Full wwPDB EM Validation Report ⓘ

Jun 9, 2025 – 09:36 PM JST

PDB ID	:	8ZY6 / pdb_00008zy6
EMDB ID	:	EMD-60557
Title	:	Sarbecovirus GX2013 Spike Trimer in a Locked Conformation
Authors	:	Wang, J.; Xiong, X.
Deposited on	:	2024-06-16
Resolution	:	3.30 Å(reported)

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

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

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

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

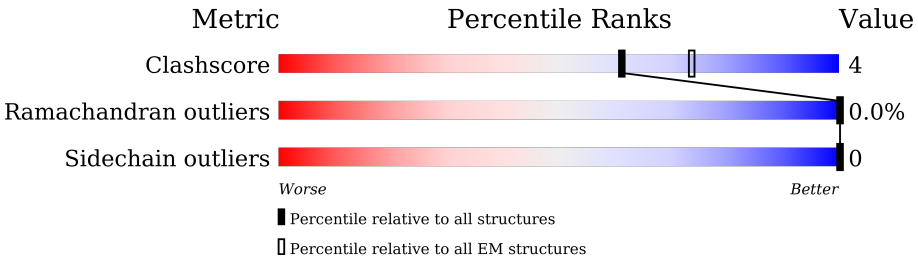
EMDB validation analysis	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.30 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	1256	73% 10% 17%
1	B	1256	74% 9% 17%
1	C	1256	74% 9% 17%
2	D	2	100%
2	E	2	100%
2	F	2	50% 50%
2	G	2	100%
2	H	2	100%
2	I	2	100%

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

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 25275 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	C	1041	Total	C	N	O	S	0	0
			8131	5168	1357	1563	43		
1	A	1041	Total	C	N	O	S	0	0
			8131	5168	1357	1563	43		
1	B	1041	Total	C	N	O	S	0	0
			8131	5168	1357	1563	43		

There are 237 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1178	GLY	-	expression tag	UNP A0A0U1WHJ8
C	1179	SER	-	expression tag	UNP A0A0U1WHJ8
C	1180	GLY	-	expression tag	UNP A0A0U1WHJ8
C	1181	TYR	-	expression tag	UNP A0A0U1WHJ8
C	1182	ILE	-	expression tag	UNP A0A0U1WHJ8
C	1183	PRO	-	expression tag	UNP A0A0U1WHJ8
C	1184	GLU	-	expression tag	UNP A0A0U1WHJ8
C	1185	ALA	-	expression tag	UNP A0A0U1WHJ8
C	1186	PRO	-	expression tag	UNP A0A0U1WHJ8
C	1187	ARG	-	expression tag	UNP A0A0U1WHJ8
C	1188	ASP	-	expression tag	UNP A0A0U1WHJ8
C	1189	GLY	-	expression tag	UNP A0A0U1WHJ8
C	1190	GLN	-	expression tag	UNP A0A0U1WHJ8
C	1191	ALA	-	expression tag	UNP A0A0U1WHJ8
C	1192	TYR	-	expression tag	UNP A0A0U1WHJ8
C	1193	VAL	-	expression tag	UNP A0A0U1WHJ8
C	1194	ARG	-	expression tag	UNP A0A0U1WHJ8
C	1195	LYS	-	expression tag	UNP A0A0U1WHJ8
C	1196	ASP	-	expression tag	UNP A0A0U1WHJ8
C	1197	GLY	-	expression tag	UNP A0A0U1WHJ8
C	1198	GLU	-	expression tag	UNP A0A0U1WHJ8
C	1199	TRP	-	expression tag	UNP A0A0U1WHJ8
C	1200	VAL	-	expression tag	UNP A0A0U1WHJ8
C	1201	LEU	-	expression tag	UNP A0A0U1WHJ8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1202	LEU	-	expression tag	UNP A0A0U1WHJ8
C	1203	SER	-	expression tag	UNP A0A0U1WHJ8
C	1204	THR	-	expression tag	UNP A0A0U1WHJ8
C	1205	PHE	-	expression tag	UNP A0A0U1WHJ8
C	1206	LEU	-	expression tag	UNP A0A0U1WHJ8
C	1207	LEU	-	expression tag	UNP A0A0U1WHJ8
C	1208	GLU	-	expression tag	UNP A0A0U1WHJ8
C	1209	VAL	-	expression tag	UNP A0A0U1WHJ8
C	1210	LEU	-	expression tag	UNP A0A0U1WHJ8
C	1211	PHE	-	expression tag	UNP A0A0U1WHJ8
C	1212	GLN	-	expression tag	UNP A0A0U1WHJ8
C	1213	GLY	-	expression tag	UNP A0A0U1WHJ8
C	1214	PRO	-	expression tag	UNP A0A0U1WHJ8
C	1215	GLY	-	expression tag	UNP A0A0U1WHJ8
C	1216	HIS	-	expression tag	UNP A0A0U1WHJ8
C	1217	HIS	-	expression tag	UNP A0A0U1WHJ8
C	1218	HIS	-	expression tag	UNP A0A0U1WHJ8
C	1219	HIS	-	expression tag	UNP A0A0U1WHJ8
C	1220	HIS	-	expression tag	UNP A0A0U1WHJ8
C	1221	HIS	-	expression tag	UNP A0A0U1WHJ8
C	1222	HIS	-	expression tag	UNP A0A0U1WHJ8
C	1223	HIS	-	expression tag	UNP A0A0U1WHJ8
C	1224	SER	-	expression tag	UNP A0A0U1WHJ8
C	1225	ALA	-	expression tag	UNP A0A0U1WHJ8
C	1226	TRP	-	expression tag	UNP A0A0U1WHJ8
C	1227	SER	-	expression tag	UNP A0A0U1WHJ8
C	1228	HIS	-	expression tag	UNP A0A0U1WHJ8
C	1229	PRO	-	expression tag	UNP A0A0U1WHJ8
C	1230	GLN	-	expression tag	UNP A0A0U1WHJ8
C	1231	PHE	-	expression tag	UNP A0A0U1WHJ8
C	1232	GLU	-	expression tag	UNP A0A0U1WHJ8
C	1233	LYS	-	expression tag	UNP A0A0U1WHJ8
C	1234	GLY	-	expression tag	UNP A0A0U1WHJ8
C	1235	GLY	-	expression tag	UNP A0A0U1WHJ8
C	1236	GLY	-	expression tag	UNP A0A0U1WHJ8
C	1237	SER	-	expression tag	UNP A0A0U1WHJ8
C	1238	GLY	-	expression tag	UNP A0A0U1WHJ8
C	1239	GLY	-	expression tag	UNP A0A0U1WHJ8
C	1240	GLY	-	expression tag	UNP A0A0U1WHJ8
C	1241	GLY	-	expression tag	UNP A0A0U1WHJ8
C	1242	SER	-	expression tag	UNP A0A0U1WHJ8
C	1243	GLY	-	expression tag	UNP A0A0U1WHJ8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1244	GLY	-	expression tag	UNP A0A0U1WHJ8
C	1245	SER	-	expression tag	UNP A0A0U1WHJ8
C	1246	ALA	-	expression tag	UNP A0A0U1WHJ8
C	1247	TRP	-	expression tag	UNP A0A0U1WHJ8
C	1248	SER	-	expression tag	UNP A0A0U1WHJ8
C	1249	HIS	-	expression tag	UNP A0A0U1WHJ8
C	1250	PRO	-	expression tag	UNP A0A0U1WHJ8
C	1251	GLN	-	expression tag	UNP A0A0U1WHJ8
C	1252	PHE	-	expression tag	UNP A0A0U1WHJ8
C	1253	GLU	-	expression tag	UNP A0A0U1WHJ8
C	1254	LYS	-	expression tag	UNP A0A0U1WHJ8
C	1255	SER	-	expression tag	UNP A0A0U1WHJ8
C	1256	ALA	-	expression tag	UNP A0A0U1WHJ8
A	1178	GLY	-	expression tag	UNP A0A0U1WHJ8
A	1179	SER	-	expression tag	UNP A0A0U1WHJ8
A	1180	GLY	-	expression tag	UNP A0A0U1WHJ8
A	1181	TYR	-	expression tag	UNP A0A0U1WHJ8
A	1182	ILE	-	expression tag	UNP A0A0U1WHJ8
A	1183	PRO	-	expression tag	UNP A0A0U1WHJ8
A	1184	GLU	-	expression tag	UNP A0A0U1WHJ8
A	1185	ALA	-	expression tag	UNP A0A0U1WHJ8
A	1186	PRO	-	expression tag	UNP A0A0U1WHJ8
A	1187	ARG	-	expression tag	UNP A0A0U1WHJ8
A	1188	ASP	-	expression tag	UNP A0A0U1WHJ8
A	1189	GLY	-	expression tag	UNP A0A0U1WHJ8
A	1190	GLN	-	expression tag	UNP A0A0U1WHJ8
A	1191	ALA	-	expression tag	UNP A0A0U1WHJ8
A	1192	TYR	-	expression tag	UNP A0A0U1WHJ8
A	1193	VAL	-	expression tag	UNP A0A0U1WHJ8
A	1194	ARG	-	expression tag	UNP A0A0U1WHJ8
A	1195	LYS	-	expression tag	UNP A0A0U1WHJ8
A	1196	ASP	-	expression tag	UNP A0A0U1WHJ8
A	1197	GLY	-	expression tag	UNP A0A0U1WHJ8
A	1198	GLU	-	expression tag	UNP A0A0U1WHJ8
A	1199	TRP	-	expression tag	UNP A0A0U1WHJ8
A	1200	VAL	-	expression tag	UNP A0A0U1WHJ8
A	1201	LEU	-	expression tag	UNP A0A0U1WHJ8
A	1202	LEU	-	expression tag	UNP A0A0U1WHJ8
A	1203	SER	-	expression tag	UNP A0A0U1WHJ8
A	1204	THR	-	expression tag	UNP A0A0U1WHJ8
A	1205	PHE	-	expression tag	UNP A0A0U1WHJ8
A	1206	LEU	-	expression tag	UNP A0A0U1WHJ8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1207	LEU	-	expression tag	UNP A0A0U1WHJ8
A	1208	GLU	-	expression tag	UNP A0A0U1WHJ8
A	1209	VAL	-	expression tag	UNP A0A0U1WHJ8
A	1210	LEU	-	expression tag	UNP A0A0U1WHJ8
A	1211	PHE	-	expression tag	UNP A0A0U1WHJ8
A	1212	GLN	-	expression tag	UNP A0A0U1WHJ8
A	1213	GLY	-	expression tag	UNP A0A0U1WHJ8
A	1214	PRO	-	expression tag	UNP A0A0U1WHJ8
A	1215	GLY	-	expression tag	UNP A0A0U1WHJ8
A	1216	HIS	-	expression tag	UNP A0A0U1WHJ8
A	1217	HIS	-	expression tag	UNP A0A0U1WHJ8
A	1218	HIS	-	expression tag	UNP A0A0U1WHJ8
A	1219	HIS	-	expression tag	UNP A0A0U1WHJ8
A	1220	HIS	-	expression tag	UNP A0A0U1WHJ8
A	1221	HIS	-	expression tag	UNP A0A0U1WHJ8
A	1222	HIS	-	expression tag	UNP A0A0U1WHJ8
A	1223	HIS	-	expression tag	UNP A0A0U1WHJ8
A	1224	SER	-	expression tag	UNP A0A0U1WHJ8
A	1225	ALA	-	expression tag	UNP A0A0U1WHJ8
A	1226	TRP	-	expression tag	UNP A0A0U1WHJ8
A	1227	SER	-	expression tag	UNP A0A0U1WHJ8
A	1228	HIS	-	expression tag	UNP A0A0U1WHJ8
A	1229	PRO	-	expression tag	UNP A0A0U1WHJ8
A	1230	GLN	-	expression tag	UNP A0A0U1WHJ8
A	1231	PHE	-	expression tag	UNP A0A0U1WHJ8
A	1232	GLU	-	expression tag	UNP A0A0U1WHJ8
A	1233	LYS	-	expression tag	UNP A0A0U1WHJ8
A	1234	GLY	-	expression tag	UNP A0A0U1WHJ8
A	1235	GLY	-	expression tag	UNP A0A0U1WHJ8
A	1236	GLY	-	expression tag	UNP A0A0U1WHJ8
A	1237	SER	-	expression tag	UNP A0A0U1WHJ8
A	1238	GLY	-	expression tag	UNP A0A0U1WHJ8
A	1239	GLY	-	expression tag	UNP A0A0U1WHJ8
A	1240	GLY	-	expression tag	UNP A0A0U1WHJ8
A	1241	GLY	-	expression tag	UNP A0A0U1WHJ8
A	1242	SER	-	expression tag	UNP A0A0U1WHJ8
A	1243	GLY	-	expression tag	UNP A0A0U1WHJ8
A	1244	GLY	-	expression tag	UNP A0A0U1WHJ8
A	1245	SER	-	expression tag	UNP A0A0U1WHJ8
A	1246	ALA	-	expression tag	UNP A0A0U1WHJ8
A	1247	TRP	-	expression tag	UNP A0A0U1WHJ8
A	1248	SER	-	expression tag	UNP A0A0U1WHJ8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1249	HIS	-	expression tag	UNP A0A0U1WHJ8
A	1250	PRO	-	expression tag	UNP A0A0U1WHJ8
A	1251	GLN	-	expression tag	UNP A0A0U1WHJ8
A	1252	PHE	-	expression tag	UNP A0A0U1WHJ8
A	1253	GLU	-	expression tag	UNP A0A0U1WHJ8
A	1254	LYS	-	expression tag	UNP A0A0U1WHJ8
A	1255	SER	-	expression tag	UNP A0A0U1WHJ8
A	1256	ALA	-	expression tag	UNP A0A0U1WHJ8
B	1178	GLY	-	expression tag	UNP A0A0U1WHJ8
B	1179	SER	-	expression tag	UNP A0A0U1WHJ8
B	1180	GLY	-	expression tag	UNP A0A0U1WHJ8
B	1181	TYR	-	expression tag	UNP A0A0U1WHJ8
B	1182	ILE	-	expression tag	UNP A0A0U1WHJ8
B	1183	PRO	-	expression tag	UNP A0A0U1WHJ8
B	1184	GLU	-	expression tag	UNP A0A0U1WHJ8
B	1185	ALA	-	expression tag	UNP A0A0U1WHJ8
B	1186	PRO	-	expression tag	UNP A0A0U1WHJ8
B	1187	ARG	-	expression tag	UNP A0A0U1WHJ8
B	1188	ASP	-	expression tag	UNP A0A0U1WHJ8
B	1189	GLY	-	expression tag	UNP A0A0U1WHJ8
B	1190	GLN	-	expression tag	UNP A0A0U1WHJ8
B	1191	ALA	-	expression tag	UNP A0A0U1WHJ8
B	1192	TYR	-	expression tag	UNP A0A0U1WHJ8
B	1193	VAL	-	expression tag	UNP A0A0U1WHJ8
B	1194	ARG	-	expression tag	UNP A0A0U1WHJ8
B	1195	LYS	-	expression tag	UNP A0A0U1WHJ8
B	1196	ASP	-	expression tag	UNP A0A0U1WHJ8
B	1197	GLY	-	expression tag	UNP A0A0U1WHJ8
B	1198	GLU	-	expression tag	UNP A0A0U1WHJ8
B	1199	TRP	-	expression tag	UNP A0A0U1WHJ8
B	1200	VAL	-	expression tag	UNP A0A0U1WHJ8
B	1201	LEU	-	expression tag	UNP A0A0U1WHJ8
B	1202	LEU	-	expression tag	UNP A0A0U1WHJ8
B	1203	SER	-	expression tag	UNP A0A0U1WHJ8
B	1204	THR	-	expression tag	UNP A0A0U1WHJ8
B	1205	PHE	-	expression tag	UNP A0A0U1WHJ8
B	1206	LEU	-	expression tag	UNP A0A0U1WHJ8
B	1207	LEU	-	expression tag	UNP A0A0U1WHJ8
B	1208	GLU	-	expression tag	UNP A0A0U1WHJ8
B	1209	VAL	-	expression tag	UNP A0A0U1WHJ8
B	1210	LEU	-	expression tag	UNP A0A0U1WHJ8
B	1211	PHE	-	expression tag	UNP A0A0U1WHJ8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1212	GLN	-	expression tag	UNP A0A0U1WHJ8
B	1213	GLY	-	expression tag	UNP A0A0U1WHJ8
B	1214	PRO	-	expression tag	UNP A0A0U1WHJ8
B	1215	GLY	-	expression tag	UNP A0A0U1WHJ8
B	1216	HIS	-	expression tag	UNP A0A0U1WHJ8
B	1217	HIS	-	expression tag	UNP A0A0U1WHJ8
B	1218	HIS	-	expression tag	UNP A0A0U1WHJ8
B	1219	HIS	-	expression tag	UNP A0A0U1WHJ8
B	1220	HIS	-	expression tag	UNP A0A0U1WHJ8
B	1221	HIS	-	expression tag	UNP A0A0U1WHJ8
B	1222	HIS	-	expression tag	UNP A0A0U1WHJ8
B	1223	HIS	-	expression tag	UNP A0A0U1WHJ8
B	1224	SER	-	expression tag	UNP A0A0U1WHJ8
B	1225	ALA	-	expression tag	UNP A0A0U1WHJ8
B	1226	TRP	-	expression tag	UNP A0A0U1WHJ8
B	1227	SER	-	expression tag	UNP A0A0U1WHJ8
B	1228	HIS	-	expression tag	UNP A0A0U1WHJ8
B	1229	PRO	-	expression tag	UNP A0A0U1WHJ8
B	1230	GLN	-	expression tag	UNP A0A0U1WHJ8
B	1231	PHE	-	expression tag	UNP A0A0U1WHJ8
B	1232	GLU	-	expression tag	UNP A0A0U1WHJ8
B	1233	LYS	-	expression tag	UNP A0A0U1WHJ8
B	1234	GLY	-	expression tag	UNP A0A0U1WHJ8
B	1235	GLY	-	expression tag	UNP A0A0U1WHJ8
B	1236	GLY	-	expression tag	UNP A0A0U1WHJ8
B	1237	SER	-	expression tag	UNP A0A0U1WHJ8
B	1238	GLY	-	expression tag	UNP A0A0U1WHJ8
B	1239	GLY	-	expression tag	UNP A0A0U1WHJ8
B	1240	GLY	-	expression tag	UNP A0A0U1WHJ8
B	1241	GLY	-	expression tag	UNP A0A0U1WHJ8
B	1242	SER	-	expression tag	UNP A0A0U1WHJ8
B	1243	GLY	-	expression tag	UNP A0A0U1WHJ8
B	1244	GLY	-	expression tag	UNP A0A0U1WHJ8
B	1245	SER	-	expression tag	UNP A0A0U1WHJ8
B	1246	ALA	-	expression tag	UNP A0A0U1WHJ8
B	1247	TRP	-	expression tag	UNP A0A0U1WHJ8
B	1248	SER	-	expression tag	UNP A0A0U1WHJ8
B	1249	HIS	-	expression tag	UNP A0A0U1WHJ8
B	1250	PRO	-	expression tag	UNP A0A0U1WHJ8
B	1251	GLN	-	expression tag	UNP A0A0U1WHJ8
B	1252	PHE	-	expression tag	UNP A0A0U1WHJ8
B	1253	GLU	-	expression tag	UNP A0A0U1WHJ8

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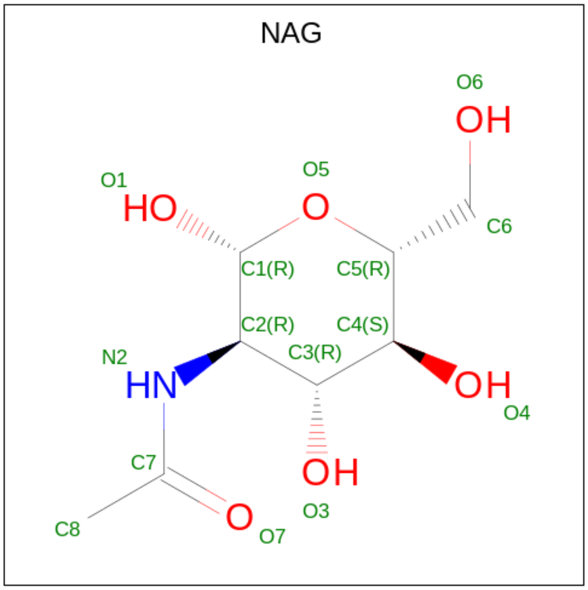
Chain	Residue	Modelled	Actual	Comment	Reference
B	1254	LYS	-	expression tag	UNP A0A0U1WHJ8
B	1255	SER	-	expression tag	UNP A0A0U1WHJ8
B	1256	ALA	-	expression tag	UNP A0A0U1WHJ8

- 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		

- 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	C	1	Total C N O 14 8 1 5	0
3	C	1	Total C N O 14 8 1 5	0
3	C	1	Total C N O 14 8 1 5	0
3	C	1	Total C N O 14 8 1 5	0
3	C	1	Total C N O 14 8 1 5	0
3	C	1	Total C N O 14 8 1 5	0
3	C	1	Total C N O 14 8 1 5	0
3	C	1	Total C N O 14 8 1 5	0
3	C	1	Total C N O 14 8 1 5	0
3	C	1	Total C N O 14 8 1 5	0
3	C	1	Total C N O 14 8 1 5	0
3	C	1	Total C N O 14 8 1 5	0
3	C	1	Total C N O 14 8 1 5	0
3	C	1	Total C N O 14 8 1 5	0

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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	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	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

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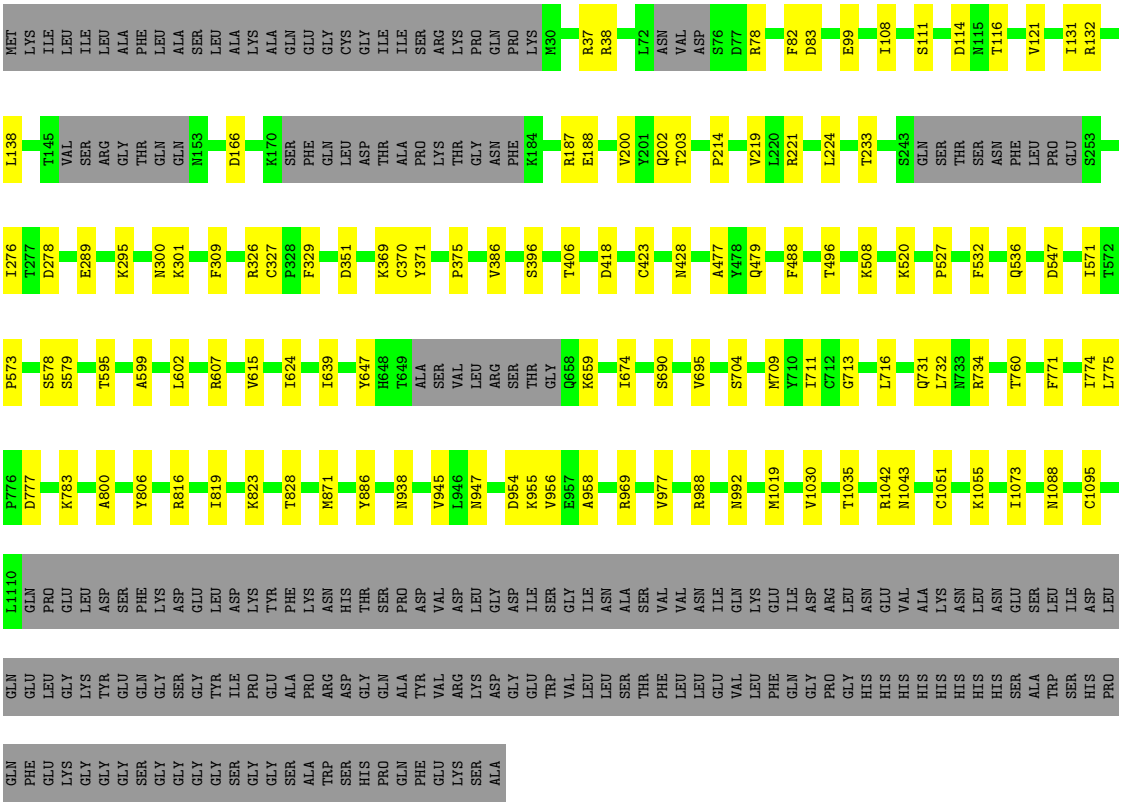
Mol	Chain	Residues	Atoms				AltConf
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	

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.

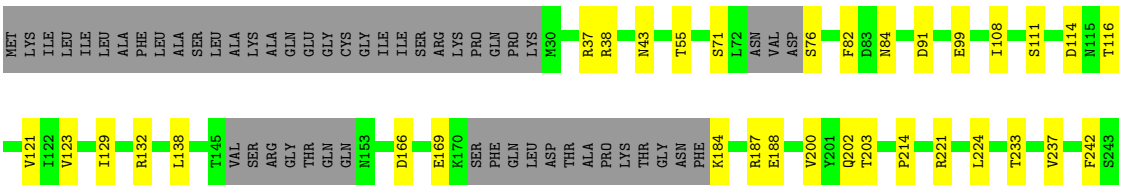
- Molecule 1: Spike glycoprotein

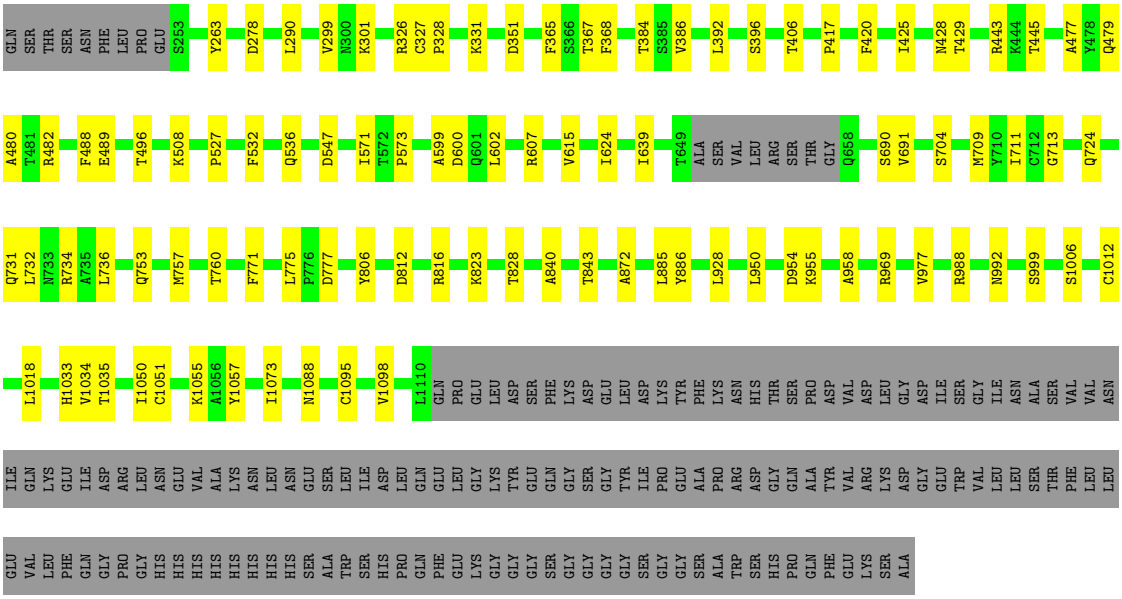
Chain C:



- Molecule 1: Spike glycoprotein

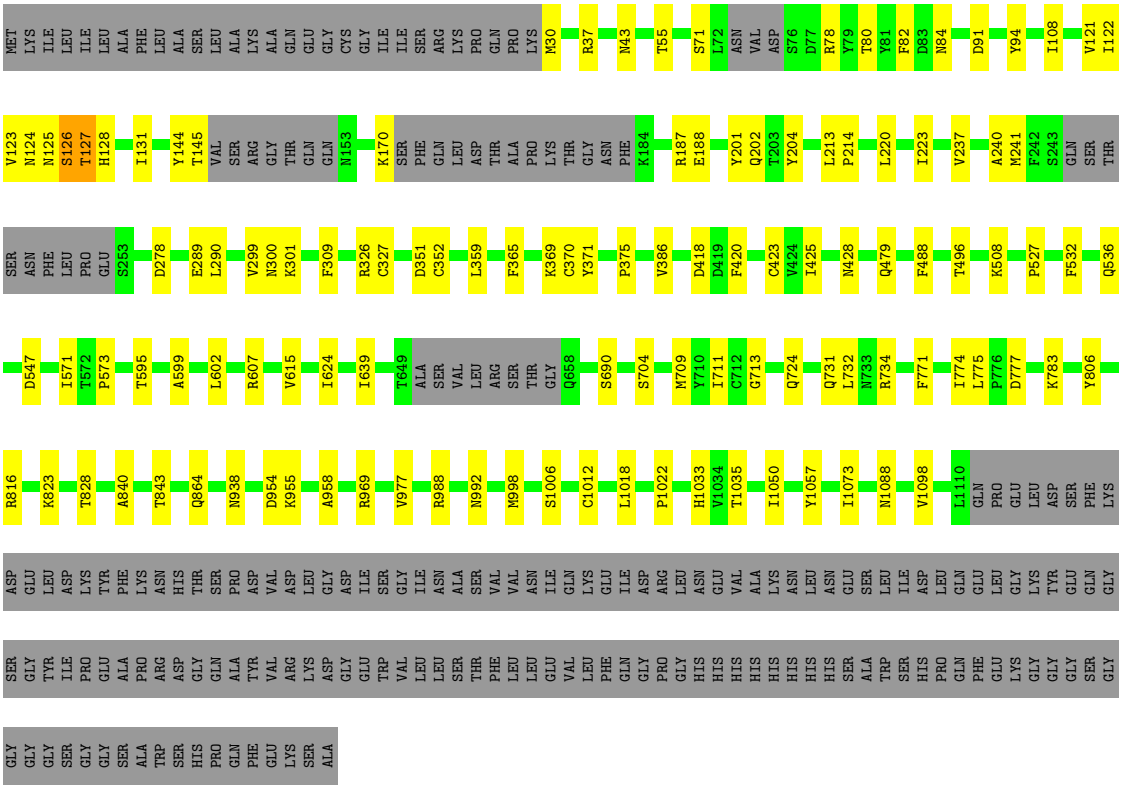
Chain A:





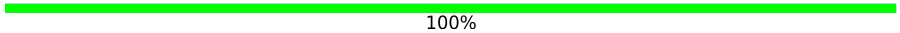
• Molecule 1: Spike glycoprotein

Chain B:

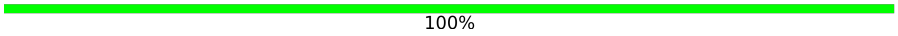


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:



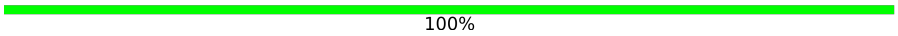
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E: 

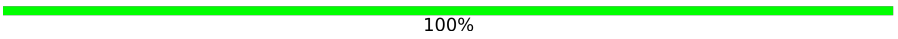
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F: 

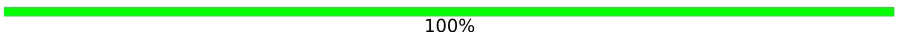
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

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

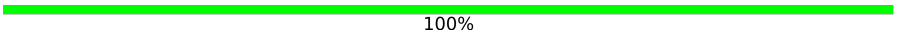
Chain I: 

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

Chain J: 

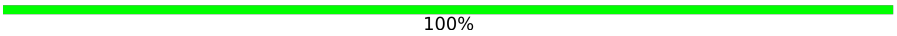
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:



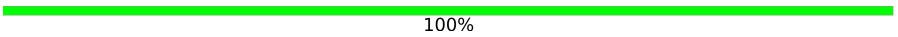
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:



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

Chain M:

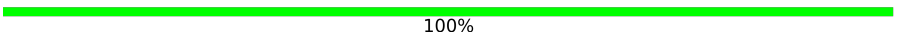


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:

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

Chain O:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	122098	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)	200	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.17	0/8305	0.42	0/11293
1	B	0.19	0/8305	0.48	6/11293 (0.1%)
1	C	0.16	0/8305	0.42	1/11293 (0.0%)
All	All	0.17	0/24915	0.44	7/33879 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	127	THR	N-CA-C	-9.22	99.94	112.94
1	C	595	THR	N-CA-C	-6.78	106.20	114.75
1	B	420	PHE	CA-C-N	-6.71	111.56	120.95
1	B	420	PHE	C-N-CA	-6.71	111.56	120.95
1	B	123	VAL	N-CA-CB	-5.61	106.17	112.45
1	B	595	THR	N-CA-C	-5.52	108.33	114.62
1	B	126	SER	CB-CA-C	-5.40	110.37	116.63

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	8131	0	7921	78	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	8131	0	7921	75	0
1	C	8131	0	7921	71	0
2	D	28	0	25	0	0
2	E	28	0	25	0	0
2	F	28	0	25	0	0
2	G	28	0	25	0	0
2	H	28	0	25	0	0
2	I	28	0	25	0	0
2	J	28	0	25	0	0
2	K	28	0	25	0	0
2	L	28	0	25	0	0
2	M	28	0	25	0	0
2	N	28	0	25	0	0
2	O	28	0	25	0	0
3	A	182	0	169	0	0
3	B	168	0	156	0	0
3	C	196	0	182	0	0
All	All	25275	0	24570	211	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 4.

All (211) 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:B:126:SER:CB	1:B:128:HIS:HD2	1.25	1.45
1:B:126:SER:HB3	1:B:128:HIS:CD2	1.52	1.40
1:B:126:SER:CB	1:B:128:HIS:CD2	2.08	1.33
1:B:126:SER:OG	1:B:128:HIS:CD2	2.18	0.95
1:B:126:SER:HB3	1:B:128:HIS:HD2	0.61	0.77
1:B:128:HIS:HA	1:B:170:LYS:C	2.16	0.71
1:B:126:SER:HG	1:B:128:HIS:CD2	2.08	0.71
1:A:1006:SER:H	1:A:1018:LEU:HD23	1.57	0.69
1:A:955:LYS:HA	1:A:958:ALA:HB3	1.74	0.69
1:C:200:VAL:HB	1:C:224:LEU:HB2	1.74	0.69
1:A:200:VAL:HB	1:A:224:LEU:HB2	1.75	0.68
1:A:84:ASN:ND2	1:A:237:VAL:O	2.31	0.64
1:A:351:ASP:H	1:A:496:THR:HB	1.64	0.63
1:C:351:ASP:H	1:C:496:THR:HB	1.63	0.63
1:C:695:VAL:HG12	1:C:1030:VAL:HG22	1.79	0.63
1:B:351:ASP:H	1:B:496:THR:HB	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1006:SER:H	1:B:1018:LEU:HD23	1.64	0.63
1:B:955:LYS:HA	1:B:958:ALA:HB3	1.82	0.61
1:B:326:ARG:NH1	1:B:327:CYS:O	2.34	0.60
1:C:78:ARG:HG2	1:C:82:PHE:HB2	1.84	0.60
1:C:1042:ARG:NH1	1:C:1043:ASN:OD1	2.35	0.60
1:A:806:TYR:HD1	1:A:823:LYS:HD3	1.68	0.59
1:B:428:ASN:ND2	1:B:479:GLN:OE1	2.35	0.59
1:A:886:TYR:HB3	1:B:1098:VAL:HG12	1.84	0.58
1:C:886:TYR:HB3	1:A:1098:VAL:HG12	1.85	0.58
1:A:326:ARG:NH1	1:A:327:CYS:O	2.36	0.58
1:B:988:ARG:NH1	1:B:992:ASN:OD1	2.37	0.58
1:C:988:ARG:NH1	1:C:992:ASN:OD1	2.37	0.57
1:A:132:ARG:NH1	1:A:166:ASP:OD2	2.38	0.56
1:A:872:ALA:HB2	1:A:885:LEU:HD22	1.86	0.56
1:B:145:THR:OG1	1:B:241:MET:SD	2.63	0.56
1:C:132:ARG:NH1	1:C:166:ASP:OD2	2.39	0.56
1:B:711:ILE:O	1:B:969:ARG:NH1	2.38	0.56
1:C:871:MET:HE1	1:C:1019:MET:HE1	1.87	0.56
1:A:428:ASN:ND2	1:A:479:GLN:OE1	2.39	0.55
1:C:599:ALA:HA	1:C:602:LEU:HD12	1.89	0.55
1:A:988:ARG:NH1	1:A:992:ASN:OD1	2.40	0.55
1:C:301:LYS:HG3	1:C:573:PRO:HA	1.89	0.55
1:B:30:MET:SD	1:B:30:MET:N	2.81	0.55
1:B:998:MET:HE1	1:B:1022:PRO:HG3	1.89	0.55
1:C:711:ILE:O	1:C:969:ARG:NH1	2.37	0.54
1:A:76:SER:N	1:A:242:PHE:O	2.40	0.54
1:A:711:ILE:O	1:A:969:ARG:NH1	2.37	0.54
1:C:326:ARG:NH1	1:C:327:CYS:O	2.40	0.53
1:B:301:LYS:HG3	1:B:573:PRO:HA	1.90	0.53
1:C:955:LYS:HA	1:C:958:ALA:HB3	1.90	0.53
1:C:38:ARG:NH1	1:C:188:GLU:OE2	2.41	0.53
1:C:1042:ARG:NH1	1:C:1043:ASN:O	2.41	0.53
1:A:443:ARG:NH1	1:A:445:THR:O	2.41	0.53
1:C:704:SER:OG	1:C:828:THR:OG1	2.27	0.53
1:A:532:PHE:HB3	1:A:536:GLN:HB3	1.91	0.52
1:B:599:ALA:HA	1:B:602:LEU:HD12	1.91	0.52
1:B:704:SER:OG	1:B:828:THR:OG1	2.27	0.52
1:B:126:SER:OG	1:B:127:THR:N	2.43	0.52
1:C:571:ILE:HD13	1:C:639:ILE:HD12	1.91	0.52
1:A:600:ASP:OD1	1:A:600:ASP:N	2.42	0.52
1:A:38:ARG:NH1	1:A:188:GLU:OE2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:SER:HB3	1:A:477:ALA:HB1	1.92	0.51
1:A:704:SER:OG	1:A:828:THR:OG1	2.28	0.51
1:A:99:GLU:OE2	1:A:187:ARG:NH1	2.41	0.51
1:A:108:ILE:HG21	1:A:138:LEU:HD11	1.93	0.51
1:C:108:ILE:HG12	1:C:121:VAL:HG12	1.93	0.51
1:B:731:GLN:OE1	1:B:734:ARG:NH1	2.39	0.51
1:A:301:LYS:HG3	1:A:573:PRO:HA	1.92	0.50
1:C:532:PHE:HB3	1:C:536:GLN:HB3	1.93	0.50
1:A:760:THR:HG23	1:A:775:LEU:HD23	1.94	0.50
1:B:369:LYS:NZ	1:B:371:TYR:OH	2.39	0.50
1:B:122:ILE:HG23	1:B:131:ILE:HG12	1.94	0.50
1:C:369:LYS:NZ	1:C:371:TYR:OH	2.39	0.50
1:C:396:SER:HB3	1:C:477:ALA:HB1	1.94	0.50
1:C:731:GLN:OE1	1:C:734:ARG:NH1	2.40	0.50
1:A:71:SER:HA	1:A:82:PHE:HB3	1.94	0.49
1:A:114:ASP:HB2	1:A:116:THR:HG22	1.93	0.49
1:B:777:ASP:OD1	1:B:777:ASP:N	2.45	0.49
1:C:760:THR:HG23	1:C:775:LEU:HD23	1.95	0.49
1:A:816:ARG:NH2	1:B:547:ASP:OD2	2.44	0.49
1:A:571:ILE:HD13	1:A:639:ILE:HD12	1.95	0.49
1:B:806:TYR:HD1	1:B:823:LYS:HD3	1.77	0.49
1:B:213:LEU:HD12	1:B:214:PRO:HD2	1.95	0.49
1:C:508:LYS:HD3	1:C:527:PRO:HD3	1.95	0.49
1:B:571:ILE:HD13	1:B:639:ILE:HD12	1.95	0.48
1:C:806:TYR:HD1	1:C:823:LYS:HD3	1.78	0.48
1:C:428:ASN:ND2	1:C:479:GLN:OE1	2.40	0.48
1:C:99:GLU:OE2	1:C:187:ARG:NH1	2.46	0.48
1:A:111:SER:HA	1:A:233:THR:HG22	1.95	0.48
1:A:731:GLN:OE1	1:A:734:ARG:NH1	2.39	0.48
1:C:674:ILE:HD11	1:B:864:GLN:HB3	1.94	0.47
1:C:774:ILE:HG13	1:C:775:LEU:HD12	1.97	0.47
1:A:599:ALA:HA	1:A:602:LEU:HD12	1.96	0.47
1:B:202:GLN:HE22	1:B:223:ILE:HG21	1.78	0.47
1:B:732:LEU:HD22	1:B:977:VAL:HG21	1.96	0.47
1:C:38:ARG:HH21	1:C:214:PRO:HB2	1.79	0.47
1:B:290:LEU:HD21	1:B:299:VAL:HG11	1.94	0.47
1:A:91:ASP:OD1	1:A:91:ASP:N	2.46	0.47
1:B:690:SER:OG	1:B:1035:THR:OG1	2.33	0.47
1:B:94:TYR:OH	1:B:188:GLU:OE1	2.25	0.47
1:A:732:LEU:HD22	1:A:977:VAL:HG21	1.97	0.47
1:B:108:ILE:HG12	1:B:121:VAL:HG12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:202:GLN:O	1:C:221:ARG:NH1	2.48	0.46
1:A:691:VAL:HG22	1:A:1034:VAL:HG22	1.97	0.46
1:C:289:GLU:HG3	1:C:309:PHE:HB2	1.96	0.46
1:A:328:PRO:HB2	1:A:331:LYS:HB2	1.97	0.46
1:C:326:ARG:HH22	1:C:329:PHE:HD1	1.63	0.46
1:B:532:PHE:HB3	1:B:536:GLN:HB3	1.97	0.46
1:B:709:MET:HA	1:B:713:GLY:HA2	1.97	0.46
1:C:777:ASP:OD1	1:C:777:ASP:N	2.48	0.46
1:B:43:ASN:HD21	1:B:55:THR:HG21	1.81	0.46
1:C:956:VAL:CG2	1:B:418:ASP:HB3	2.46	0.46
1:B:187:ARG:HG2	1:B:204:TYR:HD1	1.79	0.46
1:C:709:MET:HA	1:C:713:GLY:HA2	1.98	0.46
1:B:289:GLU:HG3	1:B:309:PHE:HB2	1.98	0.46
1:C:406:THR:HG22	1:B:375:PRO:HB2	1.97	0.46
1:A:38:ARG:HH21	1:A:214:PRO:HB2	1.81	0.46
1:A:417:PRO:HG2	1:A:420:PHE:HB2	1.98	0.45
1:B:615:VAL:HG23	1:B:624:ILE:HG12	1.98	0.45
1:C:111:SER:HA	1:C:233:THR:HG22	1.98	0.45
1:A:43:ASN:HD21	1:A:55:THR:HG21	1.82	0.45
1:A:1073:ILE:HD13	1:A:1088:ASN:HB3	1.98	0.45
1:B:1012:CYS:HB3	1:B:1033:HIS:CE1	2.51	0.45
1:A:384:THR:OG1	1:A:489:GLU:O	2.30	0.45
1:C:816:ARG:NH2	1:A:547:ASP:OD2	2.50	0.45
1:B:37:ARG:NH2	1:B:278:ASP:OD1	2.49	0.45
1:C:800:ALA:HB3	1:C:819:ILE:HG21	1.98	0.45
1:C:615:VAL:HG23	1:C:624:ILE:HG12	1.99	0.45
1:A:1012:CYS:HB3	1:A:1033:HIS:CE1	2.52	0.45
1:C:954:ASP:N	1:C:954:ASP:OD1	2.48	0.45
1:C:108:ILE:HG21	1:C:138:LEU:HD11	1.98	0.44
1:A:508:LYS:HD3	1:A:527:PRO:HD3	1.99	0.44
1:A:709:MET:HA	1:A:713:GLY:HA2	1.98	0.44
1:C:300:ASN:OD1	1:C:301:LYS:N	2.50	0.44
1:A:429:THR:HG21	1:A:482:ARG:HD2	1.98	0.44
1:C:83:ASP:N	1:C:83:ASP:OD1	2.50	0.44
1:B:78:ARG:NH2	1:B:240:ALA:O	2.50	0.44
1:B:201:TYR:HB3	1:B:220:LEU:HB3	1.99	0.44
1:B:954:ASP:OD1	1:B:954:ASP:N	2.46	0.44
1:A:386:VAL:HG22	1:A:488:PHE:HB3	1.98	0.44
1:A:202:GLN:O	1:A:221:ARG:NH1	2.50	0.44
1:C:647:TYR:O	1:C:659:LYS:NZ	2.50	0.44
1:A:771:PHE:HB3	1:A:775:LEU:HD13	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:954:ASP:N	1:A:954:ASP:OD1	2.49	0.44
1:A:367:THR:O	1:A:425:ILE:HD12	2.18	0.44
1:B:300:ASN:OD1	1:B:301:LYS:N	2.50	0.44
1:B:71:SER:HA	1:B:82:PHE:HB3	2.00	0.44
1:A:615:VAL:HG23	1:A:624:ILE:HG12	1.99	0.43
1:B:125:ASN:O	1:B:128:HIS:N	2.50	0.43
1:C:938:ASN:OD1	1:B:724:GLN:NE2	2.52	0.43
1:B:365:PHE:CG	1:B:425:ILE:HD11	2.54	0.43
1:C:188:GLU:HB2	1:C:203:THR:HG22	2.00	0.43
1:C:771:PHE:HB3	1:C:775:LEU:HD13	2.01	0.43
1:A:690:SER:OG	1:A:1035:THR:OG1	2.34	0.43
1:A:724:GLN:NE2	1:B:938:ASN:OD1	2.51	0.43
1:A:1051:CYS:HB2	1:A:1095:CYS:HB2	1.90	0.43
1:C:716:LEU:HD12	1:A:263:TYR:HE2	1.82	0.43
1:B:124:ASN:O	1:B:144:TYR:HE2	2.01	0.43
1:A:121:VAL:HG12	1:A:123:VAL:HG22	2.00	0.43
1:A:365:PHE:HB3	1:A:425:ILE:HD11	1.99	0.43
1:B:386:VAL:HG22	1:B:488:PHE:HB3	2.01	0.43
1:A:188:GLU:HB2	1:A:203:THR:HG22	2.00	0.43
1:B:125:ASN:O	1:B:126:SER:HB3	2.18	0.43
1:C:547:ASP:OD2	1:B:816:ARG:NH2	2.52	0.42
1:C:578:SER:OG	1:C:579:SER:N	2.52	0.42
1:C:945:VAL:HG22	1:C:947:ASN:H	1.83	0.42
1:A:777:ASP:OD1	1:A:777:ASP:N	2.49	0.42
1:B:327:CYS:HB3	1:B:352:CYS:HB3	1.75	0.42
1:C:375:PRO:HB2	1:A:406:THR:HG22	2.00	0.42
1:B:78:ARG:HH22	1:B:241:MET:HA	1.84	0.42
1:C:121:VAL:O	1:C:131:ILE:HA	2.19	0.42
1:B:840:ALA:HA	1:B:843:THR:HG22	2.02	0.42
1:C:114:ASP:HB2	1:C:116:THR:HG22	2.01	0.42
1:A:812:ASP:OD1	1:A:812:ASP:N	2.47	0.42
1:B:774:ILE:HG13	1:B:775:LEU:HD12	2.02	0.42
1:C:520:LYS:HB3	1:C:520:LYS:HE2	1.84	0.42
1:C:418:ASP:OD2	1:A:955:LYS:HE3	2.18	0.42
1:A:290:LEU:HD21	1:A:299:VAL:HG11	2.01	0.42
1:A:757:MET:HE3	1:A:757:MET:HB3	1.95	0.42
1:A:928:LEU:HD23	1:A:928:LEU:HA	1.89	0.42
1:C:732:LEU:HD22	1:C:977:VAL:HG21	2.02	0.42
1:A:840:ALA:HA	1:A:843:THR:HG22	2.02	0.42
1:B:84:ASN:ND2	1:B:237:VAL:O	2.53	0.42
1:C:219:VAL:HG11	1:C:276:ILE:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:690:SER:OG	1:C:1035:THR:OG1	2.37	0.41
1:C:783:LYS:HA	1:C:783:LYS:HD2	1.86	0.41
1:B:359:LEU:HD13	1:B:365:PHE:HZ	1.85	0.41
1:B:508:LYS:HD3	1:B:527:PRO:HD3	2.02	0.41
1:C:37:ARG:NH2	1:C:278:ASP:OD1	2.51	0.41
1:B:91:ASP:OD1	1:B:91:ASP:N	2.48	0.41
1:B:124:ASN:C	1:B:144:TYR:HE2	2.28	0.41
1:A:368:PHE:CD1	1:A:425:ILE:HD13	2.55	0.41
1:A:1055:LYS:HB2	1:A:1055:LYS:HE3	1.86	0.41
1:A:37:ARG:NH2	1:A:278:ASP:OD1	2.52	0.41
1:C:1051:CYS:HB2	1:C:1095:CYS:HB2	1.85	0.41
1:A:129:ILE:HD11	1:A:169:GLU:HB3	2.03	0.41
1:A:392:LEU:HD11	1:A:480:ALA:HB1	2.02	0.41
1:B:602:LEU:O	1:B:607:ARG:NH2	2.48	0.41
1:B:1073:ILE:HD13	1:B:1088:ASN:HB3	2.01	0.41
1:A:950:LEU:HD23	1:A:950:LEU:HA	1.92	0.41
1:A:1050:ILE:HG13	1:A:1057:TYR:HB2	2.02	0.41
1:B:771:PHE:HB3	1:B:775:LEU:HD13	2.01	0.41
1:C:1055:LYS:HB2	1:C:1055:LYS:HE3	1.86	0.41
1:B:1050:ILE:HG13	1:B:1057:TYR:HB2	2.02	0.41
1:C:386:VAL:HG22	1:C:488:PHE:HB3	2.02	0.41
1:A:753:GLN:OE1	1:A:999:SER:OG	2.35	0.41
1:C:602:LEU:O	1:C:607:ARG:NH2	2.47	0.40
1:A:736:LEU:HD23	1:A:736:LEU:HA	1.92	0.40
1:B:783:LYS:HA	1:B:783:LYS:HD2	1.90	0.40
1:C:1073:ILE:HD13	1:C:1088:ASN:HB3	2.02	0.40
1:A:602:LEU:O	1:A:607:ARG:NH2	2.47	0.40
1:C:295:LYS:HB3	1:C:295:LYS:HE2	1.89	0.40
1:A:184:LYS:HD3	1:A:184:LYS:HA	1.97	0.40
1:B:370:CYS:HA	1:B:423:CYS:HA	2.02	0.40
1:C:370:CYS:HA	1:C:423:CYS:HA	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1029/1256 (82%)	987 (96%)	42 (4%)	0	100	100
1	B	1029/1256 (82%)	993 (96%)	35 (3%)	1 (0%)	48	76
1	C	1029/1256 (82%)	990 (96%)	39 (4%)	0	100	100
All	All	3087/3768 (82%)	2970 (96%)	116 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	80	THR

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	905/1084 (84%)	905 (100%)	0	100	100
1	B	905/1084 (84%)	905 (100%)	0	100	100
1	C	905/1084 (84%)	905 (100%)	0	100	100
All	All	2715/3252 (84%)	2715 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	515	ASN
1	C	628	HIS
1	C	748	GLN
1	C	773	GLN
1	C	870	GLN
1	C	902	GLN
1	C	961	GLN

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Mol	Chain	Res	Type
1	C	1040	GLN
1	A	208	ASN
1	A	471	ASN
1	A	473	ASN
1	A	724	GLN
1	A	934	GLN
1	A	961	GLN
1	A	974	GLN
1	A	1005	GLN
1	A	1077	ASN
1	B	128	HIS
1	B	162	ASN
1	B	471	ASN
1	B	473	ASN
1	B	882	GLN
1	B	918	GLN
1	B	922	ASN
1	B	961	GLN
1	B	974	GLN
1	B	1017	HIS

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)

24 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	D	1	2	14,14,15	0.20	0	17,19,21	0.42	0
2	NAG	D	2	2	14,14,15	0.37	0	17,19,21	0.49	0
2	NAG	E	1	2,1	14,14,15	0.21	0	17,19,21	0.43	0
2	NAG	E	2	2	14,14,15	0.26	0	17,19,21	0.45	0
2	NAG	F	1	2,1	14,14,15	0.35	0	17,19,21	0.66	1 (5%)
2	NAG	F	2	2	14,14,15	0.27	0	17,19,21	0.46	0
2	NAG	G	1	2	14,14,15	0.22	0	17,19,21	0.43	0
2	NAG	G	2	2	14,14,15	0.25	0	17,19,21	0.43	0
2	NAG	H	1	2	14,14,15	0.22	0	17,19,21	0.44	0
2	NAG	H	2	2	14,14,15	0.37	0	17,19,21	0.49	0
2	NAG	I	1	2,1	14,14,15	0.22	0	17,19,21	0.43	0
2	NAG	I	2	2	14,14,15	0.26	0	17,19,21	0.44	0
2	NAG	J	1	2,1	14,14,15	0.37	0	17,19,21	0.68	1 (5%)
2	NAG	J	2	2	14,14,15	0.29	0	17,19,21	0.48	0
2	NAG	K	1	2	14,14,15	0.22	0	17,19,21	0.44	0
2	NAG	K	2	2	14,14,15	0.26	0	17,19,21	0.44	0
2	NAG	L	1	2	14,14,15	0.23	0	17,19,21	0.44	0
2	NAG	L	2	2	14,14,15	0.39	0	17,19,21	0.48	0
2	NAG	M	1	2,1	14,14,15	0.22	0	17,19,21	0.44	0
2	NAG	M	2	2	14,14,15	0.26	0	17,19,21	0.45	0
2	NAG	N	1	2,1	14,14,15	0.33	0	17,19,21	0.67	1 (5%)
2	NAG	N	2	2	14,14,15	0.26	0	17,19,21	0.47	0
2	NAG	O	1	2	14,14,15	0.24	0	17,19,21	0.43	0
2	NAG	O	2	2	14,14,15	0.25	0	17,19,21	0.44	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	D	1	2	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	3/6/23/26	0/1/1/1
2	NAG	E	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	NAG	F	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
2	NAG	G	1	2	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1
2	NAG	H	1	2	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	H	2	2	-	3/6/23/26	0/1/1/1
2	NAG	I	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	I	2	2	-	2/6/23/26	0/1/1/1
2	NAG	J	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	J	2	2	-	2/6/23/26	0/1/1/1
2	NAG	K	1	2	-	0/6/23/26	0/1/1/1
2	NAG	K	2	2	-	2/6/23/26	0/1/1/1
2	NAG	L	1	2	-	0/6/23/26	0/1/1/1
2	NAG	L	2	2	-	2/6/23/26	0/1/1/1
2	NAG	M	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	M	2	2	-	2/6/23/26	0/1/1/1
2	NAG	N	1	2,1	-	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	2	-	0/6/23/26	0/1/1/1
2	NAG	O	2	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	1	NAG	C1-O5-C5	2.28	115.28	112.19
2	N	1	NAG	C1-O5-C5	2.27	115.26	112.19
2	F	1	NAG	C1-O5-C5	2.20	115.17	112.19

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1	NAG	O5-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6
2	O	2	NAG	O5-C5-C6-O6
2	K	2	NAG	O5-C5-C6-O6
2	I	2	NAG	O5-C5-C6-O6
2	M	1	NAG	O5-C5-C6-O6
2	M	2	NAG	O5-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
2	O	2	NAG	C4-C5-C6-O6
2	G	2	NAG	C4-C5-C6-O6

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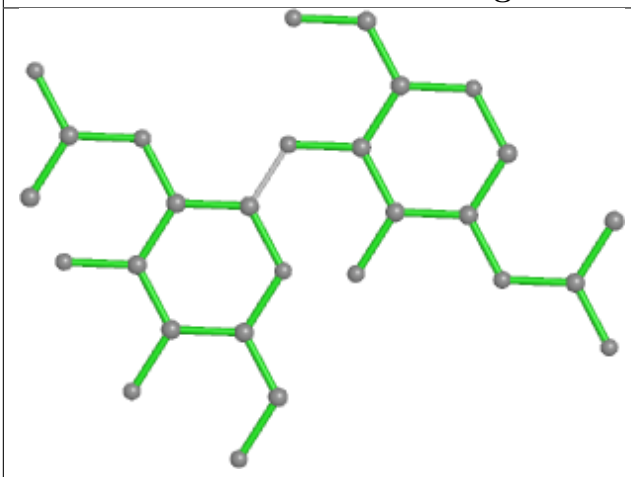
Mol	Chain	Res	Type	Atoms
2	K	2	NAG	C4-C5-C6-O6
2	M	1	NAG	C4-C5-C6-O6
2	I	1	NAG	O5-C5-C6-O6
2	I	2	NAG	C4-C5-C6-O6
2	D	2	NAG	C8-C7-N2-C2
2	D	2	NAG	O7-C7-N2-C2
2	H	2	NAG	C8-C7-N2-C2
2	H	2	NAG	O7-C7-N2-C2
2	L	2	NAG	C8-C7-N2-C2
2	L	2	NAG	O7-C7-N2-C2
2	F	2	NAG	O5-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	M	2	NAG	C4-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
2	I	1	NAG	C4-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
2	J	2	NAG	O5-C5-C6-O6
2	N	2	NAG	O5-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
2	H	1	NAG	O5-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	J	2	NAG	C4-C5-C6-O6
2	H	2	NAG	C4-C5-C6-O6
2	N	2	NAG	C4-C5-C6-O6

There are no ring outliers.

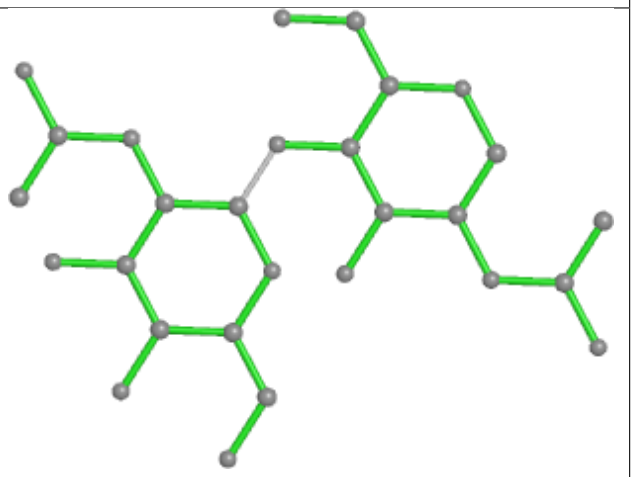
No monomer is involved in short contacts.

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

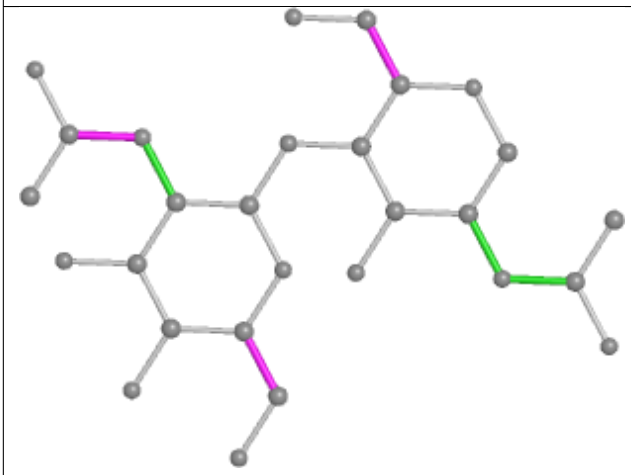
Oligosaccharide Chain D



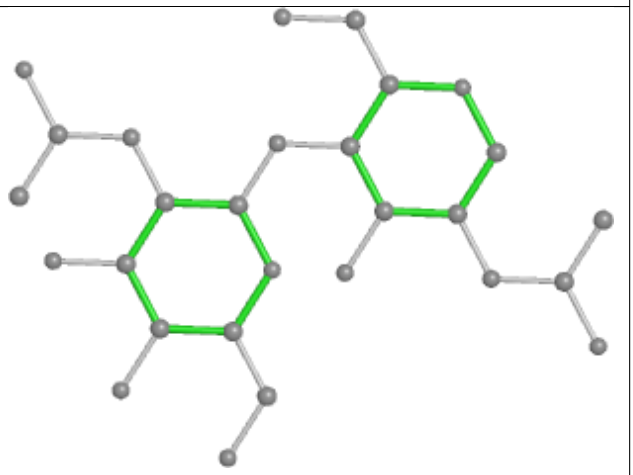
Bond lengths



Bond angles

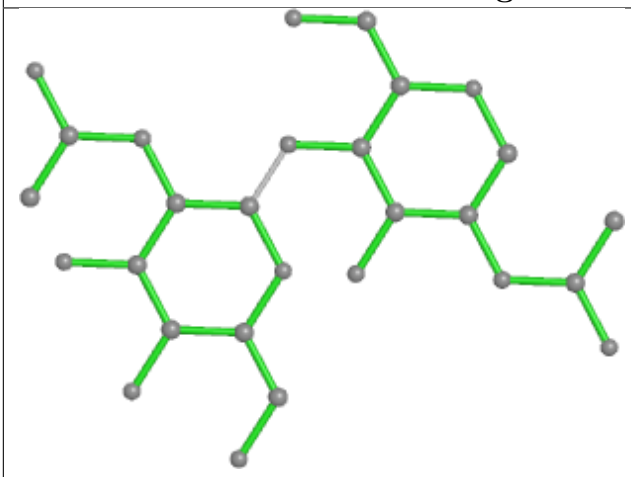


Torsions

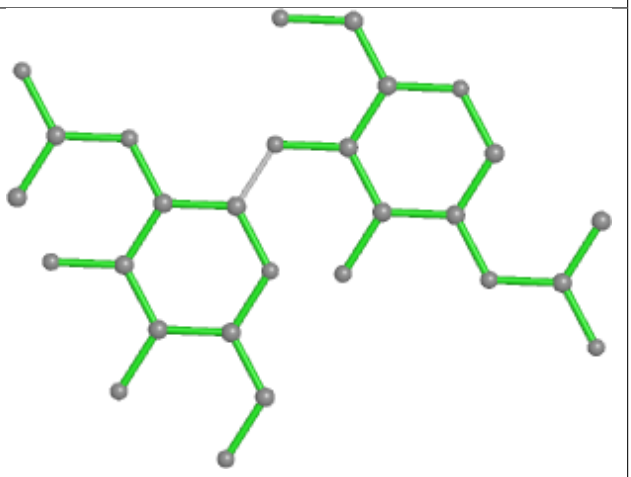


Rings

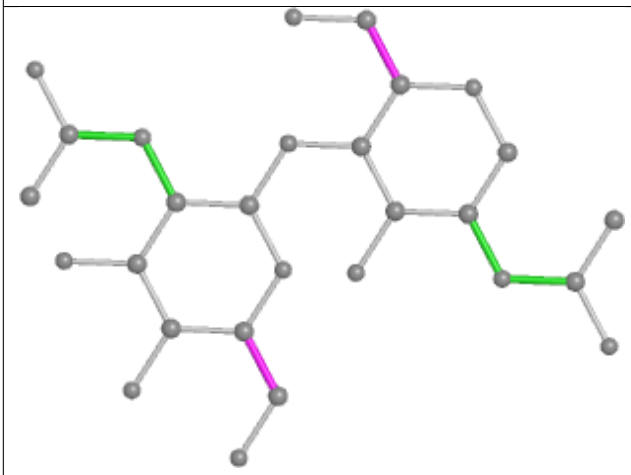
Oligosaccharide Chain E



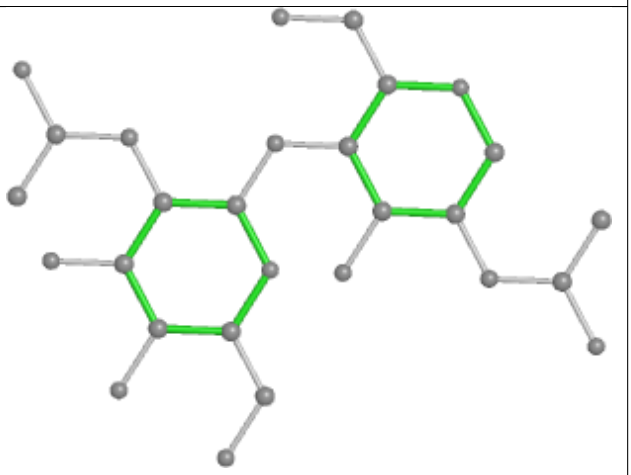
Bond lengths



Bond angles

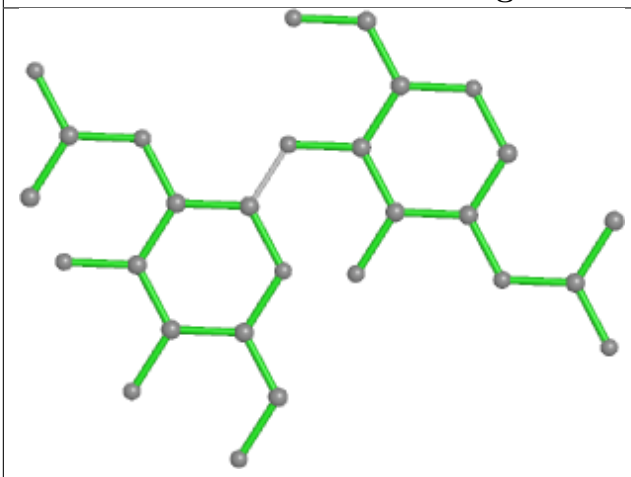


Torsions

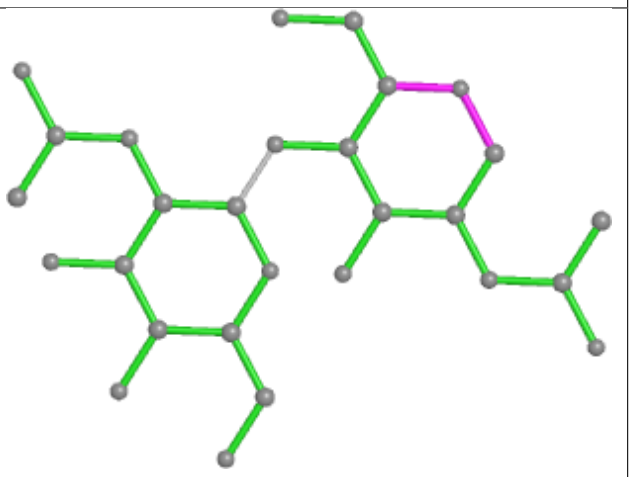


Rings

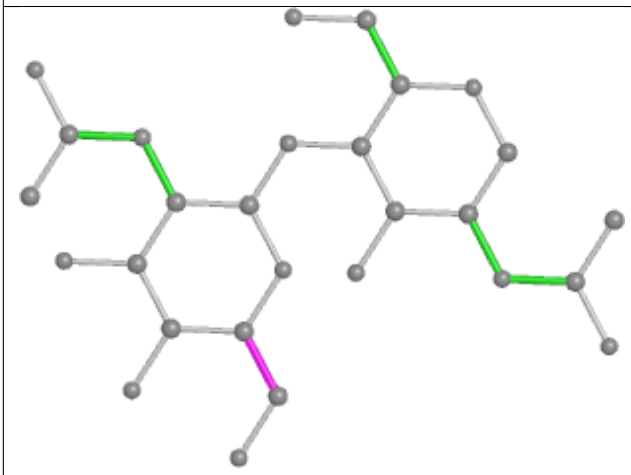
Oligosaccharide Chain F



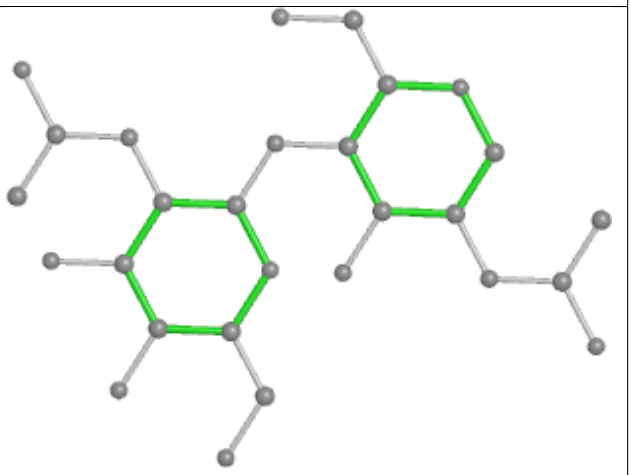
Bond lengths



Bond angles

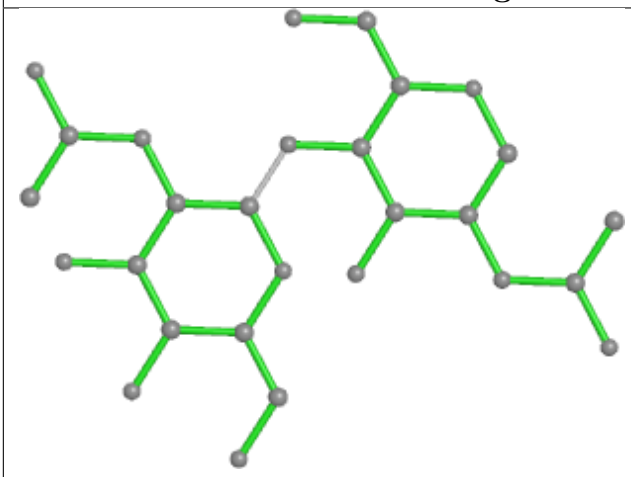


Torsions

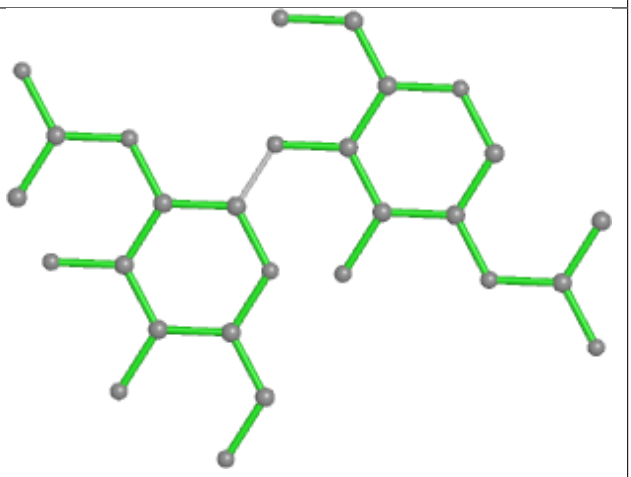


Rings

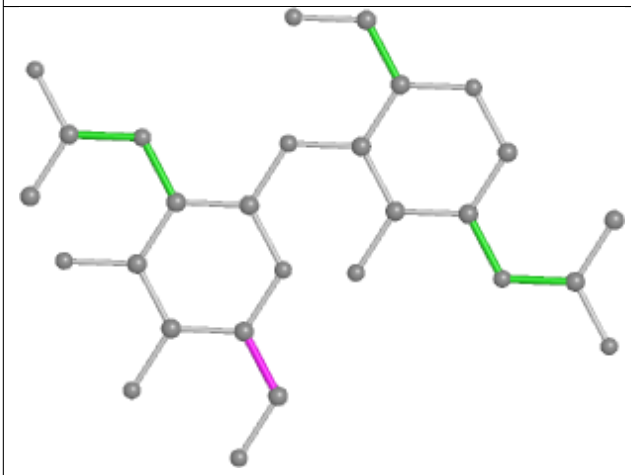
Oligosaccharide Chain G



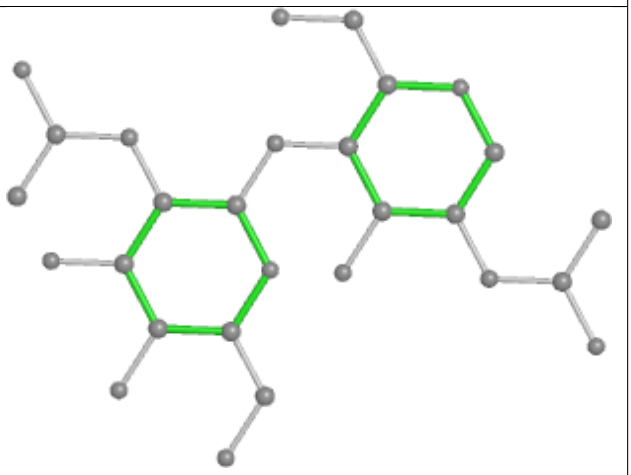
Bond lengths



Bond angles

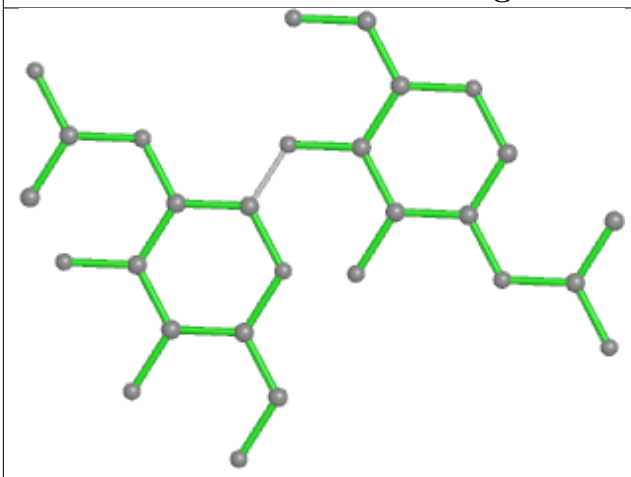


Torsions

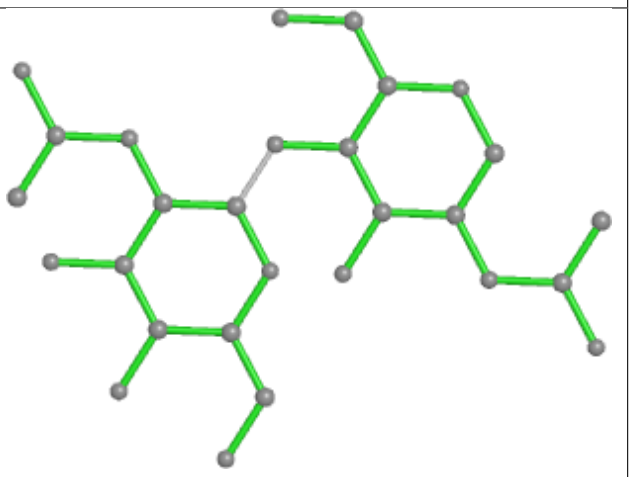


Rings

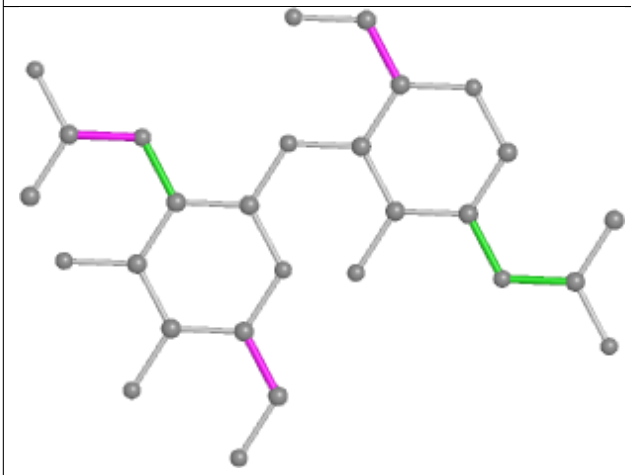
Oligosaccharide Chain H



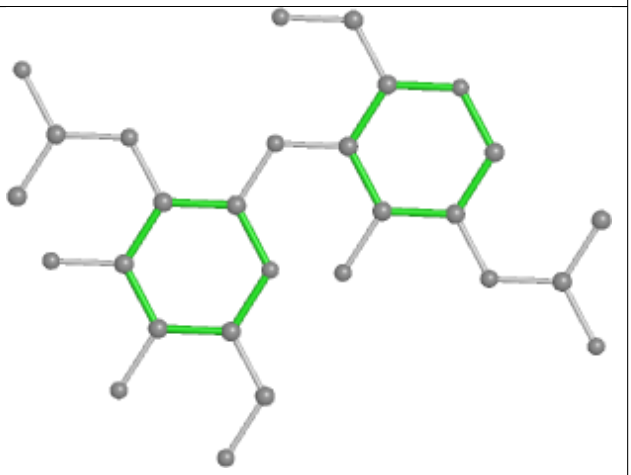
Bond lengths



Bond angles

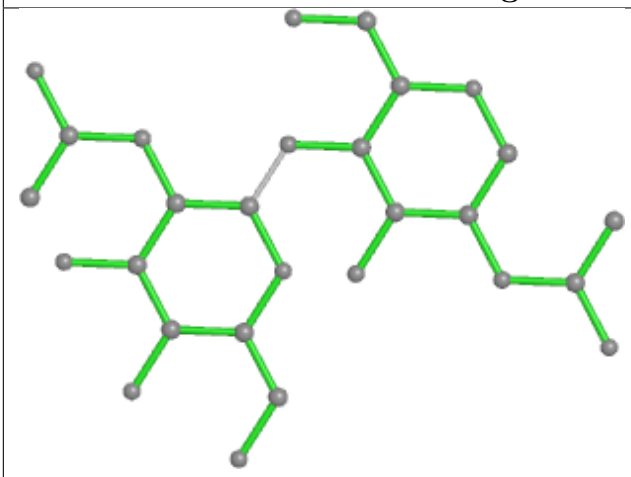


Torsions

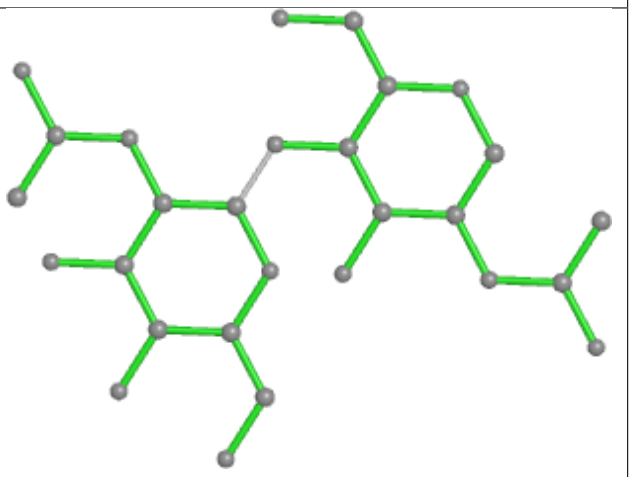


Rings

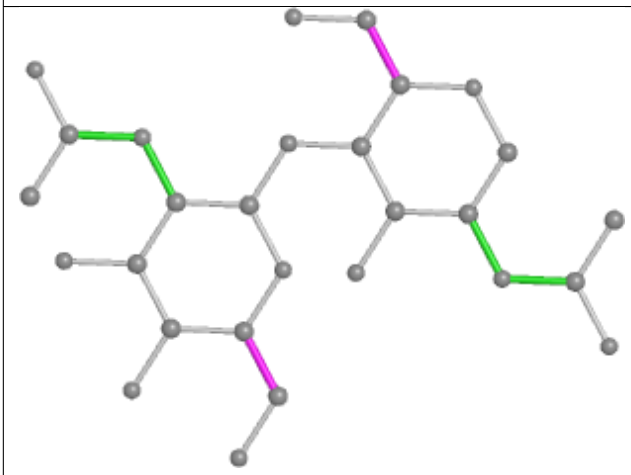
Oligosaccharide Chain I



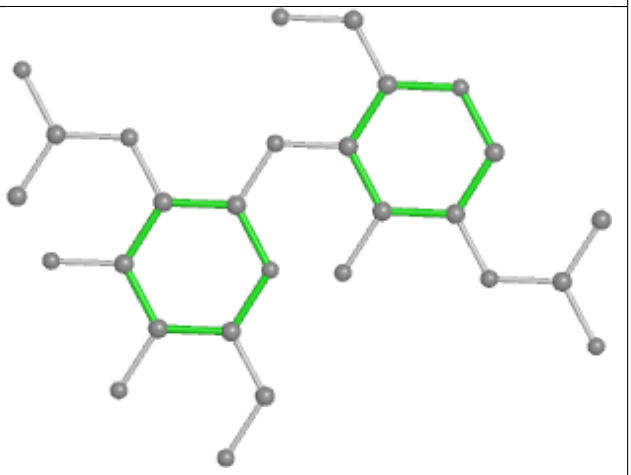
Bond lengths



Bond angles

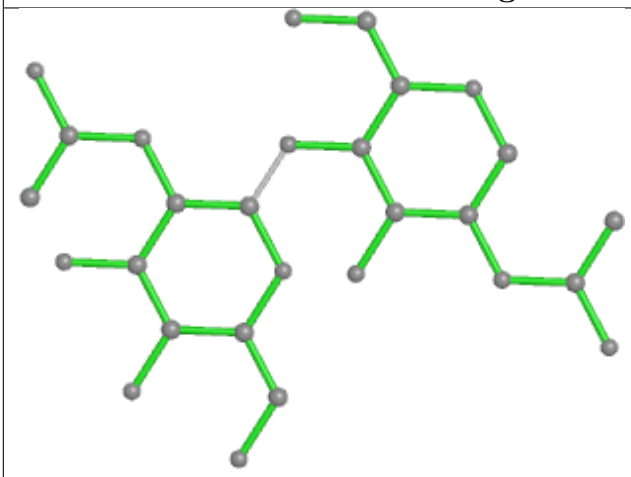


Torsions

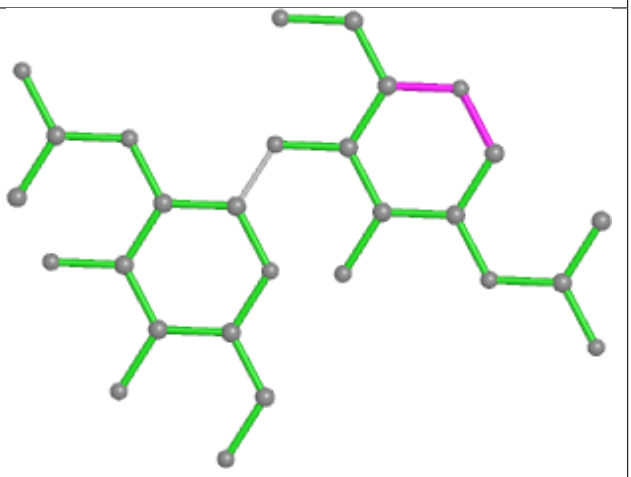


Rings

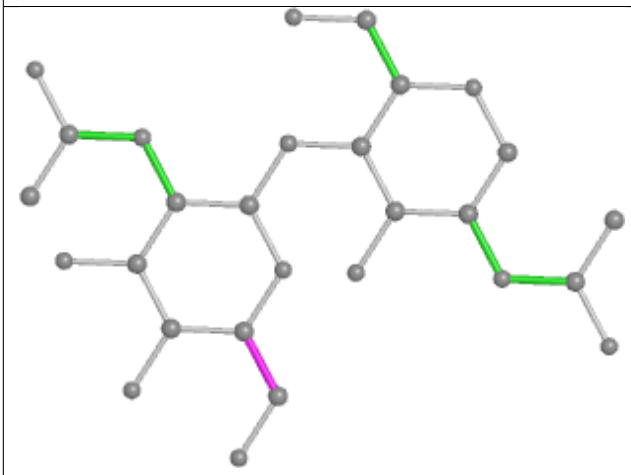
Oligosaccharide Chain J



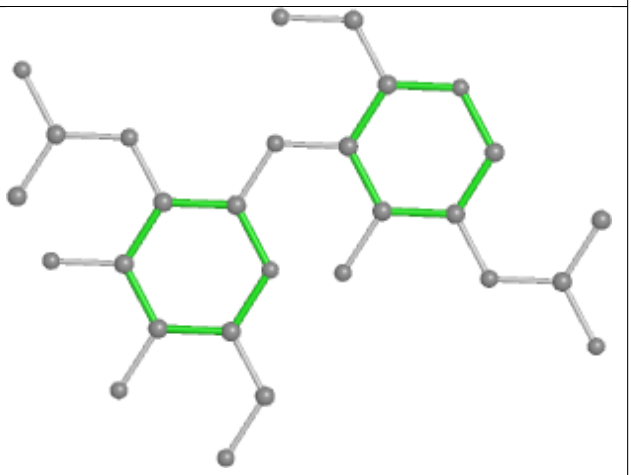
Bond lengths



Bond angles

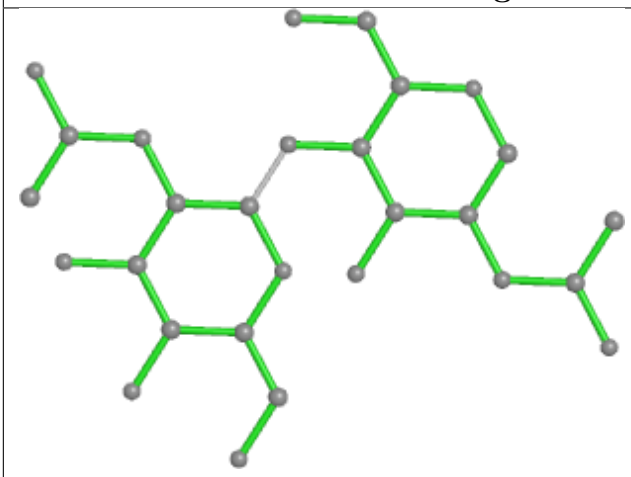


Torsions

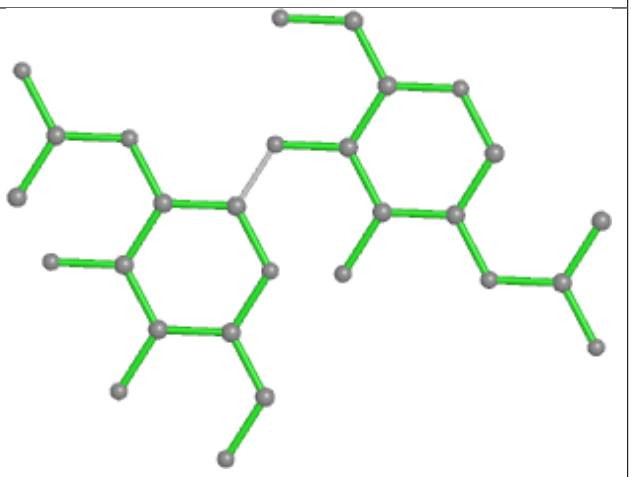


Rings

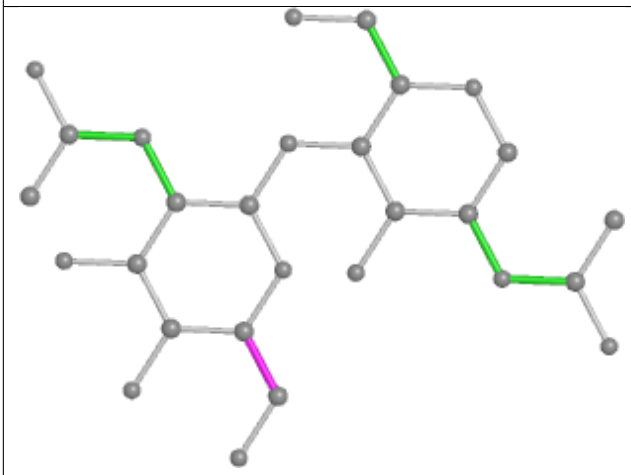
Oligosaccharide Chain K



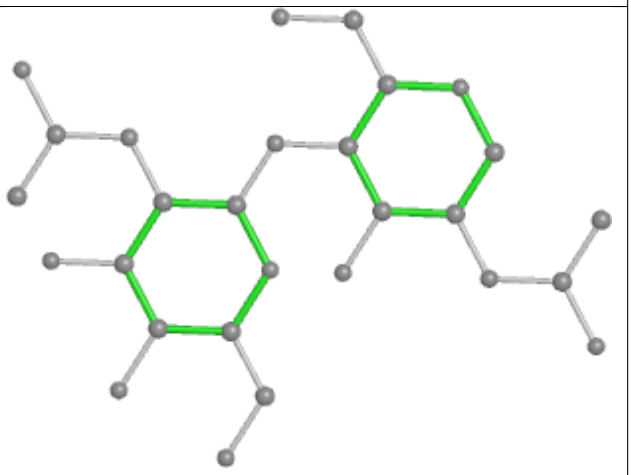
Bond lengths



Bond angles

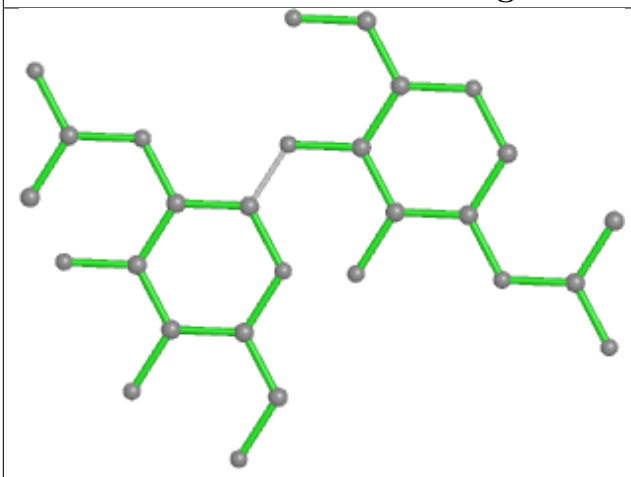


Torsions

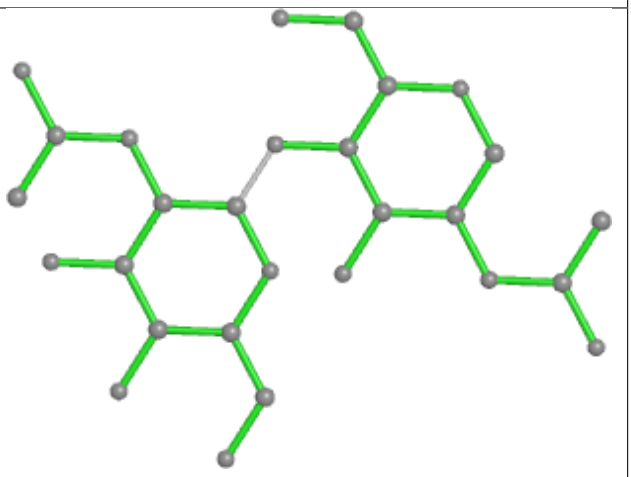


Rings

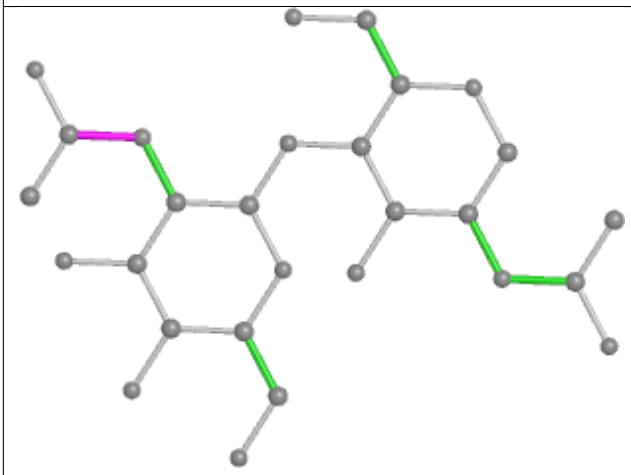
Oligosaccharide Chain L



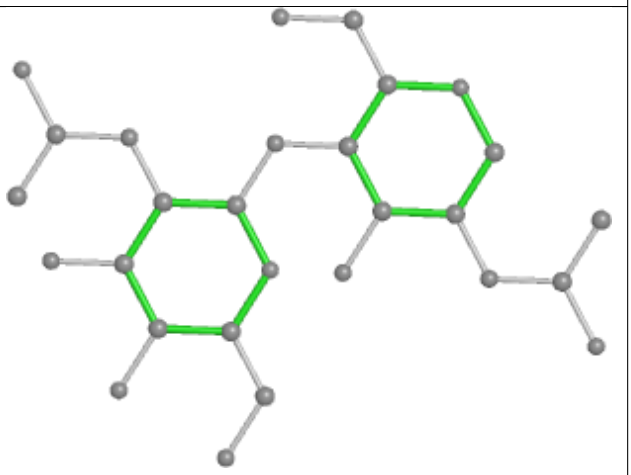
Bond lengths



Bond angles

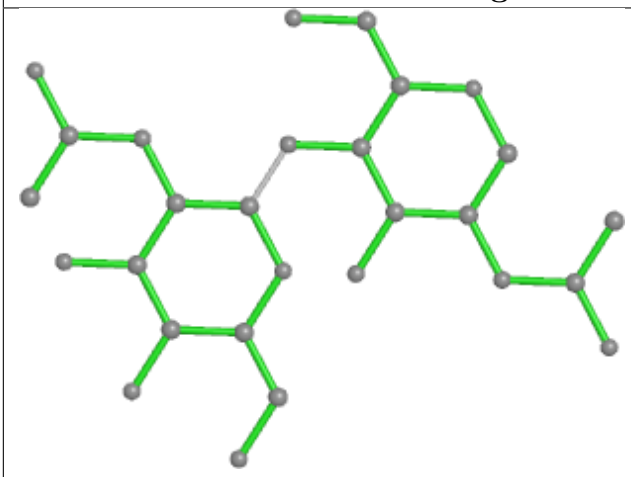


Torsions

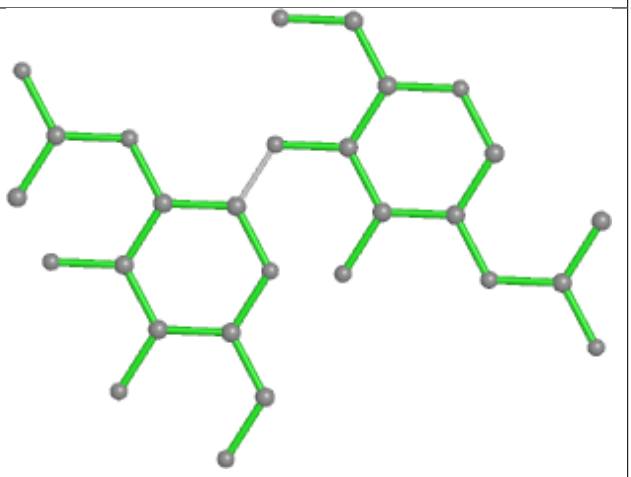


Rings

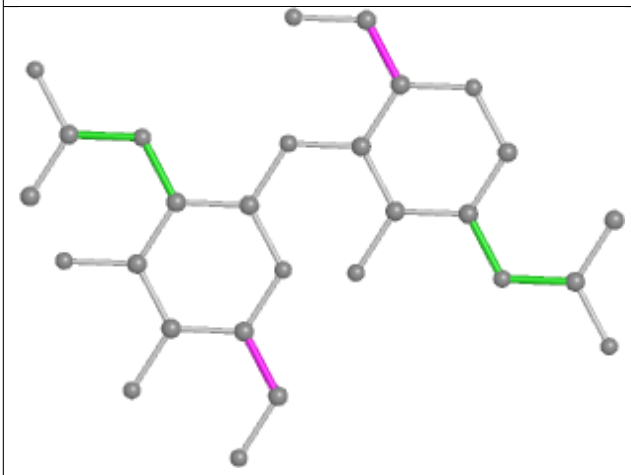
Oligosaccharide Chain M



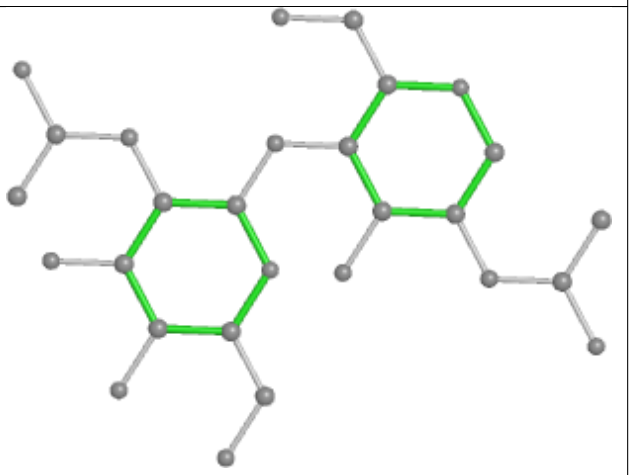
Bond lengths



Bond angles

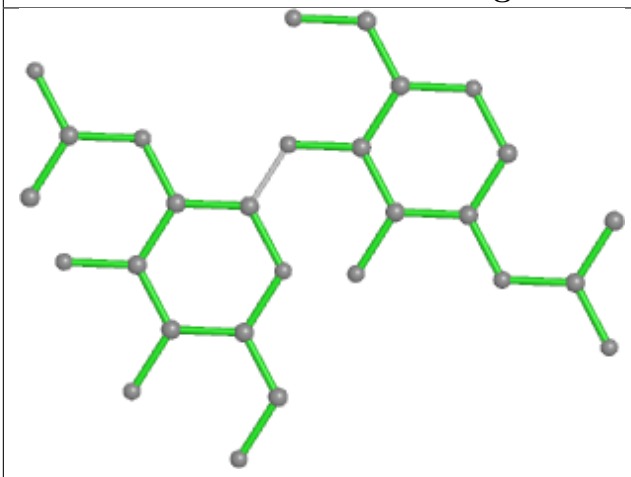


Torsions

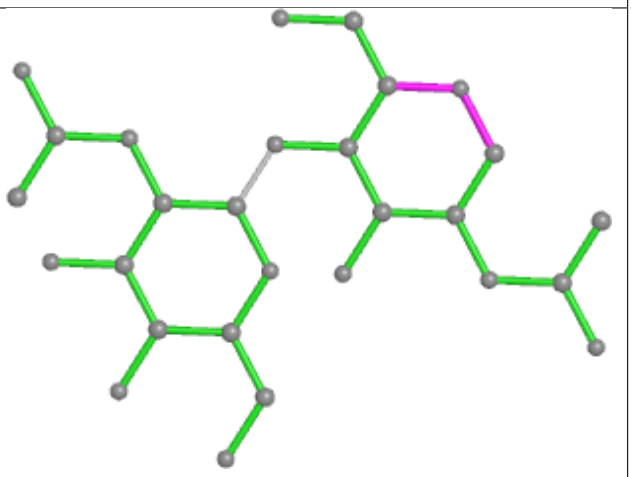


Rings

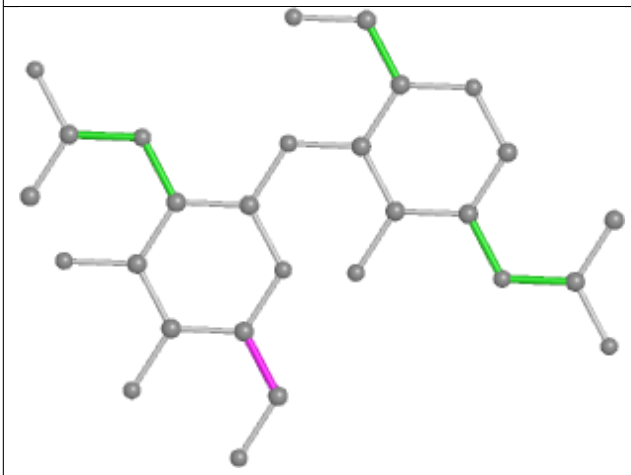
Oligosaccharide Chain N



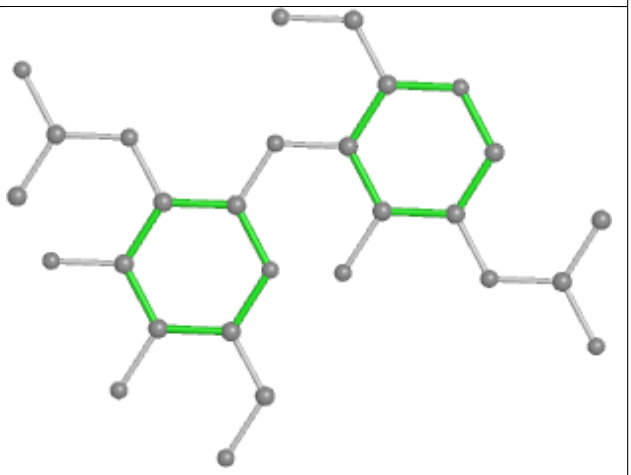
Bond lengths



Bond angles

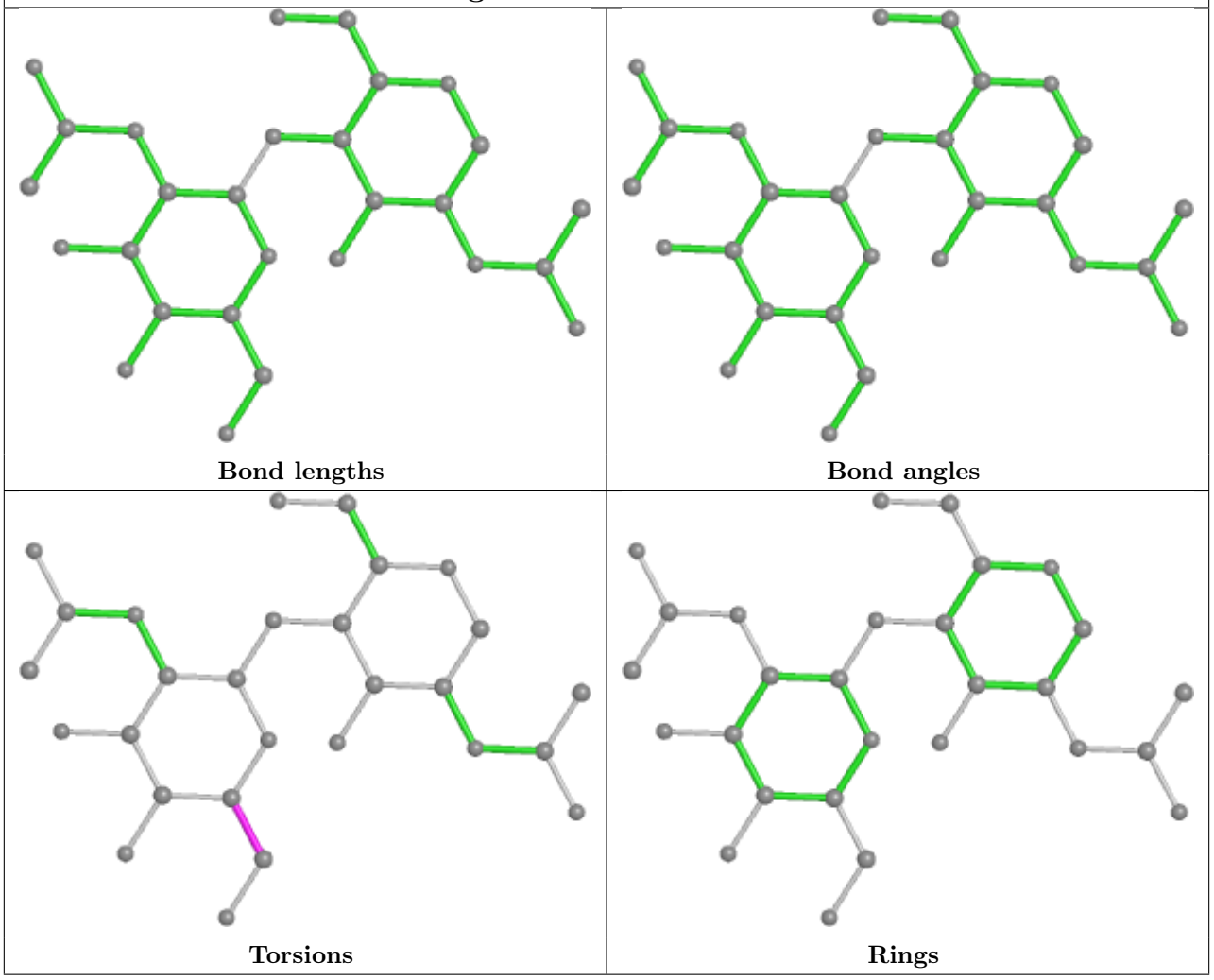


Torsions



Rings

Oligosaccharide Chain O



5.6 Ligand geometry (i)

39 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	C	1303	1	14,14,15	0.39	0	17,19,21	0.87	1 (5%)
3	NAG	A	1302	-	14,14,15	0.21	0	17,19,21	0.48	0
3	NAG	A	1305	-	14,14,15	0.23	0	17,19,21	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	A	1308	-	14,14,15	0.22	0	17,19,21	0.44	0
3	NAG	B	1309	-	14,14,15	0.22	0	17,19,21	0.45	0
3	NAG	C	1301	1	14,14,15	0.25	0	17,19,21	0.47	0
3	NAG	A	1313	1	14,14,15	0.42	0	17,19,21	0.75	1 (5%)
3	NAG	C	1304	1	14,14,15	0.25	0	17,19,21	0.43	0
3	NAG	B	1301	1	14,14,15	0.26	0	17,19,21	0.48	0
3	NAG	B	1304	1	14,14,15	0.24	0	17,19,21	0.44	0
3	NAG	B	1303	1	14,14,15	0.38	0	17,19,21	0.82	1 (5%)
3	NAG	A	1303	1	14,14,15	0.37	0	17,19,21	0.87	1 (5%)
3	NAG	B	1306	1	14,14,15	0.24	0	17,19,21	0.46	0
3	NAG	A	1306	1	14,14,15	0.25	0	17,19,21	0.45	0
3	NAG	A	1309	-	14,14,15	0.22	0	17,19,21	0.45	0
3	NAG	B	1305	-	14,14,15	0.23	0	17,19,21	0.44	0
3	NAG	C	1312	1	14,14,15	0.27	0	17,19,21	0.39	0
3	NAG	C	1313	1	14,14,15	0.41	0	17,19,21	0.76	1 (5%)
3	NAG	B	1308	-	14,14,15	0.22	0	17,19,21	0.45	0
3	NAG	A	1312	1	14,14,15	0.28	0	17,19,21	0.39	0
3	NAG	C	1302	-	14,14,15	0.22	0	17,19,21	0.49	0
3	NAG	C	1310	1	14,14,15	0.23	0	17,19,21	0.46	0
3	NAG	C	1314	-	14,14,15	0.27	0	17,19,21	0.43	0
3	NAG	A	1304	1	14,14,15	0.24	0	17,19,21	0.43	0
3	NAG	C	1311	-	14,14,15	0.27	0	17,19,21	0.43	0
3	NAG	C	1306	1	14,14,15	0.25	0	17,19,21	0.48	0
3	NAG	A	1310	1	14,14,15	0.22	0	17,19,21	0.45	0
3	NAG	B	1312	1	14,14,15	0.33	0	17,19,21	0.77	1 (5%)
3	NAG	C	1305	-	14,14,15	0.22	0	17,19,21	0.44	0
3	NAG	C	1307	1	14,14,15	0.28	0	17,19,21	0.56	0
3	NAG	C	1308	-	14,14,15	0.22	0	17,19,21	0.45	0
3	NAG	B	1307	1	14,14,15	0.28	0	17,19,21	0.56	0
3	NAG	B	1302	-	14,14,15	0.22	0	17,19,21	0.47	0
3	NAG	A	1301	1	14,14,15	0.25	0	17,19,21	0.47	0
3	NAG	B	1311	1	14,14,15	0.28	0	17,19,21	0.39	0
3	NAG	A	1311	-	14,14,15	0.25	0	17,19,21	0.42	0
3	NAG	C	1309	-	14,14,15	0.22	0	17,19,21	0.44	0
3	NAG	A	1307	1	14,14,15	0.30	0	17,19,21	0.55	0
3	NAG	B	1310	1	14,14,15	0.27	0	17,19,21	0.44	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	1303	1	-	3/6/23/26	0/1/1/1
3	NAG	A	1302	-	-	4/6/23/26	0/1/1/1
3	NAG	A	1305	-	-	2/6/23/26	0/1/1/1
3	NAG	A	1308	-	-	2/6/23/26	0/1/1/1
3	NAG	B	1309	-	-	2/6/23/26	0/1/1/1
3	NAG	C	1301	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1313	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1304	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1301	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1304	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1303	1	-	3/6/23/26	0/1/1/1
3	NAG	A	1303	1	-	3/6/23/26	0/1/1/1
3	NAG	B	1306	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1306	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1309	-	-	2/6/23/26	0/1/1/1
3	NAG	B	1305	-	-	2/6/23/26	0/1/1/1
3	NAG	C	1312	1	-	1/6/23/26	0/1/1/1
3	NAG	C	1313	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1308	-	-	2/6/23/26	0/1/1/1
3	NAG	A	1312	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1302	-	-	2/6/23/26	0/1/1/1
3	NAG	C	1310	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1314	-	-	1/6/23/26	0/1/1/1
3	NAG	A	1304	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1311	-	-	1/6/23/26	0/1/1/1
3	NAG	C	1306	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1310	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1312	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1305	-	-	2/6/23/26	0/1/1/1
3	NAG	C	1307	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1308	-	-	2/6/23/26	0/1/1/1
3	NAG	B	1307	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1302	-	-	4/6/23/26	0/1/1/1
3	NAG	A	1301	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1311	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1311	-	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	1309	-	-	2/6/23/26	0/1/1/1
3	NAG	A	1307	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1310	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1312	NAG	C2-N2-C7	2.52	126.49	122.90
3	C	1313	NAG	C2-N2-C7	2.48	126.43	122.90
3	A	1313	NAG	C2-N2-C7	2.46	126.41	122.90
3	B	1303	NAG	C2-N2-C7	2.44	126.38	122.90
3	C	1303	NAG	C2-N2-C7	2.41	126.33	122.90
3	A	1303	NAG	C2-N2-C7	2.40	126.33	122.90

There are no chirality outliers.

All (75) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1308	NAG	C4-C5-C6-O6
3	C	1306	NAG	O5-C5-C6-O6
3	C	1310	NAG	O5-C5-C6-O6
3	A	1303	NAG	O5-C5-C6-O6
3	A	1306	NAG	O5-C5-C6-O6
3	B	1310	NAG	O5-C5-C6-O6
3	C	1303	NAG	O5-C5-C6-O6
3	B	1302	NAG	O5-C5-C6-O6
3	B	1306	NAG	O5-C5-C6-O6
3	A	1308	NAG	C4-C5-C6-O6
3	A	1309	NAG	C4-C5-C6-O6
3	B	1309	NAG	C4-C5-C6-O6
3	B	1305	NAG	O5-C5-C6-O6
3	A	1305	NAG	O5-C5-C6-O6
3	C	1309	NAG	C4-C5-C6-O6
3	B	1310	NAG	C4-C5-C6-O6
3	A	1310	NAG	O5-C5-C6-O6
3	C	1303	NAG	C4-C5-C6-O6
3	C	1310	NAG	C4-C5-C6-O6
3	C	1305	NAG	O5-C5-C6-O6
3	B	1308	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	A	1303	NAG	C4-C5-C6-O6
3	A	1306	NAG	C4-C5-C6-O6
3	A	1307	NAG	C4-C5-C6-O6
3	B	1302	NAG	C4-C5-C6-O6
3	B	1306	NAG	C4-C5-C6-O6
3	B	1303	NAG	O5-C5-C6-O6
3	C	1309	NAG	O5-C5-C6-O6
3	C	1307	NAG	C4-C5-C6-O6
3	C	1308	NAG	C4-C5-C6-O6
3	A	1309	NAG	O5-C5-C6-O6
3	B	1309	NAG	O5-C5-C6-O6
3	C	1306	NAG	C4-C5-C6-O6
3	A	1310	NAG	C4-C5-C6-O6
3	B	1307	NAG	C4-C5-C6-O6
3	C	1305	NAG	C4-C5-C6-O6
3	B	1303	NAG	C4-C5-C6-O6
3	B	1305	NAG	C4-C5-C6-O6
3	C	1302	NAG	C8-C7-N2-C2
3	C	1302	NAG	O7-C7-N2-C2
3	A	1302	NAG	C8-C7-N2-C2
3	A	1302	NAG	O7-C7-N2-C2
3	B	1302	NAG	C8-C7-N2-C2
3	B	1302	NAG	O7-C7-N2-C2
3	A	1305	NAG	C4-C5-C6-O6
3	A	1308	NAG	O5-C5-C6-O6
3	A	1307	NAG	O5-C5-C6-O6
3	C	1308	NAG	O5-C5-C6-O6
3	A	1312	NAG	O5-C5-C6-O6
3	B	1311	NAG	O5-C5-C6-O6
3	C	1307	NAG	O5-C5-C6-O6
3	C	1313	NAG	O5-C5-C6-O6
3	B	1307	NAG	O5-C5-C6-O6
3	B	1312	NAG	O5-C5-C6-O6
3	C	1301	NAG	C4-C5-C6-O6
3	A	1313	NAG	O5-C5-C6-O6
3	C	1301	NAG	O5-C5-C6-O6
3	A	1311	NAG	O5-C5-C6-O6
3	B	1301	NAG	C4-C5-C6-O6
3	C	1314	NAG	O5-C5-C6-O6
3	A	1302	NAG	C4-C5-C6-O6
3	C	1311	NAG	O5-C5-C6-O6
3	B	1301	NAG	O5-C5-C6-O6

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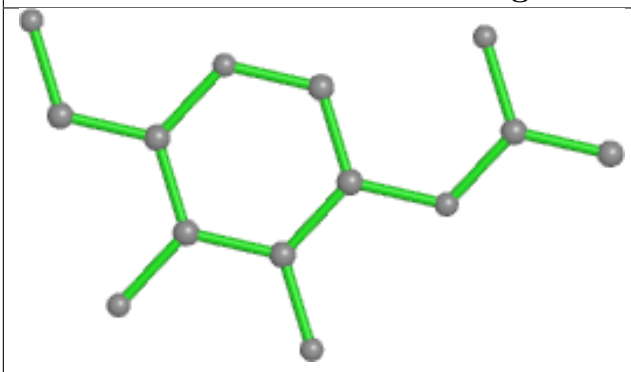
Mol	Chain	Res	Type	Atoms
3	C	1312	NAG	O5-C5-C6-O6
3	A	1301	NAG	C4-C5-C6-O6
3	A	1301	NAG	O5-C5-C6-O6
3	A	1302	NAG	O5-C5-C6-O6
3	A	1312	NAG	C4-C5-C6-O6
3	B	1311	NAG	C4-C5-C6-O6
3	C	1303	NAG	C3-C2-N2-C7
3	C	1313	NAG	C3-C2-N2-C7
3	A	1303	NAG	C3-C2-N2-C7
3	A	1313	NAG	C3-C2-N2-C7
3	B	1303	NAG	C3-C2-N2-C7
3	B	1312	NAG	C3-C2-N2-C7

There are no ring outliers.

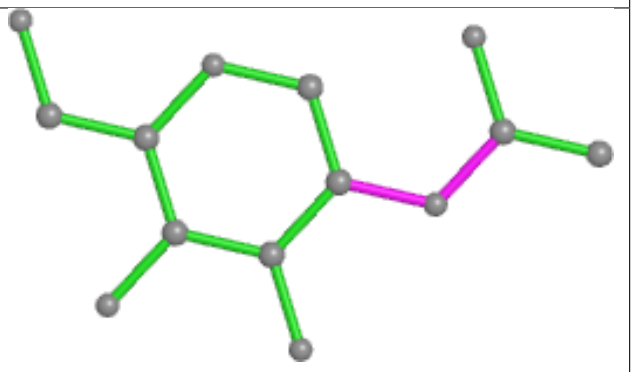
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

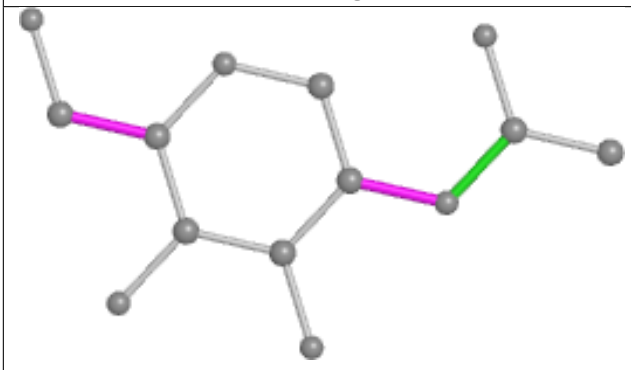
Ligand NAG C 1303



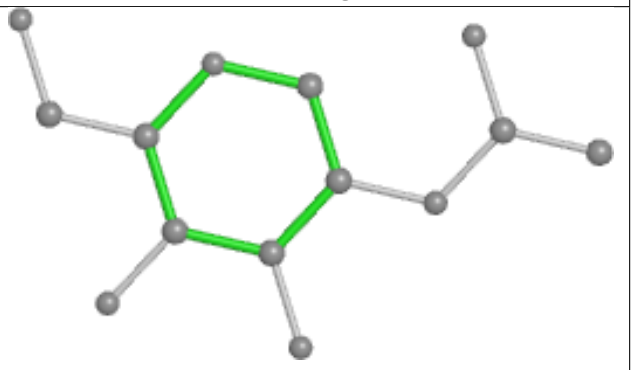
Bond lengths



Bond angles

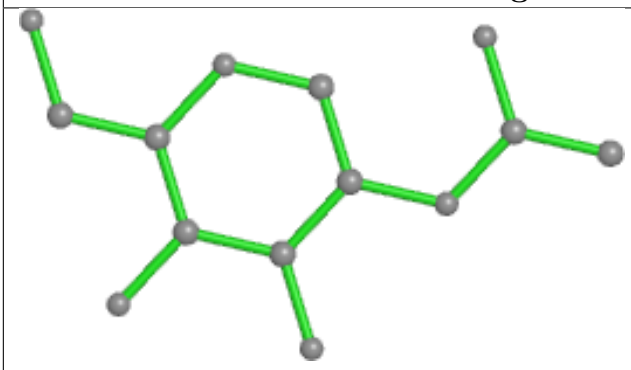


Torsions

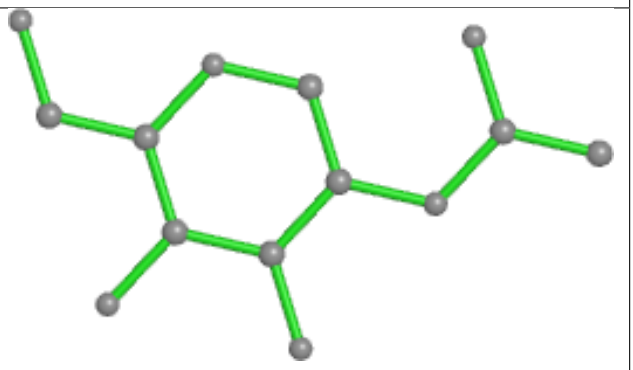


Rings

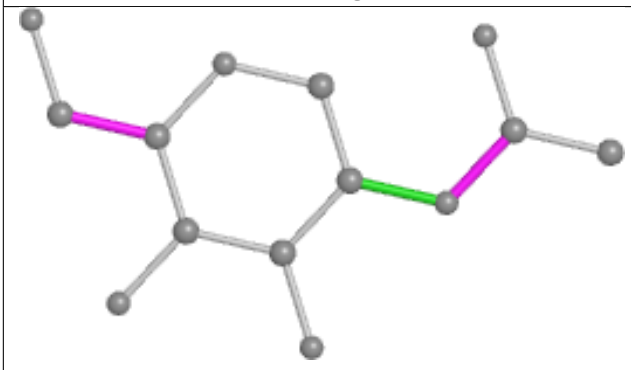
Ligand NAG A 1302



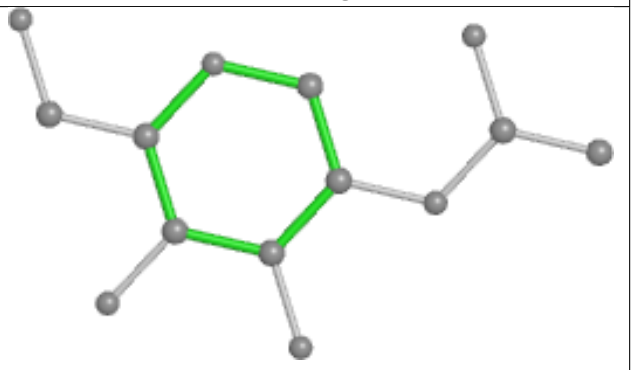
Bond lengths



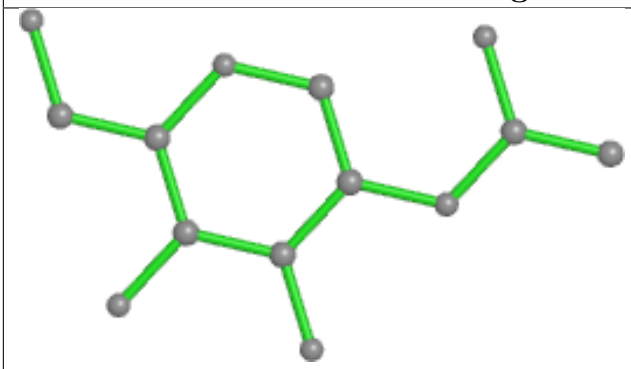
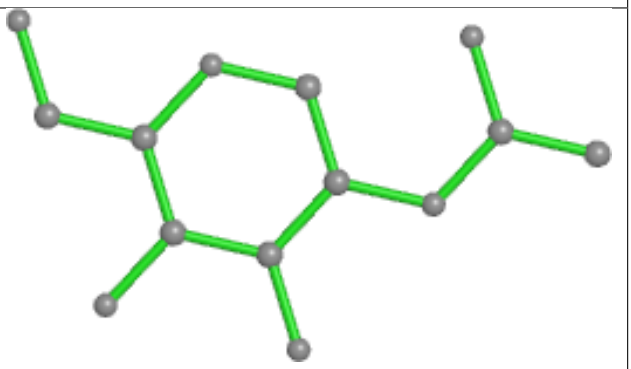
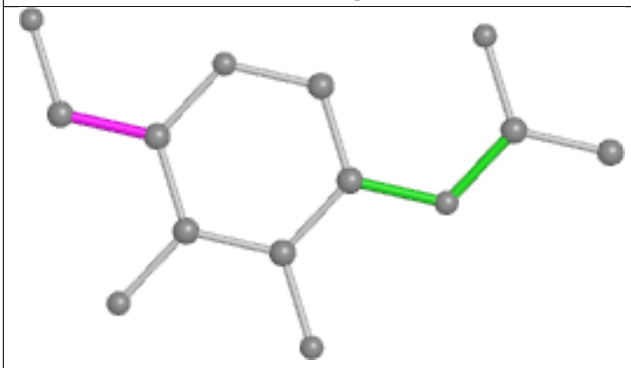
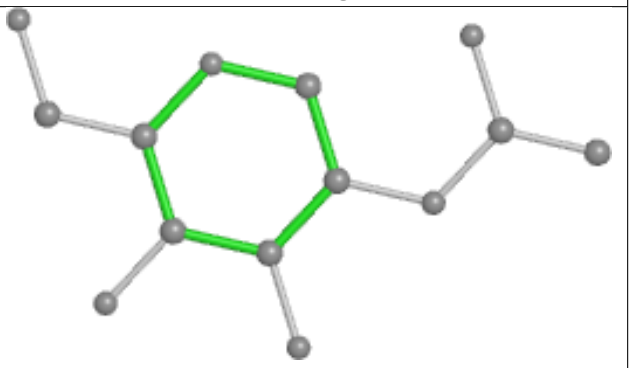
Bond angles

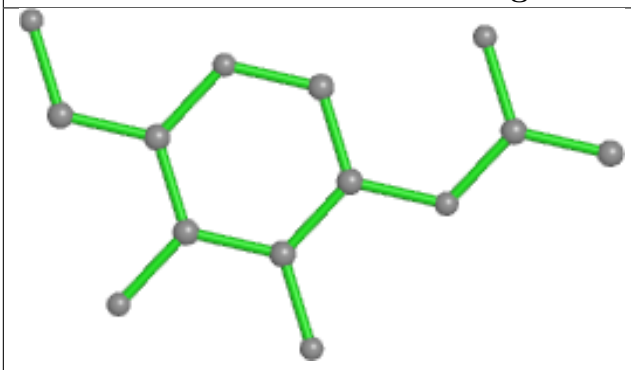
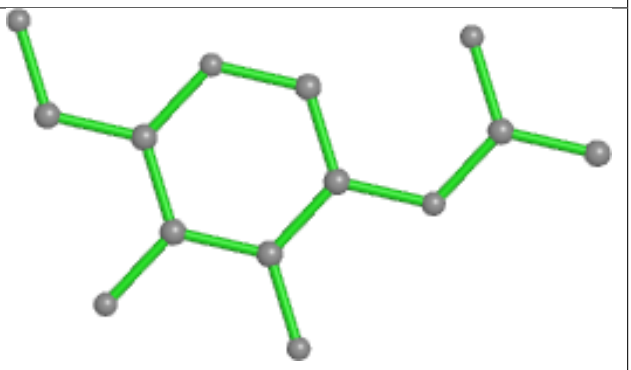
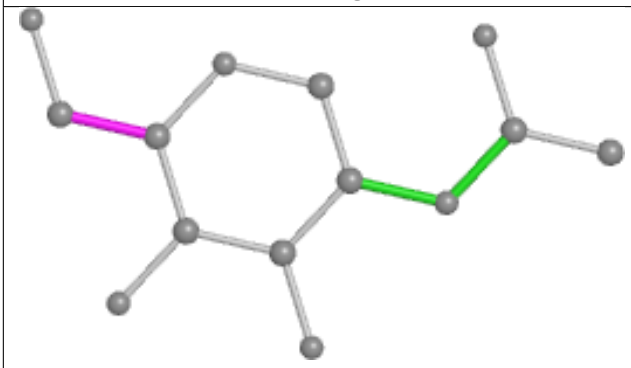
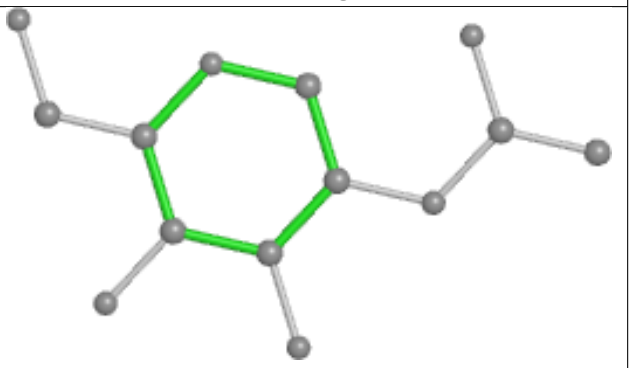


Torsions

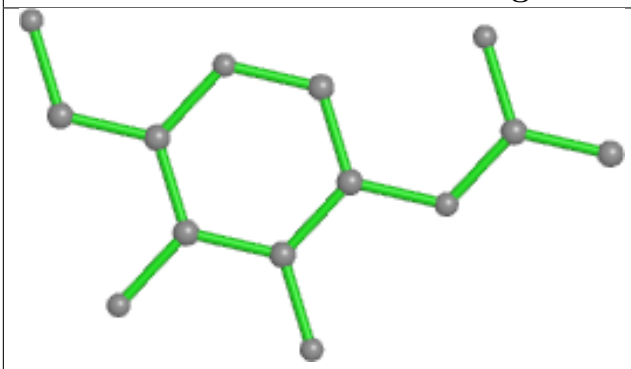


Rings

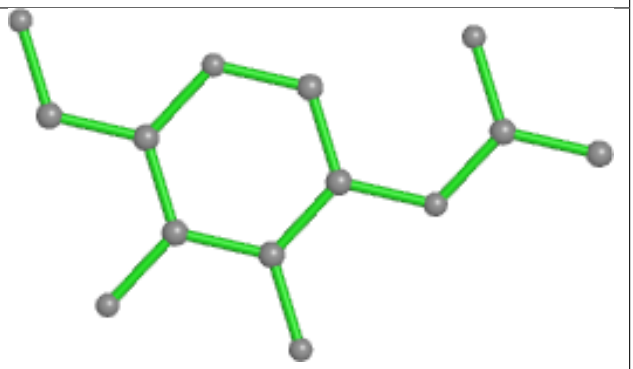
Ligand NAG A 1305	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG A 1308	
 Bond lengths	 Bond angles
 Torsions	 Rings

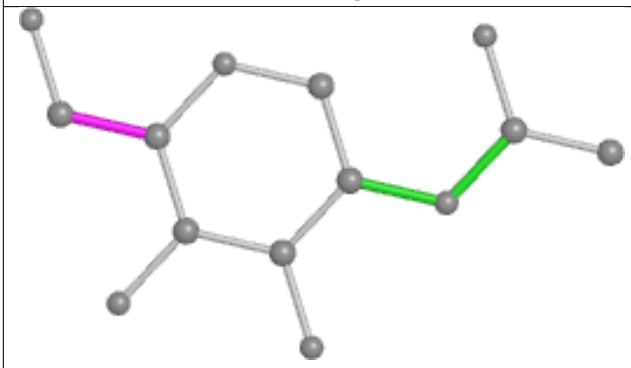
Ligand NAG B 1309



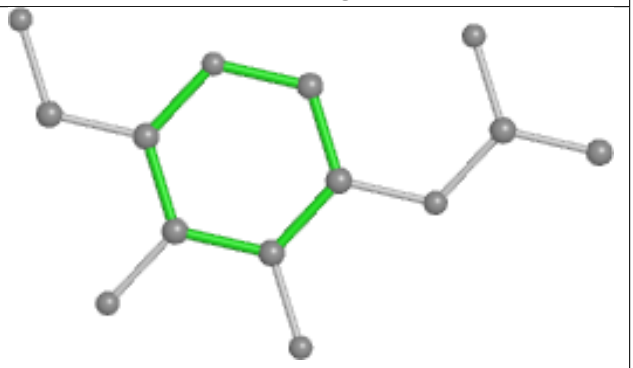
Bond lengths



Bond angles

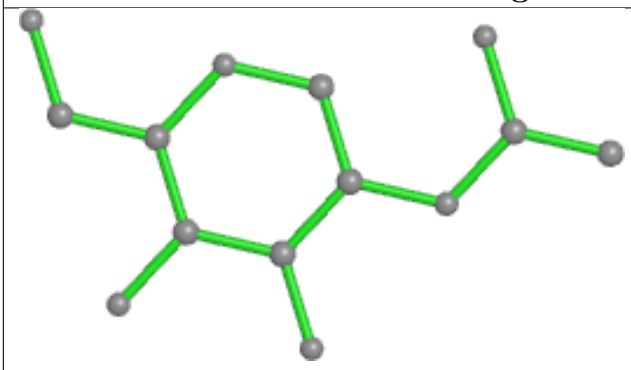


Torsions

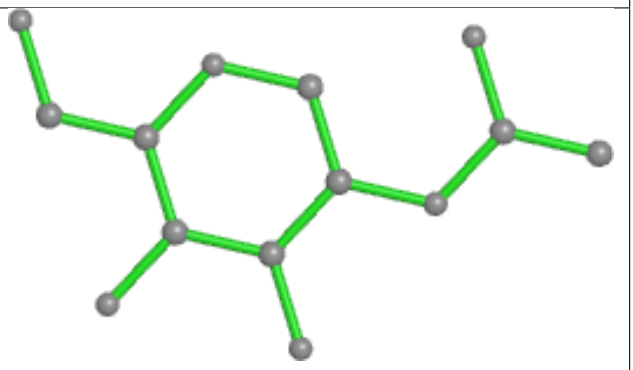


Rings

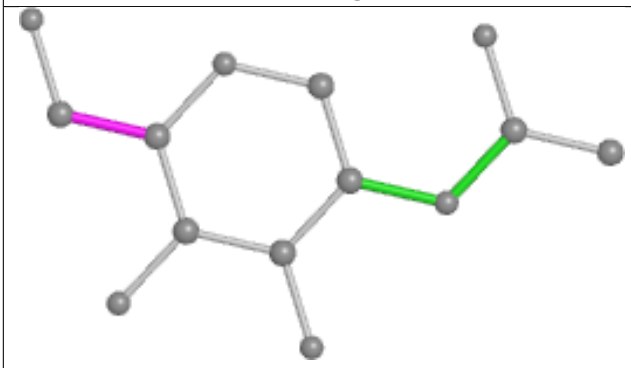
Ligand NAG C 1301



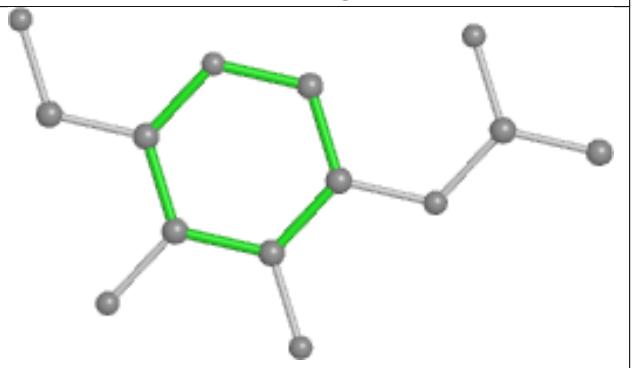
Bond lengths



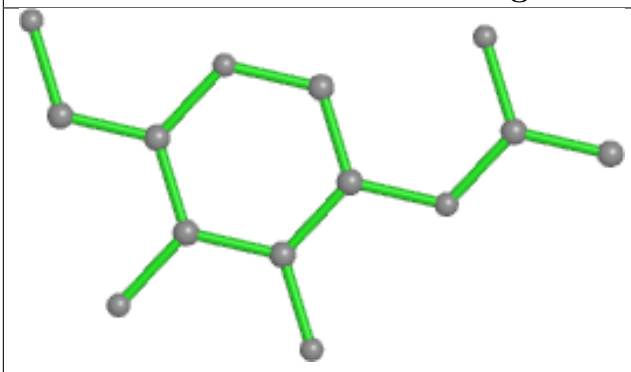
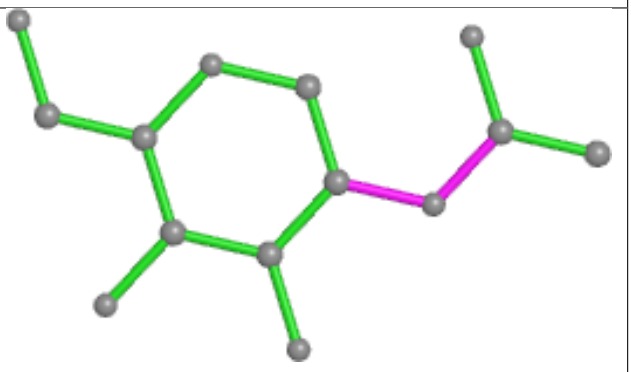
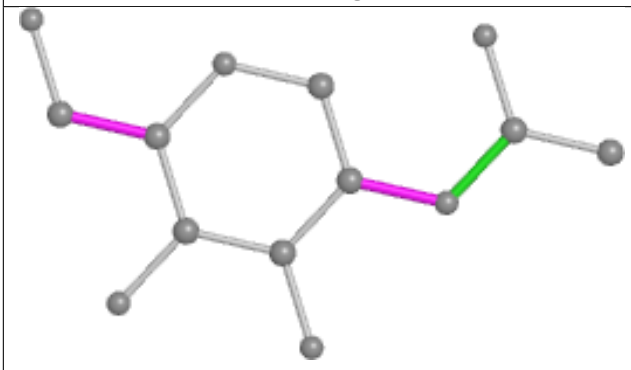
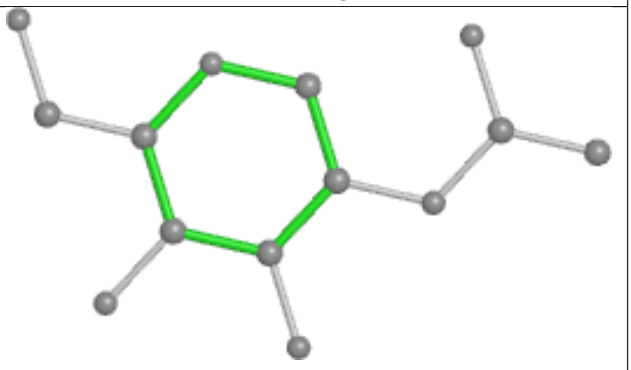
Bond angles

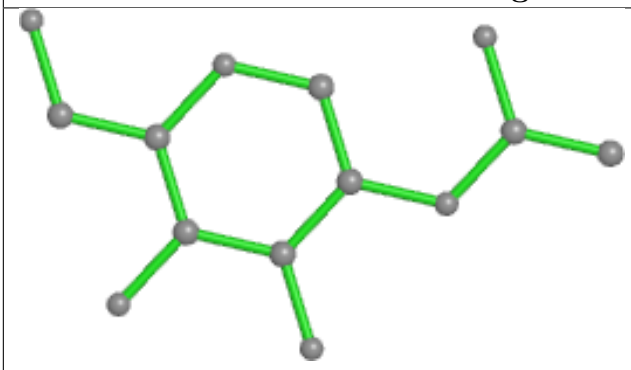
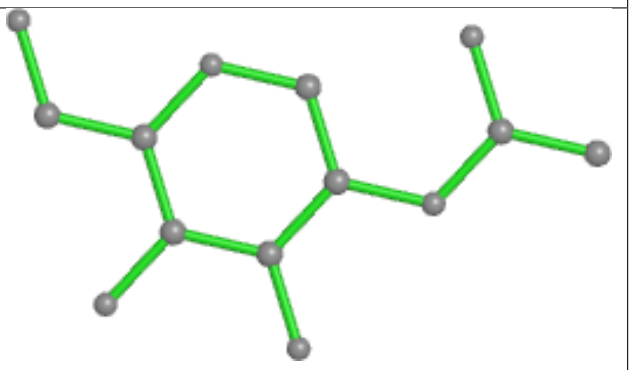
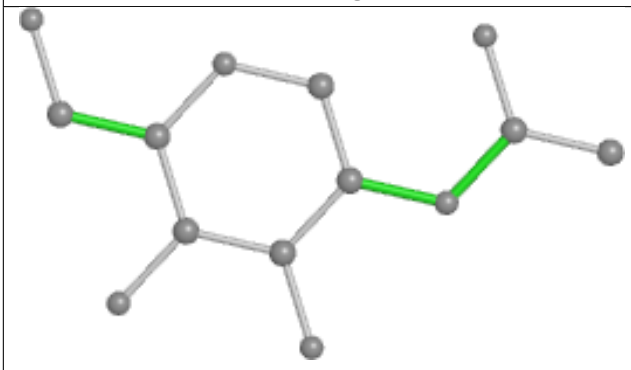
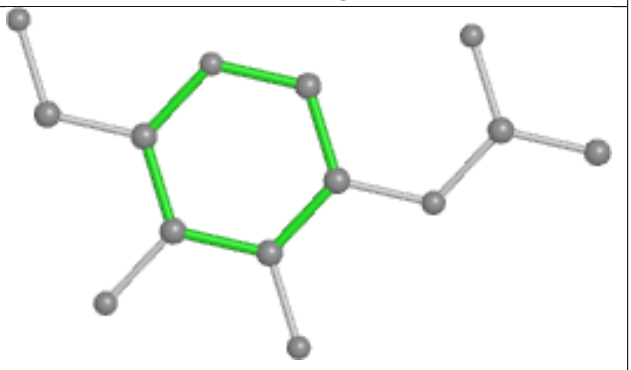


Torsions

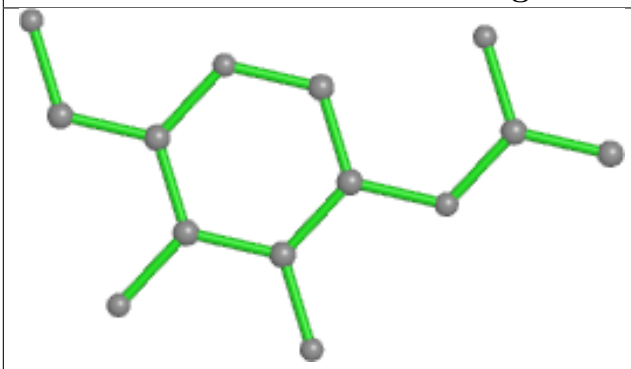


Rings

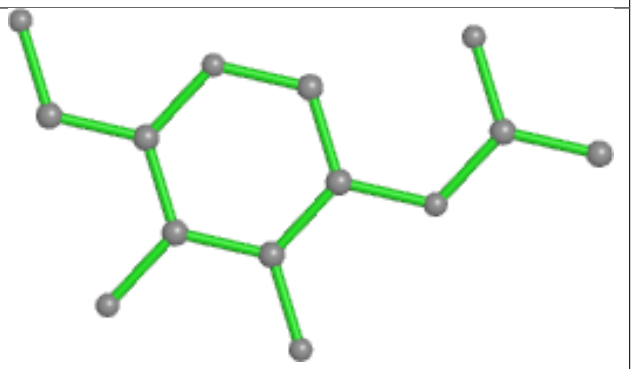
Ligand NAG A 1313	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG C 1304	
 Bond lengths	 Bond angles
 Torsions	 Rings

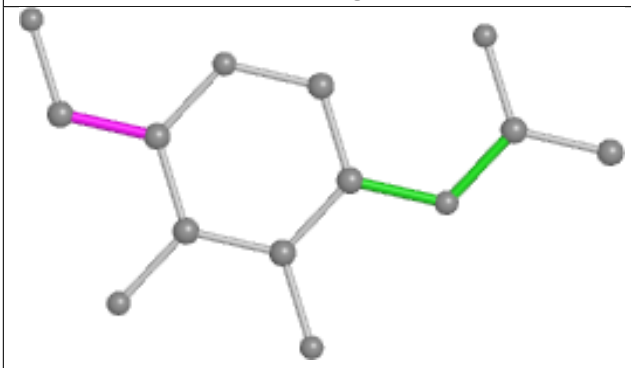
Ligand NAG B 1301



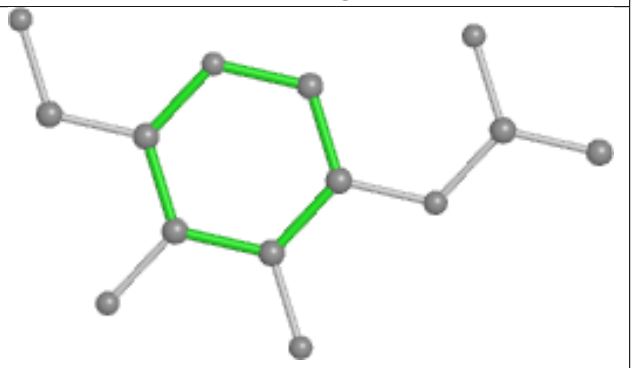
Bond lengths



Bond angles

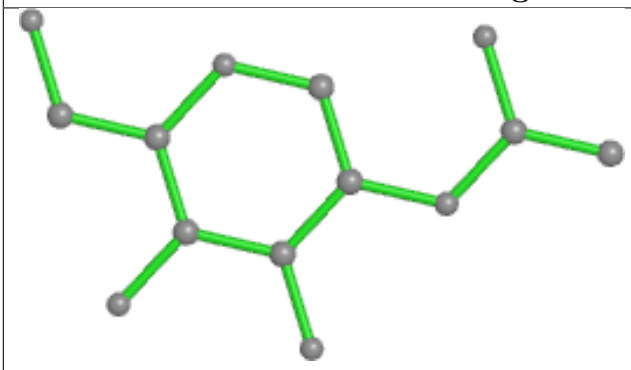


Torsions

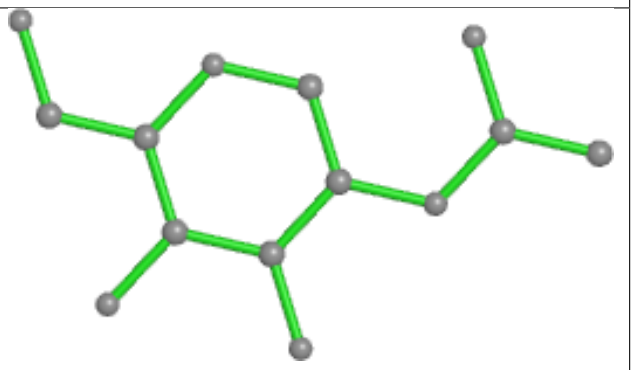


Rings

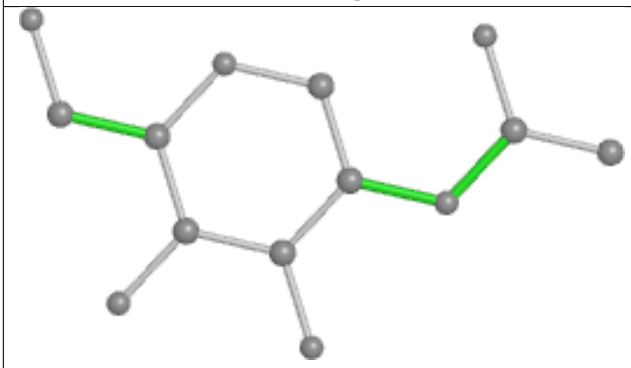
Ligand NAG B 1304



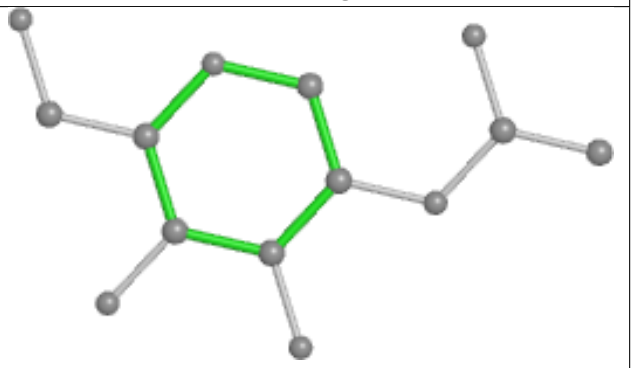
Bond lengths



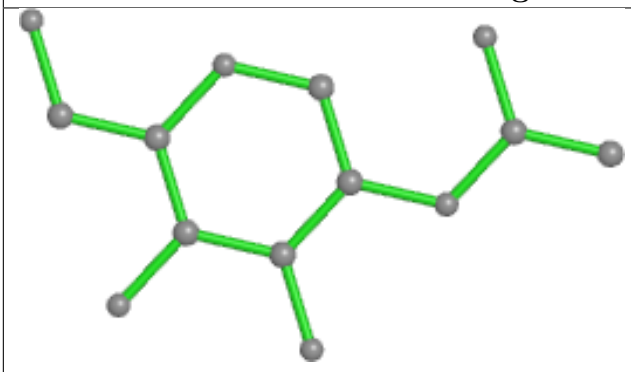
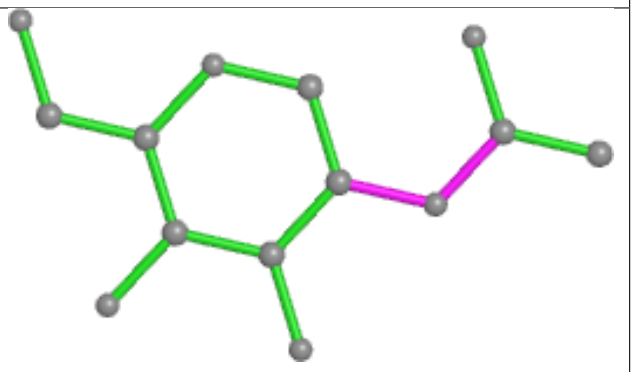
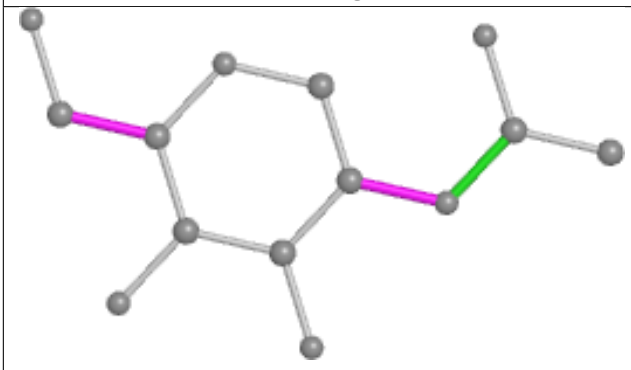
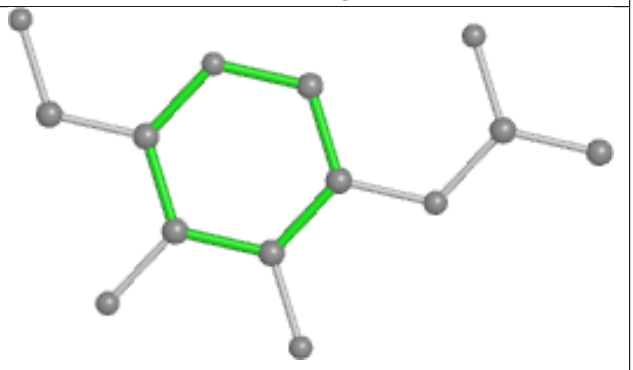
Bond angles

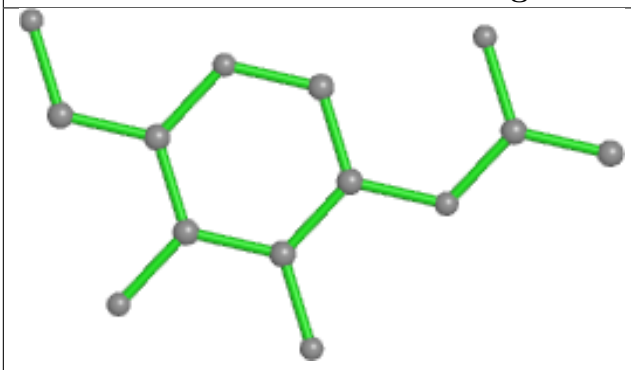
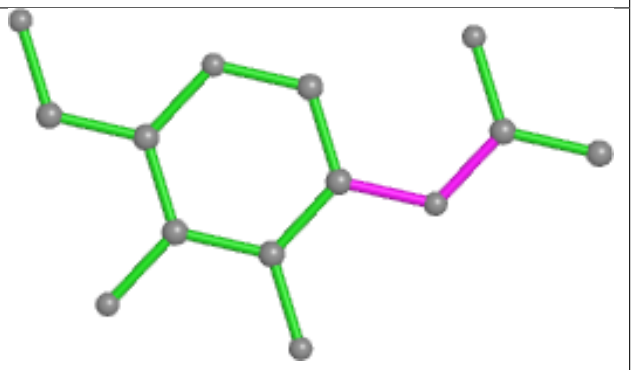
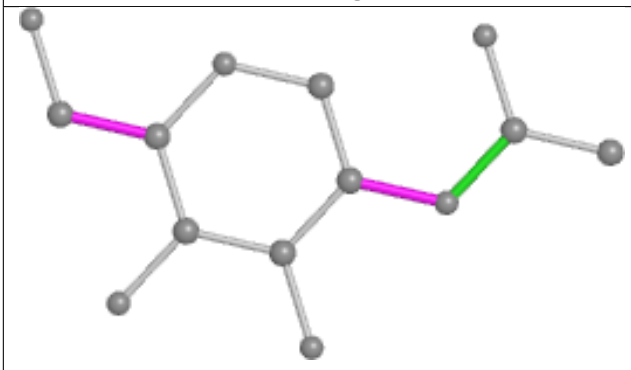
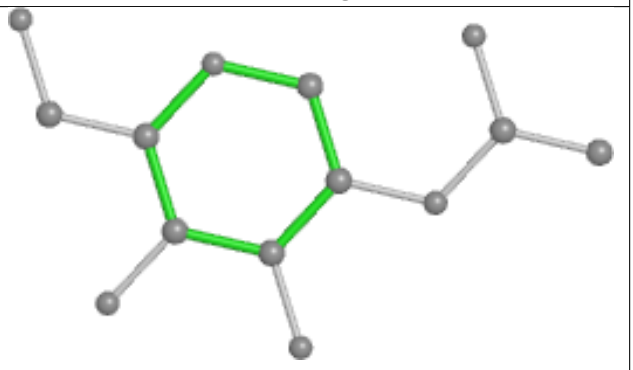


Torsions

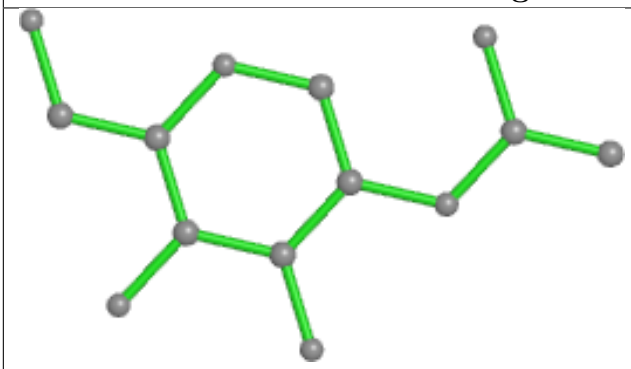


Rings

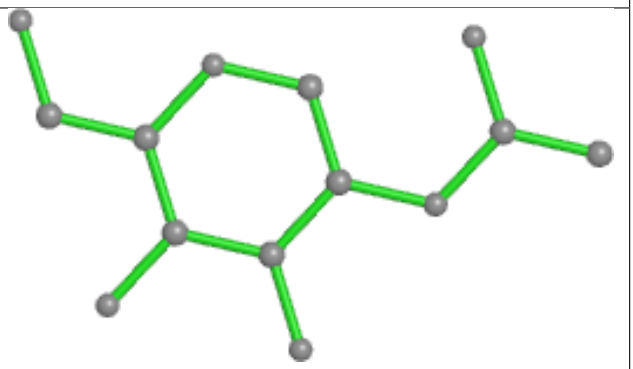
Ligand NAG B 1303	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG A 1303	
 Bond lengths	 Bond angles
 Torsions	 Rings

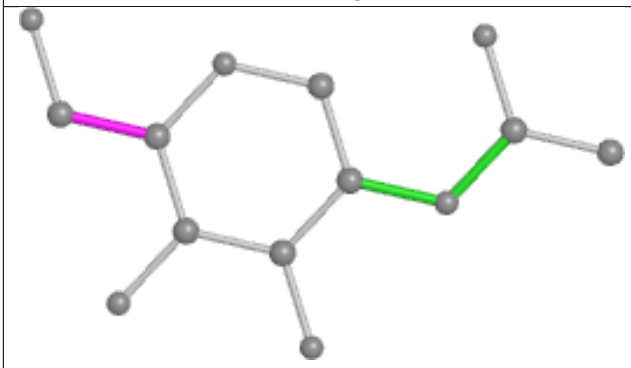
Ligand NAG B 1306



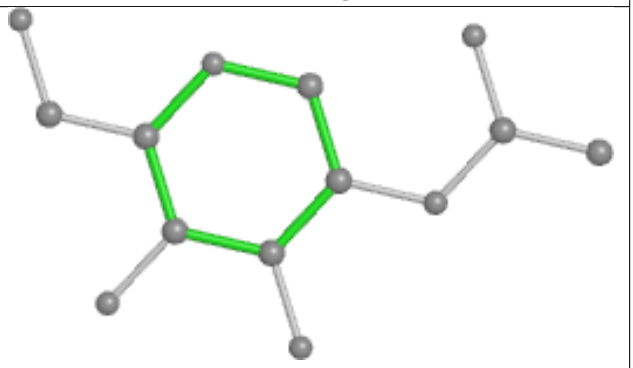
Bond lengths



Bond angles

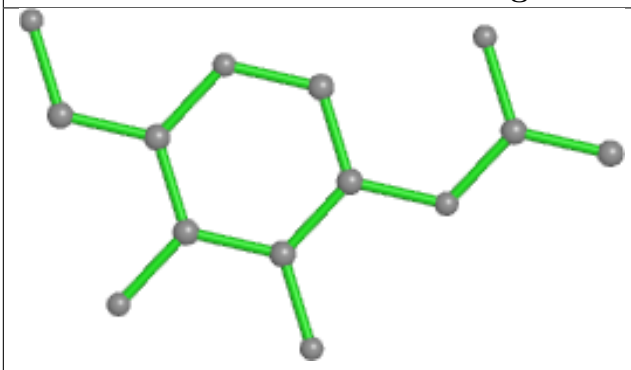


Torsions

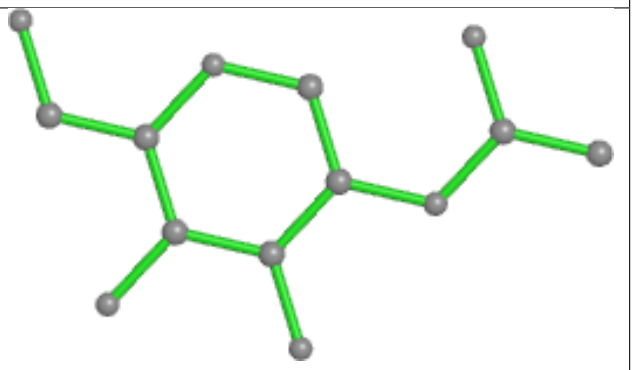


Rings

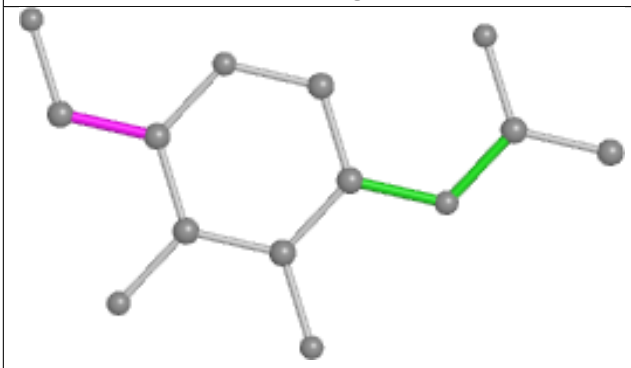
Ligand NAG A 1306



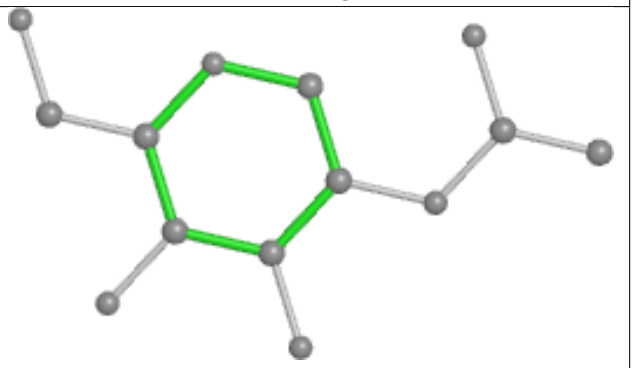
Bond lengths



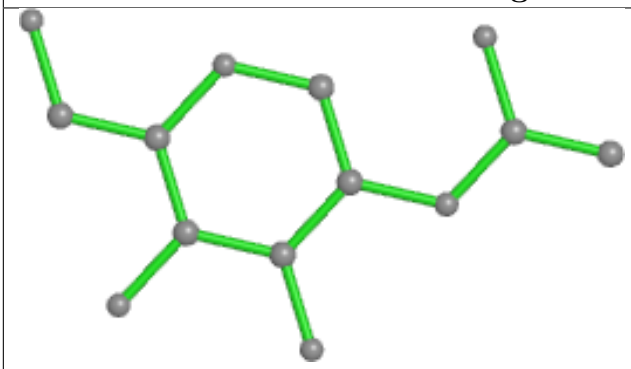
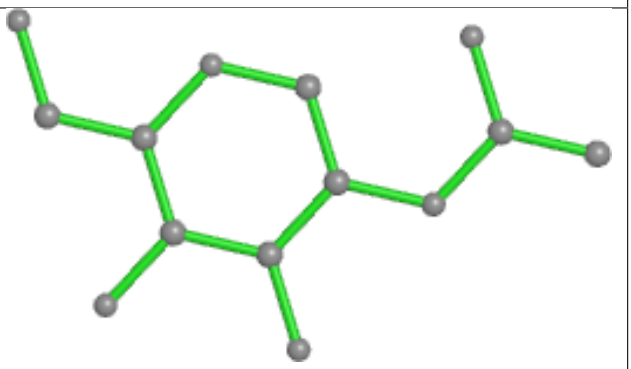
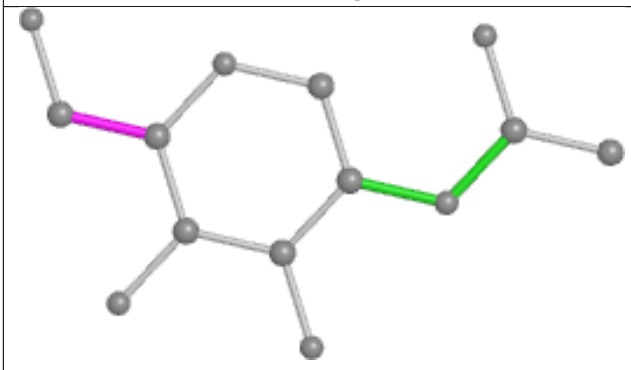
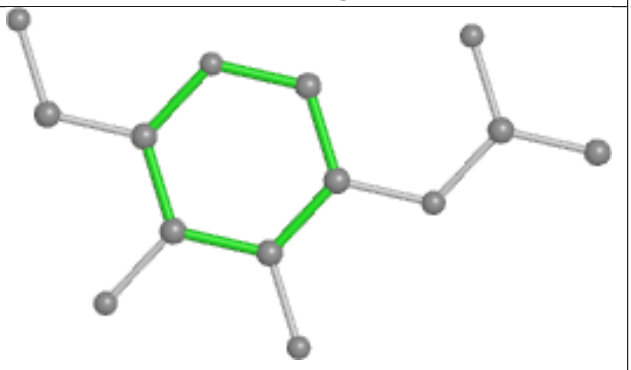
Bond angles

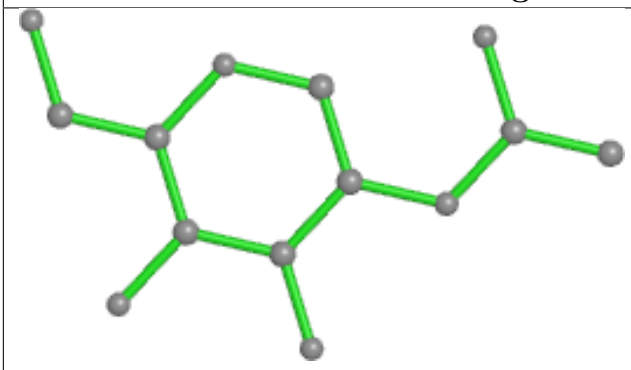
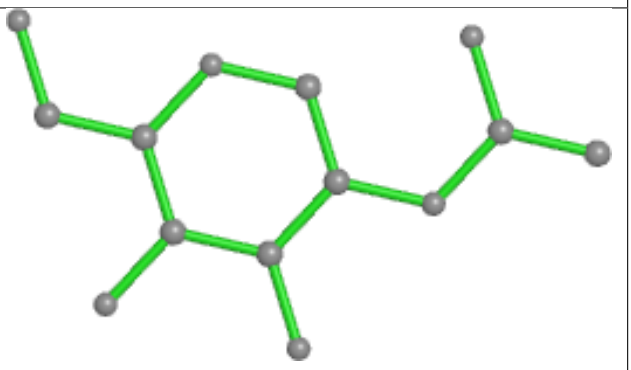
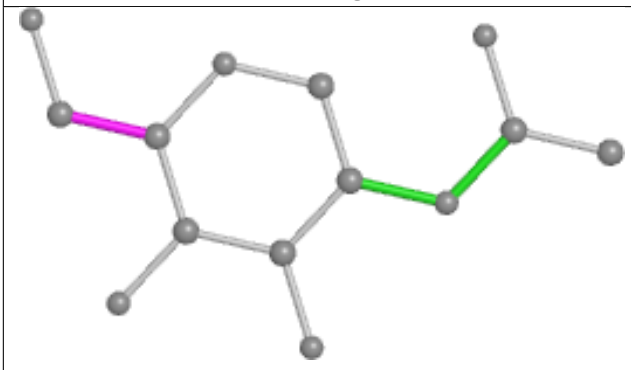
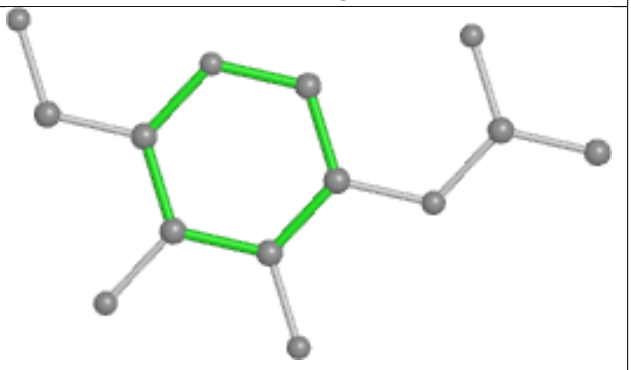


Torsions

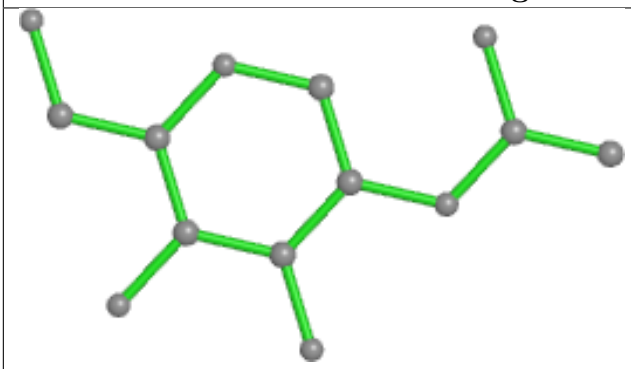


Rings

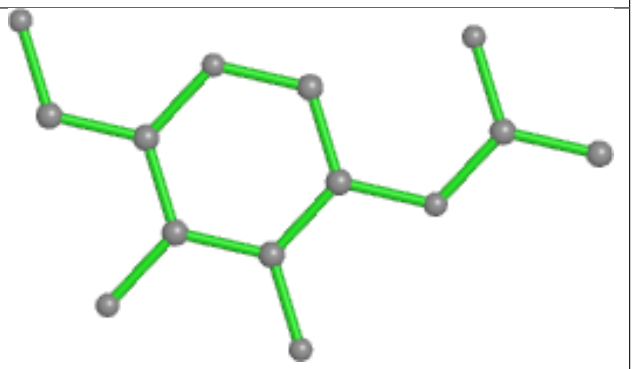
Ligand NAG A 1309	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG B 1305	
 Bond lengths	 Bond angles
 Torsions	 Rings

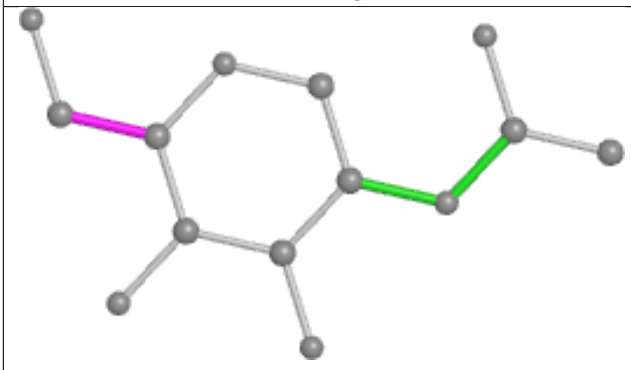
Ligand NAG C 1312



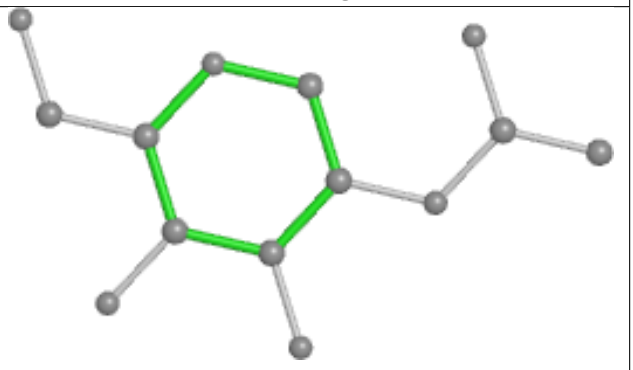
Bond lengths



Bond angles

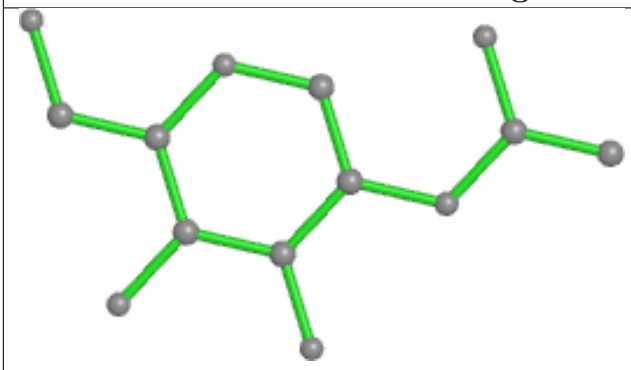


Torsions

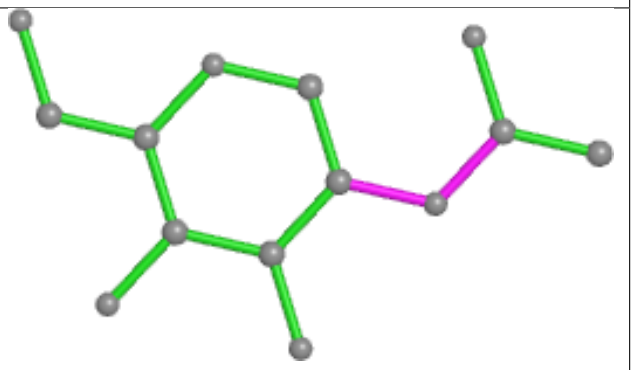


Rings

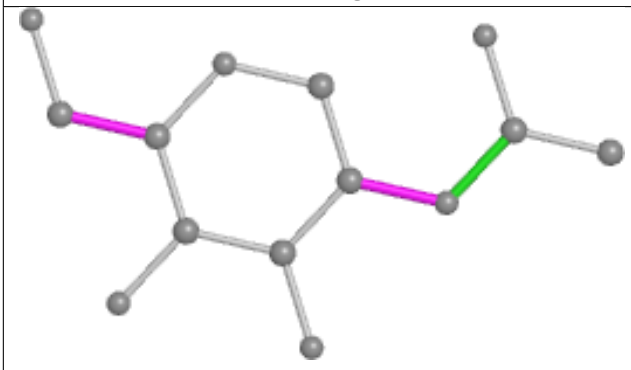
Ligand NAG C 1313



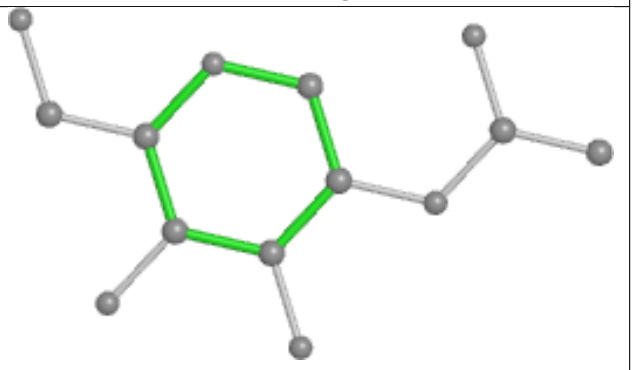
Bond lengths



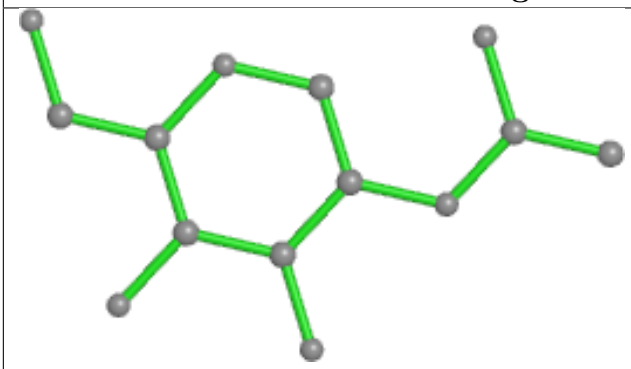
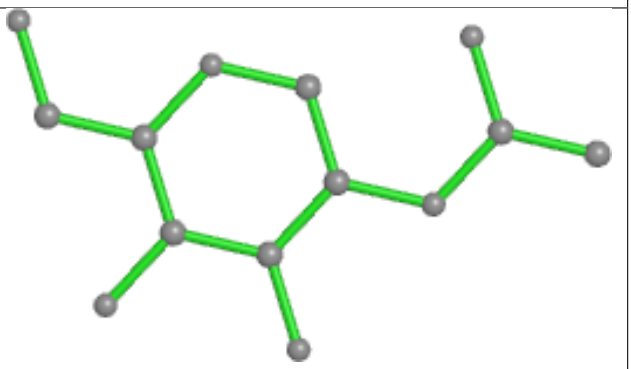
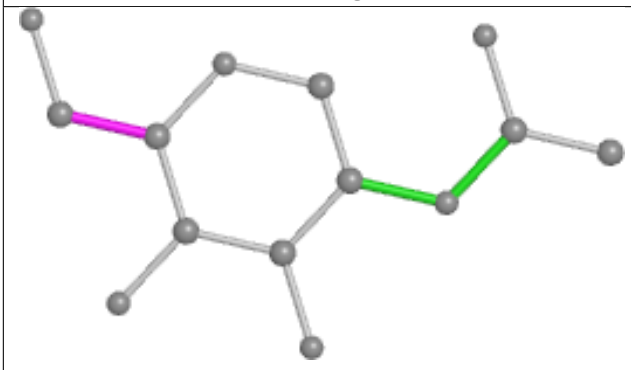
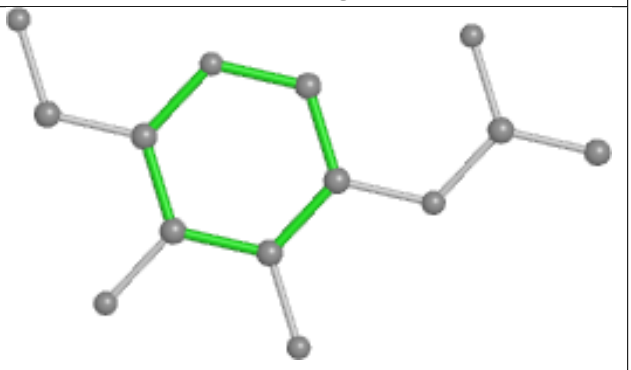
Bond angles

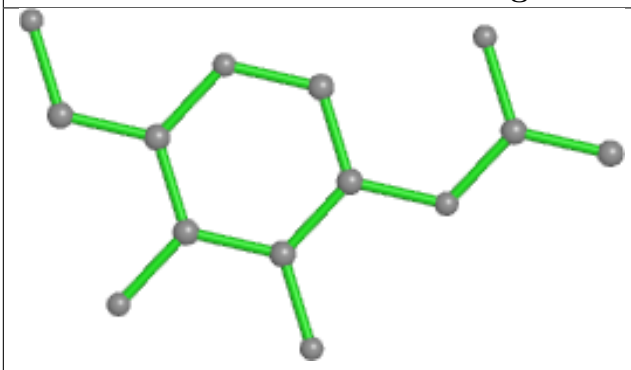
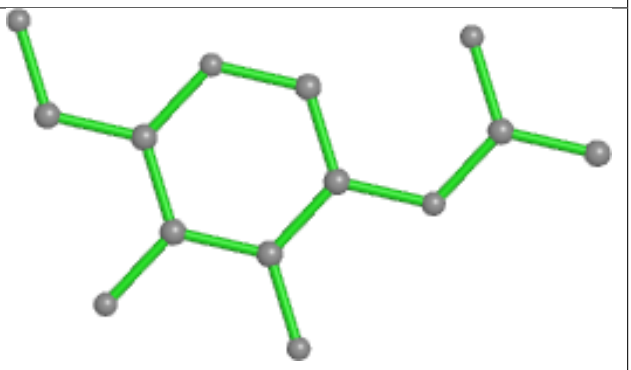
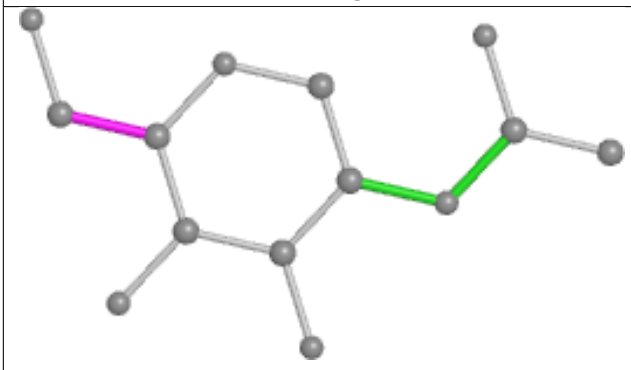
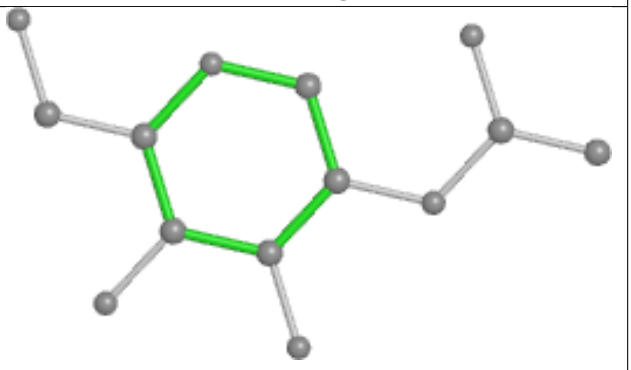


Torsions

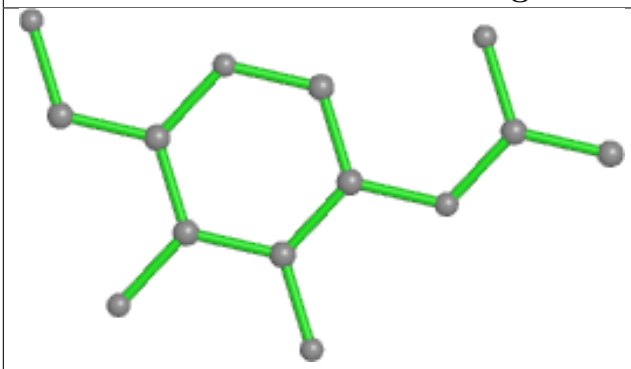


Rings

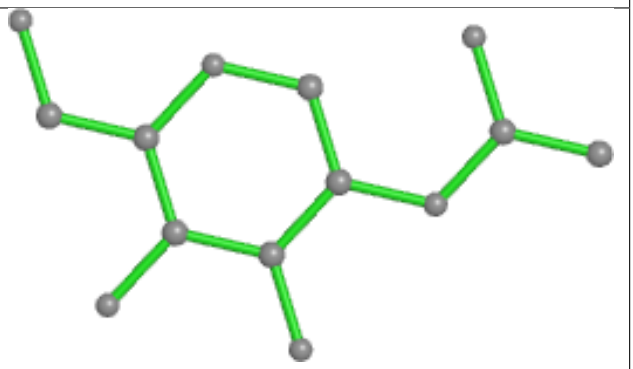
Ligand NAG B 1308	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG A 1312	
 Bond lengths	 Bond angles
 Torsions	 Rings

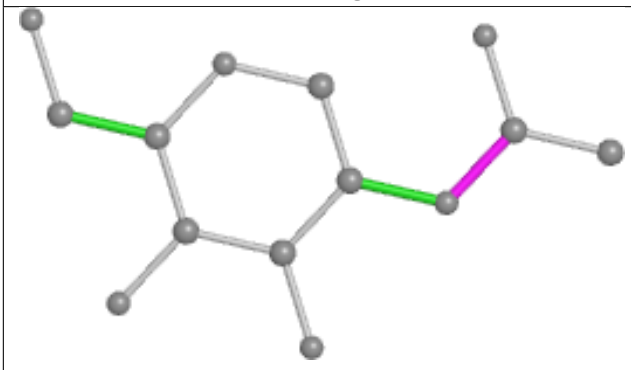
Ligand NAG C 1302



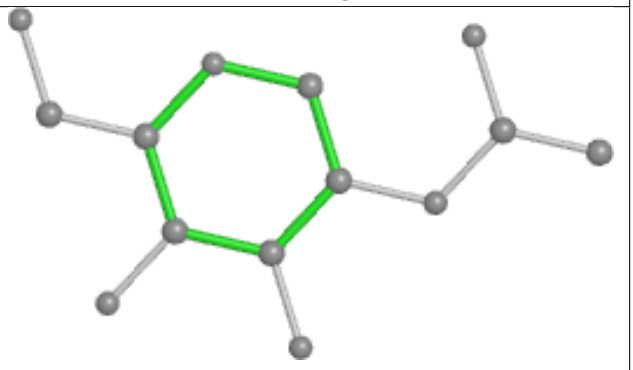
Bond lengths



Bond angles

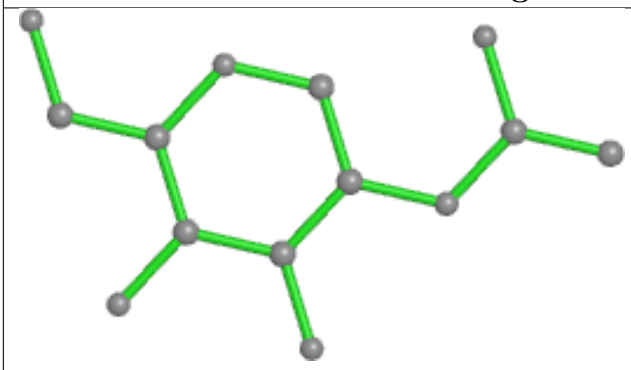


Torsions

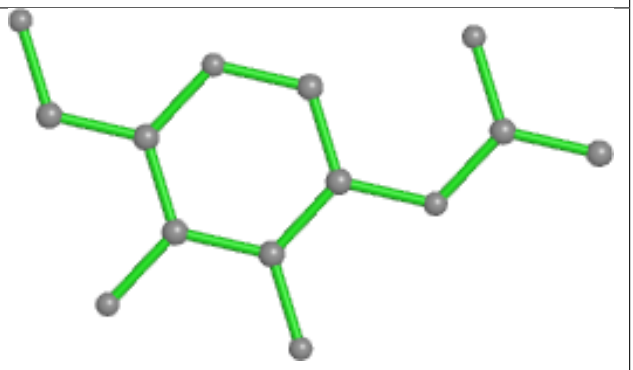


Rings

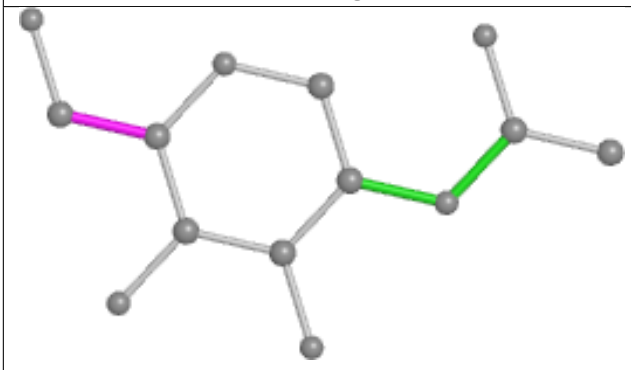
Ligand NAG C 1310



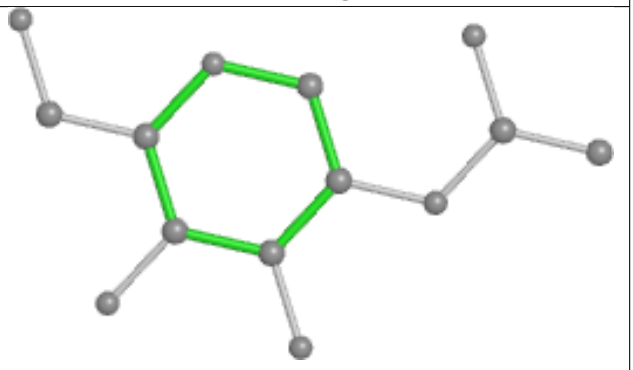
Bond lengths



Bond angles

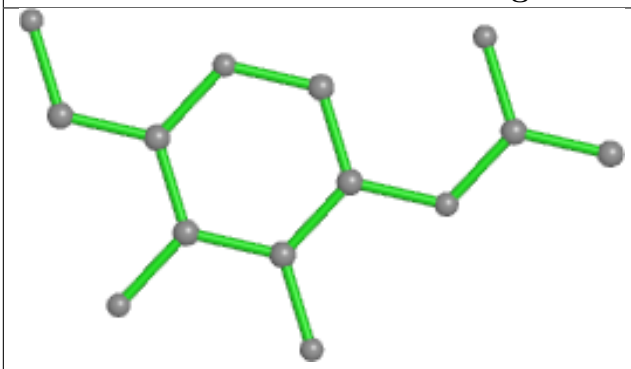


Torsions

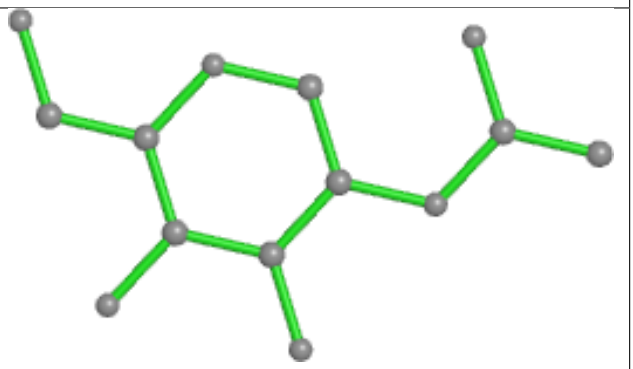


Rings

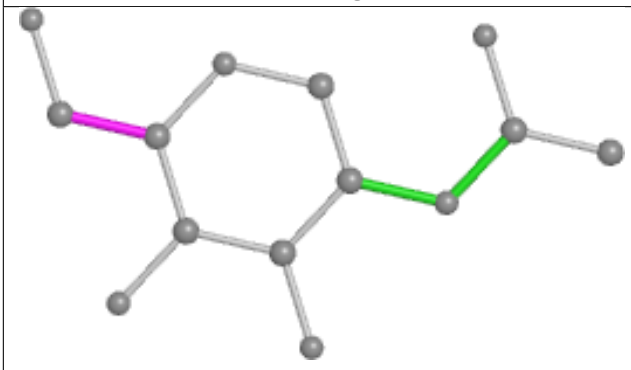
Ligand NAG C 1314



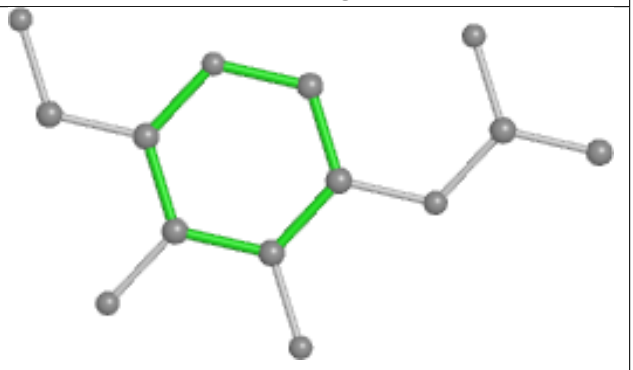
Bond lengths



Bond angles

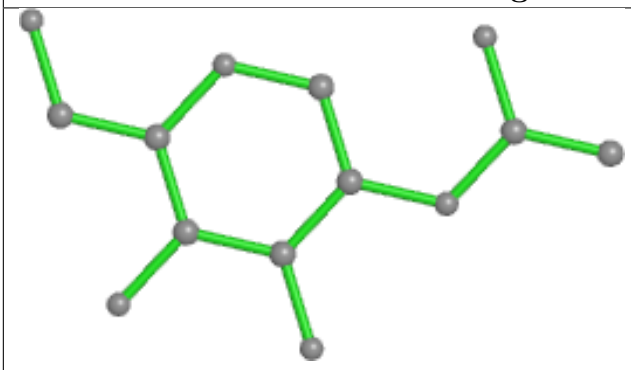


Torsions

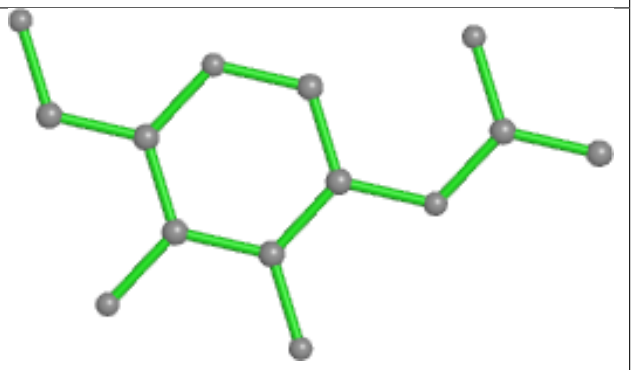


Rings

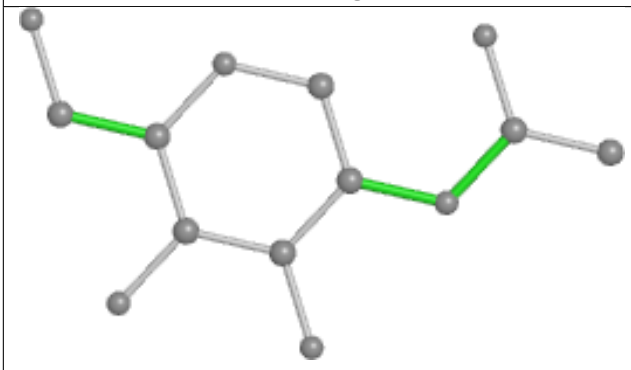
Ligand NAG A 1304



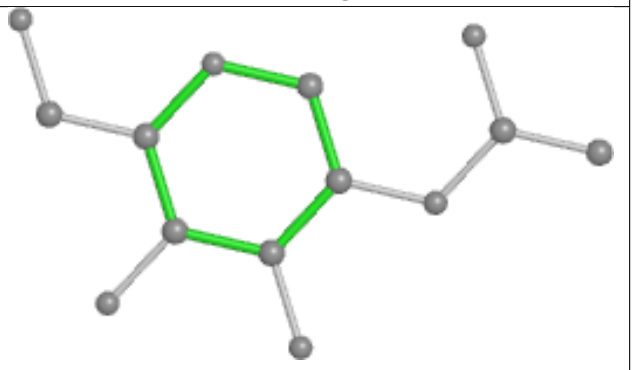
Bond lengths



Bond angles

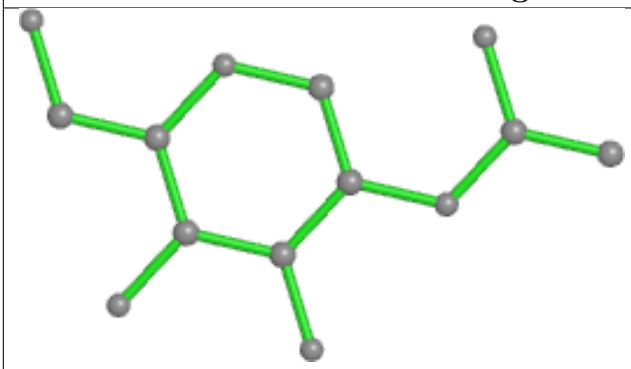


Torsions

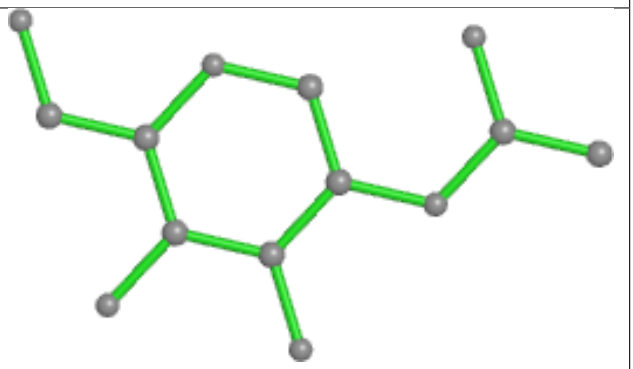


Rings

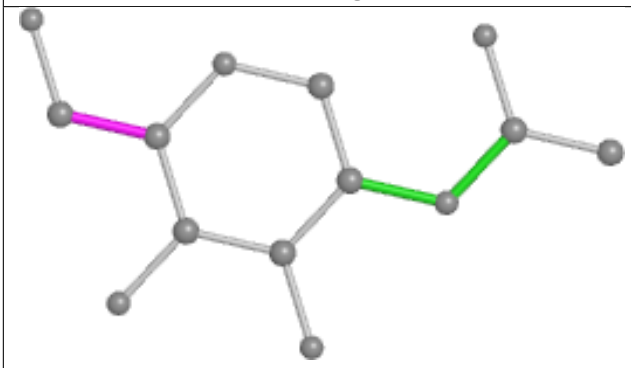
Ligand NAG C 1311



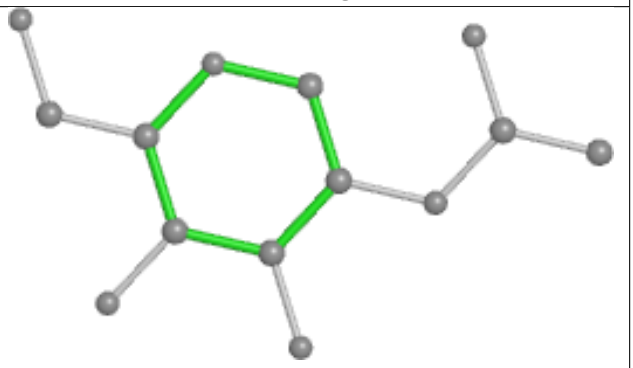
Bond lengths



Bond angles

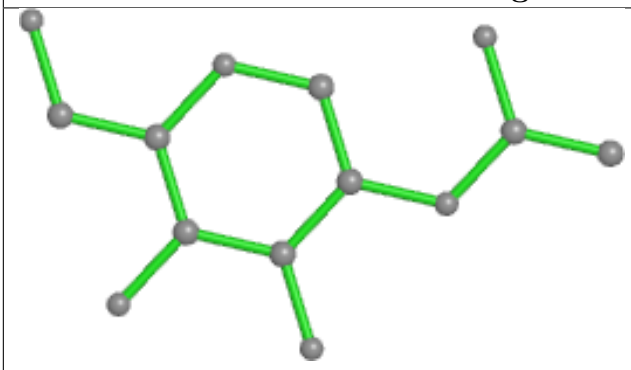


Torsions

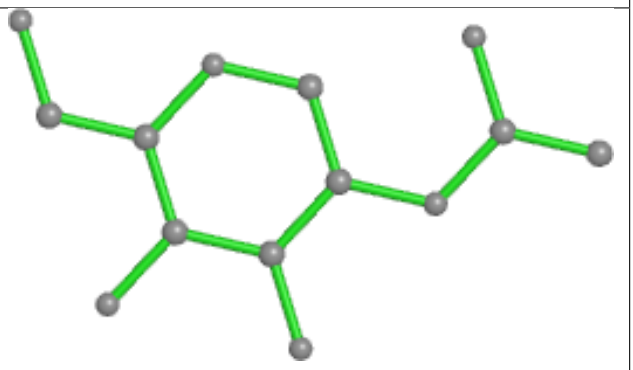


Rings

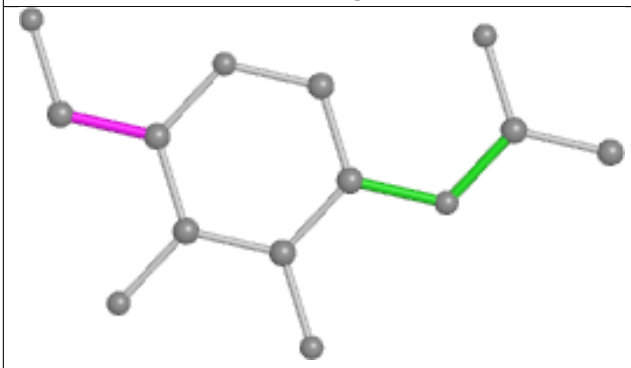
Ligand NAG C 1306



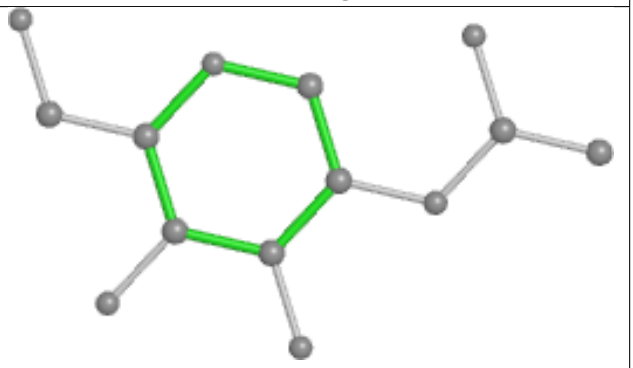
Bond lengths



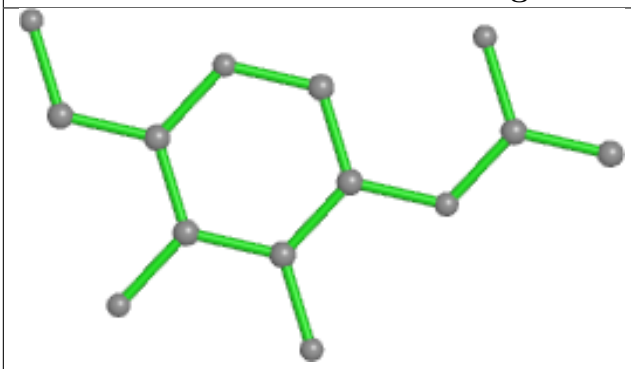
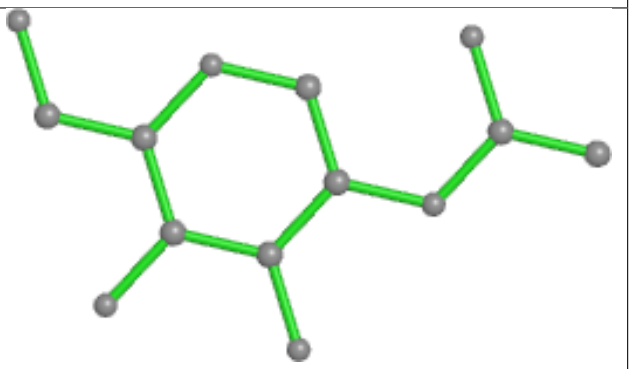
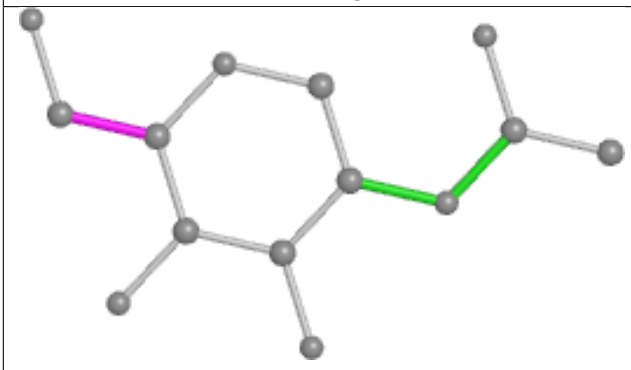
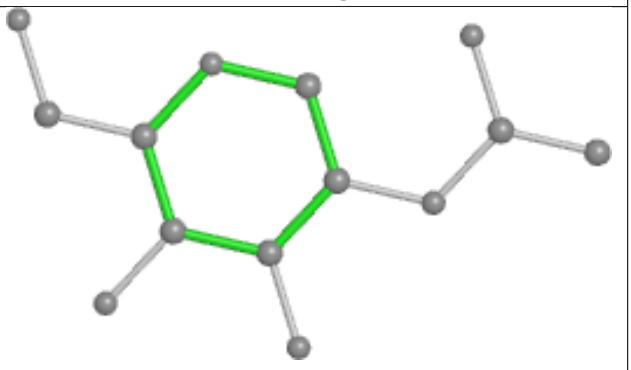
Bond angles

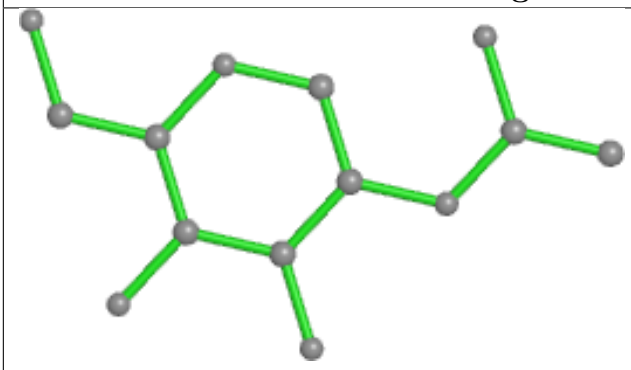
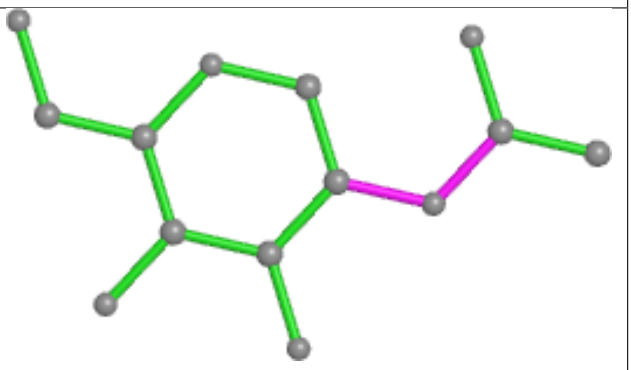
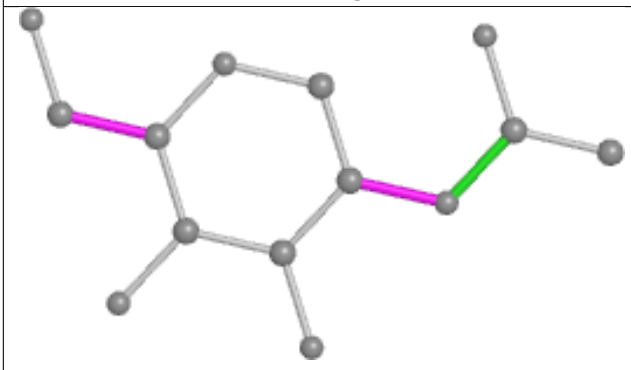
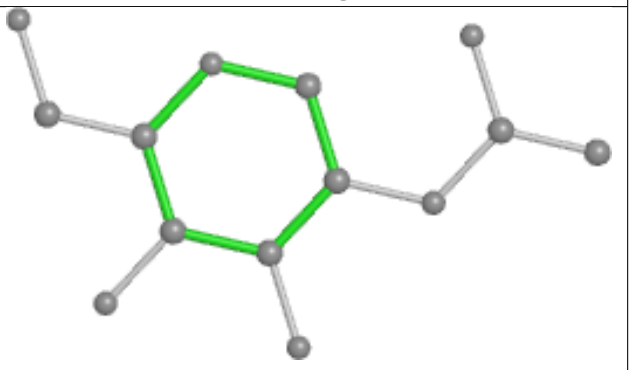


Torsions

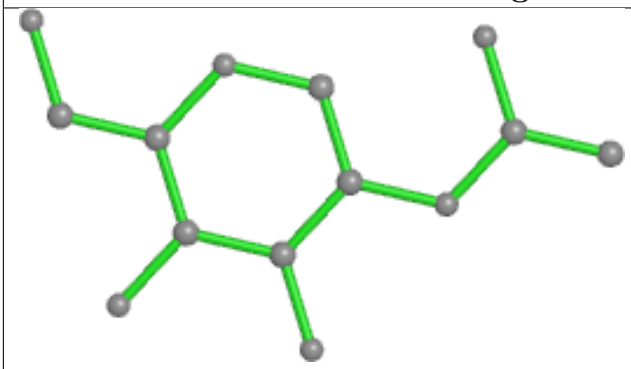


Rings

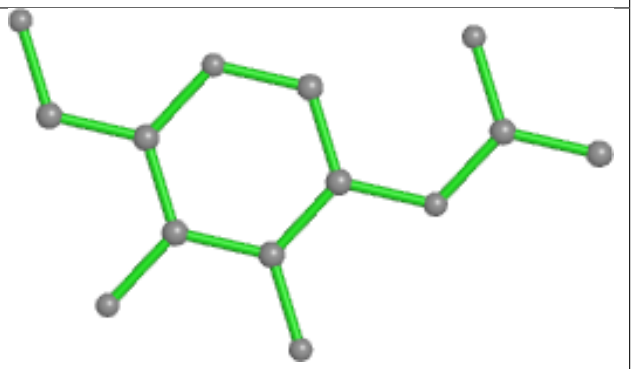
Ligand NAG A 1310	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG B 1312	
 Bond lengths	 Bond angles
 Torsions	 Rings

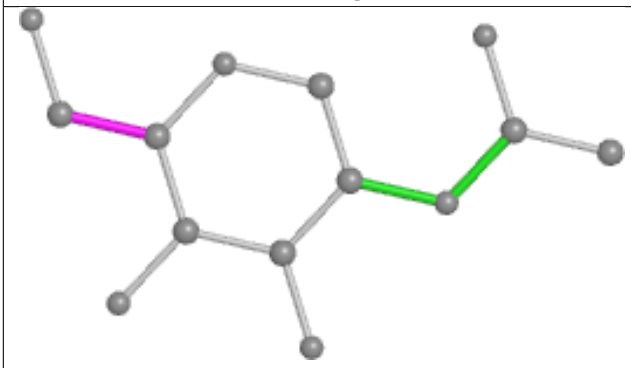
Ligand NAG C 1305



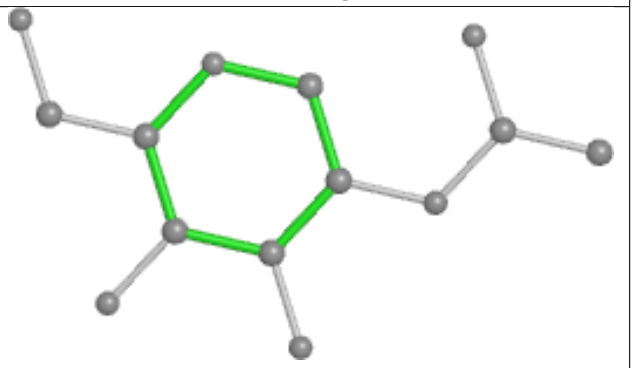
Bond lengths



Bond angles

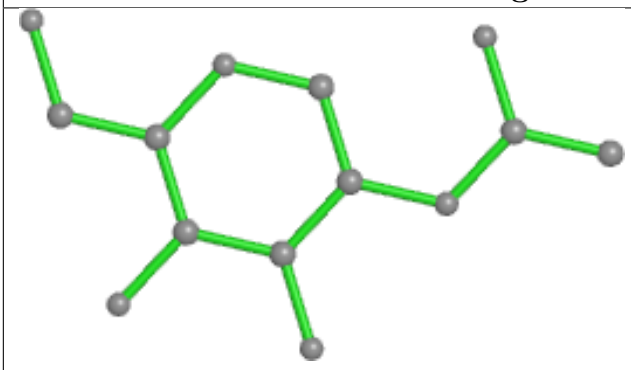


Torsions

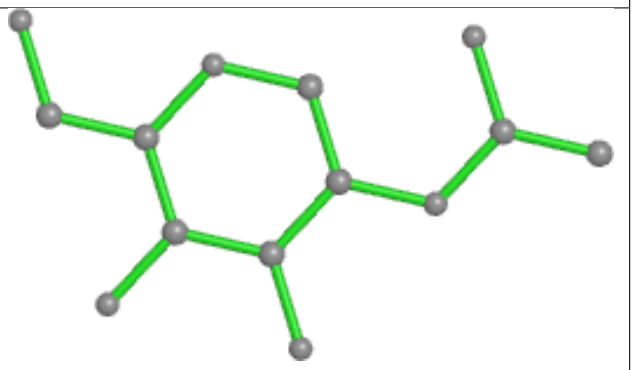


Rings

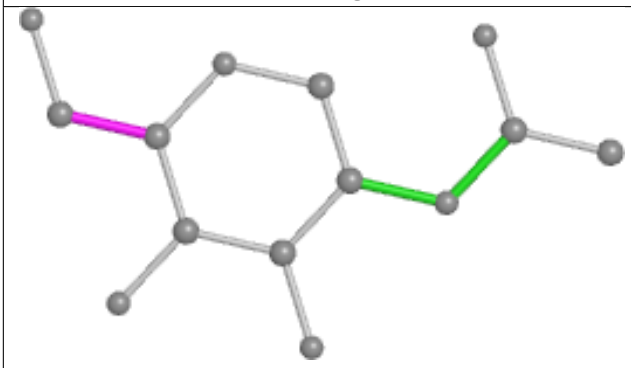
Ligand NAG C 1307



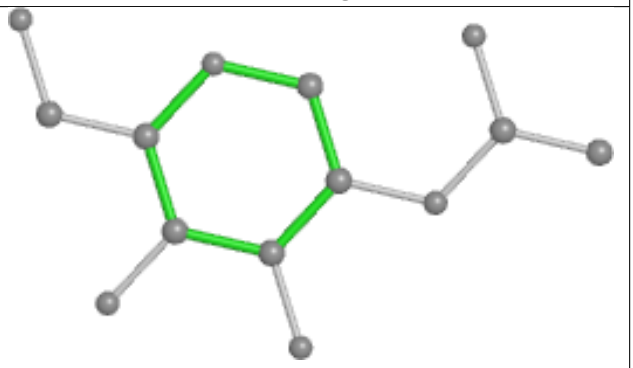
Bond lengths



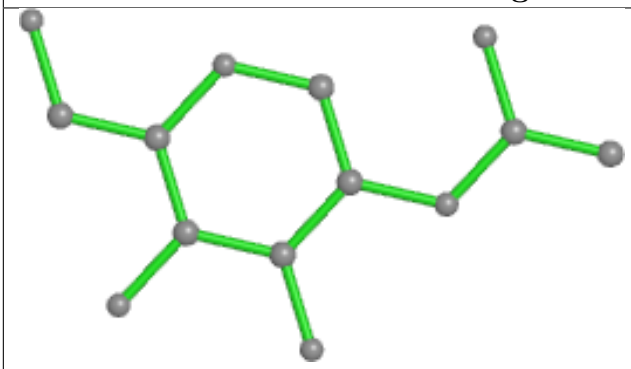
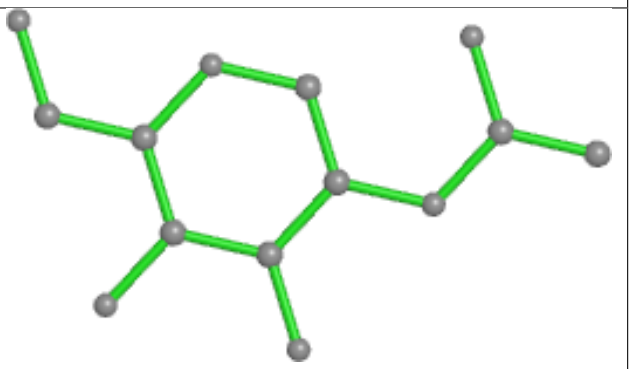
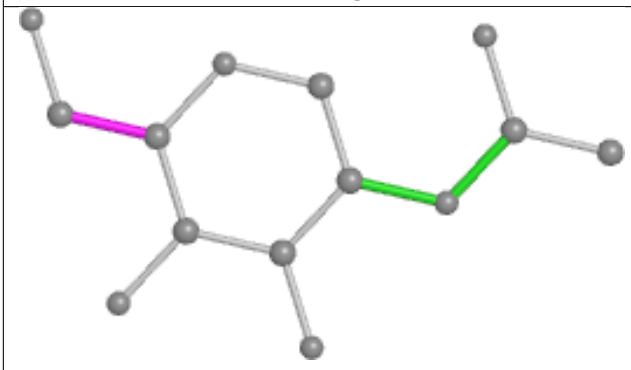
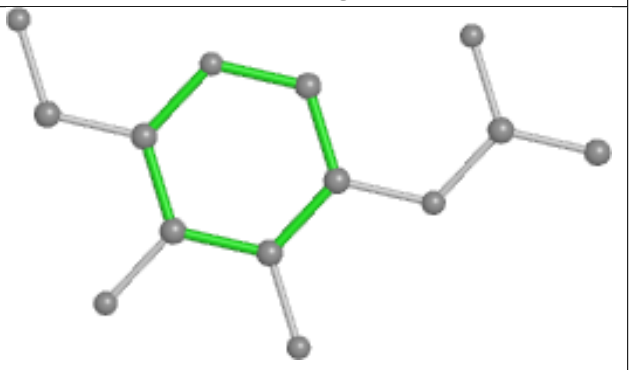
Bond angles

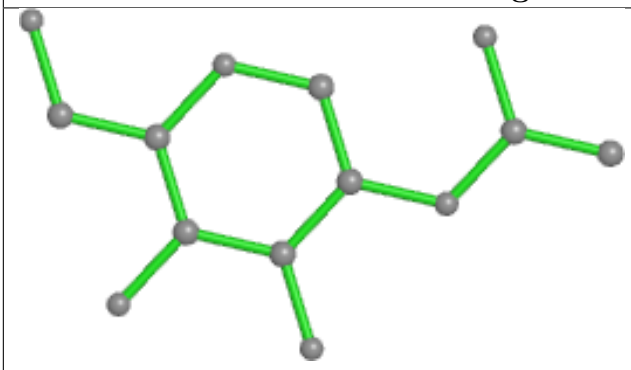
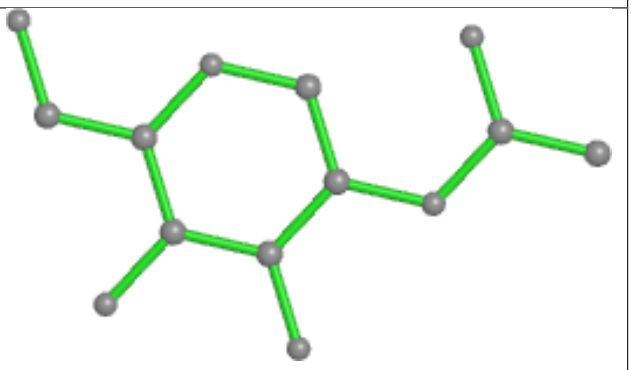
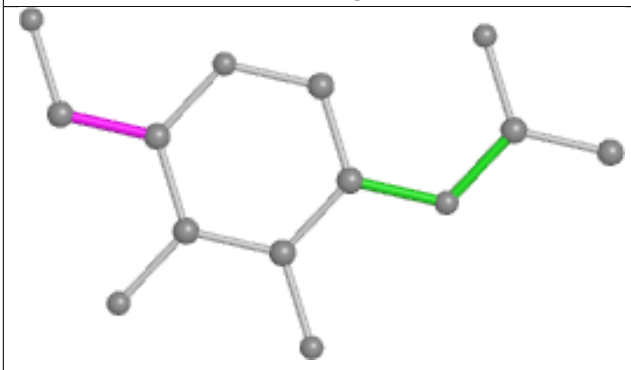
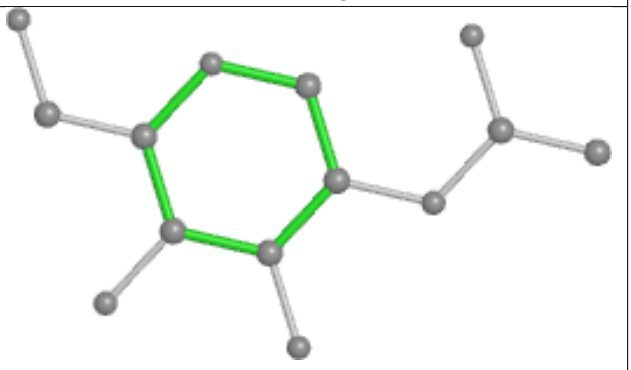


Torsions

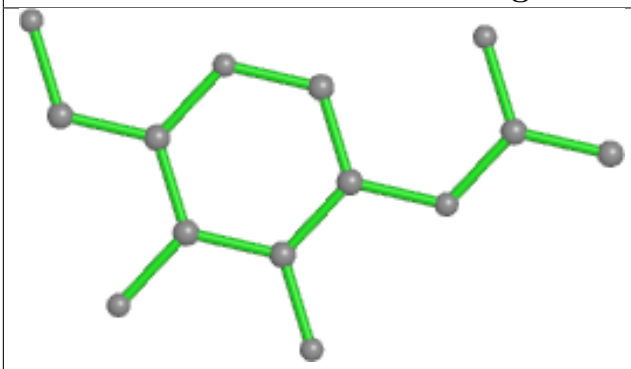


Rings

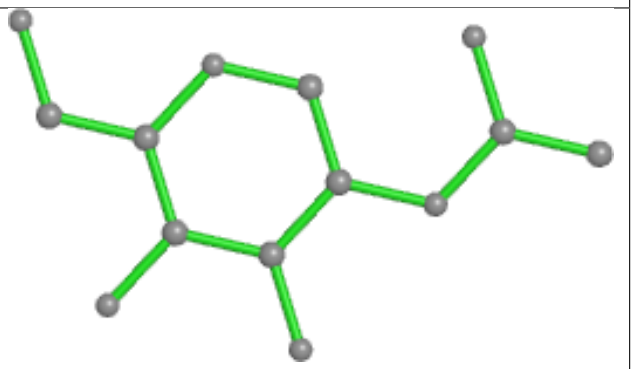
Ligand NAG C 1308	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG B 1307	
 Bond lengths	 Bond angles
 Torsions	 Rings

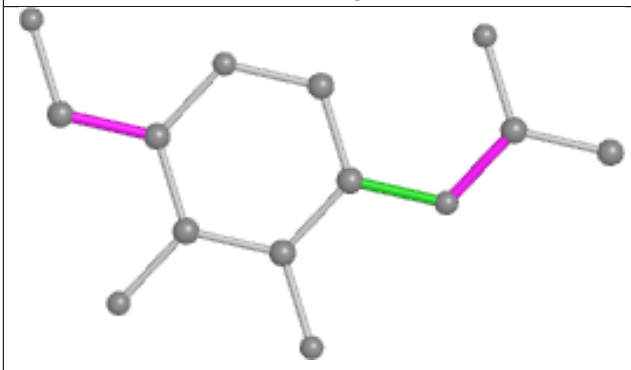
Ligand NAG B 1302



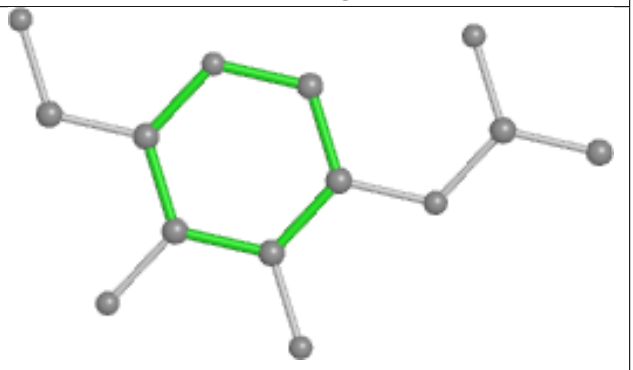
Bond lengths



Bond angles

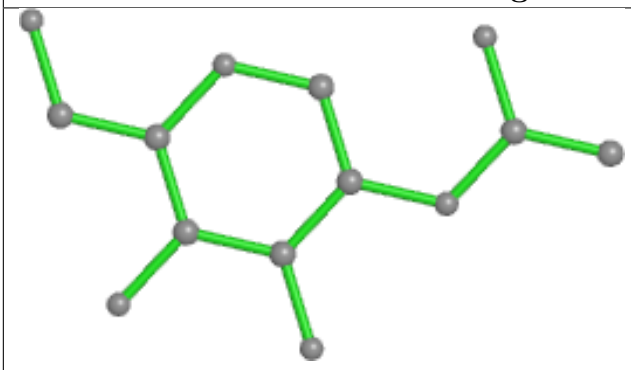


Torsions

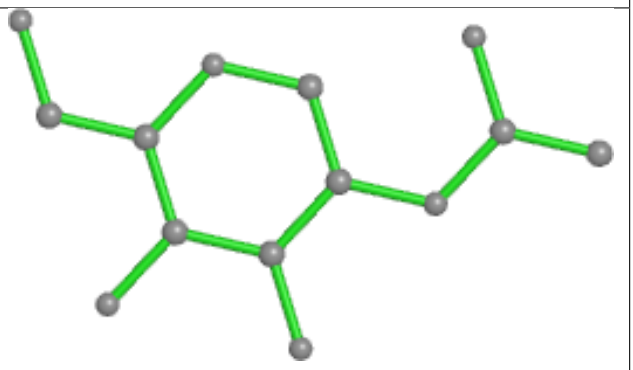


Rings

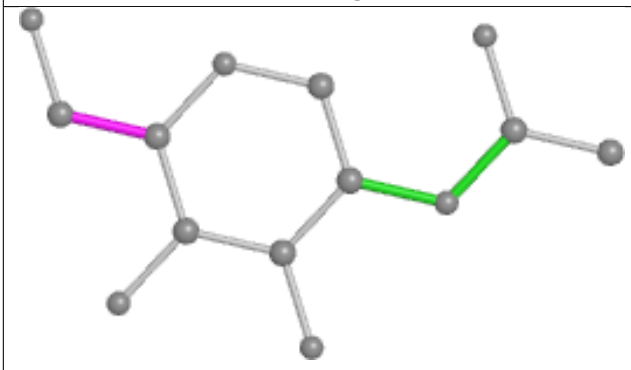
Ligand NAG A 1301



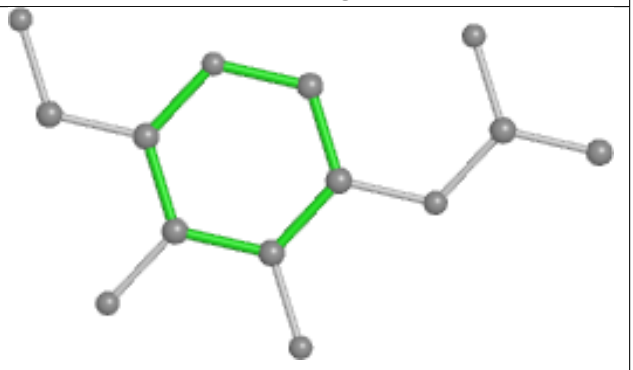
Bond lengths



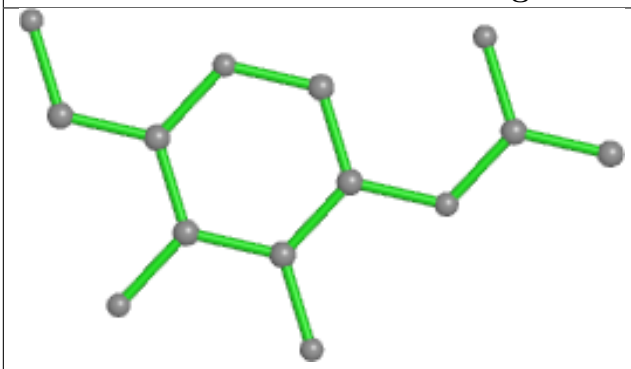
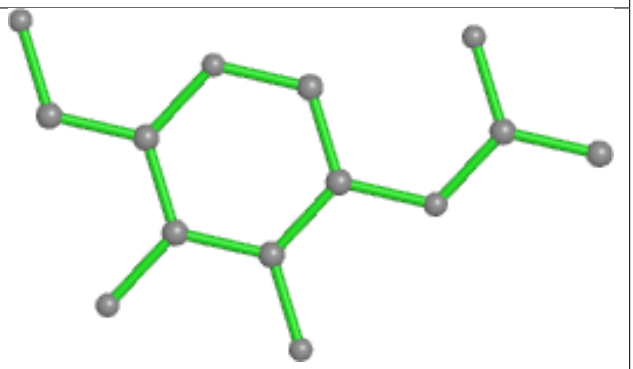
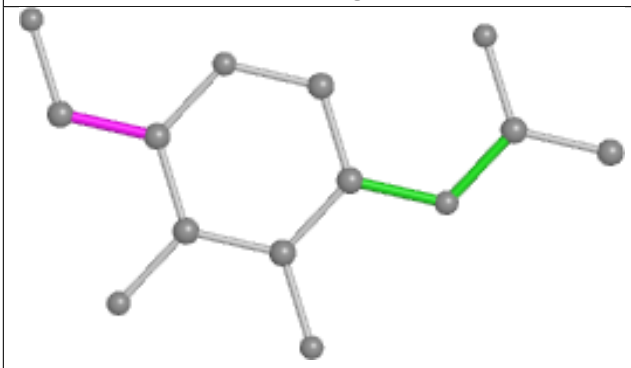
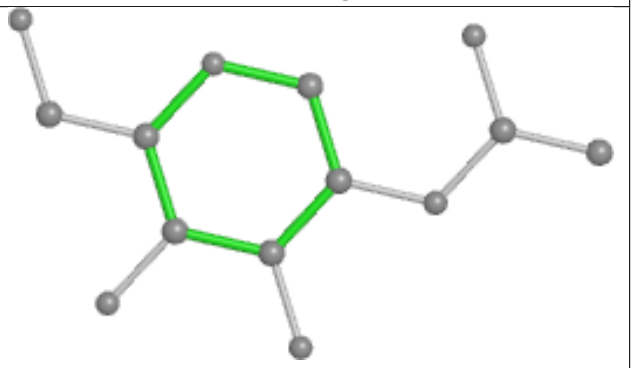
Bond angles

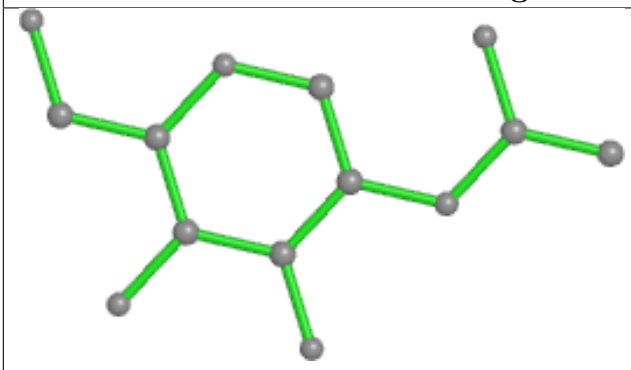
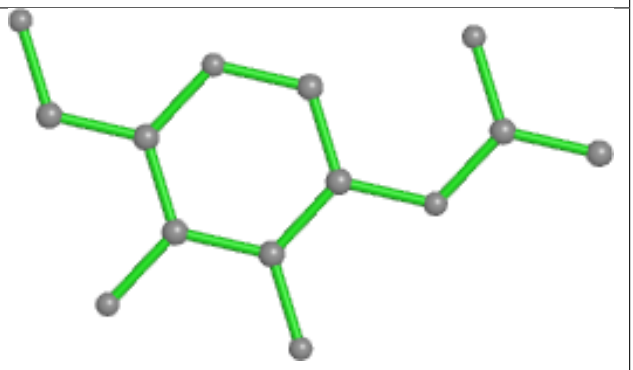
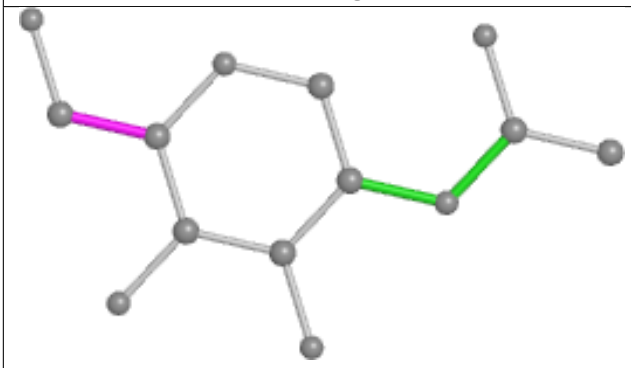
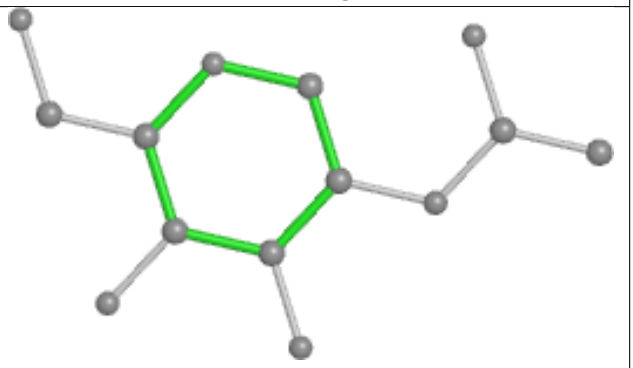


Torsions

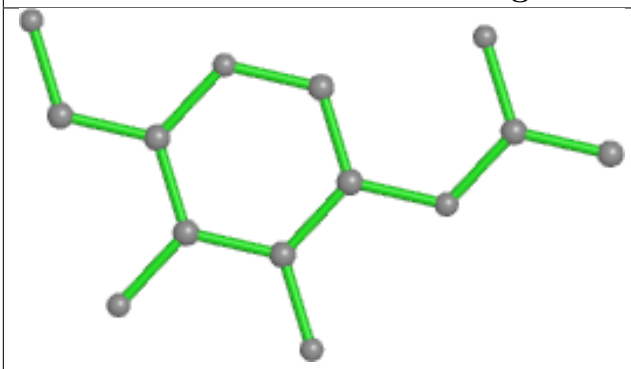


Rings

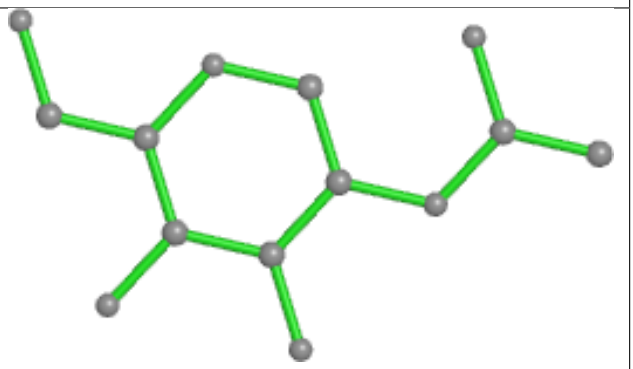
Ligand NAG B 1311	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand NAG A 1311	
	
Bond lengths	Bond angles
	
Torsions	Rings

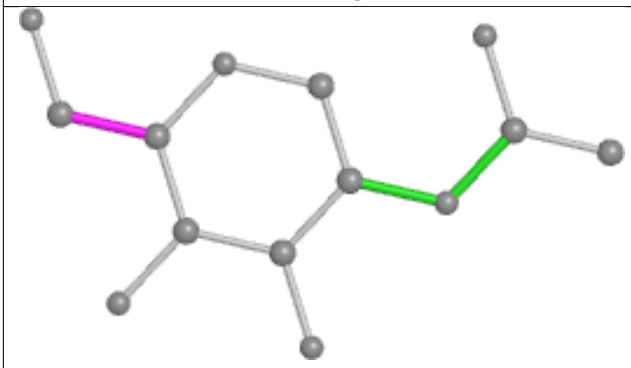
Ligand NAG C 1309



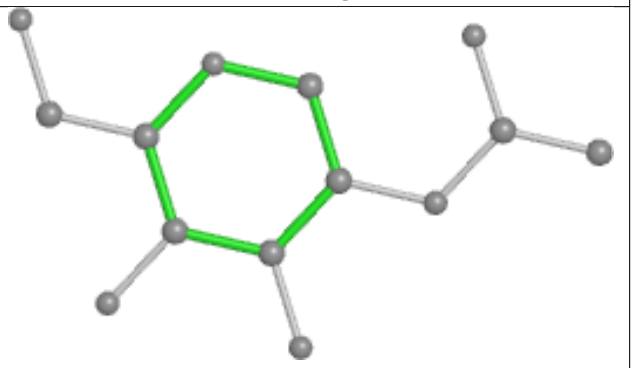
Bond lengths



Bond angles

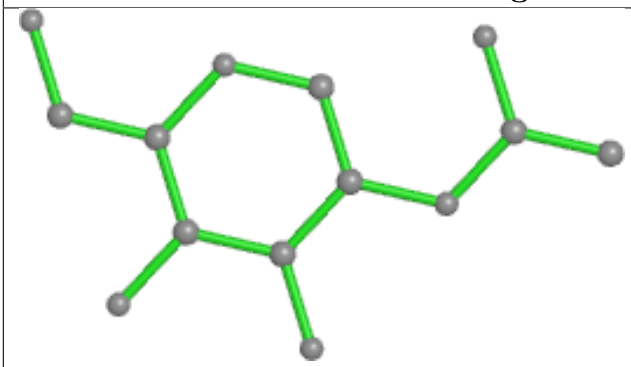


Torsions

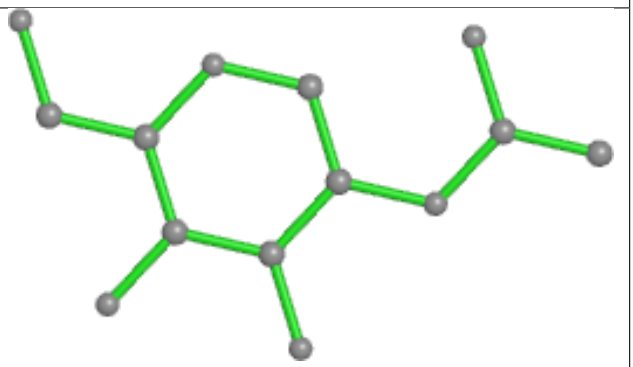


Rings

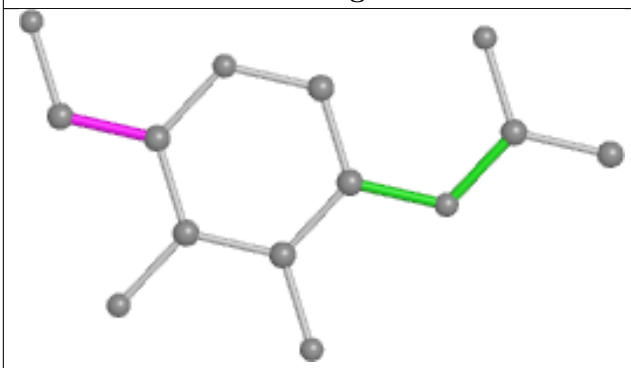
Ligand NAG A 1307



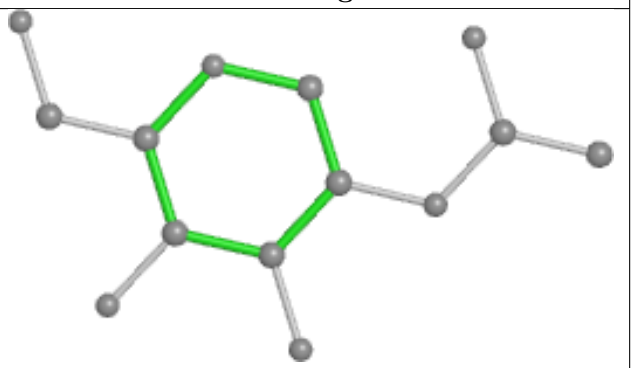
Bond lengths



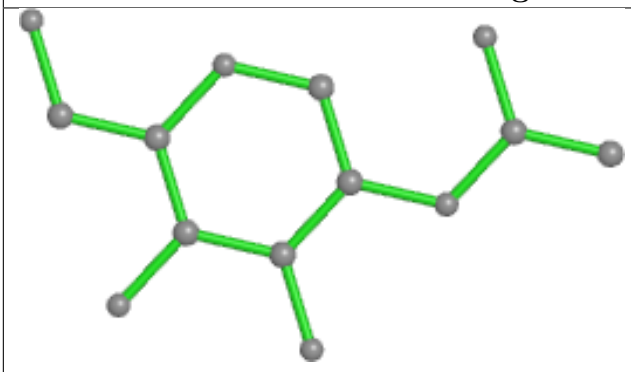
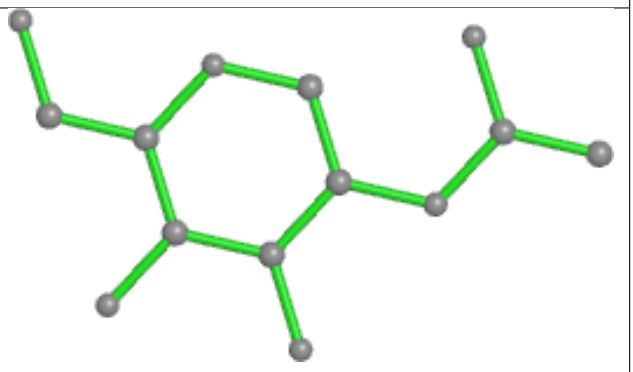
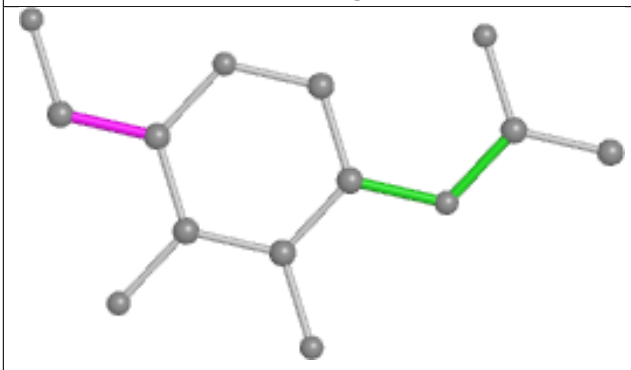
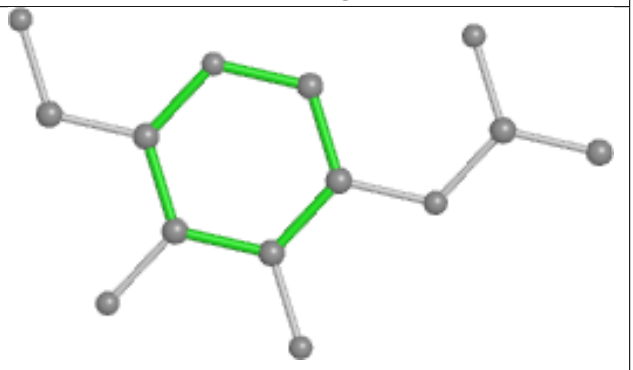
Bond angles



Torsions



Rings

Ligand NAG B 1310	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.