wwPDB EM Validation Summary Report

Jun 9, 2025 – 09:52 PM JST

PDB ID	:	8ZY4 / pdb_00008zy4
EMDB ID	:	EMD-60555
Title	:	Sarbecovirus YN2013 Spike Trimer in a Locked Conformation
Authors	:	Wang, J.; Xiong, X.
Deposited on	:	2024-06-16
Resolution	:	2.53 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:

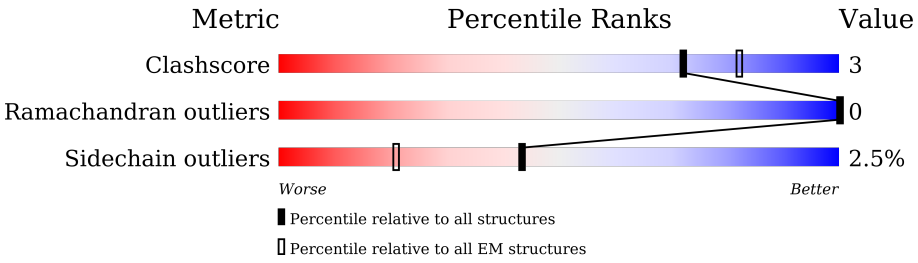
EMDB validation analysis	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal 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 2.53 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	1247	77% 9% 14%
1	B	1247	78% 8% 14%
1	C	1247	78% 8% 14%
2	D	2	100%
2	E	2	100%
2	F	2	100%
2	G	2	50% 50%
2	H	2	50% 50%
2	I	2	50% 50%

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

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 26181 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	1073	Total	C	N	O	S	0	0
			8344	5313	1395	1596	40		
1	B	1073	Total	C	N	O	S	0	0
			8350	5316	1398	1596	40		
1	C	1073	Total	C	N	O	S	0	0
			8350	5316	1398	1596	40		

There are 243 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	946	PRO	LYS	engineered mutation	UNP A0A0U1WJY8
A	947	PRO	VAL	engineered mutation	UNP A0A0U1WJY8
A	1169	GLY	-	expression tag	UNP A0A0U1WJY8
A	1170	SER	-	expression tag	UNP A0A0U1WJY8
A	1171	GLY	-	expression tag	UNP A0A0U1WJY8
A	1172	TYR	-	expression tag	UNP A0A0U1WJY8
A	1173	ILE	-	expression tag	UNP A0A0U1WJY8
A	1174	PRO	-	expression tag	UNP A0A0U1WJY8
A	1175	GLU	-	expression tag	UNP A0A0U1WJY8
A	1176	ALA	-	expression tag	UNP A0A0U1WJY8
A	1177	PRO	-	expression tag	UNP A0A0U1WJY8
A	1178	ARG	-	expression tag	UNP A0A0U1WJY8
A	1179	ASP	-	expression tag	UNP A0A0U1WJY8
A	1180	GLY	-	expression tag	UNP A0A0U1WJY8
A	1181	GLN	-	expression tag	UNP A0A0U1WJY8
A	1182	ALA	-	expression tag	UNP A0A0U1WJY8
A	1183	TYR	-	expression tag	UNP A0A0U1WJY8
A	1184	VAL	-	expression tag	UNP A0A0U1WJY8
A	1185	ARG	-	expression tag	UNP A0A0U1WJY8
A	1186	LYS	-	expression tag	UNP A0A0U1WJY8
A	1187	ASP	-	expression tag	UNP A0A0U1WJY8
A	1188	GLY	-	expression tag	UNP A0A0U1WJY8
A	1189	GLU	-	expression tag	UNP A0A0U1WJY8
A	1190	TRP	-	expression tag	UNP A0A0U1WJY8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1191	VAL	-	expression tag	UNP A0A0U1WJY8
A	1192	LEU	-	expression tag	UNP A0A0U1WJY8
A	1193	LEU	-	expression tag	UNP A0A0U1WJY8
A	1194	SER	-	expression tag	UNP A0A0U1WJY8
A	1195	THR	-	expression tag	UNP A0A0U1WJY8
A	1196	PHE	-	expression tag	UNP A0A0U1WJY8
A	1197	LEU	-	expression tag	UNP A0A0U1WJY8
A	1198	LEU	-	expression tag	UNP A0A0U1WJY8
A	1199	GLU	-	expression tag	UNP A0A0U1WJY8
A	1200	VAL	-	expression tag	UNP A0A0U1WJY8
A	1201	LEU	-	expression tag	UNP A0A0U1WJY8
A	1202	PHE	-	expression tag	UNP A0A0U1WJY8
A	1203	GLN	-	expression tag	UNP A0A0U1WJY8
A	1204	GLY	-	expression tag	UNP A0A0U1WJY8
A	1205	PRO	-	expression tag	UNP A0A0U1WJY8
A	1206	GLY	-	expression tag	UNP A0A0U1WJY8
A	1207	HIS	-	expression tag	UNP A0A0U1WJY8
A	1208	HIS	-	expression tag	UNP A0A0U1WJY8
A	1209	HIS	-	expression tag	UNP A0A0U1WJY8
A	1210	HIS	-	expression tag	UNP A0A0U1WJY8
A	1211	HIS	-	expression tag	UNP A0A0U1WJY8
A	1212	HIS	-	expression tag	UNP A0A0U1WJY8
A	1213	HIS	-	expression tag	UNP A0A0U1WJY8
A	1214	HIS	-	expression tag	UNP A0A0U1WJY8
A	1215	SER	-	expression tag	UNP A0A0U1WJY8
A	1216	ALA	-	expression tag	UNP A0A0U1WJY8
A	1217	TRP	-	expression tag	UNP A0A0U1WJY8
A	1218	SER	-	expression tag	UNP A0A0U1WJY8
A	1219	HIS	-	expression tag	UNP A0A0U1WJY8
A	1220	PRO	-	expression tag	UNP A0A0U1WJY8
A	1221	GLN	-	expression tag	UNP A0A0U1WJY8
A	1222	PHE	-	expression tag	UNP A0A0U1WJY8
A	1223	GLU	-	expression tag	UNP A0A0U1WJY8
A	1224	LYS	-	expression tag	UNP A0A0U1WJY8
A	1225	GLY	-	expression tag	UNP A0A0U1WJY8
A	1226	GLY	-	expression tag	UNP A0A0U1WJY8
A	1227	GLY	-	expression tag	UNP A0A0U1WJY8
A	1228	SER	-	expression tag	UNP A0A0U1WJY8
A	1229	GLY	-	expression tag	UNP A0A0U1WJY8
A	1230	GLY	-	expression tag	UNP A0A0U1WJY8
A	1231	GLY	-	expression tag	UNP A0A0U1WJY8
A	1232	GLY	-	expression tag	UNP A0A0U1WJY8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1233	SER	-	expression tag	UNP A0A0U1WJY8
A	1234	GLY	-	expression tag	UNP A0A0U1WJY8
A	1235	GLY	-	expression tag	UNP A0A0U1WJY8
A	1236	SER	-	expression tag	UNP A0A0U1WJY8
A	1237	ALA	-	expression tag	UNP A0A0U1WJY8
A	1238	TRP	-	expression tag	UNP A0A0U1WJY8
A	1239	SER	-	expression tag	UNP A0A0U1WJY8
A	1240	HIS	-	expression tag	UNP A0A0U1WJY8
A	1241	PRO	-	expression tag	UNP A0A0U1WJY8
A	1242	GLN	-	expression tag	UNP A0A0U1WJY8
A	1243	PHE	-	expression tag	UNP A0A0U1WJY8
A	1244	GLU	-	expression tag	UNP A0A0U1WJY8
A	1245	LYS	-	expression tag	UNP A0A0U1WJY8
A	1246	SER	-	expression tag	UNP A0A0U1WJY8
A	1247	ALA	-	expression tag	UNP A0A0U1WJY8
B	946	PRO	LYS	engineered mutation	UNP A0A0U1WJY8
B	947	PRO	VAL	engineered mutation	UNP A0A0U1WJY8
B	1169	GLY	-	expression tag	UNP A0A0U1WJY8
B	1170	SER	-	expression tag	UNP A0A0U1WJY8
B	1171	GLY	-	expression tag	UNP A0A0U1WJY8
B	1172	TYR	-	expression tag	UNP A0A0U1WJY8
B	1173	ILE	-	expression tag	UNP A0A0U1WJY8
B	1174	PRO	-	expression tag	UNP A0A0U1WJY8
B	1175	GLU	-	expression tag	UNP A0A0U1WJY8
B	1176	ALA	-	expression tag	UNP A0A0U1WJY8
B	1177	PRO	-	expression tag	UNP A0A0U1WJY8
B	1178	ARG	-	expression tag	UNP A0A0U1WJY8
B	1179	ASP	-	expression tag	UNP A0A0U1WJY8
B	1180	GLY	-	expression tag	UNP A0A0U1WJY8
B	1181	GLN	-	expression tag	UNP A0A0U1WJY8
B	1182	ALA	-	expression tag	UNP A0A0U1WJY8
B	1183	TYR	-	expression tag	UNP A0A0U1WJY8
B	1184	VAL	-	expression tag	UNP A0A0U1WJY8
B	1185	ARG	-	expression tag	UNP A0A0U1WJY8
B	1186	LYS	-	expression tag	UNP A0A0U1WJY8
B	1187	ASP	-	expression tag	UNP A0A0U1WJY8
B	1188	GLY	-	expression tag	UNP A0A0U1WJY8
B	1189	GLU	-	expression tag	UNP A0A0U1WJY8
B	1190	TRP	-	expression tag	UNP A0A0U1WJY8
B	1191	VAL	-	expression tag	UNP A0A0U1WJY8
B	1192	LEU	-	expression tag	UNP A0A0U1WJY8
B	1193	LEU	-	expression tag	UNP A0A0U1WJY8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1194	SER	-	expression tag	UNP A0A0U1WJY8
B	1195	THR	-	expression tag	UNP A0A0U1WJY8
B	1196	PHE	-	expression tag	UNP A0A0U1WJY8
B	1197	LEU	-	expression tag	UNP A0A0U1WJY8
B	1198	LEU	-	expression tag	UNP A0A0U1WJY8
B	1199	GLU	-	expression tag	UNP A0A0U1WJY8
B	1200	VAL	-	expression tag	UNP A0A0U1WJY8
B	1201	LEU	-	expression tag	UNP A0A0U1WJY8
B	1202	PHE	-	expression tag	UNP A0A0U1WJY8
B	1203	GLN	-	expression tag	UNP A0A0U1WJY8
B	1204	GLY	-	expression tag	UNP A0A0U1WJY8
B	1205	PRO	-	expression tag	UNP A0A0U1WJY8
B	1206	GLY	-	expression tag	UNP A0A0U1WJY8
B	1207	HIS	-	expression tag	UNP A0A0U1WJY8
B	1208	HIS	-	expression tag	UNP A0A0U1WJY8
B	1209	HIS	-	expression tag	UNP A0A0U1WJY8
B	1210	HIS	-	expression tag	UNP A0A0U1WJY8
B	1211	HIS	-	expression tag	UNP A0A0U1WJY8
B	1212	HIS	-	expression tag	UNP A0A0U1WJY8
B	1213	HIS	-	expression tag	UNP A0A0U1WJY8
B	1214	HIS	-	expression tag	UNP A0A0U1WJY8
B	1215	SER	-	expression tag	UNP A0A0U1WJY8
B	1216	ALA	-	expression tag	UNP A0A0U1WJY8
B	1217	TRP	-	expression tag	UNP A0A0U1WJY8
B	1218	SER	-	expression tag	UNP A0A0U1WJY8
B	1219	HIS	-	expression tag	UNP A0A0U1WJY8
B	1220	PRO	-	expression tag	UNP A0A0U1WJY8
B	1221	GLN	-	expression tag	UNP A0A0U1WJY8
B	1222	PHE	-	expression tag	UNP A0A0U1WJY8
B	1223	GLU	-	expression tag	UNP A0A0U1WJY8
B	1224	LYS	-	expression tag	UNP A0A0U1WJY8
B	1225	GLY	-	expression tag	UNP A0A0U1WJY8
B	1226	GLY	-	expression tag	UNP A0A0U1WJY8
B	1227	GLY	-	expression tag	UNP A0A0U1WJY8
B	1228	SER	-	expression tag	UNP A0A0U1WJY8
B	1229	GLY	-	expression tag	UNP A0A0U1WJY8
B	1230	GLY	-	expression tag	UNP A0A0U1WJY8
B	1231	GLY	-	expression tag	UNP A0A0U1WJY8
B	1232	GLY	-	expression tag	UNP A0A0U1WJY8
B	1233	SER	-	expression tag	UNP A0A0U1WJY8
B	1234	GLY	-	expression tag	UNP A0A0U1WJY8
B	1235	GLY	-	expression tag	UNP A0A0U1WJY8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1236	SER	-	expression tag	UNP A0A0U1WJY8
B	1237	ALA	-	expression tag	UNP A0A0U1WJY8
B	1238	TRP	-	expression tag	UNP A0A0U1WJY8
B	1239	SER	-	expression tag	UNP A0A0U1WJY8
B	1240	HIS	-	expression tag	UNP A0A0U1WJY8
B	1241	PRO	-	expression tag	UNP A0A0U1WJY8
B	1242	GLN	-	expression tag	UNP A0A0U1WJY8
B	1243	PHE	-	expression tag	UNP A0A0U1WJY8
B	1244	GLU	-	expression tag	UNP A0A0U1WJY8
B	1245	LYS	-	expression tag	UNP A0A0U1WJY8
B	1246	SER	-	expression tag	UNP A0A0U1WJY8
B	1247	ALA	-	expression tag	UNP A0A0U1WJY8
C	946	PRO	LYS	engineered mutation	UNP A0A0U1WJY8
C	947	PRO	VAL	engineered mutation	UNP A0A0U1WJY8
C	1169	GLY	-	expression tag	UNP A0A0U1WJY8
C	1170	SER	-	expression tag	UNP A0A0U1WJY8
C	1171	GLY	-	expression tag	UNP A0A0U1WJY8
C	1172	TYR	-	expression tag	UNP A0A0U1WJY8
C	1173	ILE	-	expression tag	UNP A0A0U1WJY8
C	1174	PRO	-	expression tag	UNP A0A0U1WJY8
C	1175	GLU	-	expression tag	UNP A0A0U1WJY8
C	1176	ALA	-	expression tag	UNP A0A0U1WJY8
C	1177	PRO	-	expression tag	UNP A0A0U1WJY8
C	1178	ARG	-	expression tag	UNP A0A0U1WJY8
C	1179	ASP	-	expression tag	UNP A0A0U1WJY8
C	1180	GLY	-	expression tag	UNP A0A0U1WJY8
C	1181	GLN	-	expression tag	UNP A0A0U1WJY8
C	1182	ALA	-	expression tag	UNP A0A0U1WJY8
C	1183	TYR	-	expression tag	UNP A0A0U1WJY8
C	1184	VAL	-	expression tag	UNP A0A0U1WJY8
C	1185	ARG	-	expression tag	UNP A0A0U1WJY8
C	1186	LYS	-	expression tag	UNP A0A0U1WJY8
C	1187	ASP	-	expression tag	UNP A0A0U1WJY8
C	1188	GLY	-	expression tag	UNP A0A0U1WJY8
C	1189	GLU	-	expression tag	UNP A0A0U1WJY8
C	1190	TRP	-	expression tag	UNP A0A0U1WJY8
C	1191	VAL	-	expression tag	UNP A0A0U1WJY8
C	1192	LEU	-	expression tag	UNP A0A0U1WJY8
C	1193	LEU	-	expression tag	UNP A0A0U1WJY8
C	1194	SER	-	expression tag	UNP A0A0U1WJY8
C	1195	THR	-	expression tag	UNP A0A0U1WJY8
C	1196	PHE	-	expression tag	UNP A0A0U1WJY8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1197	LEU	-	expression tag	UNP A0A0U1WJY8
C	1198	LEU	-	expression tag	UNP A0A0U1WJY8
C	1199	GLU	-	expression tag	UNP A0A0U1WJY8
C	1200	VAL	-	expression tag	UNP A0A0U1WJY8
C	1201	LEU	-	expression tag	UNP A0A0U1WJY8
C	1202	PHE	-	expression tag	UNP A0A0U1WJY8
C	1203	GLN	-	expression tag	UNP A0A0U1WJY8
C	1204	GLY	-	expression tag	UNP A0A0U1WJY8
C	1205	PRO	-	expression tag	UNP A0A0U1WJY8
C	1206	GLY	-	expression tag	UNP A0A0U1WJY8
C	1207	HIS	-	expression tag	UNP A0A0U1WJY8
C	1208	HIS	-	expression tag	UNP A0A0U1WJY8
C	1209	HIS	-	expression tag	UNP A0A0U1WJY8
C	1210	HIS	-	expression tag	UNP A0A0U1WJY8
C	1211	HIS	-	expression tag	UNP A0A0U1WJY8
C	1212	HIS	-	expression tag	UNP A0A0U1WJY8
C	1213	HIS	-	expression tag	UNP A0A0U1WJY8
C	1214	HIS	-	expression tag	UNP A0A0U1WJY8
C	1215	SER	-	expression tag	UNP A0A0U1WJY8
C	1216	ALA	-	expression tag	UNP A0A0U1WJY8
C	1217	TRP	-	expression tag	UNP A0A0U1WJY8
C	1218	SER	-	expression tag	UNP A0A0U1WJY8
C	1219	HIS	-	expression tag	UNP A0A0U1WJY8
C	1220	PRO	-	expression tag	UNP A0A0U1WJY8
C	1221	GLN	-	expression tag	UNP A0A0U1WJY8
C	1222	PHE	-	expression tag	UNP A0A0U1WJY8
C	1223	GLU	-	expression tag	UNP A0A0U1WJY8
C	1224	LYS	-	expression tag	UNP A0A0U1WJY8
C	1225	GLY	-	expression tag	UNP A0A0U1WJY8
C	1226	GLY	-	expression tag	UNP A0A0U1WJY8
C	1227	GLY	-	expression tag	UNP A0A0U1WJY8
C	1228	SER	-	expression tag	UNP A0A0U1WJY8
C	1229	GLY	-	expression tag	UNP A0A0U1WJY8
C	1230	GLY	-	expression tag	UNP A0A0U1WJY8
C	1231	GLY	-	expression tag	UNP A0A0U1WJY8
C	1232	GLY	-	expression tag	UNP A0A0U1WJY8
C	1233	SER	-	expression tag	UNP A0A0U1WJY8
C	1234	GLY	-	expression tag	UNP A0A0U1WJY8
C	1235	GLY	-	expression tag	UNP A0A0U1WJY8
C	1236	SER	-	expression tag	UNP A0A0U1WJY8
C	1237	ALA	-	expression tag	UNP A0A0U1WJY8
C	1238	TRP	-	expression tag	UNP A0A0U1WJY8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1239	SER	-	expression tag	UNP A0A0U1WJY8
C	1240	HIS	-	expression tag	UNP A0A0U1WJY8
C	1241	PRO	-	expression tag	UNP A0A0U1WJY8
C	1242	GLN	-	expression tag	UNP A0A0U1WJY8
C	1243	PHE	-	expression tag	UNP A0A0U1WJY8
C	1244	GLU	-	expression tag	UNP A0A0U1WJY8
C	1245	LYS	-	expression tag	UNP A0A0U1WJY8
C	1246	SER	-	expression tag	UNP A0A0U1WJY8
C	1247	ALA	-	expression tag	UNP A0A0U1WJY8

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

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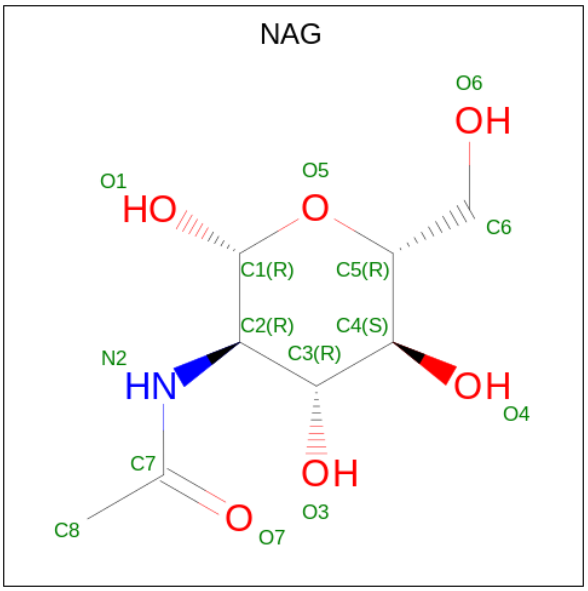
Mol	Chain	Residues	Atoms	AltConf	Trace
2	P	2	Total C N O 28 16 2 10	0	0
2	Q	2	Total C N O 28 16 2 10	0	0
2	R	2	Total C N O 28 16 2 10	0	0

- 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
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

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

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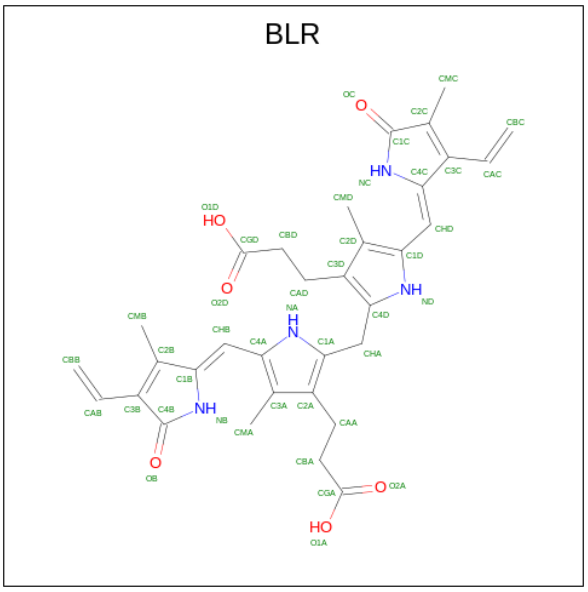
Mol	Chain	Residues	Atoms				AltConf
3	C	1	Total 14	C 8	N 1	O 5	0
3	C	1	Total 14	C 8	N 1	O 5	0
3	C	1	Total 14	C 8	N 1	O 5	0
3	C	1	Total 14	C 8	N 1	O 5	0
3	C	1	Total 14	C 8	N 1	O 5	0
3	C	1	Total 14	C 8	N 1	O 5	0
3	C	1	Total 14	C 8	N 1	O 5	0
3	C	1	Total 14	C 8	N 1	O 5	0
3	C	1	Total 14	C 8	N 1	O 5	0
3	C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

- Molecule 4 is 3-[5-[(Z)-(4-ethenyl-3-methyl-5-oxidanylidene-pyrrol-2-ylidene)methyl]-2-[[5-[(Z)-(3-ethenyl-4-methyl-5-oxidanylidene-pyrrol-2-ylidene)methyl]-3-(3-hydroxy-3-oxopropyl)-4-methyl-1H-pyrrol-2-yl]methyl]-4-methyl-1H-pyrrol-3-yl]propanoic acid (CCD ID: BLR) (formula: $C_{33}H_{36}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



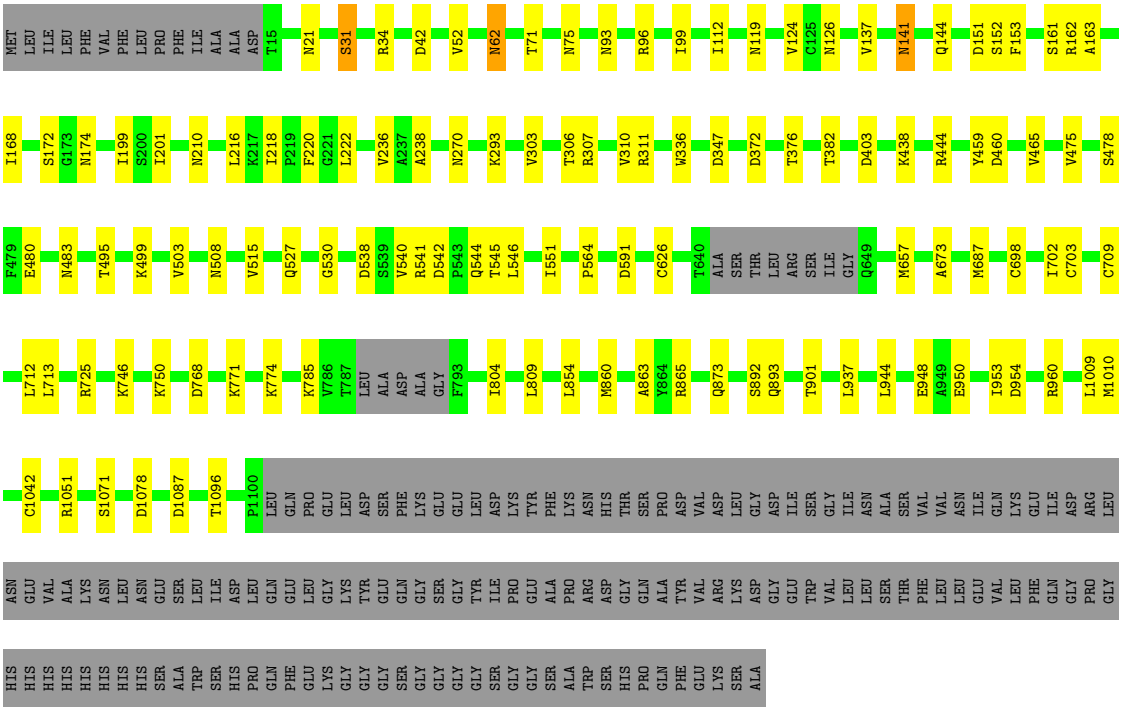
Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			43	33	4	6	
4	B	1	Total	C	N	O	0
			43	33	4	6	
4	C	1	Total	C	N	O	0
			43	33	4	6	

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.

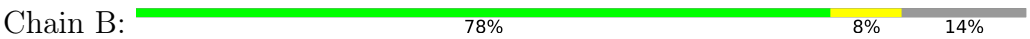
- Molecule 1: Spike glycoprotein

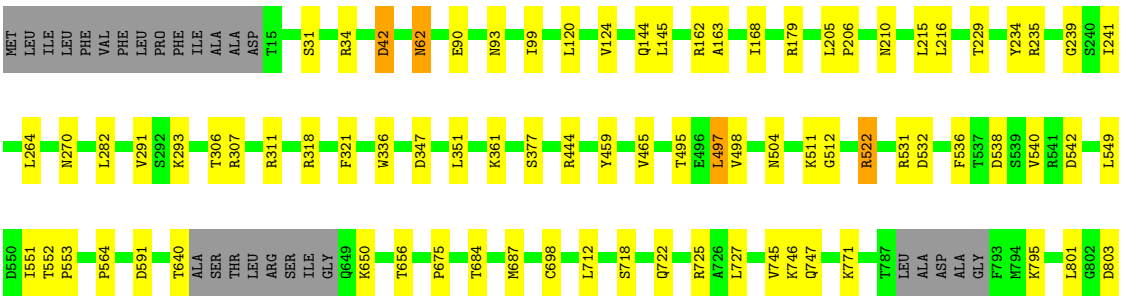
Chain A:

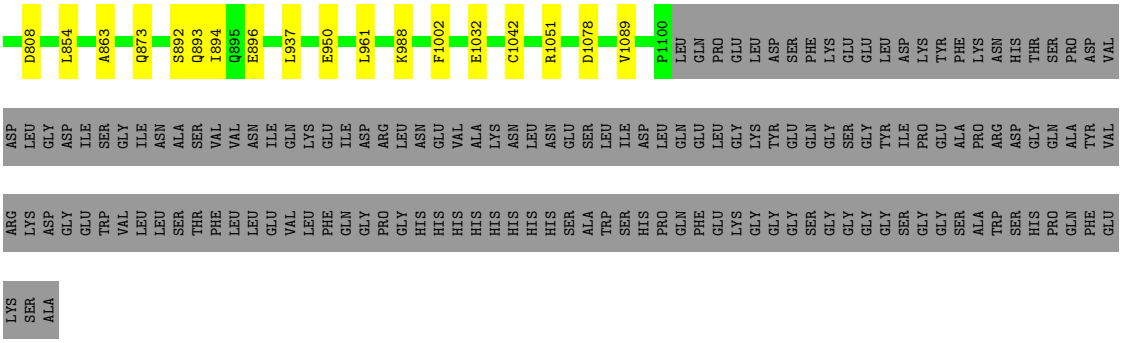


- Molecule 1: Spike glycoprotein

Chain B:

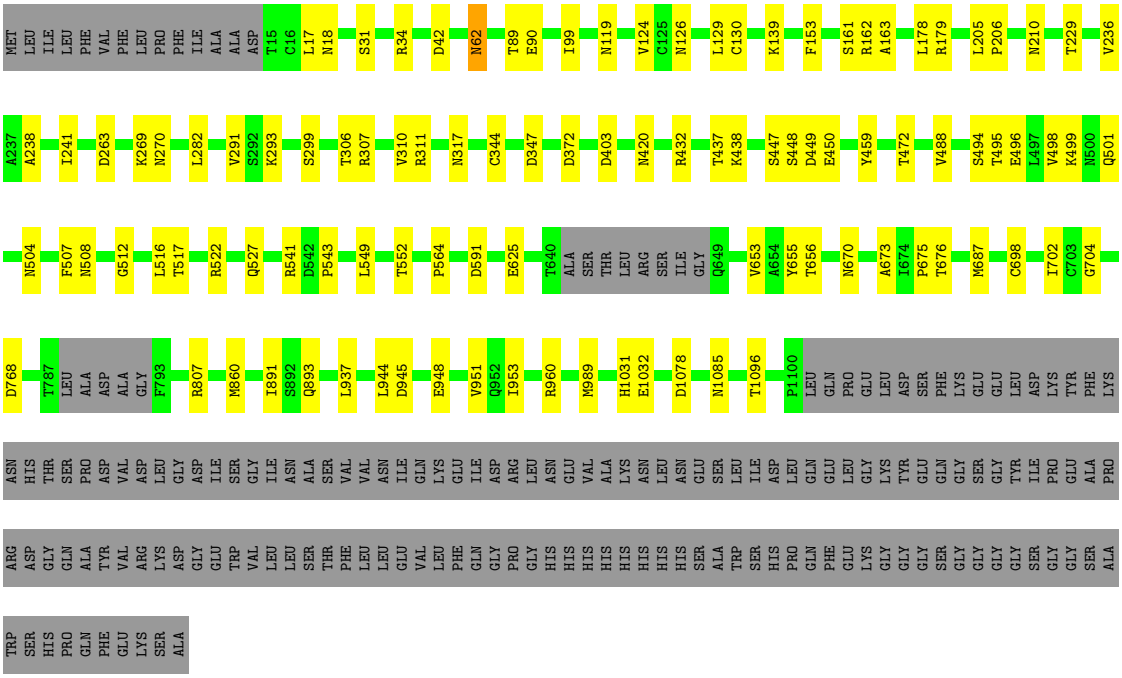






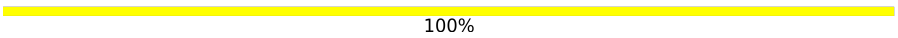
• Molecule 1: Spike glycoprotein

Chain C:



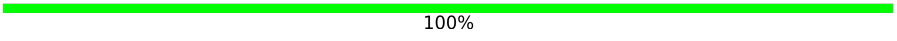
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:

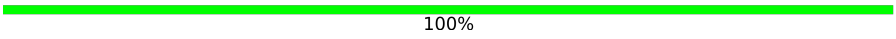


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

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: 

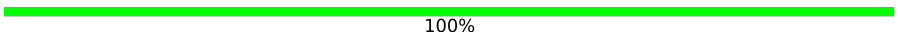
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

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

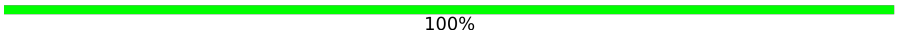
Chain M:

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

Chain N:

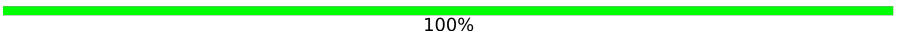
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

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:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	452110	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, BLR

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	0.14	0/8529	0.36	0/11607
1	B	0.15	0/8535	0.38	0/11614
1	C	0.14	0/8535	0.38	0/11614
All	All	0.14	0/25599	0.37	0/34835

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	8344	0	8128	59	0
1	B	8350	0	8139	55	0
1	C	8350	0	8139	53	0
2	D	28	0	25	0	0
2	E	28	0	25	0	0
2	F	28	0	25	0	0
2	G	28	0	25	0	0
2	H	28	0	25	0	0
2	I	28	0	25	0	0
2	J	28	0	25	0	0

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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	0	0
2	M	28	0	25	0	0
2	N	28	0	25	0	0
2	O	28	0	25	0	0
2	P	28	0	25	0	0
2	Q	28	0	25	0	0
2	R	28	0	25	0	0
3	A	196	0	182	0	0
3	B	196	0	182	0	0
3	C	196	0	182	0	0
4	A	43	0	34	2	0
4	B	43	0	34	2	0
4	C	43	0	34	1	0
All	All	26181	0	25429	166	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 166 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:483:ASN:HD21	1:A:530:GLY:H	1.46	0.64
1:A:126:ASN:HB2	1:A:153:PHE:HB2	1.82	0.60
1:C:702:ILE:O	1:C:960:ARG:NH1	2.37	0.58
1:C:447:SER:OG	1:C:450:GLU:OE1	2.22	0.57
1:A:293:LYS:HG3	1:A:564:PRO:HA	1.87	0.57

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	1067/1247 (86%)	1027 (96%)	40 (4%)	0	100	100
1	B	1067/1247 (86%)	1020 (96%)	47 (4%)	0	100	100
1	C	1067/1247 (86%)	1023 (96%)	44 (4%)	0	100	100
All	All	3201/3741 (86%)	3070 (96%)	131 (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	929/1072 (87%)	904 (97%)	25 (3%)	40	65
1	B	930/1072 (87%)	910 (98%)	20 (2%)	47	71
1	C	930/1072 (87%)	906 (97%)	24 (3%)	41	66
All	All	2789/3216 (87%)	2720 (98%)	69 (2%)	43	67

5 of 69 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	516	LEU
1	C	552	THR
1	C	951	VAL
1	A	1096	THR
1	A	1042	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	764	GLN
1	C	796	GLN
1	B	470	GLN
1	B	300	ASN
1	C	816	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

30 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	D	1	1,2	14,14,15	0.67	0	17,19,21	1.68	3 (17%)
2	NAG	D	2	2	14,14,15	0.70	0	17,19,21	0.95	1 (5%)
2	NAG	E	1	1,2	14,14,15	0.72	0	17,19,21	0.96	0
2	NAG	E	2	2	14,14,15	0.71	0	17,19,21	0.90	0
2	NAG	F	1	1,2	14,14,15	0.75	0	17,19,21	1.02	0
2	NAG	F	2	2	14,14,15	0.71	0	17,19,21	0.88	0
2	NAG	G	1	1,2	14,14,15	0.74	0	17,19,21	1.17	1 (5%)
2	NAG	G	2	2	14,14,15	0.71	0	17,19,21	0.86	0
2	NAG	H	1	1,2	14,14,15	0.72	0	17,19,21	1.00	1 (5%)
2	NAG	H	2	2	14,14,15	0.71	0	17,19,21	0.87	0
2	NAG	I	1	1,2	14,14,15	0.75	0	17,19,21	1.07	1 (5%)
2	NAG	I	2	2	14,14,15	0.71	0	17,19,21	0.91	0
2	NAG	J	1	1,2	14,14,15	0.68	0	17,19,21	1.50	2 (11%)
2	NAG	J	2	2	14,14,15	0.72	0	17,19,21	0.94	0
2	NAG	K	1	1,2	14,14,15	0.75	0	17,19,21	1.01	0
2	NAG	K	2	2	14,14,15	0.73	0	17,19,21	0.86	0
2	NAG	L	1	1,2	14,14,15	0.73	0	17,19,21	1.22	3 (17%)
2	NAG	L	2	2	14,14,15	0.70	0	17,19,21	0.85	0
2	NAG	M	1	1,2	14,14,15	0.72	0	17,19,21	1.03	1 (5%)
2	NAG	M	2	2	14,14,15	0.71	0	17,19,21	0.89	0
2	NAG	N	1	1,2	14,14,15	0.75	0	17,19,21	1.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	N	2	2	14,14,15	0.70	0	17,19,21	1.50	1 (5%)
2	NAG	O	1	1,2	14,14,15	0.70	0	17,19,21	0.93	0
2	NAG	O	2	2	14,14,15	0.72	0	17,19,21	0.91	0
2	NAG	P	1	1,2	14,14,15	0.70	0	17,19,21	0.91	0
2	NAG	P	2	2	14,14,15	0.70	0	17,19,21	0.88	0
2	NAG	Q	1	1,2	14,14,15	0.73	0	17,19,21	1.12	1 (5%)
2	NAG	Q	2	2	14,14,15	0.71	0	17,19,21	0.88	0
2	NAG	R	1	1,2	14,14,15	0.73	0	17,19,21	1.00	1 (5%)
2	NAG	R	2	2	14,14,15	0.72	0	17,19,21	0.88	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	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1
2	NAG	G	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1
2	NAG	H	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	1/6/23/26	0/1/1/1
2	NAG	I	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	I	2	2	-	1/6/23/26	0/1/1/1
2	NAG	J	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	J	2	2	-	0/6/23/26	0/1/1/1
2	NAG	K	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	K	2	2	-	0/6/23/26	0/1/1/1
2	NAG	L	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	L	2	2	-	0/6/23/26	0/1/1/1
2	NAG	M	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	M	2	2	-	0/6/23/26	0/1/1/1
2	NAG	N	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	N	2	2	-	2/6/23/26	0/1/1/1
2	NAG	O	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	O	2	2	-	0/6/23/26	0/1/1/1
2	NAG	P	1	1,2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	P	2	2	-	0/6/23/26	0/1/1/1
2	NAG	Q	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	Q	2	2	-	0/6/23/26	0/1/1/1
2	NAG	R	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	R	2	2	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1	NAG	C2-N2-C7	4.40	129.18	122.90
2	N	2	NAG	C2-N2-C7	4.27	128.99	122.90
2	J	1	NAG	C2-N2-C7	4.27	128.98	122.90
2	D	1	NAG	C1-O5-C5	2.94	116.18	112.19
2	G	1	NAG	C2-N2-C7	2.73	126.79	122.90

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

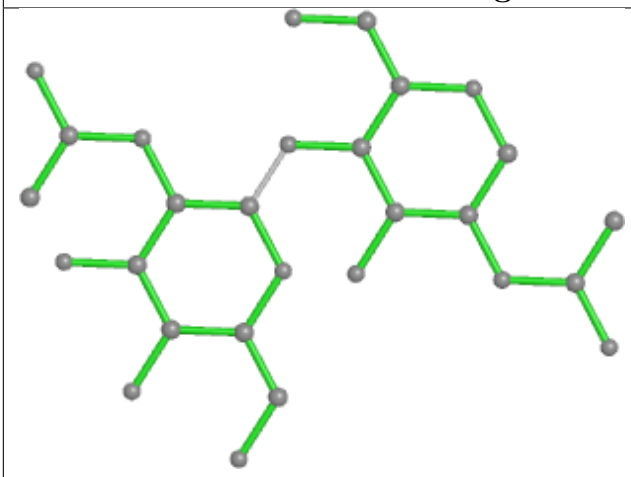
Mol	Chain	Res	Type	Atoms
2	G	1	NAG	C8-C7-N2-C2
2	G	1	NAG	O7-C7-N2-C2
2	L	1	NAG	C8-C7-N2-C2
2	L	1	NAG	O7-C7-N2-C2
2	Q	1	NAG	C8-C7-N2-C2

There are no ring outliers.

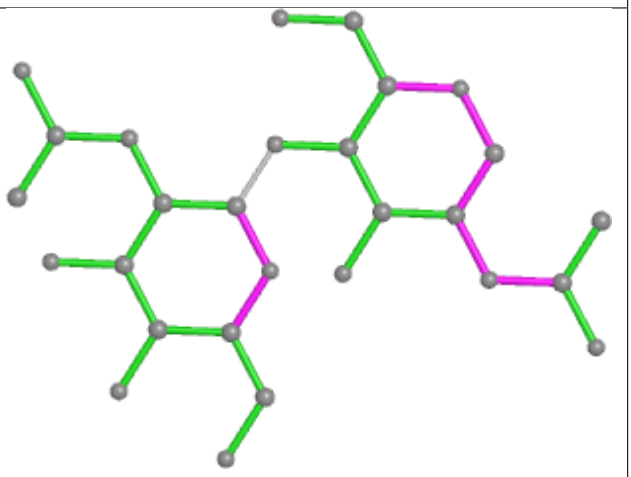
No monomer is involved in short contacts.

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

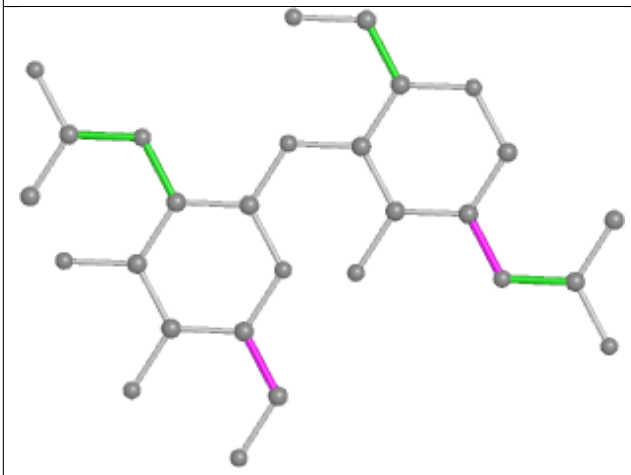
Oligosaccharide Chain D



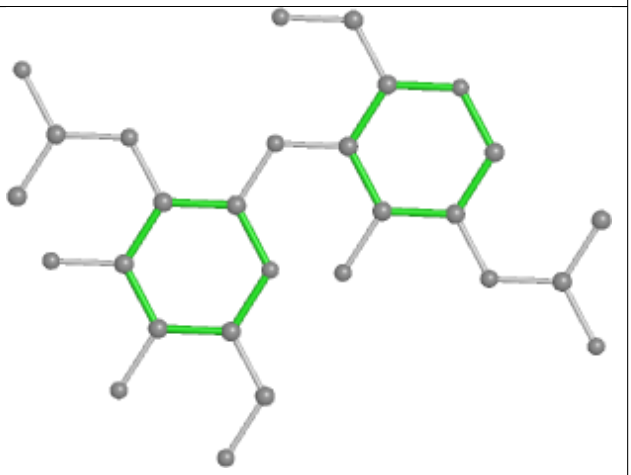
Bond lengths



Bond angles

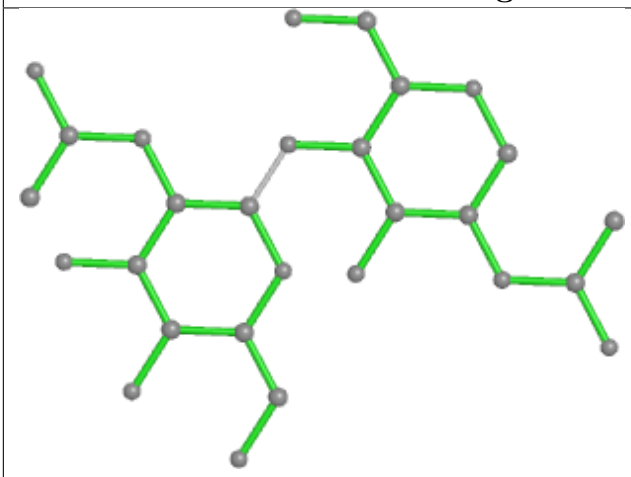


Torsions

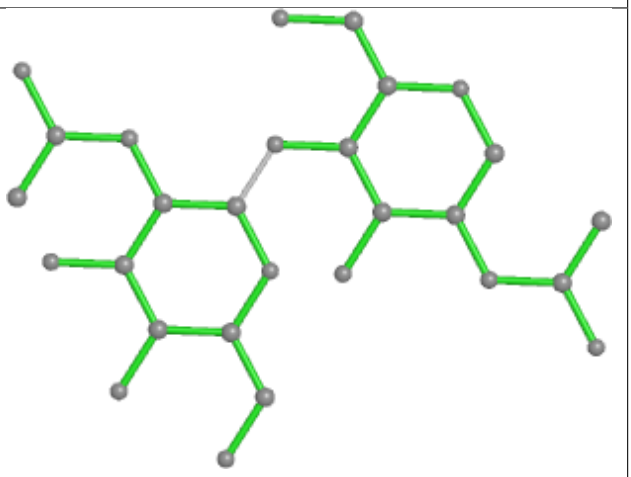


Rings

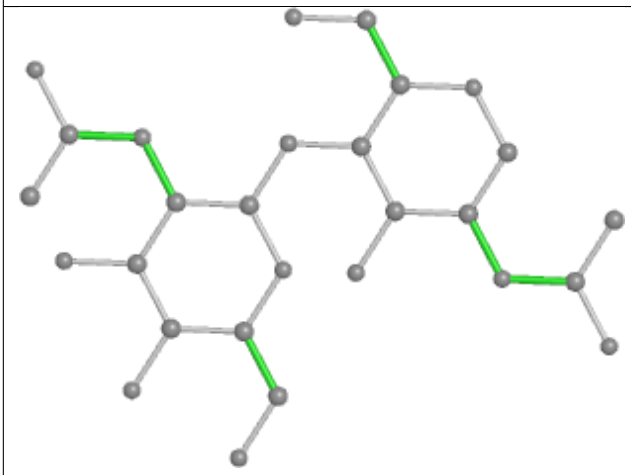
Oligosaccharide Chain E



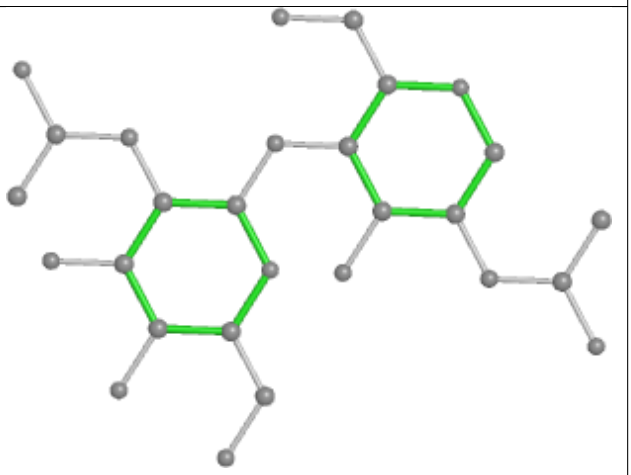
Bond lengths



Bond angles

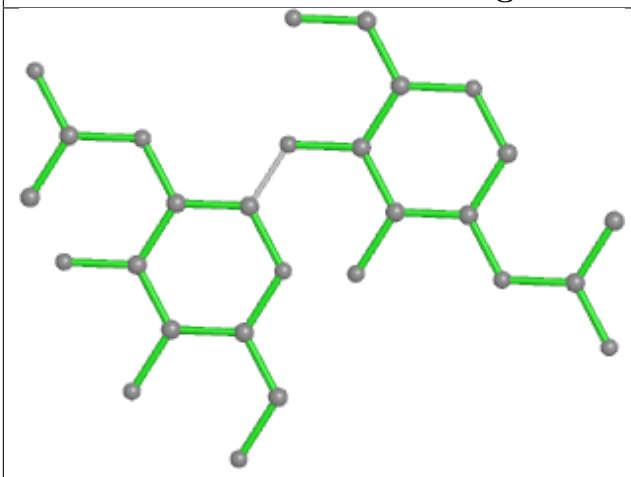


Torsions

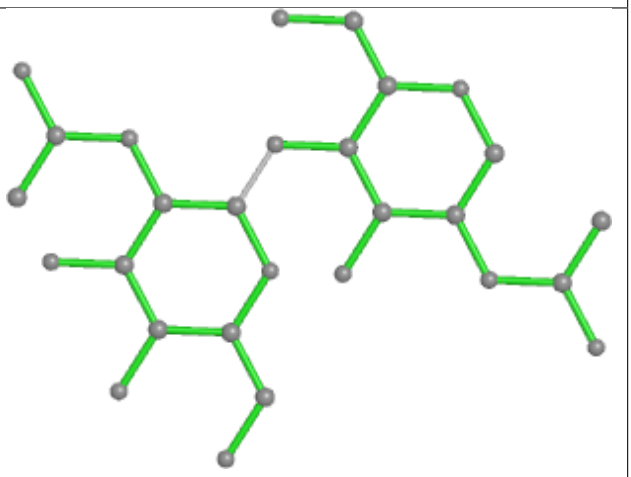


Rings

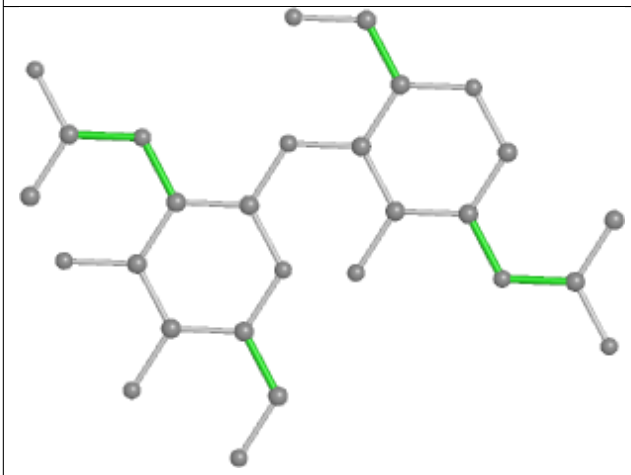
Oligosaccharide Chain F



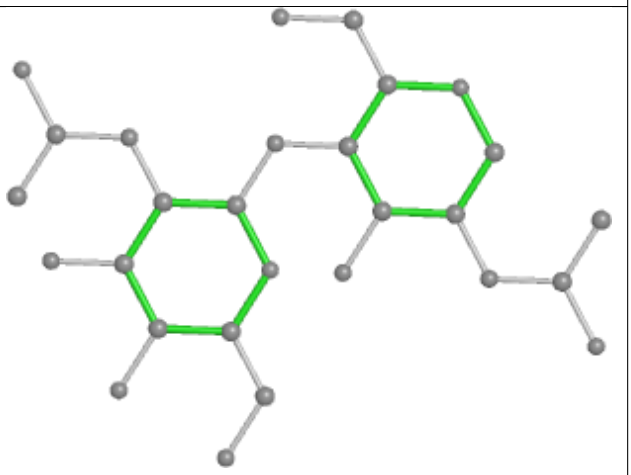
Bond lengths



Bond angles

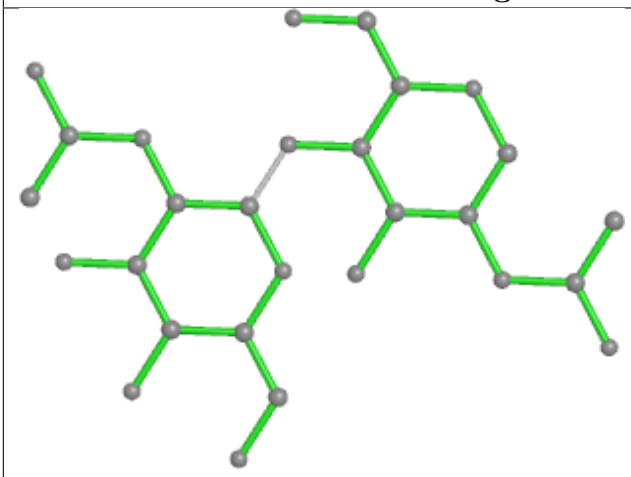


Torsions

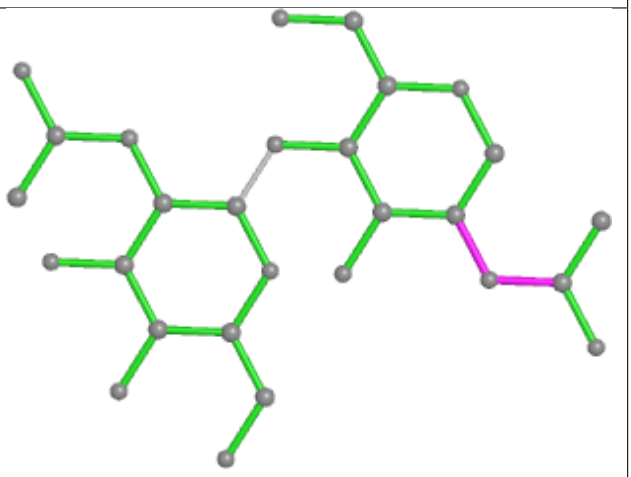


Rings

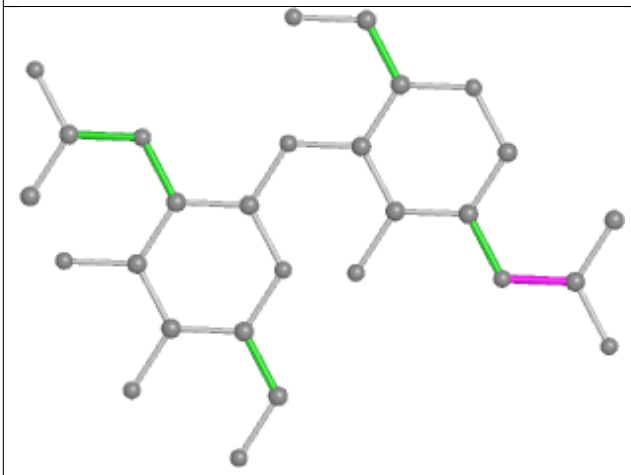
Oligosaccharide Chain G



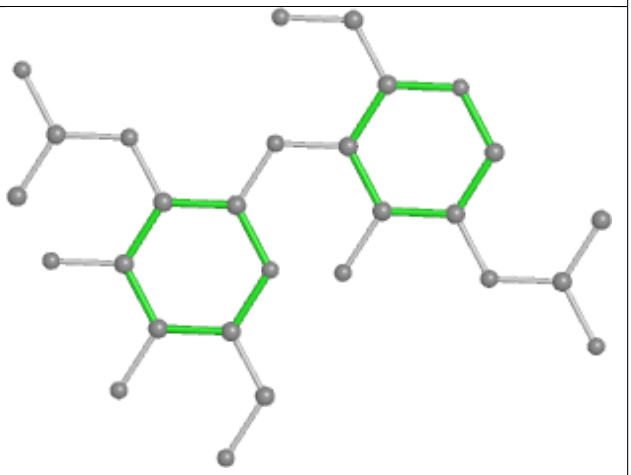
Bond lengths



Bond angles

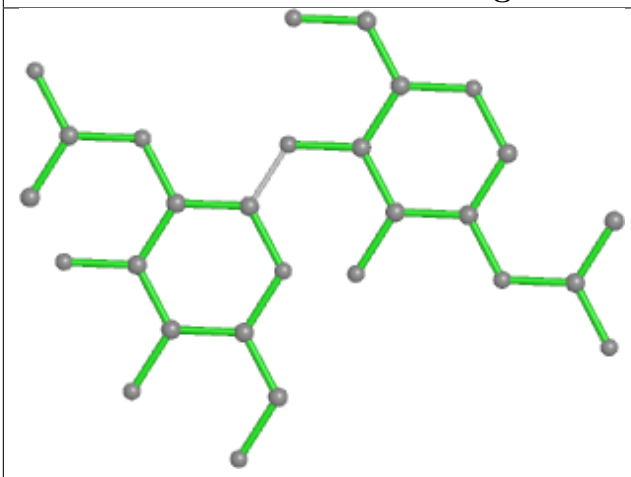


Torsions

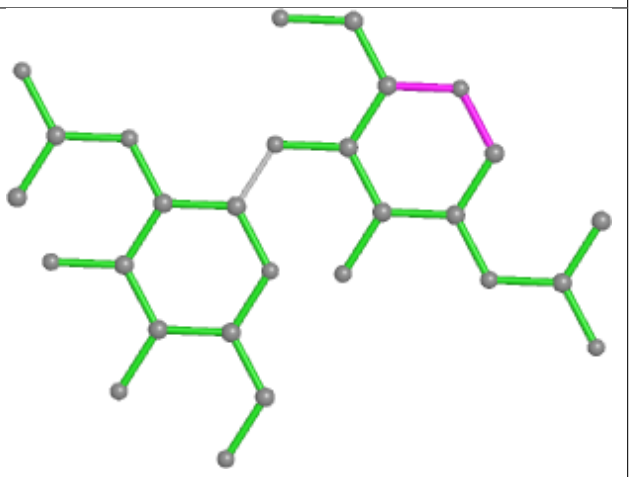


Rings

Oligosaccharide Chain H



Bond lengths



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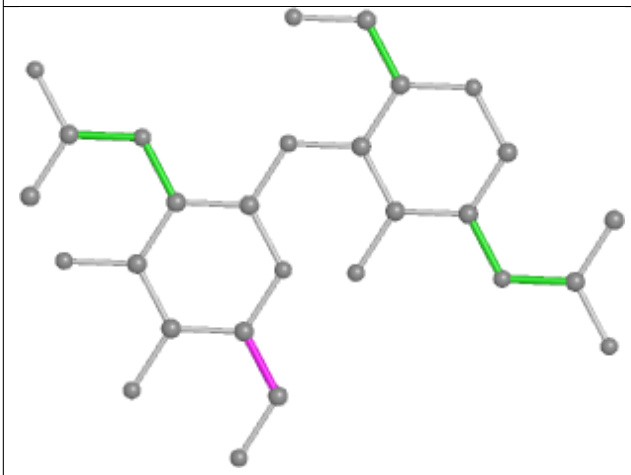

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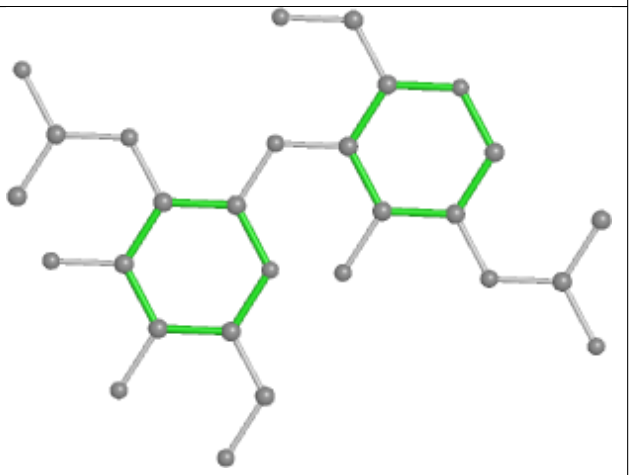
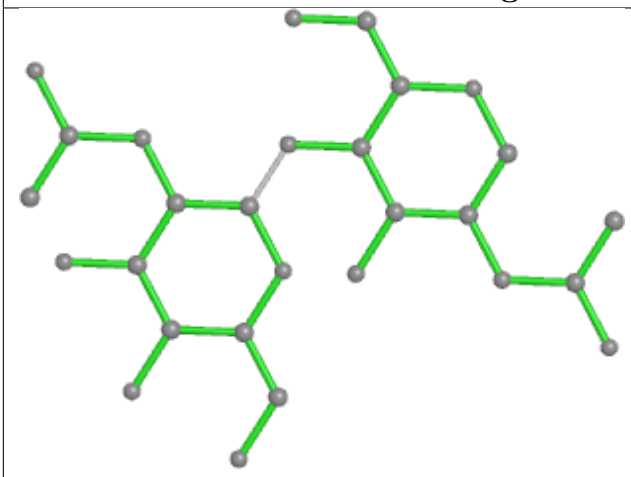


Rings

Oligosaccharide Chain I



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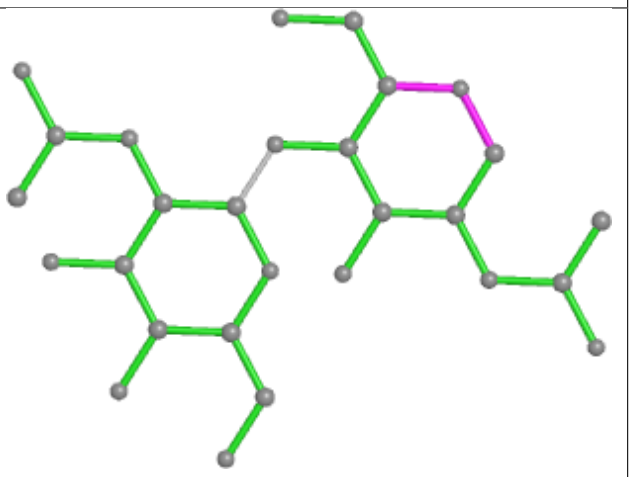
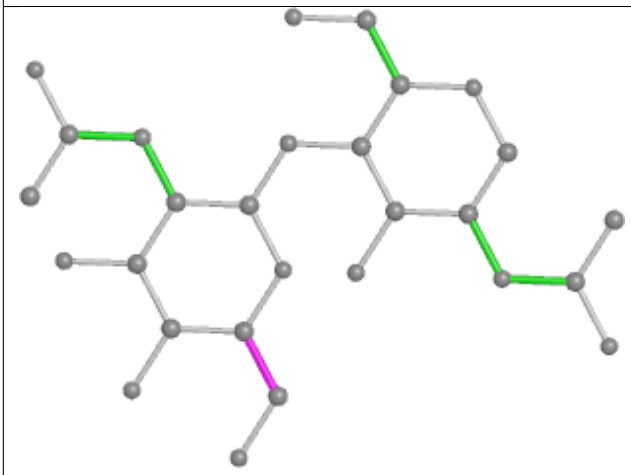


Bond angles



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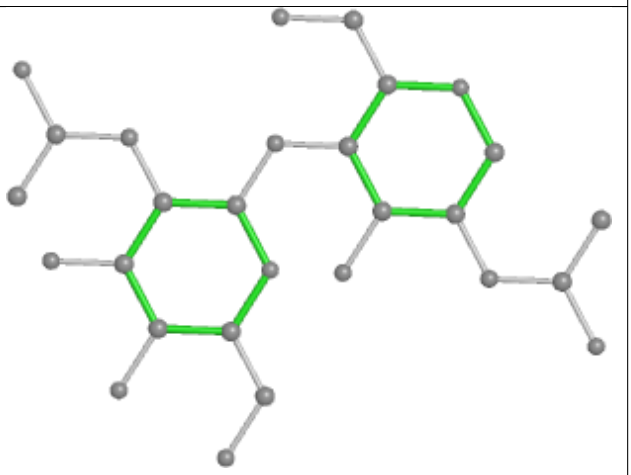
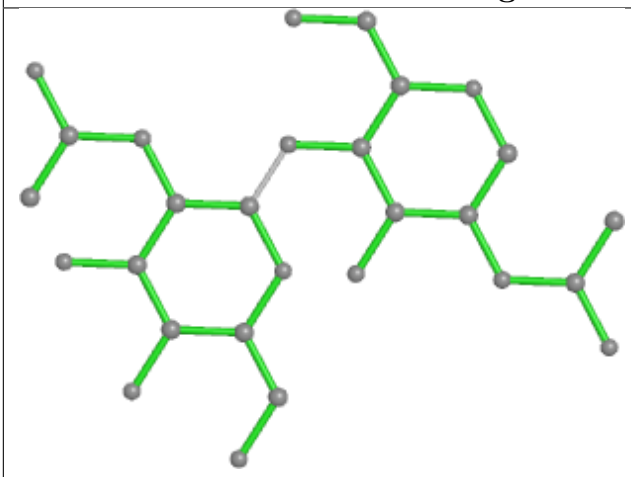
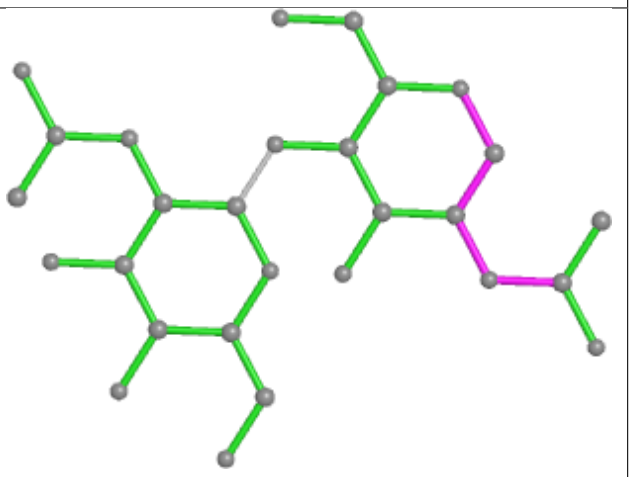


Rings

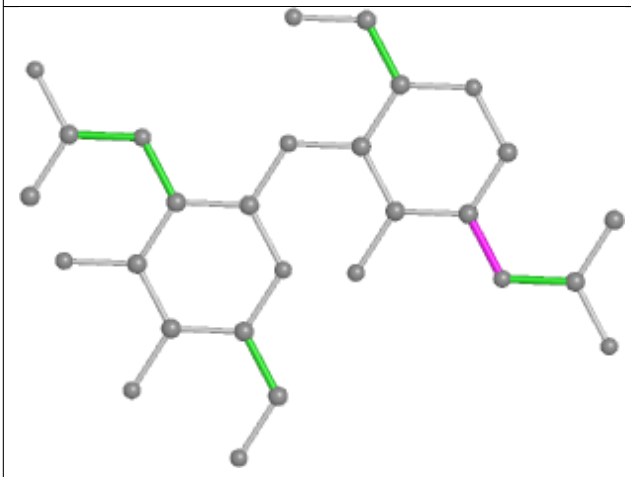
Oligosaccharide Chain J



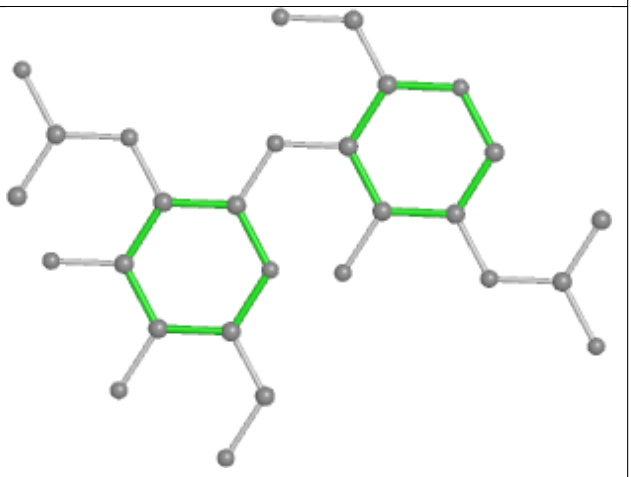
Bond lengths



Bond angles

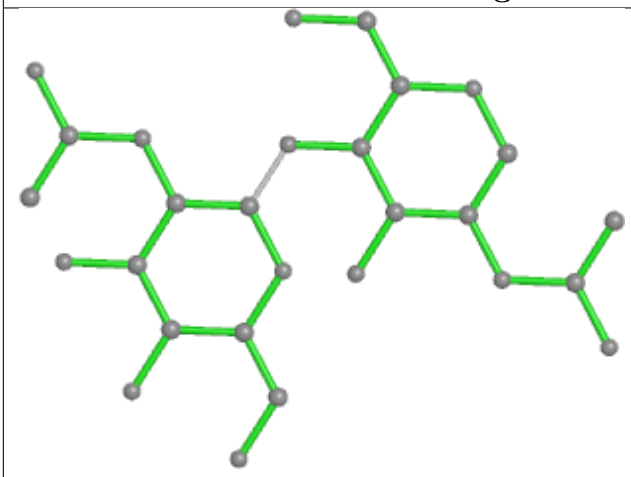


Torsions

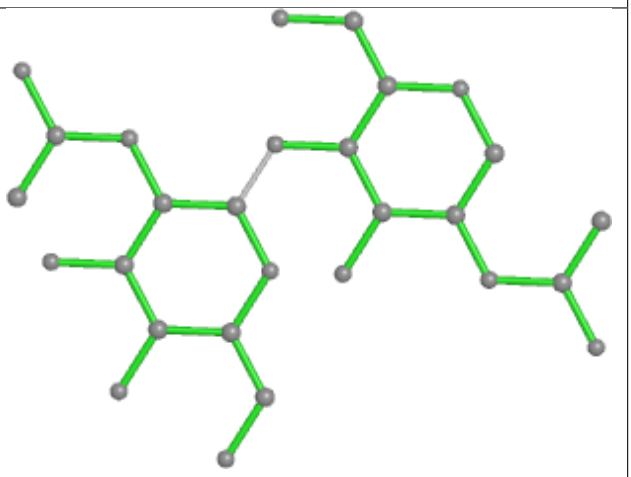


Rings

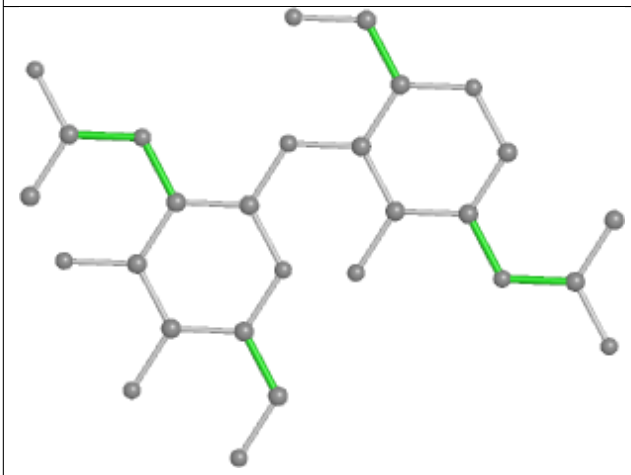
Oligosaccharide Chain K



Bond lengths



Bond angles



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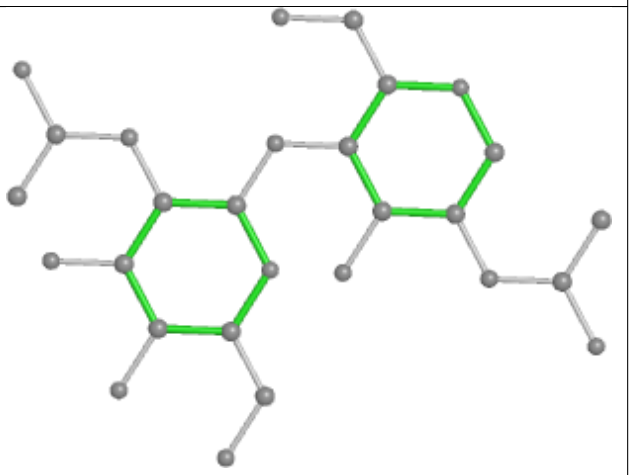
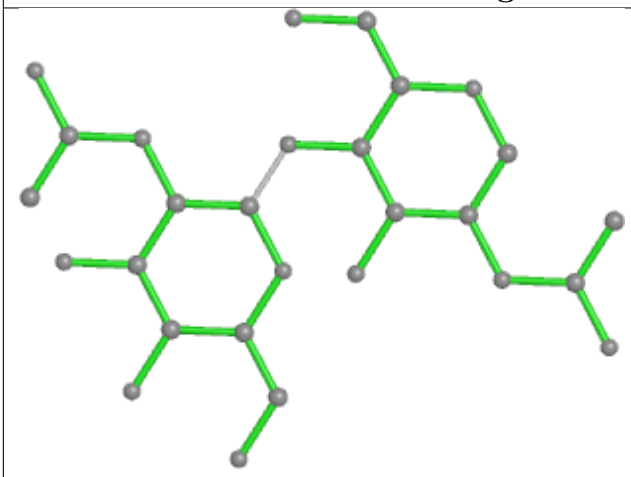
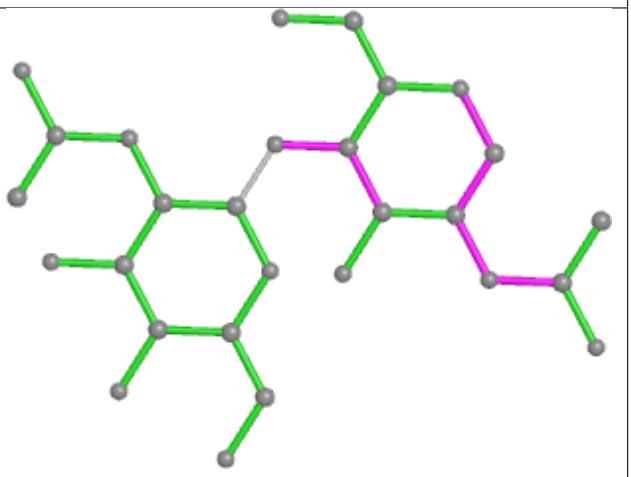


Rings

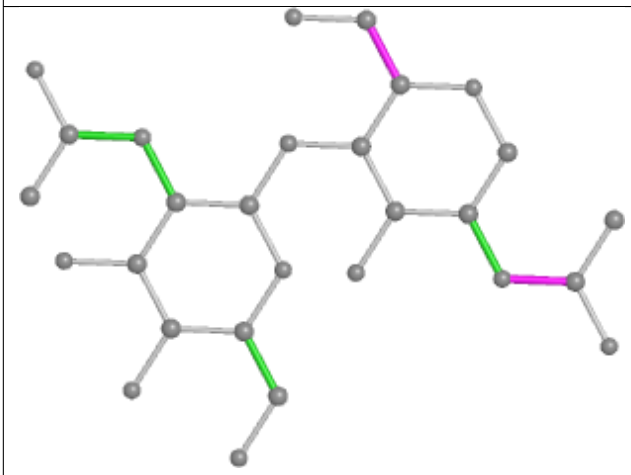
Oligosaccharide Chain L



Bond lengths



Bond angles



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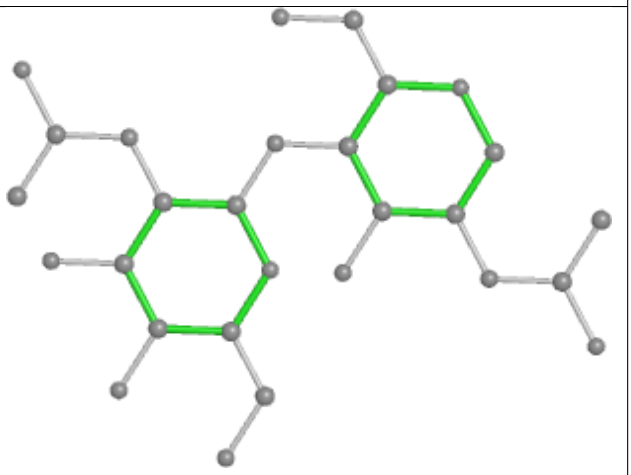
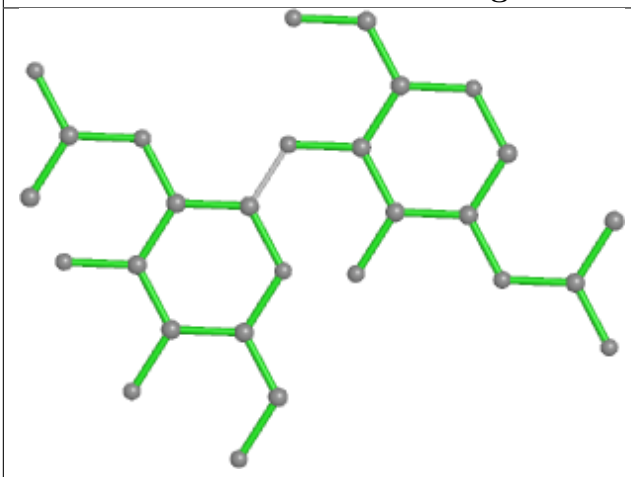
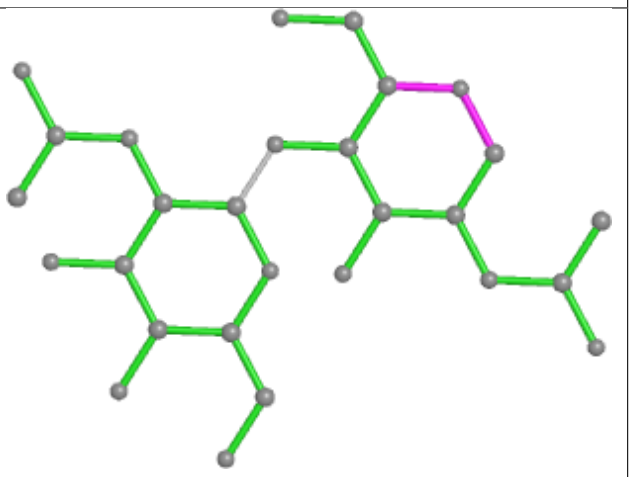


Rings

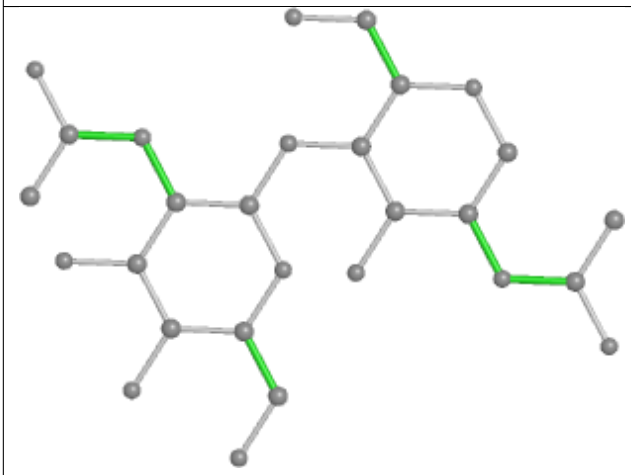
Oligosaccharide Chain M



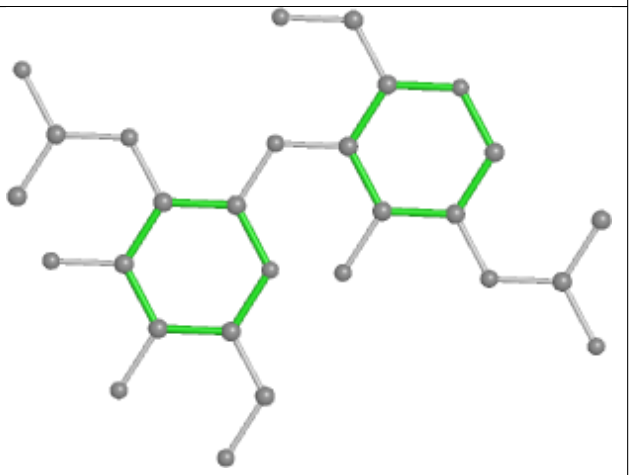
Bond lengths



Bond angles

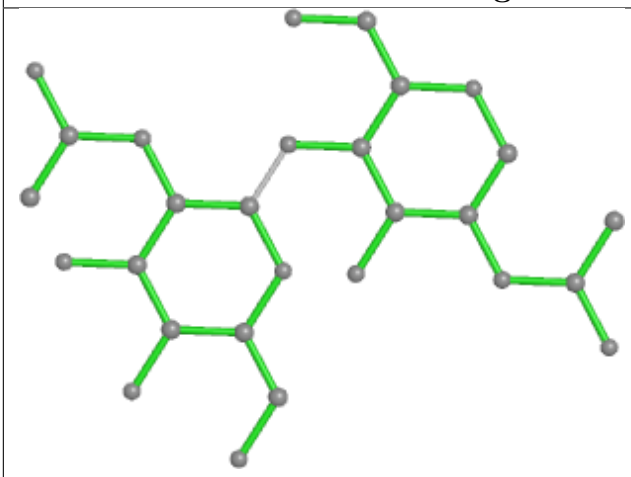


Torsions

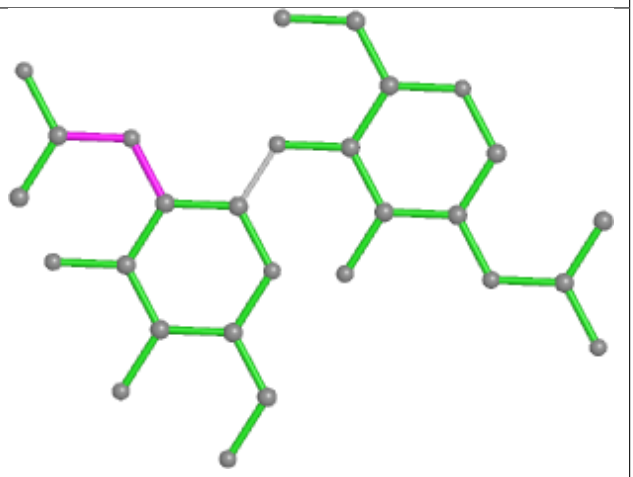


Rings

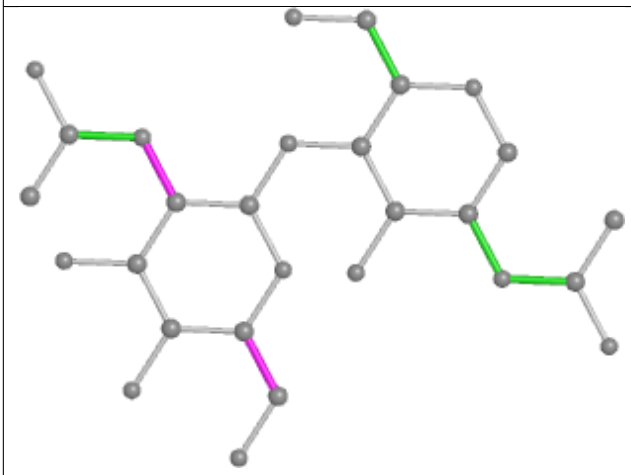
Oligosaccharide Chain N



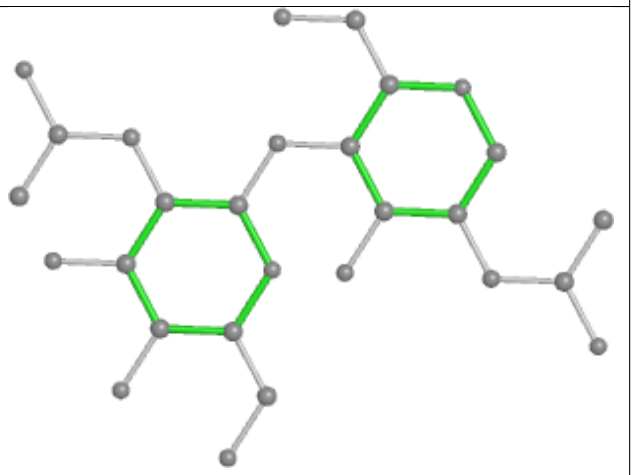
Bond lengths



Bond angles

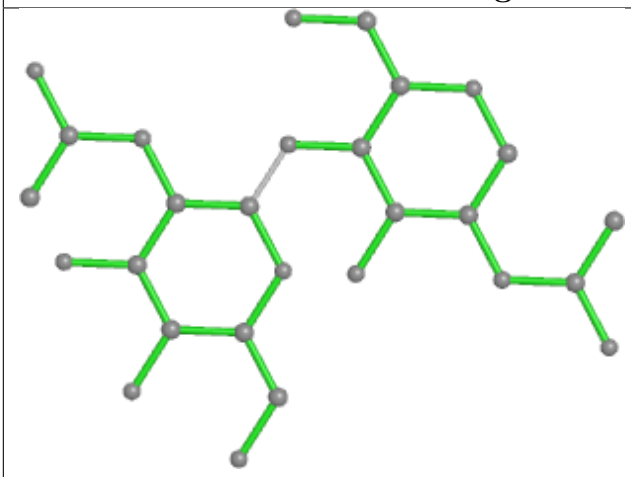


Torsions

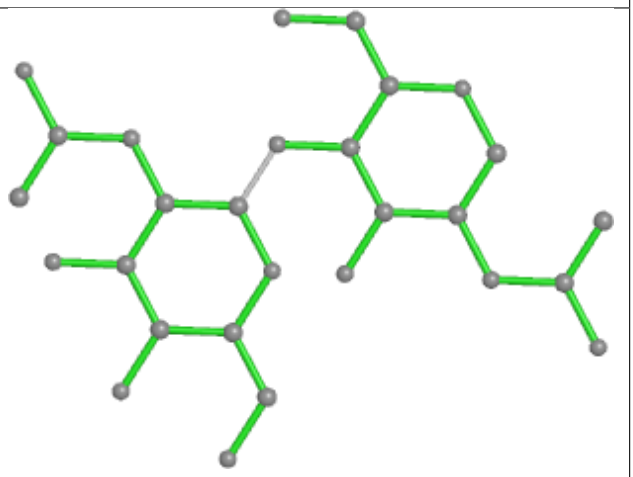


Rings

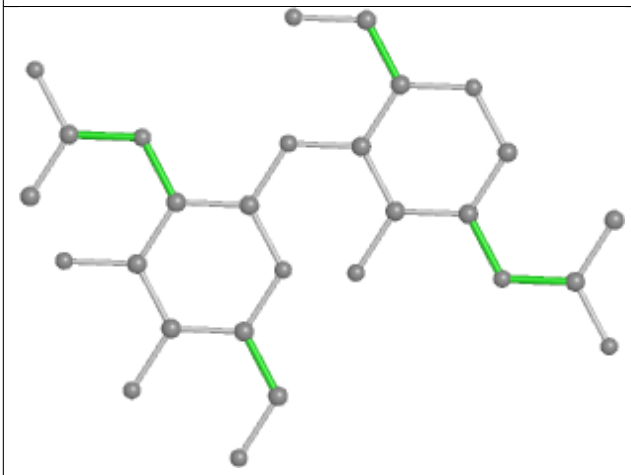
Oligosaccharide Chain O



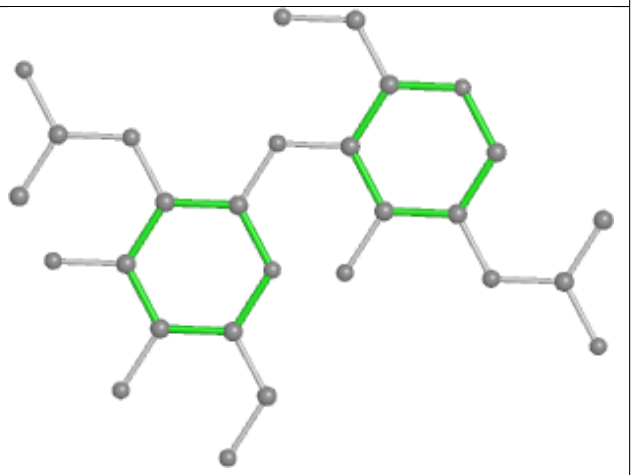
Bond lengths



Bond angles

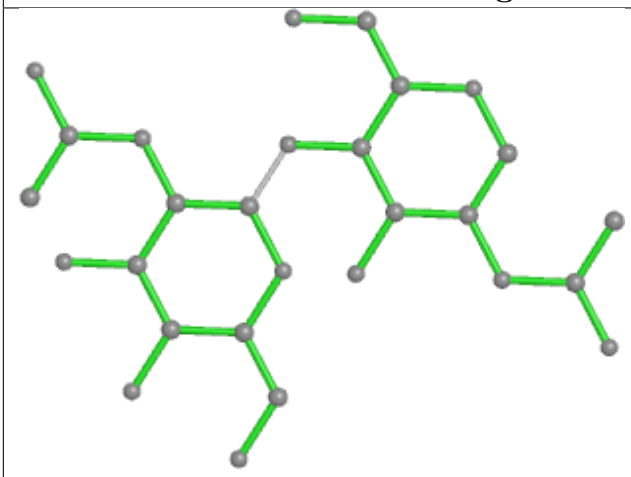


Torsions

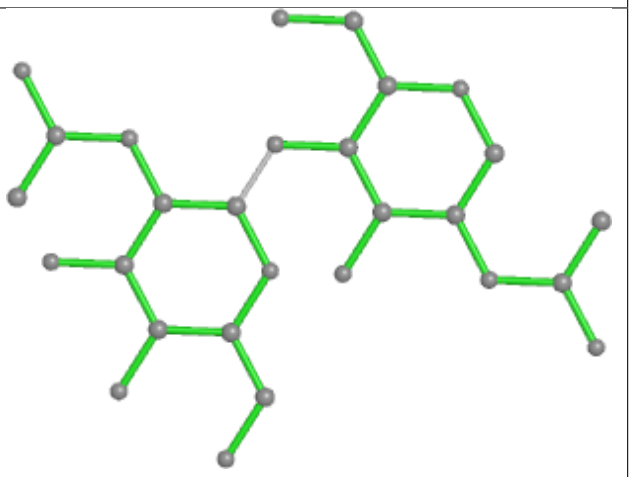


Rings

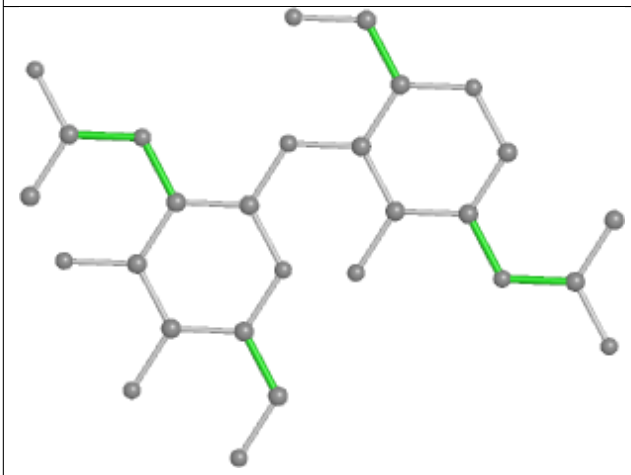
Oligosaccharide Chain P



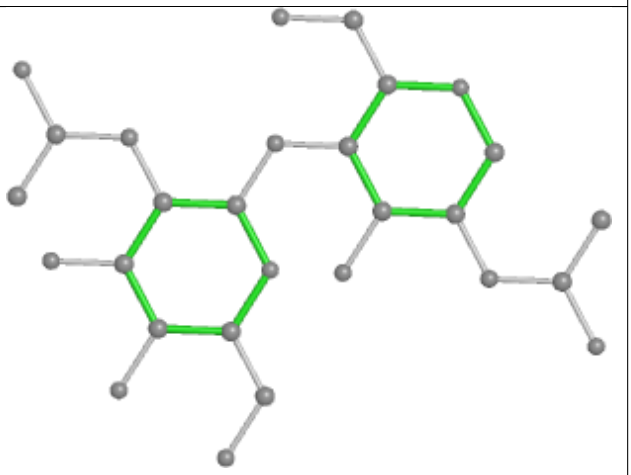
Bond lengths



Bond angles

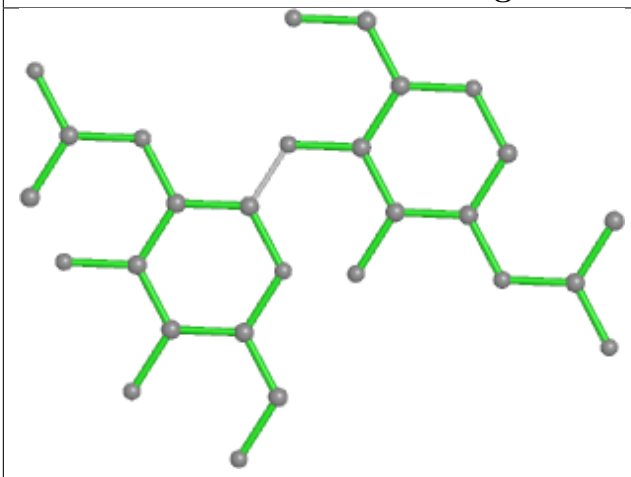


Torsions

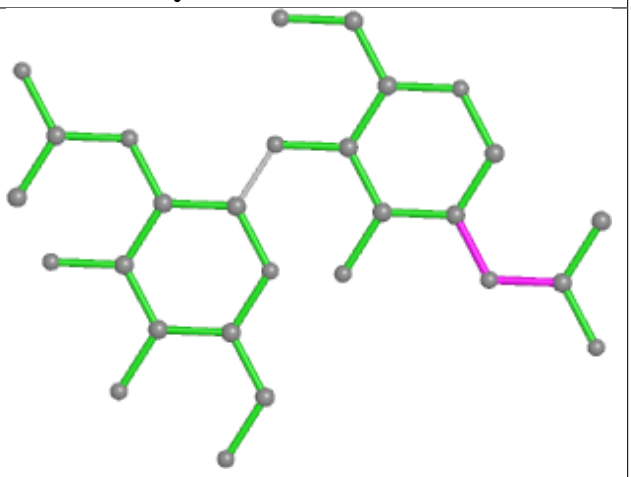


Rings

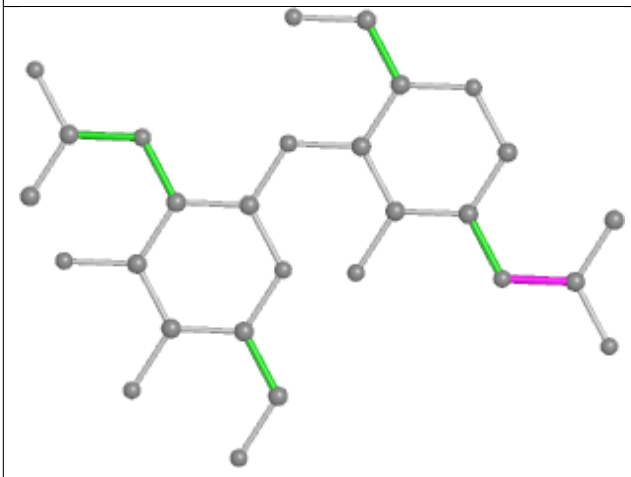
Oligosaccharide Chain Q



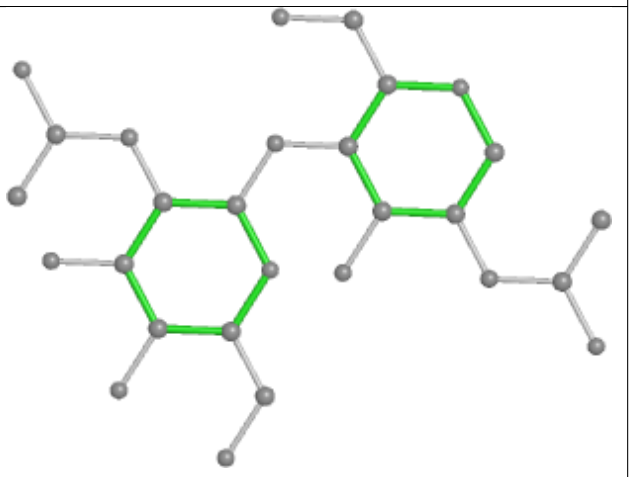
Bond lengths



Bond angles

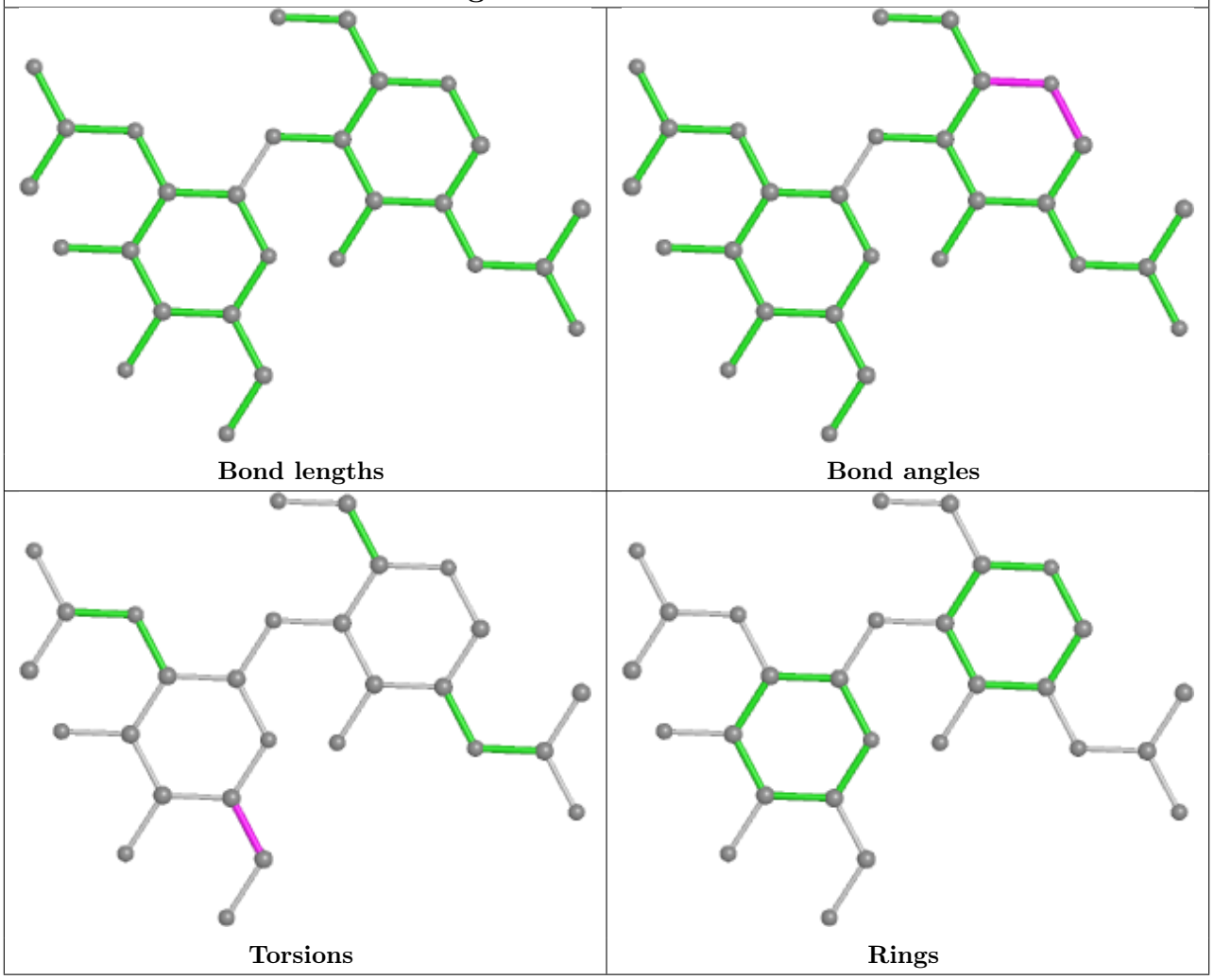


Torsions



Rings

Oligosaccharide Chain R



5.6 Ligand geometry (i)

45 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	A	1312	1	14,14,15	0.70	0	17,19,21	0.82	0
3	NAG	A	1315	1	14,14,15	0.70	0	17,19,21	1.46	2 (11%)
3	NAG	B	1311	1	14,14,15	0.73	0	17,19,21	1.47	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	B	1301	1	14,14,15	0.73	0	17,19,21	0.92	1 (5%)
3	NAG	C	1312	1	14,14,15	0.70	0	17,19,21	0.85	0
3	NAG	C	1314	1	14,14,15	0.71	0	17,19,21	0.90	1 (5%)
3	NAG	A	1310	1	14,14,15	0.70	0	17,19,21	1.46	2 (11%)
3	NAG	C	1302	1	14,14,15	0.69	0	17,19,21	1.05	1 (5%)
3	NAG	A	1303	1	14,14,15	0.73	0	17,19,21	0.97	1 (5%)
3	NAG	A	1307	1	14,14,15	0.74	0	17,19,21	1.60	2 (11%)
3	NAG	B	1314	1	14,14,15	0.70	0	17,19,21	0.90	0
3	NAG	B	1305	1	14,14,15	0.69	0	17,19,21	1.07	2 (11%)
3	NAG	B	1312	1	14,14,15	0.70	0	17,19,21	0.87	0
3	NAG	C	1307	1	14,14,15	0.73	0	17,19,21	1.55	2 (11%)
3	NAG	A	1306	1	14,14,15	0.71	0	17,19,21	0.78	0
3	NAG	C	1310	1	14,14,15	0.75	0	17,19,21	0.82	0
3	NAG	C	1306	1	14,14,15	0.73	0	17,19,21	0.95	1 (5%)
3	NAG	C	1303	1	14,14,15	0.72	0	17,19,21	1.07	1 (5%)
3	NAG	A	1311	1	14,14,15	0.71	0	17,19,21	0.87	0
3	NAG	A	1302	1	14,14,15	0.70	0	17,19,21	0.88	0
3	NAG	C	1311	1	14,14,15	0.70	0	17,19,21	1.45	2 (11%)
3	NAG	B	1310	1	14,14,15	0.68	0	17,19,21	1.17	1 (5%)
3	NAG	B	1308	1	14,14,15	0.71	0	17,19,21	1.00	1 (5%)
4	BLR	B	1315	-	40,46,46	3.65	3 (7%)	44,67,67	0.99	2 (4%)
3	NAG	B	1302	1	14,14,15	0.69	0	17,19,21	0.87	0
3	NAG	B	1304	1	14,14,15	0.66	0	17,19,21	2.53	4 (23%)
3	NAG	B	1306	1	14,14,15	0.72	0	17,19,21	0.90	1 (5%)
3	NAG	C	1305	1	14,14,15	0.69	0	17,19,21	1.10	2 (11%)
3	NAG	A	1313	1	14,14,15	0.71	0	17,19,21	0.89	0
3	NAG	C	1309	1	14,14,15	0.43	0	17,19,21	0.81	1 (5%)
3	NAG	B	1303	1	14,14,15	0.73	0	17,19,21	1.00	1 (5%)
3	NAG	A	1301	1	14,14,15	0.71	0	17,19,21	0.92	1 (5%)
3	NAG	A	1308	1	14,14,15	0.70	0	17,19,21	1.00	1 (5%)
3	NAG	B	1313	1	14,14,15	0.71	0	17,19,21	0.84	0
3	NAG	C	1304	1	14,14,15	0.69	0	17,19,21	1.02	1 (5%)
3	NAG	C	1313	1	14,14,15	0.71	0	17,19,21	0.86	0
3	NAG	B	1309	1	14,14,15	0.71	0	17,19,21	1.45	1 (5%)
4	BLR	C	1315	-	40,46,46	3.61	3 (7%)	44,67,67	1.03	3 (6%)
3	NAG	A	1304	1	14,14,15	0.71	0	17,19,21	1.02	1 (5%)
3	NAG	C	1308	1	14,14,15	0.70	0	17,19,21	0.96	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	C	1301	1	14,14,15	0.70	0	17,19,21	0.94	1 (5%)
4	BLR	A	1314	-	40,46,46	3.61	3 (7%)	44,67,67	0.99	3 (6%)
3	NAG	B	1307	1	14,14,15	0.74	0	17,19,21	1.04	1 (5%)
3	NAG	A	1309	1	14,14,15	0.76	0	17,19,21	0.82	0
3	NAG	A	1305	1	14,14,15	0.67	0	17,19,21	1.03	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	1312	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1315	1	-	1/6/23/26	0/1/1/1
3	NAG	B	1311	1	-	3/6/23/26	0/1/1/1
3	NAG	B	1301	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1312	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1314	1	-	1/6/23/26	0/1/1/1
3	NAG	A	1310	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1302	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1303	1	-	1/6/23/26	0/1/1/1
3	NAG	A	1307	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1314	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1305	1	-	3/6/23/26	0/1/1/1
3	NAG	B	1312	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1307	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1306	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1310	1	-	1/6/23/26	0/1/1/1
3	NAG	C	1306	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1303	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1311	1	-	1/6/23/26	0/1/1/1
3	NAG	A	1302	1	-	1/6/23/26	0/1/1/1
3	NAG	C	1311	1	-	1/6/23/26	0/1/1/1
3	NAG	B	1310	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1308	1	-	1/6/23/26	0/1/1/1
4	BLR	B	1315	-	-	10/24/58/58	0/4/4/4
3	NAG	B	1302	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1304	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1306	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1305	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	1313	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1309	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1303	1	-	1/6/23/26	0/1/1/1
3	NAG	A	1301	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	1313	1	-	1/6/23/26	0/1/1/1
3	NAG	C	1304	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1313	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1309	1	-	1/6/23/26	0/1/1/1
4	BLR	C	1315	-	-	10/24/58/58	0/4/4/4
3	NAG	A	1304	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1308	1	-	1/6/23/26	0/1/1/1
3	NAG	C	1301	1	-	1/6/23/26	0/1/1/1
4	BLR	A	1314	-	-	11/24/58/58	0/4/4/4
3	NAG	B	1307	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1309	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1305	1	-	2/6/23/26	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1315	BLR	CHA-C4D	-18.04	1.37	1.51
4	C	1315	BLR	CHA-C4D	-17.83	1.38	1.51
4	A	1314	BLR	CHA-C4D	-17.77	1.38	1.51
4	B	1315	BLR	CHA-C1A	-12.35	1.42	1.51
4	A	1314	BLR	CHA-C1A	-12.24	1.42	1.51

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1304	NAG	C1-O5-C5	8.76	124.06	112.19
3	A	1310	NAG	C2-N2-C7	4.28	129.00	122.90
3	C	1311	NAG	C2-N2-C7	4.26	128.97	122.90
3	A	1315	NAG	C2-N2-C7	4.25	128.96	122.90
3	A	1307	NAG	C2-N2-C7	4.25	128.96	122.90

There are no chirality outliers.

5 of 70 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1314	BLR	C2A-C1A-CHA-C4D
4	A	1314	BLR	C3D-C4D-CHA-C1A
4	A	1314	BLR	ND-C1D-CHD-C4C
4	A	1314	BLR	C2D-C1D-CHD-C4C
4	B	1315	BLR	C2A-C1A-CHA-C4D

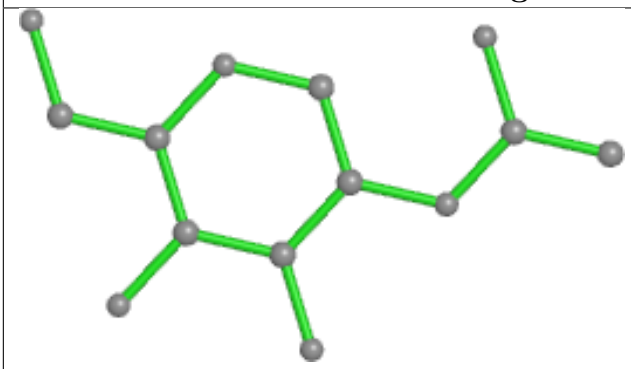
There are no ring outliers.

3 monomers are involved in 5 short contacts:

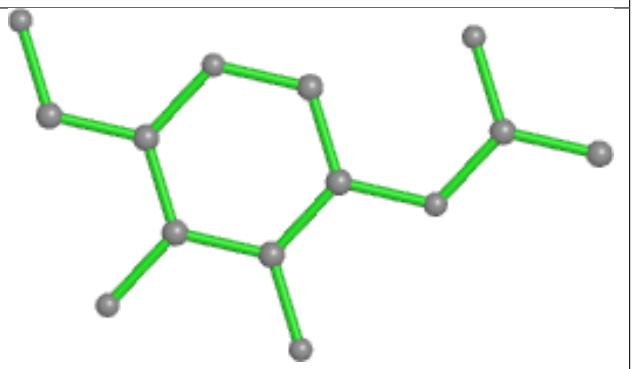
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1315	BLR	2	0
4	C	1315	BLR	1	0
4	A	1314	BLR	2	0

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.

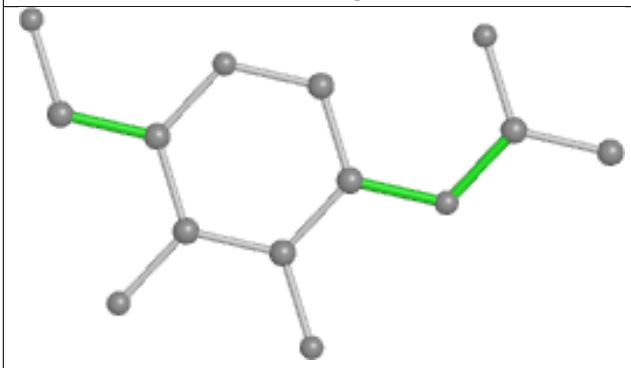
Ligand NAG A 1312



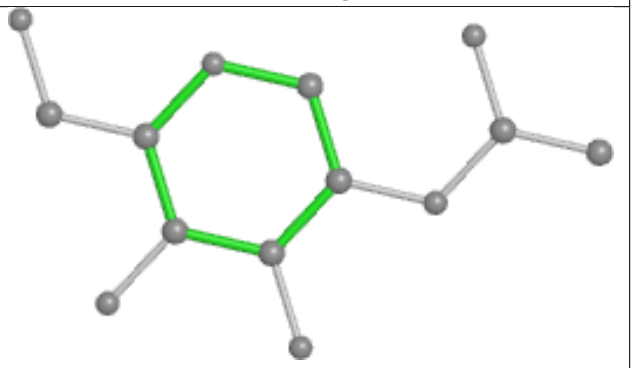
Bond lengths



Bond angles

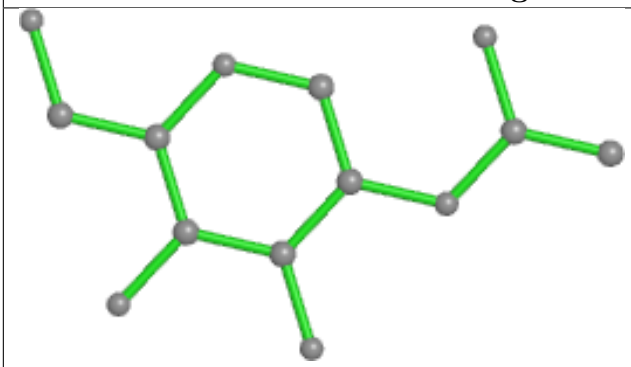


Torsions

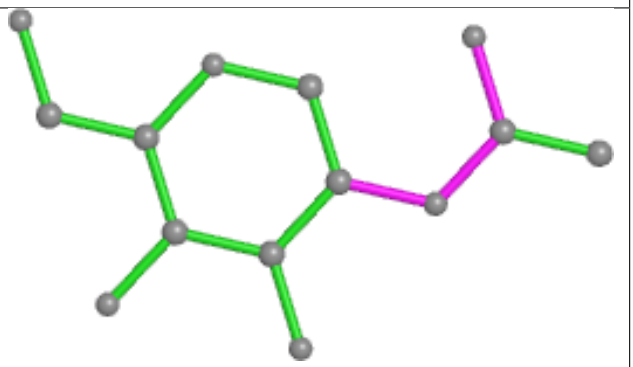


Rings

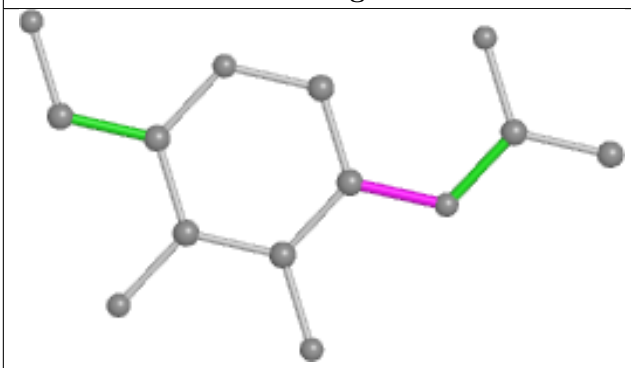
Ligand NAG A 1315



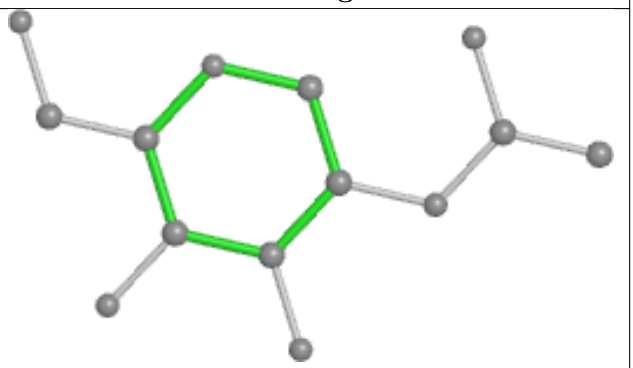
Bond lengths



Bond angles

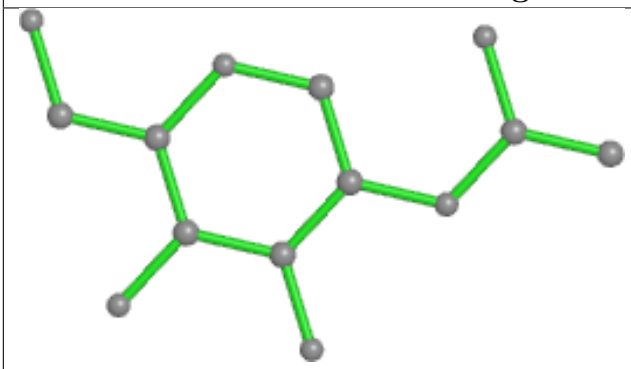


Torsions

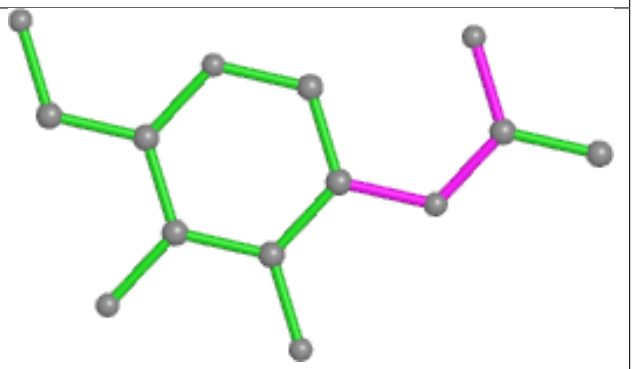


Rings

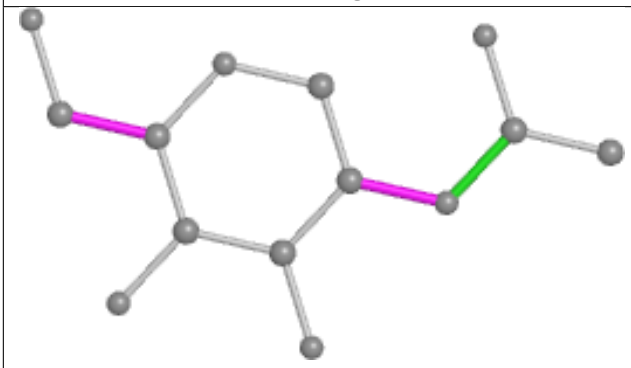
Ligand NAG B 1311



Bond lengths



Bond angles



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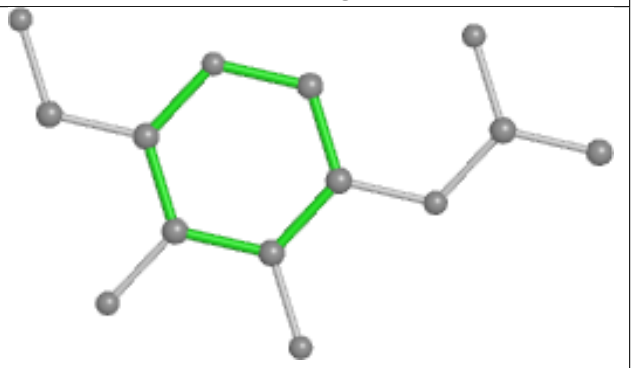

Rings

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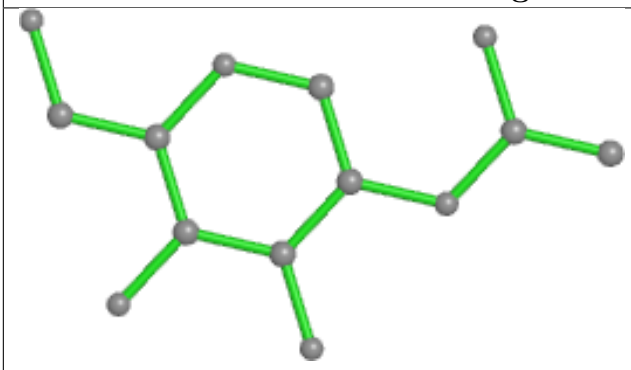

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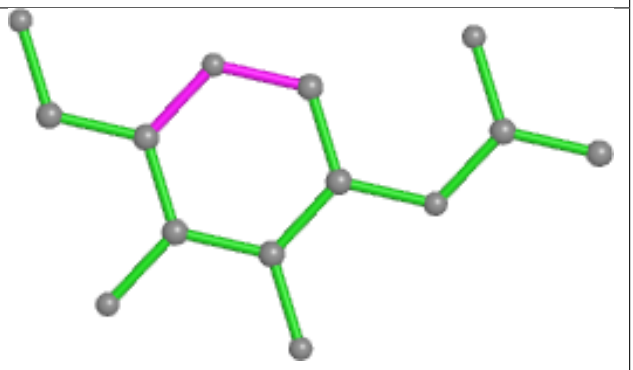

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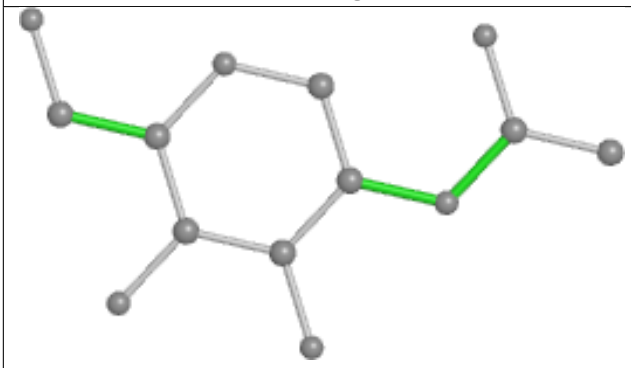

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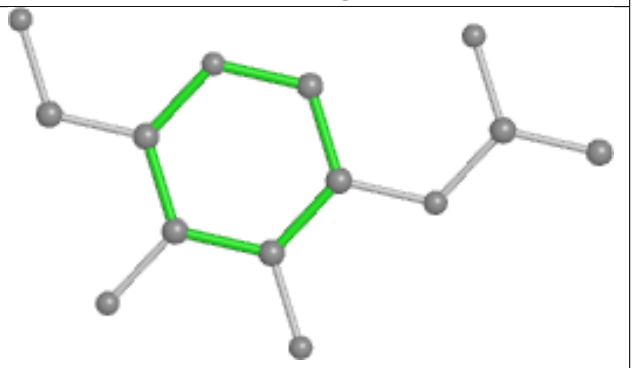
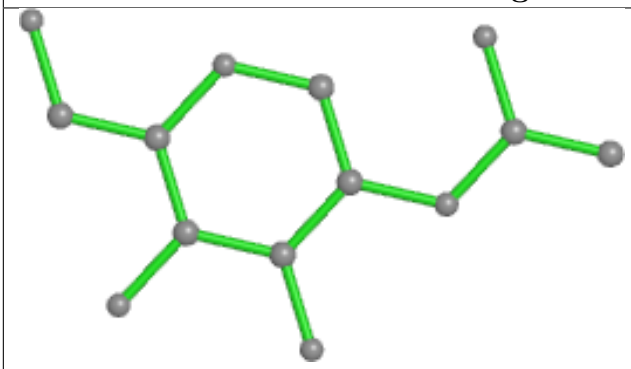


Rings

Ligand NAG C 1312



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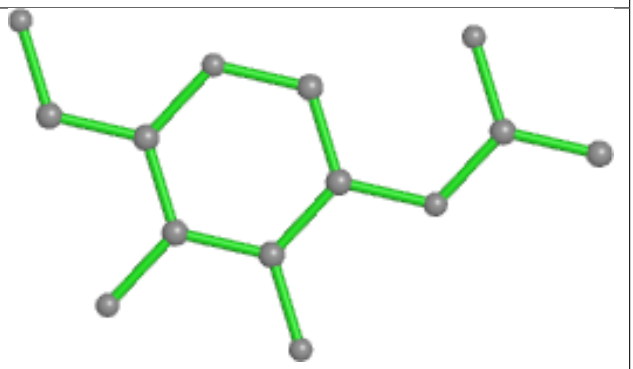

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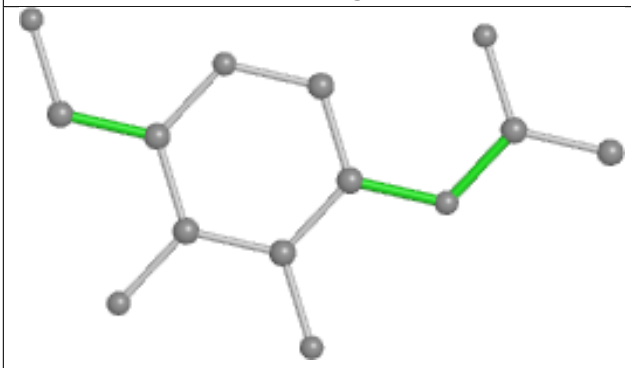

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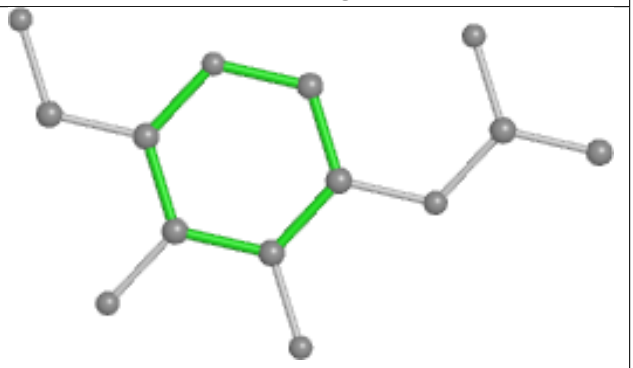

Rings

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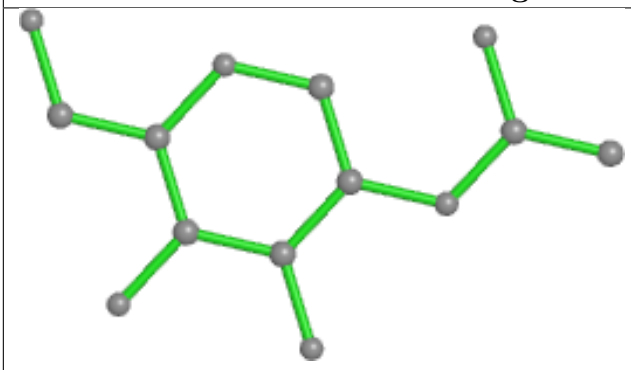

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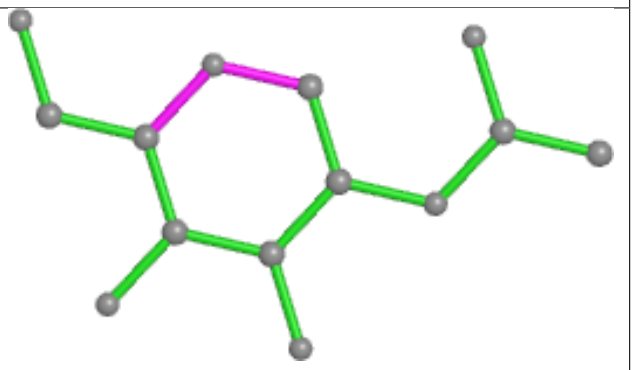

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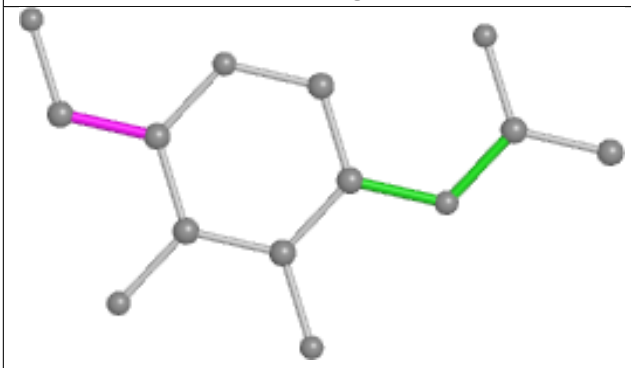

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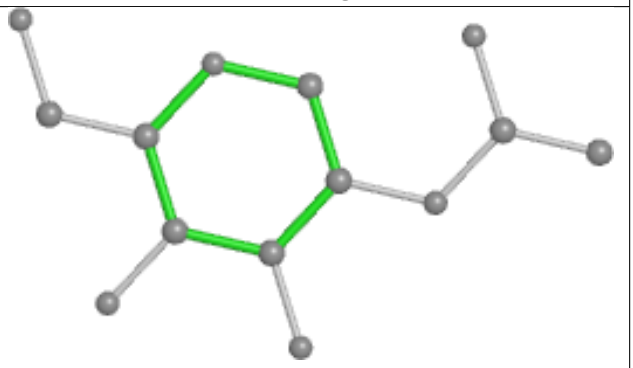
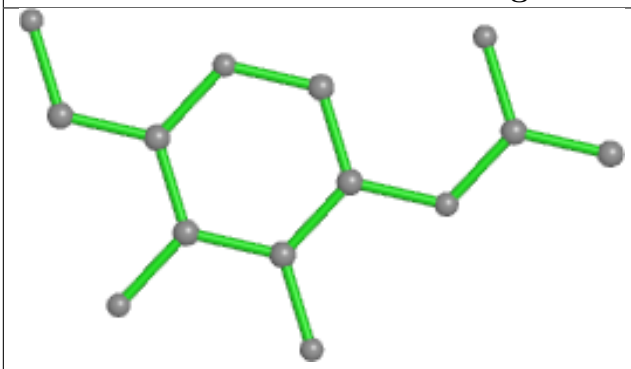


Rings

Ligand NAG A 1310



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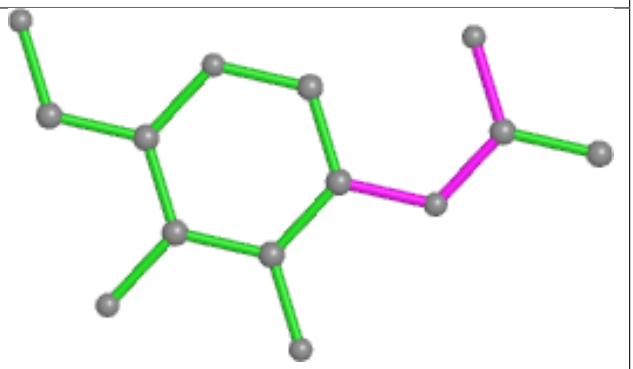

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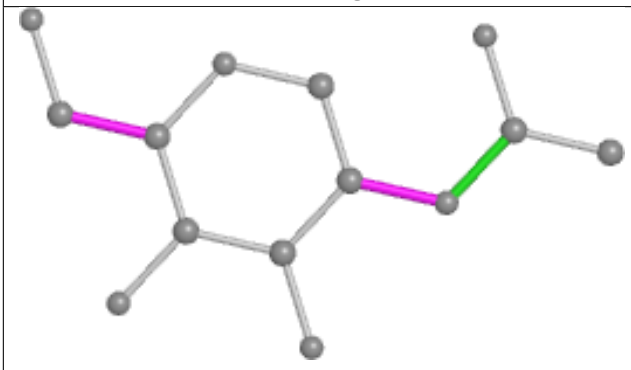

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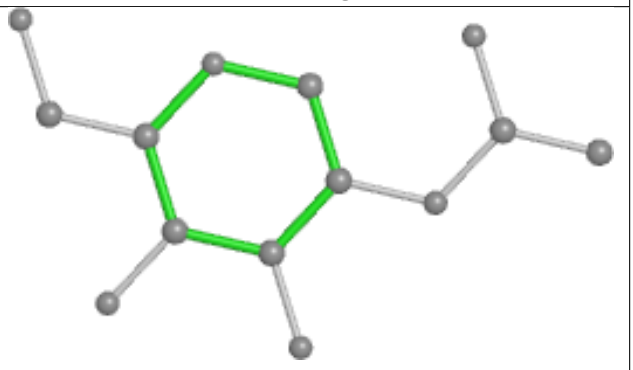

Rings

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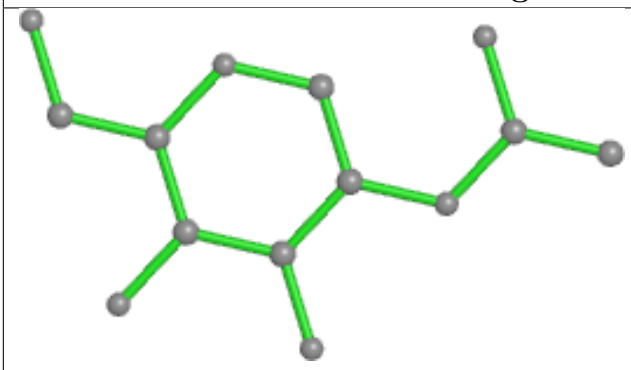

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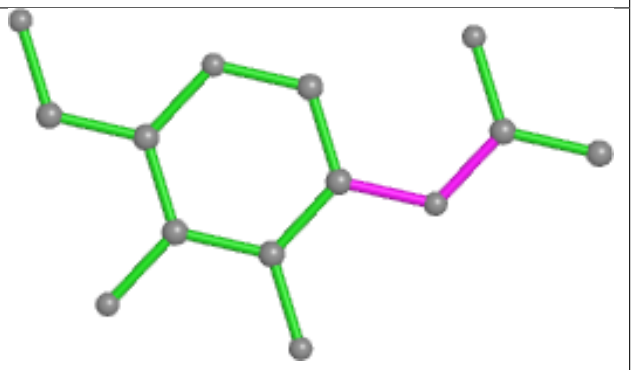

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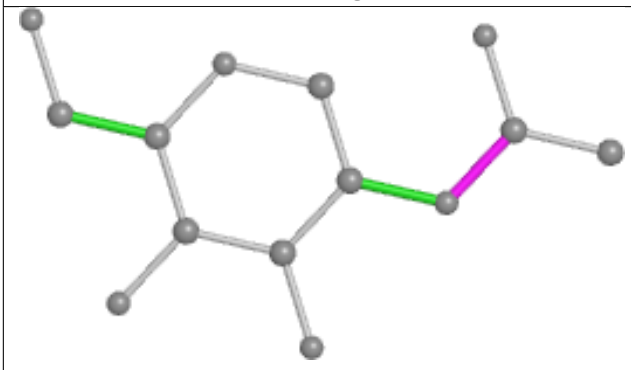

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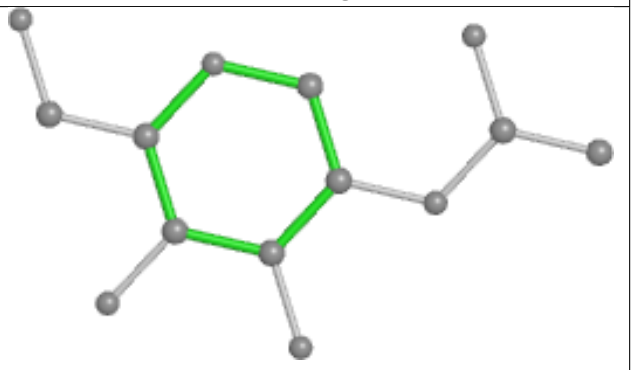

Rings

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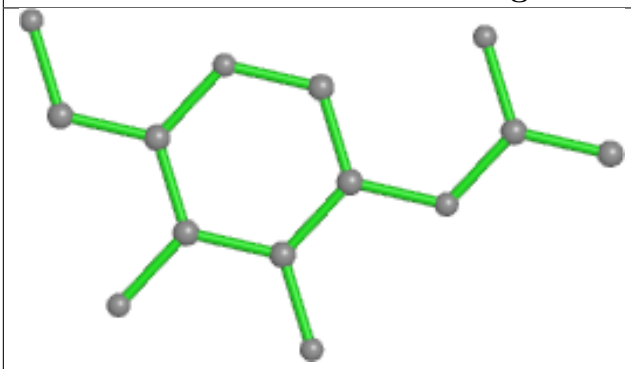

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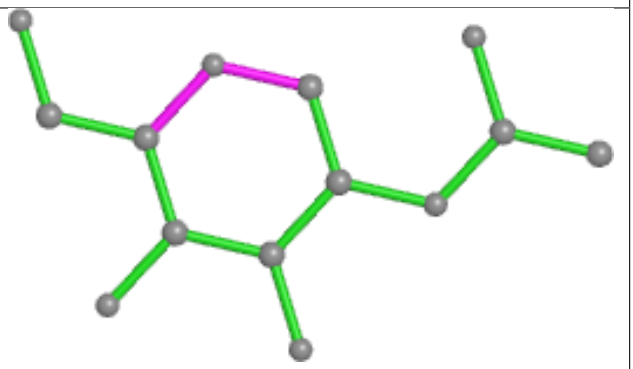

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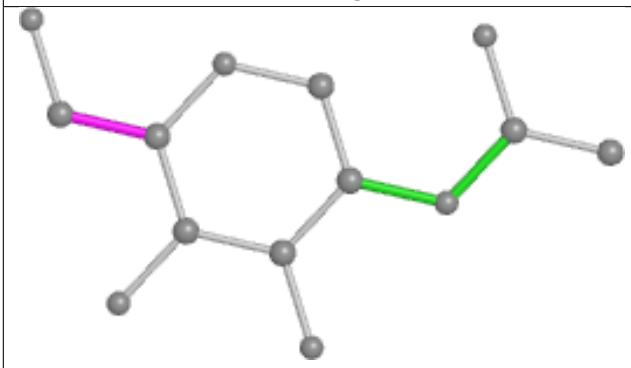

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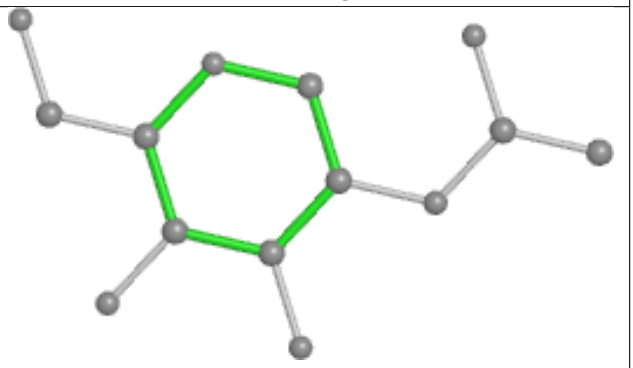

Rings

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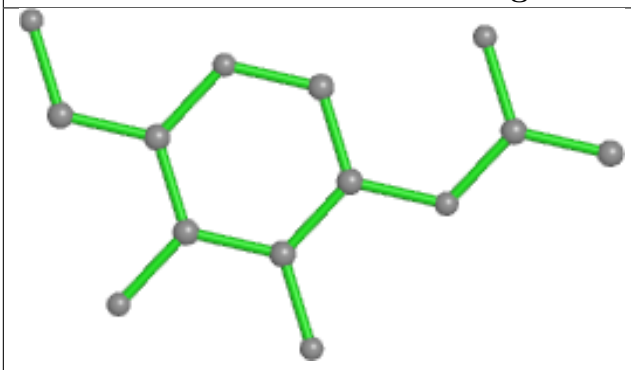

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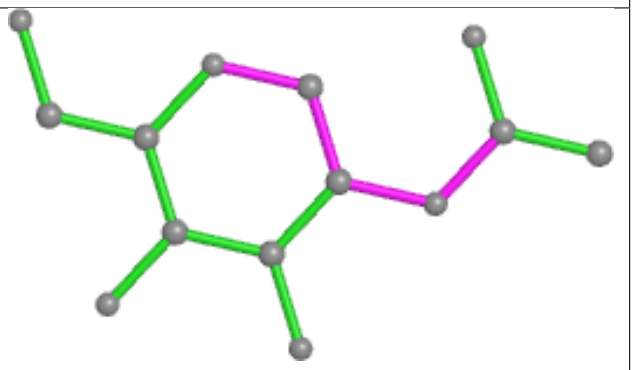

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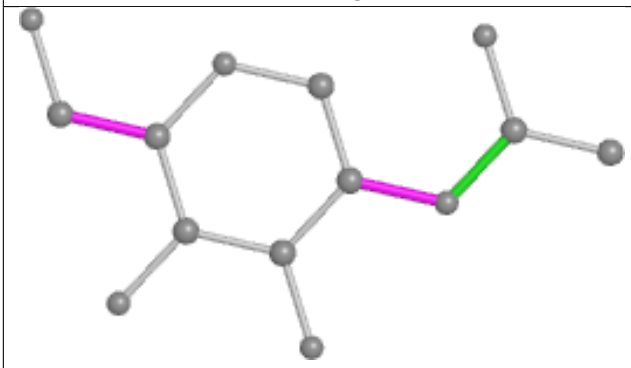

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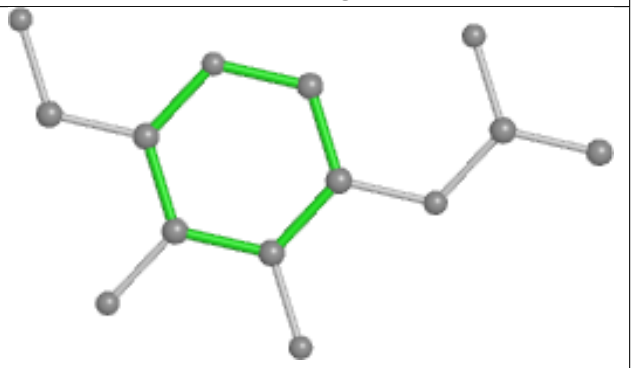

Rings

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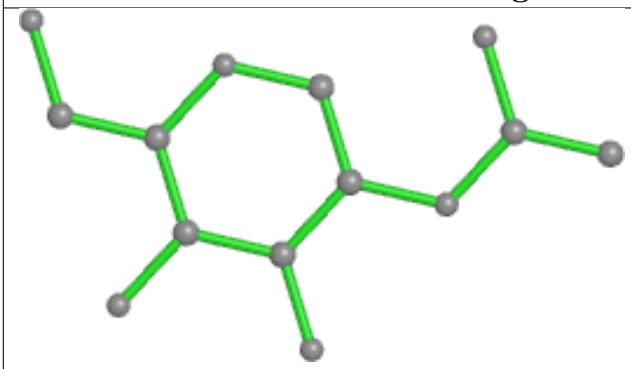

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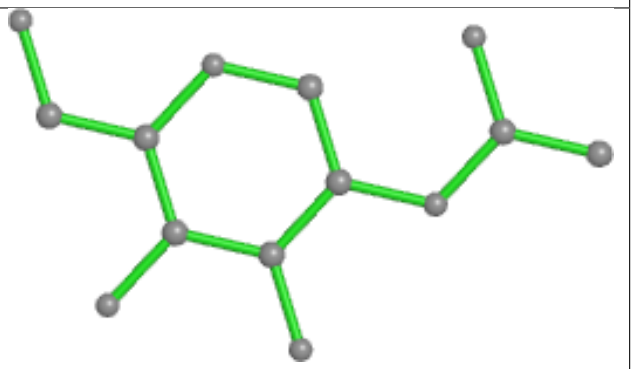

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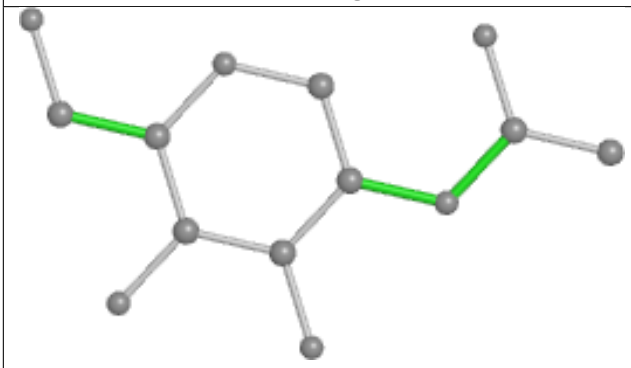

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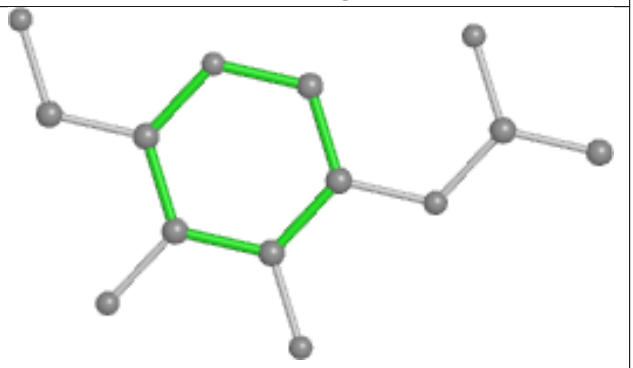

Rings

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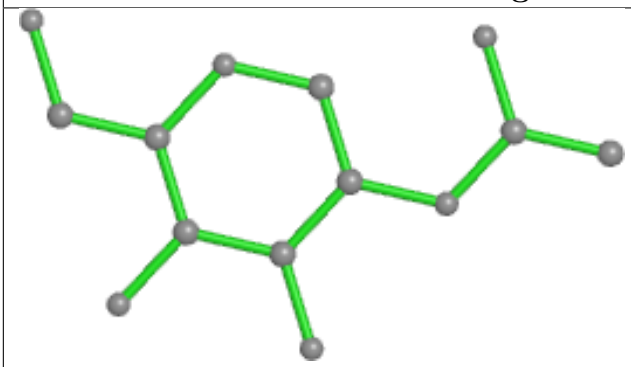

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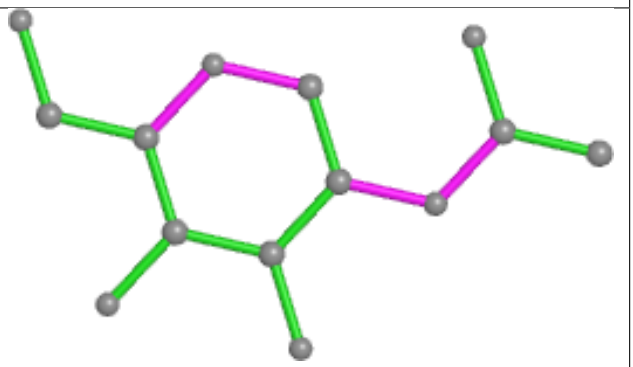
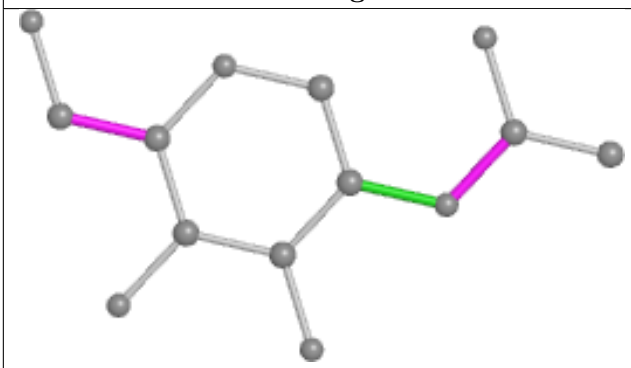


Bond angles



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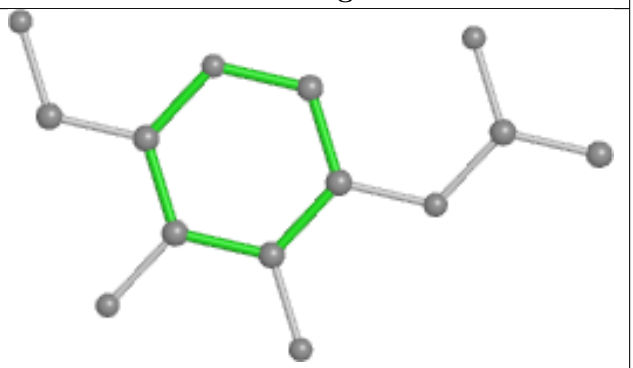

Rings

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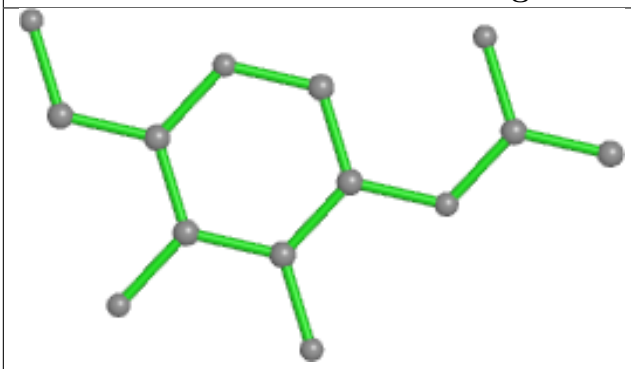

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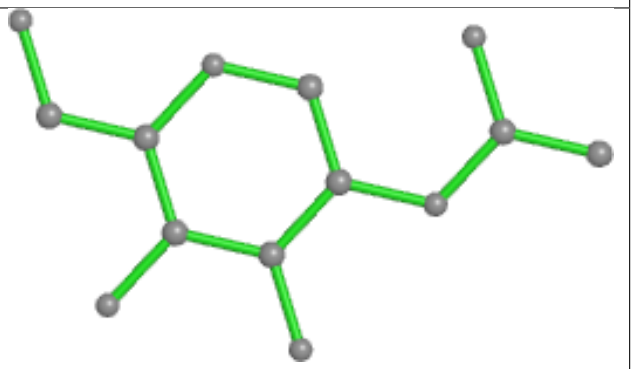
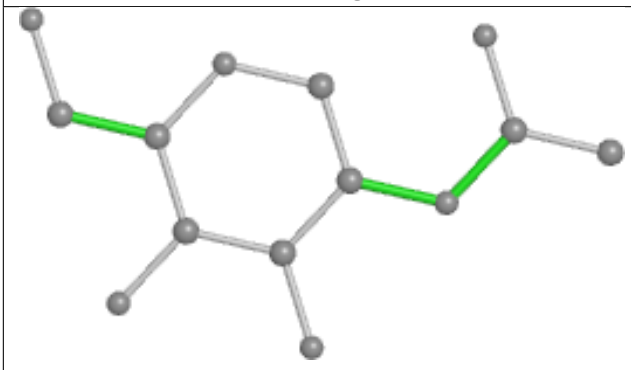


Bond angles



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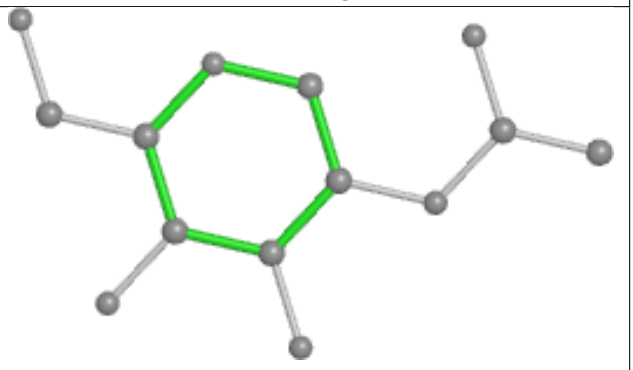
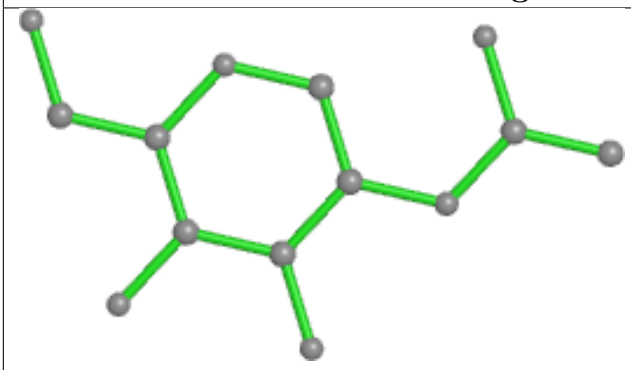


Rings

Ligand NAG C 1307



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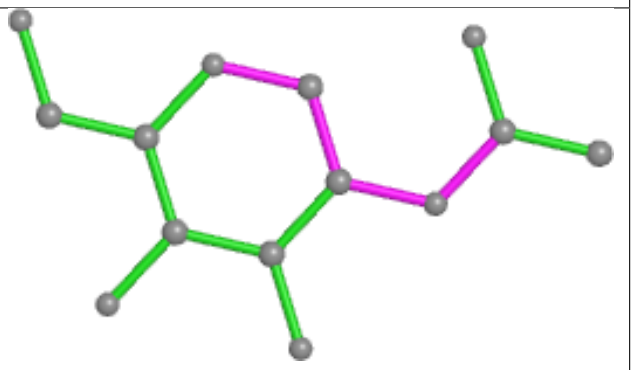
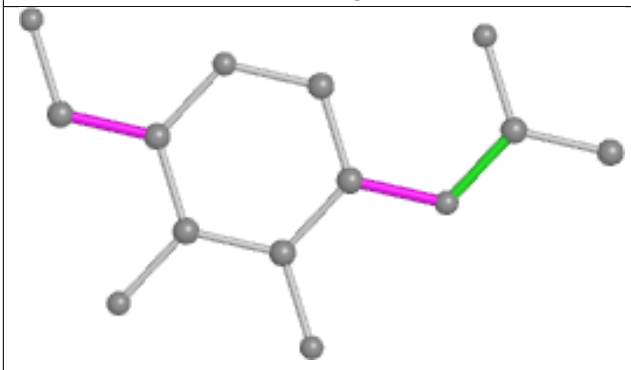


Bond angles



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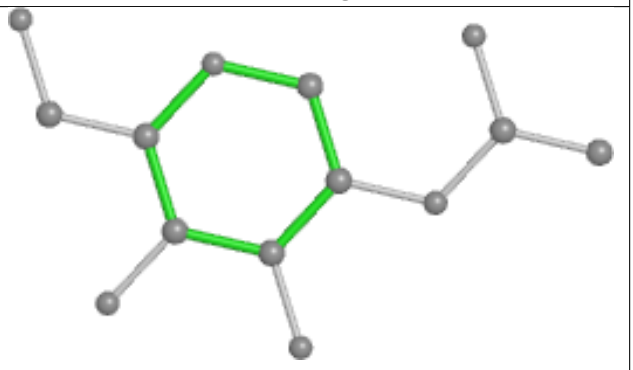

Rings

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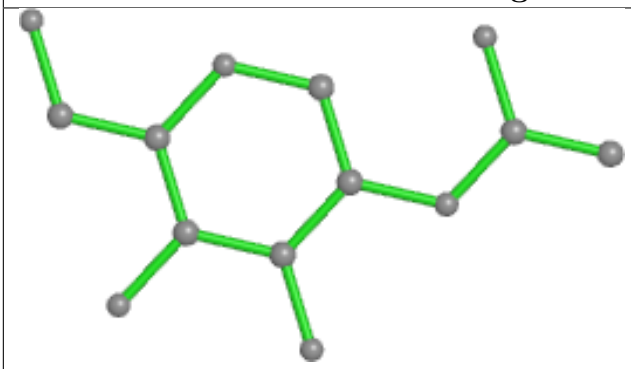

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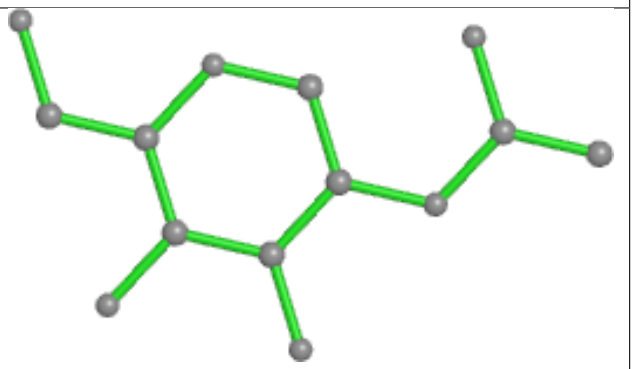
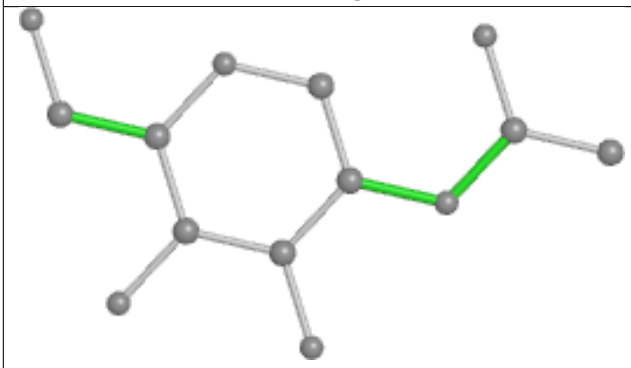


Bond angles



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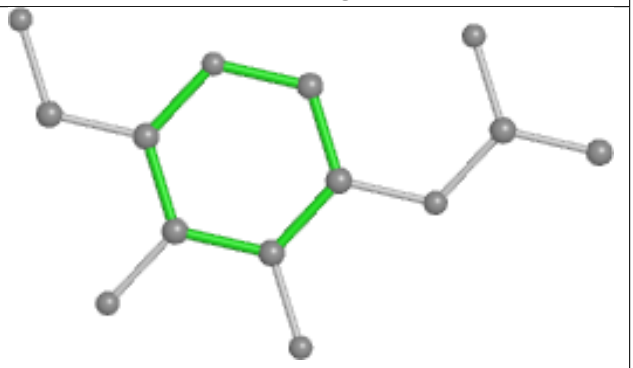
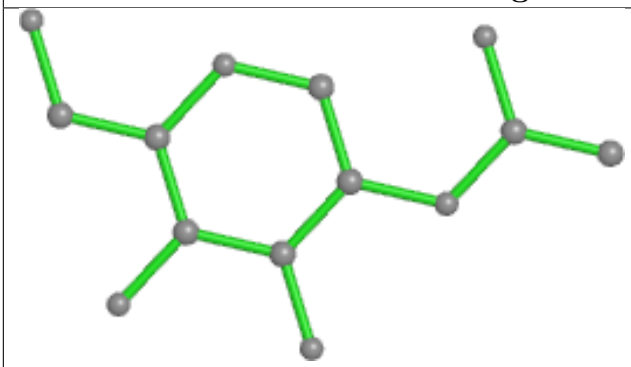


Rings

Ligand NAG C 1310



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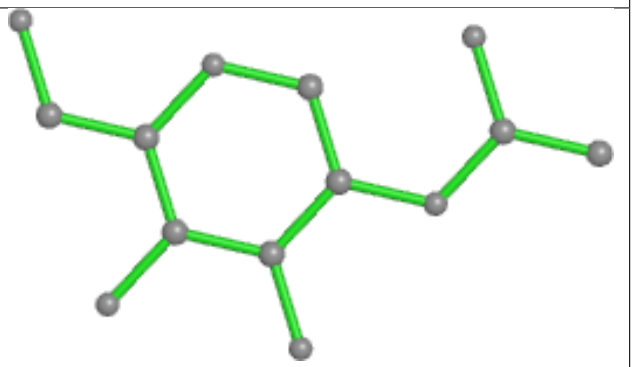

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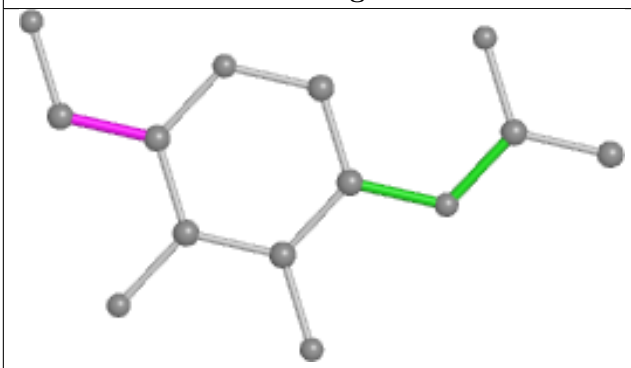

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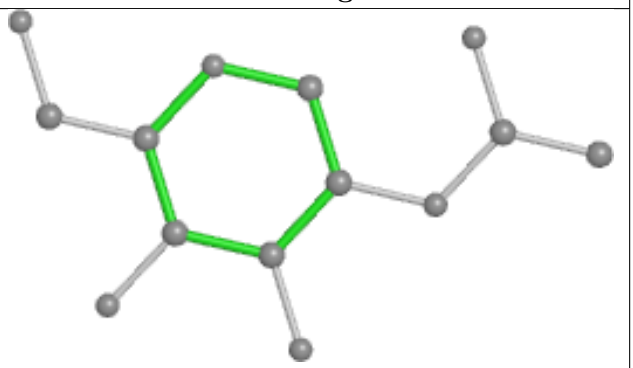
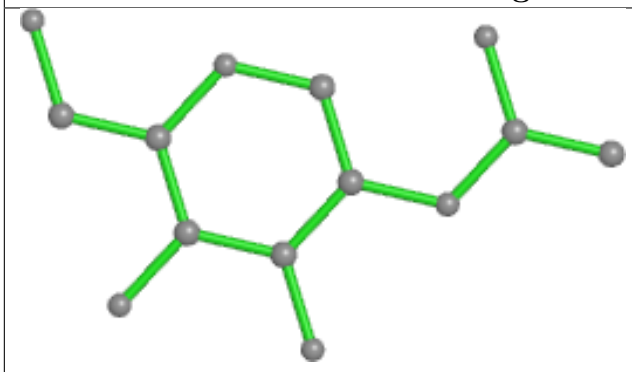


Rings

Ligand NAG C 1306



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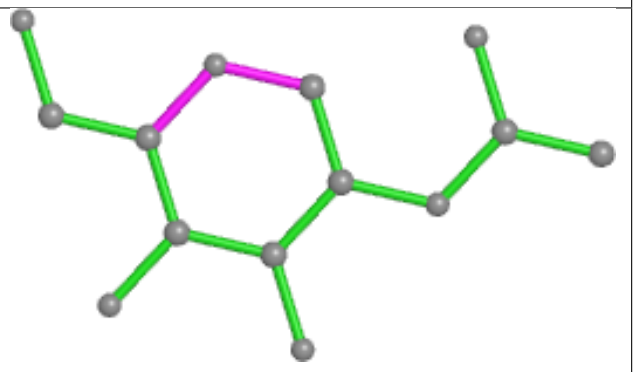

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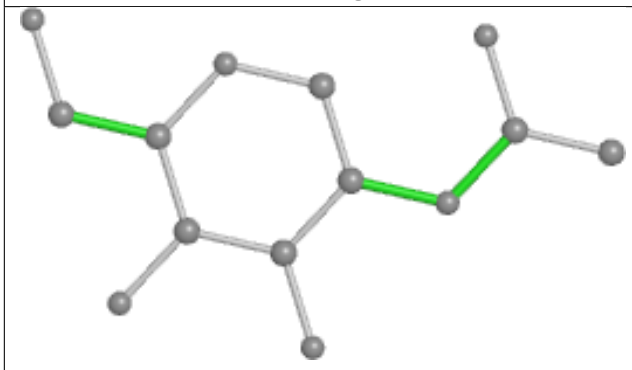

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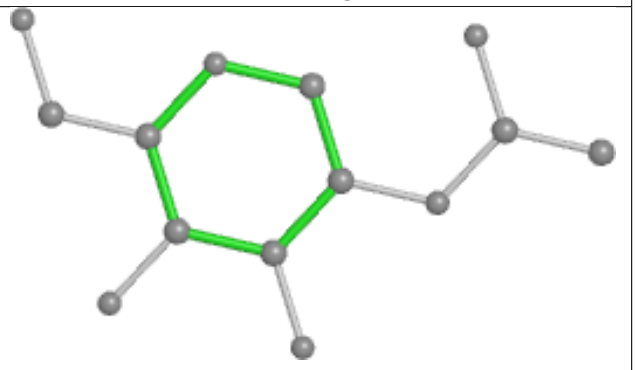
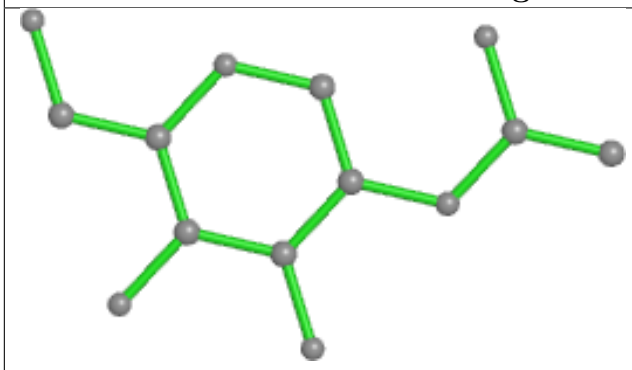


Rings

Ligand NAG C 1303



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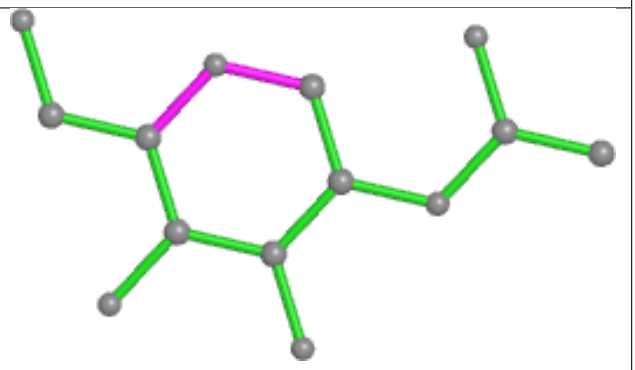

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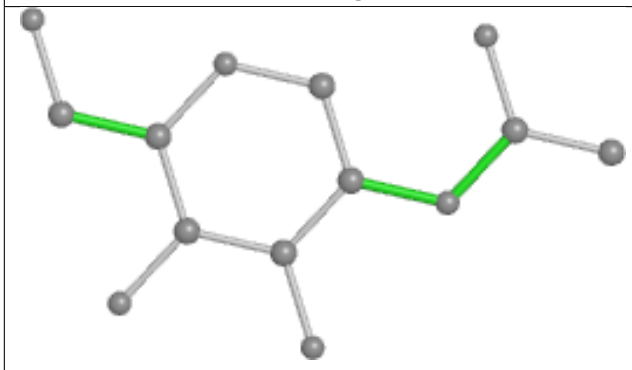

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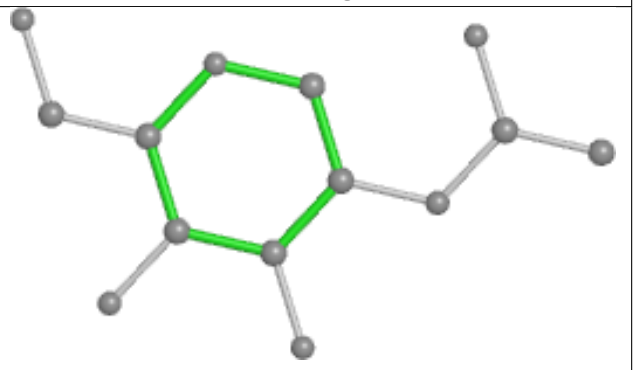
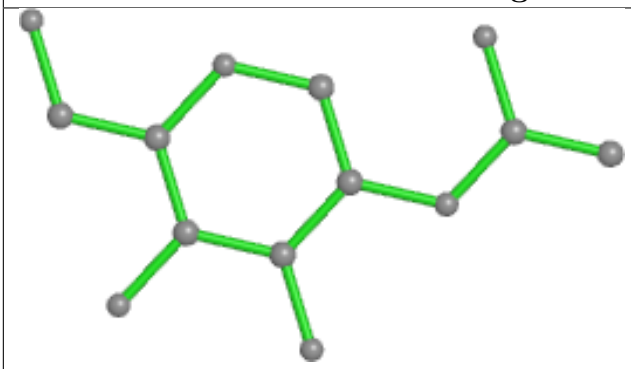


Rings

Ligand NAG A 1311



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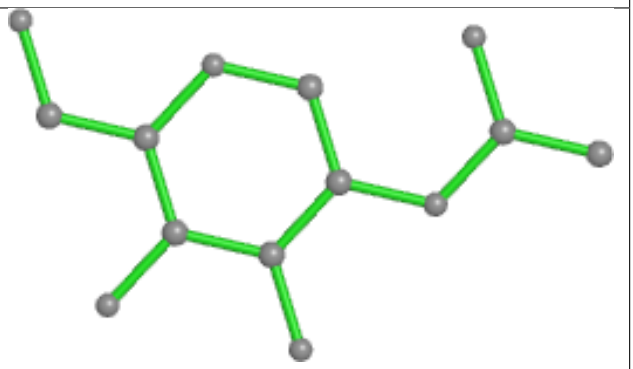

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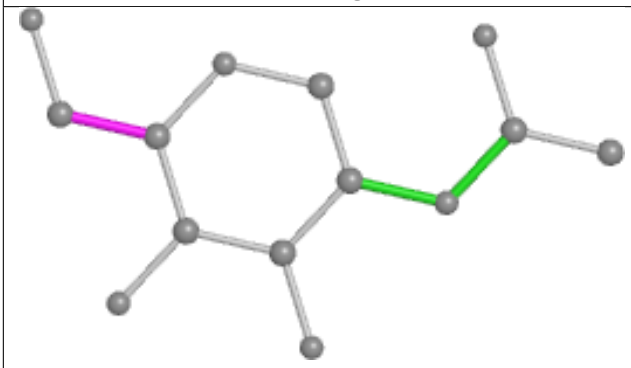

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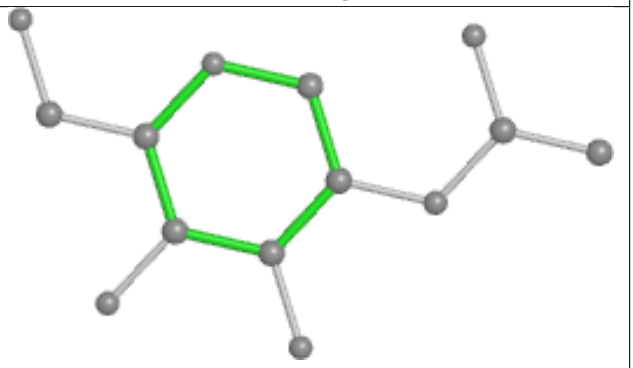

Rings

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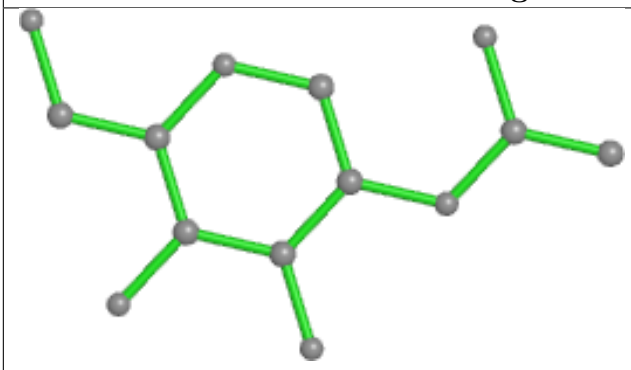

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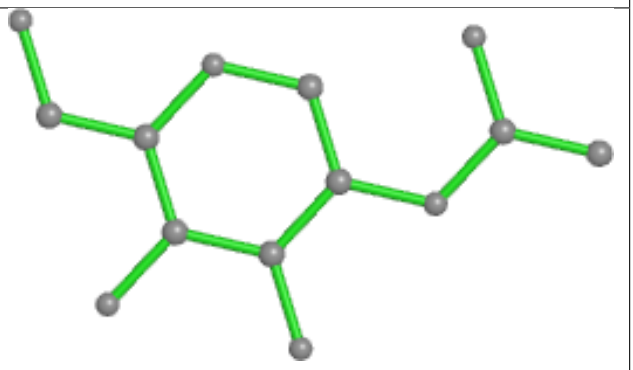
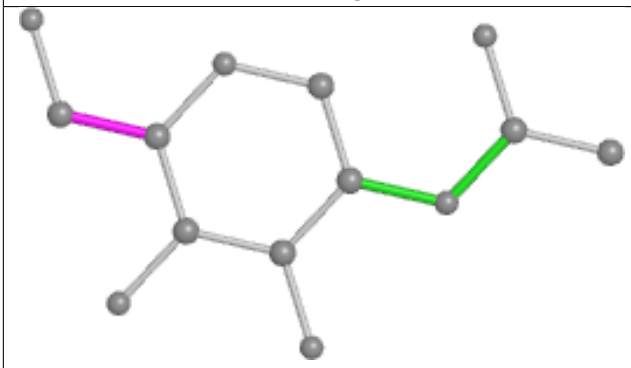


Bond angles



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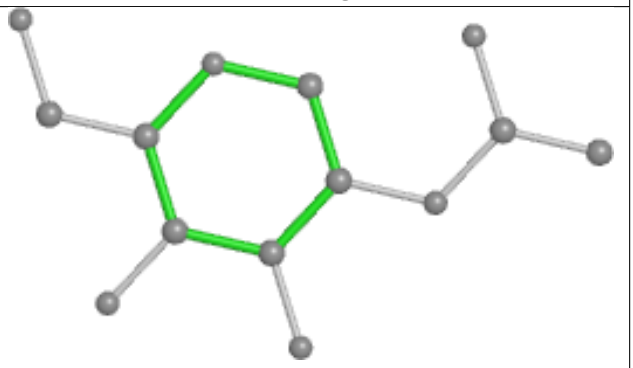

Rings

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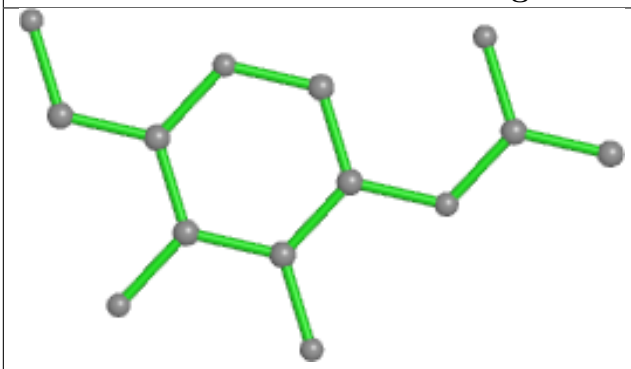

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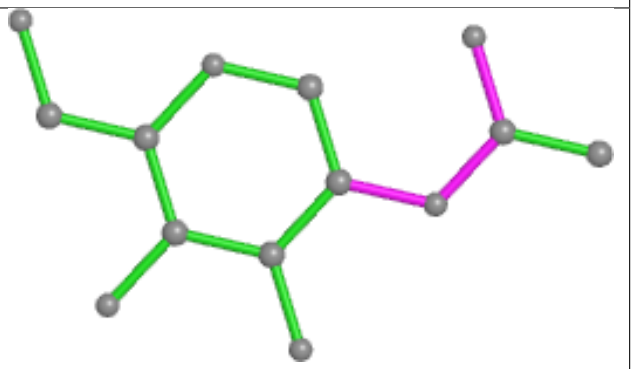

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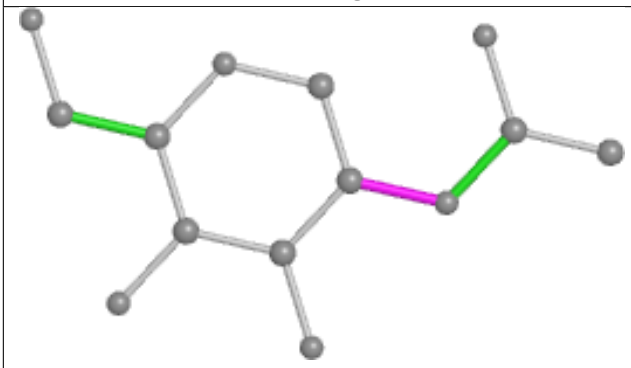

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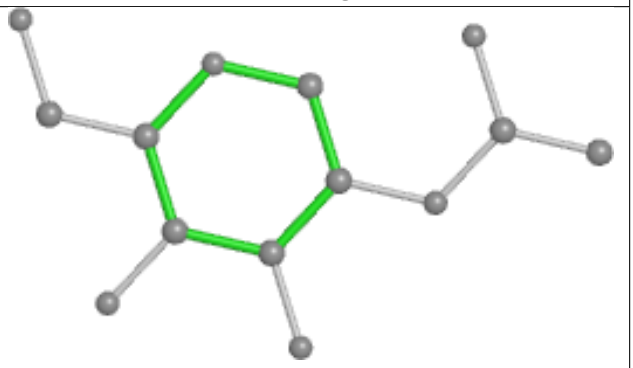

Rings

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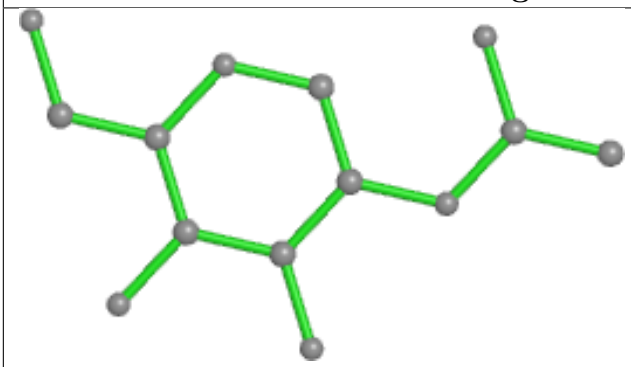

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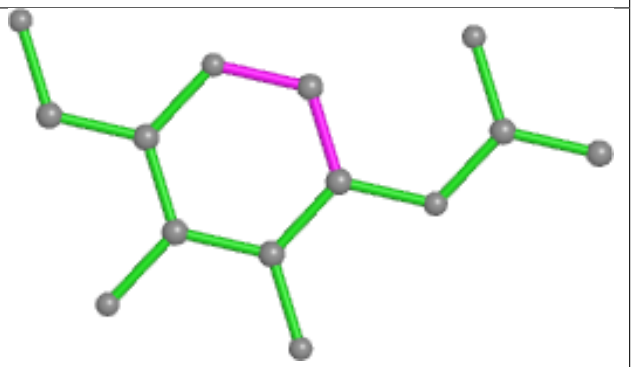

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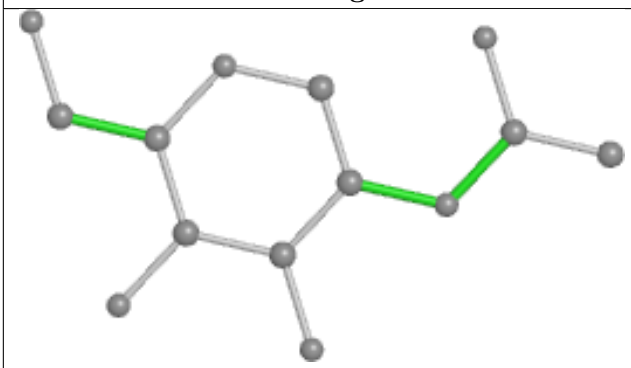

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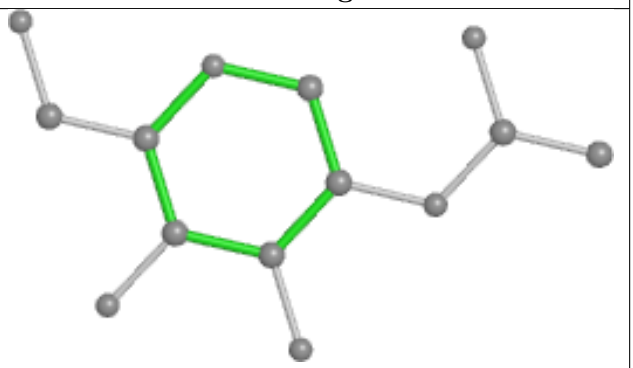

Rings

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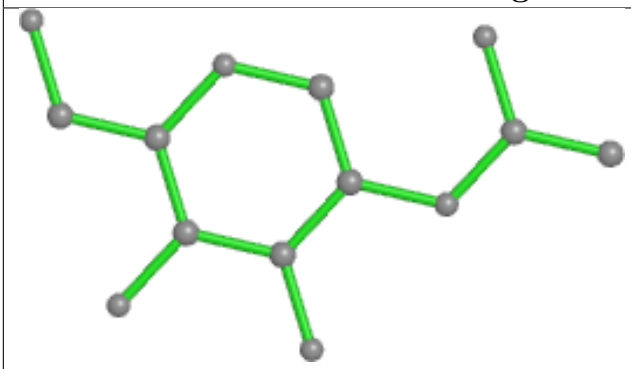

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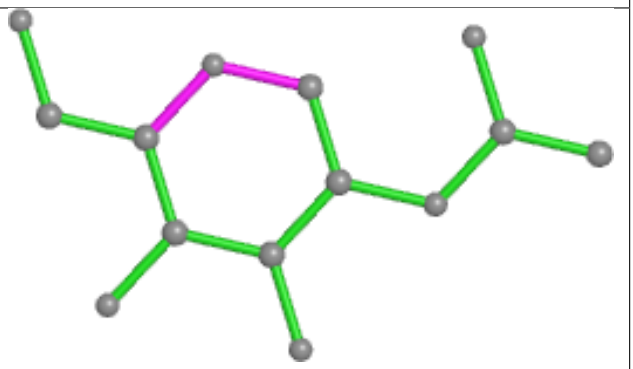

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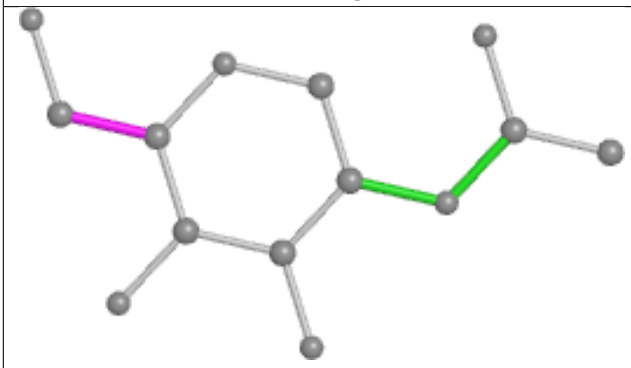

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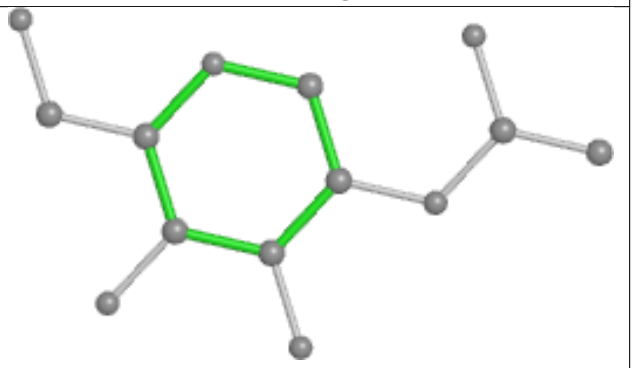

Rings

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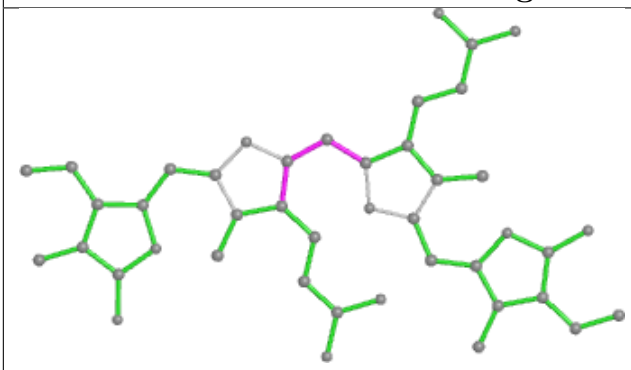

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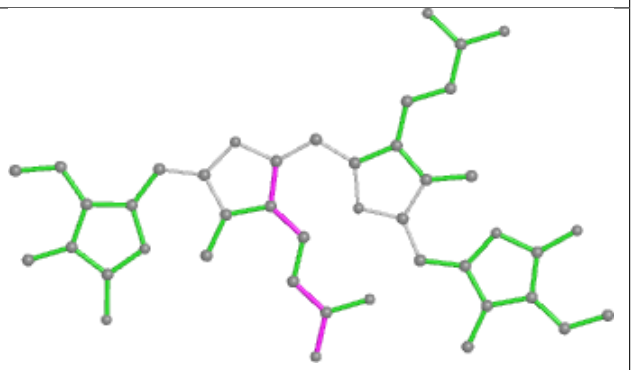
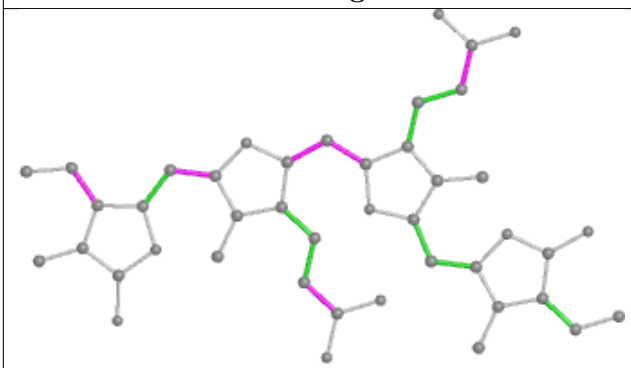


Bond angles



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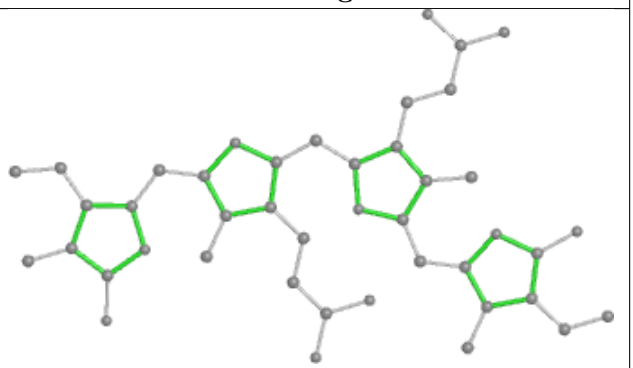

Rings

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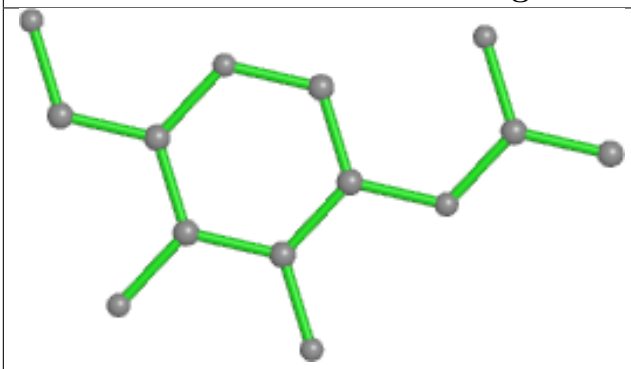

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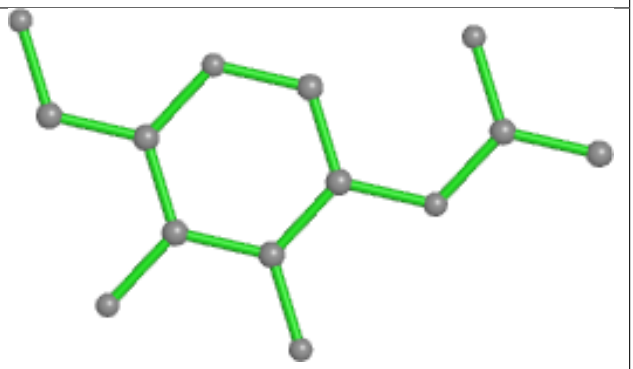

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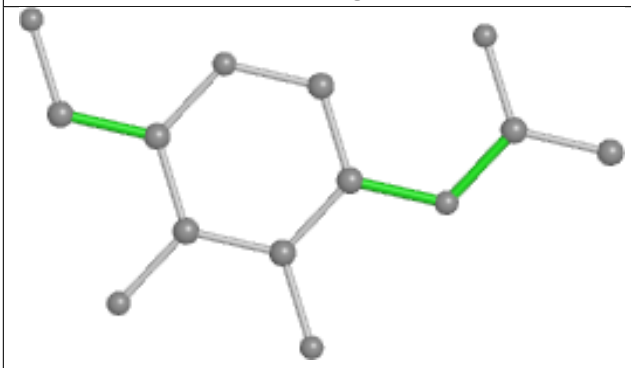

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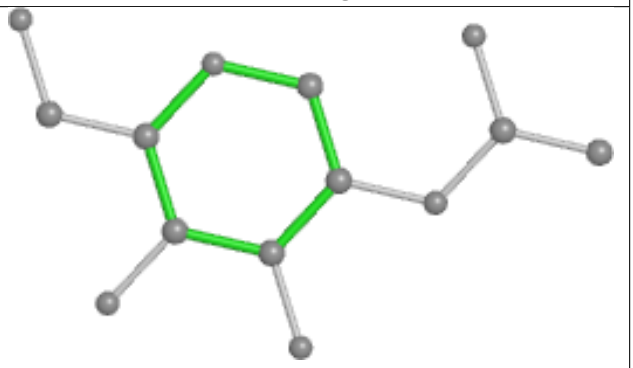

Rings

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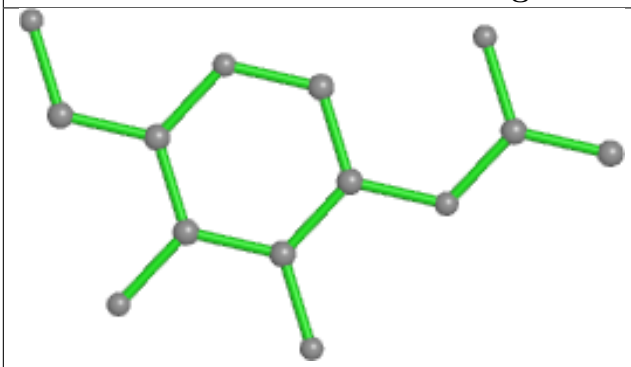

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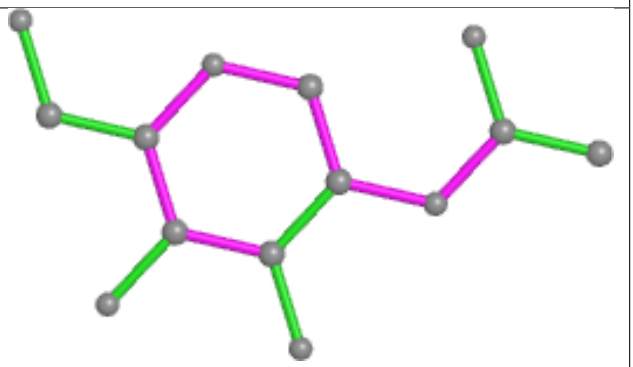
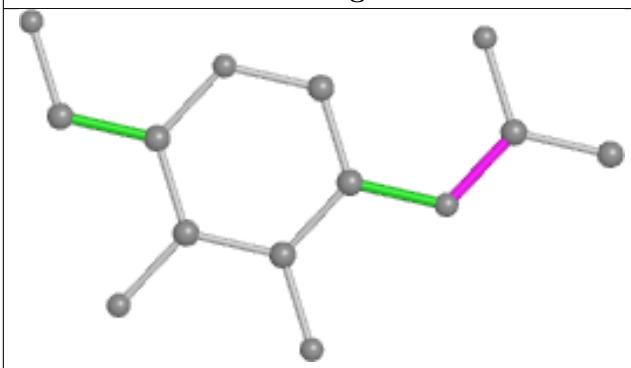


Bond angles



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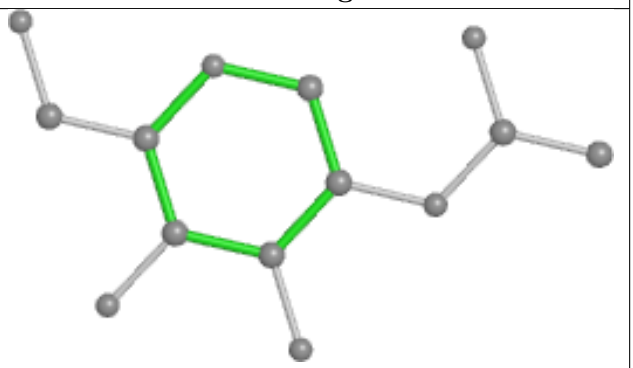

Rings

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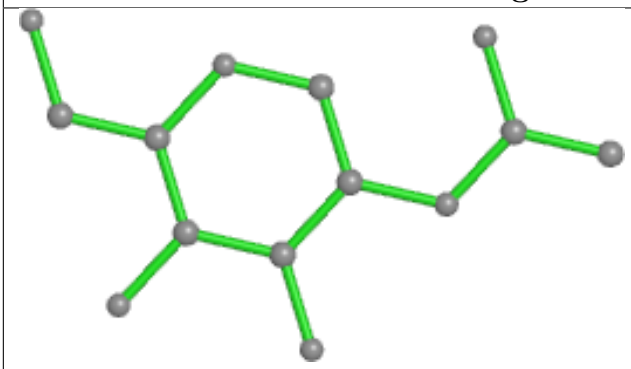

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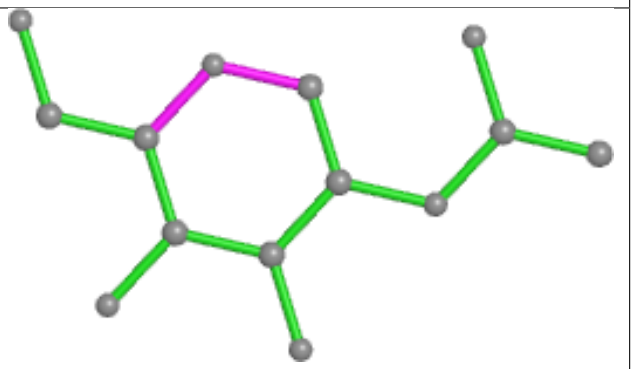
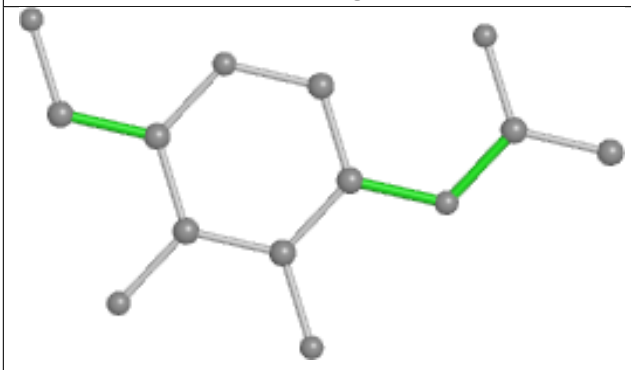
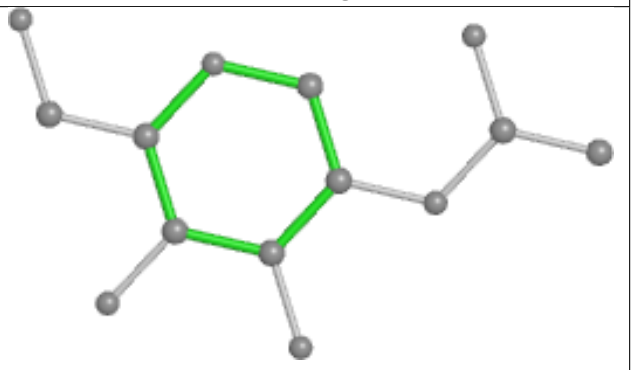


Bond angles

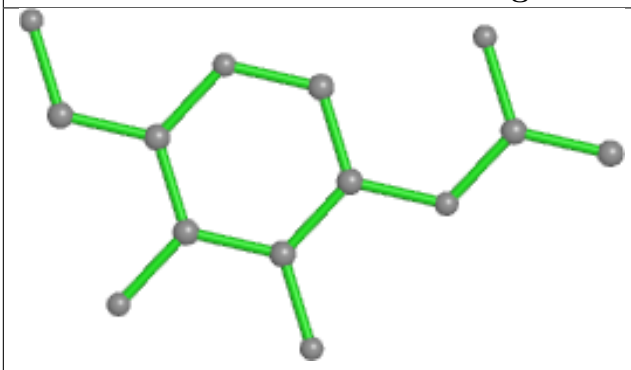


Torsions



Rings

Ligand NAG C 1305



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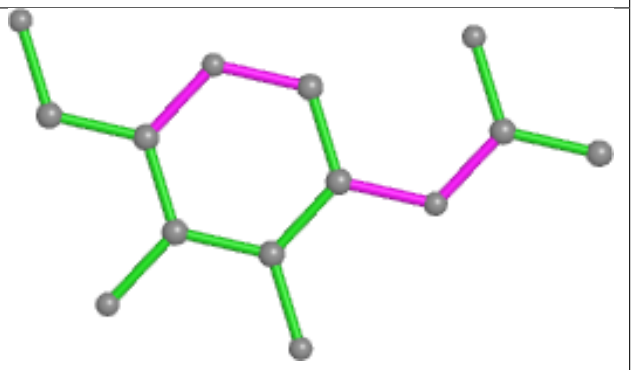

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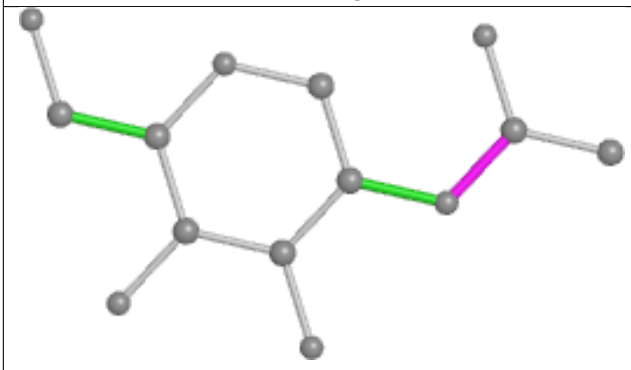

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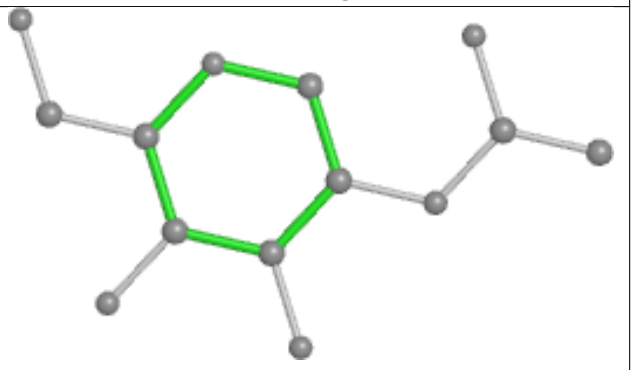
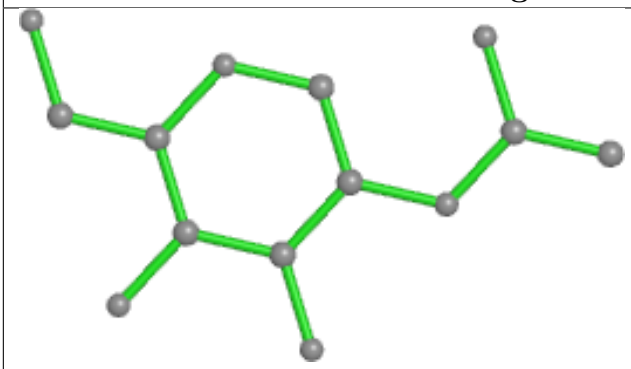


Rings

Ligand NAG A 1313



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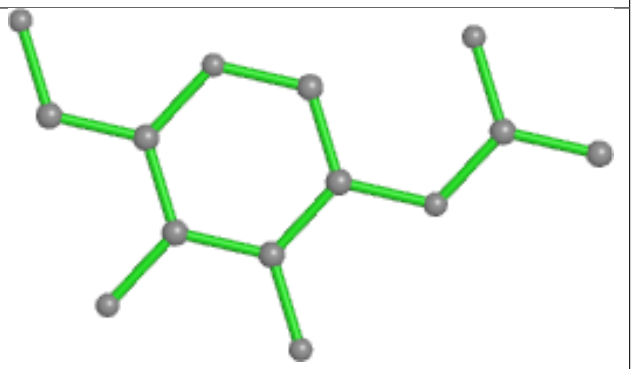

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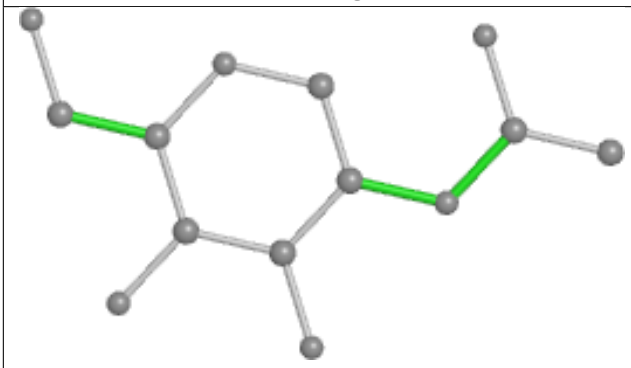

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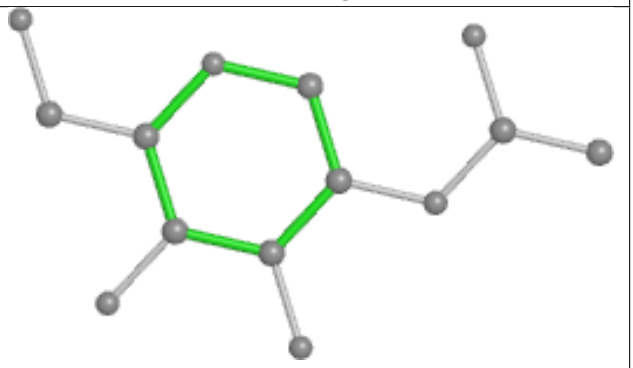
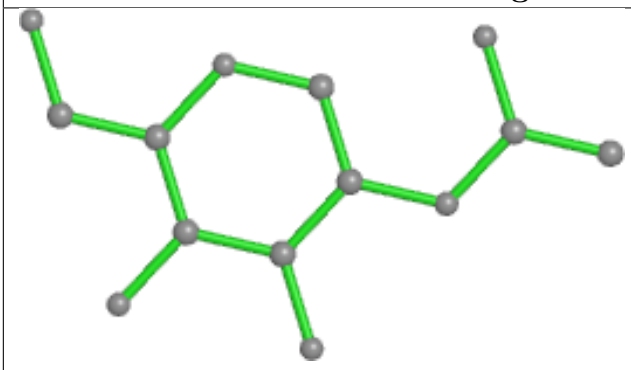


Rings

Ligand NAG C 1309



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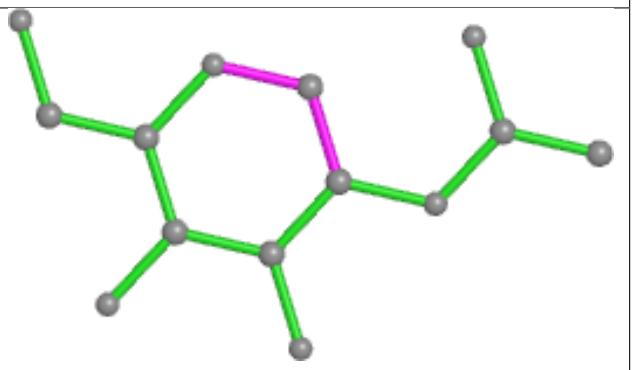

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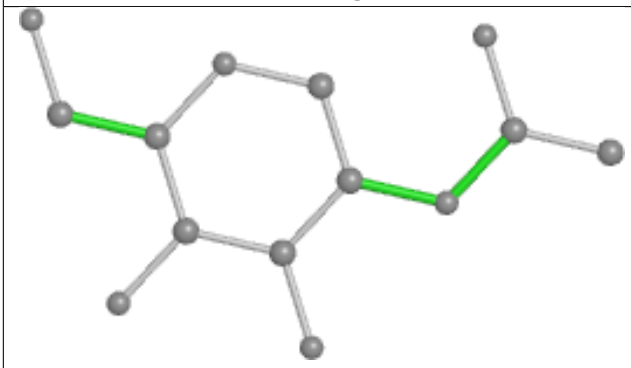

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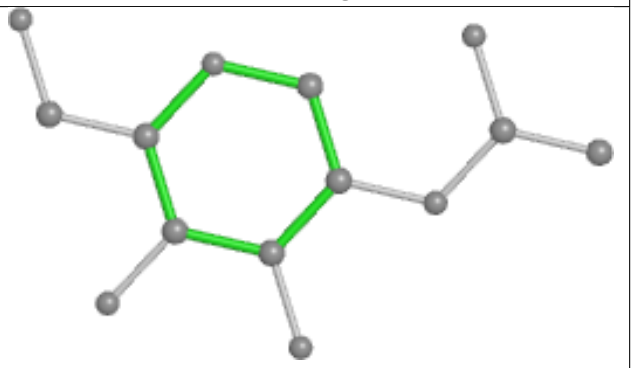

Rings

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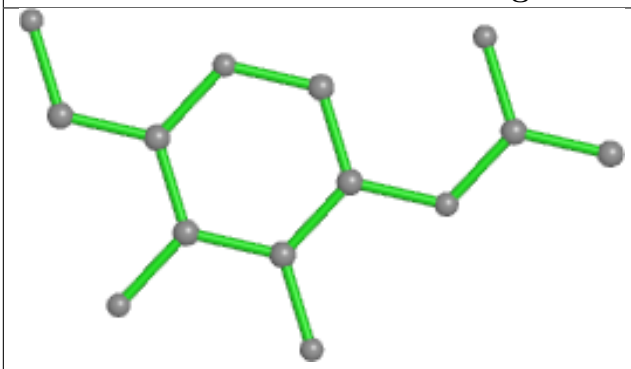

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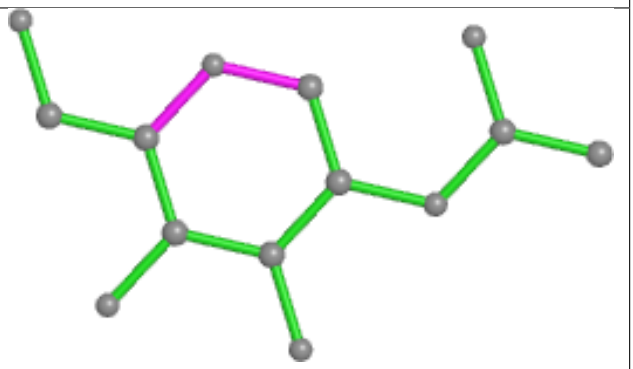

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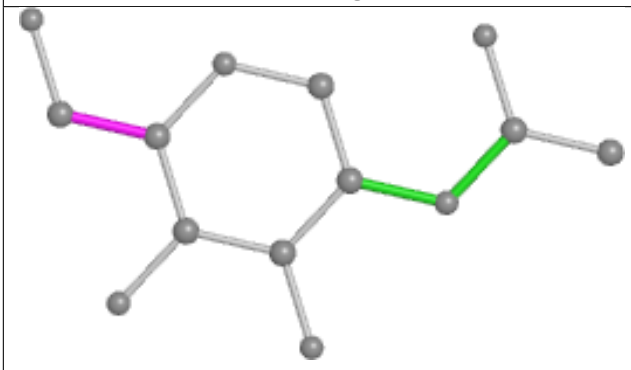

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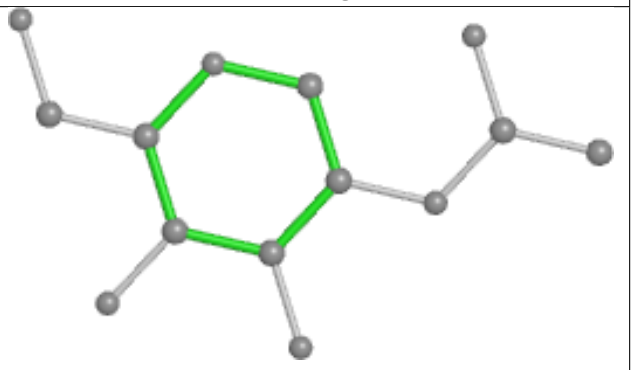

Rings

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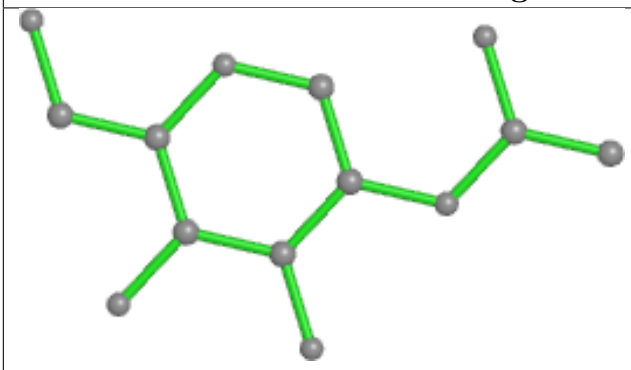

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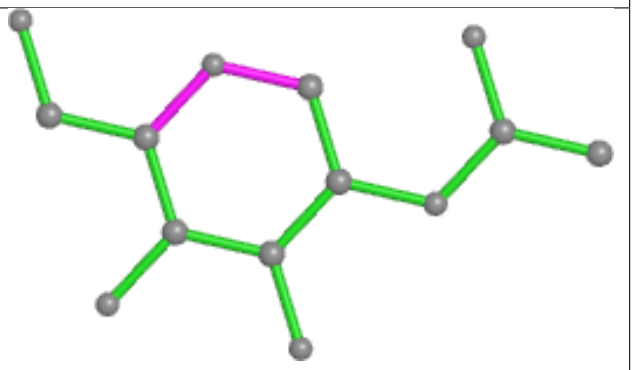

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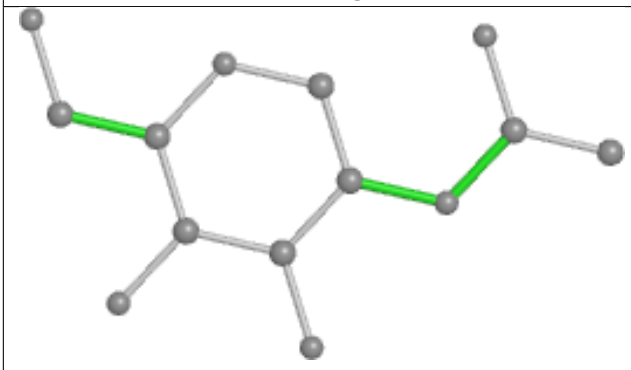

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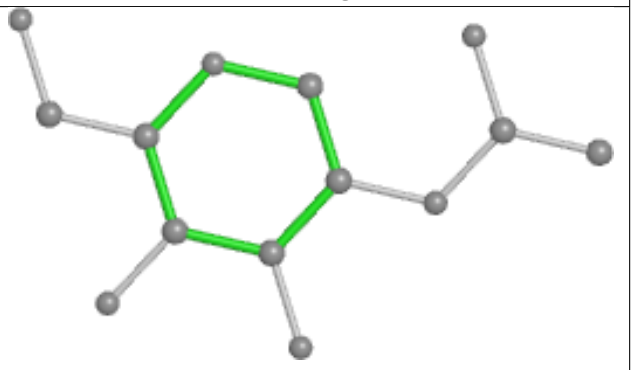

Rings

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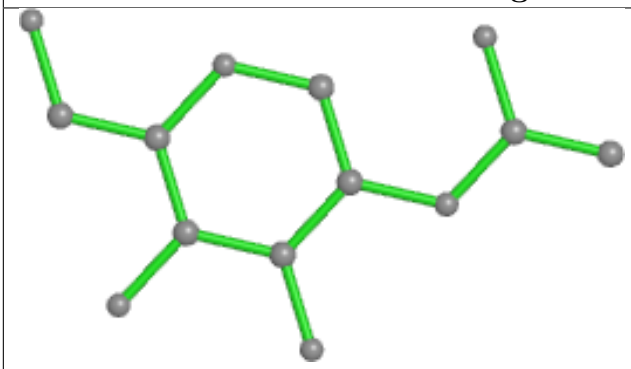

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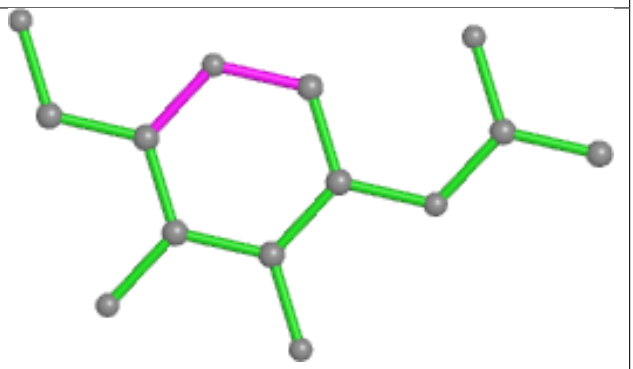

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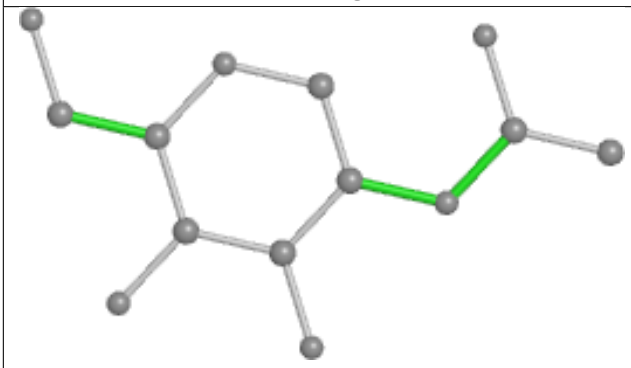

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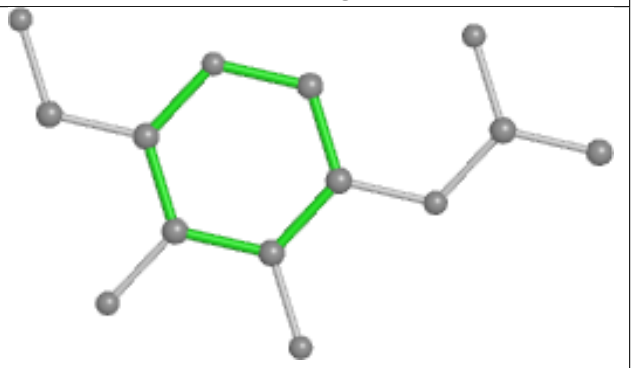

Rings

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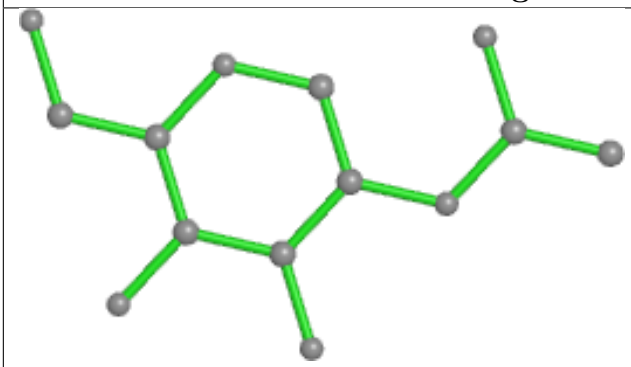

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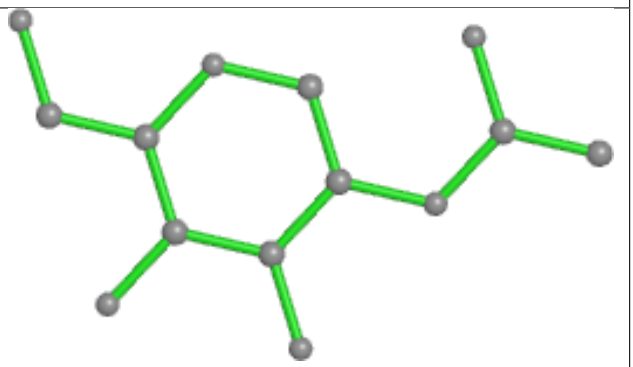

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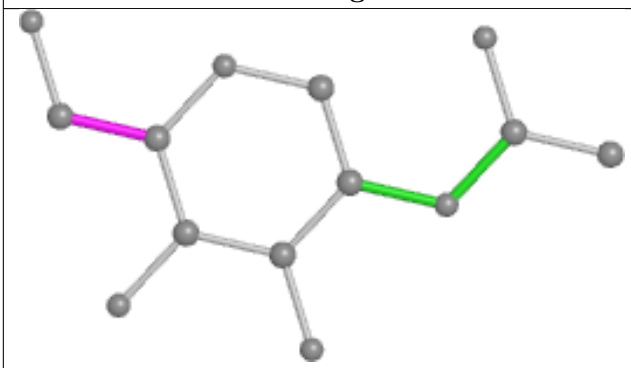

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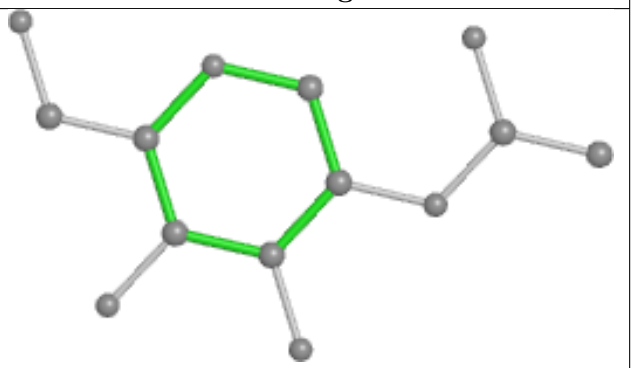
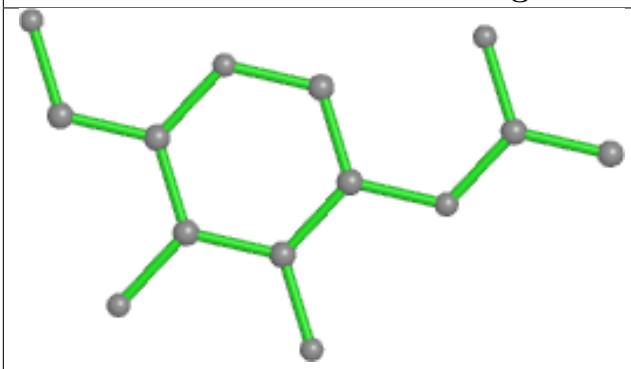


Rings

Ligand NAG C 1304



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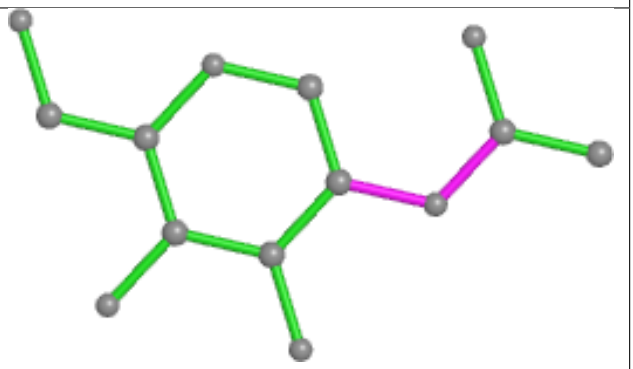

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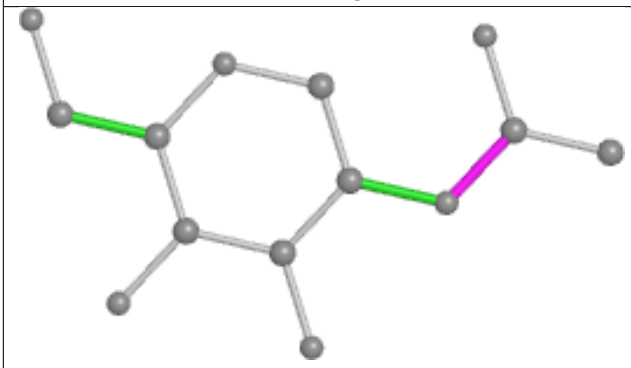

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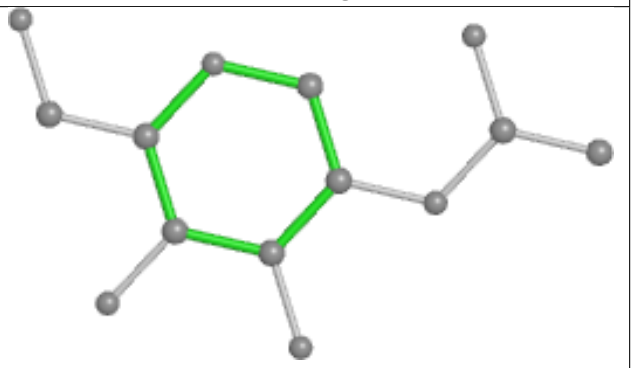

Rings

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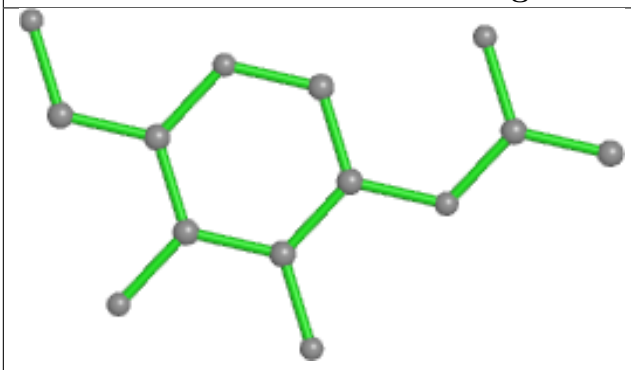

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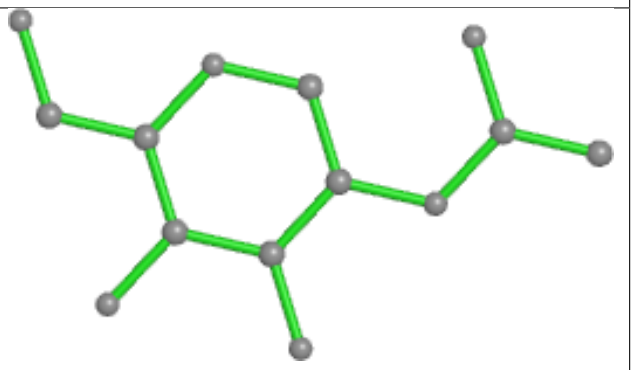

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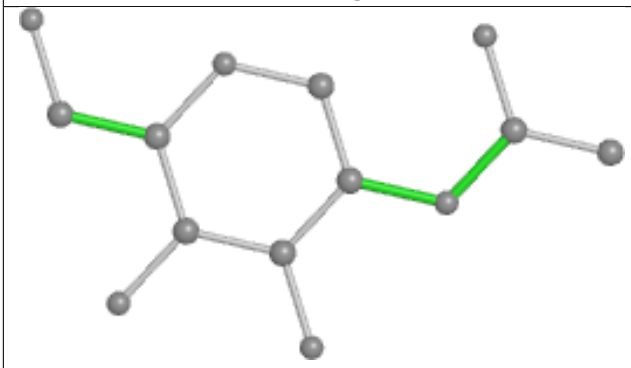

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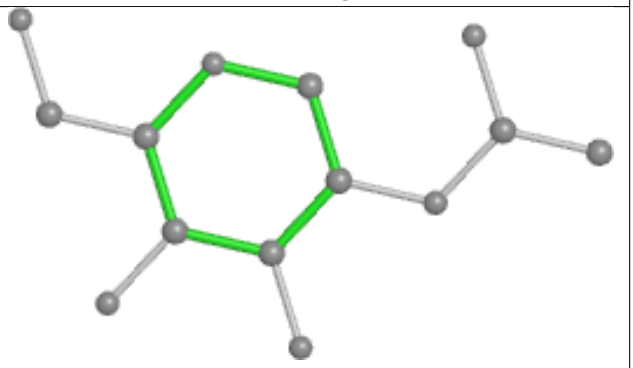
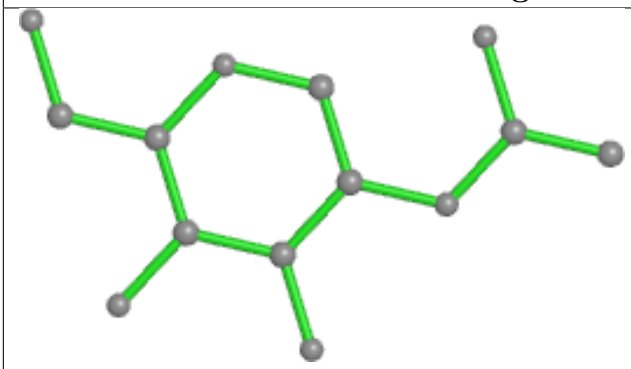


Rings

Ligand NAG B 1309



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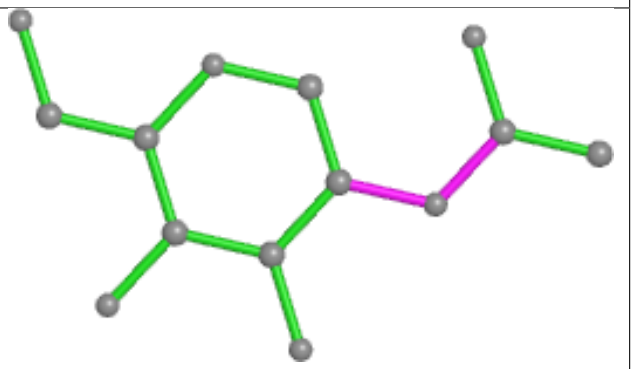
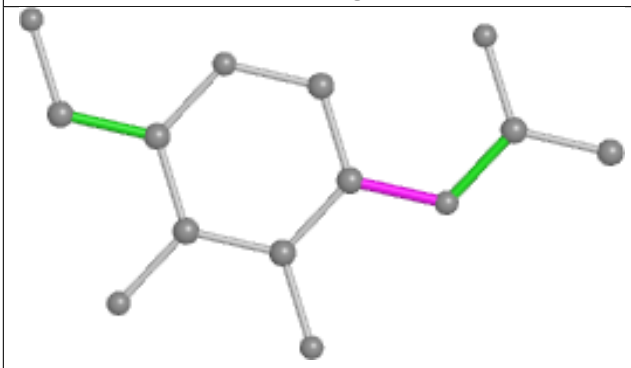


Bond angles



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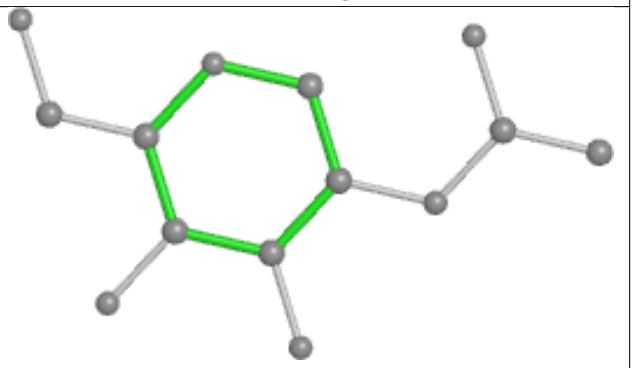

Rings

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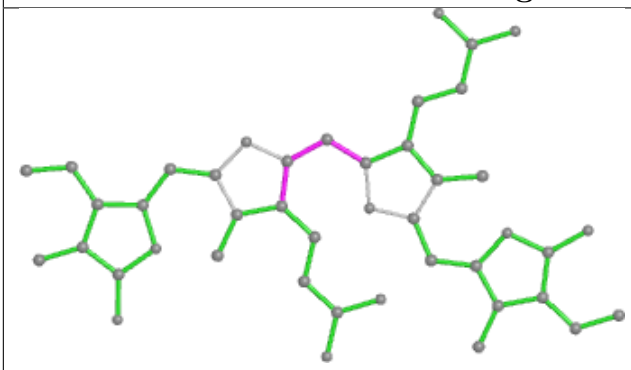

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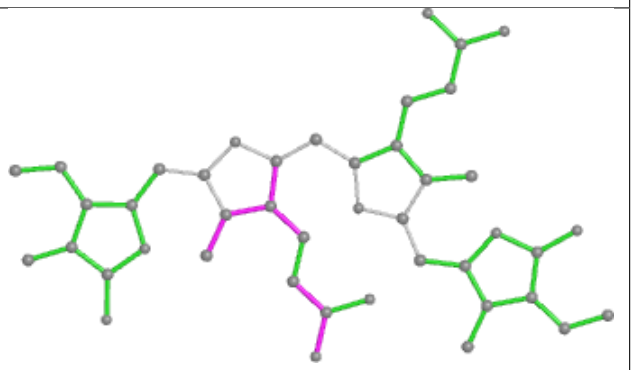
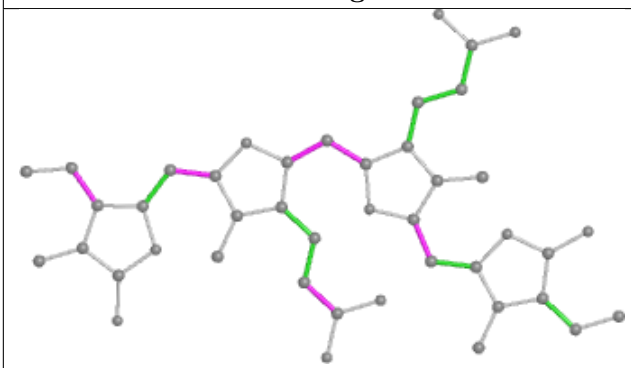


Bond angles



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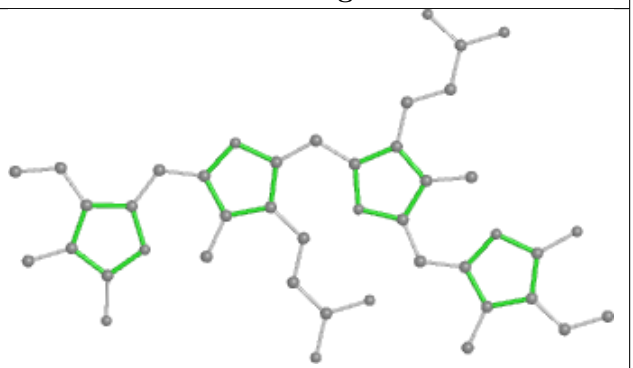
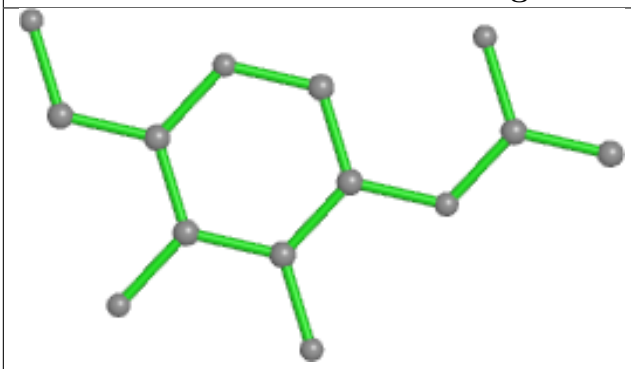


Rings

Ligand NAG A 1304



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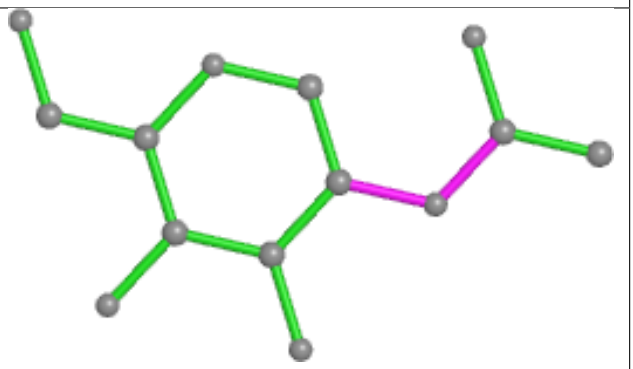
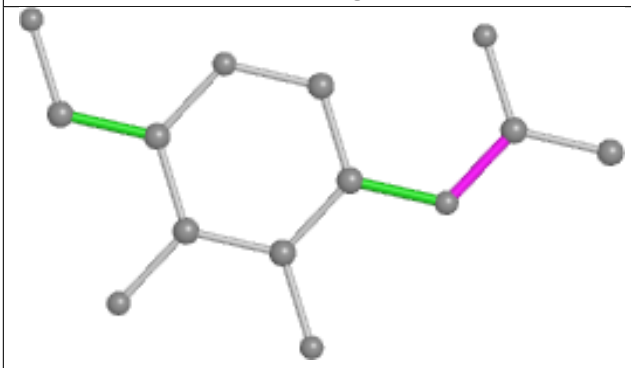


Bond angles



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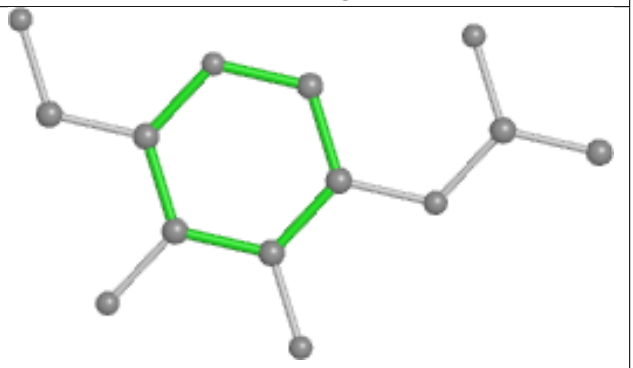

Rings

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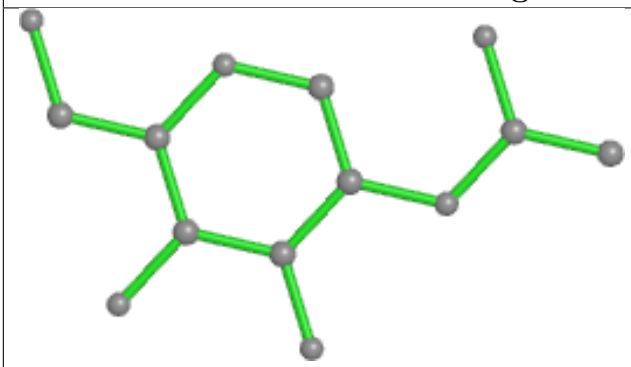
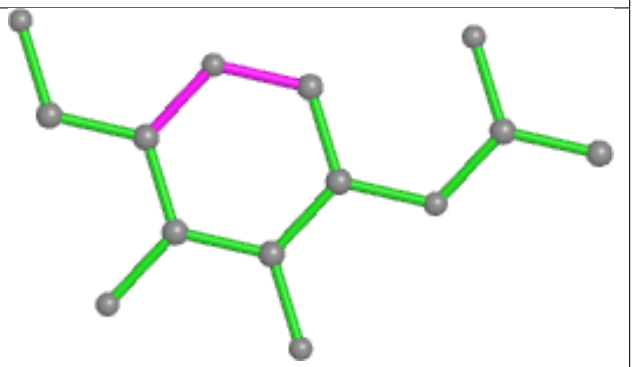
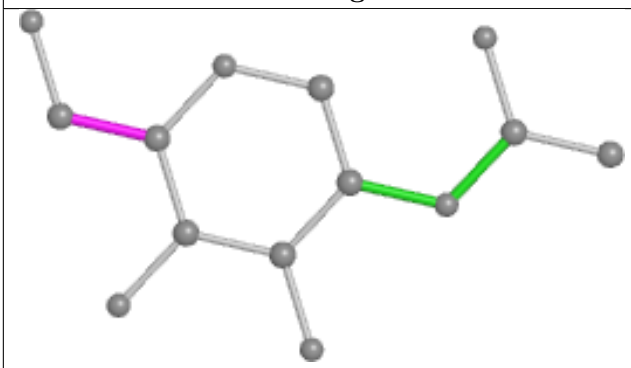


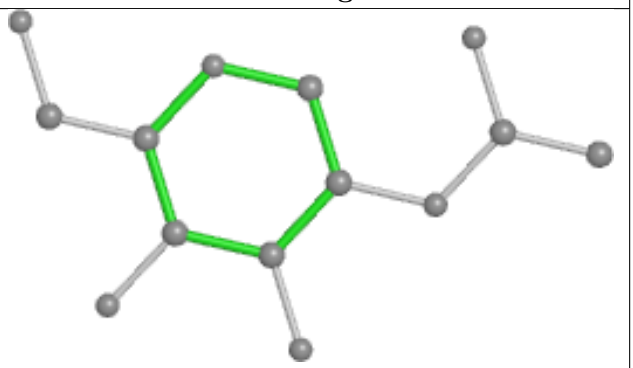
Bond lengths



Bond angles

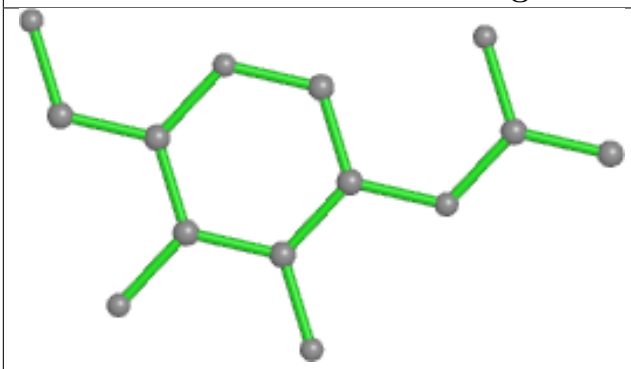


Torsions



Rings

Ligand NAG C 1301



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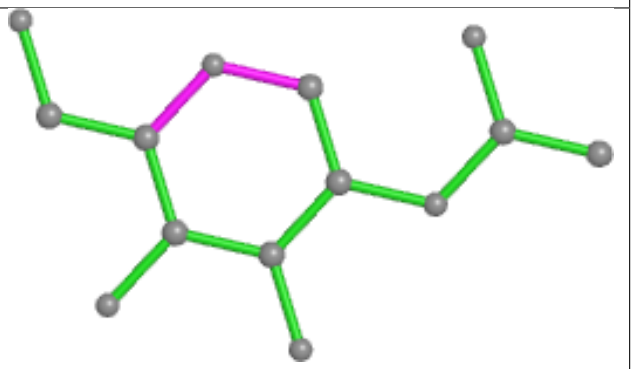
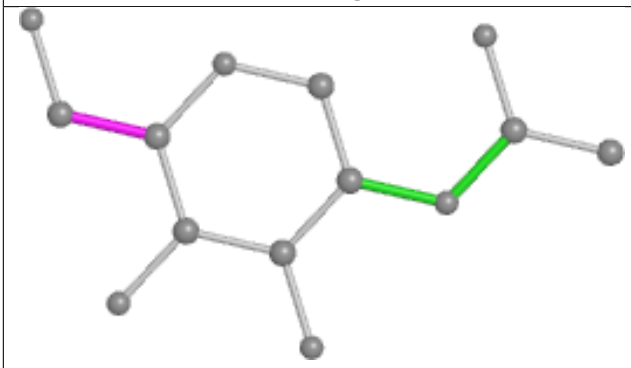


Bond angles



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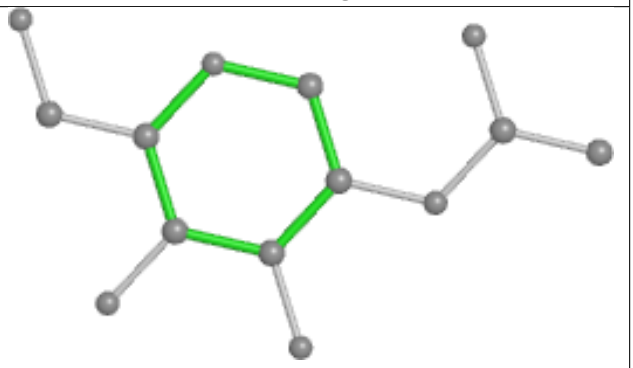
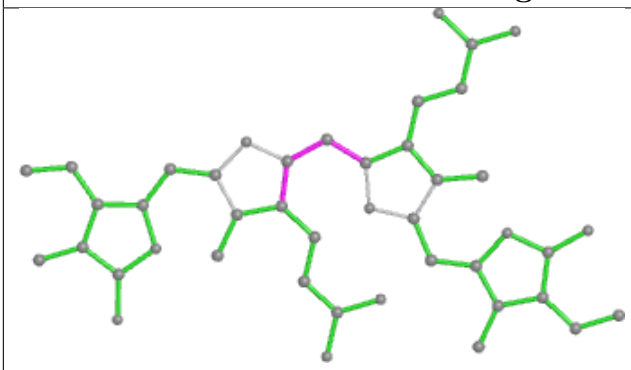


Rings

Ligand BLR A 1314



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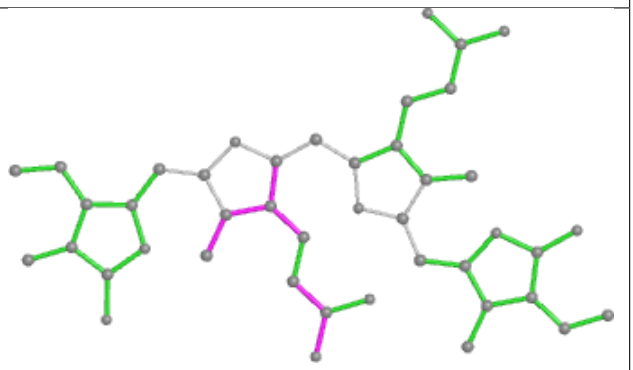
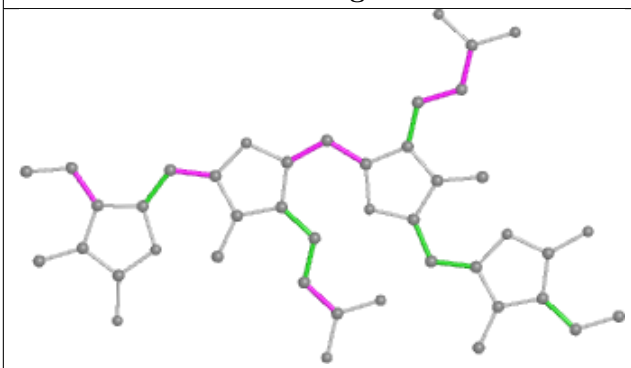
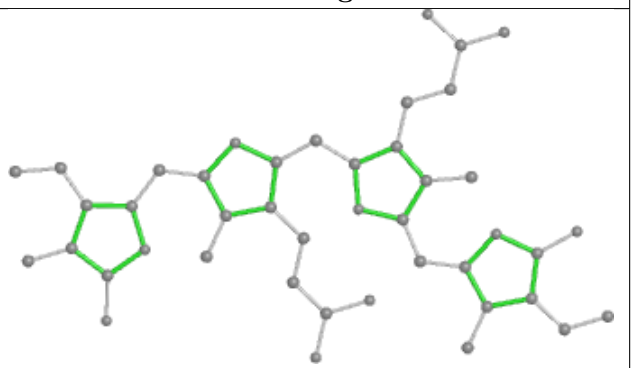


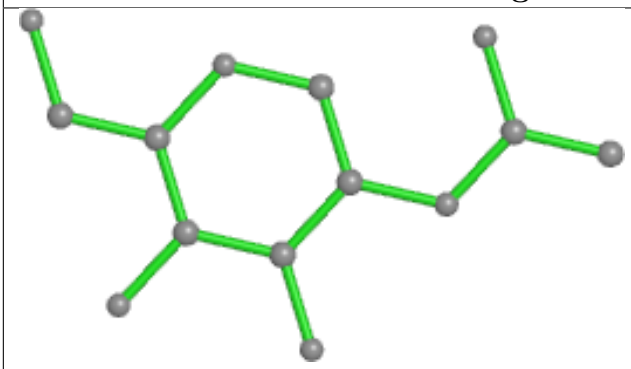
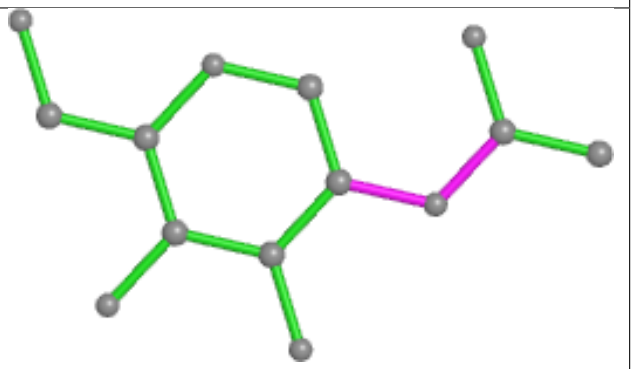
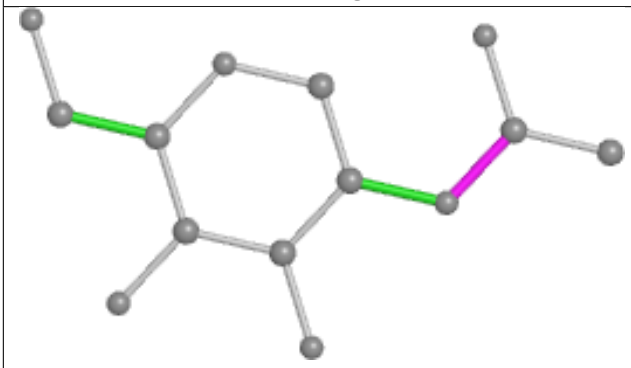
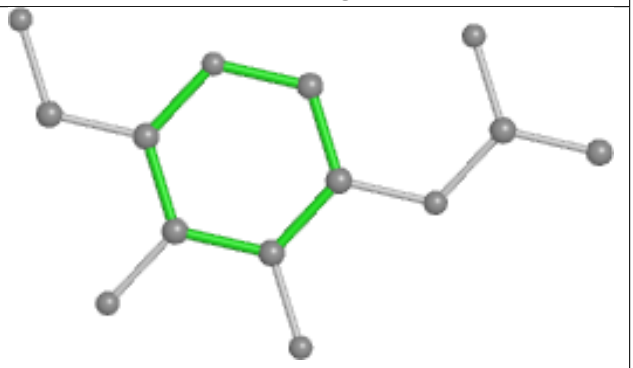
Bond angles



Torsions



Rings

Ligand NAG B 1307	
 Bond lengths	 Bond angles
 Torsions	 Rings

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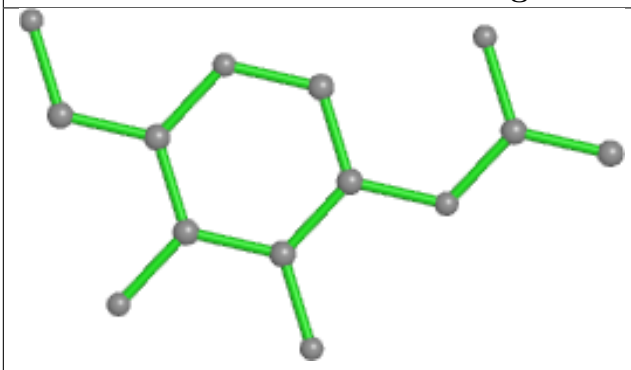
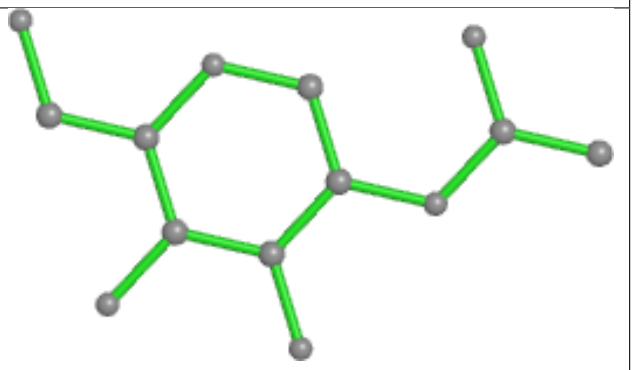
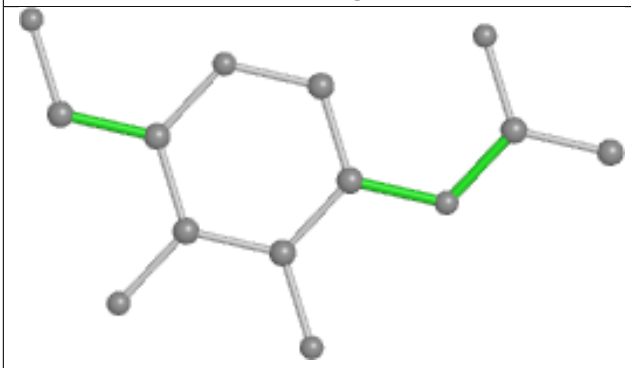
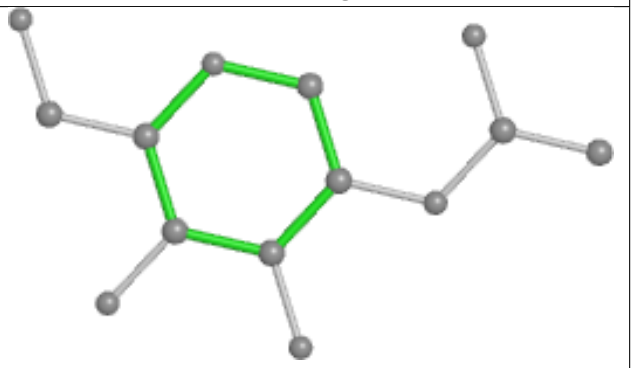
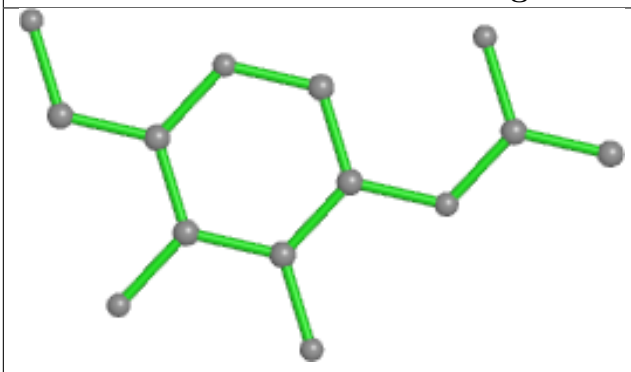
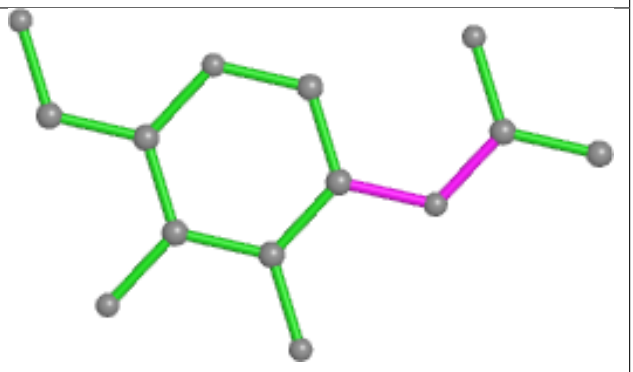
 Bond lengths	 Bond angles
 Torsions	 Rings

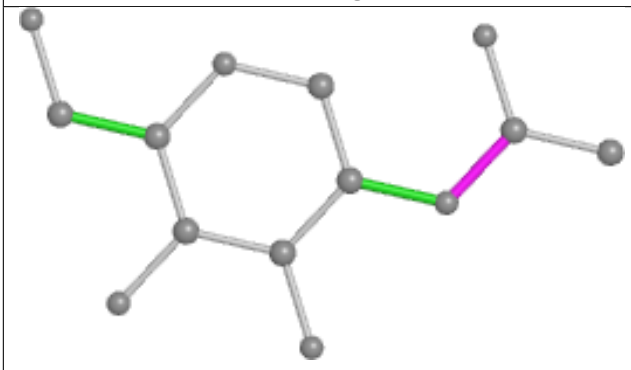
Ligand NAG A 1305



Bond lengths



Bond angles



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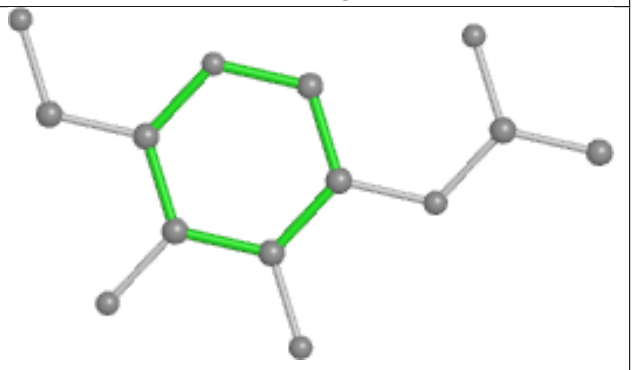

Rings

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.