Full wwPDB EM Validation Report ⓘ

Nov 22, 2022 – 02:26 AM JST

PDB ID	:	7DWY
EMDB ID	:	EMD-30889
Title	:	S protein of SARS-CoV-2 in the locked conformation
Authors	:	Yan, R.H.; Zhang, Y.Y.; Li, Y.N.; Ye, F.F.; Guo, Y.Y.; Xia, L.; Zhong, X.Y.; Chi, X.M.; Zhou, Q.
Deposited on	:	2021-01-18
Resolution	:	2.70 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:

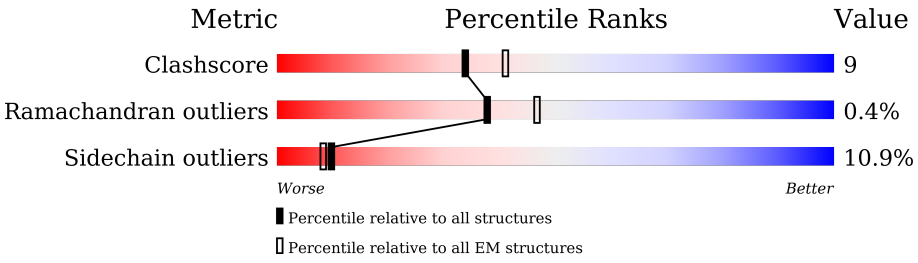
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 2.70 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1283	67% 16% 14%
1	B	1283	67% 16% 14%
1	C	1283	68% 16% 14%
2	D	2	100% 100%
2	E	2	100%
2	F	2	50% 50% 50%
2	G	2	50% 50%
2	H	2	50% 100%

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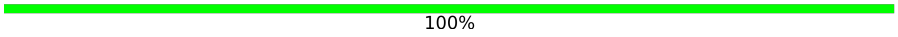
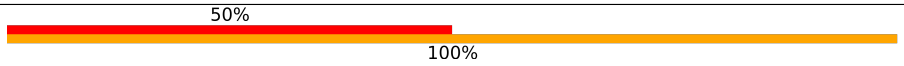
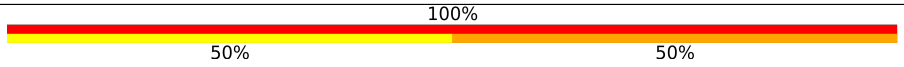
Mol	Chain	Length	Quality of chain
2	I	2	
2	J	2	
2	K	2	
2	L	2	
2	M	2	
2	N	2	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	A	1412	-	-	X	-
3	NAG	A	1413	-	-	X	-
3	NAG	B	1412	-	-	X	-
3	NAG	B	1413	-	-	X	-
3	NAG	C	1410	-	-	X	-
3	NAG	C	1411	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 26979 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	1099	Total	C	N	O	S	0	0
			8595	5483	1436	1636	40		
1	B	1099	Total	C	N	O	S	0	0
			8595	5483	1436	1636	40		
1	C	1099	Total	C	N	O	S	0	0
			8595	5483	1436	1636	40		

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
A	1274	LEU	-	expression tag	UNP P0DTC2
A	1275	GLU	-	expression tag	UNP P0DTC2
A	1276	ASP	-	expression tag	UNP P0DTC2
A	1277	TYR	-	expression tag	UNP P0DTC2
A	1278	LYS	-	expression tag	UNP P0DTC2
A	1279	ASP	-	expression tag	UNP P0DTC2
A	1280	ASP	-	expression tag	UNP P0DTC2
A	1281	ASP	-	expression tag	UNP P0DTC2
A	1282	ASP	-	expression tag	UNP P0DTC2
A	1283	LYS	-	expression tag	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	1274	LEU	-	expression tag	UNP P0DTC2
B	1275	GLU	-	expression tag	UNP P0DTC2
B	1276	ASP	-	expression tag	UNP P0DTC2
B	1277	TYR	-	expression tag	UNP P0DTC2
B	1278	LYS	-	expression tag	UNP P0DTC2
B	1279	ASP	-	expression tag	UNP P0DTC2
B	1280	ASP	-	expression tag	UNP P0DTC2
B	1281	ASP	-	expression tag	UNP P0DTC2
B	1282	ASP	-	expression tag	UNP P0DTC2
B	1283	LYS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	1274	LEU	-	expression tag	UNP P0DTC2
C	1275	GLU	-	expression tag	UNP P0DTC2
C	1276	ASP	-	expression tag	UNP P0DTC2
C	1277	TYR	-	expression tag	UNP P0DTC2
C	1278	LYS	-	expression tag	UNP P0DTC2
C	1279	ASP	-	expression tag	UNP P0DTC2
C	1280	ASP	-	expression tag	UNP P0DTC2
C	1281	ASP	-	expression tag	UNP P0DTC2
C	1282	ASP	-	expression tag	UNP P0DTC2
C	1283	LYS	-	expression tag	UNP P0DTC2

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	2	Total	C	N	O	0	0
			28	16	2	10		
2	E	2	Total	C	N	O	0	0
			28	16	2	10		
2	F	2	Total	C	N	O	0	0
			28	16	2	10		
2	G	2	Total	C	N	O	0	0
			28	16	2	10		
2	H	2	Total	C	N	O	0	0
			28	16	2	10		
2	I	2	Total	C	N	O	0	0
			28	16	2	10		
2	J	2	Total	C	N	O	0	0
			28	16	2	10		
2	K	2	Total	C	N	O	0	0
			28	16	2	10		
2	L	2	Total	C	N	O	0	0
			28	16	2	10		
2	M	2	Total	C	N	O	0	0
			28	16	2	10		

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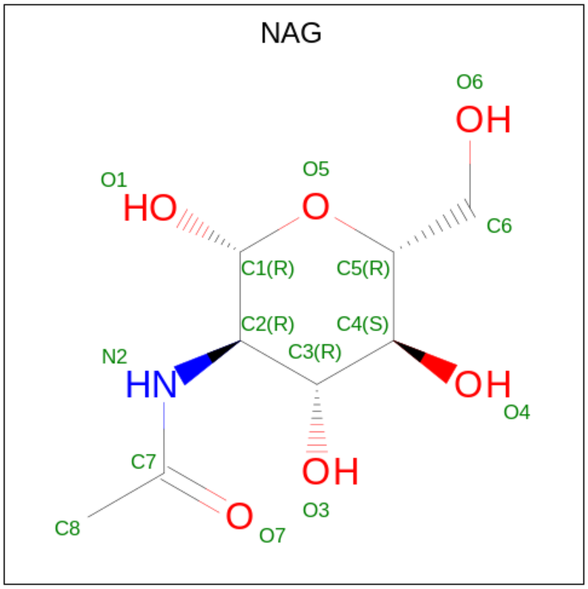
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	N	2	28	16	2	10	0	0

- Molecule 3 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
			Total	C	N	O	
3	A	1	266	152	19	95	0
3	A	1	266	152	19	95	0
3	A	1	266	152	19	95	0
3	A	1	266	152	19	95	0
3	A	1	266	152	19	95	0
3	A	1	266	152	19	95	0
3	A	1	266	152	19	95	0
3	A	1	266	152	19	95	0
3	A	1	266	152	19	95	0
3	A	1	266	152	19	95	0

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Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total 266	C 152	N 19	O 95	0
3	A	1	Total 266	C 152	N 19	O 95	0
3	A	1	Total 266	C 152	N 19	O 95	0
3	A	1	Total 266	C 152	N 19	O 95	0
3	A	1	Total 266	C 152	N 19	O 95	0
3	A	1	Total 266	C 152	N 19	O 95	0
3	A	1	Total 266	C 152	N 19	O 95	0
3	A	1	Total 266	C 152	N 19	O 95	0
3	A	1	Total 266	C 152	N 19	O 95	0
3	B	1	Total 294	C 168	N 21	O 105	0
3	B	1	Total 294	C 168	N 21	O 105	0
3	B	1	Total 294	C 168	N 21	O 105	0
3	B	1	Total 294	C 168	N 21	O 105	0
3	B	1	Total 294	C 168	N 21	O 105	0
3	B	1	Total 294	C 168	N 21	O 105	0
3	B	1	Total 294	C 168	N 21	O 105	0
3	B	1	Total 294	C 168	N 21	O 105	0
3	B	1	Total 294	C 168	N 21	O 105	0
3	B	1	Total 294	C 168	N 21	O 105	0
3	B	1	Total 294	C 168	N 21	O 105	0
3	B	1	Total 294	C 168	N 21	O 105	0

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Mol	Chain	Residues	Atoms	AltConf
3	B	1	Total C N O 294 168 21 105	0
3	B	1	Total C N O 294 168 21 105	0
3	B	1	Total C N O 294 168 21 105	0
3	B	1	Total C N O 294 168 21 105	0
3	B	1	Total C N O 294 168 21 105	0
3	B	1	Total C N O 294 168 21 105	0
3	B	1	Total C N O 294 168 21 105	0
3	B	1	Total C N O 294 168 21 105	0
3	B	1	Total C N O 294 168 21 105	0
3	C	1	Total C N O 266 152 19 95	0
3	C	1	Total C N O 266 152 19 95	0
3	C	1	Total C N O 266 152 19 95	0
3	C	1	Total C N O 266 152 19 95	0
3	C	1	Total C N O 266 152 19 95	0
3	C	1	Total C N O 266 152 19 95	0
3	C	1	Total C N O 266 152 19 95	0
3	C	1	Total C N O 266 152 19 95	0
3	C	1	Total C N O 266 152 19 95	0
3	C	1	Total C N O 266 152 19 95	0
3	C	1	Total C N O 266 152 19 95	0
3	C	1	Total C N O 266 152 19 95	0

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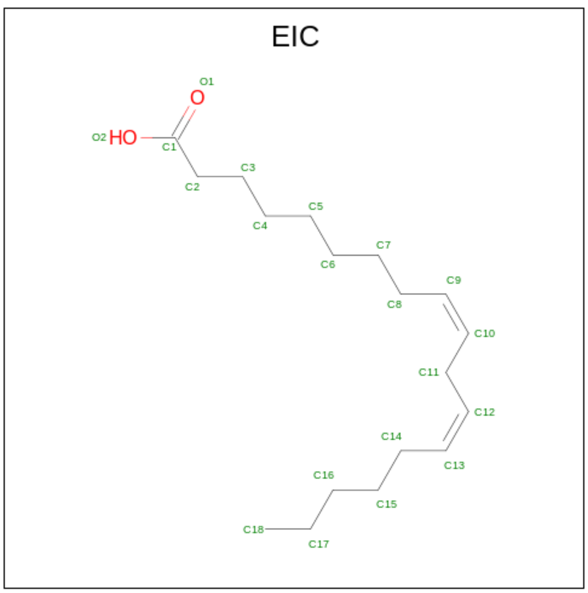
Mol	Chain	Residues	Atoms				AltConf
3	C	1	Total 266	C 152	N 19	O 95	0
3	C	1	Total 266	C 152	N 19	O 95	0
3	C	1	Total 266	C 152	N 19	O 95	0
3	C	1	Total 266	C 152	N 19	O 95	0
3	C	1	Total 266	C 152	N 19	O 95	0
3	C	1	Total 266	C 152	N 19	O 95	0
3	C	1	Total 266	C 152	N 19	O 95	0

- Molecule 4 is LINOLEIC ACID (three-letter code: EIC) (formula: $C_{18}H_{32}O_2$).



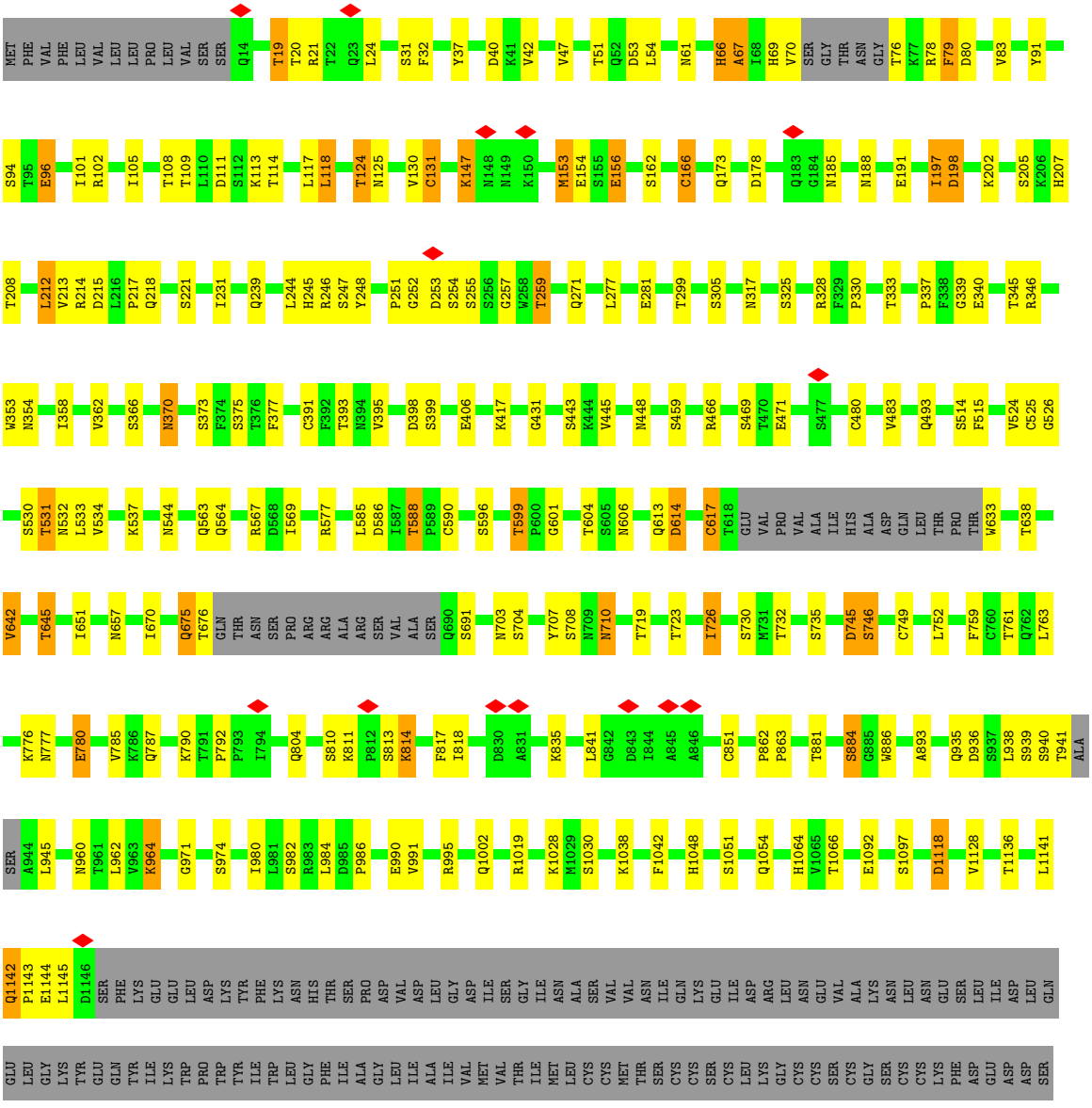
Mol	Chain	Residues	Atoms			AltConf
4	A	1	Total 20	C 18	O 2	0
4	B	1	Total 20	C 18	O 2	0
4	C	1	Total 20	C 18	O 2	0

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 and atom inclusion in map density. 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. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

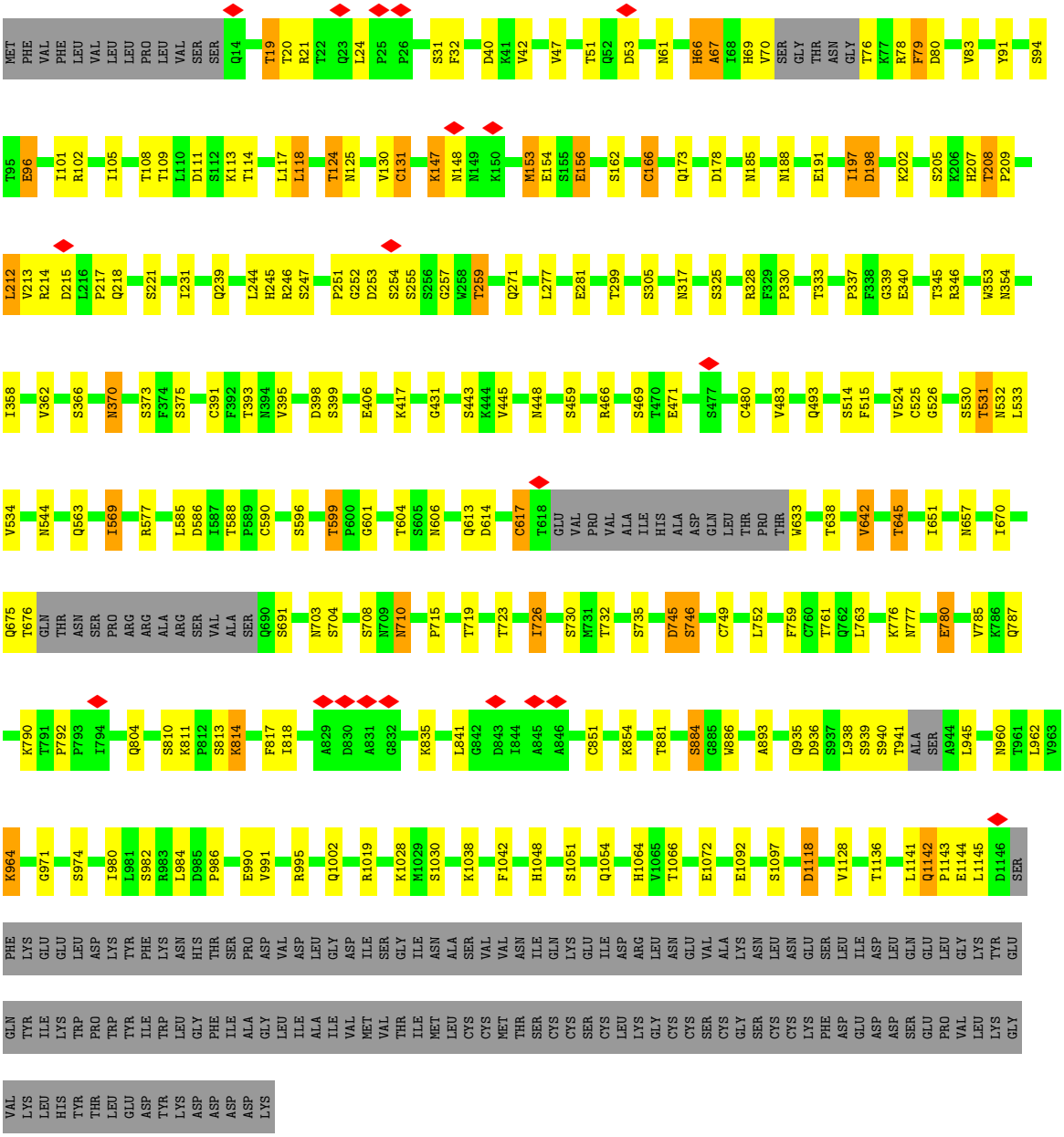
- Molecule 1: Spike glycoprotein

Chain A:



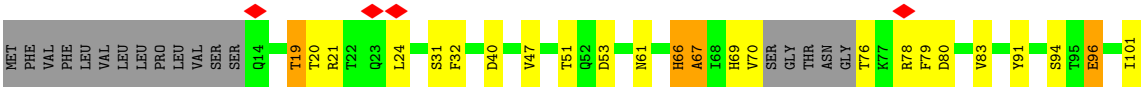
• Molecule 1: Spike glycoprotein

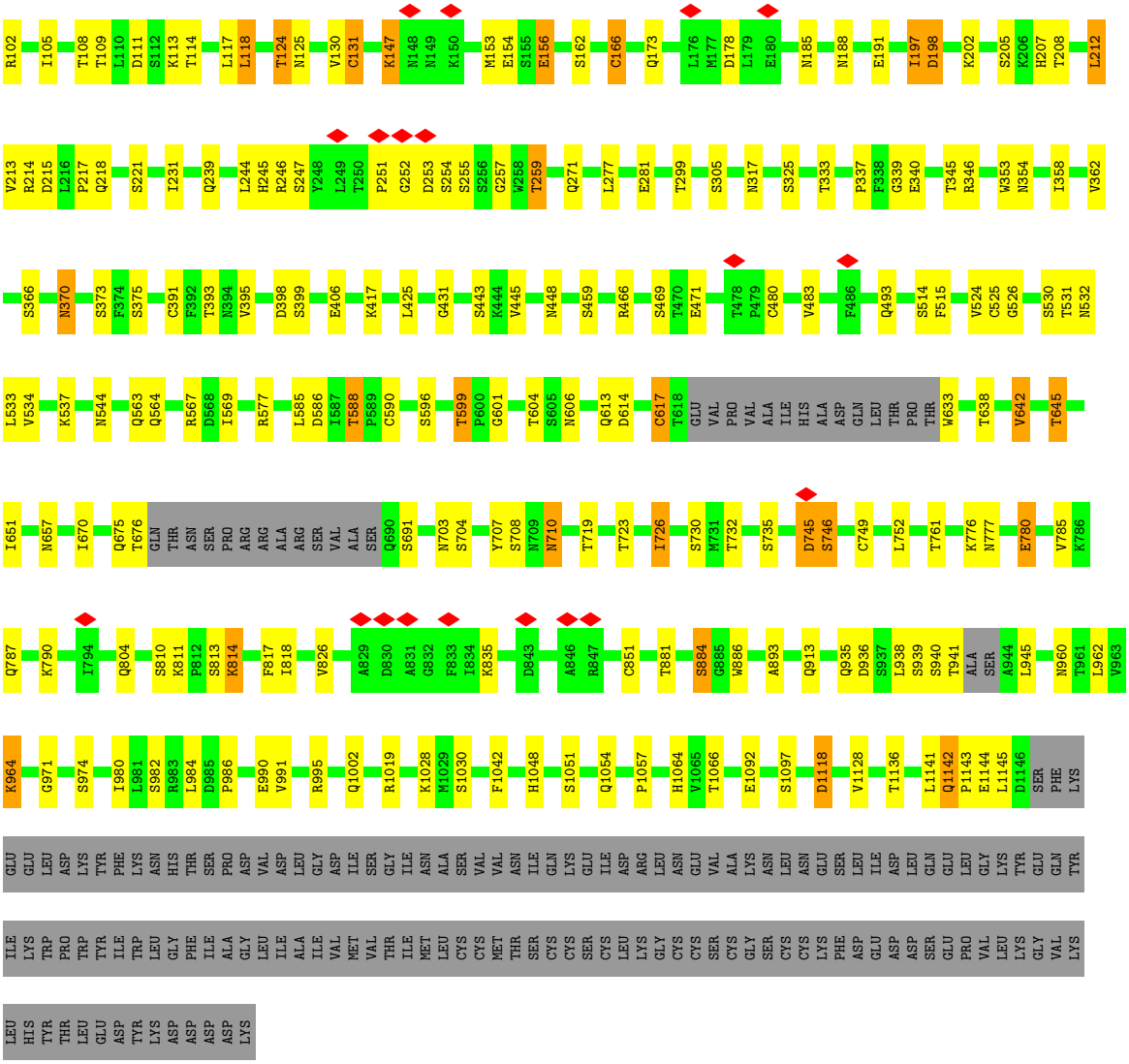
Chain B:



• Molecule 1: Spike glycoprotein

Chain C:



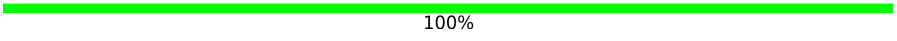


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:

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

Chain E:



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

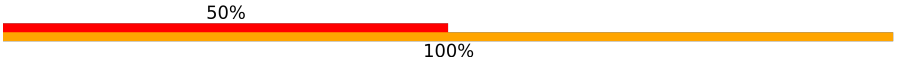
Chain F:

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

Chain G:

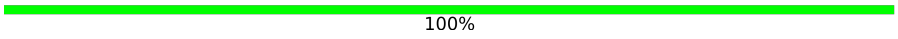
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:



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

Chain I:

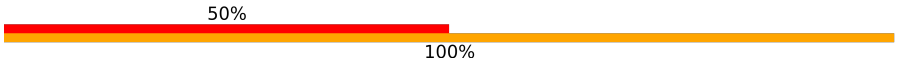


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:

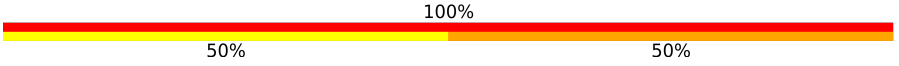
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:



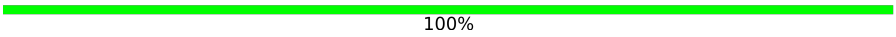
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:



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

Chain M:



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

Chain N:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	143836	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)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.202	Depositor
Minimum map value	-0.123	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	313.056, 313.056, 313.056	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.087, 1.087, 1.087	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, EIC

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	0.43	0/8795	0.49	0/11969
1	B	0.43	0/8795	0.49	0/11969
1	C	0.43	0/8795	0.49	0/11969
All	All	0.43	0/26385	0.49	0/35907

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8595	0	8351	141	0
1	B	8595	0	8351	140	0
1	C	8595	0	8351	136	0
2	D	28	0	25	1	0
2	E	28	0	25	0	0
2	F	28	0	25	1	0
2	G	28	0	25	0	0
2	H	28	0	25	1	0
2	I	28	0	25	0	0
2	J	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	K	28	0	25	1	0
2	L	28	0	25	6	0
2	M	28	0	25	0	0
2	N	28	0	25	0	0
3	A	266	0	245	35	0
3	B	294	0	270	35	0
3	C	266	0	245	30	0
4	A	20	0	31	4	0
4	B	20	0	31	4	0
4	C	20	0	31	2	0
All	All	26979	0	26181	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 9.

All (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)
3:A:1401:NAG:O4	3:A:1402:NAG:C1	1.69	1.39
3:A:1418:NAG:O4	3:A:1419:NAG:C1	1.69	1.39
3:C:1401:NAG:O4	3:C:1402:NAG:C1	1.69	1.39
3:B:1420:NAG:O4	3:B:1421:NAG:C1	1.69	1.37
3:C:1418:NAG:O4	3:C:1419:NAG:C1	1.69	1.37
3:B:1401:NAG:O4	3:B:1402:NAG:C1	1.69	1.36
3:C:1410:NAG:O4	3:C:1411:NAG:C1	1.86	1.24
3:A:1412:NAG:O4	3:A:1413:NAG:C1	1.86	1.23
3:B:1412:NAG:O4	3:B:1413:NAG:C1	1.86	1.23
3:A:1401:NAG:HO4	3:A:1402:NAG:C1	1.49	1.19
3:C:1401:NAG:HO4	3:C:1402:NAG:C1	1.48	1.18
1:C:67:ALA:HA	1:C:78:ARG:O	1.50	1.12
1:A:67:ALA:HA	1:A:78:ARG:O	1.50	1.11
1:B:67:ALA:HA	1:B:78:ARG:O	1.50	1.10
1:C:339:GLY:HA3	2:L:1:NAG:H82	1.31	1.10
1:B:339:GLY:HA3	3:B:1409:NAG:H82	1.31	1.09
1:A:339:GLY:HA3	3:A:1409:NAG:H82	1.31	1.07
1:B:339:GLY:CA	3:B:1409:NAG:H82	1.87	1.05
1:A:339:GLY:CA	3:A:1409:NAG:H82	1.87	1.05
1:B:358:ILE:CD1	4:B:1422:EIC:H182	1.84	1.05
1:C:339:GLY:CA	2:L:1:NAG:H82	1.87	1.05
1:B:358:ILE:HD13	4:B:1422:EIC:H182	1.06	1.04
1:B:339:GLY:HA3	3:B:1409:NAG:C8	1.89	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:GLY:HA3	3:A:1409:NAG:C8	1.89	1.02
1:C:339:GLY:HA3	2:L:1:NAG:C8	1.89	1.02
1:A:124:THR:HG21	3:A:1404:NAG:C8	1.90	1.01
1:B:124:THR:HG21	3:B:1404:NAG:C8	1.90	0.99
1:C:124:THR:HG21	3:C:1404:NAG:C8	1.91	0.99
1:A:131:CYS:HB3	1:A:166:CYS:HA	1.42	0.99
1:C:131:CYS:HB3	1:C:166:CYS:HA	1.42	0.98
1:B:131:CYS:HB3	1:B:166:CYS:HA	1.43	0.98
3:A:1418:NAG:HO4	3:A:1419:NAG:C1	1.78	0.93
3:A:1412:NAG:H62	3:A:1413:NAG:C7	1.99	0.93
3:C:1410:NAG:H62	3:C:1411:NAG:C7	1.99	0.92
3:B:1412:NAG:H62	3:B:1413:NAG:C7	1.99	0.91
3:B:1412:NAG:HO4	3:B:1413:NAG:C1	1.81	0.90
1:C:940:SER:O	1:C:941:THR:OG1	1.91	0.89
1:B:940:SER:O	1:B:941:THR:OG1	1.91	0.88
1:A:940:SER:O	1:A:941:THR:OG1	1.91	0.88
1:C:362:VAL:HG13	1:C:526:GLY:O	1.74	0.88
1:C:1144:GLU:C	1:C:1145:LEU:HD23	1.95	0.87
1:B:124:THR:HG21	3:B:1404:NAG:H82	1.58	0.86
1:A:362:VAL:HG13	1:A:526:GLY:O	1.74	0.86
1:A:1144:GLU:C	1:A:1145:LEU:HD23	1.95	0.86
1:B:362:VAL:HG13	1:B:526:GLY:O	1.74	0.86
1:C:124:THR:HG21	3:C:1404:NAG:H82	1.58	0.85
1:B:1144:GLU:C	1:B:1145:LEU:HD23	1.95	0.85
1:A:124:THR:HG21	3:A:1404:NAG:H82	1.58	0.84
3:A:1412:NAG:HO4	3:A:1413:NAG:C1	1.88	0.83
3:C:1418:NAG:HO4	3:C:1419:NAG:C1	1.89	0.83
1:B:358:ILE:HD13	4:B:1422:EIC:C18	2.01	0.82
1:A:817:PHE:CE2	1:A:935:GLN:NE2	2.50	0.80
1:C:817:PHE:CE2	1:C:935:GLN:NE2	2.50	0.80
1:B:817:PHE:CE2	1:B:935:GLN:NE2	2.50	0.80
1:A:131:CYS:HB3	1:A:166:CYS:CA	2.13	0.79
1:C:131:CYS:HB3	1:C:166:CYS:CA	2.12	0.79
3:B:1414:NAG:H3	3:B:1414:NAG:C8	2.13	0.79
3:A:1414:NAG:H3	3:A:1414:NAG:C8	2.13	0.78
3:C:1410:NAG:HO4	3:C:1411:NAG:C1	1.93	0.78
1:B:124:THR:HG21	3:B:1404:NAG:H83	1.65	0.78
1:B:131:CYS:HB3	1:B:166:CYS:CA	2.13	0.78
3:C:1412:NAG:H3	3:C:1412:NAG:C8	2.13	0.78
1:B:24:LEU:HB2	1:B:78:ARG:NH2	2.00	0.77
1:C:599:THR:HG23	1:C:601:GLY:H	1.49	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:599:THR:HG23	1:A:601:GLY:H	1.50	0.77
1:A:24:LEU:HB2	1:A:78:ARG:NH2	2.00	0.77
1:A:124:THR:HG21	3:A:1404:NAG:H83	1.65	0.77
1:B:599:THR:HG23	1:B:601:GLY:H	1.50	0.76
1:C:124:THR:HG21	3:C:1404:NAG:H83	1.65	0.76
1:C:24:LEU:HB2	1:C:78:ARG:NH2	2.00	0.76
1:C:124:THR:CG2	3:C:1404:NAG:C8	2.65	0.74
1:B:124:THR:CG2	3:B:1404:NAG:C8	2.65	0.74
1:C:358:ILE:HD13	4:C:1420:EIC:H172	1.68	0.74
1:C:67:ALA:CA	1:C:78:ARG:O	2.34	0.74
1:A:1144:GLU:O	1:A:1145:LEU:HD23	1.88	0.74
3:C:1412:NAG:H3	3:C:1412:NAG:H82	1.71	0.73
1:C:339:GLY:HA2	2:L:1:NAG:H82	1.70	0.73
3:C:1410:NAG:H62	3:C:1411:NAG:C8	2.19	0.73
1:A:124:THR:CG2	3:A:1404:NAG:C8	2.65	0.73
1:A:67:ALA:CA	1:A:78:ARG:O	2.34	0.73
1:A:1142:GLN:N	1:A:1142:GLN:OE1	2.21	0.73
1:B:1142:GLN:N	1:B:1142:GLN:OE1	2.21	0.73
1:A:339:GLY:HA2	3:A:1409:NAG:H82	1.70	0.72
1:B:1144:GLU:O	1:B:1145:LEU:HD23	1.88	0.72
1:C:1142:GLN:OE1	1:C:1142:GLN:N	2.21	0.72
1:C:1144:GLU:O	1:C:1145:LEU:HD23	1.88	0.72
1:A:69:HIS:HA	1:A:76:THR:O	1.89	0.72
3:B:1414:NAG:H3	3:B:1414:NAG:H82	1.71	0.72
1:A:124:THR:CG2	3:A:1404:NAG:H82	2.20	0.72
3:B:1401:NAG:HO4	3:B:1402:NAG:C1	1.99	0.72
3:A:1414:NAG:H3	3:A:1414:NAG:H82	1.71	0.72
1:B:339:GLY:HA2	3:B:1409:NAG:H82	1.70	0.72
3:B:1412:NAG:H62	3:B:1413:NAG:C8	2.19	0.72
1:A:370:ASN:N	1:A:370:ASN:OD1	2.22	0.72
1:C:370:ASN:OD1	1:C:370:ASN:N	2.22	0.72
1:B:69:HIS:HA	1:B:76:THR:O	1.89	0.71
1:C:69:HIS:HA	1:C:76:THR:O	1.89	0.71
3:A:1412:NAG:H62	3:A:1413:NAG:C8	2.19	0.71
1:B:370:ASN:OD1	1:B:370:ASN:N	2.22	0.71
1:B:124:THR:CG2	3:B:1404:NAG:H82	2.20	0.71
1:C:345:THR:HG23	1:C:346:ARG:HG3	1.72	0.71
1:B:345:THR:HG23	1:B:346:ARG:HG3	1.72	0.71
1:A:345:THR:HG23	1:A:346:ARG:HG3	1.72	0.70
1:C:124:THR:CG2	3:C:1404:NAG:H82	2.20	0.70
3:B:1420:NAG:HO4	3:B:1421:NAG:C1	2.04	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:CYS:CB	1:C:166:CYS:HA	2.20	0.70
1:B:67:ALA:CA	1:B:78:ARG:O	2.34	0.69
1:A:131:CYS:CB	1:A:166:CYS:HA	2.21	0.69
1:B:131:CYS:CB	1:B:166:CYS:HA	2.21	0.69
1:B:246:ARG:NH2	1:B:254:SER:O	2.27	0.68
1:C:246:ARG:NH2	1:C:254:SER:O	2.27	0.67
1:A:69:HIS:C	1:A:70:VAL:HG23	2.15	0.67
1:A:246:ARG:NH2	1:A:254:SER:O	2.27	0.67
1:A:1144:GLU:OE2	1:A:1144:GLU:HA	1.94	0.67
1:C:69:HIS:C	1:C:70:VAL:HG23	2.15	0.67
1:B:69:HIS:C	1:B:70:VAL:HG23	2.15	0.66
1:B:1144:GLU:OE2	1:B:1144:GLU:HA	1.94	0.66
1:C:1144:GLU:HA	1:C:1144:GLU:OE2	1.94	0.65
1:B:358:ILE:CD1	4:B:1422:EIC:C18	2.67	0.65
1:B:406:GLU:OE2	1:B:417:LYS:NZ	2.27	0.65
1:C:124:THR:CG2	3:C:1404:NAG:H83	2.28	0.64
1:C:776:LYS:O	1:C:780:GLU:HG2	1.97	0.64
1:A:406:GLU:OE2	1:A:417:LYS:NZ	2.27	0.64
1:B:776:LYS:O	1:B:780:GLU:HG2	1.97	0.64
1:A:776:LYS:O	1:A:780:GLU:HG2	1.97	0.63
1:B:817:PHE:HE2	1:B:935:GLN:NE2	1.97	0.63
1:A:817:PHE:HE2	1:A:935:GLN:NE2	1.97	0.63
1:A:124:THR:CG2	3:A:1404:NAG:H83	2.28	0.62
1:C:253:ASP:N	1:C:253:ASP:OD1	2.31	0.62
1:A:745:ASP:N	1:A:745:ASP:OD1	2.32	0.62
3:A:1412:NAG:H62	3:A:1413:NAG:H82	1.82	0.62
1:B:111:ASP:OD2	1:B:113:LYS:NZ	2.33	0.62
1:B:745:ASP:OD1	1:B:745:ASP:N	2.32	0.62
1:C:111:ASP:OD2	1:C:113:LYS:NZ	2.33	0.61
1:C:406:GLU:OE2	1:C:417:LYS:NZ	2.27	0.61
3:B:1412:NAG:H62	3:B:1413:NAG:H82	1.82	0.61
3:C:1410:NAG:H62	3:C:1411:NAG:H82	1.82	0.61
1:A:111:ASP:OD2	1:A:113:LYS:NZ	2.33	0.61
1:B:156:GLU:OE1	1:B:246:ARG:NH1	2.34	0.61
1:C:156:GLU:OE1	1:C:246:ARG:NH1	2.34	0.61
1:B:102:ARG:NH2	1:B:154:GLU:OE1	2.33	0.61
1:A:253:ASP:OD1	1:A:253:ASP:N	2.31	0.61
1:C:745:ASP:OD1	1:C:745:ASP:N	2.32	0.61
1:B:124:THR:CG2	3:B:1404:NAG:H83	2.28	0.61
1:A:156:GLU:OE1	1:A:246:ARG:NH1	2.34	0.60
1:C:102:ARG:NH2	1:C:154:GLU:OE1	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:ARG:NH2	1:A:154:GLU:OE1	2.33	0.60
1:A:70:VAL:N	1:A:76:THR:O	2.29	0.60
1:B:814:LYS:HD2	1:B:814:LYS:N	2.18	0.59
1:B:70:VAL:N	1:B:76:THR:O	2.29	0.59
1:B:253:ASP:OD1	1:B:253:ASP:N	2.31	0.59
2:H:1:NAG:H62	2:H:2:NAG:H82	1.84	0.59
1:B:69:HIS:O	1:B:70:VAL:HG23	2.03	0.59
1:C:814:LYS:HD2	1:C:814:LYS:N	2.18	0.59
1:A:69:HIS:O	1:A:70:VAL:HG23	2.03	0.59
1:A:814:LYS:N	1:A:814:LYS:HD2	2.17	0.59
1:C:69:HIS:O	1:C:70:VAL:HG23	2.03	0.59
1:C:70:VAL:N	1:C:76:THR:O	2.29	0.59
1:B:339:GLY:HA3	3:B:1409:NAG:H81	1.80	0.58
1:A:339:GLY:HA3	3:A:1409:NAG:H81	1.80	0.58
1:C:339:GLY:HA3	2:L:1:NAG:H81	1.80	0.58
1:C:817:PHE:HE2	1:C:935:GLN:NE2	1.97	0.58
1:C:777:ASN:OD1	1:C:1019:ARG:NH1	2.31	0.57
3:A:1412:NAG:C6	3:A:1413:NAG:C7	2.80	0.57
1:B:940:SER:C	1:B:941:THR:HG1	2.02	0.57
1:B:91:TYR:OH	1:B:191:GLU:OE1	2.20	0.57
1:B:124:THR:OG1	1:B:125:ASN:OD1	2.22	0.57
1:A:811:LYS:HB2	1:A:813:SER:O	2.04	0.57
1:C:811:LYS:O	1:C:814:LYS:NZ	2.38	0.57
1:A:124:THR:OG1	1:A:125:ASN:OD1	2.22	0.57
1:A:811:LYS:O	1:A:814:LYS:NZ	2.38	0.57
1:B:811:LYS:HB2	1:B:813:SER:O	2.04	0.57
1:C:124:THR:OG1	1:C:125:ASN:OD1	2.22	0.56
1:C:66:HIS:O	1:C:67:ALA:HB2	2.05	0.56
1:A:813:SER:C	1:A:814:LYS:HD2	2.26	0.56
1:B:813:SER:C	1:B:814:LYS:HD2	2.26	0.56
3:B:1419:NAG:H3	3:B:1419:NAG:H83	1.87	0.56
1:C:813:SER:C	1:C:814:LYS:HD2	2.26	0.56
2:F:2:NAG:H3	2:F:2:NAG:H83	1.87	0.56
1:B:105:ILE:HG22	1:B:118:LEU:HD12	1.88	0.56
1:B:66:HIS:O	1:B:67:ALA:HB2	2.05	0.56
1:B:777:ASN:OD1	1:B:1019:ARG:NH1	2.31	0.56
1:C:337:PRO:HB2	1:C:340:GLU:HG2	1.88	0.56
1:C:811:LYS:HB2	1:C:813:SER:O	2.04	0.56
1:A:91:TYR:OH	1:A:191:GLU:OE1	2.20	0.56
1:B:811:LYS:O	1:B:814:LYS:NZ	2.38	0.55
1:B:960:ASN:O	1:B:964:LYS:HG3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:105:ILE:HG22	1:C:118:LEU:HD12	1.88	0.55
1:C:941:THR:HG22	1:C:941:THR:O	2.06	0.55
3:C:1417:NAG:H83	3:C:1417:NAG:H3	1.87	0.55
1:A:61:ASN:OD1	3:A:1403:NAG:H82	2.07	0.55
1:A:66:HIS:O	1:A:67:ALA:HB2	2.05	0.55
1:A:777:ASN:OD1	1:A:1019:ARG:NH1	2.31	0.55
1:B:212:LEU:HD22	1:B:217:PRO:HG3	1.89	0.55
1:A:105:ILE:HG22	1:A:118:LEU:HD12	1.88	0.55
1:A:212:LEU:HD22	1:A:217:PRO:HG3	1.89	0.55
1:A:941:THR:O	1:A:941:THR:HG22	2.06	0.55
1:B:941:THR:HG22	1:B:941:THR:O	2.06	0.55
1:C:960:ASN:O	1:C:964:LYS:HG3	2.06	0.55
1:A:337:PRO:HB2	1:A:340:GLU:HG2	1.88	0.54
1:B:337:PRO:HB2	1:B:340:GLU:HG2	1.88	0.54
1:B:480:CYS:O	1:B:483:VAL:HG22	2.07	0.54
1:A:960:ASN:O	1:A:964:LYS:HG3	2.06	0.54
1:C:1142:GLN:HB2	1:C:1143:PRO:HD3	1.89	0.54
1:B:61:ASN:OD1	3:B:1403:NAG:H82	2.07	0.54
1:B:1142:GLN:HB2	1:B:1143:PRO:HD3	1.89	0.54
1:C:212:LEU:HD22	1:C:217:PRO:HG3	1.89	0.54
3:B:1417:NAG:H83	3:B:1417:NAG:H3	1.90	0.54
1:A:188:ASN:ND2	1:A:207:HIS:HE1	2.05	0.54
3:A:1417:NAG:H83	3:A:1417:NAG:H3	1.90	0.54
1:C:480:CYS:O	1:C:483:VAL:HG22	2.07	0.54
1:A:1142:GLN:HB2	1:A:1143:PRO:HD3	1.89	0.53
1:C:61:ASN:OD1	3:C:1403:NAG:H82	2.07	0.53
1:A:480:CYS:O	1:A:483:VAL:HG22	2.07	0.53
1:C:188:ASN:ND2	1:C:207:HIS:HE1	2.05	0.53
1:B:188:ASN:ND2	1:B:207:HIS:HE1	2.05	0.53
1:C:1118:ASP:OD1	1:C:1118:ASP:N	2.42	0.53
3:C:1415:NAG:H83	3:C:1415:NAG:H3	1.90	0.53
1:B:1118:ASP:N	1:B:1118:ASP:OD1	2.42	0.53
1:B:188:ASN:HD22	1:B:207:HIS:HE1	1.57	0.52
1:C:188:ASN:HD22	1:C:207:HIS:HE1	1.58	0.52
3:C:1410:NAG:C6	3:C:1411:NAG:C7	2.80	0.52
1:A:188:ASN:HD22	1:A:207:HIS:HE1	1.57	0.52
1:A:841:LEU:HD12	1:C:588:THR:HG21	1.91	0.52
1:C:1142:GLN:N	1:C:1143:PRO:CD	2.73	0.52
1:A:1142:GLN:N	1:A:1143:PRO:CD	2.73	0.51
1:B:1142:GLN:N	1:B:1143:PRO:CD	2.73	0.51
1:A:354:ASN:O	1:A:398:ASP:HA	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:792:PRO:HG3	1:C:707:TYR:HB3	1.92	0.51
3:B:1412:NAG:C6	3:B:1413:NAG:C7	2.80	0.51
1:C:354:ASN:O	1:C:398:ASP:HA	2.10	0.51
1:A:1118:ASP:OD1	1:A:1118:ASP:N	2.42	0.51
1:B:354:ASN:O	1:B:398:ASP:HA	2.10	0.51
1:B:642:VAL:HG13	1:B:651:ILE:HG12	1.93	0.51
1:B:835:LYS:HD3	1:B:851:CYS:SG	2.51	0.51
1:C:642:VAL:HG13	1:C:651:ILE:HG12	1.93	0.51
1:A:213:VAL:HG23	1:A:214:ARG:HG2	1.93	0.50
1:B:804:GLN:NE2	3:B:1416:NAG:O6	2.44	0.50
1:A:804:GLN:NE2	3:A:1416:NAG:O6	2.44	0.50
1:C:19:THR:O	1:C:20:THR:OG1	2.27	0.50
1:A:835:LYS:HD3	1:A:851:CYS:SG	2.51	0.50
1:B:32:PHE:CD2	1:B:218:GLN:HG2	2.47	0.50
1:B:213:VAL:HG23	1:B:214:ARG:HG2	1.93	0.50
1:C:835:LYS:HD3	1:C:851:CYS:SG	2.51	0.50
1:A:645:THR:CG2	1:A:670:ILE:HG13	2.42	0.50
1:B:645:THR:CG2	1:B:670:ILE:HG13	2.42	0.50
1:A:69:HIS:CE1	1:A:70:VAL:HG22	2.47	0.49
1:C:804:GLN:NE2	3:C:1414:NAG:O6	2.44	0.49
1:A:377:PHE:CE2	4:A:1420:EIC:H21	2.48	0.49
1:A:1145:LEU:HD23	1:A:1145:LEU:N	2.26	0.49
1:C:213:VAL:HG23	1:C:214:ARG:HG2	1.93	0.49
1:A:32:PHE:CD2	1:A:218:GLN:HG2	2.47	0.49
1:C:32:PHE:CD2	1:C:218:GLN:HG2	2.47	0.49
1:C:69:HIS:CE1	1:C:70:VAL:HG22	2.47	0.49
1:A:567:ARG:HD2	1:B:42:VAL:HG11	1.95	0.49
1:C:79:PHE:CZ	1:C:244:LEU:HD13	2.48	0.49
1:B:198:ASP:N	1:B:198:ASP:OD1	2.46	0.49
1:A:79:PHE:CZ	1:A:244:LEU:HD13	2.48	0.49
1:A:642:VAL:HG13	1:A:651:ILE:HG12	1.93	0.49
1:B:69:HIS:CE1	1:B:70:VAL:HG22	2.47	0.49
1:B:1145:LEU:HD23	1:B:1145:LEU:N	2.26	0.49
1:A:117:LEU:HD13	1:A:130:VAL:HG22	1.95	0.49
1:B:109:THR:OG1	1:B:114:THR:OG1	2.31	0.49
1:C:1145:LEU:HD23	1:C:1145:LEU:N	2.26	0.49
1:A:42:VAL:HG11	1:C:567:ARG:HD2	1.95	0.48
1:A:198:ASP:OD1	1:A:198:ASP:N	2.46	0.48
1:B:147:LYS:HE3	1:B:147:LYS:HB3	1.58	0.48
1:B:19:THR:O	1:B:20:THR:OG1	2.27	0.48
1:C:645:THR:CG2	1:C:670:ILE:HG13	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:117:LEU:HD13	1:C:130:VAL:HG22	1.95	0.48
1:C:940:SER:C	1:C:941:THR:HG1	2.03	0.48
1:A:533:LEU:HD21	1:A:585:LEU:HD11	1.96	0.48
1:C:91:TYR:OH	1:C:191:GLU:OE1	2.20	0.48
1:C:109:THR:OG1	1:C:114:THR:OG1	2.31	0.48
1:C:533:LEU:HD21	1:C:585:LEU:HD11	1.96	0.48
1:A:109:THR:OG1	1:A:114:THR:OG1	2.31	0.47
3:B:1414:NAG:H3	3:B:1414:NAG:H83	1.96	0.47
1:B:79:PHE:CZ	1:B:244:LEU:HD13	2.48	0.47
1:B:117:LEU:HD13	1:B:130:VAL:HG22	1.95	0.47
1:B:533:LEU:HD21	1:B:585:LEU:HD11	1.96	0.47
1:C:197:ILE:HD12	1:C:202:LYS:HD2	1.96	0.47
1:B:197:ILE:HD12	1:B:202:LYS:HD2	1.96	0.47
3:C:1408:NAG:H83	3:C:1408:NAG:O3	2.15	0.47
3:B:1408:NAG:O3	3:B:1408:NAG:H83	2.15	0.47
1:C:1051:SER:OG	1:C:1064:HIS:HD2	1.97	0.47
1:A:69:HIS:HD2	1:A:259:THR:OG1	1.98	0.47
1:A:245:HIS:HB2	1:A:259:THR:HG22	1.97	0.47
1:A:1051:SER:OG	1:A:1064:HIS:HD2	1.97	0.47
1:C:198:ASP:OD1	1:C:198:ASP:N	2.46	0.47
1:C:986:PRO:O	1:C:990:GLU:HG3	2.15	0.47
1:B:986:PRO:O	1:B:990:GLU:HG3	2.15	0.47
3:C:1412:NAG:H3	3:C:1412:NAG:H83	1.96	0.47
3:A:1408:NAG:H83	3:A:1408:NAG:O3	2.15	0.47
1:B:69:HIS:HD2	1:B:259:THR:OG1	1.98	0.47
1:B:1051:SER:OG	1:B:1064:HIS:HD2	1.97	0.47
1:A:130:VAL:HG21	1:A:231:ILE:HG22	1.97	0.46
1:A:147:LYS:HE3	1:A:147:LYS:HB3	1.58	0.46
1:B:245:HIS:HB2	1:B:259:THR:HG22	1.97	0.46
1:B:617:CYS:HB3	1:B:633:TRP:CE2	2.50	0.46
1:B:69:HIS:CG	1:B:70:VAL:HG23	2.50	0.46
1:C:69:HIS:CG	1:C:70:VAL:HG23	2.50	0.46
1:C:130:VAL:HG21	1:C:231:ILE:HG22	1.97	0.46
1:C:617:CYS:HB3	1:C:633:TRP:CE2	2.50	0.46
1:A:395:VAL:HG11	4:A:1420:EIC:H131	1.98	0.46
1:C:69:HIS:HD2	1:C:259:THR:OG1	1.97	0.46
1:C:245:HIS:HB2	1:C:259:THR:HG22	1.97	0.46
1:A:339:GLY:CA	3:A:1409:NAG:C8	2.66	0.46
1:A:197:ILE:HD12	1:A:202:LYS:HD2	1.96	0.46
3:C:1412:NAG:C8	3:C:1412:NAG:C3	2.87	0.46
2:K:1:NAG:H62	2:K:2:NAG:H82	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:ARG:HH11	1:A:79:PHE:HB3	1.81	0.45
1:A:596:SER:OG	1:A:613:GLN:OE1	2.34	0.45
1:A:938:LEU:O	1:A:940:SER:N	2.50	0.45
1:A:971:GLY:O	1:A:995:ARG:NH1	2.47	0.45
1:A:1048:HIS:HA	1:A:1066:THR:HG22	1.98	0.45
1:C:1141:LEU:O	1:C:1144:GLU:HB2	2.16	0.45
1:A:19:THR:O	1:A:20:THR:OG1	2.27	0.45
1:A:707:TYR:HB3	1:B:792:PRO:HG3	1.98	0.45
3:B:1412:NAG:H5	3:B:1413:NAG:O7	2.16	0.45
1:C:244:LEU:HA	1:C:244:LEU:HD12	1.74	0.45
1:C:1048:HIS:HA	1:C:1066:THR:HG22	1.98	0.45
1:A:986:PRO:O	1:A:990:GLU:HG3	2.15	0.45
3:A:1412:NAG:H5	3:A:1413:NAG:O7	2.16	0.45
1:C:596:SER:OG	1:C:613:GLN:OE1	2.34	0.45
1:B:938:LEU:O	1:B:940:SER:N	2.50	0.45
1:A:391:CYS:HA	1:A:525:CYS:HA	1.98	0.45
1:A:1141:LEU:O	1:A:1144:GLU:HB2	2.16	0.45
4:C:1420:EIC:H142	4:C:1420:EIC:H112	1.65	0.45
1:A:69:HIS:CG	1:A:70:VAL:HG23	2.50	0.45
1:A:532:ASN:HD22	1:A:532:ASN:N	2.14	0.45
1:A:617:CYS:HB3	1:A:633:TRP:CE2	2.50	0.45
1:B:130:VAL:HG21	1:B:231:ILE:HG22	1.97	0.45
1:B:596:SER:OG	1:B:613:GLN:OE1	2.34	0.45
1:C:83:VAL:HG22	1:C:239:GLN:NE2	2.32	0.45
1:C:395:VAL:HG21	1:C:524:VAL:HG21	1.99	0.45
1:C:710:ASN:C	1:C:710:ASN:HD22	2.20	0.45
1:C:339:GLY:CA	2:L:1:NAG:C8	2.66	0.45
1:C:353:TRP:O	1:C:466:ARG:NH1	2.50	0.45
1:C:938:LEU:O	1:C:940:SER:N	2.50	0.45
1:A:358:ILE:HD13	4:A:1420:EIC:H162	1.98	0.45
3:B:1414:NAG:C8	3:B:1414:NAG:C3	2.87	0.45
1:C:391:CYS:HA	1:C:525:CYS:HA	1.98	0.45
3:C:1410:NAG:H5	3:C:1411:NAG:O7	2.16	0.45
2:D:1:NAG:H62	2:D:2:NAG:H82	1.99	0.45
1:A:117:LEU:HD13	1:A:130:VAL:CG2	2.47	0.45
1:A:83:VAL:HG22	1:A:239:GLN:NE2	2.32	0.44
1:B:1141:LEU:O	1:B:1144:GLU:HB2	2.16	0.44
1:B:1048:HIS:HA	1:B:1066:THR:HG22	1.98	0.44
1:C:971:GLY:O	1:C:995:ARG:NH1	2.47	0.44
1:A:96:GLU:OE1	1:A:101:ILE:HD12	2.18	0.44
1:A:353:TRP:O	1:A:466:ARG:NH1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:117:LEU:HD13	1:C:130:VAL:CG2	2.47	0.44
3:C:1407:NAG:O7	3:C:1407:NAG:O3	2.32	0.44
1:B:21:ARG:HH11	1:B:79:PHE:HB3	1.81	0.44
1:B:83:VAL:HG22	1:B:239:GLN:NE2	2.32	0.44
1:C:726:ILE:HD12	1:C:945:LEU:HD22	1.99	0.44
1:A:710:ASN:HD22	1:A:710:ASN:C	2.20	0.44
1:B:532:ASN:N	1:B:532:ASN:HD22	2.14	0.44
3:B:1420:NAG:H61	3:B:1421:NAG:O7	2.18	0.44
1:C:21:ARG:HH11	1:C:79:PHE:HB3	1.81	0.44
1:C:96:GLU:OE1	1:C:101:ILE:HD12	2.18	0.44
1:C:785:VAL:HG23	1:C:787:GLN:H	1.83	0.44
1:B:117:LEU:HD13	1:B:130:VAL:CG2	2.47	0.44
1:B:130:VAL:HG21	1:B:231:ILE:CG2	2.48	0.44
1:B:971:GLY:O	1:B:995:ARG:NH1	2.47	0.44
3:C:1418:NAG:H61	3:C:1419:NAG:O7	2.18	0.44
1:A:130:VAL:HG21	1:A:231:ILE:CG2	2.48	0.44
1:B:726:ILE:HD12	1:B:945:LEU:HD22	1.99	0.44
1:C:252:GLY:HA3	1:C:257:GLY:N	2.33	0.44
1:C:532:ASN:N	1:C:532:ASN:HD22	2.15	0.44
1:A:395:VAL:HG21	1:A:524:VAL:HG21	1.99	0.44
1:A:431:GLY:HA2	1:A:515:PHE:CZ	2.53	0.44
3:A:1418:NAG:H61	3:A:1419:NAG:O7	2.18	0.44
1:B:785:VAL:HG23	1:B:787:GLN:H	1.83	0.44
1:B:339:GLY:CA	3:B:1409:NAG:C8	2.66	0.43
1:B:395:VAL:HG21	1:B:524:VAL:HG21	1.99	0.43
1:B:431:GLY:HA2	1:B:515:PHE:CZ	2.53	0.43
1:A:726:ILE:HD12	1:A:945:LEU:HD22	1.99	0.43
1:A:785:VAL:HG23	1:A:787:GLN:H	1.83	0.43
3:A:1412:NAG:HO3	3:A:1412:NAG:C7	2.30	0.43
1:B:96:GLU:OE1	1:B:101:ILE:HD12	2.18	0.43
1:B:391:CYS:HA	1:B:525:CYS:HA	1.99	0.43
1:A:78:ARG:HA	1:A:78:ARG:HD2	1.79	0.43
1:C:130:VAL:HG21	1:C:231:ILE:CG2	2.48	0.43
1:C:431:GLY:HA2	1:C:515:PHE:CZ	2.53	0.43
1:A:252:GLY:HA3	1:A:257:GLY:N	2.33	0.43
1:C:1142:GLN:N	1:C:1143:PRO:HD2	2.33	0.43
1:A:1142:GLN:N	1:A:1143:PRO:HD2	2.34	0.43
1:B:353:TRP:O	1:B:466:ARG:NH1	2.50	0.43
1:B:710:ASN:C	1:B:710:ASN:HD22	2.20	0.43
1:C:913:GLN:H	1:C:913:GLN:HG3	1.63	0.43
1:A:537:LYS:HB3	1:A:537:LYS:HE2	1.70	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1407:NAG:O7	3:A:1407:NAG:O3	2.32	0.43
1:A:328:ARG:NH1	1:A:531:THR:O	2.50	0.42
1:A:980:ILE:O	1:A:984:LEU:HB2	2.19	0.42
1:B:252:GLY:HA3	1:B:257:GLY:N	2.33	0.42
1:B:980:ILE:O	1:B:984:LEU:HB2	2.19	0.42
1:C:147:LYS:HB3	1:C:147:LYS:HE3	1.58	0.42
1:C:153:MET:CE	3:C:1405:NAG:HN2	2.32	0.42
1:A:563:GLN:O	1:A:577:ARG:NH1	2.53	0.42
1:A:153:MET:CE	3:A:1405:NAG:HN2	2.32	0.42
1:A:588:THR:HG21	1:B:841:LEU:HD12	2.02	0.42
1:B:328:ARG:NH1	1:B:531:THR:O	2.50	0.42
1:C:980:ILE:O	1:C:984:LEU:HB2	2.19	0.42
1:A:752:LEU:HD21	1:A:990:GLU:OE2	2.20	0.42
1:B:1142:GLN:N	1:B:1143:PRO:HD2	2.33	0.42
1:C:563:GLN:O	1:C:577:ARG:NH1	2.53	0.42
1:C:746:SER:HB3	1:C:749:CYS:HB3	2.02	0.42
1:A:614:ASP:OD2	1:B:854:LYS:HE3	2.19	0.42
1:B:1038:LYS:HA	1:B:1038:LYS:HD3	1.90	0.42
3:A:1414:NAG:H3	3:A:1414:NAG:H83	1.96	0.42
1:B:746:SER:HB3	1:B:749:CYS:HB3	2.02	0.42
1:C:533:LEU:HD12	1:C:533:LEU:HA	1.91	0.42
1:C:817:PHE:CE2	1:C:935:GLN:CD	2.93	0.42
1:A:564:GLN:HE21	1:A:564:GLN:HB2	1.67	0.42
1:A:938:LEU:C	1:A:940:SER:N	2.73	0.42
1:A:940:SER:C	1:A:941:THR:HG1	2.00	0.42
1:C:66:HIS:HB2	1:C:67:ALA:H	1.60	0.42
1:A:37:TYR:OH	1:A:54:LEU:O	2.25	0.41
1:A:1038:LYS:HA	1:A:1038:LYS:HD3	1.90	0.41
1:B:69:HIS:C	1:B:70:VAL:CG2	2.86	0.41
1:B:569:ILE:HD11	1:C:964:LYS:HB3	2.02	0.41
1:C:425:LEU:HD23	1:C:425:LEU:HA	1.93	0.41
1:B:703:ASN:OD1	1:B:704:SER:N	2.53	0.41
1:A:703:ASN:OD1	1:A:704:SER:N	2.53	0.41
1:A:818:ILE:HB	1:A:1054:GLN:HE21	1.86	0.41
1:B:532:ASN:N	1:B:532:ASN:ND2	2.69	0.41
1:C:537:LYS:HB3	1:C:537:LYS:HE2	1.70	0.41
1:A:78:ARG:HG3	1:A:80:ASP:OD2	2.21	0.41
1:A:759:PHE:O	1:A:763:LEU:HG	2.21	0.41
4:A:1420:EIC:H72	4:A:1420:EIC:H42	1.88	0.41
1:B:153:MET:CE	3:B:1405:NAG:HN2	2.32	0.41
1:B:938:LEU:C	1:B:940:SER:N	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:938:LEU:C	1:C:940:SER:N	2.73	0.41
1:A:675:GLN:HE21	1:A:675:GLN:HB3	1.62	0.41
1:B:78:ARG:HA	1:B:78:ARG:HD2	1.79	0.41
1:B:563:GLN:O	1:B:577:ARG:NH1	2.53	0.41
1:B:752:LEU:HD21	1:B:990:GLU:OE2	2.20	0.41
1:C:818:ILE:HB	1:C:1054:GLN:HE21	1.85	0.41
1:B:1028:LYS:NZ	1:B:1042:PHE:O	2.53	0.41
1:C:703:ASN:OD1	1:C:704:SER:N	2.53	0.41
1:A:147:LYS:HD3	1:A:248:TYR:CE1	2.56	0.41
1:B:66:HIS:HB2	1:B:67:ALA:H	1.60	0.41
1:B:818:ILE:HB	1:B:1054:GLN:HE21	1.86	0.41
1:C:78:ARG:HA	1:C:78:ARG:HD2	1.79	0.41
1:A:532:ASN:N	1:A:532:ASN:ND2	2.69	0.41
1:A:817:PHE:CE2	1:A:935:GLN:CD	2.93	0.41
1:B:130:VAL:HG12	1:B:130:VAL:O	2.21	0.41
1:B:817:PHE:CE2	1:B:935:GLN:CD	2.93	0.41
1:B:884:SER:OG	1:B:893:ALA:HB1	2.21	0.41
1:C:752:LEU:HD21	1:C:990:GLU:OE2	2.20	0.41
1:C:1142:GLN:O	1:C:1145:LEU:N	2.41	0.41
1:A:746:SER:HB3	1:A:749:CYS:HB3	2.02	0.41
1:B:153:MET:HE2	3:B:1405:NAG:H3	2.03	0.41
1:B:715:PRO:HA	1:B:1072:GLU:HA	2.03	0.41
1:B:759:PHE:O	1:B:763:LEU:HG	2.21	0.41
1:A:1028:LYS:NZ	1:A:1042:PHE:O	2.53	0.40
1:B:78:ARG:HG3	1:B:80:ASP:OD2	2.21	0.40
1:A:153:MET:HE2	3:A:1405:NAG:H3	2.03	0.40
1:A:884:SER:OG	1:A:893:ALA:HB1	2.21	0.40
1:C:564:GLN:HE21	1:C:564:GLN:HB2	1.67	0.40
1:C:884:SER:OG	1:C:893:ALA:HB1	2.21	0.40
1:B:148:ASN:OD1	1:B:148:ASN:N	2.55	0.40
1:B:208:THR:HA	1:B:209:PRO:HD3	1.92	0.40
1:B:330:PRO:HD2	1:B:525:CYS:SG	2.62	0.40
1:C:826:VAL:HB	1:C:1057:PRO:HG2	2.04	0.40
1:C:130:VAL:O	1:C:130:VAL:HG12	2.21	0.40
1:C:1028:LYS:NZ	1:C:1042:PHE:O	2.53	0.40
1:A:330:PRO:HD2	1:A:525:CYS:SG	2.62	0.40
1:A:862:PRO:HA	1:A:863:PRO:HD3	1.97	0.40
1:C:78:ARG:HG3	1:C:80:ASP:OD2	2.21	0.40
1:C:153:MET:HE2	3:C:1405:NAG:H3	2.04	0.40
1:C:532:ASN:N	1:C:532:ASN:ND2	2.69	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	1089/1283 (85%)	1026 (94%)	59 (5%)	4 (0%)	34	60
1	B	1089/1283 (85%)	1026 (94%)	59 (5%)	4 (0%)	34	60
1	C	1089/1283 (85%)	1026 (94%)	59 (5%)	4 (0%)	34	60
All	All	3267/3849 (85%)	3078 (94%)	177 (5%)	12 (0%)	38	60

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	67	ALA
1	B	67	ALA
1	C	67	ALA
1	A	939	SER
1	B	939	SER
1	C	939	SER
1	A	936	ASP
1	B	936	ASP
1	C	936	ASP
1	A	251	PRO
1	B	251	PRO
1	C	251	PRO

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	957/1122 (85%)	852 (89%)	105 (11%)	6 14
1	B	957/1122 (85%)	852 (89%)	105 (11%)	6 14
1	C	957/1122 (85%)	854 (89%)	103 (11%)	6 15
All	All	2871/3366 (85%)	2558 (89%)	313 (11%)	10 14

All (313) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	THR
1	A	31	SER
1	A	40	ASP
1	A	47	VAL
1	A	51	THR
1	A	53	ASP
1	A	66	HIS
1	A	79	PHE
1	A	94	SER
1	A	96	GLU
1	A	108	THR
1	A	118	LEU
1	A	124	THR
1	A	131	CYS
1	A	147	LYS
1	A	153	MET
1	A	156	GLU
1	A	162	SER
1	A	166	CYS
1	A	173	GLN
1	A	178	ASP
1	A	185	ASN
1	A	197	ILE
1	A	198	ASP
1	A	205	SER
1	A	208	THR
1	A	212	LEU
1	A	215	ASP
1	A	221	SER
1	A	247	SER
1	A	255	SER

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Mol	Chain	Res	Type
1	A	259	THR
1	A	271	GLN
1	A	277	LEU
1	A	281	GLU
1	A	299	THR
1	A	305	SER
1	A	317	ASN
1	A	325	SER
1	A	333	THR
1	A	366	SER
1	A	370	ASN
1	A	373	SER
1	A	375	SER
1	A	393	THR
1	A	399	SER
1	A	443	SER
1	A	445	VAL
1	A	448	ASN
1	A	459	SER
1	A	469	SER
1	A	471	GLU
1	A	493	GLN
1	A	514	SER
1	A	530	SER
1	A	531	THR
1	A	534	VAL
1	A	544	ASN
1	A	569	ILE
1	A	586	ASP
1	A	588	THR
1	A	590	CYS
1	A	599	THR
1	A	604	THR
1	A	606	ASN
1	A	614	ASP
1	A	617	CYS
1	A	638	THR
1	A	642	VAL
1	A	645	THR
1	A	657	ASN
1	A	675	GLN
1	A	676	THR

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Mol	Chain	Res	Type
1	A	691	SER
1	A	708	SER
1	A	710	ASN
1	A	719	THR
1	A	723	THR
1	A	726	ILE
1	A	730	SER
1	A	732	THR
1	A	735	SER
1	A	745	ASP
1	A	746	SER
1	A	761	THR
1	A	780	GLU
1	A	790	LYS
1	A	810	SER
1	A	814	LYS
1	A	881	THR
1	A	884	SER
1	A	886	TRP
1	A	962	LEU
1	A	964	LYS
1	A	974	SER
1	A	982	SER
1	A	991	VAL
1	A	1002	GLN
1	A	1030	SER
1	A	1092	GLU
1	A	1097	SER
1	A	1118	ASP
1	A	1128	VAL
1	A	1136	THR
1	A	1142	GLN
1	B	19	THR
1	B	31	SER
1	B	40	ASP
1	B	47	VAL
1	B	51	THR
1	B	53	ASP
1	B	66	HIS
1	B	79	PHE
1	B	94	SER
1	B	96	GLU

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Mol	Chain	Res	Type
1	B	108	THR
1	B	118	LEU
1	B	124	THR
1	B	131	CYS
1	B	147	LYS
1	B	153	MET
1	B	156	GLU
1	B	162	SER
1	B	166	CYS
1	B	173	GLN
1	B	178	ASP
1	B	185	ASN
1	B	197	ILE
1	B	198	ASP
1	B	205	SER
1	B	208	THR
1	B	212	LEU
1	B	215	ASP
1	B	221	SER
1	B	247	SER
1	B	255	SER
1	B	259	THR
1	B	271	GLN
1	B	277	LEU
1	B	281	GLU
1	B	299	THR
1	B	305	SER
1	B	317	ASN
1	B	325	SER
1	B	333	THR
1	B	366	SER
1	B	370	ASN
1	B	373	SER
1	B	375	SER
1	B	393	THR
1	B	399	SER
1	B	443	SER
1	B	445	VAL
1	B	448	ASN
1	B	459	SER
1	B	469	SER
1	B	471	GLU

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Mol	Chain	Res	Type
1	B	493	GLN
1	B	514	SER
1	B	530	SER
1	B	531	THR
1	B	534	VAL
1	B	544	ASN
1	B	569	ILE
1	B	586	ASP
1	B	588	THR
1	B	590	CYS
1	B	599	THR
1	B	604	THR
1	B	606	ASN
1	B	614	ASP
1	B	617	CYS
1	B	638	THR
1	B	642	VAL
1	B	645	THR
1	B	657	ASN
1	B	675	GLN
1	B	676	THR
1	B	691	SER
1	B	708	SER
1	B	710	ASN
1	B	719	THR
1	B	723	THR
1	B	726	ILE
1	B	730	SER
1	B	732	THR
1	B	735	SER
1	B	745	ASP
1	B	746	SER
1	B	761	THR
1	B	780	GLU
1	B	790	LYS
1	B	810	SER
1	B	814	LYS
1	B	881	THR
1	B	884	SER
1	B	886	TRP
1	B	962	LEU
1	B	964	LYS

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Mol	Chain	Res	Type
1	B	974	SER
1	B	982	SER
1	B	991	VAL
1	B	1002	GLN
1	B	1030	SER
1	B	1092	GLU
1	B	1097	SER
1	B	1118	ASP
1	B	1128	VAL
1	B	1136	THR
1	B	1142	GLN
1	C	19	THR
1	C	31	SER
1	C	40	ASP
1	C	47	VAL
1	C	51	THR
1	C	53	ASP
1	C	66	HIS
1	C	94	SER
1	C	96	GLU
1	C	108	THR
1	C	118	LEU
1	C	124	THR
1	C	131	CYS
1	C	147	LYS
1	C	156	GLU
1	C	162	SER
1	C	166	CYS
1	C	173	GLN
1	C	178	ASP
1	C	185	ASN
1	C	197	ILE
1	C	198	ASP
1	C	205	SER
1	C	208	THR
1	C	212	LEU
1	C	215	ASP
1	C	221	SER
1	C	247	SER
1	C	255	SER
1	C	259	THR
1	C	271	GLN

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Mol	Chain	Res	Type
1	C	277	LEU
1	C	281	GLU
1	C	299	THR
1	C	305	SER
1	C	317	ASN
1	C	325	SER
1	C	333	THR
1	C	366	SER
1	C	370	ASN
1	C	373	SER
1	C	375	SER
1	C	393	THR
1	C	399	SER
1	C	443	SER
1	C	445	VAL
1	C	448	ASN
1	C	459	SER
1	C	469	SER
1	C	471	GLU
1	C	493	GLN
1	C	514	SER
1	C	530	SER
1	C	531	THR
1	C	534	VAL
1	C	544	ASN
1	C	569	ILE
1	C	586	ASP
1	C	588	THR
1	C	590	CYS
1	C	599	THR
1	C	604	THR
1	C	606	ASN
1	C	614	ASP
1	C	617	CYS
1	C	638	THR
1	C	642	VAL
1	C	645	THR
1	C	657	ASN
1	C	675	GLN
1	C	676	THR
1	C	691	SER
1	C	708	SER

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Mol	Chain	Res	Type
1	C	710	ASN
1	C	719	THR
1	C	723	THR
1	C	726	ILE
1	C	730	SER
1	C	732	THR
1	C	735	SER
1	C	745	ASP
1	C	746	SER
1	C	761	THR
1	C	780	GLU
1	C	790	LYS
1	C	810	SER
1	C	814	LYS
1	C	881	THR
1	C	884	SER
1	C	886	TRP
1	C	962	LEU
1	C	964	LYS
1	C	974	SER
1	C	982	SER
1	C	991	VAL
1	C	1002	GLN
1	C	1030	SER
1	C	1092	GLU
1	C	1097	SER
1	C	1118	ASP
1	C	1128	VAL
1	C	1136	THR
1	C	1142	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (91) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	HIS
1	A	69	HIS
1	A	183	GLN
1	A	188	ASN
1	A	207	HIS
1	A	239	GLN
1	A	314	GLN
1	A	317	ASN

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Mol	Chain	Res	Type
1	A	448	ASN
1	A	450	ASN
1	A	493	GLN
1	A	498	GLN
1	A	532	ASN
1	A	544	ASN
1	A	556	ASN
1	A	564	GLN
1	A	606	ASN
1	A	613	GLN
1	A	675	GLN
1	A	710	ASN
1	A	751	ASN
1	A	804	GLN
1	A	856	ASN
1	A	919	ASN
1	A	925	ASN
1	A	1023	ASN
1	A	1036	GLN
1	A	1054	GLN
1	A	1064	HIS
1	A	1125	ASN
1	B	66	HIS
1	B	69	HIS
1	B	183	GLN
1	B	188	ASN
1	B	207	HIS
1	B	239	GLN
1	B	314	GLN
1	B	317	ASN
1	B	448	ASN
1	B	450	ASN
1	B	493	GLN
1	B	498	GLN
1	B	532	ASN
1	B	544	ASN
1	B	556	ASN
1	B	564	GLN
1	B	606	ASN
1	B	613	GLN
1	B	675	GLN
1	B	710	ASN

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Mol	Chain	Res	Type
1	B	751	ASN
1	B	804	GLN
1	B	856	ASN
1	B	919	ASN
1	B	925	ASN
1	B	935	GLN
1	B	1023	ASN
1	B	1036	GLN
1	B	1054	GLN
1	B	1064	HIS
1	B	1125	ASN
1	C	66	HIS
1	C	69	HIS
1	C	183	GLN
1	C	188	ASN
1	C	207	HIS
1	C	239	GLN
1	C	314	GLN
1	C	317	ASN
1	C	448	ASN
1	C	450	ASN
1	C	493	GLN
1	C	498	GLN
1	C	532	ASN
1	C	544	ASN
1	C	556	ASN
1	C	564	GLN
1	C	606	ASN
1	C	613	GLN
1	C	675	GLN
1	C	710	ASN
1	C	751	ASN
1	C	804	GLN
1	C	856	ASN
1	C	919	ASN
1	C	925	ASN
1	C	1023	ASN
1	C	1036	GLN
1	C	1054	GLN
1	C	1064	HIS
1	C	1125	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

22 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	1.16	1 (7%)	17,19,21	0.61	0
2	NAG	D	2	2	14,14,15	2.26	2 (14%)	17,19,21	0.97	2 (11%)
2	NAG	E	1	2,1	14,14,15	0.30	0	17,19,21	0.61	0
2	NAG	E	2	2	14,14,15	0.52	0	17,19,21	0.47	0
2	NAG	F	1	2,1	14,14,15	0.70	1 (7%)	17,19,21	0.70	0
2	NAG	F	2	2	14,14,15	0.39	0	17,19,21	1.40	3 (17%)
2	NAG	G	1	2,1	14,14,15	0.71	1 (7%)	17,19,21	0.67	0
2	NAG	G	2	2	14,14,15	0.29	0	17,19,21	0.65	0
2	NAG	H	1	2,1	14,14,15	1.16	1 (7%)	17,19,21	0.61	0
2	NAG	H	2	2	14,14,15	2.27	2 (14%)	17,19,21	0.97	2 (11%)
2	NAG	I	1	2,1	14,14,15	0.30	0	17,19,21	0.62	0
2	NAG	I	2	2	14,14,15	0.51	0	17,19,21	0.47	0
2	NAG	J	1	2,1	14,14,15	0.71	1 (7%)	17,19,21	0.67	0
2	NAG	J	2	2	14,14,15	0.29	0	17,19,21	0.65	0
2	NAG	K	1	2,1	14,14,15	1.15	1 (7%)	17,19,21	0.61	0
2	NAG	K	2	2	14,14,15	2.26	2 (14%)	17,19,21	0.97	2 (11%)
2	NAG	L	1	2,1	14,14,15	0.86	1 (7%)	17,19,21	0.55	0
2	NAG	L	2	2	14,14,15	2.94	3 (21%)	17,19,21	1.54	4 (23%)
2	NAG	M	1	2,1	14,14,15	0.29	0	17,19,21	0.61	0
2	NAG	M	2	2	14,14,15	0.51	0	17,19,21	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	N	1	2,1	14,14,15	0.71	1 (7%)	17,19,21	0.67	0
2	NAG	N	2	2	14,14,15	0.30	0	17,19,21	0.65	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	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	NAG	E	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	NAG	F	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	5/6/23/26	0/1/1/1
2	NAG	G	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	G	2	2	-	3/6/23/26	0/1/1/1
2	NAG	H	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1
2	NAG	I	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	I	2	2	-	2/6/23/26	0/1/1/1
2	NAG	J	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	J	2	2	-	3/6/23/26	0/1/1/1
2	NAG	K	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	K	2	2	-	2/6/23/26	0/1/1/1
2	NAG	L	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	L	2	2	-	2/6/23/26	0/1/1/1
2	NAG	M	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	M	2	2	-	2/6/23/26	0/1/1/1
2	NAG	N	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	N	2	2	-	3/6/23/26	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	2	NAG	O5-C1	-8.15	1.30	1.43
2	H	2	NAG	O5-C1	-7.16	1.32	1.43
2	D	2	NAG	O5-C1	-7.11	1.32	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	2	NAG	O5-C1	-7.09	1.32	1.43
2	L	2	NAG	C1-C2	-6.76	1.42	1.52
2	K	2	NAG	C1-C2	-4.45	1.45	1.52
2	H	2	NAG	C1-C2	-4.44	1.45	1.52
2	D	2	NAG	C1-C2	-4.43	1.45	1.52
2	H	1	NAG	O5-C1	-4.24	1.36	1.43
2	D	1	NAG	O5-C1	-4.23	1.37	1.43
2	K	1	NAG	O5-C1	-4.21	1.37	1.43
2	L	1	NAG	O5-C1	-2.82	1.39	1.43
2	G	1	NAG	O5-C1	-2.61	1.39	1.43
2	J	1	NAG	O5-C1	-2.60	1.39	1.43
2	N	1	NAG	O5-C1	-2.59	1.39	1.43
2	F	1	NAG	O5-C1	-2.36	1.39	1.43
2	L	2	NAG	C2-N2	-2.08	1.42	1.46

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	2	NAG	C2-N2-C7	4.43	129.22	122.90
2	L	2	NAG	C1-C2-N2	3.29	116.11	110.49
2	L	2	NAG	O5-C1-C2	3.27	116.45	111.29
2	L	2	NAG	C1-O5-C5	3.22	116.55	112.19
2	H	2	NAG	C1-C2-N2	2.52	114.79	110.49
2	D	2	NAG	C1-C2-N2	2.50	114.76	110.49
2	K	2	NAG	C1-O5-C5	2.50	115.58	112.19
2	D	2	NAG	C1-O5-C5	2.49	115.56	112.19
2	K	2	NAG	C1-C2-N2	2.48	114.72	110.49
2	H	2	NAG	C1-O5-C5	2.46	115.52	112.19
2	F	2	NAG	C1-C2-N2	2.36	114.51	110.49
2	L	2	NAG	C2-N2-C7	2.20	126.04	122.90
2	F	2	NAG	C1-O5-C5	2.07	115.00	112.19

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	2	NAG	O5-C5-C6-O6
2	H	2	NAG	O5-C5-C6-O6
2	K	2	NAG	O5-C5-C6-O6
2	G	1	NAG	O5-C5-C6-O6
2	J	1	NAG	O5-C5-C6-O6
2	N	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	G	1	NAG	C4-C5-C6-O6
2	J	1	NAG	C4-C5-C6-O6
2	N	1	NAG	C4-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	H	2	NAG	C4-C5-C6-O6
2	K	2	NAG	C4-C5-C6-O6
2	F	2	NAG	C8-C7-N2-C2
2	F	2	NAG	O7-C7-N2-C2
2	F	1	NAG	C4-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6
2	J	2	NAG	O5-C5-C6-O6
2	N	2	NAG	O5-C5-C6-O6
2	F	1	NAG	O5-C5-C6-O6
2	G	2	NAG	C4-C5-C6-O6
2	J	2	NAG	C4-C5-C6-O6
2	N	2	NAG	C4-C5-C6-O6
2	I	2	NAG	O5-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	I	2	NAG	C4-C5-C6-O6
2	M	2	NAG	C4-C5-C6-O6
2	M	2	NAG	O5-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	G	2	NAG	C3-C2-N2-C7
2	J	2	NAG	C3-C2-N2-C7
2	N	2	NAG	C3-C2-N2-C7
2	F	2	NAG	C4-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	H	1	NAG	O5-C5-C6-O6
2	K	1	NAG	O5-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
2	K	1	NAG	C1-C2-N2-C7
2	L	1	NAG	C4-C5-C6-O6
2	D	1	NAG	C1-C2-N2-C7
2	H	1	NAG	C1-C2-N2-C7
2	F	2	NAG	C3-C2-N2-C7
2	L	2	NAG	C3-C2-N2-C7
2	L	2	NAG	C1-C2-N2-C7

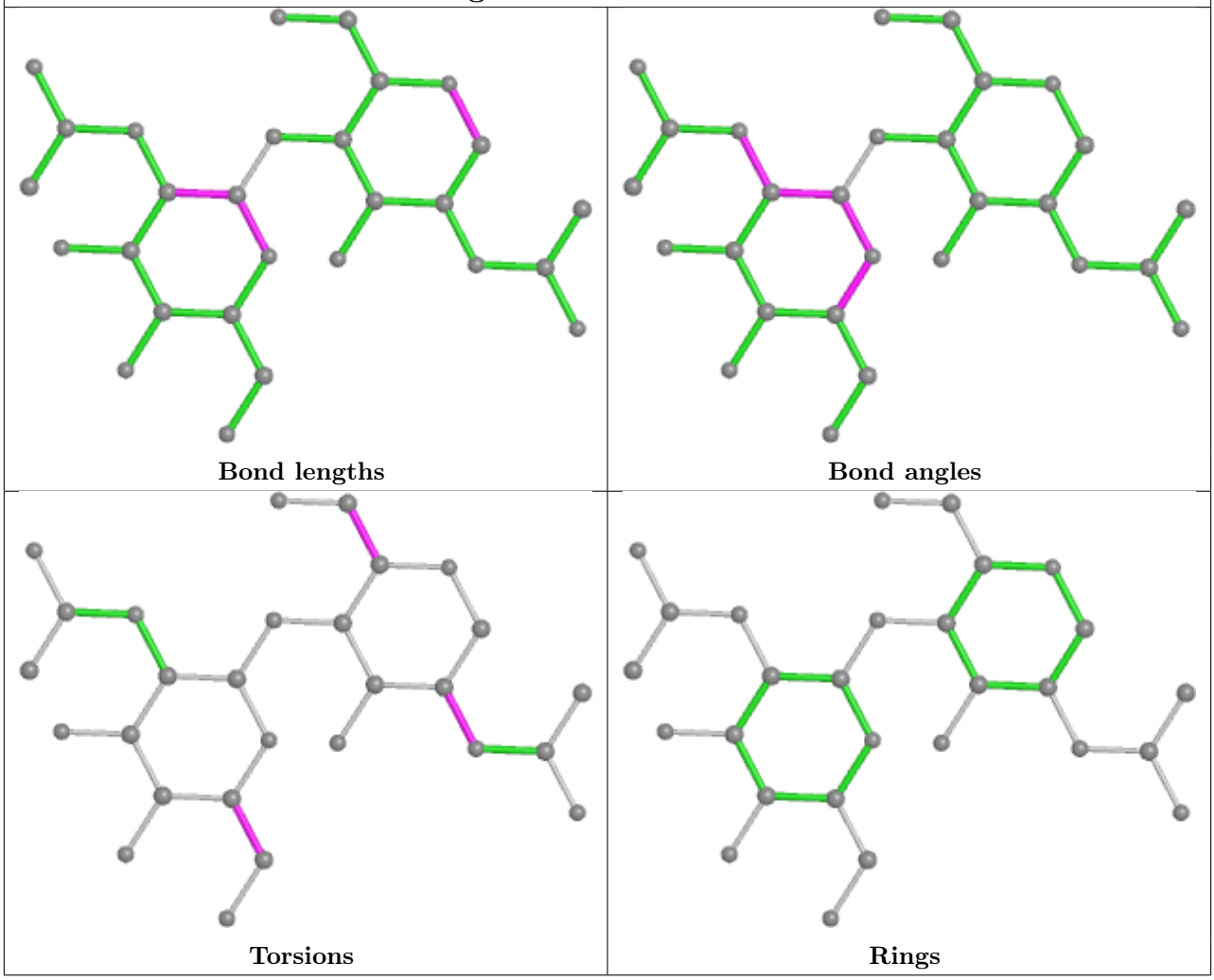
There are no ring outliers.

8 monomers are involved in 10 short contacts:

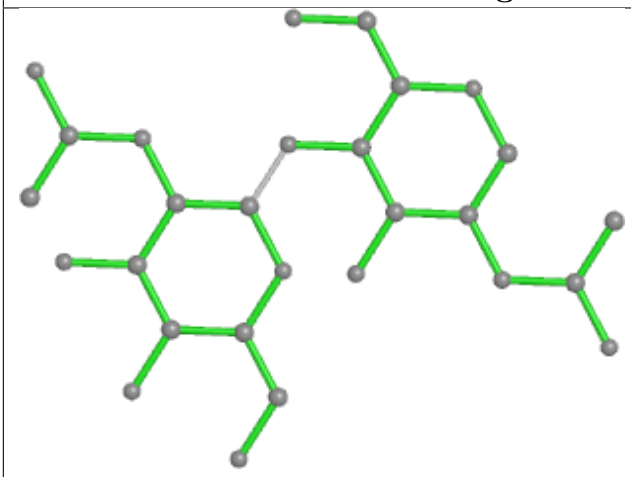
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	1	NAG	6	0
2	D	1	NAG	1	0
2	D	2	NAG	1	0
2	K	1	NAG	1	0
2	F	2	NAG	1	0
2	H	2	NAG	1	0
2	H	1	NAG	1	0
2	K	2	NAG	1	0

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

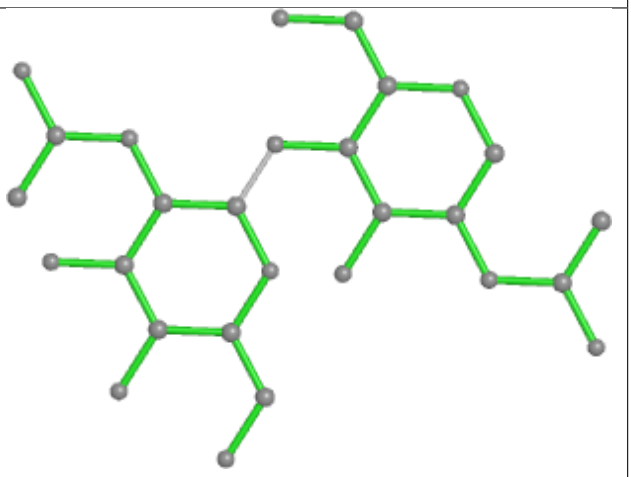
Oligosaccharide Chain D



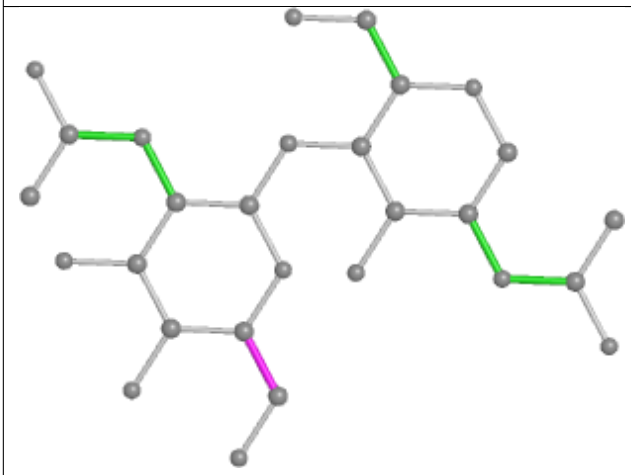
Oligosaccharide Chain E



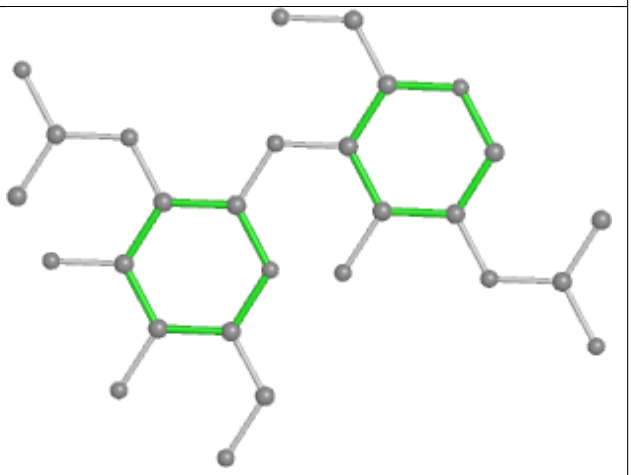
Bond lengths



Bond angles

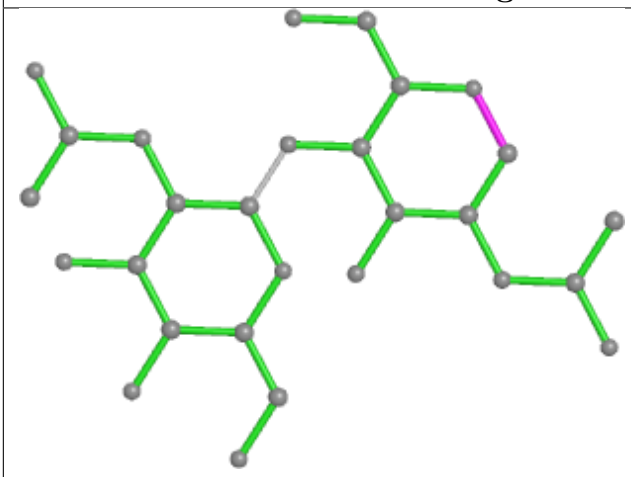


Torsions

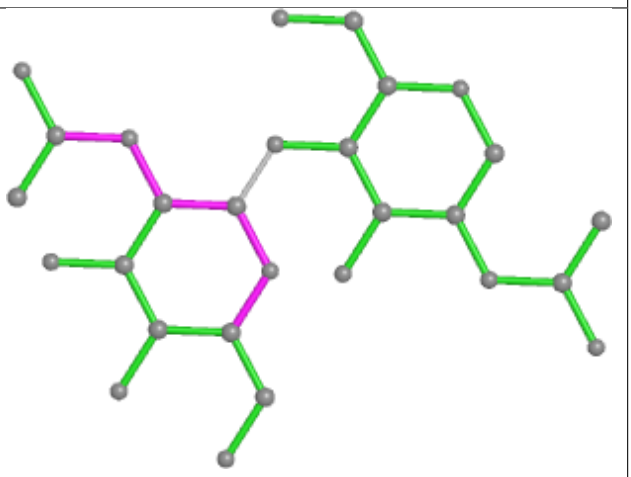


Rings

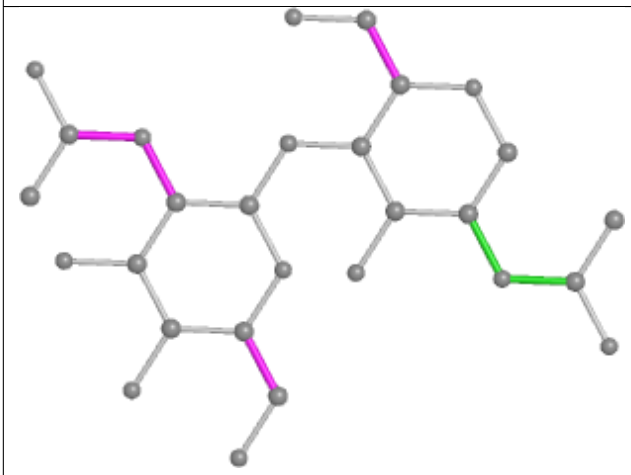
Oligosaccharide Chain F



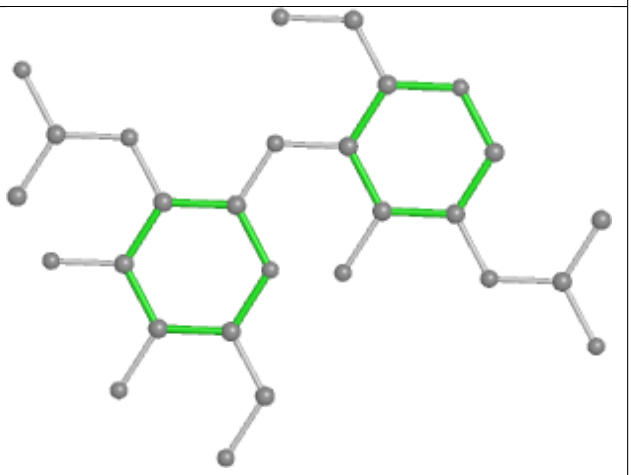
Bond lengths



Bond angles

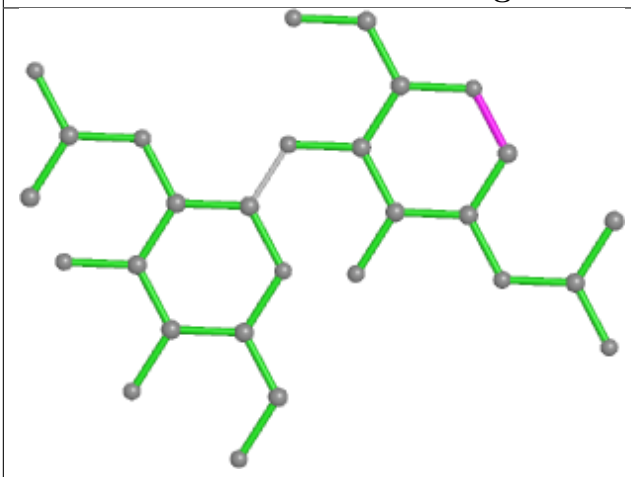


Torsions

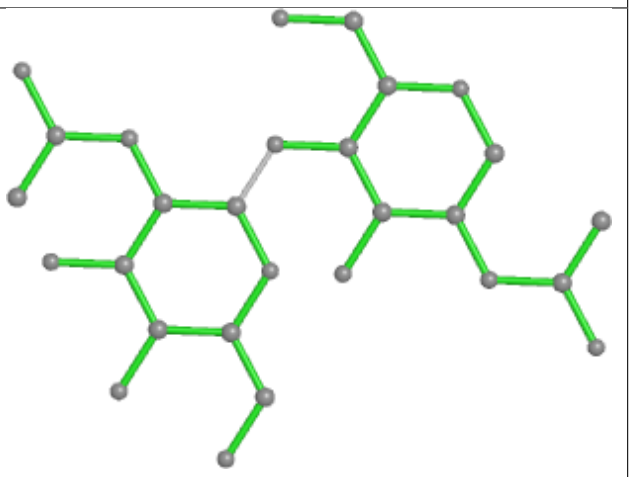


Rings

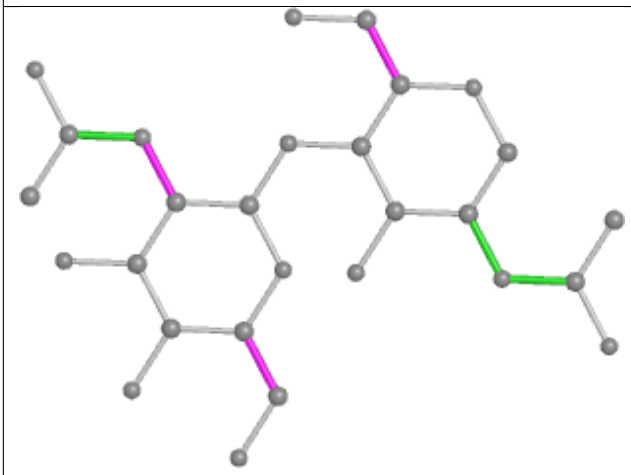
Oligosaccharide Chain G



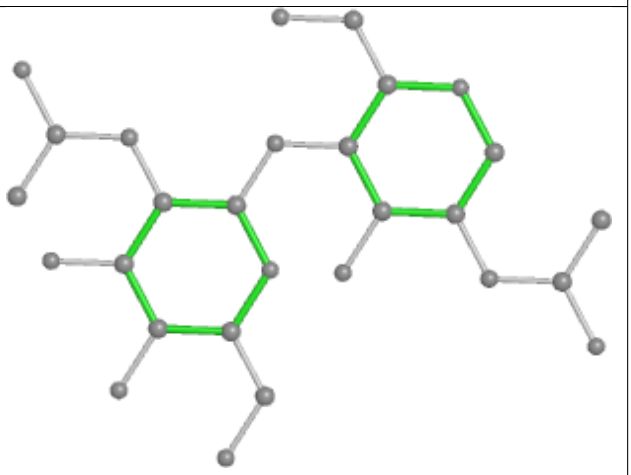
Bond lengths



Bond angles

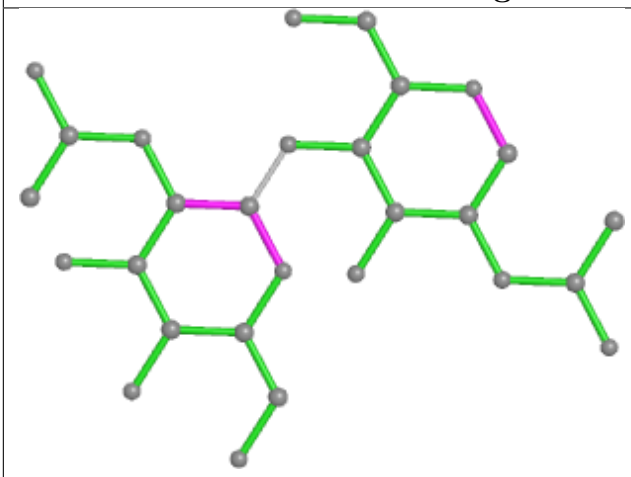


Torsions

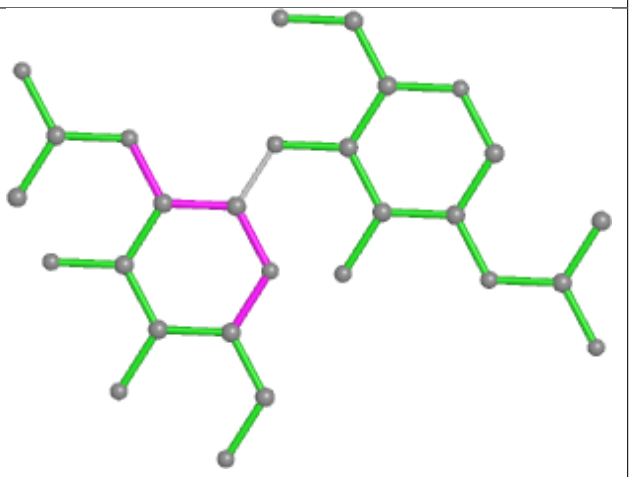


Rings

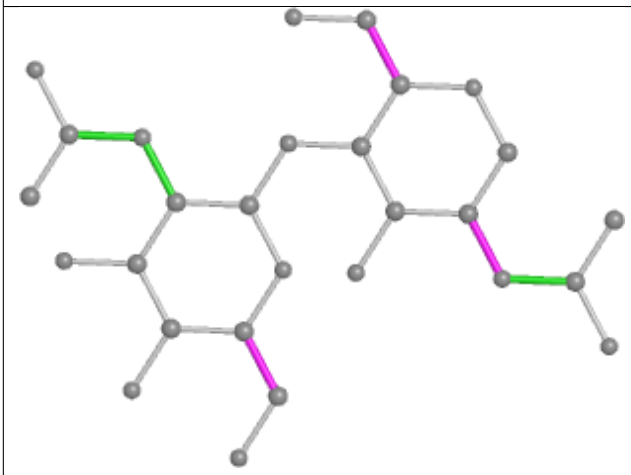
Oligosaccharide Chain H



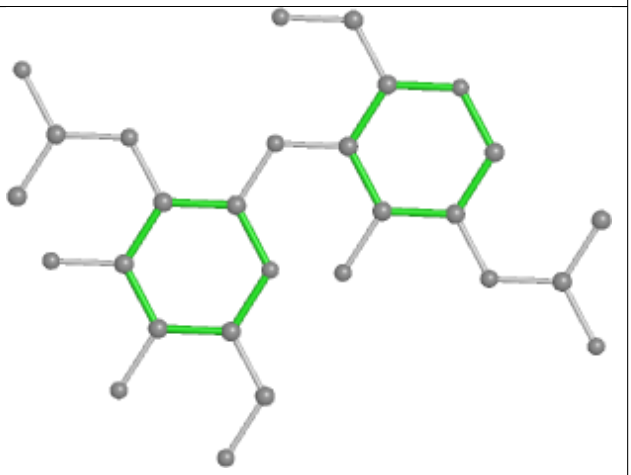
Bond lengths



Bond angles

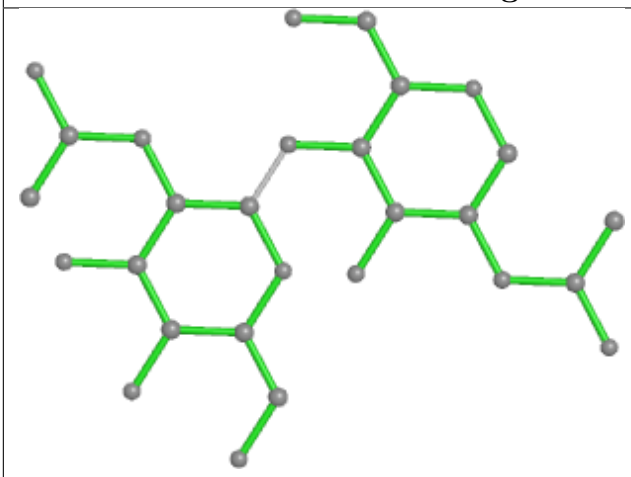


Torsions

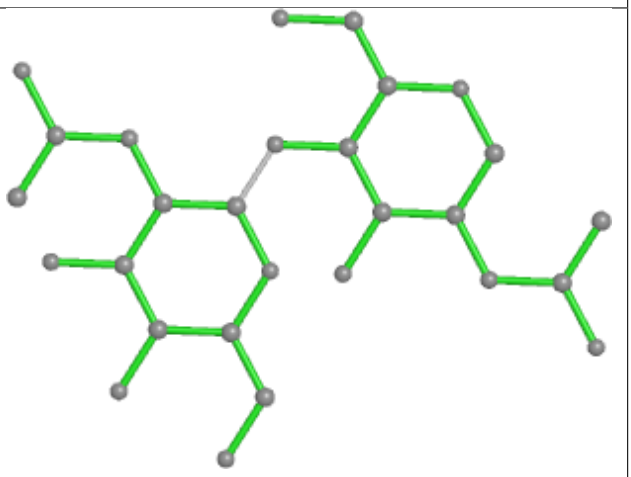


Rings

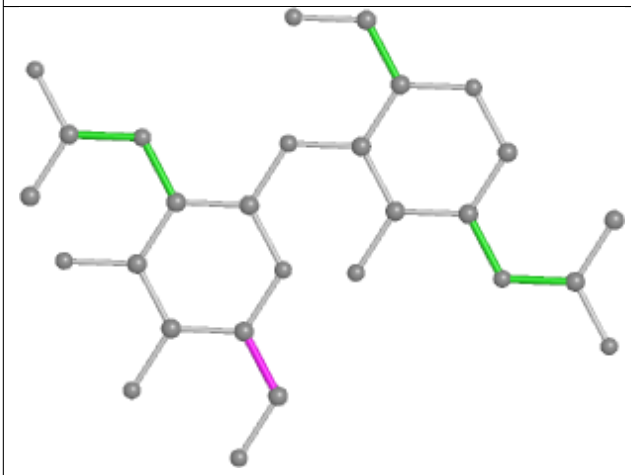
Oligosaccharide Chain I



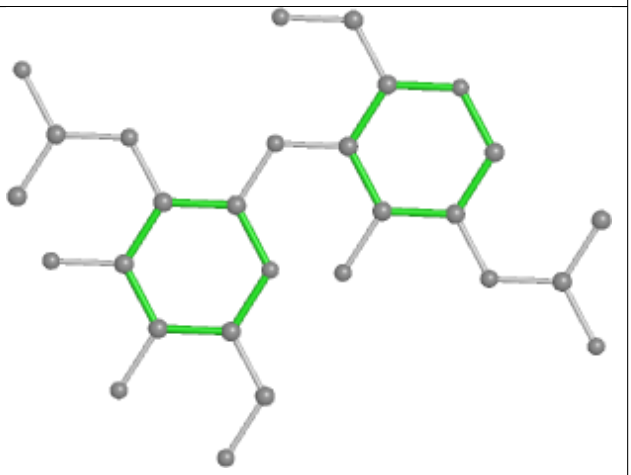
Bond lengths



Bond angles

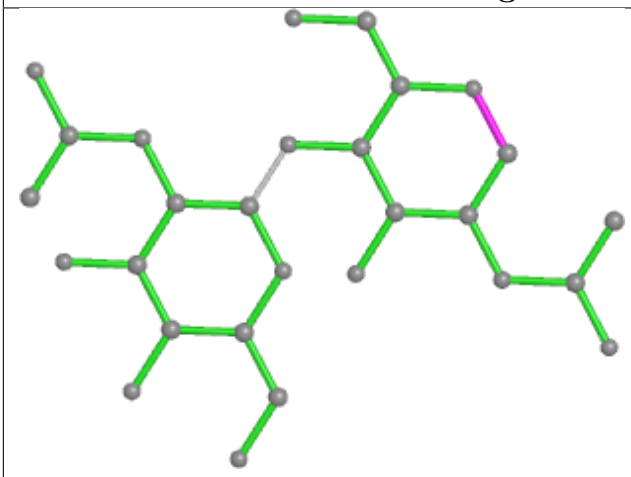


Torsions

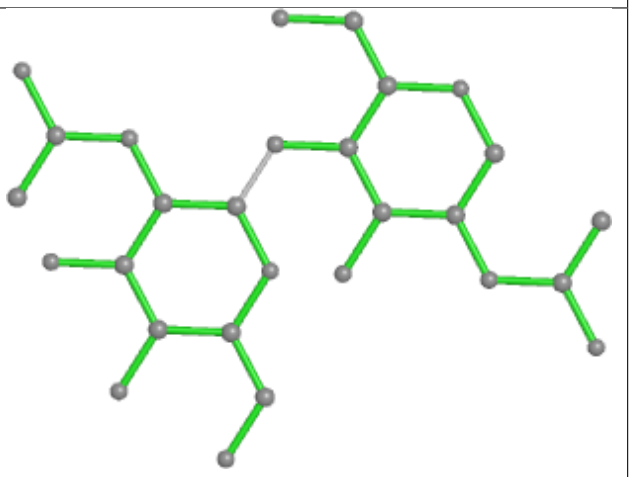


Rings

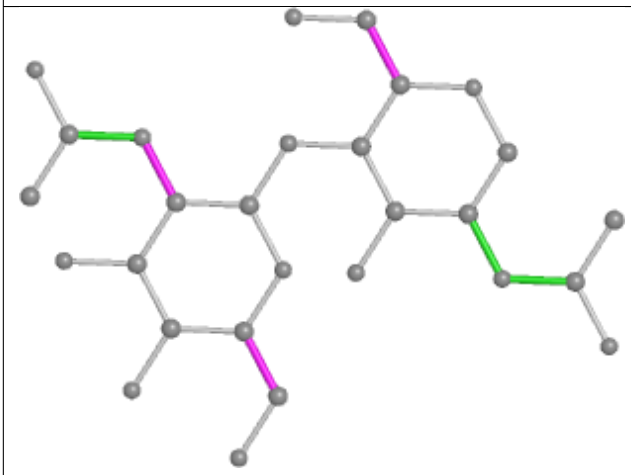
Oligosaccharide Chain J



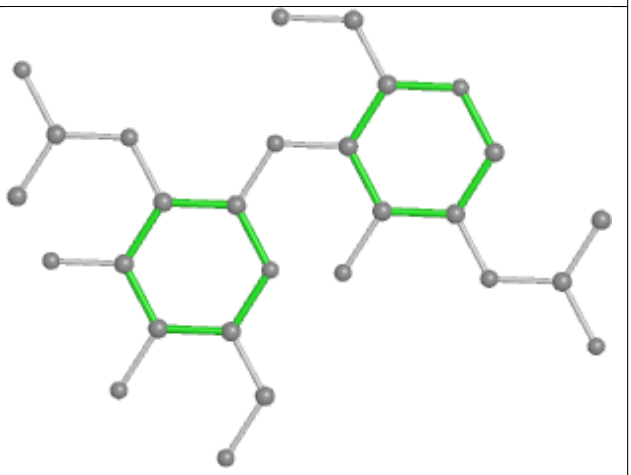
Bond lengths



Bond angles

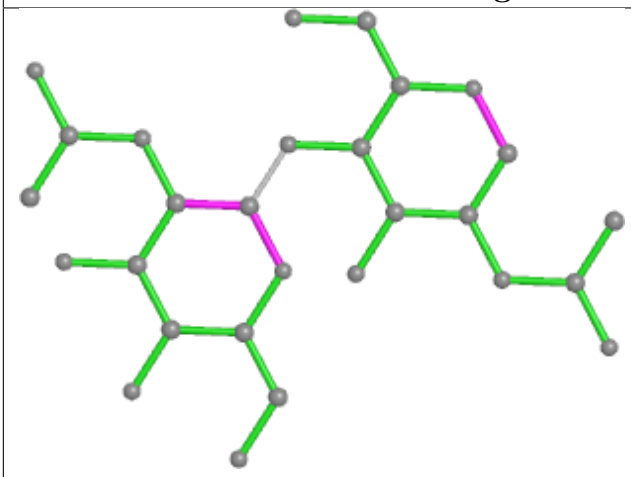


Torsions

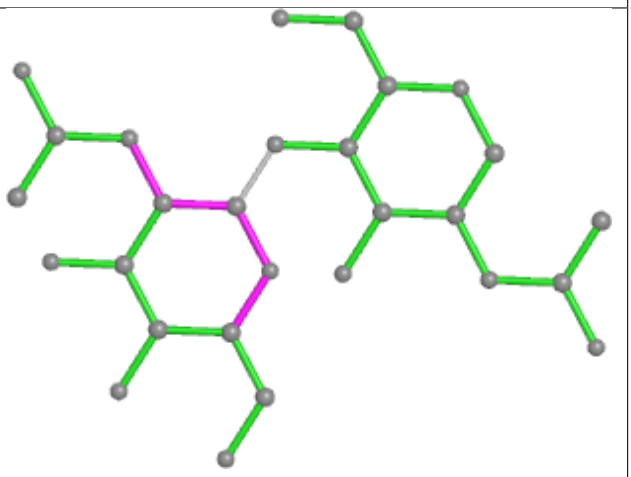


Rings

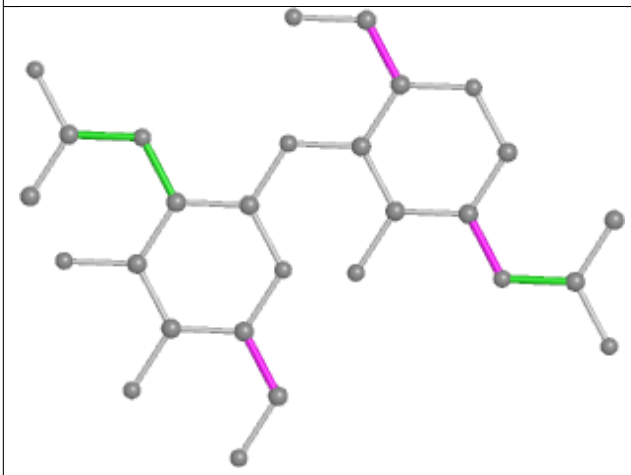
Oligosaccharide Chain K



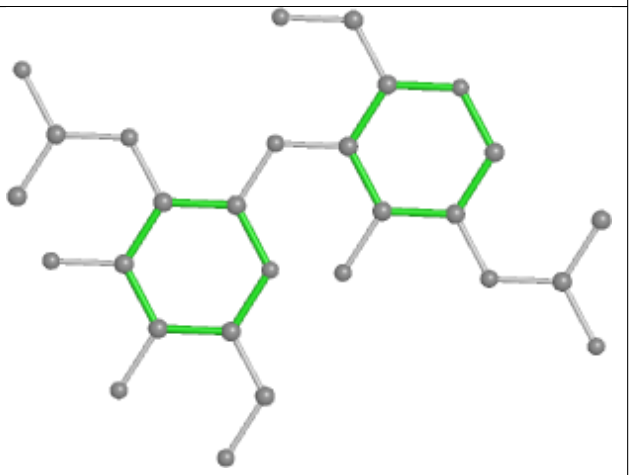
Bond lengths



Bond angles

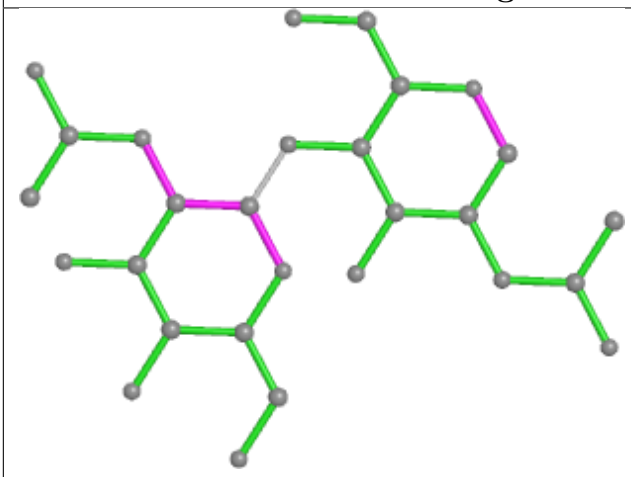


Torsions

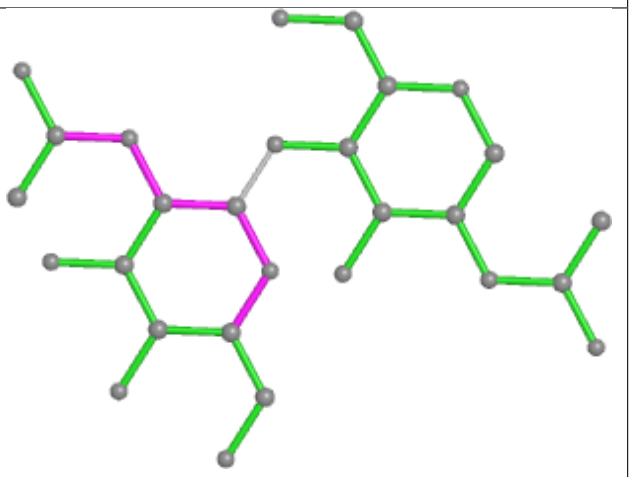


Rings

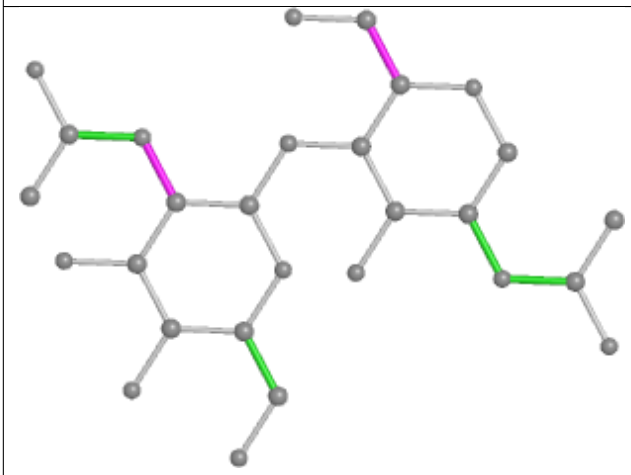
Oligosaccharide Chain L



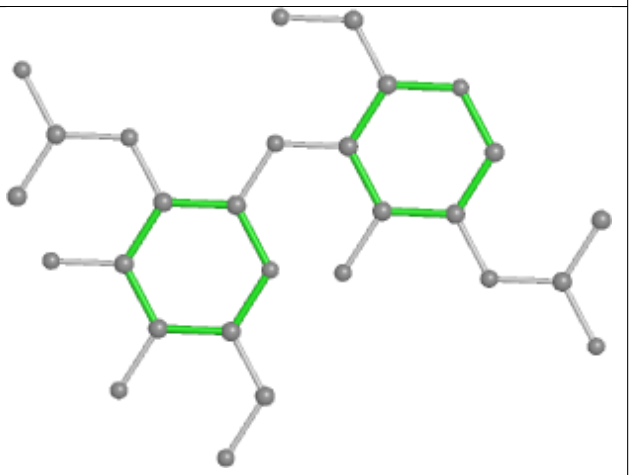
Bond lengths



Bond angles

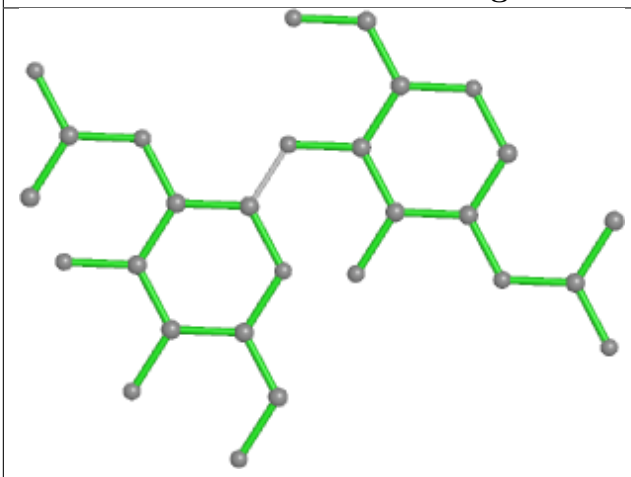


Torsions

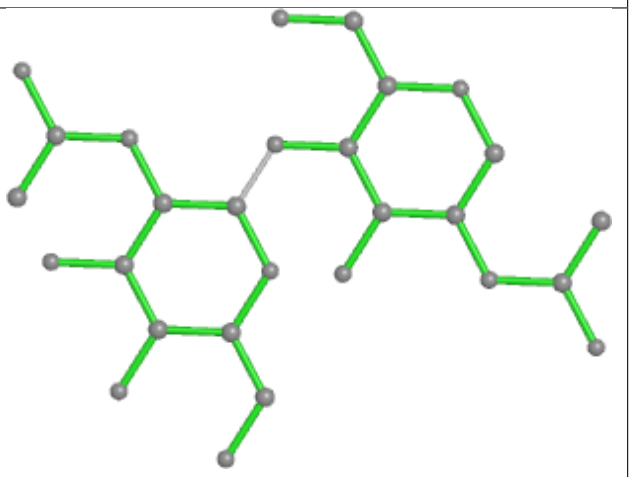


Rings

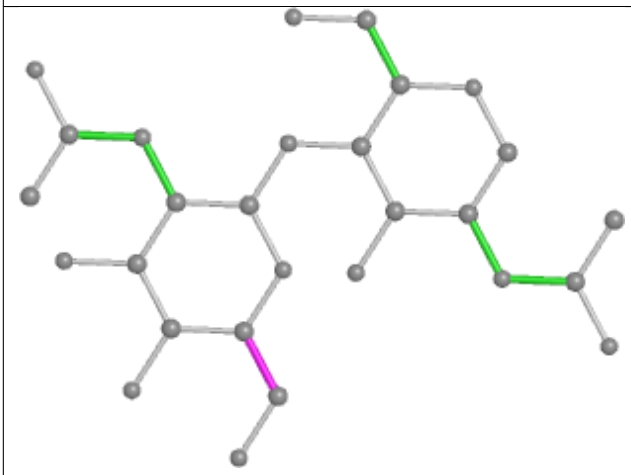
Oligosaccharide Chain M



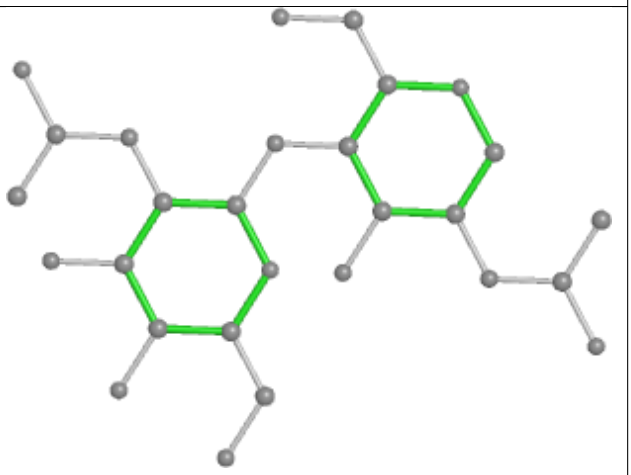
Bond lengths



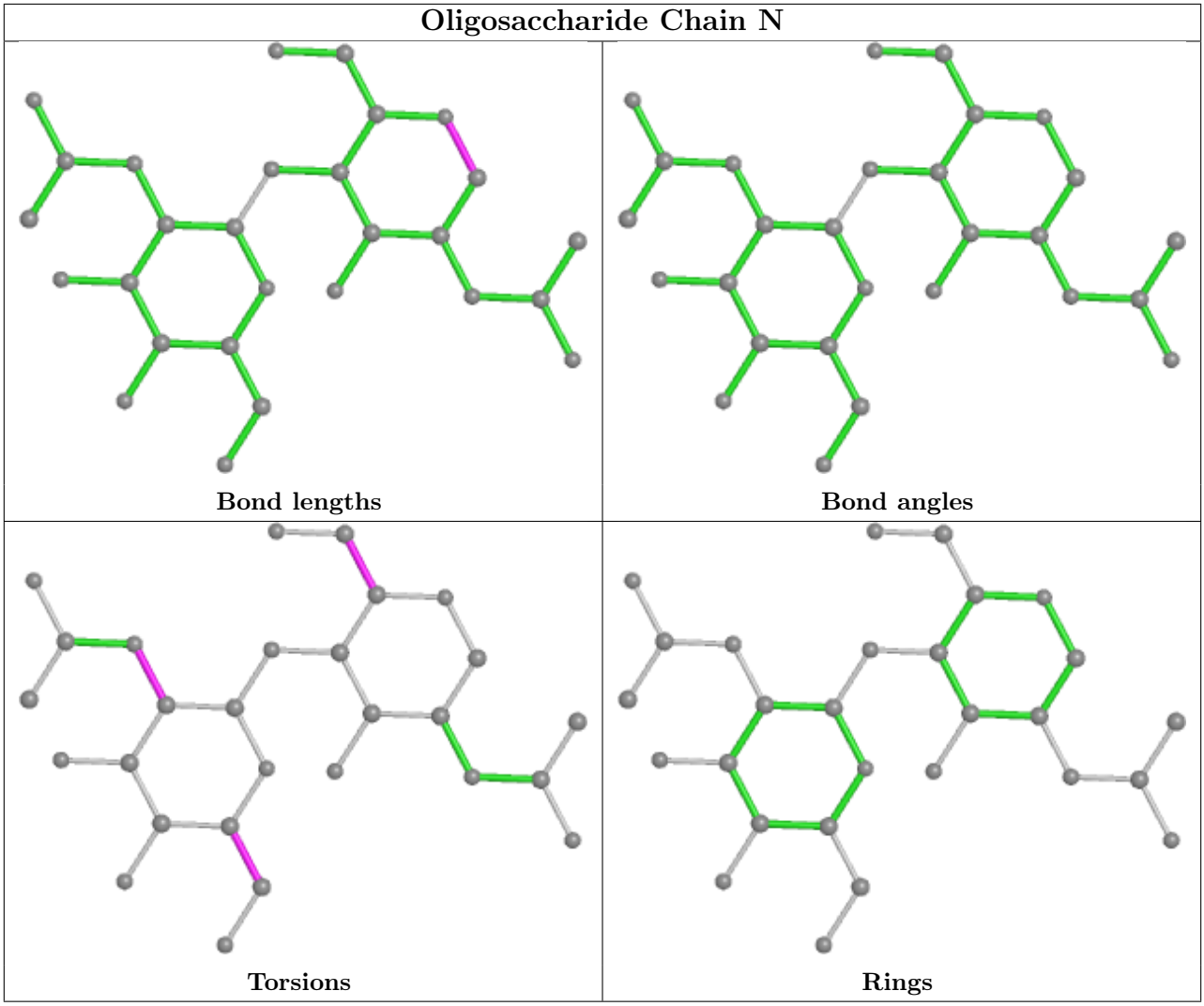
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

62 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	C	1404	1	14,14,15	0.46	0	17,19,21	0.62	0
3	NAG	A	1416	1	14,14,15	0.38	0	17,19,21	0.72	0
3	NAG	B	1411	1	14,14,15	0.61	0	17,19,21	0.74	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	C	1415	-	14,14,15	0.29	0	17,19,21	1.31	2 (11%)
3	NAG	C	1416	1	14,14,15	0.70	1 (7%)	17,19,21	0.70	0
3	NAG	B	1419	-	14,14,15	0.39	0	17,19,21	1.40	3 (17%)
4	EIC	A	1420	-	19,19,19	0.55	0	19,19,19	0.99	0
3	NAG	B	1402	-	14,14,15	0.41	0	17,19,21	1.17	2 (11%)
3	NAG	B	1413	-	14,14,15	0.41	0	17,19,21	1.16	1 (5%)
3	NAG	B	1404	1	14,14,15	0.46	0	17,19,21	0.61	0
3	NAG	C	1401	1	14,14,15	0.40	0	17,19,21	1.17	1 (5%)
3	NAG	C	1403	1	14,14,15	0.20	0	17,19,21	0.38	0
3	NAG	A	1417	-	14,14,15	0.30	0	17,19,21	1.32	2 (11%)
3	NAG	C	1412	1	14,14,15	0.29	0	17,19,21	0.62	0
3	NAG	A	1404	1	14,14,15	0.46	0	17,19,21	0.61	0
3	NAG	B	1417	-	14,14,15	0.29	0	17,19,21	1.32	2 (11%)
3	NAG	C	1408	1	14,14,15	0.29	0	17,19,21	0.63	0
3	NAG	A	1413	-	14,14,15	0.41	0	17,19,21	1.16	1 (5%)
3	NAG	A	1402	-	14,14,15	0.41	0	17,19,21	1.17	2 (11%)
3	NAG	A	1418	1	14,14,15	0.25	0	17,19,21	0.68	1 (5%)
3	NAG	B	1410	-	14,14,15	2.92	2 (14%)	17,19,21	1.53	4 (23%)
3	NAG	B	1418	1	14,14,15	0.70	1 (7%)	17,19,21	0.70	0
3	NAG	B	1405	1	14,14,15	0.41	0	17,19,21	1.17	2 (11%)
3	NAG	A	1419	-	14,14,15	0.17	0	17,19,21	0.47	0
3	NAG	A	1403	1	14,14,15	0.20	0	17,19,21	0.38	0
3	NAG	B	1412	1	14,14,15	0.29	0	17,19,21	0.63	0
4	EIC	C	1420	-	19,19,19	0.57	0	19,19,19	0.96	0
3	NAG	A	1405	1	14,14,15	0.41	0	17,19,21	1.17	2 (11%)
3	NAG	A	1410	-	14,14,15	2.93	3 (21%)	17,19,21	1.54	4 (23%)
3	NAG	A	1412	1	14,14,15	0.29	0	17,19,21	0.62	0
3	NAG	C	1411	-	14,14,15	0.42	0	17,19,21	1.16	1 (5%)
3	NAG	A	1406	1	14,14,15	0.30	0	17,19,21	0.39	0
3	NAG	A	1414	1	14,14,15	0.28	0	17,19,21	0.62	0
3	NAG	C	1413	1	14,14,15	0.51	0	17,19,21	0.35	0
3	NAG	B	1414	1	14,14,15	0.28	0	17,19,21	0.62	0
3	NAG	C	1402	-	14,14,15	0.41	0	17,19,21	1.17	2 (11%)
3	NAG	C	1418	1	14,14,15	0.26	0	17,19,21	0.67	1 (5%)
3	NAG	C	1409	1	14,14,15	0.62	0	17,19,21	0.74	1 (5%)
3	NAG	A	1411	1	14,14,15	0.62	0	17,19,21	0.74	1 (5%)
3	NAG	B	1415	1	14,14,15	0.53	0	17,19,21	0.35	0
3	NAG	C	1419	-	14,14,15	0.16	0	17,19,21	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	A	1401	1	14,14,15	0.41	0	17,19,21	1.16	2 (11%)
3	NAG	C	1417	-	14,14,15	0.41	0	17,19,21	1.40	3 (17%)
3	NAG	B	1401	1	14,14,15	0.41	0	17,19,21	1.16	2 (11%)
3	NAG	B	1421	-	14,14,15	0.16	0	17,19,21	0.47	0
3	NAG	C	1410	1	14,14,15	0.29	0	17,19,21	0.62	0
3	NAG	A	1409	1	14,14,15	0.86	1 (7%)	17,19,21	0.56	0
3	NAG	B	1403	1	14,14,15	0.20	0	17,19,21	0.38	0
3	NAG	C	1405	1	14,14,15	0.41	0	17,19,21	1.17	2 (11%)
3	NAG	C	1406	1	14,14,15	0.30	0	17,19,21	0.39	0
3	NAG	A	1415	1	14,14,15	0.52	0	17,19,21	0.35	0
3	NAG	B	1409	1	14,14,15	0.86	1 (7%)	17,19,21	0.56	0
3	NAG	B	1408	1	14,14,15	0.28	0	17,19,21	0.61	0
3	NAG	B	1406	1	14,14,15	0.31	0	17,19,21	0.39	0
3	NAG	B	1420	1	14,14,15	0.25	0	17,19,21	0.68	1 (5%)
3	NAG	C	1407	1	14,14,15	0.75	1 (7%)	17,19,21	0.60	0
3	NAG	C	1414	1	14,14,15	0.37	0	17,19,21	0.72	0
3	NAG	B	1407	1	14,14,15	0.75	1 (7%)	17,19,21	0.59	0
3	NAG	A	1408	1	14,14,15	0.29	0	17,19,21	0.62	0
3	NAG	B	1416	1	14,14,15	0.36	0	17,19,21	0.72	0
4	EIC	B	1422	-	19,19,19	0.57	0	19,19,19	0.96	0
3	NAG	A	1407	1	14,14,15	0.75	1 (7%)	17,19,21	0.59	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	1404	1	-	4/6/23/26	0/1/1/1
3	NAG	A	1416	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1411	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1415	-	-	3/6/23/26	0/1/1/1
3	NAG	C	1416	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1419	-	-	5/6/23/26	0/1/1/1
4	EIC	A	1420	-	-	11/17/17/17	-
3	NAG	B	1402	-	-	0/6/23/26	0/1/1/1
3	NAG	B	1413	-	-	0/6/23/26	0/1/1/1
3	NAG	B	1404	1	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	1401	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1403	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1417	-	-	3/6/23/26	0/1/1/1
3	NAG	C	1412	1	-	4/6/23/26	0/1/1/1
3	NAG	A	1404	1	-	4/6/23/26	0/1/1/1
3	NAG	B	1417	-	-	3/6/23/26	0/1/1/1
3	NAG	C	1408	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1413	-	-	0/6/23/26	0/1/1/1
3	NAG	A	1402	-	-	0/6/23/26	0/1/1/1
3	NAG	A	1418	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1410	-	-	2/6/23/26	0/1/1/1
3	NAG	B	1418	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1405	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1419	-	-	0/6/23/26	0/1/1/1
3	NAG	A	1403	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1412	1	-	6/6/23/26	0/1/1/1
4	EIC	C	1420	-	-	6/17/17/17	-
3	NAG	A	1405	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1410	-	-	2/6/23/26	0/1/1/1
3	NAG	A	1412	1	-	6/6/23/26	0/1/1/1
3	NAG	C	1411	-	-	0/6/23/26	0/1/1/1
3	NAG	A	1406	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1414	1	-	4/6/23/26	0/1/1/1
3	NAG	C	1413	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1414	1	-	4/6/23/26	0/1/1/1
3	NAG	C	1402	-	-	0/6/23/26	0/1/1/1
3	NAG	C	1418	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1409	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1411	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1415	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1419	-	-	0/6/23/26	0/1/1/1
3	NAG	A	1401	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1417	-	-	5/6/23/26	0/1/1/1
3	NAG	B	1401	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1421	-	-	0/6/23/26	0/1/1/1
3	NAG	C	1410	1	-	6/6/23/26	0/1/1/1
3	NAG	A	1409	1	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	1403	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1405	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1406	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1415	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1409	1	-	1/6/23/26	0/1/1/1
3	NAG	B	1408	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1406	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1420	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1407	1	-	4/6/23/26	0/1/1/1
3	NAG	C	1414	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1407	1	-	4/6/23/26	0/1/1/1
3	NAG	A	1408	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1416	1	-	2/6/23/26	0/1/1/1
4	EIC	B	1422	-	-	7/17/17/17	-
3	NAG	A	1407	1	-	4/6/23/26	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1410	NAG	O5-C1	-8.12	1.30	1.43
3	B	1410	NAG	O5-C1	-8.10	1.30	1.43
3	B	1410	NAG	C1-C2	-6.77	1.42	1.52
3	A	1410	NAG	C1-C2	-6.77	1.42	1.52
3	A	1409	NAG	O5-C1	-2.81	1.39	1.43
3	B	1409	NAG	O5-C1	-2.80	1.39	1.43
3	C	1416	NAG	O5-C1	-2.36	1.39	1.43
3	B	1418	NAG	O5-C1	-2.34	1.40	1.43
3	B	1407	NAG	C1-C2	2.05	1.55	1.52
3	A	1410	NAG	C2-N2	-2.04	1.42	1.46
3	A	1407	NAG	C1-C2	2.02	1.55	1.52
3	C	1407	NAG	C1-C2	2.01	1.55	1.52

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1417	NAG	C2-N2-C7	4.45	129.24	122.90
3	B	1419	NAG	C2-N2-C7	4.43	129.21	122.90
3	B	1417	NAG	C2-N2-C7	4.31	129.04	122.90
3	A	1417	NAG	C2-N2-C7	4.29	129.01	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1415	NAG	C2-N2-C7	4.26	128.97	122.90
3	A	1410	NAG	O5-C1-C2	3.28	116.47	111.29
3	A	1410	NAG	C1-C2-N2	3.28	116.09	110.49
3	B	1410	NAG	C1-C2-N2	3.27	116.07	110.49
3	B	1410	NAG	O5-C1-C2	3.25	116.42	111.29
3	A	1410	NAG	C1-O5-C5	3.20	116.53	112.19
3	B	1410	NAG	C1-O5-C5	3.15	116.47	112.19
3	C	1415	NAG	C1-C2-N2	2.38	114.55	110.49
3	B	1419	NAG	C1-C2-N2	2.36	114.53	110.49
3	C	1401	NAG	C8-C7-N2	2.36	120.09	116.10
3	A	1417	NAG	C1-C2-N2	2.35	114.50	110.49
3	B	1417	NAG	C1-C2-N2	2.34	114.49	110.49
3	B	1402	NAG	C8-C7-N2	2.34	120.06	116.10
3	C	1417	NAG	C1-C2-N2	2.34	114.48	110.49
3	A	1413	NAG	C8-C7-N2	2.33	120.05	116.10
3	A	1402	NAG	C8-C7-N2	2.32	120.03	116.10
3	C	1411	NAG	C8-C7-N2	2.32	120.03	116.10
3	B	1405	NAG	C8-C7-N2	2.32	120.03	116.10
3	A	1401	NAG	C8-C7-N2	2.32	120.03	116.10
3	C	1402	NAG	C8-C7-N2	2.32	120.02	116.10
3	C	1405	NAG	C8-C7-N2	2.32	120.02	116.10
3	B	1413	NAG	C8-C7-N2	2.31	120.02	116.10
3	B	1401	NAG	C8-C7-N2	2.30	120.00	116.10
3	A	1405	NAG	C8-C7-N2	2.30	120.00	116.10
3	B	1411	NAG	C1-O5-C5	2.22	115.20	112.19
3	C	1409	NAG	C1-O5-C5	2.20	115.18	112.19
3	A	1411	NAG	C1-O5-C5	2.20	115.18	112.19
3	A	1410	NAG	C2-N2-C7	2.19	126.02	122.90
3	B	1410	NAG	C2-N2-C7	2.18	126.01	122.90
3	B	1420	NAG	C1-O5-C5	2.09	115.02	112.19
3	B	1419	NAG	C1-O5-C5	2.08	115.01	112.19
3	A	1418	NAG	C1-O5-C5	2.07	115.00	112.19
3	C	1417	NAG	C1-O5-C5	2.07	114.99	112.19
3	C	1402	NAG	C2-N2-C7	-2.05	119.98	122.90
3	A	1402	NAG	C2-N2-C7	-2.04	120.00	122.90
3	C	1418	NAG	C1-O5-C5	2.04	114.96	112.19
3	A	1405	NAG	C2-N2-C7	-2.03	120.01	122.90
3	B	1401	NAG	C2-N2-C7	-2.03	120.01	122.90
3	B	1402	NAG	C2-N2-C7	-2.03	120.02	122.90
3	A	1401	NAG	C2-N2-C7	-2.02	120.03	122.90
3	B	1405	NAG	C2-N2-C7	-2.01	120.05	122.90
3	C	1405	NAG	C2-N2-C7	-2.01	120.05	122.90

There are no chirality outliers.

All (149) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1408	NAG	C8-C7-N2-C2
3	A	1408	NAG	O7-C7-N2-C2
3	A	1414	NAG	C8-C7-N2-C2
3	A	1414	NAG	O7-C7-N2-C2
3	B	1408	NAG	C8-C7-N2-C2
3	B	1408	NAG	O7-C7-N2-C2
3	B	1414	NAG	C8-C7-N2-C2
3	B	1414	NAG	O7-C7-N2-C2
3	C	1408	NAG	C8-C7-N2-C2
3	C	1408	NAG	O7-C7-N2-C2
3	C	1412	NAG	C8-C7-N2-C2
3	C	1412	NAG	O7-C7-N2-C2
3	A	1412	NAG	O5-C5-C6-O6
3	B	1412	NAG	O5-C5-C6-O6
3	C	1410	NAG	O5-C5-C6-O6
3	B	1404	NAG	C4-C5-C6-O6
3	C	1404	NAG	C4-C5-C6-O6
3	A	1404	NAG	C4-C5-C6-O6
3	A	1412	NAG	C8-C7-N2-C2
3	B	1412	NAG	C8-C7-N2-C2
3	C	1410	NAG	C8-C7-N2-C2
3	A	1407	NAG	O5-C5-C6-O6
3	B	1407	NAG	O5-C5-C6-O6
3	C	1407	NAG	O5-C5-C6-O6
3	A	1412	NAG	C4-C5-C6-O6
3	B	1412	NAG	C4-C5-C6-O6
3	C	1410	NAG	C4-C5-C6-O6
3	A	1404	NAG	O5-C5-C6-O6
3	B	1404	NAG	O5-C5-C6-O6
3	C	1404	NAG	O5-C5-C6-O6
3	A	1407	NAG	C1-C2-N2-C7
3	A	1412	NAG	C1-C2-N2-C7
3	B	1407	NAG	C1-C2-N2-C7
3	B	1412	NAG	C1-C2-N2-C7
3	C	1407	NAG	C1-C2-N2-C7
3	C	1410	NAG	C1-C2-N2-C7
3	A	1403	NAG	O5-C5-C6-O6
3	B	1403	NAG	O5-C5-C6-O6
3	C	1403	NAG	O5-C5-C6-O6
3	A	1415	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	B	1415	NAG	C4-C5-C6-O6
3	C	1413	NAG	C4-C5-C6-O6
3	A	1412	NAG	O7-C7-N2-C2
3	A	1417	NAG	C8-C7-N2-C2
3	A	1417	NAG	O7-C7-N2-C2
3	B	1412	NAG	O7-C7-N2-C2
3	B	1417	NAG	C8-C7-N2-C2
3	B	1417	NAG	O7-C7-N2-C2
3	B	1419	NAG	C8-C7-N2-C2
3	B	1419	NAG	O7-C7-N2-C2
3	C	1410	NAG	O7-C7-N2-C2
3	C	1415	NAG	C8-C7-N2-C2
3	C	1415	NAG	O7-C7-N2-C2
3	C	1417	NAG	C8-C7-N2-C2
3	C	1417	NAG	O7-C7-N2-C2
3	B	1418	NAG	C4-C5-C6-O6
3	C	1416	NAG	C4-C5-C6-O6
3	A	1415	NAG	O5-C5-C6-O6
3	B	1415	NAG	O5-C5-C6-O6
3	C	1413	NAG	O5-C5-C6-O6
3	A	1416	NAG	C4-C5-C6-O6
3	B	1416	NAG	C4-C5-C6-O6
3	C	1414	NAG	C4-C5-C6-O6
3	A	1411	NAG	O5-C5-C6-O6
3	B	1411	NAG	O5-C5-C6-O6
3	C	1409	NAG	O5-C5-C6-O6
4	A	1420	EIC	C1-C2-C3-C4
3	A	1414	NAG	O5-C5-C6-O6
3	B	1414	NAG	O5-C5-C6-O6
3	C	1412	NAG	O5-C5-C6-O6
3	B	1411	NAG	C4-C5-C6-O6
3	A	1411	NAG	C4-C5-C6-O6
3	C	1409	NAG	C4-C5-C6-O6
3	A	1407	NAG	C4-C5-C6-O6
3	B	1407	NAG	C4-C5-C6-O6
3	C	1407	NAG	C4-C5-C6-O6
3	C	1412	NAG	C1-C2-N2-C7
3	A	1416	NAG	O5-C5-C6-O6
3	B	1416	NAG	O5-C5-C6-O6
3	C	1414	NAG	O5-C5-C6-O6
3	B	1406	NAG	O5-C5-C6-O6
3	B	1418	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	C	1416	NAG	O5-C5-C6-O6
3	A	1406	NAG	O5-C5-C6-O6
4	C	1420	EIC	C4-C5-C6-C7
3	C	1406	NAG	O5-C5-C6-O6
3	A	1414	NAG	C1-C2-N2-C7
3	B	1414	NAG	C1-C2-N2-C7
4	A	1420	EIC	C5-C6-C7-C8
3	A	1406	NAG	C4-C5-C6-O6
3	B	1406	NAG	C4-C5-C6-O6
3	C	1406	NAG	C4-C5-C6-O6
4	A	1420	EIC	C13-C14-C15-C16
3	A	1418	NAG	C4-C5-C6-O6
3	B	1420	NAG	C4-C5-C6-O6
3	C	1418	NAG	C4-C5-C6-O6
3	C	1418	NAG	O5-C5-C6-O6
3	A	1418	NAG	O5-C5-C6-O6
3	B	1420	NAG	O5-C5-C6-O6
4	A	1420	EIC	C14-C15-C16-C17
4	A	1420	EIC	C15-C16-C17-C18
4	A	1420	EIC	C6-C7-C8-C9
3	A	1412	NAG	C3-C2-N2-C7
3	B	1412	NAG	C3-C2-N2-C7
3	C	1410	NAG	C3-C2-N2-C7
4	C	1420	EIC	C2-C3-C4-C5
3	B	1404	NAG	C1-C2-N2-C7
4	B	1422	EIC	C4-C5-C6-C7
4	A	1420	EIC	C10-C11-C12-C13
4	B	1422	EIC	C10-C11-C12-C13
3	A	1404	NAG	C1-C2-N2-C7
3	C	1404	NAG	C1-C2-N2-C7
4	C	1420	EIC	C5-C6-C7-C8
3	B	1403	NAG	C4-C5-C6-O6
3	A	1403	NAG	C4-C5-C6-O6
3	C	1403	NAG	C4-C5-C6-O6
4	B	1422	EIC	C15-C16-C17-C18
3	B	1419	NAG	C4-C5-C6-O6
3	C	1417	NAG	C4-C5-C6-O6
4	C	1420	EIC	O1-C1-C2-C3
4	A	1420	EIC	C9-C10-C11-C12
4	B	1422	EIC	C7-C8-C9-C10
3	B	1419	NAG	O5-C5-C6-O6
3	C	1417	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	C	1420	EIC	O2-C1-C2-C3
4	A	1420	EIC	C4-C5-C6-C7
3	A	1409	NAG	C4-C5-C6-O6
3	B	1409	NAG	C4-C5-C6-O6
4	B	1422	EIC	O1-C1-C2-C3
4	B	1422	EIC	O2-C1-C2-C3
4	C	1420	EIC	C7-C8-C9-C10
4	B	1422	EIC	C14-C15-C16-C17
3	A	1404	NAG	C3-C2-N2-C7
3	A	1407	NAG	C3-C2-N2-C7
3	A	1410	NAG	C3-C2-N2-C7
3	A	1417	NAG	C3-C2-N2-C7
3	B	1404	NAG	C3-C2-N2-C7
3	B	1407	NAG	C3-C2-N2-C7
3	B	1410	NAG	C3-C2-N2-C7
3	B	1417	NAG	C3-C2-N2-C7
3	B	1419	NAG	C3-C2-N2-C7
3	C	1404	NAG	C3-C2-N2-C7
3	C	1407	NAG	C3-C2-N2-C7
3	C	1415	NAG	C3-C2-N2-C7
3	C	1417	NAG	C3-C2-N2-C7
4	A	1420	EIC	C7-C8-C9-C10
3	B	1410	NAG	C1-C2-N2-C7
4	A	1420	EIC	C12-C13-C14-C15
3	A	1410	NAG	C1-C2-N2-C7

There are no ring outliers.

48 monomers are involved in 110 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1404	NAG	6	0
3	A	1416	NAG	1	0
3	C	1415	NAG	1	0
3	B	1419	NAG	1	0
4	A	1420	EIC	4	0
3	B	1402	NAG	2	0
3	B	1413	NAG	7	0
3	B	1404	NAG	6	0
3	C	1401	NAG	2	0
3	C	1403	NAG	1	0
3	A	1417	NAG	1	0
3	C	1412	NAG	4	0

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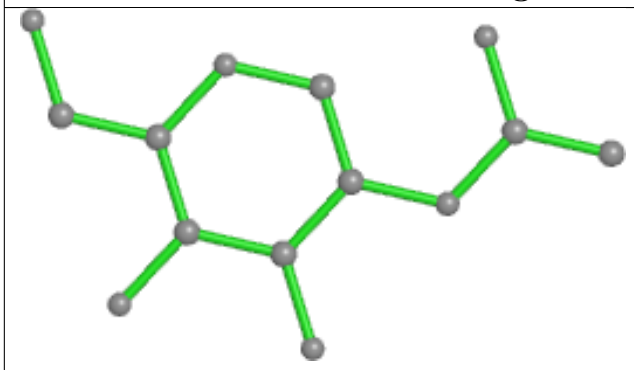
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1404	NAG	6	0
3	B	1417	NAG	1	0
3	C	1408	NAG	1	0
3	A	1413	NAG	7	0
3	A	1402	NAG	2	0
3	A	1418	NAG	3	0
3	B	1405	NAG	2	0
3	A	1419	NAG	3	0
3	A	1403	NAG	1	0
3	B	1412	NAG	7	0
4	C	1420	EIC	2	0
3	A	1405	NAG	2	0
3	A	1412	NAG	8	0
3	C	1411	NAG	7	0
3	A	1414	NAG	3	0
3	B	1414	NAG	4	0
3	C	1402	NAG	2	0
3	C	1418	NAG	3	0
3	C	1419	NAG	3	0
3	A	1401	NAG	2	0
3	C	1417	NAG	1	0
3	B	1401	NAG	2	0
3	B	1421	NAG	3	0
3	C	1410	NAG	7	0
3	A	1409	NAG	6	0
3	B	1403	NAG	1	0
3	C	1405	NAG	2	0
3	B	1409	NAG	6	0
3	B	1408	NAG	1	0
3	B	1420	NAG	3	0
3	C	1407	NAG	1	0
3	C	1414	NAG	1	0
3	A	1408	NAG	1	0
3	B	1416	NAG	1	0
4	B	1422	EIC	4	0
3	A	1407	NAG	1	0

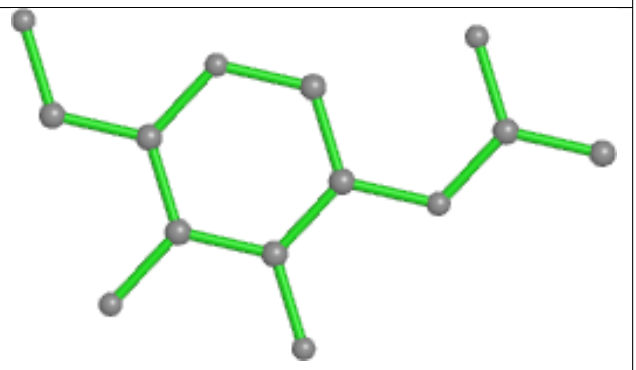
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

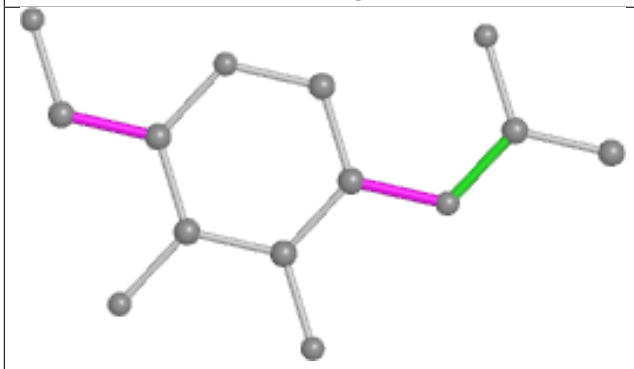
Ligand NAG C 1404



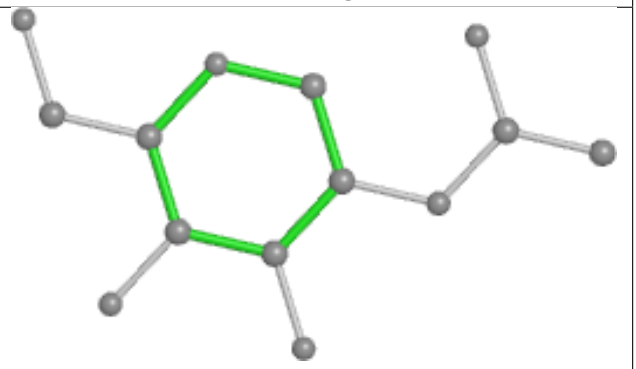
Bond lengths



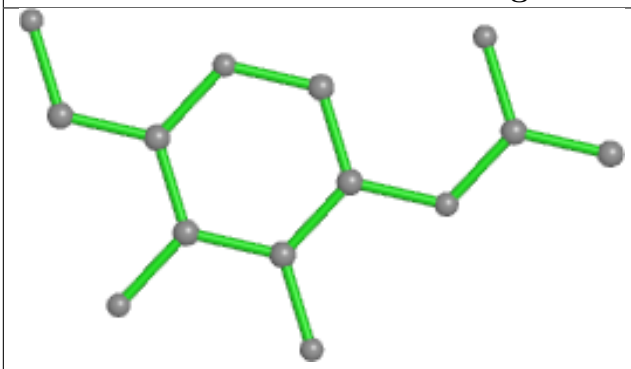
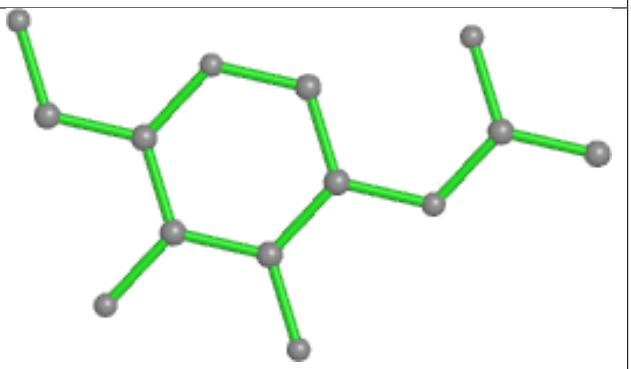
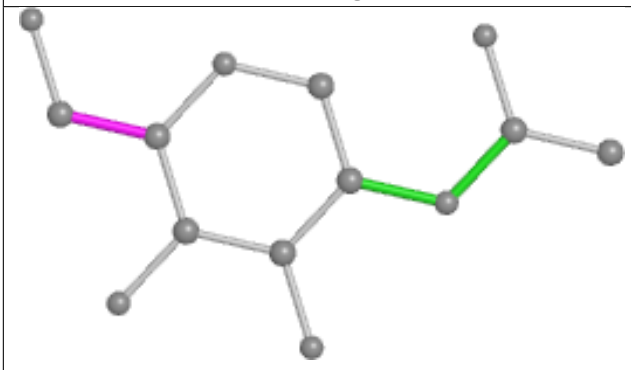
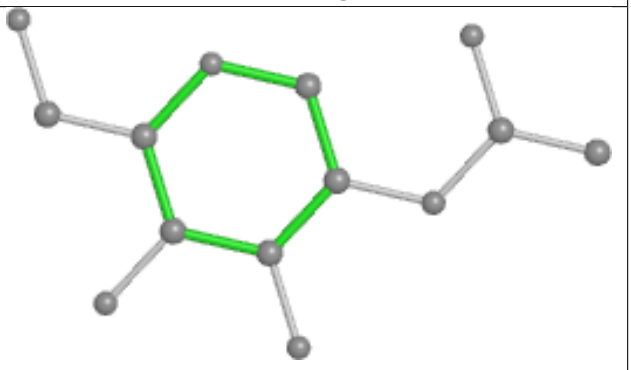
Bond angles

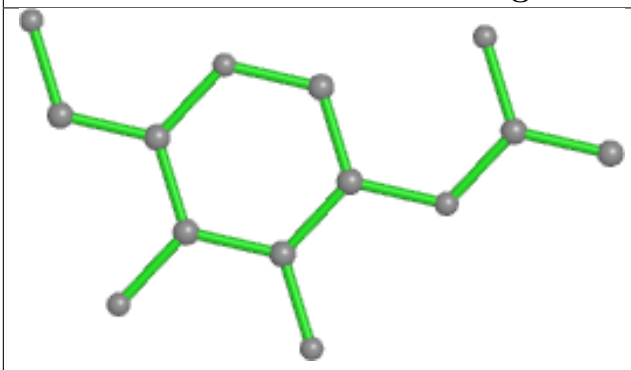
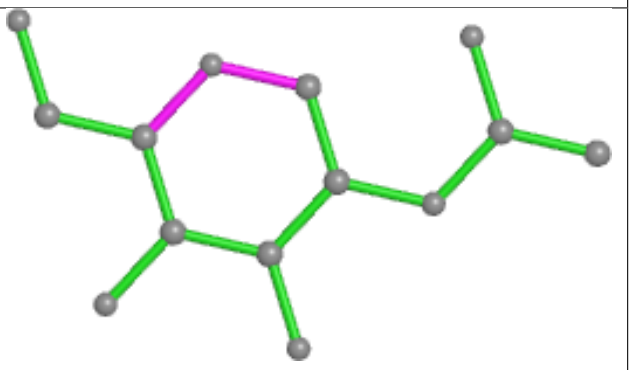
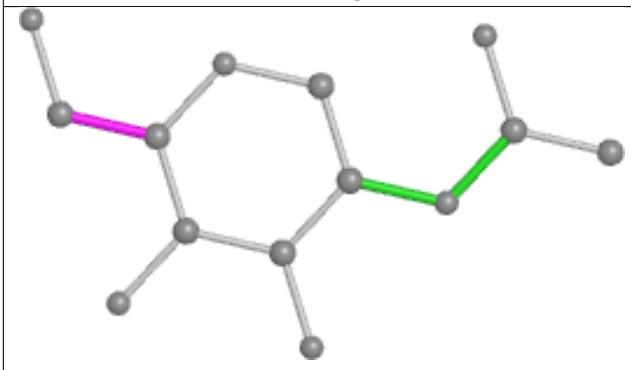
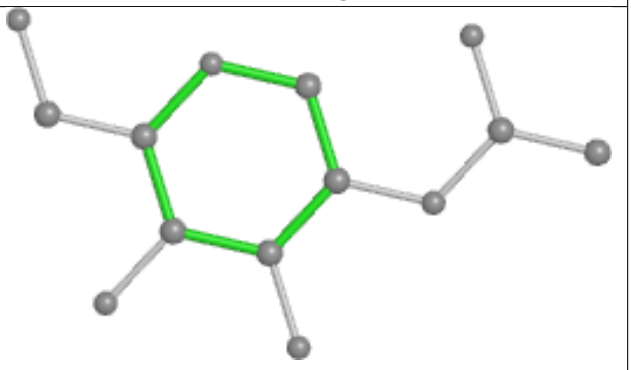


Torsions

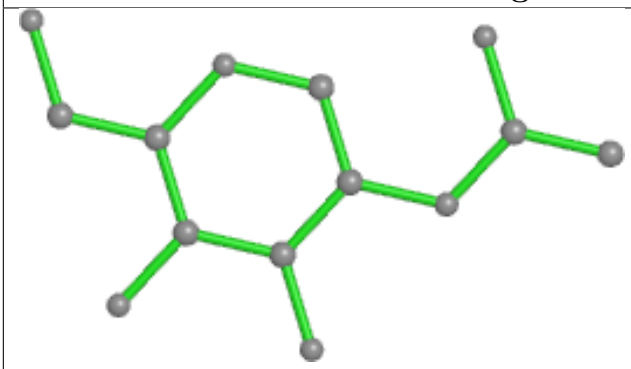


Rings

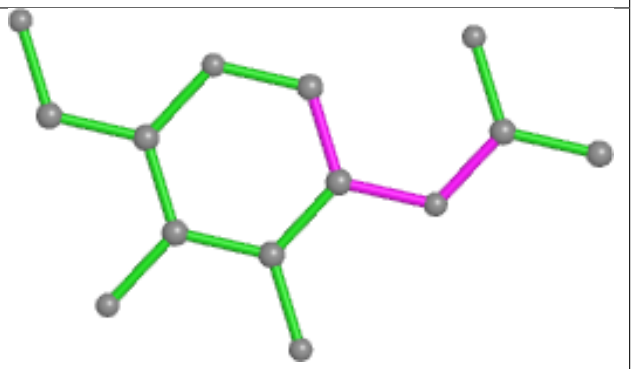
Ligand NAG A 1416	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG B 1411	
 Bond lengths	 Bond angles
 Torsions	 Rings

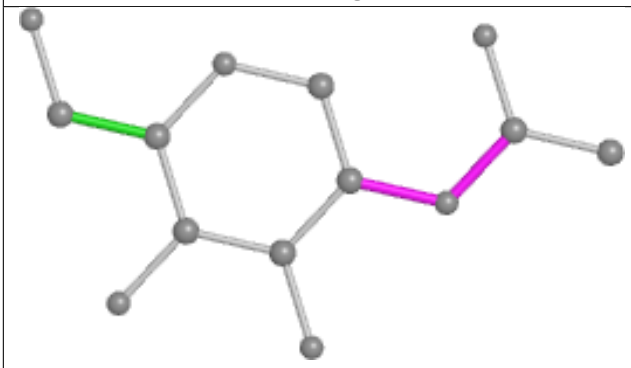
Ligand NAG C 1415



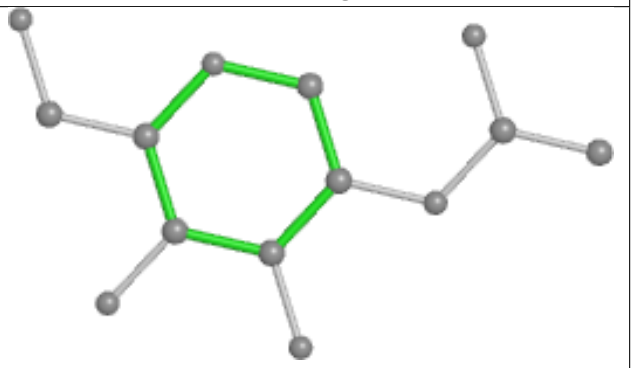
Bond lengths



Bond angles

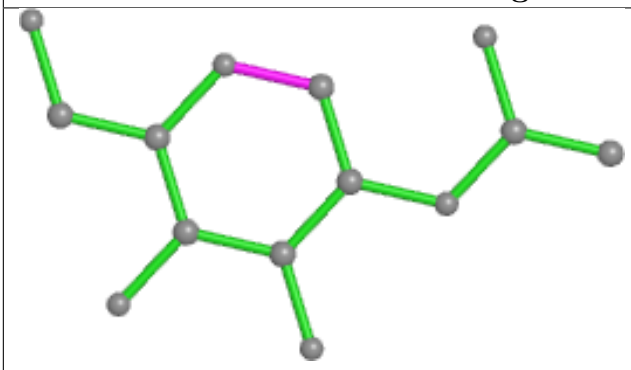


Torsions

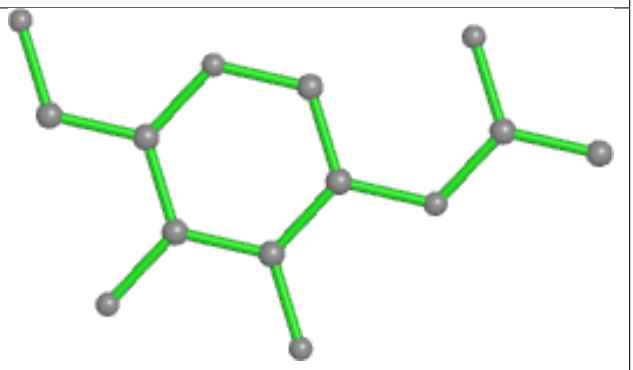


Rings

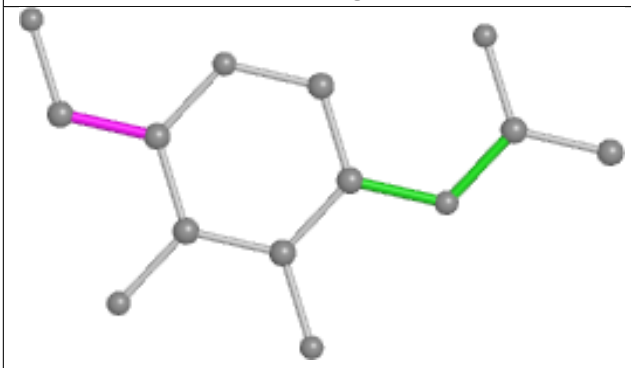
Ligand NAG C 1416



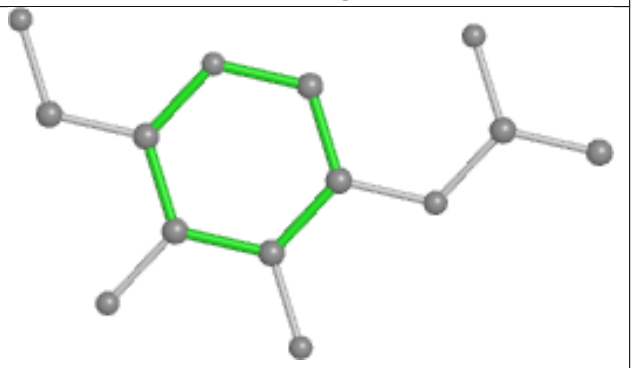
Bond lengths



Bond angles

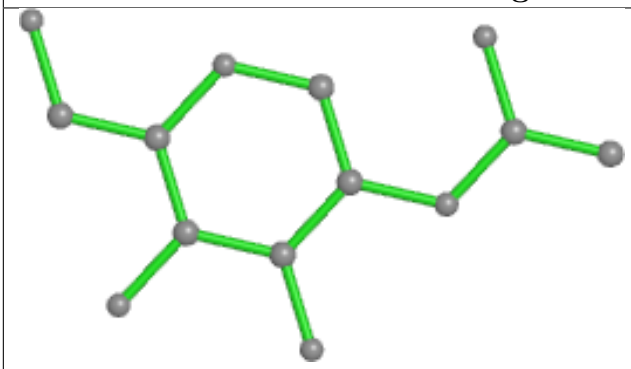


Torsions



Rings

Ligand NAG B 1419



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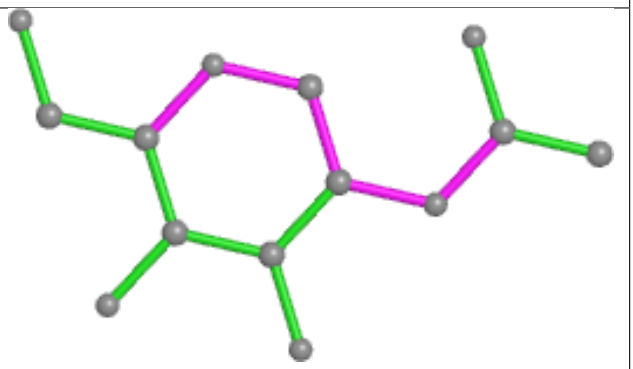
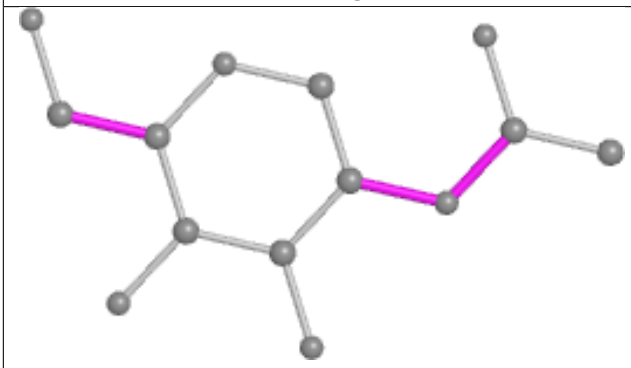
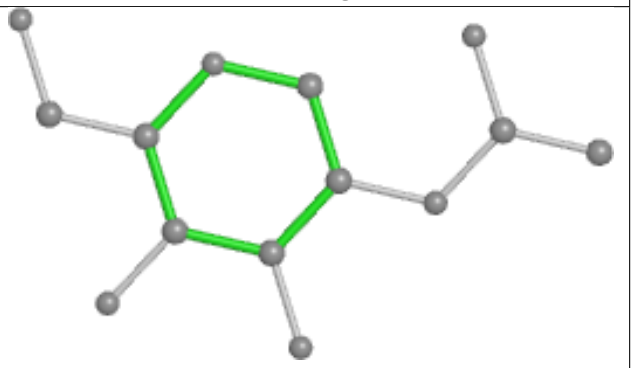


Bond angles

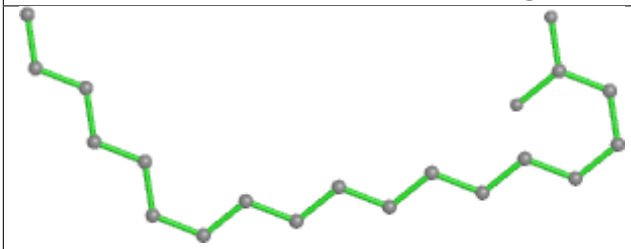


Torsions

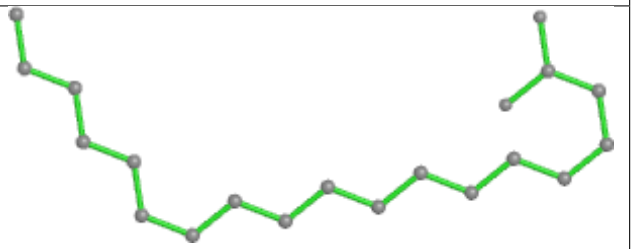


Rings

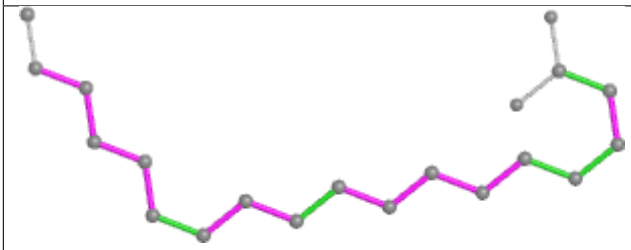
Ligand EIC A 1420



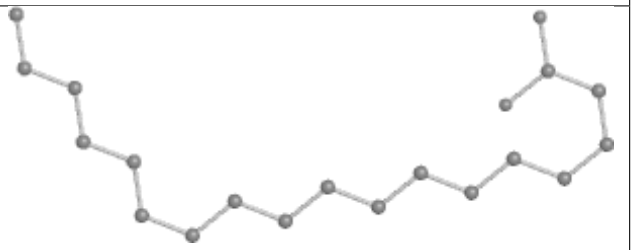
Bond lengths



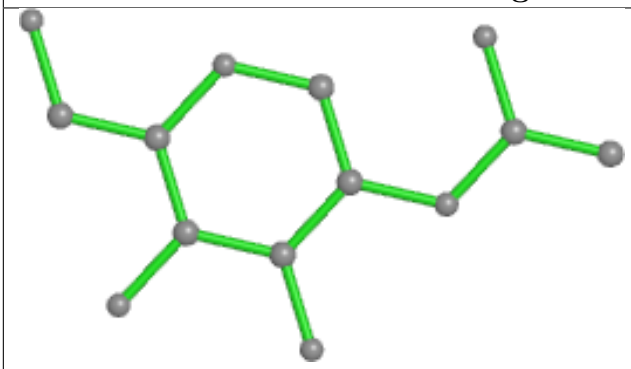
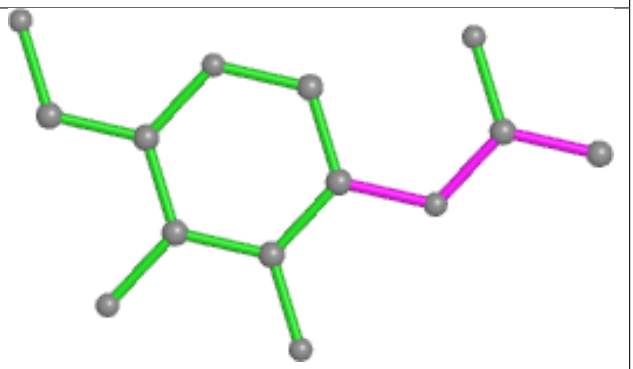
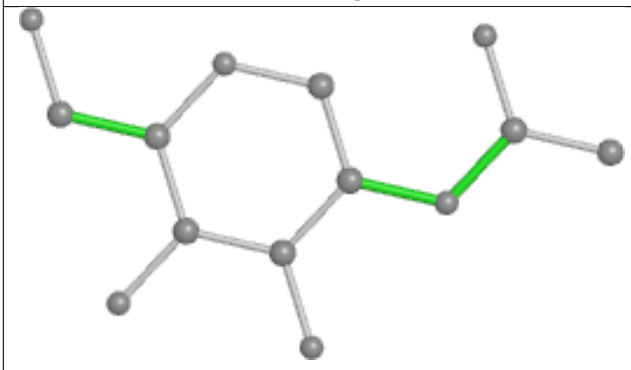
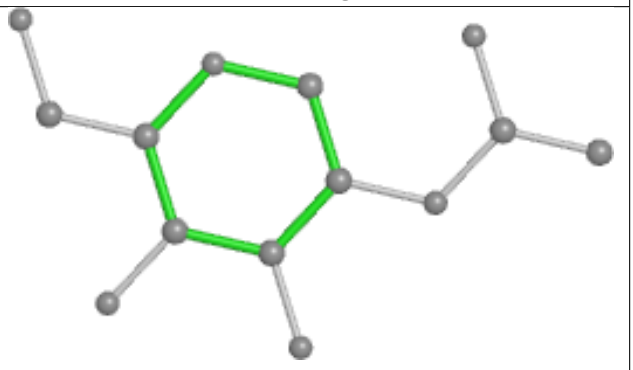
Bond angles

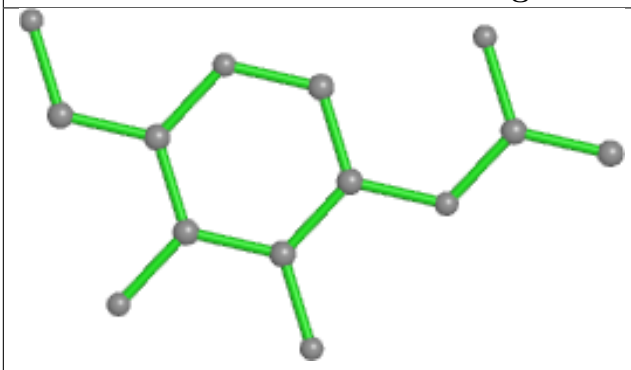
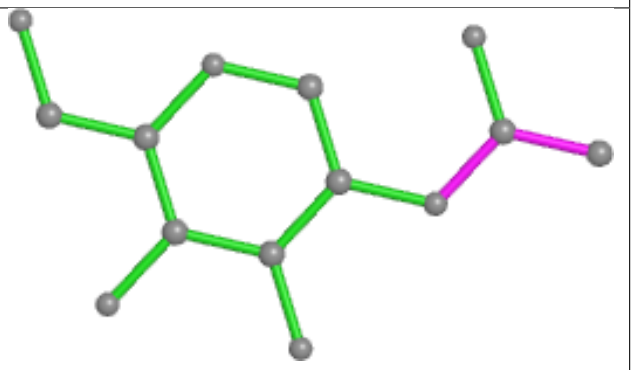
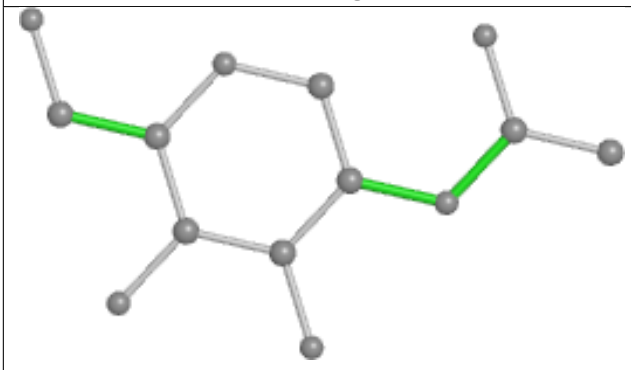
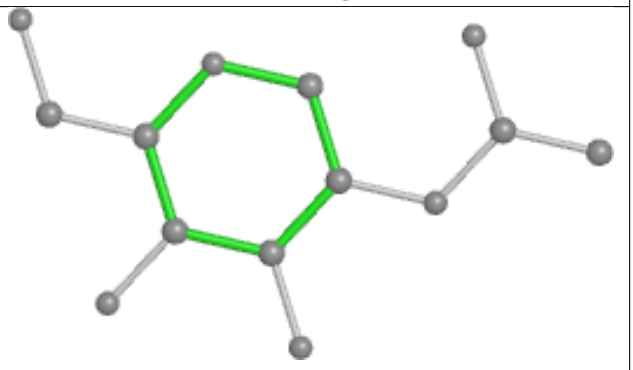


Torsions

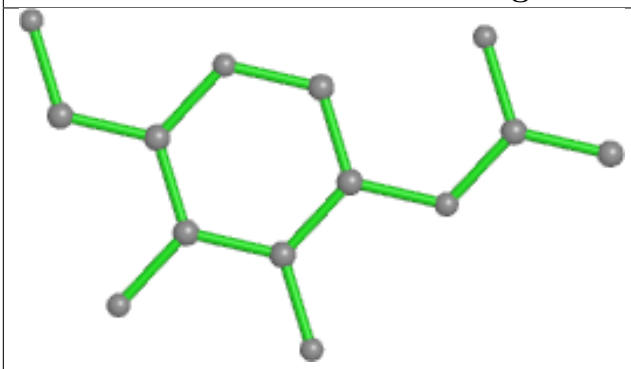


Rings

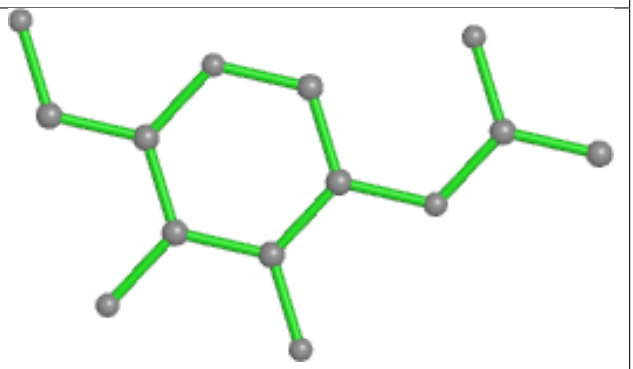
Ligand NAG B 1402	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG B 1413	
 Bond lengths	 Bond angles
 Torsions	 Rings

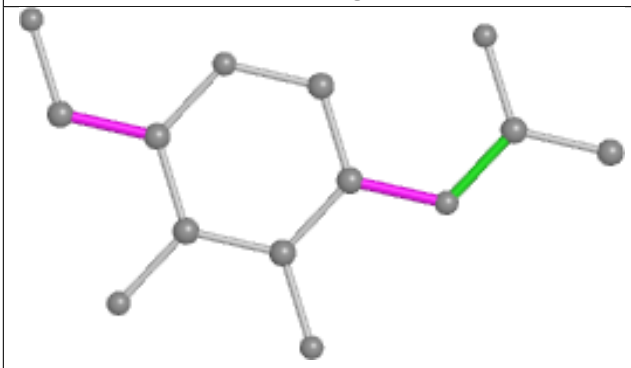
Ligand NAG B 1404



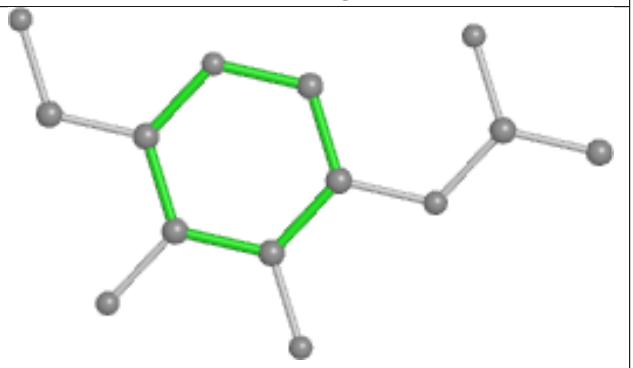
Bond lengths



Bond angles

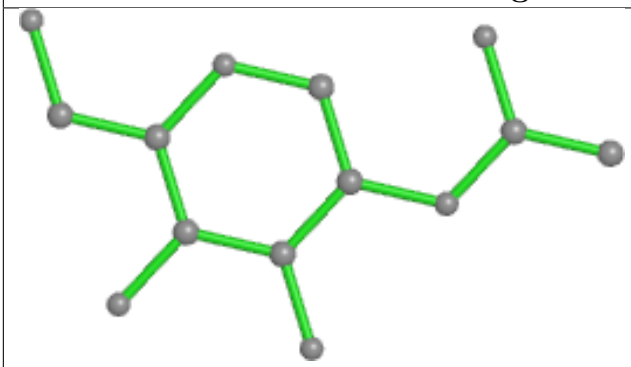


Torsions

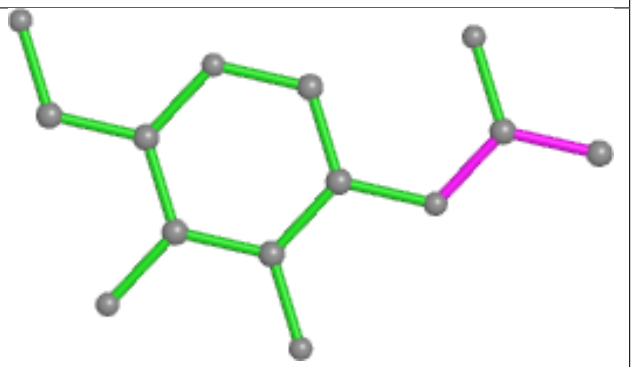


Rings

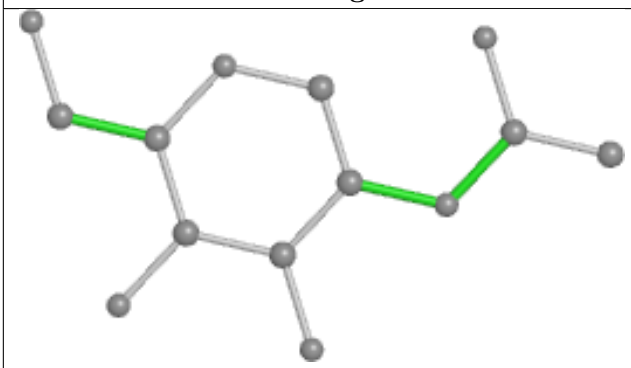
Ligand NAG C 1401



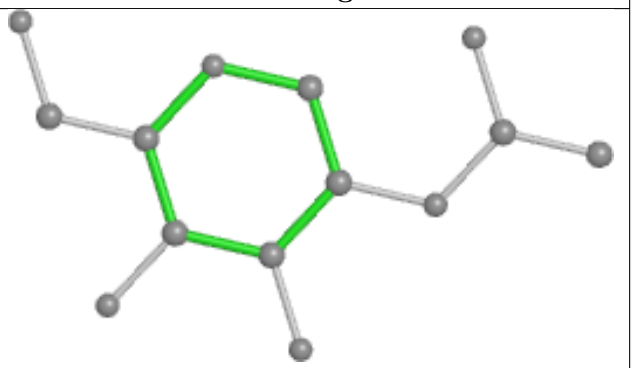
Bond lengths



Bond angles

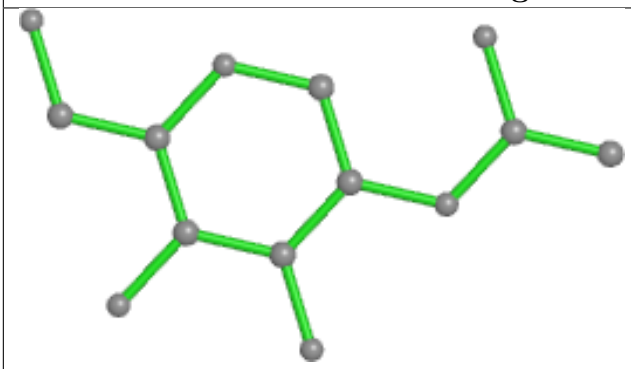


Torsions

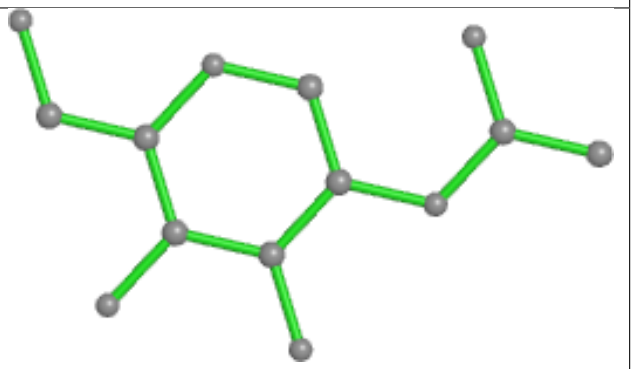


Rings

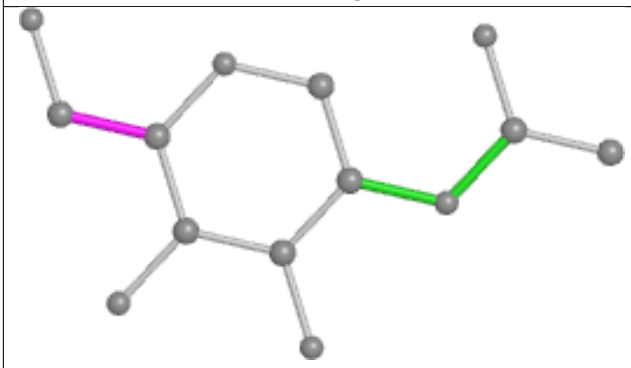
Ligand NAG C 1403



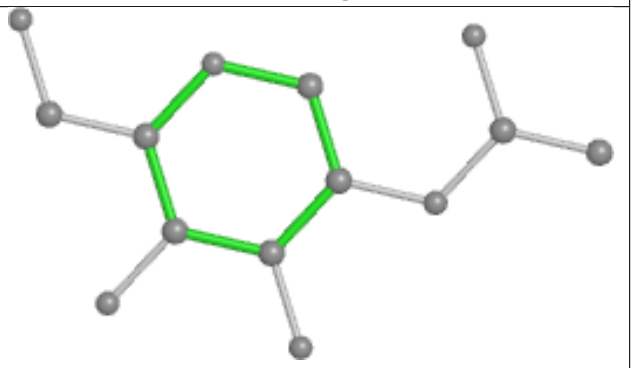
Bond lengths



Bond angles

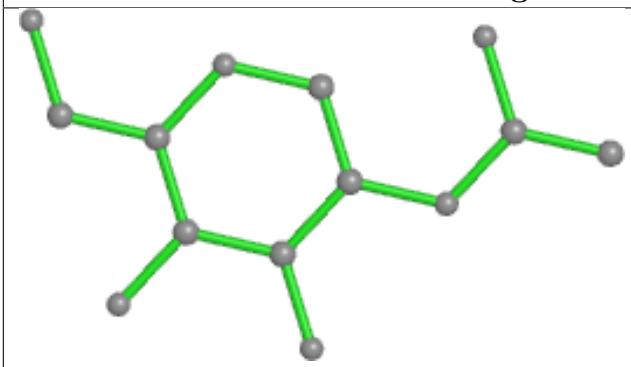


Torsions

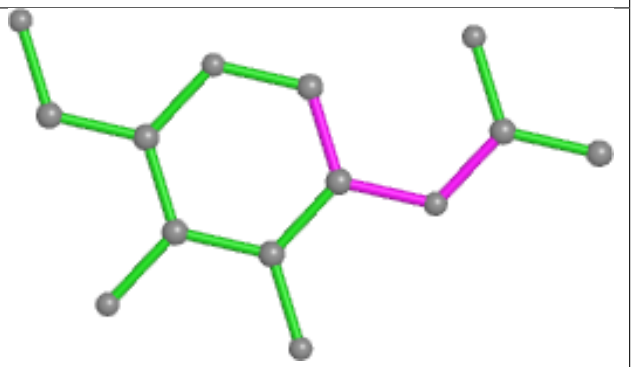


Rings

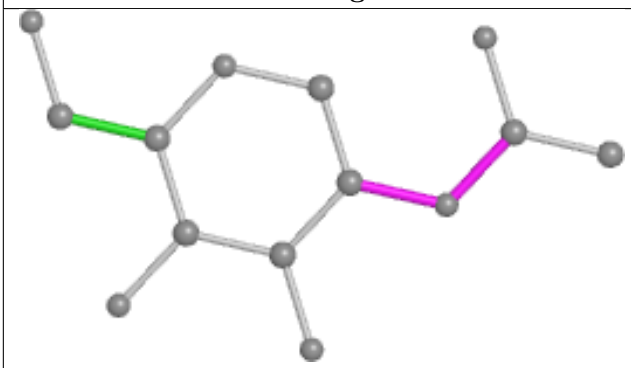
Ligand NAG A 1417



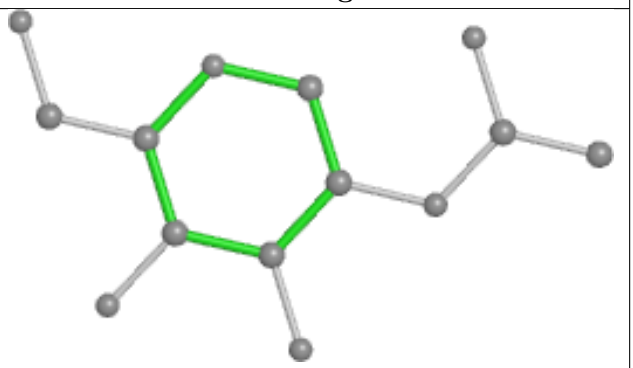
Bond lengths



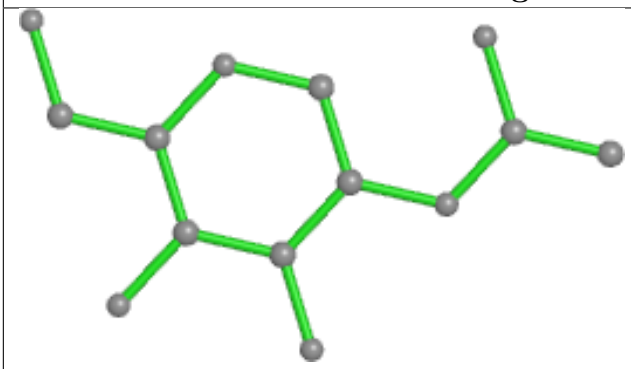
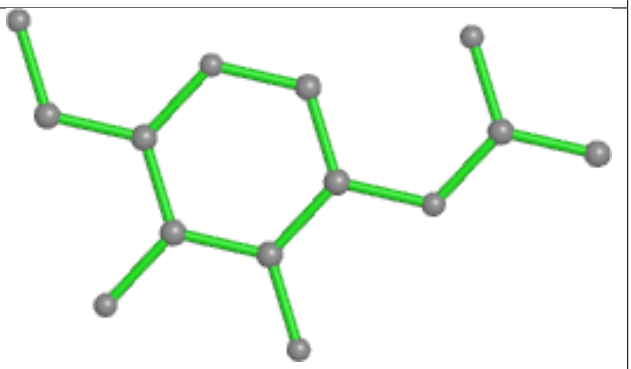
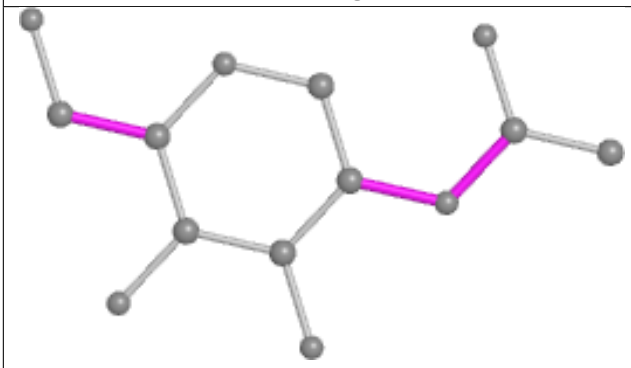
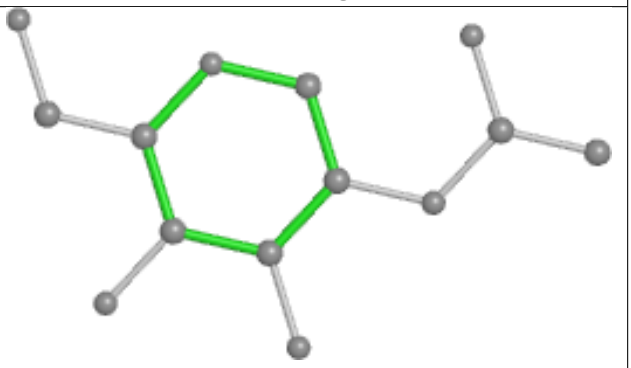
Bond angles

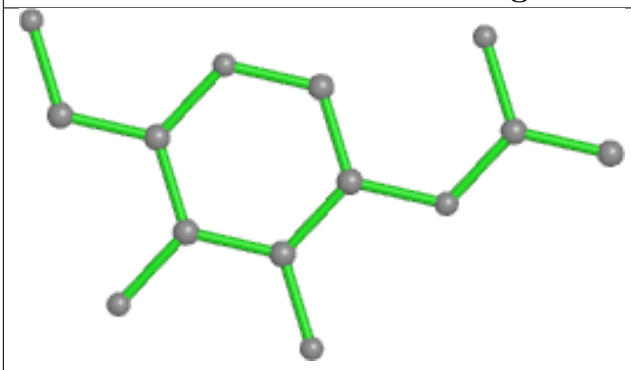
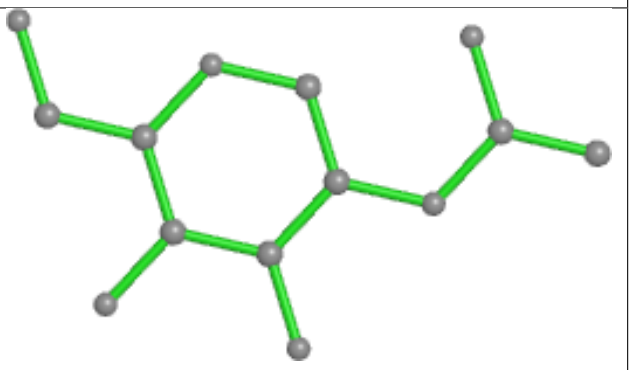
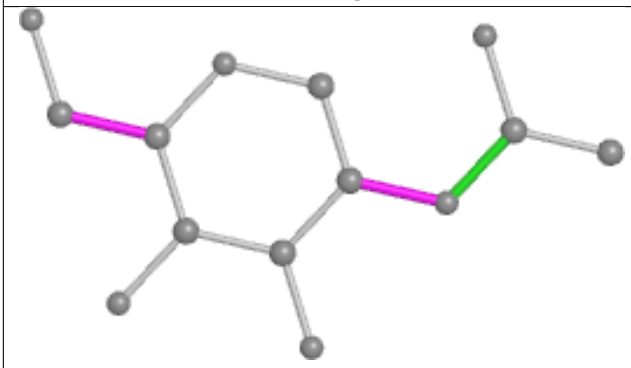
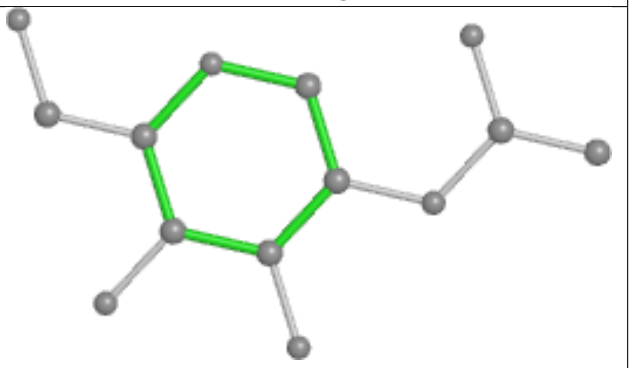


Torsions

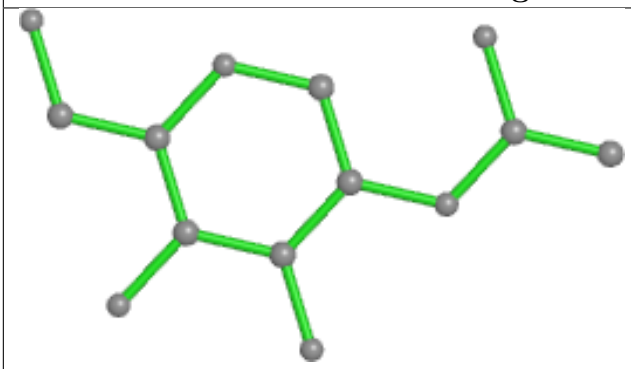


Rings

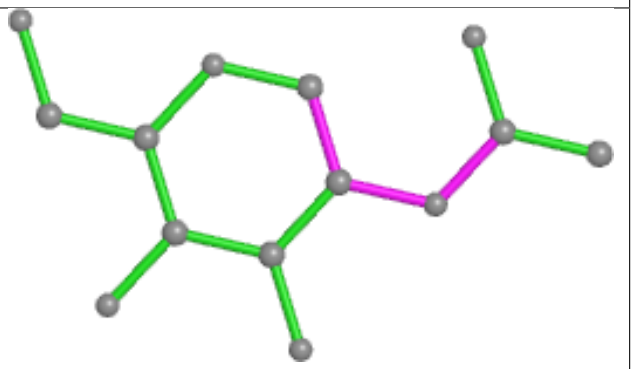
Ligand NAG C 1412	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG A 1404	
 Bond lengths	 Bond angles
 Torsions	 Rings

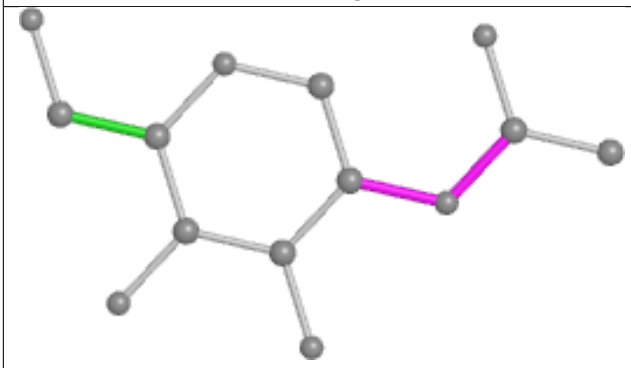
Ligand NAG B 1417



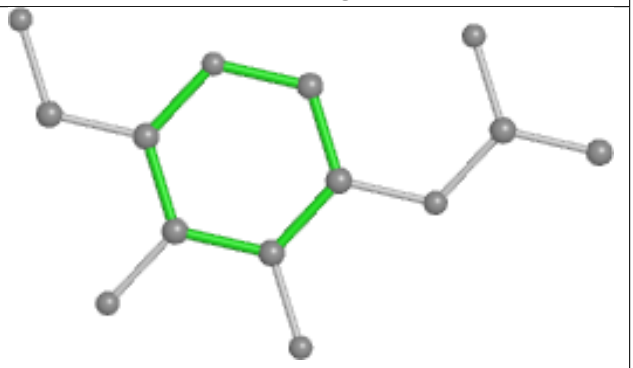
Bond lengths



Bond angles

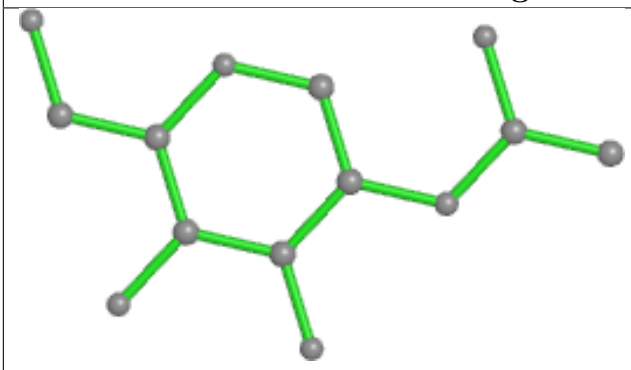


Torsions

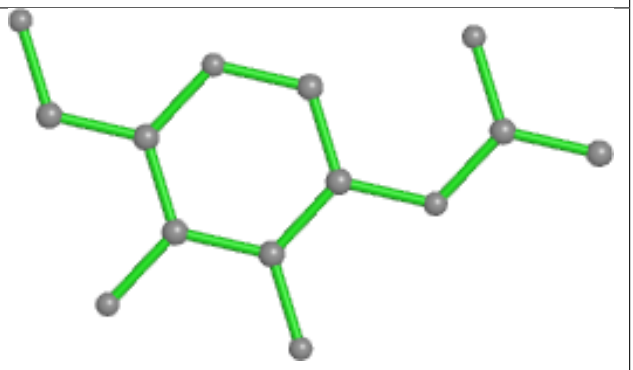


Rings

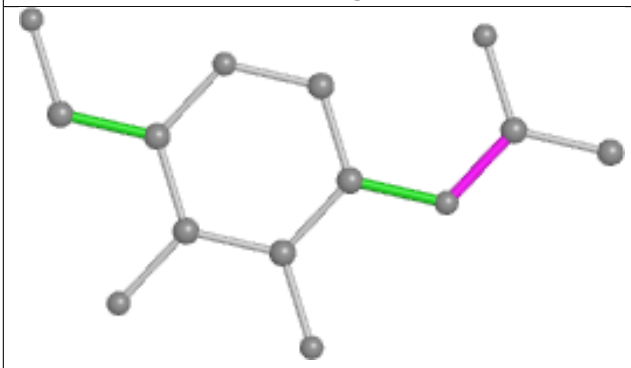
Ligand NAG C 1408



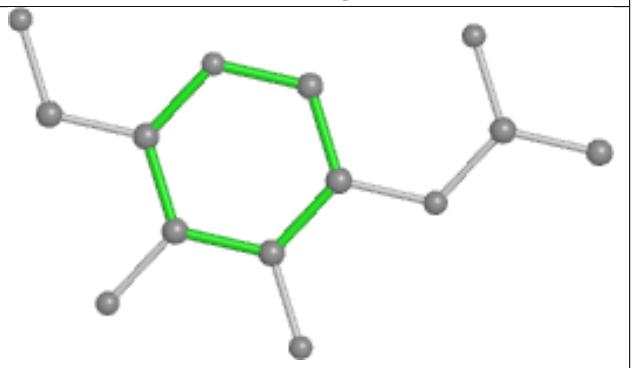
Bond lengths



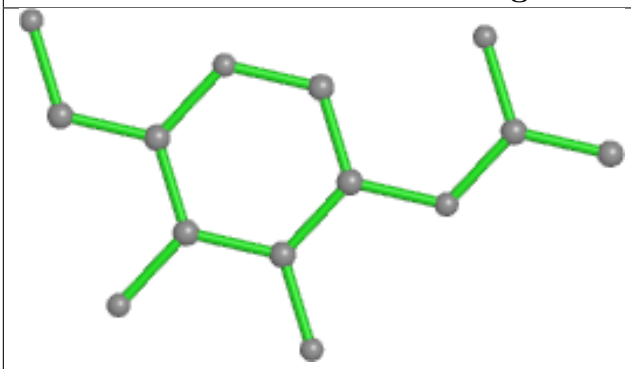
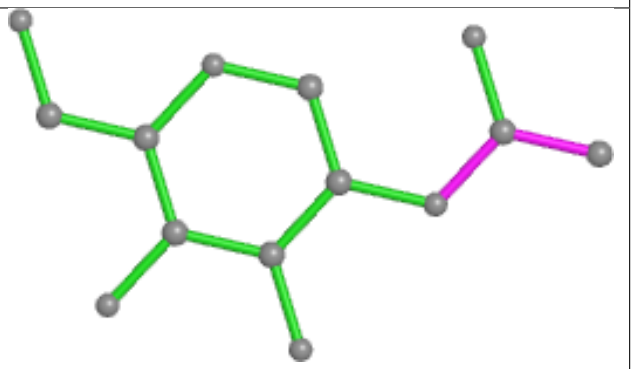
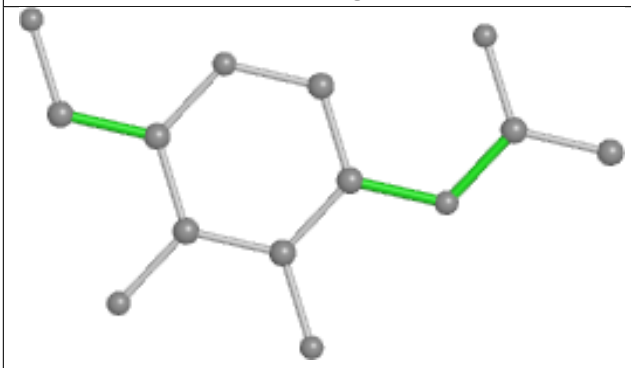
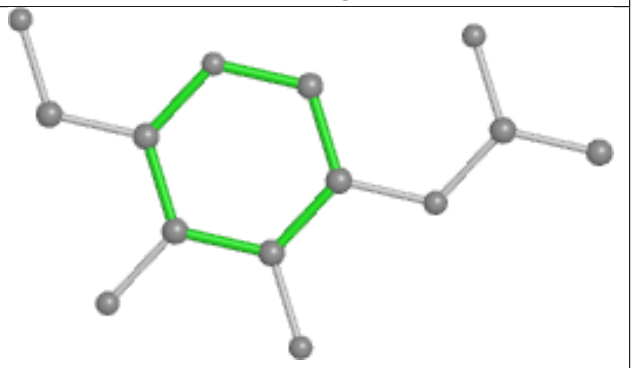
Bond angles

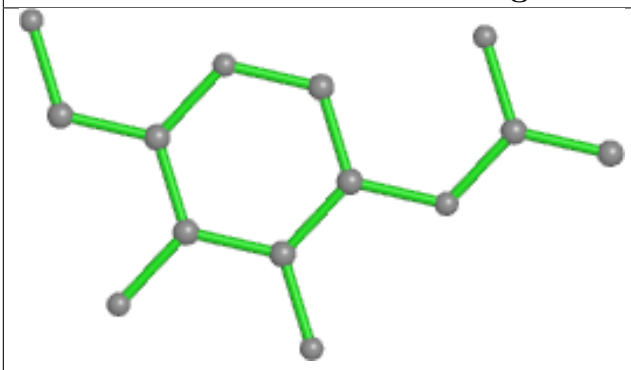
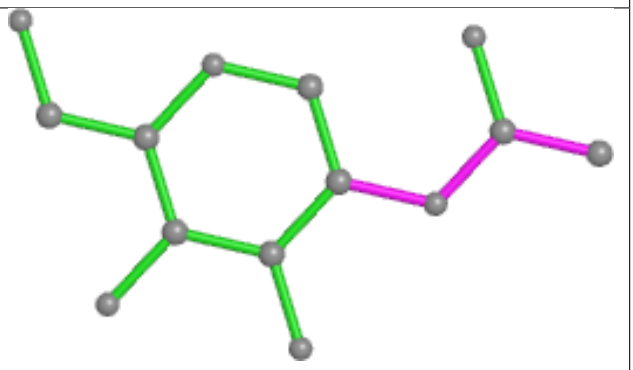
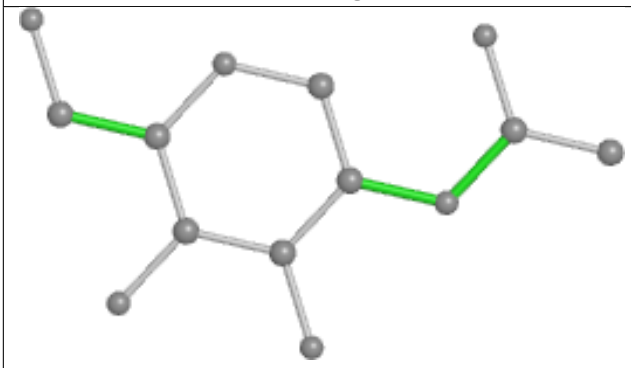
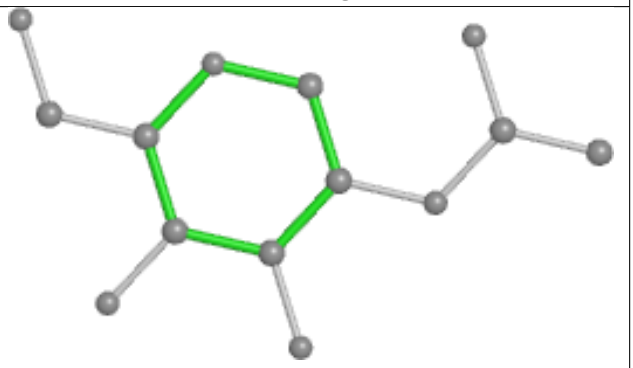


Torsions

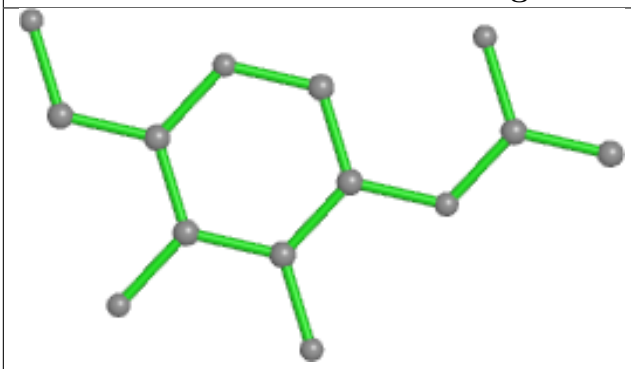


Rings

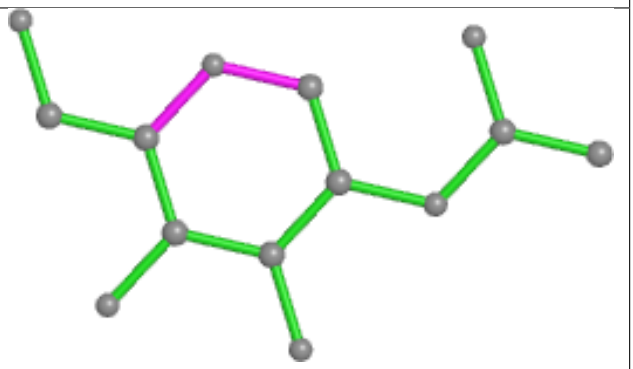
Ligand NAG A 1413	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG A 1402	
 Bond lengths	 Bond angles
 Torsions	 Rings

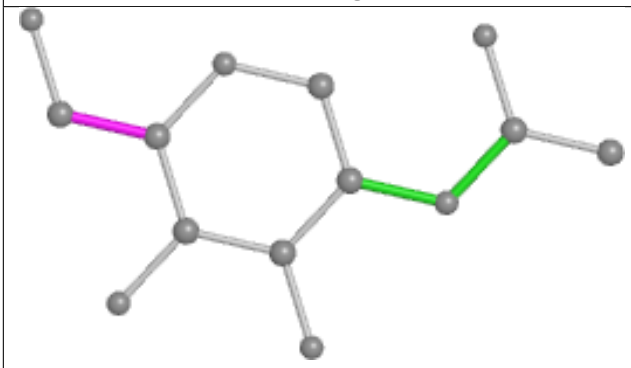
Ligand NAG A 1418



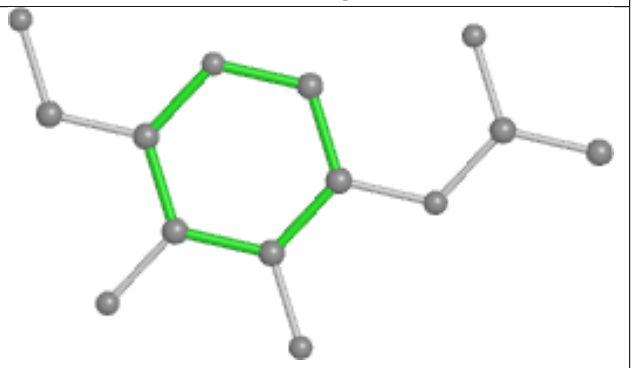
Bond lengths



Bond angles

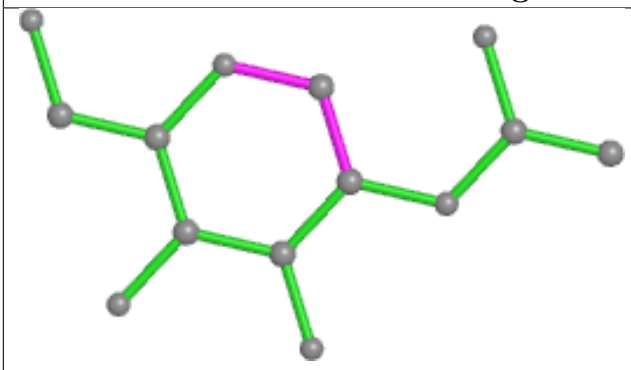


Torsions

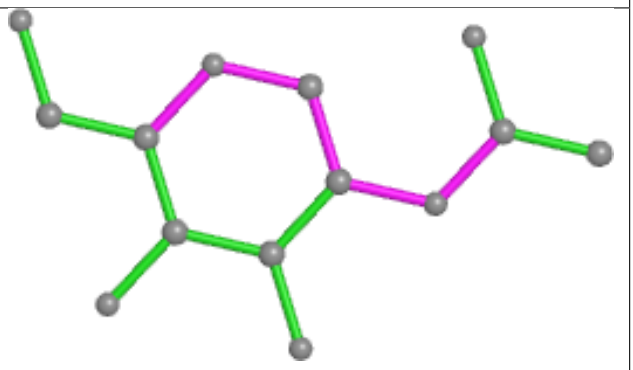


Rings

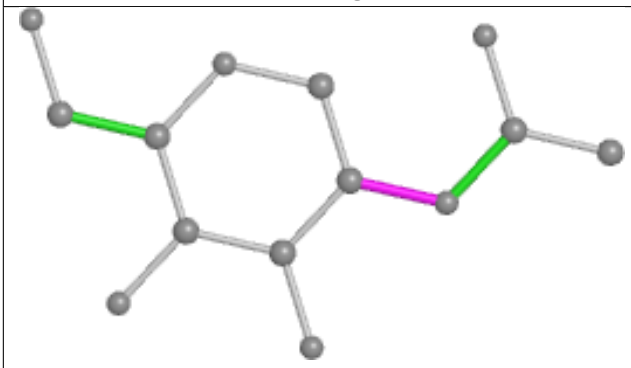
Ligand NAG B 1410



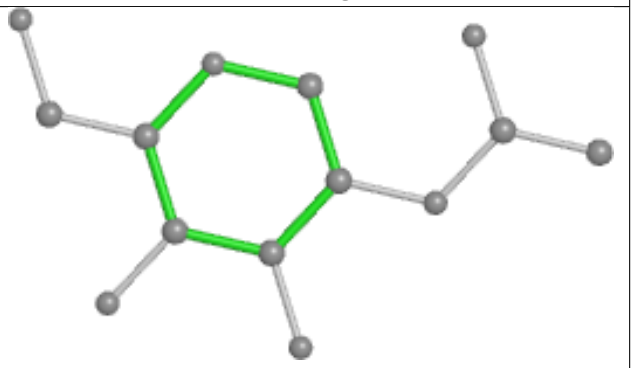
Bond lengths



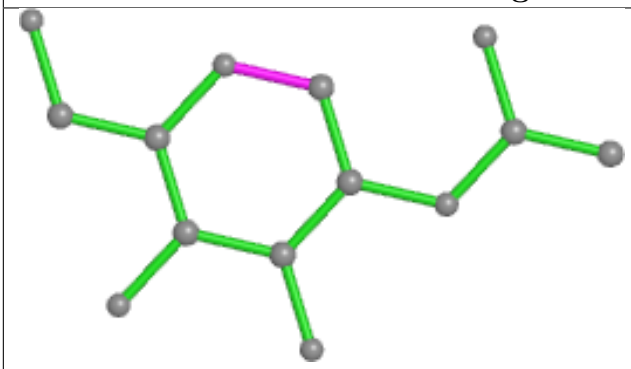
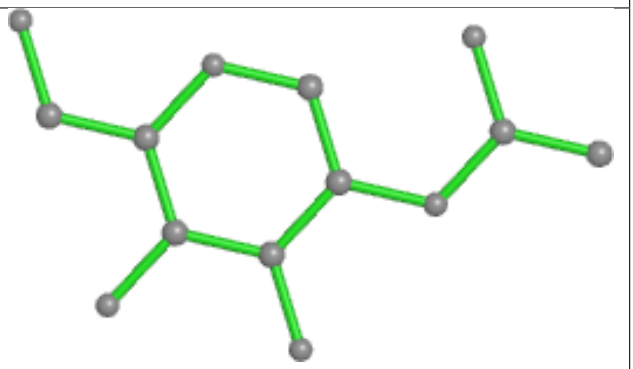
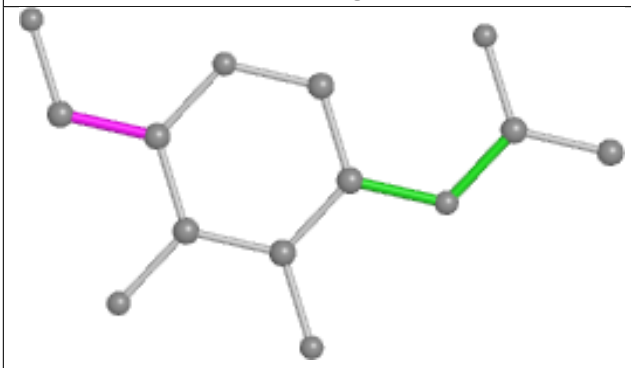
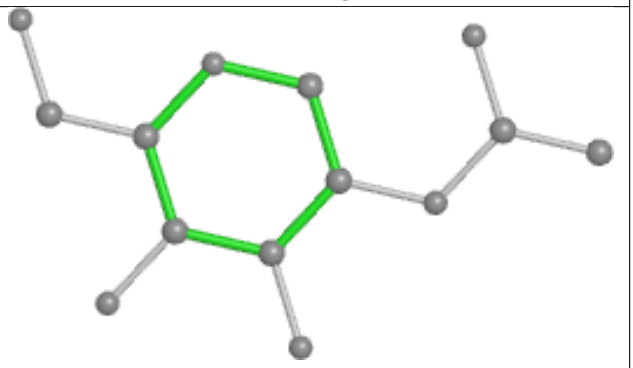
Bond angles

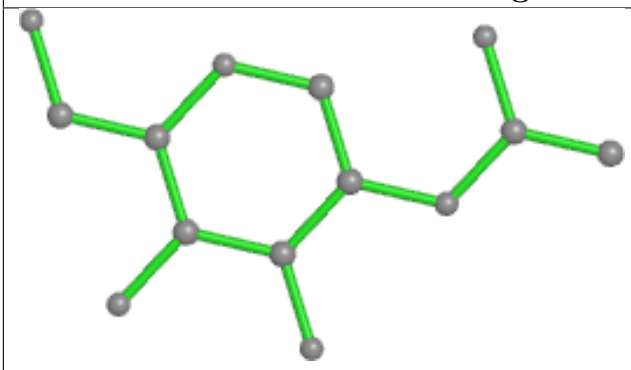
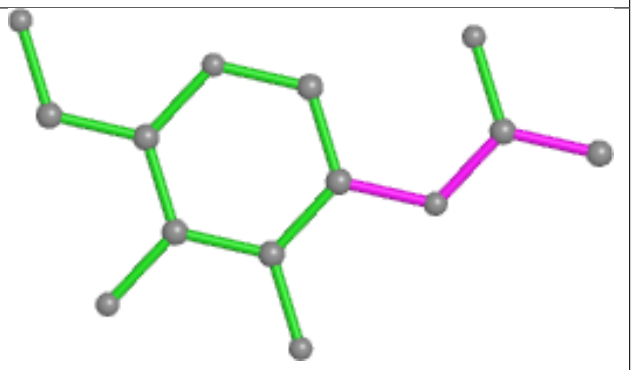
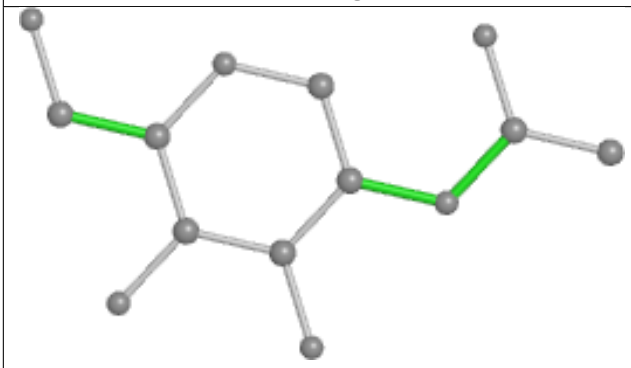
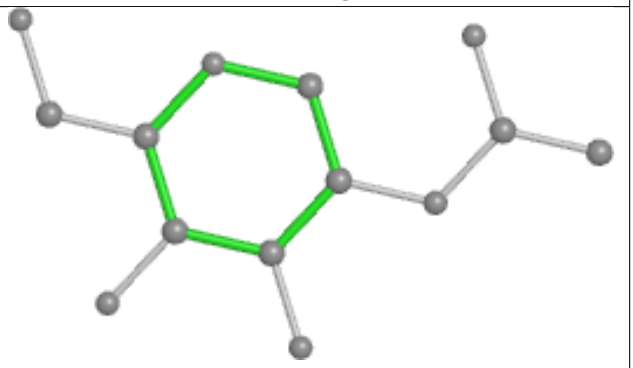


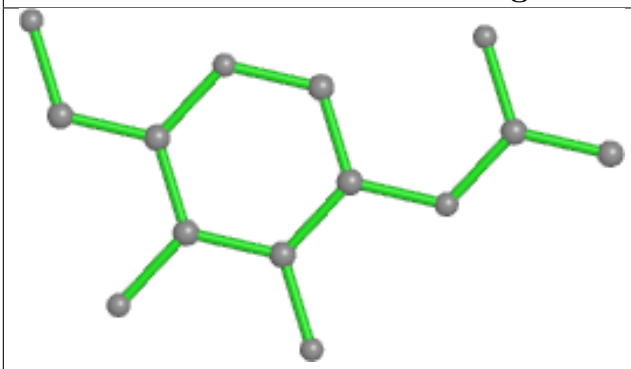
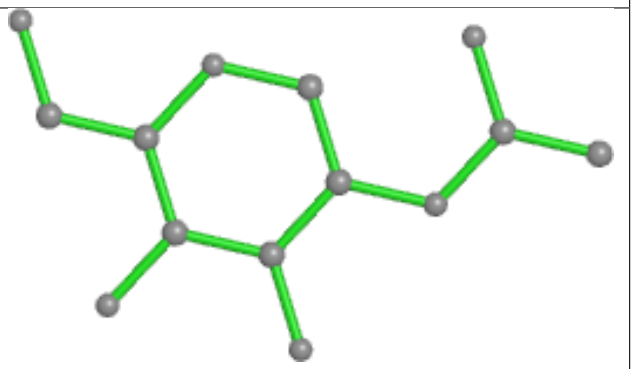
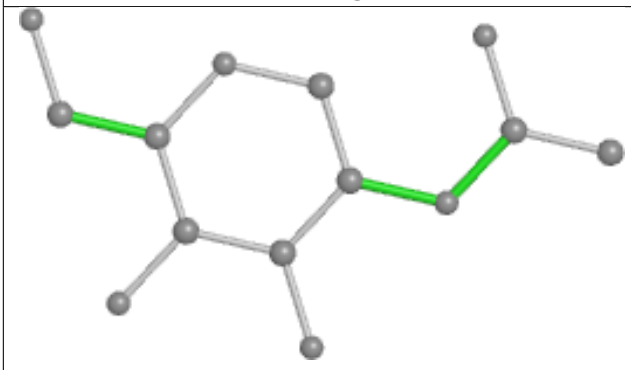
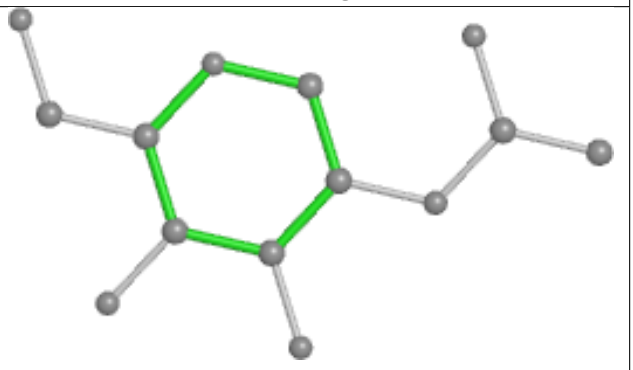
Torsions

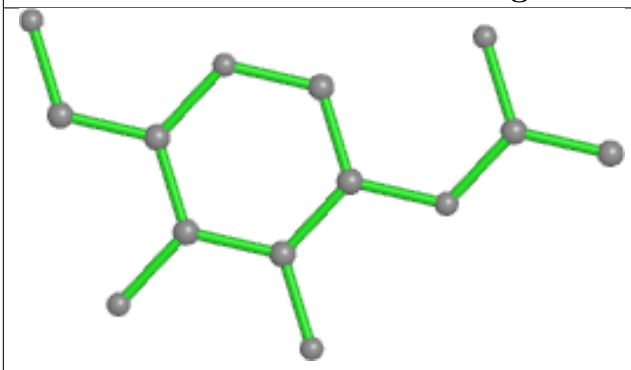
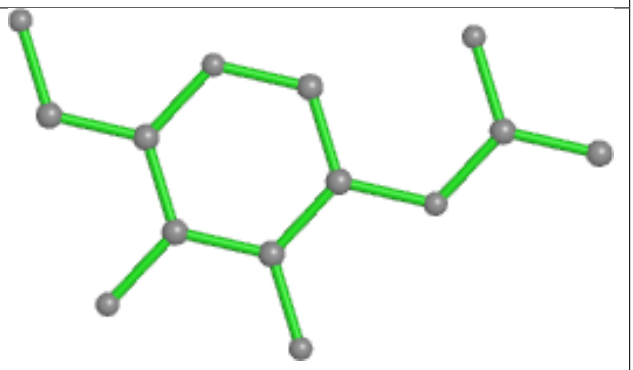
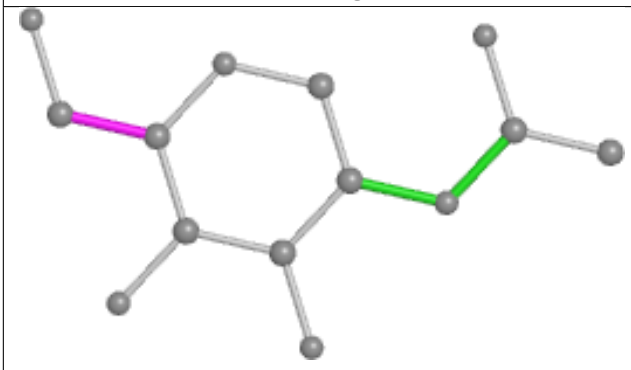
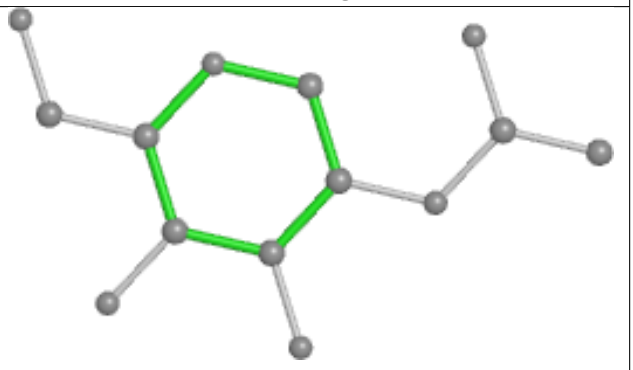


Rings

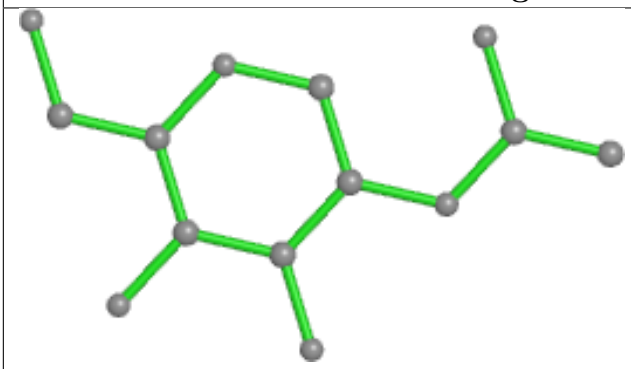
Ligand NAG B 1418	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG B 1405	
 Bond lengths	 Bond angles
 Torsions	 Rings

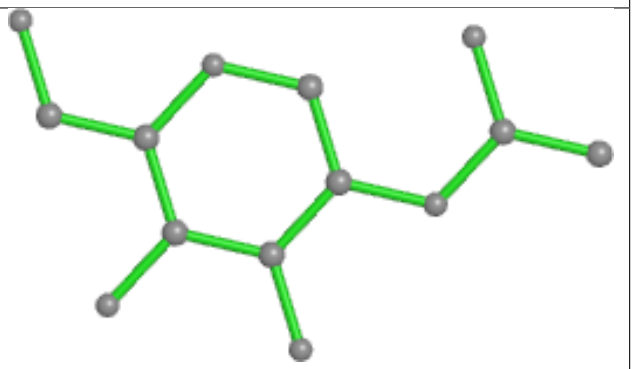
Ligand NAG A 1419	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand NAG A 1403	
	
Bond lengths	Bond angles
	
Torsions	Rings

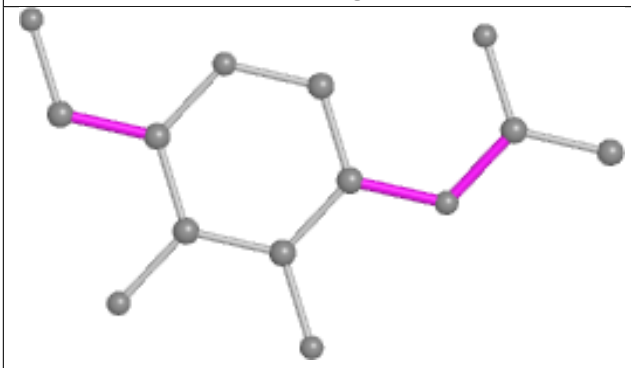
Ligand NAG B 1412



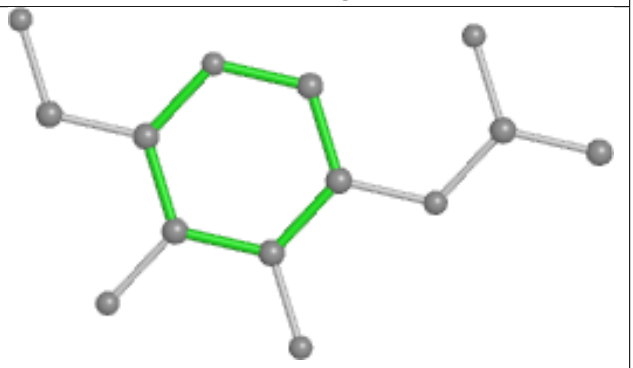
Bond lengths



Bond angles

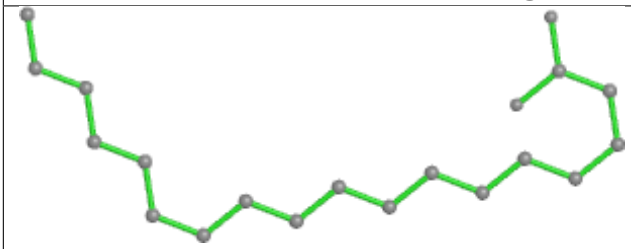


Torsions

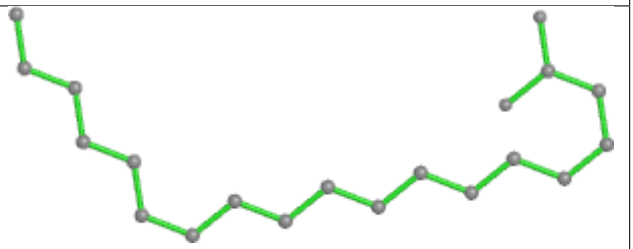


Rings

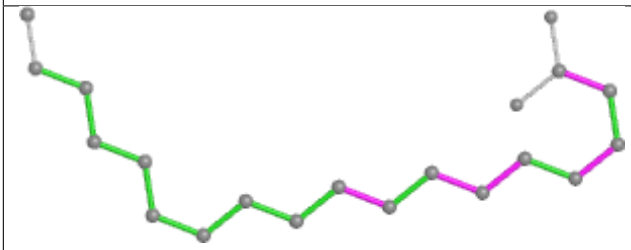
Ligand EIC C 1420



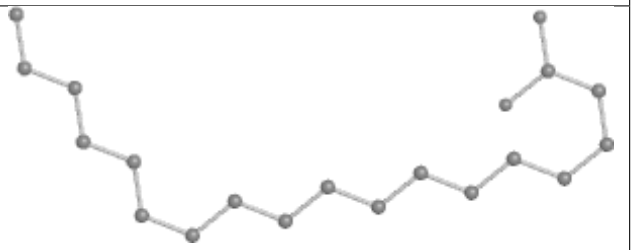
Bond lengths



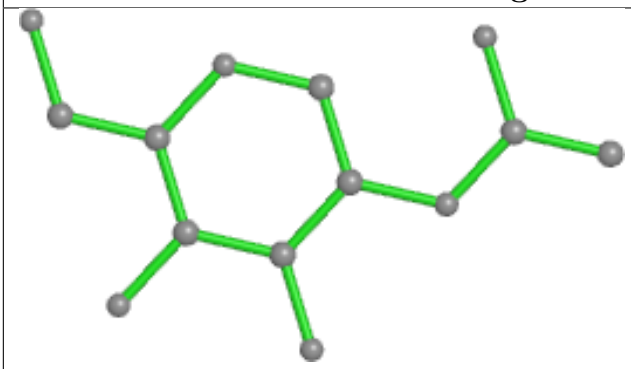
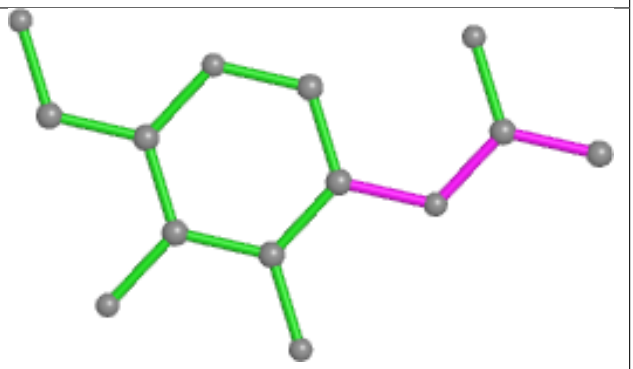
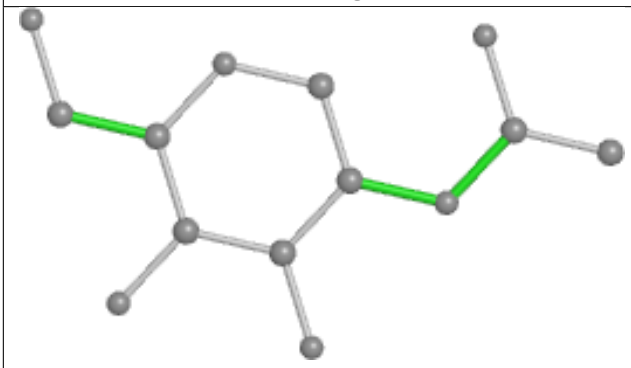
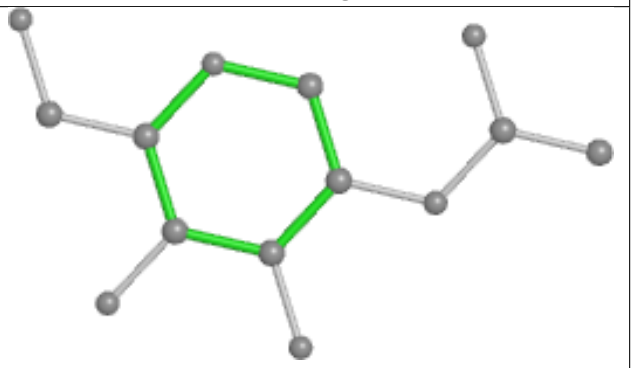
Bond angles

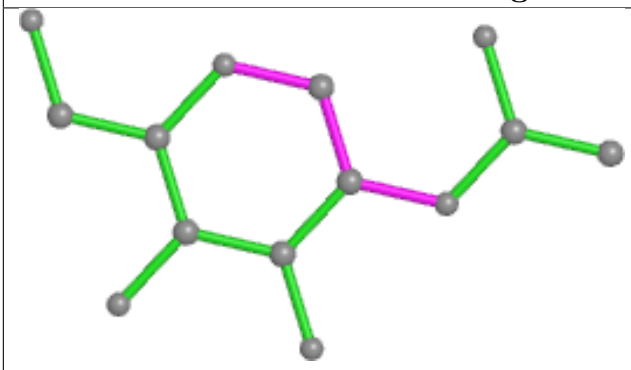
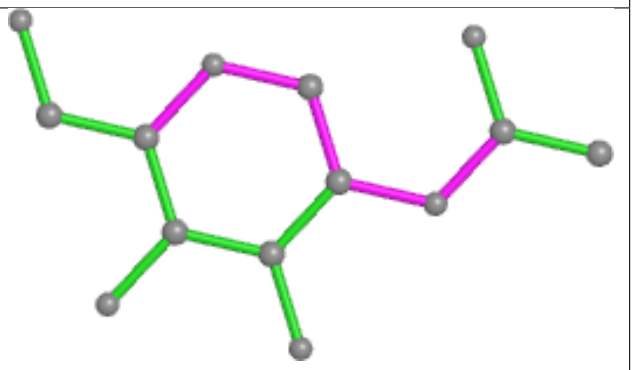
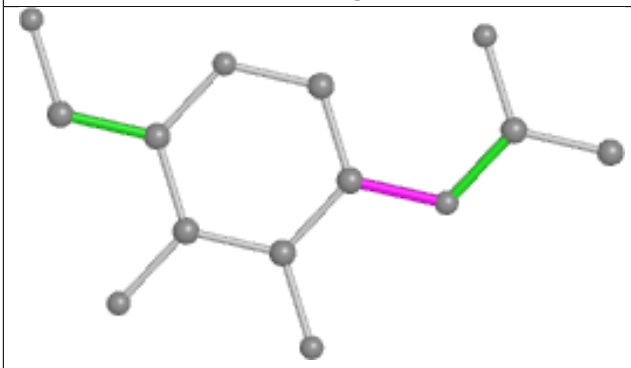
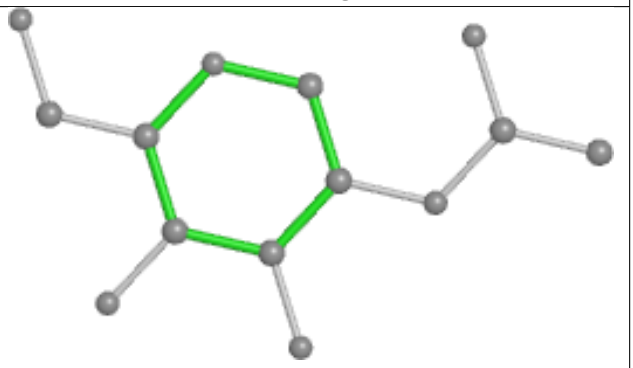


Torsions

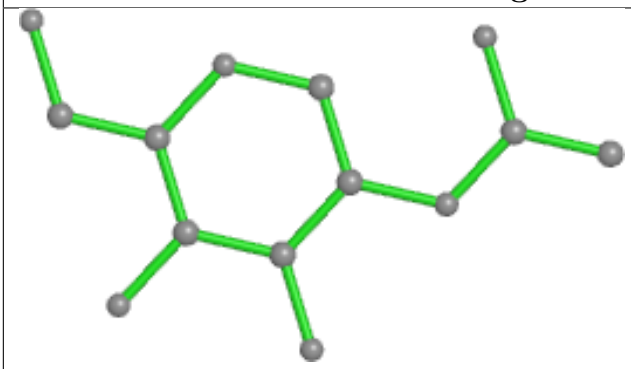


Rings

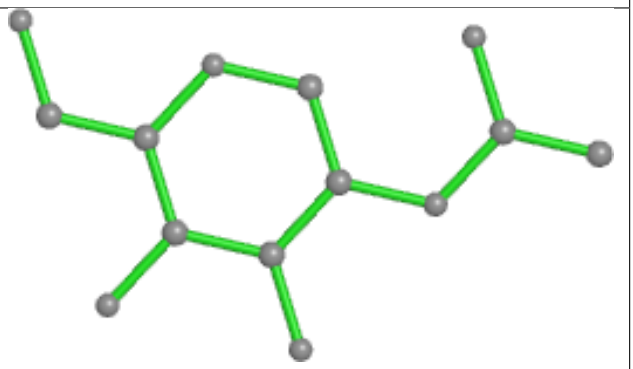
Ligand NAG A 1405	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG A 1410	
 Bond lengths	 Bond angles
 Torsions	 Rings

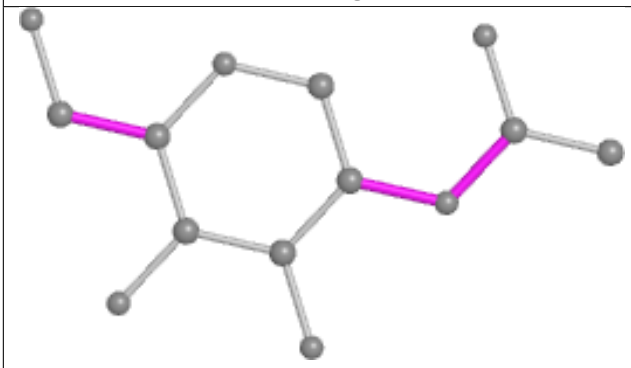
Ligand NAG A 1412



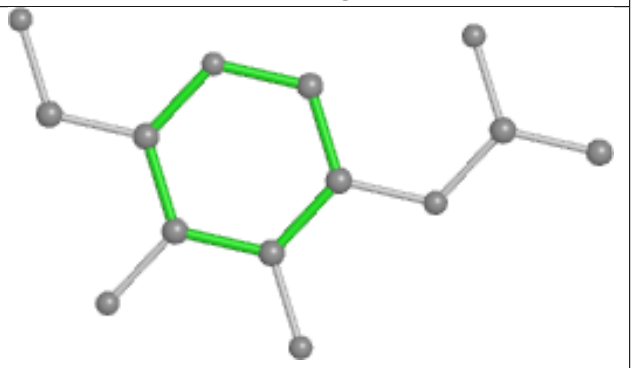
Bond lengths



Bond angles

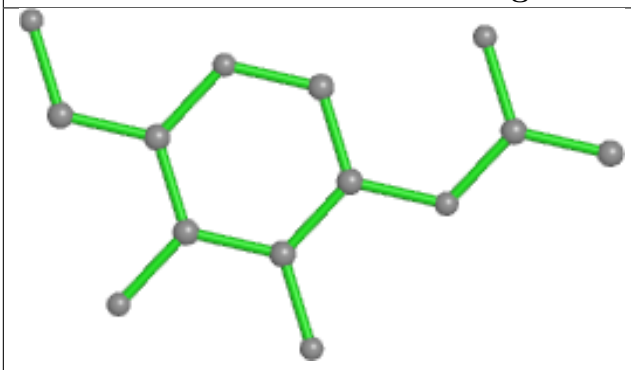


Torsions



Rings

Ligand NAG C 1411



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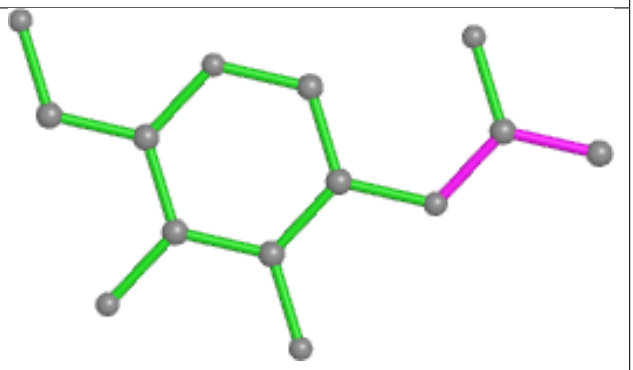
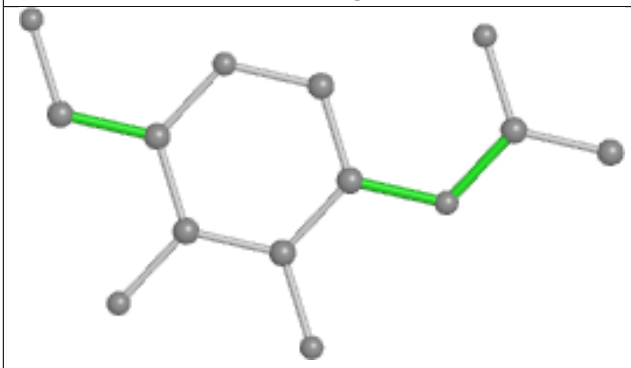


Bond angles



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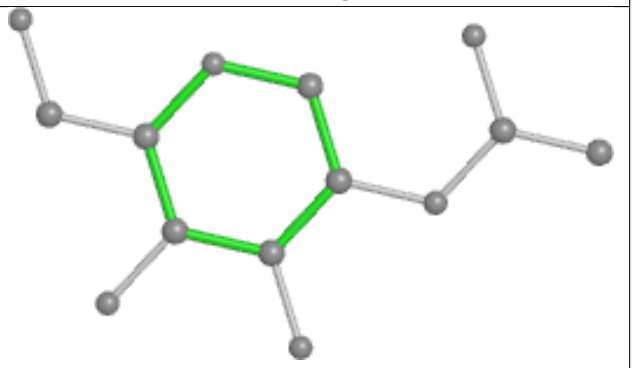
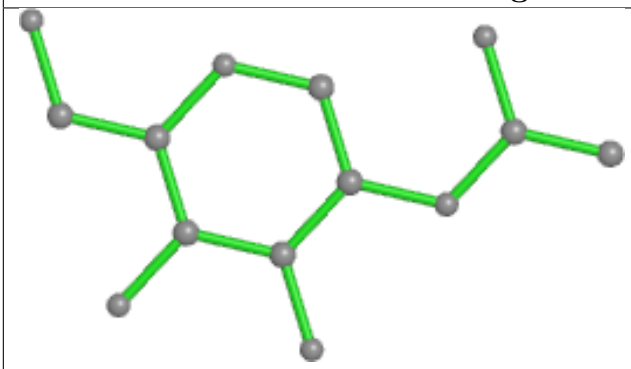


Rings

Ligand NAG A 1406



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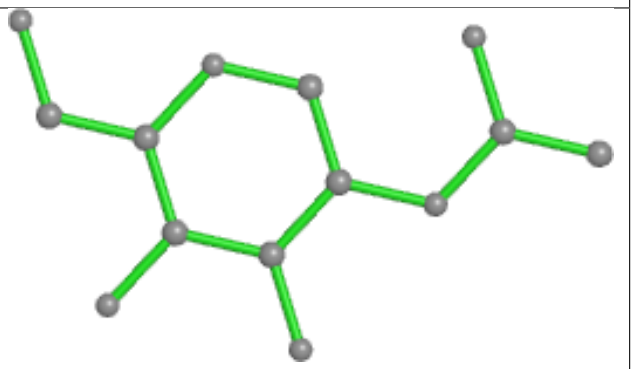
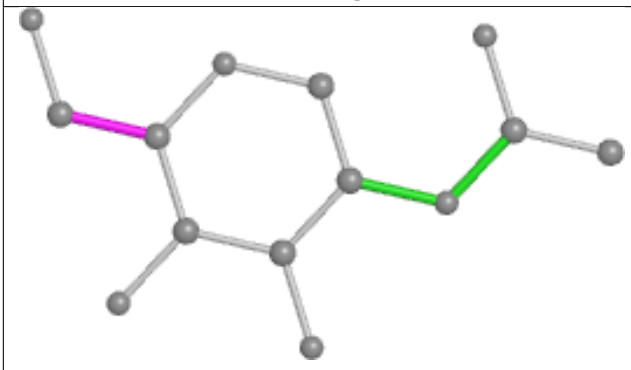


Bond angles



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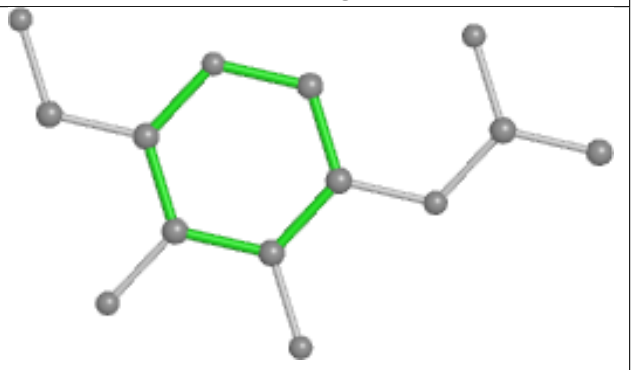
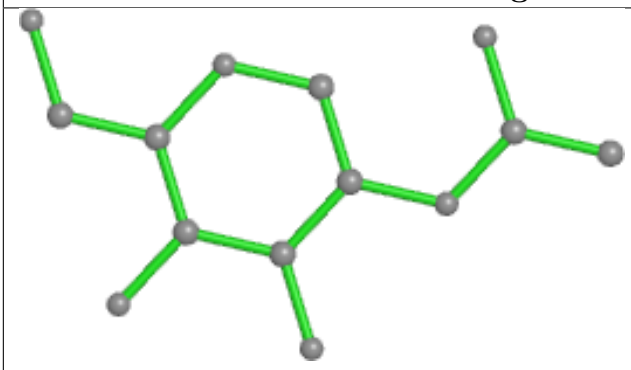


Rings

Ligand NAG A 1414



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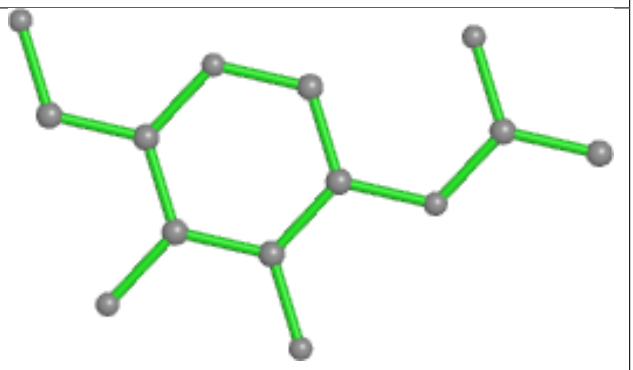
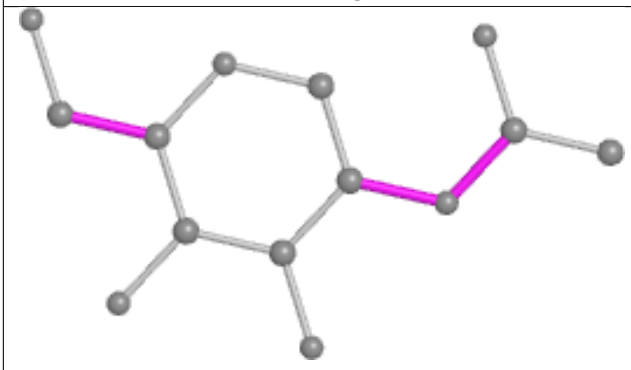


Bond angles



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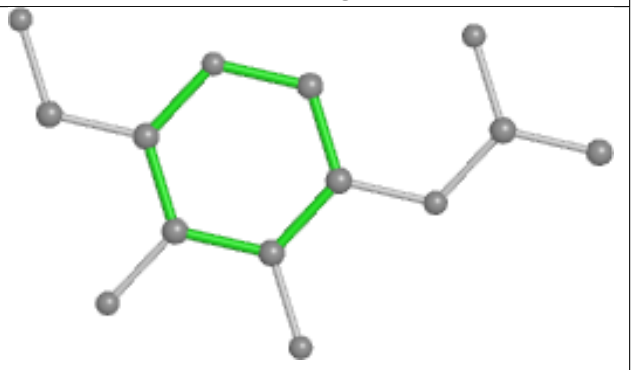
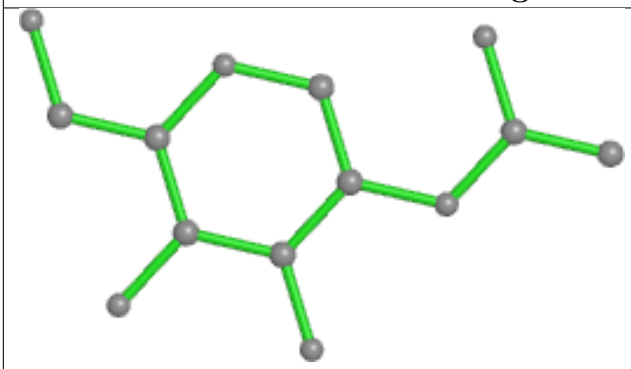


Rings

Ligand NAG C 1413



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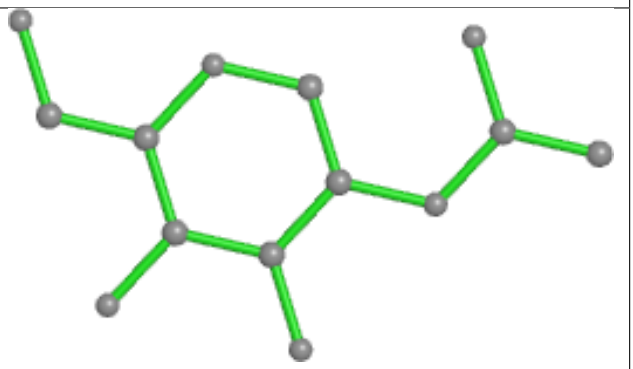
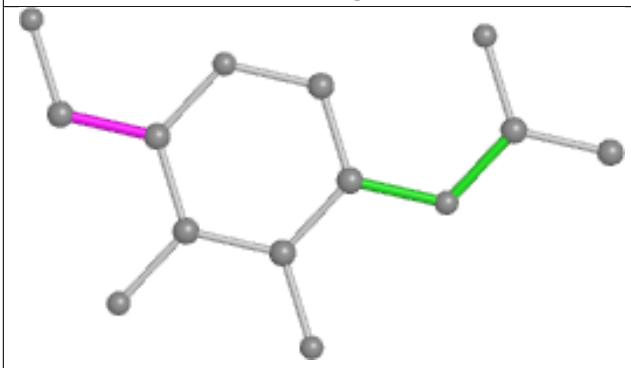


Bond angles



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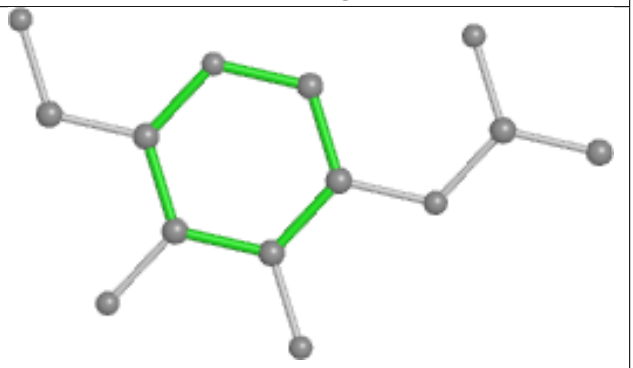
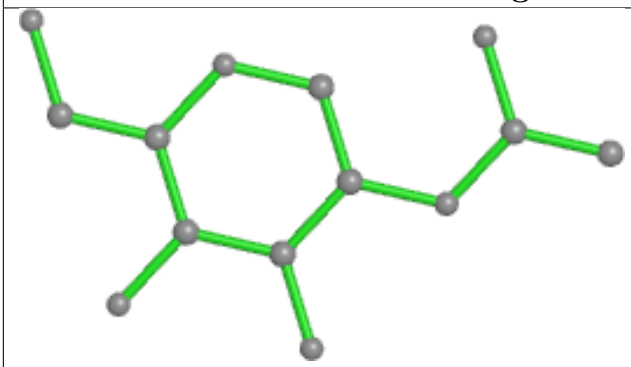


Rings

Ligand NAG B 1414



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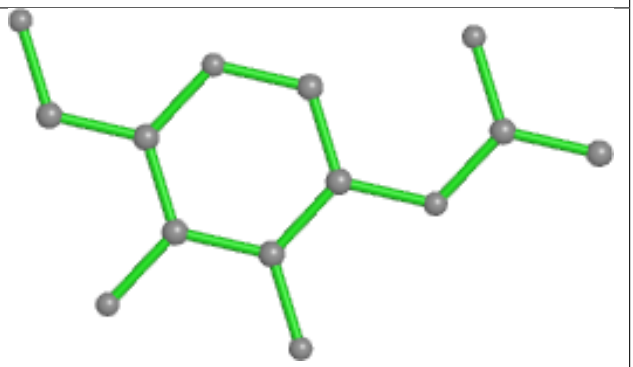
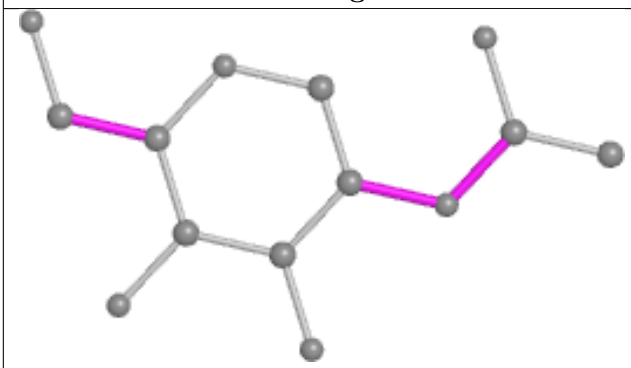


Bond angles



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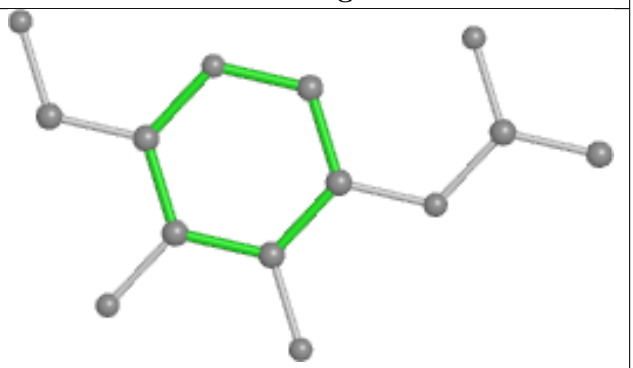
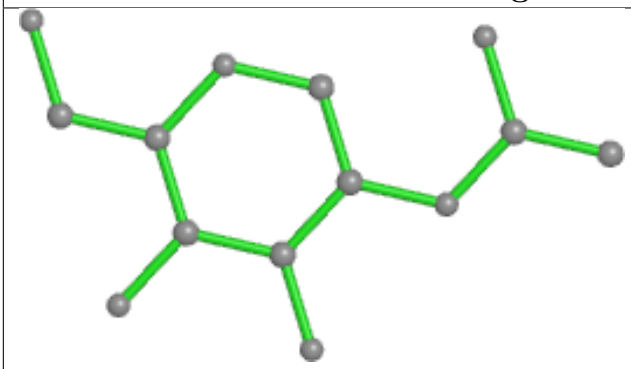


Rings

Ligand NAG C 1402



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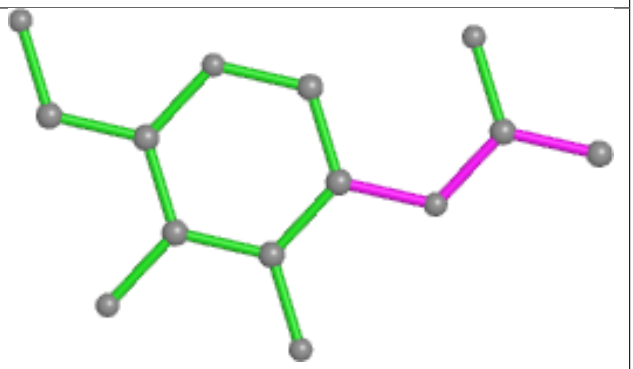
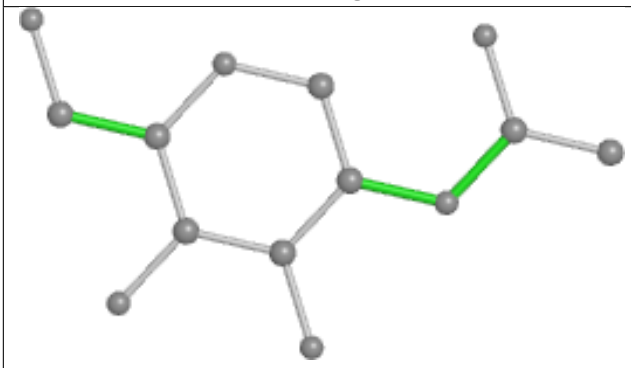
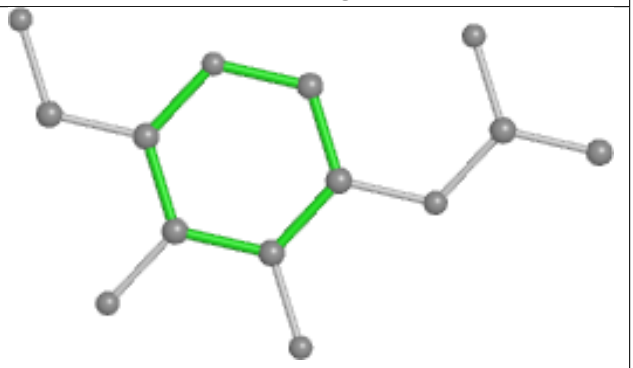


Bond angles

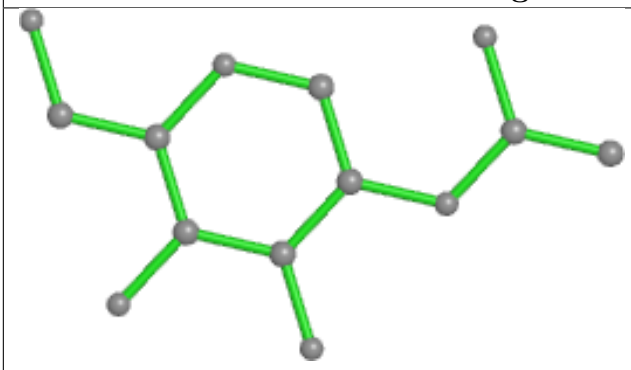


Torsions



Rings

Ligand NAG C 1418



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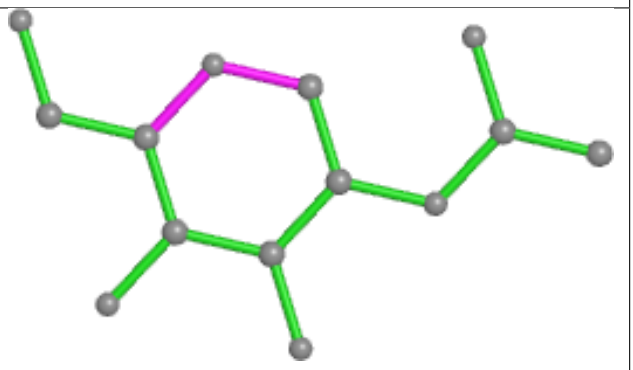
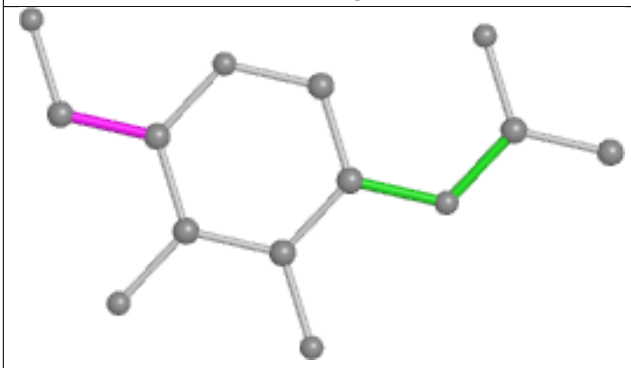


Bond angles



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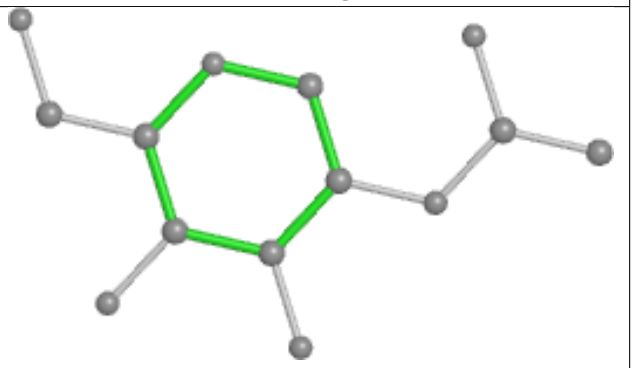
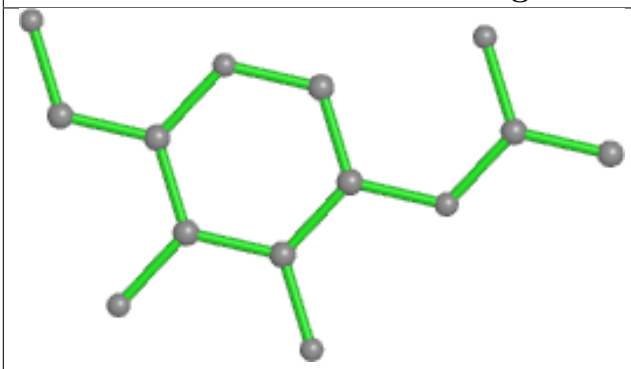
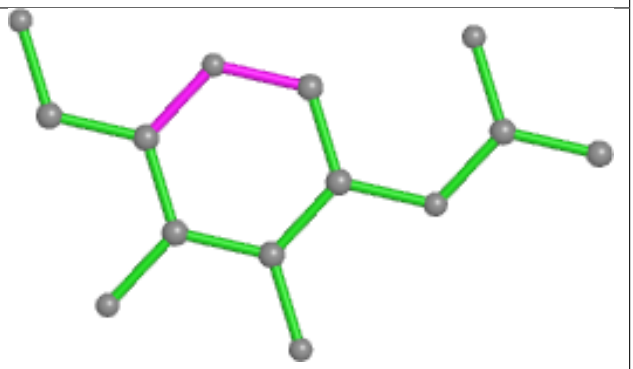
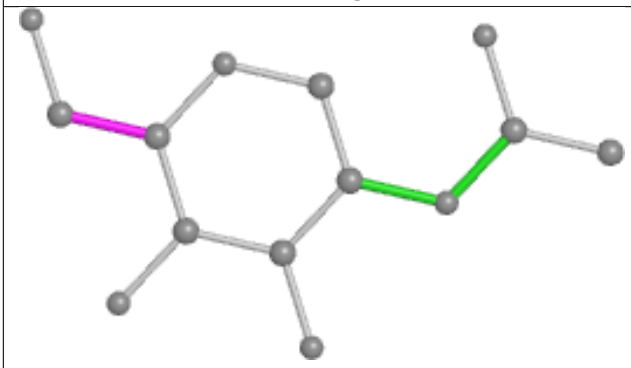
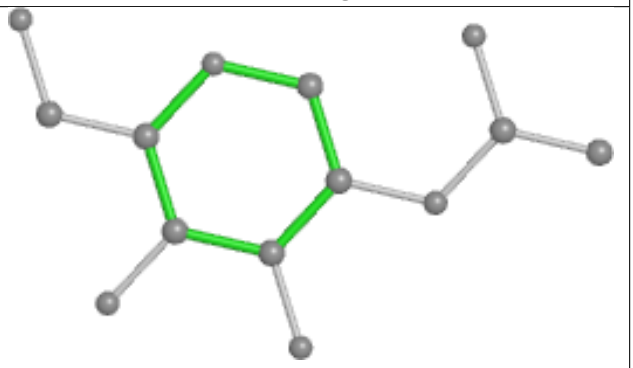
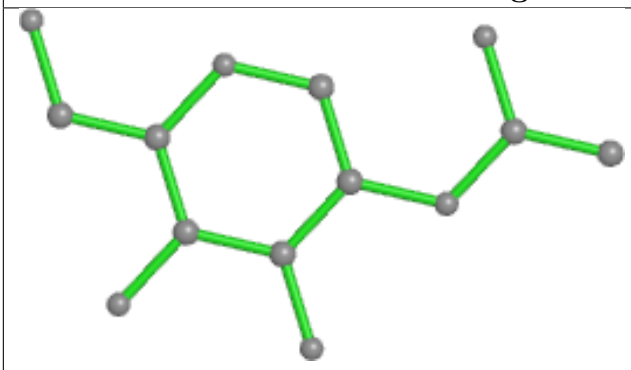
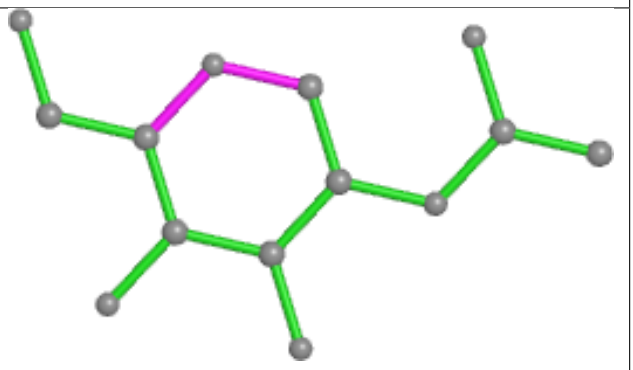
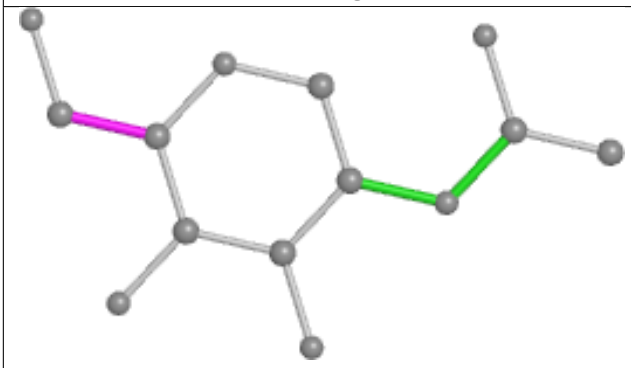
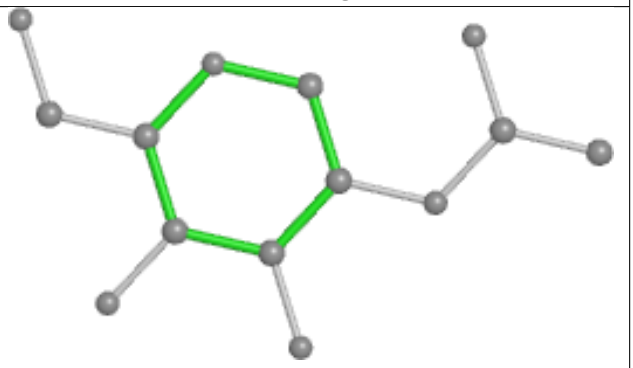
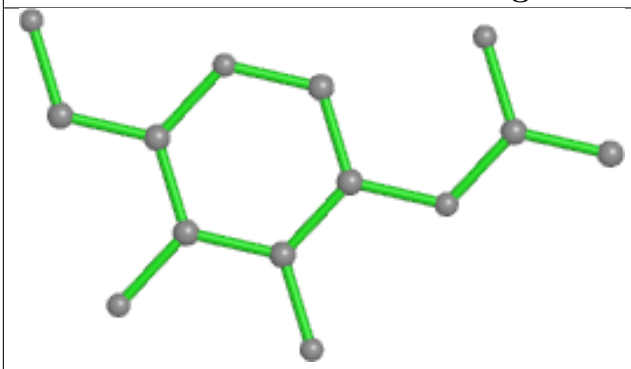


Rings

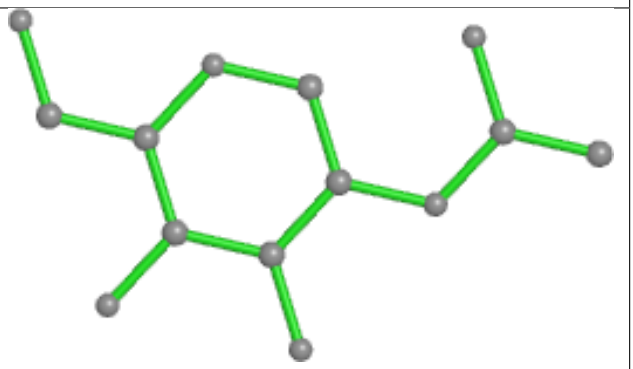
Ligand NAG C 1409	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG A 1411	
 Bond lengths	 Bond angles
 Torsions	 Rings

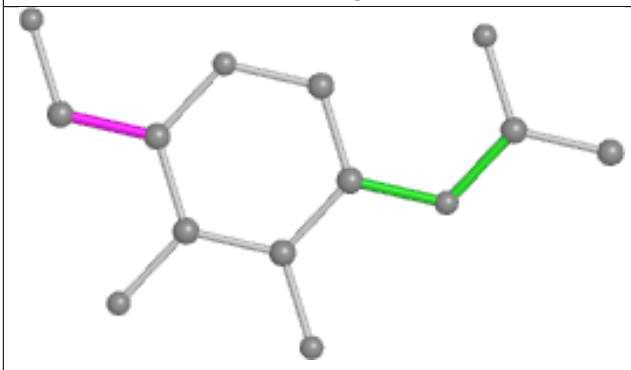
Ligand NAG B 1415



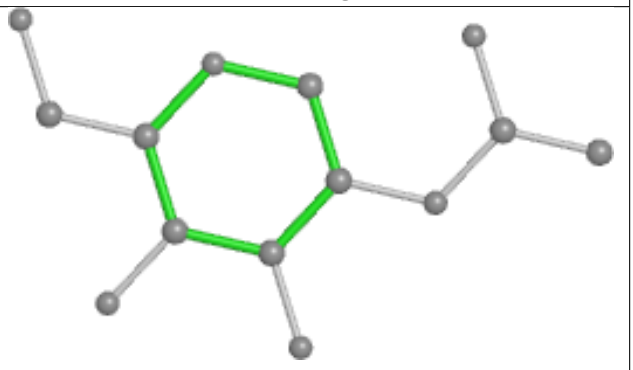
Bond lengths



Bond angles

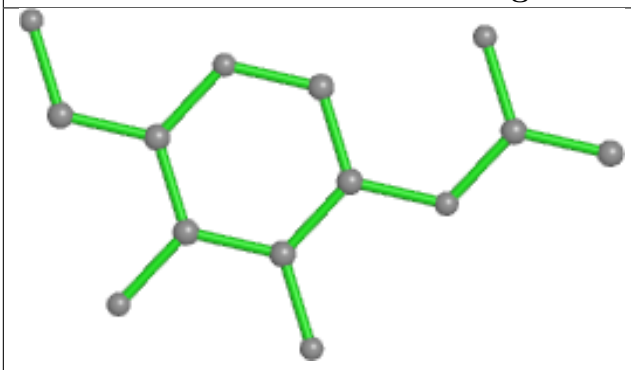


Torsions

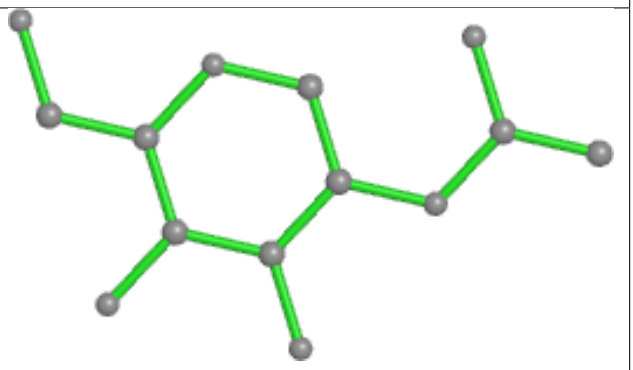


Rings

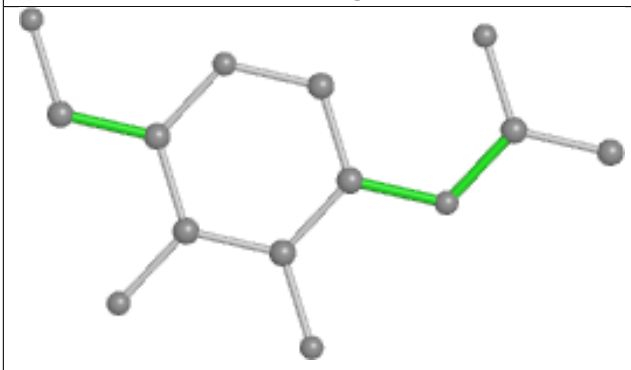
Ligand NAG C 1419



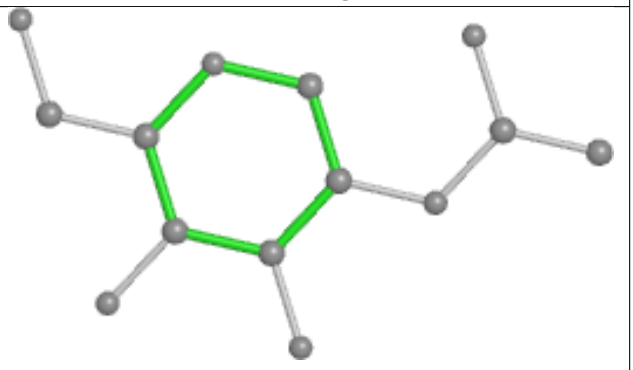
Bond lengths



Bond angles

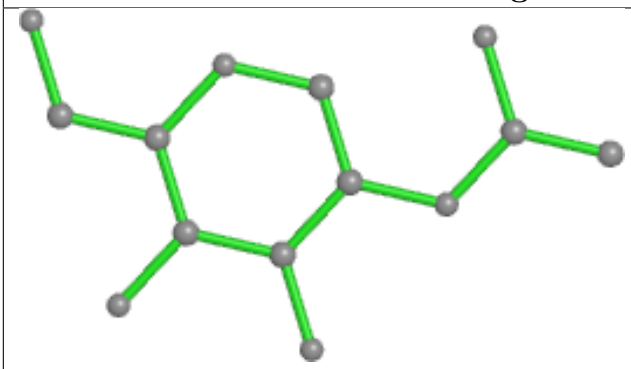


Torsions

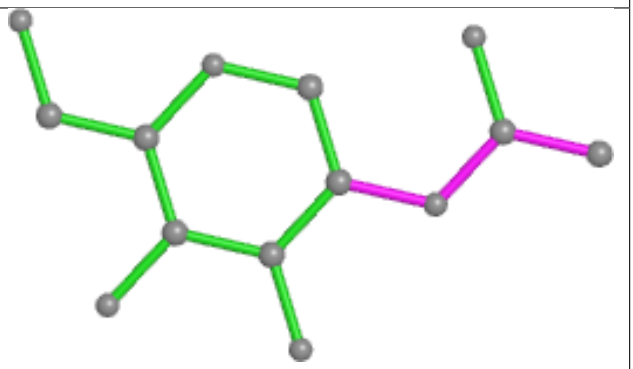


Rings

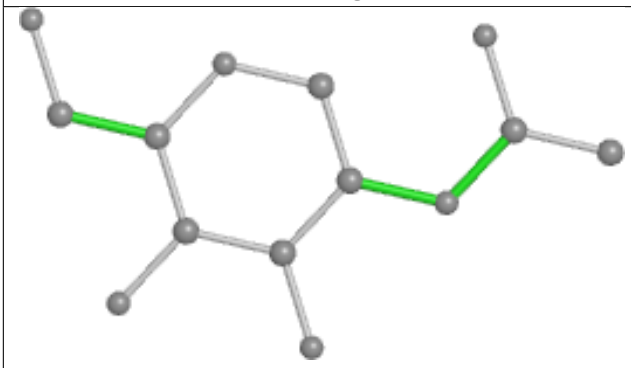
Ligand NAG A 1401



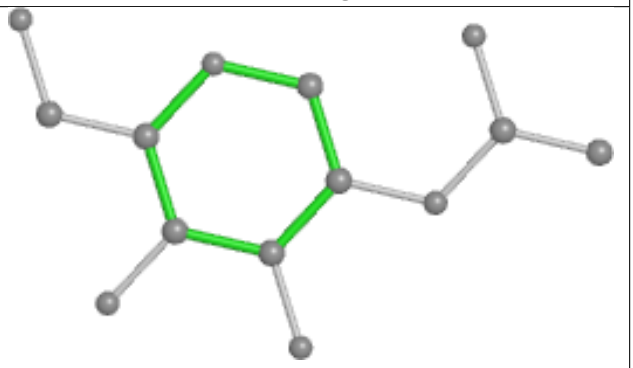
Bond lengths



Bond angles

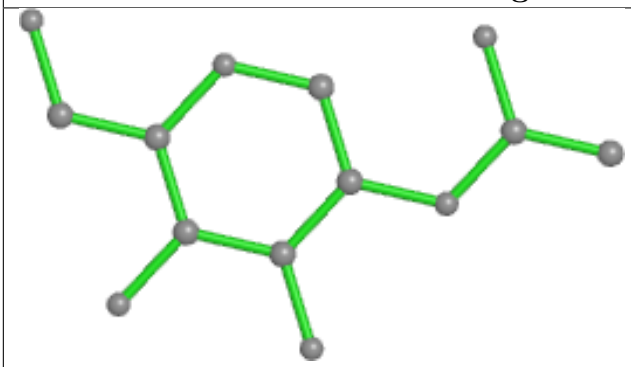


Torsions

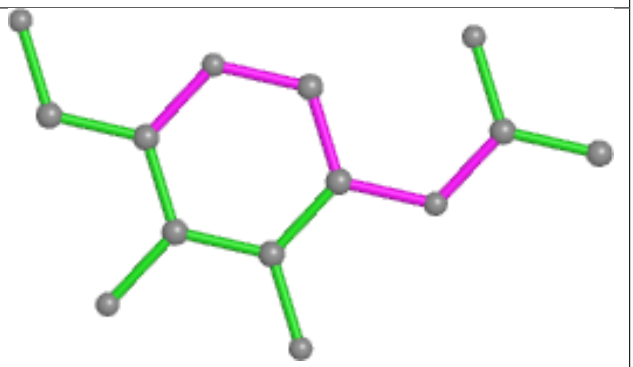


Rings

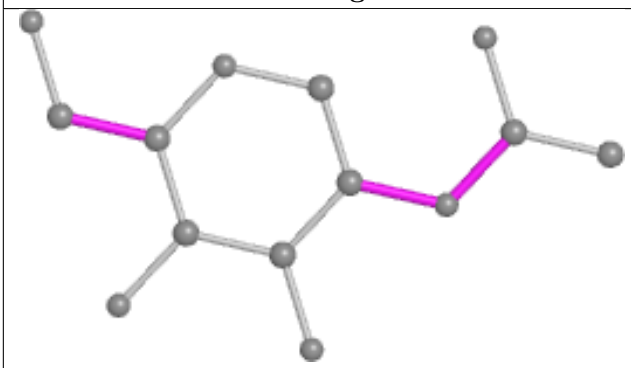
Ligand NAG C 1417



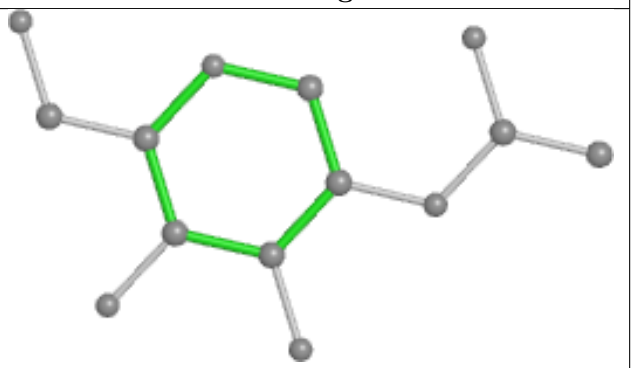
Bond lengths



Bond angles

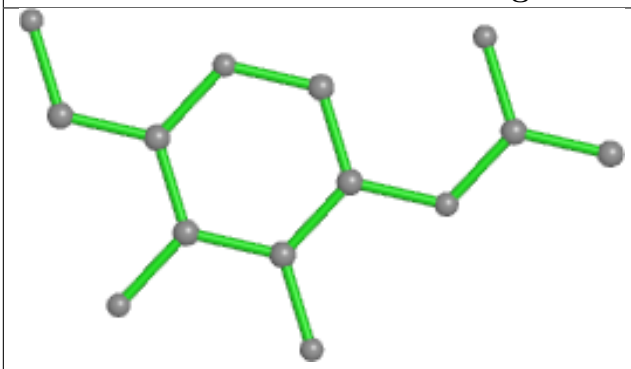


Torsions

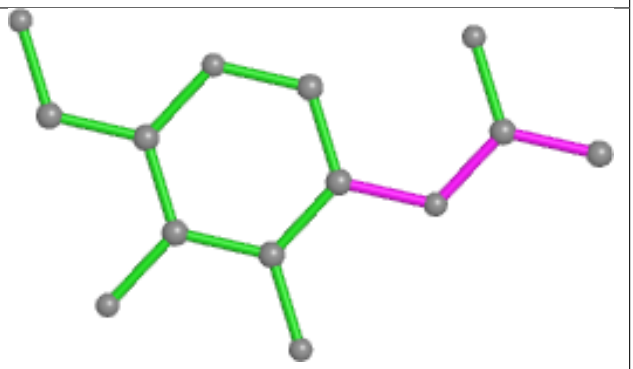


Rings

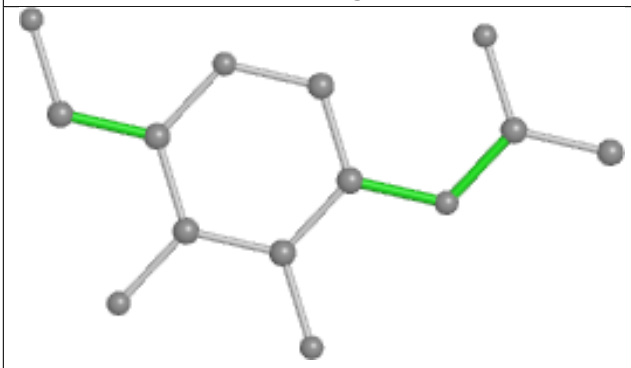
Ligand NAG B 1401



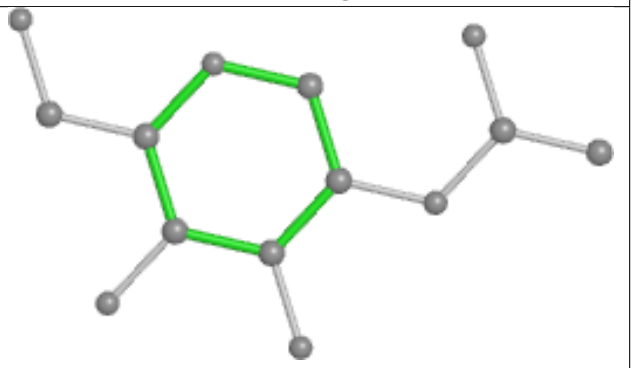
Bond lengths



Bond angles

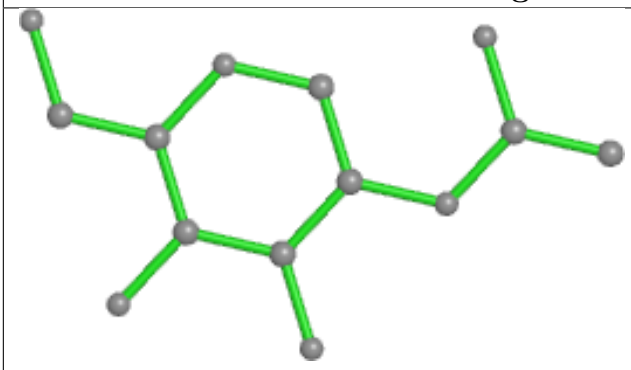


Torsions



Rings

Ligand NAG B 1421



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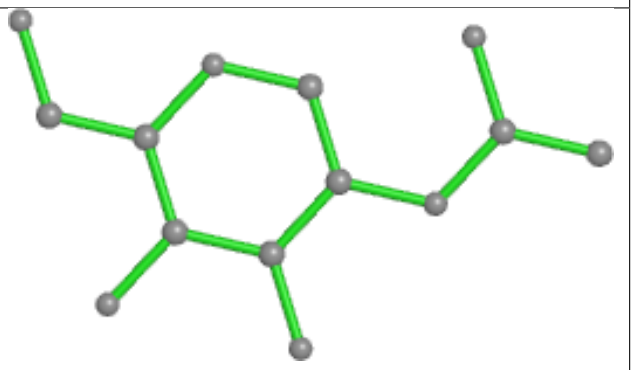
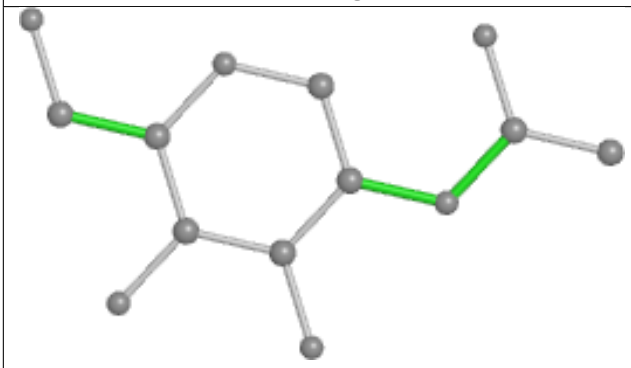


Bond angles



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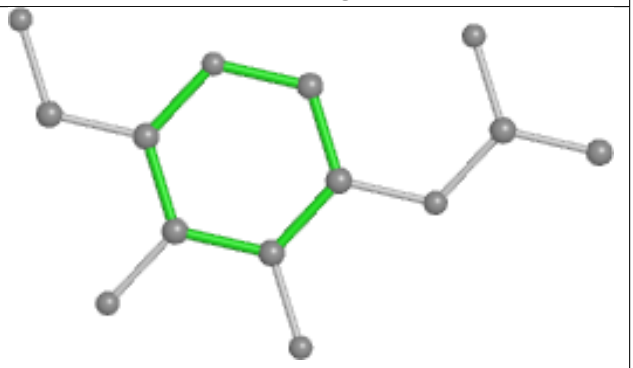
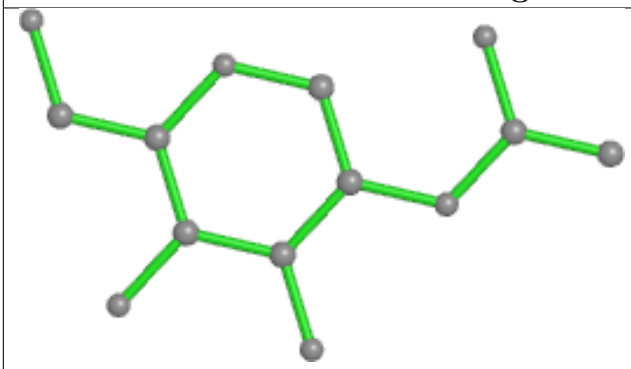
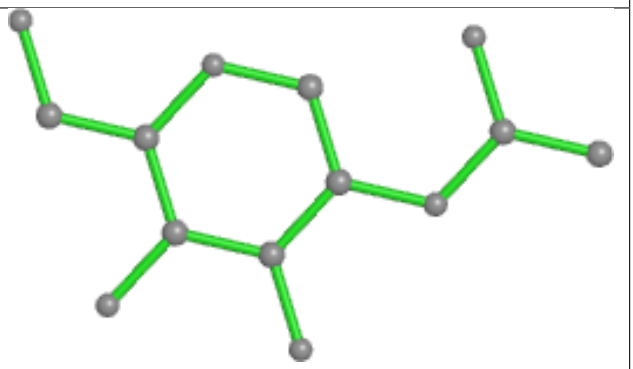


Rings

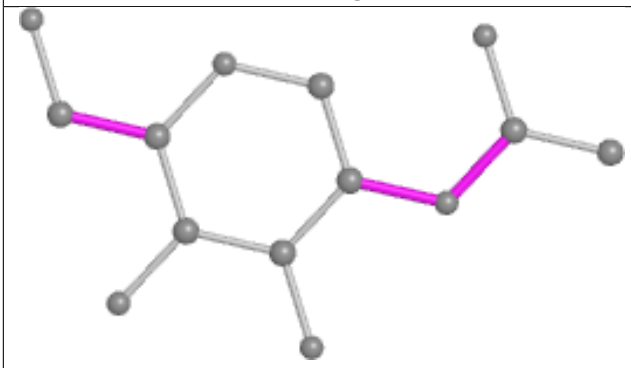
Ligand NAG C 1410



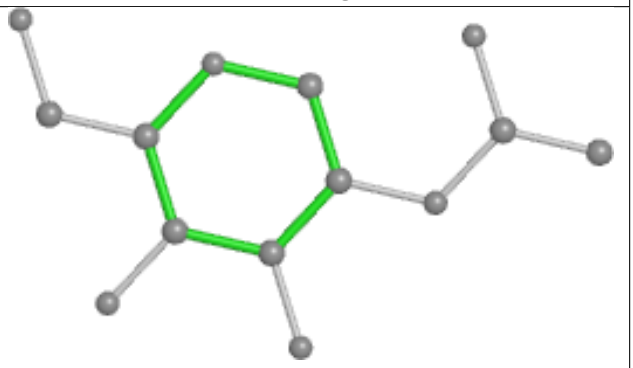
Bond lengths



Bond angles

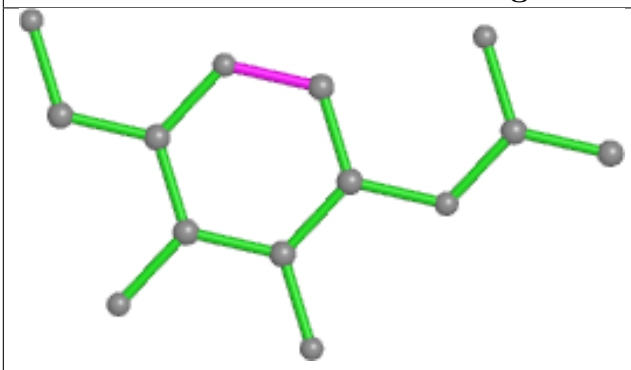


Torsions



Rings

Ligand NAG A 1409



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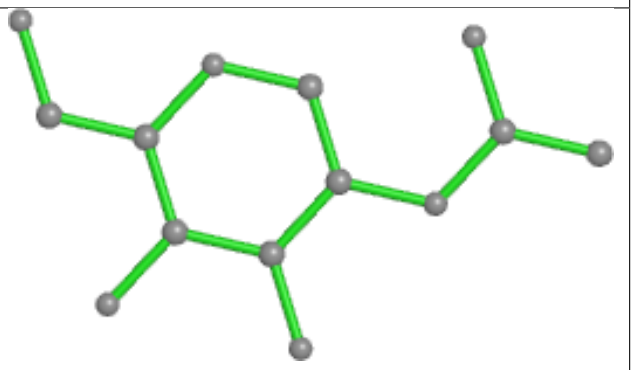
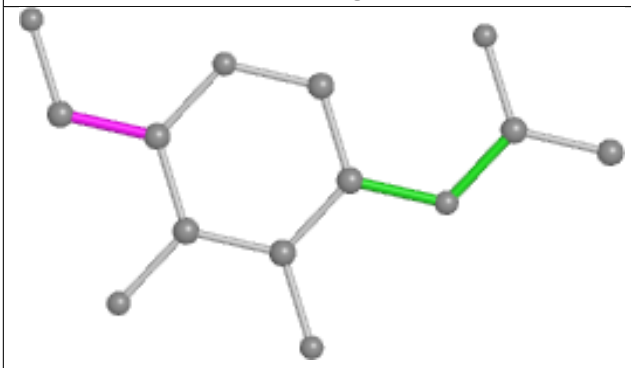
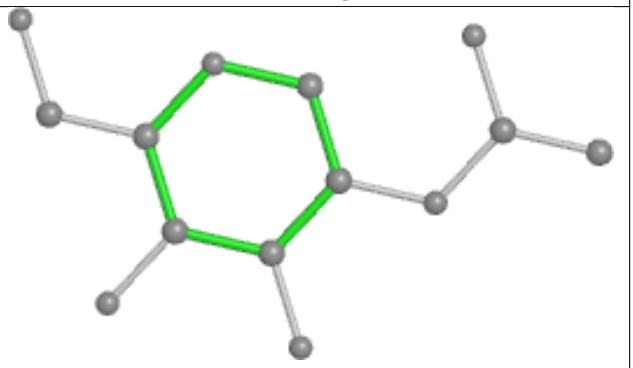


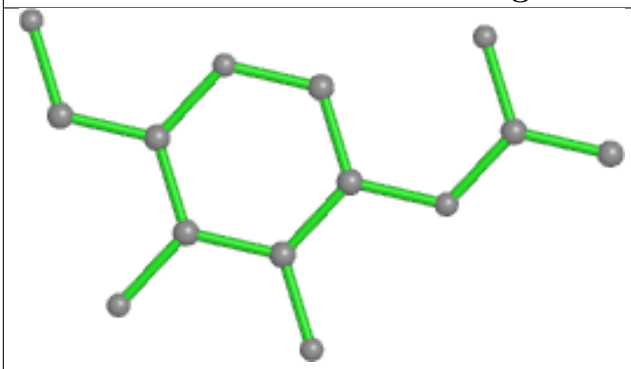
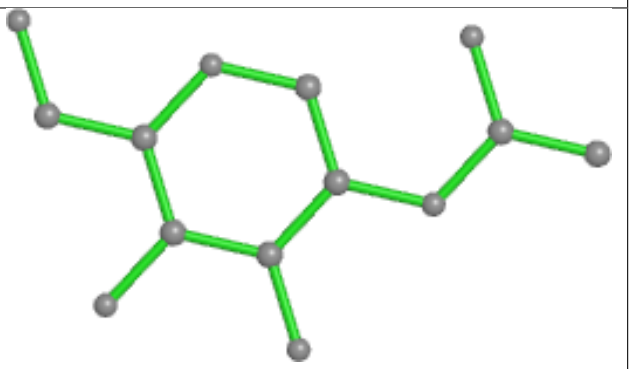
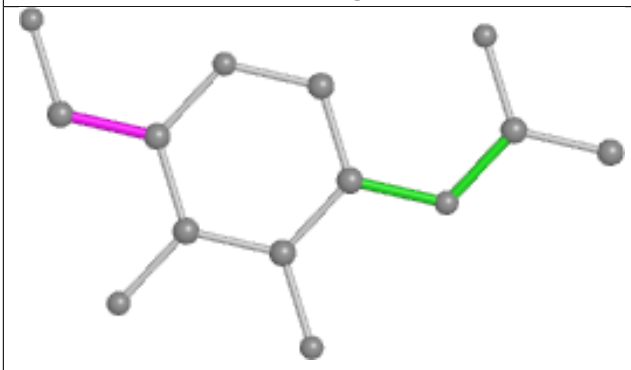
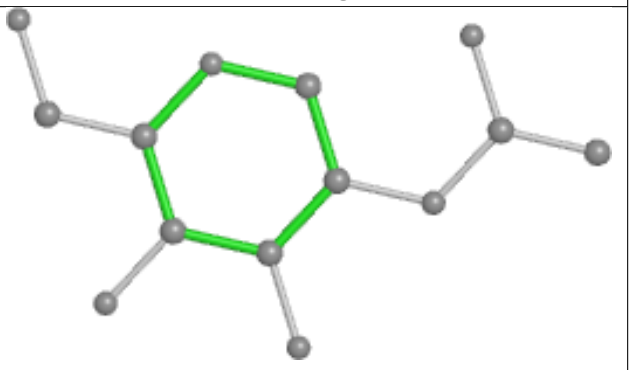
Bond angles

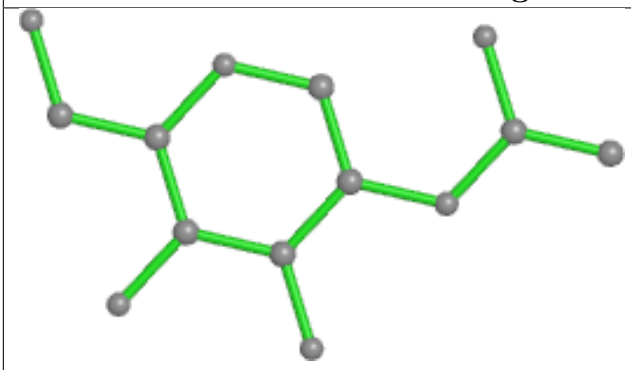
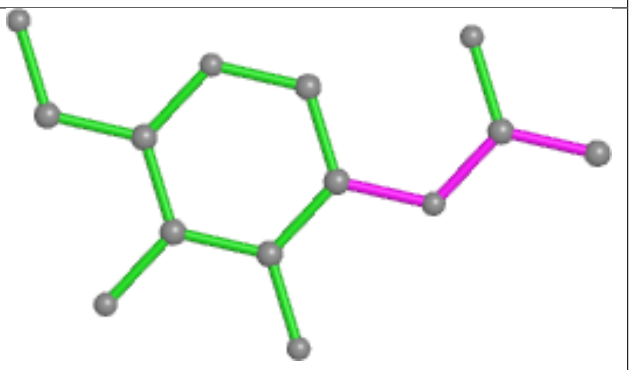
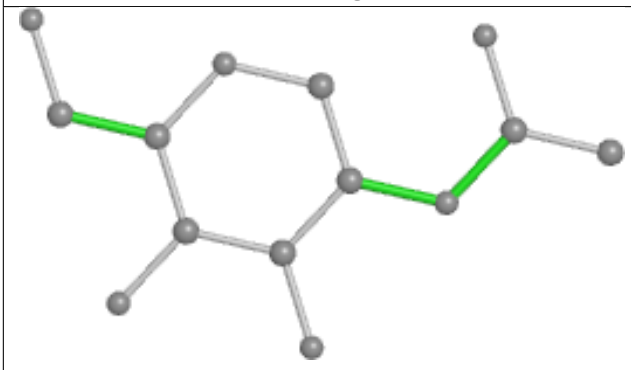
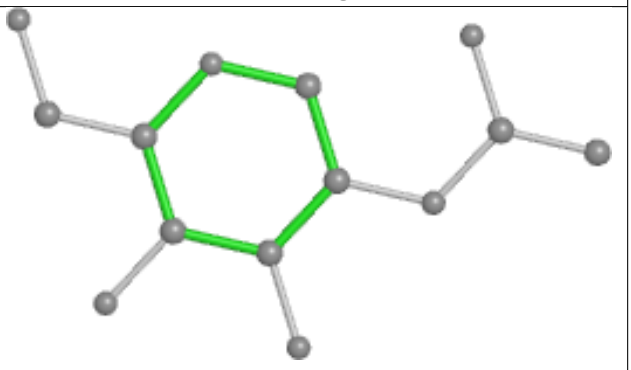


Torsions

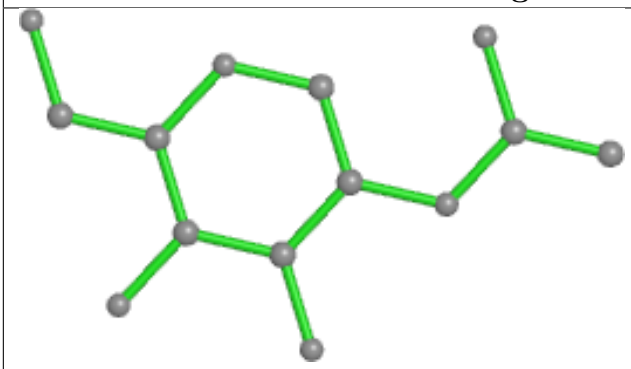


Rings

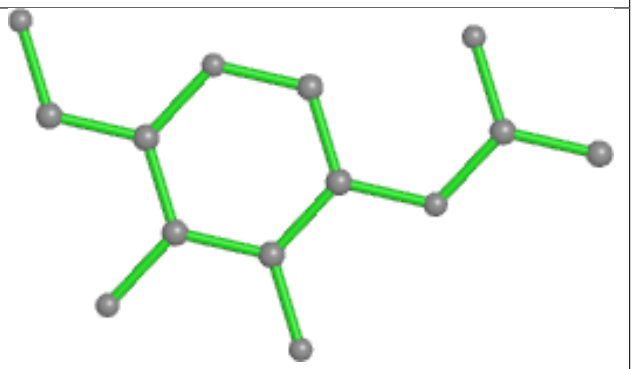
Ligand NAG B 1403	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG C 1405	
 Bond lengths	 Bond angles
 Torsions	 Rings

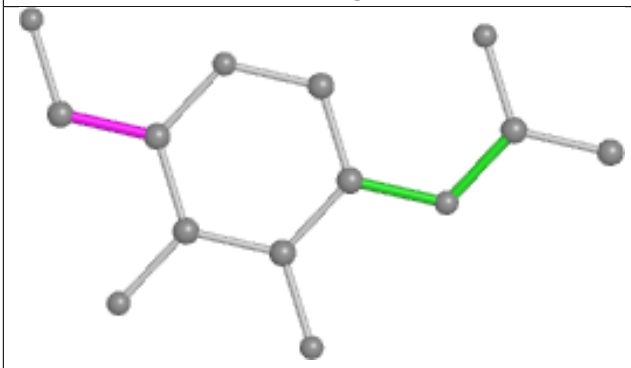
Ligand NAG C 1406



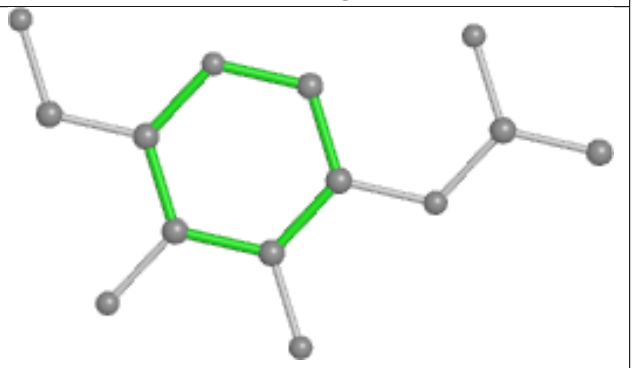
Bond lengths



Bond angles

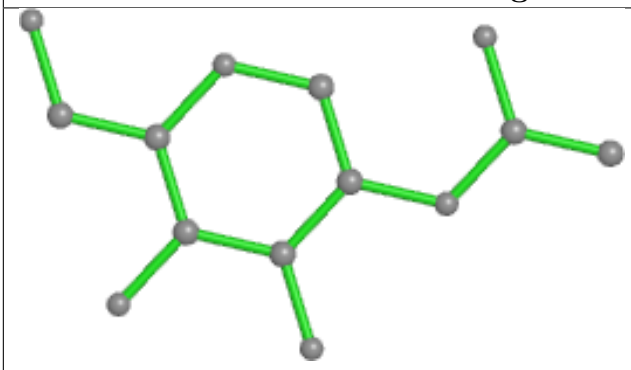


Torsions

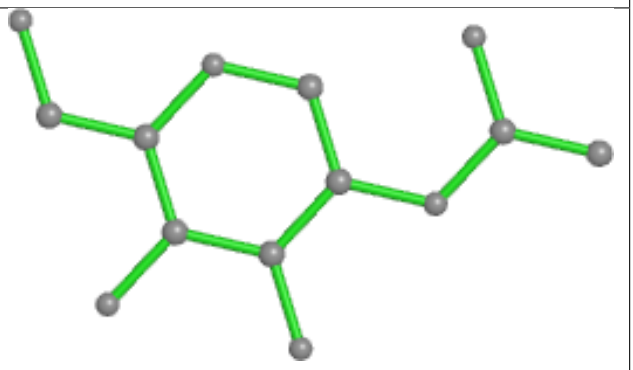


Rings

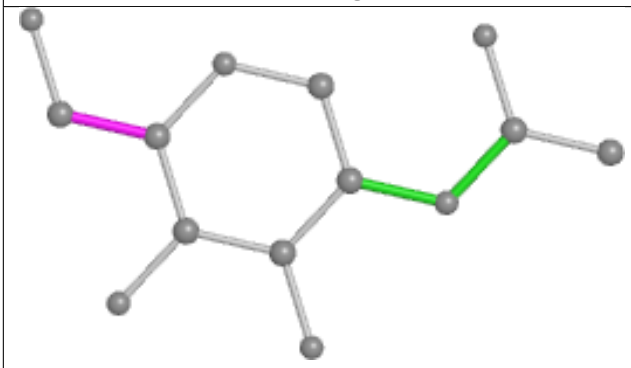
Ligand NAG A 1415



Bond lengths



Bond angles



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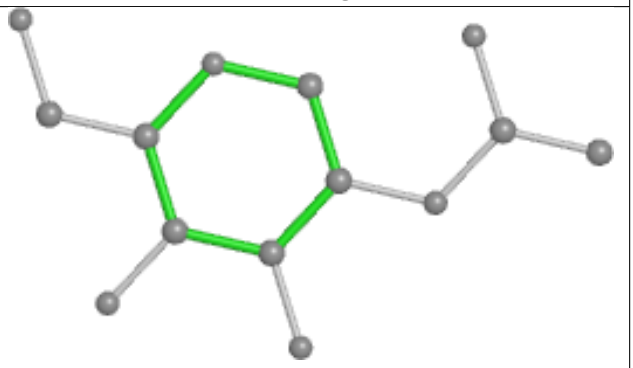
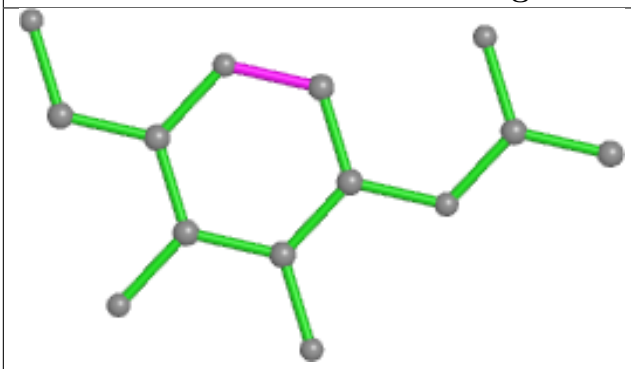


Rings

Ligand NAG B 1409



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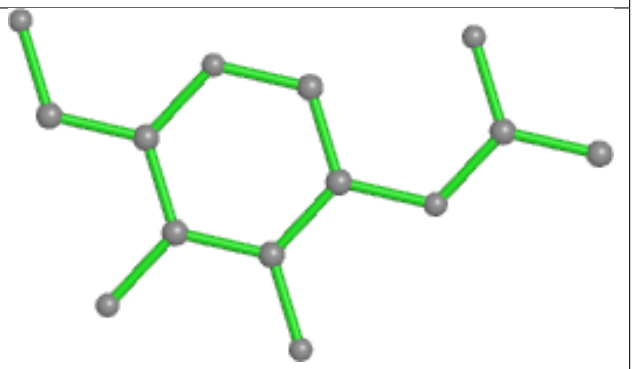
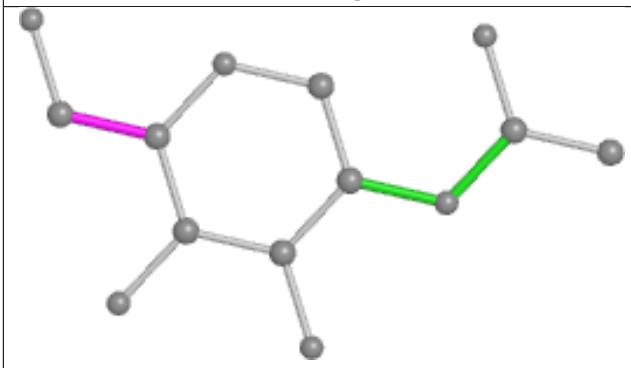
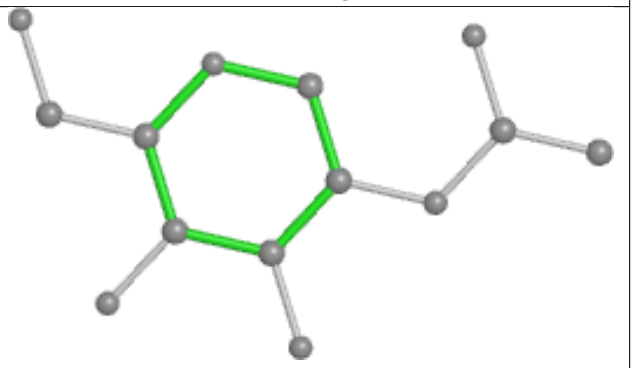


Bond angles

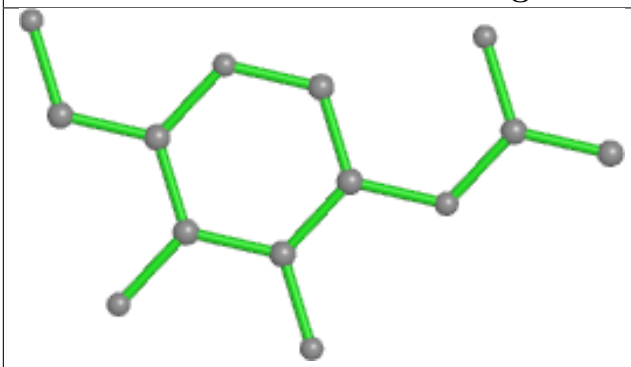


Torsions

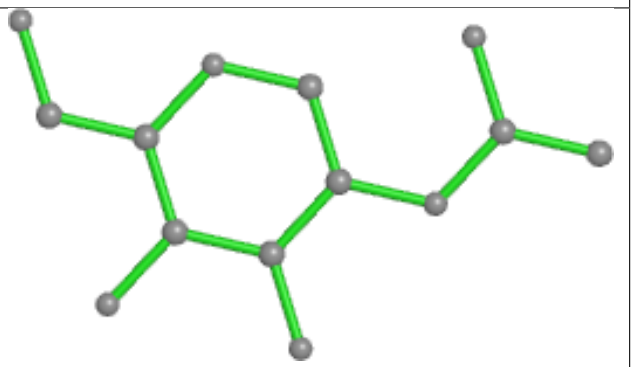


Rings

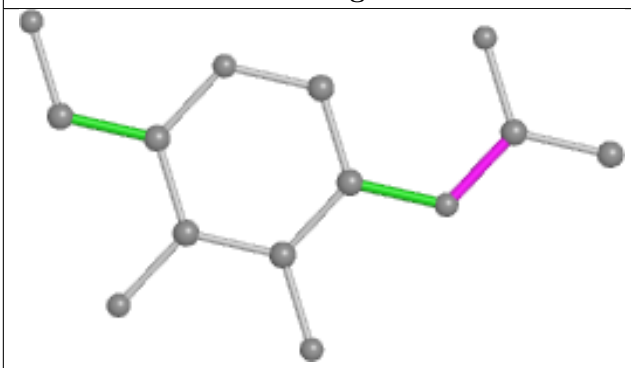
Ligand NAG B 1408



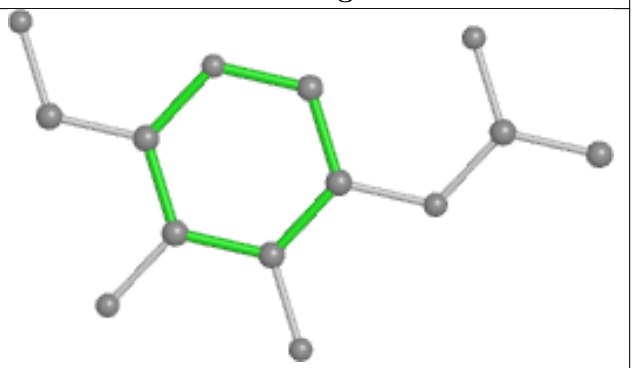
Bond lengths



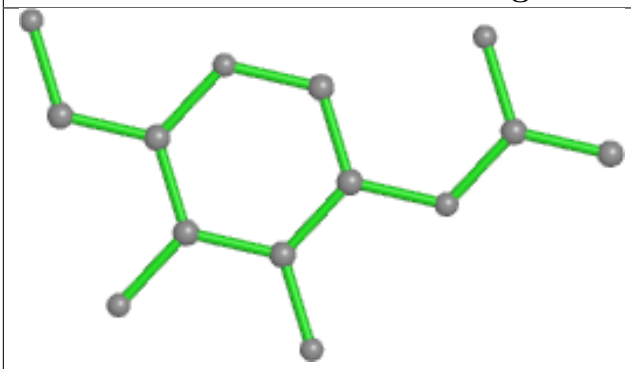
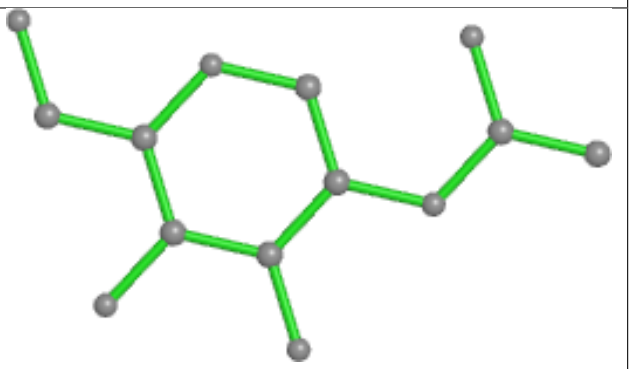
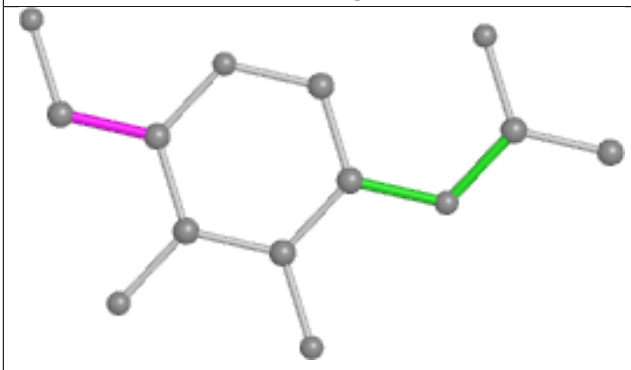
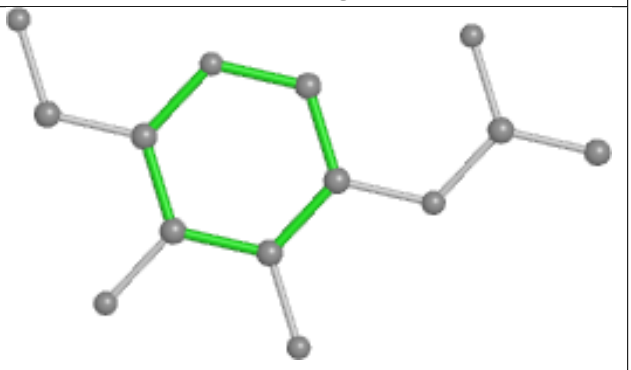
Bond angles

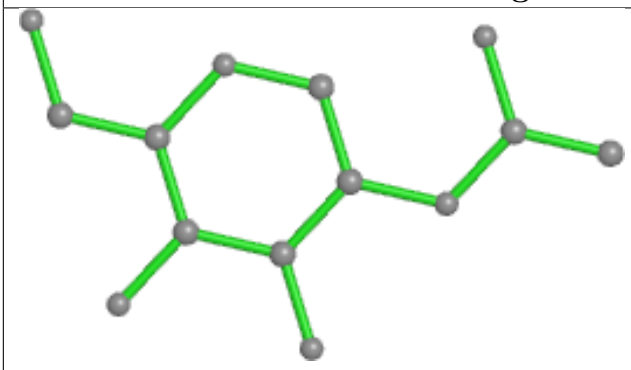
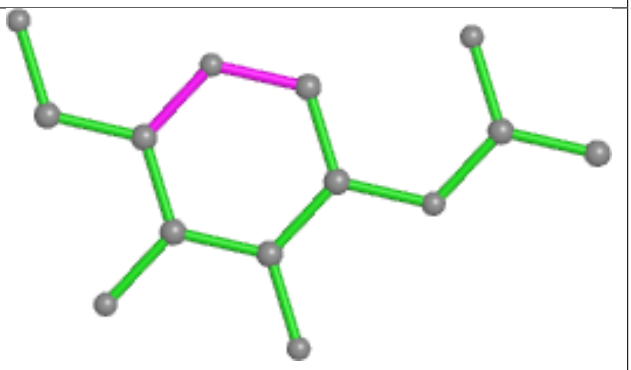
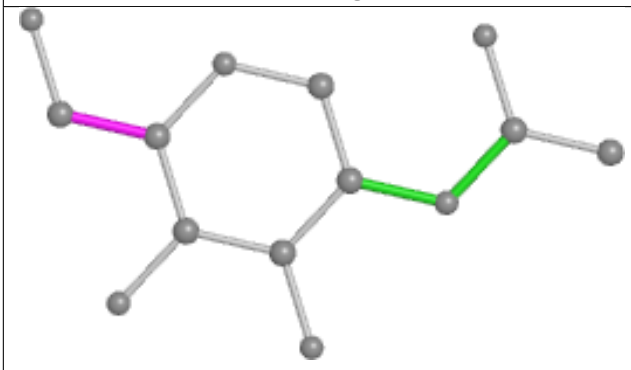
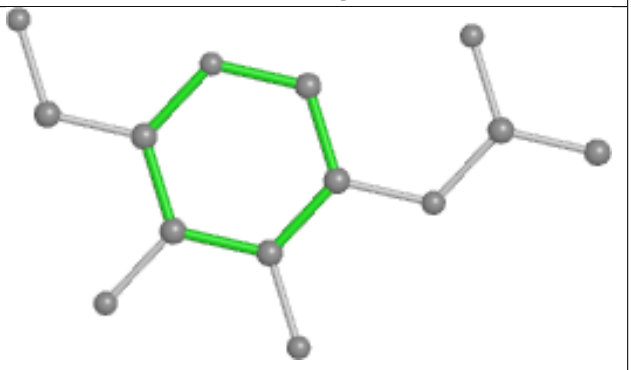


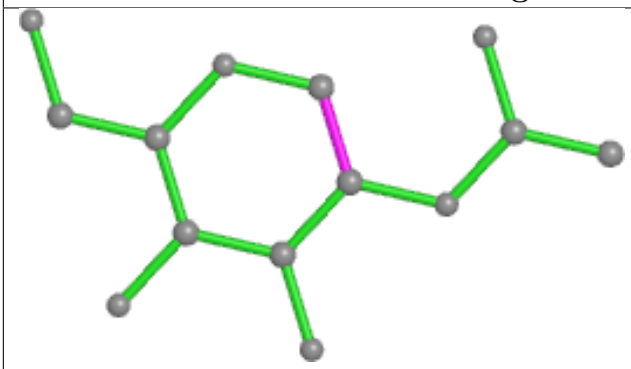
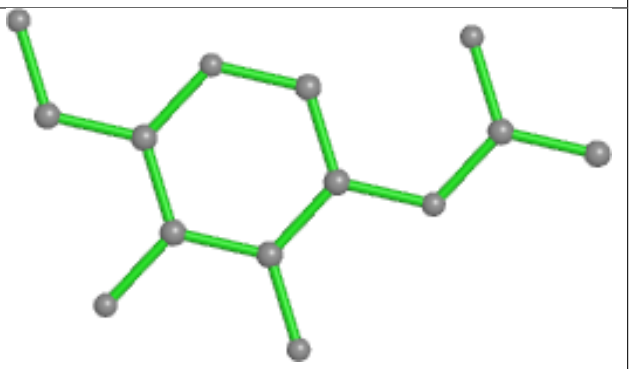
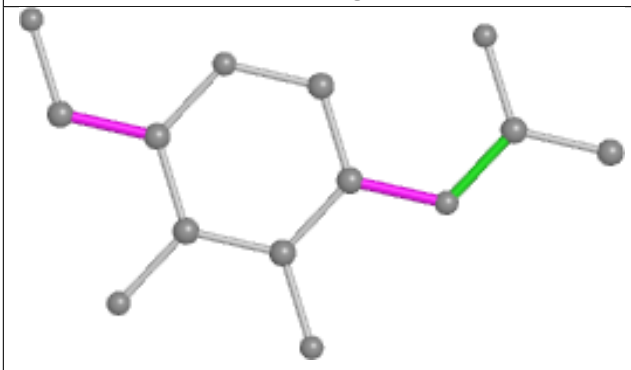
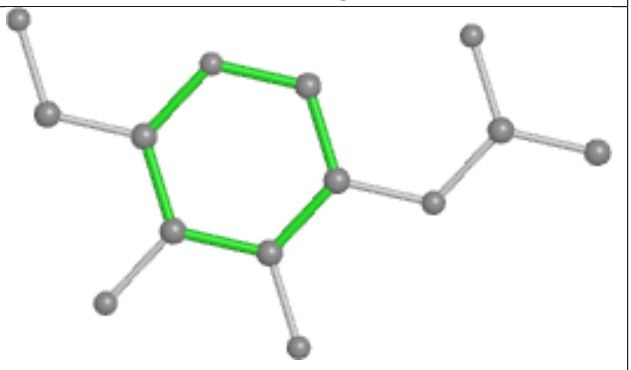
Torsions

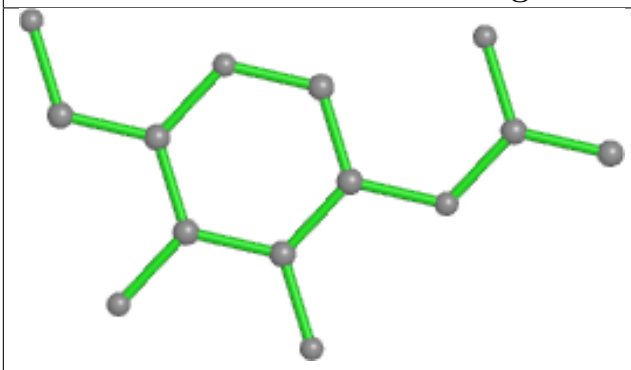
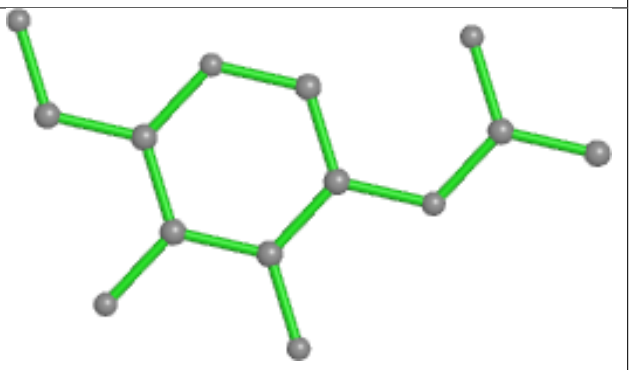
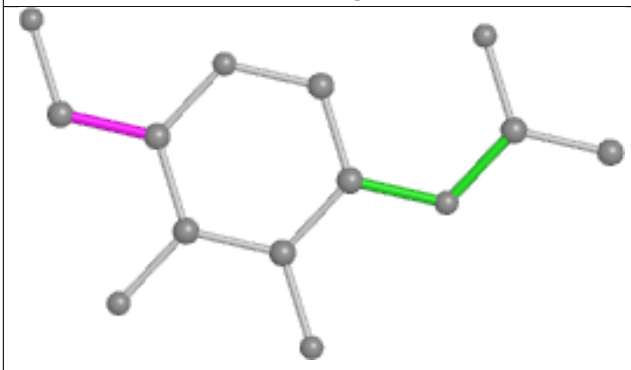
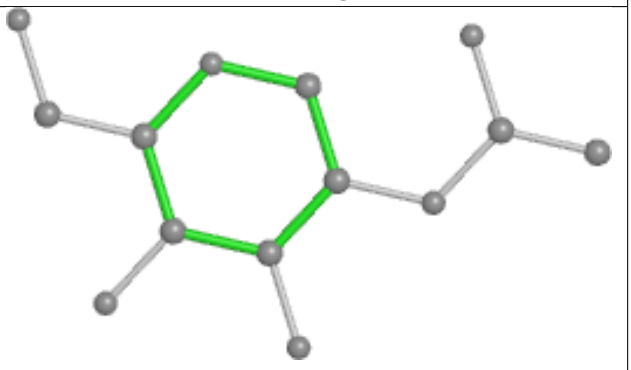


Rings

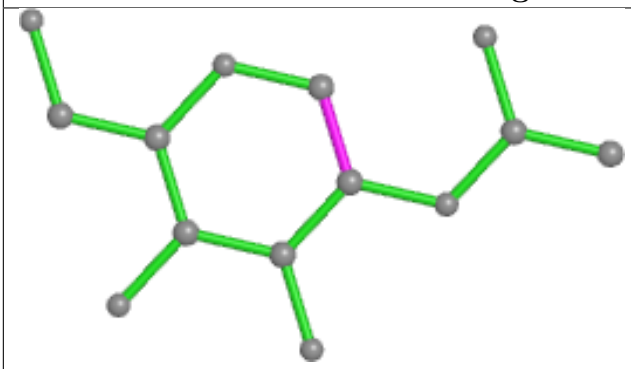
Ligand NAG B 1406	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG B 1420	
 Bond lengths	 Bond angles
 Torsions	 Rings

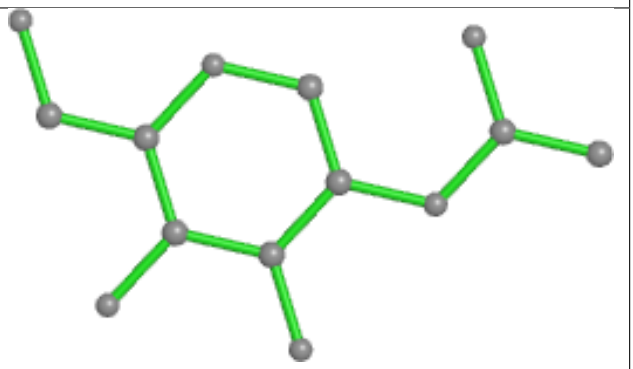
Ligand NAG C 1407	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG C 1414	
 Bond lengths	 Bond angles
 Torsions	 Rings

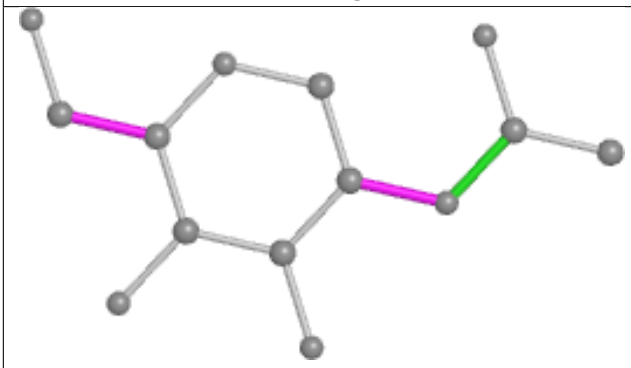
Ligand NAG B 1407



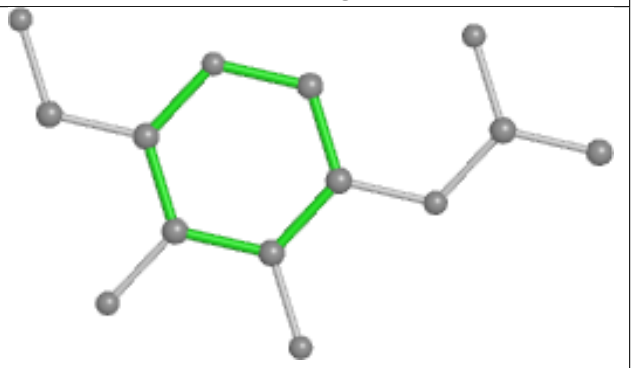
Bond lengths



Bond angles

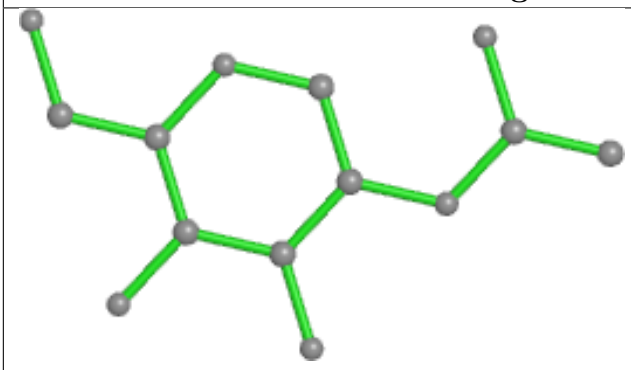


Torsions

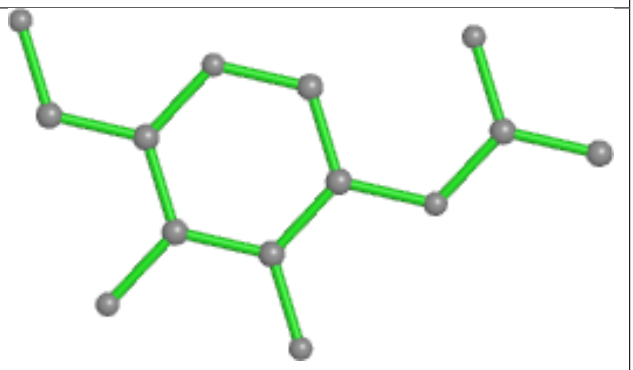


Rings

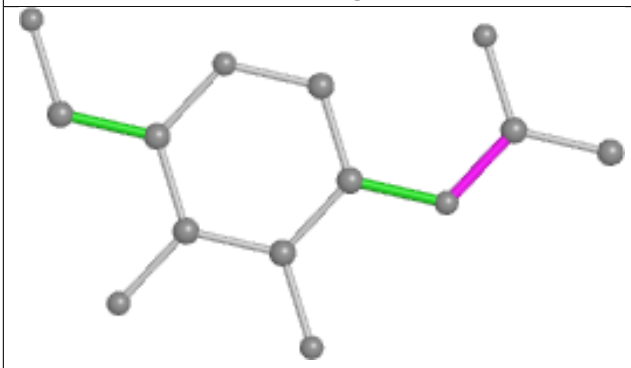
Ligand NAG A 1408



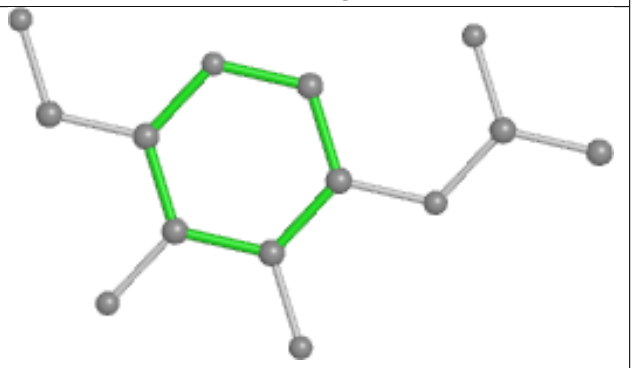
Bond lengths



Bond angles

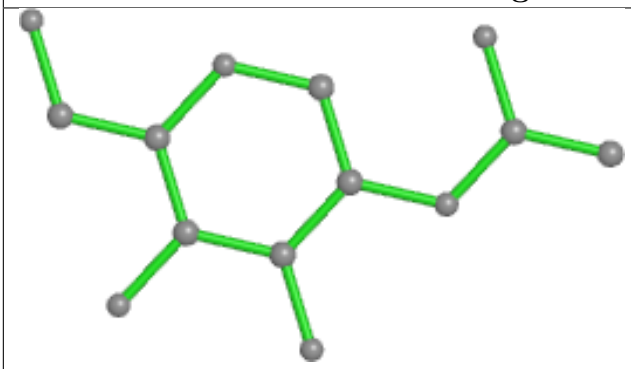


Torsions

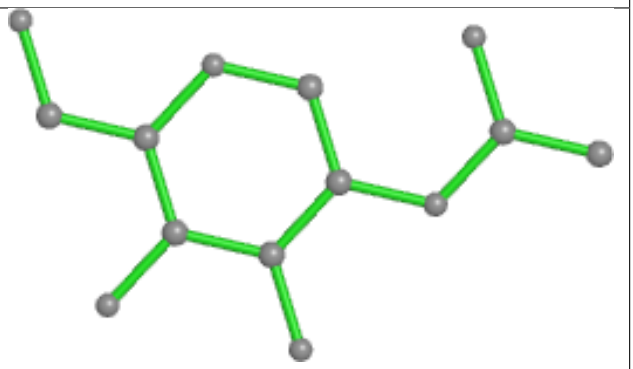


Rings

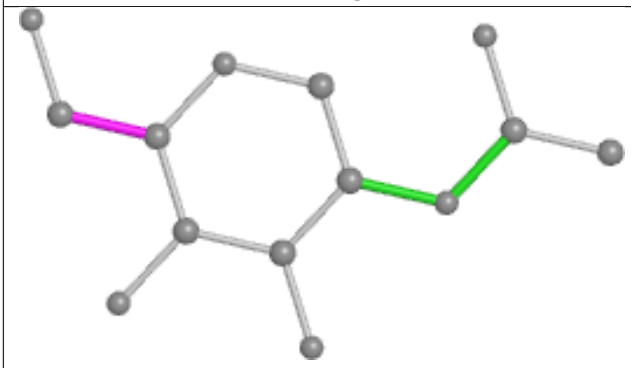
Ligand NAG B 1416



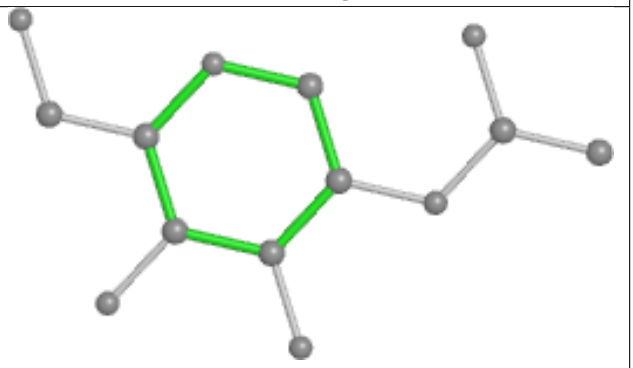
Bond lengths



Bond angles

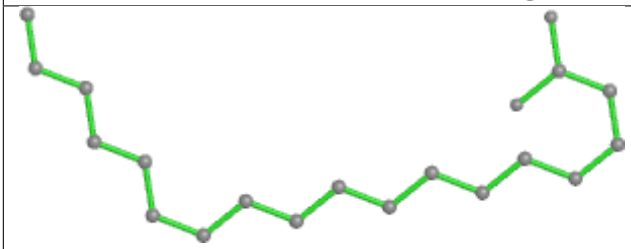


Torsions

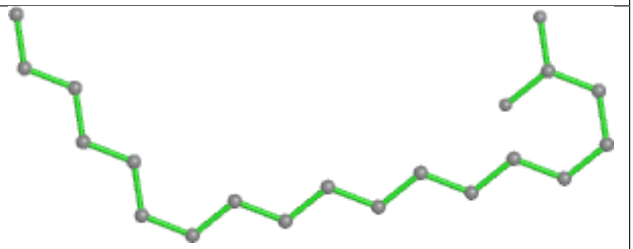


Rings

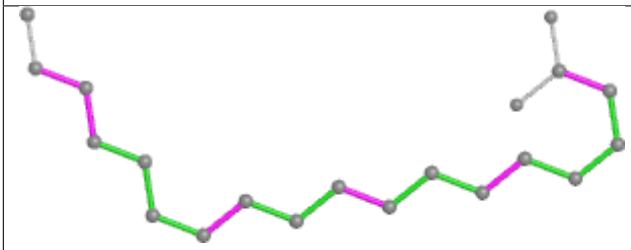
Ligand EIC B 1422



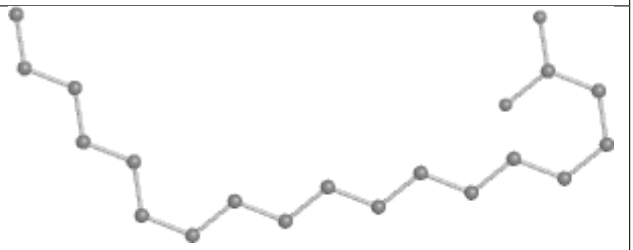
Bond lengths



Bond angles

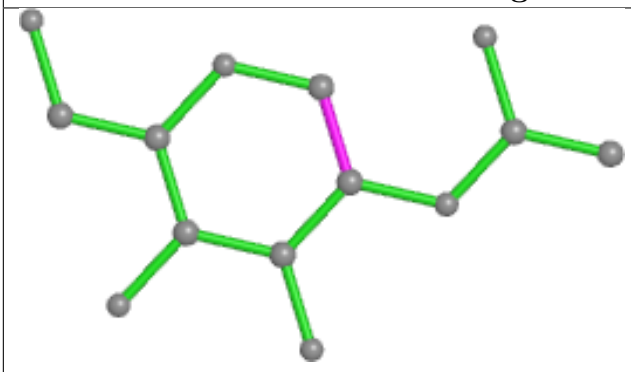


Torsions

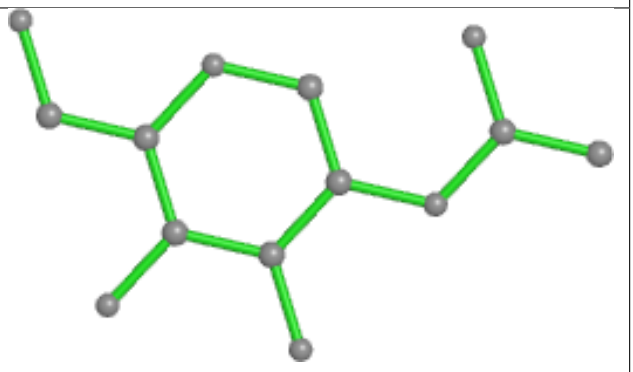


Rings

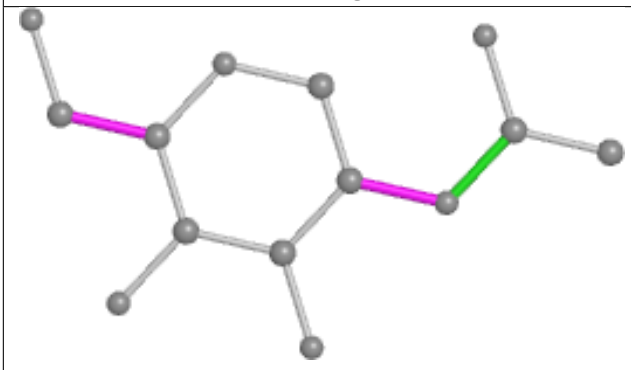
Ligand NAG A 1407



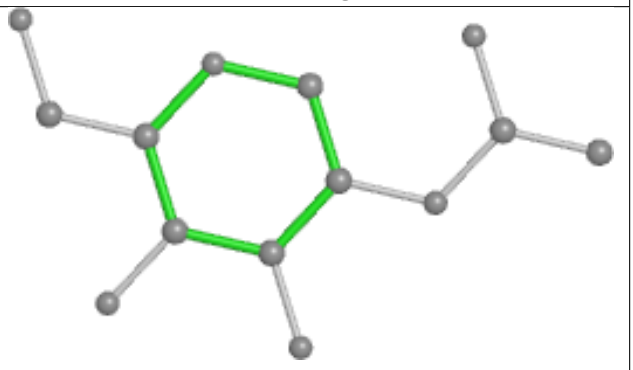
Bond lengths



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.

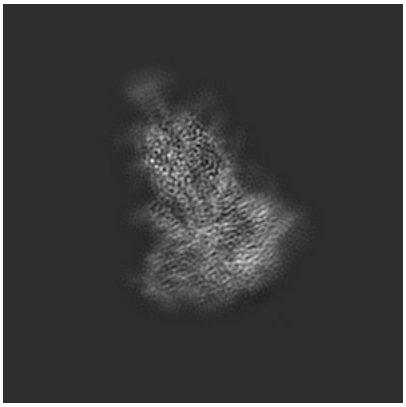
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-30889. These allow visual inspection of the internal detail of the map and identification of artifacts.

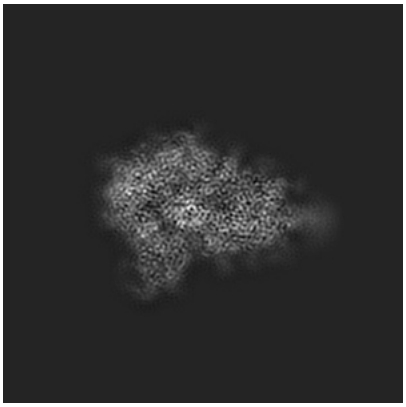
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

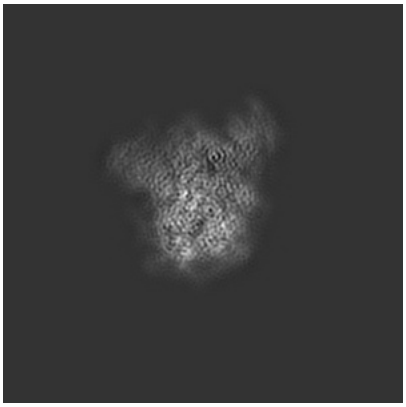
6.1.1 Primary map



X



Y

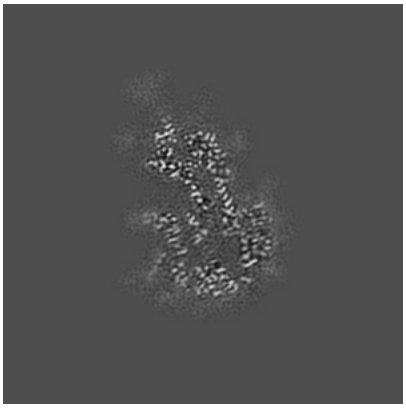


Z

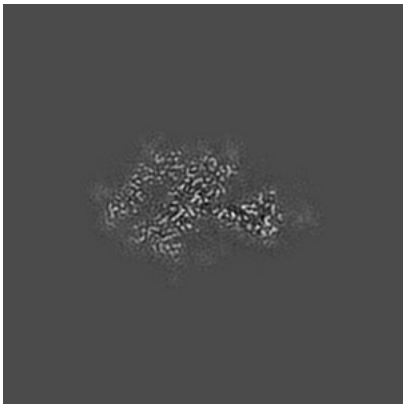
The images above show the map projected in three orthogonal directions.

6.2 Central slices

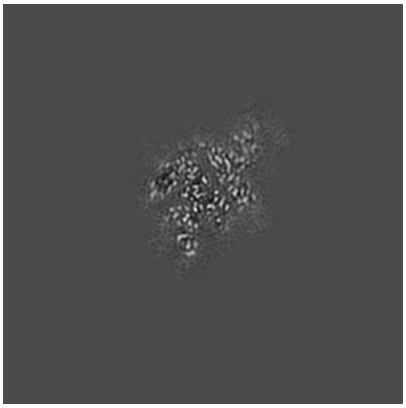
6.2.1 Primary map



X Index: 144



Y Index: 144

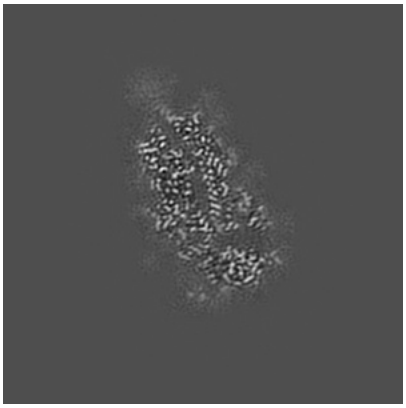


Z Index: 144

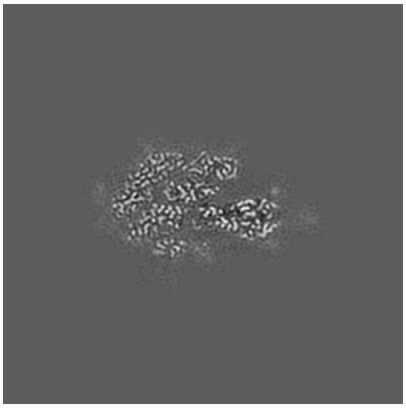
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

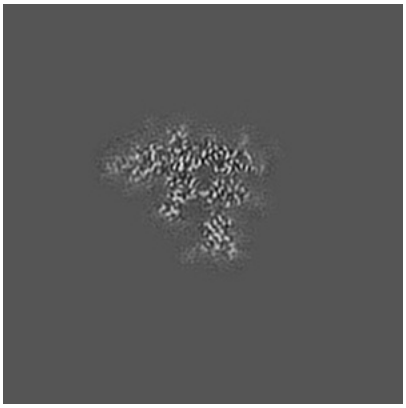
6.3.1 Primary map



X Index: 129



Y Index: 148

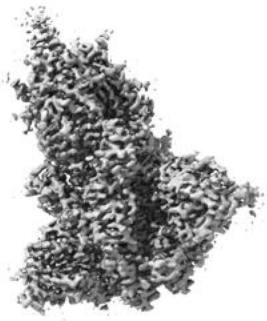


Z Index: 102

The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

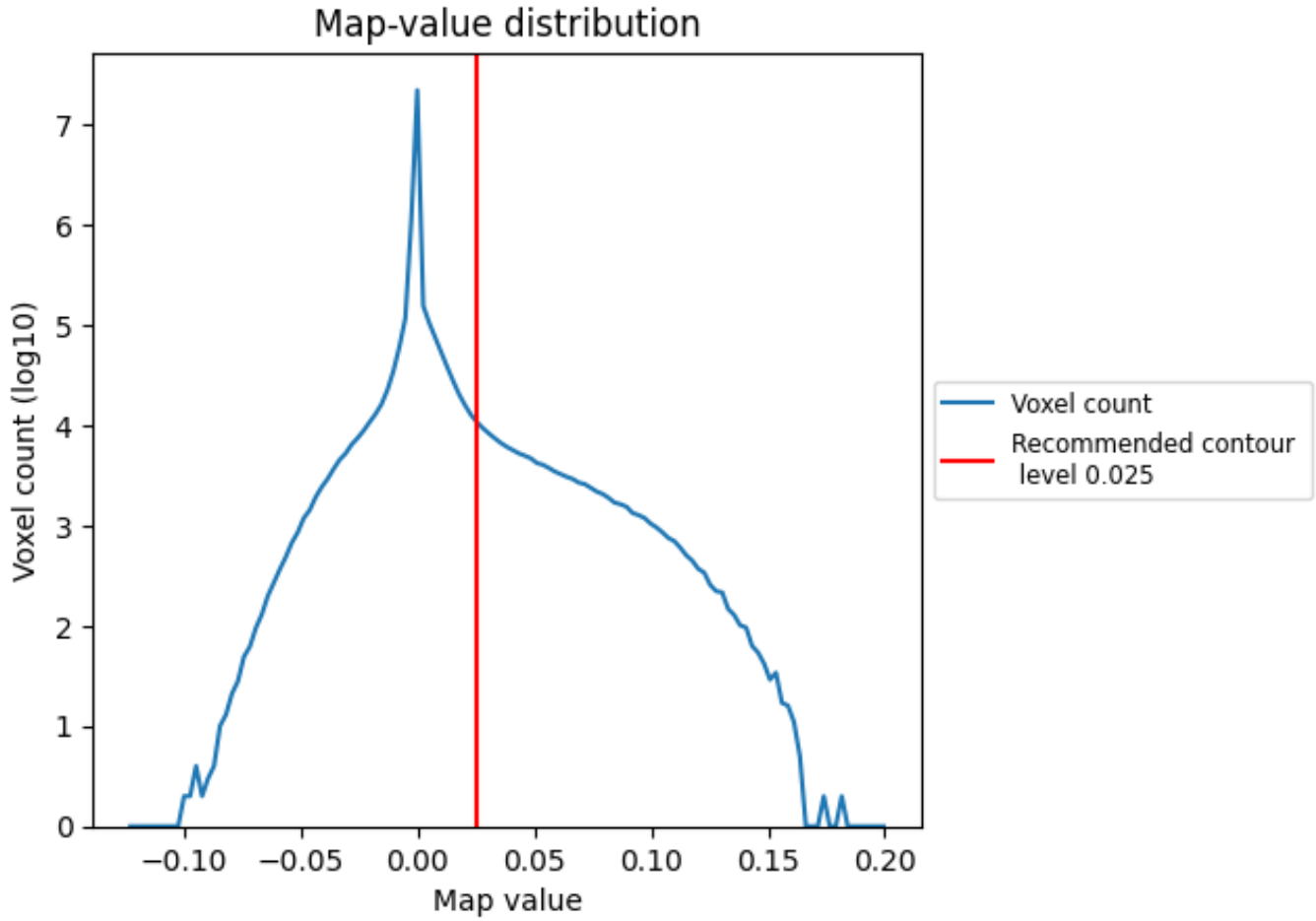
6.5 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

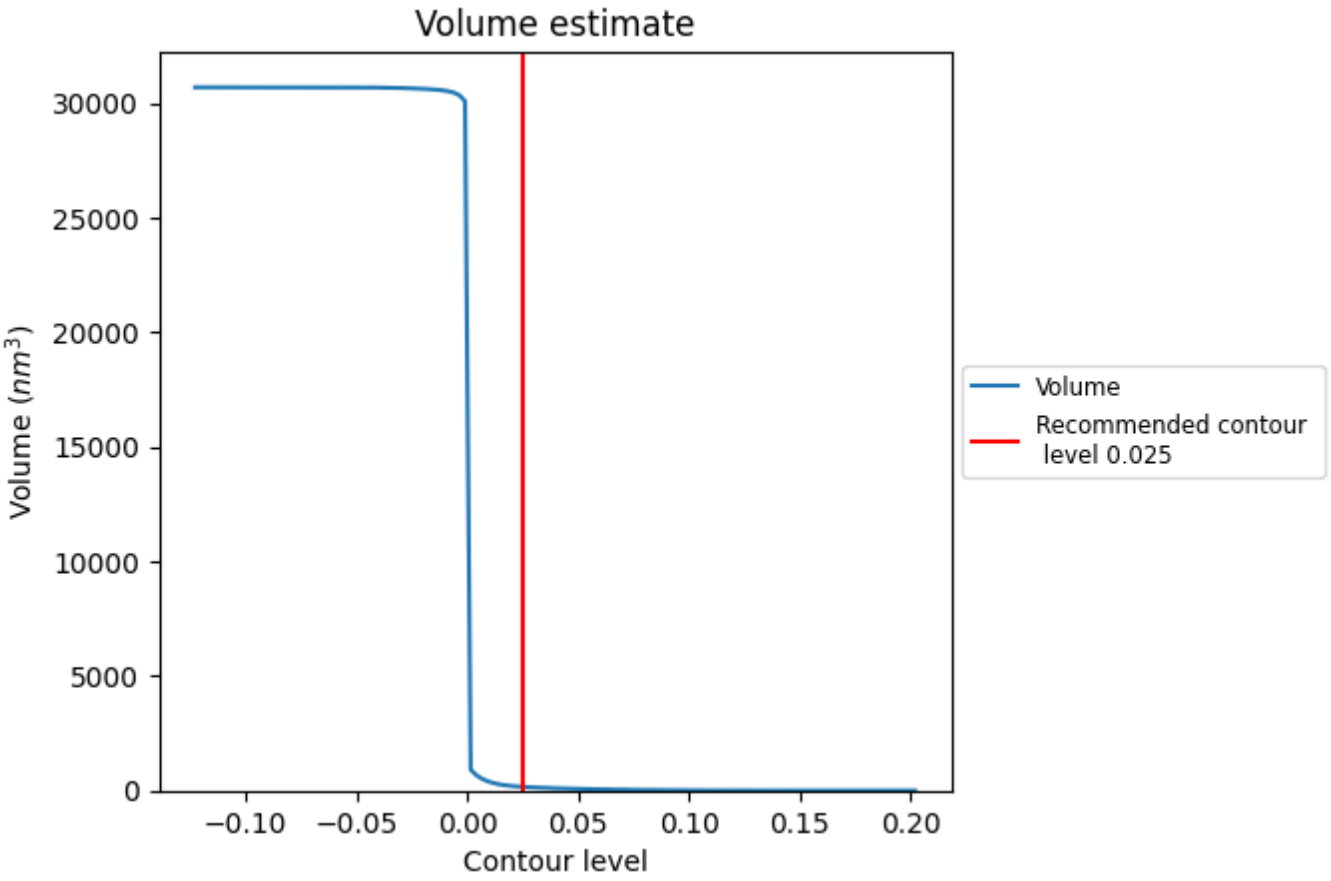
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

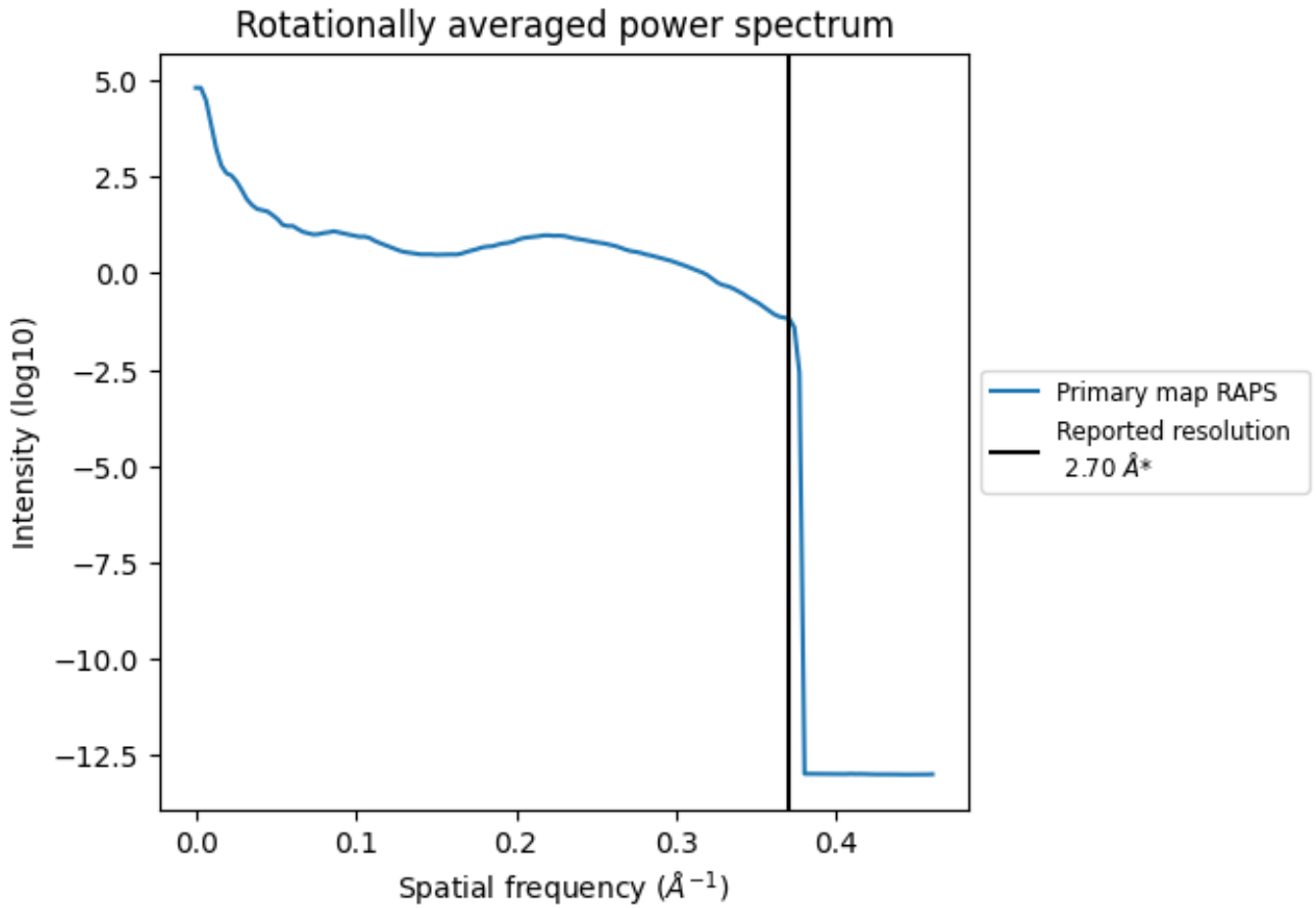
7.2 Volume estimate



The volume at the recommended contour level is 162 nm^3; this corresponds to an approximate mass of 146 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.370 $Å^{-1}$

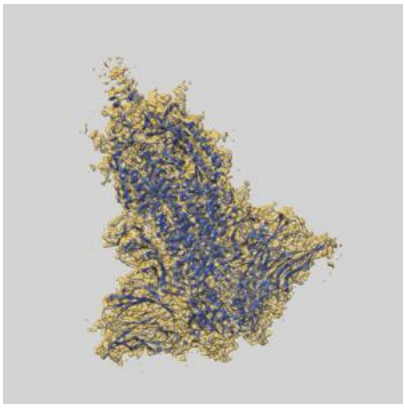
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

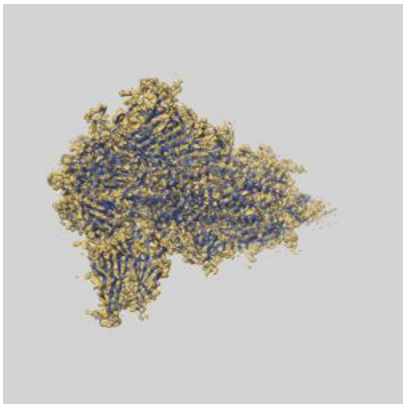
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-30889 and PDB model 7DWY. Per-residue inclusion information can be found in section 3 on page 10.

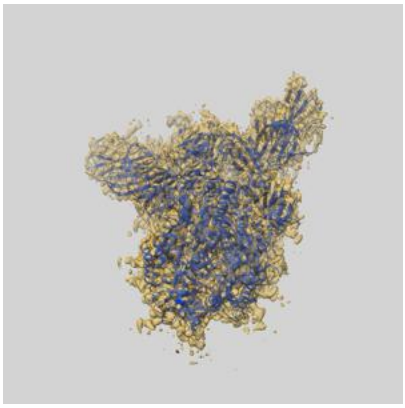
9.1 Map-model overlay



X



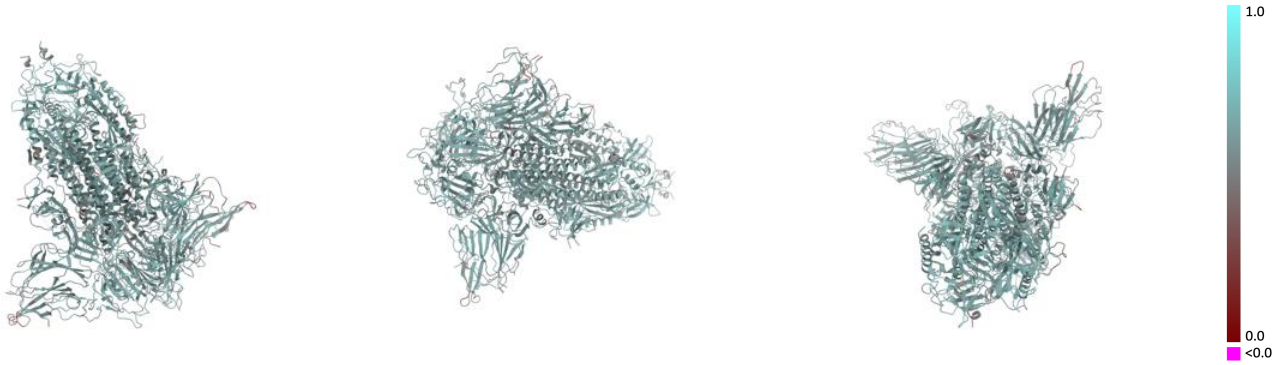
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

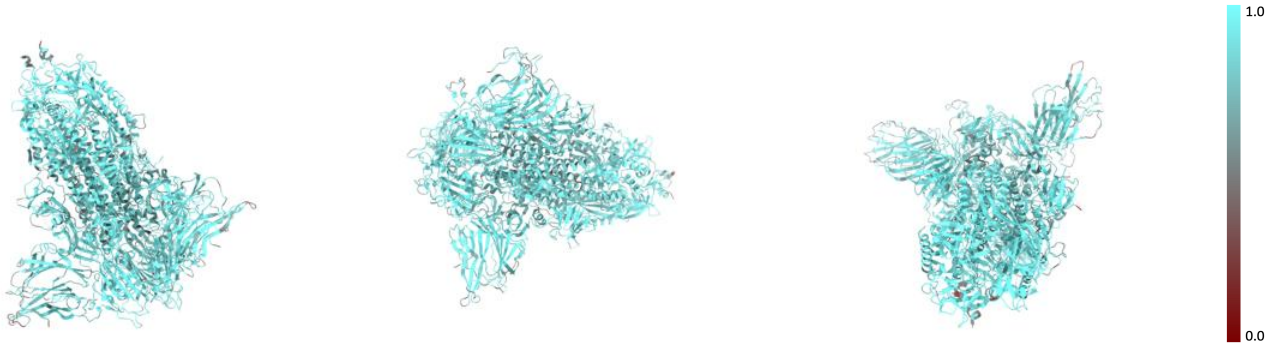
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

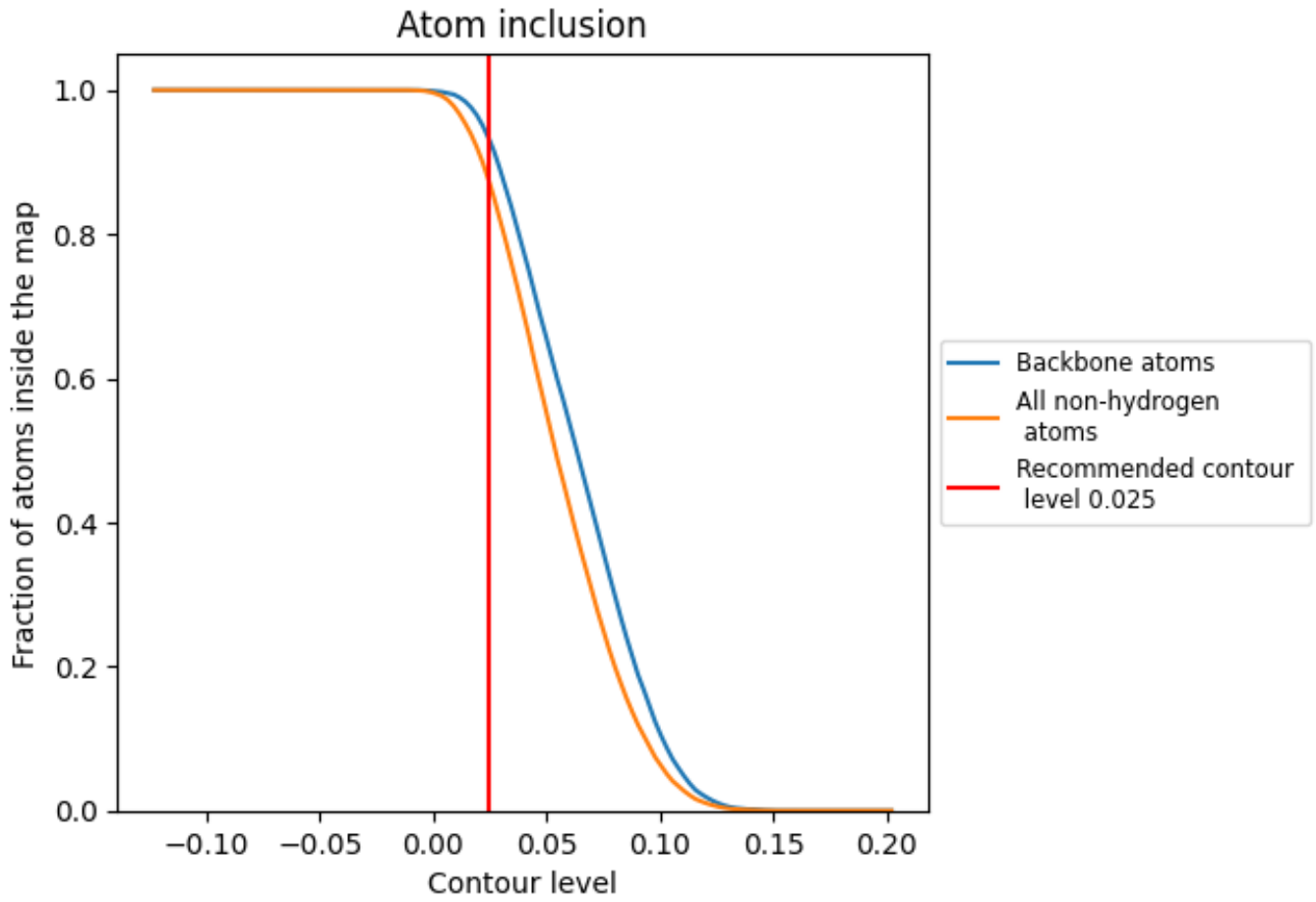
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.025).

9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 87% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8703	0.5790
A	0.8809	0.5870
B	0.8724	0.5780
C	0.8700	0.5790
D	0.1429	0.1940
E	0.7857	0.5170
F	0.5357	0.4610
G	0.6429	0.4480
H	0.2500	0.2020
I	0.7500	0.5240
J	0.6786	0.4280
K	0.2143	0.1540
L	0.2143	0.1780
M	0.7857	0.5410
N	0.7143	0.4380