Full wwPDB EM Validation Report ⓘ

Oct 7, 2024 – 02:35 PM JST

PDB ID	:	8Y1H
EMDB ID	:	EMD-38836
Title	:	The 2up formation 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	:	3.16 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:

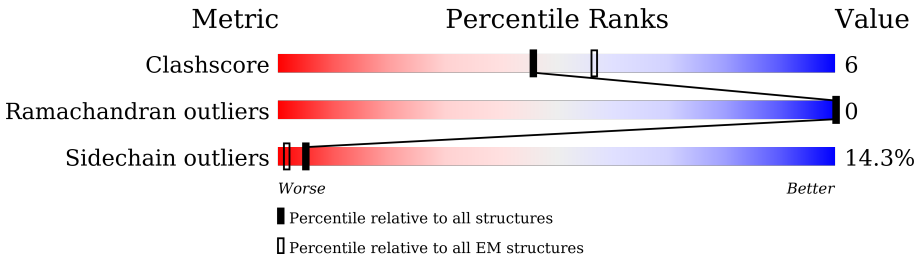
EMDB validation analysis	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 3.16 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	70% 21% • 6%
1	B	1290	70% 21% • 6%
1	C	1290	68% 22% • 6%
2	D	6	33% 67%
2	I	6	17% 67% 17%
2	N	6	33% 67%
3	E	2	100%
3	F	2	50% 50%
3	G	2	50% 50%

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

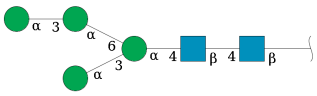
- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	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		
1	A	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
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
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

- 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.

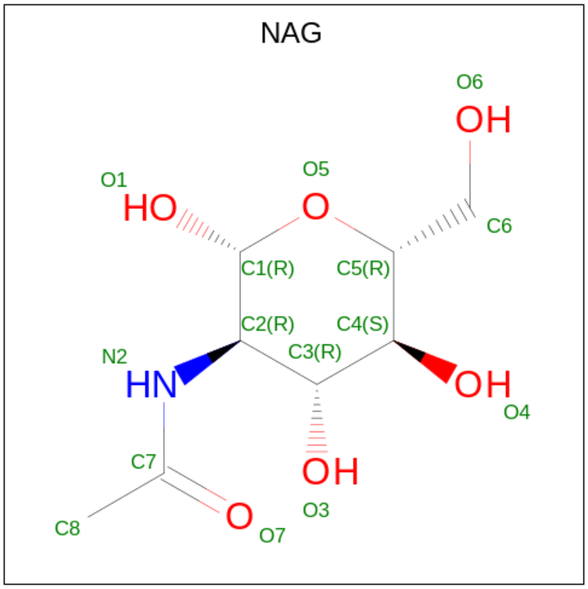


Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	6	Total	C	N	O	0	0
			72	40	2	30		
2	I	6	Total	C	N	O	0	0
			72	40	2	30		
2	N	6	Total	C	N	O	0	0
			72	40	2	30		

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

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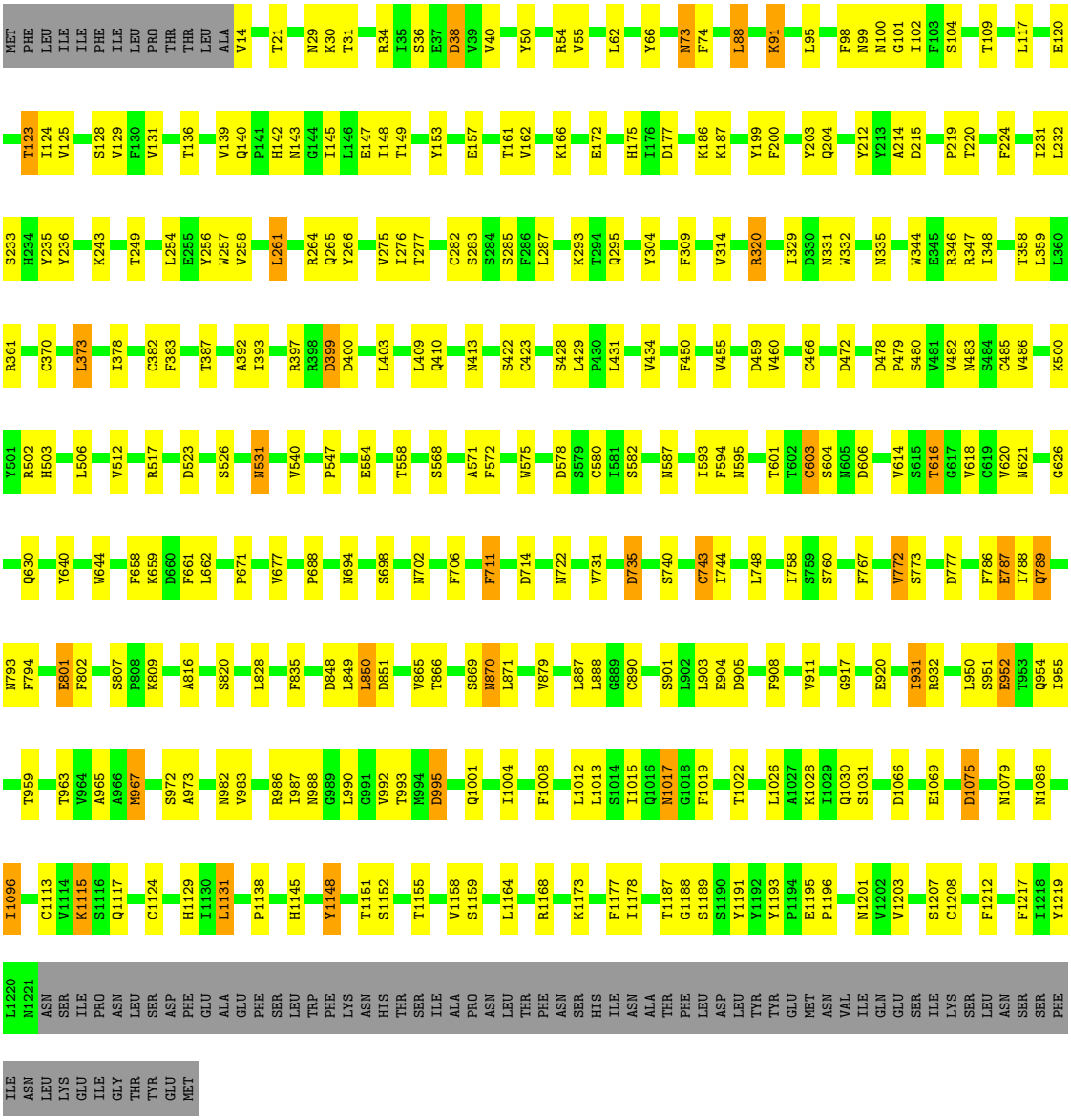
Mol	Chain	Residues	Atoms	AltConf
4	C	1	Total C N O 14 8 1 5	0
4	A	1	Total C N O 14 8 1 5	0
4	A	1	Total C N O 14 8 1 5	0
4	A	1	Total C N O 14 8 1 5	0
4	A	1	Total C N O 14 8 1 5	0
4	A	1	Total C N O 14 8 1 5	0
4	A	1	Total C N O 14 8 1 5	0
4	A	1	Total C N O 14 8 1 5	0
4	A	1	Total C N O 14 8 1 5	0
4	A	1	Total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

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.

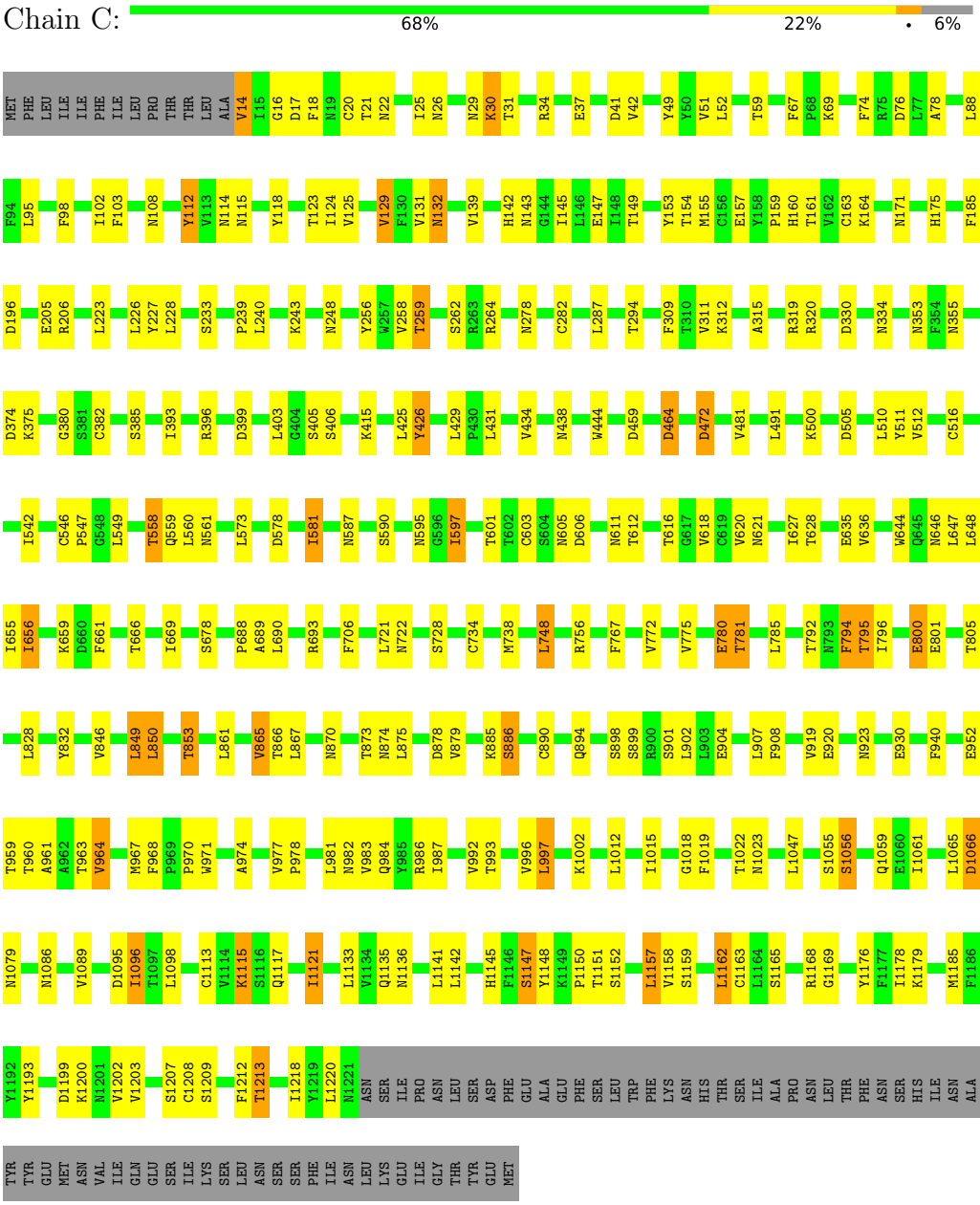
- Molecule 1: Spike glycoprotein

Chain B:



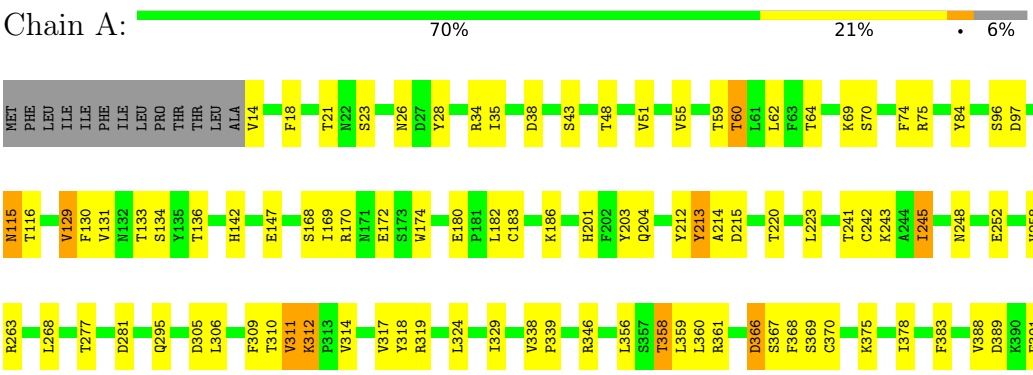
- Molecule 1: Spike glycoprotein

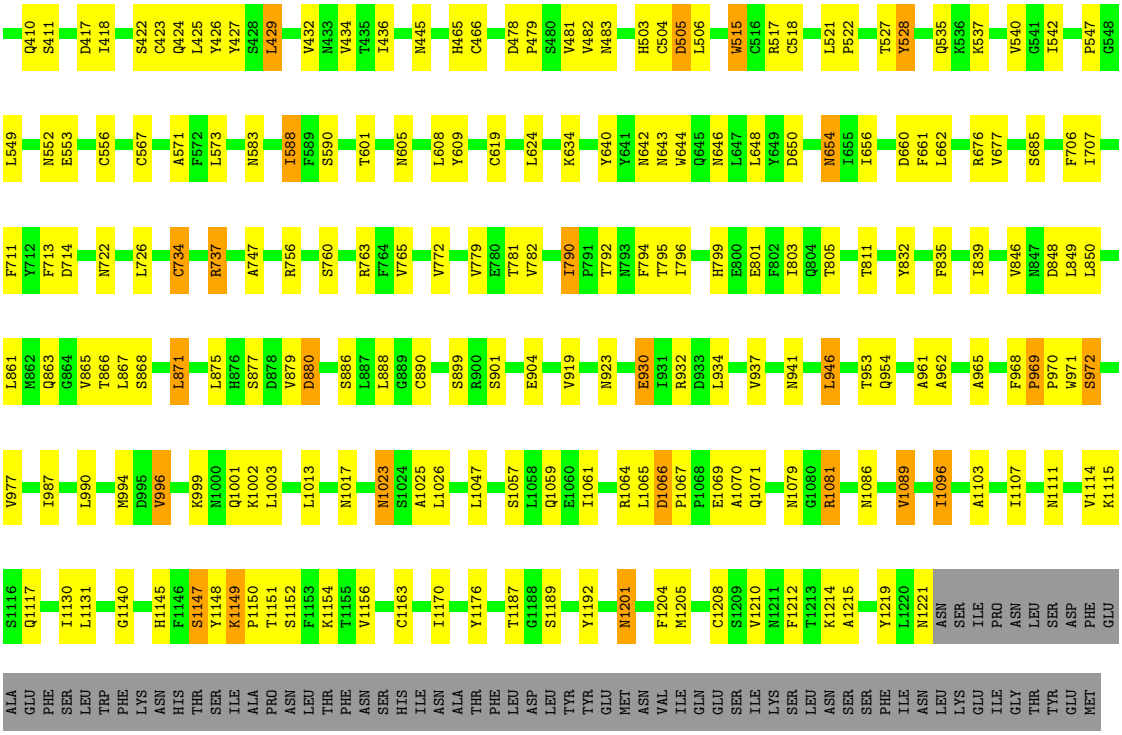
Chain C:



• Molecule 1: Spike glycoprotein

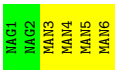
Chain A:





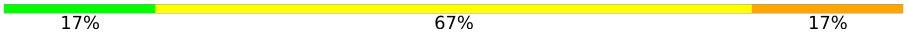
• Molecule 2: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:



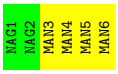
• Molecule 2: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

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

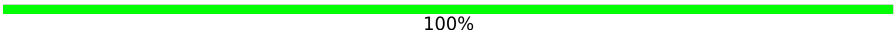
Chain F:

• 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:

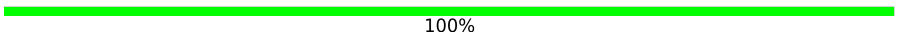


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:

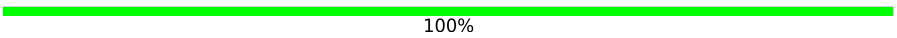
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:



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

Chain L:

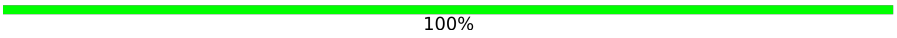


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:

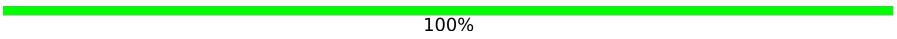
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:



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

Chain P:

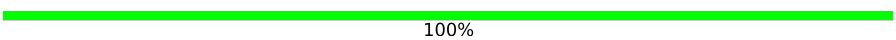


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

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	134669	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	0.32	0/9653	0.53	0/13146
1	B	0.31	0/9653	0.52	1/13146 (0.0%)
1	C	0.32	0/9653	0.54	0/13146
All	All	0.31	0/28959	0.53	1/39438 (0.0%)

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	4
1	C	0	1
All	All	0	5

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1148	TYR	CA-CB-CG	5.11	123.11	113.40

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	930	GLU	Peptide
1	A	968	PHE	Peptide
1	A	969	PRO	Peptide
1	A	972	SER	Peptide

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Mol	Chain	Res	Type	Group
1	C	968	PHE	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	9078	120	0
1	B	9425	0	9076	112	0
1	C	9425	0	9076	130	0
2	D	72	0	61	0	0
2	I	72	0	61	1	0
2	N	72	0	61	0	0
3	E	28	0	25	0	0
3	F	28	0	25	1	0
3	G	28	0	25	1	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	1	0
4	B	238	0	221	1	0
4	C	238	0	221	0	0
All	All	29541	0	28376	347	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 6.

All (347) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:ALA:HB2	1:B:220:THR:HA	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:890:CYS:H	1:A:899:SER:HB2	1.61	0.65
1:C:690:LEU:HB2	1:C:721:LEU:HB2	1.79	0.64
1:C:315:ALA:H	1:C:620:VAL:HG12	1.61	0.64
1:C:801:GLU:OE1	1:C:1145:HIS:NE2	2.31	0.64
1:A:868:SER:HB3	1:A:871:LEU:HB2	1.81	0.63
1:C:353:ASN:HB3	1:C:605:ASN:HD22	1.63	0.63
1:C:287:LEU:HB3	1:C:688:PRO:HD3	1.82	0.61
1:A:201:HIS:HB3	1:A:212:TYR:HB2	1.82	0.61
1:C:795:THR:OG1	1:C:796:ILE:N	2.32	0.61
1:C:978:PRO:O	1:C:982:ASN:N	2.30	0.61
1:C:132:ASN:N	1:C:132:ASN:OD1	2.33	0.61
1:B:62:LEU:HD13	1:B:295:GLN:HG2	1.82	0.61
1:B:348:ILE:HG23	1:B:387:THR:HG22	1.83	0.60
1:A:429:LEU:HB2	1:A:588:ILE:HD11	1.84	0.60
1:B:904:GLU:O	1:B:908:PHE:HB2	2.02	0.60
1:A:366:ASP:N	1:A:366:ASP:OD1	2.34	0.60
1:B:466:CYS:HB3	1:B:547:PRO:HD2	1.84	0.59
1:C:971:TRP:HB3	1:C:974:ALA:HB3	1.85	0.59
1:A:183:CYS:SG	1:A:186:LYS:NZ	2.76	0.58
1:C:650:ASP:HB3	1:C:656:ILE:HD11	1.84	0.58
1:A:504:CYS:HA	1:A:518:CYS:HA	1.85	0.58
1:A:518:CYS:HB2	1:A:521:LEU:HD21	1.86	0.58
1:A:1023:ASN:HD22	1:A:1025:ALA:H	1.51	0.58
1:C:92:PRO:HA	1:C:95:LEU:HB3	1.86	0.58
1:C:627:ILE:HG21	1:C:655:ILE:HD13	1.86	0.57
1:C:1165:SER:O	1:C:1168:ARG:NH2	2.37	0.57
1:A:370:CYS:HA	1:A:423:CYS:HA	1.86	0.57
1:B:793:ASN:HB3	1:B:1151:THR:HB	1.85	0.57
1:A:338:VAL:HG21	1:A:434:VAL:HG13	1.87	0.57
1:B:735:ASP:OD1	1:B:735:ASP:N	2.37	0.57
1:B:1013:LEU:O	1:B:1017:ASN:ND2	2.38	0.57
1:B:293:LYS:HE3	1:B:304:TYR:HB3	1.88	0.56
1:A:23:SER:O	1:A:170:ARG:NH1	2.39	0.56
1:B:344:TRP:NE1	1:B:413:ASN:O	2.39	0.56
1:C:920:GLU:HA	1:C:923:ASN:HD22	1.71	0.56
1:B:606:ASP:HA	3:G:1:NAG:H82	1.87	0.56
1:C:319:ARG:NH1	1:C:612:THR:O	2.38	0.56
1:C:772:VAL:HG21	1:A:867:LEU:HB2	1.86	0.56
1:B:472:ASP:N	1:B:472:ASP:OD1	2.38	0.56
1:B:1075:ASP:O	1:B:1079:ASN:ND2	2.39	0.56
1:A:832:TYR:OH	1:A:1079:ASN:ND2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:472:ASP:OD1	1:C:472:ASP:N	2.39	0.55
1:C:901:SER:OG	1:C:902:LEU:N	2.38	0.55
1:B:162:VAL:HB	1:B:172:GLU:HB2	1.89	0.55
1:B:973:ALA:HB2	1:B:1115:LYS:HE2	1.89	0.55
1:A:713:PHE:HB2	4:A:2012:NAG:H82	1.89	0.55
1:B:370:CYS:HA	1:B:423:CYS:HA	1.88	0.55
1:C:67:PHE:O	1:C:264:ARG:NH1	2.40	0.55
1:C:88:LEU:HA	1:C:91:LYS:HD3	1.87	0.55
1:C:103:PHE:HB3	1:C:259:THR:HG23	1.89	0.55
1:C:425:LEU:HB3	1:C:590:SER:HB3	1.88	0.55
1:C:1055:SER:OG	1:C:1056:SER:N	2.40	0.55
1:A:747:ALA:HB2	1:A:763:ARG:HH21	1.72	0.55
1:C:846:VAL:HG13	1:C:1096:ILE:HG13	1.89	0.55
1:A:919:VAL:O	1:A:923:ASN:ND2	2.39	0.55
1:C:767:PHE:O	1:A:954:GLN:NE2	2.39	0.54
1:B:694:ASN:HD21	1:C:919:VAL:HG13	1.72	0.54
4:B:2014:NAG:O7	1:C:870:ASN:ND2	2.41	0.54
1:C:886:SER:O	1:C:901:SER:OG	2.22	0.54
1:B:104:SER:HB2	1:B:200:PHE:HB2	1.89	0.54
1:A:213:TYR:HB3	1:A:223:LEU:HD22	1.90	0.54
1:B:123:THR:OG1	1:B:124:ILE:N	2.40	0.54
1:C:320:ARG:O	1:C:611:ASN:ND2	2.40	0.54
1:C:1066:ASP:OD1	1:C:1066:ASP:N	2.41	0.54
1:A:425:LEU:HB3	1:A:590:SER:HB3	1.89	0.54
1:B:314:VAL:HB	1:B:620:VAL:HG12	1.90	0.54
1:A:402:GLN:O	1:A:410:GLN:NE2	2.41	0.54
1:A:478:ASP:HB3	1:A:481:VAL:HG22	1.90	0.54
1:B:967:MET:SD	1:B:967:MET:N	2.78	0.53
1:C:794:PHE:HA	1:C:1150:PRO:HA	1.91	0.53
1:B:399:ASP:N	1:B:399:ASP:OD1	2.41	0.53
1:C:628:THR:OG1	1:A:1059:GLN:NE2	2.41	0.53
1:A:1147:SER:OG	1:A:1148:TYR:N	2.41	0.53
1:B:88:LEU:HA	1:B:91:LYS:HD3	1.91	0.53
1:C:14:VAL:N	1:C:157:GLU:OE1	2.41	0.53
1:A:479:PRO:O	1:A:483:ASN:ND2	2.41	0.53
1:C:959:THR:O	1:C:963:THR:OG1	2.24	0.53
1:A:339:PRO:HG2	1:A:391:PHE:HA	1.90	0.53
1:A:801:GLU:OE2	1:A:1145:HIS:NE2	2.36	0.53
1:B:397:ARG:HD3	1:B:409:LEU:HG	1.90	0.53
1:B:901:SER:H	1:B:904:GLU:HB2	1.74	0.53
1:B:1187:THR:OG1	1:B:1188:GLY:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:995:ASP:N	1:B:995:ASP:OD1	2.39	0.52
1:C:278:ASN:OD1	1:C:278:ASN:N	2.41	0.52
1:C:650:ASP:OD2	1:C:652:ASN:ND2	2.42	0.52
1:A:425:LEU:HG	1:A:427:TYR:HB3	1.91	0.52
1:C:382:CYS:HA	1:C:603:CYS:HA	1.91	0.52
1:B:147:GLU:OE2	1:B:186:LYS:NZ	2.42	0.52
1:B:422:SER:HA	1:B:593:ILE:HA	1.91	0.52
1:C:78:ALA:HB2	1:C:256:TYR:HB2	1.92	0.52
1:A:734:CYS:O	1:A:737:ARG:NH1	2.37	0.52
1:B:347:ARG:NH2	3:F:1:NAG:O6	2.43	0.52
1:C:1187:THR:OG1	1:C:1188:GLY:N	2.42	0.52
1:A:650:ASP:OD1	1:A:650:ASP:N	2.43	0.52
1:C:129:VAL:HB	1:C:131:VAL:HG22	1.92	0.52
1:B:382:CYS:HA	1:B:603:CYS:HA	1.90	0.52
1:C:160:HIS:NE2	1:C:171:ASN:O	2.43	0.52
1:B:911:VAL:HG21	1:B:1138:PRO:HG2	1.91	0.51
1:A:886:SER:O	1:A:901:SER:OG	2.28	0.51
1:B:1164:LEU:HB2	1:B:1168:ARG:HB2	1.92	0.51
1:A:996:VAL:HA	1:A:999:LYS:HB2	1.92	0.51
1:C:124:ILE:HG22	1:C:139:VAL:HB	1.93	0.51
1:B:621:ASN:HD21	1:C:1059:GLN:HE22	1.56	0.51
1:C:656:ILE:O	1:C:669:ILE:N	2.39	0.51
1:C:678:SER:OG	1:C:693:ARG:NH2	2.43	0.51
1:C:1162:LEU:HD12	1:C:1213:THR:HB	1.92	0.51
1:B:373:LEU:HD11	1:B:594:PHE:HB2	1.93	0.51
1:C:1151:THR:OG1	1:C:1152:SER:N	2.43	0.51
1:A:535:GLN:NE2	1:A:553:GLU:OE2	2.43	0.51
1:C:98:PHE:HE2	1:C:102:ILE:HG12	1.75	0.51
1:C:142:HIS:HB2	1:C:145:ILE:HB	1.92	0.51
1:B:965:ALA:O	1:B:972:SER:N	2.43	0.51
1:A:23:SER:OG	1:A:170:ARG:NH1	2.44	0.51
1:A:805:THR:H	1:A:1140:GLY:HA2	1.76	0.51
1:B:215:ASP:OD1	1:B:215:ASP:N	2.42	0.50
1:A:131:VAL:HG23	1:A:133:THR:H	1.76	0.50
1:B:698:SER:O	1:B:702:ASN:ND2	2.45	0.50
1:B:1004:ILE:O	1:B:1008:PHE:HB2	2.11	0.50
1:C:987:ILE:HG22	1:C:992:VAL:HG21	1.93	0.50
1:A:214:ALA:HB2	1:A:220:THR:HA	1.93	0.50
1:A:1163:CYS:HB3	1:A:1214:LYS:HA	1.94	0.50
1:A:356:LEU:HD13	1:A:359:LEU:HD23	1.93	0.50
1:B:531:ASN:N	1:B:531:ASN:OD1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:789:GLN:NE2	1:B:1155:THR:OG1	2.43	0.50
1:C:1158:VAL:HB	1:C:1176:TYR:HB3	1.94	0.50
1:B:199:TYR:HB2	1:B:214:ALA:HB3	1.92	0.50
1:C:904:GLU:O	1:C:908:PHE:HB2	2.11	0.50
1:C:636:VAL:O	1:C:666:THR:OG1	2.30	0.50
1:C:396:ARG:NH1	1:C:578:ASP:OD2	2.45	0.50
1:C:955:ILE:HB	1:C:1136:ASN:HD21	1.77	0.50
1:C:904:GLU:OE1	1:C:1135:GLN:NE2	2.43	0.50
1:C:597:ILE:HD11	1:A:1064:ARG:HG2	1.93	0.49
1:C:1162:LEU:HD22	1:C:1218:ILE:HD12	1.94	0.49
1:B:850:LEU:HD13	1:B:1096:ILE:HD11	1.94	0.49
1:A:356:LEU:H	1:A:605:ASN:HD22	1.60	0.49
1:A:880:ASP:OD1	1:A:880:ASP:N	2.43	0.49
1:B:580:CYS:HB2	1:B:587:ASN:H	1.77	0.49
1:B:66:TYR:HB3	1:B:261:LEU:HD13	1.93	0.49
1:B:140:GLN:NE2	1:B:172:GLU:OE2	2.45	0.49
1:B:187:LYS:HD3	1:A:324:LEU:HD11	1.95	0.49
1:A:215:ASP:N	1:A:215:ASP:OD1	2.44	0.49
1:A:375:LYS:HA	1:A:378:ILE:HD12	1.95	0.49
1:C:108:ASN:HB3	1:C:196:ASP:HA	1.94	0.49
1:C:366:ASP:HB2	1:C:426:TYR:HB3	1.94	0.49
1:B:479:PRO:O	1:B:483:ASN:ND2	2.40	0.49
1:C:405:SER:O	1:C:415:LYS:NZ	2.46	0.49
1:B:688:PRO:O	1:B:722:ASN:ND2	2.40	0.49
1:C:558:THR:OG1	1:C:561:ASN:O	2.31	0.49
1:B:786:PHE:HD2	1:B:1158:VAL:HG23	1.77	0.49
1:A:481:VAL:HB	1:A:506:LEU:HD21	1.95	0.49
1:A:38:ASP:HB3	1:A:74:PHE:HB2	1.95	0.48
1:A:901:SER:H	1:A:904:GLU:HG3	1.78	0.48
1:B:568:SER:HB2	1:B:571:ALA:HB2	1.94	0.48
1:C:30:LYS:HA	1:C:88:LEU:HD22	1.96	0.48
1:C:90:TYR:OH	1:C:159:PRO:O	2.32	0.48
1:A:319:ARG:NE	1:A:660:ASP:OD1	2.46	0.48
1:C:1019:PHE:HA	1:C:1023:ASN:HD22	1.79	0.48
1:A:346:ARG:NH2	1:A:389:ASP:OD2	2.47	0.48
1:B:992:VAL:HG13	1:B:1191:TYR:HB2	1.95	0.48
1:C:444:TRP:NE1	1:C:547:PRO:O	2.46	0.48
1:A:142:HIS:NE2	1:A:147:GLU:OE1	2.43	0.48
1:A:422:SER:OG	1:A:424:GLN:NE2	2.47	0.48
1:A:654:ASN:OD1	1:A:654:ASN:N	2.46	0.47
1:B:29:ASN:HD22	1:B:31:THR:HB	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1019:PHE:HB3	1:B:1026:LEU:HD11	1.94	0.47
1:C:385:SER:HB3	1:C:595:ASN:HB2	1.97	0.47
1:B:329:ILE:HA	1:B:332:TRP:HB3	1.96	0.47
1:C:18:PHE:HD2	2:I:1:NAG:H62	1.79	0.47
1:A:527:THR:OG1	1:A:528:TYR:N	2.47	0.47
1:C:794:PHE:HE1	1:C:1191:TYR:HB2	1.80	0.47
1:B:614:VAL:HG12	1:B:616:THR:HG22	1.97	0.47
1:A:369:SER:O	1:A:424:GLN:N	2.47	0.47
1:B:431:LEU:HD23	1:B:434:VAL:HG21	1.96	0.47
1:B:773:SER:HB2	1:C:866:THR:HG22	1.96	0.47
1:C:393:ILE:HD12	1:C:587:ASN:HB3	1.95	0.47
1:A:1107:ILE:O	1:A:1111:ASN:ND2	2.48	0.47
1:B:62:LEU:HD11	1:B:265:GLN:HE21	1.79	0.47
1:B:502:ARG:NH1	1:B:554:GLU:OE1	2.46	0.47
1:A:367:SER:HB3	1:A:426:TYR:HB2	1.97	0.47
1:C:978:PRO:HG2	1:C:981:LEU:HB2	1.97	0.46
1:C:1061:ILE:HG23	1:C:1065:LEU:HD12	1.96	0.46
1:A:26:ASN:HB2	1:A:84:TYR:HB3	1.97	0.46
1:C:689:ALA:HA	1:C:722:ASN:HB3	1.97	0.46
1:C:919:VAL:O	1:C:923:ASN:ND2	2.48	0.46
1:A:311:VAL:O	1:A:312:LYS:NZ	2.43	0.46
1:A:69:LYS:NZ	1:A:70:SER:O	2.45	0.46
1:A:407:GLY:O	1:A:411:SER:OG	2.33	0.46
1:C:907:LEU:HD11	1:C:1142:LEU:HD22	1.98	0.46
1:B:1208:CYS:HB2	1:B:1212:PHE:HD2	1.81	0.46
1:A:861:LEU:HB3	1:A:962:ALA:HB2	1.97	0.46
1:A:863:GLN:O	1:A:1115:LYS:NZ	2.48	0.46
1:B:772:VAL:HG12	1:C:865:VAL:HG13	1.98	0.46
1:B:952:GLU:HA	1:B:955:ILE:HB	1.97	0.46
1:C:118:TYR:HA	1:C:143:ASN:HD21	1.81	0.46
1:A:1047:LEU:HA	1:A:1081:ARG:HE	1.80	0.46
1:C:510:LEU:O	1:A:583:ASN:ND2	2.49	0.45
1:A:1163:CYS:HB2	1:A:1212:PHE:HB3	1.98	0.45
1:B:38:ASP:H	1:B:73:ASN:HD21	1.63	0.45
1:A:794:PHE:HA	1:A:1150:PRO:HA	1.99	0.45
1:B:743:CYS:SG	1:B:744:ILE:N	2.89	0.45
1:B:870:ASN:OD1	1:B:870:ASN:N	2.49	0.45
1:C:956:SER:O	1:C:960:THR:OG1	2.28	0.45
1:C:334:ASN:HA	1:C:429:LEU:HD11	1.98	0.45
1:A:172:GLU:OE2	1:A:174:TRP:NE1	2.48	0.45
1:C:800:GLU:HB2	1:C:1142:LEU:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:SER:OG	1:A:169:ILE:N	2.49	0.45
1:C:1169:GLY:N	1:C:1207:SER:O	2.50	0.45
1:A:937:VAL:O	1:A:941:ASN:ND2	2.40	0.45
1:B:794:PHE:HE2	1:B:1004:ILE:HD11	1.82	0.45
1:A:59:THR:OG1	1:A:60:THR:O	2.35	0.45
1:C:438:ASN:ND2	1:C:459:ASP:O	2.46	0.44
1:A:358:THR:HA	1:A:361:ARG:HG2	1.99	0.44
1:A:969:PRO:HA	1:A:971:TRP:CD2	2.52	0.44
1:B:809:LYS:NZ	1:B:851:ASP:OD1	2.44	0.44
1:A:946:LEU:HD22	1:A:946:LEU:HA	1.87	0.44
1:B:95:LEU:HA	1:B:236:TYR:HB2	1.99	0.44
1:B:393:ILE:HD12	1:B:587:ASN:HB3	1.99	0.44
1:C:781:THR:O	1:C:781:THR:OG1	2.35	0.44
1:A:129:VAL:HB	1:A:131:VAL:HG22	1.99	0.44
1:C:91:LYS:HB3	1:C:93:PRO:HG2	1.99	0.44
1:B:802:PHE:HD2	1:B:1028:LYS:HB3	1.82	0.44
1:C:464:ASP:OD1	1:C:464:ASP:N	2.49	0.44
1:C:646:ASN:OD1	1:C:646:ASN:N	2.51	0.44
1:A:62:LEU:HD22	1:A:295:GLN:HE21	1.83	0.44
1:A:245:ILE:HG13	1:A:252:GLU:HB2	2.00	0.44
1:A:338:VAL:HB	1:A:436:ILE:HA	2.00	0.44
1:B:91:LYS:HD2	1:B:91:LYS:HA	1.70	0.44
1:C:415:LYS:HB3	1:C:542:ILE:HG12	1.98	0.44
1:C:431:LEU:HD11	1:C:581:ILE:HG21	1.99	0.44
1:A:556:CYS:HA	1:A:567:CYS:HA	2.00	0.44
1:B:671:PRO:HG2	1:C:940:PHE:HD2	1.83	0.44
1:B:1159:SER:HB3	1:B:1177:PHE:HB2	2.00	0.44
1:B:98:PHE:HB3	1:B:233:SER:HA	1.99	0.43
1:C:319:ARG:HA	1:C:319:ARG:HD2	1.88	0.43
1:A:608:LEU:HD13	1:A:608:LEU:HA	1.89	0.43
1:A:1151:THR:OG1	1:A:1152:SER:N	2.51	0.43
1:B:400:ASP:O	1:B:410:GLN:NE2	2.51	0.43
1:B:959:THR:O	1:B:963:THR:OG1	2.28	0.43
1:C:986:ARG:HD2	1:C:1117:GLN:HG2	1.99	0.43
1:C:312:LYS:HD3	1:C:312:LYS:HA	1.76	0.43
1:C:983:VAL:O	1:C:987:ILE:HG13	2.18	0.43
1:A:417:ASP:HB2	1:A:542:ILE:HG21	2.00	0.43
1:B:36:SER:OG	1:B:73:ASN:ND2	2.51	0.43
1:B:161:THR:HA	1:B:172:GLU:HG3	2.01	0.43
1:B:951:SER:OG	1:B:954:GLN:OE1	2.37	0.43
1:C:850:LEU:HD13	1:C:1096:ILE:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:885:LYS:HE3	1:C:885:LYS:HB2	1.87	0.43
1:A:846:VAL:HG13	1:A:1096:ILE:HG13	2.00	0.43
1:B:777:ASP:HB3	1:B:787:GLU:HB3	2.00	0.43
1:B:901:SER:O	1:B:905:ASP:N	2.51	0.43
1:C:491:LEU:HD22	1:C:559:GLN:HB2	2.00	0.43
1:A:319:ARG:HB2	1:A:624:LEU:HD23	2.01	0.43
1:A:722:ASN:OD1	1:A:760:SER:OG	2.36	0.43
1:B:139:VAL:HG13	1:B:148:ILE:HG12	2.01	0.43
1:A:505:ASP:HB2	1:A:517:ARG:HG3	2.01	0.43
1:B:74:PHE:CG	1:B:257:TRP:HB3	2.54	0.43
1:C:16:GLY:HA3	1:C:155:MET:HB2	2.01	0.43
1:C:161:THR:OG1	1:C:239:PRO:O	2.29	0.43
1:A:203:TYR:HB3	1:A:261:LEU:HD12	2.01	0.43
1:B:243:LYS:HB2	1:B:243:LYS:HZ2	1.84	0.43
1:B:767:PHE:O	1:C:954:GLN:NE2	2.50	0.43
1:B:983:VAL:HG22	1:B:1131:LEU:HD21	2.01	0.43
1:C:785:LEU:HD12	1:C:1157:LEU:HD12	2.01	0.43
1:C:849:LEU:O	1:C:853:THR:OG1	2.35	0.43
1:B:392:ALA:HB3	1:B:460:VAL:HG11	2.01	0.43
1:A:1066:ASP:O	1:A:1070:ALA:N	2.51	0.43
1:B:1196:PRO:O	1:B:1201:ASN:ND2	2.52	0.42
1:C:163:CYS:HB3	1:C:240:LEU:HD21	2.00	0.42
1:B:378:ILE:HG23	1:B:383:PHE:HZ	1.85	0.42
1:B:711:PHE:HE1	1:B:758:ILE:HB	1.84	0.42
1:B:917:GLY:HA2	1:B:920:GLU:HG2	2.00	0.42
1:A:518:CYS:H	1:A:521:LEU:HD11	1.84	0.42
1:B:320:ARG:HH22	1:B:626:GLY:HA2	1.83	0.42
1:B:593:ILE:O	1:B:595:ASN:ND2	2.52	0.42
1:C:981:LEU:HA	1:C:984:GLN:HB2	2.01	0.42
1:A:648:LEU:HD12	1:A:648:LEU:HA	1.94	0.42
1:B:472:ASP:HB2	1:B:500:LYS:HG3	2.01	0.42
1:C:1047:LEU:O	1:C:1056:SER:OG	2.26	0.42
1:A:312:LYS:HD3	1:A:312:LYS:HA	1.85	0.42
1:C:648:LEU:HA	1:A:55:VAL:HB	2.00	0.42
1:B:109:THR:OG1	1:B:120:GLU:O	2.38	0.42
1:A:115:ASN:N	1:A:115:ASN:OD1	2.53	0.42
1:A:369:SER:HB3	1:A:424:GLN:HB2	2.00	0.42
1:A:445:ASN:OD1	1:A:549:LEU:N	2.52	0.42
1:B:801:GLU:OE2	1:B:1145:HIS:NE2	2.47	0.42
1:B:816:ALA:HA	1:B:820:SER:HA	2.01	0.42
1:C:861:LEU:HA	1:C:1115:LYS:HE3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:ILE:HG21	1:A:388:VAL:HG21	2.01	0.42
1:C:1145:HIS:O	1:C:1147:SER:OG	2.37	0.42
1:A:805:THR:HG22	1:A:1103:ALA:HA	2.02	0.42
1:B:931:ILE:HD11	1:A:656:ILE:HD12	2.01	0.42
1:B:128:SER:HB2	1:B:232:LEU:HA	2.02	0.41
1:B:1178:ILE:H	1:B:1178:ILE:HG13	1.74	0.41
1:A:466:CYS:HB3	1:A:547:PRO:HD2	2.02	0.41
1:A:865:VAL:HG21	1:A:965:ALA:HB1	2.01	0.41
1:B:982:ASN:OD1	1:B:1117:GLN:NE2	2.54	0.41
1:A:552:ASN:H	1:A:571:ALA:HB1	1.85	0.41
1:B:98:PHE:HE2	1:B:101:GLY:HA2	1.84	0.41
1:B:314:VAL:H	1:B:620:VAL:HA	1.85	0.41
1:C:780:GLU:H	1:C:780:GLU:HG2	1.70	0.41
1:A:378:ILE:HG12	1:A:383:PHE:HZ	1.85	0.41
1:A:795:THR:OG1	1:A:796:ILE:N	2.54	0.41
1:A:1170:ILE:HG22	1:A:1204:PHE:HA	2.02	0.41
1:B:98:PHE:HB2	1:B:235:TYR:HD2	1.85	0.41
1:B:965:ALA:HB1	1:B:972:SER:HB2	2.02	0.41
1:C:112:TYR:HD1	1:C:112:TYR:HA	1.73	0.41
1:C:647:LEU:O	1:A:55:VAL:N	2.49	0.41
1:C:1121:ILE:H	1:C:1121:ILE:HG13	1.65	0.41
1:A:865:VAL:HG23	1:A:972:SER:HB2	2.01	0.41
1:B:212:TYR:HB3	1:B:220:THR:HB	2.02	0.41
1:B:1178:ILE:HG12	1:B:1187:THR:HB	2.02	0.41
1:A:515:TRP:HE1	1:A:517:ARG:HD2	1.85	0.41
1:A:537:LYS:HE3	1:A:537:LYS:HB2	1.90	0.41
1:A:1201:ASN:OD1	1:A:1201:ASN:N	2.52	0.41
1:C:164:LYS:HE2	1:C:164:LYS:HB3	1.83	0.41
1:C:355:ASN:ND2	1:C:605:ASN:OD1	2.50	0.41
1:C:360:LEU:HD23	1:C:360:LEU:HA	1.95	0.41
1:C:987:ILE:HD12	1:C:997:LEU:HD21	2.03	0.41
1:A:961:ALA:O	1:A:965:ALA:HB2	2.21	0.41
1:A:1149:LYS:HA	1:A:1150:PRO:HD3	1.95	0.41
1:B:572:PHE:O	1:B:575:TRP:NE1	2.53	0.41
1:C:320:ARG:NH2	1:C:380:GLY:O	2.54	0.41
1:C:1015:ILE:HD13	1:C:1015:ILE:HA	1.86	0.41
1:C:1191:TYR:CD1	1:C:1193:TYR:HB2	2.55	0.41
1:C:832:TYR:OH	1:C:1079:ASN:ND2	2.52	0.41
1:A:1163:CYS:O	1:A:1215:ALA:N	2.46	0.41
1:B:332:TRP:HA	1:B:335:ASN:HB2	2.02	0.41
1:C:223:LEU:HD12	1:C:223:LEU:HA	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:748:LEU:H	1:C:748:LEU:HG	1.45	0.41
1:C:961:ALA:HA	1:C:964:VAL:HG12	2.02	0.41
1:A:790:ILE:HB	1:A:1192:TYR:HB2	2.03	0.41
1:A:839:ILE:HG23	1:A:1089:VAL:HG21	2.02	0.41
1:B:219:PRO:HG2	1:B:276:ILE:HD12	2.02	0.40
1:C:405:SER:OG	1:C:406:SER:N	2.54	0.40
1:C:1148:TYR:OH	1:C:1190:SER:O	2.38	0.40
1:C:1018:GLY:O	1:C:1023:ASN:ND2	2.55	0.40
1:C:1220:LEU:HD13	1:C:1220:LEU:HA	1.96	0.40
1:B:30:LYS:H	1:B:30:LYS:HG2	1.73	0.40
1:C:616:THR:HG21	1:C:635:GLU:HB2	2.03	0.40
1:A:642:ASN:OD1	1:A:643:ASN:ND2	2.54	0.40
1:A:130:PHE:HA	1:A:136:THR:HG21	2.03	0.40
1:A:1061:ILE:HG23	1:A:1065:LEU:HD12	2.03	0.40
1:C:898:SER:O	1:C:898:SER:OG	2.39	0.40
1:A:465:HIS:HE1	1:A:537:LYS:HD3	1.86	0.40
1:A:1067:PRO:O	1:A:1071:GLN:NE2	2.45	0.40
1:A:1130:ILE:HG22	1:A:1131:LEU:HG	2.04	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%)	1097 (91%)	109 (9%)	0	100	100
1	B	1206/1290 (94%)	1125 (93%)	81 (7%)	0	100	100
1	C	1206/1290 (94%)	1105 (92%)	101 (8%)	0	100	100
All	All	3618/3870 (94%)	3327 (92%)	291 (8%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1082/1159 (93%)	940 (87%)	142 (13%)	3 14
1	B	1082/1159 (93%)	924 (85%)	158 (15%)	2 11
1	C	1082/1159 (93%)	919 (85%)	163 (15%)	2 10
All	All	3246/3477 (93%)	2783 (86%)	463 (14%)	5 12

All (463) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	14	VAL
1	B	21	THR
1	B	34	ARG
1	B	38	ASP
1	B	40	VAL
1	B	50	TYR
1	B	54	ARG
1	B	55	VAL
1	B	73	ASN
1	B	88	LEU
1	B	91	LYS
1	B	99	ASN
1	B	100	ASN
1	B	102	ILE
1	B	117	LEU
1	B	123	THR
1	B	125	VAL
1	B	129	VAL
1	B	131	VAL
1	B	136	THR
1	B	142	HIS
1	B	143	ASN
1	B	145	ILE
1	B	149	THR
1	B	153	TYR
1	B	157	GLU

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Mol	Chain	Res	Type
1	B	166	LYS
1	B	175	HIS
1	B	177	ASP
1	B	203	TYR
1	B	204	GLN
1	B	224	PHE
1	B	231	ILE
1	B	249	THR
1	B	254	LEU
1	B	256	TYR
1	B	258	VAL
1	B	261	LEU
1	B	264	ARG
1	B	266	TYR
1	B	275	VAL
1	B	277	THR
1	B	282	CYS
1	B	283	SER
1	B	285	SER
1	B	287	LEU
1	B	309	PHE
1	B	320	ARG
1	B	331	ASN
1	B	346	ARG
1	B	358	THR
1	B	359	LEU
1	B	361	ARG
1	B	373	LEU
1	B	399	ASP
1	B	403	LEU
1	B	428	SER
1	B	429	LEU
1	B	450	PHE
1	B	455	VAL
1	B	459	ASP
1	B	478	ASP
1	B	480	SER
1	B	482	VAL
1	B	485	CYS
1	B	486	VAL
1	B	503	HIS
1	B	506	LEU

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Mol	Chain	Res	Type
1	B	512	VAL
1	B	517	ARG
1	B	523	ASP
1	B	526	SER
1	B	531	ASN
1	B	540	VAL
1	B	558	THR
1	B	578	ASP
1	B	582	SER
1	B	601	THR
1	B	603	CYS
1	B	604	SER
1	B	616	THR
1	B	618	VAL
1	B	630	GLN
1	B	640	TYR
1	B	644	TRP
1	B	658	PHE
1	B	659	LYS
1	B	661	PHE
1	B	662	LEU
1	B	677	VAL
1	B	706	PHE
1	B	711	PHE
1	B	714	ASP
1	B	731	VAL
1	B	735	ASP
1	B	740	SER
1	B	743	CYS
1	B	748	LEU
1	B	760	SER
1	B	772	VAL
1	B	787	GLU
1	B	788	ILE
1	B	789	GLN
1	B	801	GLU
1	B	807	SER
1	B	828	LEU
1	B	835	PHE
1	B	848	ASP
1	B	849	LEU
1	B	850	LEU

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Mol	Chain	Res	Type
1	B	865	VAL
1	B	866	THR
1	B	869	SER
1	B	870	ASN
1	B	871	LEU
1	B	879	VAL
1	B	887	LEU
1	B	888	LEU
1	B	890	CYS
1	B	903	LEU
1	B	931	ILE
1	B	932	ARG
1	B	950	LEU
1	B	952	GLU
1	B	967	MET
1	B	986	ARG
1	B	987	ILE
1	B	988	ASN
1	B	990	LEU
1	B	993	THR
1	B	995	ASP
1	B	1001	GLN
1	B	1012	LEU
1	B	1015	ILE
1	B	1017	ASN
1	B	1022	THR
1	B	1030	GLN
1	B	1031	SER
1	B	1066	ASP
1	B	1069	GLU
1	B	1075	ASP
1	B	1086	ASN
1	B	1096	ILE
1	B	1113	CYS
1	B	1115	LYS
1	B	1124	CYS
1	B	1129	HIS
1	B	1131	LEU
1	B	1148	TYR
1	B	1152	SER
1	B	1173	LYS
1	B	1189	SER

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Mol	Chain	Res	Type
1	B	1193	TYR
1	B	1195	GLU
1	B	1203	VAL
1	B	1207	SER
1	B	1217	PHE
1	B	1219	TYR
1	C	14	VAL
1	C	17	ASP
1	C	20	CYS
1	C	21	THR
1	C	22	ASN
1	C	25	ILE
1	C	26	ASN
1	C	29	ASN
1	C	30	LYS
1	C	31	THR
1	C	34	ARG
1	C	37	GLU
1	C	41	ASP
1	C	42	VAL
1	C	49	TYR
1	C	51	VAL
1	C	52	LEU
1	C	59	THR
1	C	69	LYS
1	C	74	PHE
1	C	76	ASP
1	C	91	LYS
1	C	112	TYR
1	C	114	ASN
1	C	115	ASN
1	C	123	THR
1	C	125	VAL
1	C	129	VAL
1	C	132	ASN
1	C	147	GLU
1	C	149	THR
1	C	153	TYR
1	C	154	THR
1	C	175	HIS
1	C	185	PHE
1	C	187	LYS

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Mol	Chain	Res	Type
1	C	189	PHE
1	C	205	GLU
1	C	206	ARG
1	C	226	LEU
1	C	227	TYR
1	C	228	LEU
1	C	233	SER
1	C	243	LYS
1	C	248	ASN
1	C	258	VAL
1	C	259	THR
1	C	262	SER
1	C	282	CYS
1	C	294	THR
1	C	309	PHE
1	C	311	VAL
1	C	330	ASP
1	C	373	LEU
1	C	374	ASP
1	C	375	LYS
1	C	399	ASP
1	C	403	LEU
1	C	426	TYR
1	C	434	VAL
1	C	464	ASP
1	C	472	ASP
1	C	481	VAL
1	C	500	LYS
1	C	505	ASP
1	C	511	TYR
1	C	512	VAL
1	C	516	CYS
1	C	520	CYS
1	C	527	THR
1	C	535	GLN
1	C	546	CYS
1	C	549	LEU
1	C	558	THR
1	C	560	LEU
1	C	573	LEU
1	C	581	ILE
1	C	597	ILE

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Mol	Chain	Res	Type
1	C	601	THR
1	C	606	ASP
1	C	618	VAL
1	C	621	ASN
1	C	644	TRP
1	C	652	ASN
1	C	656	ILE
1	C	659	LYS
1	C	661	PHE
1	C	706	PHE
1	C	728	SER
1	C	734	CYS
1	C	738	MET
1	C	748	LEU
1	C	756	ARG
1	C	775	VAL
1	C	780	GLU
1	C	781	THR
1	C	792	THR
1	C	794	PHE
1	C	795	THR
1	C	800	GLU
1	C	805	THR
1	C	811	THR
1	C	820	SER
1	C	821	ASN
1	C	828	LEU
1	C	849	LEU
1	C	850	LEU
1	C	853	THR
1	C	865	VAL
1	C	867	LEU
1	C	873	THR
1	C	874	ASN
1	C	875	LEU
1	C	878	ASP
1	C	879	VAL
1	C	886	SER
1	C	890	CYS
1	C	894	GLN
1	C	899	SER
1	C	930	GLU

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Mol	Chain	Res	Type
1	C	952	GLU
1	C	953	THR
1	C	964	VAL
1	C	967	MET
1	C	970	PRO
1	C	977	VAL
1	C	993	THR
1	C	996	VAL
1	C	997	LEU
1	C	1002	LYS
1	C	1012	LEU
1	C	1022	THR
1	C	1056	SER
1	C	1066	ASP
1	C	1069	GLU
1	C	1077	LEU
1	C	1086	ASN
1	C	1089	VAL
1	C	1095	ASP
1	C	1096	ILE
1	C	1098	LEU
1	C	1113	CYS
1	C	1115	LYS
1	C	1121	ILE
1	C	1133	LEU
1	C	1141	LEU
1	C	1147	SER
1	C	1157	LEU
1	C	1159	SER
1	C	1162	LEU
1	C	1163	CYS
1	C	1178	ILE
1	C	1179	LYS
1	C	1185	MET
1	C	1187	THR
1	C	1199	ASP
1	C	1200	LYS
1	C	1202	VAL
1	C	1203	VAL
1	C	1208	CYS
1	C	1209	SER
1	C	1212	PHE

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Mol	Chain	Res	Type
1	C	1213	THR
1	A	14	VAL
1	A	18	PHE
1	A	21	THR
1	A	28	TYR
1	A	34	ARG
1	A	35	ILE
1	A	43	SER
1	A	48	THR
1	A	51	VAL
1	A	60	THR
1	A	64	THR
1	A	75	ARG
1	A	96	SER
1	A	97	ASP
1	A	109	THR
1	A	112	TYR
1	A	115	ASN
1	A	116	THR
1	A	129	VAL
1	A	134	SER
1	A	180	GLU
1	A	182	LEU
1	A	204	GLN
1	A	213	TYR
1	A	241	THR
1	A	242	CYS
1	A	243	LYS
1	A	245	ILE
1	A	248	ASN
1	A	258	VAL
1	A	259	THR
1	A	263	ARG
1	A	268	LEU
1	A	277	THR
1	A	281	ASP
1	A	305	ASP
1	A	306	LEU
1	A	309	PHE
1	A	310	THR
1	A	311	VAL
1	A	312	LYS

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Mol	Chain	Res	Type
1	A	314	VAL
1	A	317	VAL
1	A	318	TYR
1	A	358	THR
1	A	360	LEU
1	A	366	ASP
1	A	368	PHE
1	A	418	ILE
1	A	429	LEU
1	A	432	VAL
1	A	482	VAL
1	A	503	HIS
1	A	505	ASP
1	A	515	TRP
1	A	522	PRO
1	A	528	TYR
1	A	540	VAL
1	A	573	LEU
1	A	588	ILE
1	A	601	THR
1	A	609	TYR
1	A	619	CYS
1	A	634	LYS
1	A	640	TYR
1	A	644	TRP
1	A	646	ASN
1	A	654	ASN
1	A	661	PHE
1	A	662	LEU
1	A	676	ARG
1	A	677	VAL
1	A	685	SER
1	A	706	PHE
1	A	707	ILE
1	A	711	PHE
1	A	714	ASP
1	A	726	LEU
1	A	734	CYS
1	A	737	ARG
1	A	756	ARG
1	A	765	VAL
1	A	772	VAL

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Mol	Chain	Res	Type
1	A	779	VAL
1	A	781	THR
1	A	782	VAL
1	A	790	ILE
1	A	792	THR
1	A	799	HIS
1	A	803	ILE
1	A	811	THR
1	A	835	PHE
1	A	848	ASP
1	A	849	LEU
1	A	850	LEU
1	A	866	THR
1	A	871	LEU
1	A	875	LEU
1	A	877	SER
1	A	879	VAL
1	A	880	ASP
1	A	888	LEU
1	A	930	GLU
1	A	932	ARG
1	A	934	LEU
1	A	946	LEU
1	A	953	THR
1	A	970	PRO
1	A	977	VAL
1	A	987	ILE
1	A	990	LEU
1	A	994	MET
1	A	996	VAL
1	A	1001	GLN
1	A	1002	LYS
1	A	1003	LEU
1	A	1013	LEU
1	A	1017	ASN
1	A	1023	ASN
1	A	1026	LEU
1	A	1057	SER
1	A	1066	ASP
1	A	1069	GLU
1	A	1081	ARG
1	A	1086	ASN

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Mol	Chain	Res	Type
1	A	1089	VAL
1	A	1096	ILE
1	A	1114	VAL
1	A	1117	GLN
1	A	1147	SER
1	A	1149	LYS
1	A	1154	LYS
1	A	1156	VAL
1	A	1176	TYR
1	A	1187	THR
1	A	1189	SER
1	A	1201	ASN
1	A	1205	MET
1	A	1208	CYS
1	A	1210	VAL
1	A	1219	TYR
1	A	1221	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	73	ASN
1	B	99	ASN
1	B	152	GLN
1	B	204	GLN
1	B	265	GLN
1	B	291	GLN
1	B	371	ASN
1	B	595	ASN
1	B	598	ASN
1	B	621	ASN
1	B	652	ASN
1	B	694	ASN
1	B	874	ASN
1	B	876	HIS
1	B	982	ASN
1	B	984	GLN
1	B	1000	ASN
1	B	1017	ASN
1	B	1045	GLN
1	B	1091	GLN
1	B	1117	GLN

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Mol	Chain	Res	Type
1	B	1122	ASN
1	B	1201	ASN
1	C	22	ASN
1	C	115	ASN
1	C	140	GLN
1	C	152	GLN
1	C	351	ASN
1	C	561	ASN
1	C	694	ASN
1	C	722	ASN
1	C	923	ASN
1	C	1045	GLN
1	C	1091	GLN
1	C	1092	GLN
1	C	1136	ASN
1	A	73	ASN
1	A	204	GLN
1	A	234	HIS
1	A	278	ASN
1	A	295	GLN
1	A	424	GLN
1	A	465	HIS
1	A	583	ASN
1	A	595	ASN
1	A	605	ASN
1	A	643	ASN
1	A	694	ASN
1	A	838	ASN
1	A	923	ASN
1	A	982	ASN
1	A	988	ASN
1	A	1023	ASN
1	A	1059	GLN
1	A	1079	ASN
1	A	1091	GLN
1	A	1111	ASN

5.3.3 RNA

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	2,1	14,14,15	0.36	0	17,19,21	0.50	0
2	NAG	D	2	2	14,14,15	0.29	0	17,19,21	0.48	0
2	MAN	D	3	2	11,11,12	1.45	2 (18%)	15,15,17	1.55	3 (20%)
2	MAN	D	4	2	11,11,12	0.94	1 (9%)	15,15,17	1.29	2 (13%)
2	MAN	D	5	2	11,11,12	0.94	0	15,15,17	0.94	1 (6%)
2	MAN	D	6	2	11,11,12	1.01	1 (9%)	15,15,17	1.47	2 (13%)
3	NAG	E	1	1,3	14,14,15	0.54	0	17,19,21	0.63	0
3	NAG	E	2	3	14,14,15	0.50	0	17,19,21	0.45	0
3	NAG	F	1	1,3	14,14,15	0.30	0	17,19,21	0.49	0
3	NAG	F	2	3	14,14,15	0.36	0	17,19,21	0.46	0
3	NAG	G	1	1,3	14,14,15	0.80	1 (7%)	17,19,21	1.08	1 (5%)
3	NAG	G	2	3	14,14,15	0.43	0	17,19,21	0.64	1 (5%)
3	NAG	H	1	1,3	14,14,15	0.28	0	17,19,21	0.55	0
3	NAG	H	2	3	14,14,15	0.32	0	17,19,21	0.48	0
2	NAG	I	1	2,1	14,14,15	0.40	0	17,19,21	0.73	1 (5%)
2	NAG	I	2	2	14,14,15	0.29	0	17,19,21	0.54	0
2	MAN	I	3	2	11,11,12	1.37	1 (9%)	15,15,17	1.75	3 (20%)
2	MAN	I	4	2	11,11,12	0.94	1 (9%)	15,15,17	1.42	2 (13%)
2	MAN	I	5	2	11,11,12	1.21	1 (9%)	15,15,17	1.52	3 (20%)
2	MAN	I	6	2	11,11,12	1.46	2 (18%)	15,15,17	2.42	4 (26%)
3	NAG	J	1	1,3	14,14,15	0.35	0	17,19,21	0.52	0
3	NAG	J	2	3	14,14,15	0.40	0	17,19,21	0.43	0
3	NAG	K	1	1,3	14,14,15	0.23	0	17,19,21	0.50	0
3	NAG	K	2	3	14,14,15	0.31	0	17,19,21	0.53	0
3	NAG	L	1	1,3	14,14,15	0.38	0	17,19,21	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	L	2	3	14,14,15	0.40	0	17,19,21	0.45	0
3	NAG	M	1	1,3	14,14,15	0.39	0	17,19,21	0.43	0
3	NAG	M	2	3	14,14,15	0.40	0	17,19,21	0.57	1 (5%)
2	NAG	N	1	2,1	14,14,15	0.28	0	17,19,21	0.42	0
2	NAG	N	2	2	14,14,15	0.36	0	17,19,21	0.50	0
2	MAN	N	3	2	11,11,12	1.82	4 (36%)	15,15,17	1.62	3 (20%)
2	MAN	N	4	2	11,11,12	1.07	0	15,15,17	1.04	1 (6%)
2	MAN	N	5	2	11,11,12	0.97	1 (9%)	15,15,17	1.29	2 (13%)
2	MAN	N	6	2	11,11,12	0.74	0	15,15,17	1.27	2 (13%)
3	NAG	O	1	1,3	14,14,15	0.37	0	17,19,21	0.60	0
3	NAG	O	2	3	14,14,15	0.31	0	17,19,21	0.39	0
3	NAG	P	1	1,3	14,14,15	0.23	0	17,19,21	0.49	0
3	NAG	P	2	3	14,14,15	0.37	0	17,19,21	0.56	0
3	NAG	Q	1	1,3	14,14,15	0.62	0	17,19,21	0.96	1 (5%)
3	NAG	Q	2	3	14,14,15	0.45	0	17,19,21	0.52	0
3	NAG	R	1	1,3	14,14,15	0.21	0	17,19,21	0.59	0
3	NAG	R	2	3	14,14,15	0.35	0	17,19,21	0.46	0

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

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

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

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	3	MAN	O5-C5	3.38	1.50	1.43
2	N	3	MAN	O5-C5	3.33	1.50	1.43
2	I	6	MAN	C1-C2	3.31	1.59	1.52
2	I	5	MAN	C1-C2	3.26	1.59	1.52
2	N	3	MAN	C1-C2	3.03	1.59	1.52
2	I	3	MAN	O5-C5	2.67	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	6	MAN	C1-C2	2.65	1.58	1.52
2	I	6	MAN	C2-C3	2.63	1.56	1.52
3	G	1	NAG	O5-C1	2.62	1.47	1.43
2	D	3	MAN	C1-C2	2.38	1.57	1.52
2	N	5	MAN	C1-C2	2.37	1.57	1.52
2	N	3	MAN	C2-C3	2.33	1.55	1.52
2	N	3	MAN	C4-C3	2.29	1.58	1.52
2	D	4	MAN	C1-C2	2.29	1.57	1.52
2	I	4	MAN	O5-C5	2.04	1.47	1.43

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	6	MAN	C1-O5-C5	6.39	120.84	112.19
2	I	3	MAN	C1-O5-C5	5.31	119.39	112.19
2	N	3	MAN	C1-O5-C5	4.57	118.38	112.19
2	I	6	MAN	C1-C2-C3	4.41	115.08	109.67
2	D	3	MAN	C1-O5-C5	4.25	117.95	112.19
2	D	6	MAN	C1-O5-C5	4.24	117.93	112.19
2	I	6	MAN	O5-C1-C2	3.88	116.75	110.77
2	N	6	MAN	C1-O5-C5	3.82	117.37	112.19
2	I	4	MAN	C1-O5-C5	3.60	117.07	112.19
2	I	5	MAN	C1-O5-C5	3.57	117.02	112.19
2	N	5	MAN	C1-O5-C5	3.42	116.83	112.19
3	G	1	NAG	C1-O5-C5	3.32	116.69	112.19
2	D	4	MAN	C1-O5-C5	3.19	116.51	112.19
3	Q	1	NAG	C1-O5-C5	3.00	116.26	112.19
2	I	5	MAN	C1-C2-C3	2.73	113.02	109.67
2	N	3	MAN	C1-C2-C3	2.52	112.77	109.67
2	N	3	MAN	O2-C2-C3	-2.49	105.14	110.14
2	D	3	MAN	O2-C2-C3	-2.42	105.28	110.14
2	D	5	MAN	O2-C2-C3	-2.32	105.49	110.14
2	N	6	MAN	O2-C2-C3	-2.32	105.49	110.14
2	D	3	MAN	C1-C2-C3	2.31	112.50	109.67
3	G	2	NAG	C1-O5-C5	2.29	115.30	112.19
2	N	4	MAN	O2-C2-C3	-2.27	105.59	110.14
2	D	4	MAN	O2-C2-C3	-2.23	105.66	110.14
2	I	5	MAN	O2-C2-C3	-2.23	105.68	110.14
2	D	6	MAN	O2-C2-C3	-2.22	105.69	110.14
2	I	6	MAN	O2-C2-C3	-2.19	105.75	110.14
2	I	3	MAN	O2-C2-C3	-2.16	105.81	110.14
2	N	5	MAN	O2-C2-C3	-2.12	105.89	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	4	MAN	O2-C2-C3	-2.11	105.91	110.14
2	I	1	NAG	C1-O5-C5	2.10	115.03	112.19
2	I	3	MAN	C2-C3-C4	2.07	114.48	110.89
3	M	2	NAG	C1-O5-C5	2.01	114.91	112.19

There are no chirality outliers.

All (62) torsion outliers are listed below:

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

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

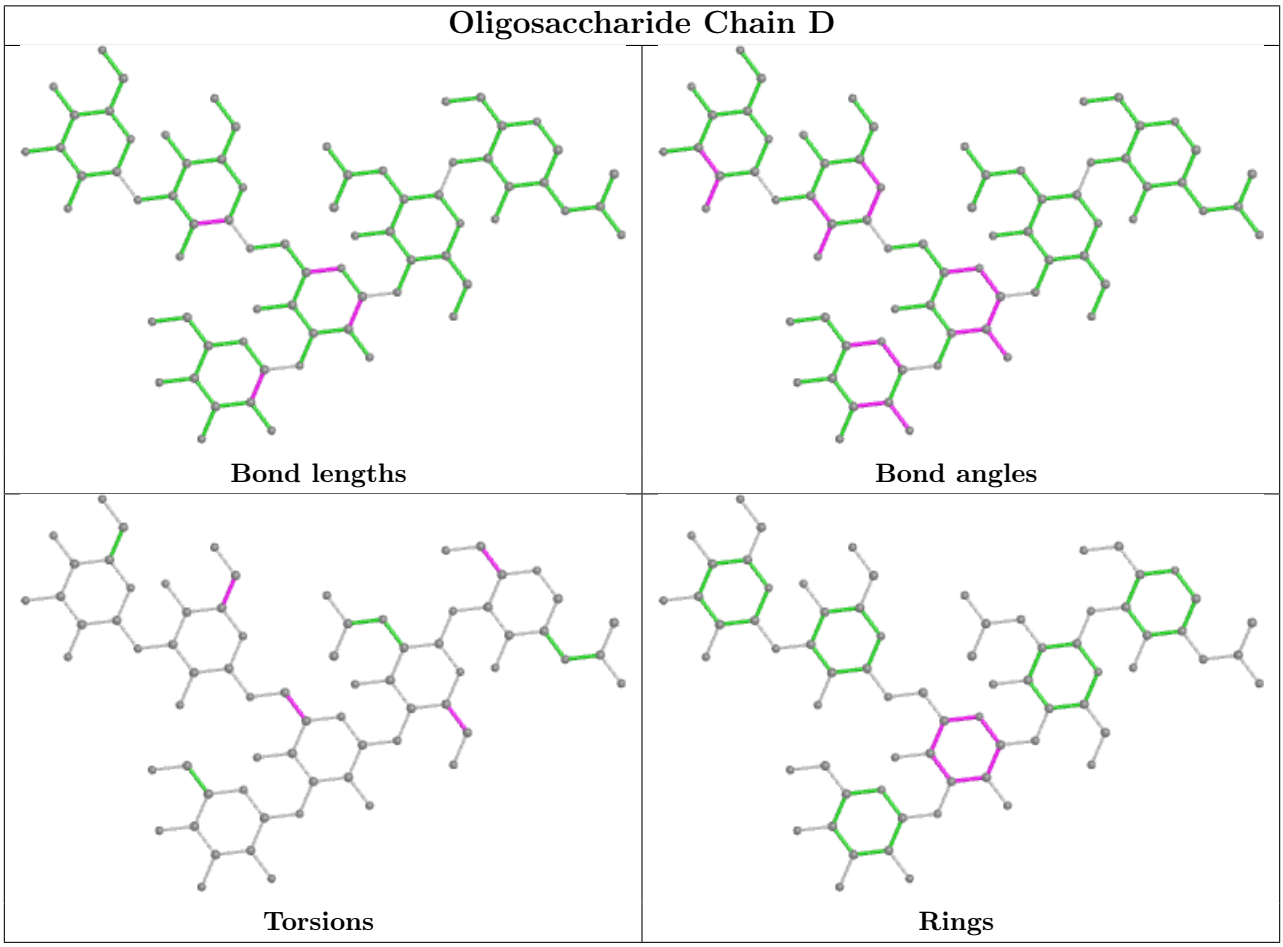
All (2) ring outliers are listed below:

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

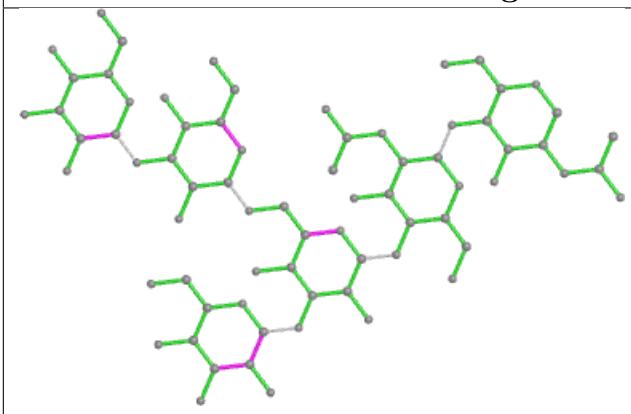
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	1	NAG	1	0
3	F	1	NAG	1	0
3	G	1	NAG	1	0

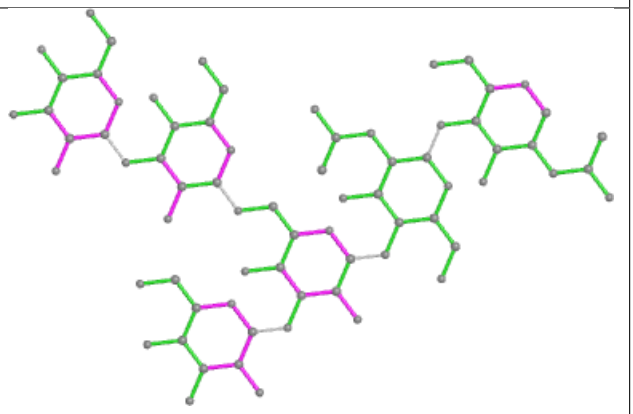
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



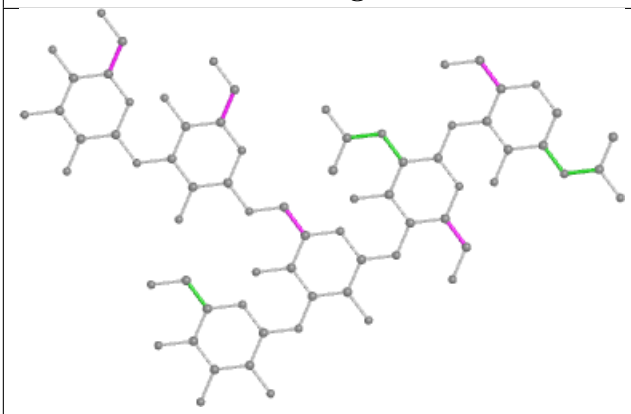
Oligosaccharide Chain I



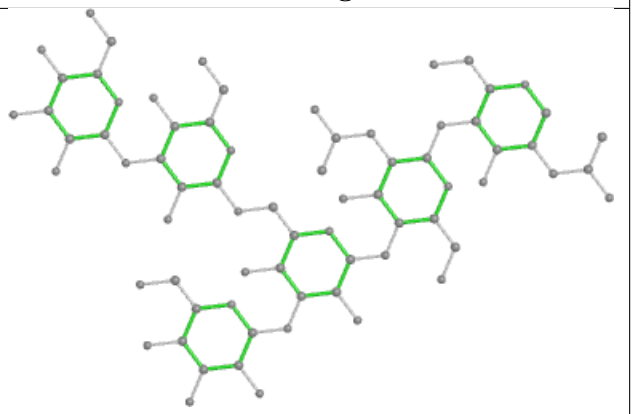
Bond lengths



Bond angles

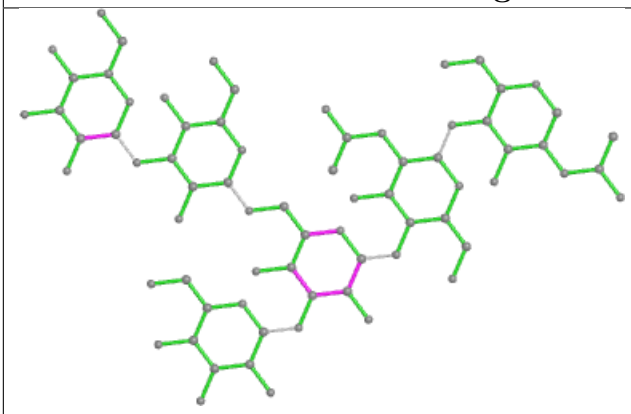


Torsions



Rings

Oligosaccharide Chain N



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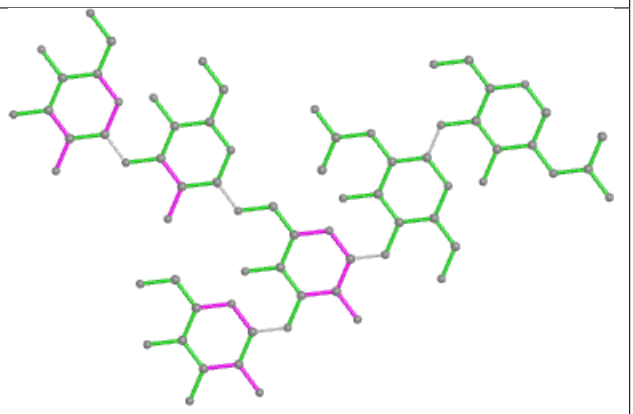
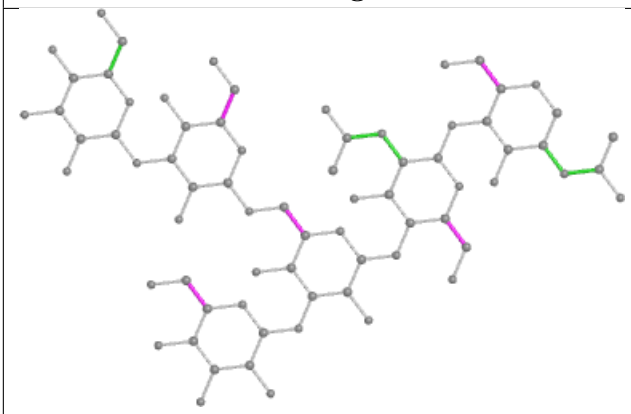


Bond angles



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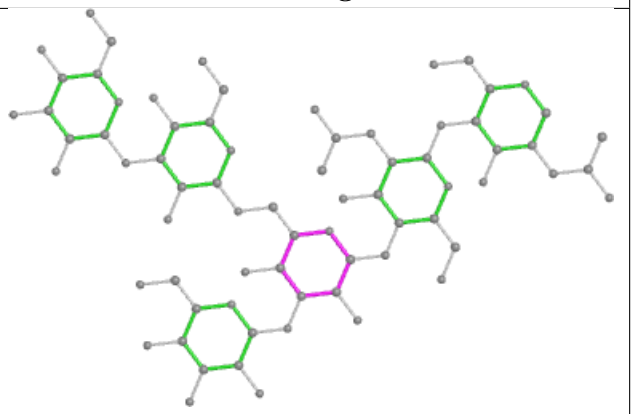
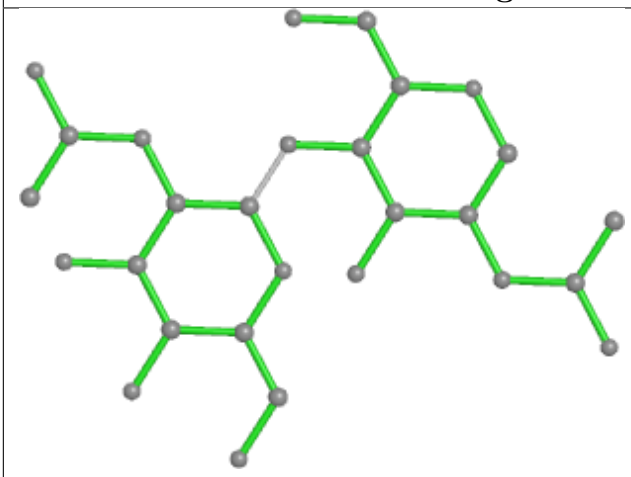


Rings

Oligosaccharide Chain E



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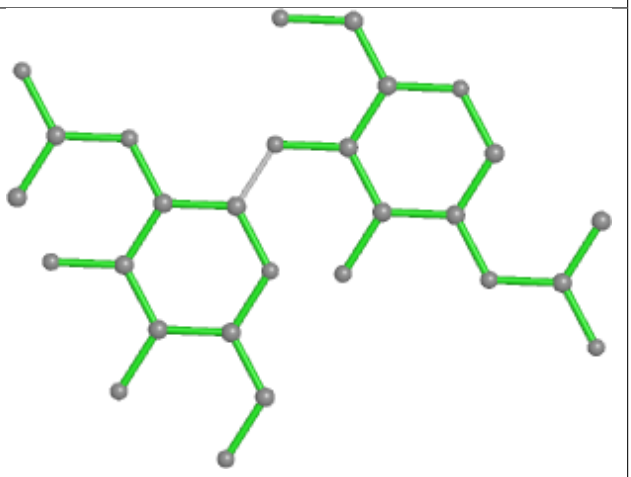
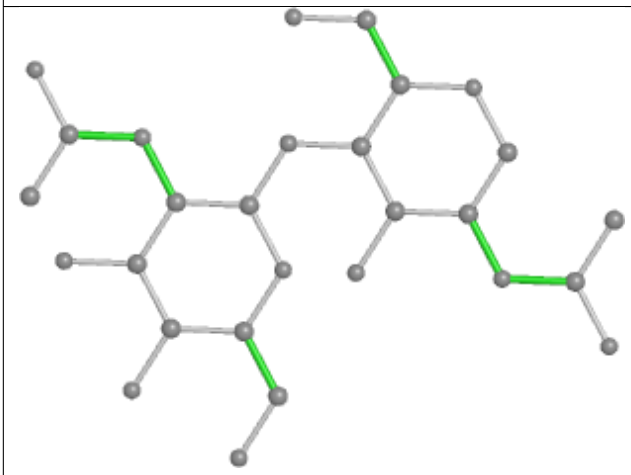


Bond angles



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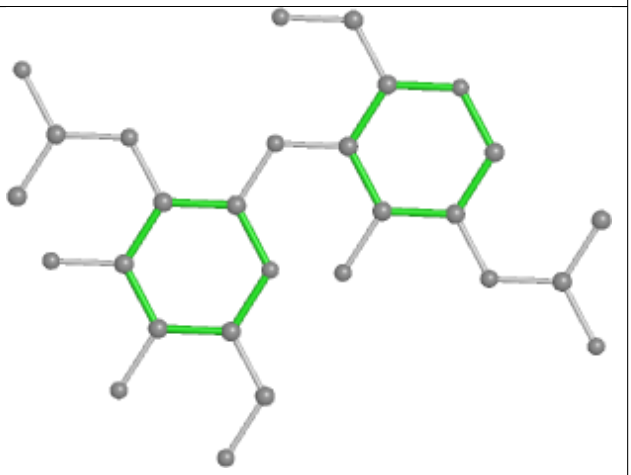
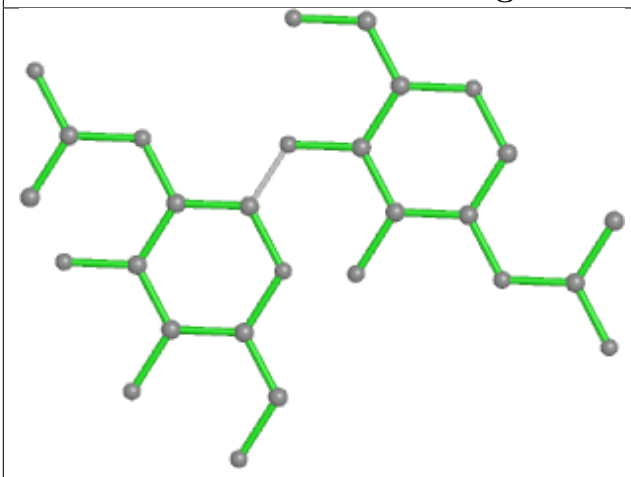
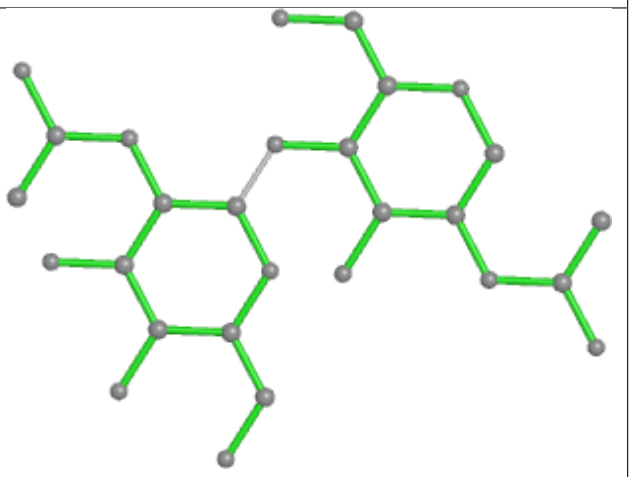


Rings

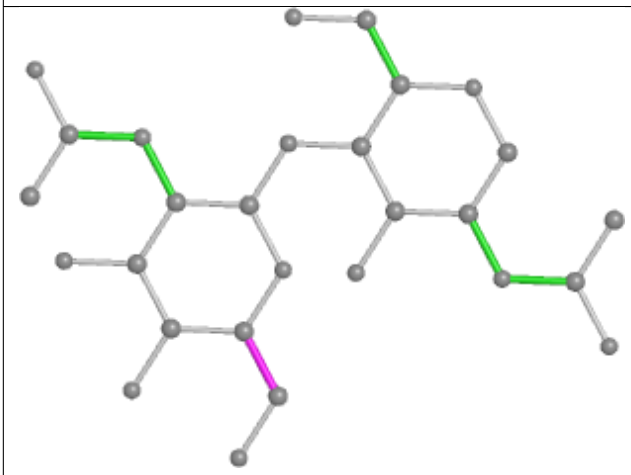
Oligosaccharide Chain F



Bond lengths



Bond angles



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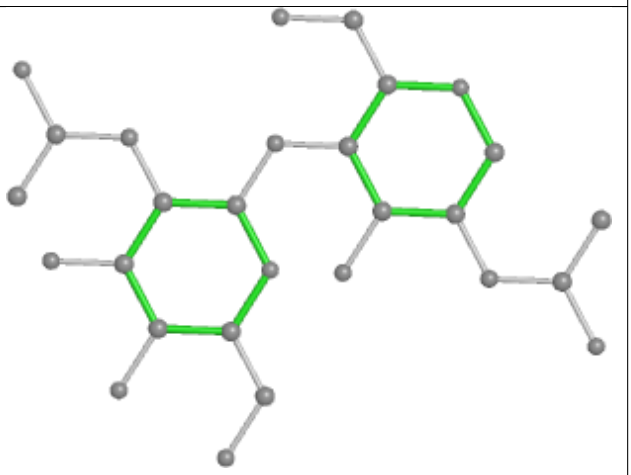
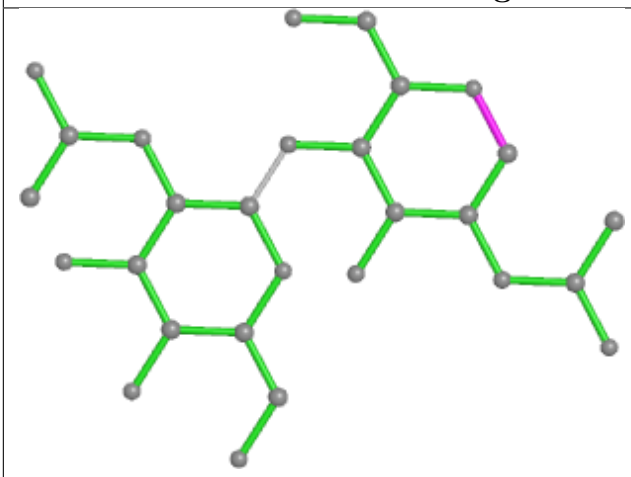
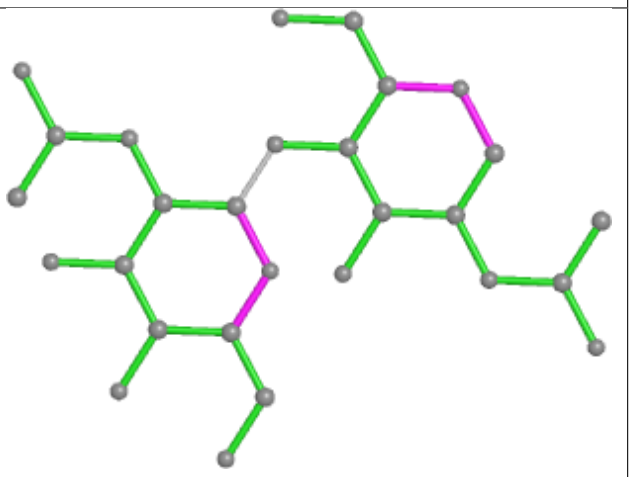


Rings

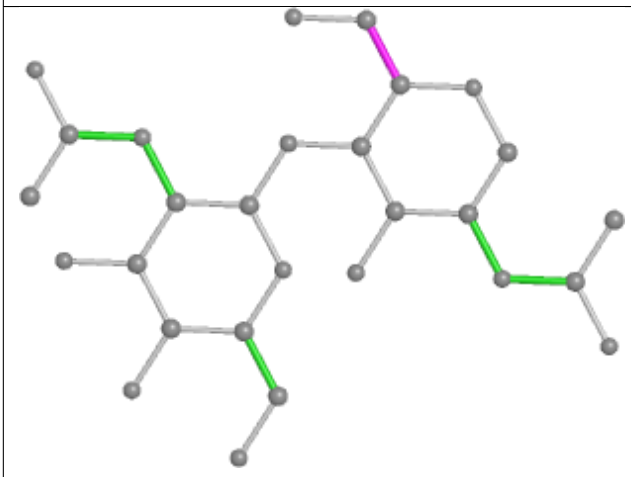
Oligosaccharide Chain G



Bond lengths



Bond angles



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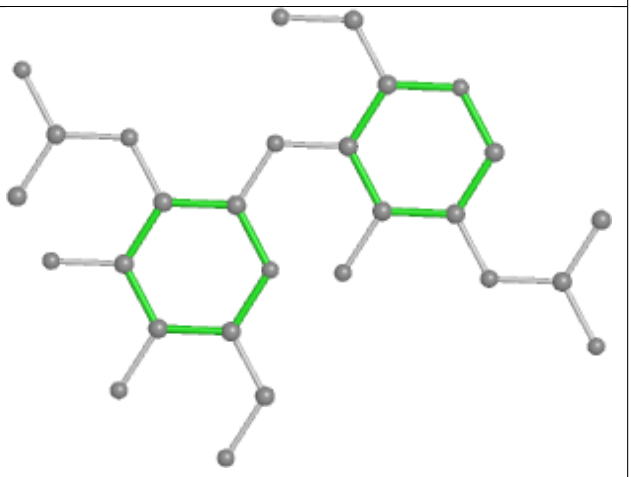
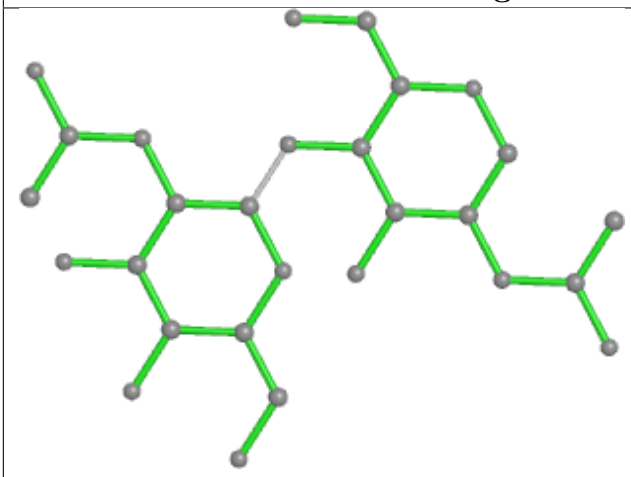
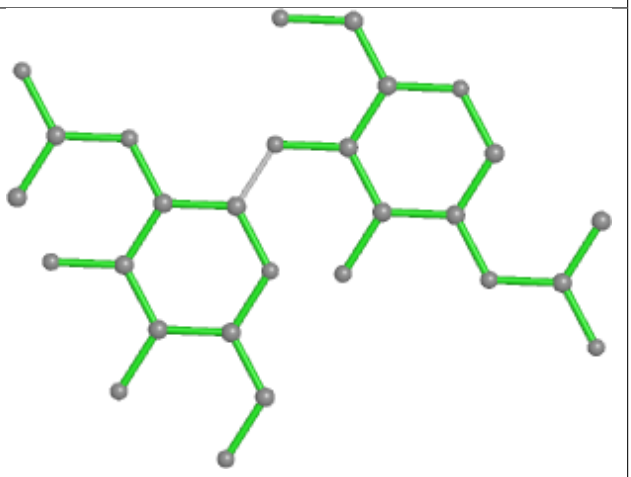


Rings

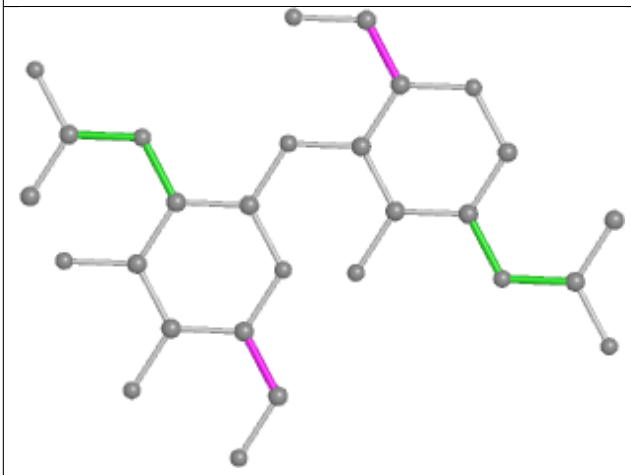
Oligosaccharide Chain H



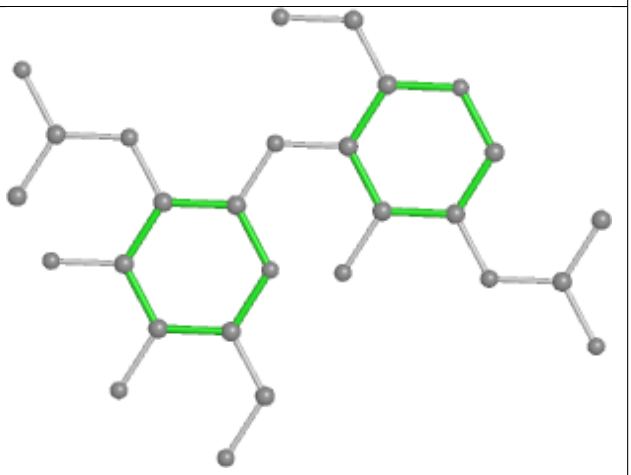
Bond lengths



Bond angles

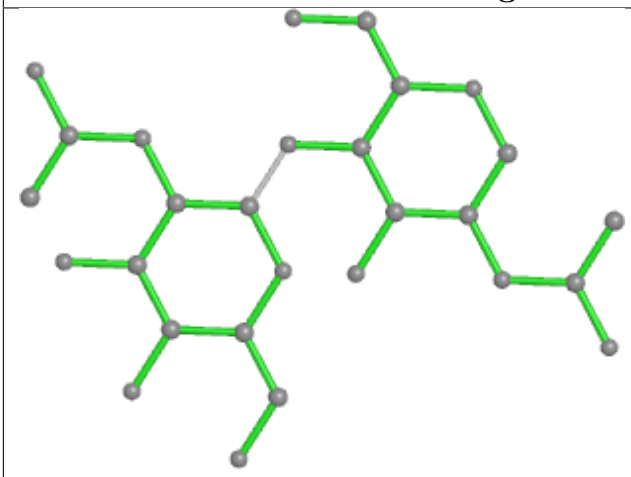


Torsions



Rings

Oligosaccharide Chain J



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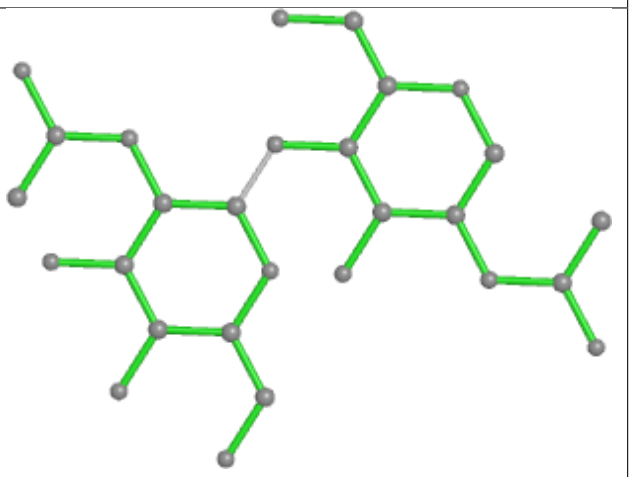
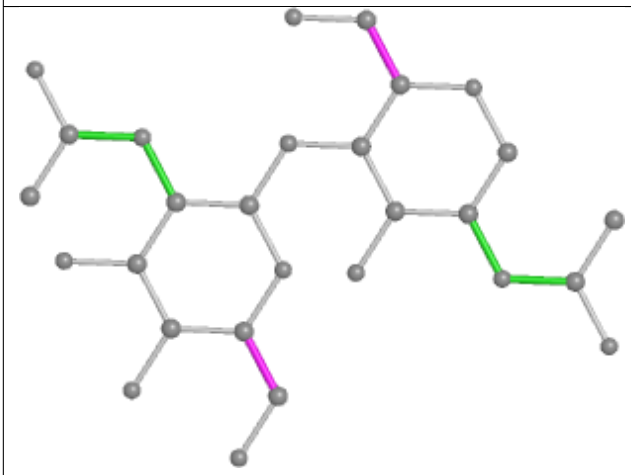


Bond angles



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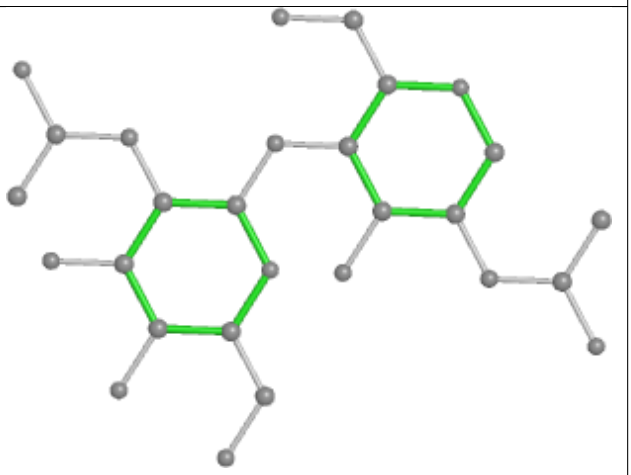
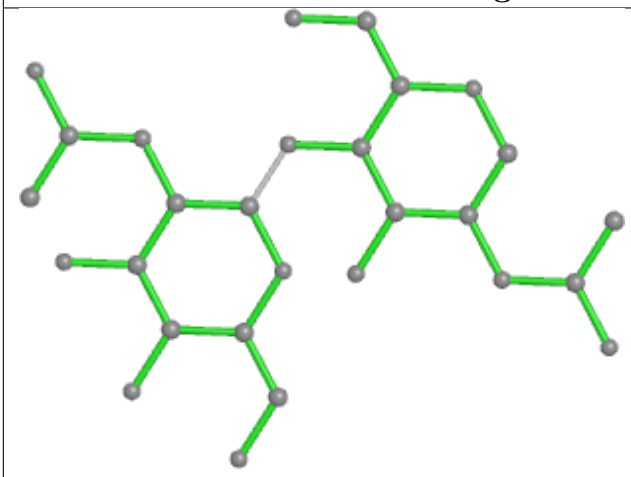


Rings

Oligosaccharide Chain K



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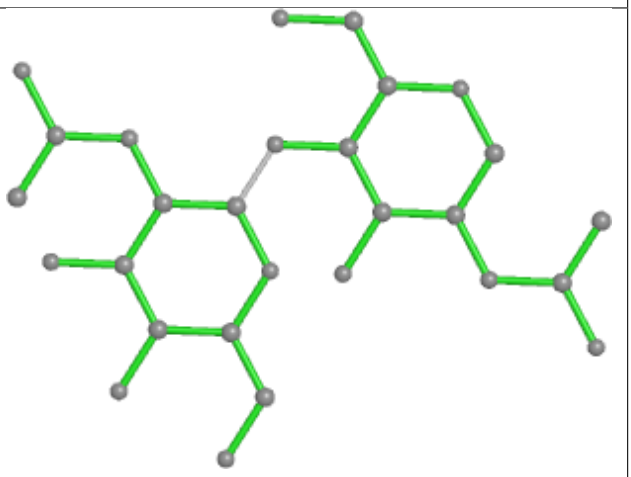
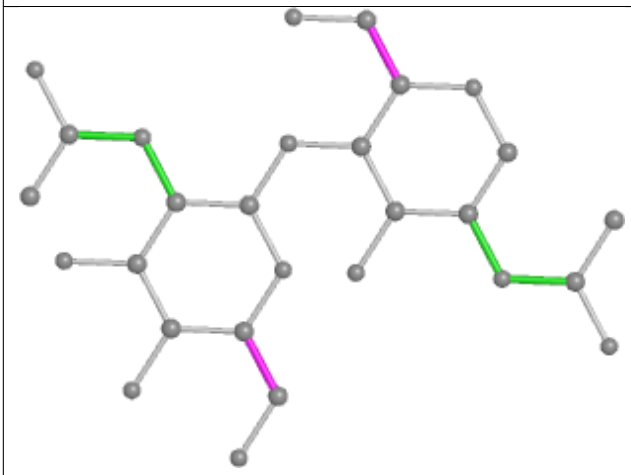


Bond angles



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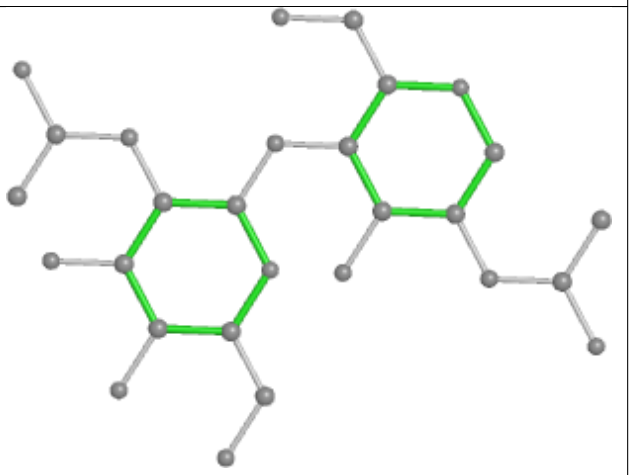
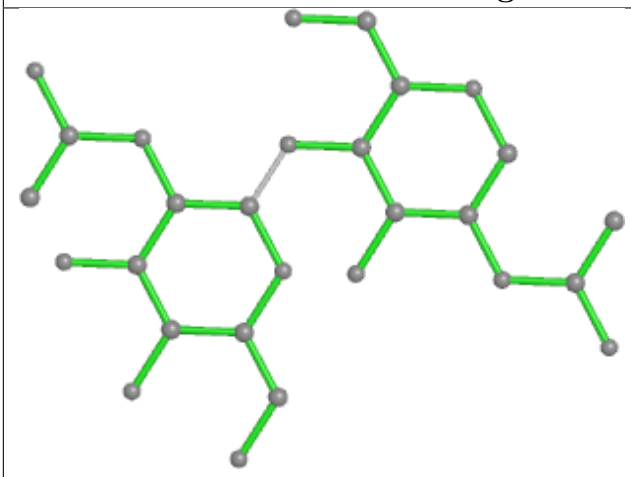


Rings

Oligosaccharide Chain L



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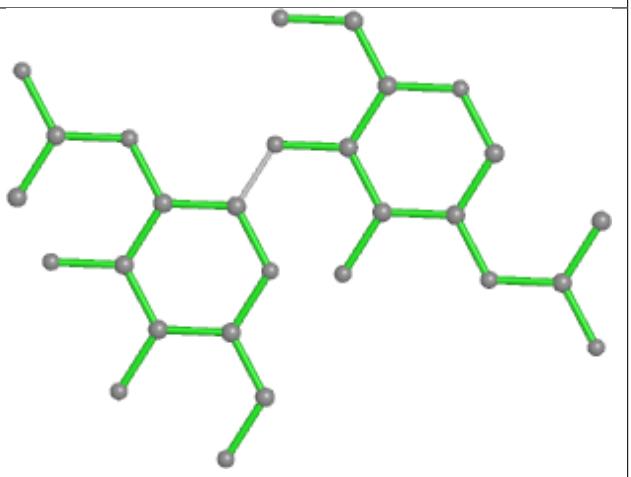
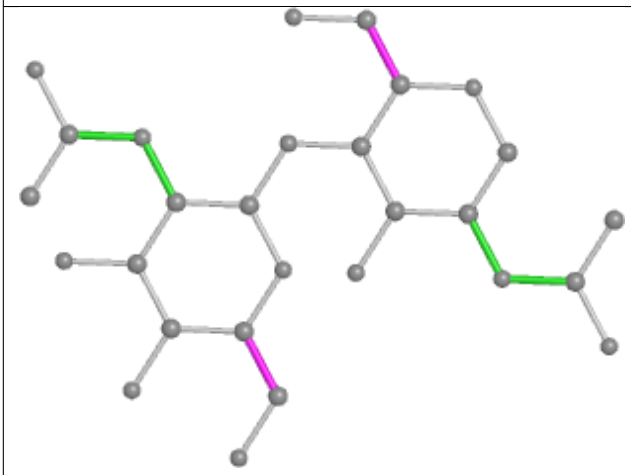


Bond angles



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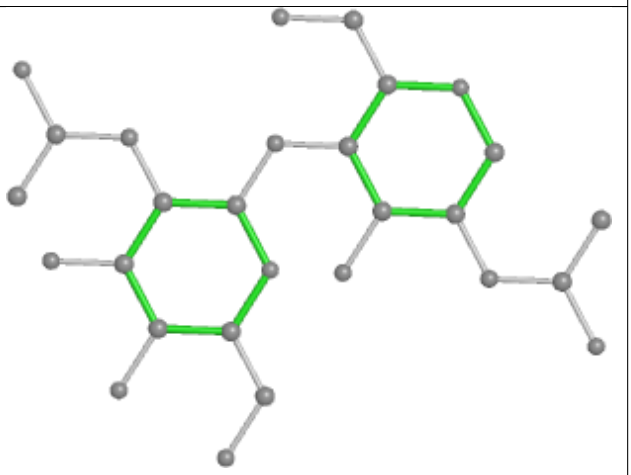
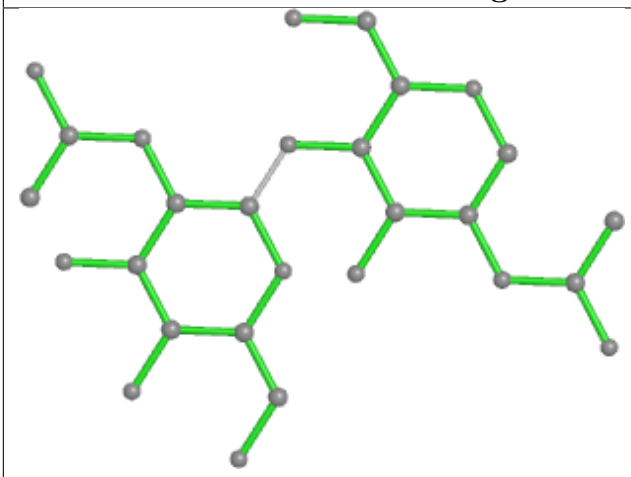
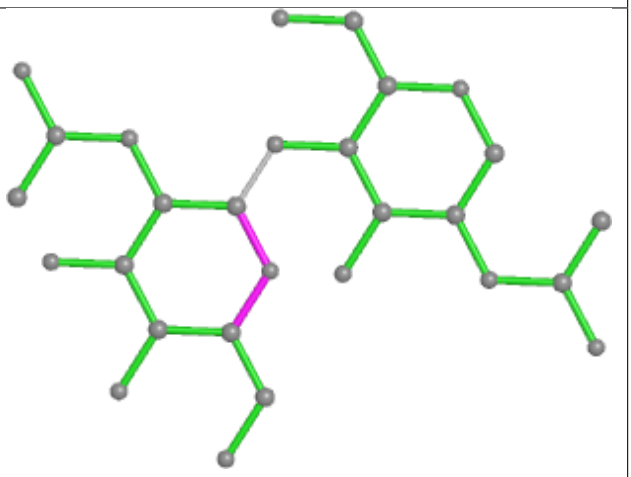


Rings

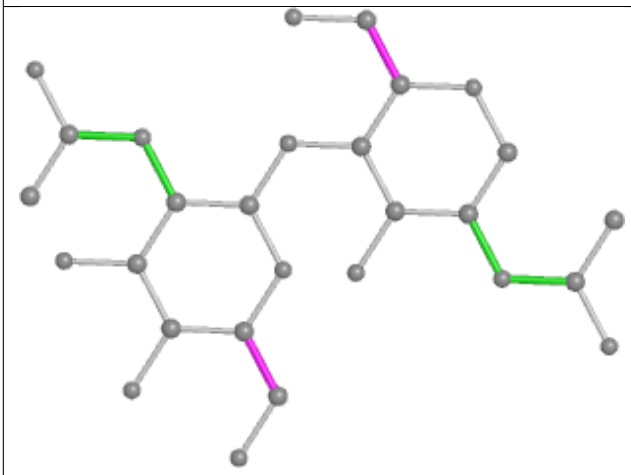
Oligosaccharide Chain M



Bond lengths



Bond angles



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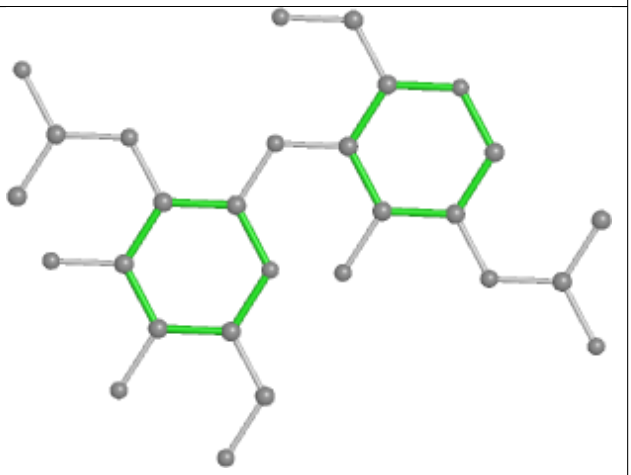
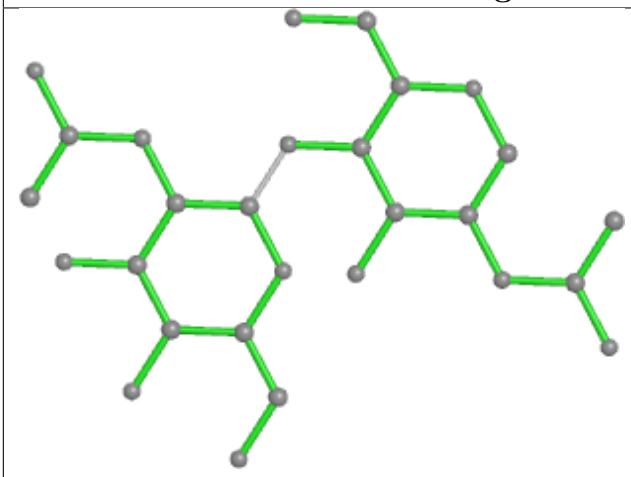
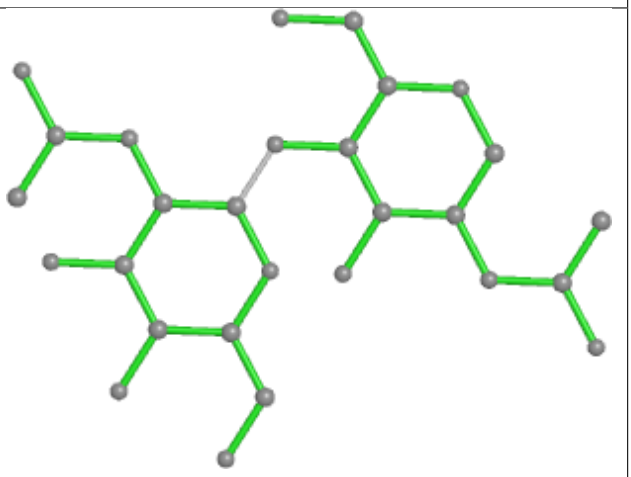


Rings

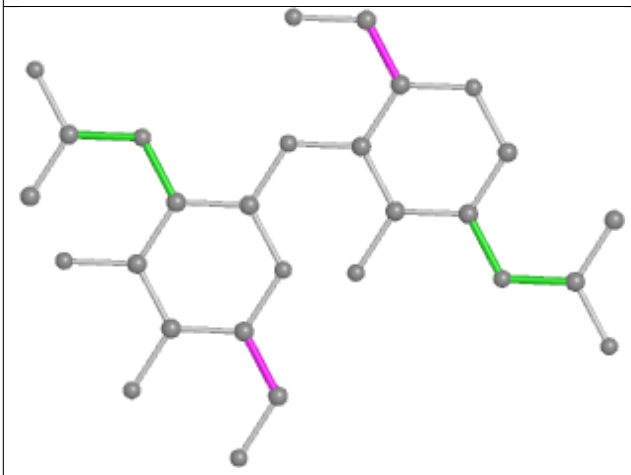
Oligosaccharide Chain O



Bond lengths



Bond angles



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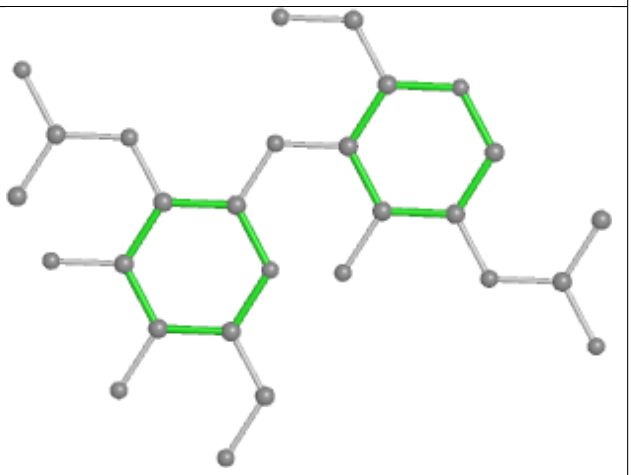
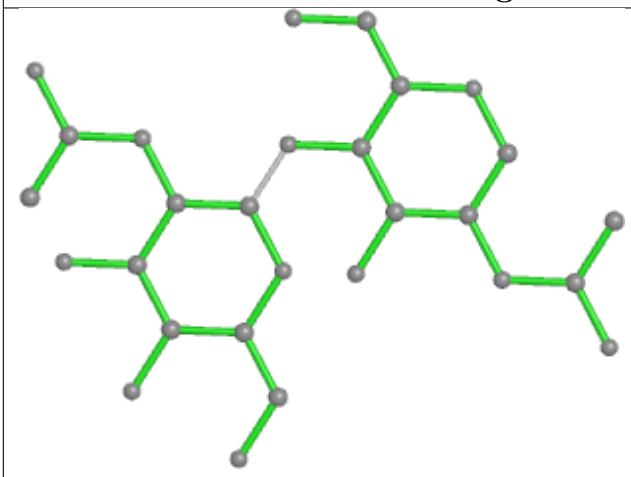
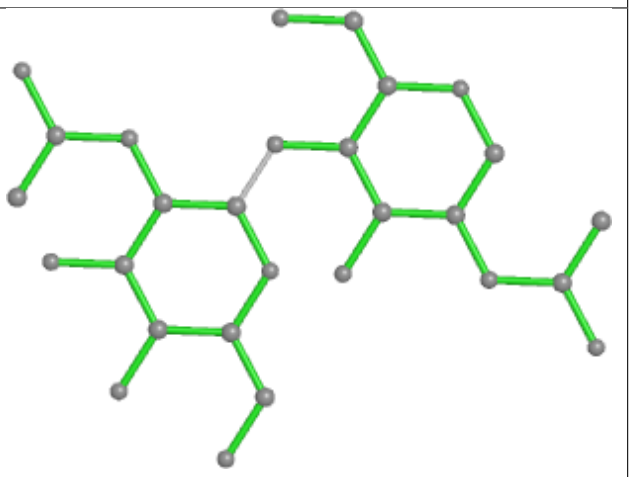
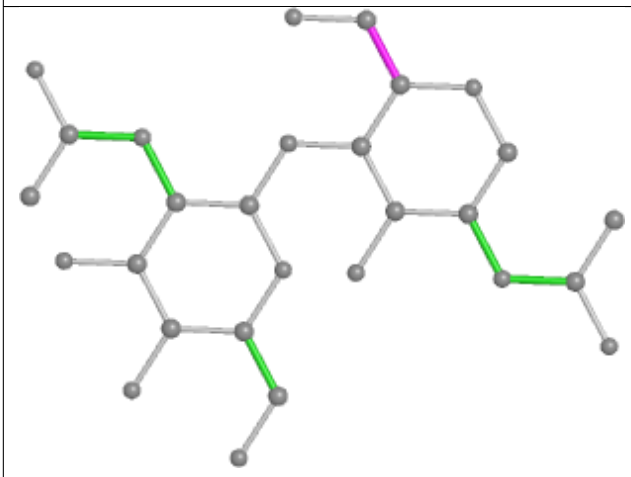
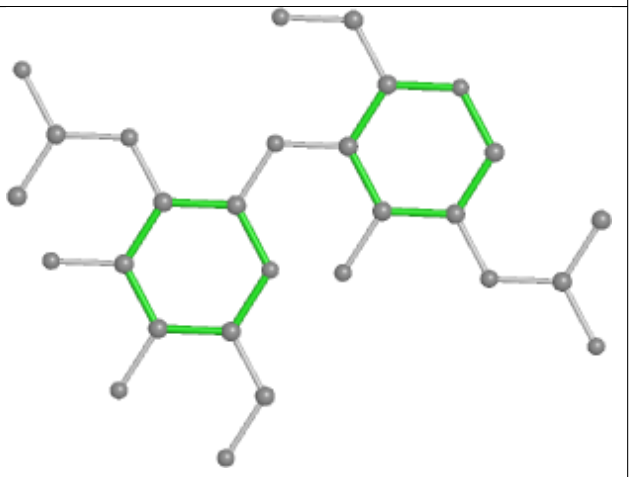
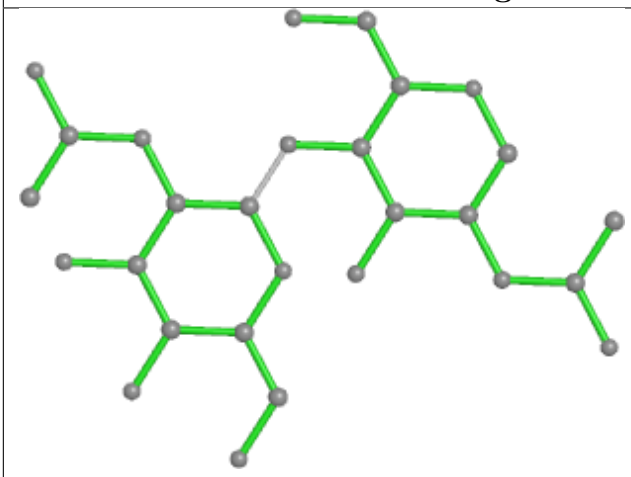


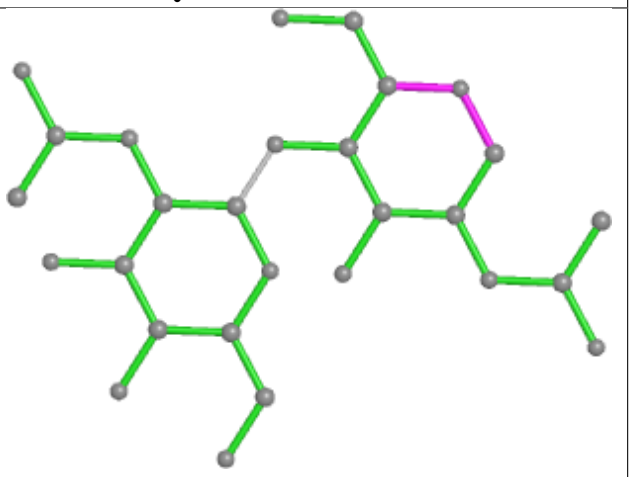
Rings

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

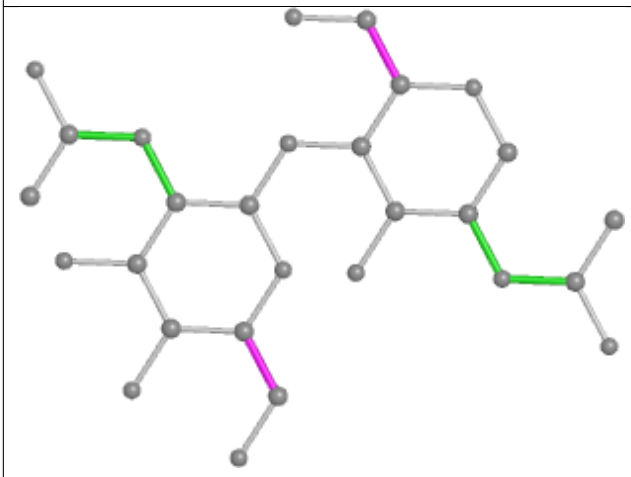
Oligosaccharide Chain Q



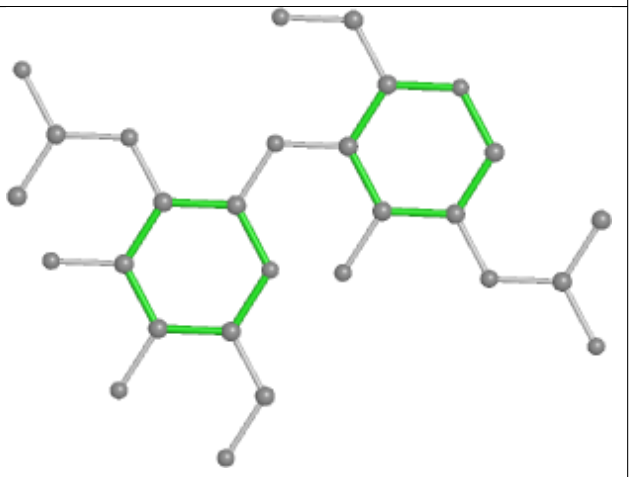
Bond lengths



Bond angles

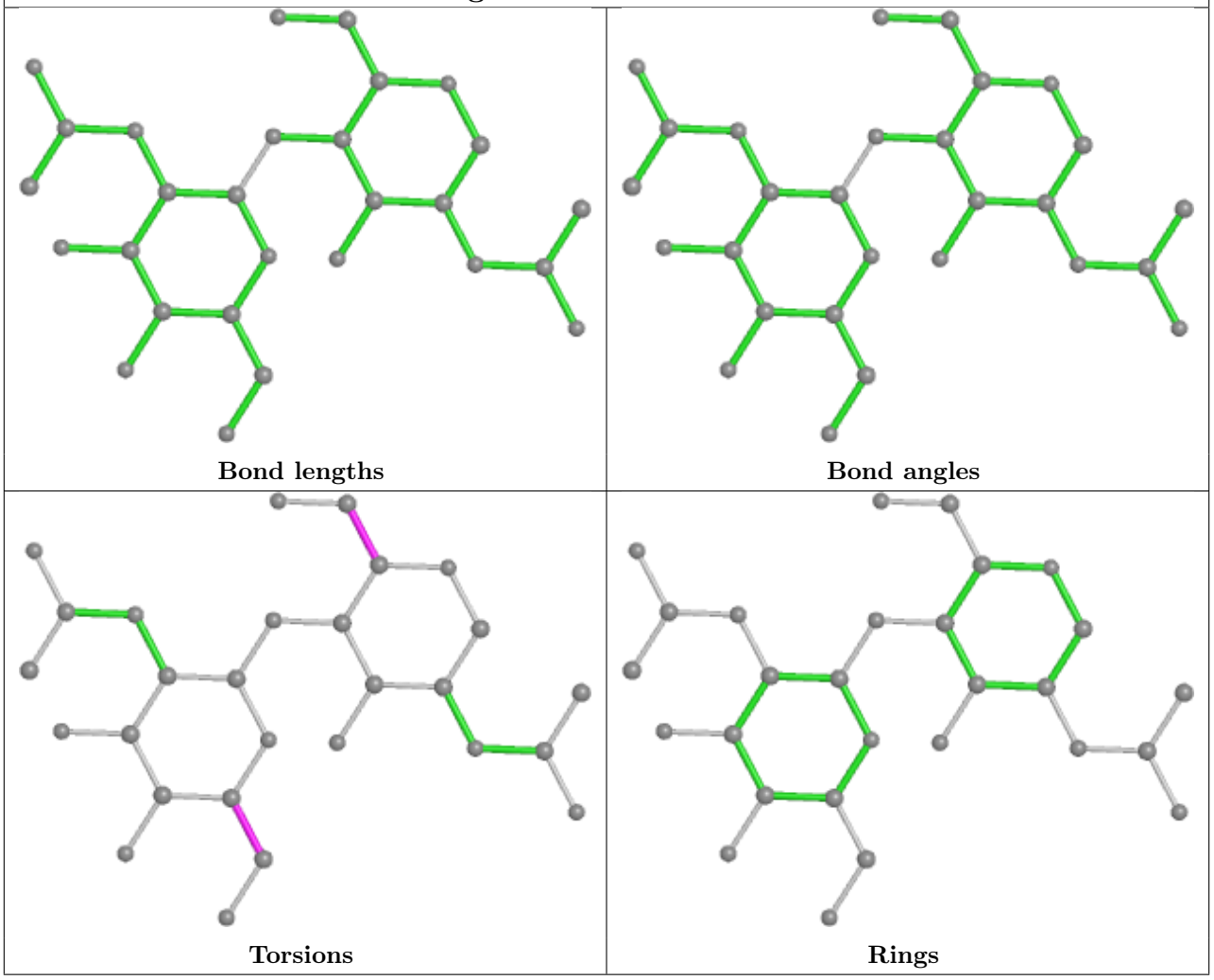


Torsions



Rings

Oligosaccharide Chain R



5.6 Ligand geometry (i)

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	B	2010	1	14,14,15	0.36	0	17,19,21	0.50	0
4	NAG	B	2016	1	14,14,15	0.27	0	17,19,21	0.57	0
4	NAG	C	2005	1	14,14,15	0.37	0	17,19,21	0.49	0
4	NAG	A	2007	1	14,14,15	0.36	0	17,19,21	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	C	2010	1	14,14,15	0.40	0	17,19,21	0.63	1 (5%)
4	NAG	A	2004	1	14,14,15	0.40	0	17,19,21	0.60	1 (5%)
4	NAG	C	2007	1	14,14,15	0.37	0	17,19,21	0.48	0
4	NAG	B	2014	1	14,14,15	0.39	0	17,19,21	0.45	0
4	NAG	B	2015	1	14,14,15	0.40	0	17,19,21	0.66	1 (5%)
4	NAG	B	2005	1	14,14,15	0.29	0	17,19,21	0.47	0
4	NAG	B	2007	1	14,14,15	0.45	0	17,19,21	0.59	1 (5%)
4	NAG	A	2014	1	14,14,15	0.49	0	17,19,21	0.51	0
4	NAG	A	2015	1	14,14,15	0.44	0	17,19,21	0.45	0
4	NAG	B	2006	1	14,14,15	0.48	0	17,19,21	0.52	0
4	NAG	C	2008	1	14,14,15	0.27	0	17,19,21	0.46	0
4	NAG	A	2002	1	14,14,15	0.54	0	17,19,21	0.50	0
4	NAG	C	2003	1	14,14,15	0.55	0	17,19,21	0.58	0
4	NAG	B	2009	1	14,14,15	0.29	0	17,19,21	0.46	0
4	NAG	C	2011	1	14,14,15	0.40	0	17,19,21	0.54	0
4	NAG	A	2013	1	14,14,15	0.55	0	17,19,21	0.33	0
4	NAG	B	2001	1	14,14,15	0.29	0	17,19,21	0.54	0
4	NAG	A	2001	1	14,14,15	0.33	0	17,19,21	0.64	1 (5%)
4	NAG	C	2012	1	14,14,15	0.29	0	17,19,21	0.44	0
4	NAG	B	2003	1	14,14,15	0.55	0	17,19,21	0.43	0
4	NAG	A	2011	1	14,14,15	0.27	0	17,19,21	0.46	0
4	NAG	C	2001	1	14,14,15	0.53	0	17,19,21	0.72	1 (5%)
4	NAG	C	2016	1	14,14,15	0.33	0	17,19,21	0.61	1 (5%)
4	NAG	A	2005	1	14,14,15	0.36	0	17,19,21	0.39	0
4	NAG	C	2006	1	14,14,15	0.38	0	17,19,21	0.47	0
4	NAG	A	2016	1	14,14,15	0.50	0	17,19,21	0.54	0
4	NAG	C	2017	1	14,14,15	0.53	0	17,19,21	0.55	0
4	NAG	C	2014	1	14,14,15	0.33	0	17,19,21	0.35	0
4	NAG	A	2008	1	14,14,15	0.32	0	17,19,21	0.48	0
4	NAG	C	2015	1	14,14,15	0.29	0	17,19,21	0.47	0
4	NAG	A	2003	1	14,14,15	0.68	0	17,19,21	0.47	0
4	NAG	A	2010	1	14,14,15	0.54	0	17,19,21	0.46	0
4	NAG	B	2017	1	14,14,15	0.41	0	17,19,21	0.55	0
4	NAG	B	2008	1	14,14,15	0.42	0	17,19,21	0.50	0
4	NAG	A	2006	1	14,14,15	0.46	0	17,19,21	0.41	0
4	NAG	A	2017	1	14,14,15	0.41	0	17,19,21	0.48	0
4	NAG	C	2002	1	14,14,15	0.44	0	17,19,21	0.57	0
4	NAG	B	2002	1	14,14,15	0.35	0	17,19,21	0.45	0
4	NAG	B	2011	1	14,14,15	0.42	0	17,19,21	0.55	0
4	NAG	C	2013	1	14,14,15	0.36	0	17,19,21	0.47	0
4	NAG	A	2012	1	14,14,15	0.24	0	17,19,21	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	A	2009	1	14,14,15	0.35	0	17,19,21	0.55	0
4	NAG	C	2009	1	14,14,15	0.31	0	17,19,21	0.65	1 (5%)
4	NAG	B	2013	1	14,14,15	0.45	0	17,19,21	0.43	0
4	NAG	B	2012	1	14,14,15	0.28	0	17,19,21	0.65	1 (5%)
4	NAG	C	2004	1	14,14,15	0.41	0	17,19,21	0.61	1 (5%)
4	NAG	B	2004	1	14,14,15	0.39	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
4	NAG	B	2010	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	2005	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	2010	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2004	1	-	1/6/23/26	0/1/1/1
4	NAG	C	2007	1	-	0/6/23/26	0/1/1/1
4	NAG	B	2014	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2015	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2005	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2007	1	-	0/6/23/26	0/1/1/1
4	NAG	A	2014	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2015	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2006	1	-	2/6/23/26	0/1/1/1
4	NAG	C	2008	1	-	0/6/23/26	0/1/1/1
4	NAG	A	2002	1	-	2/6/23/26	0/1/1/1
4	NAG	C	2003	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2009	1	-	0/6/23/26	0/1/1/1
4	NAG	C	2011	1	-	0/6/23/26	0/1/1/1
4	NAG	A	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	2001	1	-	2/6/23/26	0/1/1/1
4	NAG	C	2012	1	-	0/6/23/26	0/1/1/1
4	NAG	B	2003	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2011	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	2001	1	-	2/6/23/26	0/1/1/1
4	NAG	C	2016	1	-	0/6/23/26	0/1/1/1
4	NAG	A	2005	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	2016	1	-	1/6/23/26	0/1/1/1
4	NAG	C	2017	1	-	2/6/23/26	0/1/1/1
4	NAG	C	2014	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2008	1	-	2/6/23/26	0/1/1/1
4	NAG	C	2015	1	-	0/6/23/26	0/1/1/1
4	NAG	A	2003	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2010	1	-	1/6/23/26	0/1/1/1
4	NAG	B	2017	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2008	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2006	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2017	1	-	2/6/23/26	0/1/1/1
4	NAG	C	2002	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2002	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	2013	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2012	1	-	0/6/23/26	0/1/1/1
4	NAG	A	2009	1	-	2/6/23/26	0/1/1/1
4	NAG	C	2009	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2013	1	-	0/6/23/26	0/1/1/1
4	NAG	B	2012	1	-	2/6/23/26	0/1/1/1
4	NAG	C	2004	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2004	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	2001	NAG	C1-O5-C5	2.57	115.68	112.19
4	C	2009	NAG	C1-O5-C5	2.30	115.31	112.19
4	C	2010	NAG	C1-O5-C5	2.27	115.26	112.19
4	B	2015	NAG	C1-O5-C5	2.25	115.24	112.19
4	A	2001	NAG	C1-O5-C5	2.19	115.16	112.19
4	C	2004	NAG	C1-O5-C5	2.18	115.15	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	2004	NAG	C1-O5-C5	2.11	115.05	112.19
4	C	2016	NAG	C1-O5-C5	2.08	115.00	112.19
4	B	2007	NAG	C1-O5-C5	2.02	114.94	112.19
4	B	2012	NAG	C1-O5-C5	2.00	114.91	112.19

There are no chirality outliers.

All (73) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	2006	NAG	O5-C5-C6-O6
4	C	2002	NAG	O5-C5-C6-O6
4	A	2008	NAG	O5-C5-C6-O6
4	B	2014	NAG	C4-C5-C6-O6
4	A	2017	NAG	O5-C5-C6-O6
4	B	2003	NAG	O5-C5-C6-O6
4	B	2008	NAG	O5-C5-C6-O6
4	B	2016	NAG	O5-C5-C6-O6
4	A	2015	NAG	O5-C5-C6-O6
4	B	2010	NAG	O5-C5-C6-O6
4	C	2001	NAG	O5-C5-C6-O6
4	A	2013	NAG	O5-C5-C6-O6
4	C	2002	NAG	C4-C5-C6-O6
4	C	2013	NAG	C4-C5-C6-O6
4	A	2017	NAG	C4-C5-C6-O6
4	A	2003	NAG	C4-C5-C6-O6
4	B	2002	NAG	O5-C5-C6-O6
4	B	2015	NAG	O5-C5-C6-O6
4	A	2001	NAG	O5-C5-C6-O6
4	A	2003	NAG	O5-C5-C6-O6
4	B	2006	NAG	C4-C5-C6-O6
4	A	2008	NAG	C4-C5-C6-O6
4	B	2014	NAG	O5-C5-C6-O6
4	C	2004	NAG	O5-C5-C6-O6
4	C	2014	NAG	O5-C5-C6-O6
4	A	2005	NAG	O5-C5-C6-O6
4	A	2014	NAG	O5-C5-C6-O6
4	C	2003	NAG	O5-C5-C6-O6
4	C	2006	NAG	O5-C5-C6-O6
4	C	2010	NAG	O5-C5-C6-O6
4	A	2002	NAG	O5-C5-C6-O6
4	B	2010	NAG	C4-C5-C6-O6
4	A	2001	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	A	2005	NAG	C4-C5-C6-O6
4	A	2007	NAG	O5-C5-C6-O6
4	C	2001	NAG	C4-C5-C6-O6
4	C	2017	NAG	O5-C5-C6-O6
4	B	2003	NAG	C4-C5-C6-O6
4	B	2016	NAG	C4-C5-C6-O6
4	B	2015	NAG	C4-C5-C6-O6
4	A	2015	NAG	C4-C5-C6-O6
4	C	2009	NAG	O5-C5-C6-O6
4	C	2010	NAG	C4-C5-C6-O6
4	C	2014	NAG	C4-C5-C6-O6
4	A	2002	NAG	C4-C5-C6-O6
4	A	2014	NAG	C4-C5-C6-O6
4	B	2008	NAG	C4-C5-C6-O6
4	C	2003	NAG	C4-C5-C6-O6
4	C	2004	NAG	C4-C5-C6-O6
4	B	2011	NAG	O5-C5-C6-O6
4	B	2017	NAG	O5-C5-C6-O6
4	B	2002	NAG	C4-C5-C6-O6
4	C	2006	NAG	C4-C5-C6-O6
4	C	2009	NAG	C4-C5-C6-O6
4	C	2017	NAG	C4-C5-C6-O6
4	C	2013	NAG	O5-C5-C6-O6
4	A	2009	NAG	O5-C5-C6-O6
4	A	2013	NAG	C4-C5-C6-O6
4	A	2006	NAG	C4-C5-C6-O6
4	B	2012	NAG	C4-C5-C6-O6
4	B	2012	NAG	O5-C5-C6-O6
4	B	2001	NAG	C4-C5-C6-O6
4	B	2017	NAG	C4-C5-C6-O6
4	A	2010	NAG	O5-C5-C6-O6
4	A	2006	NAG	O5-C5-C6-O6
4	B	2011	NAG	C4-C5-C6-O6
4	A	2016	NAG	O5-C5-C6-O6
4	B	2005	NAG	C4-C5-C6-O6
4	B	2005	NAG	O5-C5-C6-O6
4	A	2009	NAG	C4-C5-C6-O6
4	B	2001	NAG	O5-C5-C6-O6
4	A	2007	NAG	C4-C5-C6-O6
4	A	2004	NAG	C4-C5-C6-O6

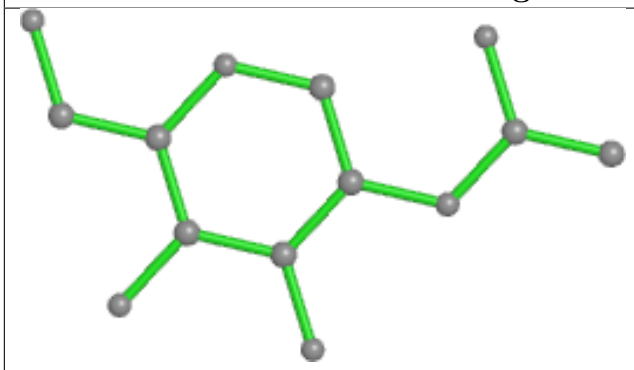
There are no ring outliers.

2 monomers are involved in 2 short contacts:

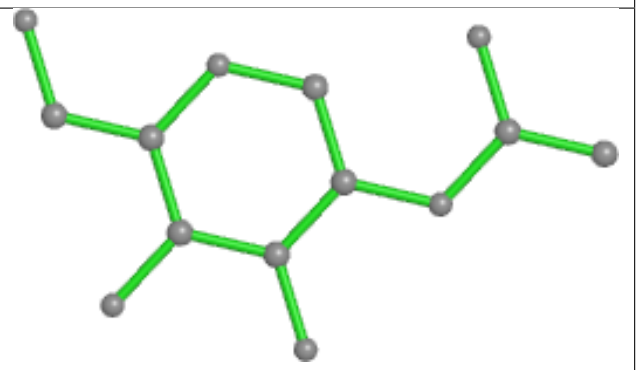
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	2014	NAG	1	0
4	A	2012	NAG	1	0

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

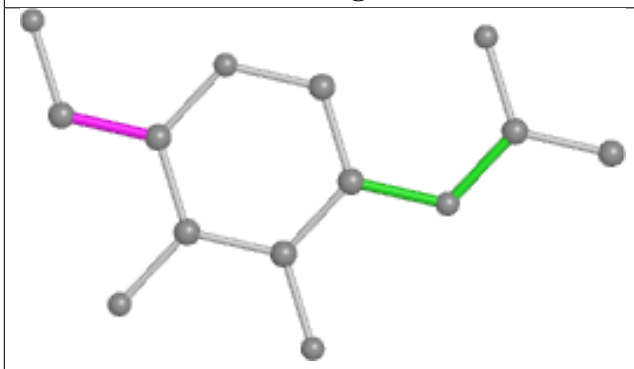
Ligand NAG B 2010



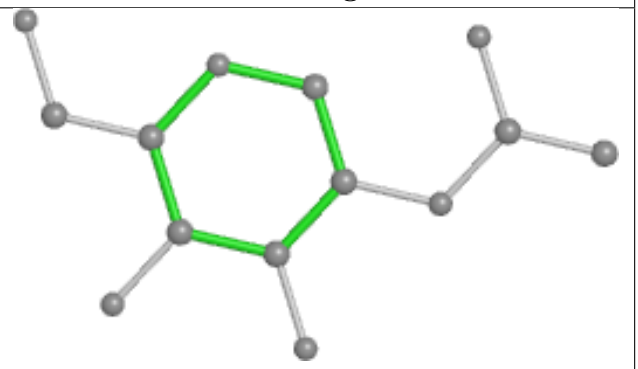
Bond lengths



Bond angles

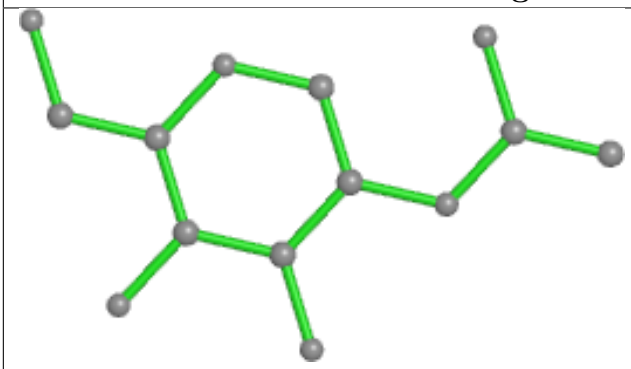


Torsions

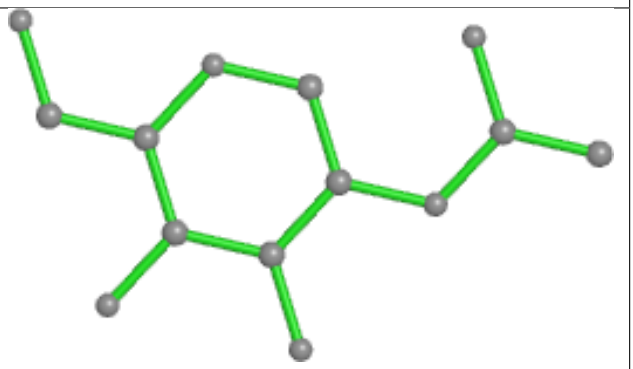


Rings

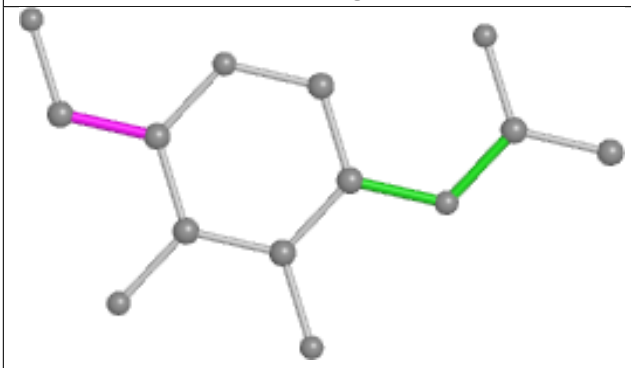
Ligand NAG B 2016



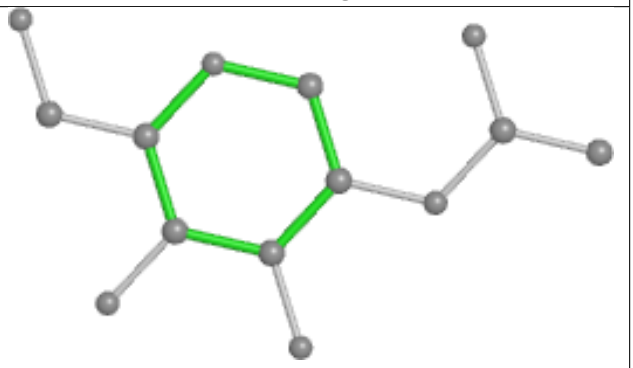
Bond lengths



Bond angles

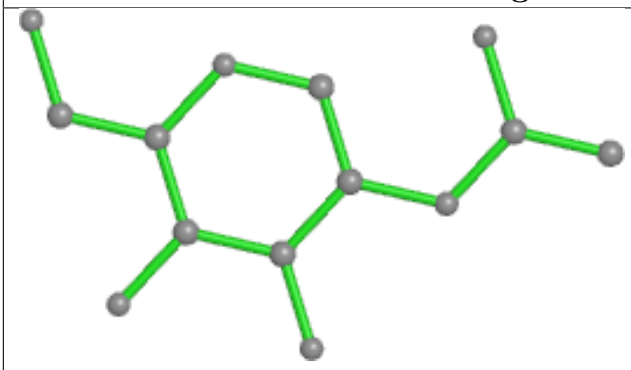


Torsions

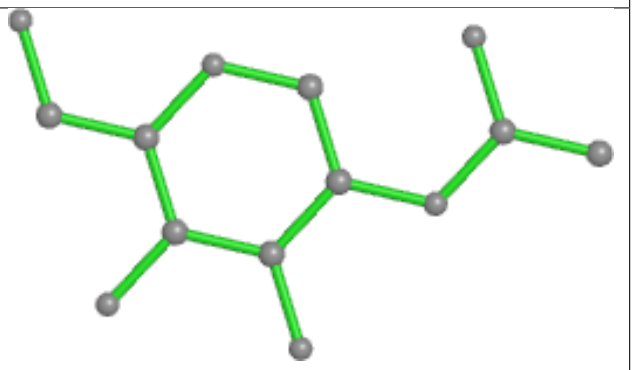


Rings

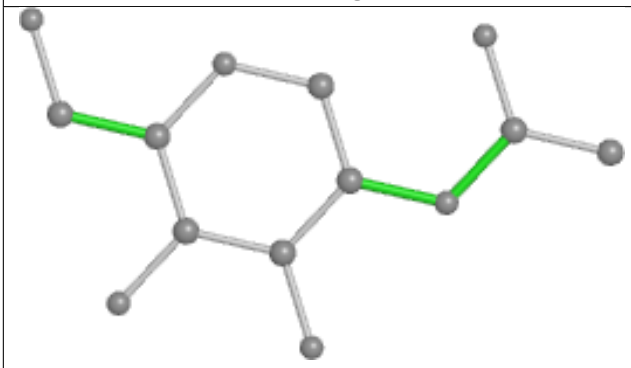
Ligand NAG C 2005



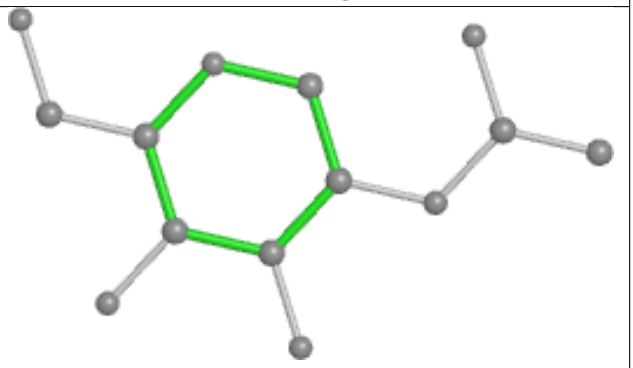
Bond lengths



Bond angles

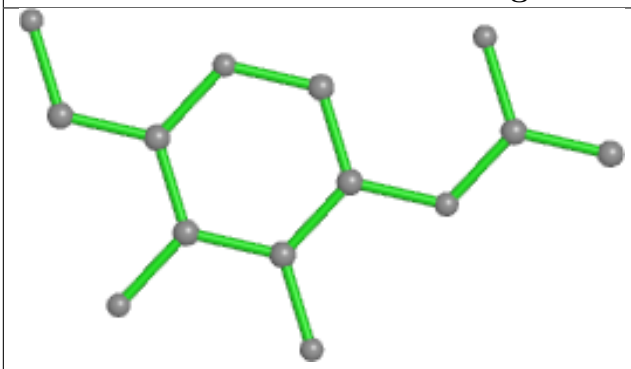


Torsions

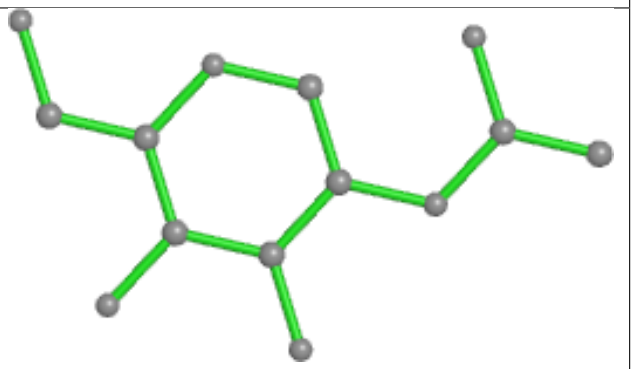


Rings

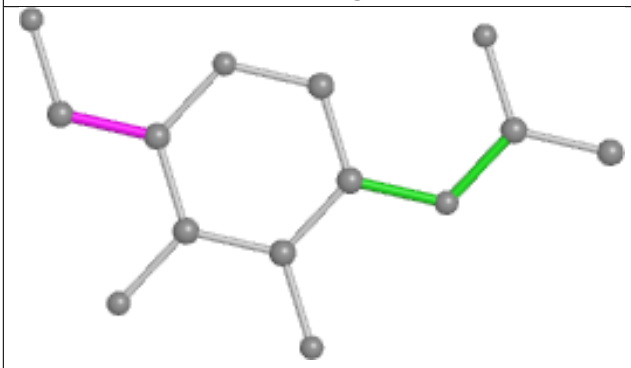
Ligand NAG A 2007



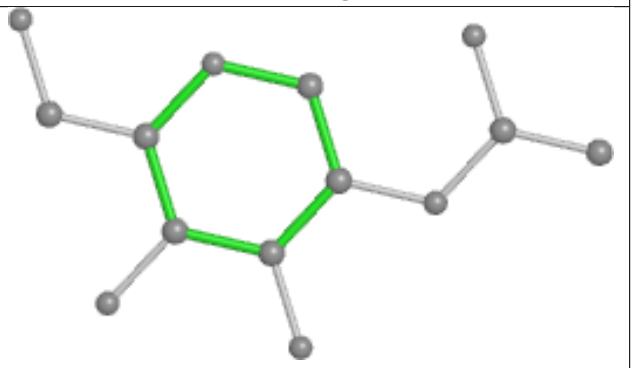
Bond lengths



Bond angles

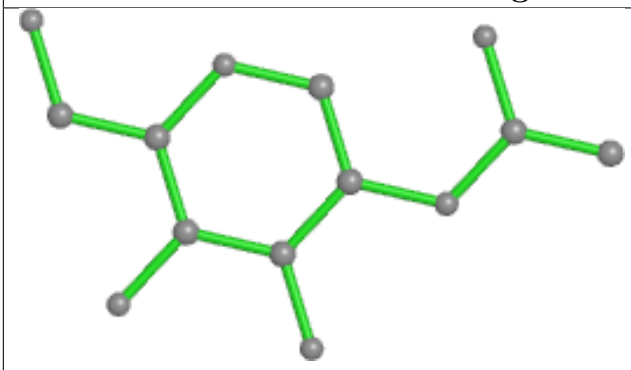


Torsions

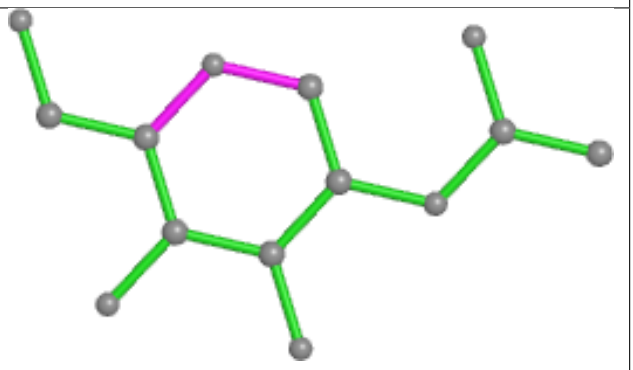


Rings

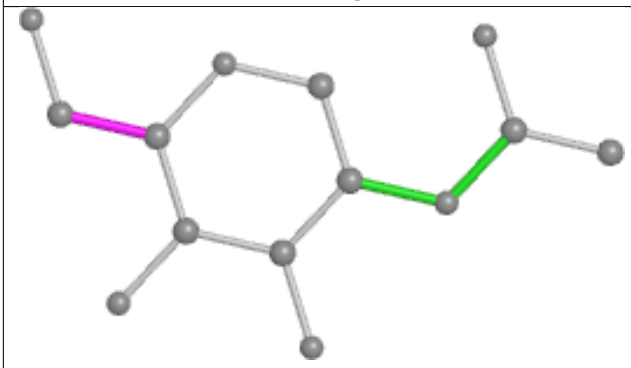
Ligand NAG C 2010



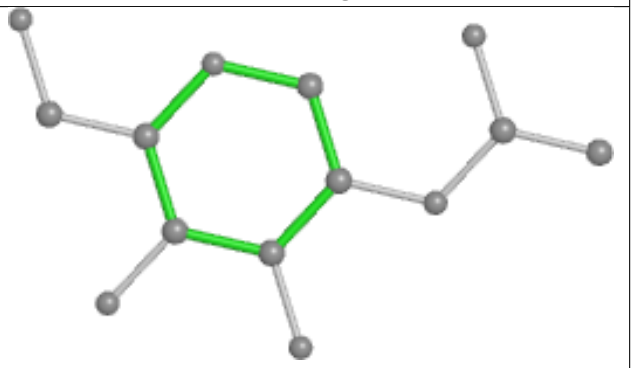
Bond lengths



Bond angles

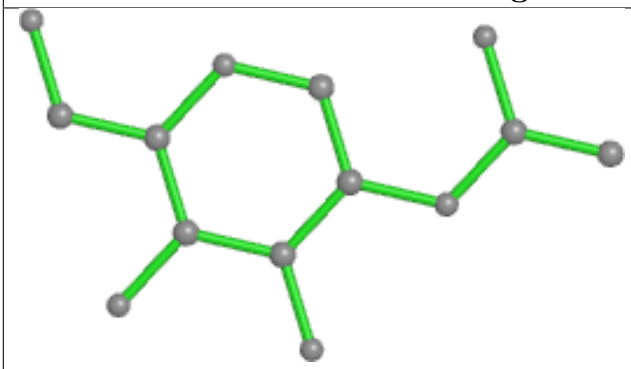


Torsions

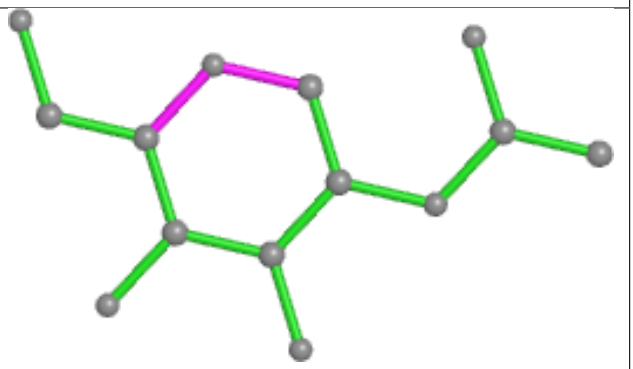


Rings

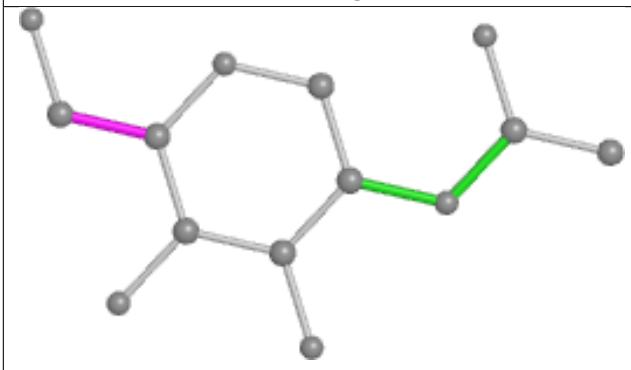
Ligand NAG A 2004



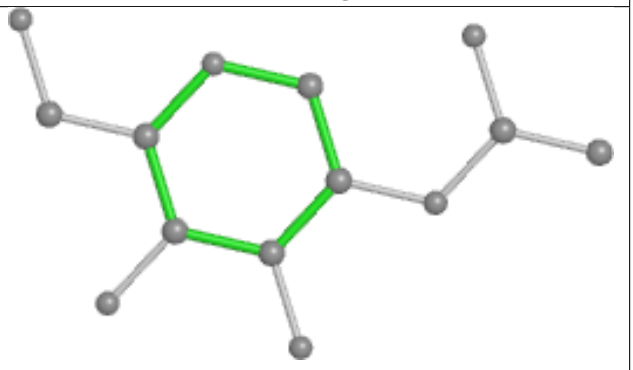
Bond lengths



Bond angles

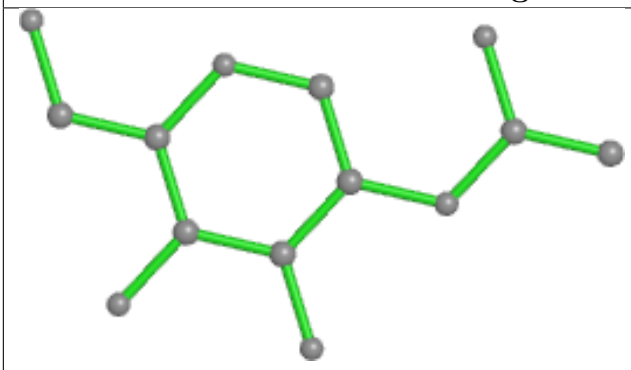


Torsions



Rings

Ligand NAG C 2007



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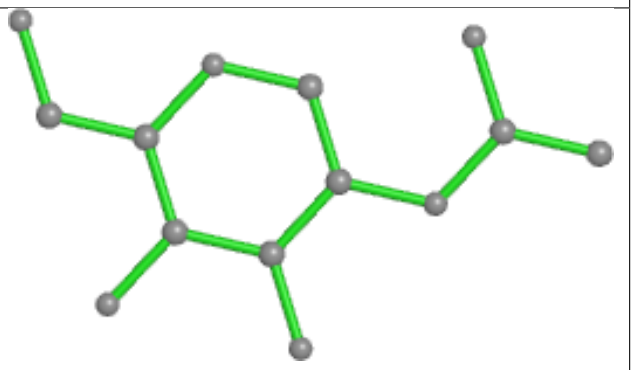
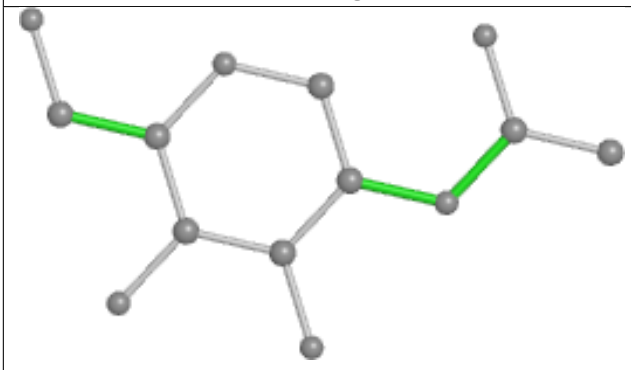


Bond angles



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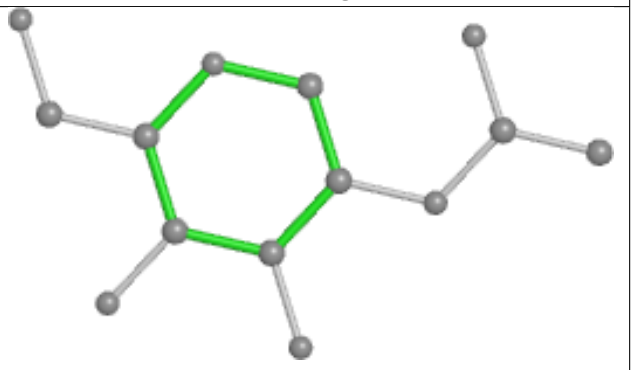
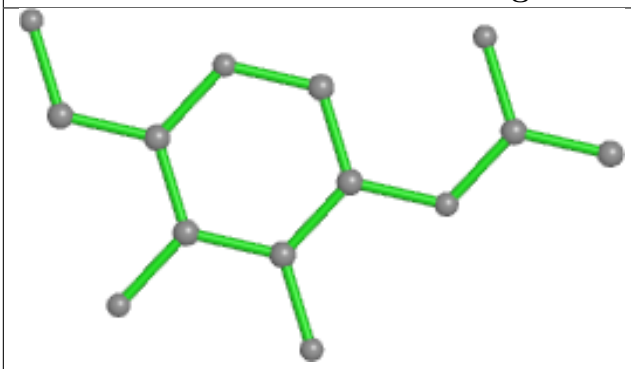
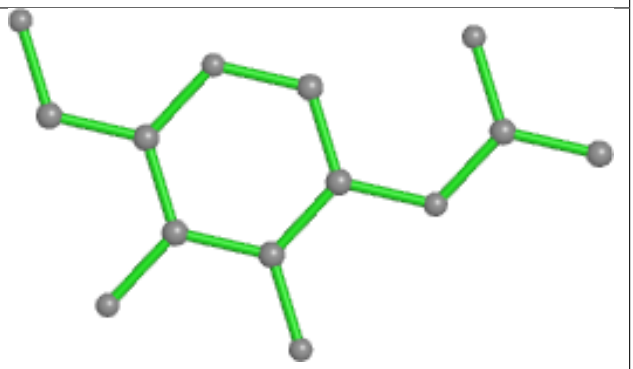
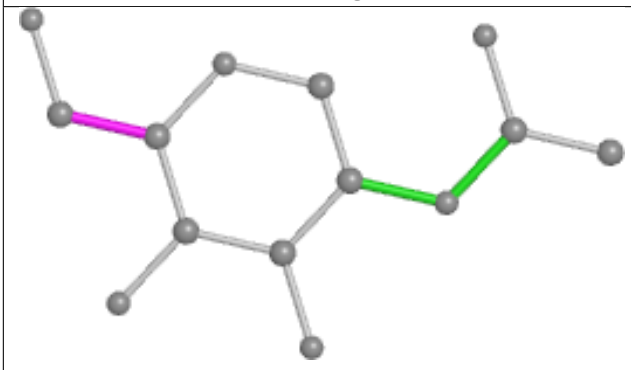
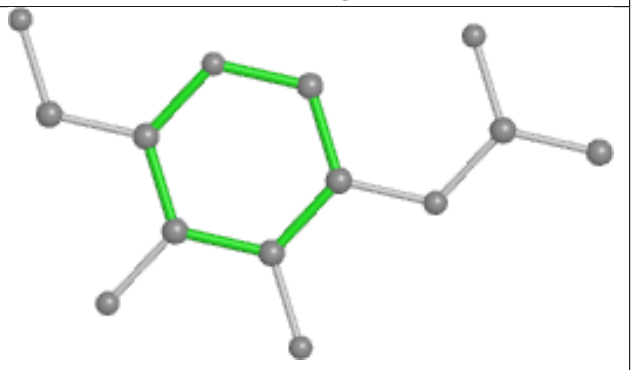
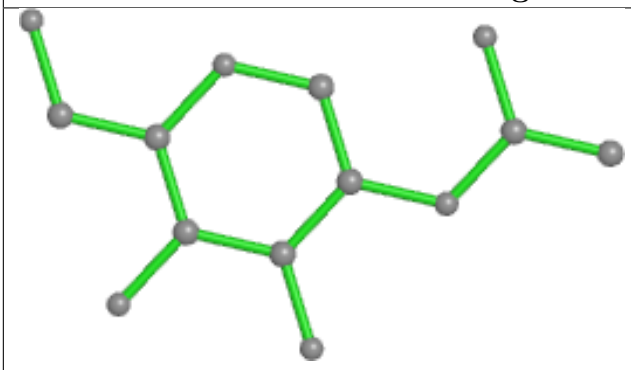
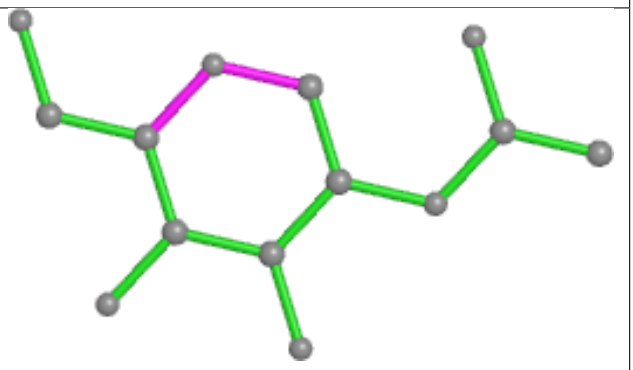
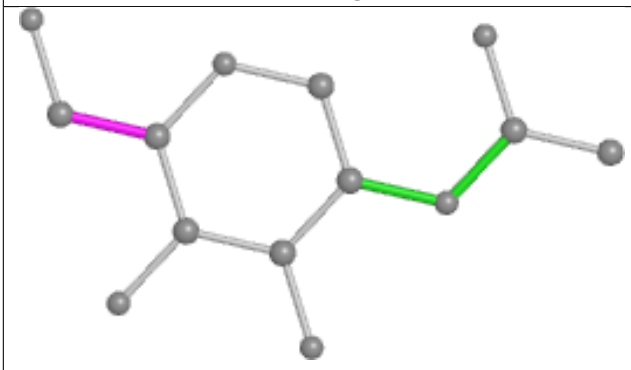
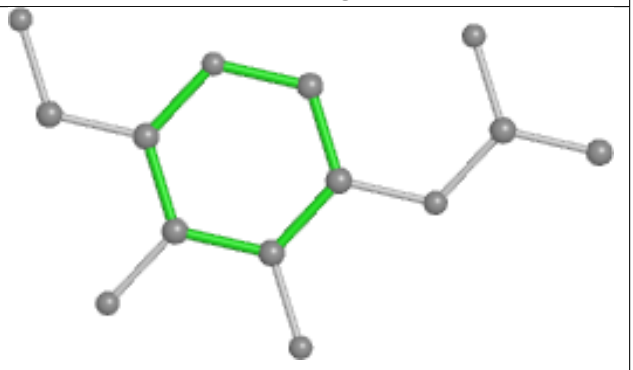
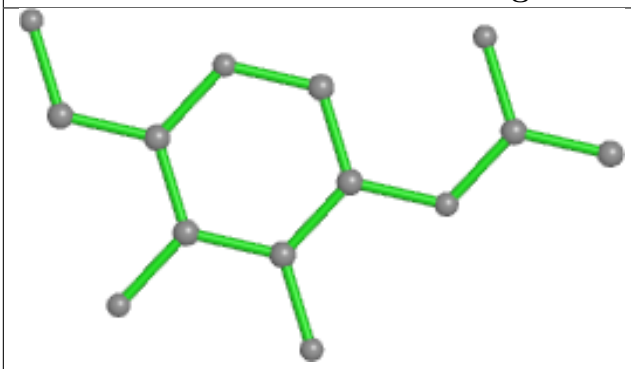


Rings

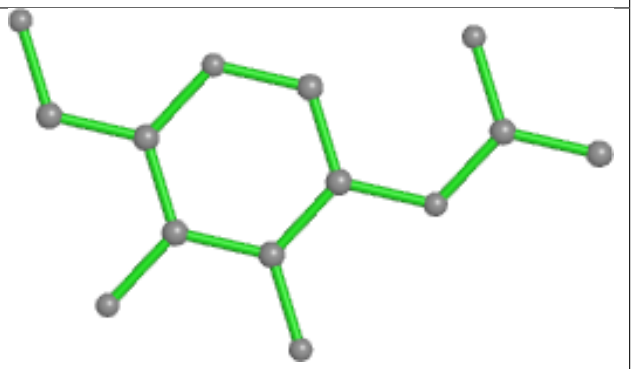
Ligand NAG B 2014	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand NAG B 2015	
	
Bond lengths	Bond angles
	
Torsions	Rings

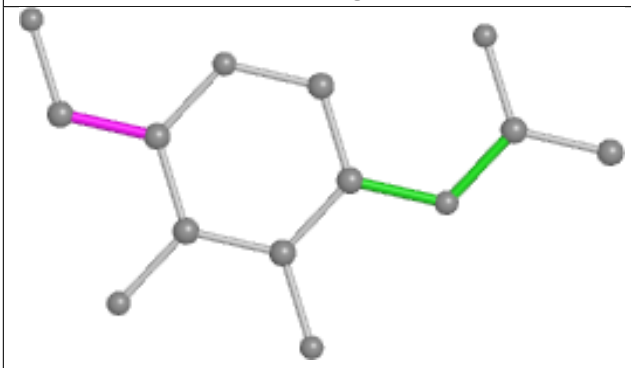
Ligand NAG B 2005



Bond lengths



Bond angles



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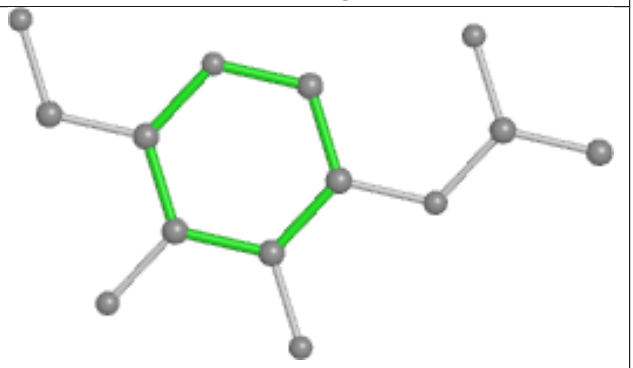
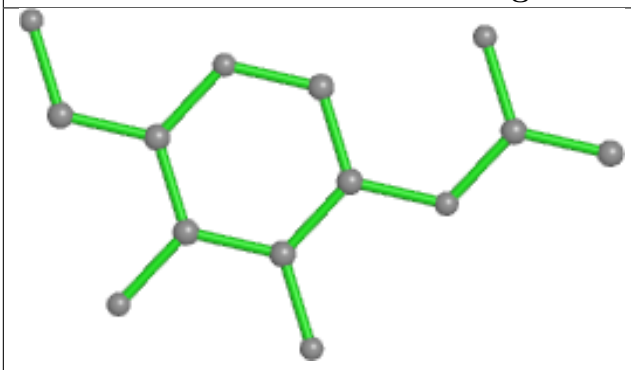


Rings

Ligand NAG B 2007



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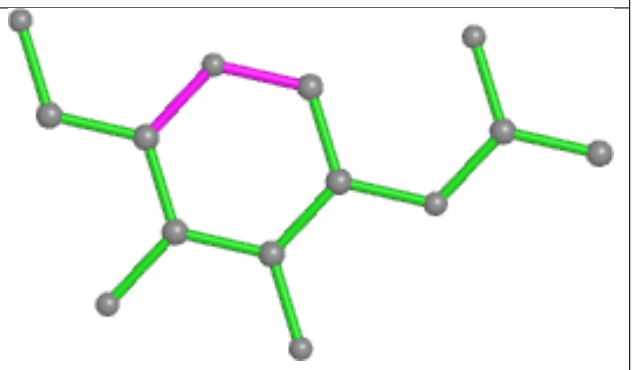
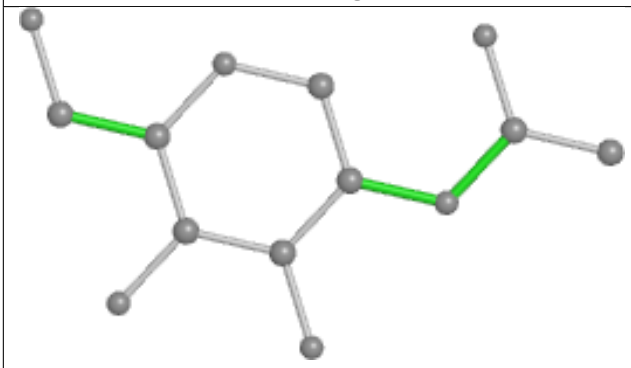


Bond angles



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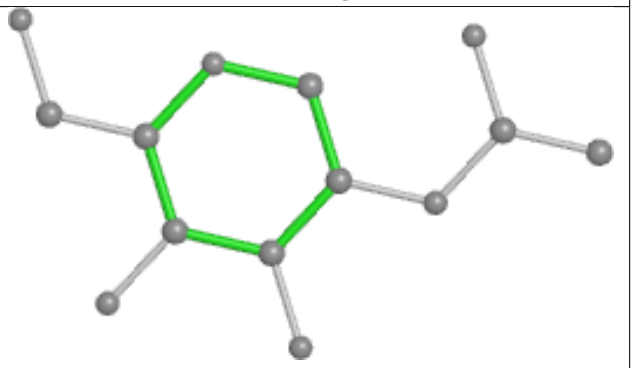
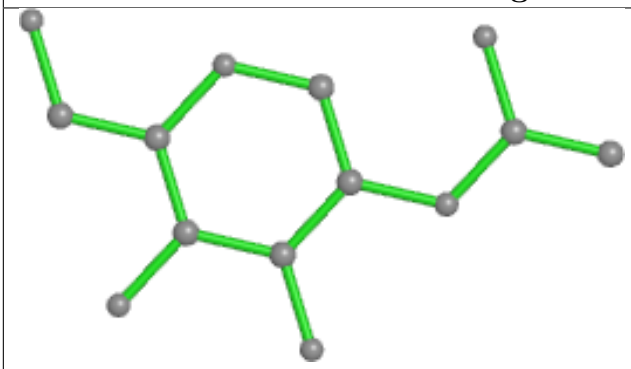


Rings

Ligand NAG A 2014



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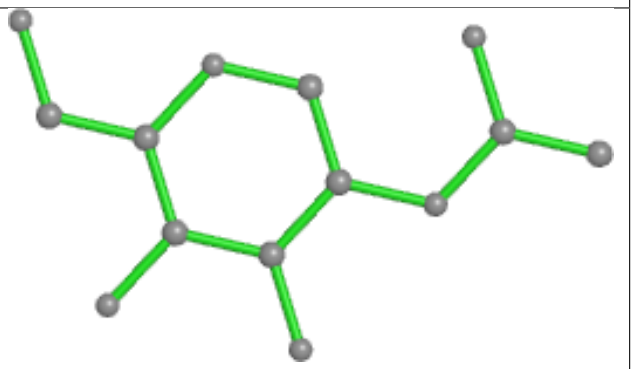
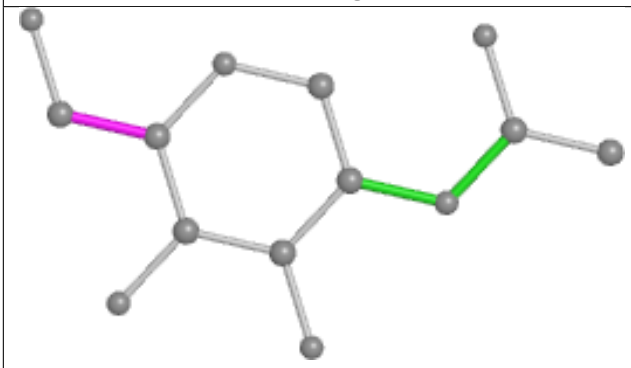


Bond angles



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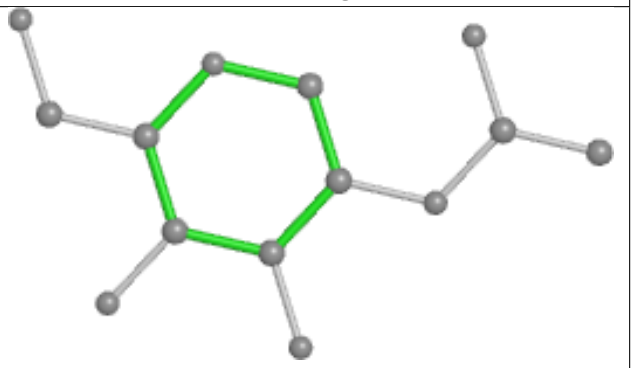
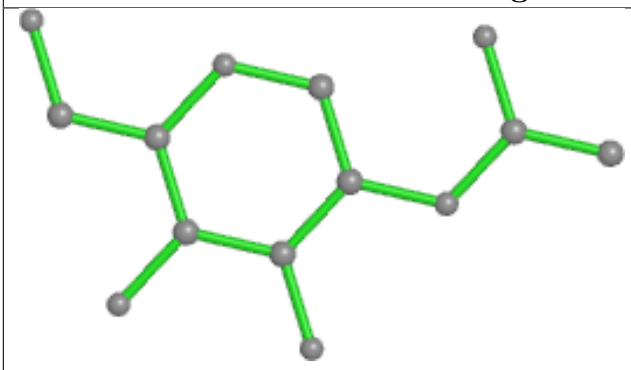


Rings

Ligand NAG A 2015



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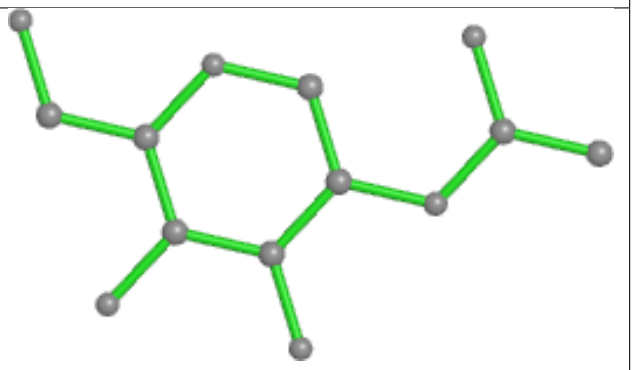
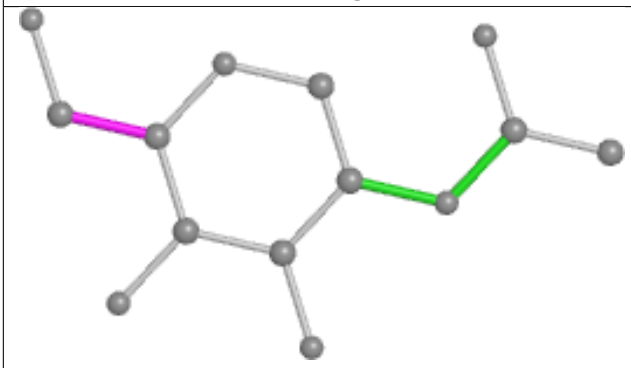


Bond angles



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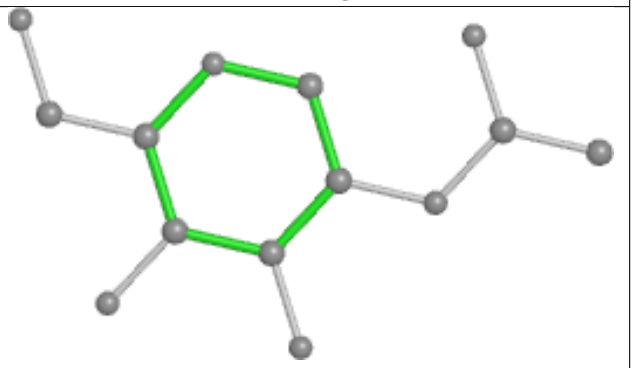
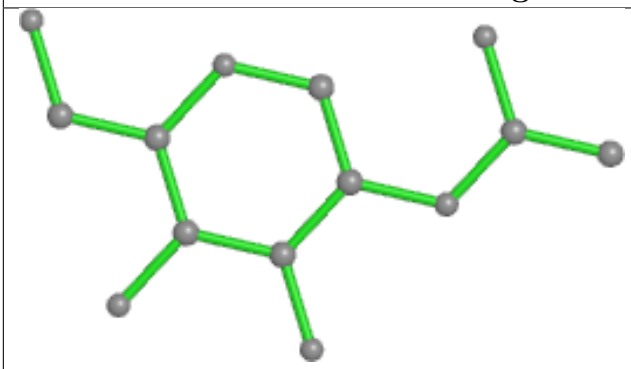


Rings

Ligand NAG B 2006



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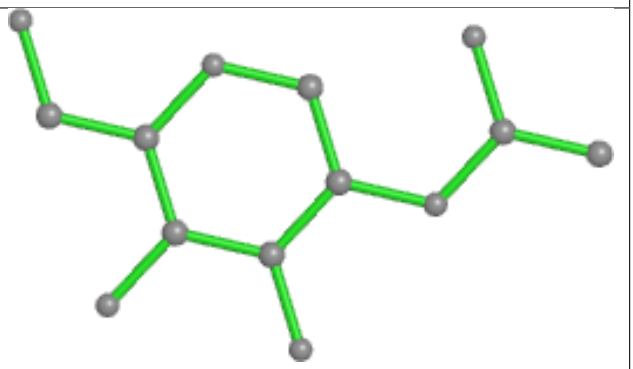
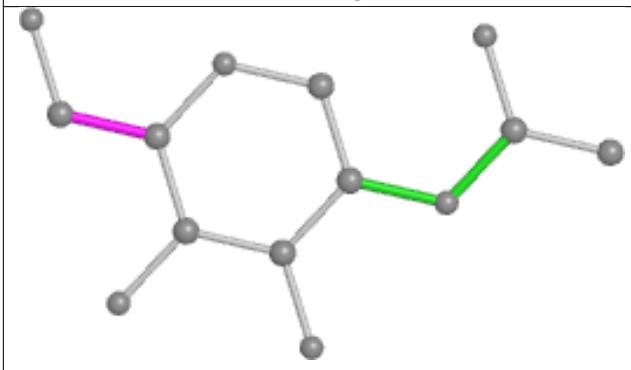


Bond angles



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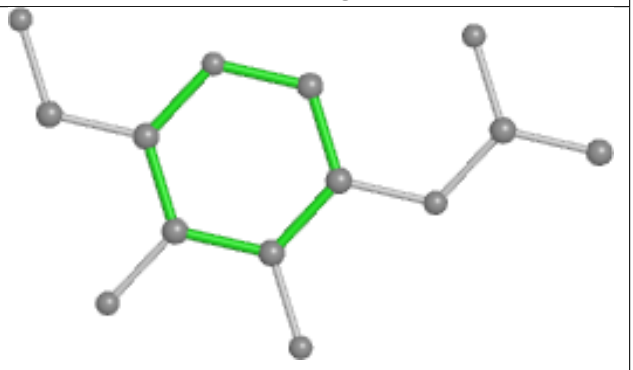
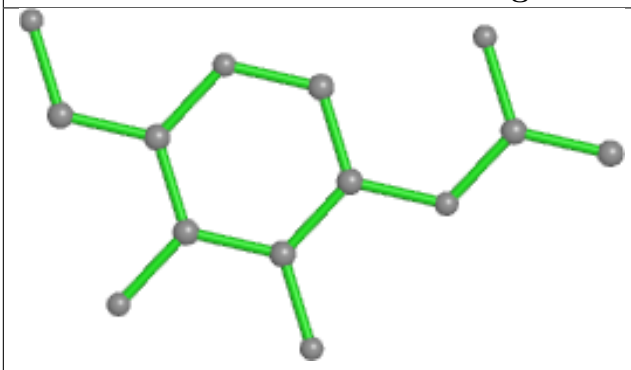


Rings

Ligand NAG C 2008



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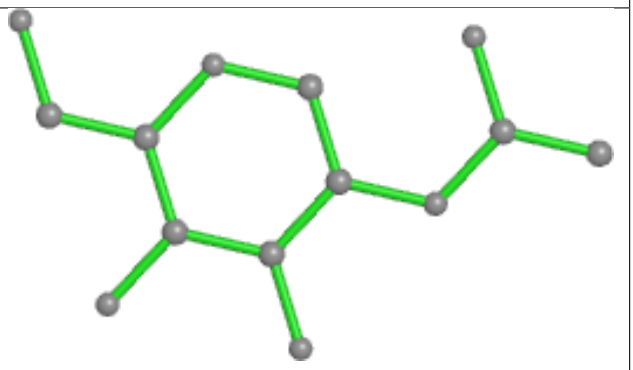
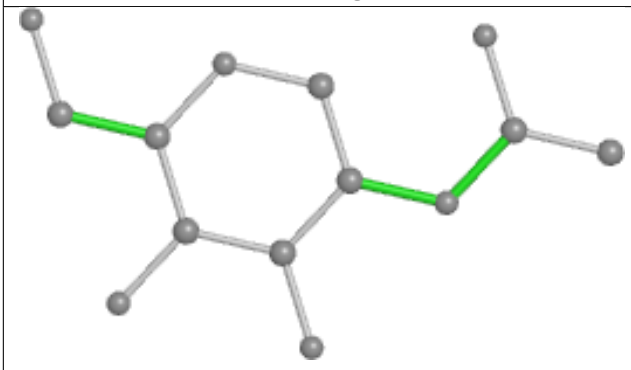
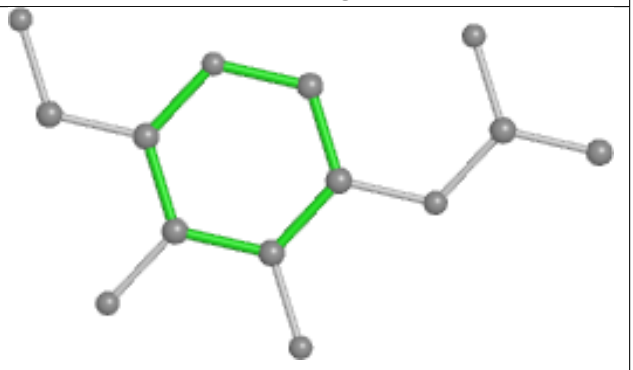


Bond angles

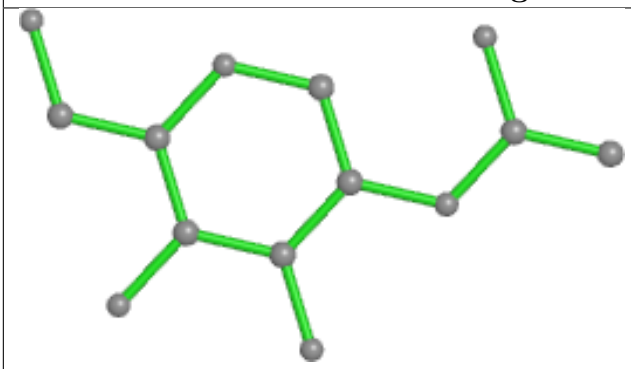


Torsions



Rings

Ligand NAG A 2002



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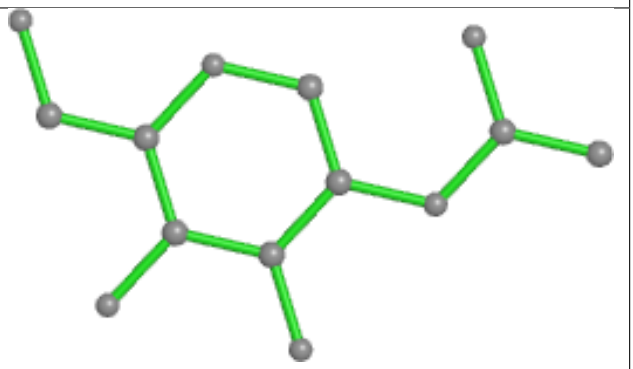
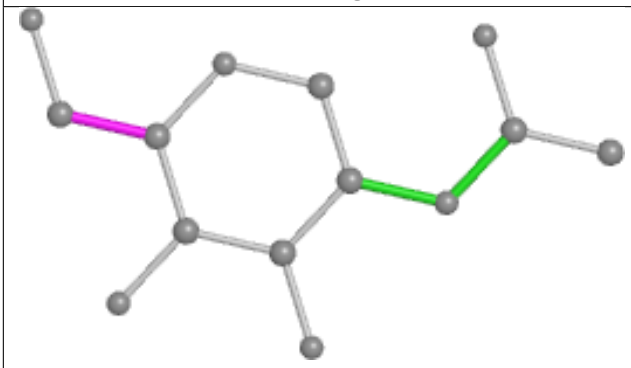


Bond angles



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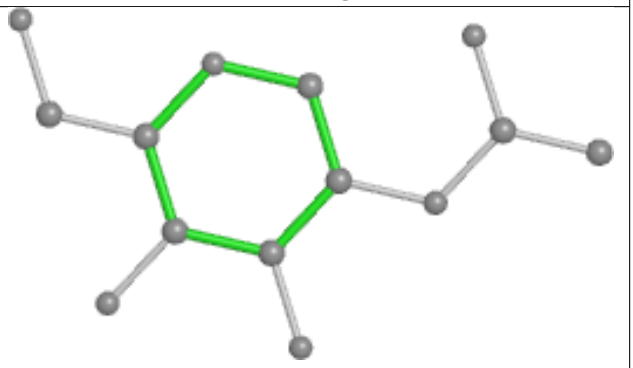
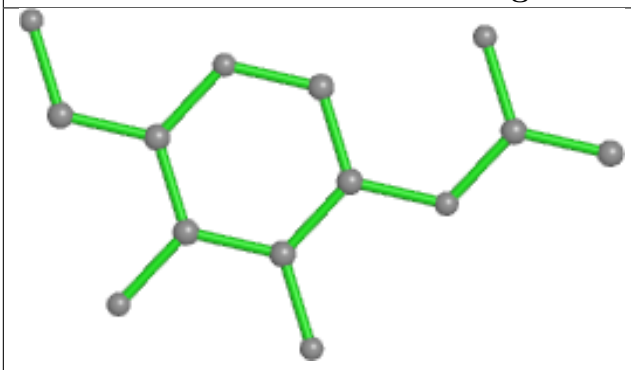


Rings

Ligand NAG C 2003



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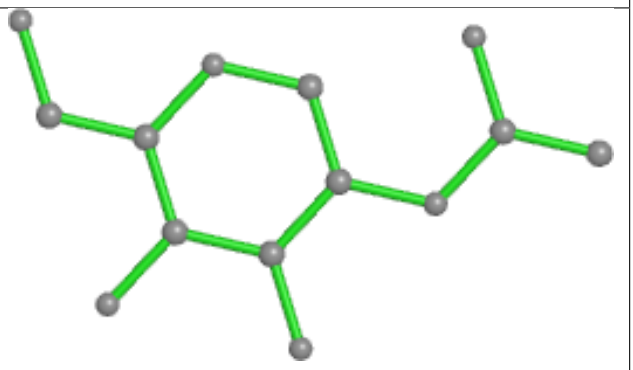

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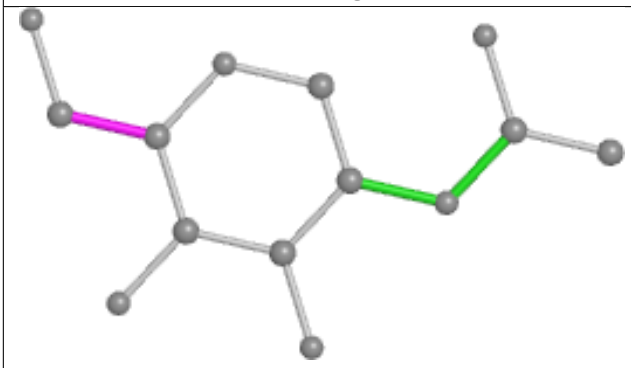

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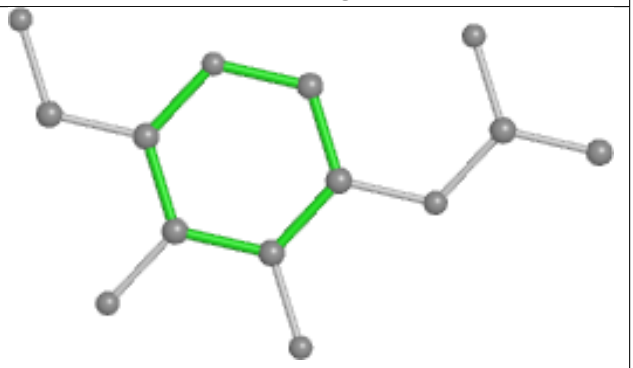
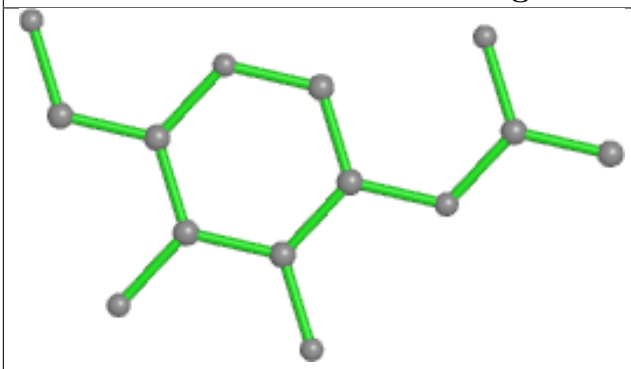


Rings

Ligand NAG B 2009



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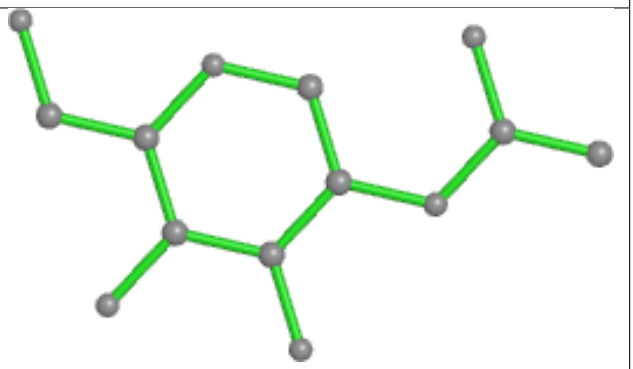
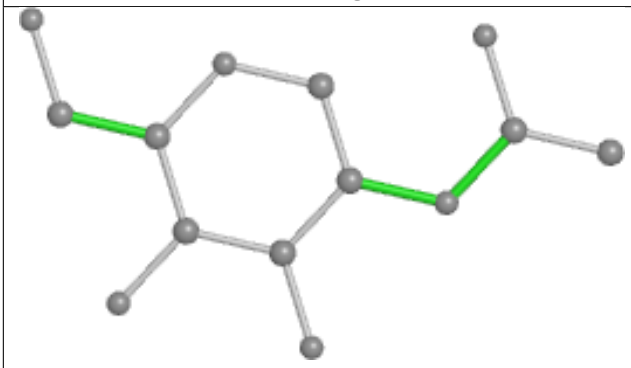
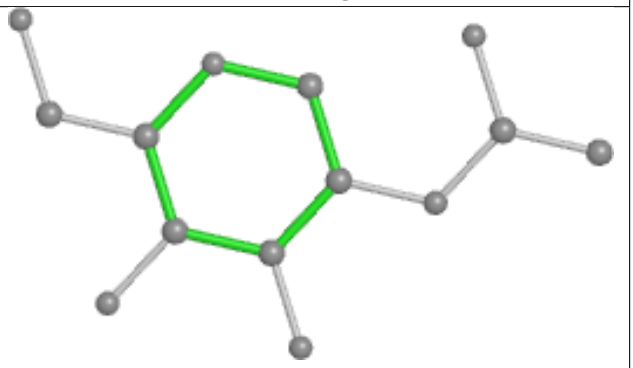


Bond angles

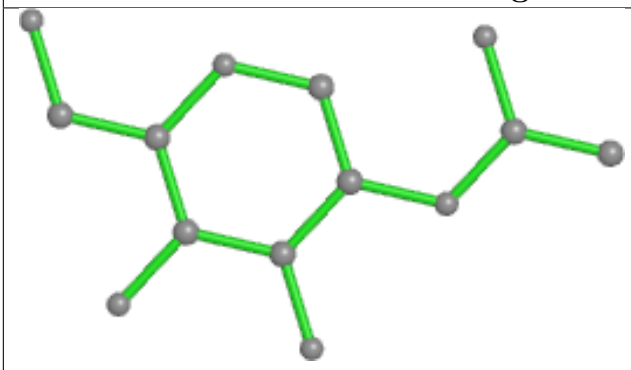


Torsions



Rings

Ligand NAG C 2011



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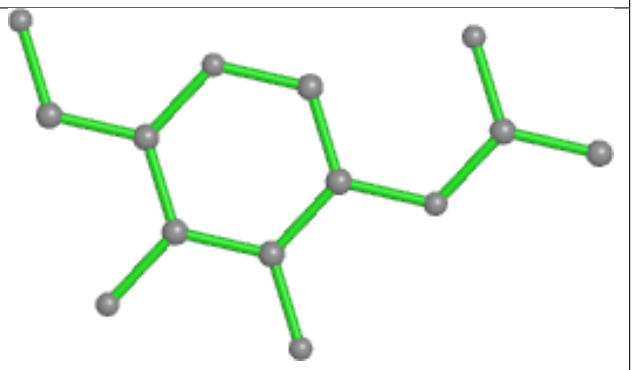
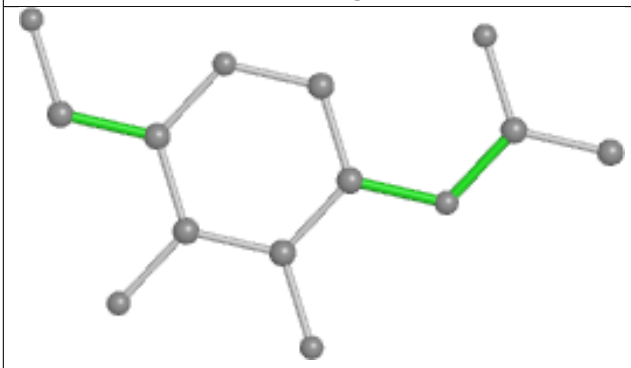


Bond angles



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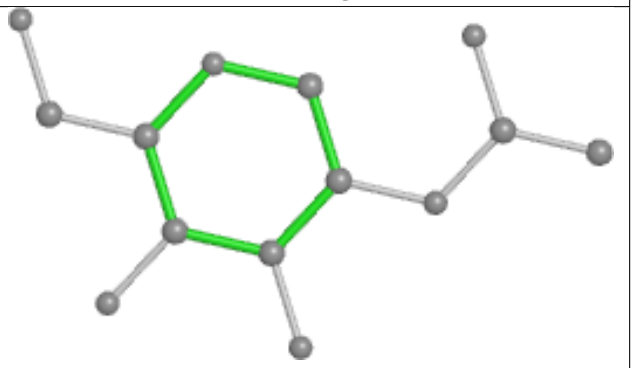
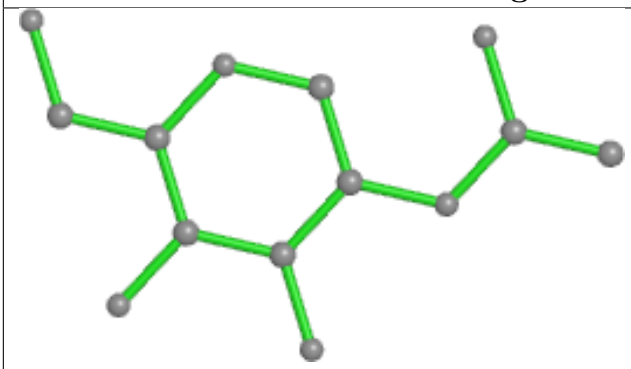


Rings

Ligand NAG A 2013



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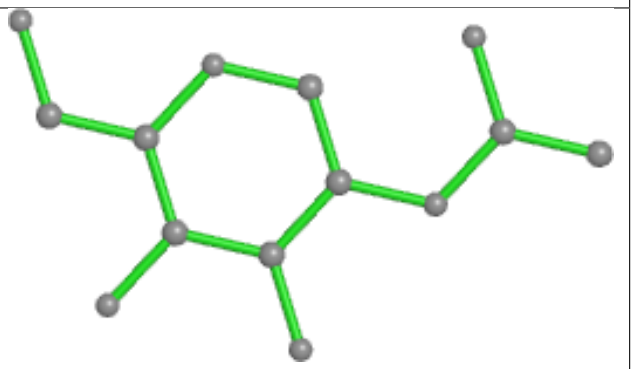
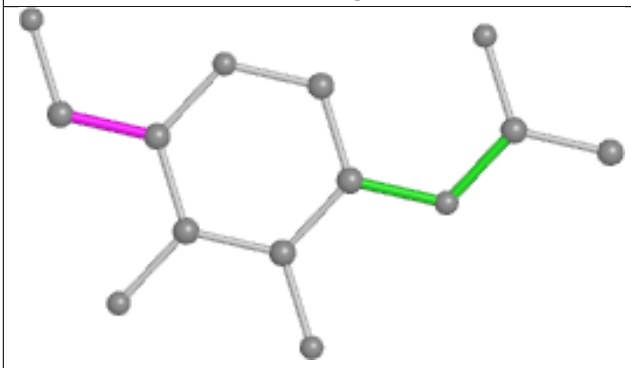
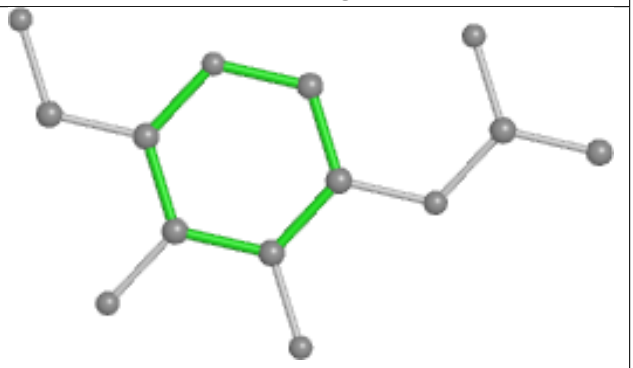


Bond angles

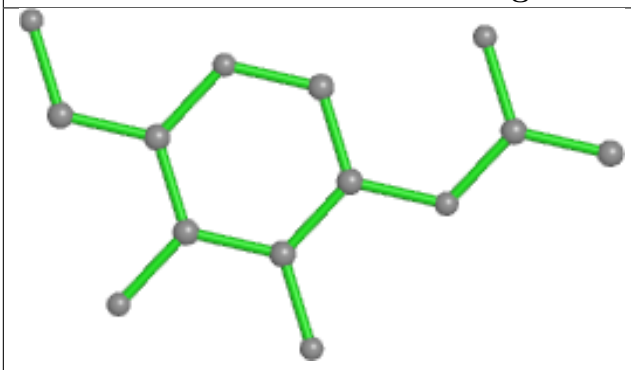


Torsions



Rings

Ligand NAG B 2001



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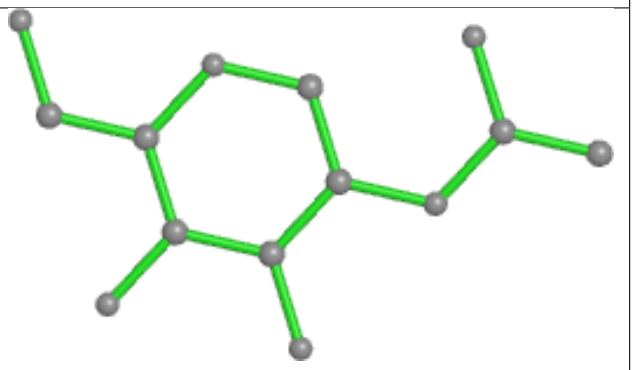

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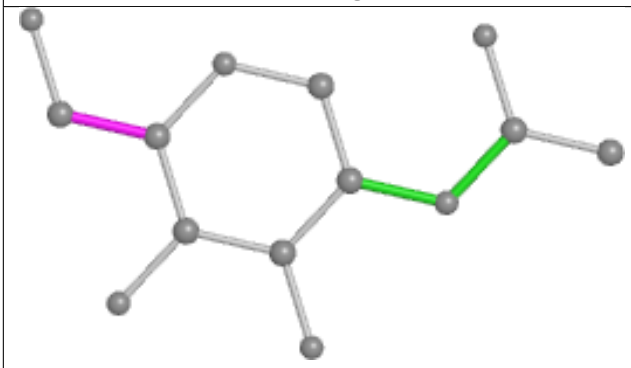

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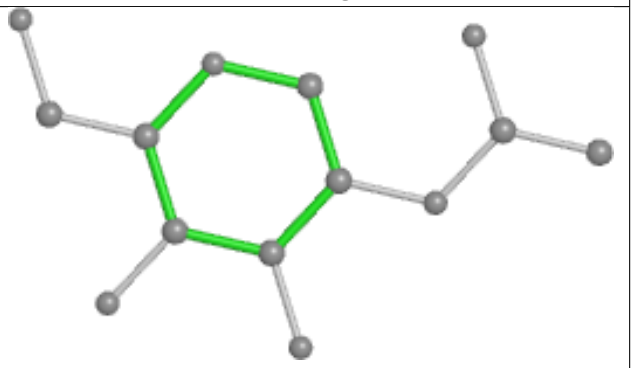
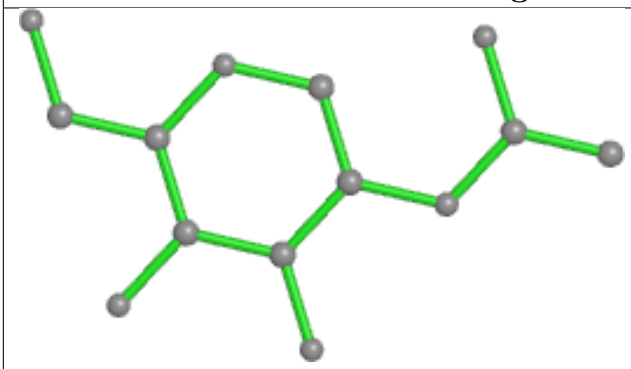


Rings

Ligand NAG A 2001



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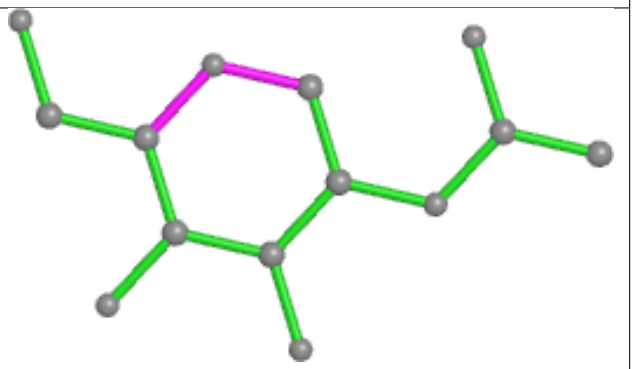

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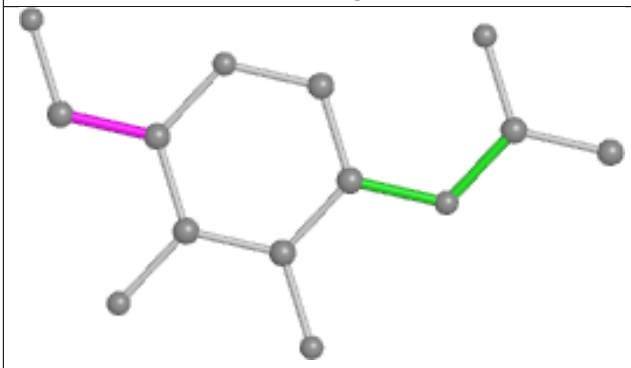

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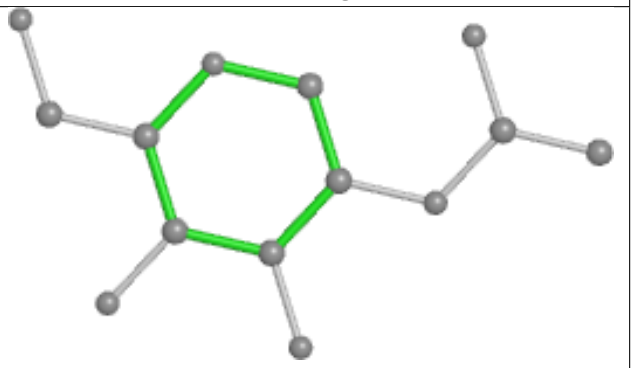
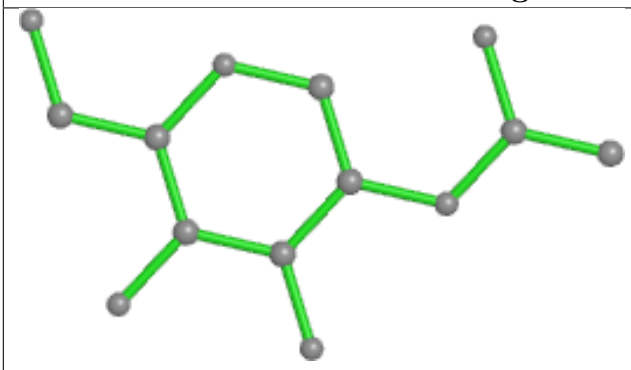


Rings

Ligand NAG C 2012



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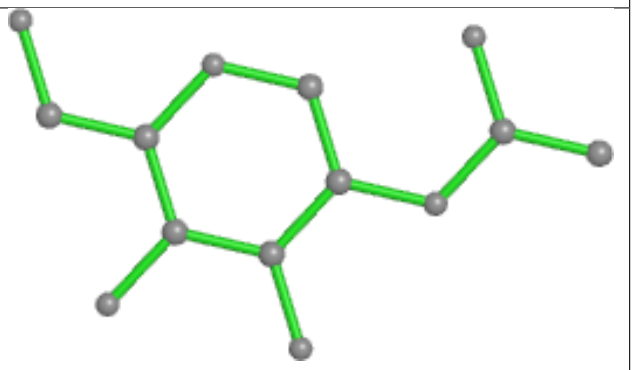
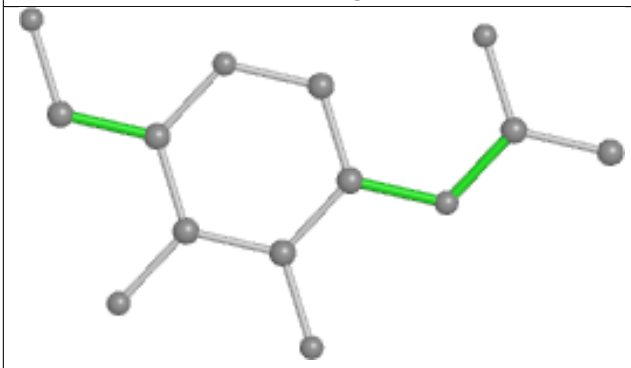


Bond angles



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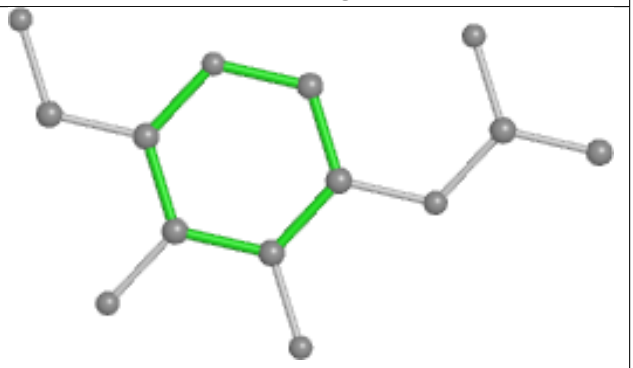
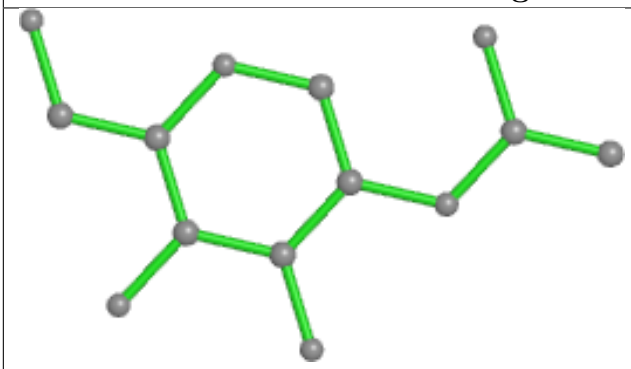


Rings

Ligand NAG B 2003



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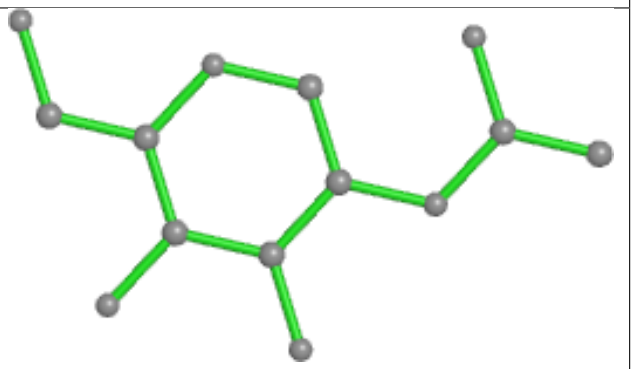

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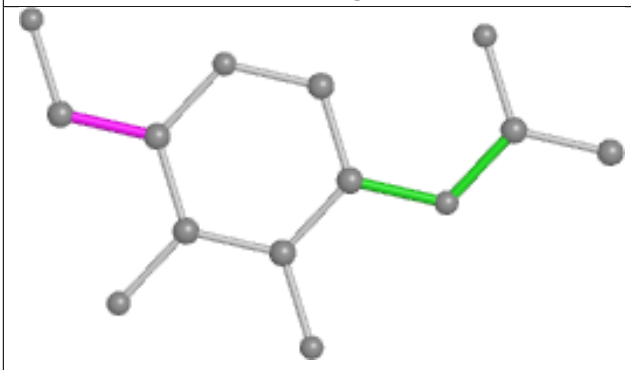

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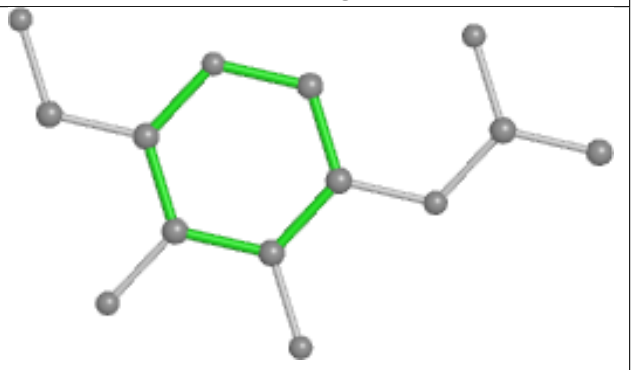
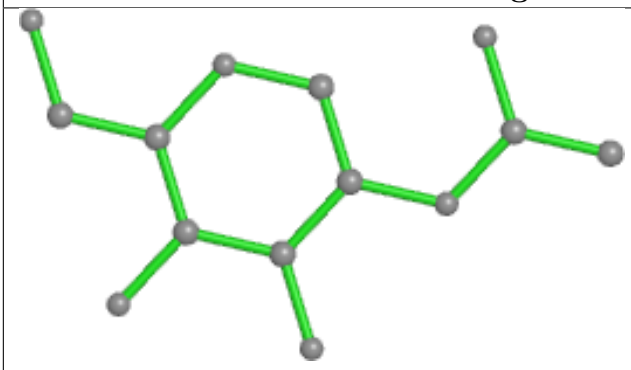


Rings

Ligand NAG A 2011



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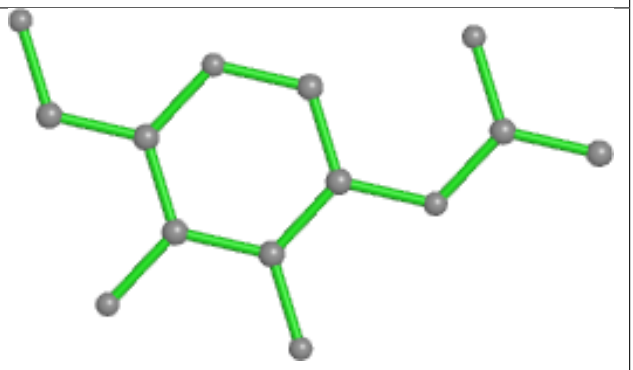

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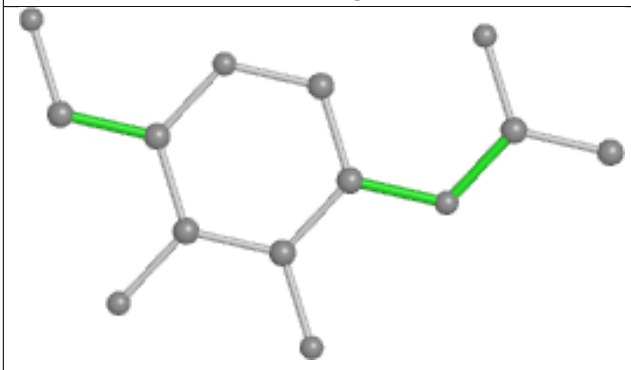

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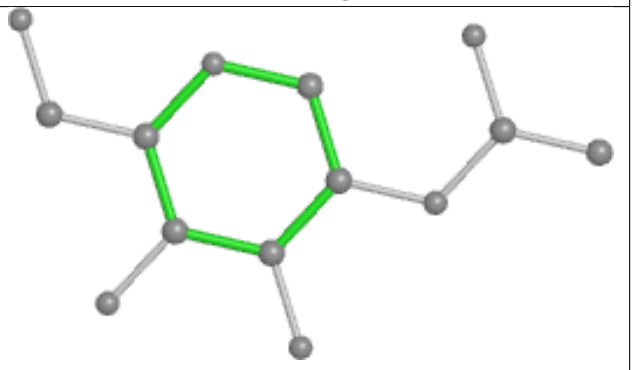
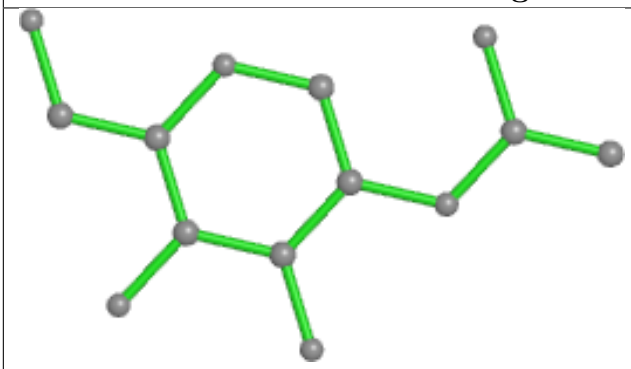


Rings

Ligand NAG C 2001



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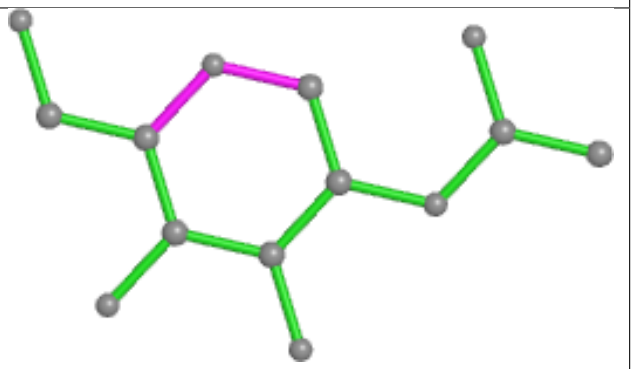

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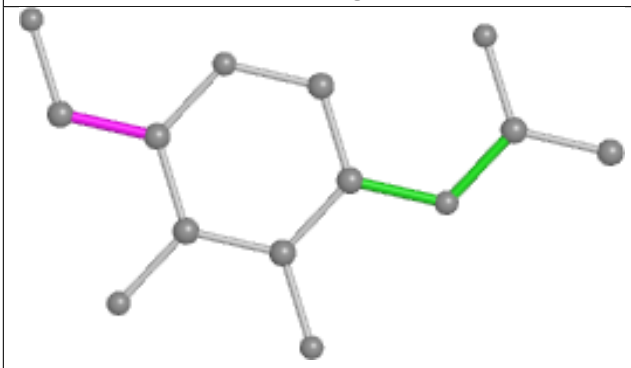

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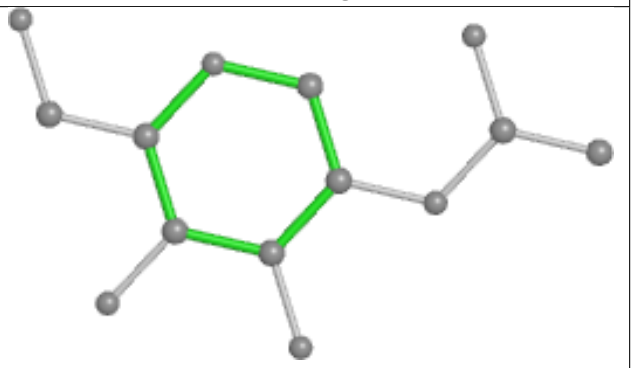
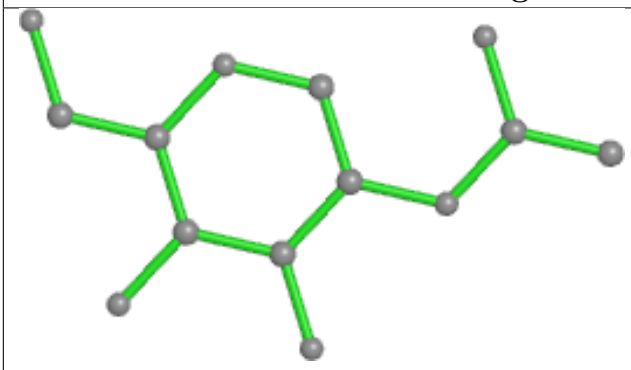


Rings

Ligand NAG C 2016



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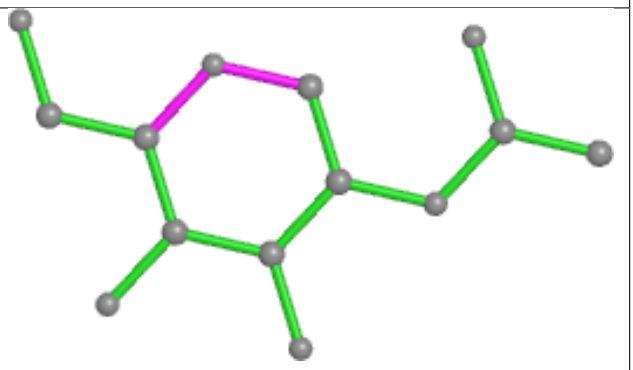

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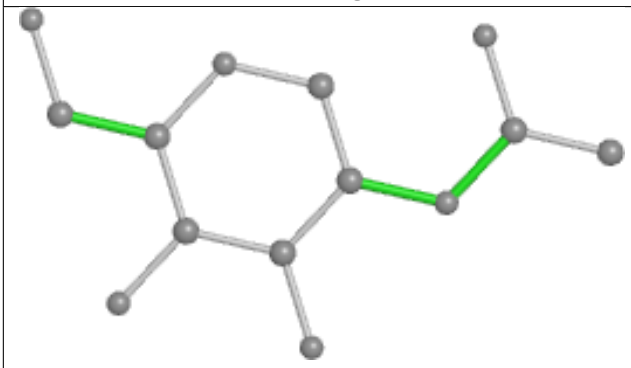

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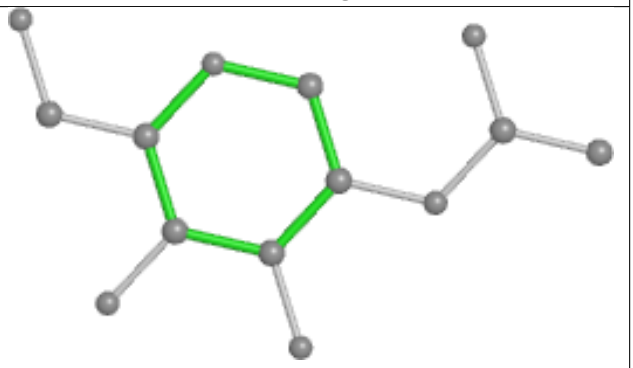
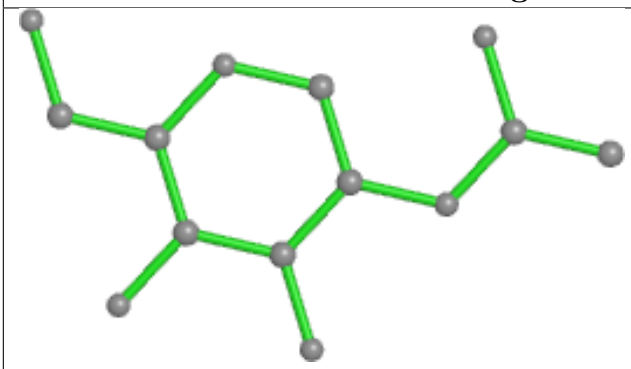


Rings

Ligand NAG A 2005



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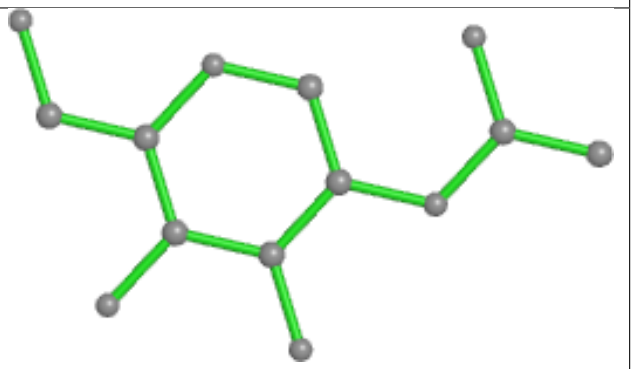
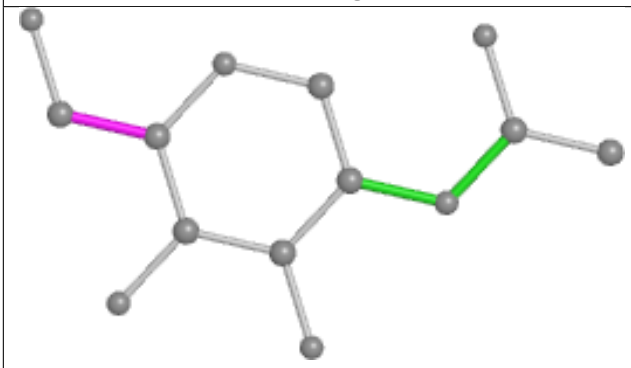


Bond angles



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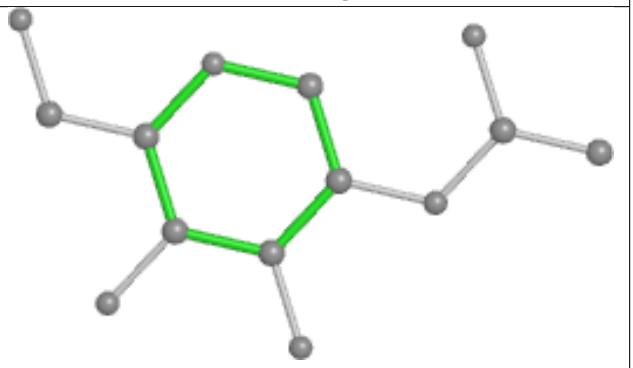
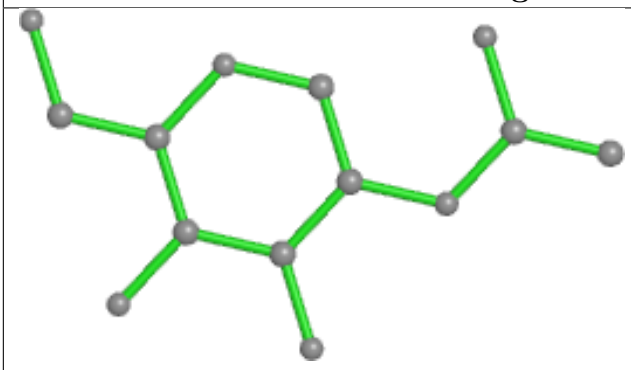


Rings

Ligand NAG C 2006



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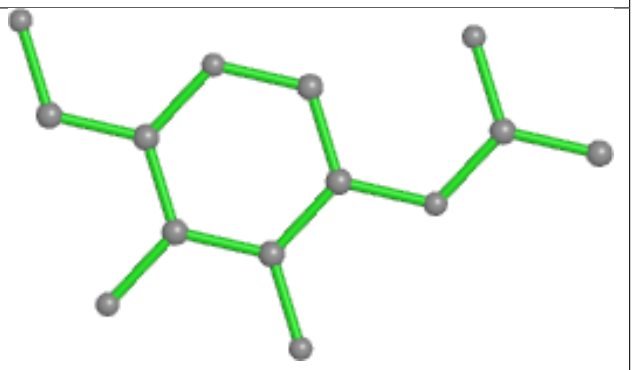
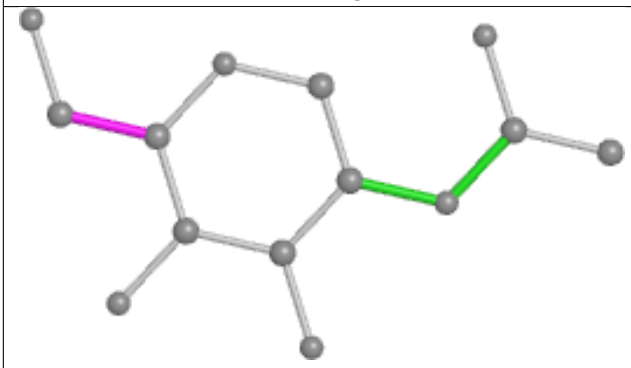
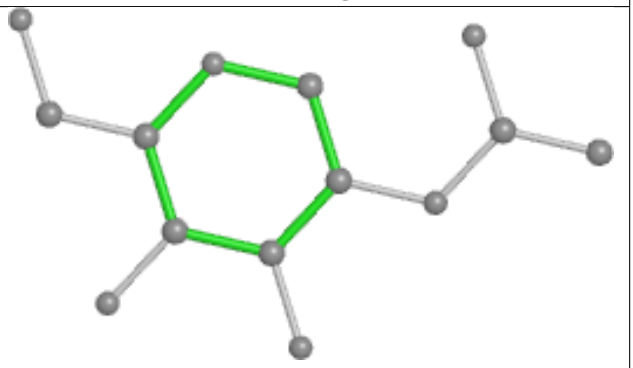


Bond angles

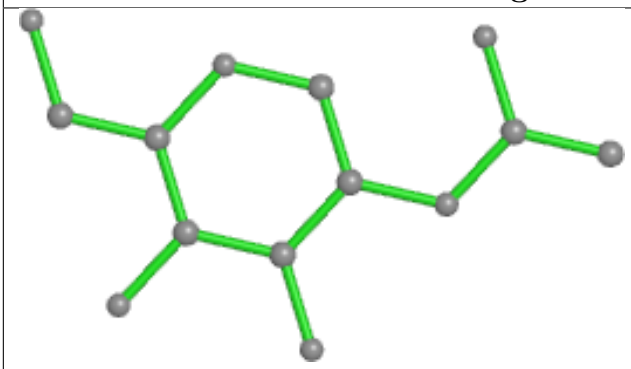


Torsions



Rings

Ligand NAG A 2016



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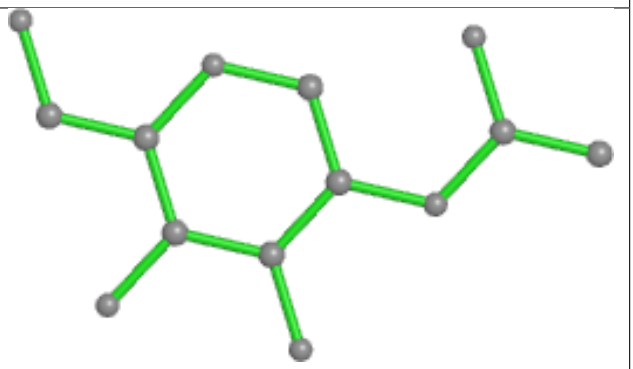

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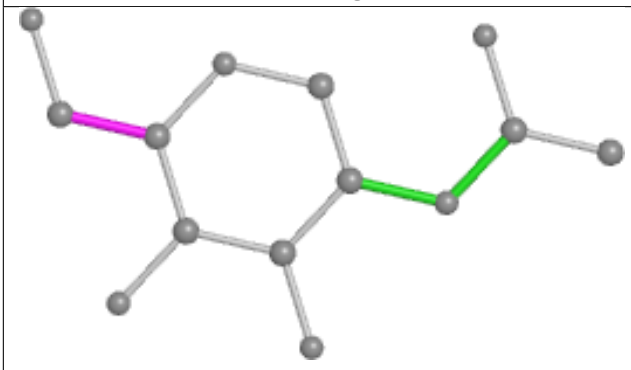

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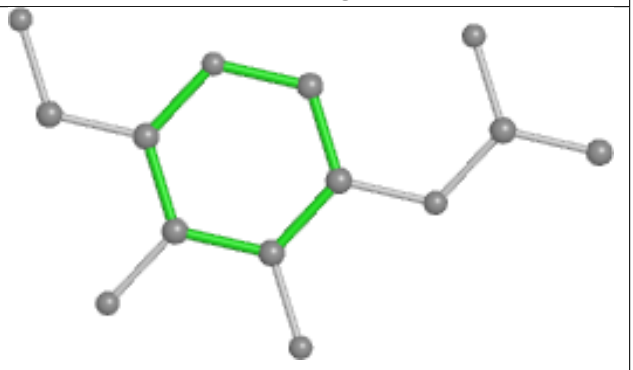

Rings

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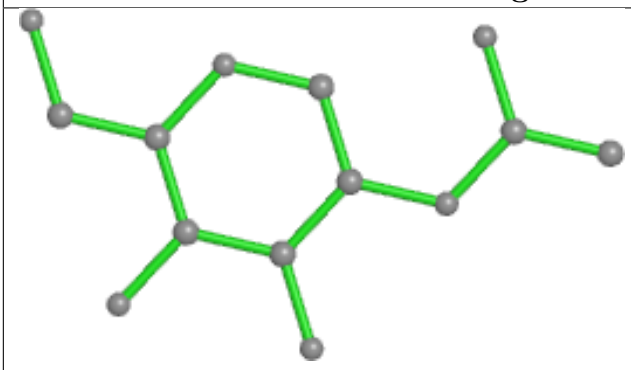

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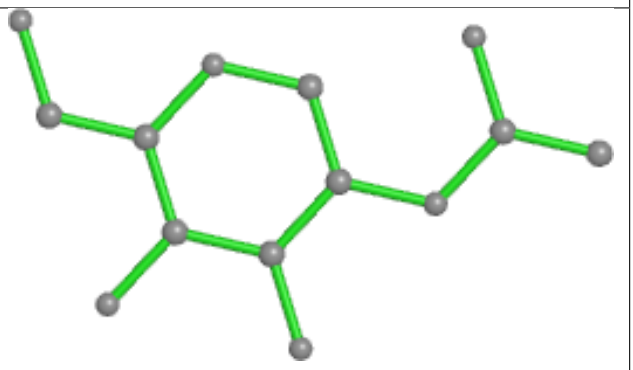
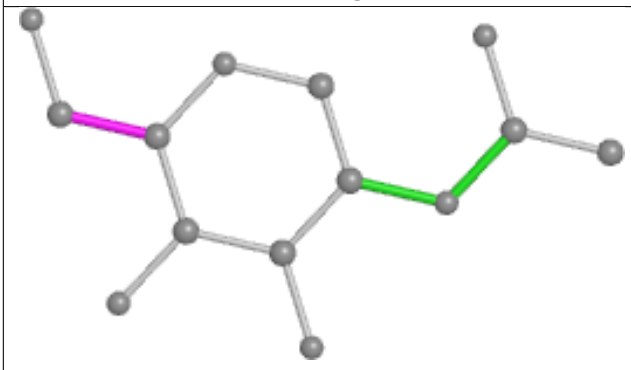


Bond angles



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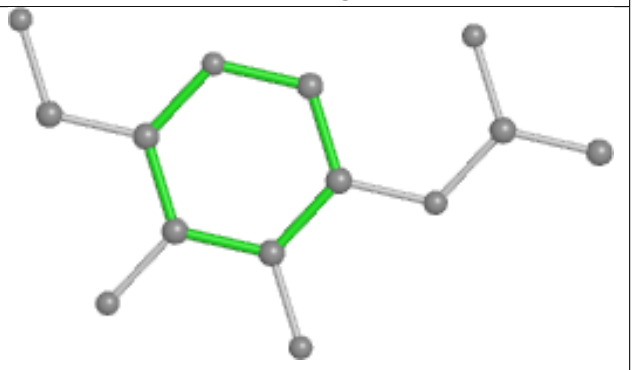
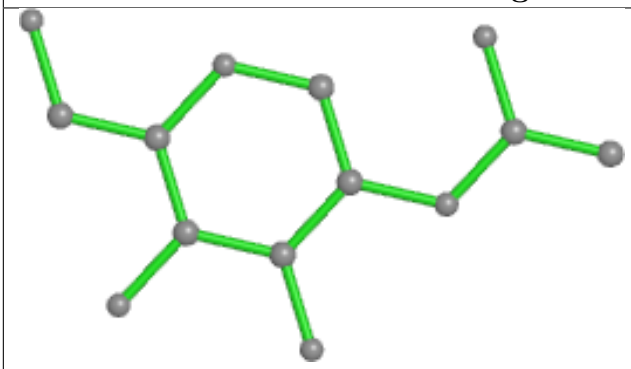


Rings

Ligand NAG C 2014



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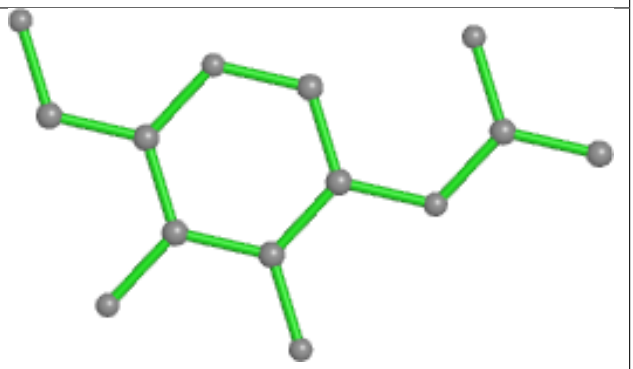

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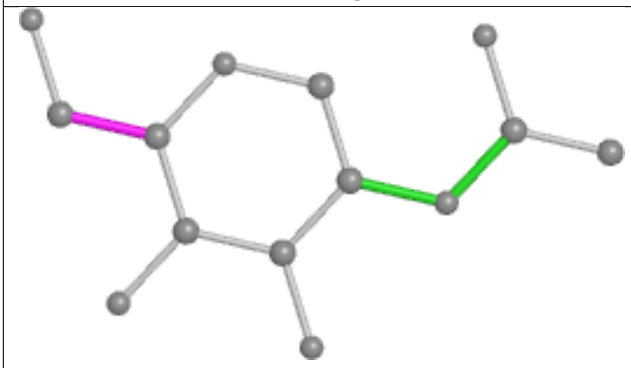

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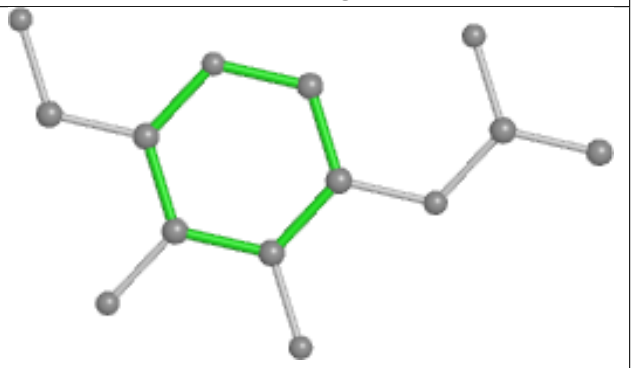
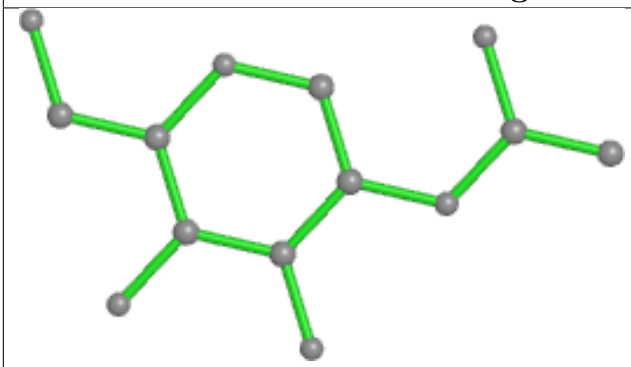


Rings

Ligand NAG A 2008



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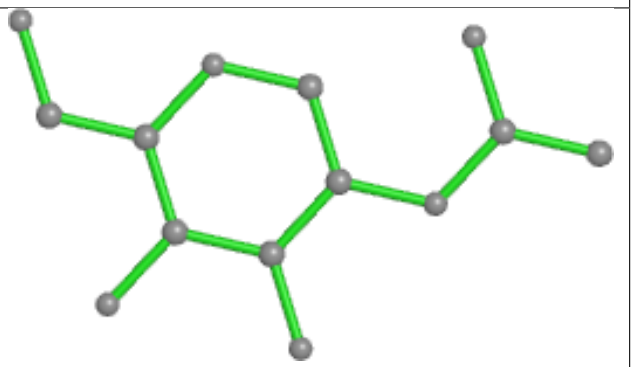
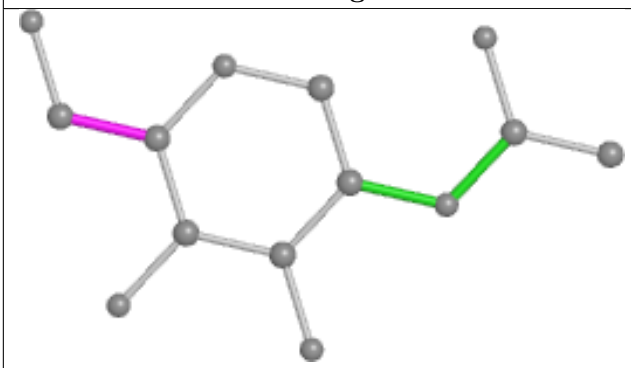


Bond angles



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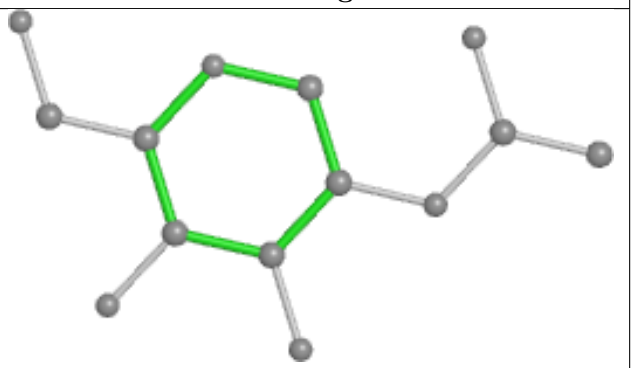
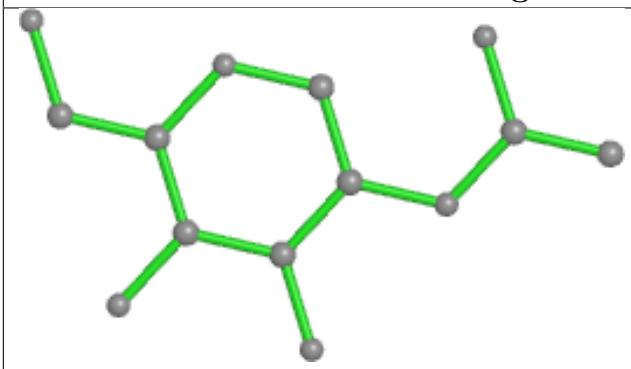


Rings

Ligand NAG C 2015



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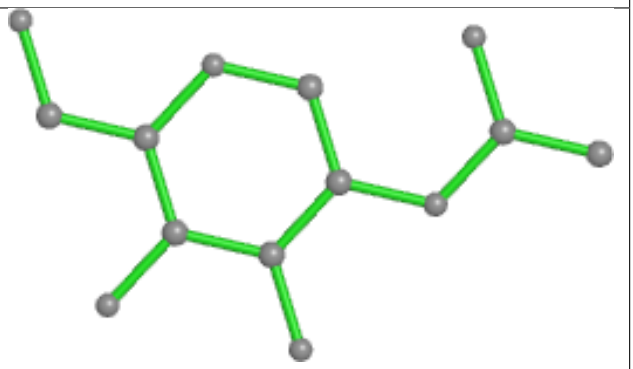
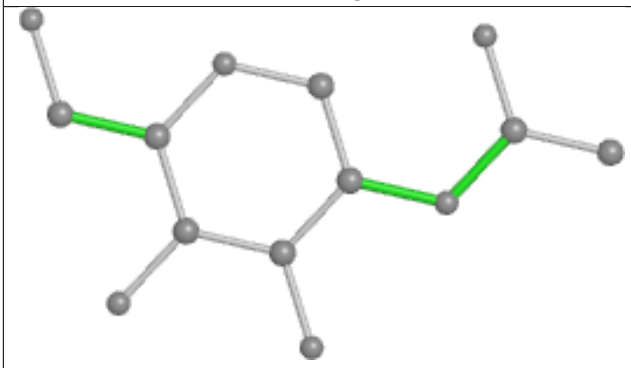
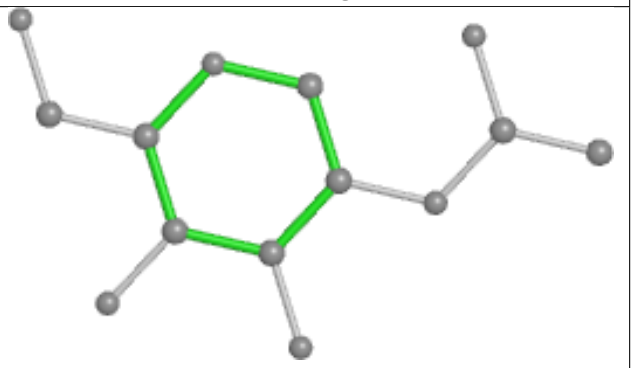


Bond angles

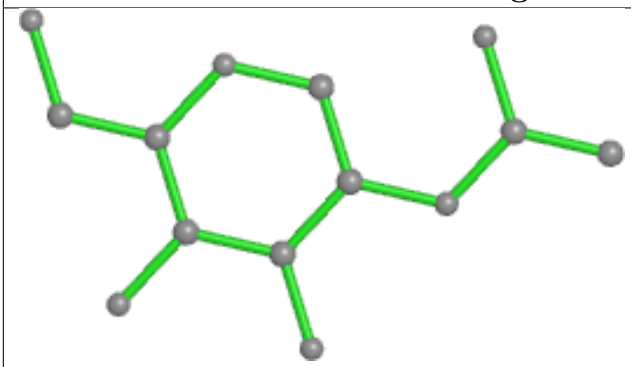


Torsions

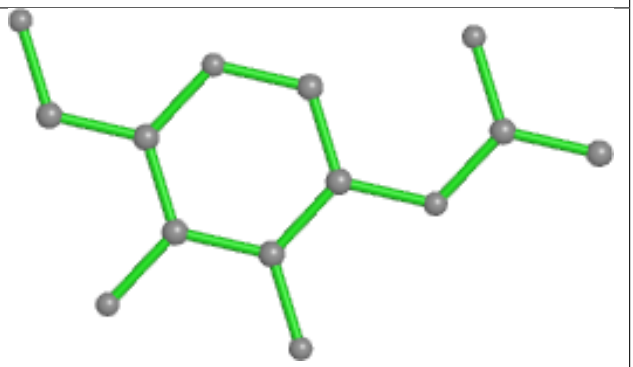


Rings

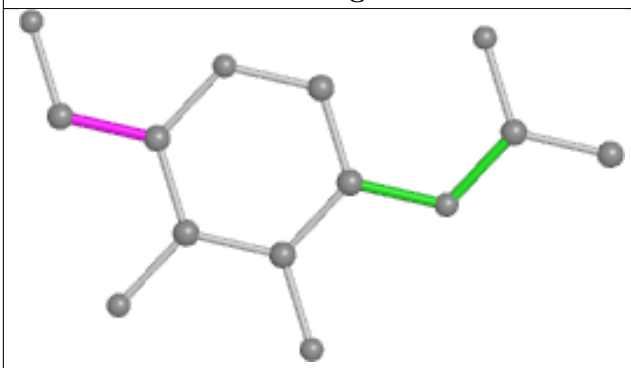
Ligand NAG A 2003



Bond lengths



Bond angles



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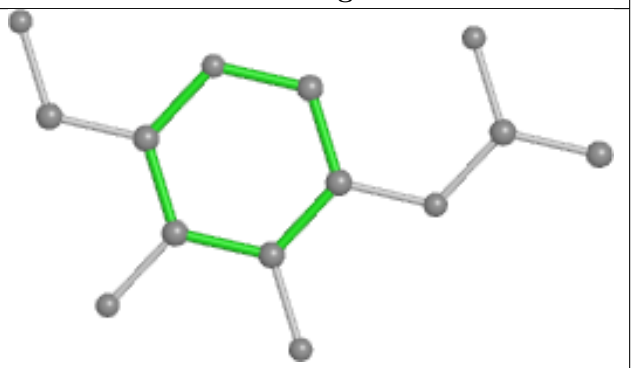
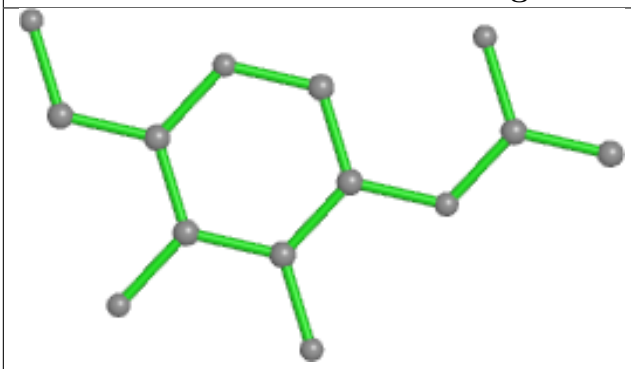


Rings

Ligand NAG A 2010



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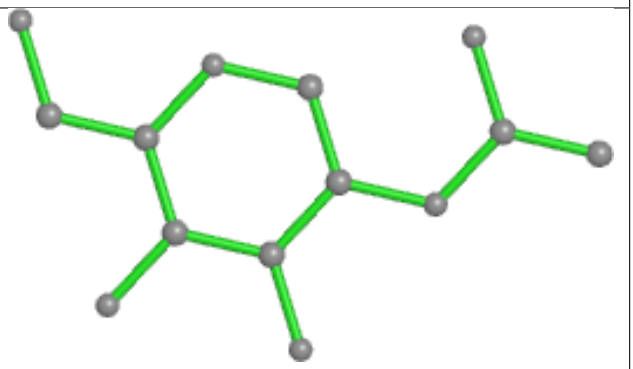
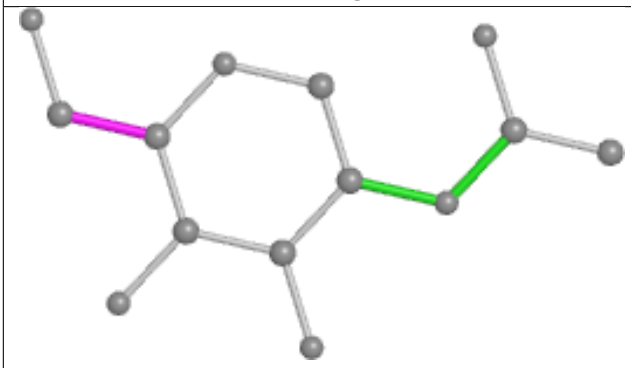


Bond angles



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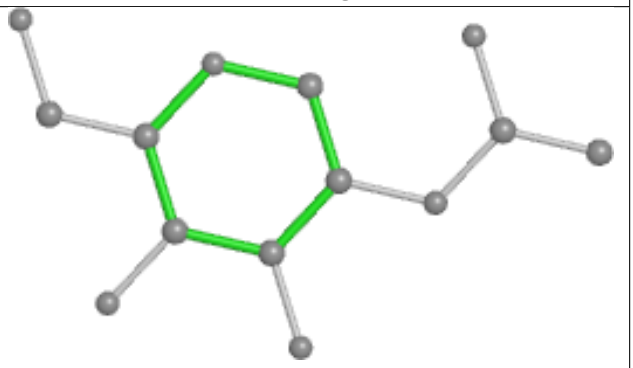
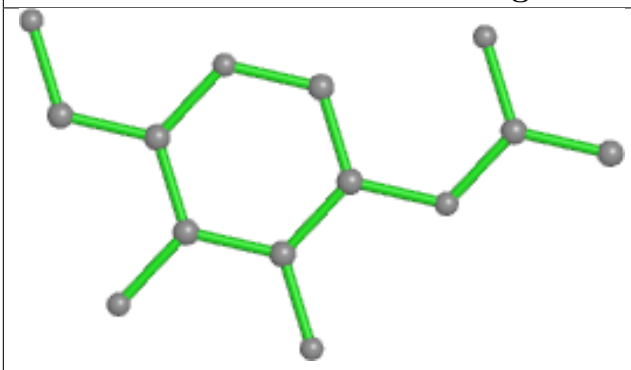


Rings

Ligand NAG B 2017



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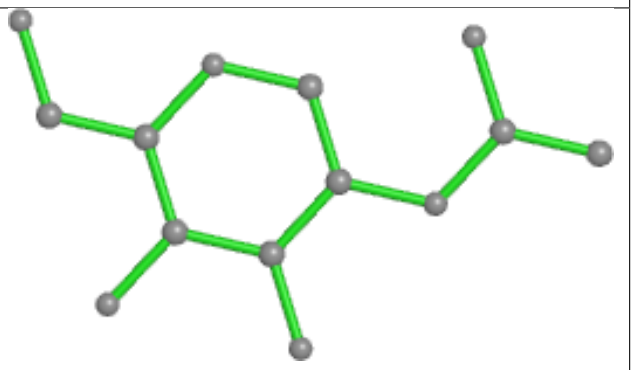
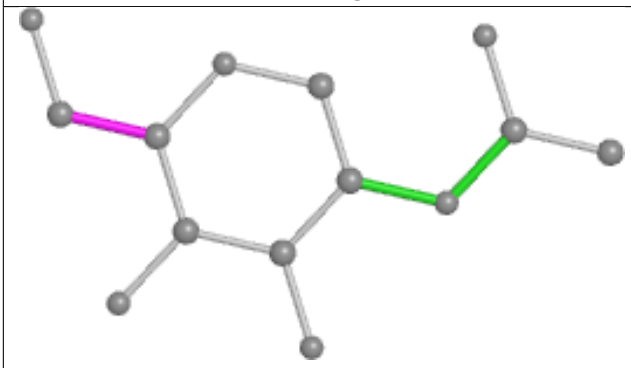


Bond angles



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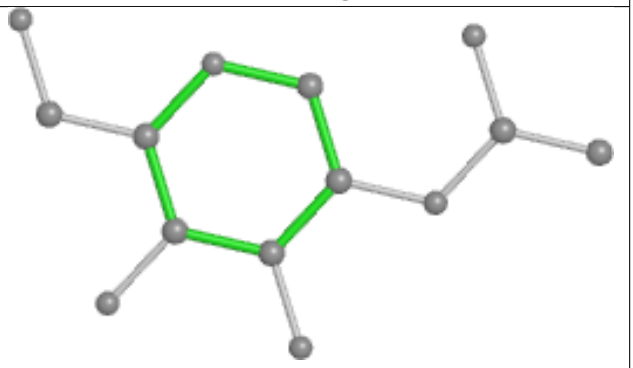
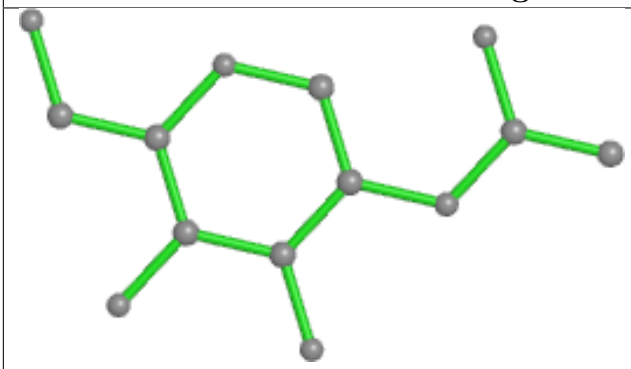
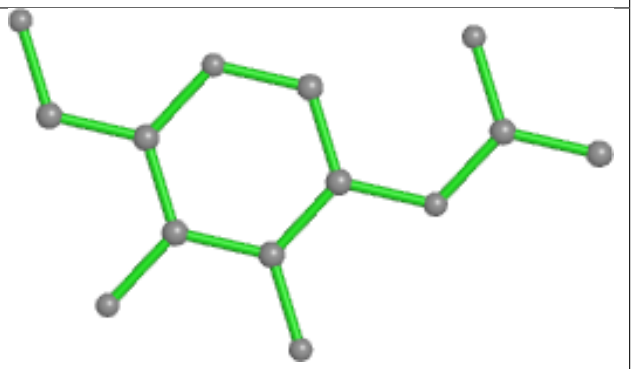
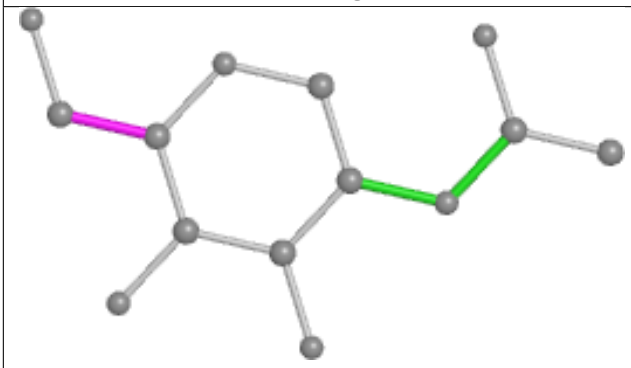
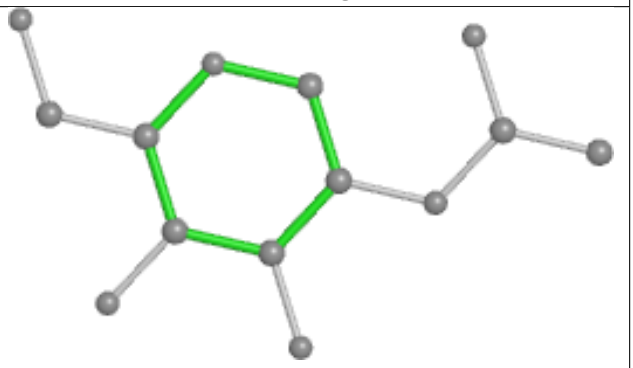
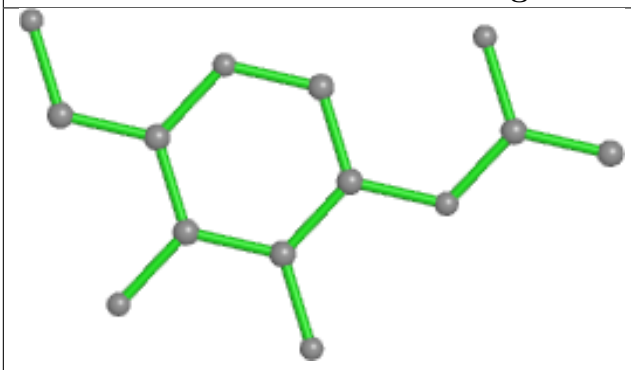
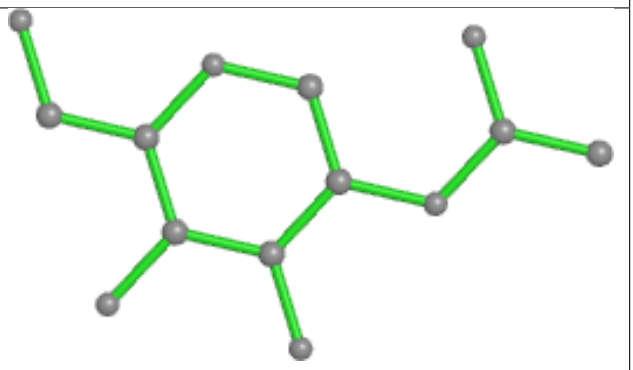
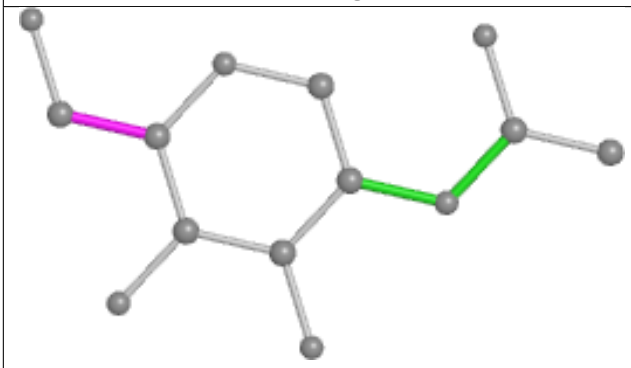
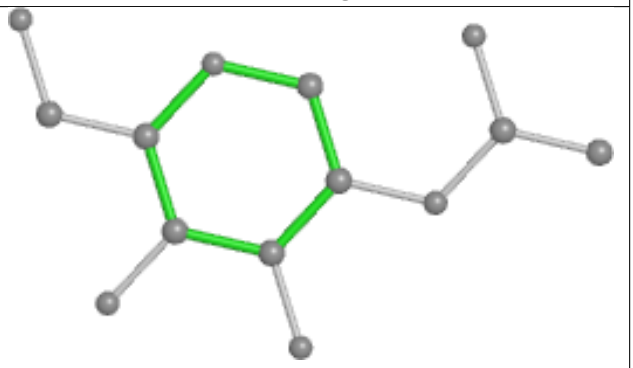
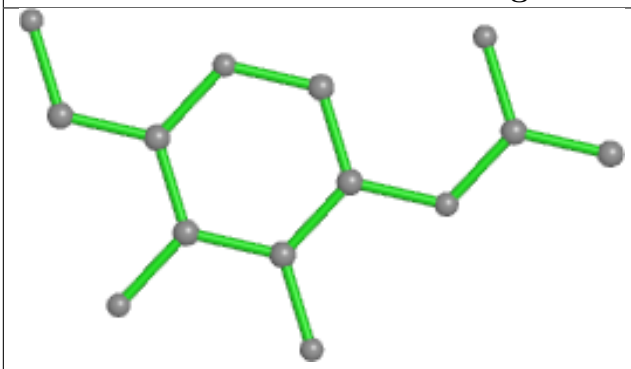


Rings

Ligand NAG B 2008	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand NAG A 2006	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand NAG A 2017



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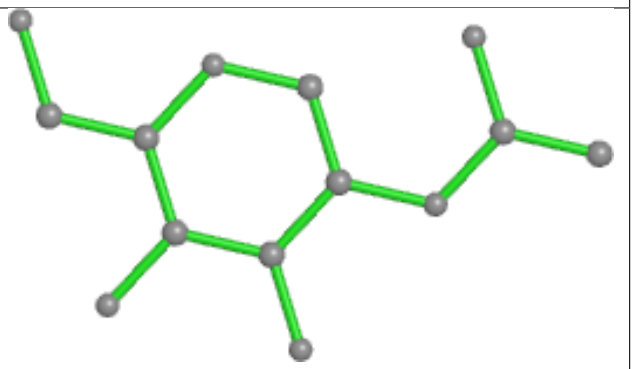
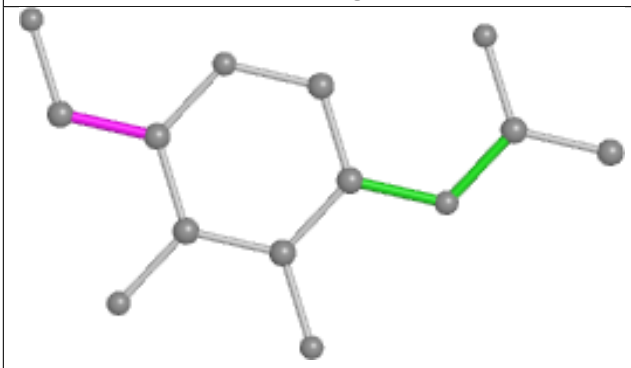


Bond angles



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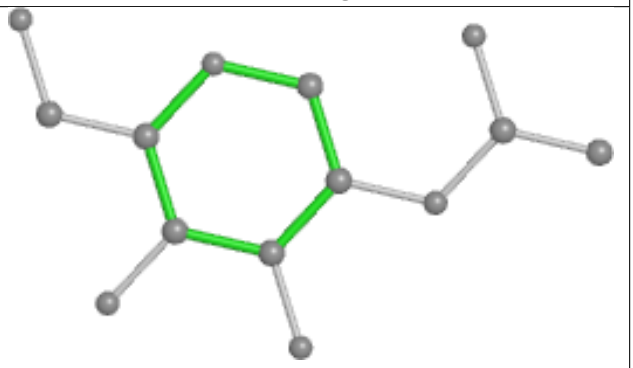
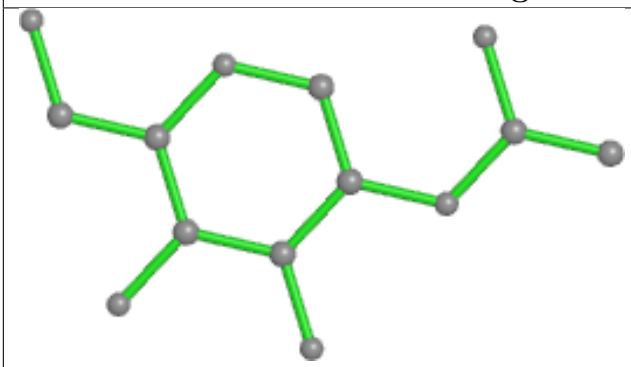


Rings

Ligand NAG C 2002



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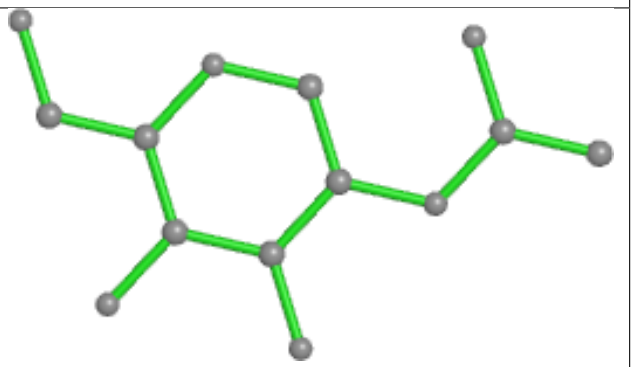

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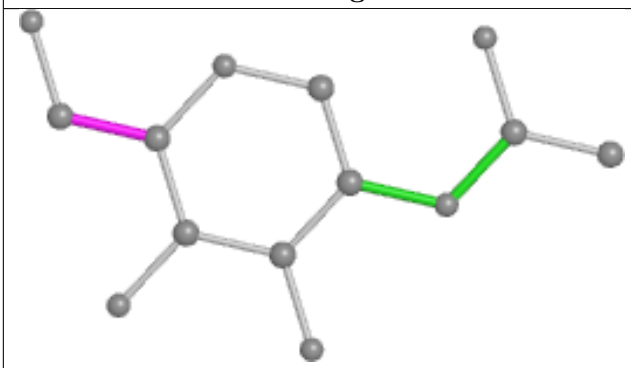

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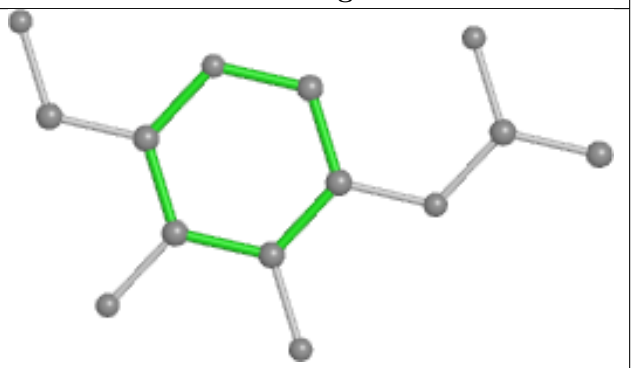
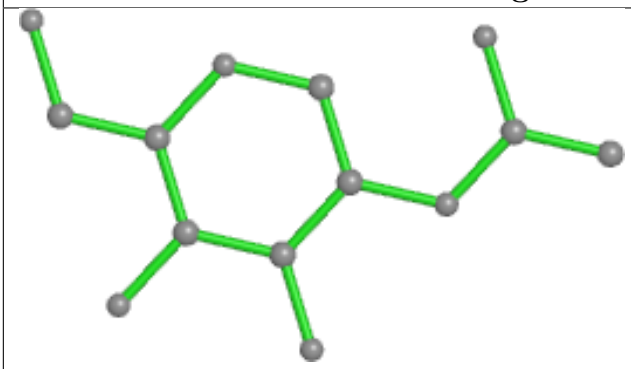


Rings

Ligand NAG B 2002



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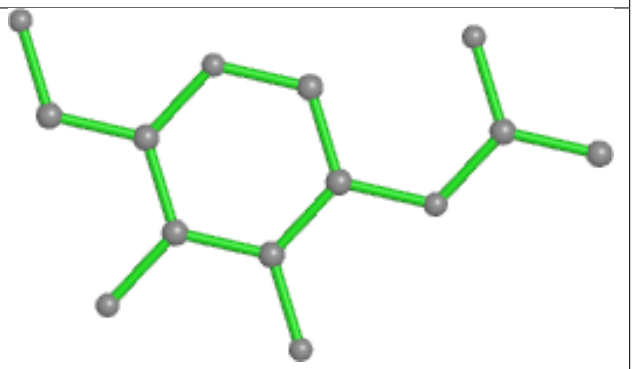

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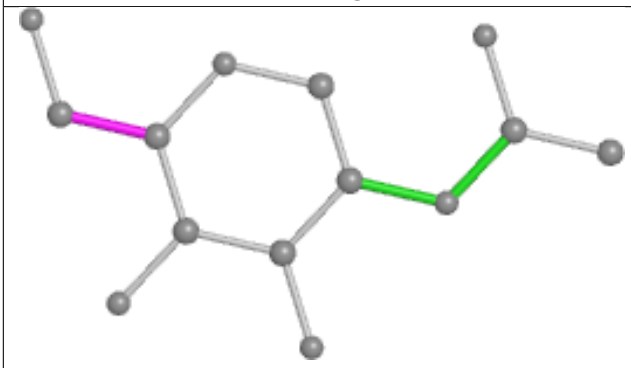

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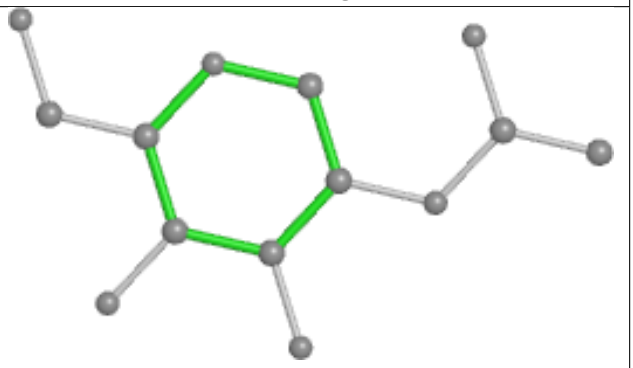
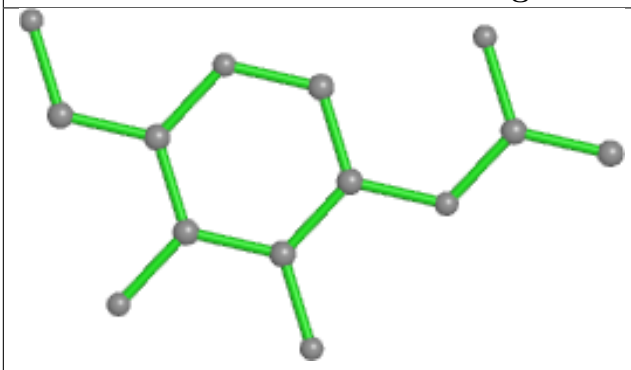


Rings

Ligand NAG B 2011



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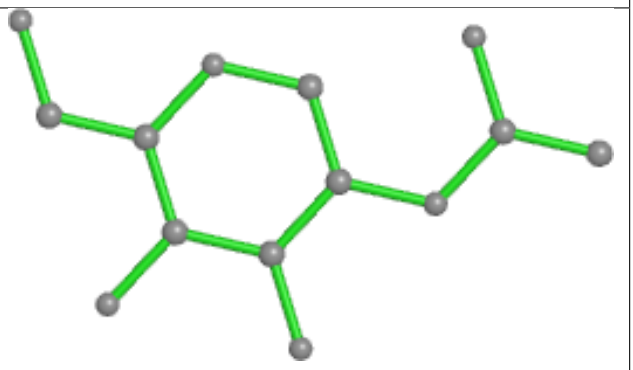
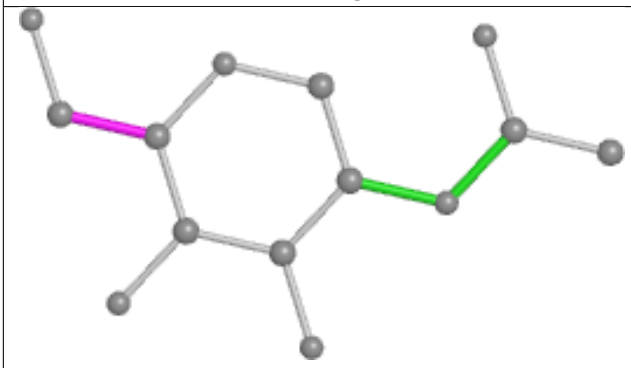


Bond angles



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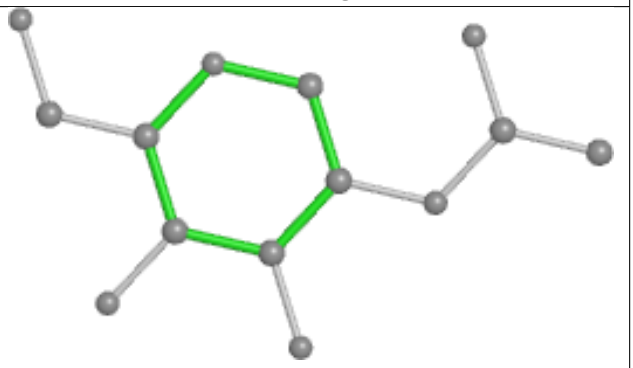
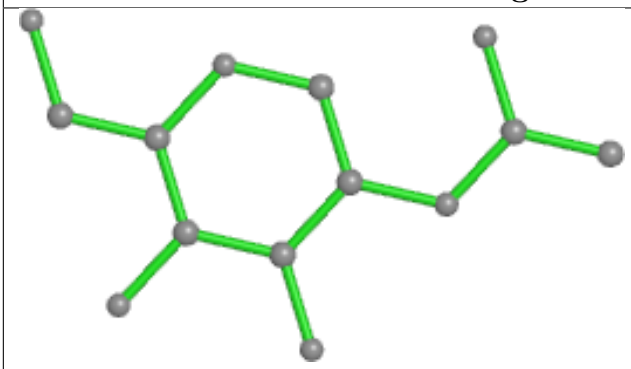


Rings

Ligand NAG C 2013



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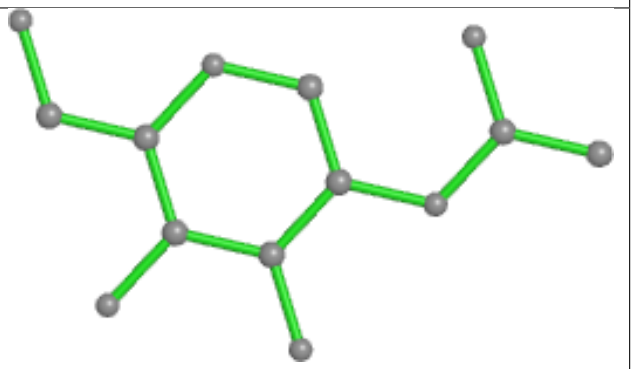

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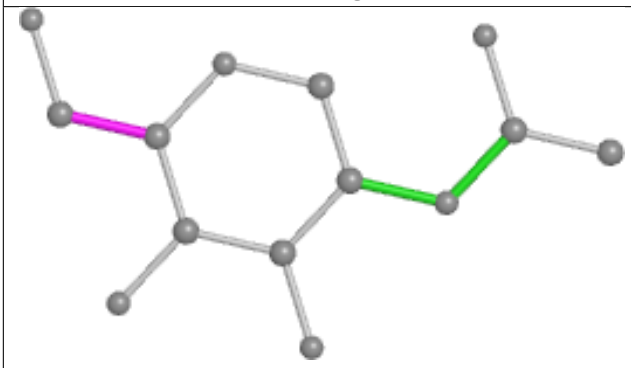

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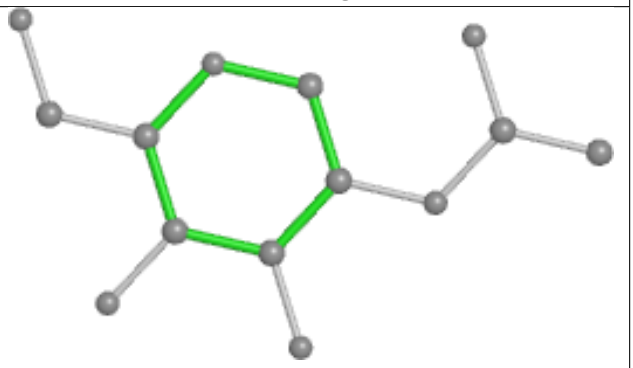
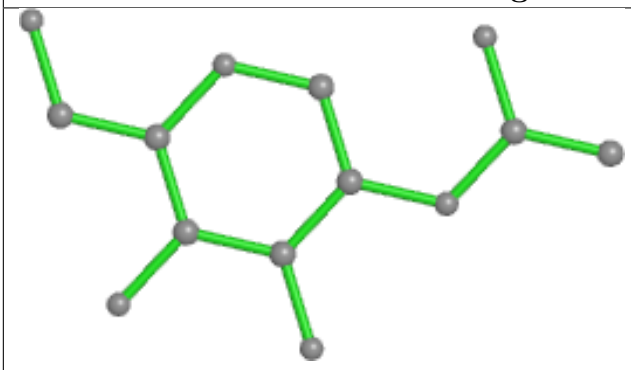


Rings

Ligand NAG A 2012



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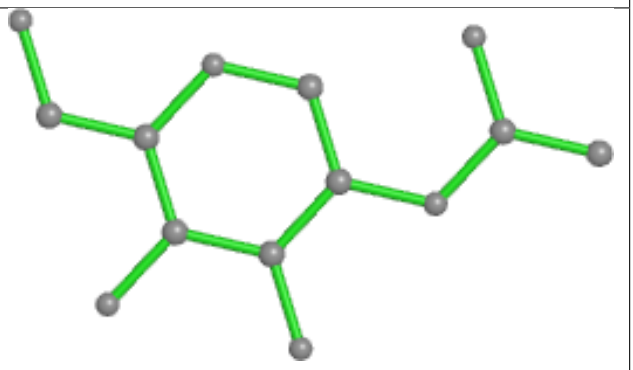
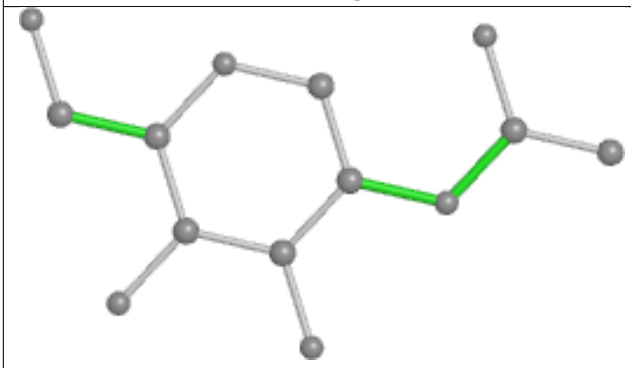


Bond angles



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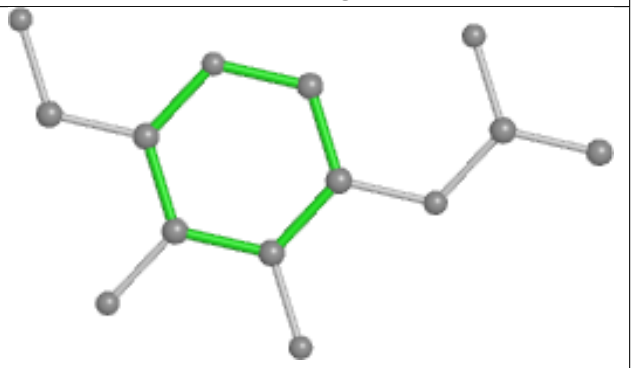
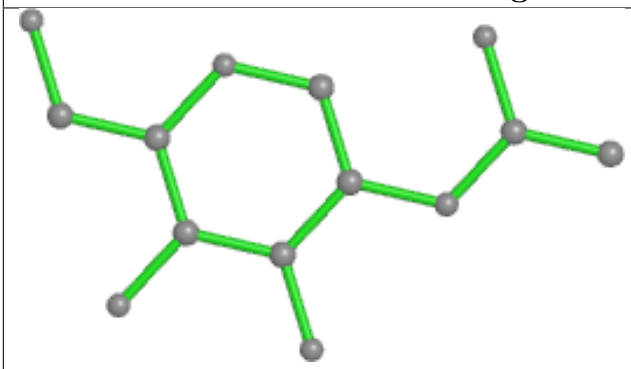
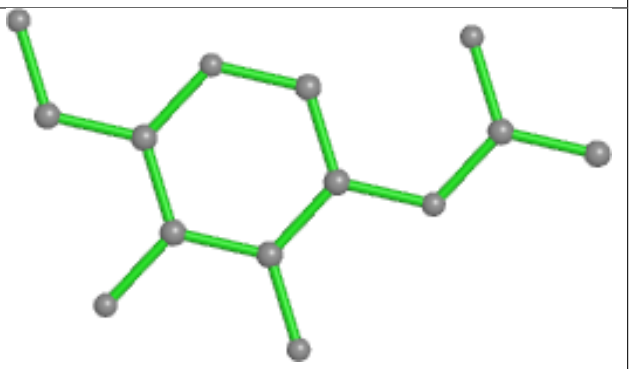
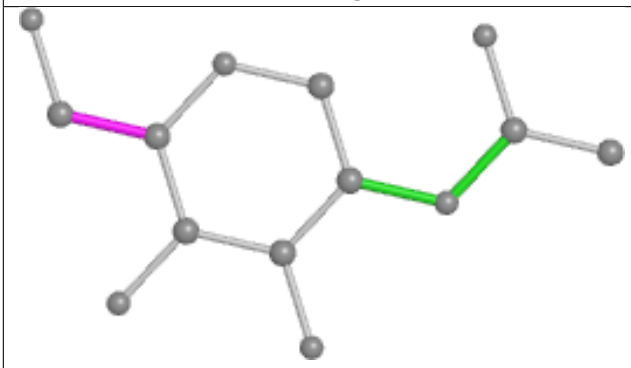
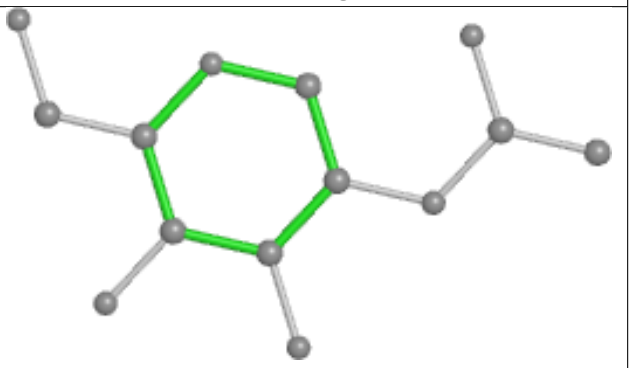
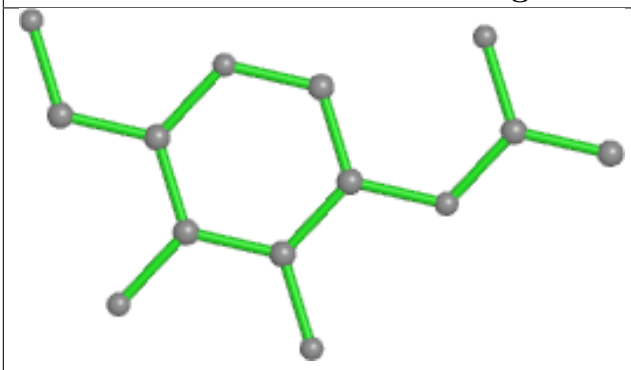
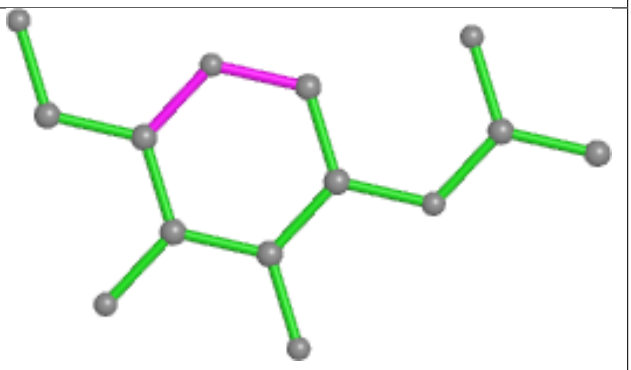
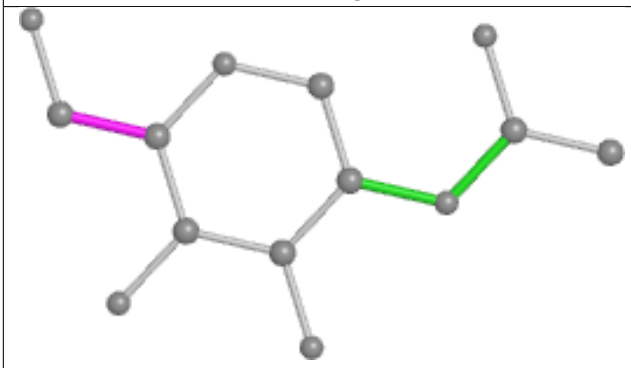
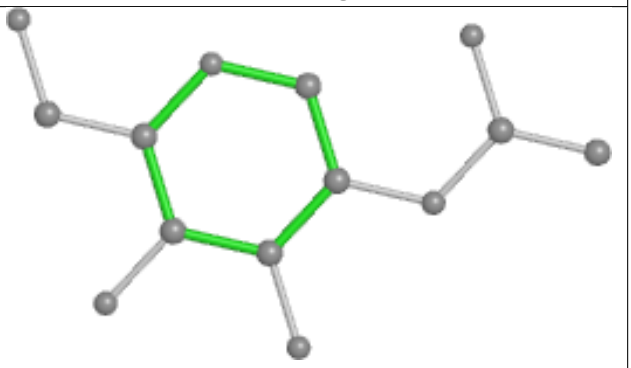
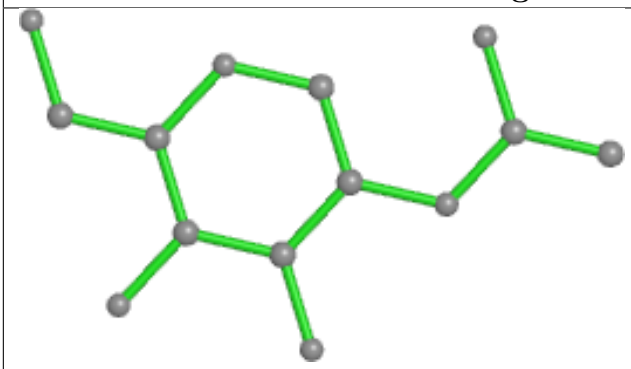


Rings

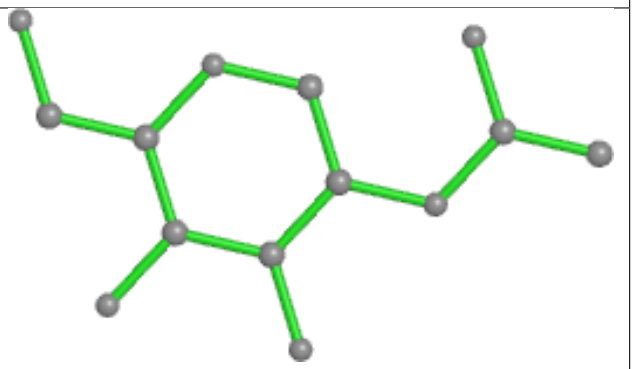
Ligand NAG A 2009	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG C 2009	
 Bond lengths	 Bond angles
 Torsions	 Rings

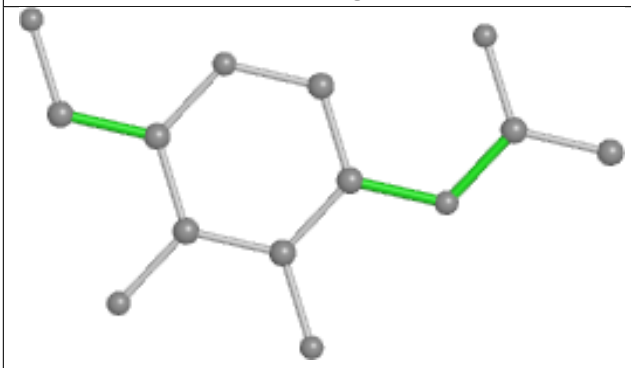
Ligand NAG B 2013



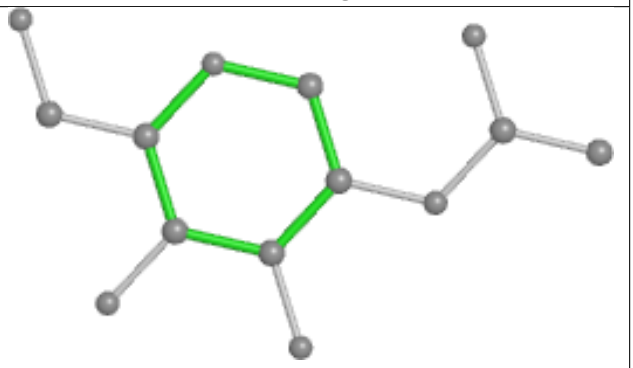
Bond lengths



Bond angles

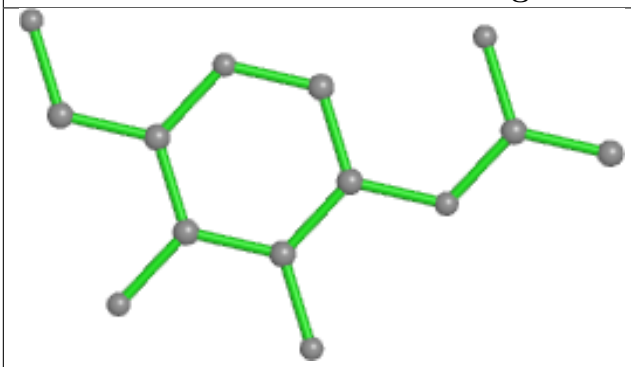


Torsions

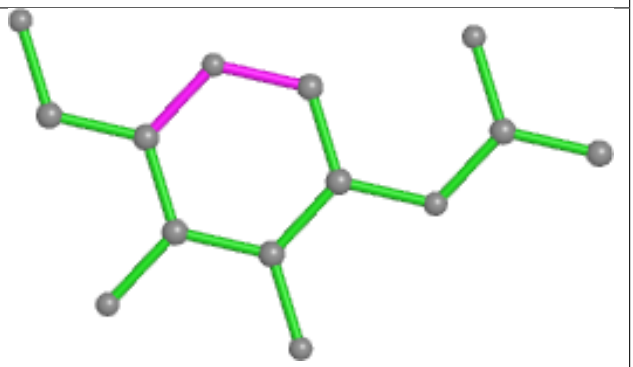


Rings

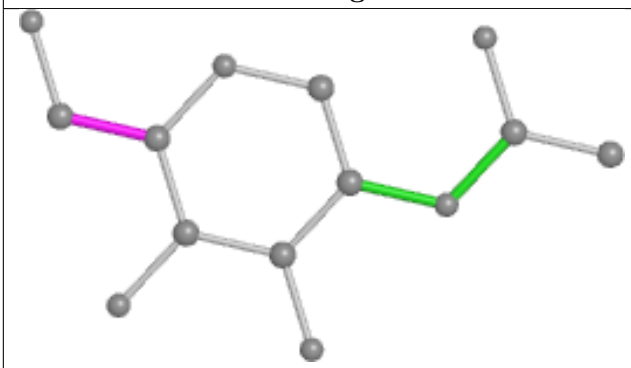
Ligand NAG B 2012



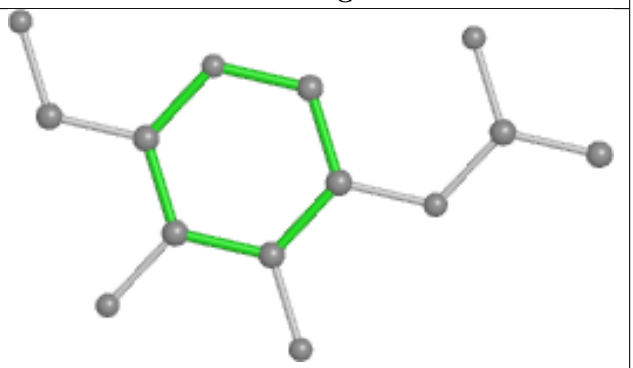
Bond lengths



Bond angles

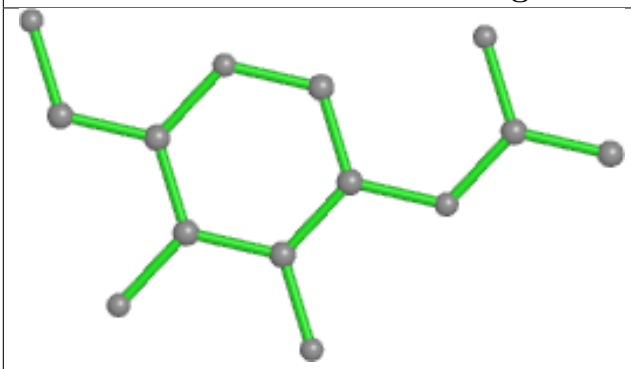


Torsions

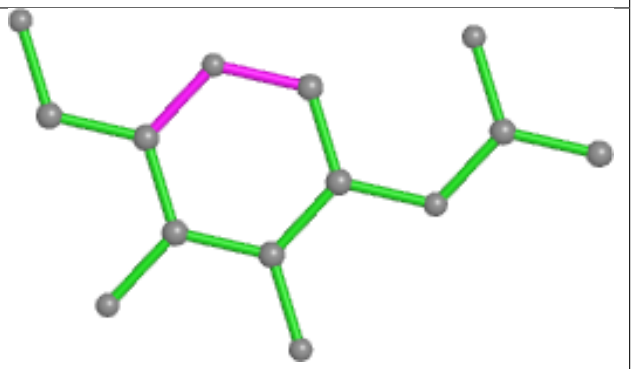


Rings

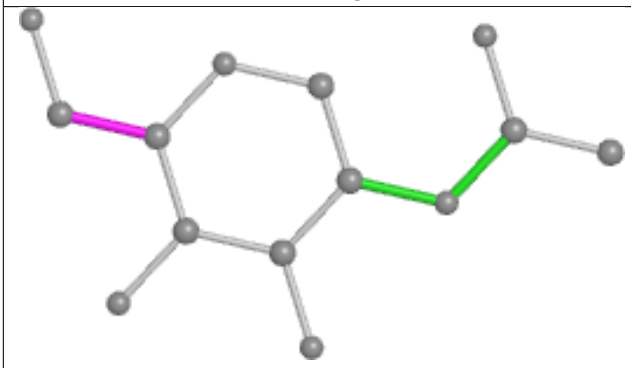
Ligand NAG C 2004



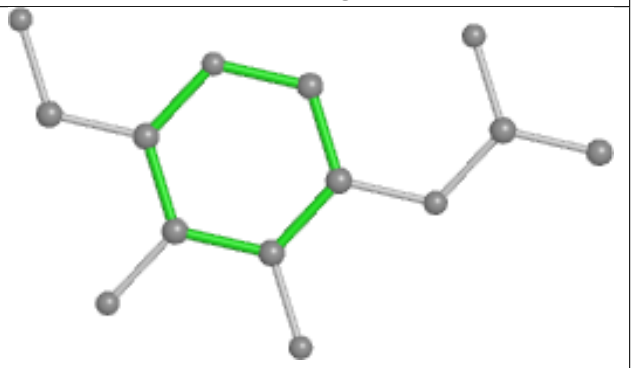
Bond lengths



Bond angles

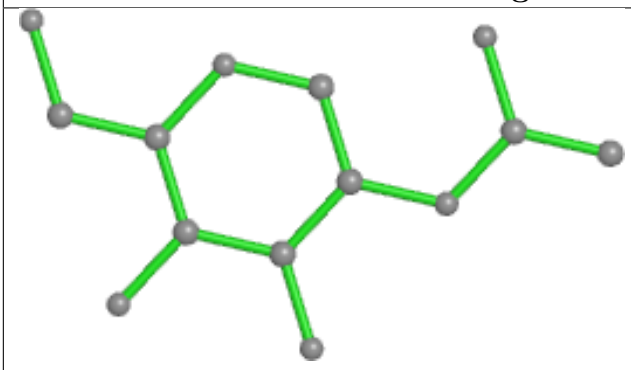


Torsions

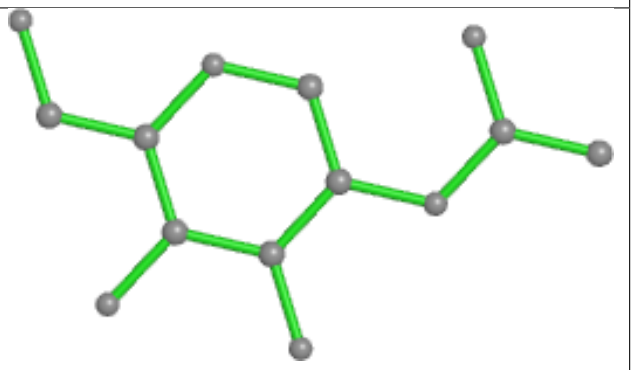


Rings

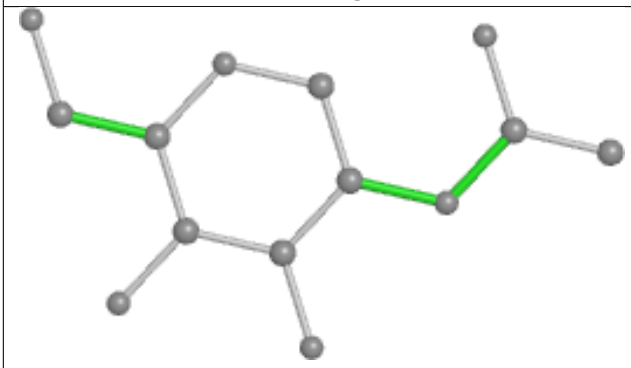
Ligand NAG B 2004



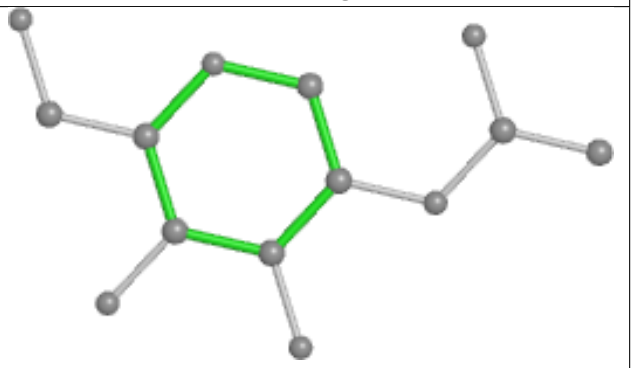
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.