



wwPDB EM Validation Summary Report ⓘ

Jul 13, 2025 – 12:27 PM JST

PDB ID : 9K6Z / pdb_00009k6z
EMDB ID : EMD-62143
Title : SARS-CoV-2 related bat coronavirus BANAL-52 spike in the locked state
Authors : Li, Q.Q.; Cai, X.; Li, X.N.; Zhang, Y.B.; Li, R.; Kang, Z.R.; Wan, D.D.;
Wang, J.X.; Yang, J.X.; Shi, J.X.; Jin, S.L.; Peng, Y.; Zang, N.; Xie, Z.K.;
Wan, Y.S.; Shang, J.
Deposited on : 2024-10-22
Resolution : 3.51 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.dev118
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
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) : 2.44

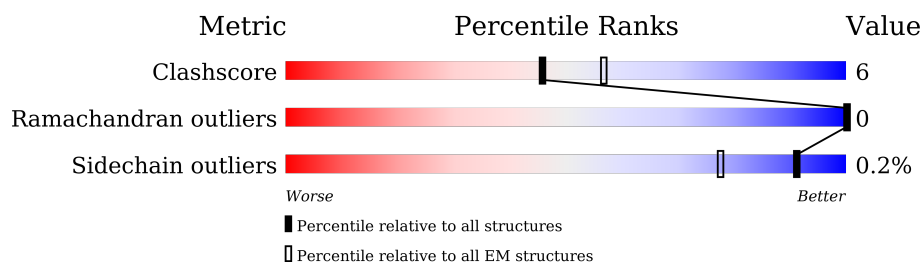
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.51 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	1247	 6% 75% 13% 12%
1	B	1247	 5% 76% 13% 12%
1	C	1247	 5% 76% 13% 12%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 26628 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	1102	Total	C	N	O	S	0	0
			8604	5487	1437	1640	40		
1	B	1102	Total	C	N	O	S	0	0
			8604	5487	1437	1640	40		
1	C	1102	Total	C	N	O	S	0	0
			8604	5487	1437	1640	40		

There are 183 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	68	ILE	LEU	conflict	UNP A0AA49X976
A	111	ASP	ASN	conflict	UNP A0AA49X976
A	147	ARG	LYS	conflict	UNP A0AA49X976
A	176	LEU	PHE	conflict	UNP A0AA49X976
A	177	MET	ILE	conflict	UNP A0AA49X976
A	222	ALA	VAL	conflict	UNP A0AA49X976
A	292	SER	ALA	conflict	UNP A0AA49X976
A	324	GLU	GLN	conflict	UNP A0AA49X976
A	346	THR	ARG	conflict	UNP A0AA49X976
A	402	VAL	ILE	conflict	UNP A0AA49X976
A	486	PHE	LEU	conflict	UNP A0AA49X976
A	554	GLU	GLN	conflict	UNP A0AA49X976
A	627	ASN	ASP	conflict	UNP A0AA49X976
A	789	GLN	PRO	conflict	UNP A0AA49X976
A	982	PRO	LYS	conflict	UNP A0AA49X976
A	983	PRO	VAL	conflict	UNP A0AA49X976
A	1080	ASP	ASN	conflict	UNP A0AA49X976
A	1107	GLU	LYS	conflict	UNP A0AA49X976
A	1160	VAL	ILE	conflict	UNP A0AA49X976
A	1163	SER	GLY	conflict	UNP A0AA49X976
A	1187	LYS	ARG	conflict	UNP A0AA49X976
A	1208	GLY	-	expression tag	UNP A0AA49X976
A	1209	SER	-	expression tag	UNP A0AA49X976
A	1210	GLY	-	expression tag	UNP A0AA49X976

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1211	SER	-	expression tag	UNP A0AA49X976
A	1212	GLY	-	expression tag	UNP A0AA49X976
A	1213	TYR	-	expression tag	UNP A0AA49X976
A	1214	ILE	-	expression tag	UNP A0AA49X976
A	1215	PRO	-	expression tag	UNP A0AA49X976
A	1216	GLU	-	expression tag	UNP A0AA49X976
A	1217	ALA	-	expression tag	UNP A0AA49X976
A	1218	PRO	-	expression tag	UNP A0AA49X976
A	1219	ARG	-	expression tag	UNP A0AA49X976
A	1220	ASP	-	expression tag	UNP A0AA49X976
A	1221	GLY	-	expression tag	UNP A0AA49X976
A	1222	GLN	-	expression tag	UNP A0AA49X976
A	1223	ALA	-	expression tag	UNP A0AA49X976
A	1224	TYR	-	expression tag	UNP A0AA49X976
A	1225	VAL	-	expression tag	UNP A0AA49X976
A	1226	ARG	-	expression tag	UNP A0AA49X976
A	1227	LYS	-	expression tag	UNP A0AA49X976
A	1228	ASP	-	expression tag	UNP A0AA49X976
A	1229	GLY	-	expression tag	UNP A0AA49X976
A	1230	GLU	-	expression tag	UNP A0AA49X976
A	1231	TRP	-	expression tag	UNP A0AA49X976
A	1232	VAL	-	expression tag	UNP A0AA49X976
A	1233	LEU	-	expression tag	UNP A0AA49X976
A	1234	LEU	-	expression tag	UNP A0AA49X976
A	1235	SER	-	expression tag	UNP A0AA49X976
A	1236	THR	-	expression tag	UNP A0AA49X976
A	1237	PHE	-	expression tag	UNP A0AA49X976
A	1238	LEU	-	expression tag	UNP A0AA49X976
A	1239	GLY	-	expression tag	UNP A0AA49X976
A	1240	HIS	-	expression tag	UNP A0AA49X976
A	1241	HIS	-	expression tag	UNP A0AA49X976
A	1242	HIS	-	expression tag	UNP A0AA49X976
A	1243	HIS	-	expression tag	UNP A0AA49X976
A	1244	HIS	-	expression tag	UNP A0AA49X976
A	1245	HIS	-	expression tag	UNP A0AA49X976
A	1246	HIS	-	expression tag	UNP A0AA49X976
A	1247	HIS	-	expression tag	UNP A0AA49X976
B	68	ILE	LEU	conflict	UNP A0AA49X976
B	111	ASP	ASN	conflict	UNP A0AA49X976
B	147	ARG	LYS	conflict	UNP A0AA49X976
B	176	LEU	PHE	conflict	UNP A0AA49X976
B	177	MET	ILE	conflict	UNP A0AA49X976

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Chain	Residue	Modelled	Actual	Comment	Reference
B	222	ALA	VAL	conflict	UNP A0AA49X976
B	292	SER	ALA	conflict	UNP A0AA49X976
B	324	GLU	GLN	conflict	UNP A0AA49X976
B	346	THR	ARG	conflict	UNP A0AA49X976
B	402	VAL	ILE	conflict	UNP A0AA49X976
B	486	PHE	LEU	conflict	UNP A0AA49X976
B	554	GLU	GLN	conflict	UNP A0AA49X976
B	627	ASN	ASP	conflict	UNP A0AA49X976
B	789	GLN	PRO	conflict	UNP A0AA49X976
B	982	PRO	LYS	conflict	UNP A0AA49X976
B	983	PRO	VAL	conflict	UNP A0AA49X976
B	1080	ASP	ASN	conflict	UNP A0AA49X976
B	1107	GLU	LYS	conflict	UNP A0AA49X976
B	1160	VAL	ILE	conflict	UNP A0AA49X976
B	1163	SER	GLY	conflict	UNP A0AA49X976
B	1187	LYS	ARG	conflict	UNP A0AA49X976
B	1208	GLY	-	expression tag	UNP A0AA49X976
B	1209	SER	-	expression tag	UNP A0AA49X976
B	1210	GLY	-	expression tag	UNP A0AA49X976
B	1211	SER	-	expression tag	UNP A0AA49X976
B	1212	GLY	-	expression tag	UNP A0AA49X976
B	1213	TYR	-	expression tag	UNP A0AA49X976
B	1214	ILE	-	expression tag	UNP A0AA49X976
B	1215	PRO	-	expression tag	UNP A0AA49X976
B	1216	GLU	-	expression tag	UNP A0AA49X976
B	1217	ALA	-	expression tag	UNP A0AA49X976
B	1218	PRO	-	expression tag	UNP A0AA49X976
B	1219	ARG	-	expression tag	UNP A0AA49X976
B	1220	ASP	-	expression tag	UNP A0AA49X976
B	1221	GLY	-	expression tag	UNP A0AA49X976
B	1222	GLN	-	expression tag	UNP A0AA49X976
B	1223	ALA	-	expression tag	UNP A0AA49X976
B	1224	TYR	-	expression tag	UNP A0AA49X976
B	1225	VAL	-	expression tag	UNP A0AA49X976
B	1226	ARG	-	expression tag	UNP A0AA49X976
B	1227	LYS	-	expression tag	UNP A0AA49X976
B	1228	ASP	-	expression tag	UNP A0AA49X976
B	1229	GLY	-	expression tag	UNP A0AA49X976
B	1230	GLU	-	expression tag	UNP A0AA49X976
B	1231	TRP	-	expression tag	UNP A0AA49X976
B	1232	VAL	-	expression tag	UNP A0AA49X976
B	1233	LEU	-	expression tag	UNP A0AA49X976

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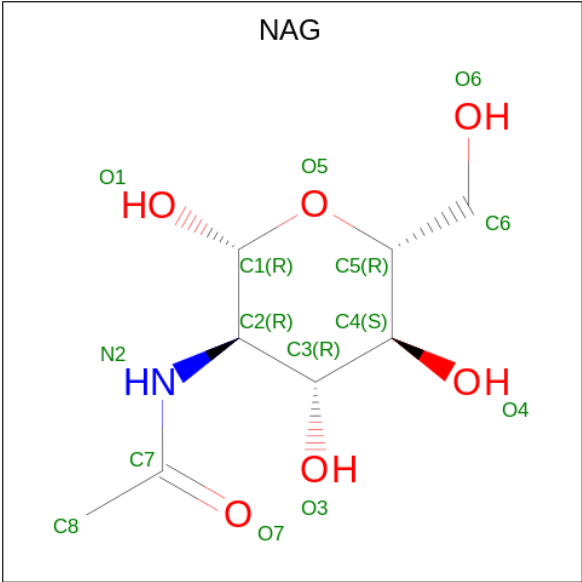
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B	1234	LEU	-	expression tag	UNP A0AA49X976
B	1235	SER	-	expression tag	UNP A0AA49X976
B	1236	THR	-	expression tag	UNP A0AA49X976
B	1237	PHE	-	expression tag	UNP A0AA49X976
B	1238	LEU	-	expression tag	UNP A0AA49X976
B	1239	GLY	-	expression tag	UNP A0AA49X976
B	1240	HIS	-	expression tag	UNP A0AA49X976
B	1241	HIS	-	expression tag	UNP A0AA49X976
B	1242	HIS	-	expression tag	UNP A0AA49X976
B	1243	HIS	-	expression tag	UNP A0AA49X976
B	1244	HIS	-	expression tag	UNP A0AA49X976
B	1245	HIS	-	expression tag	UNP A0AA49X976
B	1246	HIS	-	expression tag	UNP A0AA49X976
B	1247	HIS	-	expression tag	UNP A0AA49X976
C	68	ILE	LEU	conflict	UNP A0AA49X976
C	111	ASP	ASN	conflict	UNP A0AA49X976
C	147	ARG	LYS	conflict	UNP A0AA49X976
C	176	LEU	PHE	conflict	UNP A0AA49X976
C	177	MET	ILE	conflict	UNP A0AA49X976
C	222	ALA	VAL	conflict	UNP A0AA49X976
C	292	SER	ALA	conflict	UNP A0AA49X976
C	324	GLU	GLN	conflict	UNP A0AA49X976
C	346	THR	ARG	conflict	UNP A0AA49X976
C	402	VAL	ILE	conflict	UNP A0AA49X976
C	486	PHE	LEU	conflict	UNP A0AA49X976
C	554	GLU	GLN	conflict	UNP A0AA49X976
C	627	ASN	ASP	conflict	UNP A0AA49X976
C	789	GLN	PRO	conflict	UNP A0AA49X976
C	982	PRO	LYS	conflict	UNP A0AA49X976
C	983	PRO	VAL	conflict	UNP A0AA49X976
C	1080	ASP	ASN	conflict	UNP A0AA49X976
C	1107	GLU	LYS	conflict	UNP A0AA49X976
C	1160	VAL	ILE	conflict	UNP A0AA49X976
C	1163	SER	GLY	conflict	UNP A0AA49X976
C	1187	LYS	ARG	conflict	UNP A0AA49X976
C	1208	GLY	-	expression tag	UNP A0AA49X976
C	1209	SER	-	expression tag	UNP A0AA49X976
C	1210	GLY	-	expression tag	UNP A0AA49X976
C	1211	SER	-	expression tag	UNP A0AA49X976
C	1212	GLY	-	expression tag	UNP A0AA49X976
C	1213	TYR	-	expression tag	UNP A0AA49X976
C	1214	ILE	-	expression tag	UNP A0AA49X976

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1215	PRO	-	expression tag	UNP A0AA49X976
C	1216	GLU	-	expression tag	UNP A0AA49X976
C	1217	ALA	-	expression tag	UNP A0AA49X976
C	1218	PRO	-	expression tag	UNP A0AA49X976
C	1219	ARG	-	expression tag	UNP A0AA49X976
C	1220	ASP	-	expression tag	UNP A0AA49X976
C	1221	GLY	-	expression tag	UNP A0AA49X976
C	1222	GLN	-	expression tag	UNP A0AA49X976
C	1223	ALA	-	expression tag	UNP A0AA49X976
C	1224	TYR	-	expression tag	UNP A0AA49X976
C	1225	VAL	-	expression tag	UNP A0AA49X976
C	1226	ARG	-	expression tag	UNP A0AA49X976
C	1227	LYS	-	expression tag	UNP A0AA49X976
C	1228	ASP	-	expression tag	UNP A0AA49X976
C	1229	GLY	-	expression tag	UNP A0AA49X976
C	1230	GLU	-	expression tag	UNP A0AA49X976
C	1231	TRP	-	expression tag	UNP A0AA49X976
C	1232	VAL	-	expression tag	UNP A0AA49X976
C	1233	LEU	-	expression tag	UNP A0AA49X976
C	1234	LEU	-	expression tag	UNP A0AA49X976
C	1235	SER	-	expression tag	UNP A0AA49X976
C	1236	THR	-	expression tag	UNP A0AA49X976
C	1237	PHE	-	expression tag	UNP A0AA49X976
C	1238	LEU	-	expression tag	UNP A0AA49X976
C	1239	GLY	-	expression tag	UNP A0AA49X976
C	1240	HIS	-	expression tag	UNP A0AA49X976
C	1241	HIS	-	expression tag	UNP A0AA49X976
C	1242	HIS	-	expression tag	UNP A0AA49X976
C	1243	HIS	-	expression tag	UNP A0AA49X976
C	1244	HIS	-	expression tag	UNP A0AA49X976
C	1245	HIS	-	expression tag	UNP A0AA49X976
C	1246	HIS	-	expression tag	UNP A0AA49X976
C	1247	HIS	-	expression tag	UNP A0AA49X976

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

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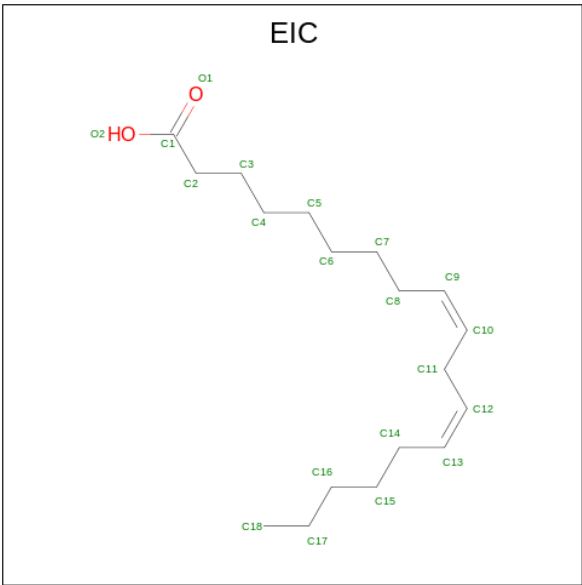
Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total 14	C 8	N 1	O 5	0
2	A	1	Total 14	C 8	N 1	O 5	0
2	A	1	Total 14	C 8	N 1	O 5	0
2	A	1	Total 14	C 8	N 1	O 5	0
2	B	1	Total 14	C 8	N 1	O 5	0
2	B	1	Total 14	C 8	N 1	O 5	0
2	B	1	Total 14	C 8	N 1	O 5	0
2	B	1	Total 14	C 8	N 1	O 5	0
2	B	1	Total 14	C 8	N 1	O 5	0
2	B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

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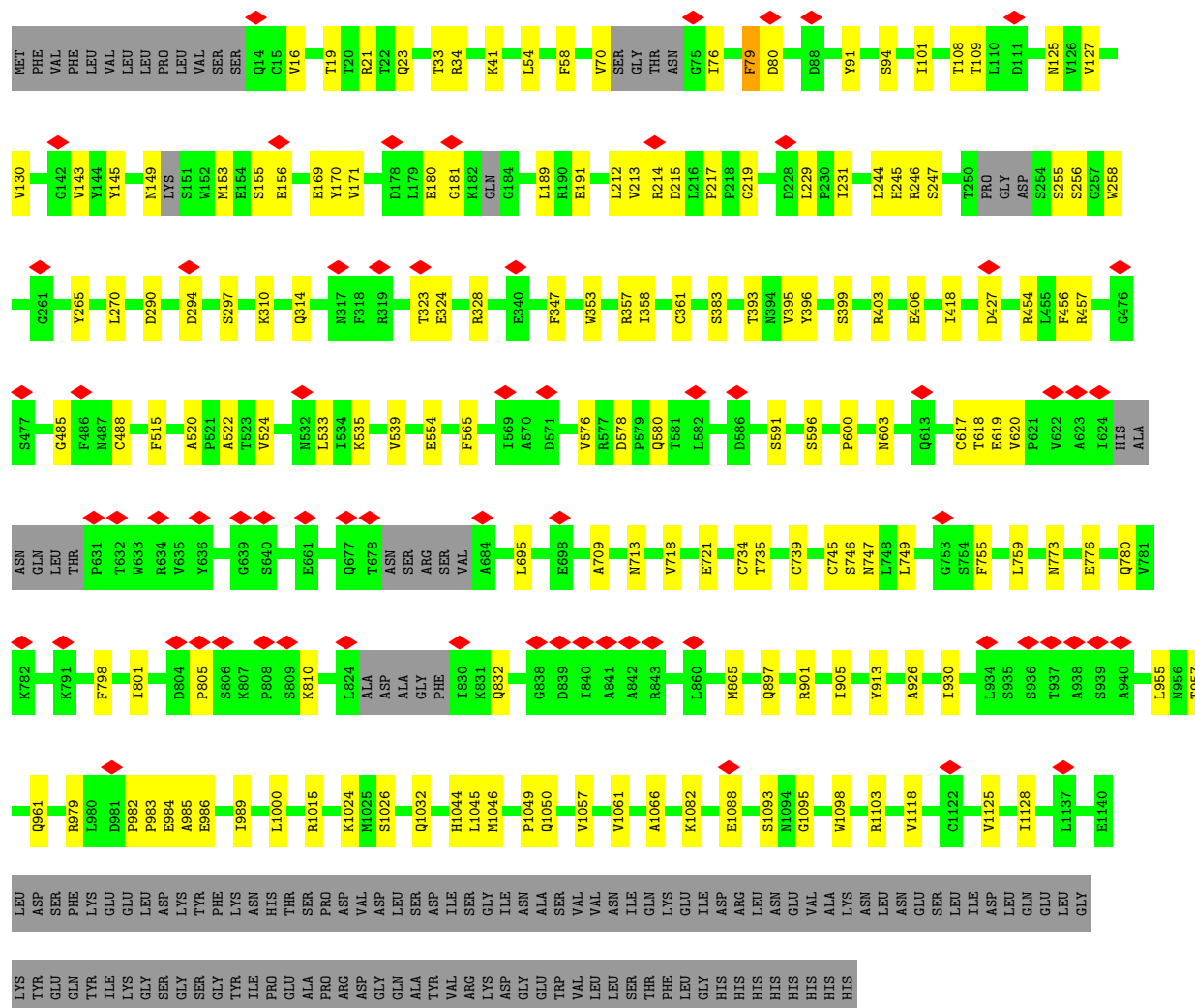
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Mol	Chain	Residues	Atoms				AltConf
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C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

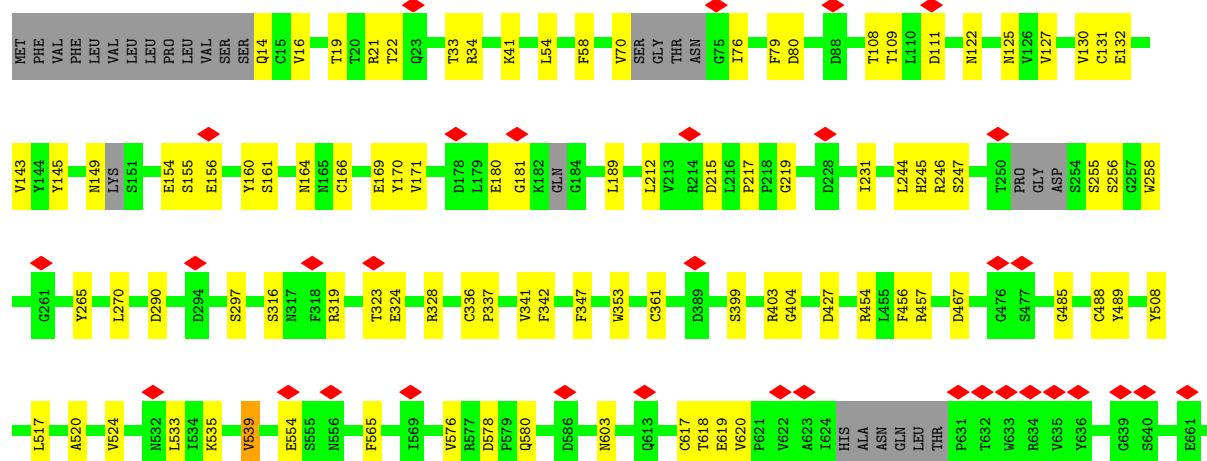
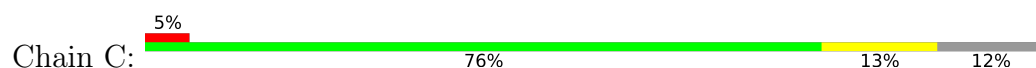
- Molecule 3 is LINOLEIC ACID (CCD ID: EIC) (formula: $C_{18}H_{32}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
3	A	1	Total	C	O	0
			20	18	2	
3	B	1	Total	C	O	0
			20	18	2	
3	C	1	Total	C	O	0
			20	18	2	



• Molecule 1: Spike glycoprotein



GLN	ALA	TYR	VAL	ARG	LYS	ASP	GLY	GLU	TRP	VAL	VAL	LEU	LEU	SER	THR	PHE	LEU	GLY	HIS	HIS	HIS	HIS	HIS																				
LEU	SER	ASP	ILE	SER	GLY	ILE	ASN	ALA	SER	SER	VAL	VAL	ASN	ASN	ILE	GLN	LYS	GLU	ILE	ASP	ARG	LEU	ASN	ASN	GLU	VAL	VAL	LYS	ASN	GLY	ASP	GLY	ASP	VAL	ASP	GLY							
R1015	K1024	K1034	H1044	L1045	M1046	Q1050	V1057	V1061	A1066	K1082	E1088	S1093	H1097	W1098	R1103	I1110	V1118	V1125	L1137	E1140	LEU	ASP	SER	PHE	LYS	GLU	GLU	LEU	ASP	LYS	TYR	PHE	LYS	ASN	HIS	THR	SER	PRO	ARG	ASP	VAL	ASP	
L824	ALA	ASP	ALA	GLY	PHE	I830	G838	D839	I840	A841	A842	R843	L861	M865	L890	Q897	R901	Y913	A926	I930	L934	S935	S936	T937	A938	S939	A940	L955	N956	T957	Q961	L973	I976	L980	D981	P982	P983	E984	A985	E986	V987	Q988	I989
Q677	T678	ASN	SER	ARG	SER	VAL	A684	L695	E698	A709	N713	V718	E721	C734	T735	M736	C739	C745	S746	N747	Y752	G753	S754	F755	L759	N773	V777	Q789	I790	K791	D792	F798	I801	D804	P805	S806	K807	P808	S809	K810	D816		

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	20175	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.172	Depositor
Minimum map value	-0.079	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.035	Depositor
Map size (Å)	424.96, 424.96, 424.96	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.66, 1.66, 1.66	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, EIC

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	0.12	0/8800	0.28	0/11976
1	B	0.11	0/8800	0.27	0/11976
1	C	0.12	0/8800	0.27	0/11976
All	All	0.11	0/26400	0.27	0/35928

There are no bond length outliers.

There are no bond angle outliers.

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	8604	0	8379	120	0
1	B	8604	0	8379	111	0
1	C	8604	0	8379	107	0
2	A	252	0	234	5	0
2	B	252	0	234	5	0
2	C	252	0	234	5	0
3	A	20	0	31	2	0
3	B	20	0	31	0	0
3	C	20	0	31	0	0
All	All	26628	0	25932	317	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 6.

The worst 5 of 317 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:391:CYS:HA	1:A:525:CYS:HB3	1.46	0.97
1:C:14:GLN:HE22	1:C:161:SER:HA	1.55	0.70
1:A:14:GLN:HE22	1:A:161:SER:HA	1.56	0.69
1:A:70:VAL:HG12	1:A:76:ILE:H	1.56	0.69
1:B:70:VAL:HG12	1:B:76:ILE:H	1.59	0.68

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	1086/1247 (87%)	1021 (94%)	65 (6%)	0	100	100
1	B	1086/1247 (87%)	1026 (94%)	60 (6%)	0	100	100
1	C	1086/1247 (87%)	1028 (95%)	58 (5%)	0	100	100
All	All	3258/3741 (87%)	3075 (94%)	183 (6%)	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	961/1088 (88%)	958 (100%)	3 (0%)	91	96
1	B	961/1088 (88%)	960 (100%)	1 (0%)	92	97
1	C	961/1088 (88%)	958 (100%)	3 (0%)	91	96
All	All	2883/3264 (88%)	2876 (100%)	7 (0%)	91	97

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	79	PHE
1	C	22	THR
1	C	816	ASP
1	C	539	VAL
1	A	539	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	783	GLN
1	C	953	GLN
1	B	1060	HIS
1	C	686	GLN
1	B	953	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

57 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	A	1302	1	14,14,15	0.23	0	17,19,21	0.38	0
2	NAG	B	1304	1	14,14,15	0.20	0	17,19,21	0.41	0
2	NAG	B	1309	1	14,14,15	0.23	0	17,19,21	0.51	0
2	NAG	B	1312	1	14,14,15	0.36	0	17,19,21	0.52	0
2	NAG	C	1316	1	14,14,15	0.24	0	17,19,21	0.47	0
2	NAG	B	1311	1	14,14,15	0.23	0	17,19,21	0.41	0
2	NAG	C	1302	1	14,14,15	0.23	0	17,19,21	0.39	0
2	NAG	C	1305	1	14,14,15	0.23	0	17,19,21	0.46	0
2	NAG	C	1309	1	14,14,15	0.23	0	17,19,21	0.49	0
2	NAG	B	1303	1	14,14,15	0.22	0	17,19,21	0.43	0
2	NAG	B	1315	1	14,14,15	0.19	0	17,19,21	0.42	0
2	NAG	A	1309	1	14,14,15	0.23	0	17,19,21	0.52	0
2	NAG	A	1306	1	14,14,15	0.20	0	17,19,21	0.47	0
2	NAG	B	1310	1	14,14,15	0.21	0	17,19,21	0.46	0
2	NAG	A	1307	1	14,14,15	0.22	0	17,19,21	0.49	0
2	NAG	A	1311	1	14,14,15	0.23	0	17,19,21	0.41	0
3	EIC	B	1319	-	19,19,19	0.59	0	19,19,19	0.56	0
2	NAG	C	1310	1	14,14,15	0.21	0	17,19,21	0.47	0
2	NAG	C	1312	1	14,14,15	0.35	0	17,19,21	0.51	0
2	NAG	A	1315	1	14,14,15	0.19	0	17,19,21	0.41	0
2	NAG	C	1318	1	14,14,15	0.22	0	17,19,21	0.44	0
2	NAG	A	1310	1	14,14,15	0.22	0	17,19,21	0.46	0
2	NAG	C	1307	1	14,14,15	0.21	0	17,19,21	0.47	0
2	NAG	C	1317	1	14,14,15	0.19	0	17,19,21	0.44	0
2	NAG	C	1306	1	14,14,15	0.20	0	17,19,21	0.45	0
2	NAG	C	1314	1	14,14,15	0.26	0	17,19,21	0.45	0
2	NAG	A	1308	1	14,14,15	0.22	0	17,19,21	0.46	0
2	NAG	A	1313	1	14,14,15	0.28	0	17,19,21	0.34	0
2	NAG	B	1314	1	14,14,15	0.25	0	17,19,21	0.45	0
2	NAG	A	1303	1	14,14,15	0.23	0	17,19,21	0.43	0
2	NAG	B	1308	1	14,14,15	0.20	0	17,19,21	0.45	0
2	NAG	B	1316	1	14,14,15	0.25	0	17,19,21	0.47	0
2	NAG	B	1302	1	14,14,15	0.24	0	17,19,21	0.39	0
2	NAG	B	1317	1	14,14,15	0.18	0	17,19,21	0.44	0
2	NAG	C	1313	1	14,14,15	0.27	0	17,19,21	0.35	0
2	NAG	B	1306	1	14,14,15	0.20	0	17,19,21	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	C	1308	1	14,14,15	0.20	0	17,19,21	0.45	0
2	NAG	A	1316	1	14,14,15	0.26	0	17,19,21	0.48	0
2	NAG	B	1305	1	14,14,15	0.24	0	17,19,21	0.45	0
2	NAG	B	1318	1	14,14,15	0.20	0	17,19,21	0.45	0
3	EIC	C	1319	-	19,19,19	0.59	0	19,19,19	0.56	0
2	NAG	B	1301	1	14,14,15	0.49	0	17,19,21	0.69	1 (5%)
2	NAG	B	1307	1	14,14,15	0.21	0	17,19,21	0.49	0
2	NAG	B	1313	1	14,14,15	0.28	0	17,19,21	0.34	0
2	NAG	A	1305	1	14,14,15	0.24	0	17,19,21	0.46	0
3	EIC	A	1319	-	19,19,19	0.59	0	19,19,19	0.57	0
2	NAG	A	1304	1	14,14,15	0.19	0	17,19,21	0.41	0
2	NAG	C	1301	1	14,14,15	0.39	0	17,19,21	0.61	1 (5%)
2	NAG	C	1315	1	14,14,15	0.20	0	17,19,21	0.41	0
2	NAG	A	1317	1	14,14,15	0.19	0	17,19,21	0.45	0
2	NAG	A	1312	1	14,14,15	0.35	0	17,19,21	0.52	0
2	NAG	A	1318	1	14,14,15	0.23	0	17,19,21	0.44	0
2	NAG	C	1311	1	14,14,15	0.24	0	17,19,21	0.41	0
2	NAG	A	1301	1	14,14,15	0.42	0	17,19,21	0.69	1 (5%)
2	NAG	A	1314	1	14,14,15	0.26	0	17,19,21	0.46	0
2	NAG	C	1304	1	14,14,15	0.20	0	17,19,21	0.39	0
2	NAG	C	1303	1	14,14,15	0.22	0	17,19,21	0.44	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	A	1302	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1304	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1309	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1312	1	-	2/6/23/26	0/1/1/1
2	NAG	C	1316	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1311	1	-	2/6/23/26	0/1/1/1
2	NAG	C	1302	1	-	2/6/23/26	0/1/1/1
2	NAG	C	1305	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1309	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1303	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1315	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1309	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	1306	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1310	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1307	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1311	1	-	1/6/23/26	0/1/1/1
3	EIC	B	1319	-	-	1/17/17/17	-
2	NAG	C	1310	1	-	2/6/23/26	0/1/1/1
2	NAG	C	1312	1	-	1/6/23/26	0/1/1/1
2	NAG	A	1315	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1318	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1310	1	-	2/6/23/26	0/1/1/1
2	NAG	C	1307	1	-	2/6/23/26	0/1/1/1
2	NAG	C	1317	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1306	1	-	2/6/23/26	0/1/1/1
2	NAG	C	1314	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1308	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1313	1	-	1/6/23/26	0/1/1/1
2	NAG	B	1314	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1303	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1308	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1316	1	-	1/6/23/26	0/1/1/1
2	NAG	B	1302	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1317	1	-	2/6/23/26	0/1/1/1
2	NAG	C	1313	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1306	1	-	2/6/23/26	0/1/1/1
2	NAG	C	1308	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1316	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1305	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1318	1	-	2/6/23/26	0/1/1/1
3	EIC	C	1319	-	-	1/17/17/17	-
2	NAG	B	1301	1	-	3/6/23/26	0/1/1/1
2	NAG	B	1307	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1313	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1305	1	-	0/6/23/26	0/1/1/1
3	EIC	A	1319	-	-	1/17/17/17	-
2	NAG	A	1304	1	-	2/6/23/26	0/1/1/1
2	NAG	C	1301	1	-	2/6/23/26	0/1/1/1
2	NAG	C	1315	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	1317	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1312	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1318	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1311	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1301	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1314	1	-	2/6/23/26	0/1/1/1
2	NAG	C	1304	1	-	2/6/23/26	0/1/1/1
2	NAG	C	1303	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1301	NAG	C1-O5-C5	2.47	115.54	112.19
2	B	1301	NAG	C1-O5-C5	2.43	115.49	112.19
2	C	1301	NAG	C1-O5-C5	2.11	115.05	112.19

There are no chirality outliers.

5 of 82 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1309	NAG	O5-C5-C6-O6
2	C	1302	NAG	C4-C5-C6-O6
2	A	1302	NAG	C4-C5-C6-O6
2	A	1301	NAG	O5-C5-C6-O6
2	C	1307	NAG	C4-C5-C6-O6

There are no ring outliers.

13 monomers are involved in 17 short contacts:

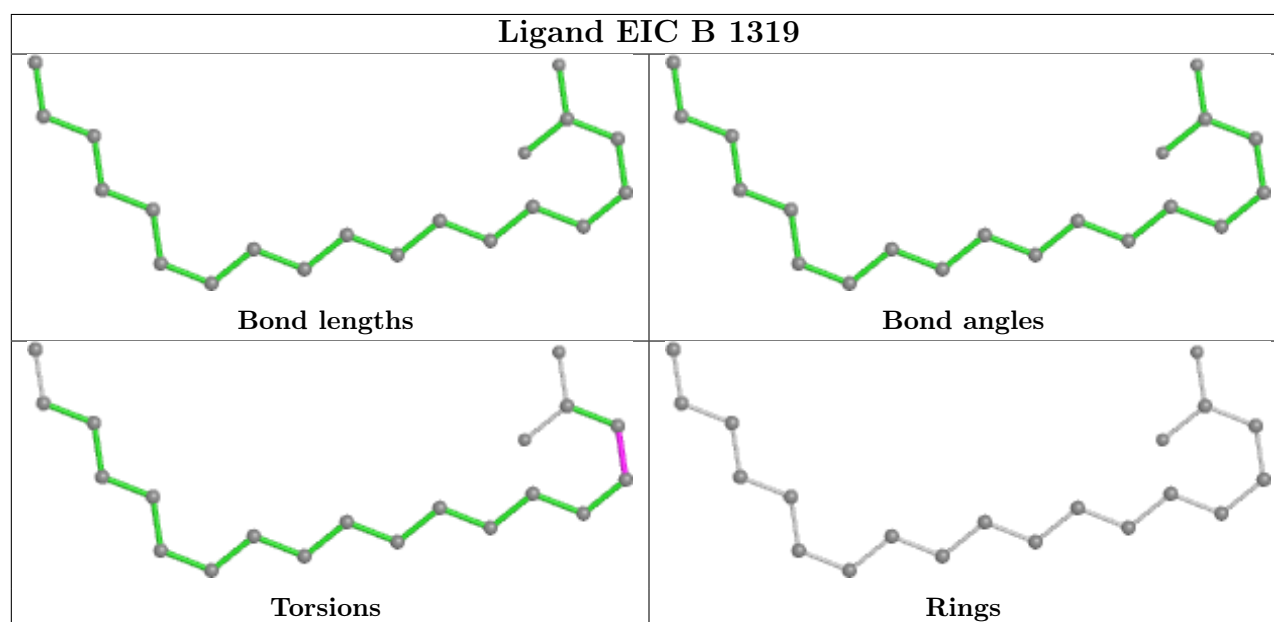
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1304	NAG	2	0
2	B	1312	NAG	1	0
2	A	1307	NAG	1	0
2	C	1312	NAG	1	0
2	C	1314	NAG	1	0
2	B	1314	NAG	1	0
2	B	1307	NAG	1	0
3	A	1319	EIC	2	0
2	A	1304	NAG	2	0

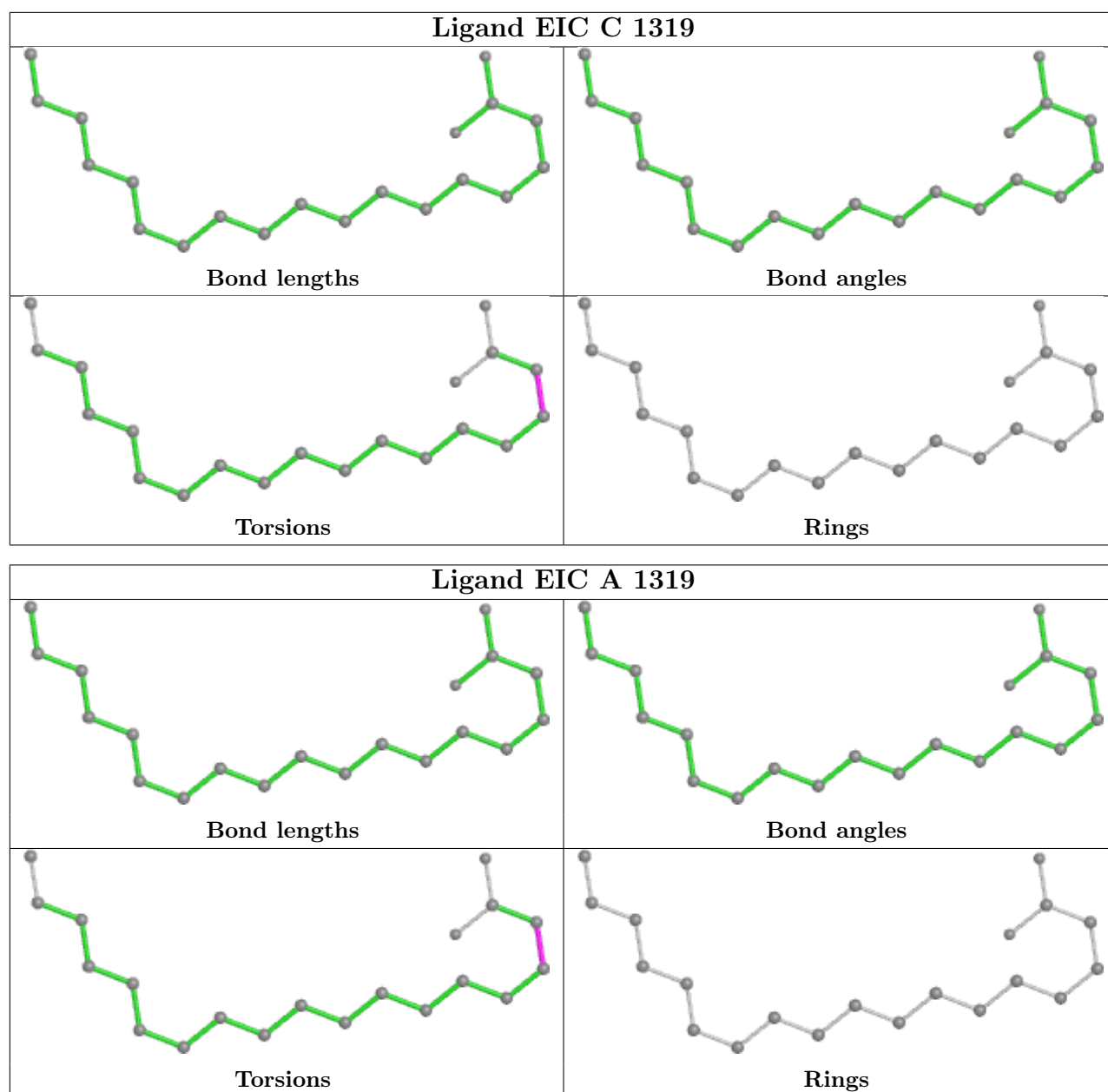
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1301	NAG	2	0
2	A	1312	NAG	1	0
2	A	1314	NAG	1	0
2	C	1304	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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.

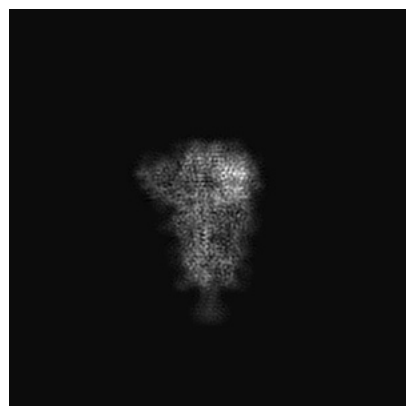
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62143. These allow visual inspection of the internal detail of the map and identification of artifacts.

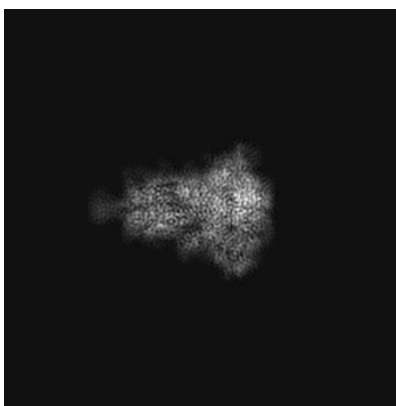
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

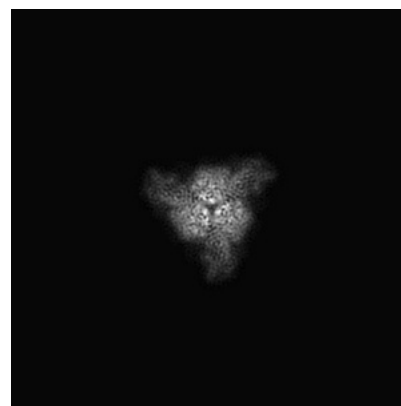
6.1.1 Primary map



X

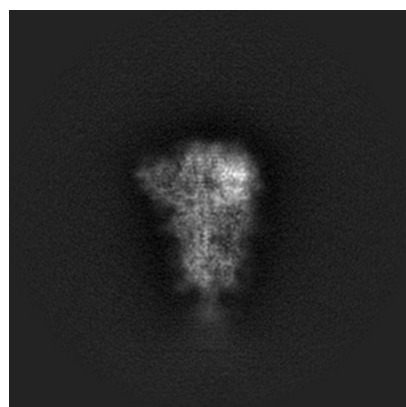


Y

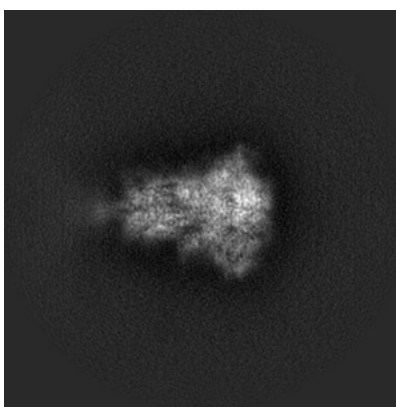


Z

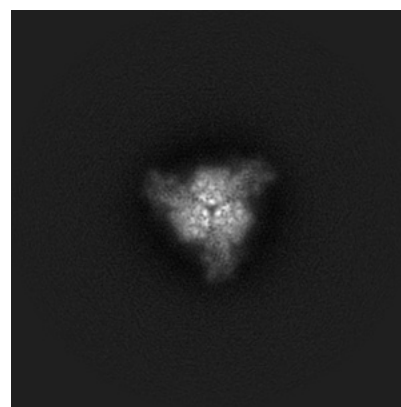
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices [i](#)

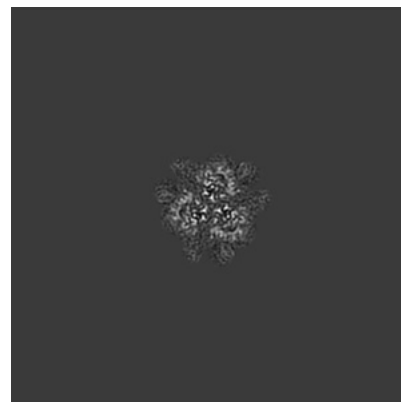
6.2.1 Primary map



X Index: 128

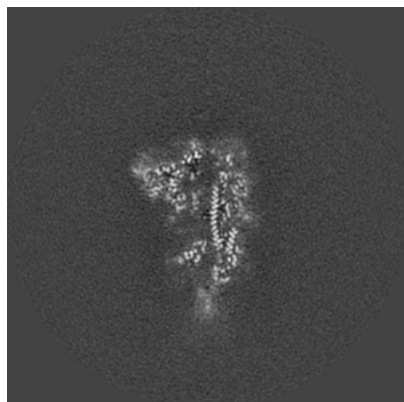


Y Index: 128

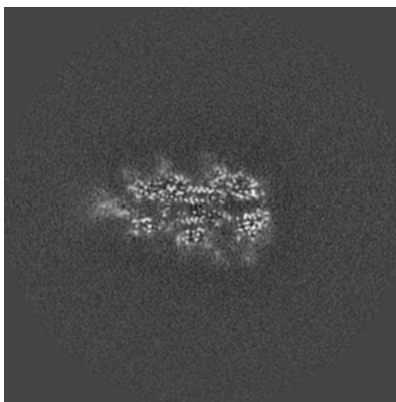


Z Index: 128

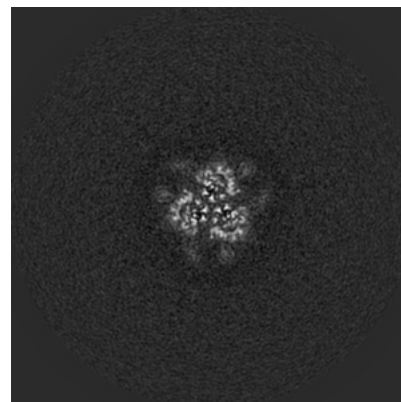
6.2.2 Raw map



X Index: 128



Y Index: 128



Z Index: 128

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

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 136

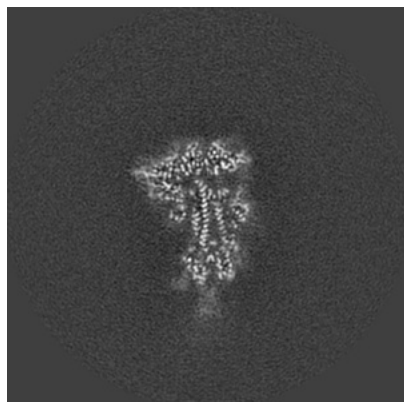


Y Index: 125

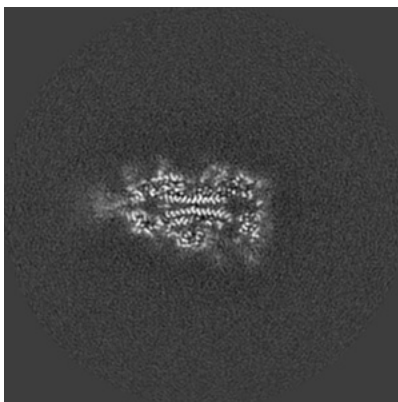


Z Index: 151

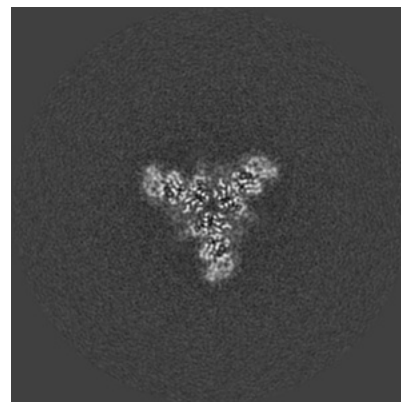
6.3.2 Raw map



X Index: 133



Y Index: 126

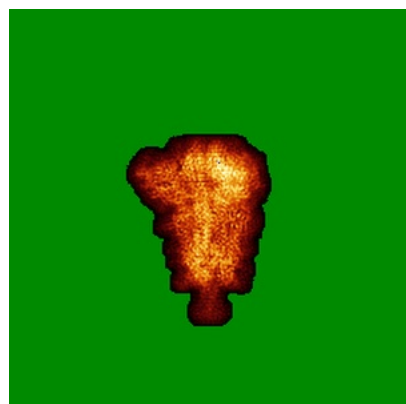


Z Index: 151

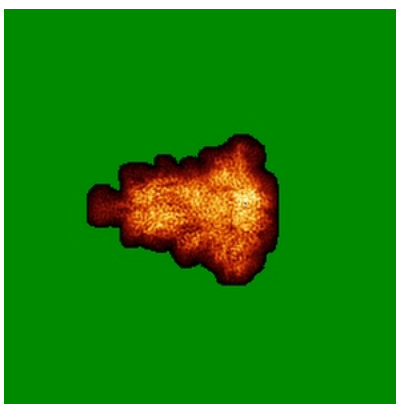
The images above show the largest variance slices of the map in three orthogonal directions.

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

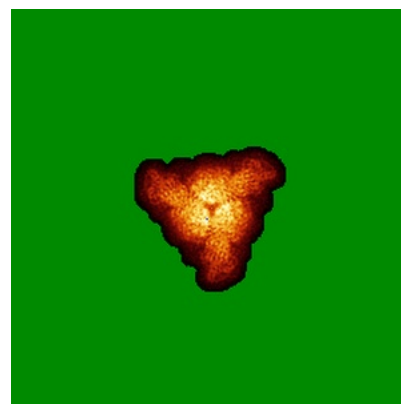
6.4.1 Primary map



X

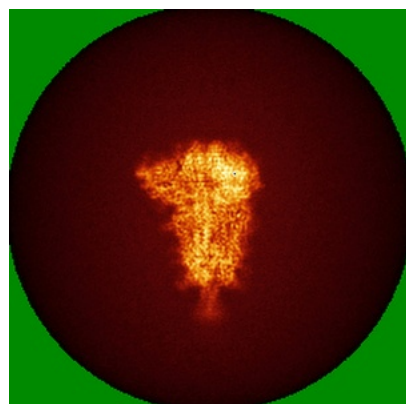


Y

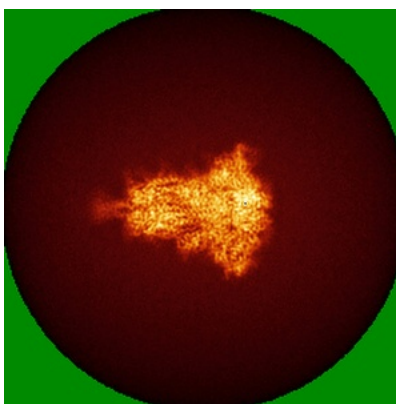


Z

6.4.2 Raw map



X



Y

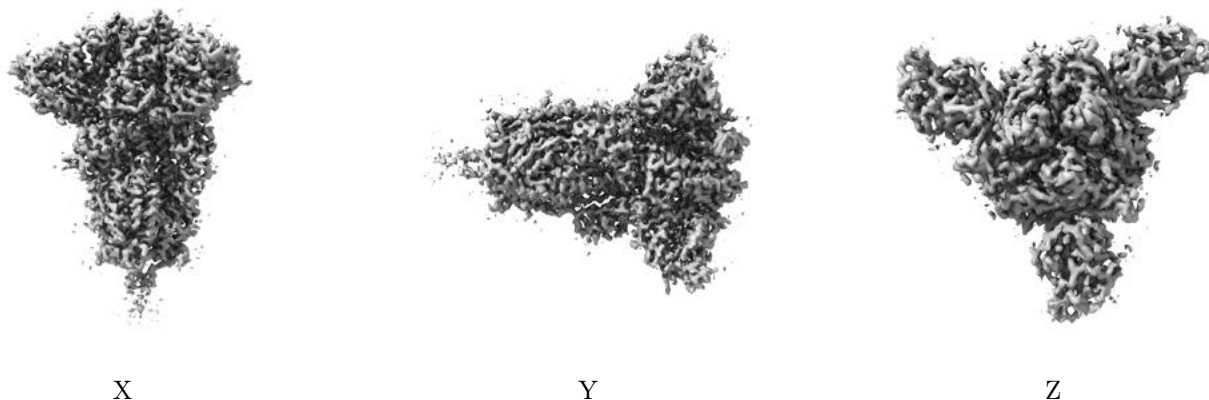


Z

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

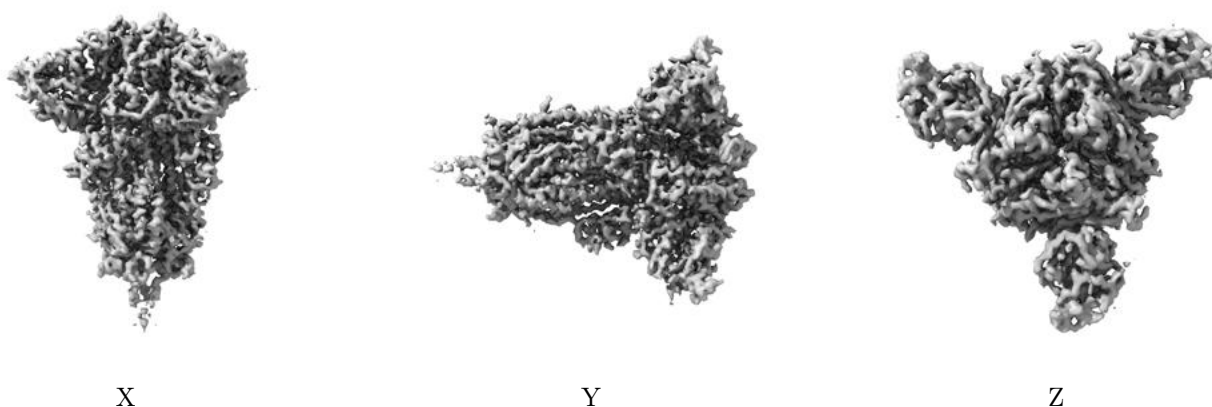
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.035. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

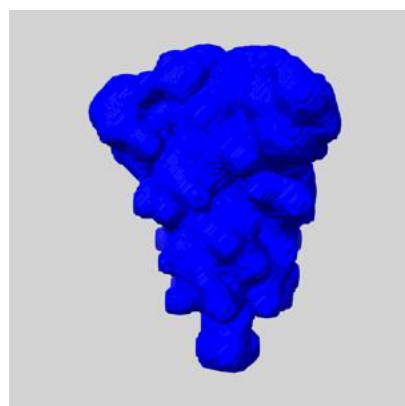
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

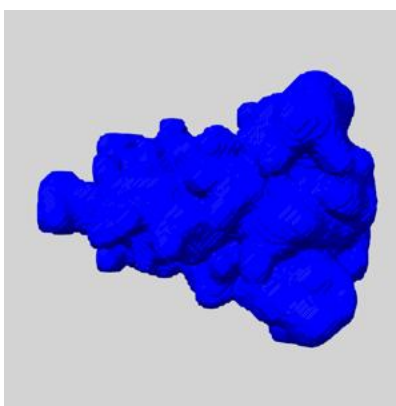
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

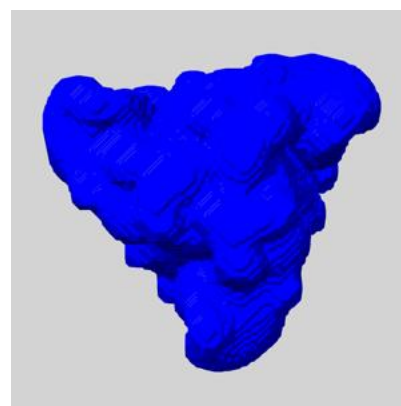
6.6.1 emd_62143_msk_1.map [i](#)



X



Y

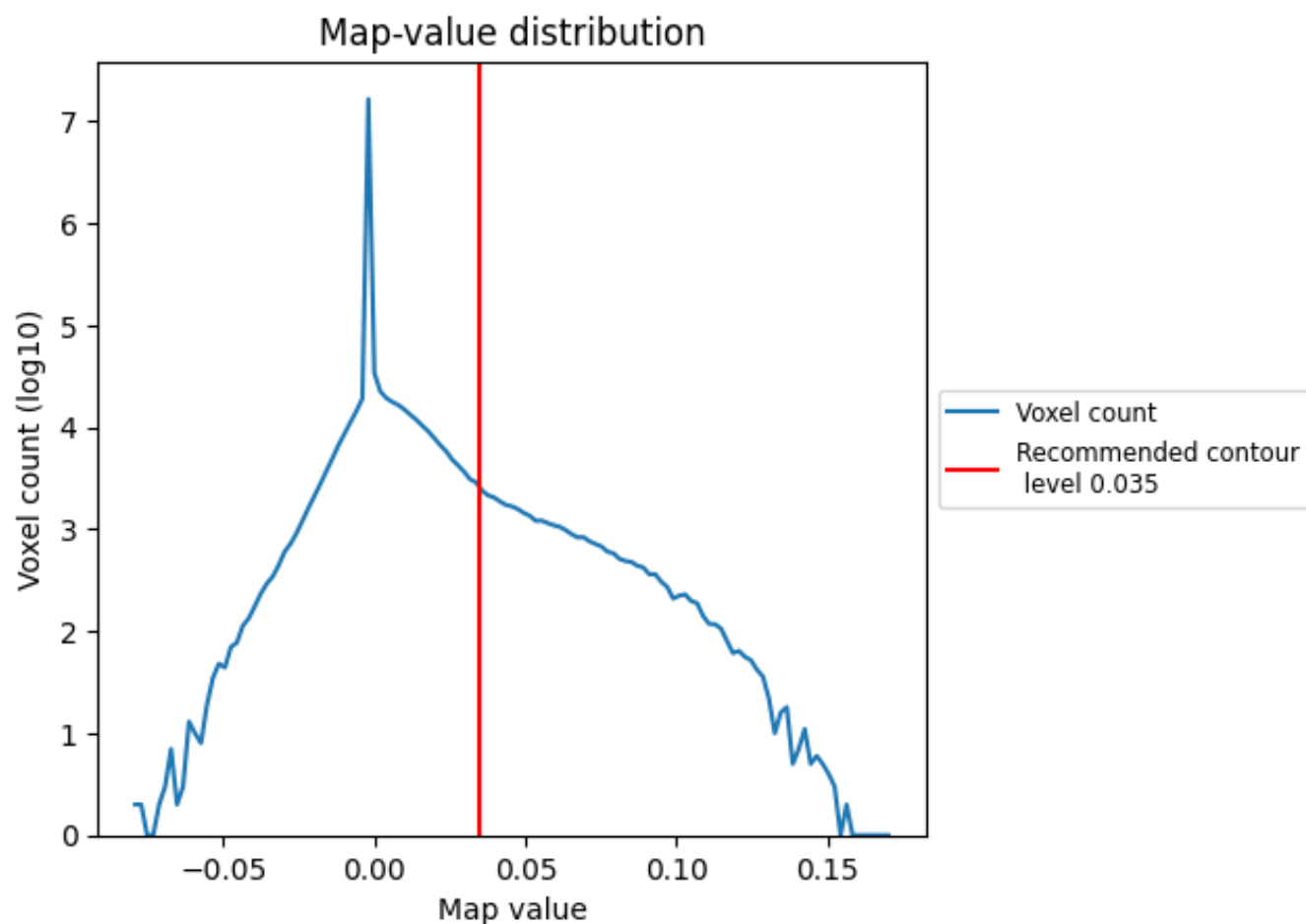


Z

7 Map analysis [i](#)

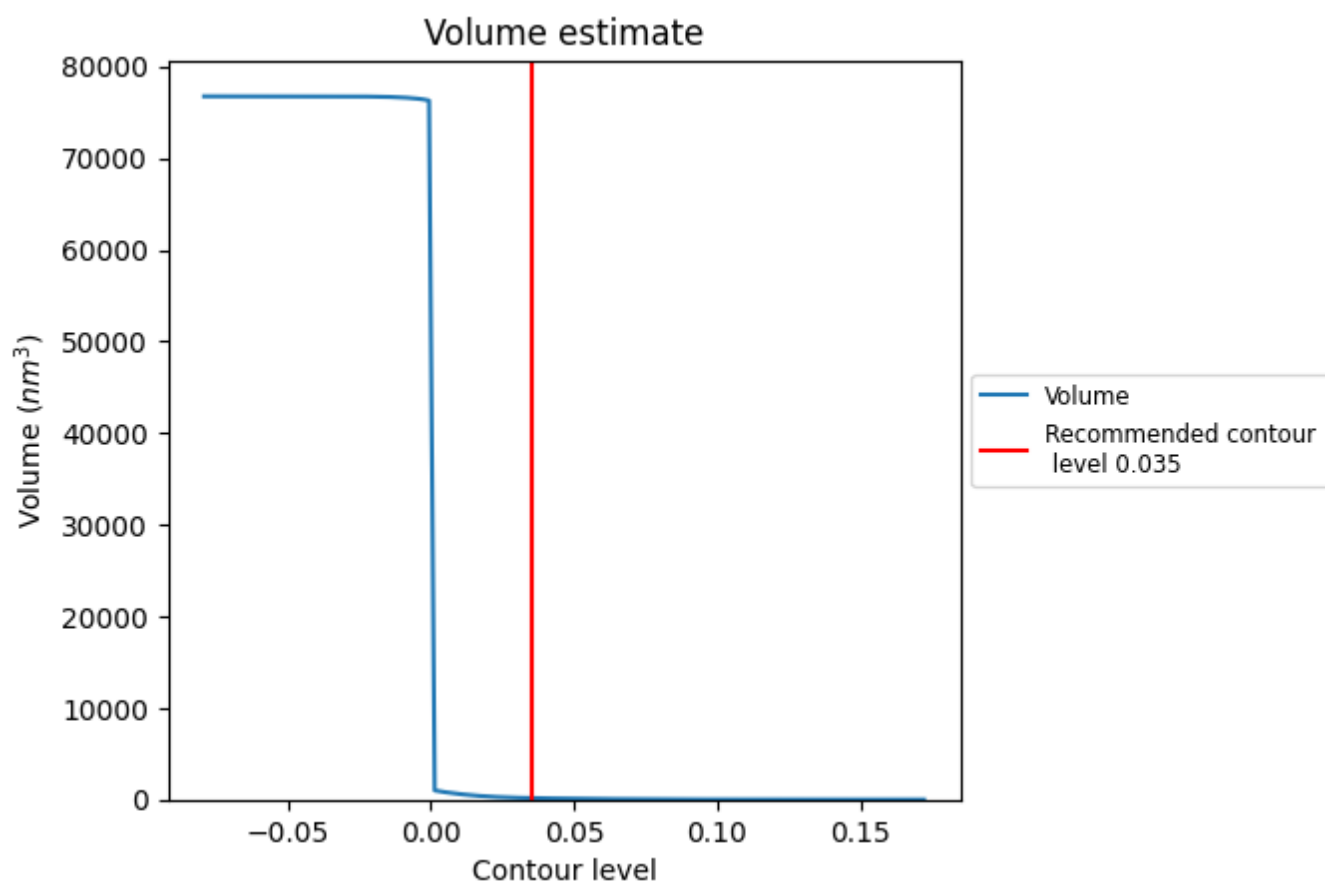
This section contains the results of statistical analysis of the map.

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.

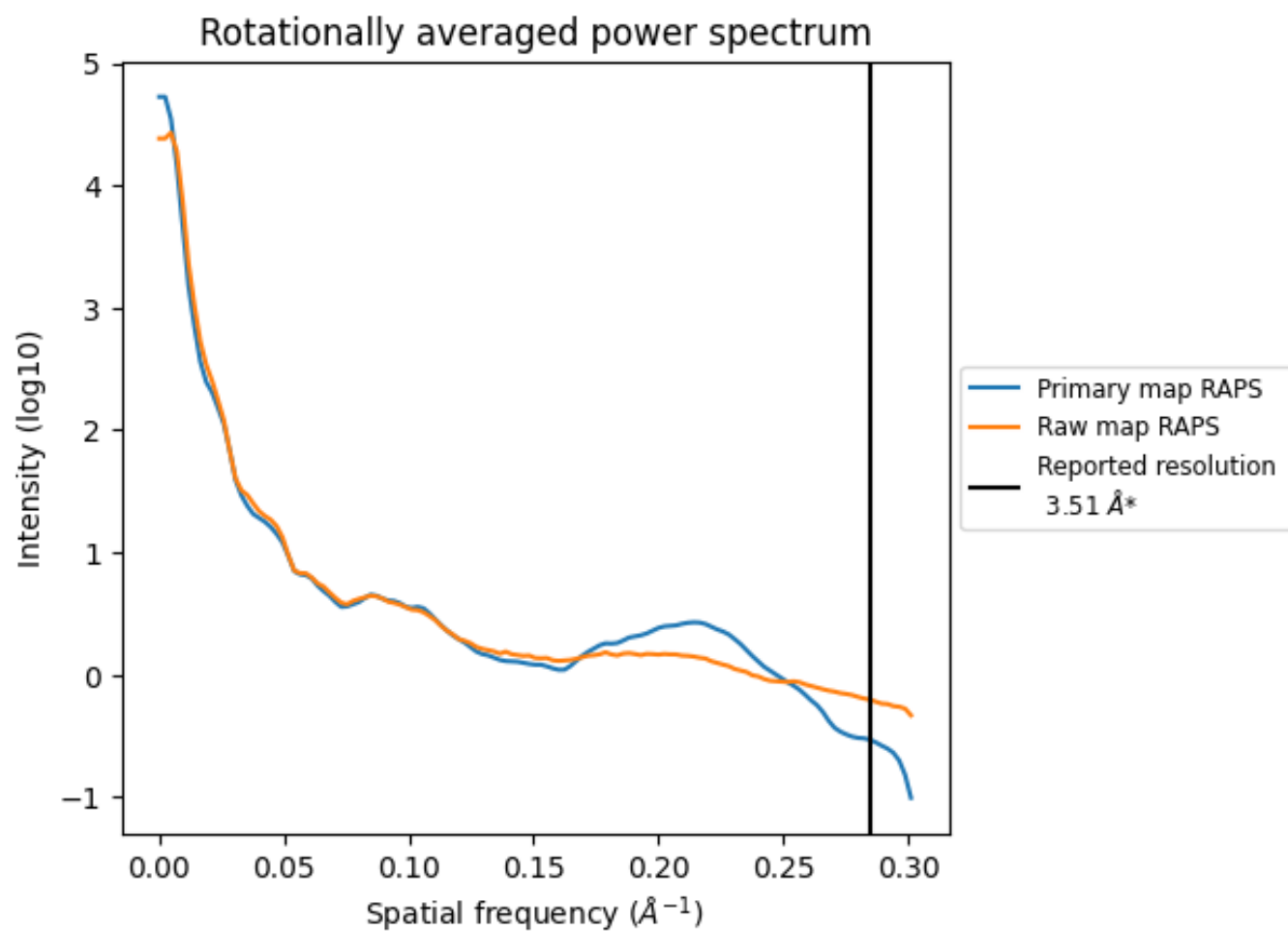
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 162 nm^3 ; this corresponds to an approximate mass of 146 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 ⓘ

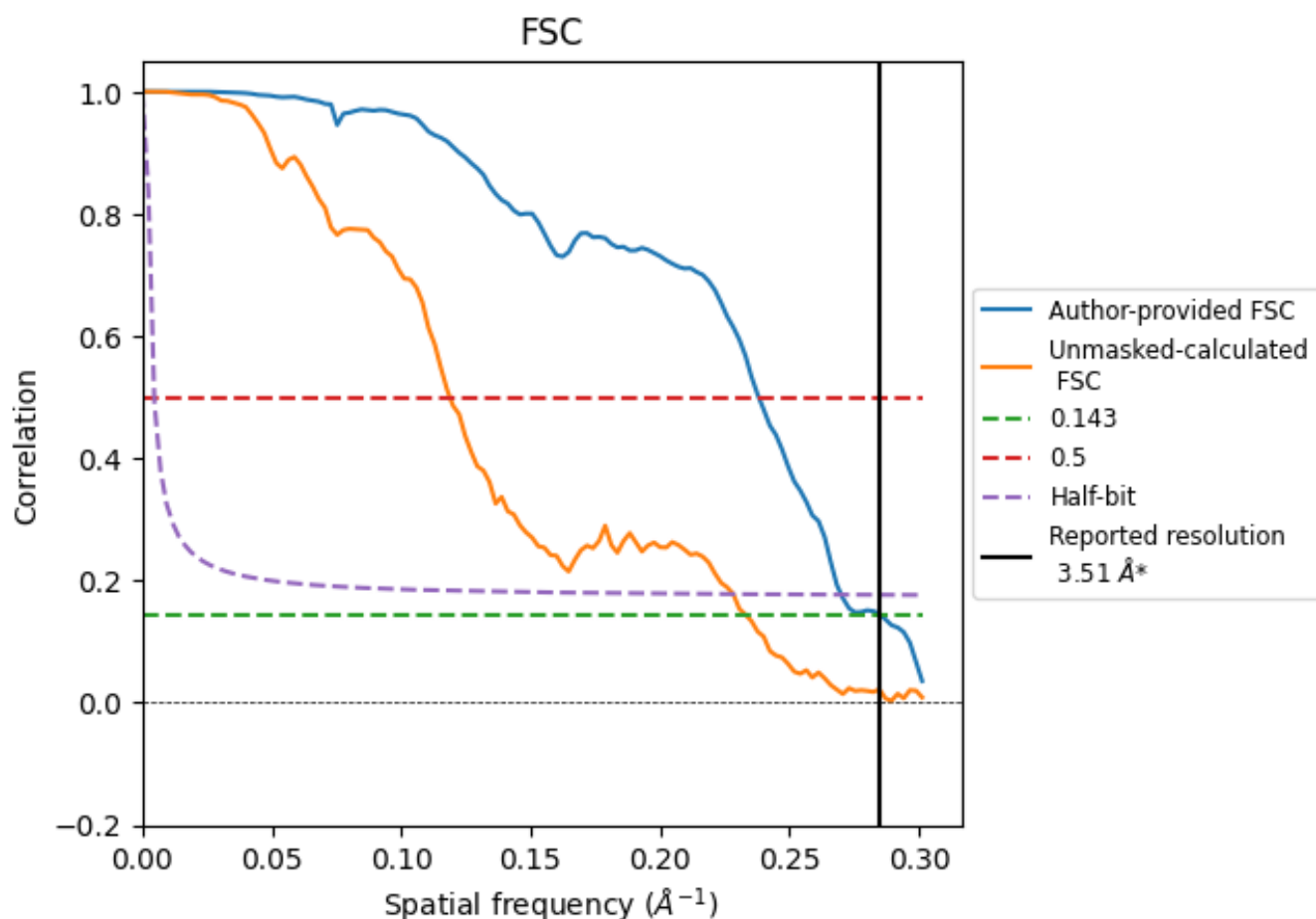


*Reported resolution corresponds to spatial frequency of 0.285 Å⁻¹

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 0.285 \AA^{-1}

8.2 Resolution estimates [i](#)

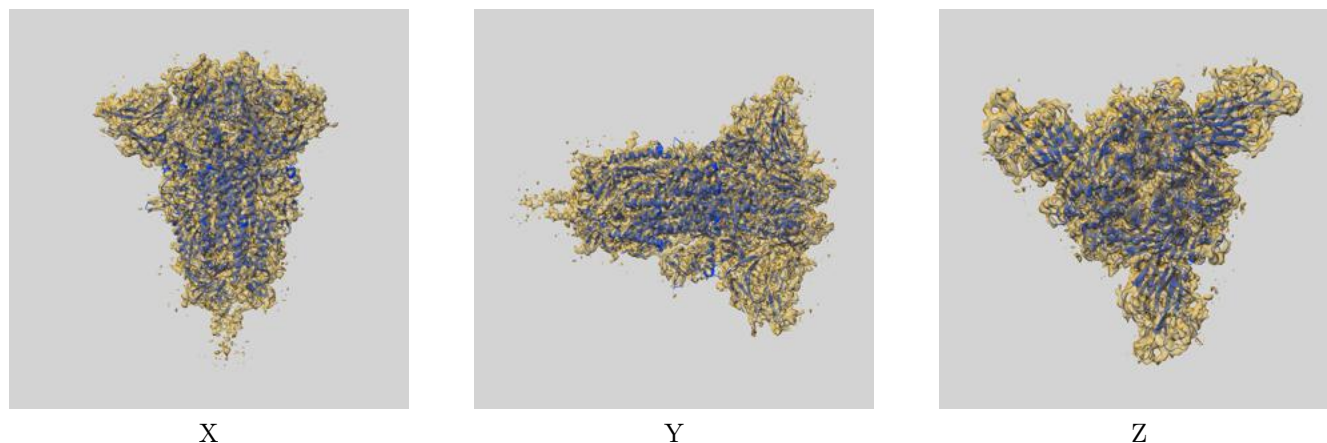
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.51	-	-
Author-provided FSC curve	3.50	4.20	3.70
Unmasked-calculated*	4.29	8.42	4.38

*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 4.29 differs from the reported value 3.51 by more than 10 %

9 Map-model fit [i](#)

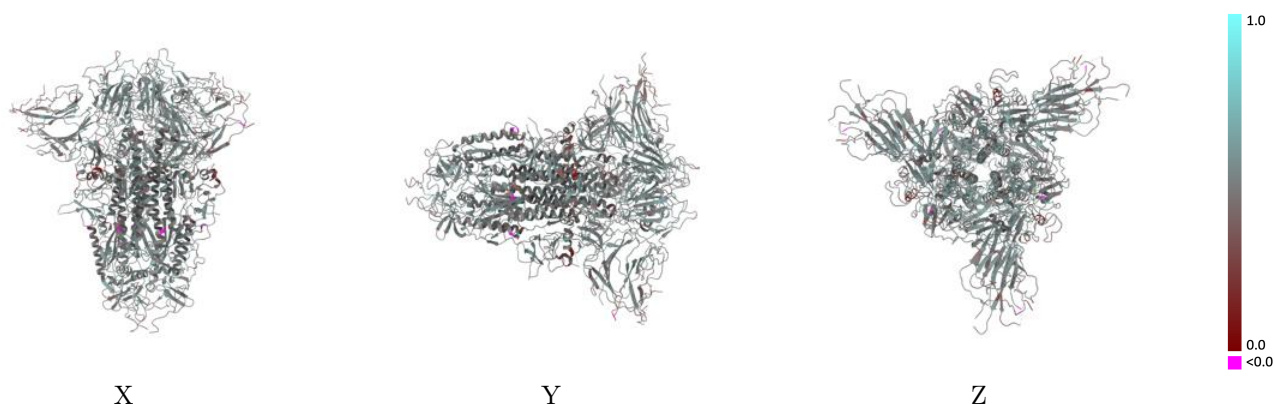
This section contains information regarding the fit between EMDB map EMD-62143 and PDB model 9K6Z. Per-residue inclusion information can be found in section [3](#) on page [12](#).

9.1 Map-model overlay [i](#)



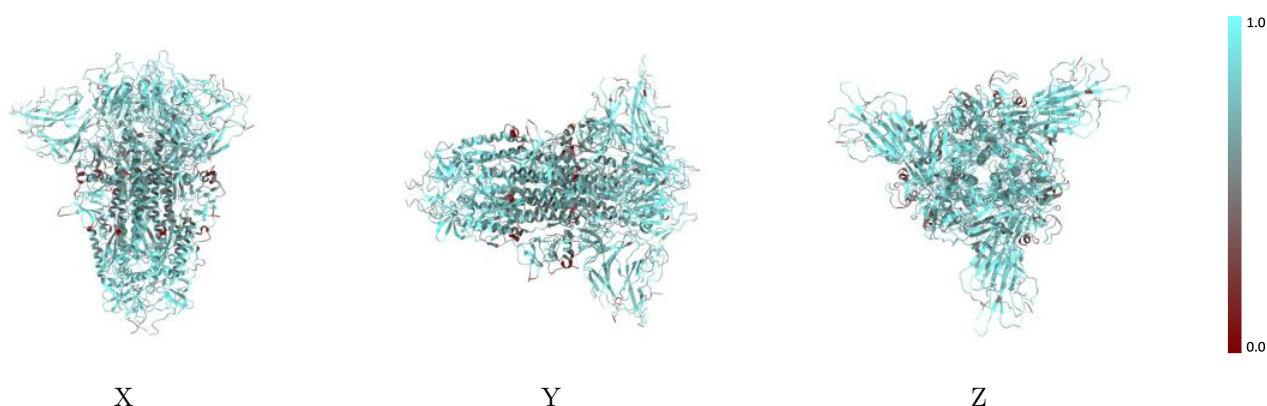
The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



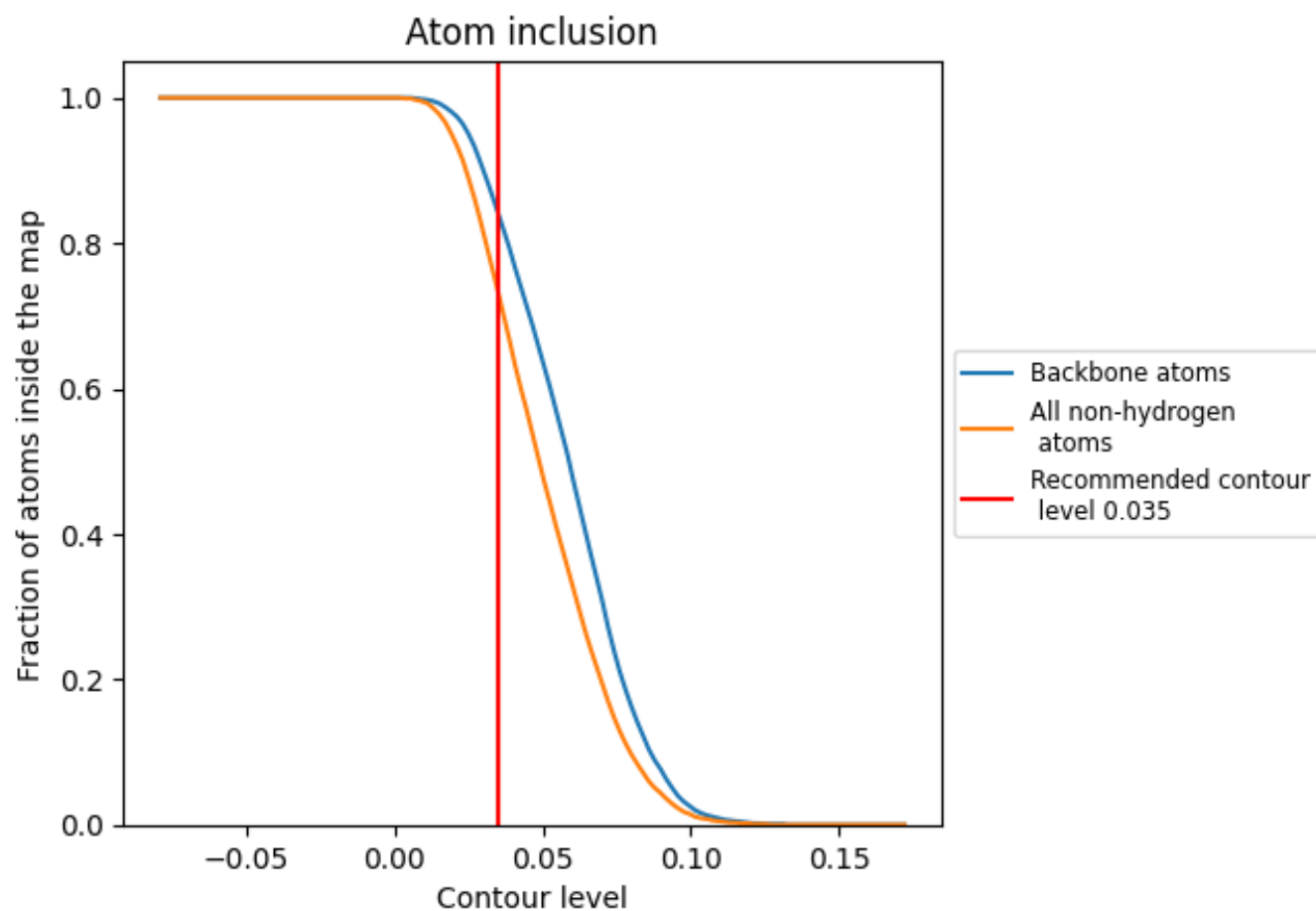
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.035).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 73% 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 (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7310	<div></div> 0.4950
A	<div></div> 0.7320	<div></div> 0.4960
B	<div></div> 0.7320	<div></div> 0.4960
C	<div></div> 0.7290	<div></div> 0.4940

