



Full wwPDB EM Validation Report ⓘ

Nov 6, 2022 – 05:21 AM EST

PDB ID : 6B3O
EMDB ID : EMD-7040
Title : Tectonic conformational changes of a coronavirus spike glycoprotein promote membrane fusion
Authors : Walls, A.C.; Tortorici, M.A.; Snijder, J.; Xiong, X.; Bosch, B.J.; Rey, F.A.; Veesler, D.
Deposited on : 2017-09-22
Resolution : 4.10 Å(reported)

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The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

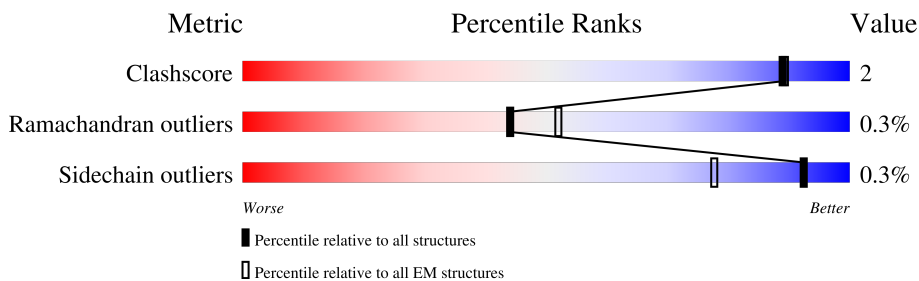
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	605	
1	B	605	
1	C	605	

2 Entry composition i

There is only 1 type of molecule in this entry. The entry contains 7980 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
			Total	C	N	O	S		
1	A	344	2660	1680	445	523	12	0	0
1	B	344	2660	1680	445	523	12	0	0
1	C	344	2660	1680	445	523	12	0	0

There are 210 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	696	MET	-	initiating methionine	UNP P11224
A	697	LYS	-	see remark 999	UNP P11224
A	698	LEU	-	see remark 999	UNP P11224
A	699	CYS	-	see remark 999	UNP P11224
A	700	ILE	-	see remark 999	UNP P11224
A	701	LEU	-	see remark 999	UNP P11224
A	702	LEU	-	see remark 999	UNP P11224
A	703	ALA	-	see remark 999	UNP P11224
A	704	VAL	-	see remark 999	UNP P11224
A	705	VAL	-	see remark 999	UNP P11224
A	706	ALA	-	see remark 999	UNP P11224
A	707	PHE	-	see remark 999	UNP P11224
A	708	VAL	-	see remark 999	UNP P11224
A	709	GLY	-	see remark 999	UNP P11224
A	710	LEU	-	see remark 999	UNP P11224
A	711	SER	-	see remark 999	UNP P11224
A	712	LEU	-	see remark 999	UNP P11224
A	713	GLY	-	see remark 999	UNP P11224
A	714	ARG	-	see remark 999	UNP P11224
A	715	SER	-	see remark 999	UNP P11224
A	716	LEU	-	see remark 999	UNP P11224
A	717	ALA	-	see remark 999	UNP P11224
A	1253	ILE	-	linker	UNP P11224
A	1254	LYS	-	linker	UNP P11224

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1255	ARG	-	see remark 999	UNP P11224
A	1256	MET	-	see remark 999	UNP P11224
A	1257	LYS	-	see remark 999	UNP P11224
A	1258	GLN	-	see remark 999	UNP P11224
A	1259	ILE	-	see remark 999	UNP P11224
A	1260	GLU	-	see remark 999	UNP P11224
A	1261	ASP	-	see remark 999	UNP P11224
A	1262	LYS	-	see remark 999	UNP P11224
A	1263	ILE	-	see remark 999	UNP P11224
A	1264	GLU	-	see remark 999	UNP P11224
A	1265	GLU	-	see remark 999	UNP P11224
A	1266	ILE	-	see remark 999	UNP P11224
A	1267	GLU	-	see remark 999	UNP P11224
A	1268	SER	-	see remark 999	UNP P11224
A	1269	LYS	-	see remark 999	UNP P11224
A	1270	GLN	-	see remark 999	UNP P11224
A	1271	LYS	-	see remark 999	UNP P11224
A	1272	LYS	-	see remark 999	UNP P11224
A	1273	ILE	-	see remark 999	UNP P11224
A	1274	GLU	-	see remark 999	UNP P11224
A	1275	ASN	-	see remark 999	UNP P11224
A	1276	GLU	-	see remark 999	UNP P11224
A	1277	ILE	-	see remark 999	UNP P11224
A	1278	ALA	-	see remark 999	UNP P11224
A	1279	ARG	-	see remark 999	UNP P11224
A	1280	ILE	-	see remark 999	UNP P11224
A	1281	LYS	-	see remark 999	UNP P11224
A	1282	LYS	-	see remark 999	UNP P11224
A	1283	ILE	-	see remark 999	UNP P11224
A	1284	LYS	-	see remark 999	UNP P11224
A	1285	LEU	-	see remark 999	UNP P11224
A	1286	VAL	-	see remark 999	UNP P11224
A	1287	PRO	-	see remark 999	UNP P11224
A	1288	ARG	-	see remark 999	UNP P11224
A	1289	GLY	-	see remark 999	UNP P11224
A	1290	SER	-	see remark 999	UNP P11224
A	1291	LEU	-	see remark 999	UNP P11224
A	1292	GLU	-	see remark 999	UNP P11224
A	1293	TRP	-	see remark 999	UNP P11224
A	1294	SER	-	see remark 999	UNP P11224
A	1295	HIS	-	see remark 999	UNP P11224
A	1296	PRO	-	see remark 999	UNP P11224

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1297	GLN	-	see remark 999	UNP P11224
A	1298	PHE	-	see remark 999	UNP P11224
A	1299	GLU	-	see remark 999	UNP P11224
A	1300	LYS	-	see remark 999	UNP P11224
B	696	MET	-	initiating methionine	UNP P11224
B	697	LYS	-	see remark 999	UNP P11224
B	698	LEU	-	see remark 999	UNP P11224
B	699	CYS	-	see remark 999	UNP P11224
B	700	ILE	-	see remark 999	UNP P11224
B	701	LEU	-	see remark 999	UNP P11224
B	702	LEU	-	see remark 999	UNP P11224
B	703	ALA	-	see remark 999	UNP P11224
B	704	VAL	-	see remark 999	UNP P11224
B	705	VAL	-	see remark 999	UNP P11224
B	706	ALA	-	see remark 999	UNP P11224
B	707	PHE	-	see remark 999	UNP P11224
B	708	VAL	-	see remark 999	UNP P11224
B	709	GLY	-	see remark 999	UNP P11224
B	710	LEU	-	see remark 999	UNP P11224
B	711	SER	-	see remark 999	UNP P11224
B	712	LEU	-	see remark 999	UNP P11224
B	713	GLY	-	see remark 999	UNP P11224
B	714	ARG	-	see remark 999	UNP P11224
B	715	SER	-	see remark 999	UNP P11224
B	716	LEU	-	see remark 999	UNP P11224
B	717	ALA	-	see remark 999	UNP P11224
B	1253	ILE	-	linker	UNP P11224
B	1254	LYS	-	linker	UNP P11224
B	1255	ARG	-	see remark 999	UNP P11224
B	1256	MET	-	see remark 999	UNP P11224
B	1257	LYS	-	see remark 999	UNP P11224
B	1258	GLN	-	see remark 999	UNP P11224
B	1259	ILE	-	see remark 999	UNP P11224
B	1260	GLU	-	see remark 999	UNP P11224
B	1261	ASP	-	see remark 999	UNP P11224
B	1262	LYS	-	see remark 999	UNP P11224
B	1263	ILE	-	see remark 999	UNP P11224
B	1264	GLU	-	see remark 999	UNP P11224
B	1265	GLU	-	see remark 999	UNP P11224
B	1266	ILE	-	see remark 999	UNP P11224
B	1267	GLU	-	see remark 999	UNP P11224
B	1268	SER	-	see remark 999	UNP P11224

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1269	LYS	-	see remark 999	UNP P11224
B	1270	GLN	-	see remark 999	UNP P11224
B	1271	LYS	-	see remark 999	UNP P11224
B	1272	LYS	-	see remark 999	UNP P11224
B	1273	ILE	-	see remark 999	UNP P11224
B	1274	GLU	-	see remark 999	UNP P11224
B	1275	ASN	-	see remark 999	UNP P11224
B	1276	GLU	-	see remark 999	UNP P11224
B	1277	ILE	-	see remark 999	UNP P11224
B	1278	ALA	-	see remark 999	UNP P11224
B	1279	ARG	-	see remark 999	UNP P11224
B	1280	ILE	-	see remark 999	UNP P11224
B	1281	LYS	-	see remark 999	UNP P11224
B	1282	LYS	-	see remark 999	UNP P11224
B	1283	ILE	-	see remark 999	UNP P11224
B	1284	LYS	-	see remark 999	UNP P11224
B	1285	LEU	-	see remark 999	UNP P11224
B	1286	VAL	-	see remark 999	UNP P11224
B	1287	PRO	-	see remark 999	UNP P11224
B	1288	ARG	-	see remark 999	UNP P11224
B	1289	GLY	-	see remark 999	UNP P11224
B	1290	SER	-	see remark 999	UNP P11224
B	1291	LEU	-	see remark 999	UNP P11224
B	1292	GLU	-	see remark 999	UNP P11224
B	1293	TRP	-	see remark 999	UNP P11224
B	1294	SER	-	see remark 999	UNP P11224
B	1295	HIS	-	see remark 999	UNP P11224
B	1296	PRO	-	see remark 999	UNP P11224
B	1297	GLN	-	see remark 999	UNP P11224
B	1298	PHE	-	see remark 999	UNP P11224
B	1299	GLU	-	see remark 999	UNP P11224
B	1300	LYS	-	see remark 999	UNP P11224
C	696	MET	-	initiating methionine	UNP P11224
C	697	LYS	-	see remark 999	UNP P11224
C	698	LEU	-	see remark 999	UNP P11224
C	699	CYS	-	see remark 999	UNP P11224
C	700	ILE	-	see remark 999	UNP P11224
C	701	LEU	-	see remark 999	UNP P11224
C	702	LEU	-	see remark 999	UNP P11224
C	703	ALA	-	see remark 999	UNP P11224
C	704	VAL	-	see remark 999	UNP P11224
C	705	VAL	-	see remark 999	UNP P11224

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Chain	Residue	Modelled	Actual	Comment	Reference
C	706	ALA	-	see remark 999	UNP P11224
C	707	PHE	-	see remark 999	UNP P11224
C	708	VAL	-	see remark 999	UNP P11224
C	709	GLY	-	see remark 999	UNP P11224
C	710	LEU	-	see remark 999	UNP P11224
C	711	SER	-	see remark 999	UNP P11224
C	712	LEU	-	see remark 999	UNP P11224
C	713	GLY	-	see remark 999	UNP P11224
C	714	ARG	-	see remark 999	UNP P11224
C	715	SER	-	see remark 999	UNP P11224
C	716	LEU	-	see remark 999	UNP P11224
C	717	ALA	-	see remark 999	UNP P11224
C	1253	ILE	-	linker	UNP P11224
C	1254	LYS	-	linker	UNP P11224
C	1255	ARG	-	see remark 999	UNP P11224
C	1256	MET	-	see remark 999	UNP P11224
C	1257	LYS	-	see remark 999	UNP P11224
C	1258	GLN	-	see remark 999	UNP P11224
C	1259	ILE	-	see remark 999	UNP P11224
C	1260	GLU	-	see remark 999	UNP P11224
C	1261	ASP	-	see remark 999	UNP P11224
C	1262	LYS	-	see remark 999	UNP P11224
C	1263	ILE	-	see remark 999	UNP P11224
C	1264	GLU	-	see remark 999	UNP P11224
C	1265	GLU	-	see remark 999	UNP P11224
C	1266	ILE	-	see remark 999	UNP P11224
C	1267	GLU	-	see remark 999	UNP P11224
C	1268	SER	-	see remark 999	UNP P11224
C	1269	LYS	-	see remark 999	UNP P11224
C	1270	GLN	-	see remark 999	UNP P11224
C	1271	LYS	-	see remark 999	UNP P11224
C	1272	LYS	-	see remark 999	UNP P11224
C	1273	ILE	-	see remark 999	UNP P11224
C	1274	GLU	-	see remark 999	UNP P11224
C	1275	ASN	-	see remark 999	UNP P11224
C	1276	GLU	-	see remark 999	UNP P11224
C	1277	ILE	-	see remark 999	UNP P11224
C	1278	ALA	-	see remark 999	UNP P11224
C	1279	ARG	-	see remark 999	UNP P11224
C	1280	ILE	-	see remark 999	UNP P11224
C	1281	LYS	-	see remark 999	UNP P11224
C	1282	LYS	-	see remark 999	UNP P11224

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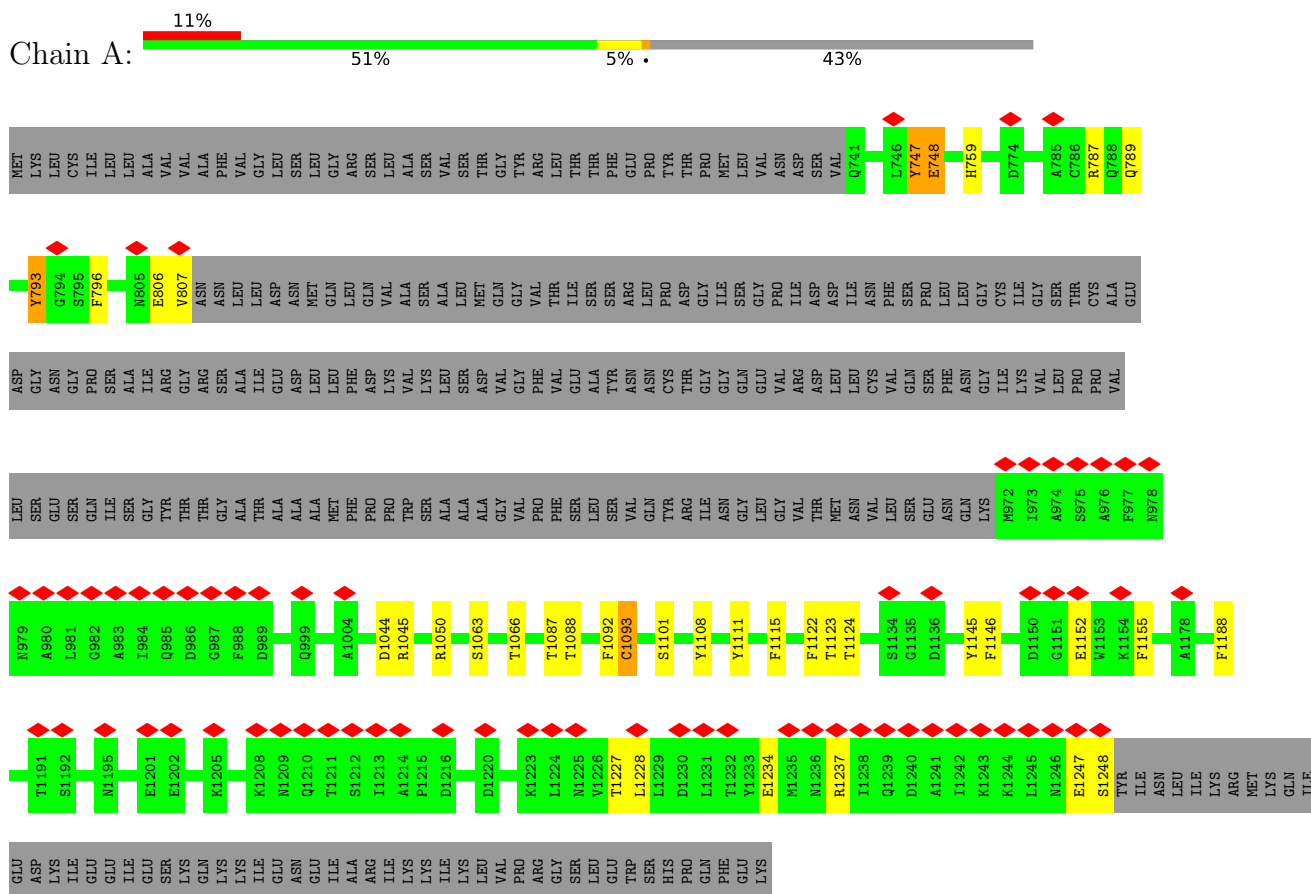
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Chain	Residue	Modelled	Actual	Comment	Reference
C	1283	ILE	-	see remark 999	UNP P11224
C	1284	LYS	-	see remark 999	UNP P11224
C	1285	LEU	-	see remark 999	UNP P11224
C	1286	VAL	-	see remark 999	UNP P11224
C	1287	PRO	-	see remark 999	UNP P11224
C	1288	ARG	-	see remark 999	UNP P11224
C	1289	GLY	-	see remark 999	UNP P11224
C	1290	SER	-	see remark 999	UNP P11224
C	1291	LEU	-	see remark 999	UNP P11224
C	1292	GLU	-	see remark 999	UNP P11224
C	1293	TRP	-	see remark 999	UNP P11224
C	1294	SER	-	see remark 999	UNP P11224
C	1295	HIS	-	see remark 999	UNP P11224
C	1296	PRO	-	see remark 999	UNP P11224
C	1297	GLN	-	see remark 999	UNP P11224
C	1298	PHE	-	see remark 999	UNP P11224
C	1299	GLU	-	see remark 999	UNP P11224
C	1300	LYS	-	see remark 999	UNP P11224

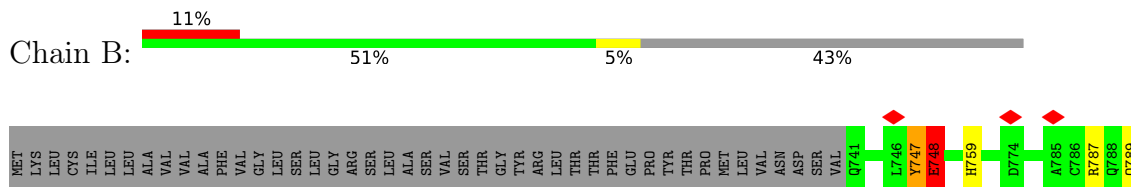
3 Residue-property plots [i](#)

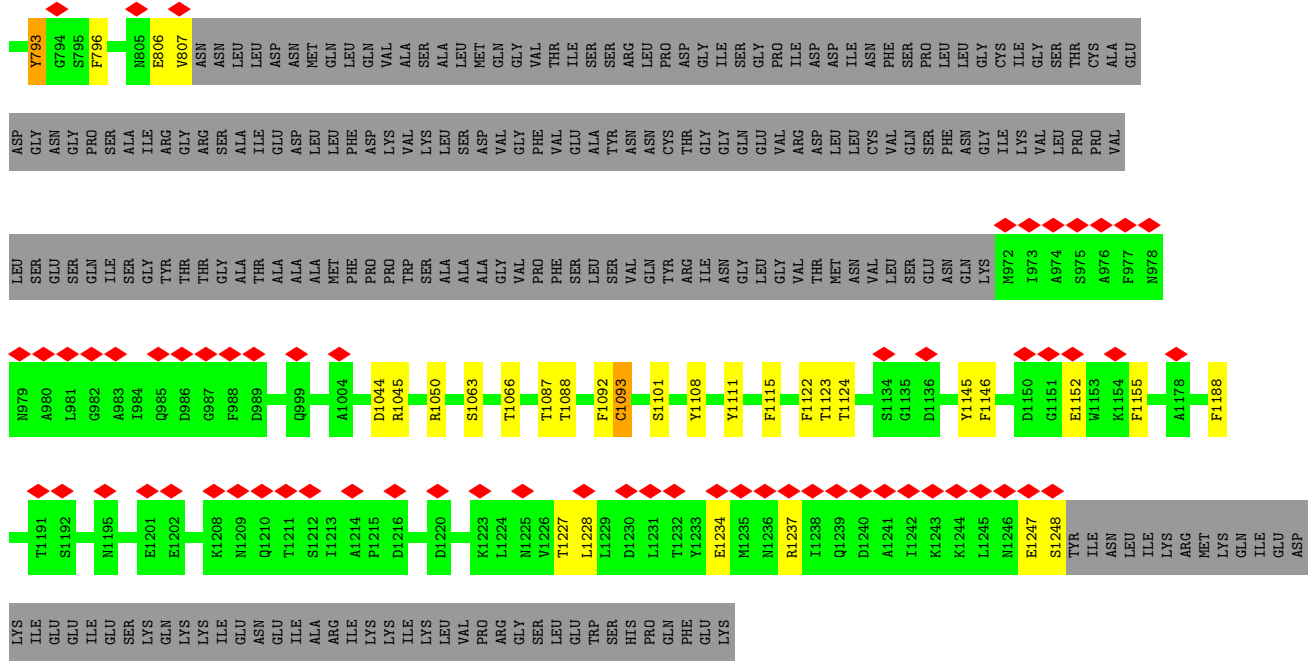
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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

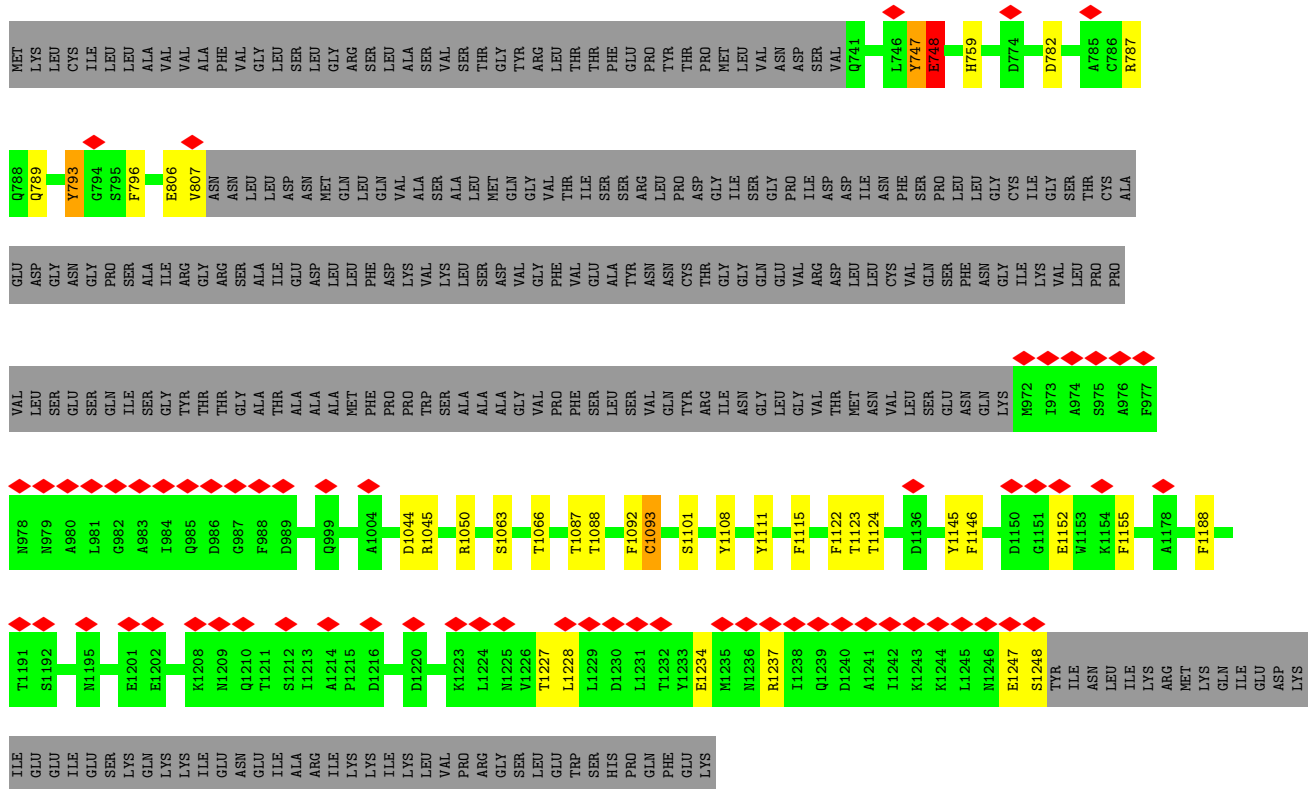


- Molecule 1: Spike glycoprotein





• Molecule 1: Spike glycoprotein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	106000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.785	Depositor
Minimum map value	-0.513	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.16	Depositor
Map size (Å)	435.2, 435.2, 435.2	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.36, 1.36, 1.36	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	1.31	13/2708 (0.5%)	0.99	12/3678 (0.3%)
1	B	1.31	14/2708 (0.5%)	0.99	12/3678 (0.3%)
1	C	1.31	14/2708 (0.5%)	0.99	12/3678 (0.3%)
All	All	1.31	41/8124 (0.5%)	0.99	36/11034 (0.3%)

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	796	PHE	CB-CG	-9.02	1.36	1.51
1	C	796	PHE	CB-CG	-9.02	1.36	1.51
1	A	796	PHE	CB-CG	-9.01	1.36	1.51
1	C	1155	PHE	CB-CG	-8.64	1.36	1.51
1	A	1155	PHE	CB-CG	-8.62	1.36	1.51
1	B	1155	PHE	CB-CG	-8.62	1.36	1.51
1	B	1093	CYS	CB-SG	-7.38	1.69	1.82
1	A	1093	CYS	CB-SG	-7.36	1.69	1.82
1	C	1093	CYS	CB-SG	-7.30	1.69	1.82
1	B	1122	PHE	CB-CG	-7.29	1.39	1.51
1	C	1122	PHE	CB-CG	-7.29	1.39	1.51
1	A	1122	PHE	CB-CG	-7.28	1.39	1.51
1	C	1115	PHE	CB-CG	-7.16	1.39	1.51
1	B	1115	PHE	CB-CG	-7.15	1.39	1.51
1	A	1115	PHE	CB-CG	-7.15	1.39	1.51
1	B	747	TYR	CB-CG	-6.69	1.41	1.51
1	C	747	TYR	CB-CG	-6.68	1.41	1.51
1	A	747	TYR	CB-CG	-6.67	1.41	1.51
1	A	1188	PHE	CB-CG	-6.06	1.41	1.51
1	C	1188	PHE	CB-CG	-6.06	1.41	1.51
1	B	1188	PHE	CB-CG	-6.05	1.41	1.51
1	B	1101	SER	CB-OG	-5.59	1.34	1.42
1	C	1101	SER	CB-OG	-5.59	1.34	1.42
1	A	1101	SER	CB-OG	-5.58	1.35	1.42
1	C	1234	GLU	CD-OE1	-5.53	1.19	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1234	GLU	CD-OE1	-5.52	1.19	1.25
1	A	1234	GLU	CD-OE1	-5.52	1.19	1.25
1	A	759	HIS	CB-CG	-5.51	1.40	1.50
1	C	759	HIS	CB-CG	-5.50	1.40	1.50
1	B	759	HIS	CB-CG	-5.49	1.40	1.50
1	B	1145	TYR	CE1-CZ	-5.22	1.31	1.38
1	A	1145	TYR	CE1-CZ	-5.21	1.31	1.38
1	C	1145	TYR	CE1-CZ	-5.20	1.31	1.38
1	C	1152	GLU	CD-OE2	-5.12	1.20	1.25
1	C	1145	TYR	CB-CG	-5.08	1.44	1.51
1	A	1145	TYR	CB-CG	-5.07	1.44	1.51
1	A	1152	GLU	CD-OE2	-5.06	1.20	1.25
1	B	1145	TYR	CB-CG	-5.05	1.44	1.51
1	B	748	GLU	CD-OE1	-5.01	1.20	1.25
1	B	1152	GLU	CD-OE2	-5.01	1.20	1.25
1	C	748	GLU	CD-OE1	-5.00	1.20	1.25

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	793	TYR	CB-CG-CD1	-9.11	115.53	121.00
1	A	793	TYR	CB-CG-CD1	-9.04	115.57	121.00
1	C	793	TYR	CB-CG-CD1	-9.04	115.58	121.00
1	C	1111	TYR	CB-CG-CD1	-8.52	115.89	121.00
1	A	1111	TYR	CB-CG-CD1	-8.49	115.91	121.00
1	B	1111	TYR	CB-CG-CD1	-8.48	115.91	121.00
1	A	1145	TYR	CB-CG-CD1	-6.58	117.05	121.00
1	B	1145	TYR	CB-CG-CD1	-6.58	117.05	121.00
1	C	1145	TYR	CB-CG-CD1	-6.58	117.06	121.00
1	C	1045	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	A	1045	ARG	NE-CZ-NH2	-5.75	117.43	120.30
1	B	1108	TYR	CB-CG-CD2	-5.68	117.59	121.00
1	B	1045	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	A	1108	TYR	CB-CG-CD2	-5.62	117.63	121.00
1	A	1050	ARG	NE-CZ-NH2	-5.61	117.50	120.30
1	B	1050	ARG	NE-CZ-NH2	-5.61	117.50	120.30
1	C	1108	TYR	CB-CG-CD2	-5.57	117.66	121.00
1	C	1050	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	A	1155	PHE	CB-CG-CD1	-5.48	116.97	120.80
1	B	1155	PHE	CB-CG-CD1	-5.47	116.97	120.80
1	C	1155	PHE	CB-CG-CD1	-5.46	116.98	120.80
1	B	1146	PHE	CB-CG-CD1	5.33	124.53	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	787	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	C	747	TYR	CB-CG-CD2	-5.33	117.80	121.00
1	A	747	TYR	CB-CG-CD2	-5.32	117.81	121.00
1	C	1146	PHE	CB-CG-CD1	5.32	124.52	120.80
1	A	1146	PHE	CB-CG-CD1	5.31	124.52	120.80
1	B	747	TYR	CB-CG-CD2	-5.29	117.83	121.00
1	A	787	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	B	787	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	A	1237	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	B	1237	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	C	1146	PHE	CB-CG-CD2	-5.19	117.17	120.80
1	C	1237	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	A	1146	PHE	CB-CG-CD2	-5.12	117.22	120.80
1	B	1146	PHE	CB-CG-CD2	-5.11	117.22	120.80

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	2660	0	2607	10	0
1	B	2660	0	2607	10	0
1	C	2660	0	2607	11	0
All	All	7980	0	7821	28	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 2.

All (28) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:806:GLU:O	1:C:807:VAL:C	2.42	0.58
1:B:806:GLU:O	1:B:807:VAL:C	2.42	0.58
1:A:806:GLU:O	1:A:807:VAL:C	2.42	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1087:THR:OG1	1:B:1088:THR:N	2.43	0.51
1:A:1087:THR:OG1	1:A:1088:THR:N	2.43	0.51
1:B:1063:SER:OG	1:C:1066:THR:OG1	2.29	0.50
1:B:789:GLN:NE2	1:B:1044:ASP:OD1	2.45	0.49
1:C:1087:THR:OG1	1:C:1088:THR:N	2.43	0.49
1:A:1066:THR:OG1	1:C:1063:SER:OG	2.29	0.49
1:A:789:GLN:NE2	1:A:1044:ASP:OD1	2.45	0.48
1:A:1063:SER:OG	1:B:1066:THR:OG1	2.29	0.48
1:C:789:GLN:NE2	1:C:1044:ASP:OD1	2.46	0.48
1:A:1123:THR:OG1	1:A:1124:THR:N	2.48	0.46
1:C:1123:THR:OG1	1:C:1124:THR:N	2.48	0.46
1:B:1227:THR:OG1	1:B:1228:LEU:N	2.50	0.44
1:B:1092:PHE:O	1:B:1093:CYS:C	2.55	0.44
1:B:1123:THR:OG1	1:B:1124:THR:N	2.48	0.44
1:A:1227:THR:OG1	1:A:1228:LEU:N	2.50	0.44
1:A:1092:PHE:O	1:A:1093:CYS:C	2.55	0.44
1:B:747:TYR:O	1:B:748:GLU:CB	2.66	0.44
1:C:1227:THR:OG1	1:C:1228:LEU:N	2.50	0.44
1:C:1247:GLU:O	1:C:1248:SER:C	2.57	0.43
1:B:1247:GLU:O	1:B:1248:SER:C	2.57	0.43
1:C:1092:PHE:O	1:C:1093:CYS:C	2.55	0.43
1:A:747:TYR:O	1:A:748:GLU:CB	2.66	0.43
1:C:747:TYR:O	1:C:748:GLU:CB	2.66	0.43
1:C:782:ASP:OD1	1:C:782:ASP:N	2.45	0.42
1:A:1247:GLU:O	1:A:1248:SER:C	2.57	0.42

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	340/605 (56%)	332 (98%)	7 (2%)	1 (0%)	41 75

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	340/605 (56%)	332 (98%)	7 (2%)	1 (0%)	41	75
1	C	340/605 (56%)	332 (98%)	7 (2%)	1 (0%)	41	75
All	All	1020/1815 (56%)	996 (98%)	21 (2%)	3 (0%)	44	75

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	748	GLU
1	B	748	GLU
1	C	748	GLU

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	295/518 (57%)	294 (100%)	1 (0%)	92	95
1	B	295/518 (57%)	294 (100%)	1 (0%)	92	95
1	C	295/518 (57%)	294 (100%)	1 (0%)	92	95
All	All	885/1554 (57%)	882 (100%)	3 (0%)	92	95

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

Mol	Chain	Res	Type
1	A	793	TYR
1	B	793	TYR
1	C	793	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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.

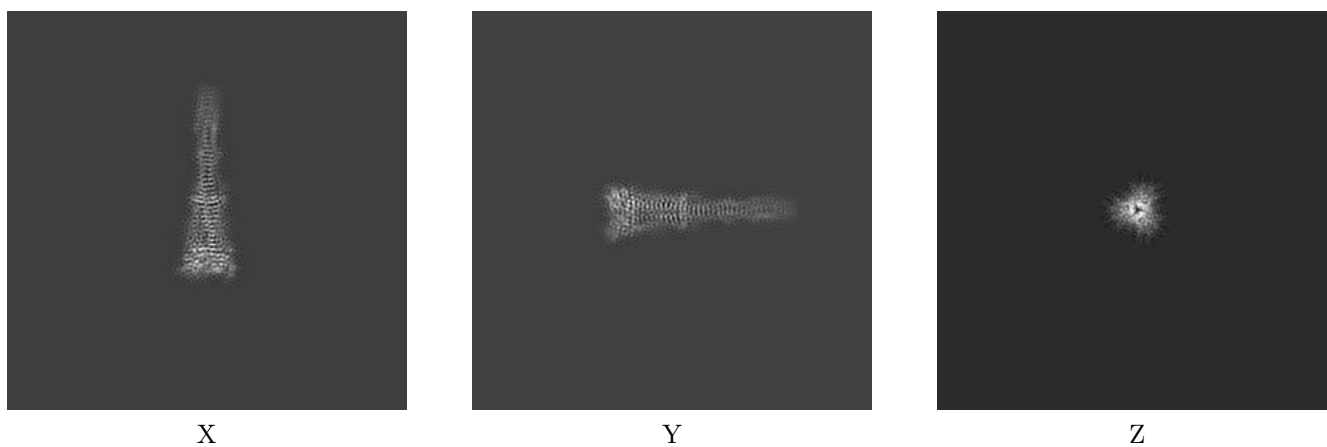
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7040. 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](#)

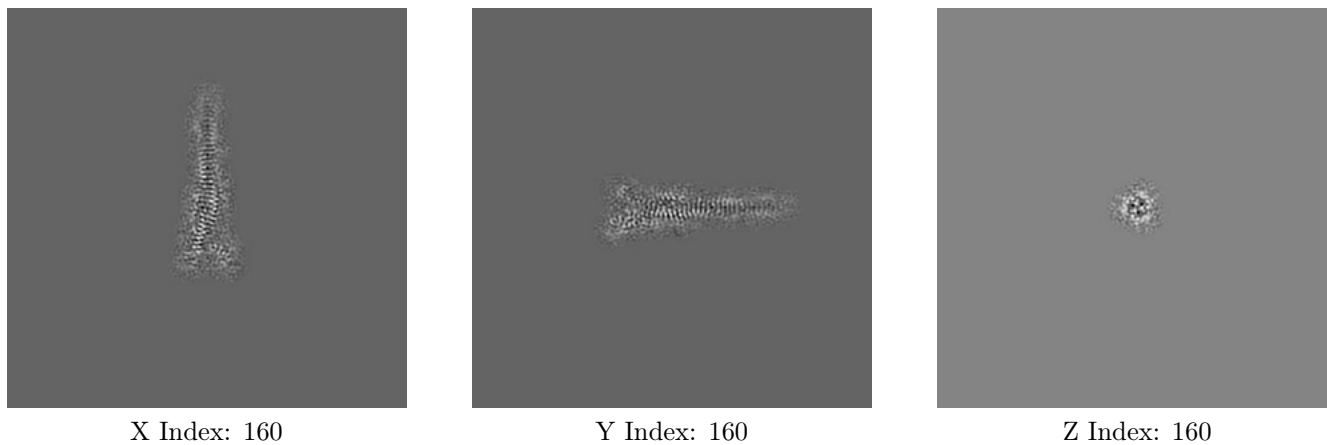
6.1.1 Primary map



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

6.2 Central slices [i](#)

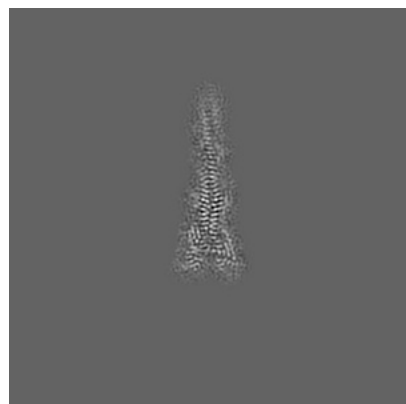
6.2.1 Primary map



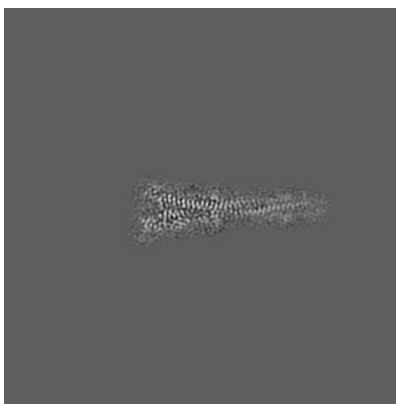
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

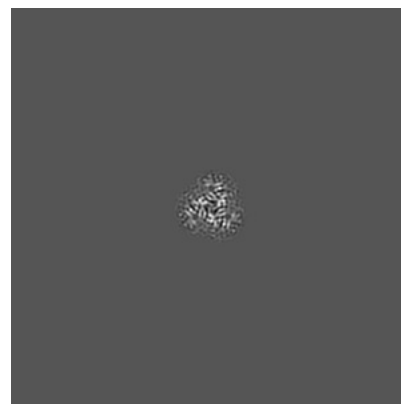
6.3.1 Primary map



X Index: 163



Y Index: 164



Z Index: 128

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.16. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

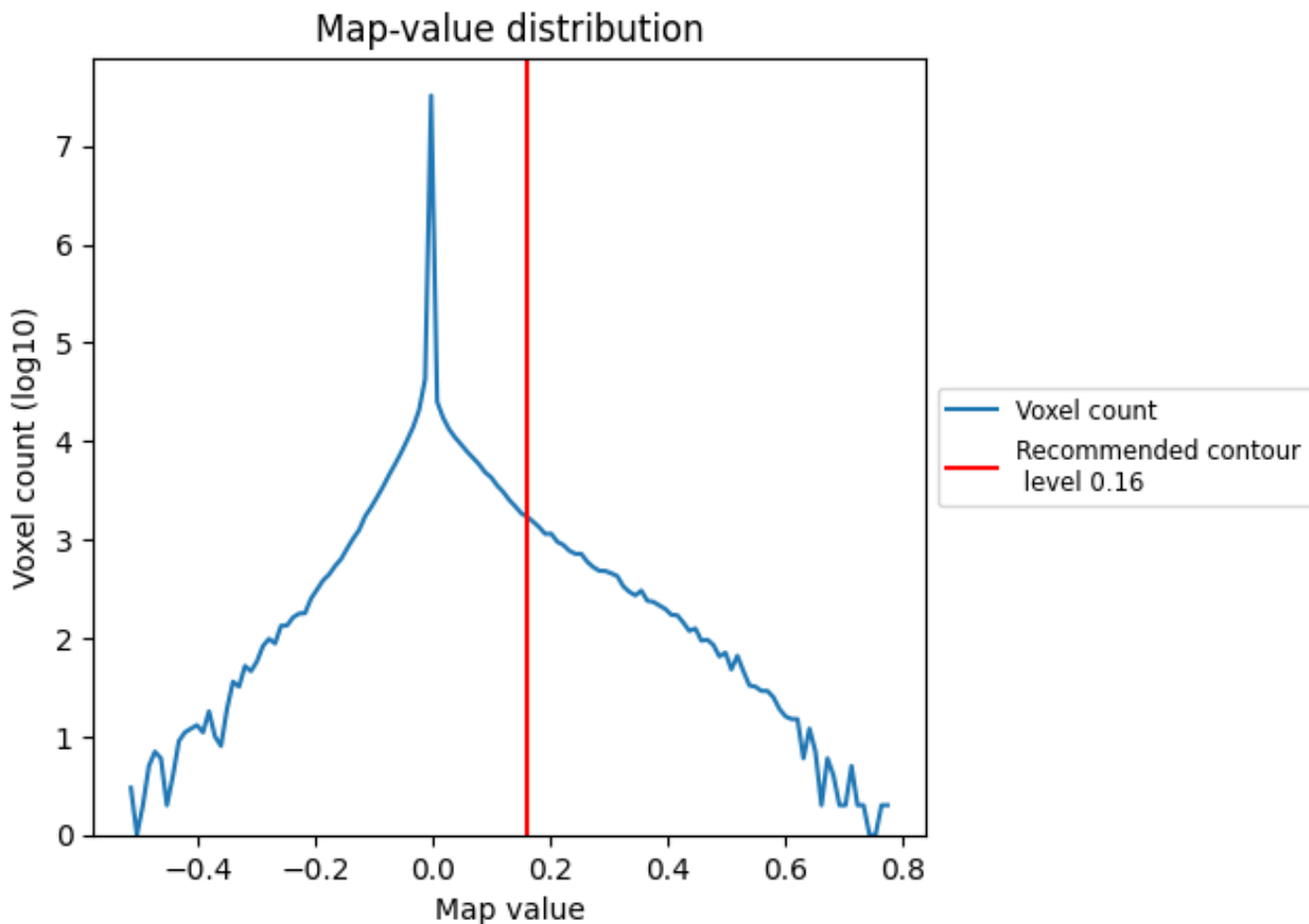
6.5 Mask visualisation

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

7 Map analysis [i](#)

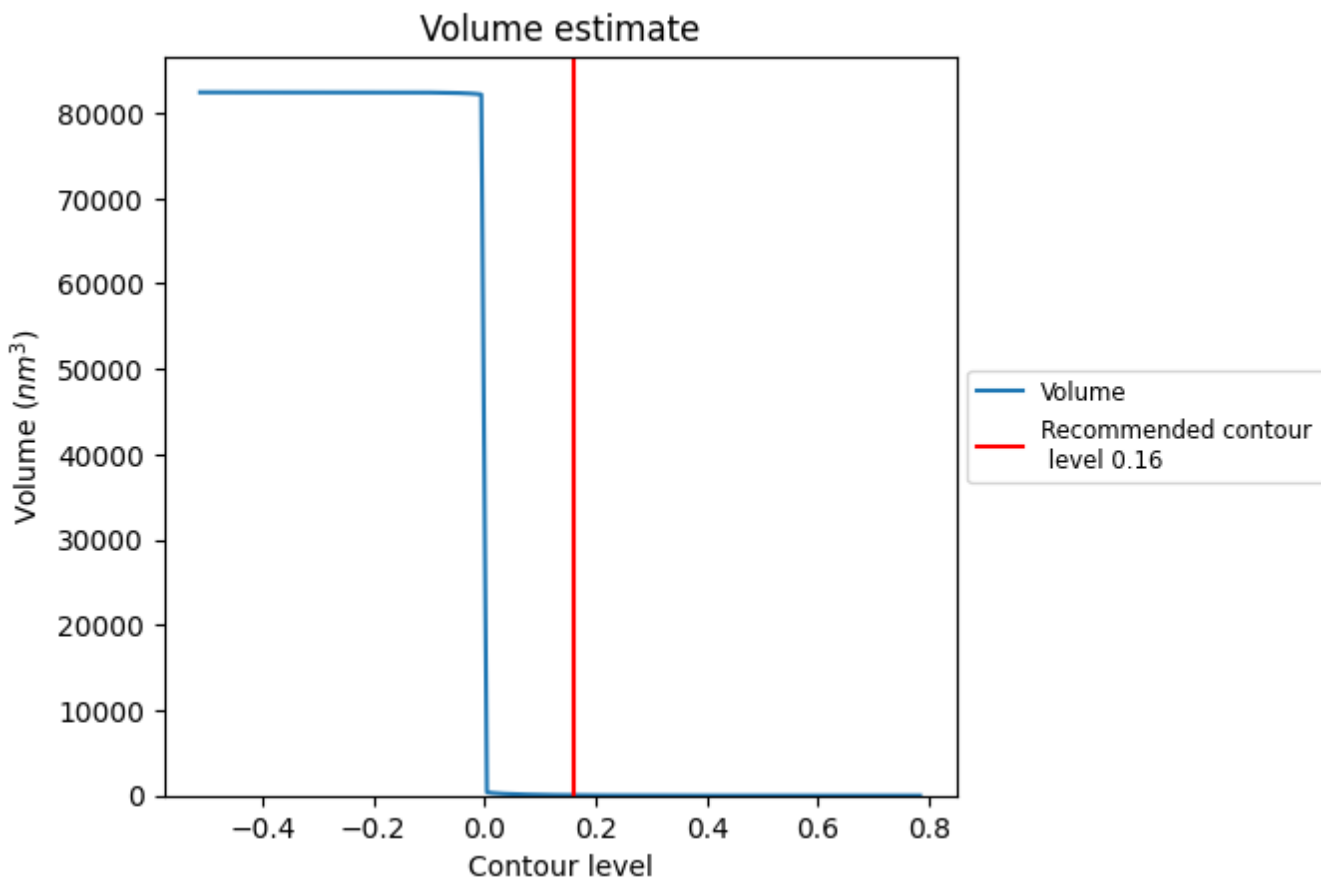
This section contains the results of statistical analysis of the map.

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.

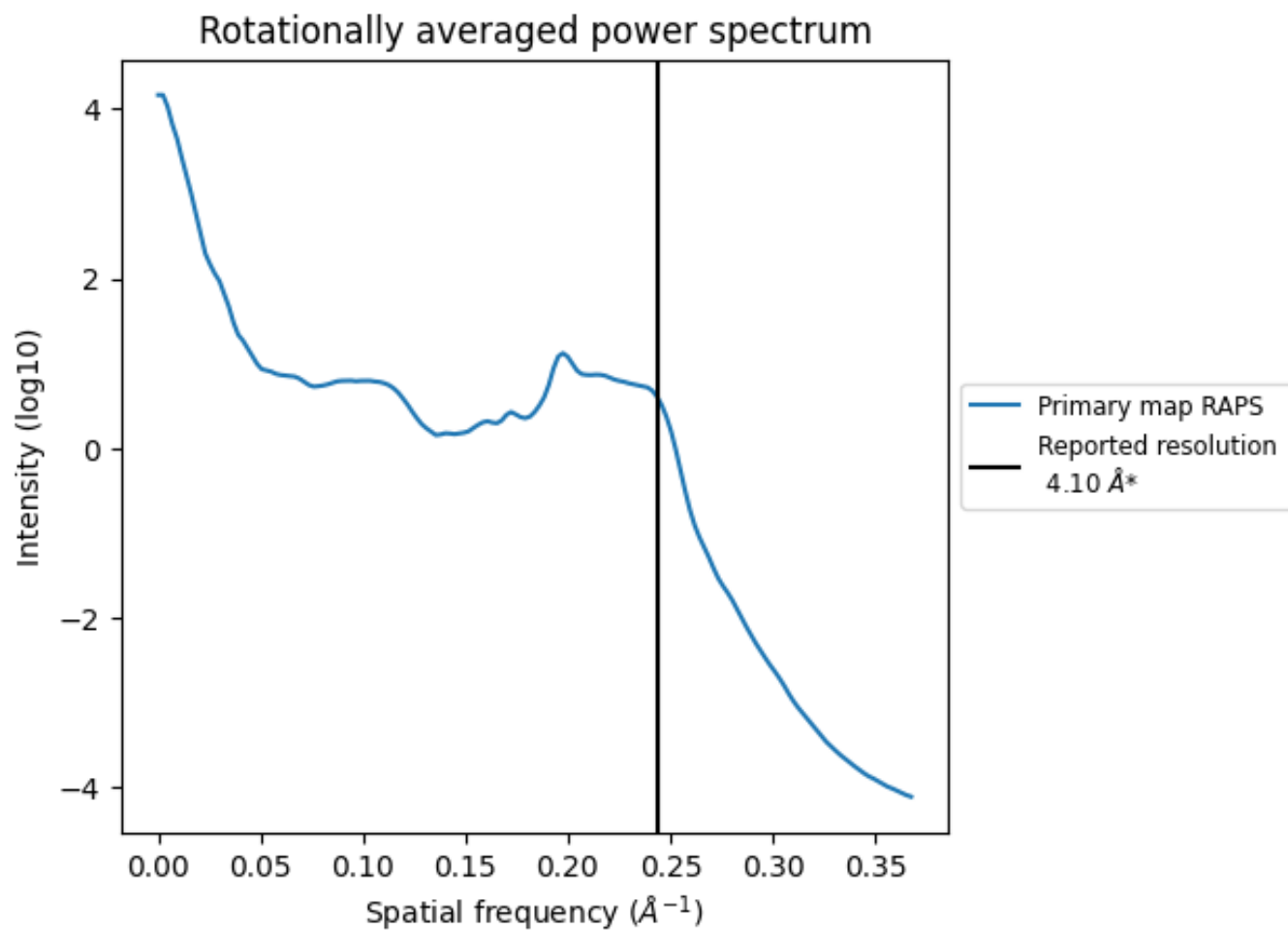
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 45 nm³; this corresponds to an approximate mass of 40 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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.244\AA^{-1}

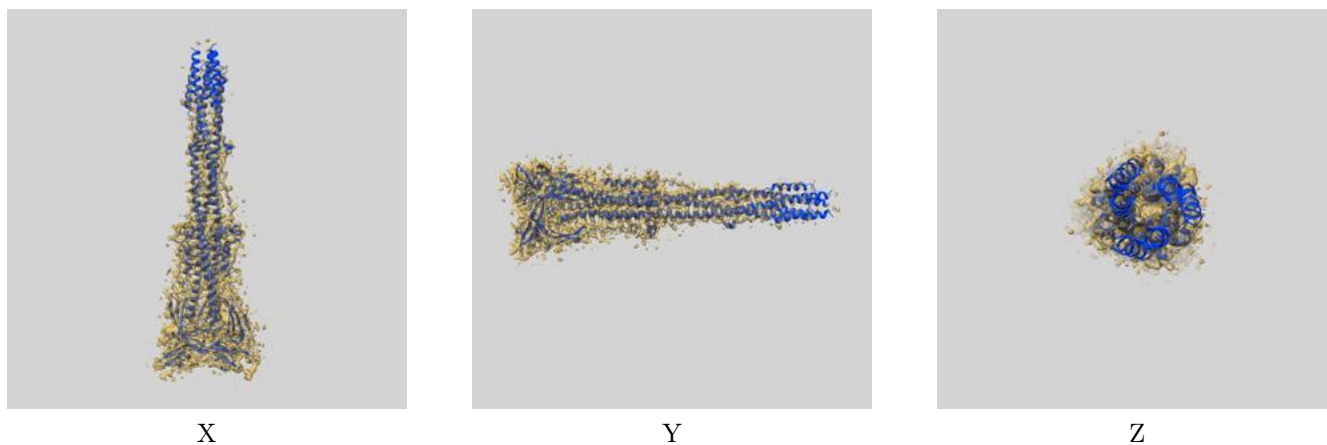
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

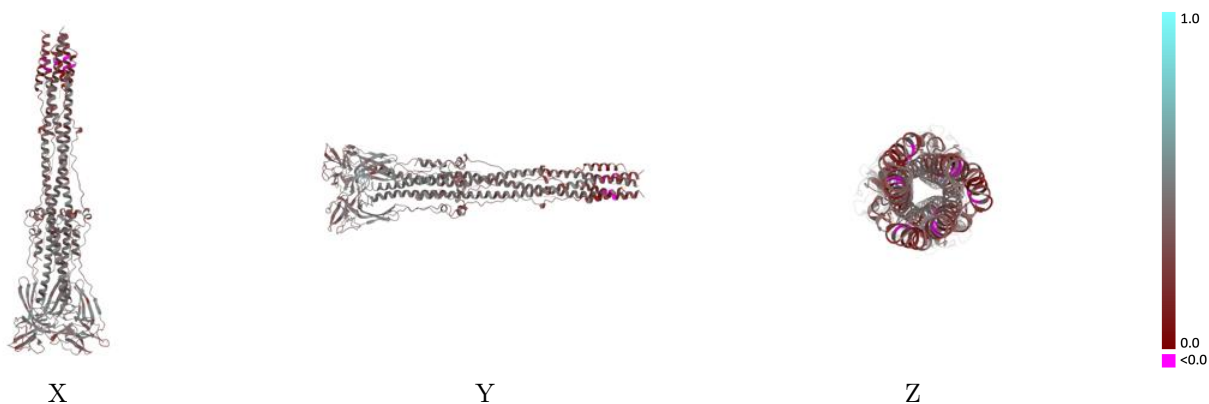
This section contains information regarding the fit between EMDB map EMD-7040 and PDB model 6B3O. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)



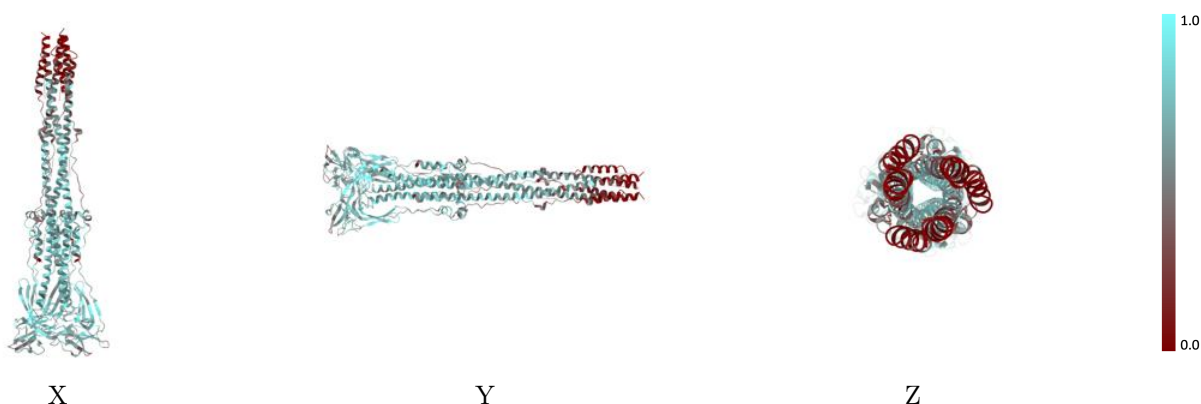
The images above show the 3D surface view of the map at the recommended contour level 0.16 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



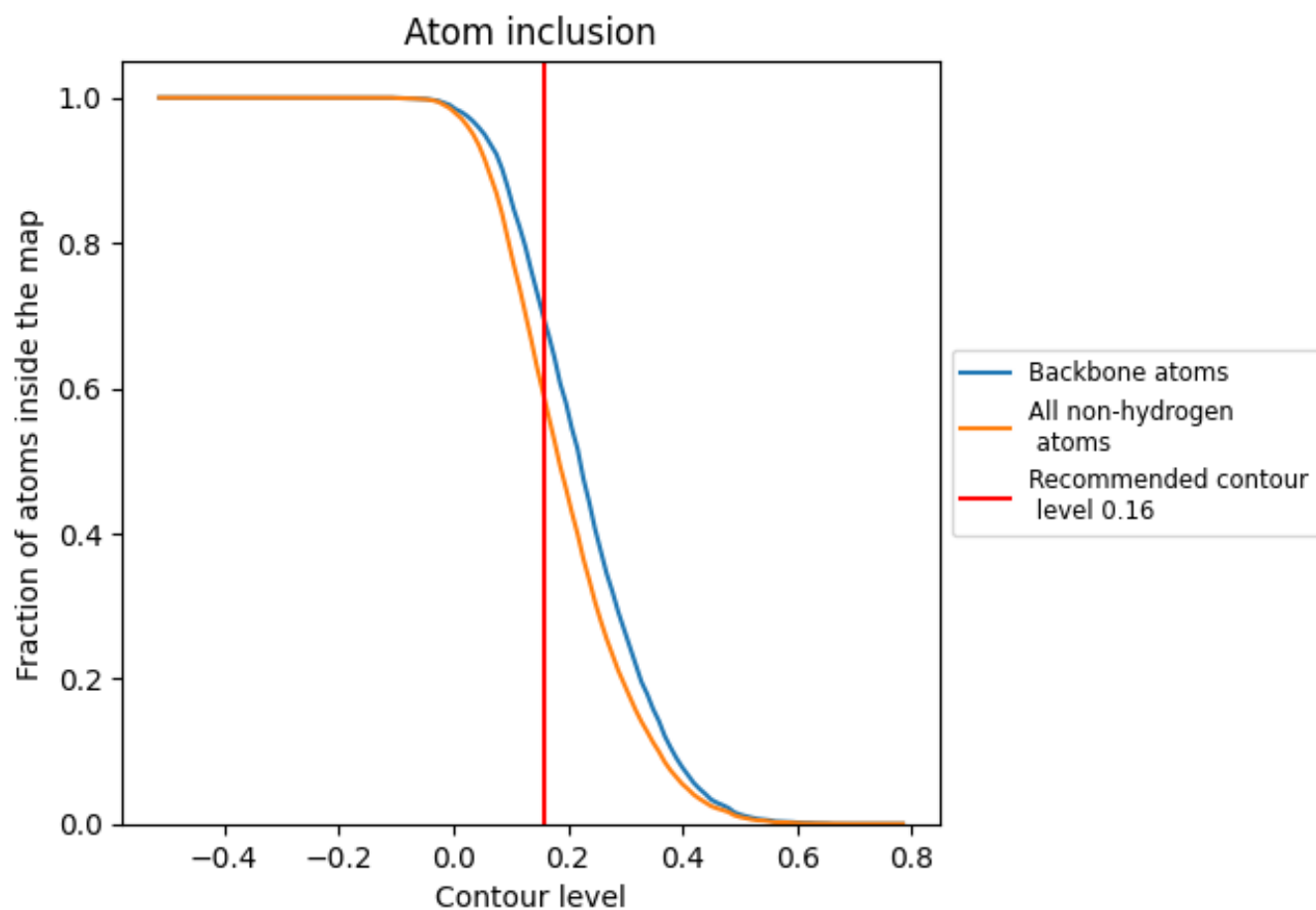
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.16).









9.4 Atom inclusion [i](#)



At the recommended contour level, 69% of all backbone atoms, 58% 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 (0.16) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5830	 0.3910
A	 0.5818	 0.3920
B	 0.5826	 0.3910
C	 0.5845	 0.3900

