Full wwPDB X-ray Structure Validation Report ⓘ

Oct 1, 2023 – 11:58 PM EDT

PDB ID	:	6MDT
Title	:	Crystal structure of the B41 SOSIP.664 Env trimer with PGT124 and 35O22 Fabs, in P63 space group
Authors	:	Kumar, S.; Sarkar, A.; Wilson, I.A.
Deposited on	:	2018-09-05
Resolution	:	3.82 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp
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:

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 3.82 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 14 unique types of molecules in this entry. The entry contains 12314 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	136	Total	C	N	O	S	0	0	0
			1077	688	181	201	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	605	CYS	THR	conflict	UNP B3UES2

- Molecule 2 is a protein called Surface protein gp120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	455	Total	C	N	O	S	0	0	0
			3562	2237	628	671	26			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	501	CYS	ALA	conflict	UNP B3UF58

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

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

- Molecule 4 is a protein called 35O22 Fab light chain.

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

- 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-(1-3)-[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	5	Total	C	N	O	0	0	0
			61	34	2	25			
7	I	5	Total	C	N	O	0	0	0
			61	34	2	25			
7	K	5	Total	C	N	O	0	0	0
			61	34	2	25			
7	Q	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 8 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-(1-4)-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	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 9 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
9	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 10 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
10	J	3	Total	C	N	O	0	0	0
			39	22	2	15			
10	M	3	Total	C	N	O	0	0	0
			39	22	2	15			
10	O	3	Total	C	N	O	0	0	0
			39	22	2	15			
10	S	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 11 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
11	N	4	Total	C	N	O	0	0	0
			50	28	2	20			
11	P	4	Total	C	N	O	0	0	0
			50	28	2	20			

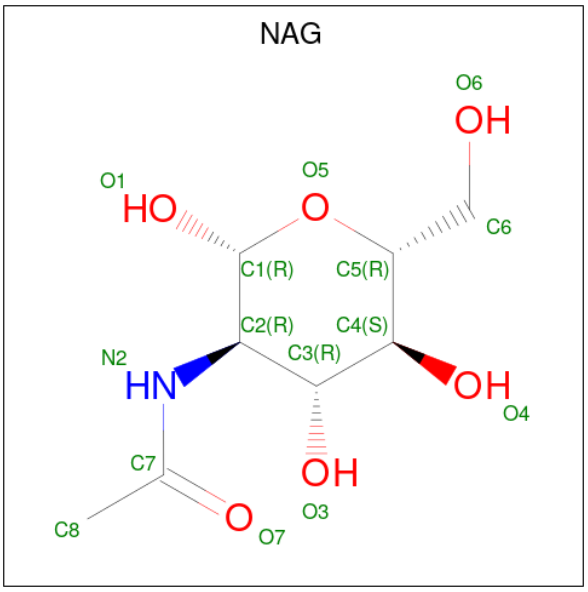
- Molecule 12 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

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

- Molecule 13 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-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
13	T	9	Total	C	N	O	0	0	0
			105	58	2	45			

- Molecule 14 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	B	1	Total C N O 14 8 1 5	0	0
14	B	1	Total C N O 14 8 1 5	0	0
14	B	1	Total C N O 14 8 1 5	0	0
14	G	1	Total C N O 14 8 1 5	0	0
14	G	1	Total C N O 14 8 1 5	0	0
14	G	1	Total C N O 14 8 1 5	0	0
14	G	1	Total C N O 14 8 1 5	0	0
14	G	1	Total C N O 14 8 1 5	0	0
14	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 63	Depositor
Cell constants a, b, c, α, β, γ	129.34Å 129.34Å 313.07Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.96 – 3.82	Depositor
% Data completeness (in resolution range)	99.9 (41.96-3.82)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.48 (at 3.76Å)	Xtriage
Refinement program	PHENIX (1.12_2829)	Depositor
R, R_{free}	0.294 , 0.311	Depositor
Wilson B-factor (Å^2)	98.9	Xtriage
Anisotropy	0.359	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.35$, $< L^2 > = 0.17$	Xtriage
Estimated twinning fraction	0.177 for h,-h-k,-l	Xtriage
Total number of atoms	12314	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 1.88% 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

62 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	7,1	14,14,15	0.58	0	17,19,21	0.65	0
7	NAG	A	2	7,3	14,14,15	0.26	0	17,19,21	1.08	1 (5%)
7	BMA	A	3	7	11,11,12	0.61	0	15,15,17	1.76	3 (20%)
7	MAN	A	4	7	11,11,12	0.56	0	15,15,17	0.88	1 (6%)
7	MAN	A	5	7	11,11,12	0.46	0	15,15,17	0.73	0
8	NAG	C	1	8,2	14,14,15	0.55	0	17,19,21	0.43	0
8	NAG	C	2	8	14,14,15	0.37	0	17,19,21	0.49	0
8	BMA	C	3	8	11,11,12	0.26	0	15,15,17	1.34	3 (20%)
8	MAN	C	4	8	11,11,12	0.92	1 (9%)	15,15,17	2.61	5 (33%)
8	MAN	C	5	8	11,11,12	0.54	0	15,15,17	1.30	2 (13%)
8	MAN	C	6	8	11,11,12	0.29	0	15,15,17	0.84	1 (6%)
8	MAN	C	7	8	11,11,12	0.25	0	15,15,17	0.97	1 (6%)
9	NAG	F	1	9,2	14,14,15	0.20	0	17,19,21	0.48	0
9	NAG	F	2	9	14,14,15	0.33	0	17,19,21	0.47	0
7	NAG	I	1	7,2	14,14,15	0.29	0	17,19,21	0.47	0
7	NAG	I	2	7	14,14,15	1.14	1 (7%)	17,19,21	1.32	1 (5%)
7	BMA	I	3	7	11,11,12	0.37	0	15,15,17	1.26	1 (6%)
7	MAN	I	4	7	11,11,12	0.44	0	15,15,17	0.87	0
7	MAN	I	5	7	11,11,12	0.36	0	15,15,17	0.77	0
10	NAG	J	1	10,2	14,14,15	0.94	1 (7%)	17,19,21	1.80	5 (29%)
10	NAG	J	2	10	14,14,15	1.02	1 (7%)	17,19,21	0.83	1 (5%)
10	BMA	J	3	10	11,11,12	0.40	0	15,15,17	0.77	0
7	NAG	K	1	7	14,14,15	1.12	1 (7%)	17,19,21	0.51	0
7	NAG	K	2	7	14,14,15	0.14	0	17,19,21	0.47	0
7	BMA	K	3	7	11,11,12	0.44	0	15,15,17	1.12	1 (6%)
7	MAN	K	4	7	11,11,12	0.58	0	15,15,17	0.93	1 (6%)
7	MAN	K	5	7	11,11,12	0.43	0	15,15,17	0.81	1 (6%)
10	NAG	M	1	10,2	14,14,15	0.72	1 (7%)	17,19,21	0.55	0
10	NAG	M	2	10	14,14,15	0.41	0	17,19,21	1.34	2 (11%)
10	BMA	M	3	10	11,11,12	0.38	0	15,15,17	0.82	0
11	NAG	N	1	11,2	14,14,15	0.29	0	17,19,21	0.53	0
11	NAG	N	2	11	14,14,15	0.38	0	17,19,21	0.55	0
11	BMA	N	3	11	11,11,12	0.72	0	15,15,17	1.20	0
11	MAN	N	4	11	11,11,12	0.81	0	15,15,17	1.38	3 (20%)
10	NAG	O	1	10,2	14,14,15	0.43	0	17,19,21	0.55	0
10	NAG	O	2	10	14,14,15	0.53	0	17,19,21	0.47	0
10	BMA	O	3	10	11,11,12	0.64	0	15,15,17	0.79	0
11	NAG	P	1	11,2	14,14,15	0.34	0	17,19,21	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	NAG	P	2	11	14,14,15	0.53	0	17,19,21	0.64	0
11	BMA	P	3	11	11,11,12	0.25	0	15,15,17	0.76	0
11	MAN	P	4	11	11,11,12	0.24	0	15,15,17	0.57	0
7	NAG	Q	1	7,2	14,14,15	0.31	0	17,19,21	0.48	0
7	NAG	Q	2	7,2	14,14,15	0.54	0	17,19,21	0.93	1 (5%)
7	BMA	Q	3	7	11,11,12	0.56	0	15,15,17	1.11	1 (6%)
7	MAN	Q	4	7	11,11,12	0.31	0	15,15,17	0.88	1 (6%)
7	MAN	Q	5	7	11,11,12	0.32	0	15,15,17	0.87	1 (6%)
12	NAG	R	1	12	14,14,15	0.64	1 (7%)	17,19,21	0.58	0
12	NAG	R	2	12	14,14,15	0.53	0	17,19,21	1.42	2 (11%)
12	BMA	R	3	12	11,11,12	0.32	0	15,15,17	0.75	0
12	MAN	R	4	12	11,11,12	0.61	0	15,15,17	0.66	0
10	NAG	S	1	10,2	14,14,15	0.33	0	17,19,21	0.51	0
10	NAG	S	2	10	14,14,15	0.37	0	17,19,21	0.60	0
10	BMA	S	3	10	11,11,12	0.41	0	15,15,17	0.85	1 (6%)
13	NAG	T	1	13	14,14,15	0.49	0	17,19,21	0.59	0
13	NAG	T	2	13	14,14,15	0.91	1 (7%)	17,19,21	0.95	1 (5%)
13	BMA	T	3	13	11,11,12	0.85	0	15,15,17	2.89	5 (33%)
13	MAN	T	4	13	11,11,12	0.36	0	15,15,17	1.70	3 (20%)
13	MAN	T	5	6,13	11,11,12	0.49	0	15,15,17	1.76	3 (20%)
13	MAN	T	6	13	11,11,12	0.24	0	15,15,17	0.75	0
13	MAN	T	7	13	11,11,12	0.32	0	15,15,17	0.92	0
13	MAN	T	8	13	11,11,12	0.36	0	15,15,17	0.69	0
13	MAN	T	9	13	11,11,12	0.43	0	15,15,17	0.85	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	7,1	-	0/6/23/26	0/1/1/1
7	NAG	A	2	7,3	-	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	-	0/2/19/22	0/1/1/1
7	MAN	A	5	7	-	2/2/19/22	0/1/1/1
8	NAG	C	1	8,2	-	2/6/23/26	0/1/1/1
8	NAG	C	2	8	-	0/6/23/26	0/1/1/1
8	BMA	C	3	8	-	2/2/19/22	0/1/1/1

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	NAG	R	1	12	-	2/6/23/26	0/1/1/1
12	NAG	R	2	12	-	5/6/23/26	0/1/1/1
12	BMA	R	3	12	-	0/2/19/22	0/1/1/1
12	MAN	R	4	12	-	1/2/19/22	0/1/1/1
10	NAG	S	1	10,2	-	2/6/23/26	0/1/1/1
10	NAG	S	2	10	-	0/6/23/26	0/1/1/1
10	BMA	S	3	10	-	0/2/19/22	0/1/1/1
13	NAG	T	1	13	-	2/6/23/26	0/1/1/1
13	NAG	T	2	13	-	1/6/23/26	0/1/1/1
13	BMA	T	3	13	-	1/2/19/22	0/1/1/1
13	MAN	T	4	13	-	2/2/19/22	0/1/1/1
13	MAN	T	5	6,13	-	0/2/19/22	0/1/1/1
13	MAN	T	6	13	-	0/2/19/22	0/1/1/1
13	MAN	T	7	13	-	2/2/19/22	0/1/1/1
13	MAN	T	8	13	-	2/2/19/22	0/1/1/1
13	MAN	T	9	13	-	0/2/19/22	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	K	1	NAG	O5-C1	-4.08	1.37	1.43
7	I	2	NAG	C1-C2	3.89	1.58	1.52
10	J	2	NAG	O5-C1	-3.60	1.38	1.43
10	J	1	NAG	O5-C1	-2.71	1.39	1.43
13	T	2	NAG	O5-C1	-2.56	1.39	1.43
8	C	4	MAN	O2-C2	2.24	1.48	1.43
12	R	1	NAG	C1-C2	2.11	1.55	1.52
10	M	1	NAG	O5-C1	-2.10	1.40	1.43

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	T	3	BMA	O5-C1-C2	7.65	122.57	110.77
8	C	4	MAN	C1-C2-C3	-6.21	102.04	109.67
13	T	3	BMA	O3-C3-C2	-5.11	100.21	109.99
8	C	4	MAN	O2-C2-C3	4.97	120.10	110.14
10	J	1	NAG	C1-O5-C5	-4.47	106.13	112.19
12	R	2	NAG	C2-N2-C7	4.46	129.26	122.90
13	T	4	MAN	C1-C2-C3	4.21	114.84	109.67
10	M	2	NAG	C1-O5-C5	4.10	117.75	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	I	2	NAG	C2-N2-C7	4.03	128.65	122.90
13	T	5	MAN	O2-C2-C1	-3.99	100.99	109.15
7	A	3	BMA	O5-C1-C2	-3.83	104.86	110.77
8	C	4	MAN	O2-C2-C1	3.59	116.50	109.15
13	T	3	BMA	O5-C5-C4	-3.57	102.14	110.83
7	I	3	BMA	O5-C5-C6	3.56	112.78	107.20
13	T	5	MAN	O3-C3-C2	-3.30	103.67	109.99
8	C	4	MAN	C6-C5-C4	-3.24	105.42	113.00
10	J	1	NAG	C2-N2-C7	3.08	127.29	122.90
7	K	3	BMA	O3-C3-C2	-3.03	104.19	109.99
13	T	5	MAN	O5-C1-C2	-2.99	106.16	110.77
7	A	3	BMA	C1-O5-C5	-2.89	108.27	112.19
7	Q	2	NAG	C2-N2-C7	2.81	126.90	122.90
8	C	7	MAN	O5-C1-C2	-2.79	106.46	110.77
13	T	3	BMA	C1-O5-C5	-2.74	108.47	112.19
13	T	4	MAN	O5-C1-C2	-2.70	106.61	110.77
13	T	3	BMA	O2-C2-C1	2.60	114.47	109.15
8	C	3	BMA	O5-C1-C2	-2.57	106.80	110.77
11	N	4	MAN	O5-C5-C6	2.53	111.18	107.20
11	N	4	MAN	C1-C2-C3	2.53	112.77	109.67
8	C	5	MAN	O5-C1-C2	-2.52	106.88	110.77
10	J	1	NAG	O4-C4-C5	-2.50	103.10	109.30
7	K	5	MAN	O5-C1-C2	-2.49	106.93	110.77
12	R	2	NAG	C1-C2-N2	2.45	114.68	110.49
7	A	2	NAG	C2-N2-C7	2.44	126.38	122.90
10	J	2	NAG	C1-O5-C5	2.38	115.42	112.19
7	Q	3	BMA	O5-C5-C6	-2.36	103.51	107.20
7	Q	5	MAN	O5-C1-C2	-2.31	107.21	110.77
13	T	4	MAN	O2-C2-C1	-2.28	104.48	109.15
8	C	6	MAN	O5-C1-C2	-2.28	107.25	110.77
10	M	2	NAG	C2-N2-C7	2.26	126.12	122.90
10	S	3	BMA	O5-C5-C6	2.24	110.72	107.20
8	C	3	BMA	C1-O5-C5	-2.23	109.17	112.19
10	J	1	NAG	C1-C2-N2	2.23	114.29	110.49
8	C	5	MAN	O5-C5-C6	2.22	110.68	107.20
7	A	3	BMA	C1-C2-C3	-2.21	106.95	109.67
13	T	2	NAG	C3-C4-C5	-2.19	106.33	110.24
11	N	4	MAN	C1-O5-C5	2.16	115.12	112.19
7	K	4	MAN	O5-C1-C2	-2.14	107.47	110.77
8	C	3	BMA	C3-C4-C5	-2.12	106.47	110.24
7	Q	4	MAN	O5-C1-C2	-2.08	107.56	110.77
8	C	4	MAN	O4-C4-C5	-2.05	104.20	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	J	1	NAG	C3-C4-C5	2.05	113.90	110.24
7	A	4	MAN	O5-C1-C2	-2.05	107.61	110.77

There are no chirality outliers.

All (88) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	J	1	NAG	C4-C5-C6-O6
11	P	1	NAG	O5-C5-C6-O6
7	K	3	BMA	C4-C5-C6-O6
8	C	4	MAN	C4-C5-C6-O6
7	Q	3	BMA	O5-C5-C6-O6
8	C	1	NAG	O5-C5-C6-O6
8	C	7	MAN	O5-C5-C6-O6
10	S	1	NAG	O5-C5-C6-O6
13	T	4	MAN	O5-C5-C6-O6
8	C	6	MAN	O5-C5-C6-O6
10	J	1	NAG	O5-C5-C6-O6
10	M	1	NAG	O5-C5-C6-O6
11	P	2	NAG	O5-C5-C6-O6
13	T	8	MAN	O5-C5-C6-O6
7	Q	3	BMA	C4-C5-C6-O6
8	C	4	MAN	O5-C5-C6-O6
7	I	3	BMA	O5-C5-C6-O6
7	I	5	MAN	O5-C5-C6-O6
7	K	3	BMA	O5-C5-C6-O6
10	J	1	NAG	C1-C2-N2-C7
10	O	2	NAG	C1-C2-N2-C7
11	P	1	NAG	C1-C2-N2-C7
8	C	1	NAG	C4-C5-C6-O6
11	P	1	NAG	C4-C5-C6-O6
10	M	1	NAG	C4-C5-C6-O6
13	T	8	MAN	C4-C5-C6-O6
7	I	2	NAG	C8-C7-N2-C2
7	I	2	NAG	O7-C7-N2-C2
7	Q	1	NAG	C8-C7-N2-C2
7	Q	1	NAG	O7-C7-N2-C2
10	M	1	NAG	C8-C7-N2-C2
10	M	1	NAG	O7-C7-N2-C2
11	N	2	NAG	C8-C7-N2-C2
11	N	2	NAG	O7-C7-N2-C2
12	R	1	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
12	R	1	NAG	O7-C7-N2-C2
12	R	2	NAG	C8-C7-N2-C2
12	R	2	NAG	O7-C7-N2-C2
13	T	1	NAG	C8-C7-N2-C2
13	T	1	NAG	O7-C7-N2-C2
8	C	5	MAN	O5-C5-C6-O6
11	N	4	MAN	O5-C5-C6-O6
11	N	2	NAG	C4-C5-C6-O6
7	I	3	BMA	C4-C5-C6-O6
7	A	2	NAG	C1-C2-N2-C7
11	N	1	NAG	C4-C5-C6-O6
10	J	2	NAG	O5-C5-C6-O6
9	F	2	NAG	C4-C5-C6-O6
11	P	2	NAG	C4-C5-C6-O6
8	C	5	MAN	C4-C5-C6-O6
10	S	1	NAG	C4-C5-C6-O6
7	Q	1	NAG	C4-C5-C6-O6
11	N	2	NAG	O5-C5-C6-O6
8	C	6	MAN	C4-C5-C6-O6
12	R	2	NAG	C4-C5-C6-O6
13	T	7	MAN	O5-C5-C6-O6
7	A	2	NAG	O5-C5-C6-O6
9	F	2	NAG	O5-C5-C6-O6
8	C	7	MAN	C4-C5-C6-O6
8	C	3	BMA	C4-C5-C6-O6
13	T	2	NAG	O5-C5-C6-O6
11	N	1	NAG	O5-C5-C6-O6
7	I	5	MAN	C4-C5-C6-O6
7	A	3	BMA	O5-C5-C6-O6
11	P	3	BMA	O5-C5-C6-O6
7	I	2	NAG	O5-C5-C6-O6
7	Q	1	NAG	O5-C5-C6-O6
11	N	3	BMA	O5-C5-C6-O6
10	O	2	NAG	O5-C5-C6-O6
10	O	3	BMA	O5-C5-C6-O6
10	O	1	NAG	O5-C5-C6-O6
10	M	2	NAG	O5-C5-C6-O6
12	R	4	MAN	O5-C5-C6-O6
12	R	2	NAG	O5-C5-C6-O6
10	M	2	NAG	C3-C2-N2-C7
7	I	1	NAG	C4-C5-C6-O6
10	J	2	NAG	C4-C5-C6-O6

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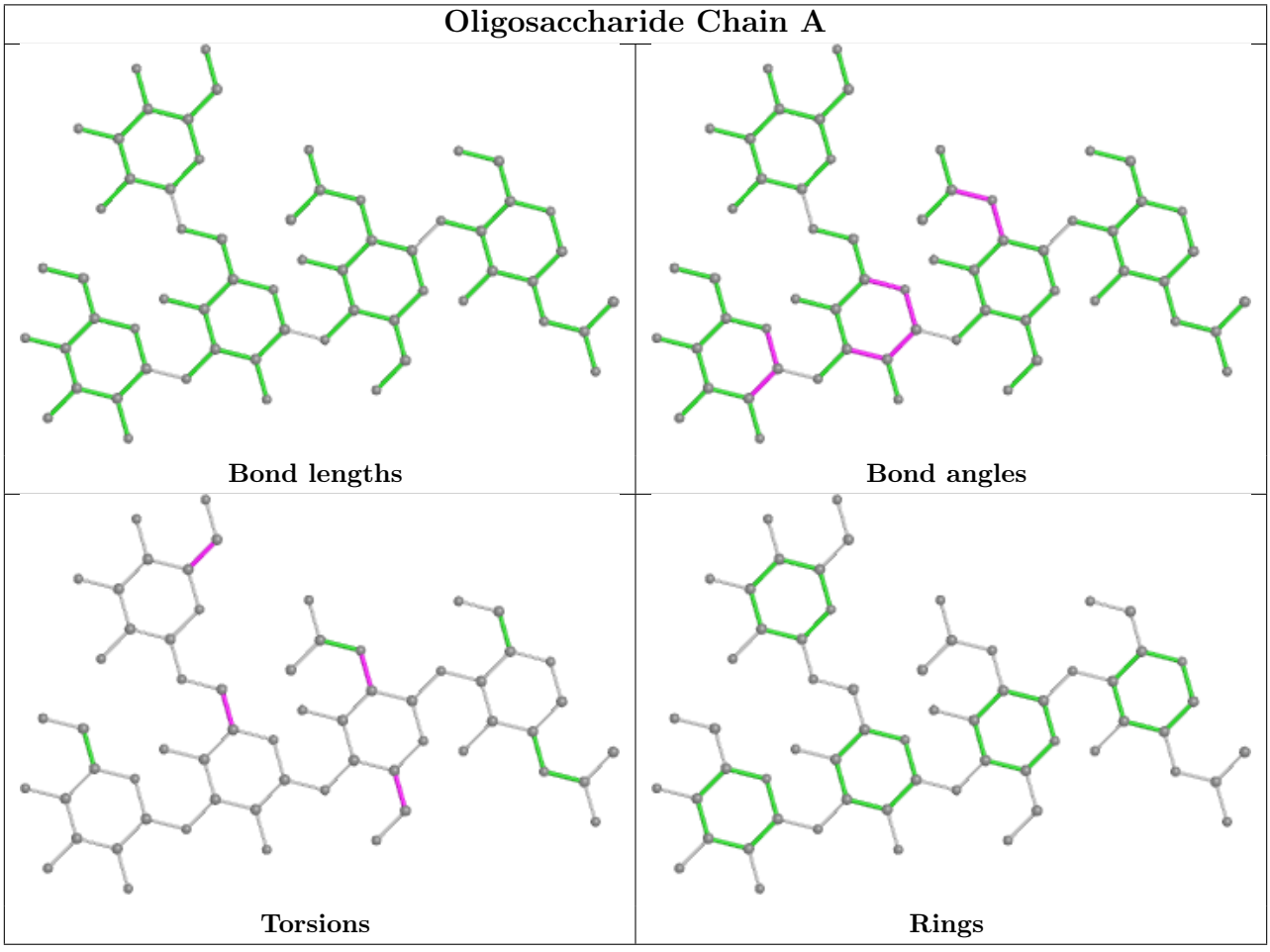
Mol	Chain	Res	Type	Atoms
13	T	7	MAN	C4-C5-C6-O6
13	T	4	MAN	C4-C5-C6-O6
13	T	3	BMA	C4-C5-C6-O6
8	C	3	BMA	O5-C5-C6-O6
7	K	1	NAG	C1-C2-N2-C7
7	I	2	NAG	C3-C2-N2-C7
10	O	2	NAG	C3-C2-N2-C7
11	P	1	NAG	C3-C2-N2-C7
7	A	5	MAN	C4-C5-C6-O6
12	R	2	NAG	C3-C2-N2-C7
7	A	5	MAN	O5-C5-C6-O6

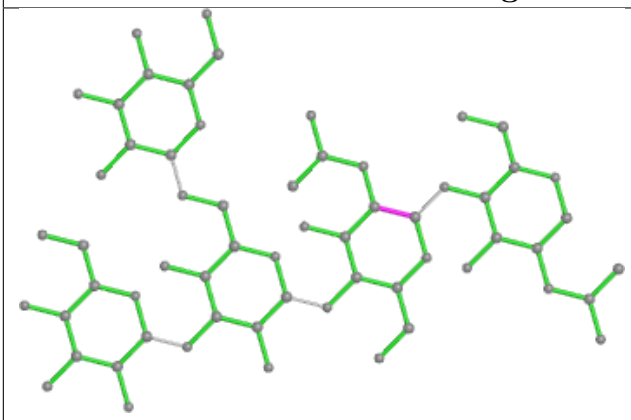
There are no ring outliers.

No monomer is involved in short contacts.

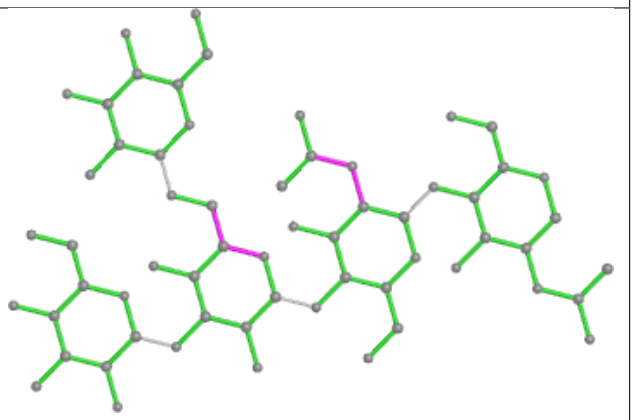
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



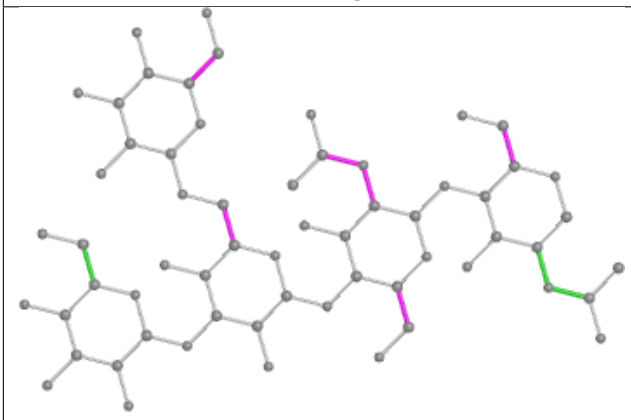
Oligosaccharide Chain I



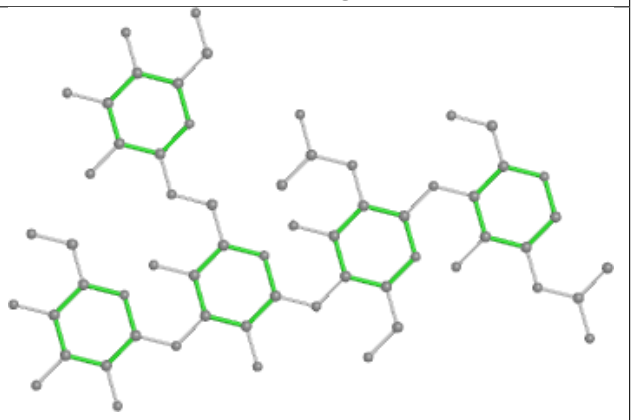
Bond lengths



Bond angles

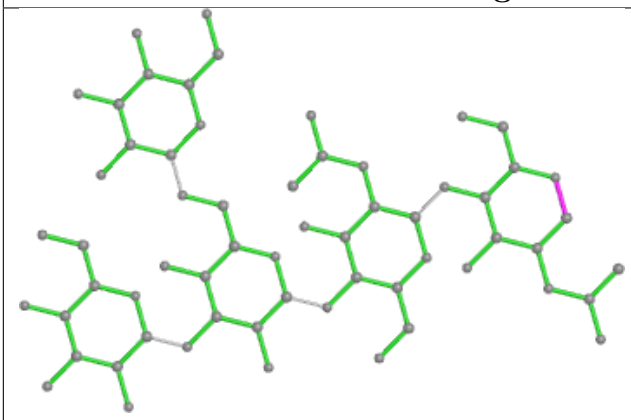


Torsions

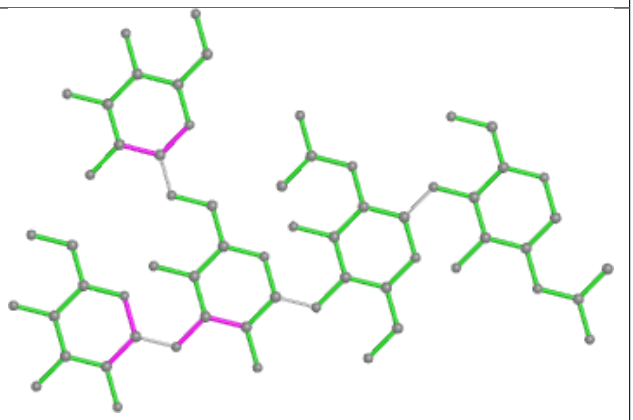


Rings

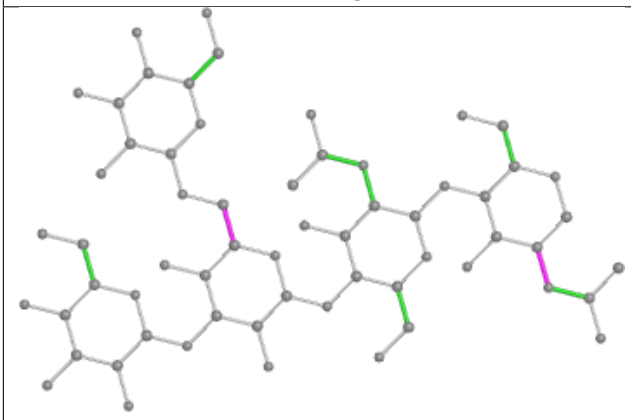
Oligosaccharide Chain K



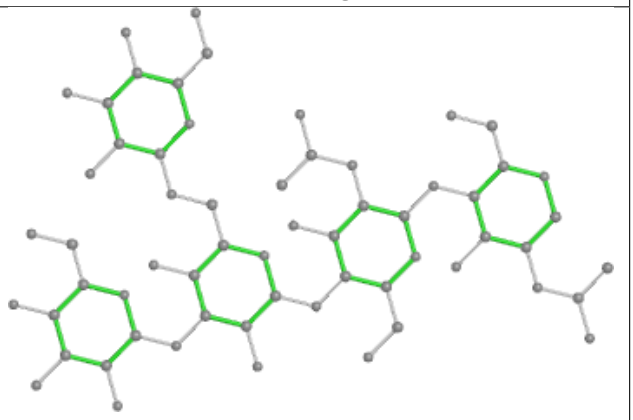
Bond lengths



Bond angles

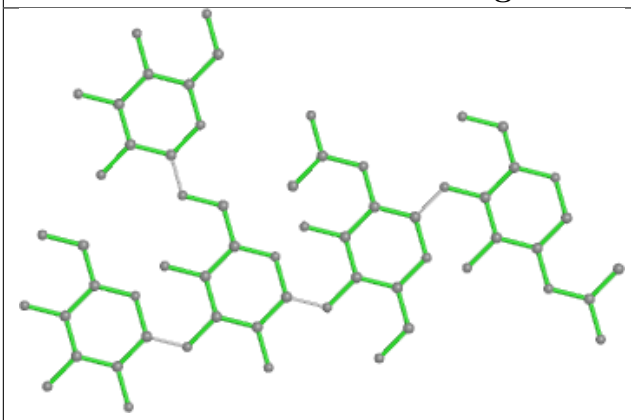


Torsions

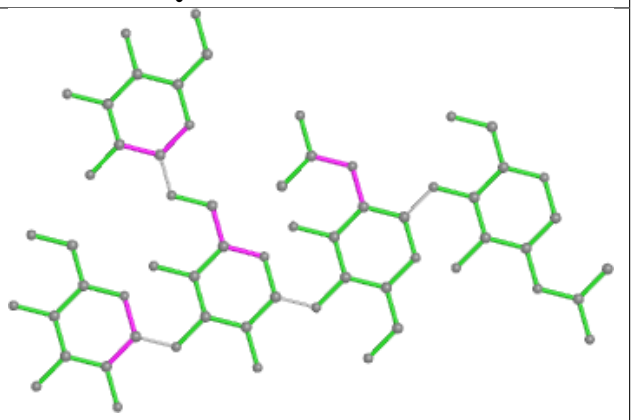


Rings

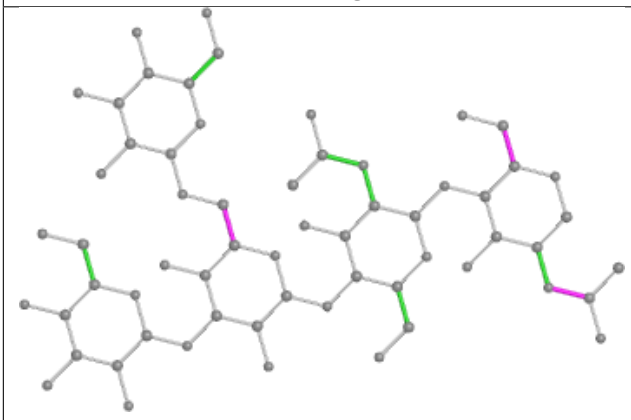
Oligosaccharide Chain Q



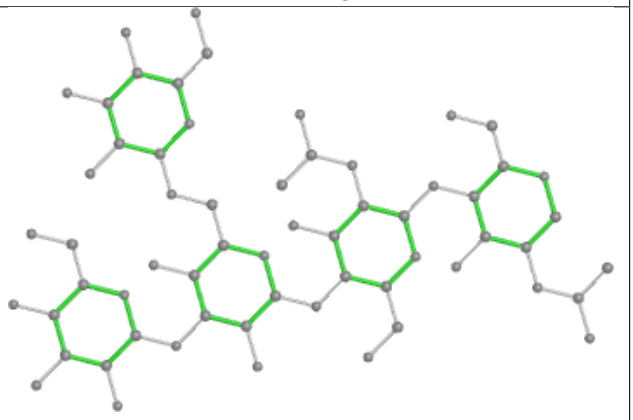
Bond lengths



Bond angles

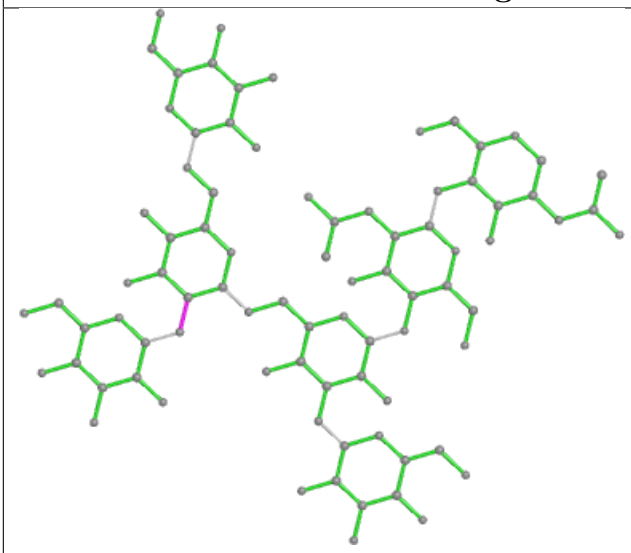


Torsions

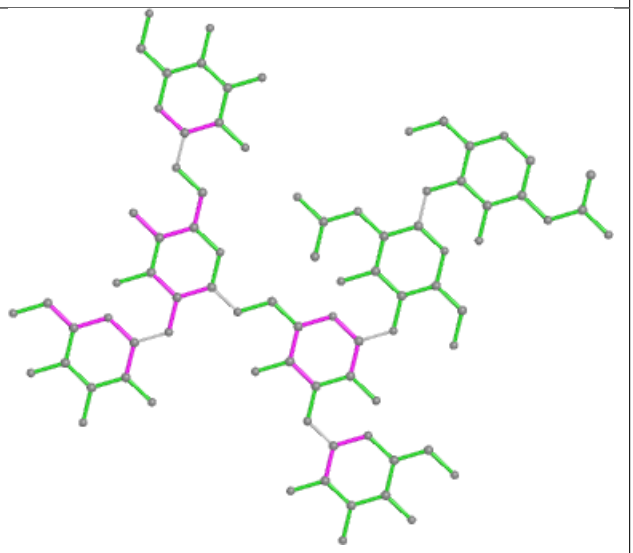


Rings

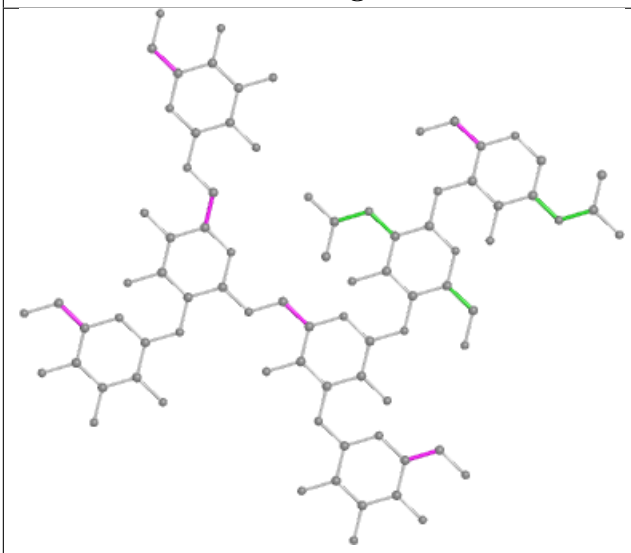
Oligosaccharide Chain C



Bond lengths



Bond angles



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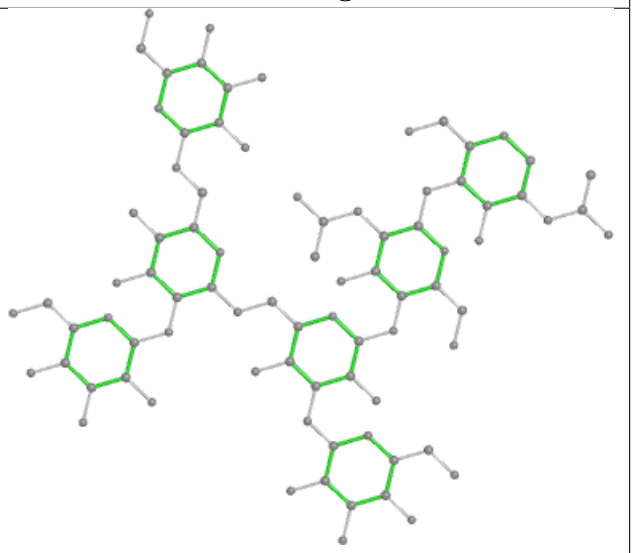
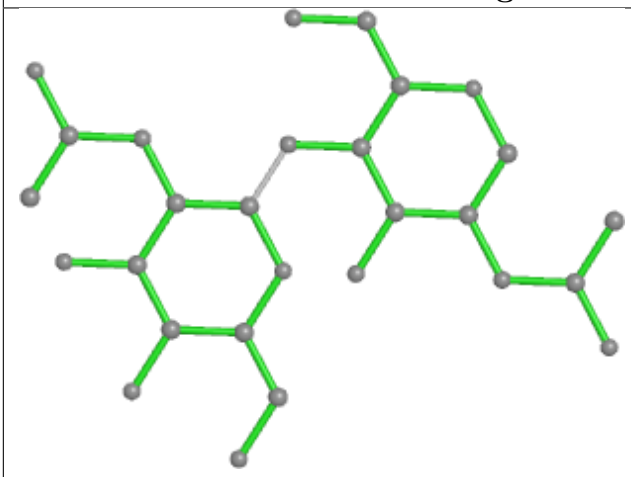
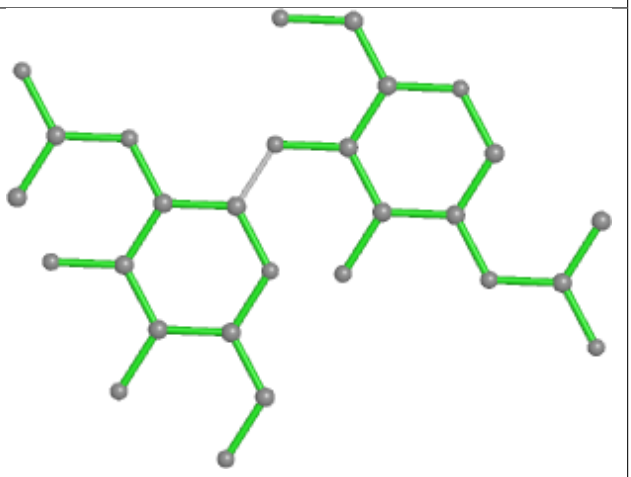


Rings

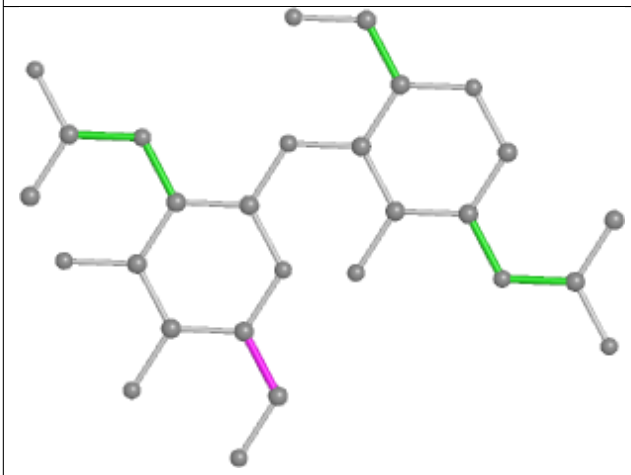
Oligosaccharide Chain F



Bond lengths



Bond angles



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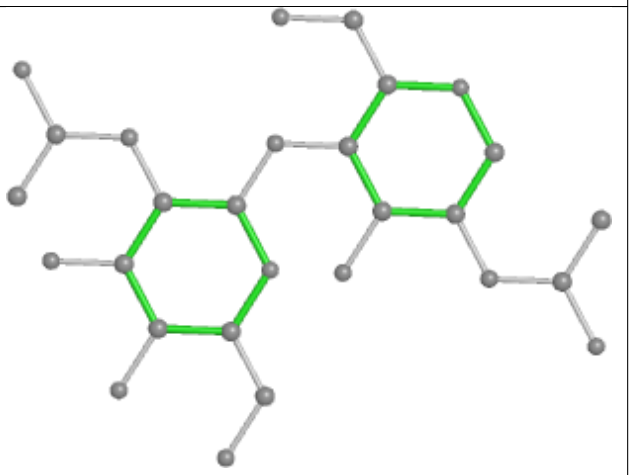
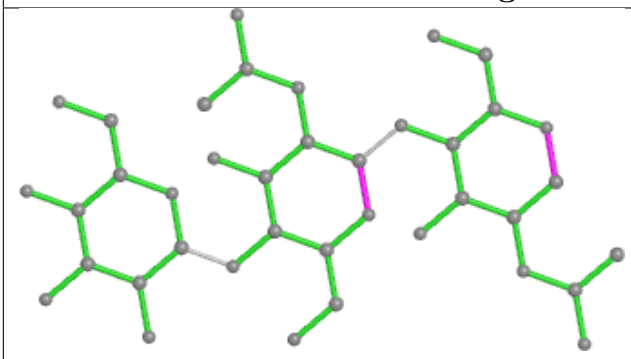
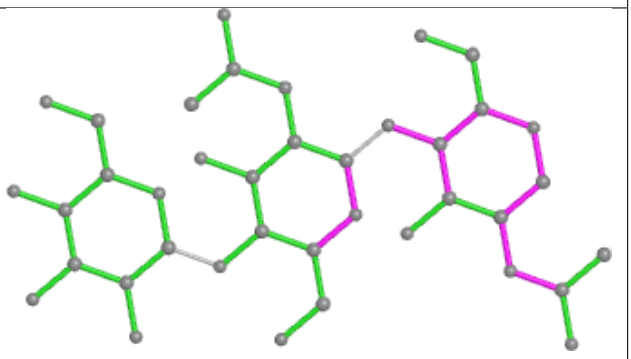


Rings

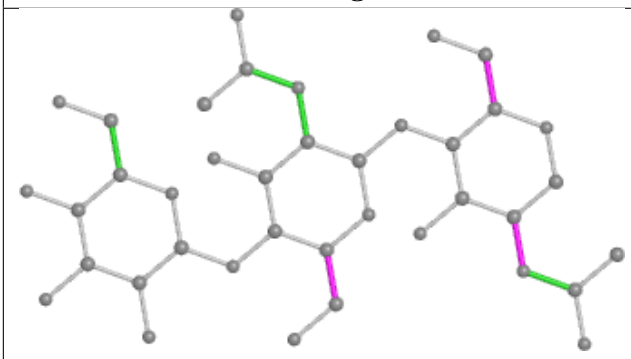
Oligosaccharide Chain J



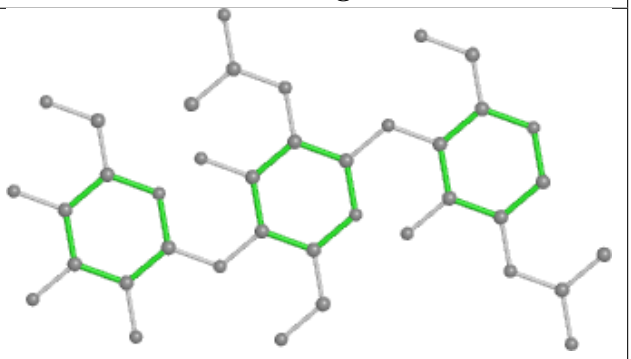
Bond lengths



Bond angles

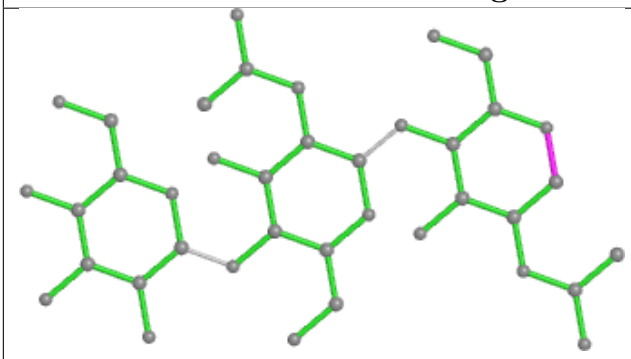


Torsions

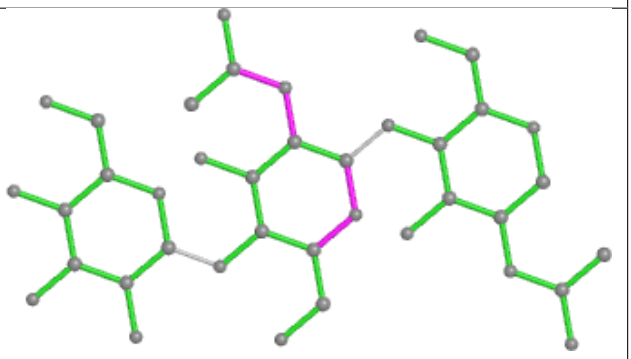


Rings

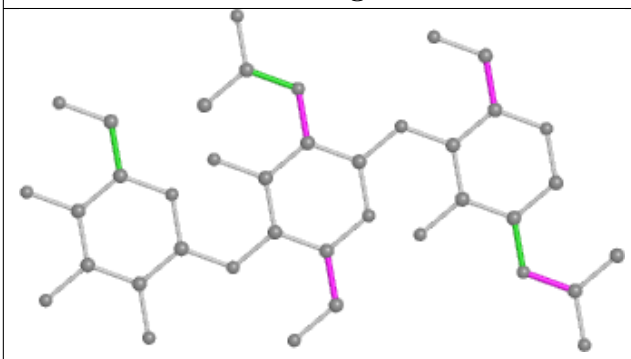
Oligosaccharide Chain M



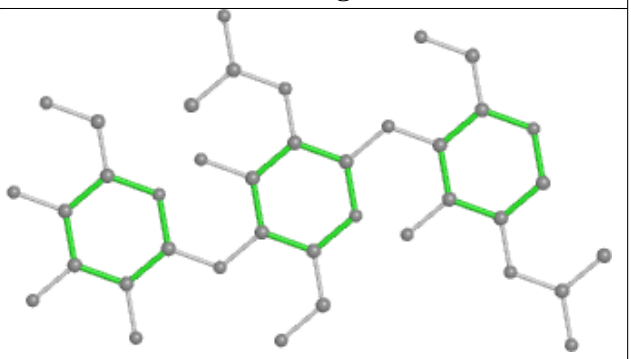
Bond lengths



Bond angles

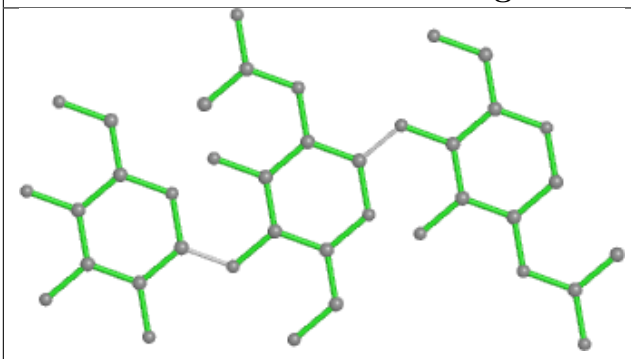


Torsions

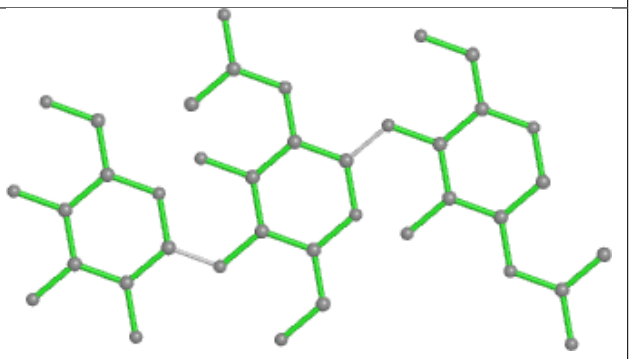


Rings

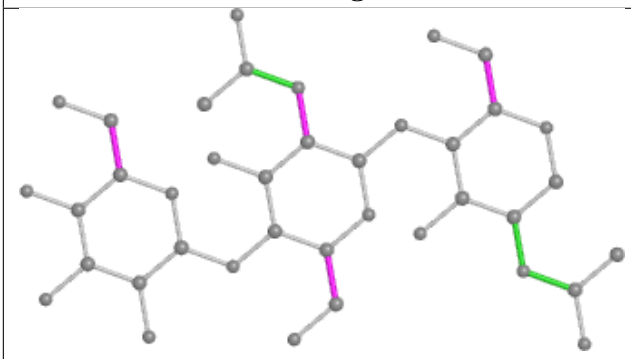
Oligosaccharide Chain O



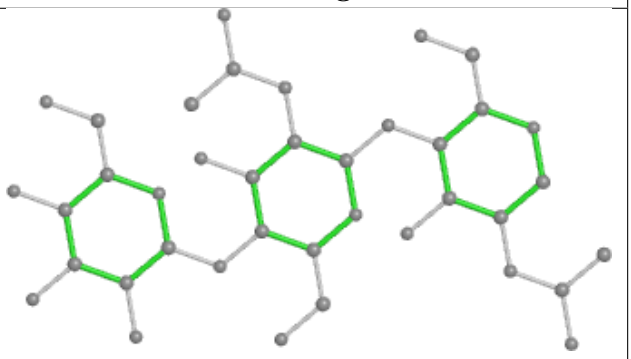
Bond lengths



Bond angles

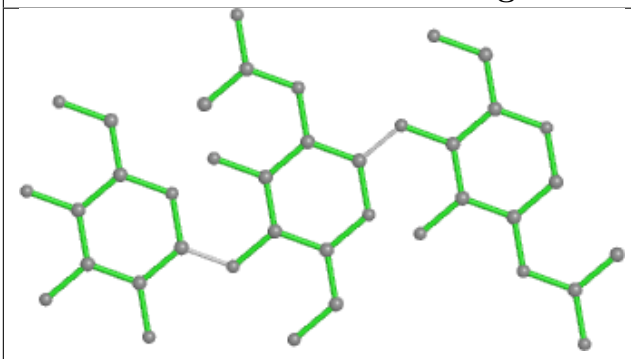


Torsions

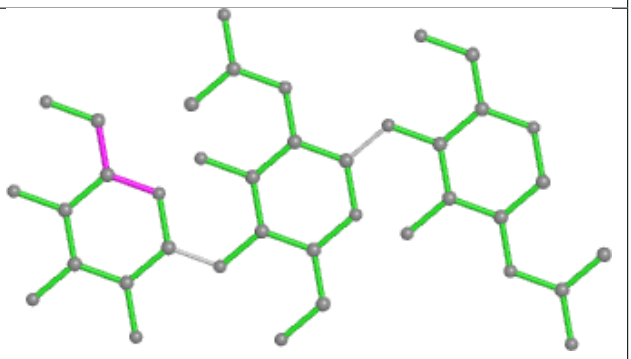


Rings

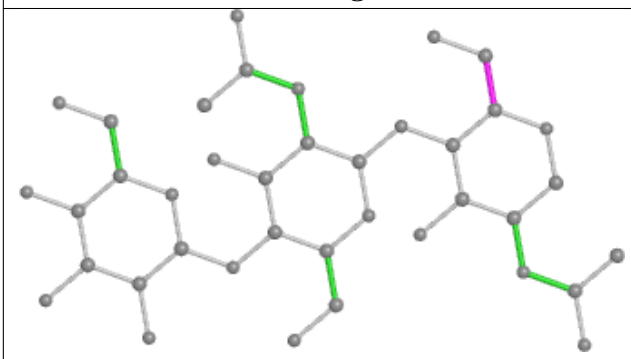
Oligosaccharide Chain S



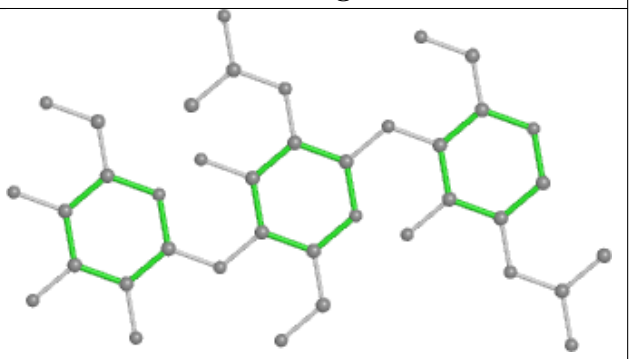
Bond lengths



Bond angles

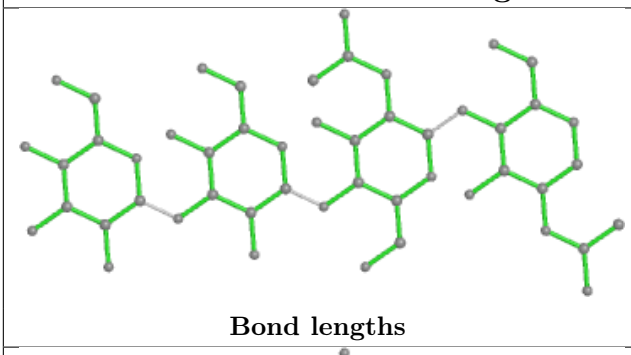


Torsions

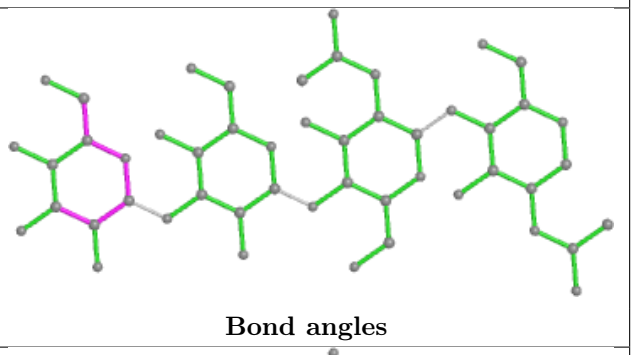


Rings

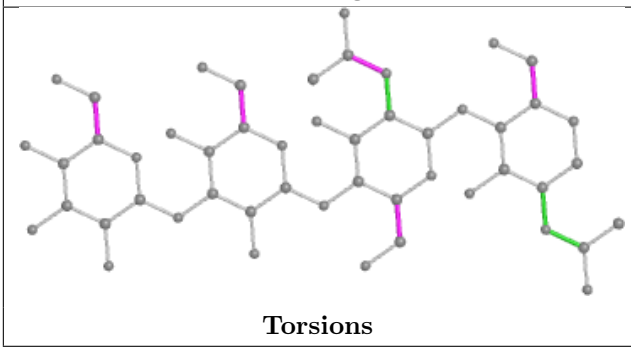
Oligosaccharide Chain N



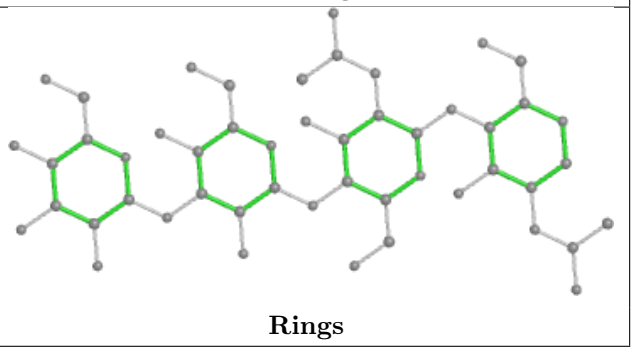
Bond lengths



Bond angles

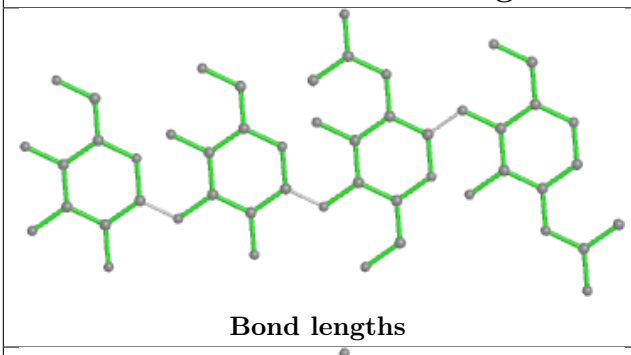


Torsions

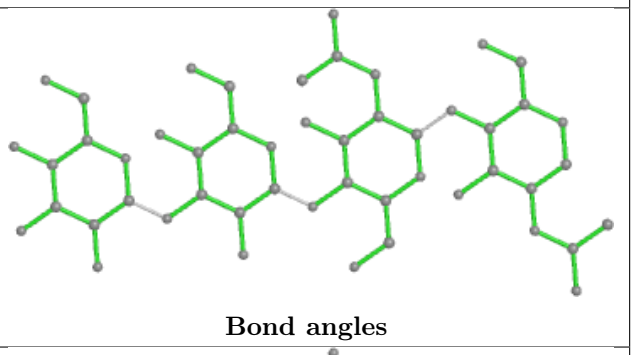


Rings

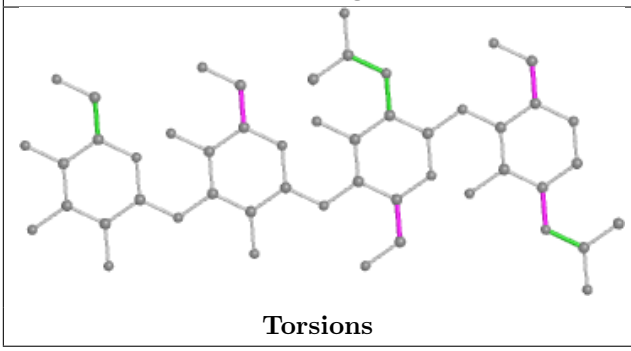
Oligosaccharide Chain P



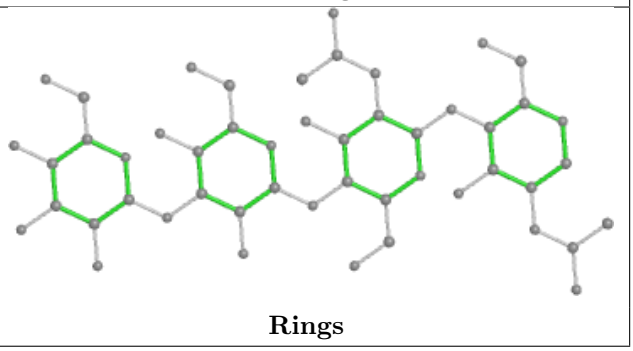
Bond lengths



Bond angles

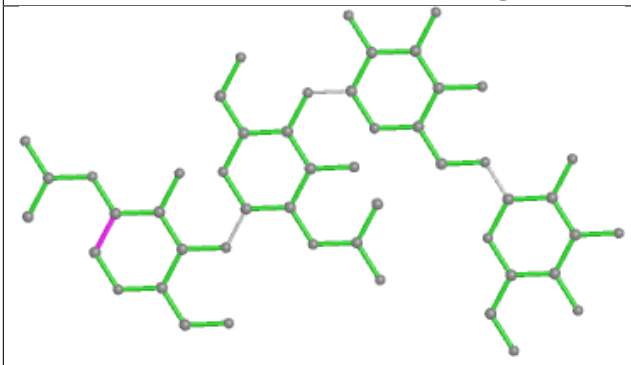


Torsions

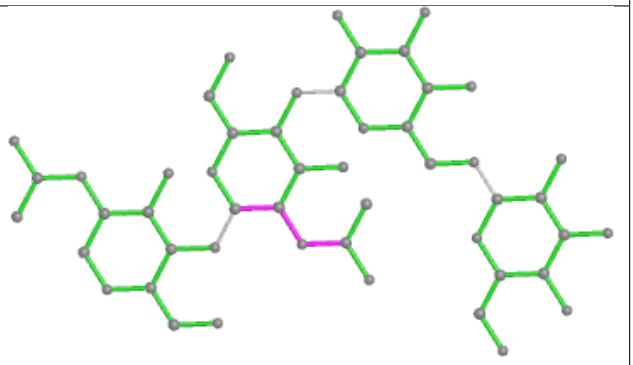


Rings

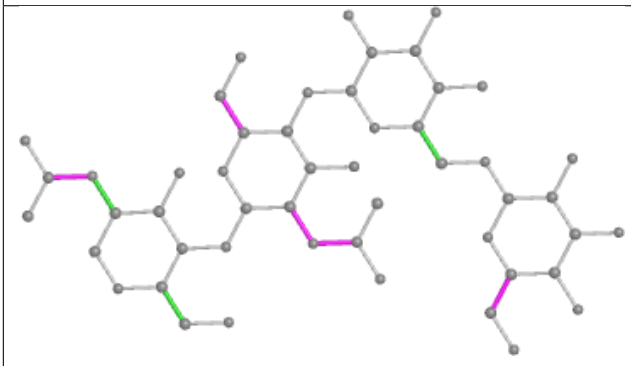
Oligosaccharide Chain R



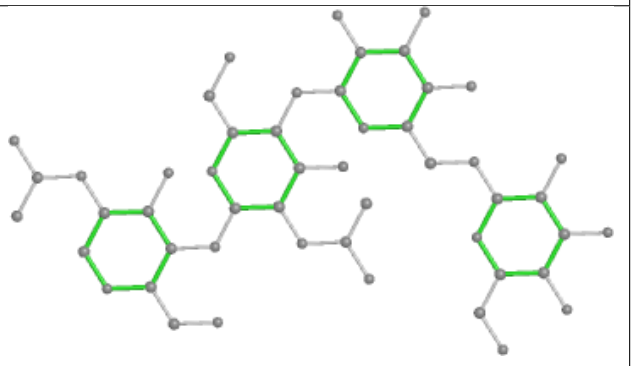
Bond lengths



Bond angles

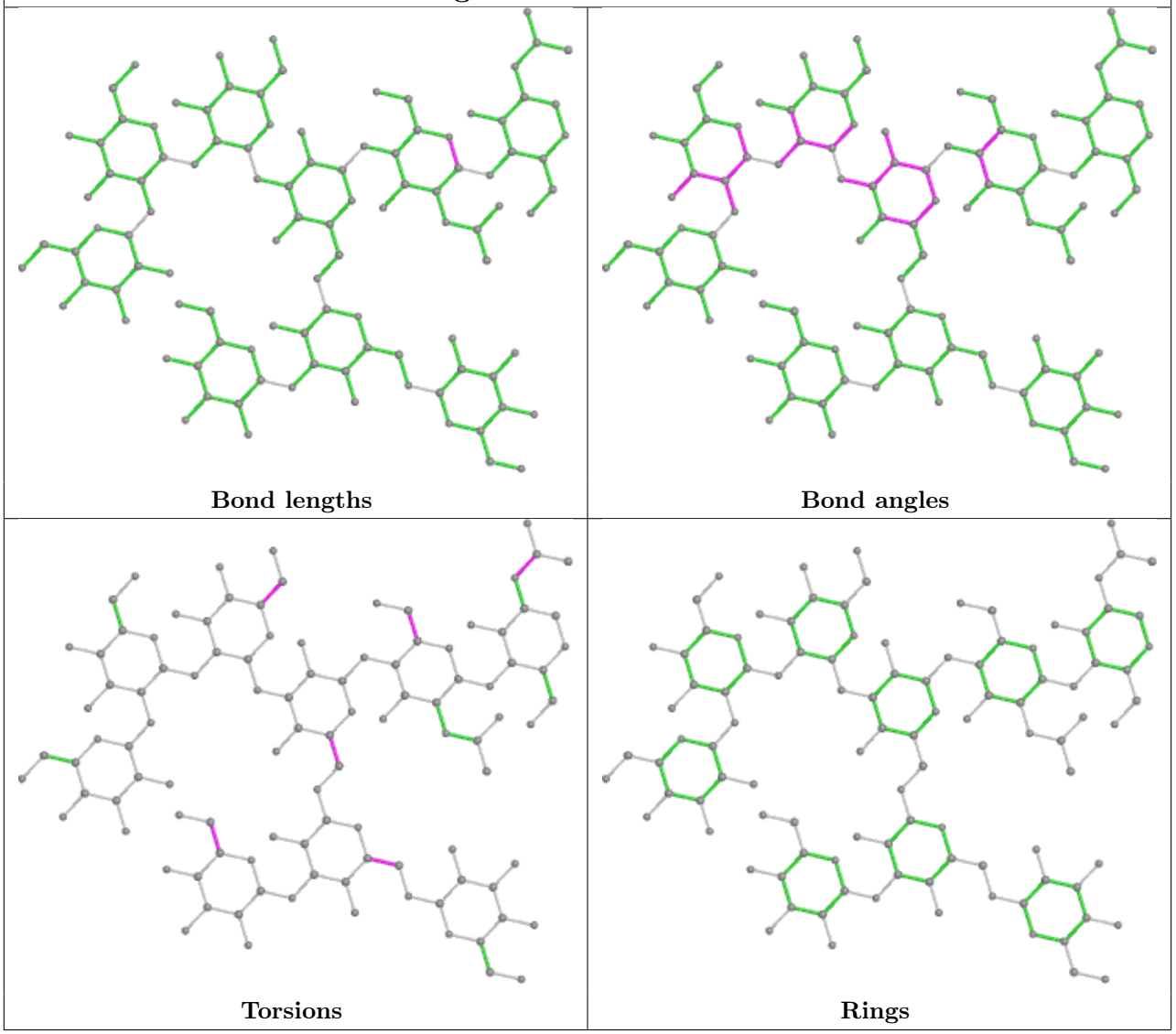


Torsions



Rings

Oligosaccharide Chain T



4.6 Ligand geometry (i)

9 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	$\#\|Z\| > 2$
14	NAG	G	610	2	14,14,15	0.36	0	17,19,21	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	NAG	G	633	2	14,14,15	0.28	0	17,19,21	0.54	0
14	NAG	B	708	1	14,14,15	0.34	0	17,19,21	0.51	0
14	NAG	G	646	2	14,14,15	0.53	0	17,19,21	0.61	1 (5%)
14	NAG	G	654	2	14,14,15	0.27	0	17,19,21	0.65	0
14	NAG	G	611	2	14,14,15	0.53	0	17,19,21	0.91	1 (5%)
14	NAG	B	701	1	14,14,15	0.22	0	17,19,21	0.40	0
14	NAG	G	625	2	14,14,15	0.26	0	17,19,21	0.34	0
14	NAG	B	707	1	14,14,15	0.51	0	17,19,21	0.41	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
14	NAG	G	610	2	-	4/6/23/26	0/1/1/1
14	NAG	G	633	2	-	2/6/23/26	0/1/1/1
14	NAG	B	708	1	-	0/6/23/26	0/1/1/1
14	NAG	G	646	2	-	2/6/23/26	0/1/1/1
14	NAG	G	654	2	-	2/6/23/26	0/1/1/1
14	NAG	G	611	2	-	0/6/23/26	0/1/1/1
14	NAG	B	701	1	-	0/6/23/26	0/1/1/1
14	NAG	G	625	2	-	0/6/23/26	0/1/1/1
14	NAG	B	707	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	G	611	NAG	C1-O5-C5	3.43	116.84	112.19
14	G	646	NAG	C1-O5-C5	2.02	114.93	112.19

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	G	654	NAG	O5-C5-C6-O6
14	G	610	NAG	C8-C7-N2-C2
14	G	610	NAG	O7-C7-N2-C2
14	G	610	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
14	G	654	NAG	C4-C5-C6-O6
14	G	610	NAG	C4-C5-C6-O6
14	G	633	NAG	C4-C5-C6-O6
14	G	633	NAG	O5-C5-C6-O6
14	G	646	NAG	O5-C5-C6-O6
14	G	646	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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

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.