wwPDB EM Validation Summary Report

Nov 20, 2022 – 09:08 PM JST

PDB ID	:	7CN4
EMDB ID	:	EMD-30416
Title	:	Cryo-EM structure of bat RaTG13 spike glycoprotein
Authors	:	Wang, X.; Zhang, S.; Qiao, S.; Yu, J.; Zeng, J.; Tian, L.
Deposited on	:	2020-07-30
Resolution	:	2.93 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:

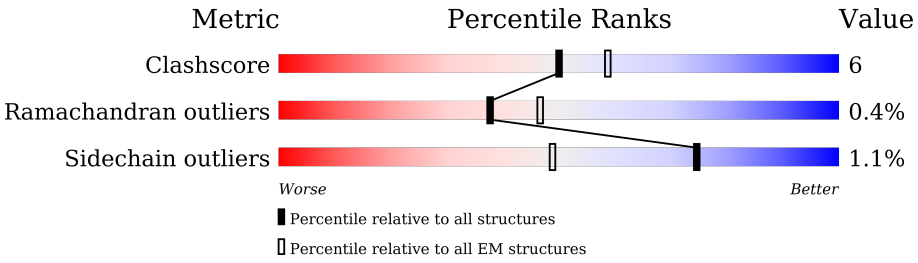
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (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 2.93 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	1267	75% 13% 12%
1	B	1267	75% 13% 12%
1	C	1267	74% 14% 12%
2	D	2	100%
2	E	2	50% 50%
2	F	2	50% 50%
2	G	2	50% 50%
2	H	2	50% 50%

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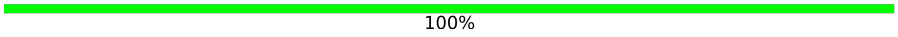
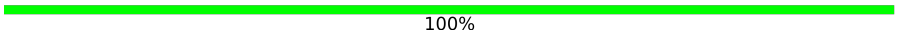
Mol	Chain	Length	Quality of chain
2	I	2	
2	J	2	
2	K	2	
2	L	2	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 26253 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	1120	Total	C	N	O	S	0	0
			8499	5411	1429	1621	38		
1	B	1120	Total	C	N	O	S	0	0
			8499	5411	1429	1621	38		
1	C	1120	Total	C	N	O	S	0	0
			8499	5411	1429	1621	38		

There are 180 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	982	PRO	LYS	engineered mutation	UNP A0A6B9WHD3
A	983	PRO	VAL	engineered mutation	UNP A0A6B9WHD3
A	1210	LEU	-	expression tag	UNP A0A6B9WHD3
A	1211	GLU	-	expression tag	UNP A0A6B9WHD3
A	1212	VAL	-	expression tag	UNP A0A6B9WHD3
A	1213	LEU	-	expression tag	UNP A0A6B9WHD3
A	1214	PHE	-	expression tag	UNP A0A6B9WHD3
A	1215	GLN	-	expression tag	UNP A0A6B9WHD3
A	1216	GLY	-	expression tag	UNP A0A6B9WHD3
A	1217	PRO	-	expression tag	UNP A0A6B9WHD3
A	1218	GLY	-	expression tag	UNP A0A6B9WHD3
A	1219	GLY	-	expression tag	UNP A0A6B9WHD3
A	1220	GLY	-	expression tag	UNP A0A6B9WHD3
A	1221	SER	-	expression tag	UNP A0A6B9WHD3
A	1222	GLY	-	expression tag	UNP A0A6B9WHD3
A	1223	GLY	-	expression tag	UNP A0A6B9WHD3
A	1224	GLY	-	expression tag	UNP A0A6B9WHD3
A	1225	SER	-	expression tag	UNP A0A6B9WHD3
A	1226	GLY	-	expression tag	UNP A0A6B9WHD3
A	1227	TYR	-	expression tag	UNP A0A6B9WHD3
A	1228	ILE	-	expression tag	UNP A0A6B9WHD3
A	1229	PRO	-	expression tag	UNP A0A6B9WHD3
A	1230	GLU	-	expression tag	UNP A0A6B9WHD3
A	1231	ALA	-	expression tag	UNP A0A6B9WHD3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1232	PRO	-	expression tag	UNP A0A6B9WHD3
A	1233	ARG	-	expression tag	UNP A0A6B9WHD3
A	1234	ASP	-	expression tag	UNP A0A6B9WHD3
A	1235	GLY	-	expression tag	UNP A0A6B9WHD3
A	1236	GLN	-	expression tag	UNP A0A6B9WHD3
A	1237	ALA	-	expression tag	UNP A0A6B9WHD3
A	1238	TYR	-	expression tag	UNP A0A6B9WHD3
A	1239	VAL	-	expression tag	UNP A0A6B9WHD3
A	1240	ARG	-	expression tag	UNP A0A6B9WHD3
A	1241	LYS	-	expression tag	UNP A0A6B9WHD3
A	1242	ASP	-	expression tag	UNP A0A6B9WHD3
A	1243	GLY	-	expression tag	UNP A0A6B9WHD3
A	1244	GLU	-	expression tag	UNP A0A6B9WHD3
A	1245	TRP	-	expression tag	UNP A0A6B9WHD3
A	1246	VAL	-	expression tag	UNP A0A6B9WHD3
A	1247	LEU	-	expression tag	UNP A0A6B9WHD3
A	1248	LEU	-	expression tag	UNP A0A6B9WHD3
A	1249	SER	-	expression tag	UNP A0A6B9WHD3
A	1250	THR	-	expression tag	UNP A0A6B9WHD3
A	1251	PHE	-	expression tag	UNP A0A6B9WHD3
A	1252	LEU	-	expression tag	UNP A0A6B9WHD3
A	1253	GLY	-	expression tag	UNP A0A6B9WHD3
A	1254	HIS	-	expression tag	UNP A0A6B9WHD3
A	1255	HIS	-	expression tag	UNP A0A6B9WHD3
A	1256	HIS	-	expression tag	UNP A0A6B9WHD3
A	1257	HIS	-	expression tag	UNP A0A6B9WHD3
A	1258	HIS	-	expression tag	UNP A0A6B9WHD3
A	1259	HIS	-	expression tag	UNP A0A6B9WHD3
A	1260	TRP	-	expression tag	UNP A0A6B9WHD3
A	1261	SER	-	expression tag	UNP A0A6B9WHD3
A	1262	HIS	-	expression tag	UNP A0A6B9WHD3
A	1263	PRO	-	expression tag	UNP A0A6B9WHD3
A	1264	GLN	-	expression tag	UNP A0A6B9WHD3
A	1265	PHE	-	expression tag	UNP A0A6B9WHD3
A	1266	GLU	-	expression tag	UNP A0A6B9WHD3
A	1267	LYS	-	expression tag	UNP A0A6B9WHD3
B	982	PRO	LYS	engineered mutation	UNP A0A6B9WHD3
B	983	PRO	VAL	engineered mutation	UNP A0A6B9WHD3
B	1210	LEU	-	expression tag	UNP A0A6B9WHD3
B	1211	GLU	-	expression tag	UNP A0A6B9WHD3
B	1212	VAL	-	expression tag	UNP A0A6B9WHD3
B	1213	LEU	-	expression tag	UNP A0A6B9WHD3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1214	PHE	-	expression tag	UNP A0A6B9WHD3
B	1215	GLN	-	expression tag	UNP A0A6B9WHD3
B	1216	GLY	-	expression tag	UNP A0A6B9WHD3
B	1217	PRO	-	expression tag	UNP A0A6B9WHD3
B	1218	GLY	-	expression tag	UNP A0A6B9WHD3
B	1219	GLY	-	expression tag	UNP A0A6B9WHD3
B	1220	GLY	-	expression tag	UNP A0A6B9WHD3
B	1221	SER	-	expression tag	UNP A0A6B9WHD3
B	1222	GLY	-	expression tag	UNP A0A6B9WHD3
B	1223	GLY	-	expression tag	UNP A0A6B9WHD3
B	1224	GLY	-	expression tag	UNP A0A6B9WHD3
B	1225	SER	-	expression tag	UNP A0A6B9WHD3
B	1226	GLY	-	expression tag	UNP A0A6B9WHD3
B	1227	TYR	-	expression tag	UNP A0A6B9WHD3
B	1228	ILE	-	expression tag	UNP A0A6B9WHD3
B	1229	PRO	-	expression tag	UNP A0A6B9WHD3
B	1230	GLU	-	expression tag	UNP A0A6B9WHD3
B	1231	ALA	-	expression tag	UNP A0A6B9WHD3
B	1232	PRO	-	expression tag	UNP A0A6B9WHD3
B	1233	ARG	-	expression tag	UNP A0A6B9WHD3
B	1234	ASP	-	expression tag	UNP A0A6B9WHD3
B	1235	GLY	-	expression tag	UNP A0A6B9WHD3
B	1236	GLN	-	expression tag	UNP A0A6B9WHD3
B	1237	ALA	-	expression tag	UNP A0A6B9WHD3
B	1238	TYR	-	expression tag	UNP A0A6B9WHD3
B	1239	VAL	-	expression tag	UNP A0A6B9WHD3
B	1240	ARG	-	expression tag	UNP A0A6B9WHD3
B	1241	LYS	-	expression tag	UNP A0A6B9WHD3
B	1242	ASP	-	expression tag	UNP A0A6B9WHD3
B	1243	GLY	-	expression tag	UNP A0A6B9WHD3
B	1244	GLU	-	expression tag	UNP A0A6B9WHD3
B	1245	TRP	-	expression tag	UNP A0A6B9WHD3
B	1246	VAL	-	expression tag	UNP A0A6B9WHD3
B	1247	LEU	-	expression tag	UNP A0A6B9WHD3
B	1248	LEU	-	expression tag	UNP A0A6B9WHD3
B	1249	SER	-	expression tag	UNP A0A6B9WHD3
B	1250	THR	-	expression tag	UNP A0A6B9WHD3
B	1251	PHE	-	expression tag	UNP A0A6B9WHD3
B	1252	LEU	-	expression tag	UNP A0A6B9WHD3
B	1253	GLY	-	expression tag	UNP A0A6B9WHD3
B	1254	HIS	-	expression tag	UNP A0A6B9WHD3
B	1255	HIS	-	expression tag	UNP A0A6B9WHD3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1256	HIS	-	expression tag	UNP A0A6B9WHD3
B	1257	HIS	-	expression tag	UNP A0A6B9WHD3
B	1258	HIS	-	expression tag	UNP A0A6B9WHD3
B	1259	HIS	-	expression tag	UNP A0A6B9WHD3
B	1260	TRP	-	expression tag	UNP A0A6B9WHD3
B	1261	SER	-	expression tag	UNP A0A6B9WHD3
B	1262	HIS	-	expression tag	UNP A0A6B9WHD3
B	1263	PRO	-	expression tag	UNP A0A6B9WHD3
B	1264	GLN	-	expression tag	UNP A0A6B9WHD3
B	1265	PHE	-	expression tag	UNP A0A6B9WHD3
B	1266	GLU	-	expression tag	UNP A0A6B9WHD3
B	1267	LYS	-	expression tag	UNP A0A6B9WHD3
C	982	PRO	LYS	engineered mutation	UNP A0A6B9WHD3
C	983	PRO	VAL	engineered mutation	UNP A0A6B9WHD3
C	1210	LEU	-	expression tag	UNP A0A6B9WHD3
C	1211	GLU	-	expression tag	UNP A0A6B9WHD3
C	1212	VAL	-	expression tag	UNP A0A6B9WHD3
C	1213	LEU	-	expression tag	UNP A0A6B9WHD3
C	1214	PHE	-	expression tag	UNP A0A6B9WHD3
C	1215	GLN	-	expression tag	UNP A0A6B9WHD3
C	1216	GLY	-	expression tag	UNP A0A6B9WHD3
C	1217	PRO	-	expression tag	UNP A0A6B9WHD3
C	1218	GLY	-	expression tag	UNP A0A6B9WHD3
C	1219	GLY	-	expression tag	UNP A0A6B9WHD3
C	1220	GLY	-	expression tag	UNP A0A6B9WHD3
C	1221	SER	-	expression tag	UNP A0A6B9WHD3
C	1222	GLY	-	expression tag	UNP A0A6B9WHD3
C	1223	GLY	-	expression tag	UNP A0A6B9WHD3
C	1224	GLY	-	expression tag	UNP A0A6B9WHD3
C	1225	SER	-	expression tag	UNP A0A6B9WHD3
C	1226	GLY	-	expression tag	UNP A0A6B9WHD3
C	1227	TYR	-	expression tag	UNP A0A6B9WHD3
C	1228	ILE	-	expression tag	UNP A0A6B9WHD3
C	1229	PRO	-	expression tag	UNP A0A6B9WHD3
C	1230	GLU	-	expression tag	UNP A0A6B9WHD3
C	1231	ALA	-	expression tag	UNP A0A6B9WHD3
C	1232	PRO	-	expression tag	UNP A0A6B9WHD3
C	1233	ARG	-	expression tag	UNP A0A6B9WHD3
C	1234	ASP	-	expression tag	UNP A0A6B9WHD3
C	1235	GLY	-	expression tag	UNP A0A6B9WHD3
C	1236	GLN	-	expression tag	UNP A0A6B9WHD3
C	1237	ALA	-	expression tag	UNP A0A6B9WHD3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1238	TYR	-	expression tag	UNP A0A6B9WHD3
C	1239	VAL	-	expression tag	UNP A0A6B9WHD3
C	1240	ARG	-	expression tag	UNP A0A6B9WHD3
C	1241	LYS	-	expression tag	UNP A0A6B9WHD3
C	1242	ASP	-	expression tag	UNP A0A6B9WHD3
C	1243	GLY	-	expression tag	UNP A0A6B9WHD3
C	1244	GLU	-	expression tag	UNP A0A6B9WHD3
C	1245	TRP	-	expression tag	UNP A0A6B9WHD3
C	1246	VAL	-	expression tag	UNP A0A6B9WHD3
C	1247	LEU	-	expression tag	UNP A0A6B9WHD3
C	1248	LEU	-	expression tag	UNP A0A6B9WHD3
C	1249	SER	-	expression tag	UNP A0A6B9WHD3
C	1250	THR	-	expression tag	UNP A0A6B9WHD3
C	1251	PHE	-	expression tag	UNP A0A6B9WHD3
C	1252	LEU	-	expression tag	UNP A0A6B9WHD3
C	1253	GLY	-	expression tag	UNP A0A6B9WHD3
C	1254	HIS	-	expression tag	UNP A0A6B9WHD3
C	1255	HIS	-	expression tag	UNP A0A6B9WHD3
C	1256	HIS	-	expression tag	UNP A0A6B9WHD3
C	1257	HIS	-	expression tag	UNP A0A6B9WHD3
C	1258	HIS	-	expression tag	UNP A0A6B9WHD3
C	1259	HIS	-	expression tag	UNP A0A6B9WHD3
C	1260	TRP	-	expression tag	UNP A0A6B9WHD3
C	1261	SER	-	expression tag	UNP A0A6B9WHD3
C	1262	HIS	-	expression tag	UNP A0A6B9WHD3
C	1263	PRO	-	expression tag	UNP A0A6B9WHD3
C	1264	GLN	-	expression tag	UNP A0A6B9WHD3
C	1265	PHE	-	expression tag	UNP A0A6B9WHD3
C	1266	GLU	-	expression tag	UNP A0A6B9WHD3
C	1267	LYS	-	expression tag	UNP A0A6B9WHD3

- 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
2	D	2	Total	C	N	O	0	0
			28	16	2	10		

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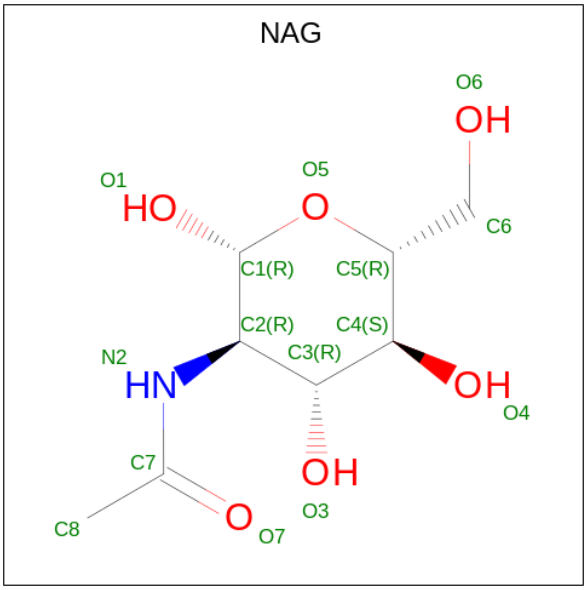
Mol	Chain	Residues	Atoms				AltConf	Trace
2	E	2	Total	C	N	O	0	0
			28	16	2	10		
2	F	2	Total	C	N	O	0	0
			28	16	2	10		
2	G	2	Total	C	N	O	0	0
			28	16	2	10		
2	H	2	Total	C	N	O	0	0
			28	16	2	10		
2	I	2	Total	C	N	O	0	0
			28	16	2	10		
2	J	2	Total	C	N	O	0	0
			28	16	2	10		
2	K	2	Total	C	N	O	0	0
			28	16	2	10		
2	L	2	Total	C	N	O	0	0
			28	16	2	10		

- 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
3	A	1	Total	C	N	O	0
			168	96	12	60	
3	A	1	Total	C	N	O	0
			168	96	12	60	
3	A	1	Total	C	N	O	0
			168	96	12	60	

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Mol	Chain	Residues	Atoms	AltConf
3	A	1	Total C N O 168 96 12 60	0
3	A	1	Total C N O 168 96 12 60	0
3	A	1	Total C N O 168 96 12 60	0
3	A	1	Total C N O 168 96 12 60	0
3	A	1	Total C N O 168 96 12 60	0
3	A	1	Total C N O 168 96 12 60	0
3	A	1	Total C N O 168 96 12 60	0
3	A	1	Total C N O 168 96 12 60	0
3	A	1	Total C N O 168 96 12 60	0
3	B	1	Total C N O 168 96 12 60	0
3	B	1	Total C N O 168 96 12 60	0
3	B	1	Total C N O 168 96 12 60	0
3	B	1	Total C N O 168 96 12 60	0
3	B	1	Total C N O 168 96 12 60	0
3	B	1	Total C N O 168 96 12 60	0
3	B	1	Total C N O 168 96 12 60	0
3	B	1	Total C N O 168 96 12 60	0
3	B	1	Total C N O 168 96 12 60	0
3	B	1	Total C N O 168 96 12 60	0
3	B	1	Total C N O 168 96 12 60	0
3	B	1	Total C N O 168 96 12 60	0

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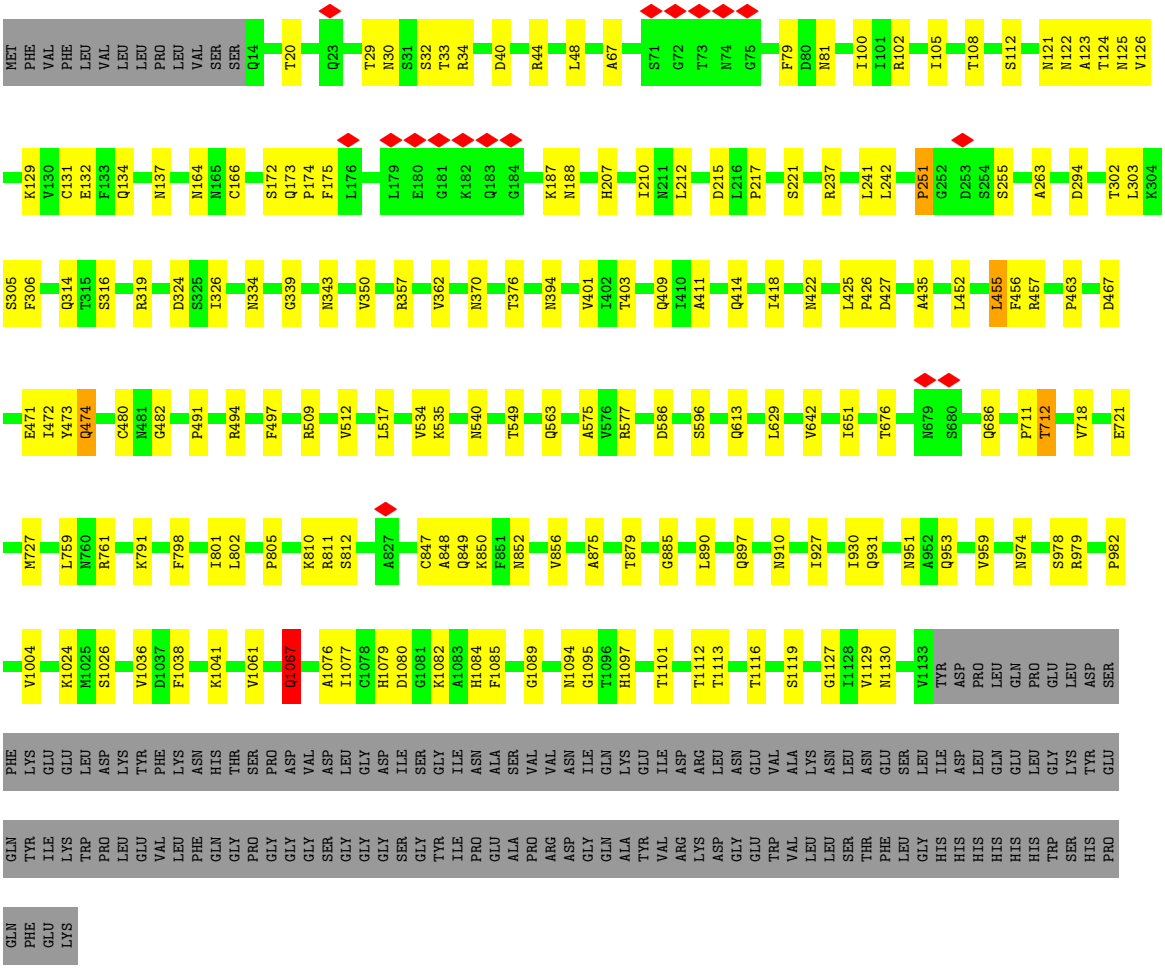
Mol	Chain	Residues	Atoms				AltConf
3	C	1	Total 168	C 96	N 12	O 60	0
3	C	1	Total 168	C 96	N 12	O 60	0
3	C	1	Total 168	C 96	N 12	O 60	0
3	C	1	Total 168	C 96	N 12	O 60	0
3	C	1	Total 168	C 96	N 12	O 60	0
3	C	1	Total 168	C 96	N 12	O 60	0
3	C	1	Total 168	C 96	N 12	O 60	0
3	C	1	Total 168	C 96	N 12	O 60	0
3	C	1	Total 168	C 96	N 12	O 60	0
3	C	1	Total 168	C 96	N 12	O 60	0
3	C	1	Total 168	C 96	N 12	O 60	0
3	C	1	Total 168	C 96	N 12	O 60	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.

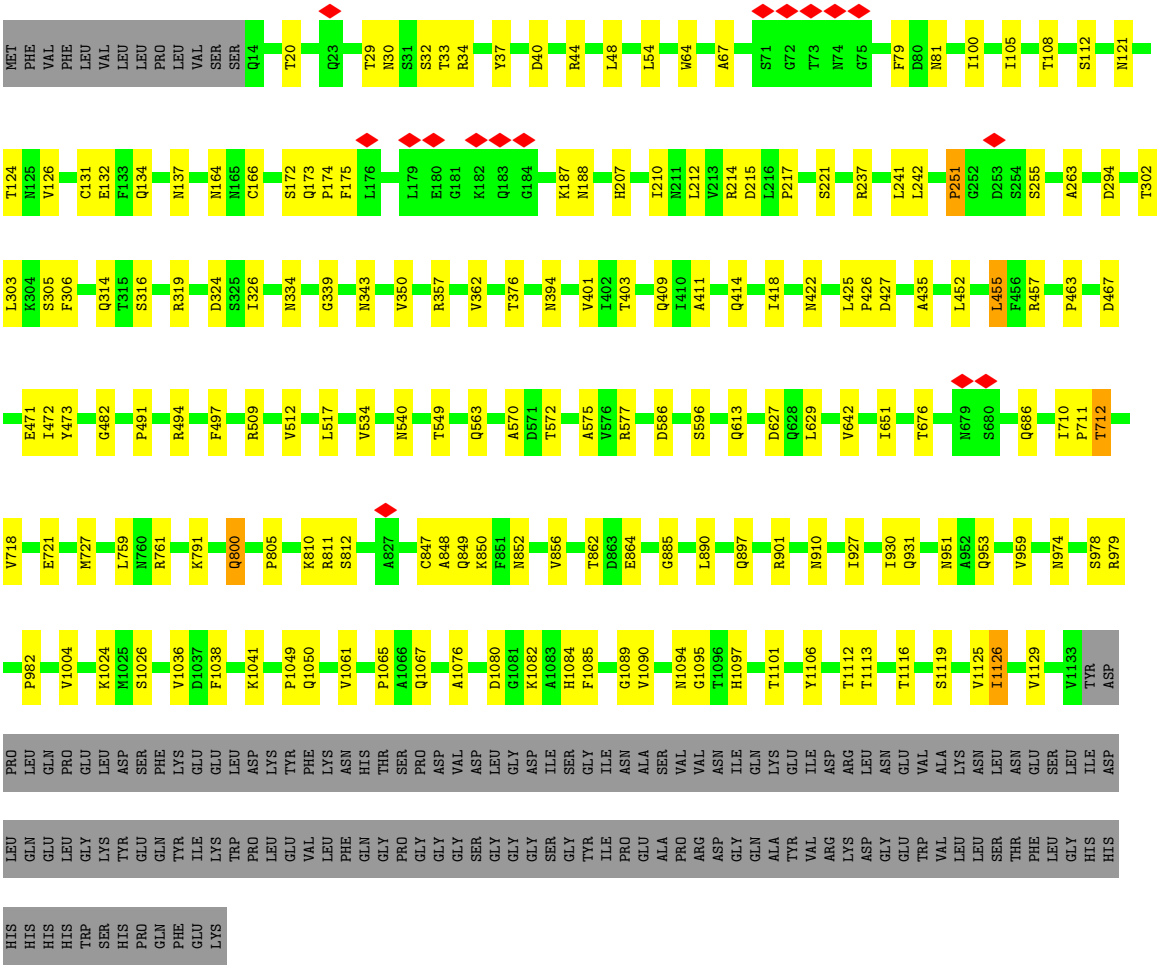
• Molecule 1: Spike glycoprotein

Chain A:



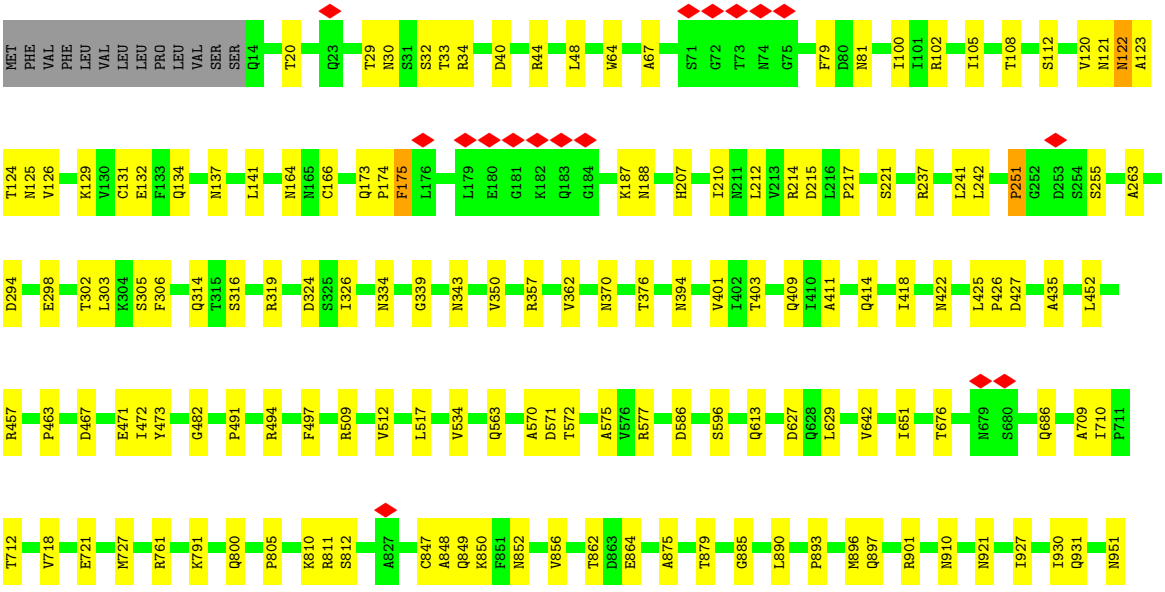
• Molecule 1: Spike glycoprotein

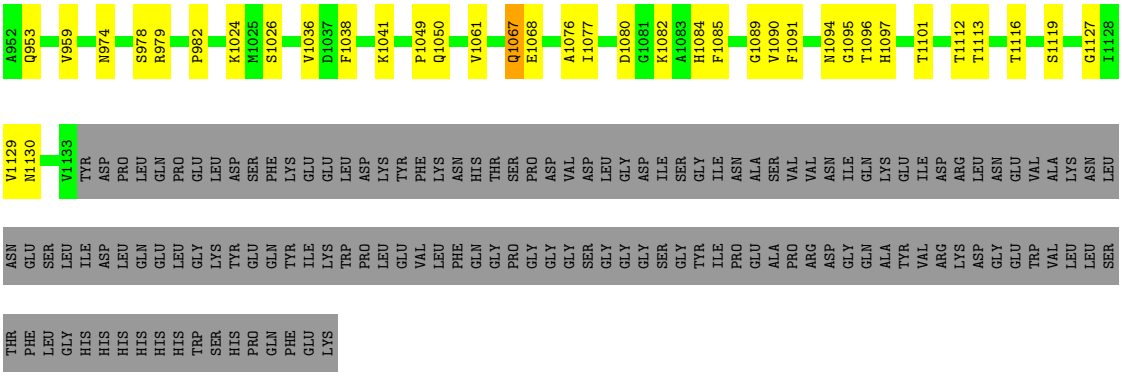
Chain B:



• Molecule 1: Spike glycoprotein

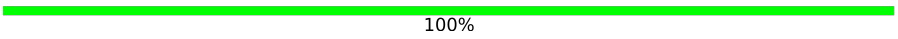
Chain C:





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

Chain D:



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

Chain E:

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

Chain F:

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

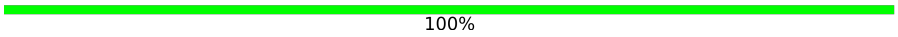
Chain G:

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

Chain H:

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

Chain I:

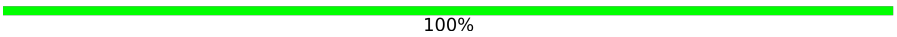


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:

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

Chain K:



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

Chain L:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	99241	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.067	Depositor
Minimum map value	-0.025	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0082	Depositor
Map size (Å)	320.41998, 320.41998, 320.41998	wwPDB
Map dimensions	296, 296, 296	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0825, 1.0825, 1.0825	Depositor

5 Model quality

5.1 Standard geometry

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	0.37	1/8690 (0.0%)	0.49	1/11852 (0.0%)
1	B	0.36	0/8690	0.49	1/11852 (0.0%)
1	C	0.36	0/8690	0.48	1/11852 (0.0%)
All	All	0.36	1/26070 (0.0%)	0.49	3/35556 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1067	GLN	C-N	6.63	1.49	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	251	PRO	N-CA-CB	6.25	110.81	103.30
1	A	251	PRO	N-CA-CB	6.25	110.80	103.30
1	B	251	PRO	N-CA-CB	6.25	110.80	103.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	8499	0	8115	113	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	8499	0	8116	110	0
1	C	8499	0	8116	117	0
2	D	28	0	25	0	0
2	E	28	0	25	1	0
2	F	28	0	25	0	0
2	G	28	0	25	0	0
2	H	28	0	25	0	0
2	I	28	0	25	0	0
2	J	28	0	25	0	0
2	K	28	0	25	0	0
2	L	28	0	25	1	0
3	A	168	0	156	3	0
3	B	168	0	156	3	0
3	C	168	0	156	3	0
All	All	26253	0	25040	306	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 306 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:847:CYS:HA	1:C:850:LYS:HB2	1.71	0.73
1:A:474:GLN:HB3	1:A:480:CYS:HB2	1.73	0.71
1:B:711:PRO:HG2	1:B:1065:PRO:HB2	1.75	0.68
1:C:326:ILE:HD11	1:C:534:VAL:H	1.63	0.63
1:B:727:MET:HB2	1:B:951:ASN:HD21	1.64	0.62

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	1118/1267 (88%)	1033 (92%)	82 (7%)	3 (0%)	41	69
1	B	1118/1267 (88%)	1036 (93%)	78 (7%)	4 (0%)	34	64
1	C	1118/1267 (88%)	1040 (93%)	73 (6%)	5 (0%)	34	64
All	All	3354/3801 (88%)	3109 (93%)	233 (7%)	12 (0%)	38	64

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	175	PHE
1	B	175	PHE
1	C	175	PHE
1	C	123	ALA
1	A	1067	GLN

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	906/1099 (82%)	895 (99%)	11 (1%)	71	89
1	B	906/1099 (82%)	897 (99%)	9 (1%)	76	91
1	C	906/1099 (82%)	897 (99%)	9 (1%)	76	91
All	All	2718/3297 (82%)	2689 (99%)	29 (1%)	74	90

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	712	THR
1	C	1068	GLU
1	B	812	SER
1	C	800	GLN
1	B	811	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	800	GLN
1	C	953	GLN
1	B	951	ASN
1	C	897	GLN
1	B	921	ASN

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)

18 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	1,2	14,14,15	0.30	0	17,19,21	0.56	0
2	NAG	D	2	2	14,14,15	0.30	0	17,19,21	0.63	0
2	NAG	E	1	1,2	14,14,15	0.45	0	17,19,21	1.51	2 (11%)
2	NAG	E	2	2	14,14,15	0.38	0	17,19,21	0.93	0
2	NAG	F	1	1,2	14,14,15	0.35	0	17,19,21	1.07	1 (5%)
2	NAG	F	2	2	14,14,15	0.29	0	17,19,21	0.62	0
2	NAG	G	1	1,2	14,14,15	0.35	0	17,19,21	1.07	1 (5%)
2	NAG	G	2	2	14,14,15	0.30	0	17,19,21	0.62	0
2	NAG	H	1	1,2	14,14,15	0.35	0	17,19,21	1.07	1 (5%)
2	NAG	H	2	2	14,14,15	0.29	0	17,19,21	0.62	0
2	NAG	I	1	1,2	14,14,15	0.30	0	17,19,21	0.55	0
2	NAG	I	2	2	14,14,15	0.29	0	17,19,21	0.63	0
2	NAG	J	1	1,2	14,14,15	0.45	0	17,19,21	1.26	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	J	2	2	14,14,15	0.32	0	17,19,21	0.61	0
2	NAG	K	1	1,2	14,14,15	0.30	0	17,19,21	0.56	0
2	NAG	K	2	2	14,14,15	0.30	0	17,19,21	0.63	0
2	NAG	L	1	1,2	14,14,15	0.39	0	17,19,21	0.92	1 (5%)
2	NAG	L	2	2	14,14,15	0.36	0	17,19,21	0.92	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	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	1/6/23/26	0/1/1/1
2	NAG	E	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	E	2	2	-	4/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
2	NAG	G	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1
2	NAG	H	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1
2	NAG	I	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	I	2	2	-	1/6/23/26	0/1/1/1
2	NAG	J	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	J	2	2	-	2/6/23/26	0/1/1/1
2	NAG	K	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	K	2	2	-	1/6/23/26	0/1/1/1
2	NAG	L	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	L	2	2	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	1	NAG	C4-C3-C2	4.22	117.20	111.02
2	F	1	NAG	O5-C1-C2	-3.62	105.58	111.29
2	G	1	NAG	O5-C1-C2	-3.61	105.58	111.29
2	H	1	NAG	O5-C1-C2	-3.61	105.59	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	1	NAG	C1-O5-C5	-3.57	107.35	112.19

There are no chirality outliers.

5 of 43 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	1	NAG	C8-C7-N2-C2
2	E	1	NAG	O7-C7-N2-C2
2	E	2	NAG	C8-C7-N2-C2
2	E	2	NAG	O7-C7-N2-C2
2	J	1	NAG	C8-C7-N2-C2

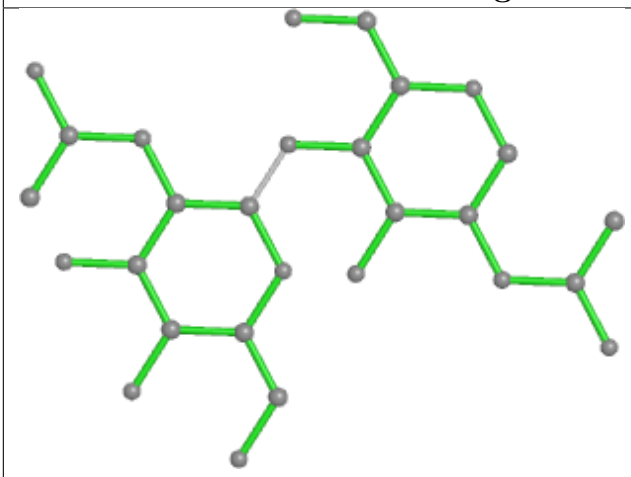
There are no ring outliers.

2 monomers are involved in 2 short contacts:

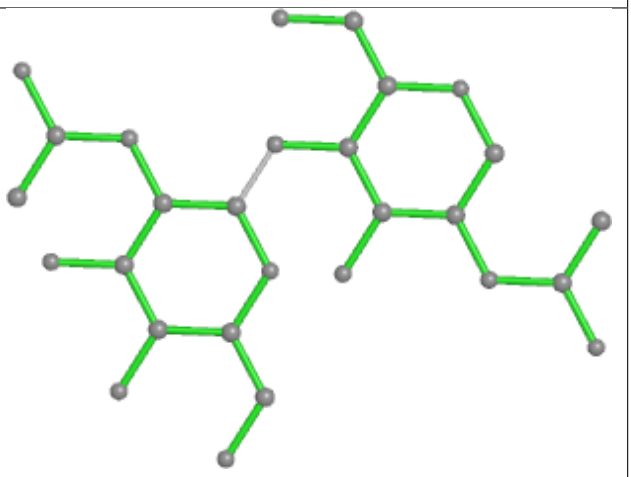
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	1	NAG	1	0
2	E	1	NAG	1	0

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

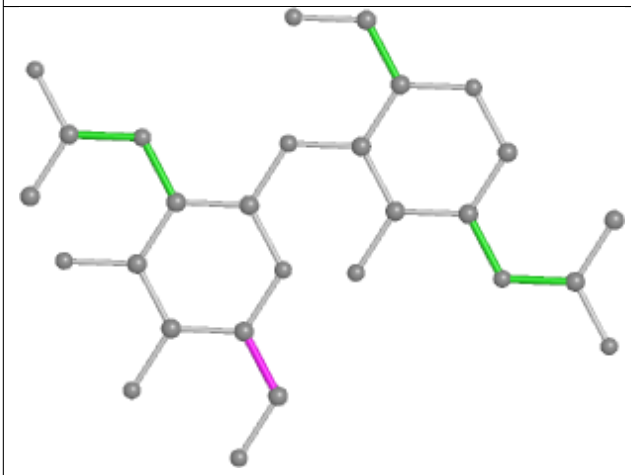
Oligosaccharide Chain D



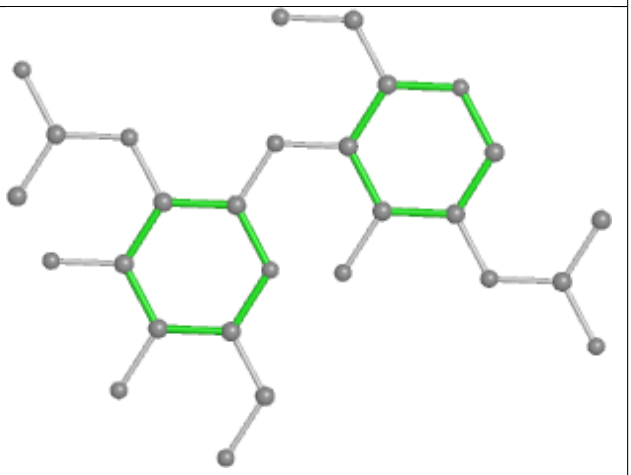
Bond lengths



Bond angles

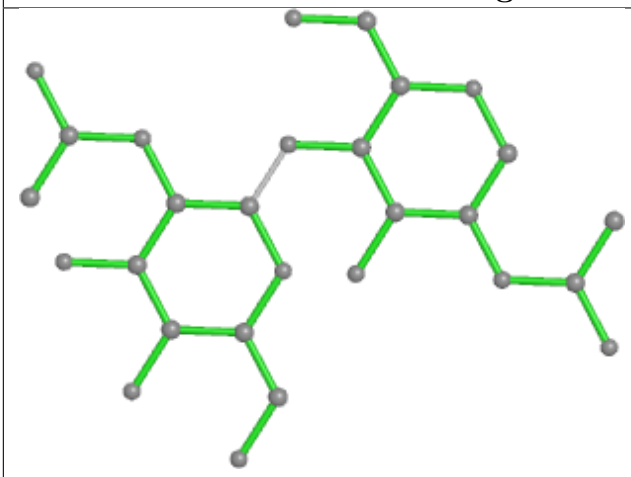


Torsions

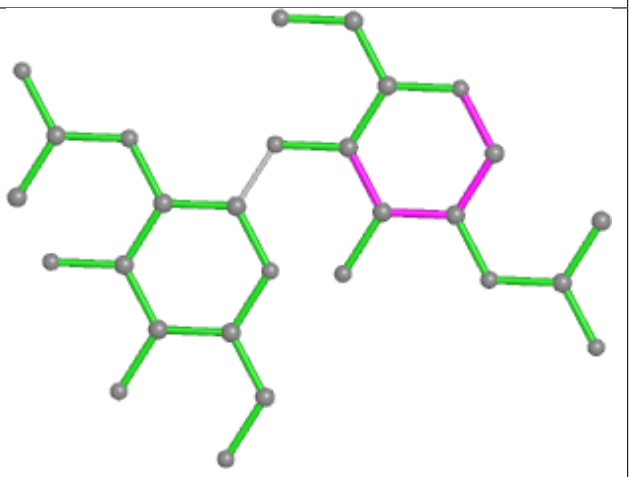


Rings

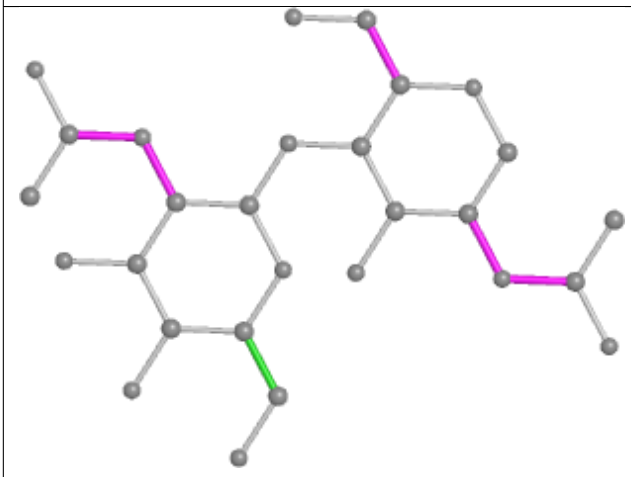
Oligosaccharide Chain E



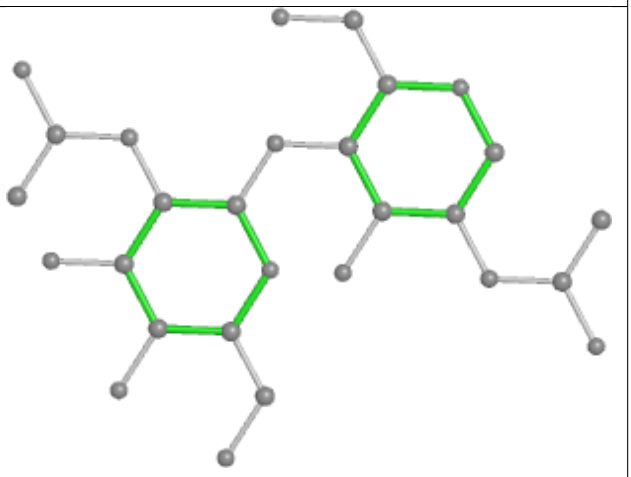
Bond lengths



Bond angles

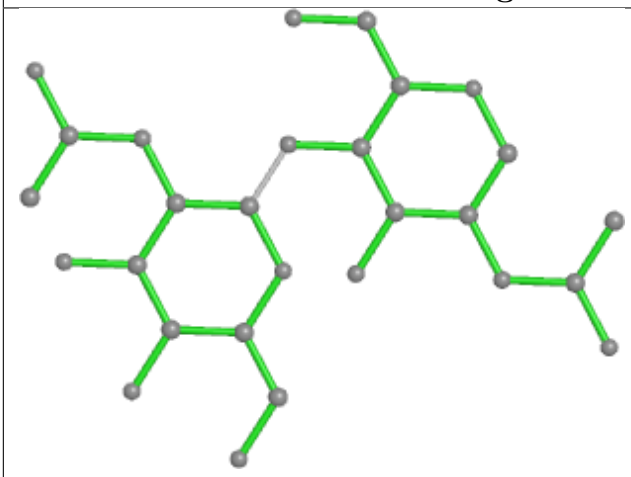


Torsions

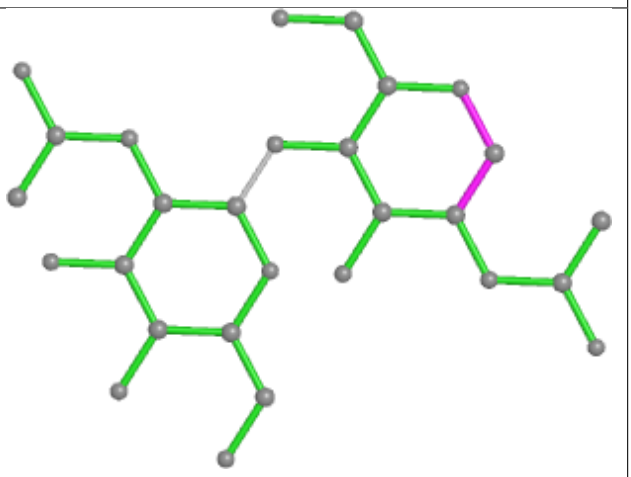


Rings

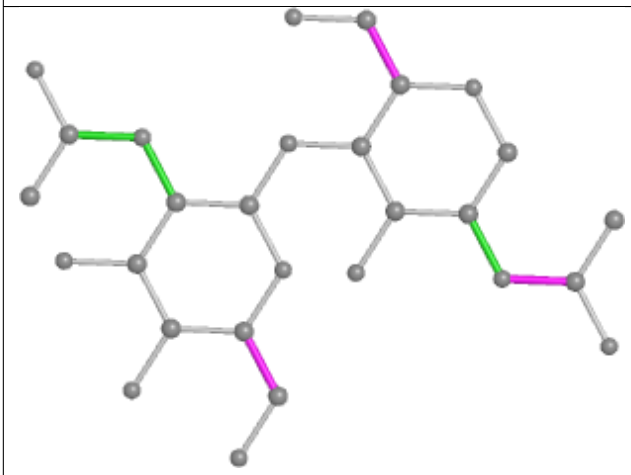
Oligosaccharide Chain F



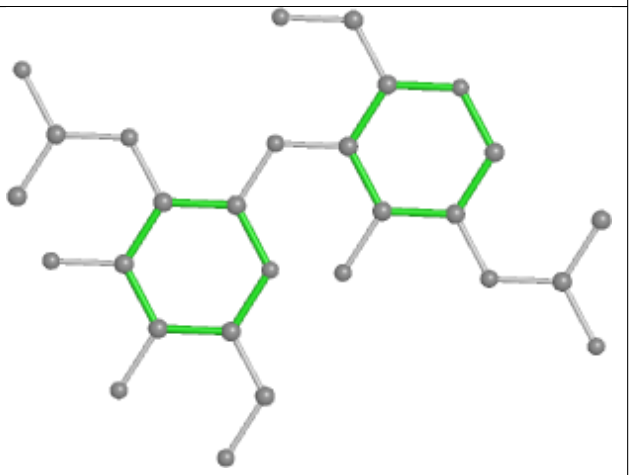
Bond lengths



Bond angles

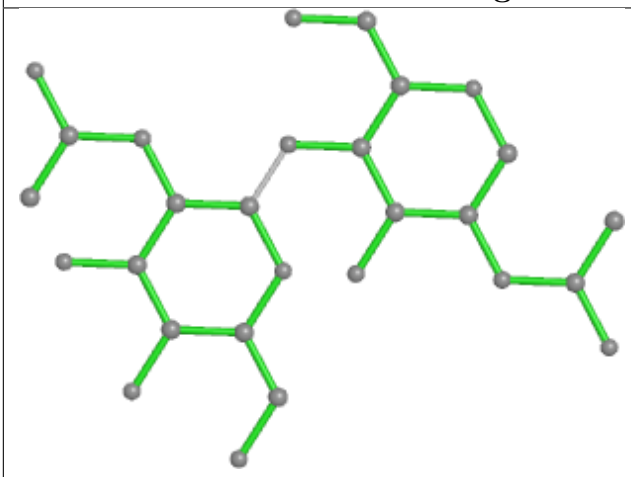


Torsions

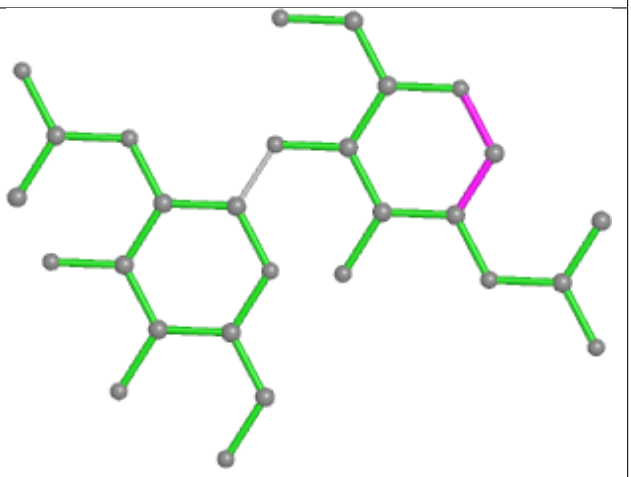


Rings

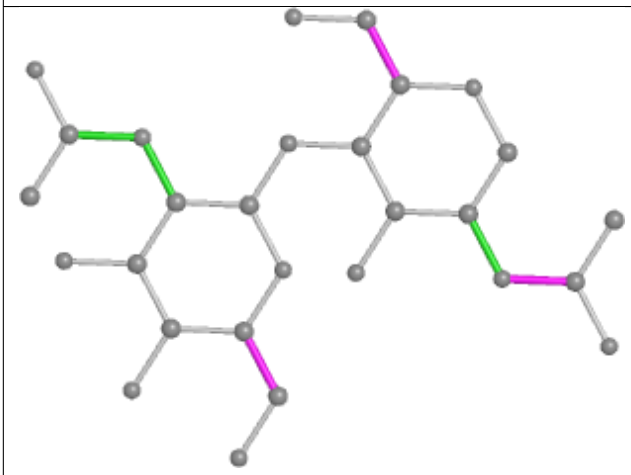
Oligosaccharide Chain G



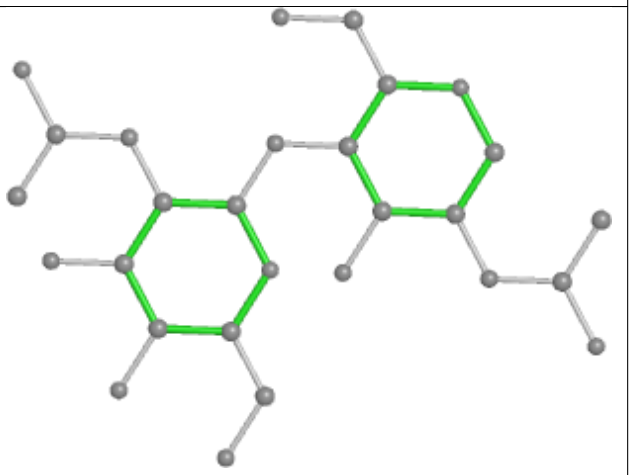
Bond lengths



Bond angles

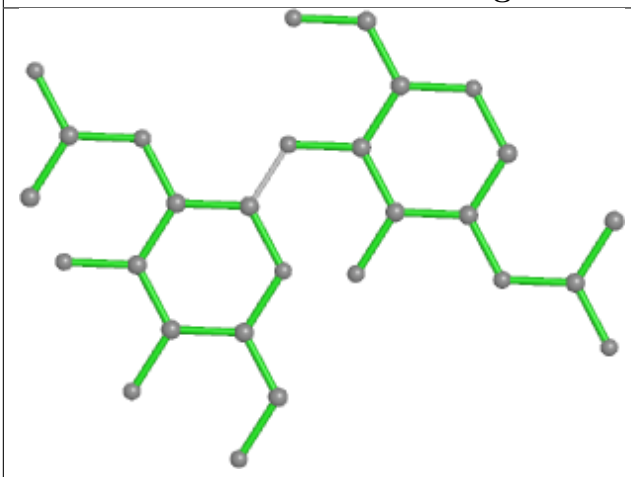


Torsions

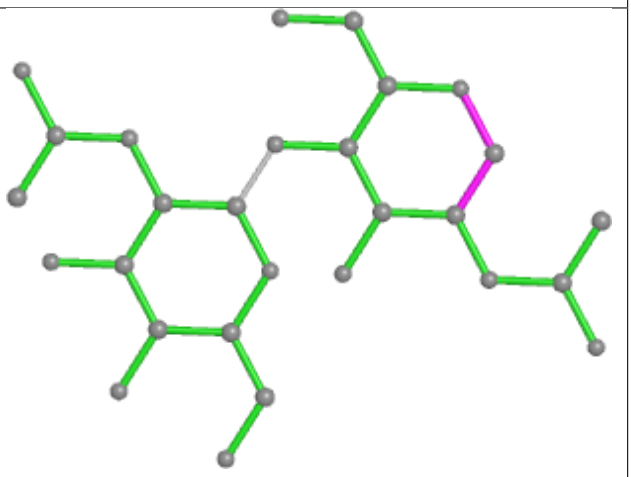


Rings

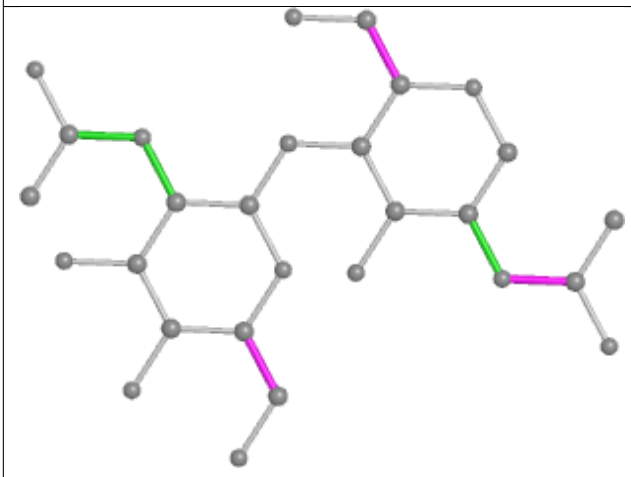
Oligosaccharide Chain H



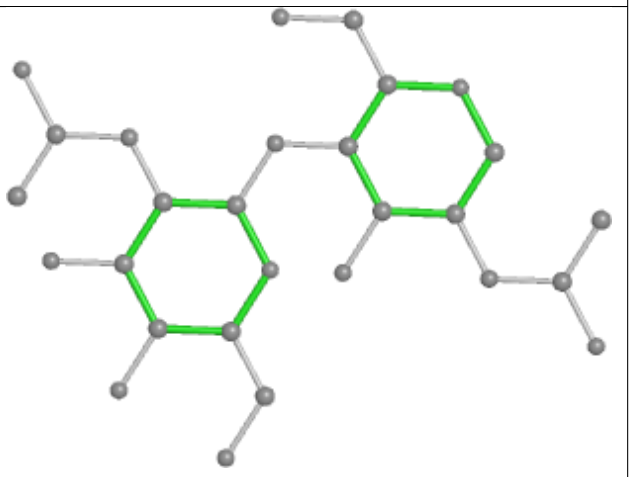
Bond lengths



Bond angles

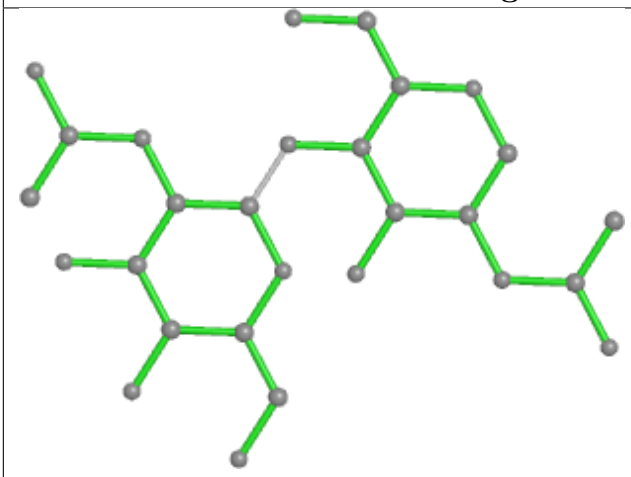


Torsions

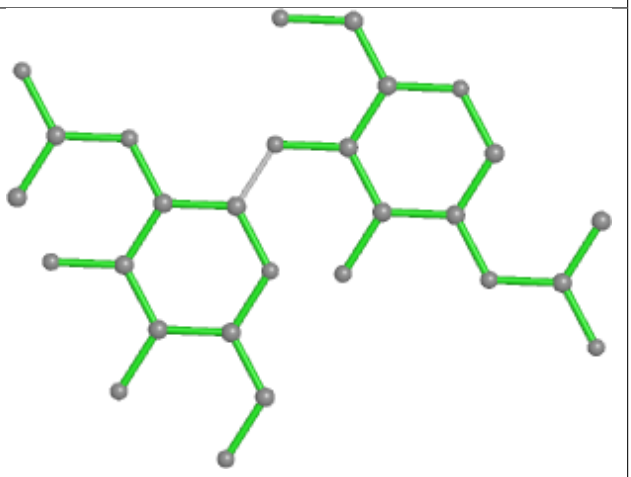


Rings

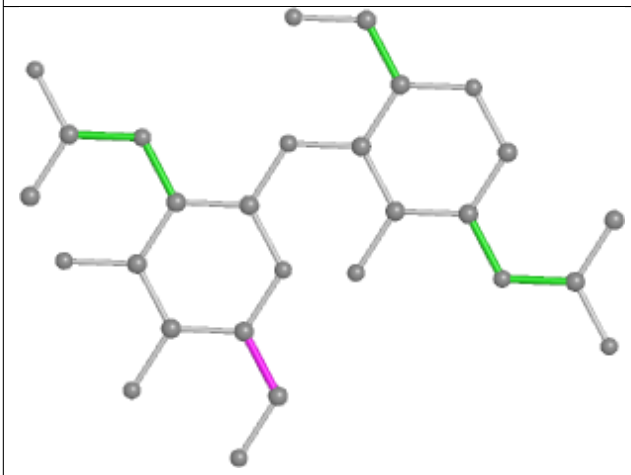
Oligosaccharide Chain I



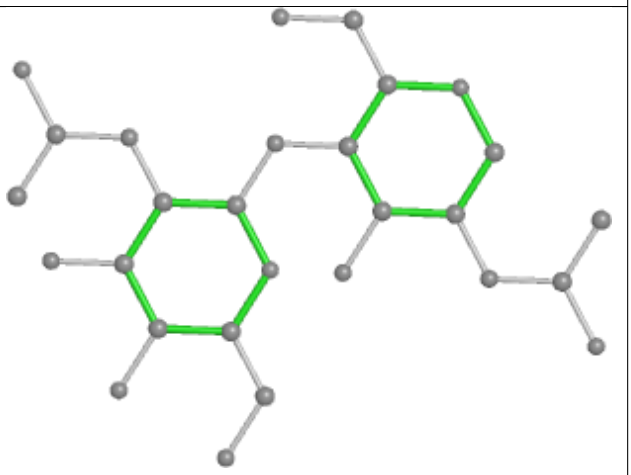
Bond lengths



Bond angles

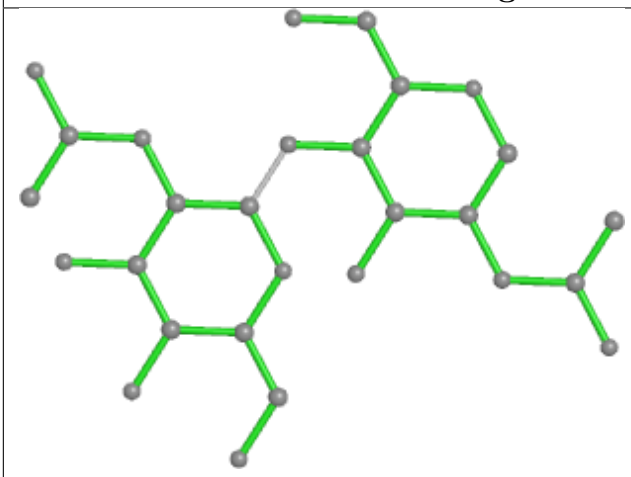


Torsions

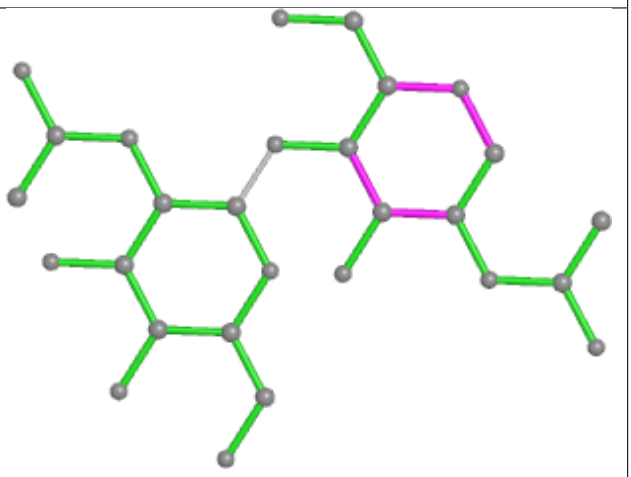


Rings

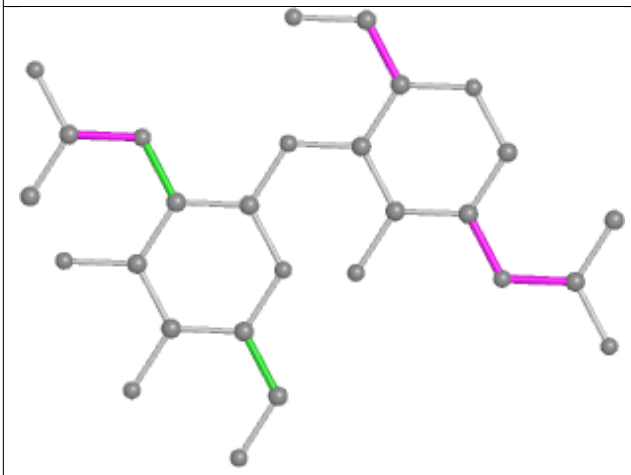
Oligosaccharide Chain J



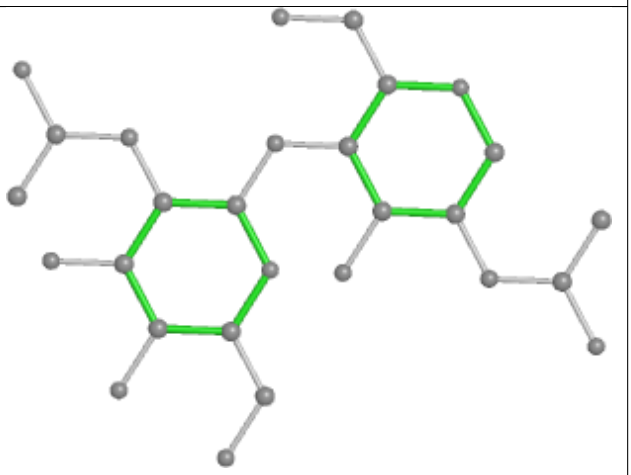
Bond lengths



Bond angles

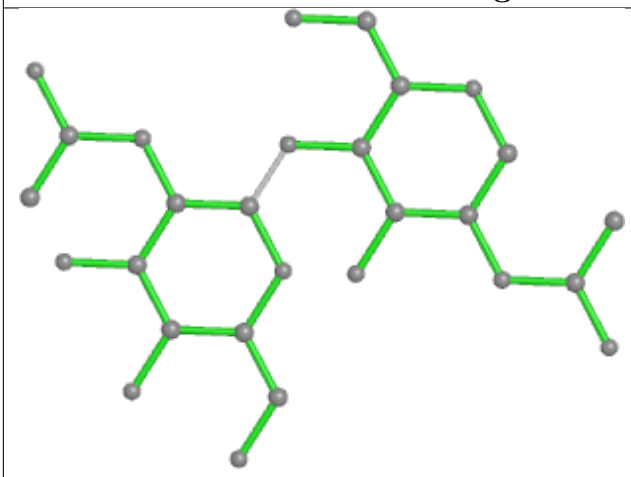


Torsions

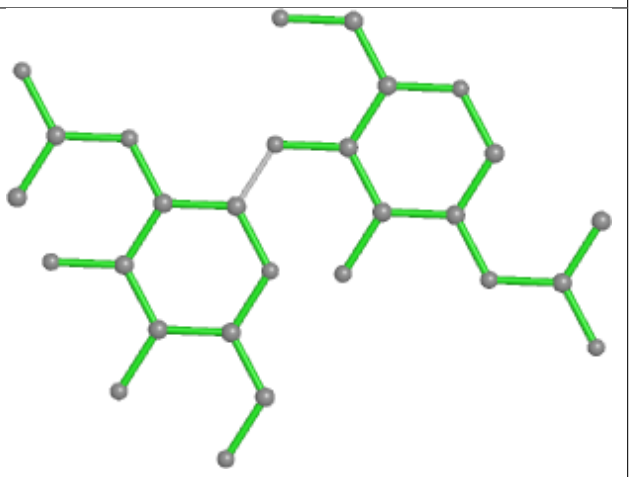


Rings

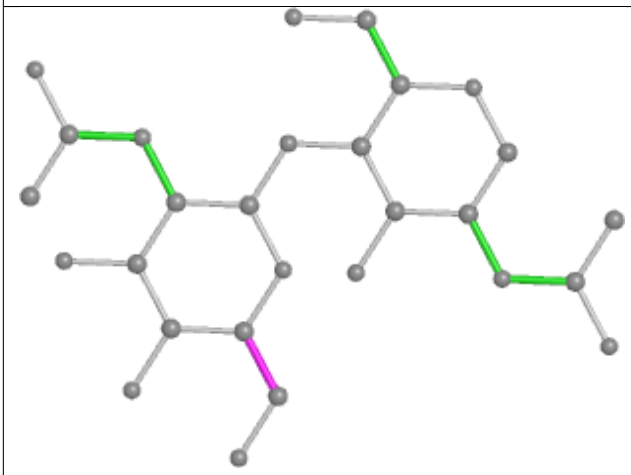
Oligosaccharide Chain K



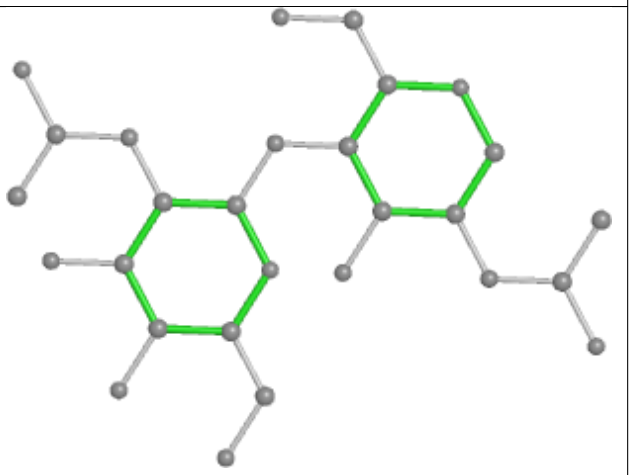
Bond lengths



Bond angles

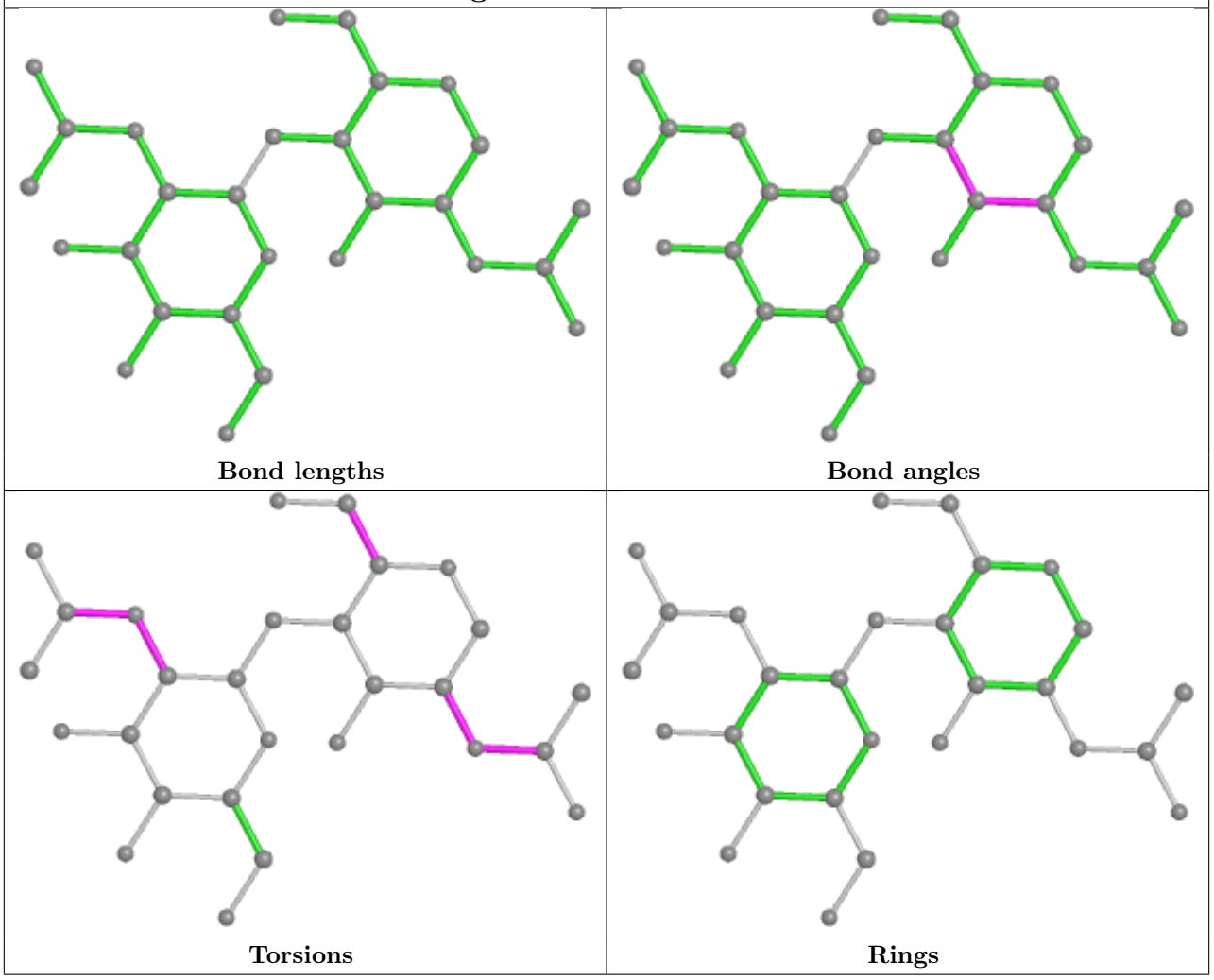


Torsions



Rings

Oligosaccharide Chain L



5.6 Ligand geometry (i)

36 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	1302	1	14,14,15	0.26	0	17,19,21	0.46	0
3	NAG	A	1311	1	14,14,15	0.40	0	17,19,21	0.82	0
3	NAG	B	1311	1	14,14,15	0.18	0	17,19,21	0.39	0
3	NAG	B	1303	1	14,14,15	0.23	0	17,19,21	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	B	1308	1	14,14,15	0.28	0	17,19,21	0.55	0
3	NAG	C	1310	1	14,14,15	0.26	0	17,19,21	0.68	0
3	NAG	C	1309	1	14,14,15	0.49	0	17,19,21	1.26	1 (5%)
3	NAG	A	1312	1	14,14,15	0.36	0	17,19,21	0.87	1 (5%)
3	NAG	A	1306	1	14,14,15	0.25	0	17,19,21	0.50	0
3	NAG	A	1304	1	14,14,15	0.39	0	17,19,21	1.29	1 (5%)
3	NAG	C	1306	1	14,14,15	0.25	0	17,19,21	0.50	0
3	NAG	B	1310	1	14,14,15	0.27	0	17,19,21	0.68	0
3	NAG	C	1307	1	14,14,15	0.16	0	17,19,21	0.51	0
3	NAG	A	1307	1	14,14,15	0.17	0	17,19,21	0.52	0
3	NAG	C	1308	1	14,14,15	0.29	0	17,19,21	0.55	0
3	NAG	B	1309	1	14,14,15	0.50	0	17,19,21	1.28	1 (5%)
3	NAG	A	1301	1	14,14,15	0.22	0	17,19,21	0.43	0
3	NAG	A	1308	1	14,14,15	0.29	0	17,19,21	0.55	0
3	NAG	A	1310	1	14,14,15	0.20	0	17,19,21	0.38	0
3	NAG	C	1301	1	14,14,15	0.22	0	17,19,21	0.43	0
3	NAG	B	1312	1	14,14,15	0.41	0	17,19,21	0.82	0
3	NAG	B	1306	1	14,14,15	0.26	0	17,19,21	0.50	0
3	NAG	A	1303	1	14,14,15	0.23	0	17,19,21	0.44	0
3	NAG	B	1307	1	14,14,15	0.16	0	17,19,21	0.52	0
3	NAG	C	1304	1	14,14,15	0.39	0	17,19,21	1.29	1 (5%)
3	NAG	B	1304	1	14,14,15	0.39	0	17,19,21	1.30	1 (5%)
3	NAG	C	1302	1	14,14,15	0.26	0	17,19,21	0.46	0
3	NAG	A	1305	1	14,14,15	0.22	0	17,19,21	0.63	0
3	NAG	B	1302	1	14,14,15	0.28	0	17,19,21	0.46	0
3	NAG	C	1311	1	14,14,15	0.20	0	17,19,21	0.38	0
3	NAG	C	1312	1	14,14,15	0.40	0	17,19,21	0.82	0
3	NAG	B	1305	1	14,14,15	0.22	0	17,19,21	0.63	0
3	NAG	C	1303	1	14,14,15	0.24	0	17,19,21	0.45	0
3	NAG	C	1305	1	14,14,15	0.21	0	17,19,21	0.63	0
3	NAG	A	1309	1	14,14,15	0.26	0	17,19,21	0.68	0
3	NAG	B	1301	1	14,14,15	0.22	0	17,19,21	0.43	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	1302	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1311	1	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	1311	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1303	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1308	1	-	4/6/23/26	0/1/1/1
3	NAG	C	1310	1	-	3/6/23/26	0/1/1/1
3	NAG	C	1309	1	-	3/6/23/26	0/1/1/1
3	NAG	A	1312	1	-	3/6/23/26	0/1/1/1
3	NAG	A	1306	1	-	4/6/23/26	0/1/1/1
3	NAG	A	1304	1	-	5/6/23/26	0/1/1/1
3	NAG	C	1306	1	-	4/6/23/26	0/1/1/1
3	NAG	B	1310	1	-	3/6/23/26	0/1/1/1
3	NAG	C	1307	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1307	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1308	1	-	4/6/23/26	0/1/1/1
3	NAG	B	1309	1	-	3/6/23/26	0/1/1/1
3	NAG	A	1301	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1308	1	-	4/6/23/26	0/1/1/1
3	NAG	A	1310	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1301	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1312	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1306	1	-	4/6/23/26	0/1/1/1
3	NAG	A	1303	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1307	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1304	1	-	5/6/23/26	0/1/1/1
3	NAG	B	1304	1	-	5/6/23/26	0/1/1/1
3	NAG	C	1302	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1305	1	-	3/6/23/26	0/1/1/1
3	NAG	B	1302	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1311	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1312	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1305	1	-	3/6/23/26	0/1/1/1
3	NAG	C	1303	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1305	1	-	3/6/23/26	0/1/1/1
3	NAG	A	1309	1	-	3/6/23/26	0/1/1/1
3	NAG	B	1301	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1304	NAG	C2-N2-C7	4.32	129.06	122.90
3	C	1304	NAG	C2-N2-C7	4.29	129.01	122.90
3	A	1304	NAG	C2-N2-C7	4.29	129.01	122.90
3	B	1309	NAG	C2-N2-C7	3.74	128.22	122.90
3	C	1309	NAG	C2-N2-C7	3.64	128.09	122.90

There are no chirality outliers.

5 of 96 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1309	NAG	C1-C2-N2-C7
3	B	1309	NAG	C8-C7-N2-C2
3	B	1309	NAG	O7-C7-N2-C2
3	C	1309	NAG	C1-C2-N2-C7
3	C	1309	NAG	C8-C7-N2-C2

There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1304	NAG	1	0
3	A	1301	NAG	2	0
3	C	1301	NAG	2	0
3	C	1304	NAG	1	0
3	B	1304	NAG	1	0
3	B	1301	NAG	2	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.

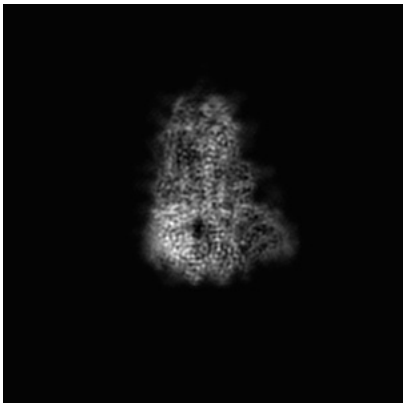
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-30416. These allow visual inspection of the internal detail of the map and identification of artifacts.

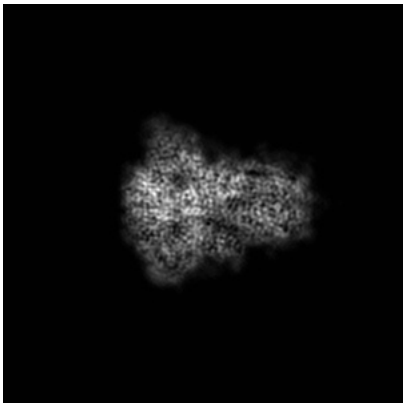
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

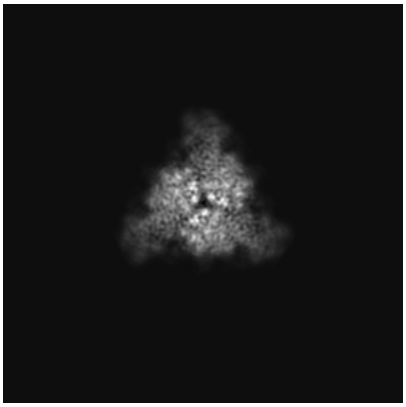
6.1.1 Primary map



X



Y

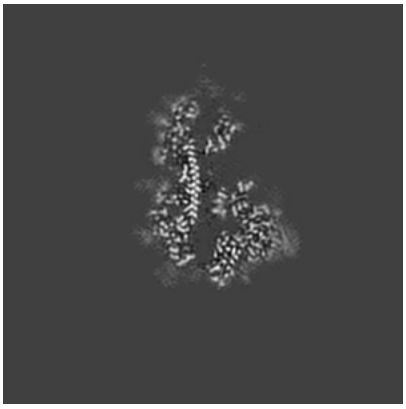


Z

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

6.2 Central slices

6.2.1 Primary map



X Index: 148

Y Index: 148

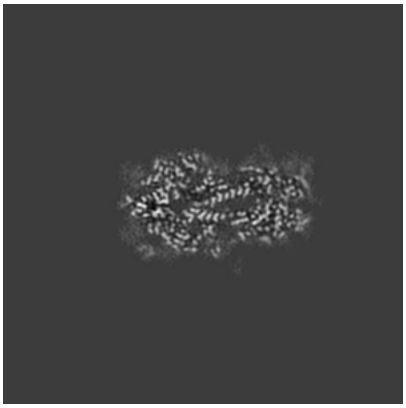
Z Index: 148

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: 156



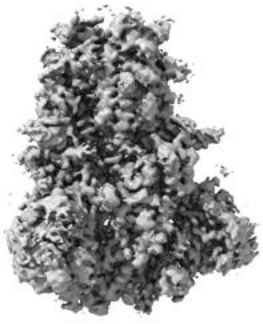
Y Index: 159

Z Index: 117

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 0.0082. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

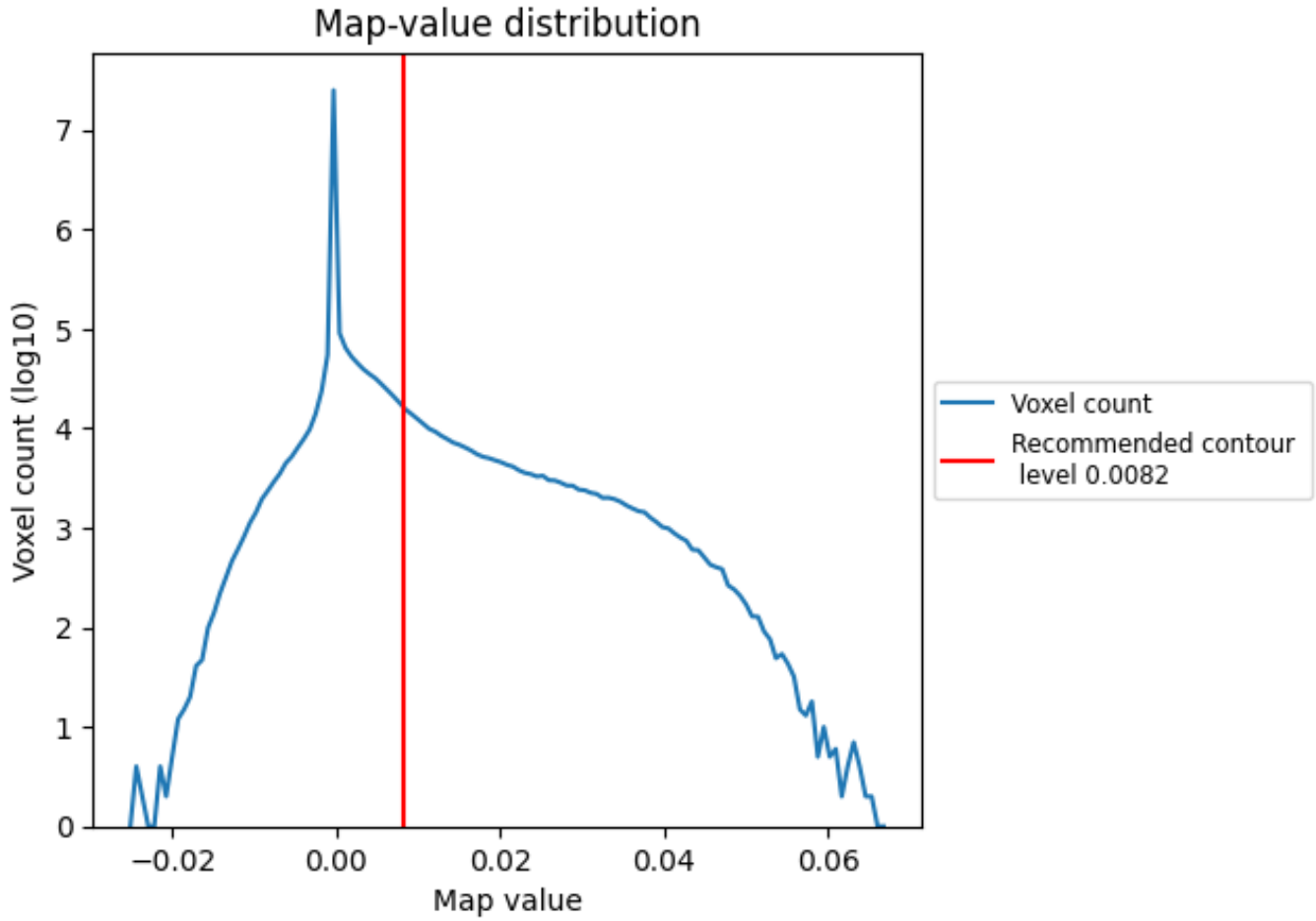
6.5 Mask visualisation (i)

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

7 Map analysis

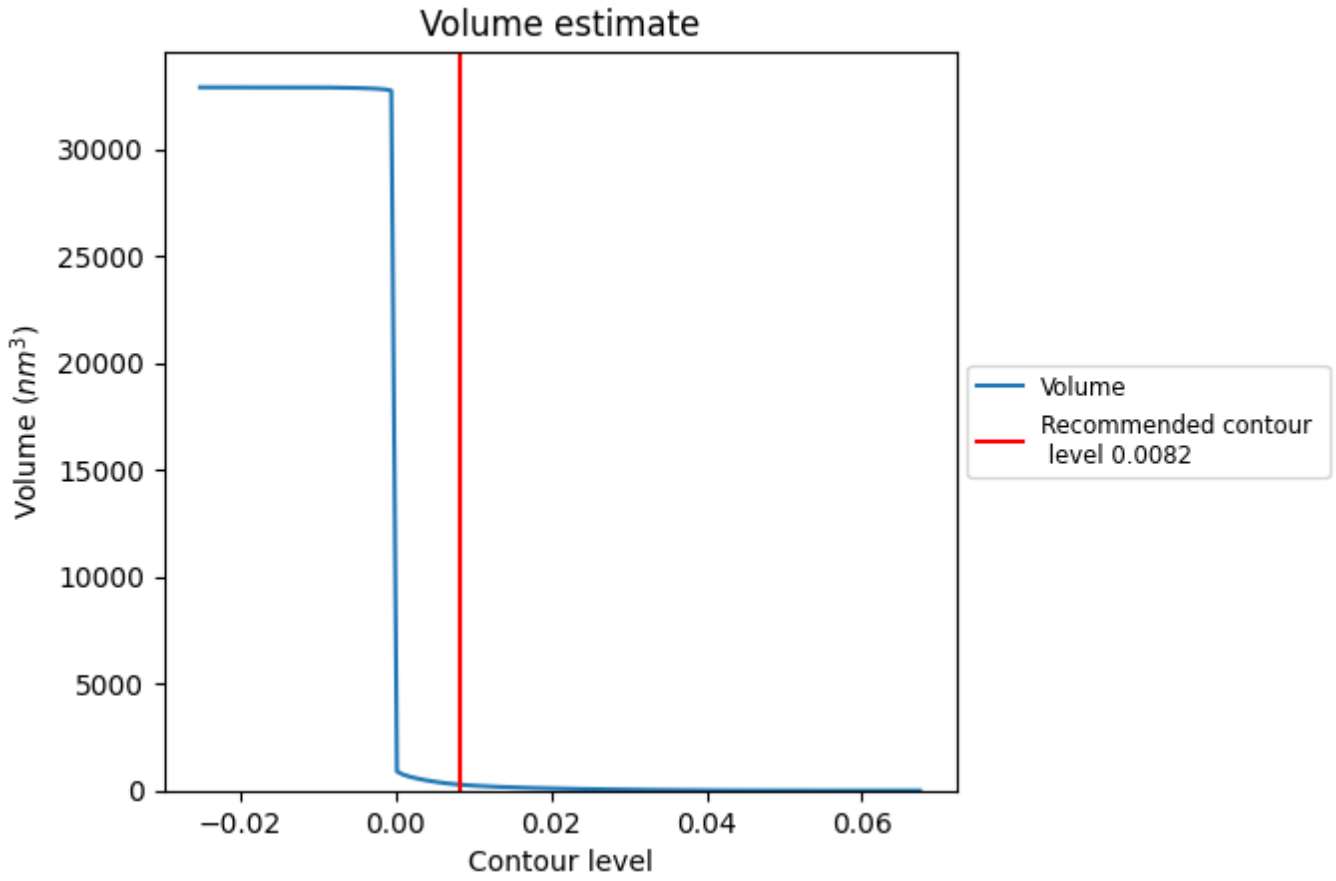
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

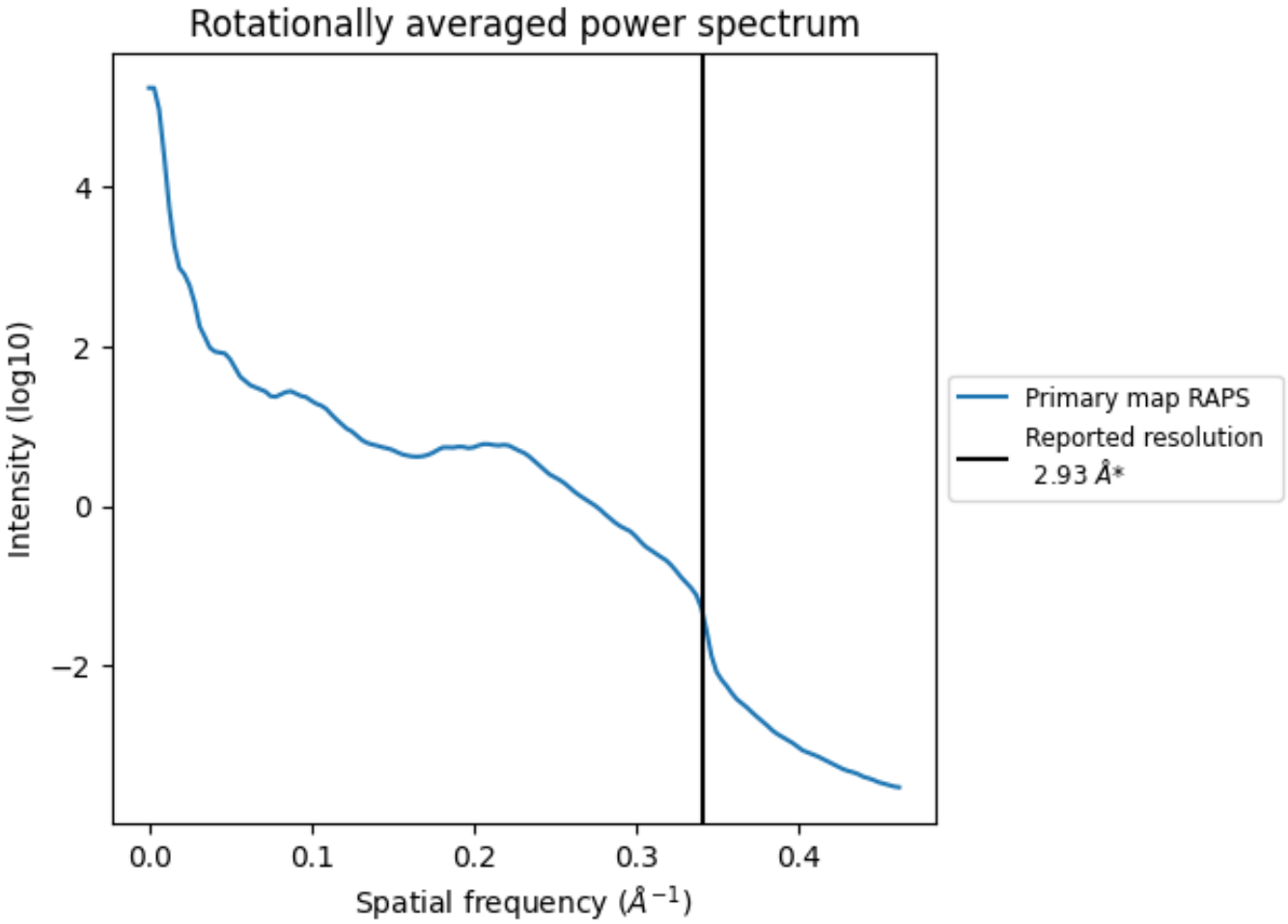
7.2 Volume estimate (i)



The volume at the recommended contour level is 279 nm^3; this corresponds to an approximate mass of 252 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)

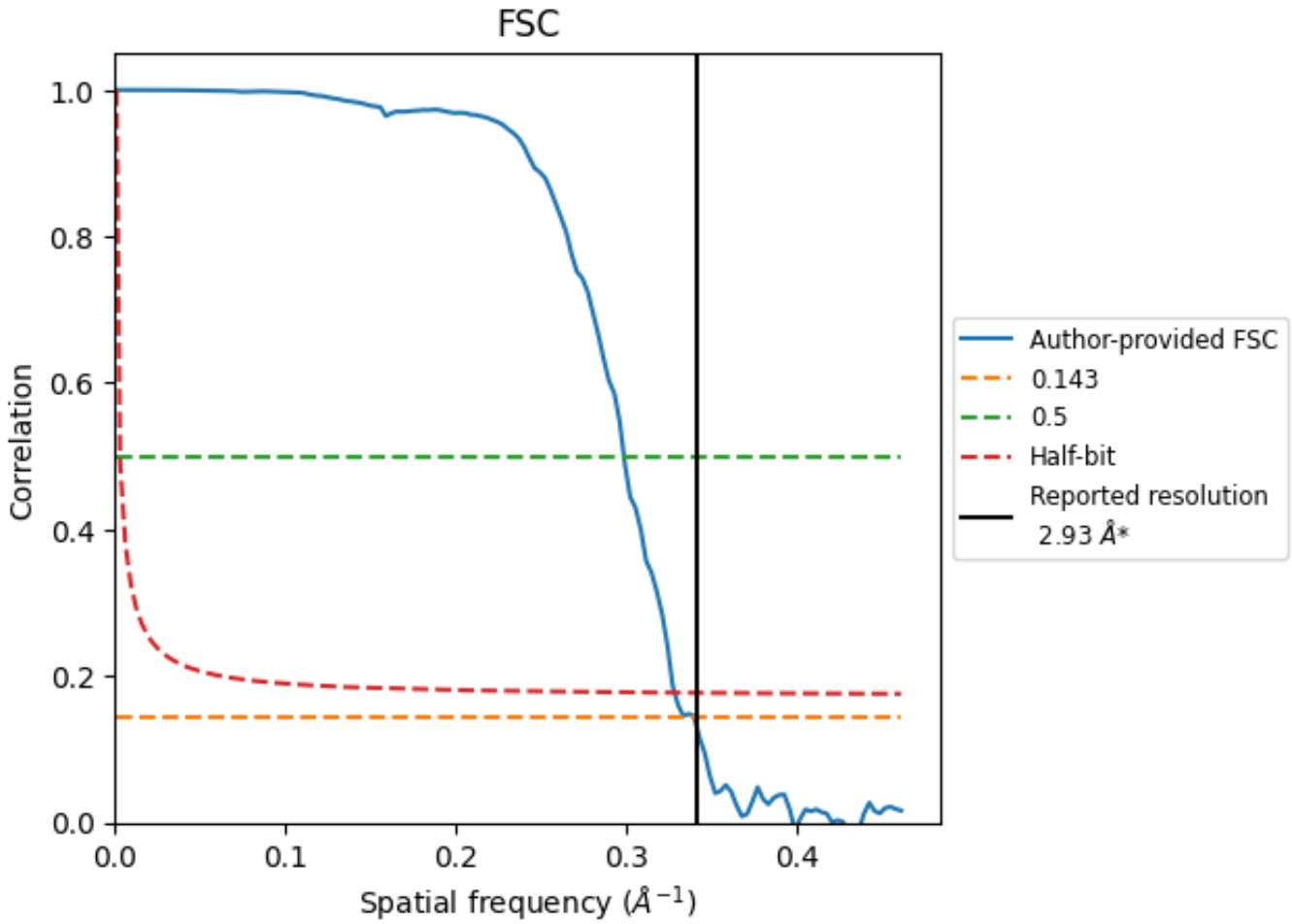


*Reported resolution corresponds to spatial frequency of 0.341 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.341 Å^{-1}

8.2 Resolution estimates (i)

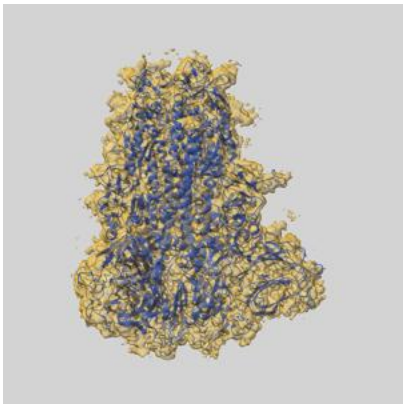
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.93	-	-
Author-provided FSC curve	2.94	3.34	3.04
Unmasked-calculated*	-	-	-

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

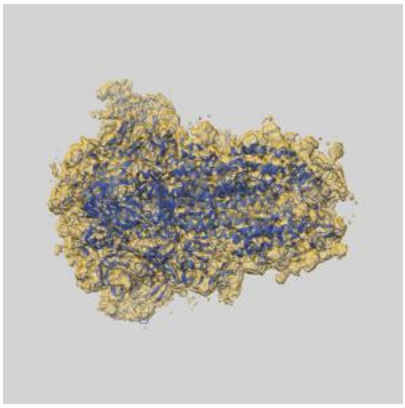
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-30416 and PDB model 7CN4. Per-residue inclusion information can be found in section 3 on page 12.

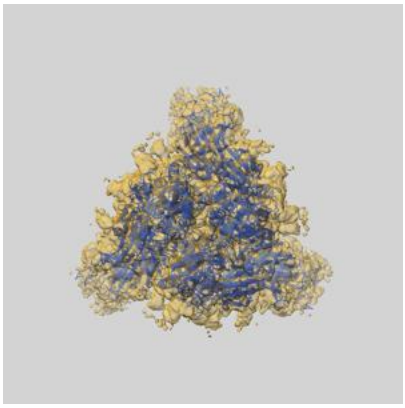
9.1 Map-model overlay



X



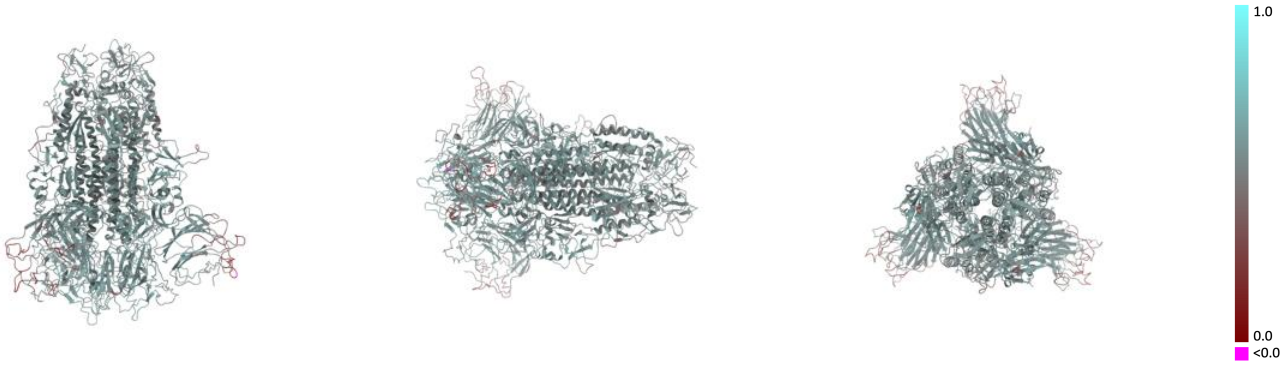
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0082 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.

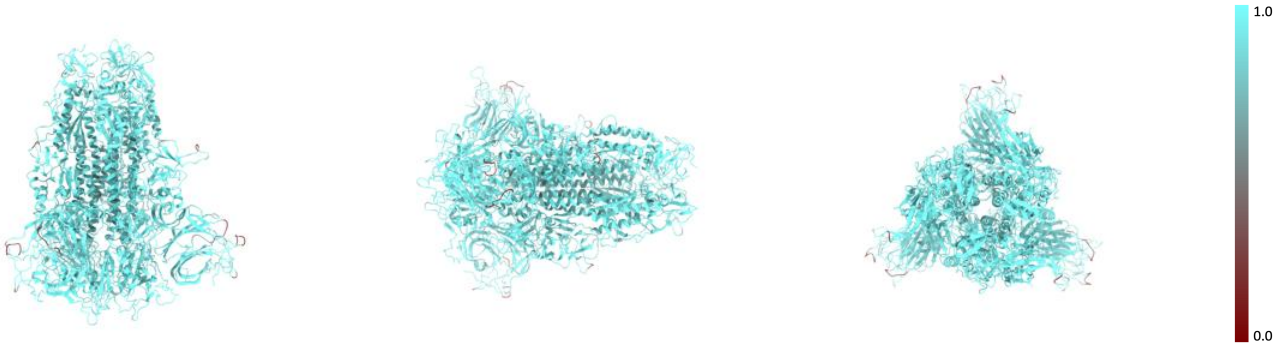
9.2 Q-score mapped to coordinate model (i)



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.

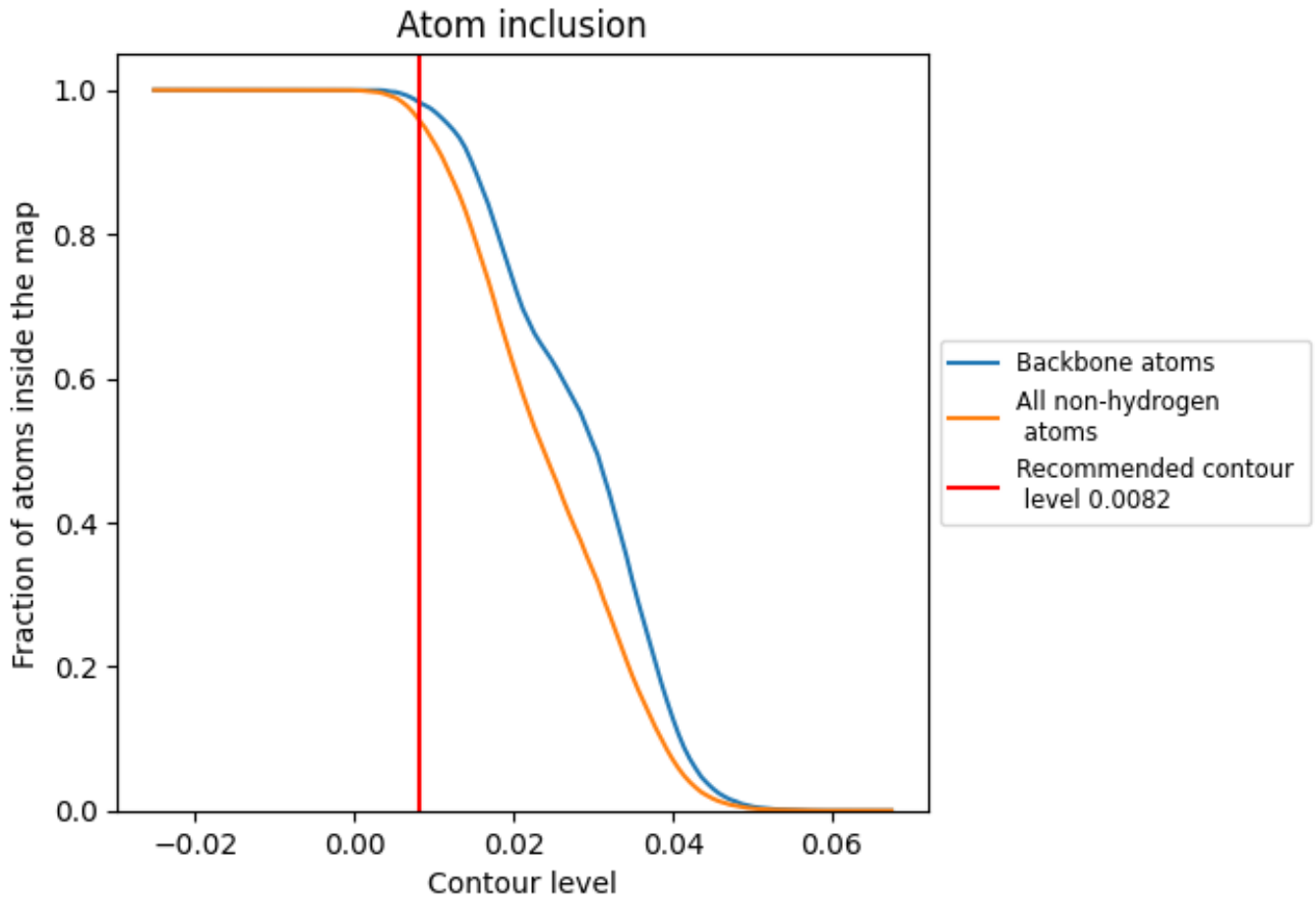
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0082).

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

The table lists the average atom inclusion at the recommended contour level (0.0082) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9575	0.5440
A	0.9573	0.5440
B	0.9585	0.5440
C	0.9582	0.5450
D	0.9643	0.5090
E	0.8929	0.3880
F	0.8929	0.4840
G	0.8929	0.4980
H	0.8929	0.4980
I	0.9643	0.5110
J	0.7857	0.2090
K	0.9643	0.5120
L	0.9286	0.3830