wwPDB X-ray Structure Validation Summary Report (i)

Oct 3, 2023 – 03:52 AM EDT

PDB ID	:	6TZB
Title	:	Crystal structure of the A/Hong Kong/1/1968 (H3N2) influenza virus hemagglutinin in complex with 6'-SLNLN
Authors	:	Wu, N.C.; Wilson, I.A.
Deposited on	:	2019-08-12
Resolution	:	2.24 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

MolProbity	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.24 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 12998 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Hemagglutinin HA1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	321	2479	1552	438	476	13	0	0	0
1	C	317	2443	1531	429	470	13	0	0	0
1	E	317	2443	1531	429	470	13	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	PRO	-	expression tag	UNP Q91MA7
A	10	GLY	-	expression tag	UNP Q91MA7
C	9	PRO	-	expression tag	UNP Q91MA7
C	10	GLY	-	expression tag	UNP Q91MA7
E	9	PRO	-	expression tag	UNP Q91MA7
E	10	GLY	-	expression tag	UNP Q91MA7

- Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	172	1391	863	243	279	6	0	0	0
2	D	171	1382	858	241	277	6	0	0	0
2	F	171	1382	858	241	277	6	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	123	GLY	ARG	conflict	UNP H9XC94
D	123	GLY	ARG	conflict	UNP H9XC94

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	123	GLY	ARG	conflict	UNP H9XC94

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	G	3	39	22	2	15	0	0	0
3	H	3	39	22	2	15	0	0	0
3	L	3	39	22	2	15	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	I	2	28	16	2	10	0	0	0
4	N	2	28	16	2	10	0	0	0
4	P	2	28	16	2	10	0	0	0

- Molecule 5 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	J	5	71	39	3	29	0	0	0
5	Q	5	71	39	3	29	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
6	K	4	50	28	2	20	0	0	0

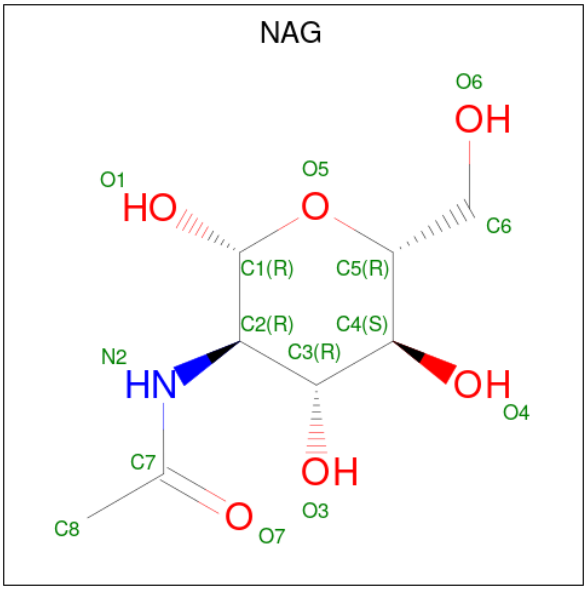
- Molecule 7 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galacto pyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
7	M	3	46	25	2	19	0	0	0

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranos e-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gluco pyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
8	O	4	50	28	2	20	0	0	0

- Molecule 9 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				ZeroOcc	AltConf
			Total	C	N	O		
9	A	1	14	8	1	5	0	0
9	C	1	14	8	1	5	0	0
9	C	1	14	8	1	5	0	0
9	D	1	14	8	1	5	0	0
9	E	1	14	8	1	5	0	0

- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	175	Total O 175 175	0	0
10	B	97	Total O 97 97	0	0
10	C	183	Total O 183 183	0	0
10	D	111	Total O 111 111	0	0
10	E	264	Total O 264 264	0	0
10	F	89	Total O 89 89	0	0

MolProbity and EDS failed to run properly - this section is therefore empty.

3 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	210.40Å 132.17Å 72.47Å 90.00° 97.93° 90.00°	Depositor
Resolution (Å)	39.75 – 2.24	Depositor
% Data completeness (in resolution range)	99.5 (39.75-2.24)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.91 (at 2.24Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.157 , 0.207	Depositor
Wilson B-factor (Å^2)	37.2	Xtriage
Anisotropy	0.121	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12998	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality (i)

4.1 Standard geometry (i)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts (i)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles (i)

4.3.1 Protein backbone (i)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains (i)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA (i)

MolProbity failed to run properly - this section is therefore empty.

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

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

4.5 Carbohydrates (i)

36 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	G	1	3,1	14,14,15	0.28	0	17,19,21	0.37	0
3	NAG	G	2	3	14,14,15	0.28	0	17,19,21	0.57	0
3	BMA	G	3	3	11,11,12	0.82	0	15,15,17	0.78	0
3	NAG	H	1	3,1	14,14,15	0.47	0	17,19,21	0.64	0
3	NAG	H	2	3	14,14,15	0.28	0	17,19,21	0.50	0
3	BMA	H	3	3	11,11,12	1.04	1 (9%)	15,15,17	1.68	3 (20%)
4	NAG	I	1	1,4	14,14,15	0.34	0	17,19,21	0.61	0
4	NAG	I	2	4	14,14,15	0.49	0	17,19,21	0.37	0
5	NAG	J	1	5	15,15,15	0.13	0	21,21,21	0.33	0
5	GAL	J	2	5	11,11,12	1.11	2 (18%)	15,15,17	1.62	2 (13%)
5	NAG	J	3	5	14,14,15	0.55	0	17,19,21	0.83	1 (5%)
5	GAL	J	4	5	11,11,12	0.87	0	15,15,17	1.05	1 (6%)
5	SIA	J	5	5	20,20,21	2.11	3 (15%)	24,28,31	1.43	4 (16%)
6	NAG	K	1	1,6	14,14,15	0.48	0	17,19,21	0.58	0
6	NAG	K	2	6	14,14,15	0.28	0	17,19,21	0.60	0
6	BMA	K	3	6	11,11,12	1.41	2 (18%)	15,15,17	1.79	4 (26%)
6	MAN	K	4	6	11,11,12	1.41	3 (27%)	15,15,17	1.54	2 (13%)
3	NAG	L	1	3,1	14,14,15	0.75	1 (7%)	17,19,21	0.36	0
3	NAG	L	2	3	14,14,15	0.20	0	17,19,21	0.54	0
3	BMA	L	3	3	11,11,12	0.87	0	15,15,17	0.73	0
7	NAG	M	1	7	15,15,15	0.45	0	21,21,21	0.51	0
7	GAL	M	2	7	11,11,12	0.64	0	15,15,17	1.06	2 (13%)
7	SIA	M	3	7	20,20,21	2.13	2 (10%)	24,28,31	1.41	4 (16%)
4	NAG	N	1	1,4	14,14,15	0.34	0	17,19,21	0.84	1 (5%)
4	NAG	N	2	4	14,14,15	0.33	0	17,19,21	0.51	0
8	NAG	O	1	8,1	14,14,15	0.31	0	17,19,21	0.73	1 (5%)
8	NAG	O	2	8	14,14,15	0.64	0	17,19,21	0.56	0
8	BMA	O	3	8	11,11,12	0.89	1 (9%)	15,15,17	1.57	3 (20%)
8	MAN	O	4	8	11,11,12	0.97	0	15,15,17	1.19	1 (6%)
4	NAG	P	1	1,4	14,14,15	0.62	1 (7%)	17,19,21	0.62	0
4	NAG	P	2	4	14,14,15	0.42	0	17,19,21	0.41	0
5	NAG	Q	1	5	15,15,15	0.19	0	21,21,21	0.18	0
5	GAL	Q	2	5	11,11,12	0.59	0	15,15,17	0.93	0
5	NAG	Q	3	5	14,14,15	0.74	1 (7%)	17,19,21	0.59	0
5	GAL	Q	4	5	11,11,12	0.71	0	15,15,17	1.52	3 (20%)
5	SIA	Q	5	5	20,20,21	2.28	3 (15%)	24,28,31	1.16	1 (4%)

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	G	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	BMA	G	3	3	-	1/2/19/22	0/1/1/1
3	NAG	H	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	2/6/23/26	0/1/1/1
3	BMA	H	3	3	-	2/2/19/22	0/1/1/1
4	NAG	I	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	I	2	4	-	1/6/23/26	0/1/1/1
5	NAG	J	1	5	-	0/6/26/26	0/1/1/1
5	GAL	J	2	5	-	2/2/19/22	0/1/1/1
5	NAG	J	3	5	-	0/6/23/26	0/1/1/1
5	GAL	J	4	5	-	2/2/19/22	0/1/1/1
5	SIA	J	5	5	-	5/18/34/38	0/1/1/1
6	NAG	K	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	K	2	6	-	2/6/23/26	0/1/1/1
6	BMA	K	3	6	-	0/2/19/22	0/1/1/1
6	MAN	K	4	6	-	2/2/19/22	0/1/1/1
3	NAG	L	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	L	2	3	-	2/6/23/26	0/1/1/1
3	BMA	L	3	3	-	0/2/19/22	0/1/1/1
7	NAG	M	1	7	-	2/6/26/26	0/1/1/1
7	GAL	M	2	7	-	1/2/19/22	0/1/1/1
7	SIA	M	3	7	-	1/18/34/38	0/1/1/1
4	NAG	N	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	N	2	4	-	0/6/23/26	0/1/1/1
8	NAG	O	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	O	2	8	-	1/6/23/26	0/1/1/1
8	BMA	O	3	8	-	2/2/19/22	0/1/1/1
8	MAN	O	4	8	-	2/2/19/22	0/1/1/1
4	NAG	P	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	P	2	4	-	0/6/23/26	0/1/1/1
5	NAG	Q	1	5	-	0/6/26/26	0/1/1/1
5	GAL	Q	2	5	-	0/2/19/22	0/1/1/1
5	NAG	Q	3	5	-	0/6/23/26	0/1/1/1
5	GAL	Q	4	5	-	0/2/19/22	0/1/1/1
5	SIA	Q	5	5	-	0/18/34/38	0/1/1/1

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	Q	5	SIA	C2-C1	8.94	1.60	1.52
7	M	3	SIA	C2-C1	7.76	1.59	1.52
5	J	5	SIA	C2-C1	7.62	1.59	1.52
6	K	3	BMA	C1-C2	3.84	1.61	1.52
5	J	5	SIA	O6-C2	3.41	1.48	1.43

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	J	2	GAL	C1-C2-C3	4.95	115.75	109.67
6	K	4	MAN	C1-O5-C5	4.22	117.92	112.19
6	K	3	BMA	C1-C2-C3	4.06	114.65	109.67
7	M	3	SIA	O1A-C1-C2	-3.76	113.69	122.57
5	Q	4	GAL	C1-O5-C5	3.71	117.22	112.19

There are no chirality outliers.

5 of 37 torsion outliers are listed below:

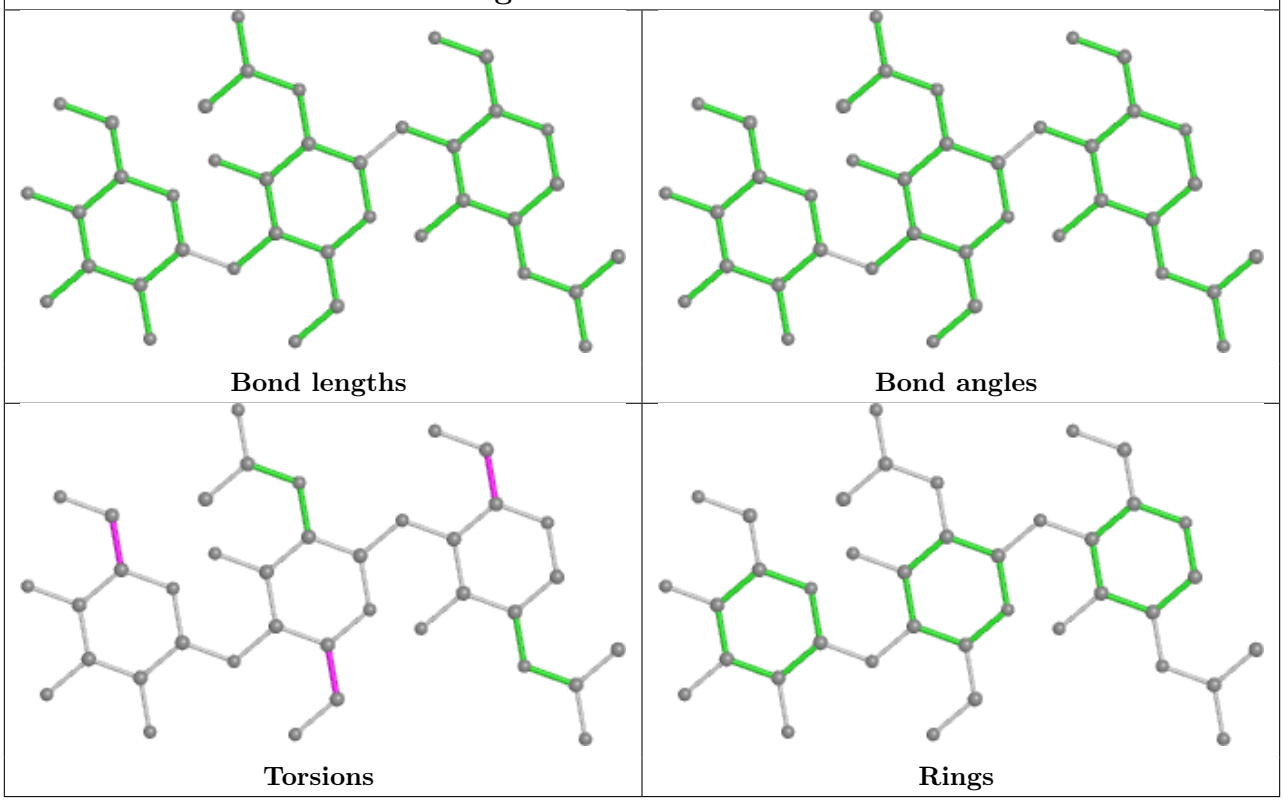
Mol	Chain	Res	Type	Atoms
6	K	2	NAG	O5-C5-C6-O6
3	L	2	NAG	O5-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
5	J	4	GAL	O5-C5-C6-O6
6	K	2	NAG	C4-C5-C6-O6

There are no ring outliers.

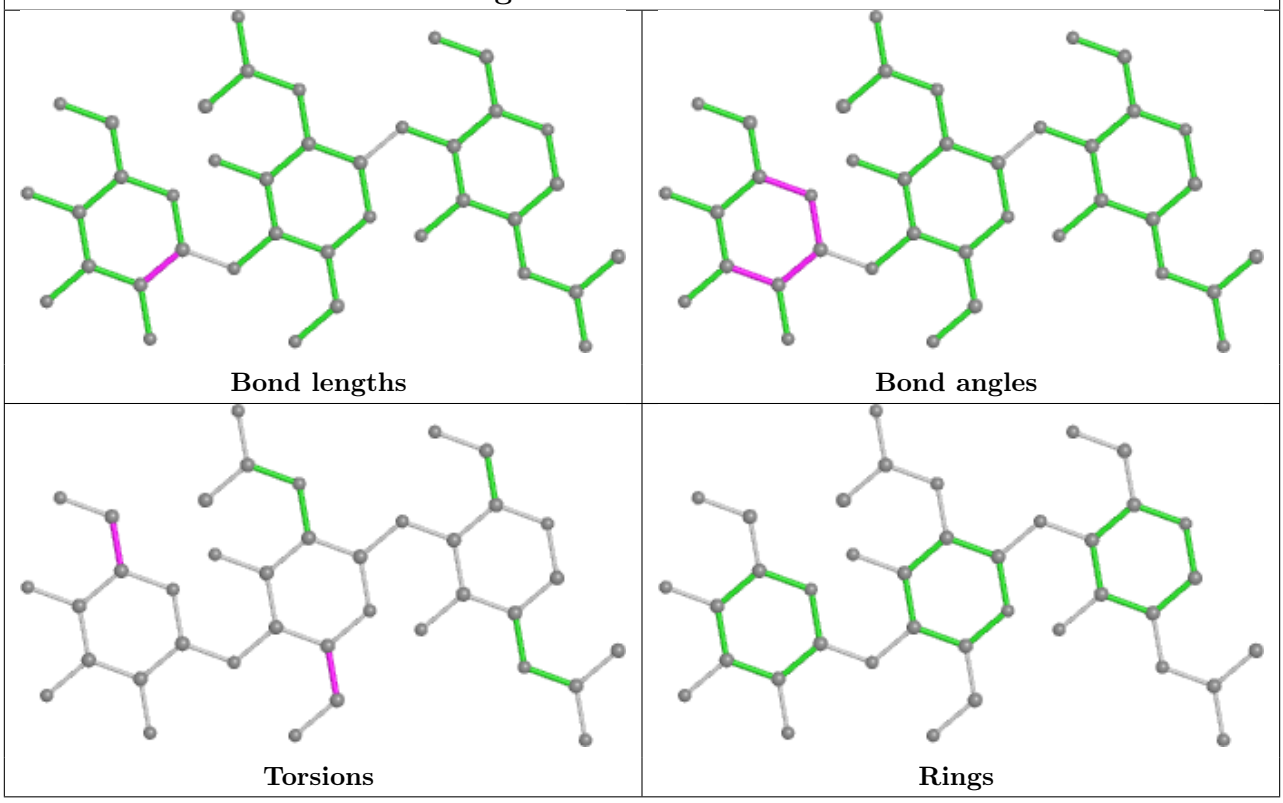
No monomer is involved in short contacts.

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

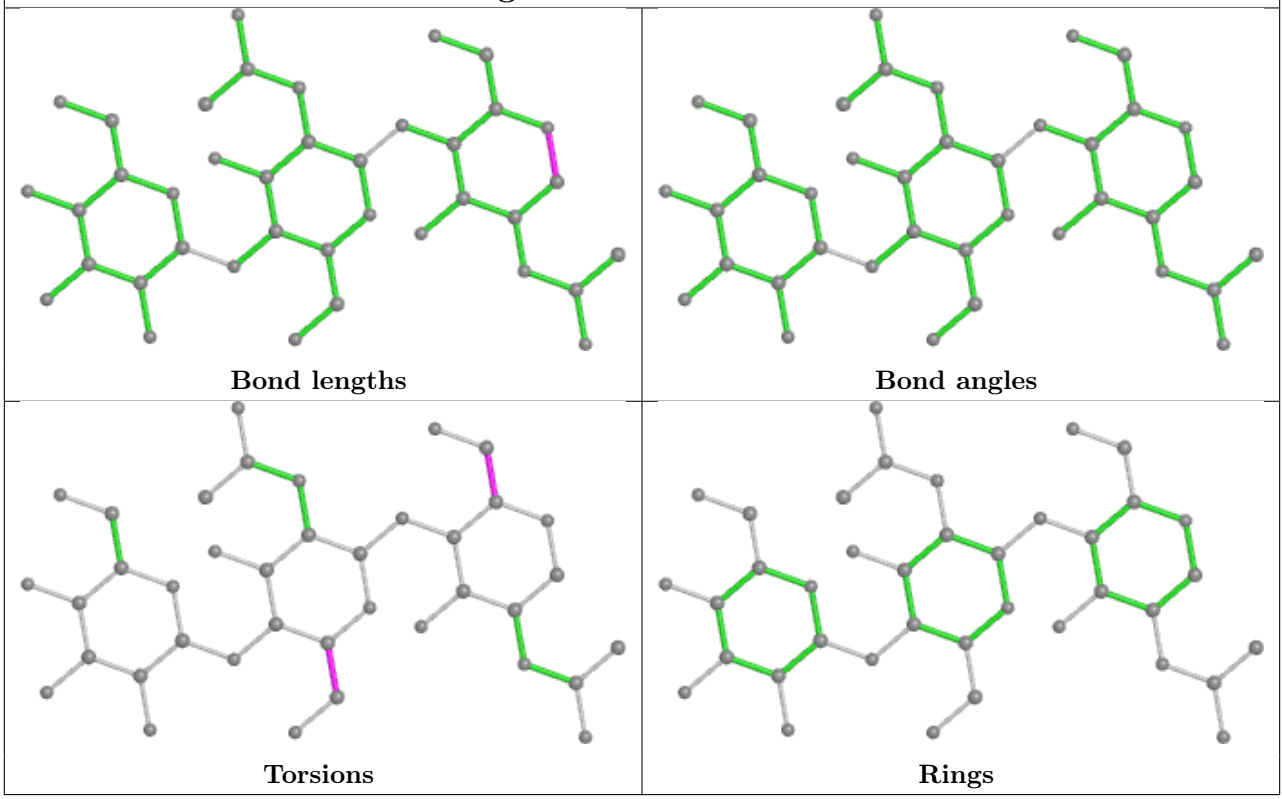
Oligosaccharide Chain G



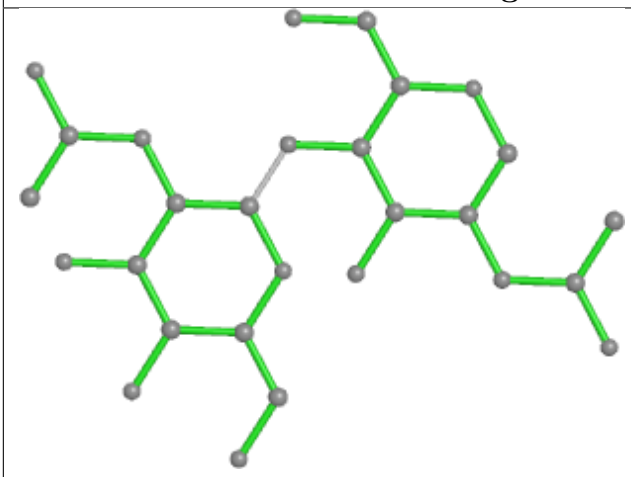
Oligosaccharide Chain H



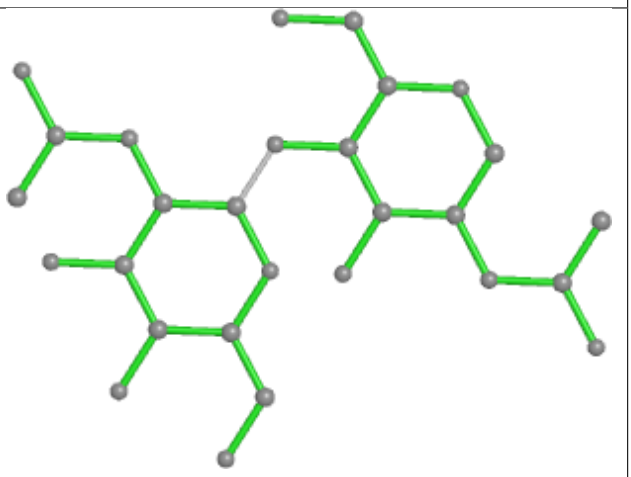
Oligosaccharide Chain L



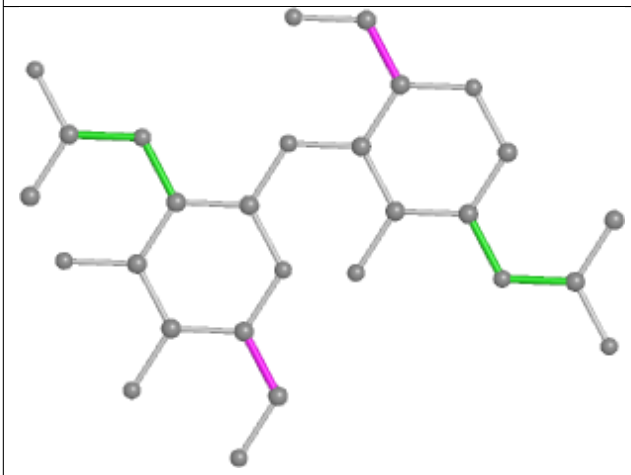
Oligosaccharide Chain I



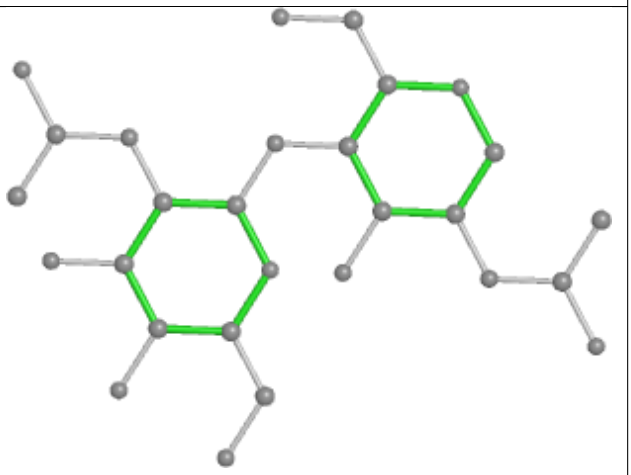
Bond lengths



Bond angles

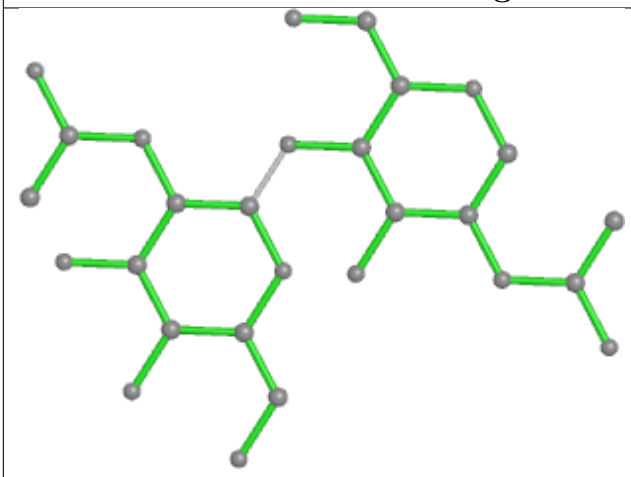


Torsions

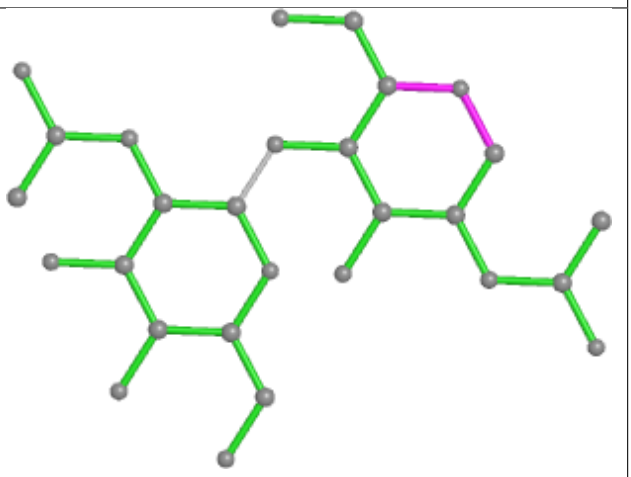


Rings

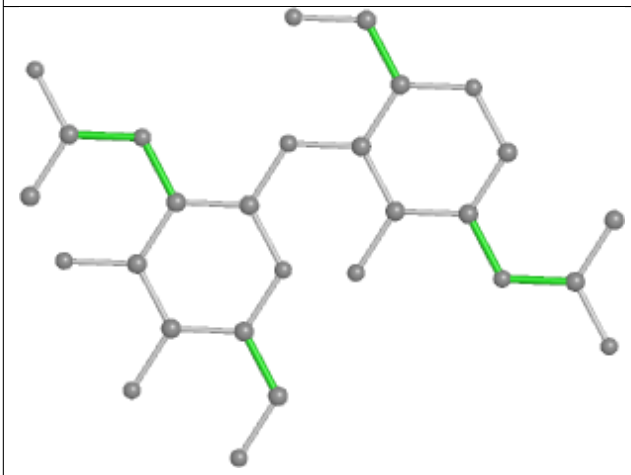
Oligosaccharide Chain N



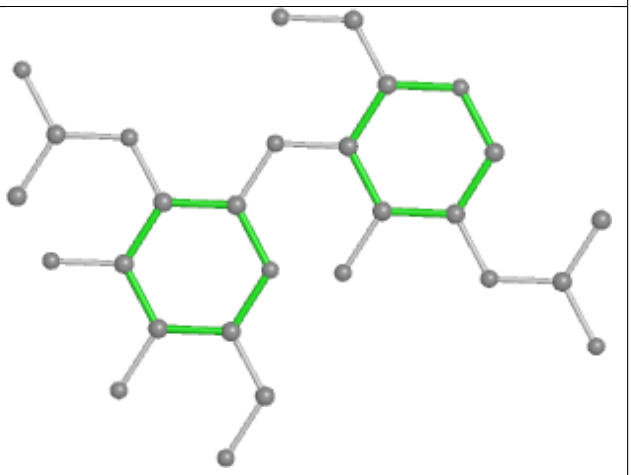
Bond lengths



Bond angles

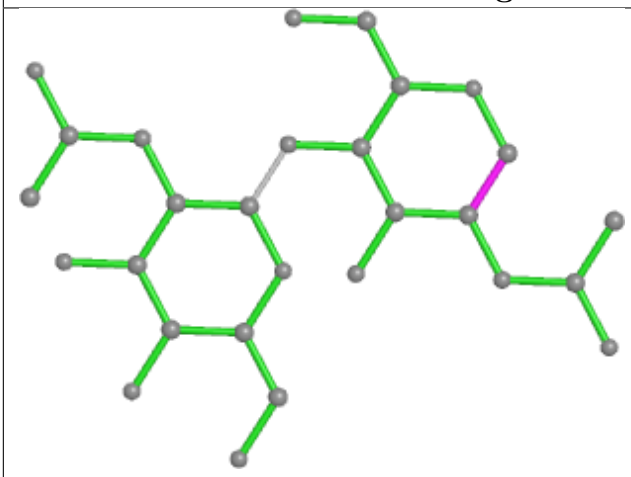


Torsions

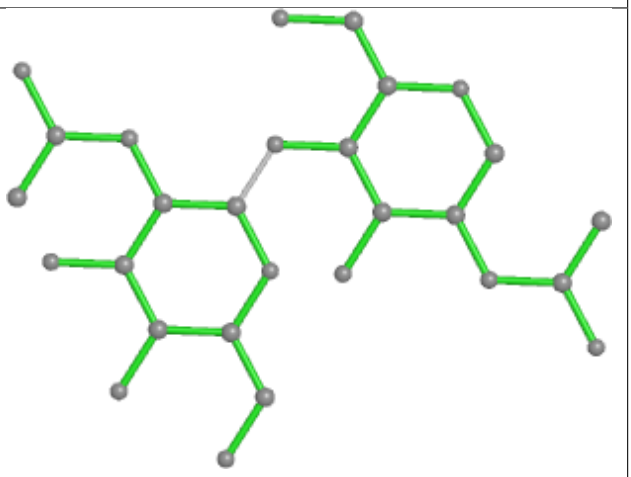


Rings

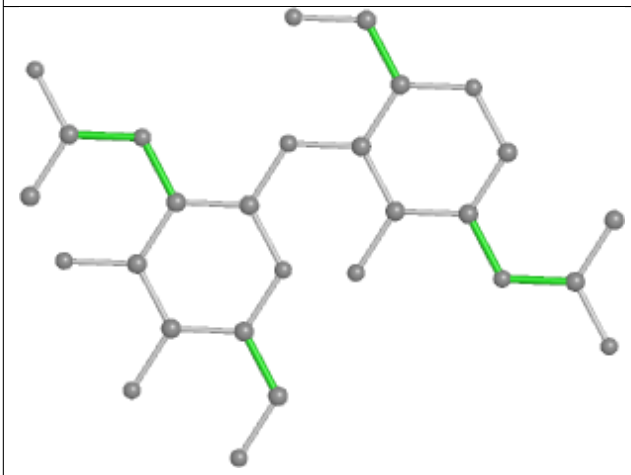
Oligosaccharide Chain P



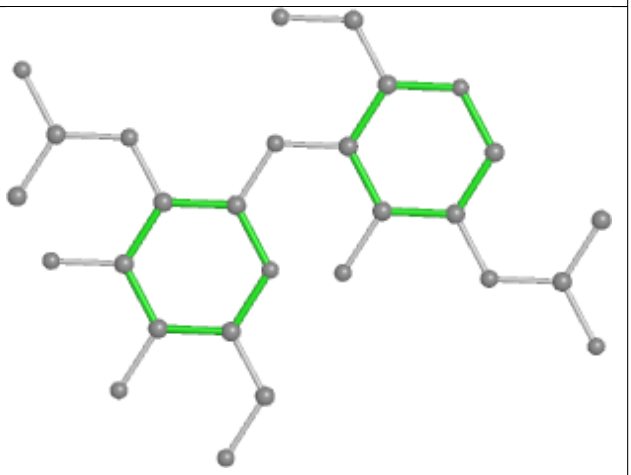
Bond lengths



Bond angles

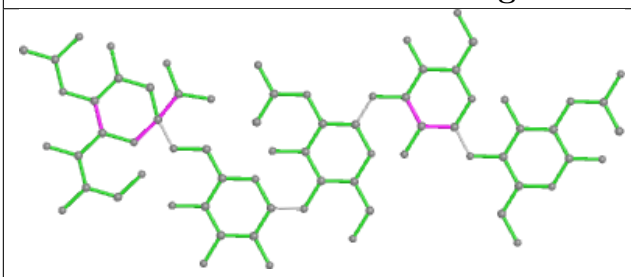


Torsions

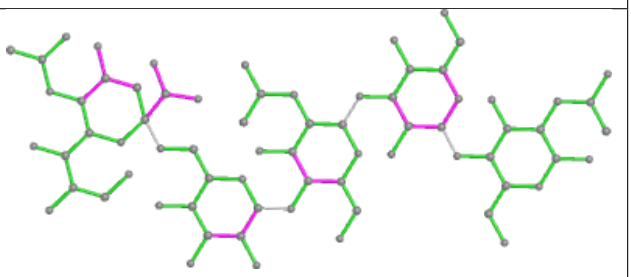


Rings

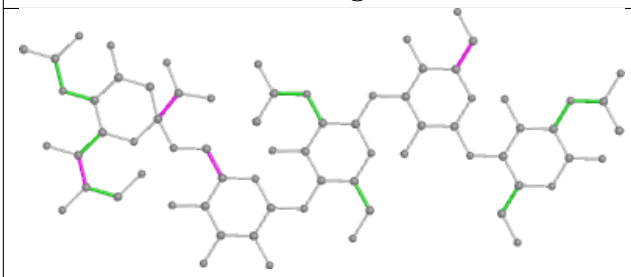
Oligosaccharide Chain J



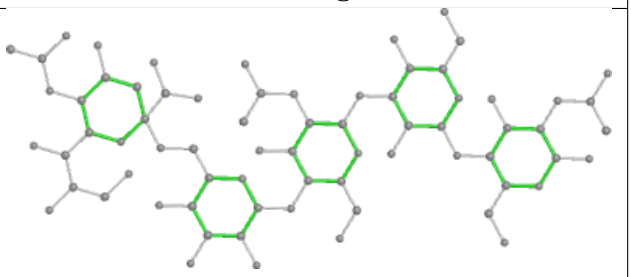
Bond lengths



Bond angles

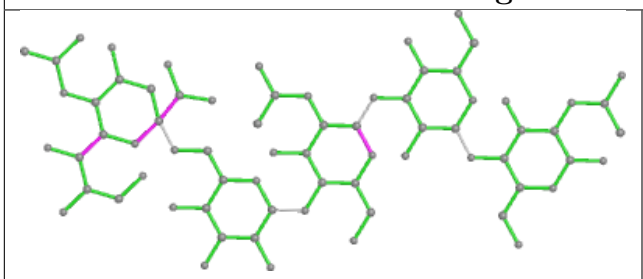


Torsions

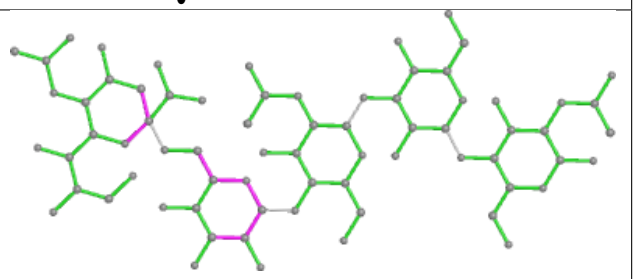


Rings

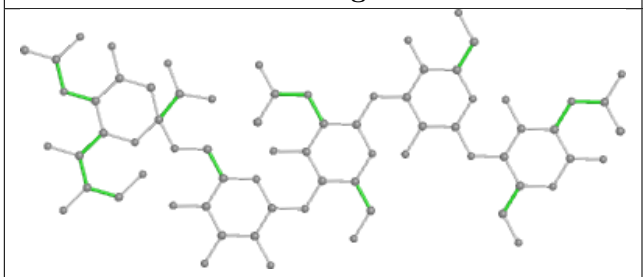
Oligosaccharide Chain Q



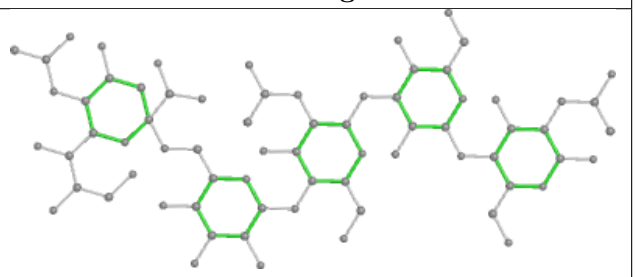
Bond lengths



Bond angles

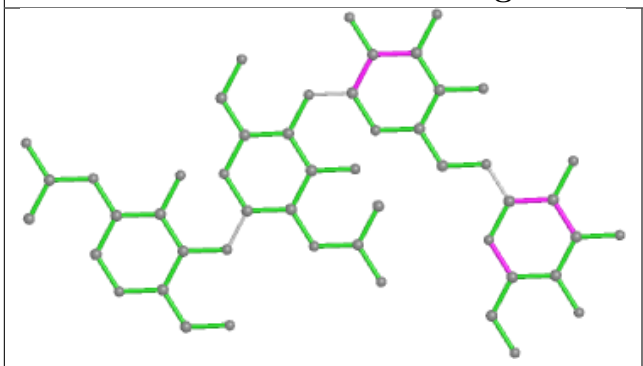


Torsions

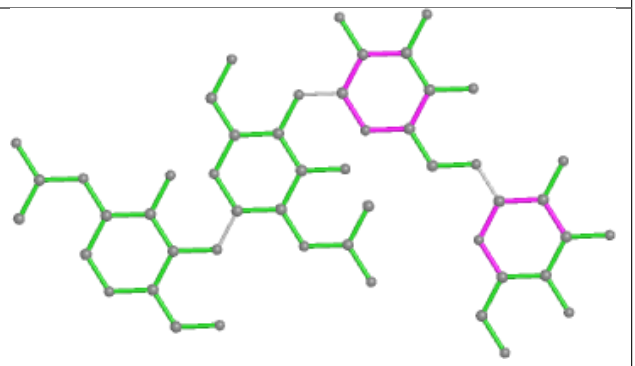


Rings

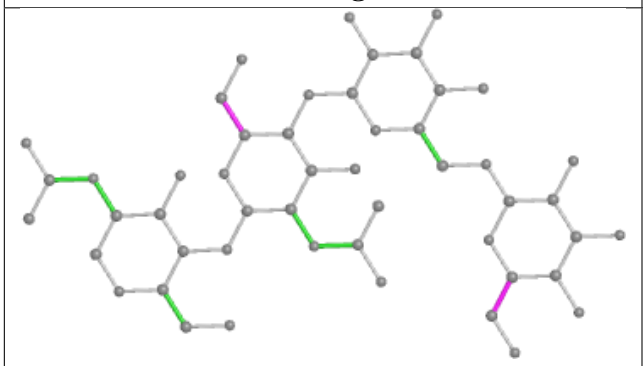
Oligosaccharide Chain K



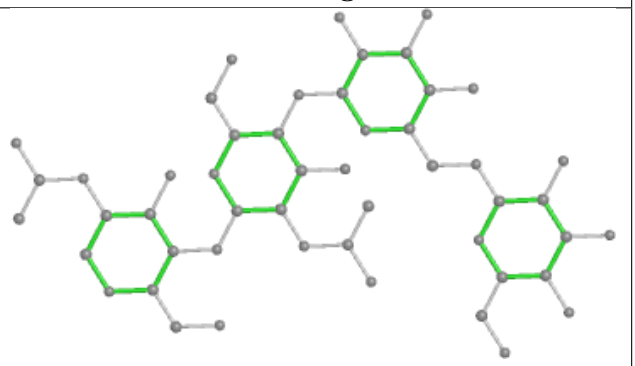
Bond lengths



Bond angles

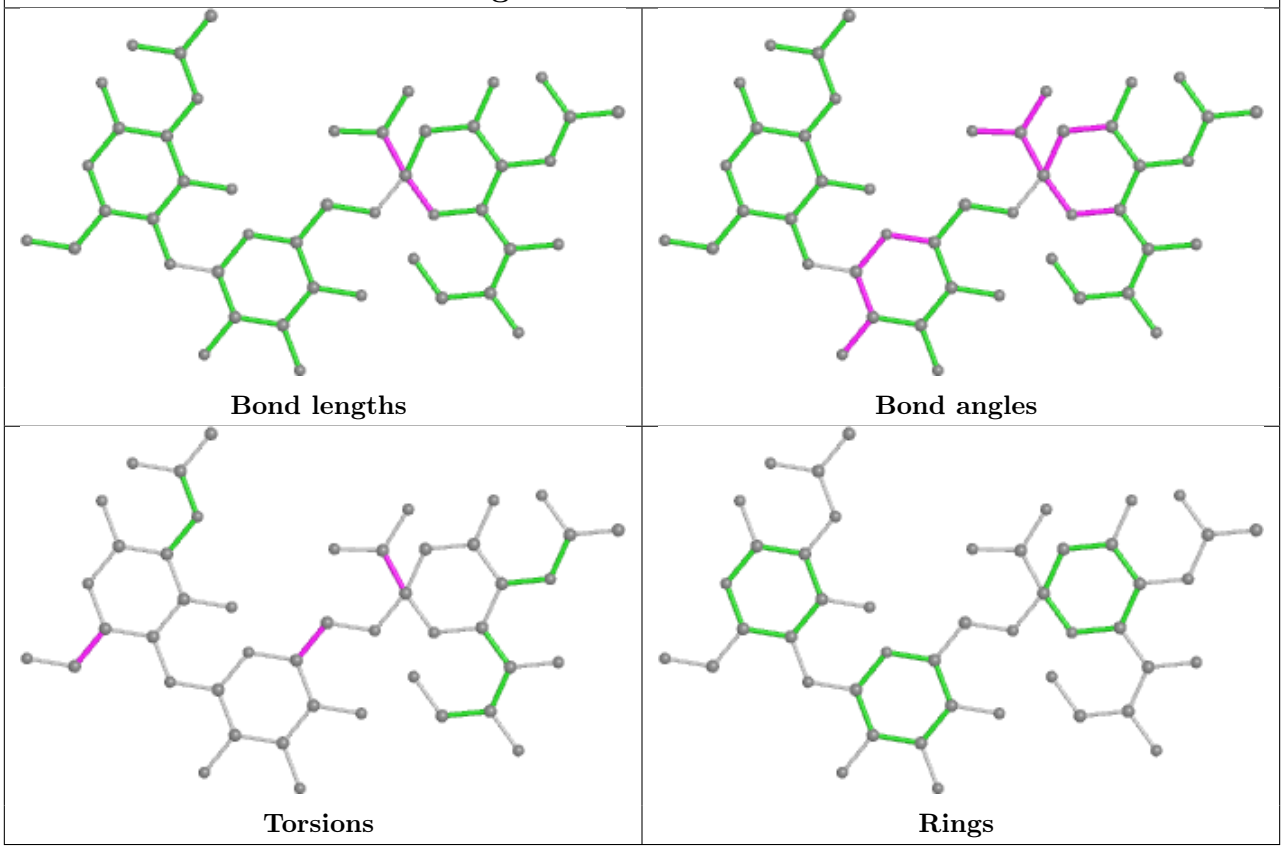


Torsions

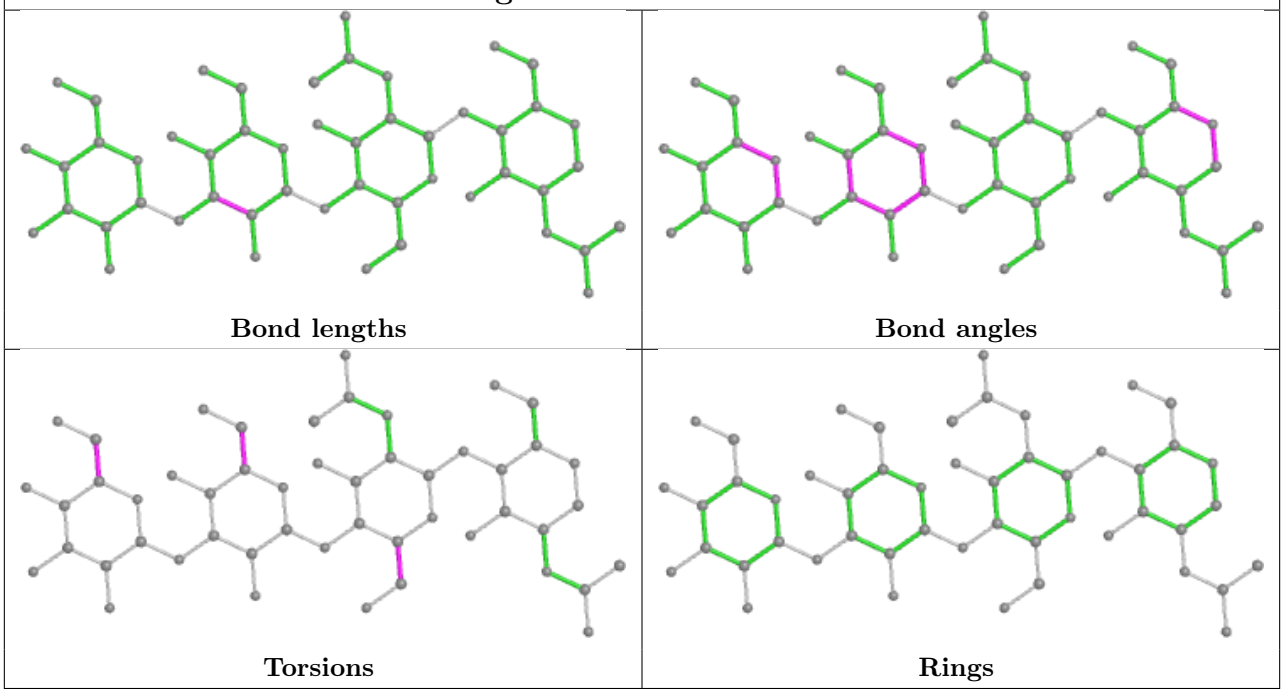


Rings

Oligosaccharide Chain M



Oligosaccharide Chain O



4.6 Ligand geometry (i)

5 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	$\#\|Z\| > 2$
9	NAG	E	509	1	14,14,15	0.96	2 (14%)	17,19,21	0.72	0
9	NAG	C	502	1	14,14,15	1.07	1 (7%)	17,19,21	1.66	1 (5%)
9	NAG	A	404	1	14,14,15	0.74	1 (7%)	17,19,21	0.74	1 (5%)
9	NAG	D	201	2	14,14,15	0.94	2 (14%)	17,19,21	0.61	0
9	NAG	C	501	1	14,14,15	0.86	1 (7%)	17,19,21	1.34	1 (5%)

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
9	NAG	E	509	1	-	2/6/23/26	0/1/1/1
9	NAG	C	502	1	-	0/6/23/26	0/1/1/1
9	NAG	A	404	1	-	2/6/23/26	0/1/1/1
9	NAG	D	201	2	-	3/6/23/26	0/1/1/1
9	NAG	C	501	1	-	2/6/23/26	0/1/1/1

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	502	NAG	O5-C1	3.86	1.49	1.43
9	C	501	NAG	O5-C1	3.03	1.48	1.43
9	E	509	NAG	O5-C1	2.87	1.48	1.43
9	D	201	NAG	C1-C2	2.63	1.56	1.52
9	A	404	NAG	O5-C1	2.57	1.47	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	C	502	NAG	C1-O5-C5	6.33	120.77	112.19
9	C	501	NAG	C1-O5-C5	5.16	119.19	112.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	404	NAG	C1-O5-C5	2.40	115.44	112.19

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

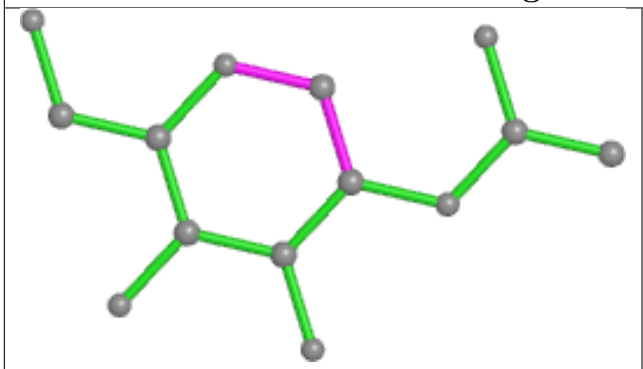
Mol	Chain	Res	Type	Atoms
9	E	509	NAG	O5-C5-C6-O6
9	D	201	NAG	O5-C5-C6-O6
9	D	201	NAG	C4-C5-C6-O6
9	E	509	NAG	C4-C5-C6-O6
9	A	404	NAG	O5-C5-C6-O6

There are no ring outliers.

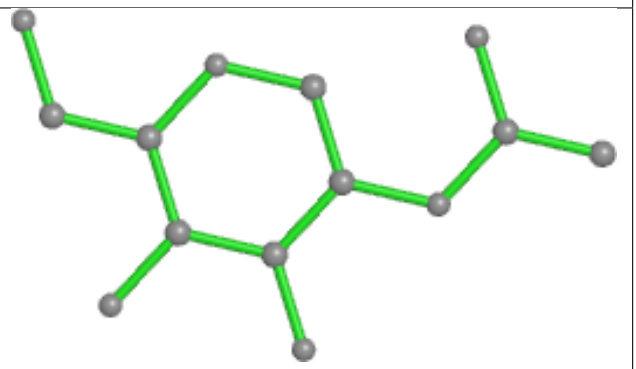
No monomer is involved in short contacts.

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

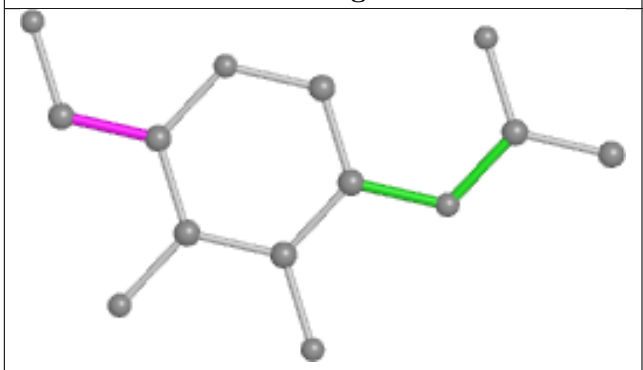
Ligand NAG E 509



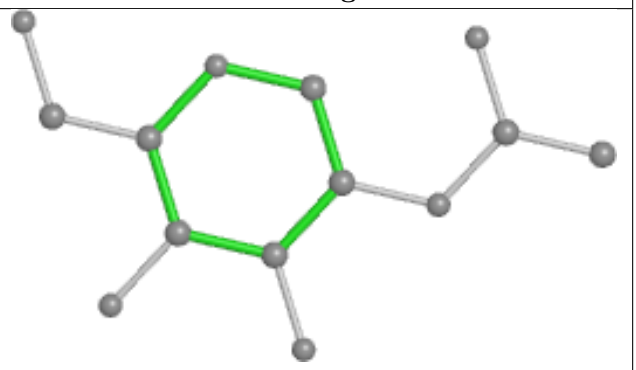
Bond lengths



Bond angles

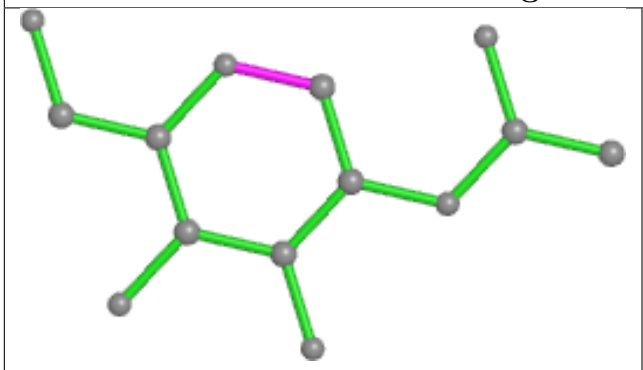


Torsions

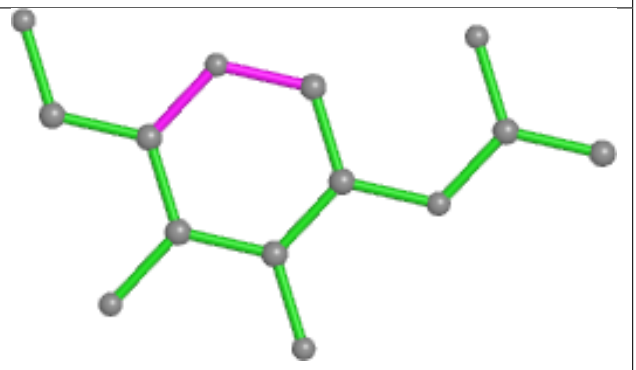


Rings

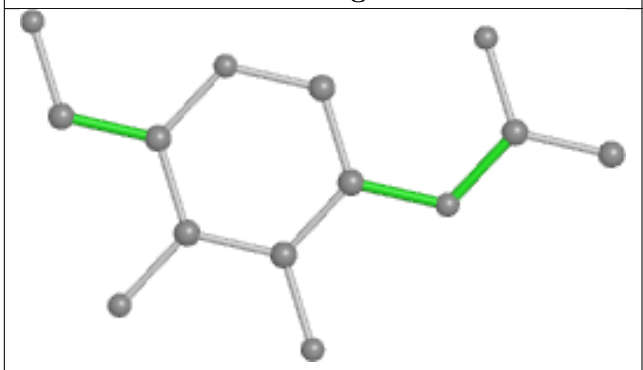
Ligand NAG C 502



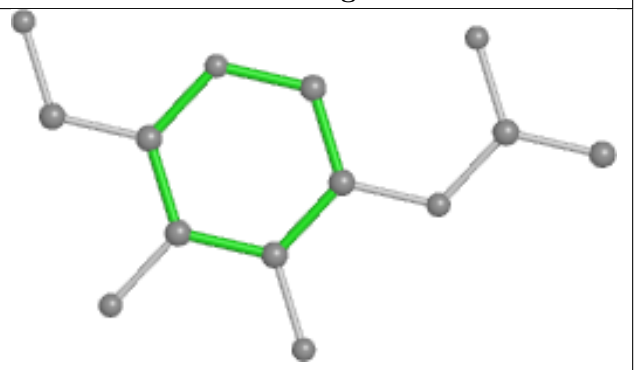
Bond lengths



Bond angles

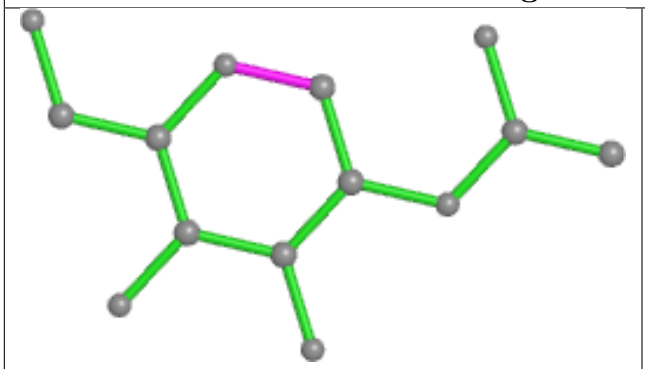


Torsions

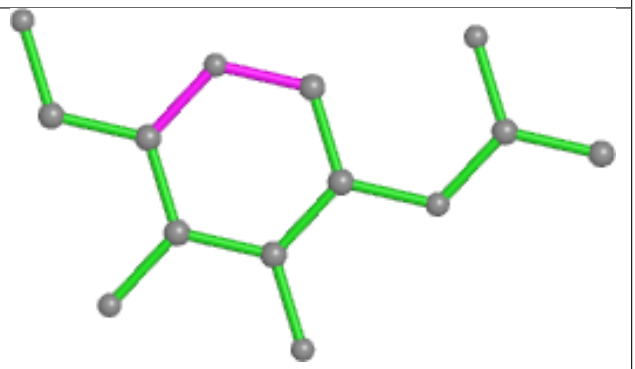


Rings

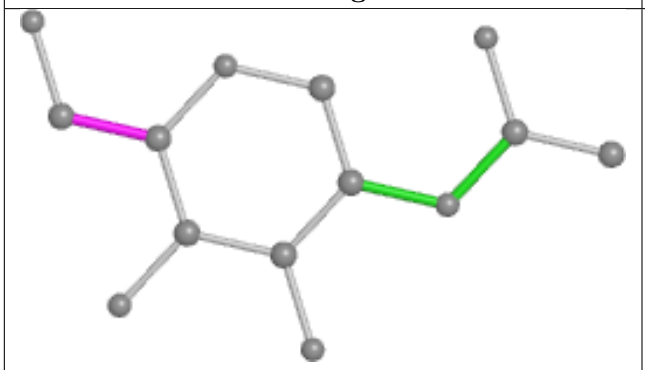
Ligand NAG A 404



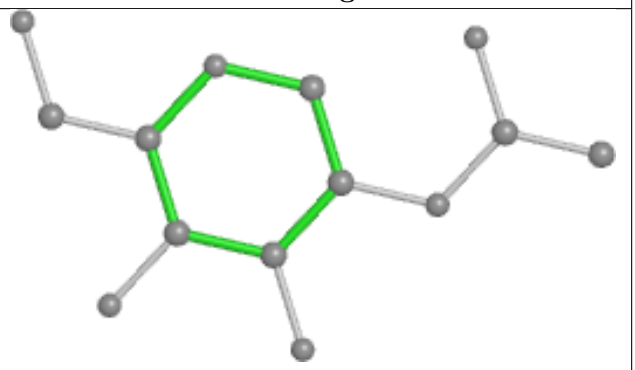
Bond lengths



Bond angles

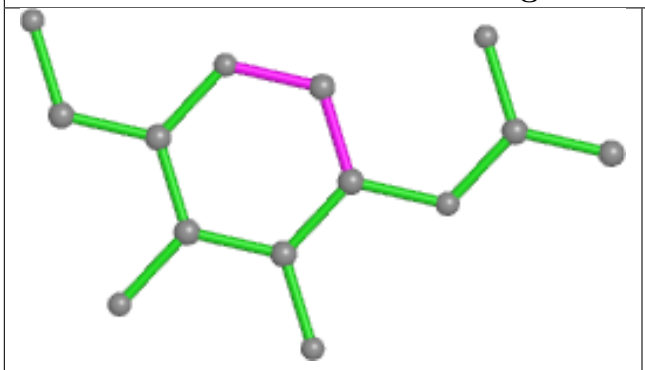


Torsions

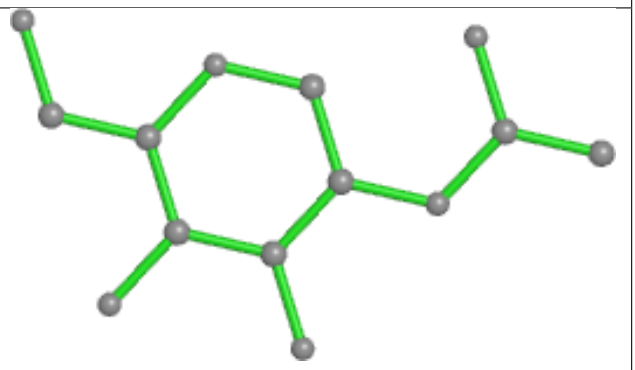


Rings

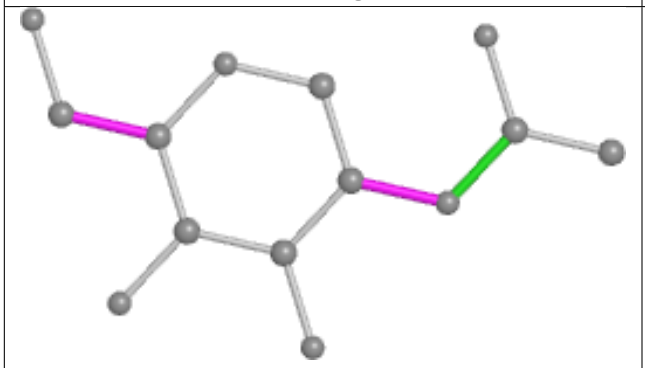
Ligand NAG D 201



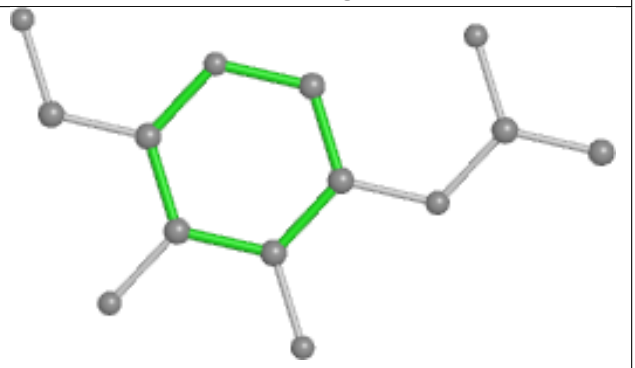
Bond lengths



Bond angles

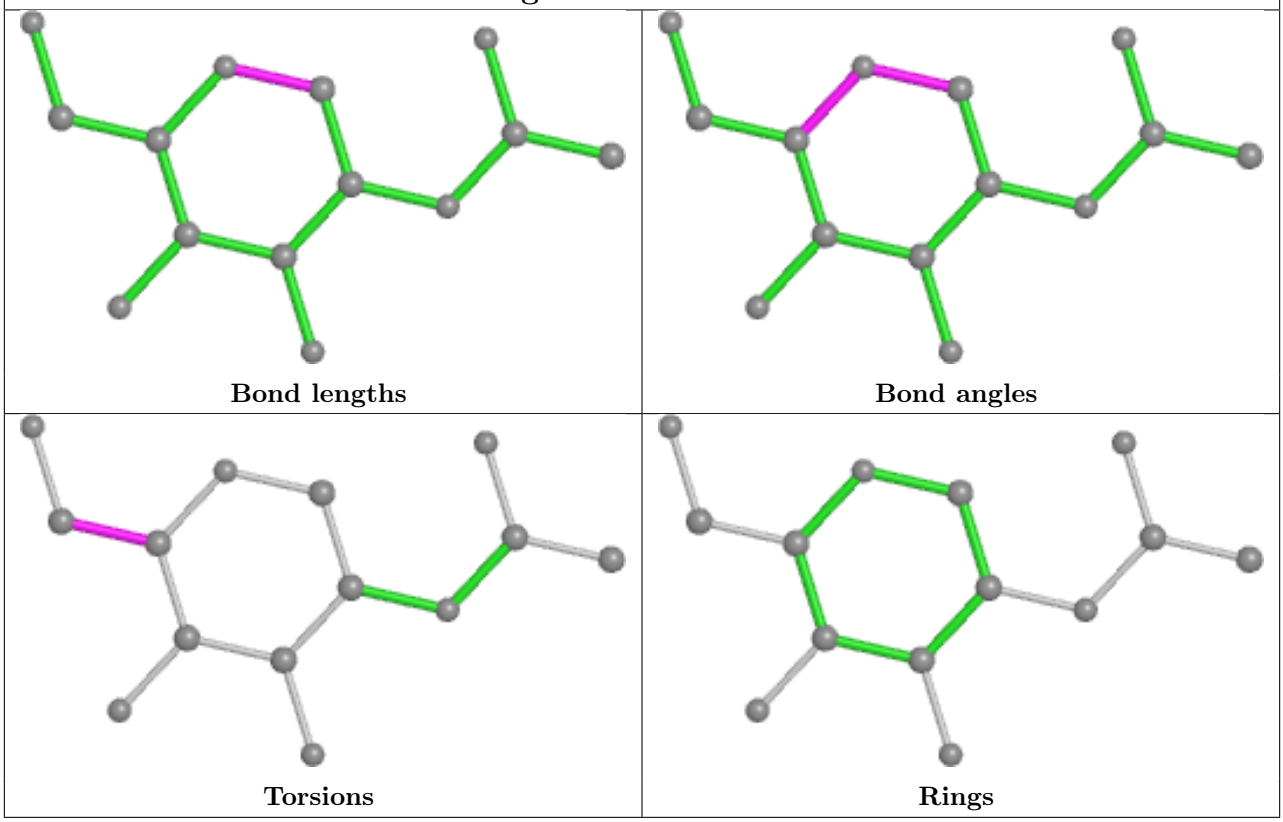


Torsions



Rings

Ligand NAG C 501



4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

5 Fit of model and data (i)

5.1 Protein, DNA and RNA chains (i)

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates (i)

EDS failed to run properly - this section is therefore empty.

5.4 Ligands (i)

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers (i)

EDS failed to run properly - this section is therefore empty.