wwPDB EM Validation Summary Report

Dec 17, 2022 – 10:00 pm GMT

PDB ID	:	6ZP5
EMDB ID	:	EMD-11336
Title	:	SARS-CoV-2 spike in prefusion state (flexibility analysis, 1-up closed conformation)
Authors	:	Martinez, M.; Marabini, R.; Carazo, J.M.
Deposited on	:	2020-07-08
Resolution	:	3.10 Å(reported)
Based on initial model	:	6ZOW

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

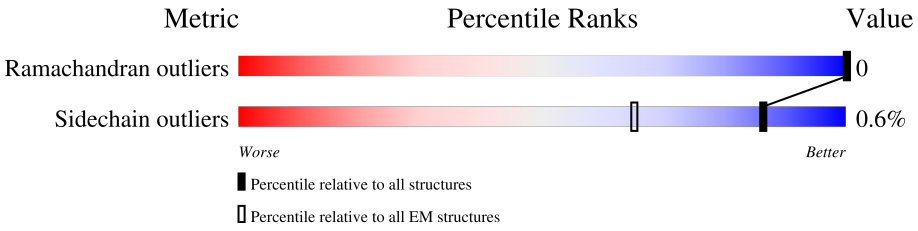
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
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	1288	5%, 76%, 23%
1	B	1288	73%, 27%
1	C	1288	72%, 28%
2	D	2	50%, 100%
2	G	2	50%, 50%
2	H	2	100%
2	I	2	100%
2	J	2	50%, 100%
2	K	2	100%

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Mol	Chain	Length	Quality of chain
2	L	2	100%
2	M	2	50% 50%
2	P	2	100%
2	S	2	50% 50%
2	T	2	50% 50%
2	V	2	50% 50%
2	X	2	100%
2	Z	2	50% 50%
2	c	2	50% 50%
2	d	2	50% 100%
3	E	4	75% 25%
3	F	4	75% 25%
3	R	4	50% 50%
3	U	4	75% 25%
4	N	3	67% 33%
4	O	3	33% 100%
4	W	3	33% 33% 67%
4	Y	3	100%
4	a	3	33% 67% 33%
4	b	3	67% 33%
5	Q	3	33% 67%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	W	2	X	-	-	-
6	NAG	C	1302	X	-	-	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 23615 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	988	Total	C	N	O	S	0	0
			7709	4918	1282	1475	34		
1	B	943	Total	C	N	O	S	0	0
			7367	4704	1223	1408	32		
1	C	930	Total	C	N	O	S	0	0
			7243	4621	1203	1387	32		

There are 255 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	655	GLY	ARG	engineered mutation	UNP P0DTC2
A	656	SER	ARG	engineered mutation	UNP P0DTC2
A	658	SER	ARG	engineered mutation	UNP P0DTC2
A	959	PRO	LYS	engineered mutation	UNP P0DTC2
A	960	PRO	VAL	engineered mutation	UNP P0DTC2
A	1182	GLY	-	expression tag	UNP P0DTC2
A	1183	SER	-	expression tag	UNP P0DTC2
A	1184	GLY	-	expression tag	UNP P0DTC2
A	1185	TYR	-	expression tag	UNP P0DTC2
A	1186	ILE	-	expression tag	UNP P0DTC2
A	1187	PRO	-	expression tag	UNP P0DTC2
A	1188	GLU	-	expression tag	UNP P0DTC2
A	1189	ALA	-	expression tag	UNP P0DTC2
A	1190	PRO	-	expression tag	UNP P0DTC2
A	1191	ARG	-	expression tag	UNP P0DTC2
A	1192	ASP	-	expression tag	UNP P0DTC2
A	1193	GLY	-	expression tag	UNP P0DTC2
A	1194	GLN	-	expression tag	UNP P0DTC2
A	1195	ALA	-	expression tag	UNP P0DTC2
A	1196	TYR	-	expression tag	UNP P0DTC2
A	1197	VAL	-	expression tag	UNP P0DTC2
A	1198	ARG	-	expression tag	UNP P0DTC2
A	1199	LYS	-	expression tag	UNP P0DTC2
A	1200	ASP	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1201	GLY	-	expression tag	UNP P0DTC2
A	1202	GLU	-	expression tag	UNP P0DTC2
A	1203	TRP	-	expression tag	UNP P0DTC2
A	1204	VAL	-	expression tag	UNP P0DTC2
A	1205	LEU	-	expression tag	UNP P0DTC2
A	1206	LEU	-	expression tag	UNP P0DTC2
A	1207	SER	-	expression tag	UNP P0DTC2
A	1208	THR	-	expression tag	UNP P0DTC2
A	1209	PHE	-	expression tag	UNP P0DTC2
A	1210	LEU	-	expression tag	UNP P0DTC2
A	1211	GLY	-	expression tag	UNP P0DTC2
A	1212	ARG	-	expression tag	UNP P0DTC2
A	1213	SER	-	expression tag	UNP P0DTC2
A	1214	LEU	-	expression tag	UNP P0DTC2
A	1215	GLU	-	expression tag	UNP P0DTC2
A	1216	VAL	-	expression tag	UNP P0DTC2
A	1217	LEU	-	expression tag	UNP P0DTC2
A	1218	PHE	-	expression tag	UNP P0DTC2
A	1219	GLN	-	expression tag	UNP P0DTC2
A	1220	GLY	-	expression tag	UNP P0DTC2
A	1221	PRO	-	expression tag	UNP P0DTC2
A	1222	GLY	-	expression tag	UNP P0DTC2
A	1223	HIS	-	expression tag	UNP P0DTC2
A	1224	HIS	-	expression tag	UNP P0DTC2
A	1225	HIS	-	expression tag	UNP P0DTC2
A	1226	HIS	-	expression tag	UNP P0DTC2
A	1227	HIS	-	expression tag	UNP P0DTC2
A	1228	HIS	-	expression tag	UNP P0DTC2
A	1229	HIS	-	expression tag	UNP P0DTC2
A	1230	HIS	-	expression tag	UNP P0DTC2
A	1231	SER	-	expression tag	UNP P0DTC2
A	1232	ALA	-	expression tag	UNP P0DTC2
A	1233	TRP	-	expression tag	UNP P0DTC2
A	1234	SER	-	expression tag	UNP P0DTC2
A	1235	HIS	-	expression tag	UNP P0DTC2
A	1236	PRO	-	expression tag	UNP P0DTC2
A	1237	GLN	-	expression tag	UNP P0DTC2
A	1238	PHE	-	expression tag	UNP P0DTC2
A	1239	GLU	-	expression tag	UNP P0DTC2
A	1240	LYS	-	expression tag	UNP P0DTC2
A	1241	GLY	-	expression tag	UNP P0DTC2
A	1242	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1243	GLY	-	expression tag	UNP P0DTC2
A	1244	SER	-	expression tag	UNP P0DTC2
A	1245	GLY	-	expression tag	UNP P0DTC2
A	1246	GLY	-	expression tag	UNP P0DTC2
A	1247	GLY	-	expression tag	UNP P0DTC2
A	1248	GLY	-	expression tag	UNP P0DTC2
A	1249	SER	-	expression tag	UNP P0DTC2
A	1250	GLY	-	expression tag	UNP P0DTC2
A	1251	GLY	-	expression tag	UNP P0DTC2
A	1252	SER	-	expression tag	UNP P0DTC2
A	1253	ALA	-	expression tag	UNP P0DTC2
A	1254	TRP	-	expression tag	UNP P0DTC2
A	1255	SER	-	expression tag	UNP P0DTC2
A	1256	HIS	-	expression tag	UNP P0DTC2
A	1257	PRO	-	expression tag	UNP P0DTC2
A	1258	GLN	-	expression tag	UNP P0DTC2
A	1259	PHE	-	expression tag	UNP P0DTC2
A	1260	GLU	-	expression tag	UNP P0DTC2
A	1261	LYS	-	expression tag	UNP P0DTC2
B	509F	GLY	ARG	engineered mutation	UNP P0DTC2
B	509G	SER	ARG	engineered mutation	UNP P0DTC2
B	509I	SER	ARG	engineered mutation	UNP P0DTC2
B	783	PRO	LYS	engineered mutation	UNP P0DTC2
B	784	PRO	VAL	engineered mutation	UNP P0DTC2
B	1006	GLY	-	expression tag	UNP P0DTC2
B	1007	SER	-	expression tag	UNP P0DTC2
B	1008	GLY	-	expression tag	UNP P0DTC2
B	1009	TYR	-	expression tag	UNP P0DTC2
B	1010	ILE	-	expression tag	UNP P0DTC2
B	1011	PRO	-	expression tag	UNP P0DTC2
B	1012	GLU	-	expression tag	UNP P0DTC2
B	1013	ALA	-	expression tag	UNP P0DTC2
B	1014	PRO	-	expression tag	UNP P0DTC2
B	1015	ARG	-	expression tag	UNP P0DTC2
B	1016	ASP	-	expression tag	UNP P0DTC2
B	1017	GLY	-	expression tag	UNP P0DTC2
B	1018	GLN	-	expression tag	UNP P0DTC2
B	1019	ALA	-	expression tag	UNP P0DTC2
B	1020	TYR	-	expression tag	UNP P0DTC2
B	1021	VAL	-	expression tag	UNP P0DTC2
B	1022	ARG	-	expression tag	UNP P0DTC2
B	1023	LYS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1024	ASP	-	expression tag	UNP P0DTC2
B	1025	GLY	-	expression tag	UNP P0DTC2
B	1026	GLU	-	expression tag	UNP P0DTC2
B	1027	TRP	-	expression tag	UNP P0DTC2
B	1028	VAL	-	expression tag	UNP P0DTC2
B	1029	LEU	-	expression tag	UNP P0DTC2
B	1030	LEU	-	expression tag	UNP P0DTC2
B	1031	SER	-	expression tag	UNP P0DTC2
B	1032	THR	-	expression tag	UNP P0DTC2
B	1033	PHE	-	expression tag	UNP P0DTC2
B	1034	LEU	-	expression tag	UNP P0DTC2
B	1035	GLY	-	expression tag	UNP P0DTC2
B	1036	ARG	-	expression tag	UNP P0DTC2
B	1037	SER	-	expression tag	UNP P0DTC2
B	1038	LEU	-	expression tag	UNP P0DTC2
B	1039	GLU	-	expression tag	UNP P0DTC2
B	1040	VAL	-	expression tag	UNP P0DTC2
B	1041	LEU	-	expression tag	UNP P0DTC2
B	1042	PHE	-	expression tag	UNP P0DTC2
B	1043	GLN	-	expression tag	UNP P0DTC2
B	1044	GLY	-	expression tag	UNP P0DTC2
B	1045	PRO	-	expression tag	UNP P0DTC2
B	1046	GLY	-	expression tag	UNP P0DTC2
B	1047	HIS	-	expression tag	UNP P0DTC2
B	1048	HIS	-	expression tag	UNP P0DTC2
B	1049	HIS	-	expression tag	UNP P0DTC2
B	1050	HIS	-	expression tag	UNP P0DTC2
B	1051	HIS	-	expression tag	UNP P0DTC2
B	1052	HIS	-	expression tag	UNP P0DTC2
B	1053	HIS	-	expression tag	UNP P0DTC2
B	1054	HIS	-	expression tag	UNP P0DTC2
B	1055	SER	-	expression tag	UNP P0DTC2
B	1056	ALA	-	expression tag	UNP P0DTC2
B	1057	TRP	-	expression tag	UNP P0DTC2
B	1058	SER	-	expression tag	UNP P0DTC2
B	1059	HIS	-	expression tag	UNP P0DTC2
B	1060	PRO	-	expression tag	UNP P0DTC2
B	1061	GLN	-	expression tag	UNP P0DTC2
B	1062	PHE	-	expression tag	UNP P0DTC2
B	1063	GLU	-	expression tag	UNP P0DTC2
B	1064	LYS	-	expression tag	UNP P0DTC2
B	1065	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1066	GLY	-	expression tag	UNP P0DTC2
B	1067	GLY	-	expression tag	UNP P0DTC2
B	1068	SER	-	expression tag	UNP P0DTC2
B	1069	GLY	-	expression tag	UNP P0DTC2
B	1070	GLY	-	expression tag	UNP P0DTC2
B	1071	GLY	-	expression tag	UNP P0DTC2
B	1072	GLY	-	expression tag	UNP P0DTC2
B	1073	SER	-	expression tag	UNP P0DTC2
B	1074	GLY	-	expression tag	UNP P0DTC2
B	1075	GLY	-	expression tag	UNP P0DTC2
B	1076	SER	-	expression tag	UNP P0DTC2
B	1077	ALA	-	expression tag	UNP P0DTC2
B	1078	TRP	-	expression tag	UNP P0DTC2
B	1079	SER	-	expression tag	UNP P0DTC2
B	1080	HIS	-	expression tag	UNP P0DTC2
B	1081	PRO	-	expression tag	UNP P0DTC2
B	1082	GLN	-	expression tag	UNP P0DTC2
B	1083	PHE	-	expression tag	UNP P0DTC2
B	1084	GLU	-	expression tag	UNP P0DTC2
B	1085	LYS	-	expression tag	UNP P0DTC2
C	656	GLY	ARG	engineered mutation	UNP P0DTC2
C	657	SER	ARG	engineered mutation	UNP P0DTC2
C	659	SER	ARG	engineered mutation	UNP P0DTC2
C	960	PRO	LYS	engineered mutation	UNP P0DTC2
C	961	PRO	VAL	engineered mutation	UNP P0DTC2
C	1183	GLY	-	expression tag	UNP P0DTC2
C	1184	SER	-	expression tag	UNP P0DTC2
C	1185	GLY	-	expression tag	UNP P0DTC2
C	1186	TYR	-	expression tag	UNP P0DTC2
C	1187	ILE	-	expression tag	UNP P0DTC2
C	1188	PRO	-	expression tag	UNP P0DTC2
C	1189	GLU	-	expression tag	UNP P0DTC2
C	1190	ALA	-	expression tag	UNP P0DTC2
C	1191	PRO	-	expression tag	UNP P0DTC2
C	1192	ARG	-	expression tag	UNP P0DTC2
C	1193	ASP	-	expression tag	UNP P0DTC2
C	1194	GLY	-	expression tag	UNP P0DTC2
C	1195	GLN	-	expression tag	UNP P0DTC2
C	1196	ALA	-	expression tag	UNP P0DTC2
C	1197	TYR	-	expression tag	UNP P0DTC2
C	1198	VAL	-	expression tag	UNP P0DTC2
C	1199	ARG	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1200	LYS	-	expression tag	UNP P0DTC2
C	1201	ASP	-	expression tag	UNP P0DTC2
C	1202	GLY	-	expression tag	UNP P0DTC2
C	1203	GLU	-	expression tag	UNP P0DTC2
C	1204	TRP	-	expression tag	UNP P0DTC2
C	1205	VAL	-	expression tag	UNP P0DTC2
C	1206	LEU	-	expression tag	UNP P0DTC2
C	1207	LEU	-	expression tag	UNP P0DTC2
C	1208	SER	-	expression tag	UNP P0DTC2
C	1209	THR	-	expression tag	UNP P0DTC2
C	1210	PHE	-	expression tag	UNP P0DTC2
C	1211	LEU	-	expression tag	UNP P0DTC2
C	1212	GLY	-	expression tag	UNP P0DTC2
C	1213	ARG	-	expression tag	UNP P0DTC2
C	1214	SER	-	expression tag	UNP P0DTC2
C	1215	LEU	-	expression tag	UNP P0DTC2
C	1216	GLU	-	expression tag	UNP P0DTC2
C	1217	VAL	-	expression tag	UNP P0DTC2
C	1218	LEU	-	expression tag	UNP P0DTC2
C	1219	PHE	-	expression tag	UNP P0DTC2
C	1220	GLN	-	expression tag	UNP P0DTC2
C	1221	GLY	-	expression tag	UNP P0DTC2
C	1222	PRO	-	expression tag	UNP P0DTC2
C	1223	GLY	-	expression tag	UNP P0DTC2
C	1224	HIS	-	expression tag	UNP P0DTC2
C	1225	HIS	-	expression tag	UNP P0DTC2
C	1226	HIS	-	expression tag	UNP P0DTC2
C	1227	HIS	-	expression tag	UNP P0DTC2
C	1228	HIS	-	expression tag	UNP P0DTC2
C	1229	HIS	-	expression tag	UNP P0DTC2
C	1230	HIS	-	expression tag	UNP P0DTC2
C	1231	HIS	-	expression tag	UNP P0DTC2
C	1232	SER	-	expression tag	UNP P0DTC2
C	1233	ALA	-	expression tag	UNP P0DTC2
C	1234	TRP	-	expression tag	UNP P0DTC2
C	1235	SER	-	expression tag	UNP P0DTC2
C	1236	HIS	-	expression tag	UNP P0DTC2
C	1237	PRO	-	expression tag	UNP P0DTC2
C	1238	GLN	-	expression tag	UNP P0DTC2
C	1239	PHE	-	expression tag	UNP P0DTC2
C	1240	GLU	-	expression tag	UNP P0DTC2
C	1241	LYS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1242	GLY	-	expression tag	UNP P0DTC2
C	1243	GLY	-	expression tag	UNP P0DTC2
C	1244	GLY	-	expression tag	UNP P0DTC2
C	1245	SER	-	expression tag	UNP P0DTC2
C	1246	GLY	-	expression tag	UNP P0DTC2
C	1247	GLY	-	expression tag	UNP P0DTC2
C	1248	GLY	-	expression tag	UNP P0DTC2
C	1249	GLY	-	expression tag	UNP P0DTC2
C	1250	SER	-	expression tag	UNP P0DTC2
C	1251	GLY	-	expression tag	UNP P0DTC2
C	1252	GLY	-	expression tag	UNP P0DTC2
C	1253	SER	-	expression tag	UNP P0DTC2
C	1254	ALA	-	expression tag	UNP P0DTC2
C	1255	TRP	-	expression tag	UNP P0DTC2
C	1256	SER	-	expression tag	UNP P0DTC2
C	1257	HIS	-	expression tag	UNP P0DTC2
C	1258	PRO	-	expression tag	UNP P0DTC2
C	1259	GLN	-	expression tag	UNP P0DTC2
C	1260	PHE	-	expression tag	UNP P0DTC2
C	1261	GLU	-	expression tag	UNP P0DTC2
C	1262	LYS	-	expression tag	UNP P0DTC2

- 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
			30	16	2	12		
2	G	2	Total	C	N	O	0	0
			30	16	2	12		
2	H	2	Total	C	N	O	0	0
			30	16	2	12		
2	I	2	Total	C	N	O	0	0
			30	16	2	12		
2	J	2	Total	C	N	O	0	0
			30	16	2	12		
2	K	2	Total	C	N	O	0	0
			30	16	2	12		

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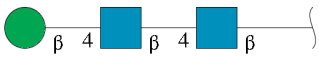
Mol	Chain	Residues	Atoms				AltConf	Trace
2	L	2	Total	C	N	O	0	0
			30	16	2	12		
2	M	2	Total	C	N	O	0	0
			30	16	2	12		
2	P	2	Total	C	N	O	0	0
			30	16	2	12		
2	S	2	Total	C	N	O	0	0
			30	16	2	12		
2	T	2	Total	C	N	O	0	0
			30	16	2	12		
2	V	2	Total	C	N	O	0	0
			30	16	2	12		
2	X	2	Total	C	N	O	0	0
			30	16	2	12		
2	Z	2	Total	C	N	O	0	0
			30	16	2	12		
2	c	2	Total	C	N	O	0	0
			30	16	2	12		
2	d	2	Total	C	N	O	0	0
			30	16	2	12		

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

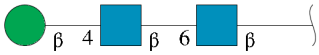
Mol	Chain	Residues	Atoms				AltConf	Trace
3	E	4	Total	C	N	O	0	0
			54	28	2	24		
3	F	4	Total	C	N	O	0	0
			54	28	2	24		
3	R	4	Total	C	N	O	0	0
			54	28	2	24		
3	U	4	Total	C	N	O	0	0
			54	28	2	24		

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



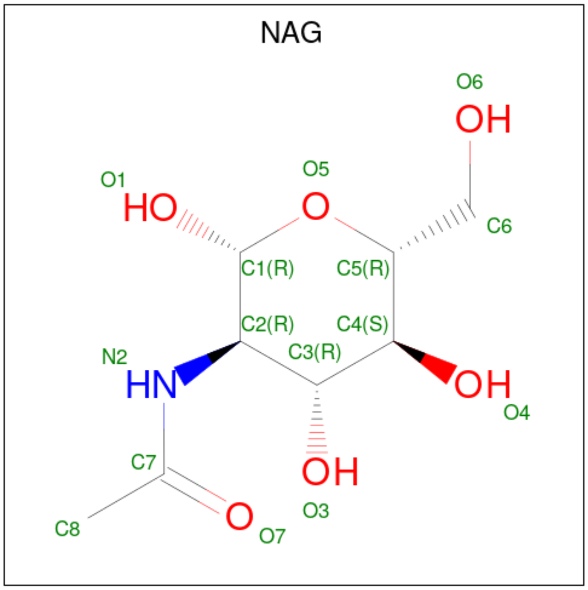
Mol	Chain	Residues	Atoms				AltConf	Trace
4	N	3	Total	C	N	O	0	0
			42	22	2	18		
4	O	3	Total	C	N	O	0	0
			42	22	2	18		
4	W	3	Total	C	N	O	0	0
			42	22	2	18		
4	Y	3	Total	C	N	O	0	0
			42	22	2	18		
4	a	3	Total	C	N	O	0	0
			42	22	2	18		
4	b	3	Total	C	N	O	0	0
			42	22	2	18		

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
5	Q	3	Total	C	N	O	0	0
			42	22	2	18		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	AltConf
6	A	1	Total C N O 90 48 6 36	0
6	A	1	Total C N O 90 48 6 36	0
6	A	1	Total C N O 90 48 6 36	0
6	A	1	Total C N O 90 48 6 36	0
6	A	1	Total C N O 90 48 6 36	0
6	A	1	Total C N O 90 48 6 36	0
6	B	1	Total C N O 120 64 8 48	0
6	B	1	Total C N O 120 64 8 48	0
6	B	1	Total C N O 120 64 8 48	0
6	B	1	Total C N O 120 64 8 48	0
6	B	1	Total C N O 120 64 8 48	0
6	B	1	Total C N O 120 64 8 48	0
6	B	1	Total C N O 120 64 8 48	0
6	B	1	Total C N O 120 64 8 48	0

Continued on next page...

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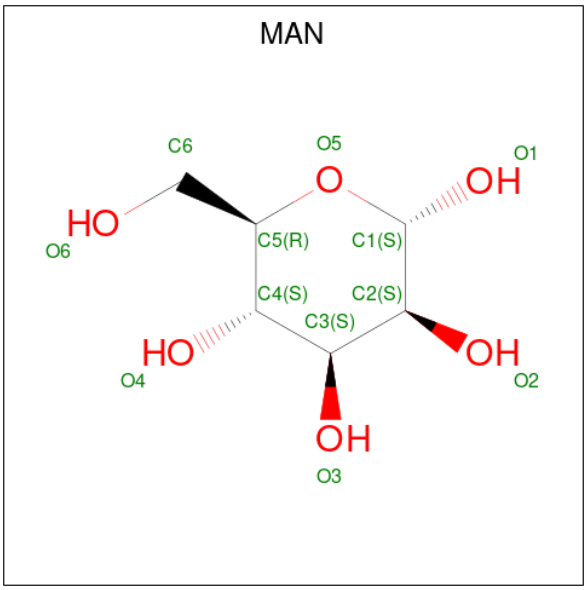
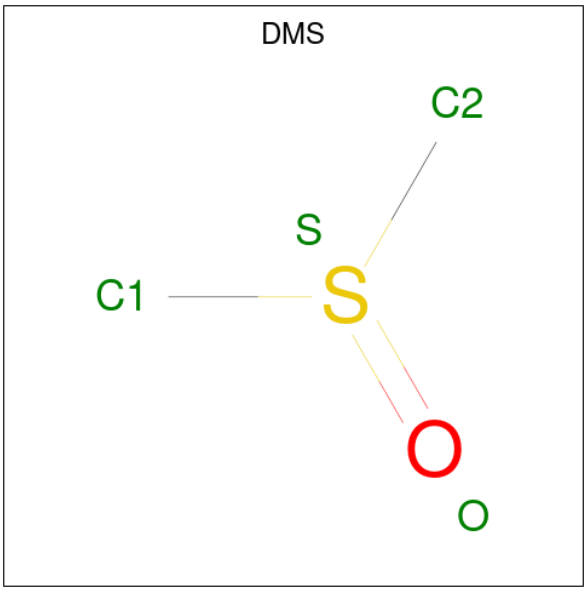
Mol	Chain	Residues	Atoms	AltConf
6	C	1	Total C N O 60 32 4 24	0
6	C	1	Total C N O 60 32 4 24	0
6	C	1	Total C N O 60 32 4 24	0
6	C	1	Total C N O 60 32 4 24	0

- Molecule 7 is alpha-D-mannopyranose (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms	AltConf
7	A	1	Total C O 12 6 6	0
7	C	1	Total C O 12 6 6	0

- Molecule 8 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



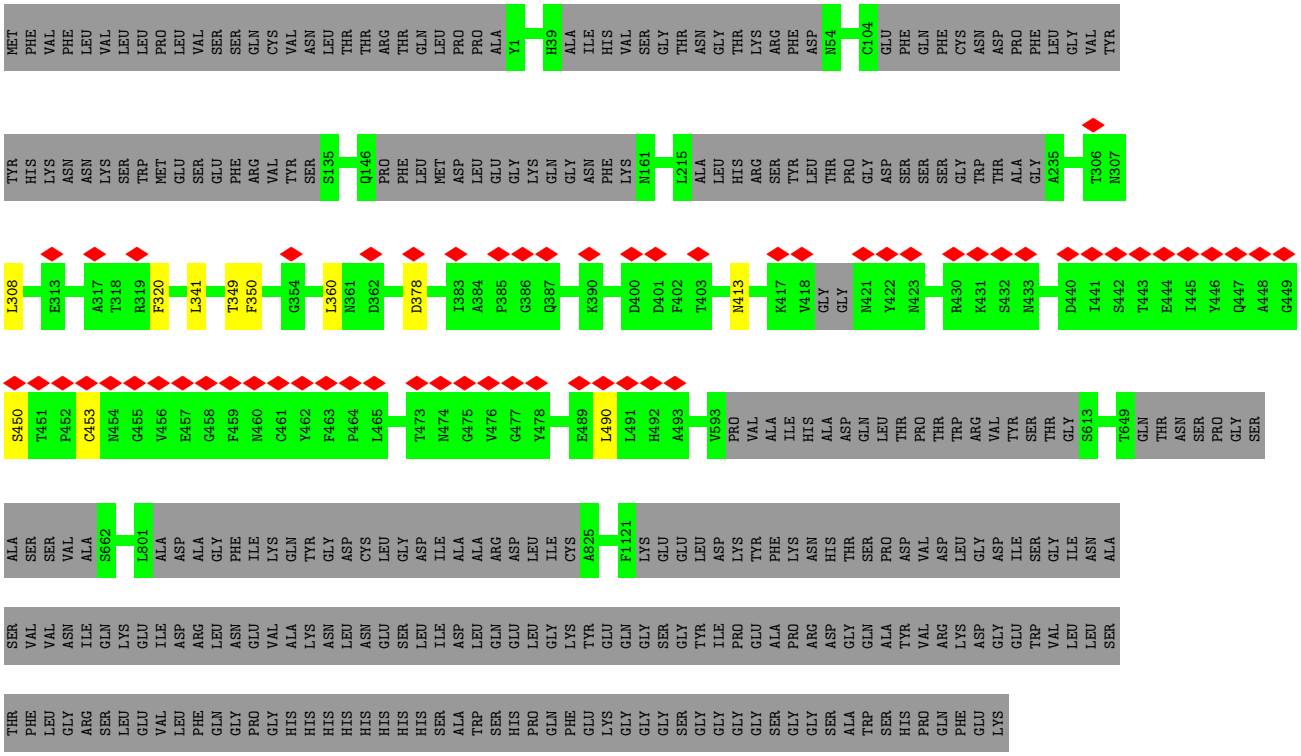
Mol	Chain	Residues	Atoms				AltConf
8	A	1	Total	C	O	S	0
			12	6	3	3	
8	A	1	Total	C	O	S	0
			12	6	3	3	
8	A	1	Total	C	O	S	0
			12	6	3	3	

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.

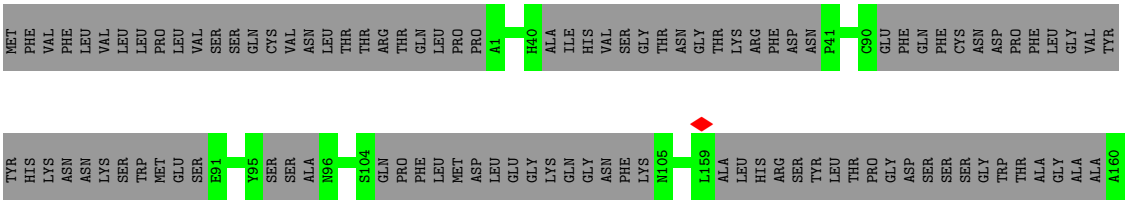
• Molecule 1: Spike glycoprotein

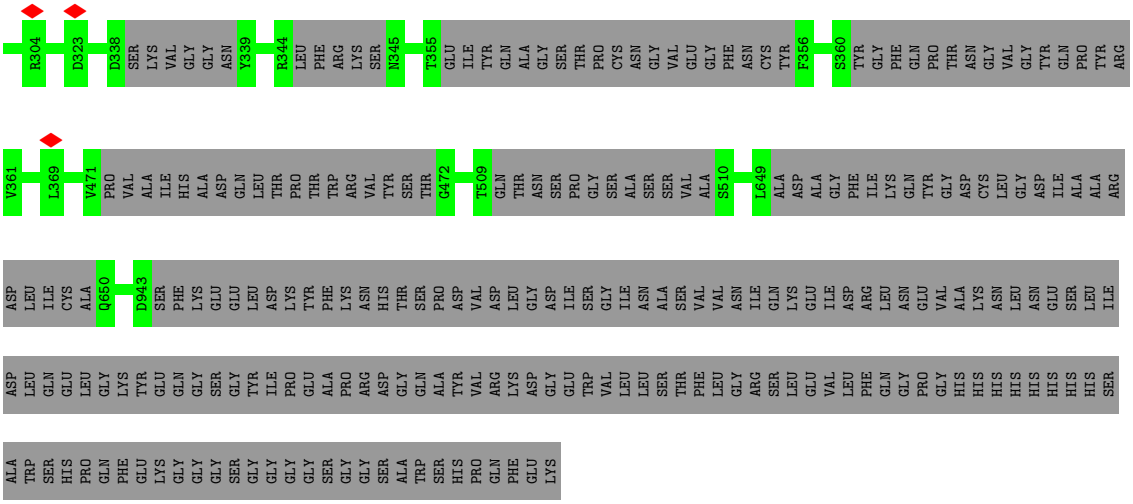
Chain A:



• Molecule 1: Spike glycoprotein

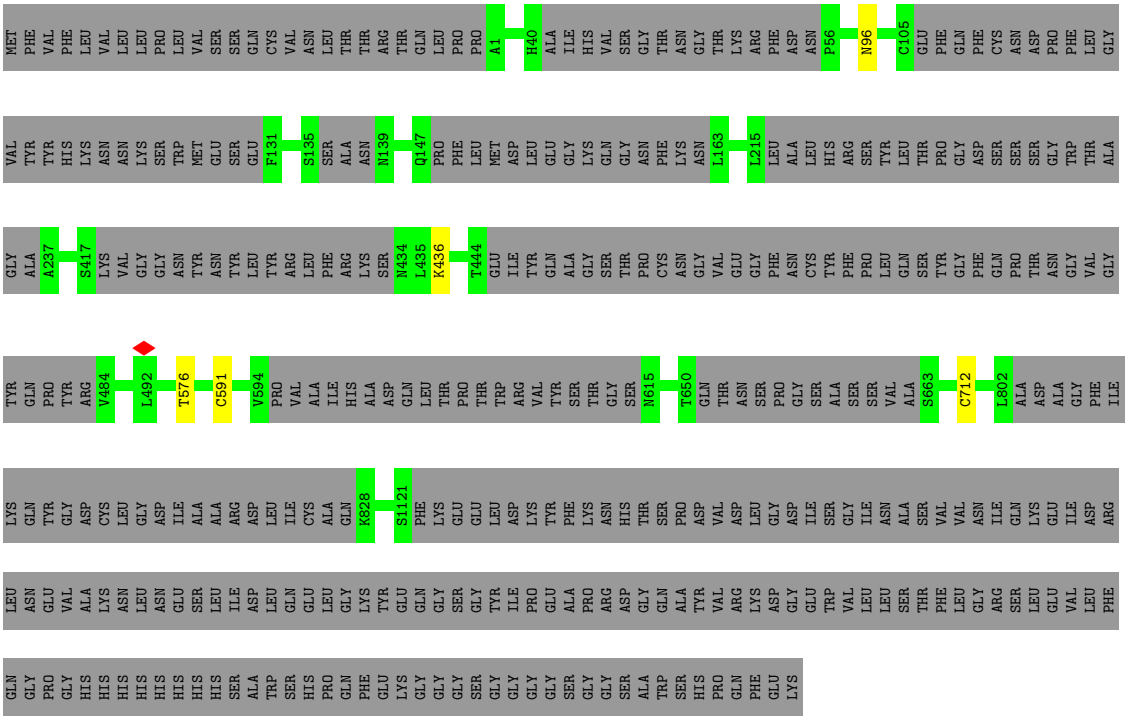
Chain B:





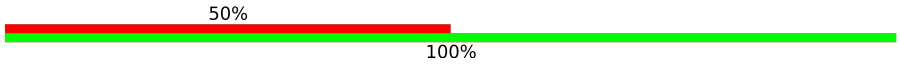
• Molecule 1: Spike glycoprotein

Chain C:



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

Chain D:

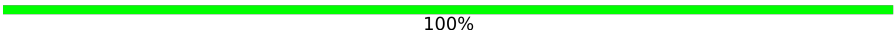


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:

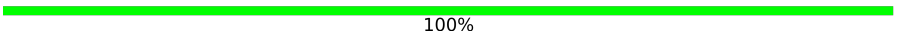
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:



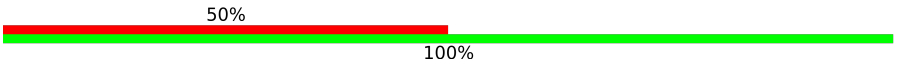
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:



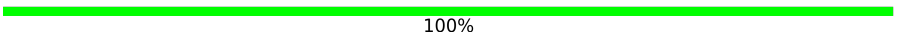
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:



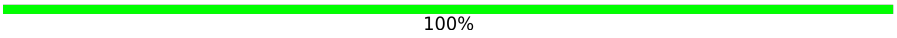
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:



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

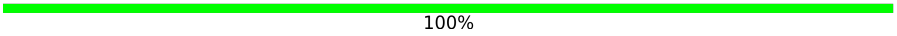
Chain L:



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

Chain M: 

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

Chain P: 

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

Chain S: 

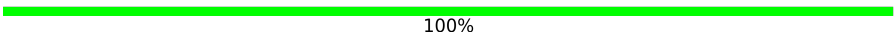
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T: 

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

Chain V: 

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

Chain X: 

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

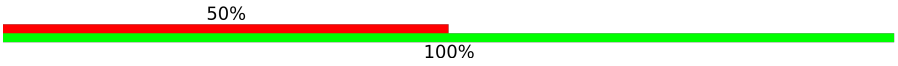
Chain Z: 

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

Chain c:

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

Chain d:



• Molecule 3: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

• Molecule 3: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:

• Molecule 3: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:

• Molecule 3: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

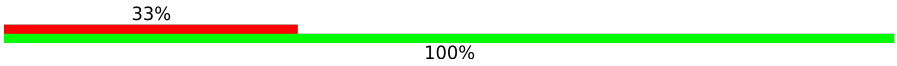
Chain U:

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

Chain N:

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

Chain O:

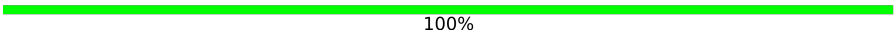


• Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:

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

Chain Y:



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

Chain a:

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

Chain b:

• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:


NAG1
NAG2
BMA3

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	45000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	36	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	1.655	Depositor
Minimum map value	-0.621	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.035	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	452.30396, 452.30396, 452.30396	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0469999, 1.0469999, 1.0469999	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, DMS, BMA, 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	0.47	1/7877 (0.0%)	0.52	3/10717 (0.0%)
1	B	0.36	0/7522	0.48	0/10229
1	C	0.37	0/7395	0.50	1/10059 (0.0%)
All	All	0.40	1/22794 (0.0%)	0.50	4/31005 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	308	LEU	C-N	28.50	1.99	1.34

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	308	LEU	O-C-N	-19.82	90.99	122.70
1	A	308	LEU	CA-C-N	10.42	140.13	117.20
1	A	308	LEU	C-N-CA	6.40	137.71	121.70
1	C	712	CYS	CA-CB-SG	5.15	123.27	114.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles

5.3.1 Protein backbone

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	968/1288 (75%)	924 (96%)	44 (4%)	0	100	100
1	B	917/1288 (71%)	903 (98%)	14 (2%)	0	100	100
1	C	908/1288 (70%)	882 (97%)	26 (3%)	0	100	100
All	All	2793/3864 (72%)	2709 (97%)	84 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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	865/1113 (78%)	855 (99%)	10 (1%)	71	88
1	B	829/1113 (74%)	829 (100%)	0	100	100
1	C	816/1113 (73%)	812 (100%)	4 (0%)	88	94
All	All	2510/3339 (75%)	2496 (99%)	14 (1%)	86	94

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	450	SER
1	A	453	CYS
1	C	591	CYS
1	C	436	LYS
1	C	576	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 49 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	710	GLN
1	C	317	ASN
1	B	751	GLN
1	B	903	GLN
1	C	537	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)

69 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	D	1	2,1	15,15,15	0.33	0	21,21,21	0.15	0
2	NAG	D	2	2	15,15,15	0.34	0	21,21,21	0.11	0
3	NAG	E	1	3,1	15,15,15	0.35	0	21,21,21	0.17	0
3	NAG	E	2	3	15,15,15	0.32	0	21,21,21	0.28	0
3	BMA	E	3	3	12,12,12	0.52	0	17,17,17	0.74	0
3	MAN	E	4	3	12,12,12	0.64	0	17,17,17	1.26	1 (5%)
3	NAG	F	1	3,1	15,15,15	0.36	0	21,21,21	0.18	0
3	NAG	F	2	3	15,15,15	0.40	0	21,21,21	0.60	0
3	BMA	F	3	3	12,12,12	0.56	0	17,17,17	0.67	0
3	MAN	F	4	3	12,12,12	0.61	0	17,17,17	1.17	2 (11%)
2	NAG	G	1	2,1	15,15,15	0.34	0	21,21,21	0.20	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	G	2	2	15,15,15	0.49	0	21,21,21	0.89	2 (9%)
2	NAG	H	1	2,1	15,15,15	0.34	0	21,21,21	0.28	0
2	NAG	H	2	2	15,15,15	0.35	0	21,21,21	0.27	0
2	NAG	I	1	2,1	15,15,15	0.32	0	21,21,21	0.12	0
2	NAG	I	2	2	15,15,15	0.33	0	21,21,21	0.12	0
2	NAG	J	1	2,1	15,15,15	0.35	0	21,21,21	0.33	0
2	NAG	J	2	2	15,15,15	0.35	0	21,21,21	0.13	0
2	NAG	K	1	2,1	15,15,15	0.34	0	21,21,21	0.28	0
2	NAG	K	2	2	15,15,15	0.32	0	21,21,21	0.14	0
2	NAG	L	1	2,1	15,15,15	0.34	0	21,21,21	0.27	0
2	NAG	L	2	2	15,15,15	0.59	0	21,21,21	0.31	0
2	NAG	M	1	2,1	15,15,15	0.58	0	21,21,21	0.50	0
2	NAG	M	2	2	15,15,15	0.61	0	21,21,21	0.97	2 (9%)
4	NAG	N	1	4,1	15,15,15	0.35	0	21,21,21	0.15	0
4	NAG	N	2	4	15,15,15	0.43	0	21,21,21	0.89	2 (9%)
4	BMA	N	3	4	12,12,12	0.51	0	17,17,17	0.70	0
4	NAG	O	1	4	15,15,15	0.40	0	21,21,21	0.40	0
4	NAG	O	2	4	15,15,15	0.33	0	21,21,21	0.27	0
4	BMA	O	3	4	12,12,12	0.62	0	17,17,17	0.65	0
2	NAG	P	1	2	15,15,15	0.44	0	21,21,21	0.50	0
2	NAG	P	2	2	15,15,15	0.37	0	21,21,21	0.27	0
5	NAG	Q	1	5	15,15,15	0.42	0	21,21,21	0.95	2 (9%)
5	NAG	Q	2	5	15,15,15	0.52	0	21,21,21	0.62	0
5	BMA	Q	3	5	12,12,12	1.26	2 (16%)	17,17,17	0.71	0
3	NAG	R	1	3,1	15,15,15	0.35	0	21,21,21	0.23	0
3	NAG	R	2	3	15,15,15	0.34	0	21,21,21	0.39	0
3	BMA	R	3	3	12,12,12	0.81	1 (8%)	17,17,17	0.88	1 (5%)
3	MAN	R	4	3	12,12,12	0.59	0	17,17,17	0.89	2 (11%)
2	NAG	S	1	2	15,15,15	0.84	1 (6%)	21,21,21	1.65	5 (23%)
2	NAG	S	2	2	15,15,15	0.47	0	21,21,21	0.32	0
2	NAG	T	1	2	15,15,15	0.41	0	21,21,21	0.94	2 (9%)
2	NAG	T	2	2	15,15,15	0.54	0	21,21,21	0.32	0
3	NAG	U	1	3	15,15,15	0.35	0	21,21,21	0.18	0
3	NAG	U	2	3	15,15,15	0.34	0	21,21,21	0.20	0
3	BMA	U	3	3	12,12,12	0.51	0	17,17,17	0.57	0
3	MAN	U	4	3	12,12,12	0.82	0	17,17,17	1.54	2 (11%)
2	NAG	V	1	2	15,15,15	0.33	0	21,21,21	0.24	0
2	NAG	V	2	2	15,15,15	0.49	0	21,21,21	0.89	2 (9%)
4	NAG	W	1	4	15,15,15	0.40	0	21,21,21	0.47	0
4	NAG	W	2	4	15,15,15	0.54	0	21,21,21	1.81	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	BMA	W	3	4	12,12,12	0.66	0	17,17,17	0.85	1 (5%)
2	NAG	X	1	2	15,15,15	0.33	0	21,21,21	0.19	0
2	NAG	X	2	2	15,15,15	0.42	0	21,21,21	0.24	0
4	NAG	Y	1	4,1	15,15,15	0.33	0	21,21,21	0.17	0
4	NAG	Y	2	4	15,15,15	0.32	0	21,21,21	0.24	0
4	BMA	Y	3	4	12,12,12	0.63	0	17,17,17	0.65	0
2	NAG	Z	1	2	15,15,15	0.41	0	21,21,21	0.90	2 (9%)
2	NAG	Z	2	2	15,15,15	0.34	0	21,21,21	0.18	0
4	NAG	a	1	4,1	15,15,15	0.41	0	21,21,21	0.86	0
4	NAG	a	2	4	15,15,15	0.42	0	21,21,21	0.32	0
4	BMA	a	3	4	12,12,12	0.59	0	17,17,17	0.85	1 (5%)
4	NAG	b	1	4	15,15,15	0.47	0	21,21,21	0.94	2 (9%)
4	NAG	b	2	4	15,15,15	0.31	0	21,21,21	0.34	0
4	BMA	b	3	4	12,12,12	0.63	0	17,17,17	0.70	0
2	NAG	c	1	2	15,15,15	0.41	0	21,21,21	0.82	1 (4%)
2	NAG	c	2	2	15,15,15	0.39	0	21,21,21	0.34	0
2	NAG	d	1	2	15,15,15	0.35	0	21,21,21	0.29	0
2	NAG	d	2	2	15,15,15	0.43	0	21,21,21	0.25	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	D	1	2,1	-	1/6/26/26	0/1/1/1
2	NAG	D	2	2	-	0/6/26/26	0/1/1/1
3	NAG	E	1	3,1	-	2/6/26/26	0/1/1/1
3	NAG	E	2	3	-	0/6/26/26	0/1/1/1
3	BMA	E	3	3	-	0/2/22/22	0/1/1/1
3	MAN	E	4	3	-	0/2/22/22	0/1/1/1
3	NAG	F	1	3,1	-	1/6/26/26	0/1/1/1
3	NAG	F	2	3	-	4/6/26/26	0/1/1/1
3	BMA	F	3	3	-	1/2/22/22	0/1/1/1
3	MAN	F	4	3	-	0/2/22/22	0/1/1/1
2	NAG	G	1	2,1	-	0/6/26/26	0/1/1/1
2	NAG	G	2	2	-	4/6/26/26	0/1/1/1
2	NAG	H	1	2,1	-	2/6/26/26	0/1/1/1
2	NAG	H	2	2	-	2/6/26/26	0/1/1/1
2	NAG	I	1	2,1	-	2/6/26/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	I	2	2	-	0/6/26/26	0/1/1/1
2	NAG	J	1	2,1	-	2/6/26/26	0/1/1/1
2	NAG	J	2	2	-	2/6/26/26	0/1/1/1
2	NAG	K	1	2,1	-	2/6/26/26	0/1/1/1
2	NAG	K	2	2	-	2/6/26/26	0/1/1/1
2	NAG	L	1	2,1	-	2/6/26/26	0/1/1/1
2	NAG	L	2	2	-	1/6/26/26	0/1/1/1
2	NAG	M	1	2,1	-	4/6/26/26	0/1/1/1
2	NAG	M	2	2	-	4/6/26/26	0/1/1/1
4	NAG	N	1	4,1	-	0/6/26/26	0/1/1/1
4	NAG	N	2	4	-	4/6/26/26	0/1/1/1
4	BMA	N	3	4	-	2/2/22/22	0/1/1/1
4	NAG	O	1	4	-	4/6/26/26	0/1/1/1
4	NAG	O	2	4	-	0/6/26/26	0/1/1/1
4	BMA	O	3	4	-	0/2/22/22	0/1/1/1
2	NAG	P	1	2	-	2/6/26/26	0/1/1/1
2	NAG	P	2	2	-	2/6/26/26	0/1/1/1
5	NAG	Q	1	5	-	6/6/26/26	0/1/1/1
5	NAG	Q	2	5	-	2/6/26/26	0/1/1/1
5	BMA	Q	3	5	-	0/2/22/22	0/1/1/1
3	NAG	R	1	3,1	-	0/6/26/26	0/1/1/1
3	NAG	R	2	3	-	0/6/26/26	0/1/1/1
3	BMA	R	3	3	-	1/2/22/22	0/1/1/1
3	MAN	R	4	3	-	1/2/22/22	0/1/1/1
2	NAG	S	1	2	-	5/6/26/26	0/1/1/1
2	NAG	S	2	2	-	1/6/26/26	0/1/1/1
2	NAG	T	1	2	-	6/6/26/26	0/1/1/1
2	NAG	T	2	2	-	1/6/26/26	0/1/1/1
3	NAG	U	1	3	-	2/6/26/26	0/1/1/1
3	NAG	U	2	3	-	0/6/26/26	0/1/1/1
3	BMA	U	3	3	-	2/2/22/22	0/1/1/1
3	MAN	U	4	3	-	0/2/22/22	0/1/1/1
2	NAG	V	1	2	-	2/6/26/26	0/1/1/1
2	NAG	V	2	2	-	6/6/26/26	0/1/1/1
4	NAG	W	1	4	-	0/6/26/26	0/1/1/1
4	NAG	W	2	4	1/1/6/7	4/6/26/26	0/1/1/1
4	BMA	W	3	4	-	2/2/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	X	1	2	-	2/6/26/26	0/1/1/1
2	NAG	X	2	2	-	4/6/26/26	0/1/1/1
4	NAG	Y	1	4,1	-	0/6/26/26	0/1/1/1
4	NAG	Y	2	4	-	2/6/26/26	0/1/1/1
4	BMA	Y	3	4	-	1/2/22/22	0/1/1/1
2	NAG	Z	1	2	-	4/6/26/26	0/1/1/1
2	NAG	Z	2	2	-	2/6/26/26	0/1/1/1
4	NAG	a	1	4,1	-	3/6/26/26	0/1/1/1
4	NAG	a	2	4	-	4/6/26/26	0/1/1/1
4	BMA	a	3	4	-	0/2/22/22	0/1/1/1
4	NAG	b	1	4	-	5/6/26/26	0/1/1/1
4	NAG	b	2	4	-	0/6/26/26	0/1/1/1
4	BMA	b	3	4	-	0/2/22/22	0/1/1/1
2	NAG	c	1	2	-	4/6/26/26	0/1/1/1
2	NAG	c	2	2	-	1/6/26/26	0/1/1/1
2	NAG	d	1	2	-	0/6/26/26	0/1/1/1
2	NAG	d	2	2	-	3/6/26/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	Q	3	BMA	C4-C5	3.02	1.59	1.53
2	S	1	NAG	O5-C1	-2.76	1.36	1.42
3	R	3	BMA	C1-C2	2.16	1.57	1.52
5	Q	3	BMA	O5-C1	2.02	1.48	1.42

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	W	2	NAG	O1-C1-O5	8.22	135.04	110.38
3	U	4	MAN	O1-C1-O5	-5.00	95.38	110.38
2	S	1	NAG	C3-C4-C5	4.33	117.97	110.24
3	E	4	MAN	O1-C1-O5	-4.11	98.05	110.38
3	F	4	MAN	O1-C1-O5	-3.80	98.97	110.38

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	W	2	NAG	C1

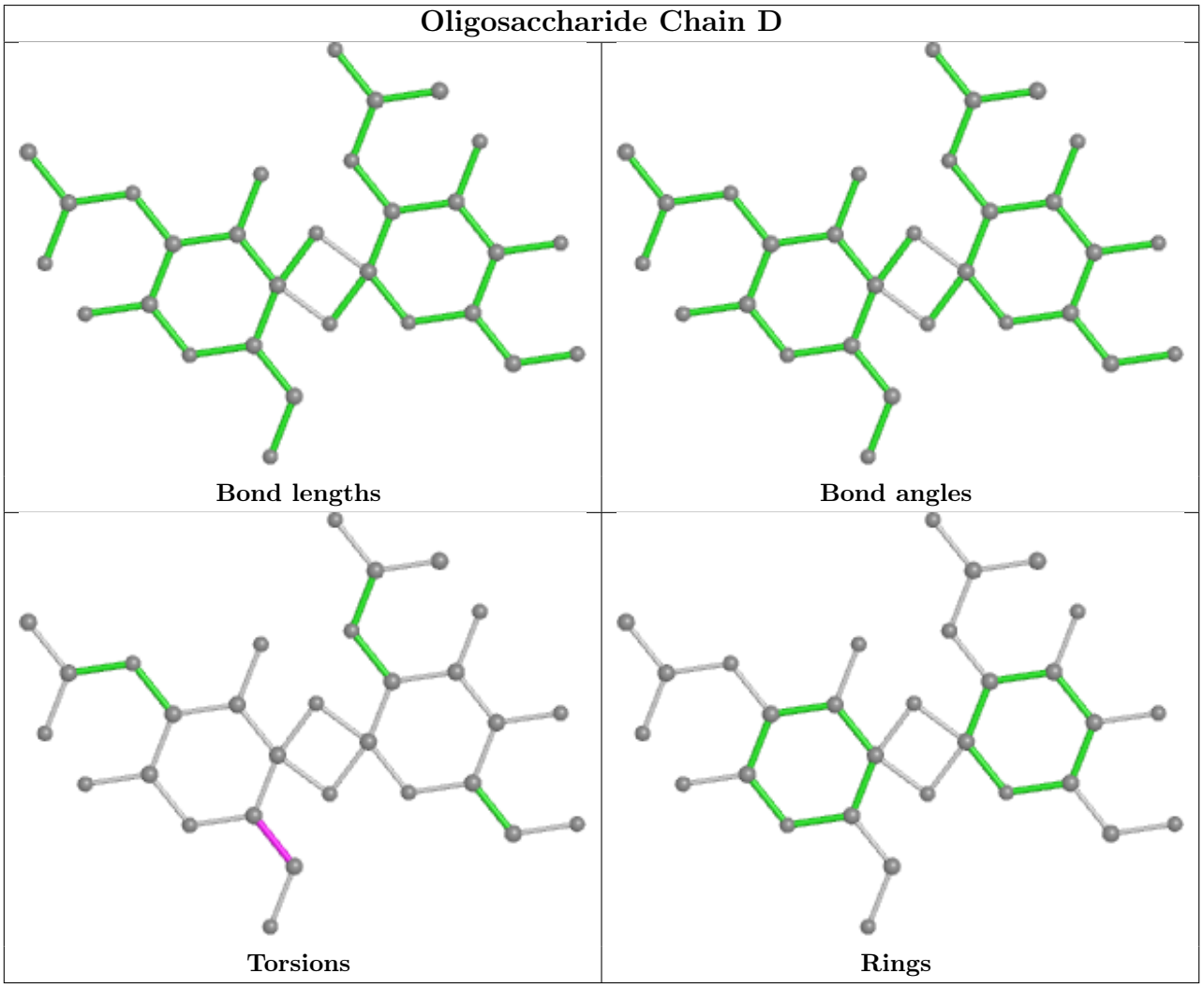
5 of 128 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	V	1	NAG	C1-C2-N2-C7
2	d	2	NAG	C1-C2-N2-C7
4	O	1	NAG	C1-C2-N2-C7
4	W	2	NAG	O5-C5-C6-O6
2	K	1	NAG	C4-C5-C6-O6

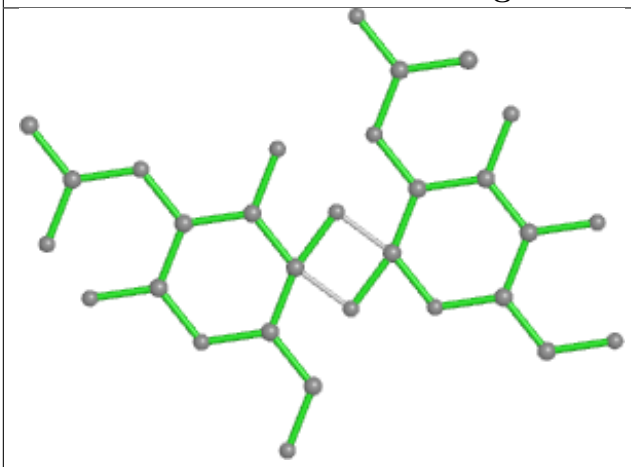
There are no ring outliers.

No monomer is involved in short contacts.

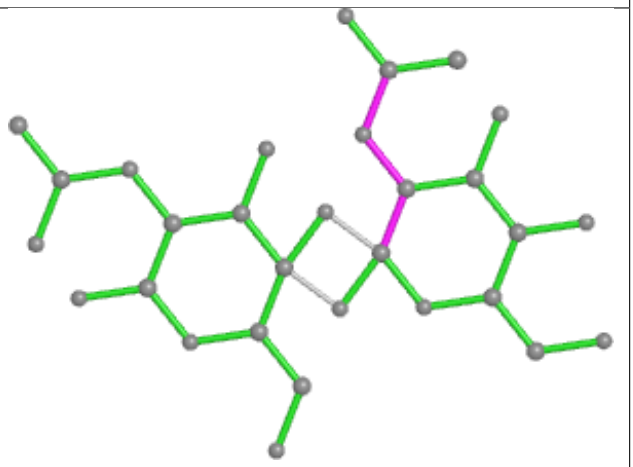
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



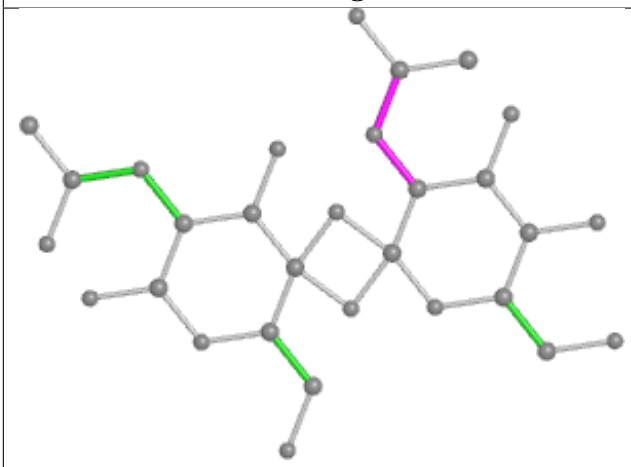
Oligosaccharide Chain G



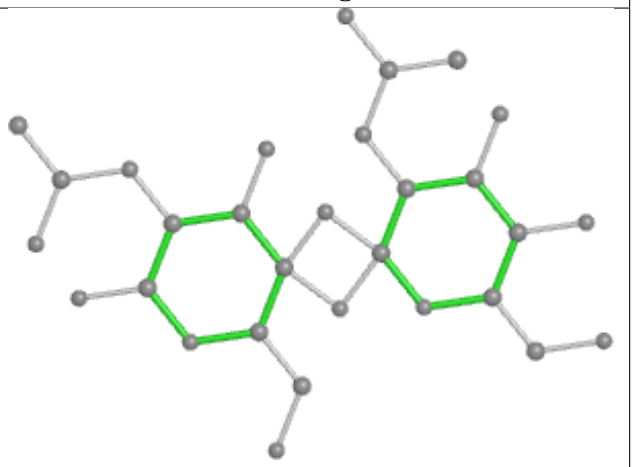
Bond lengths



Bond angles

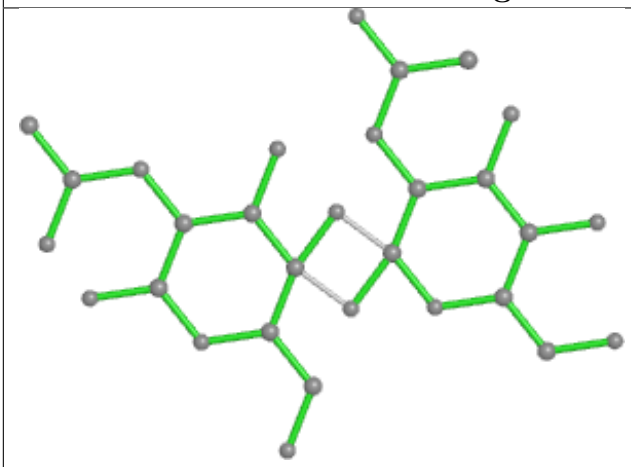


Torsions

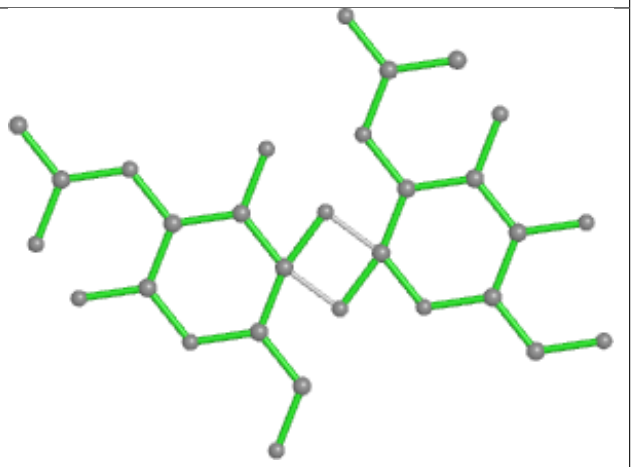


Rings

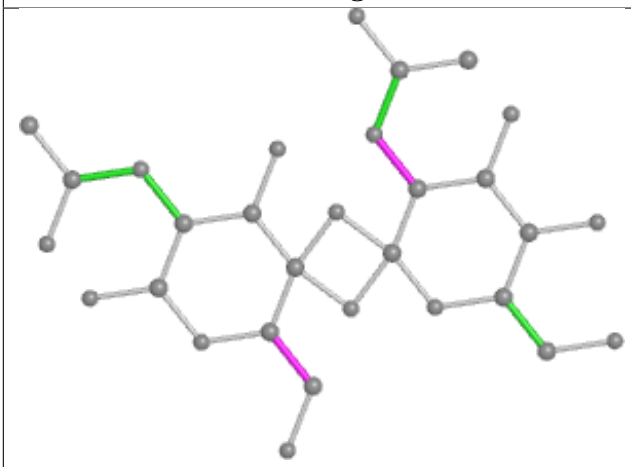
Oligosaccharide Chain H



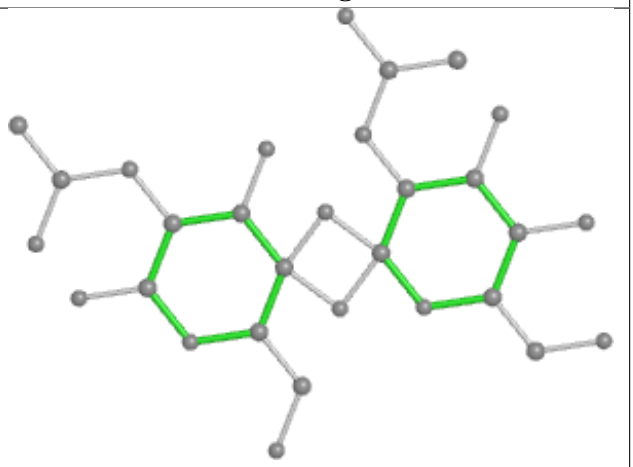
Bond lengths



Bond angles

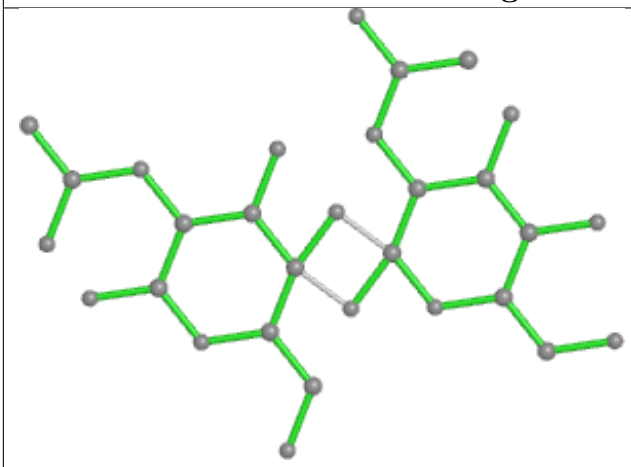


Torsions

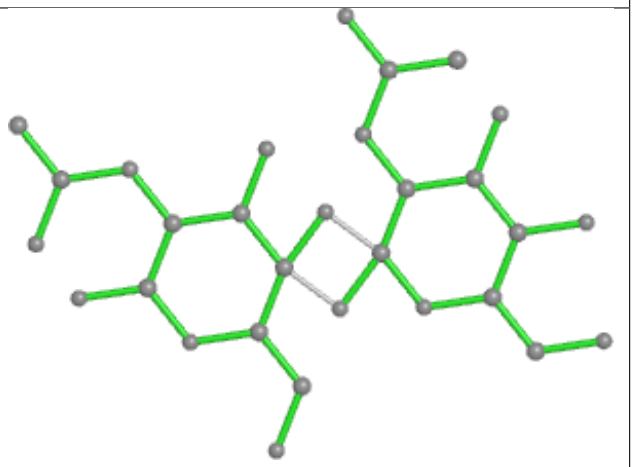


Rings

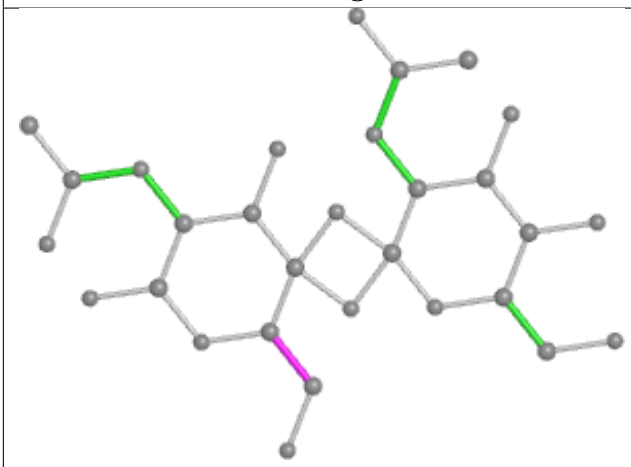
Oligosaccharide Chain I



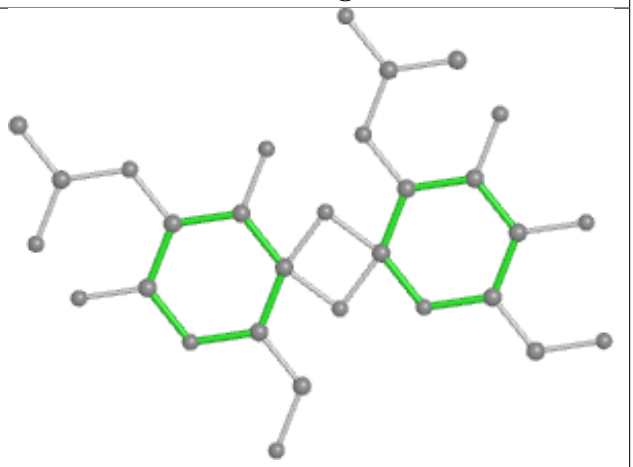
Bond lengths



Bond angles

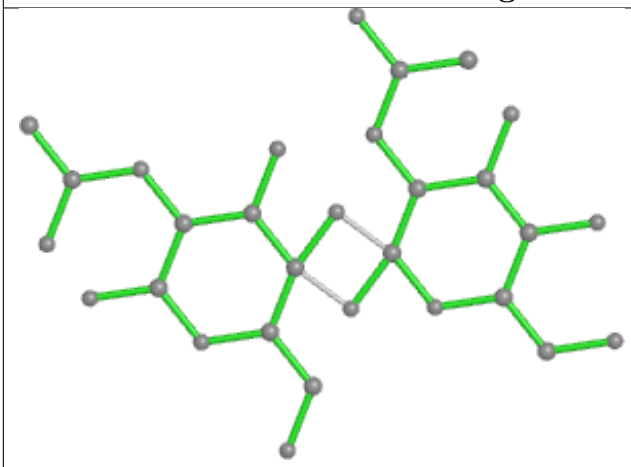


Torsions

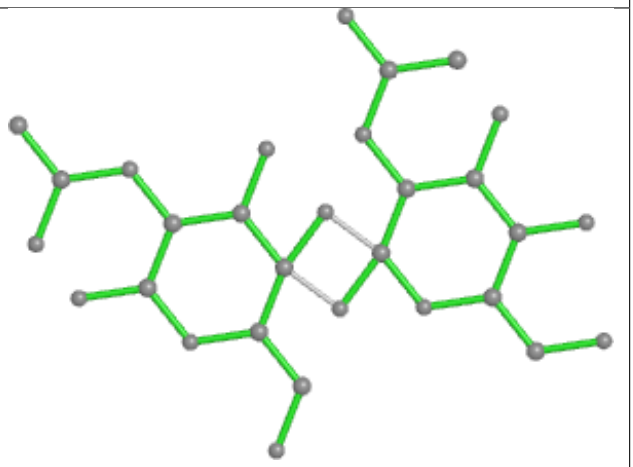


Rings

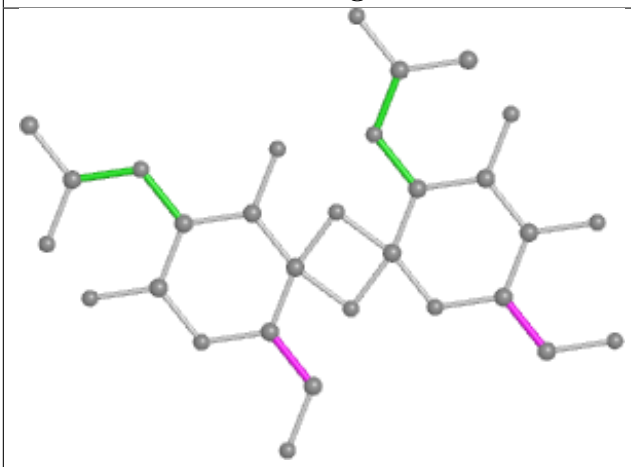
Oligosaccharide Chain J



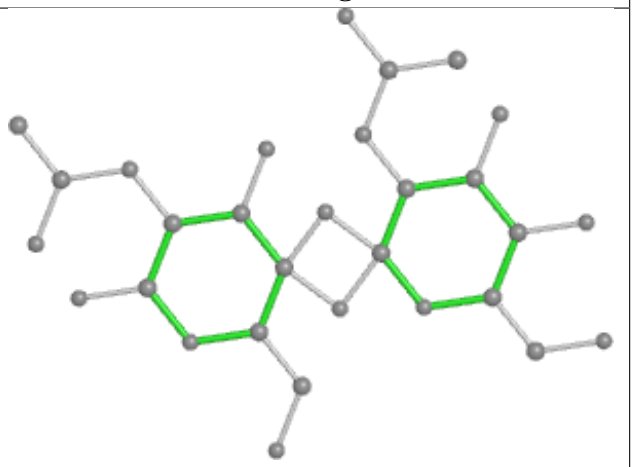
Bond lengths



Bond angles

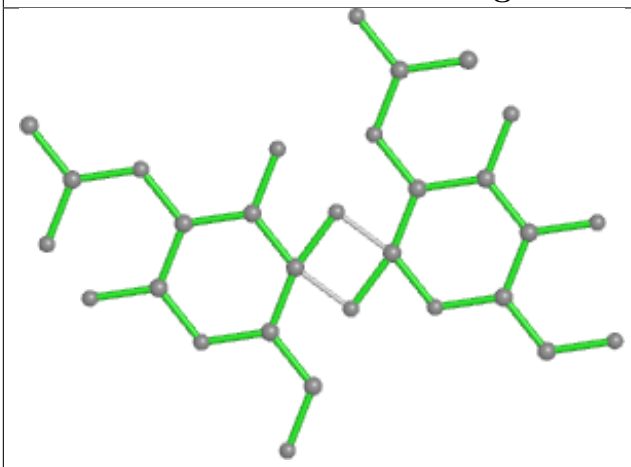


Torsions

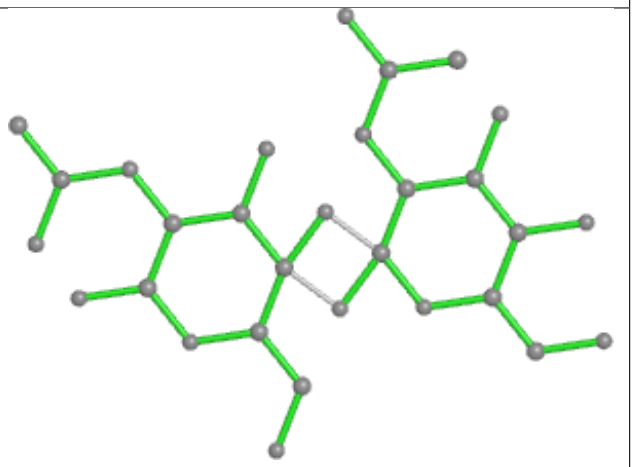


Rings

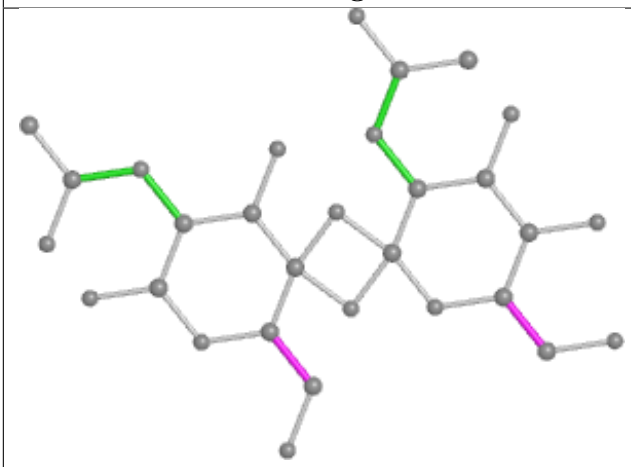
Oligosaccharide Chain K



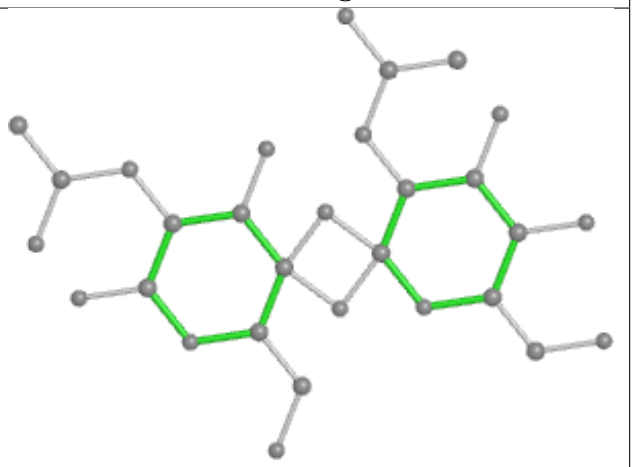
Bond lengths



Bond angles

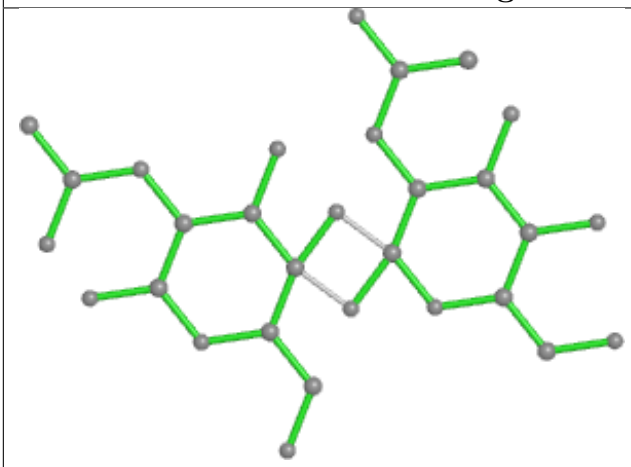


Torsions

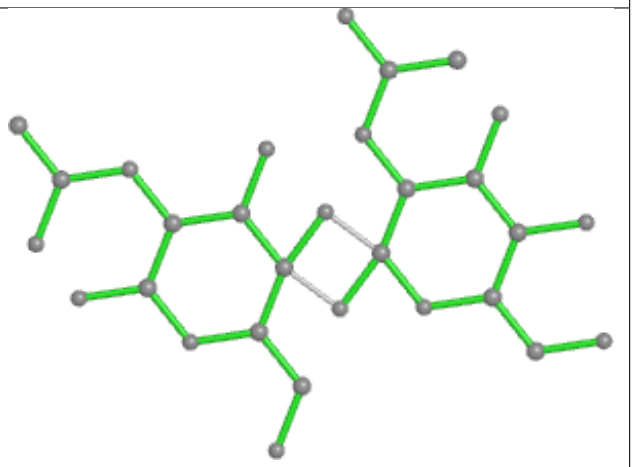


Rings

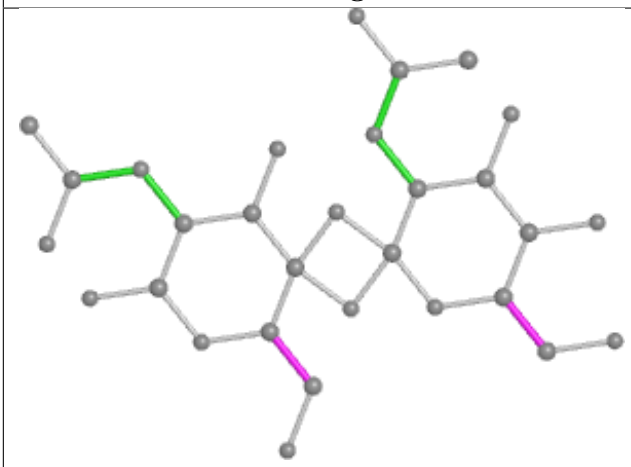
Oligosaccharide Chain L



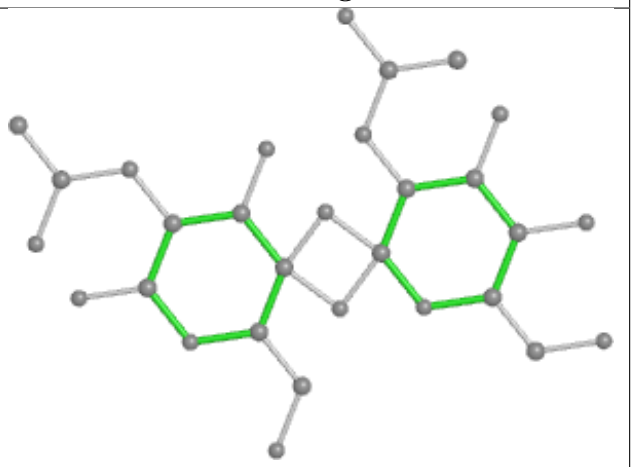
Bond lengths



Bond angles

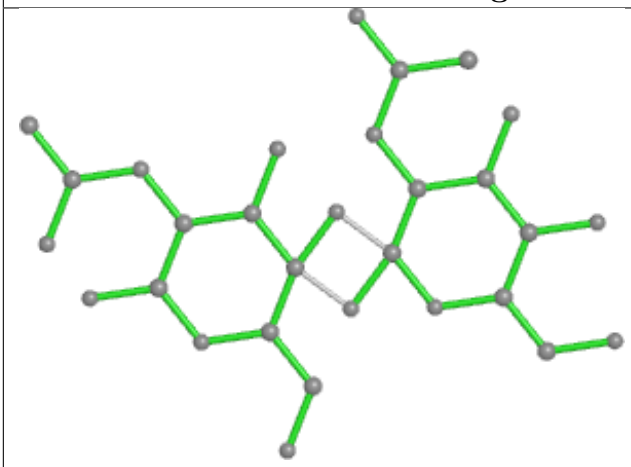


Torsions

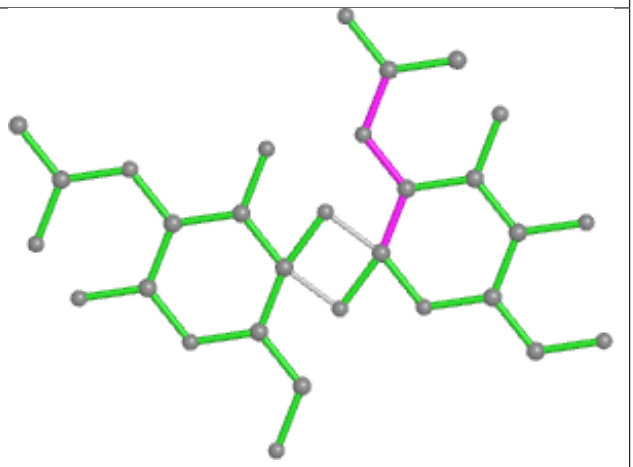


Rings

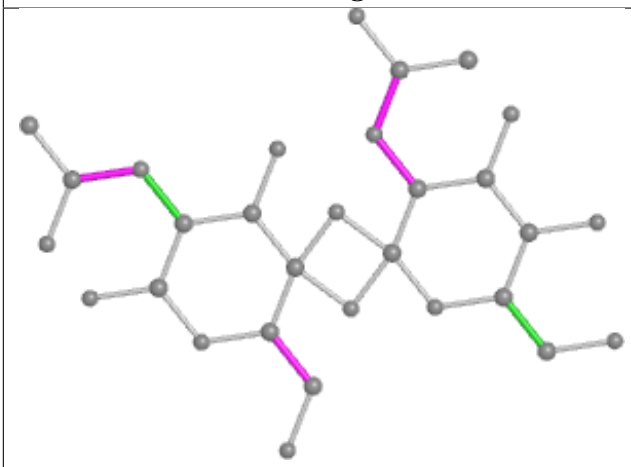
Oligosaccharide Chain M



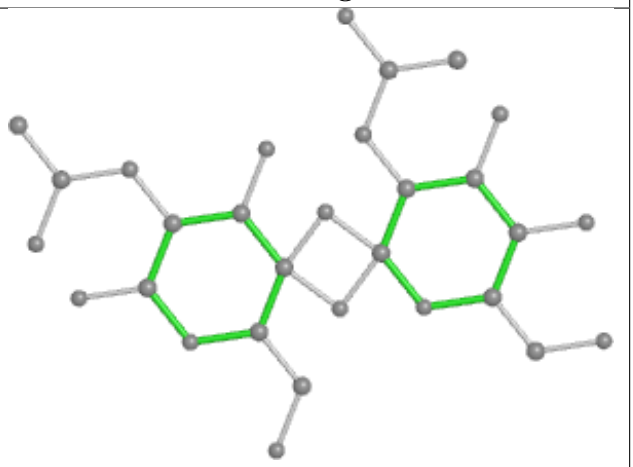
Bond lengths



Bond angles

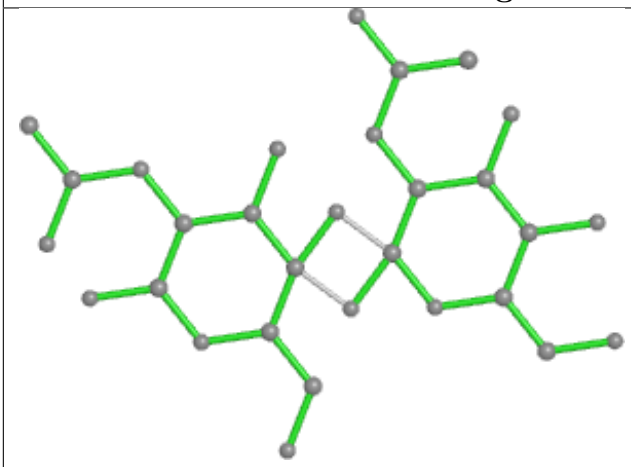


Torsions



Rings

Oligosaccharide Chain P



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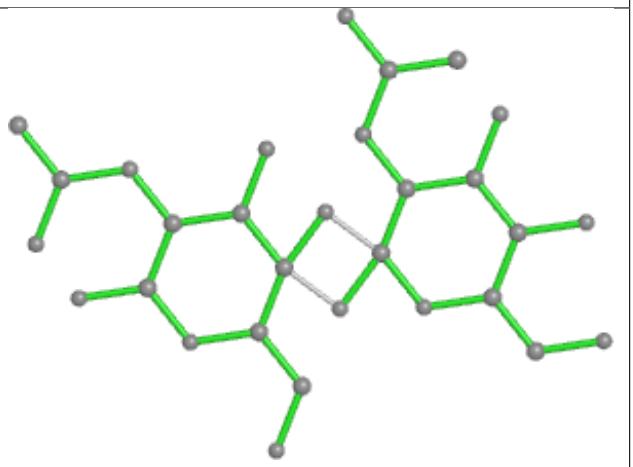
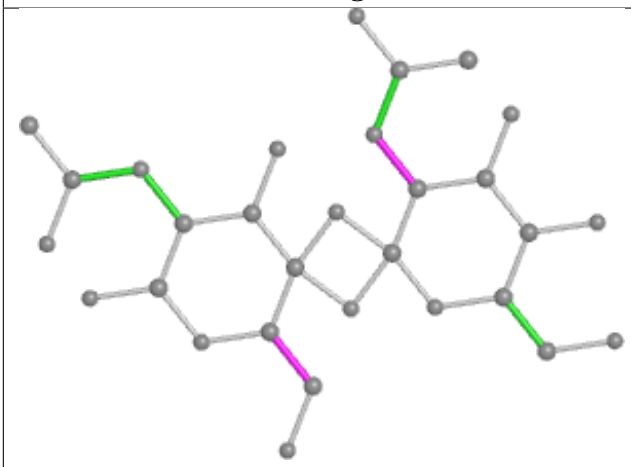


Bond angles



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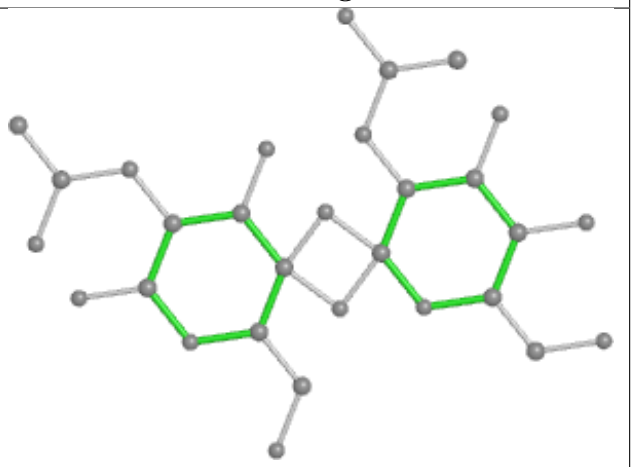
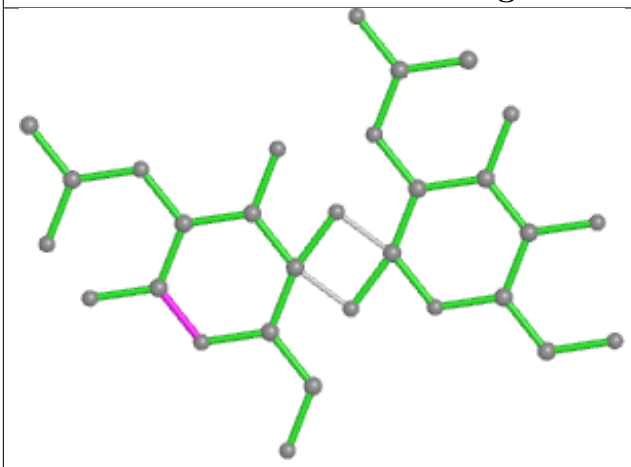


Rings

Oligosaccharide Chain S



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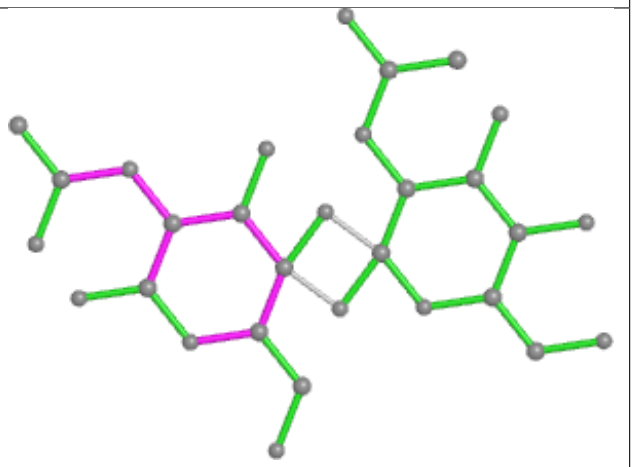
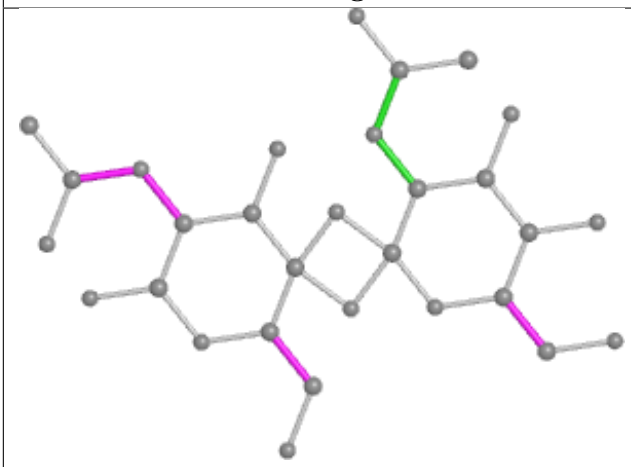


Bond angles



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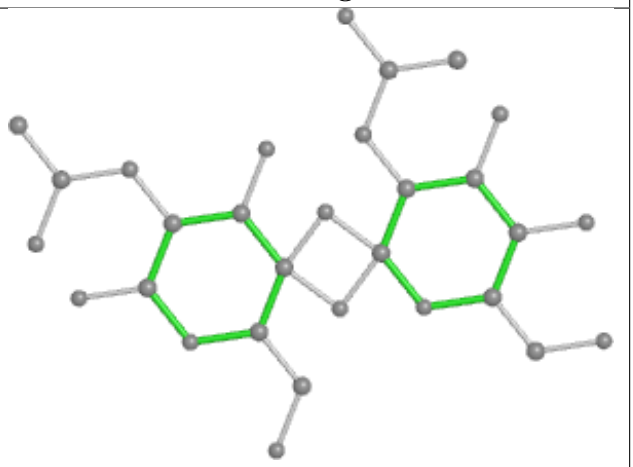
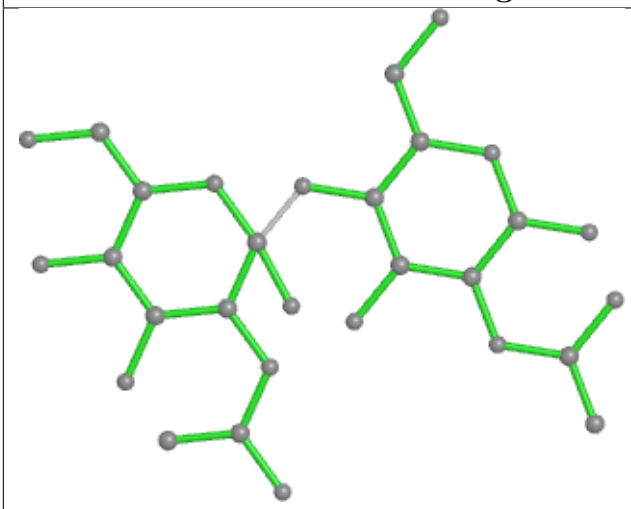


Rings

Oligosaccharide Chain T



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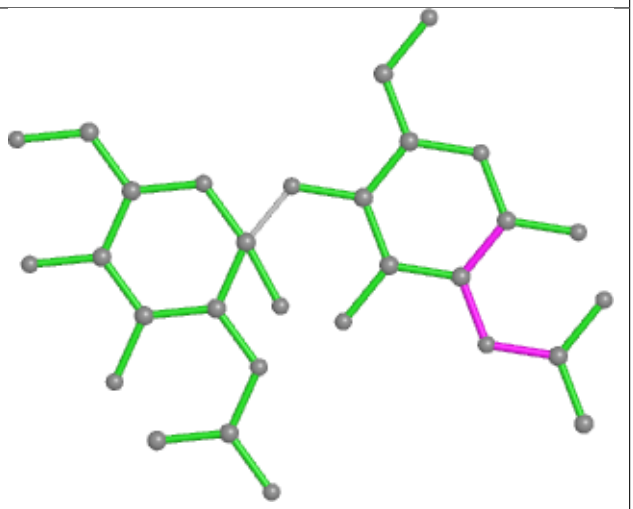
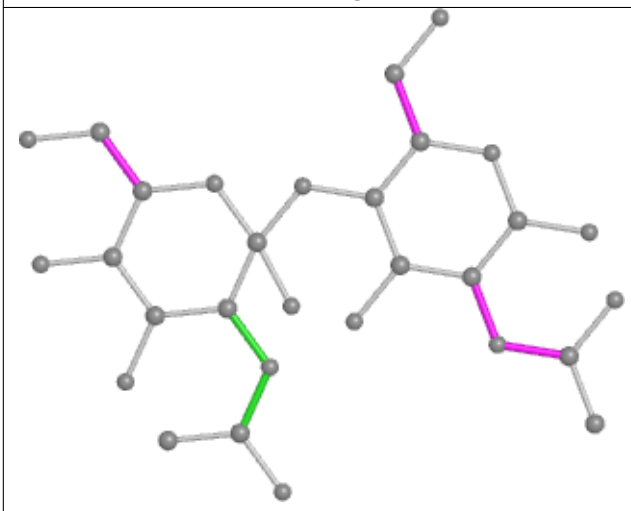


Bond angles



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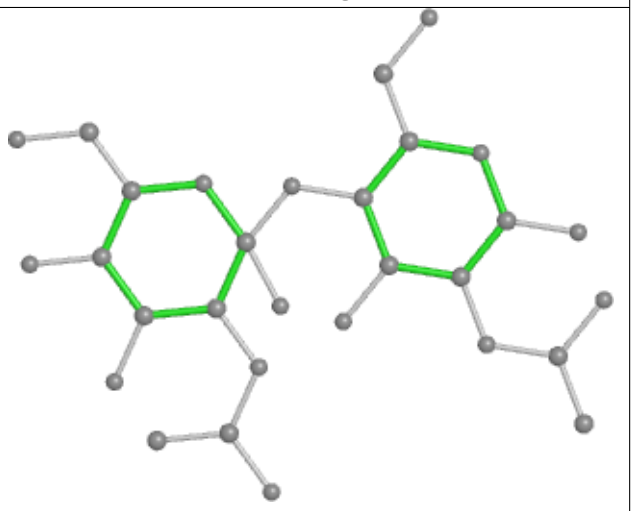
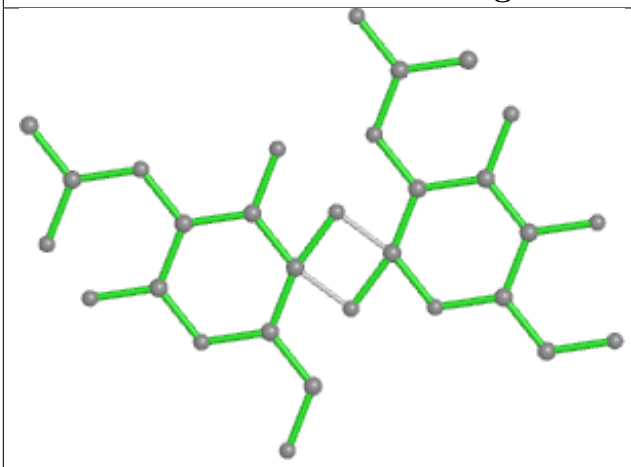


Rings

Oligosaccharide Chain V



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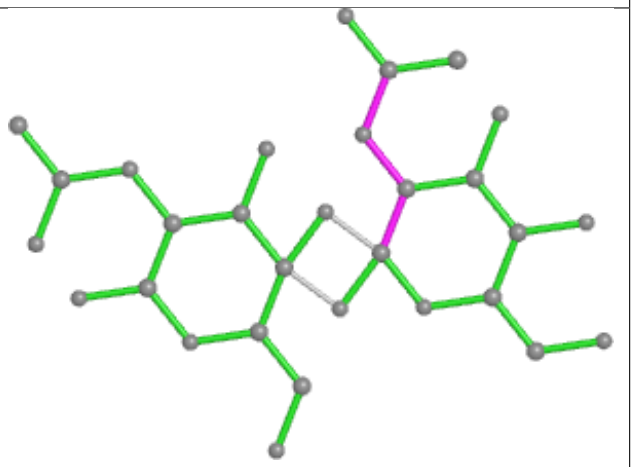
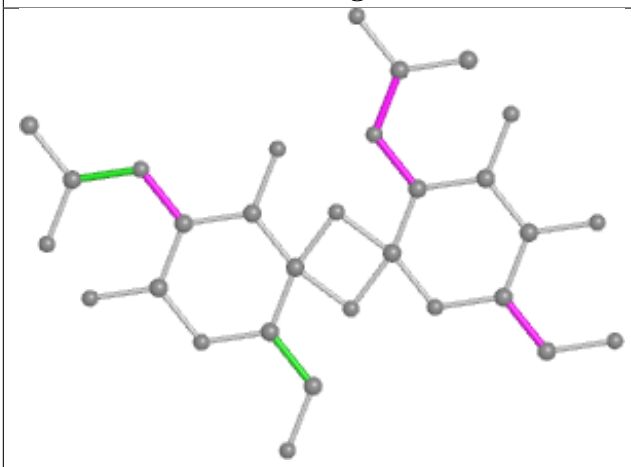


Bond angles



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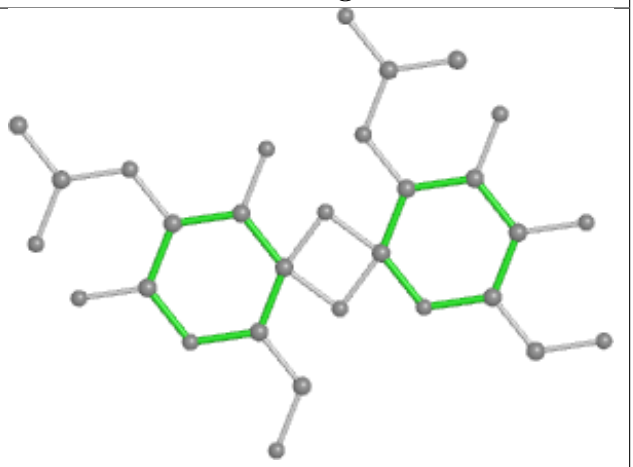
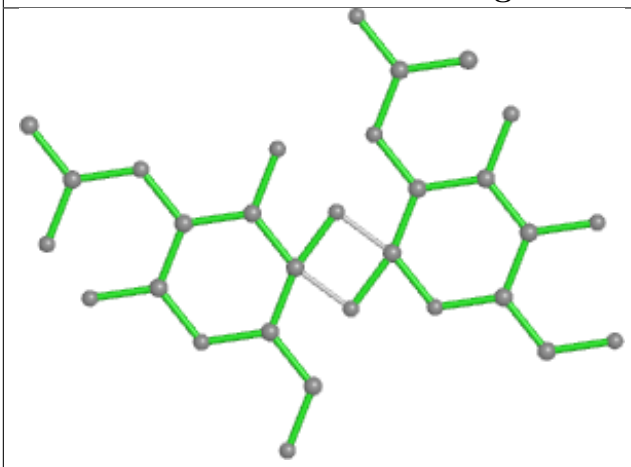


Rings

Oligosaccharide Chain X



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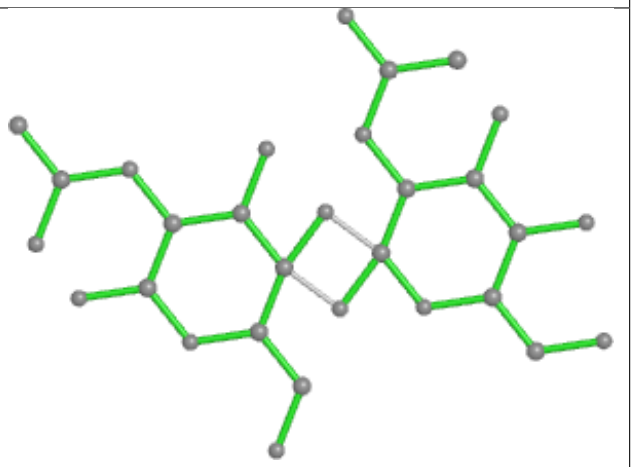
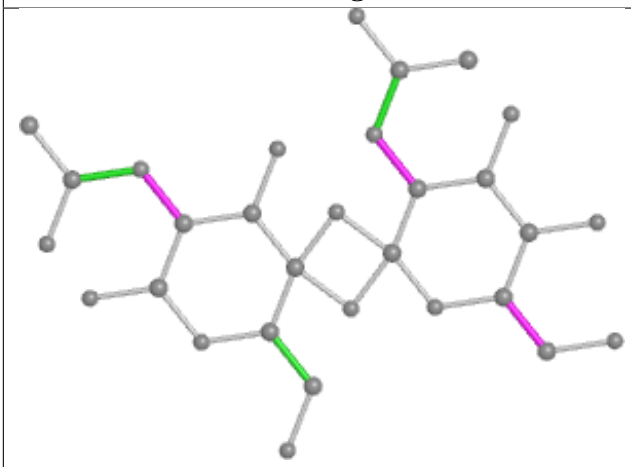


Bond angles



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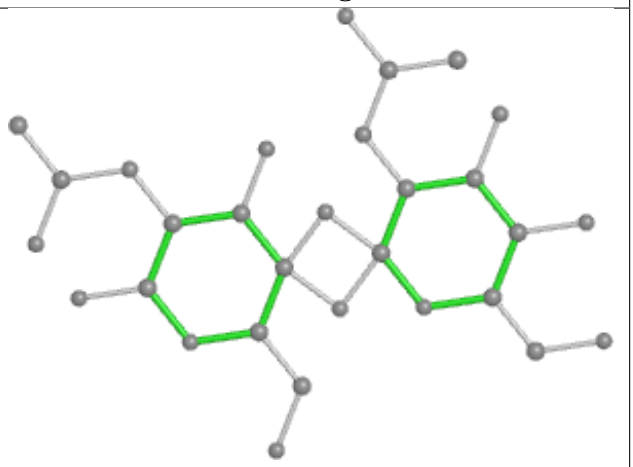
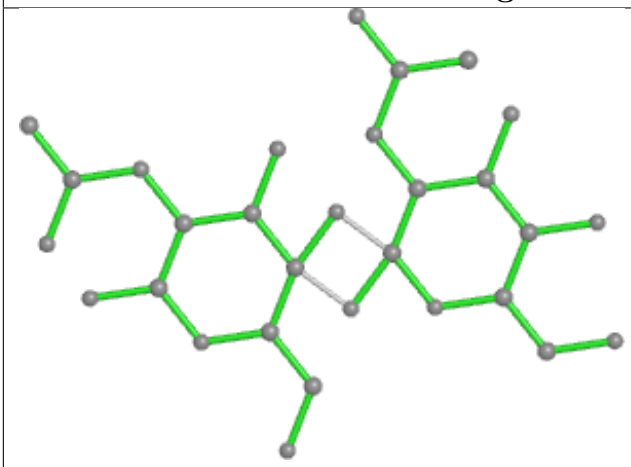


Rings

Oligosaccharide Chain Z



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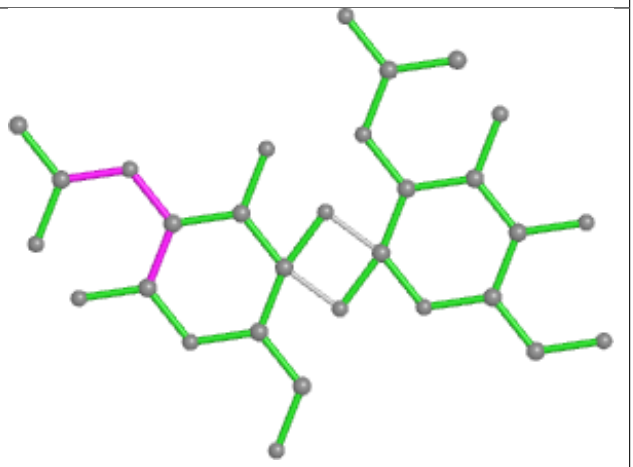
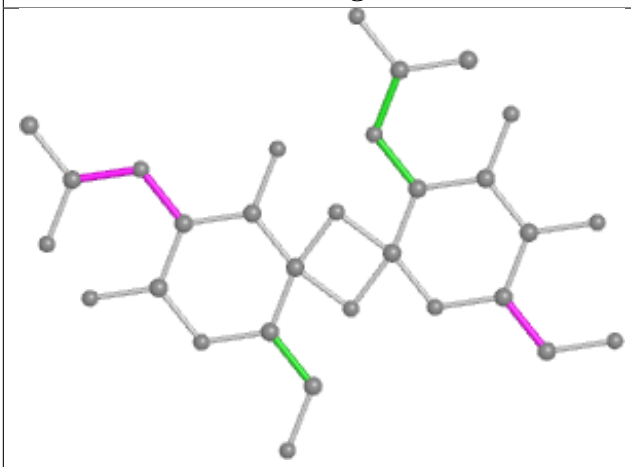


Bond angles



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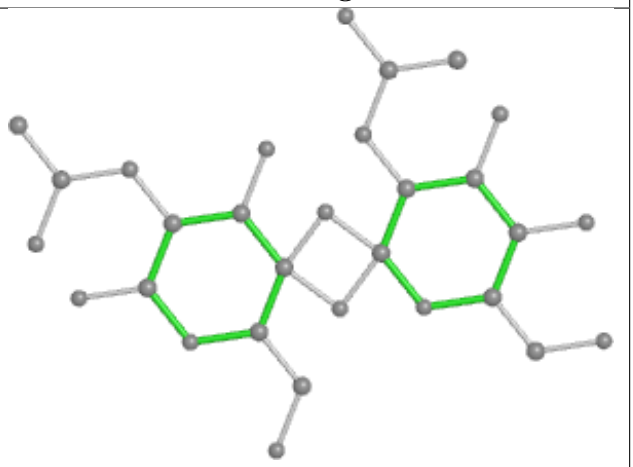
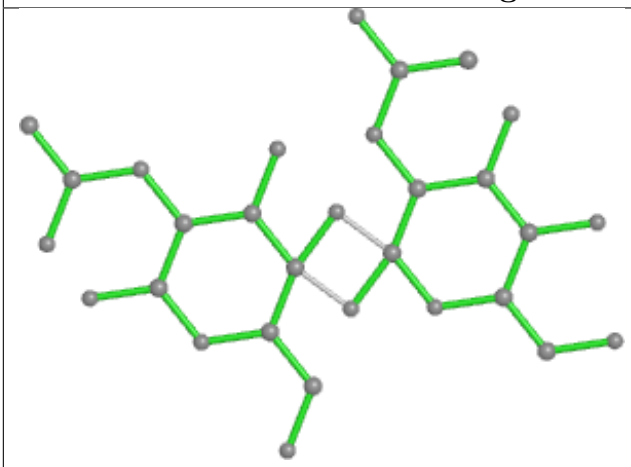


Rings

Oligosaccharide Chain c



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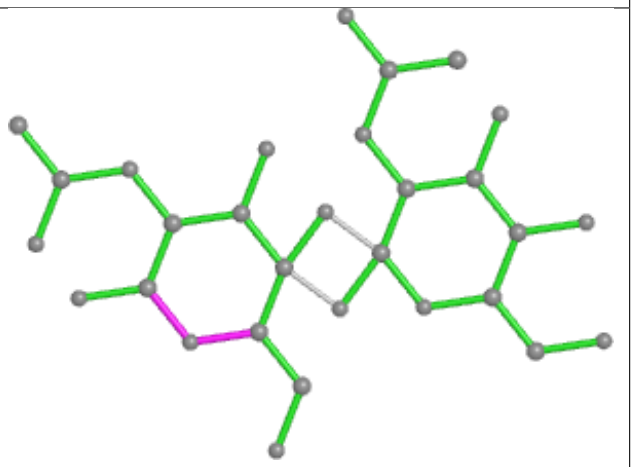
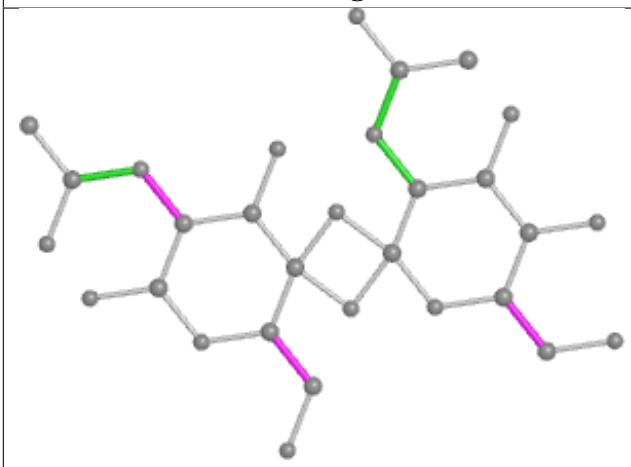


Bond angles



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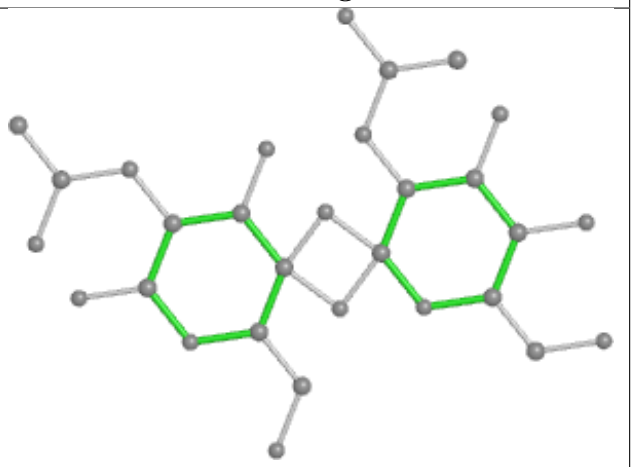
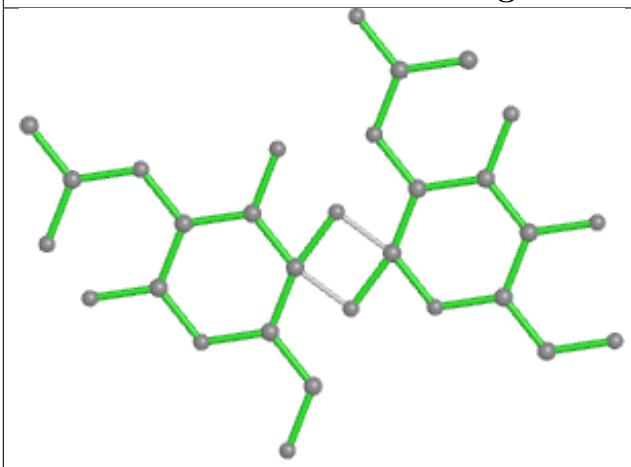


Rings

Oligosaccharide Chain d



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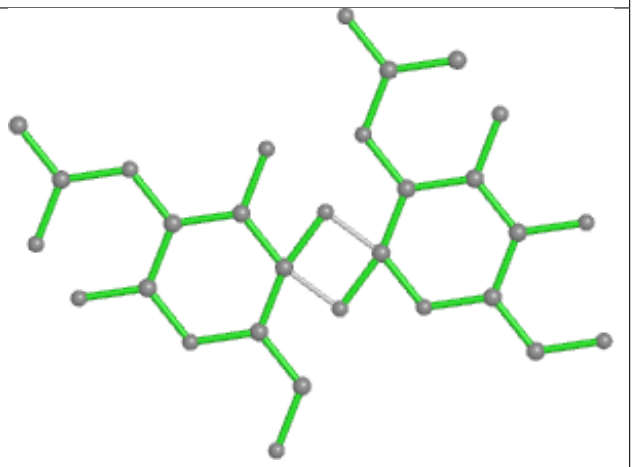
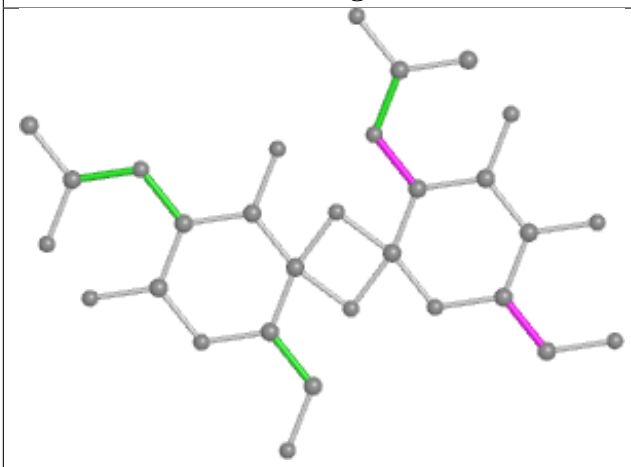


Bond angles



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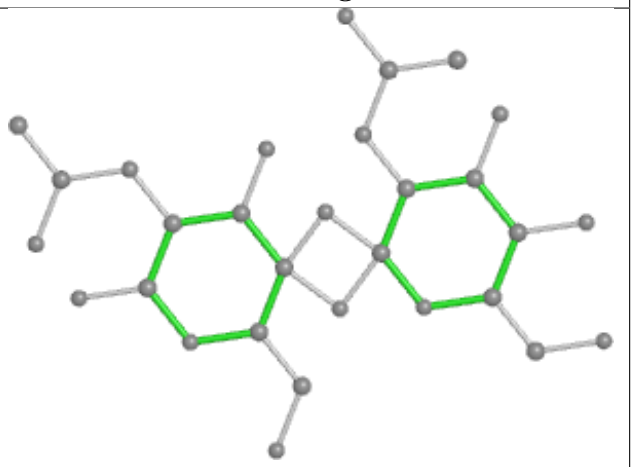
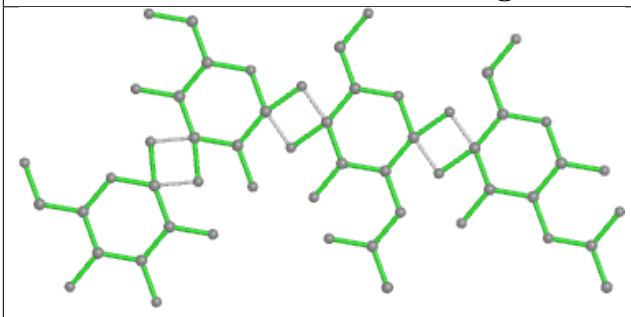


Rings

Oligosaccharide Chain E



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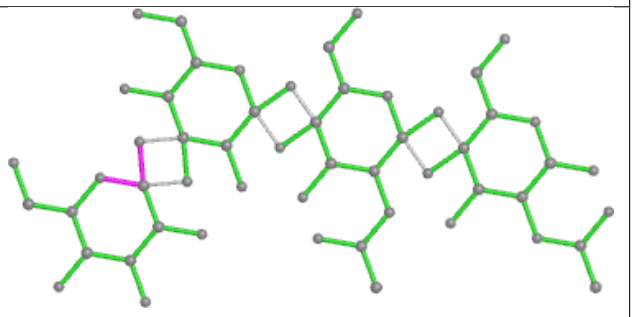
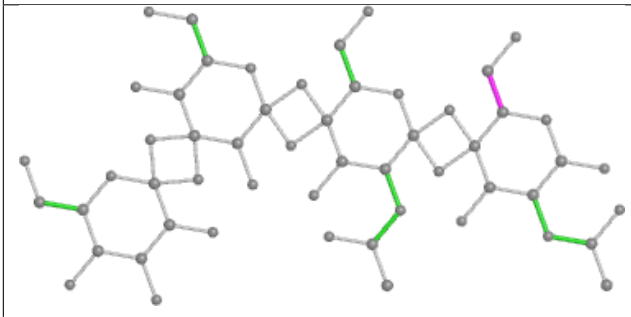
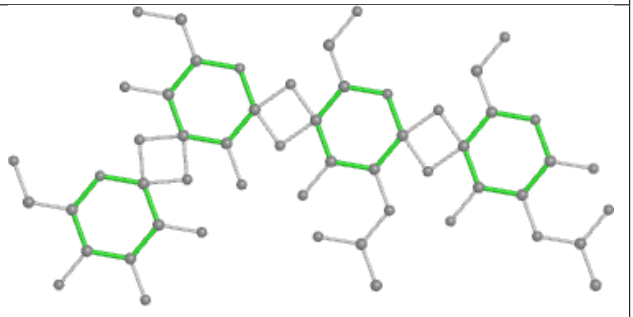


Bond angles

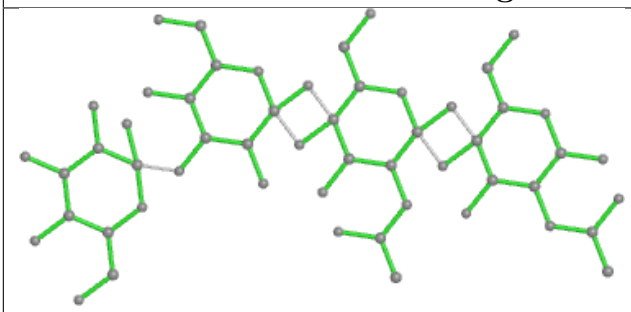


Torsions



Rings

Oligosaccharide Chain F



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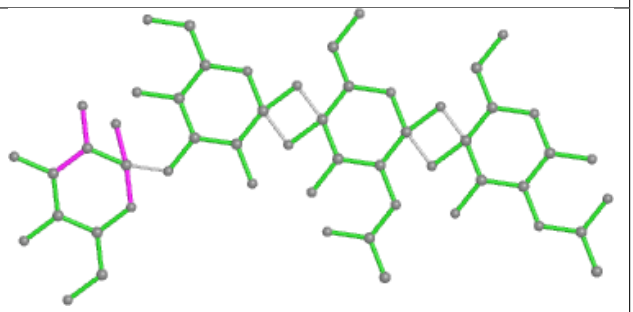
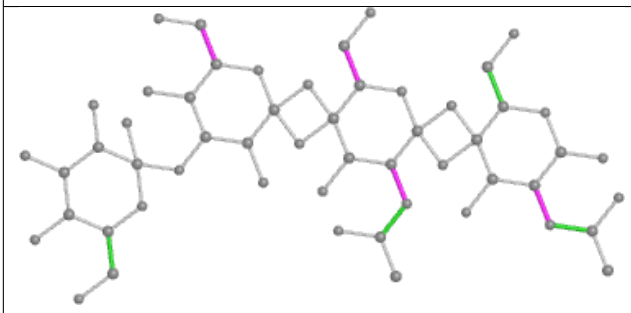


Bond angles



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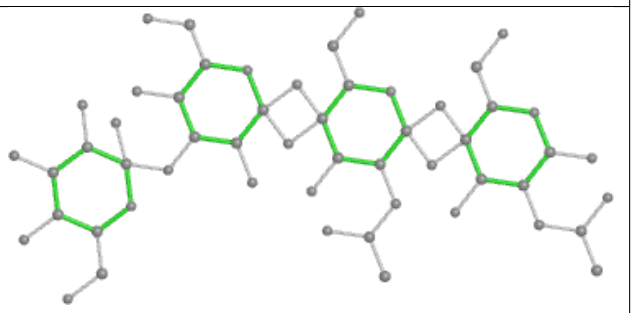
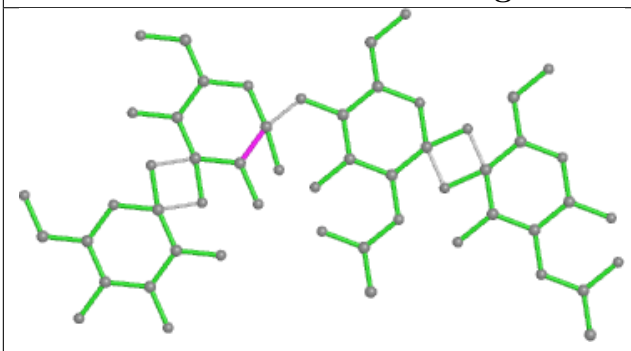


Rings

Oligosaccharide Chain R



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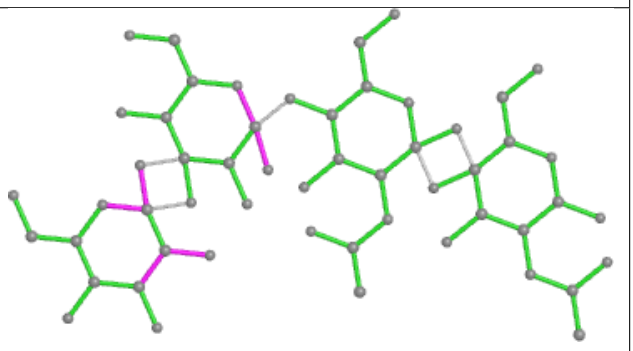
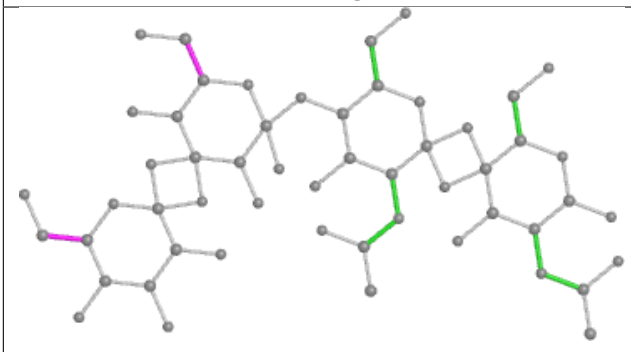


Bond angles



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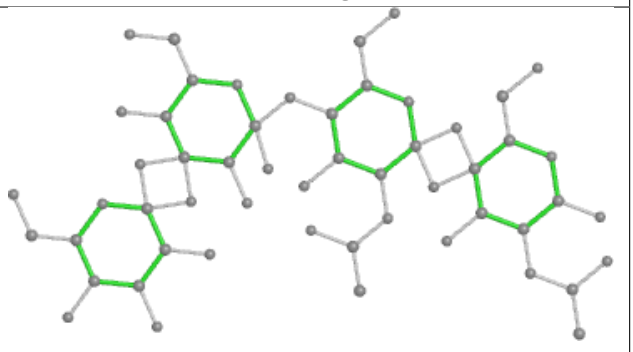
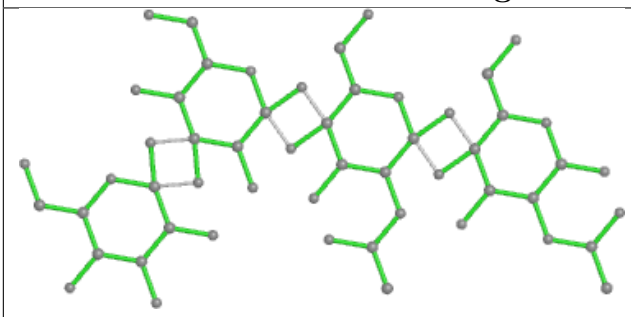


Rings

Oligosaccharide Chain U



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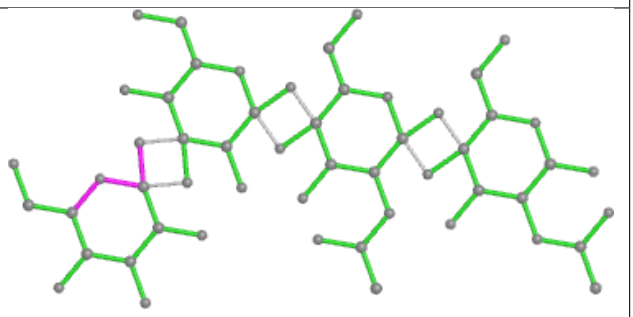
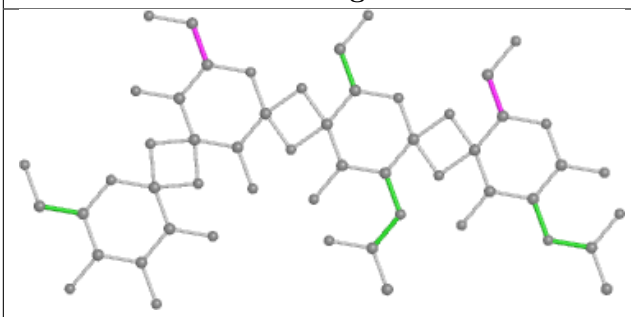
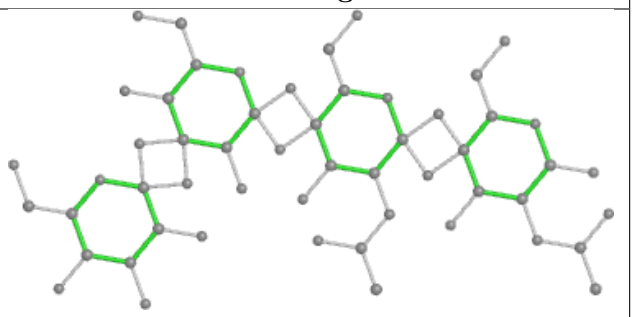


Bond angles

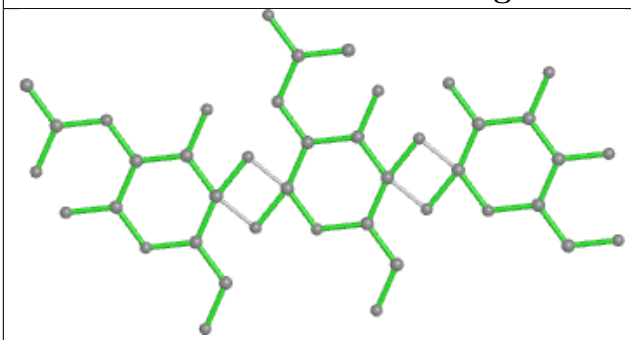


Torsions

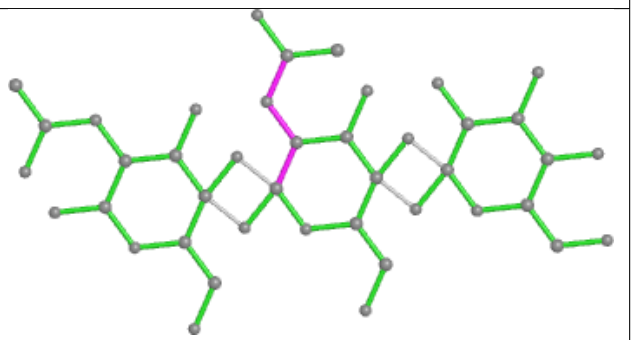


Rings

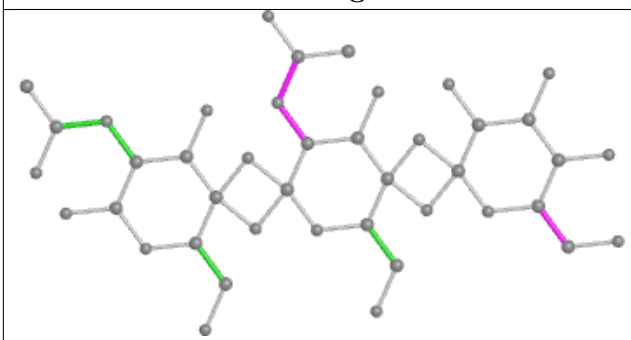
Oligosaccharide Chain N



Bond lengths



Bond angles



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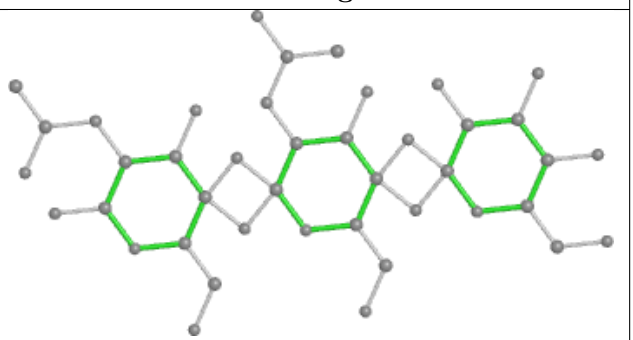
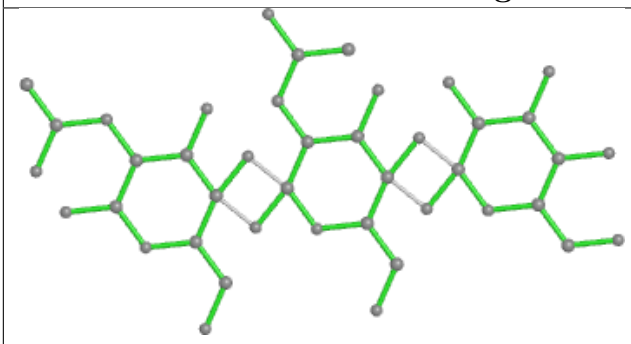
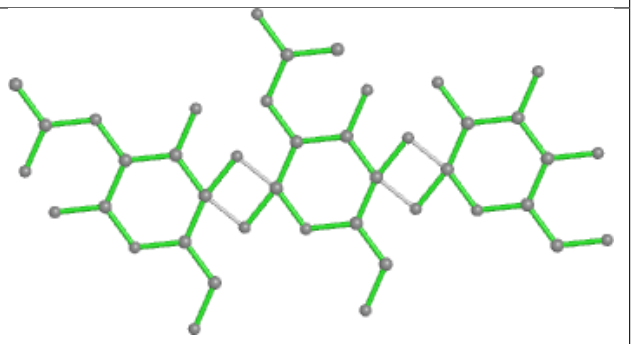
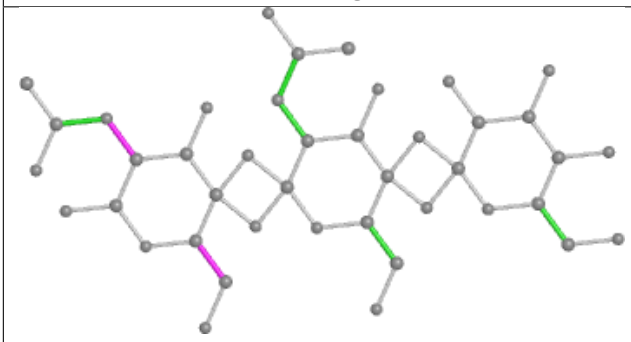
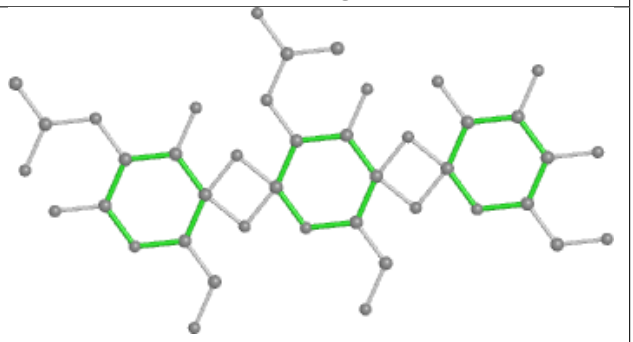
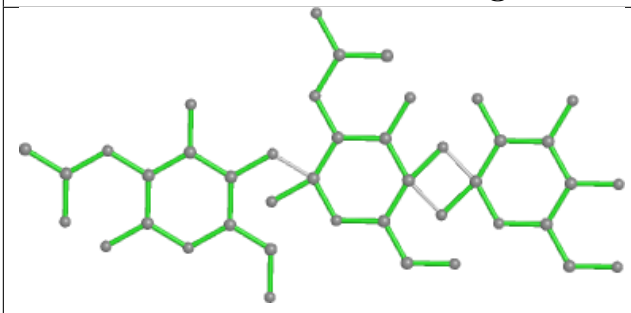
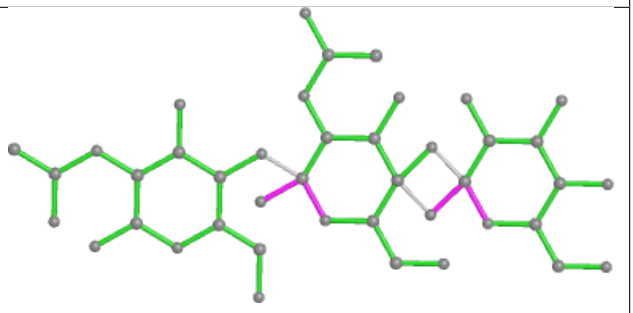
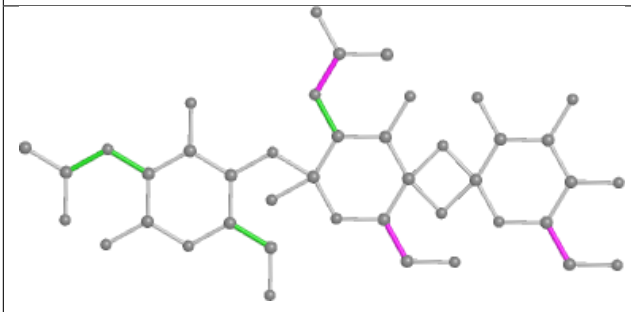
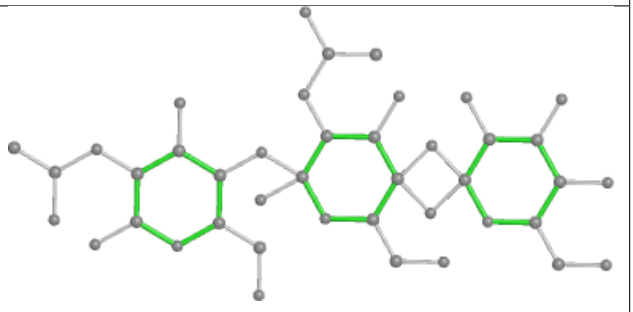
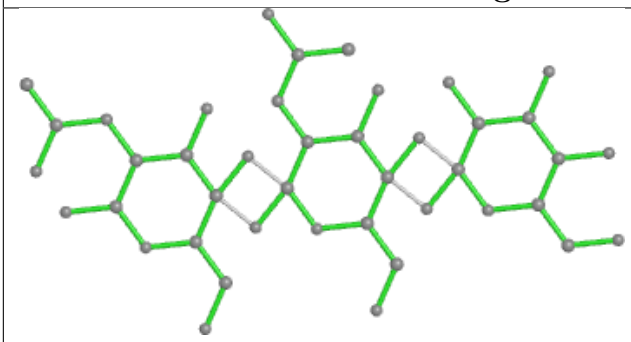


Rings

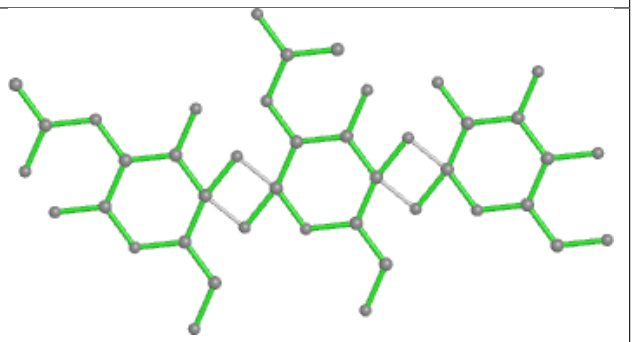
Oligosaccharide Chain O	
	
Bond lengths	Bond angles
	
Torsions	Rings

Oligosaccharide Chain W	
	
Bond lengths	Bond angles
	
Torsions	Rings

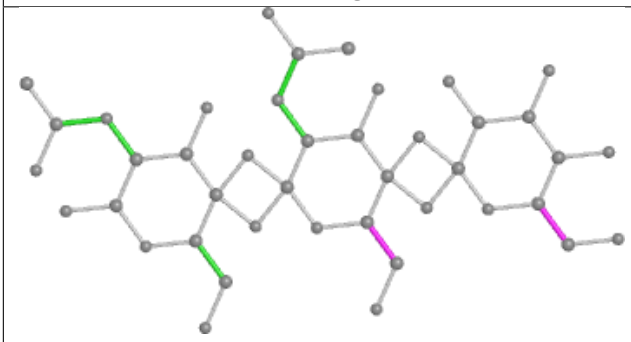
Oligosaccharide Chain Y



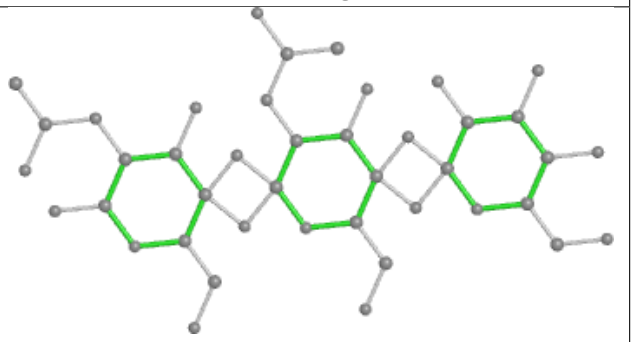
Bond lengths



Bond angles

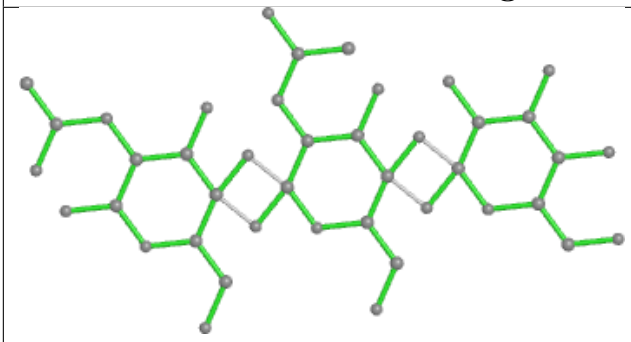


Torsions

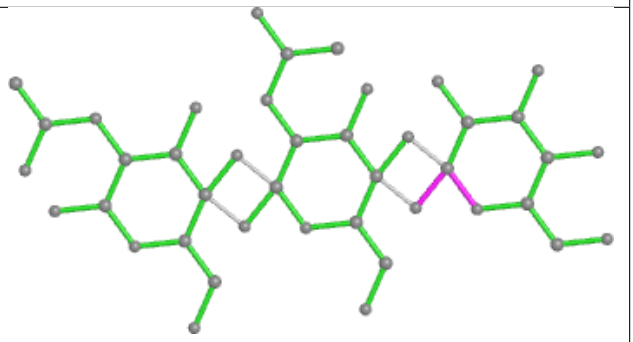


Rings

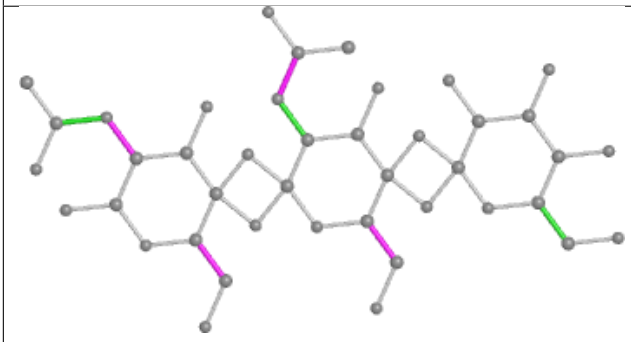
Oligosaccharide Chain a



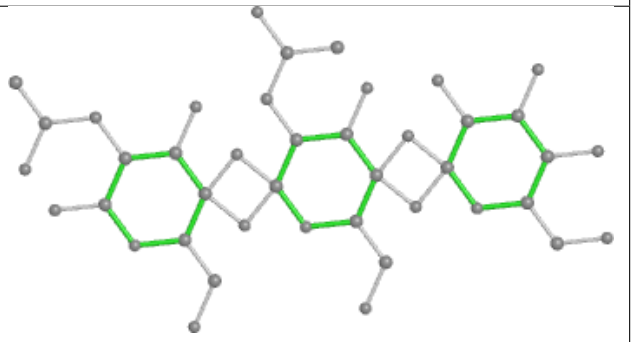
Bond lengths



Bond angles

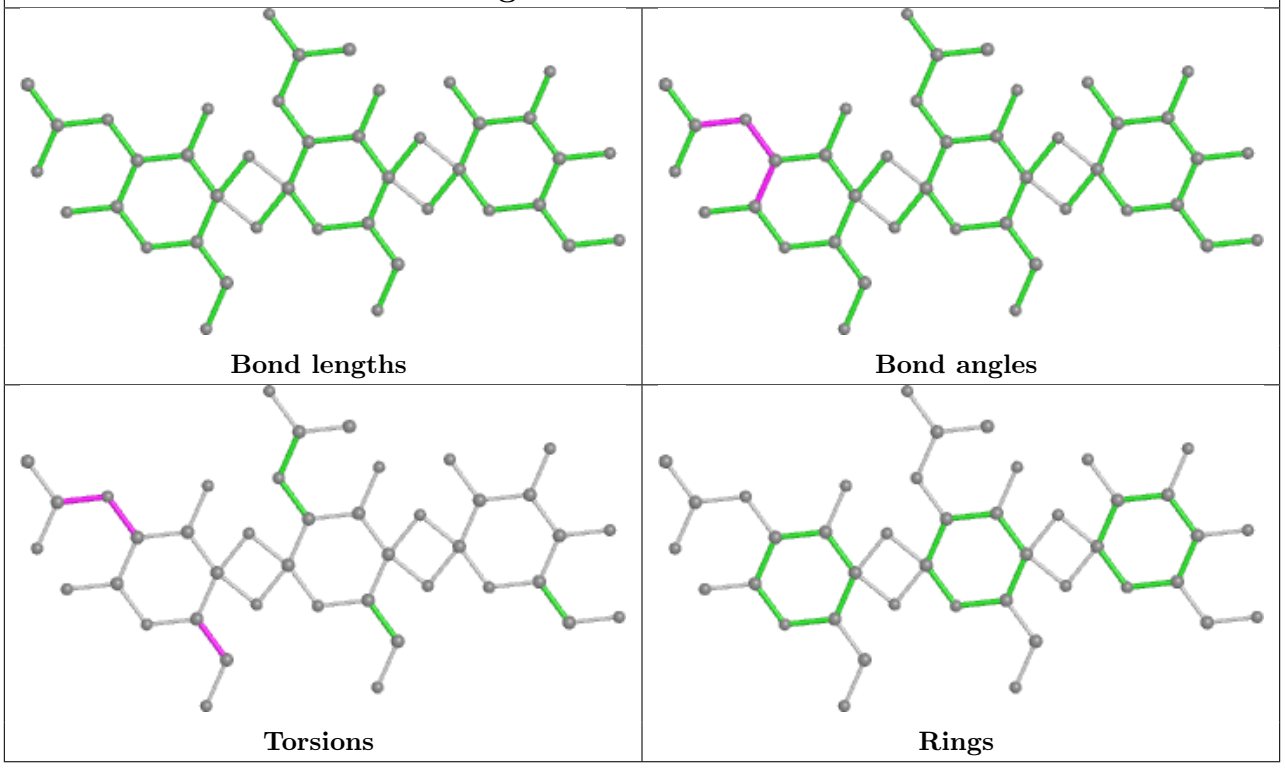


Torsions

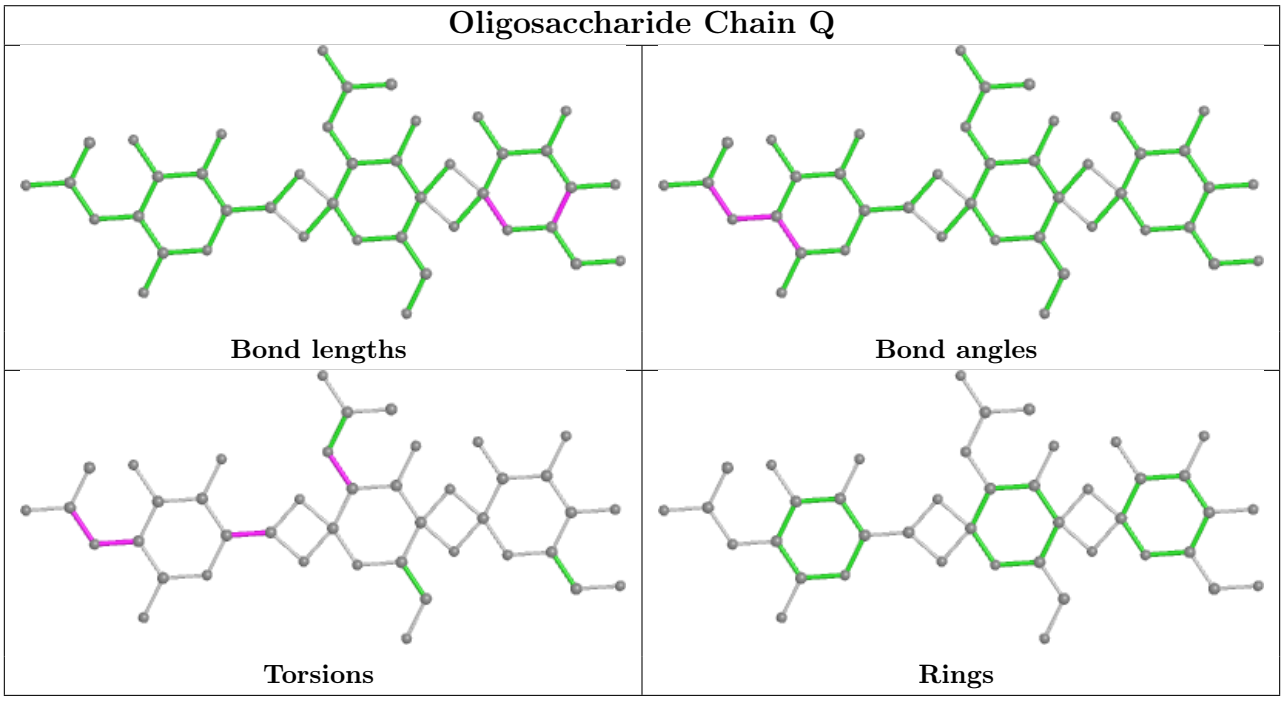


Rings

Oligosaccharide Chain b



Oligosaccharide Chain Q



5.6 Ligand geometry (i)

23 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	$\#\|Z\| > 2$
6	NAG	B	1102	1	15,15,15	0.42	0	21,21,21	0.29	0
6	NAG	B	1103	-	15,15,15	0.42	0	21,21,21	0.90	2 (9%)
6	NAG	A	1306	1	15,15,15	0.33	0	21,21,21	0.16	0
8	DMS	A	1309	-	3,3,3	0.67	0	3,3,3	0.51	0
6	NAG	B	1106	1	15,15,15	0.51	0	21,21,21	0.42	0
6	NAG	A	1303	1	15,15,15	0.33	0	21,21,21	0.12	0
6	NAG	A	1301	1	15,15,15	0.73	1 (6%)	21,21,21	0.62	0
7	MAN	C	1304	-	12,12,12	0.58	0	17,17,17	1.31	1 (5%)
6	NAG	B	1104	-	15,15,15	0.48	0	21,21,21	0.34	0
8	DMS	A	1310	-	3,3,3	0.66	0	3,3,3	1.13	0
6	NAG	B	1108	1	15,15,15	0.32	0	21,21,21	0.25	0
7	MAN	A	1307	-	12,12,12	0.57	0	17,17,17	1.32	2 (11%)
6	NAG	A	1304	-	15,15,15	0.33	0	21,21,21	0.13	0
6	NAG	C	1301	-	15,15,15	0.34	0	21,21,21	0.11	0
6	NAG	B	1105	-	15,15,15	0.36	0	21,21,21	0.13	0
6	NAG	B	1107	1	15,15,15	0.62	0	21,21,21	0.25	0
6	NAG	C	1303	1	15,15,15	0.91	1 (6%)	21,21,21	0.48	0
6	NAG	C	1305	-	15,15,15	0.48	0	21,21,21	0.30	0
6	NAG	A	1302	1	15,15,15	0.35	0	21,21,21	0.16	0
6	NAG	C	1302	-	15,15,15	0.73	1 (6%)	21,21,21	0.46	0
6	NAG	B	1101	1	15,15,15	0.33	0	21,21,21	0.41	0
8	DMS	A	1308	-	3,3,3	0.66	0	3,3,3	0.48	0
6	NAG	A	1305	-	15,15,15	0.43	0	21,21,21	0.89	2 (9%)

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
6	NAG	B	1102	1	-	4/6/26/26	0/1/1/1
6	NAG	B	1103	-	-	6/6/26/26	0/1/1/1
6	NAG	A	1306	1	-	2/6/26/26	0/1/1/1
6	NAG	B	1106	1	-	0/6/26/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	A	1303	1	-	2/6/26/26	0/1/1/1
6	NAG	A	1301	1	-	2/6/26/26	0/1/1/1
7	MAN	C	1304	-	-	0/2/22/22	0/1/1/1
6	NAG	B	1104	-	-	3/6/26/26	0/1/1/1
6	NAG	B	1108	1	-	3/6/26/26	0/1/1/1
7	MAN	A	1307	-	-	0/2/22/22	0/1/1/1
6	NAG	A	1304	-	-	2/6/26/26	0/1/1/1
6	NAG	C	1301	-	-	2/6/26/26	0/1/1/1
6	NAG	B	1105	-	-	0/6/26/26	0/1/1/1
6	NAG	B	1107	1	-	2/6/26/26	0/1/1/1
6	NAG	C	1303	1	-	2/6/26/26	0/1/1/1
6	NAG	C	1305	-	-	0/6/26/26	0/1/1/1
6	NAG	A	1302	1	-	0/6/26/26	0/1/1/1
6	NAG	C	1302	-	1/1/6/7	2/6/26/26	0/1/1/1
6	NAG	B	1101	1	-	4/6/26/26	0/1/1/1
6	NAG	A	1305	-	-	5/6/26/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1303	NAG	C1-C2	2.94	1.56	1.52
6	A	1301	NAG	C1-C2	2.41	1.55	1.52
6	C	1302	NAG	O5-C1	2.07	1.48	1.42

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	1307	MAN	O1-C1-O5	-4.35	97.32	110.38
7	C	1304	MAN	O1-C1-O5	-4.34	97.36	110.38
6	B	1103	NAG	C1-C2-N2	2.82	114.00	110.73
6	A	1305	NAG	C1-C2-N2	2.78	113.95	110.73
6	A	1305	NAG	C2-N2-C7	2.50	129.25	123.18

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	C	1302	NAG	C1

5 of 41 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	1102	NAG	C1-C2-N2-C7
6	A	1306	NAG	O5-C5-C6-O6
6	C	1303	NAG	O5-C5-C6-O6
6	A	1303	NAG	O5-C5-C6-O6
6	A	1304	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	498:CYS	C	499:GLY	N	2.83
1	A	308:LEU	C	309:CYS	N	1.99

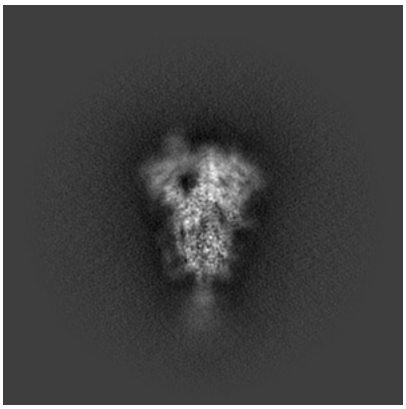
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-11336. These allow visual inspection of the internal detail of the map and identification of artifacts.

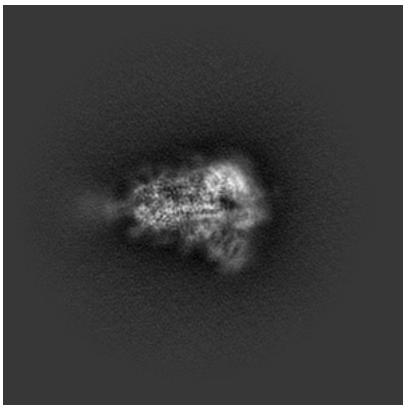
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

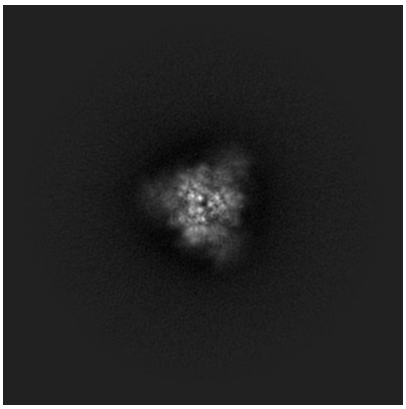
6.1.1 Primary map



X

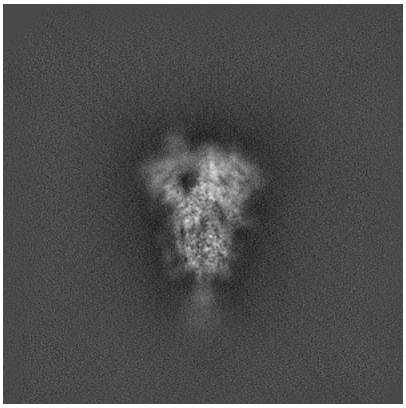


Y

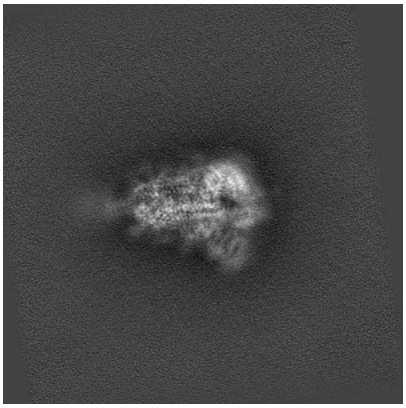


Z

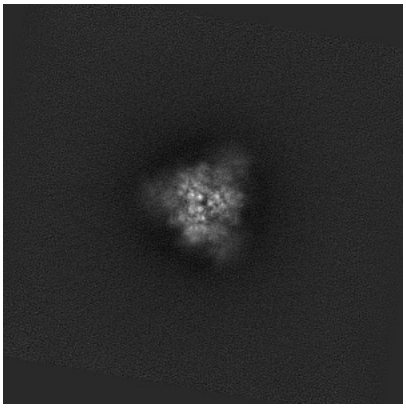
6.1.2 Raw map



X



Y

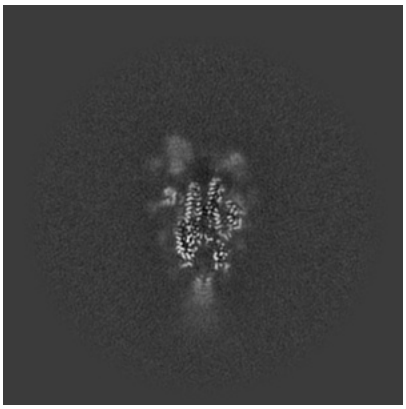


Z

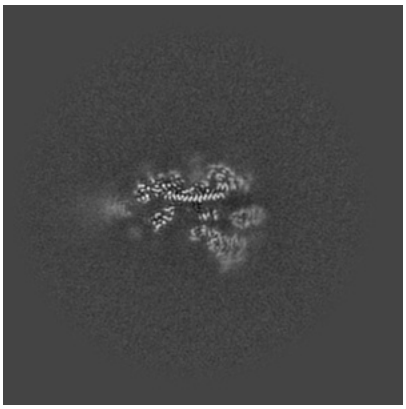
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

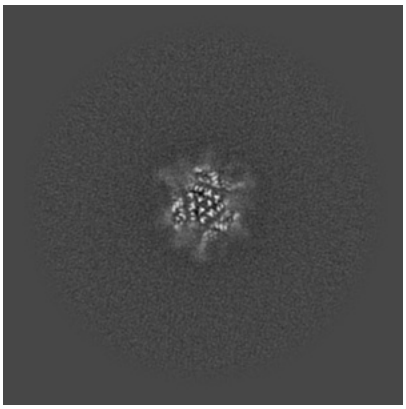
6.2.1 Primary map



X Index: 216

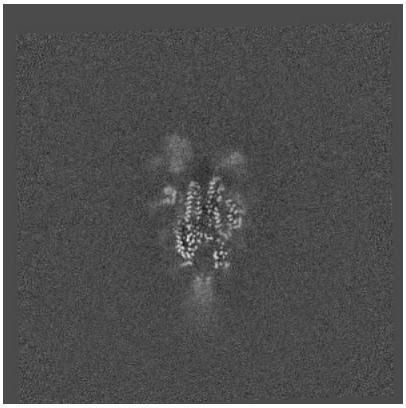


Y Index: 216

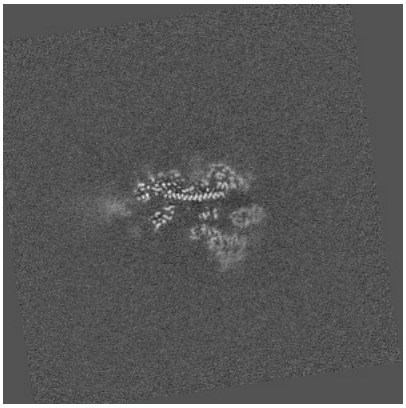


Z Index: 216

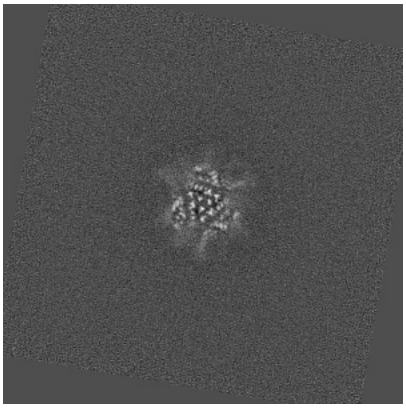
6.2.2 Raw map



X Index: 216



Y Index: 216

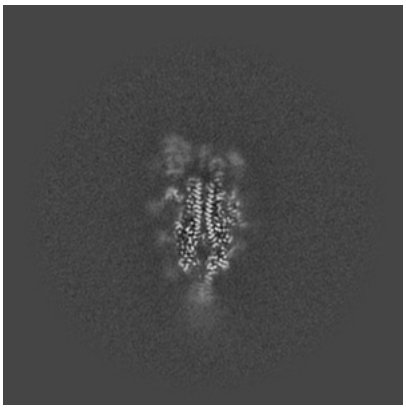


Z Index: 216

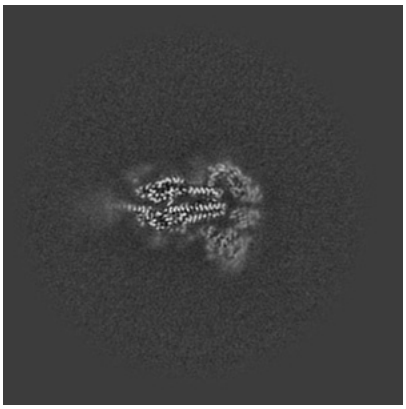
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

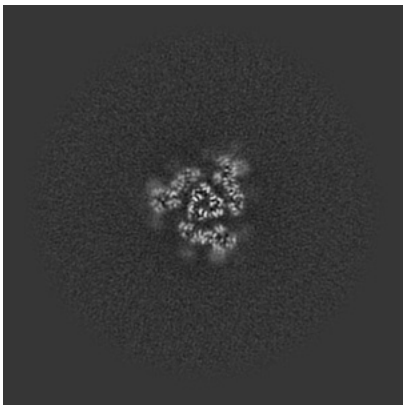
6.3.1 Primary map



X Index: 212

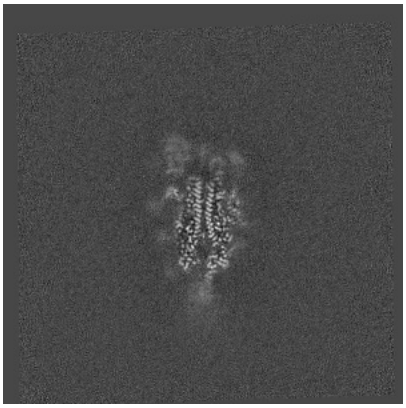


Y Index: 224

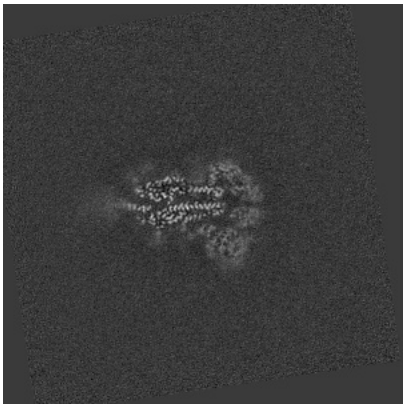


Z Index: 231

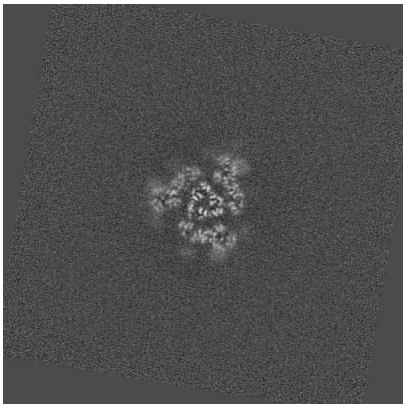
6.3.2 Raw map



X Index: 212



Y Index: 223

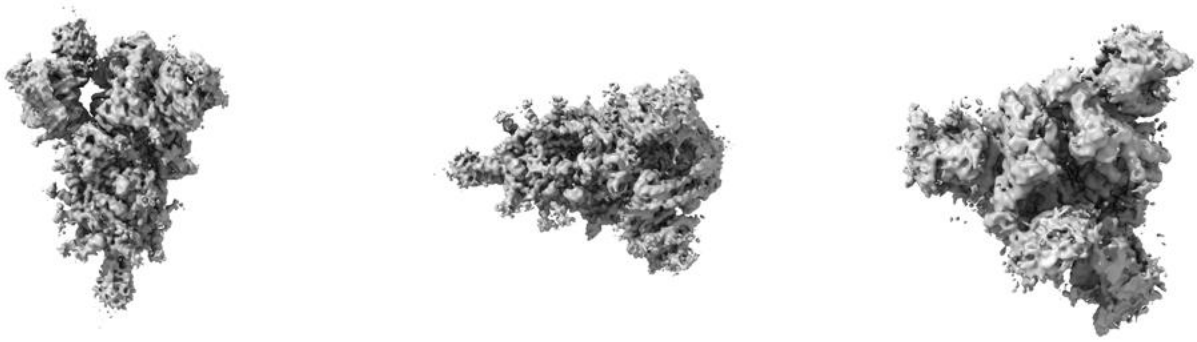


Z Index: 231

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

6.4 Orthogonal surface views (i)

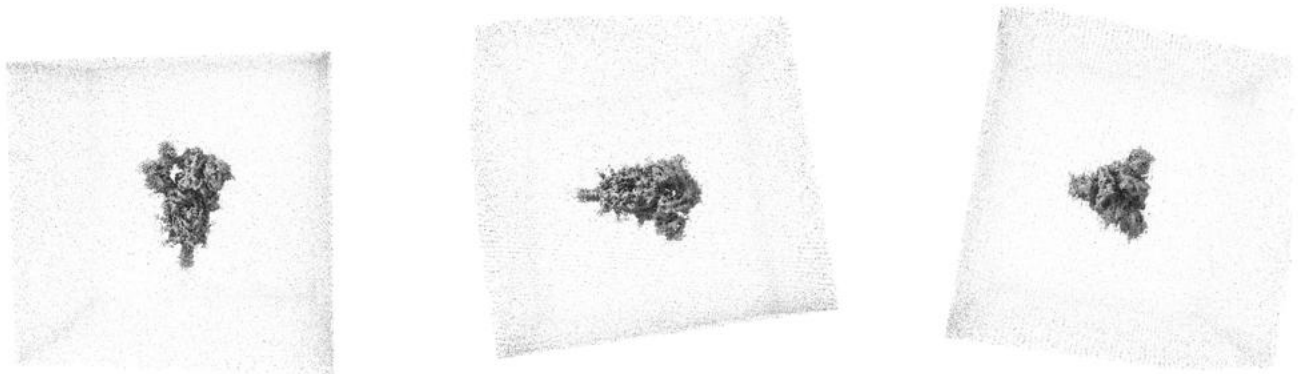
6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



X Y Z

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

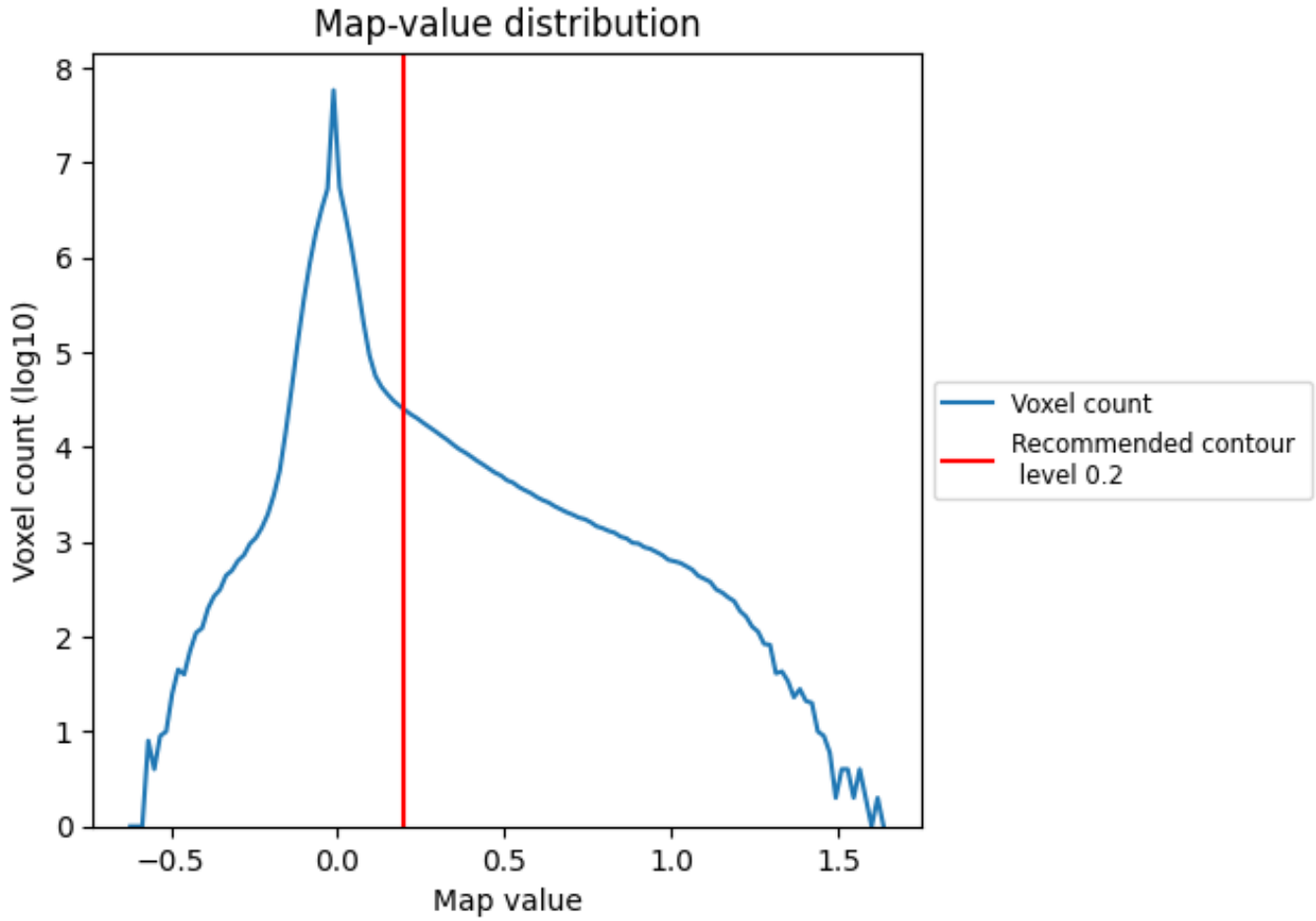
6.5 Mask visualisation (i)

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

7 Map analysis

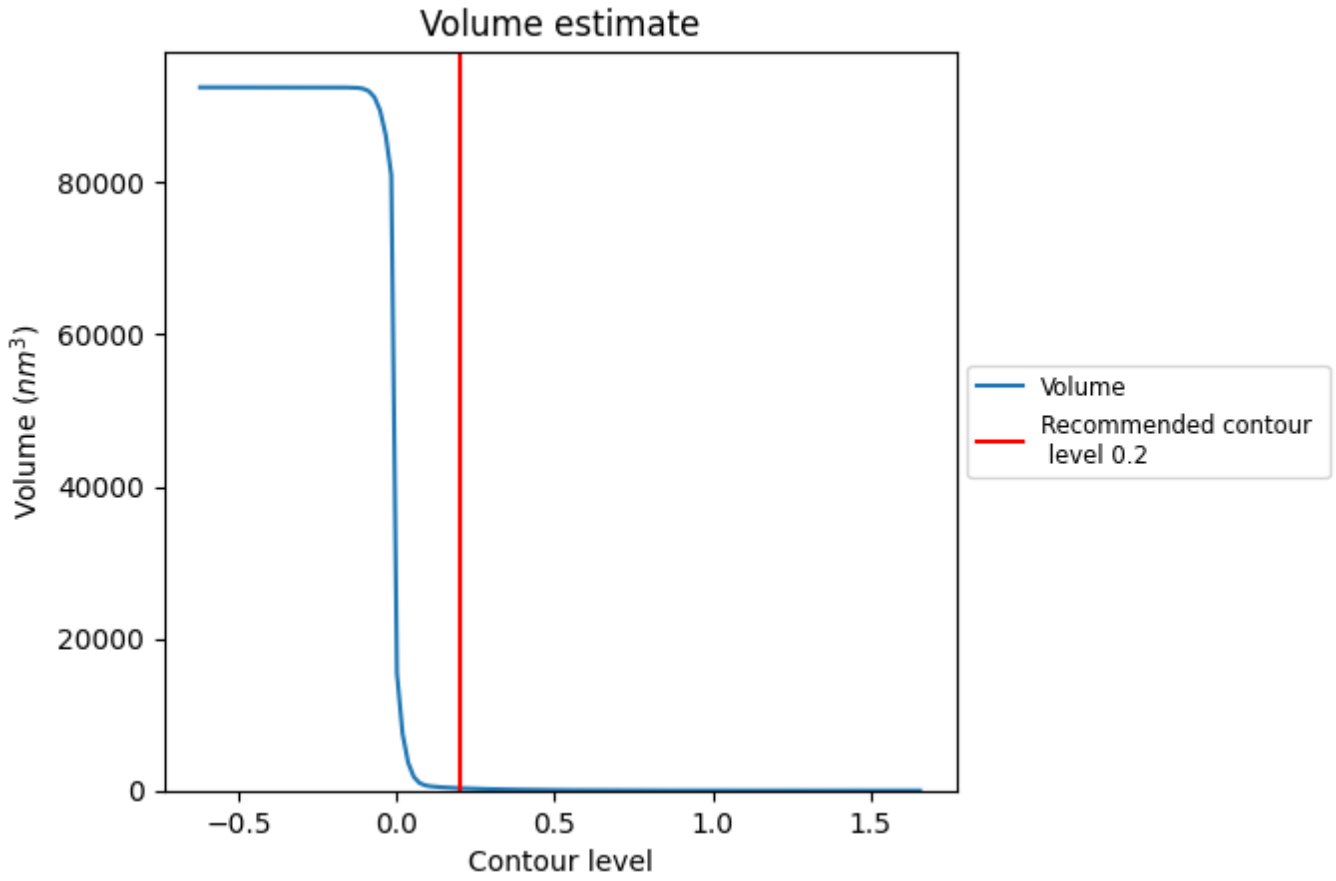
This section contains the results of statistical analysis of the map.

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.

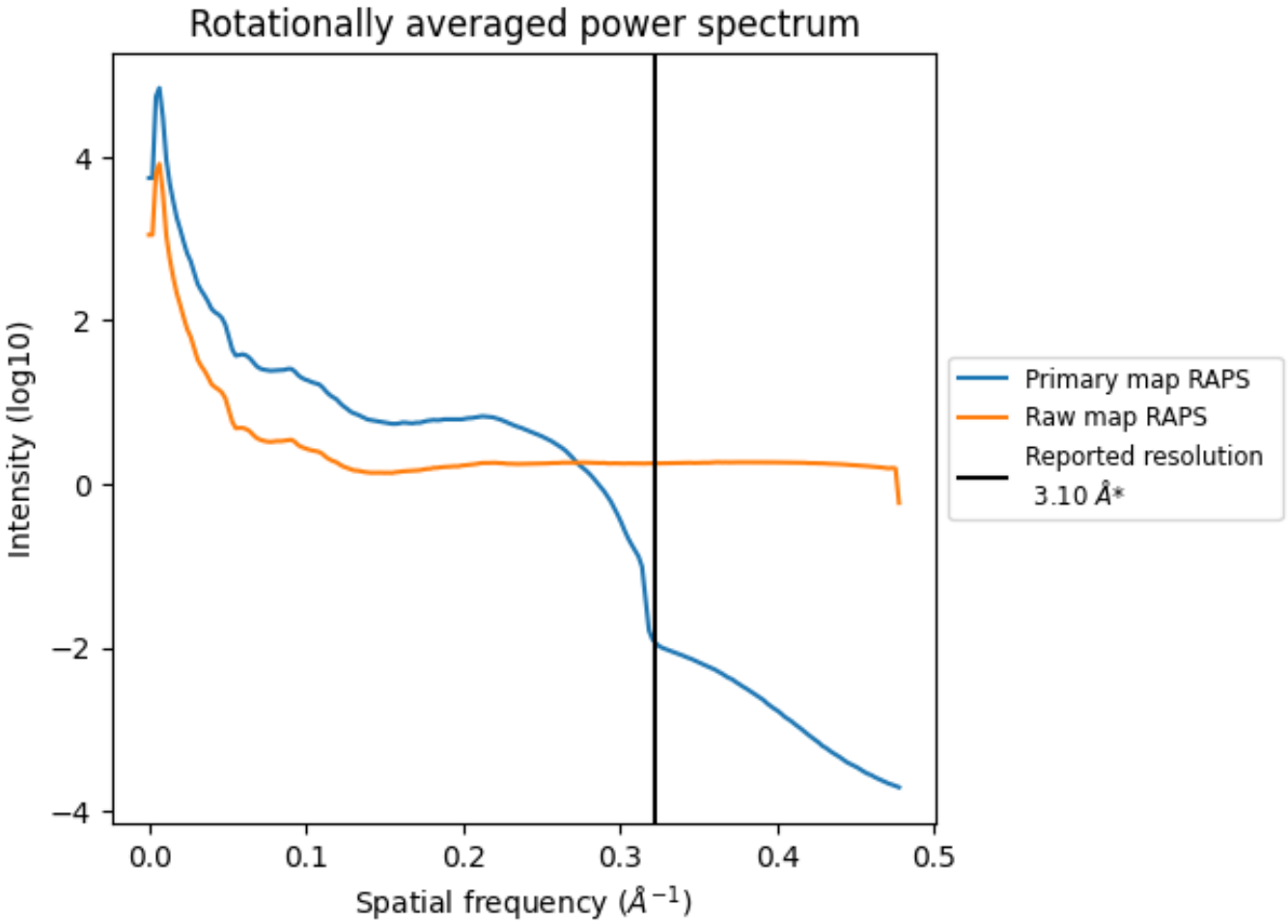
7.2 Volume estimate (i)



The volume at the recommended contour level is 313 nm^3; this corresponds to an approximate mass of 283 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)

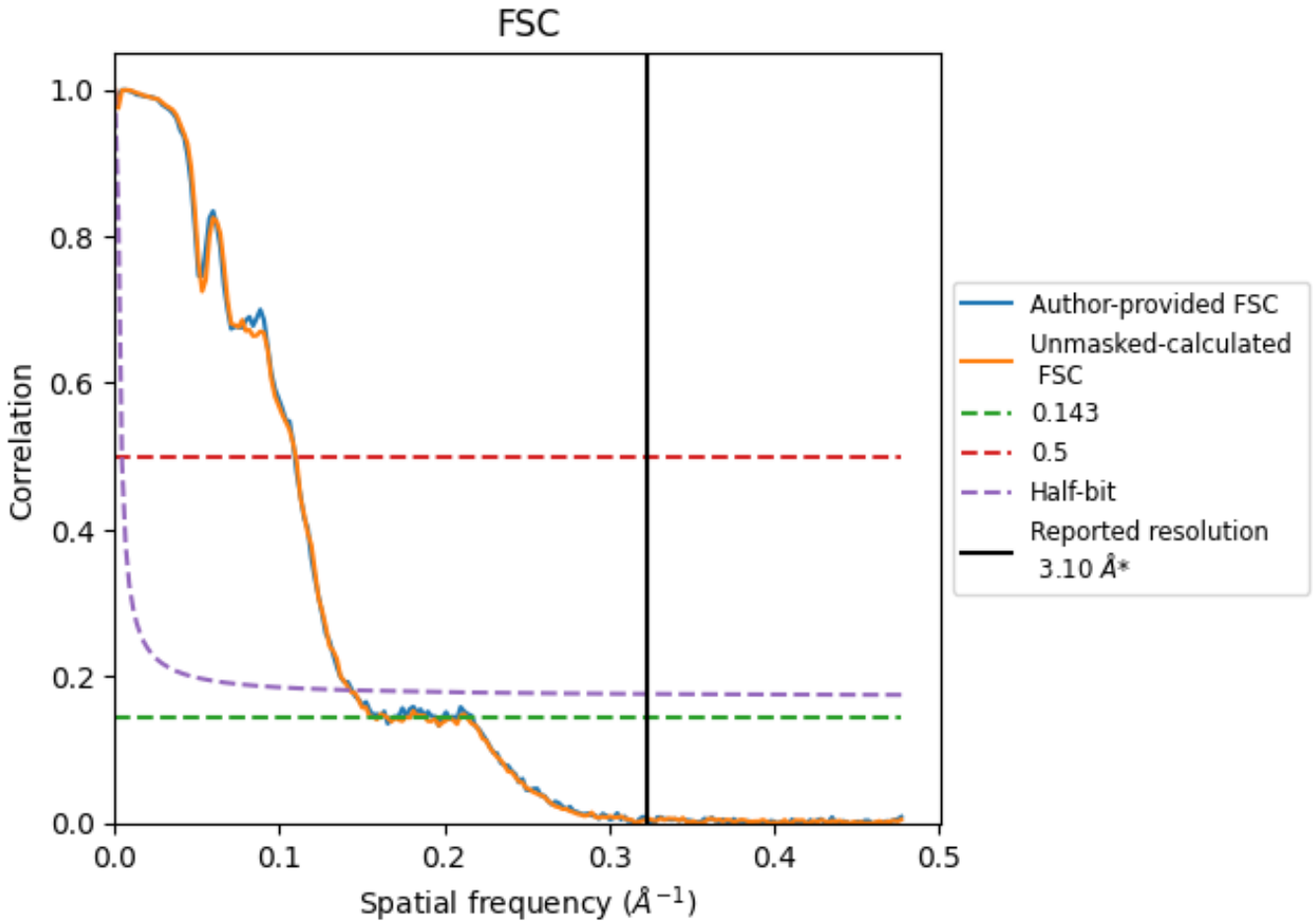


*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

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 0.323 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	6.07	9.15	6.94
Unmasked-calculated*	6.34	9.10	7.00

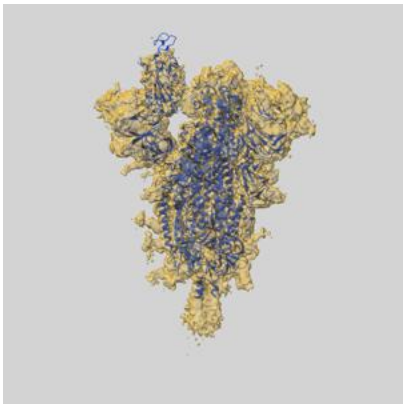
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 6.07 differs from the reported value 3.1 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.34 differs from the reported value 3.1 by more than 10 %

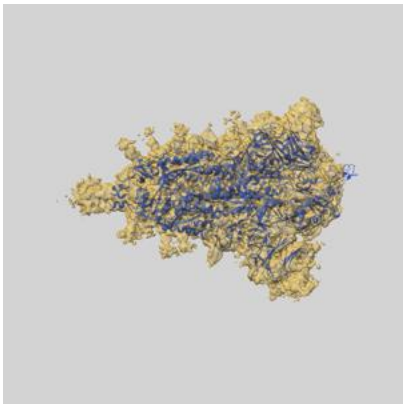
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-11336 and PDB model 6ZP5. Per-residue inclusion information can be found in section 3 on page 16.

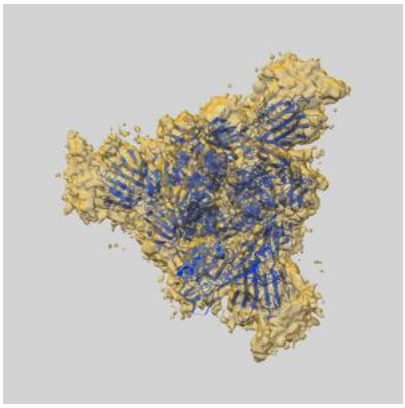
9.1 Map-model overlay



X



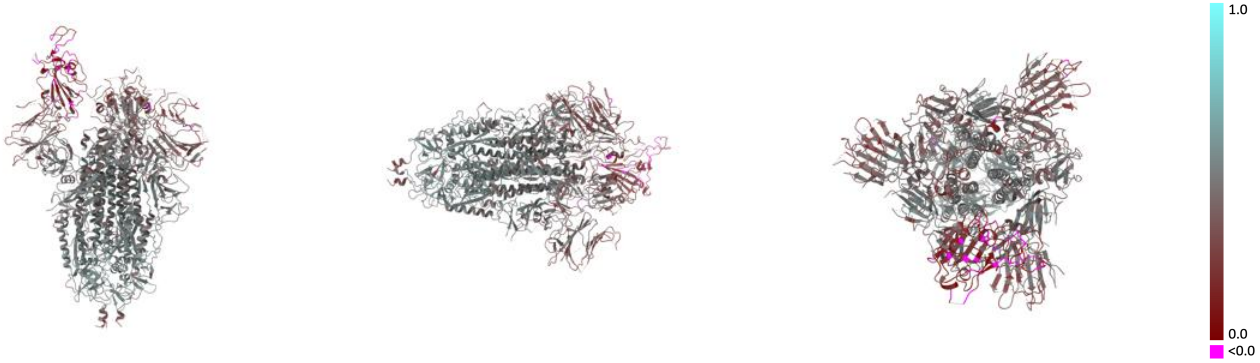
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.2 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.

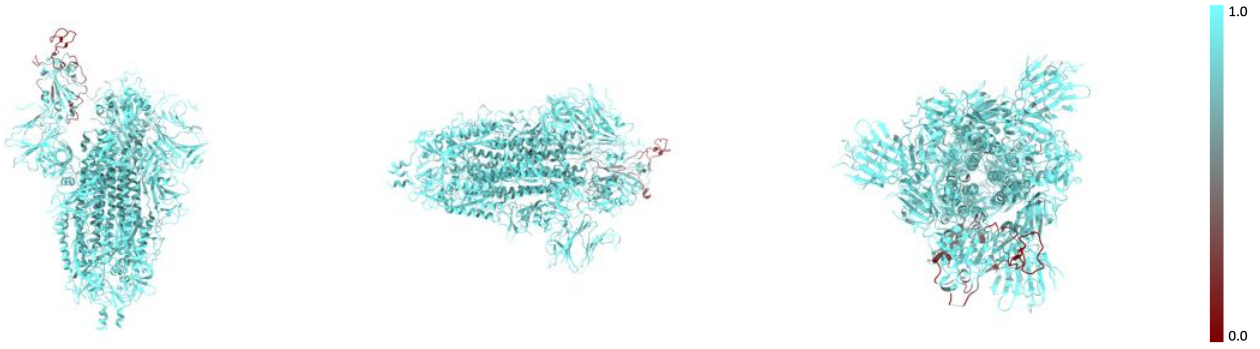
9.2 Q-score mapped to coordinate model (i)



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.

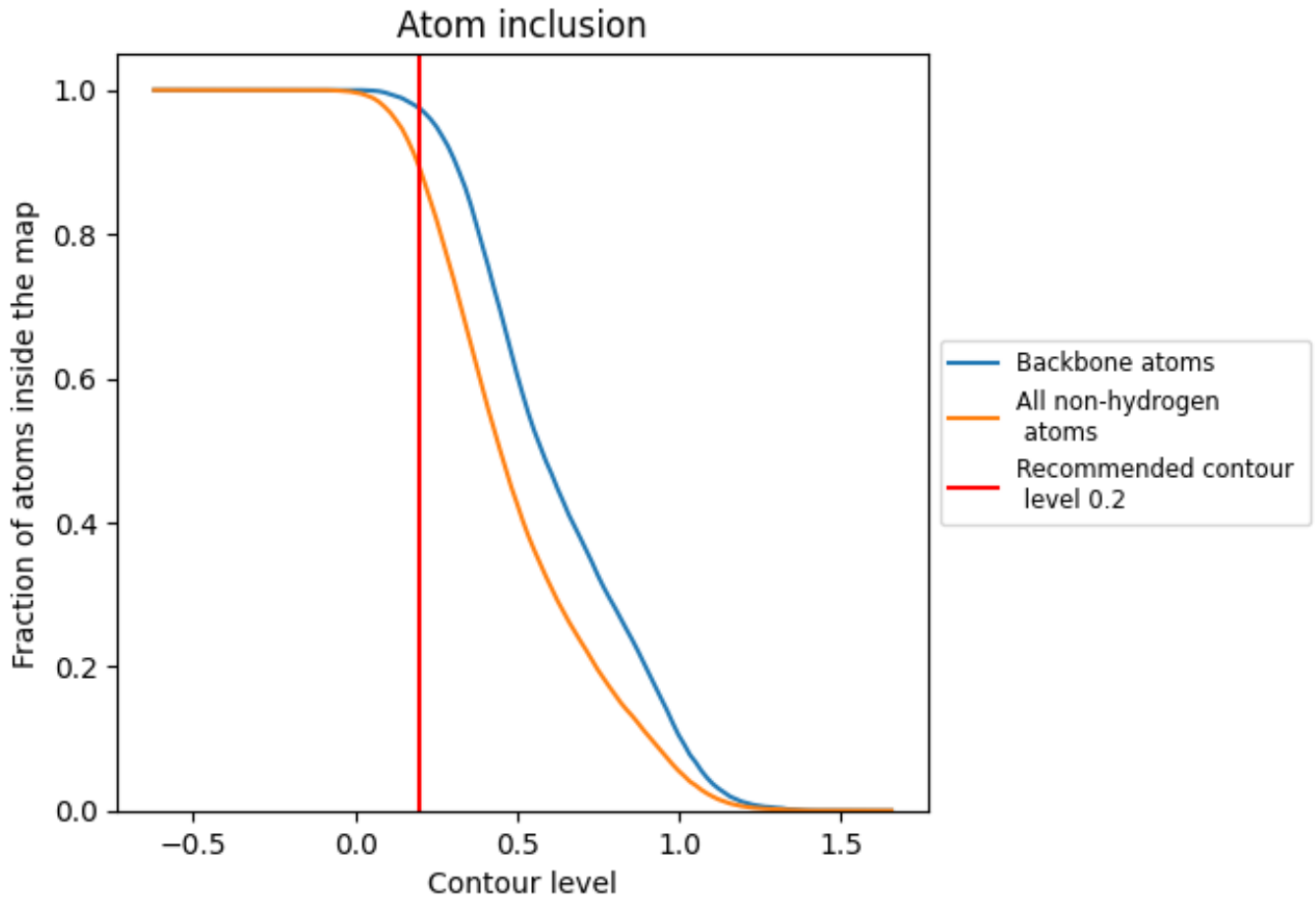
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.2).

9.4 Atom inclusion (i)



At the recommended contour level, 97% of all backbone atoms, 89% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8900	0.4170
A	0.8572	0.3960
B	0.9099	0.4270
C	0.9211	0.4370
D	0.4667	0.2950
E	0.9074	0.4320
F	0.7407	0.3080
G	0.8000	0.4620
H	0.9333	0.4330
I	0.9333	0.4210
J	0.5000	0.2630
K	0.8667	0.3340
L	0.7333	0.2970
M	0.8667	0.4220
N	0.9286	0.3710
O	0.6190	0.3230
P	0.9667	0.4170
Q	0.9524	0.3850
R	0.9074	0.4180
S	0.6667	0.2840
T	0.7333	0.1980
U	0.7593	0.3200
V	0.9333	0.4130
W	0.4762	0.3130
X	0.8667	0.3650
Y	0.9286	0.4750
Z	0.8333	0.4100
a	0.5000	0.1940
b	0.8095	0.3060
c	0.7000	0.3490
d	0.3667	0.3010