Full wwPDB EM Validation Report

Nov 13, 2024 – 10:57 AM JST

PDB ID	:	8Y1F
EMDB ID	:	EMD-38834
Title	:	The closed conformation of the HKU1-B S protein in the apo state
Authors	:	Xia, L.Y.; Zhang, Y.Y.; Zhou, Q.
Deposited on	:	2024-01-24
Resolution	:	2.80 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:

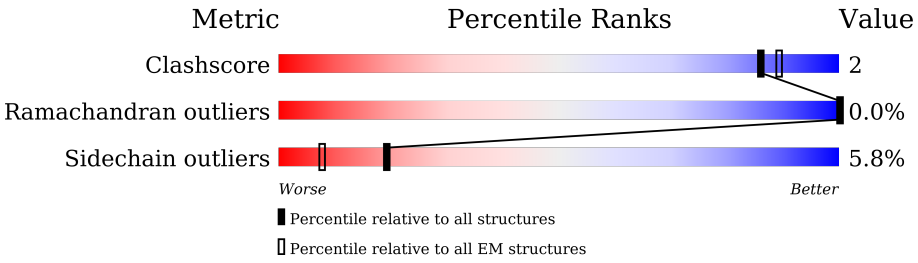
EMDB validation analysis	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance

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

The reported resolution of this entry is 2.80 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	1290	83% 10% • 6%
1	B	1290	84% 9% • 6%
1	C	1290	84% 9% • 6%
2	D	6	33% 67%
2	I	6	33% 67%
2	N	6	33% 67%
3	E	2	100%
3	F	2	50% 50%
3	G	2	100%

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

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 29541 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

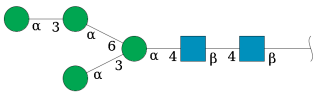
- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1208	Total	C	N	O	S	0	0
			9425	6003	1551	1814	57		
1	B	1208	Total	C	N	O	S	0	0
			9425	6003	1551	1814	57		
1	C	1208	Total	C	N	O	S	0	0
			9425	6003	1551	1814	57		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	752	GLY	ARG	conflict	UNP Q14EB0
A	753	SER	ARG	conflict	UNP Q14EB0
A	754	ALA	LYS	conflict	UNP Q14EB0
A	755	SER	ARG	conflict	UNP Q14EB0
A	1067	PRO	ASN	conflict	UNP Q14EB0
A	1068	PRO	LEU	conflict	UNP Q14EB0
B	752	GLY	ARG	conflict	UNP Q14EB0
B	753	SER	ARG	conflict	UNP Q14EB0
B	754	ALA	LYS	conflict	UNP Q14EB0
B	755	SER	ARG	conflict	UNP Q14EB0
B	1067	PRO	ASN	conflict	UNP Q14EB0
B	1068	PRO	LEU	conflict	UNP Q14EB0
C	752	GLY	ARG	conflict	UNP Q14EB0
C	753	SER	ARG	conflict	UNP Q14EB0
C	754	ALA	LYS	conflict	UNP Q14EB0
C	755	SER	ARG	conflict	UNP Q14EB0
C	1067	PRO	ASN	conflict	UNP Q14EB0
C	1068	PRO	LEU	conflict	UNP Q14EB0

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

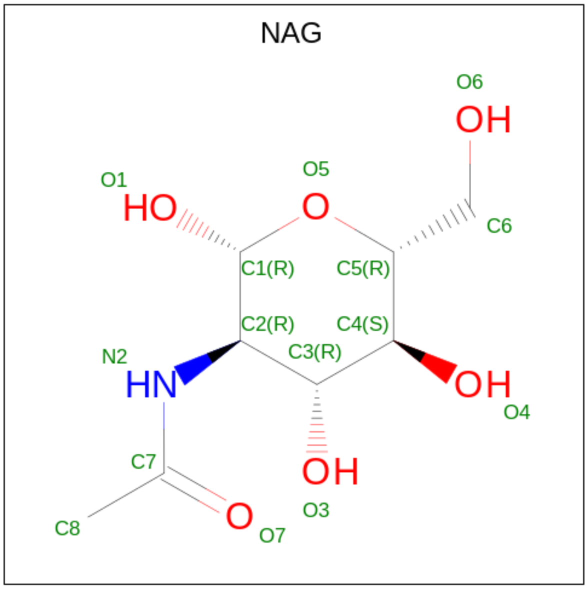


Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	6	Total	C	N	O	0	0
			72	40	2	30		
2	I	6	Total	C	N	O	0	0
			72	40	2	30		
2	N	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 3 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
3	E	2	Total	C	N	O	0	0
			28	16	2	10		
3	F	2	Total	C	N	O	0	0
			28	16	2	10		
3	G	2	Total	C	N	O	0	0
			28	16	2	10		
3	H	2	Total	C	N	O	0	0
			28	16	2	10		
3	J	2	Total	C	N	O	0	0
			28	16	2	10		
3	K	2	Total	C	N	O	0	0
			28	16	2	10		
3	L	2	Total	C	N	O	0	0
			28	16	2	10		
3	M	2	Total	C	N	O	0	0
			28	16	2	10		
3	O	2	Total	C	N	O	0	0
			28	16	2	10		
3	P	2	Total	C	N	O	0	0
			28	16	2	10		
3	Q	2	Total	C	N	O	0	0
			28	16	2	10		
3	R	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



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

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

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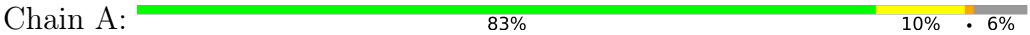
Mol	Chain	Residues	Atoms				AltConf
4	B	1	Total 14	C 8	N 1	O 5	0
4	C	1	Total 14	C 8	N 1	O 5	0
4	C	1	Total 14	C 8	N 1	O 5	0
4	C	1	Total 14	C 8	N 1	O 5	0
4	C	1	Total 14	C 8	N 1	O 5	0
4	C	1	Total 14	C 8	N 1	O 5	0
4	C	1	Total 14	C 8	N 1	O 5	0
4	C	1	Total 14	C 8	N 1	O 5	0
4	C	1	Total 14	C 8	N 1	O 5	0
4	C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

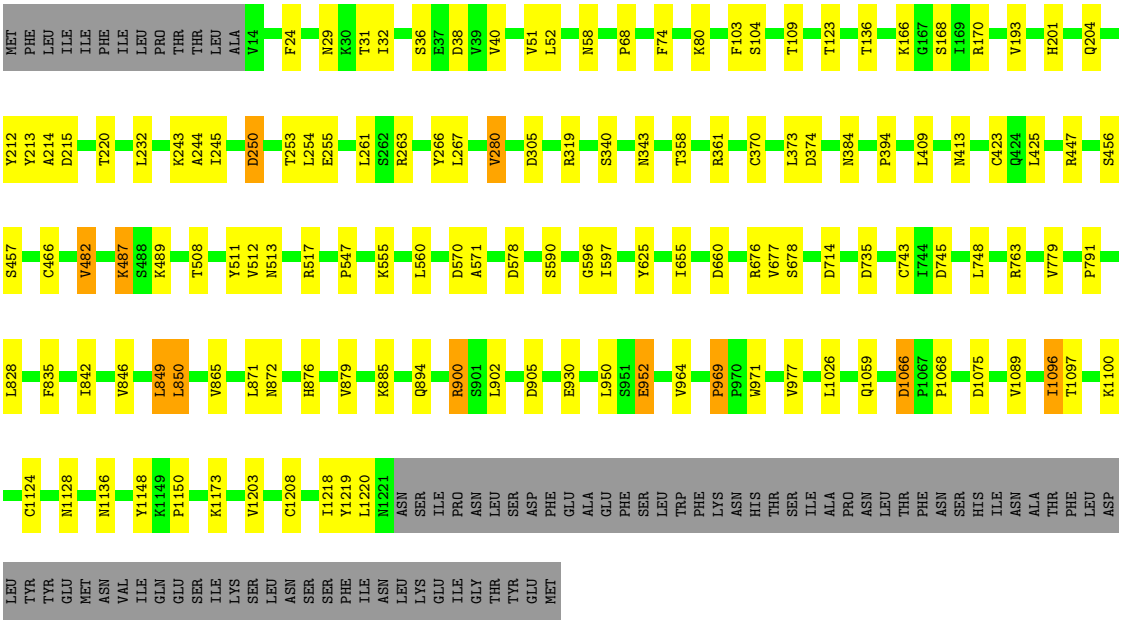
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Spike glycoprotein

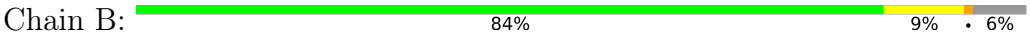
Chain A:

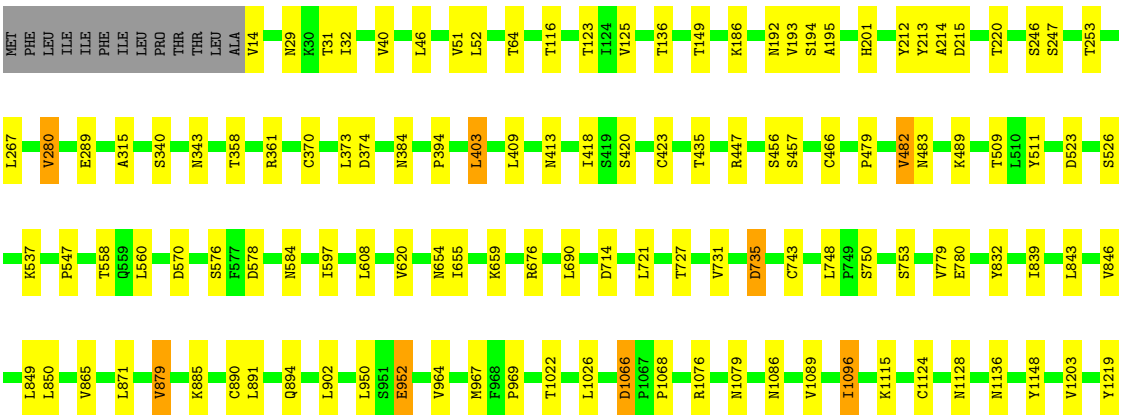


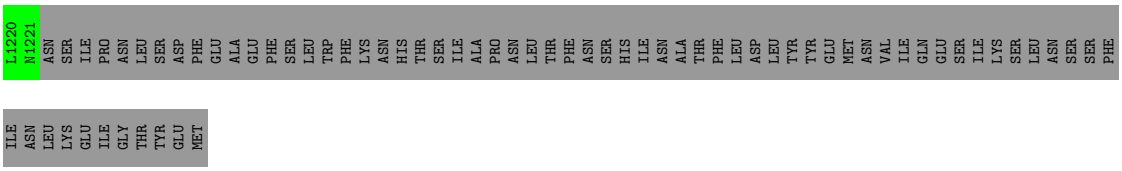


- Molecule 1: Spike glycoprotein

Chain B:

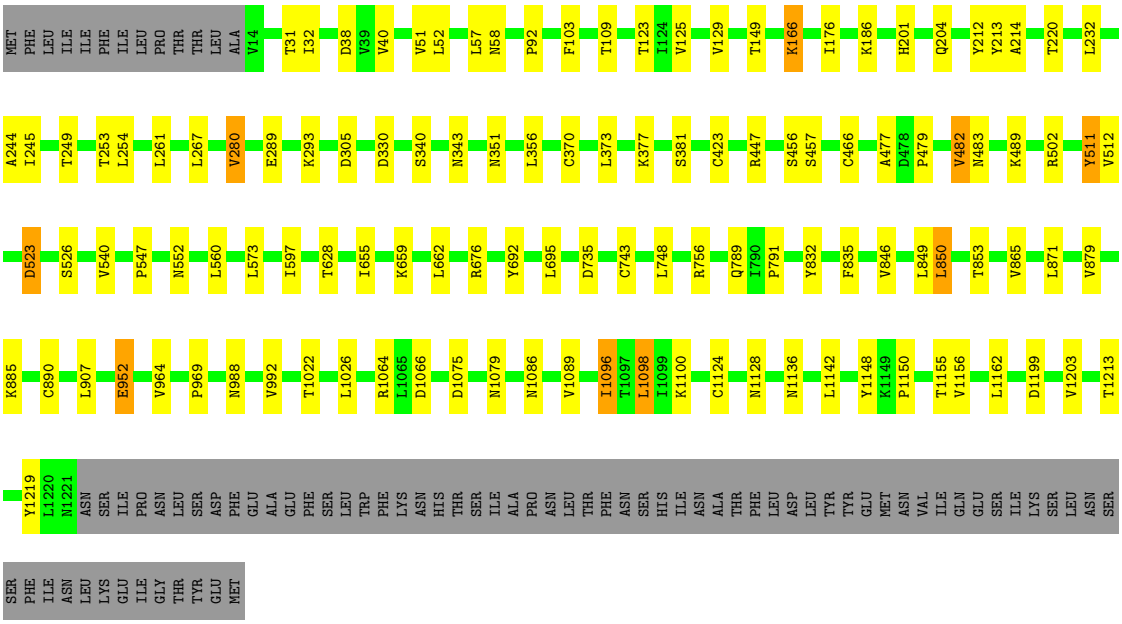






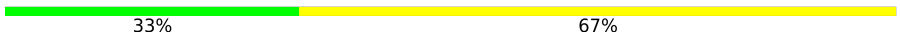
• Molecule 1: Spike glycoprotein

Chain C:



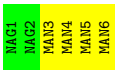
• Molecule 2: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:



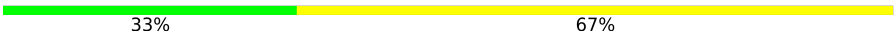
• Molecule 2: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:



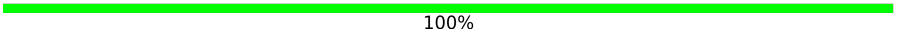
• Molecule 2: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:



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

Chain E:

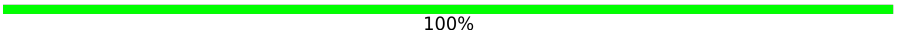


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:

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

Chain G:

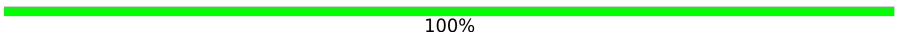


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:

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

Chain J:

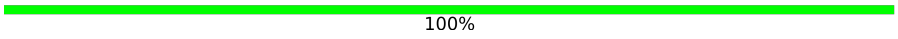


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:

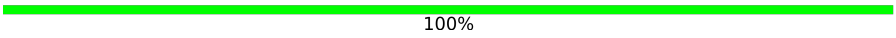
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:



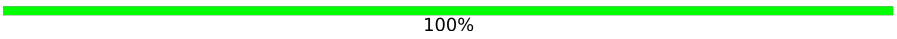
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:



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

Chain O:

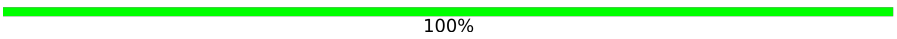


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:

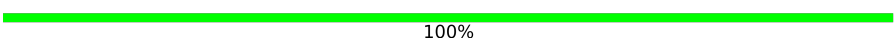
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:



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

Chain R:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	104714	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, 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	0.29	0/9653	0.49	0/13146
1	B	0.29	0/9653	0.48	0/13146
1	C	0.29	0/9653	0.49	0/13146
All	All	0.29	0/28959	0.49	0/39438

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	2
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	969	PRO	Peptide
1	B	969	PRO	Peptide
1	C	92	PRO	Peptide
1	C	969	PRO	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9425	0	9076	47	0
1	B	9425	0	9076	34	0
1	C	9425	0	9076	39	0
2	D	72	0	61	0	0
2	I	72	0	61	0	0
2	N	72	0	61	0	0
3	E	28	0	25	0	0
3	F	28	0	25	0	0
3	G	28	0	25	0	0
3	H	28	0	25	0	0
3	J	28	0	25	0	0
3	K	28	0	25	0	0
3	L	28	0	25	0	0
3	M	28	0	25	0	0
3	O	28	0	25	0	0
3	P	28	0	25	0	0
3	Q	28	0	25	0	0
3	R	28	0	25	0	0
4	A	238	0	221	0	0
4	B	238	0	221	0	0
4	C	238	0	221	0	0
All	All	29541	0	28374	116	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 2.

All (116) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:201:HIS:HB2	1:C:212:TYR:HB2	1.72	0.70
1:B:201:HIS:HB2	1:B:212:TYR:HB2	1.77	0.67
1:A:201:HIS:HB2	1:A:212:TYR:HB2	1.80	0.64
1:A:872:ASN:H	1:A:876:HIS:HD2	1.46	0.62
1:B:214:ALA:HB2	1:B:220:THR:HA	1.84	0.58
1:C:214:ALA:HB2	1:C:220:THR:HA	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:846:VAL:HG13	1:B:1096:ILE:HG13	1.86	0.57
1:B:456:SER:OG	1:B:457:SER:N	2.37	0.56
1:B:735:ASP:OD1	1:B:735:ASP:N	2.34	0.56
1:C:692:TYR:HB3	1:C:695:LEU:HD12	1.89	0.55
1:C:523:ASP:N	1:C:523:ASP:OD1	2.40	0.55
1:C:1128:ASN:HB3	1:C:1148:TYR:HB3	1.89	0.55
1:B:479:PRO:O	1:B:483:ASN:ND2	2.41	0.53
1:A:1066:ASP:HB3	1:A:1068:PRO:HD2	1.91	0.52
1:A:1128:ASN:HB3	1:A:1148:TYR:HB3	1.91	0.52
1:B:832:TYR:OH	1:B:1079:ASN:ND2	2.42	0.52
1:B:1128:ASN:HB3	1:B:1148:TYR:HB3	1.90	0.52
1:A:846:VAL:HG13	1:A:1096:ILE:HG13	1.91	0.52
1:C:789:GLN:NE2	1:C:1155:THR:OG1	2.43	0.52
1:A:952:GLU:HG3	1:A:1136:ASN:HD21	1.75	0.52
1:C:846:VAL:HG13	1:C:1096:ILE:HG13	1.91	0.52
1:B:952:GLU:HG3	1:B:1136:ASN:HD21	1.76	0.51
1:B:149:THR:HG22	1:B:186:LYS:HG3	1.91	0.51
1:A:900:ARG:NH1	1:A:905:ASP:OD1	2.43	0.51
1:A:214:ALA:HB2	1:A:220:THR:HA	1.92	0.51
1:B:1076:ARG:NH2	1:C:1075:ASP:OD2	2.41	0.51
1:C:166:LYS:HD2	1:C:244:ALA:HB3	1.92	0.50
1:A:38:ASP:HB3	1:A:74:PHE:HB2	1.93	0.50
1:C:466:CYS:HB3	1:C:547:PRO:HD2	1.93	0.49
1:A:215:ASP:N	1:A:215:ASP:OD1	2.45	0.49
1:A:1097:THR:HG23	1:C:1098:LEU:HD13	1.94	0.49
1:B:370:CYS:HA	1:B:423:CYS:HA	1.95	0.48
1:C:482:VAL:O	1:C:489:LYS:NZ	2.46	0.48
1:C:523:ASP:OD1	1:C:526:SER:OG	2.29	0.48
1:B:466:CYS:HB3	1:B:547:PRO:HD2	1.95	0.48
1:C:479:PRO:O	1:C:483:ASN:ND2	2.47	0.48
1:A:735:ASP:OD1	1:A:735:ASP:N	2.43	0.48
1:C:988:ASN:ND2	1:C:992:VAL:O	2.46	0.48
1:A:625:TYR:OH	1:A:660:ASP:OD1	2.30	0.48
1:B:315:ALA:H	1:B:620:VAL:HG12	1.79	0.48
1:C:850:LEU:HD13	1:C:1096:ILE:HD11	1.96	0.48
1:A:902:LEU:HA	1:A:905:ASP:HB2	1.96	0.47
1:C:109:THR:HG21	1:C:254:LEU:HD23	1.94	0.47
1:B:409:LEU:HA	1:B:413:ASN:HD22	1.78	0.47
1:A:340:SER:OG	1:A:343:ASN:OD1	2.30	0.47
1:A:394:PRO:HB3	1:A:578:ASP:HB3	1.96	0.47
1:C:149:THR:HG22	1:C:186:LYS:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:508:THR:HG23	1:A:513:ASN:HA	1.96	0.47
1:B:523:ASP:OD1	1:B:526:SER:OG	2.27	0.46
1:C:1199:ASP:OD1	1:C:1199:ASP:N	2.44	0.46
1:A:267:LEU:HB3	1:A:280:VAL:HG13	1.98	0.46
1:B:879:VAL:HG21	1:B:967:MET:HB3	1.97	0.46
1:C:370:CYS:HA	1:C:423:CYS:HA	1.97	0.46
1:B:597:ILE:HD13	1:C:1064:ARG:HG2	1.98	0.46
1:B:690:LEU:HD12	1:B:721:LEU:HD12	1.97	0.46
1:A:168:SER:HA	1:A:243:LYS:HB2	1.97	0.46
1:C:791:PRO:HB3	1:C:1150:PRO:HB3	1.98	0.46
1:B:246:SER:OG	1:B:247:SER:N	2.47	0.45
1:B:570:ASP:OD1	1:B:570:ASP:N	2.48	0.45
1:C:907:LEU:HD11	1:C:1142:LEU:HD22	1.99	0.45
1:C:456:SER:OG	1:C:457:SER:N	2.49	0.45
1:A:68:PRO:O	1:A:266:TYR:OH	2.31	0.45
1:A:1059:GLN:NE2	1:C:628:THR:OG1	2.50	0.45
1:B:192:ASN:HB3	1:B:195:ALA:HB2	1.99	0.45
1:A:109:THR:HG21	1:A:254:LEU:HD23	1.99	0.44
1:B:267:LEU:HB3	1:B:280:VAL:HG13	1.98	0.44
1:A:1218:ILE:HG23	1:A:1220:LEU:HD23	1.98	0.44
1:B:358:THR:HA	1:B:361:ARG:HG2	1.99	0.44
1:C:267:LEU:HB3	1:C:280:VAL:HG13	1.98	0.44
1:C:511:TYR:HD2	1:C:512:VAL:HG23	1.83	0.44
1:B:750:SER:H	1:B:753:SER:HB2	1.83	0.43
1:C:552:ASN:HB2	1:C:573:LEU:HD11	2.00	0.43
1:B:537:LYS:HE3	1:B:537:LYS:HB2	1.83	0.43
1:C:477:ALA:HA	1:C:502:ARG:HB3	2.00	0.43
1:A:409:LEU:HA	1:A:413:ASN:HD22	1.83	0.43
1:A:482:VAL:O	1:A:489:LYS:NZ	2.51	0.43
1:A:513:ASN:OD1	1:A:513:ASN:N	2.41	0.43
1:B:403:LEU:HD13	1:B:418:ILE:HG22	2.00	0.43
1:B:394:PRO:HB3	1:B:578:ASP:HB3	1.99	0.43
1:C:293:LYS:HE3	1:C:293:LYS:HB2	1.86	0.43
1:A:466:CYS:HB3	1:A:547:PRO:HD2	2.00	0.42
1:A:358:THR:HA	1:A:361:ARG:HG2	2.01	0.42
1:C:204:GLN:HE22	1:C:232:LEU:H	1.67	0.42
1:A:791:PRO:HB3	1:A:1150:PRO:HB3	2.01	0.42
1:C:377:LYS:O	1:C:381:SER:OG	2.37	0.42
1:A:103:PHE:HB2	1:A:261:LEU:HD21	2.01	0.42
1:A:969:PRO:HA	1:A:971:TRP:CE2	2.55	0.42
1:B:340:SER:OG	1:B:343:ASN:OD1	2.31	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1173:LYS:HE2	1:A:1173:LYS:HB3	1.87	0.42
1:C:756:ARG:HD3	1:C:756:ARG:HA	1.93	0.41
1:C:340:SER:OG	1:C:343:ASN:OD1	2.29	0.41
1:A:370:CYS:HA	1:A:423:CYS:HA	2.02	0.41
1:A:842:ILE:HG21	1:A:1089:VAL:HG13	2.02	0.41
1:A:850:LEU:HD13	1:A:1096:ILE:HD11	2.00	0.41
1:B:482:VAL:HG13	1:B:489:LYS:HZ2	1.86	0.41
1:A:745:ASP:OD2	1:A:763:ARG:NH2	2.42	0.41
1:C:832:TYR:OH	1:C:1079:ASN:ND2	2.52	0.41
1:B:1066:ASP:HB3	1:B:1068:PRO:HD2	2.02	0.41
1:A:204:GLN:HE22	1:A:232:LEU:H	1.69	0.41
1:A:384:ASN:HD22	1:A:596:GLY:HA3	1.86	0.41
1:A:425:LEU:HB3	1:A:590:SER:HB3	2.03	0.41
1:C:103:PHE:HB2	1:C:261:LEU:HD21	2.03	0.41
1:A:166:LYS:HD2	1:A:244:ALA:HB3	2.03	0.41
1:A:849:LEU:HD12	1:A:849:LEU:HA	1.95	0.41
1:A:1100:LYS:HE2	1:A:1100:LYS:HB3	1.84	0.40
1:B:839:ILE:HG23	1:B:1089:VAL:HG21	2.03	0.40
1:A:487:LYS:HD3	1:A:512:VAL:HG21	2.03	0.40
1:A:24:PHE:HB2	1:A:170:ARG:HH12	1.85	0.40
1:B:215:ASP:OD1	1:B:215:ASP:N	2.52	0.40
1:B:843:LEU:HD23	1:B:843:LEU:HA	1.93	0.40
1:C:952:GLU:HG3	1:C:1136:ASN:HD21	1.87	0.40
1:A:456:SER:OG	1:A:457:SER:N	2.54	0.40
1:A:555:LYS:HB2	1:A:571:ALA:HB2	2.03	0.40
1:C:853:THR:HG21	1:C:1100:LYS:HG2	2.02	0.40
1:A:80:LYS:HE3	1:A:245:ILE:HG22	2.03	0.40
1:C:1162:LEU:HD23	1:C:1213:THR:HB	2.03	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	1206/1290 (94%)	1156 (96%)	49 (4%)	1 (0%)	48 77
1	B	1206/1290 (94%)	1147 (95%)	59 (5%)	0	100 100
1	C	1206/1290 (94%)	1146 (95%)	60 (5%)	0	100 100
All	All	3618/3870 (94%)	3449 (95%)	168 (5%)	1 (0%)	100 100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	250	ASP

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	1082/1159 (93%)	1021 (94%)	61 (6%)	17 47
1	B	1082/1159 (93%)	1014 (94%)	68 (6%)	15 42
1	C	1082/1159 (93%)	1023 (94%)	59 (6%)	18 47
All	All	3246/3477 (93%)	3058 (94%)	188 (6%)	19 45

All (188) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	A	31	THR
1	A	32	ILE
1	A	36	SER
1	A	40	VAL
1	A	51	VAL
1	A	52	LEU
1	A	58	ASN
1	A	104	SER
1	A	123	THR
1	A	136	THR
1	A	193	VAL

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Mol	Chain	Res	Type
1	A	213	TYR
1	A	250	ASP
1	A	253	THR
1	A	255	GLU
1	A	263	ARG
1	A	280	VAL
1	A	305	ASP
1	A	319	ARG
1	A	373	LEU
1	A	374	ASP
1	A	447	ARG
1	A	482	VAL
1	A	487	LYS
1	A	511	TYR
1	A	517	ARG
1	A	560	LEU
1	A	570	ASP
1	A	597	ILE
1	A	655	ILE
1	A	676	ARG
1	A	677	VAL
1	A	678	SER
1	A	714	ASP
1	A	743	CYS
1	A	748	LEU
1	A	779	VAL
1	A	828	LEU
1	A	835	PHE
1	A	849	LEU
1	A	850	LEU
1	A	865	VAL
1	A	871	LEU
1	A	879	VAL
1	A	885	LYS
1	A	894	GLN
1	A	900	ARG
1	A	930	GLU
1	A	950	LEU
1	A	952	GLU
1	A	964	VAL
1	A	977	VAL
1	A	1026	LEU

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Mol	Chain	Res	Type
1	A	1066	ASP
1	A	1075	ASP
1	A	1096	ILE
1	A	1124	CYS
1	A	1203	VAL
1	A	1208	CYS
1	A	1219	TYR
1	B	14	VAL
1	B	29	ASN
1	B	31	THR
1	B	32	ILE
1	B	40	VAL
1	B	46	LEU
1	B	51	VAL
1	B	52	LEU
1	B	64	THR
1	B	116	THR
1	B	123	THR
1	B	125	VAL
1	B	136	THR
1	B	193	VAL
1	B	194	SER
1	B	213	TYR
1	B	253	THR
1	B	280	VAL
1	B	289	GLU
1	B	373	LEU
1	B	374	ASP
1	B	384	ASN
1	B	403	LEU
1	B	420	SER
1	B	435	THR
1	B	447	ARG
1	B	482	VAL
1	B	509	THR
1	B	511	TYR
1	B	558	THR
1	B	560	LEU
1	B	576	SER
1	B	584	ASN
1	B	608	LEU
1	B	654	ASN

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Mol	Chain	Res	Type
1	B	655	ILE
1	B	659	LYS
1	B	676	ARG
1	B	714	ASP
1	B	727	THR
1	B	731	VAL
1	B	735	ASP
1	B	743	CYS
1	B	748	LEU
1	B	779	VAL
1	B	780	GLU
1	B	849	LEU
1	B	850	LEU
1	B	865	VAL
1	B	871	LEU
1	B	879	VAL
1	B	885	LYS
1	B	890	CYS
1	B	891	LEU
1	B	894	GLN
1	B	902	LEU
1	B	950	LEU
1	B	952	GLU
1	B	964	VAL
1	B	1022	THR
1	B	1026	LEU
1	B	1066	ASP
1	B	1086	ASN
1	B	1096	ILE
1	B	1115	LYS
1	B	1124	CYS
1	B	1203	VAL
1	B	1219	TYR
1	C	31	THR
1	C	32	ILE
1	C	38	ASP
1	C	40	VAL
1	C	51	VAL
1	C	52	LEU
1	C	57	LEU
1	C	58	ASN
1	C	123	THR

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Mol	Chain	Res	Type
1	C	125	VAL
1	C	129	VAL
1	C	166	LYS
1	C	176	ILE
1	C	213	TYR
1	C	245	ILE
1	C	249	THR
1	C	253	THR
1	C	280	VAL
1	C	289	GLU
1	C	305	ASP
1	C	330	ASP
1	C	351	ASN
1	C	356	LEU
1	C	373	LEU
1	C	447	ARG
1	C	482	VAL
1	C	511	TYR
1	C	523	ASP
1	C	540	VAL
1	C	560	LEU
1	C	597	ILE
1	C	655	ILE
1	C	659	LYS
1	C	662	LEU
1	C	676	ARG
1	C	735	ASP
1	C	743	CYS
1	C	748	LEU
1	C	835	PHE
1	C	849	LEU
1	C	850	LEU
1	C	865	VAL
1	C	871	LEU
1	C	879	VAL
1	C	885	LYS
1	C	890	CYS
1	C	952	GLU
1	C	964	VAL
1	C	1022	THR
1	C	1026	LEU
1	C	1066	ASP

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Mol	Chain	Res	Type
1	C	1086	ASN
1	C	1089	VAL
1	C	1096	ILE
1	C	1098	LEU
1	C	1124	CYS
1	C	1156	VAL
1	C	1203	VAL
1	C	1219	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	ASN
1	A	204	GLN
1	A	384	ASN
1	A	630	GLN
1	A	876	HIS
1	A	984	GLN
1	A	1001	GLN
1	A	1059	GLN
1	A	1079	ASN
1	A	1091	GLN
1	A	1136	ASN
1	A	1180	GLN
1	B	204	GLN
1	B	353	ASN
1	B	561	ASN
1	B	630	GLN
1	B	984	GLN
1	B	1001	GLN
1	B	1079	ASN
1	B	1091	GLN
1	B	1136	ASN
1	C	204	GLN
1	C	630	GLN
1	C	789	GLN
1	C	894	GLN
1	C	954	GLN
1	C	984	GLN
1	C	1001	GLN
1	C	1059	GLN
1	C	1079	ASN

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Mol	Chain	Res	Type
1	C	1091	GLN
1	C	1136	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

42 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	D	1	1,2	14,14,15	0.22	0	17,19,21	0.54	0
2	NAG	D	2	2	14,14,15	0.24	0	17,19,21	0.53	0
2	MAN	D	3	2	11,11,12	1.25	1 (9%)	15,15,17	1.83	3 (20%)
2	MAN	D	4	2	11,11,12	0.88	1 (9%)	15,15,17	1.36	2 (13%)
2	MAN	D	5	2	11,11,12	0.75	0	15,15,17	1.12	2 (13%)
2	MAN	D	6	2	11,11,12	0.86	1 (9%)	15,15,17	1.38	2 (13%)
3	NAG	E	1	3,1	14,14,15	0.28	0	17,19,21	0.51	0
3	NAG	E	2	3	14,14,15	0.33	0	17,19,21	0.48	0
3	NAG	F	1	3,1	14,14,15	0.24	0	17,19,21	0.45	0
3	NAG	F	2	3	14,14,15	0.32	0	17,19,21	0.64	1 (5%)
3	NAG	G	1	3,1	14,14,15	0.28	0	17,19,21	0.48	0
3	NAG	G	2	3	14,14,15	0.29	0	17,19,21	0.50	0
3	NAG	H	1	3,1	14,14,15	0.24	0	17,19,21	0.51	0
3	NAG	H	2	3	14,14,15	0.31	0	17,19,21	0.52	0
2	NAG	I	1	1,2	14,14,15	0.28	0	17,19,21	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	I	2	2	14,14,15	0.24	0	17,19,21	0.53	0
2	MAN	I	3	2	11,11,12	1.39	1 (9%)	15,15,17	1.79	3 (20%)
2	MAN	I	4	2	11,11,12	0.80	0	15,15,17	1.16	2 (13%)
2	MAN	I	5	2	11,11,12	0.78	0	15,15,17	1.09	2 (13%)
2	MAN	I	6	2	11,11,12	0.75	0	15,15,17	1.34	2 (13%)
3	NAG	J	1	3,1	14,14,15	0.33	0	17,19,21	0.51	0
3	NAG	J	2	3	14,14,15	0.40	0	17,19,21	0.46	0
3	NAG	K	1	3,1	14,14,15	0.24	0	17,19,21	0.46	0
3	NAG	K	2	3	14,14,15	0.34	0	17,19,21	0.57	1 (5%)
3	NAG	L	1	3,1	14,14,15	0.23	0	17,19,21	0.45	0
3	NAG	L	2	3	14,14,15	0.30	0	17,19,21	0.53	0
3	NAG	M	1	3,1	14,14,15	0.27	0	17,19,21	0.54	0
3	NAG	M	2	3	14,14,15	0.33	0	17,19,21	0.45	0
2	NAG	N	1	1,2	14,14,15	0.23	0	17,19,21	0.58	0
2	NAG	N	2	2	14,14,15	0.25	0	17,19,21	0.50	0
2	MAN	N	3	2	11,11,12	1.37	2 (18%)	15,15,17	1.76	3 (20%)
2	MAN	N	4	2	11,11,12	0.82	0	15,15,17	1.29	2 (13%)
2	MAN	N	5	2	11,11,12	0.85	0	15,15,17	0.98	2 (13%)
2	MAN	N	6	2	11,11,12	0.86	1 (9%)	15,15,17	1.31	2 (13%)
3	NAG	O	1	3,1	14,14,15	0.31	0	17,19,21	0.55	0
3	NAG	O	2	3	14,14,15	0.43	0	17,19,21	0.45	0
3	NAG	P	1	3,1	14,14,15	0.24	0	17,19,21	0.46	0
3	NAG	P	2	3	14,14,15	0.31	0	17,19,21	0.58	1 (5%)
3	NAG	Q	1	3,1	14,14,15	0.22	0	17,19,21	0.45	0
3	NAG	Q	2	3	14,14,15	0.28	0	17,19,21	0.54	0
3	NAG	R	1	3,1	14,14,15	0.25	0	17,19,21	0.57	0
3	NAG	R	2	3	14,14,15	0.32	0	17,19,21	0.53	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	D	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	MAN	D	3	2	-	0/2/19/22	0/1/1/1
2	MAN	D	4	2	-	2/2/19/22	0/1/1/1
2	MAN	D	5	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MAN	D	6	2	-	2/2/19/22	0/1/1/1
3	NAG	E	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	NAG	F	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	NAG	G	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1
3	NAG	H	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	H	2	3	-	2/6/23/26	0/1/1/1
2	NAG	I	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	I	2	2	-	2/6/23/26	0/1/1/1
2	MAN	I	3	2	-	2/2/19/22	1/1/1/1
2	MAN	I	4	2	-	0/2/19/22	0/1/1/1
2	MAN	I	5	2	-	2/2/19/22	0/1/1/1
2	MAN	I	6	2	-	2/2/19/22	0/1/1/1
3	NAG	J	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	J	2	3	-	2/6/23/26	0/1/1/1
3	NAG	K	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	K	2	3	-	2/6/23/26	0/1/1/1
3	NAG	L	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	L	2	3	-	0/6/23/26	0/1/1/1
3	NAG	M	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	M	2	3	-	2/6/23/26	0/1/1/1
2	NAG	N	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	N	2	2	-	2/6/23/26	0/1/1/1
2	MAN	N	3	2	-	0/2/19/22	0/1/1/1
2	MAN	N	4	2	-	2/2/19/22	0/1/1/1
2	MAN	N	5	2	-	0/2/19/22	0/1/1/1
2	MAN	N	6	2	-	2/2/19/22	0/1/1/1
3	NAG	O	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	O	2	3	-	2/6/23/26	0/1/1/1
3	NAG	P	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	P	2	3	-	2/6/23/26	0/1/1/1
3	NAG	Q	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	R	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	R	2	3	-	1/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	3	MAN	O5-C5	3.31	1.50	1.43
2	D	3	MAN	O5-C5	2.65	1.48	1.43
2	N	3	MAN	O5-C5	2.36	1.48	1.43
2	N	3	MAN	C1-C2	2.25	1.57	1.52
2	N	6	MAN	C1-C2	2.13	1.57	1.52
2	D	4	MAN	C1-C2	2.08	1.56	1.52
2	D	6	MAN	O5-C5	2.01	1.47	1.43

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	3	MAN	C1-O5-C5	5.44	119.56	112.19
2	N	3	MAN	C1-O5-C5	5.32	119.40	112.19
2	I	3	MAN	C1-O5-C5	5.06	119.04	112.19
2	D	6	MAN	C1-O5-C5	4.39	118.14	112.19
2	I	6	MAN	C1-O5-C5	4.28	118.00	112.19
2	D	4	MAN	C1-O5-C5	3.80	117.34	112.19
2	N	6	MAN	C1-O5-C5	3.77	117.30	112.19
2	N	4	MAN	C1-O5-C5	3.51	116.95	112.19
2	D	5	MAN	C1-O5-C5	3.16	116.48	112.19
2	I	4	MAN	C1-O5-C5	3.16	116.48	112.19
2	I	3	MAN	C1-C2-C3	3.10	113.48	109.67
2	I	5	MAN	C1-O5-C5	3.05	116.32	112.19
2	N	5	MAN	C1-O5-C5	2.51	115.59	112.19
2	D	3	MAN	O2-C2-C3	-2.44	105.25	110.14
2	I	3	MAN	O2-C2-C3	-2.42	105.30	110.14
2	D	6	MAN	O2-C2-C3	-2.33	105.46	110.14
2	D	3	MAN	C2-C3-C4	2.31	114.90	110.89
2	N	4	MAN	O2-C2-C3	-2.29	105.54	110.14
3	F	2	NAG	C1-O5-C5	2.28	115.29	112.19
2	D	5	MAN	O2-C2-C3	-2.27	105.60	110.14
2	N	3	MAN	O2-C2-C3	-2.25	105.63	110.14
2	I	6	MAN	O2-C2-C3	-2.24	105.65	110.14
2	I	4	MAN	O2-C2-C3	-2.21	105.71	110.14
2	N	6	MAN	O2-C2-C3	-2.18	105.77	110.14
2	I	5	MAN	O2-C2-C3	-2.16	105.81	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	4	MAN	O2-C2-C3	-2.15	105.82	110.14
2	N	3	MAN	C2-C3-C4	2.12	114.57	110.89
2	N	5	MAN	O2-C2-C3	-2.08	105.97	110.14
3	P	2	NAG	C1-O5-C5	2.04	114.96	112.19
3	K	2	NAG	C1-O5-C5	2.00	114.90	112.19

There are no chirality outliers.

All (66) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	N	1	NAG	O5-C5-C6-O6
2	N	4	MAN	O5-C5-C6-O6
2	N	2	NAG	O5-C5-C6-O6
3	O	2	NAG	O5-C5-C6-O6
3	P	2	NAG	O5-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	N	1	NAG	C4-C5-C6-O6
2	N	2	NAG	C4-C5-C6-O6
3	O	2	NAG	C4-C5-C6-O6
2	N	6	MAN	O5-C5-C6-O6
3	R	1	NAG	O5-C5-C6-O6
3	H	2	NAG	O5-C5-C6-O6
2	N	4	MAN	C4-C5-C6-O6
3	M	1	NAG	C4-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
3	Q	1	NAG	C4-C5-C6-O6
3	P	1	NAG	C4-C5-C6-O6
3	O	1	NAG	O5-C5-C6-O6
2	N	6	MAN	C4-C5-C6-O6
3	H	2	NAG	C4-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
3	O	1	NAG	C4-C5-C6-O6
3	P	2	NAG	C4-C5-C6-O6
3	M	1	NAG	O5-C5-C6-O6
3	R	1	NAG	C4-C5-C6-O6
2	I	1	NAG	O5-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
2	D	4	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	I	1	NAG	C4-C5-C6-O6
2	I	3	MAN	C4-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
2	I	5	MAN	C4-C5-C6-O6
3	Q	1	NAG	O5-C5-C6-O6
2	I	3	MAN	O5-C5-C6-O6
3	P	1	NAG	O5-C5-C6-O6
2	I	2	NAG	C4-C5-C6-O6
3	K	2	NAG	O5-C5-C6-O6
3	Q	2	NAG	O5-C5-C6-O6
3	K	2	NAG	C4-C5-C6-O6
3	Q	2	NAG	C4-C5-C6-O6
2	I	6	MAN	C4-C5-C6-O6
2	I	5	MAN	O5-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
3	K	1	NAG	C4-C5-C6-O6
3	M	2	NAG	C4-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
3	L	1	NAG	C4-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
3	M	2	NAG	O5-C5-C6-O6
2	I	6	MAN	O5-C5-C6-O6
3	J	2	NAG	C4-C5-C6-O6
3	J	2	NAG	O5-C5-C6-O6
3	J	1	NAG	C4-C5-C6-O6
3	J	1	NAG	O5-C5-C6-O6
2	I	2	NAG	O5-C5-C6-O6
2	D	6	MAN	C4-C5-C6-O6
3	K	1	NAG	O5-C5-C6-O6
2	D	6	MAN	O5-C5-C6-O6
3	L	1	NAG	O5-C5-C6-O6
3	H	1	NAG	C4-C5-C6-O6
2	D	4	MAN	C4-C5-C6-O6
3	R	2	NAG	C4-C5-C6-O6

All (1) ring outliers are listed below:

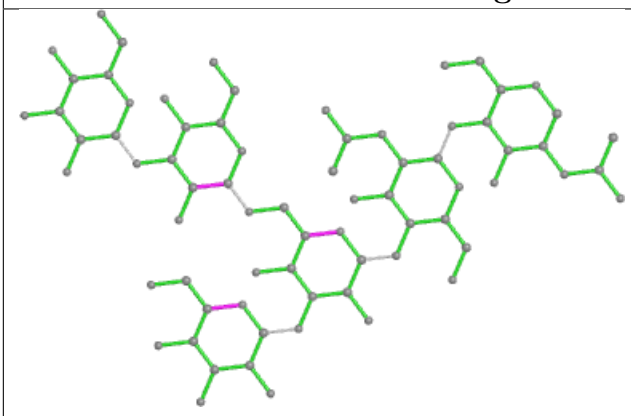
Mol	Chain	Res	Type	Atoms
2	I	3	MAN	C1-C2-C3-C4-C5-O5

No monomer is involved in short contacts.

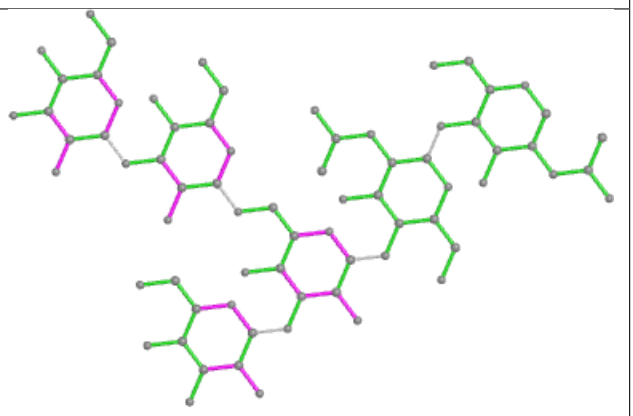
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for oligosaccharide.

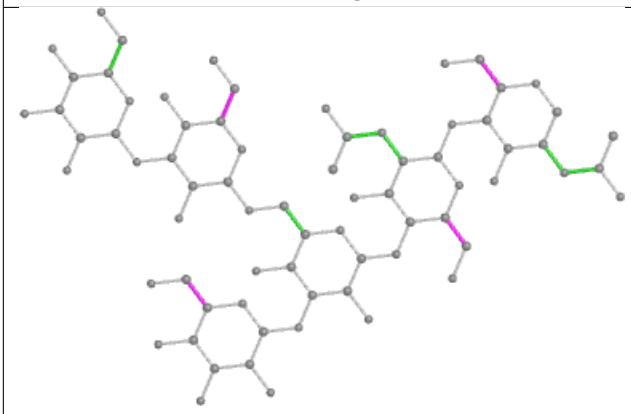
Oligosaccharide Chain D



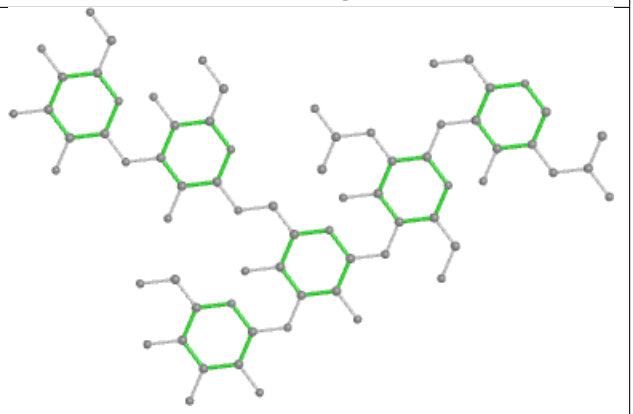
Bond lengths



Bond angles

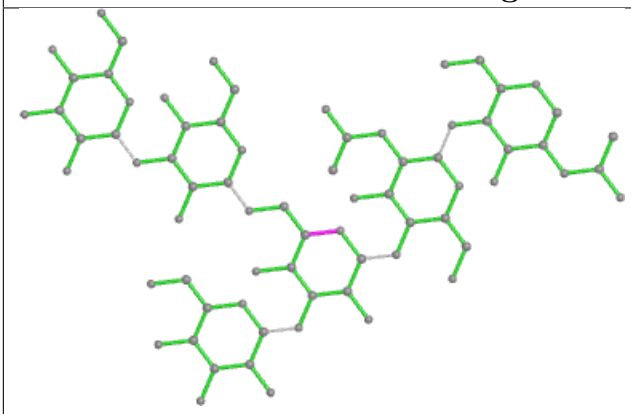


Torsions

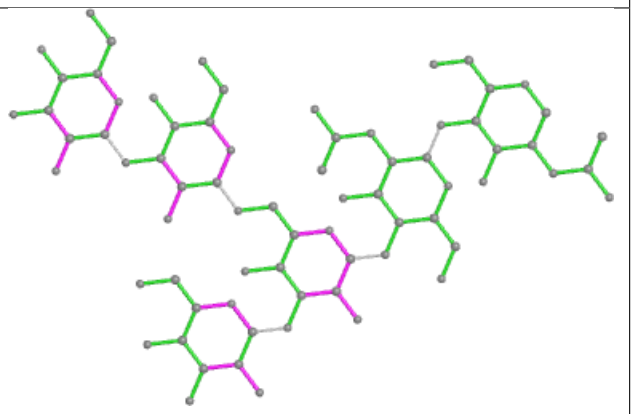


Rings

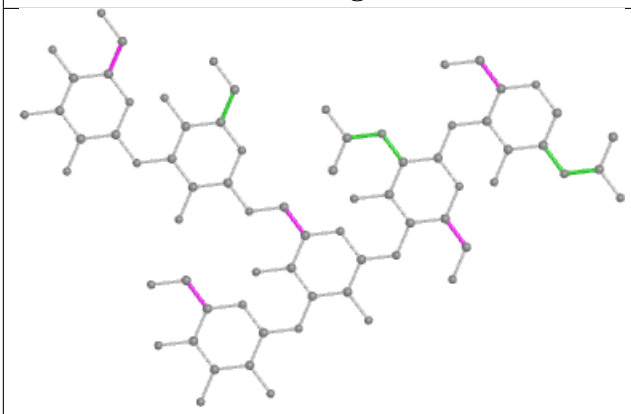
Oligosaccharide Chain I



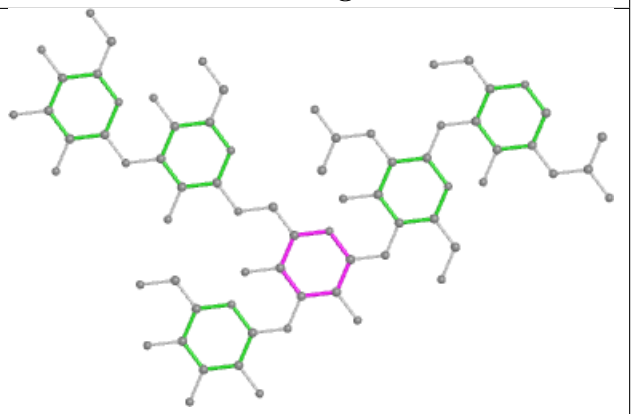
Bond lengths



Bond angles

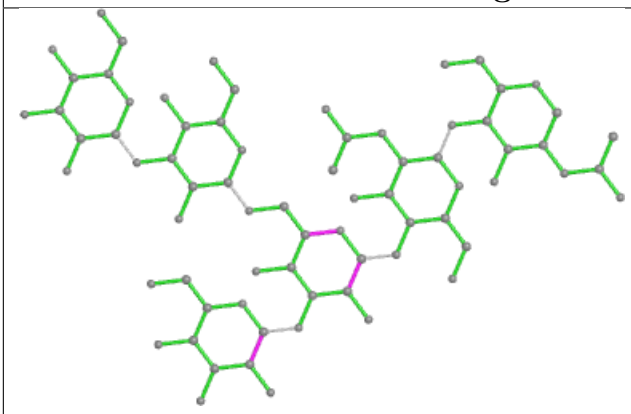


Torsions

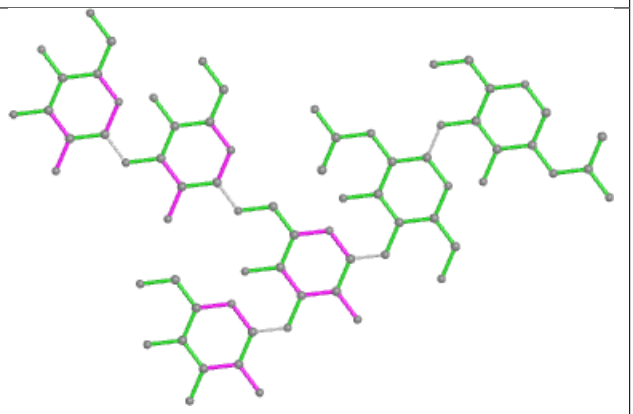


Rings

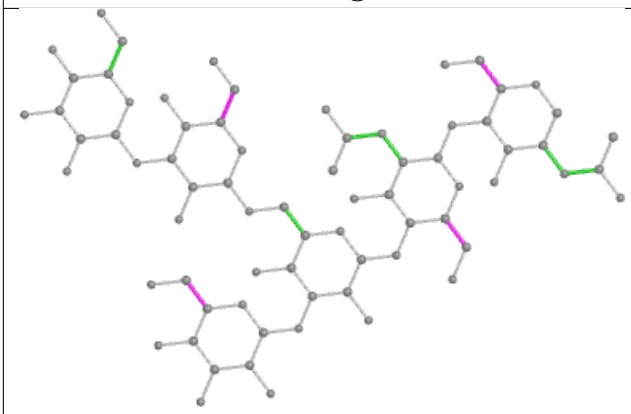
Oligosaccharide Chain N



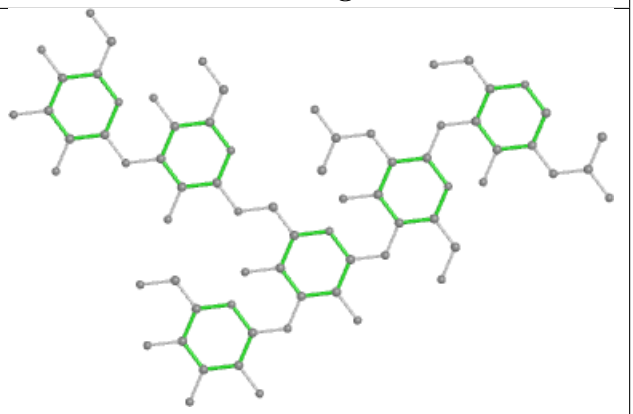
Bond lengths



Bond angles

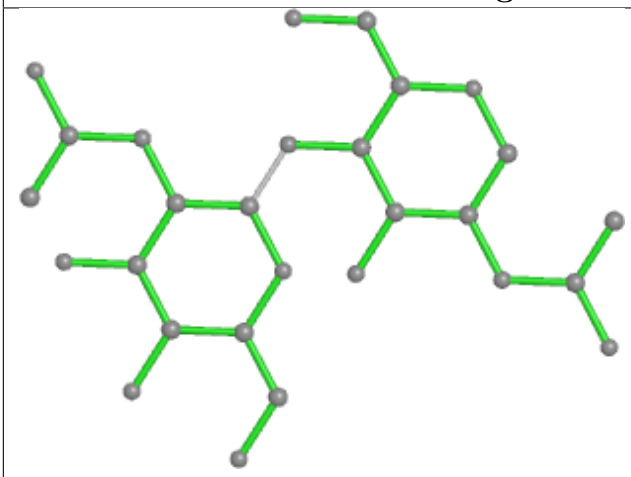


Torsions

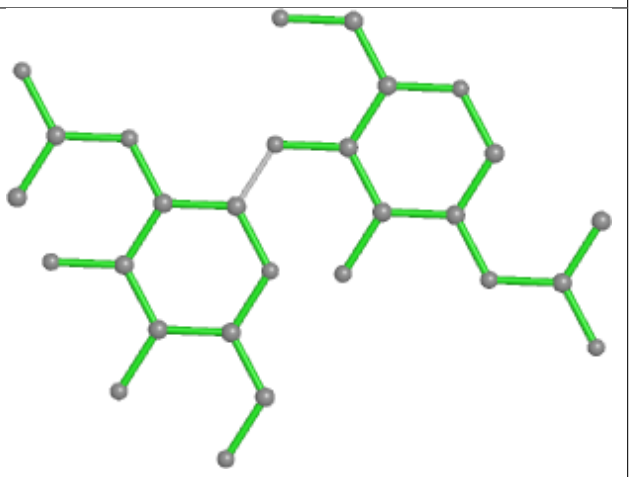


Rings

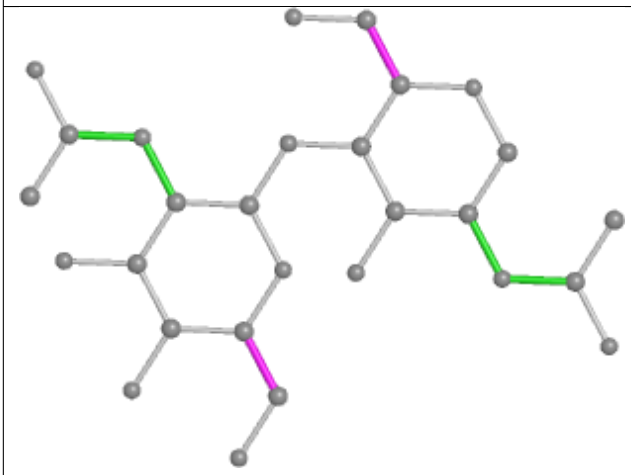
Oligosaccharide Chain E



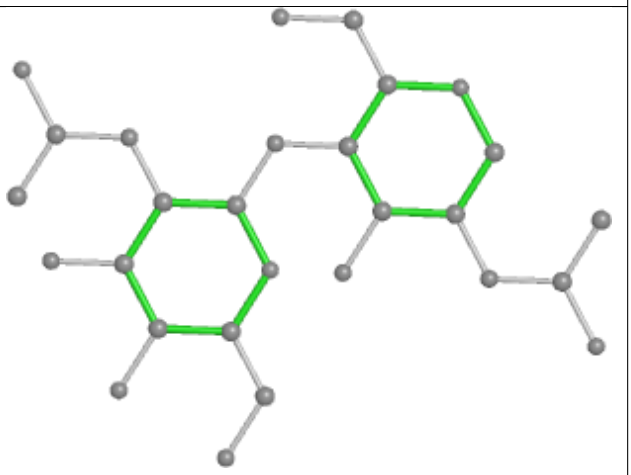
Bond lengths



Bond angles

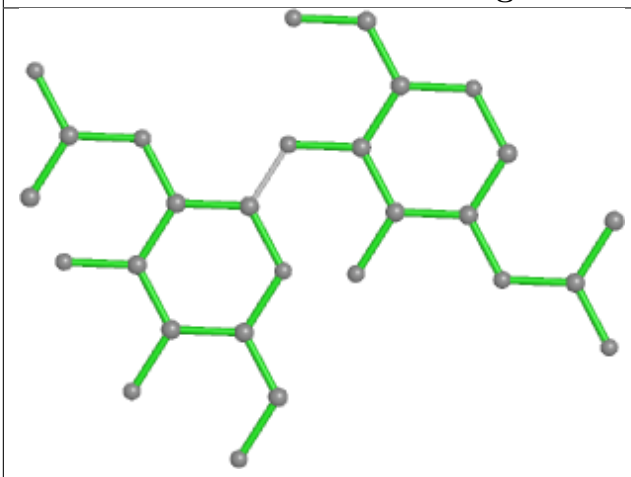


Torsions

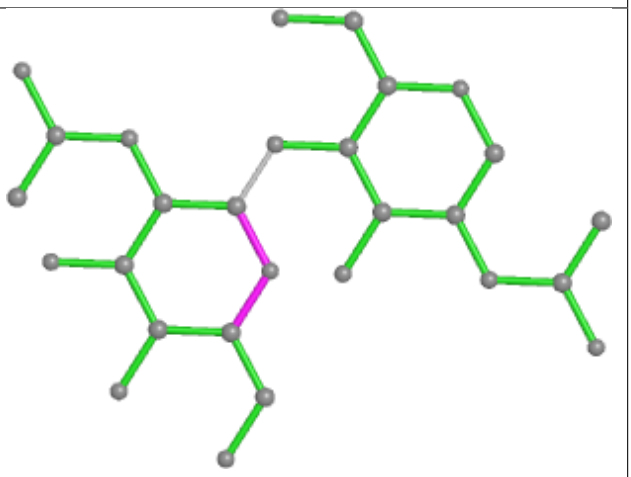


Rings

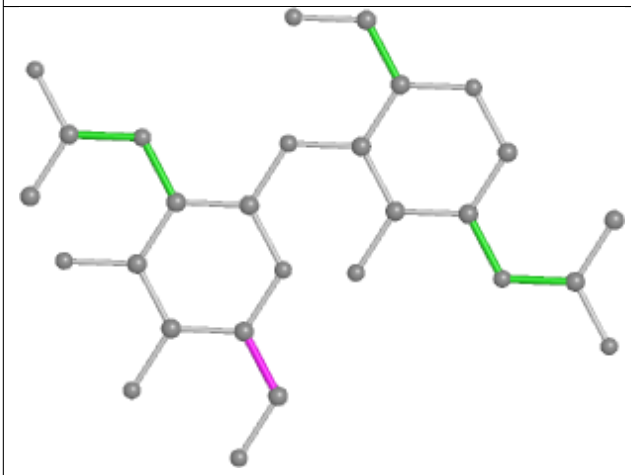
Oligosaccharide Chain F



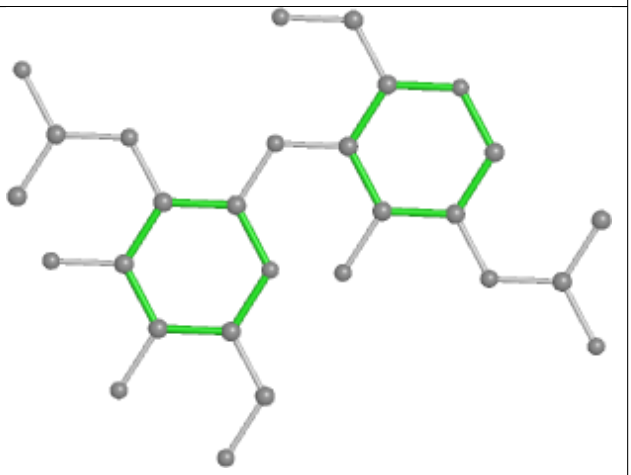
Bond lengths



Bond angles

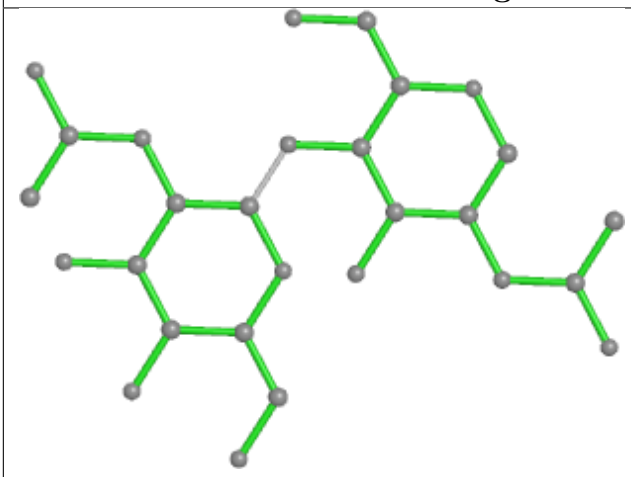


Torsions

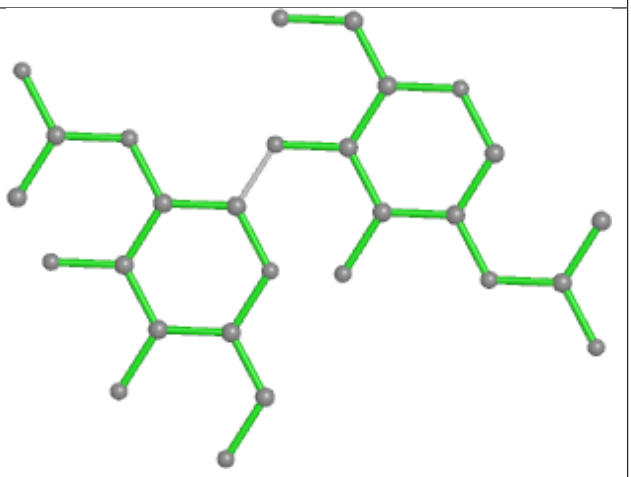


Rings

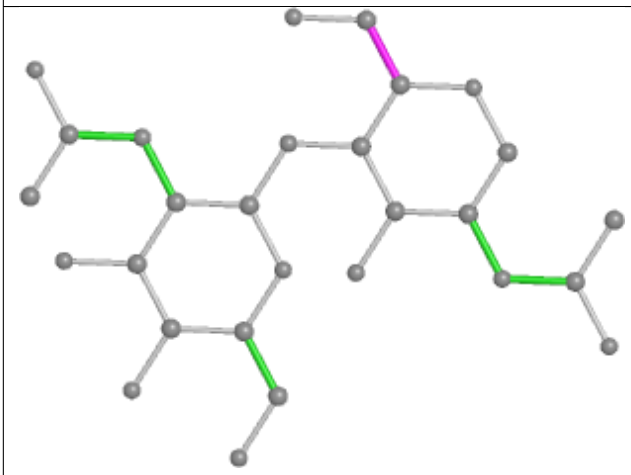
Oligosaccharide Chain G



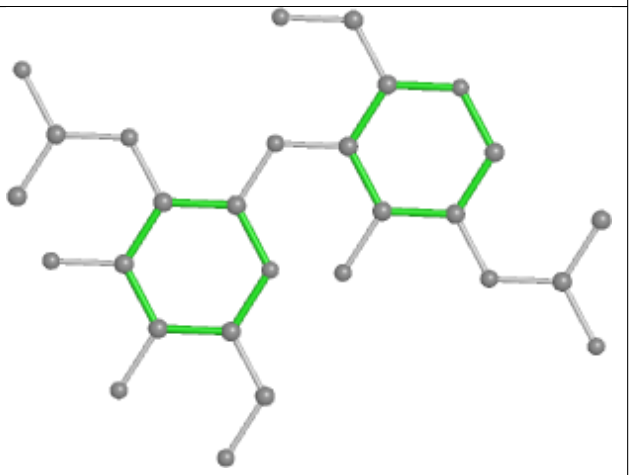
Bond lengths



Bond angles

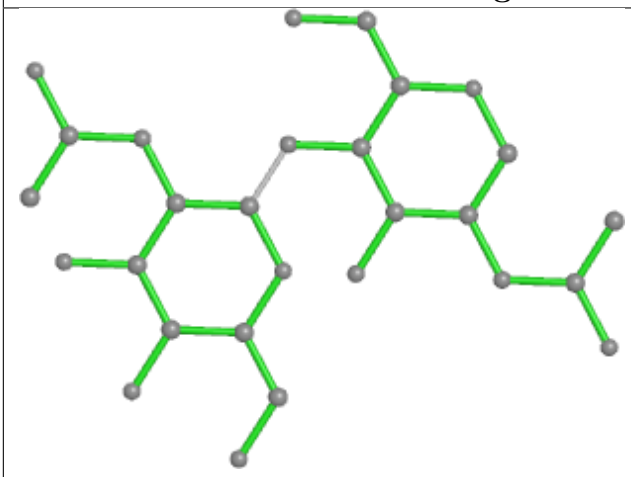


Torsions

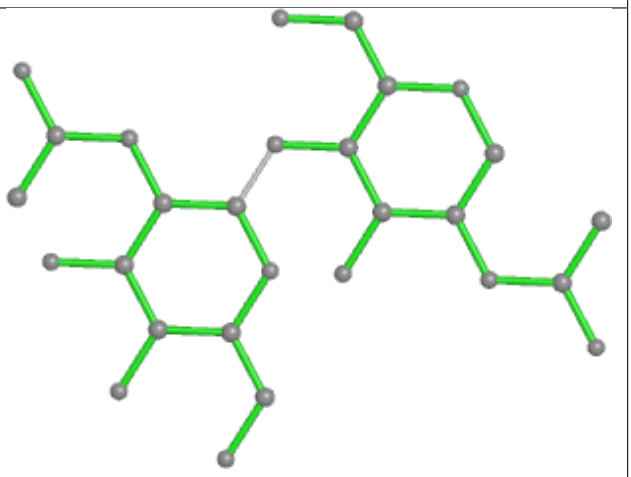


Rings

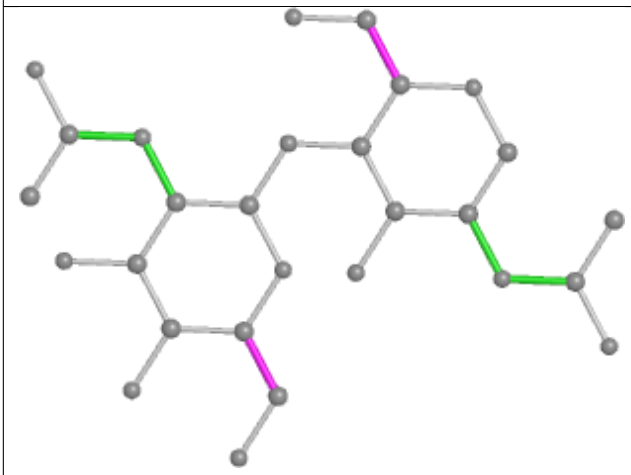
Oligosaccharide Chain H



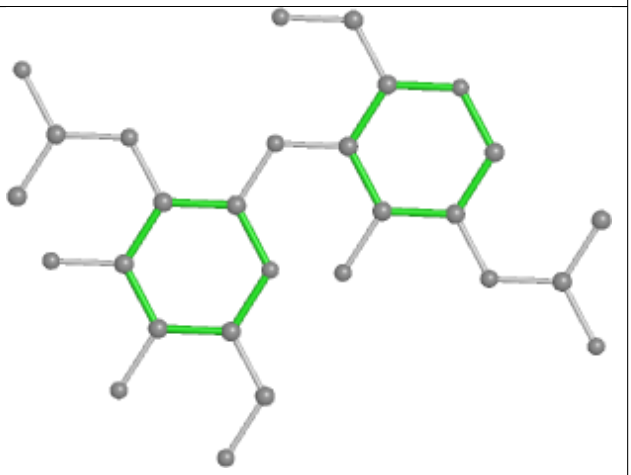
Bond lengths



Bond angles

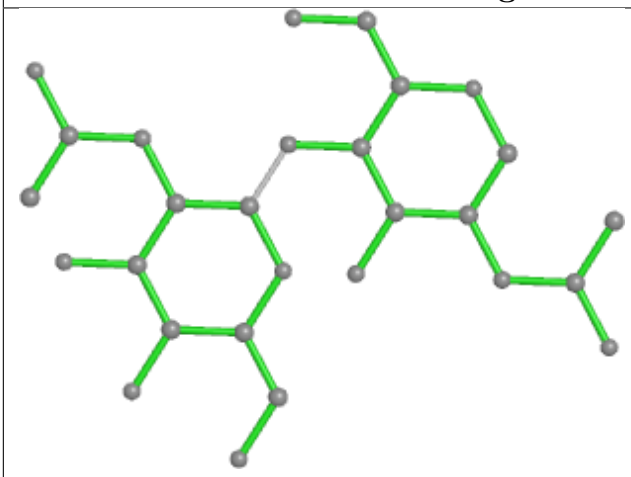


Torsions

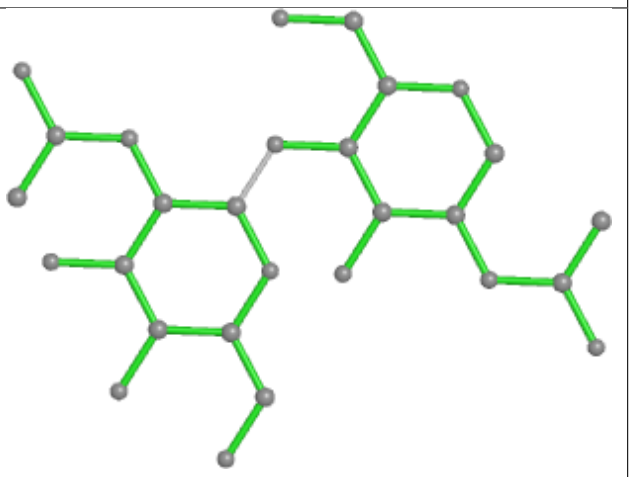


Rings

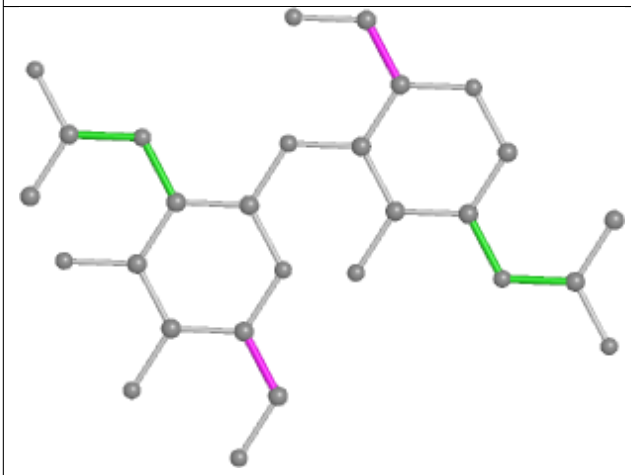
Oligosaccharide Chain J



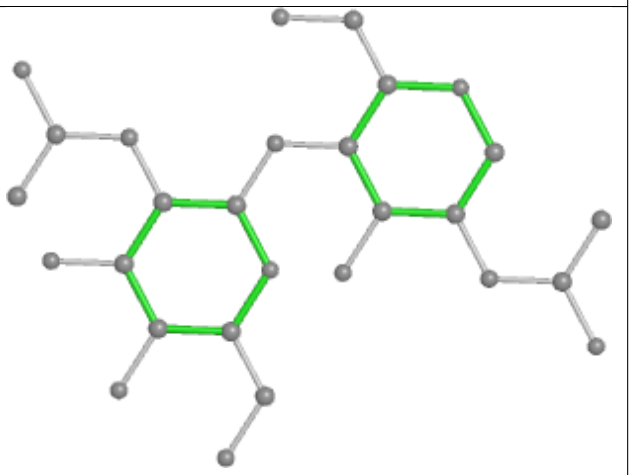
Bond lengths



Bond angles

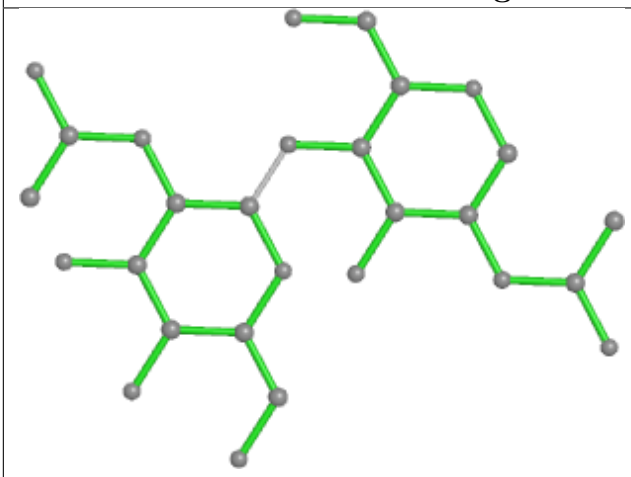


Torsions

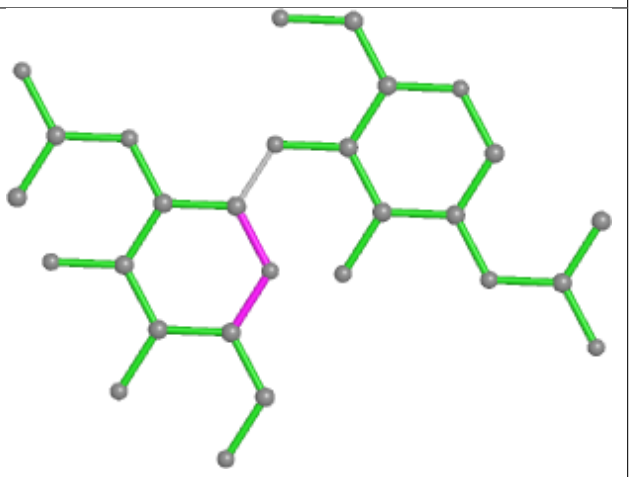


Rings

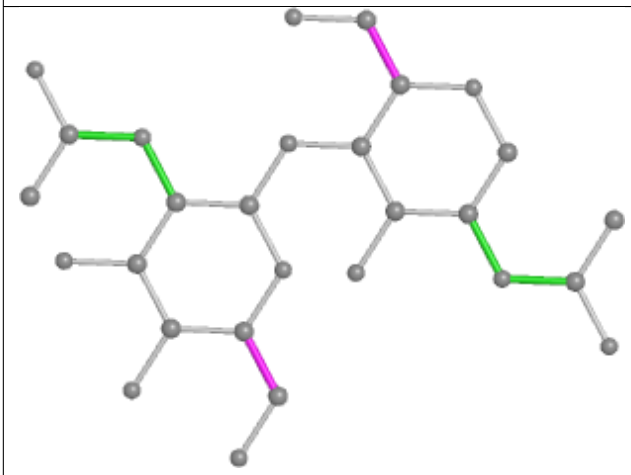
Oligosaccharide Chain K



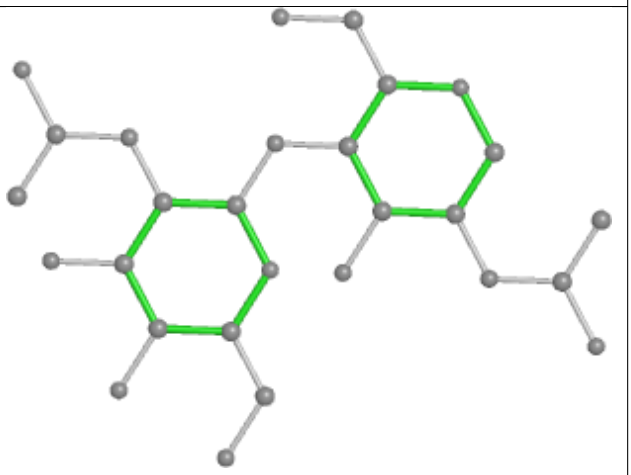
Bond lengths



Bond angles

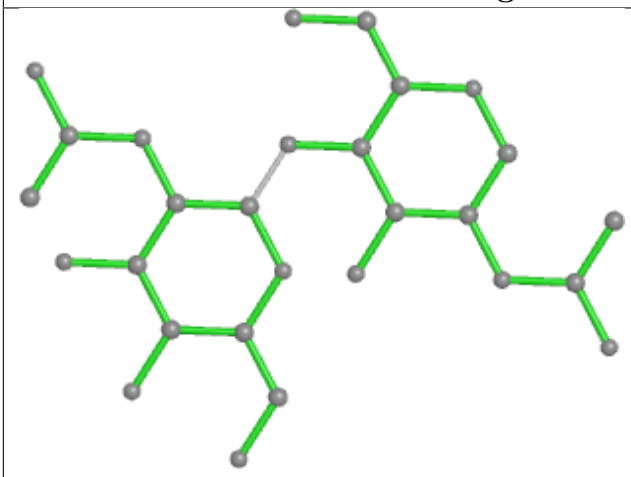


Torsions

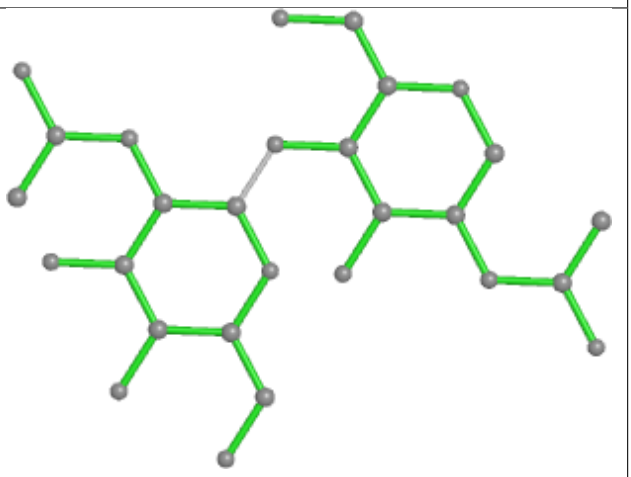


Rings

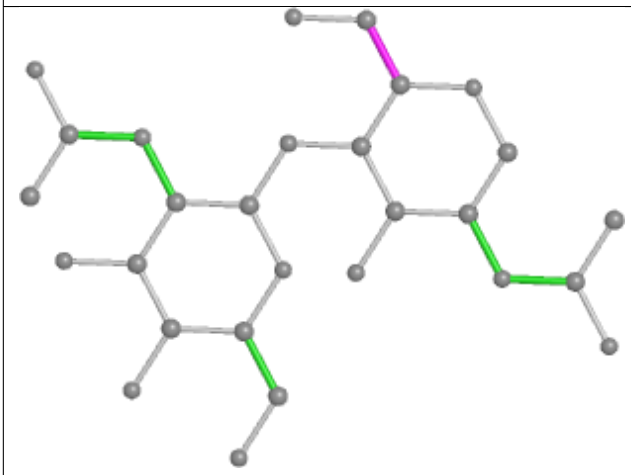
Oligosaccharide Chain L



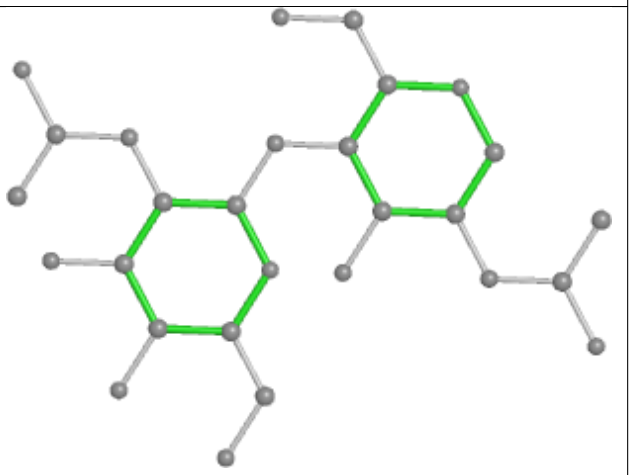
Bond lengths



Bond angles

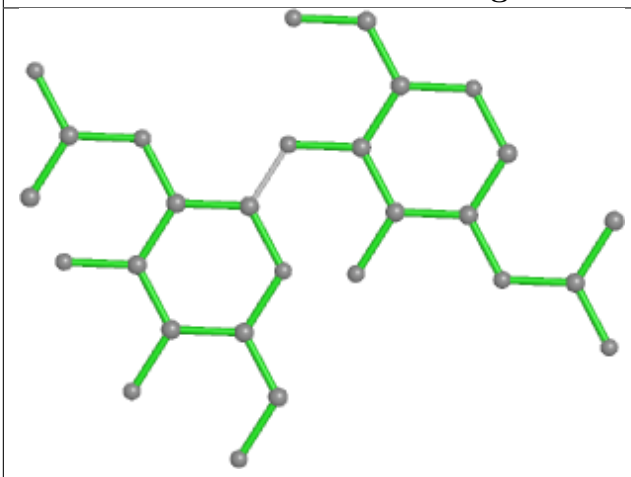


Torsions

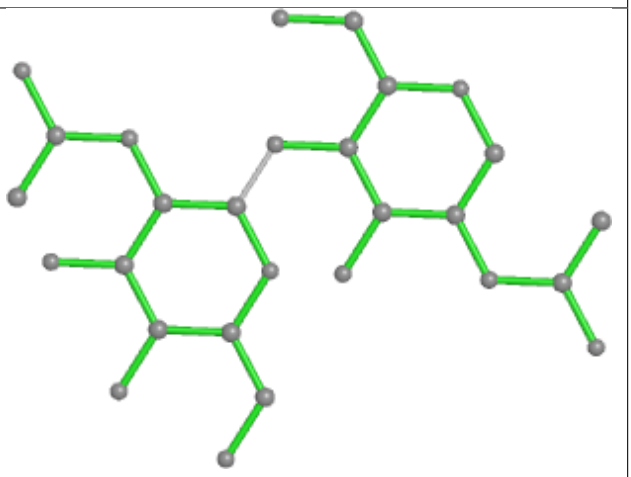


Rings

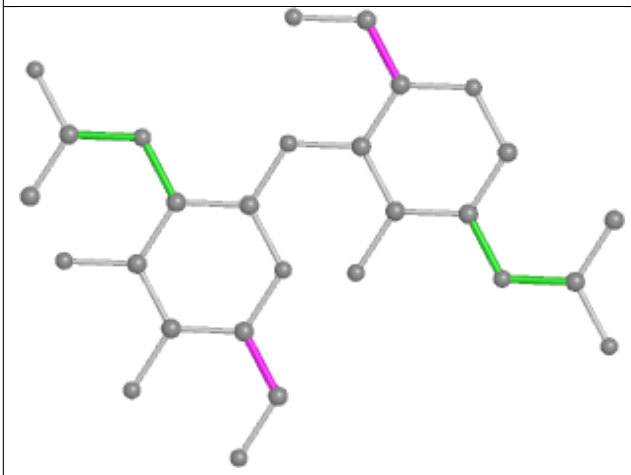
Oligosaccharide Chain M



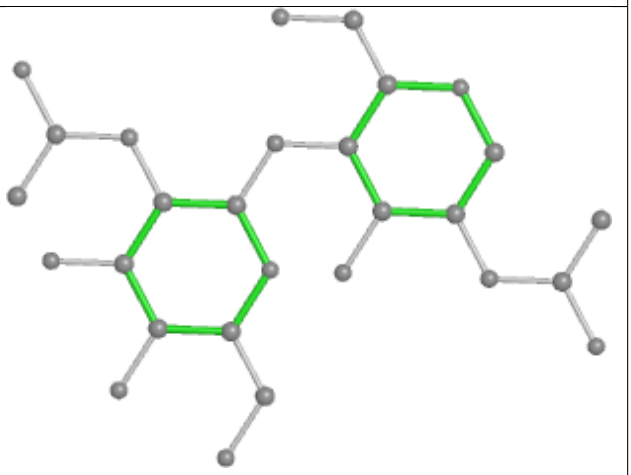
Bond lengths



Bond angles

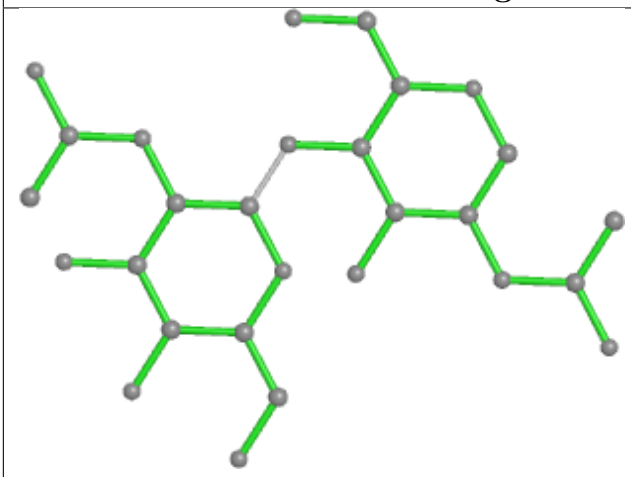


Torsions

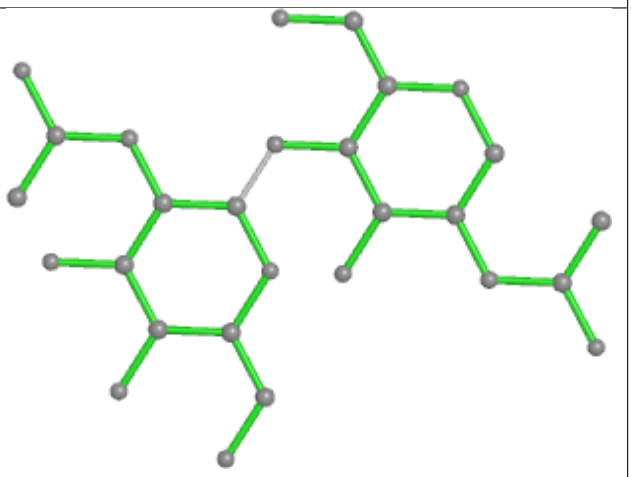


Rings

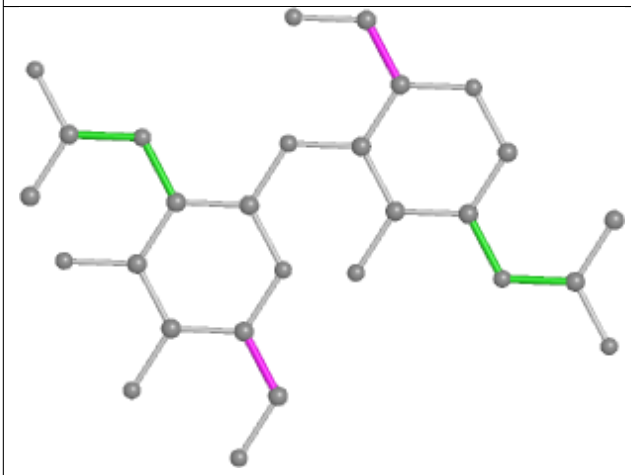
Oligosaccharide Chain O



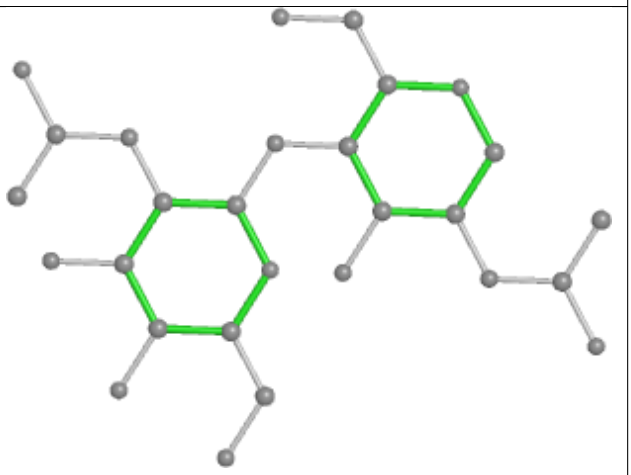
Bond lengths



Bond angles

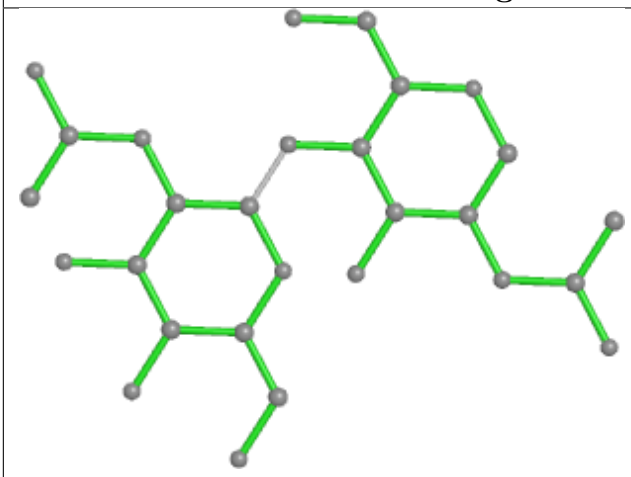


Torsions

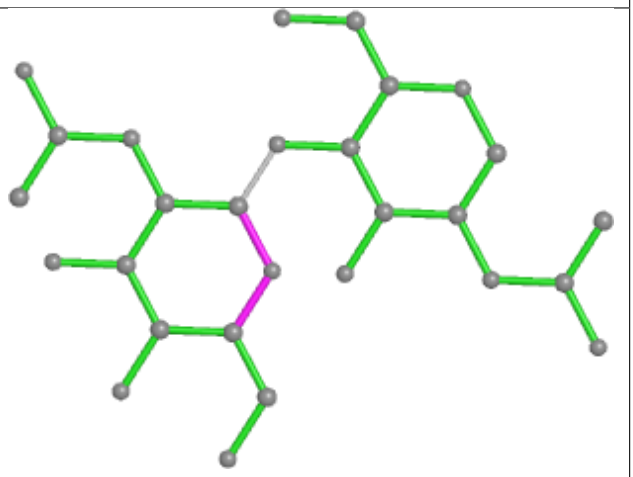


Rings

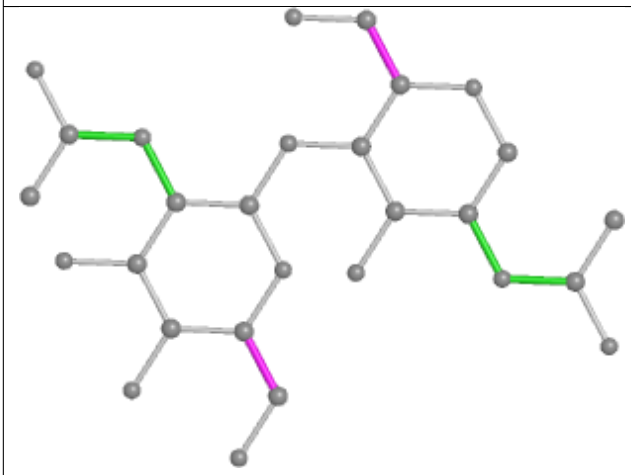
Oligosaccharide Chain P



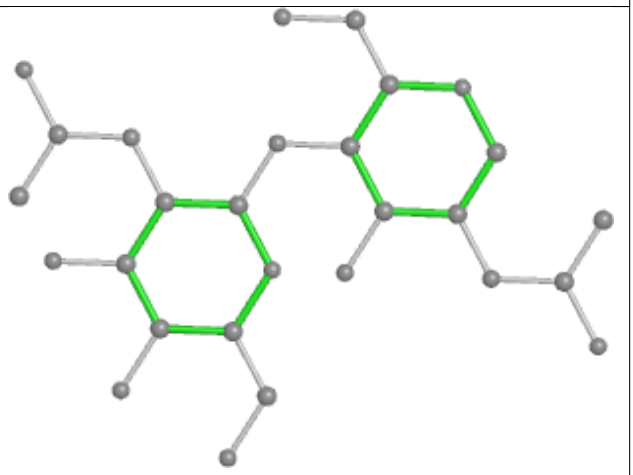
Bond lengths



Bond angles

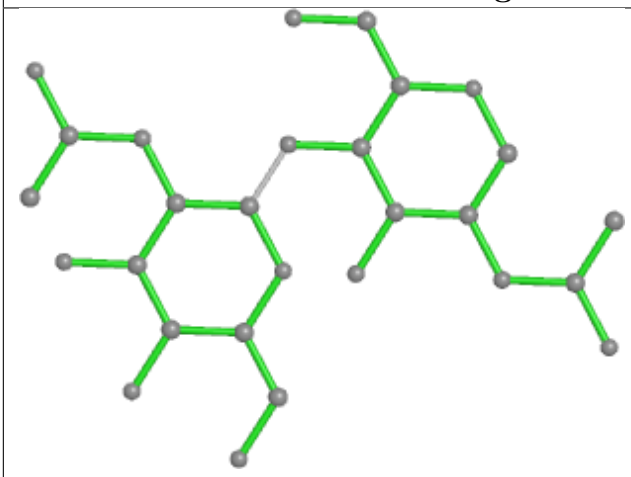


Torsions

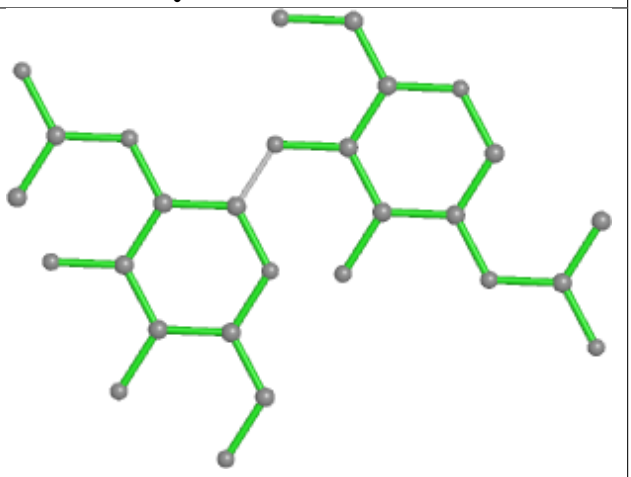


Rings

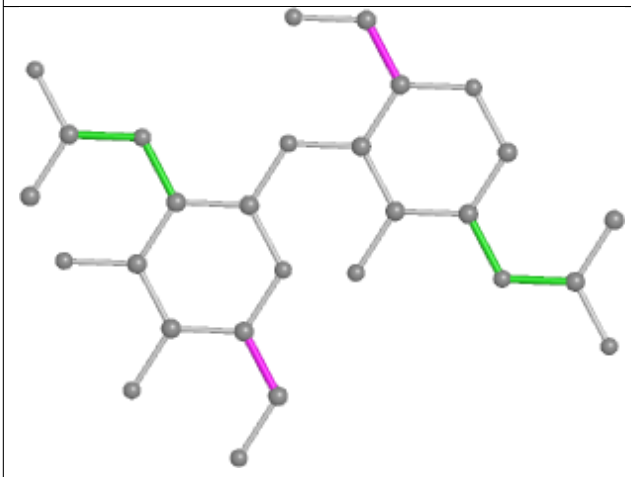
Oligosaccharide Chain Q



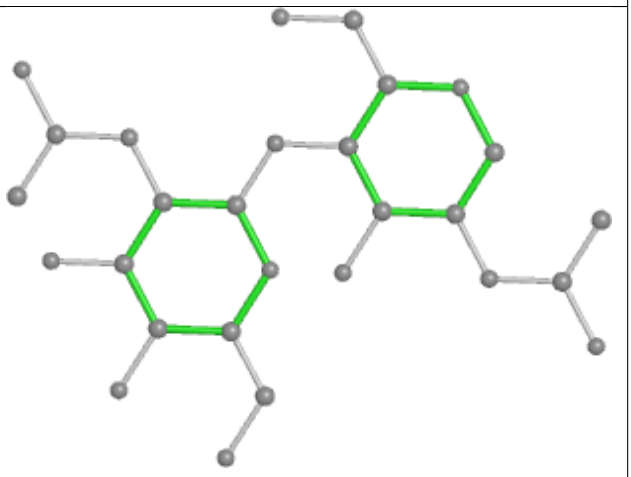
Bond lengths



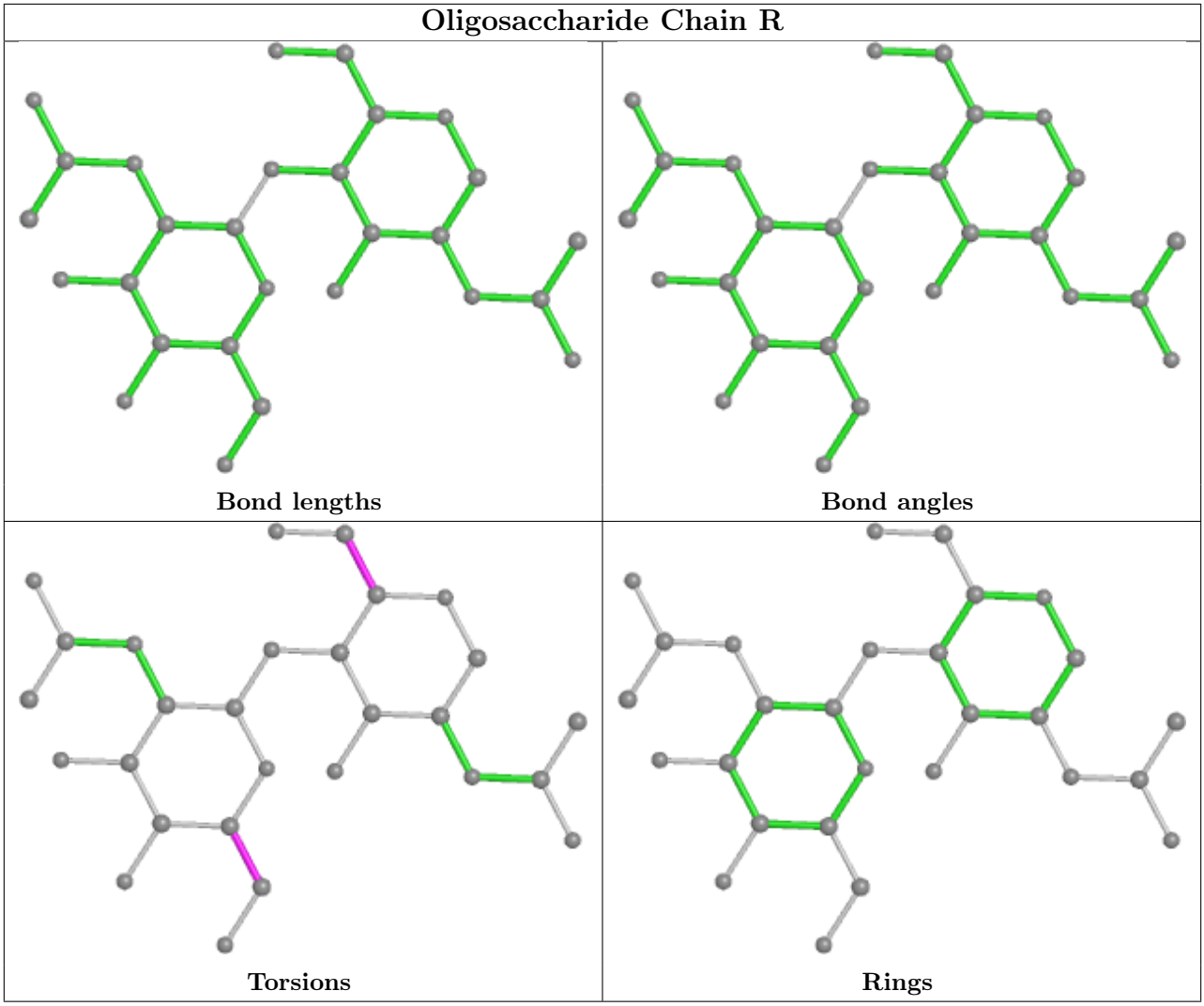
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

51 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	C	2016	1	14,14,15	0.40	0	17,19,21	0.56	0
4	NAG	B	2013	1	14,14,15	0.27	0	17,19,21	0.49	0
4	NAG	B	2012	1	14,14,15	0.35	0	17,19,21	0.59	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	B	2016	1	14,14,15	0.41	0	17,19,21	0.54	0
4	NAG	C	2003	1	14,14,15	0.42	0	17,19,21	0.39	0
4	NAG	C	2006	1	14,14,15	0.37	0	17,19,21	0.47	0
4	NAG	A	2009	1	14,14,15	0.35	0	17,19,21	0.59	1 (5%)
4	NAG	A	2012	1	14,14,15	0.30	0	17,19,21	0.61	1 (5%)
4	NAG	A	2010	1	14,14,15	0.35	0	17,19,21	0.41	0
4	NAG	B	2009	1	14,14,15	0.30	0	17,19,21	0.58	0
4	NAG	A	2002	1	14,14,15	0.48	0	17,19,21	0.49	0
4	NAG	C	2014	1	14,14,15	0.46	0	17,19,21	0.50	0
4	NAG	C	2009	1	14,14,15	0.33	0	17,19,21	0.59	1 (5%)
4	NAG	C	2010	1	14,14,15	0.33	0	17,19,21	0.37	0
4	NAG	C	2011	1	14,14,15	0.36	0	17,19,21	0.55	0
4	NAG	B	2002	1	14,14,15	0.50	0	17,19,21	0.53	0
4	NAG	A	2013	1	14,14,15	0.40	0	17,19,21	0.43	0
4	NAG	B	2010	1	14,14,15	0.34	0	17,19,21	0.39	0
4	NAG	A	2016	1	14,14,15	0.38	0	17,19,21	0.60	1 (5%)
4	NAG	A	2007	1	14,14,15	0.36	0	17,19,21	0.51	0
4	NAG	C	2008	1	14,14,15	0.48	0	17,19,21	0.60	1 (5%)
4	NAG	A	2005	1	14,14,15	0.37	0	17,19,21	0.52	0
4	NAG	B	2006	1	14,14,15	0.33	0	17,19,21	0.47	0
4	NAG	A	2015	1	14,14,15	0.32	0	17,19,21	0.53	0
4	NAG	A	2017	1	14,14,15	0.41	0	17,19,21	0.51	0
4	NAG	C	2005	1	14,14,15	0.31	0	17,19,21	0.53	0
4	NAG	B	2007	1	14,14,15	0.41	0	17,19,21	0.58	1 (5%)
4	NAG	C	2004	1	14,14,15	0.32	0	17,19,21	0.52	0
4	NAG	C	2017	1	14,14,15	0.32	0	17,19,21	0.51	0
4	NAG	C	2012	1	14,14,15	0.34	0	17,19,21	0.57	0
4	NAG	B	2005	1	14,14,15	0.40	0	17,19,21	0.52	0
4	NAG	B	2015	1	14,14,15	0.38	0	17,19,21	0.54	0
4	NAG	B	2003	1	14,14,15	0.47	0	17,19,21	0.39	0
4	NAG	B	2017	1	14,14,15	0.37	0	17,19,21	0.52	0
4	NAG	A	2014	1	14,14,15	0.33	0	17,19,21	0.43	0
4	NAG	B	2014	1	14,14,15	0.45	0	17,19,21	0.48	0
4	NAG	C	2007	1	14,14,15	0.41	0	17,19,21	0.45	0
4	NAG	C	2013	1	14,14,15	0.31	0	17,19,21	0.44	0
4	NAG	B	2001	1	14,14,15	0.51	0	17,19,21	0.52	0
4	NAG	A	2008	1	14,14,15	0.37	0	17,19,21	0.57	0
4	NAG	A	2003	1	14,14,15	0.44	0	17,19,21	0.40	0
4	NAG	A	2001	1	14,14,15	0.41	0	17,19,21	0.49	0
4	NAG	A	2011	1	14,14,15	0.32	0	17,19,21	0.56	0
4	NAG	B	2011	1	14,14,15	0.43	0	17,19,21	0.65	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	C	2001	1	14,14,15	0.41	0	17,19,21	0.50	0
4	NAG	C	2015	1	14,14,15	0.32	0	17,19,21	0.53	0
4	NAG	C	2002	1	14,14,15	0.50	0	17,19,21	0.53	0
4	NAG	A	2006	1	14,14,15	0.36	0	17,19,21	0.47	0
4	NAG	A	2004	1	14,14,15	0.38	0	17,19,21	0.54	0
4	NAG	B	2008	1	14,14,15	0.42	0	17,19,21	0.58	0
4	NAG	B	2004	1	14,14,15	0.34	0	17,19,21	0.49	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	2016	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2013	1	-	1/6/23/26	0/1/1/1
4	NAG	B	2012	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2016	1	-	2/6/23/26	0/1/1/1
4	NAG	C	2003	1	-	2/6/23/26	0/1/1/1
4	NAG	C	2006	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2009	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2012	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2010	1	-	0/6/23/26	0/1/1/1
4	NAG	B	2009	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2002	1	-	2/6/23/26	0/1/1/1
4	NAG	C	2014	1	-	2/6/23/26	0/1/1/1
4	NAG	C	2009	1	-	2/6/23/26	0/1/1/1
4	NAG	C	2010	1	-	1/6/23/26	0/1/1/1
4	NAG	C	2011	1	-	0/6/23/26	0/1/1/1
4	NAG	B	2002	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2013	1	-	1/6/23/26	0/1/1/1
4	NAG	B	2010	1	-	1/6/23/26	0/1/1/1
4	NAG	A	2016	1	-	0/6/23/26	0/1/1/1
4	NAG	A	2007	1	-	2/6/23/26	0/1/1/1
4	NAG	C	2008	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2005	1	-	1/6/23/26	0/1/1/1
4	NAG	B	2006	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2015	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2017	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	2005	1	-	0/6/23/26	0/1/1/1
4	NAG	B	2007	1	-	1/6/23/26	0/1/1/1
4	NAG	C	2004	1	-	2/6/23/26	0/1/1/1
4	NAG	C	2017	1	-	0/6/23/26	0/1/1/1
4	NAG	C	2012	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2005	1	-	0/6/23/26	0/1/1/1
4	NAG	B	2015	1	-	0/6/23/26	0/1/1/1
4	NAG	B	2003	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2017	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2014	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2014	1	-	2/6/23/26	0/1/1/1
4	NAG	C	2007	1	-	2/6/23/26	0/1/1/1
4	NAG	C	2013	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2001	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2008	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2003	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2001	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2011	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2011	1	-	2/6/23/26	0/1/1/1
4	NAG	C	2001	1	-	1/6/23/26	0/1/1/1
4	NAG	C	2015	1	-	0/6/23/26	0/1/1/1
4	NAG	C	2002	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2006	1	-	0/6/23/26	0/1/1/1
4	NAG	A	2004	1	-	1/6/23/26	0/1/1/1
4	NAG	B	2008	1	-	0/6/23/26	0/1/1/1
4	NAG	B	2004	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	2011	NAG	C1-O5-C5	2.28	115.28	112.19
4	C	2008	NAG	C1-O5-C5	2.11	115.06	112.19
4	A	2012	NAG	C1-O5-C5	2.08	115.01	112.19
4	A	2009	NAG	C1-O5-C5	2.07	115.00	112.19
4	B	2012	NAG	C1-O5-C5	2.07	115.00	112.19
4	A	2016	NAG	C1-O5-C5	2.06	114.99	112.19
4	C	2009	NAG	C1-O5-C5	2.04	114.96	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	2007	NAG	C1-O5-C5	2.01	114.91	112.19

There are no chirality outliers.

All (74) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2012	NAG	O5-C5-C6-O6
4	A	2015	NAG	O5-C5-C6-O6
4	C	2014	NAG	O5-C5-C6-O6
4	B	2002	NAG	O5-C5-C6-O6
4	B	2004	NAG	O5-C5-C6-O6
4	A	2008	NAG	O5-C5-C6-O6
4	A	2011	NAG	O5-C5-C6-O6
4	B	2014	NAG	O5-C5-C6-O6
4	C	2002	NAG	O5-C5-C6-O6
4	C	2016	NAG	O5-C5-C6-O6
4	A	2017	NAG	O5-C5-C6-O6
4	B	2001	NAG	O5-C5-C6-O6
4	C	2009	NAG	O5-C5-C6-O6
4	A	2011	NAG	C4-C5-C6-O6
4	A	2012	NAG	C4-C5-C6-O6
4	B	2002	NAG	C4-C5-C6-O6
4	B	2003	NAG	O5-C5-C6-O6
4	B	2004	NAG	C4-C5-C6-O6
4	A	2007	NAG	O5-C5-C6-O6
4	C	2004	NAG	O5-C5-C6-O6
4	B	2001	NAG	C4-C5-C6-O6
4	B	2011	NAG	C4-C5-C6-O6
4	A	2003	NAG	O5-C5-C6-O6
4	C	2013	NAG	O5-C5-C6-O6
4	A	2014	NAG	C4-C5-C6-O6
4	C	2014	NAG	C4-C5-C6-O6
4	B	2016	NAG	O5-C5-C6-O6
4	C	2007	NAG	O5-C5-C6-O6
4	C	2008	NAG	O5-C5-C6-O6
4	B	2017	NAG	O5-C5-C6-O6
4	B	2014	NAG	C4-C5-C6-O6
4	C	2002	NAG	C4-C5-C6-O6
4	A	2015	NAG	C4-C5-C6-O6
4	B	2011	NAG	O5-C5-C6-O6
4	C	2013	NAG	C4-C5-C6-O6
4	C	2006	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	B	2017	NAG	C4-C5-C6-O6
4	A	2008	NAG	C4-C5-C6-O6
4	B	2003	NAG	C4-C5-C6-O6
4	C	2004	NAG	C4-C5-C6-O6
4	C	2007	NAG	C4-C5-C6-O6
4	C	2016	NAG	C4-C5-C6-O6
4	C	2008	NAG	C4-C5-C6-O6
4	C	2009	NAG	C4-C5-C6-O6
4	A	2014	NAG	O5-C5-C6-O6
4	A	2003	NAG	C4-C5-C6-O6
4	A	2017	NAG	C4-C5-C6-O6
4	C	2003	NAG	O5-C5-C6-O6
4	C	2012	NAG	O5-C5-C6-O6
4	A	2001	NAG	C4-C5-C6-O6
4	B	2016	NAG	C4-C5-C6-O6
4	C	2012	NAG	C4-C5-C6-O6
4	B	2012	NAG	O5-C5-C6-O6
4	B	2012	NAG	C4-C5-C6-O6
4	C	2006	NAG	C4-C5-C6-O6
4	B	2006	NAG	O5-C5-C6-O6
4	A	2007	NAG	C4-C5-C6-O6
4	A	2001	NAG	O5-C5-C6-O6
4	B	2007	NAG	O5-C5-C6-O6
4	B	2009	NAG	O5-C5-C6-O6
4	C	2003	NAG	C4-C5-C6-O6
4	B	2009	NAG	C4-C5-C6-O6
4	A	2002	NAG	C4-C5-C6-O6
4	C	2001	NAG	O5-C5-C6-O6
4	A	2013	NAG	O5-C5-C6-O6
4	B	2013	NAG	O5-C5-C6-O6
4	B	2010	NAG	O5-C5-C6-O6
4	A	2002	NAG	O5-C5-C6-O6
4	A	2009	NAG	C4-C5-C6-O6
4	A	2009	NAG	O5-C5-C6-O6
4	B	2006	NAG	C4-C5-C6-O6
4	C	2010	NAG	C4-C5-C6-O6
4	A	2005	NAG	C4-C5-C6-O6
4	A	2004	NAG	C4-C5-C6-O6

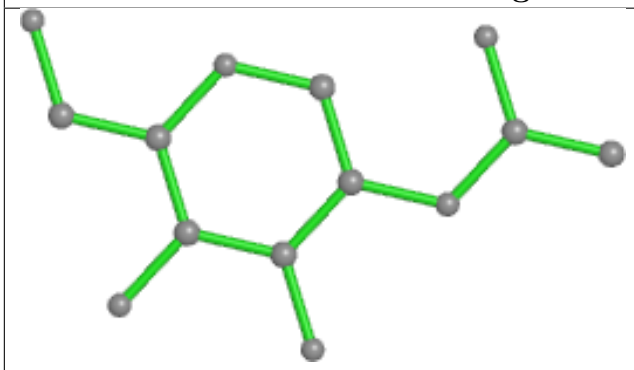
There are no ring outliers.

No monomer is involved in short contacts.

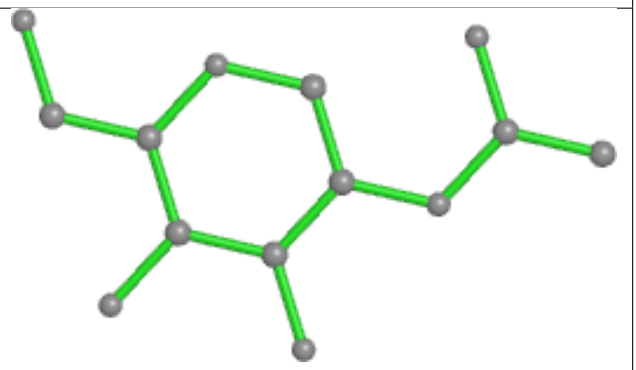
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for 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.

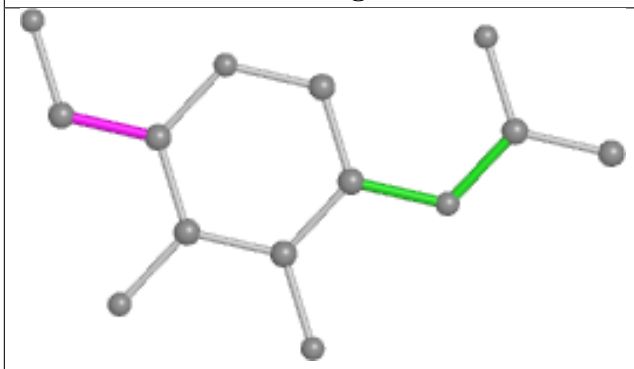
Ligand NAG C 2016



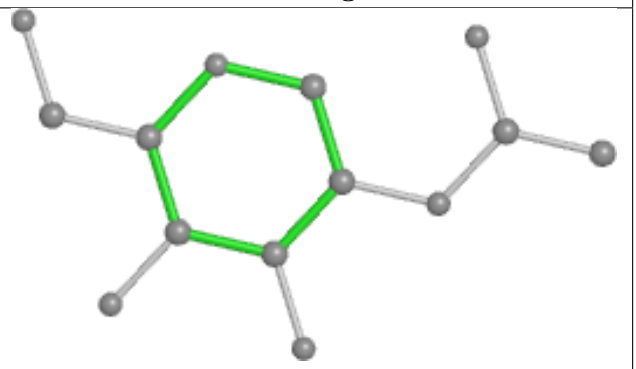
Bond lengths



Bond angles

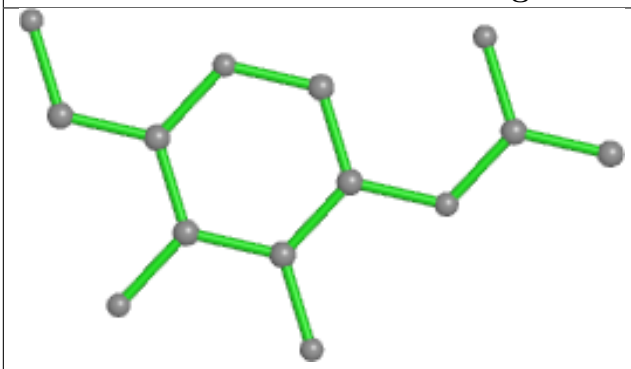


Torsions

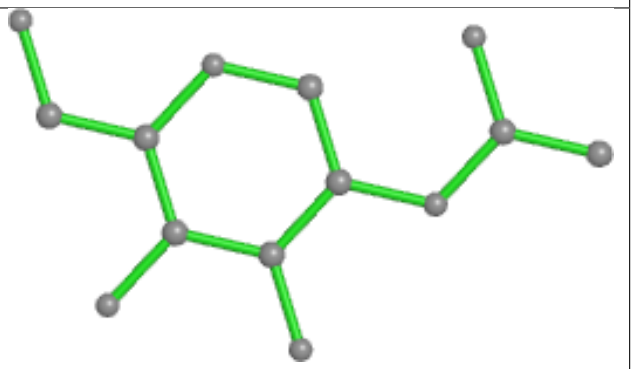


Rings

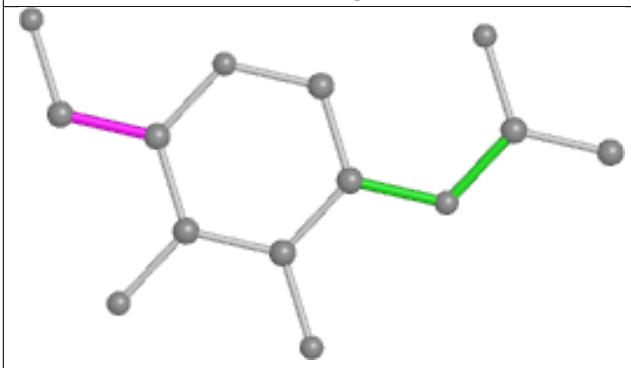
Ligand NAG B 2013



Bond lengths



Bond angles



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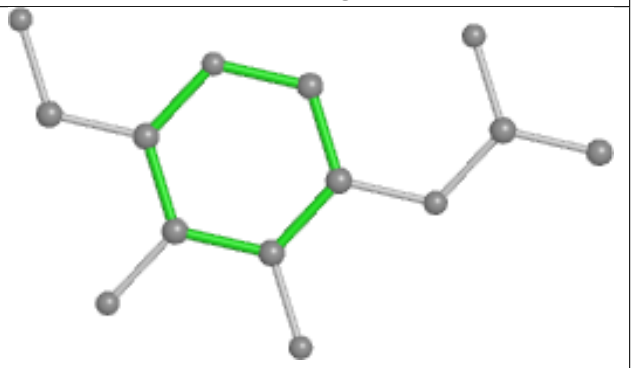
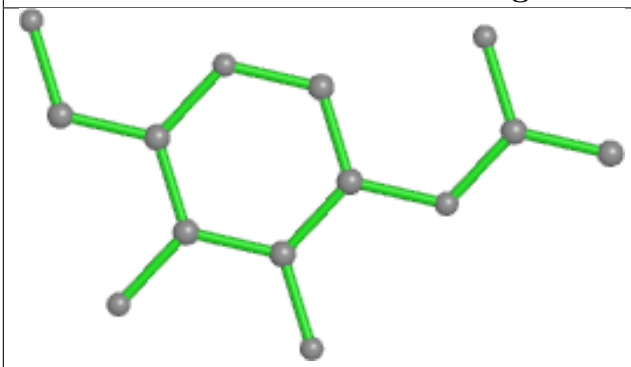


Rings

Ligand NAG B 2012



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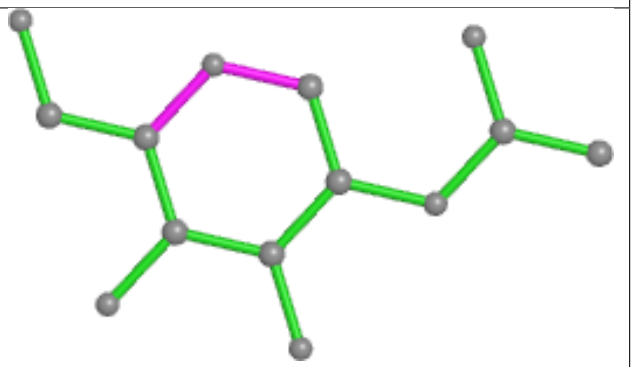
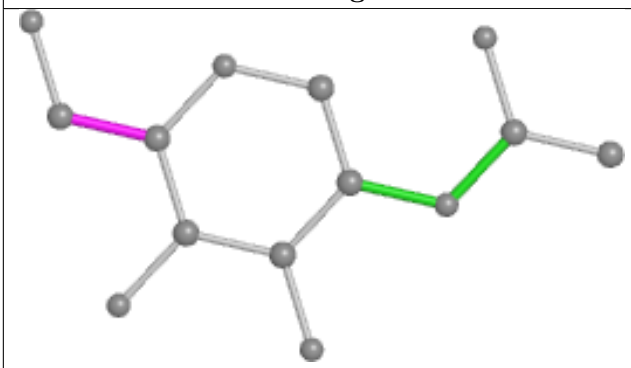
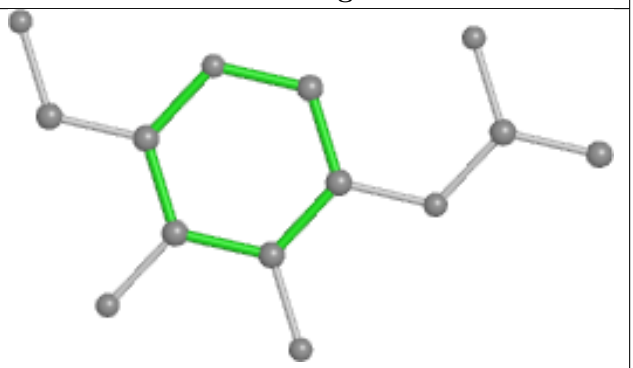


Bond angles

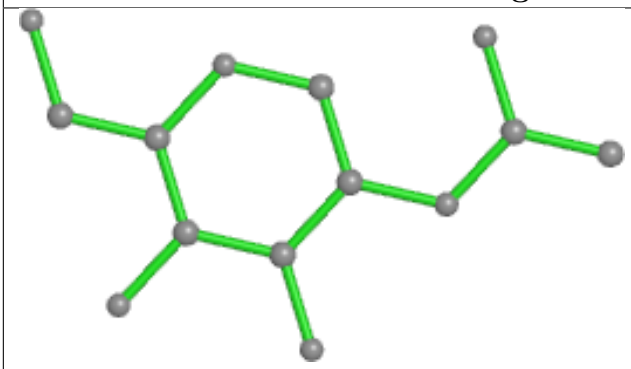


Torsions

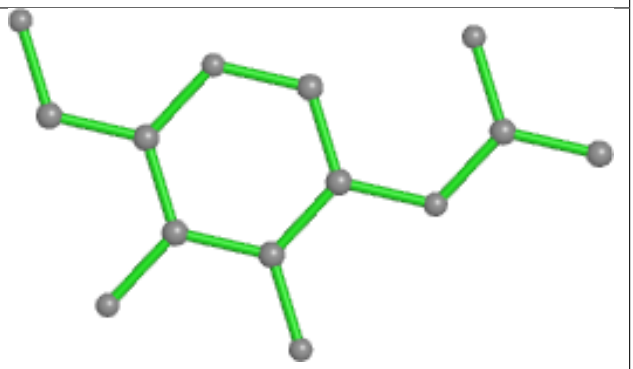


Rings

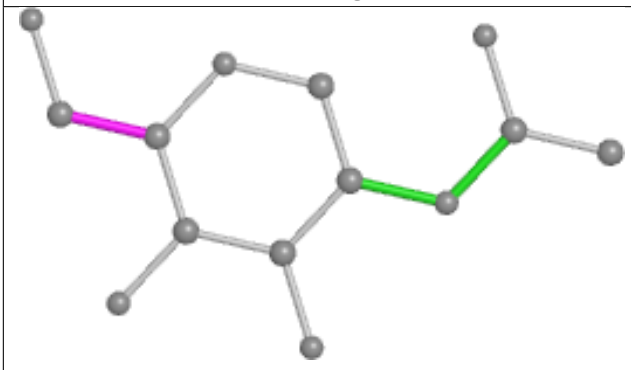
Ligand NAG B 2016



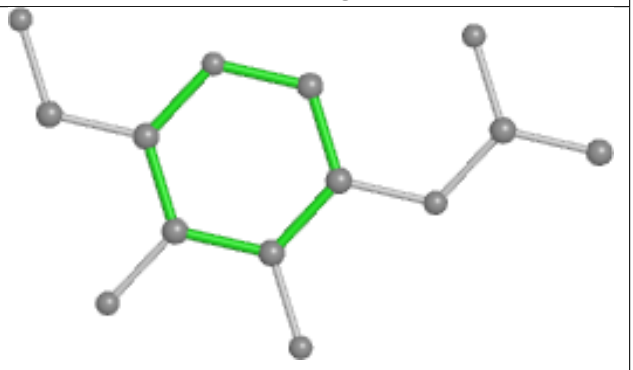
Bond lengths



Bond angles

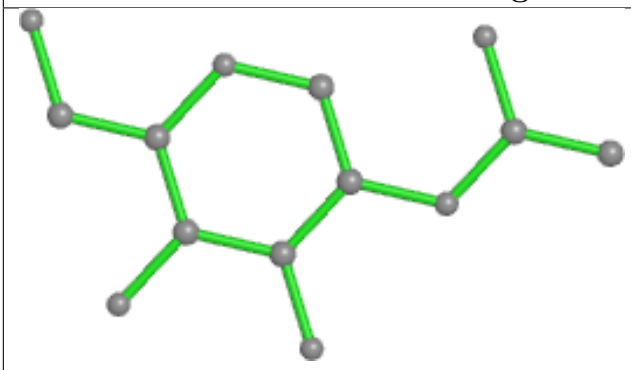


Torsions



Rings

Ligand NAG C 2003



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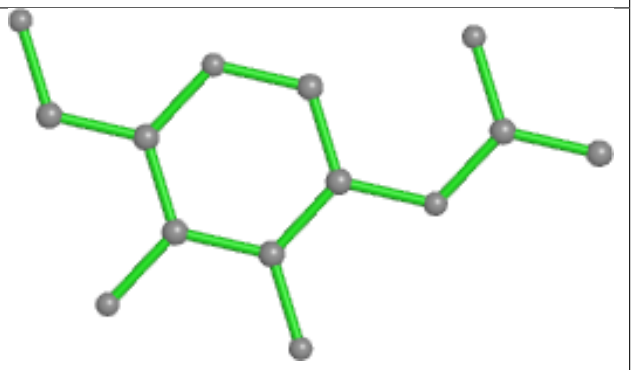
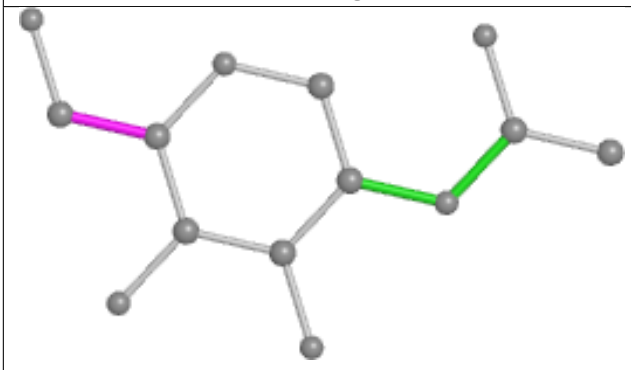


Bond angles



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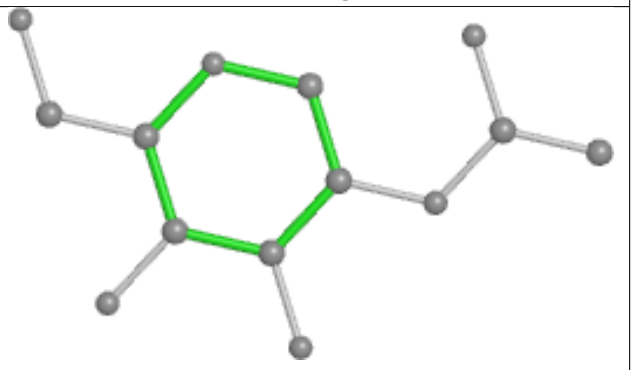
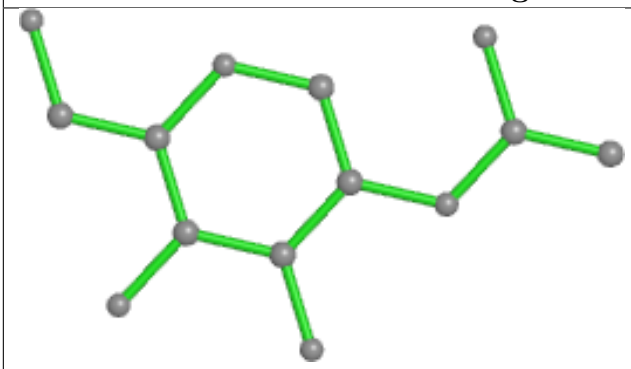


Rings

Ligand NAG C 2006



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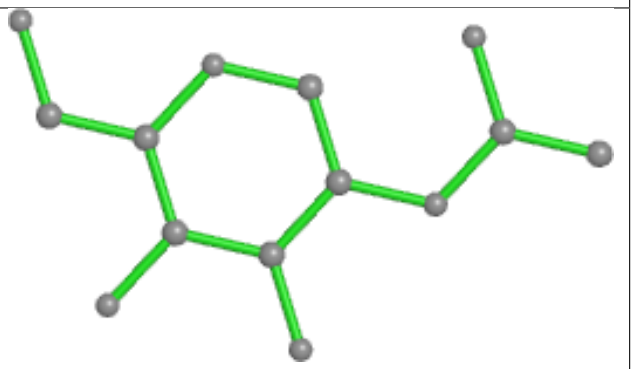
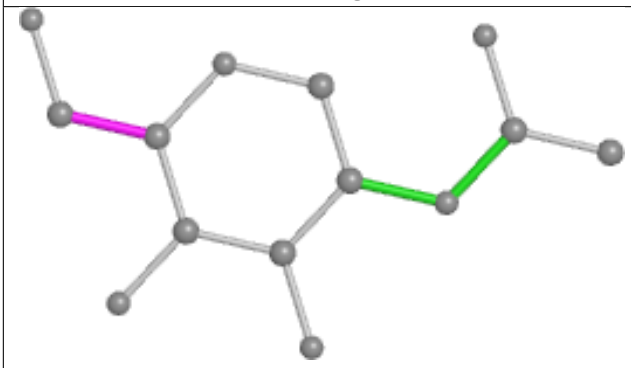


Bond angles



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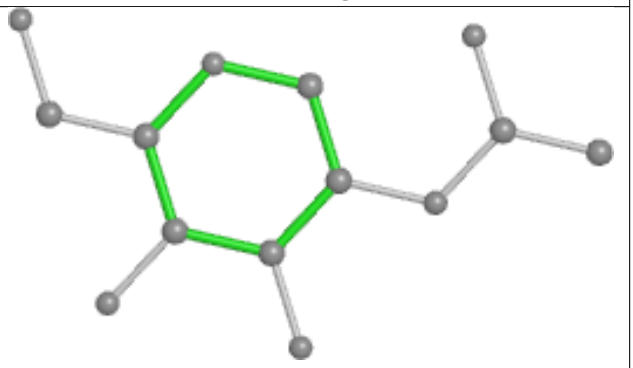
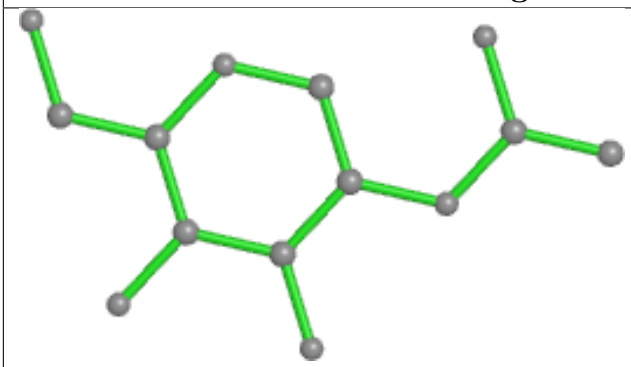


Rings

Ligand NAG A 2009



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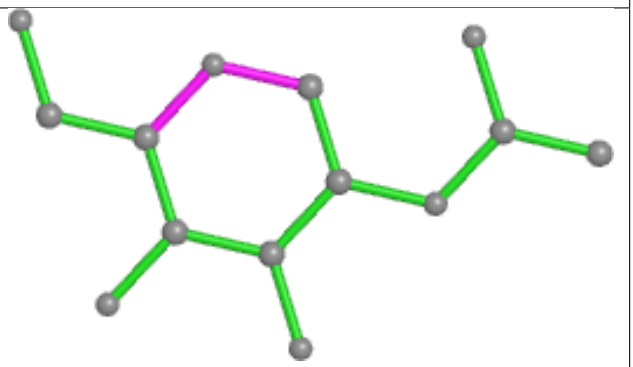

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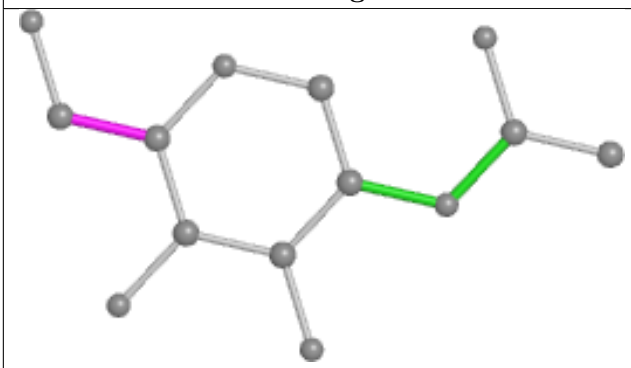

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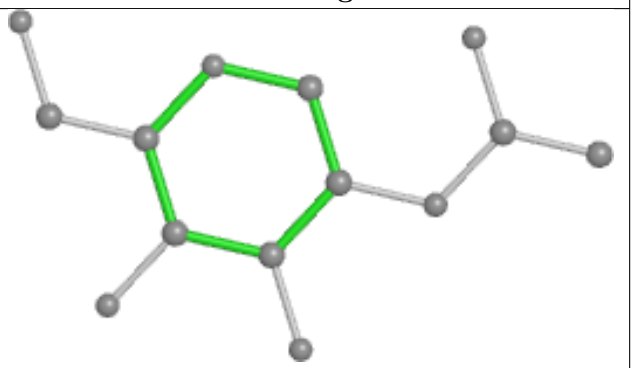
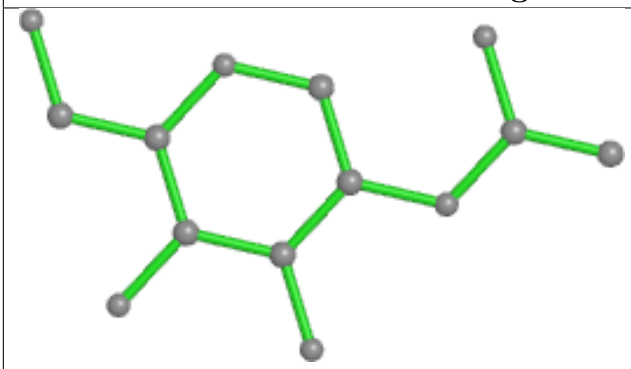


Rings

Ligand NAG A 2012



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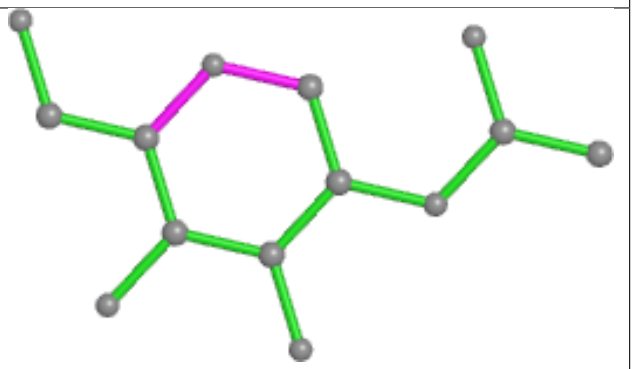

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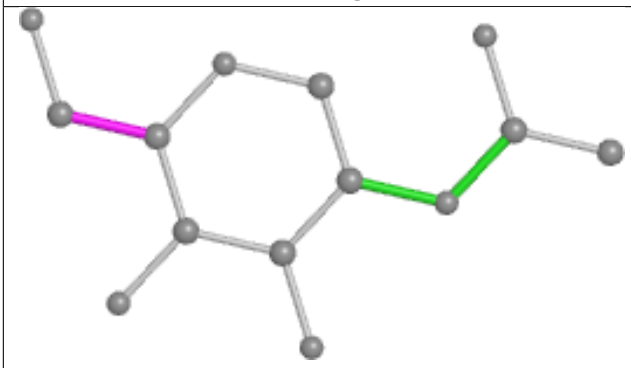
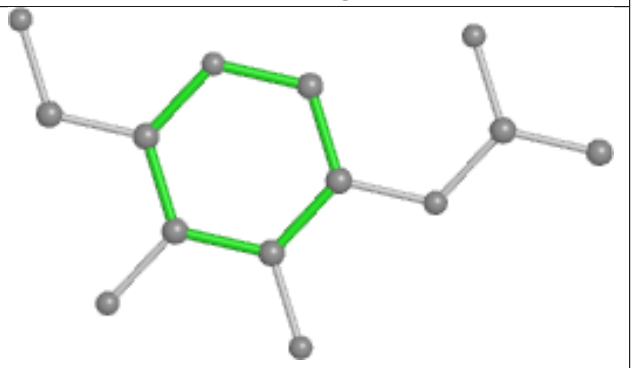
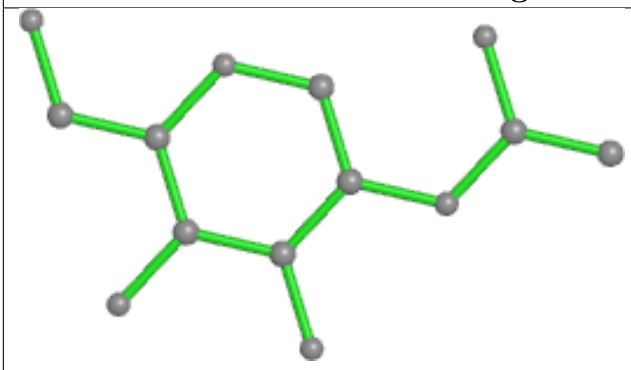


Torsions

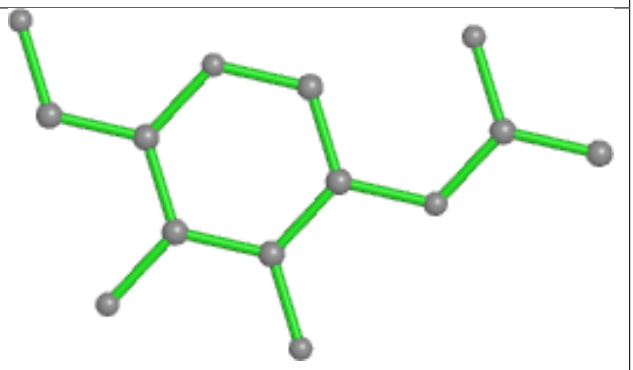


Rings

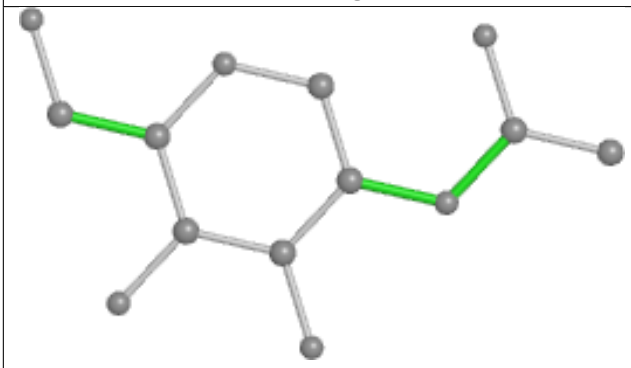
Ligand NAG A 2010



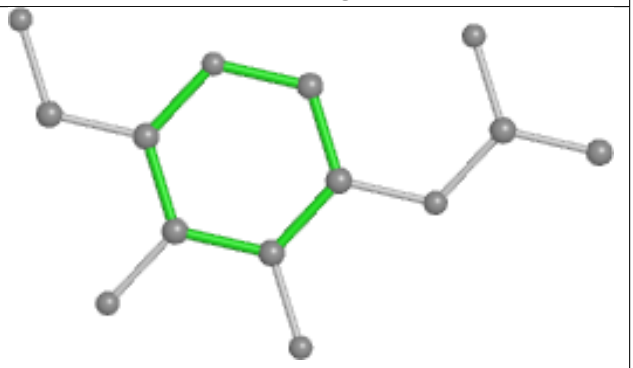
Bond lengths



Bond angles

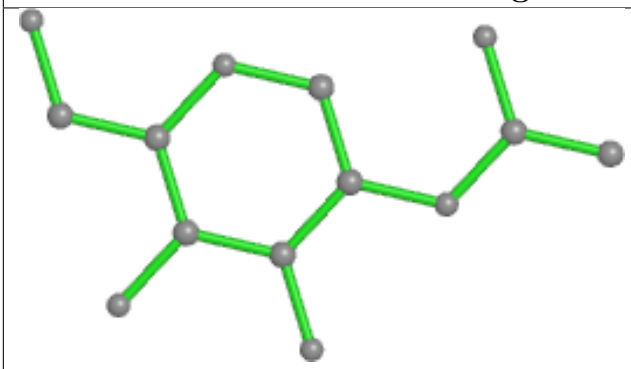


Torsions

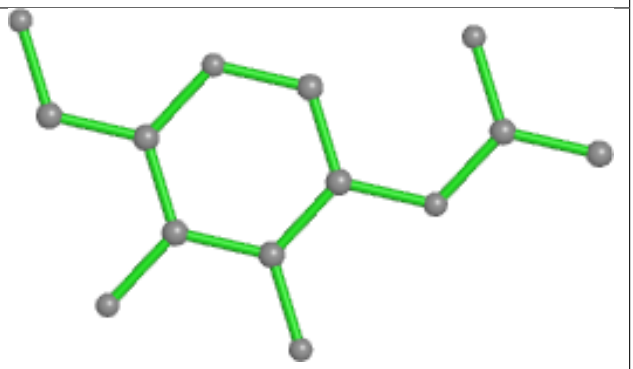


Rings

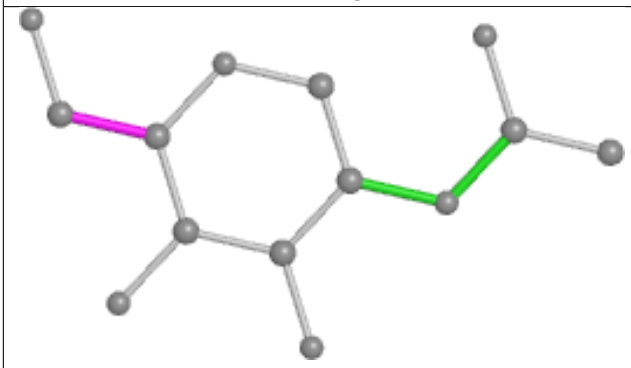
Ligand NAG B 2009



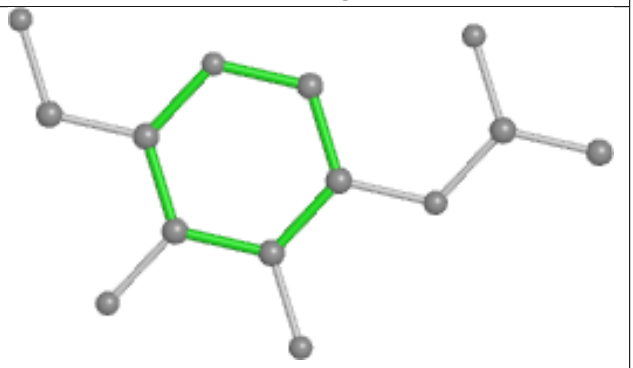
Bond lengths



Bond angles

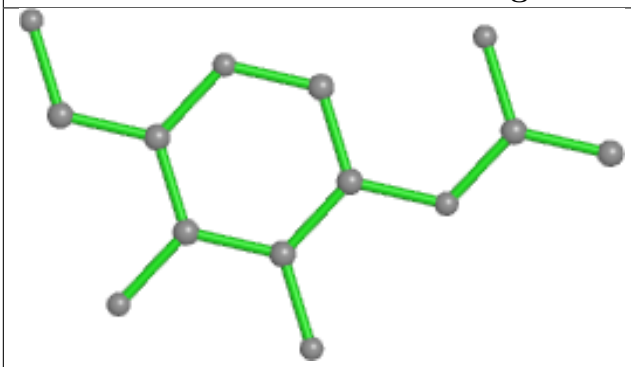


Torsions



Rings

Ligand NAG A 2002



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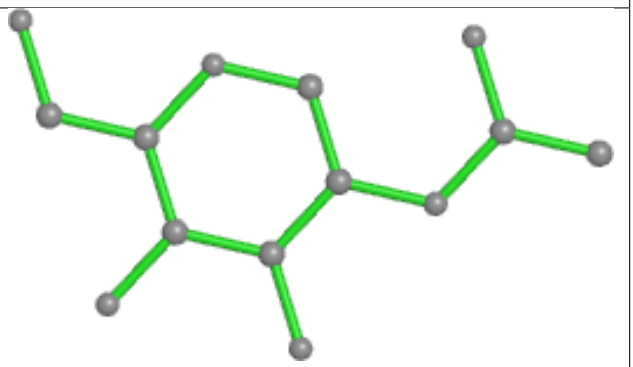

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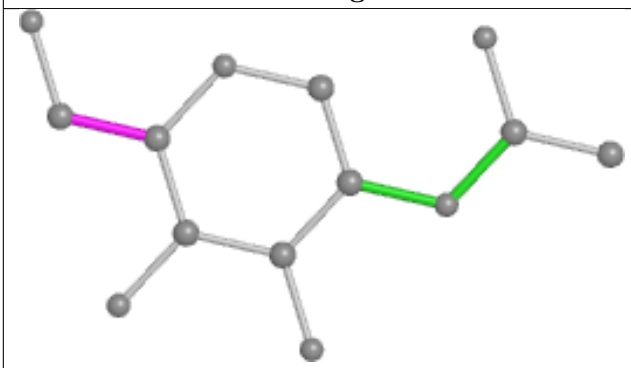

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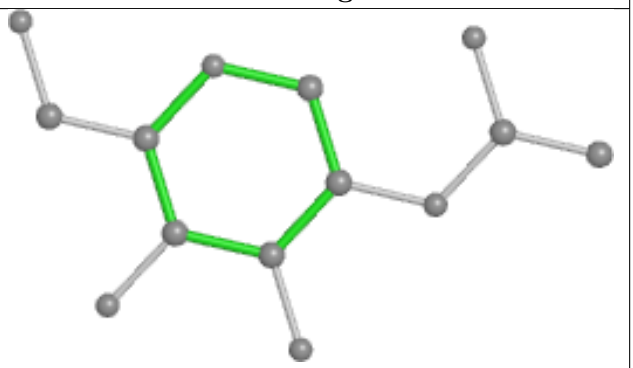
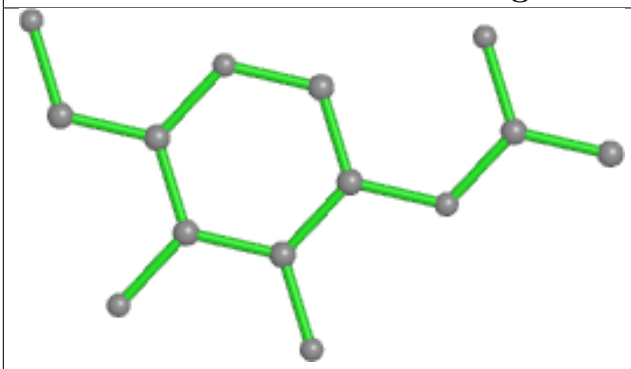


Rings

Ligand NAG C 2014



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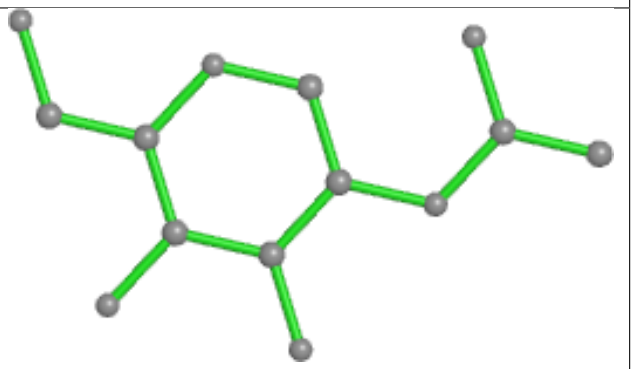

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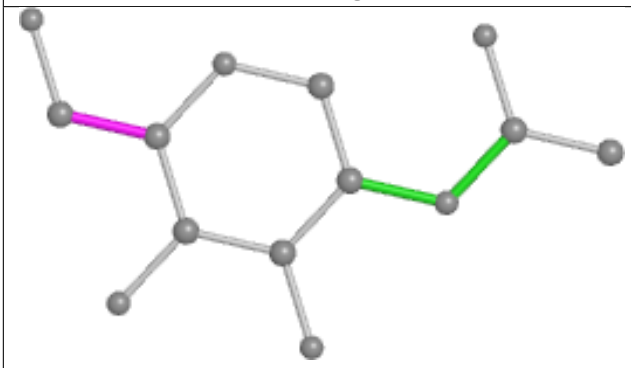

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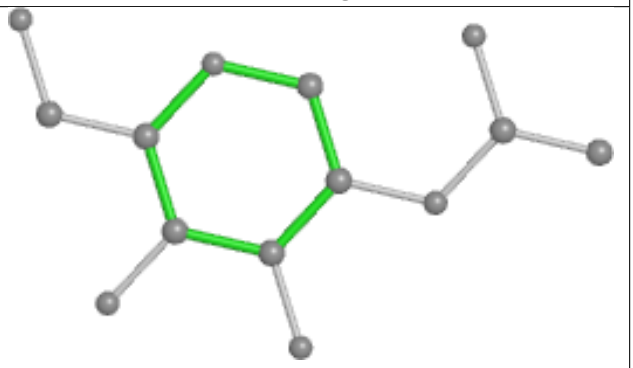
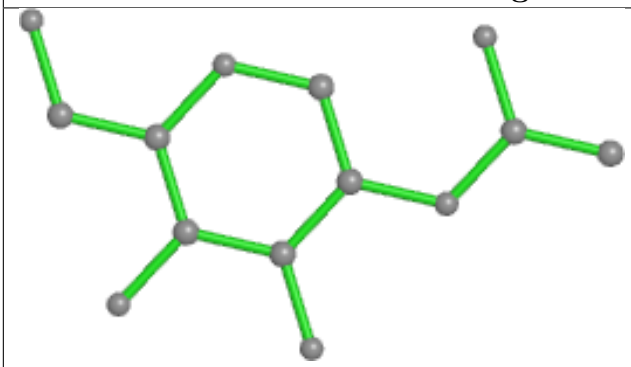


Rings

Ligand NAG C 2009



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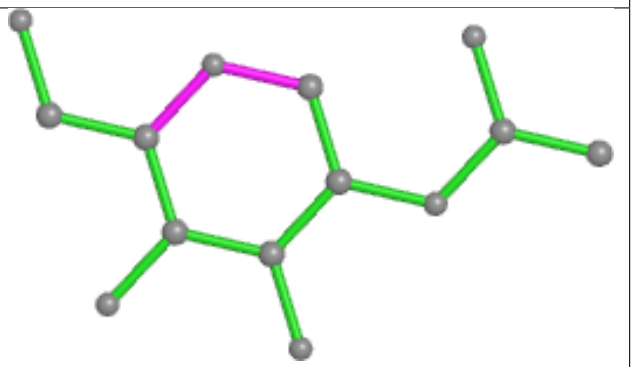

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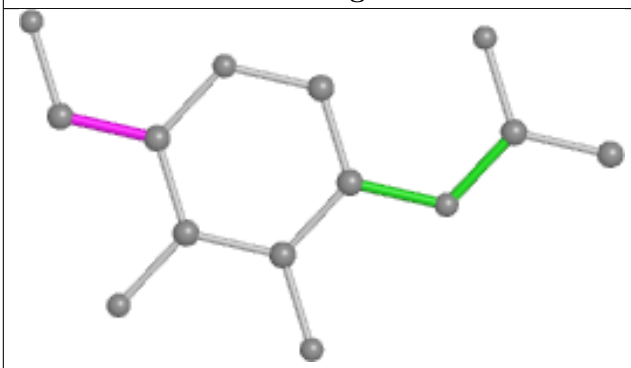

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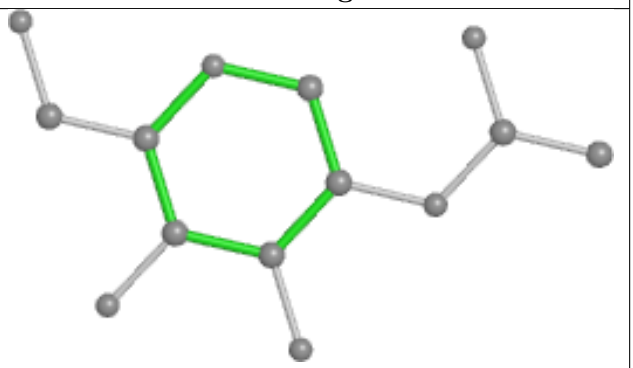
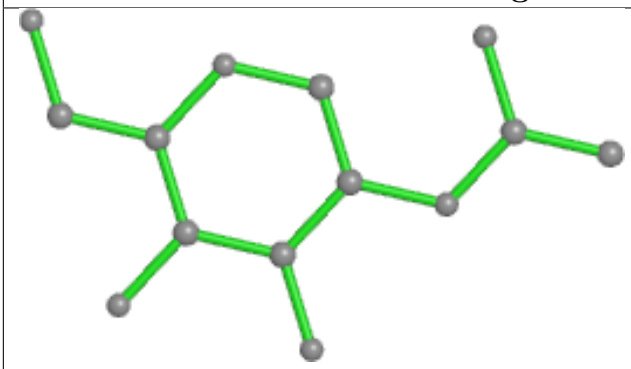


Rings

Ligand NAG C 2010



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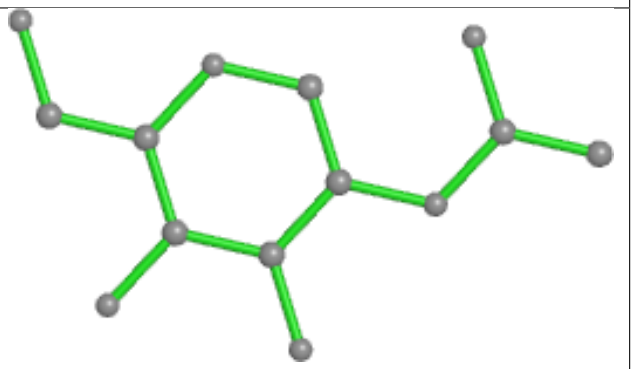

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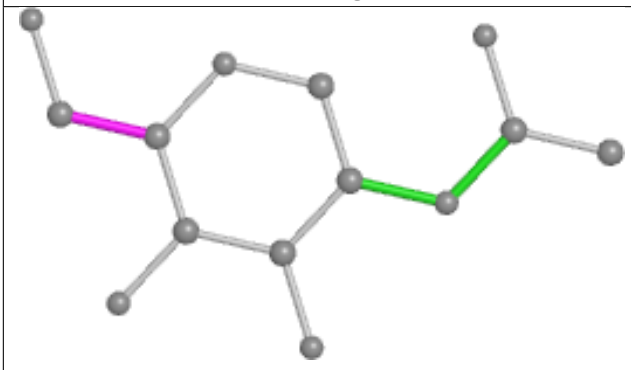

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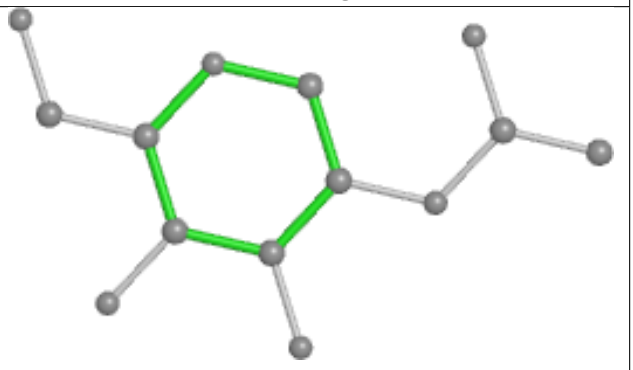
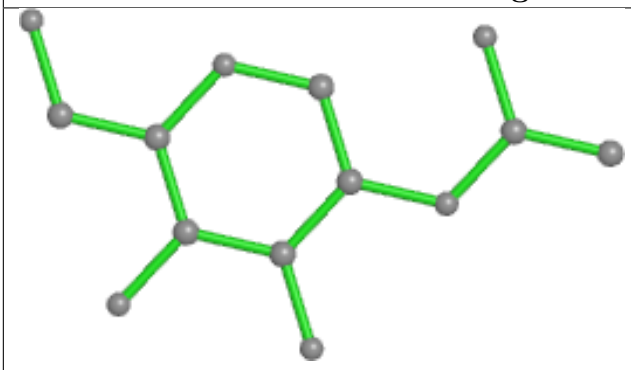


Rings

Ligand NAG C 2011



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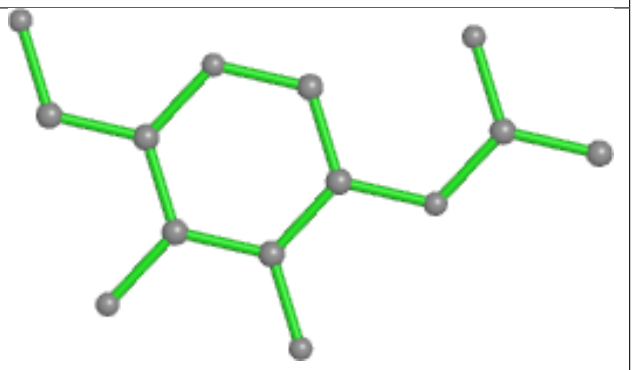

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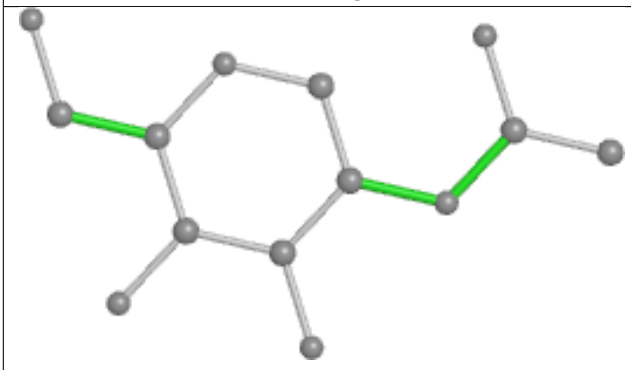

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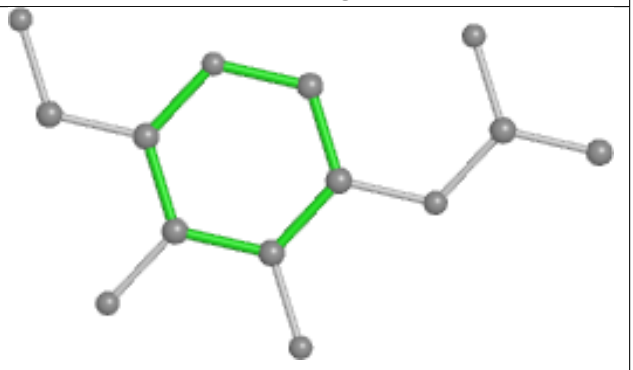
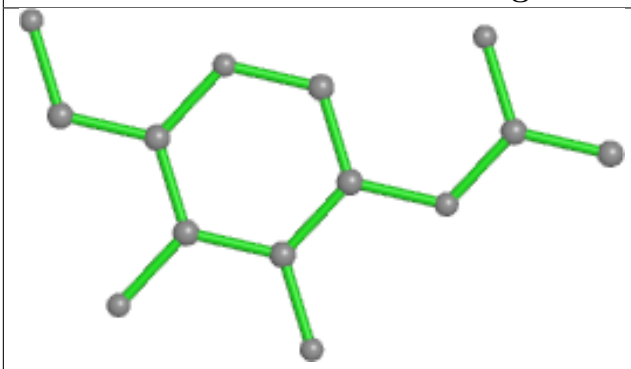


Rings

Ligand NAG B 2002



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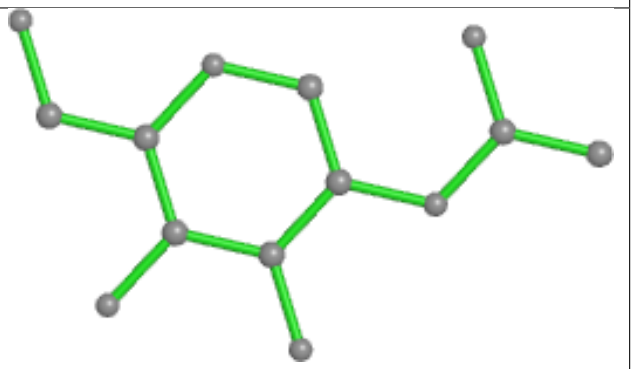

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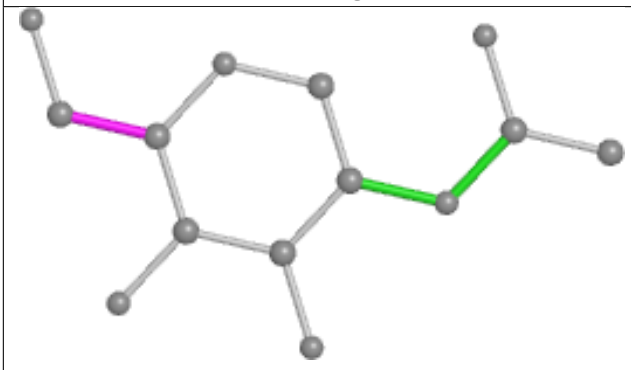

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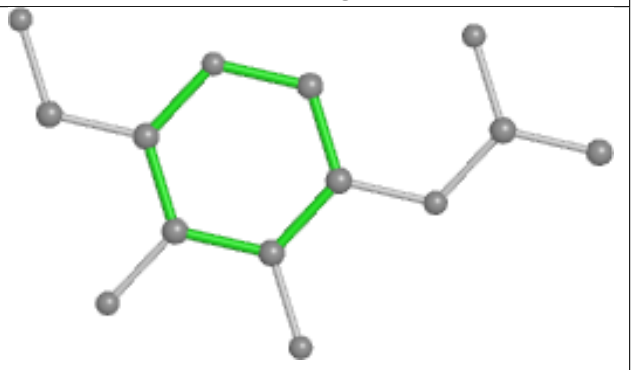
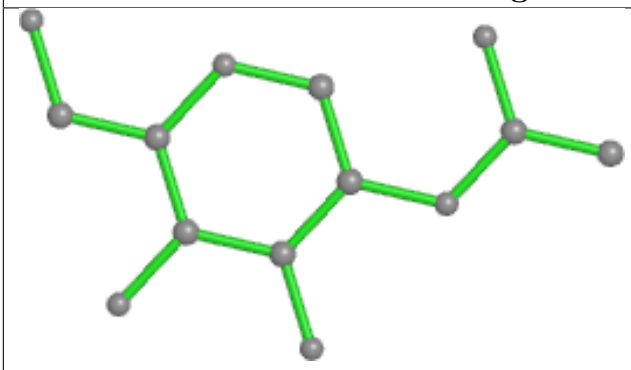


Rings

Ligand NAG A 2013



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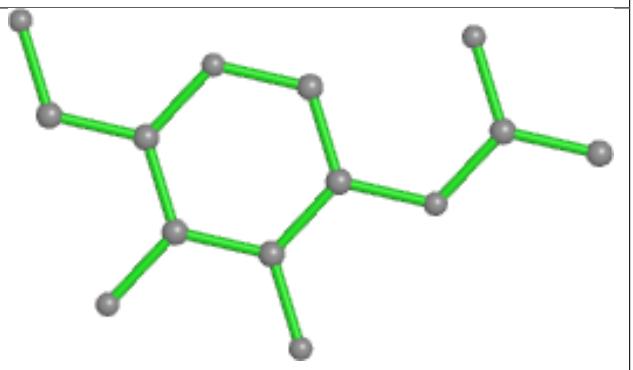

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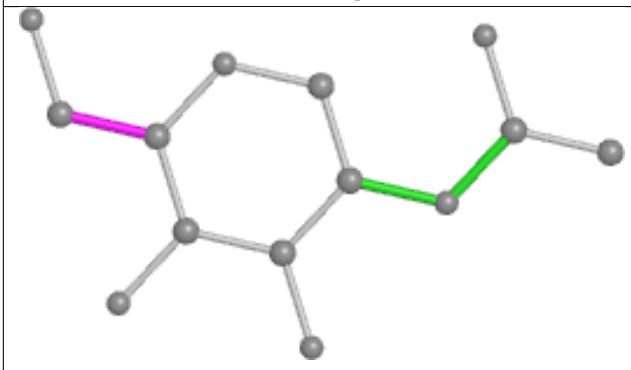

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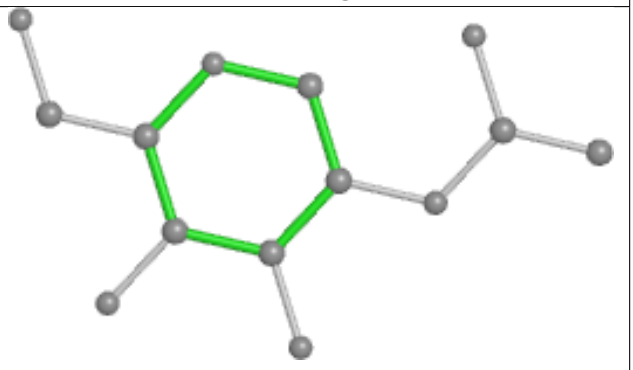
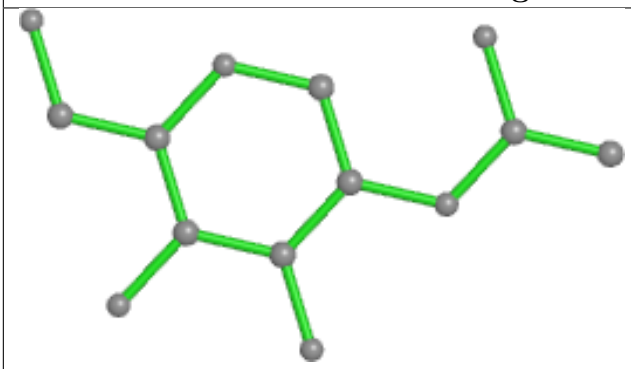


Rings

Ligand NAG B 2010



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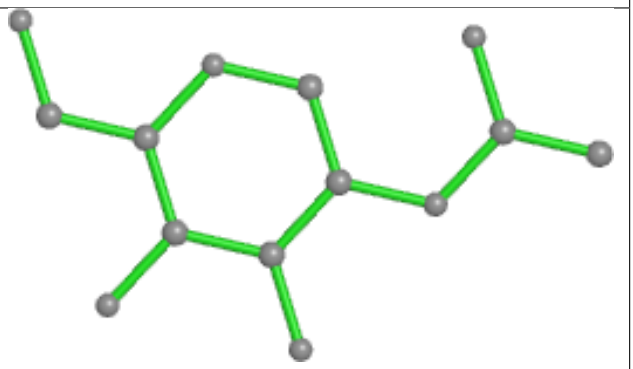

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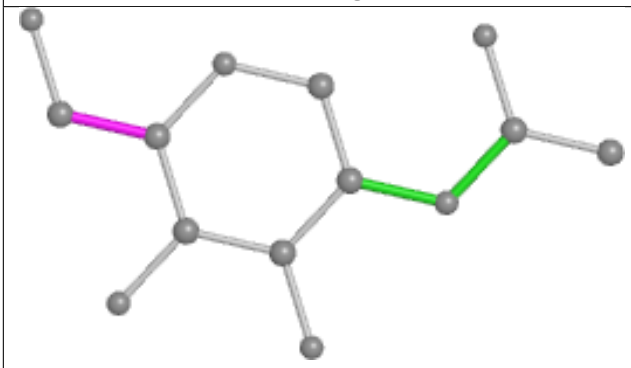

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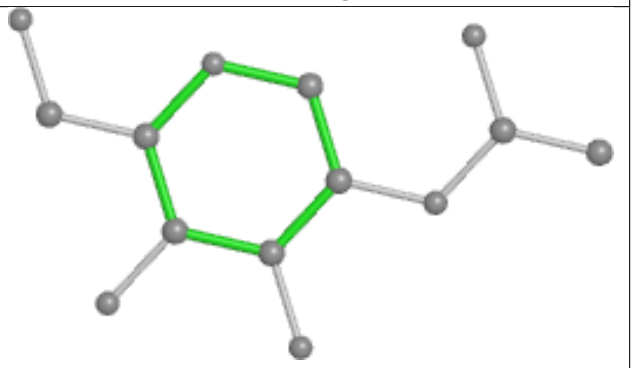
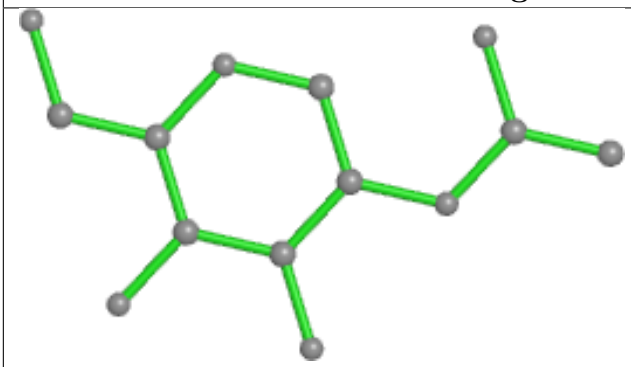


Rings

Ligand NAG A 2016



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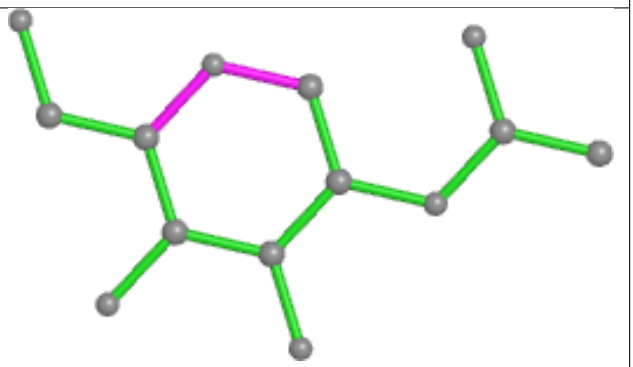
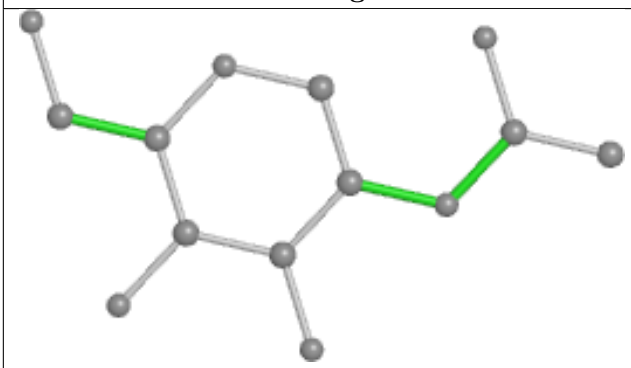


Bond angles



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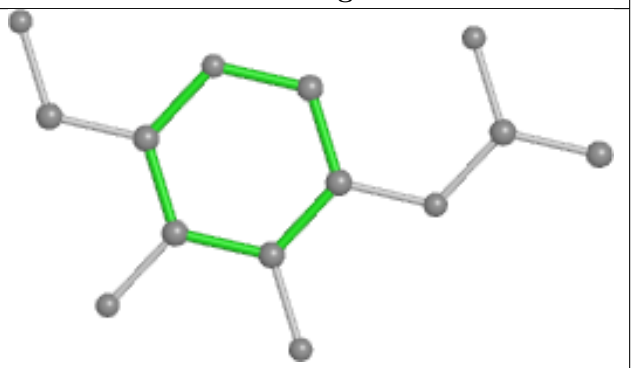
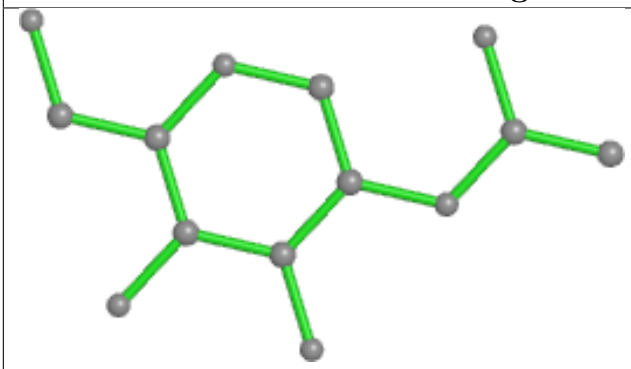


Rings

Ligand NAG A 2007



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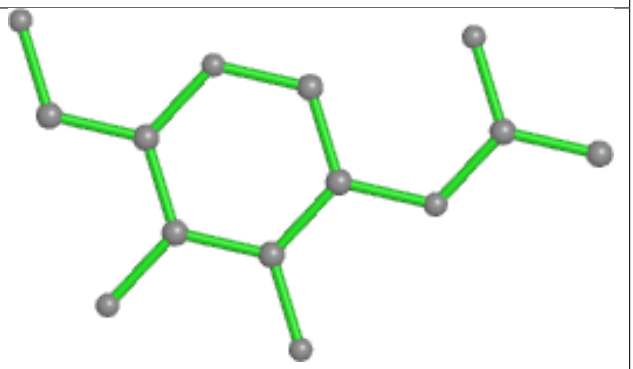

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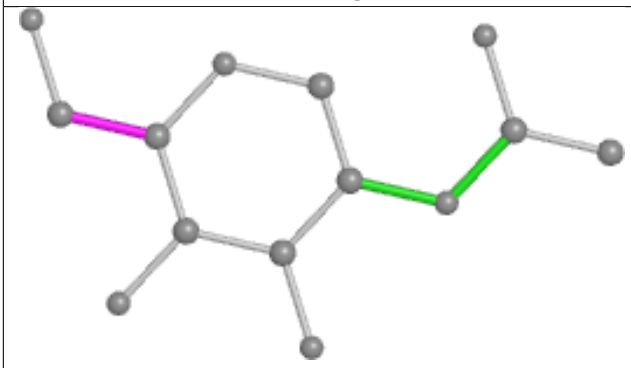

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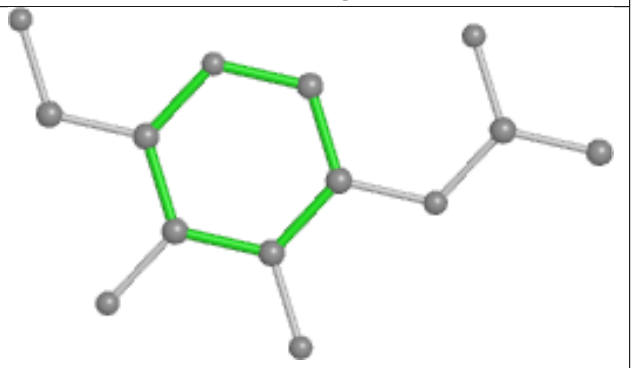
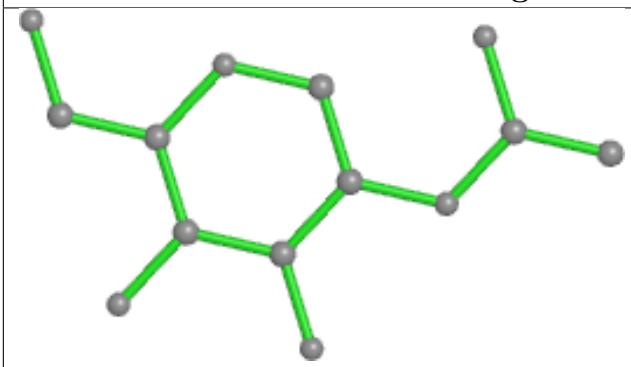


Rings

Ligand NAG C 2008



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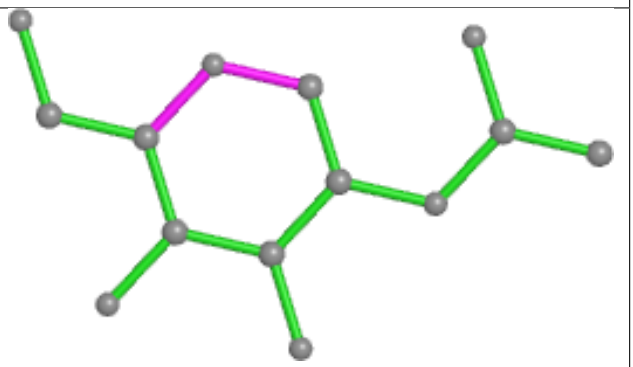

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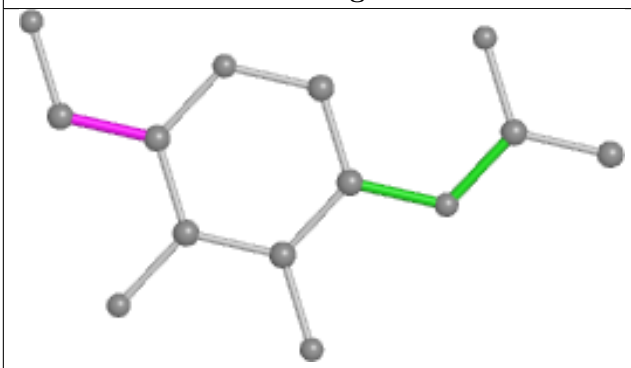

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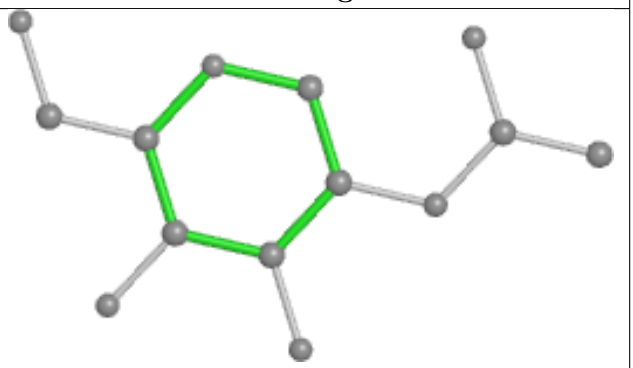
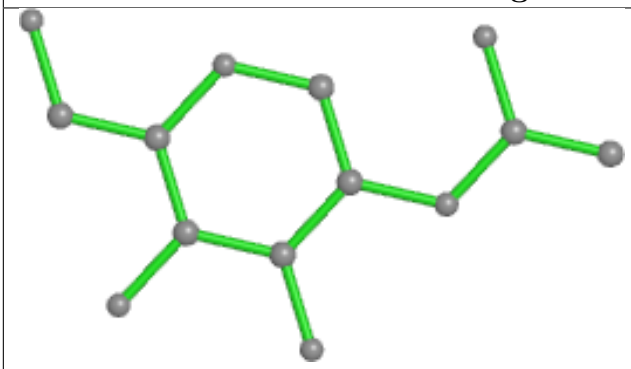


Rings

Ligand NAG A 2005



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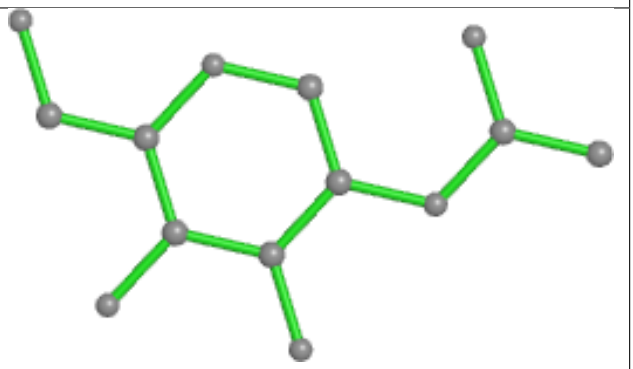

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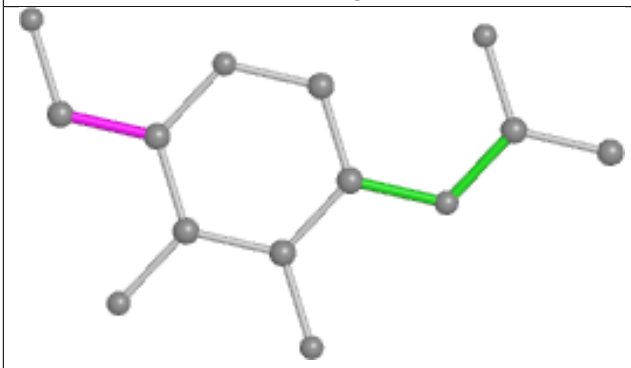

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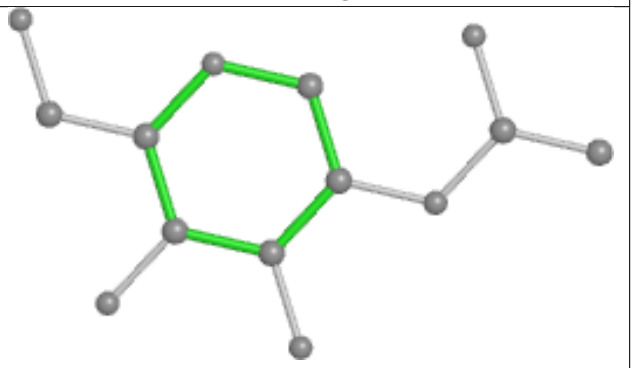
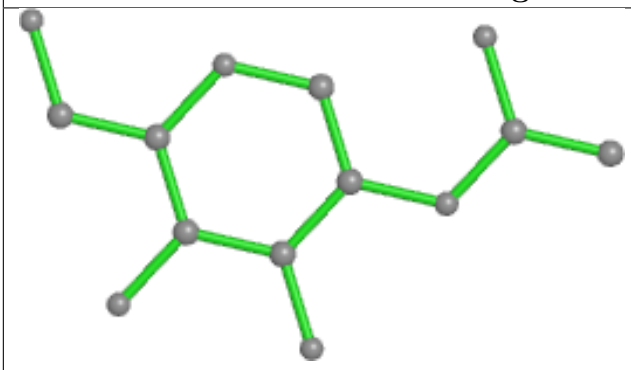


Rings

Ligand NAG B 2006



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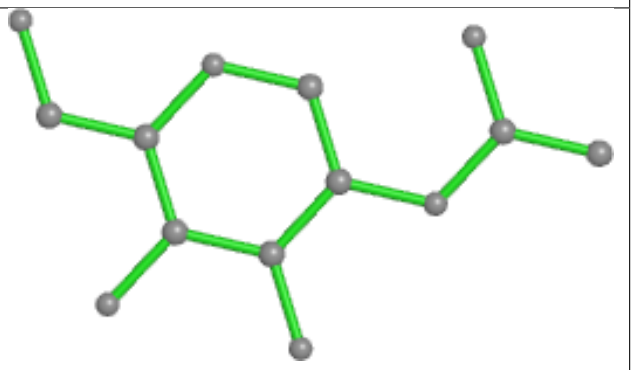
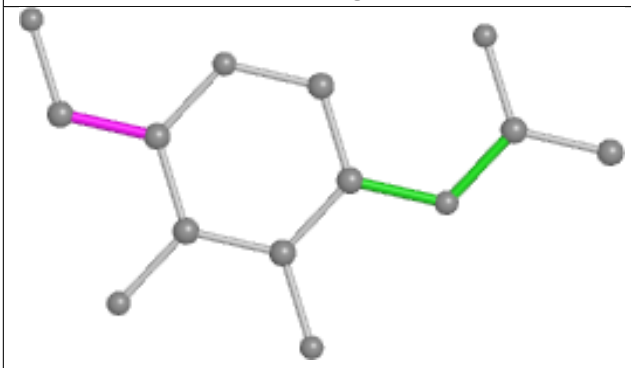


Bond angles



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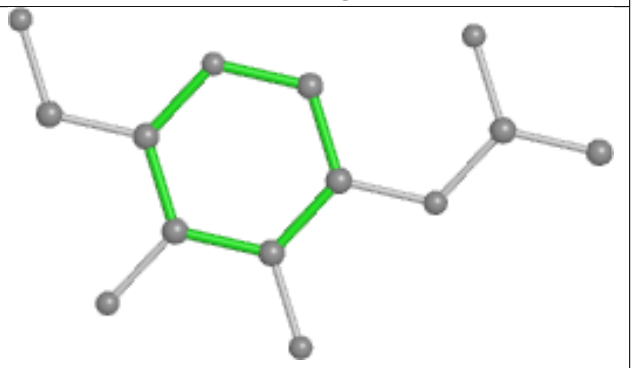
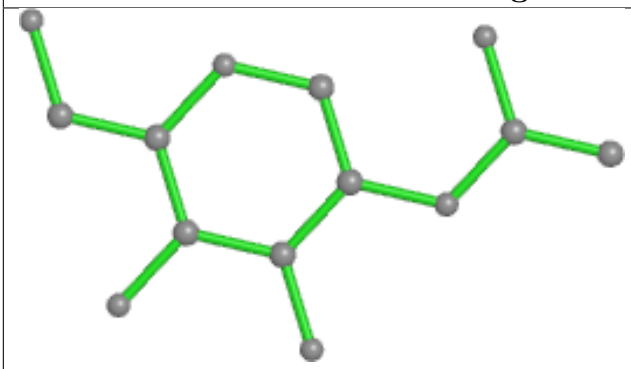
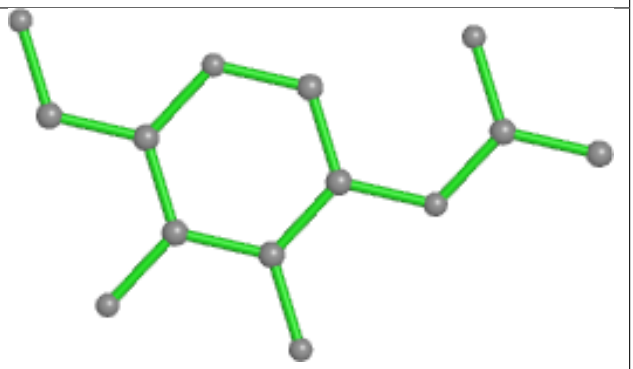


Rings

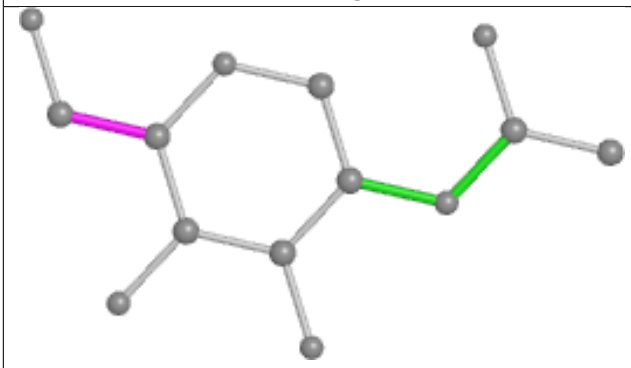
Ligand NAG A 2015



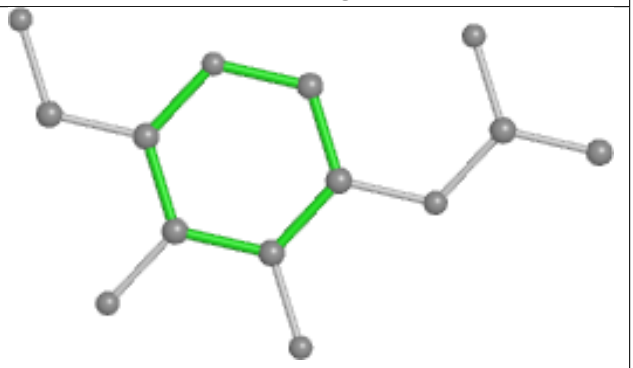
Bond lengths



Bond angles

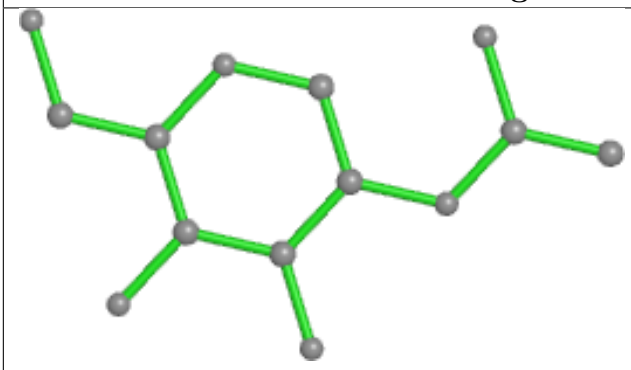


Torsions



Rings

Ligand NAG A 2017



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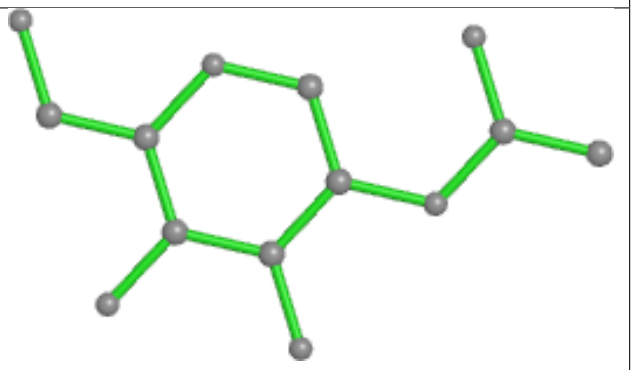

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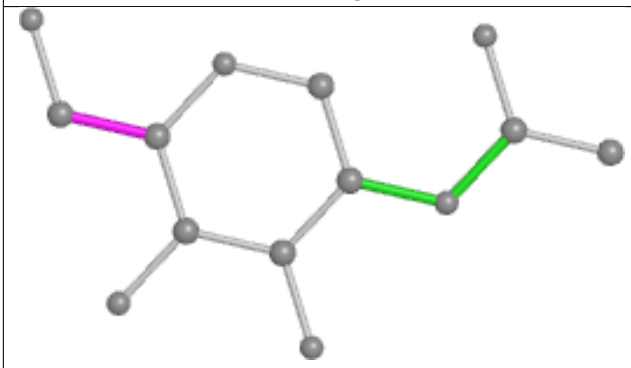

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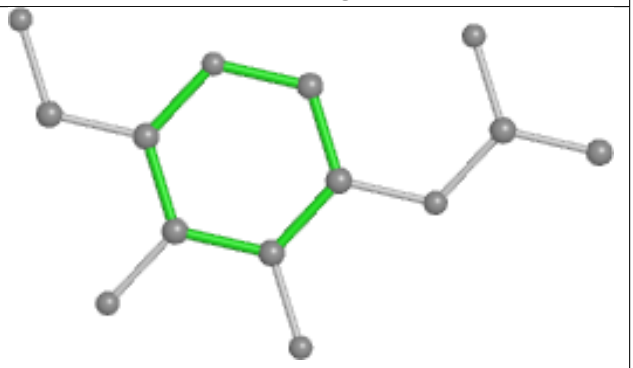
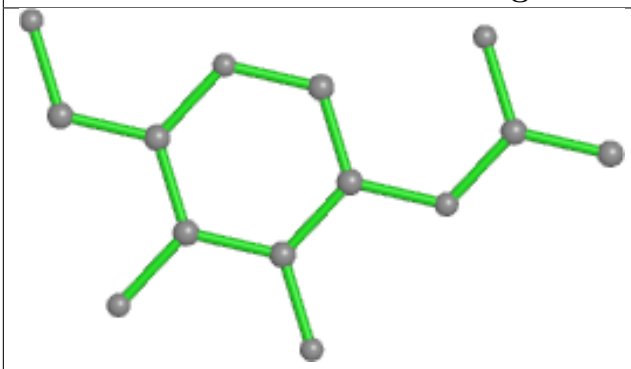


Rings

Ligand NAG C 2005



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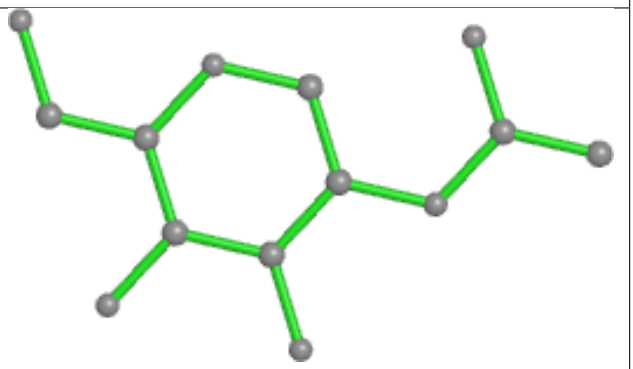

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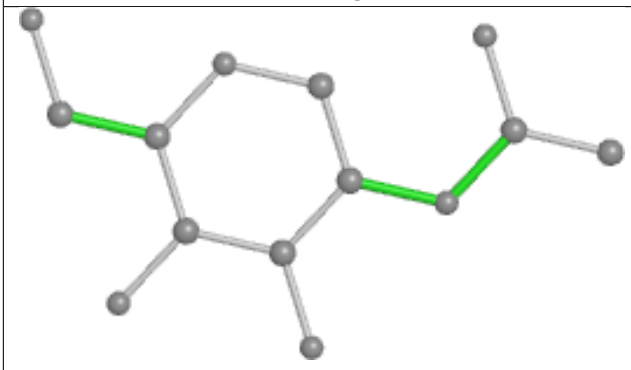

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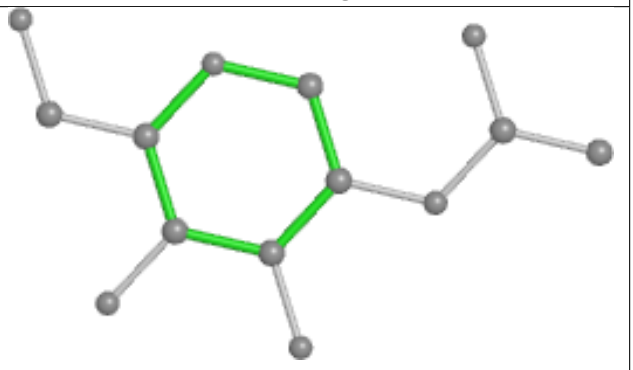
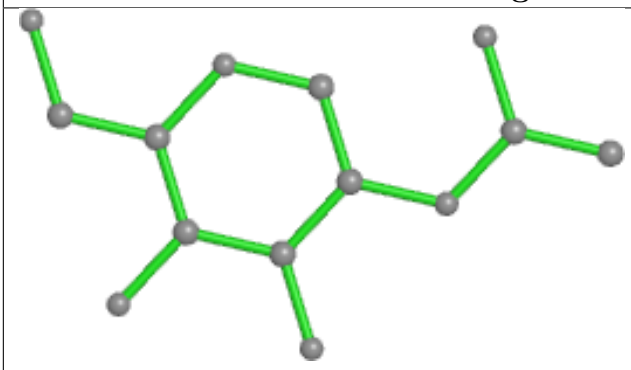


Rings

Ligand NAG B 2007



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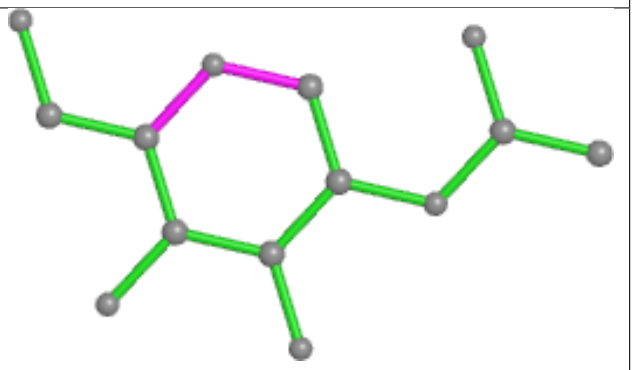

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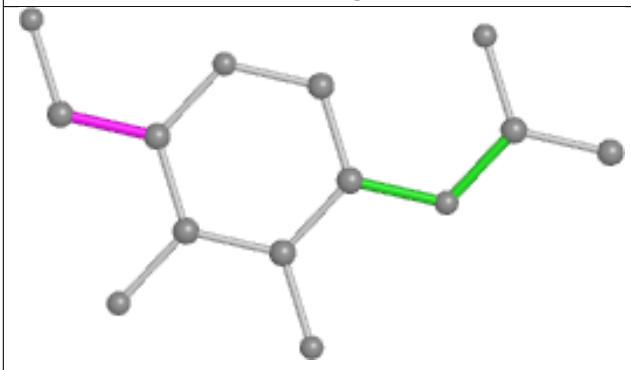

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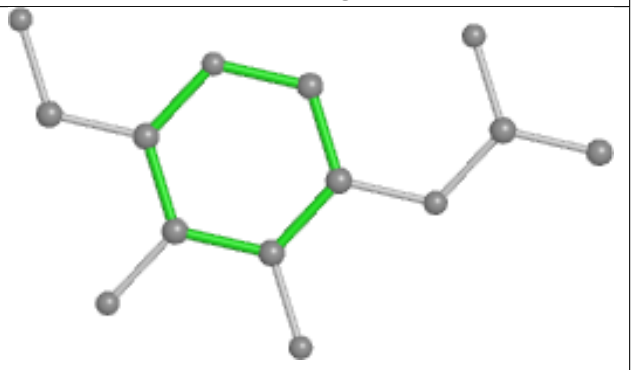
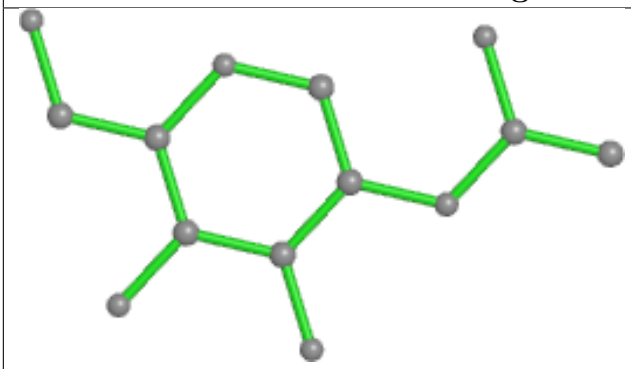


Rings

Ligand NAG C 2004



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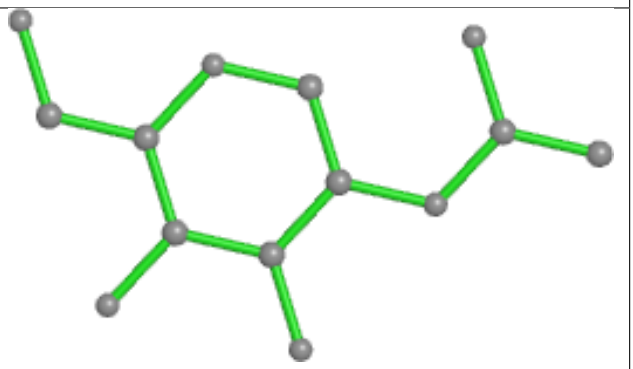

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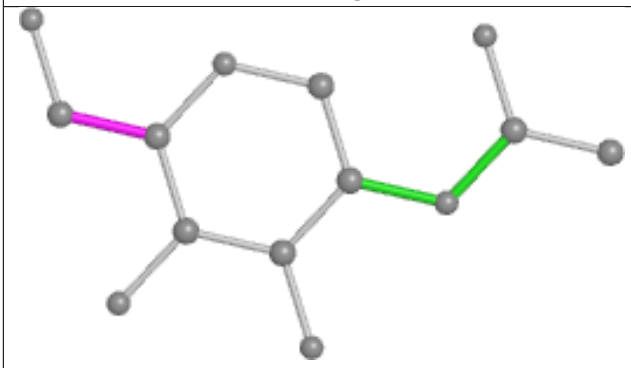

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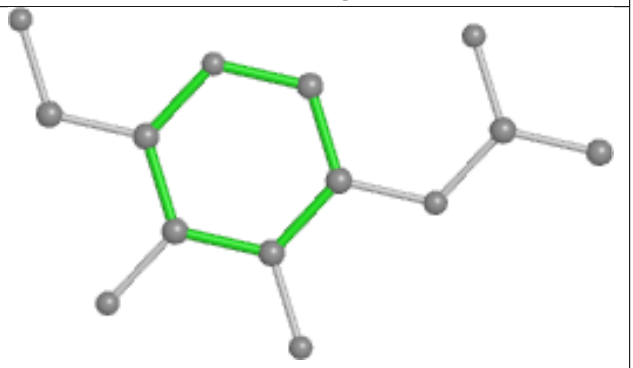
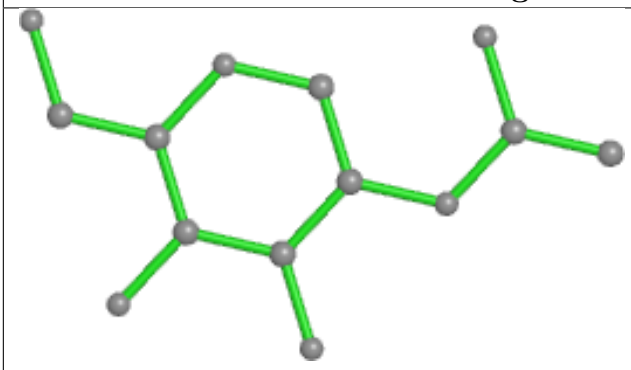


Rings

Ligand NAG C 2017



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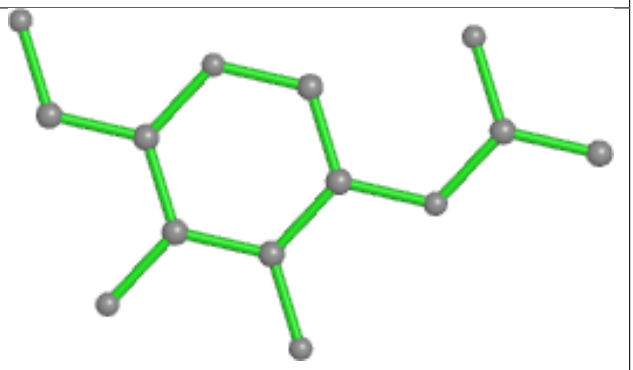

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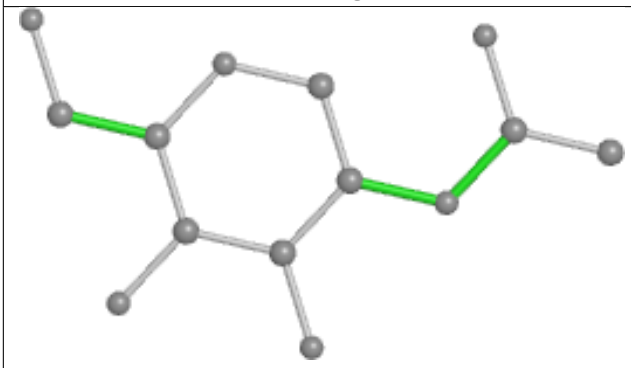

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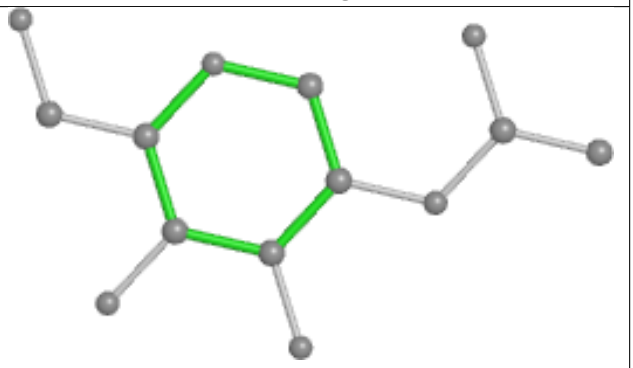
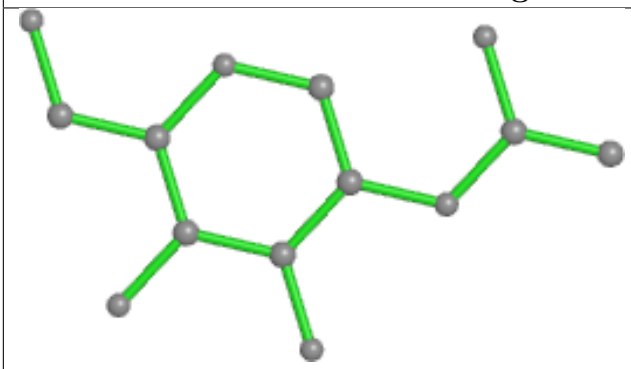


Rings

Ligand NAG C 2012



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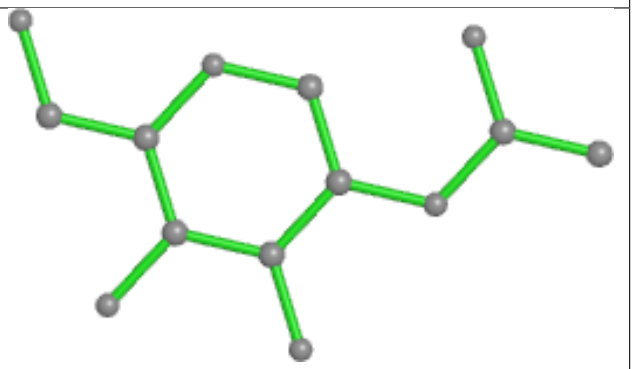

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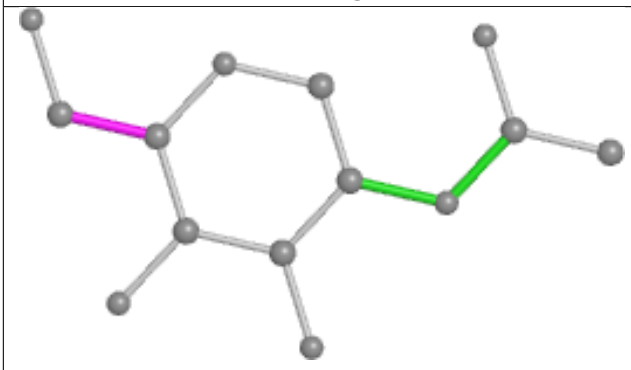

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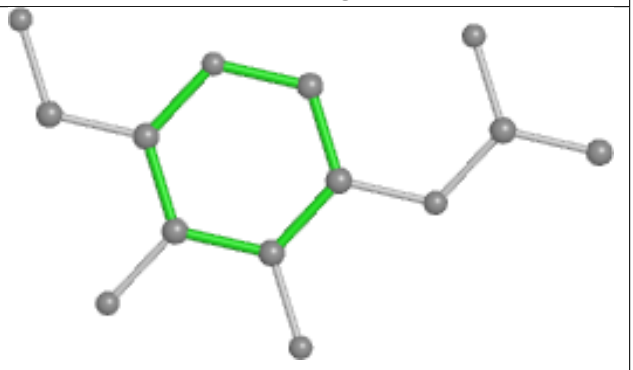
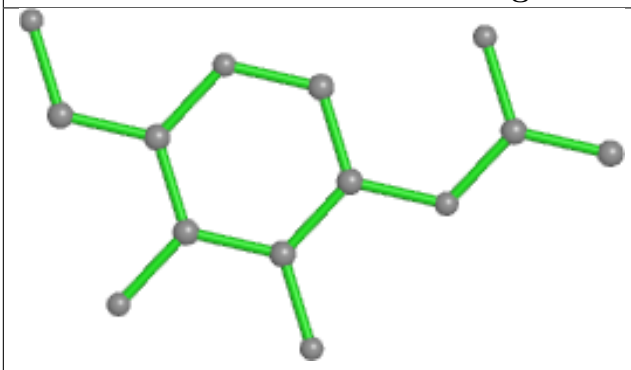


Rings

Ligand NAG B 2005



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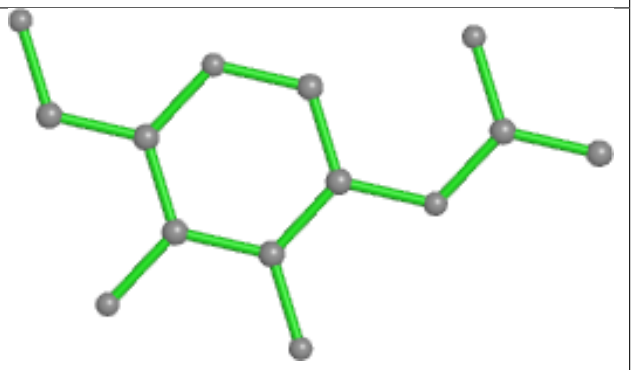

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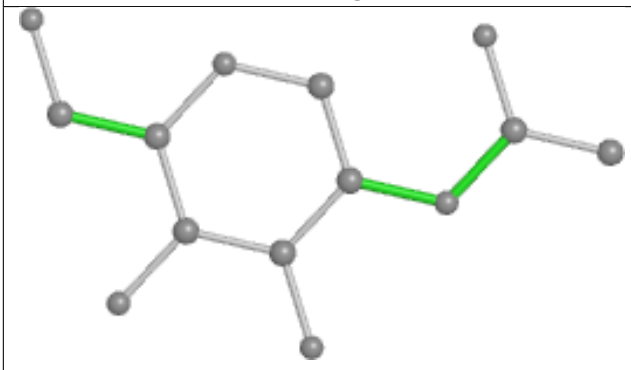

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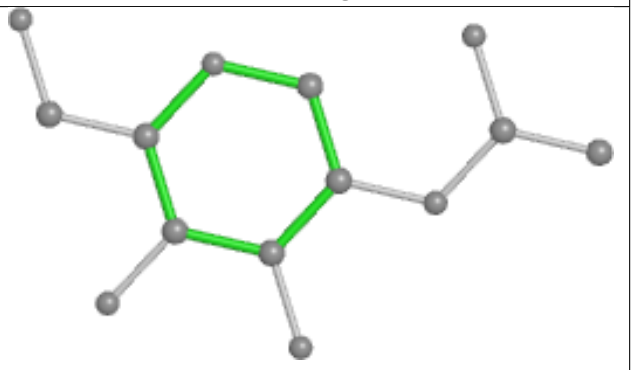
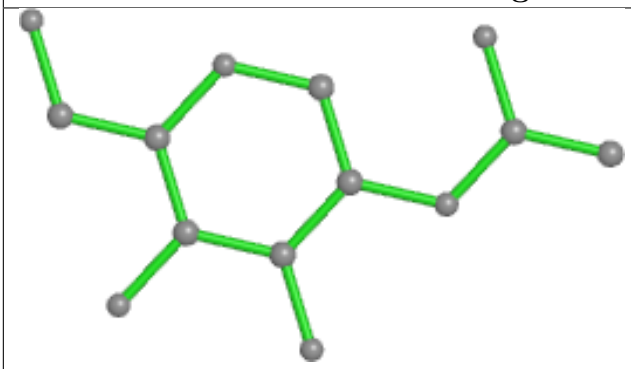


Rings

Ligand NAG B 2015



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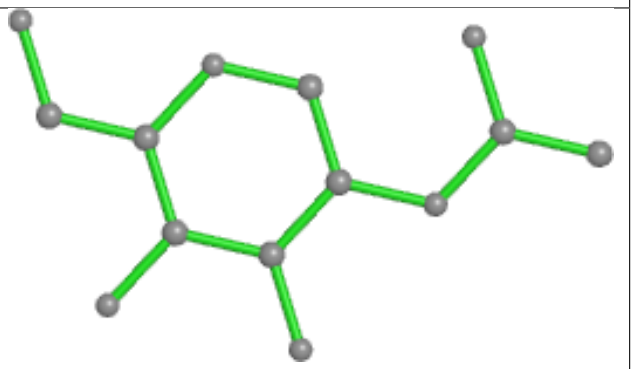

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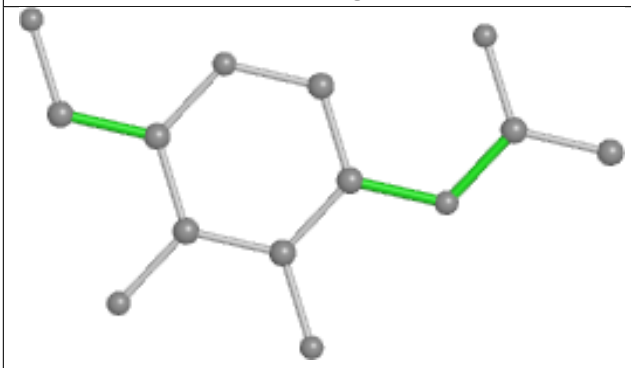

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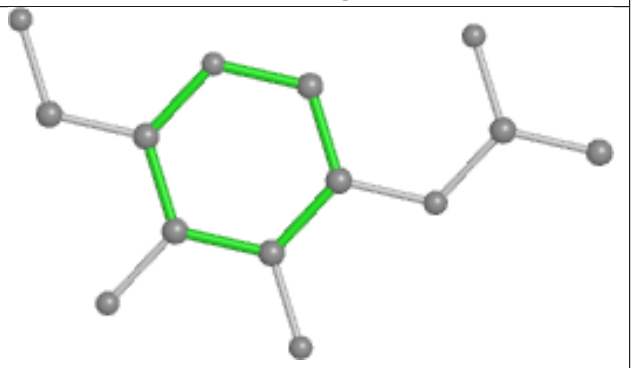
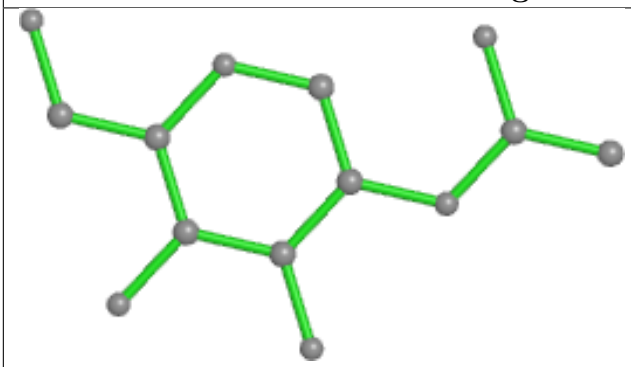


Rings

Ligand NAG B 2003



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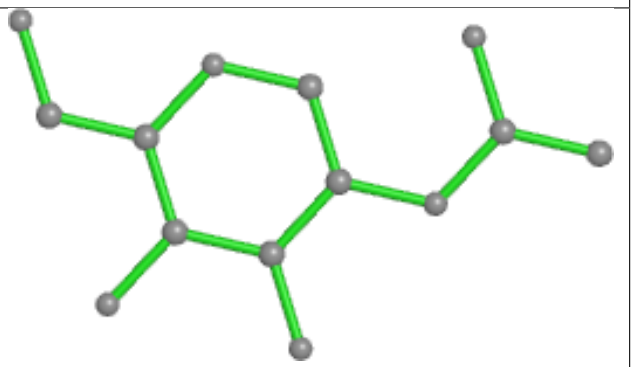

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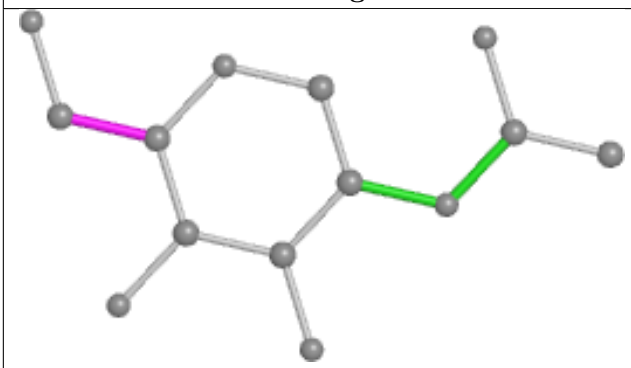

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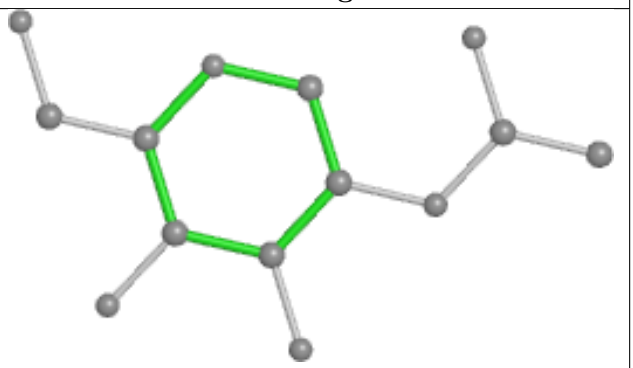
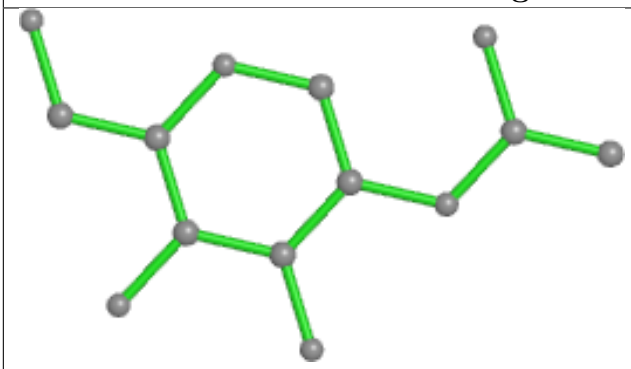


Rings

Ligand NAG B 2017



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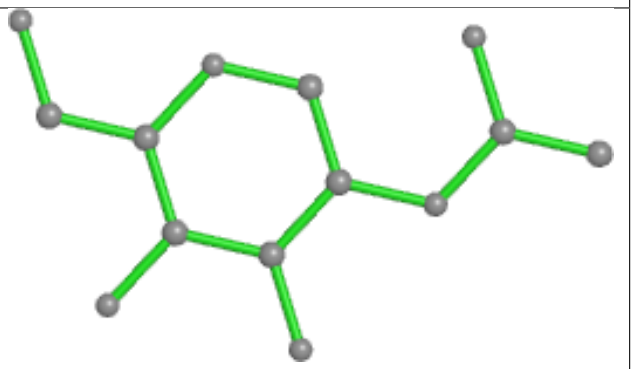

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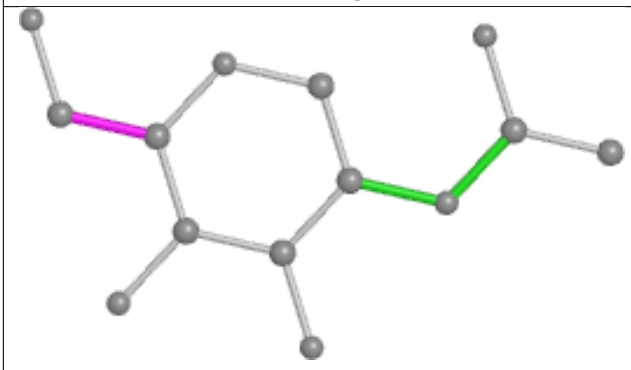

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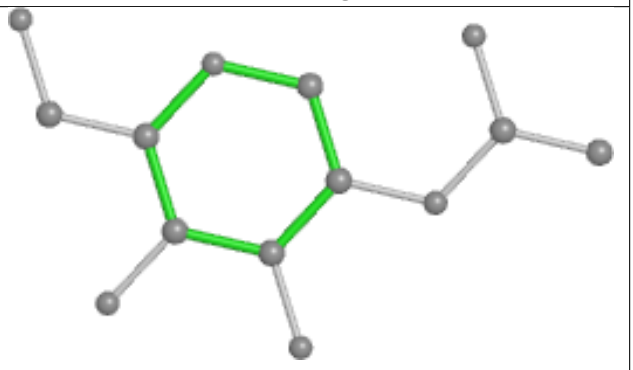
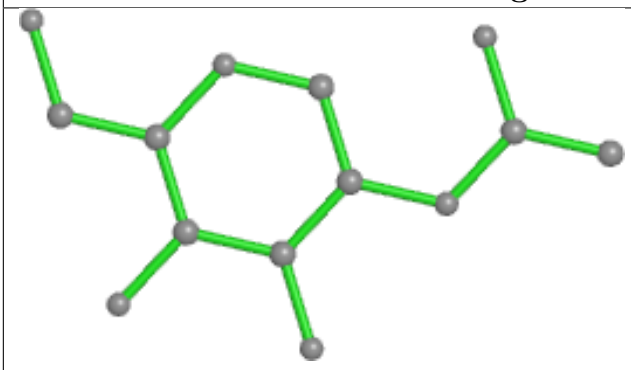


Rings

Ligand NAG A 2014



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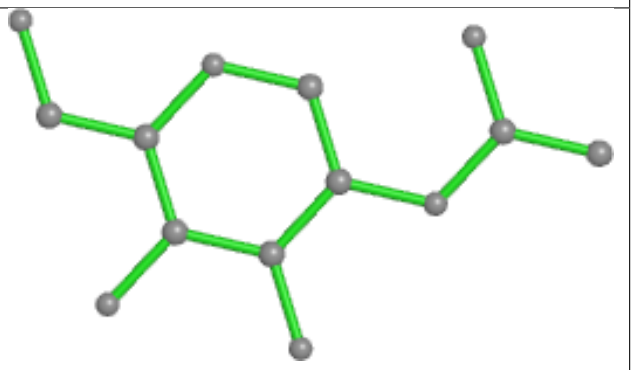

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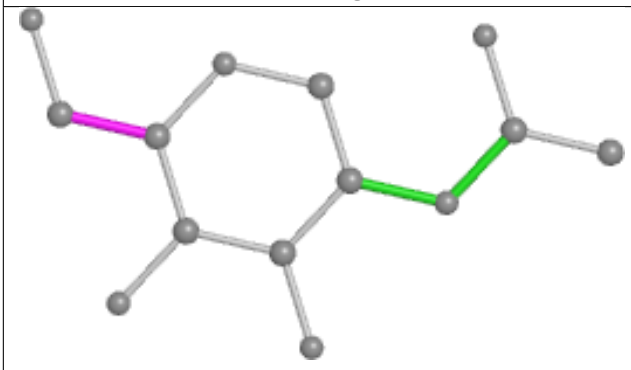

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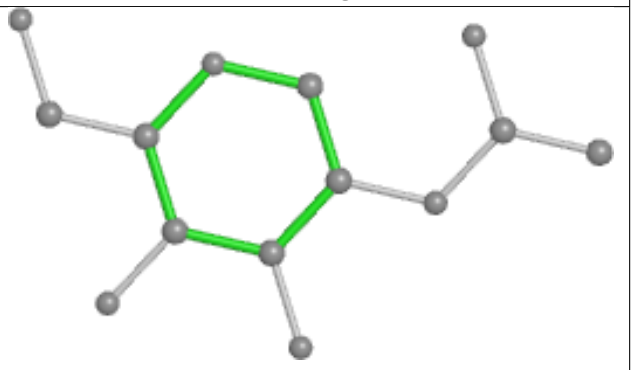
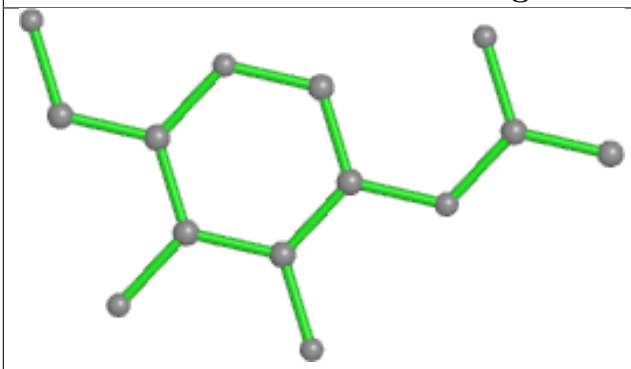


Rings

Ligand NAG B 2014



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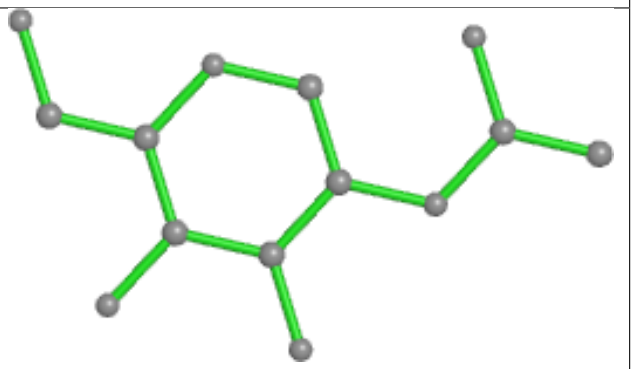

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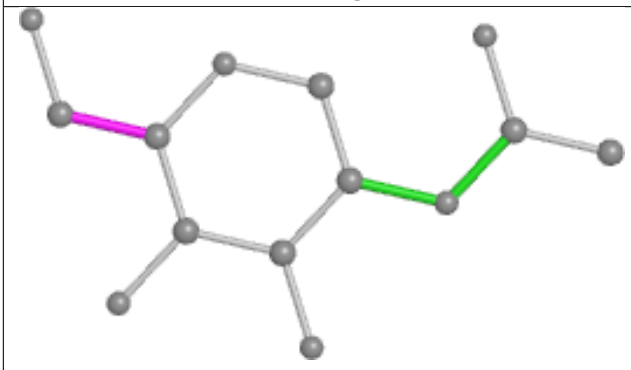

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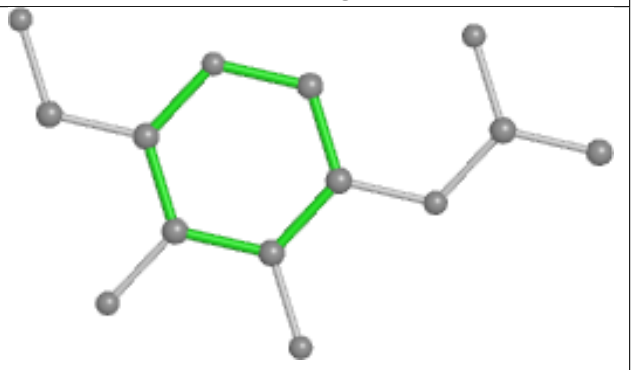
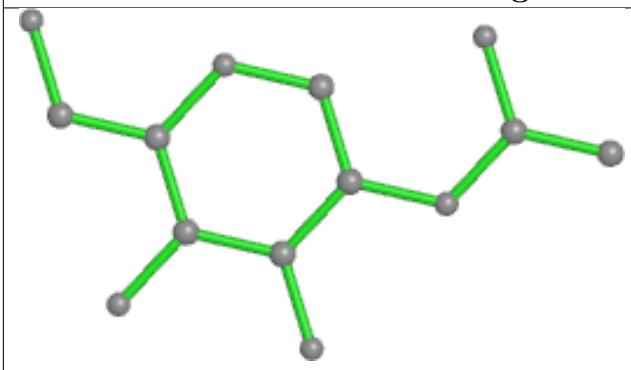


Rings

Ligand NAG C 2007



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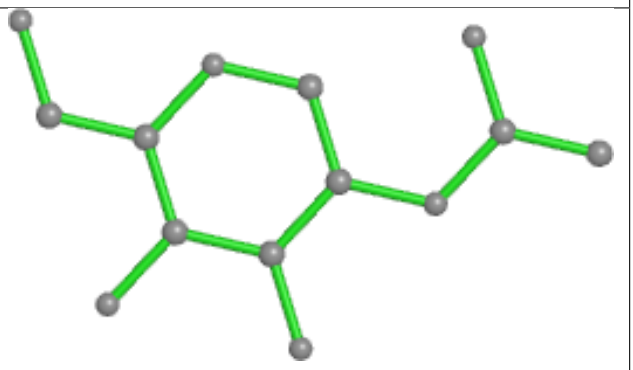

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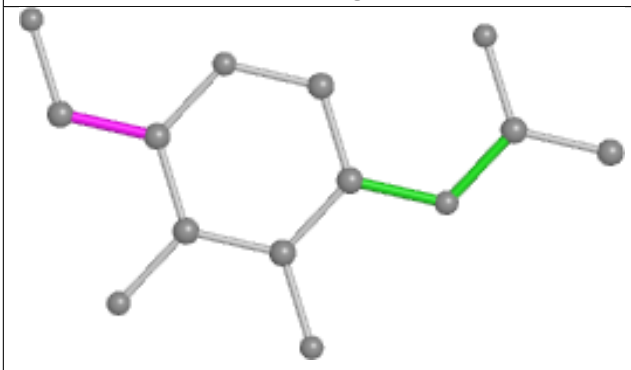

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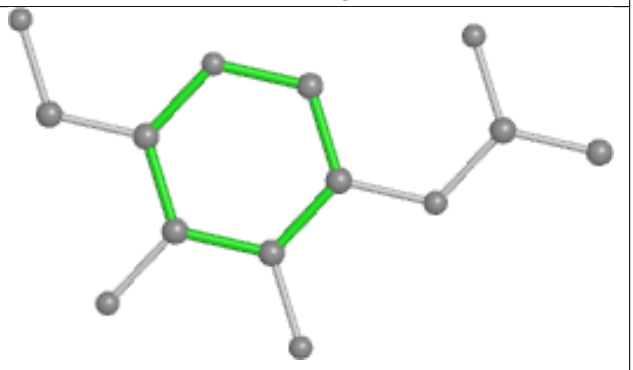
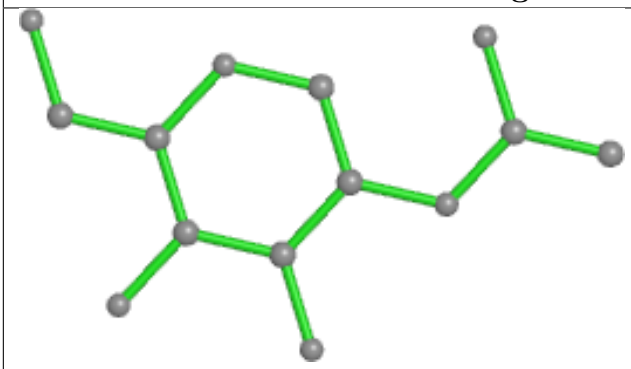


Rings

Ligand NAG C 2013



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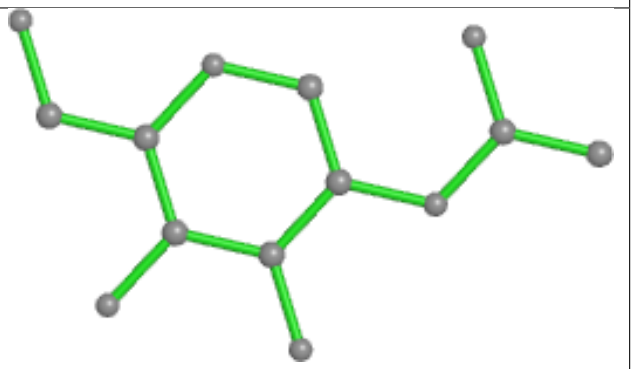

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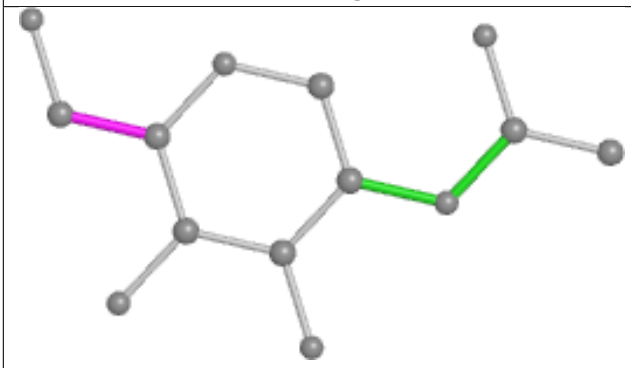
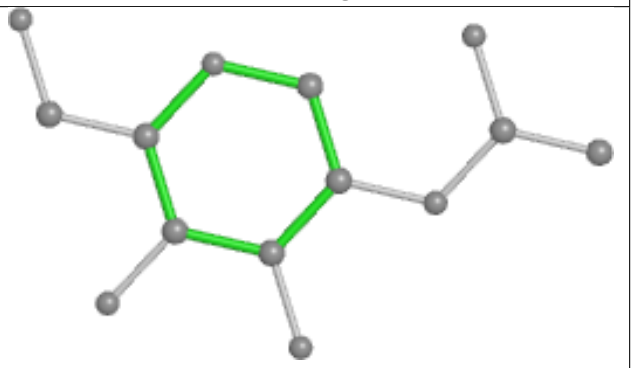
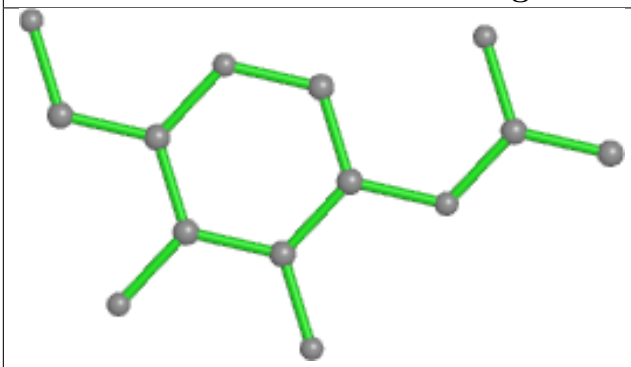


Torsions

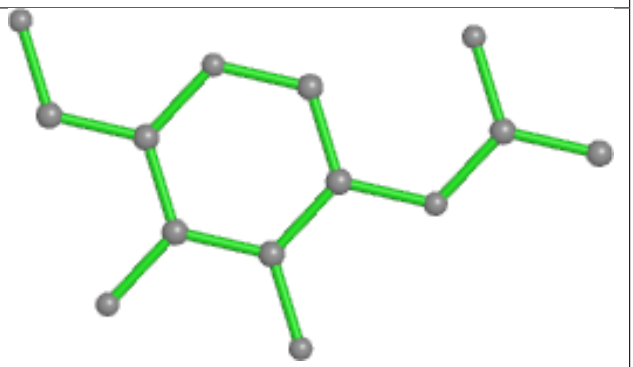


Rings

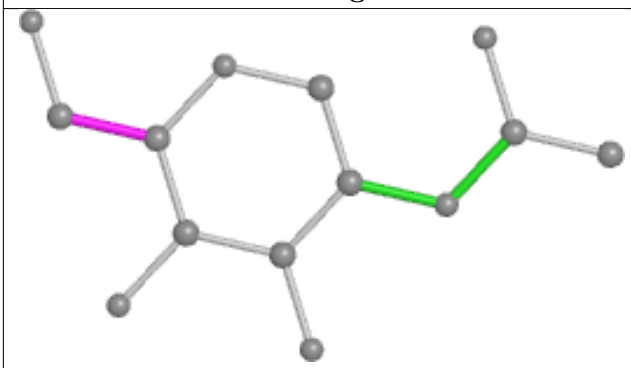
Ligand NAG B 2001



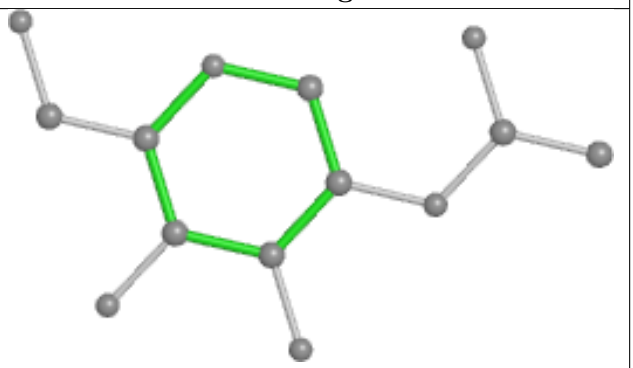
Bond lengths



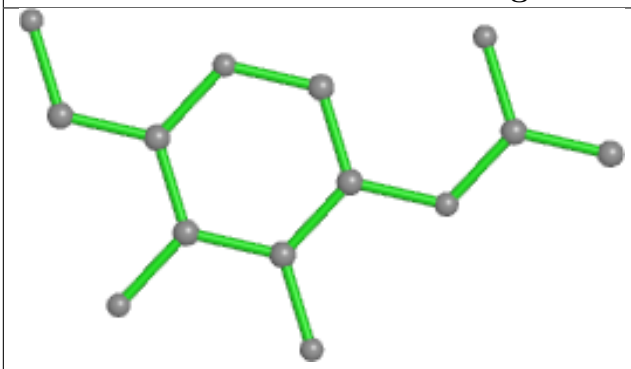
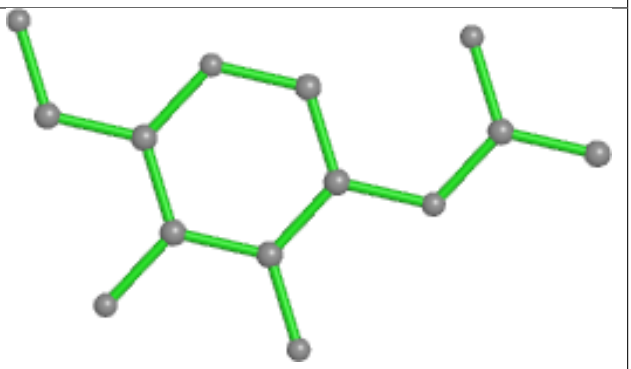
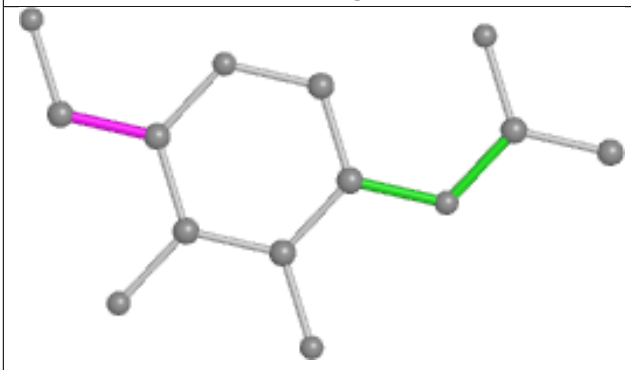
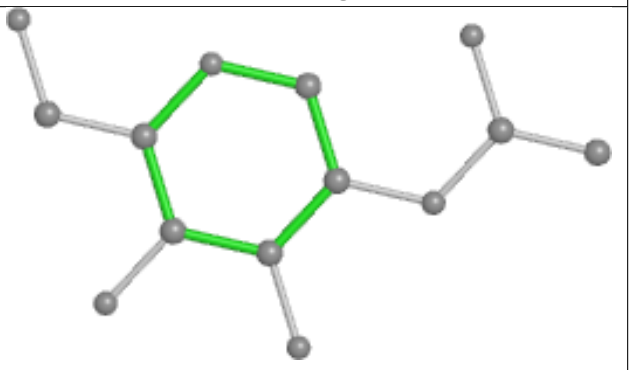
Bond angles

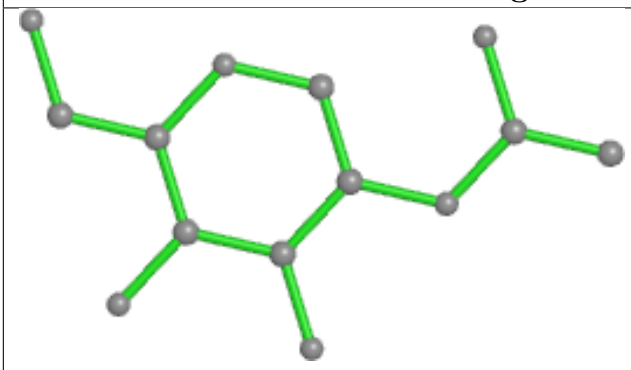
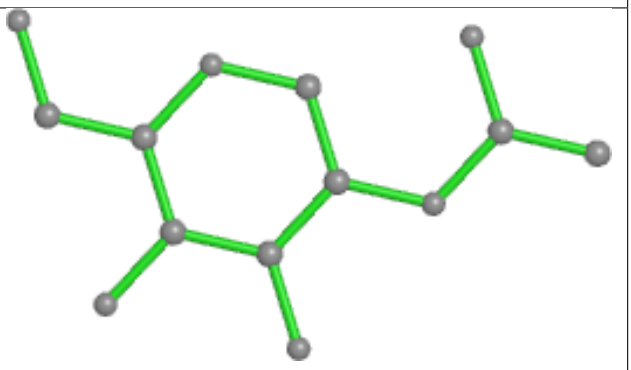
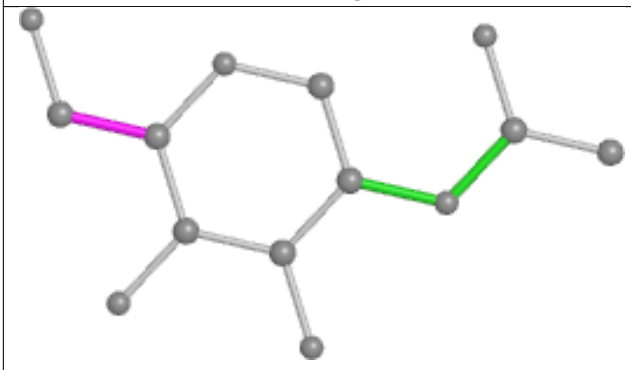
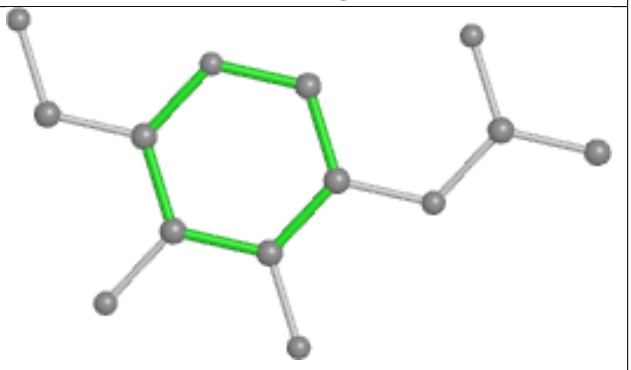


Torsions

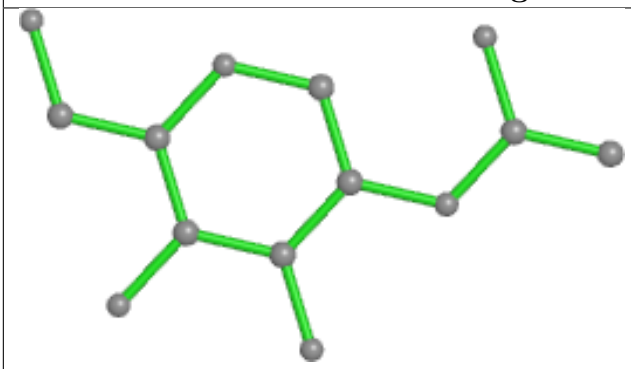


Rings

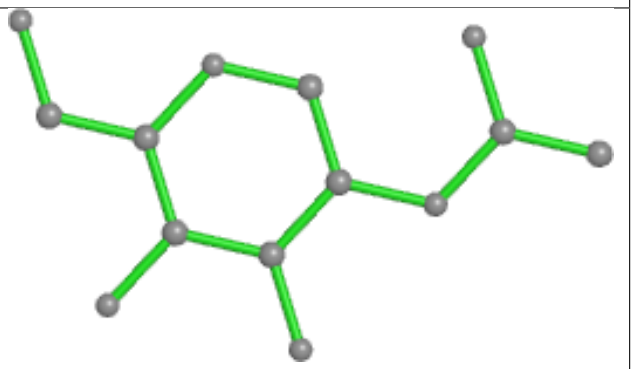
Ligand NAG A 2008	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG A 2003	
 Bond lengths	 Bond angles
 Torsions	 Rings

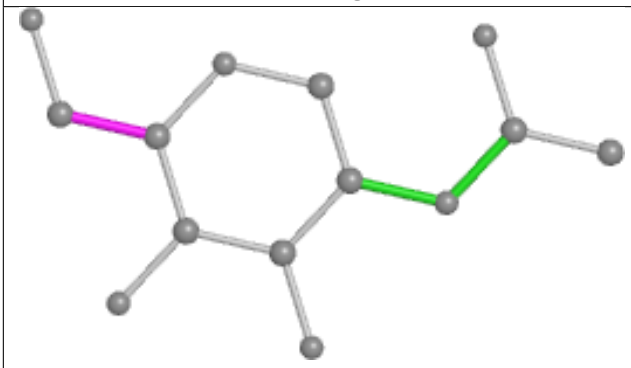
Ligand NAG A 2001



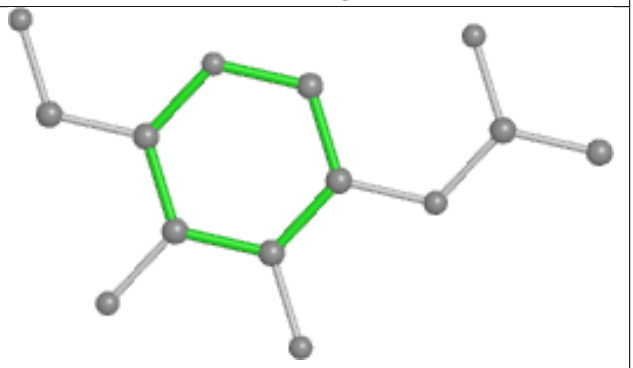
Bond lengths



Bond angles

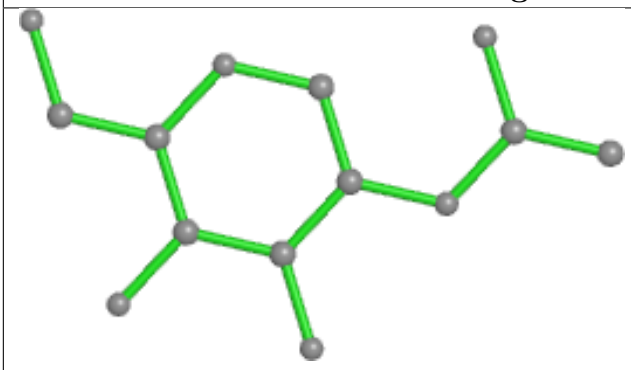


Torsions



Rings

Ligand NAG A 2011



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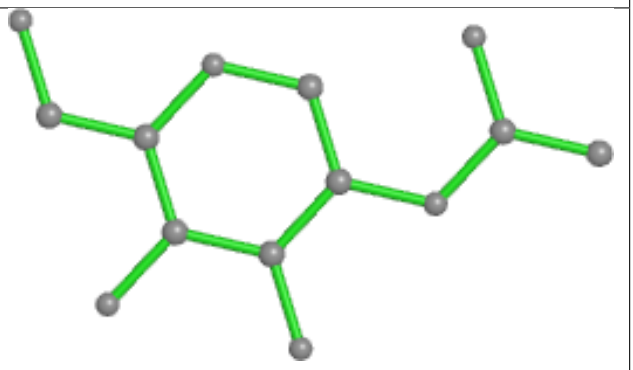

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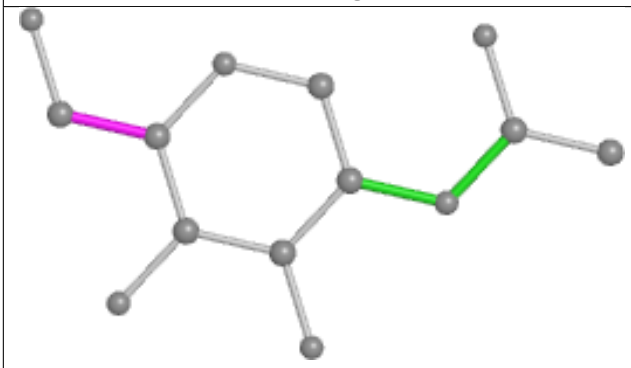

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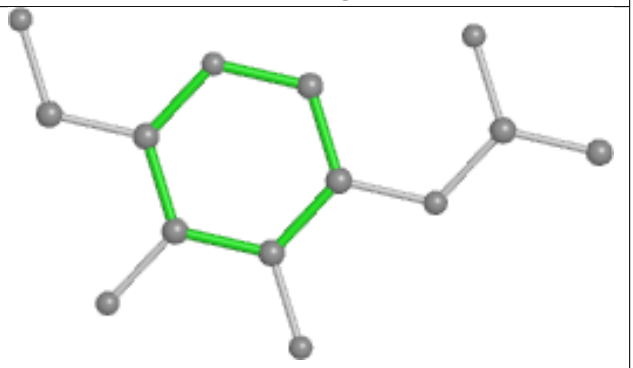
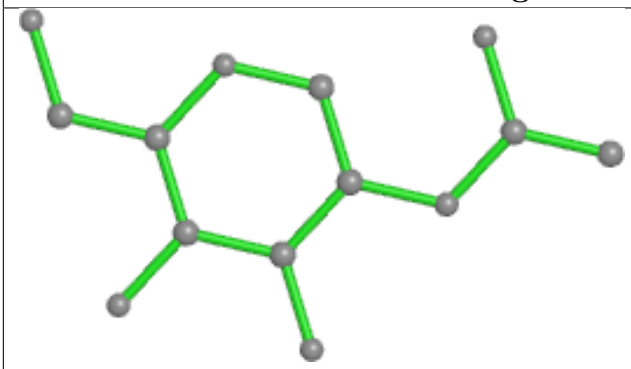


Rings

Ligand NAG B 2011



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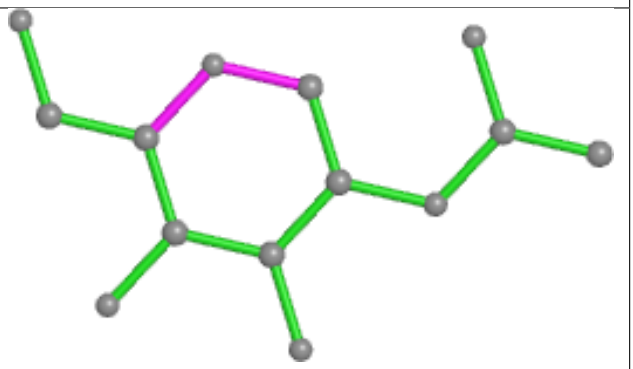

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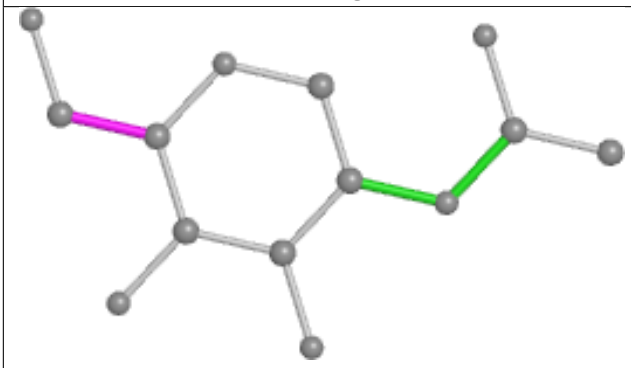

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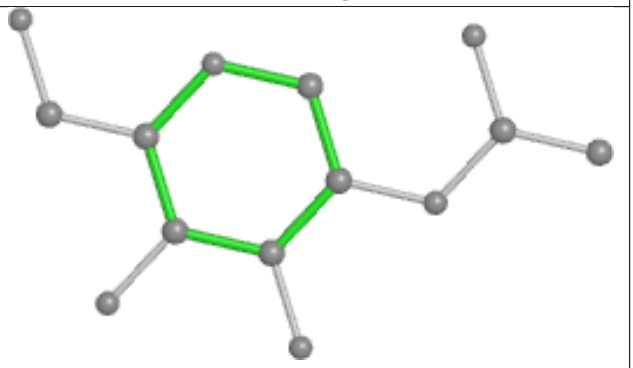
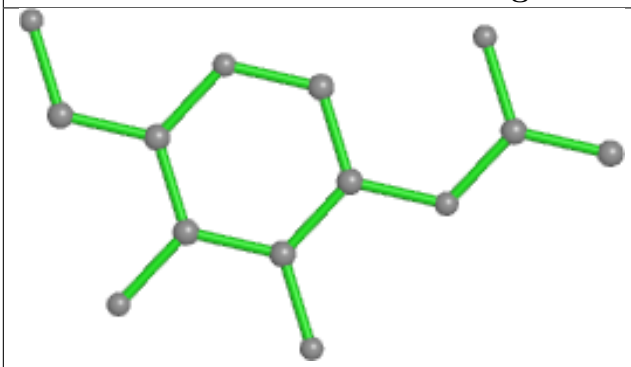


Rings

Ligand NAG C 2001



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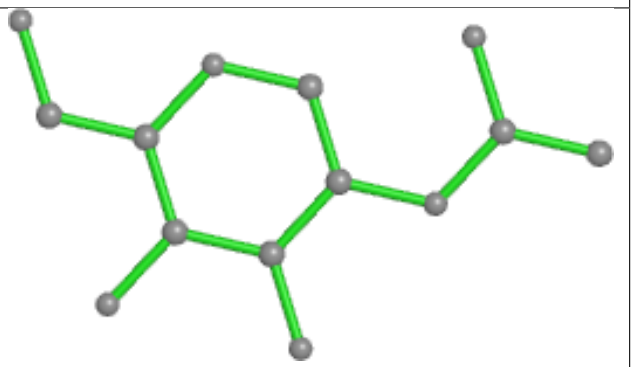
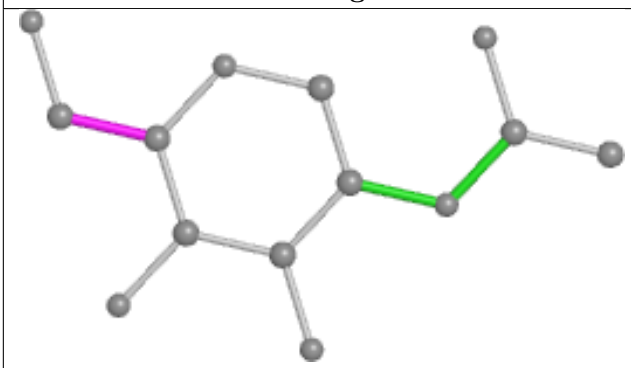


Bond angles



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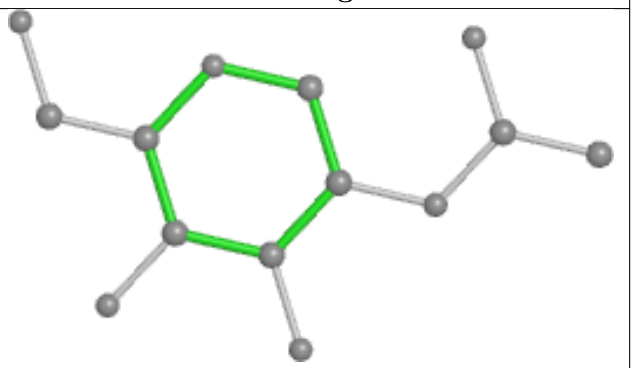
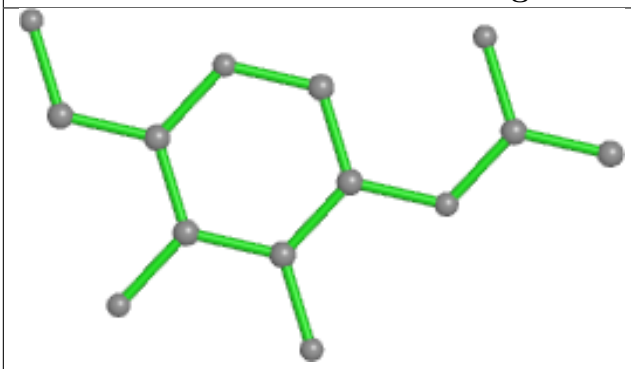


Rings

Ligand NAG C 2015



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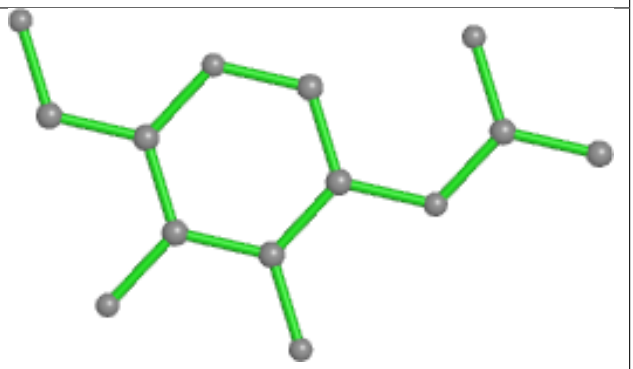
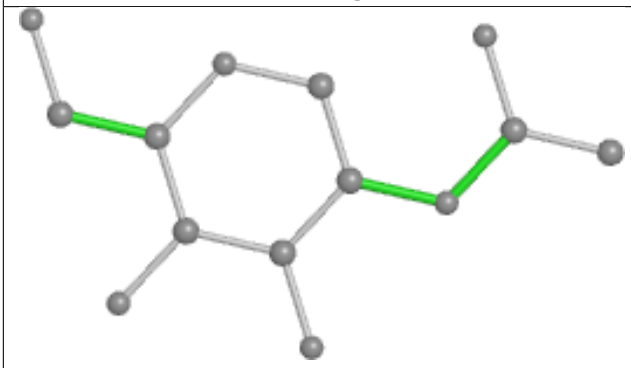


Bond angles



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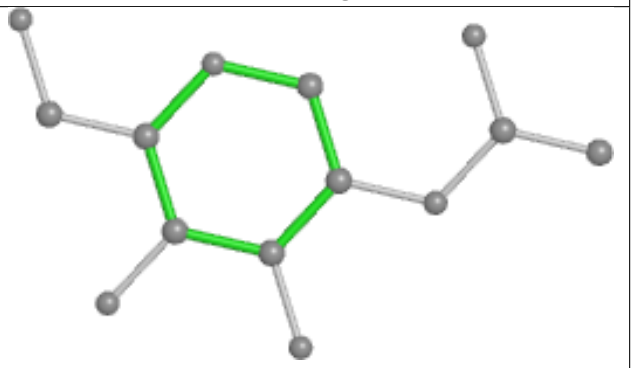
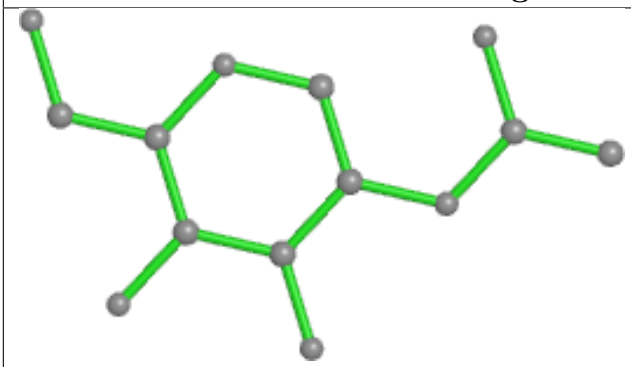
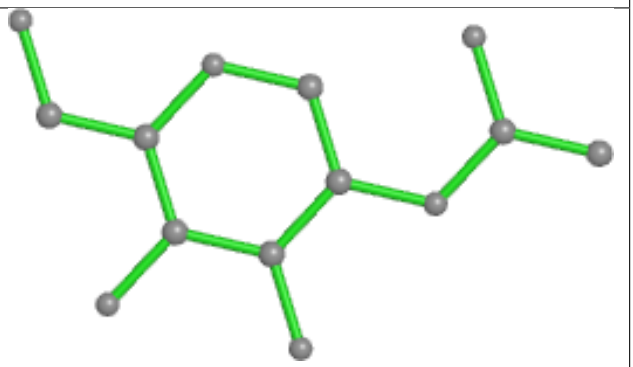


Rings

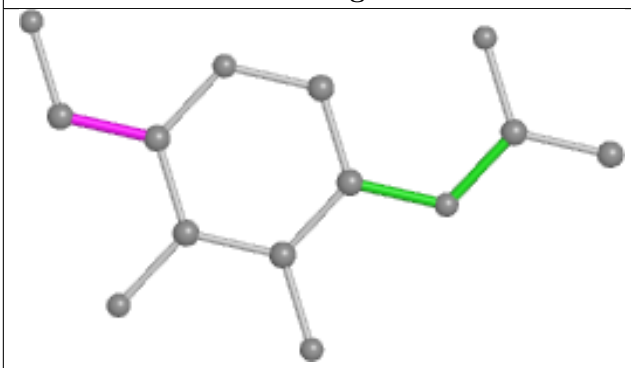
Ligand NAG C 2002



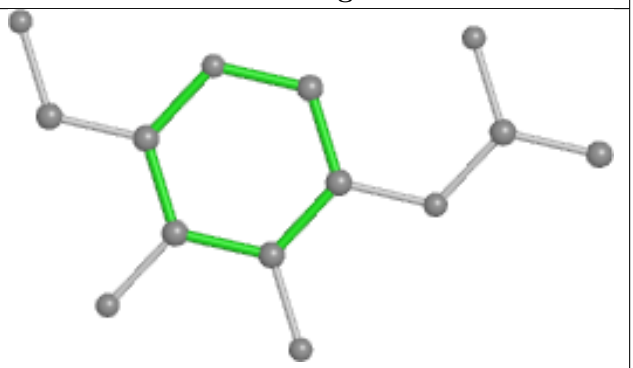
Bond lengths



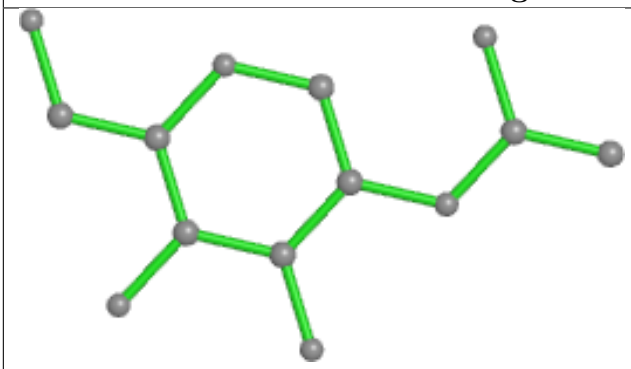
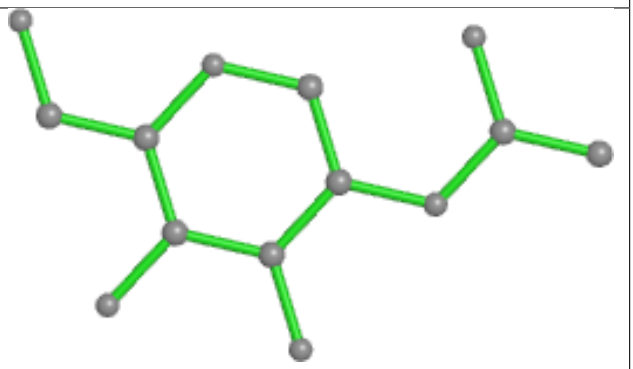
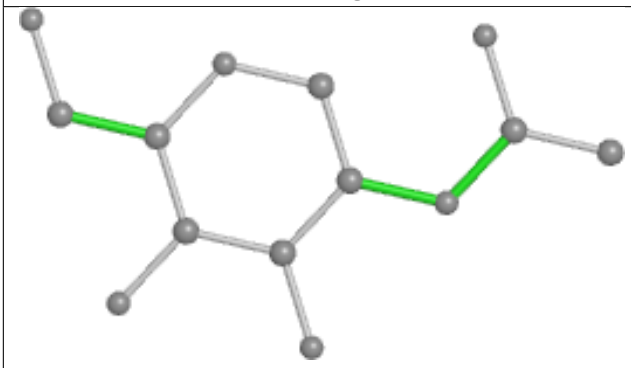
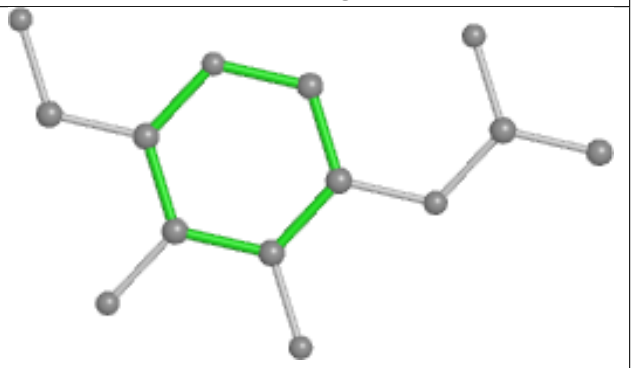
Bond angles

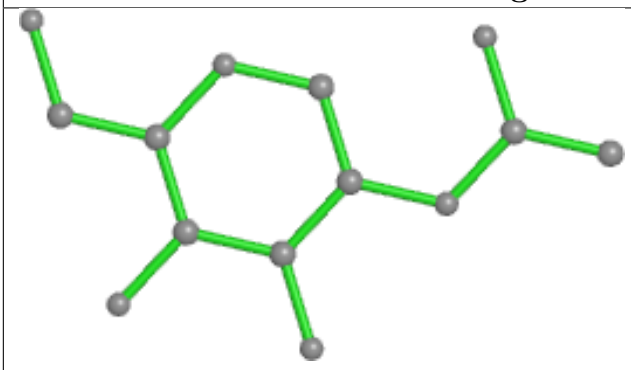
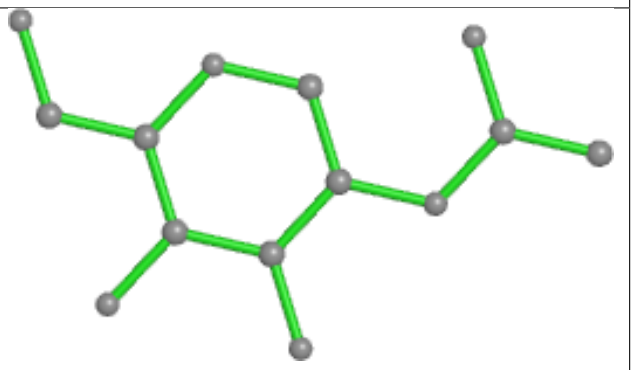
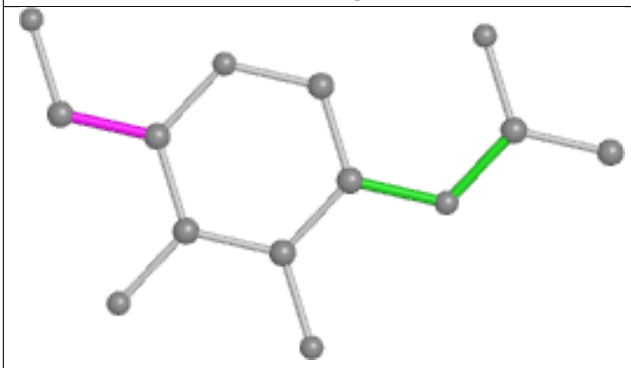
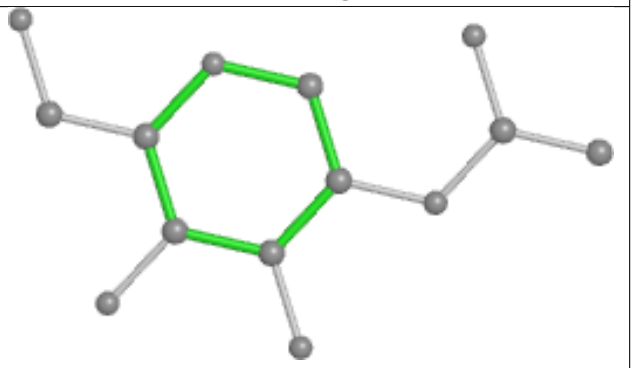


Torsions

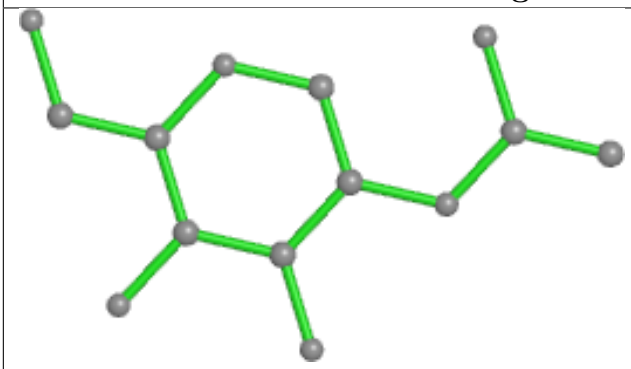


Rings

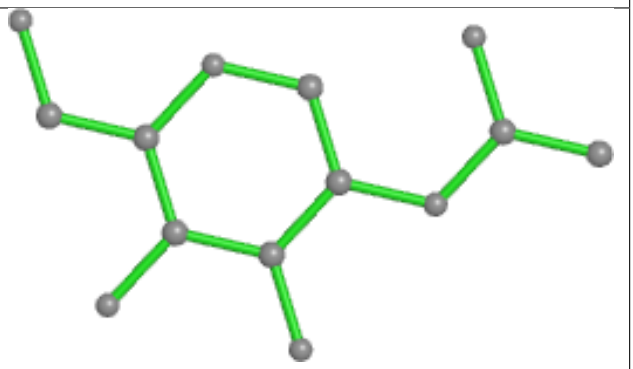
Ligand NAG A 2006	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand NAG A 2004	
	
Bond lengths	Bond angles
	
Torsions	Rings

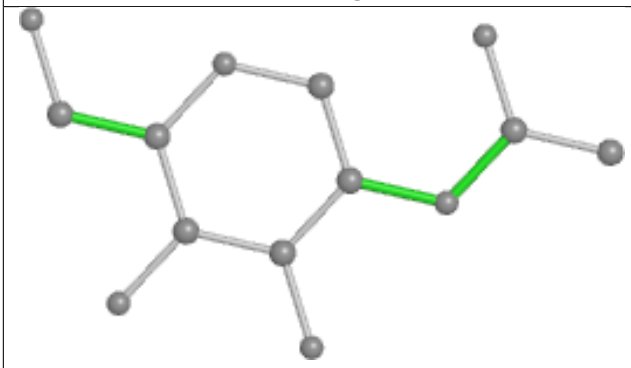
Ligand NAG B 2008



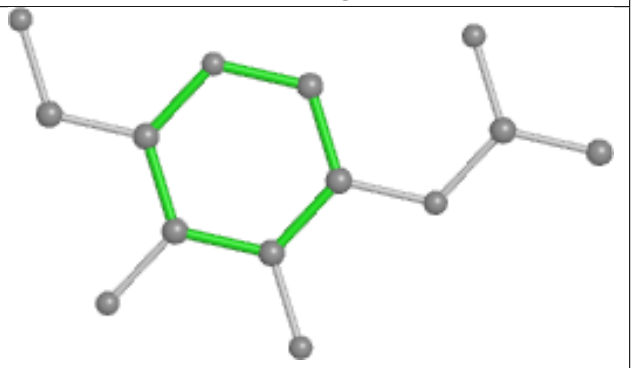
Bond lengths



Bond angles

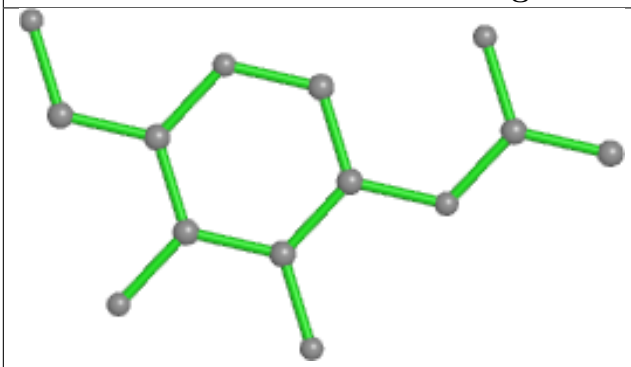


Torsions

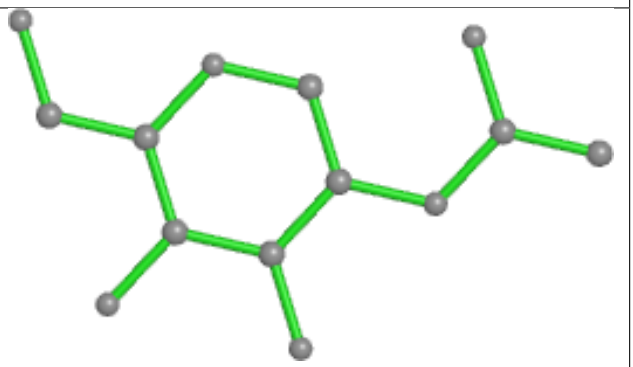


Rings

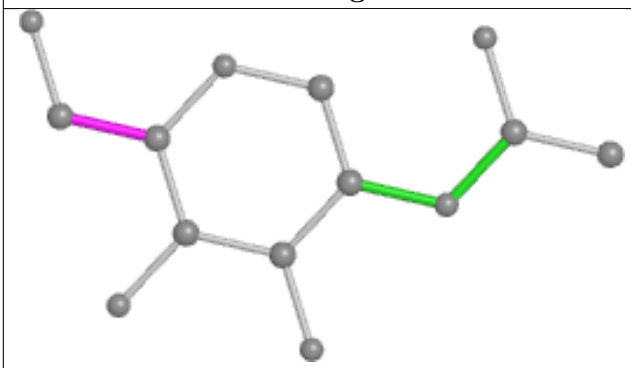
Ligand NAG B 2004



Bond lengths



Bond angles



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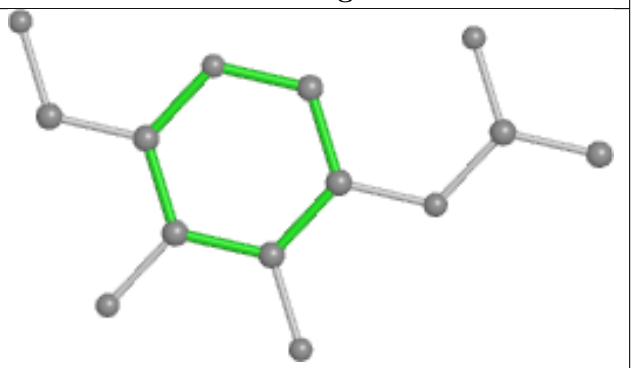

Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.