



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 4, 2022 – 08:34 PM EDT

PDB ID : 5T3X
Title : 3.9 Angstrom Crystal Structure of a Fully and Natively Glycosylated BG505
SOSIP.664 HIV-1 Env Trimer in Complex with the Broadly Neutralizing An-
tibodies IOMA and 10-1074.
Authors : Gristick, H.B.; Bjorkman, P.J.
Deposited on : 2016-08-26
Resolution : 3.90 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 ⓘ symbol.

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)	:	2.27

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.90 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

There are 23 unique types of molecules in this entry. The entry contains 12620 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 Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	126	Total	C	N	O	S	0	0	0
			1001	633	172	190	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	559	PRO	ILE	engineered mutation	UNP Q2N0S6
B	605	CYS	THR	engineered mutation	UNP Q2N0S6

- Molecule 2 is a protein called Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	449	Total	C	N	O	S	0	0	0
			3532	2217	623	665	27			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	332	ASN	THR	engineered mutation	UNP Q2N0S6
G	501	CYS	ALA	engineered mutation	UNP Q2N0S6
G	509	ARG	-	expression tag	UNP Q2N0S6
G	510	ARG	-	expression tag	UNP Q2N0S6
G	512	ARG	-	expression tag	UNP Q2N0S6
G	513	ARG	-	expression tag	UNP Q2N0S6

- Molecule 3 is a protein called 10-1074 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	230	Total	C	N	O	S	0	0	0
			1753	1108	293	345	7			

- Molecule 4 is a protein called 10-1074 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	211	Total	C	N	O	S	0	0	0
			1607	1006	281	314	6			

- Molecule 5 is a protein called IOMA Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	D	229	Total	C	N	O	S	0	0	0
			1742	1100	298	332	12			

- Molecule 6 is a protein called IOMA Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	E	210	Total	C	N	O	S	0	0	0
			1558	976	261	317	4			

- Molecule 7 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	A	2	Total	C	N	O	0	0	0
			24	14	1	9			

- Molecule 8 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	C	4	Total	C	N	O	0	0	0
			49	28	2	19			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	F	3	Total	C	N	O	0	0	0
			38	22	2	14			

- 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	I	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 11 is an oligosaccharide called beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)]alpha-D-mannopyranose-(1-3)-[beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)]-[beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	J	13	Total	C	N	O	0	0	0
			160	90	6	64			

- Molecule 12 is an oligosaccharide called beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	K	10	Total	C	N	O	0	0	0
			121	68	4	49			

- Molecule 13 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-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	M	9	Total	C	N	O	0	0	0
			120	67	5	48			

- Molecule 14 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
14	N	2	Total	C	N	O	0	0	0
			28	16	2	10			
14	Q	2	Total	C	N	O	0	0	0
			28	16	2	10			

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

- Molecule 15 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-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
15	O	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 16 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
16	P	16	Total	C	N	O	0	0	0
			214	120	9	85			

- Molecule 17 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-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
17	R	7	Total	C	N	O	0	0	0
			89	50	4	35			

- Molecule 18 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[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
18	S	10	Total	C	N	O	0	0	0
			116	64	2	50			

- Molecule 19 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[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
19	U	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 20 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
20	V	5	Total	C	N	O	0	0	0
			61	34	2	25			

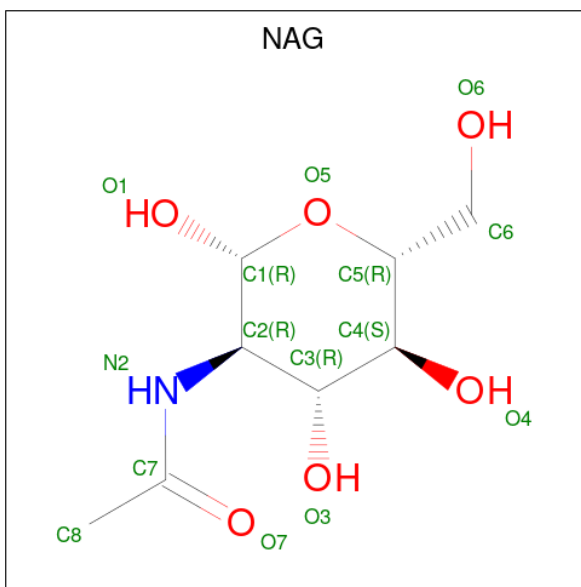
- Molecule 21 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	W	6	Total	C	N	O	0	0	0
			71	40	2	29			

- Molecule 22 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
22	X	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 23 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
23	G	1	14	8	1	5	0	0

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

3 Data and refinement statistics

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

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	217.51Å 217.51Å 156.01Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	80.63 – 3.90	Depositor
% Data completeness (in resolution range)	99.9 (80.63-3.90)	Depositor
R_{merge}	0.35	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.02 (at 3.89Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.296 , 0.331	Depositor
Wilson B-factor (Å ²)	134.0	Xtriage
Anisotropy	0.071	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.075 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.160 for k,h,-l	Depositor
Outliers	0 of 25075 reflections	Xtriage
Total number of atoms	12620	wwPDB-VP
Average B, all atoms (Å ²)	302.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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](#)

113 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	0.28	0	17,19,21	0.81	0
7	FUC	A	2	7	10,10,11	0.75	0	14,14,16	0.89	0
8	NAG	C	1	1,8	14,14,15	0.34	0	17,19,21	1.51	2 (11%)
8	NAG	C	2	8	14,14,15	0.31	0	17,19,21	1.03	1 (5%)
8	BMA	C	3	8	11,11,12	0.26	0	15,15,17	0.74	0
8	FUC	C	4	8	10,10,11	0.68	0	14,14,16	0.84	0
9	NAG	F	1	2,9	14,14,15	0.31	0	17,19,21	0.95	1 (5%)
9	NAG	F	2	9	14,14,15	0.28	0	17,19,21	0.66	0
9	FUC	F	3	9	10,10,11	0.73	0	14,14,16	0.93	0
10	NAG	I	1	2,10	14,14,15	0.43	0	17,19,21	1.41	4 (23%)
10	NAG	I	2	10	14,14,15	0.32	0	17,19,21	0.94	0
10	BMA	I	3	10	11,11,12	0.25	0	15,15,17	0.84	0
11	NAG	J	1	11,2	14,14,15	0.38	0	17,19,21	0.85	1 (5%)
11	GAL	J	10	11	11,11,12	0.24	0	15,15,17	0.77	0
11	NAG	J	11	11	14,14,15	0.33	0	17,19,21	0.85	0
11	GAL	J	12	11	11,11,12	0.26	0	15,15,17	0.79	0
11	FUC	J	13	11	10,10,11	0.70	0	14,14,16	0.84	0
11	NAG	J	2	11	14,14,15	0.36	0	17,19,21	1.08	2 (11%)
11	BMA	J	3	11	11,11,12	0.46	0	15,15,17	1.38	3 (20%)
11	MAN	J	4	11	11,11,12	0.40	0	15,15,17	1.92	3 (20%)
11	NAG	J	5	11	14,14,15	0.47	0	17,19,21	1.30	1 (5%)
11	GAL	J	6	11	11,11,12	0.25	0	15,15,17	0.79	0
11	NAG	J	7	11	14,14,15	0.31	0	17,19,21	1.08	1 (5%)
11	MAN	J	8	11	11,11,12	0.50	0	15,15,17	1.89	2 (13%)
11	NAG	J	9	11	14,14,15	0.35	0	17,19,21	1.10	2 (11%)
12	NAG	K	1	2,12	14,14,15	0.47	0	17,19,21	1.35	2 (11%)
12	FUC	K	10	12	10,10,11	0.71	0	14,14,16	0.93	0
12	NAG	K	2	12	14,14,15	0.57	0	17,19,21	2.21	4 (23%)
12	BMA	K	3	12	11,11,12	0.36	0	15,15,17	1.64	3 (20%)
12	MAN	K	4	12	11,11,12	0.39	0	15,15,17	1.08	2 (13%)
12	NAG	K	5	12	14,14,15	0.34	0	17,19,21	1.01	1 (5%)
12	GAL	K	6	12	11,11,12	0.28	0	15,15,17	0.78	0
12	MAN	K	7	12	11,11,12	0.25	0	15,15,17	1.05	1 (6%)
12	NAG	K	8	12	14,14,15	0.25	0	17,19,21	0.63	0
12	GAL	K	9	12	11,11,12	0.25	0	15,15,17	0.79	0
13	NAG	M	1	2,13	14,14,15	0.56	0	17,19,21	2.53	7 (41%)
13	NAG	M	2	13	14,14,15	0.69	0	17,19,21	1.96	5 (29%)
13	BMA	M	3	13	11,11,12	0.54	0	15,15,17	1.54	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	MAN	M	4	13	11,11,12	0.40	0	15,15,17	1.50	3 (20%)
13	NAG	M	5	13	14,14,15	0.33	0	17,19,21	0.84	1 (5%)
13	GAL	M	6	13	11,11,12	0.26	0	15,15,17	0.89	0
13	SIA	M	7	13	17,20,21	0.87	0	21,28,31	1.29	1 (4%)
13	MAN	M	8	13	11,11,12	0.26	0	15,15,17	1.09	1 (6%)
13	NAG	M	9	13	14,14,15	0.26	0	17,19,21	0.69	0
14	NAG	N	1	2,14	14,14,15	0.33	0	17,19,21	1.38	2 (11%)
14	NAG	N	2	14	14,14,15	0.25	0	17,19,21	0.79	0
15	NAG	O	1	15,2	14,14,15	0.37	0	17,19,21	0.85	0
15	NAG	O	2	15	14,14,15	0.30	0	17,19,21	1.23	2 (11%)
15	BMA	O	3	15	11,11,12	0.32	0	15,15,17	0.87	0
15	MAN	O	4	15	11,11,12	0.25	0	15,15,17	0.91	0
15	MAN	O	5	15	11,11,12	0.29	0	15,15,17	0.84	0
15	MAN	O	6	15	11,11,12	0.28	0	15,15,17	0.85	1 (6%)
15	MAN	O	7	15	11,11,12	0.34	0	15,15,17	0.92	1 (6%)
16	NAG	P	1	2,16	14,14,15	0.48	0	17,19,21	1.23	2 (11%)
16	NAG	P	10	16	14,14,15	0.39	0	17,19,21	1.43	4 (23%)
16	GAL	P	11	16	11,11,12	0.29	0	15,15,17	1.12	1 (6%)
16	SIA	P	12	16	17,20,21	0.87	0	21,28,31	1.32	1 (4%)
16	NAG	P	13	16	14,14,15	0.45	0	17,19,21	1.10	2 (11%)
16	GAL	P	14	16	11,11,12	0.25	0	15,15,17	0.93	1 (6%)
16	NAG	P	15	16	14,14,15	0.54	0	17,19,21	1.22	2 (11%)
16	FUC	P	16	16	10,10,11	0.62	0	14,14,16	0.92	0
16	NAG	P	2	16	14,14,15	0.30	0	17,19,21	1.08	3 (17%)
16	BMA	P	3	16	11,11,12	0.43	0	15,15,17	1.84	7 (46%)
16	MAN	P	4	16	11,11,12	0.36	0	15,15,17	1.66	5 (33%)
16	NAG	P	5	16	14,14,15	0.28	0	17,19,21	0.58	0
16	GAL	P	6	16	11,11,12	0.26	0	15,15,17	0.78	0
16	SIA	P	7	16	17,20,21	0.88	0	21,28,31	1.29	2 (9%)
16	NAG	P	8	16	14,14,15	0.28	0	17,19,21	0.68	0
16	MAN	P	9	16	11,11,12	0.93	0	15,15,17	3.01	10 (66%)
14	NAG	Q	1	2,14	14,14,15	0.36	0	17,19,21	0.77	0
14	NAG	Q	2	14	14,14,15	0.29	0	17,19,21	0.71	0
17	NAG	R	1	2,17	14,14,15	0.48	0	17,19,21	1.80	5 (29%)
17	NAG	R	2	17	14,14,15	0.36	0	17,19,21	0.91	2 (11%)
17	BMA	R	3	17	11,11,12	0.30	0	15,15,17	1.03	1 (6%)
17	MAN	R	4	17	11,11,12	0.28	0	15,15,17	1.12	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	NAG	R	5	17	14,14,15	0.30	0	17,19,21	0.45	0
17	MAN	R	6	17	11,11,12	0.26	0	15,15,17	0.89	0
17	NAG	R	7	17	14,14,15	0.27	0	17,19,21	0.70	0
18	NAG	S	1	2,18	14,14,15	0.30	0	17,19,21	0.75	0
18	MAN	S	10	18	11,11,12	0.27	0	15,15,17	0.80	0
18	NAG	S	2	18	14,14,15	0.25	0	17,19,21	1.33	2 (11%)
18	BMA	S	3	18	11,11,12	0.32	0	15,15,17	0.98	1 (6%)
18	MAN	S	4	18	11,11,12	0.35	0	15,15,17	1.49	2 (13%)
18	MAN	S	5	18	11,11,12	0.34	0	15,15,17	1.38	2 (13%)
18	MAN	S	6	18	11,11,12	0.22	0	15,15,17	1.02	1 (6%)
18	MAN	S	7	18	11,11,12	0.25	0	15,15,17	1.28	2 (13%)
18	MAN	S	8	18	11,11,12	0.46	0	15,15,17	1.34	1 (6%)
18	MAN	S	9	18	11,11,12	0.23	0	15,15,17	0.88	1 (6%)
14	NAG	T	1	2,14	14,14,15	0.35	0	17,19,21	0.67	0
14	NAG	T	2	14	14,14,15	0.31	0	17,19,21	0.65	0
19	NAG	U	1	19,2	14,14,15	0.53	0	17,19,21	2.17	4 (23%)
19	NAG	U	2	19	14,14,15	0.45	0	17,19,21	1.83	3 (17%)
19	BMA	U	3	19	11,11,12	0.40	0	15,15,17	1.27	2 (13%)
19	MAN	U	4	19	11,11,12	0.39	0	15,15,17	0.99	1 (6%)
19	MAN	U	5	19	11,11,12	0.27	0	15,15,17	0.88	0
19	MAN	U	6	19	11,11,12	0.28	0	15,15,17	0.87	0
19	MAN	U	7	19	11,11,12	0.32	0	15,15,17	0.86	1 (6%)
20	NAG	V	1	2,20	14,14,15	0.32	0	17,19,21	1.27	3 (17%)
20	NAG	V	2	20	14,14,15	0.61	0	17,19,21	1.78	5 (29%)
20	BMA	V	3	20	11,11,12	0.35	0	15,15,17	1.17	2 (13%)
20	MAN	V	4	20	11,11,12	0.28	0	15,15,17	0.81	1 (6%)
20	MAN	V	5	20	11,11,12	0.28	0	15,15,17	0.77	0
21	NAG	W	1	2,21	14,14,15	0.36	0	17,19,21	1.00	0
21	NAG	W	2	21	14,14,15	0.28	0	17,19,21	0.82	0
21	BMA	W	3	21	11,11,12	0.46	0	15,15,17	1.59	2 (13%)
21	MAN	W	4	21	11,11,12	0.27	0	15,15,17	0.80	1 (6%)
21	MAN	W	5	21	11,11,12	0.27	0	15,15,17	0.84	0
21	FUC	W	6	21	10,10,11	0.90	0	14,14,16	1.07	1 (7%)
22	NAG	X	1	22,2	14,14,15	0.29	0	17,19,21	1.17	1 (5%)
22	NAG	X	2	22	14,14,15	0.58	0	17,19,21	2.14	6 (35%)
22	BMA	X	3	22	11,11,12	0.32	0	15,15,17	1.15	2 (13%)
22	MAN	X	4	22	11,11,12	0.25	0	15,15,17	0.73	0
22	MAN	X	5	22	11,11,12	0.25	0	15,15,17	0.77	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	-	0/6/23/26	0/1/1/1
7	FUC	A	2	7	-	-	0/1/1/1
8	NAG	C	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	C	2	8	-	1/6/23/26	0/1/1/1
8	BMA	C	3	8	-	0/2/19/22	0/1/1/1
8	FUC	C	4	8	-	-	0/1/1/1
9	NAG	F	1	2,9	-	2/6/23/26	0/1/1/1
9	NAG	F	2	9	-	2/6/23/26	0/1/1/1
9	FUC	F	3	9	-	-	0/1/1/1
10	NAG	I	1	2,10	-	1/6/23/26	0/1/1/1
10	NAG	I	2	10	-	2/6/23/26	0/1/1/1
10	BMA	I	3	10	-	0/2/19/22	0/1/1/1
11	NAG	J	1	11,2	-	0/6/23/26	0/1/1/1
11	GAL	J	10	11	-	0/2/19/22	0/1/1/1
11	NAG	J	11	11	-	2/6/23/26	0/1/1/1
11	GAL	J	12	11	-	0/2/19/22	0/1/1/1
11	FUC	J	13	11	-	-	0/1/1/1
11	NAG	J	2	11	-	1/6/23/26	0/1/1/1
11	BMA	J	3	11	-	2/2/19/22	0/1/1/1
11	MAN	J	4	11	-	0/2/19/22	0/1/1/1
11	NAG	J	5	11	-	0/6/23/26	0/1/1/1
11	GAL	J	6	11	-	0/2/19/22	0/1/1/1
11	NAG	J	7	11	-	0/6/23/26	0/1/1/1
11	MAN	J	8	11	-	0/2/19/22	0/1/1/1
11	NAG	J	9	11	-	2/6/23/26	0/1/1/1
12	NAG	K	1	2,12	-	2/6/23/26	0/1/1/1
12	FUC	K	10	12	-	-	0/1/1/1
12	NAG	K	2	12	-	4/6/23/26	0/1/1/1
12	BMA	K	3	12	-	2/2/19/22	0/1/1/1
12	MAN	K	4	12	-	0/2/19/22	0/1/1/1
12	NAG	K	5	12	-	0/6/23/26	0/1/1/1
12	GAL	K	6	12	-	0/2/19/22	0/1/1/1
12	MAN	K	7	12	-	2/2/19/22	0/1/1/1
12	NAG	K	8	12	-	2/6/23/26	0/1/1/1
12	GAL	K	9	12	-	0/2/19/22	0/1/1/1
13	NAG	M	1	2,13	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	NAG	M	2	13	-	3/6/23/26	0/1/1/1
13	BMA	M	3	13	-	2/2/19/22	0/1/1/1
13	MAN	M	4	13	-	2/2/19/22	0/1/1/1
13	NAG	M	5	13	-	2/6/23/26	0/1/1/1
13	GAL	M	6	13	-	2/2/19/22	0/1/1/1
13	SIA	M	7	13	-	2/14/34/38	0/1/1/1
13	MAN	M	8	13	-	0/2/19/22	0/1/1/1
13	NAG	M	9	13	-	2/6/23/26	0/1/1/1
14	NAG	N	1	2,14	-	0/6/23/26	0/1/1/1
14	NAG	N	2	14	-	2/6/23/26	0/1/1/1
15	NAG	O	1	15,2	-	2/6/23/26	0/1/1/1
15	NAG	O	2	15	-	1/6/23/26	0/1/1/1
15	BMA	O	3	15	-	1/2/19/22	0/1/1/1
15	MAN	O	4	15	-	0/2/19/22	0/1/1/1
15	MAN	O	5	15	-	1/2/19/22	0/1/1/1
15	MAN	O	6	15	-	2/2/19/22	0/1/1/1
15	MAN	O	7	15	-	2/2/19/22	0/1/1/1
16	NAG	P	1	2,16	-	2/6/23/26	0/1/1/1
16	NAG	P	10	16	-	4/6/23/26	0/1/1/1
16	GAL	P	11	16	-	0/2/19/22	0/1/1/1
16	SIA	P	12	16	-	0/14/34/38	0/1/1/1
16	NAG	P	13	16	-	2/6/23/26	0/1/1/1
16	GAL	P	14	16	-	0/2/19/22	0/1/1/1
16	NAG	P	15	16	-	1/6/23/26	0/1/1/1
16	FUC	P	16	16	-	-	0/1/1/1
16	NAG	P	2	16	-	1/6/23/26	0/1/1/1
16	BMA	P	3	16	-	2/2/19/22	0/1/1/1
16	MAN	P	4	16	-	2/2/19/22	0/1/1/1
16	NAG	P	5	16	-	2/6/23/26	0/1/1/1
16	GAL	P	6	16	-	2/2/19/22	0/1/1/1
16	SIA	P	7	16	-	0/14/34/38	0/1/1/1
16	NAG	P	8	16	-	0/6/23/26	0/1/1/1
16	MAN	P	9	16	-	0/2/19/22	0/1/1/1
14	NAG	Q	1	2,14	-	1/6/23/26	0/1/1/1
14	NAG	Q	2	14	-	0/6/23/26	0/1/1/1
17	NAG	R	1	2,17	-	0/6/23/26	0/1/1/1
17	NAG	R	2	17	-	2/6/23/26	0/1/1/1
17	BMA	R	3	17	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	MAN	R	4	17	-	0/2/19/22	0/1/1/1
17	NAG	R	5	17	-	2/6/23/26	0/1/1/1
17	MAN	R	6	17	-	2/2/19/22	0/1/1/1
17	NAG	R	7	17	-	4/6/23/26	0/1/1/1
18	NAG	S	1	2,18	-	0/6/23/26	0/1/1/1
18	MAN	S	10	18	-	0/2/19/22	0/1/1/1
18	NAG	S	2	18	-	1/6/23/26	0/1/1/1
18	BMA	S	3	18	-	0/2/19/22	0/1/1/1
18	MAN	S	4	18	-	0/2/19/22	0/1/1/1
18	MAN	S	5	18	-	1/2/19/22	0/1/1/1
18	MAN	S	6	18	-	0/2/19/22	0/1/1/1
18	MAN	S	7	18	-	0/2/19/22	0/1/1/1
18	MAN	S	8	18	-	2/2/19/22	0/1/1/1
18	MAN	S	9	18	-	0/2/19/22	0/1/1/1
14	NAG	T	1	2,14	-	0/6/23/26	0/1/1/1
14	NAG	T	2	14	-	2/6/23/26	0/1/1/1
19	NAG	U	1	19,2	-	0/6/23/26	0/1/1/1
19	NAG	U	2	19	-	2/6/23/26	0/1/1/1
19	BMA	U	3	19	-	0/2/19/22	0/1/1/1
19	MAN	U	4	19	-	1/2/19/22	0/1/1/1
19	MAN	U	5	19	-	1/2/19/22	0/1/1/1
19	MAN	U	6	19	-	0/2/19/22	0/1/1/1
19	MAN	U	7	19	-	1/2/19/22	0/1/1/1
20	NAG	V	1	2,20	-	2/6/23/26	0/1/1/1
20	NAG	V	2	20	-	1/6/23/26	0/1/1/1
20	BMA	V	3	20	-	0/2/19/22	0/1/1/1
20	MAN	V	4	20	-	0/2/19/22	0/1/1/1
20	MAN	V	5	20	-	0/2/19/22	0/1/1/1
21	NAG	W	1	2,21	-	0/6/23/26	0/1/1/1
21	NAG	W	2	21	-	1/6/23/26	0/1/1/1
21	BMA	W	3	21	-	0/2/19/22	0/1/1/1
21	MAN	W	4	21	-	0/2/19/22	0/1/1/1
21	MAN	W	5	21	-	0/2/19/22	0/1/1/1
21	FUC	W	6	21	-	-	0/1/1/1
22	NAG	X	1	22,2	-	2/6/23/26	0/1/1/1
22	NAG	X	2	22	-	2/6/23/26	0/1/1/1
22	BMA	X	3	22	-	0/2/19/22	0/1/1/1
22	MAN	X	4	22	-	2/2/19/22	0/1/1/1
22	MAN	X	5	22	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 159 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	K	2	NAG	C2-N2-C7	6.75	132.51	122.90
19	U	1	NAG	O4-C4-C5	6.20	124.69	109.30
13	M	1	NAG	O3-C3-C2	-5.98	97.10	109.47
22	X	2	NAG	O4-C4-C3	-5.64	97.31	110.35
11	J	8	MAN	O2-C2-C3	5.51	121.17	110.14

There are no chirality outliers.

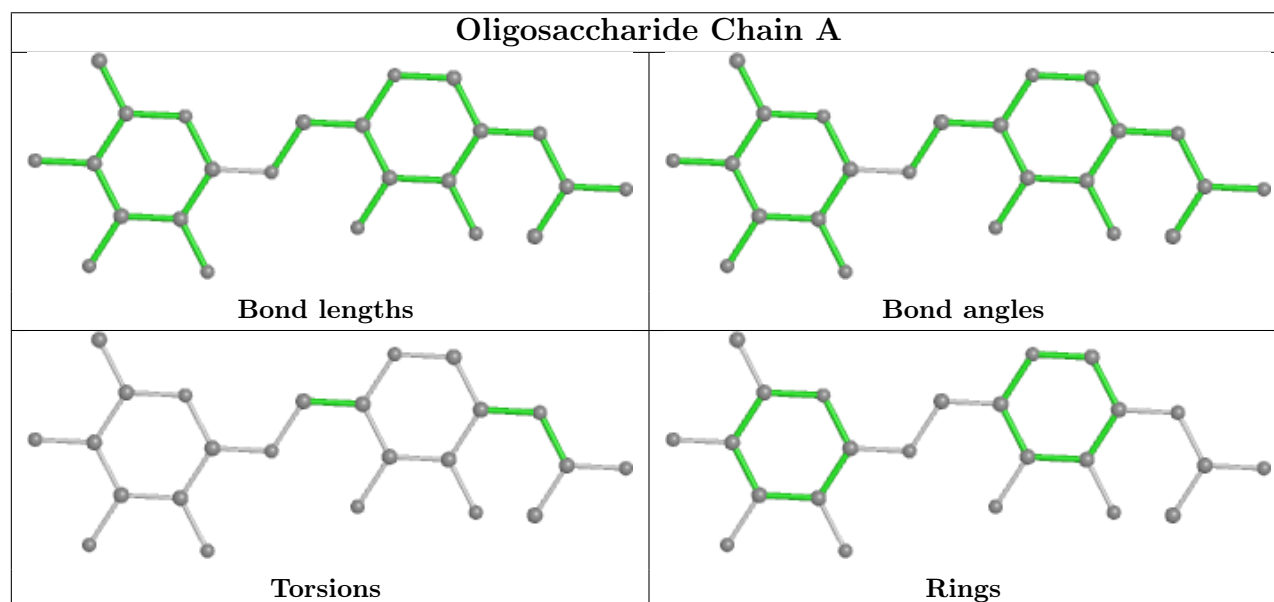
5 of 105 torsion outliers are listed below:

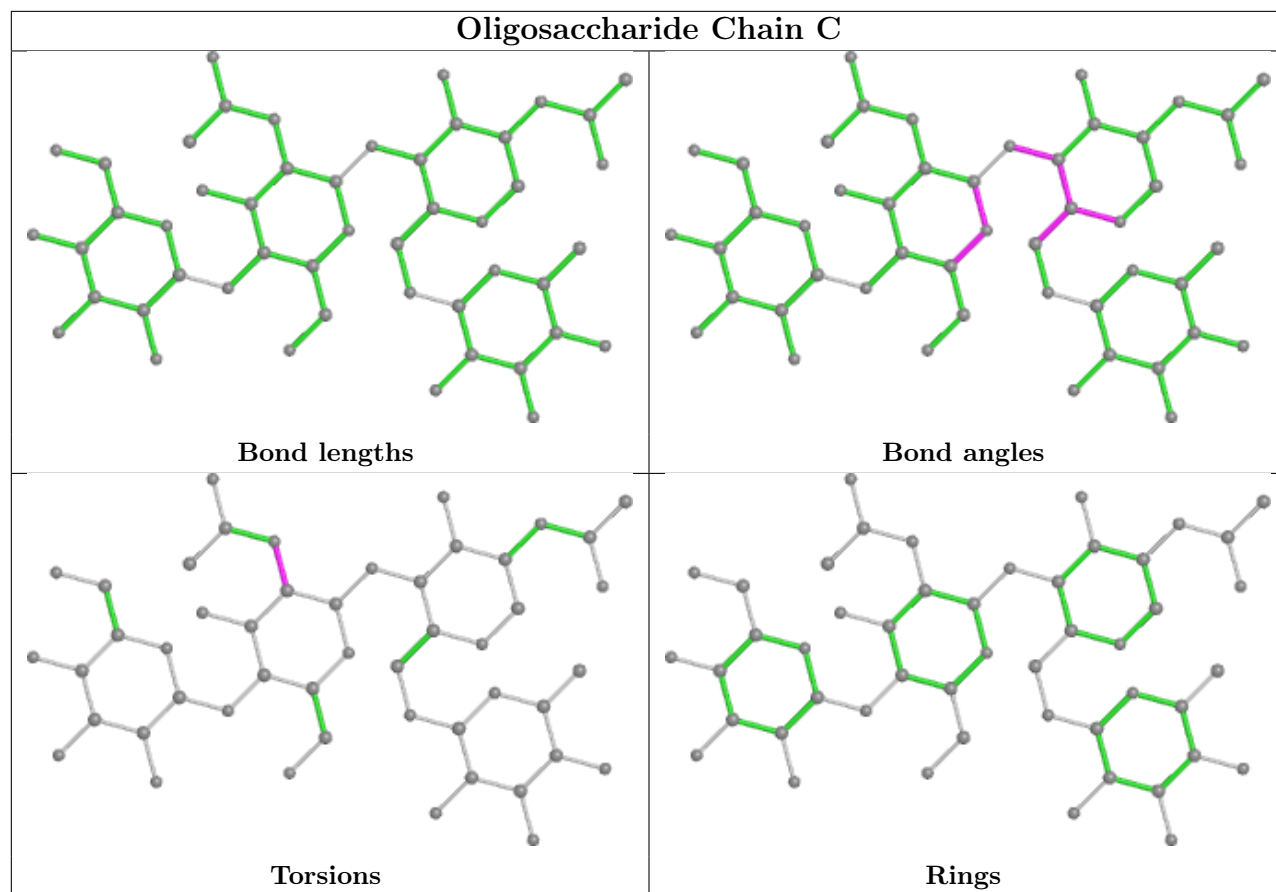
Mol	Chain	Res	Type	Atoms
16	P	3	BMA	O5-C5-C6-O6
13	M	3	BMA	O5-C5-C6-O6
13	M	4	MAN	O5-C5-C6-O6
16	P	6	GAL	O5-C5-C6-O6
12	K	3	BMA	O5-C5-C6-O6

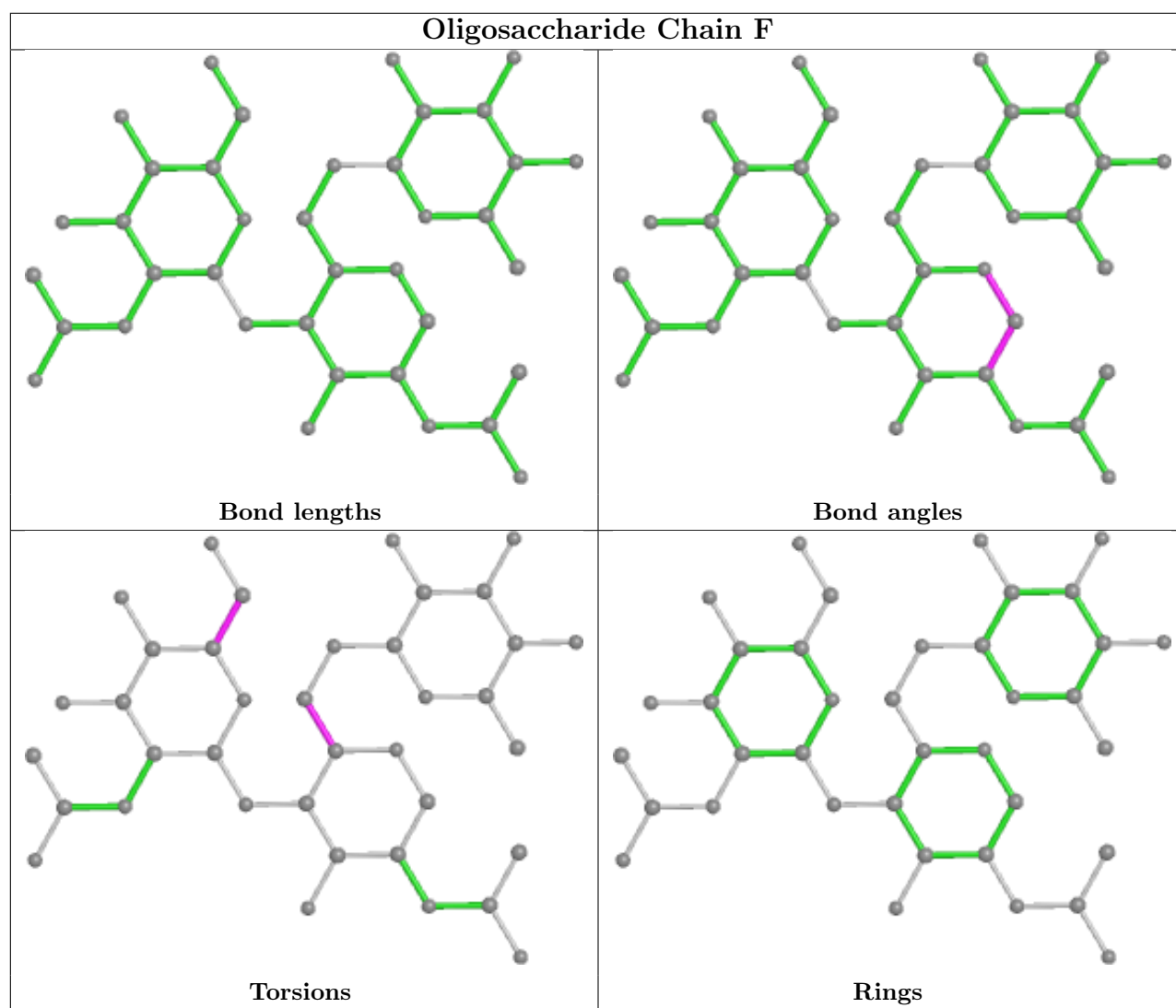
There are no ring outliers.

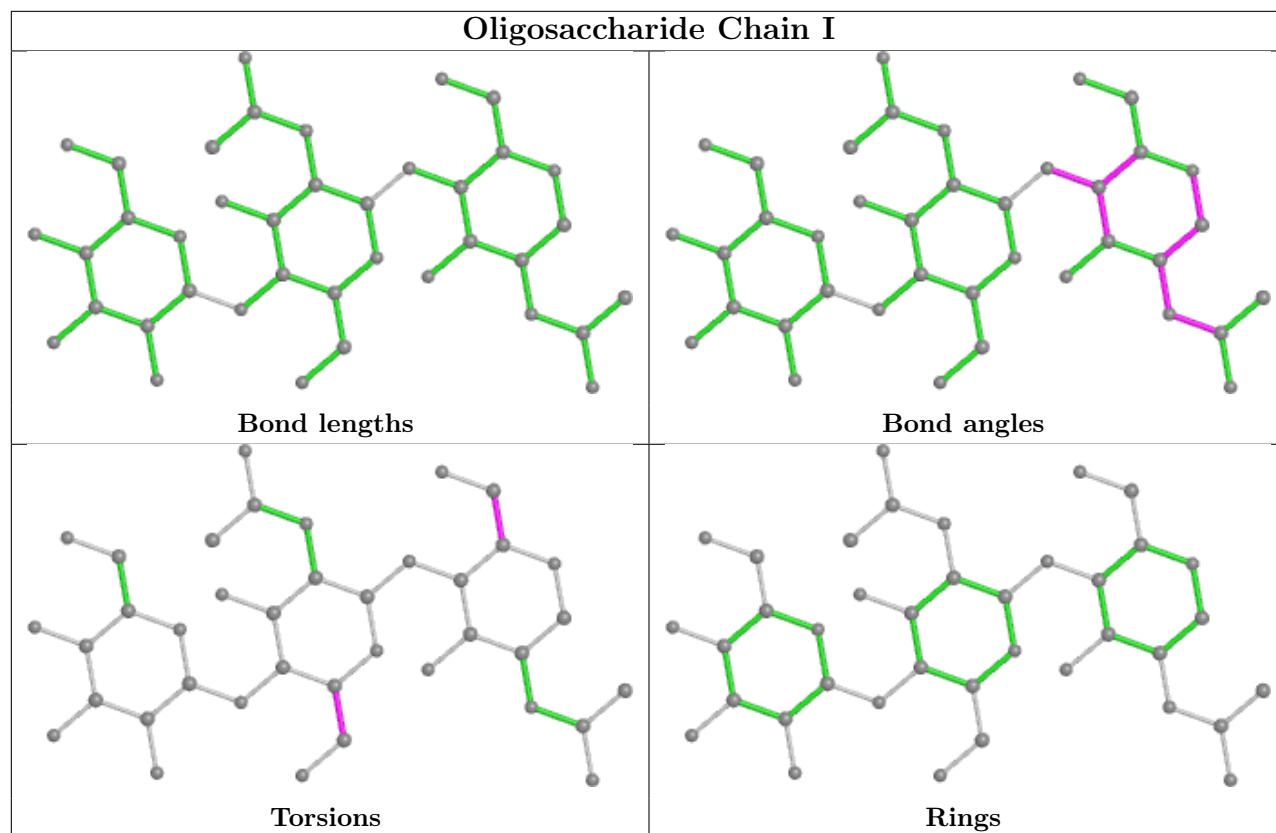
No monomer is involved in short contacts.

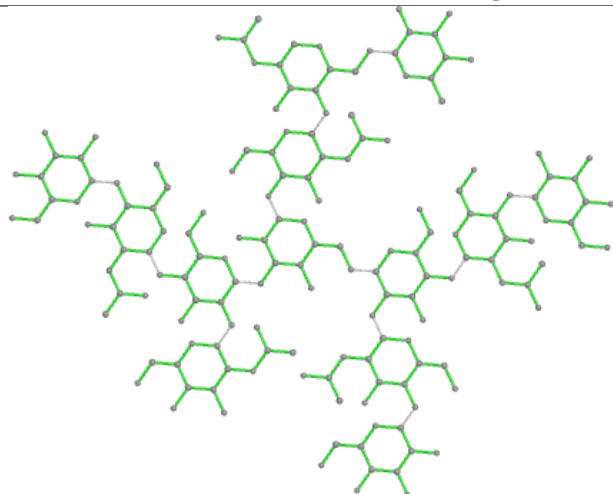
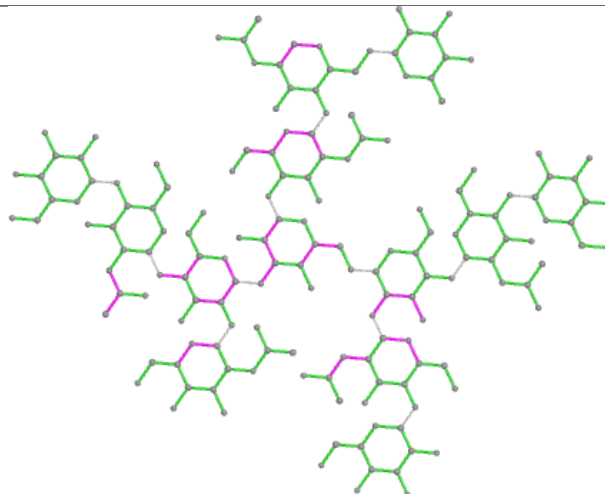
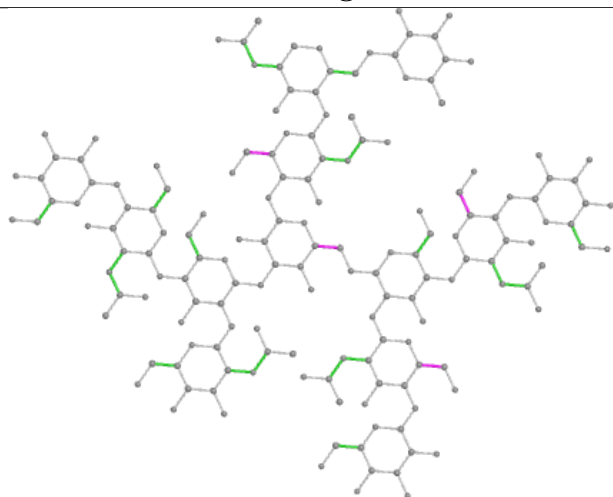
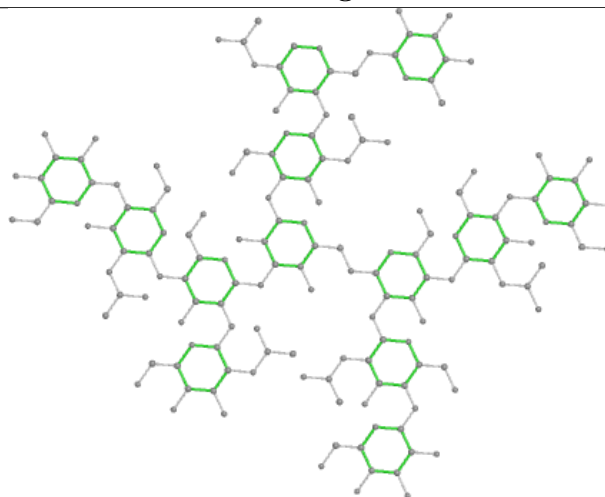
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

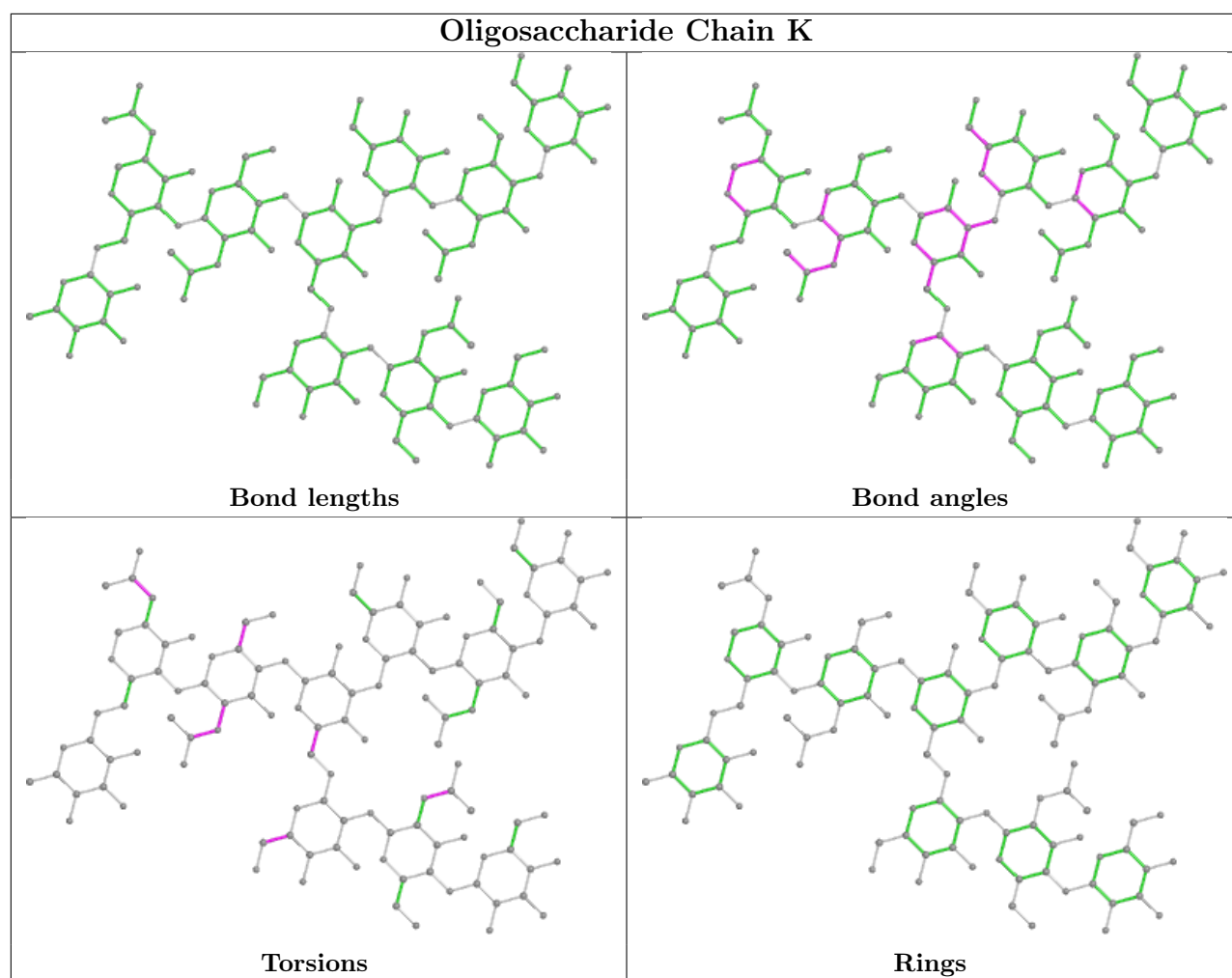


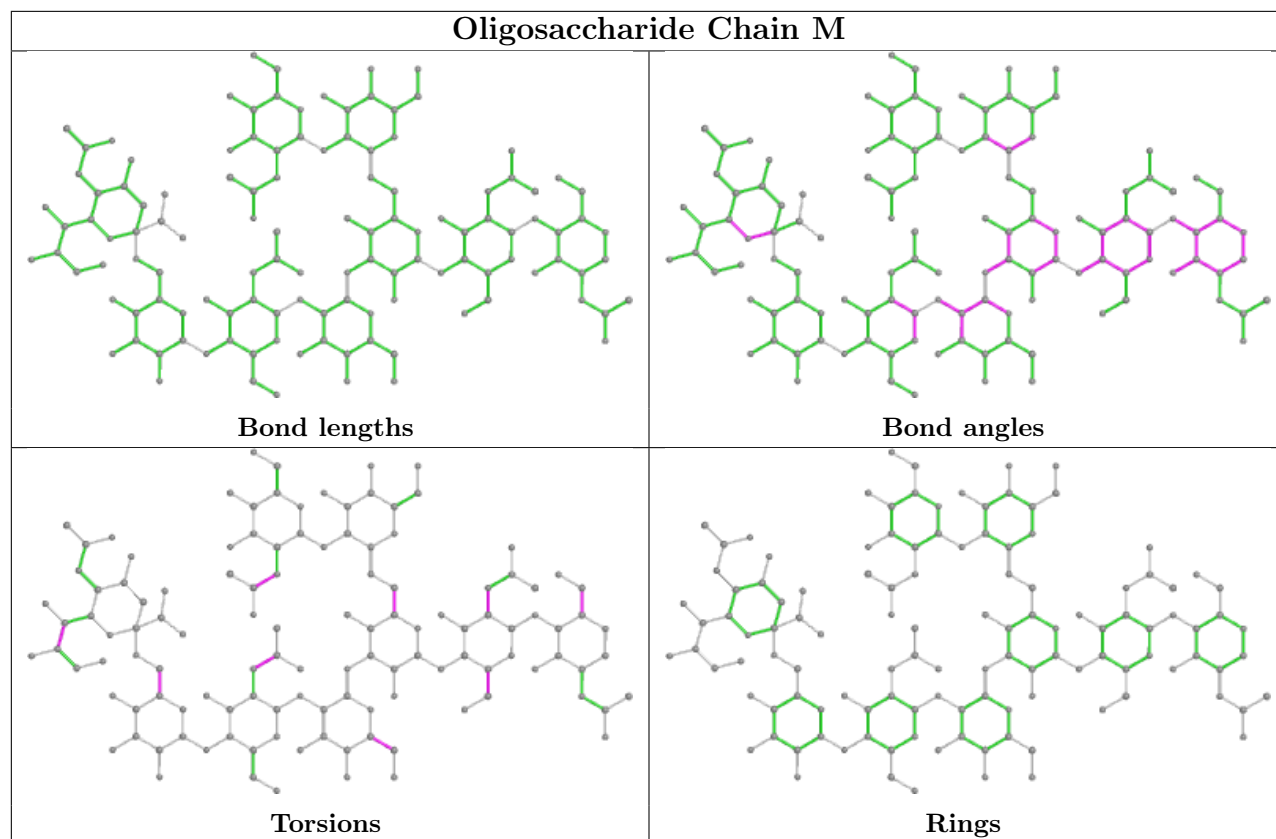


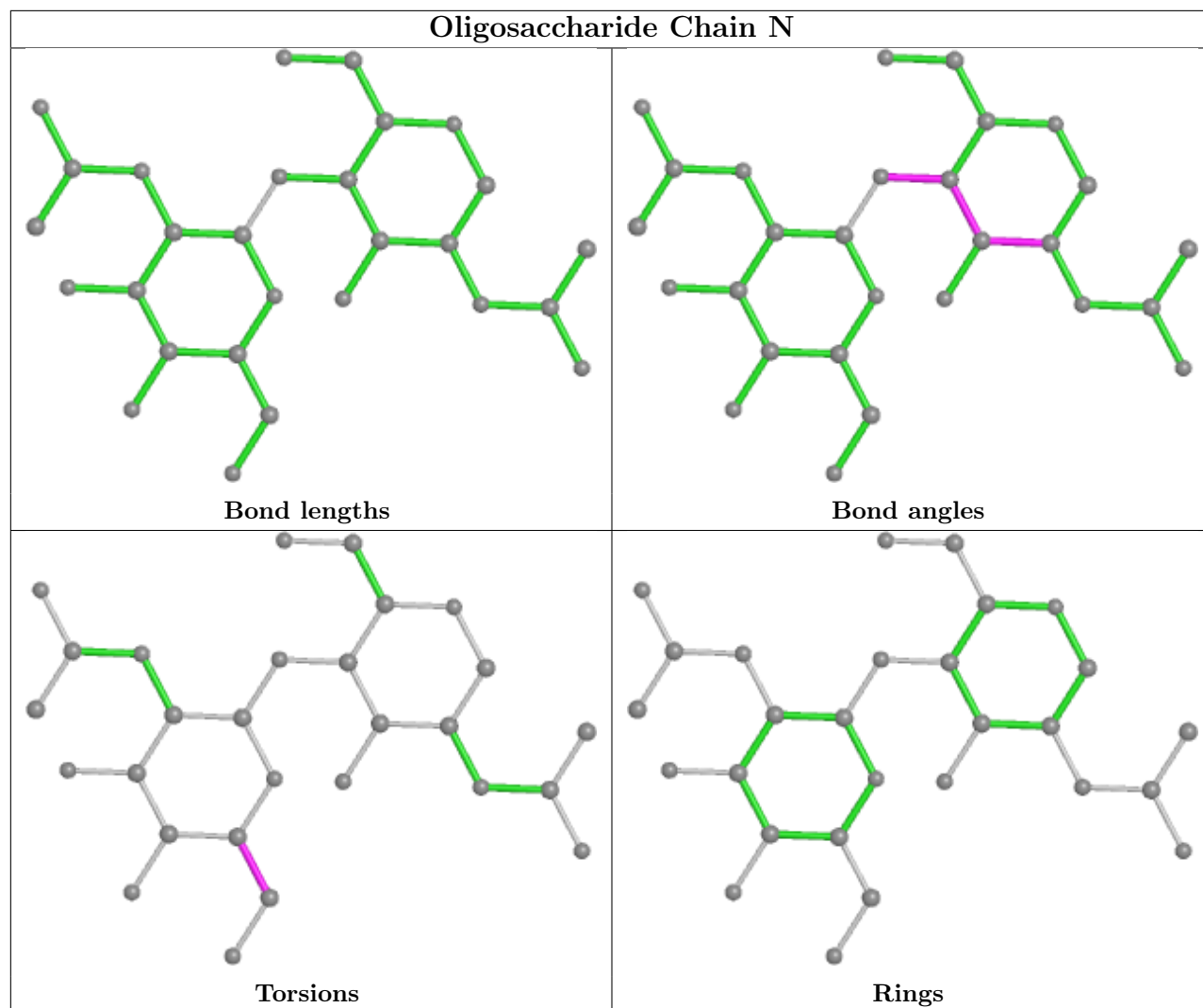


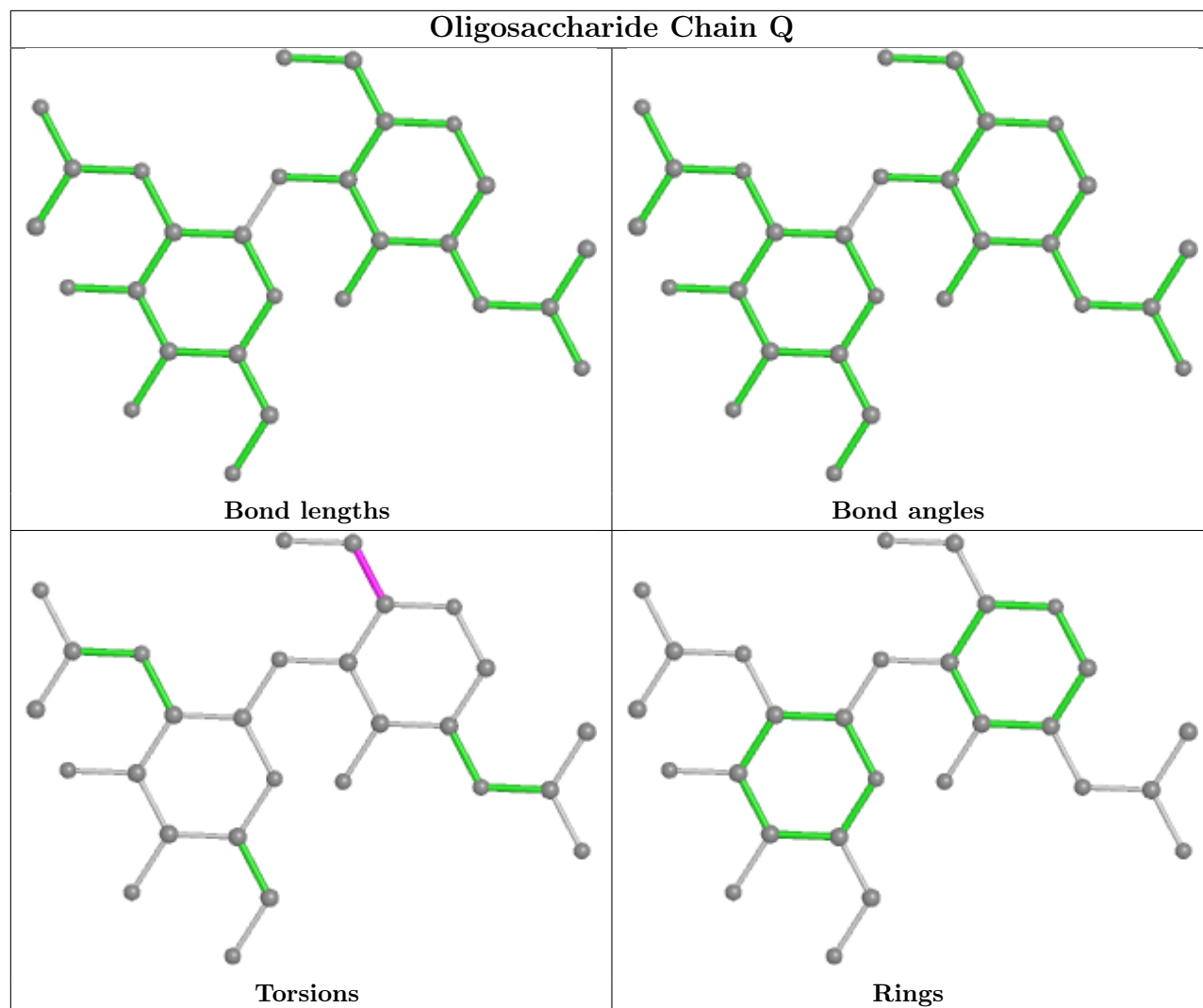


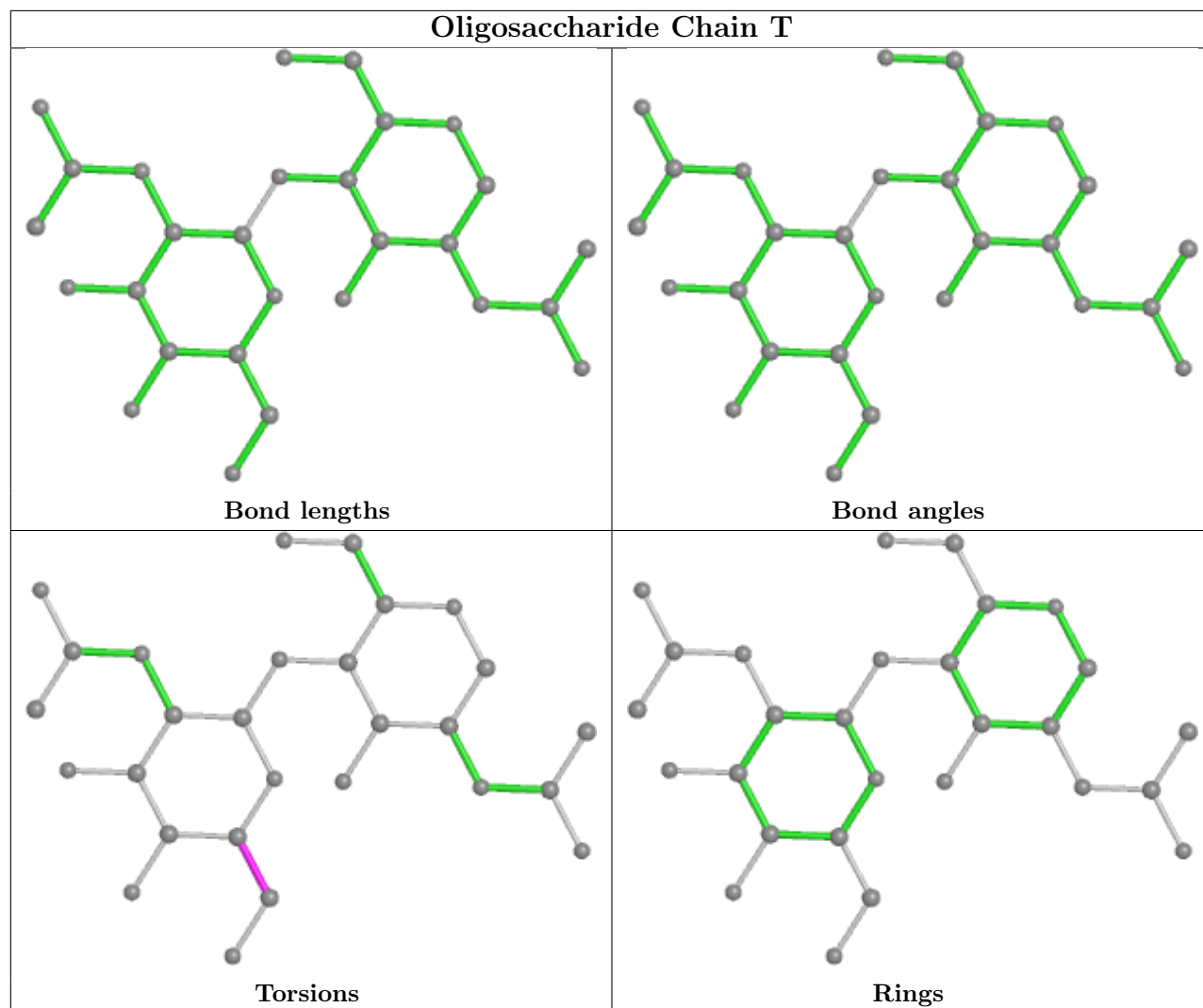
Oligosaccharide Chain J**Bond lengths****Bond angles****Torsions****Rings**

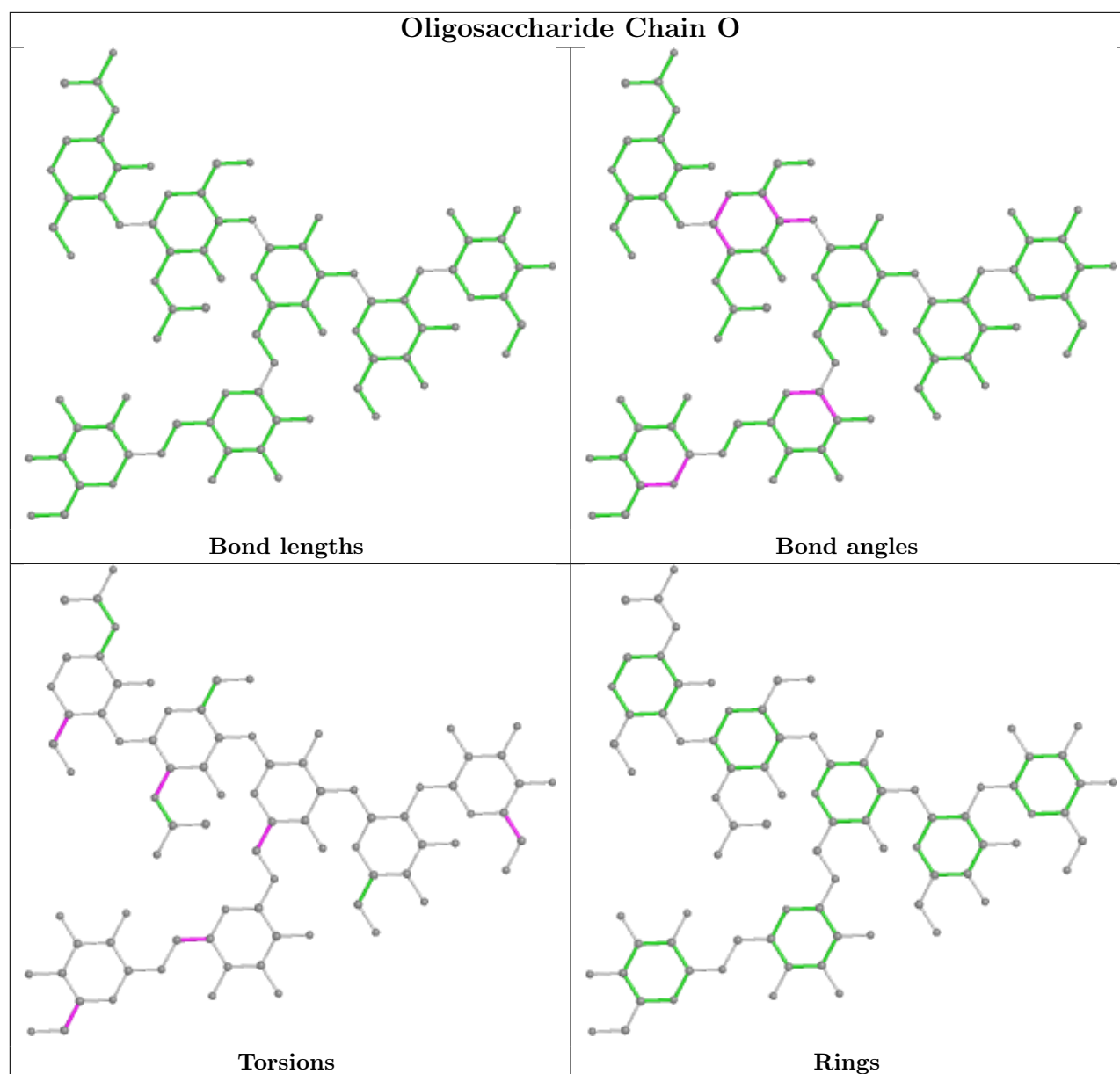


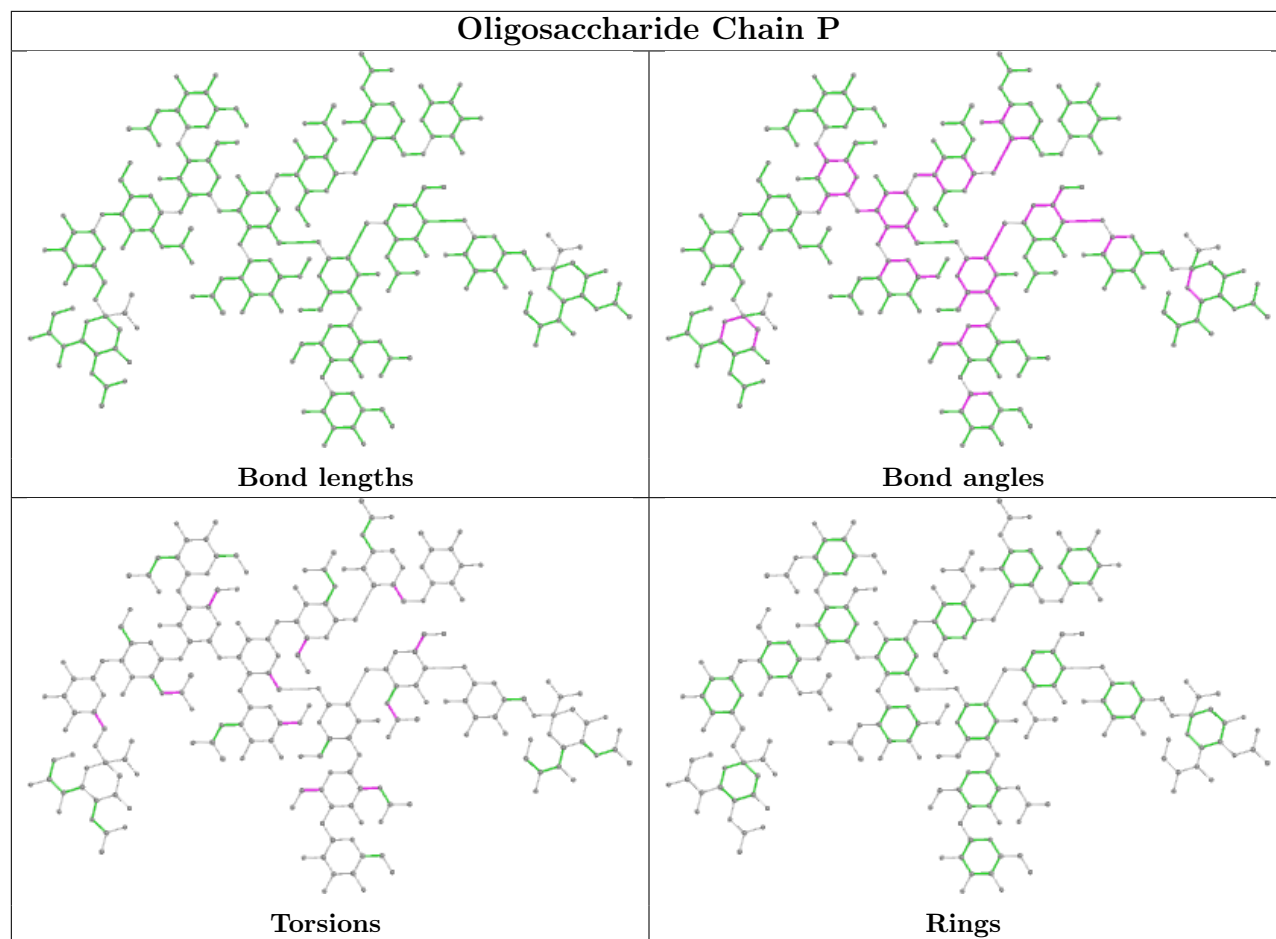


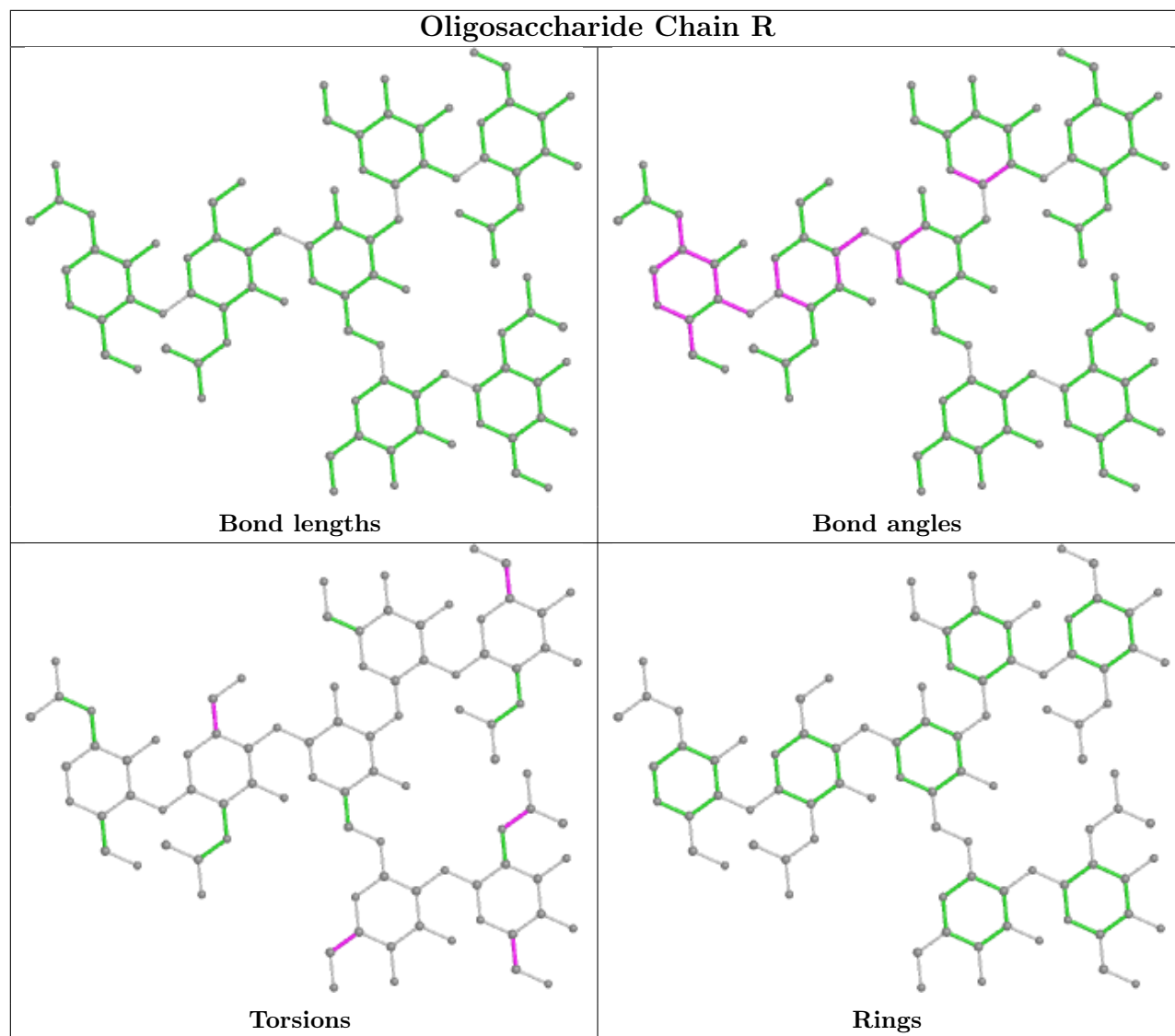


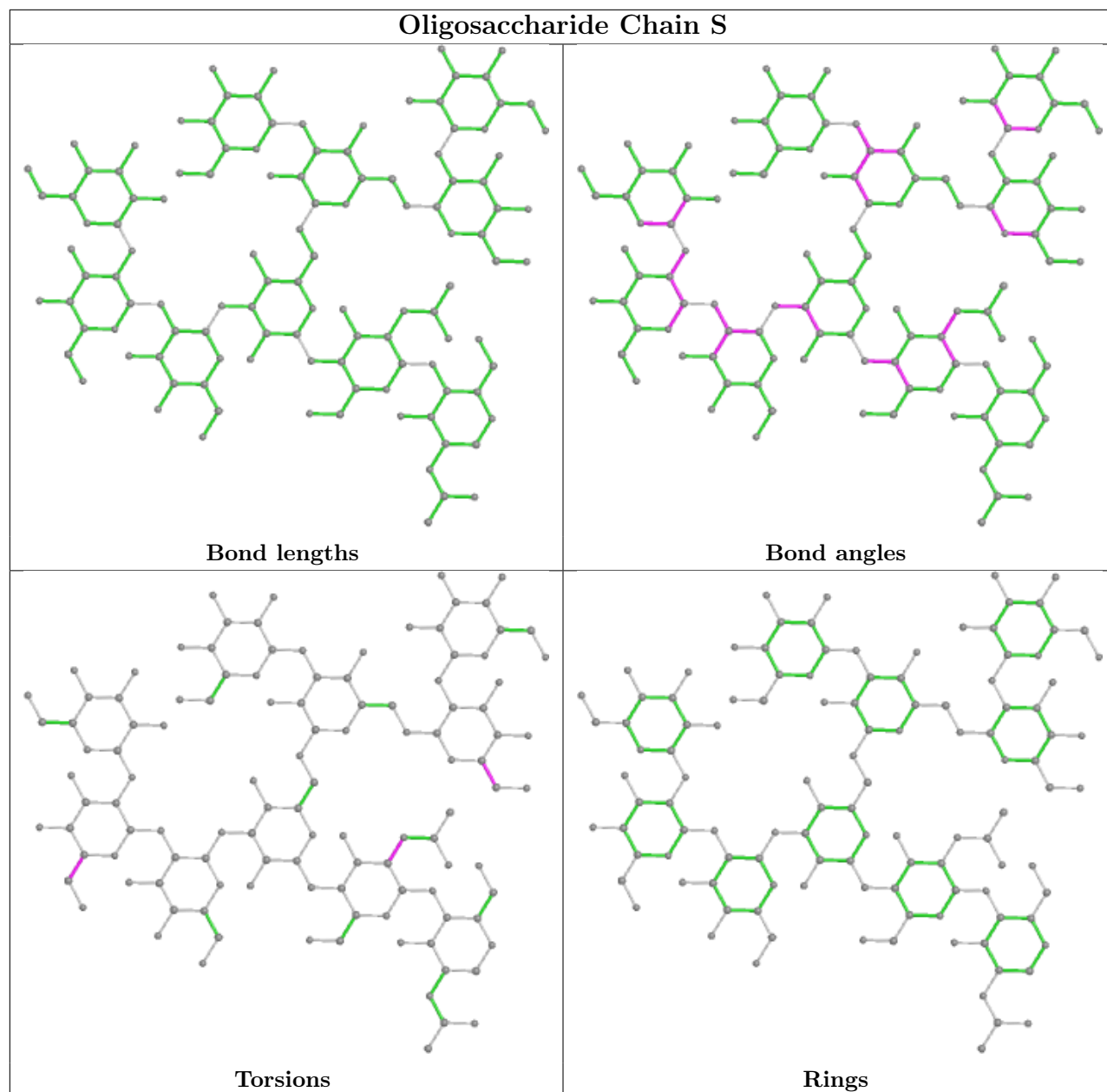


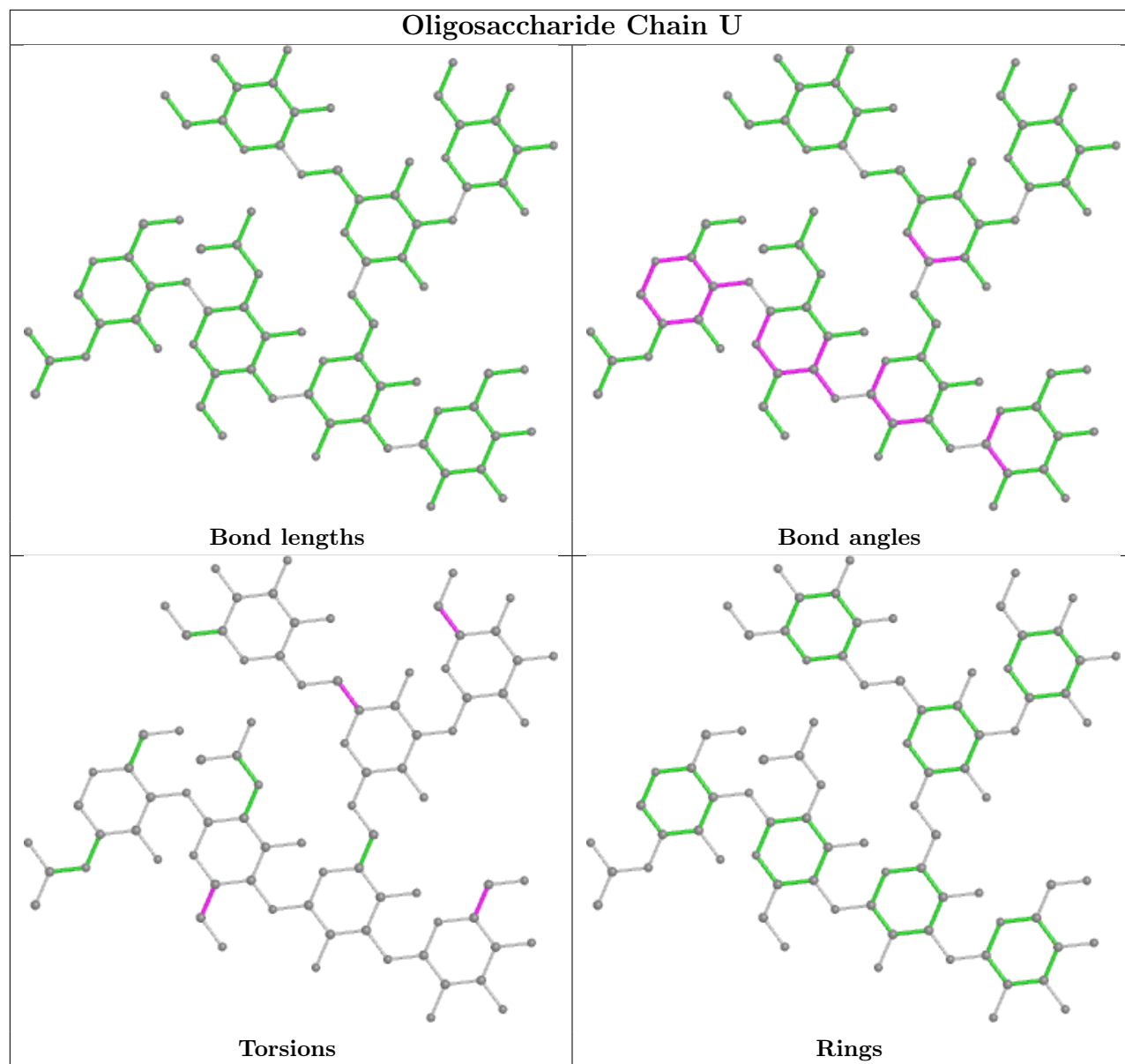


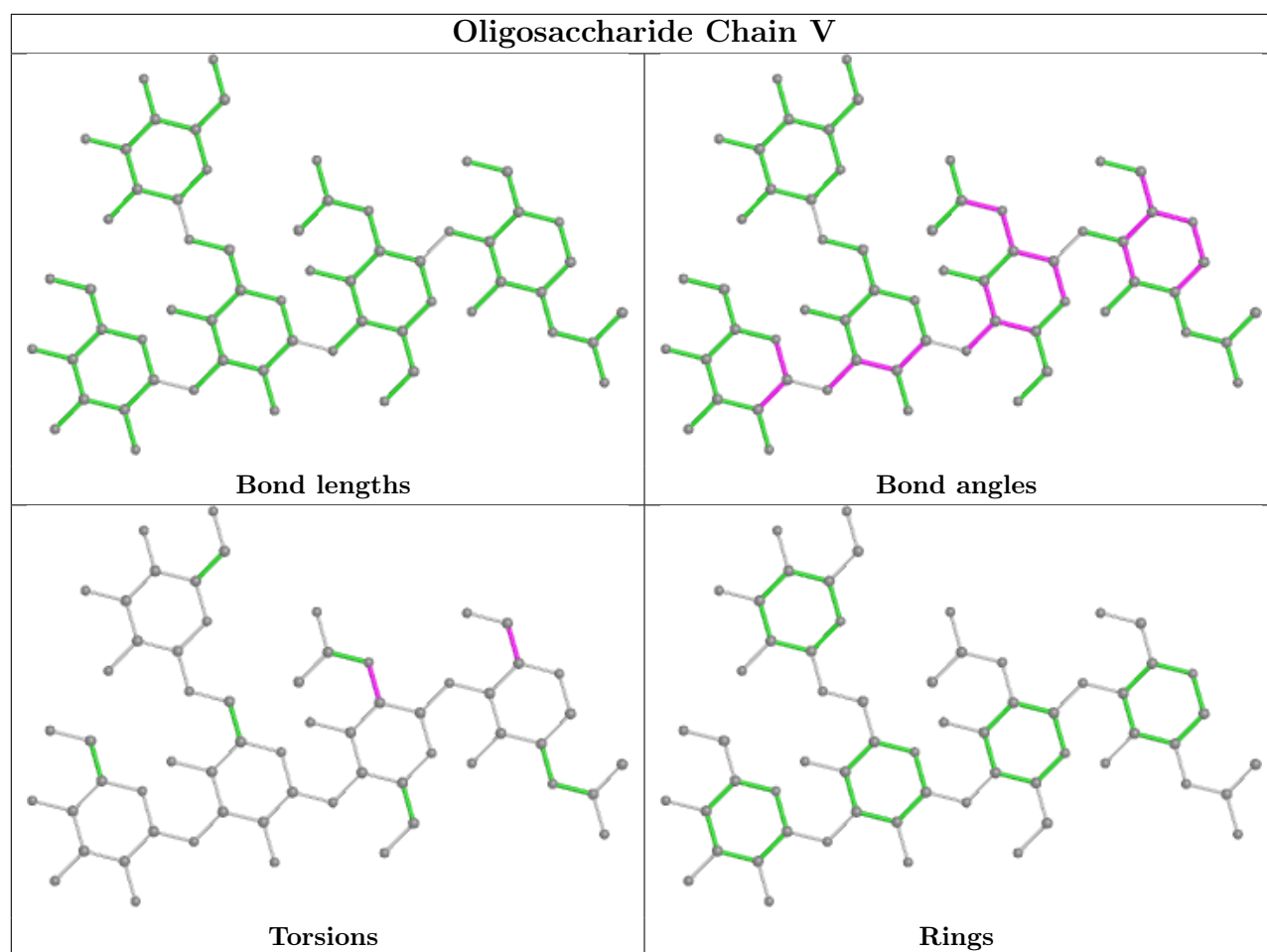




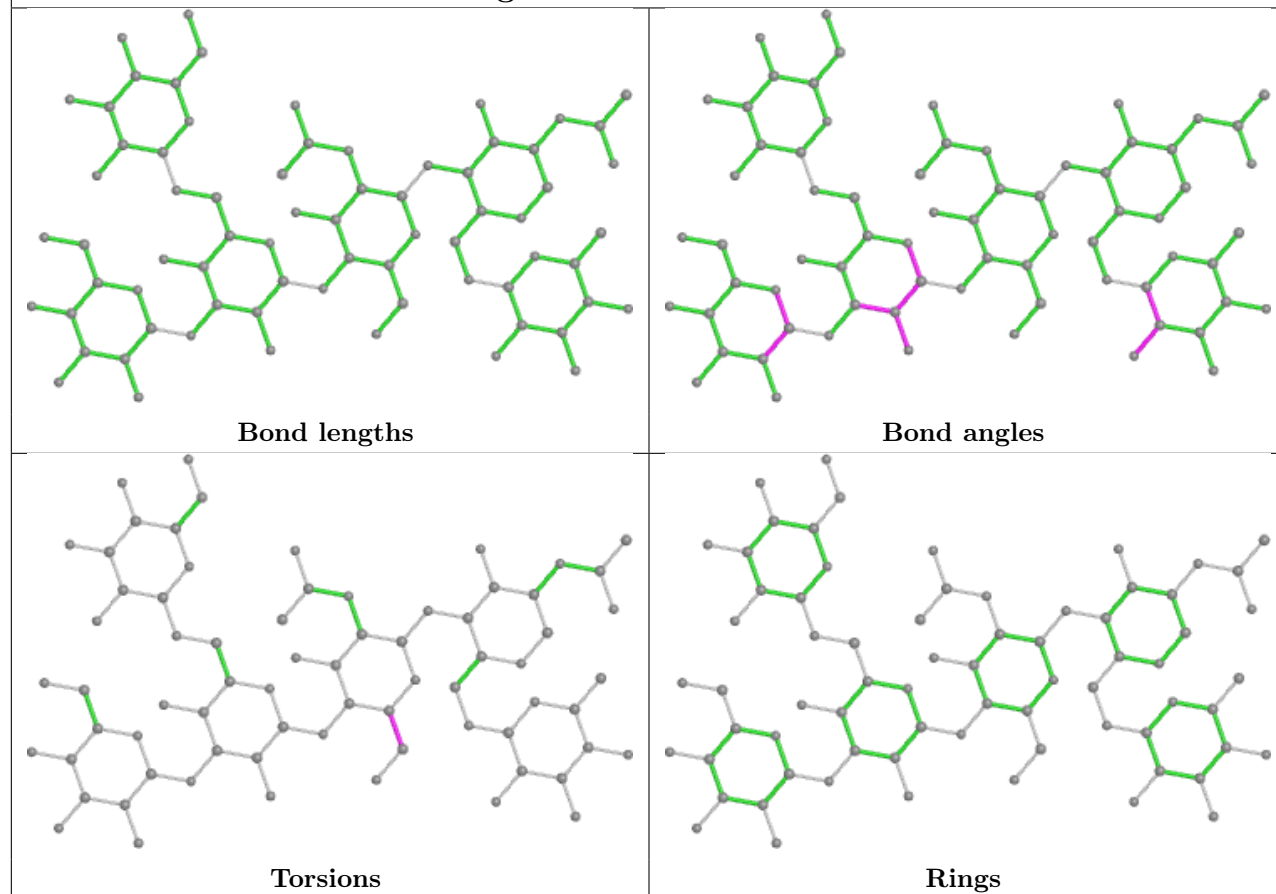




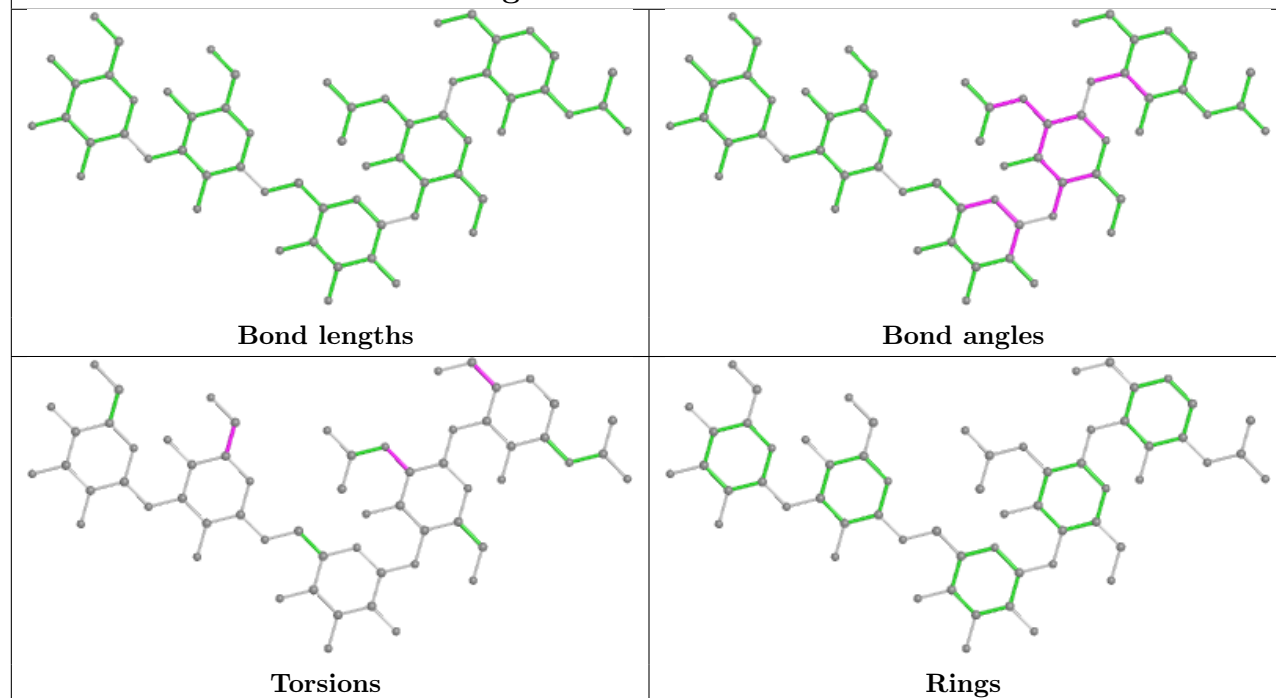




Oligosaccharide Chain W



Oligosaccharide Chain X



4.6 Ligand geometry

1 ligand is 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	$\# Z > 2$
23	NAG	G	3390	2	14,14,15	0.32	0	17,19,21	0.64	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
23	NAG	G	3390	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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

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.