wwPDB EM Validation Summary Report (i)

Dec 18, 2022 – 05:04 am GMT

PDB ID	:	7A4N
EMDB ID	:	EMD-11639
Title	:	Cryo-EM structure of a prefusion stabilized SARS-CoV-2 Spike (D614N, R682S, R685G, A892P, A942P and V987P)(S-closed trimer)
Authors	:	Rutten, L.; Renault, L.L.R.; Juraszek, J.; Langedijk, J.P.M.
Deposited on	:	2020-08-20
Resolution	:	2.75 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 (i) 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 (i)) were used in the production of this report:

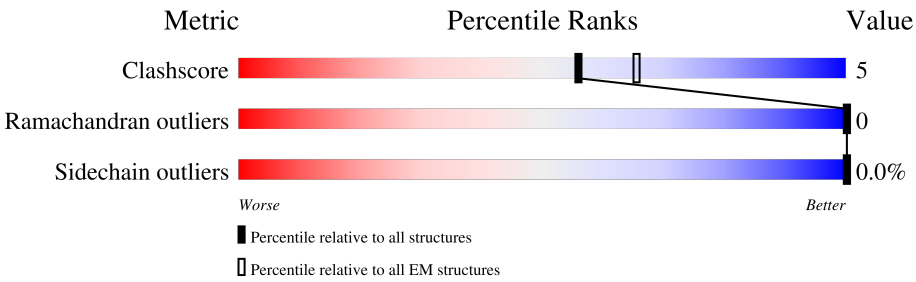
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.75 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 <=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	1297	65% 9% 26%
1	B	1297	66% 8% 26%
1	C	1297	63% 11% 26%
2	D	2	100%
2	E	2	100%
2	F	2	100%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 22809 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,Fibritin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	963	7511	4808	1241	1430	32	5	0
1	B	963	7502	4801	1241	1428	32	6	0
1	C	963	7502	4799	1238	1433	32	6	0

There are 207 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	614	ASN	ASP	engineered mutation	UNP P0DTC2
A	682	SER	ARG	engineered mutation	UNP P0DTC2
A	685	GLY	ARG	engineered mutation	UNP P0DTC2
A	892	PRO	ALA	engineered mutation	UNP P0DTC2
A	942	PRO	ALA	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
A	1209	GLY	-	linker	UNP P0DTC2
A	1210	SER	-	linker	UNP P0DTC2
A	1232	LEU	PHE	conflict	UNP P10104
A	1238	GLY	-	expression tag	UNP P10104
A	1239	ARG	-	expression tag	UNP P10104
A	1240	SER	-	expression tag	UNP P10104
A	1241	LEU	-	expression tag	UNP P10104
A	1242	GLU	-	expression tag	UNP P10104
A	1243	VAL	-	expression tag	UNP P10104
A	1244	LEU	-	expression tag	UNP P10104
A	1245	PHE	-	expression tag	UNP P10104
A	1246	GLN	-	expression tag	UNP P10104
A	1247	GLY	-	expression tag	UNP P10104
A	1248	PRO	-	expression tag	UNP P10104
A	1249	GLY	-	expression tag	UNP P10104
A	1250	SER	-	expression tag	UNP P10104
A	1251	LEU	-	expression tag	UNP P10104
A	1252	PRO	-	expression tag	UNP P10104

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1253	GLU	-	expression tag	UNP P10104
A	1254	THR	-	expression tag	UNP P10104
A	1255	GLY	-	expression tag	UNP P10104
A	1256	GLY	-	expression tag	UNP P10104
A	1257	GLY	-	expression tag	UNP P10104
A	1258	SER	-	expression tag	UNP P10104
A	1259	ASP	-	expression tag	UNP P10104
A	1260	TYR	-	expression tag	UNP P10104
A	1261	LYS	-	expression tag	UNP P10104
A	1262	ASP	-	expression tag	UNP P10104
A	1263	ASP	-	expression tag	UNP P10104
A	1264	ASP	-	expression tag	UNP P10104
A	1265	ASP	-	expression tag	UNP P10104
A	1266	LYS	-	expression tag	UNP P10104
A	1267	GLY	-	expression tag	UNP P10104
A	1268	GLY	-	expression tag	UNP P10104
A	1269	GLY	-	expression tag	UNP P10104
A	1270	GLY	-	expression tag	UNP P10104
A	1271	SER	-	expression tag	UNP P10104
A	1272	GLY	-	expression tag	UNP P10104
A	1273	GLY	-	expression tag	UNP P10104
A	1274	GLY	-	expression tag	UNP P10104
A	1275	GLY	-	expression tag	UNP P10104
A	1276	SER	-	expression tag	UNP P10104
A	1277	GLY	-	expression tag	UNP P10104
A	1278	GLY	-	expression tag	UNP P10104
A	1279	GLY	-	expression tag	UNP P10104
A	1280	GLY	-	expression tag	UNP P10104
A	1281	SER	-	expression tag	UNP P10104
A	1282	GLY	-	expression tag	UNP P10104
A	1283	GLY	-	expression tag	UNP P10104
A	1284	GLY	-	expression tag	UNP P10104
A	1285	GLY	-	expression tag	UNP P10104
A	1286	SER	-	expression tag	UNP P10104
A	1287	GLY	-	expression tag	UNP P10104
A	1288	GLY	-	expression tag	UNP P10104
A	1289	GLY	-	expression tag	UNP P10104
A	1290	GLY	-	expression tag	UNP P10104
A	1291	SER	-	expression tag	UNP P10104
A	1292	HIS	-	expression tag	UNP P10104
A	1293	HIS	-	expression tag	UNP P10104
A	1294	HIS	-	expression tag	UNP P10104

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1295	HIS	-	expression tag	UNP P10104
A	1296	HIS	-	expression tag	UNP P10104
A	1297	HIS	-	expression tag	UNP P10104
B	614	ASN	ASP	engineered mutation	UNP P0DTC2
B	682	SER	ARG	engineered mutation	UNP P0DTC2
B	685	GLY	ARG	engineered mutation	UNP P0DTC2
B	892	PRO	ALA	engineered mutation	UNP P0DTC2
B	942	PRO	ALA	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	1209	GLY	-	linker	UNP P0DTC2
B	1210	SER	-	linker	UNP P0DTC2
B	1232	LEU	PHE	conflict	UNP P10104
B	1238	GLY	-	expression tag	UNP P10104
B	1239	ARG	-	expression tag	UNP P10104
B	1240	SER	-	expression tag	UNP P10104
B	1241	LEU	-	expression tag	UNP P10104
B	1242	GLU	-	expression tag	UNP P10104
B	1243	VAL	-	expression tag	UNP P10104
B	1244	LEU	-	expression tag	UNP P10104
B	1245	PHE	-	expression tag	UNP P10104
B	1246	GLN	-	expression tag	UNP P10104
B	1247	GLY	-	expression tag	UNP P10104
B	1248	PRO	-	expression tag	UNP P10104
B	1249	GLY	-	expression tag	UNP P10104
B	1250	SER	-	expression tag	UNP P10104
B	1251	LEU	-	expression tag	UNP P10104
B	1252	PRO	-	expression tag	UNP P10104
B	1253	GLU	-	expression tag	UNP P10104
B	1254	THR	-	expression tag	UNP P10104
B	1255	GLY	-	expression tag	UNP P10104
B	1256	GLY	-	expression tag	UNP P10104
B	1257	GLY	-	expression tag	UNP P10104
B	1258	SER	-	expression tag	UNP P10104
B	1259	ASP	-	expression tag	UNP P10104
B	1260	TYR	-	expression tag	UNP P10104
B	1261	LYS	-	expression tag	UNP P10104
B	1262	ASP	-	expression tag	UNP P10104
B	1263	ASP	-	expression tag	UNP P10104
B	1264	ASP	-	expression tag	UNP P10104
B	1265	ASP	-	expression tag	UNP P10104
B	1266	LYS	-	expression tag	UNP P10104
B	1267	GLY	-	expression tag	UNP P10104

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1268	GLY	-	expression tag	UNP P10104
B	1269	GLY	-	expression tag	UNP P10104
B	1270	GLY	-	expression tag	UNP P10104
B	1271	SER	-	expression tag	UNP P10104
B	1272	GLY	-	expression tag	UNP P10104
B	1273	GLY	-	expression tag	UNP P10104
B	1274	GLY	-	expression tag	UNP P10104
B	1275	GLY	-	expression tag	UNP P10104
B	1276	SER	-	expression tag	UNP P10104
B	1277	GLY	-	expression tag	UNP P10104
B	1278	GLY	-	expression tag	UNP P10104
B	1279	GLY	-	expression tag	UNP P10104
B	1280	GLY	-	expression tag	UNP P10104
B	1281	SER	-	expression tag	UNP P10104
B	1282	GLY	-	expression tag	UNP P10104
B	1283	GLY	-	expression tag	UNP P10104
B	1284	GLY	-	expression tag	UNP P10104
B	1285	GLY	-	expression tag	UNP P10104
B	1286	SER	-	expression tag	UNP P10104
B	1287	GLY	-	expression tag	UNP P10104
B	1288	GLY	-	expression tag	UNP P10104
B	1289	GLY	-	expression tag	UNP P10104
B	1290	GLY	-	expression tag	UNP P10104
B	1291	SER	-	expression tag	UNP P10104
B	1292	HIS	-	expression tag	UNP P10104
B	1293	HIS	-	expression tag	UNP P10104
B	1294	HIS	-	expression tag	UNP P10104
B	1295	HIS	-	expression tag	UNP P10104
B	1296	HIS	-	expression tag	UNP P10104
B	1297	HIS	-	expression tag	UNP P10104
C	614	ASN	ASP	engineered mutation	UNP P0DTC2
C	682	SER	ARG	engineered mutation	UNP P0DTC2
C	685	GLY	ARG	engineered mutation	UNP P0DTC2
C	892	PRO	ALA	engineered mutation	UNP P0DTC2
C	942	PRO	ALA	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	1209	GLY	-	linker	UNP P0DTC2
C	1210	SER	-	linker	UNP P0DTC2
C	1232	LEU	PHE	conflict	UNP P10104
C	1238	GLY	-	expression tag	UNP P10104
C	1239	ARG	-	expression tag	UNP P10104
C	1240	SER	-	expression tag	UNP P10104

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1241	LEU	-	expression tag	UNP P10104
C	1242	GLU	-	expression tag	UNP P10104
C	1243	VAL	-	expression tag	UNP P10104
C	1244	LEU	-	expression tag	UNP P10104
C	1245	PHE	-	expression tag	UNP P10104
C	1246	GLN	-	expression tag	UNP P10104
C	1247	GLY	-	expression tag	UNP P10104
C	1248	PRO	-	expression tag	UNP P10104
C	1249	GLY	-	expression tag	UNP P10104
C	1250	SER	-	expression tag	UNP P10104
C	1251	LEU	-	expression tag	UNP P10104
C	1252	PRO	-	expression tag	UNP P10104
C	1253	GLU	-	expression tag	UNP P10104
C	1254	THR	-	expression tag	UNP P10104
C	1255	GLY	-	expression tag	UNP P10104
C	1256	GLY	-	expression tag	UNP P10104
C	1257	GLY	-	expression tag	UNP P10104
C	1258	SER	-	expression tag	UNP P10104
C	1259	ASP	-	expression tag	UNP P10104
C	1260	TYR	-	expression tag	UNP P10104
C	1261	LYS	-	expression tag	UNP P10104
C	1262	ASP	-	expression tag	UNP P10104
C	1263	ASP	-	expression tag	UNP P10104
C	1264	ASP	-	expression tag	UNP P10104
C	1265	ASP	-	expression tag	UNP P10104
C	1266	LYS	-	expression tag	UNP P10104
C	1267	GLY	-	expression tag	UNP P10104
C	1268	GLY	-	expression tag	UNP P10104
C	1269	GLY	-	expression tag	UNP P10104
C	1270	GLY	-	expression tag	UNP P10104
C	1271	SER	-	expression tag	UNP P10104
C	1272	GLY	-	expression tag	UNP P10104
C	1273	GLY	-	expression tag	UNP P10104
C	1274	GLY	-	expression tag	UNP P10104
C	1275	GLY	-	expression tag	UNP P10104
C	1276	SER	-	expression tag	UNP P10104
C	1277	GLY	-	expression tag	UNP P10104
C	1278	GLY	-	expression tag	UNP P10104
C	1279	GLY	-	expression tag	UNP P10104
C	1280	GLY	-	expression tag	UNP P10104
C	1281	SER	-	expression tag	UNP P10104
C	1282	GLY	-	expression tag	UNP P10104

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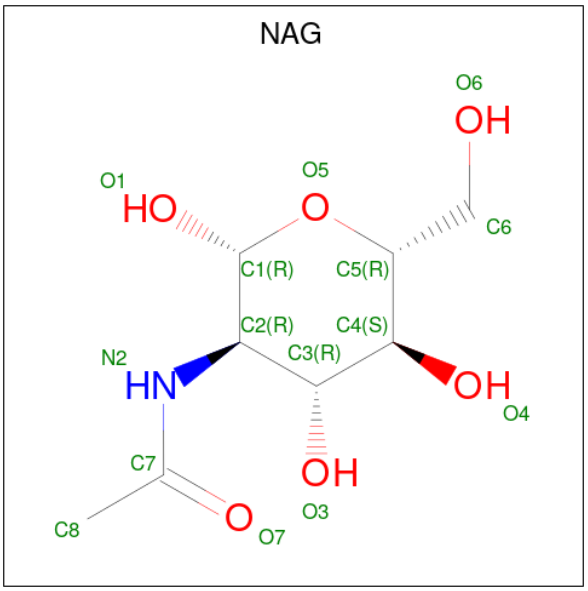
Chain	Residue	Modelled	Actual	Comment	Reference
C	1283	GLY	-	expression tag	UNP P10104
C	1284	GLY	-	expression tag	UNP P10104
C	1285	GLY	-	expression tag	UNP P10104
C	1286	SER	-	expression tag	UNP P10104
C	1287	GLY	-	expression tag	UNP P10104
C	1288	GLY	-	expression tag	UNP P10104
C	1289	GLY	-	expression tag	UNP P10104
C	1290	GLY	-	expression tag	UNP P10104
C	1291	SER	-	expression tag	UNP P10104
C	1292	HIS	-	expression tag	UNP P10104
C	1293	HIS	-	expression tag	UNP P10104
C	1294	HIS	-	expression tag	UNP P10104
C	1295	HIS	-	expression tag	UNP P10104
C	1296	HIS	-	expression tag	UNP P10104
C	1297	HIS	-	expression tag	UNP P10104

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	D	2	28	16	2	10	0	0
2	E	2	28	16	2	10	0	0
2	F	2	28	16	2	10	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
3	A	1	70	40	5	25	0
			Total	C	N	O	
3	A	1	70	40	5	25	0
			Total	C	N	O	
3	A	1	70	40	5	25	0
			Total	C	N	O	
3	A	1	70	40	5	25	0
			Total	C	N	O	
3	A	1	70	40	5	25	0
			Total	C	N	O	
3	B	1	70	40	5	25	0
			Total	C	N	O	
3	B	1	70	40	5	25	0
			Total	C	N	O	
3	B	1	70	40	5	25	0
			Total	C	N	O	
3	B	1	70	40	5	25	0
			Total	C	N	O	
3	B	1	70	40	5	25	0
			Total	C	N	O	
3	C	1	70	40	5	25	0
			Total	C	N	O	
3	C	1	70	40	5	25	0
			Total	C	N	O	
3	C	1	70	40	5	25	0
			Total	C	N	O	
3	C	1	70	40	5	25	0

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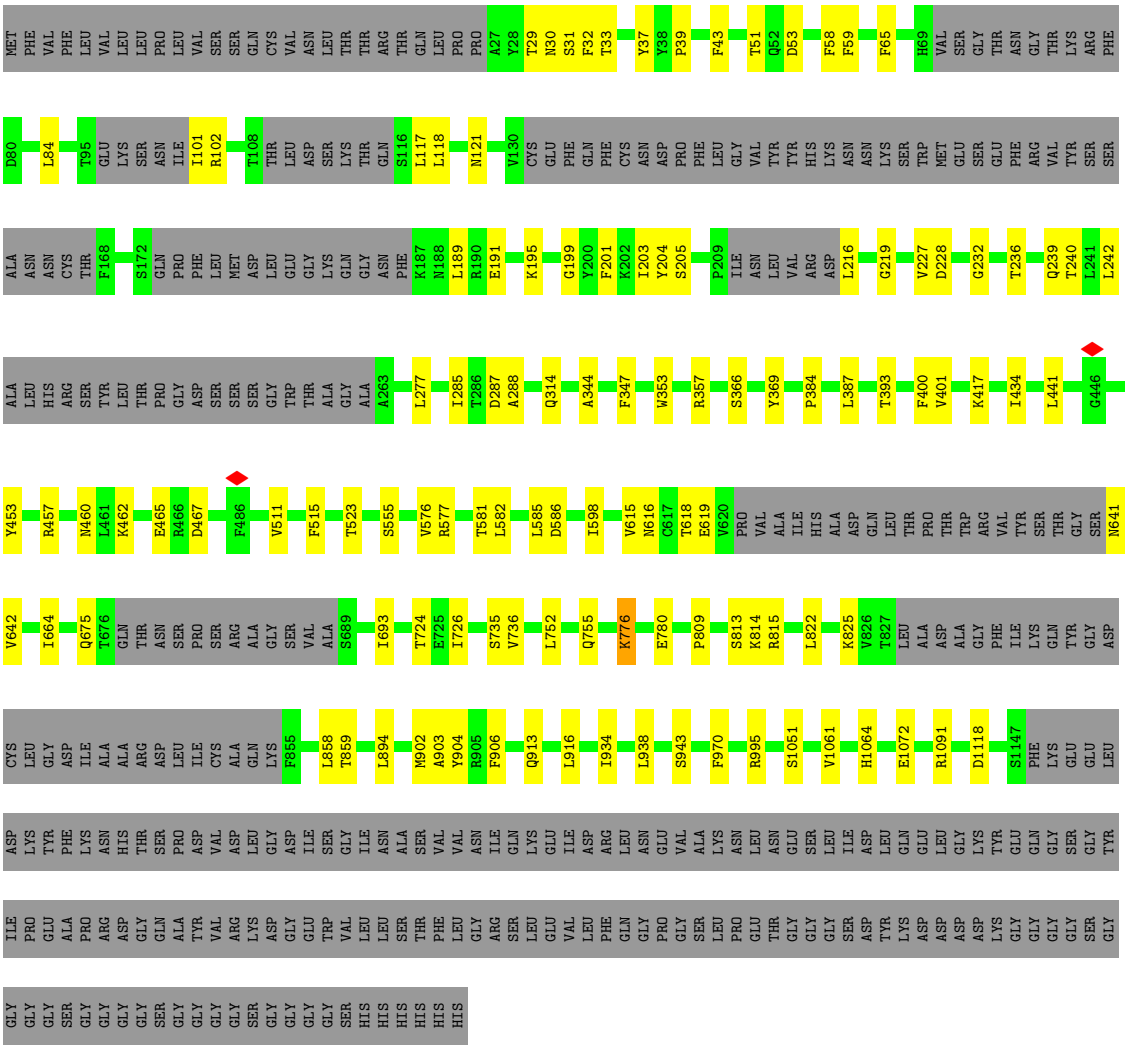
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
3	C	1	70	40	5	25	0

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.

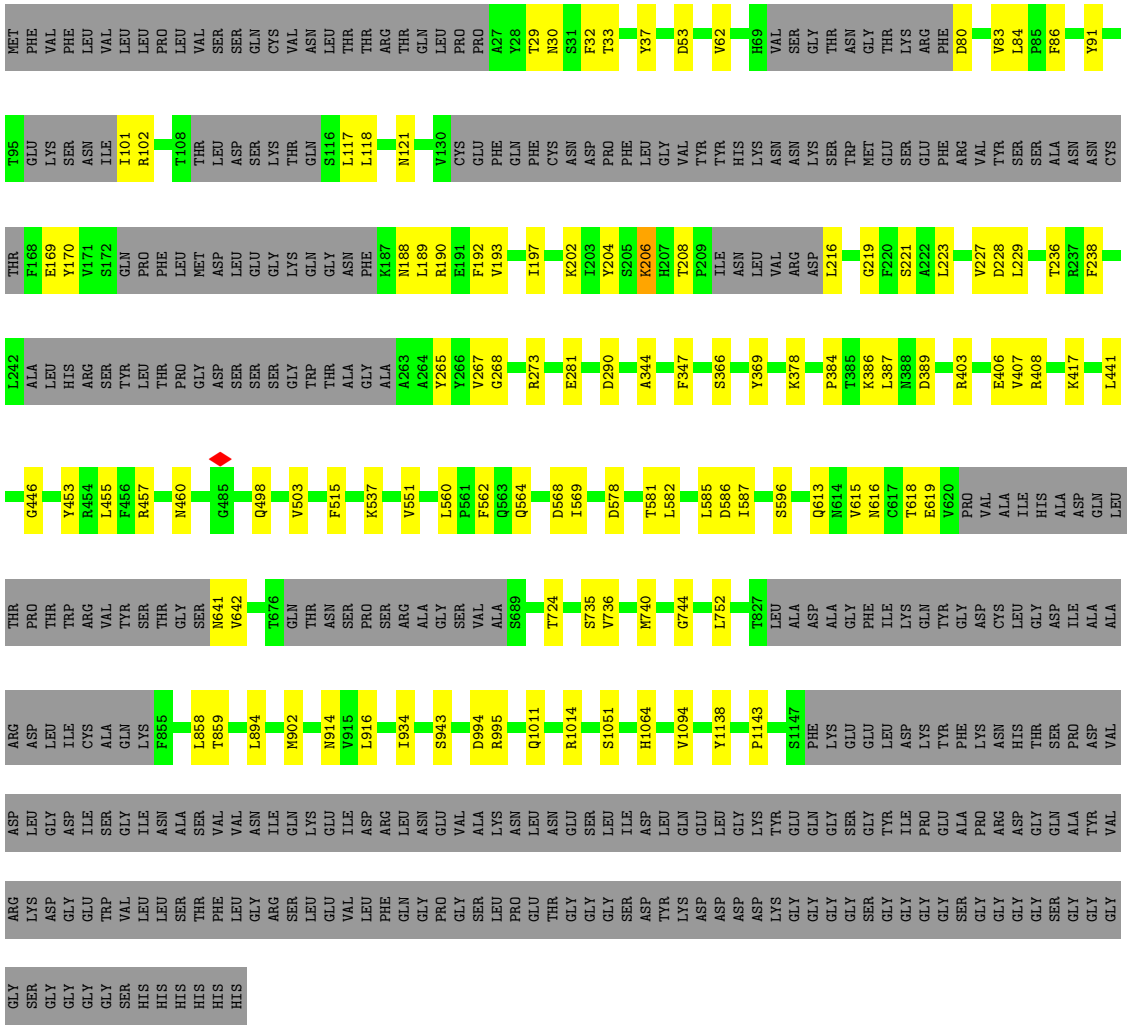
• Molecule 1: Spike glycoprotein,Fibritin

Chain A: 65% 9% 26%



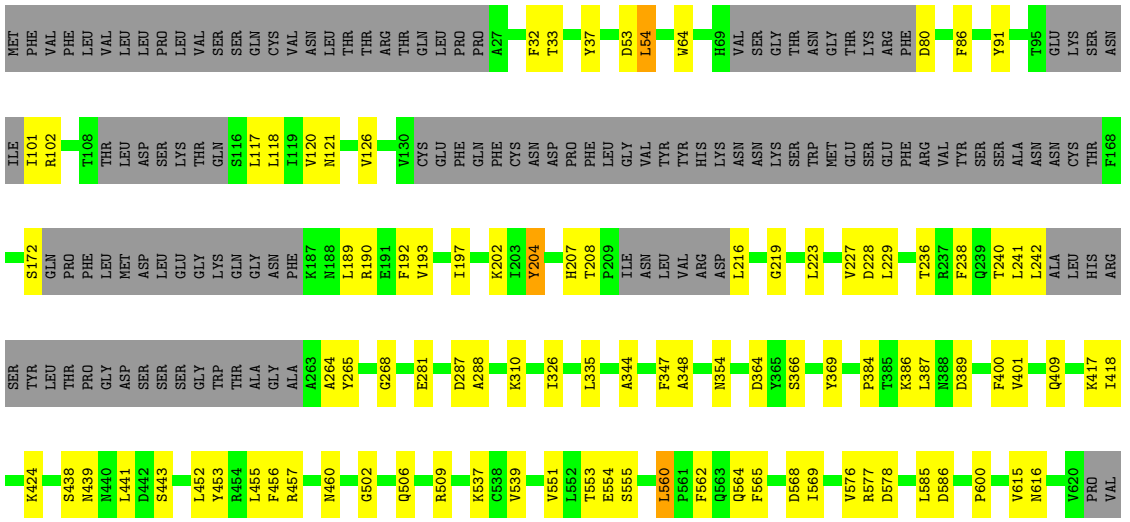
• Molecule 1: Spike glycoprotein,Fibritin

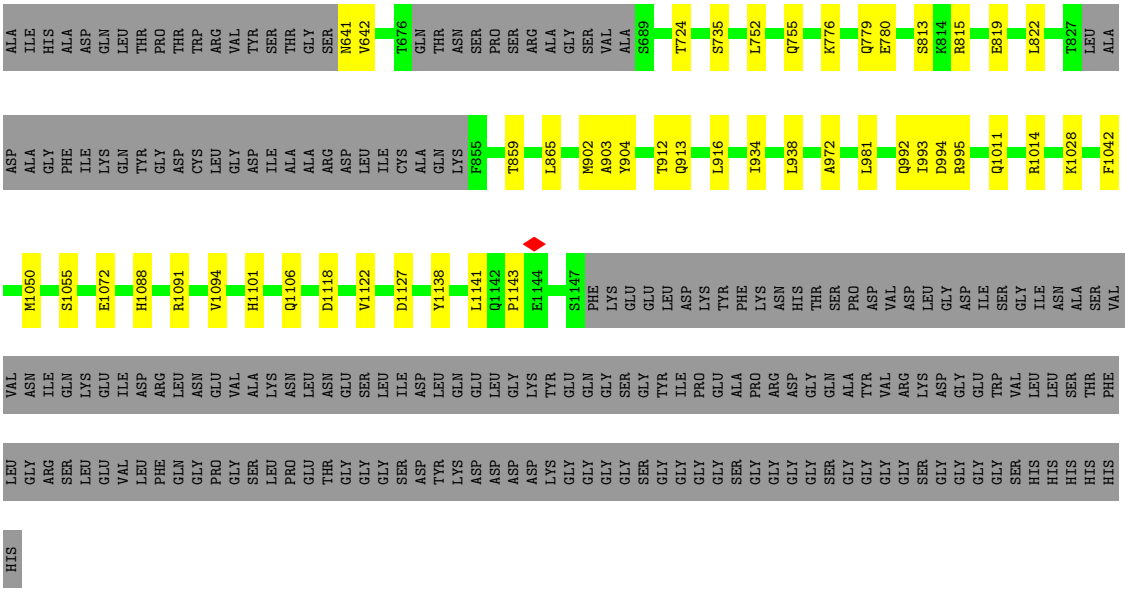
Chain B: 66% 8% 26%



- Molecule 1: Spike glycoprotein,Fibritin

Chain C: 63% 11% 26%





• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D: 100%

NAG1
NAG2

• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E: 100%

NAG1
NAG2

• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F: 100%

NAG1
NAG2

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	315000	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 ($e^-/Å^2$)	65	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.137	Depositor
Minimum map value	-0.065	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.006	Depositor
Map size (Å)	374.528, 374.528, 374.528	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.836, 0.836, 0.836	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	0.38	0/7694	0.53	4/10471 (0.0%)
1	B	0.38	0/7686	0.53	3/10460 (0.0%)
1	C	0.39	0/7686	0.56	10/10461 (0.1%)
All	All	0.38	0/23066	0.54	17/31392 (0.1%)

There are no bond length outliers.

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	776	LYS	CD-CE-NZ	12.49	140.43	111.70
1	B	206	LYS	CD-CE-NZ	12.46	140.35	111.70
1	C	424	LYS	CD-CE-NZ	12.29	139.97	111.70
1	B	378	LYS	CD-CE-NZ	-10.79	86.87	111.70
1	C	1127	ASP	CB-CG-OD2	-7.13	111.88	118.30

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	7511	0	7339	78	0
1	B	7502	0	7327	73	0
1	C	7502	0	7325	89	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	28	0	25	0	0
2	E	28	0	25	0	0
2	F	28	0	25	0	0
3	A	70	0	65	0	0
3	B	70	0	65	0	0
3	C	70	0	65	1	0
All	All	22809	0	22261	234	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 5.

The worst 5 of 234 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:A:902:MET:HG3	1:A:916:LEU:CD1	2.05	0.86
1:C:568:ASP:OD1	1:C:569:ILE:N	2.12	0.83
1:C:776:LYS:NZ	1:C:780:GLU:OE1	2.14	0.81
1:A:236:THR:O	1:A:236:THR:HG22	1.81	0.81
1:B:403:ARG:HD3	1:B:406:GLU:OE1	1.80	0.81

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	946/1297 (73%)	912 (96%)	34 (4%)	0	100	100
1	B	947/1297 (73%)	907 (96%)	40 (4%)	0	100	100
1	C	947/1297 (73%)	908 (96%)	39 (4%)	0	100	100
All	All	2840/3891 (73%)	2727 (96%)	113 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	840/1112 (76%)	840 (100%)	0	100	100
1	B	837/1112 (75%)	837 (100%)	0	100	100
1	C	840/1112 (76%)	839 (100%)	1 (0%)	93	96
All	All	2517/3336 (75%)	2516 (100%)	1 (0%)	100	100

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

Mol	Chain	Res	Type
1	C	204	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	913	GLN
1	B	1071	GLN
1	C	1101	HIS
1	C	764	ASN
1	C	1088	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

6 monosaccharides 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	1	2,1	14,14,15	0.32	0	17,19,21	0.42	0
2	NAG	D	2	2	14,14,15	0.27	0	17,19,21	0.38	0
2	NAG	E	1	2,1	14,14,15	0.25	0	17,19,21	0.52	0
2	NAG	E	2	2	14,14,15	0.27	0	17,19,21	0.38	0
2	NAG	F	1	2,1	14,14,15	0.25	0	17,19,21	0.60	0
2	NAG	F	2	2	14,14,15	0.22	0	17,19,21	0.41	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	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	NAG	E	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	NAG	F	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	2	NAG	O5-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6

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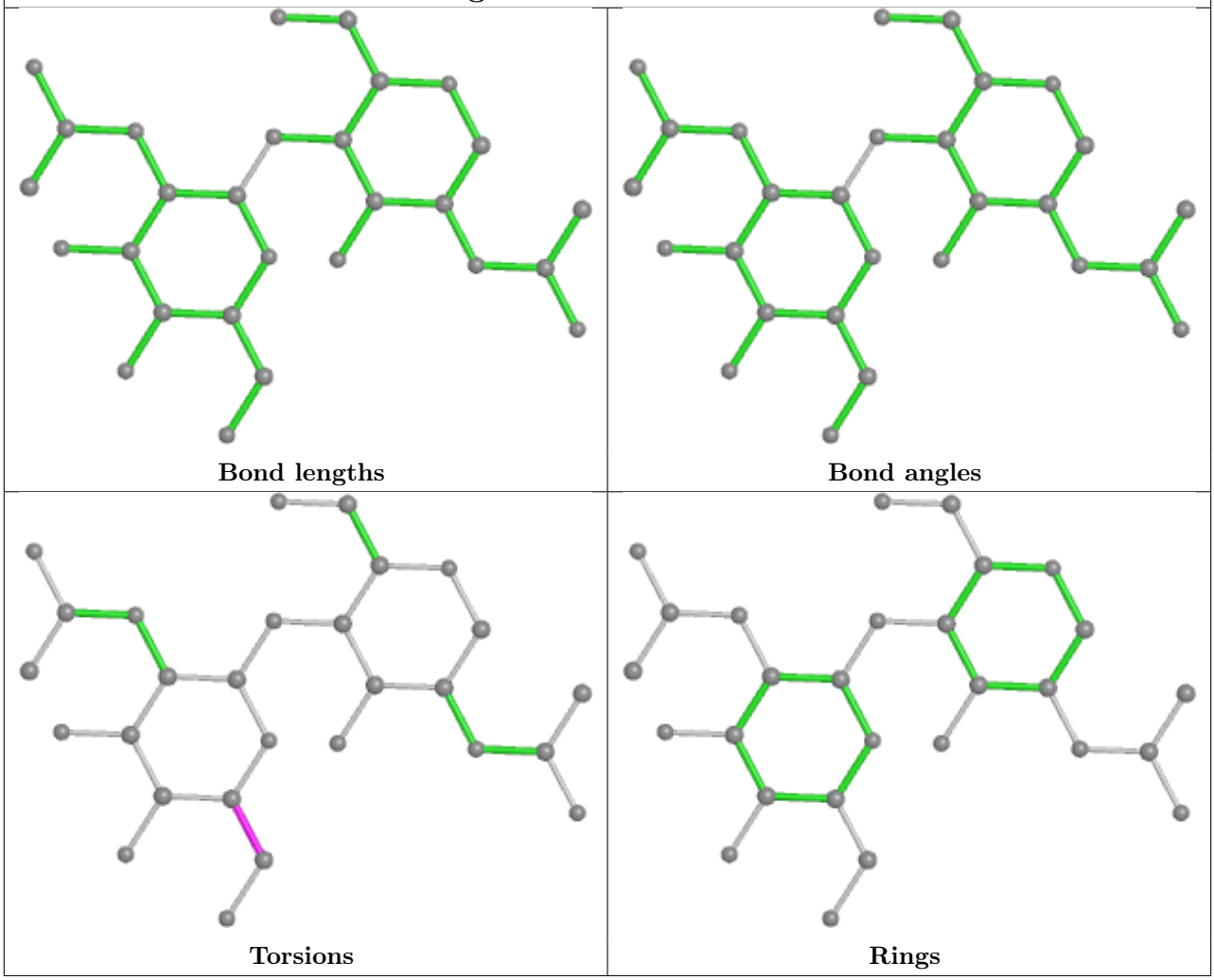
Mol	Chain	Res	Type	Atoms
2	F	2	NAG	C4-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6

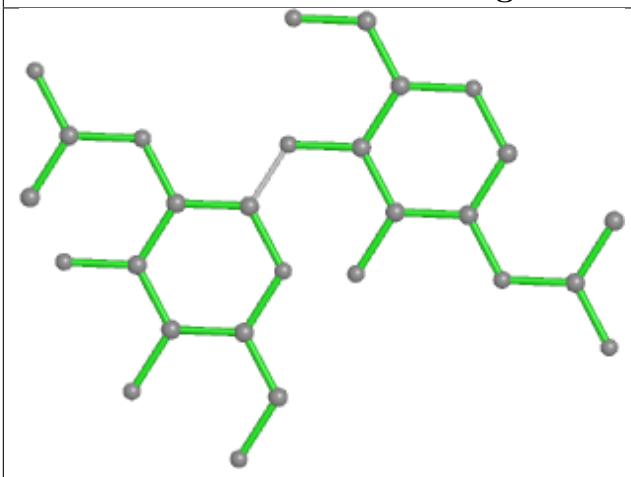
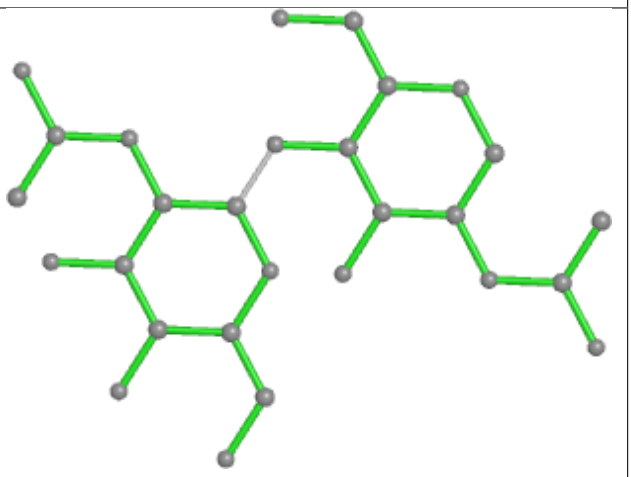
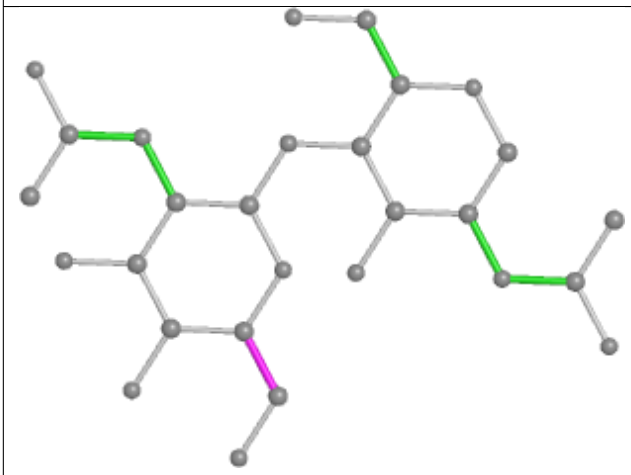
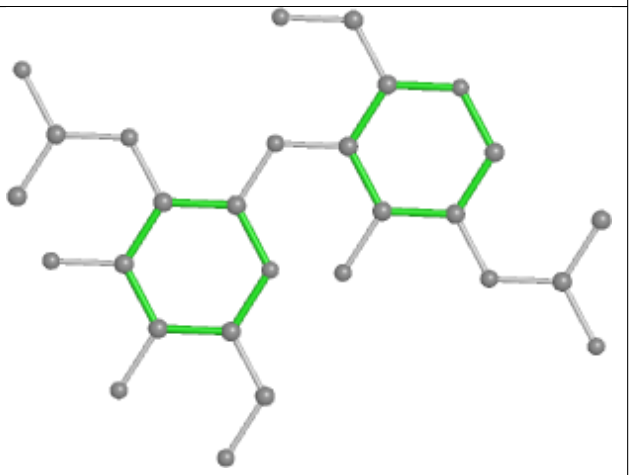
There are no ring outliers.

No monomer is involved in short contacts.

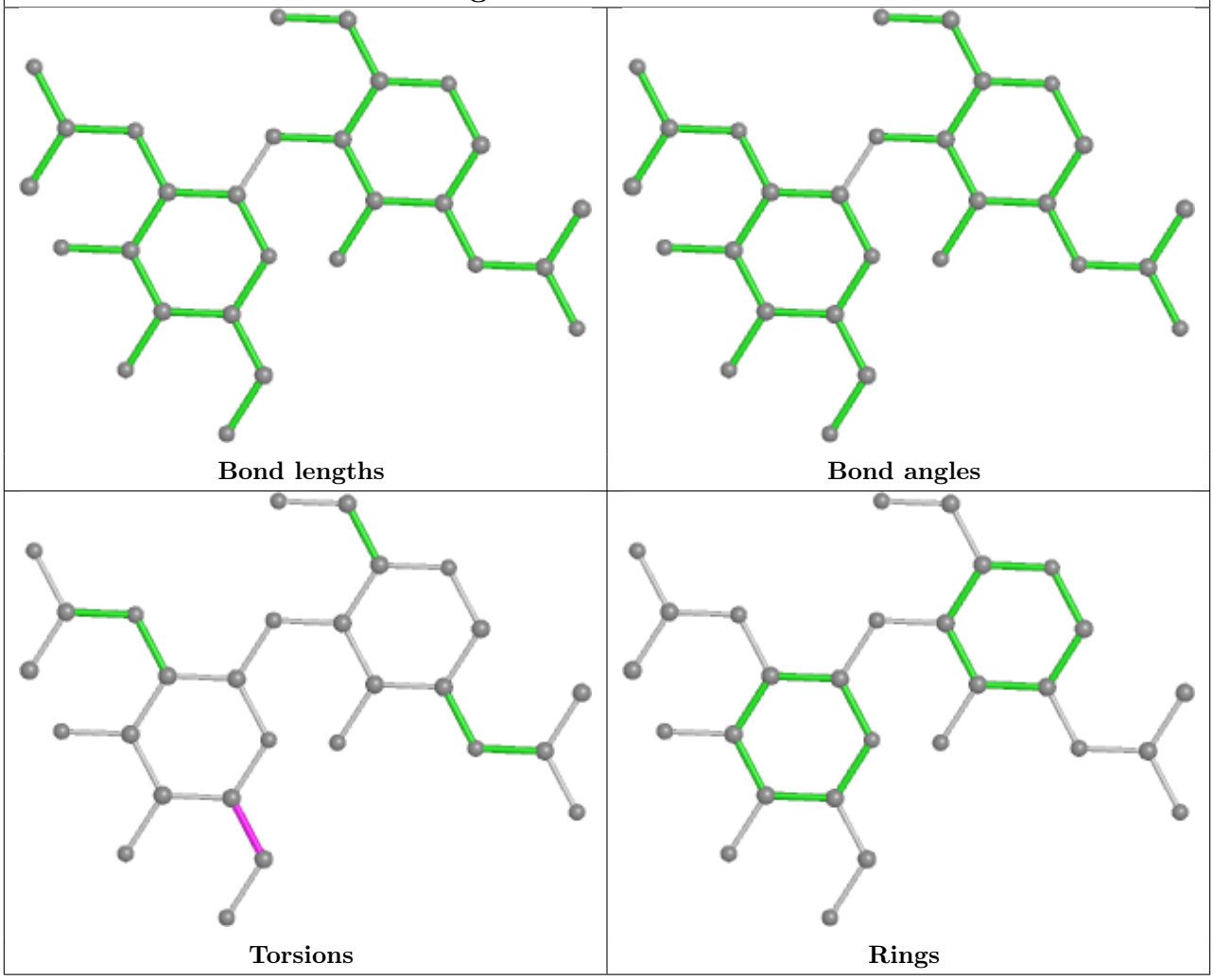
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

Oligosaccharide Chain D



Oligosaccharide Chain E	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain F



5.6 Ligand geometry (i)

15 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	$\#\|Z\| > 2$
3	NAG	A	1304	1	14,14,15	0.21	0	17,19,21	0.52	0
3	NAG	C	1302	1	14,14,15	0.25	0	17,19,21	0.60	0
3	NAG	C	1304	1	14,14,15	0.25	0	17,19,21	0.36	0
3	NAG	A	1301	1	14,14,15	0.21	0	17,19,21	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	B	1303	1	14,14,15	0.21	0	17,19,21	0.62	1 (5%)
3	NAG	C	1303	1	14,14,15	0.22	0	17,19,21	0.43	0
3	NAG	B	1305	1	14,14,15	0.21	0	17,19,21	0.52	0
3	NAG	B	1302	1	14,14,15	0.18	0	17,19,21	0.46	0
3	NAG	B	1304	1	14,14,15	0.26	0	17,19,21	0.55	0
3	NAG	A	1305	1	14,14,15	0.16	0	17,19,21	0.58	0
3	NAG	C	1305	1	14,14,15	0.15	0	17,19,21	0.60	0
3	NAG	C	1301	1	14,14,15	0.24	0	17,19,21	0.46	0
3	NAG	A	1302	1	14,14,15	0.28	0	17,19,21	0.60	0
3	NAG	A	1303	1	14,14,15	0.30	0	17,19,21	0.47	0
3	NAG	B	1301	1	14,14,15	0.30	0	17,19,21	0.35	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
3	NAG	A	1304	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1302	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1304	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1301	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1303	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1303	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1305	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1302	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1304	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1305	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1305	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1301	1	-	1/6/23/26	0/1/1/1
3	NAG	A	1302	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1303	1	-	1/6/23/26	0/1/1/1
3	NAG	B	1301	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1303	NAG	C1-O5-C5	2.09	115.03	112.19

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1305	NAG	O5-C5-C6-O6
3	B	1304	NAG	O5-C5-C6-O6
3	C	1305	NAG	O5-C5-C6-O6
3	A	1301	NAG	O5-C5-C6-O6
3	C	1303	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1304	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.

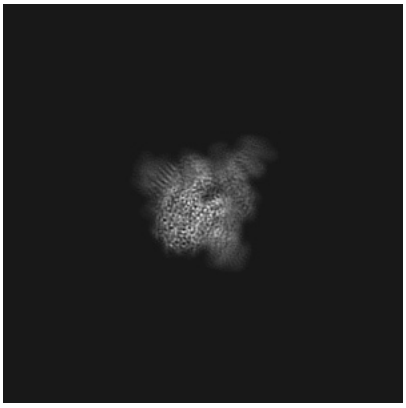
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-11639. These allow visual inspection of the internal detail of the map and identification of artifacts.

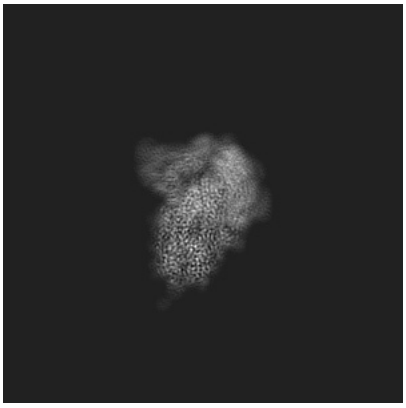
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

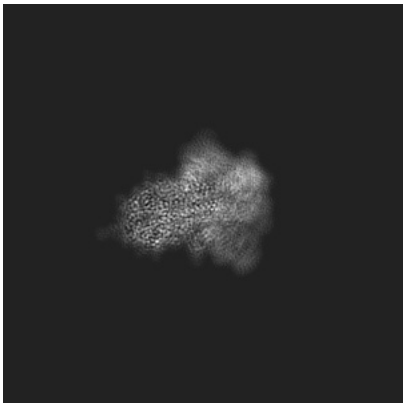
6.1.1 Primary map



X



Y

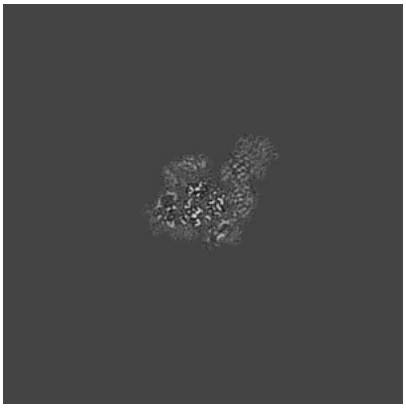


Z

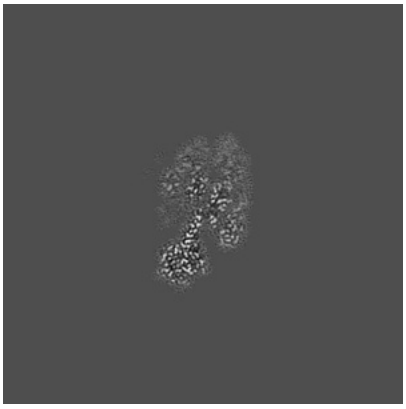
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map



X Index: 224



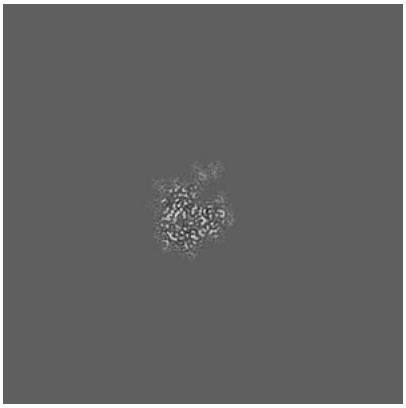
Y Index: 224

Z Index: 224

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

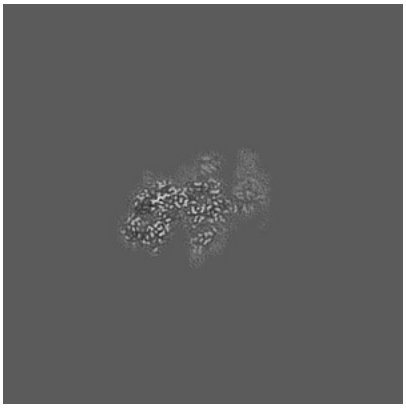
6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 176

Y Index: 212

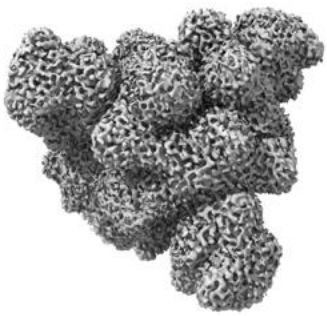


Z Index: 215

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 0.006. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

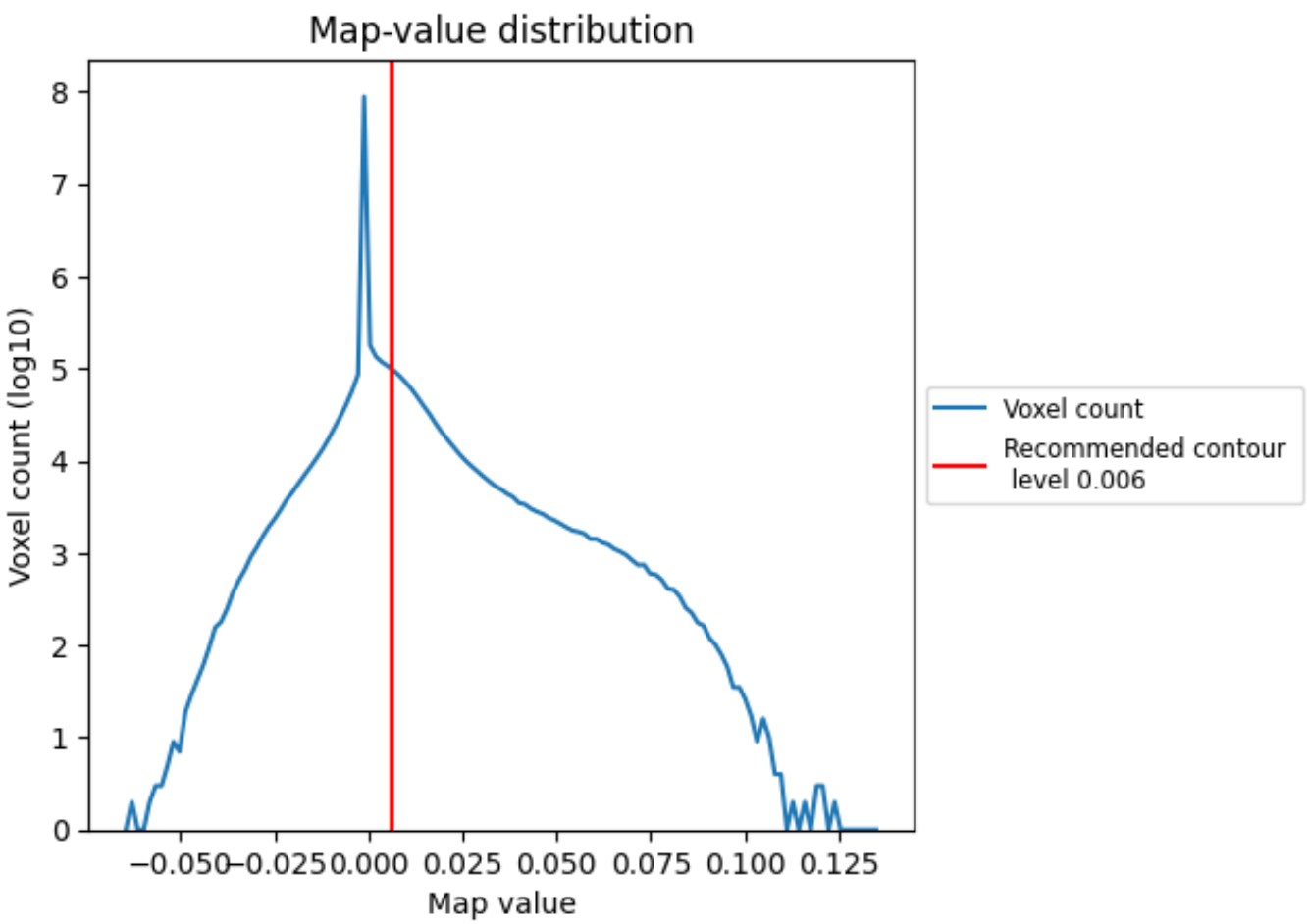
6.5 Mask visualisation (i)

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

7 Map analysis (i)

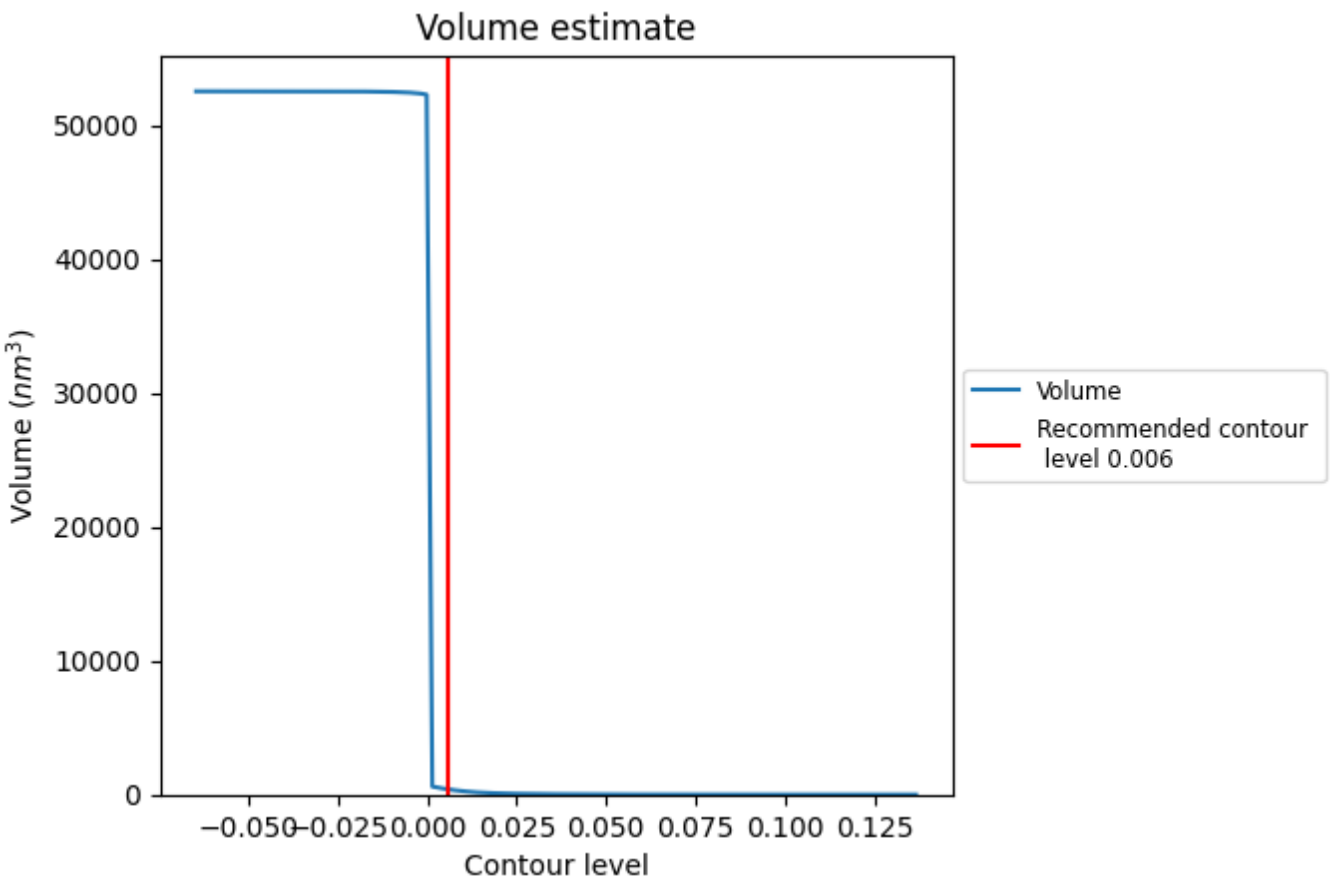
This section contains the results of statistical analysis of the map.

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.

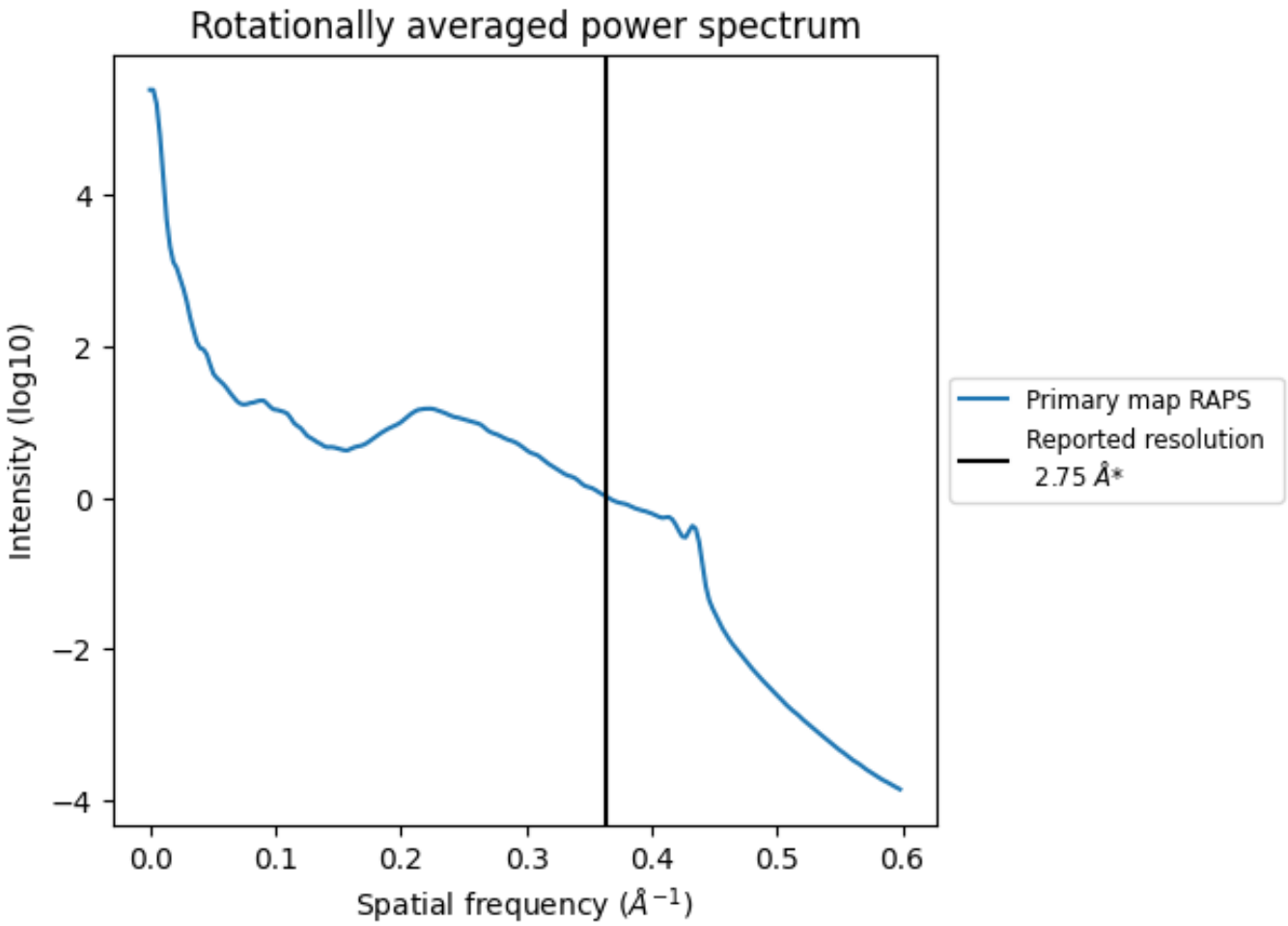
7.2 Volume estimate (i)



The volume at the recommended contour level is 390 nm^3; this corresponds to an approximate mass of 352 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)

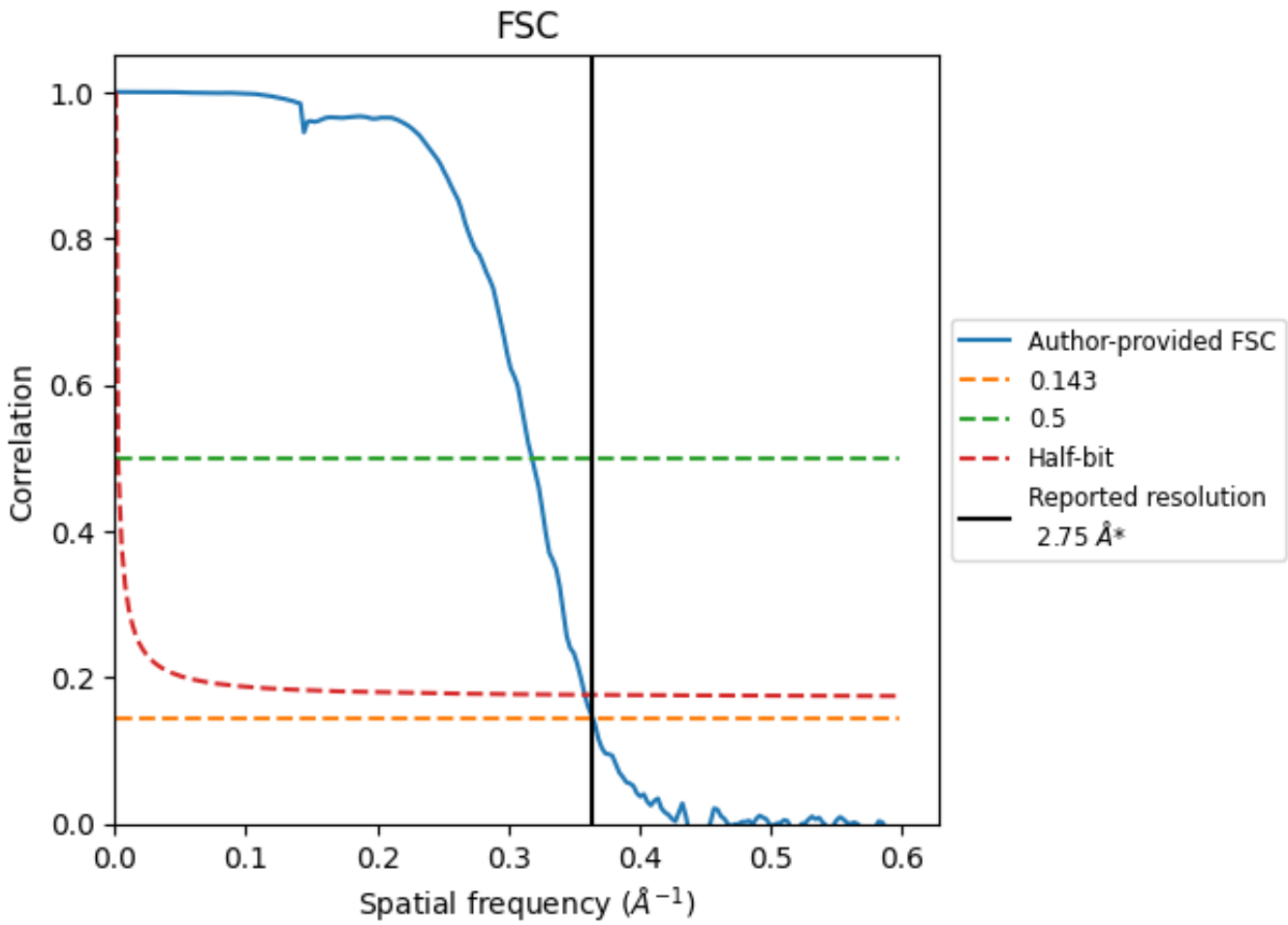


*Reported resolution corresponds to spatial frequency of 0.364 Å^{-1}

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 0.364 Å^{-1}

8.2 Resolution estimates (i)

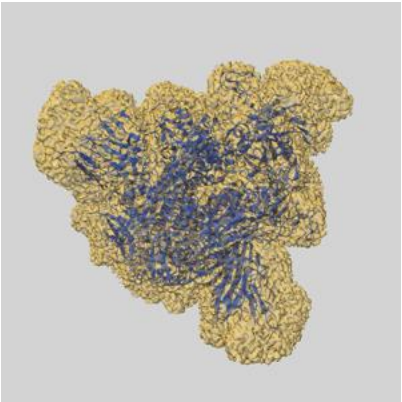
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.75	-	-
Author-provided FSC curve	2.74	3.15	2.79
Unmasked-calculated*	-	-	-

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

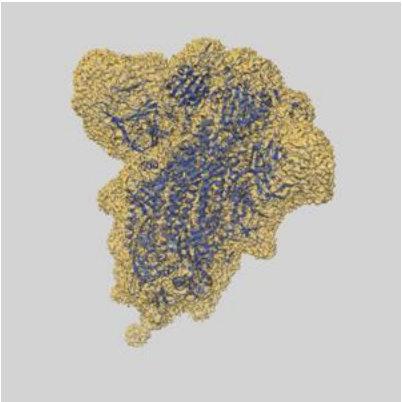
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-11639 and PDB model 7A4N. Per-residue inclusion information can be found in section 3 on page 11.

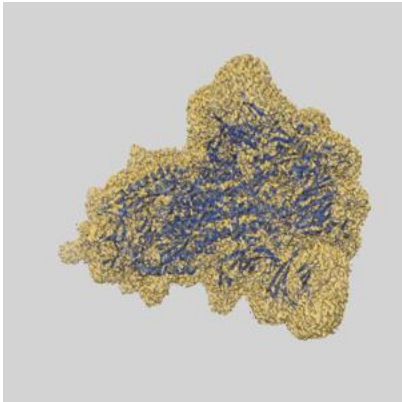
9.1 Map-model overlay (i)



X



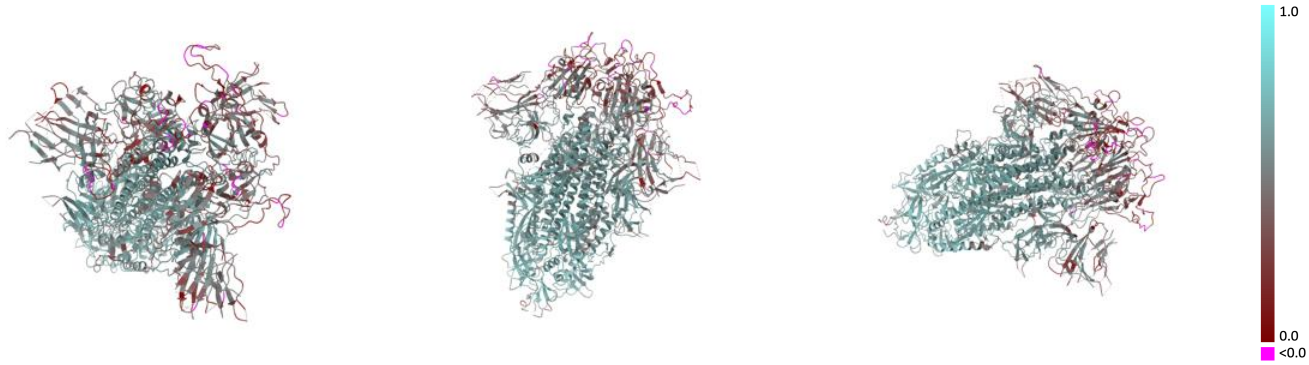
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.006 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.

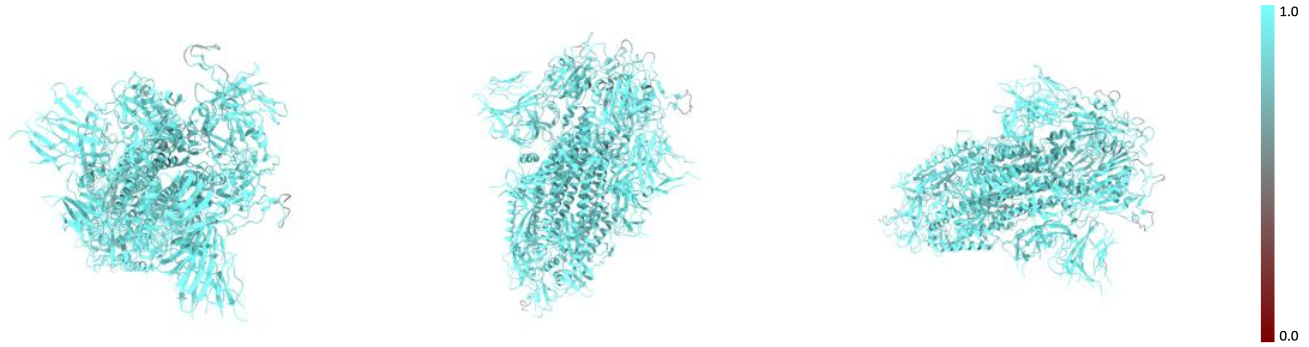
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

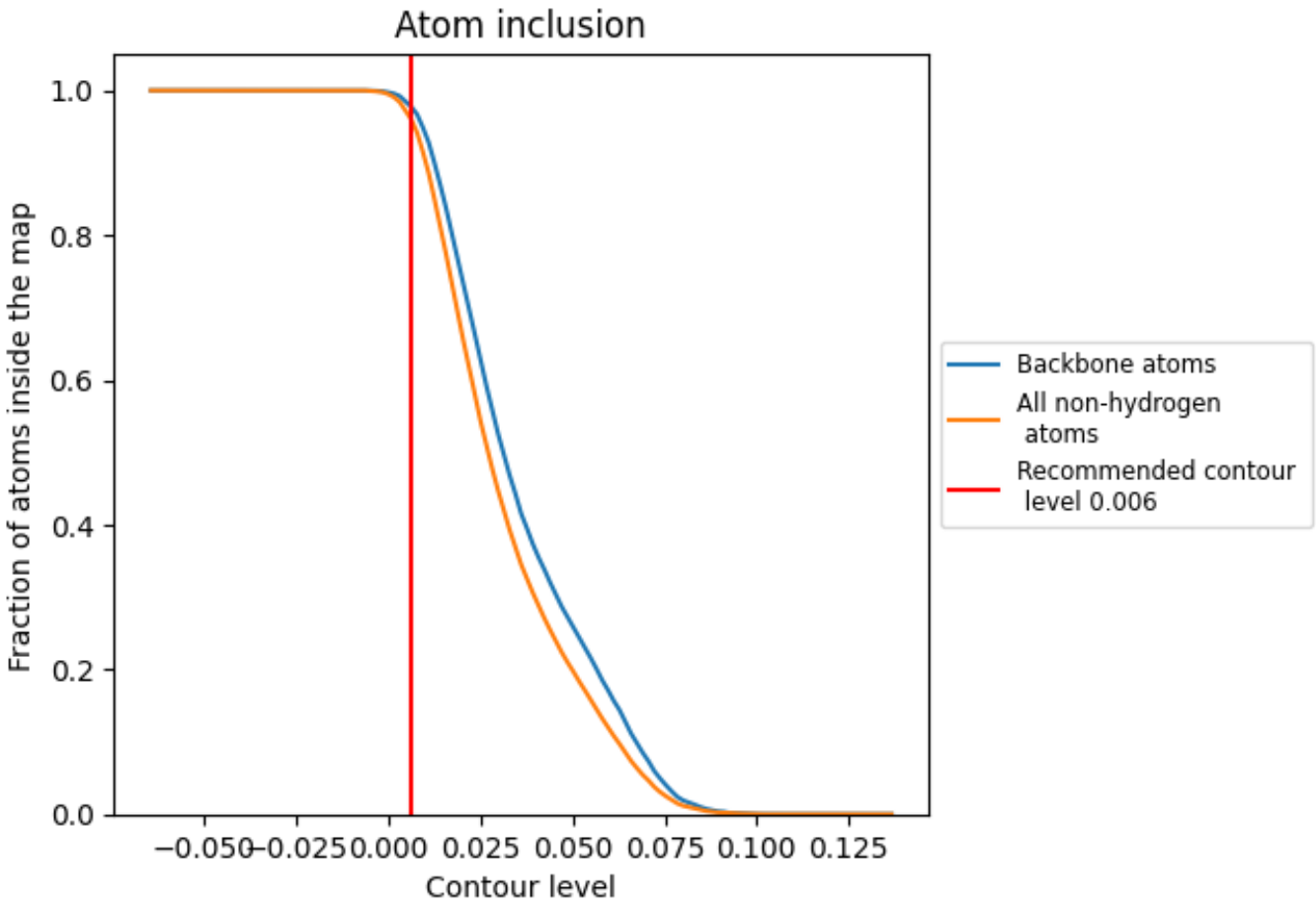
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.006).

9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9617	0.5210
A	0.9599	0.5180
B	0.9661	0.5290
C	0.9590	0.5170
D	0.9643	0.5000
E	0.9643	0.5080
F	0.9643	0.4920