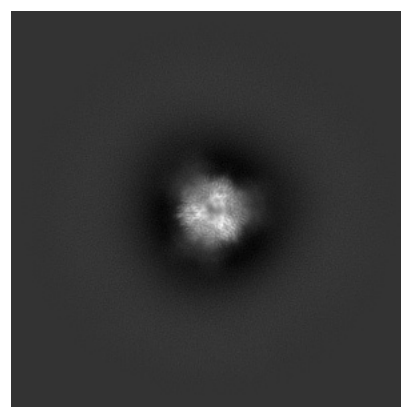
6.1.1 Primary map



X



Y

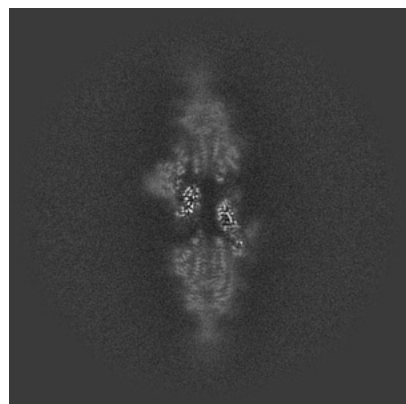


Z

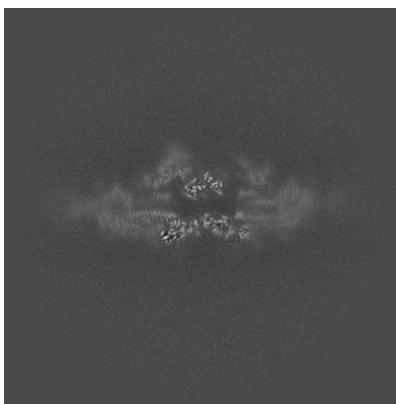
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

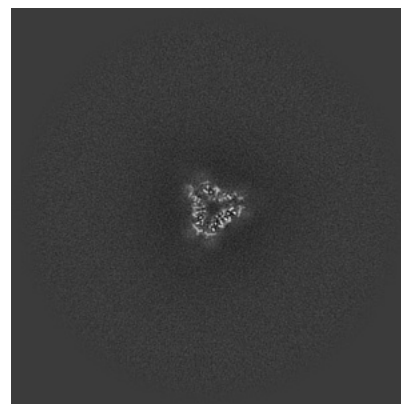
6.2.1 Primary map



X Index: 200



Y Index: 200

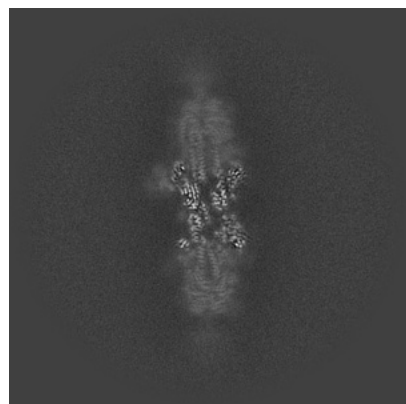


Z Index: 200

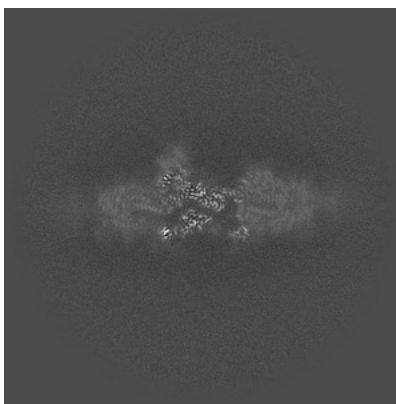
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

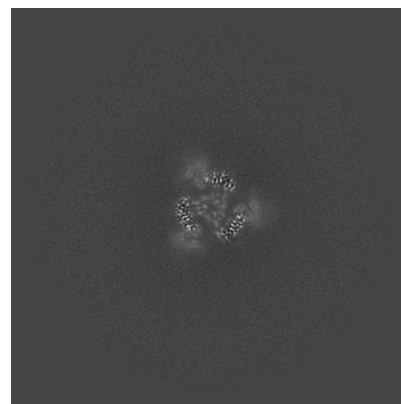
6.3.1 Primary map



X Index: 210



Y Index: 188

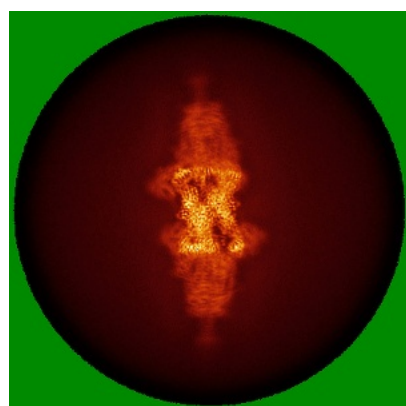


Z Index: 163

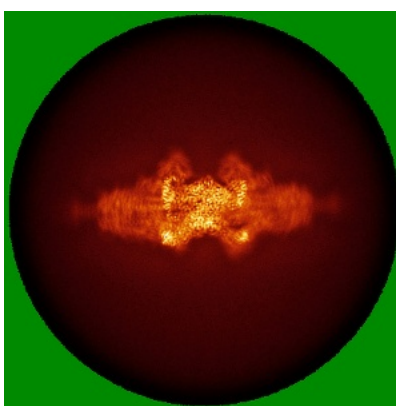
The images above show the largest variance slices of the map in three orthogonal directions.

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

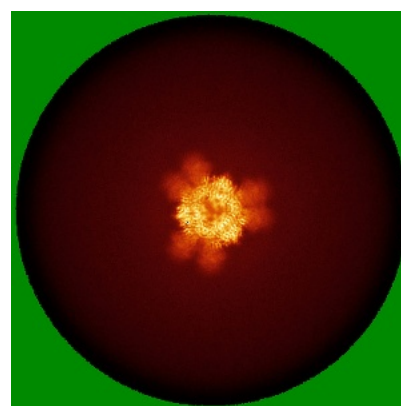
6.4.1 Primary map



X



Y

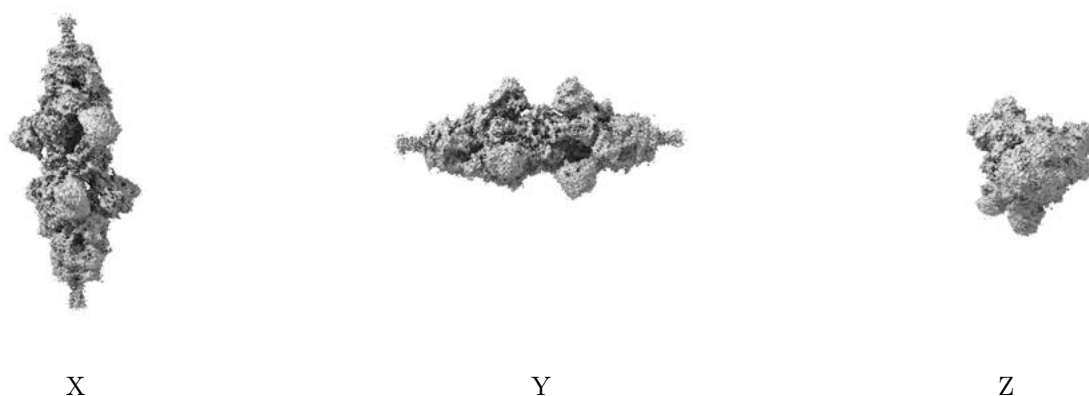


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.136. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

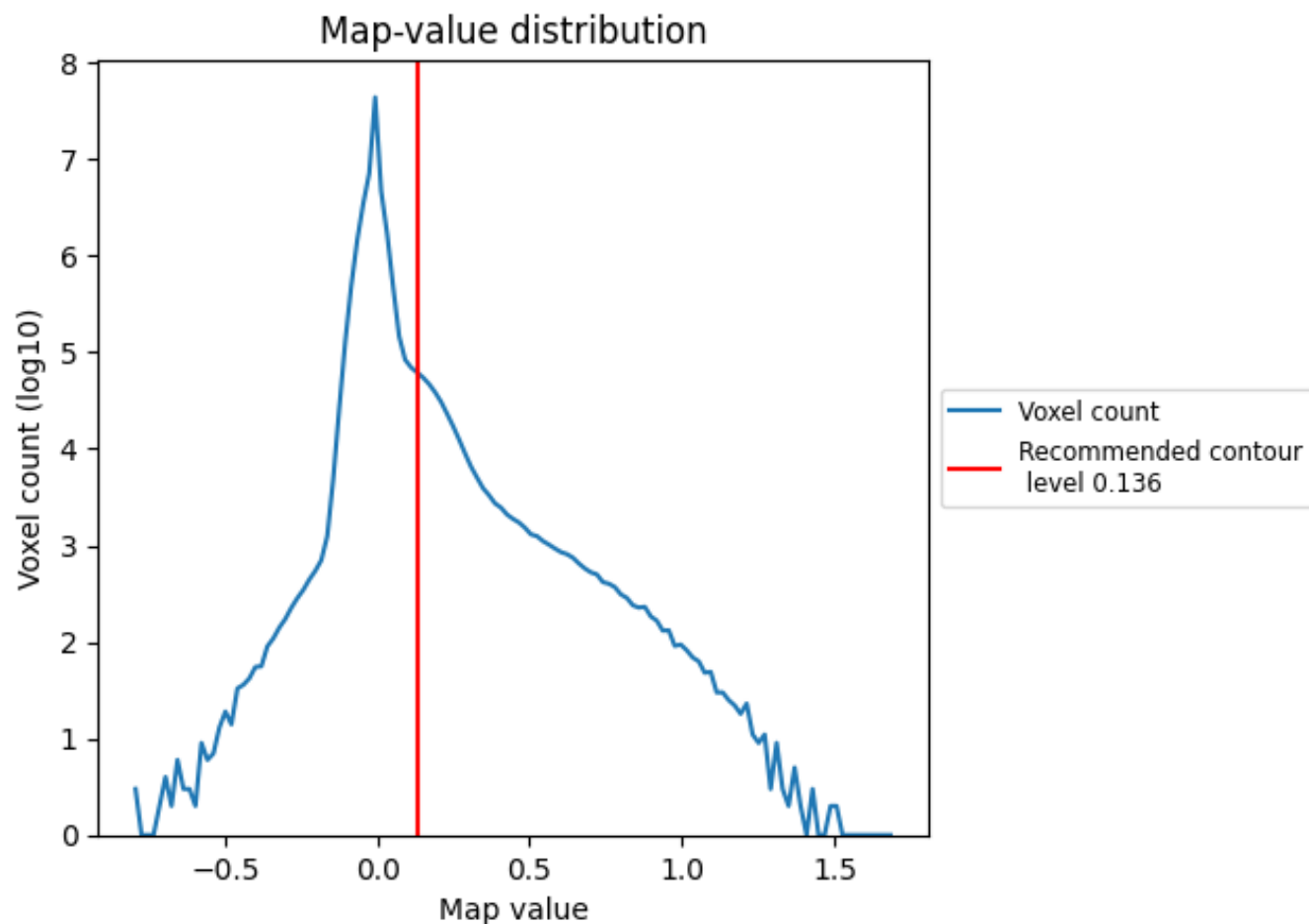
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

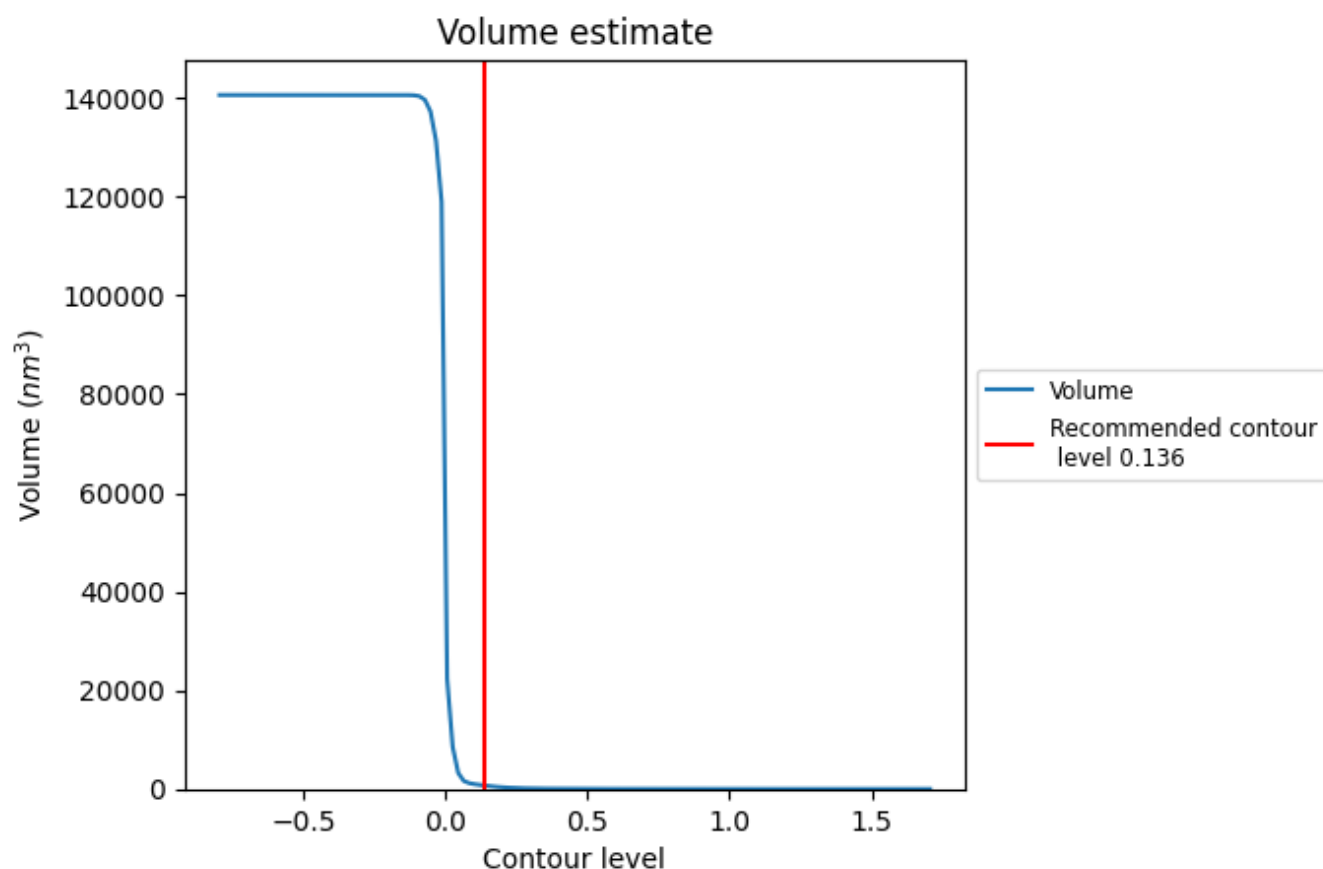
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

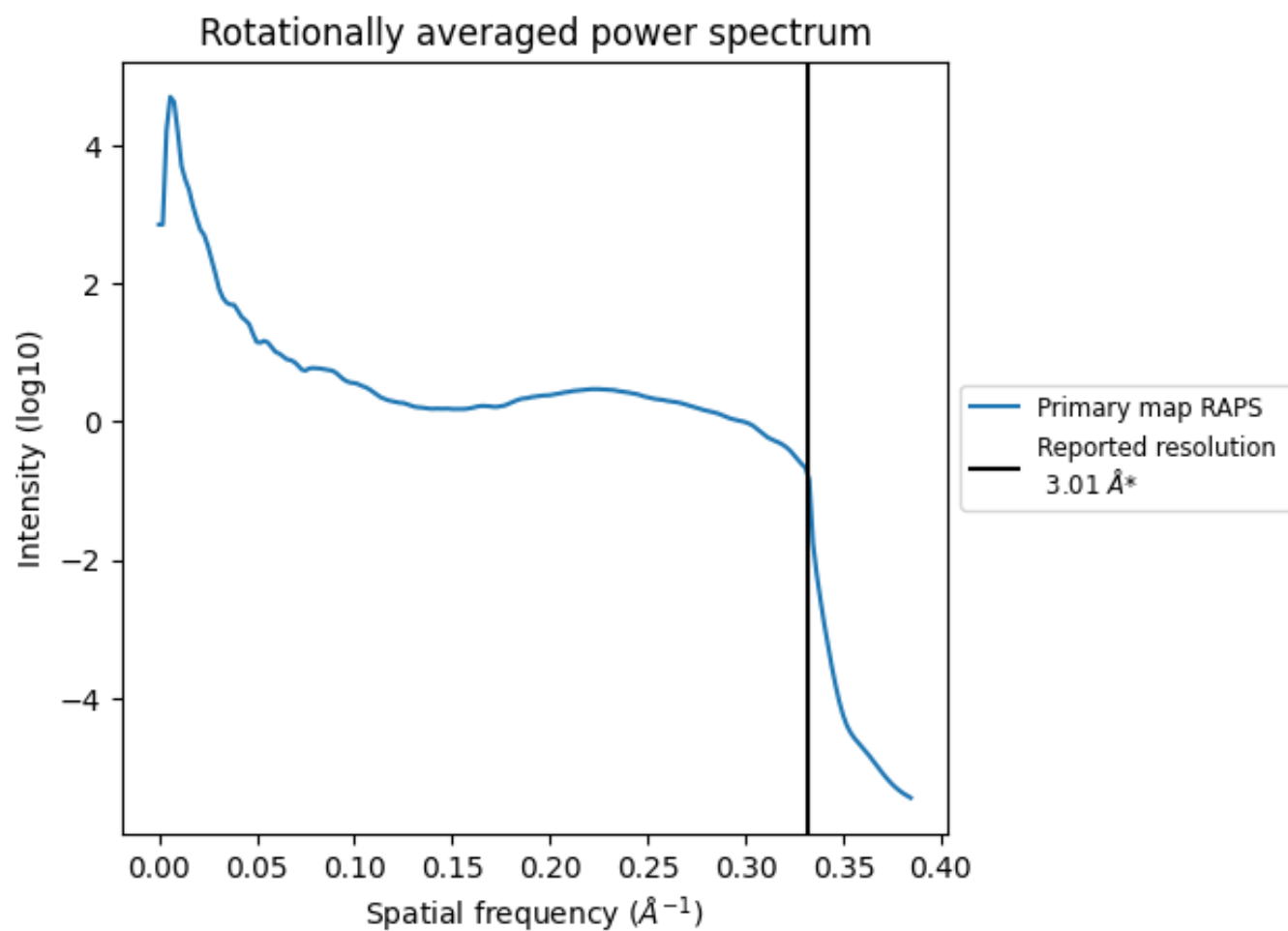
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 716 nm^3 ; this corresponds to an approximate mass of 647 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 ⓘ

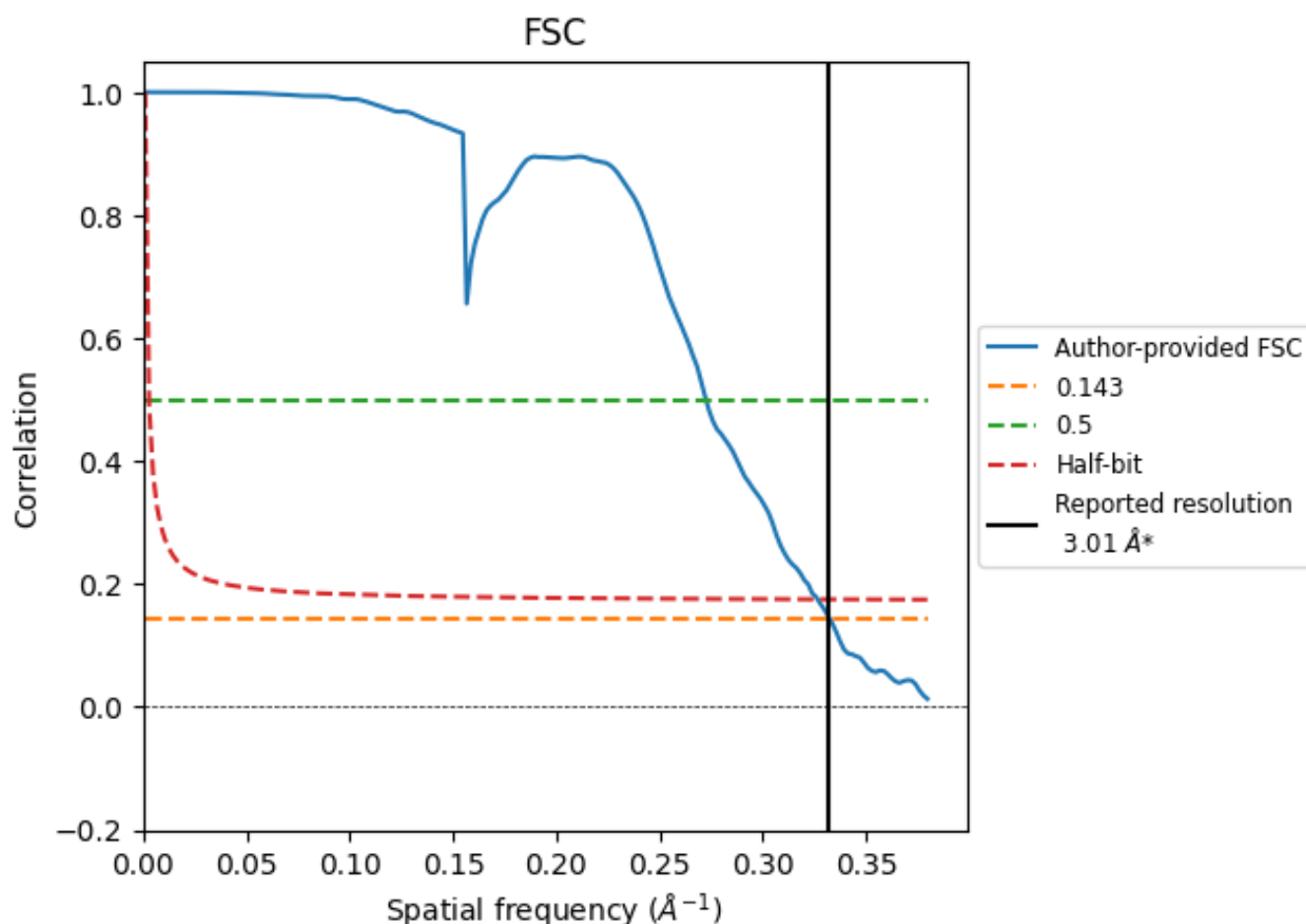


*Reported resolution corresponds to spatial frequency of 0.332 Å⁻¹

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 0.332 Å⁻¹

8.2 Resolution estimates [i](#)

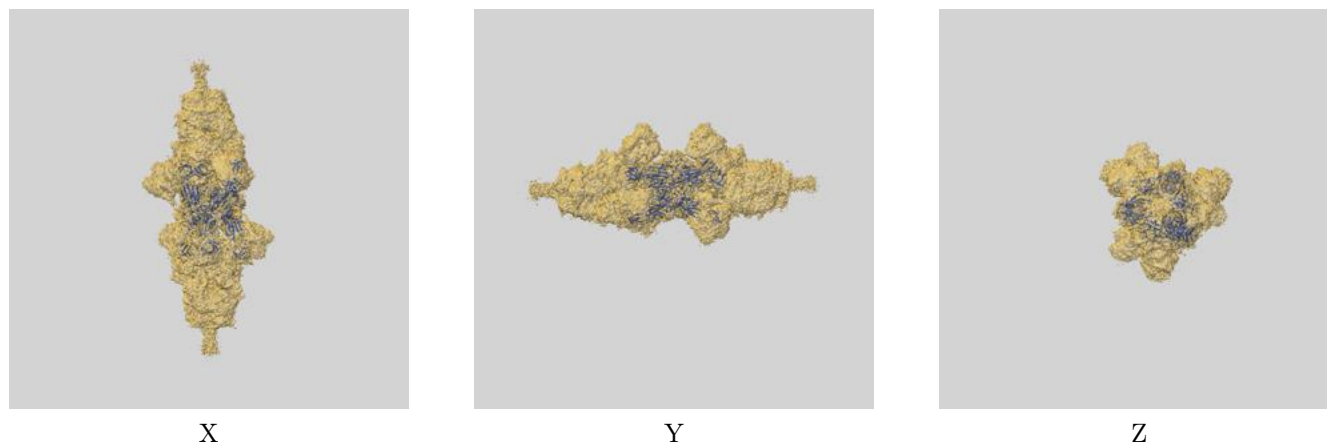
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.01	-	-
Author-provided FSC curve	3.01	3.67	3.06
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

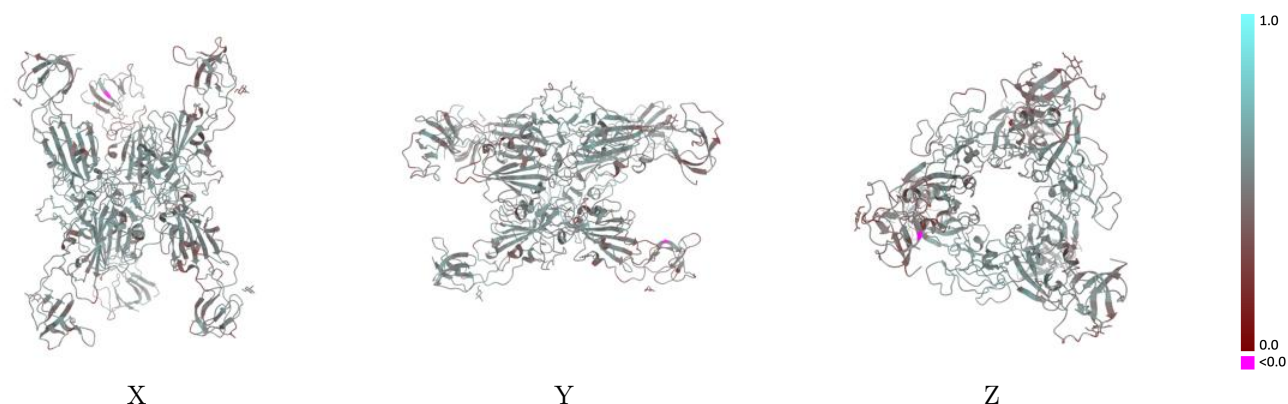
This section contains information regarding the fit between EMDB map EMD-25861 and PDB model 7TF4. Per-residue inclusion information can be found in section [3](#) on page [20](#).

9.1 Map-model overlay [i](#)



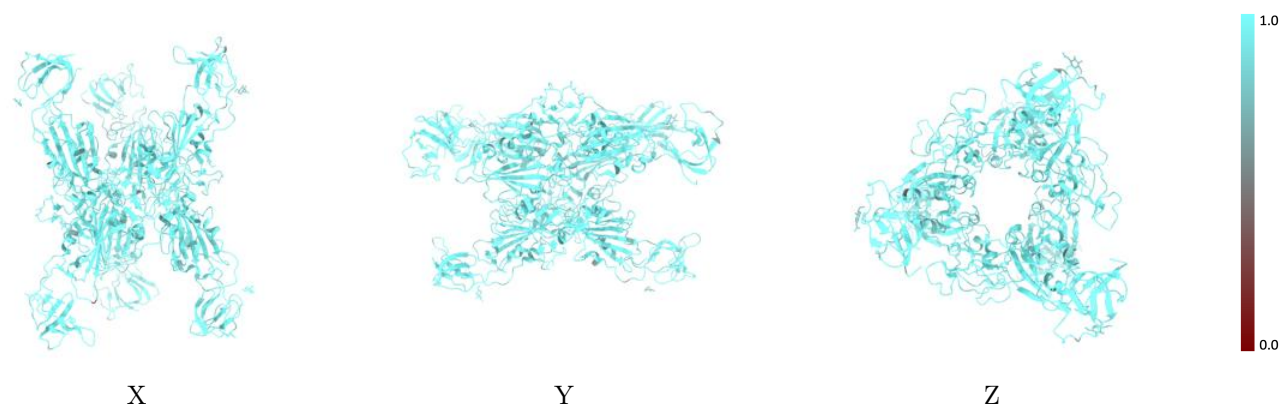
The images above show the 3D surface view of the map at the recommended contour level 0.136 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



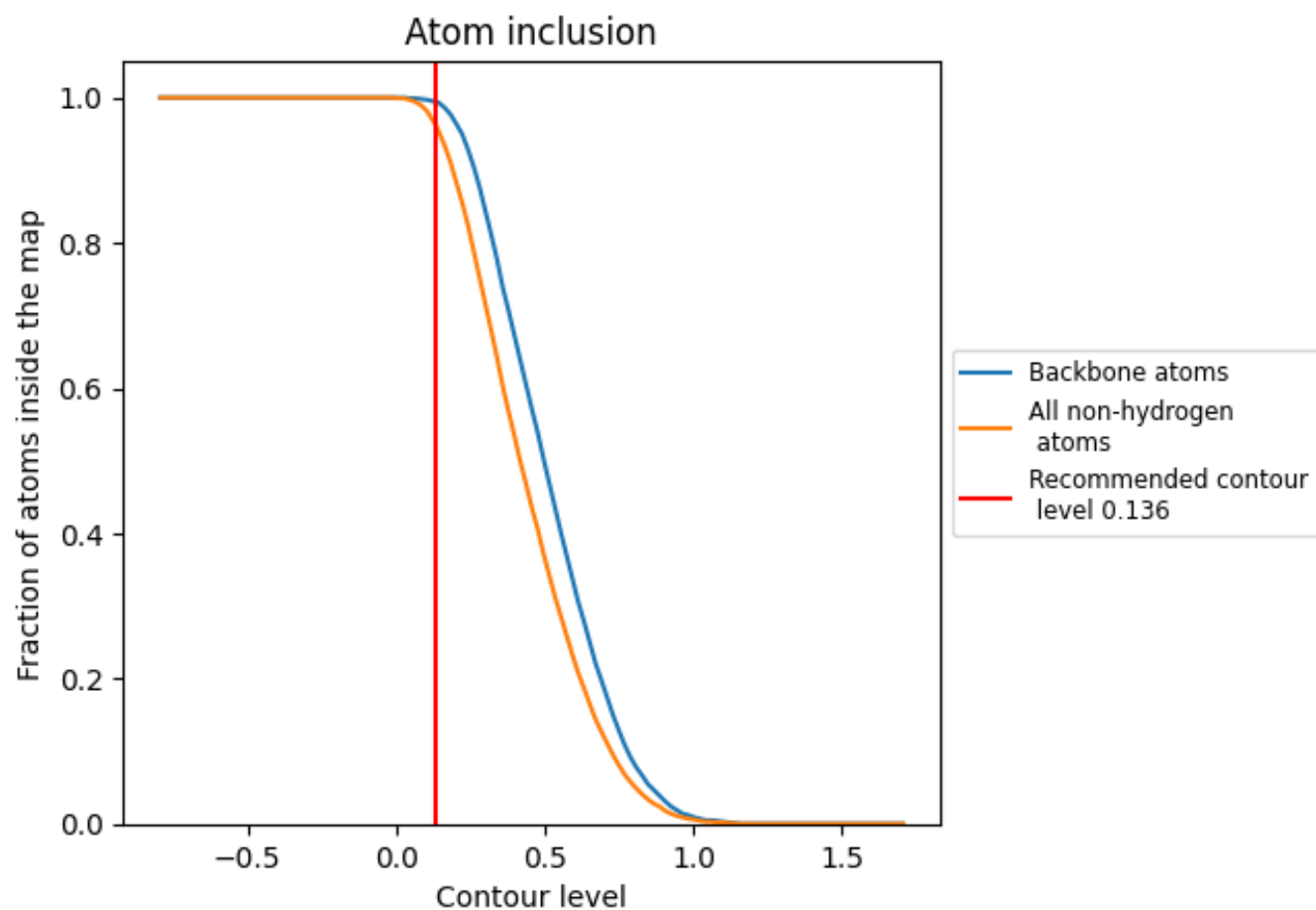
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.136).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 96% 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 (0.136) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9600	0.4970
A	0.9680	0.5080
B	0.9570	0.4800
C	0.9680	0.5200
D	0.9610	0.4990
E	0.9640	0.5220
F	0.9410	0.4570

1.0

0.0

<0.0