wwPDB X-ray Structure Validation Summary Report (i)

Oct 2, 2023 – 12:33 AM EDT

PDB ID	:	6MCO
Title	:	Crystal structure of the B41 SOSIP.664 Env trimer with PGT124 and 35O22 Fabs, in P23 space group
Authors	:	Kumar, S.; Sarkar, A.; Wilson, I.A.
Deposited on	:	2018-08-31
Resolution	:	3.53 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 (i)) were used in the production of this report:

MolProbity	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
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 3.53 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 16 unique types of molecules in this entry. The entry contains 12268 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 Transmembrane protein gp41.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	133	Total	C	N	O	S	0	0	0
			1058	675	178	198	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	605	CYS	THR	conflict	UNP B3UF08

- Molecule 2 is a protein called 35O22 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	240	Total	C	N	O	S	0	0	0
			1813	1150	303	352	8			

- Molecule 3 is a protein called 35O22 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	213	Total	C	N	O	S	0	0	0
			1615	1012	267	328	8			

- Molecule 4 is a protein called Surface protein gp120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	456	Total	C	N	O	S	0	0	0
			3576	2244	632	674	26			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	501	CYS	ALA	conflict	UNP B3UES2

- Molecule 5 is a protein called PGT124 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	H	231	Total	C	N	O	S	0	0	0
			1754	1111	293	345	5			

- Molecule 6 is a protein called PGT124 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	L	211	Total	C	N	O	S	0	0	0
			1601	1008	271	317	5			

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[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
7	A	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 8 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
8	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
8	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
8	Q	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	F	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 10 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
10	J	4	Total C N O 50 28 2 20	0	0	0
10	M	4	Total C N O 50 28 2 20	0	0	0

- Molecule 11 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
11	K	3	Total C N O 39 22 2 15	0	0	0
11	N	3	Total C N O 39 22 2 15	0	0	0
11	O	3	Total C N O 39 22 2 15	0	0	0
11	U	3	Total C N O 39 22 2 15	0	0	0

- Molecule 12 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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
12	P	8	Total C N O 94 52 2 40	0	0	0

- Molecule 13 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-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
13	R	4	Total C N O 50 28 2 20	0	0	0

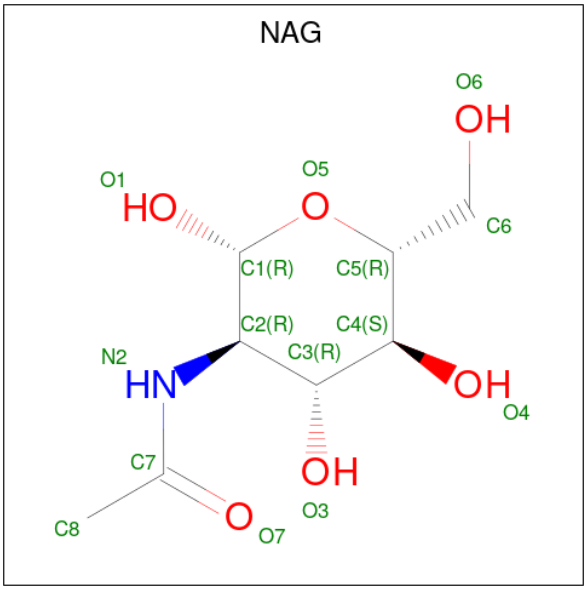
- Molecule 14 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
14	S	5	Total C N O 61 34 2 25	0	0	0

- Molecule 15 is an oligosaccharide called beta-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

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

- Molecule 16 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	B	1	Total C N O 14 8 1 5	0	0
16	B	1	Total C N O 14 8 1 5	0	0
16	G	1	Total C N O 14 8 1 5	0	0
16	G	1	Total C N O 14 8 1 5	0	0
16	G	1	Total C N O 14 8 1 5	0	0
16	G	1	Total C N O 14 8 1 5	0	0
16	G	1	Total C N O 14 8 1 5	0	0
16	G	1	Total C N O 14 8 1 5	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	P 2 3	Depositor
Cell constants a, b, c, α, β, γ	212.33Å 212.33Å 212.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.05 – 3.53	Depositor
% Data completeness (in resolution range)	99.7 (50.05-3.53)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.22 (at 3.48Å)	Xtriage
Refinement program	PHENIX (1.12_2829)	Depositor
R, R_{free}	0.306 , 0.322	Depositor
Wilson B-factor (Å^2)	106.1	Xtriage
Anisotropy	0.000	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.023 for l,-k,h	Xtriage
Total number of atoms	12268	wwPDB-VP
Average B, all atoms (Å^2)	124.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.96% 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

4.1 Standard geometry

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

4.2 Too-close contacts

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

4.3 Torsion angles

4.3.1 Protein backbone

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

4.3.2 Protein sidechains

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

4.3.3 RNA

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

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

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

4.5 Carbohydrates

59 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	$\#\|Z\|>2$
7	NAG	A	1	1,7	14,14,15	0.33	0	17,19,21	1.05	2 (11%)
7	NAG	A	2	7	14,14,15	0.28	0	17,19,21	1.31	1 (5%)
7	BMA	A	3	7	11,11,12	0.51	0	15,15,17	1.86	6 (40%)
7	MAN	A	4	7	11,11,12	1.27	1 (9%)	15,15,17	0.92	1 (6%)
7	MAN	A	5	7	11,11,12	1.22	0	15,15,17	0.86	0
7	MAN	A	6	7	11,11,12	0.79	0	15,15,17	1.19	2 (13%)
8	NAG	C	1	1,8	14,14,15	0.40	0	17,19,21	1.40	2 (11%)
8	NAG	C	2	8	14,14,15	0.34	0	17,19,21	0.65	1 (5%)
9	NAG	F	1	9,4	14,14,15	0.37	0	17,19,21	1.08	1 (5%)
9	NAG	F	2	9,2	14,14,15	0.64	0	17,19,21	1.11	1 (5%)
9	BMA	F	3	9	11,11,12	0.45	0	15,15,17	1.19	1 (6%)
9	MAN	F	4	9	11,11,12	2.12	4 (36%)	15,15,17	1.68	4 (26%)
9	MAN	F	5	9	11,11,12	0.81	1 (9%)	15,15,17	1.25	2 (13%)
9	MAN	F	6	9	11,11,12	0.56	0	15,15,17	1.25	2 (13%)
9	MAN	F	7	9	11,11,12	0.71	0	15,15,17	0.91	1 (6%)
8	NAG	I	1	8,4	14,14,15	0.30	0	17,19,21	0.73	0
8	NAG	I	2	8	14,14,15	0.29	0	17,19,21	0.69	0
10	NAG	J	1	10,4	14,14,15	0.34	0	17,19,21	0.86	0
10	NAG	J	2	10	14,14,15	0.42	0	17,19,21	1.67	3 (17%)
10	BMA	J	3	10	11,11,12	0.30	0	15,15,17	0.76	0
10	MAN	J	4	10	11,11,12	0.73	0	15,15,17	0.96	2 (13%)
11	NAG	K	1	11,4	14,14,15	0.35	0	17,19,21	0.86	0
11	NAG	K	2	11	14,14,15	0.48	0	17,19,21	1.50	2 (11%)
11	BMA	K	3	11	11,11,12	0.23	0	15,15,17	0.66	0
10	NAG	M	1	10,4	14,14,15	0.30	0	17,19,21	0.75	0
10	NAG	M	2	10	14,14,15	0.33	0	17,19,21	0.79	0
10	BMA	M	3	10	11,11,12	0.28	0	15,15,17	0.66	0
10	MAN	M	4	10	11,11,12	0.83	0	15,15,17	1.15	2 (13%)
11	NAG	N	1	11,4	14,14,15	0.35	0	17,19,21	0.93	1 (5%)
11	NAG	N	2	11	14,14,15	0.32	0	17,19,21	0.73	0
11	BMA	N	3	11	11,11,12	0.27	0	15,15,17	0.82	0
11	NAG	O	1	11,4	14,14,15	0.28	0	17,19,21	0.59	0
11	NAG	O	2	11	14,14,15	0.28	0	17,19,21	0.92	1 (5%)
11	BMA	O	3	11	11,11,12	0.30	0	15,15,17	0.83	0
12	NAG	P	1	12,4	14,14,15	0.29	0	17,19,21	1.24	2 (11%)
12	NAG	P	2	12	14,14,15	0.34	0	17,19,21	1.17	2 (11%)
12	BMA	P	3	12	11,11,12	0.66	0	15,15,17	1.74	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	MAN	P	4	12	11,11,12	0.87	1 (9%)	15,15,17	1.72	3 (20%)
12	MAN	P	5	12	11,11,12	1.02	0	15,15,17	1.52	2 (13%)
12	MAN	P	6	12	11,11,12	0.77	0	15,15,17	1.13	2 (13%)
12	MAN	P	7	12	11,11,12	0.80	0	15,15,17	0.90	1 (6%)
12	MAN	P	8	12	11,11,12	0.92	0	15,15,17	0.99	0
8	NAG	Q	1	8,4	14,14,15	0.35	0	17,19,21	1.06	2 (11%)
8	NAG	Q	2	8	14,14,15	0.29	0	17,19,21	0.93	0
13	NAG	R	1	13,4	14,14,15	0.30	0	17,19,21	0.99	2 (11%)
13	NAG	R	2	13	14,14,15	0.40	0	17,19,21	0.88	1 (5%)
13	BMA	R	3	13	11,11,12	0.43	0	15,15,17	0.97	1 (6%)
13	MAN	R	4	13	11,11,12	0.87	0	15,15,17	0.96	2 (13%)
14	NAG	S	1	14,4	14,14,15	0.27	0	17,19,21	0.66	0
14	NAG	S	2	14	14,14,15	0.33	0	17,19,21	0.66	0
14	BMA	S	3	14	11,11,12	0.33	0	15,15,17	0.88	0
14	MAN	S	4	14	11,11,12	0.77	0	15,15,17	0.88	1 (6%)
14	MAN	S	5	14	11,11,12	0.63	0	15,15,17	1.08	2 (13%)
15	NAG	T	1	15,4	14,14,15	0.38	0	17,19,21	0.93	0
15	NAG	T	2	15	14,14,15	0.55	0	17,19,21	1.99	4 (23%)
15	BMA	T	3	15	11,11,12	0.29	0	15,15,17	0.85	0
11	NAG	U	1	11,4	14,14,15	0.31	0	17,19,21	0.77	0
11	NAG	U	2	11	14,14,15	0.29	0	17,19,21	0.71	0
11	BMA	U	3	11	11,11,12	0.28	0	15,15,17	0.84	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
7	NAG	A	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	A	2	7	-	2/6/23/26	0/1/1/1
7	BMA	A	3	7	-	1/2/19/22	0/1/1/1
7	MAN	A	4	7	-	2/2/19/22	0/1/1/1
7	MAN	A	5	7	-	2/2/19/22	0/1/1/1
7	MAN	A	6	7	-	0/2/19/22	0/1/1/1
8	NAG	C	1	1,8	-	4/6/23/26	0/1/1/1
8	NAG	C	2	8	-	0/6/23/26	0/1/1/1
9	NAG	F	1	9,4	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	F	2	9,2	-	2/6/23/26	0/1/1/1
9	BMA	F	3	9	-	1/2/19/22	0/1/1/1
9	MAN	F	4	9	-	2/2/19/22	0/1/1/1
9	MAN	F	5	9	-	0/2/19/22	0/1/1/1
9	MAN	F	6	9	-	1/2/19/22	0/1/1/1
9	MAN	F	7	9	-	2/2/19/22	0/1/1/1
8	NAG	I	1	8,4	-	0/6/23/26	0/1/1/1
8	NAG	I	2	8	-	1/6/23/26	0/1/1/1
10	NAG	J	1	10,4	-	0/6/23/26	0/1/1/1
10	NAG	J	2	10	-	4/6/23/26	0/1/1/1
10	BMA	J	3	10	-	2/2/19/22	0/1/1/1
10	MAN	J	4	10	-	2/2/19/22	0/1/1/1
11	NAG	K	1	11,4	-	3/6/23/26	0/1/1/1
11	NAG	K	2	11	-	6/6/23/26	0/1/1/1
11	BMA	K	3	11	-	0/2/19/22	0/1/1/1
10	NAG	M	1	10,4	-	1/6/23/26	0/1/1/1
10	NAG	M	2	10	-	0/6/23/26	0/1/1/1
10	BMA	M	3	10	-	2/2/19/22	0/1/1/1
10	MAN	M	4	10	-	1/2/19/22	0/1/1/1
11	NAG	N	1	11,4	-	4/6/23/26	0/1/1/1
11	NAG	N	2	11	-	3/6/23/26	0/1/1/1
11	BMA	N	3	11	-	0/2/19/22	0/1/1/1
11	NAG	O	1	11,4	-	0/6/23/26	0/1/1/1
11	NAG	O	2	11	-	4/6/23/26	0/1/1/1
11	BMA	O	3	11	-	0/2/19/22	0/1/1/1
12	NAG	P	1	12,4	-	3/6/23/26	0/1/1/1
12	NAG	P	2	12	-	1/6/23/26	0/1/1/1
12	BMA	P	3	12	-	0/2/19/22	0/1/1/1
12	MAN	P	4	12	-	2/2/19/22	0/1/1/1
12	MAN	P	5	12	-	0/2/19/22	0/1/1/1
12	MAN	P	6	12	-	2/2/19/22	0/1/1/1
12	MAN	P	7	12	-	2/2/19/22	0/1/1/1
12	MAN	P	8	12	-	0/2/19/22	0/1/1/1
8	NAG	Q	1	8,4	-	3/6/23/26	0/1/1/1
8	NAG	Q	2	8	-	4/6/23/26	0/1/1/1
13	NAG	R	1	13,4	-	4/6/23/26	0/1/1/1
13	NAG	R	2	13	-	2/6/23/26	0/1/1/1
13	BMA	R	3	13	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	MAN	R	4	13	-	1/2/19/22	0/1/1/1
14	NAG	S	1	14,4	-	2/6/23/26	0/1/1/1
14	NAG	S	2	14	-	2/6/23/26	0/1/1/1
14	BMA	S	3	14	-	2/2/19/22	0/1/1/1
14	MAN	S	4	14	-	0/2/19/22	0/1/1/1
14	MAN	S	5	14	-	0/2/19/22	0/1/1/1
15	NAG	T	1	15,4	-	2/6/23/26	0/1/1/1
15	NAG	T	2	15	-	5/6/23/26	0/1/1/1
15	BMA	T	3	15	-	2/2/19/22	0/1/1/1
11	NAG	U	1	11,4	-	1/6/23/26	0/1/1/1
11	NAG	U	2	11	-	0/6/23/26	0/1/1/1
11	BMA	U	3	11	-	0/2/19/22	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	F	4	MAN	O2-C2	4.24	1.52	1.43
9	F	4	MAN	O5-C1	-3.35	1.38	1.43
9	F	4	MAN	C2-C3	3.17	1.57	1.52
7	A	4	MAN	O5-C1	-3.03	1.38	1.43
9	F	5	MAN	C1-C2	2.57	1.58	1.52

The worst 5 of 68 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	T	2	NAG	C2-N2-C7	5.67	130.98	122.90
10	J	2	NAG	C2-N2-C7	5.08	130.14	122.90
12	P	3	BMA	O3-C3-C2	-4.70	101.00	109.99
12	P	4	MAN	C1-O5-C5	4.41	118.17	112.19
12	P	5	MAN	C1-C2-C3	-4.22	104.48	109.67

There are no chirality outliers.

5 of 99 torsion outliers are listed below:

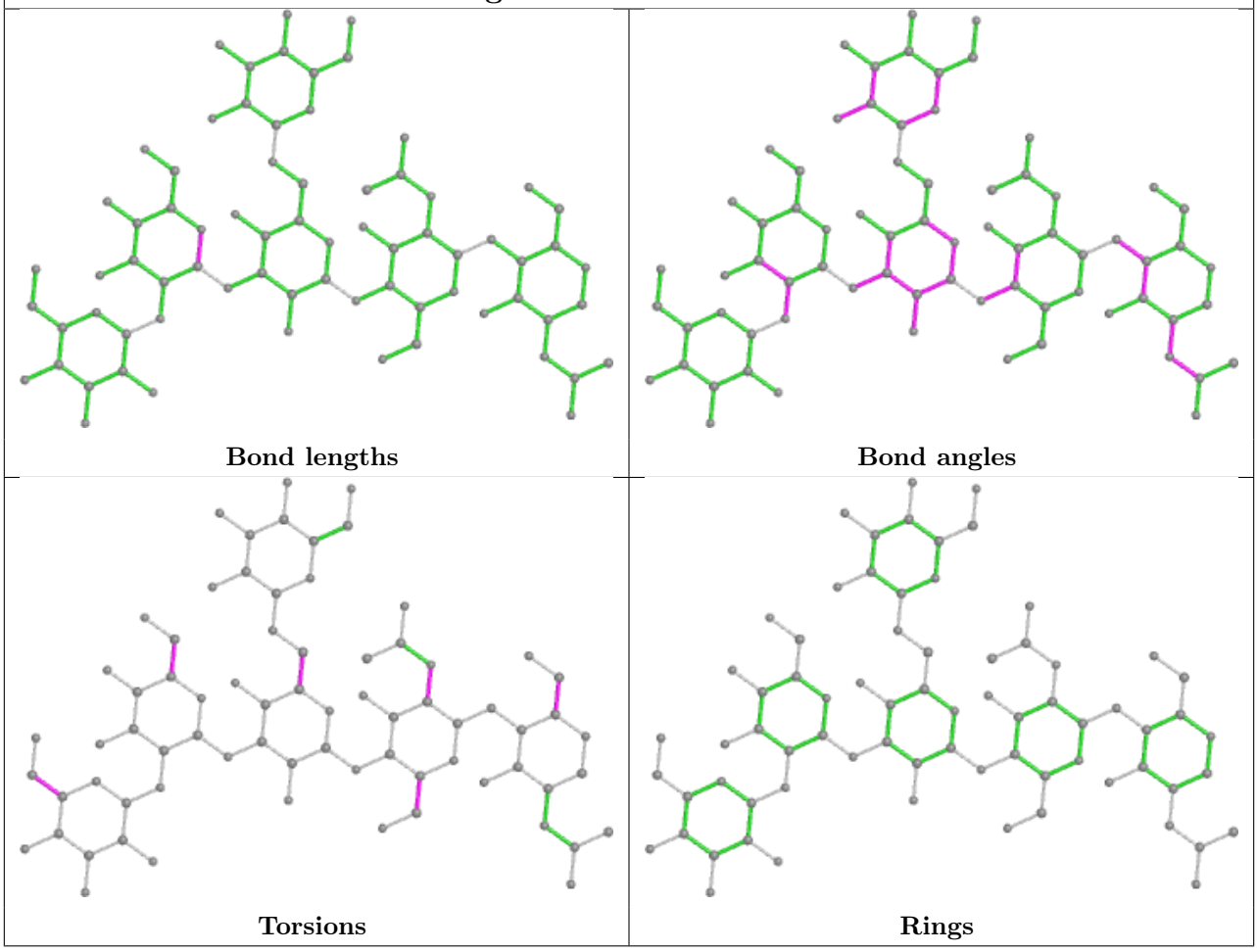
Mol	Chain	Res	Type	Atoms
8	Q	1	NAG	O7-C7-N2-C2
8	Q	2	NAG	C3-C2-N2-C7
10	J	2	NAG	C3-C2-N2-C7
10	J	2	NAG	C8-C7-N2-C2
10	J	2	NAG	O7-C7-N2-C2

There are no ring outliers.

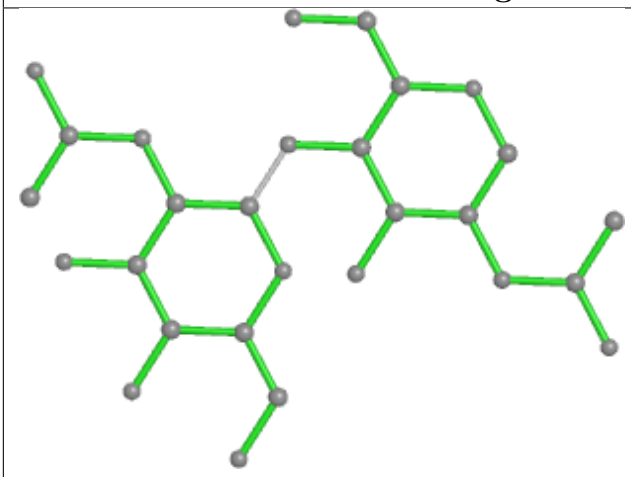
No monomer is involved in short contacts.

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

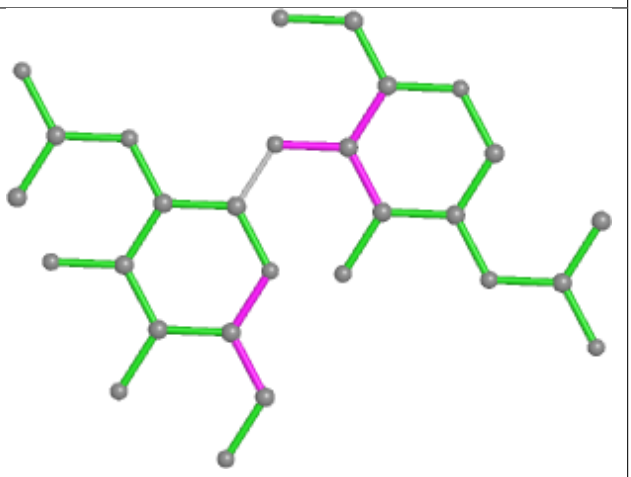
Oligosaccharide Chain A



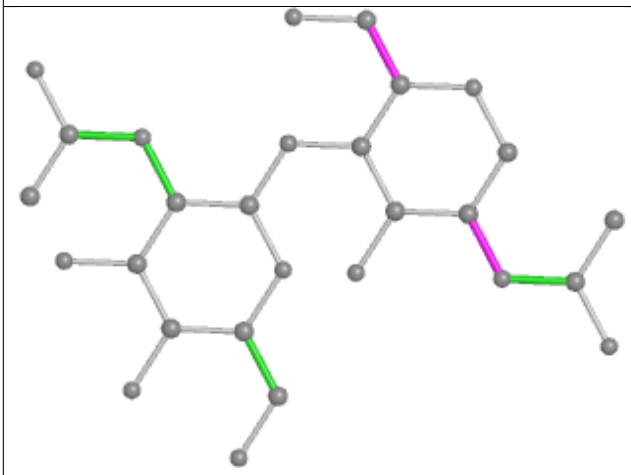
Oligosaccharide Chain C



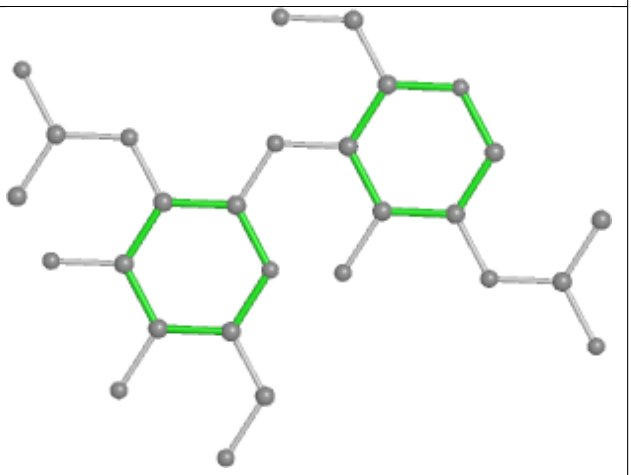
Bond lengths



Bond angles

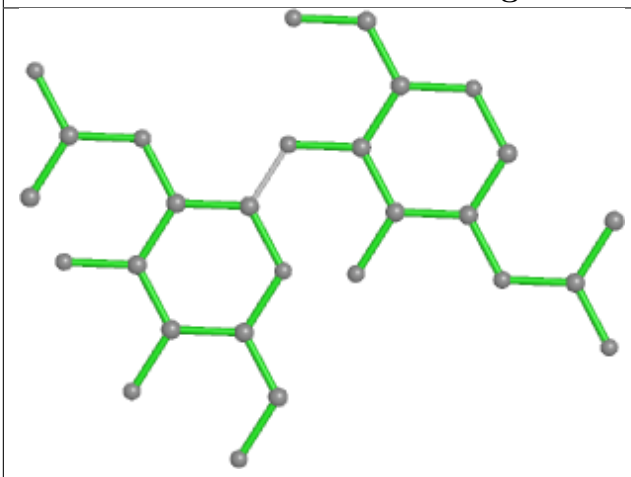


Torsions

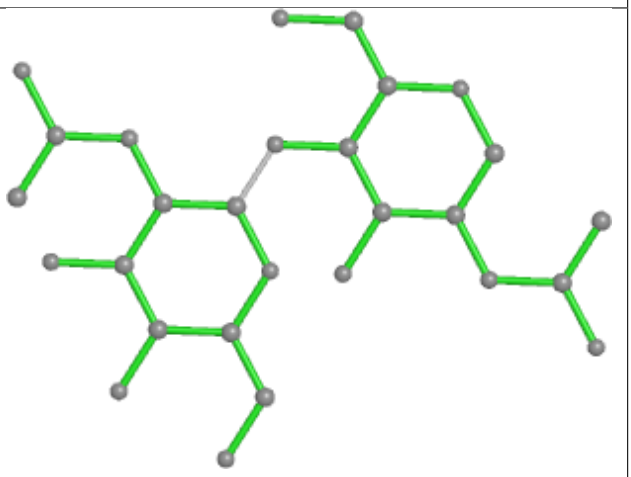


Rings

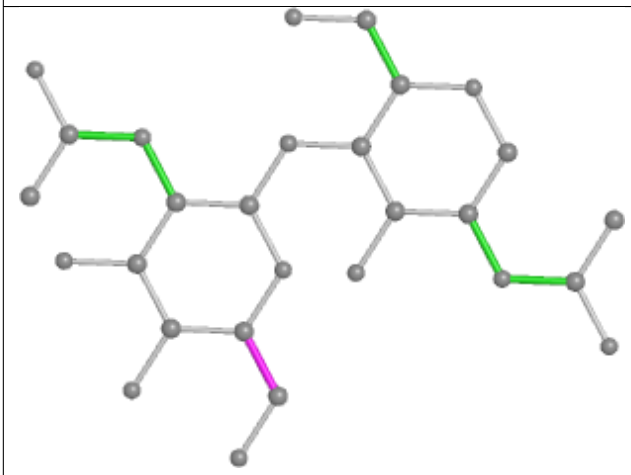
Oligosaccharide Chain I



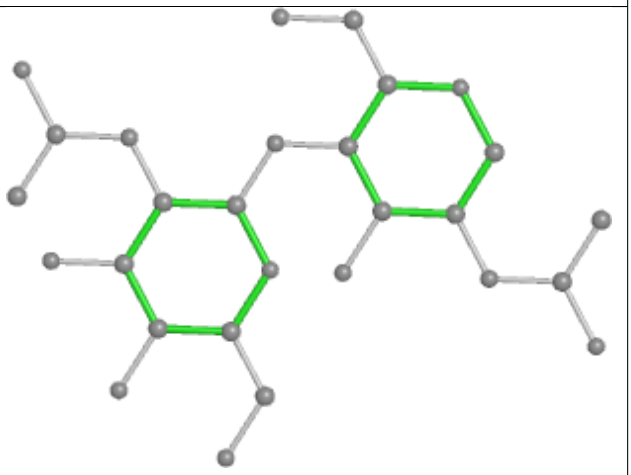
Bond lengths



Bond angles

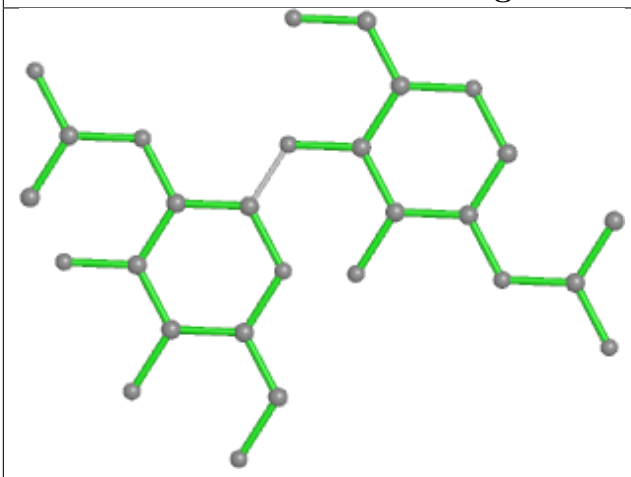


Torsions

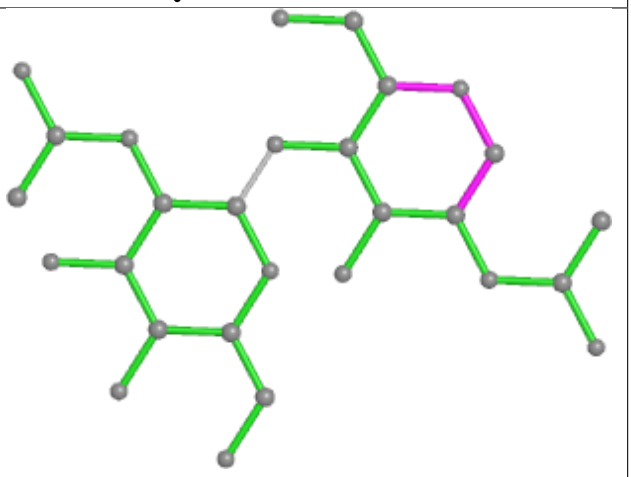


Rings

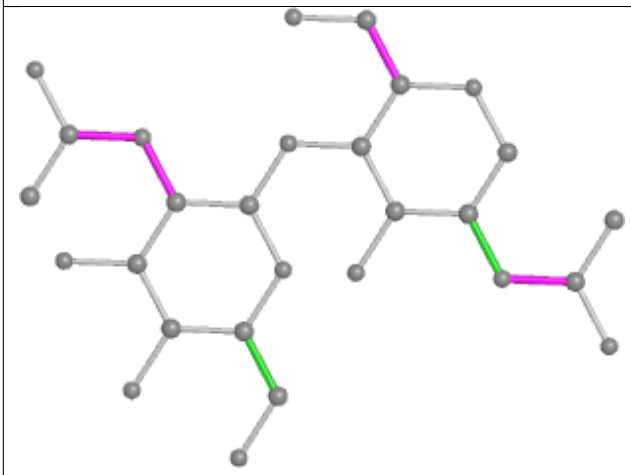
Oligosaccharide Chain Q



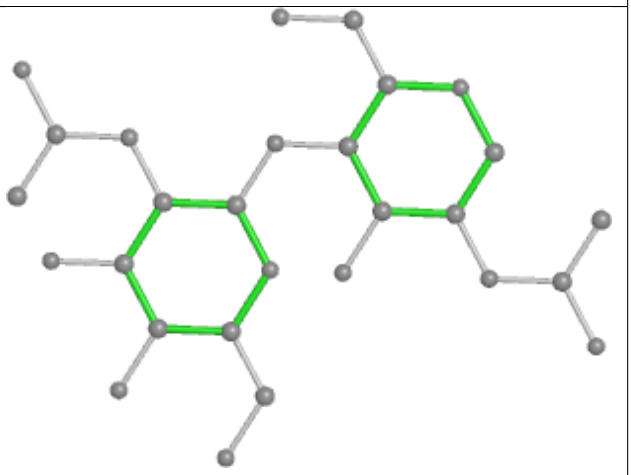
Bond lengths



Bond angles

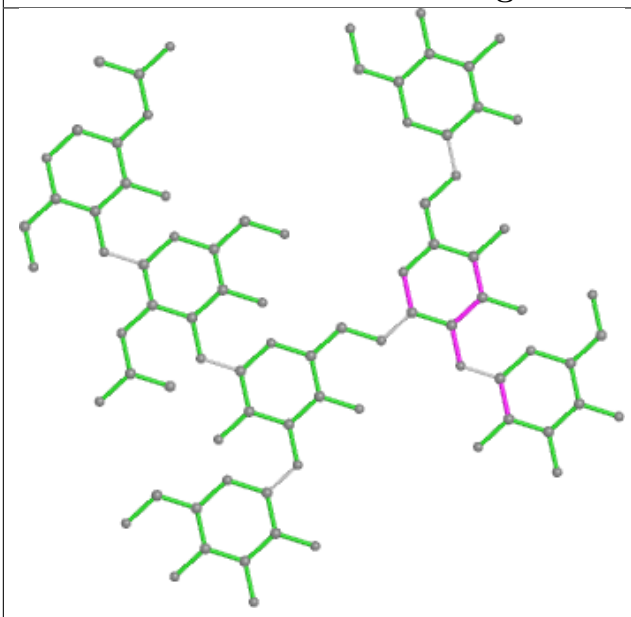


Torsions

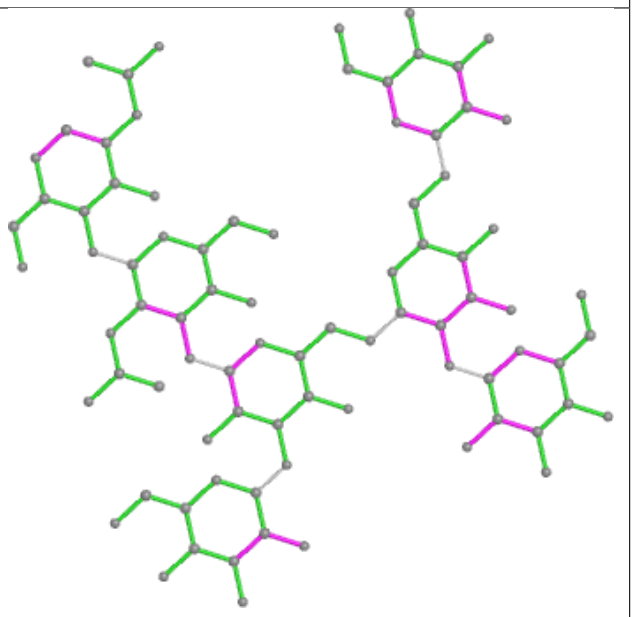


Rings

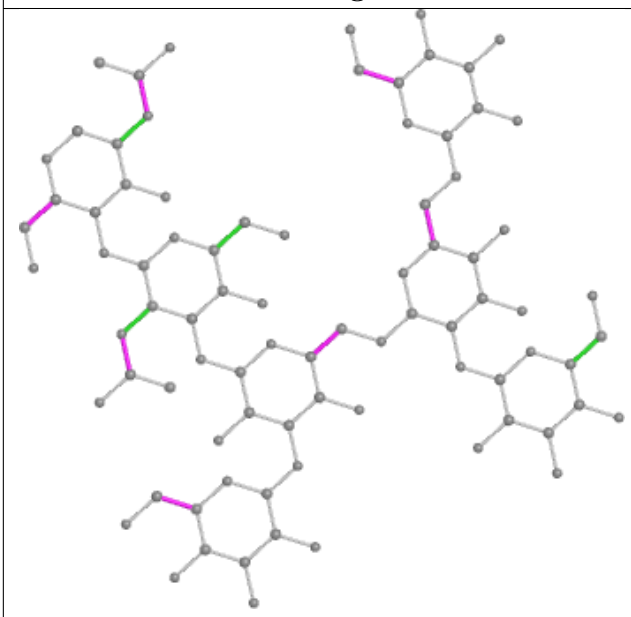
Oligosaccharide Chain F



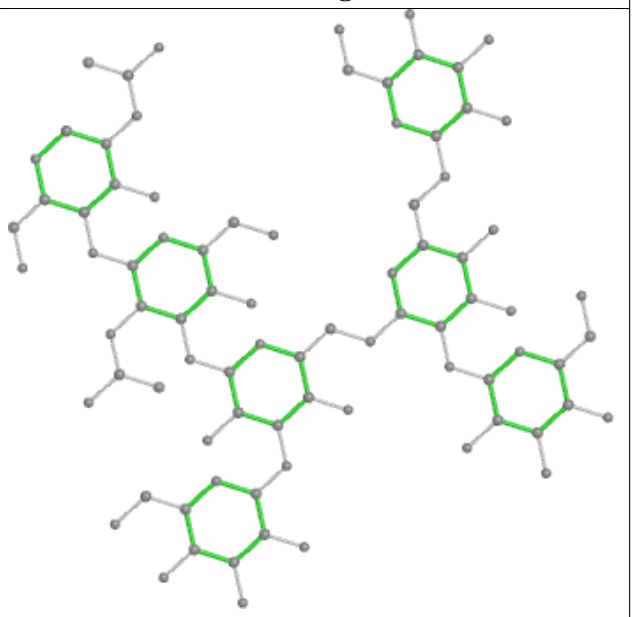
Bond lengths



Bond angles

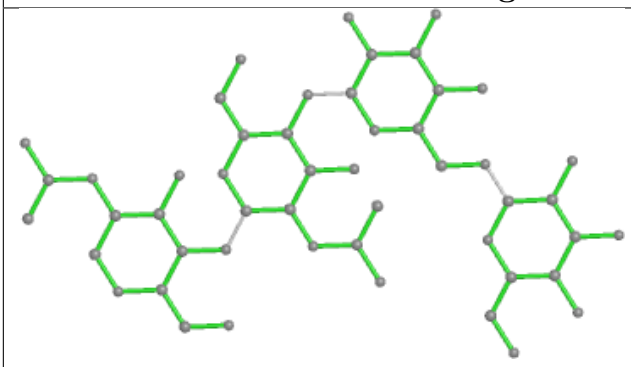


Torsions

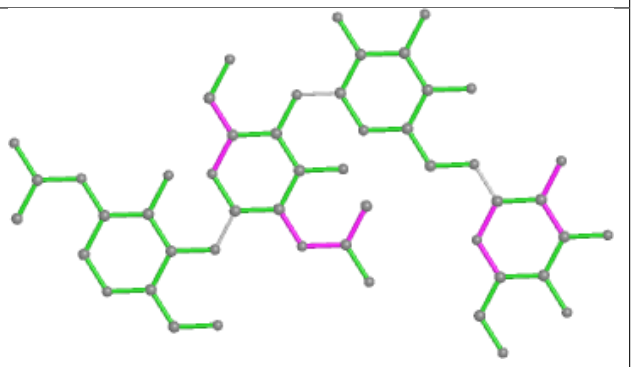


Rings

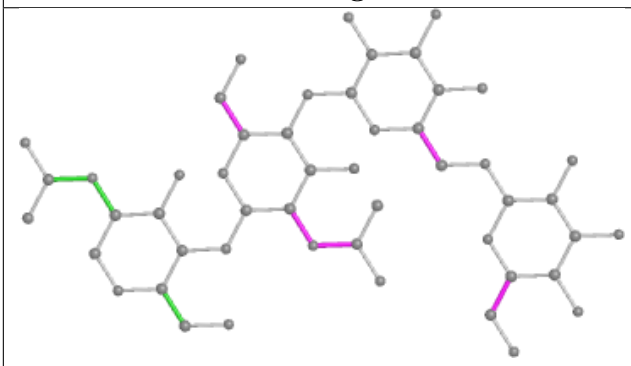
Oligosaccharide Chain J



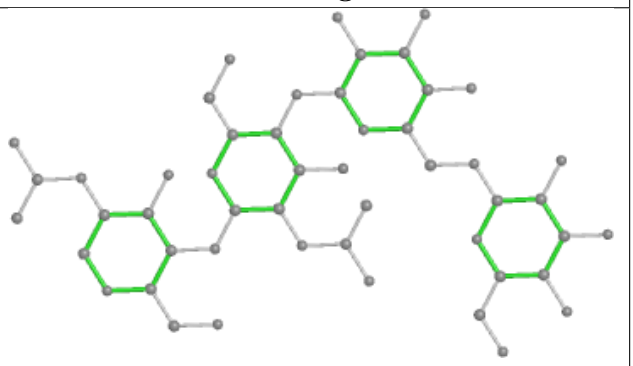
Bond lengths



Bond angles

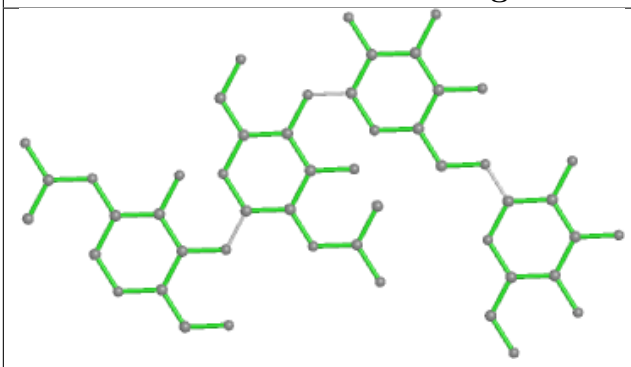


Torsions

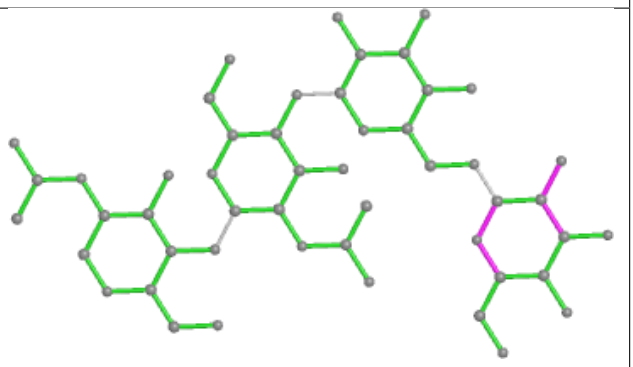


Rings

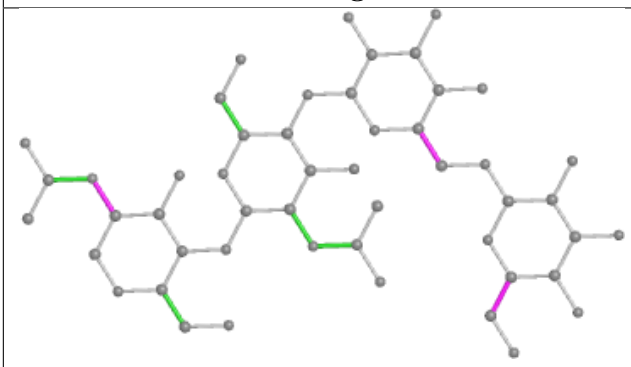
Oligosaccharide Chain M



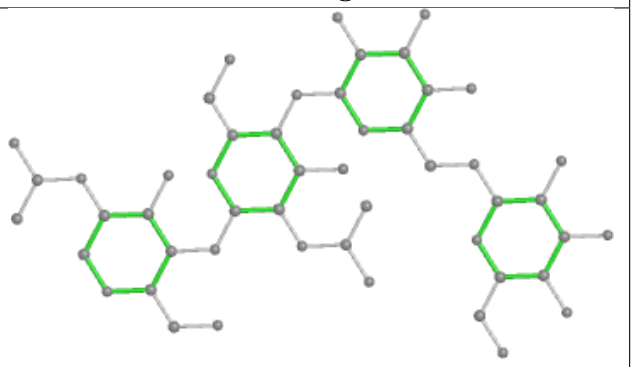
Bond lengths



Bond angles

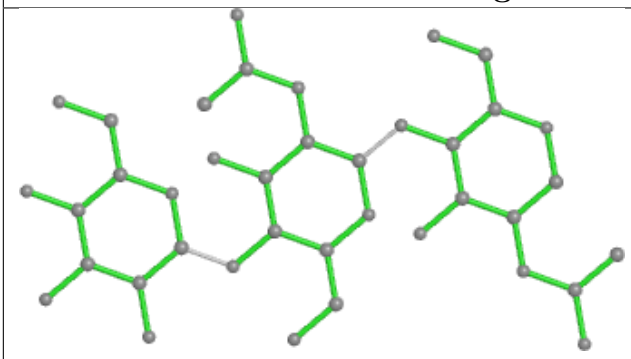


Torsions

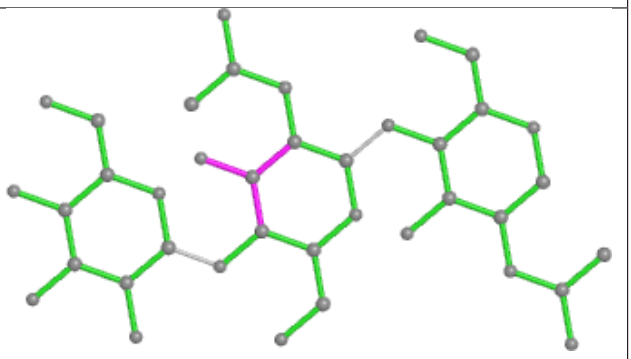


Rings

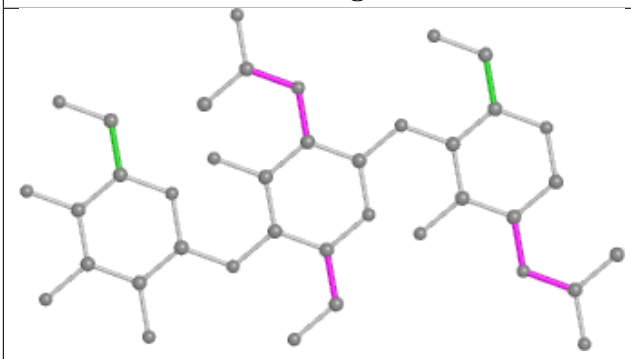
Oligosaccharide Chain K



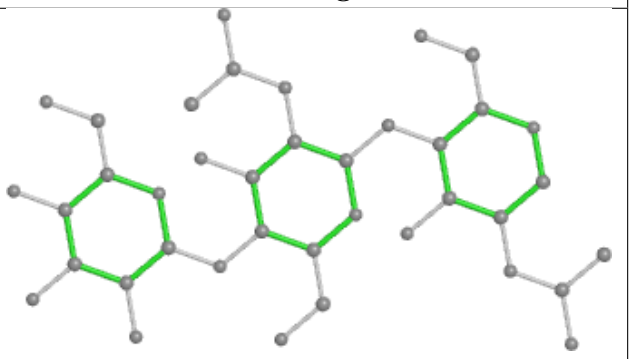
Bond lengths



Bond angles

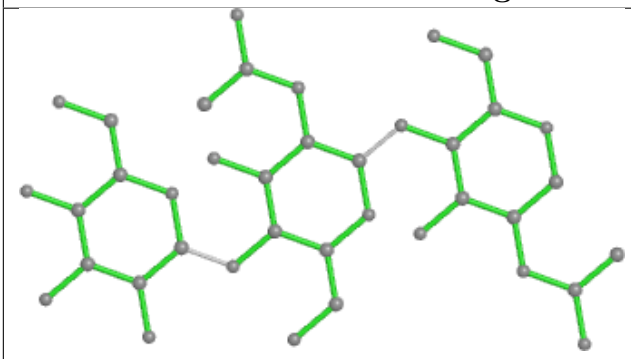


Torsions

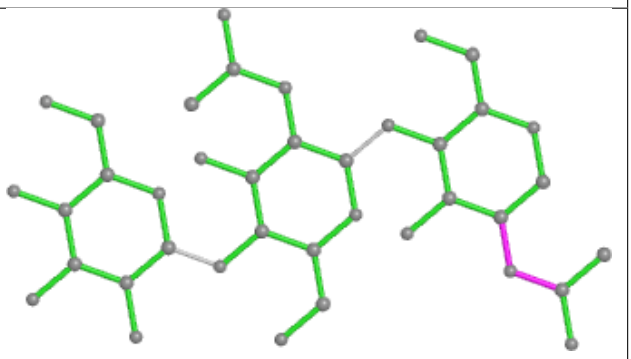


Rings

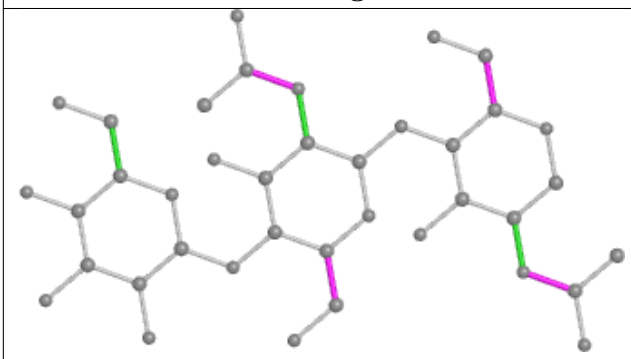
Oligosaccharide Chain N



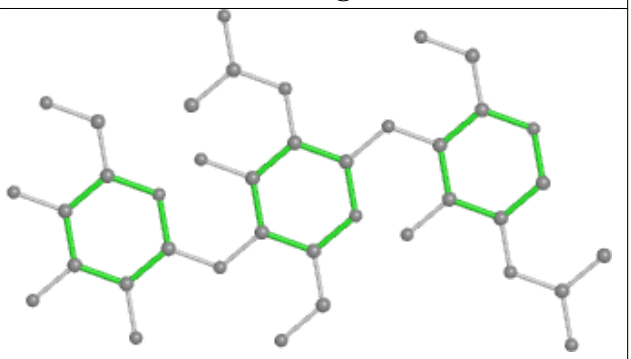
Bond lengths



Bond angles

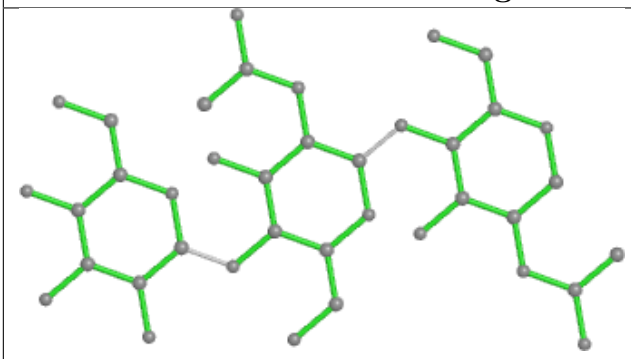


Torsions

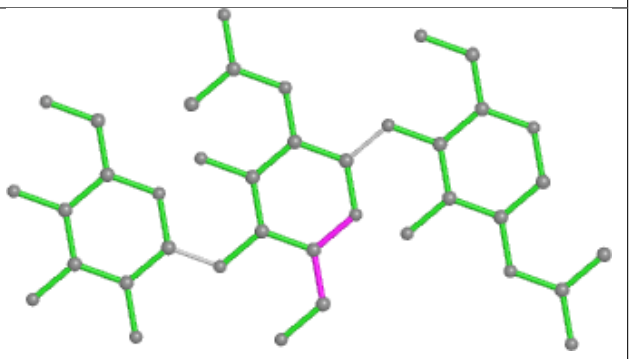


Rings

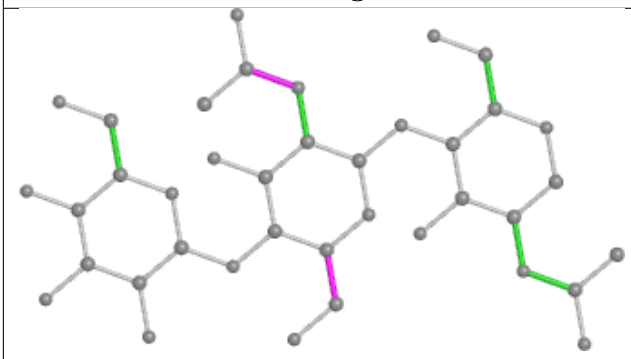
Oligosaccharide Chain O



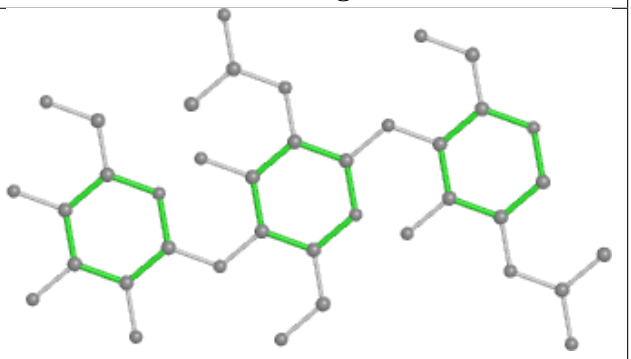
Bond lengths



Bond angles

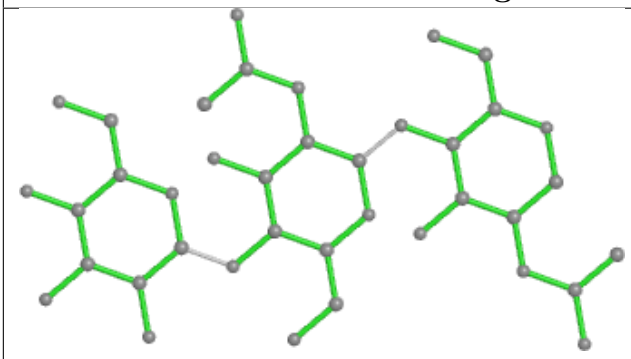


Torsions

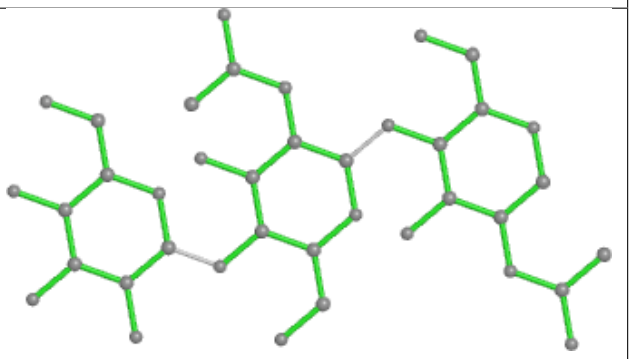


Rings

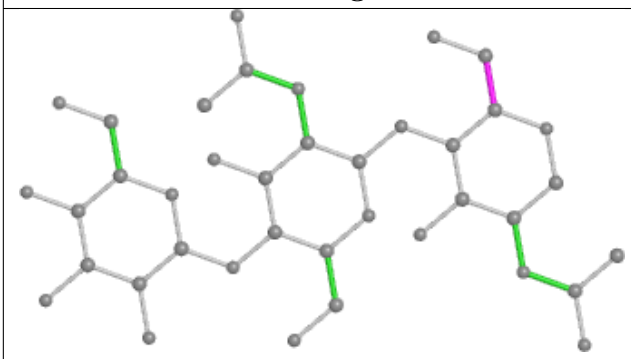
Oligosaccharide Chain U



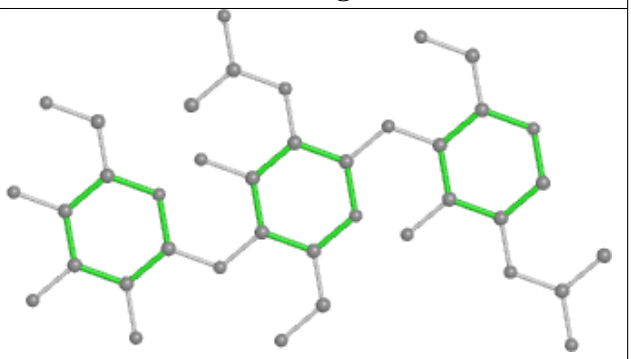
Bond lengths



Bond angles

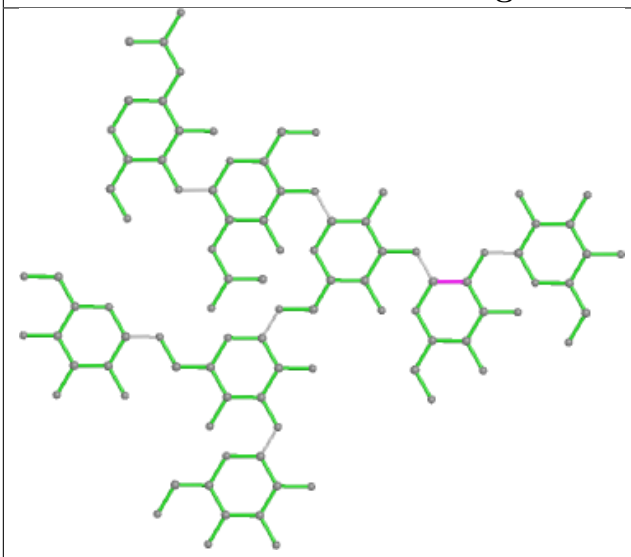


Torsions

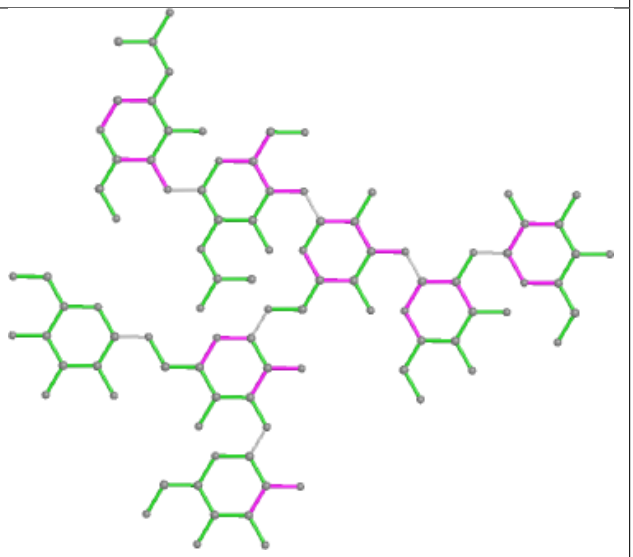


Rings

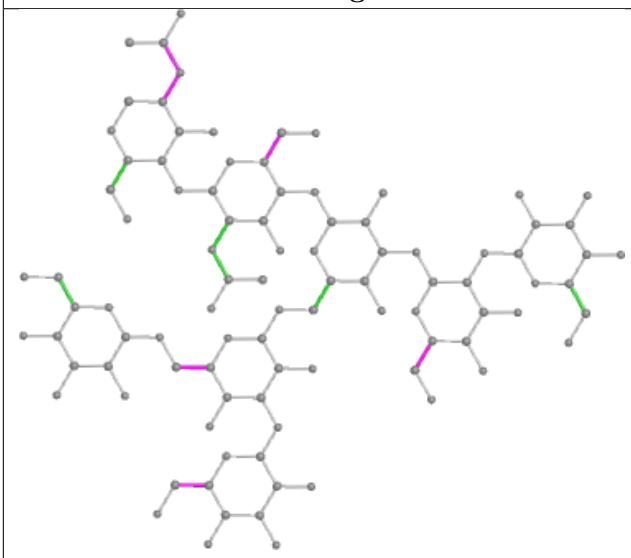
Oligosaccharide Chain P



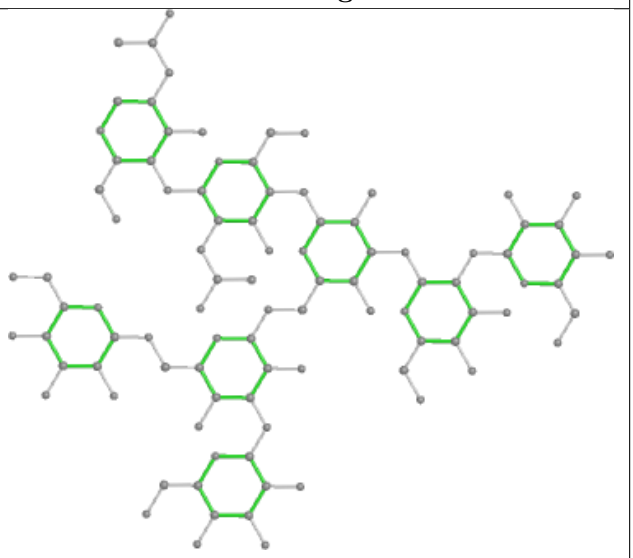
Bond lengths



Bond angles

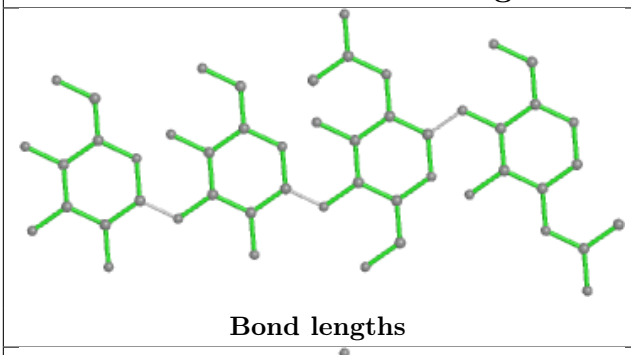


Torsions

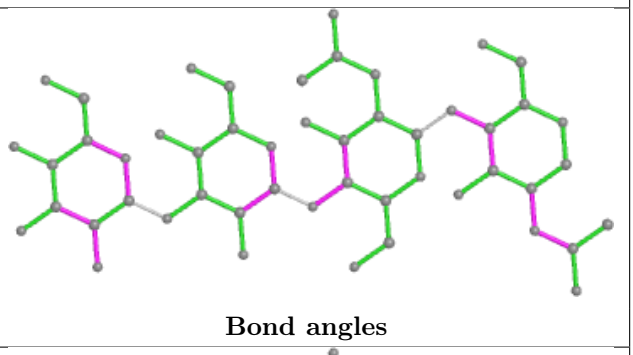


Rings

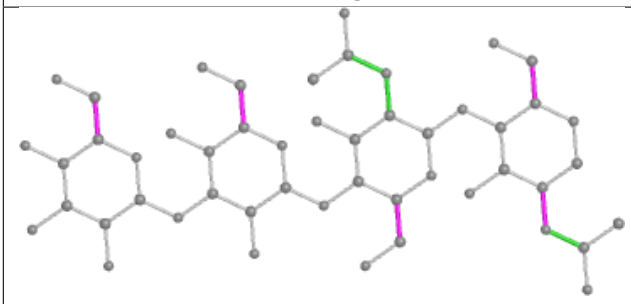
Oligosaccharide Chain R



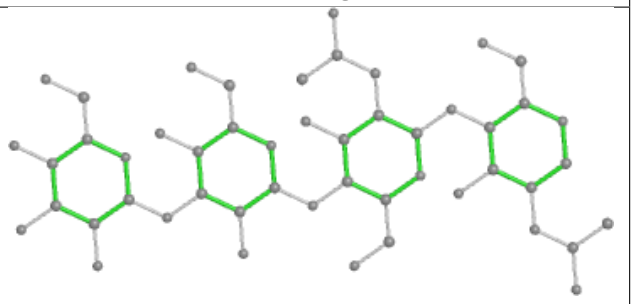
Bond lengths



Bond angles

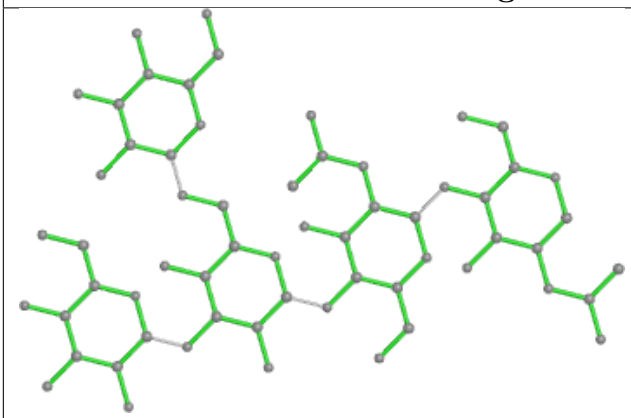


Torsions

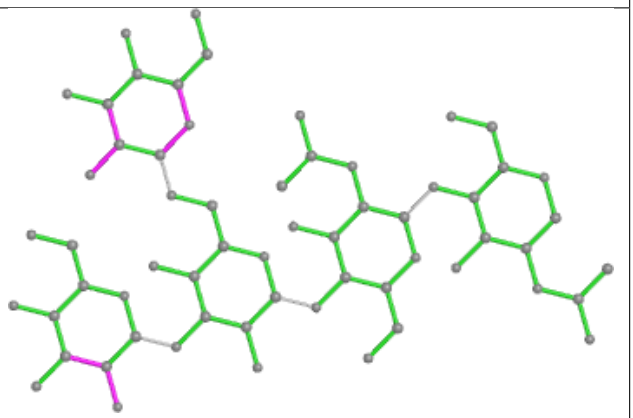


Rings

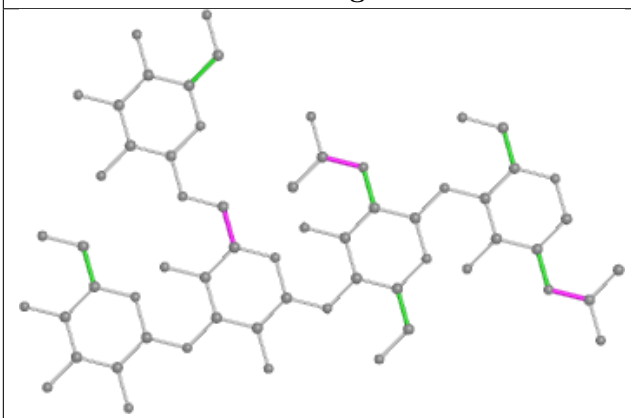
Oligosaccharide Chain S



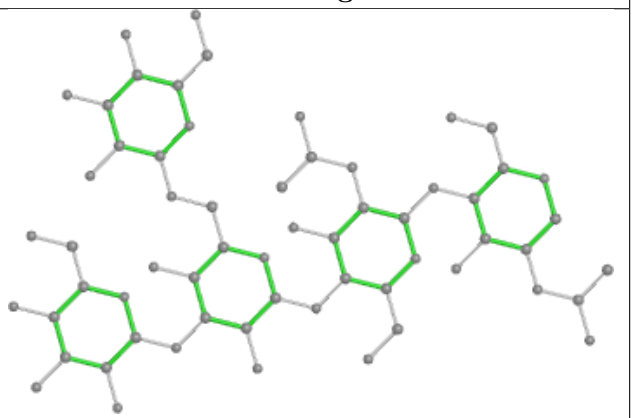
Bond lengths



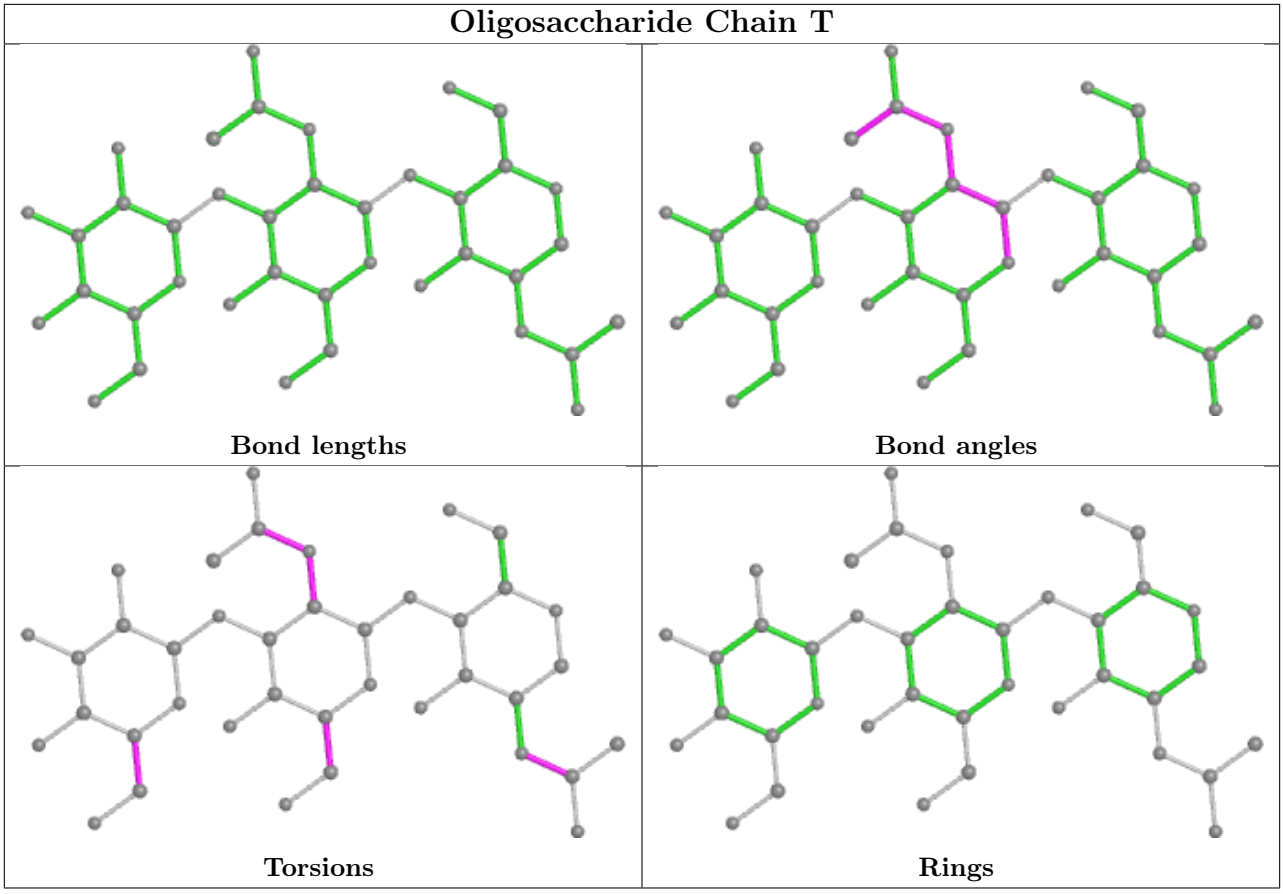
Bond angles



Torsions



Rings



4.6 Ligand geometry (i)

8 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	$\#\|Z\| > 2$
16	NAG	G	631	4	14,14,15	0.29	0	17,19,21	0.66	0
16	NAG	G	616	4	14,14,15	0.27	0	17,19,21	0.57	0
16	NAG	G	650	4	14,14,15	0.49	0	17,19,21	1.94	3 (17%)
16	NAG	G	643	4	14,14,15	0.27	0	17,19,21	0.63	0
16	NAG	G	604	4	14,14,15	0.30	0	17,19,21	0.74	0
16	NAG	B	701	1	14,14,15	0.26	0	17,19,21	0.84	1 (5%)
16	NAG	B	708	1	14,14,15	0.27	0	17,19,21	0.62	0
16	NAG	G	603	4	14,14,15	0.28	0	17,19,21	0.73	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
16	NAG	G	631	4	-	0/6/23/26	0/1/1/1
16	NAG	G	616	4	-	0/6/23/26	0/1/1/1
16	NAG	G	650	4	-	3/6/23/26	0/1/1/1
16	NAG	G	643	4	-	0/6/23/26	0/1/1/1
16	NAG	G	604	4	-	0/6/23/26	0/1/1/1
16	NAG	B	701	1	-	0/6/23/26	0/1/1/1
16	NAG	B	708	1	-	1/6/23/26	0/1/1/1
16	NAG	G	603	4	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	G	650	NAG	C2-N2-C7	6.18	131.70	122.90
16	G	650	NAG	C8-C7-N2	3.11	121.36	116.10
16	G	650	NAG	C1-O5-C5	2.21	115.19	112.19
16	B	701	NAG	O5-C5-C6	2.03	110.38	107.20

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	G	603	NAG	C8-C7-N2-C2
16	G	650	NAG	C8-C7-N2-C2
16	G	650	NAG	O7-C7-N2-C2
16	G	603	NAG	O7-C7-N2-C2
16	B	708	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers

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

5.1 Protein, DNA and RNA chains

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

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

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

5.3 Carbohydrates

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

5.4 Ligands

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

5.5 Other polymers

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