wwPDB EM Validation Summary Report (i)

Nov 14, 2022 – 08:05 PM EST

PDB ID	:	7KE4
EMDB ID	:	EMD-22831
Title	:	SARS-CoV-2 D614G 3 RBD down Spike Protein Trimer without the P986-P987 stabilizing mutations (S-GSAS-D614G Sub-class)
Authors	:	Gobeil, S.; Acharya, P.
Deposited on	:	2020-10-10
Resolution	:	3.21 Å(reported)

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

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

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

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

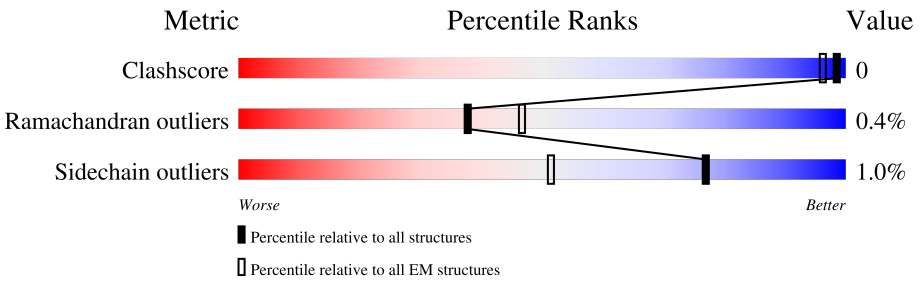
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 3.21 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	1288	72% • 25%
1	B	1288	72% • 25%
1	C	1288	72% • 25%
2	D	2	50% 100%
2	E	2	100%
2	F	2	100%
2	G	2	100%
2	H	2	100%

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Mol	Chain	Length	Quality of chain
2	I	2	100%
2	J	2	100%
2	K	2	100%
2	L	2	100%
2	M	2	100%
2	N	2	100%
2	O	2	100%
2	P	2	100%
2	Q	2	100%
2	R	2	100%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 23684 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	972	7602	4860	1263	1446	33	0	0
1	B	972	7602	4860	1263	1446	33	0	0
1	C	972	7598	4858	1263	1444	33	0	0

There are 252 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	614	GLY	ASP	engineered mutation	UNP P0DTC2
A	682	GLY	ARG	engineered mutation	UNP P0DTC2
A	683	SER	ARG	engineered mutation	UNP P0DTC2
A	685	SER	ARG	engineered mutation	UNP P0DTC2
A	1209	GLY	-	expression tag	UNP P0DTC2
A	1210	SER	-	expression tag	UNP P0DTC2
A	1211	GLY	-	expression tag	UNP P0DTC2
A	1212	TYR	-	expression tag	UNP P0DTC2
A	1213	ILE	-	expression tag	UNP P0DTC2
A	1214	PRO	-	expression tag	UNP P0DTC2
A	1215	GLU	-	expression tag	UNP P0DTC2
A	1216	ALA	-	expression tag	UNP P0DTC2
A	1217	PRO	-	expression tag	UNP P0DTC2
A	1218	ARG	-	expression tag	UNP P0DTC2
A	1219	ASP	-	expression tag	UNP P0DTC2
A	1220	GLY	-	expression tag	UNP P0DTC2
A	1221	GLN	-	expression tag	UNP P0DTC2
A	1222	ALA	-	expression tag	UNP P0DTC2
A	1223	TYR	-	expression tag	UNP P0DTC2
A	1224	VAL	-	expression tag	UNP P0DTC2
A	1225	ARG	-	expression tag	UNP P0DTC2
A	1226	LYS	-	expression tag	UNP P0DTC2
A	1227	ASP	-	expression tag	UNP P0DTC2
A	1228	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1229	GLU	-	expression tag	UNP P0DTC2
A	1230	TRP	-	expression tag	UNP P0DTC2
A	1231	VAL	-	expression tag	UNP P0DTC2
A	1232	LEU	-	expression tag	UNP P0DTC2
A	1233	LEU	-	expression tag	UNP P0DTC2
A	1234	SER	-	expression tag	UNP P0DTC2
A	1235	THR	-	expression tag	UNP P0DTC2
A	1236	PHE	-	expression tag	UNP P0DTC2
A	1237	LEU	-	expression tag	UNP P0DTC2
A	1238	GLY	-	expression tag	UNP P0DTC2
A	1239	ARG	-	expression tag	UNP P0DTC2
A	1240	SER	-	expression tag	UNP P0DTC2
A	1241	LEU	-	expression tag	UNP P0DTC2
A	1242	GLU	-	expression tag	UNP P0DTC2
A	1243	VAL	-	expression tag	UNP P0DTC2
A	1244	LEU	-	expression tag	UNP P0DTC2
A	1245	PHE	-	expression tag	UNP P0DTC2
A	1246	GLN	-	expression tag	UNP P0DTC2
A	1247	GLY	-	expression tag	UNP P0DTC2
A	1248	PRO	-	expression tag	UNP P0DTC2
A	1249	GLY	-	expression tag	UNP P0DTC2
A	1250	HIS	-	expression tag	UNP P0DTC2
A	1251	HIS	-	expression tag	UNP P0DTC2
A	1252	HIS	-	expression tag	UNP P0DTC2
A	1253	HIS	-	expression tag	UNP P0DTC2
A	1254	HIS	-	expression tag	UNP P0DTC2
A	1255	HIS	-	expression tag	UNP P0DTC2
A	1256	HIS	-	expression tag	UNP P0DTC2
A	1257	HIS	-	expression tag	UNP P0DTC2
A	1258	SER	-	expression tag	UNP P0DTC2
A	1259	ALA	-	expression tag	UNP P0DTC2
A	1260	TRP	-	expression tag	UNP P0DTC2
A	1261	SER	-	expression tag	UNP P0DTC2
A	1262	HIS	-	expression tag	UNP P0DTC2
A	1263	PRO	-	expression tag	UNP P0DTC2
A	1264	GLN	-	expression tag	UNP P0DTC2
A	1265	PHE	-	expression tag	UNP P0DTC2
A	1266	GLU	-	expression tag	UNP P0DTC2
A	1267	LYS	-	expression tag	UNP P0DTC2
A	1268	GLY	-	expression tag	UNP P0DTC2
A	1269	GLY	-	expression tag	UNP P0DTC2
A	1270	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1271	SER	-	expression tag	UNP P0DTC2
A	1272	GLY	-	expression tag	UNP P0DTC2
A	1273	GLY	-	expression tag	UNP P0DTC2
A	1274	GLY	-	expression tag	UNP P0DTC2
A	1275	GLY	-	expression tag	UNP P0DTC2
A	1276	SER	-	expression tag	UNP P0DTC2
A	1277	GLY	-	expression tag	UNP P0DTC2
A	1278	GLY	-	expression tag	UNP P0DTC2
A	1279	SER	-	expression tag	UNP P0DTC2
A	1280	ALA	-	expression tag	UNP P0DTC2
A	1281	TRP	-	expression tag	UNP P0DTC2
A	1282	SER	-	expression tag	UNP P0DTC2
A	1283	HIS	-	expression tag	UNP P0DTC2
A	1284	PRO	-	expression tag	UNP P0DTC2
A	1285	GLN	-	expression tag	UNP P0DTC2
A	1286	PHE	-	expression tag	UNP P0DTC2
A	1287	GLU	-	expression tag	UNP P0DTC2
A	1288	LYS	-	expression tag	UNP P0DTC2
B	614	GLY	ASP	engineered mutation	UNP P0DTC2
B	682	GLY	ARG	engineered mutation	UNP P0DTC2
B	683	SER	ARG	engineered mutation	UNP P0DTC2
B	685	SER	ARG	engineered mutation	UNP P0DTC2
B	1209	GLY	-	expression tag	UNP P0DTC2
B	1210	SER	-	expression tag	UNP P0DTC2
B	1211	GLY	-	expression tag	UNP P0DTC2
B	1212	TYR	-	expression tag	UNP P0DTC2
B	1213	ILE	-	expression tag	UNP P0DTC2
B	1214	PRO	-	expression tag	UNP P0DTC2
B	1215	GLU	-	expression tag	UNP P0DTC2
B	1216	ALA	-	expression tag	UNP P0DTC2
B	1217	PRO	-	expression tag	UNP P0DTC2
B	1218	ARG	-	expression tag	UNP P0DTC2
B	1219	ASP	-	expression tag	UNP P0DTC2
B	1220	GLY	-	expression tag	UNP P0DTC2
B	1221	GLN	-	expression tag	UNP P0DTC2
B	1222	ALA	-	expression tag	UNP P0DTC2
B	1223	TYR	-	expression tag	UNP P0DTC2
B	1224	VAL	-	expression tag	UNP P0DTC2
B	1225	ARG	-	expression tag	UNP P0DTC2
B	1226	LYS	-	expression tag	UNP P0DTC2
B	1227	ASP	-	expression tag	UNP P0DTC2
B	1228	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1229	GLU	-	expression tag	UNP P0DTC2
B	1230	TRP	-	expression tag	UNP P0DTC2
B	1231	VAL	-	expression tag	UNP P0DTC2
B	1232	LEU	-	expression tag	UNP P0DTC2
B	1233	LEU	-	expression tag	UNP P0DTC2
B	1234	SER	-	expression tag	UNP P0DTC2
B	1235	THR	-	expression tag	UNP P0DTC2
B	1236	PHE	-	expression tag	UNP P0DTC2
B	1237	LEU	-	expression tag	UNP P0DTC2
B	1238	GLY	-	expression tag	UNP P0DTC2
B	1239	ARG	-	expression tag	UNP P0DTC2
B	1240	SER	-	expression tag	UNP P0DTC2
B	1241	LEU	-	expression tag	UNP P0DTC2
B	1242	GLU	-	expression tag	UNP P0DTC2
B	1243	VAL	-	expression tag	UNP P0DTC2
B	1244	LEU	-	expression tag	UNP P0DTC2
B	1245	PHE	-	expression tag	UNP P0DTC2
B	1246	GLN	-	expression tag	UNP P0DTC2
B	1247	GLY	-	expression tag	UNP P0DTC2
B	1248	PRO	-	expression tag	UNP P0DTC2
B	1249	GLY	-	expression tag	UNP P0DTC2
B	1250	HIS	-	expression tag	UNP P0DTC2
B	1251	HIS	-	expression tag	UNP P0DTC2
B	1252	HIS	-	expression tag	UNP P0DTC2
B	1253	HIS	-	expression tag	UNP P0DTC2
B	1254	HIS	-	expression tag	UNP P0DTC2
B	1255	HIS	-	expression tag	UNP P0DTC2
B	1256	HIS	-	expression tag	UNP P0DTC2
B	1257	HIS	-	expression tag	UNP P0DTC2
B	1258	SER	-	expression tag	UNP P0DTC2
B	1259	ALA	-	expression tag	UNP P0DTC2
B	1260	TRP	-	expression tag	UNP P0DTC2
B	1261	SER	-	expression tag	UNP P0DTC2
B	1262	HIS	-	expression tag	UNP P0DTC2
B	1263	PRO	-	expression tag	UNP P0DTC2
B	1264	GLN	-	expression tag	UNP P0DTC2
B	1265	PHE	-	expression tag	UNP P0DTC2
B	1266	GLU	-	expression tag	UNP P0DTC2
B	1267	LYS	-	expression tag	UNP P0DTC2
B	1268	GLY	-	expression tag	UNP P0DTC2
B	1269	GLY	-	expression tag	UNP P0DTC2
B	1270	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1271	SER	-	expression tag	UNP P0DTC2
B	1272	GLY	-	expression tag	UNP P0DTC2
B	1273	GLY	-	expression tag	UNP P0DTC2
B	1274	GLY	-	expression tag	UNP P0DTC2
B	1275	GLY	-	expression tag	UNP P0DTC2
B	1276	SER	-	expression tag	UNP P0DTC2
B	1277	GLY	-	expression tag	UNP P0DTC2
B	1278	GLY	-	expression tag	UNP P0DTC2
B	1279	SER	-	expression tag	UNP P0DTC2
B	1280	ALA	-	expression tag	UNP P0DTC2
B	1281	TRP	-	expression tag	UNP P0DTC2
B	1282	SER	-	expression tag	UNP P0DTC2
B	1283	HIS	-	expression tag	UNP P0DTC2
B	1284	PRO	-	expression tag	UNP P0DTC2
B	1285	GLN	-	expression tag	UNP P0DTC2
B	1286	PHE	-	expression tag	UNP P0DTC2
B	1287	GLU	-	expression tag	UNP P0DTC2
B	1288	LYS	-	expression tag	UNP P0DTC2
C	614	GLY	ASP	engineered mutation	UNP P0DTC2
C	682	GLY	ARG	engineered mutation	UNP P0DTC2
C	683	SER	ARG	engineered mutation	UNP P0DTC2
C	685	SER	ARG	engineered mutation	UNP P0DTC2
C	1209	GLY	-	expression tag	UNP P0DTC2
C	1210	SER	-	expression tag	UNP P0DTC2
C	1211	GLY	-	expression tag	UNP P0DTC2
C	1212	TYR	-	expression tag	UNP P0DTC2
C	1213	ILE	-	expression tag	UNP P0DTC2
C	1214	PRO	-	expression tag	UNP P0DTC2
C	1215	GLU	-	expression tag	UNP P0DTC2
C	1216	ALA	-	expression tag	UNP P0DTC2
C	1217	PRO	-	expression tag	UNP P0DTC2
C	1218	ARG	-	expression tag	UNP P0DTC2
C	1219	ASP	-	expression tag	UNP P0DTC2
C	1220	GLY	-	expression tag	UNP P0DTC2
C	1221	GLN	-	expression tag	UNP P0DTC2
C	1222	ALA	-	expression tag	UNP P0DTC2
C	1223	TYR	-	expression tag	UNP P0DTC2
C	1224	VAL	-	expression tag	UNP P0DTC2
C	1225	ARG	-	expression tag	UNP P0DTC2
C	1226	LYS	-	expression tag	UNP P0DTC2
C	1227	ASP	-	expression tag	UNP P0DTC2
C	1228	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1229	GLU	-	expression tag	UNP P0DTC2
C	1230	TRP	-	expression tag	UNP P0DTC2
C	1231	VAL	-	expression tag	UNP P0DTC2
C	1232	LEU	-	expression tag	UNP P0DTC2
C	1233	LEU	-	expression tag	UNP P0DTC2
C	1234	SER	-	expression tag	UNP P0DTC2
C	1235	THR	-	expression tag	UNP P0DTC2
C	1236	PHE	-	expression tag	UNP P0DTC2
C	1237	LEU	-	expression tag	UNP P0DTC2
C	1238	GLY	-	expression tag	UNP P0DTC2
C	1239	ARG	-	expression tag	UNP P0DTC2
C	1240	SER	-	expression tag	UNP P0DTC2
C	1241	LEU	-	expression tag	UNP P0DTC2
C	1242	GLU	-	expression tag	UNP P0DTC2
C	1243	VAL	-	expression tag	UNP P0DTC2
C	1244	LEU	-	expression tag	UNP P0DTC2
C	1245	PHE	-	expression tag	UNP P0DTC2
C	1246	GLN	-	expression tag	UNP P0DTC2
C	1247	GLY	-	expression tag	UNP P0DTC2
C	1248	PRO	-	expression tag	UNP P0DTC2
C	1249	GLY	-	expression tag	UNP P0DTC2
C	1250	HIS	-	expression tag	UNP P0DTC2
C	1251	HIS	-	expression tag	UNP P0DTC2
C	1252	HIS	-	expression tag	UNP P0DTC2
C	1253	HIS	-	expression tag	UNP P0DTC2
C	1254	HIS	-	expression tag	UNP P0DTC2
C	1255	HIS	-	expression tag	UNP P0DTC2
C	1256	HIS	-	expression tag	UNP P0DTC2
C	1257	HIS	-	expression tag	UNP P0DTC2
C	1258	SER	-	expression tag	UNP P0DTC2
C	1259	ALA	-	expression tag	UNP P0DTC2
C	1260	TRP	-	expression tag	UNP P0DTC2
C	1261	SER	-	expression tag	UNP P0DTC2
C	1262	HIS	-	expression tag	UNP P0DTC2
C	1263	PRO	-	expression tag	UNP P0DTC2
C	1264	GLN	-	expression tag	UNP P0DTC2
C	1265	PHE	-	expression tag	UNP P0DTC2
C	1266	GLU	-	expression tag	UNP P0DTC2
C	1267	LYS	-	expression tag	UNP P0DTC2
C	1268	GLY	-	expression tag	UNP P0DTC2
C	1269	GLY	-	expression tag	UNP P0DTC2
C	1270	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1271	SER	-	expression tag	UNP P0DTC2
C	1272	GLY	-	expression tag	UNP P0DTC2
C	1273	GLY	-	expression tag	UNP P0DTC2
C	1274	GLY	-	expression tag	UNP P0DTC2
C	1275	GLY	-	expression tag	UNP P0DTC2
C	1276	SER	-	expression tag	UNP P0DTC2
C	1277	GLY	-	expression tag	UNP P0DTC2
C	1278	GLY	-	expression tag	UNP P0DTC2
C	1279	SER	-	expression tag	UNP P0DTC2
C	1280	ALA	-	expression tag	UNP P0DTC2
C	1281	TRP	-	expression tag	UNP P0DTC2
C	1282	SER	-	expression tag	UNP P0DTC2
C	1283	HIS	-	expression tag	UNP P0DTC2
C	1284	PRO	-	expression tag	UNP P0DTC2
C	1285	GLN	-	expression tag	UNP P0DTC2
C	1286	PHE	-	expression tag	UNP P0DTC2
C	1287	GLU	-	expression tag	UNP P0DTC2
C	1288	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
			Total	C	N	O		
2	D	2	28	16	2	10	0	0
2	E	2	28	16	2	10	0	0
2	F	2	28	16	2	10	0	0
2	G	2	28	16	2	10	0	0
2	H	2	28	16	2	10	0	0
2	I	2	28	16	2	10	0	0
2	J	2	28	16	2	10	0	0

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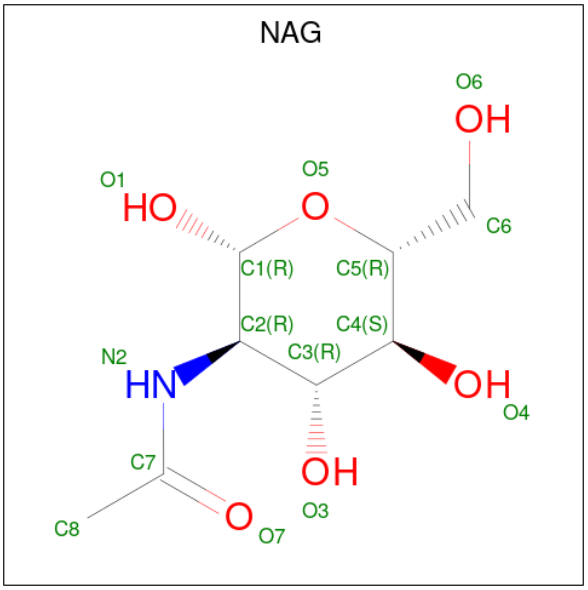
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	K	2	28	16	2	10	0	0
			Total	C	N	O		
2	L	2	28	16	2	10	0	0
			Total	C	N	O		
2	M	2	28	16	2	10	0	0
			Total	C	N	O		
2	N	2	28	16	2	10	0	0
			Total	C	N	O		
2	O	2	28	16	2	10	0	0
			Total	C	N	O		
2	P	2	28	16	2	10	0	0
			Total	C	N	O		
2	Q	2	28	16	2	10	0	0
			Total	C	N	O		
2	R	2	28	16	2	10	0	0

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



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
3	A	1	154	88	11	55	0
			Total	C	N	O	
3	A	1	154	88	11	55	0
			Total	C	N	O	
3	A	1	154	88	11	55	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
3	A	1	154	88	11	55	0
3	A	1	154	88	11	55	0
3	A	1	154	88	11	55	0
3	A	1	154	88	11	55	0
3	A	1	154	88	11	55	0
3	A	1	154	88	11	55	0
3	A	1	154	88	11	55	0
3	A	1	154	88	11	55	0
3	B	1	154	88	11	55	0
3	B	1	154	88	11	55	0
3	B	1	154	88	11	55	0
3	B	1	154	88	11	55	0
3	B	1	154	88	11	55	0
3	B	1	154	88	11	55	0
3	B	1	154	88	11	55	0
3	B	1	154	88	11	55	0
3	B	1	154	88	11	55	0
3	B	1	154	88	11	55	0
3	C	1	154	88	11	55	0
3	C	1	154	88	11	55	0

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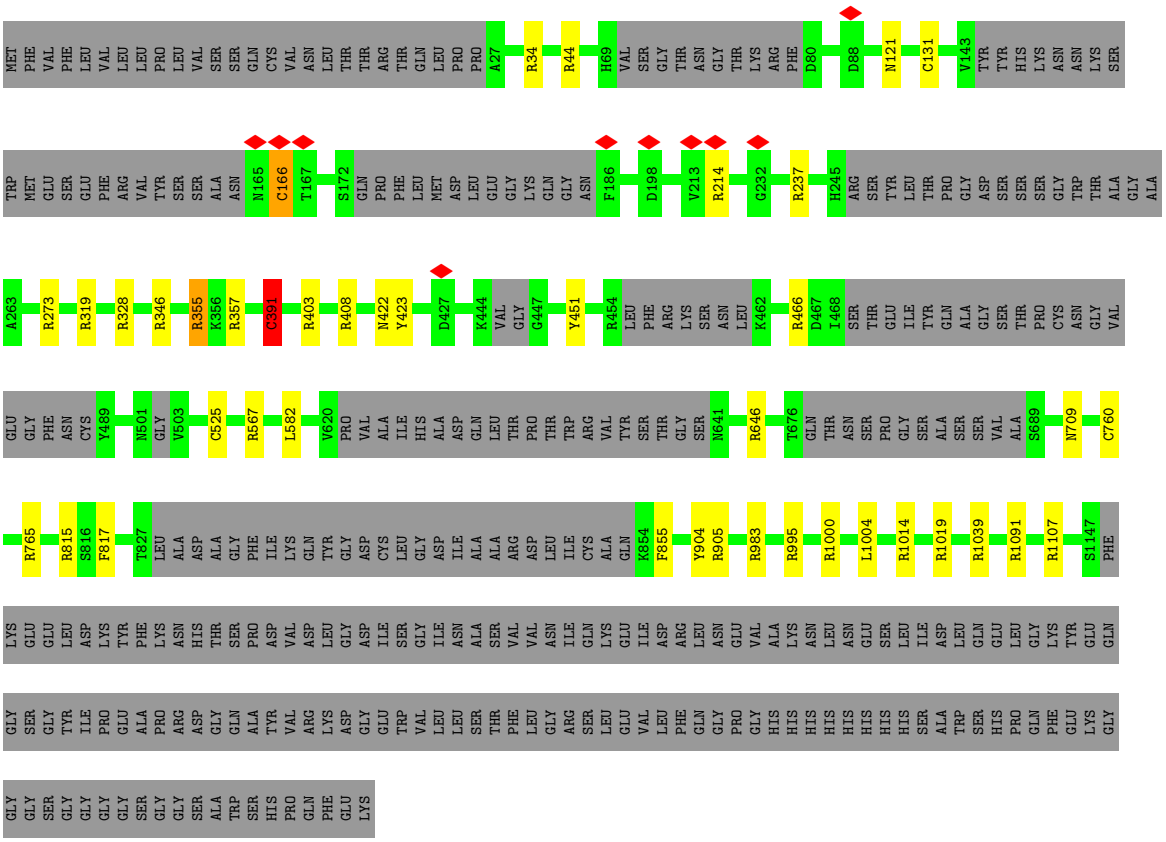
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
3	C	1	154	88	11	55	0
3	C	1	154	88	11	55	0
3	C	1	154	88	11	55	0
3	C	1	154	88	11	55	0
3	C	1	154	88	11	55	0
3	C	1	154	88	11	55	0
3	C	1	154	88	11	55	0
3	C	1	154	88	11	55	0
3	C	1	154	88	11	55	0

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.

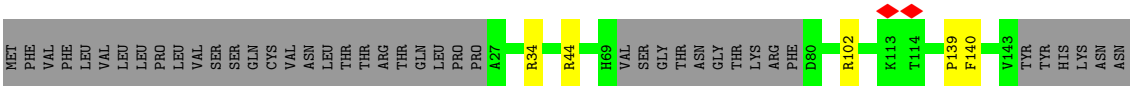
- Molecule 1: Spike glycoprotein

Chain A:



- Molecule 1: Spike glycoprotein

Chain B:



LYS SER TRP MET GLU SER GLU PHE ARG VAL TYR SER SER ALA ASN N165 C166 S172 GLN PRO PHE LEU MET ASP LEU GLU GLY LYS GLN GLY ASN F186 R190 D198 R214 G232 R237 H245 ARG SER TYR LEU THR PRO GLY ASP SER SER SER GLY TRP THR ALA

GLY ALA A263 Y266 Y269 R273 T274 F275 R319 R328 R346 R355 S366 C391 R403 G413 I418 N422 D427 D428 F429 K444 VAL GLY G447 R454 LEU PHE ARG LYS SER ASN LEU K462 R466 D467 I468 SER THR GLU ILE TYR GLN

ALA GLY SER THR PRO CYS ASN GLY VAL GLU GLY PHE ASN CYS Y489 N501 GLY V503 G504 Y505 C525 R567 R577 N603 V620 PRO VAL ALA ILE HIS ALA ASP GLN LEU THR PRO THR TRP ARG VAL TYR SER THR GLY SER N641 T676 GLN THR ASN SER PRO GLY

SER ALA SER SER VAL ALA S689 N709 I726 C760 R765 R815 T827 LEU ALA ASP ALA GLY PHE ILE LYS GLN TYR GLY ASP CYS LEU GLY ASP ILE ALA ALA ARG ASP LEU ILE CYS ALA GLN K854 Y904 L948 R983 R995 R1000 L1004 R1014

R1019 R1107 D1127 S1147 PHE LYS GLU GLU LEU ASP LYS TYR PHE LYS ASN HIS THR SER PRO ASP VAL ASP LEU GLY ASP ILE SER GLY ILE ASN ALA ALA SER VAL VAL ASN ILE GLN LYS GLU ILE ASP ARG LEU ASN GLU VAL ALA LYS ASN LEU ASN GLU SER LEU ILE ASP

LEU GLN GLU LEU GLY LYS TYR GLU GLN GLY SER GLY TYR ILE PRO GLU ALA PRO ARG ASP GLY GLN ALA TYR VAL ARG LYS ASP GLY GLU TRP VAL LEU LEU SER THR PHE LEU GLY ARG SER LEU GLU VAL LEU PHE GLN GLY PRO GLY HIS HIS HIS HIS HIS HIS HIS HIS SER ALA

TRP SER HIS PRO GLN PHE GLU LYS GLY GLY GLY SER GLY GLY GLY GLY SER GLY GLY SER ALA TRP SER HIS PRO GLN PHE GLU LYS

- Molecule 1: Spike glycoprotein

Chain C:

MET PHE VAL PHE LEU VAL LEU LEU PRO LEU VAL SER SER GLN CYS VAL ASN LEU THR THR ARG THR GLN LEU PRO PRO A27 R34 R44 H69 VAL SER GLY THR ASN GLY THR LYS ARG PHE D80 L84 R102 V143 TYR TYR HIS LYS ASN ASN LYS SER TRP MET

GLU SER GLU PHE ARG VAL TYR SER SER SER ALA ASN N165 C166 S172 GLN PRO PHE LEU MET ASP LEU GLU GLY LYS GLN GLY ASN F186 R190 D198 R214 Q218 R237 F238 H245 ARG SER TYR LEU THR PRO GLY ASP SER SER SER GLY TRP THR ALA GLY ALA A263

R273 N317 F318 R319 E324 R328 R346 R355 K356 R357 C391 Y396 R408 T415 D427 K444 VAL GLY G447 Y451 R454 LEU PHE ARG LYS SER ASN LEU K462 R466 D467 I468 SER THR GLU ILE TYR GLN ALA GLY SER THR PRO CYS ASN

GLY VAL GLU GLY PHE ASN CYS Y489 T500 N501 GLY V503 R509 C525 N536 R567 D571 T581 L582 V620 PRO VAL ALA ILE HIS ALA ASP GLN LEU THR PRO THR TRP ARG VAL TYR SER THR GLY SER N641 R646 T676 GLN THR ASN SER PRO GLY SER

ALA SER SER VAL ALA S689 N709 C760 R815 T827 LEU ALA ASP ALA GLY PHE ILE LYS GLN TYR GLY ASP CYS LEU GLY ASP ILE ALA ALA ARG ASP LEU ILE CYS ALA GLN K854 Y904 R983 R995 L1004 R1014 R1019 R1039 C1043 H1048

R1091 R1107 L1145 D1146 S1147 PHE LYS GLU GLU LEU ASP LYS TYR PHE LYS ASN HIS THR SER PRO ASP VAL ASP LEU GLY ASP ILE SER GLY ILE ASN ALA ALA SER VAL VAL ASN ILE GLN LYS GLU ILE ASP ARG LEU ASN GLU VAL ALA LYS ASN LEU ASN GLU SER LEU ILE ASP LEU

GLN GLU LEU GLY LYS TYR GLU GLN GLY SER GLY TYR ILE PRO GLU ALA PRO ARG ASP GLY GLN ALA TYR VAL ARG LYS ASP GLY GLU TRP VAL LEU LEU SER THR PHE LEU GLY ARG SER LEU GLU VAL LEU PHE GLN GLY PRO GLY HIS HIS HIS HIS HIS HIS HIS HIS SER ALA TRP

SER HIS PRO GLN PHE GLU LYS GLY GLY GLY SER GLY GLY GLY GLY SER GLY GLY SER ALA TRP SER HIS PRO GLN PHE GLU LYS

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

Chain D: 50% 100%

NAG1 NAG2

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

Chain E: 100%

NAG1 NAG2

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

Chain F: 100%

NAG1 NAG2

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

Chain G: 100%

NAG1 NAG2

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

Chain H: 100%

NAG1 NAG2

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

Chain I: 100%

NAG1 NAG2

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

Chain J: 100%

NAG1
NAG2

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

Chain K: 100%

NAG1
NAG2

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

Chain L: 100%

NAG1
NAG2

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

Chain M: 100%

NAG1
NAG2

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

Chain N: 100%

NAG1
NAG2

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

Chain O: 100%

NAG1
NAG2

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

Chain P: 100%

NAG1
NAG2

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

Chain Q: 100%

NAG1
NAG2

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

Chain R: 100%

NAG1
NAG2

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	182326	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 ($e^-/Å^2$)	51.8	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	1.829	Depositor
Minimum map value	-0.935	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.049	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	317.4, 317.4, 317.4	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.058, 1.058, 1.058	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.65	0/7768	0.97	31/10563 (0.3%)
1	B	0.64	0/7768	0.95	26/10563 (0.2%)
1	C	0.65	0/7764	0.97	28/10558 (0.3%)
All	All	0.65	0/23300	0.96	85/31684 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	3
1	C	0	4
All	All	0	10

There are no bond length outliers.

The worst 5 of 85 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	273	ARG	NE-CZ-NH1	9.02	124.81	120.30
1	A	273	ARG	NE-CZ-NH1	8.36	124.48	120.30
1	C	319	ARG	NE-CZ-NH1	8.01	124.30	120.30
1	C	328	ARG	NE-CZ-NH1	8.00	124.30	120.30
1	A	403	ARG	NE-CZ-NH1	7.96	124.28	120.30

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	355	ARG	Sidechain
1	A	391	CYS	Peptide
1	A	423	TYR	Sidechain
1	B	266	TYR	Sidechain
1	B	269	TYR	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7602	0	7421	1	0
1	B	7602	0	7420	2	0
1	C	7598	0	7417	2	0
2	D	28	0	25	0	0
2	E	28	0	25	0	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	0	0
2	M	28	0	25	0	0
2	N	28	0	25	0	0
2	O	28	0	25	0	0
2	P	28	0	25	0	0
2	Q	28	0	25	0	0
2	R	28	0	25	0	0
3	A	154	0	143	0	0
3	B	154	0	143	0	0
3	C	154	0	143	0	0
All	All	23684	0	23062	5	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 0.

All (5) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:CYS:HB2	1:A:525:CYS:HA	1.93	0.51
1:B:391:CYS:HB2	1:B:525:CYS:HA	1.92	0.51
1:C:391:CYS:HB2	1:C:525:CYS:HA	1.94	0.50
1:B:726:ILE:HG22	1:B:948:LEU:HD13	1.97	0.47
1:C:1043:CYS:HB3	1:C:1048:HIS:CD2	2.55	0.41

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	948/1288 (74%)	878 (93%)	67 (7%)	3 (0%)	41	74
1	B	948/1288 (74%)	879 (93%)	65 (7%)	4 (0%)	34	69
1	C	948/1288 (74%)	886 (94%)	59 (6%)	3 (0%)	41	74
All	All	2844/3864 (74%)	2643 (93%)	191 (7%)	10 (0%)	38	69

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	855	PHE
1	C	582	LEU
1	C	709	ASN
1	A	709	ASN
1	B	709	ASN

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	851/1112 (76%)	844 (99%)	7 (1%)	81	92
1	B	851/1112 (76%)	841 (99%)	10 (1%)	71	87
1	C	850/1112 (76%)	842 (99%)	8 (1%)	78	90
All	All	2552/3336 (76%)	2527 (99%)	25 (1%)	77	89

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	760	CYS
1	C	84	LEU
1	C	1145	LEU
1	B	1127	ASP
1	C	218	GLN

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

30 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	1.48	4 (28%)	17,19,21	0.85	1 (5%)
2	NAG	D	2	2	14,14,15	1.41	3 (21%)	17,19,21	1.13	1 (5%)
2	NAG	E	1	1,2	14,14,15	1.14	1 (7%)	17,19,21	0.78	0
2	NAG	E	2	2	14,14,15	1.16	2 (14%)	17,19,21	0.60	0
2	NAG	F	1	1,2	14,14,15	1.15	2 (14%)	17,19,21	0.58	0
2	NAG	F	2	2	14,14,15	1.26	2 (14%)	17,19,21	0.81	1 (5%)
2	NAG	G	1	1,2	14,14,15	1.24	1 (7%)	17,19,21	0.95	0
2	NAG	G	2	2	14,14,15	1.15	2 (14%)	17,19,21	0.63	0
2	NAG	H	1	1,2	14,14,15	1.28	2 (14%)	17,19,21	0.65	0
2	NAG	H	2	2	14,14,15	1.22	2 (14%)	17,19,21	0.73	0
2	NAG	I	1	1,2	14,14,15	1.18	1 (7%)	17,19,21	0.73	0
2	NAG	I	2	2	14,14,15	1.16	1 (7%)	17,19,21	0.61	0
2	NAG	J	1	1,2	14,14,15	1.18	2 (14%)	17,19,21	0.75	1 (5%)
2	NAG	J	2	2	14,14,15	1.20	1 (7%)	17,19,21	0.81	1 (5%)
2	NAG	K	1	1,2	14,14,15	1.24	1 (7%)	17,19,21	1.06	1 (5%)
2	NAG	K	2	2	14,14,15	1.22	2 (14%)	17,19,21	0.68	0
2	NAG	L	1	1,2	14,14,15	1.34	3 (21%)	17,19,21	0.99	0
2	NAG	L	2	2	14,14,15	1.23	2 (14%)	17,19,21	0.66	0
2	NAG	M	1	1,2	14,14,15	1.31	3 (21%)	17,19,21	0.53	0
2	NAG	M	2	2	14,14,15	1.22	2 (14%)	17,19,21	0.84	1 (5%)
2	NAG	N	1	1,2	14,14,15	1.23	1 (7%)	17,19,21	1.03	1 (5%)
2	NAG	N	2	2	14,14,15	1.20	2 (14%)	17,19,21	0.68	0
2	NAG	O	1	1,2	14,14,15	1.13	1 (7%)	17,19,21	0.73	0
2	NAG	O	2	2	14,14,15	1.13	1 (7%)	17,19,21	0.69	0
2	NAG	P	1	1,2	14,14,15	1.25	2 (14%)	17,19,21	0.72	0
2	NAG	P	2	2	14,14,15	1.28	2 (14%)	17,19,21	0.77	0
2	NAG	Q	1	1,2	14,14,15	1.17	2 (14%)	17,19,21	0.72	0
2	NAG	Q	2	2	14,14,15	1.26	2 (14%)	17,19,21	0.95	1 (5%)
2	NAG	R	1	1,2	14,14,15	1.39	4 (28%)	17,19,21	0.90	1 (5%)
2	NAG	R	2	2	14,14,15	1.35	2 (14%)	17,19,21	0.70	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	-	2/6/23/26	0/1/1/1
2	NAG	E	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1
2	NAG	G	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1
2	NAG	H	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	0/6/23/26	0/1/1/1
2	NAG	I	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	I	2	2	-	0/6/23/26	0/1/1/1
2	NAG	J	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	J	2	2	-	0/6/23/26	0/1/1/1
2	NAG	K	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	K	2	2	-	0/6/23/26	0/1/1/1
2	NAG	L	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	L	2	2	-	0/6/23/26	0/1/1/1
2	NAG	M	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	M	2	2	-	0/6/23/26	0/1/1/1
2	NAG	N	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	N	2	2	-	0/6/23/26	0/1/1/1
2	NAG	O	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	O	2	2	-	0/6/23/26	0/1/1/1
2	NAG	P	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	P	2	2	-	0/6/23/26	0/1/1/1
2	NAG	Q	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	Q	2	2	-	0/6/23/26	0/1/1/1
2	NAG	R	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	R	2	2	-	0/6/23/26	0/1/1/1

The worst 5 of 58 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	R	2	NAG	O5-C5	2.88	1.49	1.43
2	D	2	NAG	O5-C1	2.83	1.48	1.43
2	R	1	NAG	O5-C5	2.81	1.49	1.43
2	P	2	NAG	O5-C5	2.77	1.49	1.43
2	Q	2	NAG	O5-C5	2.77	1.49	1.43

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	2	NAG	C1-O5-C5	3.86	117.42	112.19
2	M	2	NAG	C1-O5-C5	2.57	115.67	112.19
2	Q	2	NAG	C1-O5-C5	2.48	115.55	112.19
2	R	1	NAG	C1-O5-C5	2.36	115.40	112.19
2	J	2	NAG	C1-O5-C5	2.36	115.38	112.19

There are no chirality outliers.

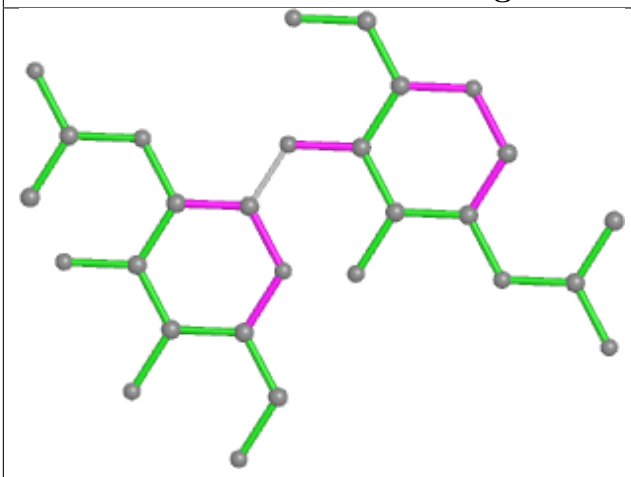
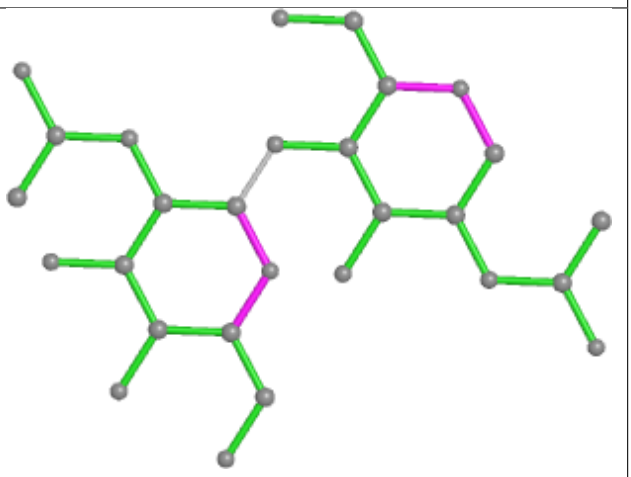
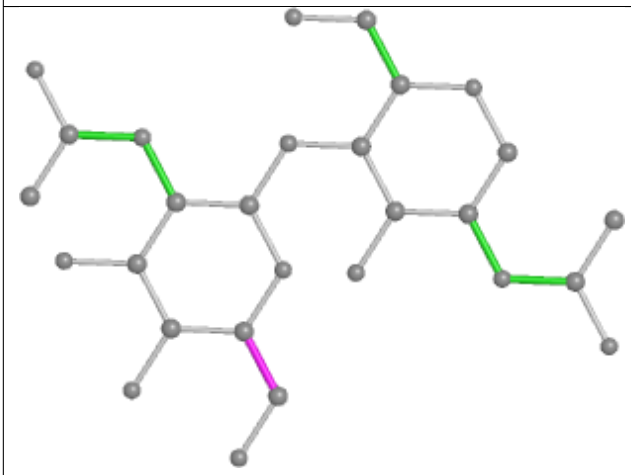
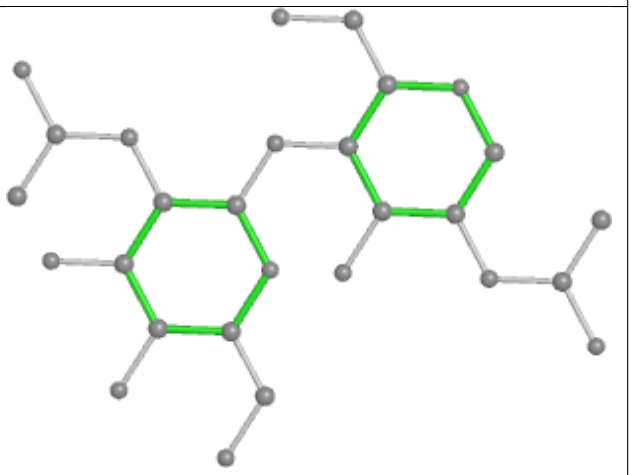
5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	2	NAG	O5-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	Q	1	NAG	O5-C5-C6-O6
2	J	1	NAG	O5-C5-C6-O6
2	F	1	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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

Oligosaccharide Chain D	
 Bond lengths	 Bond angles
 Torsions	 Rings

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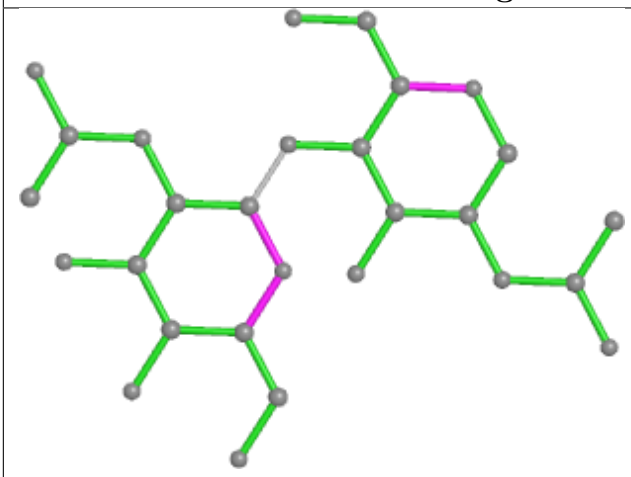
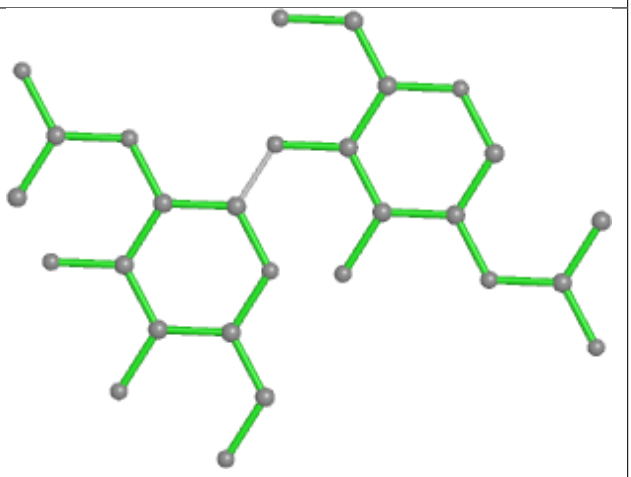
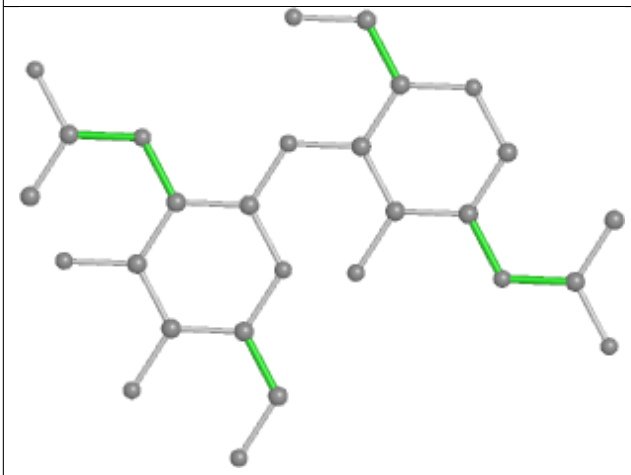
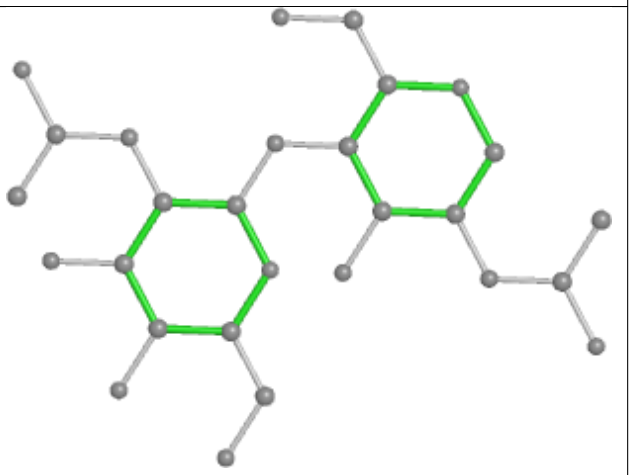
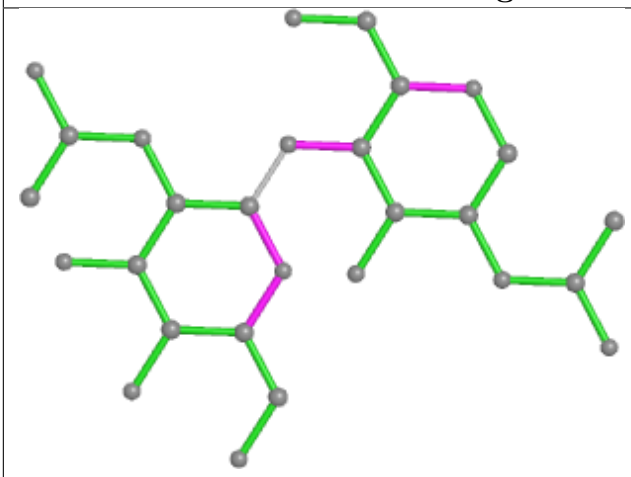
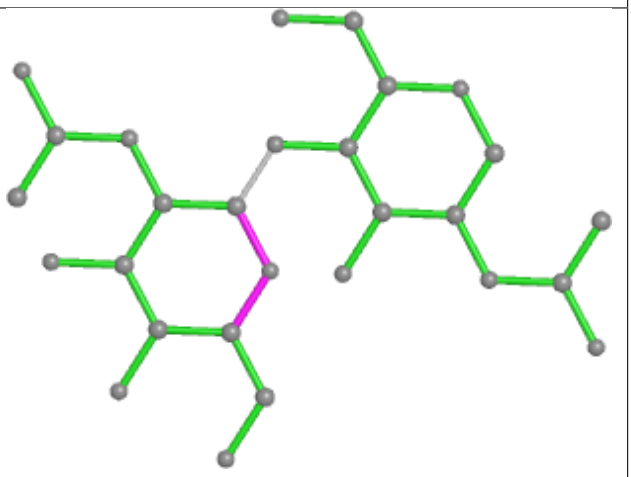
 Bond lengths	 Bond angles
 Torsions	 Rings

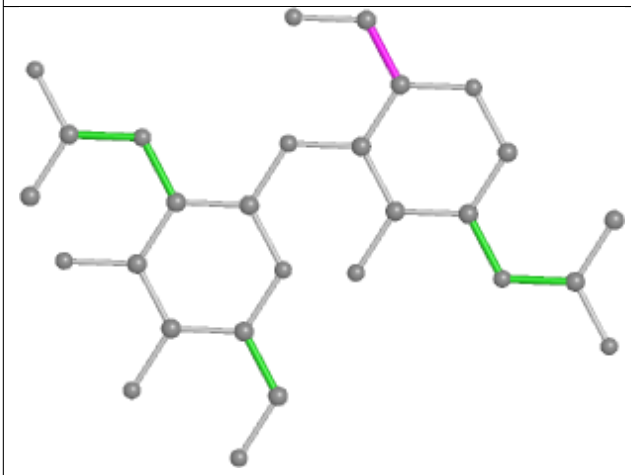
Oligosaccharide Chain F



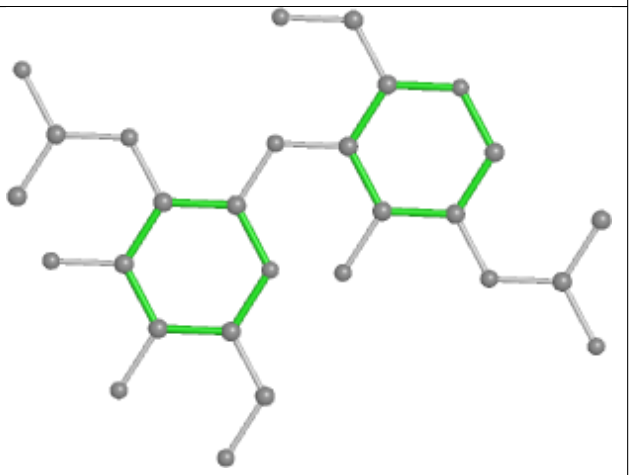
Bond lengths



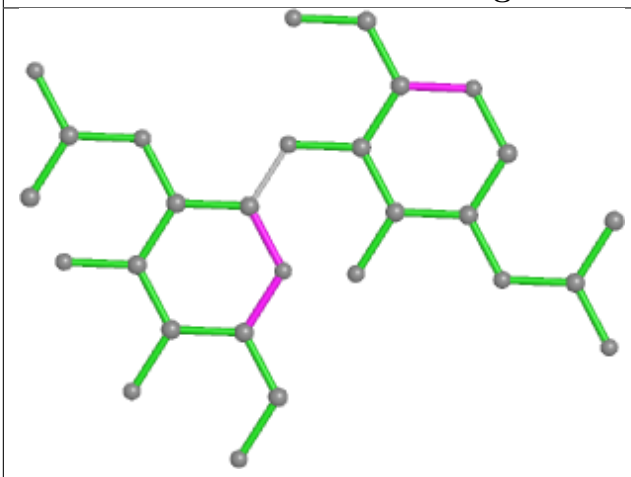
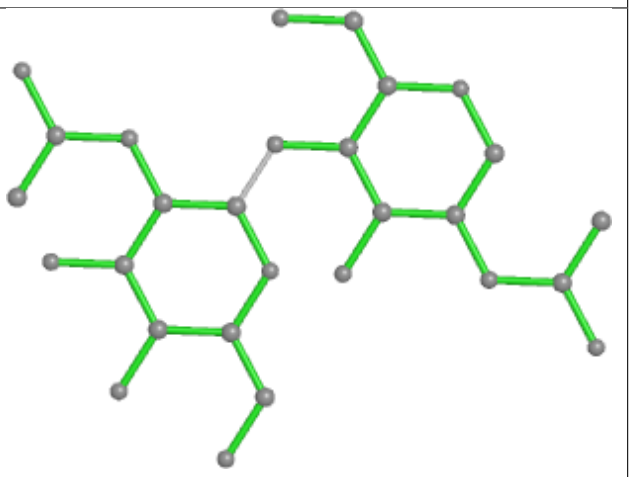
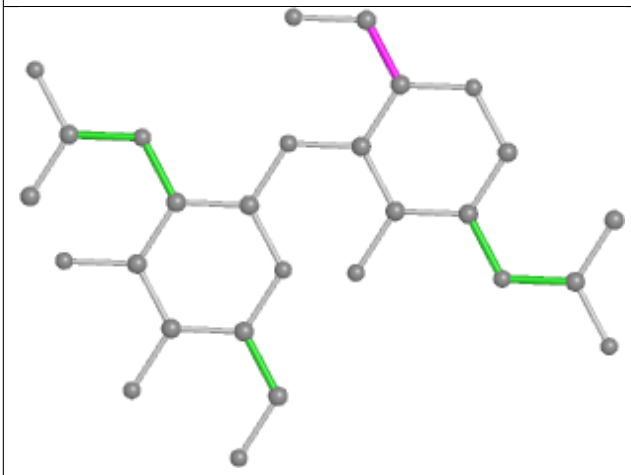
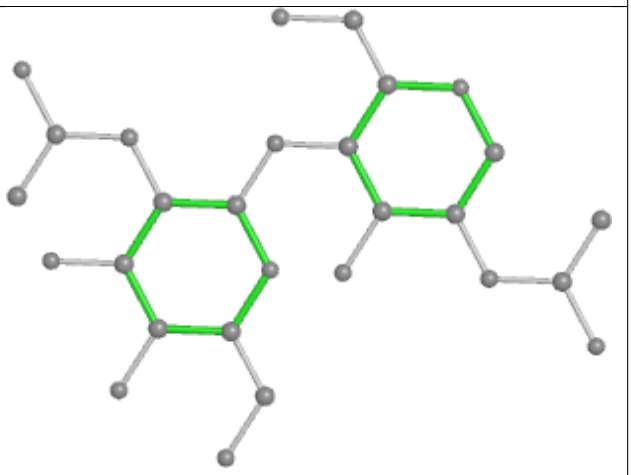
Bond angles

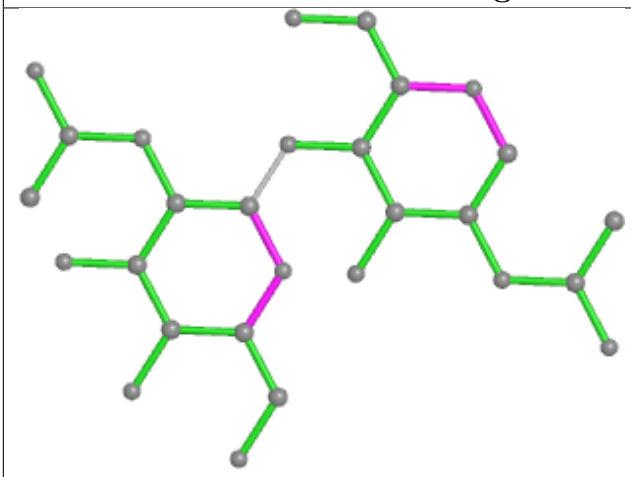
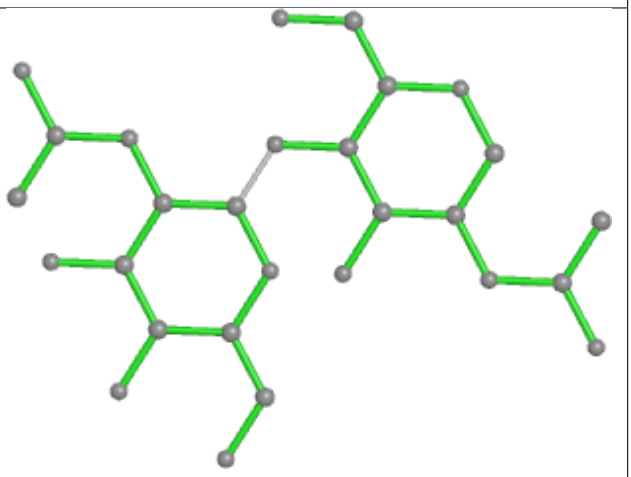
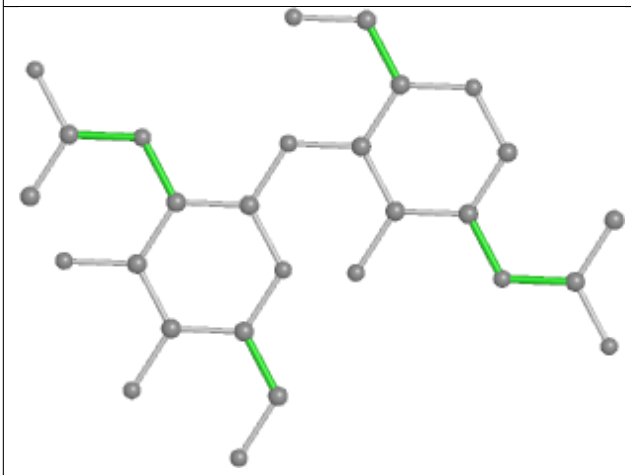
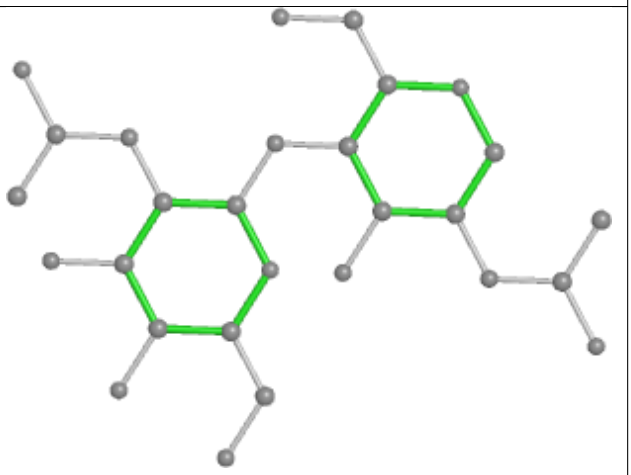


Torsions

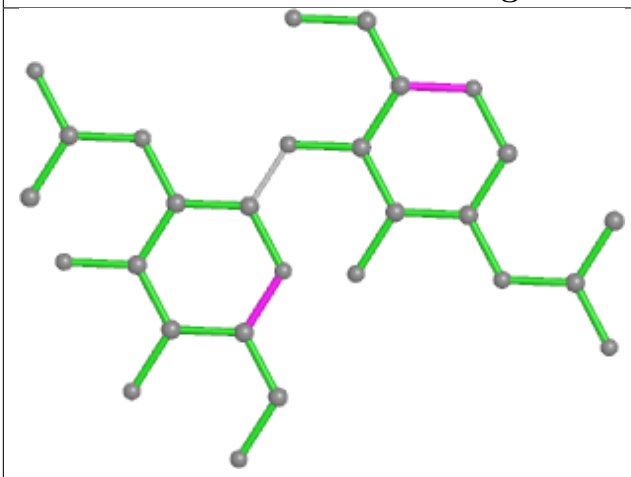


Rings

Oligosaccharide Chain G	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain H	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain I



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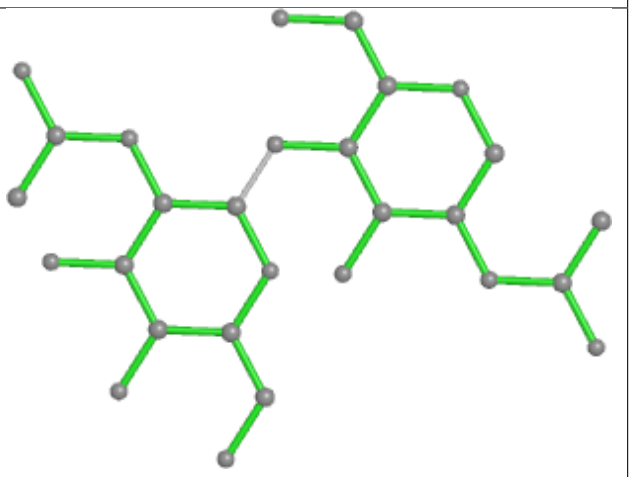

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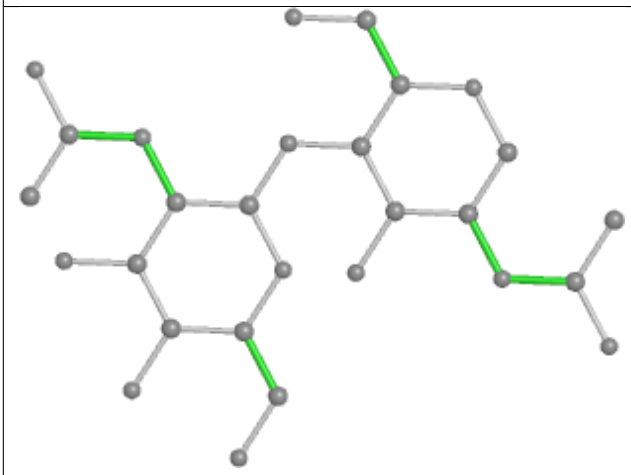

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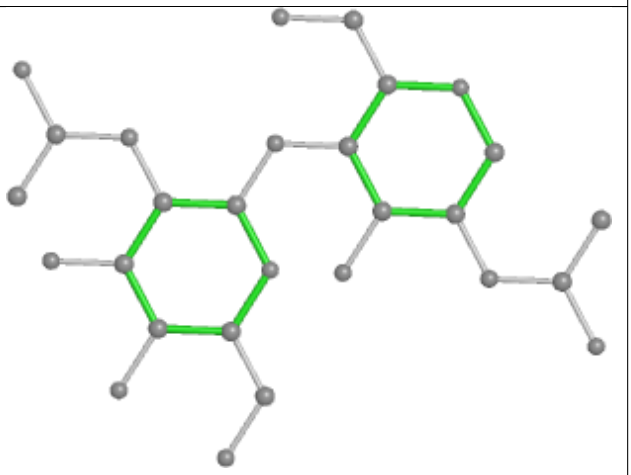
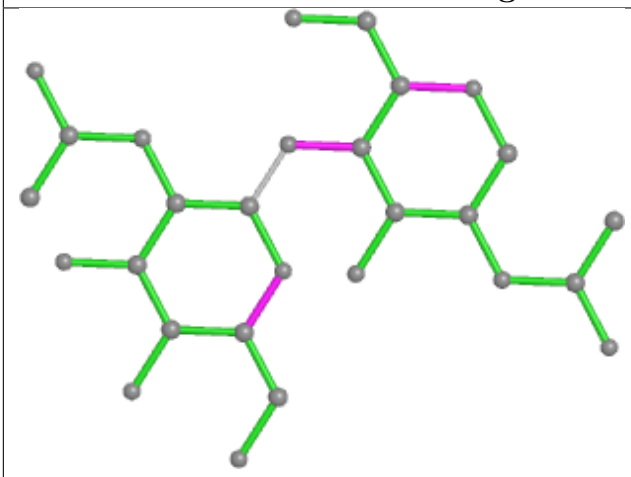


Rings

Oligosaccharide Chain J



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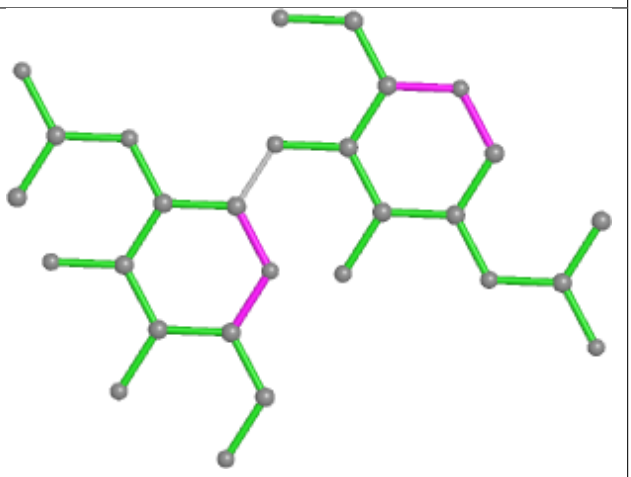

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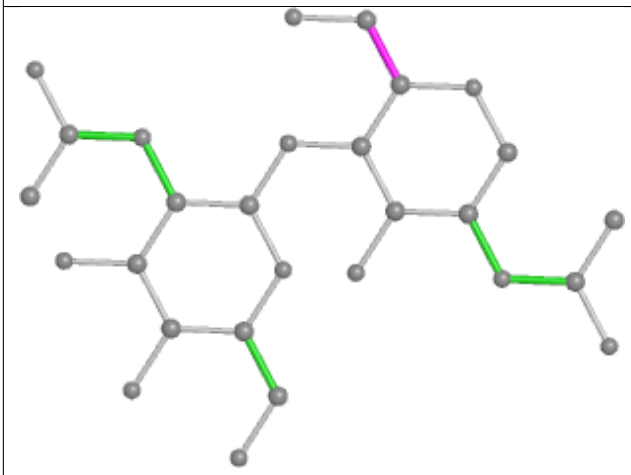

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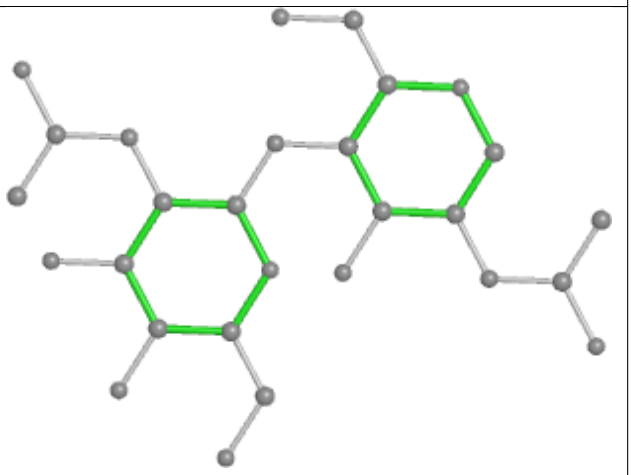
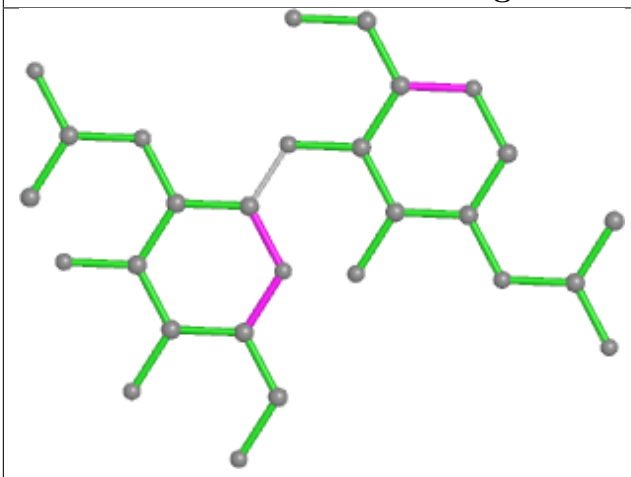
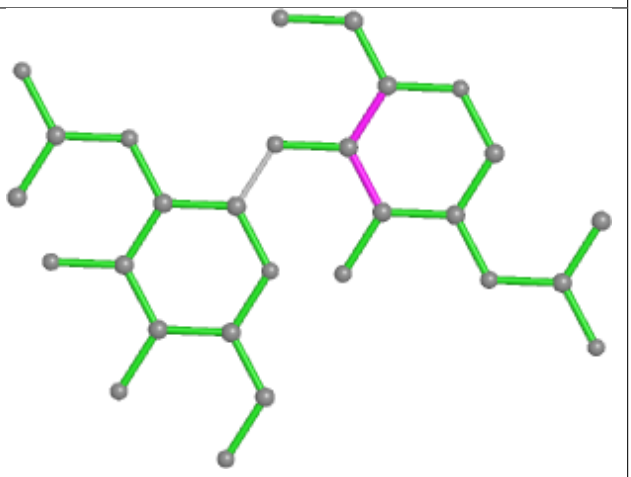


Rings

Oligosaccharide Chain K



Bond lengths



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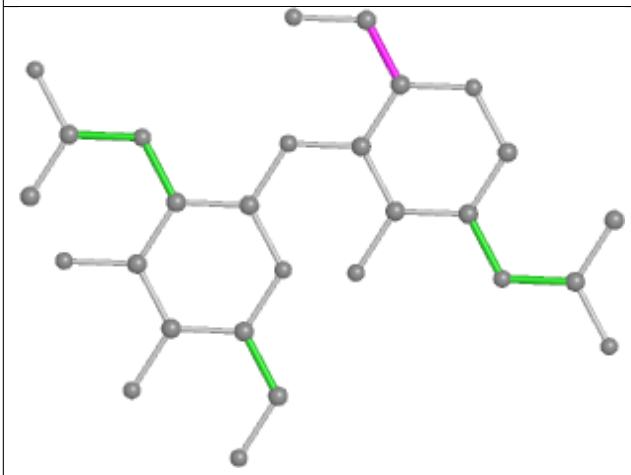
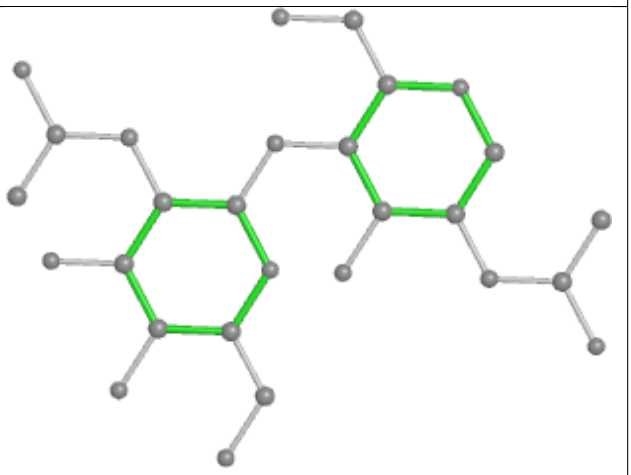
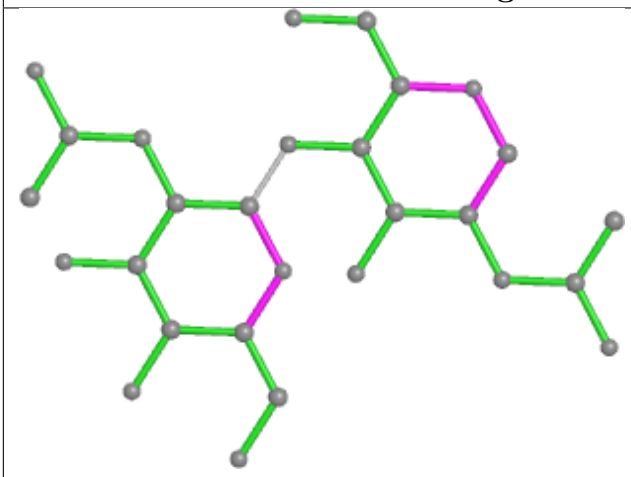
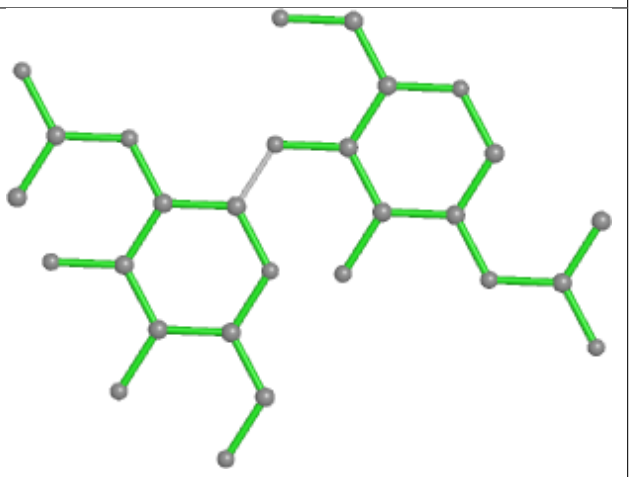
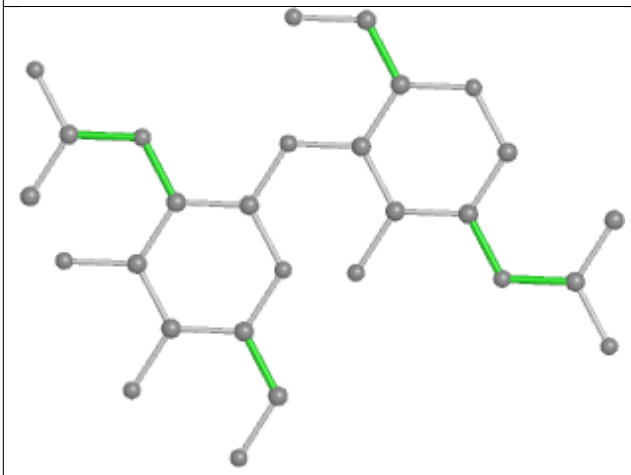
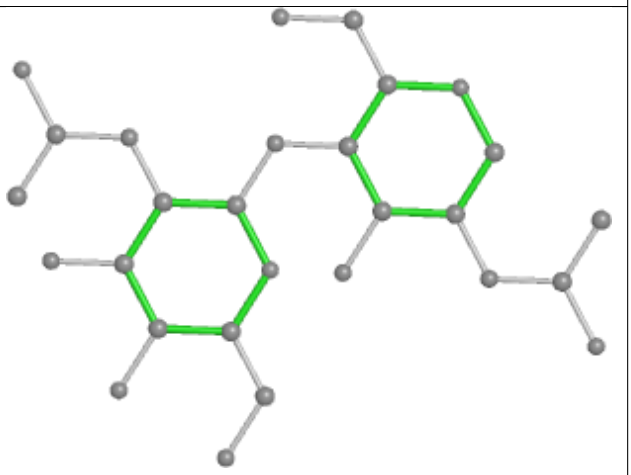
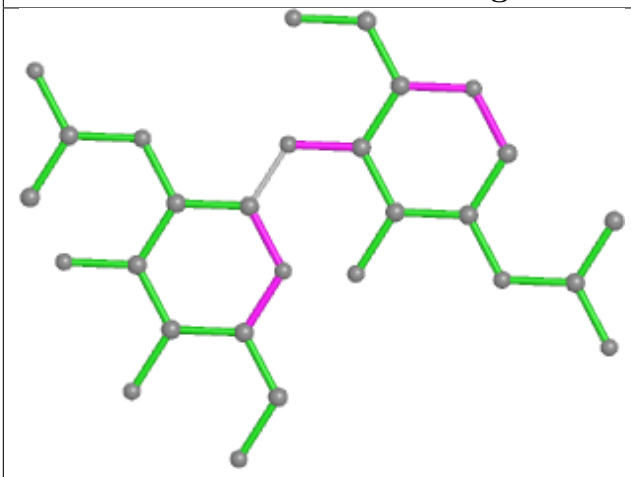
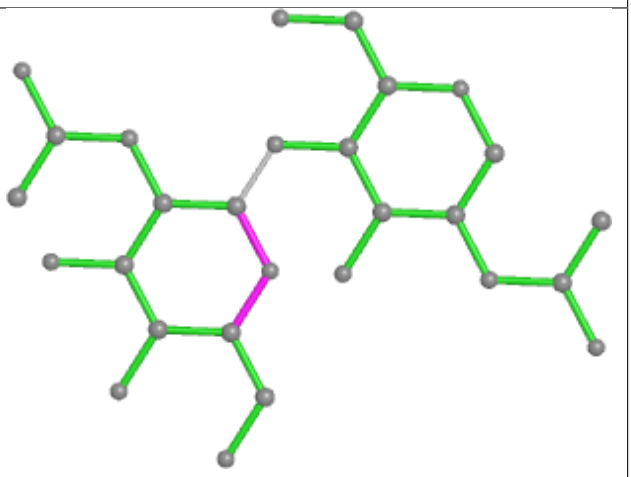
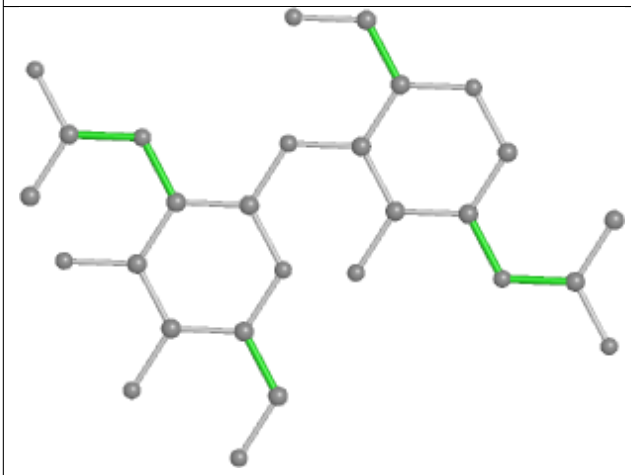
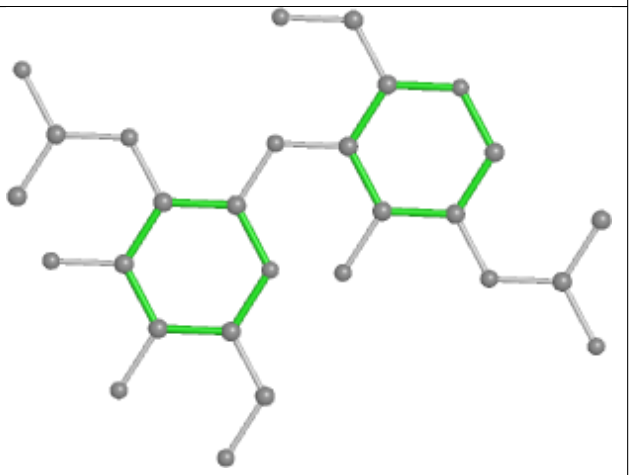


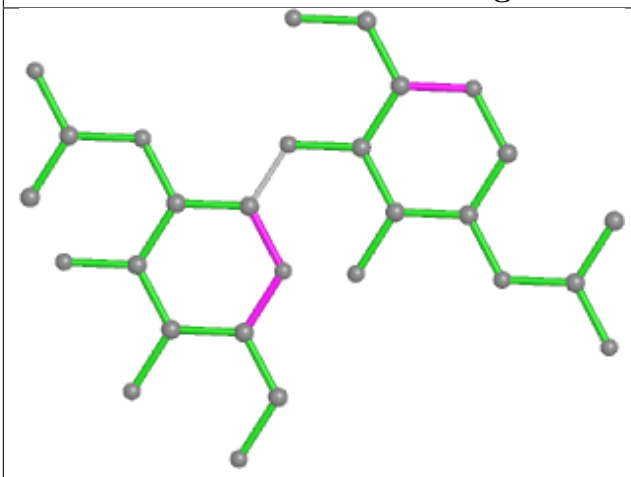
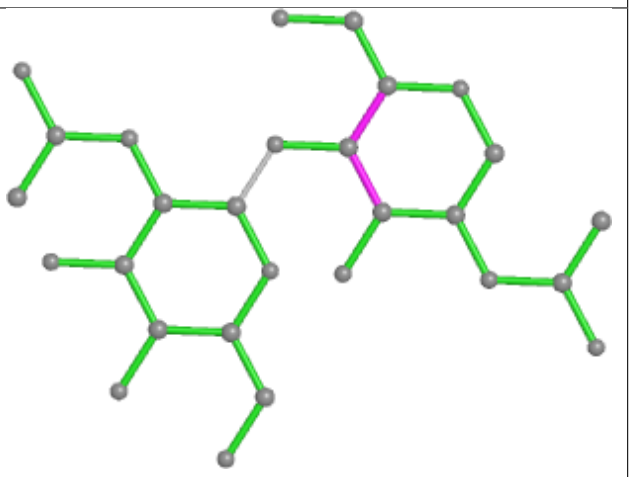
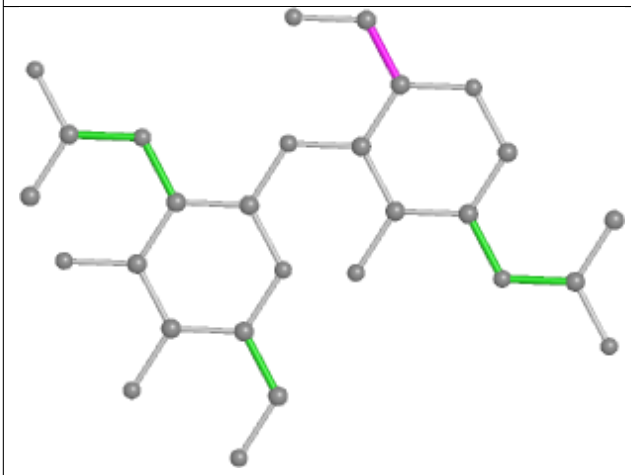
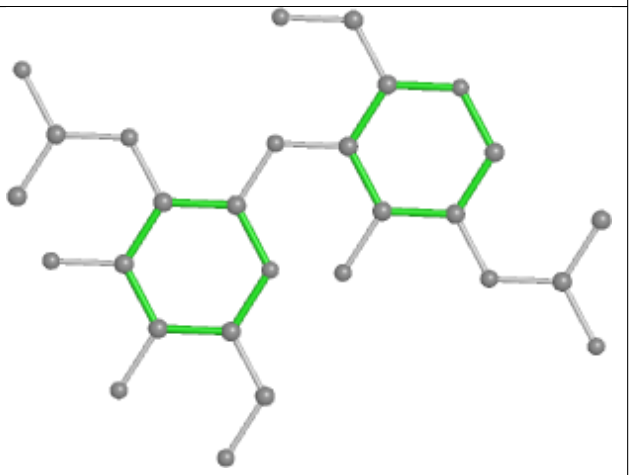
Torsions

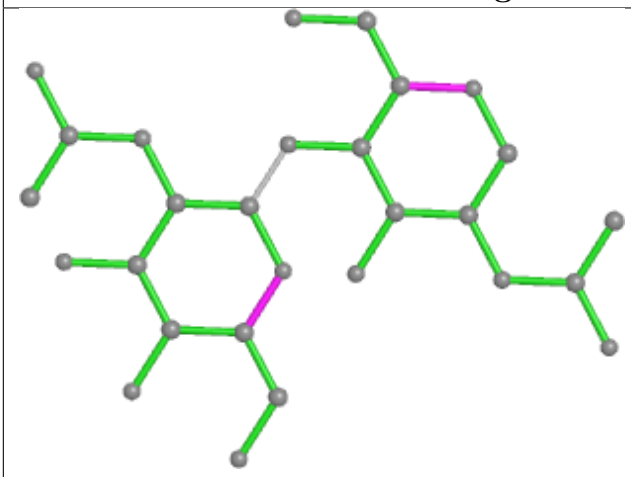
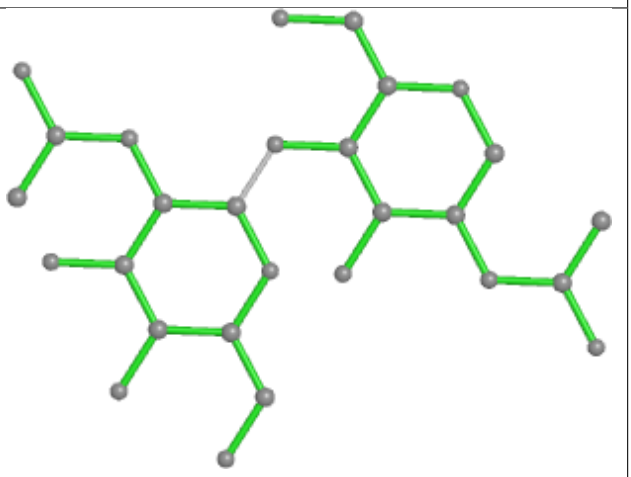
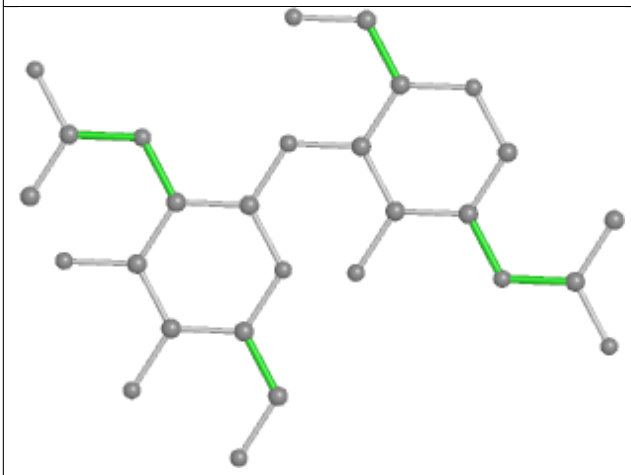
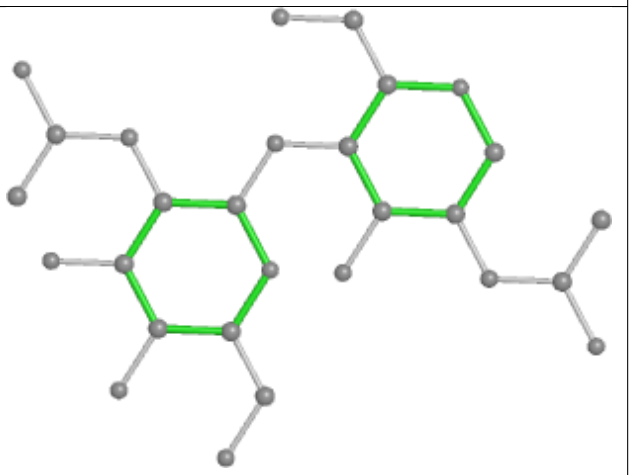


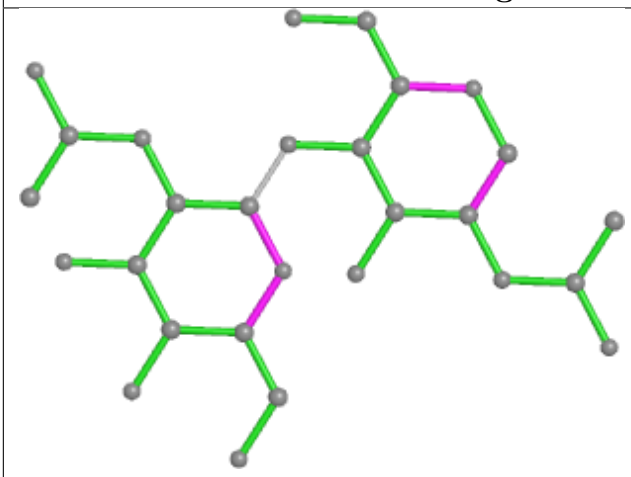
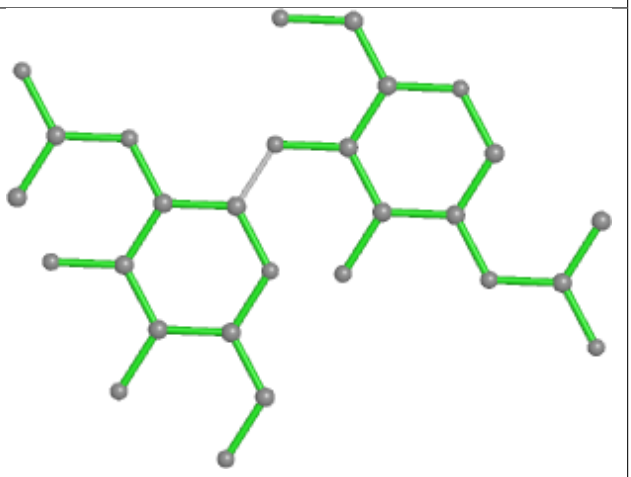
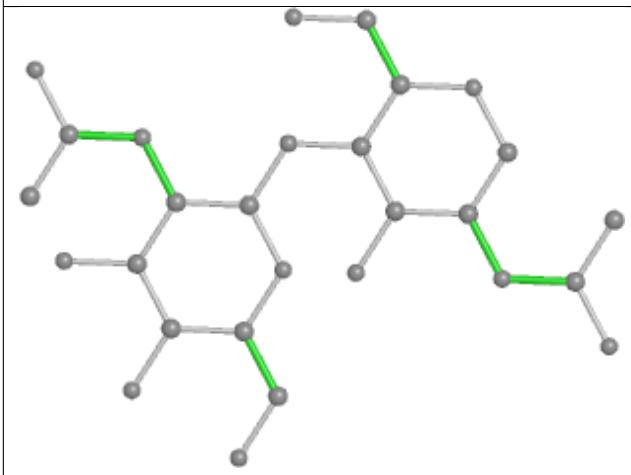
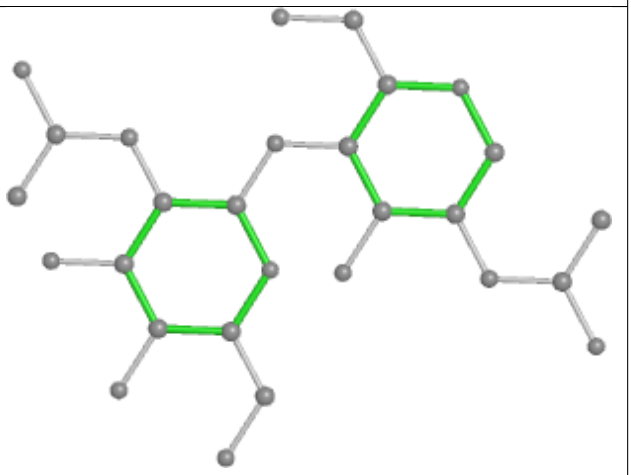
Rings

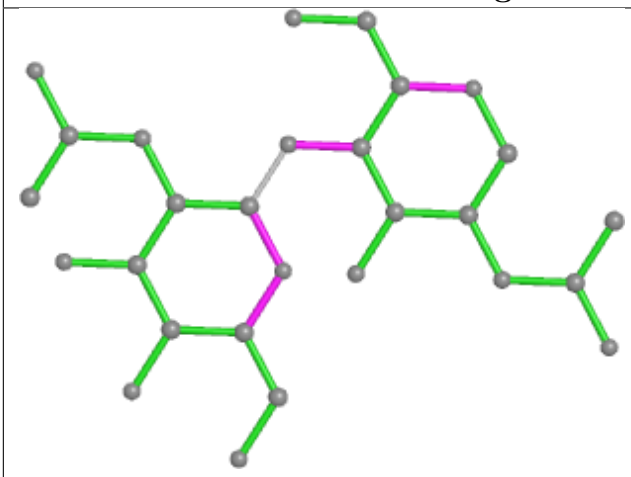
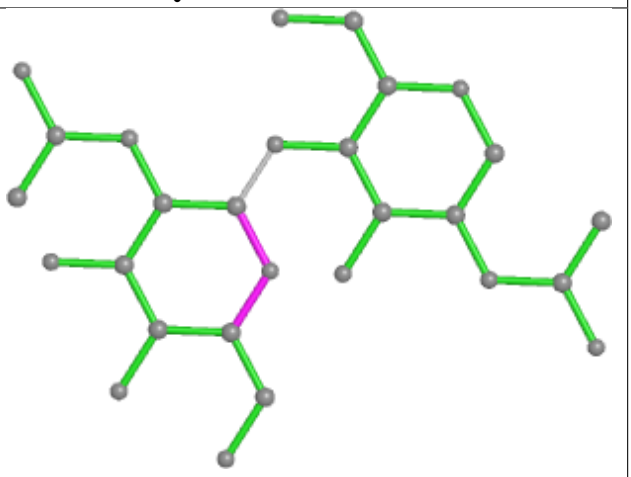
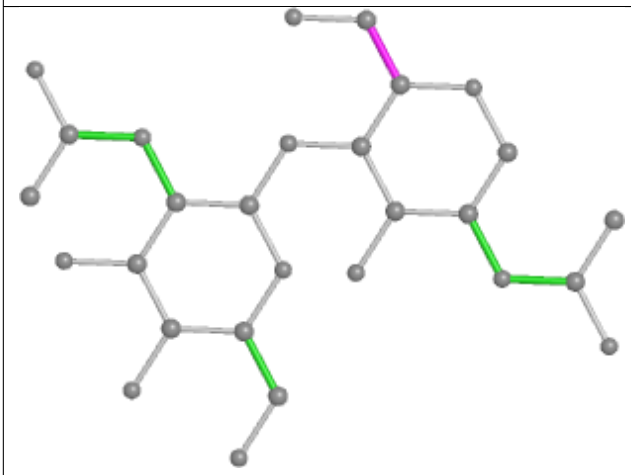
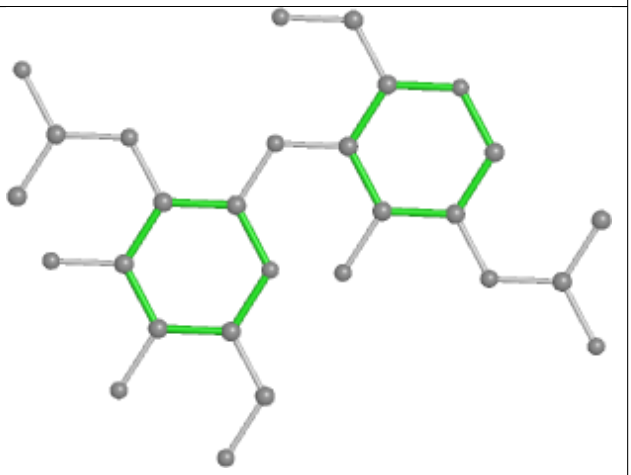
Oligosaccharide Chain L	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain M	
 Bond lengths	 Bond angles
 Torsions	 Rings

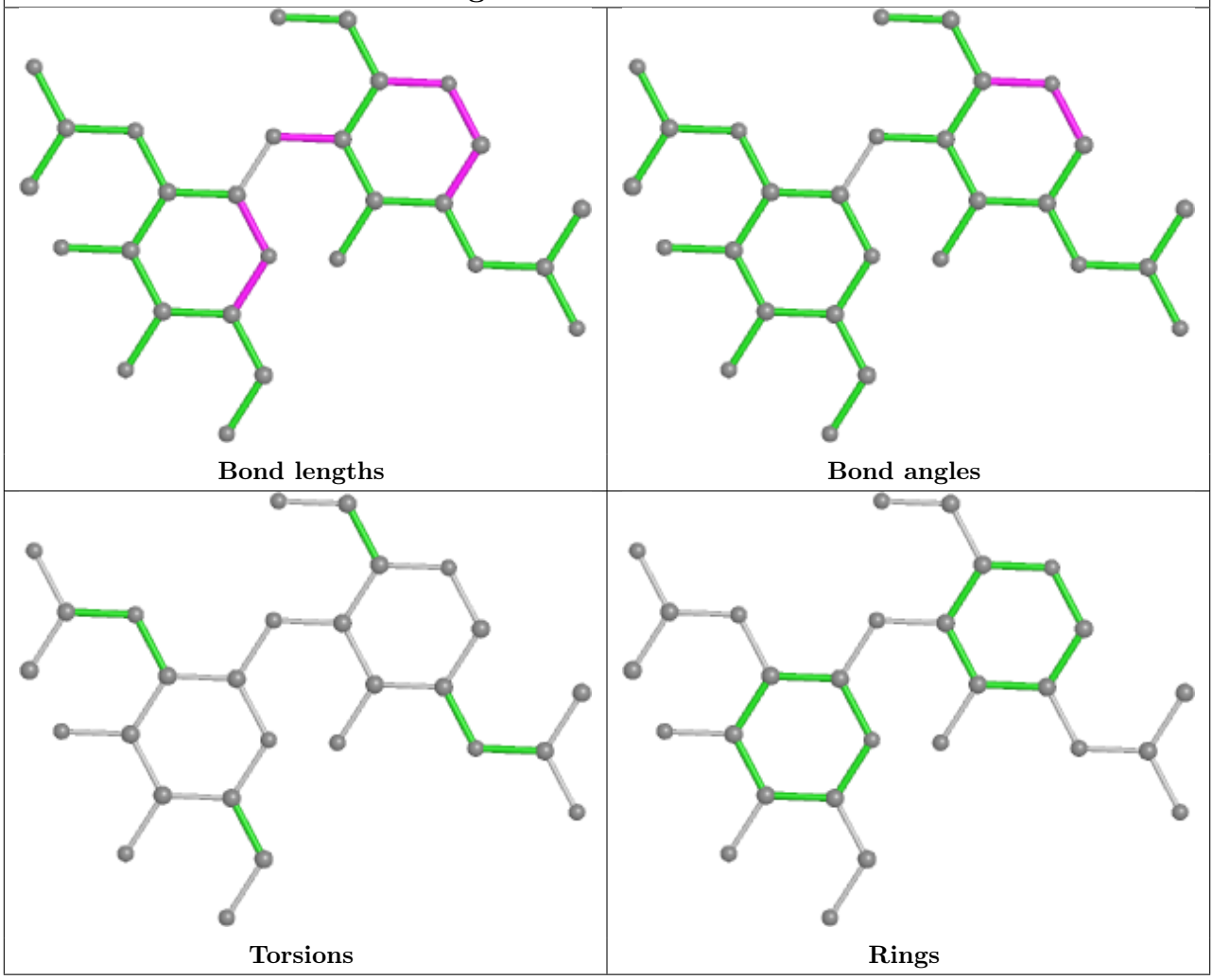
Oligosaccharide Chain N	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain O	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain P	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain Q	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain R



5.6 Ligand geometry (i)

33 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	B	1304	1	14,14,15	1.20	1 (7%)	17,19,21	0.68	0
3	NAG	B	1309	1	14,14,15	1.23	2 (14%)	17,19,21	0.70	0
3	NAG	A	1301	1	14,14,15	1.28	2 (14%)	17,19,21	0.85	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	B	1306	1	14,14,15	1.27	3 (21%)	17,19,21	0.89	1 (5%)
3	NAG	A	1309	1	14,14,15	1.13	1 (7%)	17,19,21	0.84	0
3	NAG	C	1307	1	14,14,15	1.64	2 (14%)	17,19,21	1.26	1 (5%)
3	NAG	B	1311	1	14,14,15	1.64	2 (14%)	17,19,21	0.77	0
3	NAG	A	1310	1	14,14,15	1.16	1 (7%)	17,19,21	0.72	0
3	NAG	B	1302	1	14,14,15	1.26	2 (14%)	17,19,21	0.73	0
3	NAG	B	1308	1	14,14,15	1.24	1 (7%)	17,19,21	0.98	1 (5%)
3	NAG	A	1311	1	14,14,15	1.66	2 (14%)	17,19,21	0.83	0
3	NAG	A	1308	1	14,14,15	1.30	2 (14%)	17,19,21	0.73	0
3	NAG	C	1310	1	14,14,15	1.21	1 (7%)	17,19,21	0.86	1 (5%)
3	NAG	C	1306	1	14,14,15	1.20	1 (7%)	17,19,21	0.84	1 (5%)
3	NAG	B	1301	1	14,14,15	1.25	2 (14%)	17,19,21	0.84	1 (5%)
3	NAG	B	1310	1	14,14,15	1.27	2 (14%)	17,19,21	0.65	0
3	NAG	A	1302	1	14,14,15	1.25	2 (14%)	17,19,21	0.73	0
3	NAG	B	1303	1	14,14,15	1.28	1 (7%)	17,19,21	0.71	0
3	NAG	B	1307	1	14,14,15	1.25	2 (14%)	17,19,21	0.59	0
3	NAG	A	1303	1	14,14,15	1.32	3 (21%)	17,19,21	0.64	0
3	NAG	A	1304	1	14,14,15	1.32	2 (14%)	17,19,21	0.74	1 (5%)
3	NAG	A	1305	1	14,14,15	1.24	2 (14%)	17,19,21	0.77	0
3	NAG	A	1306	1	14,14,15	1.31	3 (21%)	17,19,21	0.65	0
3	NAG	C	1311	1	14,14,15	1.27	2 (14%)	17,19,21	0.77	0
3	NAG	C	1309	1	14,14,15	1.23	2 (14%)	17,19,21	0.63	0
3	NAG	C	1302	1	14,14,15	1.27	2 (14%)	17,19,21	0.87	1 (5%)
3	NAG	A	1307	1	14,14,15	1.25	1 (7%)	17,19,21	0.82	0
3	NAG	C	1305	1	14,14,15	1.34	3 (21%)	17,19,21	0.77	0
3	NAG	C	1304	1	14,14,15	1.23	1 (7%)	17,19,21	0.70	0
3	NAG	C	1303	1	14,14,15	1.14	1 (7%)	17,19,21	0.66	0
3	NAG	C	1301	1	14,14,15	1.27	2 (14%)	17,19,21	0.70	0
3	NAG	B	1305	1	14,14,15	1.17	1 (7%)	17,19,21	0.95	1 (5%)
3	NAG	C	1308	1	14,14,15	1.21	1 (7%)	17,19,21	0.73	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	B	1304	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1309	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1301	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1306	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1309	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1307	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1311	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1310	1	-	1/6/23/26	0/1/1/1
3	NAG	B	1302	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1308	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1311	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1308	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1310	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1306	1	-	1/6/23/26	0/1/1/1
3	NAG	B	1301	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1310	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1302	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1303	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1307	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1303	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1304	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1305	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1306	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1311	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1309	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1302	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1307	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1305	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1304	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1303	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1301	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1305	1	-	1/6/23/26	0/1/1/1
3	NAG	C	1308	1	-	0/6/23/26	0/1/1/1

The worst 5 of 58 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1311	NAG	C1-C2	4.37	1.58	1.52
3	A	1311	NAG	C1-C2	4.33	1.58	1.52
3	C	1307	NAG	C1-C2	4.33	1.58	1.52
3	A	1308	NAG	O5-C5	2.91	1.49	1.43
3	B	1303	NAG	O5-C5	2.88	1.49	1.43

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1307	NAG	C1-O5-C5	4.25	117.96	112.19
3	B	1305	NAG	C1-O5-C5	2.85	116.05	112.19
3	B	1301	NAG	C1-O5-C5	2.78	115.96	112.19
3	B	1308	NAG	C1-O5-C5	2.69	115.83	112.19
3	C	1310	NAG	C1-O5-C5	2.61	115.73	112.19

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1306	NAG	O5-C5-C6-O6
3	B	1305	NAG	O5-C5-C6-O6
3	A	1310	NAG	O5-C5-C6-O6
3	B	1308	NAG	C4-C5-C6-O6
3	B	1308	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)

There are no chain breaks in this entry.

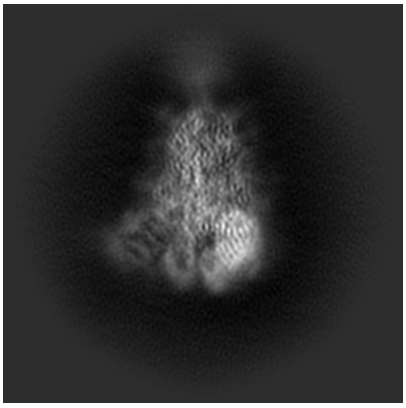
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-22831. These allow visual inspection of the internal detail of the map and identification of artifacts.

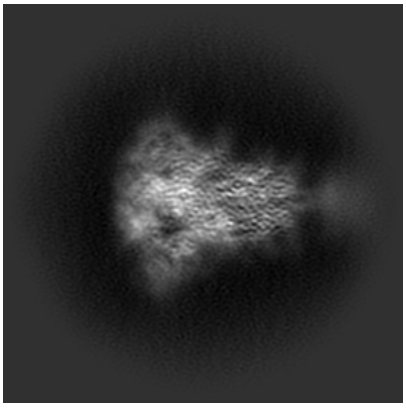
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

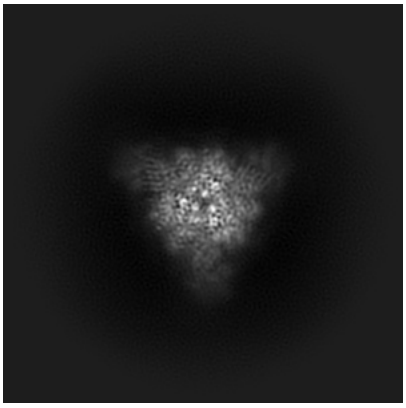
6.1.1 Primary map



X



Y

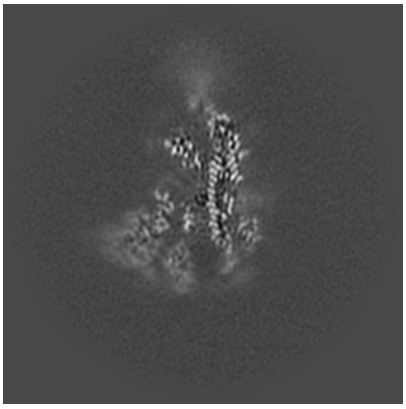


Z

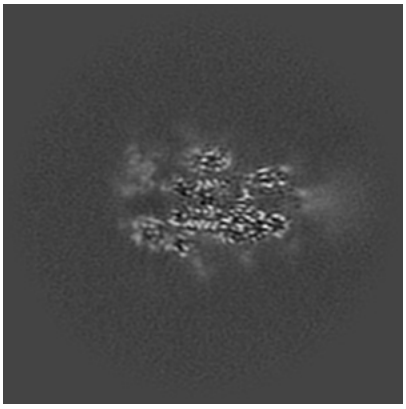
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

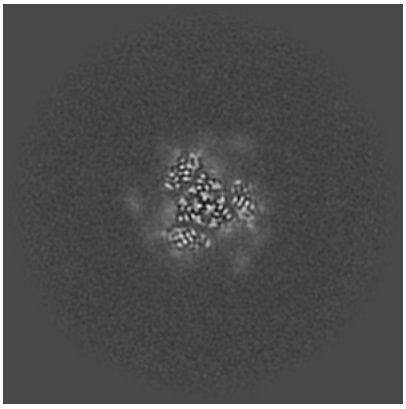
6.2.1 Primary map



X Index: 150



Y Index: 150

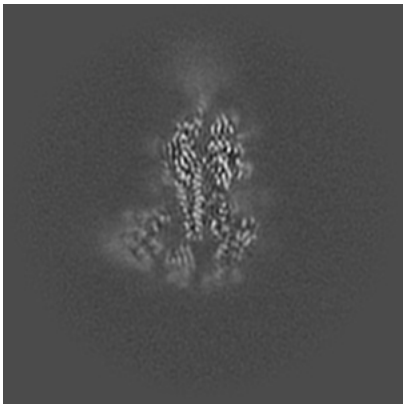


Z Index: 150

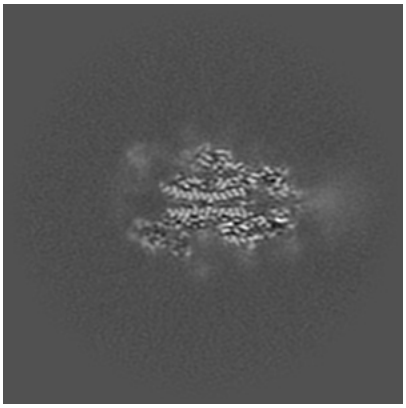
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

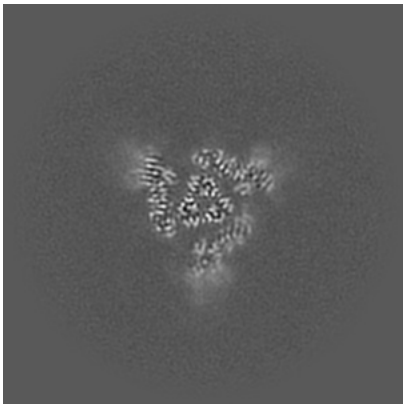
6.3.1 Primary map



X Index: 156



Y Index: 146

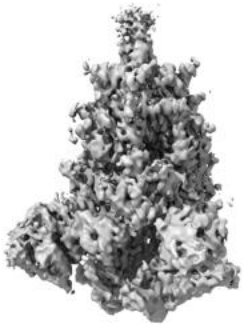


Z Index: 131

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.

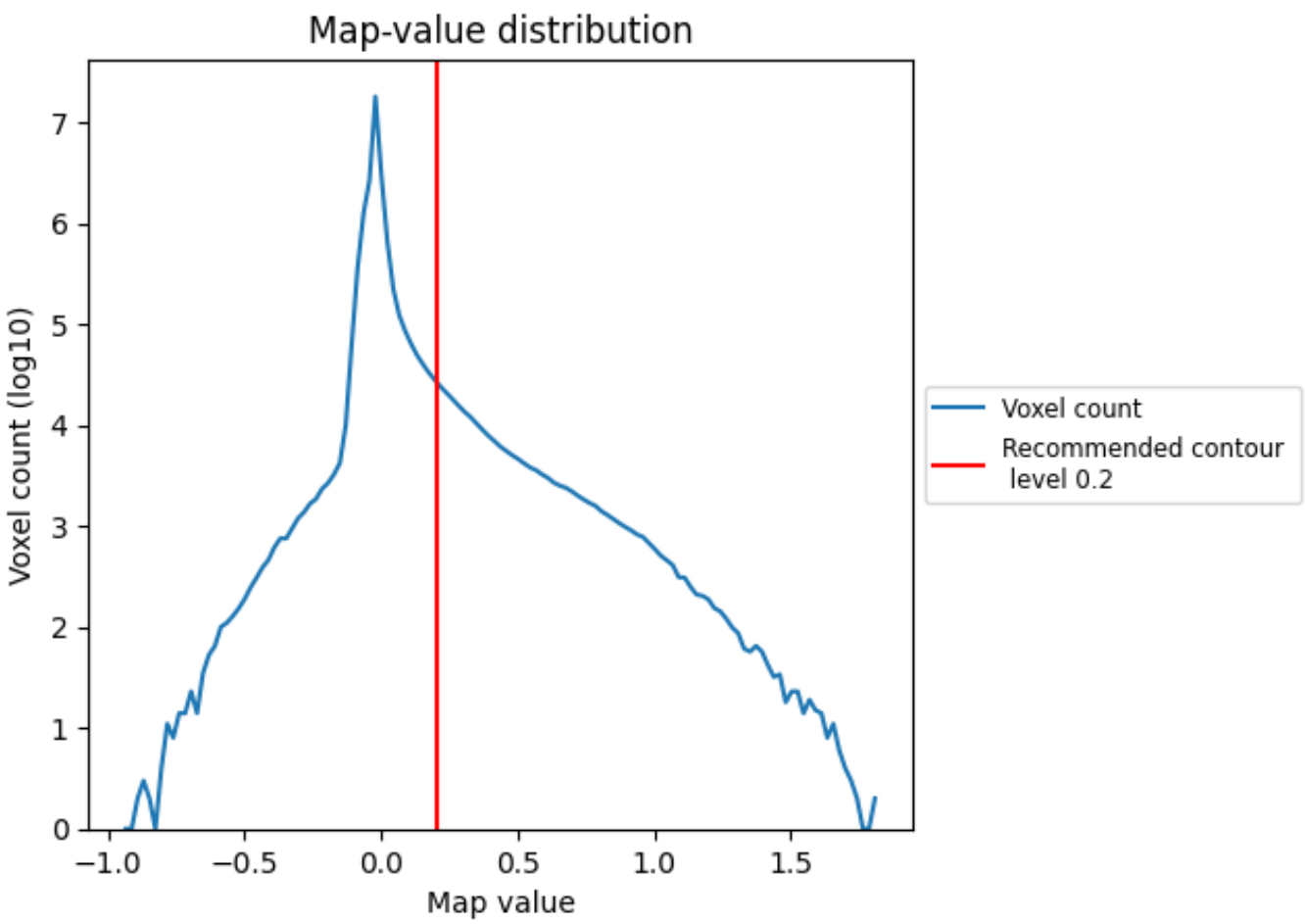
6.5 Mask visualisation (i)

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

7 Map analysis (i)

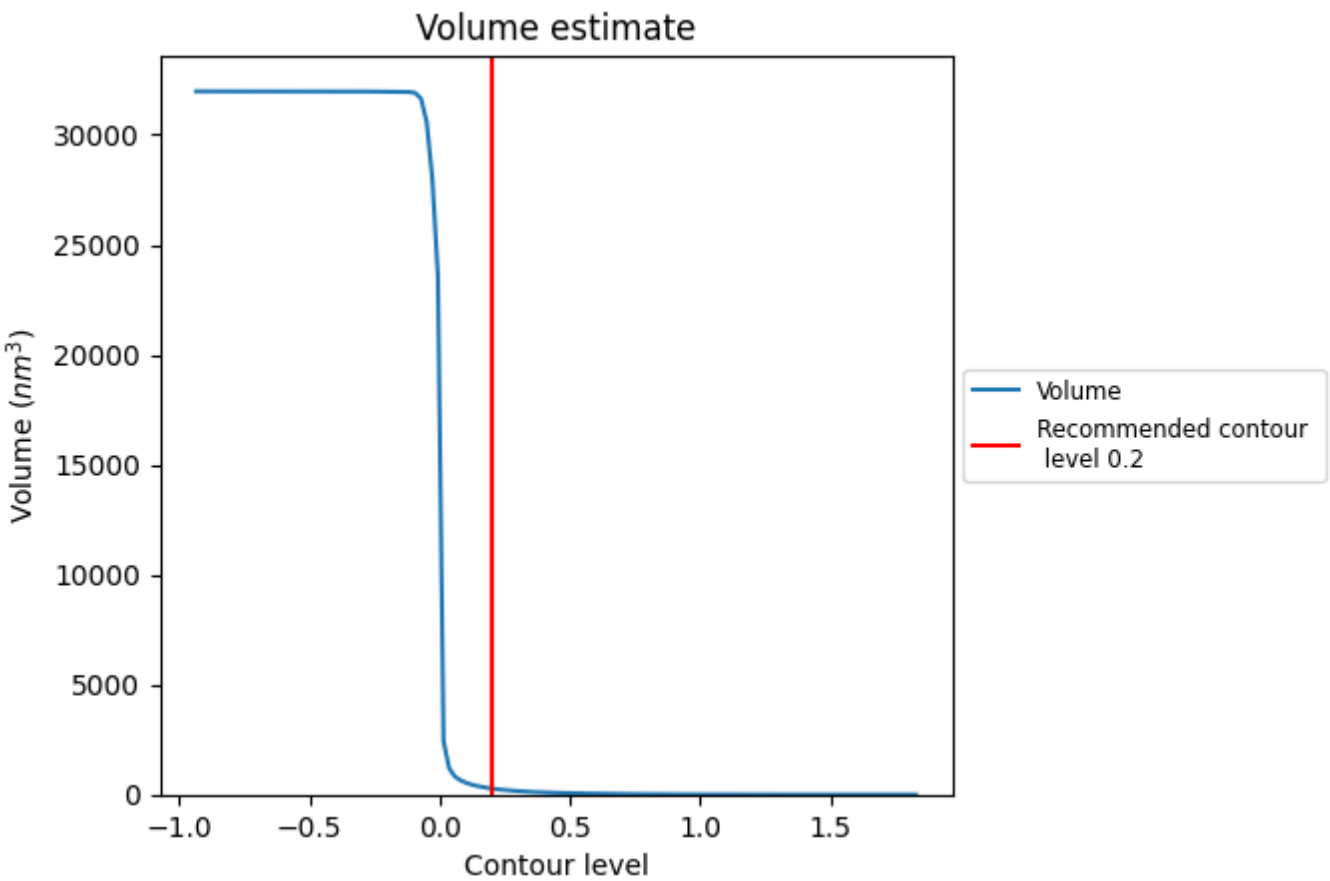
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

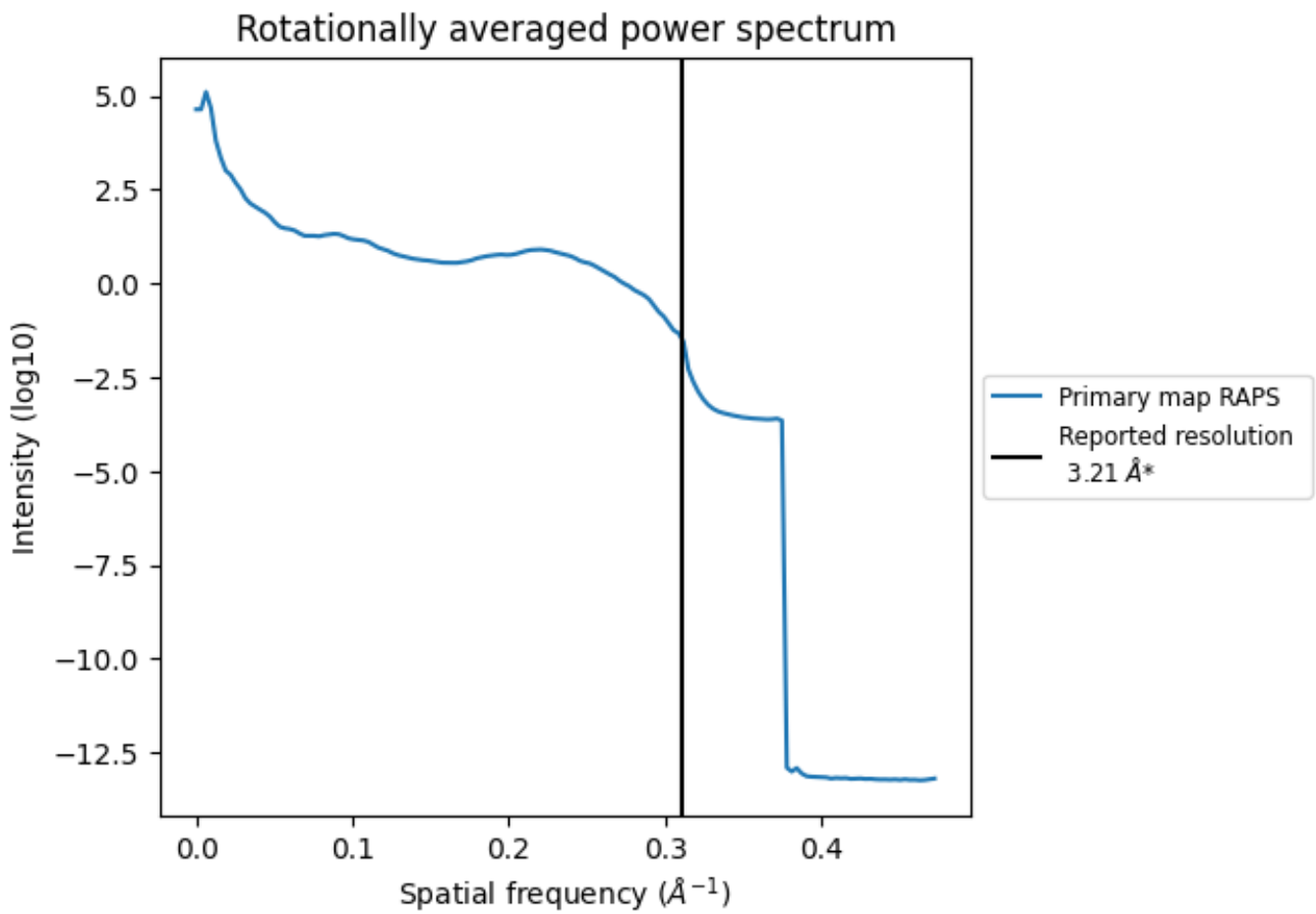
7.2 Volume estimate (i)



The volume at the recommended contour level is 275 nm^3; this corresponds to an approximate mass of 248 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 0.312 Å^{-1}

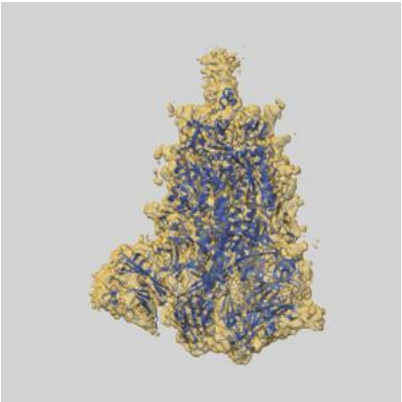
8 Fourier-Shell correlation (i)

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

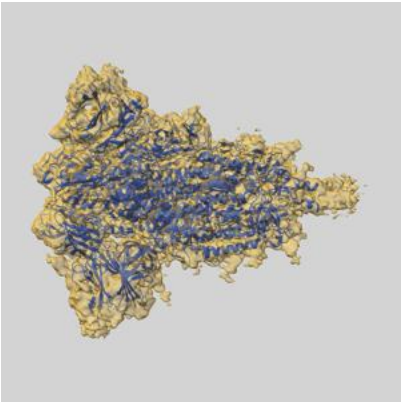
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-22831 and PDB model 7KE4. Per-residue inclusion information can be found in section 3 on page 14.

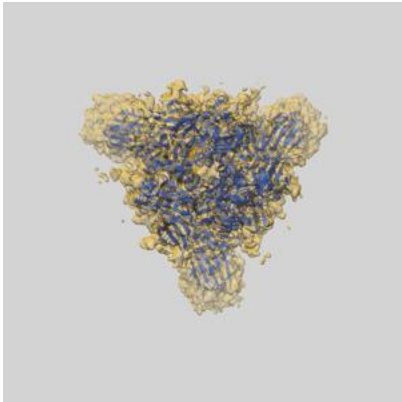
9.1 Map-model overlay (i)



X



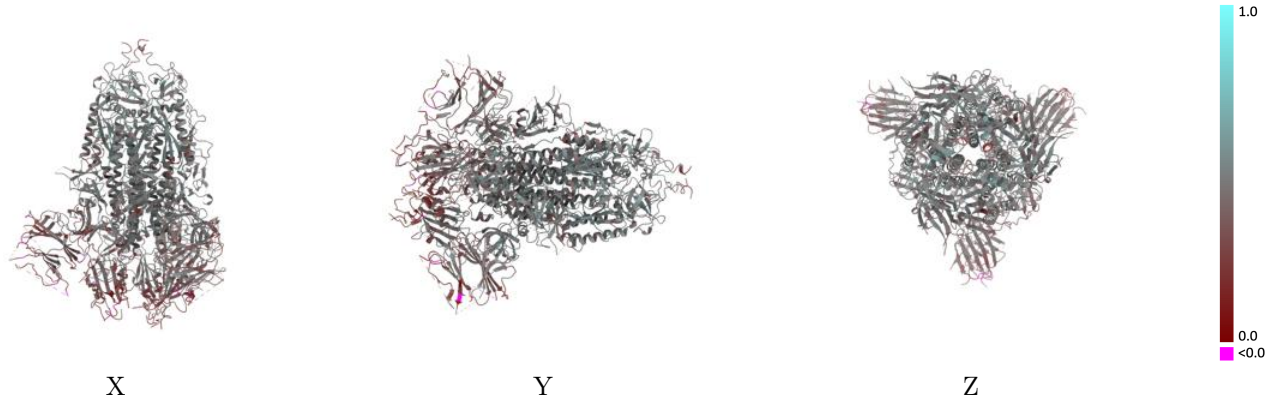
Y



Z

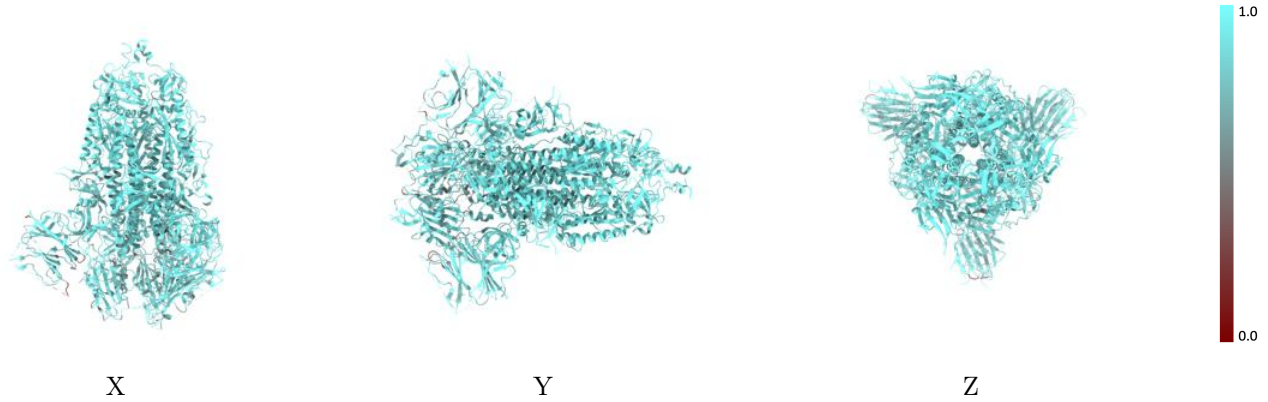
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



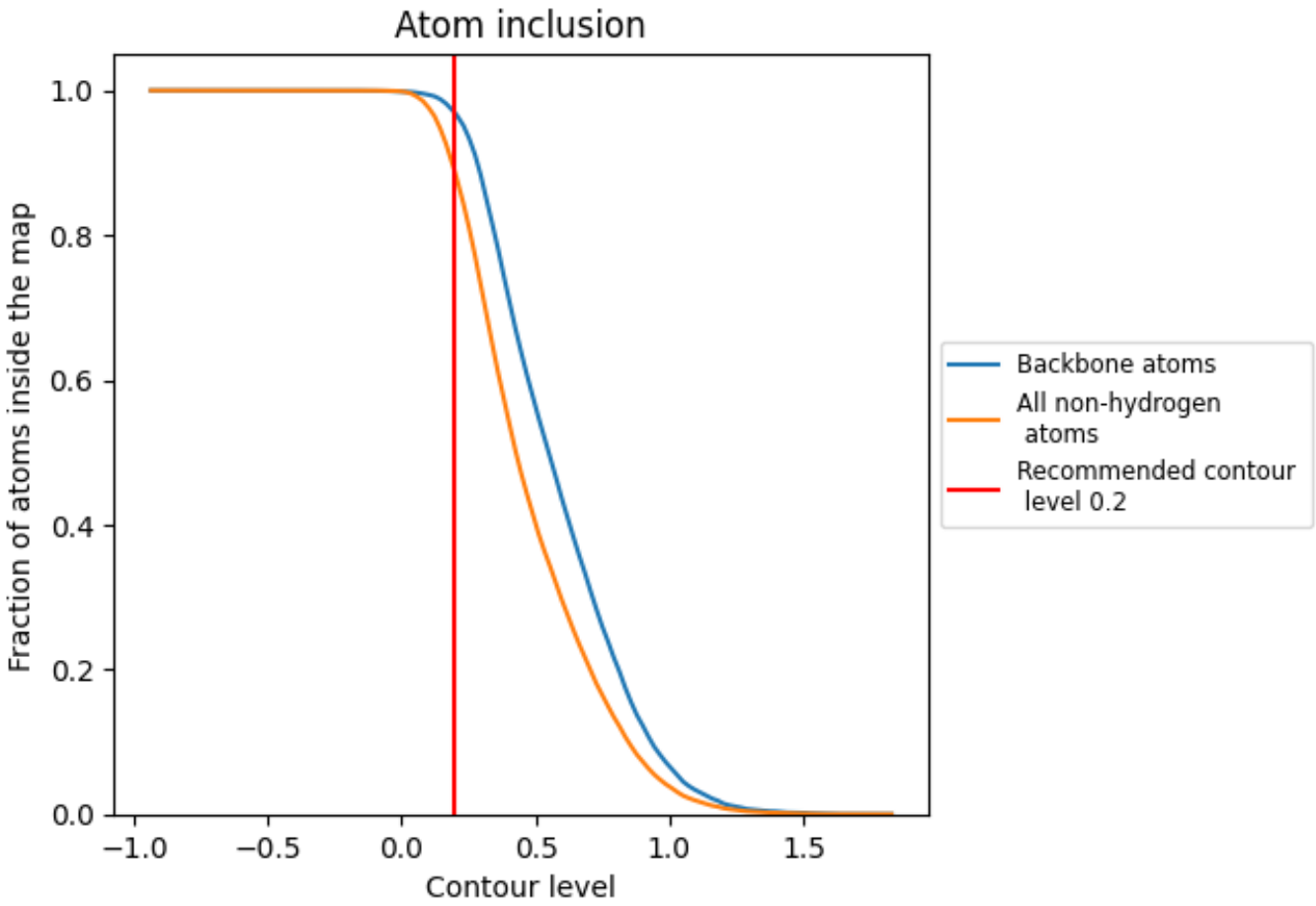
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.2).

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 (i)

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	0.8864	0.4270
A	0.8895	0.4230
B	0.8914	0.4370
C	0.8843	0.4220
D	0.2500	0.1130
E	0.9286	0.4980
F	0.7857	0.4120
G	0.8929	0.4260
H	0.8214	0.4350
I	0.9286	0.4920
J	0.8571	0.4100
K	0.8571	0.4020
L	0.5000	0.3170
M	0.8214	0.4480
N	0.8571	0.3810
O	0.9643	0.4560
P	0.8571	0.4240
Q	0.8214	0.4120
R	0.4643	0.3220