wwPDB EM Validation Summary Report

Feb 19, 2025 – 08:16 PM JST

PDB ID	:	8ZY1
EMDB ID	:	EMD-60552
Title	:	Sarbecovirus BM48-31 Spike Trimer in a Locked Conformation
Authors	:	Wang, J.; Xiong, X.
Deposited on	:	2024-06-16
Resolution	:	3.10 Å(reported)

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

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

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

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

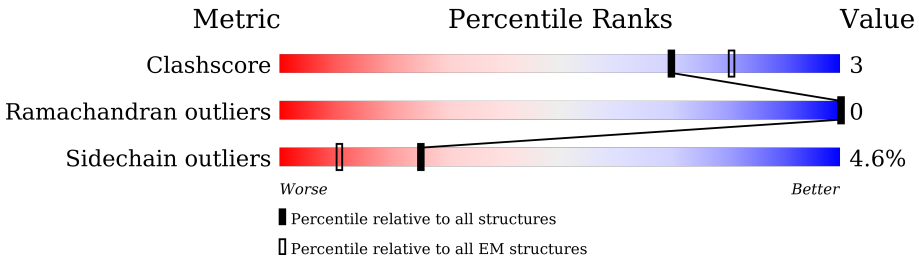
EMDB validation analysis	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.2

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 3.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
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	1273	75% 9% 15%
1	B	1273	74% 10% • 15%
1	C	1273	75% 9% 15%
2	D	2	50% 50%
2	F	2	100%
2	G	2	50% 50%
2	I	2	100%
2	J	2	100%
2	L	2	100%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	E	4	
3	H	4	
3	K	4	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 26025 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	1076	Total	C	N	O	S	0	0
			8367	5331	1393	1597	46		
1	B	1076	Total	C	N	O	S	0	0
			8367	5331	1393	1597	46		
1	C	1076	Total	C	N	O	S	0	0
			8367	5331	1393	1597	46		

There are 237 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1195	GLY	-	expression tag	UNP E0XIZ3
A	1196	SER	-	expression tag	UNP E0XIZ3
A	1197	GLY	-	expression tag	UNP E0XIZ3
A	1198	TYR	-	expression tag	UNP E0XIZ3
A	1199	ILE	-	expression tag	UNP E0XIZ3
A	1200	PRO	-	expression tag	UNP E0XIZ3
A	1201	GLU	-	expression tag	UNP E0XIZ3
A	1202	ALA	-	expression tag	UNP E0XIZ3
A	1203	PRO	-	expression tag	UNP E0XIZ3
A	1204	ARG	-	expression tag	UNP E0XIZ3
A	1205	ASP	-	expression tag	UNP E0XIZ3
A	1206	GLY	-	expression tag	UNP E0XIZ3
A	1207	GLN	-	expression tag	UNP E0XIZ3
A	1208	ALA	-	expression tag	UNP E0XIZ3
A	1209	TYR	-	expression tag	UNP E0XIZ3
A	1210	VAL	-	expression tag	UNP E0XIZ3
A	1211	ARG	-	expression tag	UNP E0XIZ3
A	1212	LYS	-	expression tag	UNP E0XIZ3
A	1213	ASP	-	expression tag	UNP E0XIZ3
A	1214	GLY	-	expression tag	UNP E0XIZ3
A	1215	GLU	-	expression tag	UNP E0XIZ3
A	1216	TRP	-	expression tag	UNP E0XIZ3
A	1217	VAL	-	expression tag	UNP E0XIZ3
A	1218	LEU	-	expression tag	UNP E0XIZ3

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	1219	LEU	-	expression tag	UNP E0XIZ3
A	1220	SER	-	expression tag	UNP E0XIZ3
A	1221	THR	-	expression tag	UNP E0XIZ3
A	1222	PHE	-	expression tag	UNP E0XIZ3
A	1223	LEU	-	expression tag	UNP E0XIZ3
A	1224	LEU	-	expression tag	UNP E0XIZ3
A	1225	GLU	-	expression tag	UNP E0XIZ3
A	1226	VAL	-	expression tag	UNP E0XIZ3
A	1227	LEU	-	expression tag	UNP E0XIZ3
A	1228	PHE	-	expression tag	UNP E0XIZ3
A	1229	GLN	-	expression tag	UNP E0XIZ3
A	1230	GLY	-	expression tag	UNP E0XIZ3
A	1231	PRO	-	expression tag	UNP E0XIZ3
A	1232	GLY	-	expression tag	UNP E0XIZ3
A	1233	HIS	-	expression tag	UNP E0XIZ3
A	1234	HIS	-	expression tag	UNP E0XIZ3
A	1235	HIS	-	expression tag	UNP E0XIZ3
A	1236	HIS	-	expression tag	UNP E0XIZ3
A	1237	HIS	-	expression tag	UNP E0XIZ3
A	1238	HIS	-	expression tag	UNP E0XIZ3
A	1239	HIS	-	expression tag	UNP E0XIZ3
A	1240	HIS	-	expression tag	UNP E0XIZ3
A	1241	SER	-	expression tag	UNP E0XIZ3
A	1242	ALA	-	expression tag	UNP E0XIZ3
A	1243	TRP	-	expression tag	UNP E0XIZ3
A	1244	SER	-	expression tag	UNP E0XIZ3
A	1245	HIS	-	expression tag	UNP E0XIZ3
A	1246	PRO	-	expression tag	UNP E0XIZ3
A	1247	GLN	-	expression tag	UNP E0XIZ3
A	1248	PHE	-	expression tag	UNP E0XIZ3
A	1249	GLU	-	expression tag	UNP E0XIZ3
A	1250	LYS	-	expression tag	UNP E0XIZ3
A	1251	GLY	-	expression tag	UNP E0XIZ3
A	1252	GLY	-	expression tag	UNP E0XIZ3
A	1253	GLY	-	expression tag	UNP E0XIZ3
A	1254	SER	-	expression tag	UNP E0XIZ3
A	1255	GLY	-	expression tag	UNP E0XIZ3
A	1256	GLY	-	expression tag	UNP E0XIZ3
A	1257	GLY	-	expression tag	UNP E0XIZ3
A	1258	GLY	-	expression tag	UNP E0XIZ3
A	1259	SER	-	expression tag	UNP E0XIZ3
A	1260	GLY	-	expression tag	UNP E0XIZ3

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	1261	GLY	-	expression tag	UNP E0XIZ3
A	1262	SER	-	expression tag	UNP E0XIZ3
A	1263	ALA	-	expression tag	UNP E0XIZ3
A	1264	TRP	-	expression tag	UNP E0XIZ3
A	1265	SER	-	expression tag	UNP E0XIZ3
A	1266	HIS	-	expression tag	UNP E0XIZ3
A	1267	PRO	-	expression tag	UNP E0XIZ3
A	1268	GLN	-	expression tag	UNP E0XIZ3
A	1269	PHE	-	expression tag	UNP E0XIZ3
A	1270	GLU	-	expression tag	UNP E0XIZ3
A	1271	LYS	-	expression tag	UNP E0XIZ3
A	1272	SER	-	expression tag	UNP E0XIZ3
A	1273	ALA	-	expression tag	UNP E0XIZ3
B	1195	GLY	-	expression tag	UNP E0XIZ3
B	1196	SER	-	expression tag	UNP E0XIZ3
B	1197	GLY	-	expression tag	UNP E0XIZ3
B	1198	TYR	-	expression tag	UNP E0XIZ3
B	1199	ILE	-	expression tag	UNP E0XIZ3
B	1200	PRO	-	expression tag	UNP E0XIZ3
B	1201	GLU	-	expression tag	UNP E0XIZ3
B	1202	ALA	-	expression tag	UNP E0XIZ3
B	1203	PRO	-	expression tag	UNP E0XIZ3
B	1204	ARG	-	expression tag	UNP E0XIZ3
B	1205	ASP	-	expression tag	UNP E0XIZ3
B	1206	GLY	-	expression tag	UNP E0XIZ3
B	1207	GLN	-	expression tag	UNP E0XIZ3
B	1208	ALA	-	expression tag	UNP E0XIZ3
B	1209	TYR	-	expression tag	UNP E0XIZ3
B	1210	VAL	-	expression tag	UNP E0XIZ3
B	1211	ARG	-	expression tag	UNP E0XIZ3
B	1212	LYS	-	expression tag	UNP E0XIZ3
B	1213	ASP	-	expression tag	UNP E0XIZ3
B	1214	GLY	-	expression tag	UNP E0XIZ3
B	1215	GLU	-	expression tag	UNP E0XIZ3
B	1216	TRP	-	expression tag	UNP E0XIZ3
B	1217	VAL	-	expression tag	UNP E0XIZ3
B	1218	LEU	-	expression tag	UNP E0XIZ3
B	1219	LEU	-	expression tag	UNP E0XIZ3
B	1220	SER	-	expression tag	UNP E0XIZ3
B	1221	THR	-	expression tag	UNP E0XIZ3
B	1222	PHE	-	expression tag	UNP E0XIZ3
B	1223	LEU	-	expression tag	UNP E0XIZ3

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	1224	LEU	-	expression tag	UNP E0XIZ3
B	1225	GLU	-	expression tag	UNP E0XIZ3
B	1226	VAL	-	expression tag	UNP E0XIZ3
B	1227	LEU	-	expression tag	UNP E0XIZ3
B	1228	PHE	-	expression tag	UNP E0XIZ3
B	1229	GLN	-	expression tag	UNP E0XIZ3
B	1230	GLY	-	expression tag	UNP E0XIZ3
B	1231	PRO	-	expression tag	UNP E0XIZ3
B	1232	GLY	-	expression tag	UNP E0XIZ3
B	1233	HIS	-	expression tag	UNP E0XIZ3
B	1234	HIS	-	expression tag	UNP E0XIZ3
B	1235	HIS	-	expression tag	UNP E0XIZ3
B	1236	HIS	-	expression tag	UNP E0XIZ3
B	1237	HIS	-	expression tag	UNP E0XIZ3
B	1238	HIS	-	expression tag	UNP E0XIZ3
B	1239	HIS	-	expression tag	UNP E0XIZ3
B	1240	HIS	-	expression tag	UNP E0XIZ3
B	1241	SER	-	expression tag	UNP E0XIZ3
B	1242	ALA	-	expression tag	UNP E0XIZ3
B	1243	TRP	-	expression tag	UNP E0XIZ3
B	1244	SER	-	expression tag	UNP E0XIZ3
B	1245	HIS	-	expression tag	UNP E0XIZ3
B	1246	PRO	-	expression tag	UNP E0XIZ3
B	1247	GLN	-	expression tag	UNP E0XIZ3
B	1248	PHE	-	expression tag	UNP E0XIZ3
B	1249	GLU	-	expression tag	UNP E0XIZ3
B	1250	LYS	-	expression tag	UNP E0XIZ3
B	1251	GLY	-	expression tag	UNP E0XIZ3
B	1252	GLY	-	expression tag	UNP E0XIZ3
B	1253	GLY	-	expression tag	UNP E0XIZ3
B	1254	SER	-	expression tag	UNP E0XIZ3
B	1255	GLY	-	expression tag	UNP E0XIZ3
B	1256	GLY	-	expression tag	UNP E0XIZ3
B	1257	GLY	-	expression tag	UNP E0XIZ3
B	1258	GLY	-	expression tag	UNP E0XIZ3
B	1259	SER	-	expression tag	UNP E0XIZ3
B	1260	GLY	-	expression tag	UNP E0XIZ3
B	1261	GLY	-	expression tag	UNP E0XIZ3
B	1262	SER	-	expression tag	UNP E0XIZ3
B	1263	ALA	-	expression tag	UNP E0XIZ3
B	1264	TRP	-	expression tag	UNP E0XIZ3
B	1265	SER	-	expression tag	UNP E0XIZ3

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	1266	HIS	-	expression tag	UNP E0XIZ3
B	1267	PRO	-	expression tag	UNP E0XIZ3
B	1268	GLN	-	expression tag	UNP E0XIZ3
B	1269	PHE	-	expression tag	UNP E0XIZ3
B	1270	GLU	-	expression tag	UNP E0XIZ3
B	1271	LYS	-	expression tag	UNP E0XIZ3
B	1272	SER	-	expression tag	UNP E0XIZ3
B	1273	ALA	-	expression tag	UNP E0XIZ3
C	1195	GLY	-	expression tag	UNP E0XIZ3
C	1196	SER	-	expression tag	UNP E0XIZ3
C	1197	GLY	-	expression tag	UNP E0XIZ3
C	1198	TYR	-	expression tag	UNP E0XIZ3
C	1199	ILE	-	expression tag	UNP E0XIZ3
C	1200	PRO	-	expression tag	UNP E0XIZ3
C	1201	GLU	-	expression tag	UNP E0XIZ3
C	1202	ALA	-	expression tag	UNP E0XIZ3
C	1203	PRO	-	expression tag	UNP E0XIZ3
C	1204	ARG	-	expression tag	UNP E0XIZ3
C	1205	ASP	-	expression tag	UNP E0XIZ3
C	1206	GLY	-	expression tag	UNP E0XIZ3
C	1207	GLN	-	expression tag	UNP E0XIZ3
C	1208	ALA	-	expression tag	UNP E0XIZ3
C	1209	TYR	-	expression tag	UNP E0XIZ3
C	1210	VAL	-	expression tag	UNP E0XIZ3
C	1211	ARG	-	expression tag	UNP E0XIZ3
C	1212	LYS	-	expression tag	UNP E0XIZ3
C	1213	ASP	-	expression tag	UNP E0XIZ3
C	1214	GLY	-	expression tag	UNP E0XIZ3
C	1215	GLU	-	expression tag	UNP E0XIZ3
C	1216	TRP	-	expression tag	UNP E0XIZ3
C	1217	VAL	-	expression tag	UNP E0XIZ3
C	1218	LEU	-	expression tag	UNP E0XIZ3
C	1219	LEU	-	expression tag	UNP E0XIZ3
C	1220	SER	-	expression tag	UNP E0XIZ3
C	1221	THR	-	expression tag	UNP E0XIZ3
C	1222	PHE	-	expression tag	UNP E0XIZ3
C	1223	LEU	-	expression tag	UNP E0XIZ3
C	1224	LEU	-	expression tag	UNP E0XIZ3
C	1225	GLU	-	expression tag	UNP E0XIZ3
C	1226	VAL	-	expression tag	UNP E0XIZ3
C	1227	LEU	-	expression tag	UNP E0XIZ3
C	1228	PHE	-	expression tag	UNP E0XIZ3

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	1229	GLN	-	expression tag	UNP E0XIZ3
C	1230	GLY	-	expression tag	UNP E0XIZ3
C	1231	PRO	-	expression tag	UNP E0XIZ3
C	1232	GLY	-	expression tag	UNP E0XIZ3
C	1233	HIS	-	expression tag	UNP E0XIZ3
C	1234	HIS	-	expression tag	UNP E0XIZ3
C	1235	HIS	-	expression tag	UNP E0XIZ3
C	1236	HIS	-	expression tag	UNP E0XIZ3
C	1237	HIS	-	expression tag	UNP E0XIZ3
C	1238	HIS	-	expression tag	UNP E0XIZ3
C	1239	HIS	-	expression tag	UNP E0XIZ3
C	1240	HIS	-	expression tag	UNP E0XIZ3
C	1241	SER	-	expression tag	UNP E0XIZ3
C	1242	ALA	-	expression tag	UNP E0XIZ3
C	1243	TRP	-	expression tag	UNP E0XIZ3
C	1244	SER	-	expression tag	UNP E0XIZ3
C	1245	HIS	-	expression tag	UNP E0XIZ3
C	1246	PRO	-	expression tag	UNP E0XIZ3
C	1247	GLN	-	expression tag	UNP E0XIZ3
C	1248	PHE	-	expression tag	UNP E0XIZ3
C	1249	GLU	-	expression tag	UNP E0XIZ3
C	1250	LYS	-	expression tag	UNP E0XIZ3
C	1251	GLY	-	expression tag	UNP E0XIZ3
C	1252	GLY	-	expression tag	UNP E0XIZ3
C	1253	GLY	-	expression tag	UNP E0XIZ3
C	1254	SER	-	expression tag	UNP E0XIZ3
C	1255	GLY	-	expression tag	UNP E0XIZ3
C	1256	GLY	-	expression tag	UNP E0XIZ3
C	1257	GLY	-	expression tag	UNP E0XIZ3
C	1258	GLY	-	expression tag	UNP E0XIZ3
C	1259	SER	-	expression tag	UNP E0XIZ3
C	1260	GLY	-	expression tag	UNP E0XIZ3
C	1261	GLY	-	expression tag	UNP E0XIZ3
C	1262	SER	-	expression tag	UNP E0XIZ3
C	1263	ALA	-	expression tag	UNP E0XIZ3
C	1264	TRP	-	expression tag	UNP E0XIZ3
C	1265	SER	-	expression tag	UNP E0XIZ3
C	1266	HIS	-	expression tag	UNP E0XIZ3
C	1267	PRO	-	expression tag	UNP E0XIZ3
C	1268	GLN	-	expression tag	UNP E0XIZ3
C	1269	PHE	-	expression tag	UNP E0XIZ3
C	1270	GLU	-	expression tag	UNP E0XIZ3

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	1271	LYS	-	expression tag	UNP E0XIZ3
C	1272	SER	-	expression tag	UNP E0XIZ3
C	1273	ALA	-	expression tag	UNP E0XIZ3

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

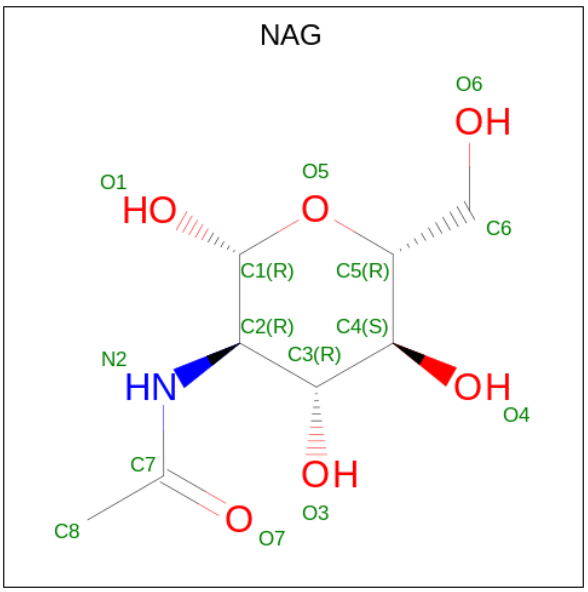
Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	2	Total	C	N	O	0	0
			28	16	2	10		
2	F	2	Total	C	N	O	0	0
			28	16	2	10		
2	G	2	Total	C	N	O	0	0
			28	16	2	10		
2	I	2	Total	C	N	O	0	0
			28	16	2	10		
2	J	2	Total	C	N	O	0	0
			28	16	2	10		
2	L	2	Total	C	N	O	0	0
			28	16	2	10		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
3	E	4	Total	C	N	O	0	0
			50	28	2	20		
3	H	4	Total	C	N	O	0	0
			50	28	2	20		
3	K	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:

$C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



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

Continued on next page...

Continued from previous page...

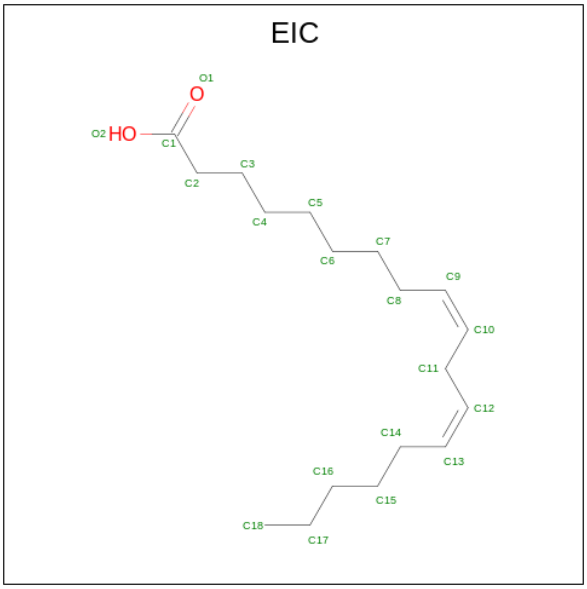
Mol	Chain	Residues	Atoms				AltConf
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4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

Continued on next page...

Continued from previous page...

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

- Molecule 5 is LINOLEIC ACID (three-letter code: EIC) (formula: $C_{18}H_{32}O_2$).



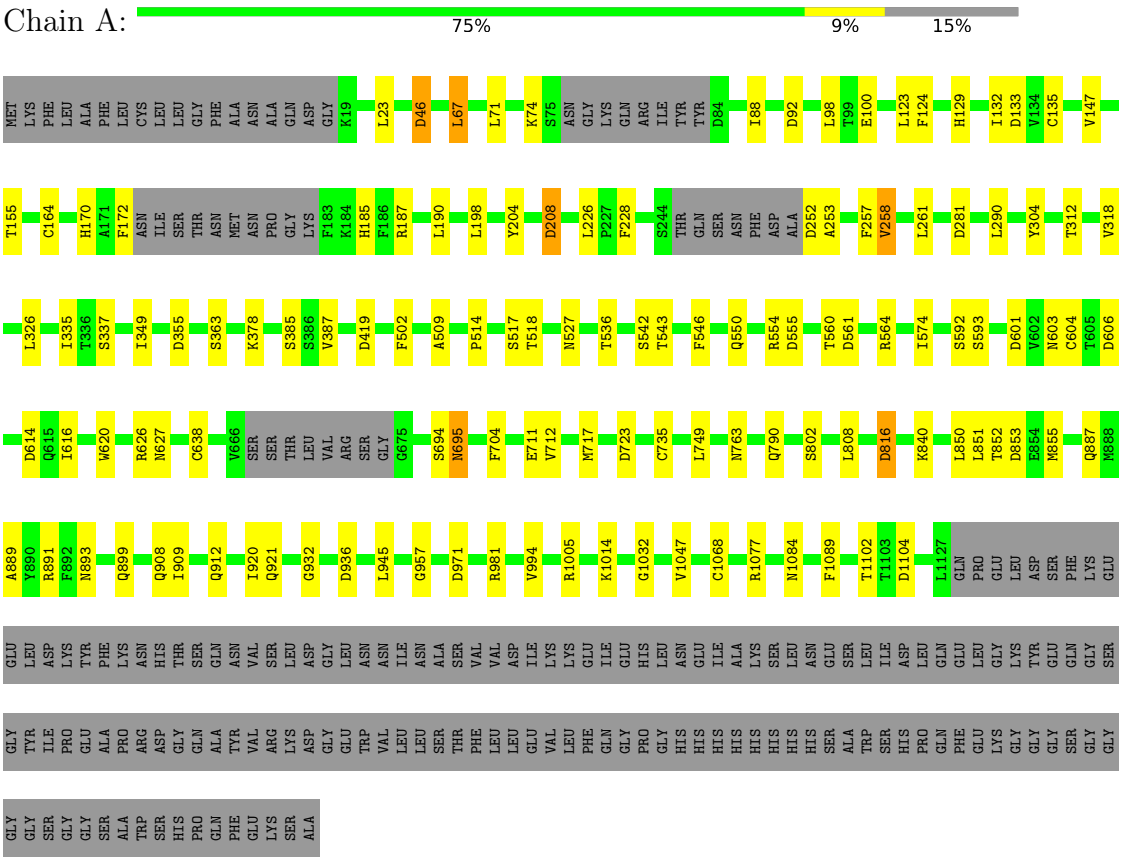
Mol	Chain	Residues	Atoms	AltConf
5	B	1	Total C O 20 18 2	0
5	C	1	Total C O 20 18 2	0
5	C	1	Total C O 20 18 2	0

3 Residue-property plots

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.

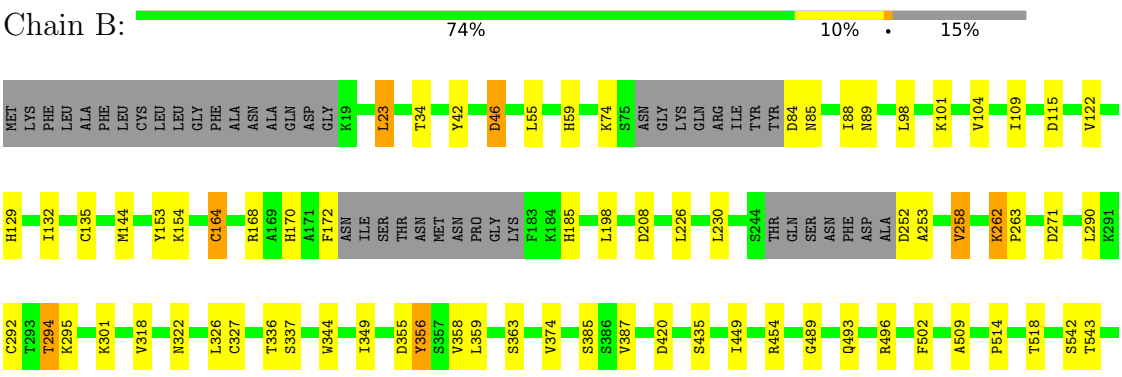
- Molecule 1: Spike glycoprotein

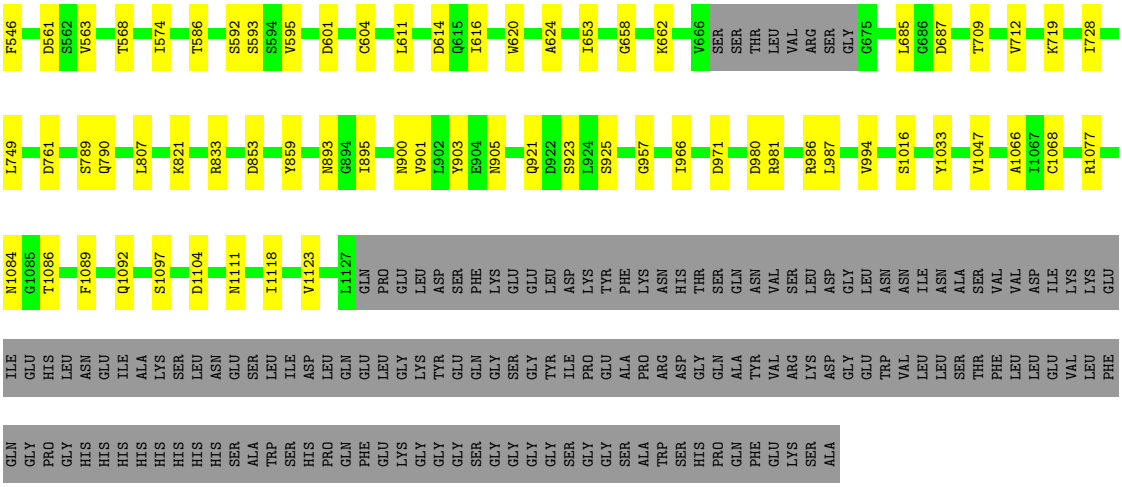
Chain A:



- Molecule 1: Spike glycoprotein

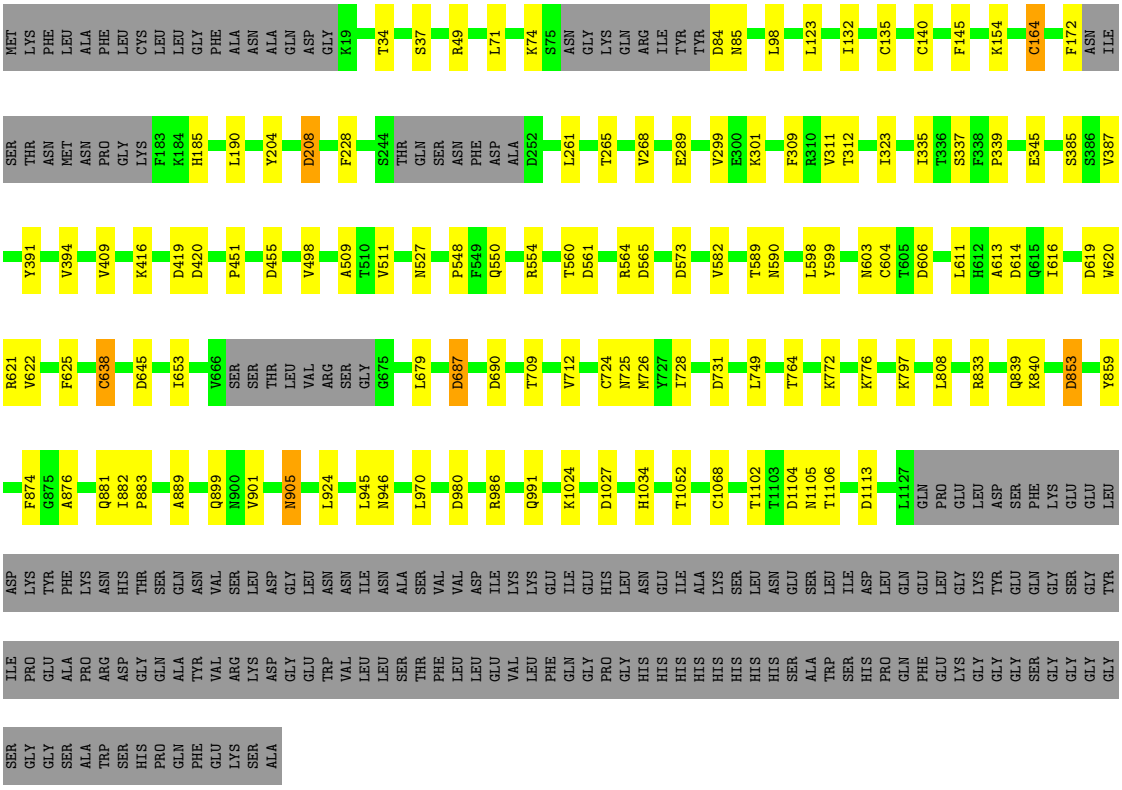
Chain B:





• Molecule 1: Spike glycoprotein

Chain C:

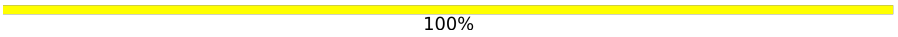


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:

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

Chain F:

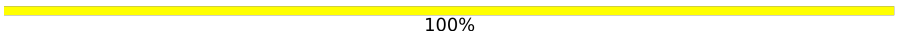


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:

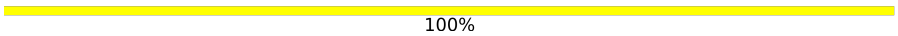
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:



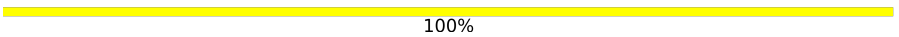
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:



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

Chain L:



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

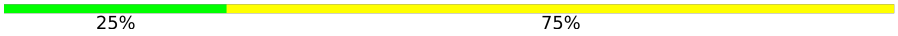
Chain E:

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

Chain H:

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

Chain K:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	79256	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN	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: MAN, EIC, NAG, BMA

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	0.26	0/8564	0.49	0/11650
1	B	0.26	0/8564	0.50	0/11650
1	C	0.26	0/8564	0.50	0/11650
All	All	0.26	0/25692	0.50	0/34950

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	8367	0	8101	60	0
1	B	8367	0	8100	62	0
1	C	8367	0	8100	58	0
2	D	28	0	25	0	0
2	F	28	0	25	0	0
2	G	28	0	25	0	0
2	I	28	0	25	0	0
2	J	28	0	25	0	0
2	L	28	0	25	0	0
3	E	50	0	43	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	50	0	43	0	0
3	K	50	0	43	0	0
4	A	182	0	169	2	0
4	B	182	0	169	1	0
4	C	182	0	169	0	0
5	B	20	0	31	0	0
5	C	40	0	62	1	0
All	All	26025	0	25180	172	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.

The worst 5 of 172 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:613:ALA:HB1	1:C:621:ARG:HG2	1.77	0.65
1:A:208:ASP:OD1	1:A:208:ASP:N	2.34	0.60
1:B:616:ILE:HD12	1:B:620:TRP:HB3	1.84	0.60
1:A:318:VAL:H	1:A:518:THR:HB	1.68	0.58
1:B:790:GLN:NE2	1:B:921:GLN:OE1	2.36	0.58

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	1066/1273 (84%)	1029 (96%)	37 (4%)	0	100	100
1	B	1066/1273 (84%)	1028 (96%)	38 (4%)	0	100	100
1	C	1066/1273 (84%)	1035 (97%)	31 (3%)	0	100	100
All	All	3198/3819 (84%)	3092 (97%)	106 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	931/1095 (85%)	895 (96%)	36 (4%)	27	58
1	B	931/1095 (85%)	883 (95%)	48 (5%)	19	48
1	C	931/1095 (85%)	886 (95%)	45 (5%)	21	51
All	All	2793/3285 (85%)	2664 (95%)	129 (5%)	25	52

5 of 129 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	726	MET
1	C	859	TYR
1	B	154	LYS
1	B	153	TYR
1	C	905	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	912	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates (i)

24 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	0.73	0	17,19,21	1.17	2 (11%)
2	NAG	D	2	2	14,14,15	0.72	0	17,19,21	0.92	0
3	NAG	E	1	1,3	14,14,15	0.74	0	17,19,21	1.00	0
3	NAG	E	2	3	14,14,15	0.72	0	17,19,21	0.99	0
3	BMA	E	3	3	11,11,12	0.89	0	15,15,17	2.36	3 (20%)
3	MAN	E	4	3	11,11,12	0.69	0	15,15,17	1.31	1 (6%)
2	NAG	F	1	1,2	14,14,15	0.69	0	17,19,21	1.51	2 (11%)
2	NAG	F	2	2	14,14,15	0.72	0	17,19,21	1.46	3 (17%)
2	NAG	G	1	1,2	14,14,15	0.73	0	17,19,21	1.27	1 (5%)
2	NAG	G	2	2	14,14,15	0.70	0	17,19,21	0.89	0
3	NAG	H	1	1,3	14,14,15	0.76	0	17,19,21	0.98	0
3	NAG	H	2	3	14,14,15	0.72	0	17,19,21	0.90	0
3	BMA	H	3	3	11,11,12	0.90	1 (9%)	15,15,17	2.45	4 (26%)
3	MAN	H	4	3	11,11,12	0.71	0	15,15,17	1.28	1 (6%)
2	NAG	I	1	1,2	14,14,15	0.71	0	17,19,21	1.50	2 (11%)
2	NAG	I	2	2	14,14,15	0.71	0	17,19,21	1.45	1 (5%)
2	NAG	J	1	1,2	14,14,15	0.72	0	17,19,21	1.31	2 (11%)
2	NAG	J	2	2	14,14,15	0.72	0	17,19,21	0.94	1 (5%)
3	NAG	K	1	1,3	14,14,15	0.76	0	17,19,21	1.01	1 (5%)
3	NAG	K	2	3	14,14,15	0.72	0	17,19,21	0.94	0
3	BMA	K	3	3	11,11,12	0.92	1 (9%)	15,15,17	2.43	5 (33%)
3	MAN	K	4	3	11,11,12	0.73	0	15,15,17	1.35	1 (6%)
2	NAG	L	1	1,2	14,14,15	0.68	0	17,19,21	1.49	1 (5%)
2	NAG	L	2	2	14,14,15	0.71	0	17,19,21	1.47	2 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	D	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	1/6/23/26	0/1/1/1
3	NAG	E	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
3	BMA	E	3	3	-	0/2/19/22	0/1/1/1
3	MAN	E	4	3	-	2/2/19/22	0/1/1/1
2	NAG	F	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	1/6/23/26	0/1/1/1
2	NAG	G	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	1/6/23/26	0/1/1/1
3	NAG	H	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	0/6/23/26	0/1/1/1
3	BMA	H	3	3	-	0/2/19/22	0/1/1/1
3	MAN	H	4	3	-	1/2/19/22	1/1/1/1
2	NAG	I	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	I	2	2	-	1/6/23/26	0/1/1/1
2	NAG	J	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	J	2	2	-	1/6/23/26	0/1/1/1
3	NAG	K	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	K	2	3	-	0/6/23/26	0/1/1/1
3	BMA	K	3	3	-	2/2/19/22	0/1/1/1
3	MAN	K	4	3	-	1/2/19/22	1/1/1/1
2	NAG	L	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	L	2	2	-	1/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	3	BMA	C2-C3	2.05	1.55	1.52
3	K	3	BMA	C2-C3	2.05	1.55	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	3	BMA	C1-O5-C5	7.44	122.27	112.19
3	K	3	BMA	C1-O5-C5	7.18	121.91	112.19
3	E	3	BMA	C1-O5-C5	7.09	121.80	112.19
2	I	1	NAG	C2-N2-C7	4.32	129.05	122.90
2	F	1	NAG	C2-N2-C7	4.31	129.04	122.90

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	4	MAN	O5-C5-C6-O6
3	E	4	MAN	C4-C5-C6-O6
3	K	3	BMA	O5-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6
2	J	2	NAG	O5-C5-C6-O6

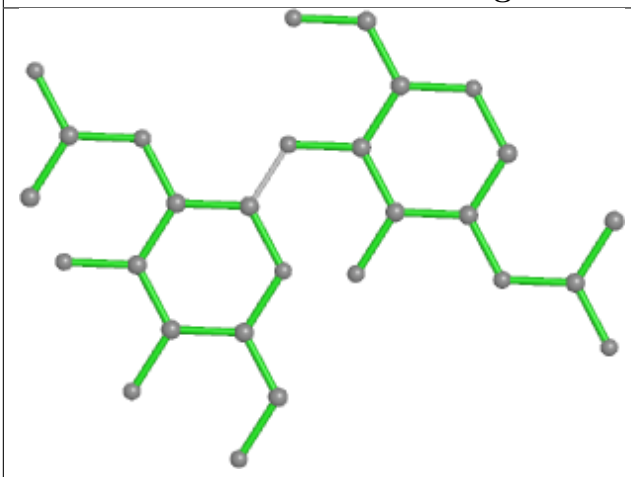
All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	4	MAN	C1-C2-C3-C4-C5-O5
3	K	4	MAN	C1-C2-C3-C4-C5-O5

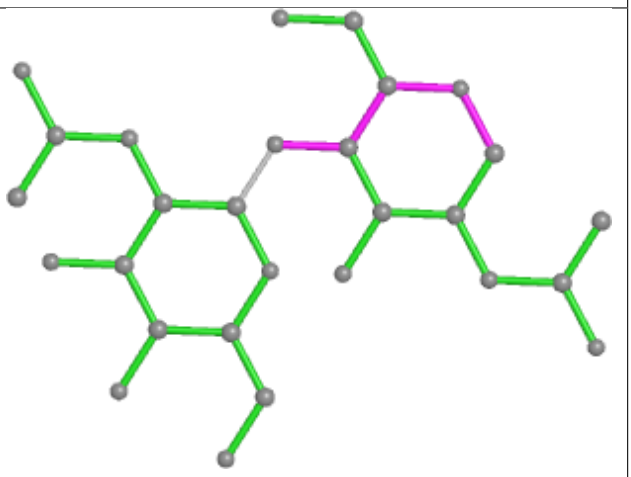
No monomer is involved in short contacts.

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

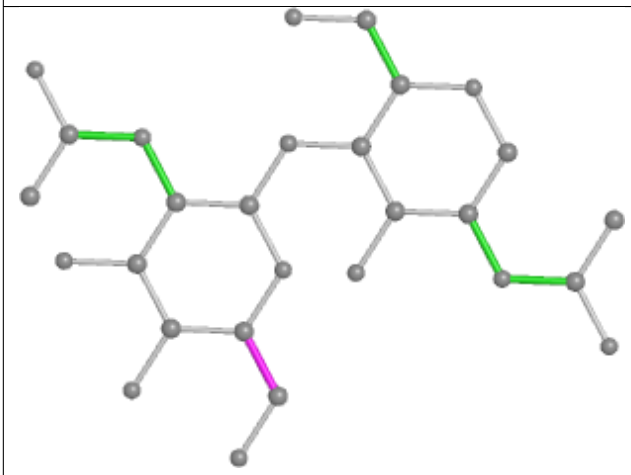
Oligosaccharide Chain D



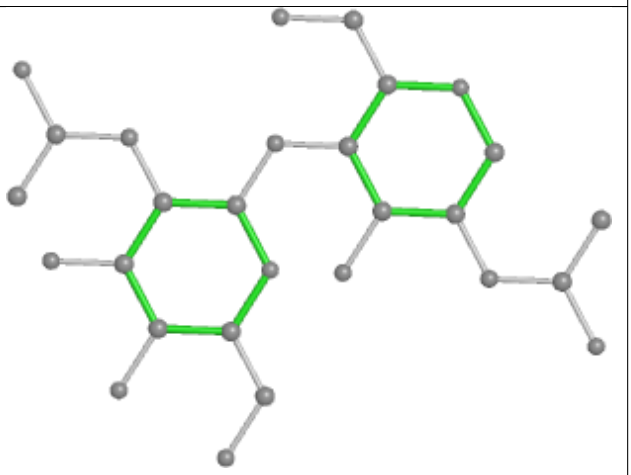
Bond lengths



Bond angles

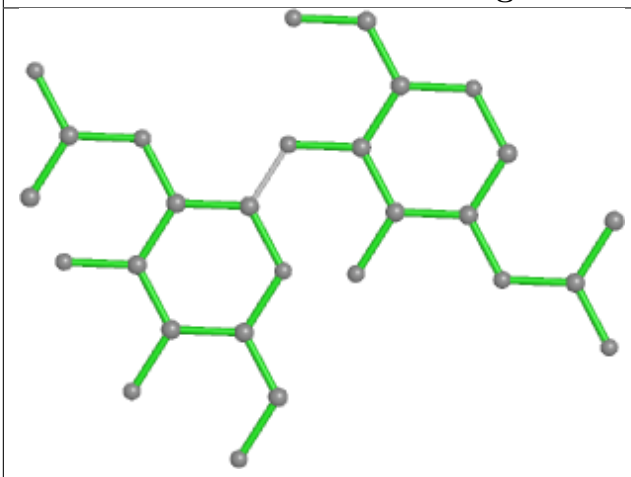


Torsions

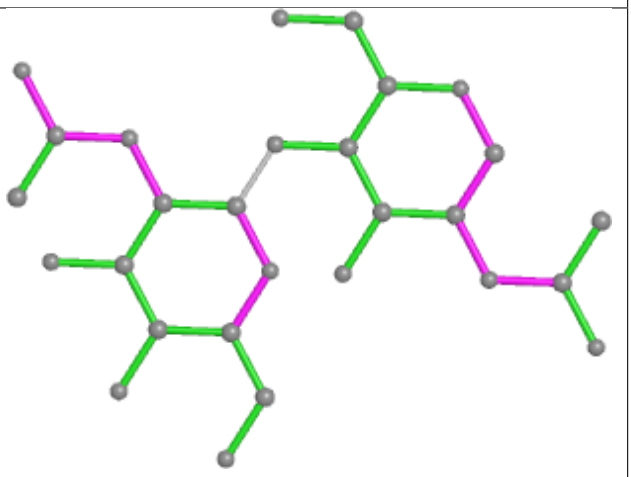


Rings

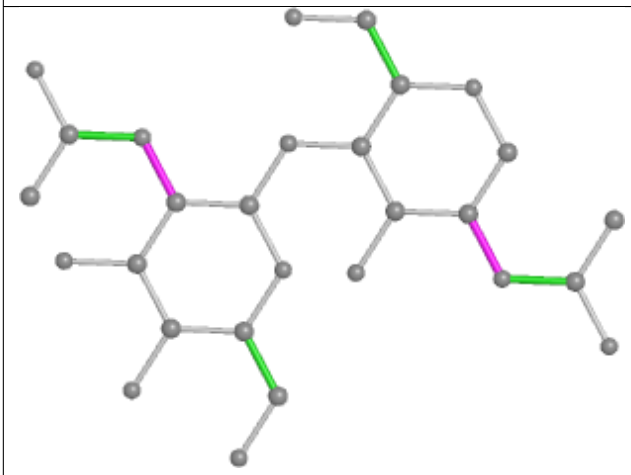
Oligosaccharide Chain F



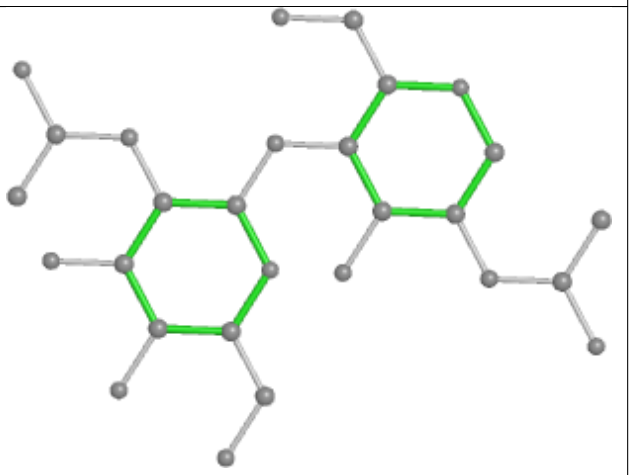
Bond lengths



Bond angles

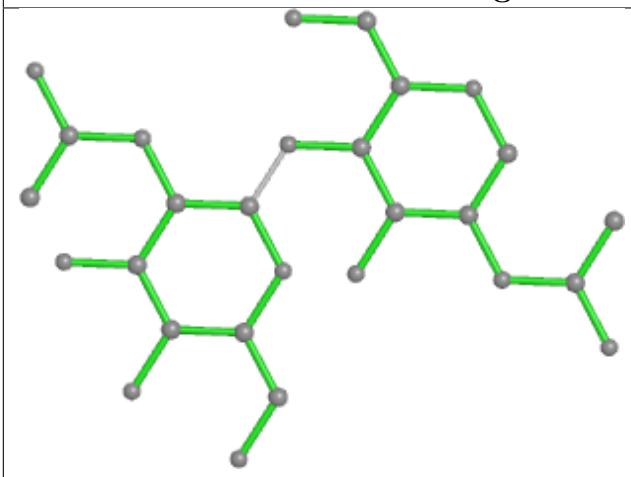


Torsions

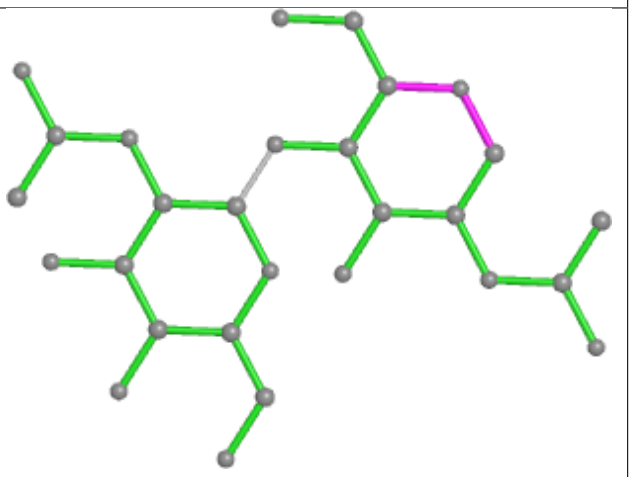


Rings

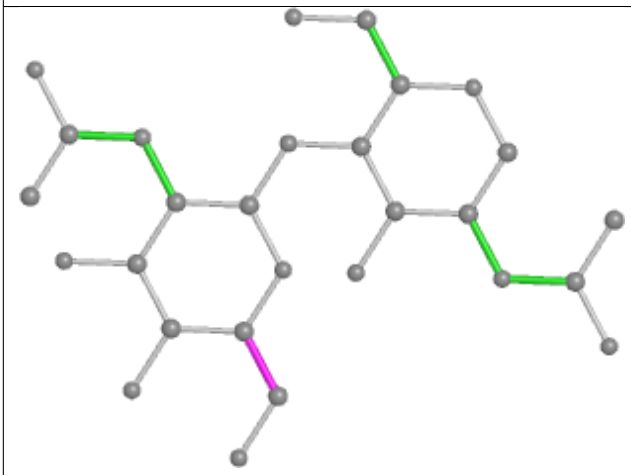
Oligosaccharide Chain G



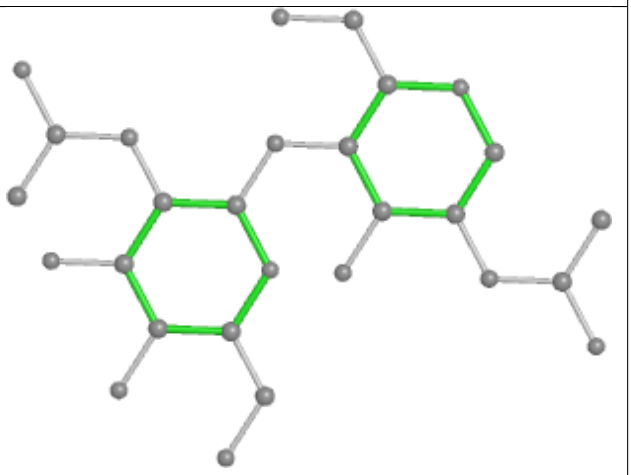
Bond lengths



Bond angles

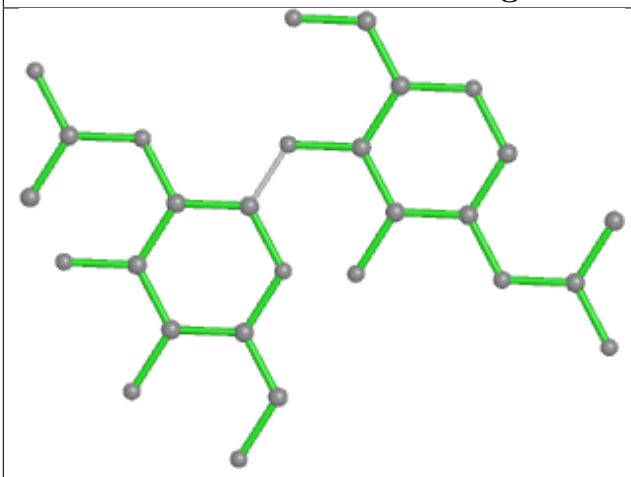


Torsions

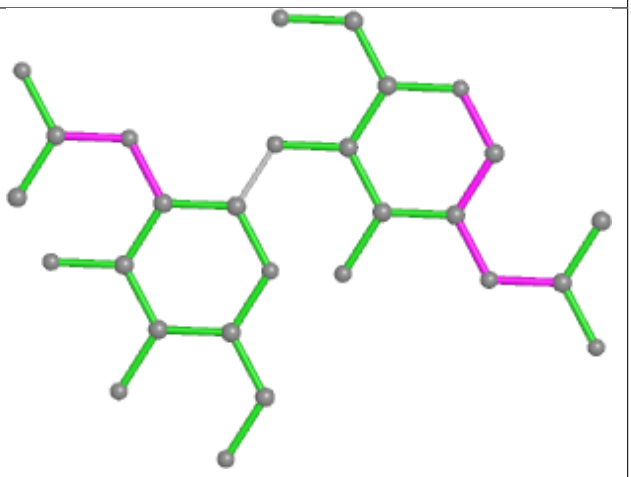


Rings

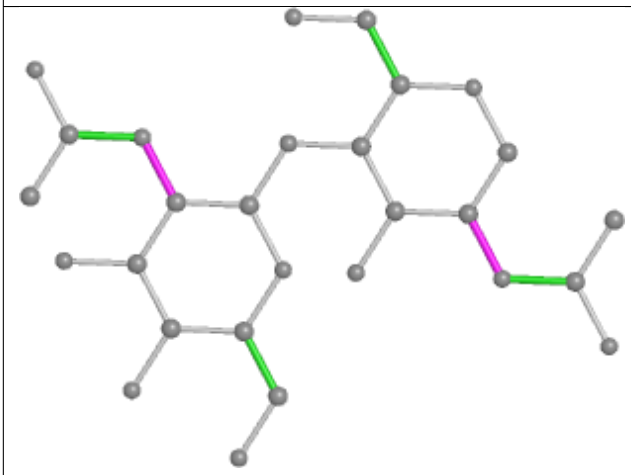
Oligosaccharide Chain I



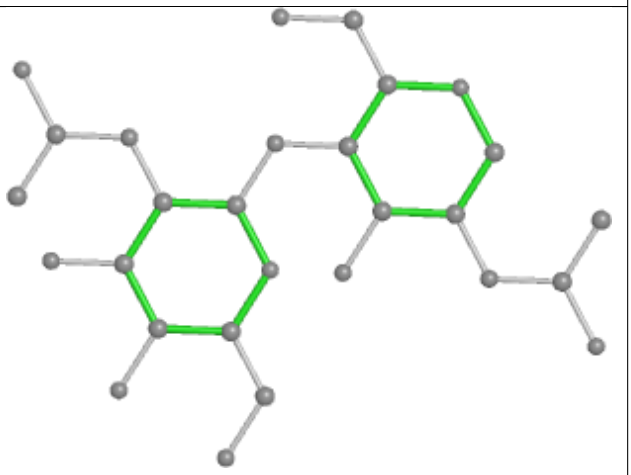
Bond lengths



Bond angles

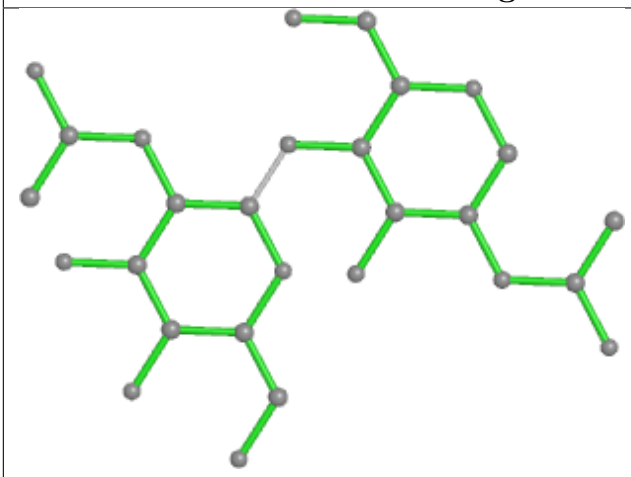


Torsions

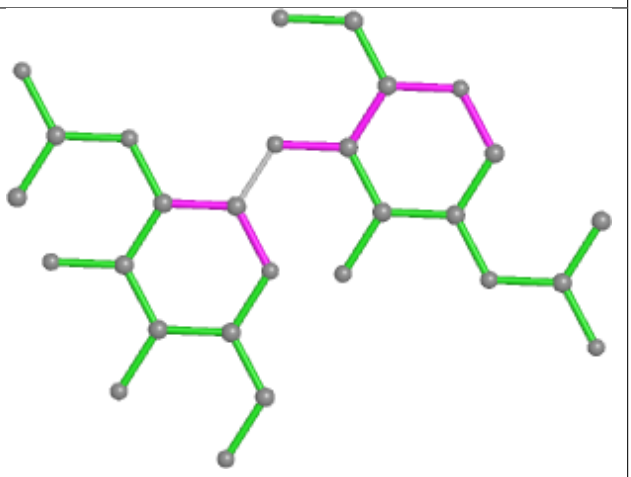


Rings

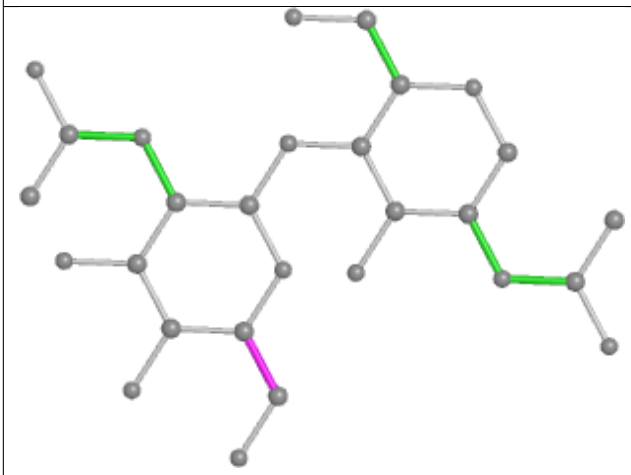
Oligosaccharide Chain J



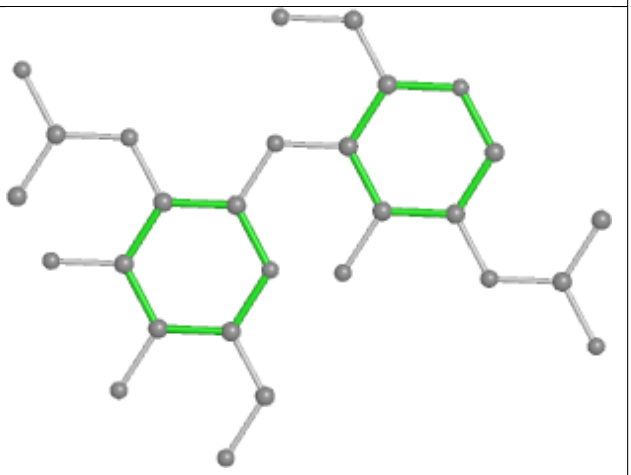
Bond lengths



Bond angles

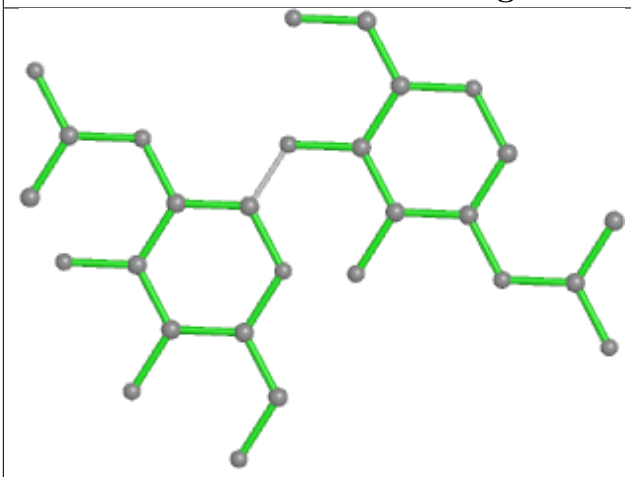


Torsions

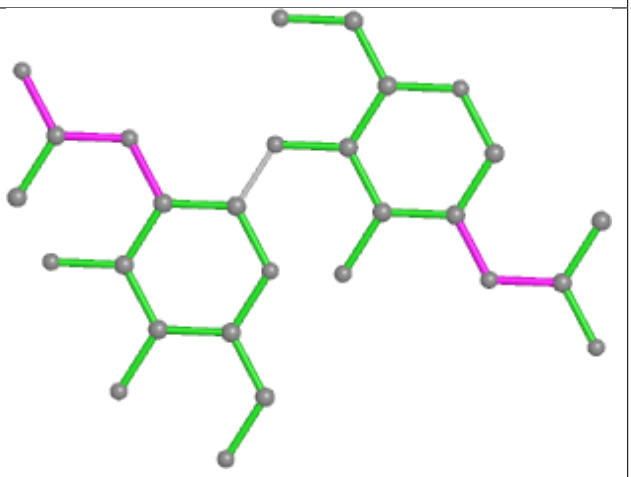


Rings

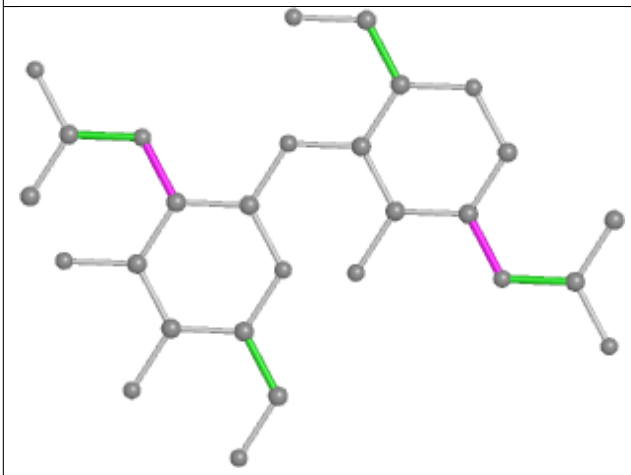
Oligosaccharide Chain L



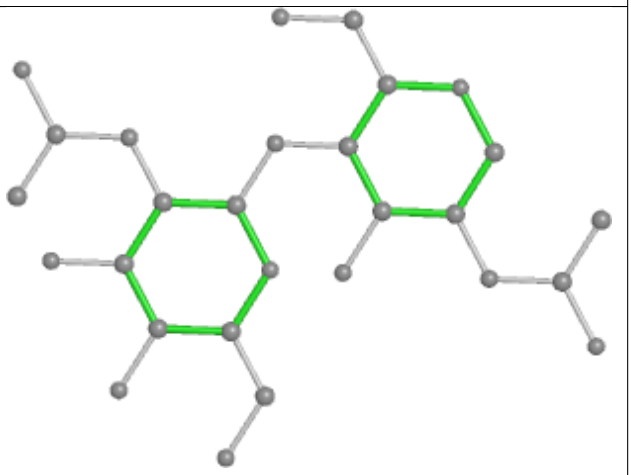
Bond lengths



Bond angles

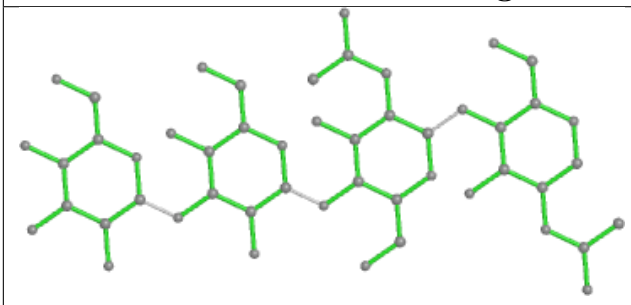


Torsions

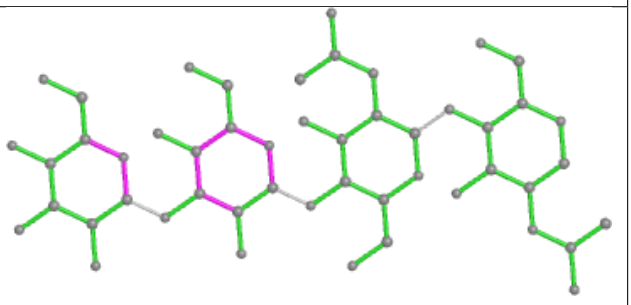


Rings

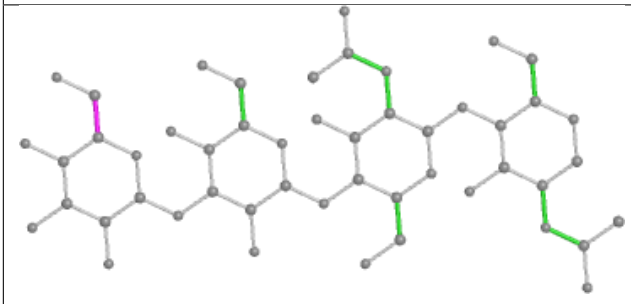
Oligosaccharide Chain E



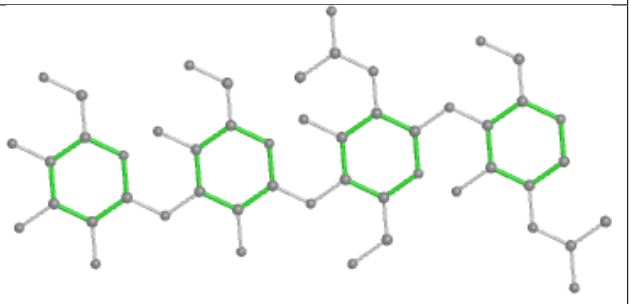
Bond lengths



Bond angles

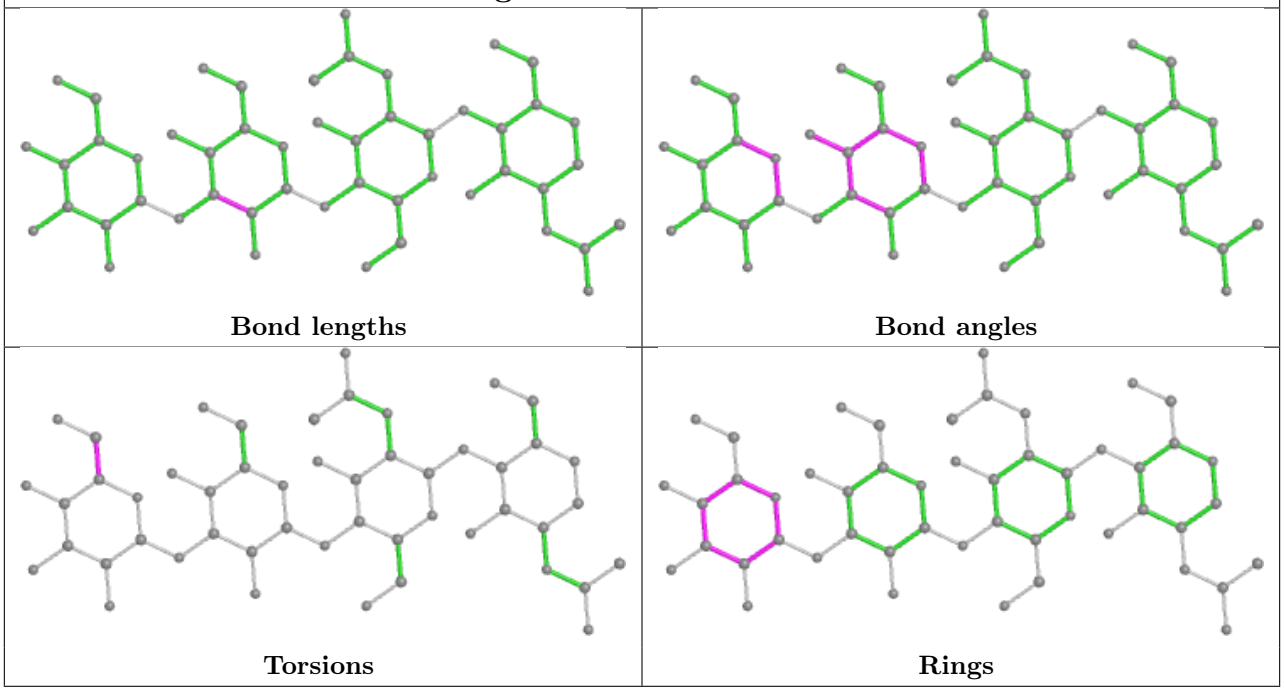


Torsions

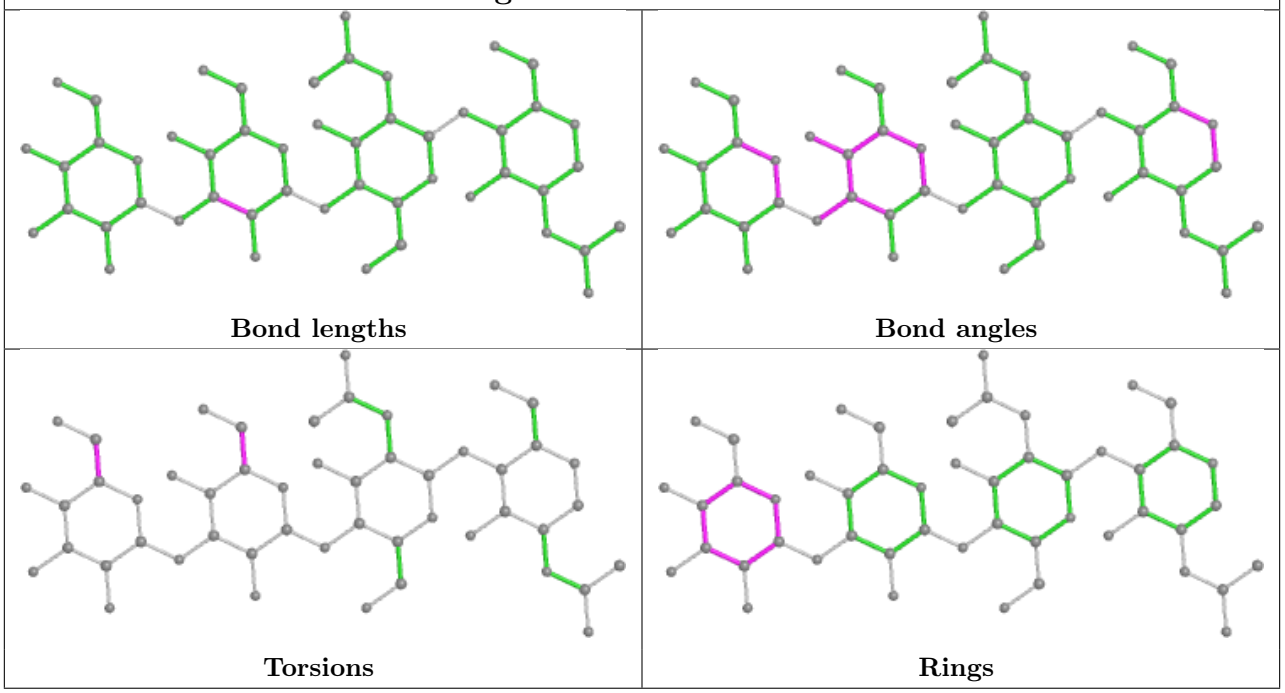


Rings

Oligosaccharide Chain H



Oligosaccharide Chain K



5.6 Ligand geometry (i)

42 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	$\#\|Z\| > 2$
4	NAG	B	1302	-	14,14,15	0.71	0	17,19,21	0.86	0
4	NAG	A	1309	1	14,14,15	0.72	0	17,19,21	1.59	2 (11%)
4	NAG	C	1304	-	14,14,15	0.71	0	17,19,21	0.84	0
4	NAG	A	1310	1	14,14,15	0.73	0	17,19,21	0.84	0
4	NAG	B	1303	-	14,14,15	0.71	0	17,19,21	0.82	0
4	NAG	A	1308	1	14,14,15	0.69	0	17,19,21	0.87	0
4	NAG	A	1312	1	14,14,15	0.73	0	17,19,21	0.85	0
4	NAG	B	1309	1	14,14,15	0.69	0	17,19,21	0.88	0
4	NAG	A	1305	1	14,14,15	0.74	0	17,19,21	0.99	1 (5%)
4	NAG	B	1310	1	14,14,15	0.73	0	17,19,21	1.48	3 (17%)
4	NAG	A	1311	1	14,14,15	0.70	0	17,19,21	1.45	1 (5%)
4	NAG	B	1306	1	14,14,15	0.72	0	17,19,21	0.95	1 (5%)
4	NAG	C	1313	1	14,14,15	0.69	0	17,19,21	1.50	2 (11%)
4	NAG	A	1303	1	14,14,15	0.72	0	17,19,21	0.87	0
4	NAG	C	1305	1	14,14,15	0.70	0	17,19,21	0.84	0
4	NAG	B	1313	1	14,14,15	0.71	0	17,19,21	0.91	0
4	NAG	C	1310	1	14,14,15	0.69	0	17,19,21	0.97	1 (5%)
4	NAG	B	1305	-	14,14,15	0.71	0	17,19,21	0.83	0
4	NAG	B	1304	1	14,14,15	0.73	0	17,19,21	0.89	0
4	NAG	C	1307	1	14,14,15	0.70	0	17,19,21	0.92	1 (5%)
4	NAG	B	1311	1	14,14,15	0.72	0	17,19,21	0.92	0
4	NAG	C	1308	-	14,14,15	0.73	0	17,19,21	0.82	0
4	NAG	B	1312	1	14,14,15	0.69	0	17,19,21	1.46	1 (5%)
5	EIC	B	1301	-	19,19,19	0.60	0	19,19,19	0.56	0
4	NAG	C	1315	1	14,14,15	0.73	0	17,19,21	0.83	0
4	NAG	C	1314	1	14,14,15	0.70	0	17,19,21	0.94	1 (5%)
5	EIC	C	1301	-	19,19,19	0.58	0	19,19,19	0.55	0
4	NAG	A	1313	-	14,14,15	0.71	0	17,19,21	0.80	0
4	NAG	A	1301	-	14,14,15	0.73	0	17,19,21	0.83	0
4	NAG	A	1306	-	14,14,15	0.72	0	17,19,21	0.86	0
4	NAG	B	1314	1	14,14,15	0.71	0	17,19,21	0.91	1 (5%)
4	NAG	A	1307	-	14,14,15	0.69	0	17,19,21	1.12	2 (11%)
4	NAG	C	1309	-	14,14,15	0.71	0	17,19,21	0.91	1 (5%)
4	NAG	B	1307	-	14,14,15	0.71	0	17,19,21	0.83	0
4	NAG	A	1302	-	14,14,15	0.70	0	17,19,21	0.82	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	B	1308	-	14,14,15	0.71	0	17,19,21	0.87	0
4	NAG	C	1303	-	14,14,15	0.72	0	17,19,21	0.85	0
4	NAG	C	1306	-	14,14,15	0.69	0	17,19,21	0.82	0
4	NAG	A	1304	-	14,14,15	0.72	0	17,19,21	0.85	0
4	NAG	C	1311	1	14,14,15	0.73	0	17,19,21	1.54	2 (11%)
4	NAG	C	1312	1	14,14,15	0.72	0	17,19,21	0.91	0
5	EIC	C	1302	-	19,19,19	0.59	0	19,19,19	0.58	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
4	NAG	B	1302	-	-	0/6/23/26	0/1/1/1
4	NAG	A	1309	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1304	-	-	0/6/23/26	0/1/1/1
4	NAG	A	1310	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1303	-	-	0/6/23/26	0/1/1/1
4	NAG	A	1308	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1312	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1309	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1305	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1310	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1311	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1306	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1313	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1303	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1305	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1313	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1310	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1305	-	-	0/6/23/26	0/1/1/1
4	NAG	B	1304	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1307	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1311	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1308	-	-	0/6/23/26	0/1/1/1
4	NAG	B	1312	1	-	1/6/23/26	0/1/1/1
5	EIC	B	1301	-	-	6/17/17/17	-
4	NAG	C	1315	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1314	1	-	0/6/23/26	0/1/1/1
5	EIC	C	1301	-	-	2/17/17/17	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1313	-	-	0/6/23/26	0/1/1/1
4	NAG	A	1301	-	-	1/6/23/26	0/1/1/1
4	NAG	A	1306	-	-	0/6/23/26	0/1/1/1
4	NAG	B	1314	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1307	-	-	1/6/23/26	0/1/1/1
4	NAG	C	1309	-	-	1/6/23/26	0/1/1/1
4	NAG	B	1307	-	-	0/6/23/26	0/1/1/1
4	NAG	A	1302	-	-	0/6/23/26	0/1/1/1
4	NAG	B	1308	-	-	1/6/23/26	0/1/1/1
4	NAG	C	1303	-	-	0/6/23/26	0/1/1/1
4	NAG	C	1306	-	-	0/6/23/26	0/1/1/1
4	NAG	A	1304	-	-	0/6/23/26	0/1/1/1
4	NAG	C	1311	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1312	1	-	0/6/23/26	0/1/1/1
5	EIC	C	1302	-	-	3/17/17/17	-

There are no bond length outliers.

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	1313	NAG	C2-N2-C7	4.30	129.02	122.90
4	B	1312	NAG	C2-N2-C7	4.30	129.02	122.90
4	A	1309	NAG	C2-N2-C7	4.28	128.99	122.90
4	A	1311	NAG	C2-N2-C7	4.27	128.99	122.90
4	C	1311	NAG	C2-N2-C7	4.14	128.80	122.90

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	1301	EIC	C9-C10-C11-C12
4	A	1312	NAG	O5-C5-C6-O6
5	C	1302	EIC	C2-C3-C4-C5
5	C	1301	EIC	C6-C7-C8-C9
5	B	1301	EIC	C1-C2-C3-C4

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1302	NAG	1	0

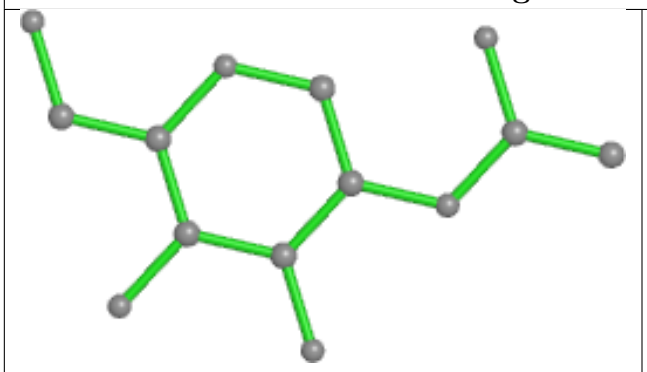
Continued on next page...

Continued from previous page...

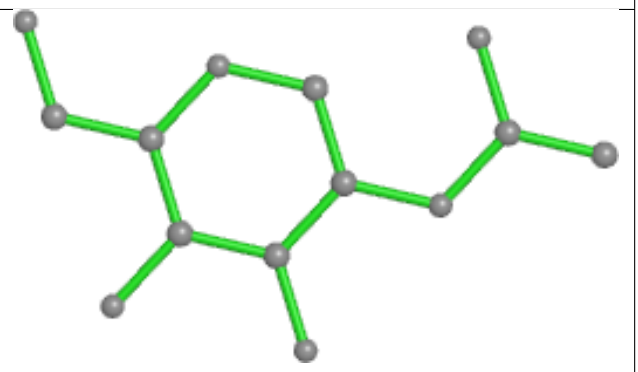
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1310	NAG	1	0
4	A	1302	NAG	1	0
5	C	1302	EIC	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

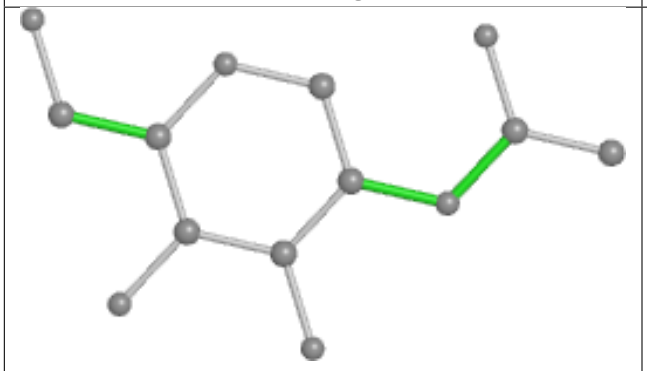
Ligand NAG B 1302



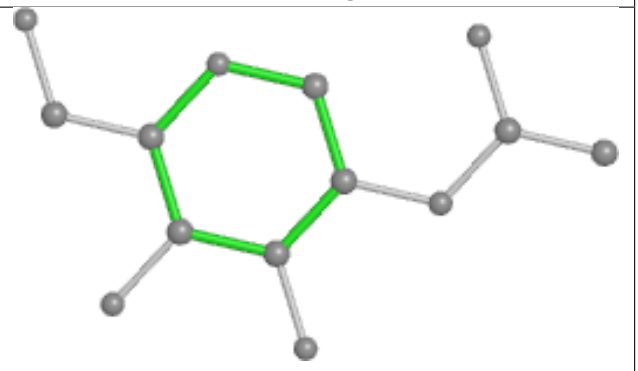
Bond lengths



Bond angles

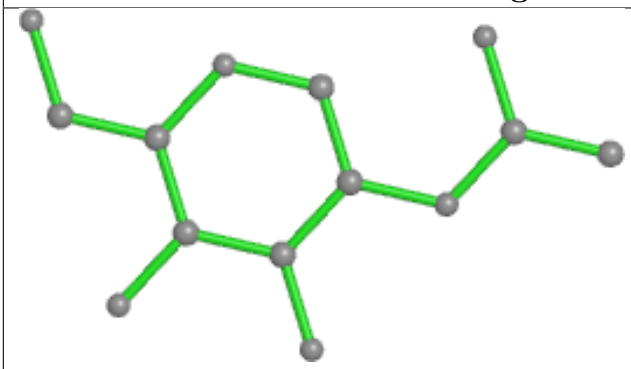


Torsions

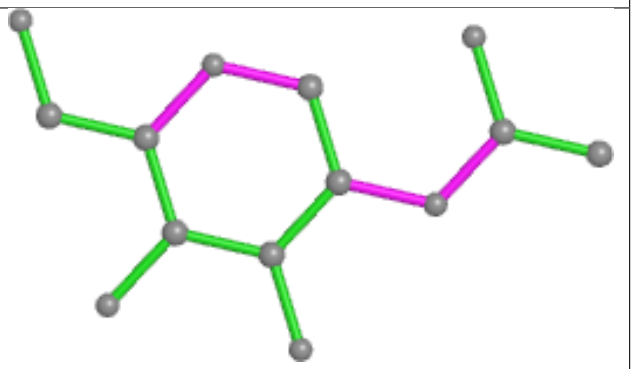


Rings

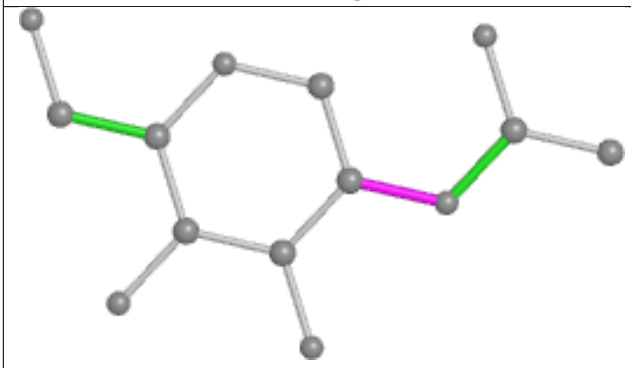
Ligand NAG A 1309



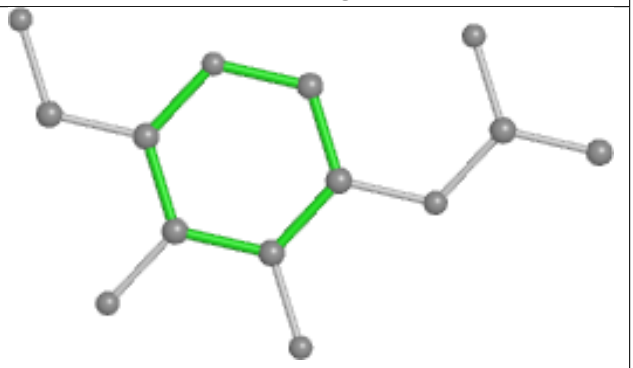
Bond lengths



Bond angles

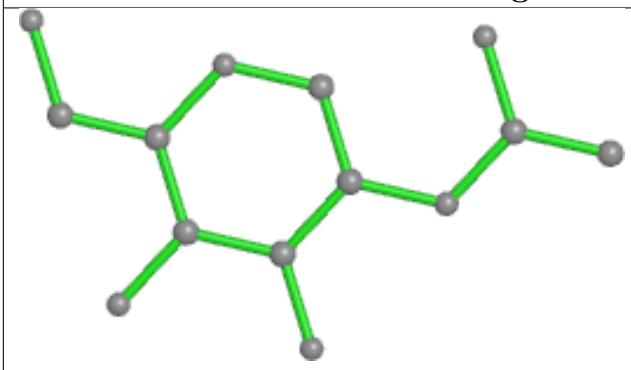


Torsions

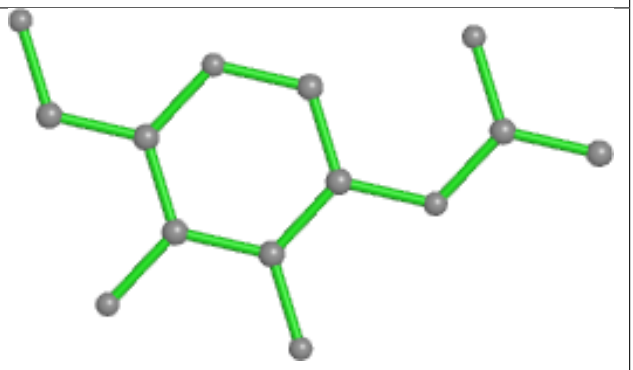


Rings

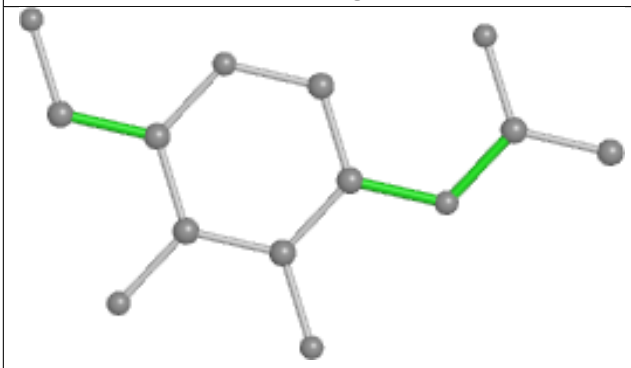
Ligand NAG C 1304



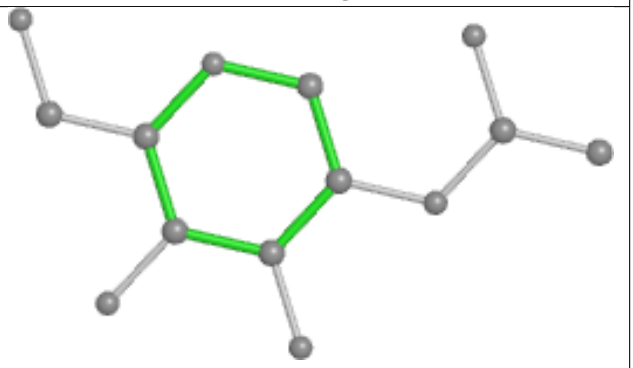
Bond lengths



Bond angles

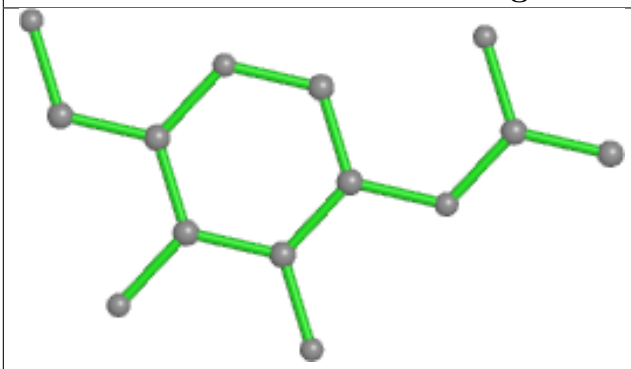


Torsions

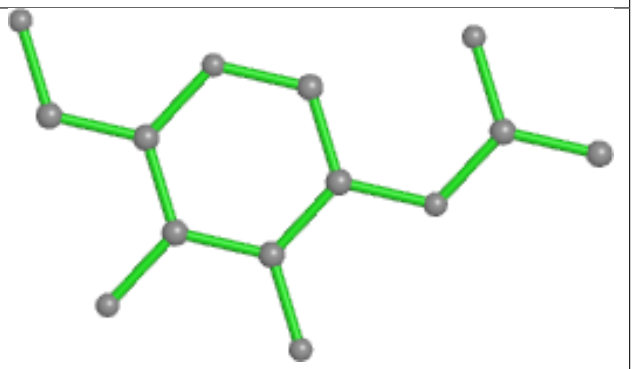


Rings

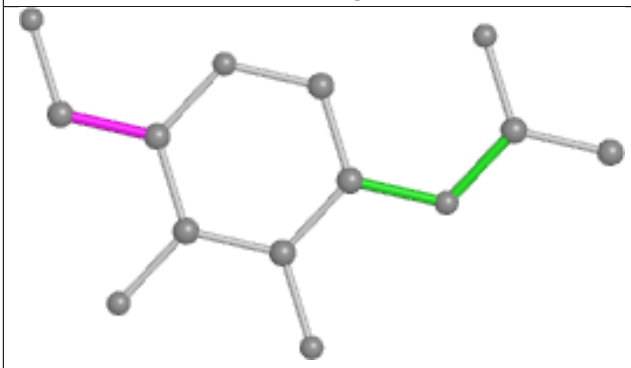
Ligand NAG A 1310



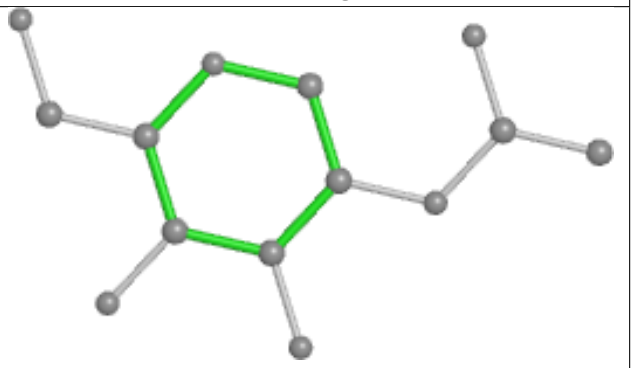
Bond lengths



Bond angles

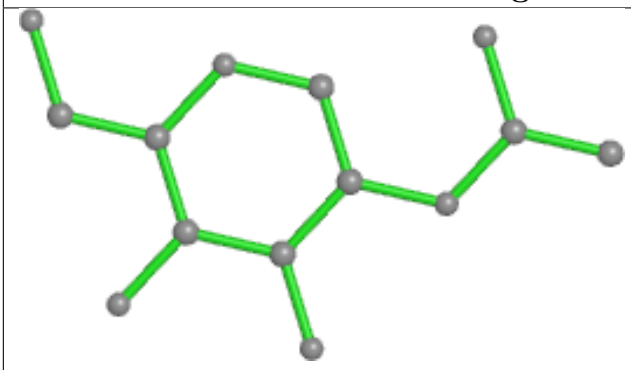


Torsions

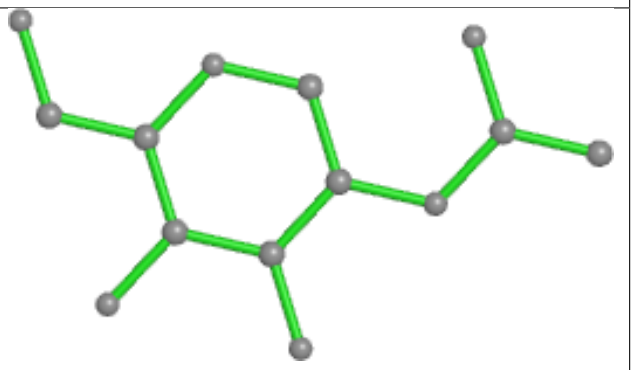


Rings

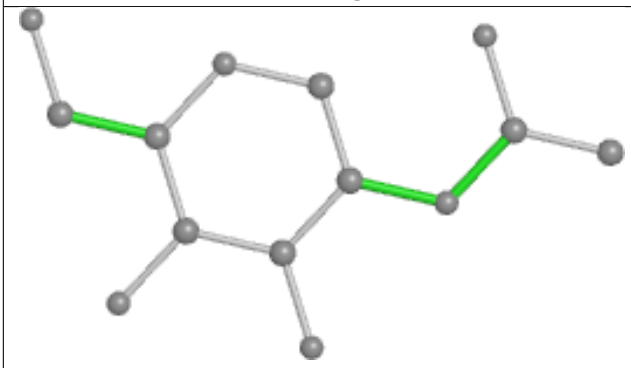
Ligand NAG B 1303



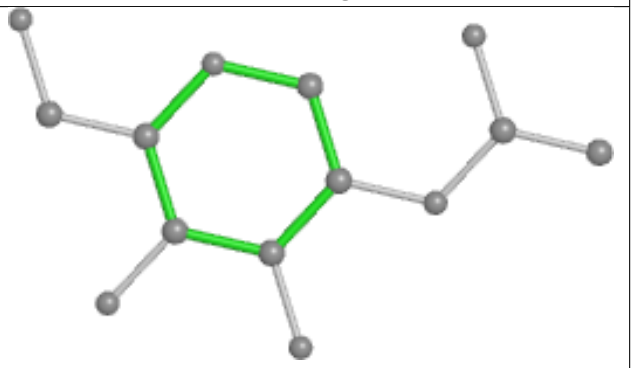
Bond lengths



Bond angles

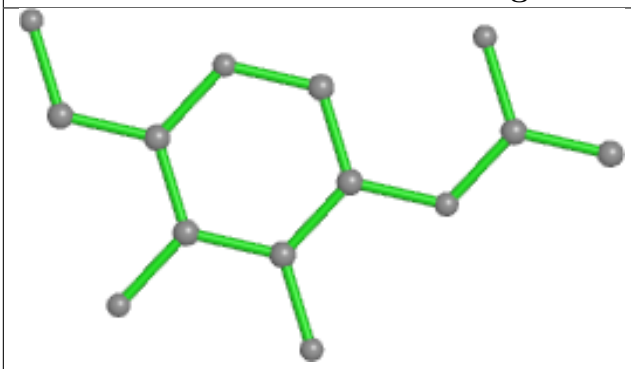


Torsions

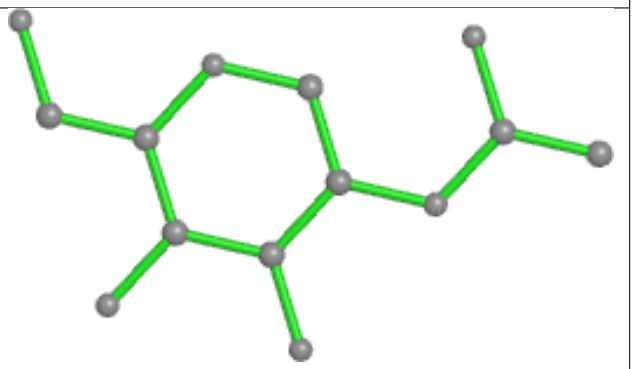


Rings

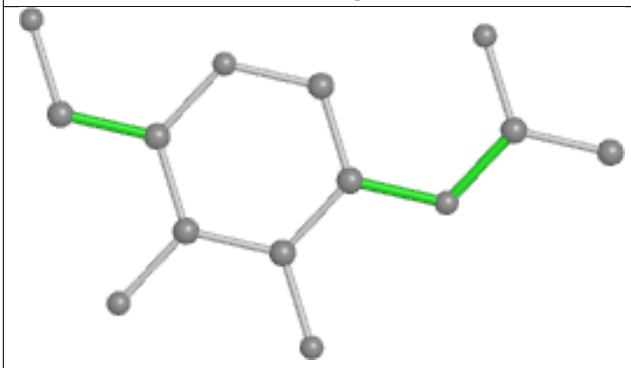
Ligand NAG A 1308



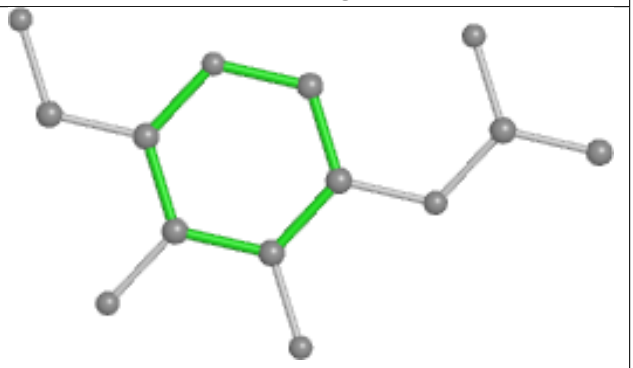
Bond lengths



Bond angles

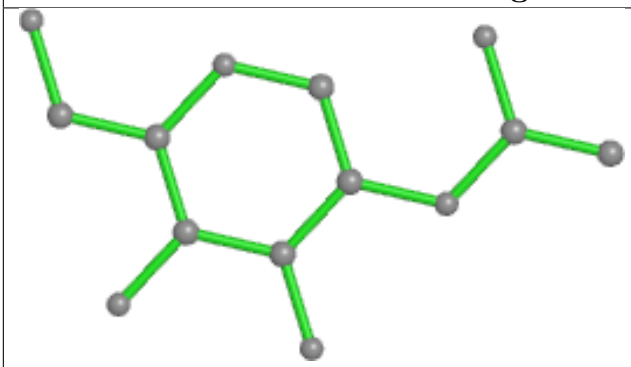


Torsions

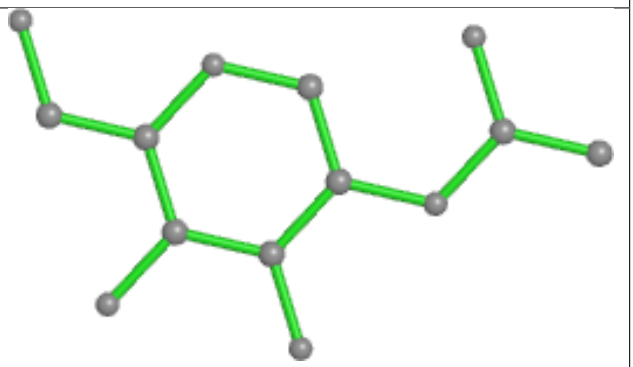


Rings

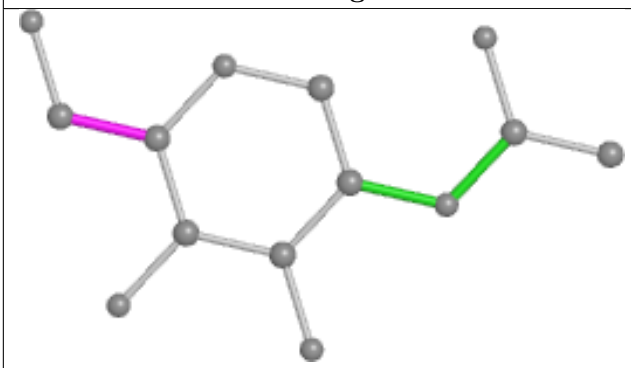
Ligand NAG A 1312



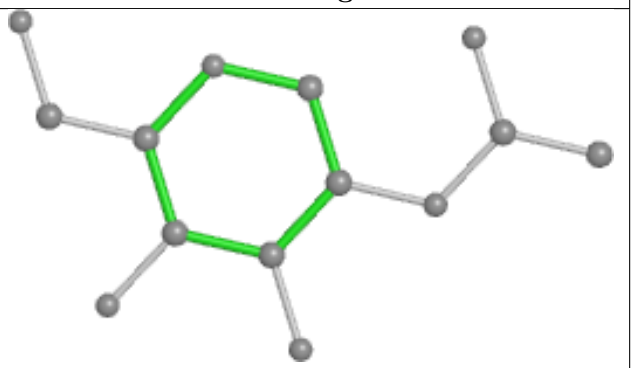
Bond lengths



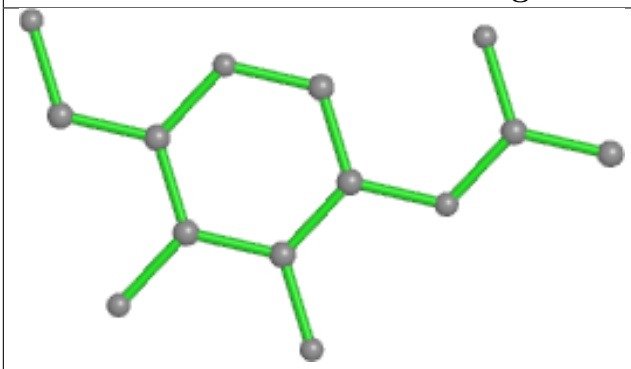
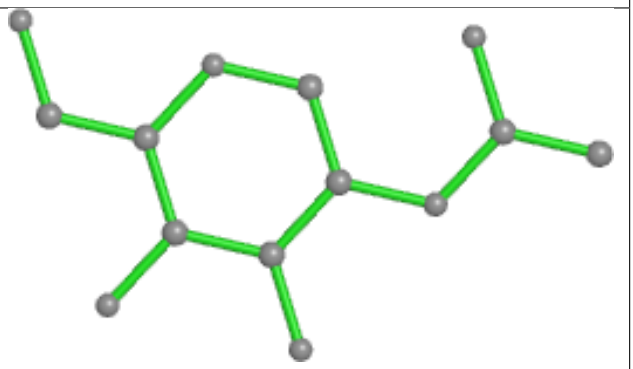
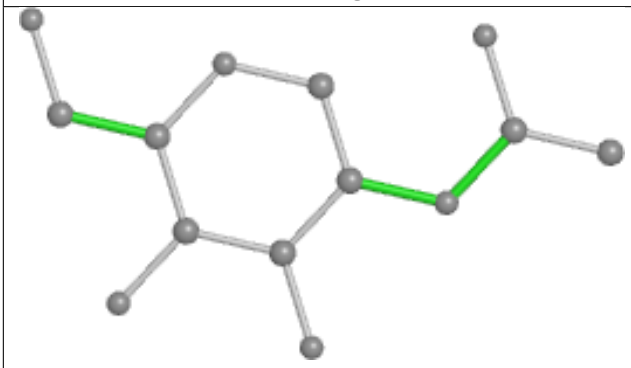
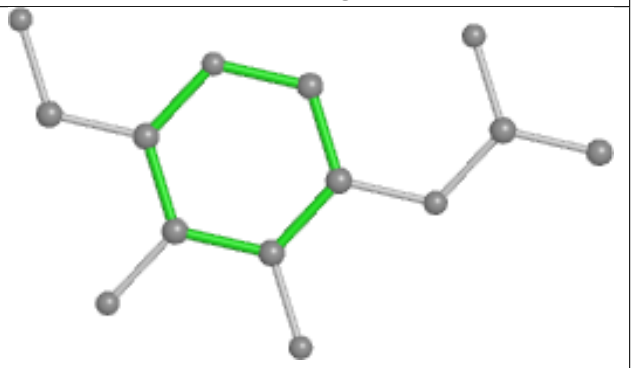
Bond angles

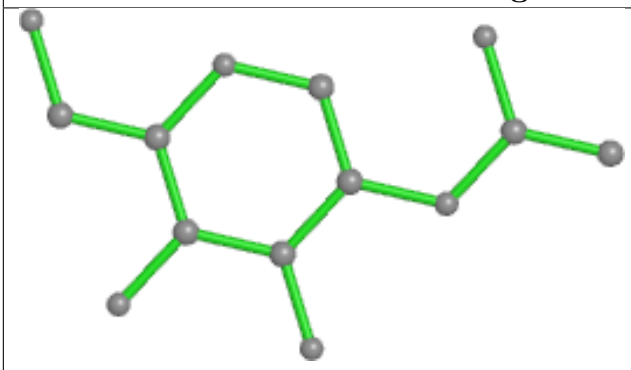
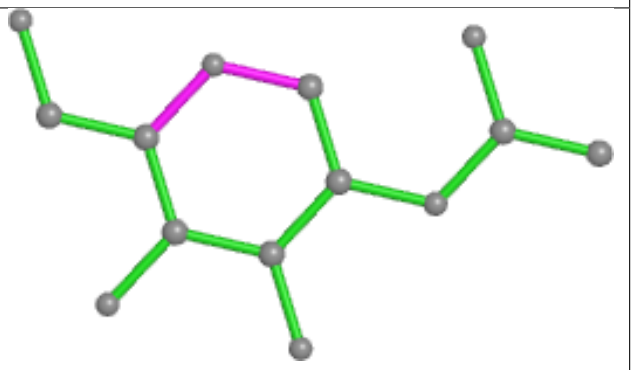
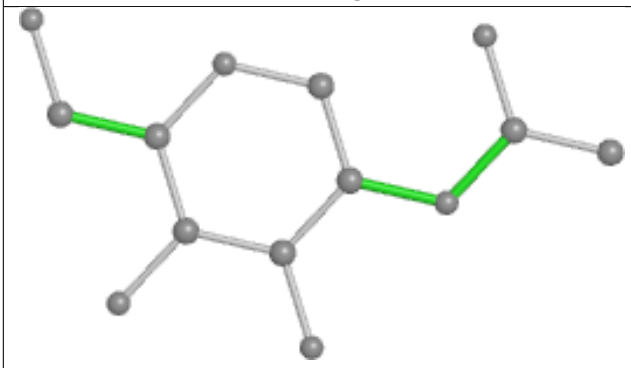
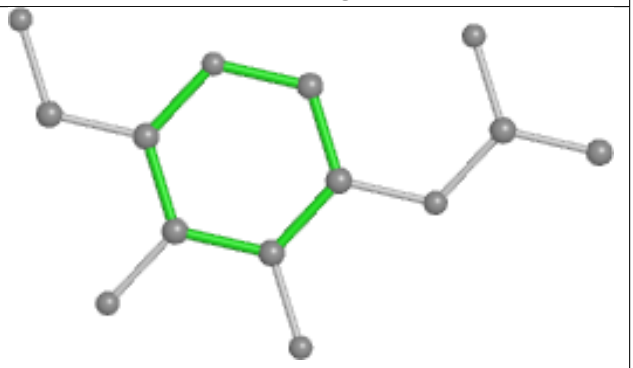


Torsions

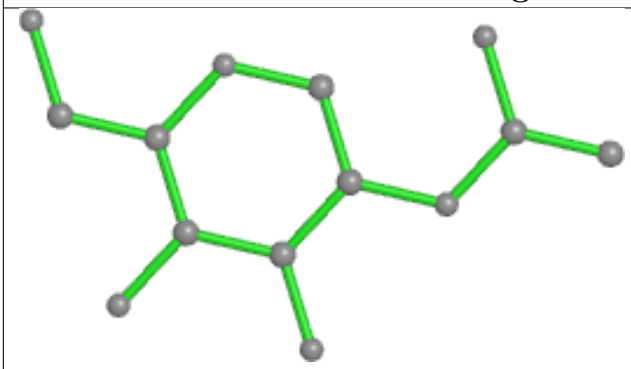


Rings

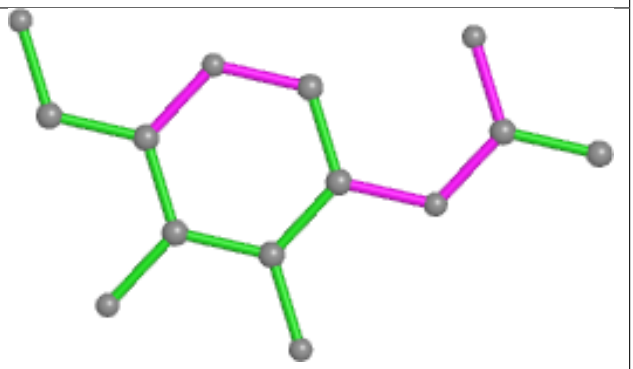
Ligand NAG B 1309	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand NAG A 1305	
	
Bond lengths	Bond angles
	
Torsions	Rings

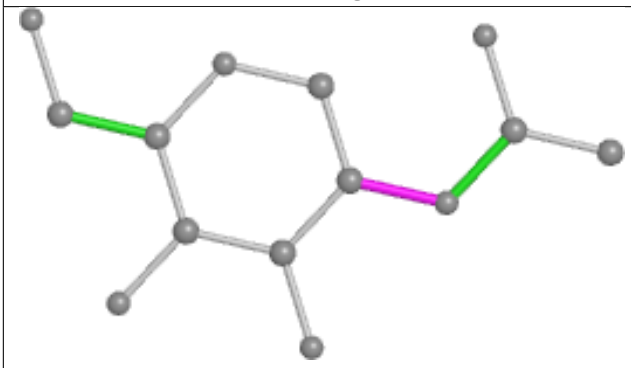
Ligand NAG B 1310



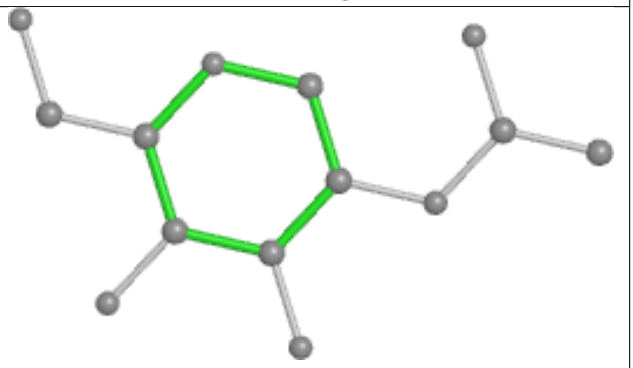
Bond lengths



Bond angles

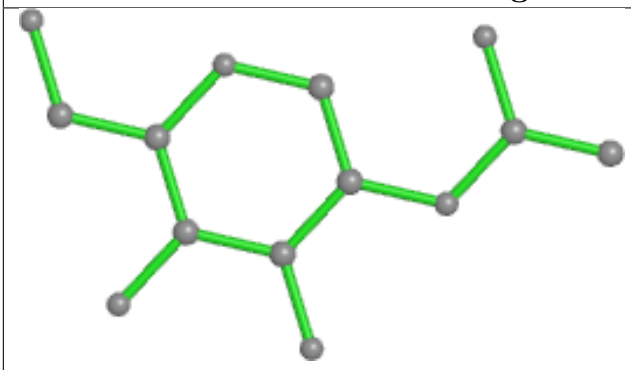


Torsions

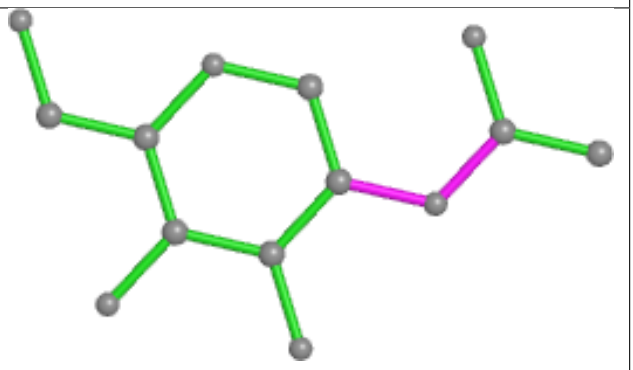


Rings

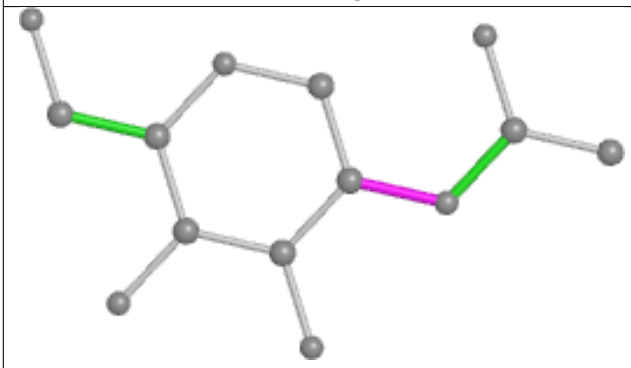
Ligand NAG A 1311



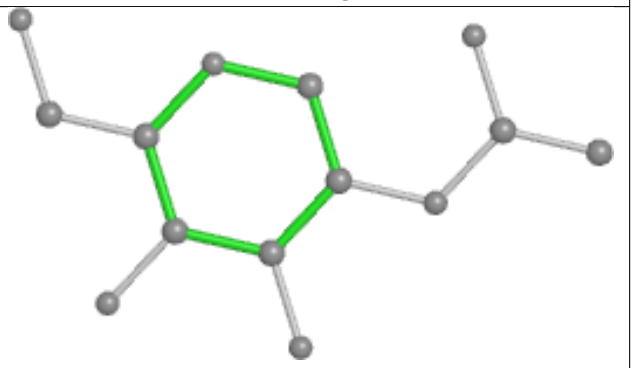
Bond lengths



Bond angles

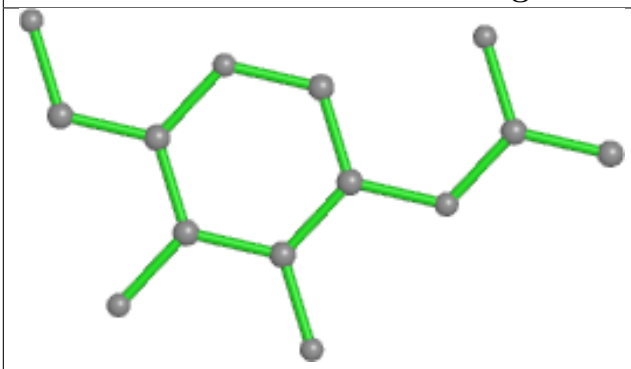


Torsions

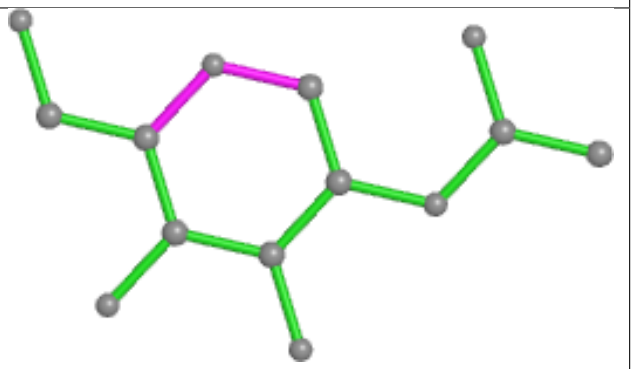


Rings

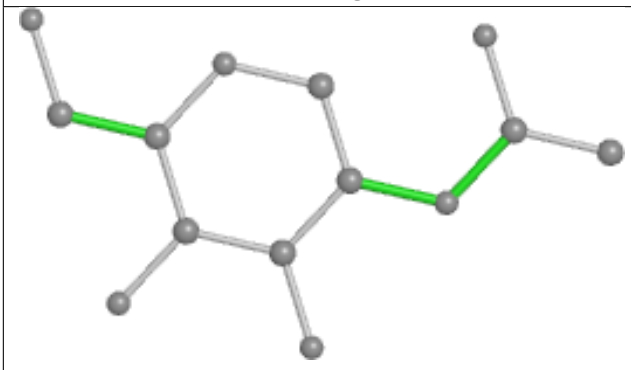
Ligand NAG B 1306



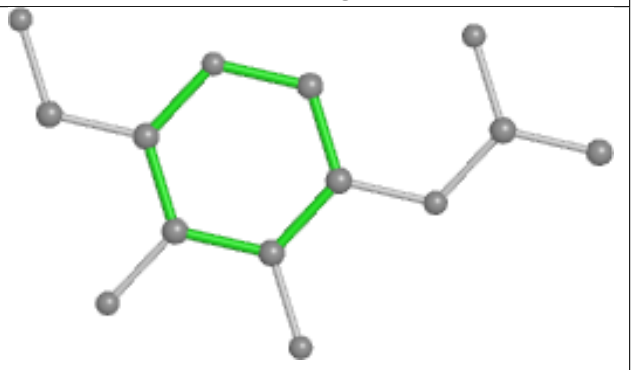
Bond lengths



Bond angles

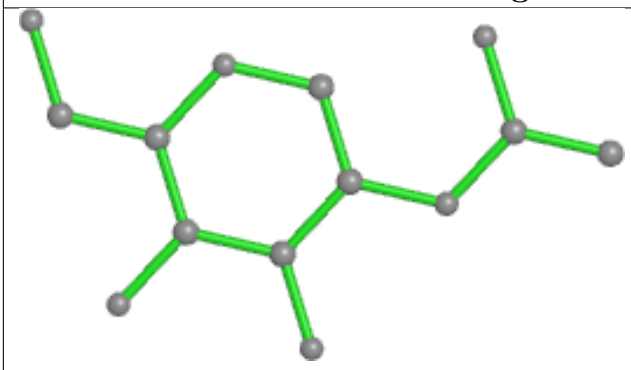


Torsions

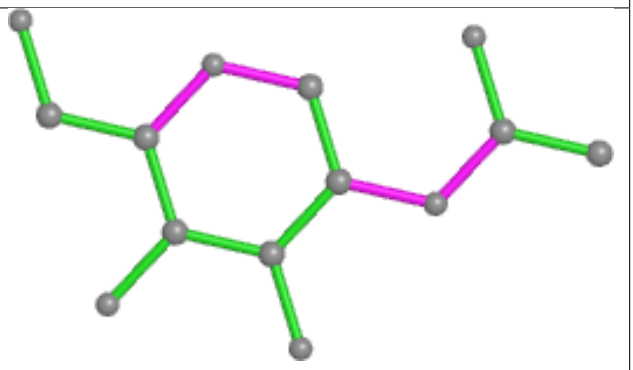


Rings

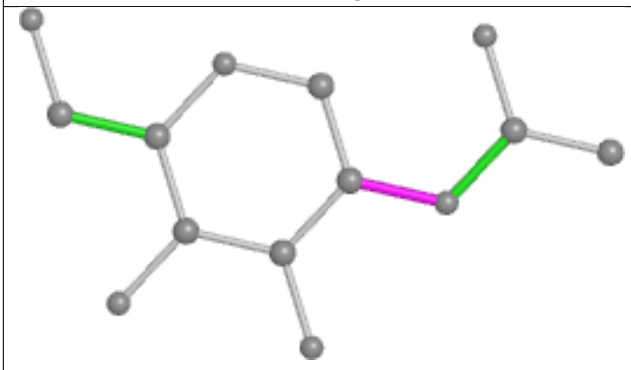
Ligand NAG C 1313



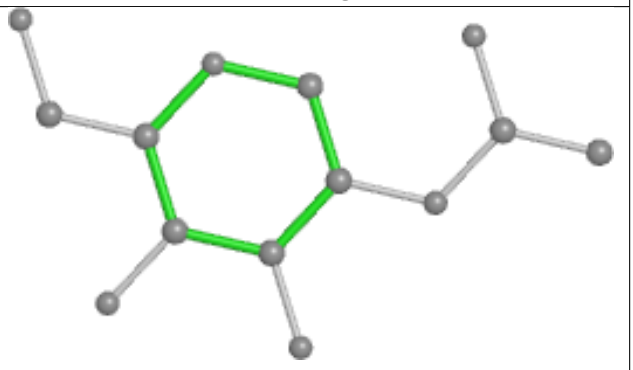
Bond lengths



Bond angles

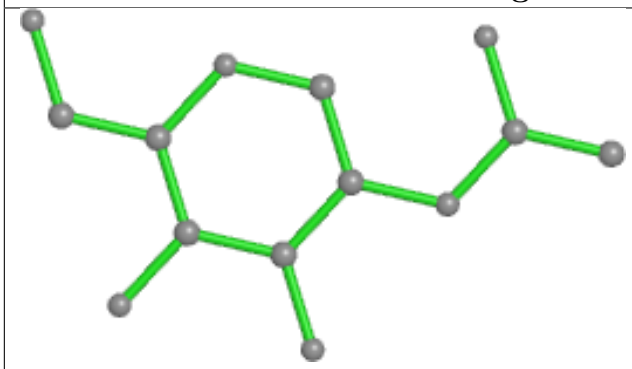


Torsions

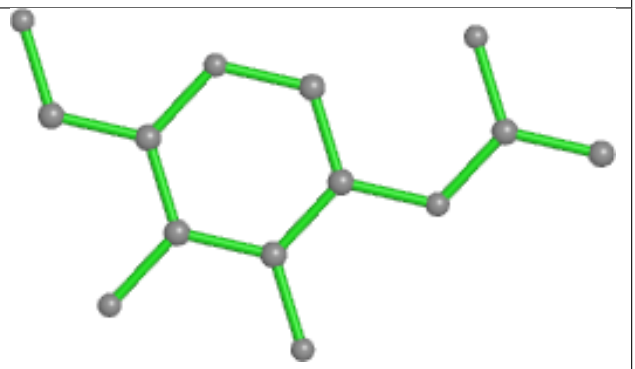


Rings

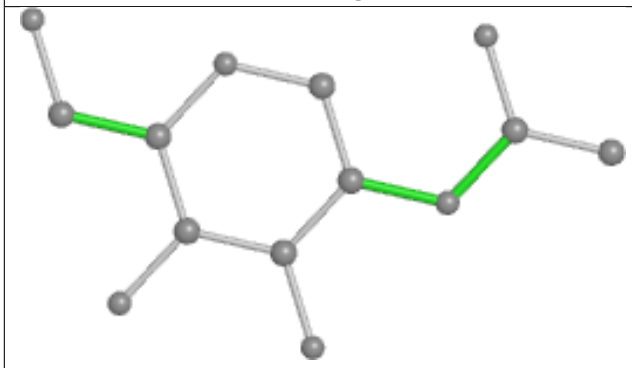
Ligand NAG A 1303



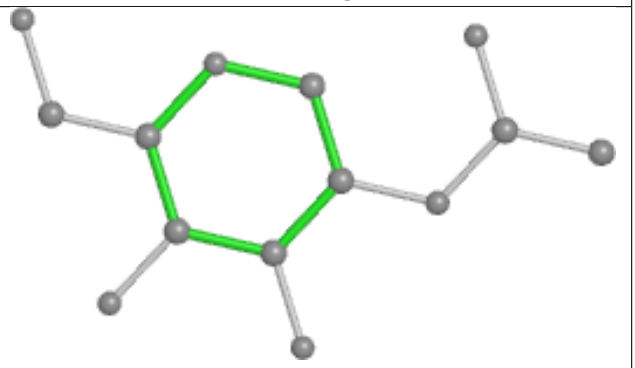
Bond lengths



Bond angles

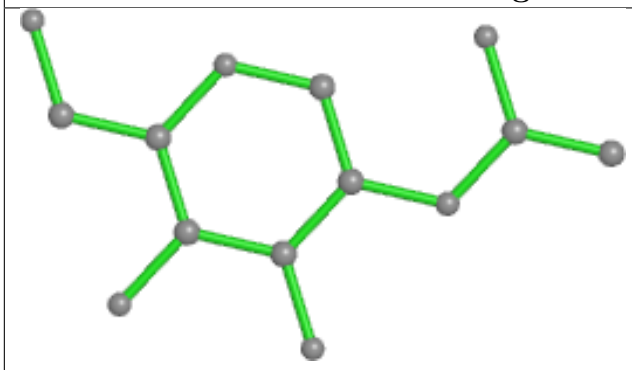


Torsions

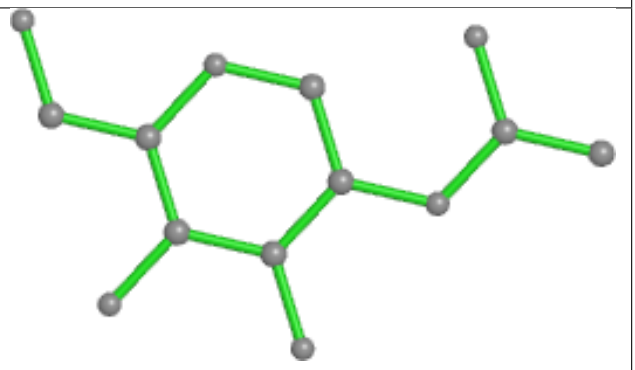


Rings

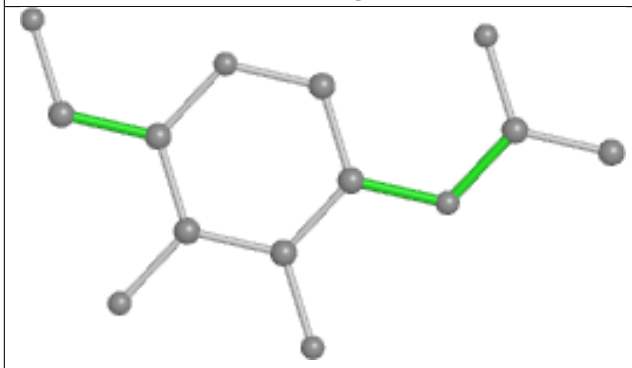
Ligand NAG C 1305



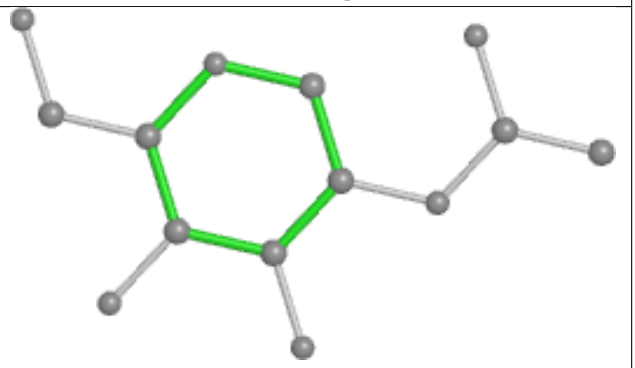
Bond lengths



Bond angles

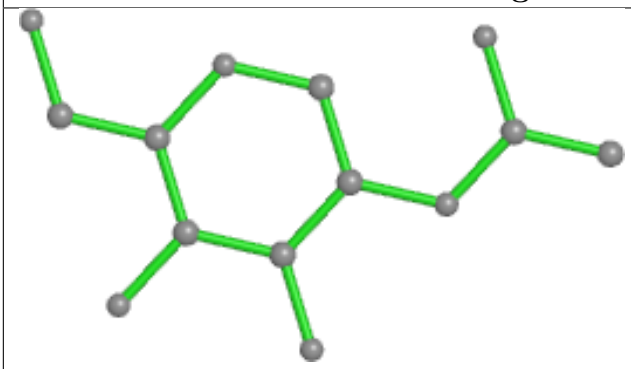


Torsions

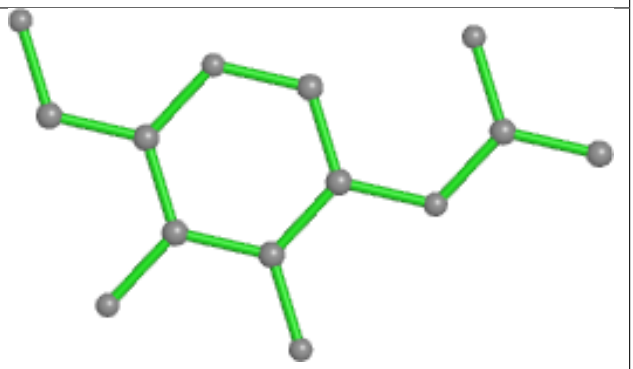


Rings

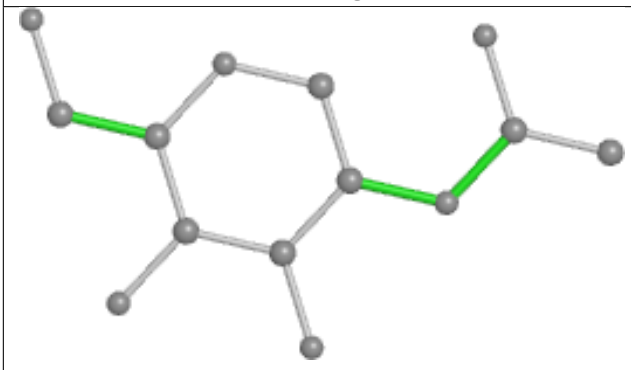
Ligand NAG B 1313



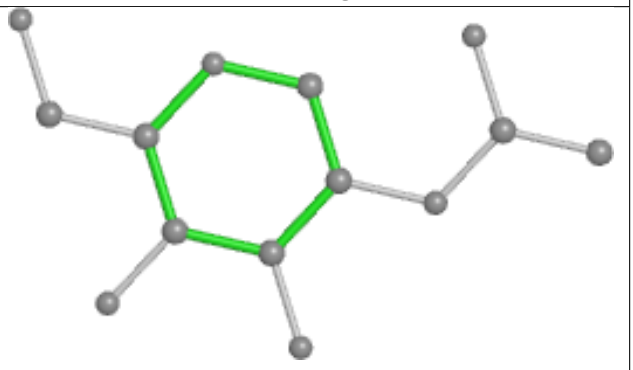
Bond lengths



Bond angles

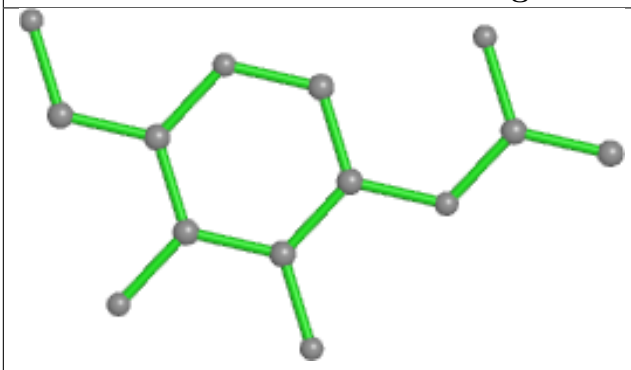


Torsions

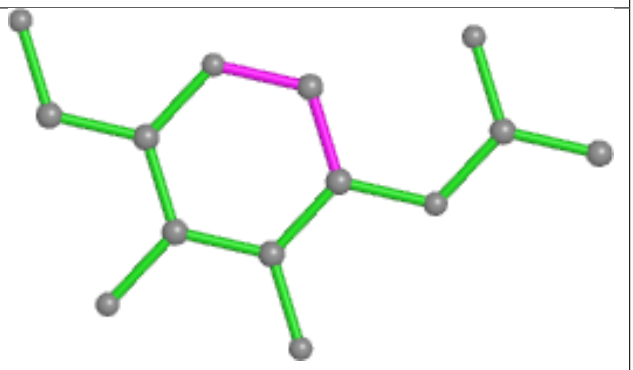


Rings

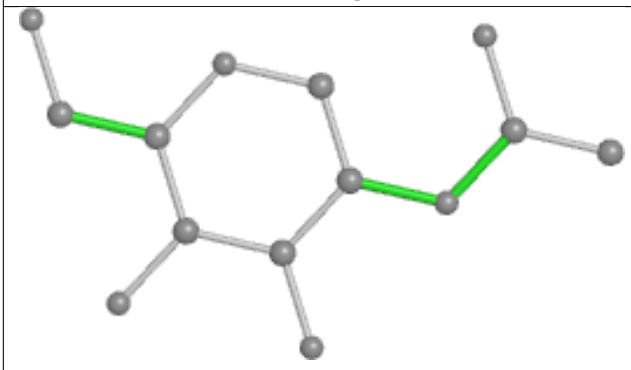
Ligand NAG C 1310



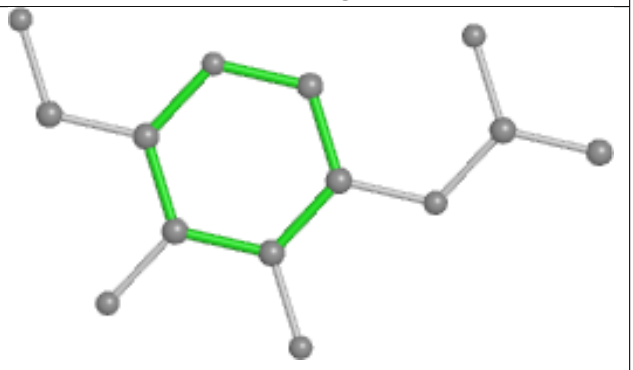
Bond lengths



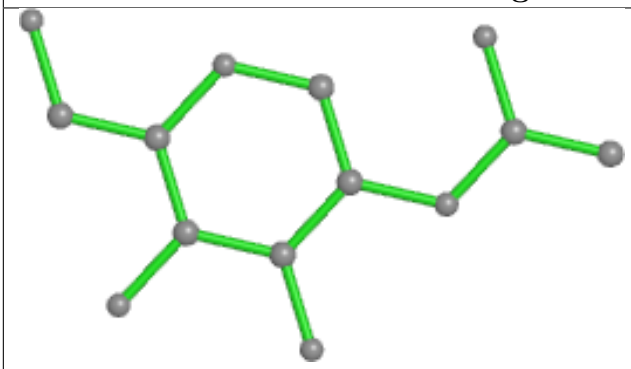
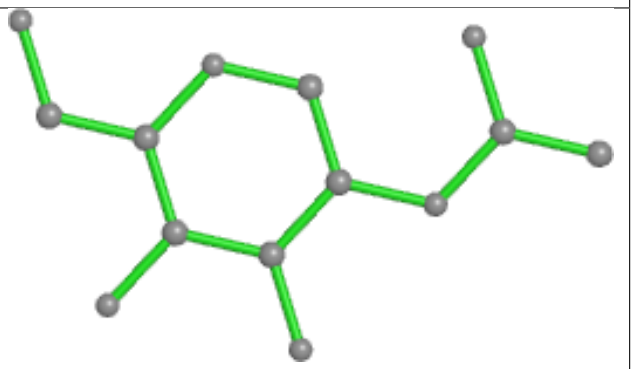
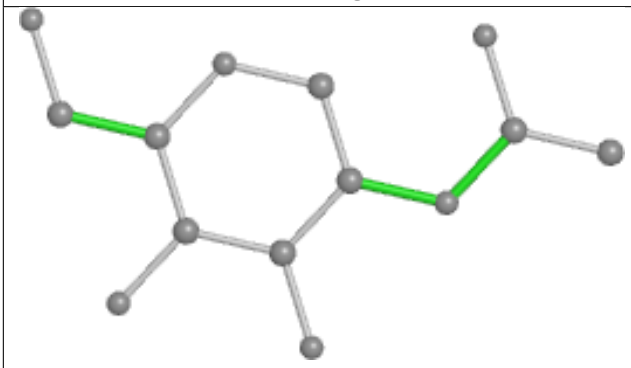
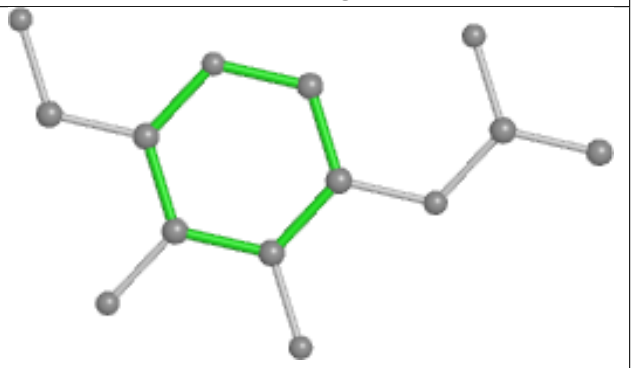
Bond angles

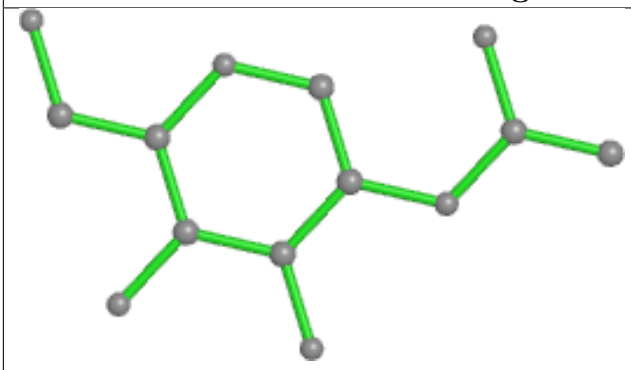
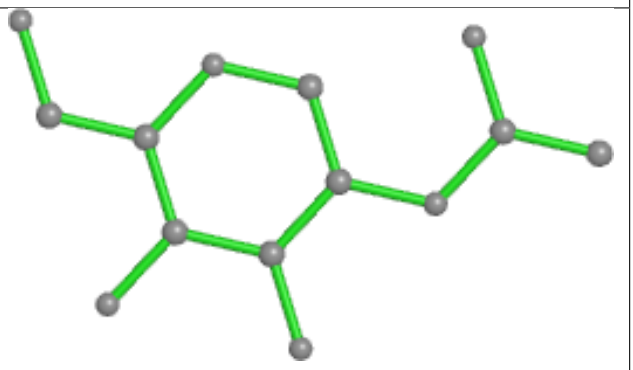
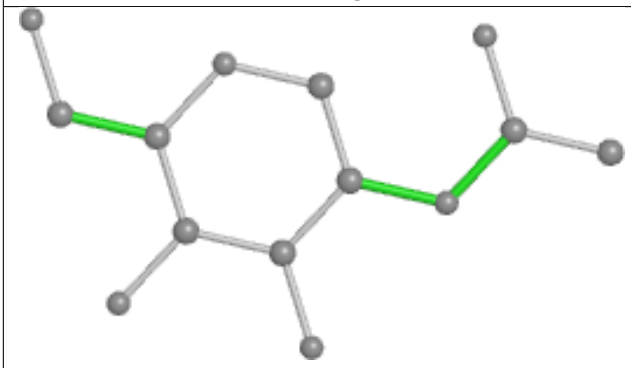
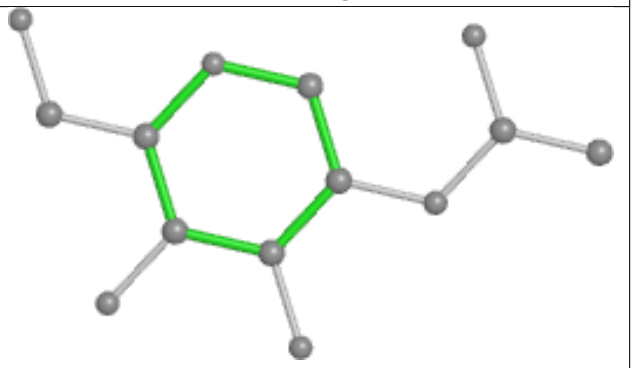


Torsions

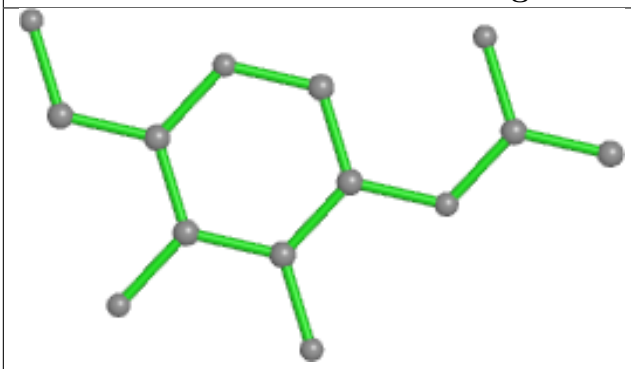


Rings

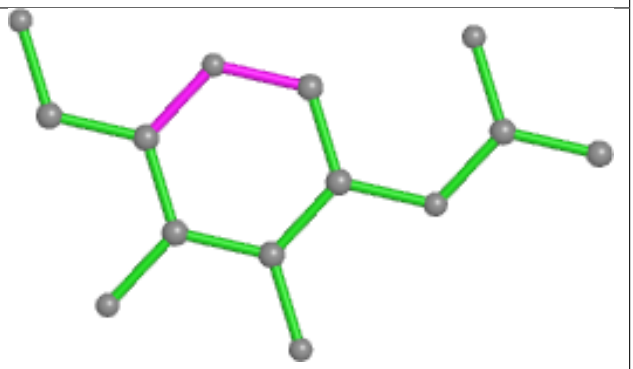
Ligand NAG B 1305	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand NAG B 1304	
	
Bond lengths	Bond angles
	
Torsions	Rings

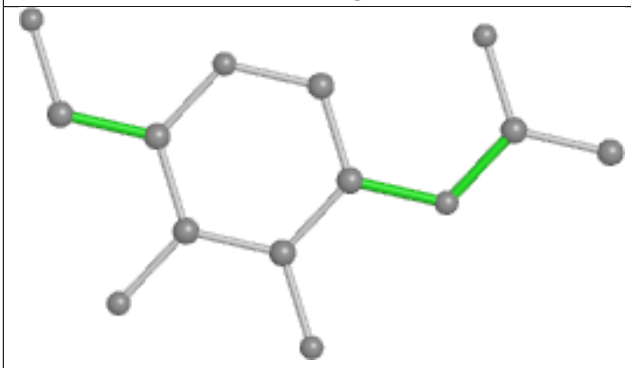
Ligand NAG C 1307



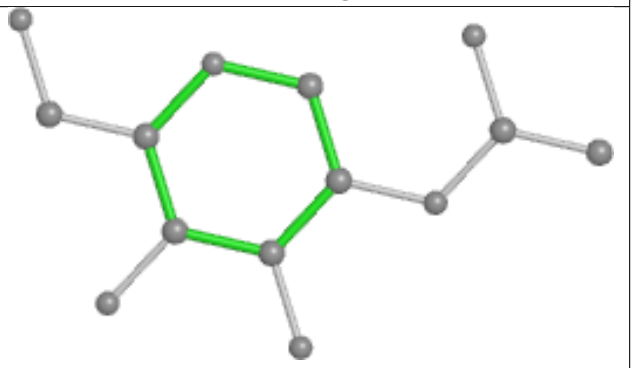
Bond lengths



Bond angles

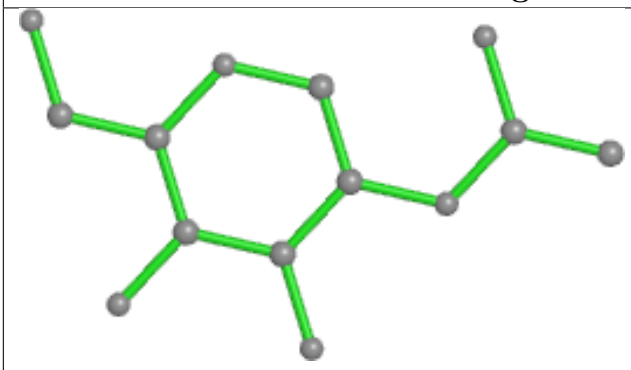


Torsions

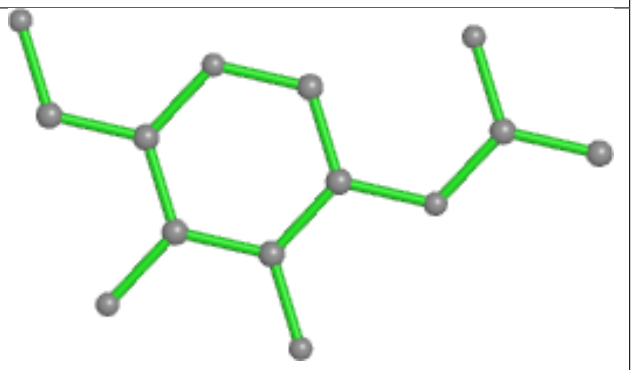


Rings

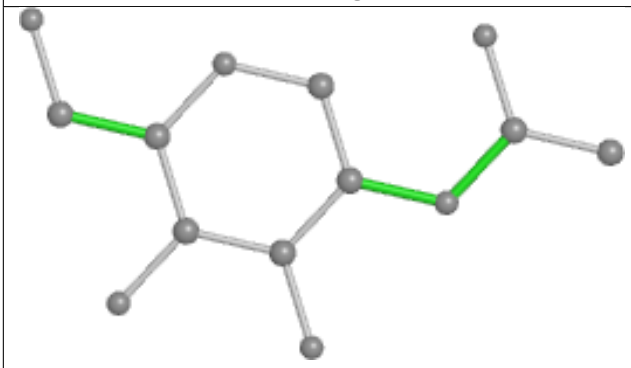
Ligand NAG B 1311



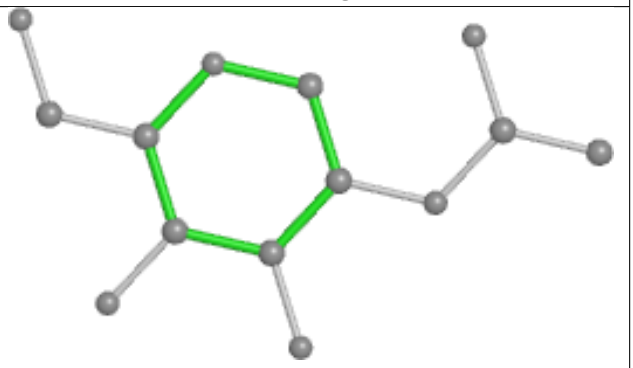
Bond lengths



Bond angles

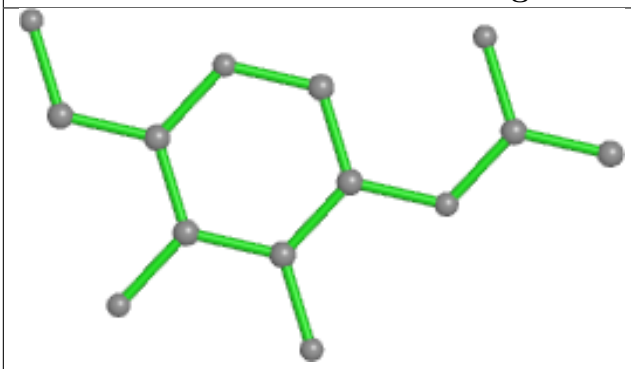


Torsions

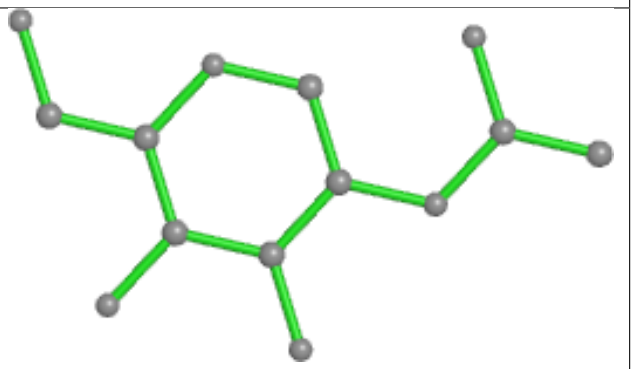


Rings

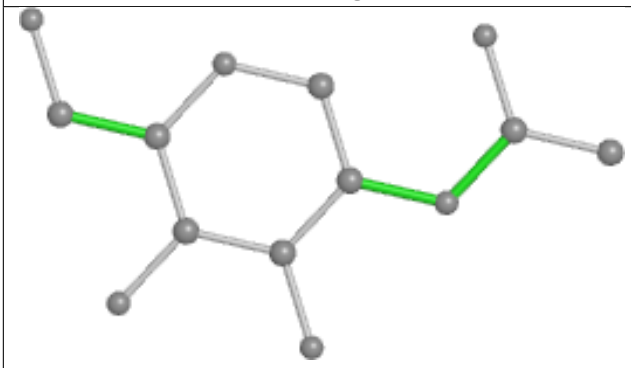
Ligand NAG C 1308



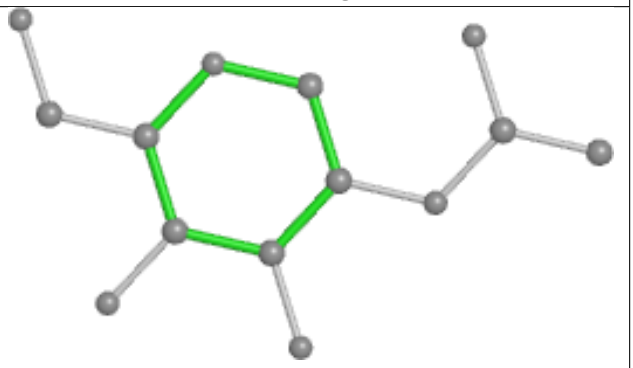
Bond lengths



Bond angles

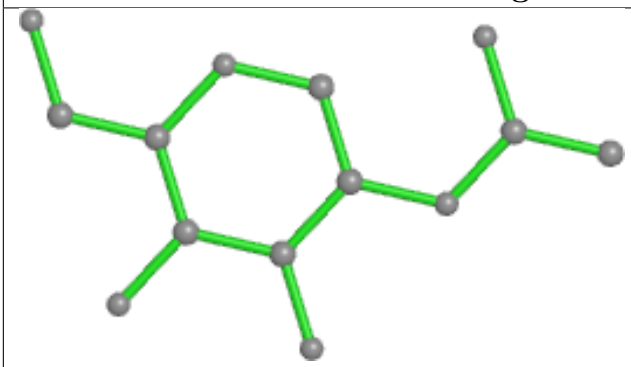


Torsions

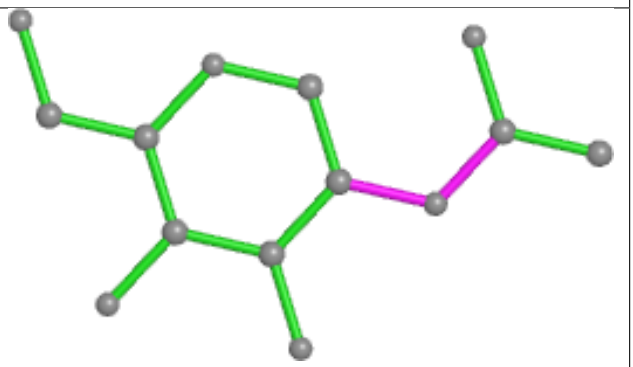


Rings

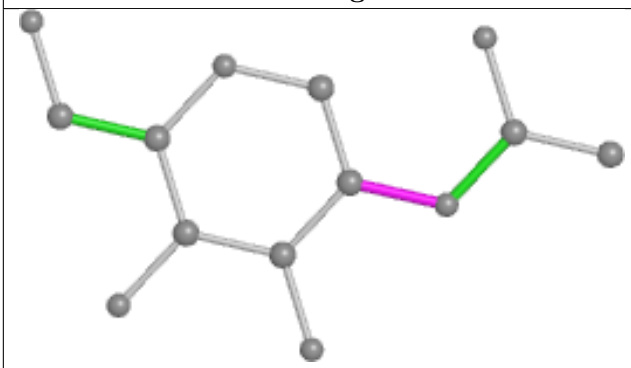
Ligand NAG B 1312



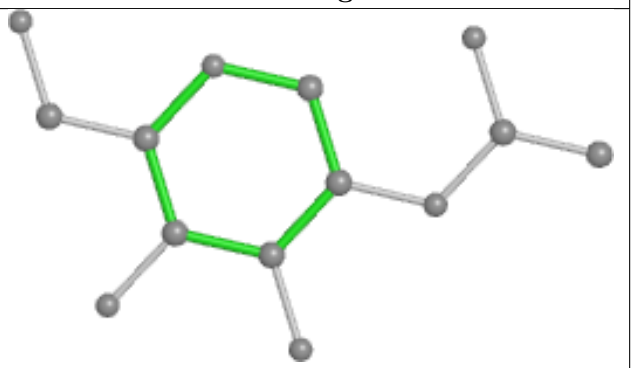
Bond lengths



Bond angles

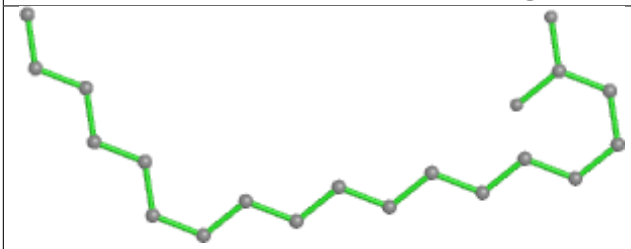


Torsions

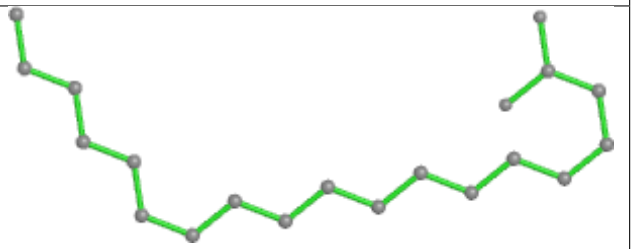


Rings

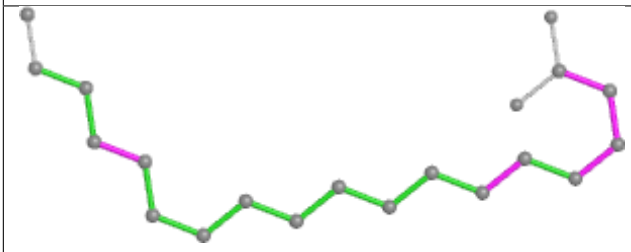
Ligand EIC B 1301



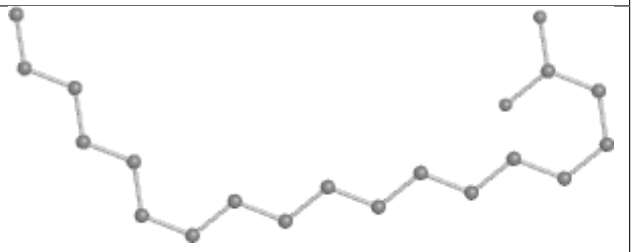
Bond lengths



Bond angles

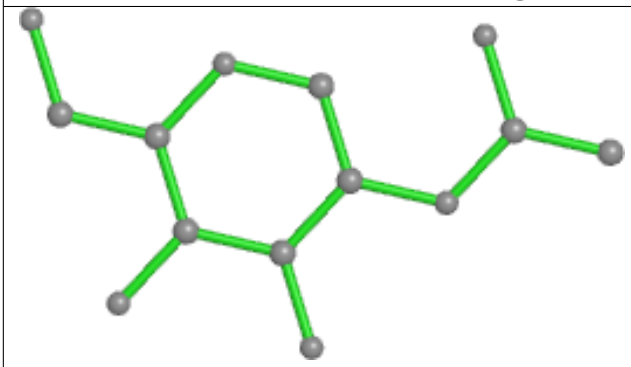


Torsions

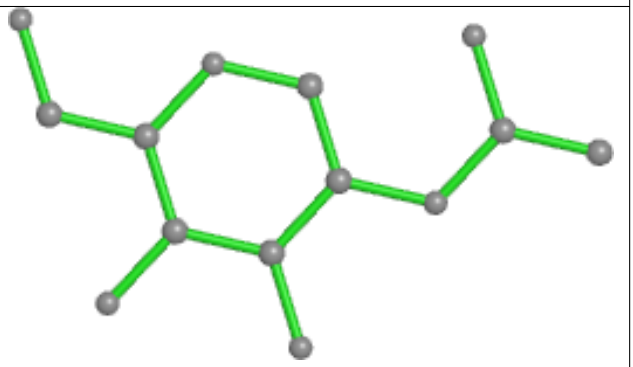


Rings

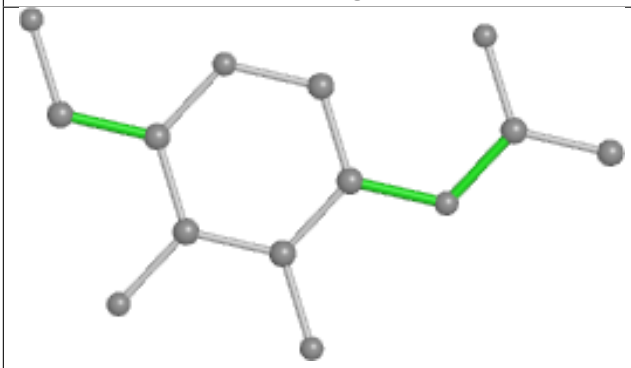
Ligand NAG C 1315



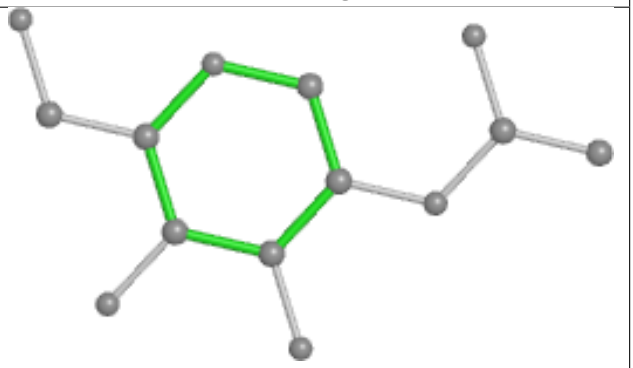
Bond lengths



Bond angles

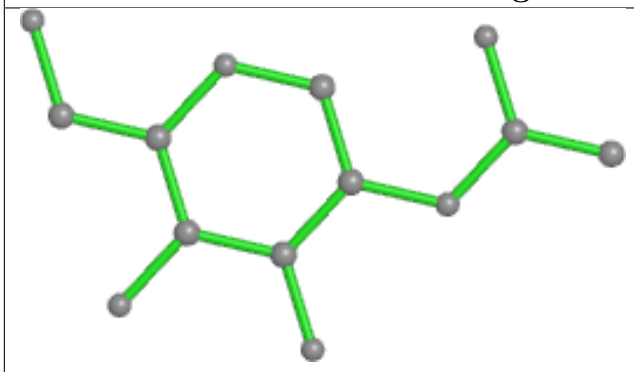


Torsions

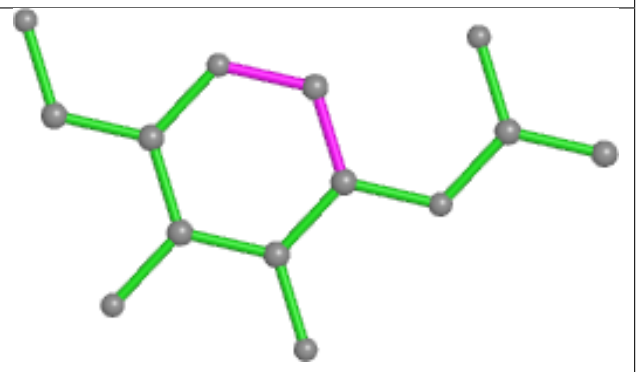


Rings

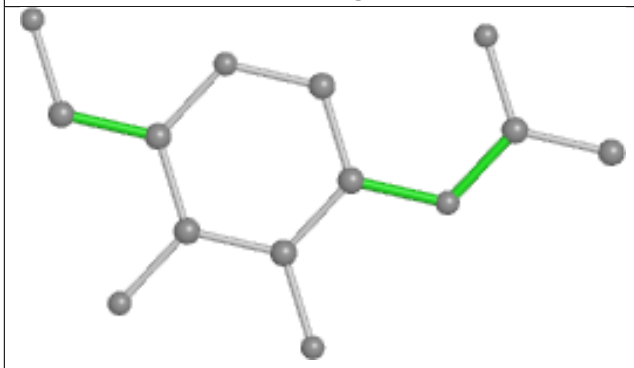
Ligand NAG C 1314



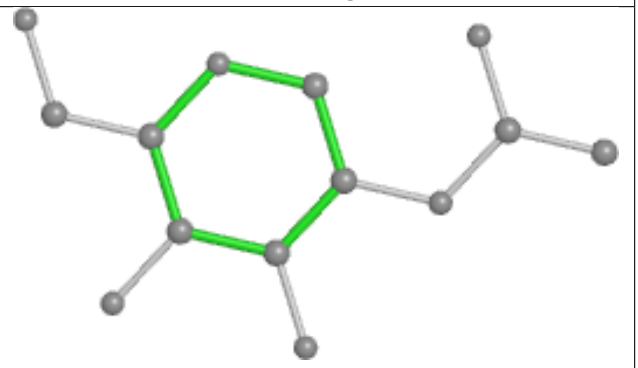
Bond lengths



Bond angles

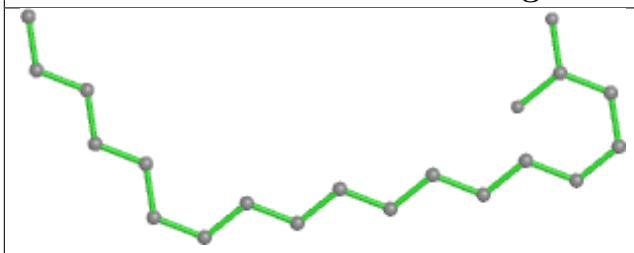


Torsions

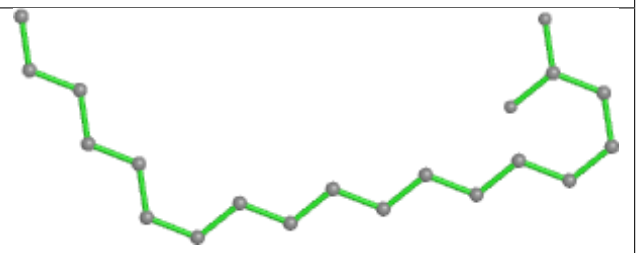


Rings

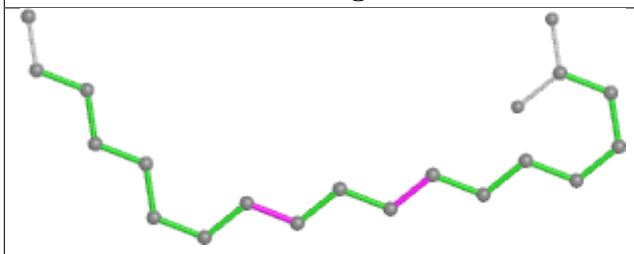
Ligand EIC C 1301



Bond lengths



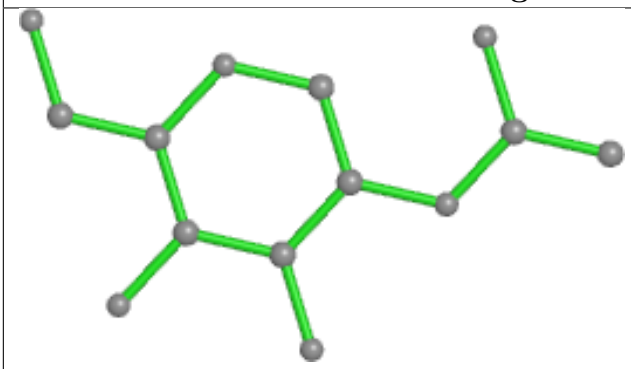
Bond angles



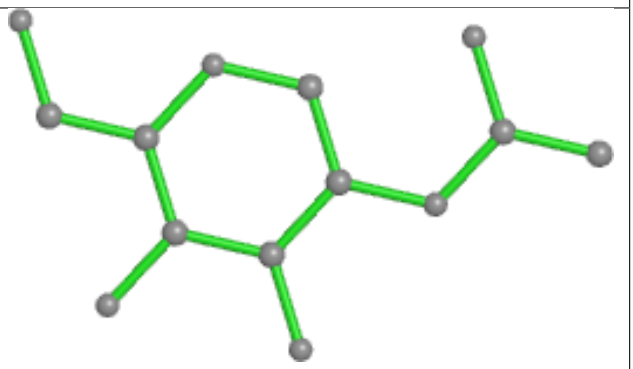
Torsions

Rings

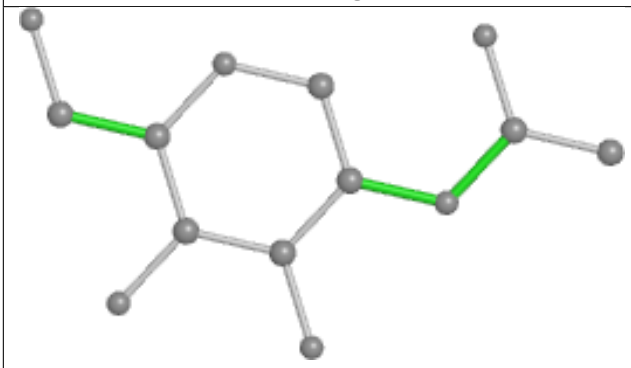
Ligand NAG A 1313



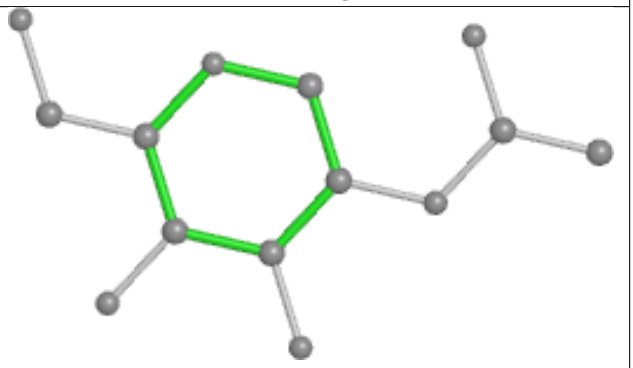
Bond lengths



Bond angles

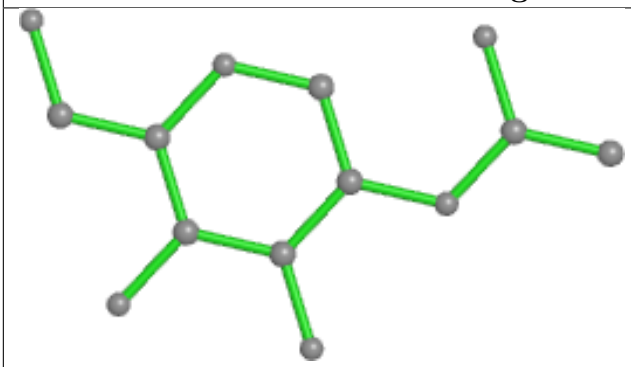


Torsions

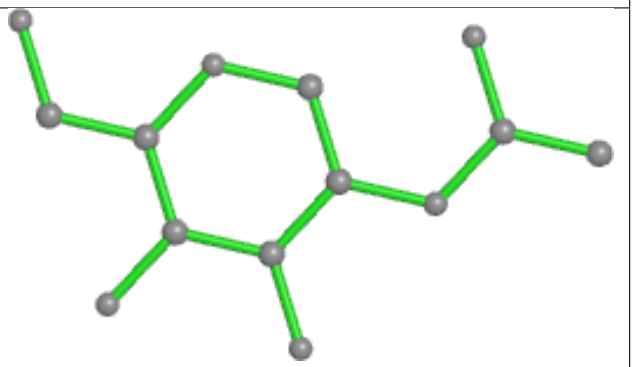


Rings

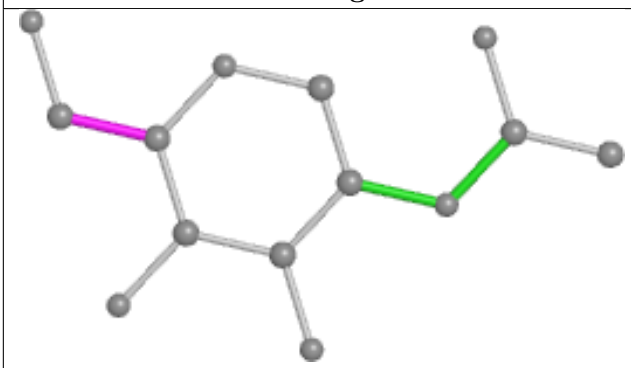
Ligand NAG A 1301



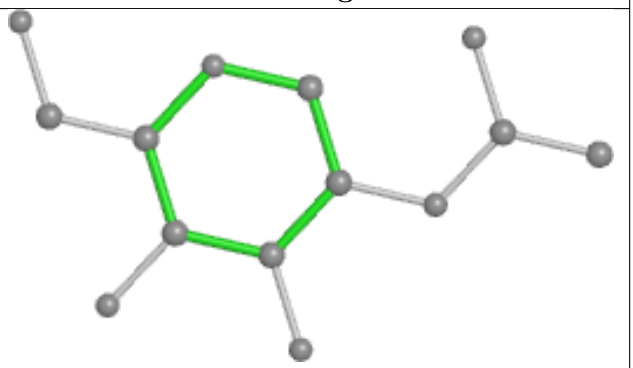
Bond lengths



Bond angles

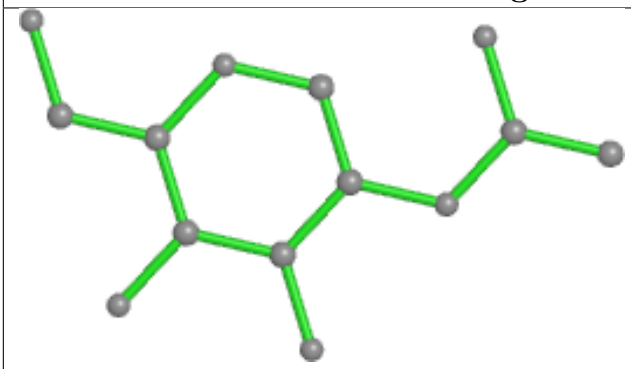


Torsions

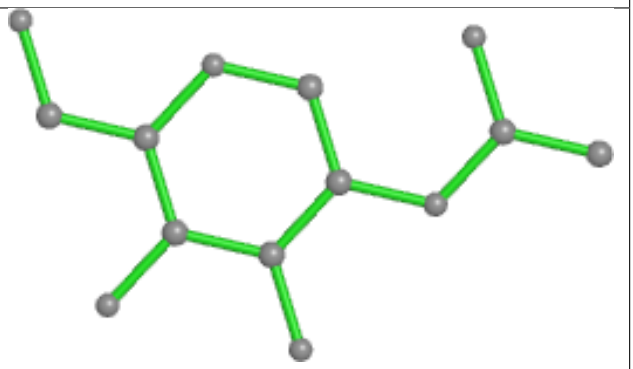


Rings

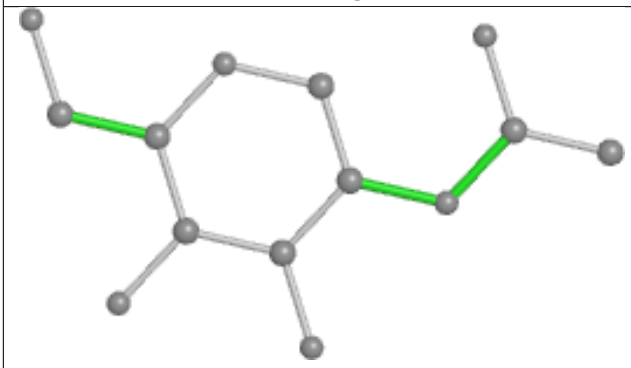
Ligand NAG A 1306



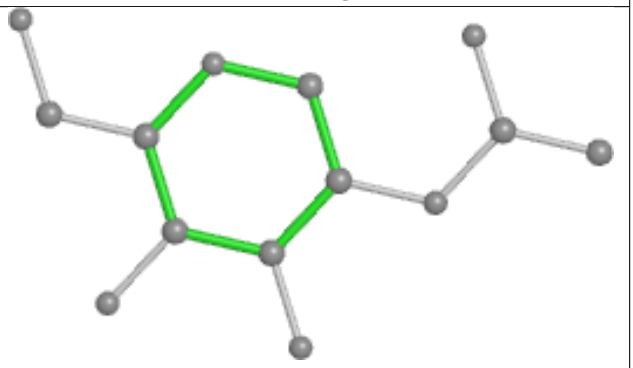
Bond lengths



Bond angles

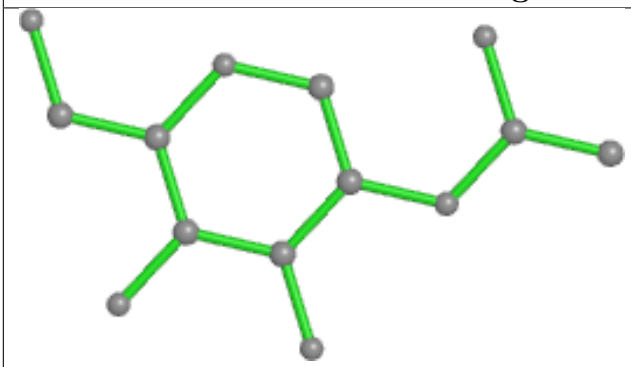


Torsions

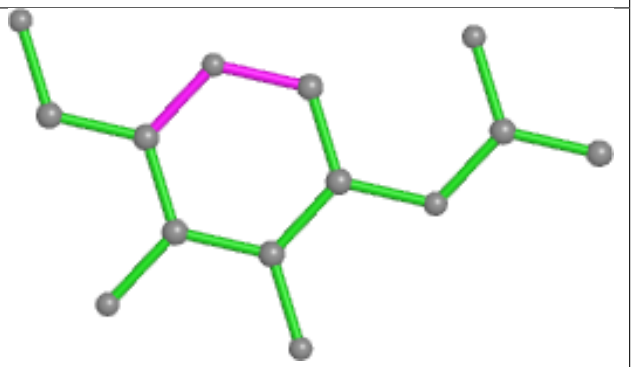


Rings

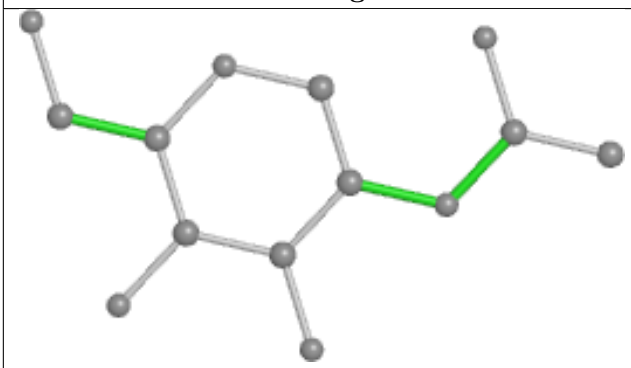
Ligand NAG B 1314



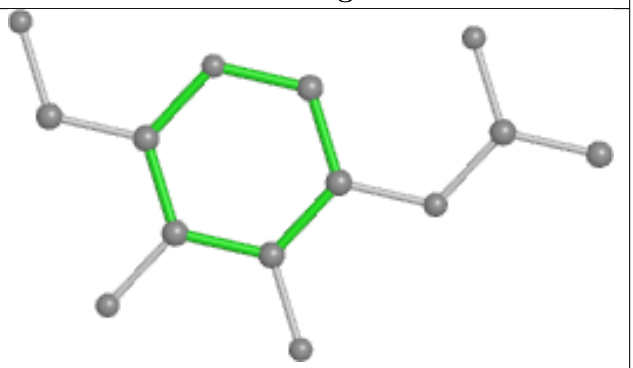
Bond lengths



Bond angles

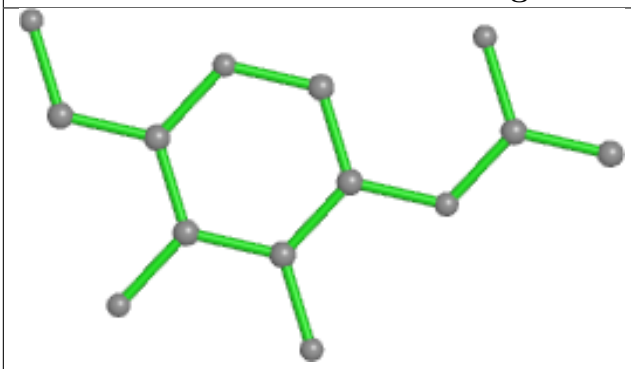


Torsions

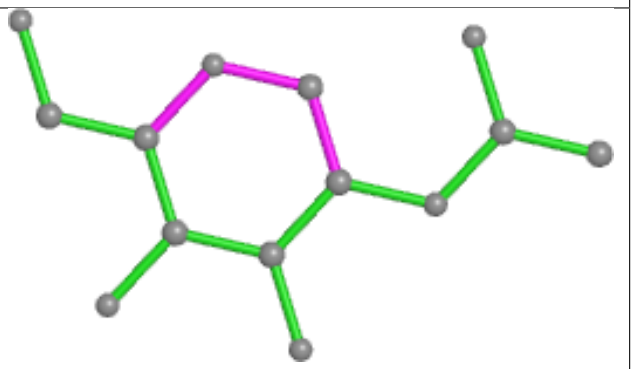


Rings

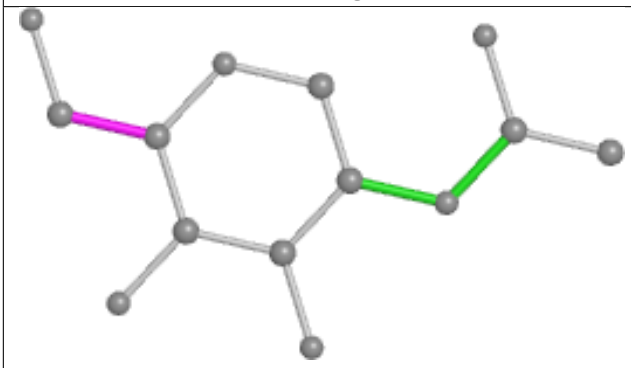
Ligand NAG A 1307



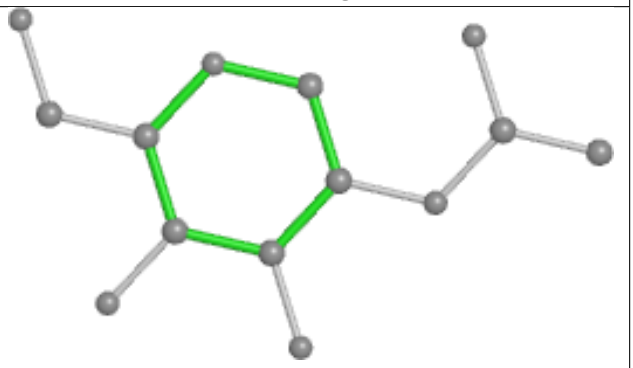
Bond lengths



Bond angles

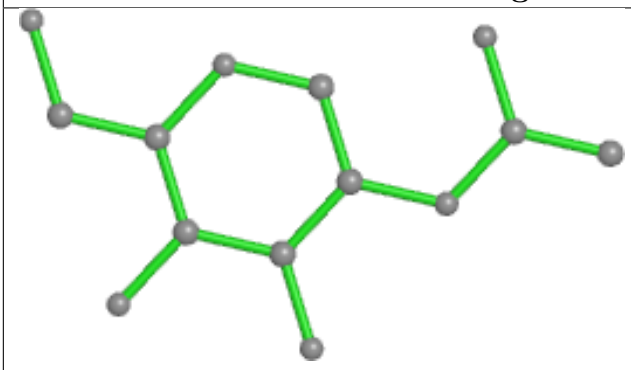


Torsions

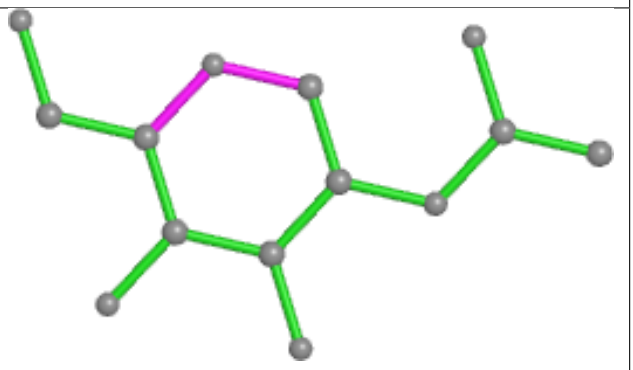


Rings

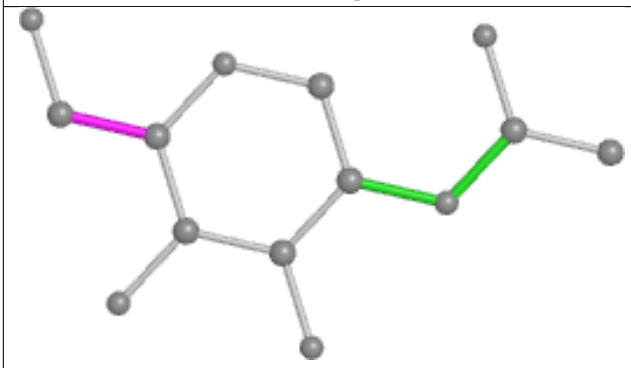
Ligand NAG C 1309



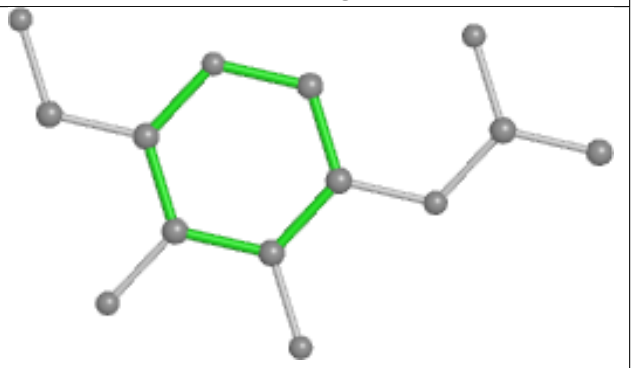
Bond lengths



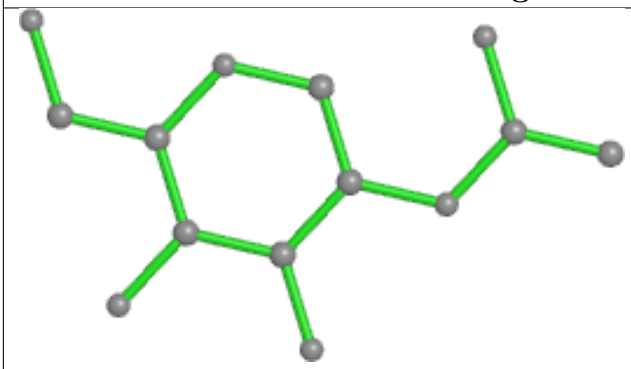
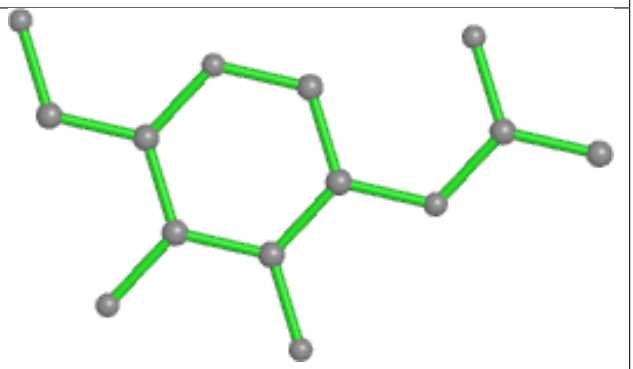
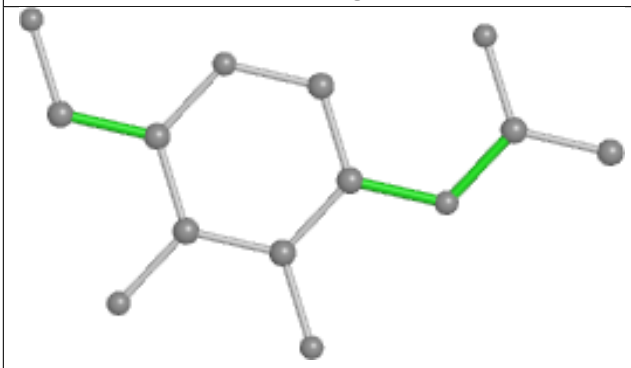
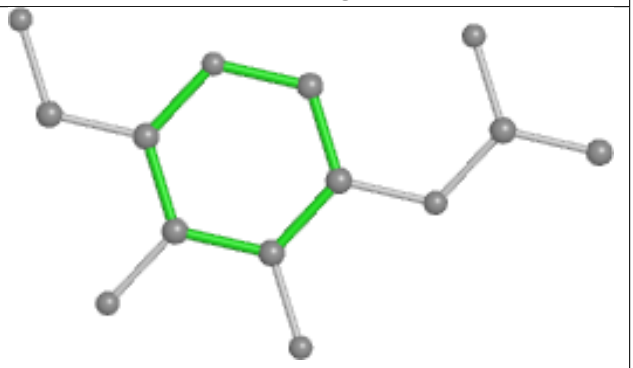
Bond angles

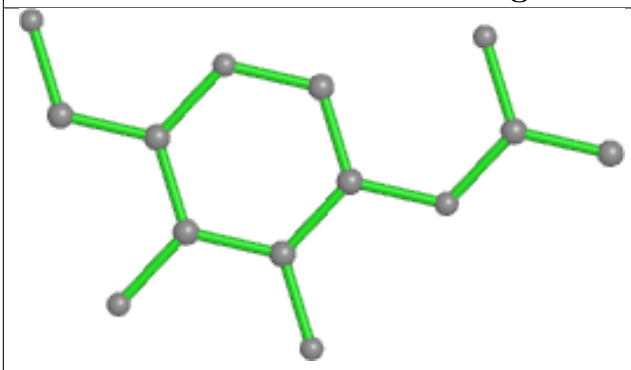
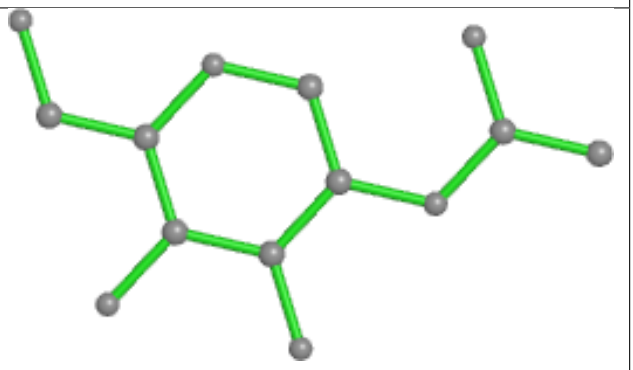
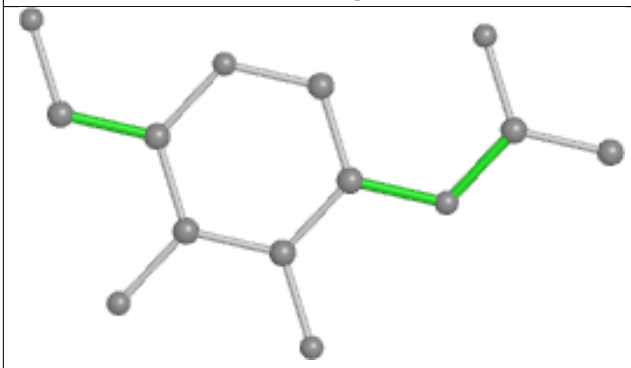
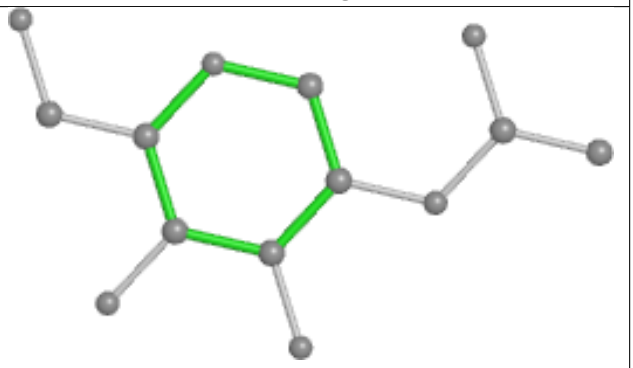


Torsions

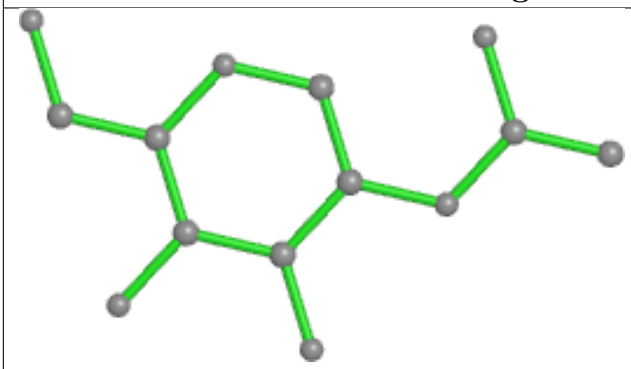


Rings

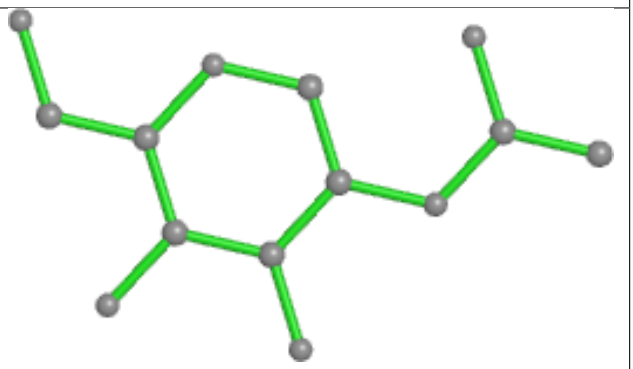
Ligand NAG B 1307	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand NAG A 1302	
	
Bond lengths	Bond angles
	
Torsions	Rings

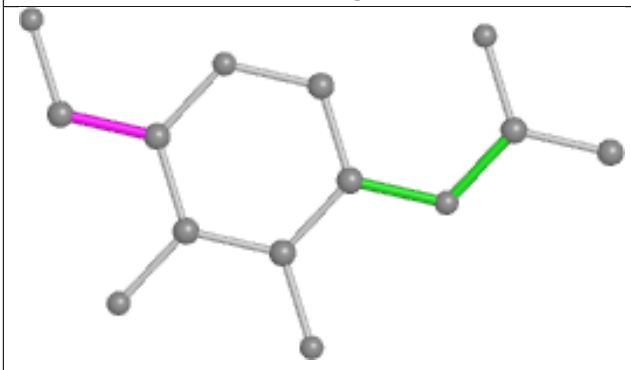
Ligand NAG B 1308



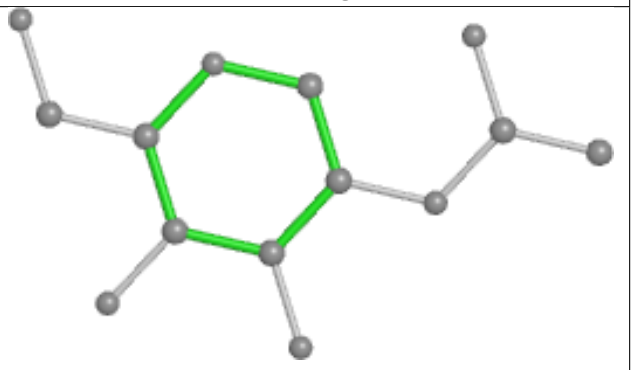
Bond lengths



Bond angles

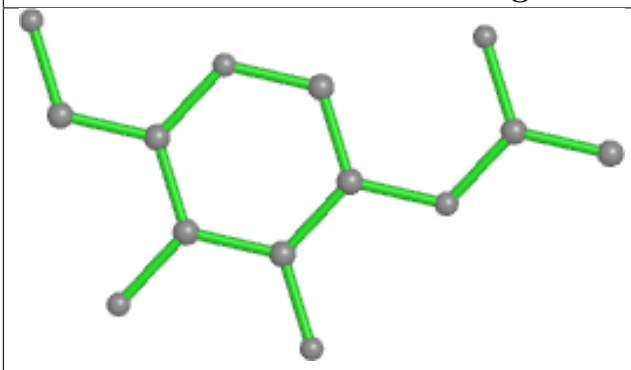


Torsions

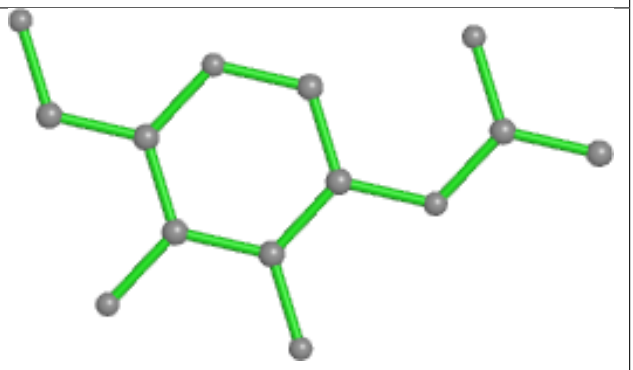


Rings

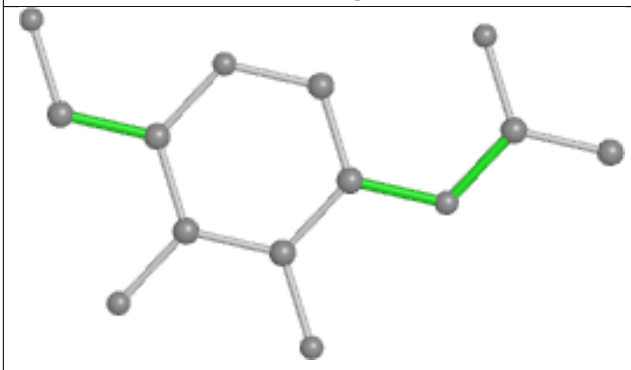
Ligand NAG C 1303



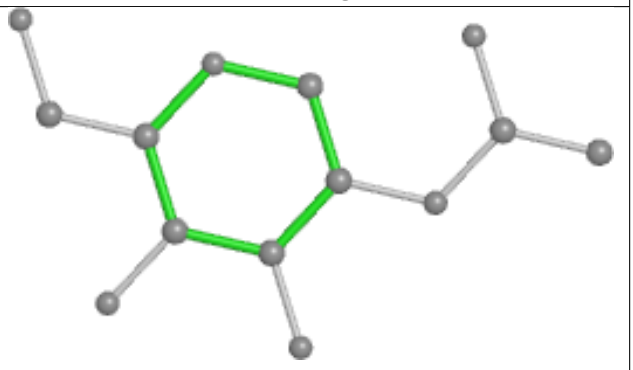
Bond lengths



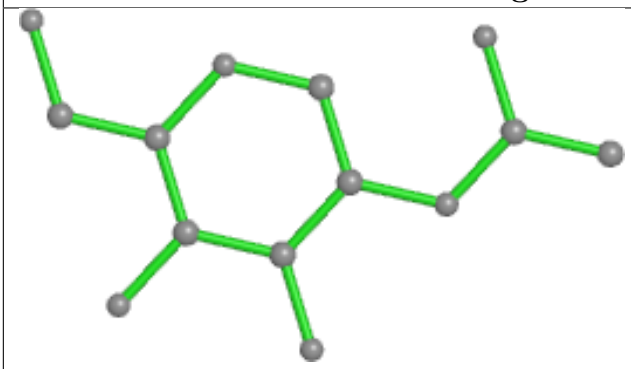
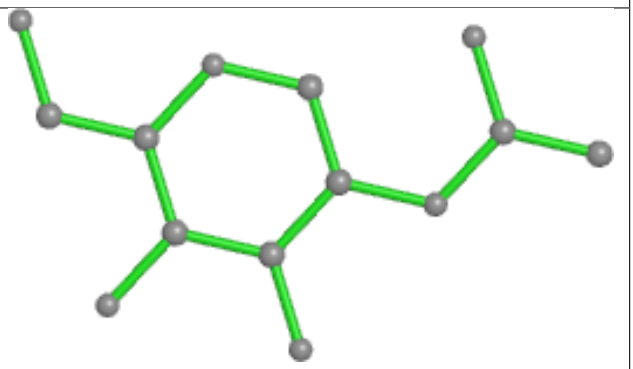
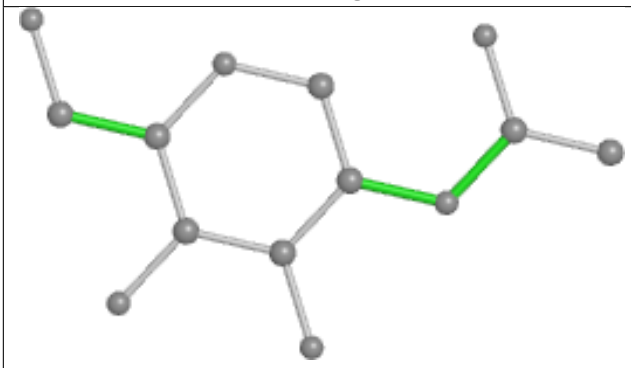
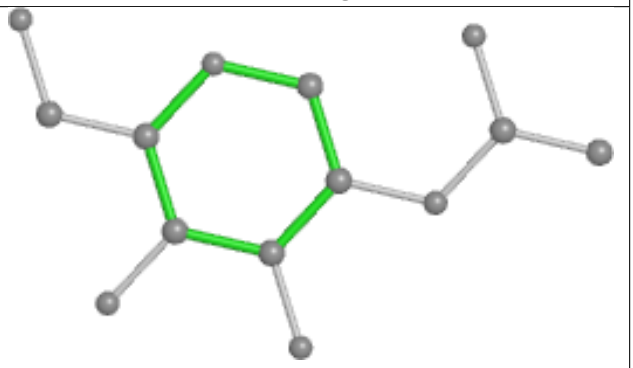
Bond angles

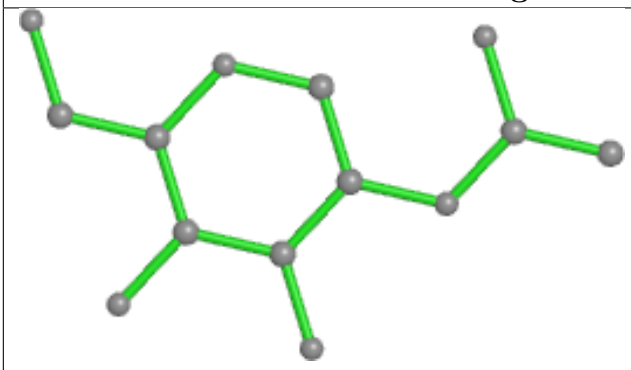
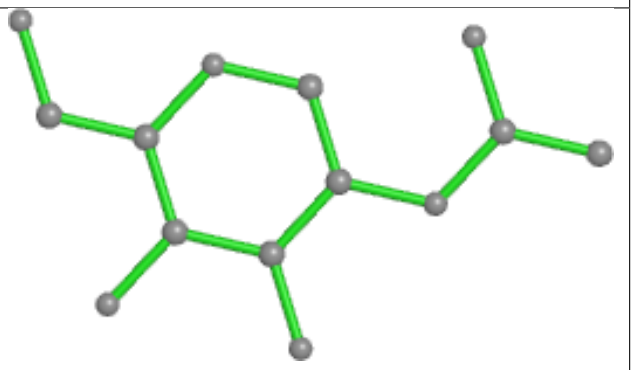
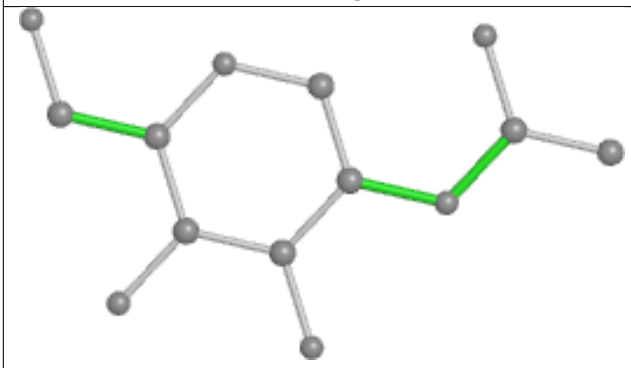
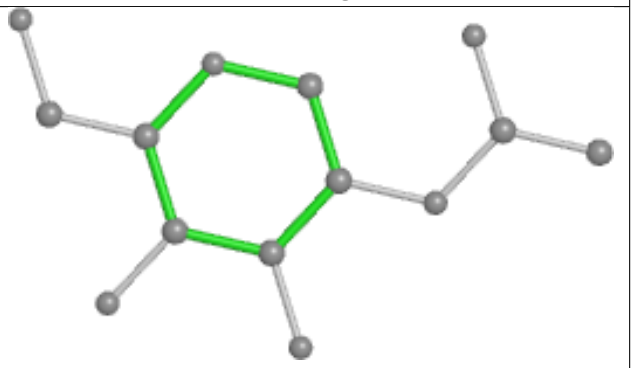


Torsions

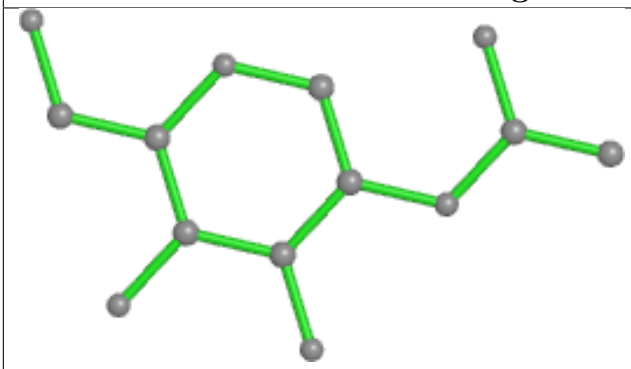


Rings

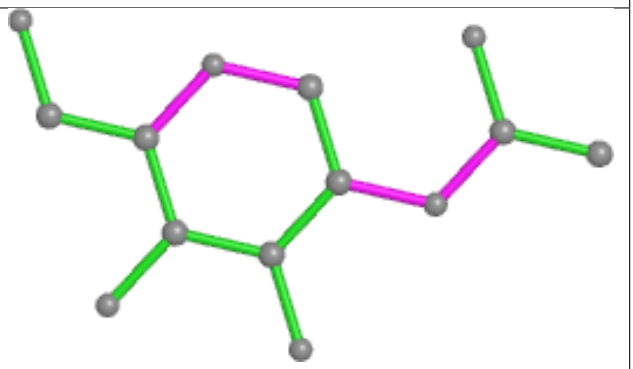
Ligand NAG C 1306	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG A 1304	
 Bond lengths	 Bond angles
 Torsions	 Rings

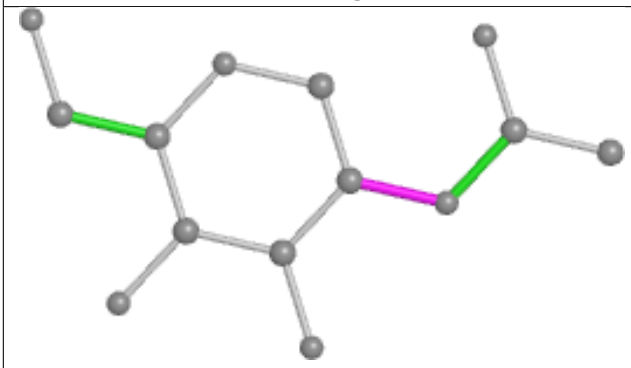
Ligand NAG C 1311



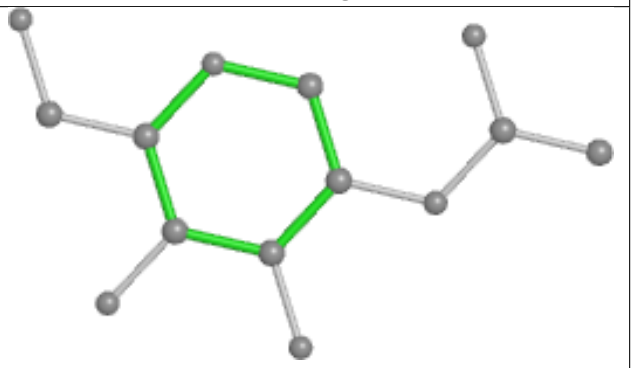
Bond lengths



Bond angles

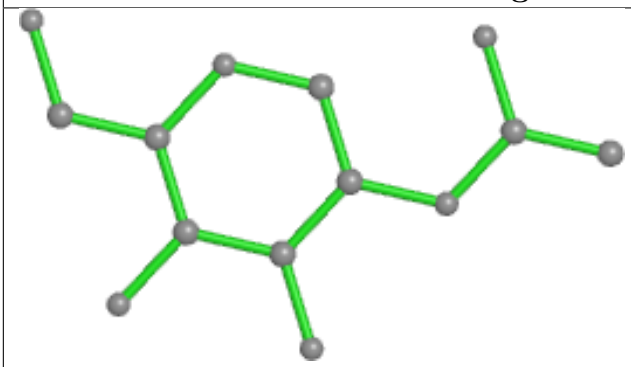


Torsions

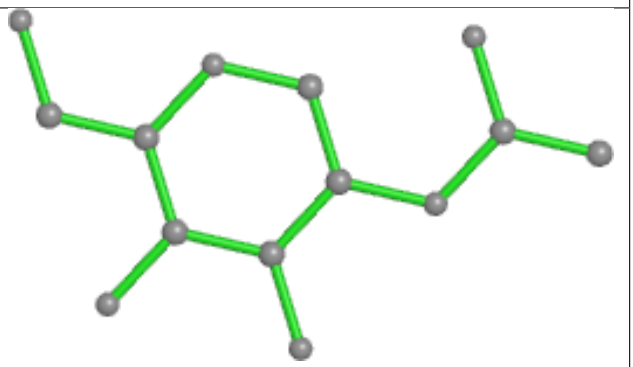


Rings

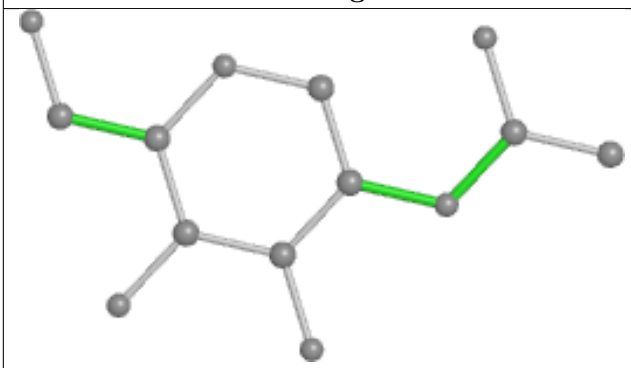
Ligand NAG C 1312



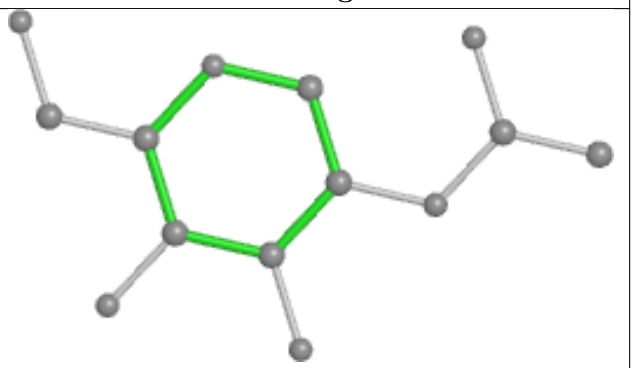
Bond lengths



Bond angles

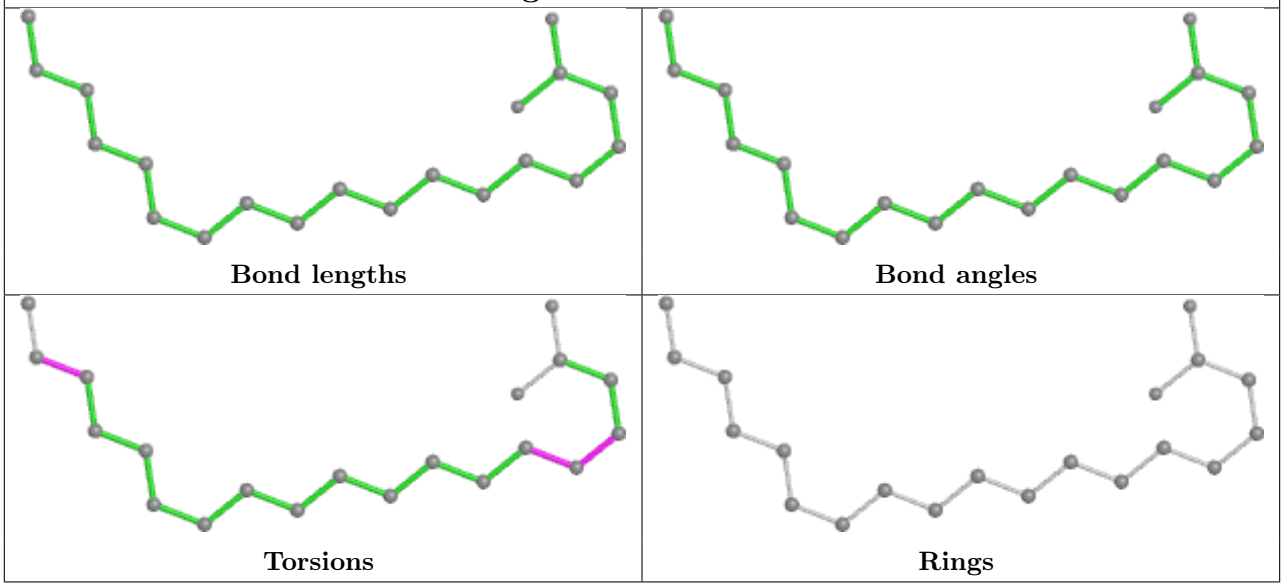


Torsions



Rings

Ligand EIC C 1302



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.