



## wwPDB EM Validation Summary Report ⓘ

Nov 7, 2022 – 04:08 PM EST

PDB ID : 6CUE  
EMDB ID : EMD-7621  
Title : Cryo-EM structure at 4.0 Å resolution of vaccine-elicited antibody vFP7.04 in complex with HIV-1 Env BG505 DS-SOSIP, and antibodies VRC03 and PGT122  
Authors : Acharya, P.; Carragher, B.; Potter, C.S.; Kwong, P.D.  
Deposited on : 2018-03-26  
Resolution : 4.00 Å (reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

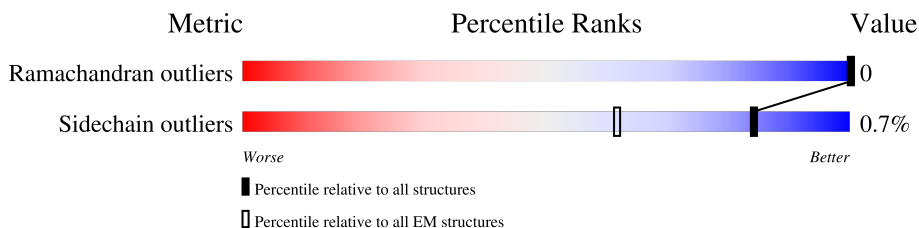
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	2	473	95% . .
1	C	473	95% .
1	c	473	95% . .
2	1	153	84% . 14%
2	D	153	85% . 14%
2	d	153	85% . 14%
3	3	118	25% 99% .
3	H	118	22% 99% .
3	h	118	23% 99% .

















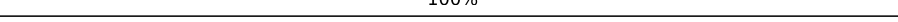


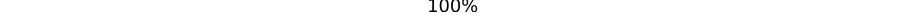





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Mol	Chain	Length	Quality of chain
4	4	112	67% 99%
4	L	112	67% 99%
4	l	112	69% 99%
5	5	132	12% 100%
5	M	132	14% 100%
5	m	132	15% 100%
6	6	107	7% 100%
6	N	107	7% 100%
6	n	107	7% 100%
7	7	129	99%
7	Q	129	99%
7	q	129	99%
8	8	102	95% 5%
8	R	102	97%
8	r	102	97%
9	9	2	50% 50%
9	A	2	50% 50%
9	F	2	50% 50%
9	G	2	100%
9	J	2	50% 50%
9	K	2	100%
9	P	2	100%
9	T	2	50% 50%
9	V	2	50% 50%
9	Y	2	50% 50%


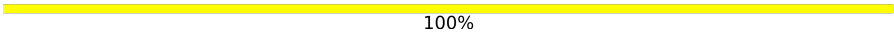
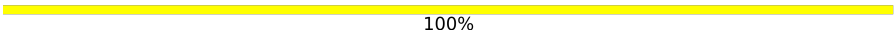
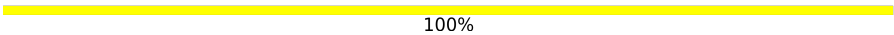
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Mol	Chain	Length	Quality of chain
9	Z	2	 100%
9	b	2	 100%
9	e	2	 50% 50%
9	g	2	 100%
9	j	2	 50% 50%
9	o	2	 50% 50%
9	t	2	 50% 50%
9	u	2	 100%
9	w	2	 100%
9	x	2	 100%
9	z	2	 50% 50%
10	B	3	 33% 67%
10	E	3	 100%
10	O	3	 67% 33%
10	W	3	 33% 67%
10	X	3	 100%
10	f	3	 67% 33%
10	p	3	 33% 67%
10	s	3	 100%
10	y	3	 67% 33%
11	I	5	 20% 80%
11	a	5	 40% 60%
11	v	5	 60% 40%
12	0	5	 20% 80%
12	S	5	 20% 80%

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Mol	Chain	Length	Quality of chain
12	i	5	 20% 80%
13	AA	4	 100%
13	U	4	 100%
13	k	4	 100%

## 2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 31692 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	c	453	3564	2233	630	671	30	0	0
1	2	453	3564	2233	630	671	30	0	0
1	C	453	3564	2233	630	671	30	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c	201	CYS	ILE	conflict	UNP Q2N0S6
c	332	ASN	THR	conflict	UNP Q2N0S6
c	433	CYS	ALA	conflict	UNP Q2N0S6
c	501	CYS	ALA	conflict	UNP Q2N0S6
2	201	CYS	ILE	conflict	UNP Q2N0S6
2	332	ASN	THR	conflict	UNP Q2N0S6
2	433	CYS	ALA	conflict	UNP Q2N0S6
2	501	CYS	ALA	conflict	UNP Q2N0S6
C	201	CYS	ILE	conflict	UNP Q2N0S6
C	332	ASN	THR	conflict	UNP Q2N0S6
C	433	CYS	ALA	conflict	UNP Q2N0S6
C	501	CYS	ALA	conflict	UNP Q2N0S6

- Molecule 2 is a protein called Envelope glycoprotein gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1	132	1034	654	178	196	6	0	0
2	D	132	1034	654	178	196	6	0	0
2	d	132	1034	654	178	196	6	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	605	CYS	THR	conflict	UNP Q2N0S7
D	605	CYS	THR	conflict	UNP Q2N0S7
d	605	CYS	THR	conflict	UNP Q2N0S7

- Molecule 3 is a protein called vFP7.04 Heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	117	Total	C	N	O	S	0	0
			919	589	149	176	5		
3	H	117	Total	C	N	O	S	0	0
			919	589	149	176	5		
3	h	117	Total	C	N	O	S	0	0
			919	589	149	176	5		

- Molecule 4 is a protein called vFP7.04 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	111	Total	C	N	O	S	0	0
			853	540	145	165	3		
4	L	111	Total	C	N	O	S	0	0
			853	540	145	165	3		
4	l	111	Total	C	N	O	S	0	0
			853	540	145	165	3		

- Molecule 5 is a protein called PGT122 heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	132	Total	C	N	O	S	0	0
			1047	669	180	195	3		
5	M	132	Total	C	N	O	S	0	0
			1047	669	180	195	3		
5	m	132	Total	C	N	O	S	0	0
			1047	669	180	195	3		

- Molecule 6 is a protein called PGT122 Light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	107	Total	C	N	O	S	0	0
			817	512	141	162	2		
6	N	107	Total	C	N	O	S	0	0
			817	512	141	162	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	n	107	817	512	141	162	2	0	0

- Molecule 7 is a protein called VRC03 Heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	7	129	1029	660	176	187	6	0	0
7	Q	129	1029	660	176	187	6	0	0
7	q	129	1029	660	176	187	6	0	0

- Molecule 8 is a protein called VRC03 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	8	102	802	510	137	152	3	0	0
8	R	102	802	510	137	152	3	0	0
8	r	102	802	510	137	152	3	0	0

- 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				AltConf	Trace
			Total	C	N	O		
9	A	2	28	16	2	10	0	0
9	F	2	28	16	2	10	0	0
9	G	2	28	16	2	10	0	0
9	J	2	28	16	2	10	0	0
9	K	2	28	16	2	10	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	P	2	28	16	2	10	0	0
9	T	2	28	16	2	10	0	0
9	V	2	28	16	2	10	0	0
9	Y	2	28	16	2	10	0	0
9	Z	2	28	16	2	10	0	0
9	b	2	28	16	2	10	0	0
9	e	2	28	16	2	10	0	0
9	g	2	28	16	2	10	0	0
9	j	2	28	16	2	10	0	0
9	o	2	28	16	2	10	0	0
9	t	2	28	16	2	10	0	0
9	u	2	28	16	2	10	0	0
9	w	2	28	16	2	10	0	0
9	x	2	28	16	2	10	0	0
9	z	2	28	16	2	10	0	0
9	9	2	28	16	2	10	0	0

- 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.



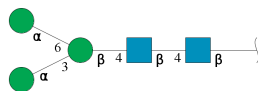
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	B	3	39	22	2	15	0	0

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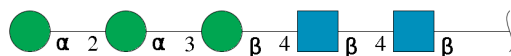
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	E	3	Total 39	C 22	N 2	O 15	0	0
10	O	3	Total 39	C 22	N 2	O 15	0	0
10	W	3	Total 39	C 22	N 2	O 15	0	0
10	X	3	Total 39	C 22	N 2	O 15	0	0
10	f	3	Total 39	C 22	N 2	O 15	0	0
10	p	3	Total 39	C 22	N 2	O 15	0	0
10	s	3	Total 39	C 22	N 2	O 15	0	0
10	y	3	Total 39	C 22	N 2	O 15	0	0

- Molecule 11 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				AltConf	Trace
			Total	C	N	O		
11	I	5	Total 61	C 34	N 2	O 25	0	0
11	a	5	Total 61	C 34	N 2	O 25	0	0
11	v	5	Total 61	C 34	N 2	O 25	0	0

- Molecule 12 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-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.



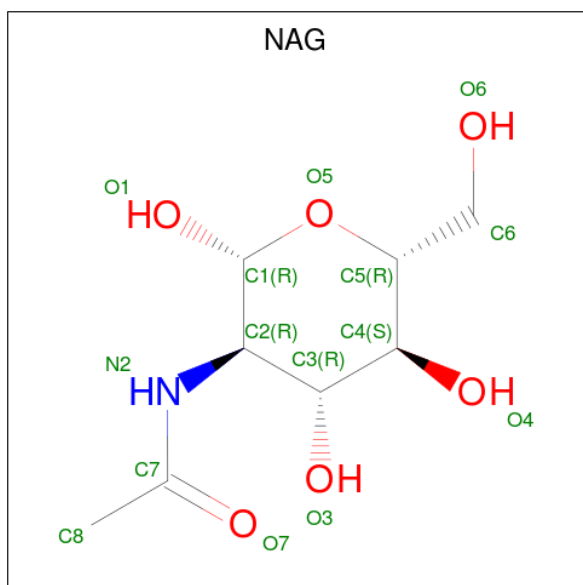
Mol	Chain	Residues	Atoms				AltConf	Trace
12	S	5	Total	C	N	O	0	0
			61	34	2	25		
12	i	5	Total	C	N	O	0	0
			61	34	2	25		
12	0	5	Total	C	N	O	0	0
			61	34	2	25		

- 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				AltConf	Trace
13	U	4	Total	C	N	O	0	0
			50	28	2	20		
13	k	4	Total	C	N	O	0	0
			50	28	2	20		
13	AA	4	Total	C	N	O	0	0
			50	28	2	20		

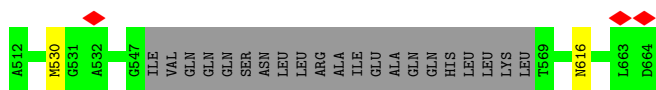
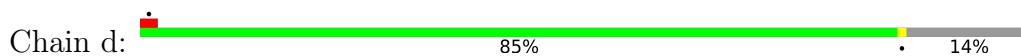
- Molecule 14 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



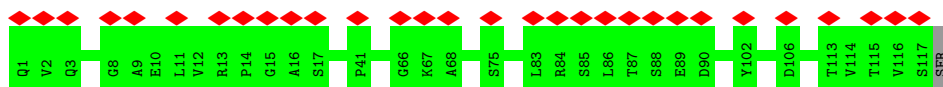
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>				<b>AltConf</b>
14	c	1	Total 14	C 8	N 1	O 5	0
14	2	1	Total 14	C 8	N 1	O 5	0
14	C	1	Total 14	C 8	N 1	O 5	0



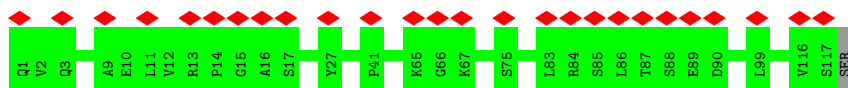
• Molecule 2: Envelope glycoprotein gp41



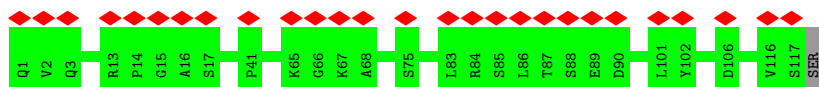
• Molecule 3: vFP7.04 Heavy chain



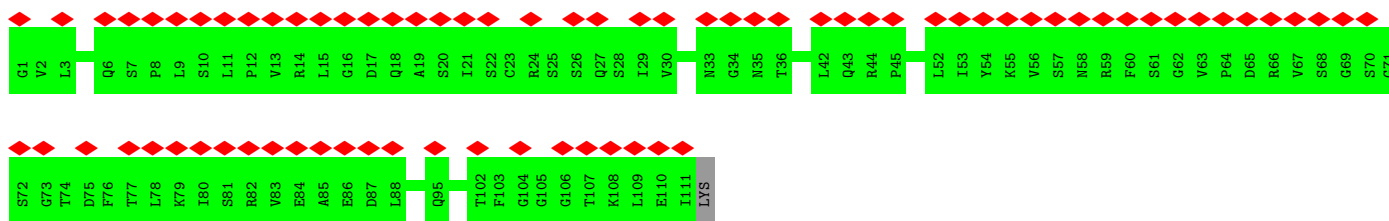
• Molecule 3: vFP7.04 Heavy chain



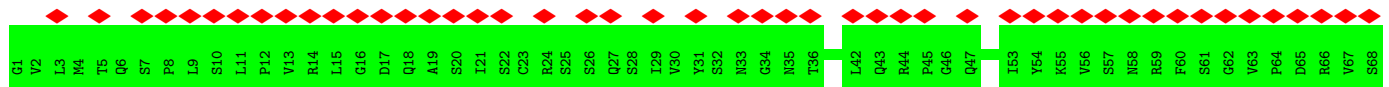
• Molecule 3: vFP7.04 Heavy chain



• Molecule 4: vFP7.04 light chain

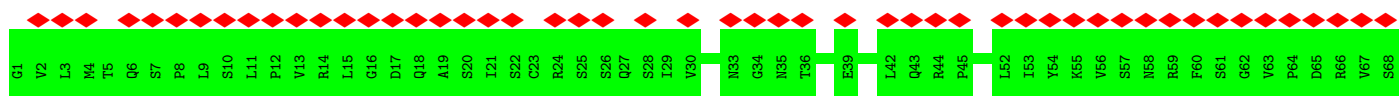


• Molecule 4: vFP7.04 light chain

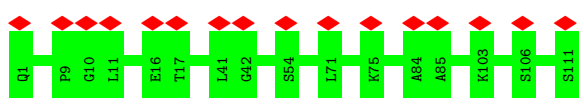




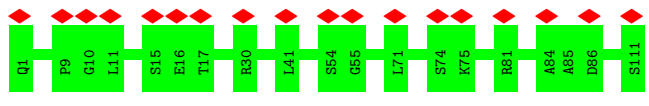
• Molecule 4: vFP7.04 light chain



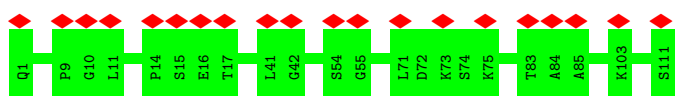
• Molecule 5: PGT122 heavy Chain



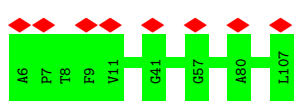
• Molecule 5: PGT122 heavy Chain



• Molecule 5: PGT122 heavy Chain

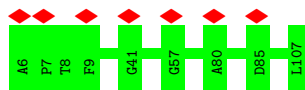


• Molecule 6: PGT122 Light chain

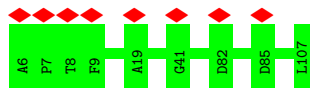


• Molecule 6: PGT122 Light chain

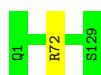




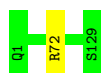
- Molecule 6: PGT122 Light chain



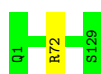
- Molecule 7: VRC03 Heavy chain



- Molecule 7: VRC03 Heavy chain



- Molecule 7: VRC03 Heavy chain



- Molecule 8: VRC03 light chain



- Molecule 8: VRC03 light chain



- Molecule 8: VRC03 light chain







- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:  50% 50%



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:  50% 50%



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:  50% 50%



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:  100%



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:  100%



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e:  50% 50%



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain g:  100%

MAG1  
MAG2

- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain j:  50% 50%MAG1  
MAG2

- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain o:  50% 50%MAG1  
MAG2

- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain t:  50% 50%MAG1  
MAG2

- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain u:  100%MAG1  
MAG2

- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain w:  100%MAG1  
MAG2

- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain x:  100%MAG1  
MAG2

- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain z:  50% 50%




- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 9:  50% 50%



- Molecule 10: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:  33% 67%



- Molecule 10: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  100%



- Molecule 10: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:  67% 33%



- Molecule 10: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:  33% 67%



- Molecule 10: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:  100%

MAG1  
MAG2  
BMA3

- Molecule 10: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain f:  67% 33%

MAG1  
MAG2  
BMA3

- Molecule 10: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain p:  33% 67%

MAG1  
MAG2  
BMA3

- Molecule 10: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain s:  100%

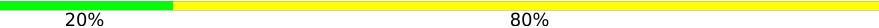
MAG1  
MAG2  
BMA3

- Molecule 10: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain y:  67% 33%

MAG1  
MAG2  
BMA3

- Molecule 11: 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

Chain I:  20% 80%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5

- Molecule 11: 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

Chain a:  40% 60%

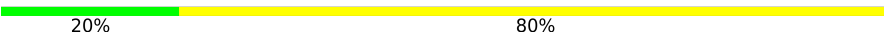
MAG1  
MAG2  
BMA3  
MAN4  
MAN5

- Molecule 11: 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

Chain v:  60% 40%



- Molecule 12: alpha-D-mannopyranose-(1-2)-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

Chain S:  20% 80%



- Molecule 12: alpha-D-mannopyranose-(1-2)-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

Chain i:  20% 80%



- Molecule 12: alpha-D-mannopyranose-(1-2)-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

Chain 0:  20% 80%



- Molecule 13: 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

Chain U:  100%



- Molecule 13: 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

Chain k:  100%



- Molecule 13: 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

Chain AA:

100%

MAG1  
MAG2  
BMA3  
MAN4

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	64580	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	53.11	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	5.517	Depositor
Minimum map value	-2.315	Depositor
Average map value	0.015	Depositor
Map value standard deviation	0.141	Depositor
Recommended contour level	1.04	Depositor
Map size (Å)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, BMA, NAG

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  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	2	0.43	0/3638	0.60	0/4939
1	C	0.44	0/3638	0.59	0/4939
1	c	0.45	0/3638	0.60	0/4939
2	1	0.40	0/1052	0.59	0/1427
2	D	0.41	0/1052	0.58	0/1427
2	d	0.43	0/1052	0.58	0/1427
3	3	0.33	0/943	0.56	0/1282
3	H	0.32	0/943	0.55	0/1282
3	h	0.32	0/943	0.56	0/1282
4	4	0.31	0/872	0.51	0/1181
4	L	0.31	0/872	0.54	0/1181
4	l	0.30	0/872	0.54	0/1181
5	5	0.31	0/1076	0.56	0/1465
5	M	0.32	0/1076	0.58	0/1465
5	m	0.32	0/1076	0.57	0/1465
6	6	0.35	0/839	0.55	0/1149
6	N	0.36	0/839	0.55	0/1149
6	n	0.35	0/839	0.55	0/1149
7	7	0.50	0/1062	0.59	0/1447
7	Q	0.53	0/1062	0.59	0/1447
7	q	0.51	0/1062	0.57	0/1447
8	8	0.43	0/820	0.66	0/1107
8	R	0.43	0/820	0.66	0/1107
8	r	0.41	0/820	0.66	0/1107
All	All	0.41	0/30906	0.58	0/41991

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	2	0	1
1	c	0	1
8	8	0	3
8	R	0	1
8	r	0	1
All	All	0	7

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	2	77	THR	Peptide
8	8	50	ASP	Peptide
8	8	83	PHE	Peptide
8	8	90	GLN	Peptide
1	c	77	THR	Peptide

## 5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	2	447/473 (94%)	410 (92%)	37 (8%)	0	100	100
1	C	447/473 (94%)	412 (92%)	35 (8%)	0	100	100
1	c	447/473 (94%)	414 (93%)	33 (7%)	0	100	100
2	1	128/153 (84%)	120 (94%)	8 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	128/153 (84%)	121 (94%)	7 (6%)	0	100	100
2	d	128/153 (84%)	121 (94%)	7 (6%)	0	100	100
3	3	115/118 (98%)	102 (89%)	13 (11%)	0	100	100
3	H	115/118 (98%)	108 (94%)	7 (6%)	0	100	100
3	h	115/118 (98%)	107 (93%)	8 (7%)	0	100	100
4	4	109/112 (97%)	100 (92%)	9 (8%)	0	100	100
4	L	109/112 (97%)	100 (92%)	9 (8%)	0	100	100
4	l	109/112 (97%)	98 (90%)	11 (10%)	0	100	100
5	5	130/132 (98%)	118 (91%)	12 (9%)	0	100	100
5	M	130/132 (98%)	117 (90%)	13 (10%)	0	100	100
5	m	130/132 (98%)	120 (92%)	10 (8%)	0	100	100
6	6	105/107 (98%)	96 (91%)	9 (9%)	0	100	100
6	N	105/107 (98%)	97 (92%)	8 (8%)	0	100	100
6	n	105/107 (98%)	95 (90%)	10 (10%)	0	100	100
7	7	127/129 (98%)	121 (95%)	6 (5%)	0	100	100
7	Q	127/129 (98%)	121 (95%)	6 (5%)	0	100	100
7	q	127/129 (98%)	120 (94%)	7 (6%)	0	100	100
8	8	100/102 (98%)	93 (93%)	7 (7%)	0	100	100
8	R	100/102 (98%)	95 (95%)	5 (5%)	0	100	100
8	r	100/102 (98%)	96 (96%)	4 (4%)	0	100	100
All	All	3783/3978 (95%)	3502 (93%)	281 (7%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	2	405/422 (96%)	402 (99%)	3 (1%)	84	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	405/422 (96%)	403 (100%)	2 (0%)	88	93
1	c	405/422 (96%)	403 (100%)	2 (0%)	88	93
2	1	110/129 (85%)	107 (97%)	3 (3%)	44	66
2	D	110/129 (85%)	108 (98%)	2 (2%)	59	77
2	d	110/129 (85%)	108 (98%)	2 (2%)	59	77
3	3	99/100 (99%)	99 (100%)	0	100	100
3	H	99/100 (99%)	99 (100%)	0	100	100
3	h	99/100 (99%)	99 (100%)	0	100	100
4	4	96/97 (99%)	96 (100%)	0	100	100
4	L	96/97 (99%)	96 (100%)	0	100	100
4	l	96/97 (99%)	96 (100%)	0	100	100
5	5	116/116 (100%)	116 (100%)	0	100	100
5	M	116/116 (100%)	116 (100%)	0	100	100
5	m	116/116 (100%)	116 (100%)	0	100	100
6	6	89/89 (100%)	89 (100%)	0	100	100
6	N	89/89 (100%)	89 (100%)	0	100	100
6	n	89/89 (100%)	89 (100%)	0	100	100
7	7	109/110 (99%)	108 (99%)	1 (1%)	78	88
7	Q	109/110 (99%)	108 (99%)	1 (1%)	78	88
7	q	109/110 (99%)	108 (99%)	1 (1%)	78	88
8	8	86/86 (100%)	84 (98%)	2 (2%)	50	70
8	R	86/86 (100%)	84 (98%)	2 (2%)	50	70
8	r	86/86 (100%)	84 (98%)	2 (2%)	50	70
All	All	3330/3447 (97%)	3307 (99%)	23 (1%)	84	90

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	616	ASN
8	R	80	ARG
8	R	45	ARG
2	d	530	MET
1	C	444	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
4	L	58	ASN
5	m	76	ASN
4	L	95	GLN
7	q	118	GLN
3	h	43	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

111 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$
12	NAG	0	1	1,12	14,14,15	0.53	0	17,19,21	0.57	0
12	NAG	0	2	12	14,14,15	0.27	0	17,19,21	1.09	1 (5%)
12	BMA	0	3	12	11,11,12	1.39	2 (18%)	15,15,17	1.33	2 (13%)
12	MAN	0	4	12	11,11,12	0.86	1 (9%)	15,15,17	1.56	2 (13%)
12	MAN	0	5	12	11,11,12	0.69	0	15,15,17	1.03	2 (13%)
9	NAG	9	1	1,9	14,14,15	0.35	0	17,19,21	0.98	1 (5%)
9	NAG	9	2	9	14,14,15	0.26	0	17,19,21	0.51	0
9	NAG	A	1	1,9	14,14,15	0.59	0	17,19,21	0.97	1 (5%)
9	NAG	A	2	9	14,14,15	0.36	0	17,19,21	0.56	0
13	NAG	AA	1	1,13	14,14,15	0.25	0	17,19,21	0.78	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
13	NAG	AA	2	13	14,14,15	0.41	0	17,19,21	1.00	2 (11%)
13	BMA	AA	3	13	11,11,12	1.20	1 (9%)	15,15,17	0.93	0
13	MAN	AA	4	13	11,11,12	0.92	1 (9%)	15,15,17	1.41	2 (13%)
10	NAG	B	1	10,1	14,14,15	0.36	0	17,19,21	0.60	0
10	NAG	B	2	10	14,14,15	0.41	0	17,19,21	0.85	1 (5%)
10	BMA	B	3	10	11,11,12	0.92	1 (9%)	15,15,17	2.00	4 (26%)
10	NAG	E	1	10,1	14,14,15	0.38	0	17,19,21	0.51	0
10	NAG	E	2	10	14,14,15	0.28	0	17,19,21	0.46	0
10	BMA	E	3	10	11,11,12	0.70	0	15,15,17	0.82	0
9	NAG	F	1	1,9	14,14,15	0.55	0	17,19,21	0.92	1 (5%)
9	NAG	F	2	9	14,14,15	0.23	0	17,19,21	0.47	0
9	NAG	G	1	1,9	14,14,15	0.44	0	17,19,21	0.47	0
9	NAG	G	2	9	14,14,15	0.31	0	17,19,21	0.52	0
11	NAG	I	1	1,11	14,14,15	0.25	0	17,19,21	0.63	1 (5%)
11	NAG	I	2	11	14,14,15	0.22	0	17,19,21	0.47	0
11	BMA	I	3	11	11,11,12	0.82	0	15,15,17	0.89	1 (6%)
11	MAN	I	4	11	11,11,12	0.78	1 (9%)	15,15,17	1.11	2 (13%)
11	MAN	I	5	11	11,11,12	0.86	0	15,15,17	1.04	2 (13%)
9	NAG	J	1	1,9	14,14,15	0.26	0	17,19,21	0.55	0
9	NAG	J	2	9	14,14,15	0.51	0	17,19,21	0.60	1 (5%)
9	NAG	K	1	1,9	14,14,15	0.19	0	17,19,21	0.52	0
9	NAG	K	2	9	14,14,15	0.23	0	17,19,21	0.51	0
10	NAG	O	1	10,1	14,14,15	0.54	0	17,19,21	0.57	0
10	NAG	O	2	10	14,14,15	0.25	0	17,19,21	0.47	0
10	BMA	O	3	10	11,11,12	1.07	1 (9%)	15,15,17	1.23	2 (13%)
9	NAG	P	1	1,9	14,14,15	0.31	0	17,19,21	0.56	0
9	NAG	P	2	9	14,14,15	0.36	0	17,19,21	0.44	0
12	NAG	S	1	1,12	14,14,15	0.58	0	17,19,21	0.60	0
12	NAG	S	2	12	14,14,15	0.25	0	17,19,21	1.11	1 (5%)
12	BMA	S	3	12	11,11,12	1.39	3 (27%)	15,15,17	1.22	1 (6%)
12	MAN	S	4	12	11,11,12	0.82	1 (9%)	15,15,17	1.42	2 (13%)
12	MAN	S	5	12	11,11,12	0.68	0	15,15,17	1.06	2 (13%)
9	NAG	T	1	1,9	14,14,15	0.24	0	17,19,21	1.00	1 (5%)
9	NAG	T	2	9	14,14,15	0.31	0	17,19,21	0.54	0
13	NAG	U	1	1,13	14,14,15	0.36	0	17,19,21	0.82	1 (5%)
13	NAG	U	2	13	14,14,15	0.41	0	17,19,21	1.12	2 (11%)
13	BMA	U	3	13	11,11,12	1.27	1 (9%)	15,15,17	0.90	0
13	MAN	U	4	13	11,11,12	0.96	1 (9%)	15,15,17	1.41	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	NAG	V	1	1,9	14,14,15	0.48	0	17,19,21	1.00	1 (5%)
9	NAG	V	2	9	14,14,15	0.32	0	17,19,21	0.58	0
10	NAG	W	1	10,1	14,14,15	0.28	0	17,19,21	0.52	0
10	NAG	W	2	10	14,14,15	0.51	0	17,19,21	0.96	1 (5%)
10	BMA	W	3	10	11,11,12	0.72	0	15,15,17	1.69	4 (26%)
10	NAG	X	1	10,1	14,14,15	0.37	0	17,19,21	0.52	0
10	NAG	X	2	10	14,14,15	0.25	0	17,19,21	0.42	0
10	BMA	X	3	10	11,11,12	0.78	0	15,15,17	0.79	0
9	NAG	Y	1	1,9	14,14,15	0.67	1 (7%)	17,19,21	0.96	1 (5%)
9	NAG	Y	2	9	14,14,15	0.24	0	17,19,21	0.43	0
9	NAG	Z	1	1,9	14,14,15	0.31	0	17,19,21	0.43	0
9	NAG	Z	2	9	14,14,15	0.34	0	17,19,21	0.55	0
11	NAG	a	1	1,11	14,14,15	0.26	0	17,19,21	0.56	0
11	NAG	a	2	11	14,14,15	0.27	0	17,19,21	0.49	0
11	BMA	a	3	11	11,11,12	0.68	0	15,15,17	0.88	1 (6%)
11	MAN	a	4	11	11,11,12	0.81	1 (9%)	15,15,17	1.20	2 (13%)
11	MAN	a	5	11	11,11,12	0.81	0	15,15,17	1.07	2 (13%)
9	NAG	b	1	1,9	14,14,15	0.21	0	17,19,21	0.58	0
9	NAG	b	2	9	14,14,15	0.46	0	17,19,21	0.55	0
9	NAG	e	1	1,9	14,14,15	0.19	0	17,19,21	0.61	1 (5%)
9	NAG	e	2	9	14,14,15	0.26	0	17,19,21	0.47	0
10	NAG	f	1	10,1	14,14,15	0.53	0	17,19,21	0.56	0
10	NAG	f	2	10	14,14,15	0.32	0	17,19,21	0.51	0
10	BMA	f	3	10	11,11,12	0.99	1 (9%)	15,15,17	1.24	2 (13%)
9	NAG	g	1	1,9	14,14,15	0.34	0	17,19,21	0.54	0
9	NAG	g	2	9	14,14,15	0.31	0	17,19,21	0.46	0
12	NAG	i	1	1,12	14,14,15	0.59	0	17,19,21	0.59	0
12	NAG	i	2	12	14,14,15	0.27	0	17,19,21	1.11	1 (5%)
12	BMA	i	3	12	11,11,12	1.34	1 (9%)	15,15,17	1.29	1 (6%)
12	MAN	i	4	12	11,11,12	0.84	1 (9%)	15,15,17	1.48	2 (13%)
12	MAN	i	5	12	11,11,12	0.76	0	15,15,17	1.00	2 (13%)
9	NAG	j	1	1,9	14,14,15	0.27	0	17,19,21	0.97	1 (5%)
9	NAG	j	2	9	14,14,15	0.28	0	17,19,21	0.55	0
13	NAG	k	1	1,13	14,14,15	0.26	0	17,19,21	0.78	1 (5%)
13	NAG	k	2	13	14,14,15	0.39	0	17,19,21	0.98	2 (11%)
13	BMA	k	3	13	11,11,12	1.09	1 (9%)	15,15,17	0.81	0
13	MAN	k	4	13	11,11,12	0.81	1 (9%)	15,15,17	1.23	2 (13%)
9	NAG	o	1	1,9	14,14,15	0.41	0	17,19,21	1.00	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	NAG	o	2	9	14,14,15	0.33	0	17,19,21	0.54	0
10	NAG	p	1	10,1	14,14,15	0.25	0	17,19,21	0.55	0
10	NAG	p	2	10	14,14,15	0.46	0	17,19,21	0.95	1 (5%)
10	BMA	p	3	10	11,11,12	0.69	0	15,15,17	1.58	3 (20%)
10	NAG	s	1	10,1	14,14,15	0.41	0	17,19,21	0.52	0
10	NAG	s	2	10	14,14,15	0.26	0	17,19,21	0.46	0
10	BMA	s	3	10	11,11,12	0.73	0	15,15,17	0.79	0
9	NAG	t	1	1,9	14,14,15	0.56	0	17,19,21	0.99	1 (5%)
9	NAG	t	2	9	14,14,15	0.27	0	17,19,21	0.41	0
9	NAG	u	1	1,9	14,14,15	0.24	0	17,19,21	0.45	0
9	NAG	u	2	9	14,14,15	0.33	0	17,19,21	0.53	0
11	NAG	v	1	1,11	14,14,15	0.30	0	17,19,21	0.55	0
11	NAG	v	2	11	14,14,15	0.23	0	17,19,21	0.44	0
11	BMA	v	3	11	11,11,12	0.75	0	15,15,17	0.88	0
11	MAN	v	4	11	11,11,12	0.90	1 (9%)	15,15,17	1.31	2 (13%)
11	MAN	v	5	11	11,11,12	0.89	0	15,15,17	0.92	1 (6%)
9	NAG	w	1	1,9	14,14,15	0.26	0	17,19,21	0.51	0
9	NAG	w	2	9	14,14,15	0.57	0	17,19,21	0.57	0
9	NAG	x	1	1,9	14,14,15	0.18	0	17,19,21	0.55	0
9	NAG	x	2	9	14,14,15	0.27	0	17,19,21	0.46	0
10	NAG	y	1	10,1	14,14,15	0.40	0	17,19,21	0.53	0
10	NAG	y	2	10	14,14,15	0.28	0	17,19,21	0.51	0
10	BMA	y	3	10	11,11,12	1.13	1 (9%)	15,15,17	1.26	1 (6%)
9	NAG	z	1	1,9	14,14,15	0.42	0	17,19,21	0.72	1 (5%)
9	NAG	z	2	9	14,14,15	0.30	0	17,19,21	0.49	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
12	NAG	0	1	1,12	-	0/6/23/26	0/1/1/1
12	NAG	0	2	12	-	3/6/23/26	0/1/1/1
12	BMA	0	3	12	-	0/2/19/22	0/1/1/1
12	MAN	0	4	12	-	0/2/19/22	0/1/1/1
12	MAN	0	5	12	-	1/2/19/22	0/1/1/1
9	NAG	9	1	1,9	-	3/6/23/26	0/1/1/1
9	NAG	9	2	9	-	0/6/23/26	0/1/1/1
9	NAG	A	1	1,9	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	A	2	9	-	2/6/23/26	0/1/1/1
13	NAG	AA	1	1,13	-	2/6/23/26	0/1/1/1
13	NAG	AA	2	13	-	2/6/23/26	0/1/1/1
13	BMA	AA	3	13	-	0/2/19/22	0/1/1/1
13	MAN	AA	4	13	-	2/2/19/22	0/1/1/1
10	NAG	B	1	10,1	-	2/6/23/26	0/1/1/1
10	NAG	B	2	10	-	2/6/23/26	0/1/1/1
10	BMA	B	3	10	-	2/2/19/22	0/1/1/1
10	NAG	E	1	10,1	-	2/6/23/26	0/1/1/1
10	NAG	E	2	10	-	2/6/23/26	0/1/1/1
10	BMA	E	3	10	-	0/2/19/22	0/1/1/1
9	NAG	F	1	1,9	-	3/6/23/26	0/1/1/1
9	NAG	F	2	9	-	2/6/23/26	0/1/1/1
9	NAG	G	1	1,9	-	2/6/23/26	0/1/1/1
9	NAG	G	2	9	-	2/6/23/26	0/1/1/1
11	NAG	I	1	1,11	-	0/6/23/26	0/1/1/1
11	NAG	I	2	11	-	2/6/23/26	0/1/1/1
11	BMA	I	3	11	-	0/2/19/22	0/1/1/1
11	MAN	I	4	11	-	1/2/19/22	0/1/1/1
11	MAN	I	5	11	-	0/2/19/22	0/1/1/1
9	NAG	J	1	1,9	-	2/6/23/26	0/1/1/1
9	NAG	J	2	9	-	2/6/23/26	0/1/1/1
9	NAG	K	1	1,9	-	1/6/23/26	0/1/1/1
9	NAG	K	2	9	-	0/6/23/26	0/1/1/1
10	NAG	O	1	10,1	-	2/6/23/26	0/1/1/1
10	NAG	O	2	10	-	2/6/23/26	0/1/1/1
10	BMA	O	3	10	-	2/2/19/22	0/1/1/1
9	NAG	P	1	1,9	-	0/6/23/26	0/1/1/1
9	NAG	P	2	9	-	2/6/23/26	0/1/1/1
12	NAG	S	1	1,12	-	0/6/23/26	0/1/1/1
12	NAG	S	2	12	-	3/6/23/26	0/1/1/1
12	BMA	S	3	12	-	0/2/19/22	0/1/1/1
12	MAN	S	4	12	-	0/2/19/22	0/1/1/1
12	MAN	S	5	12	-	1/2/19/22	0/1/1/1
9	NAG	T	1	1,9	-	2/6/23/26	0/1/1/1
9	NAG	T	2	9	-	2/6/23/26	0/1/1/1
13	NAG	U	1	1,13	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	NAG	U	2	13	-	0/6/23/26	0/1/1/1
13	BMA	U	3	13	-	0/2/19/22	0/1/1/1
13	MAN	U	4	13	-	1/2/19/22	0/1/1/1
9	NAG	V	1	1,9	-	1/6/23/26	0/1/1/1
9	NAG	V	2	9	-	2/6/23/26	0/1/1/1
10	NAG	W	1	10,1	-	2/6/23/26	0/1/1/1
10	NAG	W	2	10	-	2/6/23/26	0/1/1/1
10	BMA	W	3	10	-	2/2/19/22	0/1/1/1
10	NAG	X	1	10,1	-	1/6/23/26	0/1/1/1
10	NAG	X	2	10	-	2/6/23/26	0/1/1/1
10	BMA	X	3	10	-	2/2/19/22	0/1/1/1
9	NAG	Y	1	1,9	-	2/6/23/26	0/1/1/1
9	NAG	Y	2	9	-	2/6/23/26	0/1/1/1
9	NAG	Z	1	1,9	-	2/6/23/26	0/1/1/1
9	NAG	Z	2	9	-	2/6/23/26	0/1/1/1
11	NAG	a	1	1,11	-	2/6/23/26	0/1/1/1
11	NAG	a	2	11	-	2/6/23/26	0/1/1/1
11	BMA	a	3	11	-	1/2/19/22	0/1/1/1
11	MAN	a	4	11	-	1/2/19/22	0/1/1/1
11	MAN	a	5	11	-	0/2/19/22	0/1/1/1
9	NAG	b	1	1,9	-	2/6/23/26	0/1/1/1
9	NAG	b	2	9	-	2/6/23/26	0/1/1/1
9	NAG	e	1	1,9	-	1/6/23/26	0/1/1/1
9	NAG	e	2	9	-	2/6/23/26	0/1/1/1
10	NAG	f	1	10,1	-	2/6/23/26	0/1/1/1
10	NAG	f	2	10	-	2/6/23/26	0/1/1/1
10	BMA	f	3	10	-	2/2/19/22	0/1/1/1
9	NAG	g	1	1,9	-	2/6/23/26	0/1/1/1
9	NAG	g	2	9	-	0/6/23/26	0/1/1/1
12	NAG	i	1	1,12	-	0/6/23/26	0/1/1/1
12	NAG	i	2	12	-	3/6/23/26	0/1/1/1
12	BMA	i	3	12	-	0/2/19/22	0/1/1/1
12	MAN	i	4	12	-	0/2/19/22	0/1/1/1
12	MAN	i	5	12	-	1/2/19/22	0/1/1/1
9	NAG	j	1	1,9	-	2/6/23/26	0/1/1/1
9	NAG	j	2	9	-	2/6/23/26	0/1/1/1
13	NAG	k	1	1,13	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	NAG	k	2	13	-	2/6/23/26	0/1/1/1
13	BMA	k	3	13	-	0/2/19/22	0/1/1/1
13	MAN	k	4	13	-	2/2/19/22	0/1/1/1
9	NAG	o	1	1,9	-	3/6/23/26	0/1/1/1
9	NAG	o	2	9	-	2/6/23/26	0/1/1/1
10	NAG	p	1	10,1	-	2/6/23/26	0/1/1/1
10	NAG	p	2	10	-	0/6/23/26	0/1/1/1
10	BMA	p	3	10	-	1/2/19/22	0/1/1/1
10	NAG	s	1	10,1	-	1/6/23/26	0/1/1/1
10	NAG	s	2	10	-	0/6/23/26	0/1/1/1
10	BMA	s	3	10	-	2/2/19/22	0/1/1/1
9	NAG	t	1	1,9	-	2/6/23/26	0/1/1/1
9	NAG	t	2	9	-	2/6/23/26	0/1/1/1
9	NAG	u	1	1,9	-	2/6/23/26	0/1/1/1
9	NAG	u	2	9	-	2/6/23/26	0/1/1/1
11	NAG	v	1	1,11	-	1/6/23/26	0/1/1/1
11	NAG	v	2	11	-	2/6/23/26	0/1/1/1
11	BMA	v	3	11	-	2/2/19/22	0/1/1/1
11	MAN	v	4	11	-	1/2/19/22	0/1/1/1
11	MAN	v	5	11	-	0/2/19/22	0/1/1/1
9	NAG	w	1	1,9	-	1/6/23/26	0/1/1/1
9	NAG	w	2	9	-	2/6/23/26	0/1/1/1
9	NAG	x	1	1,9	-	1/6/23/26	0/1/1/1
9	NAG	x	2	9	-	2/6/23/26	0/1/1/1
10	NAG	y	1	10,1	-	2/6/23/26	0/1/1/1
10	NAG	y	2	10	-	2/6/23/26	0/1/1/1
10	BMA	y	3	10	-	2/2/19/22	0/1/1/1
9	NAG	z	1	1,9	-	2/6/23/26	0/1/1/1
9	NAG	z	2	9	-	0/6/23/26	0/1/1/1

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	y	3	BMA	C1-C2	2.85	1.58	1.52
10	O	3	BMA	C1-C2	2.83	1.58	1.52
11	v	4	MAN	C1-C2	2.69	1.58	1.52
12	o	3	BMA	C2-C3	2.62	1.56	1.52
12	i	3	BMA	C2-C3	2.61	1.56	1.52

The worst 5 of 79 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	3	BMA	C1-O5-C5	4.97	118.92	112.19
12	0	4	MAN	C1-O5-C5	4.74	118.62	112.19
10	W	3	BMA	C1-O5-C5	4.63	118.46	112.19
13	AA	4	MAN	C1-O5-C5	4.50	118.29	112.19
12	i	4	MAN	C1-O5-C5	4.42	118.19	112.19

There are no chirality outliers.

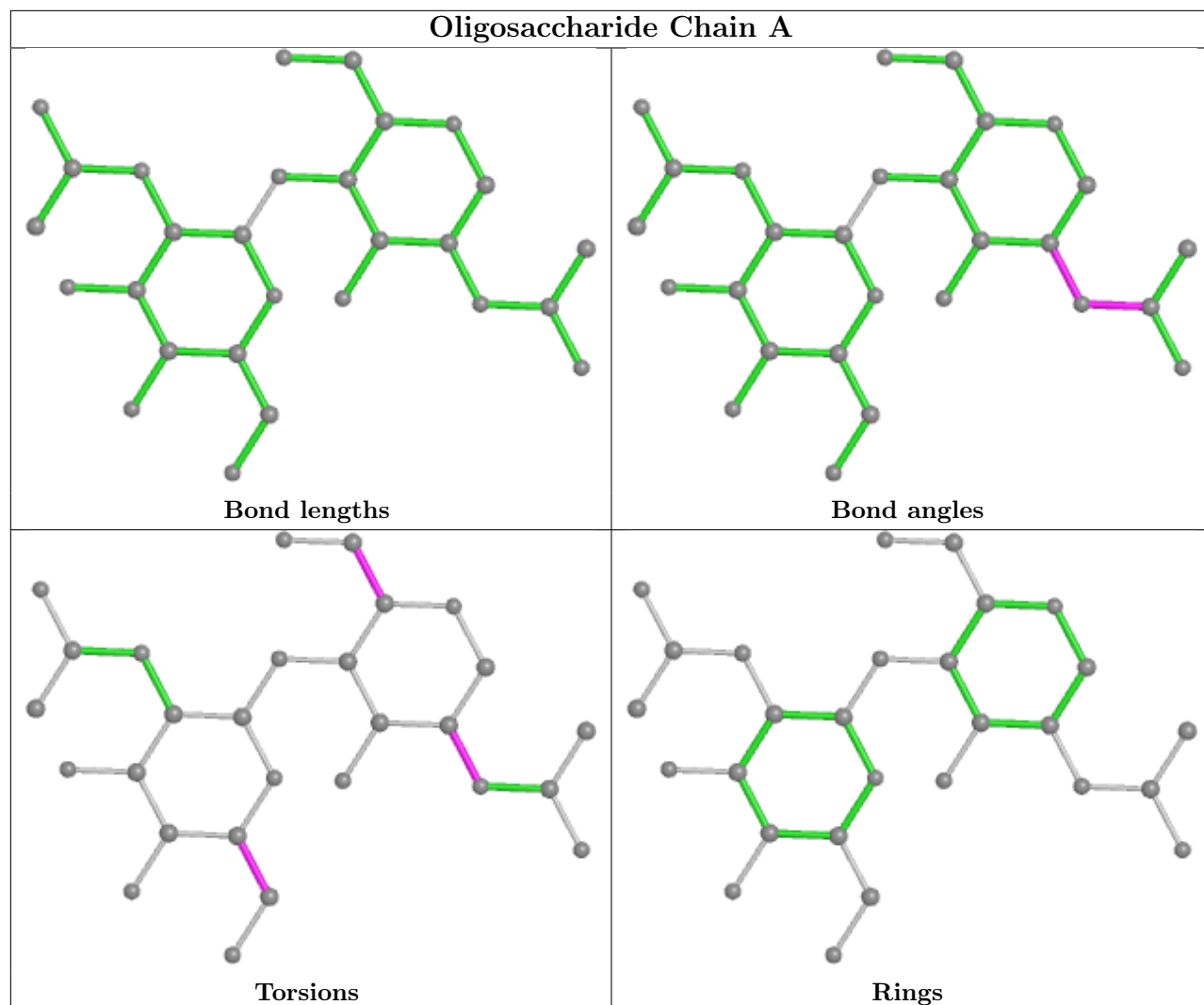
5 of 160 torsion outliers are listed below:

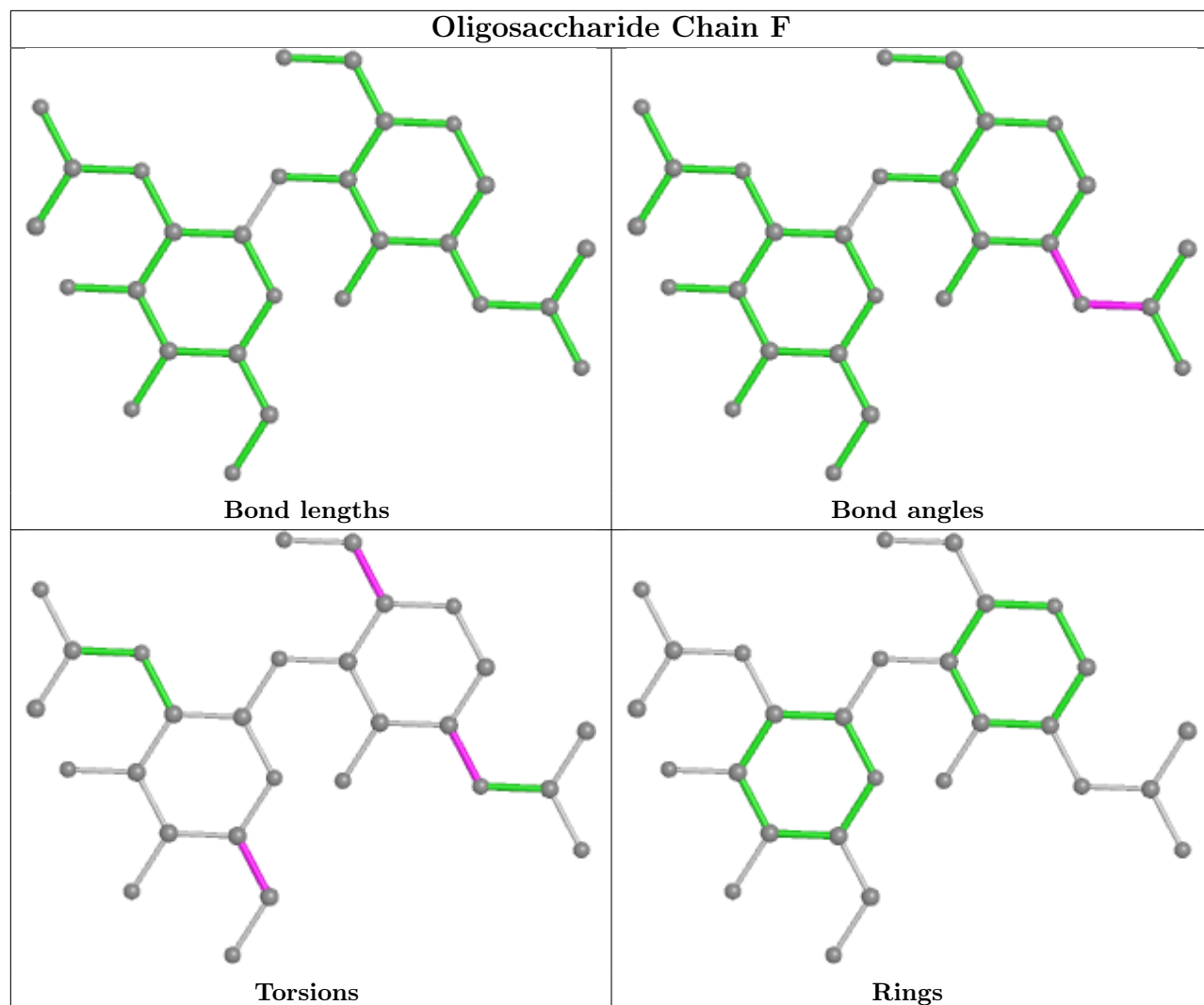
Mol	Chain	Res	Type	Atoms
9	Z	2	NAG	O5-C5-C6-O6
9	A	2	NAG	O5-C5-C6-O6
9	G	1	NAG	O5-C5-C6-O6
9	u	1	NAG	O5-C5-C6-O6
12	i	2	NAG	O5-C5-C6-O6

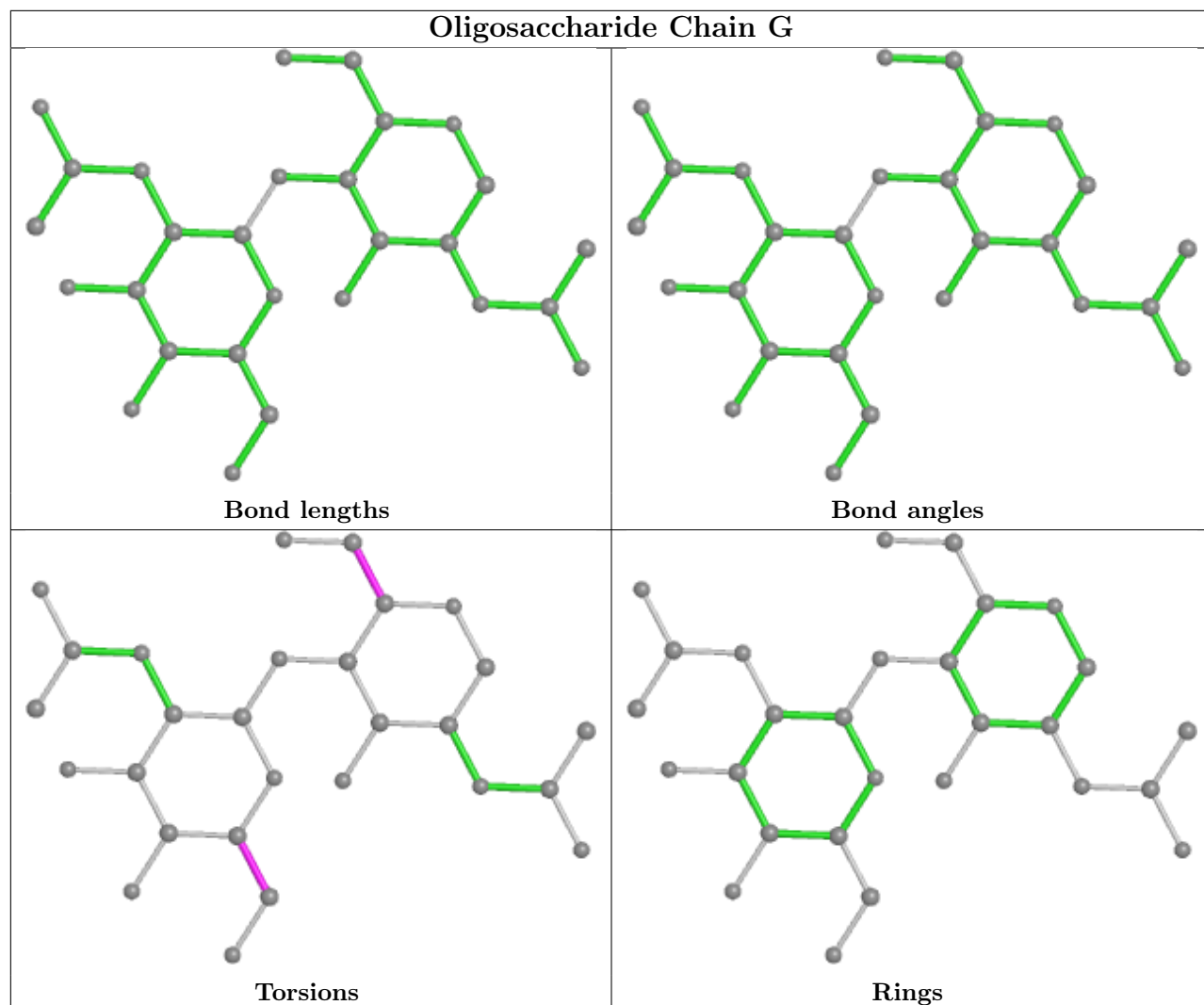
There are no ring outliers.

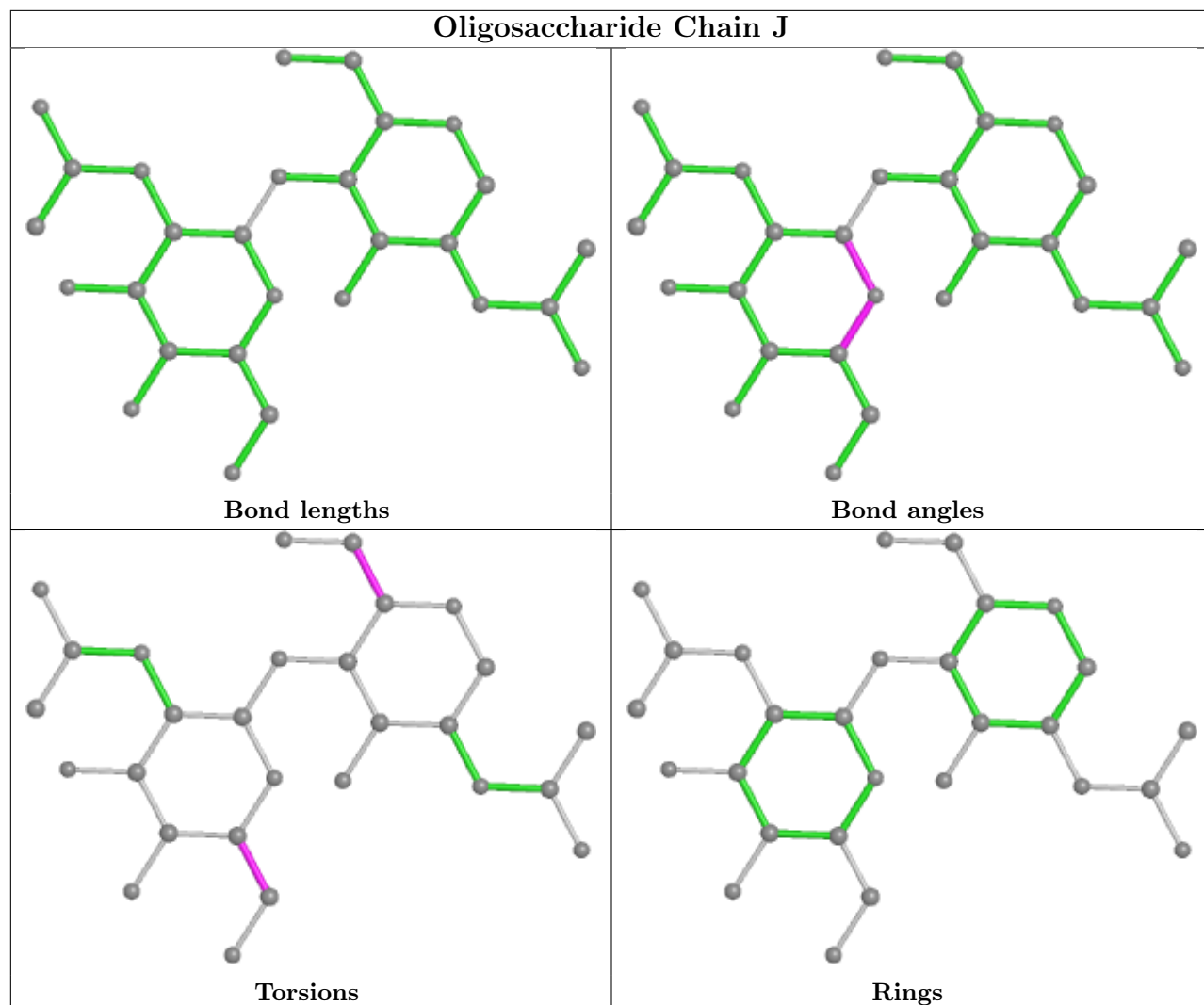
No monomer is involved in short contacts.

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

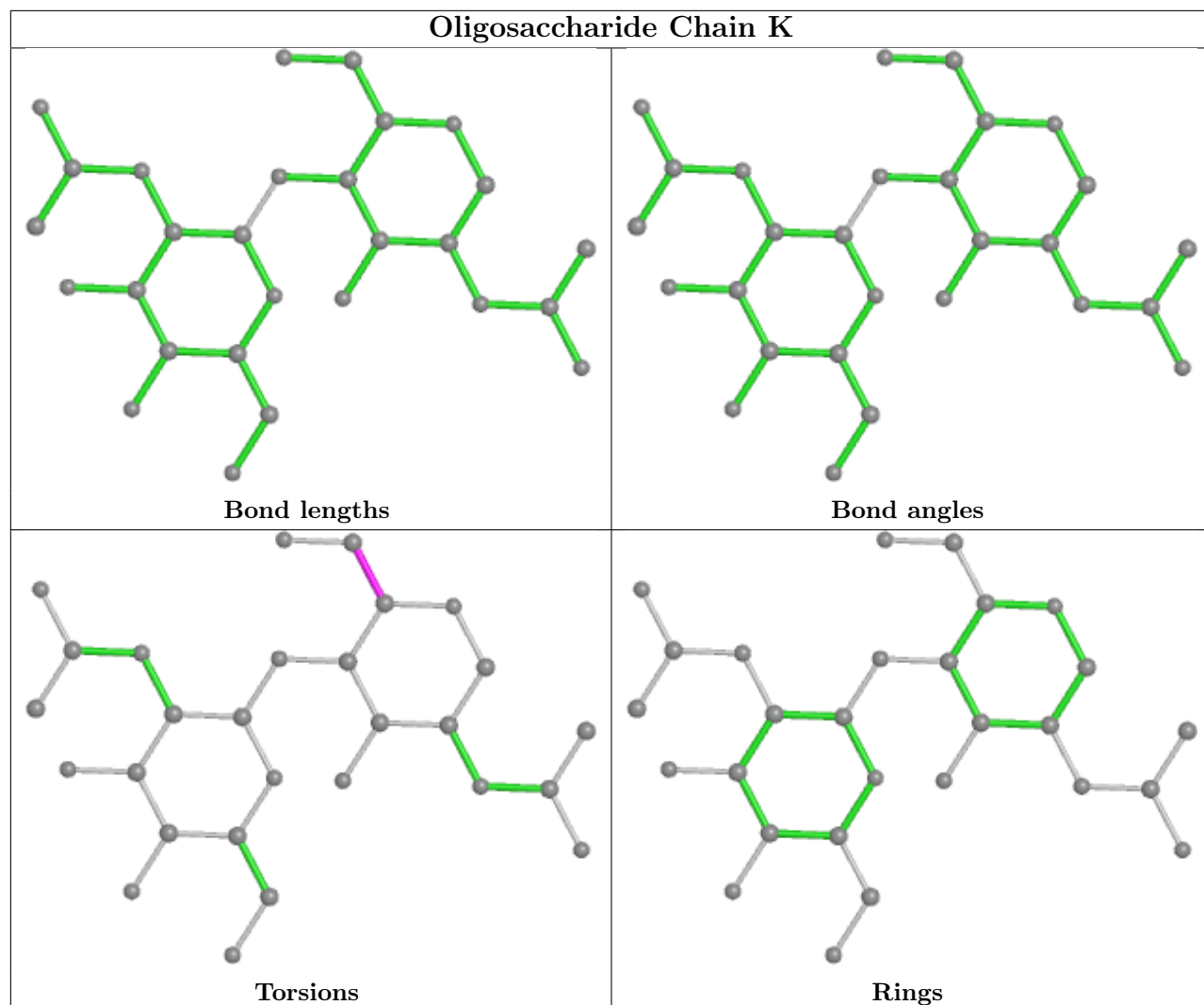


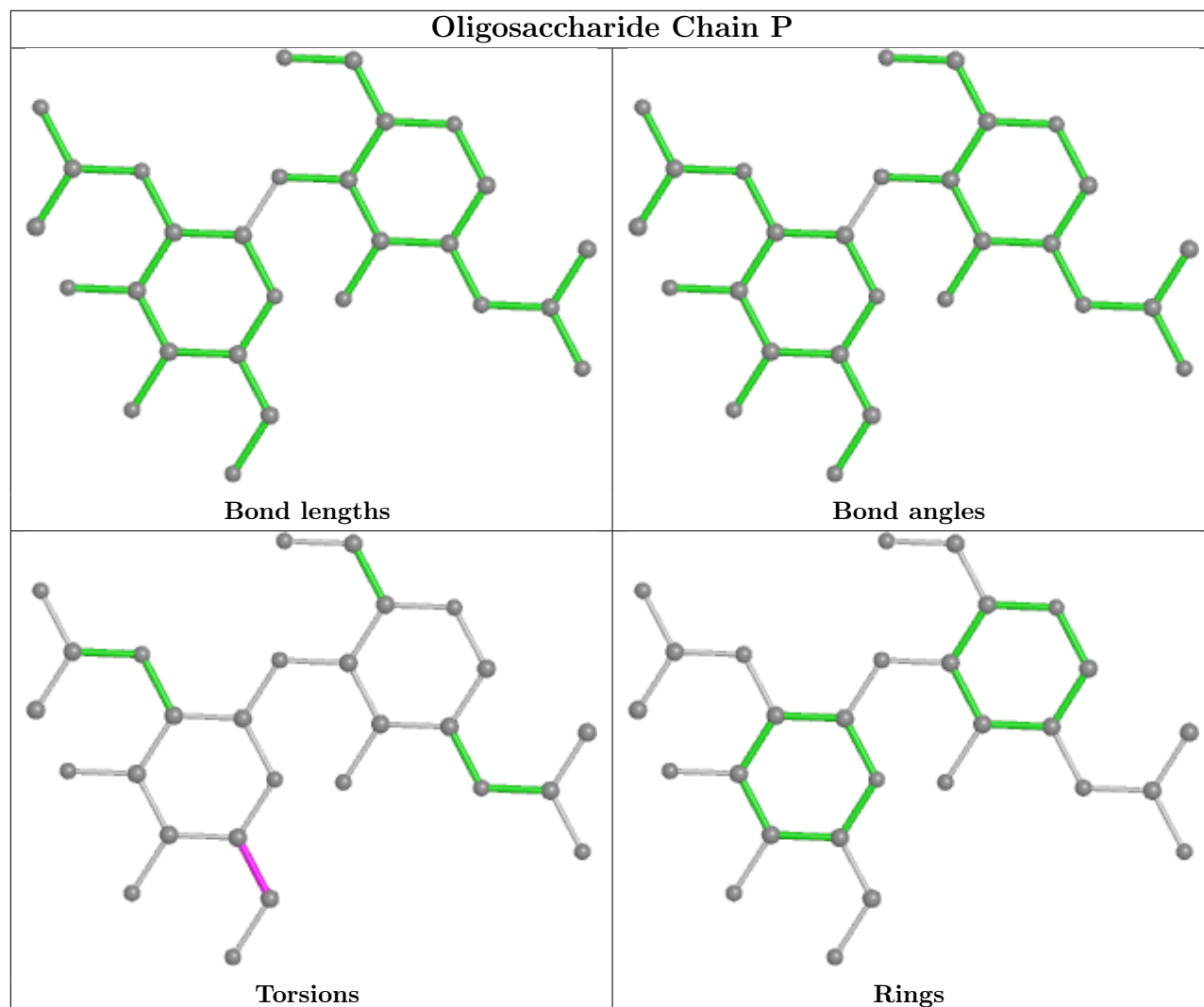


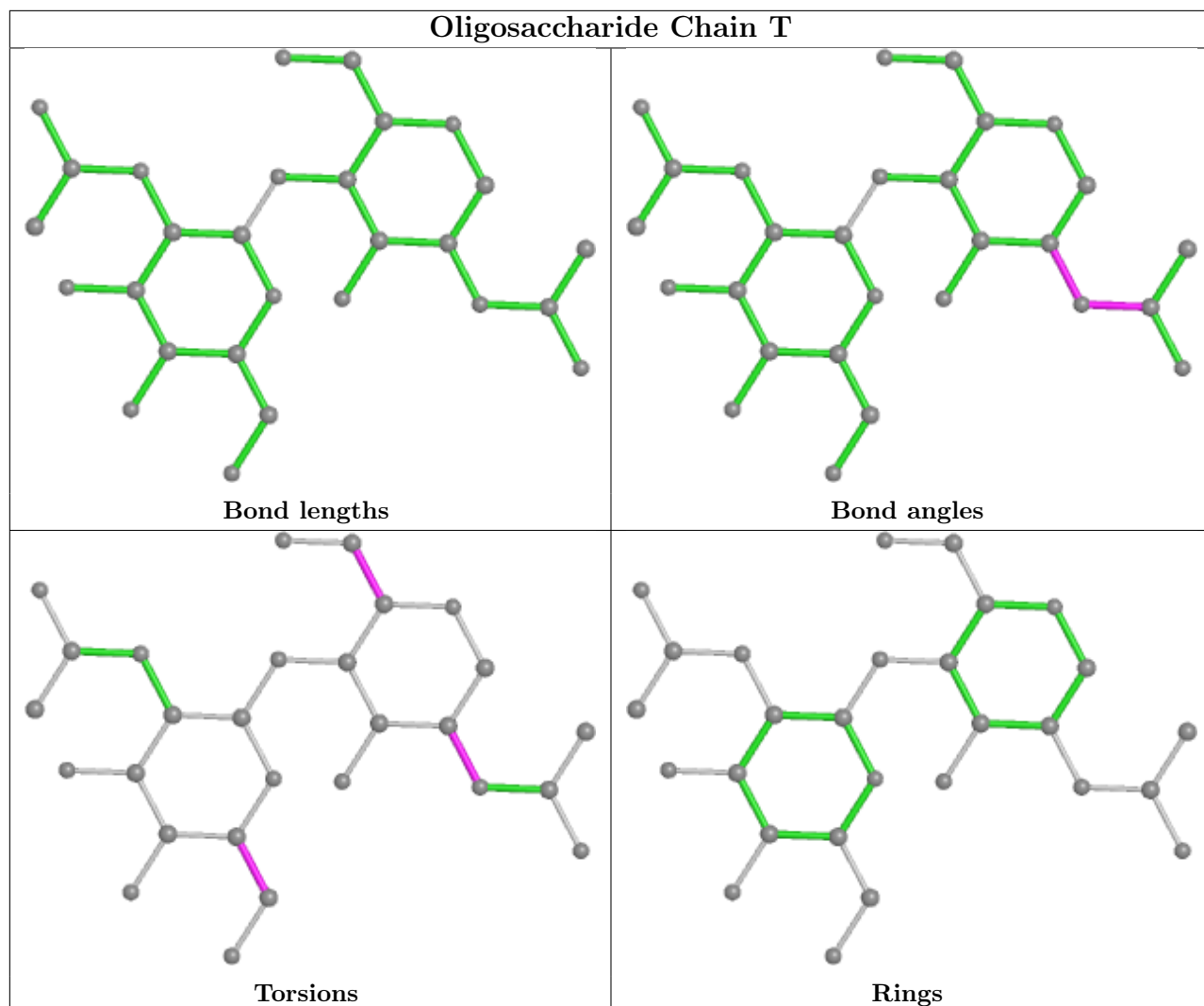


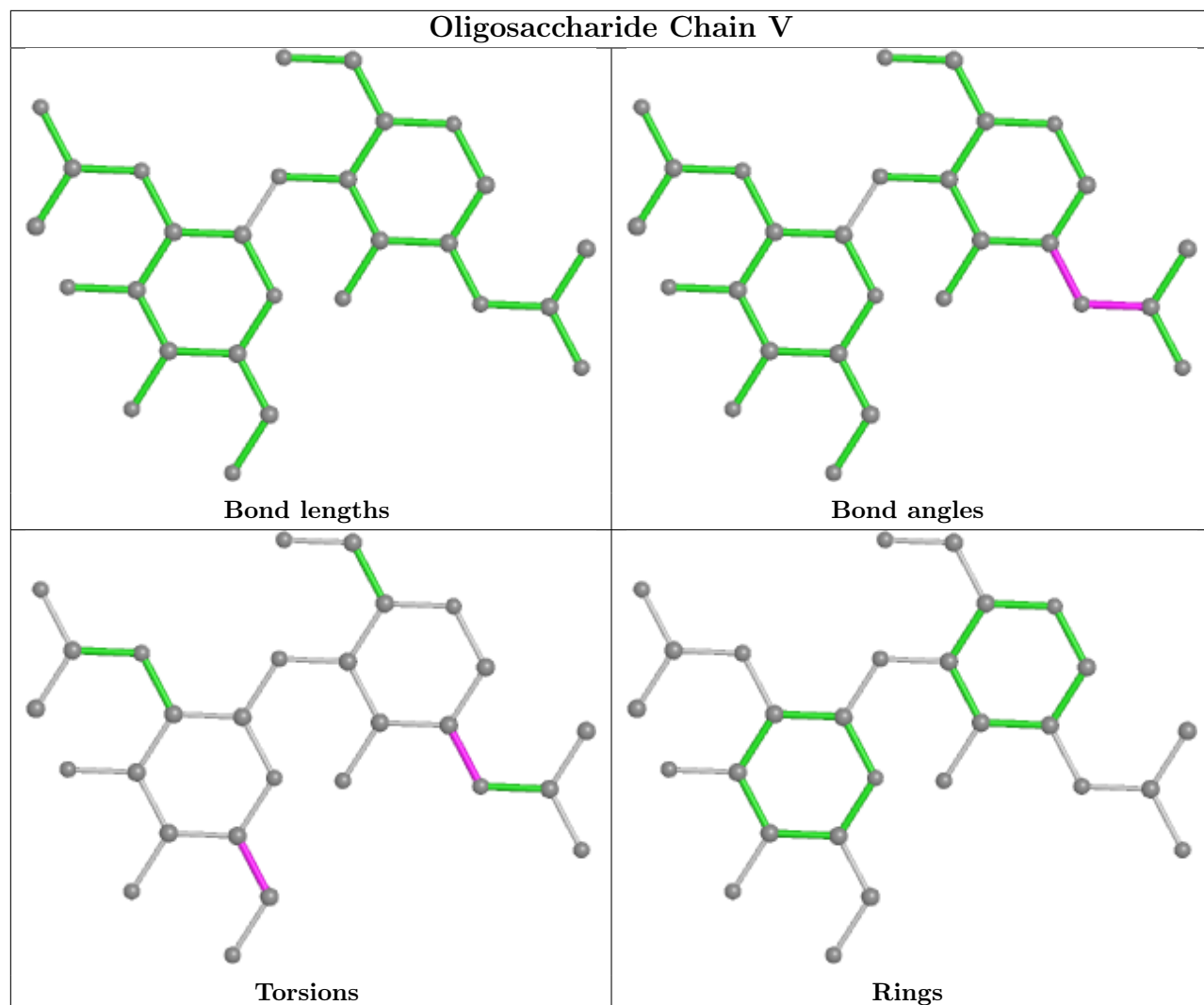


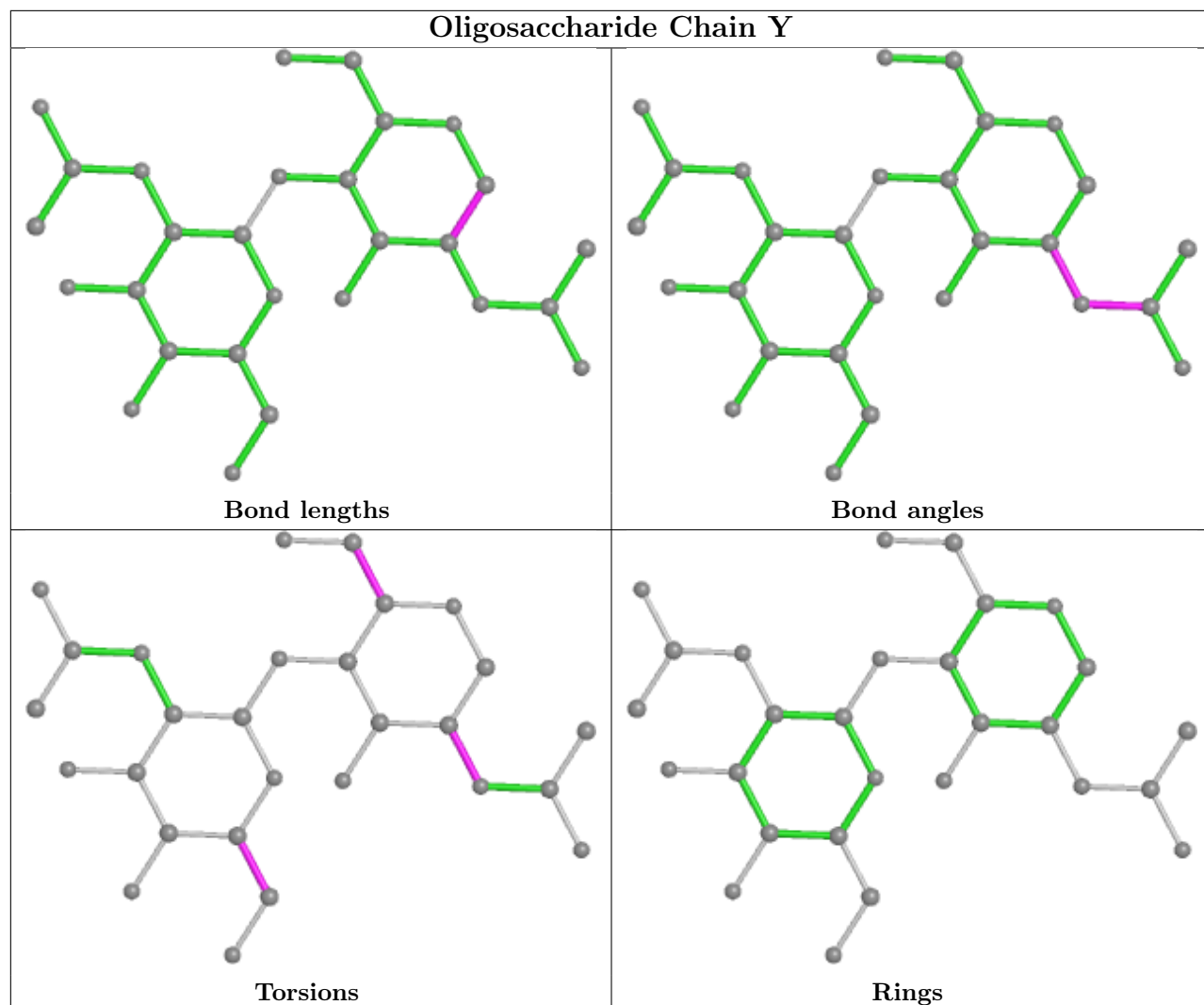


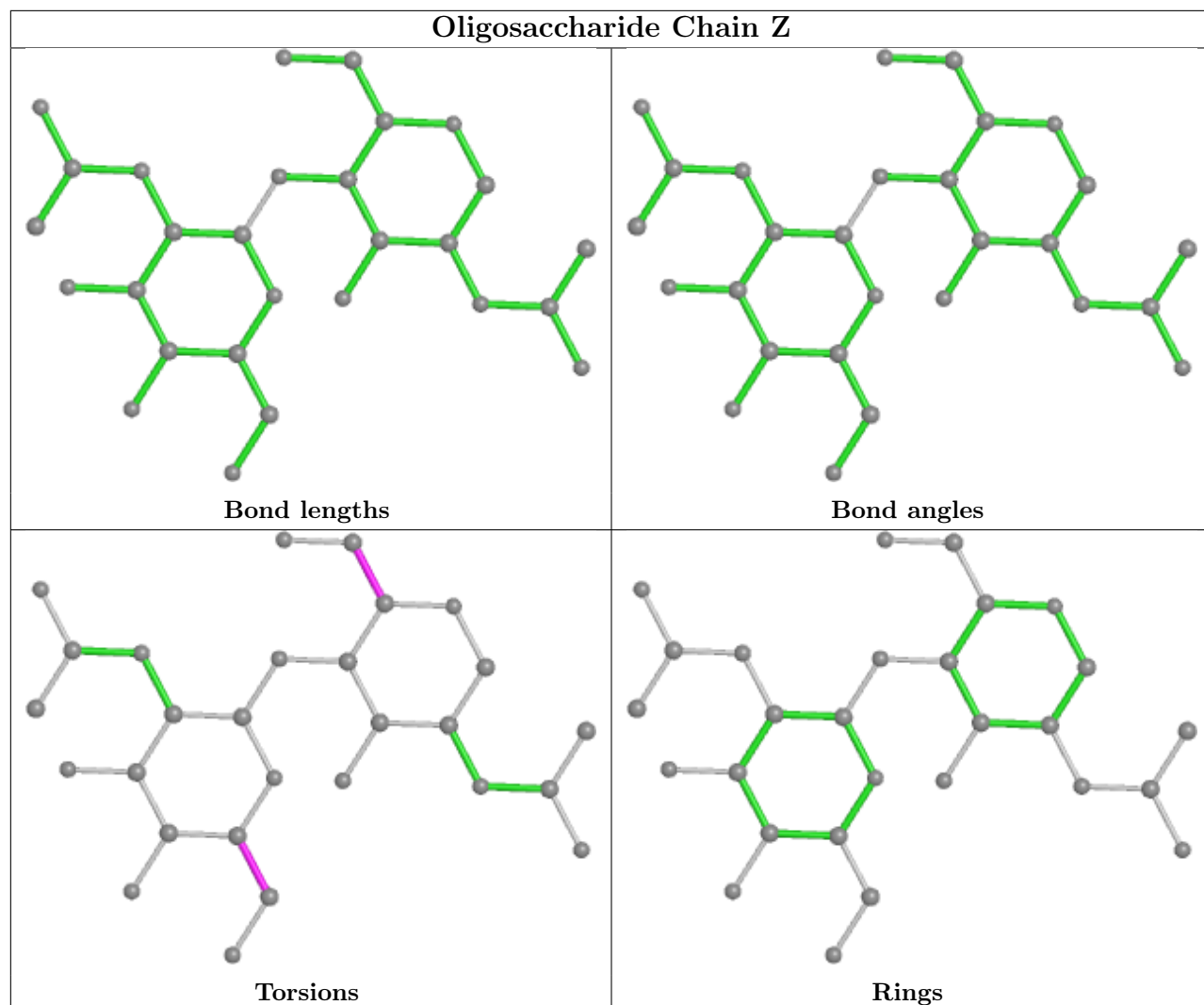


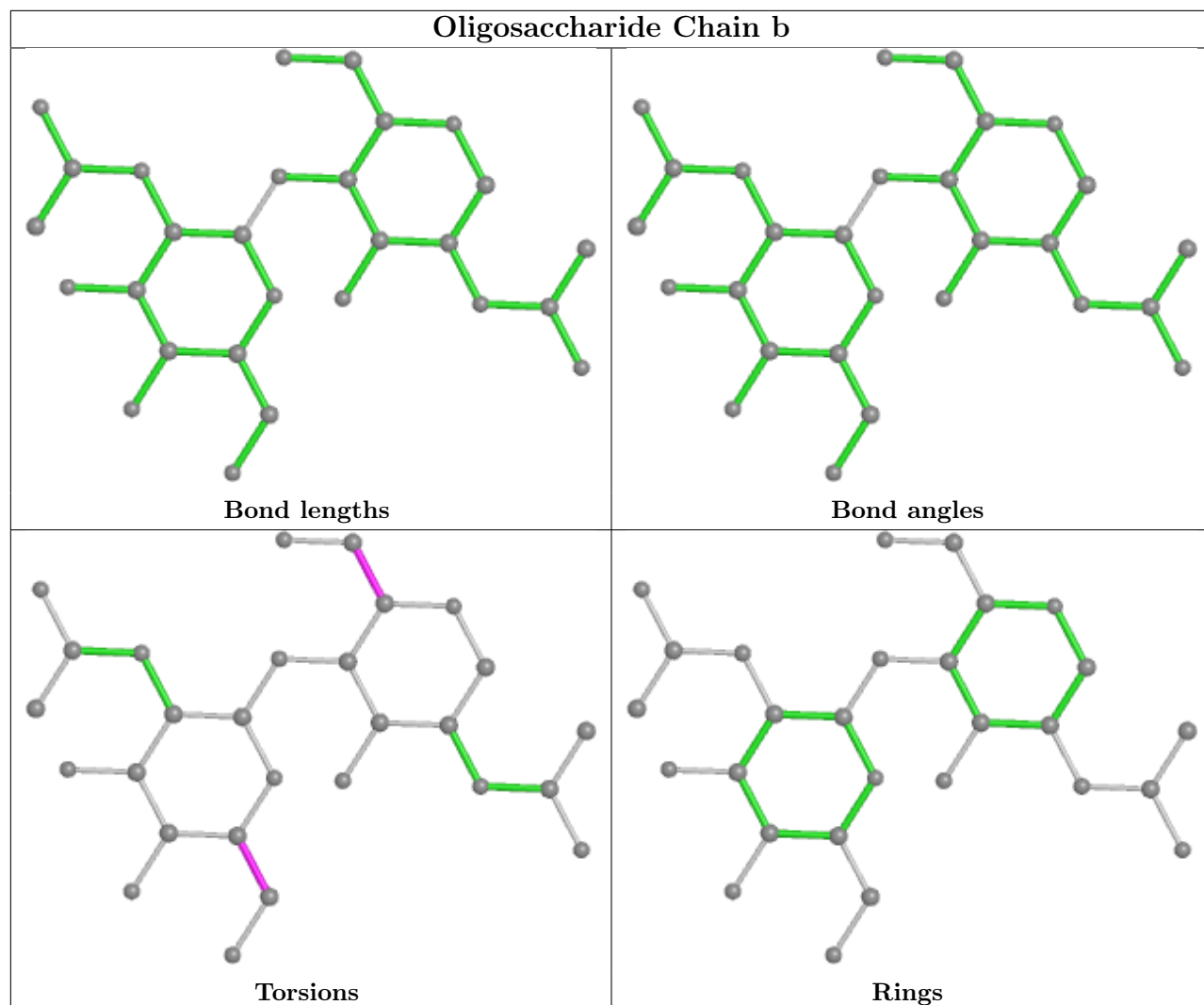


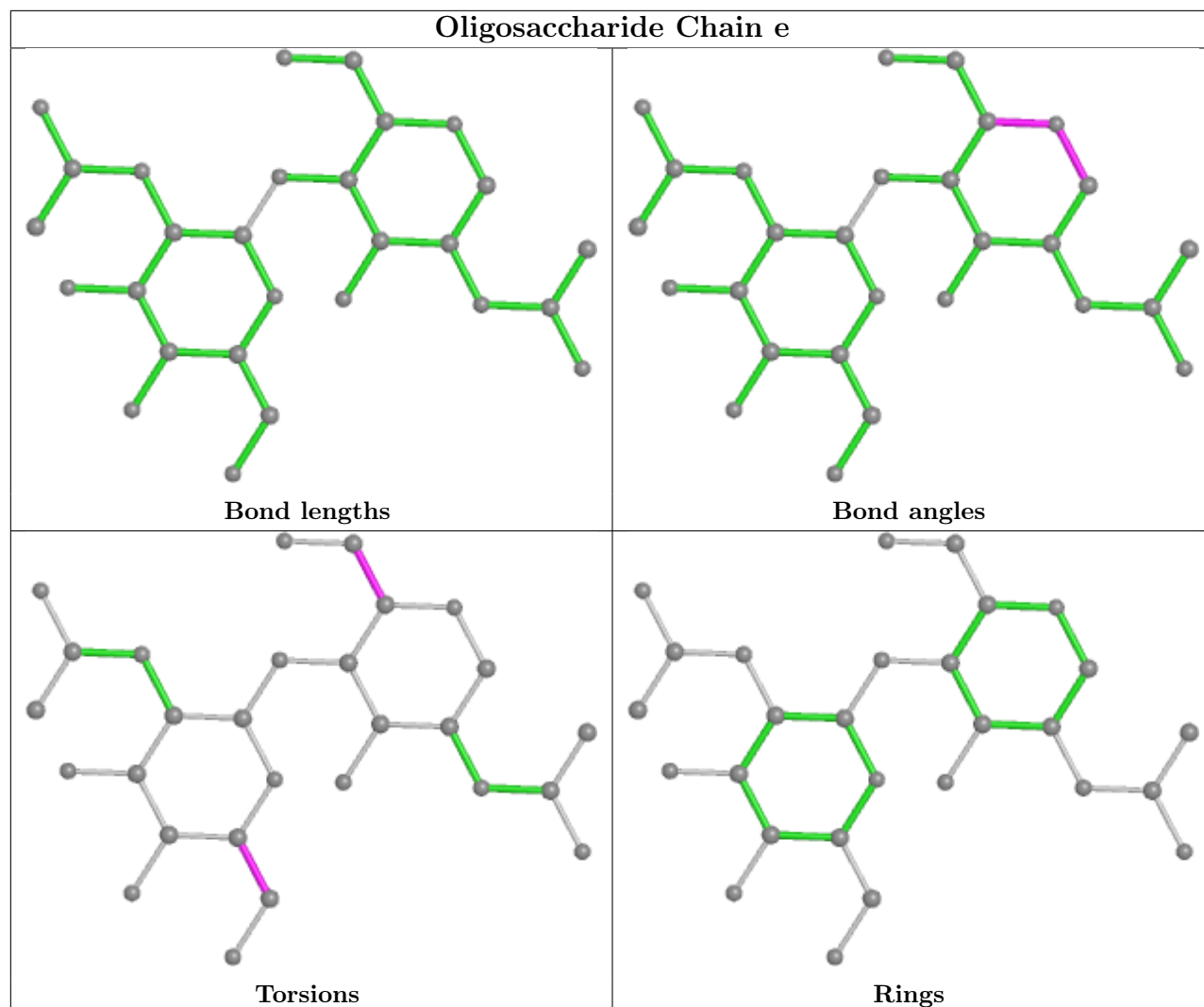




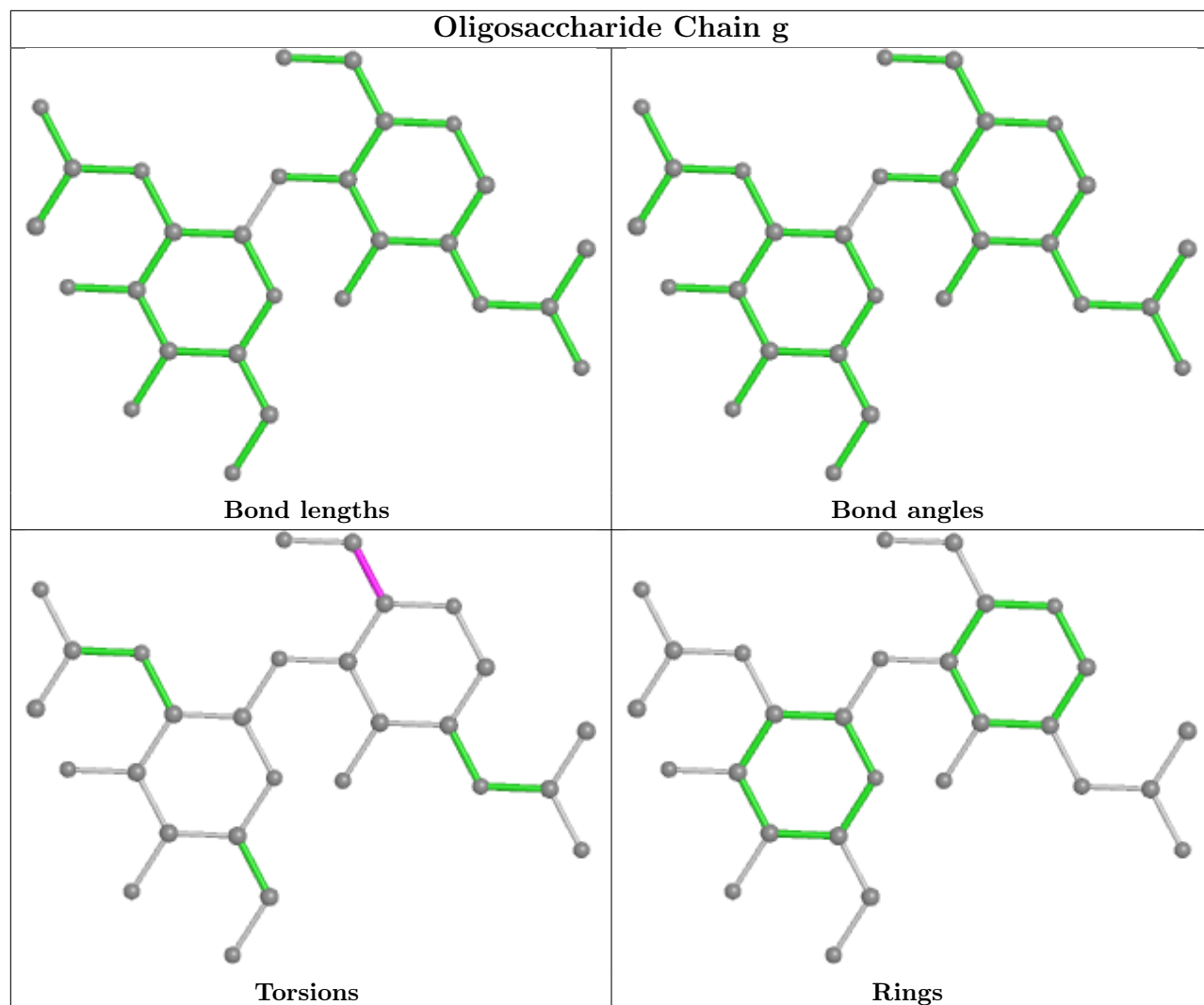


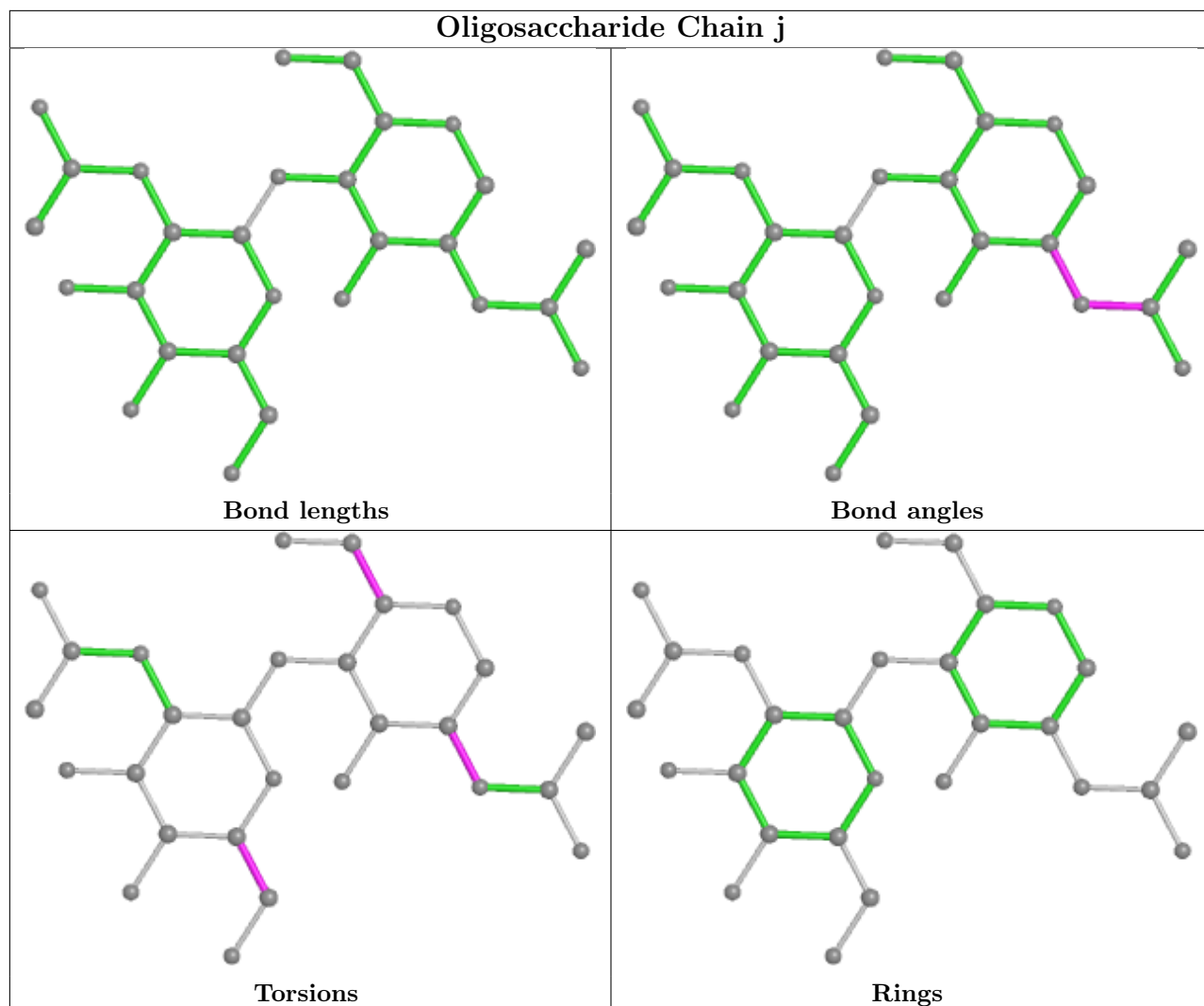


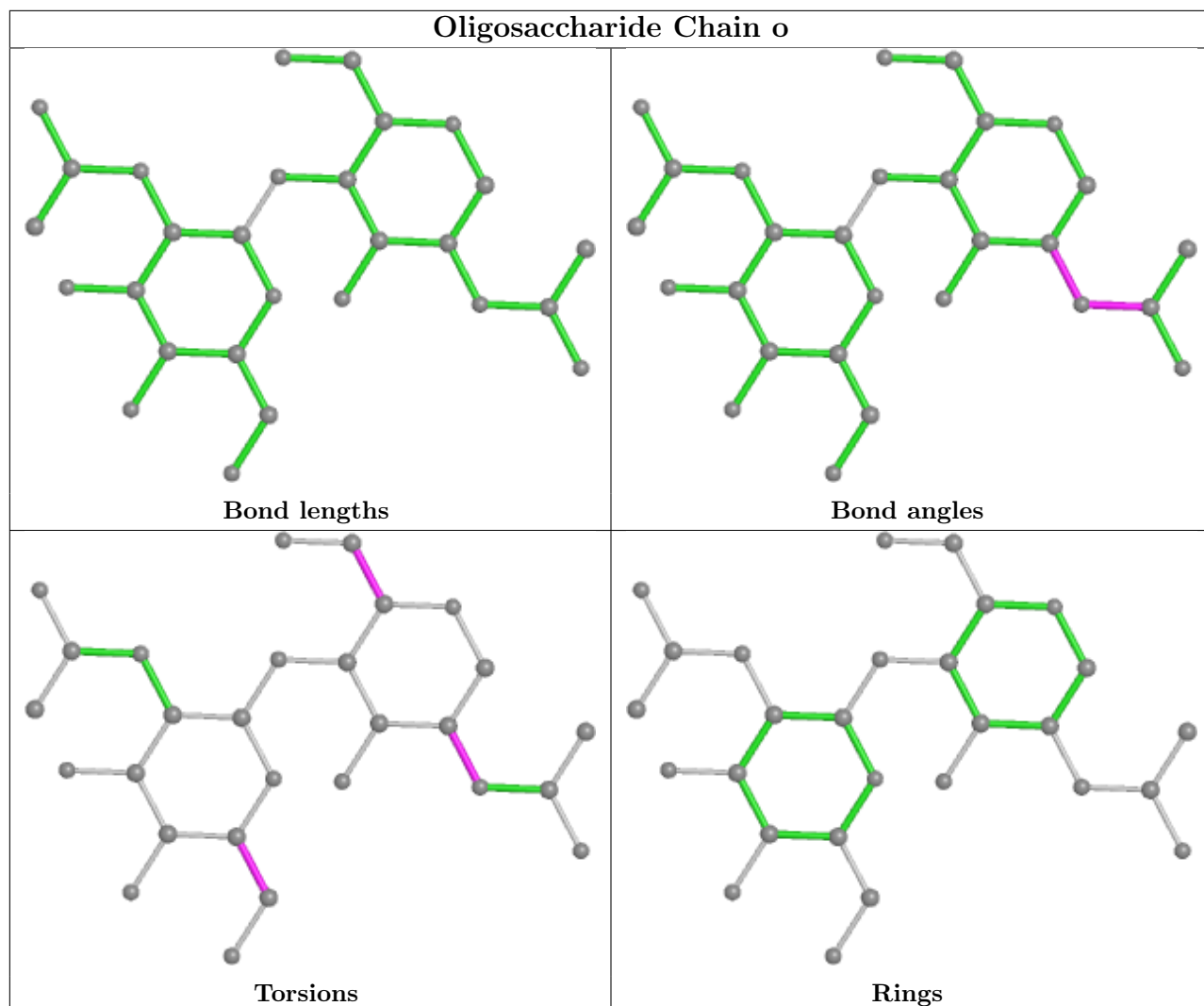


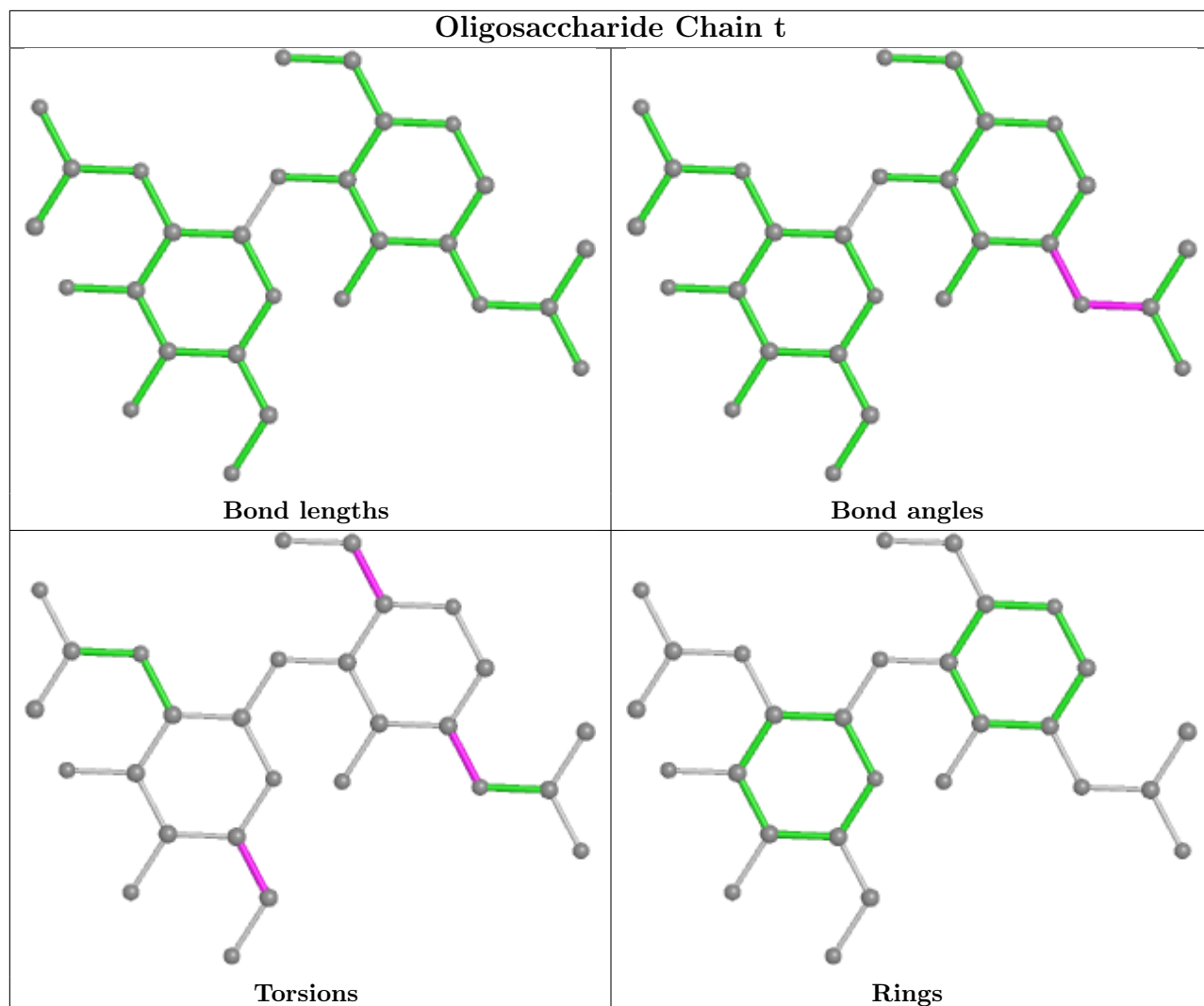


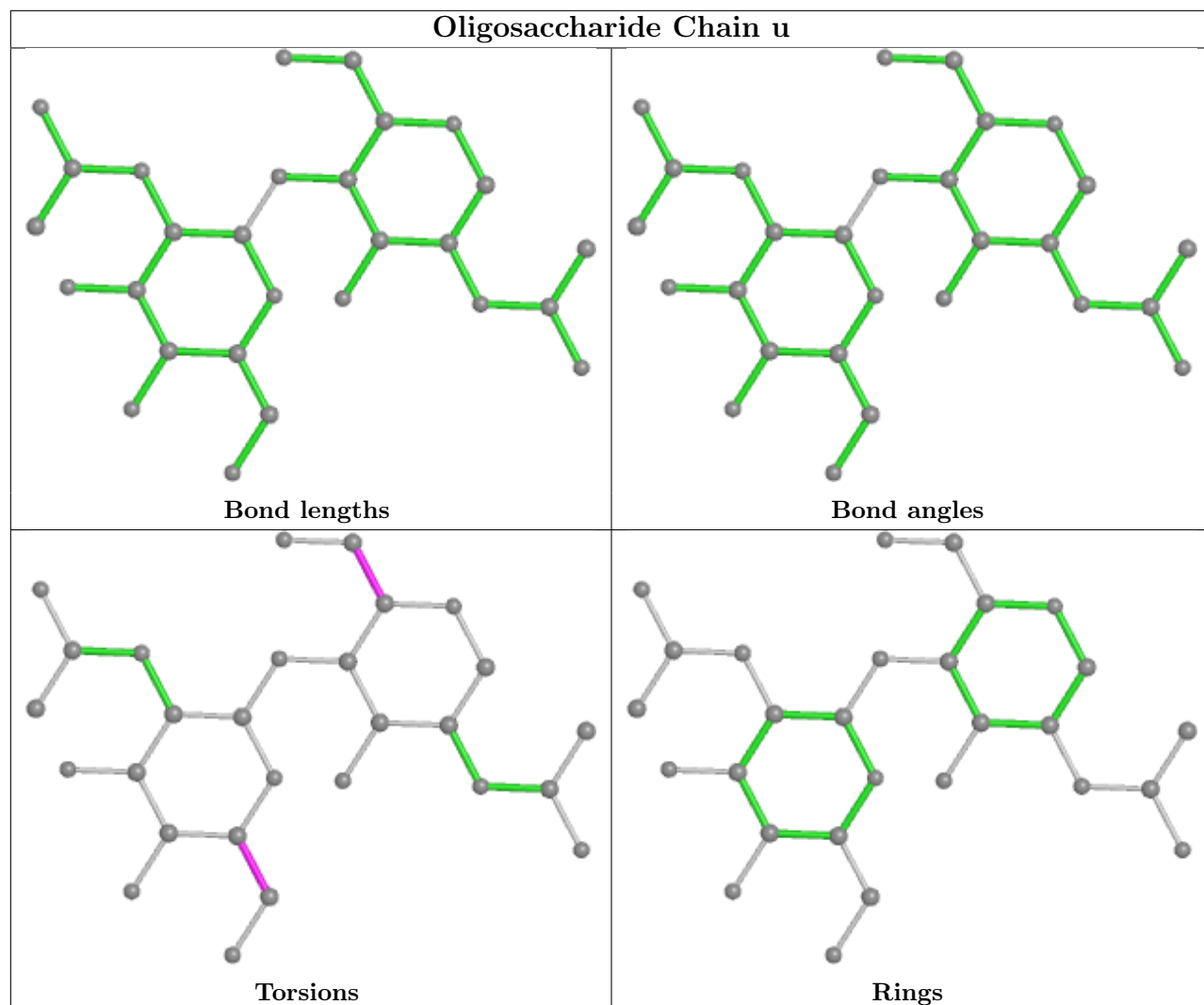


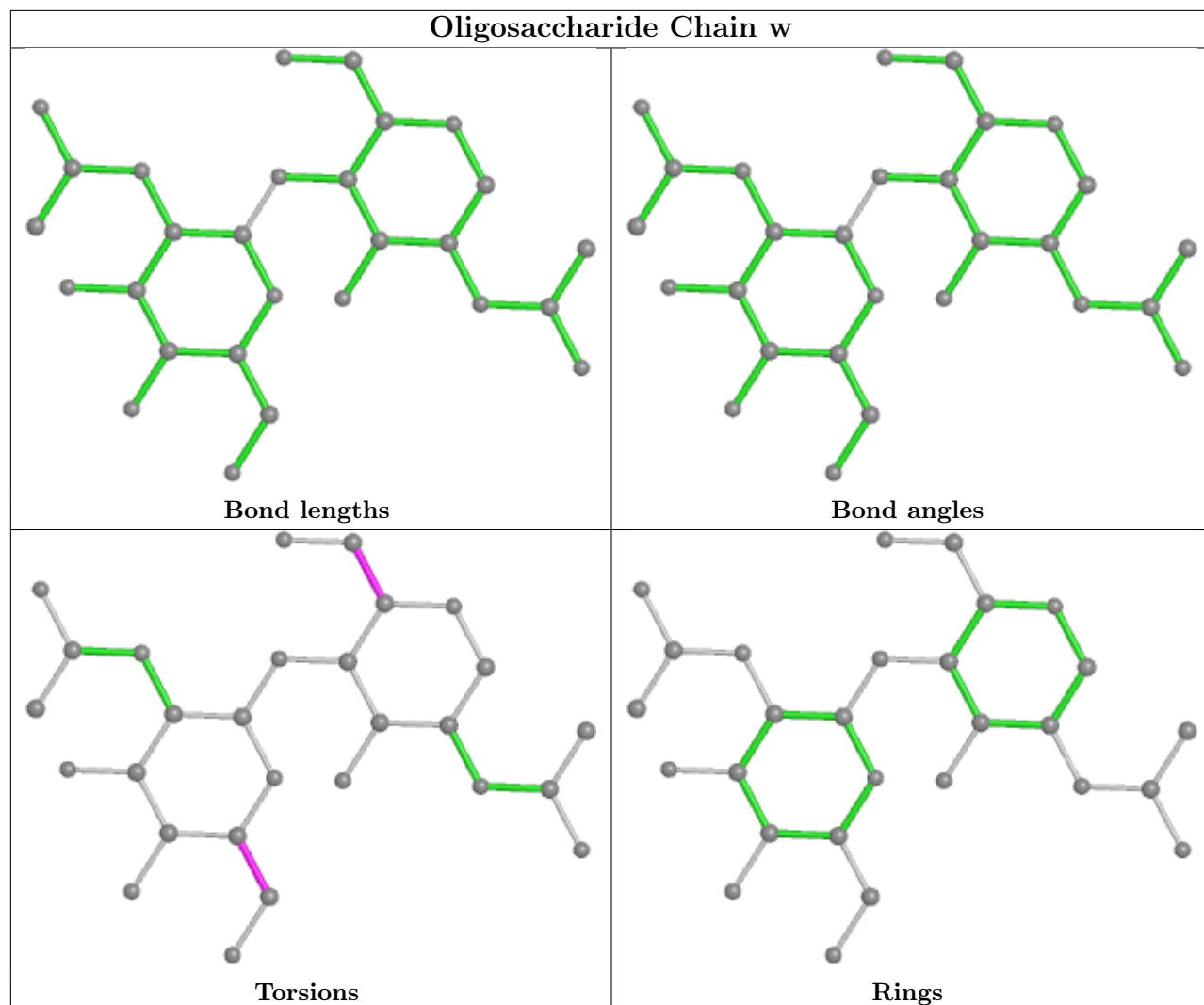


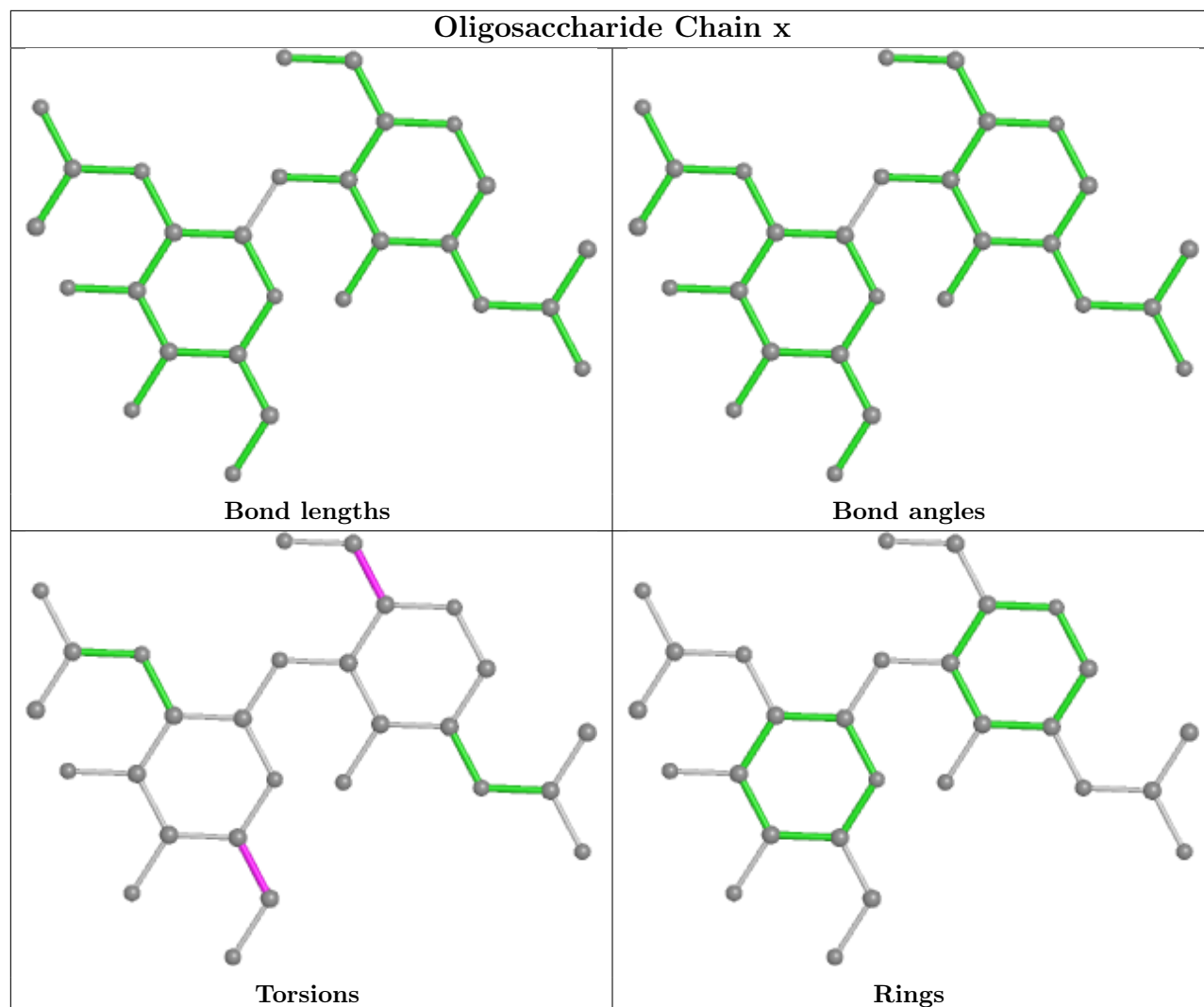


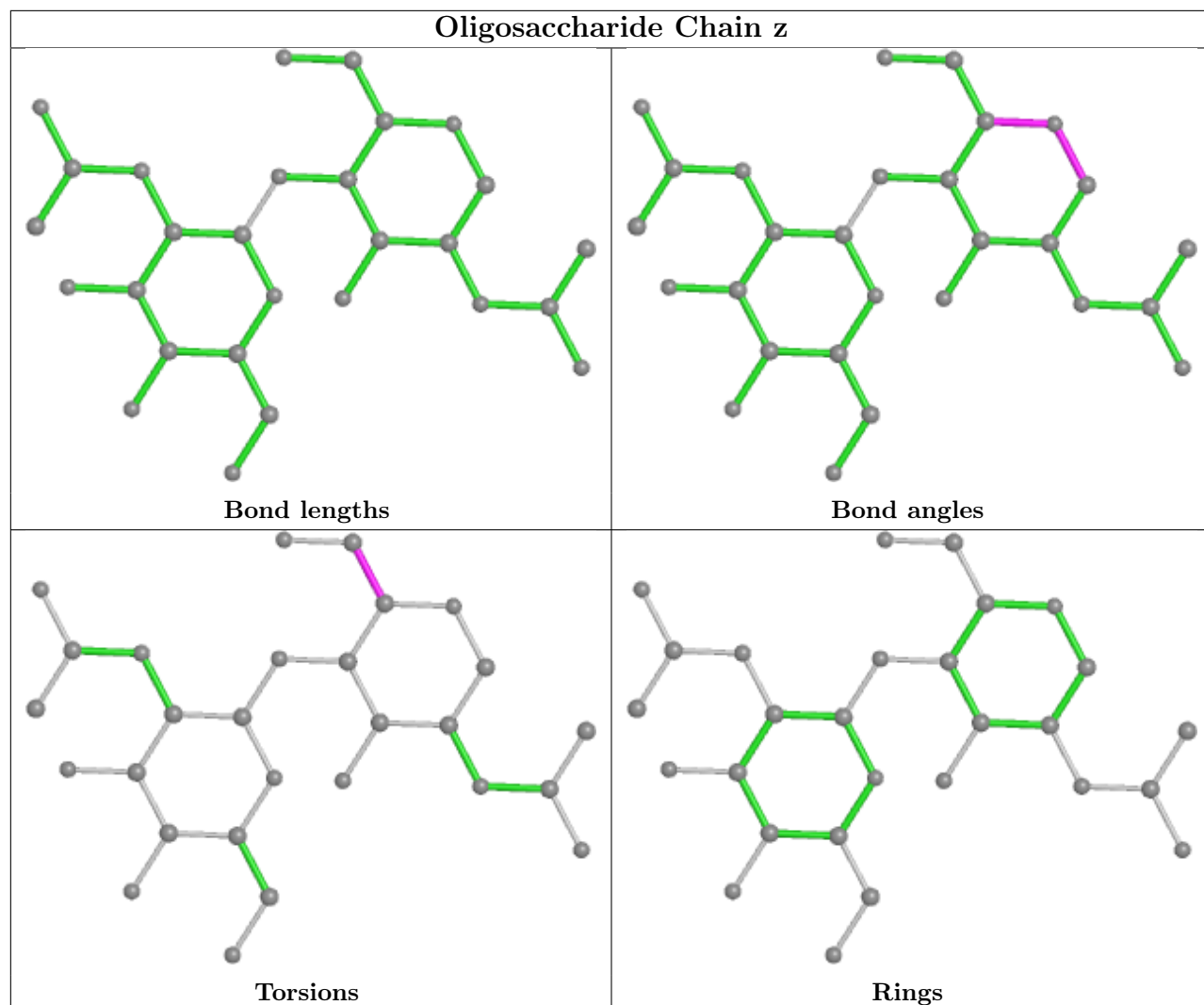




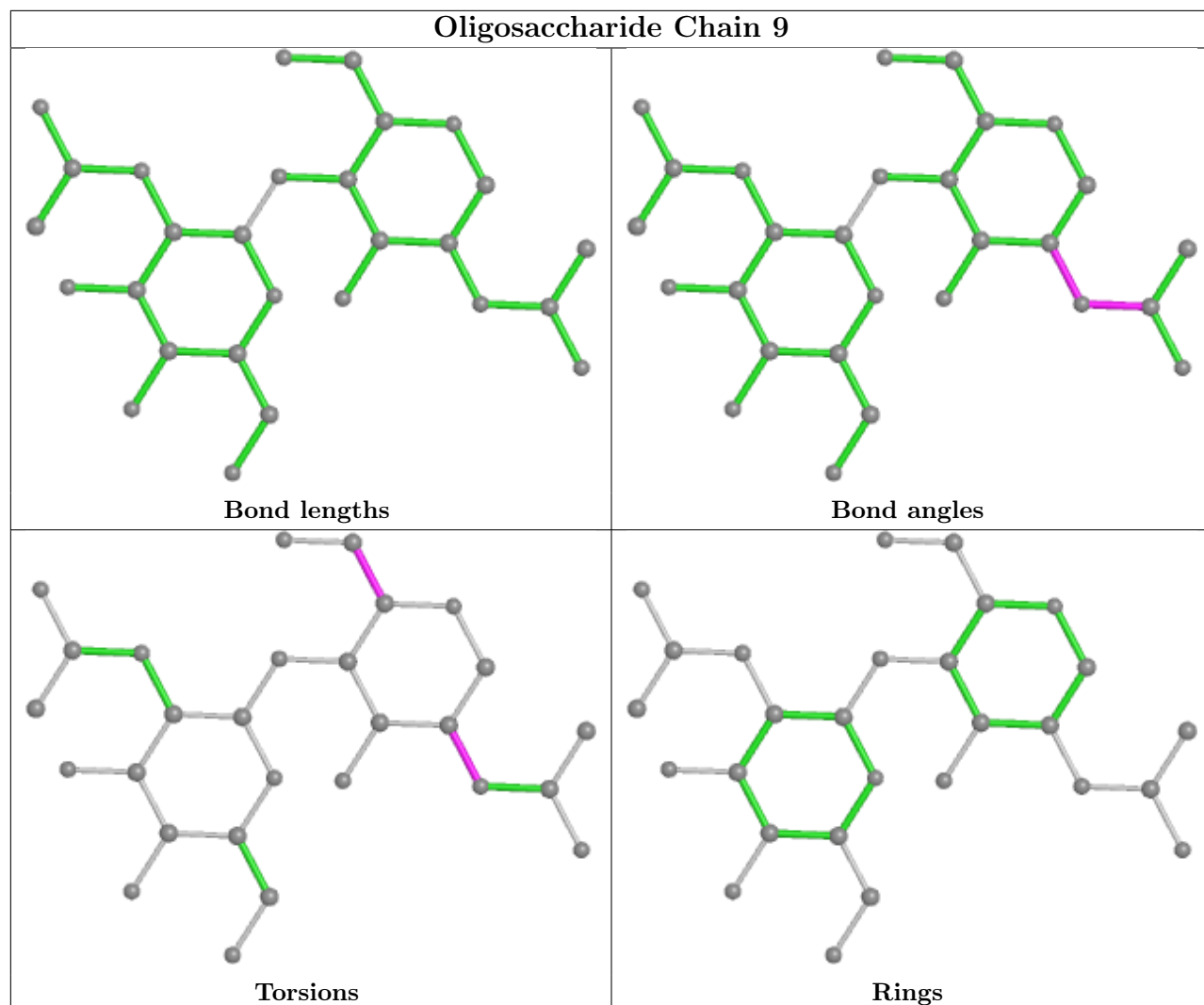


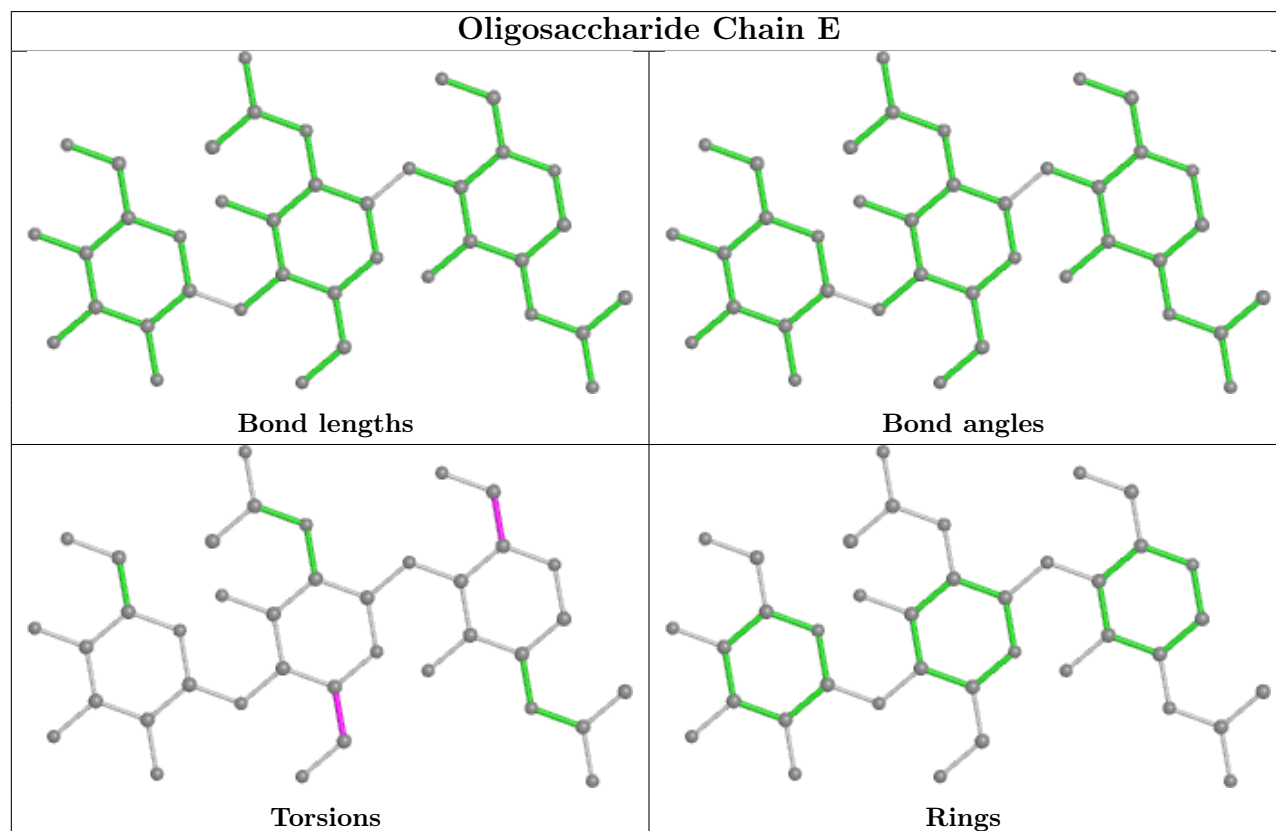
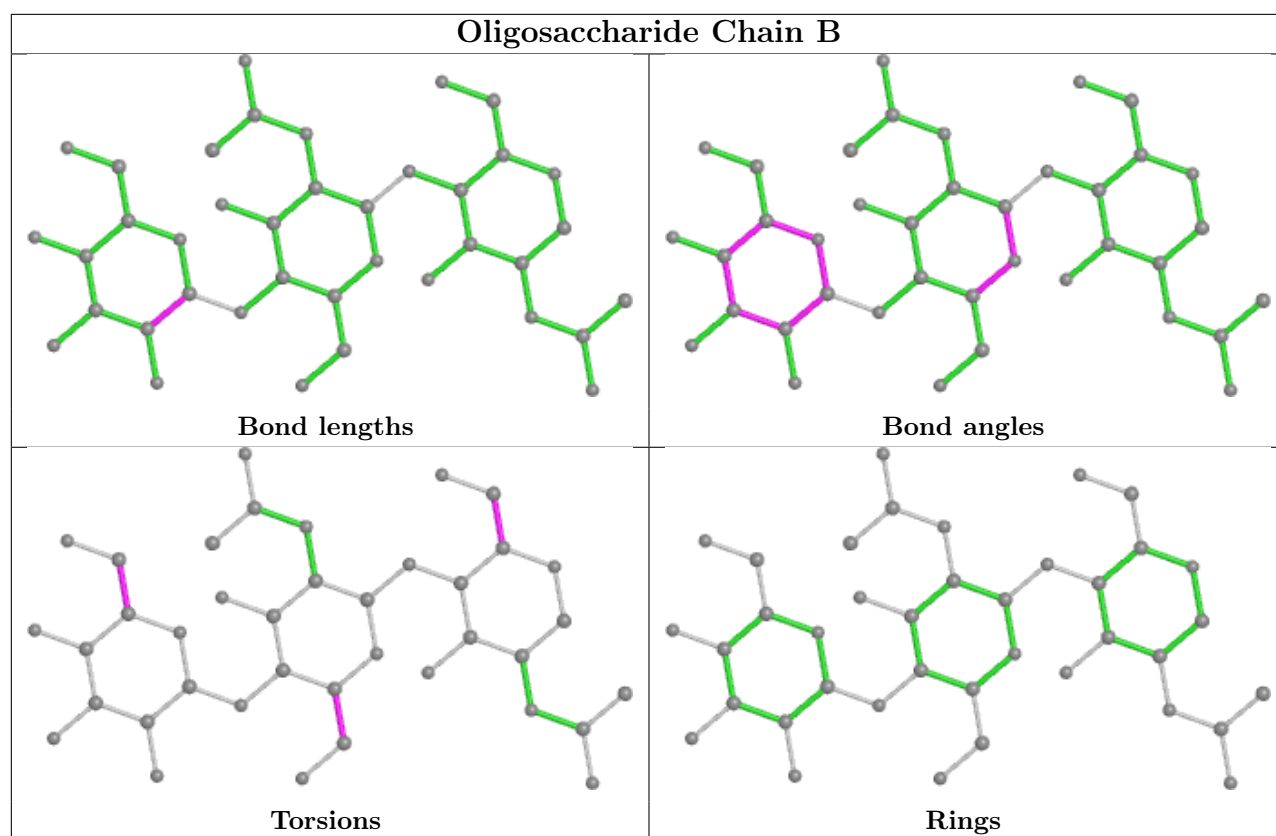


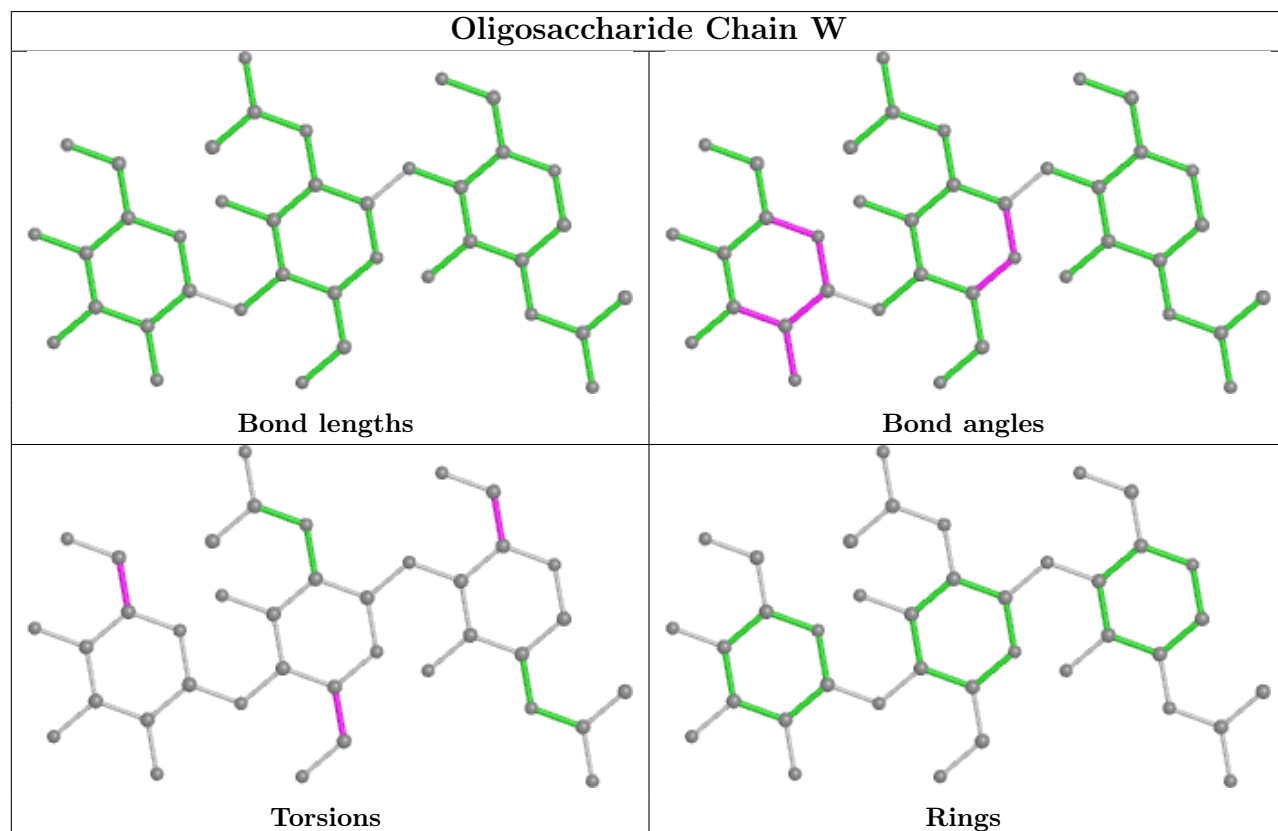
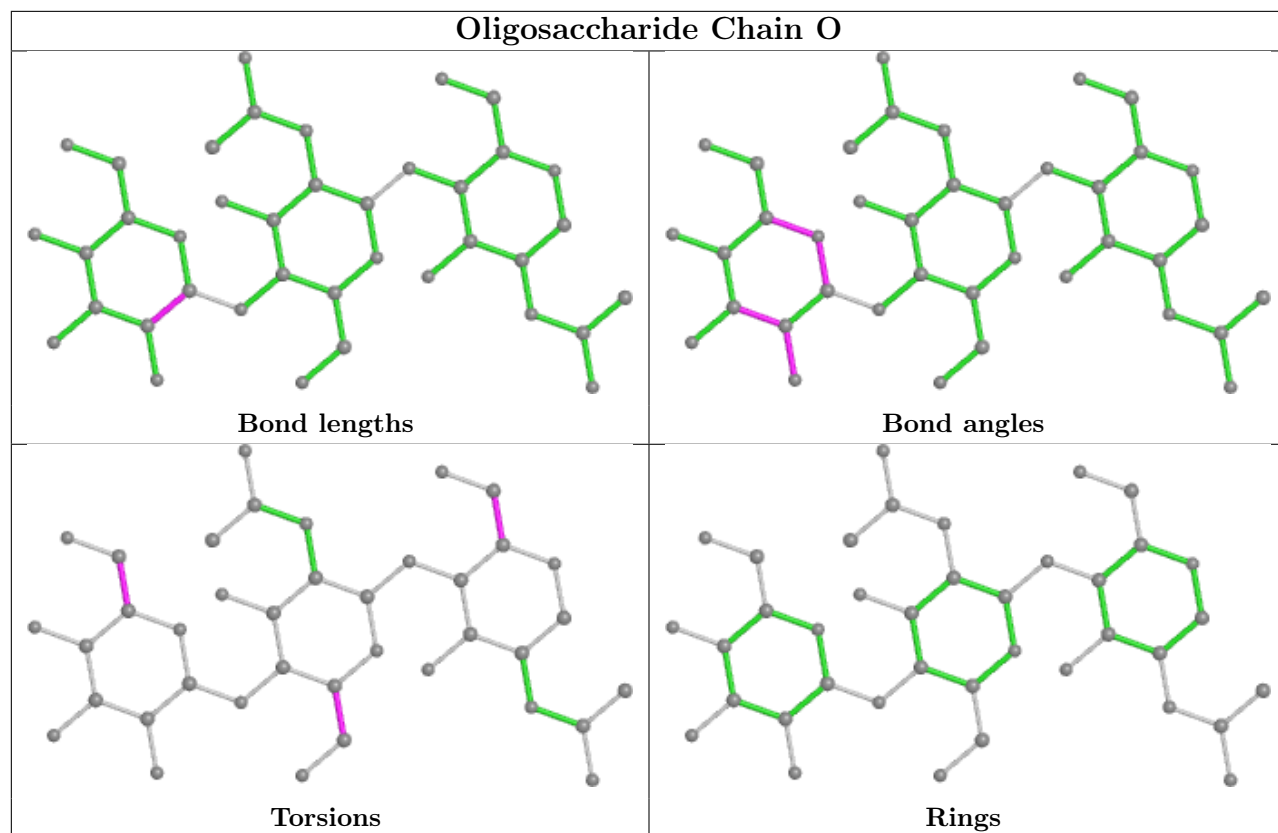


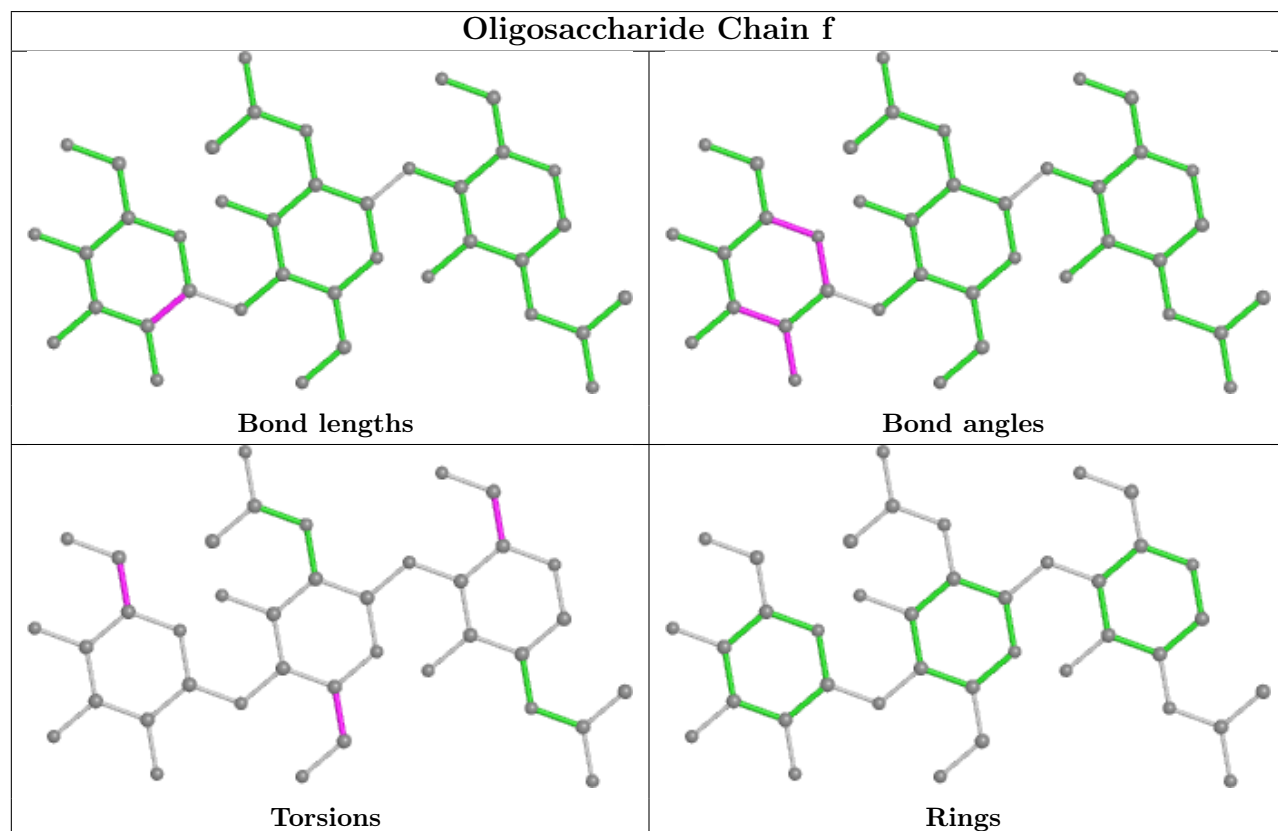
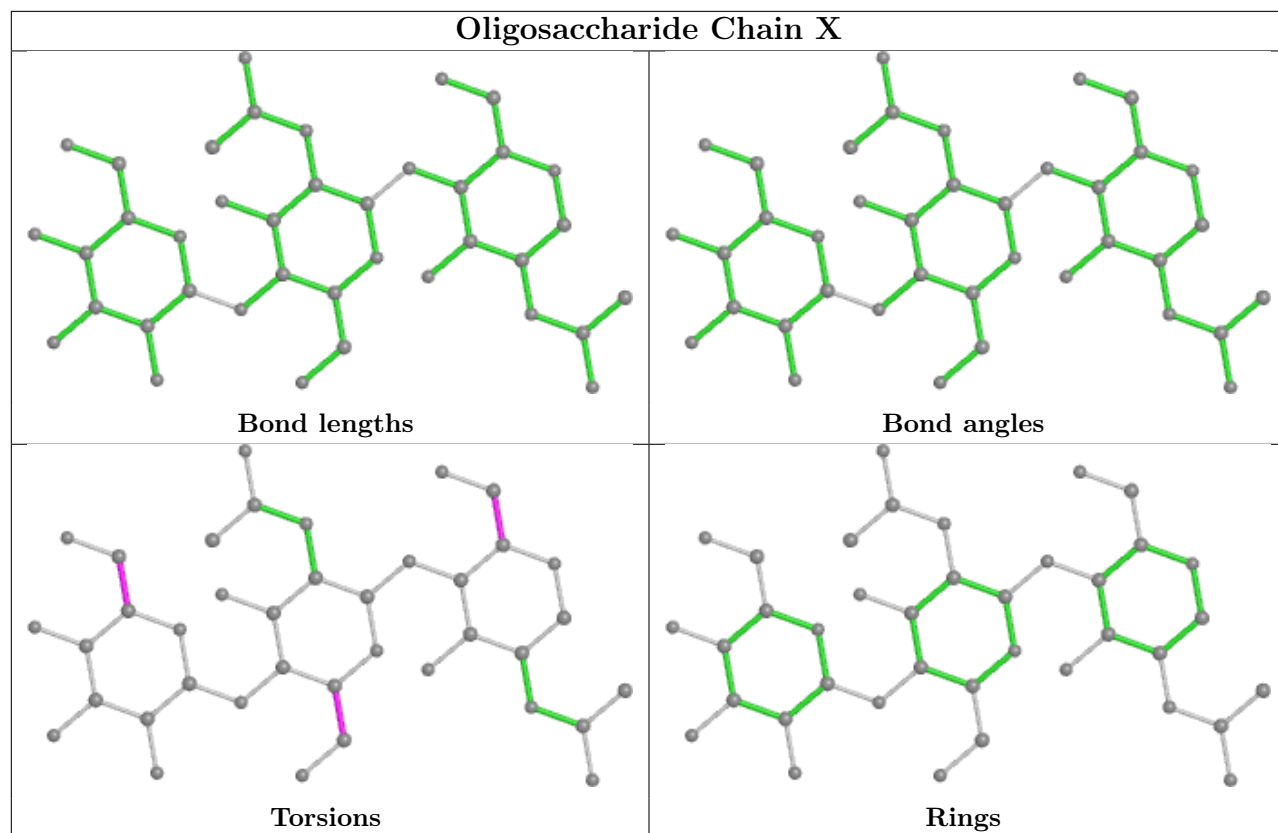


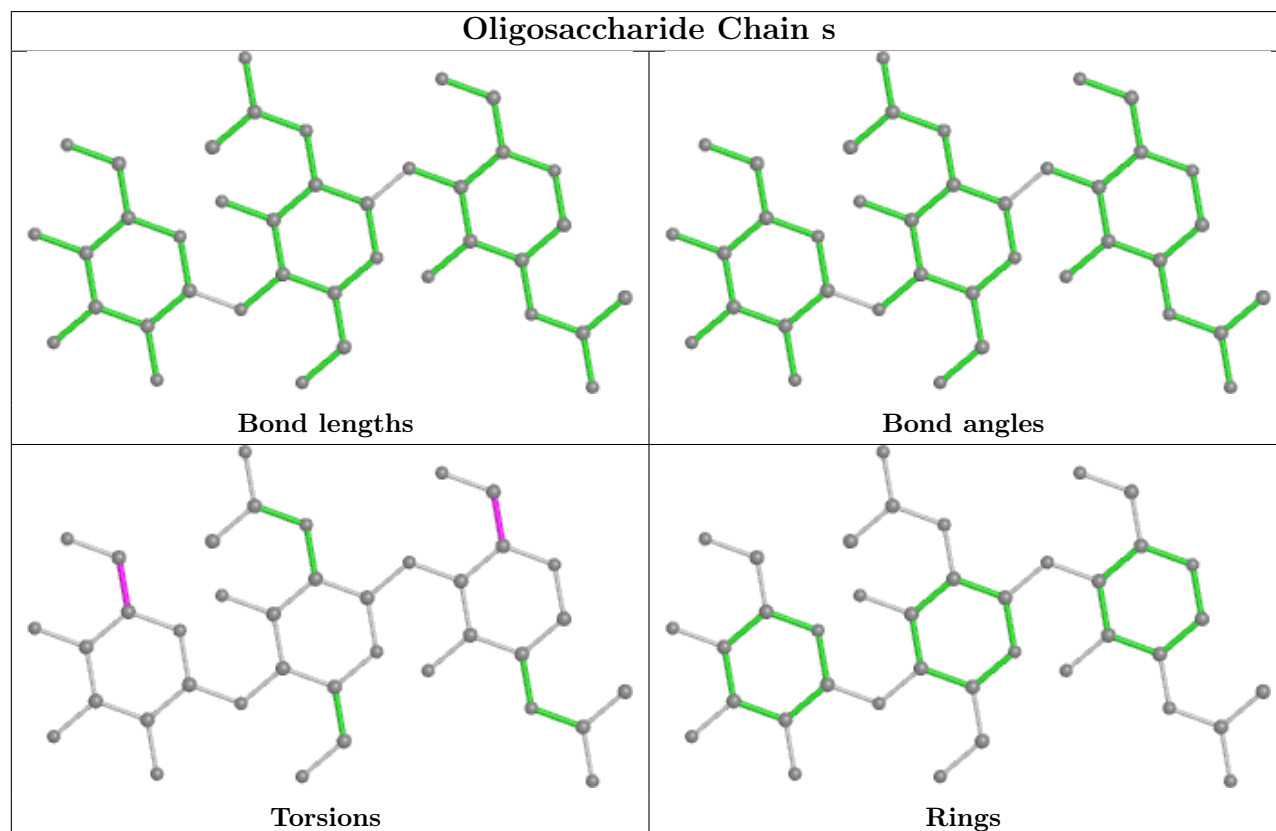
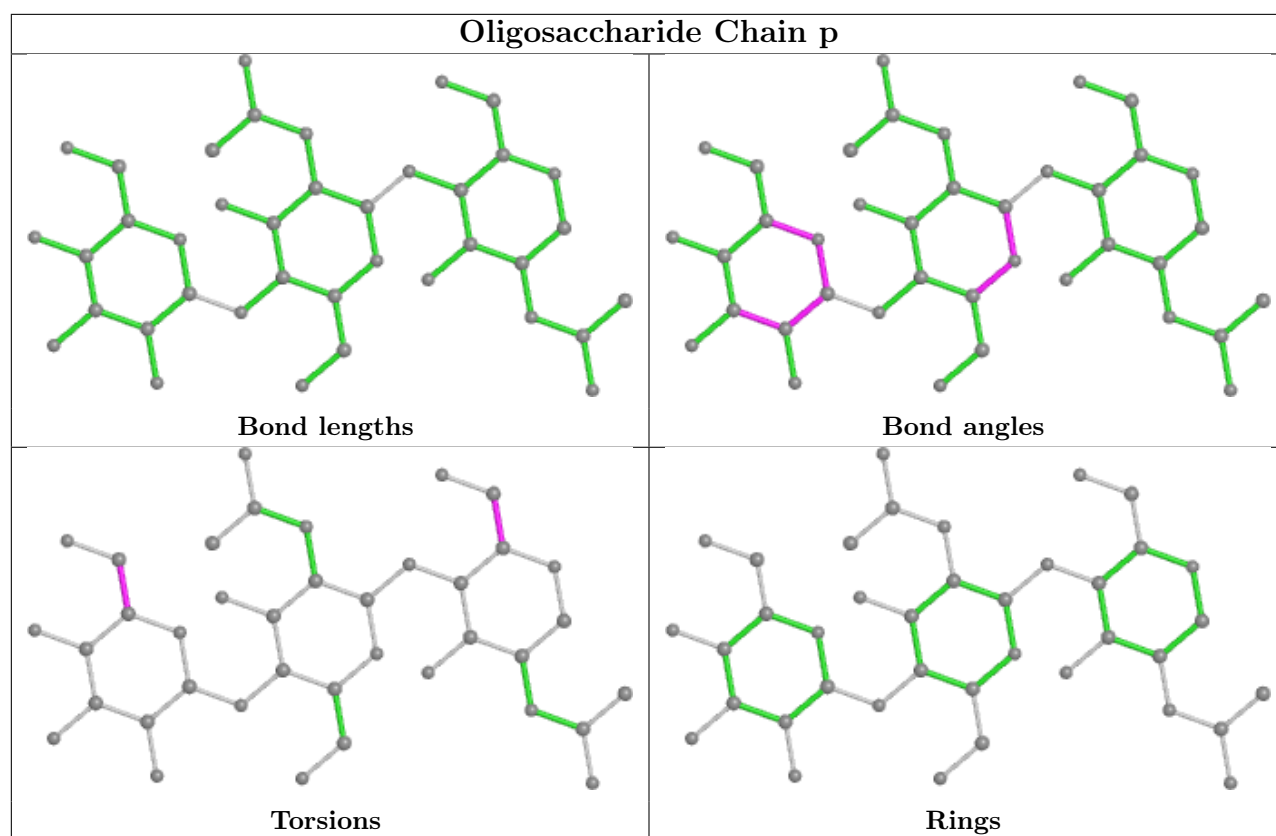


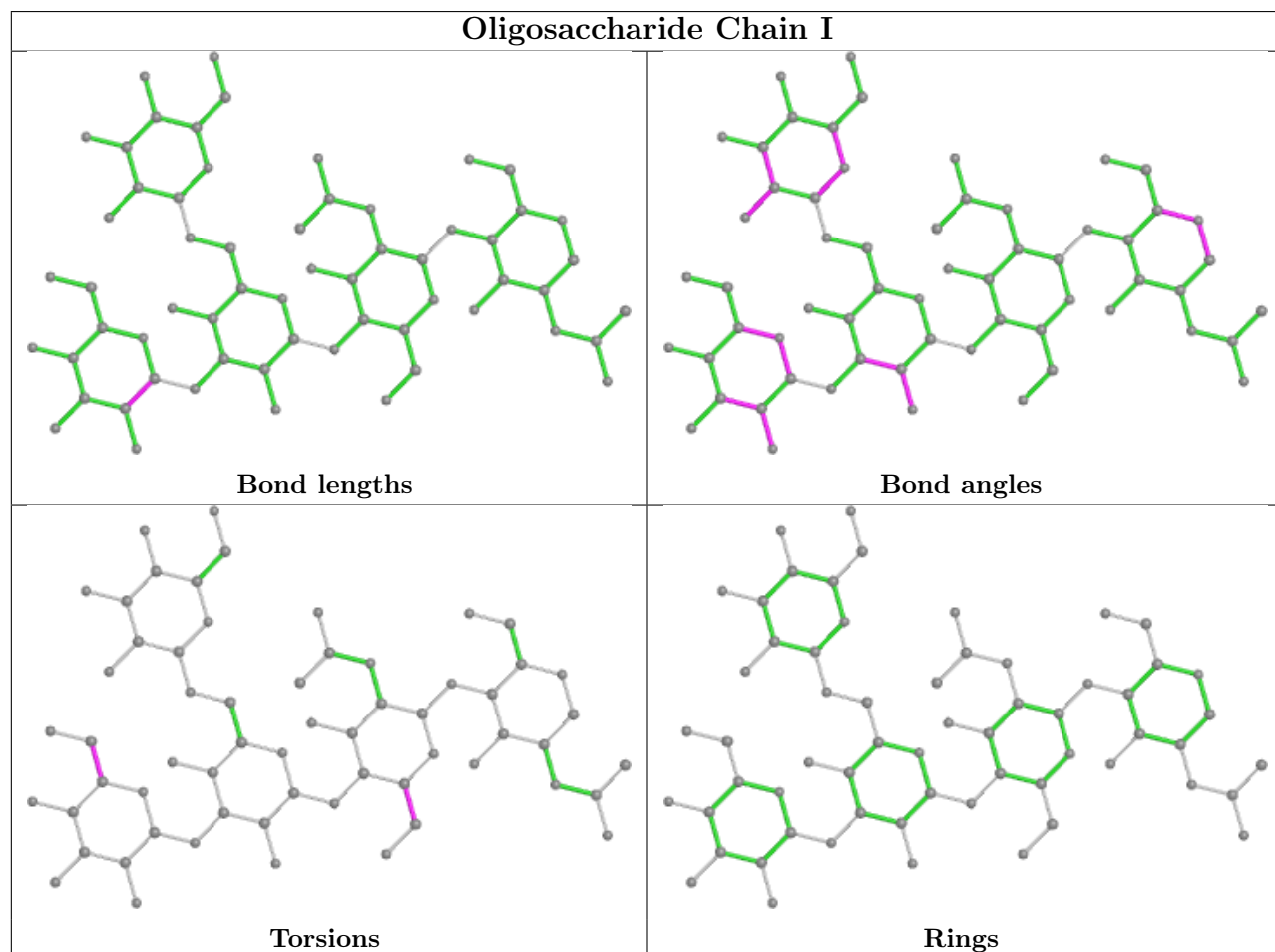
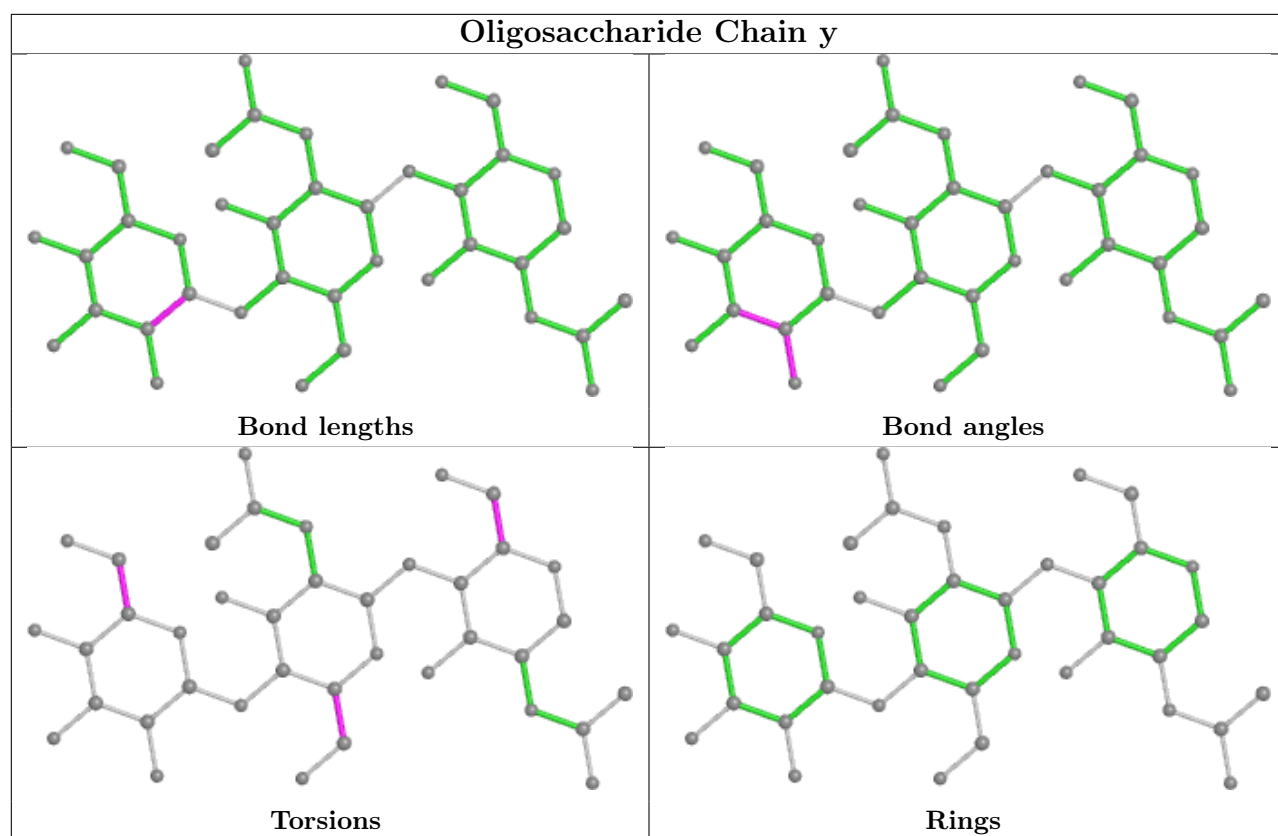


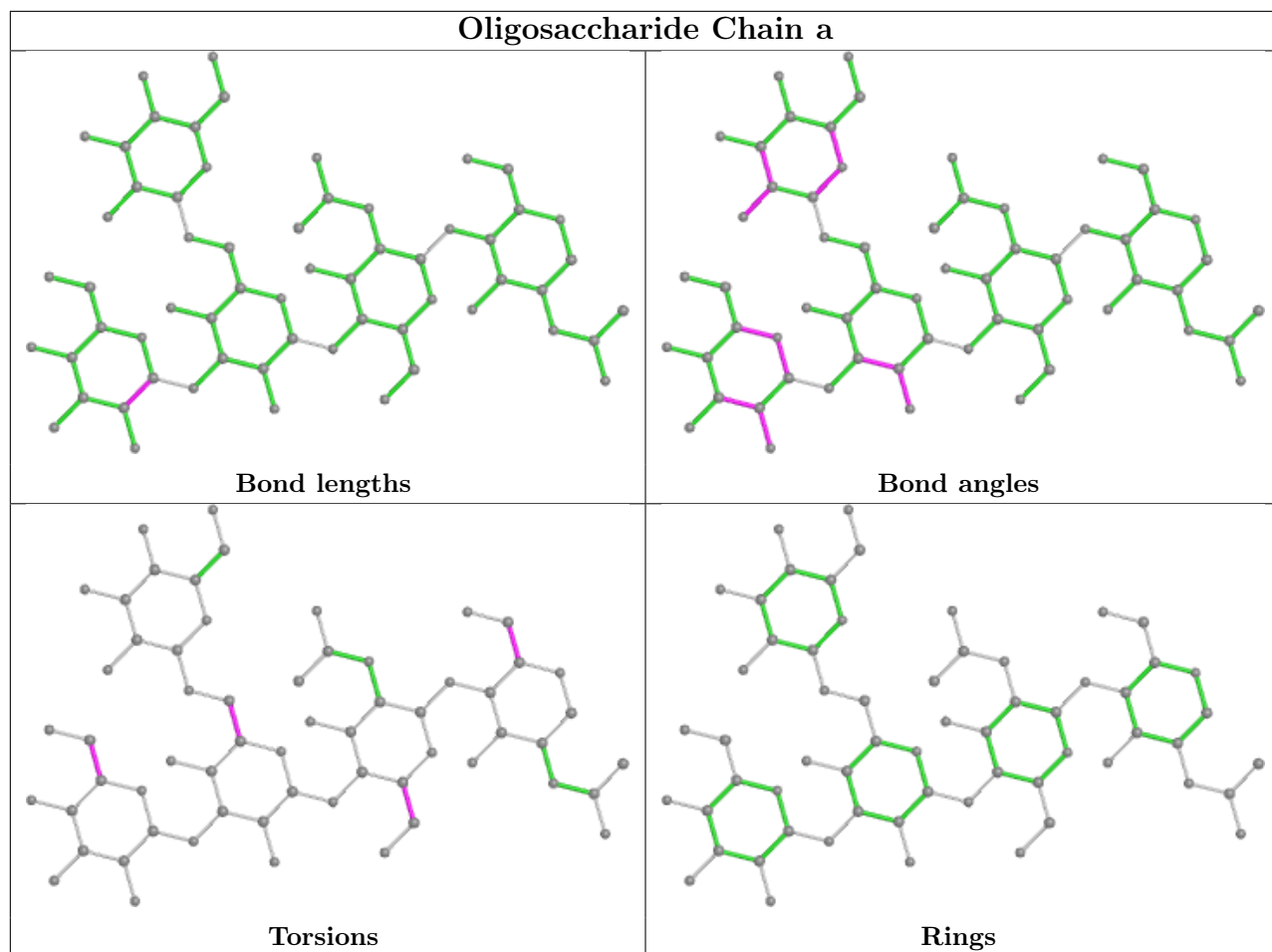


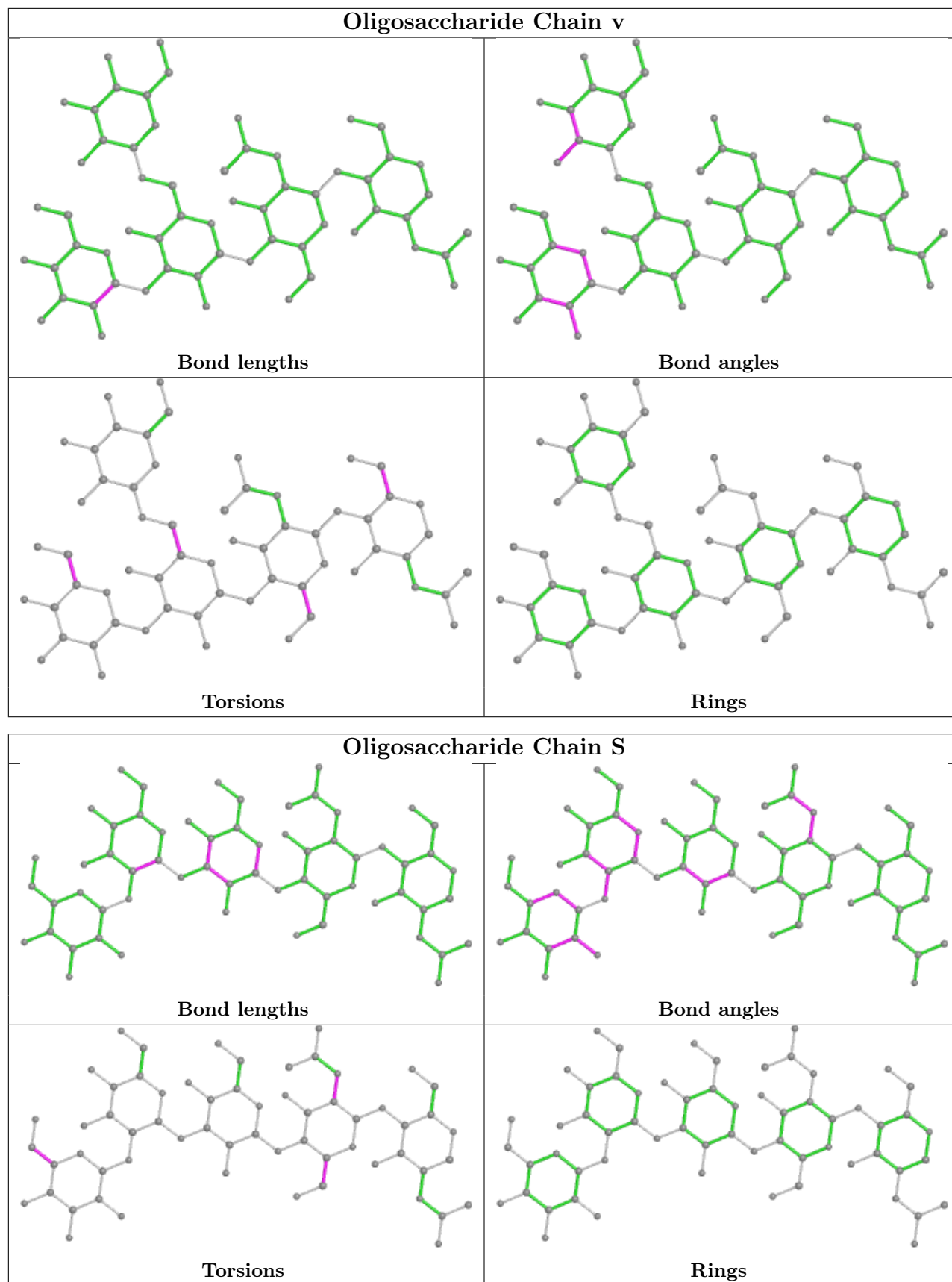




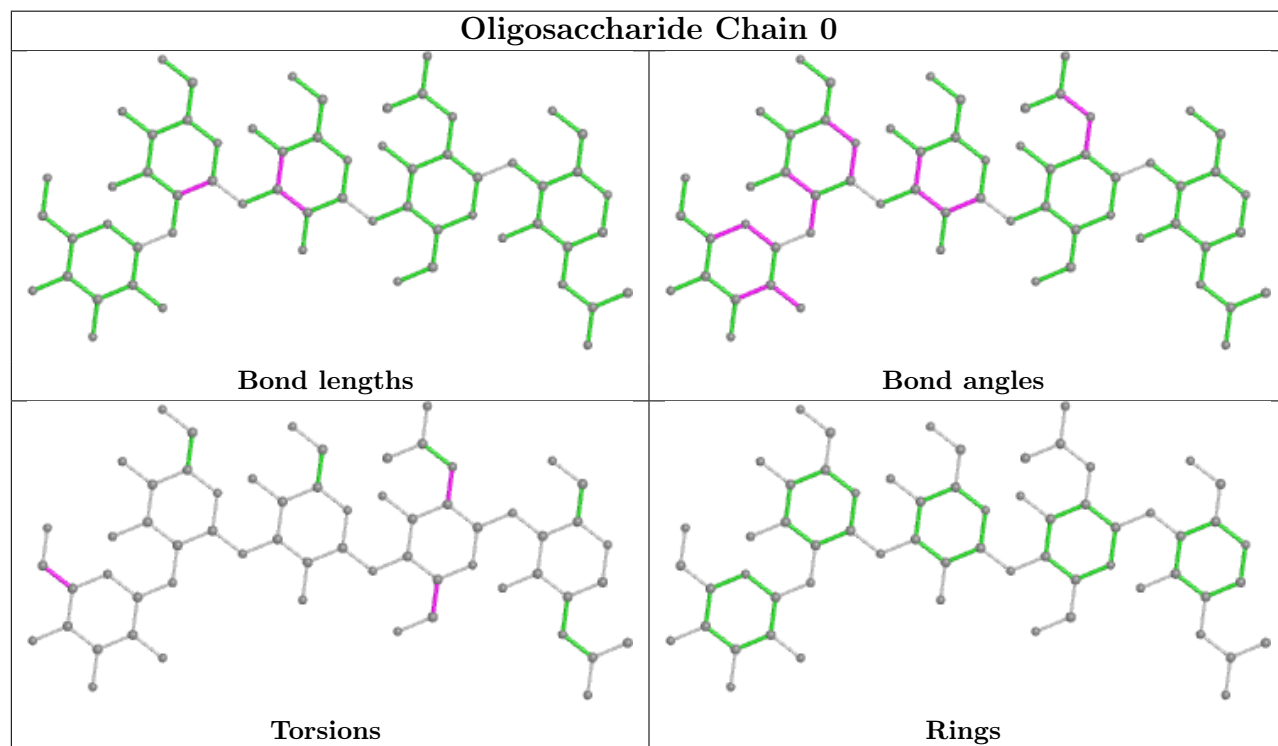
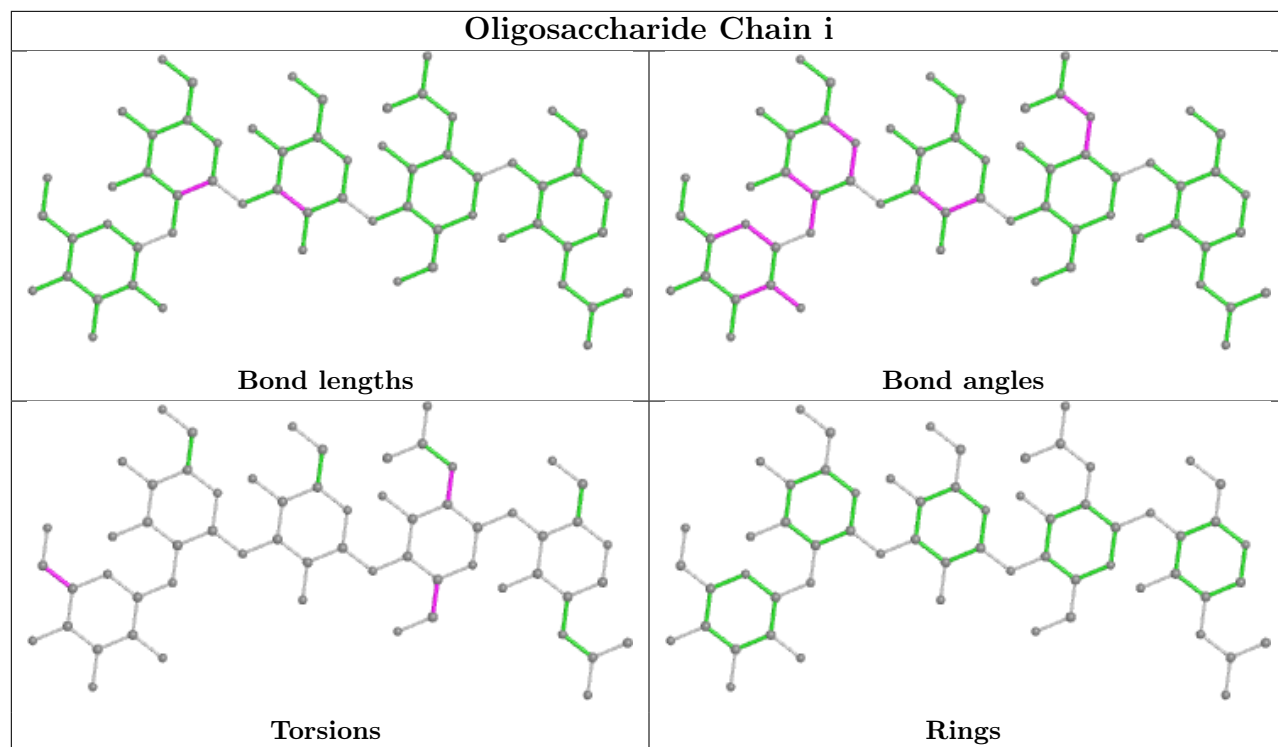


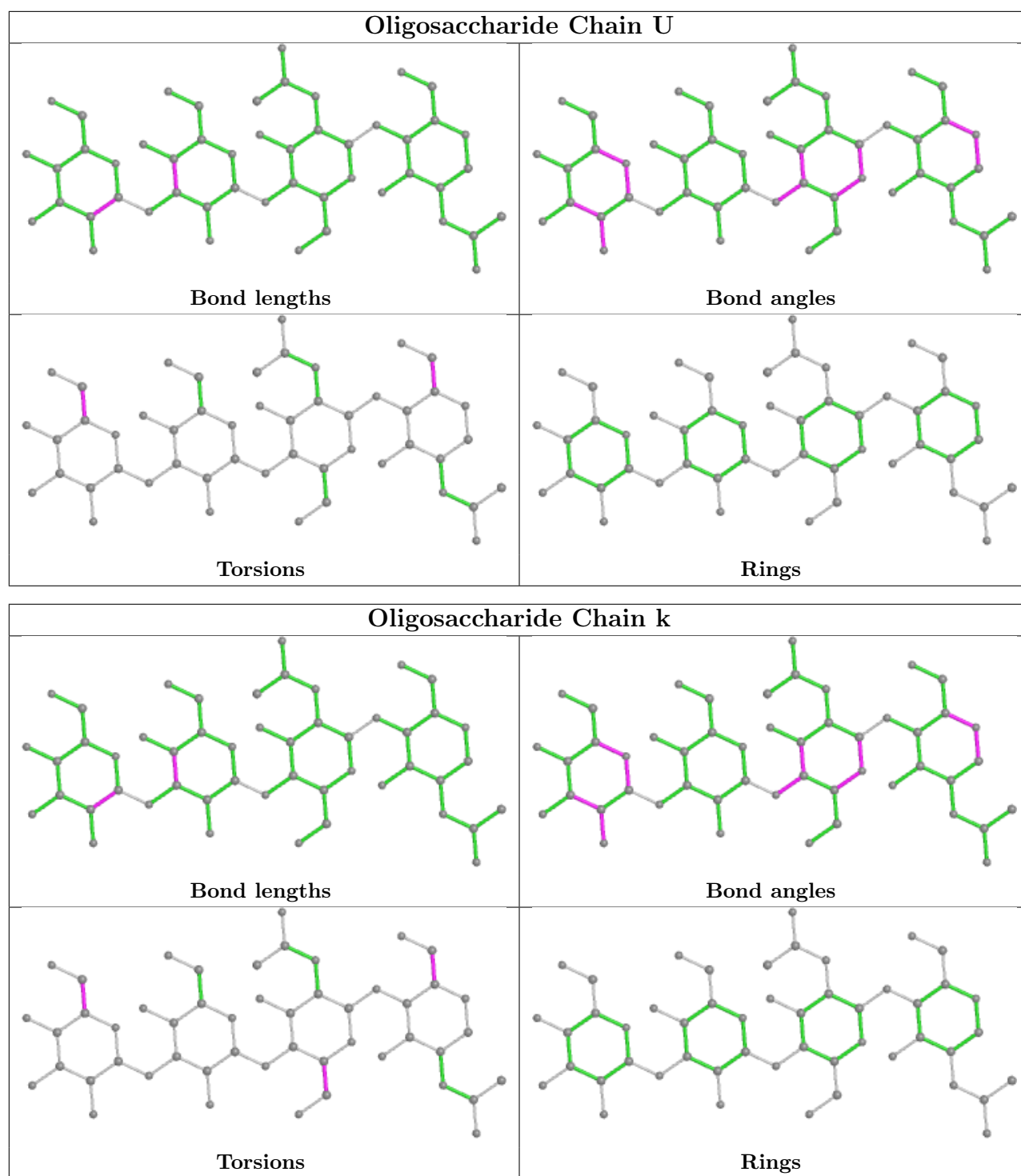


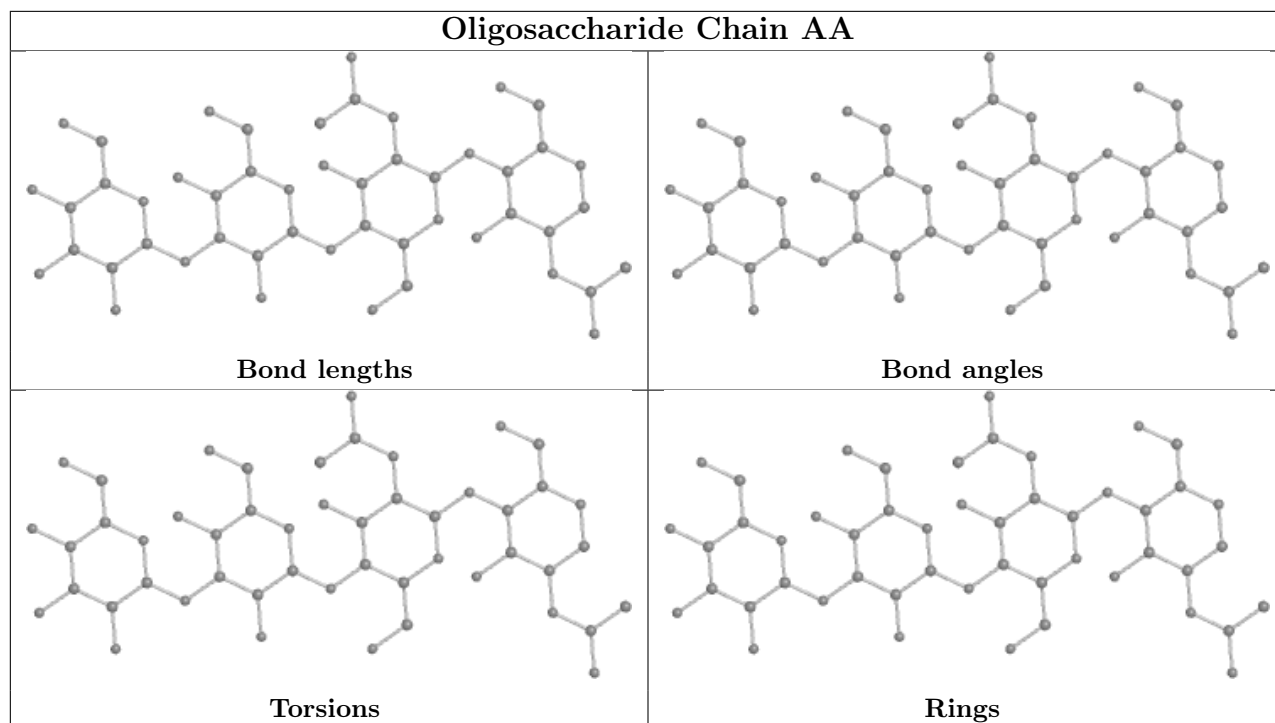












## 5.6 Ligand geometry [i](#)

3 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	2	611	1	14,14,15	0.22	0	17,19,21	0.55	0
14	NAG	c	611	1	14,14,15	0.24	0	17,19,21	0.59	0
14	NAG	C	611	1	14,14,15	0.22	0	17,19,21	0.53	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	2	611	1	-	0/6/23/26	0/1/1/1
14	NAG	c	611	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	NAG	C	611	1	-	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 (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	C	611	NAG	C4-C5-C6-O6
14	C	611	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

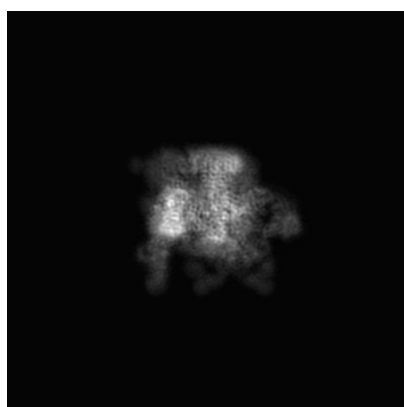
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7621. These allow visual inspection of the internal detail of the map and identification of artifacts.

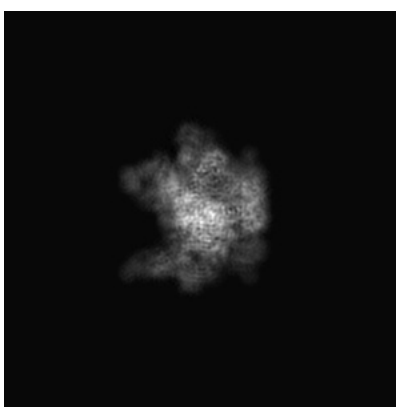
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

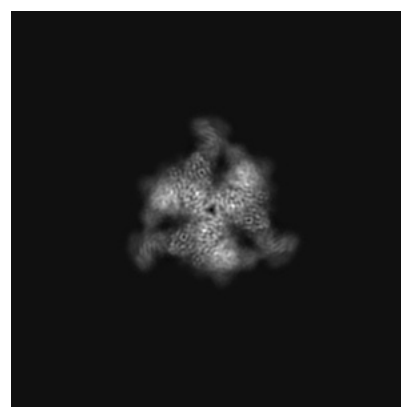
#### 6.1.1 Primary map



X



Y

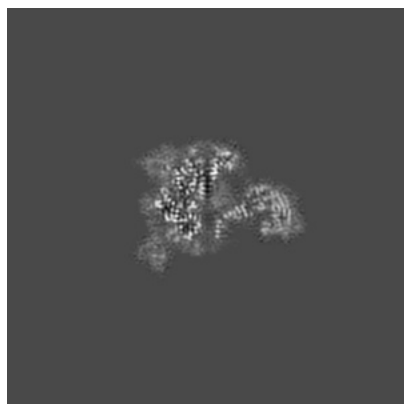


Z

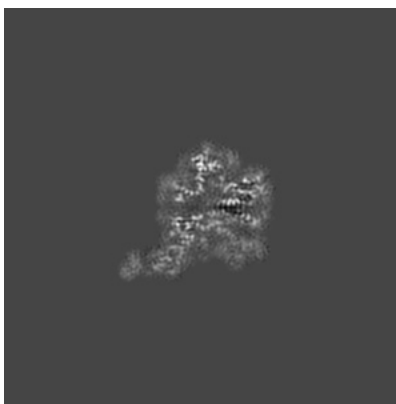
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

#### 6.2.1 Primary map



X Index: 192



Y Index: 192

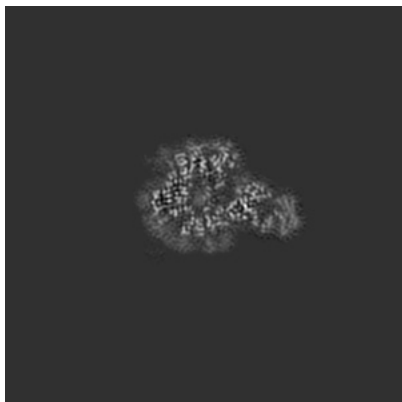


Z Index: 192

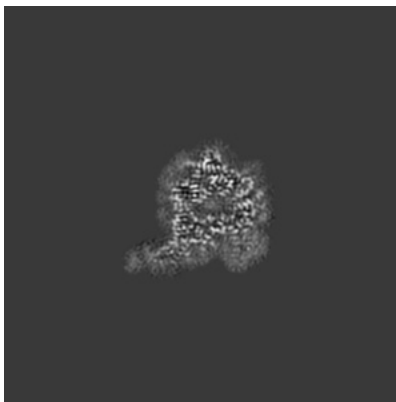
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

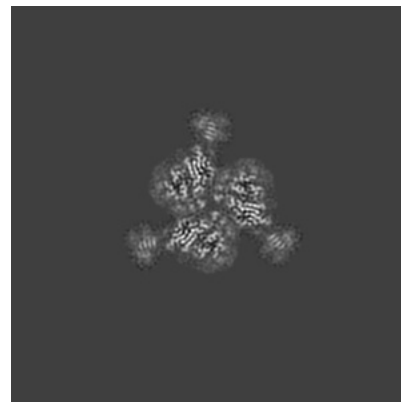
### 6.3.1 Primary map



X Index: 184



Y Index: 201

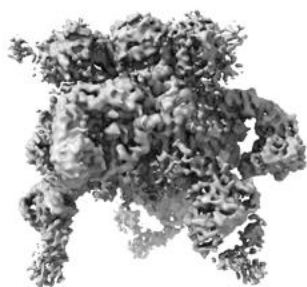


Z Index: 189

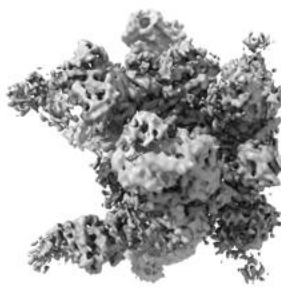
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

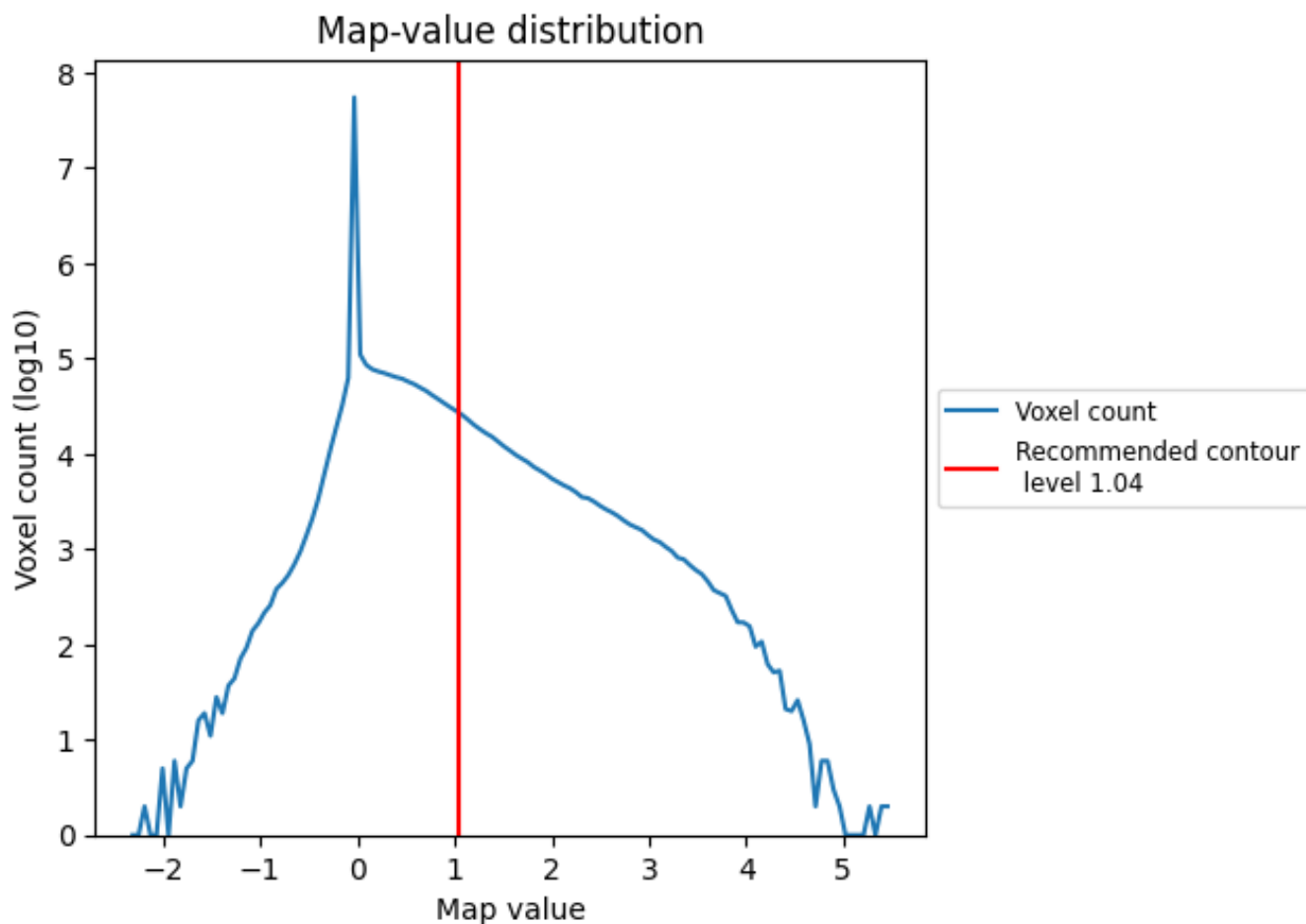
## 6.5 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis [i](#)

This section contains the results of statistical analysis of the map.

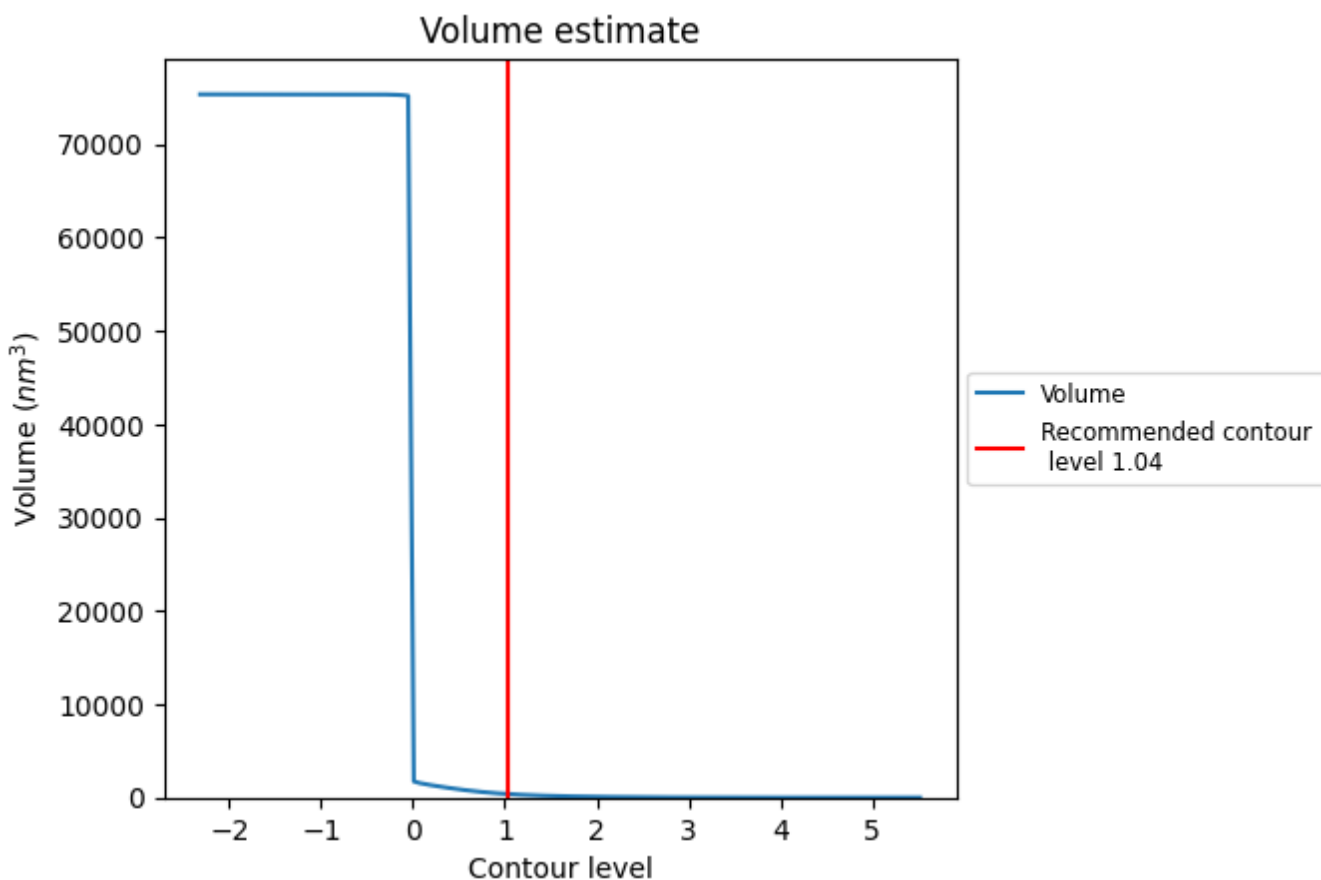
### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.



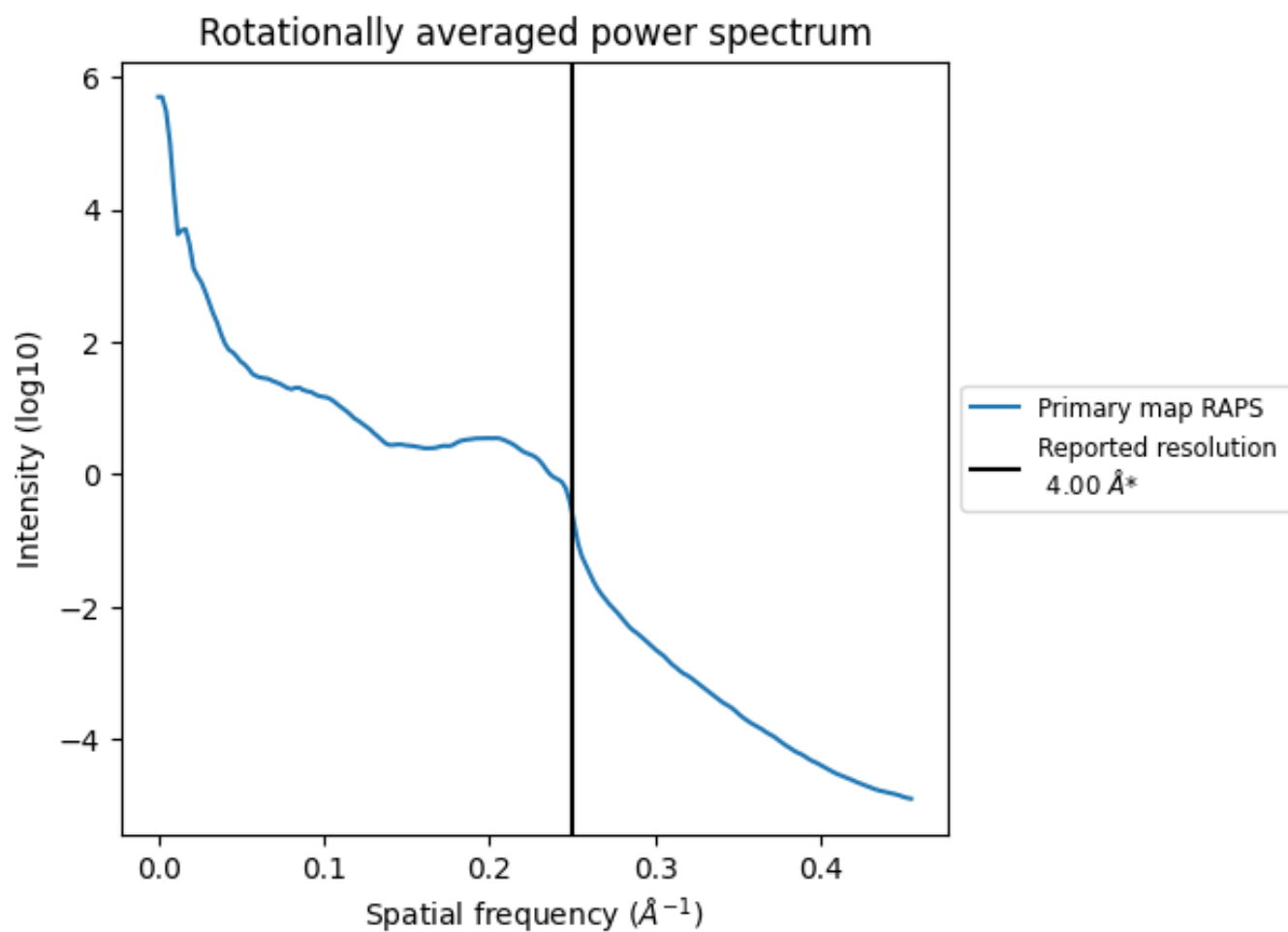
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 374 nm<sup>3</sup>; this corresponds to an approximate mass of 338 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum [i](#)



\*Reported resolution corresponds to spatial frequency of  $0.250 \text{\AA}^{-1}$

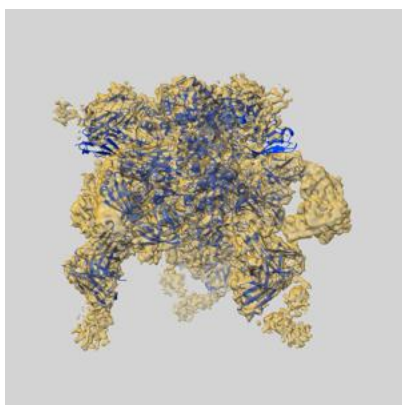
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

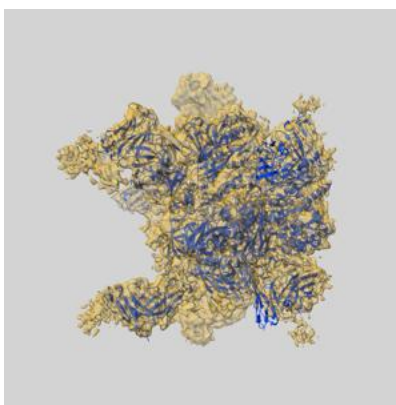
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-7621 and PDB model 6CUE. Per-residue inclusion information can be found in section 3 on page 13.

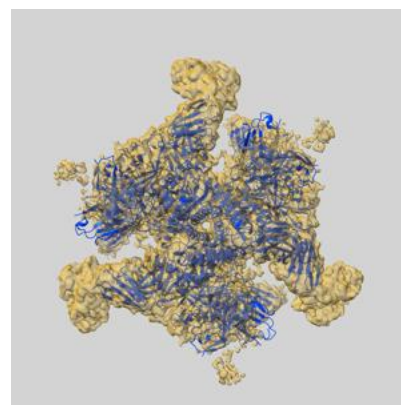
### 9.1 Map-model overlay [i](#)



X



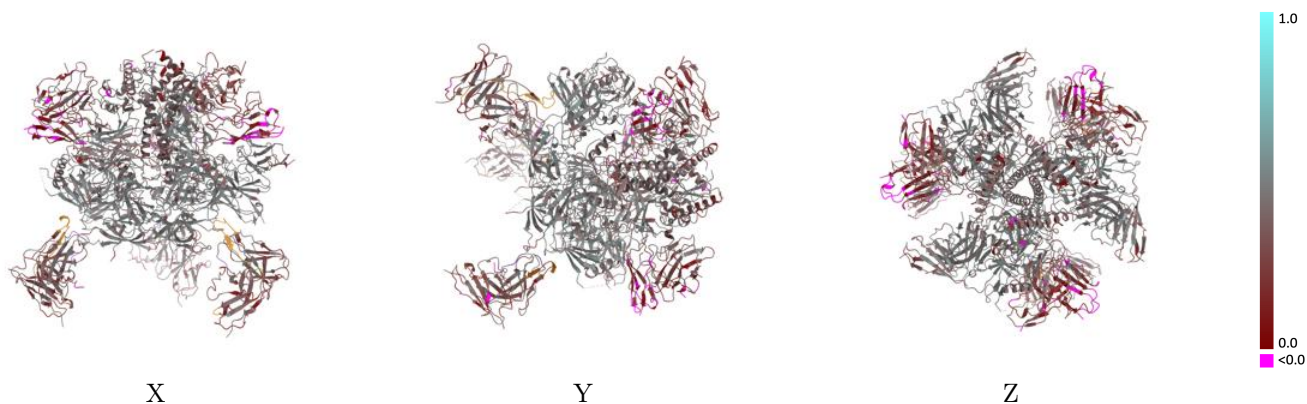
Y



Z

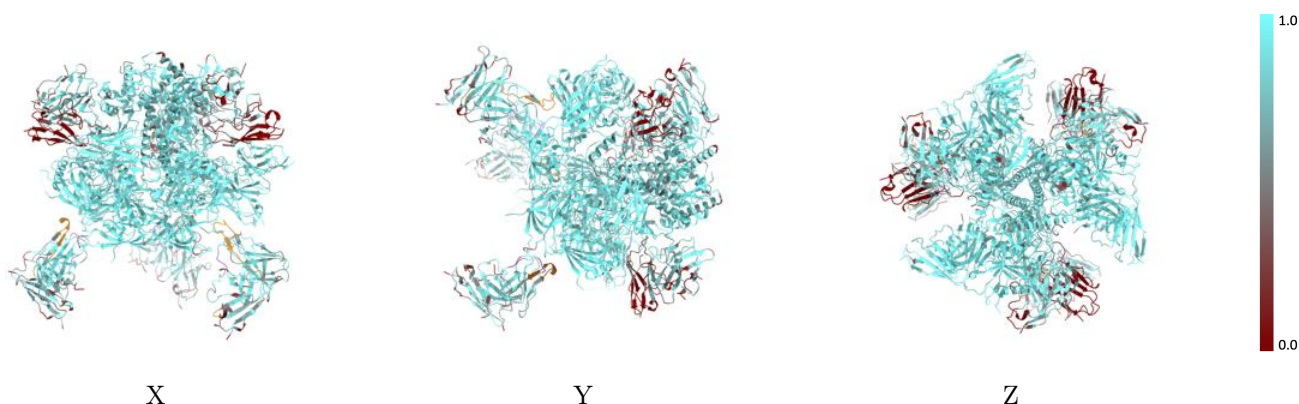
The images above show the 3D surface view of the map at the recommended contour level 1.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



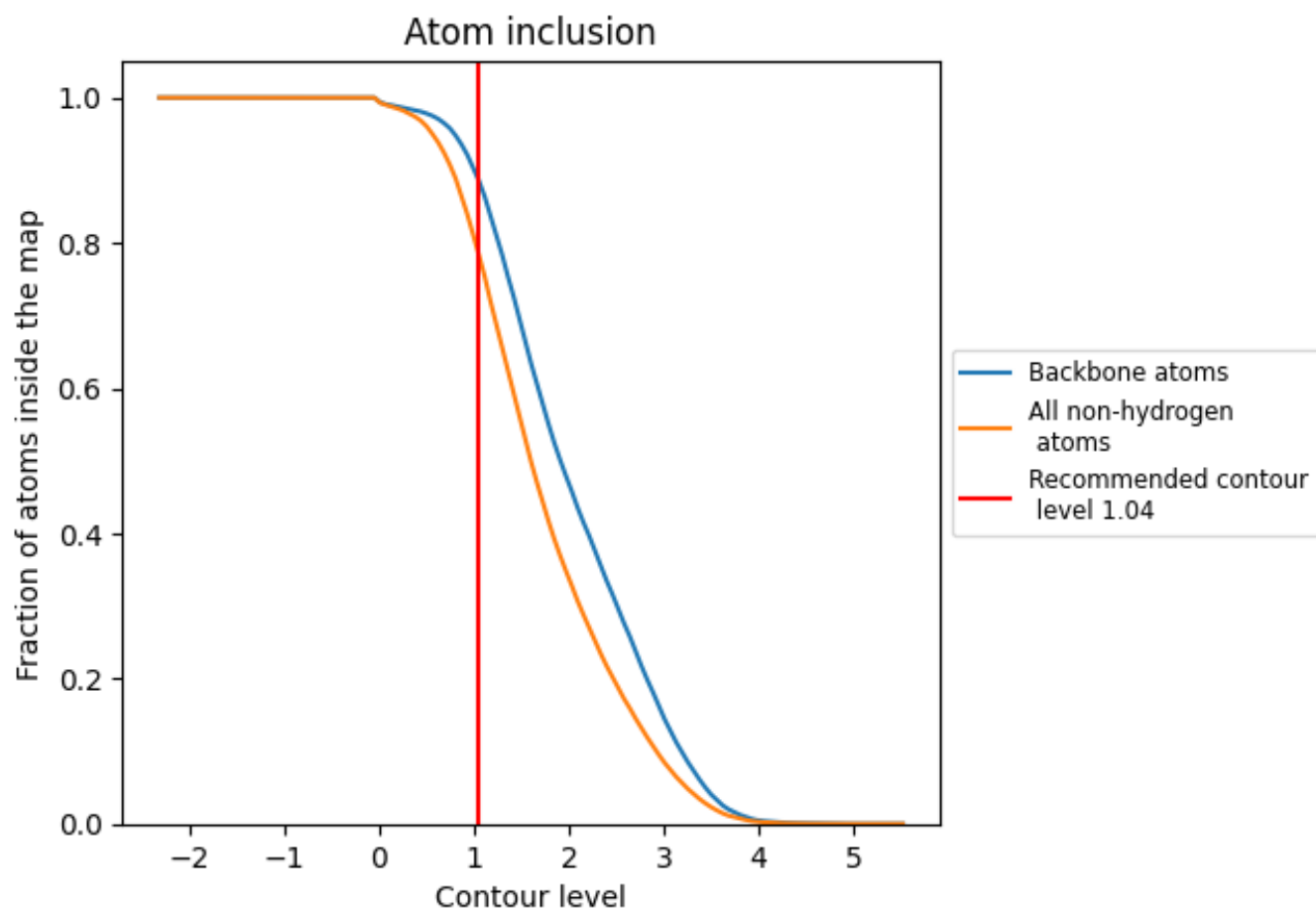
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1.04).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 79% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary



























































The table lists the average atom inclusion at the recommended contour level (1.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7887	 0.3790
0	 0.9836	 0.4710
1	 0.8521	 0.3820
2	 0.8947	 0.4460
3	 0.6356	 0.2630
4	 0.2941	 0.1720
5	 0.7123	 0.3140
6	 0.7387	 0.3450
7	 0.9049	 0.4600
8	 0.8927	 0.4120
9	 0.6786	 0.2950
A	 0.7857	 0.3410
AA	 0.8400	 0.4550
B	 0.7436	 0.4020
C	 0.8933	 0.4420
D	 0.8590	 0.3760
E	 0.9231	 0.4560
F	 0.7500	 0.4130
G	 0.9286	 0.4670
H	 0.6300	 0.2690
I	 0.8525	 0.4440
J	 0.8214	 0.4690
K	 0.7143	 0.3940
L	 0.2845	 0.1770
M	 0.7162	 0.3330
N	 0.7663	 0.3530
O	 0.8974	 0.4330
P	 0.8929	 0.4590
Q	 0.9089	 0.4600
R	 0.8902	 0.4050
S	 0.9672	 0.4810
T	 0.7143	 0.3650
U	 0.8200	 0.4590
V	 0.7500	 0.3570
W	 0.7692	 0.4270



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Chain	Atom inclusion	Q-score
X	 0.8974	 0.4580
Y	 0.8214	 0.3910
Z	 0.8929	 0.4660
a	 0.8689	 0.4540
b	 0.8571	 0.4850
c	 0.8916	 0.4420
d	 0.8590	 0.3800
e	 0.6786	 0.4220
f	 0.9231	 0.4460
g	 0.9643	 0.4800
h	 0.6256	 0.2590
i	 0.9836	 0.4800
j	 0.6786	 0.3430
k	 0.8200	 0.4530
l	 0.2857	 0.1580
m	 0.7016	 0.3250
n	 0.7638	 0.3500
o	 0.7857	 0.3610
p	 0.6923	 0.4100
q	 0.9109	 0.4590
r	 0.8902	 0.4060
s	 0.9231	 0.4660
t	 0.8214	 0.3930
u	 0.9286	 0.4660
v	 0.8689	 0.4380
w	 0.8571	 0.4610
x	 0.6786	 0.4160
y	 0.9487	 0.4580
z	 0.9286	 0.4430