Full wwPDB EM Validation Report ⓘ

Jun 9, 2025 – 09:40 PM JST

PDB ID	:	8ZY7 / pdb_00008zy7
EMDB ID	:	EMD-60558
Title	:	Sarbecovirus HeB2013 Spike Trimer in a Locked Conformation
Authors	:	Wang, J.; Xiong, X.
Deposited on	:	2024-06-16
Resolution	:	3.45 Å(reported)

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

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

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

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

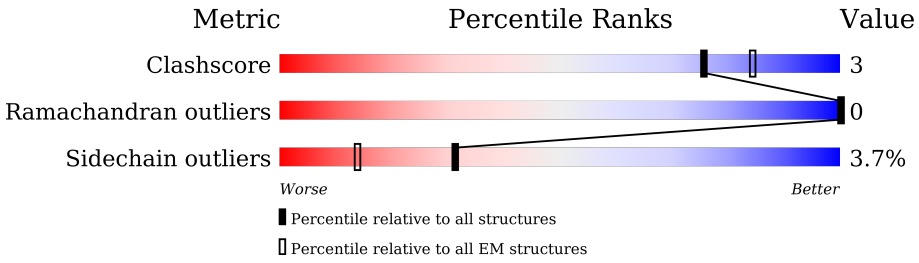
EMDB validation analysis	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance

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

The reported resolution of this entry is 3.45 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	1255	76% 9% 15%
1	B	1255	76% 8% • 15%
1	C	1255	77% 8% 15%
2	D	2	50% 50%
2	E	2	50% 50%
2	F	2	100%
2	G	2	100%
2	H	2	100%
2	I	2	50% 50%

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Mol	Chain	Length	Quality of chain
2	J	2	100%
2	K	2	50% 50%
2	L	2	50% 50%
2	M	2	100%
2	N	2	100%
2	O	2	50% 50%
2	P	2	50% 50%
2	Q	2	100%
2	R	2	100%
2	S	2	100%
2	T	2	100%
2	U	2	50% 50%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 25890 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	1065	Total	C	N	O	S	0	0
			8306	5294	1376	1594	42		
1	B	1065	Total	C	N	O	S	0	0
			8309	5295	1377	1595	42		
1	C	1065	Total	C	N	O	S	0	0
			8309	5295	1377	1595	42		

There are 246 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	29	ILE	THR	conflict	UNP A0A0U1WHK9
A	612	PRO	SER	conflict	UNP A0A0U1WHK9
A	1069	PHE	SER	conflict	UNP A0A0U1WHK9
A	1177	GLY	-	expression tag	UNP A0A0U1WHK9
A	1178	SER	-	expression tag	UNP A0A0U1WHK9
A	1179	GLY	-	expression tag	UNP A0A0U1WHK9
A	1180	TYR	-	expression tag	UNP A0A0U1WHK9
A	1181	ILE	-	expression tag	UNP A0A0U1WHK9
A	1182	PRO	-	expression tag	UNP A0A0U1WHK9
A	1183	GLU	-	expression tag	UNP A0A0U1WHK9
A	1184	ALA	-	expression tag	UNP A0A0U1WHK9
A	1185	PRO	-	expression tag	UNP A0A0U1WHK9
A	1186	ARG	-	expression tag	UNP A0A0U1WHK9
A	1187	ASP	-	expression tag	UNP A0A0U1WHK9
A	1188	GLY	-	expression tag	UNP A0A0U1WHK9
A	1189	GLN	-	expression tag	UNP A0A0U1WHK9
A	1190	ALA	-	expression tag	UNP A0A0U1WHK9
A	1191	TYR	-	expression tag	UNP A0A0U1WHK9
A	1192	VAL	-	expression tag	UNP A0A0U1WHK9
A	1193	ARG	-	expression tag	UNP A0A0U1WHK9
A	1194	LYS	-	expression tag	UNP A0A0U1WHK9
A	1195	ASP	-	expression tag	UNP A0A0U1WHK9
A	1196	GLY	-	expression tag	UNP A0A0U1WHK9
A	1197	GLU	-	expression tag	UNP A0A0U1WHK9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1198	TRP	-	expression tag	UNP A0A0U1WHK9
A	1199	VAL	-	expression tag	UNP A0A0U1WHK9
A	1200	LEU	-	expression tag	UNP A0A0U1WHK9
A	1201	LEU	-	expression tag	UNP A0A0U1WHK9
A	1202	SER	-	expression tag	UNP A0A0U1WHK9
A	1203	THR	-	expression tag	UNP A0A0U1WHK9
A	1204	PHE	-	expression tag	UNP A0A0U1WHK9
A	1205	LEU	-	expression tag	UNP A0A0U1WHK9
A	1206	LEU	-	expression tag	UNP A0A0U1WHK9
A	1207	GLU	-	expression tag	UNP A0A0U1WHK9
A	1208	VAL	-	expression tag	UNP A0A0U1WHK9
A	1209	LEU	-	expression tag	UNP A0A0U1WHK9
A	1210	PHE	-	expression tag	UNP A0A0U1WHK9
A	1211	GLN	-	expression tag	UNP A0A0U1WHK9
A	1212	GLY	-	expression tag	UNP A0A0U1WHK9
A	1213	PRO	-	expression tag	UNP A0A0U1WHK9
A	1214	GLY	-	expression tag	UNP A0A0U1WHK9
A	1215	HIS	-	expression tag	UNP A0A0U1WHK9
A	1216	HIS	-	expression tag	UNP A0A0U1WHK9
A	1217	HIS	-	expression tag	UNP A0A0U1WHK9
A	1218	HIS	-	expression tag	UNP A0A0U1WHK9
A	1219	HIS	-	expression tag	UNP A0A0U1WHK9
A	1220	HIS	-	expression tag	UNP A0A0U1WHK9
A	1221	HIS	-	expression tag	UNP A0A0U1WHK9
A	1222	HIS	-	expression tag	UNP A0A0U1WHK9
A	1223	SER	-	expression tag	UNP A0A0U1WHK9
A	1224	ALA	-	expression tag	UNP A0A0U1WHK9
A	1225	TRP	-	expression tag	UNP A0A0U1WHK9
A	1226	SER	-	expression tag	UNP A0A0U1WHK9
A	1227	HIS	-	expression tag	UNP A0A0U1WHK9
A	1228	PRO	-	expression tag	UNP A0A0U1WHK9
A	1229	GLN	-	expression tag	UNP A0A0U1WHK9
A	1230	PHE	-	expression tag	UNP A0A0U1WHK9
A	1231	GLU	-	expression tag	UNP A0A0U1WHK9
A	1232	LYS	-	expression tag	UNP A0A0U1WHK9
A	1233	GLY	-	expression tag	UNP A0A0U1WHK9
A	1234	GLY	-	expression tag	UNP A0A0U1WHK9
A	1235	GLY	-	expression tag	UNP A0A0U1WHK9
A	1236	SER	-	expression tag	UNP A0A0U1WHK9
A	1237	GLY	-	expression tag	UNP A0A0U1WHK9
A	1238	GLY	-	expression tag	UNP A0A0U1WHK9
A	1239	GLY	-	expression tag	UNP A0A0U1WHK9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1240	GLY	-	expression tag	UNP A0A0U1WHK9
A	1241	SER	-	expression tag	UNP A0A0U1WHK9
A	1242	GLY	-	expression tag	UNP A0A0U1WHK9
A	1243	GLY	-	expression tag	UNP A0A0U1WHK9
A	1244	SER	-	expression tag	UNP A0A0U1WHK9
A	1245	ALA	-	expression tag	UNP A0A0U1WHK9
A	1246	TRP	-	expression tag	UNP A0A0U1WHK9
A	1247	SER	-	expression tag	UNP A0A0U1WHK9
A	1248	HIS	-	expression tag	UNP A0A0U1WHK9
A	1249	PRO	-	expression tag	UNP A0A0U1WHK9
A	1250	GLN	-	expression tag	UNP A0A0U1WHK9
A	1251	PHE	-	expression tag	UNP A0A0U1WHK9
A	1252	GLU	-	expression tag	UNP A0A0U1WHK9
A	1253	LYS	-	expression tag	UNP A0A0U1WHK9
A	1254	SER	-	expression tag	UNP A0A0U1WHK9
A	1255	ALA	-	expression tag	UNP A0A0U1WHK9
B	29	ILE	THR	conflict	UNP A0A0U1WHK9
B	612	PRO	SER	conflict	UNP A0A0U1WHK9
B	1069	PHE	SER	conflict	UNP A0A0U1WHK9
B	1177	GLY	-	expression tag	UNP A0A0U1WHK9
B	1178	SER	-	expression tag	UNP A0A0U1WHK9
B	1179	GLY	-	expression tag	UNP A0A0U1WHK9
B	1180	TYR	-	expression tag	UNP A0A0U1WHK9
B	1181	ILE	-	expression tag	UNP A0A0U1WHK9
B	1182	PRO	-	expression tag	UNP A0A0U1WHK9
B	1183	GLU	-	expression tag	UNP A0A0U1WHK9
B	1184	ALA	-	expression tag	UNP A0A0U1WHK9
B	1185	PRO	-	expression tag	UNP A0A0U1WHK9
B	1186	ARG	-	expression tag	UNP A0A0U1WHK9
B	1187	ASP	-	expression tag	UNP A0A0U1WHK9
B	1188	GLY	-	expression tag	UNP A0A0U1WHK9
B	1189	GLN	-	expression tag	UNP A0A0U1WHK9
B	1190	ALA	-	expression tag	UNP A0A0U1WHK9
B	1191	TYR	-	expression tag	UNP A0A0U1WHK9
B	1192	VAL	-	expression tag	UNP A0A0U1WHK9
B	1193	ARG	-	expression tag	UNP A0A0U1WHK9
B	1194	LYS	-	expression tag	UNP A0A0U1WHK9
B	1195	ASP	-	expression tag	UNP A0A0U1WHK9
B	1196	GLY	-	expression tag	UNP A0A0U1WHK9
B	1197	GLU	-	expression tag	UNP A0A0U1WHK9
B	1198	TRP	-	expression tag	UNP A0A0U1WHK9
B	1199	VAL	-	expression tag	UNP A0A0U1WHK9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1200	LEU	-	expression tag	UNP A0A0U1WHK9
B	1201	LEU	-	expression tag	UNP A0A0U1WHK9
B	1202	SER	-	expression tag	UNP A0A0U1WHK9
B	1203	THR	-	expression tag	UNP A0A0U1WHK9
B	1204	PHE	-	expression tag	UNP A0A0U1WHK9
B	1205	LEU	-	expression tag	UNP A0A0U1WHK9
B	1206	LEU	-	expression tag	UNP A0A0U1WHK9
B	1207	GLU	-	expression tag	UNP A0A0U1WHK9
B	1208	VAL	-	expression tag	UNP A0A0U1WHK9
B	1209	LEU	-	expression tag	UNP A0A0U1WHK9
B	1210	PHE	-	expression tag	UNP A0A0U1WHK9
B	1211	GLN	-	expression tag	UNP A0A0U1WHK9
B	1212	GLY	-	expression tag	UNP A0A0U1WHK9
B	1213	PRO	-	expression tag	UNP A0A0U1WHK9
B	1214	GLY	-	expression tag	UNP A0A0U1WHK9
B	1215	HIS	-	expression tag	UNP A0A0U1WHK9
B	1216	HIS	-	expression tag	UNP A0A0U1WHK9
B	1217	HIS	-	expression tag	UNP A0A0U1WHK9
B	1218	HIS	-	expression tag	UNP A0A0U1WHK9
B	1219	HIS	-	expression tag	UNP A0A0U1WHK9
B	1220	HIS	-	expression tag	UNP A0A0U1WHK9
B	1221	HIS	-	expression tag	UNP A0A0U1WHK9
B	1222	HIS	-	expression tag	UNP A0A0U1WHK9
B	1223	SER	-	expression tag	UNP A0A0U1WHK9
B	1224	ALA	-	expression tag	UNP A0A0U1WHK9
B	1225	TRP	-	expression tag	UNP A0A0U1WHK9
B	1226	SER	-	expression tag	UNP A0A0U1WHK9
B	1227	HIS	-	expression tag	UNP A0A0U1WHK9
B	1228	PRO	-	expression tag	UNP A0A0U1WHK9
B	1229	GLN	-	expression tag	UNP A0A0U1WHK9
B	1230	PHE	-	expression tag	UNP A0A0U1WHK9
B	1231	GLU	-	expression tag	UNP A0A0U1WHK9
B	1232	LYS	-	expression tag	UNP A0A0U1WHK9
B	1233	GLY	-	expression tag	UNP A0A0U1WHK9
B	1234	GLY	-	expression tag	UNP A0A0U1WHK9
B	1235	GLY	-	expression tag	UNP A0A0U1WHK9
B	1236	SER	-	expression tag	UNP A0A0U1WHK9
B	1237	GLY	-	expression tag	UNP A0A0U1WHK9
B	1238	GLY	-	expression tag	UNP A0A0U1WHK9
B	1239	GLY	-	expression tag	UNP A0A0U1WHK9
B	1240	GLY	-	expression tag	UNP A0A0U1WHK9
B	1241	SER	-	expression tag	UNP A0A0U1WHK9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1242	GLY	-	expression tag	UNP A0A0U1WHK9
B	1243	GLY	-	expression tag	UNP A0A0U1WHK9
B	1244	SER	-	expression tag	UNP A0A0U1WHK9
B	1245	ALA	-	expression tag	UNP A0A0U1WHK9
B	1246	TRP	-	expression tag	UNP A0A0U1WHK9
B	1247	SER	-	expression tag	UNP A0A0U1WHK9
B	1248	HIS	-	expression tag	UNP A0A0U1WHK9
B	1249	PRO	-	expression tag	UNP A0A0U1WHK9
B	1250	GLN	-	expression tag	UNP A0A0U1WHK9
B	1251	PHE	-	expression tag	UNP A0A0U1WHK9
B	1252	GLU	-	expression tag	UNP A0A0U1WHK9
B	1253	LYS	-	expression tag	UNP A0A0U1WHK9
B	1254	SER	-	expression tag	UNP A0A0U1WHK9
B	1255	ALA	-	expression tag	UNP A0A0U1WHK9
C	29	ILE	THR	conflict	UNP A0A0U1WHK9
C	612	PRO	SER	conflict	UNP A0A0U1WHK9
C	1069	PHE	SER	conflict	UNP A0A0U1WHK9
C	1177	GLY	-	expression tag	UNP A0A0U1WHK9
C	1178	SER	-	expression tag	UNP A0A0U1WHK9
C	1179	GLY	-	expression tag	UNP A0A0U1WHK9
C	1180	TYR	-	expression tag	UNP A0A0U1WHK9
C	1181	ILE	-	expression tag	UNP A0A0U1WHK9
C	1182	PRO	-	expression tag	UNP A0A0U1WHK9
C	1183	GLU	-	expression tag	UNP A0A0U1WHK9
C	1184	ALA	-	expression tag	UNP A0A0U1WHK9
C	1185	PRO	-	expression tag	UNP A0A0U1WHK9
C	1186	ARG	-	expression tag	UNP A0A0U1WHK9
C	1187	ASP	-	expression tag	UNP A0A0U1WHK9
C	1188	GLY	-	expression tag	UNP A0A0U1WHK9
C	1189	GLN	-	expression tag	UNP A0A0U1WHK9
C	1190	ALA	-	expression tag	UNP A0A0U1WHK9
C	1191	TYR	-	expression tag	UNP A0A0U1WHK9
C	1192	VAL	-	expression tag	UNP A0A0U1WHK9
C	1193	ARG	-	expression tag	UNP A0A0U1WHK9
C	1194	LYS	-	expression tag	UNP A0A0U1WHK9
C	1195	ASP	-	expression tag	UNP A0A0U1WHK9
C	1196	GLY	-	expression tag	UNP A0A0U1WHK9
C	1197	GLU	-	expression tag	UNP A0A0U1WHK9
C	1198	TRP	-	expression tag	UNP A0A0U1WHK9
C	1199	VAL	-	expression tag	UNP A0A0U1WHK9
C	1200	LEU	-	expression tag	UNP A0A0U1WHK9
C	1201	LEU	-	expression tag	UNP A0A0U1WHK9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1202	SER	-	expression tag	UNP A0A0U1WHK9
C	1203	THR	-	expression tag	UNP A0A0U1WHK9
C	1204	PHE	-	expression tag	UNP A0A0U1WHK9
C	1205	LEU	-	expression tag	UNP A0A0U1WHK9
C	1206	LEU	-	expression tag	UNP A0A0U1WHK9
C	1207	GLU	-	expression tag	UNP A0A0U1WHK9
C	1208	VAL	-	expression tag	UNP A0A0U1WHK9
C	1209	LEU	-	expression tag	UNP A0A0U1WHK9
C	1210	PHE	-	expression tag	UNP A0A0U1WHK9
C	1211	GLN	-	expression tag	UNP A0A0U1WHK9
C	1212	GLY	-	expression tag	UNP A0A0U1WHK9
C	1213	PRO	-	expression tag	UNP A0A0U1WHK9
C	1214	GLY	-	expression tag	UNP A0A0U1WHK9
C	1215	HIS	-	expression tag	UNP A0A0U1WHK9
C	1216	HIS	-	expression tag	UNP A0A0U1WHK9
C	1217	HIS	-	expression tag	UNP A0A0U1WHK9
C	1218	HIS	-	expression tag	UNP A0A0U1WHK9
C	1219	HIS	-	expression tag	UNP A0A0U1WHK9
C	1220	HIS	-	expression tag	UNP A0A0U1WHK9
C	1221	HIS	-	expression tag	UNP A0A0U1WHK9
C	1222	HIS	-	expression tag	UNP A0A0U1WHK9
C	1223	SER	-	expression tag	UNP A0A0U1WHK9
C	1224	ALA	-	expression tag	UNP A0A0U1WHK9
C	1225	TRP	-	expression tag	UNP A0A0U1WHK9
C	1226	SER	-	expression tag	UNP A0A0U1WHK9
C	1227	HIS	-	expression tag	UNP A0A0U1WHK9
C	1228	PRO	-	expression tag	UNP A0A0U1WHK9
C	1229	GLN	-	expression tag	UNP A0A0U1WHK9
C	1230	PHE	-	expression tag	UNP A0A0U1WHK9
C	1231	GLU	-	expression tag	UNP A0A0U1WHK9
C	1232	LYS	-	expression tag	UNP A0A0U1WHK9
C	1233	GLY	-	expression tag	UNP A0A0U1WHK9
C	1234	GLY	-	expression tag	UNP A0A0U1WHK9
C	1235	GLY	-	expression tag	UNP A0A0U1WHK9
C	1236	SER	-	expression tag	UNP A0A0U1WHK9
C	1237	GLY	-	expression tag	UNP A0A0U1WHK9
C	1238	GLY	-	expression tag	UNP A0A0U1WHK9
C	1239	GLY	-	expression tag	UNP A0A0U1WHK9
C	1240	GLY	-	expression tag	UNP A0A0U1WHK9
C	1241	SER	-	expression tag	UNP A0A0U1WHK9
C	1242	GLY	-	expression tag	UNP A0A0U1WHK9
C	1243	GLY	-	expression tag	UNP A0A0U1WHK9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1244	SER	-	expression tag	UNP A0A0U1WHK9
C	1245	ALA	-	expression tag	UNP A0A0U1WHK9
C	1246	TRP	-	expression tag	UNP A0A0U1WHK9
C	1247	SER	-	expression tag	UNP A0A0U1WHK9
C	1248	HIS	-	expression tag	UNP A0A0U1WHK9
C	1249	PRO	-	expression tag	UNP A0A0U1WHK9
C	1250	GLN	-	expression tag	UNP A0A0U1WHK9
C	1251	PHE	-	expression tag	UNP A0A0U1WHK9
C	1252	GLU	-	expression tag	UNP A0A0U1WHK9
C	1253	LYS	-	expression tag	UNP A0A0U1WHK9
C	1254	SER	-	expression tag	UNP A0A0U1WHK9
C	1255	ALA	-	expression tag	UNP A0A0U1WHK9

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

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

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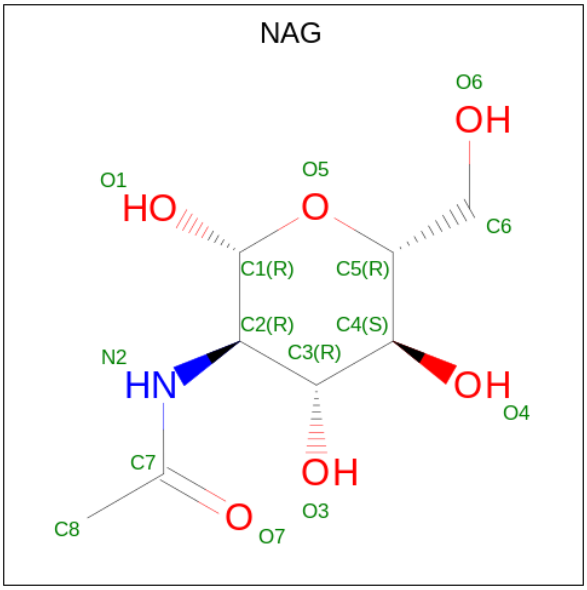
Mol	Chain	Residues	Atoms	AltConf	Trace
2	N	2	Total C N O 28 16 2 10	0	0
2	O	2	Total C N O 28 16 2 10	0	0
2	P	2	Total C N O 28 16 2 10	0	0
2	Q	2	Total C N O 28 16 2 10	0	0
2	R	2	Total C N O 28 16 2 10	0	0
2	S	2	Total C N O 28 16 2 10	0	0
2	T	2	Total C N O 28 16 2 10	0	0
2	U	2	Total C N O 28 16 2 10	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



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

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

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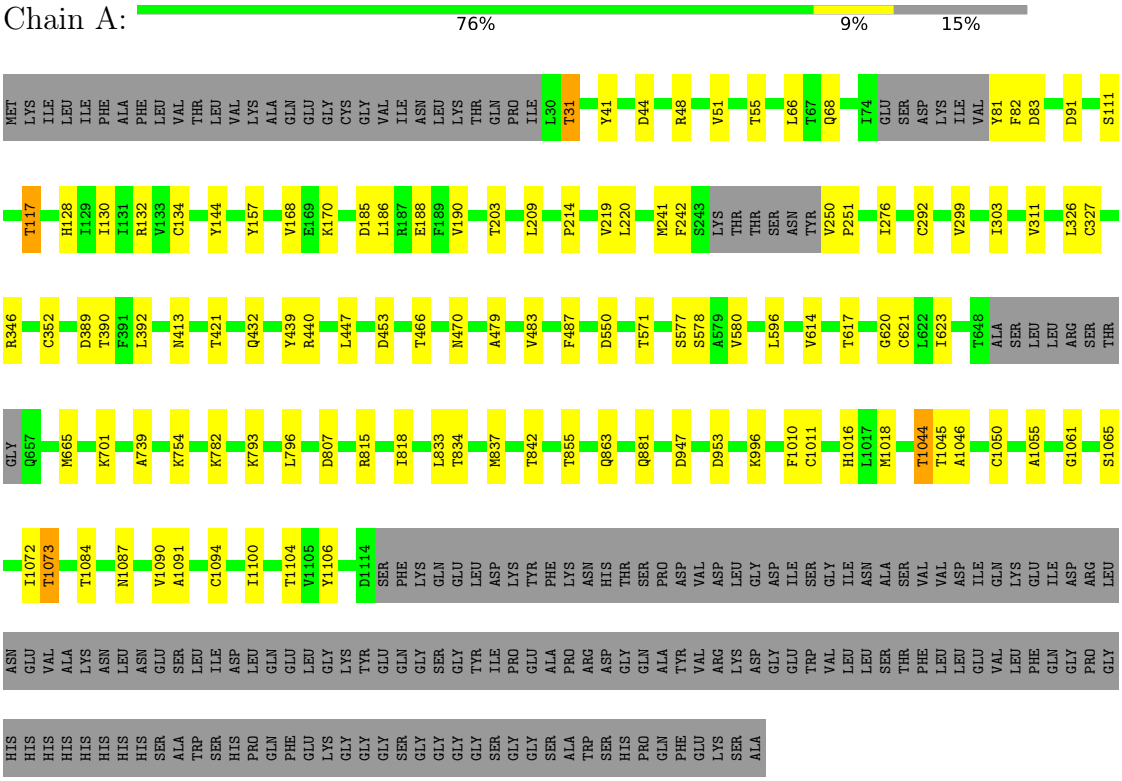
Mol	Chain	Residues	Atoms	AltConf
3	C	1	Total C N O 14 8 1 5	0
3	C	1	Total C N O 14 8 1 5	0
3	C	1	Total C N O 14 8 1 5	0
3	C	1	Total C N O 14 8 1 5	0
3	C	1	Total C N O 14 8 1 5	0
3	C	1	Total C N O 14 8 1 5	0
3	C	1	Total C N O 14 8 1 5	0
3	C	1	Total C N O 14 8 1 5	0
3	C	1	Total C N O 14 8 1 5	0

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. 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

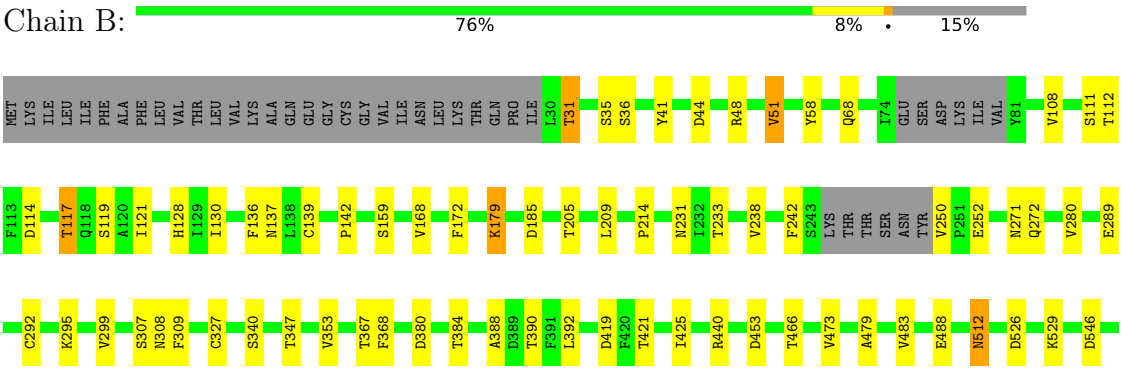
- Molecule 1: Spike glycoprotein

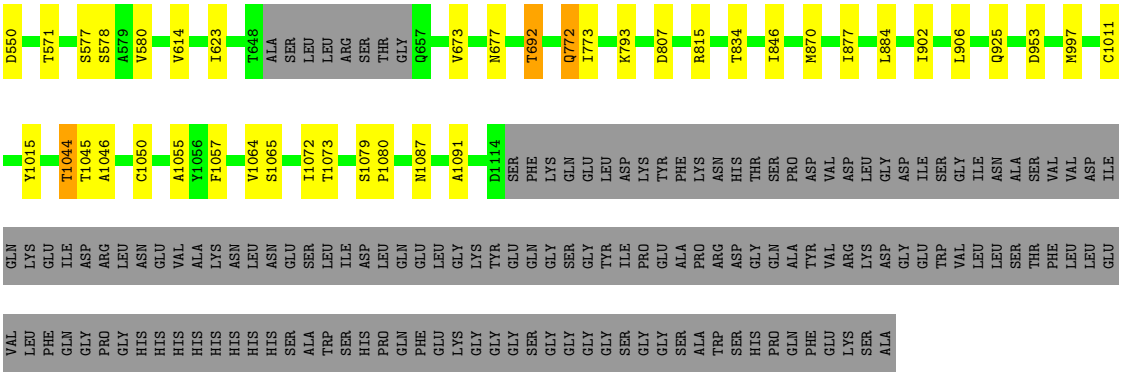
Chain A:



- Molecule 1: Spike glycoprotein

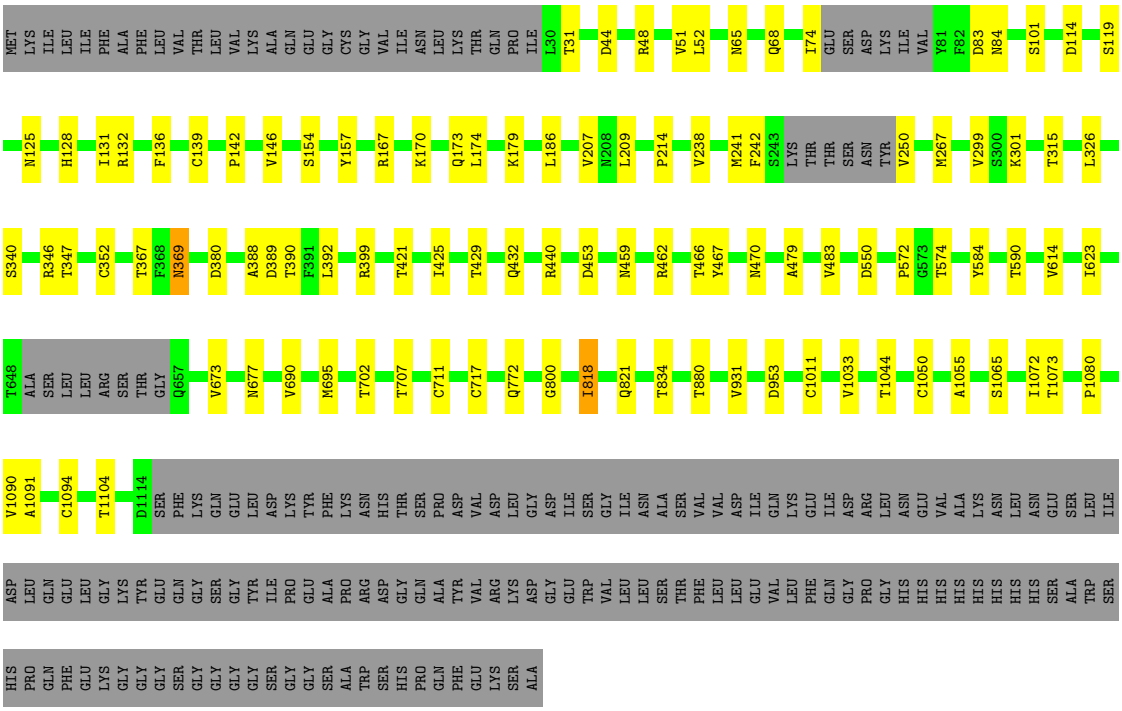
Chain B:





• Molecule 1: Spike glycoprotein

Chain C:



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

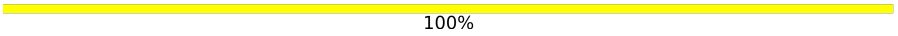
Chain D:

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

Chain E:

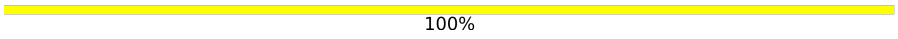
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:



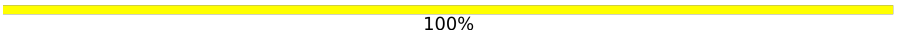
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



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

Chain H:

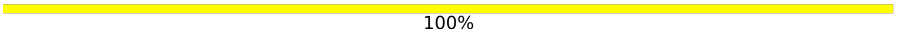


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:

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

Chain J:



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

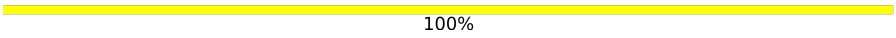
Chain K:

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

Chain L:

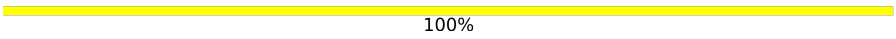
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:



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

Chain N:



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

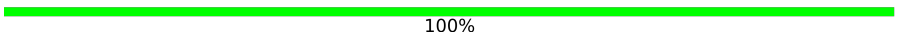
Chain O:

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

Chain P:

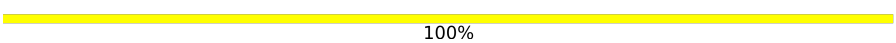
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:

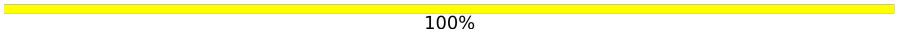


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

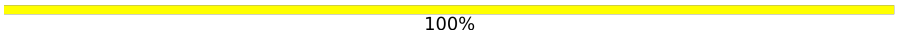
Chain R:



• 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 U: 

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	125937	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.12	0/8492	0.32	0/11557
1	B	0.13	0/8495	0.34	0/11561
1	C	0.13	0/8495	0.32	0/11561
All	All	0.13	0/25482	0.33	0/34679

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	8306	0	8083	50	0
1	B	8309	0	8087	54	0
1	C	8309	0	8088	44	0
2	D	28	0	25	1	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	K	28	0	25	0	0
2	L	28	0	25	1	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	1	0
2	Q	28	0	25	0	0
2	R	28	0	25	0	0
2	S	28	0	25	0	0
2	T	28	0	25	0	0
2	U	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	25890	0	25137	146	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 3.

All (146) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:392:LEU:HD11	1:C:479:ALA:HB1	1.83	0.61
1:A:242:PHE:O	1:A:250:VAL:N	2.36	0.59
1:A:1061:GLY:HA3	1:A:1073:THR:O	2.04	0.58
1:A:881:GLN:HE21	1:B:1057:PHE:HB3	1.69	0.57
1:B:526:ASP:OD1	1:B:526:ASP:N	2.38	0.57
1:A:392:LEU:HD11	1:A:479:ALA:HB1	1.86	0.56
1:B:119:SER:HB2	1:B:136:PHE:HD2	1.70	0.56
1:B:390:THR:HG22	1:B:483:VAL:HG22	1.87	0.56
1:A:241:MET:HG3	1:A:251:PRO:HD3	1.88	0.55
1:C:347:THR:HB	1:C:388:ALA:HB3	1.88	0.54
1:A:815:ARG:HH21	1:B:529:LYS:HZ3	1.53	0.54
1:B:35:SER:OG	1:B:36:SER:N	2.40	0.54
1:A:1055:ALA:HB3	1:A:1091:ALA:O	2.07	0.54
1:A:132:ARG:NH1	1:A:157:TYR:OH	2.41	0.54
1:A:440:ARG:NH2	1:A:453:ASP:O	2.41	0.54
1:C:690:VAL:HG22	1:C:1033:VAL:HG22	1.90	0.53
1:B:614:VAL:HG22	1:B:623:ILE:HG12	1.90	0.53
1:B:692:THR:HG23	1:B:902:ILE:HD11	1.91	0.53
1:A:834:THR:OG1	1:A:837:MET:SD	2.66	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:128:HIS:HB3	1:C:170:LYS:HA	1.92	0.52
1:B:550:ASP:OD1	1:B:550:ASP:N	2.42	0.52
1:C:186:LEU:HD23	1:C:207:VAL:HG11	1.92	0.52
1:C:550:ASP:OD1	1:C:550:ASP:N	2.38	0.52
1:A:807:ASP:OD1	1:A:807:ASP:N	2.38	0.52
1:A:209:LEU:HD11	1:A:214:PRO:HD3	1.90	0.52
1:A:413:ASN:HD21	1:A:439:TYR:HB2	1.74	0.51
1:B:440:ARG:NH2	1:B:453:ASP:O	2.43	0.51
1:C:380:ASP:OD1	1:C:380:ASP:N	2.42	0.51
1:B:1087:ASN:OD1	1:B:1087:ASN:N	2.40	0.51
1:A:947:ASP:OD1	1:A:947:ASP:N	2.41	0.51
1:C:614:VAL:HG22	1:C:623:ILE:HG12	1.92	0.51
1:B:380:ASP:OD1	1:B:380:ASP:N	2.41	0.51
1:B:392:LEU:HD11	1:B:479:ALA:HB1	1.93	0.51
1:C:1055:ALA:HB3	1:C:1091:ALA:O	2.11	0.51
1:B:209:LEU:HD11	1:B:214:PRO:HD3	1.93	0.50
1:A:130:ILE:HG22	1:A:168:VAL:HG22	1.93	0.50
1:A:1045:THR:OG1	1:A:1046:ALA:N	2.44	0.50
1:C:369:ASN:OD1	1:C:369:ASN:N	2.43	0.50
1:A:953:ASP:N	1:A:953:ASP:OD1	2.44	0.50
1:C:432:GLN:NE2	2:P:1:NAG:O7	2.43	0.50
1:A:571:THR:HB	1:A:580:VAL:HG12	1.93	0.50
1:A:1094:CYS:HB2	1:A:1100:ILE:HD13	1.94	0.50
1:A:48:ARG:HB3	1:A:51:VAL:HG11	1.94	0.50
1:A:41:TYR:HB3	1:A:220:LEU:HD12	1.93	0.49
1:C:132:ARG:NH1	1:C:157:TYR:OH	2.45	0.49
1:C:800:GLY:HA3	1:C:818:ILE:HG12	1.93	0.49
1:B:31:THR:HG23	1:B:68:GLN:HB3	1.95	0.49
1:C:114:ASP:N	1:C:114:ASP:OD1	2.46	0.49
1:B:179:LYS:HD2	1:B:252:GLU:HG2	1.95	0.48
1:A:550:ASP:N	1:A:550:ASP:OD1	2.42	0.48
1:B:130:ILE:HG22	1:B:168:VAL:HG22	1.96	0.48
1:C:83:ASP:N	1:C:83:ASP:OD1	2.45	0.48
1:C:209:LEU:HD11	1:C:214:PRO:HD3	1.96	0.48
1:C:453:ASP:N	1:C:453:ASP:OD1	2.46	0.48
1:A:996:LYS:NZ	1:A:1010:PHE:O	2.43	0.48
1:B:108:VAL:HG13	1:B:121:ILE:HG22	1.95	0.48
1:C:48:ARG:HD2	1:C:51:VAL:HG11	1.93	0.48
1:A:31:THR:HG23	1:A:68:GLN:HB3	1.96	0.48
1:A:128:HIS:CD2	1:A:170:LYS:HB3	2.49	0.48
1:B:807:ASP:OD1	1:B:807:ASP:N	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:ASP:OD1	1:A:44:ASP:N	2.45	0.47
1:A:81:TYR:HB3	1:A:82:PHE:H	1.57	0.47
1:C:677:ASN:OD1	1:C:677:ASN:N	2.45	0.47
1:B:546:ASP:OD1	1:B:546:ASP:N	2.47	0.47
1:A:470:ASN:N	1:A:470:ASN:OD1	2.47	0.47
1:B:1045:THR:OG1	1:B:1046:ALA:N	2.47	0.47
1:C:459:ASN:OD1	1:C:459:ASN:N	2.47	0.47
1:A:111:SER:HB2	1:A:117:THR:HG21	1.97	0.47
1:C:119:SER:HB2	1:C:136:PHE:HD2	1.79	0.47
1:A:614:VAL:HG22	1:A:623:ILE:HG12	1.97	0.47
1:B:384:THR:OG1	1:B:488:GLU:O	2.31	0.47
1:B:571:THR:HB	1:B:580:VAL:HG12	1.96	0.47
1:B:773:ILE:HG22	1:B:846:ILE:HD13	1.96	0.46
1:A:1044:THR:HG23	1:A:1065:SER:HB3	1.97	0.46
1:A:577:SER:OG	1:A:578:SER:N	2.49	0.46
1:C:125:ASN:OD1	1:C:128:HIS:N	2.34	0.46
1:A:701:LYS:HE3	1:A:739:ALA:HB1	1.97	0.46
1:C:711:CYS:HB3	1:C:717:CYS:HB3	1.72	0.46
1:B:368:PHE:HD1	1:B:425:ILE:HG12	1.81	0.46
1:A:432:GLN:NE2	2:D:1:NAG:O7	2.49	0.46
1:B:772:GLN:H	1:B:772:GLN:HG2	1.54	0.46
1:B:295:LYS:HB3	1:B:295:LYS:HE3	1.69	0.46
1:C:301:LYS:HG3	1:C:572:PRO:HA	1.98	0.46
1:B:347:THR:HB	1:B:388:ALA:HB3	1.98	0.45
1:B:48:ARG:HD3	1:B:51:VAL:HG11	1.97	0.45
1:C:142:PRO:HB2	1:C:238:VAL:HG12	1.97	0.45
1:C:470:ASN:N	1:C:470:ASN:OD1	2.48	0.45
1:C:346:ARG:NE	1:C:389:ASP:OD1	2.50	0.45
1:A:188:GLU:HB2	1:A:203:THR:HG22	1.98	0.45
1:C:31:THR:HG23	1:C:68:GLN:HB3	1.99	0.45
1:B:307:SER:OG	1:B:308:ASN:N	2.50	0.45
1:B:953:ASP:OD1	1:B:953:ASP:N	2.47	0.45
1:B:1079:SER:O	1:B:1079:SER:OG	2.33	0.45
1:B:815:ARG:HD3	1:B:815:ARG:HA	1.77	0.45
1:C:1073:THR:HG22	1:C:1080:PRO:HA	1.97	0.45
1:A:83:ASP:N	1:A:83:ASP:OD1	2.49	0.45
1:A:390:THR:HG22	1:A:483:VAL:HG22	1.98	0.45
1:C:390:THR:HG22	1:C:483:VAL:HG22	1.98	0.44
1:B:1073:THR:HG22	1:B:1080:PRO:HA	2.00	0.44
1:A:617:THR:OG1	1:A:620:GLY:O	2.31	0.44
1:C:173:GLN:N	1:C:173:GLN:OE1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1044:THR:HG23	1:C:1065:SER:HB3	2.00	0.44
1:B:112:THR:OG1	1:B:114:ASP:OD1	2.30	0.44
1:A:1016:HIS:NE2	1:A:1018:MET:O	2.50	0.44
1:B:142:PRO:HB2	1:B:238:VAL:HG12	1.99	0.44
1:B:44:ASP:OD1	1:B:44:ASP:N	2.47	0.43
1:B:877:ILE:HD12	1:B:1015:TYR:HB3	2.00	0.43
1:B:419:ASP:OD1	1:B:419:ASP:N	2.50	0.43
1:B:233:THR:HB	2:L:1:NAG:HN2	1.84	0.43
1:C:44:ASP:N	1:C:44:ASP:OD1	2.51	0.43
1:C:953:ASP:OD1	1:C:953:ASP:N	2.46	0.43
1:A:447:LEU:HD23	1:A:447:LEU:HA	1.92	0.43
1:B:242:PHE:O	1:B:250:VAL:N	2.52	0.43
1:C:52:LEU:HD12	1:C:52:LEU:HA	1.93	0.43
1:C:1050:CYS:HB2	1:C:1094:CYS:HB2	1.67	0.43
1:A:170:LYS:HE3	1:A:170:LYS:HB2	1.79	0.42
1:B:271:ASN:OD1	1:B:272:GLN:N	2.52	0.42
1:C:440:ARG:NH2	1:C:453:ASP:O	2.52	0.42
1:B:1055:ALA:HB3	1:B:1091:ALA:O	2.18	0.42
1:B:289:GLU:HG3	1:B:309:PHE:HB2	2.02	0.42
1:C:242:PHE:O	1:C:250:VAL:N	2.51	0.42
1:C:131:ILE:HB	1:C:167:ARG:HB3	2.02	0.42
1:A:219:VAL:HG11	1:A:276:ILE:HB	2.01	0.41
1:B:512:ASN:OD1	1:B:512:ASN:N	2.53	0.41
1:A:346:ARG:NE	1:A:389:ASP:OD1	2.54	0.41
1:B:41:TYR:OH	1:B:58:TYR:O	2.27	0.41
1:A:754:LYS:HA	1:A:754:LYS:HD2	1.90	0.41
1:A:782:LYS:HA	1:A:782:LYS:HD2	1.82	0.41
1:A:793:LYS:HE2	1:A:793:LYS:HB2	1.92	0.41
1:B:677:ASN:OD1	1:B:677:ASN:N	2.41	0.41
1:B:793:LYS:NZ	1:B:906:LEU:O	2.41	0.41
1:B:577:SER:OG	1:B:578:SER:N	2.53	0.41
1:C:52:LEU:HG	1:C:267:MET:HE2	2.02	0.41
1:A:185:ASP:OD1	1:A:185:ASP:N	2.52	0.41
1:B:997:MET:HE2	1:B:997:MET:HB2	1.93	0.40
1:B:1044:THR:HG23	1:B:1065:SER:HB3	2.03	0.40
1:C:84:ASN:OD1	1:C:84:ASN:N	2.52	0.40
1:B:185:ASP:OD1	1:B:185:ASP:N	2.53	0.40
1:C:821:GLN:HG2	1:C:931:VAL:HG21	2.02	0.40
1:A:796:LEU:HD12	1:A:796:LEU:HA	1.90	0.40
1:A:833:LEU:HD23	1:A:833:LEU:HA	1.93	0.40
1:B:111:SER:HB2	1:B:117:THR:HG21	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:462:ARG:H	1:C:462:ARG:HG2	1.74	0.40
1:A:1084:THR:HG22	1:A:1106:TYR:HB3	2.02	0.40
1:B:137:ASN:HD22	1:B:159:SER:HG	1.67	0.40
1:C:584:TYR:HE2	1:C:623:ILE:HD12	1.86	0.40

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	1057/1255 (84%)	1027 (97%)	30 (3%)	0	100	100
1	B	1057/1255 (84%)	1017 (96%)	40 (4%)	0	100	100
1	C	1057/1255 (84%)	1011 (96%)	46 (4%)	0	100	100
All	All	3171/3765 (84%)	3055 (96%)	116 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	929/1089 (85%)	895 (96%)	34 (4%)	29	59
1	B	930/1089 (85%)	898 (97%)	32 (3%)	32	61
1	C	930/1089 (85%)	894 (96%)	36 (4%)	27	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2789/3267 (85%)	2687 (96%)	102 (4%)	31 59

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	THR
1	A	55	THR
1	A	66	LEU
1	A	91	ASP
1	A	117	THR
1	A	134	CYS
1	A	144	TYR
1	A	186	LEU
1	A	190	VAL
1	A	292	CYS
1	A	299	VAL
1	A	303	ILE
1	A	311	VAL
1	A	326	LEU
1	A	327	CYS
1	A	352	CYS
1	A	421	THR
1	A	466	THR
1	A	487	PHE
1	A	596	LEU
1	A	621	CYS
1	A	665	MET
1	A	818	ILE
1	A	842	THR
1	A	855	THR
1	A	863	GLN
1	A	1011	CYS
1	A	1044	THR
1	A	1050	CYS
1	A	1072	ILE
1	A	1073	THR
1	A	1087	ASN
1	A	1090	VAL
1	A	1104	THR
1	B	31	THR
1	B	51	VAL
1	B	117	THR

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Mol	Chain	Res	Type
1	B	128	HIS
1	B	139	CYS
1	B	172	PHE
1	B	179	LYS
1	B	205	THR
1	B	231	ASN
1	B	280	VAL
1	B	292	CYS
1	B	299	VAL
1	B	327	CYS
1	B	340	SER
1	B	353	VAL
1	B	367	THR
1	B	421	THR
1	B	466	THR
1	B	473	VAL
1	B	512	ASN
1	B	673	VAL
1	B	692	THR
1	B	772	GLN
1	B	834	THR
1	B	870	MET
1	B	884	LEU
1	B	925	GLN
1	B	1011	CYS
1	B	1044	THR
1	B	1050	CYS
1	B	1064	VAL
1	B	1072	ILE
1	C	65	ASN
1	C	74	ILE
1	C	101	SER
1	C	139	CYS
1	C	146	VAL
1	C	154	SER
1	C	174	LEU
1	C	179	LYS
1	C	241	MET
1	C	299	VAL
1	C	315	THR
1	C	326	LEU
1	C	340	SER

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Mol	Chain	Res	Type
1	C	352	CYS
1	C	367	THR
1	C	369	ASN
1	C	399	ARG
1	C	421	THR
1	C	425	ILE
1	C	429	THR
1	C	466	THR
1	C	467	TYR
1	C	574	THR
1	C	590	THR
1	C	673	VAL
1	C	695	MET
1	C	702	THR
1	C	707	THR
1	C	772	GLN
1	C	818	ILE
1	C	834	THR
1	C	880	THR
1	C	1011	CYS
1	C	1072	ILE
1	C	1090	VAL
1	C	1104	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	GLN
1	A	308	ASN
1	A	428	ASN
1	A	442	HIS
1	A	881	GLN
1	A	1110	GLN
1	B	208	ASN
1	B	428	ASN
1	B	459	ASN
1	B	471	GLN
1	B	514	ASN
1	B	536	GLN
1	B	552	GLN
1	B	821	GLN
1	B	973	GLN

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Mol	Chain	Res	Type
1	B	979	GLN
1	B	1022	GLN
1	B	1081	GLN
1	B	1110	GLN
1	C	56	GLN
1	C	260	ASN
1	C	308	ASN
1	C	400	GLN
1	C	532	GLN
1	C	535	GLN
1	C	552	GLN
1	C	616	GLN
1	C	869	GLN
1	C	890	GLN
1	C	894	GLN
1	C	903	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)

36 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	D	1	1,2	14,14,15	0.72	0	17,19,21	1.47	2 (11%)
2	NAG	D	2	2	14,14,15	0.71	0	17,19,21	0.90	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	E	1	1,2	14,14,15	0.70	0	17,19,21	1.49	1 (5%)
2	NAG	E	2	2	14,14,15	0.73	0	17,19,21	0.89	0
2	NAG	F	1	1,2	14,14,15	0.69	0	17,19,21	0.93	1 (5%)
2	NAG	F	2	2	14,14,15	0.68	0	17,19,21	1.51	2 (11%)
2	NAG	G	1	1,2	14,14,15	0.70	0	17,19,21	1.27	2 (11%)
2	NAG	G	2	2	14,14,15	0.72	0	17,19,21	1.57	2 (11%)
2	NAG	H	1	1,2	14,14,15	0.79	0	17,19,21	1.26	1 (5%)
2	NAG	H	2	2	14,14,15	0.92	1 (7%)	17,19,21	1.50	1 (5%)
2	NAG	I	1	1,2	14,14,15	0.70	0	17,19,21	1.48	2 (11%)
2	NAG	I	2	2	14,14,15	0.69	0	17,19,21	0.91	0
2	NAG	J	1	1,2	14,14,15	0.70	0	17,19,21	1.58	3 (17%)
2	NAG	J	2	2	14,14,15	0.72	0	17,19,21	0.99	1 (5%)
2	NAG	K	1	1,2	14,14,15	0.72	0	17,19,21	1.60	4 (23%)
2	NAG	K	2	2	14,14,15	0.71	0	17,19,21	0.84	0
2	NAG	L	1	1,2	14,14,15	0.70	0	17,19,21	0.93	1 (5%)
2	NAG	L	2	2	14,14,15	0.69	0	17,19,21	1.52	2 (11%)
2	NAG	M	1	1,2	14,14,15	0.71	0	17,19,21	1.17	2 (11%)
2	NAG	M	2	2	14,14,15	0.70	0	17,19,21	1.55	2 (11%)
2	NAG	N	1	1,2	14,14,15	0.78	0	17,19,21	1.28	1 (5%)
2	NAG	N	2	2	14,14,15	0.92	1 (7%)	17,19,21	1.49	1 (5%)
2	NAG	O	1	1,2	14,14,15	0.71	0	17,19,21	1.52	1 (5%)
2	NAG	O	2	2	14,14,15	0.70	0	17,19,21	0.92	0
2	NAG	P	1	1,2	14,14,15	0.74	0	17,19,21	1.44	2 (11%)
2	NAG	P	2	2	14,14,15	0.74	0	17,19,21	1.01	1 (5%)
2	NAG	Q	1	1,2	14,14,15	0.73	0	17,19,21	0.93	0
2	NAG	Q	2	2	14,14,15	0.72	0	17,19,21	0.85	0
2	NAG	R	1	1,2	14,14,15	0.69	0	17,19,21	0.92	1 (5%)
2	NAG	R	2	2	14,14,15	0.68	0	17,19,21	1.56	2 (11%)
2	NAG	S	1	1,2	14,14,15	0.70	0	17,19,21	1.07	1 (5%)
2	NAG	S	2	2	14,14,15	0.72	0	17,19,21	1.51	2 (11%)
2	NAG	T	1	1,2	14,14,15	0.79	0	17,19,21	1.24	1 (5%)
2	NAG	T	2	2	14,14,15	0.94	1 (7%)	17,19,21	1.51	2 (11%)
2	NAG	U	1	1,2	14,14,15	0.70	0	17,19,21	1.52	1 (5%)
2	NAG	U	2	2	14,14,15	0.70	0	17,19,21	0.92	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	D	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	D	2	2	-	1/6/23/26	0/1/1/1
2	NAG	E	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
2	NAG	G	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1
2	NAG	H	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	H	2	2	-	1/6/23/26	0/1/1/1
2	NAG	I	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	I	2	2	-	0/6/23/26	0/1/1/1
2	NAG	J	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	J	2	2	-	1/6/23/26	0/1/1/1
2	NAG	K	1	1,2	-	1/6/23/26	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	-	2/6/23/26	0/1/1/1
2	NAG	M	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	M	2	2	-	2/6/23/26	0/1/1/1
2	NAG	N	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	N	2	2	-	1/6/23/26	0/1/1/1
2	NAG	O	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	O	2	2	-	0/6/23/26	0/1/1/1
2	NAG	P	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	P	2	2	-	1/6/23/26	0/1/1/1
2	NAG	Q	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	Q	2	2	-	1/6/23/26	0/1/1/1
2	NAG	R	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	R	2	2	-	2/6/23/26	0/1/1/1
2	NAG	S	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	S	2	2	-	1/6/23/26	0/1/1/1
2	NAG	T	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	T	2	2	-	1/6/23/26	0/1/1/1
2	NAG	U	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	U	2	2	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	2	NAG	C1-C2	2.98	1.56	1.52
2	N	2	NAG	C1-C2	2.90	1.56	1.52
2	H	2	NAG	C1-C2	2.90	1.56	1.52

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	U	1	NAG	C2-N2-C7	4.38	129.14	122.90
2	O	1	NAG	C2-N2-C7	4.37	129.13	122.90
2	K	1	NAG	C2-N2-C7	4.32	129.05	122.90
2	F	2	NAG	C2-N2-C7	4.32	129.05	122.90
2	I	1	NAG	C2-N2-C7	4.32	129.05	122.90
2	L	2	NAG	C2-N2-C7	4.31	129.03	122.90
2	P	1	NAG	C2-N2-C7	4.29	129.02	122.90
2	R	2	NAG	C2-N2-C7	4.29	129.00	122.90
2	E	1	NAG	C2-N2-C7	4.28	128.99	122.90
2	S	2	NAG	C2-N2-C7	4.26	128.97	122.90
2	D	1	NAG	C2-N2-C7	4.25	128.96	122.90
2	M	2	NAG	C2-N2-C7	4.25	128.95	122.90
2	T	2	NAG	C2-N2-C7	4.24	128.94	122.90
2	N	2	NAG	C2-N2-C7	4.21	128.90	122.90
2	G	2	NAG	C2-N2-C7	4.20	128.89	122.90
2	H	2	NAG	C2-N2-C7	4.18	128.86	122.90
2	J	1	NAG	C2-N2-C7	4.18	128.86	122.90
2	N	1	NAG	O4-C4-C3	3.98	119.54	110.35
2	H	1	NAG	O4-C4-C3	3.90	119.36	110.35
2	T	1	NAG	O4-C4-C3	3.61	118.70	110.35
2	G	1	NAG	O5-C1-C2	-3.05	106.47	111.29
2	G	2	NAG	C1-O5-C5	3.05	116.33	112.19
2	M	2	NAG	C1-O5-C5	2.78	115.95	112.19
2	M	1	NAG	O5-C1-C2	-2.63	107.14	111.29
2	R	2	NAG	C1-O5-C5	2.62	115.75	112.19
2	K	1	NAG	O5-C1-C2	-2.59	107.20	111.29
2	P	2	NAG	C1-O5-C5	2.50	115.58	112.19
2	S	1	NAG	C2-N2-C7	2.46	126.40	122.90
2	F	1	NAG	O5-C1-C2	-2.40	107.49	111.29
2	M	1	NAG	C2-N2-C7	2.39	126.30	122.90
2	G	1	NAG	C2-N2-C7	2.38	126.30	122.90
2	J	1	NAG	O5-C1-C2	-2.37	107.55	111.29
2	R	1	NAG	O5-C1-C2	-2.36	107.56	111.29
2	J	2	NAG	C1-O5-C5	2.30	115.31	112.19
2	S	2	NAG	C1-O5-C5	2.30	115.30	112.19
2	L	2	NAG	C1-O5-C5	2.30	115.30	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	1	NAG	O5-C1-C2	-2.28	107.68	111.29
2	J	1	NAG	O7-C7-N2	2.17	125.95	121.95
2	F	2	NAG	C1-O5-C5	2.17	115.13	112.19
2	K	1	NAG	O4-C4-C3	-2.16	105.35	110.35
2	D	1	NAG	O7-C7-N2	2.16	125.92	121.95
2	P	1	NAG	O7-C7-N2	2.10	125.82	121.95
2	K	1	NAG	O7-C7-N2	2.03	125.69	121.95
2	T	2	NAG	O5-C1-C2	-2.01	108.11	111.29
2	I	1	NAG	O7-C7-N2	2.00	125.63	121.95

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	1	NAG	C8-C7-N2-C2
2	G	1	NAG	O7-C7-N2-C2
2	M	1	NAG	C8-C7-N2-C2
2	M	1	NAG	O7-C7-N2-C2
2	S	1	NAG	C8-C7-N2-C2
2	S	1	NAG	O7-C7-N2-C2
2	D	2	NAG	O5-C5-C6-O6
2	T	1	NAG	C4-C5-C6-O6
2	P	2	NAG	O5-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
2	J	2	NAG	O5-C5-C6-O6
2	Q	2	NAG	O5-C5-C6-O6
2	L	2	NAG	O5-C5-C6-O6
2	R	2	NAG	O5-C5-C6-O6
2	T	1	NAG	O5-C5-C6-O6
2	H	1	NAG	O5-C5-C6-O6
2	N	1	NAG	O5-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6
2	D	1	NAG	C3-C2-N2-C7
2	E	1	NAG	C3-C2-N2-C7
2	G	2	NAG	C3-C2-N2-C7
2	J	1	NAG	C3-C2-N2-C7
2	K	1	NAG	C3-C2-N2-C7
2	M	2	NAG	C3-C2-N2-C7
2	P	1	NAG	C3-C2-N2-C7
2	S	2	NAG	C3-C2-N2-C7
2	M	2	NAG	O5-C5-C6-O6
2	F	2	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
2	H	2	NAG	C3-C2-N2-C7
2	I	1	NAG	C3-C2-N2-C7
2	L	2	NAG	C3-C2-N2-C7
2	N	2	NAG	C3-C2-N2-C7
2	O	1	NAG	C3-C2-N2-C7
2	R	2	NAG	C3-C2-N2-C7
2	T	2	NAG	C3-C2-N2-C7
2	U	1	NAG	C3-C2-N2-C7

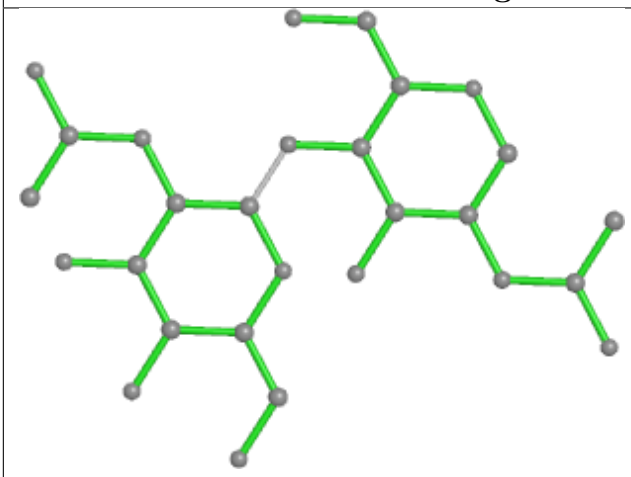
There are no ring outliers.

3 monomers are involved in 3 short contacts:

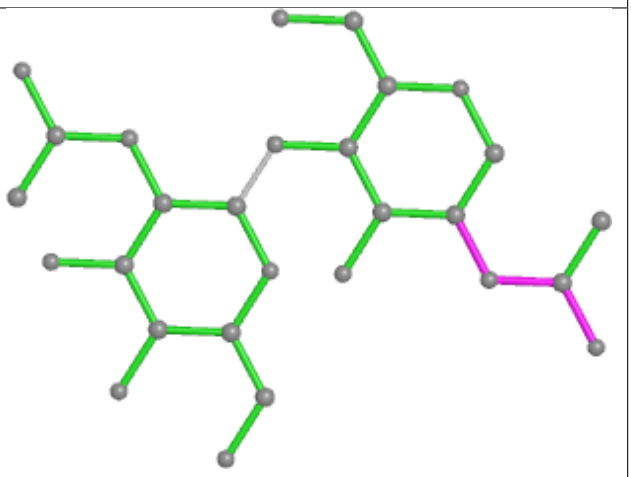
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	NAG	1	0
2	P	1	NAG	1	0
2	L	1	NAG	1	0

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

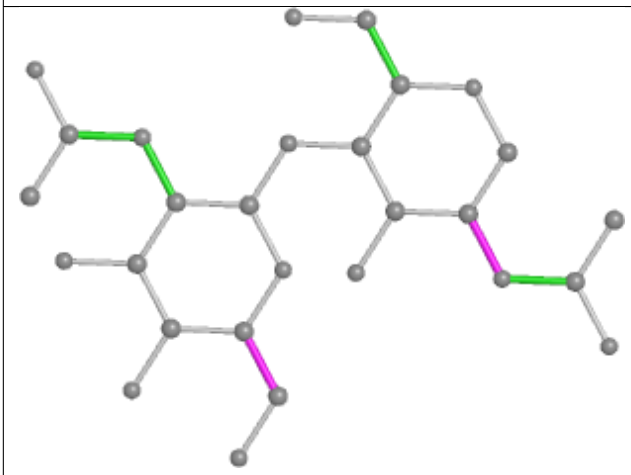
Oligosaccharide Chain D



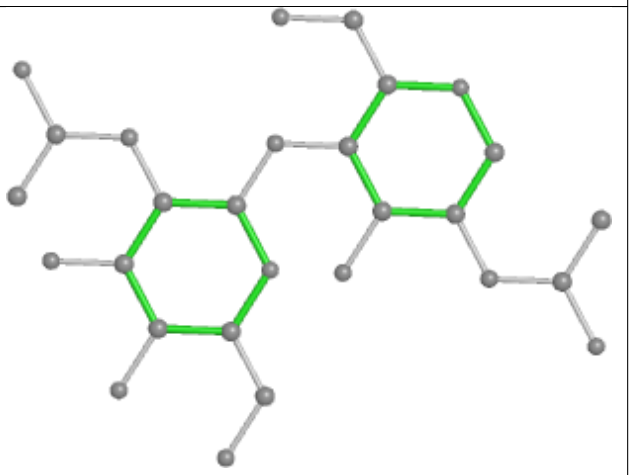
Bond lengths



Bond angles

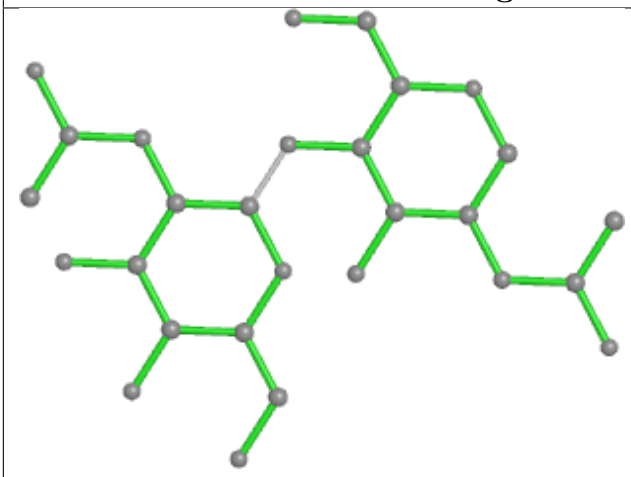


Torsions

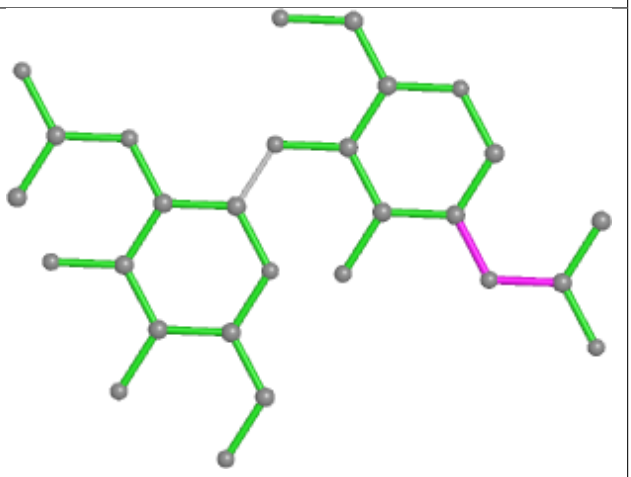


Rings

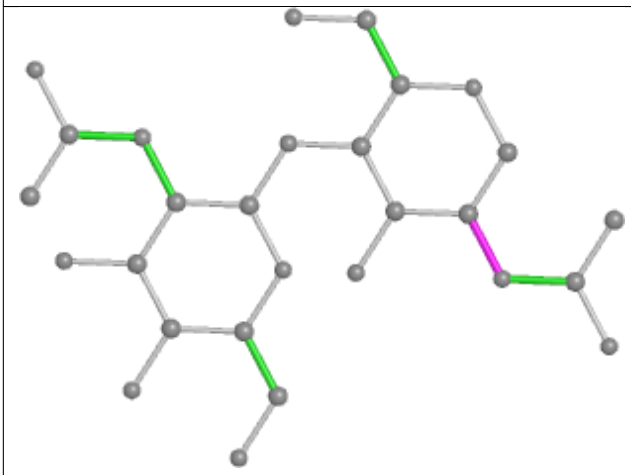
Oligosaccharide Chain E



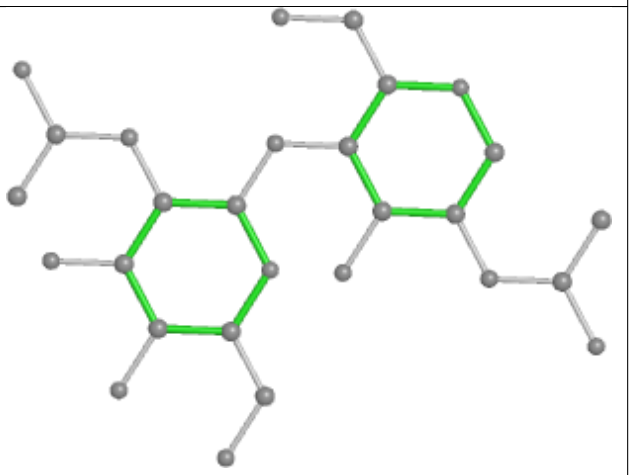
Bond lengths



Bond angles

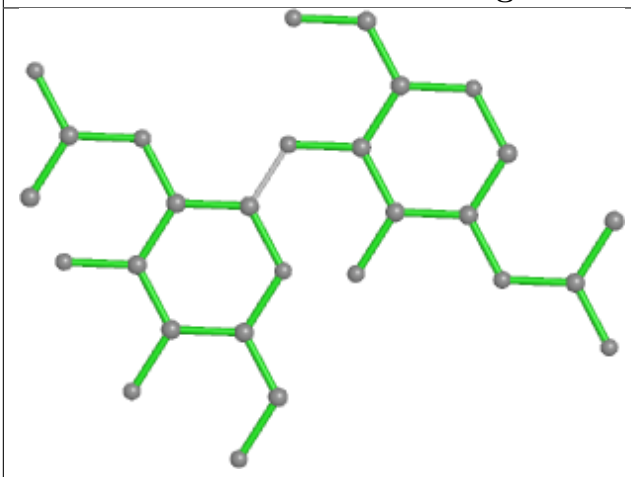


Torsions

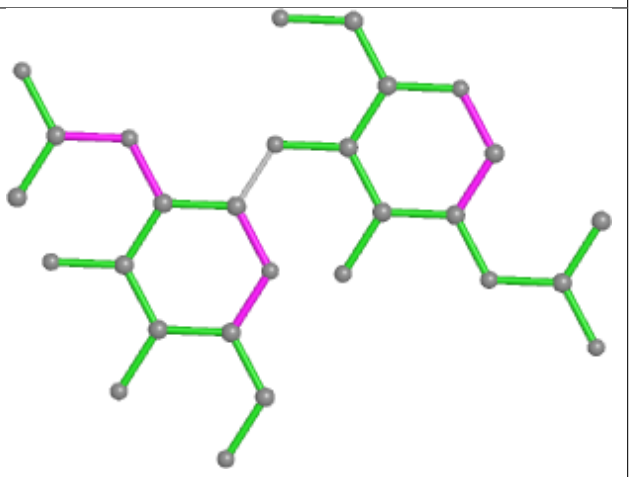


Rings

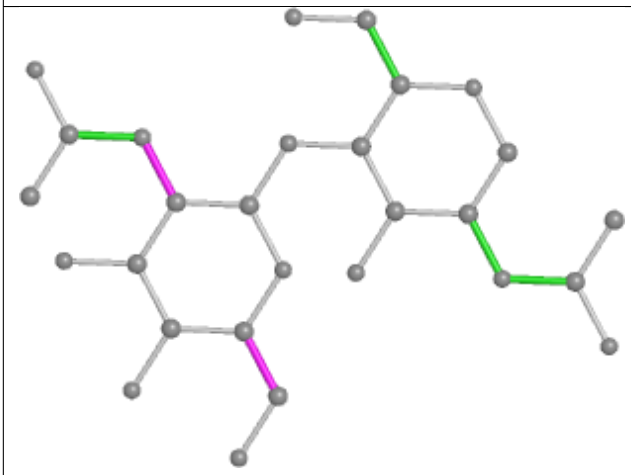
Oligosaccharide Chain F



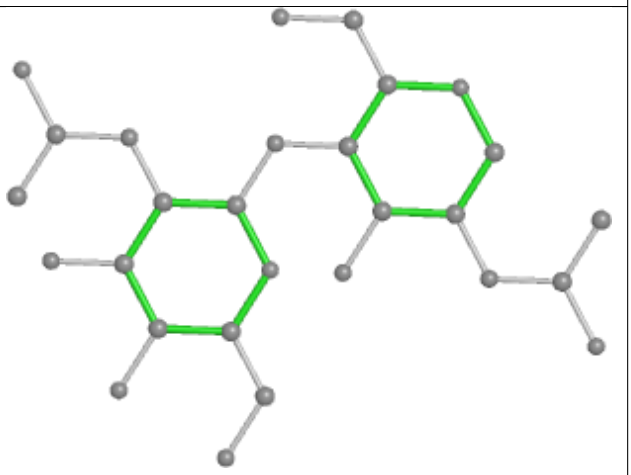
Bond lengths



Bond angles

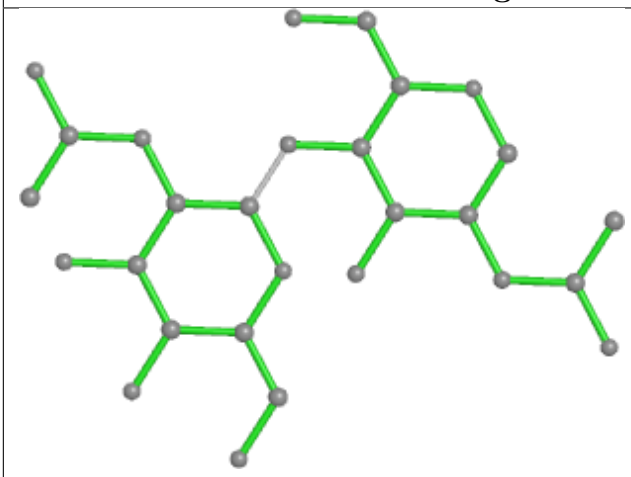


Torsions

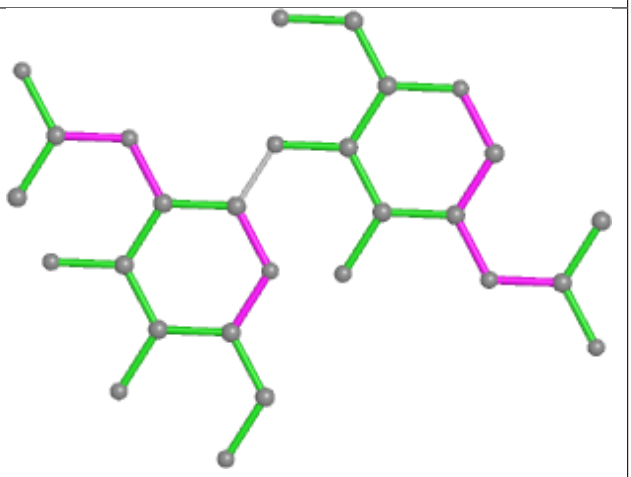


Rings

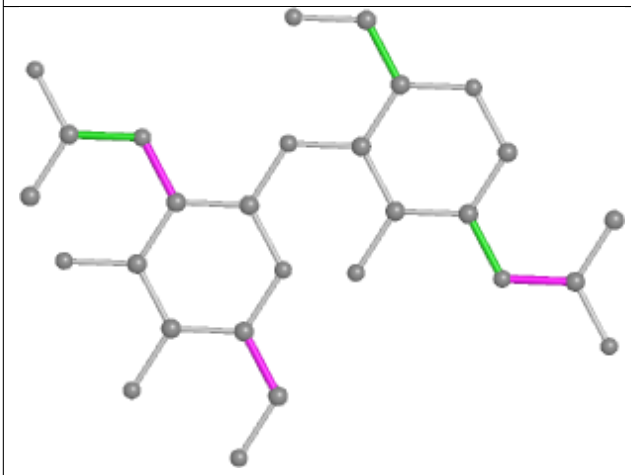
Oligosaccharide Chain G



Bond lengths



Bond angles



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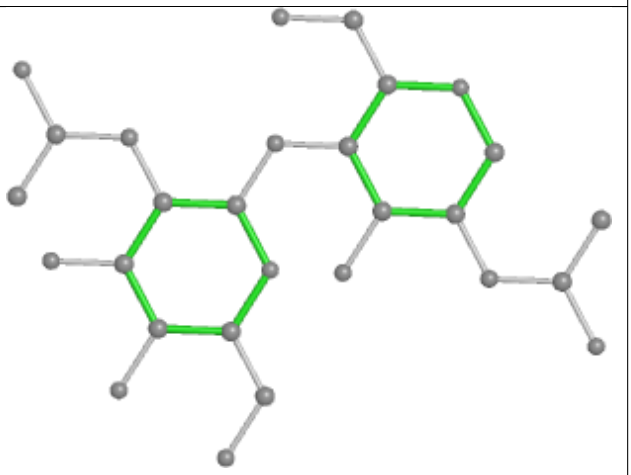
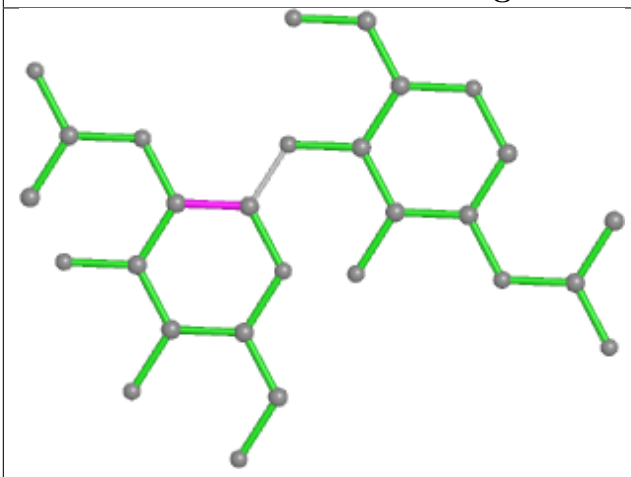
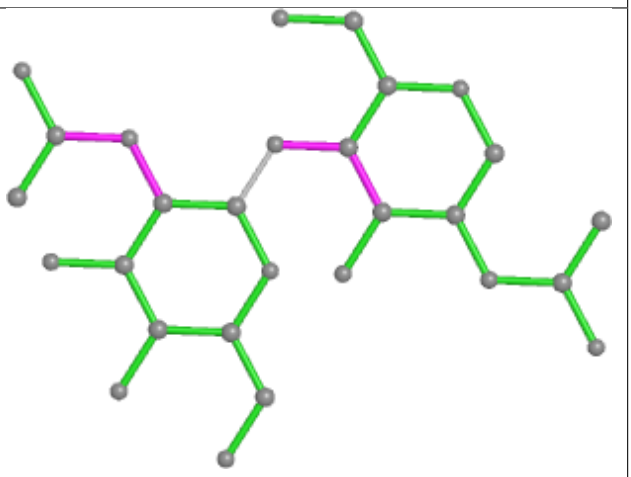


Rings

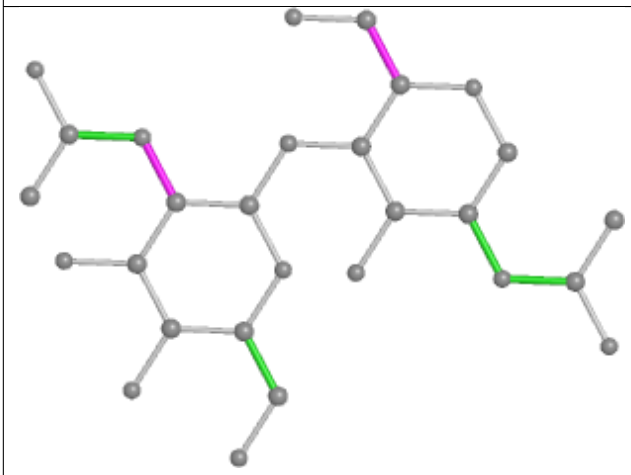
Oligosaccharide Chain H



Bond lengths



Bond angles



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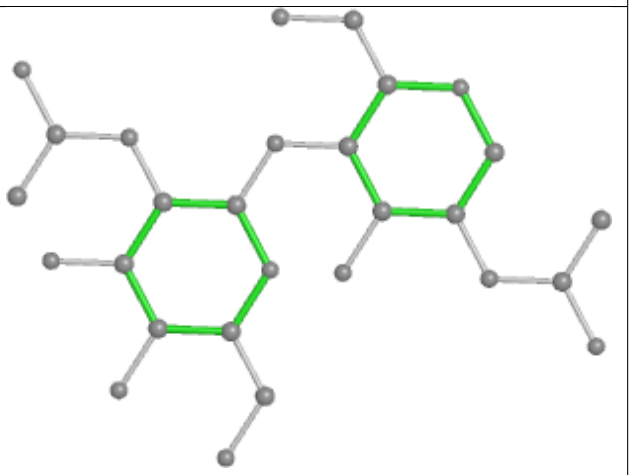
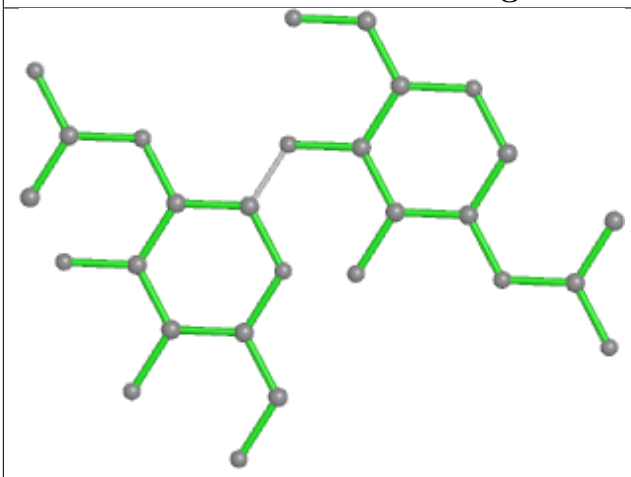


Rings

Oligosaccharide Chain I



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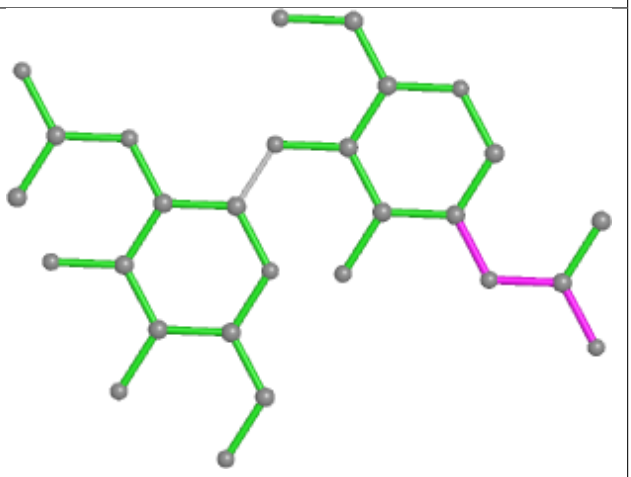
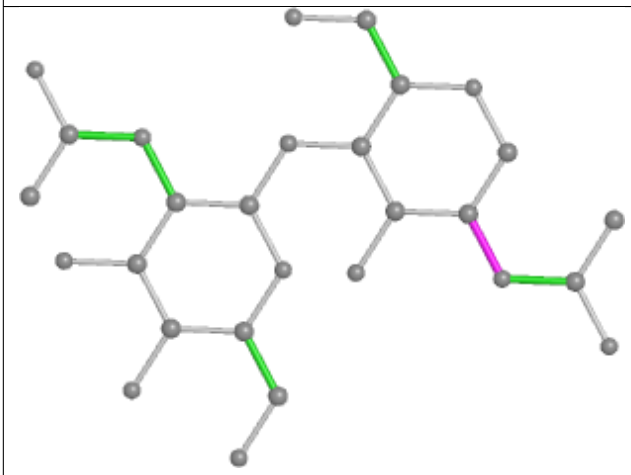
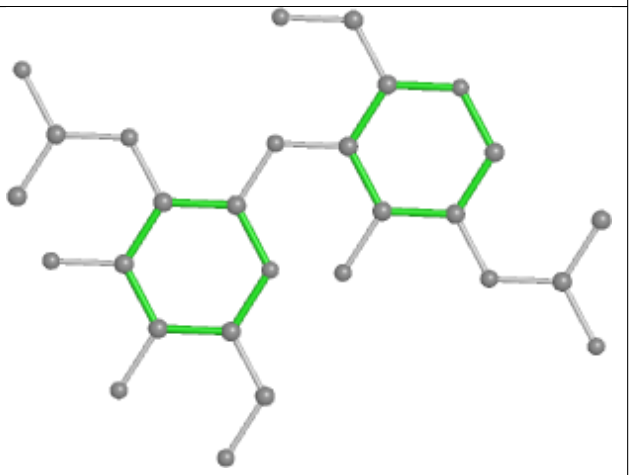


Bond angles

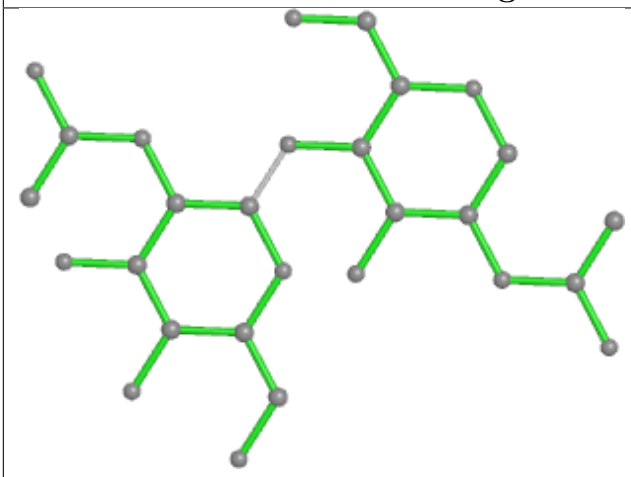


Torsions

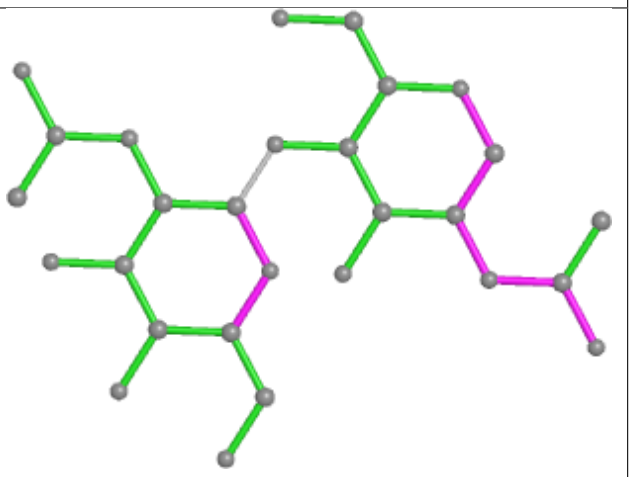


Rings

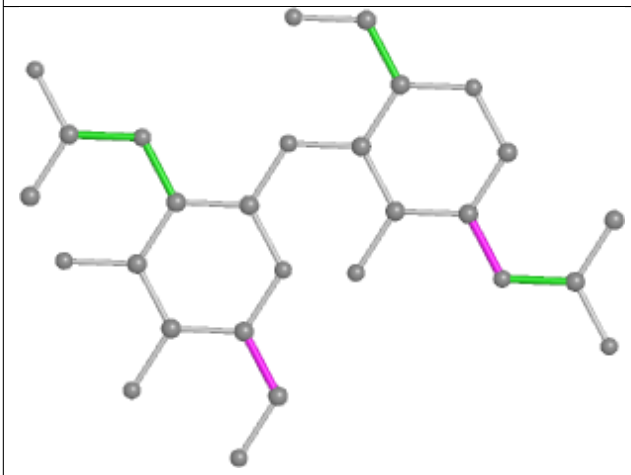
Oligosaccharide Chain J



Bond lengths



Bond angles



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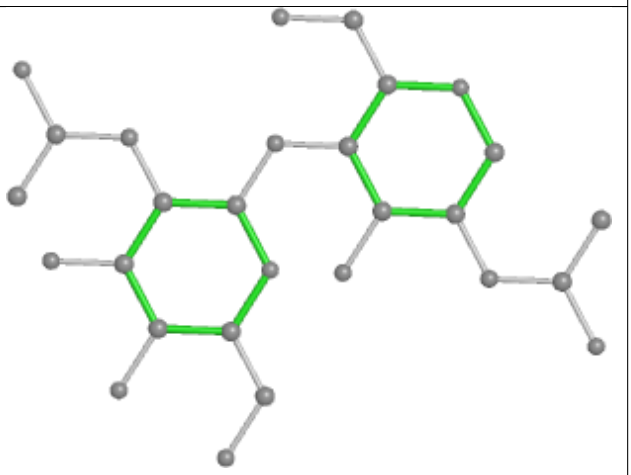
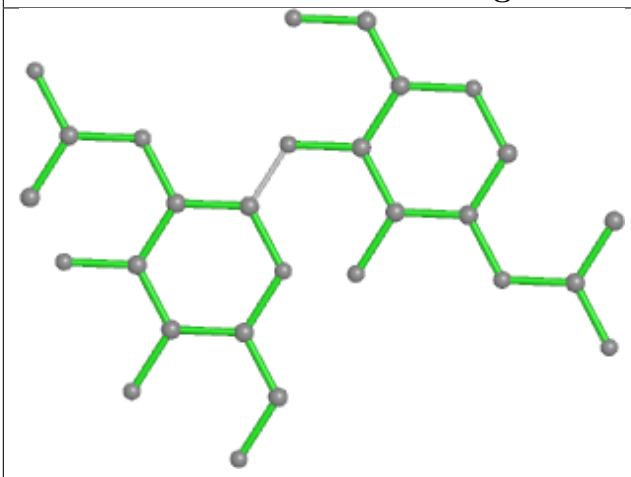
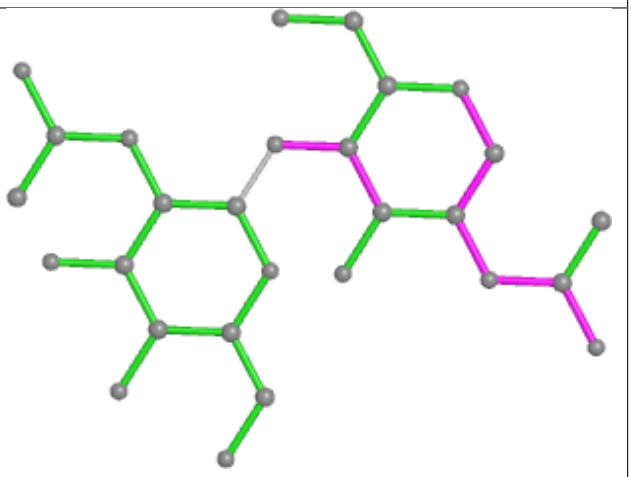


Rings

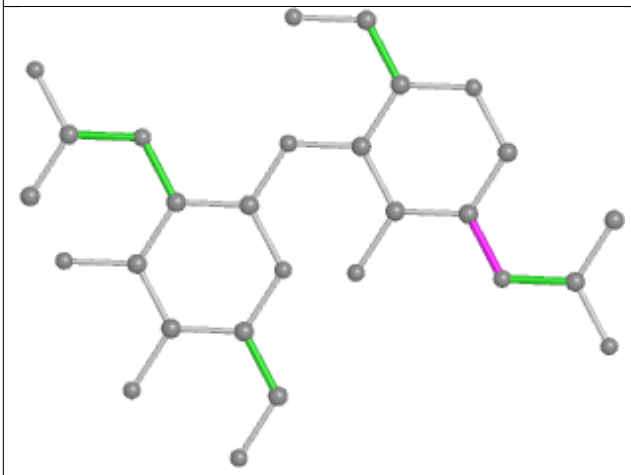
Oligosaccharide Chain K



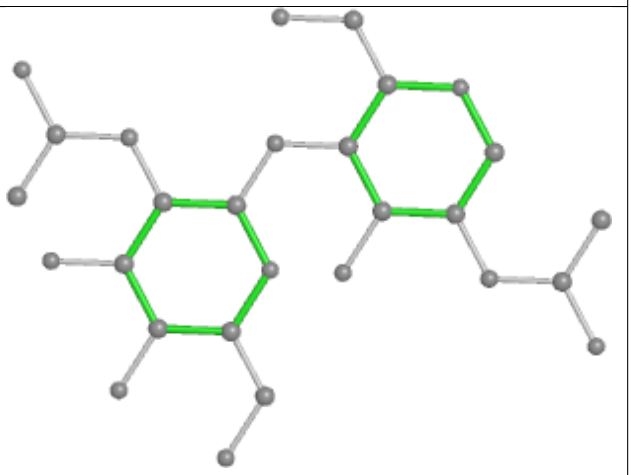
Bond lengths



Bond angles

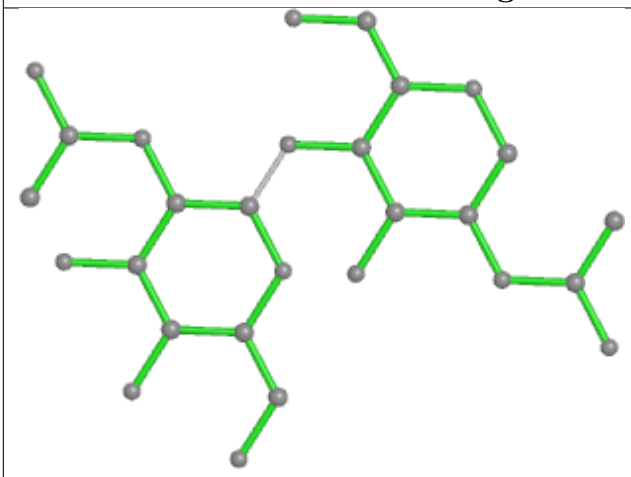


Torsions

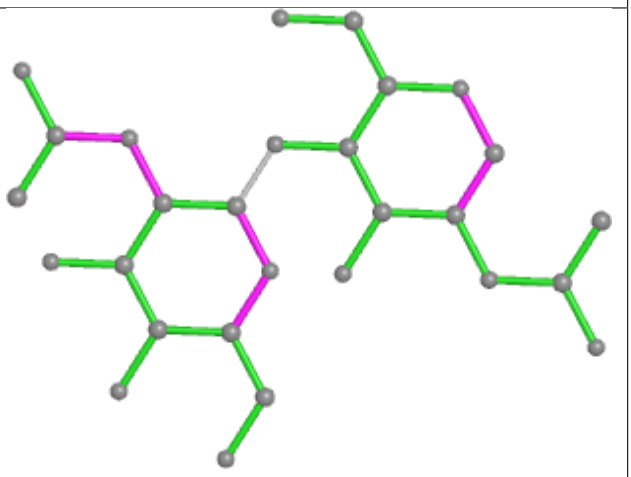


Rings

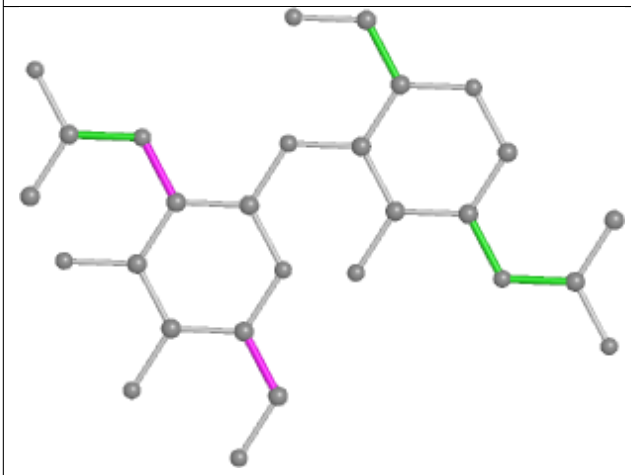
Oligosaccharide Chain L



Bond lengths



Bond angles



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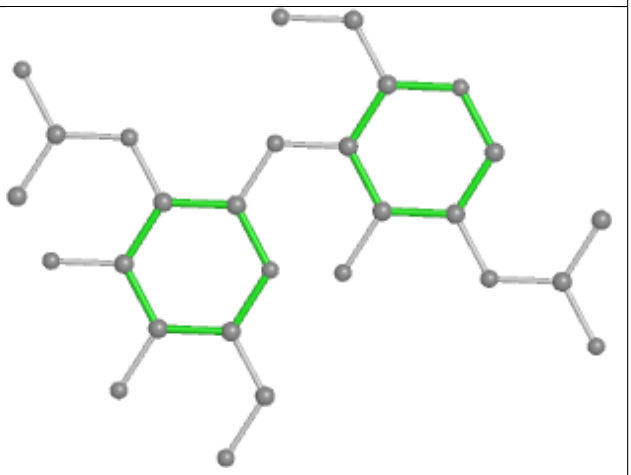
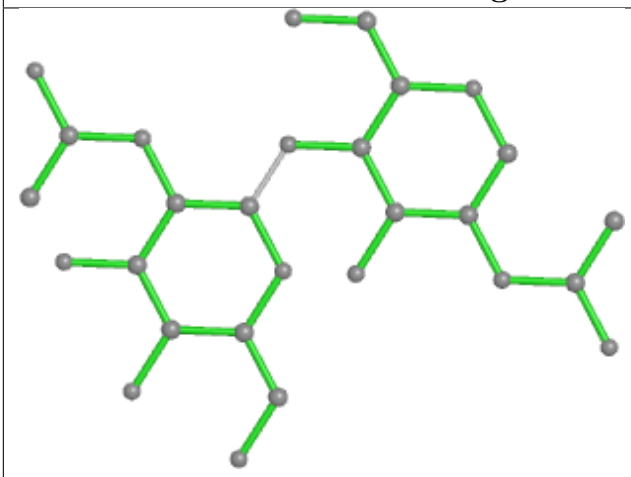
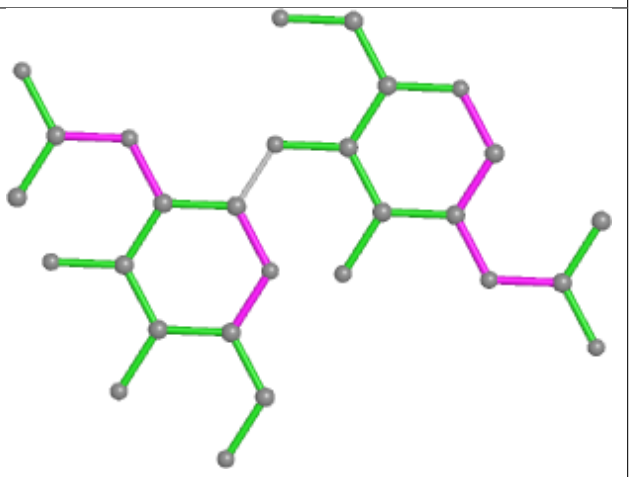


Rings

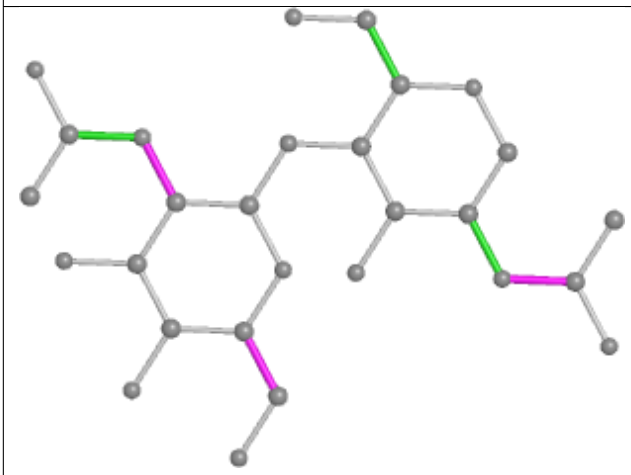
Oligosaccharide Chain M



Bond lengths



Bond angles



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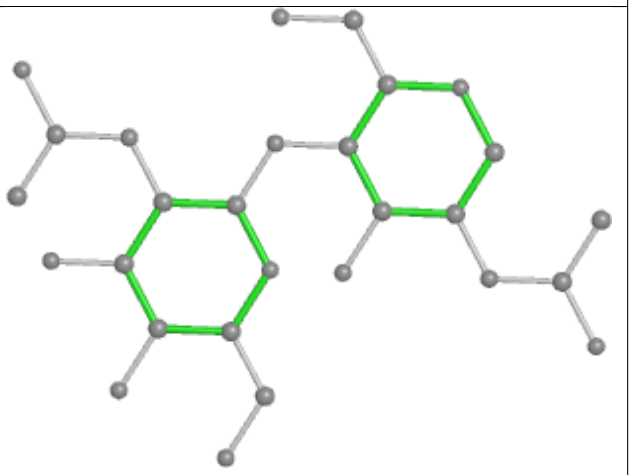
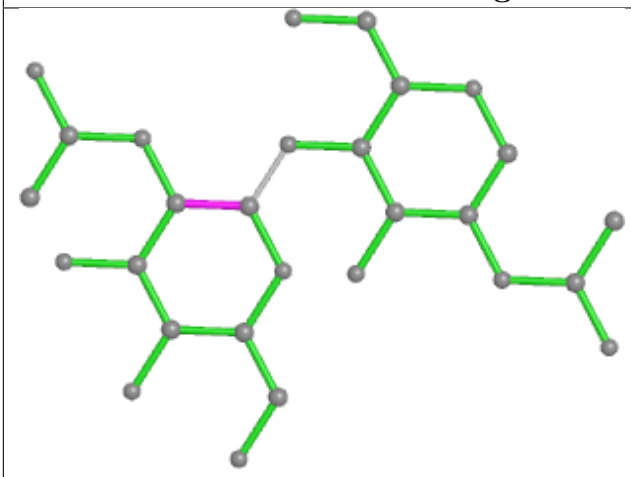
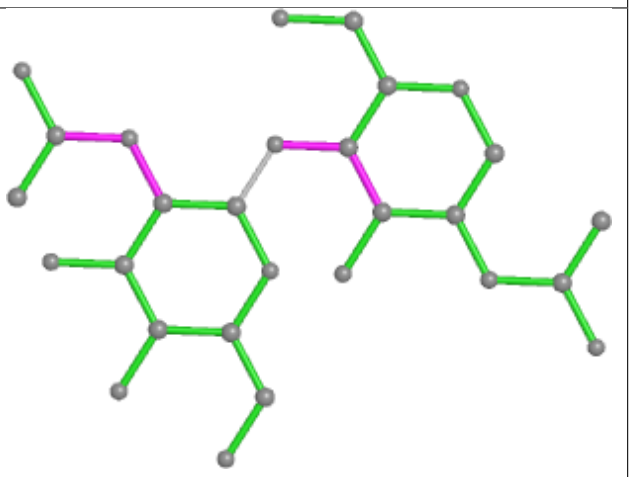
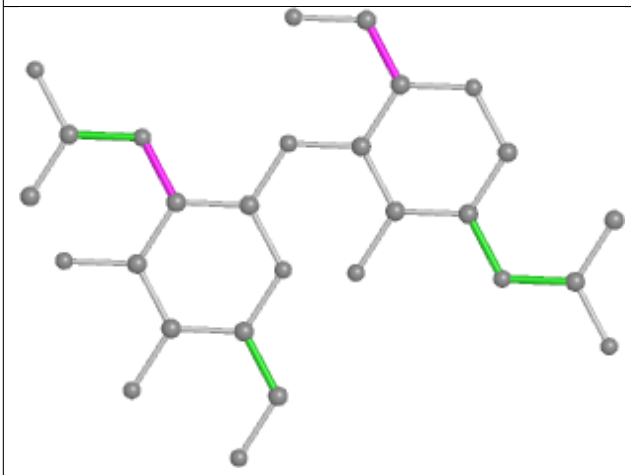
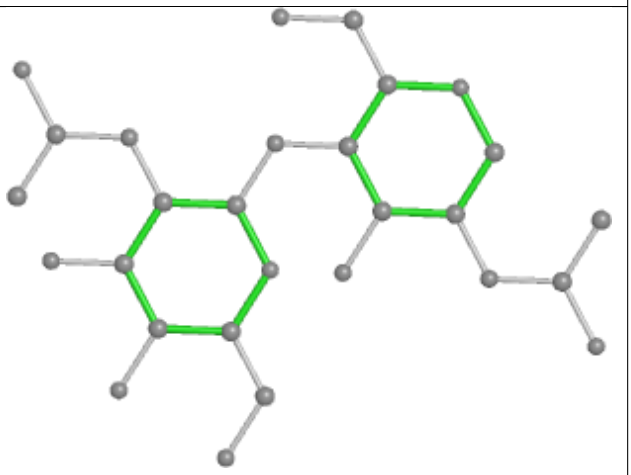
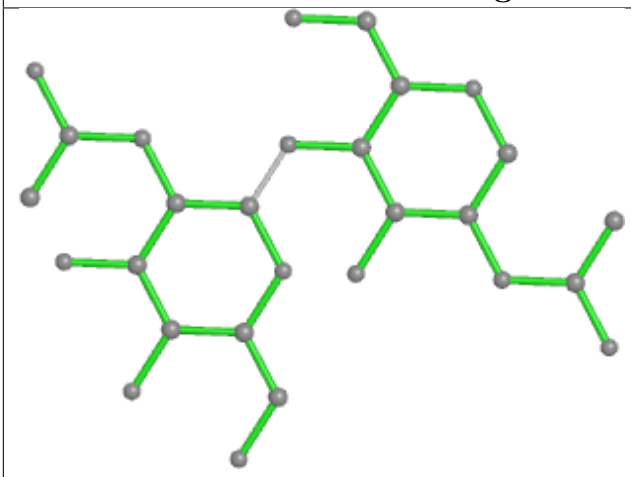


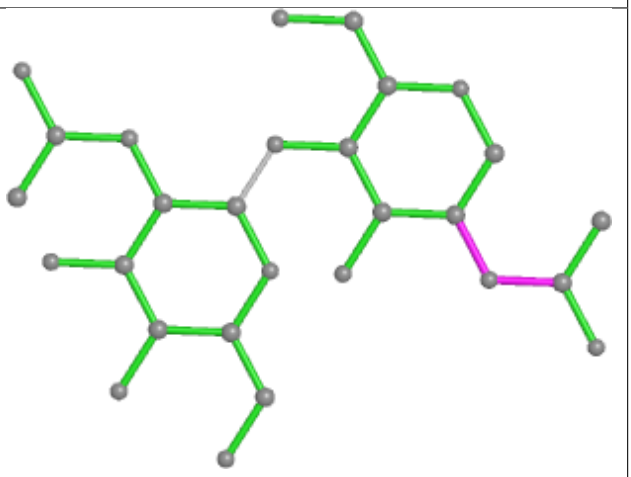
Rings

Oligosaccharide Chain N	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

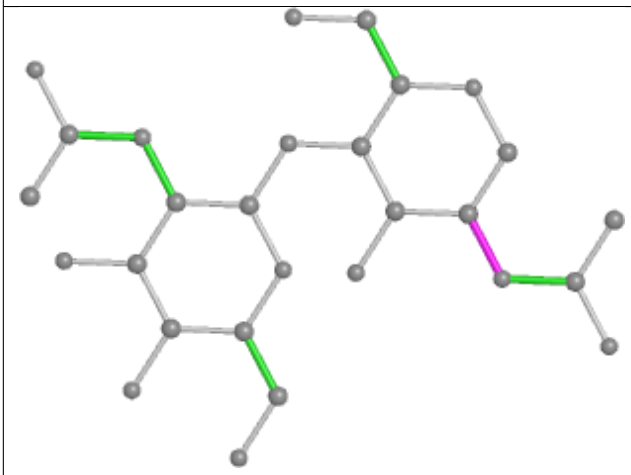
Oligosaccharide Chain O



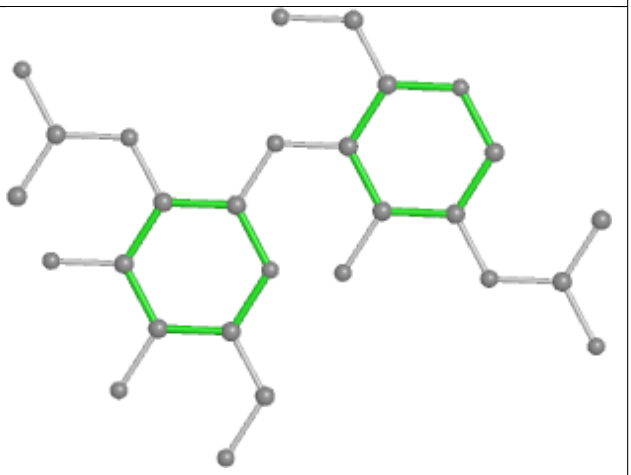
Bond lengths



Bond angles

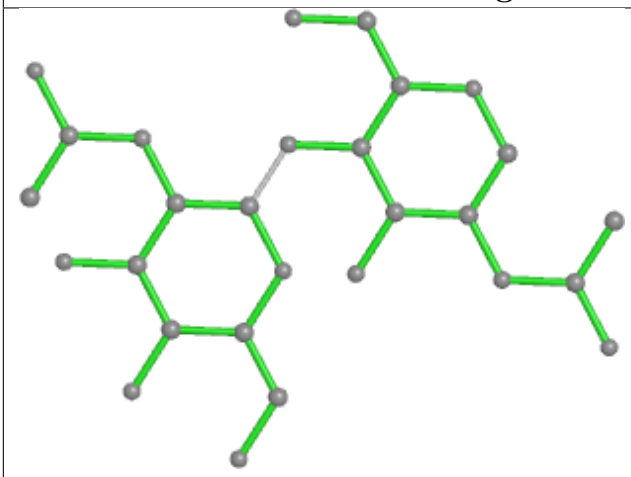


Torsions

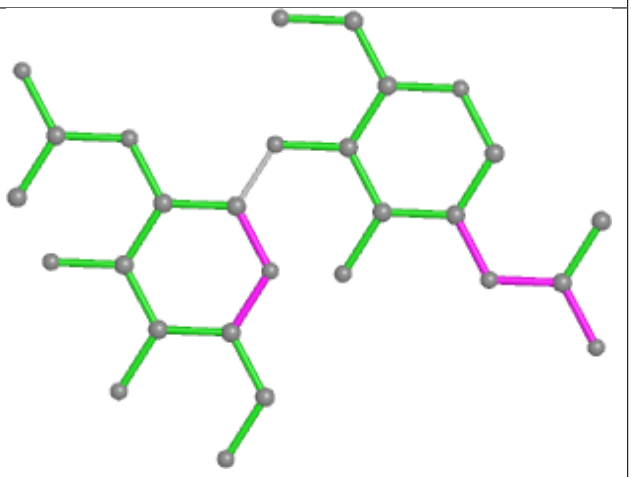


Rings

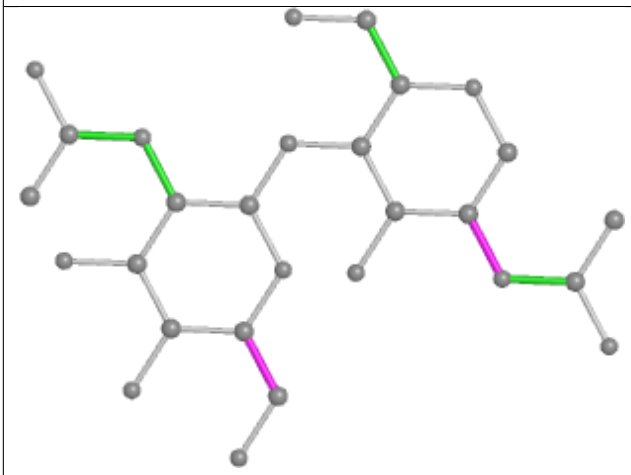
Oligosaccharide Chain P



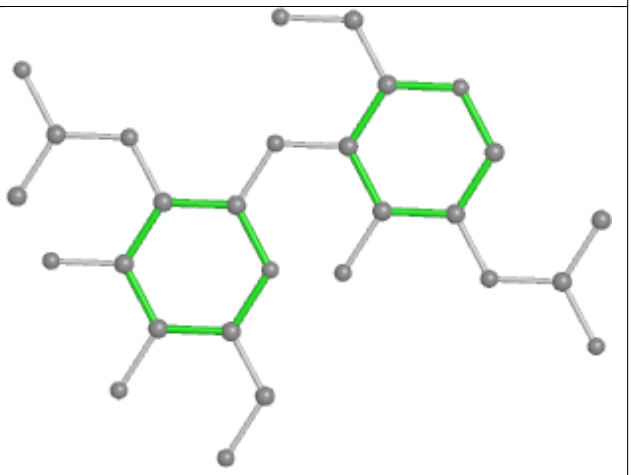
Bond lengths



Bond angles

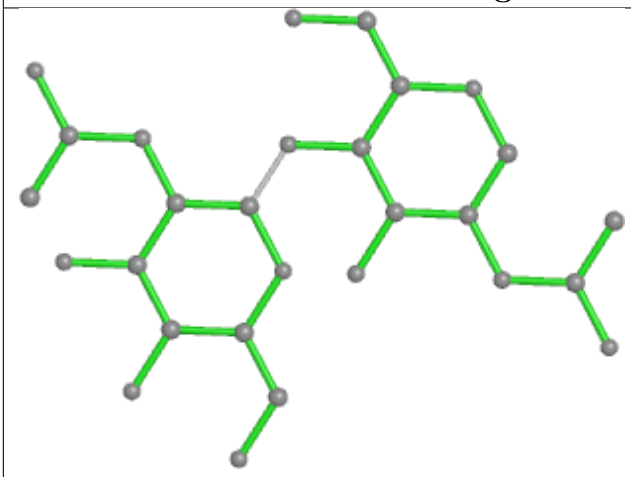


Torsions

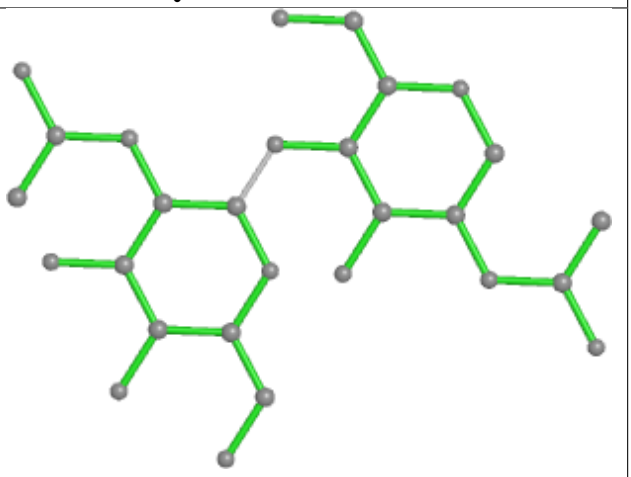


Rings

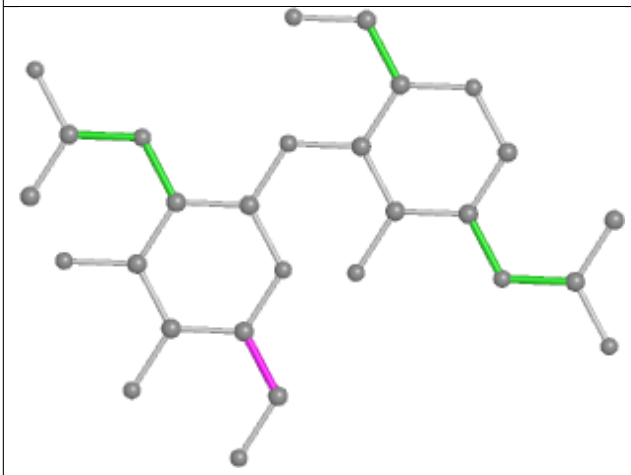
Oligosaccharide Chain Q



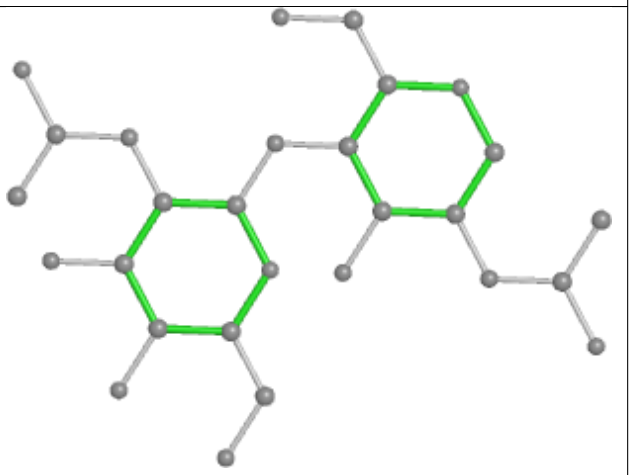
Bond lengths



Bond angles

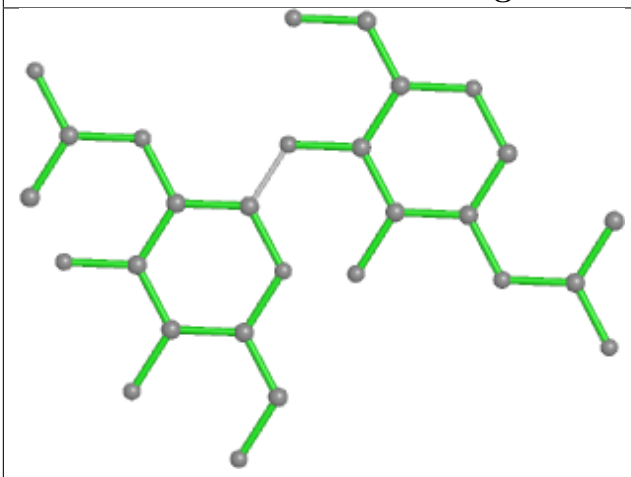


Torsions

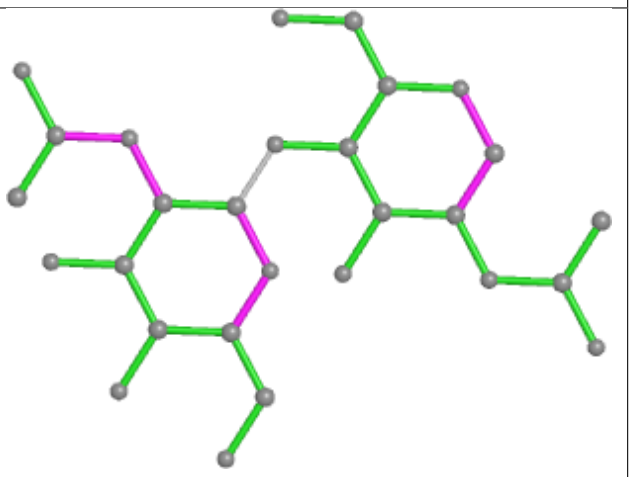


Rings

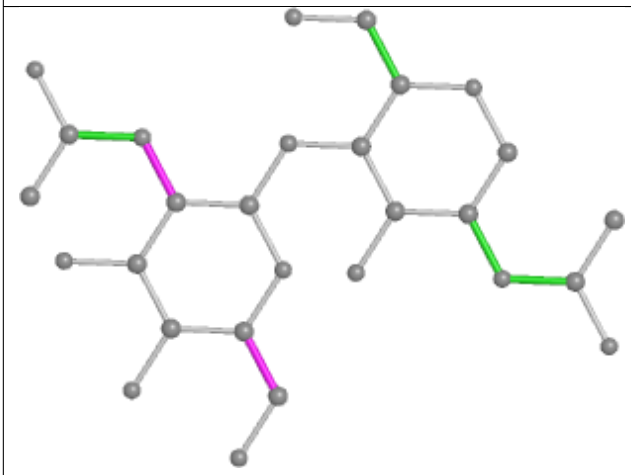
Oligosaccharide Chain R



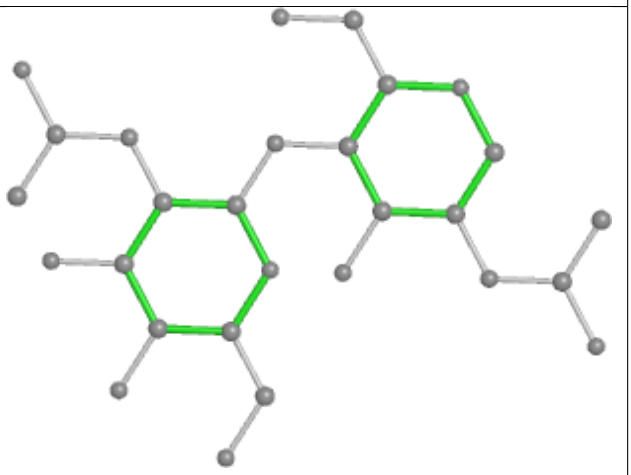
Bond lengths



Bond angles

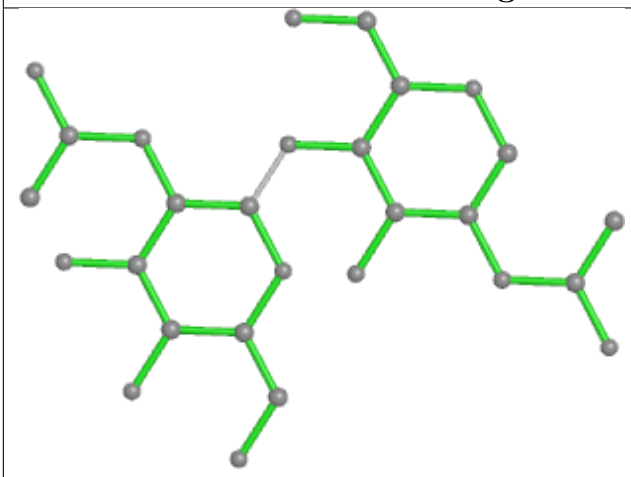


Torsions

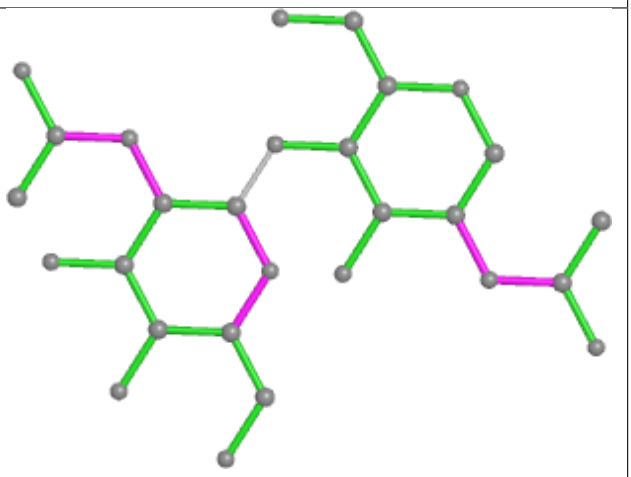


Rings

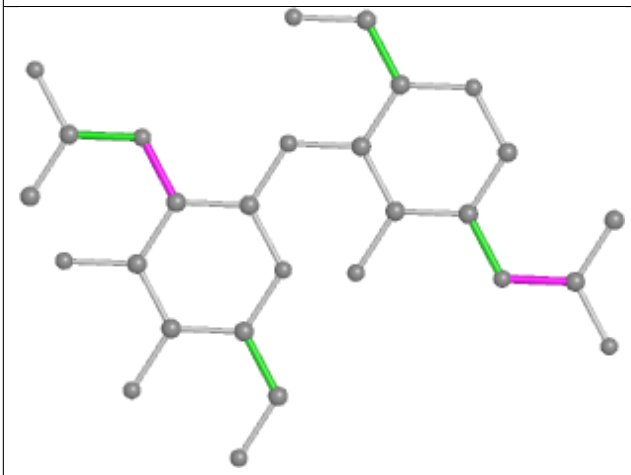
Oligosaccharide Chain S



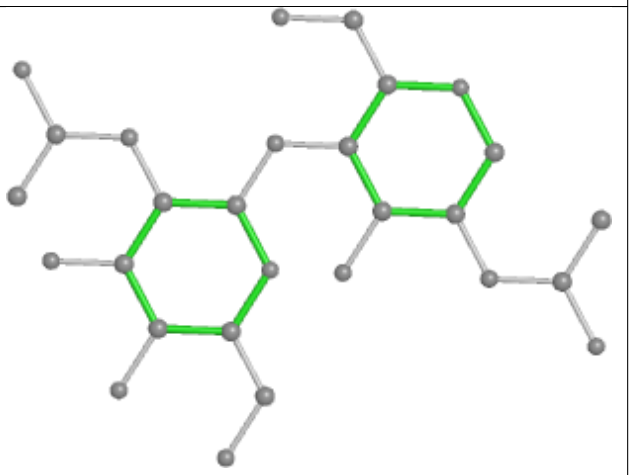
Bond lengths



Bond angles

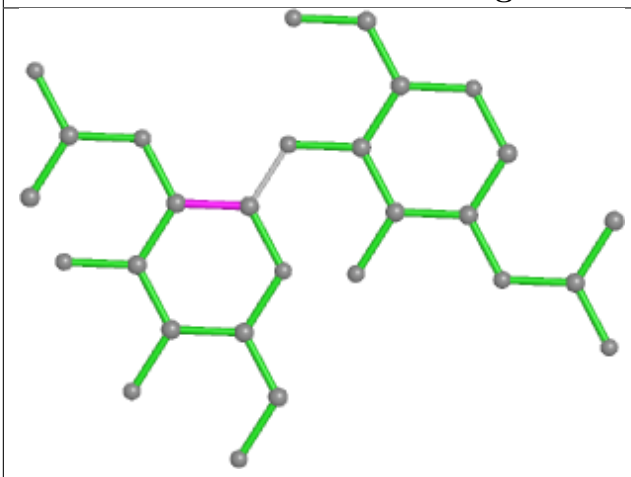


Torsions

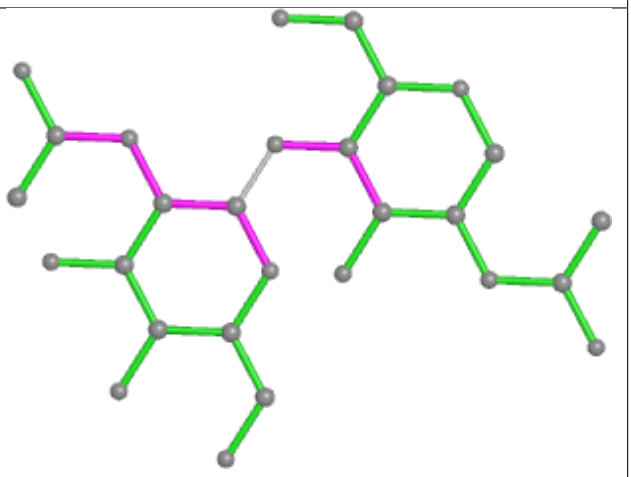


Rings

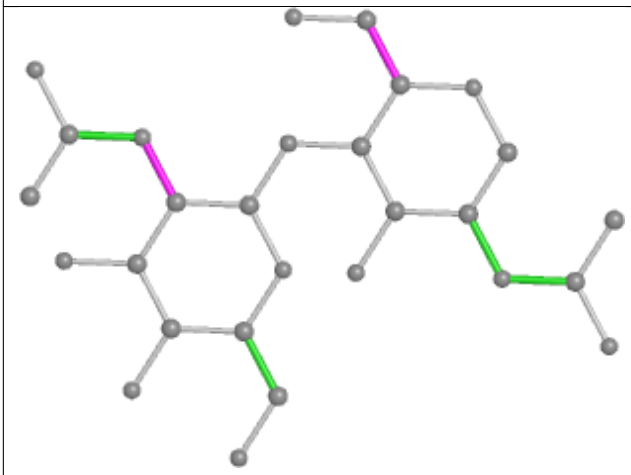
Oligosaccharide Chain T



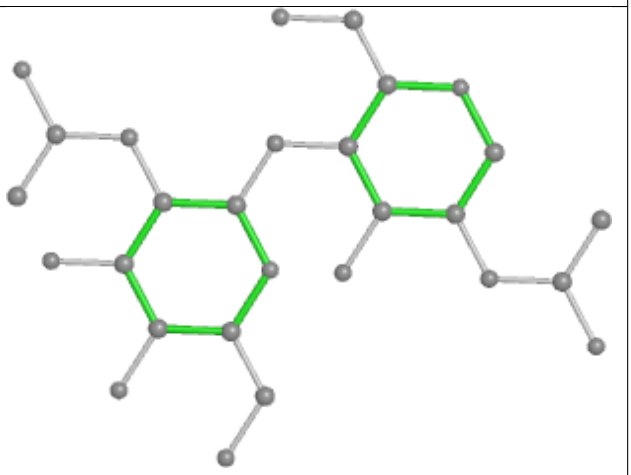
Bond lengths



Bond angles

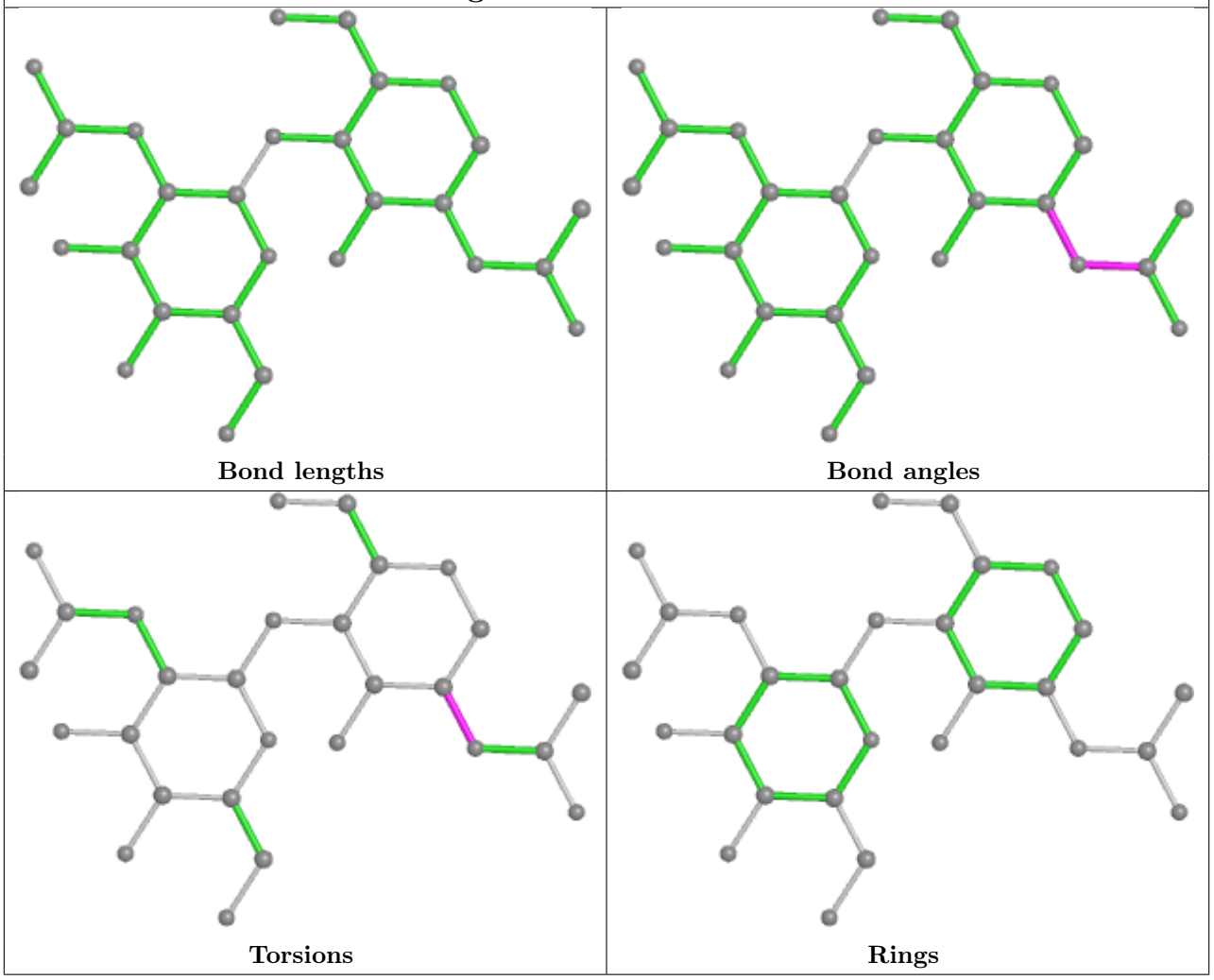


Torsions



Rings

Oligosaccharide Chain U



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	1310	1	14,14,15	0.71	0	17,19,21	0.83	0
3	NAG	A	1307	1	14,14,15	0.79	0	17,19,21	1.41	1 (5%)
3	NAG	B	1303	1	14,14,15	0.72	0	17,19,21	0.90	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	C	1306	1	14,14,15	0.69	0	17,19,21	1.03	1 (5%)
3	NAG	B	1304	1	14,14,15	0.71	0	17,19,21	1.01	1 (5%)
3	NAG	C	1305	1	14,14,15	0.77	0	17,19,21	0.85	0
3	NAG	A	1301	1	14,14,15	0.81	0	17,19,21	0.87	0
3	NAG	C	1309	1	14,14,15	0.78	0	17,19,21	1.35	1 (5%)
3	NAG	C	1311	1	14,14,15	0.72	0	17,19,21	1.52	2 (11%)
3	NAG	C	1303	1	14,14,15	0.73	0	17,19,21	0.87	0
3	NAG	A	1303	1	14,14,15	0.71	0	17,19,21	0.88	0
3	NAG	A	1308	1	14,14,15	0.72	0	17,19,21	0.83	0
3	NAG	B	1301	1	14,14,15	0.79	0	17,19,21	0.80	0
3	NAG	C	1308	-	14,14,15	0.71	0	17,19,21	0.85	0
3	NAG	C	1301	1	14,14,15	0.78	0	17,19,21	0.79	0
3	NAG	C	1310	1	14,14,15	0.70	0	17,19,21	0.84	0
3	NAG	A	1306	1	14,14,15	0.72	0	17,19,21	1.04	1 (5%)
3	NAG	B	1306	1	14,14,15	0.72	0	17,19,21	1.03	1 (5%)
3	NAG	A	1302	1	14,14,15	0.73	0	17,19,21	1.53	2 (11%)
3	NAG	A	1309	1	14,14,15	0.80	0	17,19,21	1.95	4 (23%)
3	NAG	B	1302	1	14,14,15	0.72	0	17,19,21	1.53	2 (11%)
3	NAG	C	1307	1	14,14,15	0.72	0	17,19,21	1.80	3 (17%)
3	NAG	B	1311	1	14,14,15	0.73	0	17,19,21	1.54	3 (17%)
3	NAG	B	1308	1	14,14,15	0.71	0	17,19,21	0.80	0
3	NAG	A	1304	1	14,14,15	0.71	0	17,19,21	1.01	1 (5%)
3	NAG	B	1309	1	14,14,15	0.77	0	17,19,21	1.20	1 (5%)
3	NAG	C	1304	1	14,14,15	0.71	0	17,19,21	1.03	1 (5%)
3	NAG	A	1311	1	14,14,15	0.72	0	17,19,21	1.57	3 (17%)
3	NAG	B	1305	1	14,14,15	0.79	1 (7%)	17,19,21	2.86	6 (35%)
3	NAG	B	1307	1	14,14,15	0.72	0	17,19,21	1.37	2 (11%)
3	NAG	A	1310	1	14,14,15	0.70	0	17,19,21	0.83	0
3	NAG	C	1302	1	14,14,15	0.73	0	17,19,21	1.54	2 (11%)
3	NAG	A	1305	1	14,14,15	0.82	0	17,19,21	0.98	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	1310	1	-	0/6/23/26	0/1/1/1

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1305	NAG	C1-C2	2.38	1.55	1.52

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1305	NAG	C1-O5-C5	7.91	122.91	112.19
3	B	1305	NAG	C2-N2-C7	6.09	131.58	122.90
3	A	1309	NAG	C1-O5-C5	5.08	119.07	112.19
3	B	1302	NAG	C2-N2-C7	4.36	129.11	122.90
3	C	1302	NAG	C2-N2-C7	4.35	129.10	122.90
3	A	1302	NAG	C2-N2-C7	4.31	129.04	122.90
3	A	1307	NAG	C2-N2-C7	4.31	129.03	122.90
3	C	1311	NAG	C2-N2-C7	4.29	129.01	122.90
3	C	1307	NAG	C2-N2-C7	4.29	129.01	122.90
3	B	1311	NAG	C2-N2-C7	4.25	128.95	122.90
3	A	1311	NAG	C2-N2-C7	4.21	128.90	122.90
3	B	1307	NAG	C2-N2-C7	4.21	128.90	122.90
3	A	1309	NAG	C2-N2-C7	4.15	128.82	122.90
3	C	1307	NAG	C1-O5-C5	4.05	117.68	112.19
3	C	1309	NAG	C1-O5-C5	3.88	117.44	112.19
3	B	1309	NAG	C1-O5-C5	3.24	116.58	112.19
3	B	1305	NAG	C1-C2-N2	-3.10	105.19	110.49
3	B	1305	NAG	C3-C4-C5	-3.02	104.86	110.24
3	A	1306	NAG	C2-N2-C7	2.71	126.77	122.90
3	B	1306	NAG	C2-N2-C7	2.66	126.69	122.90
3	C	1304	NAG	C2-N2-C7	2.57	126.56	122.90
3	B	1304	NAG	C2-N2-C7	2.55	126.53	122.90
3	A	1304	NAG	C2-N2-C7	2.49	126.45	122.90
3	B	1305	NAG	O4-C4-C3	-2.46	104.67	110.35
3	A	1311	NAG	C1-O5-C5	2.45	115.52	112.19
3	C	1306	NAG	C2-N2-C7	2.44	126.38	122.90
3	B	1305	NAG	O4-C4-C5	2.35	115.14	109.30
3	B	1311	NAG	C1-O5-C5	2.34	115.36	112.19
3	C	1307	NAG	O7-C7-N2	2.34	126.25	121.95
3	A	1309	NAG	C3-C4-C5	-2.27	106.19	110.24
3	B	1302	NAG	O5-C1-C2	-2.26	107.71	111.29
3	A	1302	NAG	O5-C1-C2	-2.12	107.93	111.29
3	A	1311	NAG	O7-C7-N2	2.11	125.83	121.95
3	B	1311	NAG	O7-C7-N2	2.08	125.78	121.95
3	C	1302	NAG	O5-C1-C2	-2.08	108.00	111.29
3	B	1307	NAG	O7-C7-N2	2.07	125.75	121.95
3	C	1311	NAG	O7-C7-N2	2.04	125.70	121.95
3	A	1309	NAG	O5-C1-C2	2.03	114.49	111.29

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1305	NAG	C1-C2-N2-C7
3	A	1304	NAG	C8-C7-N2-C2
3	A	1304	NAG	O7-C7-N2-C2
3	A	1306	NAG	C8-C7-N2-C2
3	A	1306	NAG	O7-C7-N2-C2
3	A	1309	NAG	C8-C7-N2-C2
3	A	1309	NAG	O7-C7-N2-C2
3	B	1304	NAG	C8-C7-N2-C2
3	B	1304	NAG	O7-C7-N2-C2
3	B	1306	NAG	C8-C7-N2-C2
3	B	1306	NAG	O7-C7-N2-C2
3	C	1304	NAG	C8-C7-N2-C2
3	C	1304	NAG	O7-C7-N2-C2
3	C	1306	NAG	C8-C7-N2-C2
3	C	1306	NAG	O7-C7-N2-C2
3	C	1306	NAG	O5-C5-C6-O6
3	A	1306	NAG	O5-C5-C6-O6
3	B	1307	NAG	O5-C5-C6-O6
3	C	1305	NAG	O5-C5-C6-O6
3	C	1307	NAG	O5-C5-C6-O6
3	B	1305	NAG	O5-C5-C6-O6
3	B	1306	NAG	O5-C5-C6-O6
3	A	1302	NAG	C3-C2-N2-C7
3	A	1307	NAG	C3-C2-N2-C7
3	A	1311	NAG	C3-C2-N2-C7
3	B	1302	NAG	C3-C2-N2-C7
3	B	1305	NAG	C3-C2-N2-C7
3	B	1307	NAG	C3-C2-N2-C7
3	B	1311	NAG	C3-C2-N2-C7
3	C	1302	NAG	C3-C2-N2-C7
3	C	1307	NAG	C3-C2-N2-C7
3	C	1311	NAG	C3-C2-N2-C7

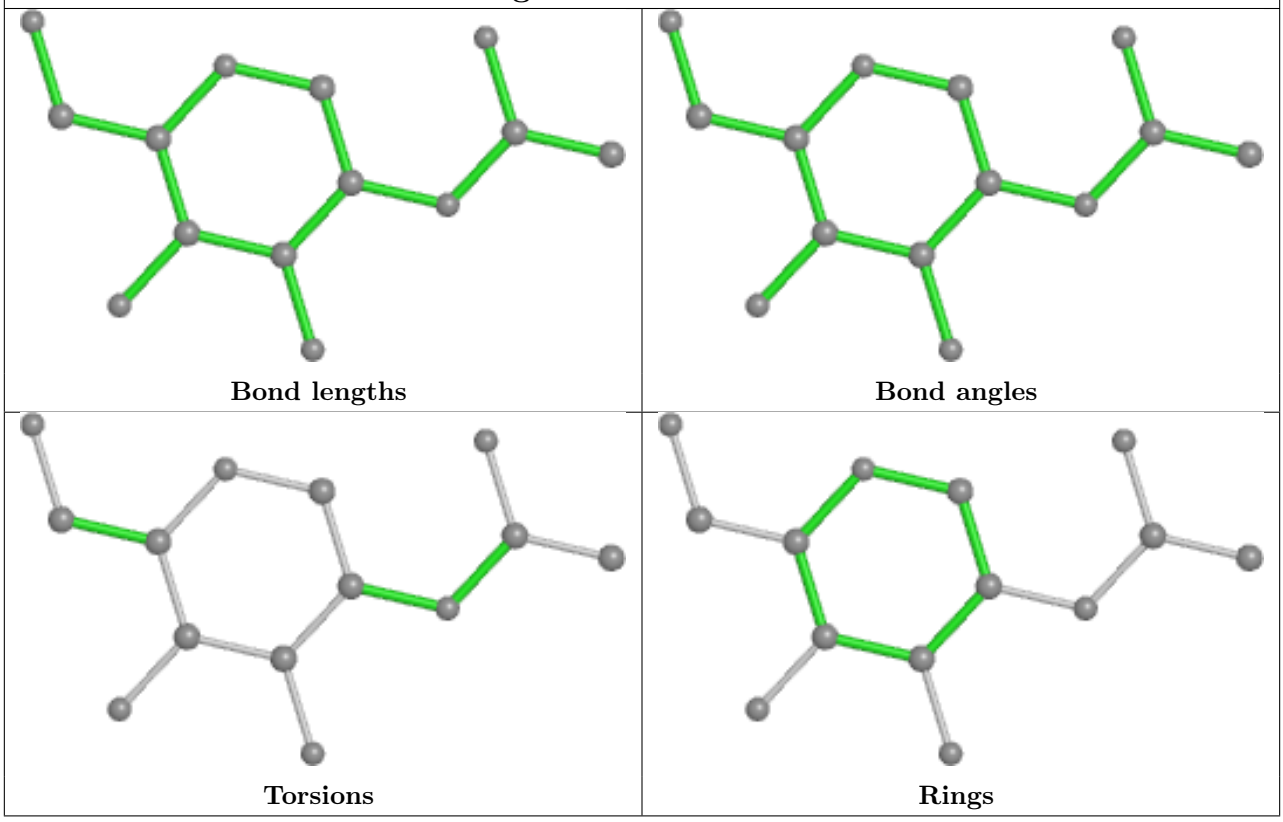
There are no ring outliers.

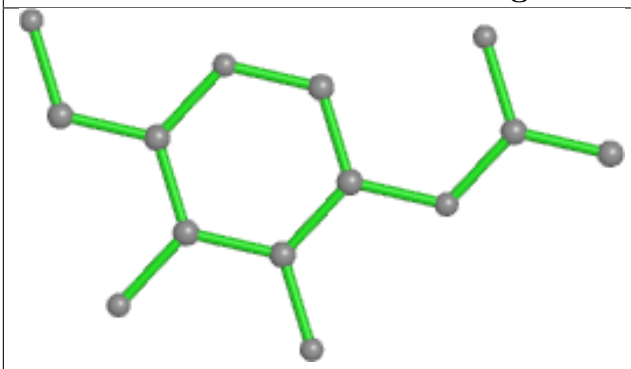
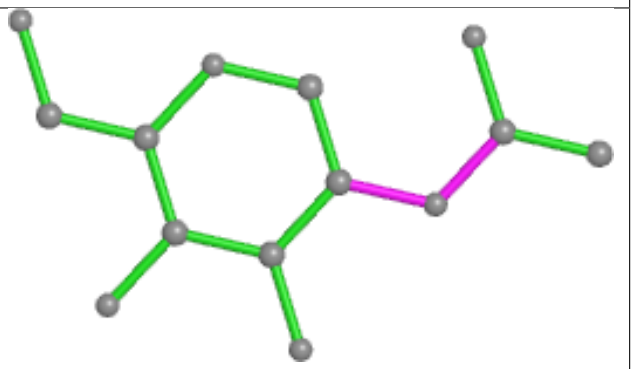
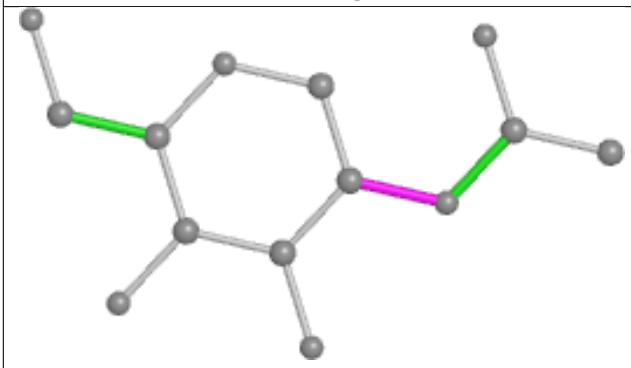
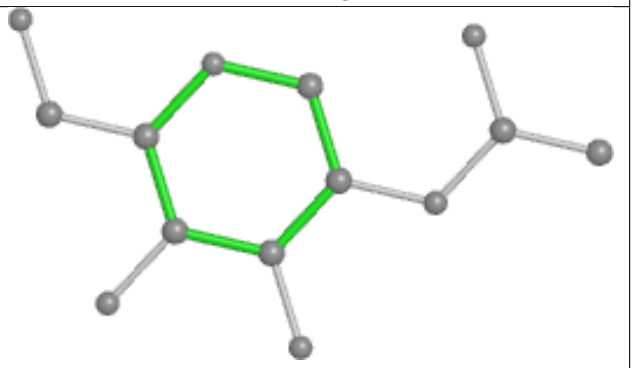
No monomer is involved in short contacts.

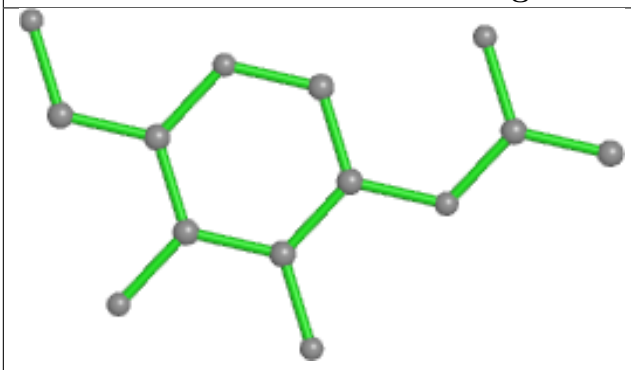
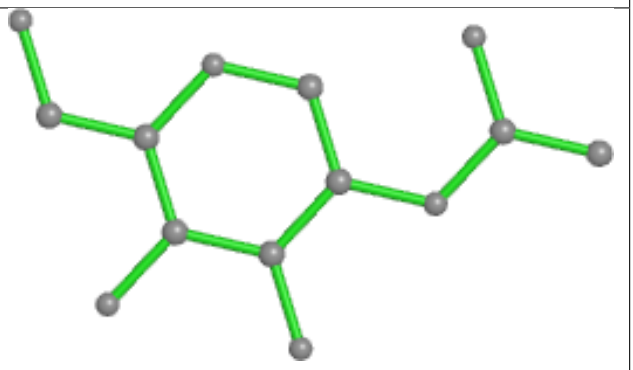
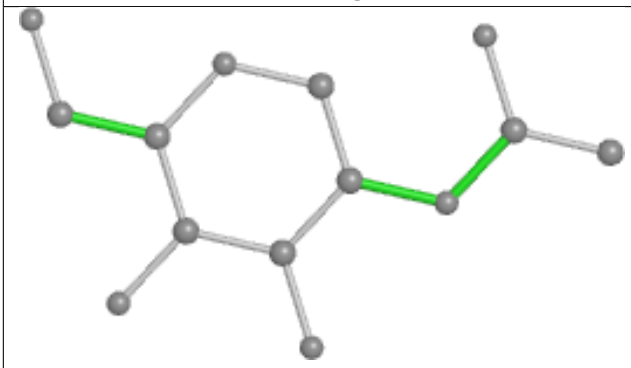
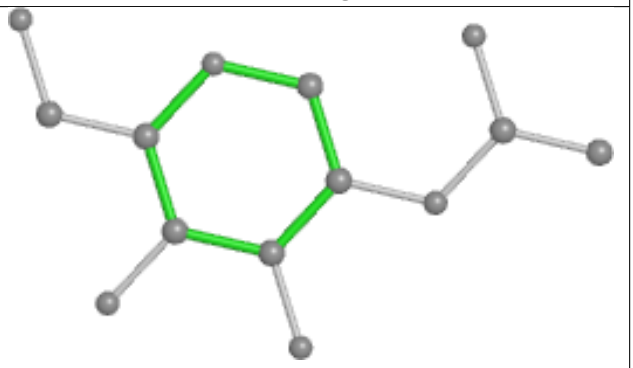
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

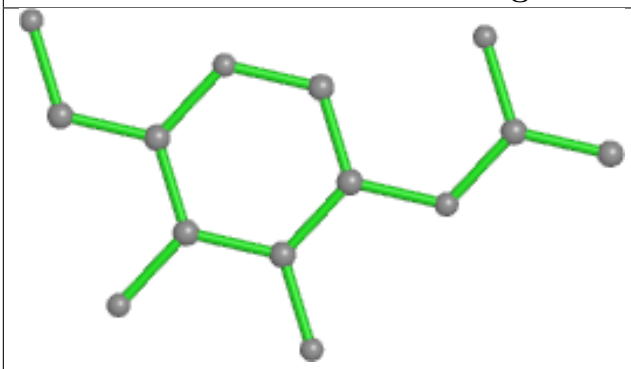
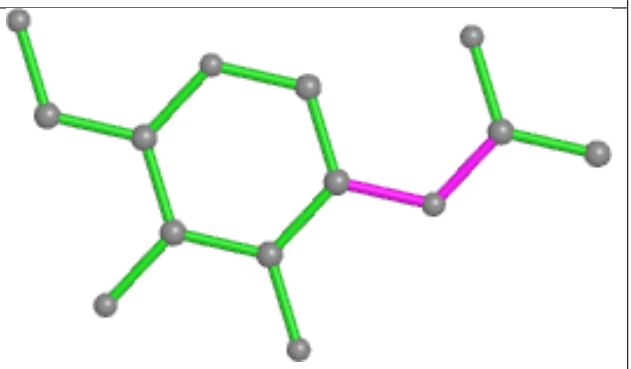
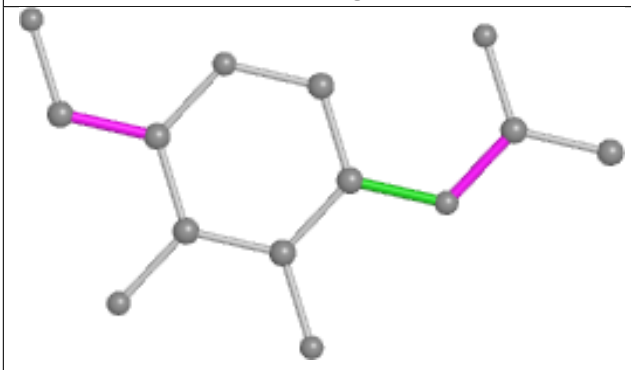
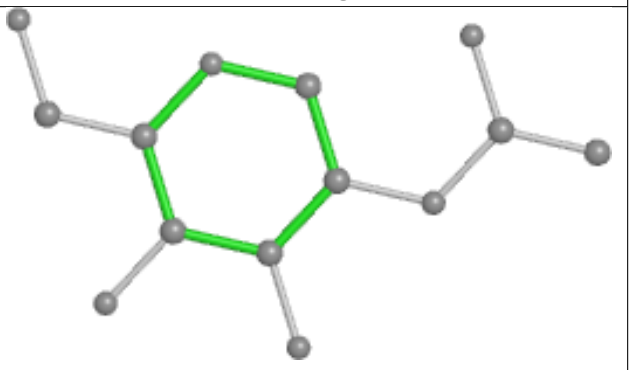
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

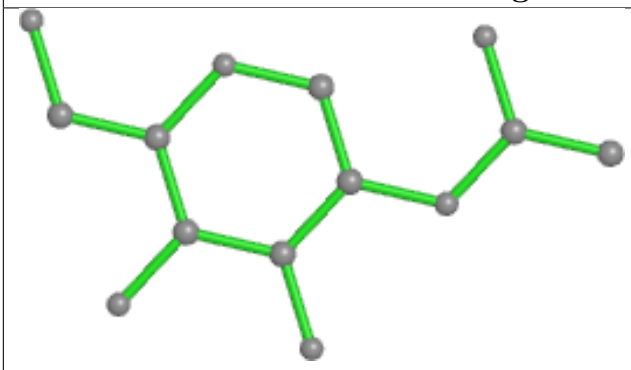
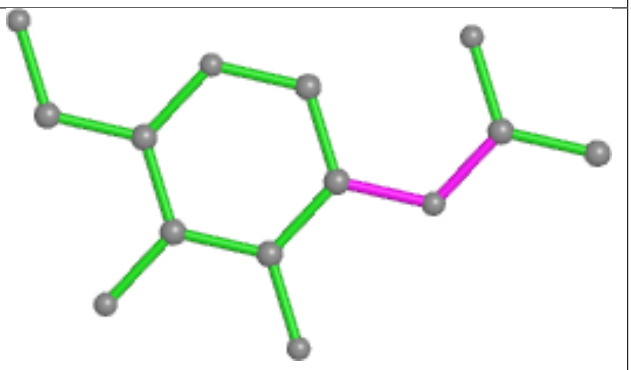
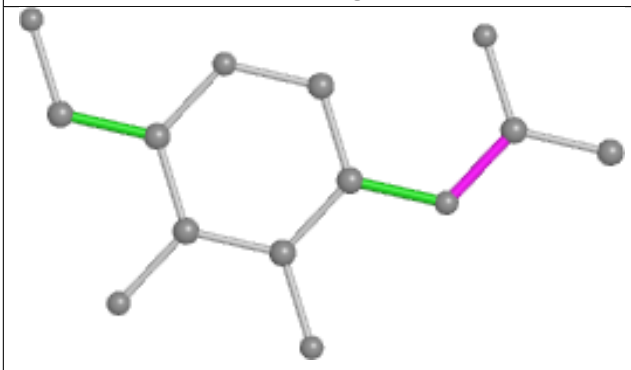
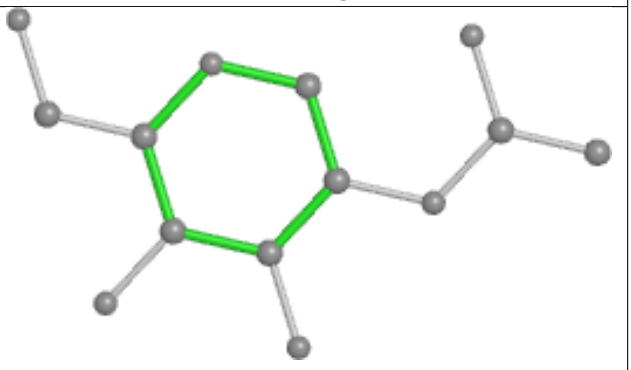
Ligand NAG B 1310



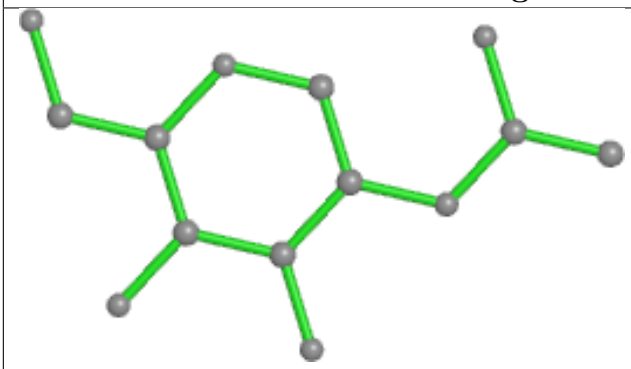
Ligand NAG A 1307	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG B 1303	
 Bond lengths	 Bond angles
 Torsions	 Rings

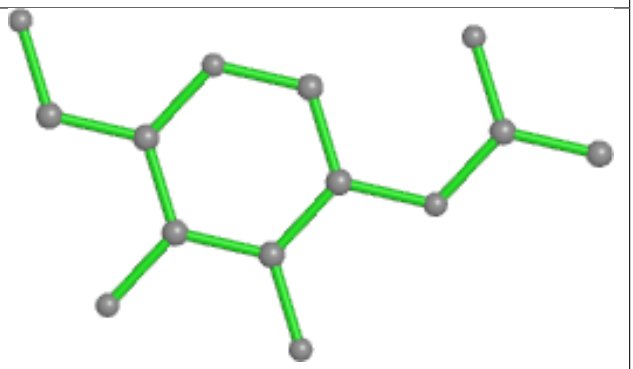
Ligand NAG C 1306	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG B 1304	
 Bond lengths	 Bond angles
 Torsions	 Rings

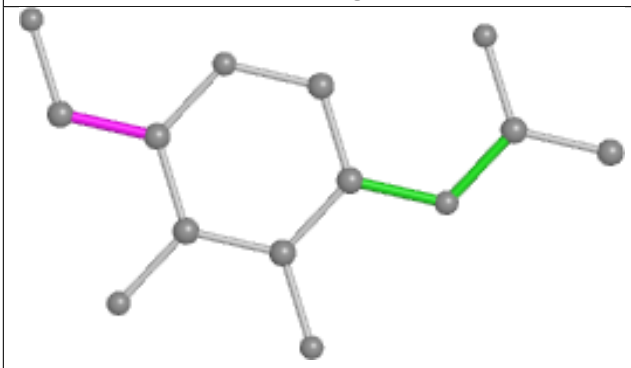
Ligand NAG C 1305



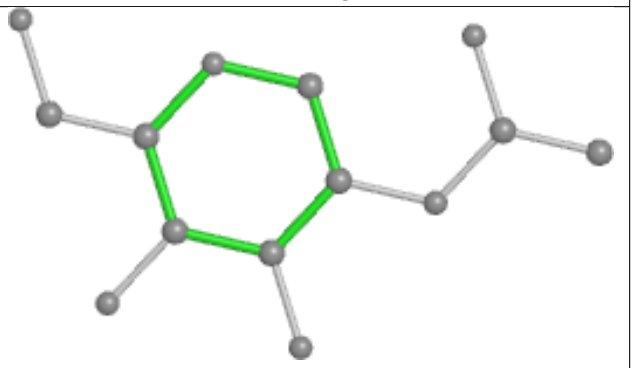
Bond lengths



Bond angles

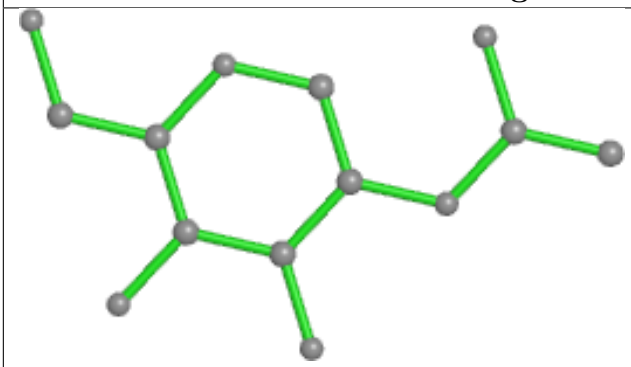


Torsions



Rings

Ligand NAG A 1301



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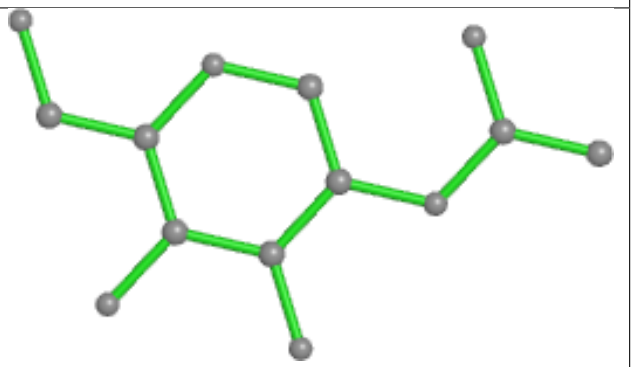
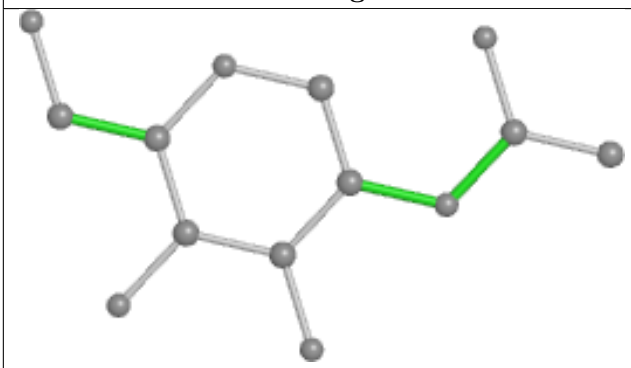


Bond angles



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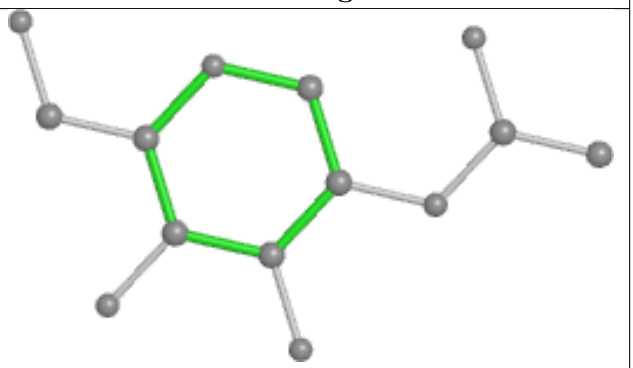
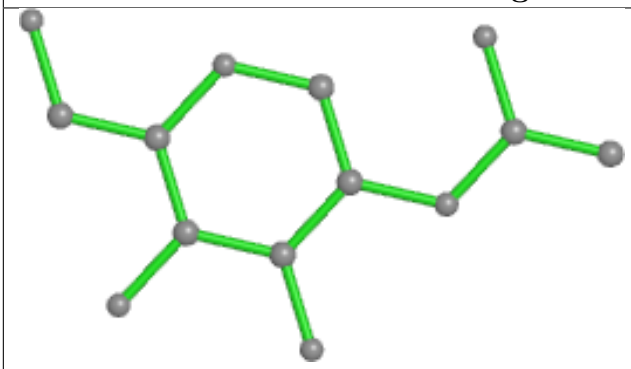
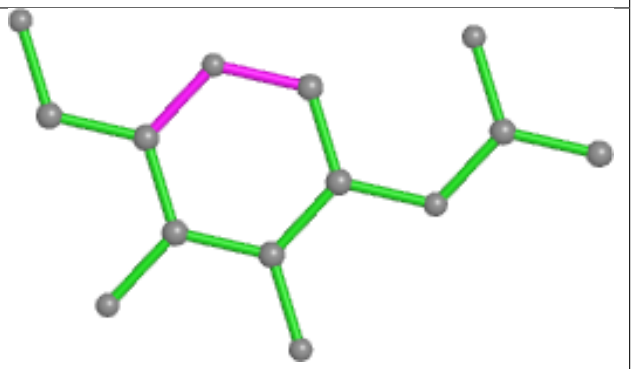


Rings

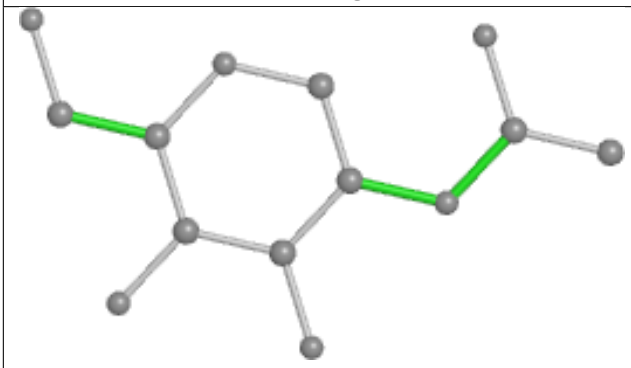
Ligand NAG C 1309



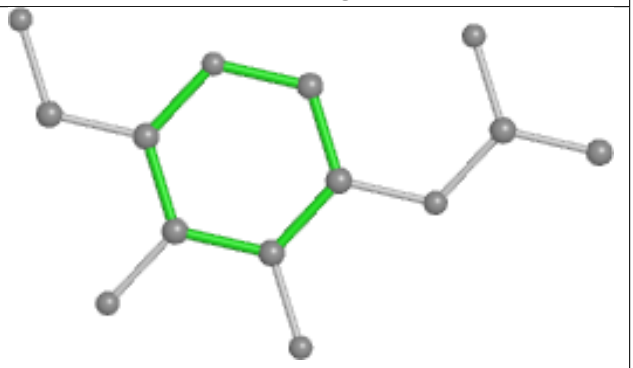
Bond lengths



Bond angles

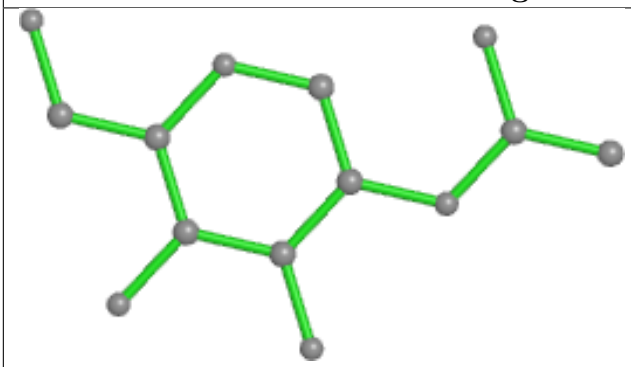


Torsions

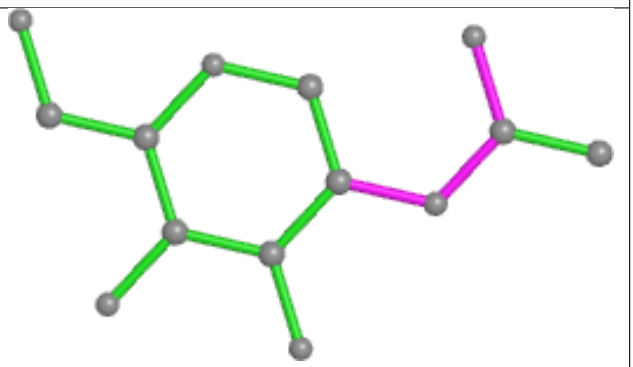


Rings

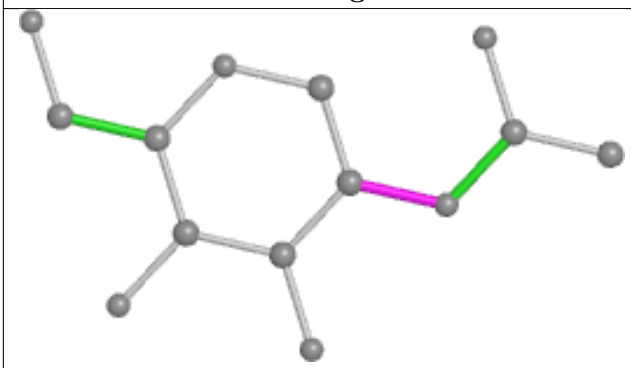
Ligand NAG C 1311



Bond lengths



Bond angles



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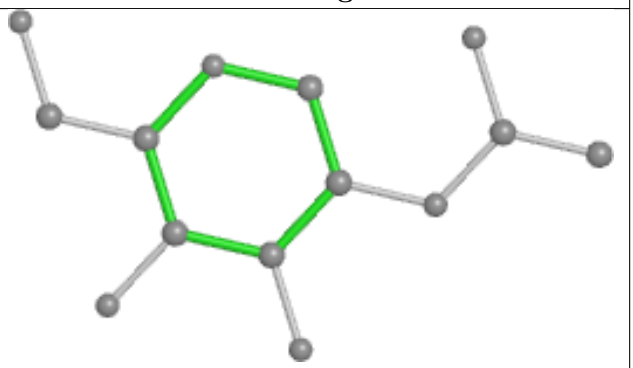
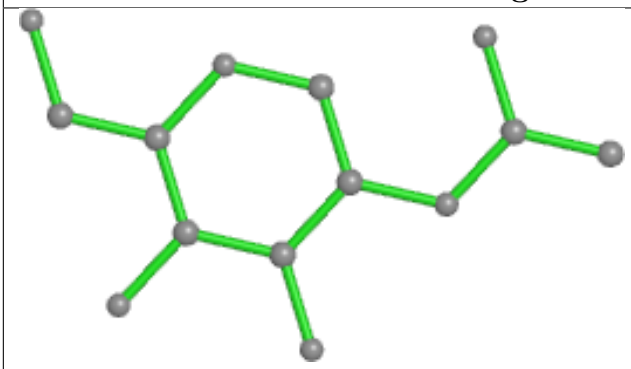
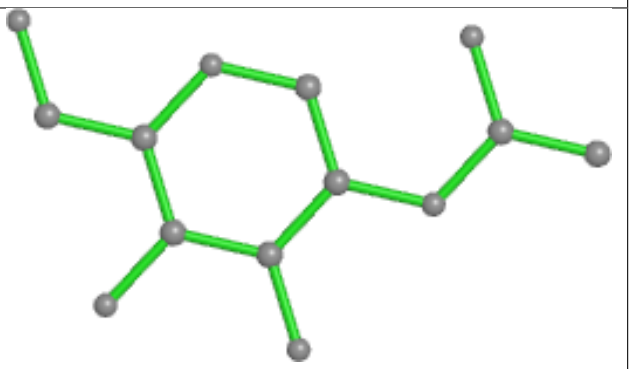
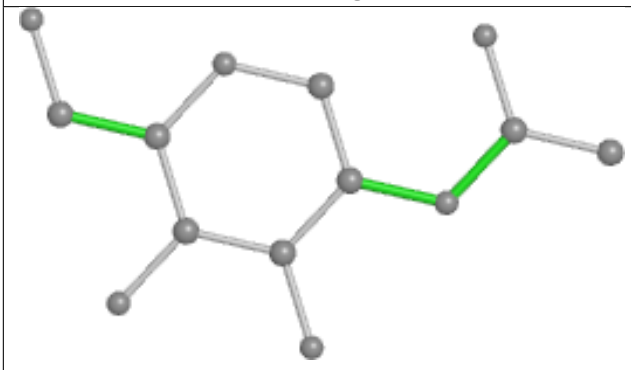
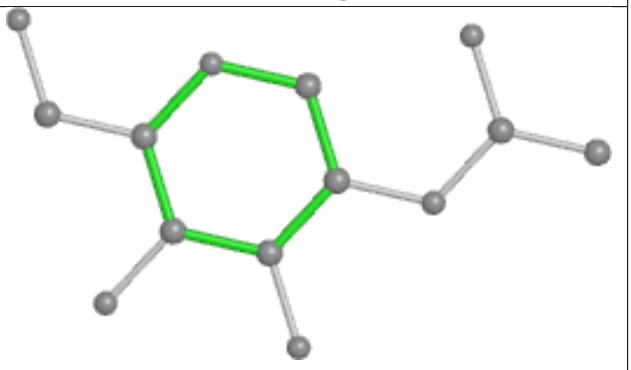
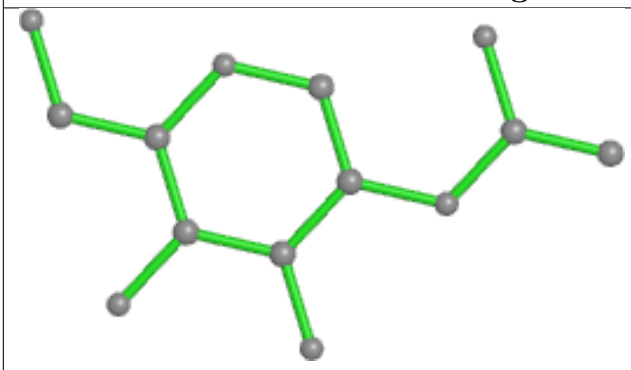
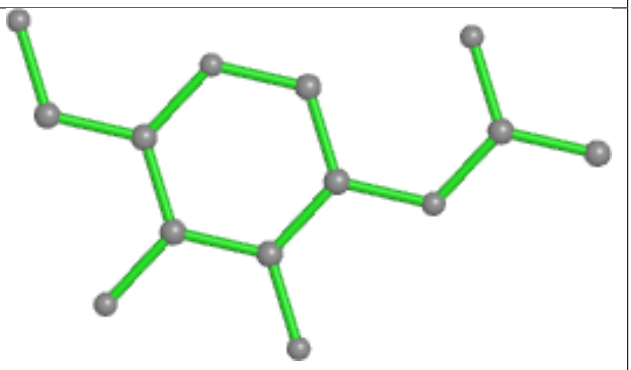
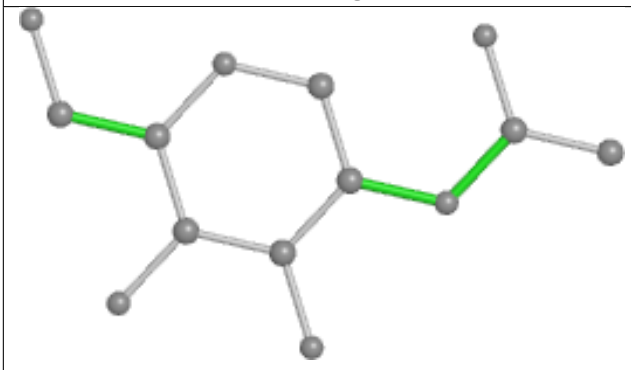
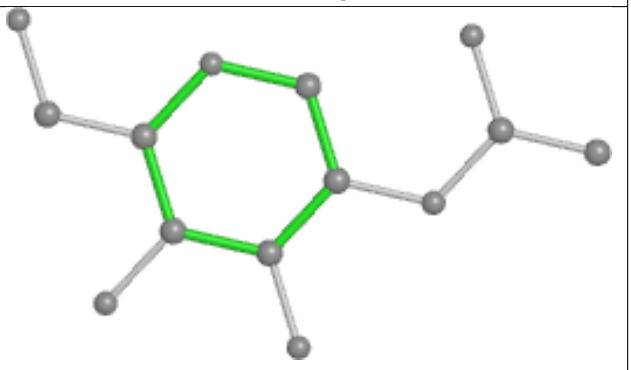
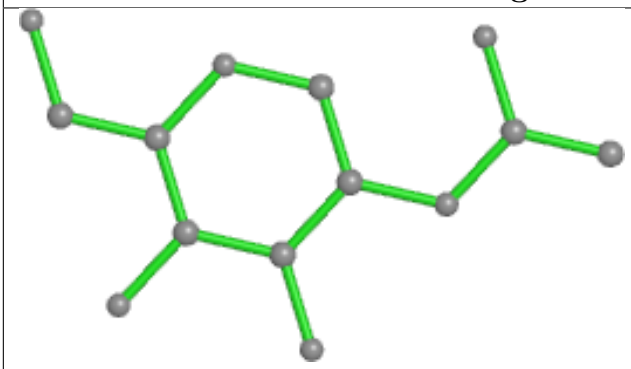
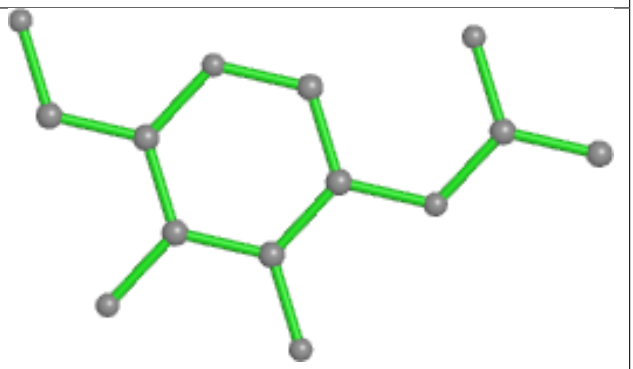
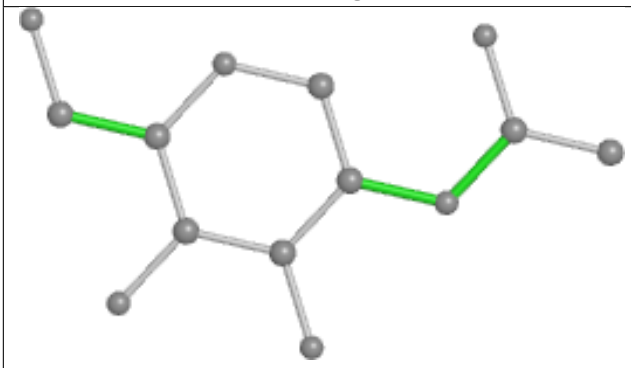
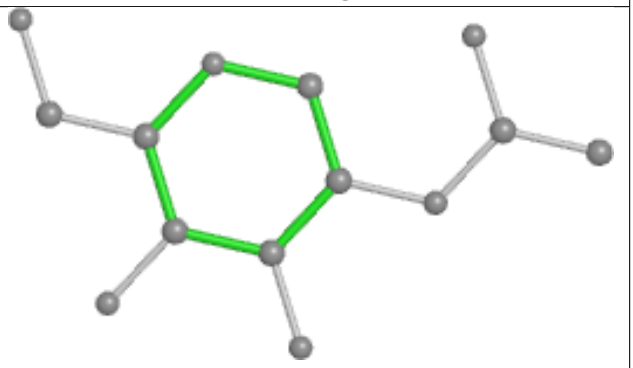
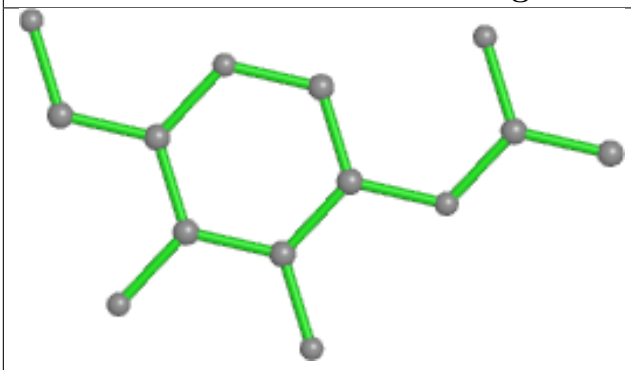
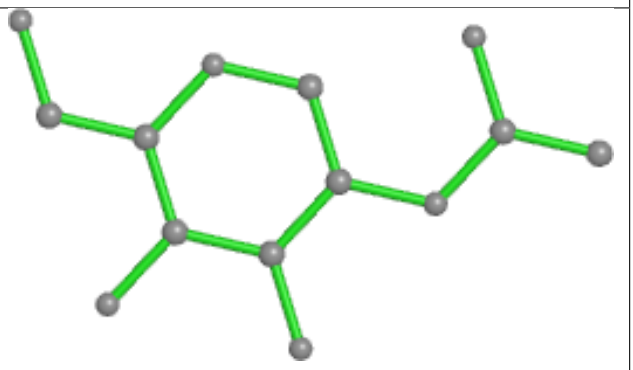
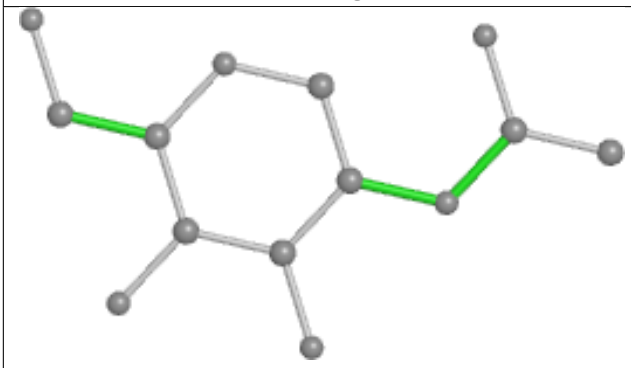
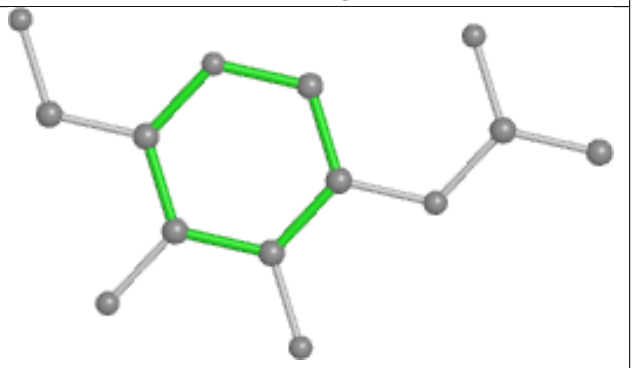


Rings

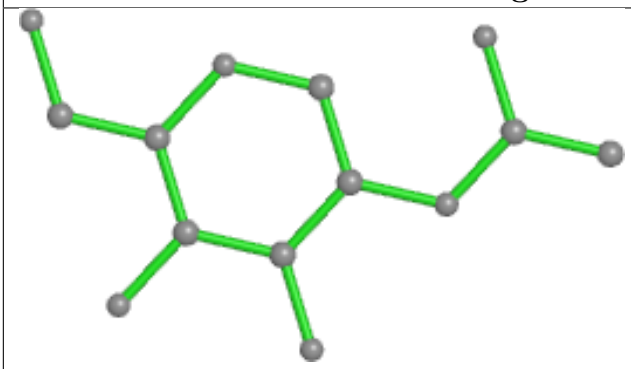
Ligand NAG C 1303	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG A 1303	
 Bond lengths	 Bond angles
 Torsions	 Rings

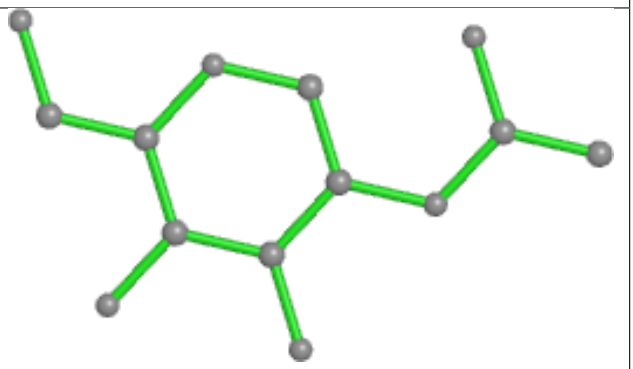
Ligand NAG A 1308	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand NAG B 1301	
	
Bond lengths	Bond angles
	
Torsions	Rings

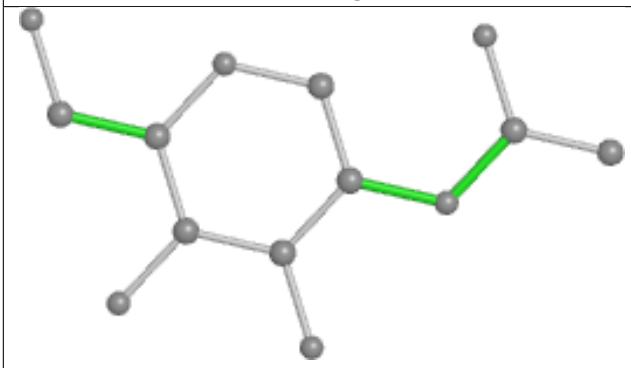
Ligand NAG C 1308



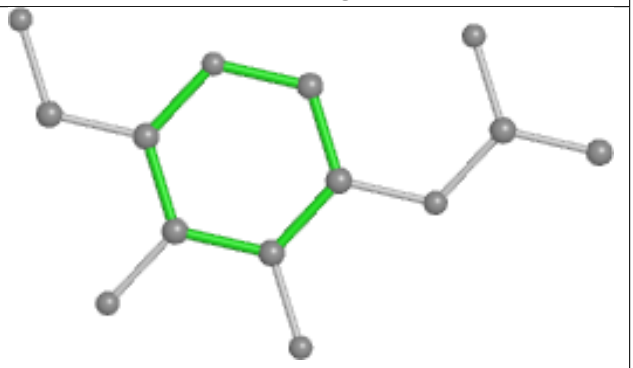
Bond lengths



Bond angles

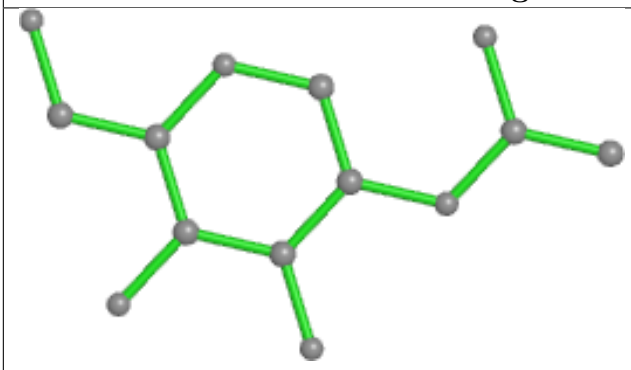


Torsions

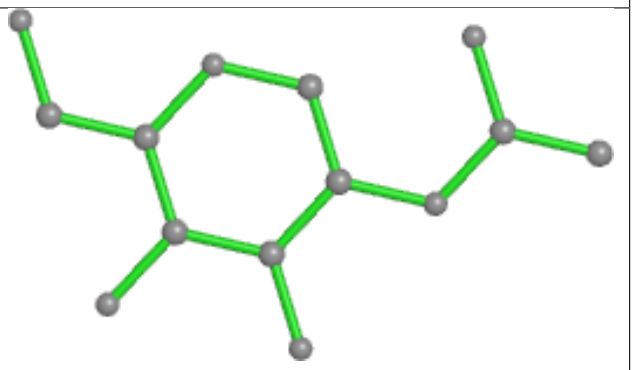


Rings

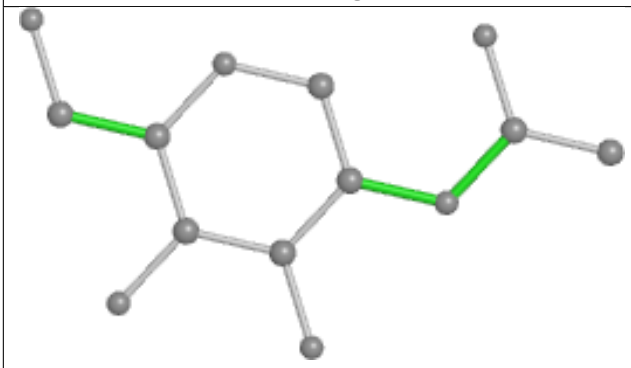
Ligand NAG C 1301



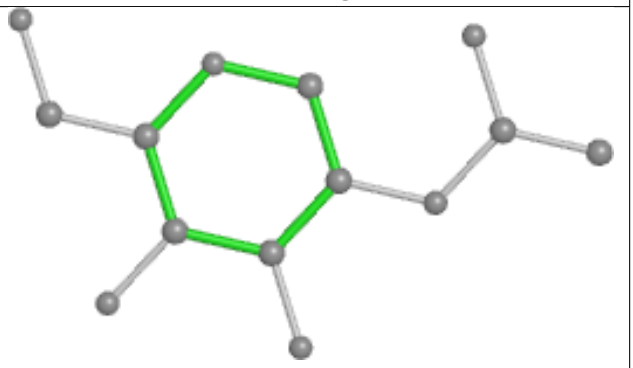
Bond lengths



Bond angles

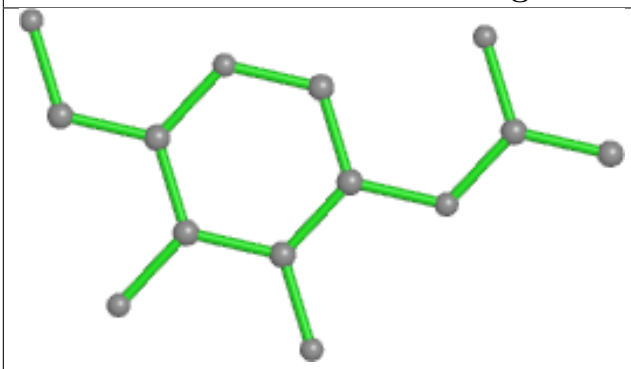


Torsions

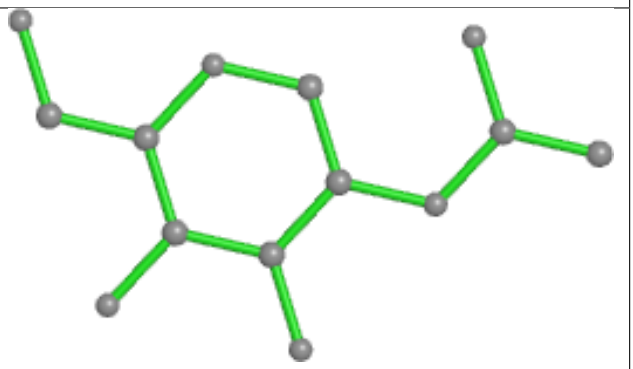


Rings

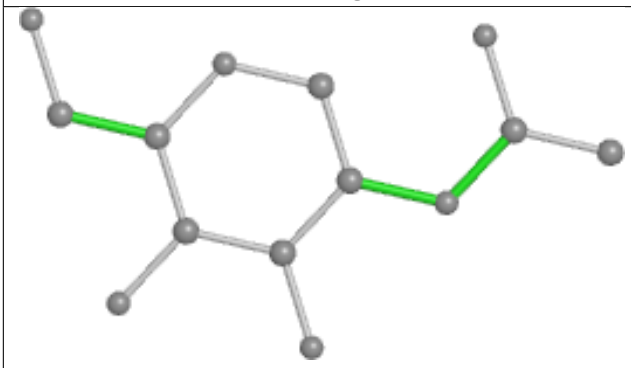
Ligand NAG C 1310



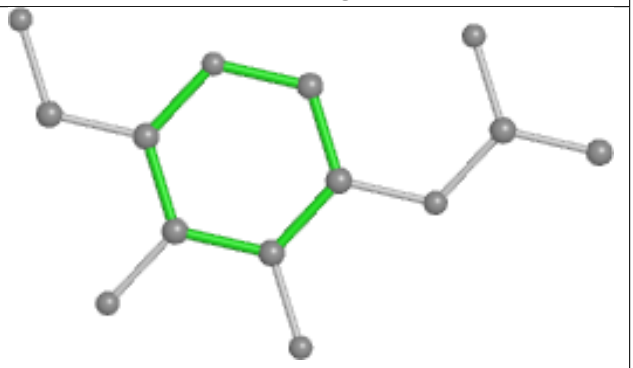
Bond lengths



Bond angles

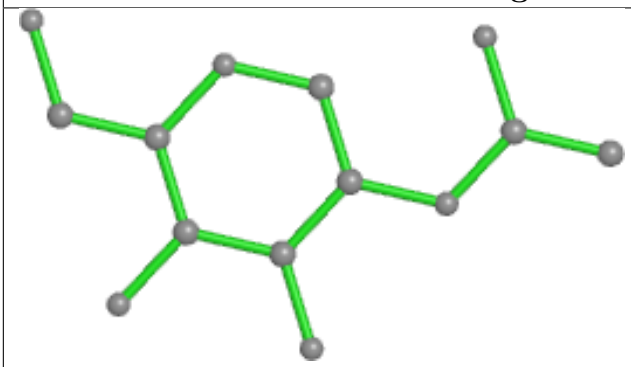


Torsions

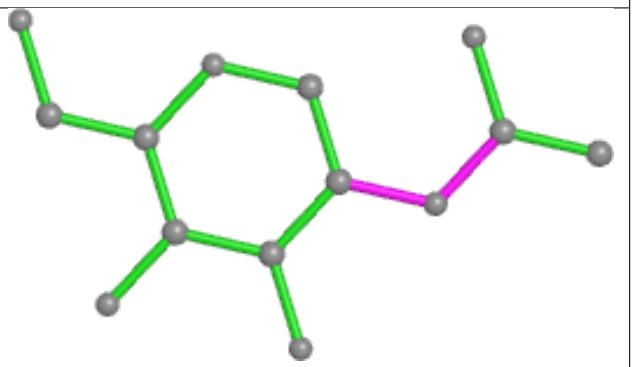


Rings

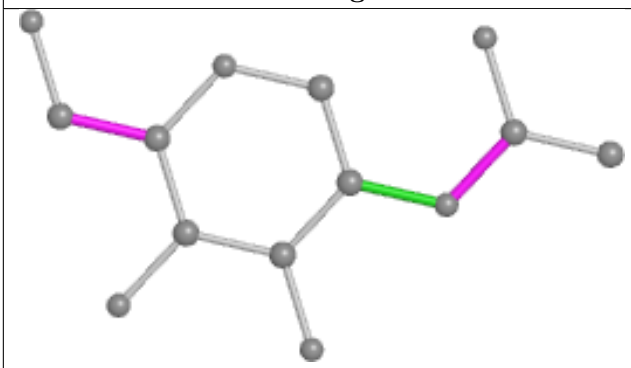
Ligand NAG A 1306



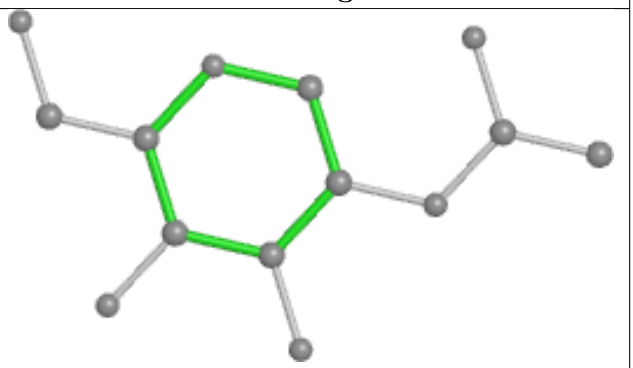
Bond lengths



Bond angles

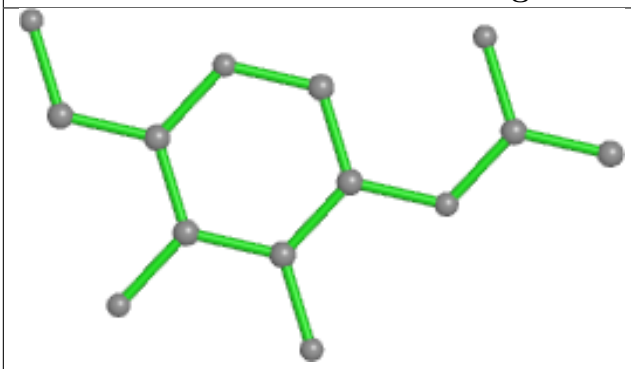


Torsions

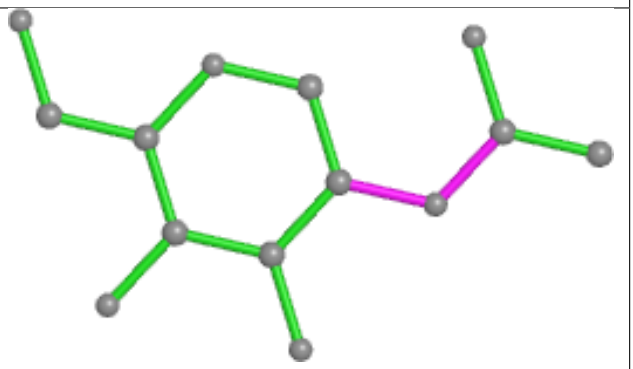


Rings

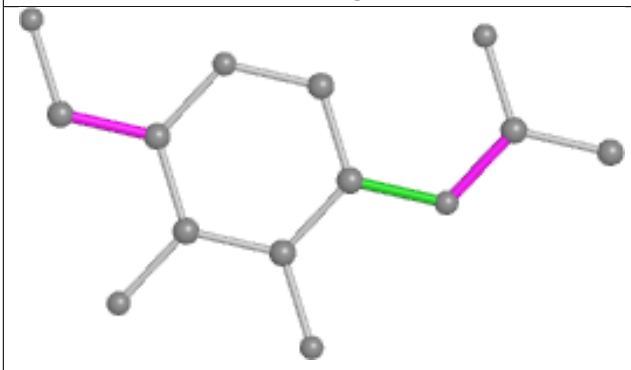
Ligand NAG B 1306



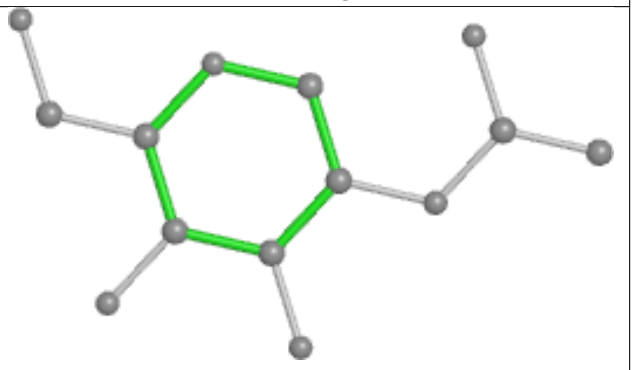
Bond lengths



Bond angles

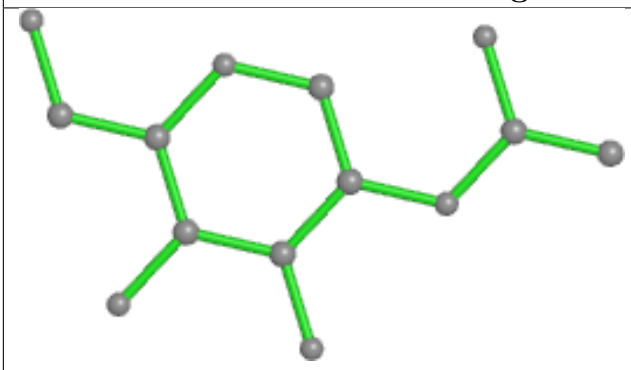


Torsions

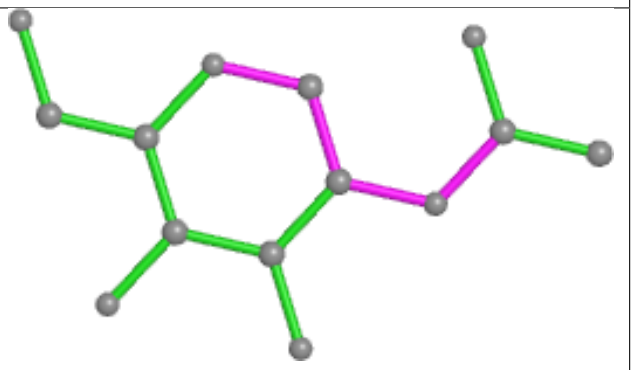


Rings

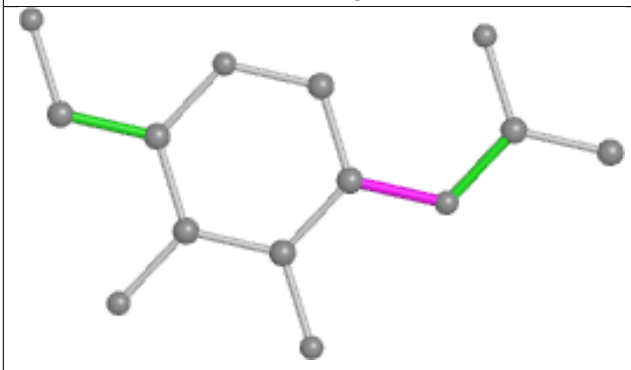
Ligand NAG A 1302



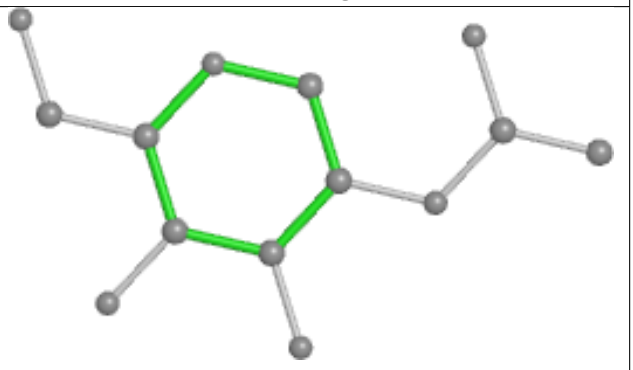
Bond lengths



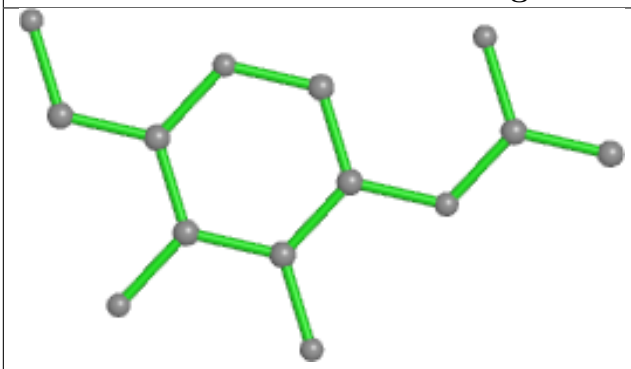
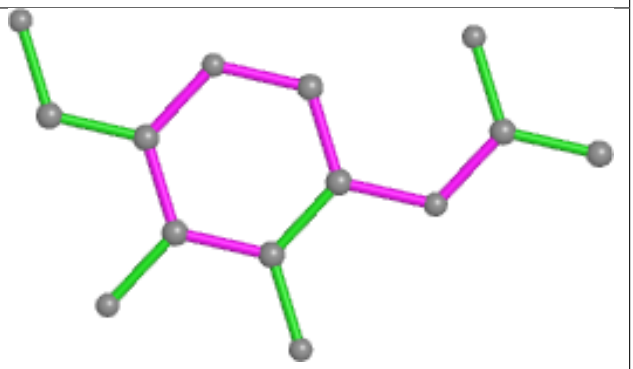
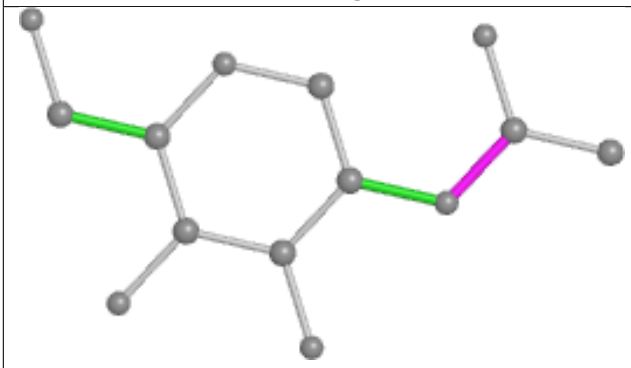
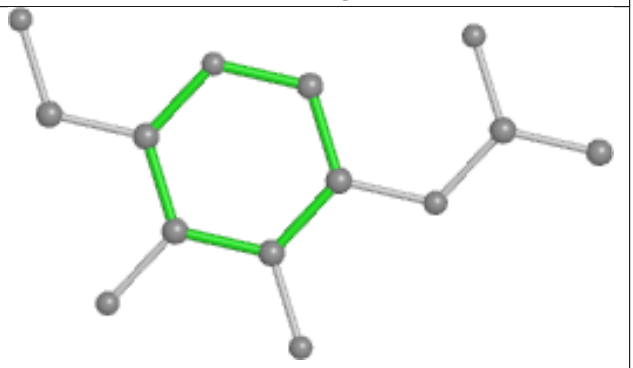
Bond angles

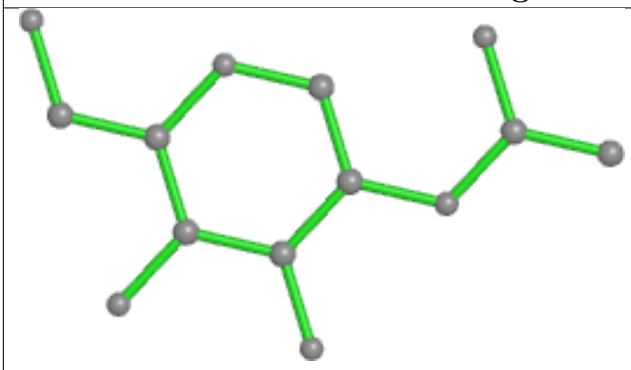
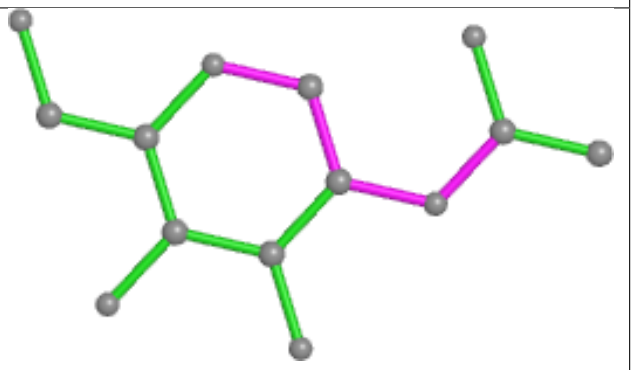
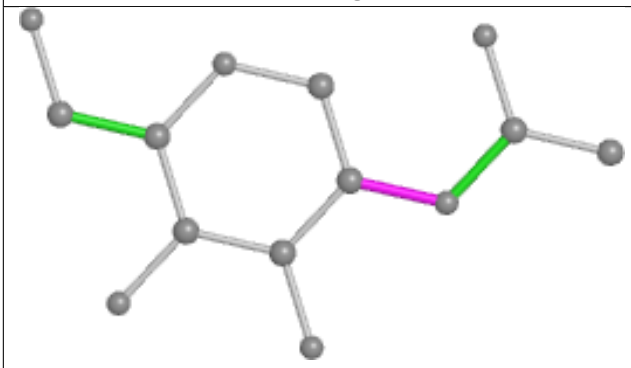
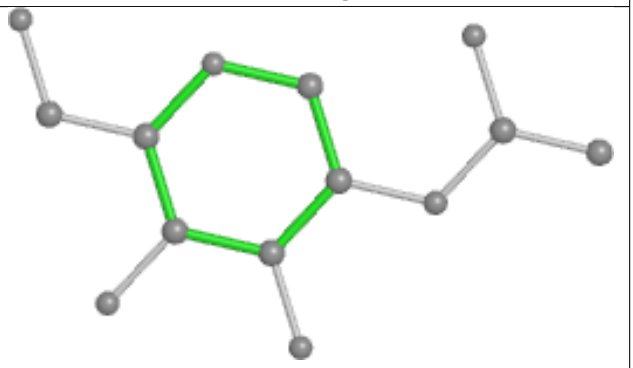


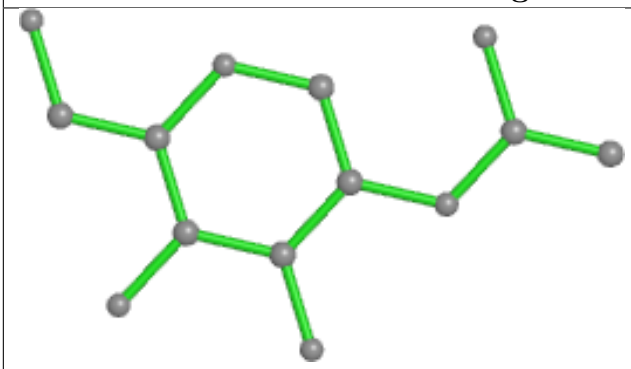
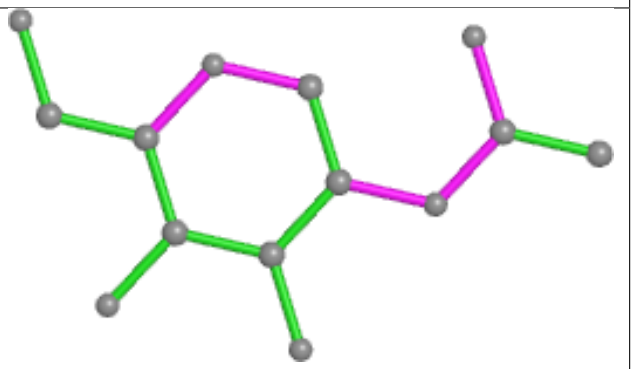
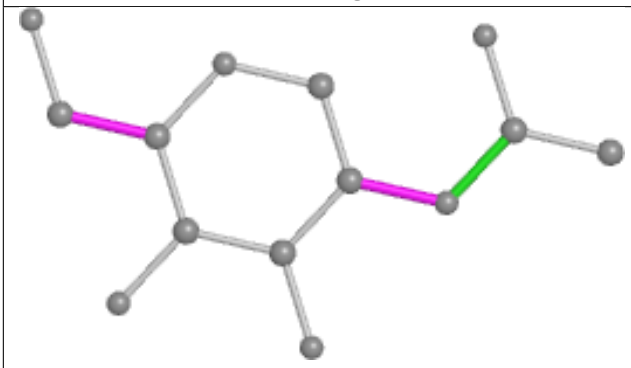
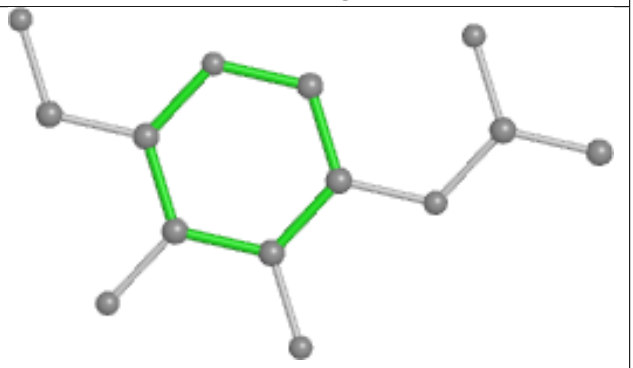
Torsions

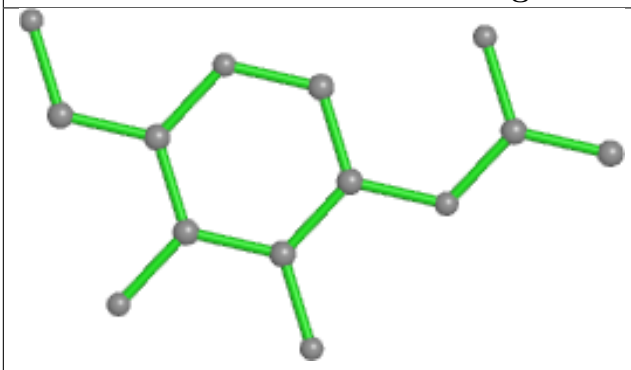
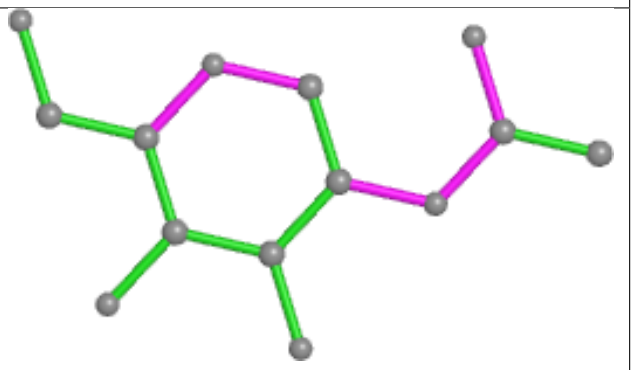
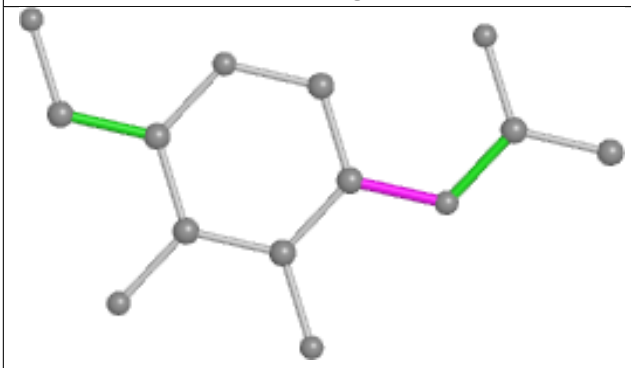
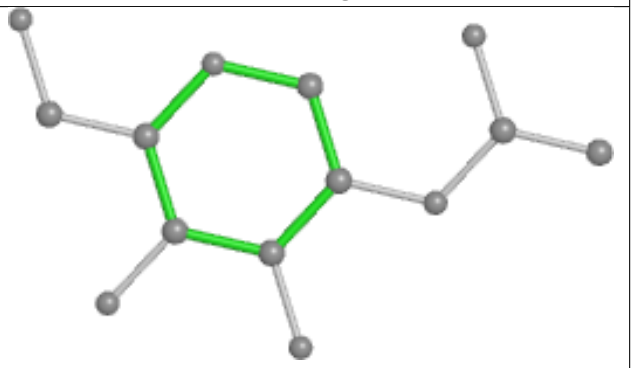


Rings

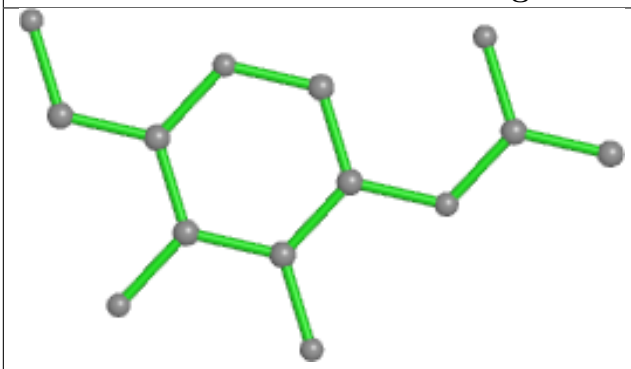
Ligand NAG A 1309	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG B 1302	
 Bond lengths	 Bond angles
 Torsions	 Rings

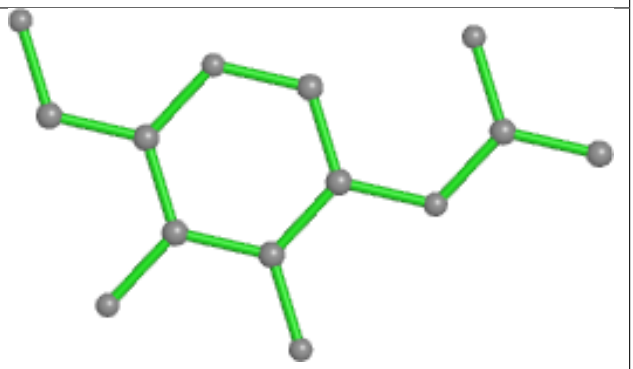
Ligand NAG C 1307	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG B 1311	
 Bond lengths	 Bond angles
 Torsions	 Rings

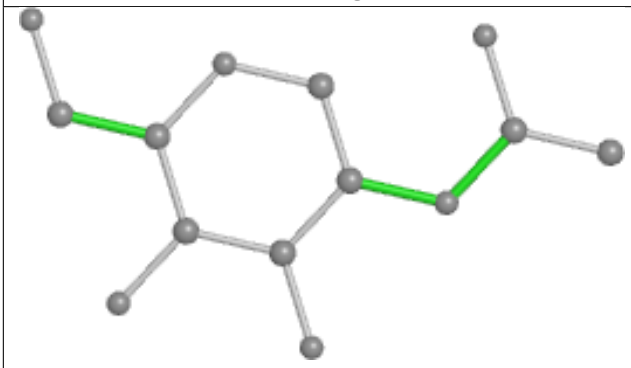
Ligand NAG B 1308



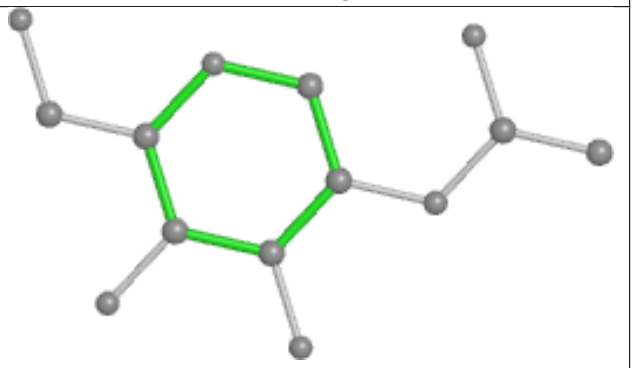
Bond lengths



Bond angles

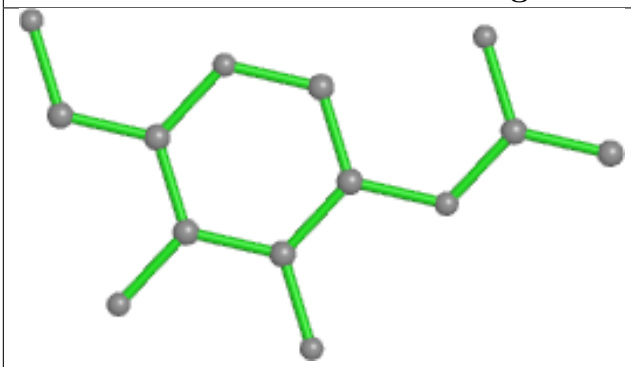


Torsions

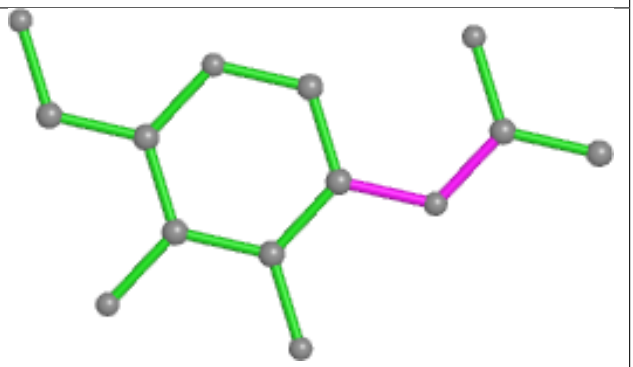


Rings

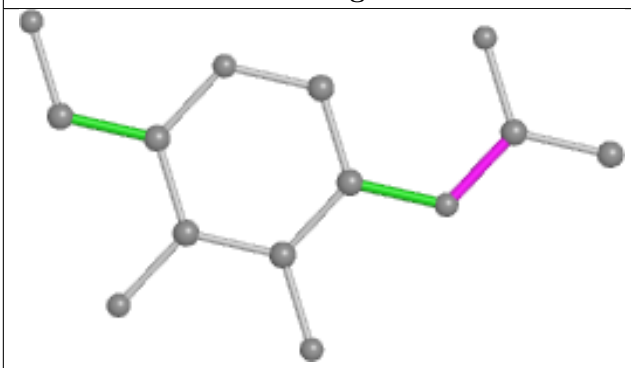
Ligand NAG A 1304



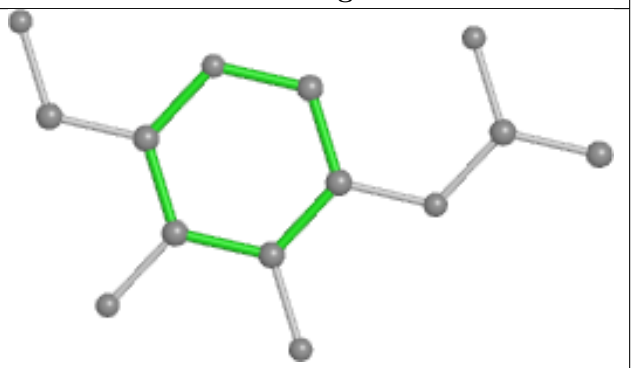
Bond lengths



Bond angles

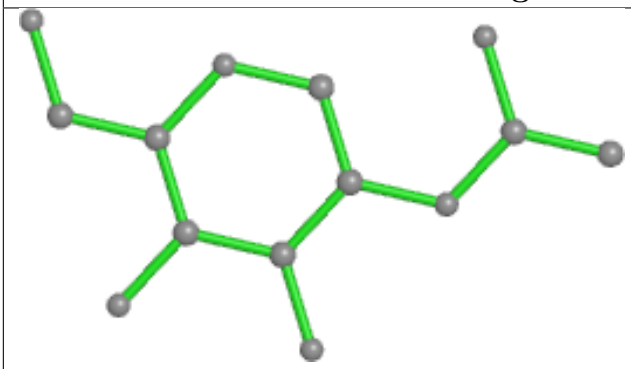


Torsions

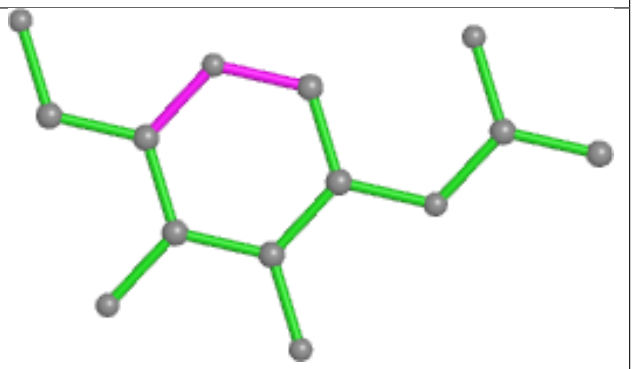


Rings

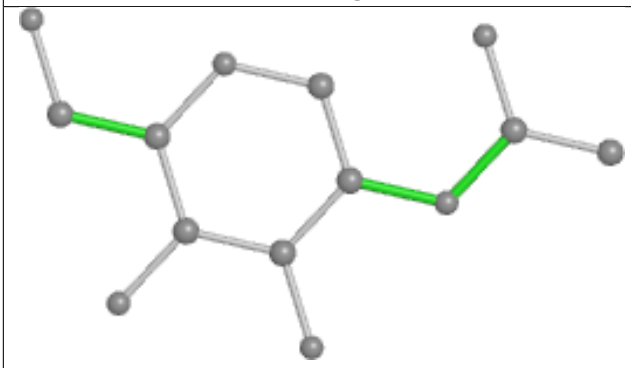
Ligand NAG B 1309



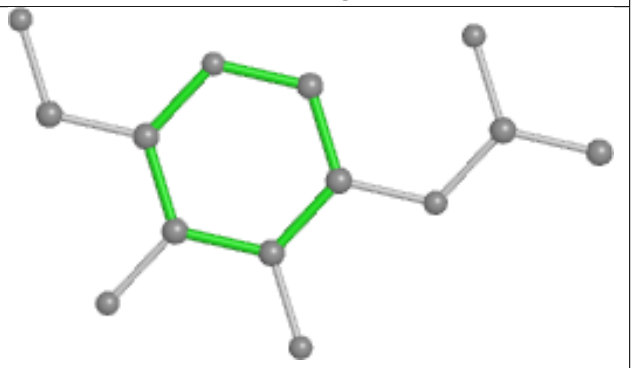
Bond lengths



Bond angles

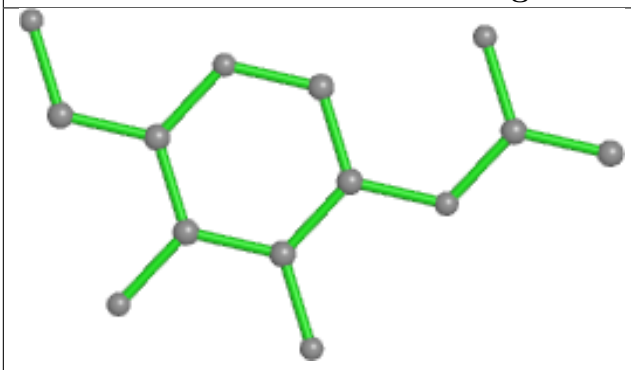


Torsions

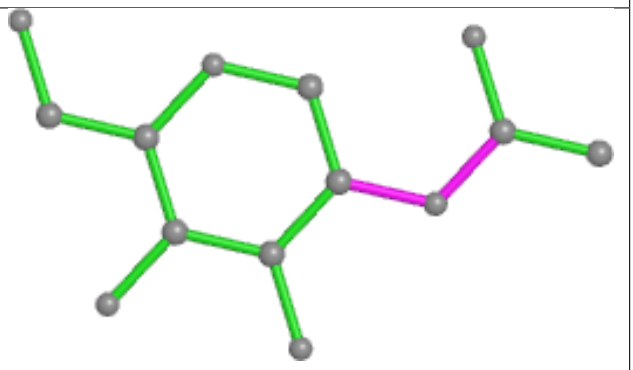


Rings

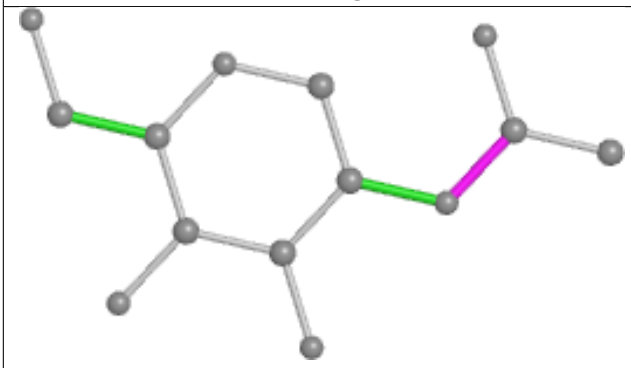
Ligand NAG C 1304



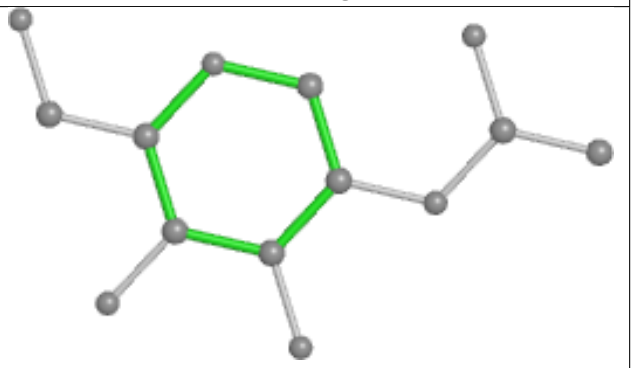
Bond lengths



Bond angles

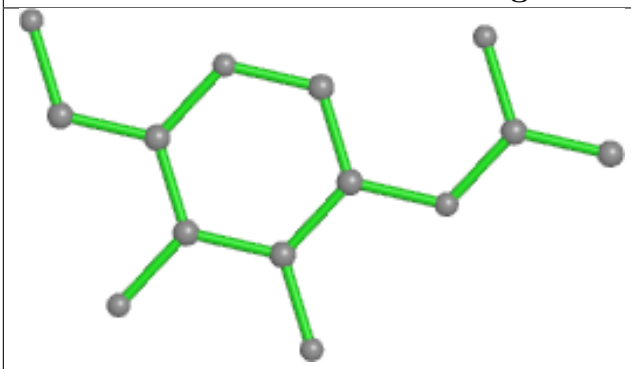


Torsions

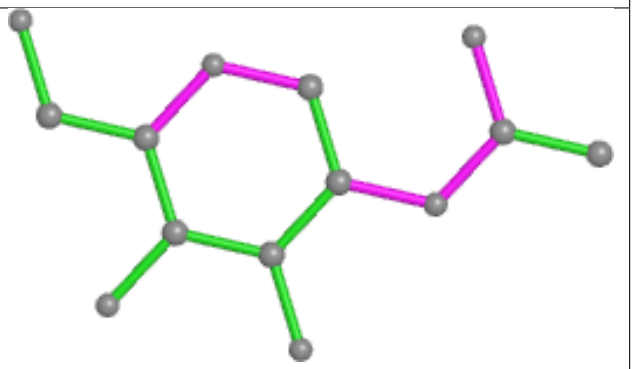


Rings

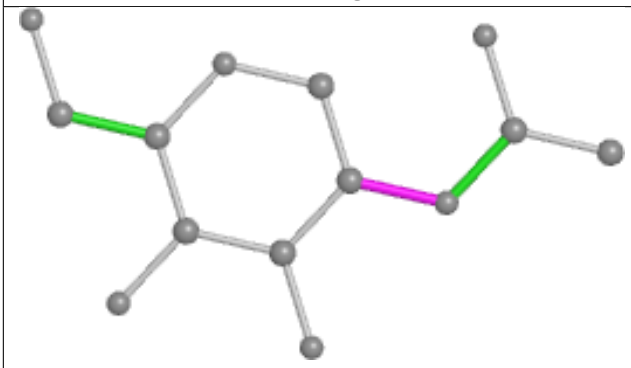
Ligand NAG A 1311



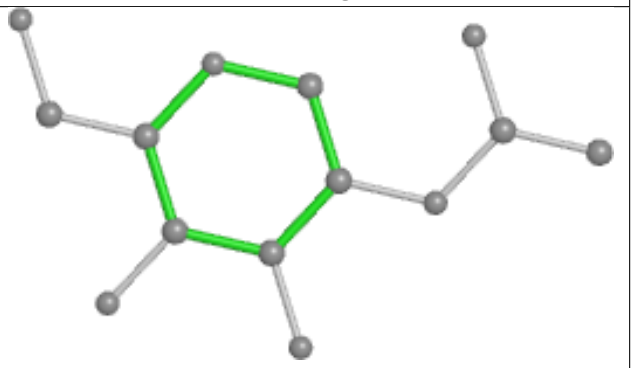
Bond lengths



Bond angles

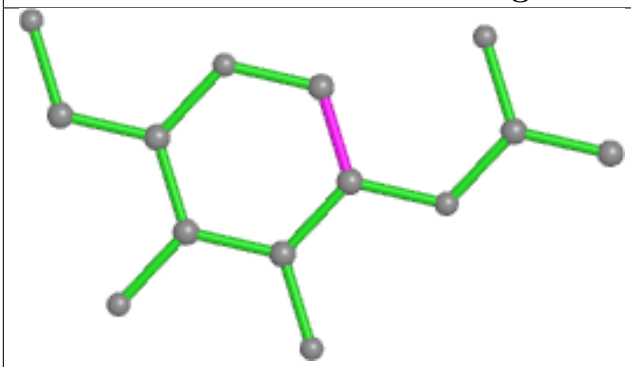


Torsions

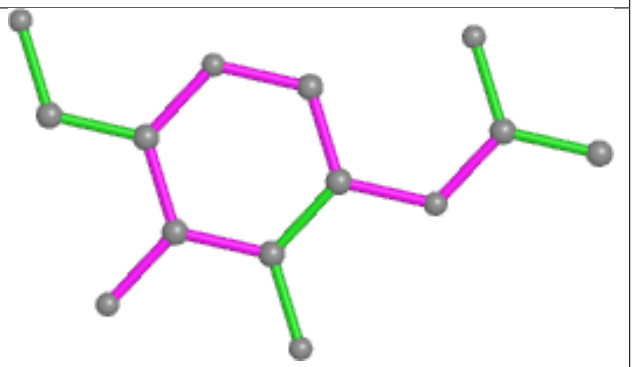


Rings

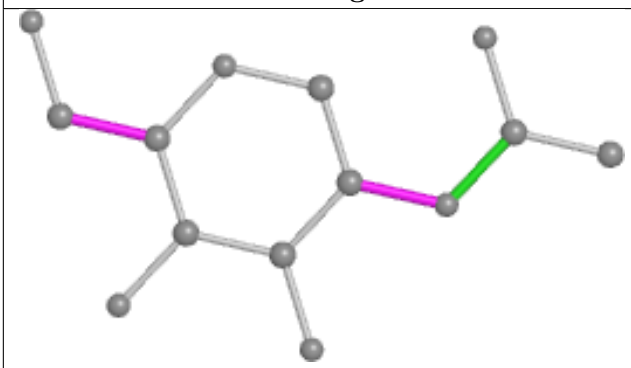
Ligand NAG B 1305



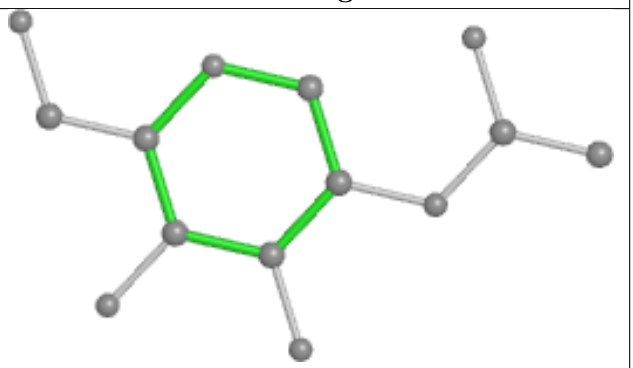
Bond lengths



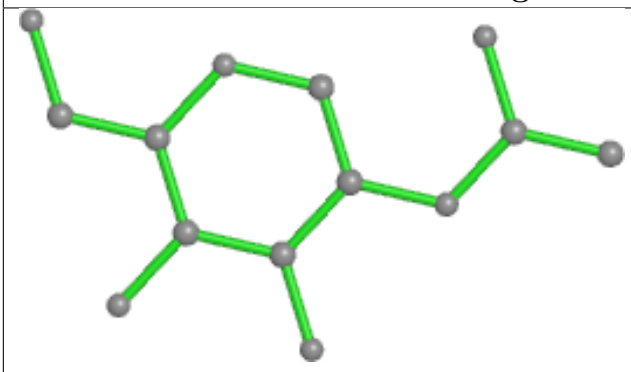
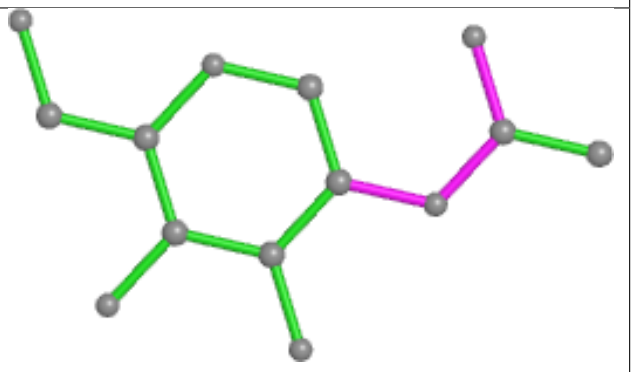
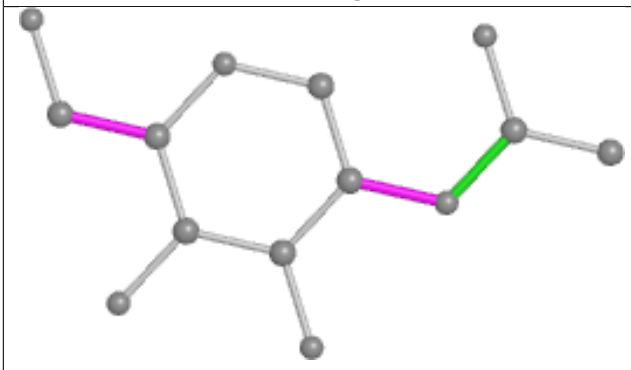
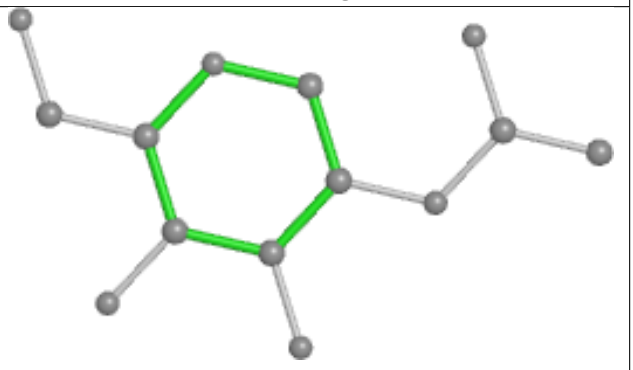
Bond angles

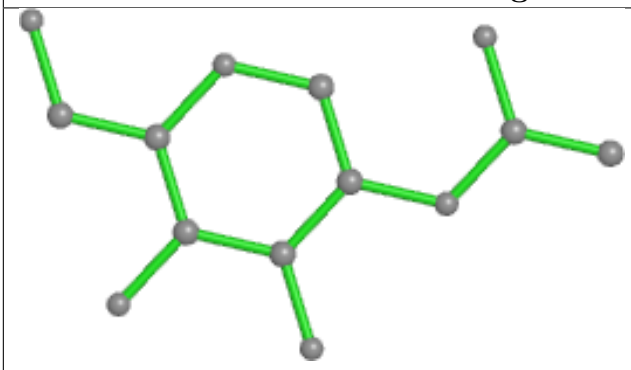
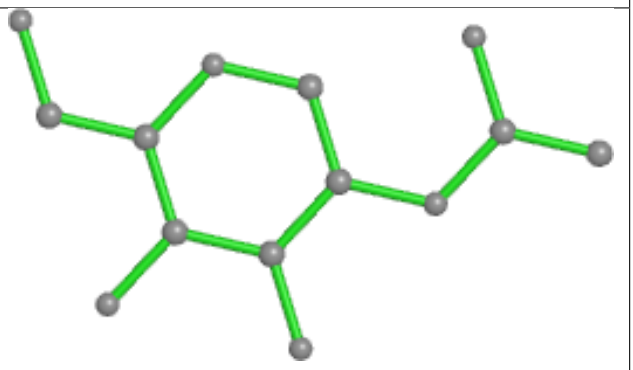
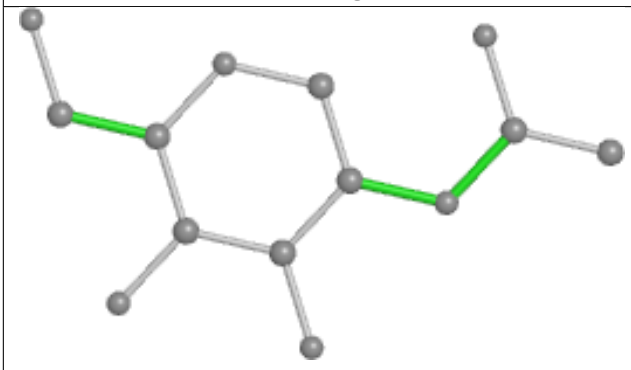
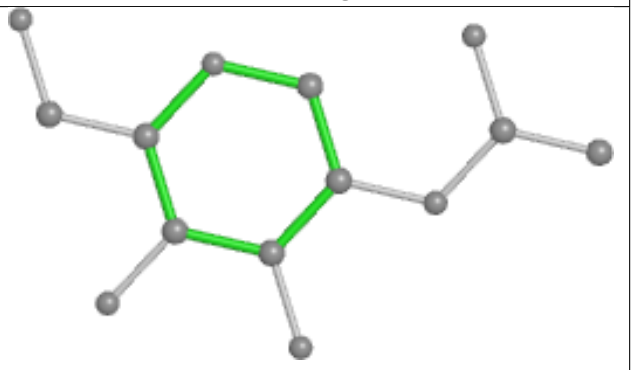


Torsions

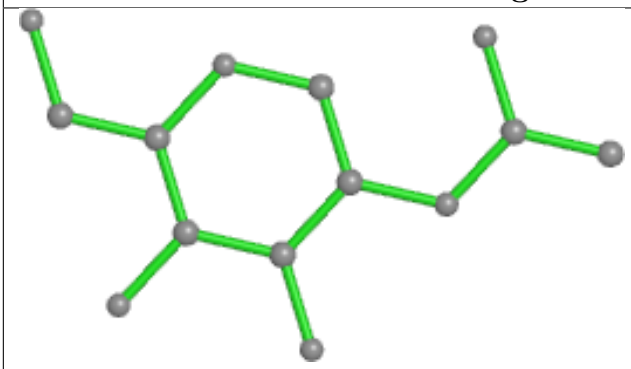


Rings

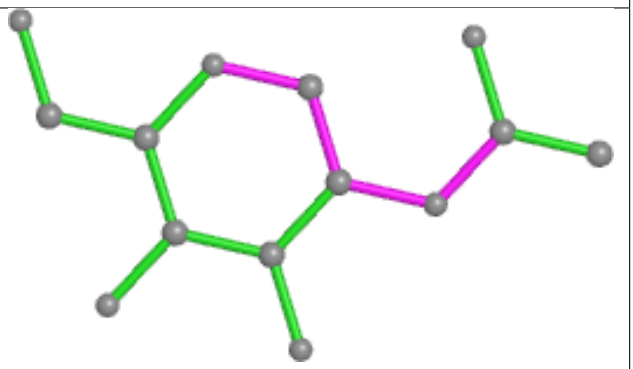
Ligand NAG B 1307	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG A 1310	
 Bond lengths	 Bond angles
 Torsions	 Rings

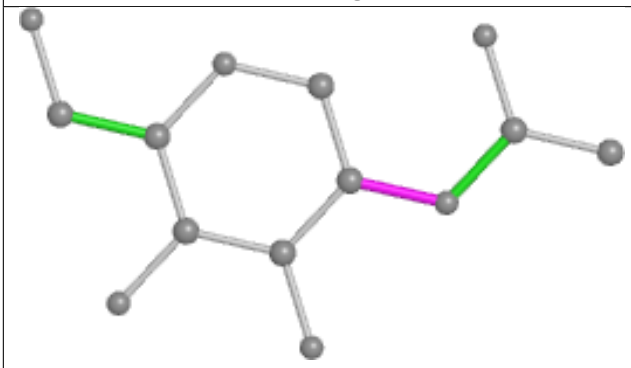
Ligand NAG C 1302



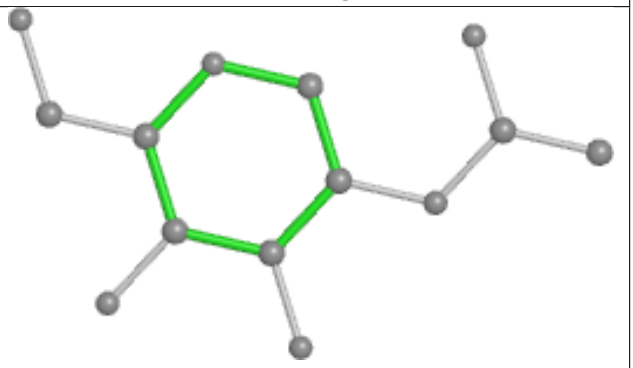
Bond lengths



Bond angles

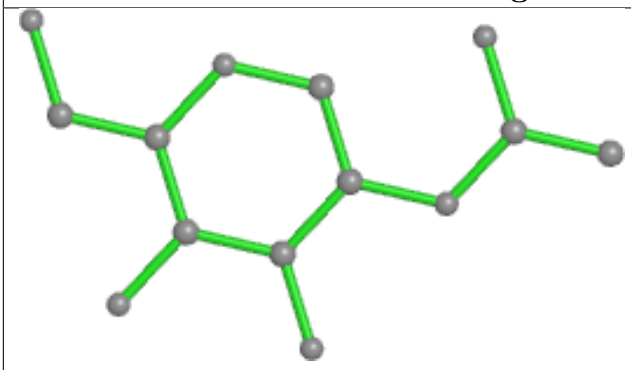


Torsions

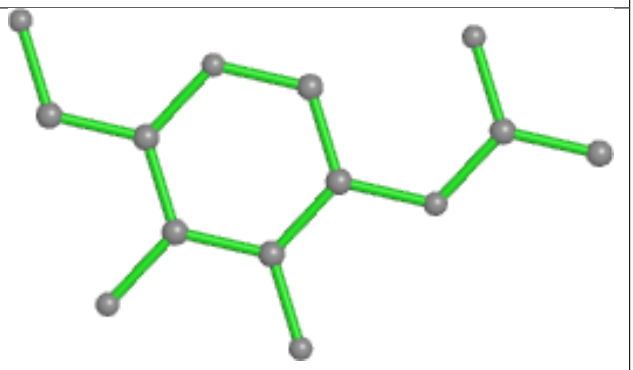


Rings

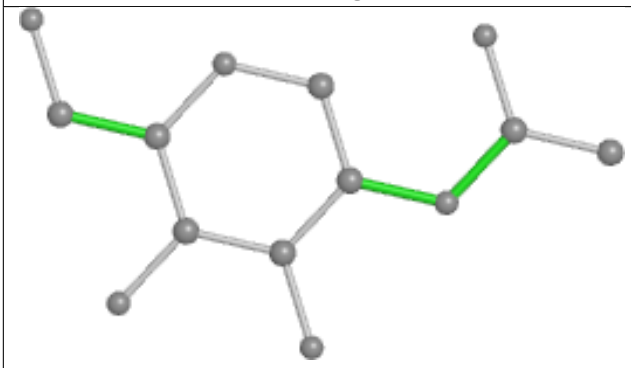
Ligand NAG A 1305



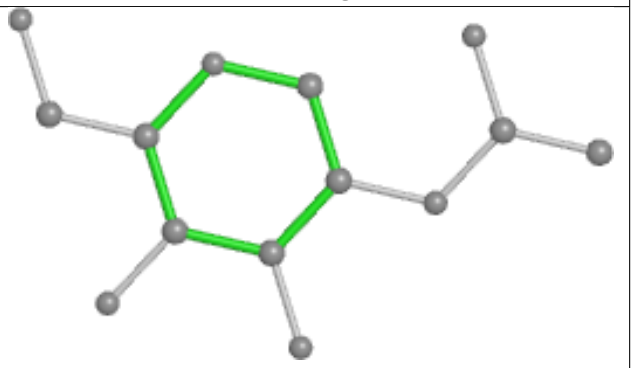
Bond lengths



Bond angles



Torsions



Rings

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.