wwPDB EM Validation Summary Report

Oct 22, 2024 – 12:36 AM JST

PDB ID	:	8WLO
EMDB ID	:	EMD-37626
Title	:	Cryo-EM structure of SARS-CoV-2 prototype spike protein in complex with hippopotamus ACE2
Authors	:	Han, P.; Yang, R.R.; Li, S.H.
Deposited on	:	2023-09-30
Resolution	:	2.62 Å(reported)

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

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

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

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

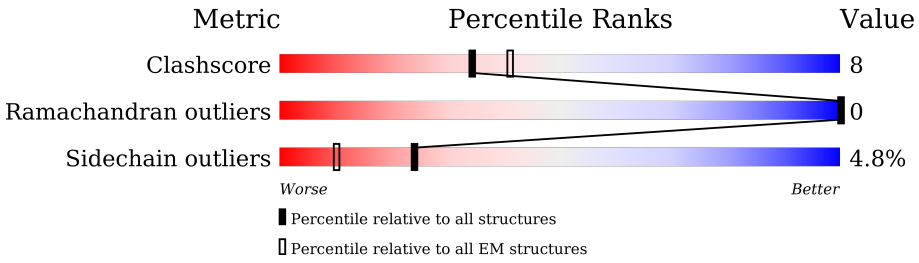
EMDB validation analysis	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.62 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	1217	73% 13% • 13%
1	B	1217	68% 17% • 13%
1	C	1217	69% 18% • 12%
2	E	597	74% 24% •
3	D	2	100%
3	F	2	100%
3	G	2	100%
3	H	2	50% 50%
3	I	2	100%

Continued on next page...

Continued from previous page...

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

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 30464 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1061	Total	C	N	O	S	0	0
			8290	5290	1383	1580	37		
1	B	1061	Total	C	N	O	S	0	0
			8292	5292	1383	1579	38		
1	C	1065	Total	C	N	O	S	0	0
			8322	5312	1388	1584	38		

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	682	GLY	ARG	engineered mutation	UNP P0DTC2
A	683	SER	ARG	engineered mutation	UNP P0DTC2
A	685	SER	ARG	engineered mutation	UNP P0DTC2
A	817	PRO	PHE	engineered mutation	UNP P0DTC2
A	892	PRO	ALA	engineered mutation	UNP P0DTC2
A	899	PRO	ALA	engineered mutation	UNP P0DTC2
A	942	PRO	ALA	engineered mutation	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	682	GLY	ARG	engineered mutation	UNP P0DTC2
B	683	SER	ARG	engineered mutation	UNP P0DTC2
B	685	SER	ARG	engineered mutation	UNP P0DTC2
B	817	PRO	PHE	engineered mutation	UNP P0DTC2
B	892	PRO	ALA	engineered mutation	UNP P0DTC2
B	899	PRO	ALA	engineered mutation	UNP P0DTC2
B	942	PRO	ALA	engineered mutation	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	682	GLY	ARG	engineered mutation	UNP P0DTC2
C	683	SER	ARG	engineered mutation	UNP P0DTC2
C	685	SER	ARG	engineered mutation	UNP P0DTC2
C	817	PRO	PHE	engineered mutation	UNP P0DTC2
C	892	PRO	ALA	engineered mutation	UNP P0DTC2
C	899	PRO	ALA	engineered mutation	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	942	PRO	ALA	engineered mutation	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2

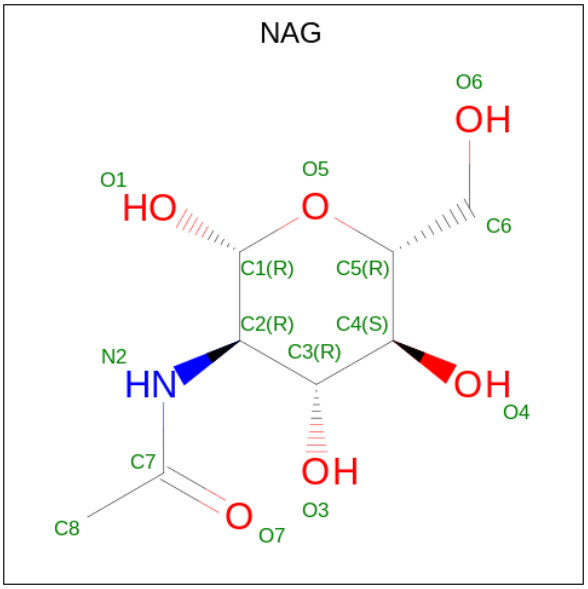
- Molecule 2 is a protein called Angiotensin-converting enzyme.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	597	Total	C	N	O	S	0	0
			4873	3110	805	929	29		

- 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	D	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	I	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	N	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		

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



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

Continued on next page...

Continued from previous page...

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

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

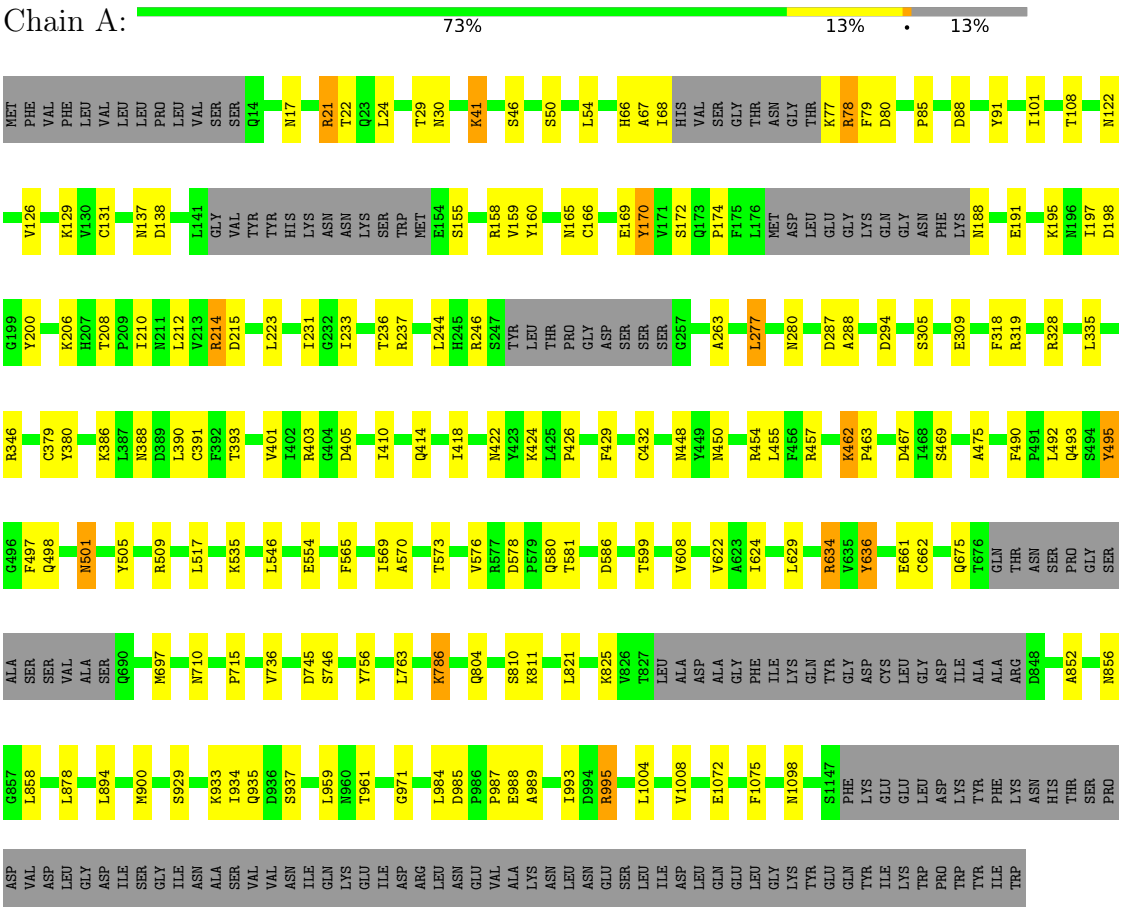
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
5	E	1	1	1	0

3 Residue-property plots (i)

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

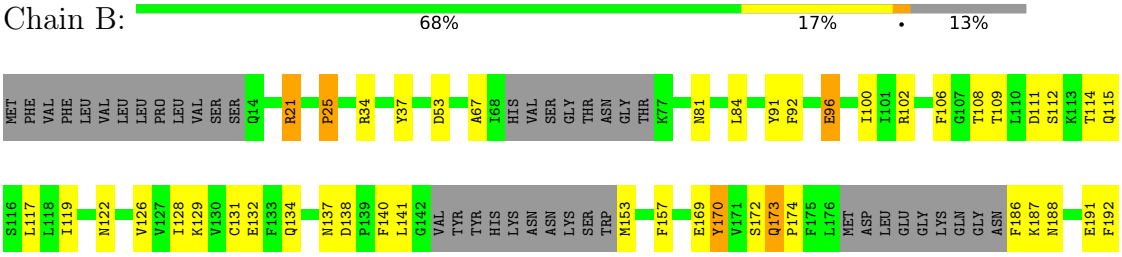
- Molecule 1: Spike glycoprotein

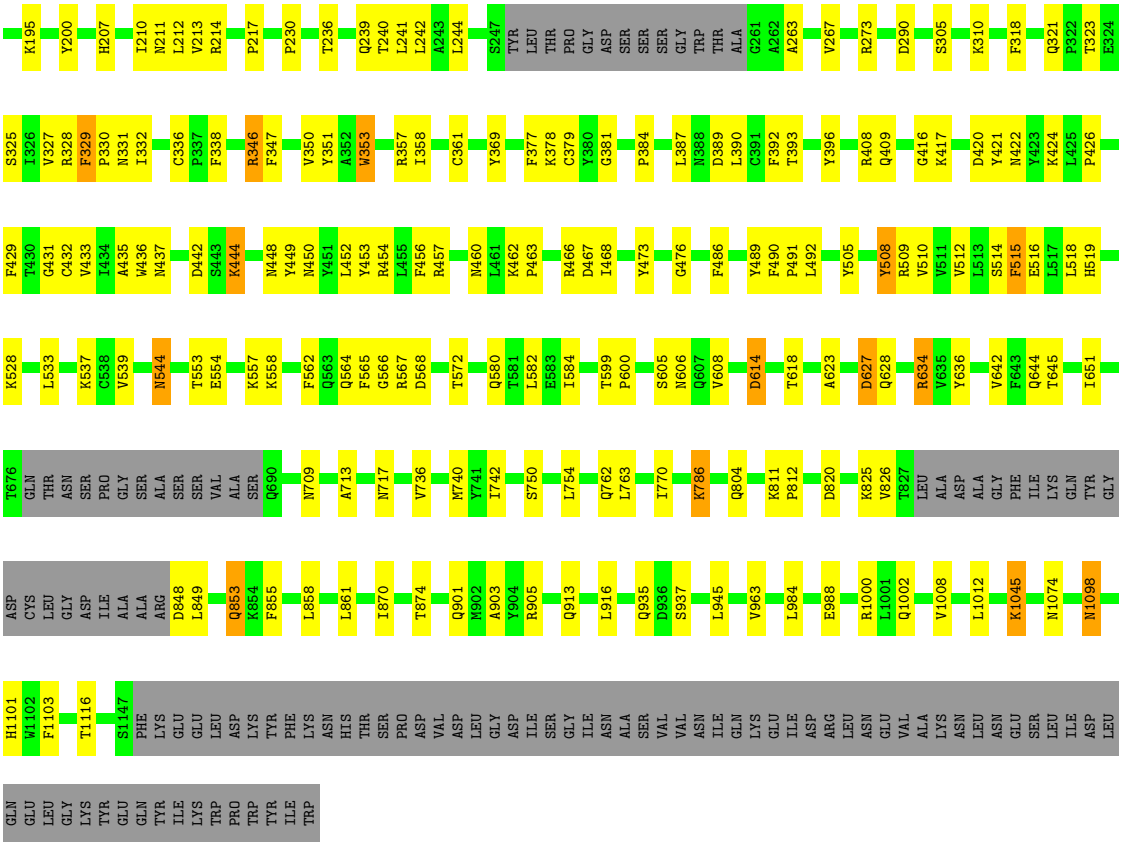
Chain A:



- Molecule 1: Spike glycoprotein

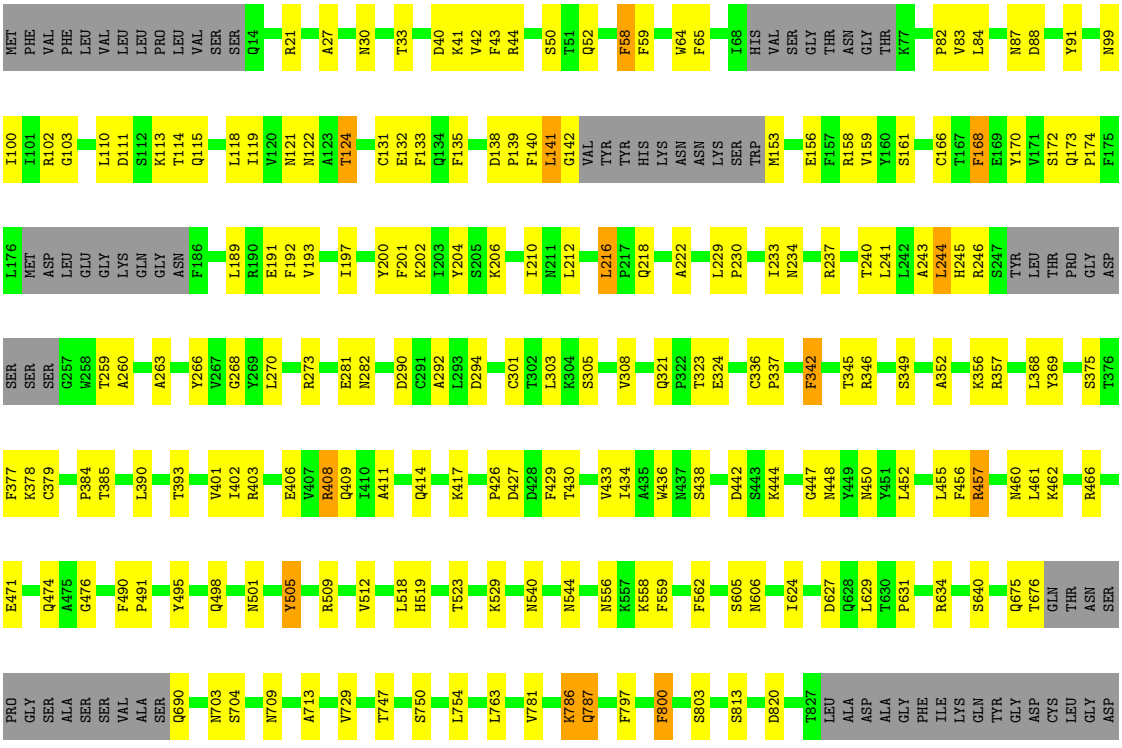
Chain B:

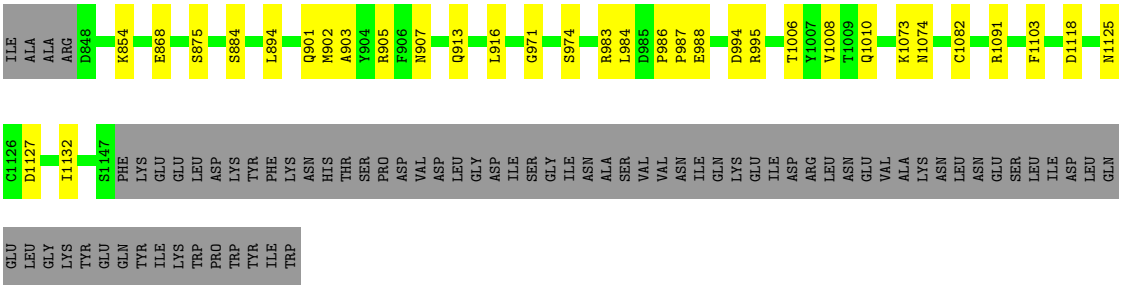




• Molecule 1: Spike glycoprotein

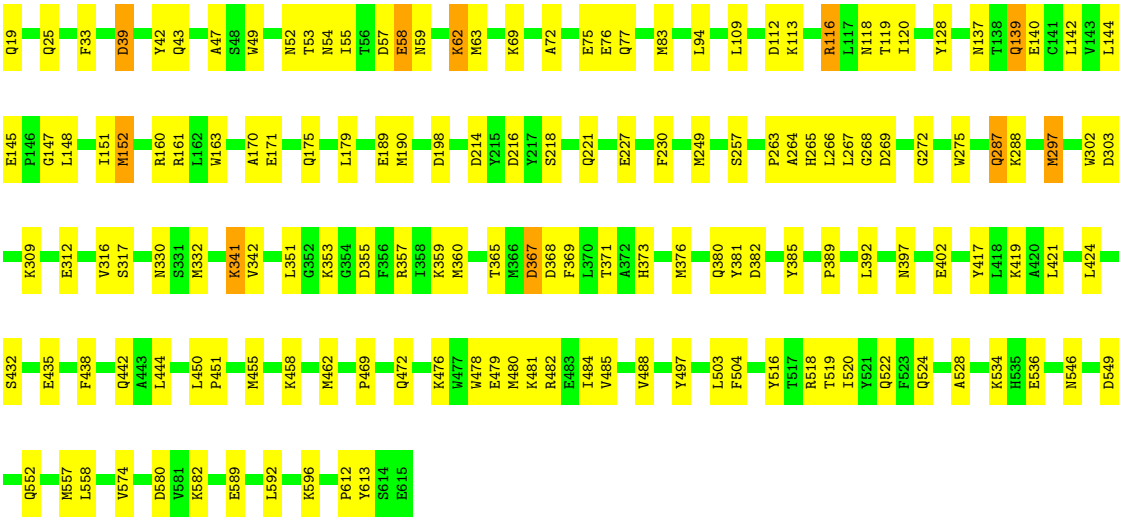
Chain C:





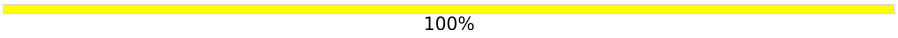
• Molecule 2: Angiotensin-converting enzyme

Chain E:



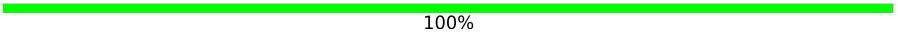
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:



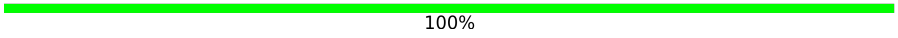
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:



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

Chain G:

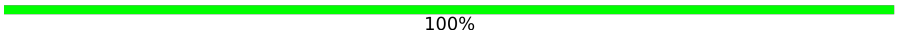


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:

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

Chain I:



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

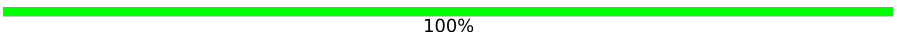
Chain J:

• 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 N:

• 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:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	227185	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 ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	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: NAG, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.26	0/8483	0.50	0/11556
1	B	0.29	1/8484 (0.0%)	0.54	5/11553 (0.0%)
1	C	0.26	0/8516	0.51	0/11598
2	E	0.26	0/5007	0.51	1/6793 (0.0%)
All	All	0.27	1/30490 (0.0%)	0.51	6/41500 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	384	PRO	CG-CD	-6.06	1.30	1.50

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	384	PRO	CA-N-CD	-12.36	94.20	111.50
1	B	384	PRO	N-CD-CG	-8.94	89.79	103.20
1	B	25	PRO	CA-N-CD	-7.01	101.68	111.50
1	B	614	ASP	CB-CG-OD2	5.12	122.91	118.30
2	E	216	ASP	CB-CG-OD1	5.09	122.88	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8290	0	8084	106	0
1	B	8292	0	8089	142	0
1	C	8322	0	8120	133	0
2	E	4873	0	4641	99	0
3	D	28	0	25	1	0
3	F	28	0	25	0	0
3	G	28	0	25	0	0
3	H	28	0	25	1	0
3	I	28	0	25	0	0
3	J	28	0	25	1	0
3	K	28	0	25	3	0
3	L	28	0	25	0	0
3	M	28	0	25	1	0
3	N	28	0	25	1	0
3	O	28	0	25	2	0
3	P	28	0	25	1	0
4	A	84	0	78	1	0
4	B	168	0	156	6	0
4	C	98	0	91	3	0
5	E	1	0	0	0	0
All	All	30464	0	29559	473	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 8.

The worst 5 of 473 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:498:GLN:H	1:A:501:ASN:HD21	1.22	0.88
1:B:396:TYR:HB2	1:B:514:SER:HB3	1.66	0.78
1:A:462:LYS:HE2	1:A:462:LYS:H	1.49	0.77
1:C:110:LEU:HD22	1:C:237:ARG:HH21	1.53	0.73
2:E:128:TYR:HE2	2:E:504:PHE:HA	1.54	0.72

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	1047/1217 (86%)	1023 (98%)	24 (2%)	0	100	100
1	B	1047/1217 (86%)	996 (95%)	51 (5%)	0	100	100
1	C	1051/1217 (86%)	1013 (96%)	38 (4%)	0	100	100
2	E	595/597 (100%)	586 (98%)	9 (2%)	0	100	100
All	All	3740/4248 (88%)	3618 (97%)	122 (3%)	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	930/1065 (87%)	897 (96%)	33 (4%)	31	55
1	B	931/1065 (87%)	880 (94%)	51 (6%)	18	37
1	C	933/1065 (88%)	884 (95%)	49 (5%)	19	38
2	E	526/526 (100%)	501 (95%)	25 (5%)	21	42
All	All	3320/3721 (89%)	3162 (95%)	158 (5%)	24	42

5 of 158 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	471	GLU
2	E	214	ASP
1	C	518	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	875	SER
2	E	367	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 50 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	978	ASN
1	C	501	ASN
2	E	599	ASN
1	C	23	GLN
1	C	314	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

24 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	D	1	3,1	14,14,15	0.27	0	17,19,21	0.54	0
3	NAG	D	2	3	14,14,15	0.27	0	17,19,21	0.41	0
3	NAG	F	1	3,1	14,14,15	0.20	0	17,19,21	0.51	0
3	NAG	F	2	3	14,14,15	0.22	0	17,19,21	0.47	0
3	NAG	G	1	3,1	14,14,15	0.43	0	17,19,21	0.41	0
3	NAG	G	2	3	14,14,15	0.28	0	17,19,21	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	H	1	3,1	14,14,15	0.34	0	17,19,21	0.68	1 (5%)
3	NAG	H	2	3	14,14,15	0.24	0	17,19,21	0.43	0
3	NAG	I	1	3,1	14,14,15	0.23	0	17,19,21	0.59	0
3	NAG	I	2	3	14,14,15	0.27	0	17,19,21	0.37	0
3	NAG	J	1	3,1	14,14,15	0.37	0	17,19,21	0.53	0
3	NAG	J	2	3	14,14,15	0.19	0	17,19,21	0.46	0
3	NAG	K	1	3,1	14,14,15	0.36	0	17,19,21	0.55	0
3	NAG	K	2	3	14,14,15	0.20	0	17,19,21	0.42	0
3	NAG	L	1	3,1	14,14,15	0.27	0	17,19,21	0.57	0
3	NAG	L	2	3	14,14,15	0.20	0	17,19,21	0.45	0
3	NAG	M	1	3,1	14,14,15	0.43	0	17,19,21	1.31	2 (11%)
3	NAG	M	2	3	14,14,15	0.19	0	17,19,21	0.43	0
3	NAG	N	1	3,1	14,14,15	0.28	0	17,19,21	0.48	0
3	NAG	N	2	3	14,14,15	0.25	0	17,19,21	0.43	0
3	NAG	O	1	3,1	14,14,15	0.38	0	17,19,21	1.27	2 (11%)
3	NAG	O	2	3	14,14,15	0.22	0	17,19,21	0.42	0
3	NAG	P	1	3,1	14,14,15	0.94	1 (7%)	17,19,21	1.79	3 (17%)
3	NAG	P	2	3	14,14,15	0.28	0	17,19,21	0.54	0

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

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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	L	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	L	2	3	-	0/6/23/26	0/1/1/1
3	NAG	M	1	3,1	-	5/6/23/26	0/1/1/1
3	NAG	M	2	3	-	0/6/23/26	0/1/1/1
3	NAG	N	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	N	2	3	-	2/6/23/26	0/1/1/1
3	NAG	O	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	O	2	3	-	0/6/23/26	0/1/1/1
3	NAG	P	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	P	2	3	-	3/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	1	NAG	O5-C1	3.13	1.48	1.43

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	P	1	NAG	C1-O5-C5	5.08	119.08	112.19
3	O	1	NAG	C2-N2-C7	4.33	129.06	122.90
3	P	1	NAG	C2-N2-C7	4.32	129.06	122.90
3	M	1	NAG	C2-N2-C7	4.32	129.05	122.90
3	O	1	NAG	C1-C2-N2	2.17	114.19	110.49

There are no chirality outliers.

5 of 47 torsion outliers are listed below:

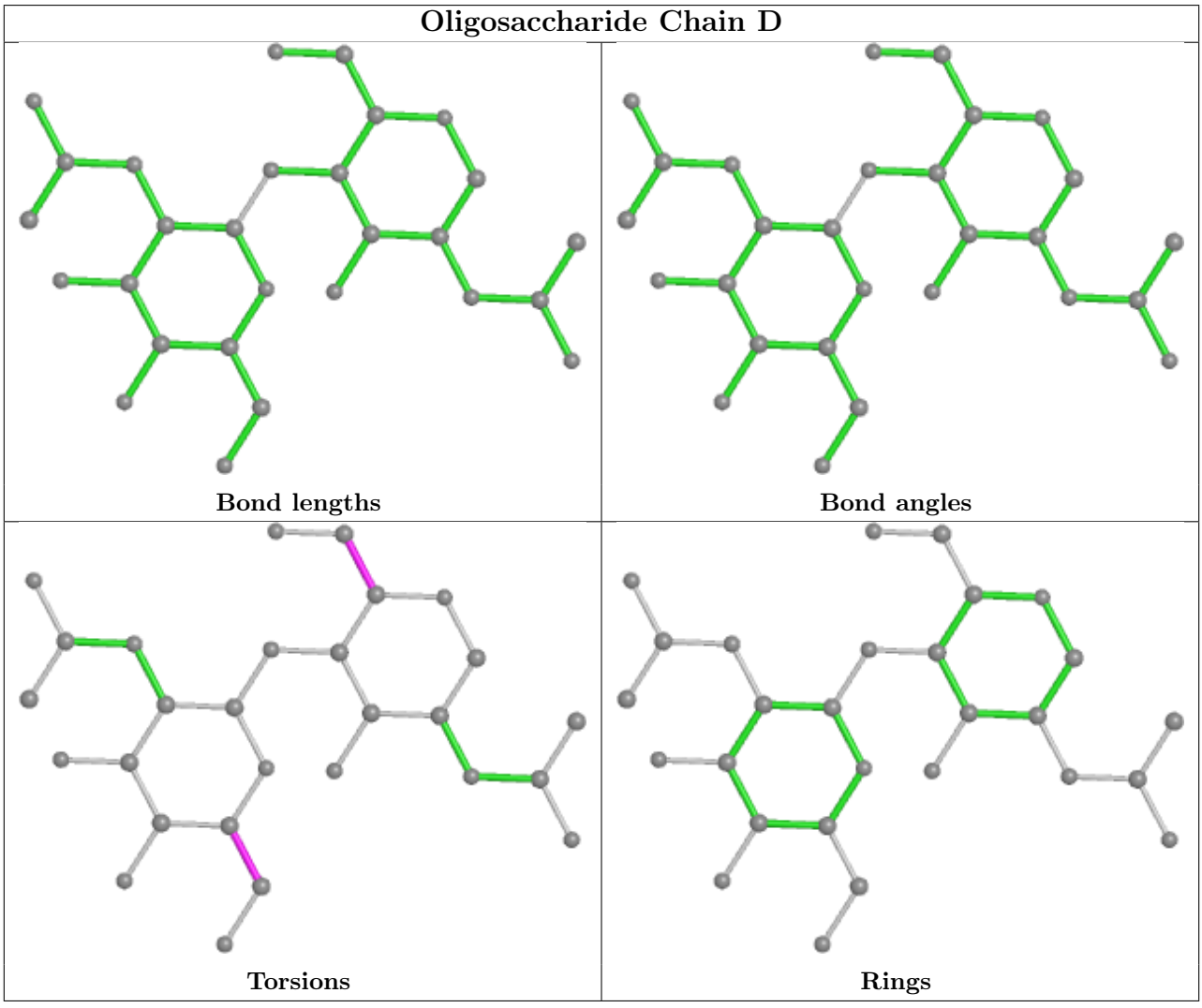
Mol	Chain	Res	Type	Atoms
3	G	2	NAG	C4-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
3	D	1	NAG	C4-C5-C6-O6
3	I	1	NAG	O5-C5-C6-O6
3	N	2	NAG	O5-C5-C6-O6

There are no ring outliers.

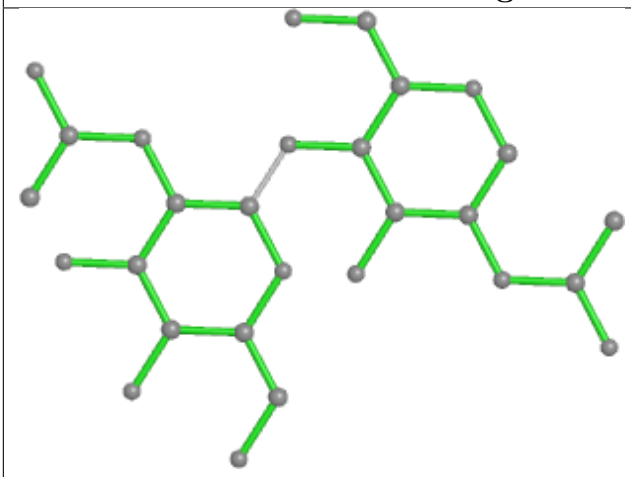
9 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	N	1	NAG	1	0
3	D	1	NAG	1	0
3	J	1	NAG	1	0
3	D	2	NAG	1	0
3	O	1	NAG	2	0
3	H	1	NAG	1	0
3	K	1	NAG	3	0
3	M	1	NAG	1	0
3	P	1	NAG	1	0

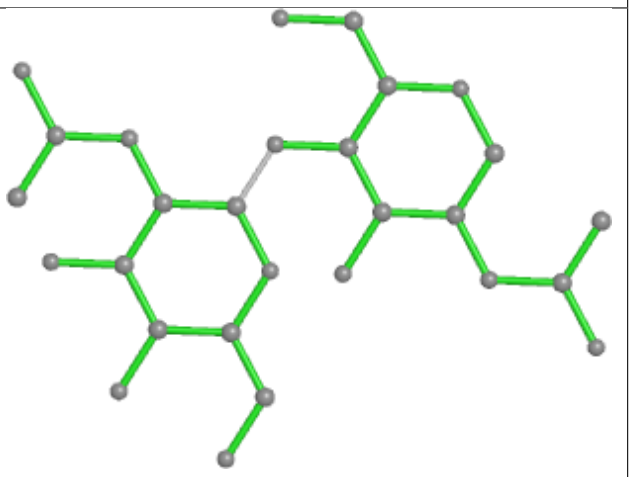
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



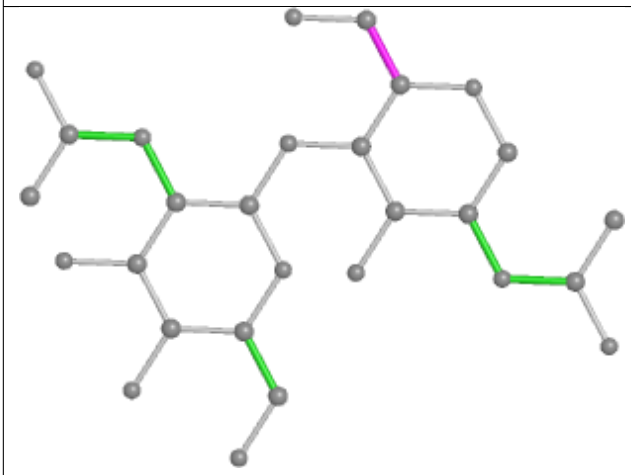
Oligosaccharide Chain F



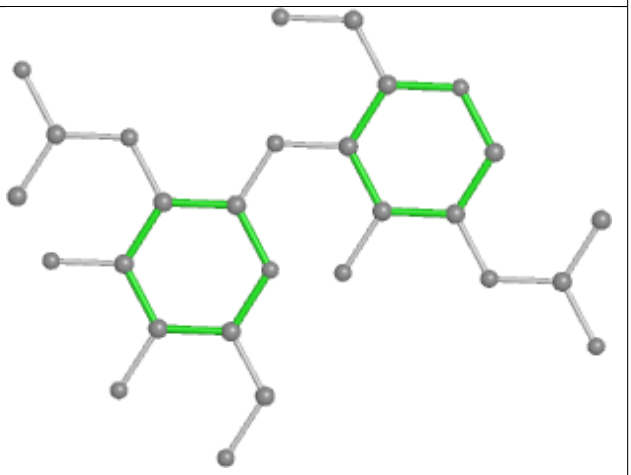
Bond lengths



Bond angles

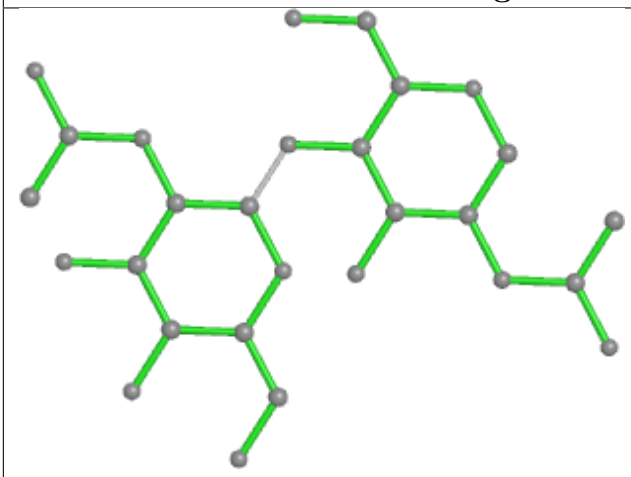


Torsions

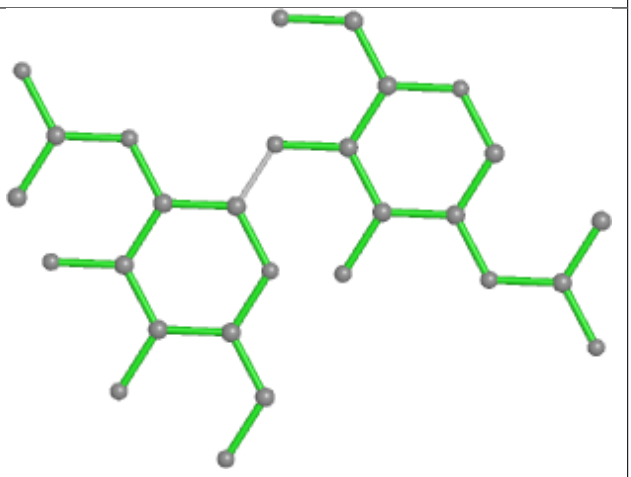


Rings

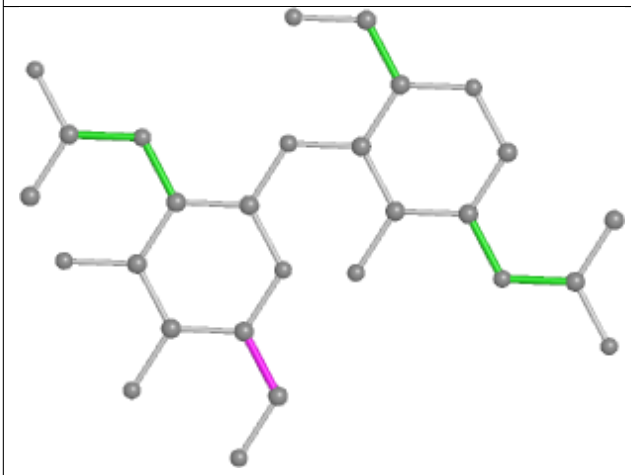
Oligosaccharide Chain G



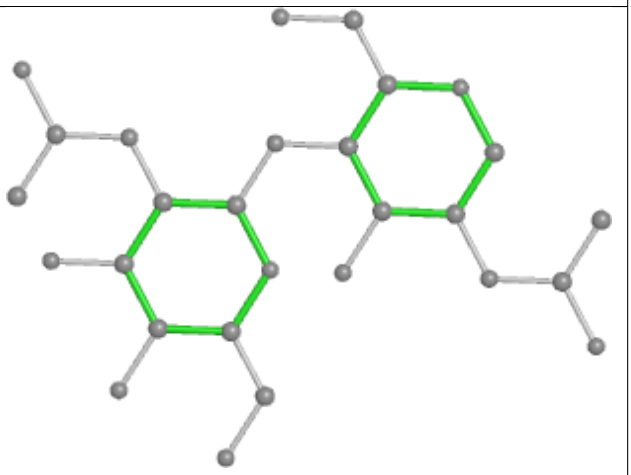
Bond lengths



Bond angles

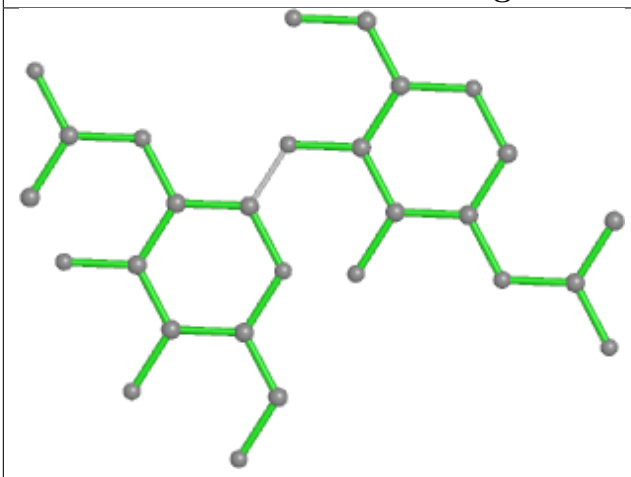


Torsions

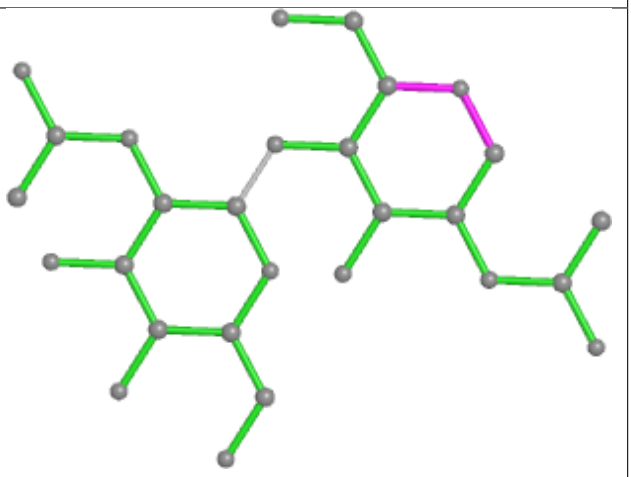


Rings

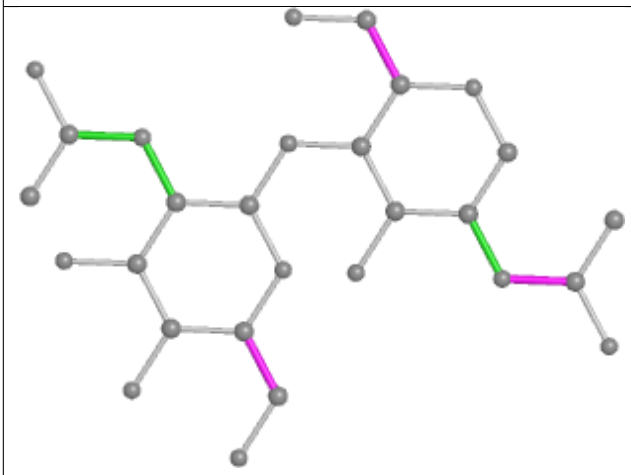
Oligosaccharide Chain H



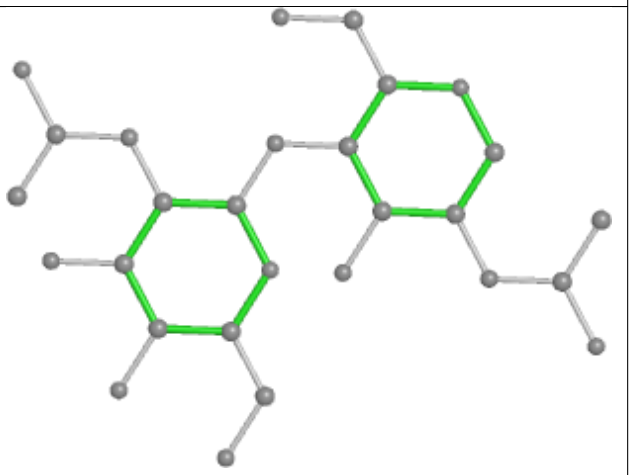
Bond lengths



Bond angles

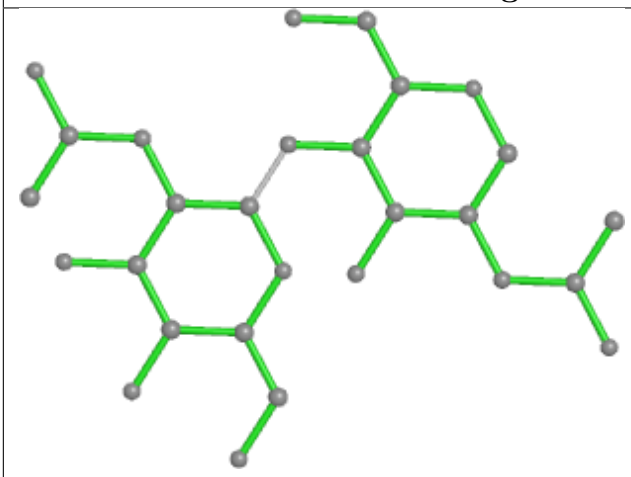


Torsions

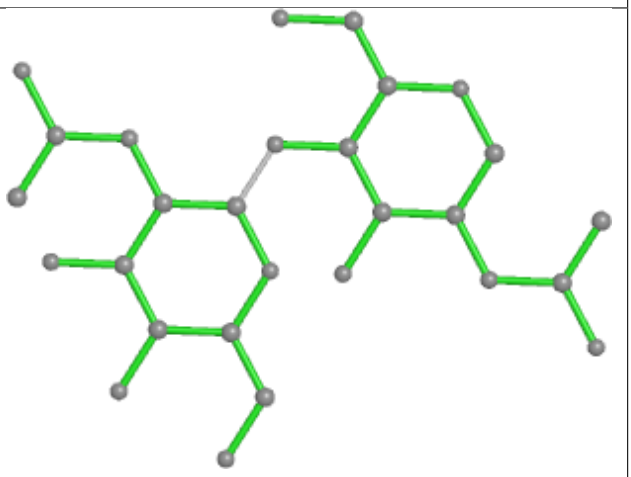


Rings

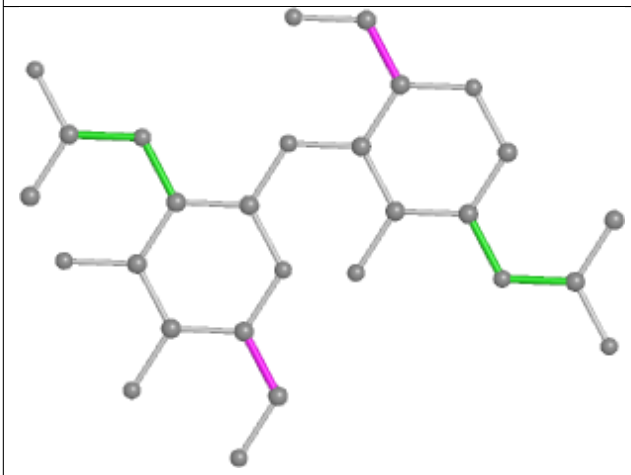
Oligosaccharide Chain I



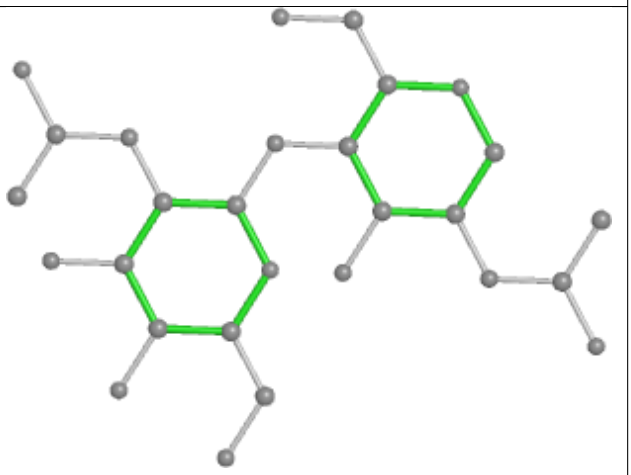
Bond lengths



Bond angles

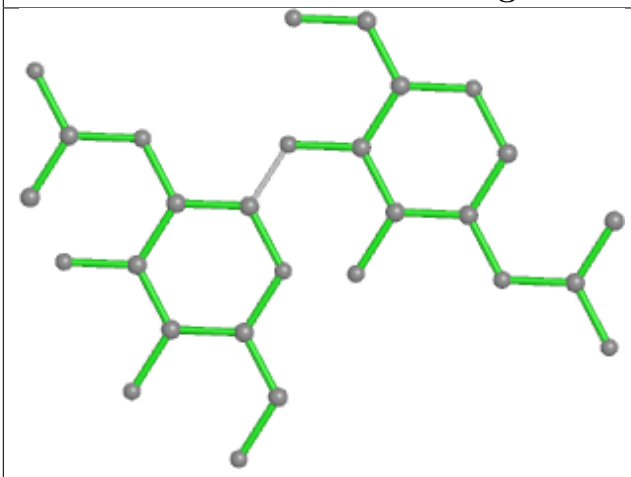


Torsions

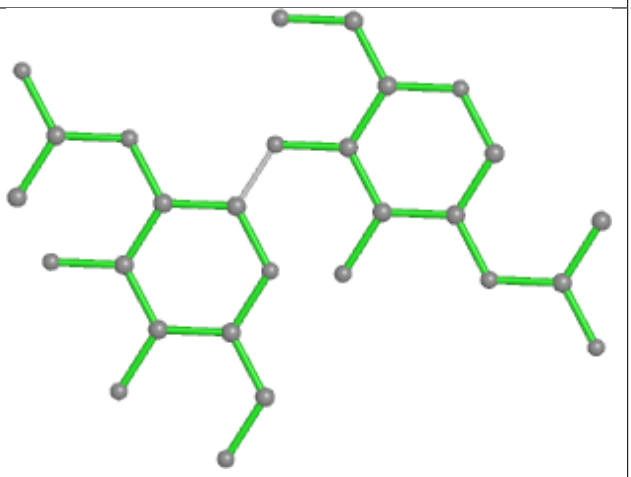


Rings

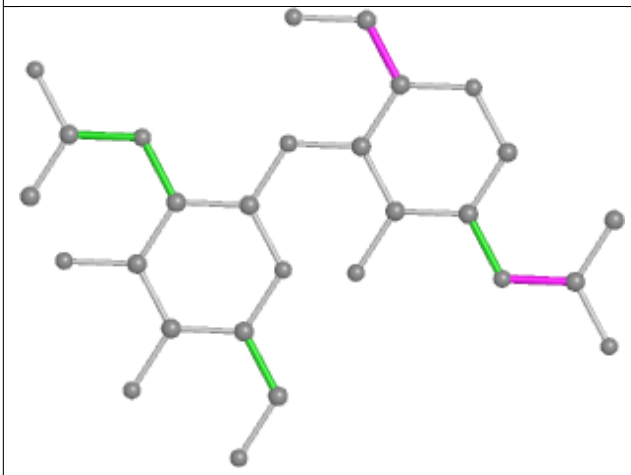
Oligosaccharide Chain J



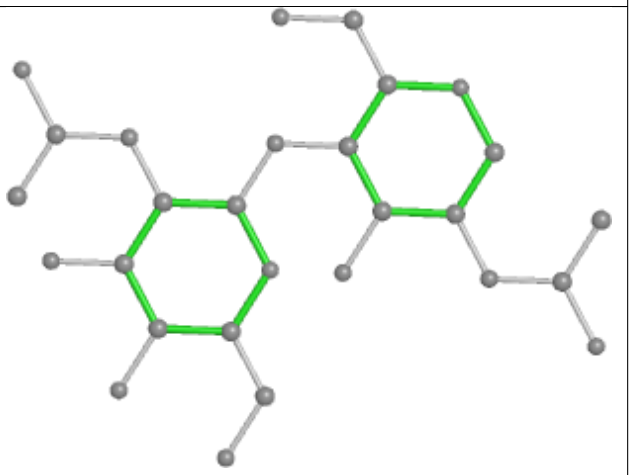
Bond lengths



Bond angles

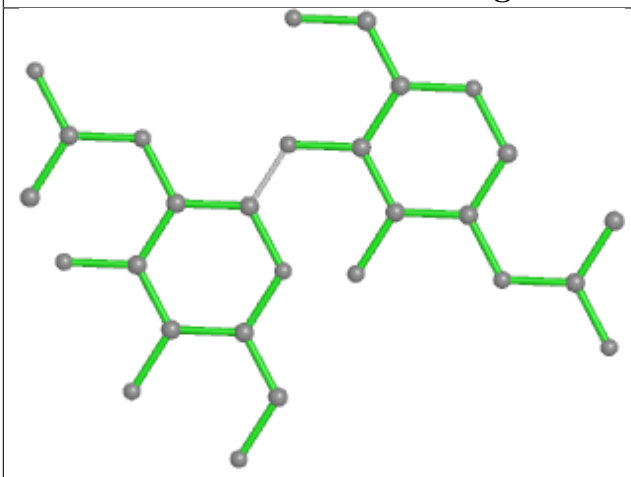


Torsions

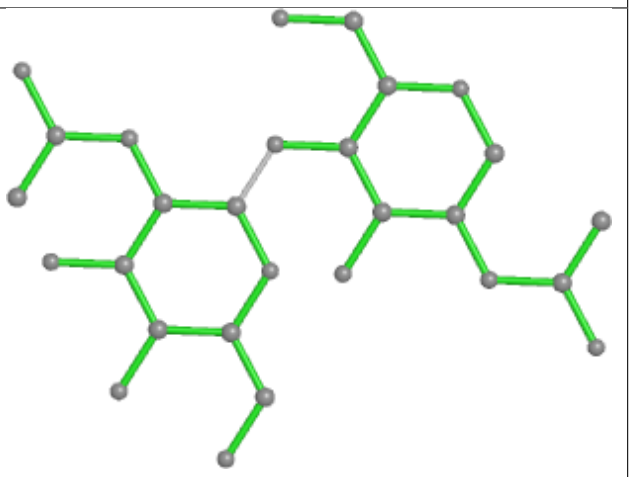


Rings

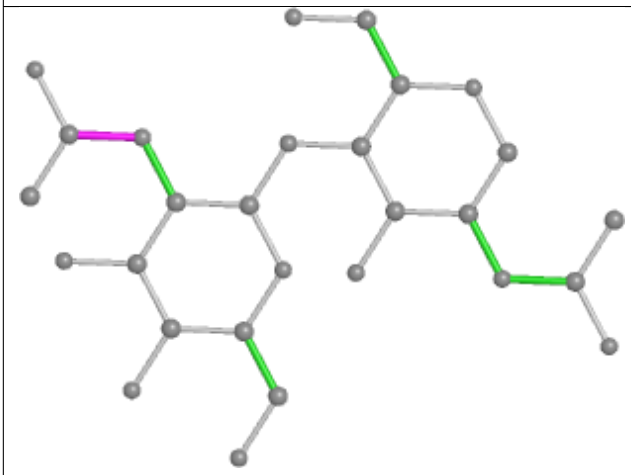
Oligosaccharide Chain K



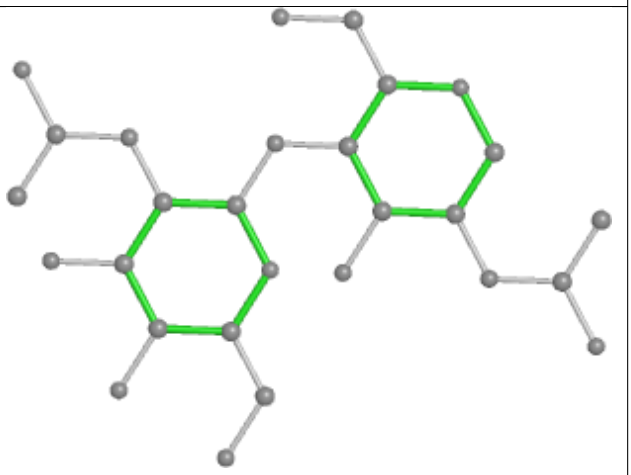
Bond lengths



Bond angles

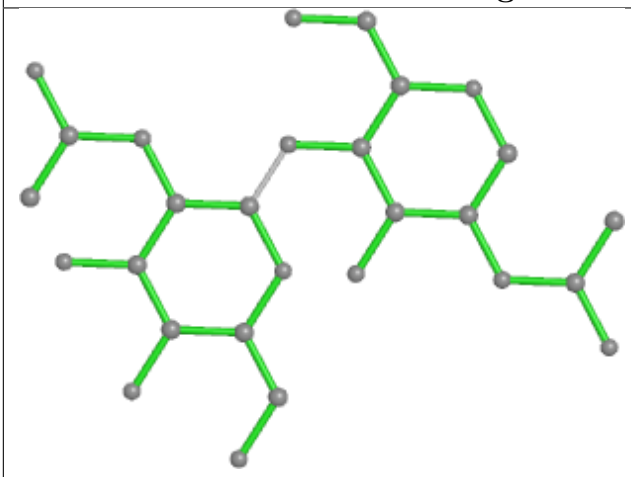


Torsions

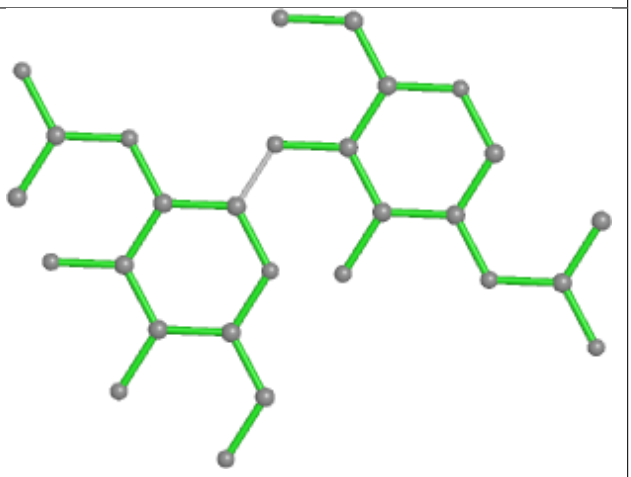


Rings

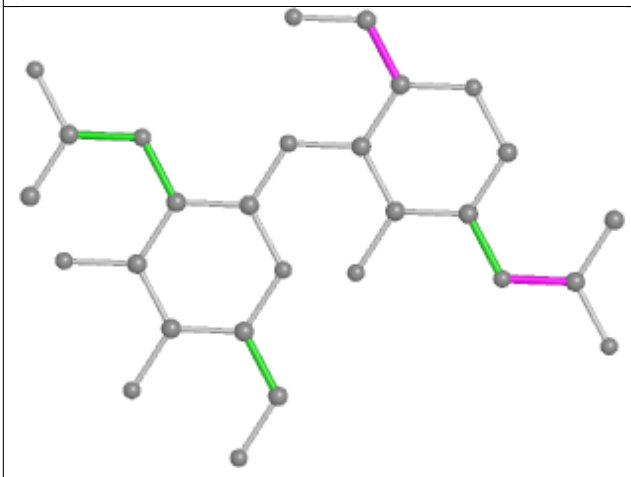
Oligosaccharide Chain L



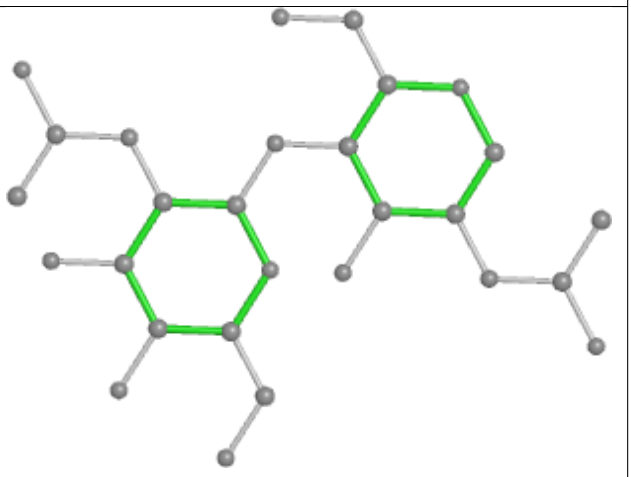
Bond lengths



Bond angles

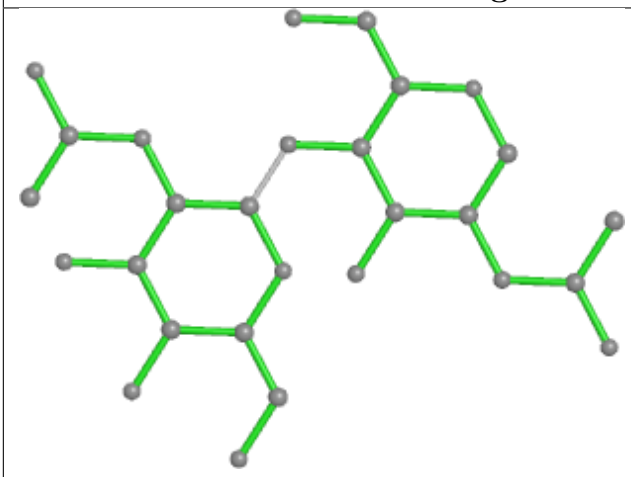


Torsions

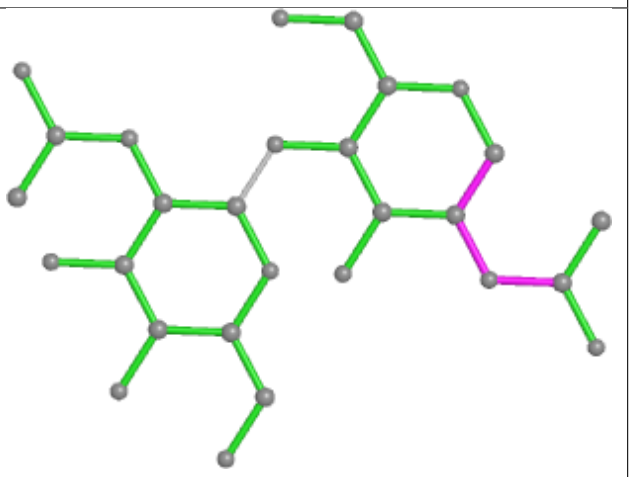


Rings

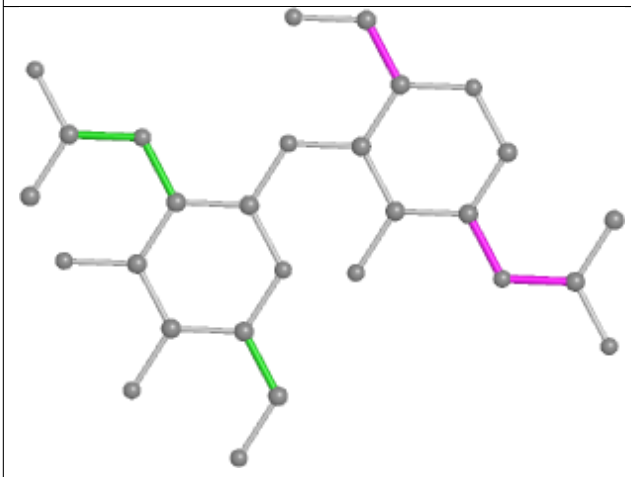
Oligosaccharide Chain M



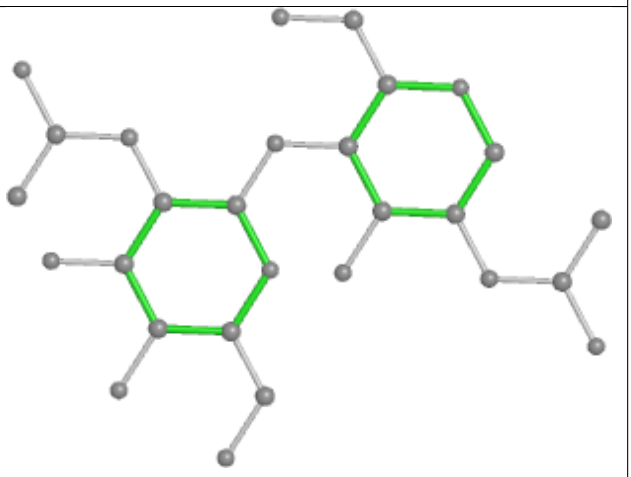
Bond lengths



Bond angles

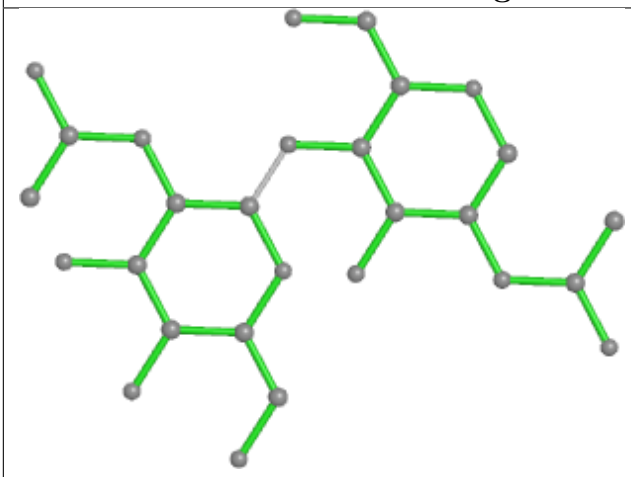


Torsions

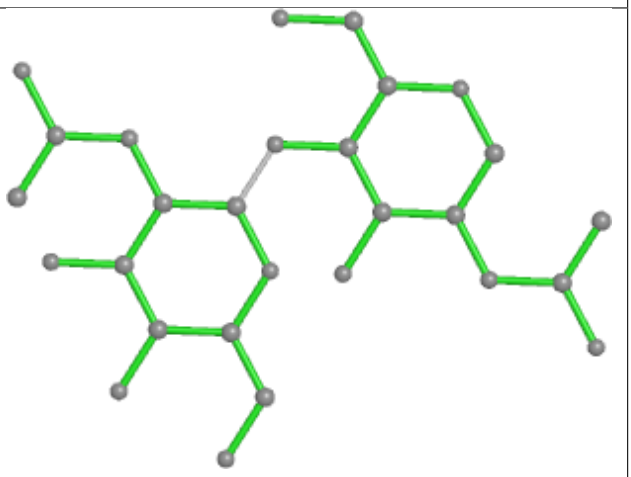


Rings

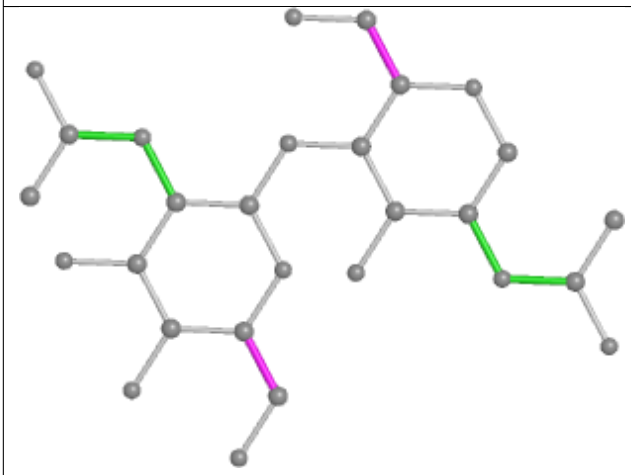
Oligosaccharide Chain N



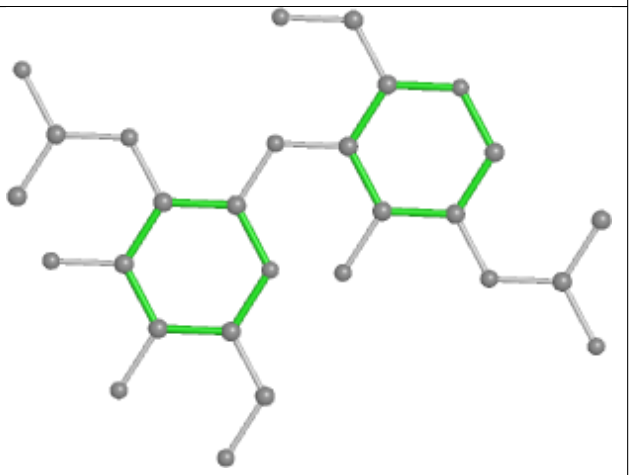
Bond lengths



Bond angles

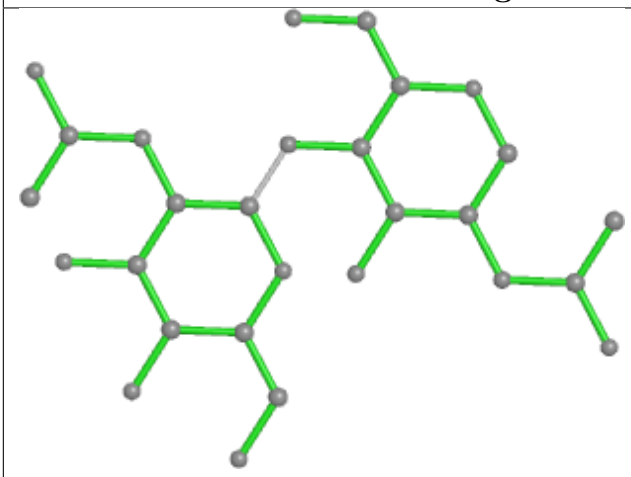


Torsions

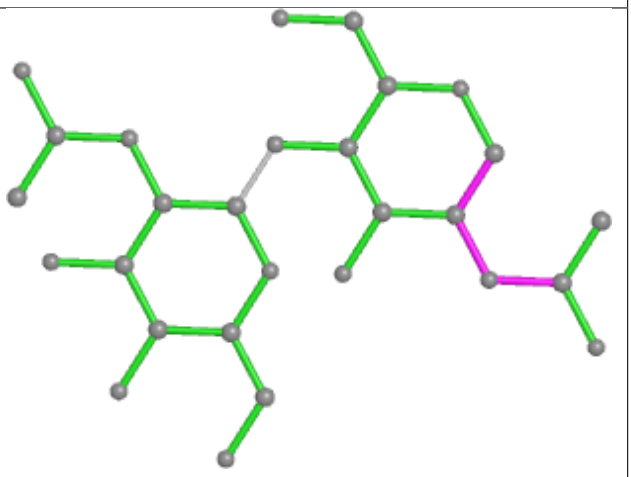


Rings

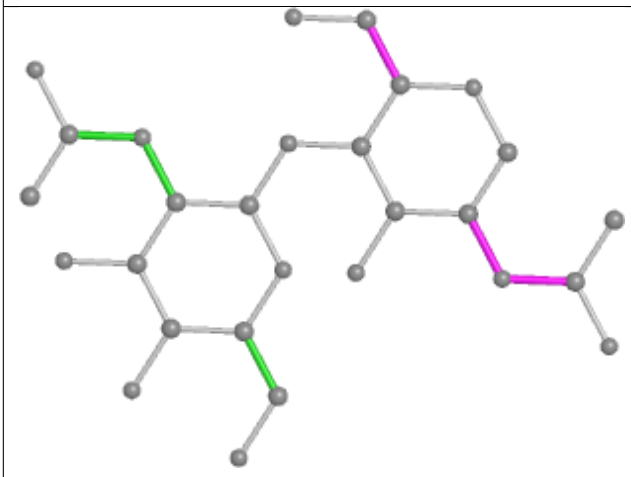
Oligosaccharide Chain O



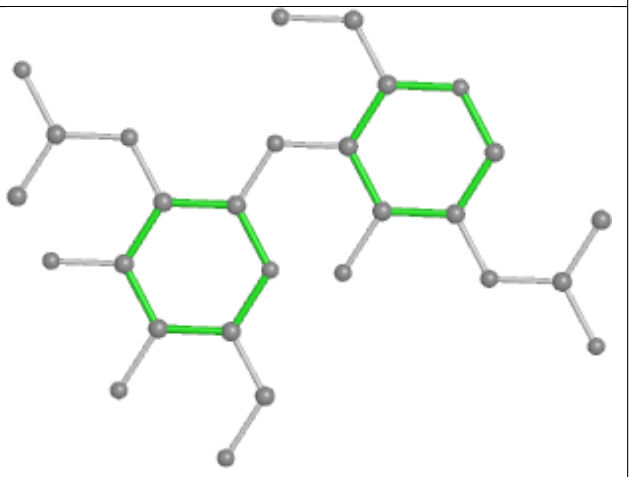
Bond lengths



Bond angles

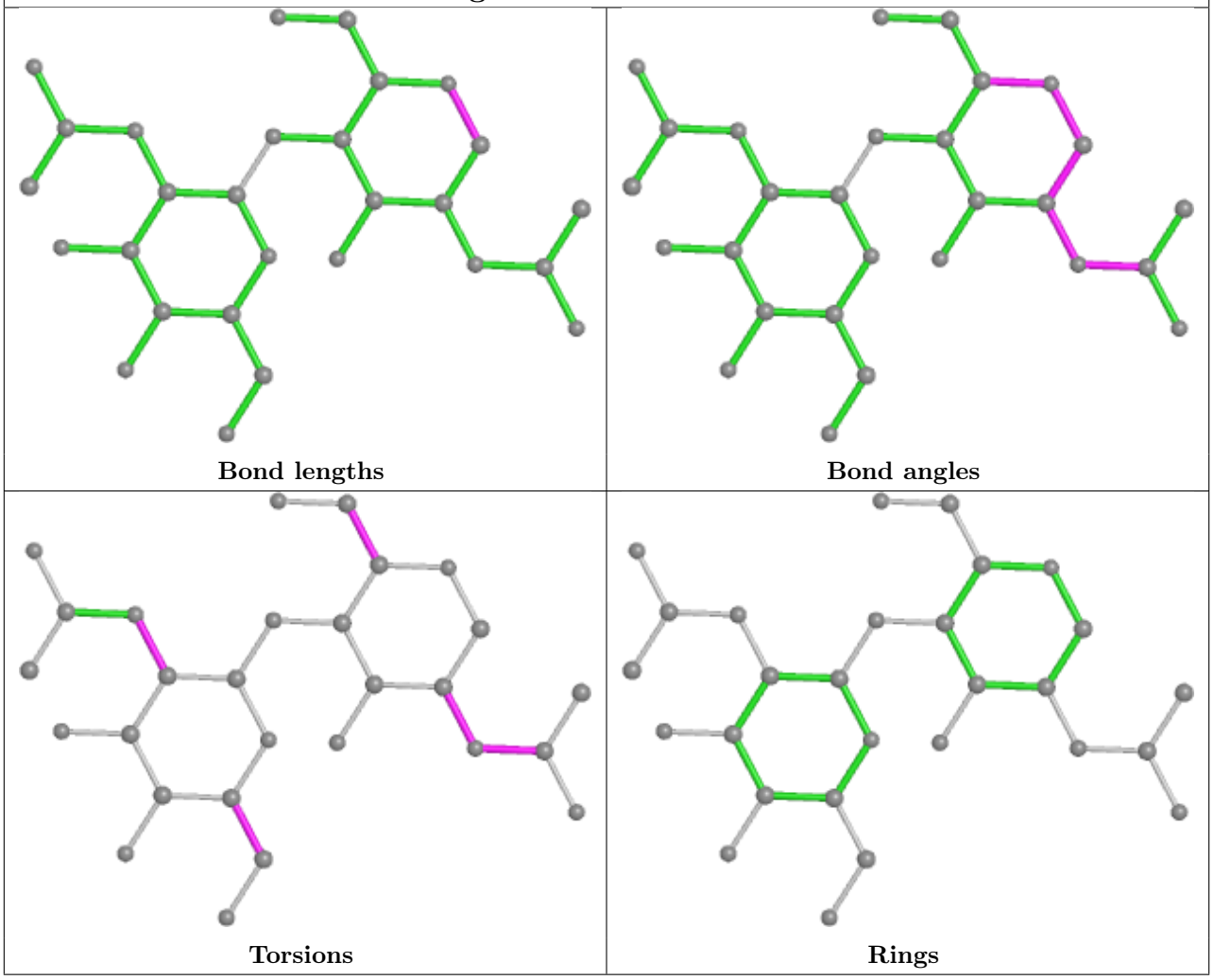


Torsions



Rings

Oligosaccharide Chain P



5.6 Ligand geometry (i)

Of 26 ligands modelled in this entry, 1 is monoatomic - leaving 25 for Mogul analysis.

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	A	1303	1	14,14,15	0.25	0	17,19,21	0.35	0
4	NAG	B	1302	1	14,14,15	0.21	0	17,19,21	0.42	0
4	NAG	B	1308	1	14,14,15	0.28	0	17,19,21	0.35	0
4	NAG	B	1303	1	14,14,15	0.22	0	17,19,21	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	B	1309	1	14,14,15	0.69	1 (7%)	17,19,21	1.25	1 (5%)
4	NAG	B	1311	1	14,14,15	0.45	0	17,19,21	1.27	1 (5%)
4	NAG	C	1303	1	14,14,15	0.24	0	17,19,21	0.42	0
4	NAG	B	1305	1	14,14,15	0.55	0	17,19,21	0.52	0
4	NAG	B	1307	1	14,14,15	0.40	0	17,19,21	0.61	1 (5%)
4	NAG	C	1301	1	14,14,15	0.24	0	17,19,21	0.36	0
4	NAG	A	1305	1	14,14,15	0.19	0	17,19,21	0.34	0
4	NAG	B	1310	1	14,14,15	0.20	0	17,19,21	0.37	0
4	NAG	A	1301	1	14,14,15	0.24	0	17,19,21	0.44	0
4	NAG	B	1304	1	14,14,15	0.44	0	17,19,21	0.39	0
4	NAG	C	1304	1	14,14,15	0.21	0	17,19,21	0.48	0
4	NAG	C	1302	1	14,14,15	0.25	0	17,19,21	0.43	0
4	NAG	A	1302	1	14,14,15	0.83	1 (7%)	17,19,21	1.03	1 (5%)
4	NAG	B	1306	1	14,14,15	0.26	0	17,19,21	0.47	0
4	NAG	B	1301	1	14,14,15	0.20	0	17,19,21	0.49	0
4	NAG	C	1306	1	14,14,15	0.21	0	17,19,21	0.35	0
4	NAG	A	1304	1	14,14,15	0.21	0	17,19,21	0.44	0
4	NAG	A	1306	1	14,14,15	0.23	0	17,19,21	0.45	0
4	NAG	C	1305	1	14,14,15	0.49	0	17,19,21	0.57	0
4	NAG	C	1307	1	14,14,15	0.88	1 (7%)	17,19,21	0.87	1 (5%)
4	NAG	B	1312	1	14,14,15	0.54	0	17,19,21	0.60	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	A	1303	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1302	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1308	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1303	1	-	4/6/23/26	0/1/1/1
4	NAG	B	1309	1	-	3/6/23/26	0/1/1/1
4	NAG	B	1311	1	-	5/6/23/26	0/1/1/1
4	NAG	C	1303	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1305	1	-	4/6/23/26	0/1/1/1
4	NAG	B	1307	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1301	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1305	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1310	1	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1302	NAG	O5-C1	2.68	1.48	1.43
4	C	1307	NAG	O5-C1	2.67	1.48	1.43
4	B	1309	NAG	C1-C2	2.29	1.55	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1311	NAG	C2-N2-C7	4.29	129.00	122.90
4	B	1309	NAG	C2-N2-C7	4.23	128.93	122.90
4	A	1302	NAG	C1-O5-C5	3.86	117.42	112.19
4	C	1307	NAG	C1-O5-C5	3.38	116.77	112.19
4	B	1307	NAG	C1-O5-C5	2.10	115.04	112.19

There are no chirality outliers.

5 of 48 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1302	NAG	C4-C5-C6-O6
4	B	1312	NAG	C4-C5-C6-O6
4	B	1305	NAG	C4-C5-C6-O6
4	B	1312	NAG	O5-C5-C6-O6
4	B	1305	NAG	O5-C5-C6-O6

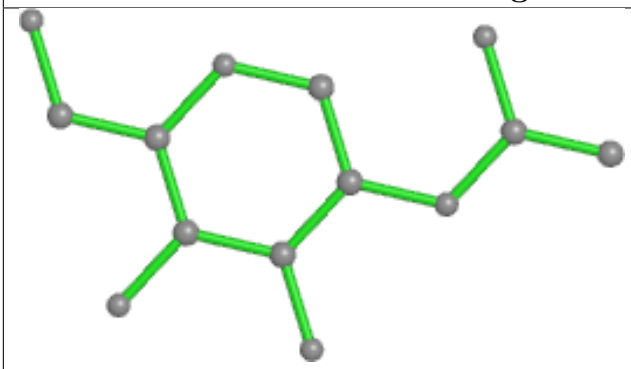
There are no ring outliers.

7 monomers are involved in 10 short contacts:

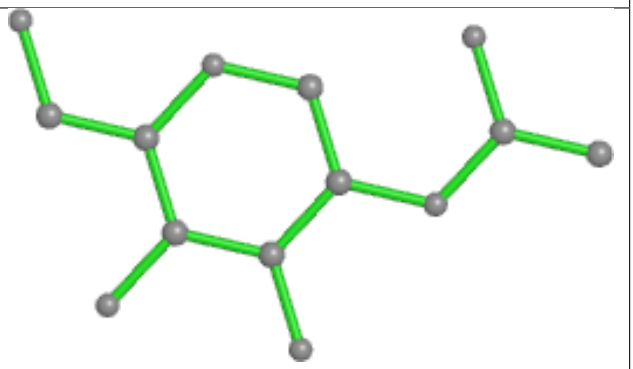
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1309	NAG	3	0
4	B	1311	NAG	1	0
4	C	1303	NAG	2	0
4	B	1305	NAG	1	0
4	B	1307	NAG	1	0
4	A	1306	NAG	1	0
4	C	1305	NAG	1	0

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.

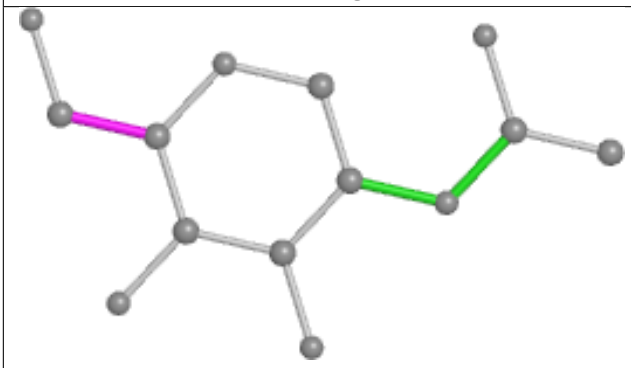
Ligand NAG A 1303



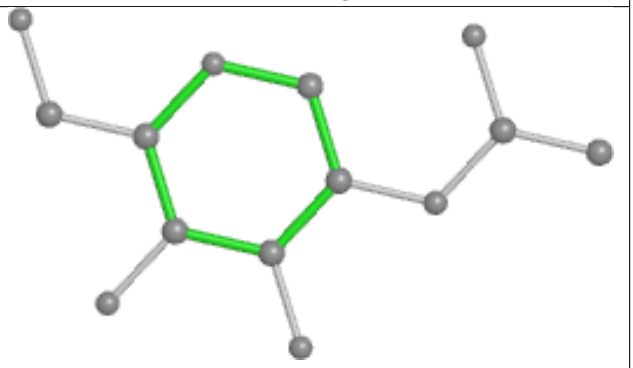
Bond lengths



Bond angles

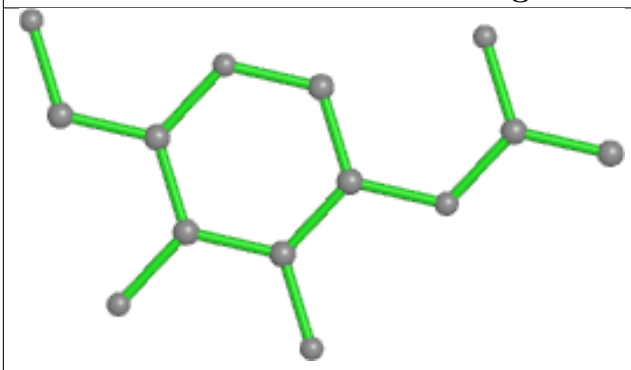


Torsions

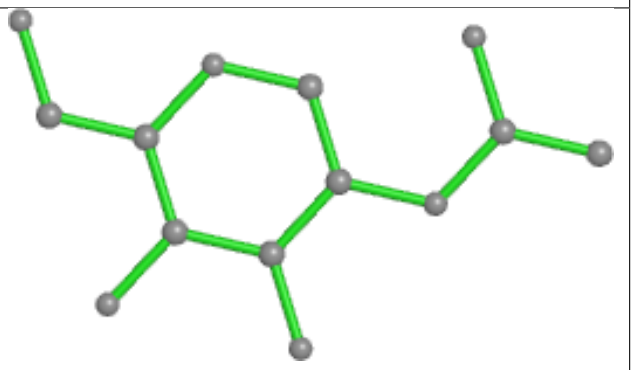


Rings

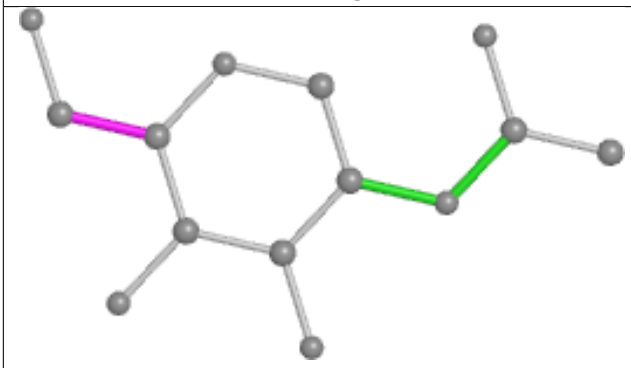
Ligand NAG B 1302



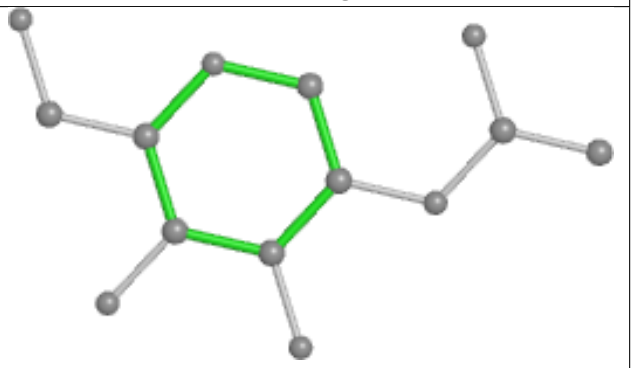
Bond lengths



Bond angles

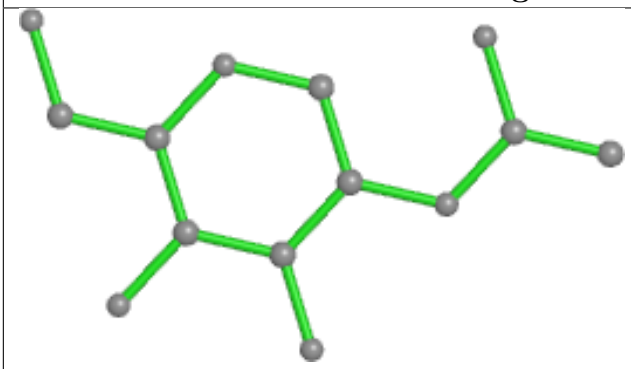


Torsions

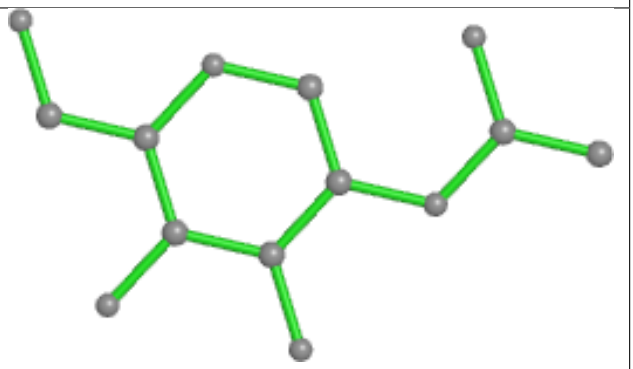


Rings

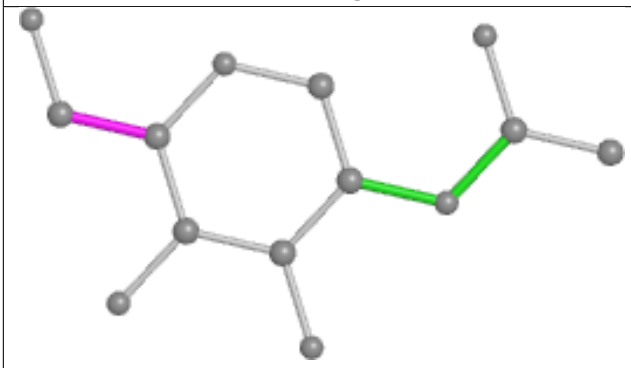
Ligand NAG B 1308



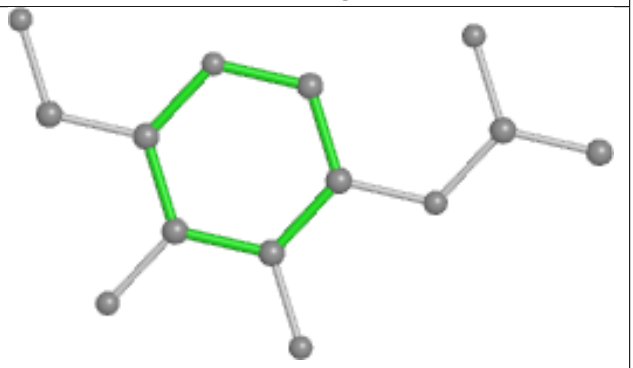
Bond lengths



Bond angles

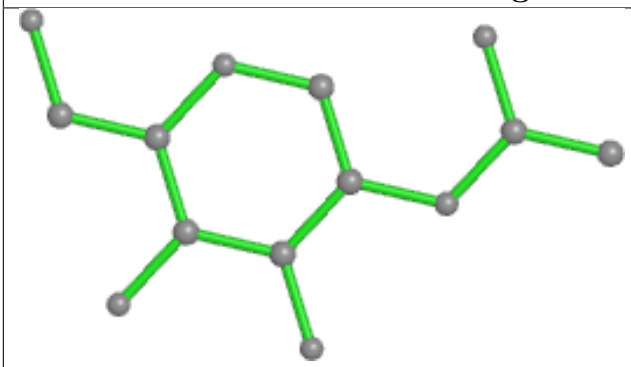


Torsions

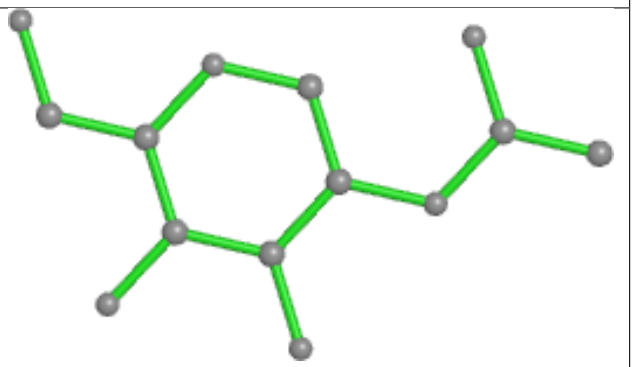


Rings

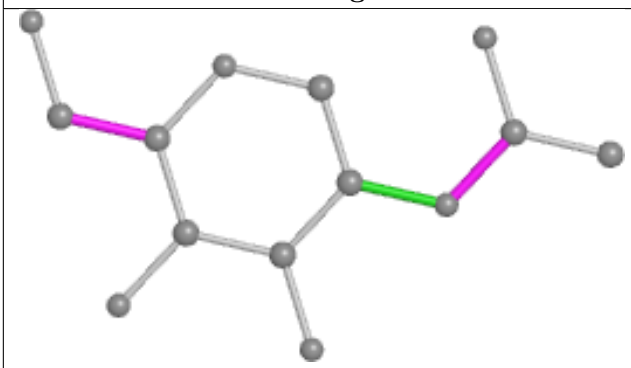
Ligand NAG B 1303



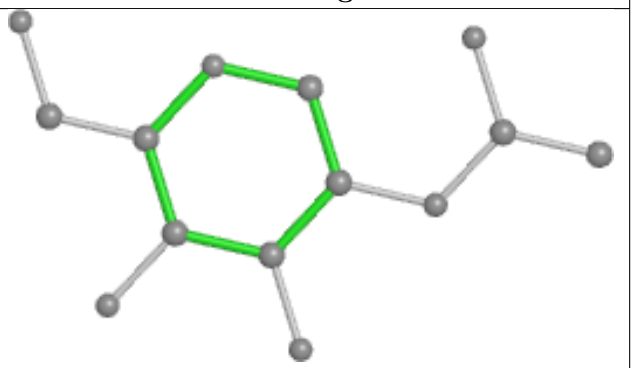
Bond lengths



Bond angles

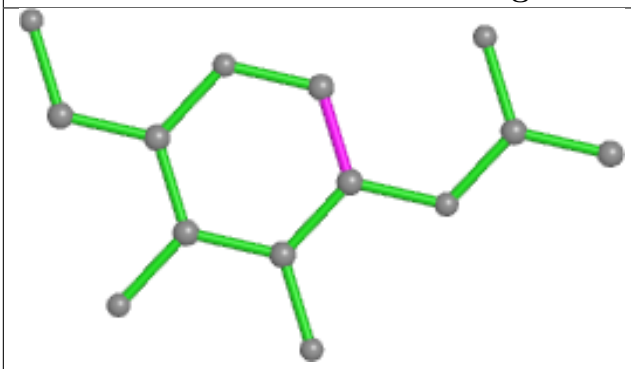


Torsions

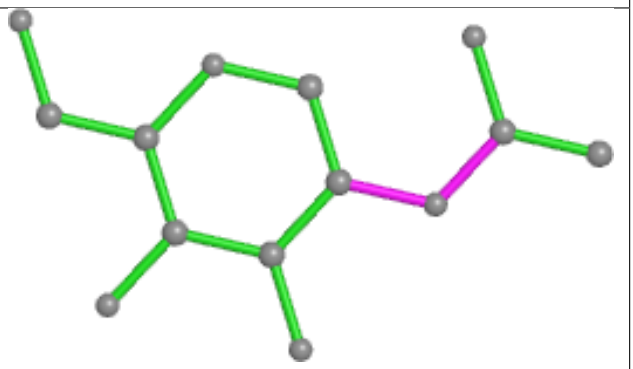


Rings

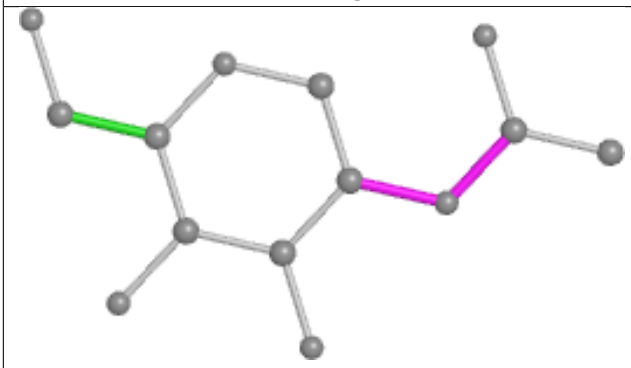
Ligand NAG B 1309



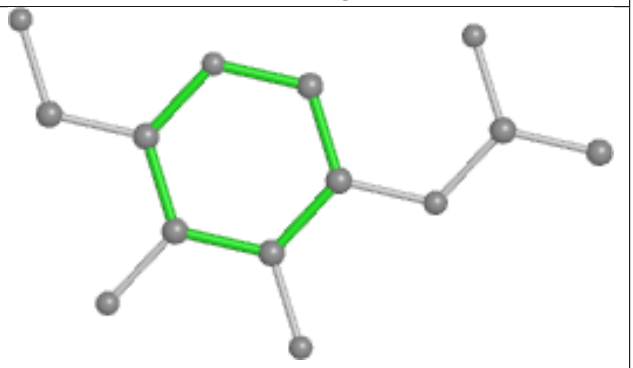
Bond lengths



Bond angles

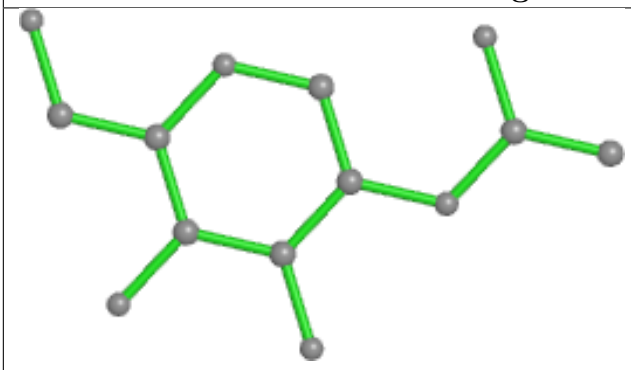


Torsions

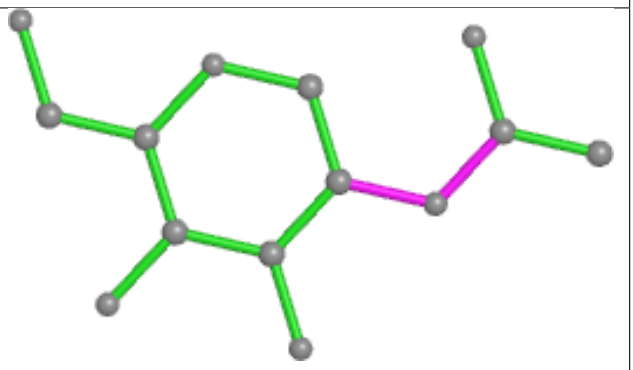


Rings

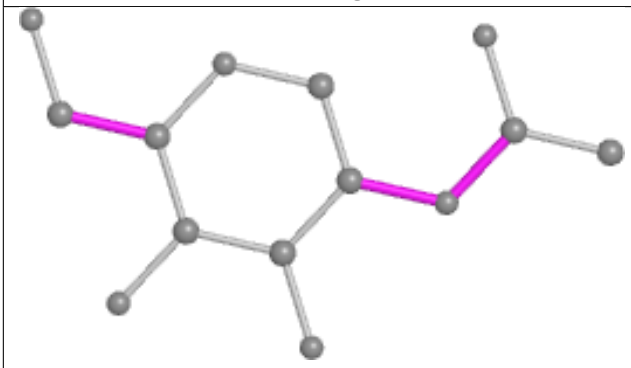
Ligand NAG B 1311



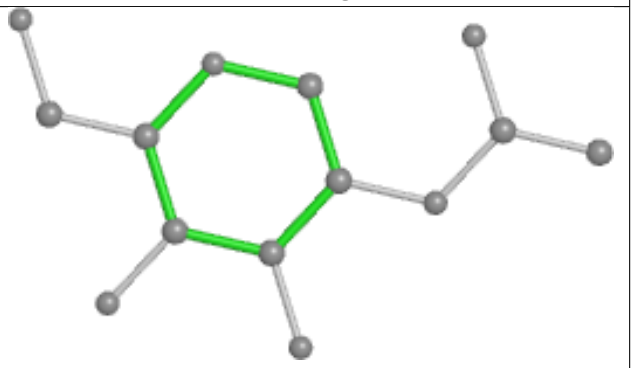
Bond lengths



Bond angles

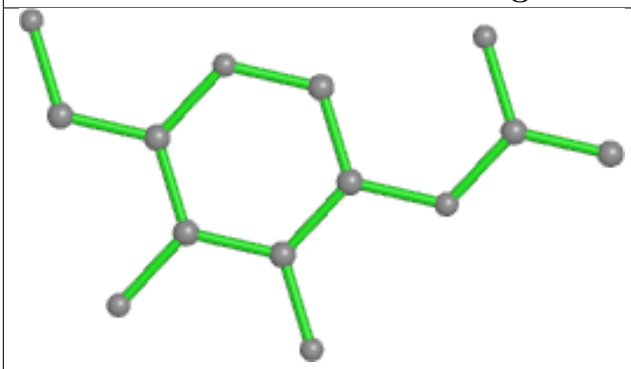


Torsions

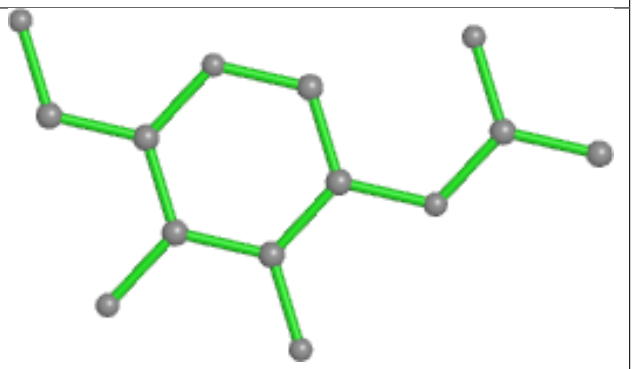


Rings

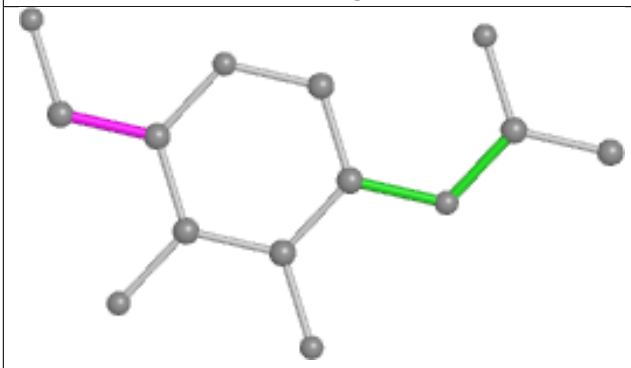
Ligand NAG C 1303



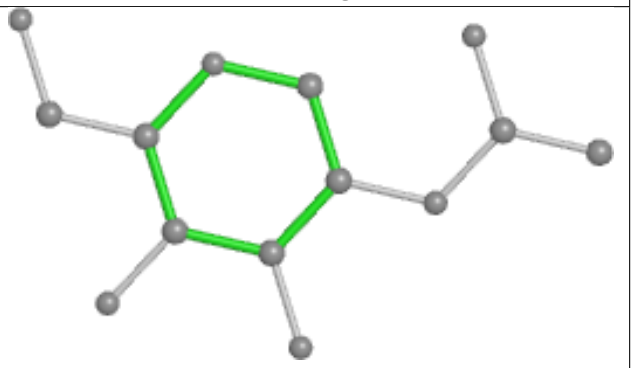
Bond lengths



Bond angles

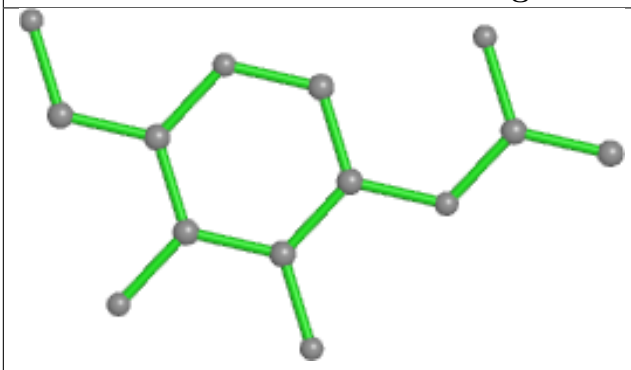


Torsions

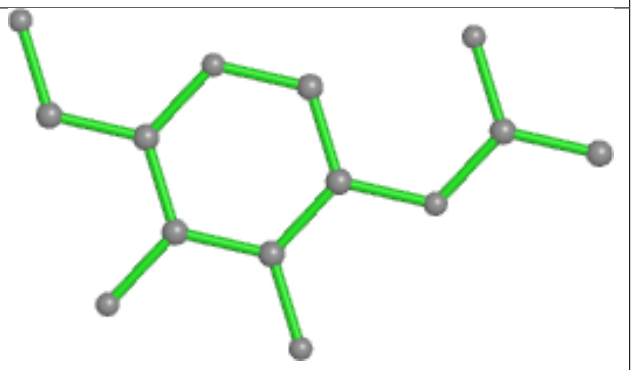


Rings

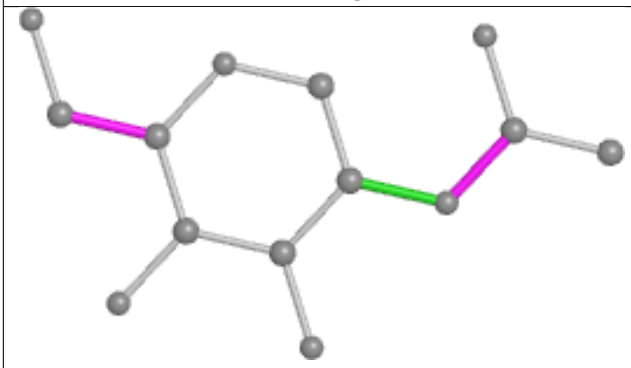
Ligand NAG B 1305



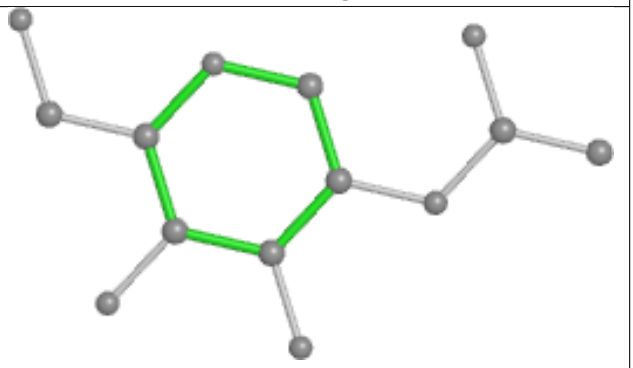
Bond lengths



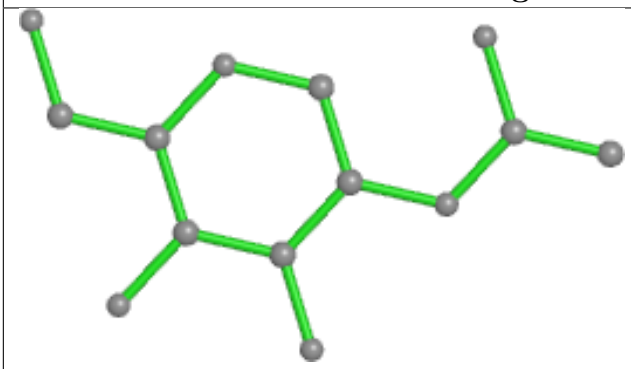
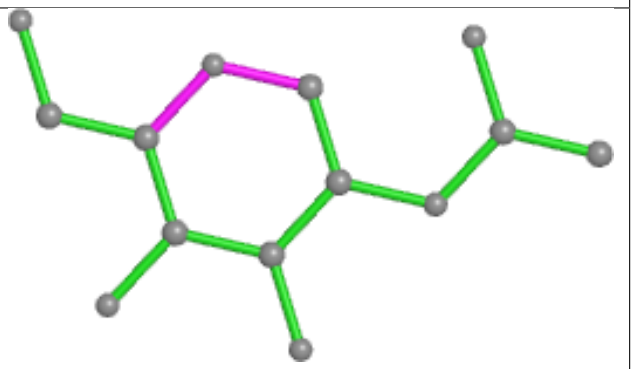
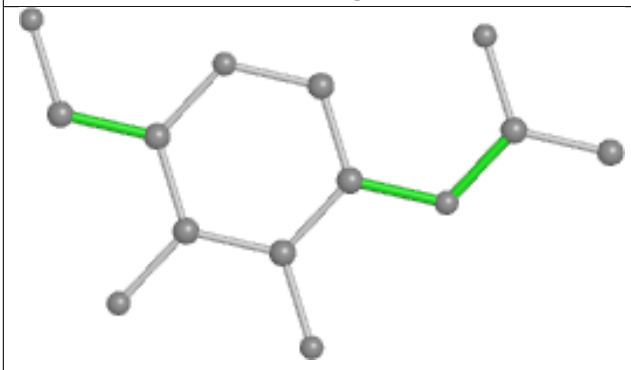
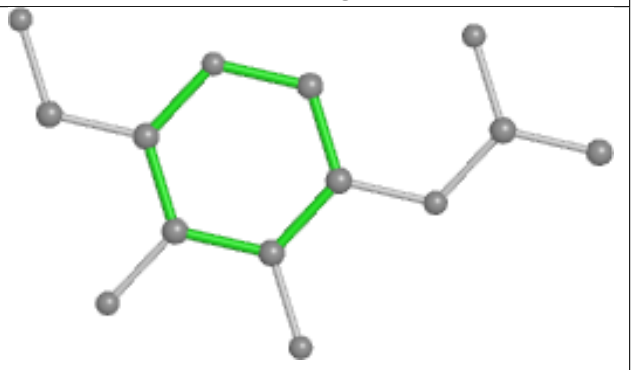
Bond angles

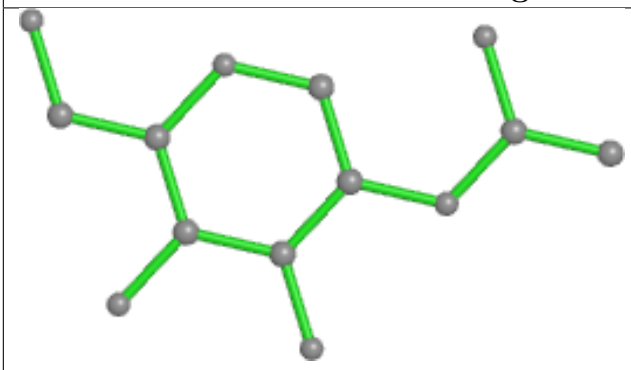
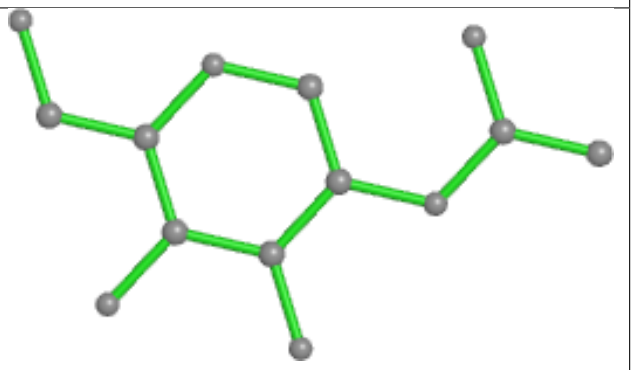
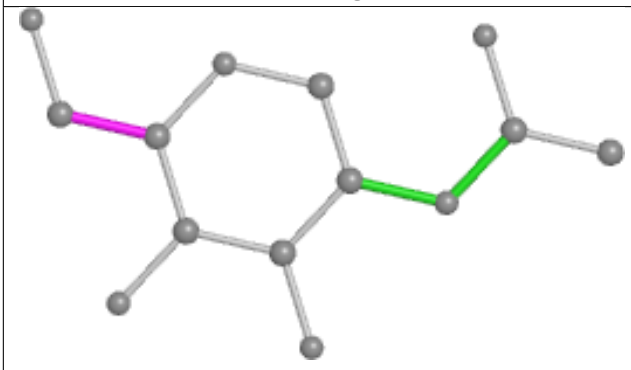
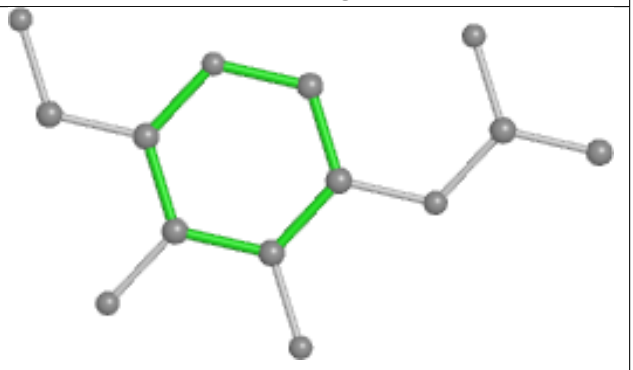


Torsions

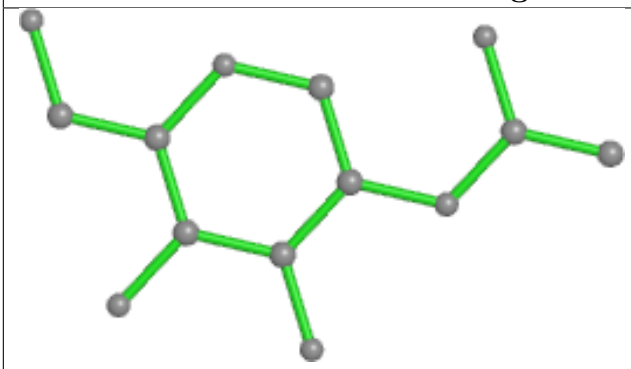


Rings

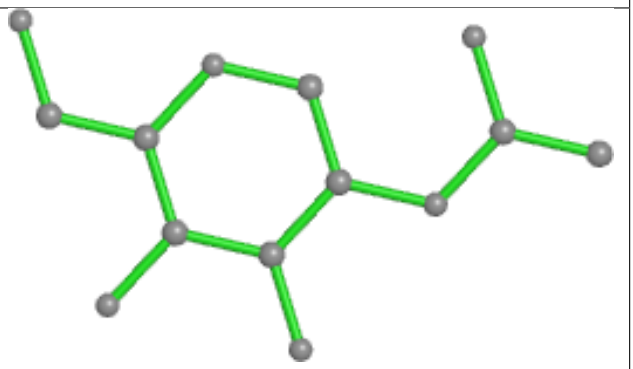
Ligand NAG B 1307	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG C 1301	
 Bond lengths	 Bond angles
 Torsions	 Rings

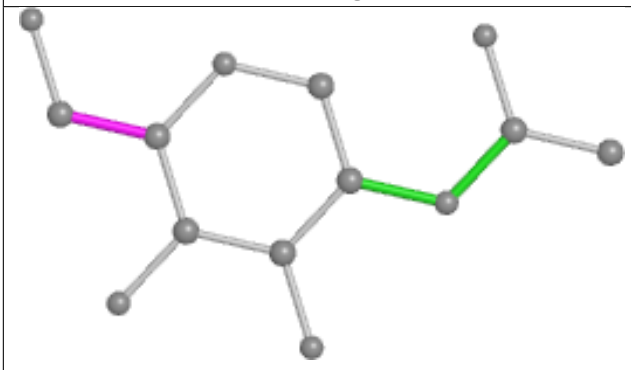
Ligand NAG A 1305



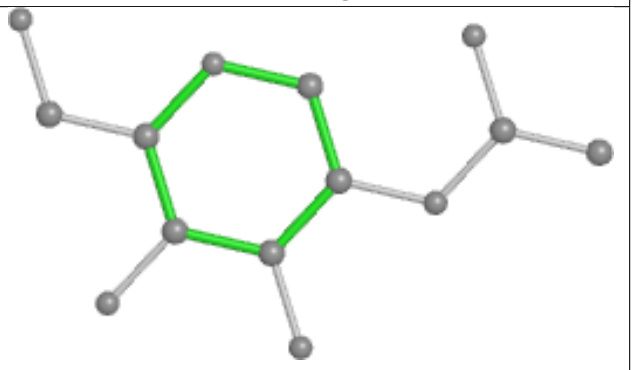
Bond lengths



Bond angles

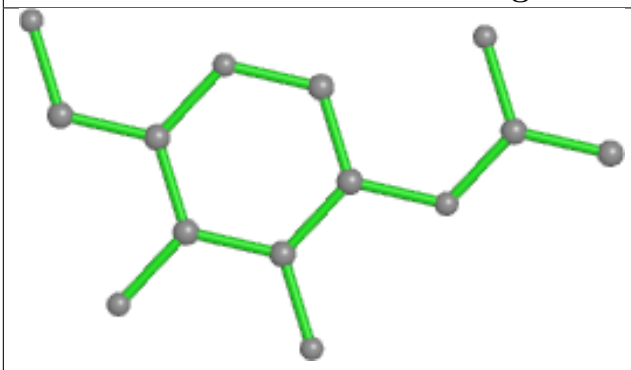


Torsions

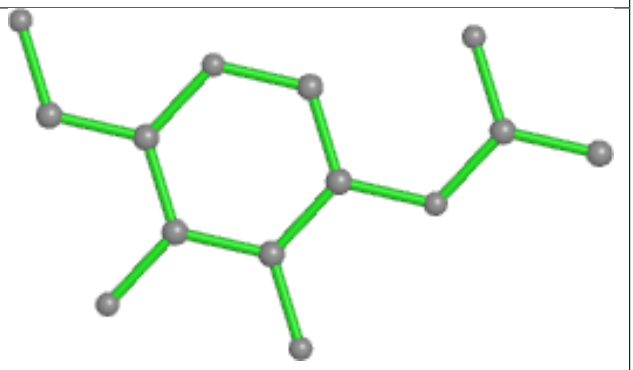


Rings

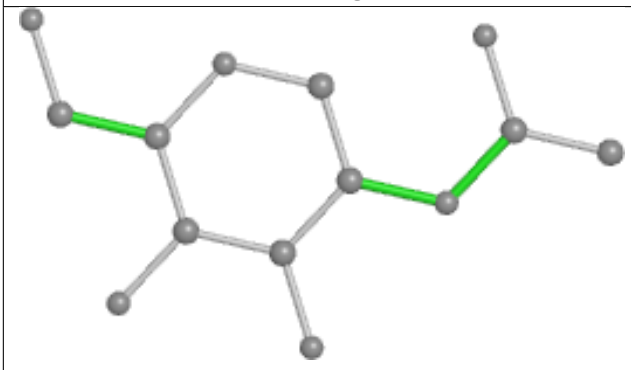
Ligand NAG B 1310



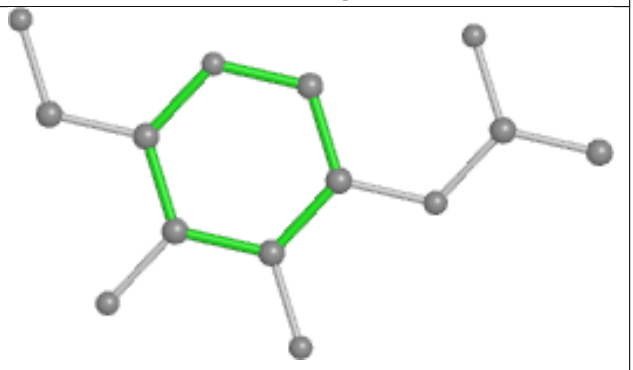
Bond lengths



Bond angles

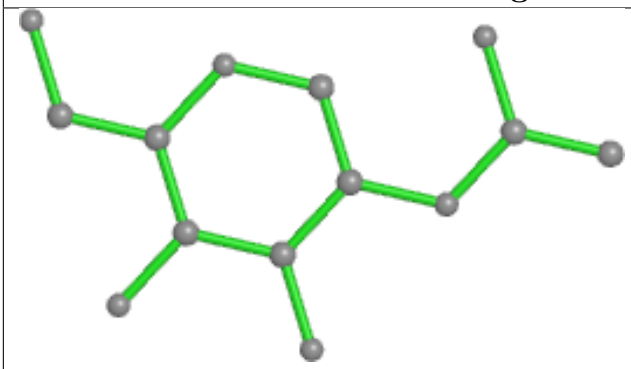


Torsions

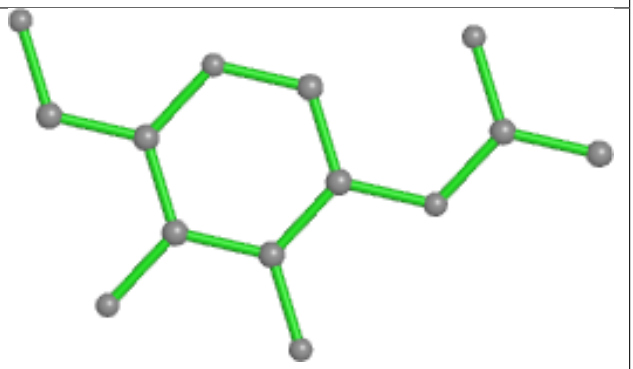


Rings

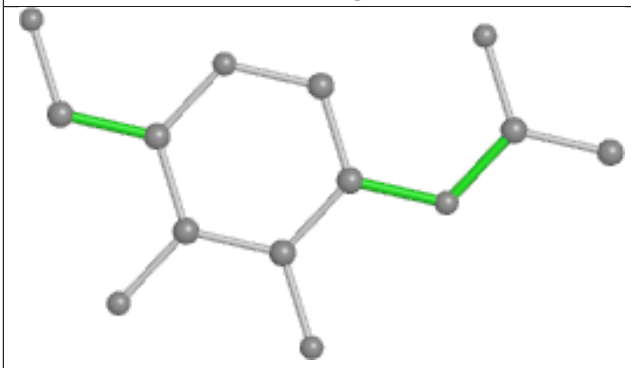
Ligand NAG A 1301



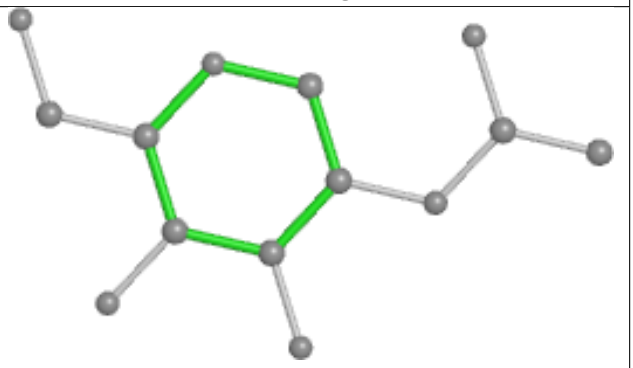
Bond lengths



Bond angles

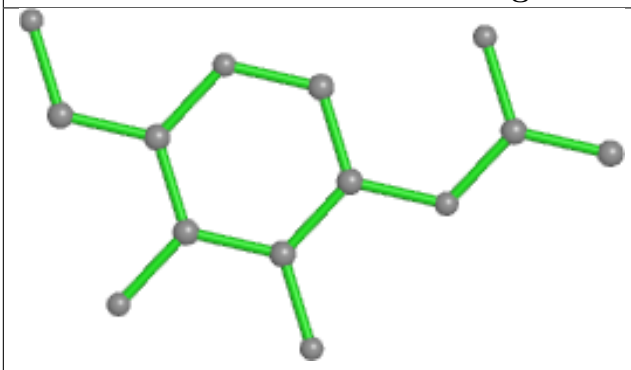


Torsions

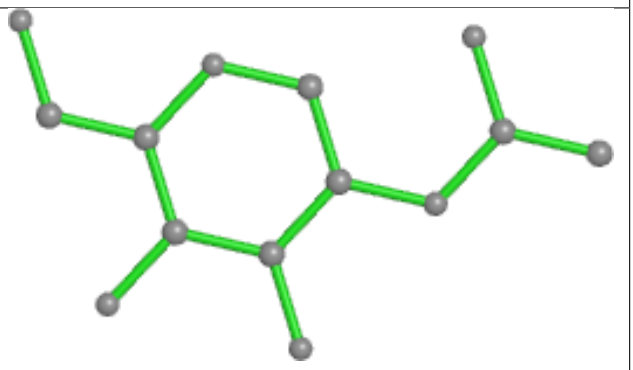


Rings

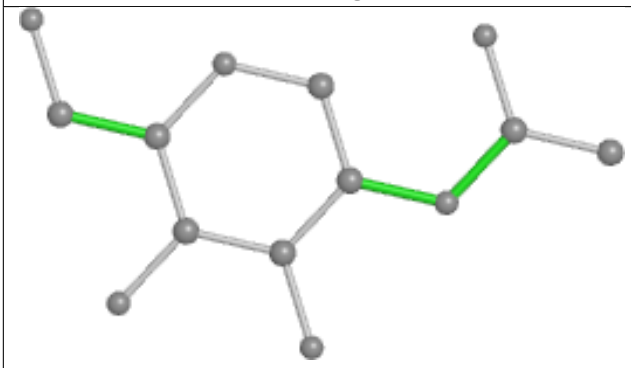
Ligand NAG B 1304



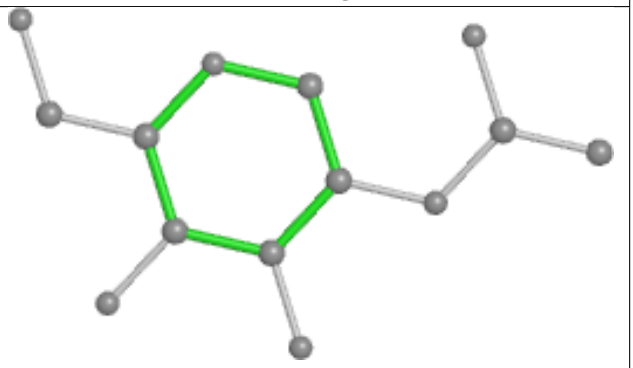
Bond lengths



Bond angles

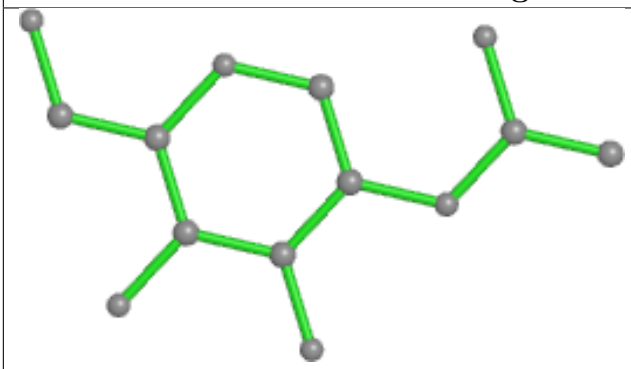


Torsions

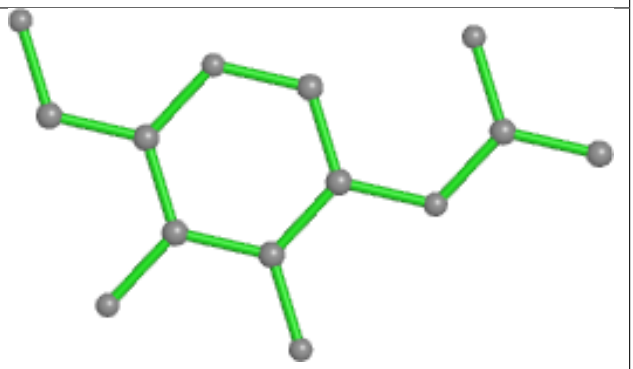


Rings

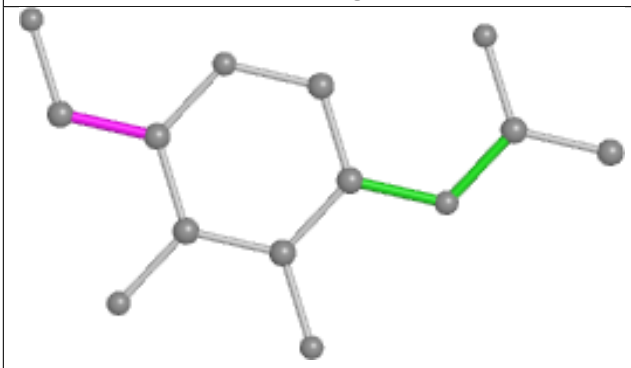
Ligand NAG C 1304



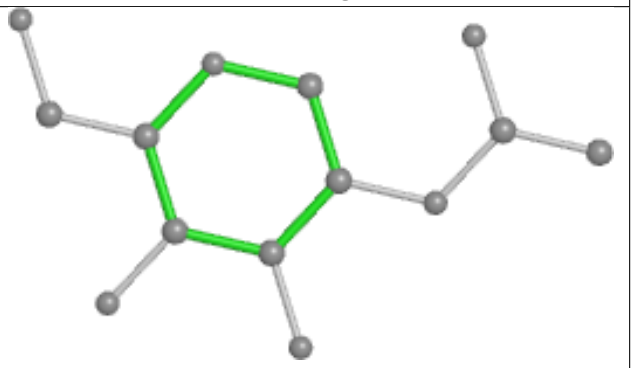
Bond lengths



Bond angles

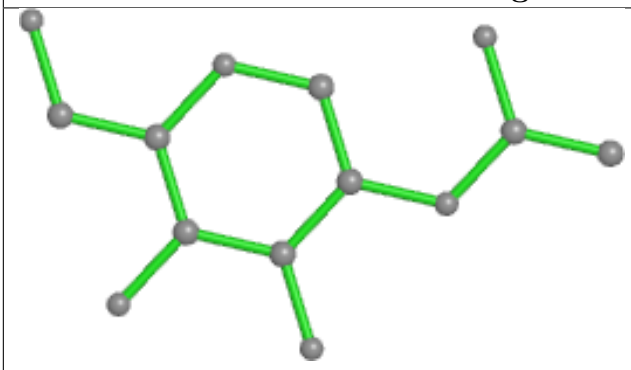


Torsions

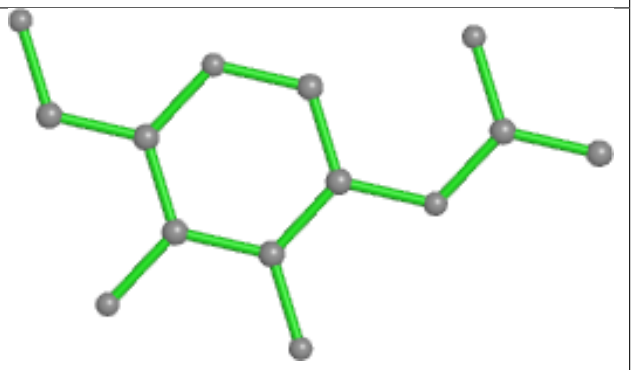


Rings

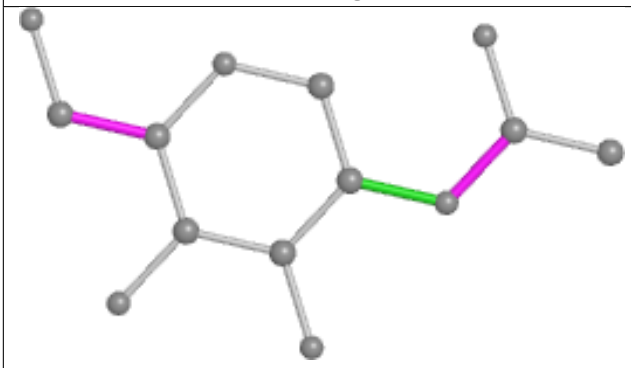
Ligand NAG C 1302



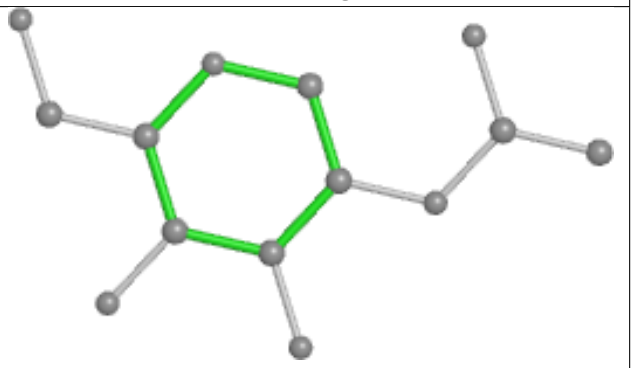
Bond lengths



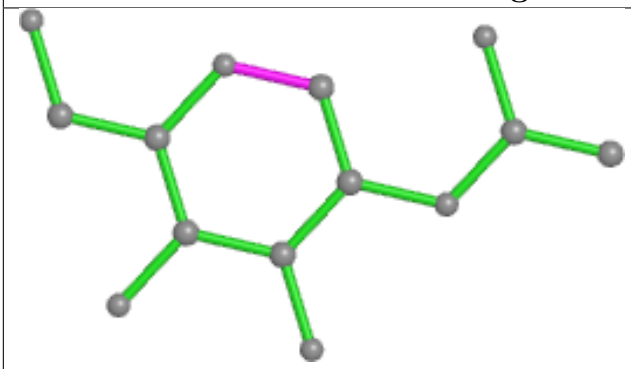
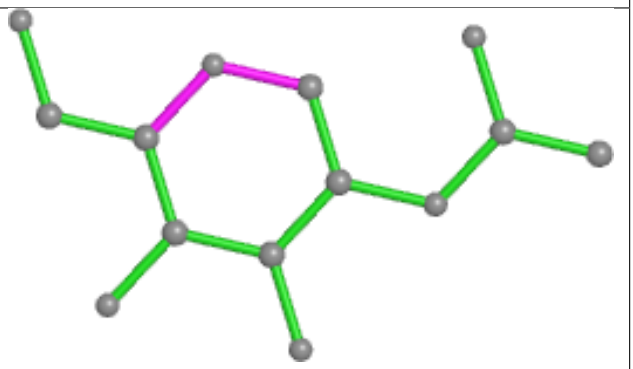
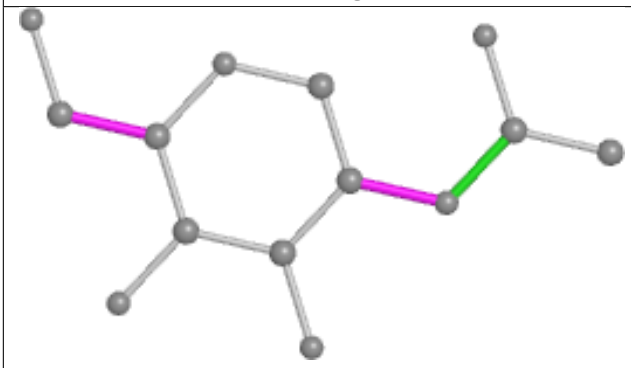
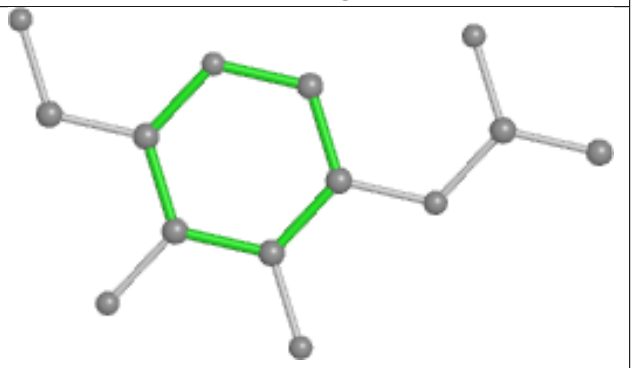
Bond angles

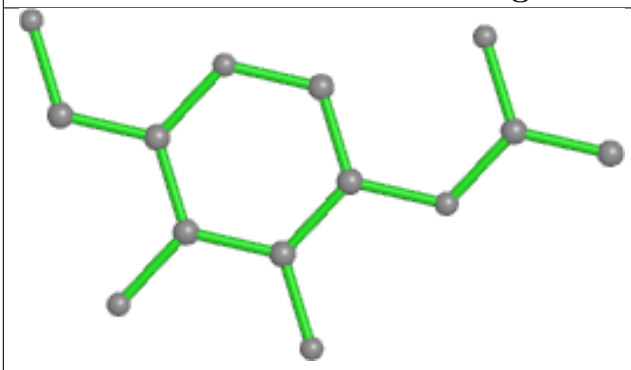
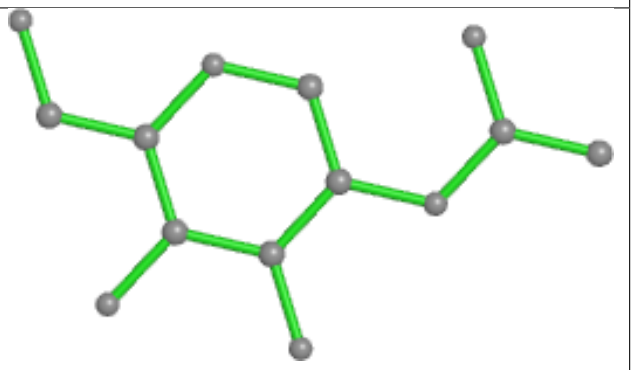
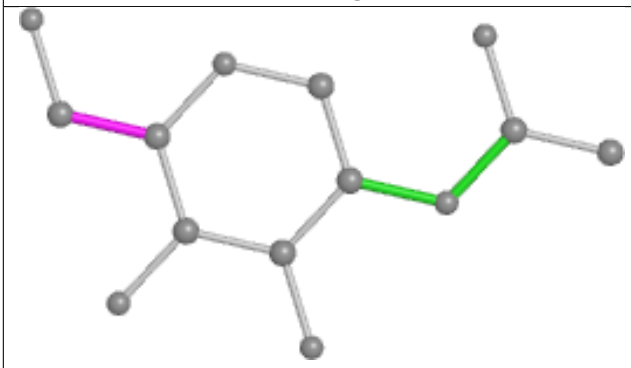
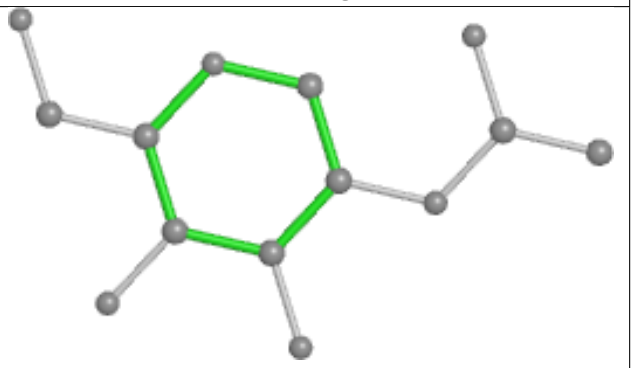


Torsions

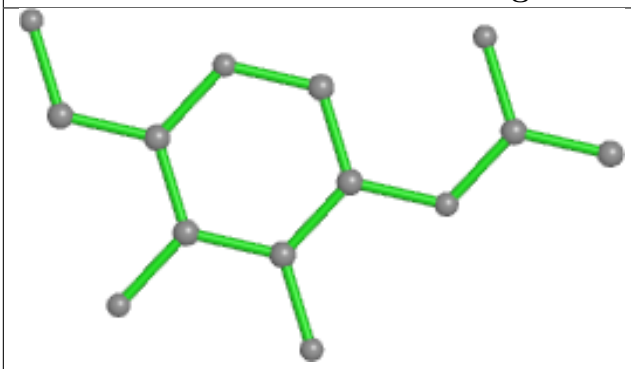


Rings

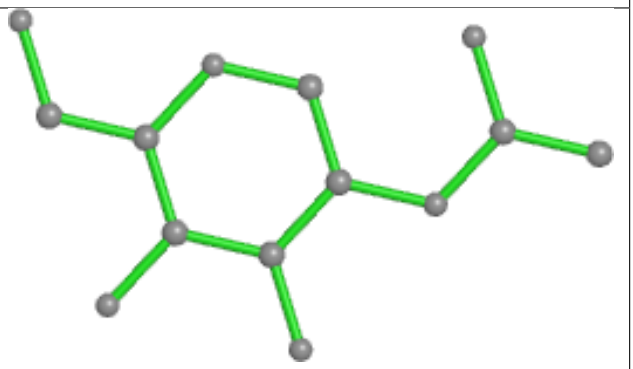
Ligand NAG A 1302	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG B 1306	
 Bond lengths	 Bond angles
 Torsions	 Rings

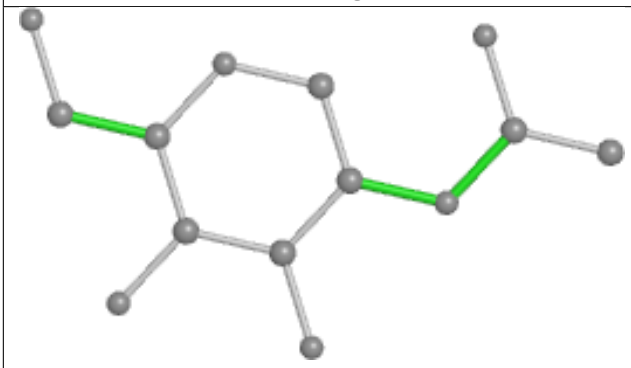
Ligand NAG B 1301



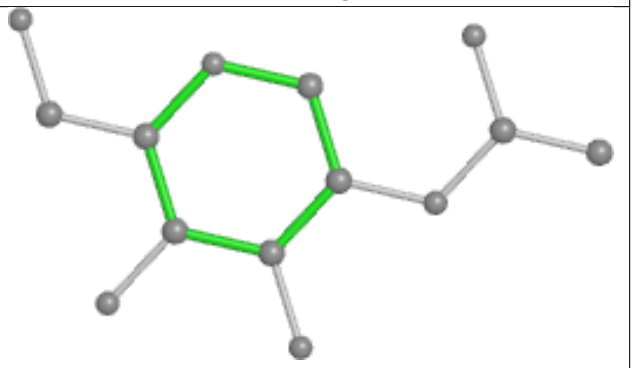
Bond lengths



Bond angles

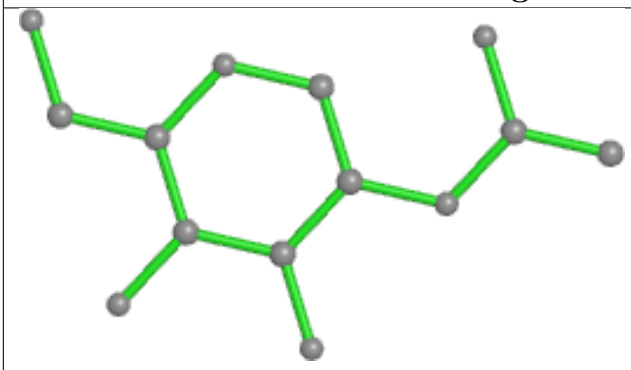


Torsions

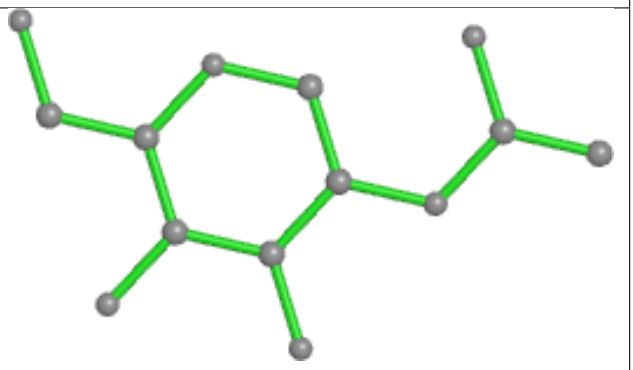


Rings

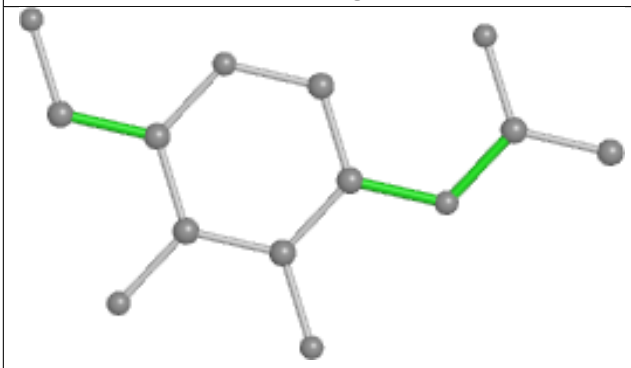
Ligand NAG C 1306



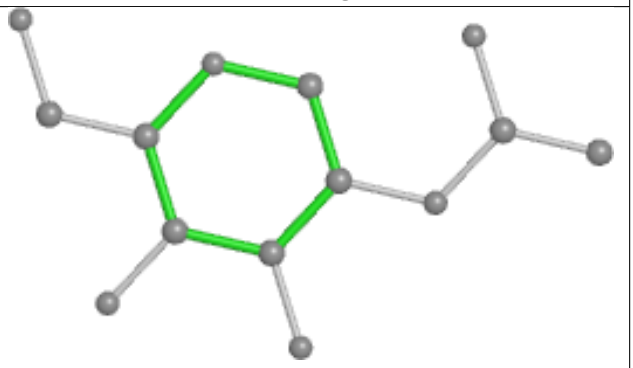
Bond lengths



Bond angles

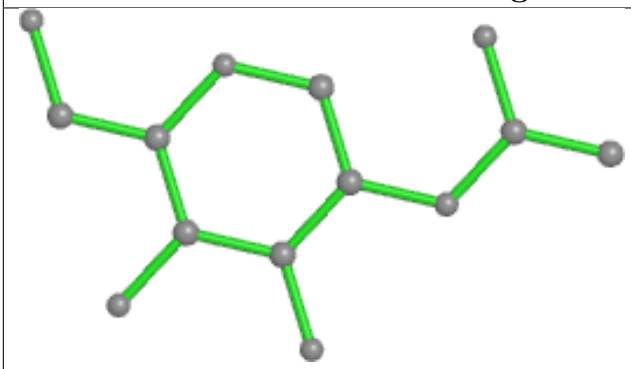


Torsions

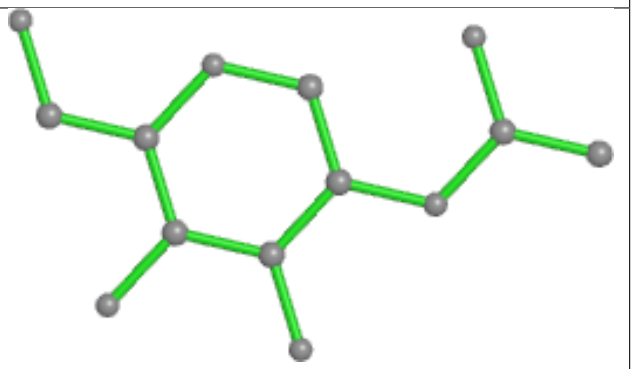


Rings

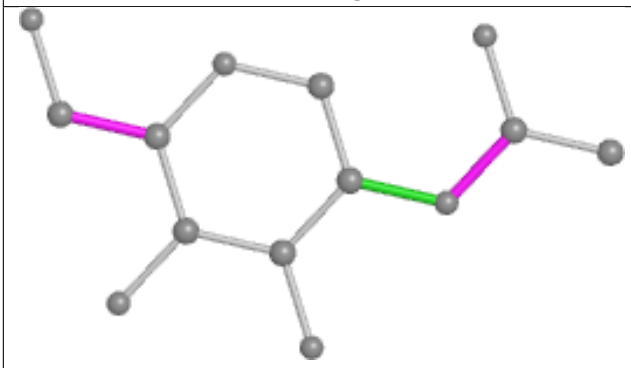
Ligand NAG A 1304



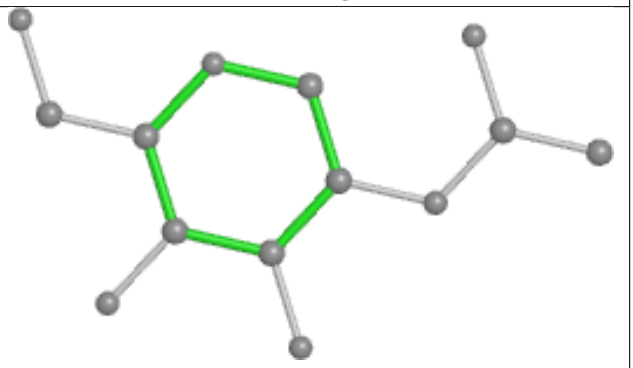
Bond lengths



Bond angles

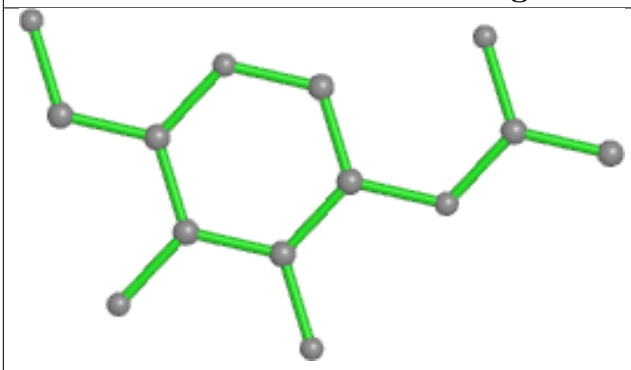


Torsions

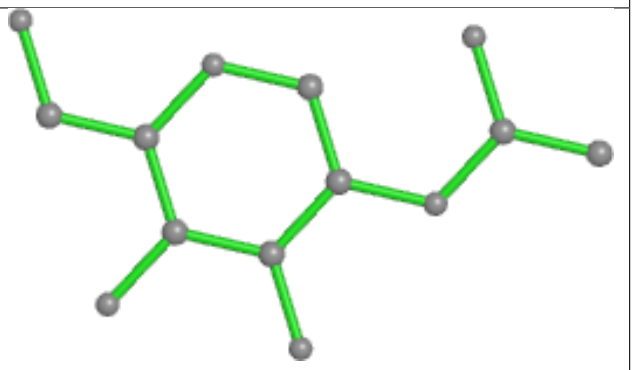


Rings

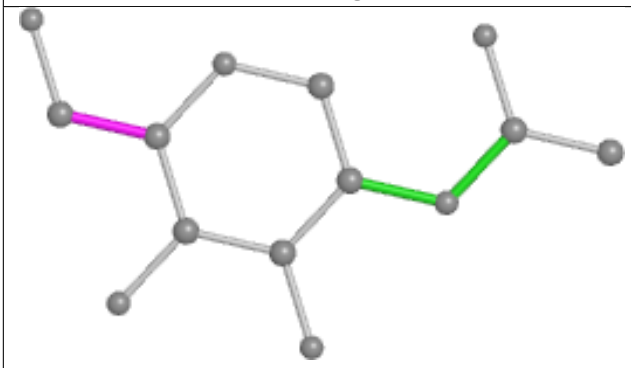
Ligand NAG A 1306



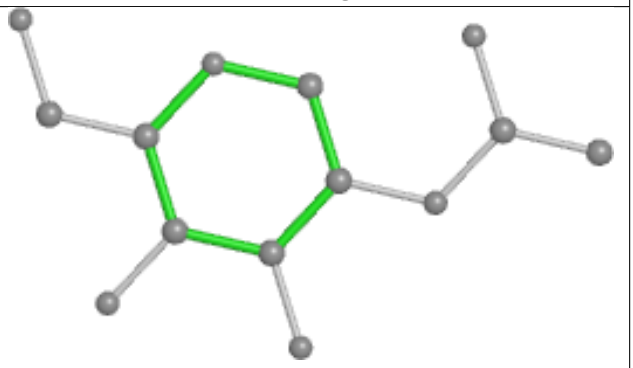
Bond lengths



Bond angles

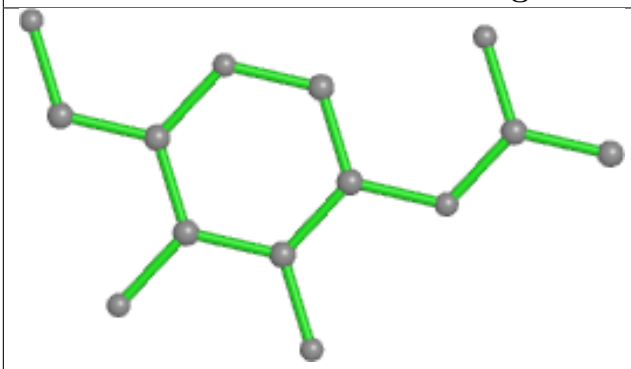


Torsions

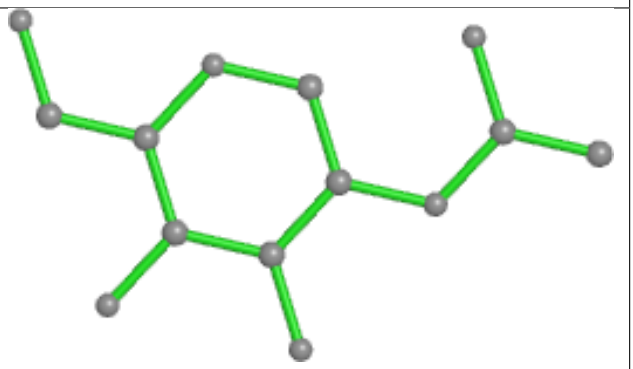


Rings

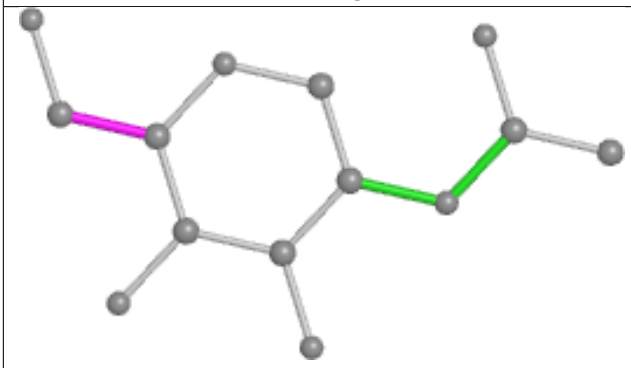
Ligand NAG C 1305



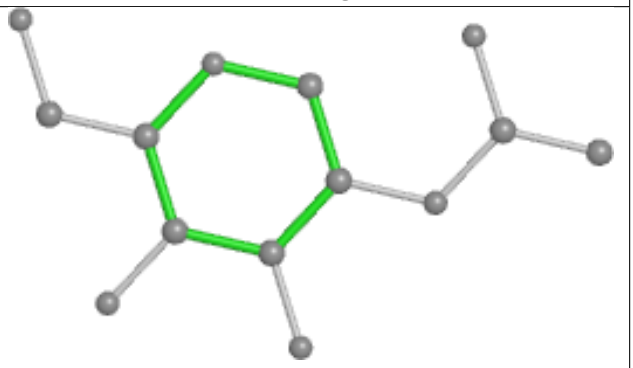
Bond lengths



Bond angles

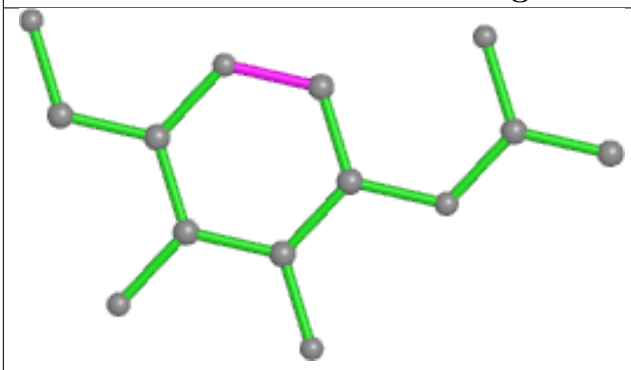


Torsions

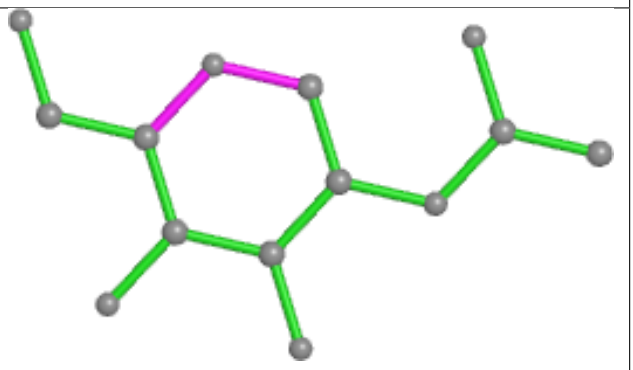


Rings

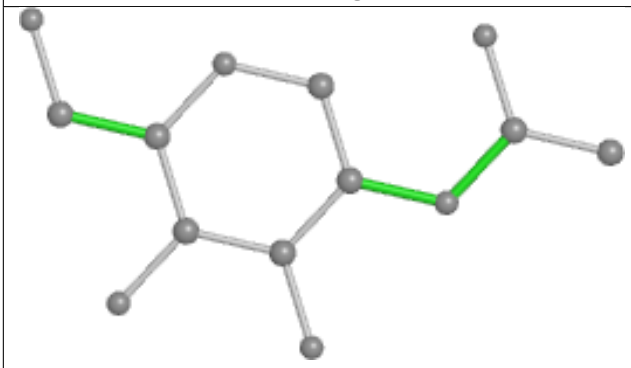
Ligand NAG C 1307



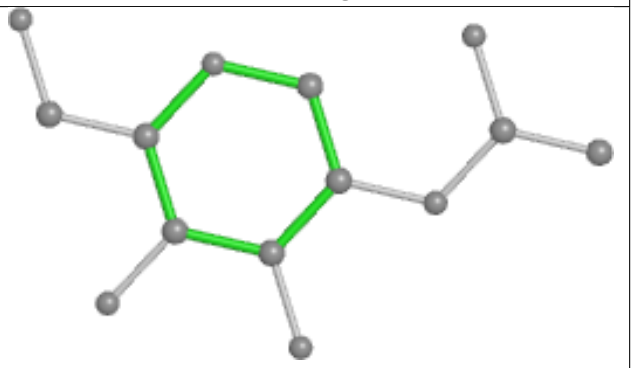
Bond lengths



Bond angles

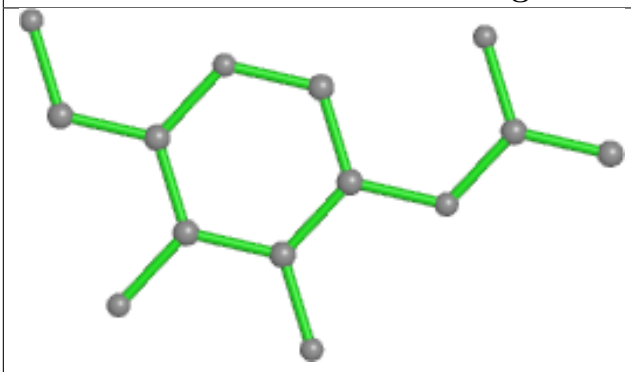


Torsions

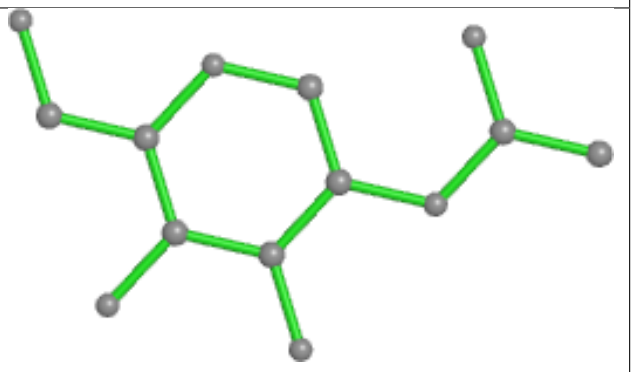


Rings

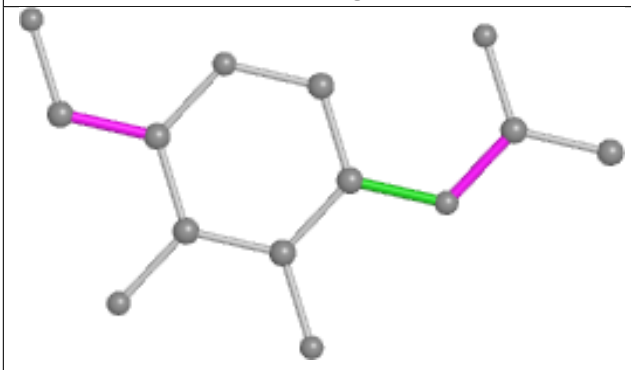
Ligand NAG B 1312



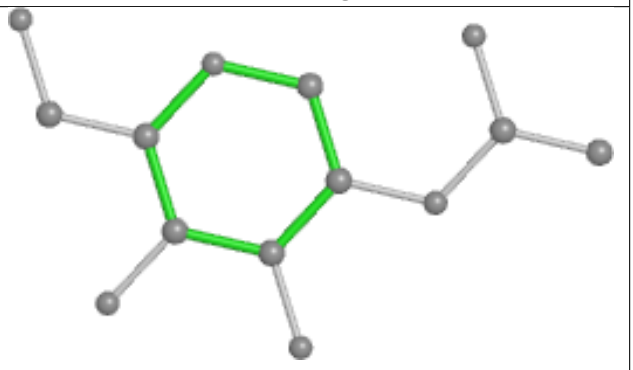
Bond lengths



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.