



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 5, 2023 – 09:13 AM EDT

PDB ID : 6W03
Title : Crystal Structure of HIV-1 BG505 DS-SOSIP.3mut Prefusion Env Trimer in Complex with Human Antibodies 3H109L and 35O22 at 3.3 Angstrom
Authors : Lai, Y.-T.; Kwong, P.D.
Deposited on : 2020-02-28
Resolution : 2.40 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)
Xtrriage (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

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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 13 unique types of molecules in this entry. The entry contains 10096 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 gp41.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	124	988	627	170	185	6	0	0	0

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 35O22 scFv heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	128	994	628	169	192	5	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	112	851	533	141	171	6	0	0	0

- Molecule 4 is a protein called Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	G	427	3365	2121	592	622	30	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	145	ALA	ASN	engineered mutation	UNP Q2N0S6
G	201	CYS	ILE	engineered mutation	UNP Q2N0S6

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Chain	Residue	Modelled	Actual	Comment	Reference
G	302	MET	ASN	engineered mutation	UNP Q2N0S6
G	320	LEU	THR	engineered mutation	UNP Q2N0S6
G	329	PRO	ALA	engineered mutation	UNP Q2N0S6
G	332	ASN	THR	engineered mutation	UNP Q2N0S6
G	433	CYS	ALA	engineered mutation	UNP Q2N0S6
G	501	CYS	ALA	engineered mutation	UNP Q2N0S6
G	508	ARG	-	expression tag	UNP Q2N0S6
G	509	ARG	-	expression tag	UNP Q2N0S6
G	510	ARG	-	expression tag	UNP Q2N0S6
G	511	ARG	-	expression tag	UNP Q2N0S6
G	512	ARG	-	expression tag	UNP Q2N0S6
G	513	ARG	-	expression tag	UNP Q2N0S6

- Molecule 5 is a protein called 3H109L Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	H	227	1721	1096	279	340	6	0	0	0

- Molecule 6 is a protein called 3H109L Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	L	211	1604	1009	276	312	7	0	0	0

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

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

- 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
			Total	C	N	O			
8	C	2	28	16	2	10	0	0	0
8	F	2	28	16	2	10	0	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
8	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
8	K	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 9 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
9	M	5	Total	C	N	O	0	0	0
			61	34	2	25			

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

- Molecule 11 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-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.

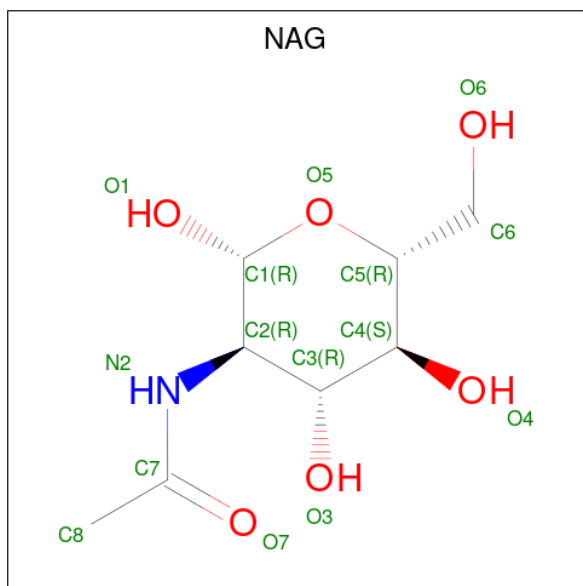
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	O	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 12 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
12	P	10	Total	C	N	O	0	0	0
			116	64	2	50			

- Molecule 13 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG)

(formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
13	B	1	Total 14	8	1	5	0	0
13	B	1	Total 14	8	1	5	0	0
13	G	1	Total 14	8	1	5	0	0
13	G	1	Total 14	8	1	5	0	0
13	G	1	Total 14	8	1	5	0	0
13	G	1	Total 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	P 63	Depositor
Cell constants a, b, c, α , β , γ	131.39Å 131.39Å 315.34Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.80 – 2.40	Depositor
% Data completeness (in resolution range)	29.4 (39.80-2.40)	Depositor
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.00 (at 2.37Å)	Xtrriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.230 , 0.273	Depositor
Wilson B-factor (Å ²)	31.6	Xtrriage
Anisotropy	0.046	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.057 for h,-h-k,-l	Xtrriage
Total number of atoms	10096	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.44% 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](#)

39 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	7,4	14,14,15	0.26	0	17,19,21	0.50	0
7	NAG	A	2	7	14,14,15	0.25	0	17,19,21	0.46	0
7	BMA	A	3	7	11,11,12	1.09	1 (9%)	15,15,17	1.16	2 (13%)
7	MAN	A	4	7	11,11,12	0.60	0	15,15,17	1.02	2 (13%)
8	NAG	C	1	4,8	14,14,15	0.94	1 (7%)	17,19,21	1.66	1 (5%)
8	NAG	C	2	8	14,14,15	0.23	0	17,19,21	0.42	0
8	NAG	F	1	4,8	14,14,15	0.25	0	17,19,21	0.44	0
8	NAG	F	2	8	14,14,15	0.27	0	17,19,21	0.38	0
8	NAG	I	1	4,8	14,14,15	0.30	0	17,19,21	0.45	0
8	NAG	I	2	8	14,14,15	0.24	0	17,19,21	0.47	0
8	NAG	J	1	4,8	14,14,15	0.29	0	17,19,21	0.48	0
8	NAG	J	2	8	14,14,15	0.27	0	17,19,21	0.37	0
8	NAG	K	1	4,8	14,14,15	0.21	0	17,19,21	0.48	0
8	NAG	K	2	8	14,14,15	0.24	0	17,19,21	0.47	0
9	NAG	M	1	4,9	14,14,15	0.25	0	17,19,21	0.41	0
9	NAG	M	2	9	14,14,15	0.22	0	17,19,21	0.37	0
9	BMA	M	3	9	11,11,12	0.76	0	15,15,17	0.88	0
9	MAN	M	4	9	11,11,12	0.84	1 (9%)	15,15,17	1.24	2 (13%)
9	MAN	M	5	9	11,11,12	0.78	1 (9%)	15,15,17	1.19	2 (13%)
10	NAG	N	1	10,4	14,14,15	0.33	0	17,19,21	0.45	0
10	NAG	N	2	10	14,14,15	0.21	0	17,19,21	0.50	0
10	BMA	N	3	10	11,11,12	0.66	0	15,15,17	0.78	0
10	MAN	N	4	10	11,11,12	1.08	1 (9%)	15,15,17	1.57	4 (26%)
11	NAG	O	1	4,11	14,14,15	0.30	0	17,19,21	0.44	0
11	NAG	O	2	11	14,14,15	0.43	0	17,19,21	1.28	1 (5%)
11	BMA	O	3	11	11,11,12	0.64	0	15,15,17	0.72	0
11	MAN	O	4	11	11,11,12	1.14	1 (9%)	15,15,17	1.33	3 (20%)
11	MAN	O	5	11	11,11,12	1.56	1 (9%)	15,15,17	1.79	3 (20%)
11	MAN	O	6	11	11,11,12	0.67	0	15,15,17	0.96	2 (13%)
12	NAG	P	1	12,4	14,14,15	0.36	0	17,19,21	1.47	2 (11%)
12	MAN	P	10	12	11,11,12	0.97	0	15,15,17	1.14	1 (6%)
12	NAG	P	2	12	14,14,15	0.25	0	17,19,21	0.47	0
12	BMA	P	3	12	11,11,12	0.95	1 (9%)	15,15,17	0.87	0
12	MAN	P	4	12	11,11,12	0.76	1 (9%)	15,15,17	1.44	2 (13%)
12	MAN	P	5	12	11,11,12	0.85	0	15,15,17	1.12	2 (13%)
12	MAN	P	6	12	11,11,12	0.79	0	15,15,17	0.86	1 (6%)
12	MAN	P	7	12	11,11,12	0.71	0	15,15,17	0.96	2 (13%)
12	MAN	P	8	12	11,11,12	0.71	0	15,15,17	0.99	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	MAN	P	9	12	11,11,12	0.78	1 (9%)	15,15,17	1.30	2 (13%)

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	7,4	-	0/6/23/26	0/1/1/1
7	NAG	A	2	7	-	2/6/23/26	0/1/1/1
7	BMA	A	3	7	-	0/2/19/22	0/1/1/1
7	MAN	A	4	7	-	2/2/19/22	0/1/1/1
8	NAG	C	1	4,8	-	4/6/23/26	0/1/1/1
8	NAG	C	2	8	-	0/6/23/26	0/1/1/1
8	NAG	F	1	4,8	-	2/6/23/26	0/1/1/1
8	NAG	F	2	8	-	0/6/23/26	0/1/1/1
8	NAG	I	1	4,8	-	2/6/23/26	0/1/1/1
8	NAG	I	2	8	-	0/6/23/26	0/1/1/1
8	NAG	J	1	4,8	-	2/6/23/26	0/1/1/1
8	NAG	J	2	8	-	0/6/23/26	0/1/1/1
8	NAG	K	1	4,8	-	2/6/23/26	0/1/1/1
8	NAG	K	2	8	-	2/6/23/26	0/1/1/1
9	NAG	M	1	4,9	-	0/6/23/26	0/1/1/1
9	NAG	M	2	9	-	0/6/23/26	0/1/1/1
9	BMA	M	3	9	-	2/2/19/22	0/1/1/1
9	MAN	M	4	9	-	0/2/19/22	0/1/1/1
9	MAN	M	5	9	-	2/2/19/22	0/1/1/1
10	NAG	N	1	10,4	-	0/6/23/26	0/1/1/1
10	NAG	N	2	10	-	1/6/23/26	0/1/1/1
10	BMA	N	3	10	-	0/2/19/22	0/1/1/1
10	MAN	N	4	10	-	0/2/19/22	0/1/1/1
11	NAG	O	1	4,11	-	0/6/23/26	0/1/1/1
11	NAG	O	2	11	-	5/6/23/26	0/1/1/1
11	BMA	O	3	11	-	2/2/19/22	0/1/1/1
11	MAN	O	4	11	-	2/2/19/22	0/1/1/1
11	MAN	O	5	11	-	1/2/19/22	0/1/1/1
11	MAN	O	6	11	-	0/2/19/22	0/1/1/1
12	NAG	P	1	12,4	-	3/6/23/26	0/1/1/1
12	MAN	P	10	12	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	NAG	P	2	12	-	2/6/23/26	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	-	0/2/19/22	0/1/1/1
12	MAN	P	7	12	-	0/2/19/22	0/1/1/1
12	MAN	P	8	12	-	2/2/19/22	0/1/1/1
12	MAN	P	9	12	-	2/2/19/22	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	O	5	MAN	C1-C2	4.35	1.62	1.52
8	C	1	NAG	O5-C1	3.38	1.49	1.43
10	N	4	MAN	C1-C2	2.97	1.59	1.52
11	O	4	MAN	O5-C1	-2.58	1.39	1.43
9	M	4	MAN	C1-C2	2.44	1.57	1.52
12	P	9	MAN	C1-C2	2.29	1.57	1.52
9	M	5	MAN	C1-C2	2.27	1.57	1.52
12	P	4	MAN	C1-C2	2.05	1.56	1.52
7	A	3	BMA	C4-C3	2.04	1.57	1.52
12	P	3	BMA	O5-C1	-2.04	1.40	1.43

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	1	NAG	C1-O5-C5	6.44	120.92	112.19
12	P	1	NAG	C2-N2-C7	4.59	129.43	122.90
11	O	2	NAG	C2-N2-C7	4.31	129.04	122.90
11	O	5	MAN	C1-C2-C3	4.17	114.80	109.67
11	O	5	MAN	C1-O5-C5	4.00	117.61	112.19
12	P	4	MAN	C1-O5-C5	3.99	117.59	112.19
12	P	9	MAN	C1-O5-C5	3.74	117.27	112.19
10	N	4	MAN	C1-O5-C5	3.63	117.11	112.19
11	O	4	MAN	C3-C4-C5	2.92	115.45	110.24
9	M	5	MAN	C1-O5-C5	2.90	116.12	112.19
12	P	8	MAN	C1-O5-C5	2.78	115.96	112.19
10	N	4	MAN	C1-C2-C3	2.77	113.07	109.67
9	M	4	MAN	C1-O5-C5	2.71	115.86	112.19
7	A	4	MAN	C1-O5-C5	2.66	115.80	112.19
7	A	3	BMA	C2-C3-C4	2.53	115.27	110.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	P	1	NAG	C1-C2-N2	2.50	114.76	110.49
12	P	5	MAN	O2-C2-C3	-2.49	105.16	110.14
12	P	4	MAN	O2-C2-C3	-2.43	105.27	110.14
11	O	6	MAN	C1-O5-C5	2.34	115.36	112.19
10	N	4	MAN	O5-C1-C2	2.32	114.36	110.77
11	O	4	MAN	O2-C2-C3	-2.29	105.54	110.14
12	P	7	MAN	C1-O5-C5	2.29	115.30	112.19
12	P	10	MAN	O2-C2-C3	-2.28	105.57	110.14
11	O	5	MAN	O2-C2-C3	-2.28	105.58	110.14
7	A	4	MAN	O2-C2-C3	-2.25	105.62	110.14
12	P	9	MAN	O2-C2-C3	-2.25	105.64	110.14
11	O	6	MAN	O2-C2-C3	-2.21	105.70	110.14
10	N	4	MAN	O2-C2-C3	-2.19	105.74	110.14
12	P	7	MAN	O2-C2-C3	-2.18	105.77	110.14
9	M	5	MAN	O2-C2-C3	-2.17	105.80	110.14
7	A	3	BMA	C3-C4-C5	2.13	114.05	110.24
9	M	4	MAN	O2-C2-C3	-2.13	105.88	110.14
12	P	5	MAN	C1-C2-C3	2.06	112.20	109.67
12	P	6	MAN	O2-C2-C3	-2.04	106.05	110.14
11	O	4	MAN	C2-C3-C4	2.03	114.41	110.89

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	O	2	NAG	O5-C5-C6-O6
8	K	2	NAG	O5-C5-C6-O6
11	O	3	BMA	O5-C5-C6-O6
9	M	3	BMA	C4-C5-C6-O6
12	P	2	NAG	O5-C5-C6-O6
7	A	2	NAG	O5-C5-C6-O6
7	A	4	MAN	O5-C5-C6-O6
8	K	2	NAG	C4-C5-C6-O6
11	O	2	NAG	C4-C5-C6-O6
8	C	1	NAG	O5-C5-C6-O6
8	J	1	NAG	O5-C5-C6-O6
11	O	3	BMA	C4-C5-C6-O6
7	A	2	NAG	C4-C5-C6-O6
9	M	3	BMA	O5-C5-C6-O6
8	J	1	NAG	C4-C5-C6-O6
12	P	2	NAG	C4-C5-C6-O6
12	P	4	MAN	O5-C5-C6-O6

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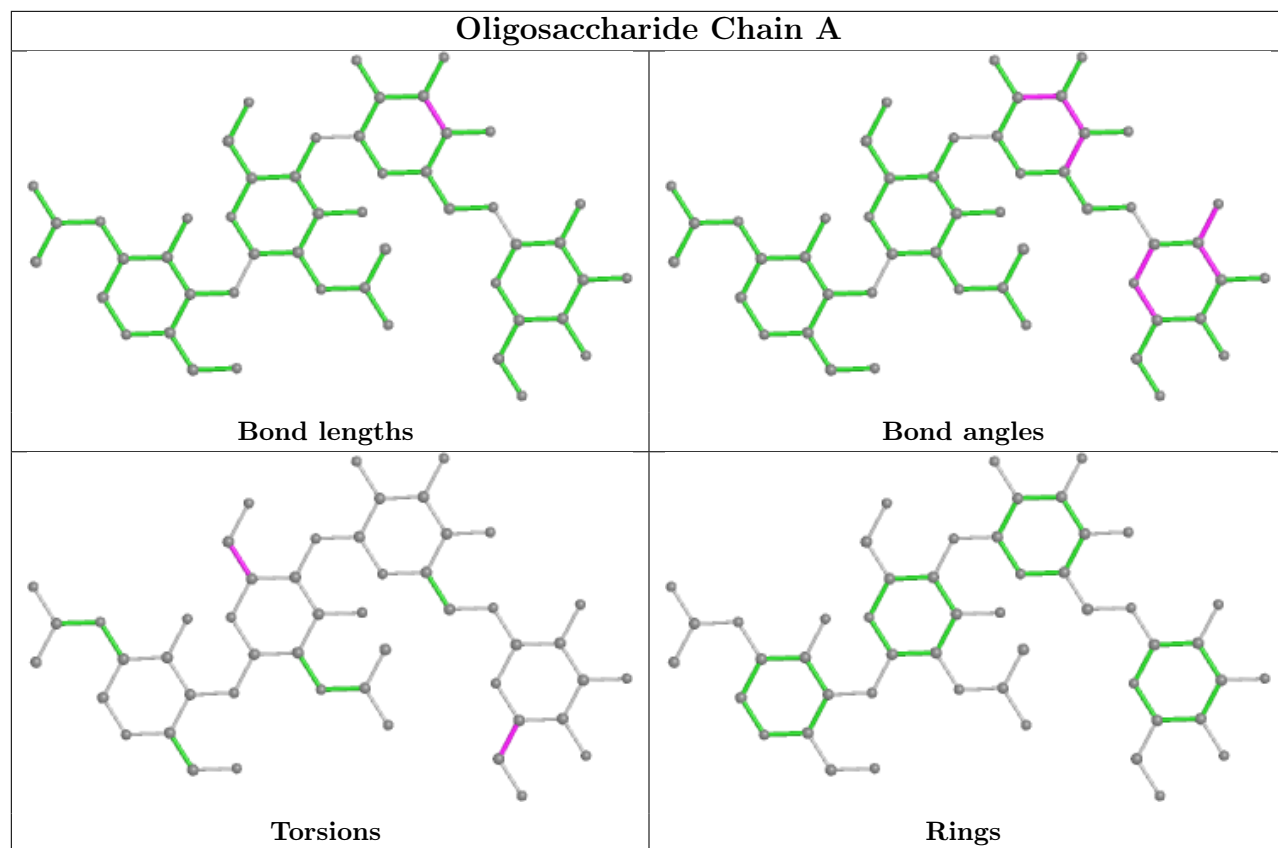
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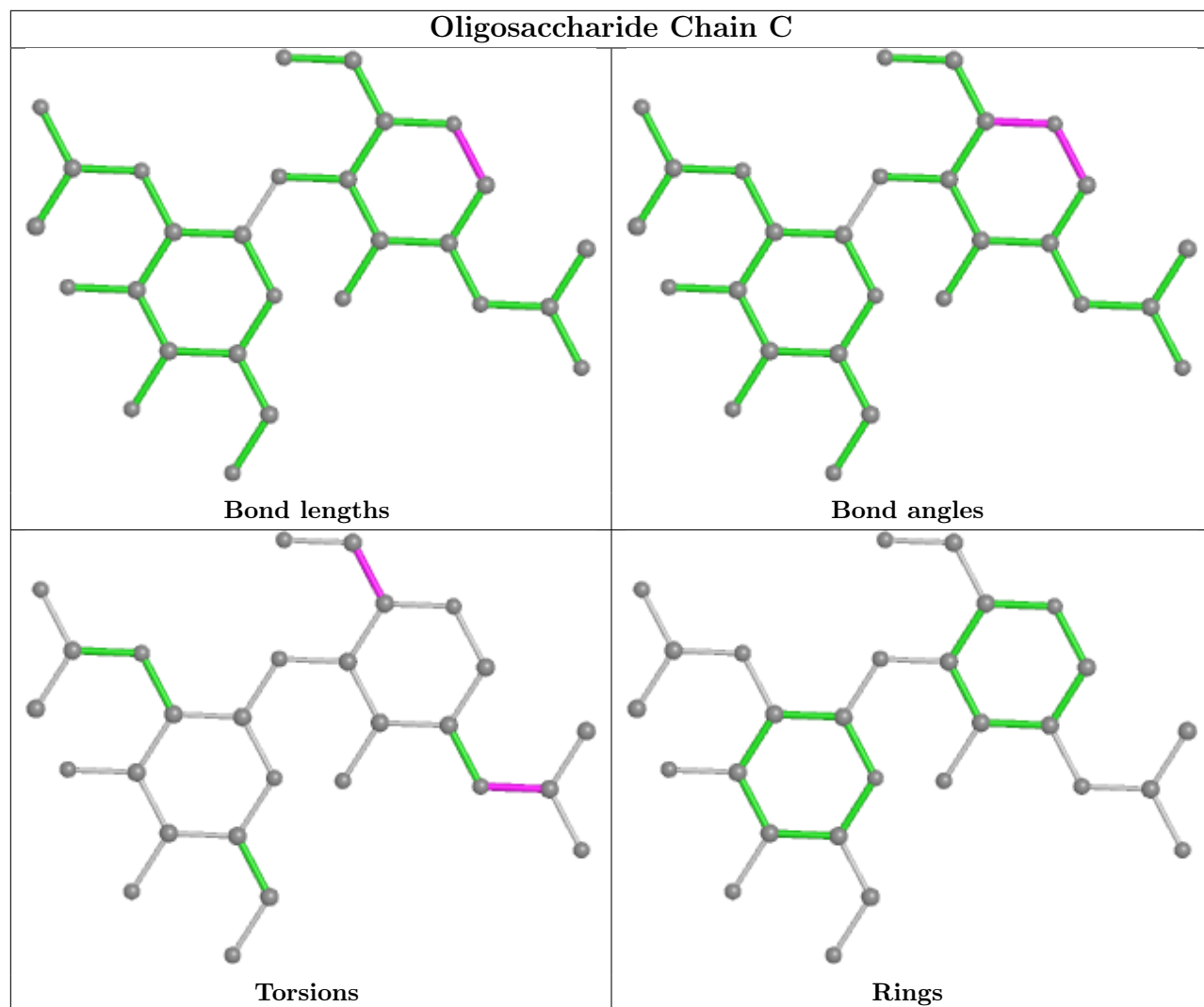
Mol	Chain	Res	Type	Atoms
8	C	1	NAG	C8-C7-N2-C2
8	C	1	NAG	O7-C7-N2-C2
11	O	2	NAG	C8-C7-N2-C2
11	O	2	NAG	O7-C7-N2-C2
12	P	1	NAG	C8-C7-N2-C2
12	P	1	NAG	O7-C7-N2-C2
7	A	4	MAN	C4-C5-C6-O6
11	O	4	MAN	O5-C5-C6-O6
8	I	1	NAG	O5-C5-C6-O6
12	P	4	MAN	C4-C5-C6-O6
9	M	5	MAN	C4-C5-C6-O6
11	O	4	MAN	C4-C5-C6-O6
8	C	1	NAG	C4-C5-C6-O6
9	M	5	MAN	O5-C5-C6-O6
12	P	10	MAN	C4-C5-C6-O6
12	P	8	MAN	O5-C5-C6-O6
8	K	1	NAG	C4-C5-C6-O6
8	K	1	NAG	O5-C5-C6-O6
12	P	10	MAN	O5-C5-C6-O6
11	O	5	MAN	O5-C5-C6-O6
8	I	1	NAG	C4-C5-C6-O6
8	F	1	NAG	C4-C5-C6-O6
8	F	1	NAG	O5-C5-C6-O6
12	P	9	MAN	C4-C5-C6-O6
10	N	2	NAG	C4-C5-C6-O6
12	P	8	MAN	C4-C5-C6-O6
11	O	2	NAG	C3-C2-N2-C7
12	P	1	NAG	C3-C2-N2-C7
12	P	9	MAN	O5-C5-C6-O6

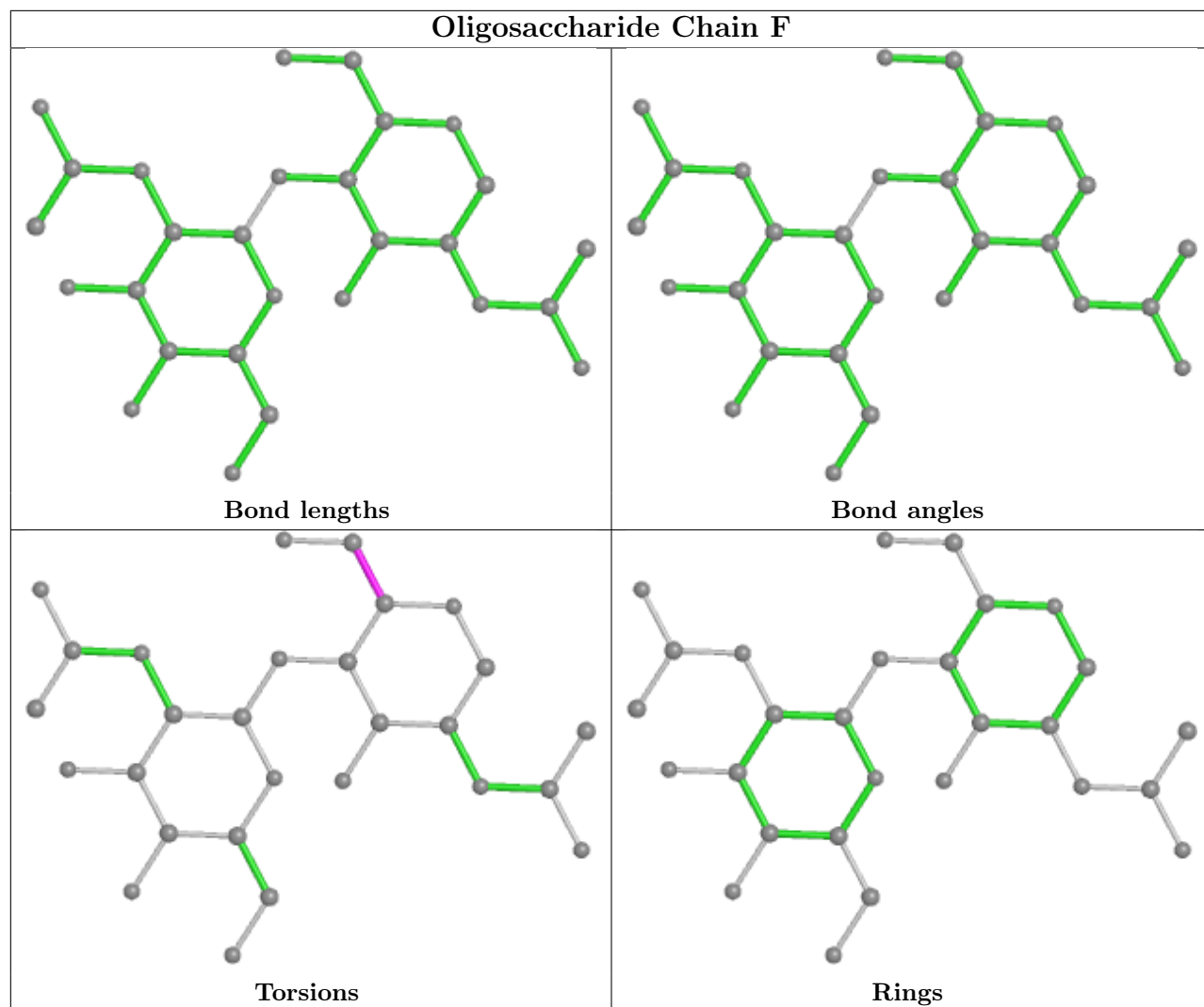
There are no ring outliers.

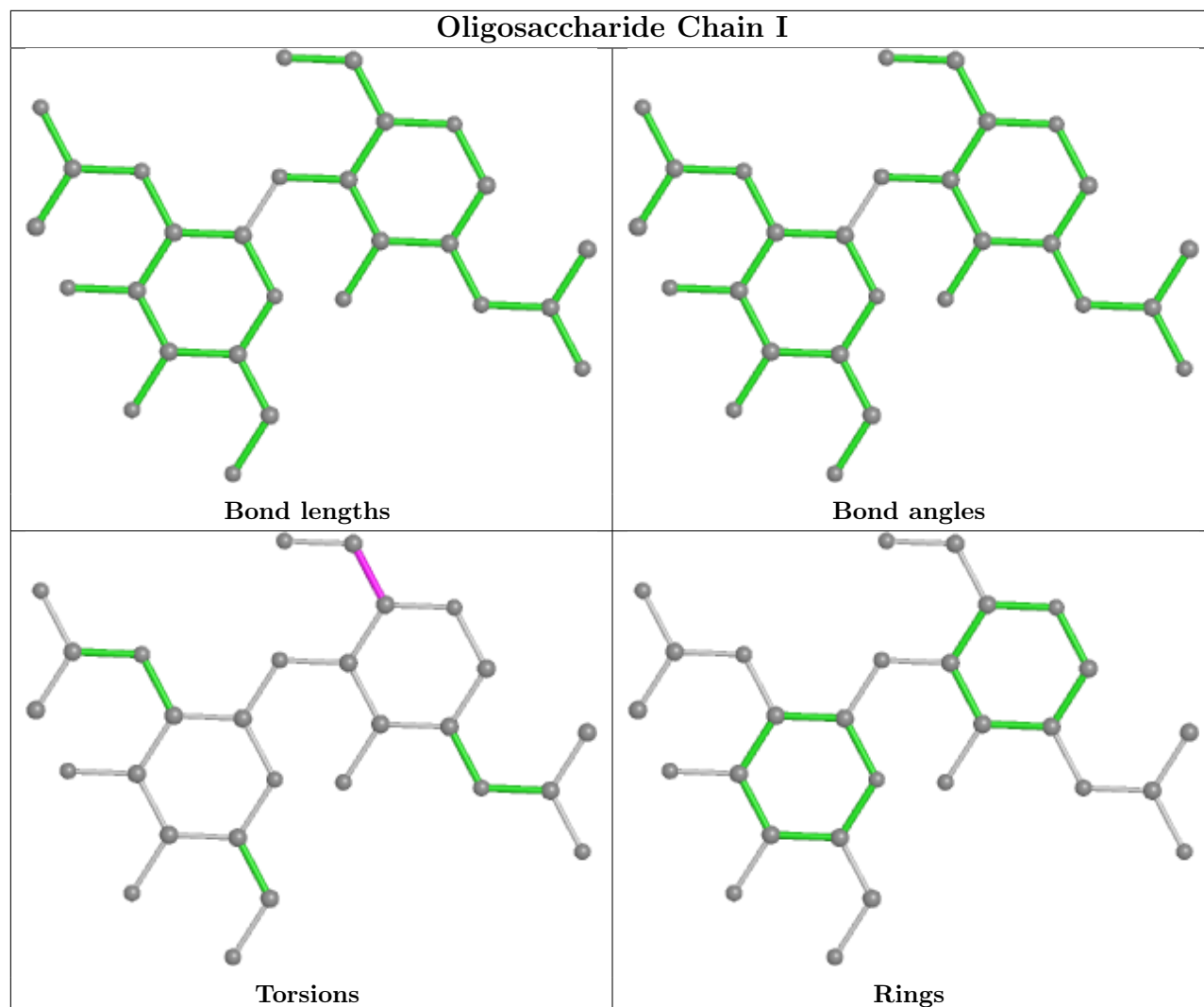
No monomer is involved in short contacts.

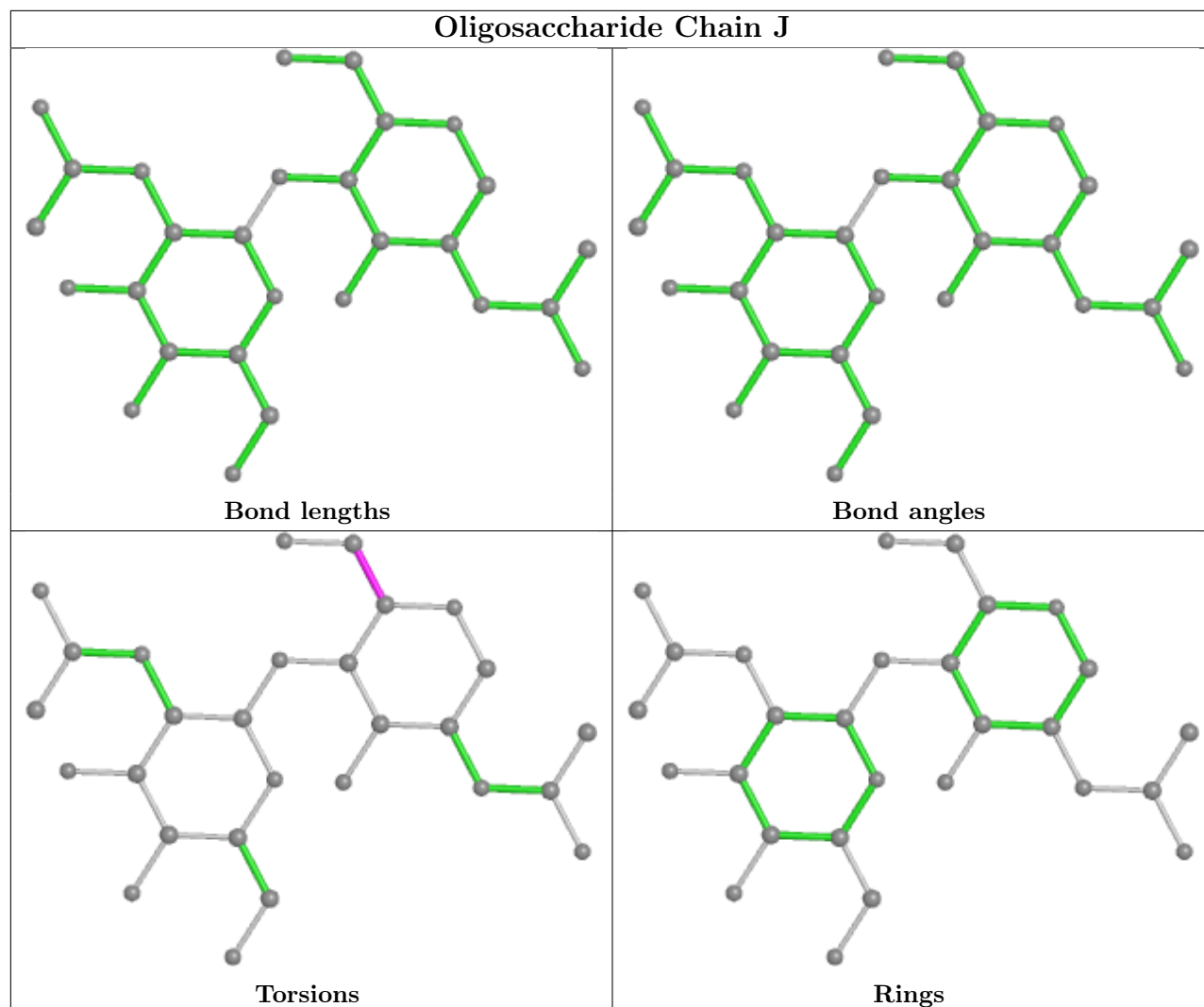
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

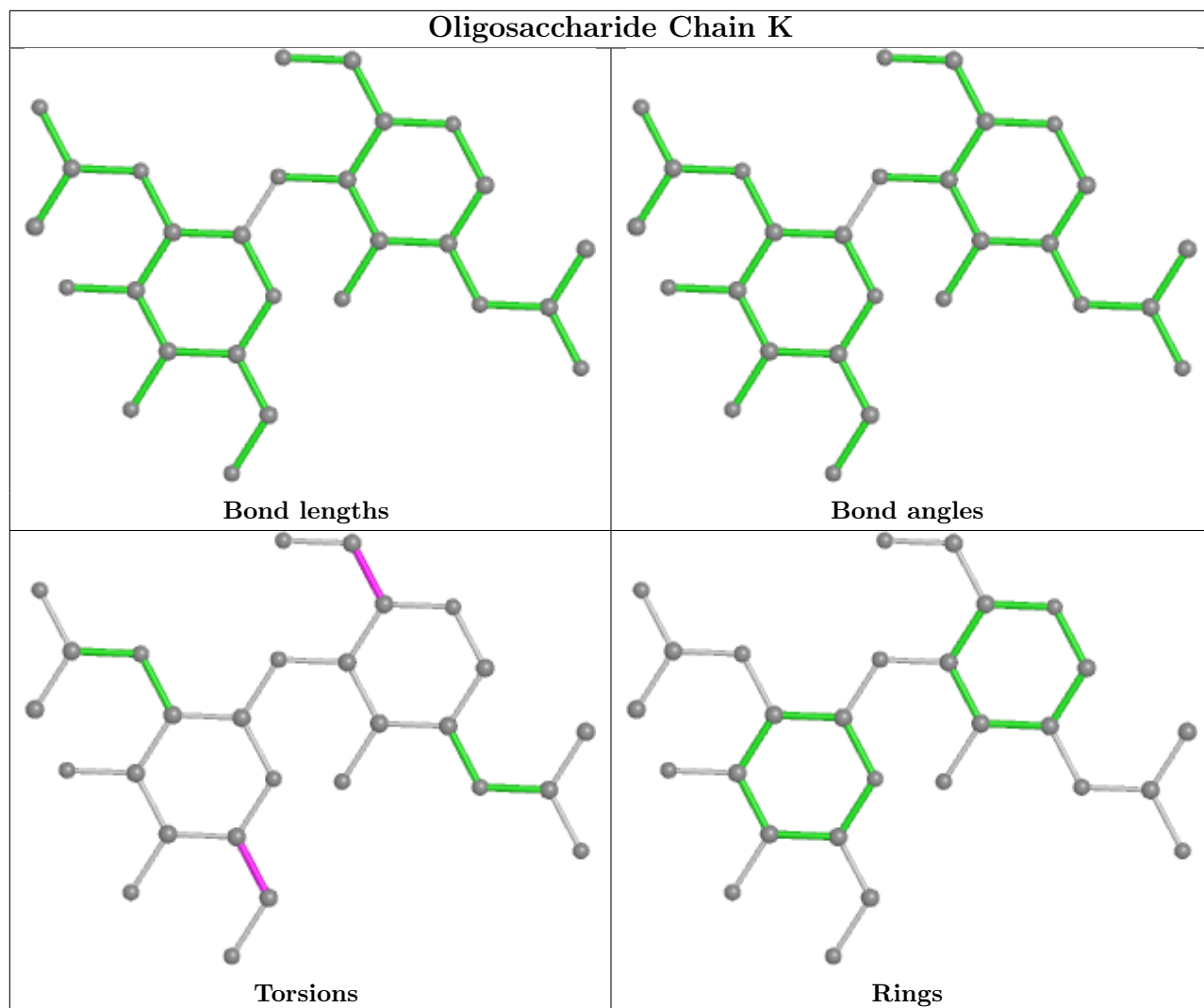


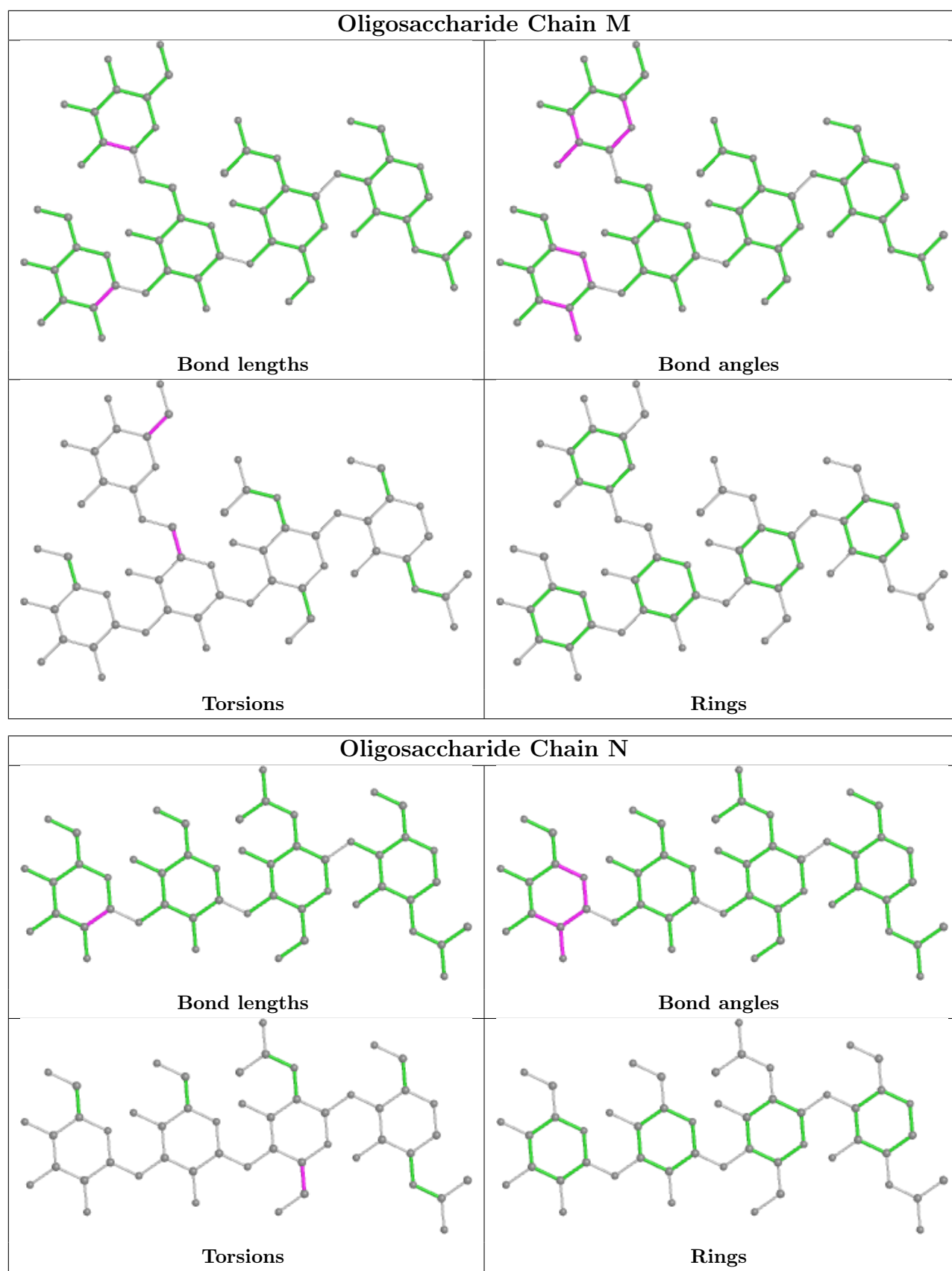


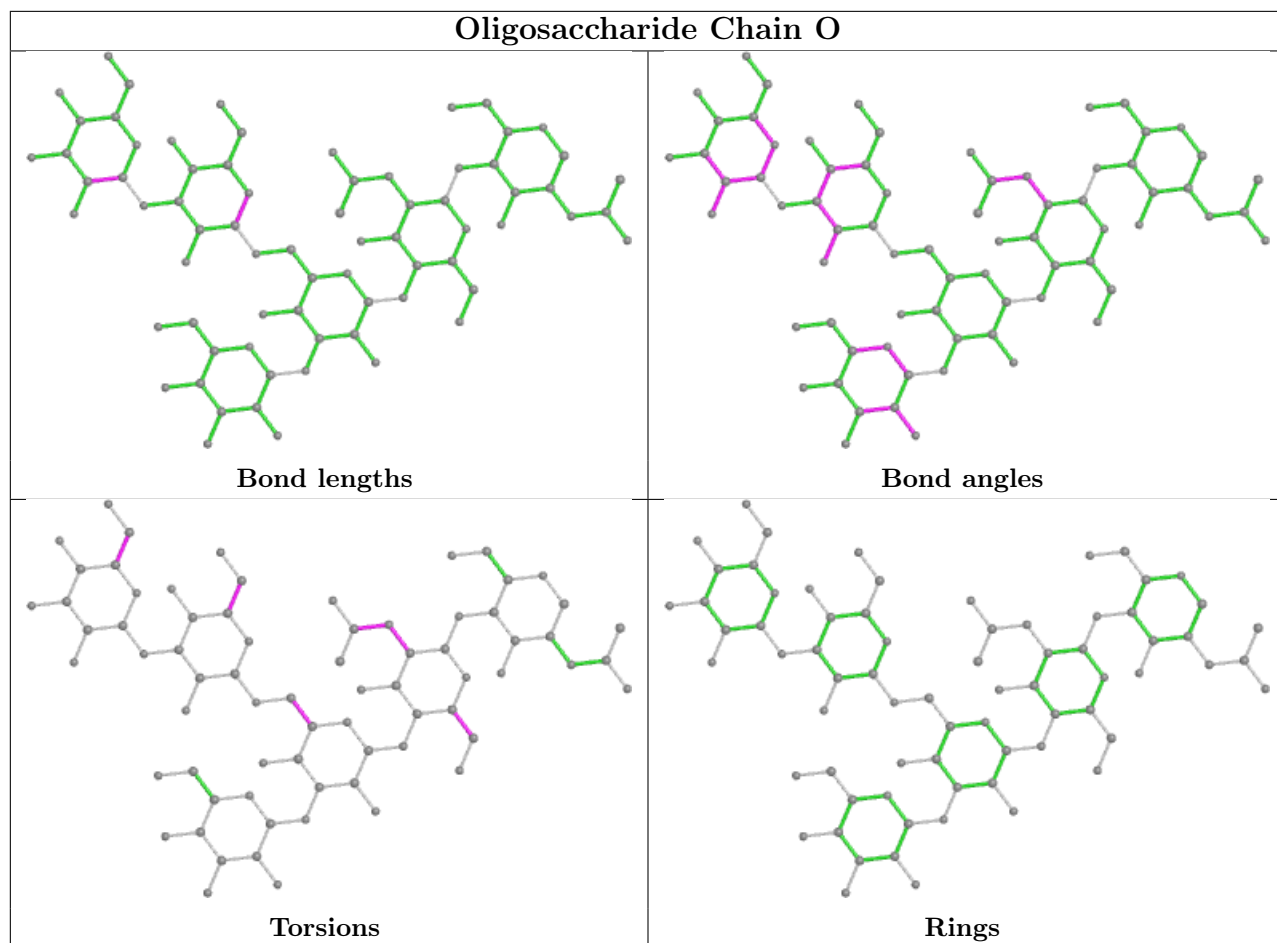


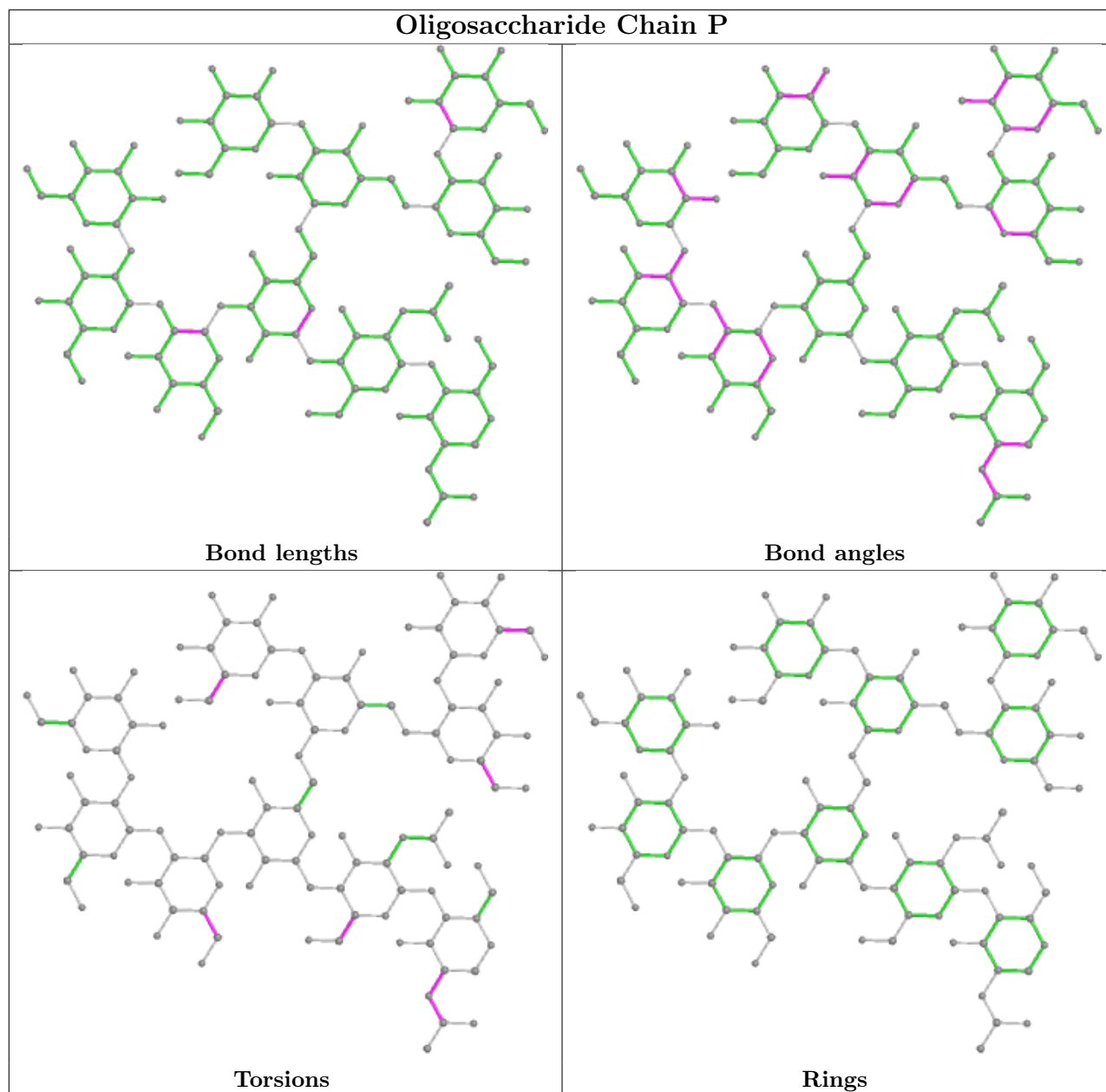












4.6 Ligand geometry [i](#)

6 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
13	NAG	G	611	4	14,14,15	0.24	0	17,19,21	0.53	0
13	NAG	G	608	4	14,14,15	0.25	0	17,19,21	0.43	0
13	NAG	G	607	4	14,14,15	0.32	0	17,19,21	0.45	0
13	NAG	B	701	1	14,14,15	0.25	0	17,19,21	0.47	0
13	NAG	B	702	1	14,14,15	0.35	0	17,19,21	0.54	0
13	NAG	G	612	4	14,14,15	0.27	0	17,19,21	0.45	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	NAG	G	611	4	-	2/6/23/26	0/1/1/1
13	NAG	G	608	4	-	0/6/23/26	0/1/1/1
13	NAG	G	607	4	-	1/6/23/26	0/1/1/1
13	NAG	B	701	1	-	1/6/23/26	0/1/1/1
13	NAG	B	702	1	-	0/6/23/26	0/1/1/1
13	NAG	G	612	4	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	G	612	NAG	O5-C5-C6-O6
13	G	611	NAG	O5-C5-C6-O6
13	G	612	NAG	C4-C5-C6-O6
13	G	611	NAG	C4-C5-C6-O6
13	B	701	NAG	O5-C5-C6-O6
13	G	607	NAG	O5-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

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.