



wwPDB EM Validation Summary Report ⓘ

Oct 6, 2024 – 08:23 AM EDT

PDB ID : 8T20
EMDB ID : EMD-40976
Title : Cryo-EM structure of mink variant Y453F trimeric spike protein bound to two mink ACE2 receptors
Authors : Ahn, H.M.; Calderon, B.; Fan, X.; Gao, Y.; Horgan, N.; Zhou, B.; Liang, B.
Deposited on : 2023-06-05
Resolution : 3.36 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

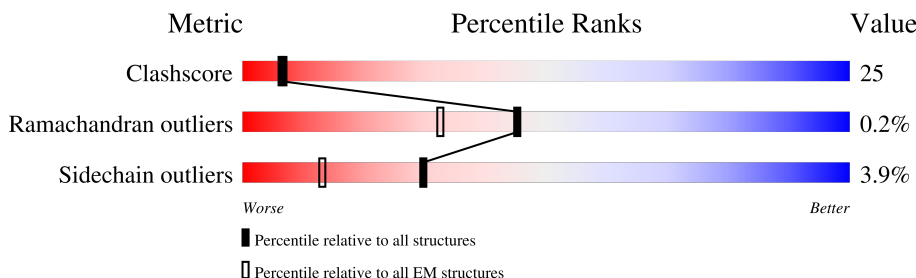
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.36 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	1269	
1	B	1269	
1	C	1269	
2	D	771	
2	E	771	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 32612 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	1001	Total	C	N	O	S	0	0
			7810	4990	1297	1488	35		
1	B	962	Total	C	N	O	S	0	0
			7497	4790	1243	1430	34		
1	C	962	Total	C	N	O	S	0	0
			7497	4790	1243	1430	34		

There are 228 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	453	PHE	TYR	variant	UNP P0DTC2
A	614	GLY	ASP	engineered mutation	UNP P0DTC2
A	682	GLY	ARG	engineered mutation	UNP P0DTC2
A	683	SER	ARG	engineered mutation	UNP P0DTC2
A	685	SER	ARG	engineered mutation	UNP P0DTC2
A	817	PRO	PHE	engineered mutation	UNP P0DTC2
A	892	PRO	ALA	engineered mutation	UNP P0DTC2
A	899	PRO	ALA	engineered mutation	UNP P0DTC2
A	942	PRO	ALA	engineered mutation	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
A	1209	GLY	-	expression tag	UNP P0DTC2
A	1210	SER	-	expression tag	UNP P0DTC2
A	1211	GLY	-	expression tag	UNP P0DTC2
A	1212	SER	-	expression tag	UNP P0DTC2
A	1213	GLY	-	expression tag	UNP P0DTC2
A	1214	SER	-	expression tag	UNP P0DTC2
A	1215	GLY	-	expression tag	UNP P0DTC2
A	1216	SER	-	expression tag	UNP P0DTC2
A	1217	GLY	-	expression tag	UNP P0DTC2
A	1218	TYR	-	expression tag	UNP P0DTC2
A	1219	ILE	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1220	PRO	-	expression tag	UNP P0DTC2
A	1221	GLU	-	expression tag	UNP P0DTC2
A	1222	ALA	-	expression tag	UNP P0DTC2
A	1223	PRO	-	expression tag	UNP P0DTC2
A	1224	ARG	-	expression tag	UNP P0DTC2
A	1225	ASP	-	expression tag	UNP P0DTC2
A	1226	GLY	-	expression tag	UNP P0DTC2
A	1227	GLN	-	expression tag	UNP P0DTC2
A	1228	ALA	-	expression tag	UNP P0DTC2
A	1229	TYR	-	expression tag	UNP P0DTC2
A	1230	VAL	-	expression tag	UNP P0DTC2
A	1231	ARG	-	expression tag	UNP P0DTC2
A	1232	LYS	-	expression tag	UNP P0DTC2
A	1233	ASP	-	expression tag	UNP P0DTC2
A	1234	GLY	-	expression tag	UNP P0DTC2
A	1235	GLU	-	expression tag	UNP P0DTC2
A	1236	TRP	-	expression tag	UNP P0DTC2
A	1237	VAL	-	expression tag	UNP P0DTC2
A	1238	LEU	-	expression tag	UNP P0DTC2
A	1239	LEU	-	expression tag	UNP P0DTC2
A	1240	SER	-	expression tag	UNP P0DTC2
A	1241	THR	-	expression tag	UNP P0DTC2
A	1242	PHE	-	expression tag	UNP P0DTC2
A	1243	LEU	-	expression tag	UNP P0DTC2
A	1244	GLY	-	expression tag	UNP P0DTC2
A	1245	SER	-	expression tag	UNP P0DTC2
A	1246	GLY	-	expression tag	UNP P0DTC2
A	1247	SER	-	expression tag	UNP P0DTC2
A	1248	GLY	-	expression tag	UNP P0DTC2
A	1249	SER	-	expression tag	UNP P0DTC2
A	1250	GLY	-	expression tag	UNP P0DTC2
A	1251	HIS	-	expression tag	UNP P0DTC2
A	1252	HIS	-	expression tag	UNP P0DTC2
A	1253	HIS	-	expression tag	UNP P0DTC2
A	1254	HIS	-	expression tag	UNP P0DTC2
A	1255	HIS	-	expression tag	UNP P0DTC2
A	1256	HIS	-	expression tag	UNP P0DTC2
A	1257	GLY	-	expression tag	UNP P0DTC2
A	1258	LEU	-	expression tag	UNP P0DTC2
A	1259	ASN	-	expression tag	UNP P0DTC2
A	1260	ASP	-	expression tag	UNP P0DTC2
A	1261	ILE	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1262	PHE	-	expression tag	UNP P0DTC2
A	1263	GLU	-	expression tag	UNP P0DTC2
A	1264	ALA	-	expression tag	UNP P0DTC2
A	1265	GLN	-	expression tag	UNP P0DTC2
A	1266	LYS	-	expression tag	UNP P0DTC2
A	1267	ILE	-	expression tag	UNP P0DTC2
A	1268	GLU	-	expression tag	UNP P0DTC2
A	1269	TRP	-	expression tag	UNP P0DTC2
A	1270	HIS	-	expression tag	UNP P0DTC2
A	1271	GLU	-	expression tag	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	453	PHE	TYR	variant	UNP P0DTC2
B	614	GLY	ASP	engineered mutation	UNP P0DTC2
B	682	GLY	ARG	engineered mutation	UNP P0DTC2
B	683	SER	ARG	engineered mutation	UNP P0DTC2
B	685	SER	ARG	engineered mutation	UNP P0DTC2
B	817	PRO	PHE	engineered mutation	UNP P0DTC2
B	892	PRO	ALA	engineered mutation	UNP P0DTC2
B	899	PRO	ALA	engineered mutation	UNP P0DTC2
B	942	PRO	ALA	engineered mutation	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	1209	GLY	-	expression tag	UNP P0DTC2
B	1210	SER	-	expression tag	UNP P0DTC2
B	1211	GLY	-	expression tag	UNP P0DTC2
B	1212	SER	-	expression tag	UNP P0DTC2
B	1213	GLY	-	expression tag	UNP P0DTC2
B	1214	SER	-	expression tag	UNP P0DTC2
B	1215	GLY	-	expression tag	UNP P0DTC2
B	1216	SER	-	expression tag	UNP P0DTC2
B	1217	GLY	-	expression tag	UNP P0DTC2
B	1218	TYR	-	expression tag	UNP P0DTC2
B	1219	ILE	-	expression tag	UNP P0DTC2
B	1220	PRO	-	expression tag	UNP P0DTC2
B	1221	GLU	-	expression tag	UNP P0DTC2
B	1222	ALA	-	expression tag	UNP P0DTC2
B	1223	PRO	-	expression tag	UNP P0DTC2
B	1224	ARG	-	expression tag	UNP P0DTC2
B	1225	ASP	-	expression tag	UNP P0DTC2
B	1226	GLY	-	expression tag	UNP P0DTC2
B	1227	GLN	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1228	ALA	-	expression tag	UNP P0DTC2
B	1229	TYR	-	expression tag	UNP P0DTC2
B	1230	VAL	-	expression tag	UNP P0DTC2
B	1231	ARG	-	expression tag	UNP P0DTC2
B	1232	LYS	-	expression tag	UNP P0DTC2
B	1233	ASP	-	expression tag	UNP P0DTC2
B	1234	GLY	-	expression tag	UNP P0DTC2
B	1235	GLU	-	expression tag	UNP P0DTC2
B	1236	TRP	-	expression tag	UNP P0DTC2
B	1237	VAL	-	expression tag	UNP P0DTC2
B	1238	LEU	-	expression tag	UNP P0DTC2
B	1239	LEU	-	expression tag	UNP P0DTC2
B	1240	SER	-	expression tag	UNP P0DTC2
B	1241	THR	-	expression tag	UNP P0DTC2
B	1242	PHE	-	expression tag	UNP P0DTC2
B	1243	LEU	-	expression tag	UNP P0DTC2
B	1244	GLY	-	expression tag	UNP P0DTC2
B	1245	SER	-	expression tag	UNP P0DTC2
B	1246	GLY	-	expression tag	UNP P0DTC2
B	1247	SER	-	expression tag	UNP P0DTC2
B	1248	GLY	-	expression tag	UNP P0DTC2
B	1249	SER	-	expression tag	UNP P0DTC2
B	1250	GLY	-	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	GLY	-	expression tag	UNP P0DTC2
B	1258	LEU	-	expression tag	UNP P0DTC2
B	1259	ASN	-	expression tag	UNP P0DTC2
B	1260	ASP	-	expression tag	UNP P0DTC2
B	1261	ILE	-	expression tag	UNP P0DTC2
B	1262	PHE	-	expression tag	UNP P0DTC2
B	1263	GLU	-	expression tag	UNP P0DTC2
B	1264	ALA	-	expression tag	UNP P0DTC2
B	1265	GLN	-	expression tag	UNP P0DTC2
B	1266	LYS	-	expression tag	UNP P0DTC2
B	1267	ILE	-	expression tag	UNP P0DTC2
B	1268	GLU	-	expression tag	UNP P0DTC2
B	1269	TRP	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1270	HIS	-	expression tag	UNP P0DTC2
B	1271	GLU	-	expression tag	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	453	PHE	TYR	variant	UNP P0DTC2
C	614	GLY	ASP	engineered mutation	UNP P0DTC2
C	682	GLY	ARG	engineered mutation	UNP P0DTC2
C	683	SER	ARG	engineered mutation	UNP P0DTC2
C	685	SER	ARG	engineered mutation	UNP P0DTC2
C	817	PRO	PHE	engineered mutation	UNP P0DTC2
C	892	PRO	ALA	engineered mutation	UNP P0DTC2
C	899	PRO	ALA	engineered mutation	UNP P0DTC2
C	942	PRO	ALA	engineered mutation	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	1209	GLY	-	expression tag	UNP P0DTC2
C	1210	SER	-	expression tag	UNP P0DTC2
C	1211	GLY	-	expression tag	UNP P0DTC2
C	1212	SER	-	expression tag	UNP P0DTC2
C	1213	GLY	-	expression tag	UNP P0DTC2
C	1214	SER	-	expression tag	UNP P0DTC2
C	1215	GLY	-	expression tag	UNP P0DTC2
C	1216	SER	-	expression tag	UNP P0DTC2
C	1217	GLY	-	expression tag	UNP P0DTC2
C	1218	TYR	-	expression tag	UNP P0DTC2
C	1219	ILE	-	expression tag	UNP P0DTC2
C	1220	PRO	-	expression tag	UNP P0DTC2
C	1221	GLU	-	expression tag	UNP P0DTC2
C	1222	ALA	-	expression tag	UNP P0DTC2
C	1223	PRO	-	expression tag	UNP P0DTC2
C	1224	ARG	-	expression tag	UNP P0DTC2
C	1225	ASP	-	expression tag	UNP P0DTC2
C	1226	GLY	-	expression tag	UNP P0DTC2
C	1227	GLN	-	expression tag	UNP P0DTC2
C	1228	ALA	-	expression tag	UNP P0DTC2
C	1229	TYR	-	expression tag	UNP P0DTC2
C	1230	VAL	-	expression tag	UNP P0DTC2
C	1231	ARG	-	expression tag	UNP P0DTC2
C	1232	LYS	-	expression tag	UNP P0DTC2
C	1233	ASP	-	expression tag	UNP P0DTC2
C	1234	GLY	-	expression tag	UNP P0DTC2
C	1235	GLU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1236	TRP	-	expression tag	UNP P0DTC2
C	1237	VAL	-	expression tag	UNP P0DTC2
C	1238	LEU	-	expression tag	UNP P0DTC2
C	1239	LEU	-	expression tag	UNP P0DTC2
C	1240	SER	-	expression tag	UNP P0DTC2
C	1241	THR	-	expression tag	UNP P0DTC2
C	1242	PHE	-	expression tag	UNP P0DTC2
C	1243	LEU	-	expression tag	UNP P0DTC2
C	1244	GLY	-	expression tag	UNP P0DTC2
C	1245	SER	-	expression tag	UNP P0DTC2
C	1246	GLY	-	expression tag	UNP P0DTC2
C	1247	SER	-	expression tag	UNP P0DTC2
C	1248	GLY	-	expression tag	UNP P0DTC2
C	1249	SER	-	expression tag	UNP P0DTC2
C	1250	GLY	-	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	GLY	-	expression tag	UNP P0DTC2
C	1258	LEU	-	expression tag	UNP P0DTC2
C	1259	ASN	-	expression tag	UNP P0DTC2
C	1260	ASP	-	expression tag	UNP P0DTC2
C	1261	ILE	-	expression tag	UNP P0DTC2
C	1262	PHE	-	expression tag	UNP P0DTC2
C	1263	GLU	-	expression tag	UNP P0DTC2
C	1264	ALA	-	expression tag	UNP P0DTC2
C	1265	GLN	-	expression tag	UNP P0DTC2
C	1266	LYS	-	expression tag	UNP P0DTC2
C	1267	ILE	-	expression tag	UNP P0DTC2
C	1268	GLU	-	expression tag	UNP P0DTC2
C	1269	TRP	-	expression tag	UNP P0DTC2
C	1270	HIS	-	expression tag	UNP P0DTC2
C	1271	GLU	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called Angiotensin-converting enzyme.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	596	Total	C	N	O	S	0	0
			4904	3133	824	918	29		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	596	Total	C	N	O	S	0	0
			4904	3133	824	918	29		

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	740	GLY	-	expression tag	UNP A0A7T0Q2W2
D	741	SER	-	expression tag	UNP A0A7T0Q2W2
D	742	GLY	-	expression tag	UNP A0A7T0Q2W2
D	743	SER	-	expression tag	UNP A0A7T0Q2W2
D	744	GLY	-	expression tag	UNP A0A7T0Q2W2
D	745	SER	-	expression tag	UNP A0A7T0Q2W2
D	746	GLY	-	expression tag	UNP A0A7T0Q2W2
D	747	HIS	-	expression tag	UNP A0A7T0Q2W2
D	748	HIS	-	expression tag	UNP A0A7T0Q2W2
D	749	HIS	-	expression tag	UNP A0A7T0Q2W2
D	750	HIS	-	expression tag	UNP A0A7T0Q2W2
D	751	HIS	-	expression tag	UNP A0A7T0Q2W2
D	752	HIS	-	expression tag	UNP A0A7T0Q2W2
D	753	GLY	-	expression tag	UNP A0A7T0Q2W2
D	754	SER	-	expression tag	UNP A0A7T0Q2W2
D	755	GLY	-	expression tag	UNP A0A7T0Q2W2
D	756	SER	-	expression tag	UNP A0A7T0Q2W2
D	757	GLY	-	expression tag	UNP A0A7T0Q2W2
D	758	LEU	-	expression tag	UNP A0A7T0Q2W2
D	759	ASN	-	expression tag	UNP A0A7T0Q2W2
D	760	ASP	-	expression tag	UNP A0A7T0Q2W2
D	761	ILE	-	expression tag	UNP A0A7T0Q2W2
D	762	PHE	-	expression tag	UNP A0A7T0Q2W2
D	763	GLU	-	expression tag	UNP A0A7T0Q2W2
D	764	ALA	-	expression tag	UNP A0A7T0Q2W2
D	765	GLN	-	expression tag	UNP A0A7T0Q2W2
D	766	LYS	-	expression tag	UNP A0A7T0Q2W2
D	767	ILE	-	expression tag	UNP A0A7T0Q2W2
D	768	GLU	-	expression tag	UNP A0A7T0Q2W2
D	769	TRP	-	expression tag	UNP A0A7T0Q2W2
D	770	HIS	-	expression tag	UNP A0A7T0Q2W2
D	771	GLU	-	expression tag	UNP A0A7T0Q2W2
E	740	GLY	-	expression tag	UNP A0A7T0Q2W2
E	741	SER	-	expression tag	UNP A0A7T0Q2W2
E	742	GLY	-	expression tag	UNP A0A7T0Q2W2
E	743	SER	-	expression tag	UNP A0A7T0Q2W2

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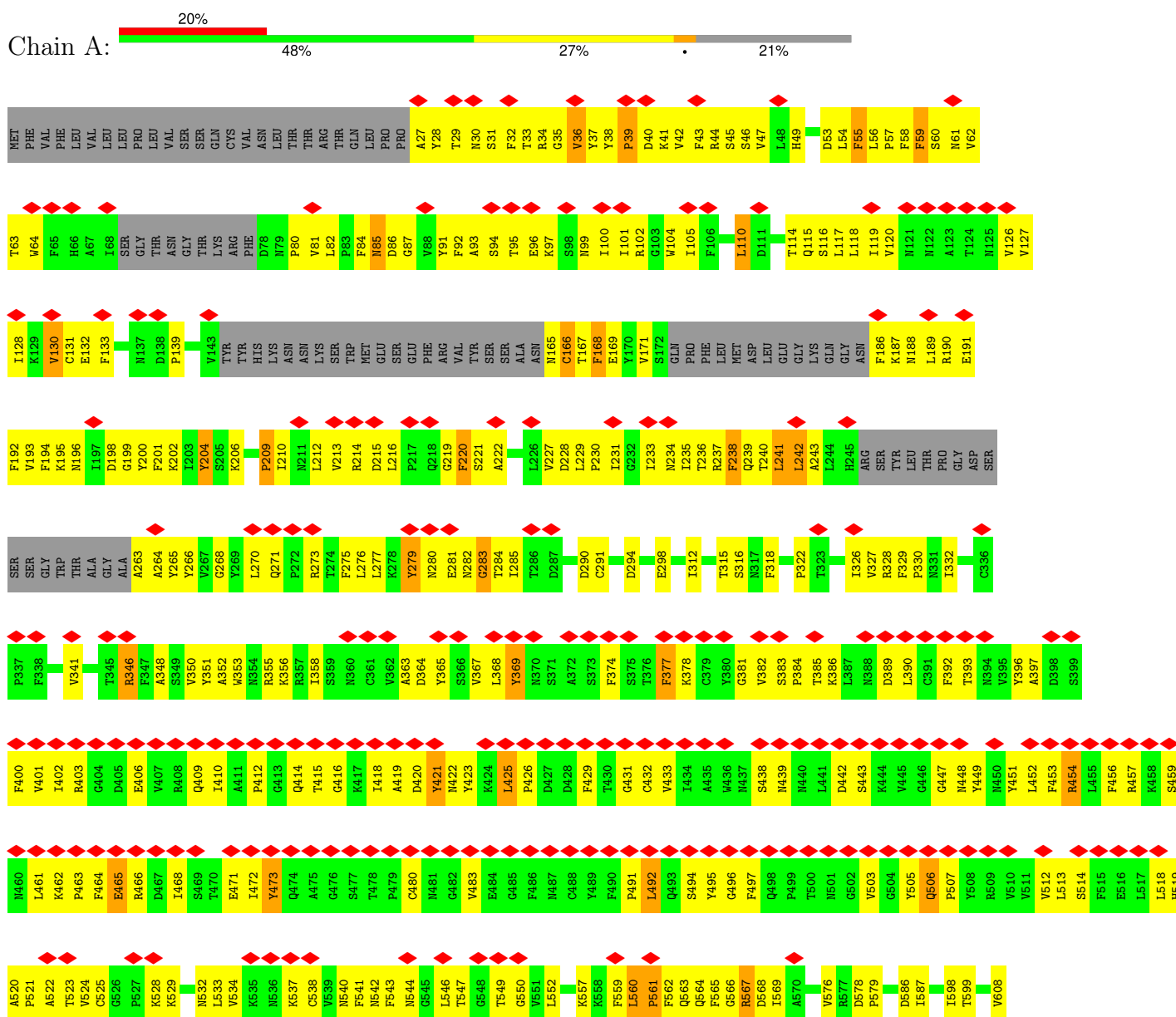
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Chain	Residue	Modelled	Actual	Comment	Reference
E	744	GLY	-	expression tag	UNP A0A7T0Q2W2
E	745	SER	-	expression tag	UNP A0A7T0Q2W2
E	746	GLY	-	expression tag	UNP A0A7T0Q2W2
E	747	HIS	-	expression tag	UNP A0A7T0Q2W2
E	748	HIS	-	expression tag	UNP A0A7T0Q2W2
E	749	HIS	-	expression tag	UNP A0A7T0Q2W2
E	750	HIS	-	expression tag	UNP A0A7T0Q2W2
E	751	HIS	-	expression tag	UNP A0A7T0Q2W2
E	752	HIS	-	expression tag	UNP A0A7T0Q2W2
E	753	GLY	-	expression tag	UNP A0A7T0Q2W2
E	754	SER	-	expression tag	UNP A0A7T0Q2W2
E	755	GLY	-	expression tag	UNP A0A7T0Q2W2
E	756	SER	-	expression tag	UNP A0A7T0Q2W2
E	757	GLY	-	expression tag	UNP A0A7T0Q2W2
E	758	LEU	-	expression tag	UNP A0A7T0Q2W2
E	759	ASN	-	expression tag	UNP A0A7T0Q2W2
E	760	ASP	-	expression tag	UNP A0A7T0Q2W2
E	761	ILE	-	expression tag	UNP A0A7T0Q2W2
E	762	PHE	-	expression tag	UNP A0A7T0Q2W2
E	763	GLU	-	expression tag	UNP A0A7T0Q2W2
E	764	ALA	-	expression tag	UNP A0A7T0Q2W2
E	765	GLN	-	expression tag	UNP A0A7T0Q2W2
E	766	LYS	-	expression tag	UNP A0A7T0Q2W2
E	767	ILE	-	expression tag	UNP A0A7T0Q2W2
E	768	GLU	-	expression tag	UNP A0A7T0Q2W2
E	769	TRP	-	expression tag	UNP A0A7T0Q2W2
E	770	HIS	-	expression tag	UNP A0A7T0Q2W2
E	771	GLU	-	expression tag	UNP A0A7T0Q2W2

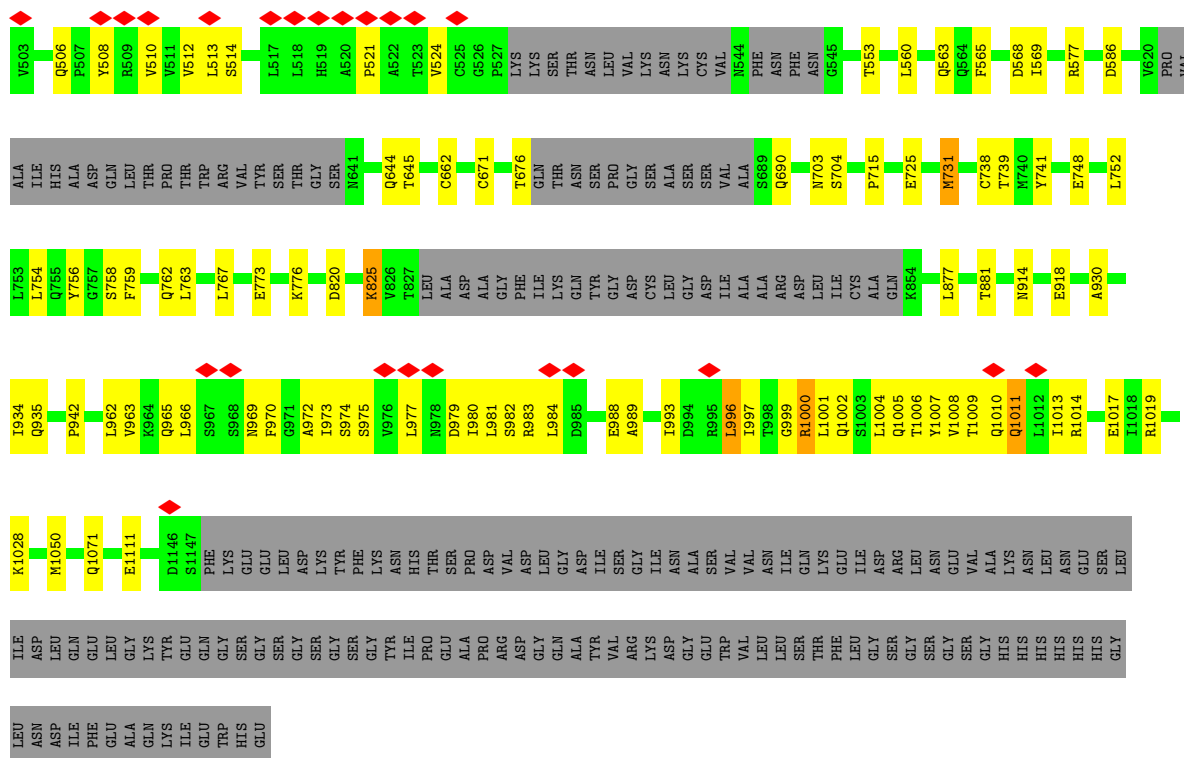
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

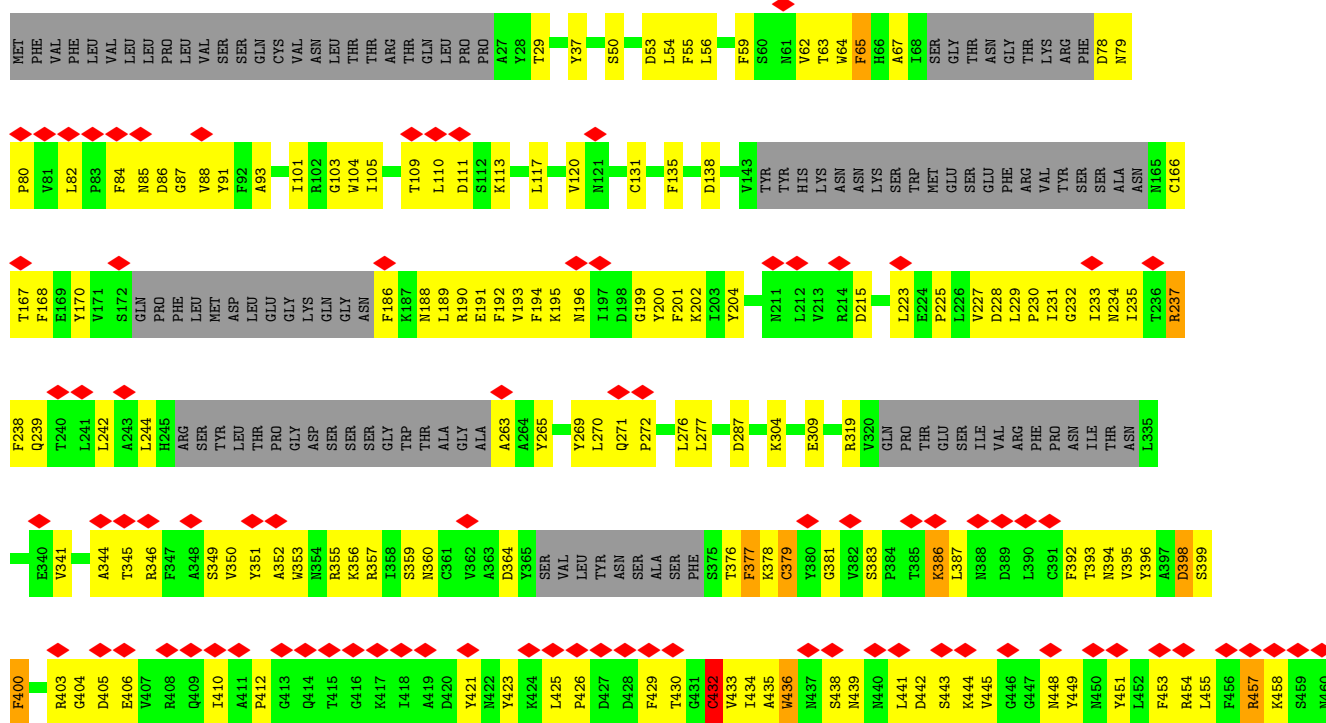
• Molecule 1: Spike glycoprotein







• Molecule 1: Spike glycoprotein



SER	GLN	N601	K541	K481	I421	C361
	THR	S602	C542	D482	G422	T362
LEU	ILE	F603	D543	D483	L423	K363
PHE	PRO	V604	I544	I484	L424	V364
LEU	PHE	G605	S545	V485	P425	T365
GLY	VAL	G605	S545	V485	P425	T365
ILE	ASP	N606	N546	G486	P426	M366
GLN	LYS	N607	S547	V487	D427	D367
PRO	ASP	N607	S547	V487	D427	D367
THR	VAL	T608	R548	E489	F428	D368
LEU	ARG	D609	E549	E489	F429	F369
GLU	VAL	W610	A550	P490	E430	L370
PRO	SER	S611	G551	L491	E430	L370
PRO	ASP	S611	G551	P492	D431	T371
TYR	LEU	P612	Q552	H493	S432	A372
GLN	LYS	Y613	K553	D494	E433	H373
PRO	PRO	A614	L554	E495	T434	H374
PRO	ARG	ASP	H555	T496	D435	E375
VAL	ILE	GLN	E556	Y497	I436	M376
GLY	SER	SER	E557	Y497	I436	M376
SER	PHE	ILE	M557	C498	G377	G377
GLY	ASN	LYS	L558	D499	H378	H378
SER	PHE	VAL	S559	P500	F438	I379
GLY	ILE	VAL	S559	P500	L439	Q380
SER	VAL	ARG	L560	A501	L440	Q380
GLY	THR	ILE	G561	A502	K441	Y381
SER	SER	SER	S662	L503	Q442	D382
HIS	PRO	LEU	R562	L503	Q442	D382
HIS	PRO	LEU	R562	L503	Q442	D382
HIS	GLU	LYS	S563	F504	A443	M383
HIS	ASN	SER	S563	F504	A443	M383
HIS	ASN	ALA	K564	H505	L444	A384
HIS	MET	ALA	K564	H505	L444	A384
HIS	SER	LEU	S665	V506	T445	Y385
HIS	SER	LEU	S665	V506	T445	Y385
GLY	ASP	GLY	W566	A507	I446	A386
SER	ILE	ILE	T567	N508	V447	A387
GLY	ILE	LYS	T567	N508	V447	A387
GLY	PRO	ALA	F568	D509	G448	Q388
SER	PRO	ALA	F568	D509	T449	P389
GLY	ARG	TRP	A569	Y510	L450	F390
LEU	ALA	GLU	L570	S511	L450	F390
LEU	ASP	TRP	L570	S511	P451	L391
ASN	ASP	ASN	E571	F512	F452	L392
ASP	VAL	ASP	R572	I513	T453	R393
ILE	GLU	GLU	V573	R514	Y454	N394
PHE	GLU	ASN	V573	R514	Y454	N394
GLU	ALA	ALA	V574	Y515	M455	G395
ALA	ILE	MET	G575	Y516	L456	A396
GLN	ARG	PHE	A576	Y516	L456	A396
ARG	ARG	THR	G576	Y516	E457	N397
LYS	LYS	PHE	T577	T517	K458	E398
ILE	SER	PHE	K577	R518	G399	G399
GLU	ARG	GLN	T578	T519	R460	F400
TRP	GLY	GLY	M579	I520	W461	H401
ARG	ARG	SER	I520	I520	M462	E402
ILE	ILE	ILE	D580	Q521	F463	A403
ASN	ASN	ALA	V581	Q522	F464	V404
ASP	ASP	TTR	R582	Q522	K465	G405
ALA	ALA	MET	L583	F523	G466	E406
PHE	PHE	ARG	L584	Q524	E467	I407
ARG	ARG	GLU	L585	F525	I468	M408
LEU	LEU	THR	L586	Q526	P469	S409
ASP	ASP	PHE	N586	E527	K470	L410
ASP	ASN	SER	T587	L528	E471	S411
ASN	LYS	LYS	F588	L529	Q472	A412
LYS	LYS	VAL	E589	C530	W473	A413
VAL	VAL	VAL	P590	Q531	M474	T414
LYS	LYS	LYS	L591	I532	Q475	P415
LYS	LYS	LYS	F592	A533	K476	N416
LYS	LYS	LYS	T593	K534	W477	H417
LYS	LYS	LYS	V594	H535	E479	L418
LYS	LYS	LYS	L595	E536	M480	K419
LYS	LYS	LYS	K596	G537		
LYS	LYS	LYS	E597	P538		
LYS	LYS	LYS	Q598	L539		
LYS	LYS	LYS	N599	Y540		
LYS	LYS	LYS	R600			

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	512723	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	49.98	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	1750	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.600	Depositor
Minimum map value	-1.876	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.062	Depositor
Recommended contour level	0.328	Depositor
Map size (Å)	568.32, 568.32, 568.32	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.11, 1.11, 1.11	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.34	0/7988	0.65	10/10873 (0.1%)
1	B	0.33	0/7665	0.56	1/10430 (0.0%)
1	C	0.33	0/7665	0.56	4/10430 (0.0%)
2	D	0.49	4/5047 (0.1%)	0.85	21/6854 (0.3%)
2	E	0.30	0/5047	0.62	2/6854 (0.0%)
All	All	0.36	4/33412 (0.0%)	0.64	38/45441 (0.1%)

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	7
1	B	0	1
2	D	0	8
2	E	0	3
All	All	0	19

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	583	PRO	CG-CD	-19.90	0.84	1.50
2	D	289	PRO	CG-CD	-8.47	1.22	1.50
2	D	426	PRO	CG-CD	-7.81	1.24	1.50
2	D	583	PRO	N-CD	7.14	1.57	1.47

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	583	PRO	N-CD-CG	-19.47	73.99	103.20
2	D	426	PRO	CA-N-CD	-12.70	93.72	111.50
2	D	289	PRO	CA-N-CD	-11.58	95.29	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	583	PRO	CA-CB-CG	-10.91	83.27	104.00
2	D	426	PRO	N-CD-CG	-10.88	86.88	103.20

There are no chirality outliers.

5 of 19 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	220	PHE	Peptide
1	A	346	ARG	Peptide
1	A	36	VAL	Peptide
1	A	506	GLN	Peptide
1	A	55	PHE	Peptide

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	7810	0	7636	482	0
1	B	7497	0	7321	261	0
1	C	7497	0	7321	222	0
2	D	4904	0	4667	399	0
2	E	4904	0	4667	280	0
All	All	32612	0	31612	1600	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 25.

The worst 5 of 1600 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1007:TYR:O	1:B:1011:GLN:HB3	1.27	1.29
1:A:1000:ARG:O	1:A:1004:LEU:HB2	1.37	1.22
1:A:1001:LEU:O	1:A:1005:GLN:HB3	1.38	1.19
2:D:484:ILE:N	2:D:607:ASN:O	1.84	1.11
1:A:961:THR:O	1:A:965:GLN:HB2	1.53	1.05

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	985/1269 (78%)	812 (82%)	171 (17%)	2 (0%)	44	71
1	B	940/1269 (74%)	837 (89%)	103 (11%)	0	100	100
1	C	940/1269 (74%)	847 (90%)	93 (10%)	0	100	100
2	D	594/771 (77%)	504 (85%)	86 (14%)	4 (1%)	19	47
2	E	594/771 (77%)	523 (88%)	69 (12%)	2 (0%)	37	65
All	All	4053/5349 (76%)	3523 (87%)	522 (13%)	8 (0%)	45	71

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	388	GLN
2	D	600	ARG
1	A	85	ASN
2	D	490	PRO
2	D	280	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	877/1101 (80%)	847 (97%)	30 (3%)	32	58
1	B	839/1101 (76%)	820 (98%)	19 (2%)	45	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	839/1101 (76%)	811 (97%)	28 (3%)	33	59
2	D	524/676 (78%)	483 (92%)	41 (8%)	10	33
2	E	524/676 (78%)	500 (95%)	24 (5%)	23	50
All	All	3603/4655 (77%)	3461 (96%)	142 (4%)	30	54

5 of 142 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	572	ARG
2	E	47	SER
2	E	374	HIS
1	B	1050	MET
1	B	1000	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
2	E	300	GLN
2	E	526	GLN
2	E	607	ASN
2	E	586	ASN
1	B	690	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 [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.

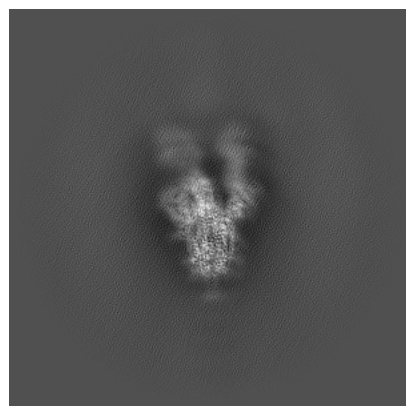
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40976. These allow visual inspection of the internal detail of the map and identification of artifacts.

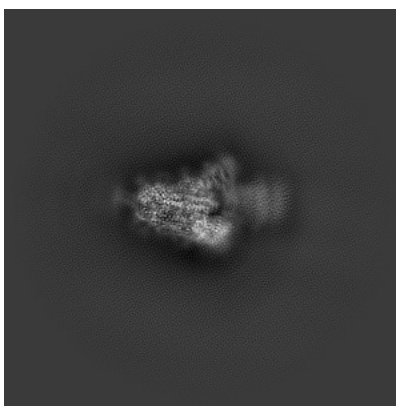
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

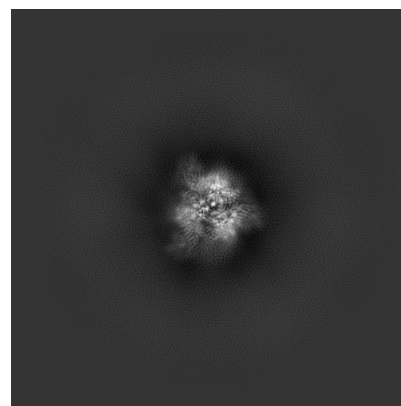
6.1.1 Primary map



X

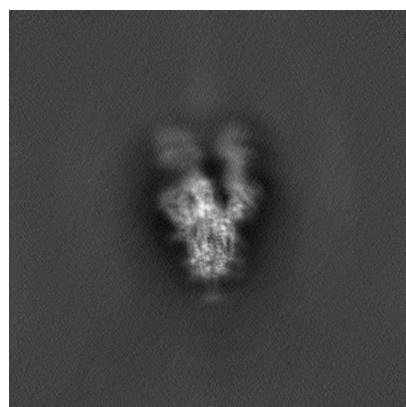


Y

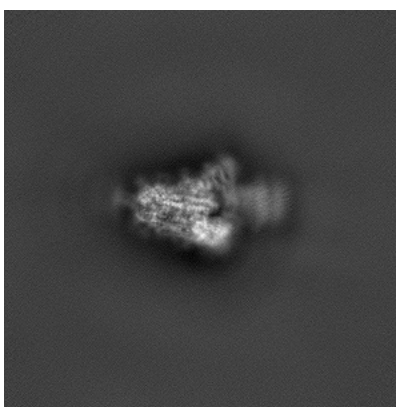


Z

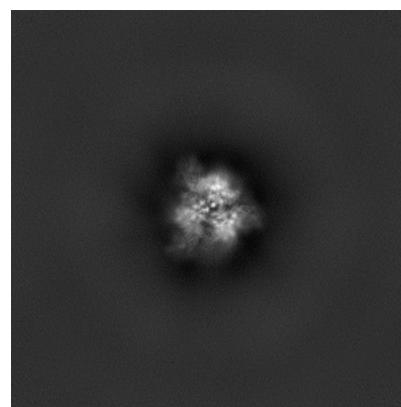
6.1.2 Raw map



X



Y

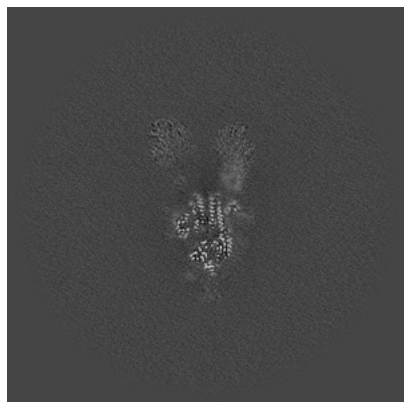


Z

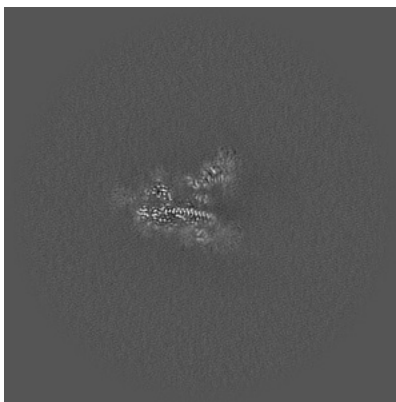
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

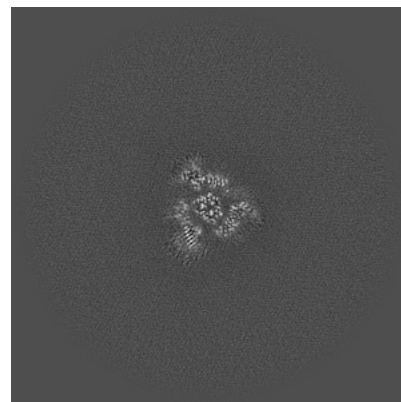
6.2.1 Primary map



X Index: 256

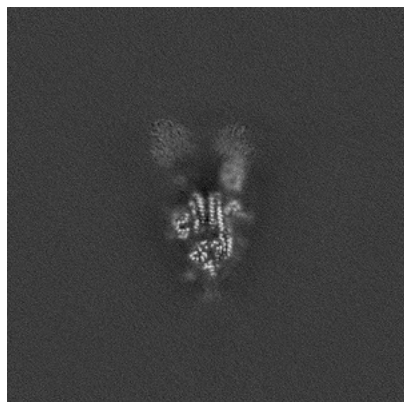


Y Index: 256

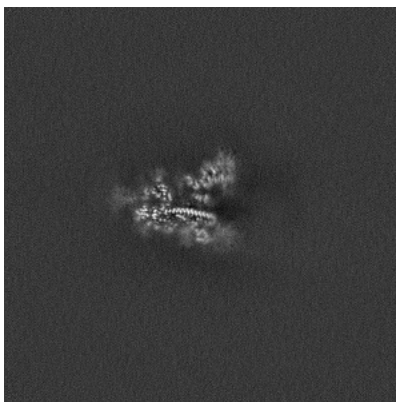


Z Index: 256

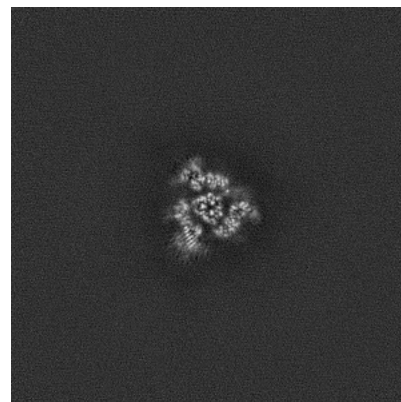
6.2.2 Raw map



X Index: 256



Y Index: 256

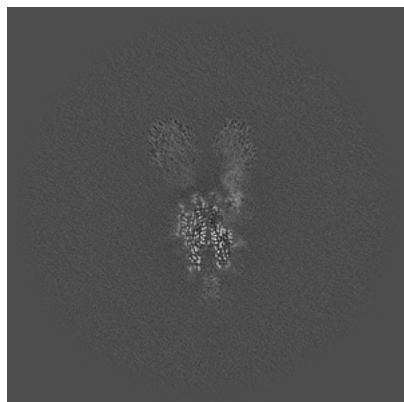


Z Index: 256

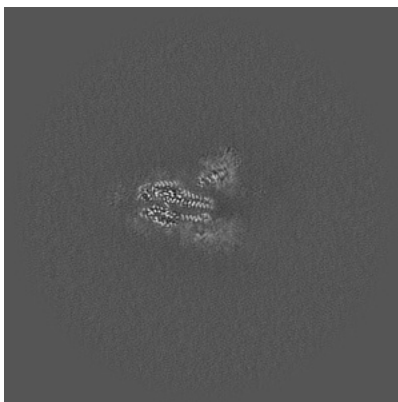
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

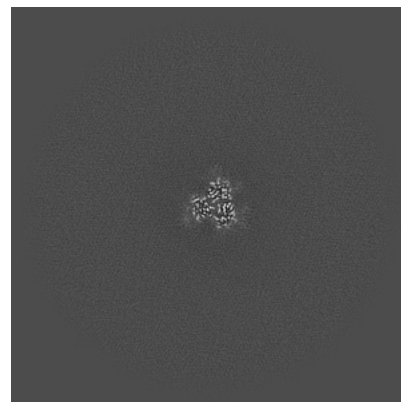
6.3.1 Primary map



X Index: 263



Y Index: 249

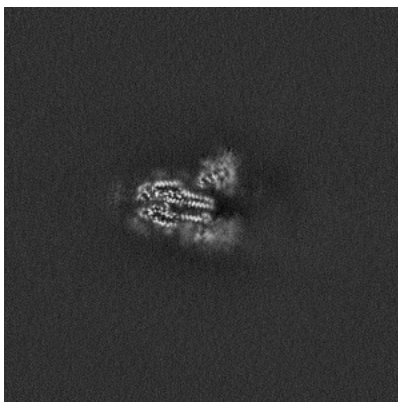


Z Index: 204

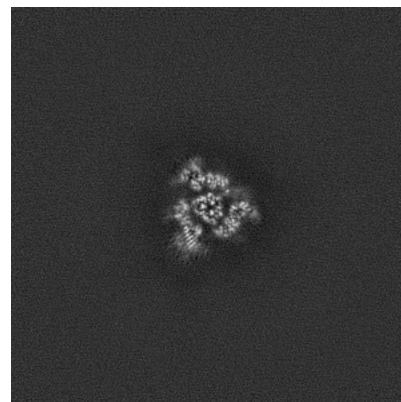
6.3.2 Raw map



X Index: 259



Y Index: 249

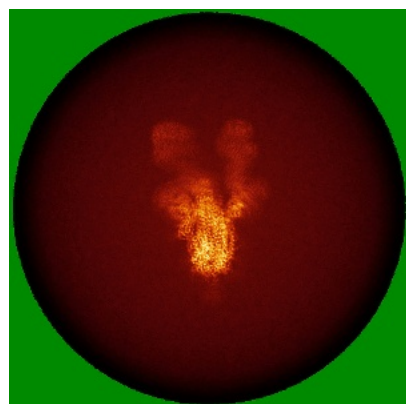


Z Index: 256

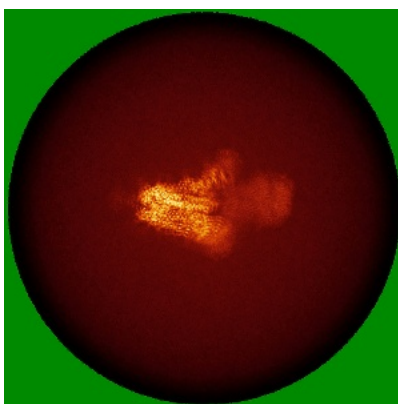
The images above show the largest variance slices of the map in three orthogonal directions.

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

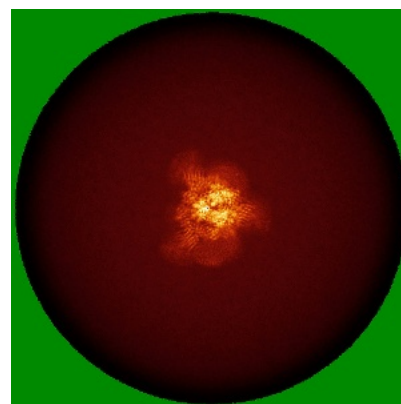
6.4.1 Primary map



X

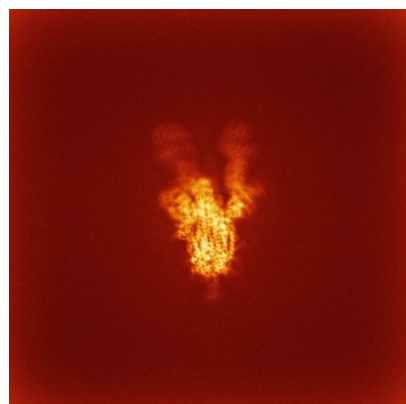


Y

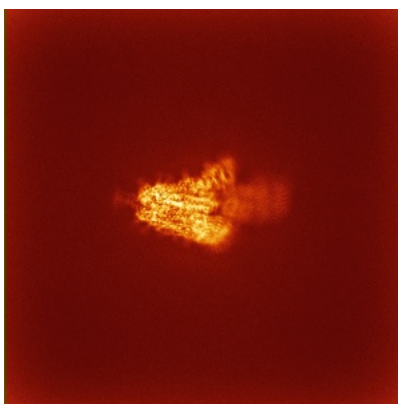


Z

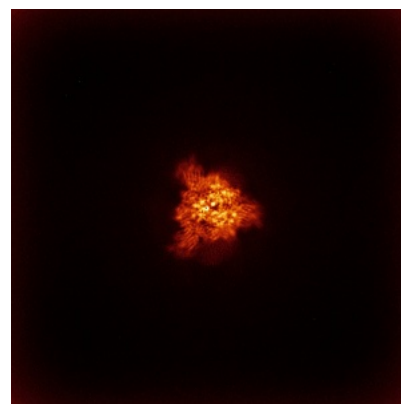
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.328. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

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

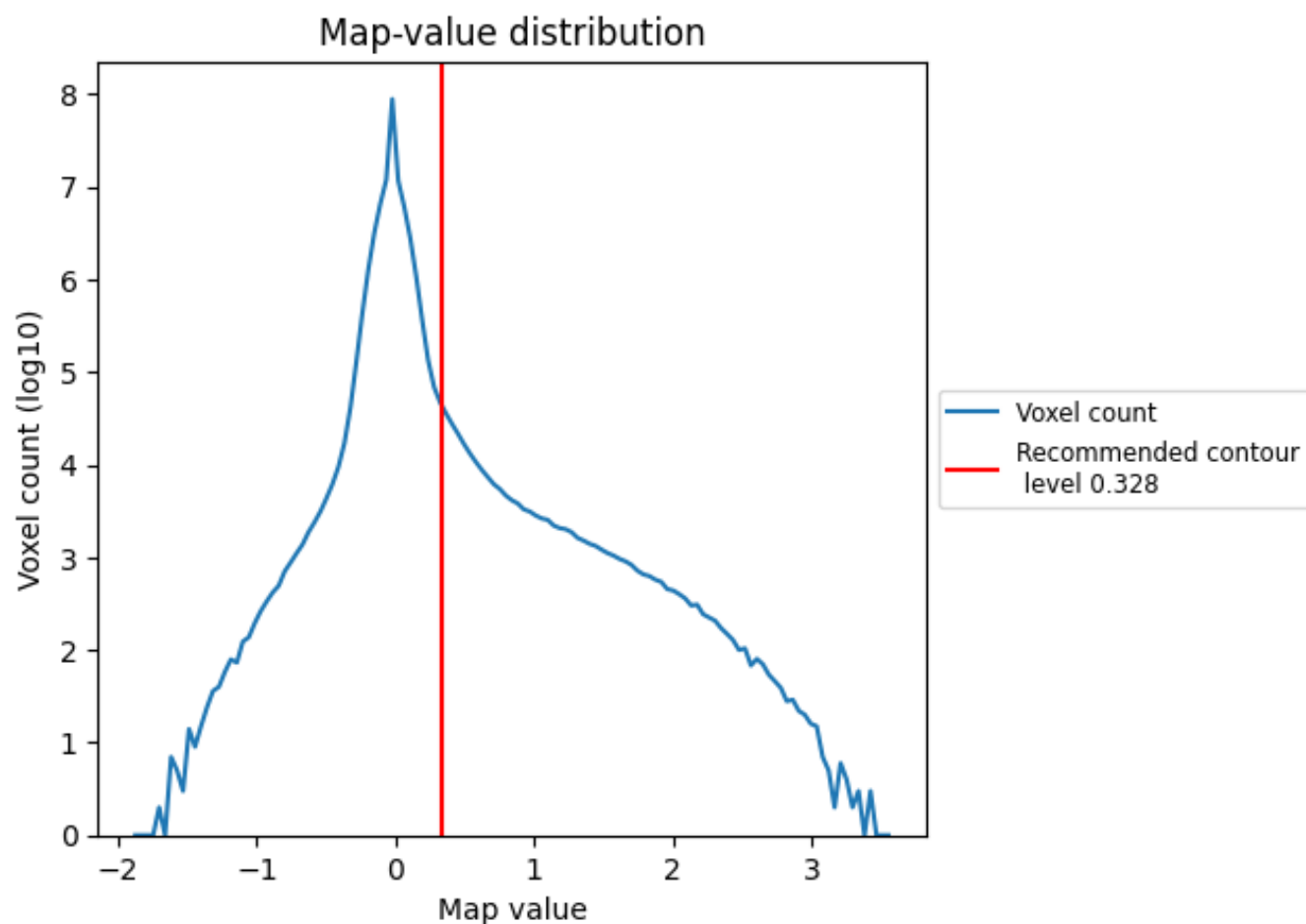
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

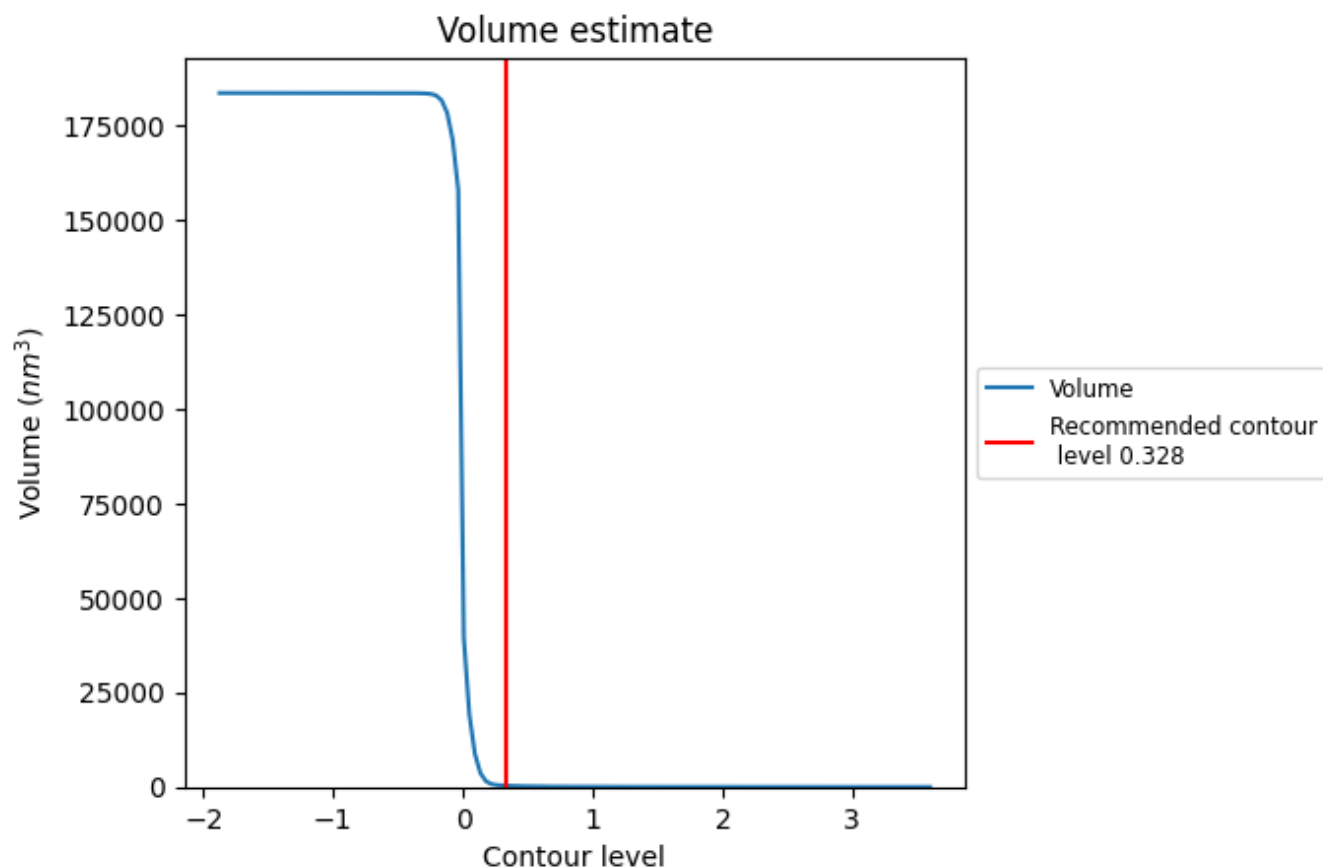
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

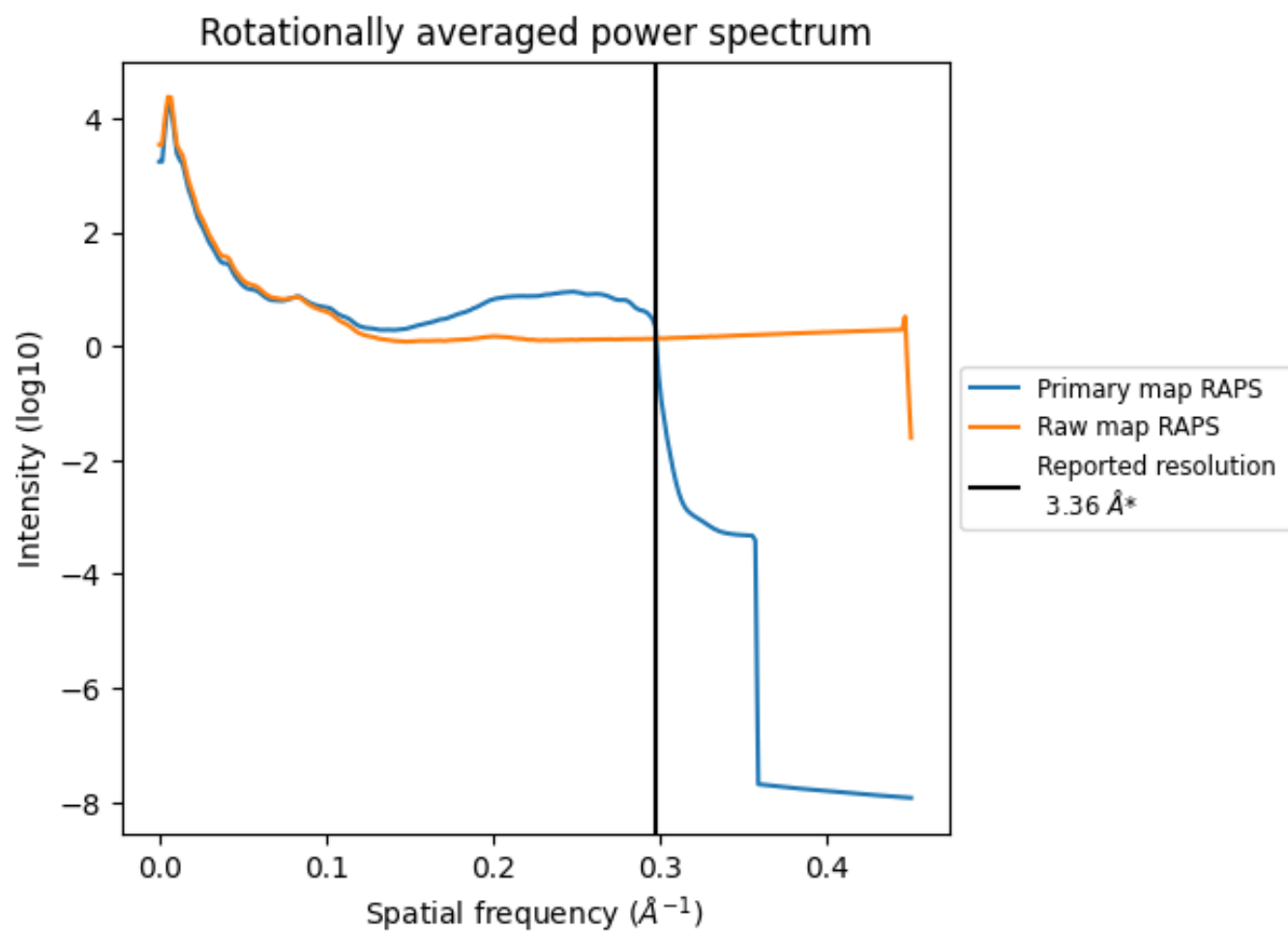
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 342 nm^3 ; this corresponds to an approximate mass of 309 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 ⓘ

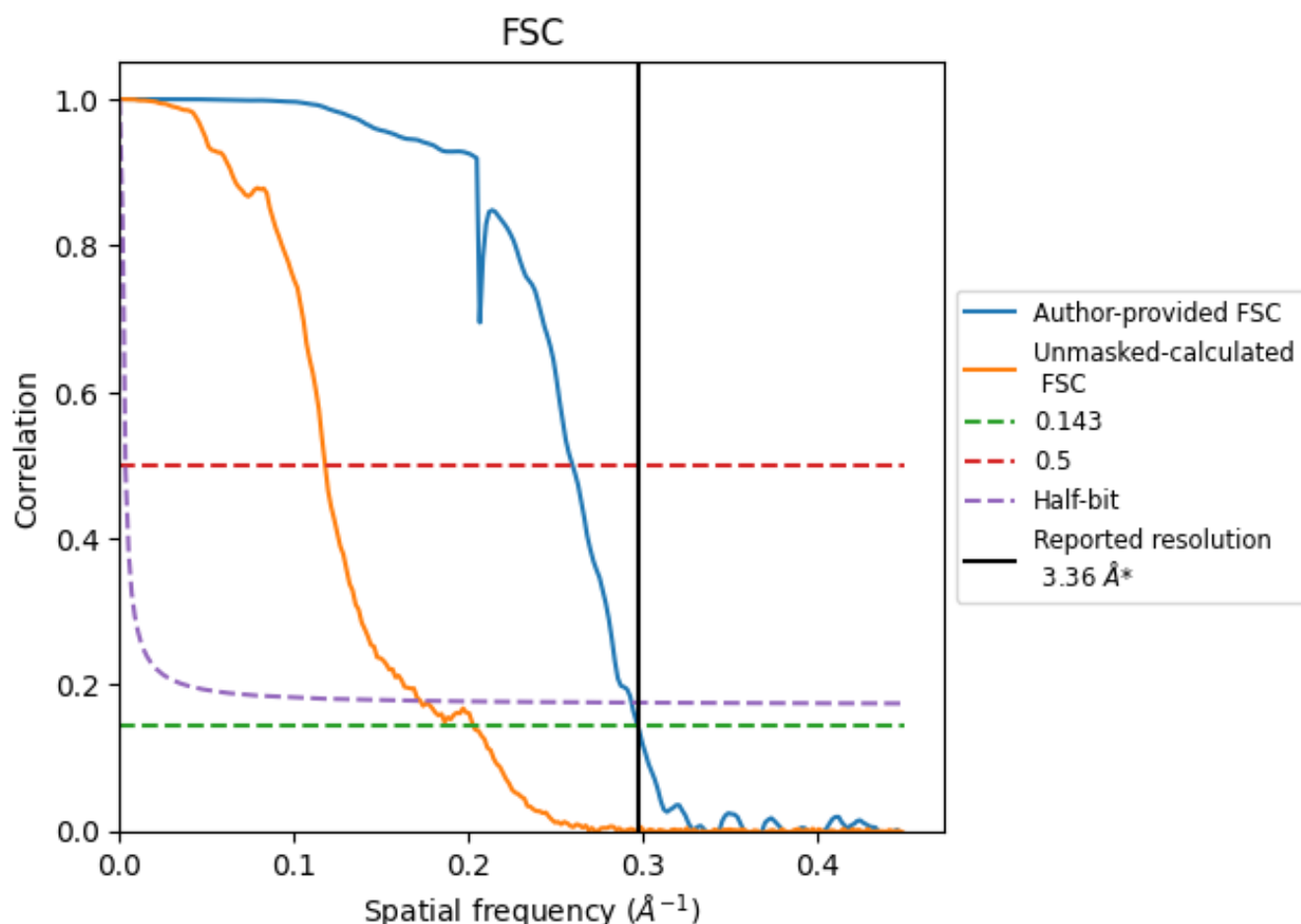


*Reported resolution corresponds to spatial frequency of 0.298 Å⁻¹

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 0.298 Å⁻¹

8.2 Resolution estimates [i](#)

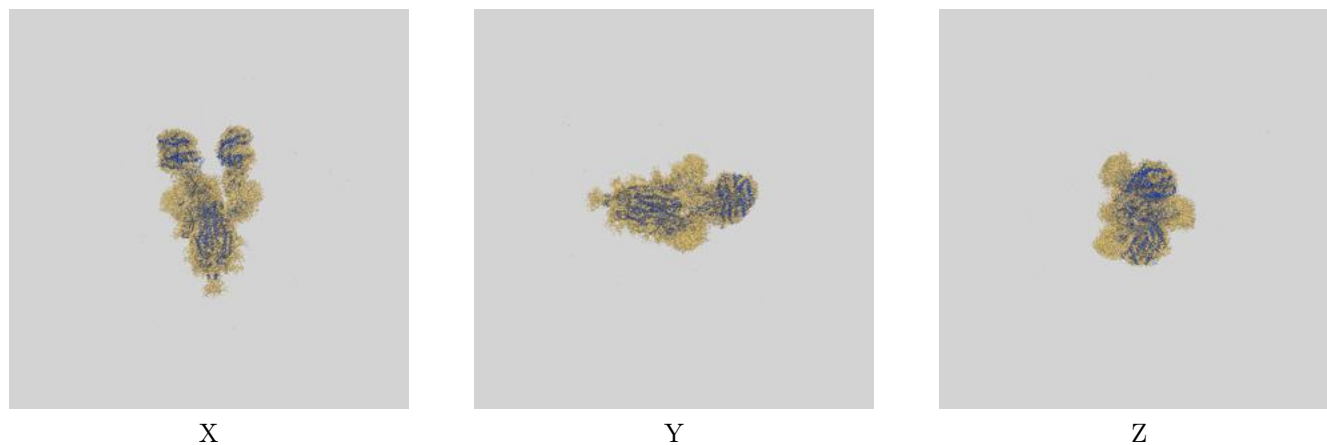
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.36	-	-
Author-provided FSC curve	3.36	3.85	3.40
Unmasked-calculated*	4.92	8.47	5.79

*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 4.92 differs from the reported value 3.36 by more than 10 %

9 Map-model fit [i](#)

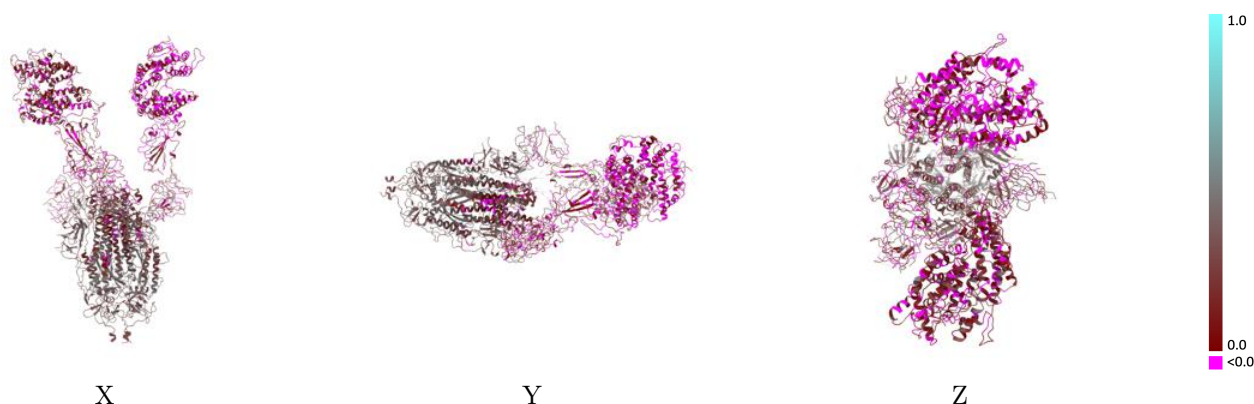
This section contains information regarding the fit between EMDB map EMD-40976 and PDB model 8T20. Per-residue inclusion information can be found in [section 3](#) on [page 11](#).

9.1 Map-model overlay [i](#)



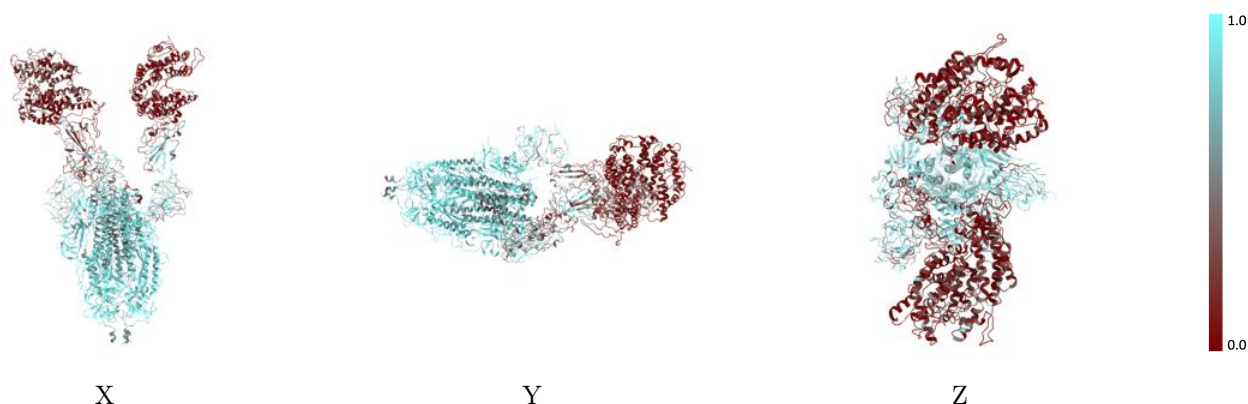
The images above show the 3D surface view of the map at the recommended contour level 0.328 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



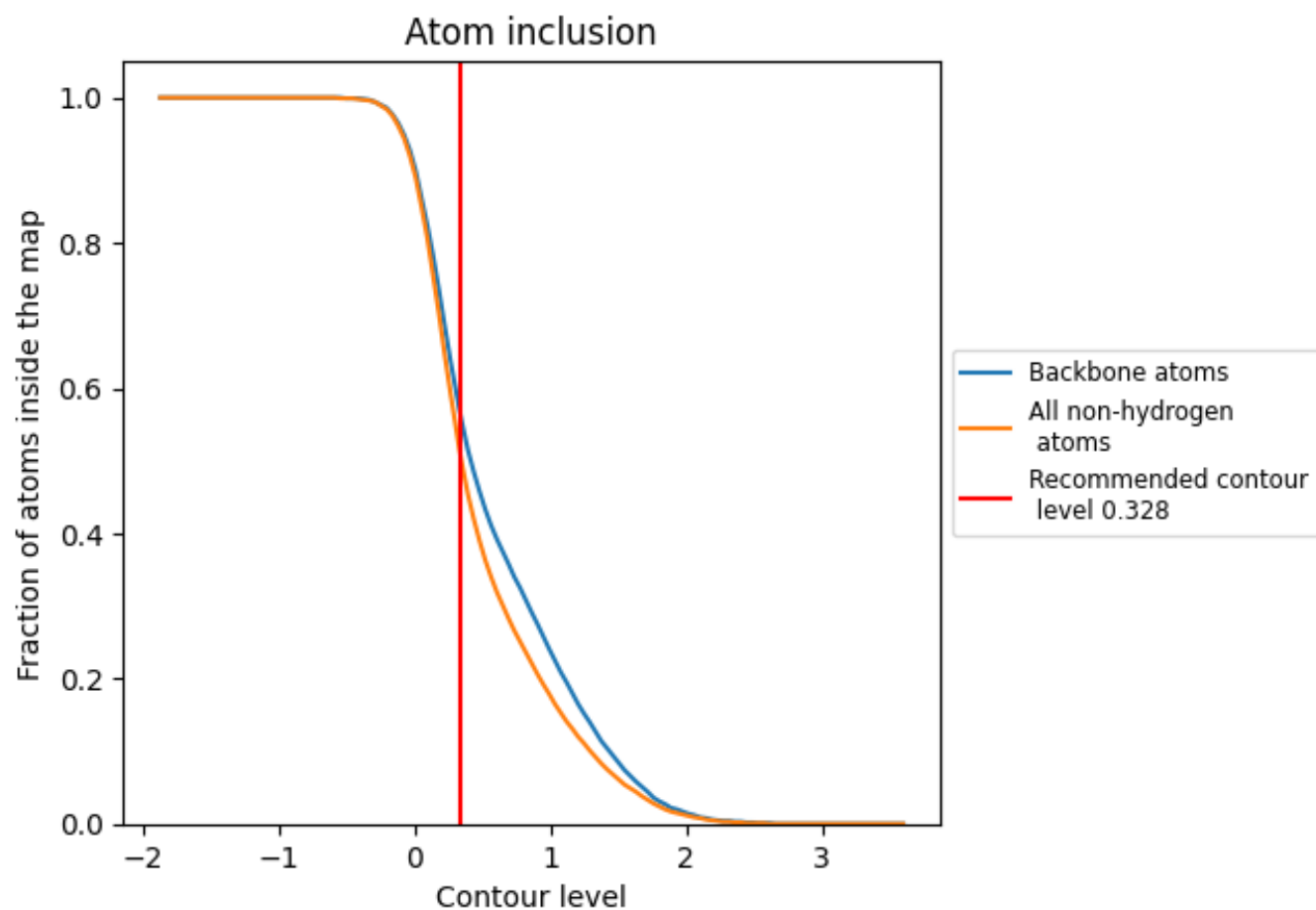
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.328).

9.4 Atom inclusion [i](#)



At the recommended contour level, 57% of all backbone atoms, 52% 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 (0.328) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.5160	<div></div> 0.1910
A	<div></div> 0.6310	<div></div> 0.2240
B	<div></div> 0.6790	<div></div> 0.2620
C	<div></div> 0.7170	<div></div> 0.2530
D	<div></div> 0.1100	<div></div> 0.0040
E	<div></div> 0.1740	<div></div> 0.1250

