



wwPDB EM Validation Summary Report ⓘ

Mar 24, 2026 – 02:21 PM UTC

PDB ID : 9ETT / pdb_00009ett
EMDB ID : EMD-19961
Title : Structure of the archaellum of *Sulfolobus acidocaldarius* strain MW039 (delta agl3 mutant).
Authors : Daum, B.; Isupov, M.N.; Gaines, M.; McLaren, M.; Mollat, C.
Deposited on : 2024-03-26
Resolution : 2.37 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

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>.

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

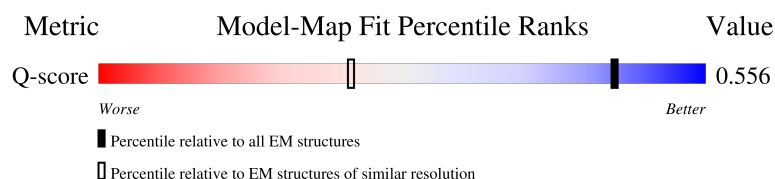
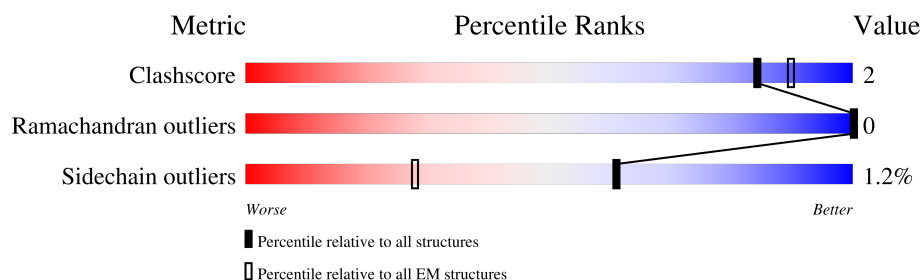
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.37 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4742 (1.87 - 2.87)

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 ≥ 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	A	293	7% 96% ..
1	B	293	6% 96% ..
1	C	293	6% 96% ..
1	D	293	6% 95% ..

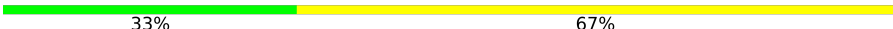
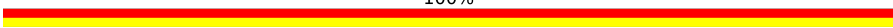
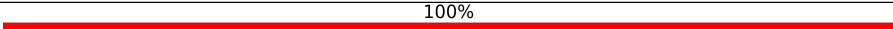
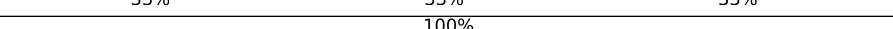
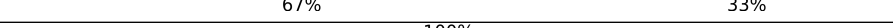
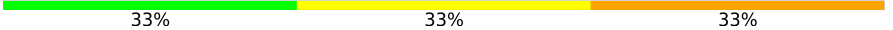
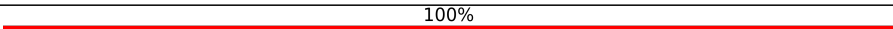
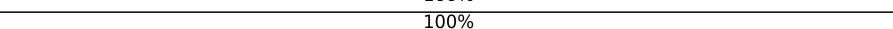
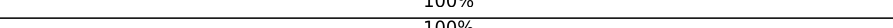
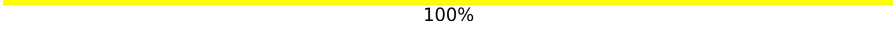
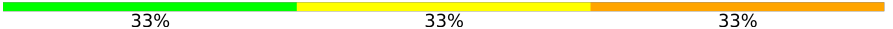
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Mol	Chain	Length	Quality of chain
1	E	293	5% 95% ..
1	F	293	5% 95% ..
1	G	293	5% 95% ..
1	H	293	5% 95% ..
1	I	293	5% 95% ..
1	J	293	5% 95% ..
1	K	293	5% 95% ..
1	L	293	5% 95% ..
1	M	293	5% 95% ..
1	N	293	5% 96% ..
1	O	293	5% 96% ..
1	P	293	6% 96% ..
1	Q	293	6% 95% ..
1	R	293	9% 96% ..
1	S	293	10% 96% ..
1	T	293	14% 96% ..
2	0	3	100% 100% 100%
2	0A	3	67% 33% 100%
2	1	3	100% 100% 100%
2	1A	3	33% 33% 33%
2	2	3	67% 33% 100%
2	2A	3	33% 67% 100%
2	3	3	33% 33% 33%
2	3A	3	33% 67% 100%
2	4	3	33% 67% 100%

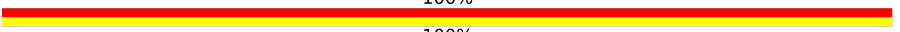
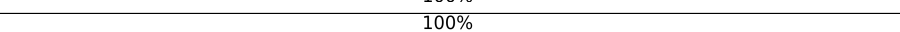
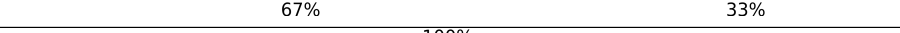
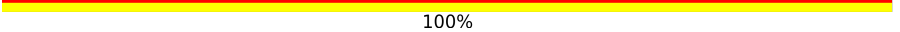
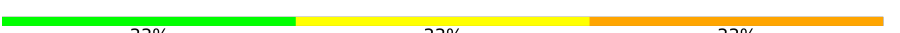
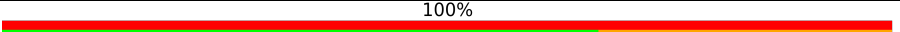
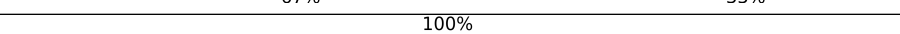
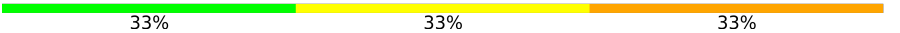
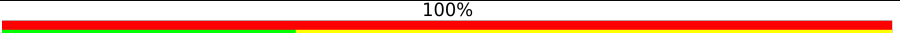
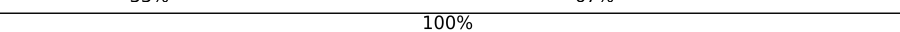
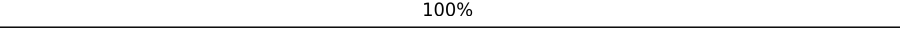
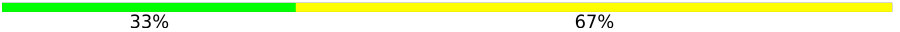
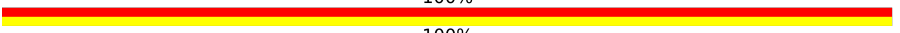
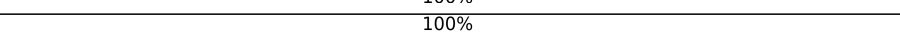
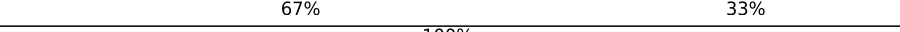
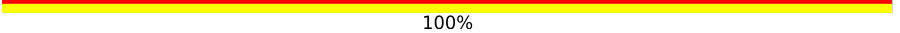
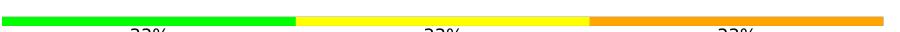
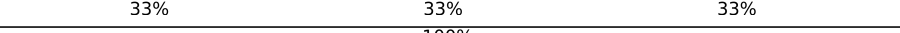
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Mol	Chain	Length	Quality of chain
2	4A	3	100% 
2	5	3	33% 
2	5A	3	100% 
2	6	3	100% 
2	6A	3	100% 
2	7	3	100% 
2	7A	3	33% 
2	8	3	100% 
2	8A	3	100% 
2	9	3	33% 
2	9A	3	67% 
2	AA	3	100% 
2	AB	3	100% 
2	BA	3	33% 
2	BB	3	100% 
2	CA	3	100% 
2	CB	3	100% 
2	DA	3	100% 
2	DB	3	33% 
2	EA	3	100% 
2	EB	3	100% 
2	FA	3	33% 
2	FB	3	67% 
2	GA	3	100% 
2	GB	3	100% 

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Mol	Chain	Length	Quality of chain
2	HA	3	 33% 67%
2	HB	3	 100%
2	IA	3	 100%
2	IB	3	 67% 33%
2	JA	3	 100%
2	JB	3	 33% 33% 33%
2	KA	3	 67% 33%
2	KB	3	 33% 67%
2	LA	3	 33% 33% 33%
2	LB	3	 67% 33%
2	MA	3	 33% 67%
2	MB	3	 100%
2	NA	3	 33% 67%
2	NB	3	 100%
2	OA	3	 100%
2	OB	3	 67% 33%
2	PA	3	 100%
2	PB	3	 33% 33% 33%
2	QA	3	 67% 33%
2	RA	3	 33% 33% 33%
2	SA	3	 33% 67%
2	TA	3	 33% 67%
2	U	3	 33% 67%
2	UA	3	 100%
2	V	3	 33% 67%

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Mol	Chain	Length	Quality of chain
2	VA	3	100%
2	W	3	100%
2	WA	3	100%
2	X	3	100%
2	XA	3	33%
2	Y	3	67%
2	YA	3	33%
2	Z	3	33%
2	ZA	3	67%
2	a	3	33%
2	aA	3	100%
2	b	3	33%
2	bA	3	100%
2	c	3	100%
2	cA	3	67%
2	d	3	100%
2	dA	3	33%
2	e	3	67%
2	eA	3	33%
2	f	3	33%
2	fA	3	67%
2	g	3	33%
2	gA	3	100%
2	h	3	33%
2	hA	3	100%

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Mol	Chain	Length	Quality of chain
2	i	3	100%
2	iA	3	100%
2	j	3	100%
2	jA	3	100%
2	k	3	100%
2	kA	3	100%
2	l	3	100%
2	lA	3	100%
2	m	3	100%
2	mA	3	100%
2	n	3	100%
2	nA	3	100%
2	o	3	100%
2	oA	3	100%
2	p	3	100%
2	pA	3	100%
2	q	3	100%
2	qA	3	100%
2	r	3	100%
2	rA	3	100%
2	s	3	100%
2	sA	3	100%
2	t	3	100%
2	tA	3	100%
2	u	3	100%

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Mol	Chain	Length	Quality of chain
2	uA	3	100% 67% 33%
2	v	3	100% 100%
2	vA	3	33% 33% 33%
2	w	3	100% 67% 33%
2	wA	3	33% 67%
2	x	3	33% 33% 33%
2	xA	3	33% 67%
2	y	3	100% 33% 67%
2	yA	3	100% 100%
2	z	3	33% 67%
2	zA	3	100% 100%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 48800 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 Flagellin.

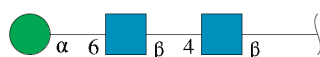
Mol	Chain	Residues	Atoms					AltConf	Trace
1	H	293	Total 2206	C 1430	N 340	O 433	S 3	0	0
1	A	293	Total 2206	C 1430	N 340	O 433	S 3	0	0
1	B	293	Total 2206	C 1430	N 340	O 433	S 3	0	0
1	C	293	Total 2206	C 1430	N 340	O 433	S 3	0	0
1	D	293	Total 2206	C 1430	N 340	O 433	S 3	0	0
1	E	293	Total 2206	C 1430	N 340	O 433	S 3	0	0
1	F	293	Total 2206	C 1430	N 340	O 433	S 3	0	0
1	G	293	Total 2206	C 1430	N 340	O 433	S 3	0	0
1	I	293	Total 2206	C 1430	N 340	O 433	S 3	0	0
1	J	293	Total 2206	C 1430	N 340	O 433	S 3	0	0
1	K	293	Total 2206	C 1430	N 340	O 433	S 3	0	0
1	L	293	Total 2206	C 1430	N 340	O 433	S 3	0	0
1	M	293	Total 2206	C 1430	N 340	O 433	S 3	0	0
1	N	293	Total 2206	C 1430	N 340	O 433	S 3	0	0
1	O	293	Total 2206	C 1430	N 340	O 433	S 3	0	0
1	P	293	Total 2206	C 1430	N 340	O 433	S 3	0	0
1	Q	293	Total 2206	C 1430	N 340	O 433	S 3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	293	Total	C	N	O	S	0	0
			2206	1430	340	433	3		
1	S	293	Total	C	N	O	S	0	0
			2206	1430	340	433	3		
1	T	293	Total	C	N	O	S	0	0
			2206	1430	340	433	3		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
2	U	3	Total	C	N	O	0	0
			39	22	2	15		
2	V	3	Total	C	N	O	0	0
			39	22	2	15		
2	W	3	Total	C	N	O	0	0
			39	22	2	15		
2	X	3	Total	C	N	O	0	0
			39	22	2	15		
2	Y	3	Total	C	N	O	0	0
			39	22	2	15		
2	Z	3	Total	C	N	O	0	0
			39	22	2	15		
2	a	3	Total	C	N	O	0	0
			39	22	2	15		
2	b	3	Total	C	N	O	0	0
			39	22	2	15		
2	c	3	Total	C	N	O	0	0
			39	22	2	15		
2	d	3	Total	C	N	O	0	0
			39	22	2	15		
2	e	3	Total	C	N	O	0	0
			39	22	2	15		
2	f	3	Total	C	N	O	0	0
			39	22	2	15		
2	g	3	Total	C	N	O	0	0
			39	22	2	15		
2	h	3	Total	C	N	O	0	0
			39	22	2	15		

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Mol	Chain	Residues	Atoms				AltConf	Trace
2	i	3	Total	C	N	O	0	0
			39	22	2	15		
2	j	3	Total	C	N	O	0	0
			39	22	2	15		
2	k	3	Total	C	N	O	0	0
			39	22	2	15		
2	l	3	Total	C	N	O	0	0
			39	22	2	15		
2	m	3	Total	C	N	O	0	0
			39	22	2	15		
2	n	3	Total	C	N	O	0	0
			39	22	2	15		
2	o	3	Total	C	N	O	0	0
			39	22	2	15		
2	p	3	Total	C	N	O	0	0
			39	22	2	15		
2	q	3	Total	C	N	O	0	0
			39	22	2	15		
2	r	3	Total	C	N	O	0	0
			39	22	2	15		
2	s	3	Total	C	N	O	0	0
			39	22	2	15		
2	t	3	Total	C	N	O	0	0
			39	22	2	15		
2	u	3	Total	C	N	O	0	0
			39	22	2	15		
2	v	3	Total	C	N	O	0	0
			39	22	2	15		
2	w	3	Total	C	N	O	0	0
			39	22	2	15		
2	x	3	Total	C	N	O	0	0
			39	22	2	15		
2	y	3	Total	C	N	O	0	0
			39	22	2	15		
2	z	3	Total	C	N	O	0	0
			39	22	2	15		
2	0	3	Total	C	N	O	0	0
			39	22	2	15		
2	1	3	Total	C	N	O	0	0
			39	22	2	15		
2	2	3	Total	C	N	O	0	0
			39	22	2	15		

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Mol	Chain	Residues	Atoms				AltConf	Trace
2	3	3	Total	C	N	O	0	0
			39	22	2	15		
2	4	3	Total	C	N	O	0	0
			39	22	2	15		
2	5	3	Total	C	N	O	0	0
			39	22	2	15		
2	6	3	Total	C	N	O	0	0
			39	22	2	15		
2	7	3	Total	C	N	O	0	0
			39	22	2	15		
2	8	3	Total	C	N	O	0	0
			39	22	2	15		
2	9	3	Total	C	N	O	0	0
			39	22	2	15		
2	AA	3	Total	C	N	O	0	0
			39	22	2	15		
2	BA	3	Total	C	N	O	0	0
			39	22	2	15		
2	CA	3	Total	C	N	O	0	0
			39	22	2	15		
2	DA	3	Total	C	N	O	0	0
			39	22	2	15		
2	EA	3	Total	C	N	O	0	0
			39	22	2	15		
2	FA	3	Total	C	N	O	0	0
			39	22	2	15		
2	GA	3	Total	C	N	O	0	0
			39	22	2	15		
2	HA	3	Total	C	N	O	0	0
			39	22	2	15		
2	IA	3	Total	C	N	O	0	0
			39	22	2	15		
2	JA	3	Total	C	N	O	0	0
			39	22	2	15		
2	KA	3	Total	C	N	O	0	0
			39	22	2	15		
2	LA	3	Total	C	N	O	0	0
			39	22	2	15		
2	MA	3	Total	C	N	O	0	0
			39	22	2	15		
2	NA	3	Total	C	N	O	0	0
			39	22	2	15		

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Mol	Chain	Residues	Atoms				AltConf	Trace
2	OA	3	Total	C	N	O	0	0
			39	22	2	15		
2	PA	3	Total	C	N	O	0	0
			39	22	2	15		
2	QA	3	Total	C	N	O	0	0
			39	22	2	15		
2	RA	3	Total	C	N	O	0	0
			39	22	2	15		
2	SA	3	Total	C	N	O	0	0
			39	22	2	15		
2	TA	3	Total	C	N	O	0	0
			39	22	2	15		
2	UA	3	Total	C	N	O	0	0
			39	22	2	15		
2	VA	3	Total	C	N	O	0	0
			39	22	2	15		
2	WA	3	Total	C	N	O	0	0
			39	22	2	15		
2	XA	3	Total	C	N	O	0	0
			39	22	2	15		
2	YA	3	Total	C	N	O	0	0
			39	22	2	15		
2	ZA	3	Total	C	N	O	0	0
			39	22	2	15		
2	aA	3	Total	C	N	O	0	0
			39	22	2	15		
2	bA	3	Total	C	N	O	0	0
			39	22	2	15		
2	cA	3	Total	C	N	O	0	0
			39	22	2	15		
2	dA	3	Total	C	N	O	0	0
			39	22	2	15		
2	eA	3	Total	C	N	O	0	0
			39	22	2	15		
2	fA	3	Total	C	N	O	0	0
			39	22	2	15		
2	gA	3	Total	C	N	O	0	0
			39	22	2	15		
2	hA	3	Total	C	N	O	0	0
			39	22	2	15		
2	iA	3	Total	C	N	O	0	0
			39	22	2	15		

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Mol	Chain	Residues	Atoms				AltConf	Trace
2	jA	3	Total	C	N	O	0	0
			39	22	2	15		
2	kA	3	Total	C	N	O	0	0
			39	22	2	15		
2	lA	3	Total	C	N	O	0	0
			39	22	2	15		
2	mA	3	Total	C	N	O	0	0
			39	22	2	15		
2	nA	3	Total	C	N	O	0	0
			39	22	2	15		
2	oA	3	Total	C	N	O	0	0
			39	22	2	15		
2	pA	3	Total	C	N	O	0	0
			39	22	2	15		
2	qA	3	Total	C	N	O	0	0
			39	22	2	15		
2	rA	3	Total	C	N	O	0	0
			39	22	2	15		
2	sA	3	Total	C	N	O	0	0
			39	22	2	15		
2	tA	3	Total	C	N	O	0	0
			39	22	2	15		
2	uA	3	Total	C	N	O	0	0
			39	22	2	15		
2	vA	3	Total	C	N	O	0	0
			39	22	2	15		
2	wA	3	Total	C	N	O	0	0
			39	22	2	15		
2	xA	3	Total	C	N	O	0	0
			39	22	2	15		
2	yA	3	Total	C	N	O	0	0
			39	22	2	15		
2	zA	3	Total	C	N	O	0	0
			39	22	2	15		
2	0A	3	Total	C	N	O	0	0
			39	22	2	15		
2	1A	3	Total	C	N	O	0	0
			39	22	2	15		
2	2A	3	Total	C	N	O	0	0
			39	22	2	15		
2	3A	3	Total	C	N	O	0	0
			39	22	2	15		

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Mol	Chain	Residues	Atoms				AltConf	Trace
2	4A	3	Total	C	N	O	0	0
			39	22	2	15		
2	5A	3	Total	C	N	O	0	0
			39	22	2	15		
2	6A	3	Total	C	N	O	0	0
			39	22	2	15		
2	7A	3	Total	C	N	O	0	0
			39	22	2	15		
2	8A	3	Total	C	N	O	0	0
			39	22	2	15		
2	9A	3	Total	C	N	O	0	0
			39	22	2	15		
2	AB	3	Total	C	N	O	0	0
			39	22	2	15		
2	BB	3	Total	C	N	O	0	0
			39	22	2	15		
2	CB	3	Total	C	N	O	0	0
			39	22	2	15		
2	DB	3	Total	C	N	O	0	0
			39	22	2	15		
2	EB	3	Total	C	N	O	0	0
			39	22	2	15		
2	FB	3	Total	C	N	O	0	0
			39	22	2	15		
2	GB	3	Total	C	N	O	0	0
			39	22	2	15		
2	HB	3	Total	C	N	O	0	0
			39	22	2	15		
2	IB	3	Total	C	N	O	0	0
			39	22	2	15		
2	JB	3	Total	C	N	O	0	0
			39	22	2	15		
2	KB	3	Total	C	N	O	0	0
			39	22	2	15		
2	LB	3	Total	C	N	O	0	0
			39	22	2	15		
2	MB	3	Total	C	N	O	0	0
			39	22	2	15		
2	NB	3	Total	C	N	O	0	0
			39	22	2	15		
2	OB	3	Total	C	N	O	0	0
			39	22	2	15		

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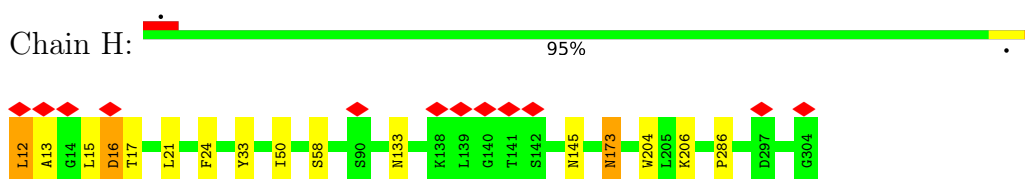
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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	PB	3	39	22	2	15	0	0

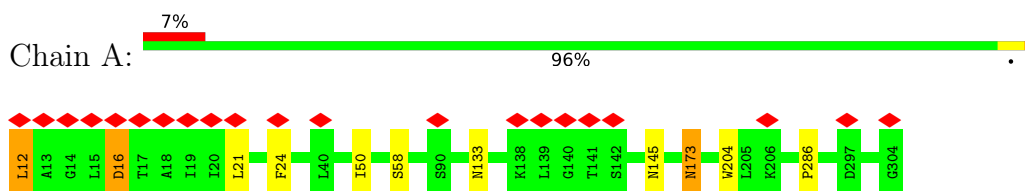
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

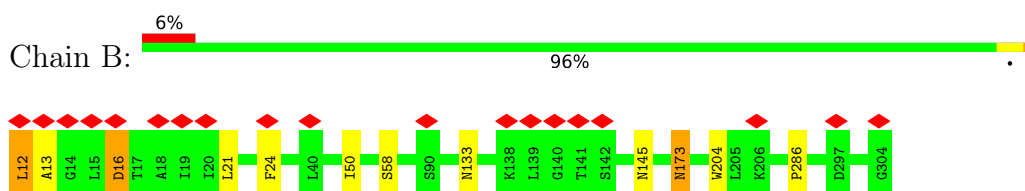
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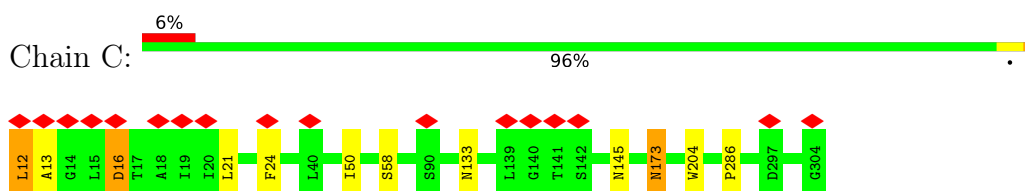
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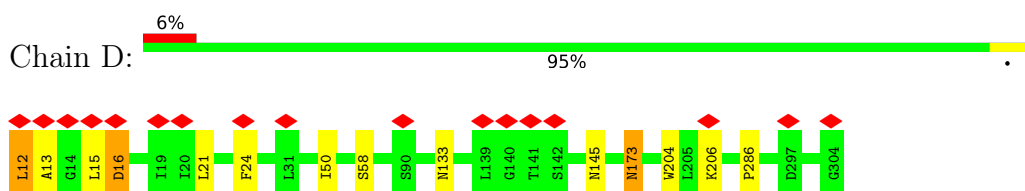
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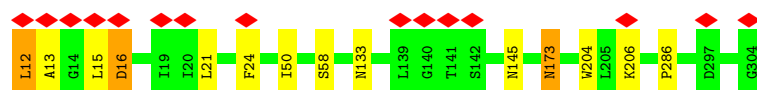
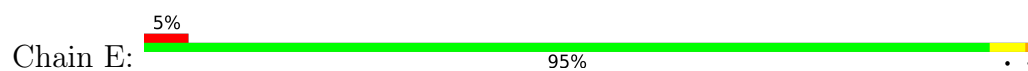
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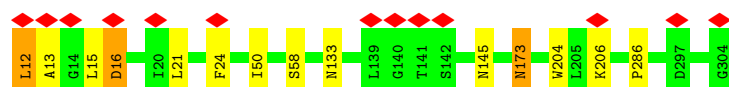
- Molecule 1: Flagellin



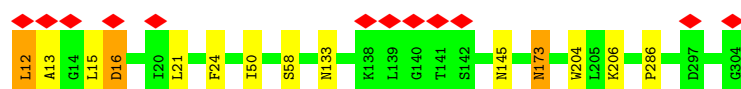
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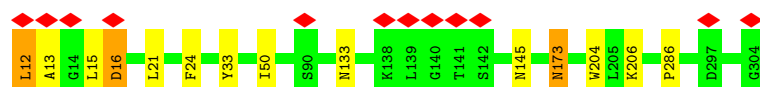
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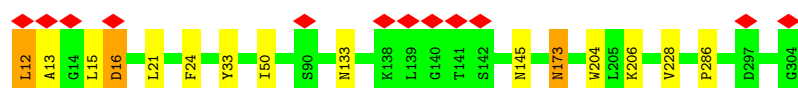
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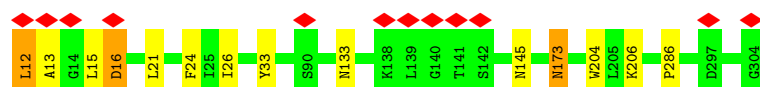
● Molecule 1: Flagellin



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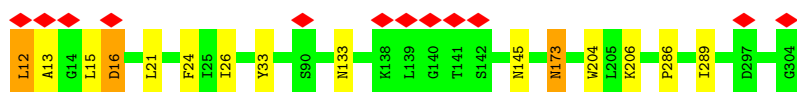


● Molecule 1: Flagellin

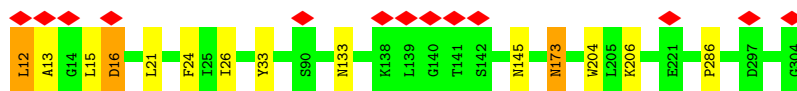


● Molecule 1: Flagellin

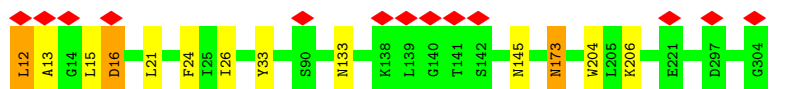




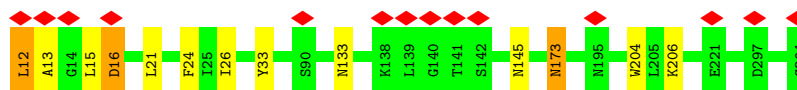
• Molecule 1: Flagellin



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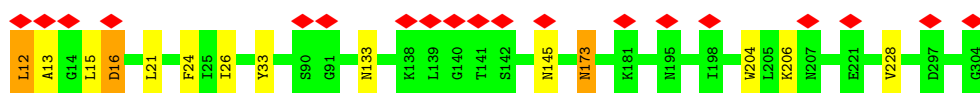
• Molecule 1: Flagellin



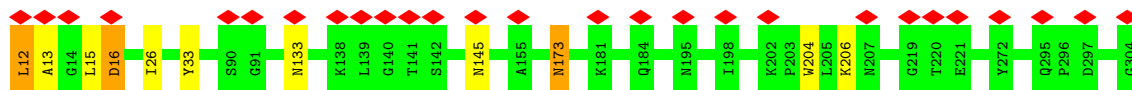
• Molecule 1: Flagellin



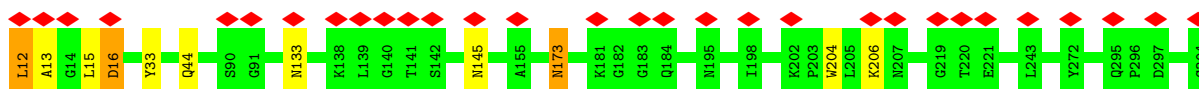
• Molecule 1: Flagellin



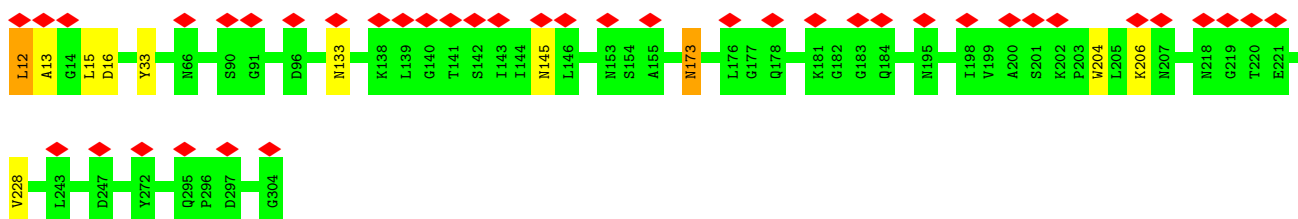
• Molecule 1: Flagellin



• Molecule 1: Flagellin



- Molecule 1: Flagellin



- Molecule 2: alpha-D-mannopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: alpha-D-mannopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: alpha-D-mannopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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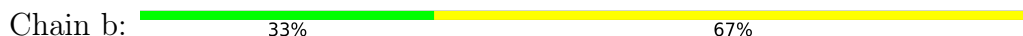
- Molecule 2: alpha-D-mannopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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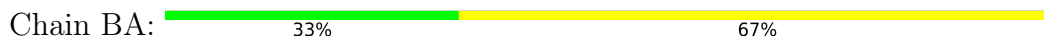
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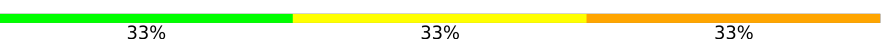


- Molecule 2: alpha-D-mannopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain KA: 



- Molecule 2: alpha-D-mannopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain LA: 



- Molecule 2: alpha-D-mannopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain MA: 

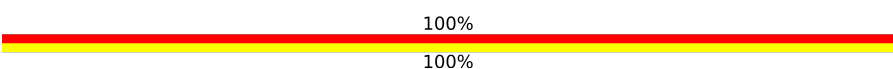


- Molecule 2: alpha-D-mannopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain NA: 

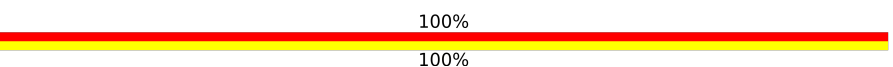


- Molecule 2: alpha-D-mannopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain OA: 



- Molecule 2: alpha-D-mannopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain PA: 



- Molecule 2: alpha-D-mannopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: alpha-D-mannopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: alpha-D-mannopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: alpha-D-mannopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: alpha-D-mannopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: alpha-D-mannopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

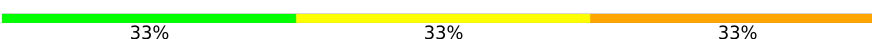


- Molecule 2: alpha-D-mannopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain WA: 



- Molecule 2: alpha-D-mannopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain XA: 



- Molecule 2: alpha-D-mannopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain YA: 



- Molecule 2: alpha-D-mannopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain ZA: 



- Molecule 2: alpha-D-mannopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain aA: 



- Molecule 2: alpha-D-mannopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain bA: 



- Molecule 2: alpha-D-mannopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: alpha-D-mannopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: alpha-D-mannopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: alpha-D-mannopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: alpha-D-mannopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



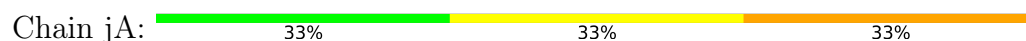
- Molecule 2: alpha-D-mannopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: alpha-D-mannopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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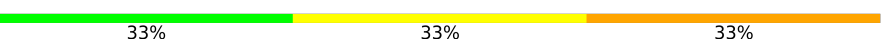


- Molecule 2: alpha-D-mannopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain OB:  100%
67% 33%



- Molecule 2: alpha-D-mannopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain PB:  33% 33% 33%



4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=107.9°, rise=5.4 Å, axial sym=C1	Depositor
Number of segments used	256869	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 ($e^-/\text{Å}^2$)	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	0.367	Depositor
Minimum map value	-0.118	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.11	Depositor
Map size (Å)	265.248, 265.248, 265.248	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.92099994, 0.92099994, 0.92099994	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, 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	A	0.55	0/2255	0.98	0/3089
1	B	0.55	0/2255	0.98	0/3089
1	C	0.55	0/2255	0.98	0/3089
1	D	0.55	0/2255	0.98	0/3089
1	E	0.55	0/2255	0.98	0/3089
1	F	0.55	0/2255	0.98	0/3089
1	G	0.55	0/2255	0.99	0/3089
1	H	0.55	0/2255	0.98	0/3089
1	I	0.55	0/2255	0.99	0/3089
1	J	0.55	0/2255	0.99	2/3089 (0.1%)
1	K	0.55	0/2255	0.99	0/3089
1	L	0.55	0/2255	0.99	0/3089
1	M	0.55	0/2255	0.99	0/3089
1	N	0.55	0/2255	0.98	0/3089
1	O	0.55	0/2255	0.98	0/3089
1	P	0.55	0/2255	0.98	0/3089
1	Q	0.55	0/2255	0.98	2/3089 (0.1%)
1	R	0.55	0/2255	0.98	0/3089
1	S	0.55	0/2255	0.98	0/3089
1	T	0.55	0/2255	0.98	2/3089 (0.1%)
All	All	0.55	0/45100	0.98	6/61780 (0.0%)

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	228	VAL	CA-C-N	5.03	127.43	120.29
1	T	228	VAL	C-N-CA	5.03	127.43	120.29
1	Q	228	VAL	CA-C-N	5.02	127.42	120.29
1	Q	228	VAL	C-N-CA	5.02	127.42	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	228	VAL	CA-C-N	5.01	127.40	120.29

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2206	0	2208	11	0
1	B	2206	0	2208	12	0
1	C	2206	0	2208	12	0
1	D	2206	0	2208	15	0
1	E	2206	0	2208	15	0
1	F	2206	0	2208	15	0
1	G	2206	0	2208	15	0
1	H	2206	0	2208	18	0
1	I	2206	0	2208	16	0
1	J	2206	0	2208	15	0
1	K	2206	0	2208	16	0
1	L	2206	0	2208	18	0
1	M	2206	0	2208	16	0
1	N	2206	0	2208	15	0
1	O	2206	0	2208	15	0
1	P	2206	0	2208	16	0
1	Q	2206	0	2208	15	0
1	R	2206	0	2208	14	0
1	S	2206	0	2208	13	0
1	T	2206	0	2208	11	0
2	0	39	0	34	0	0
2	0A	39	0	34	1	0
2	1	39	0	34	0	0
2	1A	39	0	34	3	0
2	2	39	0	34	1	0
2	2A	39	0	34	0	0
2	3	39	0	34	3	0
2	3A	39	0	34	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	4	39	0	34	0	0
2	4A	39	0	34	0	0
2	5	39	0	34	1	0
2	5A	39	0	34	0	0
2	6	39	0	34	0	0
2	6A	39	0	34	1	0
2	7	39	0	34	0	0
2	7A	39	0	34	3	0
2	8	39	0	34	1	0
2	8A	39	0	34	0	0
2	9	39	0	34	3	0
2	9A	39	0	34	1	0
2	AA	39	0	34	0	0
2	AB	39	0	34	0	0
2	BA	39	0	34	1	0
2	BB	39	0	34	0	0
2	CA	39	0	34	0	0
2	CB	39	0	34	0	0
2	DA	39	0	34	0	0
2	DB	39	0	34	3	0
2	EA	39	0	34	1	0
2	EB	39	0	34	0	0
2	FA	39	0	34	3	0
2	FB	39	0	34	1	0
2	GA	39	0	34	0	0
2	GB	39	0	34	0	0
2	HA	39	0	34	1	0
2	HB	39	0	34	0	0
2	IA	39	0	34	0	0
2	IB	39	0	34	0	0
2	JA	39	0	34	0	0
2	JB	39	0	34	3	0
2	KA	39	0	34	1	0
2	KB	39	0	34	0	0
2	LA	39	0	34	3	0
2	LB	39	0	34	1	0
2	MA	39	0	34	0	0
2	MB	39	0	34	0	0
2	NA	39	0	34	1	0
2	NB	39	0	34	0	0
2	OA	39	0	34	0	0
2	OB	39	0	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	PA	39	0	34	0	0
2	PB	39	0	34	3	0
2	QA	39	0	34	1	0
2	RA	39	0	34	3	0
2	SA	39	0	34	0	0
2	TA	39	0	34	1	0
2	U	39	0	34	0	0
2	UA	39	0	34	0	0
2	V	39	0	34	1	0
2	VA	39	0	34	0	0
2	W	39	0	34	0	0
2	WA	39	0	34	1	0
2	X	39	0	34	0	0
2	XA	39	0	34	3	0
2	Y	39	0	34	1	0
2	YA	39	0	34	0	0
2	Z	39	0	34	3	0
2	ZA	39	0	34	1	0
2	a	39	0	34	0	0
2	aA	39	0	34	0	0
2	b	39	0	34	1	0
2	bA	39	0	34	0	0
2	c	39	0	34	0	0
2	cA	39	0	34	1	0
2	d	39	0	34	0	0
2	dA	39	0	34	3	0
2	e	39	0	34	1	0
2	eA	39	0	34	0	0
2	f	39	0	34	3	0
2	fA	39	0	34	1	0
2	g	39	0	34	0	0
2	gA	39	0	34	0	0
2	h	39	0	34	1	0
2	hA	39	0	34	0	0
2	i	39	0	34	0	0
2	iA	39	0	34	1	0
2	j	39	0	34	0	0
2	jA	39	0	34	3	0
2	k	39	0	34	1	0
2	kA	39	0	34	0	0
2	l	39	0	34	3	0
2	lA	39	0	34	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	m	39	0	34	0	0
2	mA	39	0	34	0	0
2	n	39	0	34	1	0
2	nA	39	0	34	0	0
2	o	39	0	34	0	0
2	oA	39	0	34	1	0
2	p	39	0	34	0	0
2	pA	39	0	34	3	0
2	q	39	0	34	1	0
2	qA	39	0	34	0	0
2	r	39	0	34	3	0
2	rA	39	0	34	1	0
2	s	39	0	34	0	0
2	sA	39	0	34	0	0
2	t	39	0	34	1	0
2	tA	39	0	34	0	0
2	u	39	0	34	0	0
2	uA	39	0	34	1	0
2	v	39	0	34	0	0
2	vA	39	0	34	3	0
2	w	39	0	34	1	0
2	wA	39	0	34	0	0
2	x	39	0	34	3	0
2	xA	39	0	34	1	0
2	y	39	0	34	0	0
2	yA	39	0	34	0	0
2	z	39	0	34	1	0
2	zA	39	0	34	0	0
All	All	48800	0	48240	227	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

The worst 5 of 227 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:TRP:HZ2	2:f:3:MAN:HO2	1.24	0.85
1:G:204:TRP:HZ2	2:FA:3:MAN:HO2	1.25	0.84
1:K:204:TRP:HZ2	2:XA:3:MAN:HO2	1.25	0.84
1:E:204:TRP:HZ2	2:3:3:MAN:HO2	1.26	0.82
1:Q:204:TRP:HZ2	2:7A:3:MAN:HO2	1.26	0.82

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	A	291/293 (99%)	285 (98%)	6 (2%)	0	100	100
1	B	291/293 (99%)	286 (98%)	5 (2%)	0	100	100
1	C	291/293 (99%)	286 (98%)	5 (2%)	0	100	100
1	D	291/293 (99%)	286 (98%)	5 (2%)	0	100	100
1	E	291/293 (99%)	286 (98%)	5 (2%)	0	100	100
1	F	291/293 (99%)	286 (98%)	5 (2%)	0	100	100
1	G	291/293 (99%)	286 (98%)	5 (2%)	0	100	100
1	H	291/293 (99%)	286 (98%)	5 (2%)	0	100	100
1	I	291/293 (99%)	286 (98%)	5 (2%)	0	100	100
1	J	291/293 (99%)	286 (98%)	5 (2%)	0	100	100
1	K	291/293 (99%)	286 (98%)	5 (2%)	0	100	100
1	L	291/293 (99%)	286 (98%)	5 (2%)	0	100	100
1	M	291/293 (99%)	286 (98%)	5 (2%)	0	100	100
1	N	291/293 (99%)	286 (98%)	5 (2%)	0	100	100
1	O	291/293 (99%)	286 (98%)	5 (2%)	0	100	100
1	P	291/293 (99%)	286 (98%)	5 (2%)	0	100	100
1	Q	291/293 (99%)	286 (98%)	5 (2%)	0	100	100
1	R	291/293 (99%)	286 (98%)	5 (2%)	0	100	100
1	S	291/293 (99%)	286 (98%)	5 (2%)	0	100	100
1	T	291/293 (99%)	286 (98%)	5 (2%)	0	100	100
All	All	5820/5860 (99%)	5719 (98%)	101 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	A	247/247 (100%)	244 (99%)	3 (1%)	63	79
1	B	247/247 (100%)	244 (99%)	3 (1%)	63	79
1	C	247/247 (100%)	244 (99%)	3 (1%)	63	79
1	D	247/247 (100%)	244 (99%)	3 (1%)	63	79
1	E	247/247 (100%)	244 (99%)	3 (1%)	63	79
1	F	247/247 (100%)	244 (99%)	3 (1%)	63	79
1	G	247/247 (100%)	244 (99%)	3 (1%)	63	79
1	H	247/247 (100%)	244 (99%)	3 (1%)	63	79
1	I	247/247 (100%)	244 (99%)	3 (1%)	63	79
1	J	247/247 (100%)	244 (99%)	3 (1%)	63	79
1	K	247/247 (100%)	244 (99%)	3 (1%)	63	79
1	L	247/247 (100%)	244 (99%)	3 (1%)	63	79
1	M	247/247 (100%)	244 (99%)	3 (1%)	63	79
1	N	247/247 (100%)	244 (99%)	3 (1%)	63	79
1	O	247/247 (100%)	244 (99%)	3 (1%)	63	79
1	P	247/247 (100%)	244 (99%)	3 (1%)	63	79
1	Q	247/247 (100%)	244 (99%)	3 (1%)	63	79
1	R	247/247 (100%)	244 (99%)	3 (1%)	63	79
1	S	247/247 (100%)	244 (99%)	3 (1%)	63	79
1	T	247/247 (100%)	244 (99%)	3 (1%)	63	79
All	All	4940/4940 (100%)	4880 (99%)	60 (1%)	61	79

5 of 60 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	16	ASP
1	S	16	ASP
1	L	173	ASN

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Mol	Chain	Res	Type
1	S	12	LEU
1	T	173	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 76 such sidechains are listed below:

Mol	Chain	Res	Type
1	P	133	ASN
1	S	271	GLN
1	P	268	ASN
1	R	133	ASN
1	T	271	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

360 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	$\# Z > 2$
2	NAG	0	1	1,2	14,14,15	0.34	0	17,19,21	1.49	1 (5%)
2	NAG	0	2	2	14,14,15	0.51	0	17,19,21	1.97	2 (11%)
2	MAN	0	3	2	11,11,12	0.49	0	15,15,17	1.92	3 (20%)
2	NAG	0A	1	1,2	14,14,15	0.33	0	17,19,21	0.58	0
2	NAG	0A	2	2	14,14,15	0.34	0	17,19,21	0.98	1 (5%)
2	MAN	0A	3	2	11,11,12	0.32	0	15,15,17	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	1	1	1,2	14,14,15	0.48	0	17,19,21	1.45	1 (5%)
2	NAG	1	2	2	14,14,15	0.51	0	17,19,21	1.93	2 (11%)
2	MAN	1	3	2	11,11,12	0.49	0	15,15,17	1.92	3 (20%)
2	NAG	1A	1	1,2	14,14,15	0.39	0	17,19,21	1.58	1 (5%)
2	NAG	1A	2	2	14,14,15	0.30	0	17,19,21	0.70	0
2	MAN	1A	3	2	11,11,12	0.28	0	15,15,17	1.25	1 (6%)
2	NAG	2	1	1,2	14,14,15	0.32	0	17,19,21	0.58	0
2	NAG	2	2	2	14,14,15	0.34	0	17,19,21	0.98	1 (5%)
2	MAN	2	3	2	11,11,12	0.31	0	15,15,17	0.76	0
2	NAG	2A	1	1,2	14,14,15	0.24	0	17,19,21	1.51	1 (5%)
2	NAG	2A	2	2	14,14,15	0.29	0	17,19,21	0.70	1 (5%)
2	MAN	2A	3	2	11,11,12	0.25	0	15,15,17	0.53	0
2	NAG	3	1	1,2	14,14,15	0.41	0	17,19,21	1.55	1 (5%)
2	NAG	3	2	2	14,14,15	0.30	0	17,19,21	0.69	0
2	MAN	3	3	2	11,11,12	0.29	0	15,15,17	1.24	1 (6%)
2	NAG	3A	1	1,2	14,14,15	0.37	0	17,19,21	0.57	0
2	NAG	3A	2	2	14,14,15	0.52	0	17,19,21	0.64	0
2	MAN	3A	3	2	11,11,12	0.39	0	15,15,17	0.92	1 (6%)
2	NAG	4	1	1,2	14,14,15	0.26	0	17,19,21	1.54	1 (5%)
2	NAG	4	2	2	14,14,15	0.35	0	17,19,21	0.71	1 (5%)
2	MAN	4	3	2	11,11,12	0.26	0	15,15,17	0.54	0
2	NAG	4A	1	1,2	14,14,15	0.34	0	17,19,21	1.49	1 (5%)
2	NAG	4A	2	2	14,14,15	0.51	0	17,19,21	1.96	2 (11%)
2	MAN	4A	3	2	11,11,12	0.48	0	15,15,17	1.91	3 (20%)
2	NAG	5	1	1,2	14,14,15	0.37	0	17,19,21	0.61	0
2	NAG	5	2	2	14,14,15	0.54	0	17,19,21	0.62	0
2	MAN	5	3	2	11,11,12	0.41	0	15,15,17	0.90	1 (6%)
2	NAG	5A	1	1,2	14,14,15	0.48	0	17,19,21	1.43	1 (5%)
2	NAG	5A	2	2	14,14,15	0.50	0	17,19,21	1.94	2 (11%)
2	MAN	5A	3	2	11,11,12	0.49	0	15,15,17	1.92	3 (20%)
2	NAG	6	1	1,2	14,14,15	0.34	0	17,19,21	1.48	1 (5%)
2	NAG	6	2	2	14,14,15	0.52	0	17,19,21	1.95	2 (11%)
2	MAN	6	3	2	11,11,12	0.49	0	15,15,17	1.92	3 (20%)
2	NAG	6A	1	1,2	14,14,15	0.32	0	17,19,21	0.58	0
2	NAG	6A	2	2	14,14,15	0.34	0	17,19,21	0.99	1 (5%)
2	MAN	6A	3	2	11,11,12	0.30	0	15,15,17	0.78	0
2	NAG	7	1	1,2	14,14,15	0.48	0	17,19,21	1.46	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	7	2	2	14,14,15	0.50	0	17,19,21	1.95	2 (11%)
2	MAN	7	3	2	11,11,12	0.48	0	15,15,17	1.92	3 (20%)
2	NAG	7A	1	1,2	14,14,15	0.39	0	17,19,21	1.59	1 (5%)
2	NAG	7A	2	2	14,14,15	0.29	0	17,19,21	0.69	0
2	MAN	7A	3	2	11,11,12	0.28	0	15,15,17	1.25	1 (6%)
2	NAG	8	1	1,2	14,14,15	0.32	0	17,19,21	0.58	0
2	NAG	8	2	2	14,14,15	0.35	0	17,19,21	0.98	1 (5%)
2	MAN	8	3	2	11,11,12	0.31	0	15,15,17	0.77	0
2	NAG	8A	1	1,2	14,14,15	0.24	0	17,19,21	1.51	1 (5%)
2	NAG	8A	2	2	14,14,15	0.34	0	17,19,21	0.70	1 (5%)
2	MAN	8A	3	2	11,11,12	0.26	0	15,15,17	0.57	0
2	NAG	9	1	1,2	14,14,15	0.41	0	17,19,21	1.55	1 (5%)
2	NAG	9	2	2	14,14,15	0.30	0	17,19,21	0.69	0
2	MAN	9	3	2	11,11,12	0.30	0	15,15,17	1.26	1 (6%)
2	NAG	9A	1	1,2	14,14,15	0.36	0	17,19,21	0.58	0
2	NAG	9A	2	2	14,14,15	0.53	0	17,19,21	0.64	0
2	MAN	9A	3	2	11,11,12	0.40	0	15,15,17	0.90	1 (6%)
2	NAG	AA	1	1,2	14,14,15	0.24	0	17,19,21	1.54	1 (5%)
2	NAG	AA	2	2	14,14,15	0.29	0	17,19,21	0.70	1 (5%)
2	MAN	AA	3	2	11,11,12	0.26	0	15,15,17	0.51	0
2	NAG	AB	1	1,2	14,14,15	0.34	0	17,19,21	1.50	1 (5%)
2	NAG	AB	2	2	14,14,15	0.49	0	17,19,21	1.96	2 (11%)
2	MAN	AB	3	2	11,11,12	0.49	0	15,15,17	1.92	3 (20%)
2	NAG	BA	1	1,2	14,14,15	0.37	0	17,19,21	0.62	0
2	NAG	BA	2	2	14,14,15	0.53	0	17,19,21	0.64	0
2	MAN	BA	3	2	11,11,12	0.39	0	15,15,17	0.90	1 (6%)
2	NAG	BB	1	1,2	14,14,15	0.47	0	17,19,21	1.47	1 (5%)
2	NAG	BB	2	2	14,14,15	0.50	0	17,19,21	1.95	2 (11%)
2	MAN	BB	3	2	11,11,12	0.49	0	15,15,17	1.90	3 (20%)
2	NAG	CA	1	1,2	14,14,15	0.34	0	17,19,21	1.49	1 (5%)
2	NAG	CA	2	2	14,14,15	0.50	0	17,19,21	1.96	2 (11%)
2	MAN	CA	3	2	11,11,12	0.49	0	15,15,17	1.92	3 (20%)
2	NAG	CB	1	1,2	14,14,15	0.33	0	17,19,21	0.58	0
2	NAG	CB	2	2	14,14,15	0.33	0	17,19,21	0.93	1 (5%)
2	MAN	CB	3	2	11,11,12	0.30	0	15,15,17	0.80	0
2	NAG	DA	1	1,2	14,14,15	0.47	0	17,19,21	1.43	1 (5%)
2	NAG	DA	2	2	14,14,15	0.51	0	17,19,21	1.94	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MAN	DA	3	2	11,11,12	0.49	0	15,15,17	1.92	3 (20%)
2	NAG	DB	1	1,2	14,14,15	0.38	0	17,19,21	1.58	1 (5%)
2	NAG	DB	2	2	14,14,15	0.30	0	17,19,21	0.69	0
2	MAN	DB	3	2	11,11,12	0.26	0	15,15,17	1.24	2 (13%)
2	NAG	EA	1	1,2	14,14,15	0.33	0	17,19,21	0.58	0
2	NAG	EA	2	2	14,14,15	0.35	0	17,19,21	0.98	1 (5%)
2	MAN	EA	3	2	11,11,12	0.31	0	15,15,17	0.78	0
2	NAG	EB	1	1,2	14,14,15	0.25	0	17,19,21	1.53	1 (5%)
2	NAG	EB	2	2	14,14,15	0.31	0	17,19,21	0.70	1 (5%)
2	MAN	EB	3	2	11,11,12	0.27	0	15,15,17	0.60	0
2	NAG	FA	1	1,2	14,14,15	0.41	0	17,19,21	1.56	1 (5%)
2	NAG	FA	2	2	14,14,15	0.29	0	17,19,21	0.69	0
2	MAN	FA	3	2	11,11,12	0.31	0	15,15,17	1.25	1 (6%)
2	NAG	FB	1	1,2	14,14,15	0.35	0	17,19,21	0.57	0
2	NAG	FB	2	2	14,14,15	0.53	0	17,19,21	0.63	0
2	MAN	FB	3	2	11,11,12	0.40	0	15,15,17	0.91	1 (6%)
2	NAG	GA	1	1,2	14,14,15	0.25	0	17,19,21	1.53	1 (5%)
2	NAG	GA	2	2	14,14,15	0.31	0	17,19,21	0.71	1 (5%)
2	MAN	GA	3	2	11,11,12	0.25	0	15,15,17	0.60	0
2	NAG	GB	1	1,2	14,14,15	0.35	0	17,19,21	1.49	1 (5%)
2	NAG	GB	2	2	14,14,15	0.51	0	17,19,21	1.96	2 (11%)
2	MAN	GB	3	2	11,11,12	0.48	0	15,15,17	1.92	3 (20%)
2	NAG	HA	1	1,2	14,14,15	0.38	0	17,19,21	0.61	0
2	NAG	HA	2	2	14,14,15	0.53	0	17,19,21	0.64	0
2	MAN	HA	3	2	11,11,12	0.40	0	15,15,17	0.90	1 (6%)
2	NAG	HB	1	1,2	14,14,15	0.47	0	17,19,21	1.44	1 (5%)
2	NAG	HB	2	2	14,14,15	0.50	0	17,19,21	1.94	2 (11%)
2	MAN	HB	3	2	11,11,12	0.49	0	15,15,17	1.92	3 (20%)
2	NAG	IA	1	1,2	14,14,15	0.35	0	17,19,21	1.49	1 (5%)
2	NAG	IA	2	2	14,14,15	0.50	0	17,19,21	1.96	2 (11%)
2	MAN	IA	3	2	11,11,12	0.48	0	15,15,17	1.91	3 (20%)
2	NAG	IB	1	1,2	14,14,15	0.34	0	17,19,21	0.58	0
2	NAG	IB	2	2	14,14,15	0.34	0	17,19,21	0.94	1 (5%)
2	MAN	IB	3	2	11,11,12	0.32	0	15,15,17	0.81	0
2	NAG	JA	1	1,2	14,14,15	0.48	0	17,19,21	1.44	1 (5%)
2	NAG	JA	2	2	14,14,15	0.50	0	17,19,21	1.95	2 (11%)
2	MAN	JA	3	2	11,11,12	0.49	0	15,15,17	1.92	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	JB	1	1,2	14,14,15	0.40	0	17,19,21	1.58	1 (5%)
2	NAG	JB	2	2	14,14,15	0.29	0	17,19,21	0.70	0
2	MAN	JB	3	2	11,11,12	0.26	0	15,15,17	1.23	1 (6%)
2	NAG	KA	1	1,2	14,14,15	0.33	0	17,19,21	0.58	0
2	NAG	KA	2	2	14,14,15	0.34	0	17,19,21	0.99	1 (5%)
2	MAN	KA	3	2	11,11,12	0.30	0	15,15,17	0.81	0
2	NAG	KB	1	1,2	14,14,15	0.25	0	17,19,21	1.52	1 (5%)
2	NAG	KB	2	2	14,14,15	0.32	0	17,19,21	0.70	1 (5%)
2	MAN	KB	3	2	11,11,12	0.26	0	15,15,17	0.59	0
2	NAG	LA	1	1,2	14,14,15	0.42	0	17,19,21	1.57	1 (5%)
2	NAG	LA	2	2	14,14,15	0.29	0	17,19,21	0.67	0
2	MAN	LA	3	2	11,11,12	0.30	0	15,15,17	1.25	1 (6%)
2	NAG	LB	1	1,2	14,14,15	0.35	0	17,19,21	0.58	0
2	NAG	LB	2	2	14,14,15	0.53	0	17,19,21	0.64	0
2	MAN	LB	3	2	11,11,12	0.39	0	15,15,17	0.91	1 (6%)
2	NAG	MA	1	1,2	14,14,15	0.25	0	17,19,21	1.53	1 (5%)
2	NAG	MA	2	2	14,14,15	0.32	0	17,19,21	0.70	1 (5%)
2	MAN	MA	3	2	11,11,12	0.26	0	15,15,17	0.57	0
2	NAG	MB	1	1,2	14,14,15	0.34	0	17,19,21	1.49	1 (5%)
2	NAG	MB	2	2	14,14,15	0.50	0	17,19,21	1.97	2 (11%)
2	MAN	MB	3	2	11,11,12	0.49	0	15,15,17	1.91	3 (20%)
2	NAG	NA	1	1,2	14,14,15	0.38	0	17,19,21	0.60	0
2	NAG	NA	2	2	14,14,15	0.52	0	17,19,21	0.65	0
2	MAN	NA	3	2	11,11,12	0.40	0	15,15,17	0.91	1 (6%)
2	NAG	NB	1	1,2	14,14,15	0.49	0	17,19,21	1.47	1 (5%)
2	NAG	NB	2	2	14,14,15	0.51	0	17,19,21	1.93	2 (11%)
2	MAN	NB	3	2	11,11,12	0.49	0	15,15,17	1.91	3 (20%)
2	NAG	OA	1	1,2	14,14,15	0.34	0	17,19,21	1.50	1 (5%)
2	NAG	OA	2	2	14,14,15	0.51	0	17,19,21	1.96	2 (11%)
2	MAN	OA	3	2	11,11,12	0.49	0	15,15,17	1.92	3 (20%)
2	NAG	OB	1	1,2	14,14,15	0.33	0	17,19,21	0.58	0
2	NAG	OB	2	2	14,14,15	0.33	0	17,19,21	0.93	1 (5%)
2	MAN	OB	3	2	11,11,12	0.31	0	15,15,17	0.77	0
2	NAG	PA	1	1,2	14,14,15	0.49	0	17,19,21	1.46	1 (5%)
2	NAG	PA	2	2	14,14,15	0.51	0	17,19,21	1.94	2 (11%)
2	MAN	PA	3	2	11,11,12	0.50	0	15,15,17	1.91	3 (20%)
2	NAG	PB	1	1,2	14,14,15	0.39	0	17,19,21	1.58	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	PB	2	2	14,14,15	0.30	0	17,19,21	0.70	0
2	MAN	PB	3	2	11,11,12	0.26	0	15,15,17	1.24	1 (6%)
2	NAG	QA	1	1,2	14,14,15	0.32	0	17,19,21	0.58	0
2	NAG	QA	2	2	14,14,15	0.35	0	17,19,21	0.98	1 (5%)
2	MAN	QA	3	2	11,11,12	0.32	0	15,15,17	0.77	0
2	NAG	RA	1	1,2	14,14,15	0.41	0	17,19,21	1.56	1 (5%)
2	NAG	RA	2	2	14,14,15	0.30	0	17,19,21	0.69	0
2	MAN	RA	3	2	11,11,12	0.29	0	15,15,17	1.23	1 (6%)
2	NAG	SA	1	1,2	14,14,15	0.24	0	17,19,21	1.53	1 (5%)
2	NAG	SA	2	2	14,14,15	0.33	0	17,19,21	0.70	1 (5%)
2	MAN	SA	3	2	11,11,12	0.26	0	15,15,17	0.55	0
2	NAG	TA	1	1,2	14,14,15	0.38	0	17,19,21	0.59	0
2	NAG	TA	2	2	14,14,15	0.54	0	17,19,21	0.65	0
2	MAN	TA	3	2	11,11,12	0.40	0	15,15,17	0.91	1 (6%)
2	NAG	U	1	1,2	14,14,15	0.25	0	17,19,21	1.53	1 (5%)
2	NAG	U	2	2	14,14,15	0.34	0	17,19,21	0.71	1 (5%)
2	MAN	U	3	2	11,11,12	0.27	0	15,15,17	0.56	0
2	NAG	UA	1	1,2	14,14,15	0.34	0	17,19,21	1.49	1 (5%)
2	NAG	UA	2	2	14,14,15	0.51	0	17,19,21	1.95	2 (11%)
2	MAN	UA	3	2	11,11,12	0.49	0	15,15,17	1.92	3 (20%)
2	NAG	V	1	1,2	14,14,15	0.37	0	17,19,21	0.63	0
2	NAG	V	2	2	14,14,15	0.54	0	17,19,21	0.64	0
2	MAN	V	3	2	11,11,12	0.41	0	15,15,17	0.90	1 (6%)
2	NAG	VA	1	1,2	14,14,15	0.48	0	17,19,21	1.46	1 (5%)
2	NAG	VA	2	2	14,14,15	0.50	0	17,19,21	1.96	2 (11%)
2	MAN	VA	3	2	11,11,12	0.49	0	15,15,17	1.92	3 (20%)
2	NAG	W	1	1,2	14,14,15	0.35	0	17,19,21	1.49	1 (5%)
2	NAG	W	2	2	14,14,15	0.50	0	17,19,21	1.96	2 (11%)
2	MAN	W	3	2	11,11,12	0.48	0	15,15,17	1.92	3 (20%)
2	NAG	WA	1	1,2	14,14,15	0.32	0	17,19,21	0.58	0
2	NAG	WA	2	2	14,14,15	0.34	0	17,19,21	0.99	1 (5%)
2	MAN	WA	3	2	11,11,12	0.31	0	15,15,17	0.78	0
2	NAG	X	1	1,2	14,14,15	0.50	0	17,19,21	1.47	1 (5%)
2	NAG	X	2	2	14,14,15	0.50	0	17,19,21	1.95	2 (11%)
2	MAN	X	3	2	11,11,12	0.49	0	15,15,17	1.91	3 (20%)
2	NAG	XA	1	1,2	14,14,15	0.42	0	17,19,21	1.57	1 (5%)
2	NAG	XA	2	2	14,14,15	0.30	0	17,19,21	0.68	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MAN	XA	3	2	11,11,12	0.30	0	15,15,17	1.26	1 (6%)
2	NAG	Y	1	1,2	14,14,15	0.33	0	17,19,21	0.58	0
2	NAG	Y	2	2	14,14,15	0.34	0	17,19,21	0.99	1 (5%)
2	MAN	Y	3	2	11,11,12	0.30	0	15,15,17	0.79	0
2	NAG	YA	1	1,2	14,14,15	0.24	0	17,19,21	1.52	1 (5%)
2	NAG	YA	2	2	14,14,15	0.30	0	17,19,21	0.70	1 (5%)
2	MAN	YA	3	2	11,11,12	0.27	0	15,15,17	0.53	0
2	NAG	Z	1	1,2	14,14,15	0.40	0	17,19,21	1.56	1 (5%)
2	NAG	Z	2	2	14,14,15	0.30	0	17,19,21	0.68	0
2	MAN	Z	3	2	11,11,12	0.30	0	15,15,17	1.26	1 (6%)
2	NAG	ZA	1	1,2	14,14,15	0.37	0	17,19,21	0.58	0
2	NAG	ZA	2	2	14,14,15	0.54	0	17,19,21	0.63	0
2	MAN	ZA	3	2	11,11,12	0.41	0	15,15,17	0.91	1 (6%)
2	NAG	a	1	1,2	14,14,15	0.25	0	17,19,21	1.53	1 (5%)
2	NAG	a	2	2	14,14,15	0.34	0	17,19,21	0.71	1 (5%)
2	MAN	a	3	2	11,11,12	0.27	0	15,15,17	0.53	0
2	NAG	aA	1	1,2	14,14,15	0.34	0	17,19,21	1.50	1 (5%)
2	NAG	aA	2	2	14,14,15	0.50	0	17,19,21	1.96	2 (11%)
2	MAN	aA	3	2	11,11,12	0.48	0	15,15,17	1.92	3 (20%)
2	NAG	b	1	1,2	14,14,15	0.39	0	17,19,21	0.61	0
2	NAG	b	2	2	14,14,15	0.54	0	17,19,21	0.63	0
2	MAN	b	3	2	11,11,12	0.40	0	15,15,17	0.91	1 (6%)
2	NAG	bA	1	1,2	14,14,15	0.48	0	17,19,21	1.43	1 (5%)
2	NAG	bA	2	2	14,14,15	0.51	0	17,19,21	1.92	2 (11%)
2	MAN	bA	3	2	11,11,12	0.50	0	15,15,17	1.92	3 (20%)
2	NAG	c	1	1,2	14,14,15	0.33	0	17,19,21	1.49	1 (5%)
2	NAG	c	2	2	14,14,15	0.51	0	17,19,21	1.95	2 (11%)
2	MAN	c	3	2	11,11,12	0.49	0	15,15,17	1.91	3 (20%)
2	NAG	cA	1	1,2	14,14,15	0.33	0	17,19,21	0.59	0
2	NAG	cA	2	2	14,14,15	0.35	0	17,19,21	0.98	1 (5%)
2	MAN	cA	3	2	11,11,12	0.30	0	15,15,17	0.78	0
2	NAG	d	1	1,2	14,14,15	0.48	0	17,19,21	1.45	1 (5%)
2	NAG	d	2	2	14,14,15	0.50	0	17,19,21	1.96	2 (11%)
2	MAN	d	3	2	11,11,12	0.49	0	15,15,17	1.91	3 (20%)
2	NAG	dA	1	1,2	14,14,15	0.40	0	17,19,21	1.56	1 (5%)
2	NAG	dA	2	2	14,14,15	0.30	0	17,19,21	0.70	0
2	MAN	dA	3	2	11,11,12	0.30	0	15,15,17	1.26	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	e	1	1,2	14,14,15	0.32	0	17,19,21	0.58	0
2	NAG	e	2	2	14,14,15	0.35	0	17,19,21	0.99	1 (5%)
2	MAN	e	3	2	11,11,12	0.31	0	15,15,17	0.78	0
2	NAG	eA	1	1,2	14,14,15	0.24	0	17,19,21	1.52	1 (5%)
2	NAG	eA	2	2	14,14,15	0.34	0	17,19,21	0.70	1 (5%)
2	MAN	eA	3	2	11,11,12	0.25	0	15,15,17	0.56	0
2	NAG	f	1	1,2	14,14,15	0.40	0	17,19,21	1.57	1 (5%)
2	NAG	f	2	2	14,14,15	0.32	0	17,19,21	0.61	0
2	MAN	f	3	2	11,11,12	0.28	0	15,15,17	1.25	1 (6%)
2	NAG	fA	1	1,2	14,14,15	0.37	0	17,19,21	0.59	0
2	NAG	fA	2	2	14,14,15	0.53	0	17,19,21	0.65	0
2	MAN	fA	3	2	11,11,12	0.39	0	15,15,17	0.90	1 (6%)
2	NAG	g	1	1,2	14,14,15	0.25	0	17,19,21	1.53	1 (5%)
2	NAG	g	2	2	14,14,15	0.30	0	17,19,21	0.71	1 (5%)
2	MAN	g	3	2	11,11,12	0.27	0	15,15,17	0.53	0
2	NAG	gA	1	1,2	14,14,15	0.34	0	17,19,21	1.49	1 (5%)
2	NAG	gA	2	2	14,14,15	0.51	0	17,19,21	1.96	2 (11%)
2	MAN	gA	3	2	11,11,12	0.49	0	15,15,17	1.92	3 (20%)
2	NAG	h	1	1,2	14,14,15	0.37	0	17,19,21	0.60	0
2	NAG	h	2	2	14,14,15	0.55	0	17,19,21	0.62	0
2	MAN	h	3	2	11,11,12	0.41	0	15,15,17	0.91	1 (6%)
2	NAG	hA	1	1,2	14,14,15	0.47	0	17,19,21	1.45	1 (5%)
2	NAG	hA	2	2	14,14,15	0.50	0	17,19,21	1.95	2 (11%)
2	MAN	hA	3	2	11,11,12	0.49	0	15,15,17	1.91	3 (20%)
2	NAG	i	1	1,2	14,14,15	0.35	0	17,19,21	1.48	1 (5%)
2	NAG	i	2	2	14,14,15	0.51	0	17,19,21	1.96	2 (11%)
2	MAN	i	3	2	11,11,12	0.49	0	15,15,17	1.92	3 (20%)
2	NAG	iA	1	1,2	14,14,15	0.33	0	17,19,21	0.58	0
2	NAG	iA	2	2	14,14,15	0.34	0	17,19,21	0.98	1 (5%)
2	MAN	iA	3	2	11,11,12	0.30	0	15,15,17	0.79	0
2	NAG	j	1	1,2	14,14,15	0.48	0	17,19,21	1.42	1 (5%)
2	NAG	j	2	2	14,14,15	0.51	0	17,19,21	1.94	2 (11%)
2	MAN	j	3	2	11,11,12	0.49	0	15,15,17	1.92	3 (20%)
2	NAG	jA	1	1,2	14,14,15	0.41	0	17,19,21	1.57	1 (5%)
2	NAG	jA	2	2	14,14,15	0.30	0	17,19,21	0.70	0
2	MAN	jA	3	2	11,11,12	0.28	0	15,15,17	1.25	1 (6%)
2	NAG	k	1	1,2	14,14,15	0.32	0	17,19,21	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	k	2	2	14,14,15	0.34	0	17,19,21	0.99	1 (5%)
2	MAN	k	3	2	11,11,12	0.31	0	15,15,17	0.77	0
2	NAG	kA	1	1,2	14,14,15	0.24	0	17,19,21	1.52	1 (5%)
2	NAG	kA	2	2	14,14,15	0.31	0	17,19,21	0.71	1 (5%)
2	MAN	kA	3	2	11,11,12	0.26	0	15,15,17	0.60	0
2	NAG	l	1	1,2	14,14,15	0.40	0	17,19,21	1.57	1 (5%)
2	NAG	l	2	2	14,14,15	0.30	0	17,19,21	0.61	0
2	MAN	l	3	2	11,11,12	0.30	0	15,15,17	1.26	1 (6%)
2	NAG	lA	1	1,2	14,14,15	0.38	0	17,19,21	0.58	0
2	NAG	lA	2	2	14,14,15	0.54	0	17,19,21	0.63	0
2	MAN	lA	3	2	11,11,12	0.41	0	15,15,17	0.91	1 (6%)
2	NAG	m	1	1,2	14,14,15	0.23	0	17,19,21	1.53	1 (5%)
2	NAG	m	2	2	14,14,15	0.34	0	17,19,21	0.70	1 (5%)
2	MAN	m	3	2	11,11,12	0.26	0	15,15,17	0.54	0
2	NAG	mA	1	1,2	14,14,15	0.34	0	17,19,21	1.49	1 (5%)
2	NAG	mA	2	2	14,14,15	0.51	0	17,19,21	1.96	2 (11%)
2	MAN	mA	3	2	11,11,12	0.49	0	15,15,17	1.92	3 (20%)
2	NAG	n	1	1,2	14,14,15	0.37	0	17,19,21	0.62	0
2	NAG	n	2	2	14,14,15	0.54	0	17,19,21	0.62	0
2	MAN	n	3	2	11,11,12	0.41	0	15,15,17	0.91	1 (6%)
2	NAG	nA	1	1,2	14,14,15	0.47	0	17,19,21	1.43	1 (5%)
2	NAG	nA	2	2	14,14,15	0.51	0	17,19,21	1.95	2 (11%)
2	MAN	nA	3	2	11,11,12	0.49	0	15,15,17	1.92	3 (20%)
2	NAG	o	1	1,2	14,14,15	0.34	0	17,19,21	1.49	1 (5%)
2	NAG	o	2	2	14,14,15	0.50	0	17,19,21	1.95	2 (11%)
2	MAN	o	3	2	11,11,12	0.48	0	15,15,17	1.92	3 (20%)
2	NAG	oA	1	1,2	14,14,15	0.33	0	17,19,21	0.58	0
2	NAG	oA	2	2	14,14,15	0.35	0	17,19,21	0.99	1 (5%)
2	MAN	oA	3	2	11,11,12	0.31	0	15,15,17	0.81	0
2	NAG	p	1	1,2	14,14,15	0.49	0	17,19,21	1.46	1 (5%)
2	NAG	p	2	2	14,14,15	0.51	0	17,19,21	1.95	2 (11%)
2	MAN	p	3	2	11,11,12	0.50	0	15,15,17	1.90	3 (20%)
2	NAG	pA	1	1,2	14,14,15	0.41	0	17,19,21	1.57	1 (5%)
2	NAG	pA	2	2	14,14,15	0.30	0	17,19,21	0.69	0
2	MAN	pA	3	2	11,11,12	0.28	0	15,15,17	1.23	1 (6%)
2	NAG	q	1	1,2	14,14,15	0.33	0	17,19,21	0.58	0
2	NAG	q	2	2	14,14,15	0.35	0	17,19,21	0.99	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MAN	q	3	2	11,11,12	0.30	0	15,15,17	0.79	0
2	NAG	qA	1	1,2	14,14,15	0.25	0	17,19,21	1.52	1 (5%)
2	NAG	qA	2	2	14,14,15	0.32	0	17,19,21	0.70	1 (5%)
2	MAN	qA	3	2	11,11,12	0.26	0	15,15,17	0.60	0
2	NAG	r	1	1,2	14,14,15	0.40	0	17,19,21	1.57	1 (5%)
2	NAG	r	2	2	14,14,15	0.32	0	17,19,21	0.62	0
2	MAN	r	3	2	11,11,12	0.30	0	15,15,17	1.25	1 (6%)
2	NAG	rA	1	1,2	14,14,15	0.37	0	17,19,21	0.57	0
2	NAG	rA	2	2	14,14,15	0.53	0	17,19,21	0.63	0
2	MAN	rA	3	2	11,11,12	0.40	0	15,15,17	0.91	1 (6%)
2	NAG	s	1	1,2	14,14,15	0.24	0	17,19,21	1.53	1 (5%)
2	NAG	s	2	2	14,14,15	0.30	0	17,19,21	0.70	1 (5%)
2	MAN	s	3	2	11,11,12	0.26	0	15,15,17	0.60	0
2	NAG	sA	1	1,2	14,14,15	0.34	0	17,19,21	1.50	1 (5%)
2	NAG	sA	2	2	14,14,15	0.52	0	17,19,21	1.96	2 (11%)
2	MAN	sA	3	2	11,11,12	0.47	0	15,15,17	1.92	3 (20%)
2	NAG	t	1	1,2	14,14,15	0.38	0	17,19,21	0.62	0
2	NAG	t	2	2	14,14,15	0.55	0	17,19,21	0.62	0
2	MAN	t	3	2	11,11,12	0.40	0	15,15,17	0.90	1 (6%)
2	NAG	tA	1	1,2	14,14,15	0.47	0	17,19,21	1.46	1 (5%)
2	NAG	tA	2	2	14,14,15	0.50	0	17,19,21	1.93	2 (11%)
2	MAN	tA	3	2	11,11,12	0.50	0	15,15,17	1.91	3 (20%)
2	NAG	u	1	1,2	14,14,15	0.34	0	17,19,21	1.49	1 (5%)
2	NAG	u	2	2	14,14,15	0.50	0	17,19,21	1.97	2 (11%)
2	MAN	u	3	2	11,11,12	0.48	0	15,15,17	1.92	3 (20%)
2	NAG	uA	1	1,2	14,14,15	0.34	0	17,19,21	0.58	0
2	NAG	uA	2	2	14,14,15	0.35	0	17,19,21	0.99	1 (5%)
2	MAN	uA	3	2	11,11,12	0.29	0	15,15,17	0.77	0
2	NAG	v	1	1,2	14,14,15	0.47	0	17,19,21	1.43	1 (5%)
2	NAG	v	2	2	14,14,15	0.51	0	17,19,21	1.95	2 (11%)
2	MAN	v	3	2	11,11,12	0.49	0	15,15,17	1.92	3 (20%)
2	NAG	vA	1	1,2	14,14,15	0.41	0	17,19,21	1.56	1 (5%)
2	NAG	vA	2	2	14,14,15	0.28	0	17,19,21	0.71	0
2	MAN	vA	3	2	11,11,12	0.28	0	15,15,17	1.23	1 (6%)
2	NAG	w	1	1,2	14,14,15	0.33	0	17,19,21	0.58	0
2	NAG	w	2	2	14,14,15	0.34	0	17,19,21	1.00	1 (5%)
2	MAN	w	3	2	11,11,12	0.31	0	15,15,17	0.81	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	wA	1	1,2	14,14,15	0.24	0	17,19,21	1.52	1 (5%)
2	NAG	wA	2	2	14,14,15	0.32	0	17,19,21	0.69	1 (5%)
2	MAN	wA	3	2	11,11,12	0.27	0	15,15,17	0.57	0
2	NAG	x	1	1,2	14,14,15	0.42	0	17,19,21	1.55	1 (5%)
2	NAG	x	2	2	14,14,15	0.30	0	17,19,21	0.69	0
2	MAN	x	3	2	11,11,12	0.29	0	15,15,17	1.25	1 (6%)
2	NAG	xA	1	1,2	14,14,15	0.38	0	17,19,21	0.57	0
2	NAG	xA	2	2	14,14,15	0.53	0	17,19,21	0.64	0
2	MAN	xA	3	2	11,11,12	0.40	0	15,15,17	0.92	1 (6%)
2	NAG	y	1	1,2	14,14,15	0.24	0	17,19,21	1.53	1 (5%)
2	NAG	y	2	2	14,14,15	0.31	0	17,19,21	0.69	1 (5%)
2	MAN	y	3	2	11,11,12	0.26	0	15,15,17	0.59	0
2	NAG	yA	1	1,2	14,14,15	0.35	0	17,19,21	1.49	1 (5%)
2	NAG	yA	2	2	14,14,15	0.51	0	17,19,21	1.96	2 (11%)
2	MAN	yA	3	2	11,11,12	0.48	0	15,15,17	1.92	3 (20%)
2	NAG	z	1	1,2	14,14,15	0.38	0	17,19,21	0.62	0
2	NAG	z	2	2	14,14,15	0.55	0	17,19,21	0.62	0
2	MAN	z	3	2	11,11,12	0.41	0	15,15,17	0.91	1 (6%)
2	NAG	zA	1	1,2	14,14,15	0.48	0	17,19,21	1.47	1 (5%)
2	NAG	zA	2	2	14,14,15	0.50	0	17,19,21	1.97	2 (11%)
2	MAN	zA	3	2	11,11,12	0.49	0	15,15,17	1.91	3 (20%)

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
2	NAG	0	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	0	2	2	-	0/6/23/26	0/1/1/1
2	MAN	0	3	2	-	0/2/19/22	0/1/1/1
2	NAG	0A	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	0A	2	2	-	0/6/23/26	0/1/1/1
2	MAN	0A	3	2	-	2/2/19/22	0/1/1/1
2	NAG	1	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	1	2	2	-	0/6/23/26	0/1/1/1
2	MAN	1	3	2	-	0/2/19/22	0/1/1/1
2	NAG	1A	1	1,2	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	1A	2	2	-	2/6/23/26	0/1/1/1
2	MAN	1A	3	2	-	0/2/19/22	0/1/1/1
2	NAG	2	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	2	2	2	-	0/6/23/26	0/1/1/1
2	MAN	2	3	2	-	2/2/19/22	0/1/1/1
2	NAG	2A	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	2A	2	2	-	2/6/23/26	0/1/1/1
2	MAN	2A	3	2	-	0/2/19/22	0/1/1/1
2	NAG	3	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	3	2	2	-	2/6/23/26	0/1/1/1
2	MAN	3	3	2	-	0/2/19/22	0/1/1/1
2	NAG	3A	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	3A	2	2	-	0/6/23/26	0/1/1/1
2	MAN	3A	3	2	-	0/2/19/22	0/1/1/1
2	NAG	4	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	4	2	2	-	2/6/23/26	0/1/1/1
2	MAN	4	3	2	-	0/2/19/22	0/1/1/1
2	NAG	4A	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	4A	2	2	-	0/6/23/26	0/1/1/1
2	MAN	4A	3	2	-	0/2/19/22	0/1/1/1
2	NAG	5	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	5	2	2	-	0/6/23/26	0/1/1/1
2	MAN	5	3	2	-	0/2/19/22	0/1/1/1
2	NAG	5A	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	5A	2	2	-	0/6/23/26	0/1/1/1
2	MAN	5A	3	2	-	0/2/19/22	0/1/1/1
2	NAG	6	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	6	2	2	-	0/6/23/26	0/1/1/1
2	MAN	6	3	2	-	0/2/19/22	0/1/1/1
2	NAG	6A	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	6A	2	2	-	0/6/23/26	0/1/1/1
2	MAN	6A	3	2	-	2/2/19/22	0/1/1/1
2	NAG	7	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	7	2	2	-	0/6/23/26	0/1/1/1
2	MAN	7	3	2	-	0/2/19/22	0/1/1/1
2	NAG	7A	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	7A	2	2	-	2/6/23/26	0/1/1/1
2	MAN	7A	3	2	-	0/2/19/22	0/1/1/1
2	NAG	8	1	1,2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	8	2	2	-	0/6/23/26	0/1/1/1
2	MAN	8	3	2	-	2/2/19/22	0/1/1/1
2	NAG	8A	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	8A	2	2	-	2/6/23/26	0/1/1/1
2	MAN	8A	3	2	-	0/2/19/22	0/1/1/1
2	NAG	9	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	9	2	2	-	2/6/23/26	0/1/1/1
2	MAN	9	3	2	-	0/2/19/22	0/1/1/1
2	NAG	9A	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	9A	2	2	-	0/6/23/26	0/1/1/1
2	MAN	9A	3	2	-	0/2/19/22	0/1/1/1
2	NAG	AA	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	AA	2	2	-	2/6/23/26	0/1/1/1
2	MAN	AA	3	2	-	0/2/19/22	0/1/1/1
2	NAG	AB	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	AB	2	2	-	0/6/23/26	0/1/1/1
2	MAN	AB	3	2	-	0/2/19/22	0/1/1/1
2	NAG	BA	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	BA	2	2	-	0/6/23/26	0/1/1/1
2	MAN	BA	3	2	-	0/2/19/22	0/1/1/1
2	NAG	BB	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	BB	2	2	-	0/6/23/26	0/1/1/1
2	MAN	BB	3	2	-	0/2/19/22	0/1/1/1
2	NAG	CA	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	CA	2	2	-	0/6/23/26	0/1/1/1
2	MAN	CA	3	2	-	0/2/19/22	0/1/1/1
2	NAG	CB	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	CB	2	2	-	0/6/23/26	0/1/1/1
2	MAN	CB	3	2	-	2/2/19/22	0/1/1/1
2	NAG	DA	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	DA	2	2	-	0/6/23/26	0/1/1/1
2	MAN	DA	3	2	-	0/2/19/22	0/1/1/1
2	NAG	DB	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	DB	2	2	-	2/6/23/26	0/1/1/1
2	MAN	DB	3	2	-	0/2/19/22	0/1/1/1
2	NAG	EA	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	EA	2	2	-	0/6/23/26	0/1/1/1
2	MAN	EA	3	2	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	EB	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	EB	2	2	-	2/6/23/26	0/1/1/1
2	MAN	EB	3	2	-	0/2/19/22	0/1/1/1
2	NAG	FA	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	FA	2	2	-	2/6/23/26	0/1/1/1
2	MAN	FA	3	2	-	0/2/19/22	0/1/1/1
2	NAG	FB	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	FB	2	2	-	0/6/23/26	0/1/1/1
2	MAN	FB	3	2	-	0/2/19/22	0/1/1/1
2	NAG	GA	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	GA	2	2	-	2/6/23/26	0/1/1/1
2	MAN	GA	3	2	-	0/2/19/22	0/1/1/1
2	NAG	GB	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	GB	2	2	-	0/6/23/26	0/1/1/1
2	MAN	GB	3	2	-	0/2/19/22	0/1/1/1
2	NAG	HA	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	HA	2	2	-	0/6/23/26	0/1/1/1
2	MAN	HA	3	2	-	0/2/19/22	0/1/1/1
2	NAG	HB	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	HB	2	2	-	0/6/23/26	0/1/1/1
2	MAN	HB	3	2	-	0/2/19/22	0/1/1/1
2	NAG	IA	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	IA	2	2	-	0/6/23/26	0/1/1/1
2	MAN	IA	3	2	-	0/2/19/22	0/1/1/1
2	NAG	IB	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	IB	2	2	-	0/6/23/26	0/1/1/1
2	MAN	IB	3	2	-	2/2/19/22	0/1/1/1
2	NAG	JA	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	JA	2	2	-	0/6/23/26	0/1/1/1
2	MAN	JA	3	2	-	0/2/19/22	0/1/1/1
2	NAG	JB	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	JB	2	2	-	2/6/23/26	0/1/1/1
2	MAN	JB	3	2	-	0/2/19/22	0/1/1/1
2	NAG	KA	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	KA	2	2	-	0/6/23/26	0/1/1/1
2	MAN	KA	3	2	-	2/2/19/22	0/1/1/1
2	NAG	KB	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	KB	2	2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MAN	KB	3	2	-	0/2/19/22	0/1/1/1
2	NAG	LA	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	LA	2	2	-	2/6/23/26	0/1/1/1
2	MAN	LA	3	2	-	0/2/19/22	0/1/1/1
2	NAG	LB	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	LB	2	2	-	0/6/23/26	0/1/1/1
2	MAN	LB	3	2	-	0/2/19/22	0/1/1/1
2	NAG	MA	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	MA	2	2	-	2/6/23/26	0/1/1/1
2	MAN	MA	3	2	-	0/2/19/22	0/1/1/1
2	NAG	MB	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	MB	2	2	-	0/6/23/26	0/1/1/1
2	MAN	MB	3	2	-	0/2/19/22	0/1/1/1
2	NAG	NA	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	NA	2	2	-	0/6/23/26	0/1/1/1
2	MAN	NA	3	2	-	0/2/19/22	0/1/1/1
2	NAG	NB	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	NB	2	2	-	0/6/23/26	0/1/1/1
2	MAN	NB	3	2	-	0/2/19/22	0/1/1/1
2	NAG	OA	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	OA	2	2	-	0/6/23/26	0/1/1/1
2	MAN	OA	3	2	-	0/2/19/22	0/1/1/1
2	NAG	OB	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	OB	2	2	-	0/6/23/26	0/1/1/1
2	MAN	OB	3	2	-	2/2/19/22	0/1/1/1
2	NAG	PA	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	PA	2	2	-	0/6/23/26	0/1/1/1
2	MAN	PA	3	2	-	0/2/19/22	0/1/1/1
2	NAG	PB	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	PB	2	2	-	2/6/23/26	0/1/1/1
2	MAN	PB	3	2	-	0/2/19/22	0/1/1/1
2	NAG	QA	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	QA	2	2	-	0/6/23/26	0/1/1/1
2	MAN	QA	3	2	-	2/2/19/22	0/1/1/1
2	NAG	RA	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	RA	2	2	-	2/6/23/26	0/1/1/1
2	MAN	RA	3	2	-	0/2/19/22	0/1/1/1
2	NAG	SA	1	1,2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	SA	2	2	-	2/6/23/26	0/1/1/1
2	MAN	SA	3	2	-	0/2/19/22	0/1/1/1
2	NAG	TA	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	TA	2	2	-	0/6/23/26	0/1/1/1
2	MAN	TA	3	2	-	0/2/19/22	0/1/1/1
2	NAG	U	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	U	2	2	-	2/6/23/26	0/1/1/1
2	MAN	U	3	2	-	0/2/19/22	0/1/1/1
2	NAG	UA	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	UA	2	2	-	0/6/23/26	0/1/1/1
2	MAN	UA	3	2	-	0/2/19/22	0/1/1/1
2	NAG	V	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	V	2	2	-	0/6/23/26	0/1/1/1
2	MAN	V	3	2	-	0/2/19/22	0/1/1/1
2	NAG	VA	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	VA	2	2	-	0/6/23/26	0/1/1/1
2	MAN	VA	3	2	-	0/2/19/22	0/1/1/1
2	NAG	W	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	W	2	2	-	0/6/23/26	0/1/1/1
2	MAN	W	3	2	-	0/2/19/22	0/1/1/1
2	NAG	WA	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	WA	2	2	-	0/6/23/26	0/1/1/1
2	MAN	WA	3	2	-	2/2/19/22	0/1/1/1
2	NAG	X	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	X	2	2	-	0/6/23/26	0/1/1/1
2	MAN	X	3	2	-	0/2/19/22	0/1/1/1
2	NAG	XA	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	XA	2	2	-	2/6/23/26	0/1/1/1
2	MAN	XA	3	2	-	0/2/19/22	0/1/1/1
2	NAG	Y	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	Y	2	2	-	0/6/23/26	0/1/1/1
2	MAN	Y	3	2	-	2/2/19/22	0/1/1/1
2	NAG	YA	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	YA	2	2	-	2/6/23/26	0/1/1/1
2	MAN	YA	3	2	-	0/2/19/22	0/1/1/1
2	NAG	Z	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	Z	2	2	-	2/6/23/26	0/1/1/1
2	MAN	Z	3	2	-	0/2/19/22	0/1/1/1
2	NAG	ZA	1	1,2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	ZA	2	2	-	0/6/23/26	0/1/1/1
2	MAN	ZA	3	2	-	0/2/19/22	0/1/1/1
2	NAG	a	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	a	2	2	-	2/6/23/26	0/1/1/1
2	MAN	a	3	2	-	0/2/19/22	0/1/1/1
2	NAG	aA	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	aA	2	2	-	0/6/23/26	0/1/1/1
2	MAN	aA	3	2	-	0/2/19/22	0/1/1/1
2	NAG	b	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	b	2	2	-	0/6/23/26	0/1/1/1
2	MAN	b	3	2	-	0/2/19/22	0/1/1/1
2	NAG	bA	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	bA	2	2	-	0/6/23/26	0/1/1/1
2	MAN	bA	3	2	-	0/2/19/22	0/1/1/1
2	NAG	c	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	c	2	2	-	0/6/23/26	0/1/1/1
2	MAN	c	3	2	-	0/2/19/22	0/1/1/1
2	NAG	cA	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	cA	2	2	-	0/6/23/26	0/1/1/1
2	MAN	cA	3	2	-	2/2/19/22	0/1/1/1
2	NAG	d	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	d	2	2	-	0/6/23/26	0/1/1/1
2	MAN	d	3	2	-	0/2/19/22	0/1/1/1
2	NAG	dA	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	dA	2	2	-	2/6/23/26	0/1/1/1
2	MAN	dA	3	2	-	0/2/19/22	0/1/1/1
2	NAG	e	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	e	2	2	-	0/6/23/26	0/1/1/1
2	MAN	e	3	2	-	2/2/19/22	0/1/1/1
2	NAG	eA	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	eA	2	2	-	2/6/23/26	0/1/1/1
2	MAN	eA	3	2	-	0/2/19/22	0/1/1/1
2	NAG	f	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	f	2	2	-	2/6/23/26	0/1/1/1
2	MAN	f	3	2	-	0/2/19/22	0/1/1/1
2	NAG	fA	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	fA	2	2	-	0/6/23/26	0/1/1/1
2	MAN	fA	3	2	-	0/2/19/22	0/1/1/1
2	NAG	g	1	1,2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	g	2	2	-	2/6/23/26	0/1/1/1
2	MAN	g	3	2	-	0/2/19/22	0/1/1/1
2	NAG	gA	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	gA	2	2	-	0/6/23/26	0/1/1/1
2	MAN	gA	3	2	-	0/2/19/22	0/1/1/1
2	NAG	h	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	h	2	2	-	0/6/23/26	0/1/1/1
2	MAN	h	3	2	-	0/2/19/22	0/1/1/1
2	NAG	hA	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	hA	2	2	-	0/6/23/26	0/1/1/1
2	MAN	hA	3	2	-	0/2/19/22	0/1/1/1
2	NAG	i	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	i	2	2	-	0/6/23/26	0/1/1/1
2	MAN	i	3	2	-	0/2/19/22	0/1/1/1
2	NAG	iA	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	iA	2	2	-	0/6/23/26	0/1/1/1
2	MAN	iA	3	2	-	2/2/19/22	0/1/1/1
2	NAG	j	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	j	2	2	-	0/6/23/26	0/1/1/1
2	MAN	j	3	2	-	0/2/19/22	0/1/1/1
2	NAG	jA	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	jA	2	2	-	2/6/23/26	0/1/1/1
2	MAN	jA	3	2	-	0/2/19/22	0/1/1/1
2	NAG	k	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	k	2	2	-	0/6/23/26	0/1/1/1
2	MAN	k	3	2	-	2/2/19/22	0/1/1/1
2	NAG	kA	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	kA	2	2	-	2/6/23/26	0/1/1/1
2	MAN	kA	3	2	-	0/2/19/22	0/1/1/1
2	NAG	l	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	l	2	2	-	2/6/23/26	0/1/1/1
2	MAN	l	3	2	-	0/2/19/22	0/1/1/1
2	NAG	lA	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	lA	2	2	-	0/6/23/26	0/1/1/1
2	MAN	lA	3	2	-	0/2/19/22	0/1/1/1
2	NAG	m	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	m	2	2	-	2/6/23/26	0/1/1/1
2	MAN	m	3	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	mA	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	mA	2	2	-	0/6/23/26	0/1/1/1
2	MAN	mA	3	2	-	0/2/19/22	0/1/1/1
2	NAG	n	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	n	2	2	-	0/6/23/26	0/1/1/1
2	MAN	n	3	2	-	0/2/19/22	0/1/1/1
2	NAG	nA	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	nA	2	2	-	0/6/23/26	0/1/1/1
2	MAN	nA	3	2	-	0/2/19/22	0/1/1/1
2	NAG	o	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	o	2	2	-	0/6/23/26	0/1/1/1
2	MAN	o	3	2	-	0/2/19/22	0/1/1/1
2	NAG	oA	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	oA	2	2	-	0/6/23/26	0/1/1/1
2	MAN	oA	3	2	-	2/2/19/22	0/1/1/1
2	NAG	p	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	p	2	2	-	0/6/23/26	0/1/1/1
2	MAN	p	3	2	-	0/2/19/22	0/1/1/1
2	NAG	pA	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	pA	2	2	-	2/6/23/26	0/1/1/1
2	MAN	pA	3	2	-	0/2/19/22	0/1/1/1
2	NAG	q	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	q	2	2	-	0/6/23/26	0/1/1/1
2	MAN	q	3	2	-	2/2/19/22	0/1/1/1
2	NAG	qA	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	qA	2	2	-	2/6/23/26	0/1/1/1
2	MAN	qA	3	2	-	0/2/19/22	0/1/1/1
2	NAG	r	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	r	2	2	-	2/6/23/26	0/1/1/1
2	MAN	r	3	2	-	0/2/19/22	0/1/1/1
2	NAG	rA	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	rA	2	2	-	0/6/23/26	0/1/1/1
2	MAN	rA	3	2	-	0/2/19/22	0/1/1/1
2	NAG	s	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	s	2	2	-	2/6/23/26	0/1/1/1
2	MAN	s	3	2	-	0/2/19/22	0/1/1/1
2	NAG	sA	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	sA	2	2	-	0/6/23/26	0/1/1/1
2	MAN	sA	3	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	t	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	t	2	2	-	0/6/23/26	0/1/1/1
2	MAN	t	3	2	-	0/2/19/22	0/1/1/1
2	NAG	tA	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	tA	2	2	-	0/6/23/26	0/1/1/1
2	MAN	tA	3	2	-	0/2/19/22	0/1/1/1
2	NAG	u	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	u	2	2	-	0/6/23/26	0/1/1/1
2	MAN	u	3	2	-	0/2/19/22	0/1/1/1
2	NAG	uA	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	uA	2	2	-	0/6/23/26	0/1/1/1
2	MAN	uA	3	2	-	2/2/19/22	0/1/1/1
2	NAG	v	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	v	2	2	-	0/6/23/26	0/1/1/1
2	MAN	v	3	2	-	0/2/19/22	0/1/1/1
2	NAG	vA	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	vA	2	2	-	2/6/23/26	0/1/1/1
2	MAN	vA	3	2	-	0/2/19/22	0/1/1/1
2	NAG	w	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	w	2	2	-	0/6/23/26	0/1/1/1
2	MAN	w	3	2	-	2/2/19/22	0/1/1/1
2	NAG	wA	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	wA	2	2	-	2/6/23/26	0/1/1/1
2	MAN	wA	3	2	-	0/2/19/22	0/1/1/1
2	NAG	x	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	x	2	2	-	2/6/23/26	0/1/1/1
2	MAN	x	3	2	-	0/2/19/22	0/1/1/1
2	NAG	xA	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	xA	2	2	-	0/6/23/26	0/1/1/1
2	MAN	xA	3	2	-	0/2/19/22	0/1/1/1
2	NAG	y	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	y	2	2	-	2/6/23/26	0/1/1/1
2	MAN	y	3	2	-	0/2/19/22	0/1/1/1
2	NAG	yA	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	yA	2	2	-	0/6/23/26	0/1/1/1
2	MAN	yA	3	2	-	0/2/19/22	0/1/1/1
2	NAG	z	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	z	2	2	-	0/6/23/26	0/1/1/1
2	MAN	z	3	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	zA	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	zA	2	2	-	0/6/23/26	0/1/1/1
2	MAN	zA	3	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 361 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	MB	2	NAG	C1-O5-C5	6.87	121.39	112.19
2	zA	2	NAG	C1-O5-C5	6.86	121.37	112.19
2	CA	2	NAG	C1-O5-C5	6.84	121.35	112.19
2	AB	2	NAG	C1-O5-C5	6.83	121.34	112.19
2	0	2	NAG	C1-O5-C5	6.83	121.34	112.19

There are no chirality outliers.

5 of 380 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	d	1	NAG	O5-C5-C6-O6
2	v	1	NAG	O5-C5-C6-O6
2	1	1	NAG	O5-C5-C6-O6
2	7	1	NAG	O5-C5-C6-O6
2	JA	1	NAG	O5-C5-C6-O6

There are no ring outliers.

57 monomers are involved in 77 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	f	3	MAN	3	0
2	xA	2	NAG	1	0
2	PB	3	MAN	3	0
2	r	3	MAN	3	0
2	l	3	MAN	3	0
2	pA	3	MAN	3	0
2	0A	2	NAG	1	0
2	rA	2	NAG	1	0
2	iA	2	NAG	1	0
2	LB	2	NAG	1	0
2	BA	2	NAG	1	0
2	JB	3	MAN	3	0

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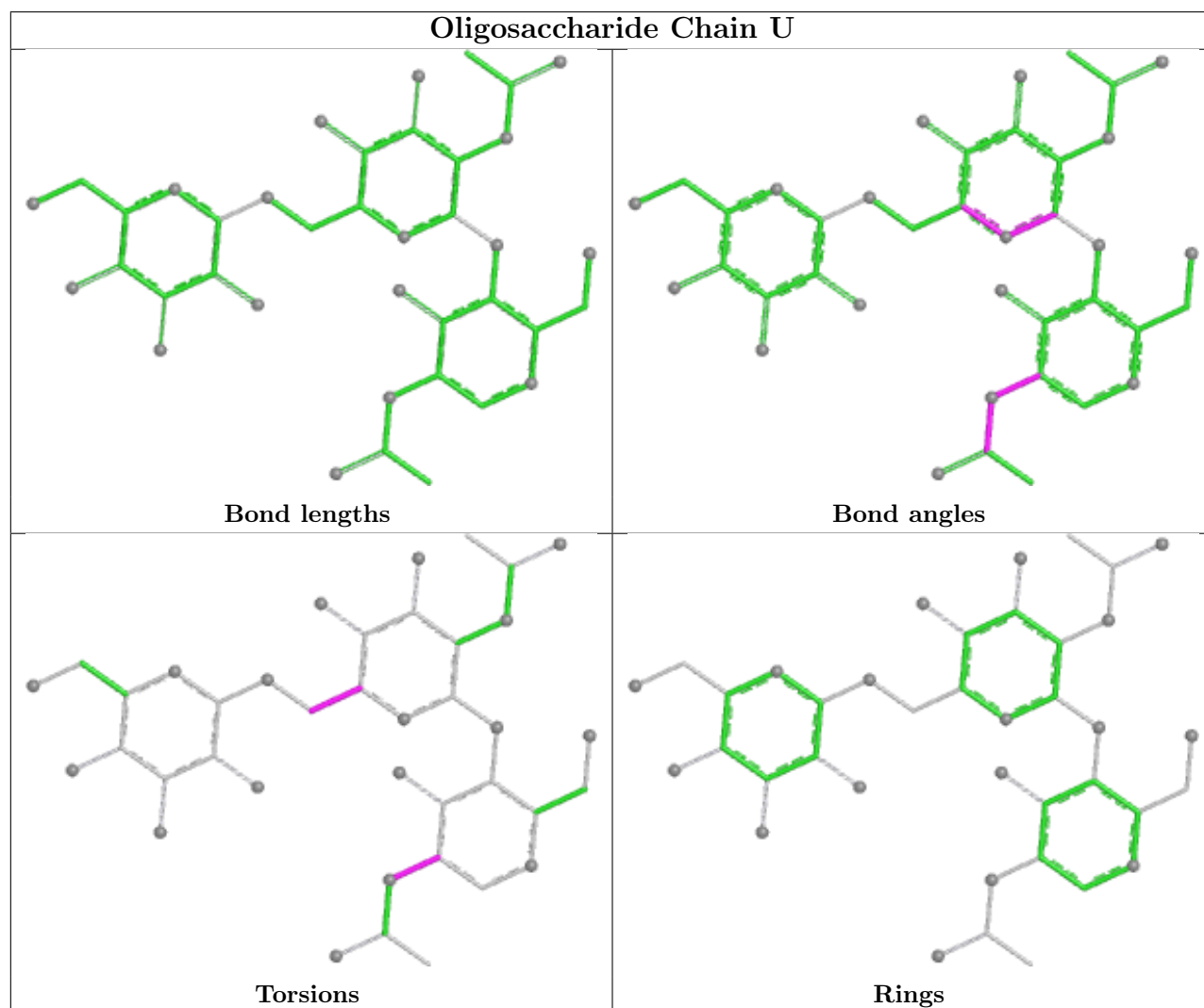
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	QA	2	NAG	1	0
2	dA	3	MAN	3	0
2	9	3	MAN	3	0
2	RA	3	MAN	3	0
2	KA	2	NAG	1	0
2	EA	2	NAG	1	0
2	e	2	NAG	1	0
2	w	2	NAG	1	0
2	7A	3	MAN	3	0
2	fA	2	NAG	1	0
2	oA	2	NAG	1	0
2	ZA	2	NAG	1	0
2	3	3	MAN	3	0
2	x	3	MAN	3	0
2	FB	2	NAG	1	0
2	WA	2	NAG	1	0
2	uA	2	NAG	1	0
2	1A	3	MAN	3	0
2	vA	3	MAN	3	0
2	2	2	NAG	1	0
2	5	2	NAG	1	0
2	6A	2	NAG	1	0
2	lA	2	NAG	1	0
2	3A	2	NAG	1	0
2	jA	3	MAN	3	0
2	9A	2	NAG	1	0
2	z	2	NAG	1	0
2	k	2	NAG	1	0
2	Y	2	NAG	1	0
2	DB	3	MAN	3	0
2	8	2	NAG	1	0
2	cA	2	NAG	1	0
2	LA	3	MAN	3	0
2	V	2	NAG	1	0
2	Z	3	MAN	3	0
2	NA	2	NAG	1	0
2	XA	3	MAN	3	0
2	q	2	NAG	1	0
2	TA	2	NAG	1	0
2	b	2	NAG	1	0
2	t	2	NAG	1	0
2	h	2	NAG	1	0

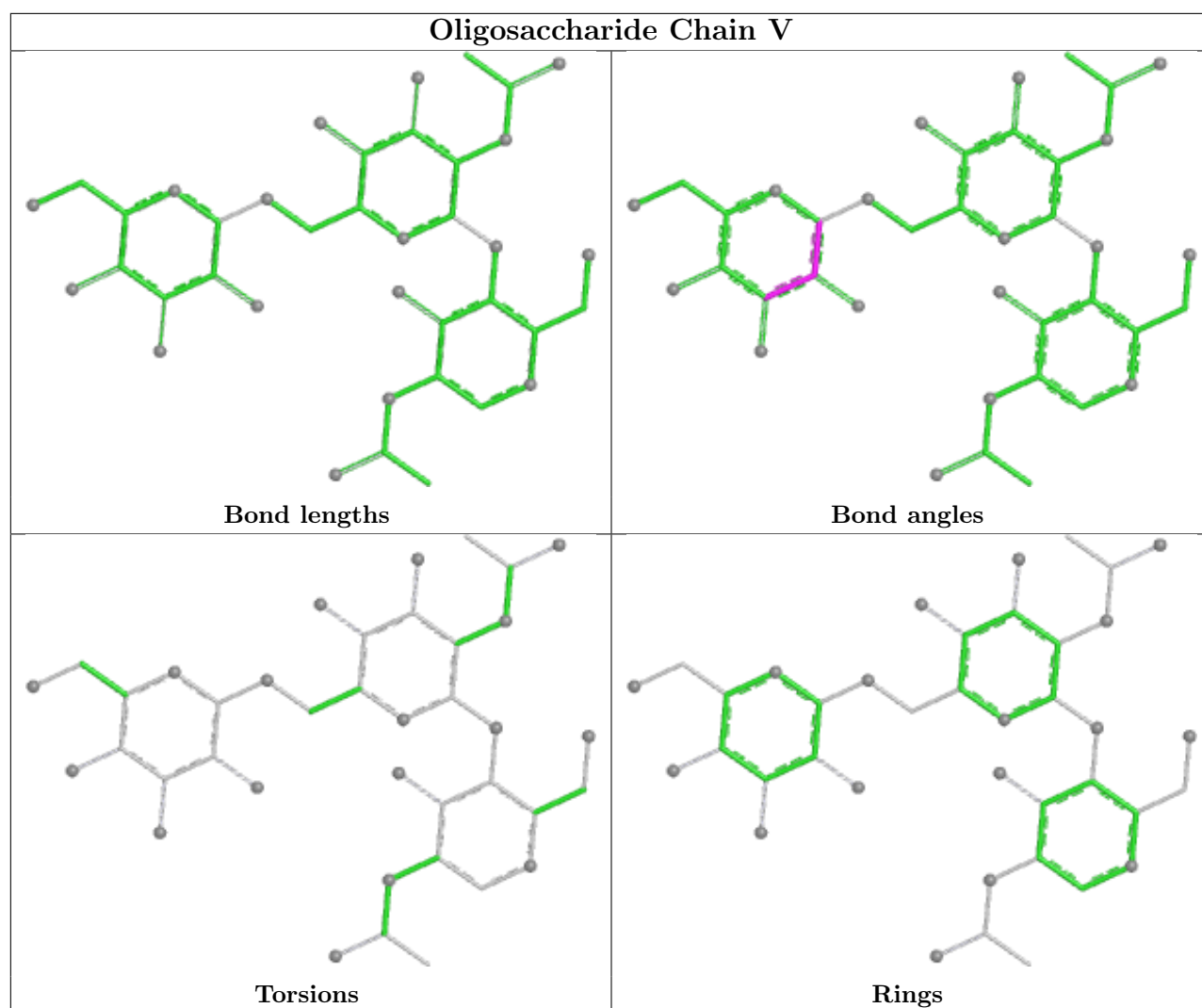
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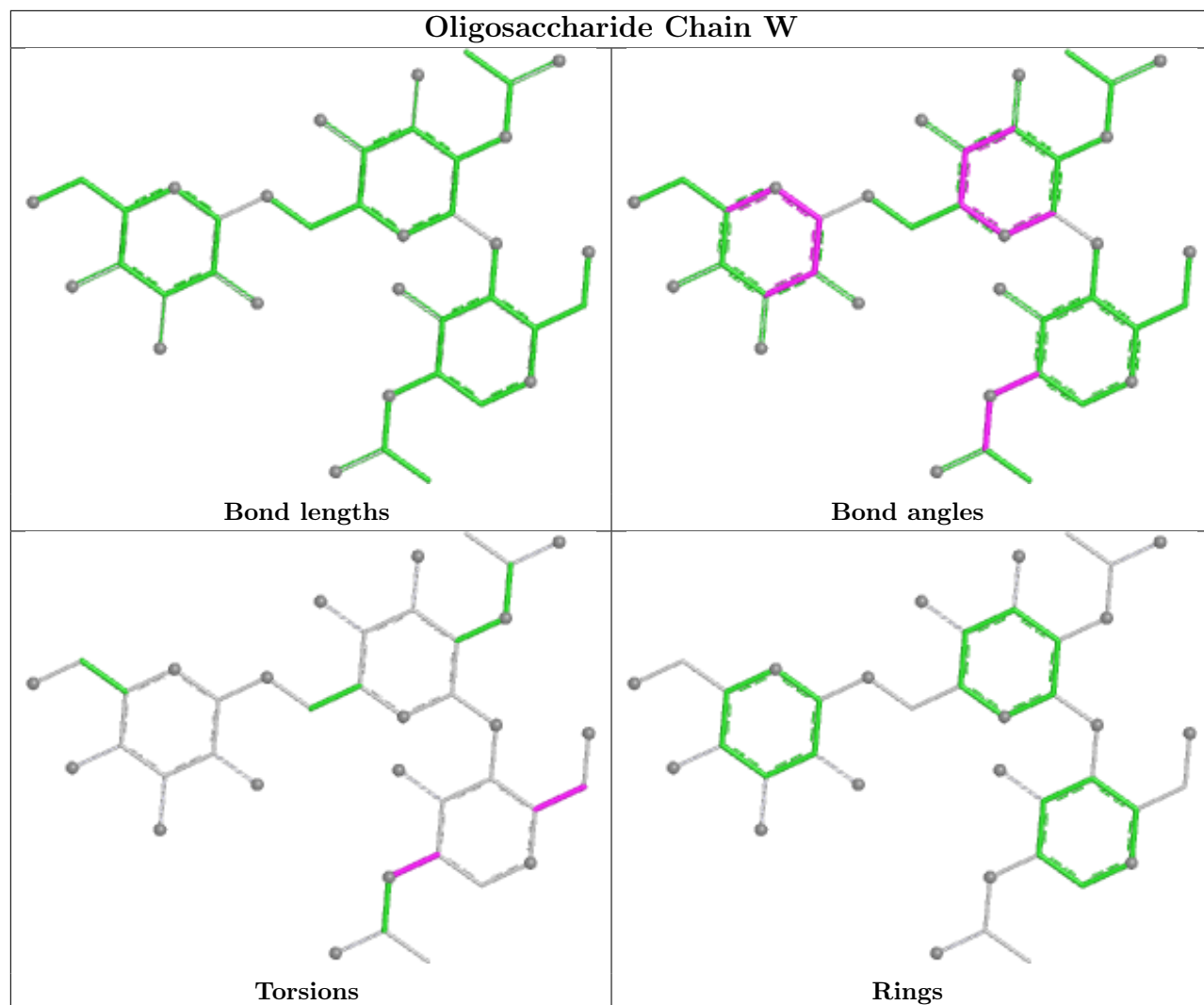
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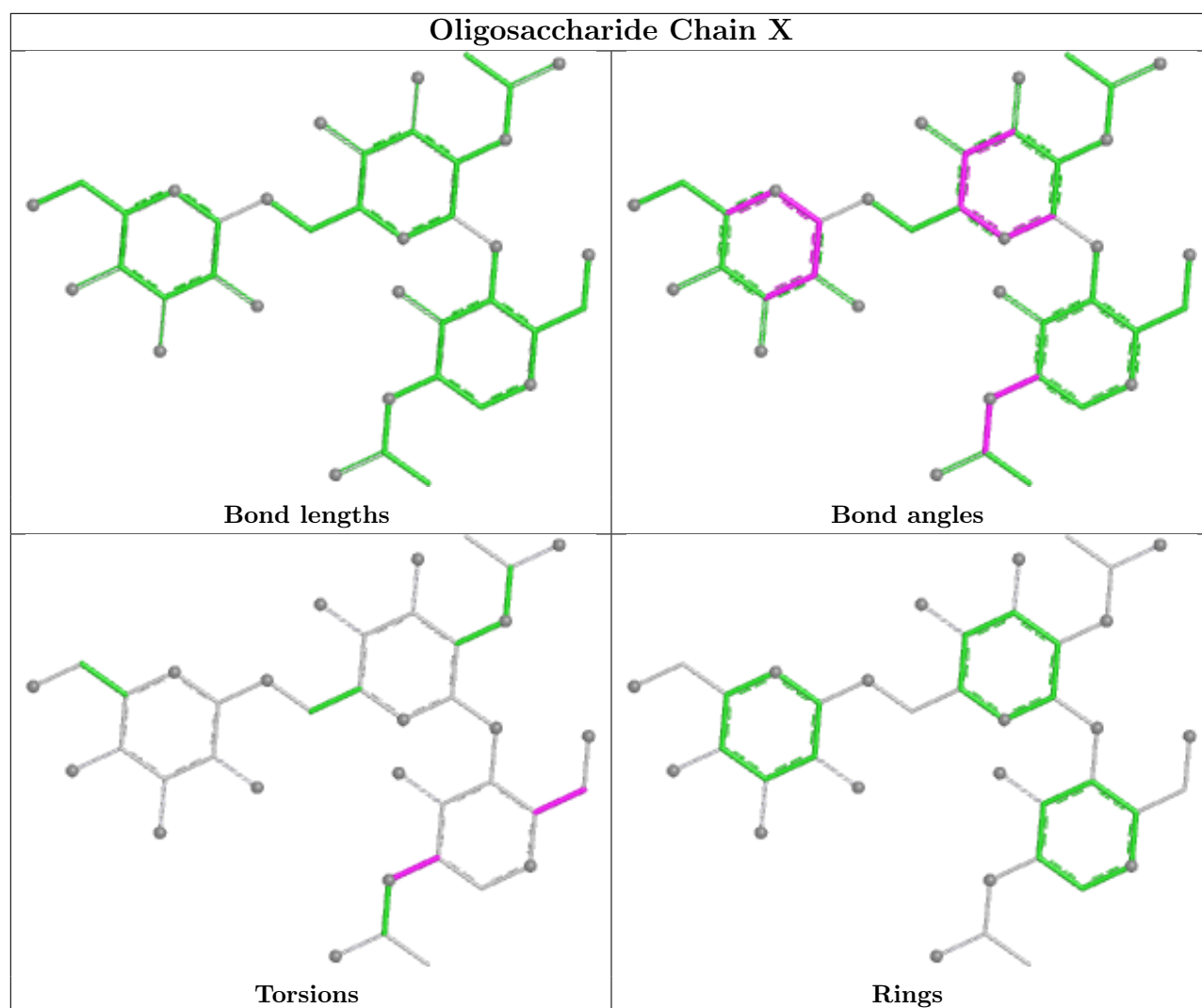
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	n	2	NAG	1	0
2	HA	2	NAG	1	0
2	FA	3	MAN	3	0

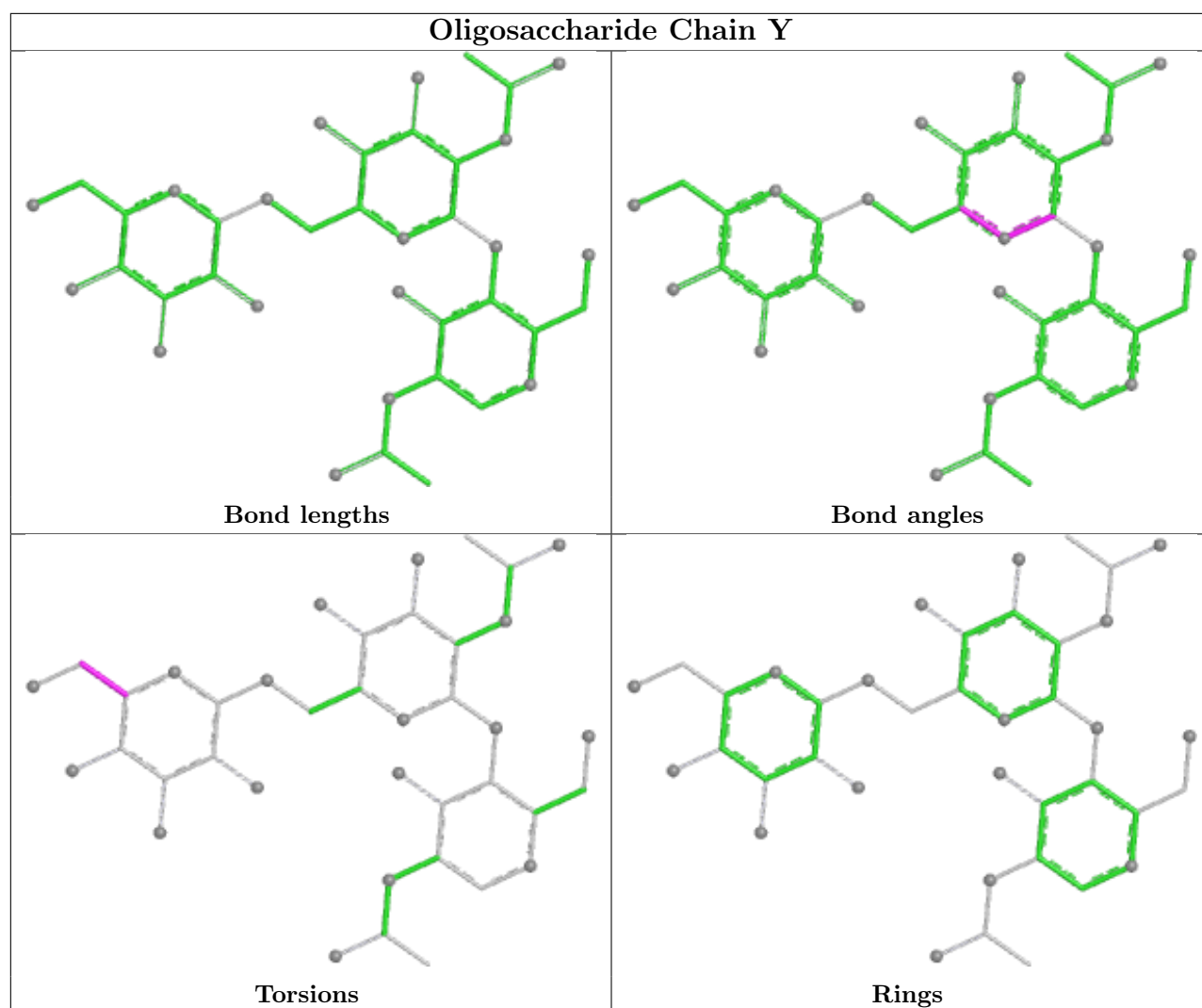
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

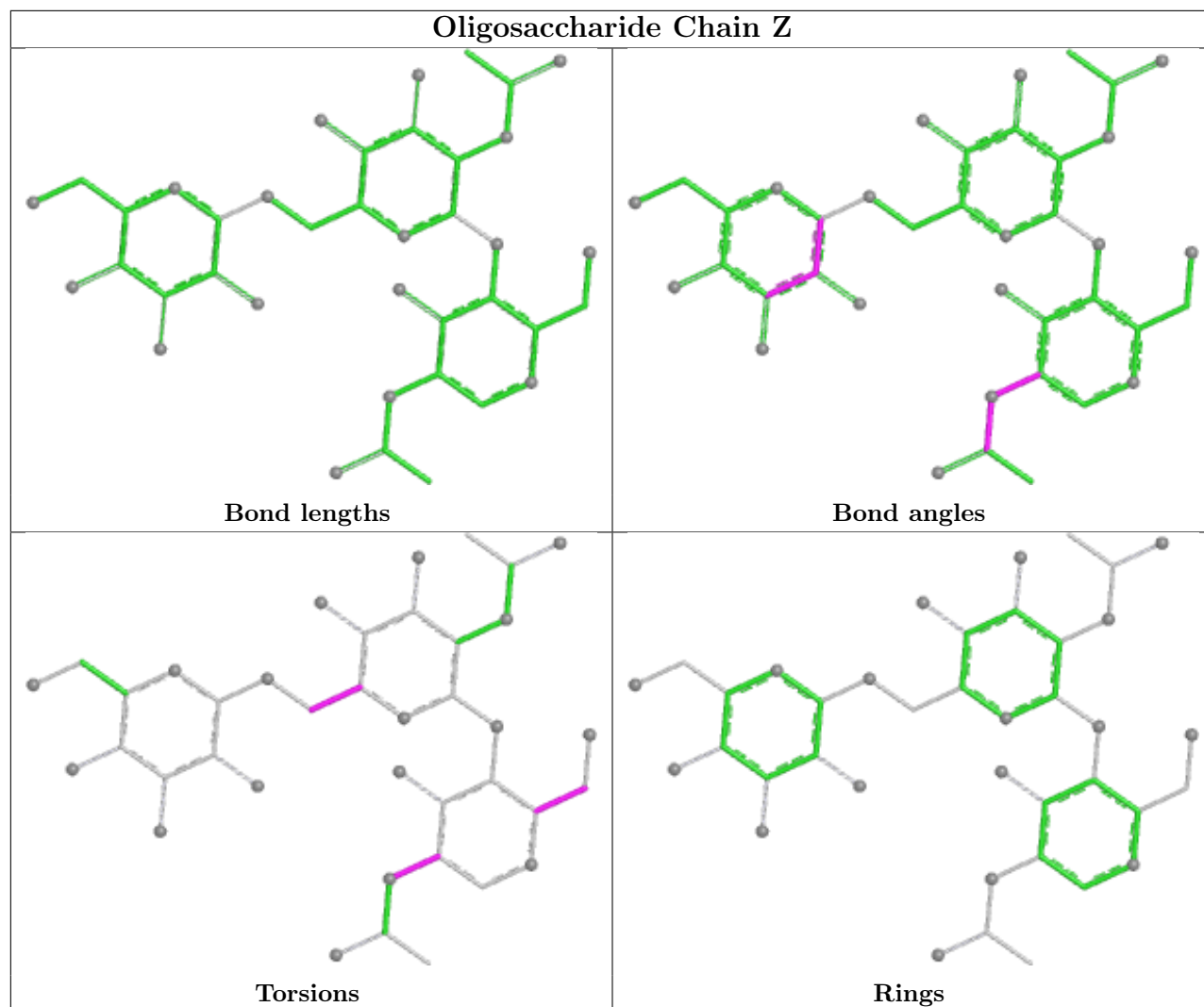


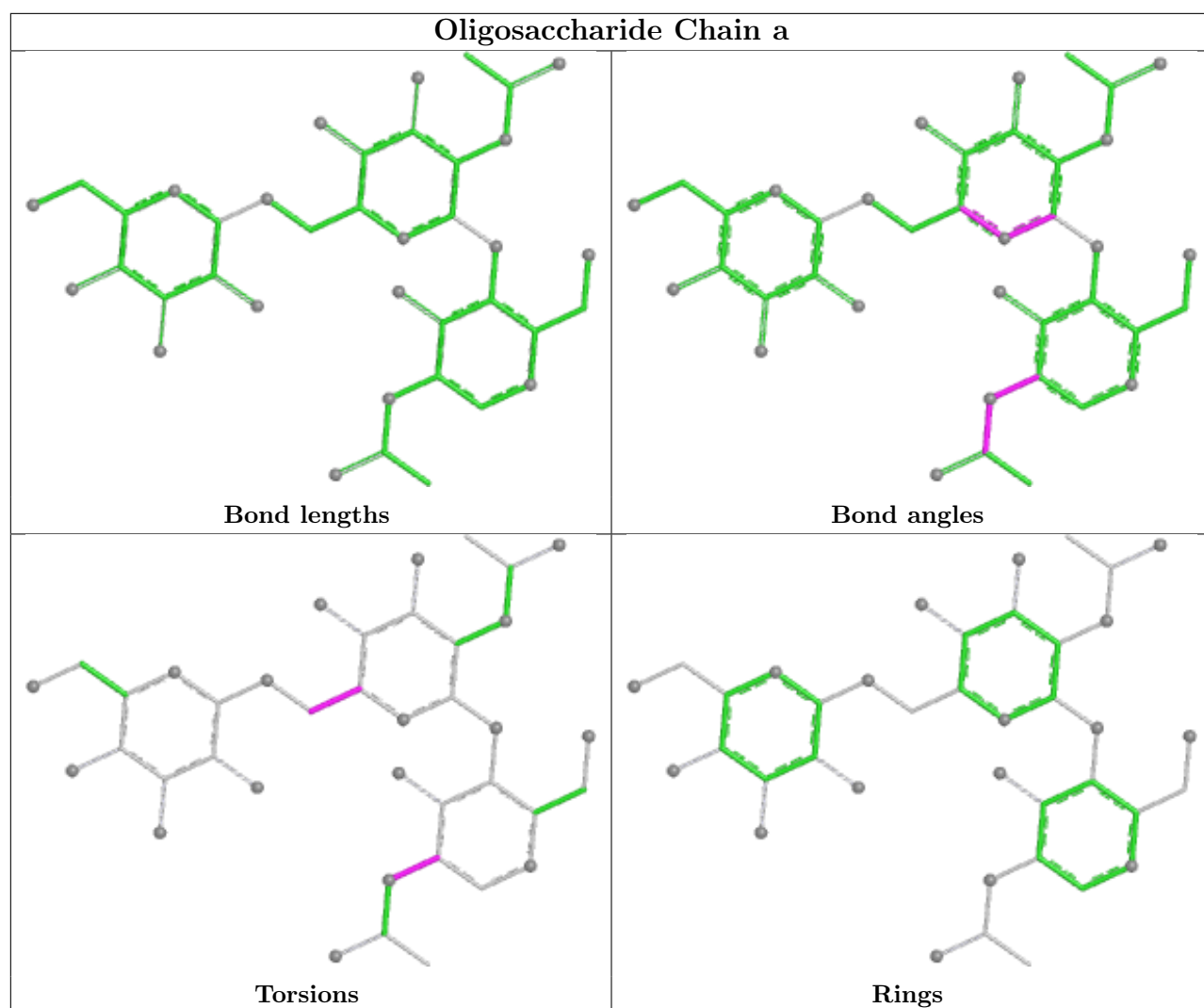


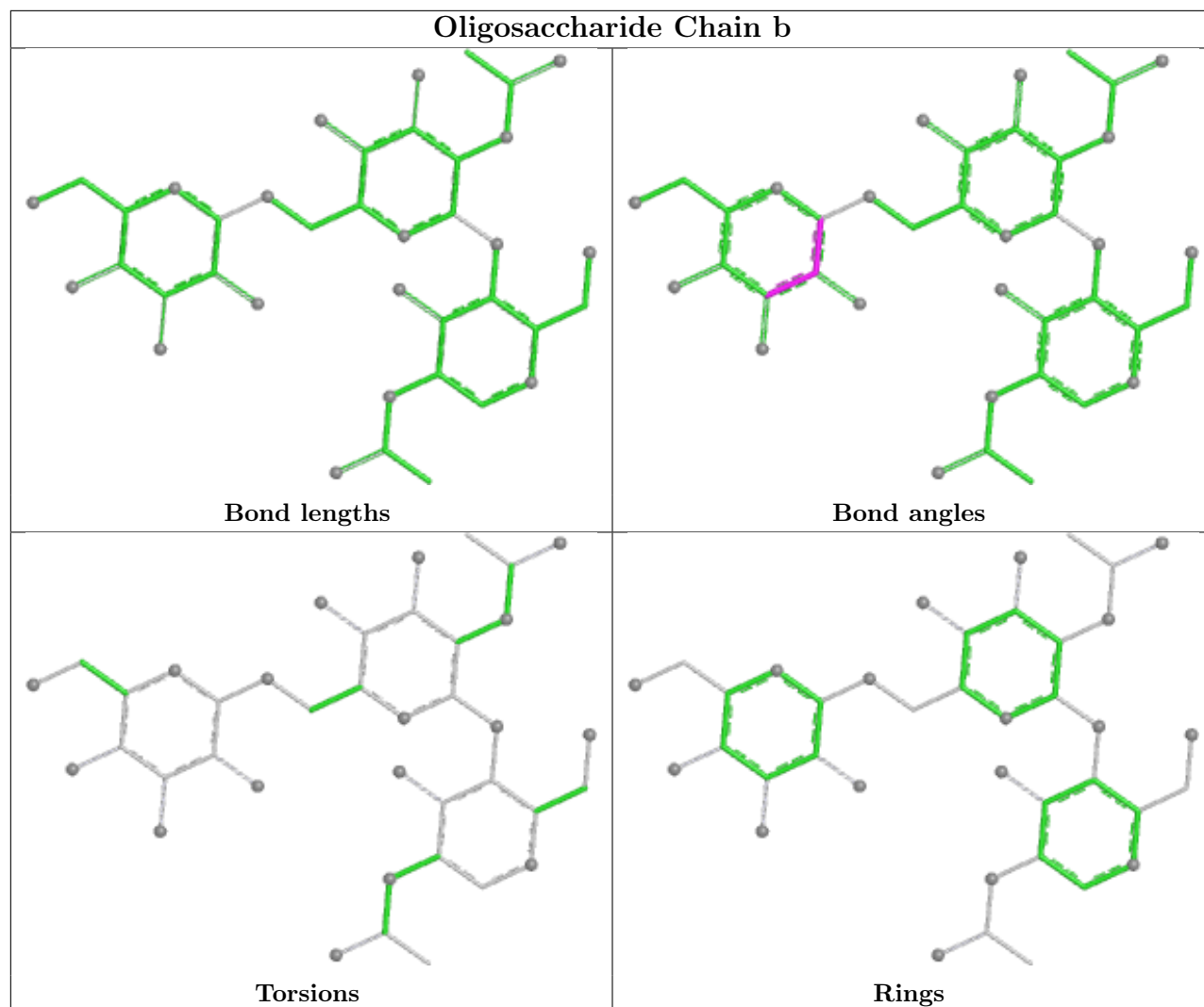


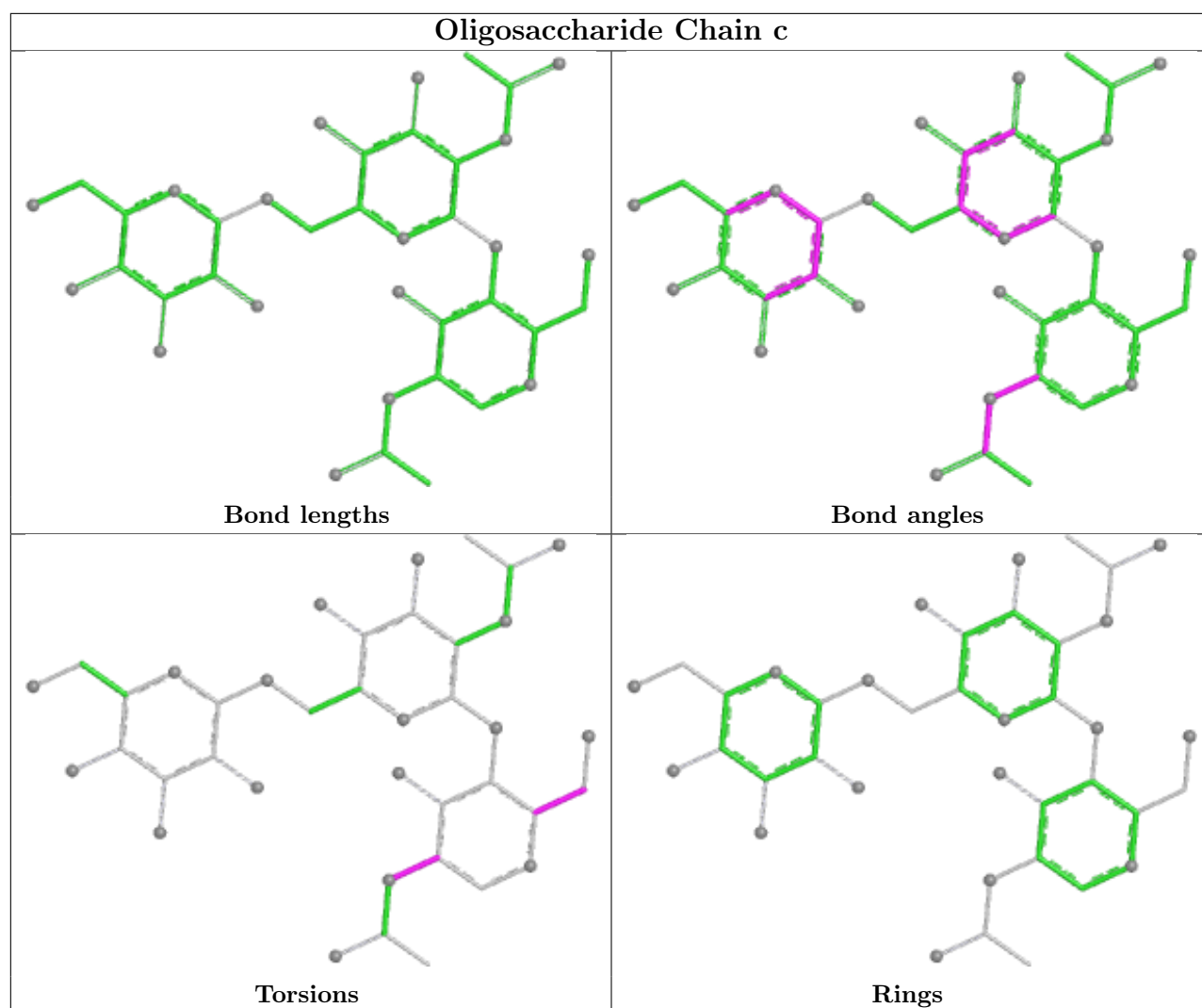


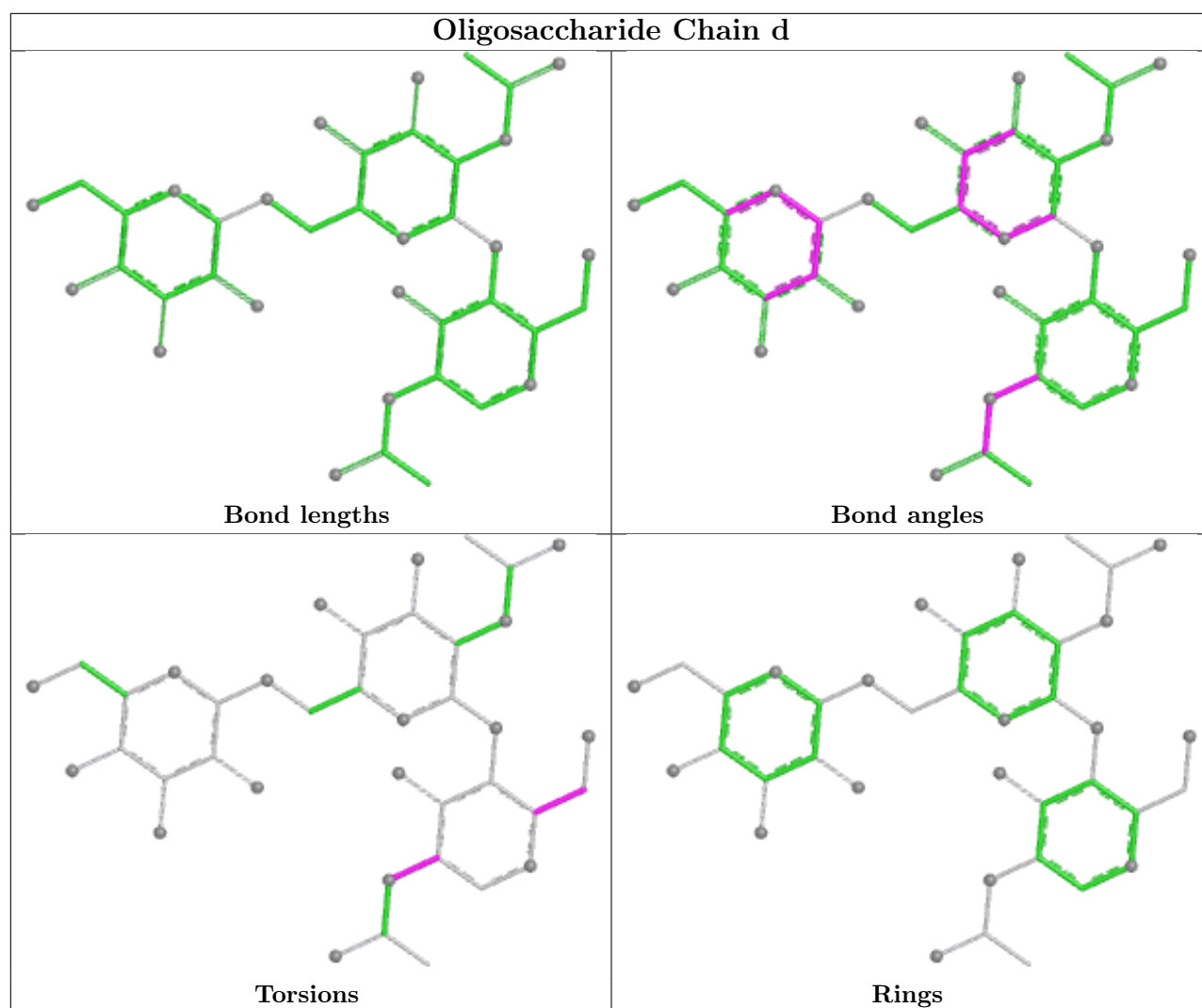


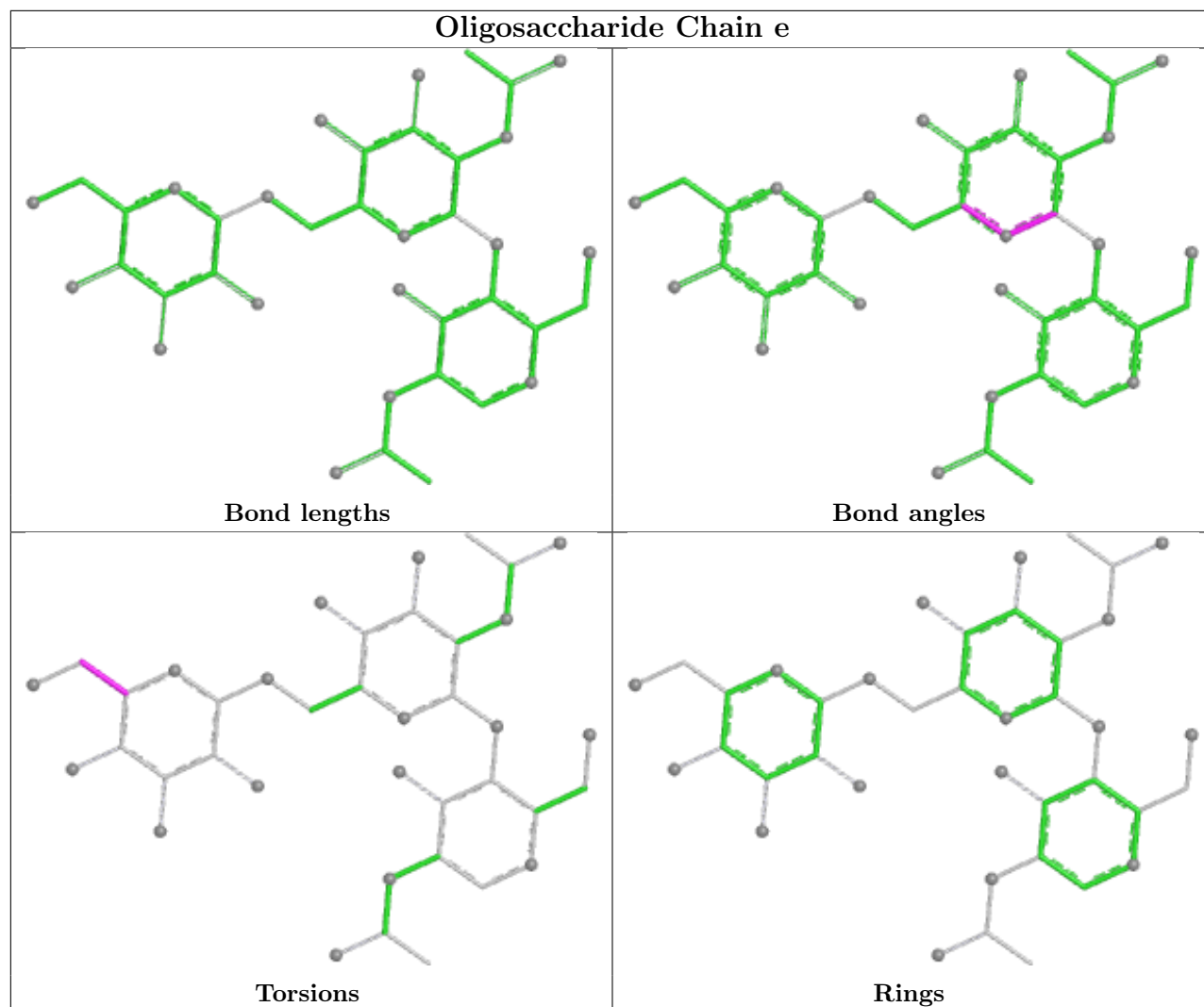


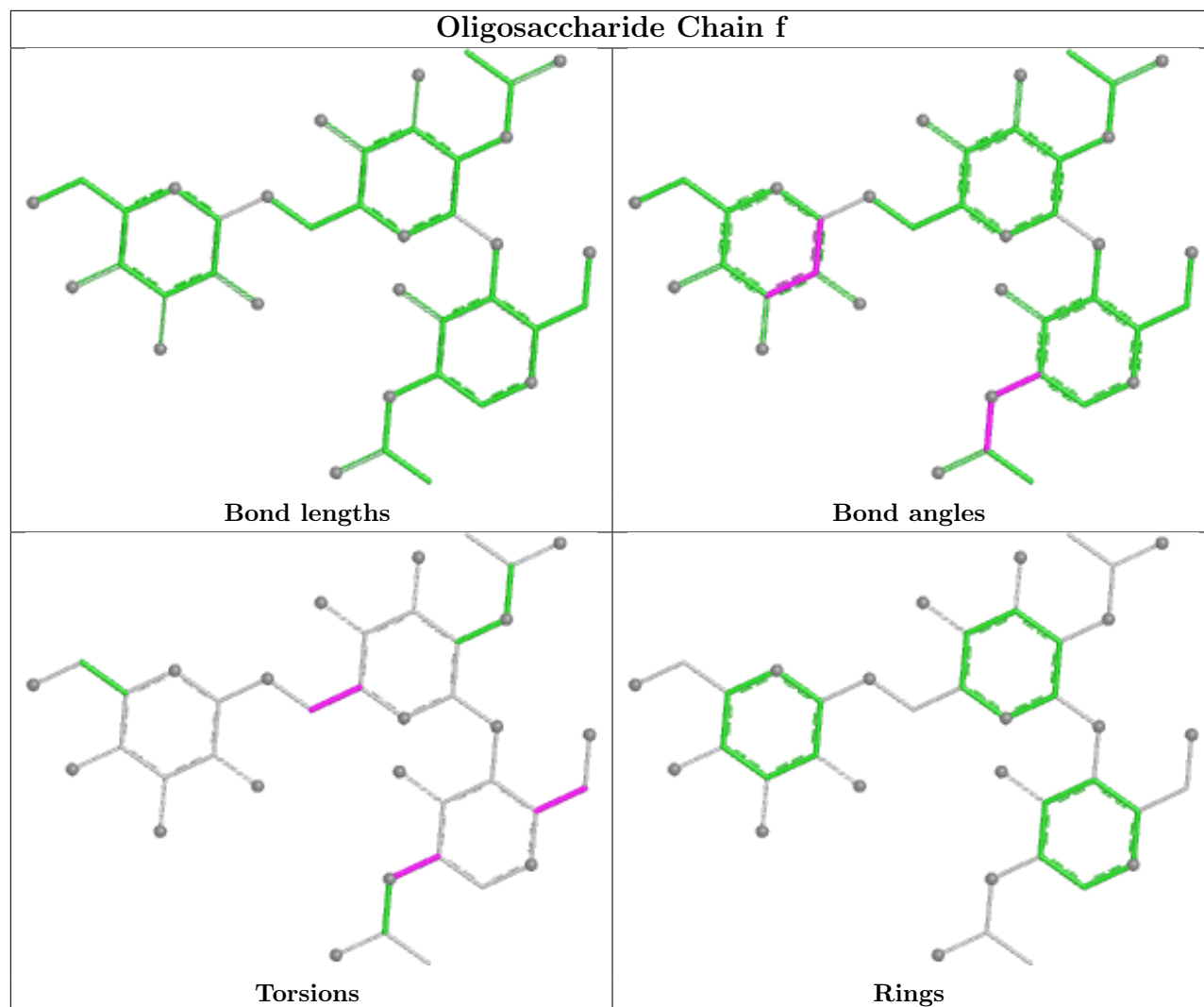


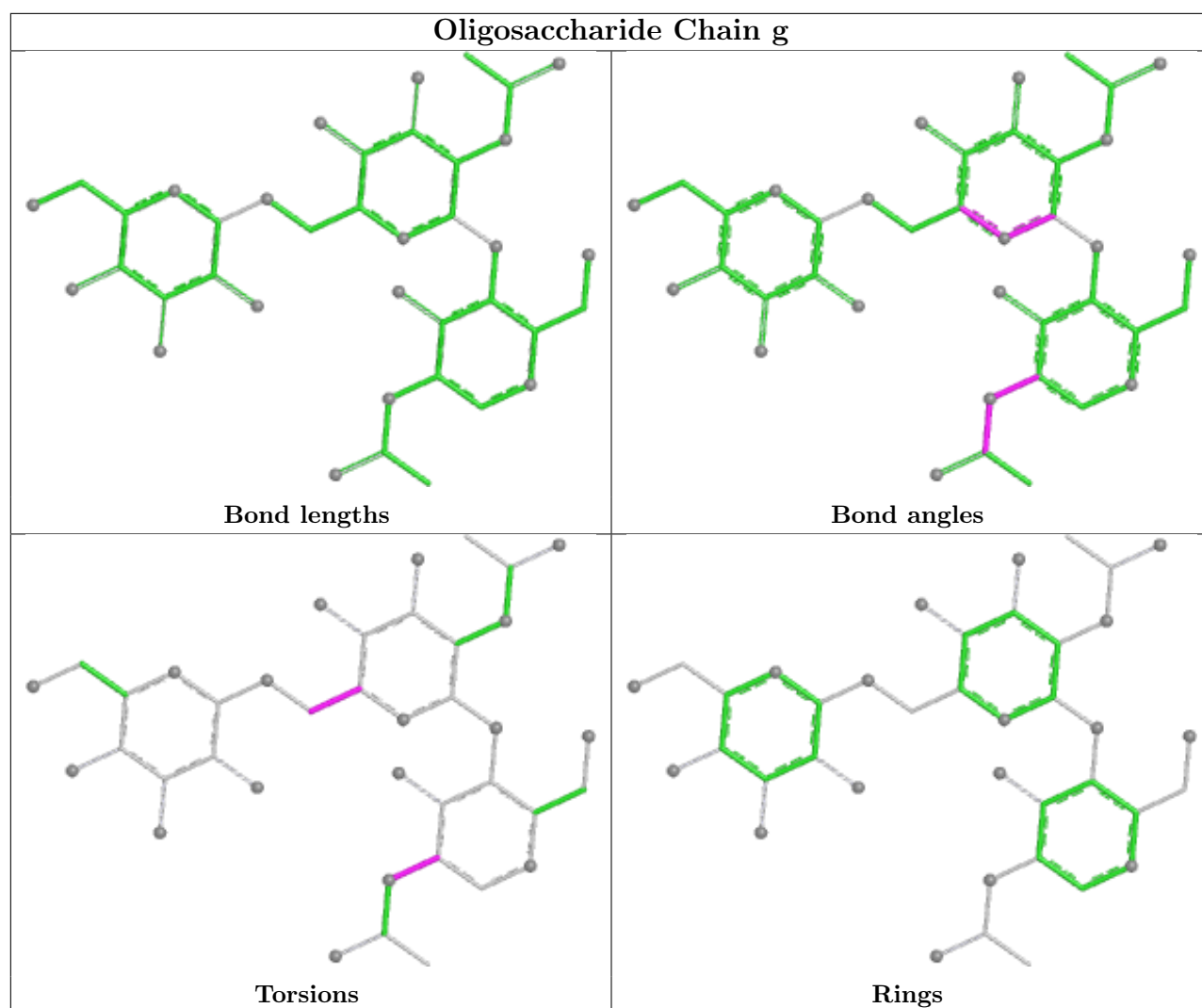


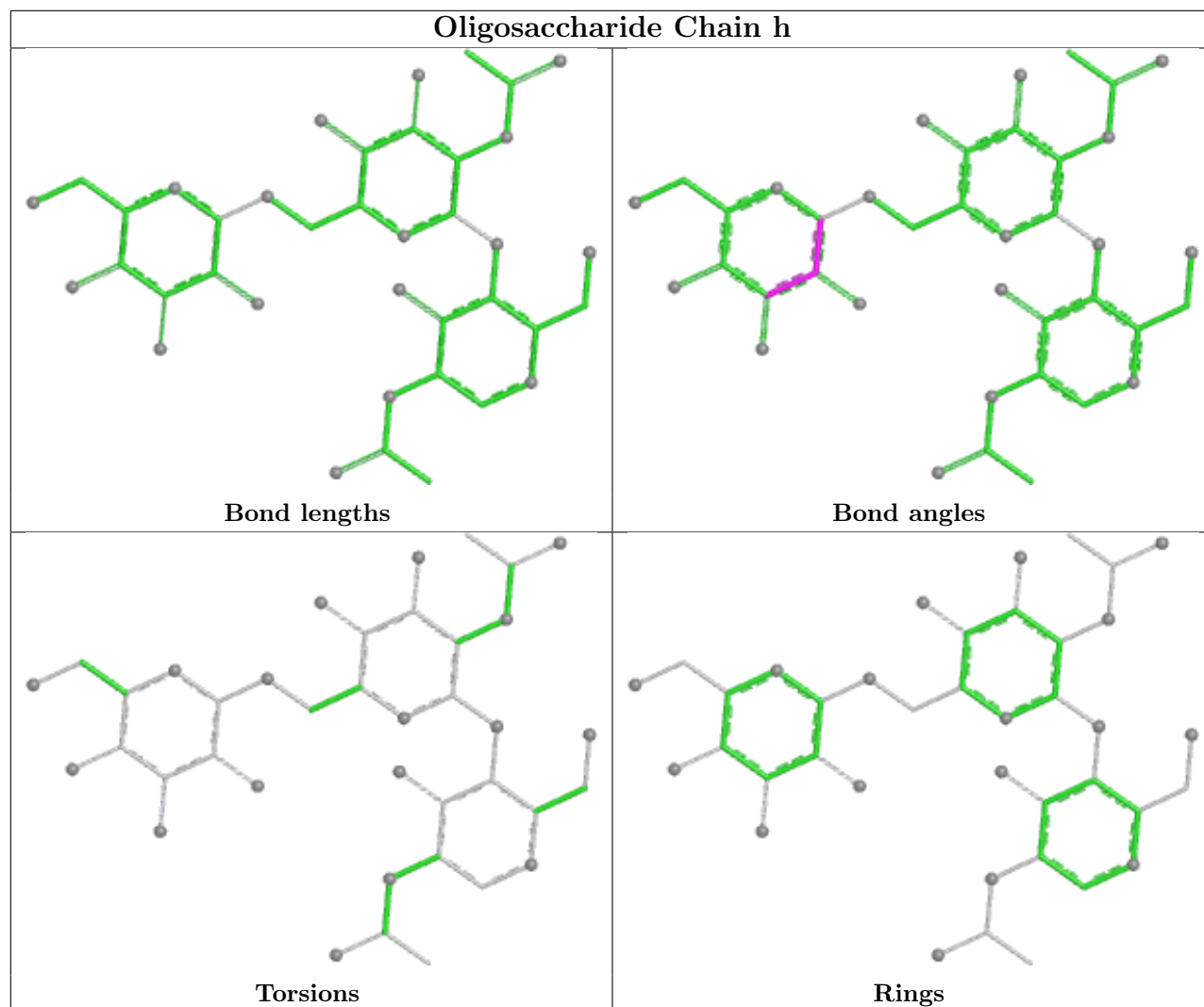


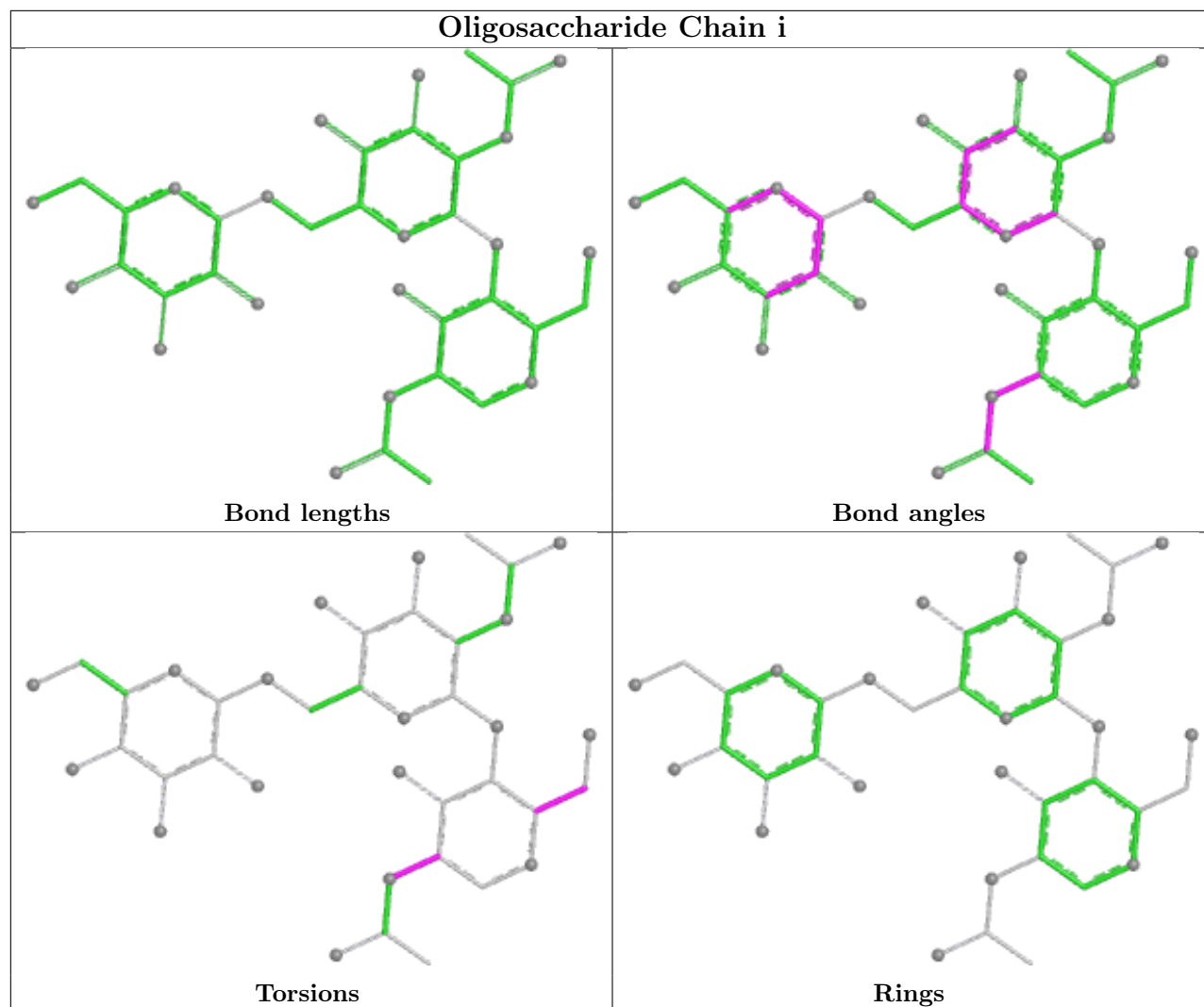


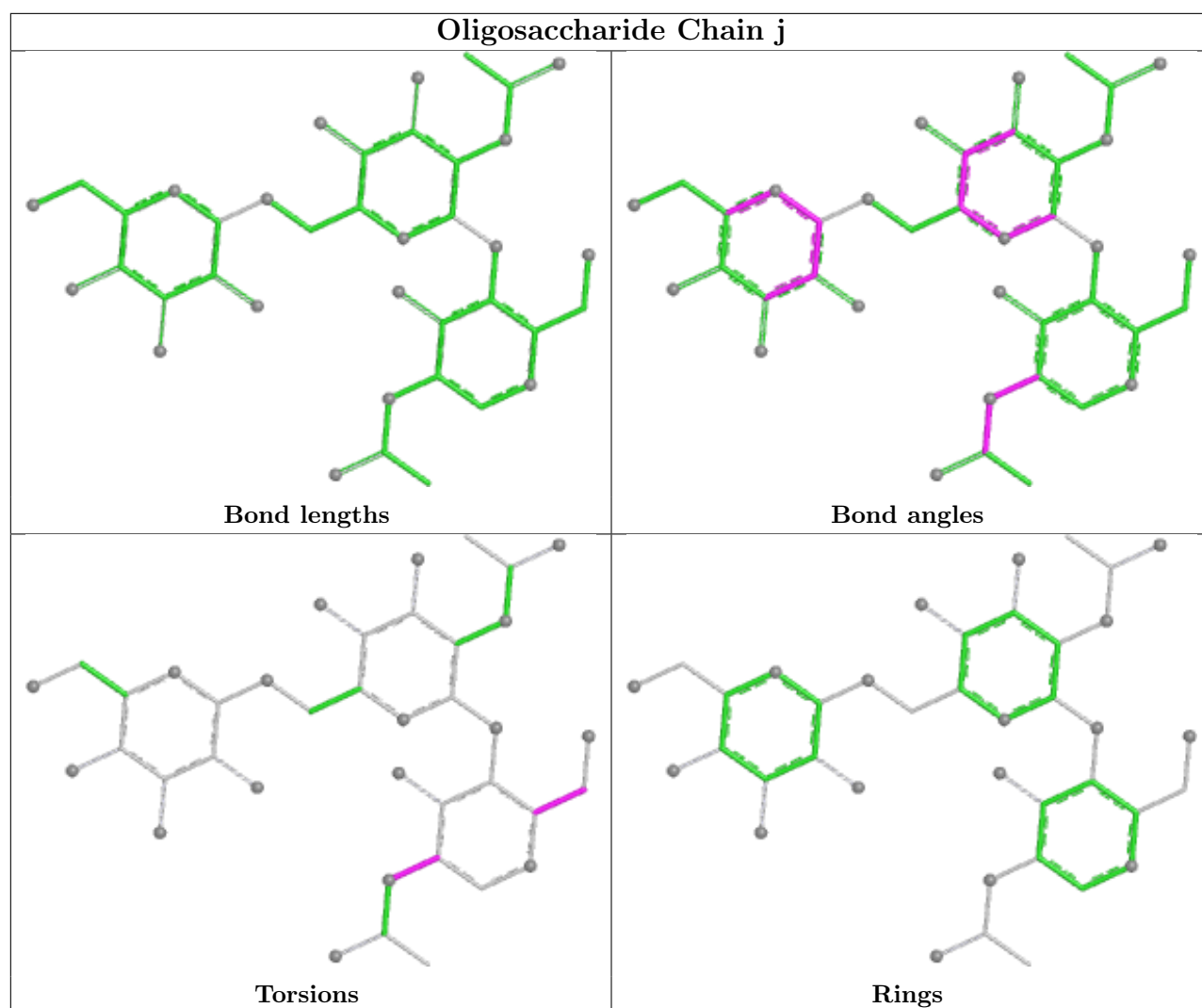


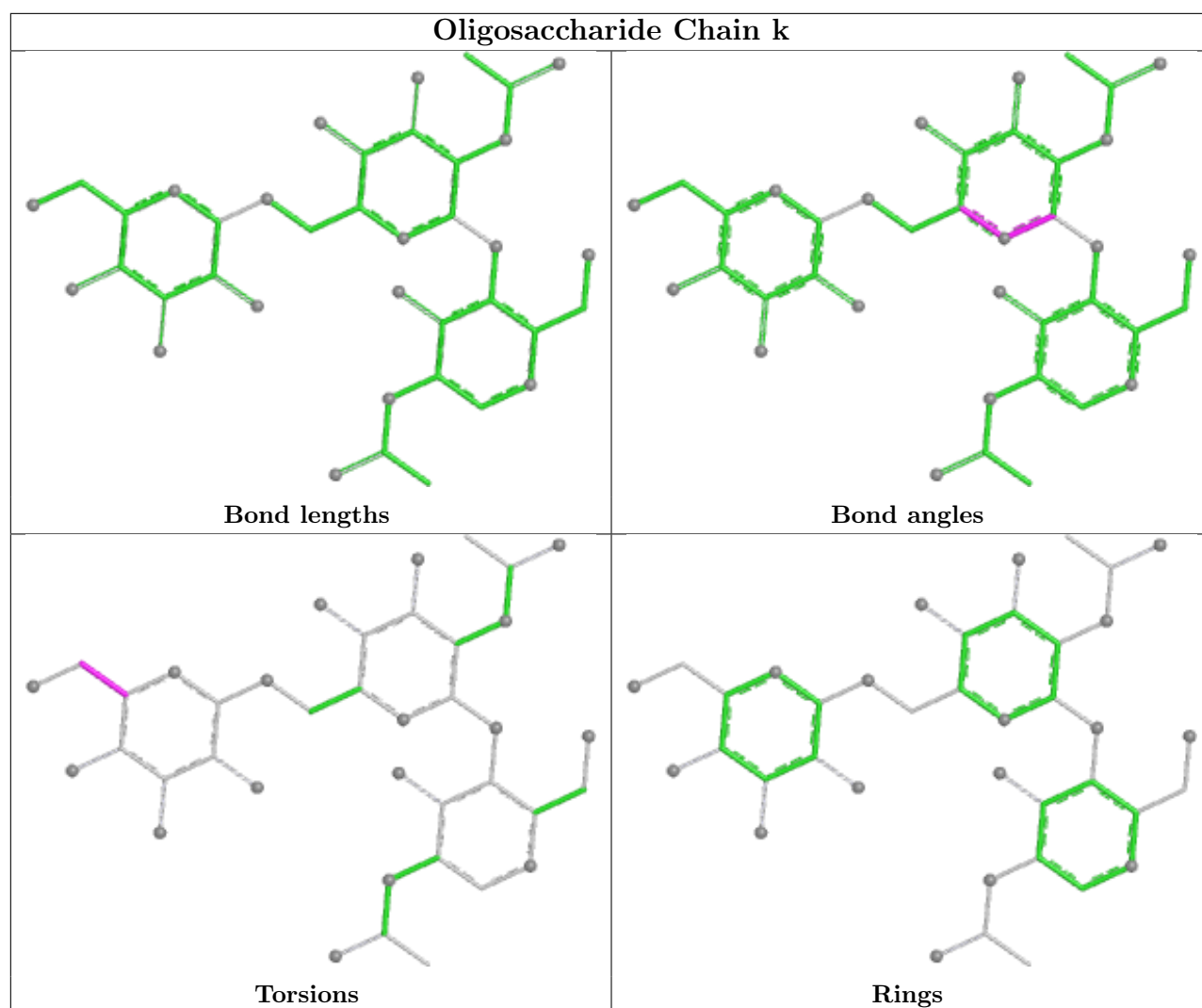


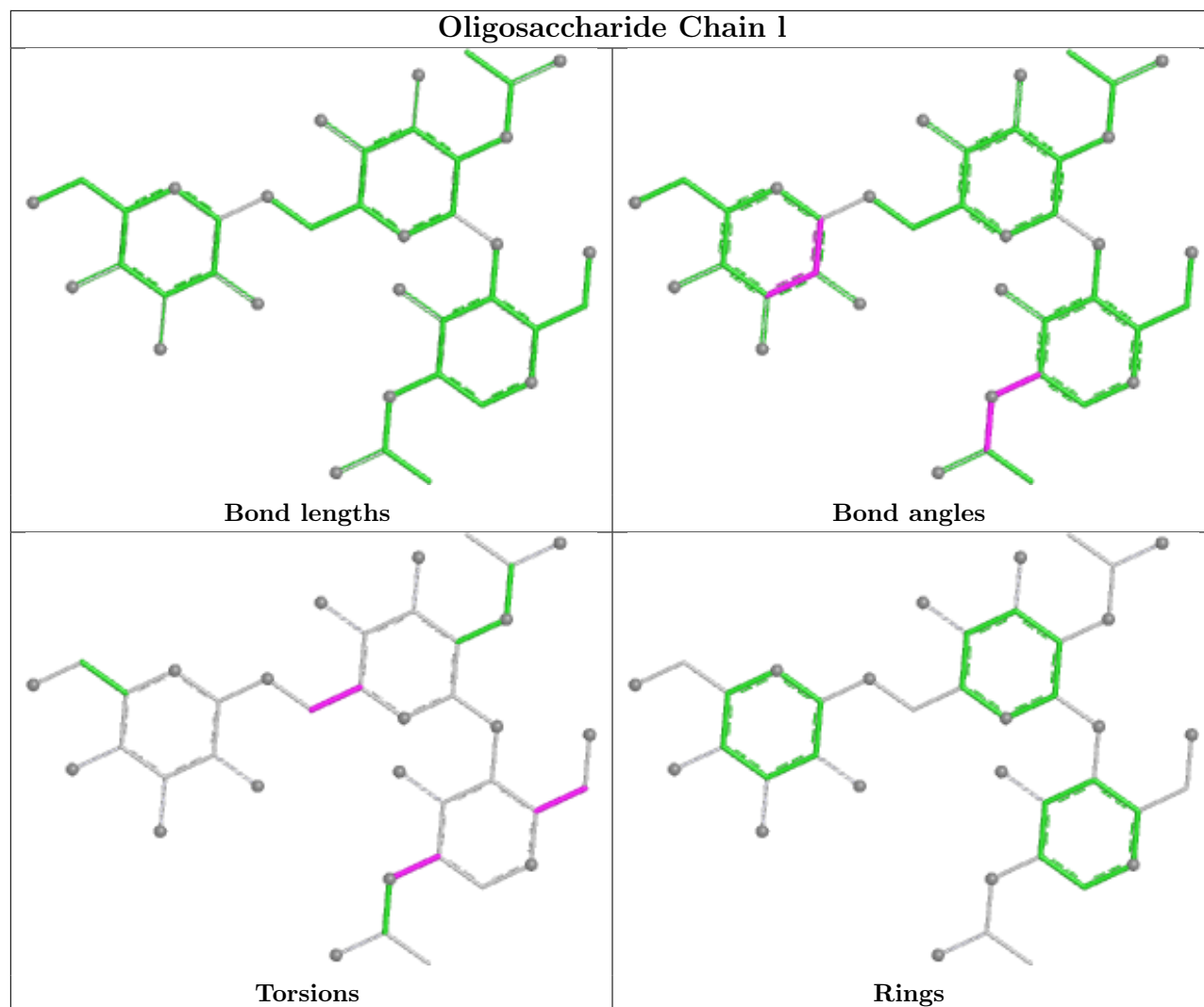


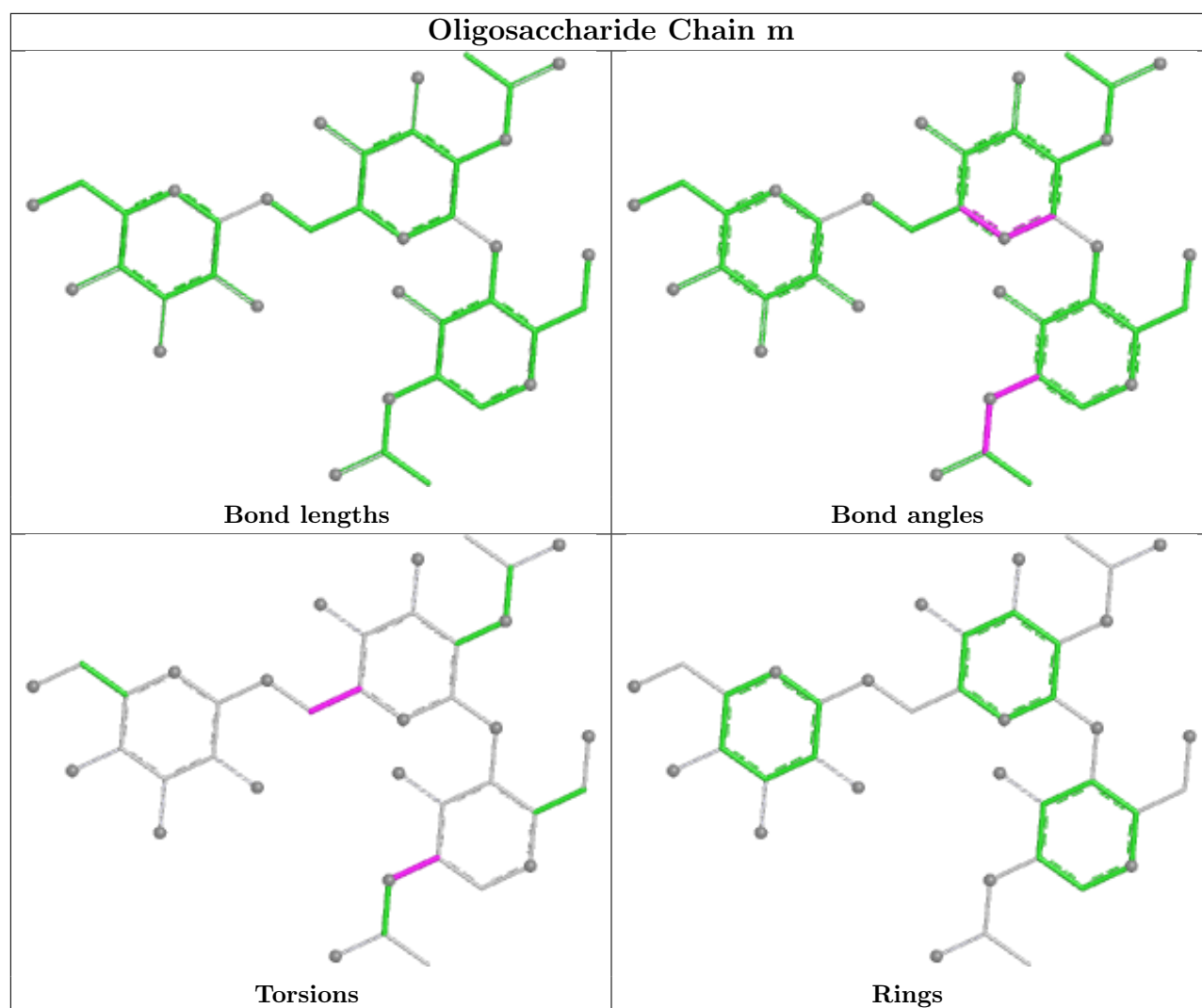


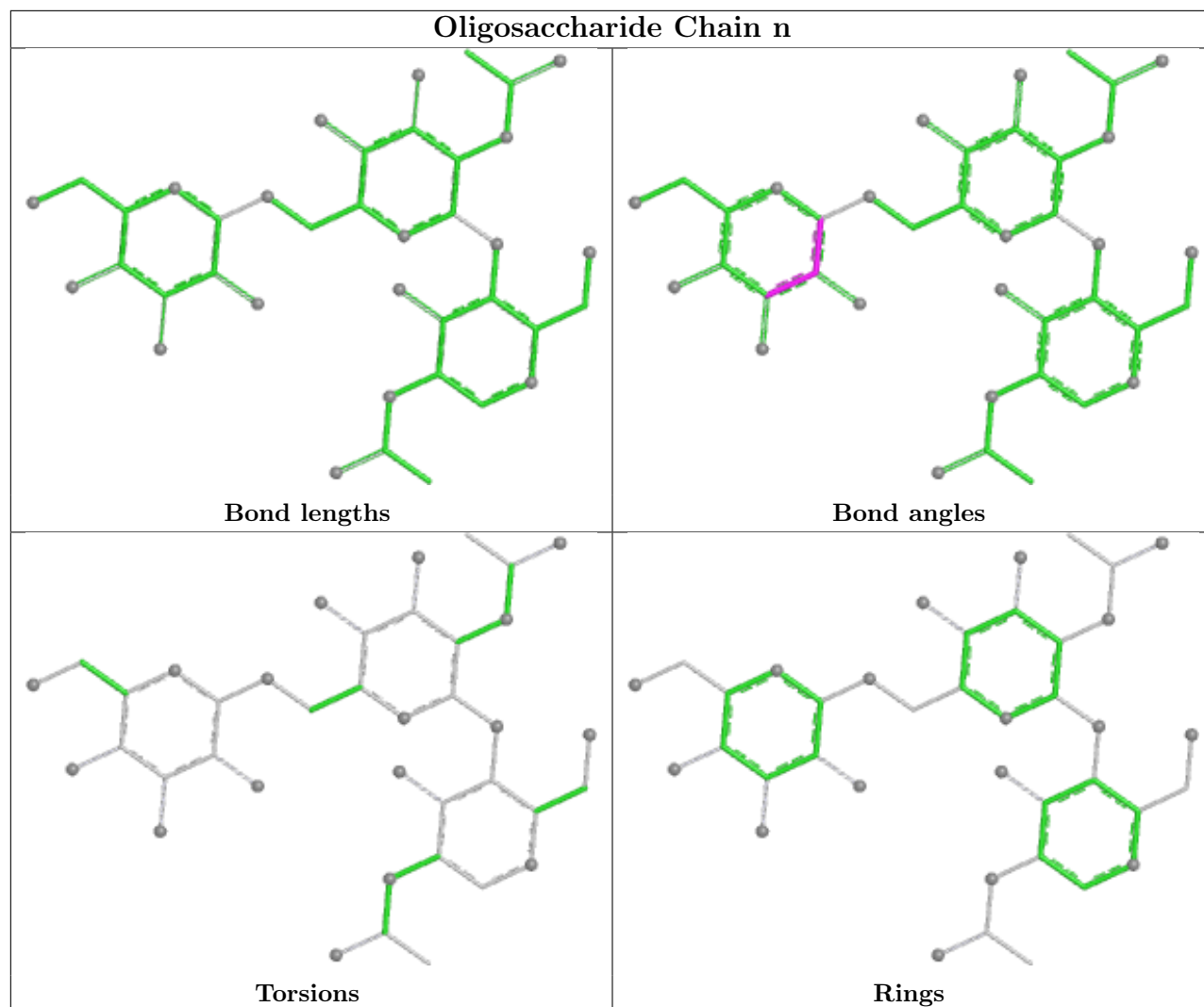


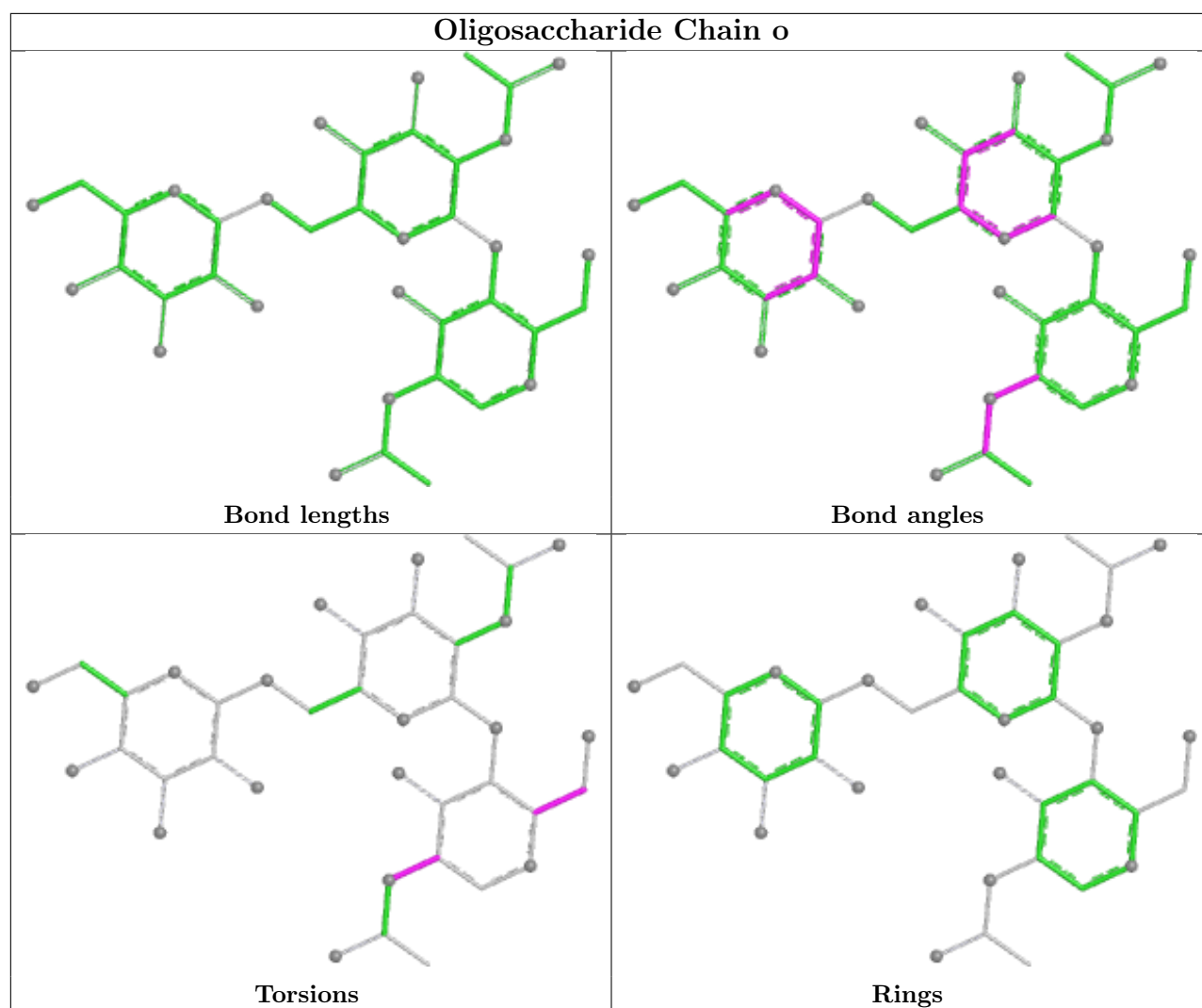


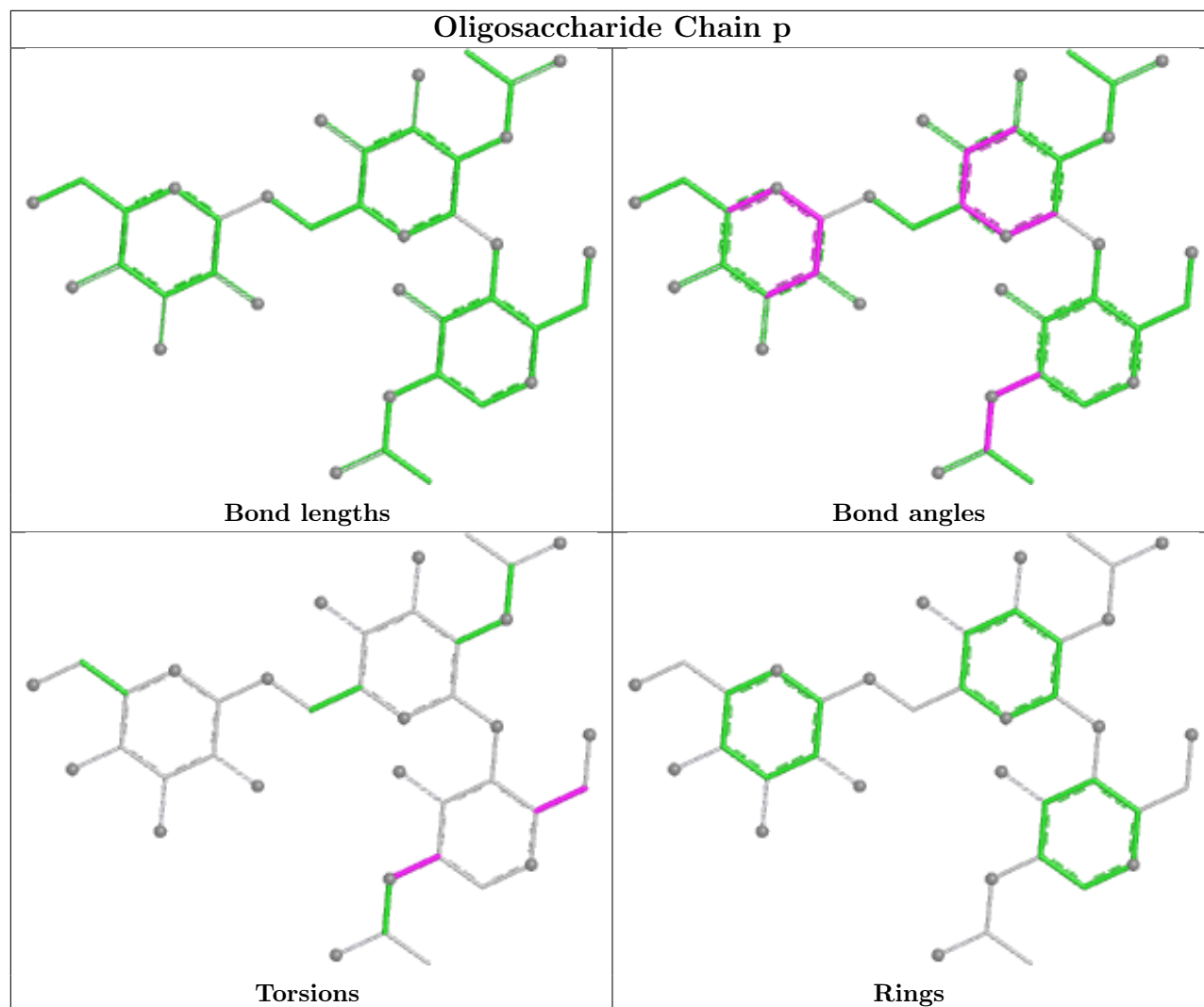


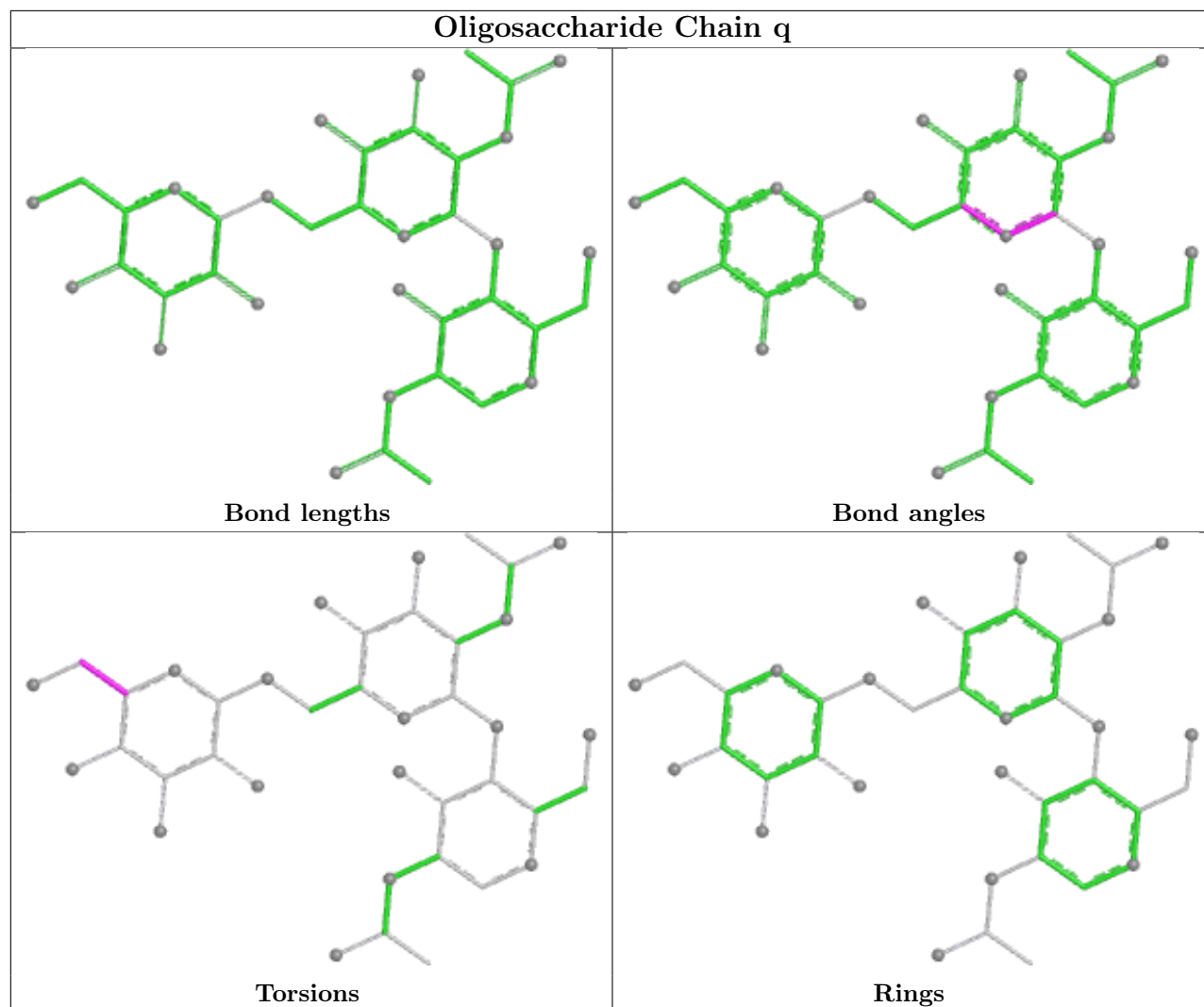


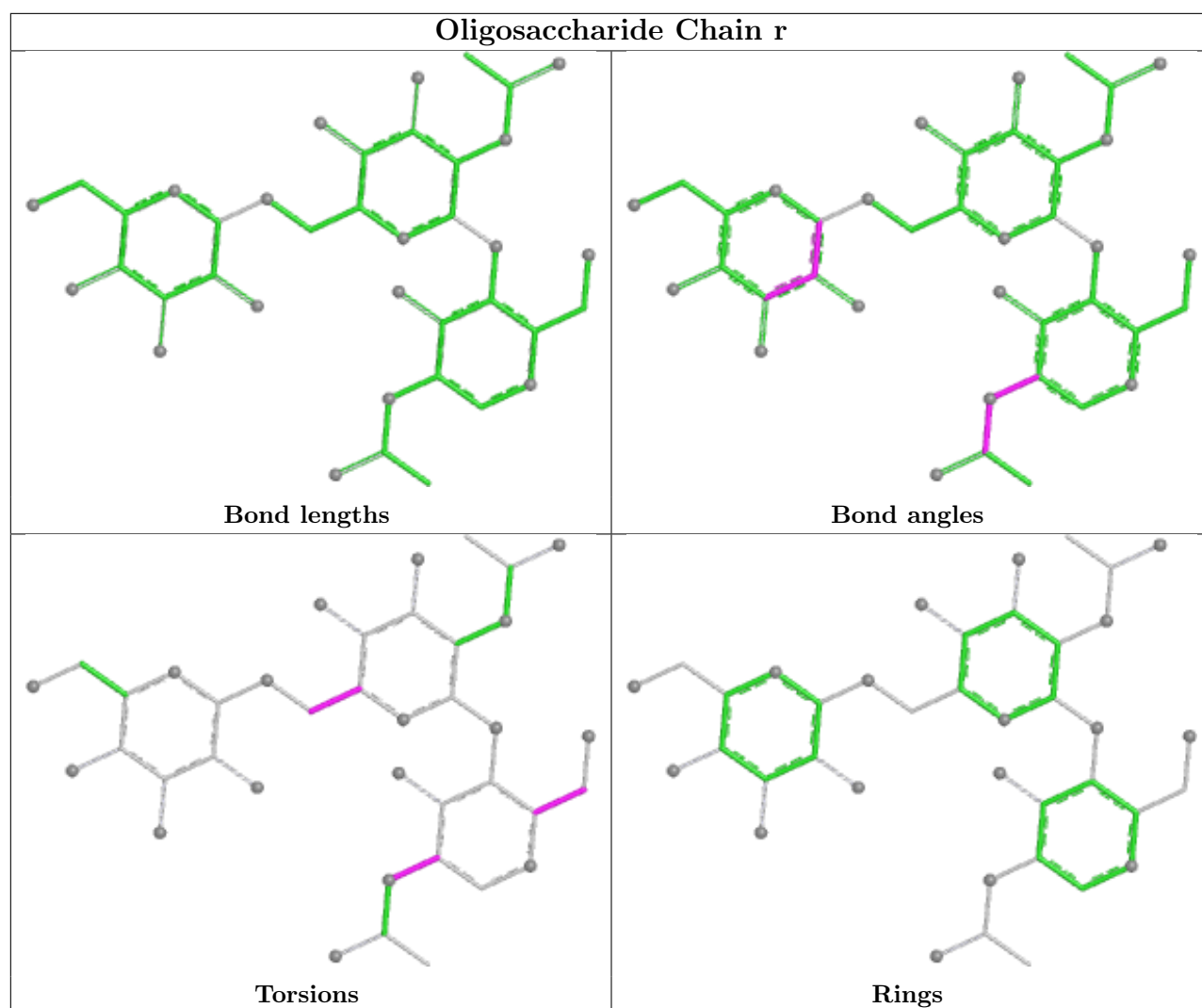


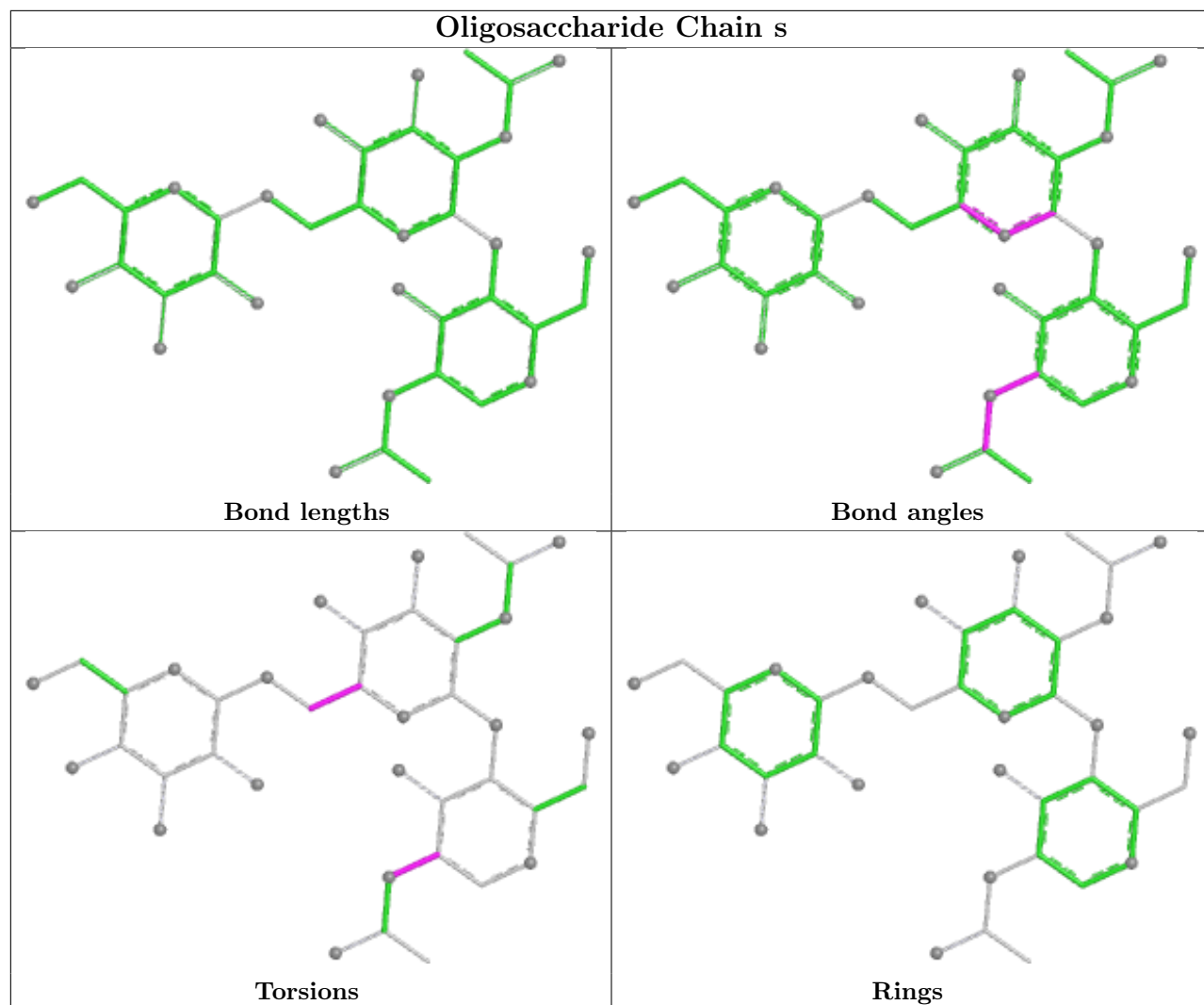


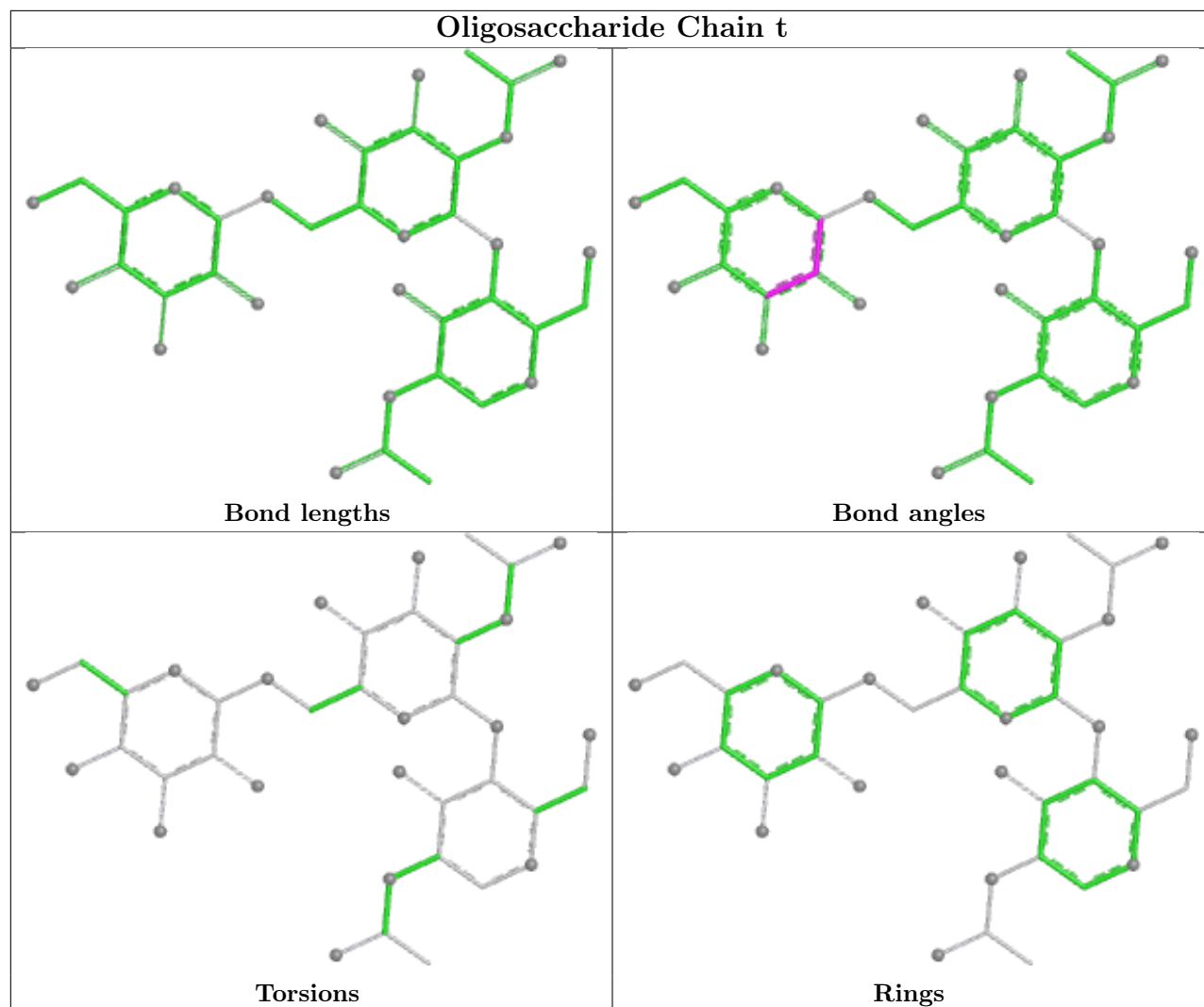


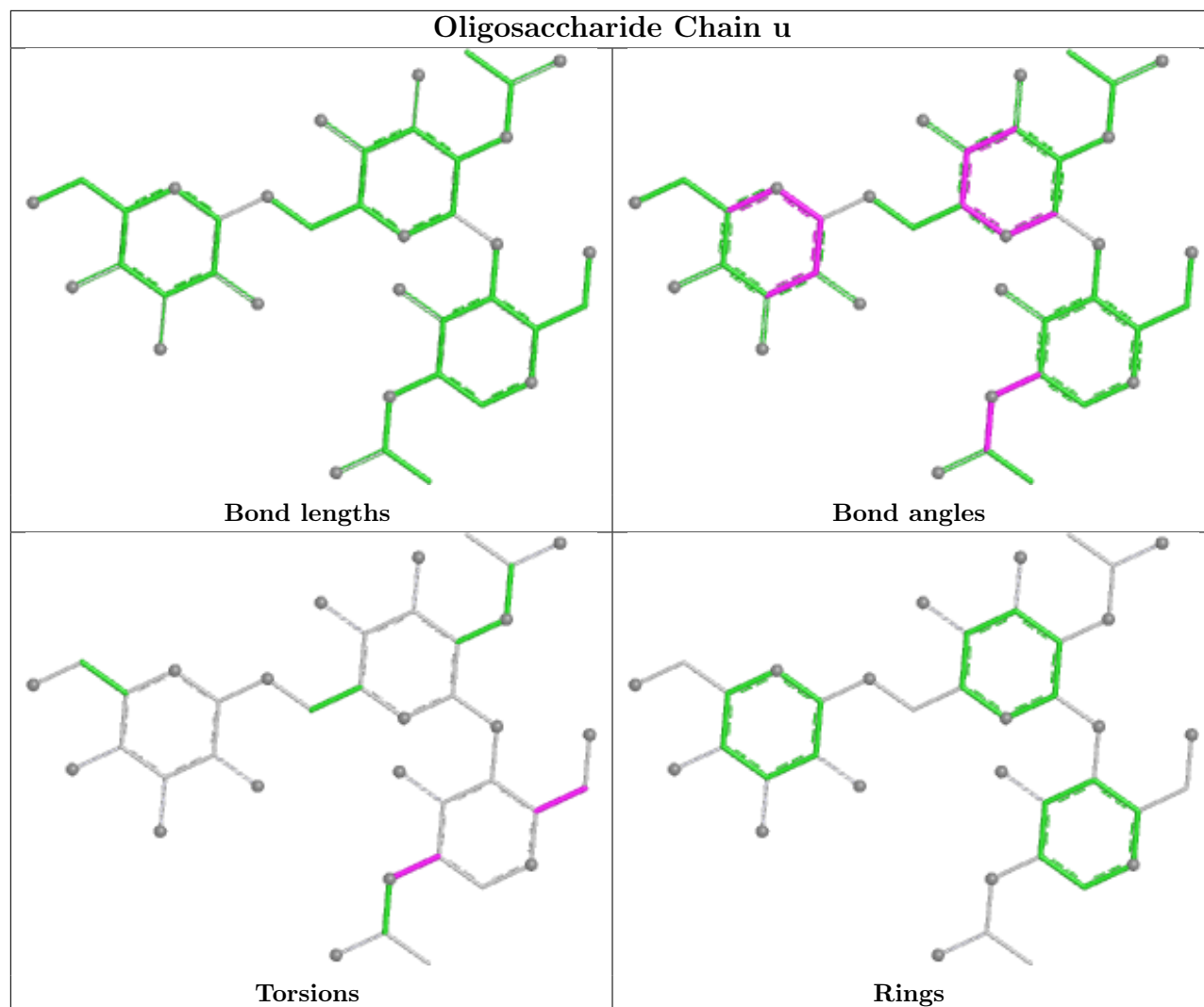


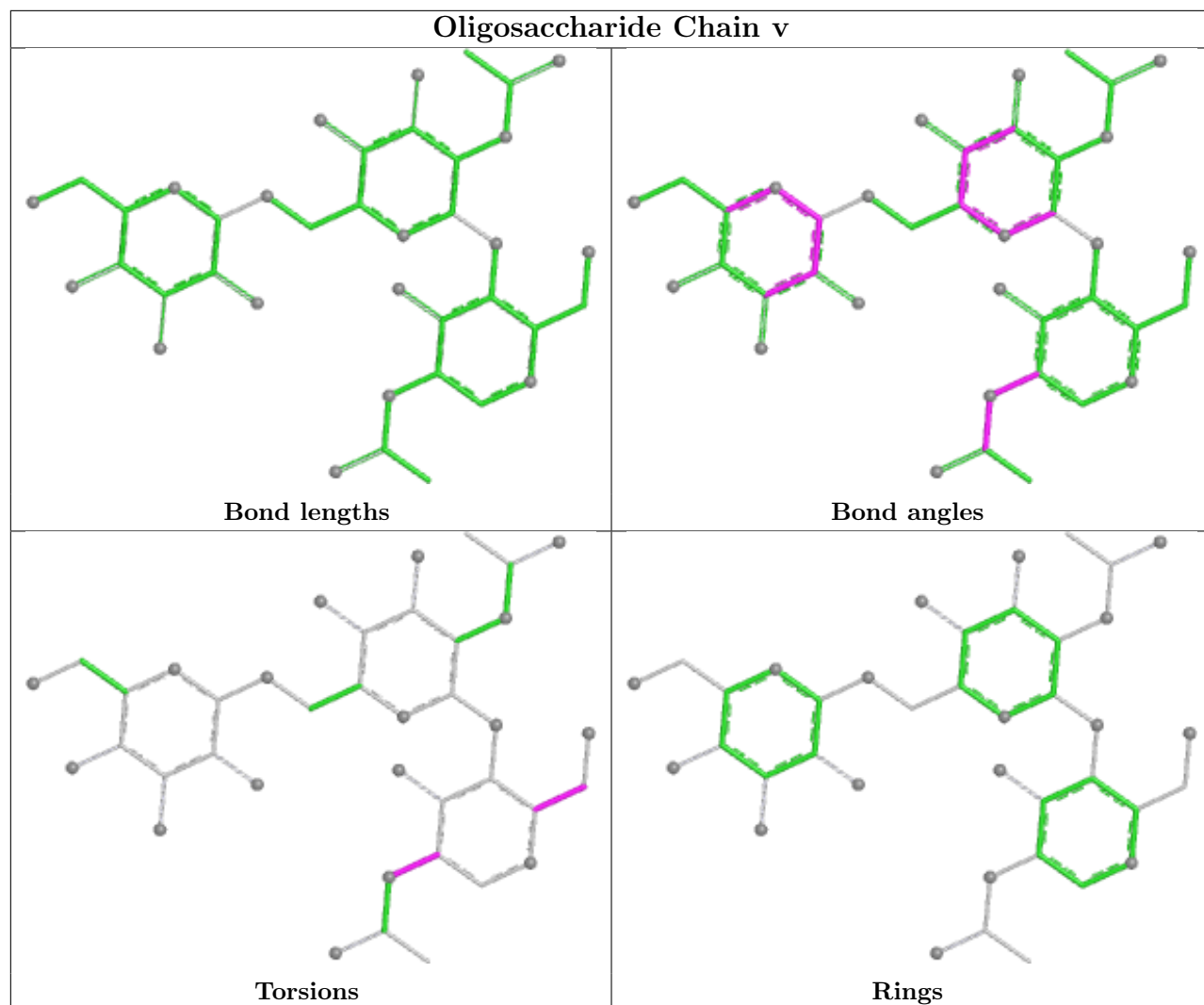


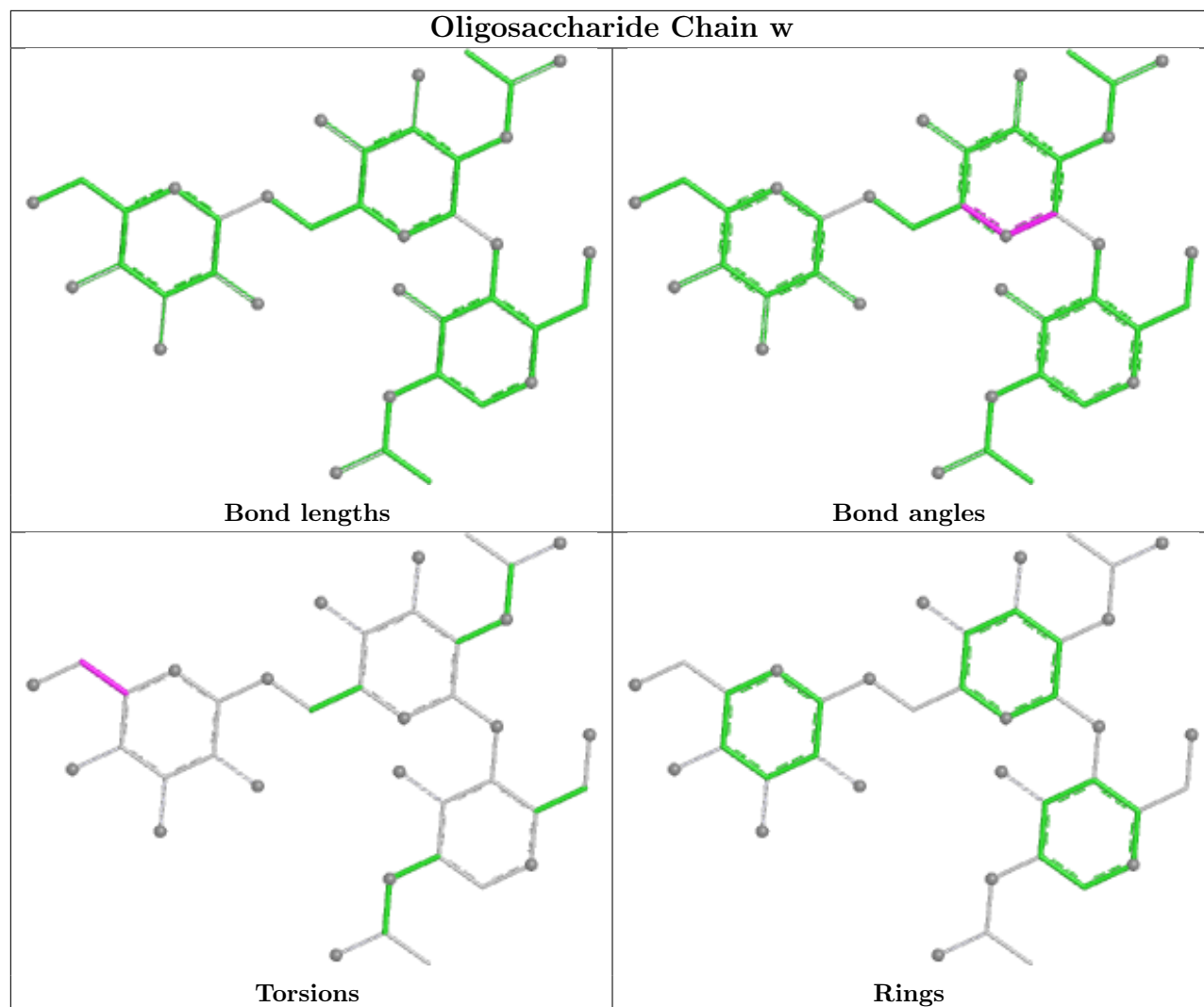


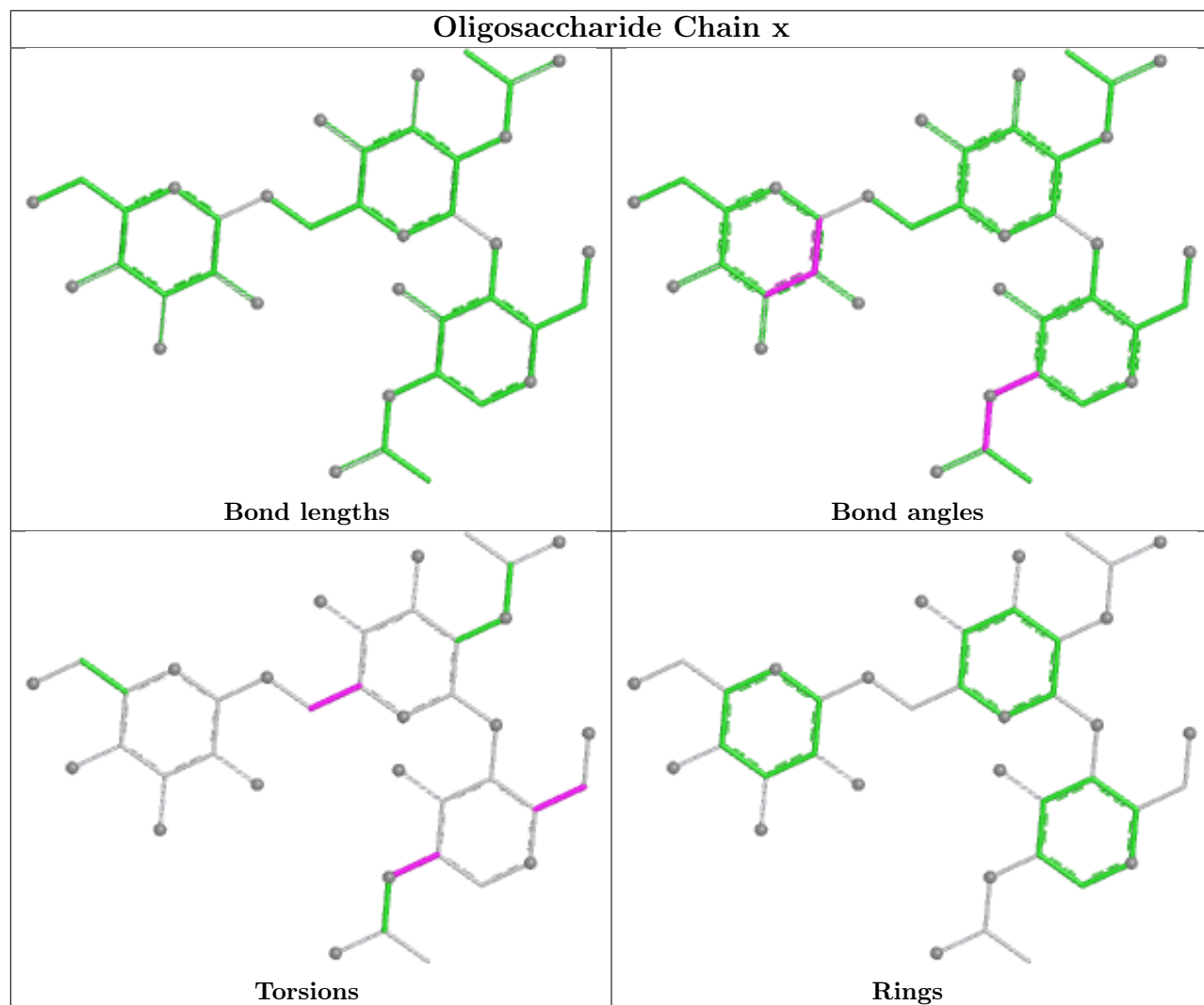


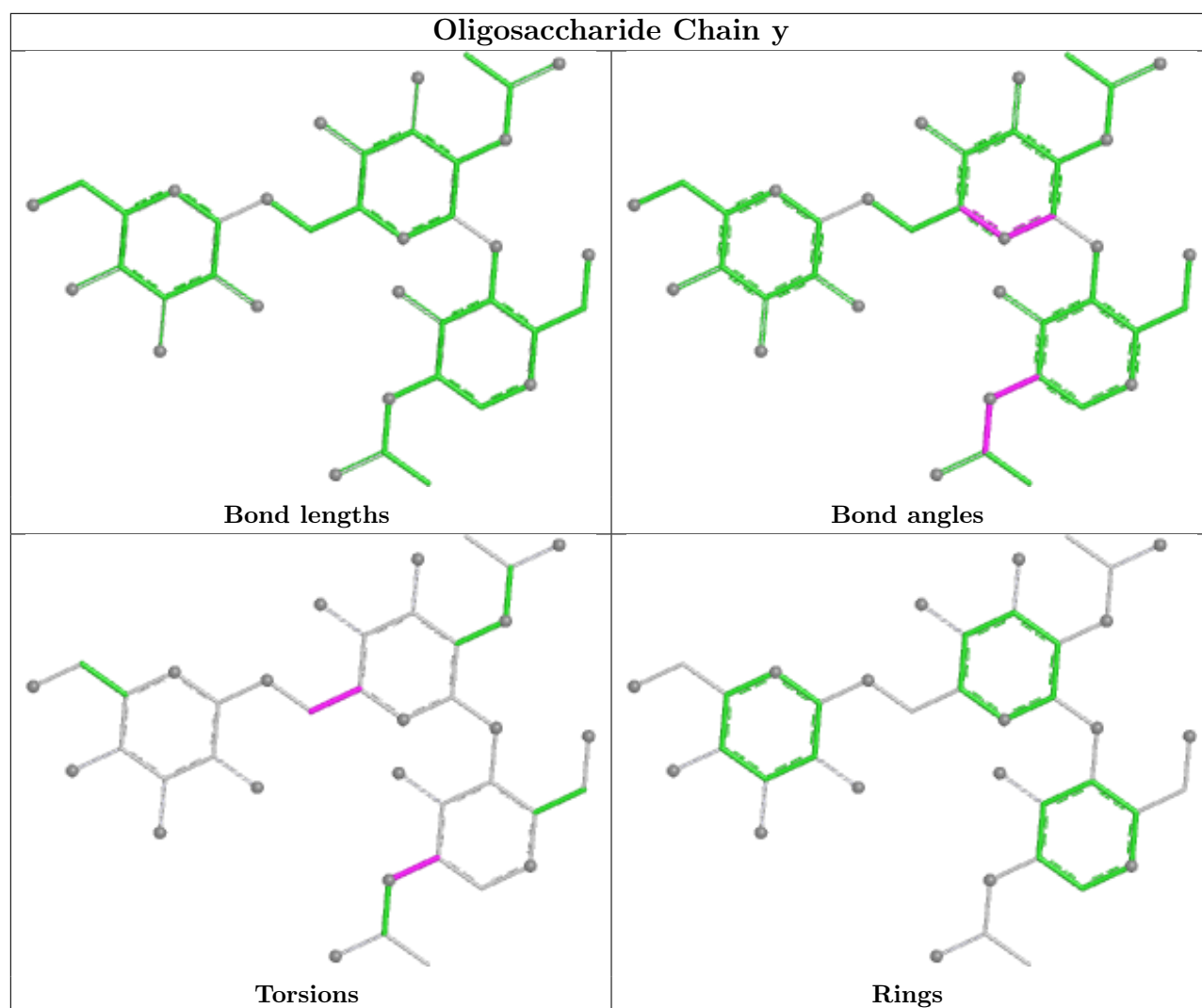


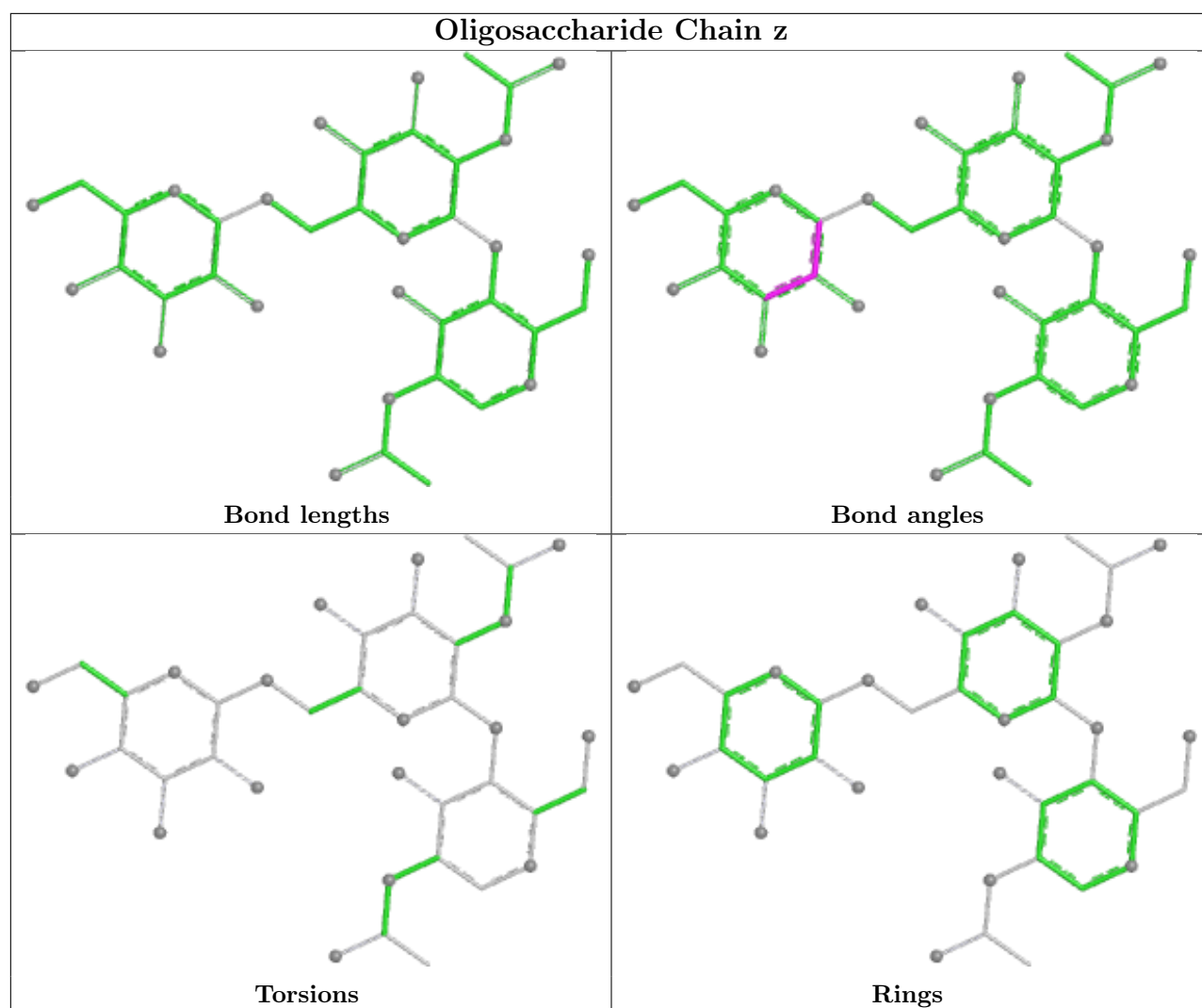


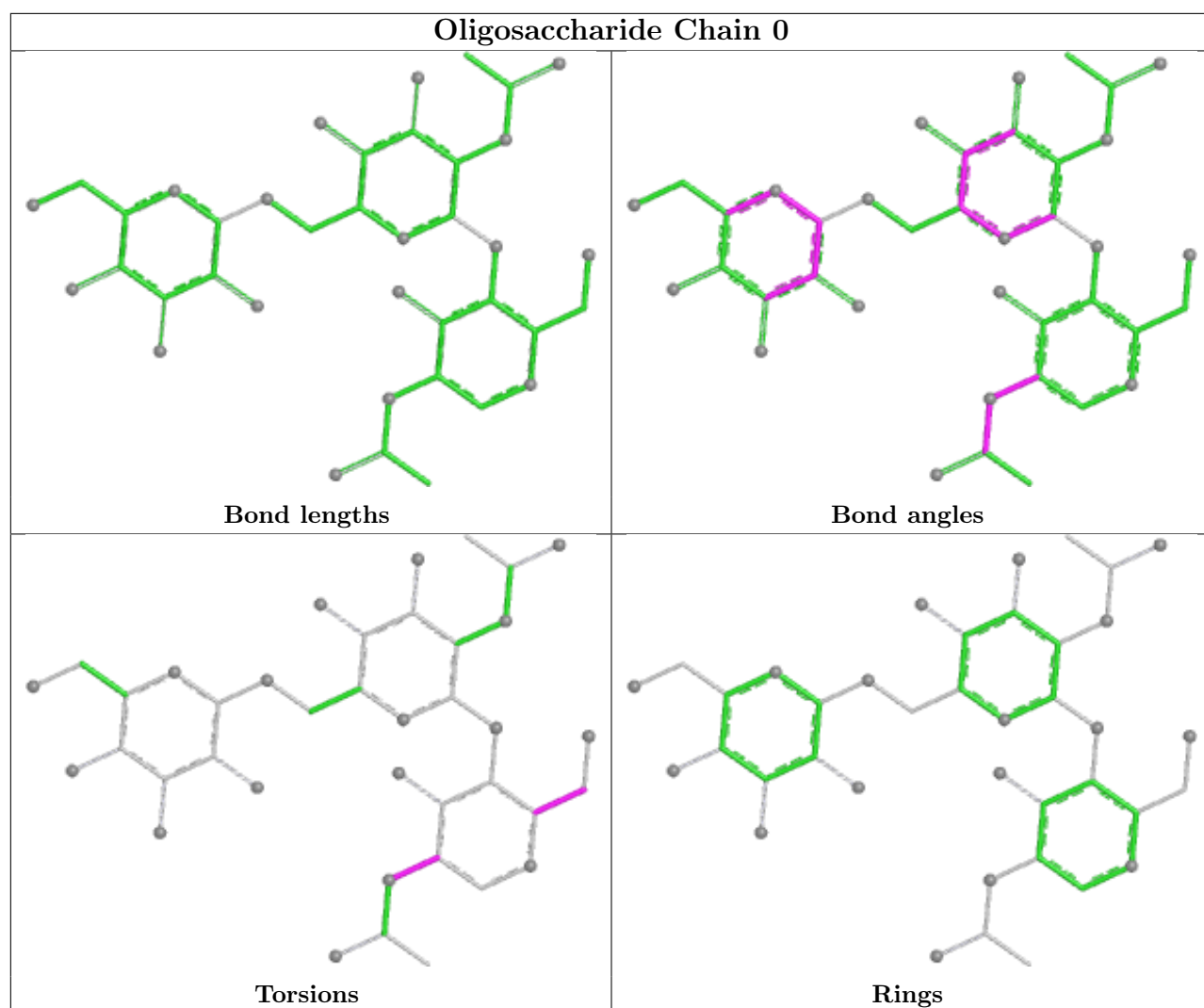


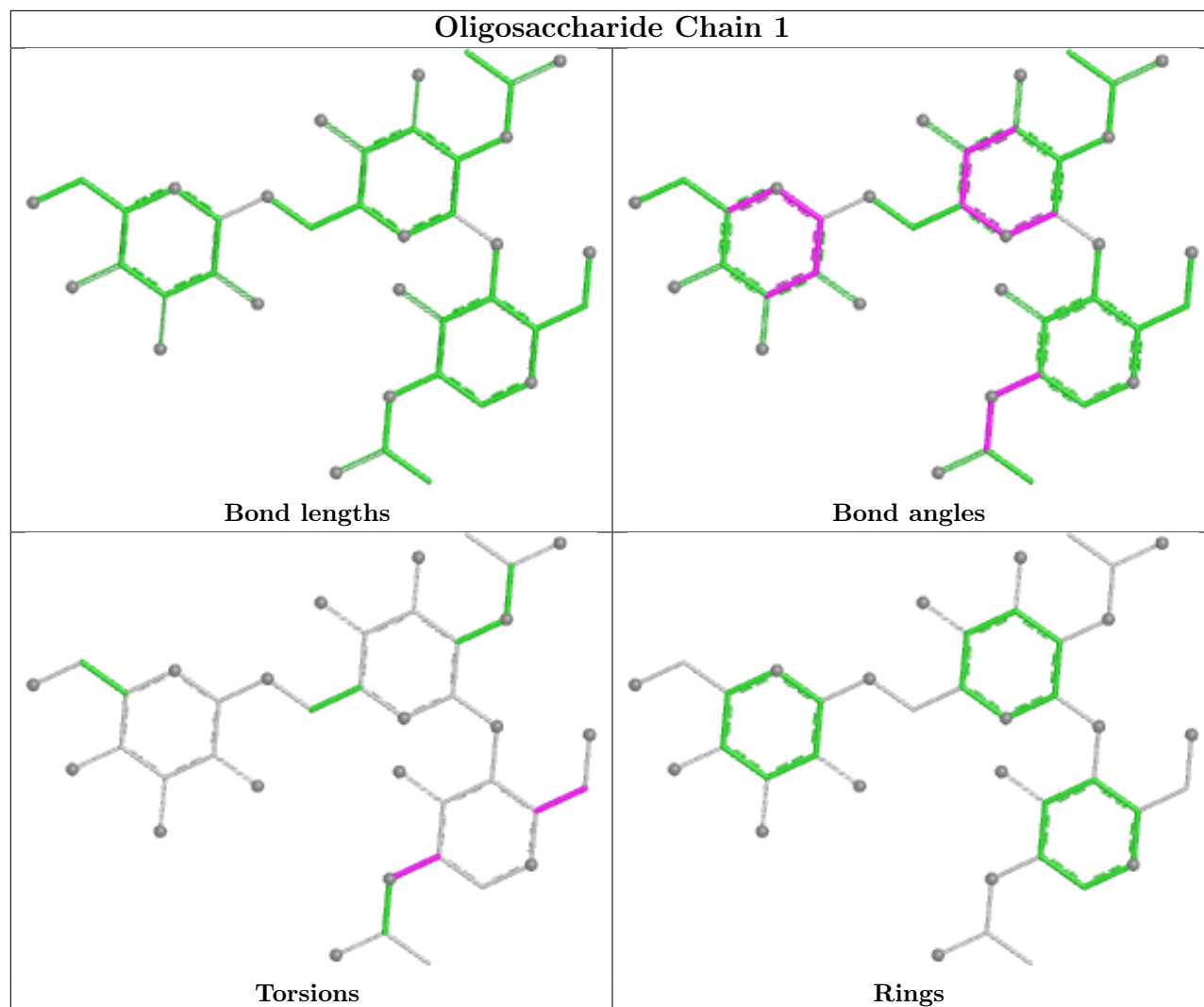


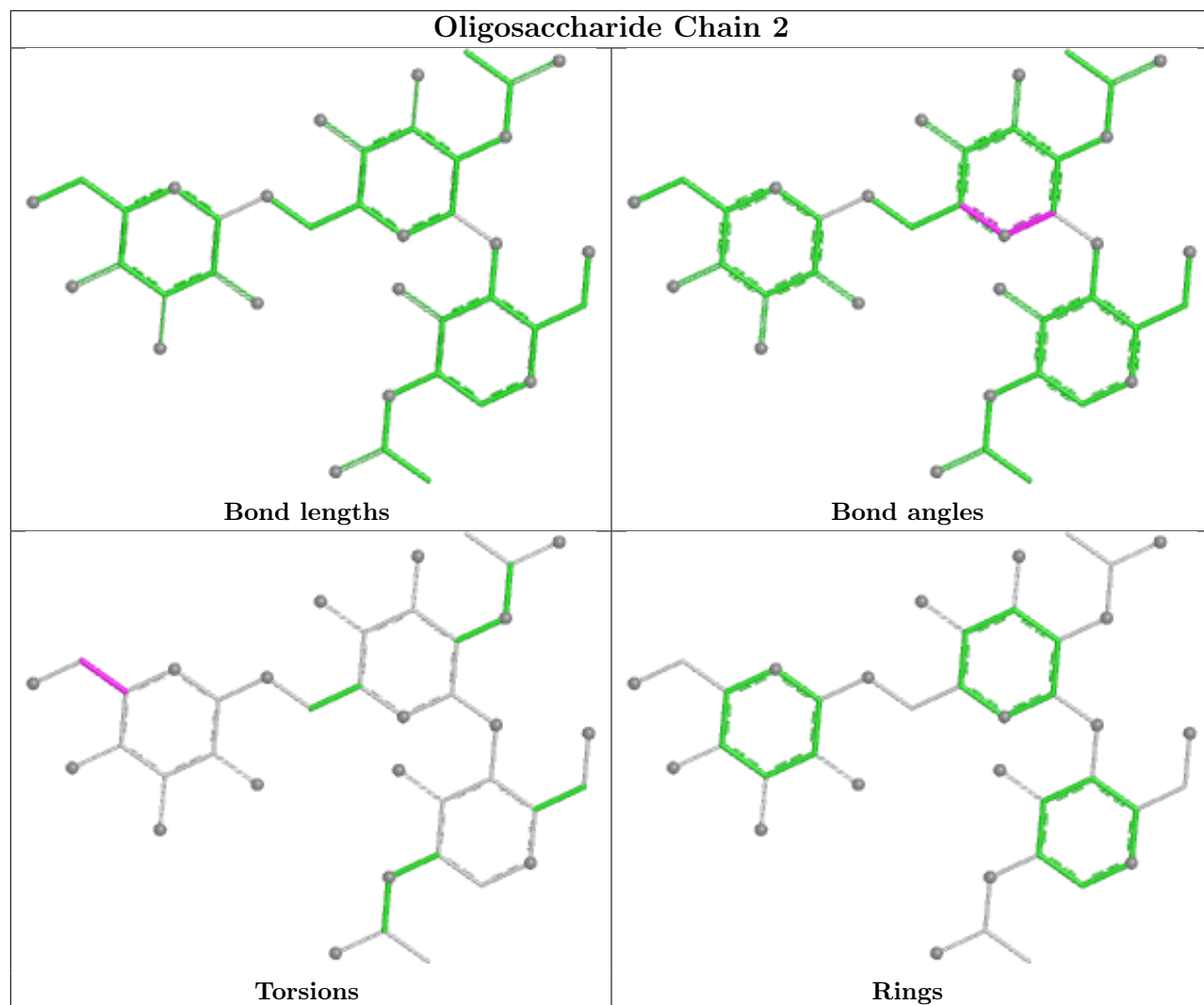


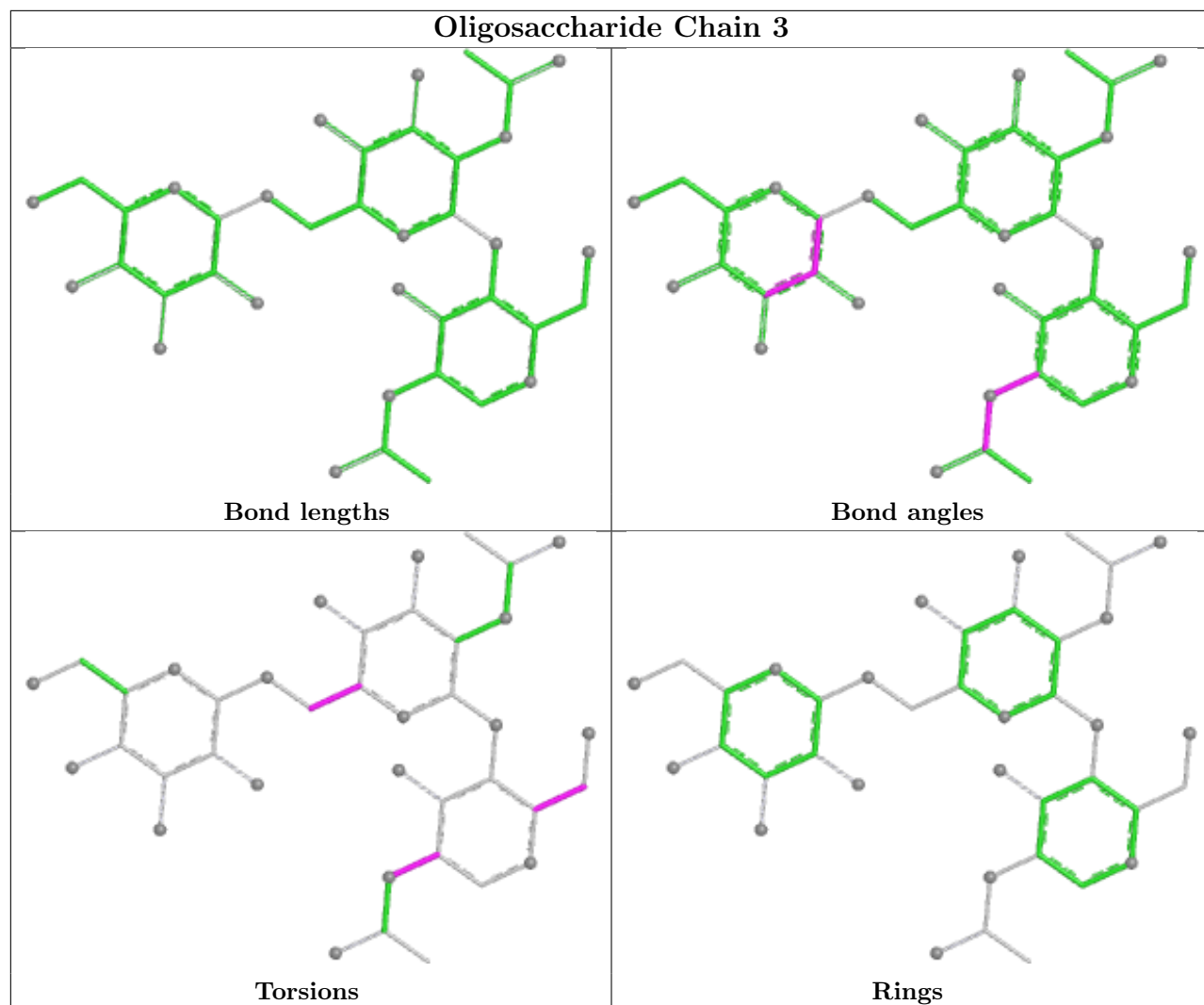


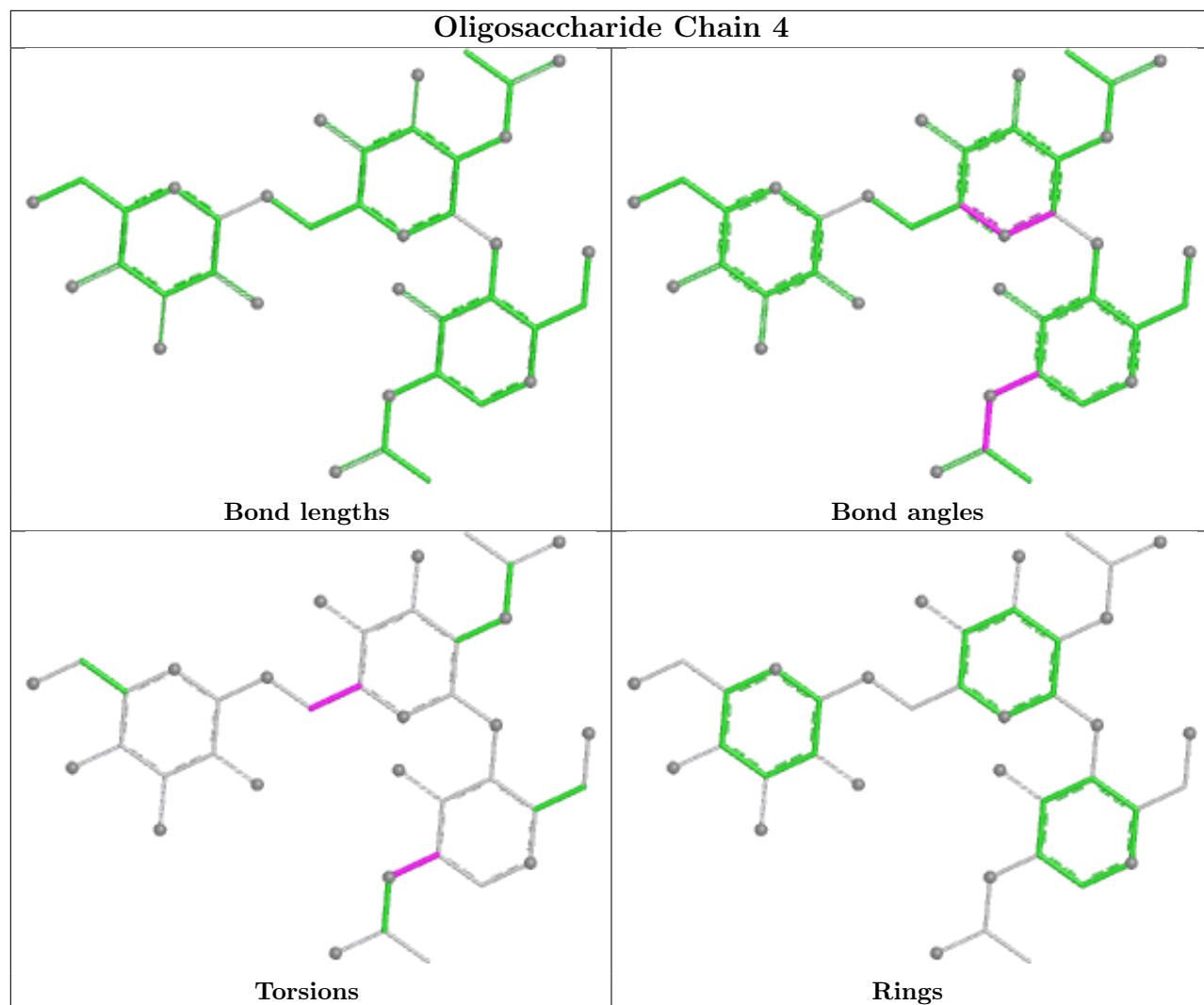


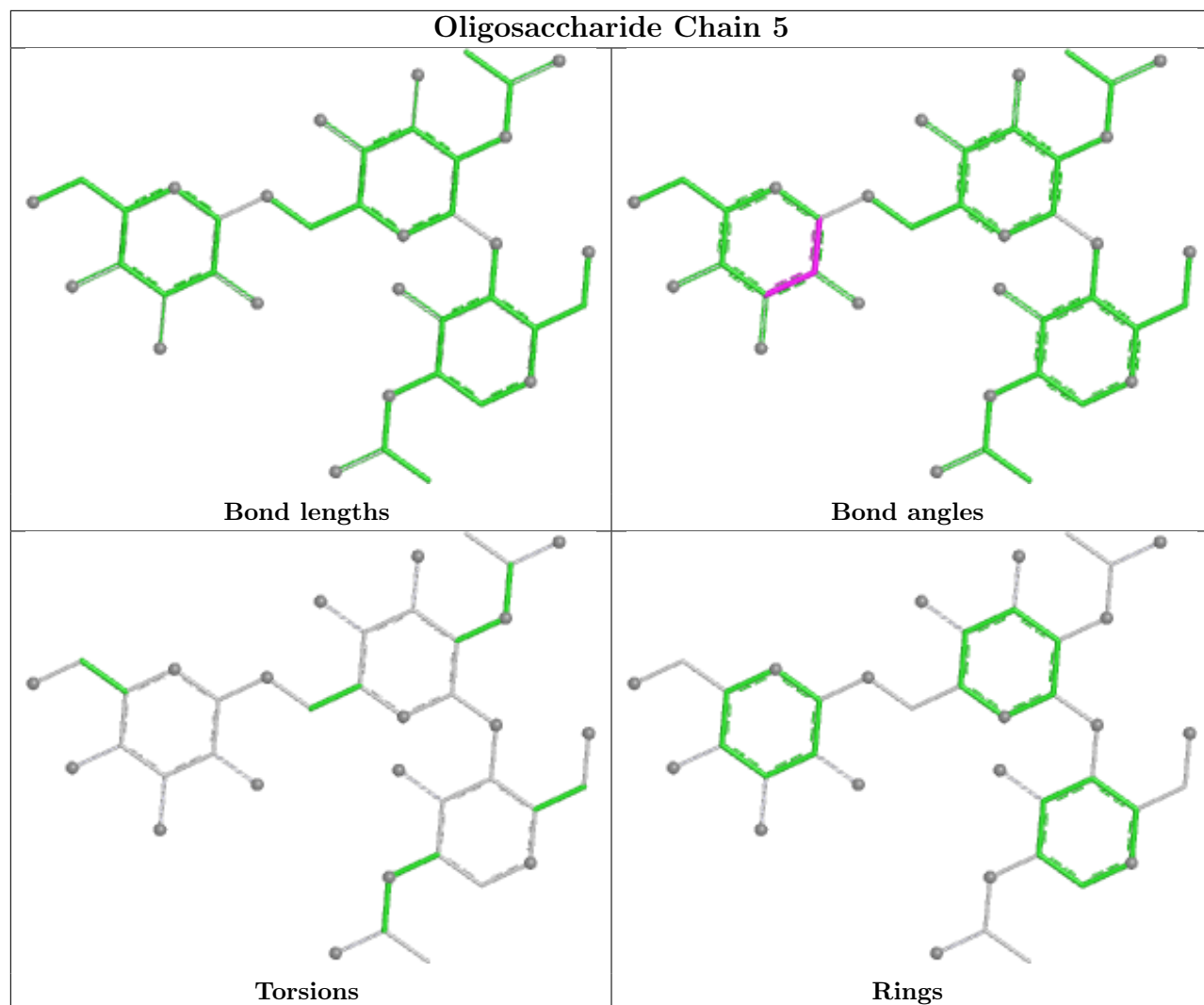


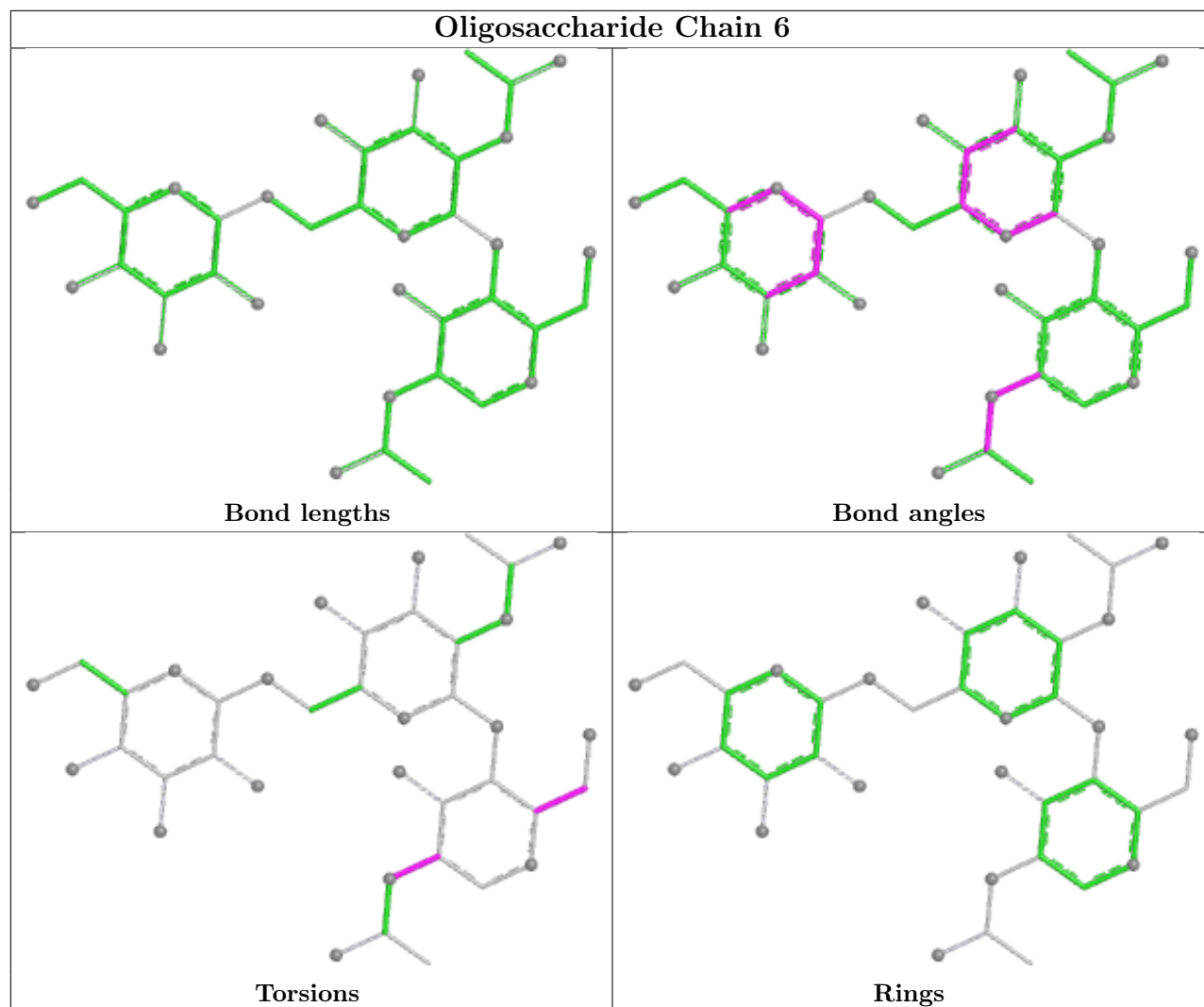


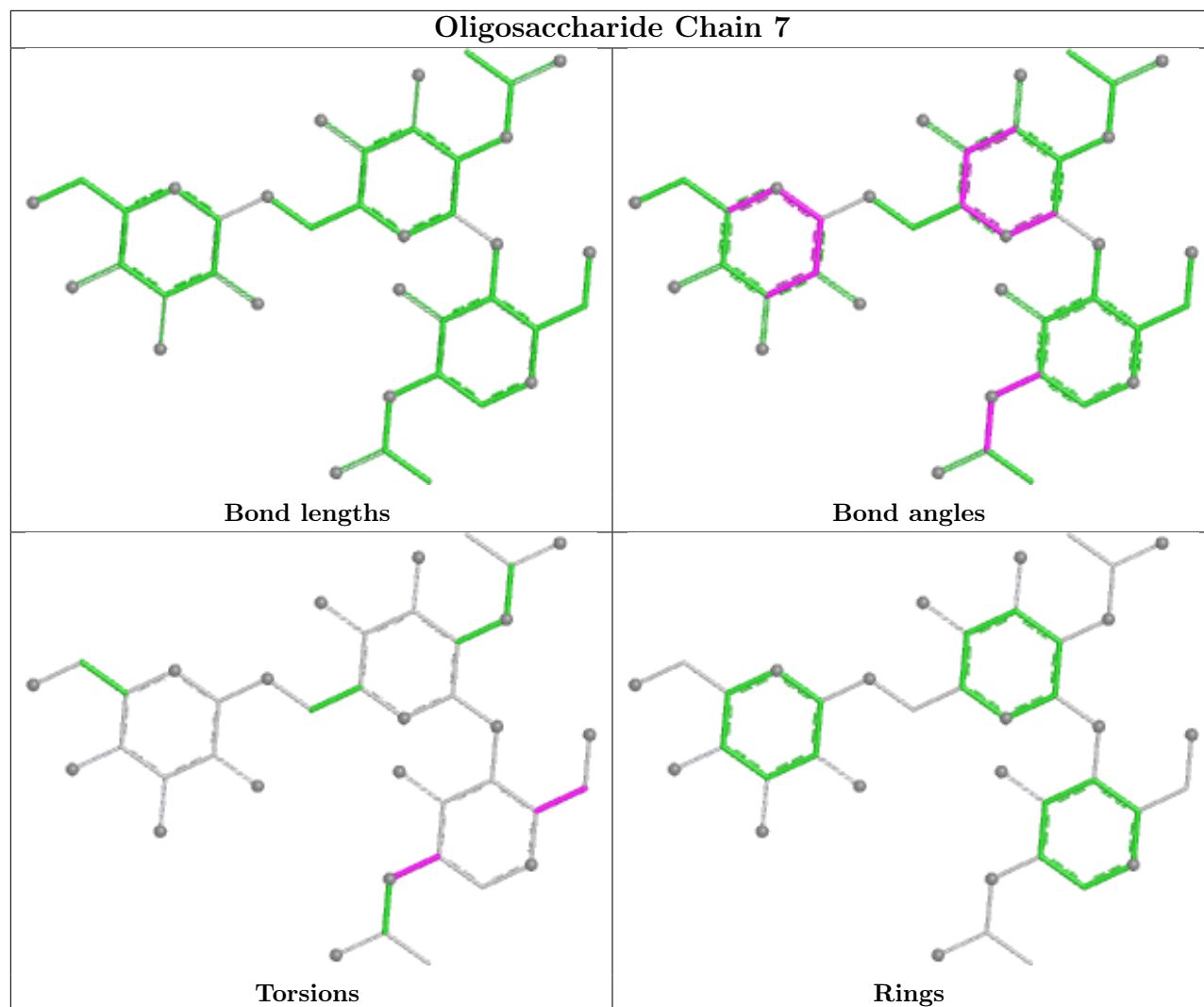


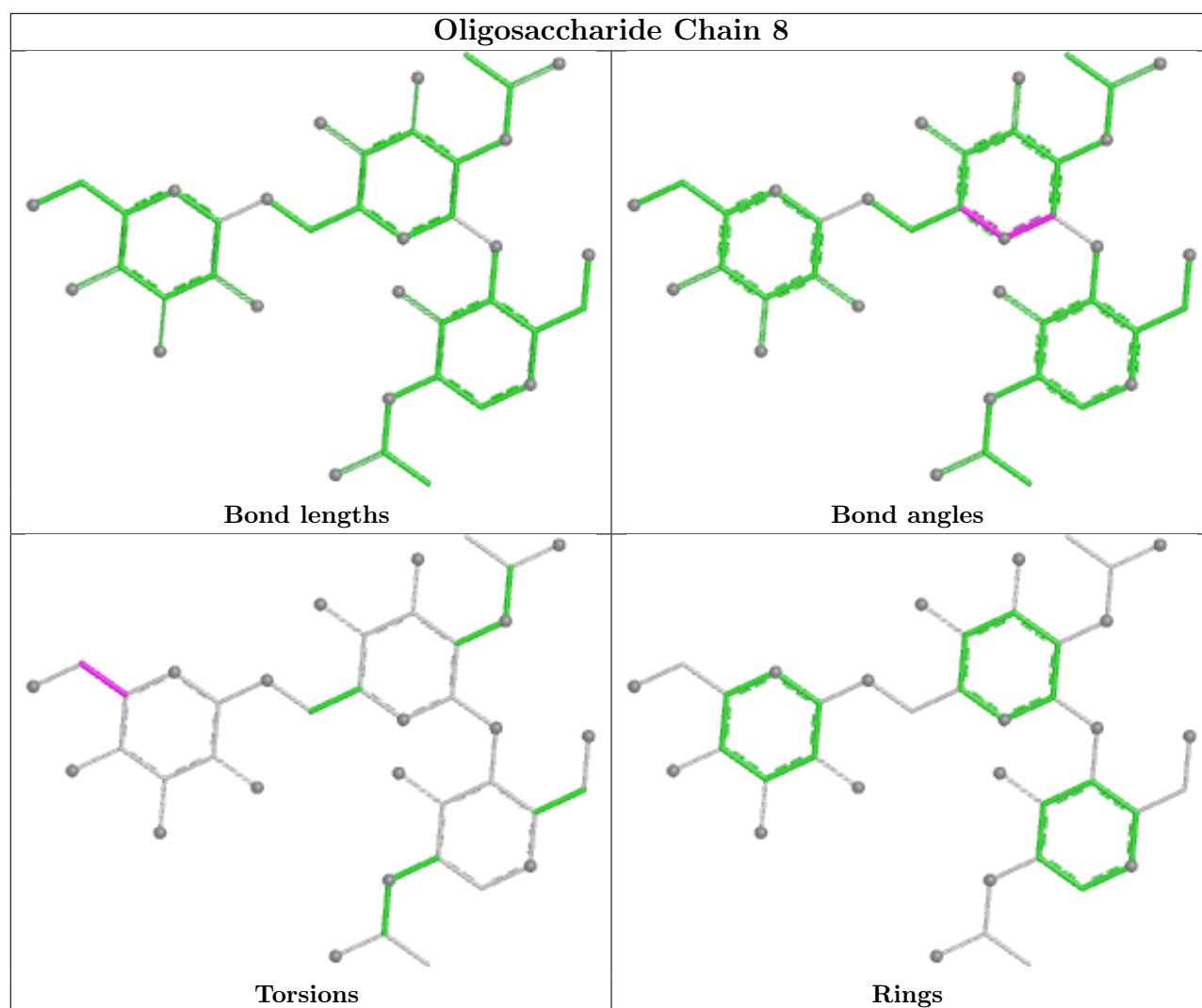




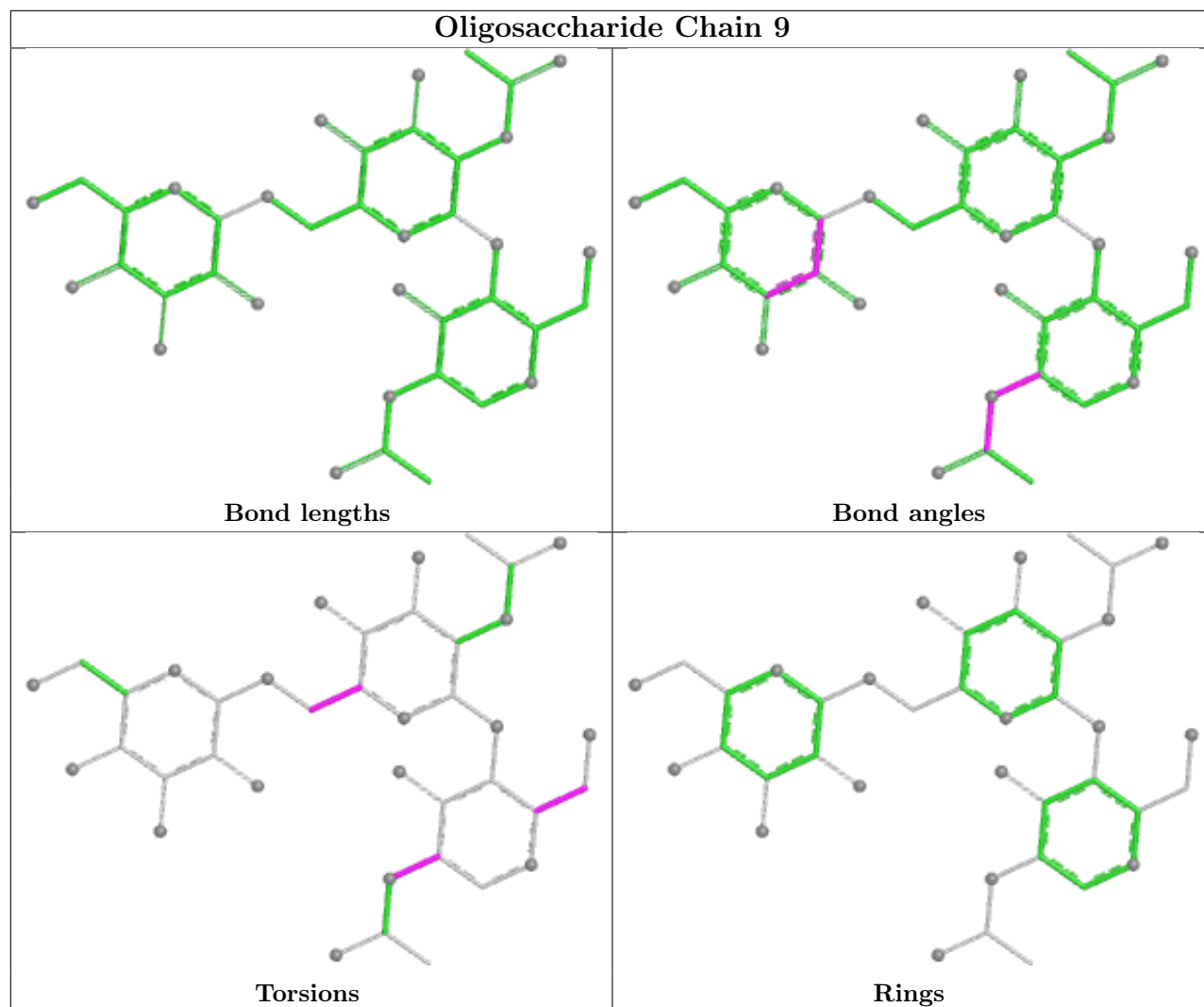


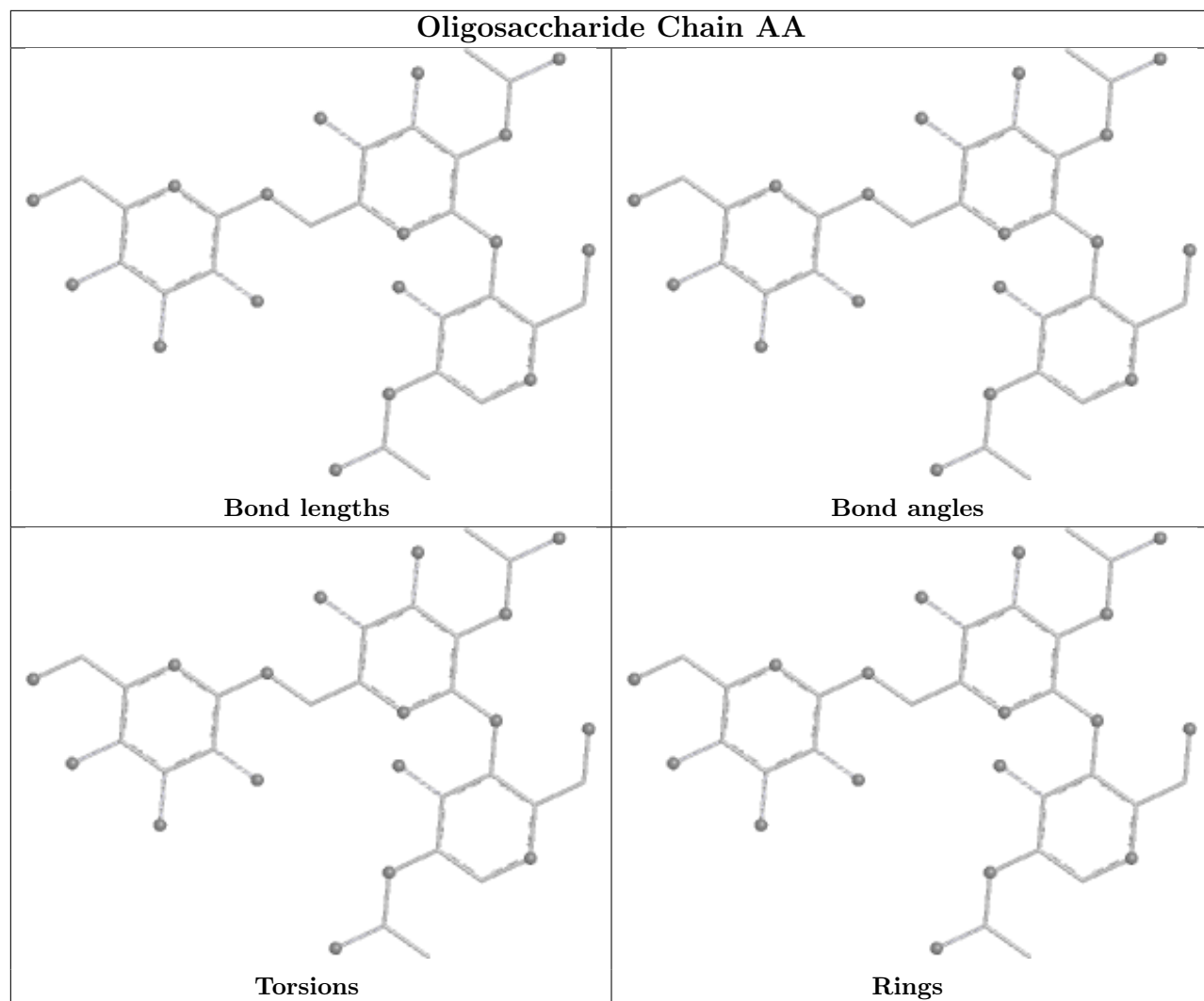


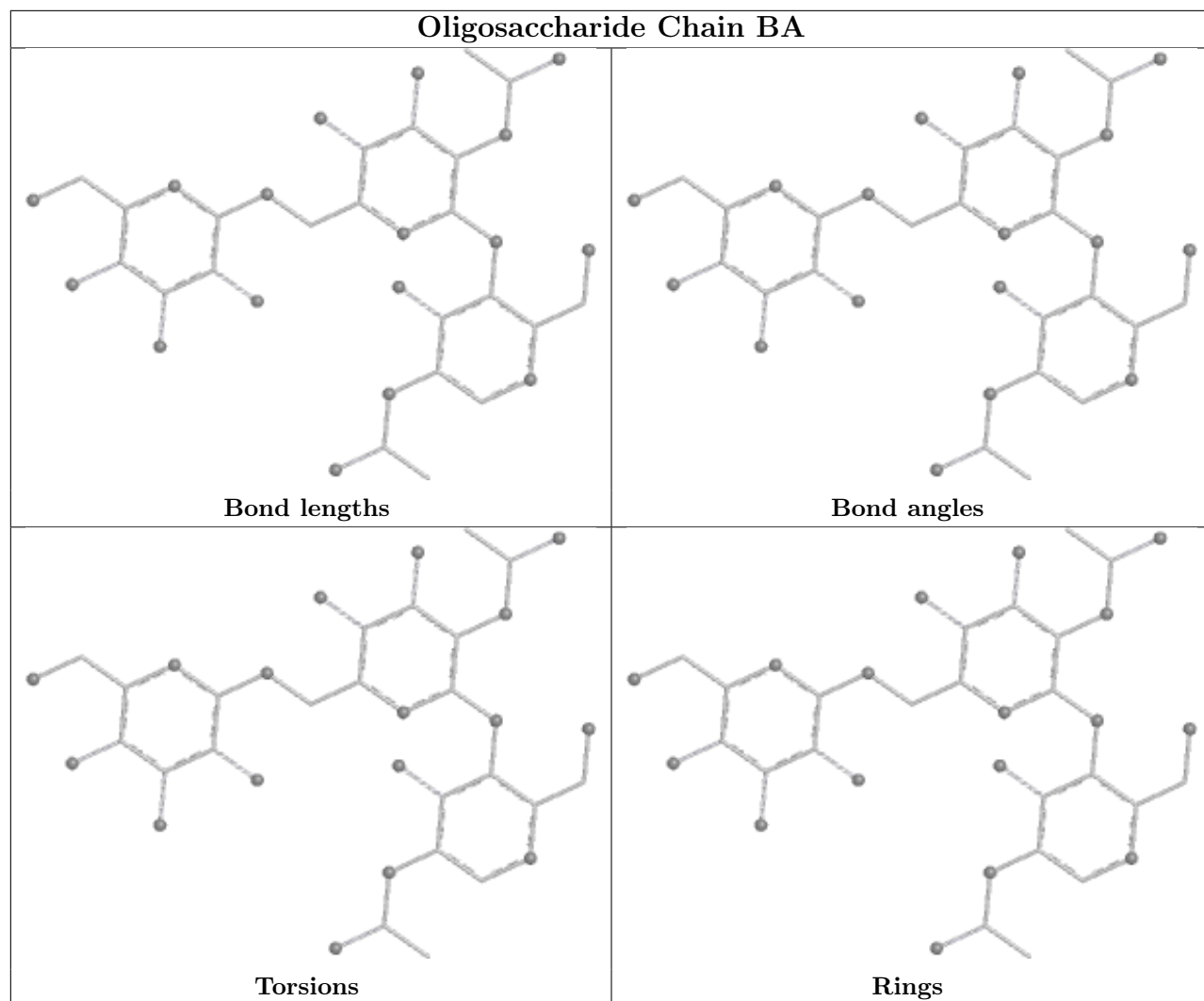


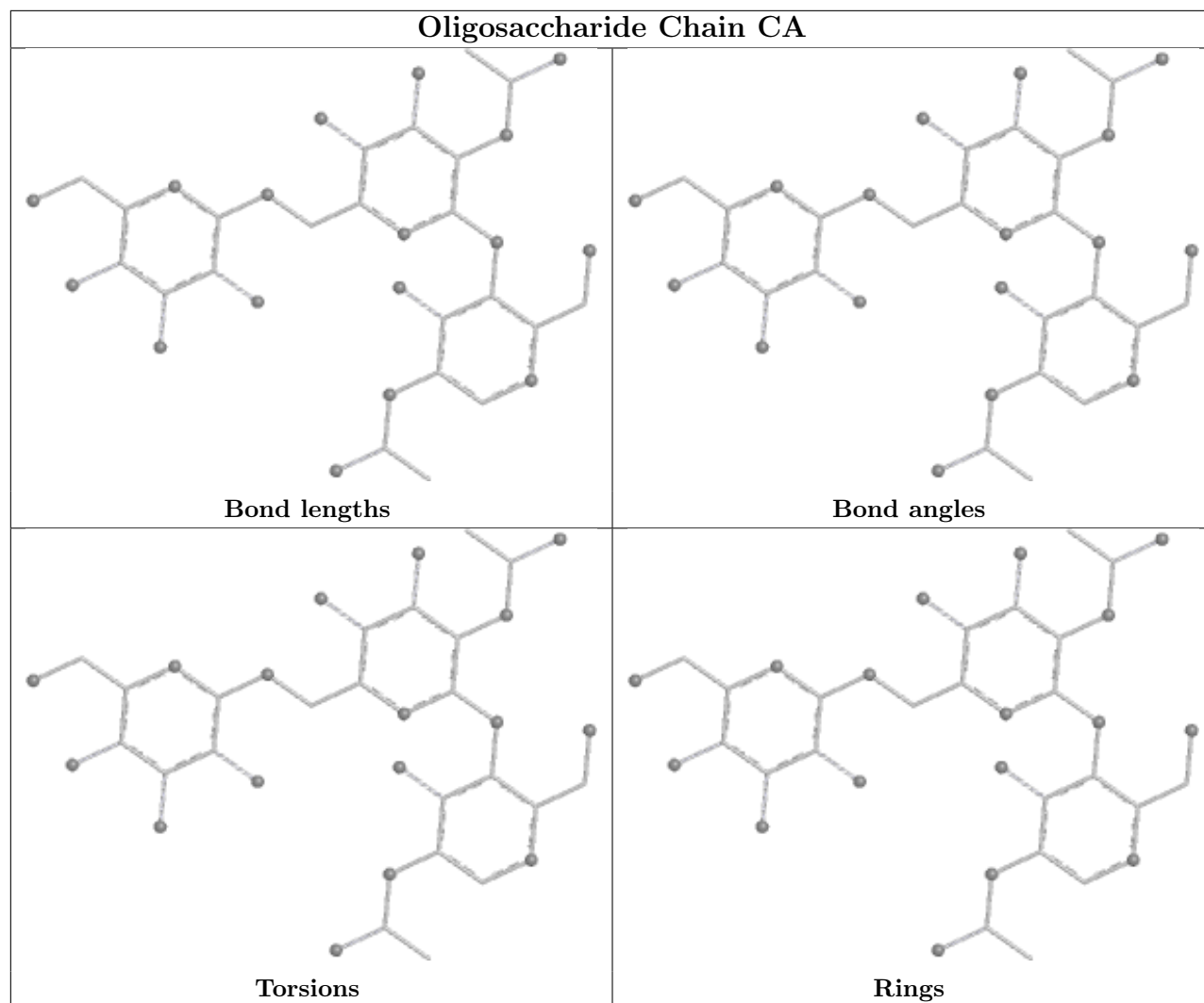


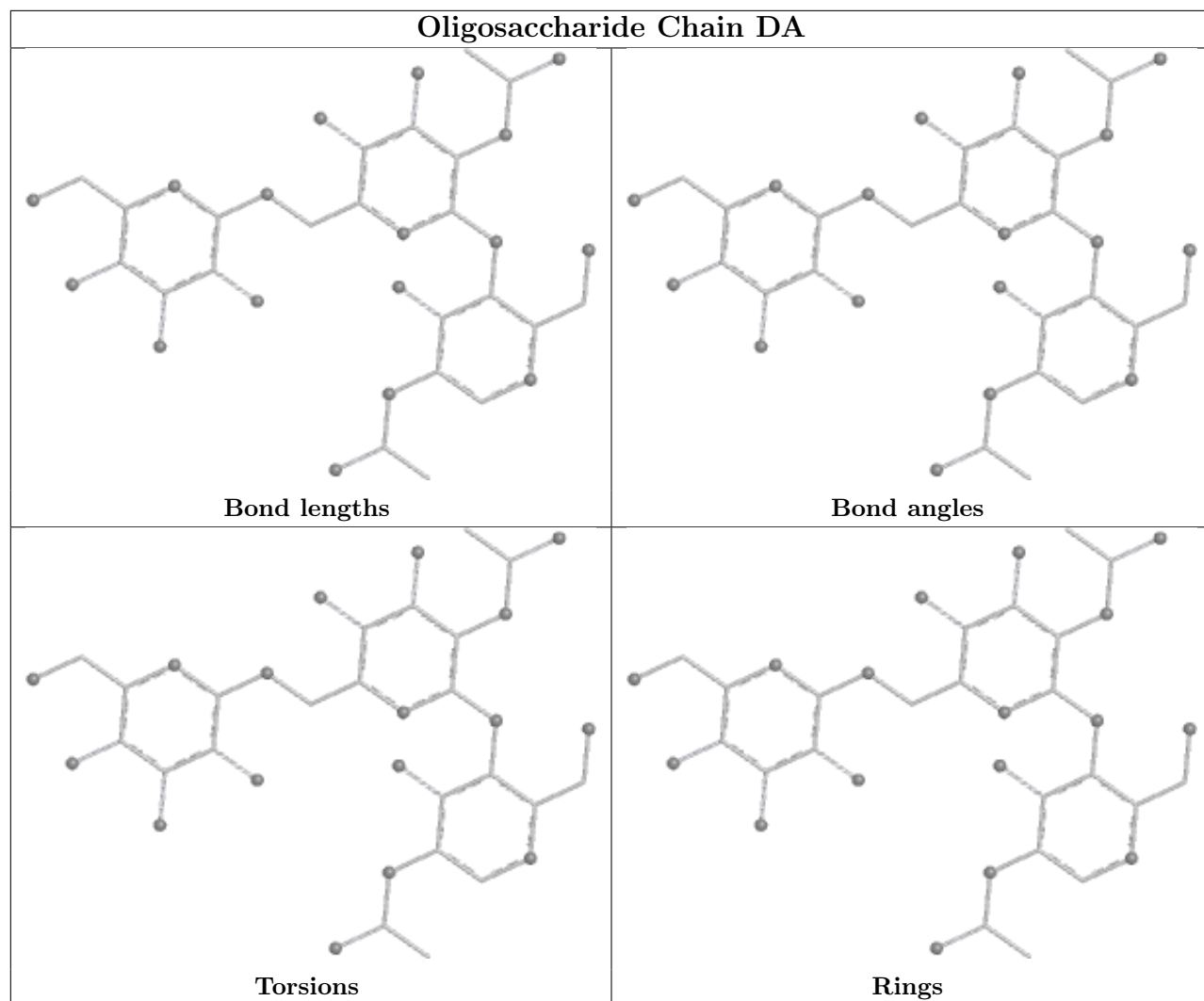
Oligosaccharide Chain 9

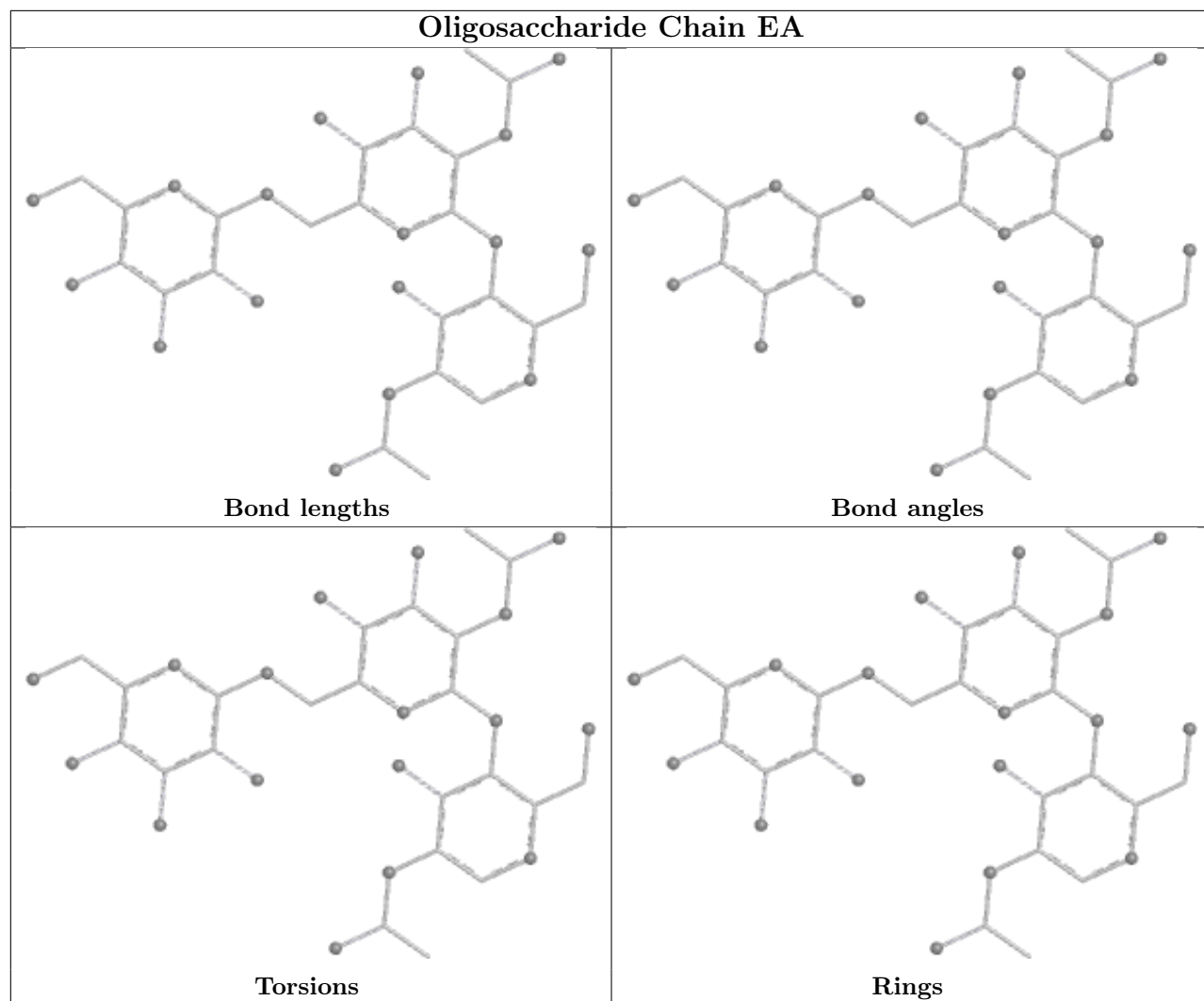


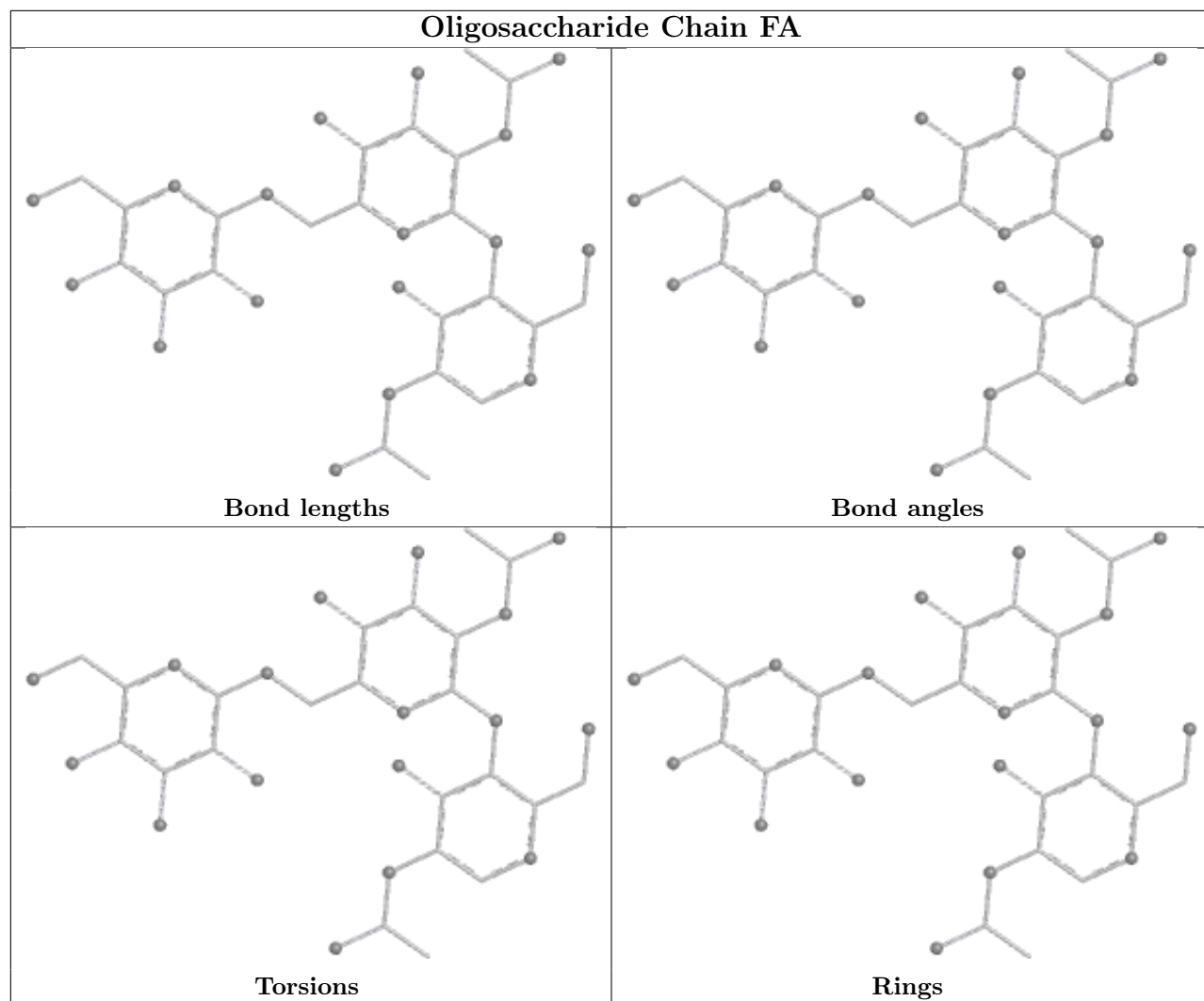
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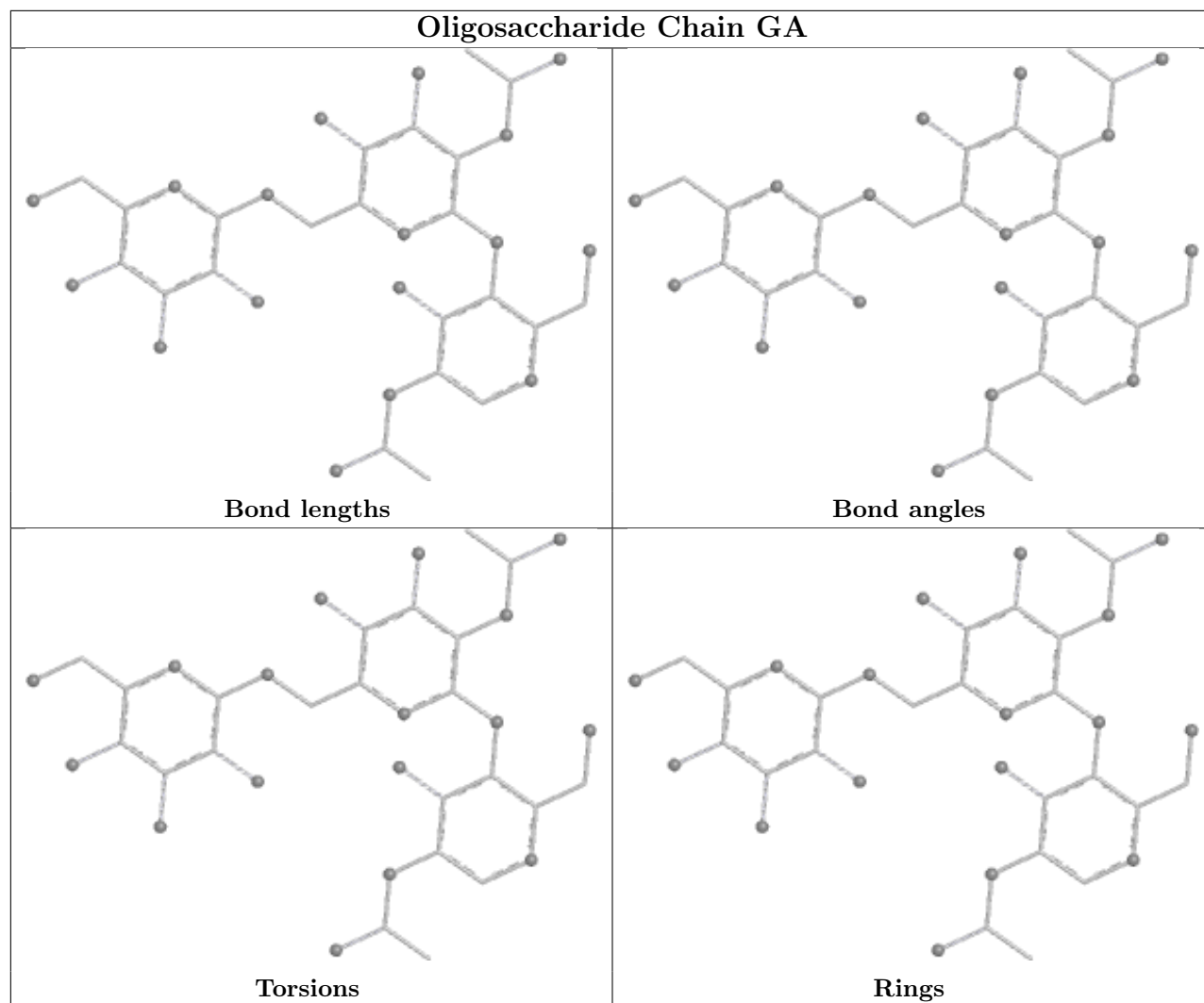
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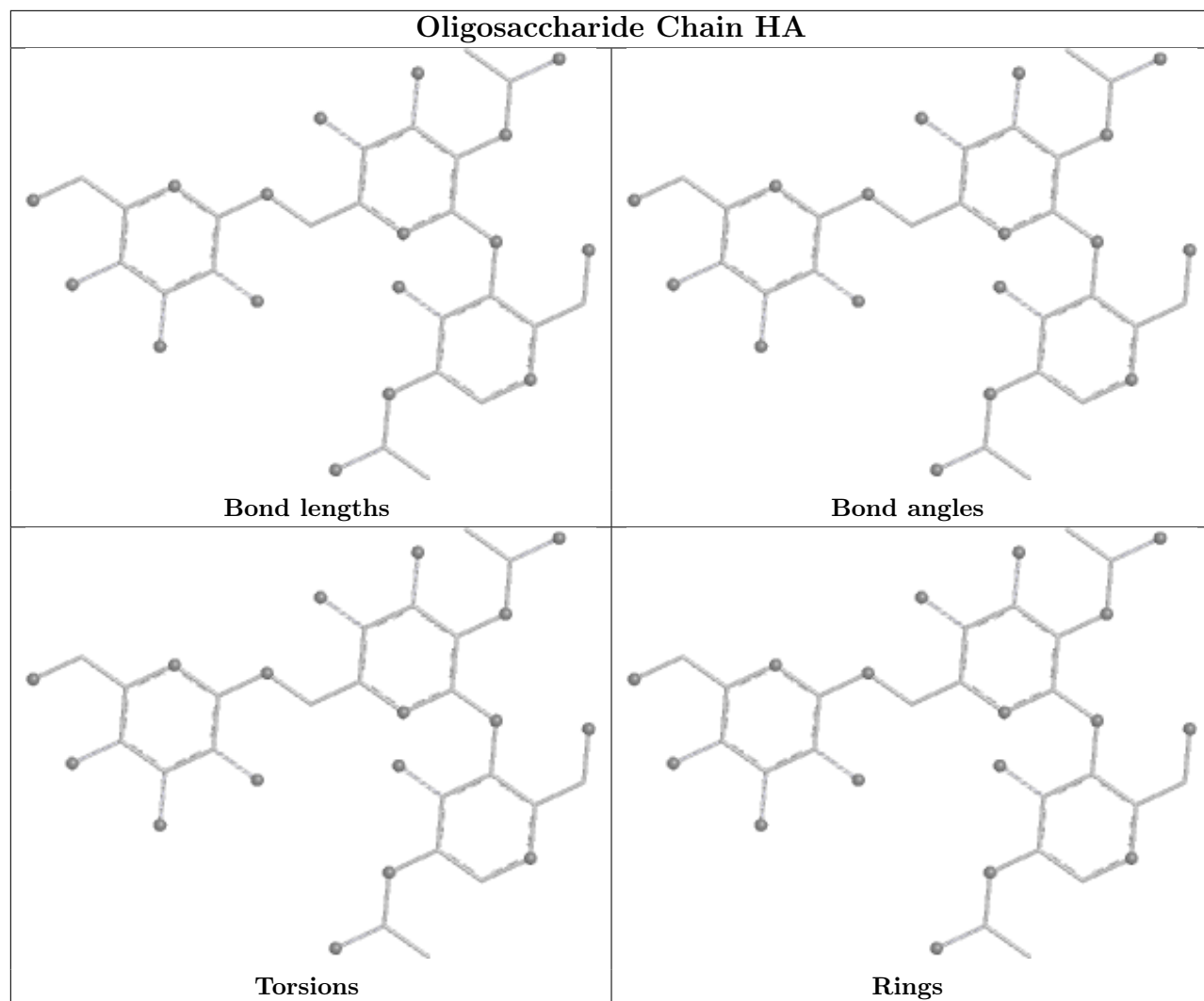
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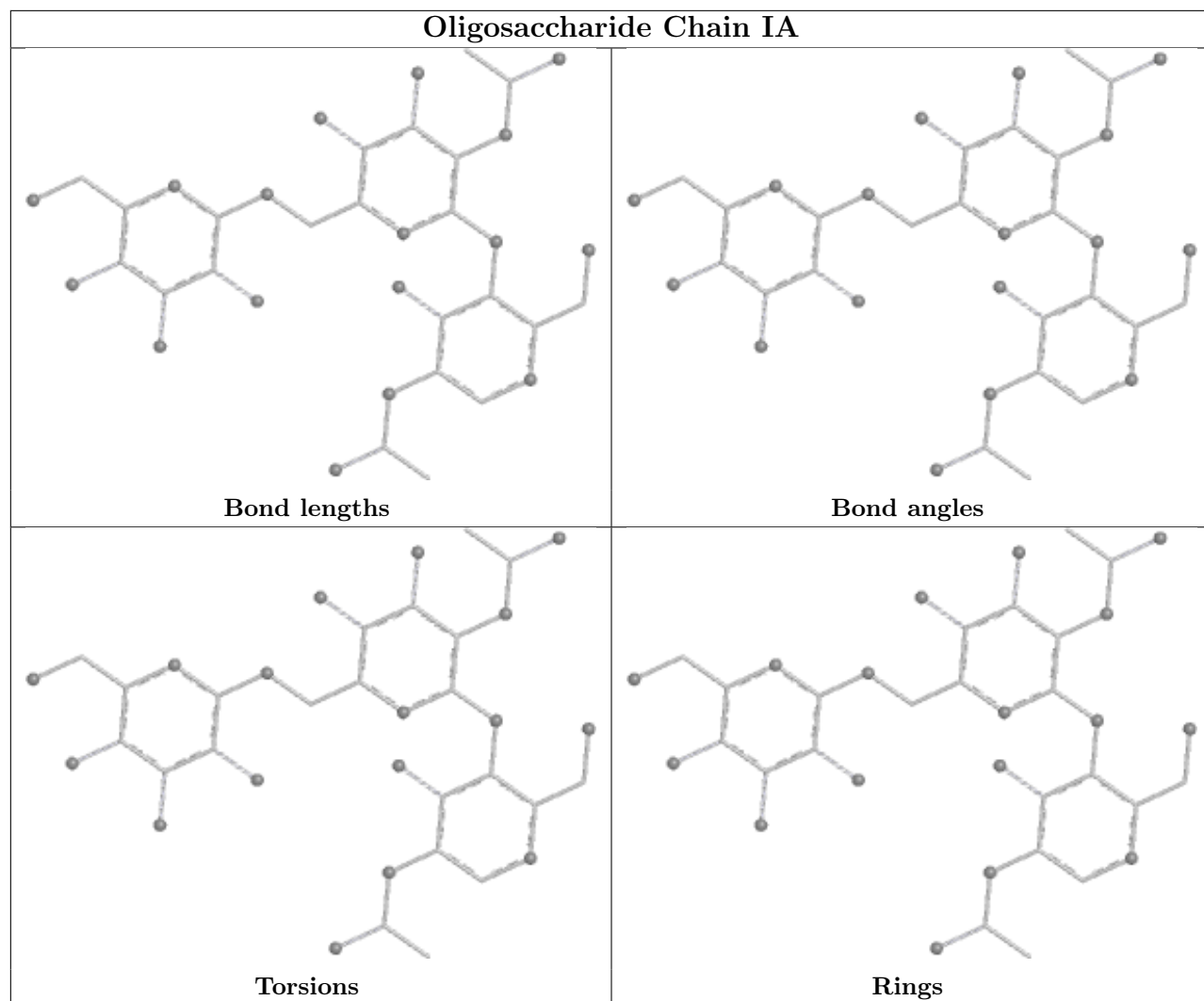
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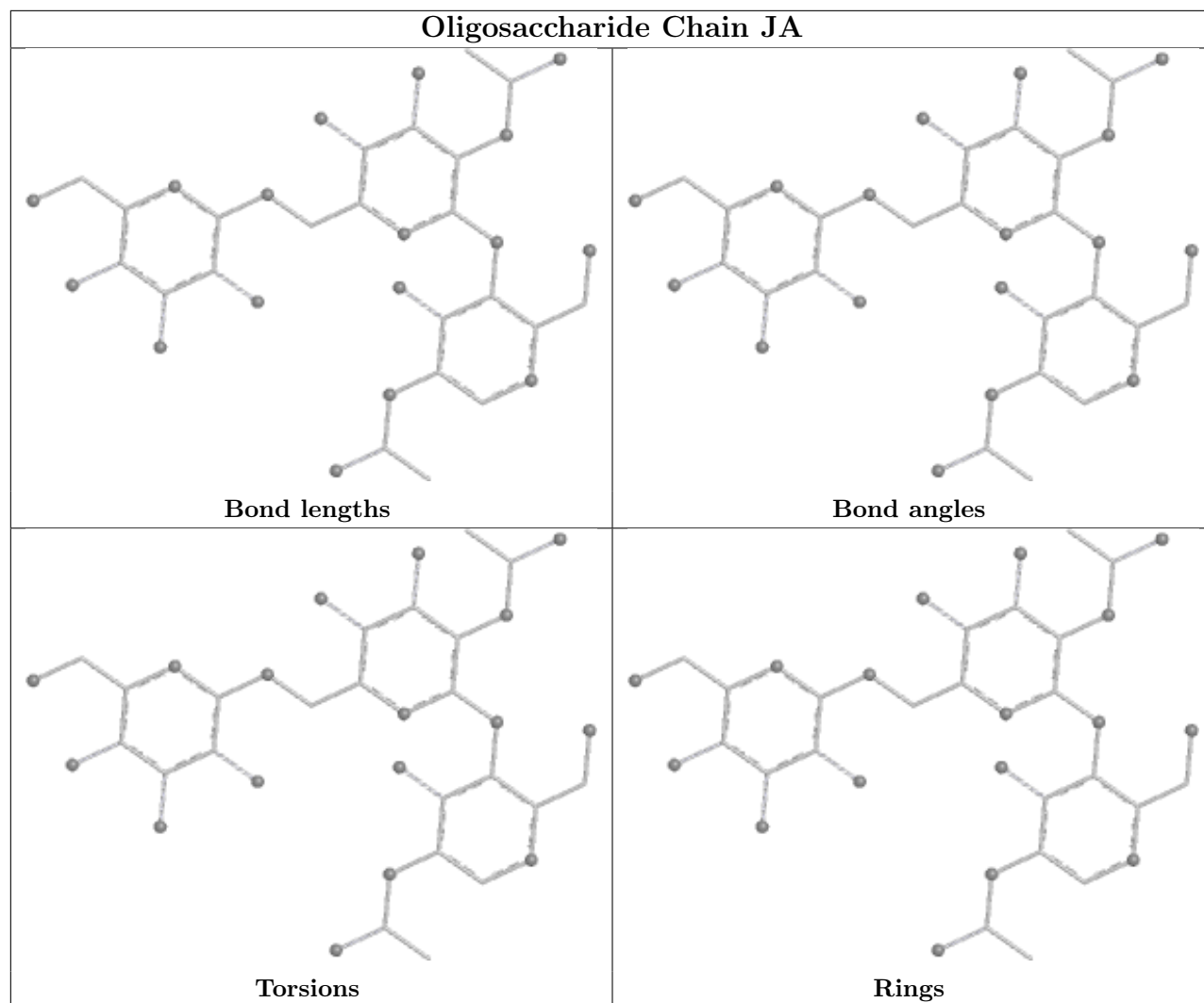
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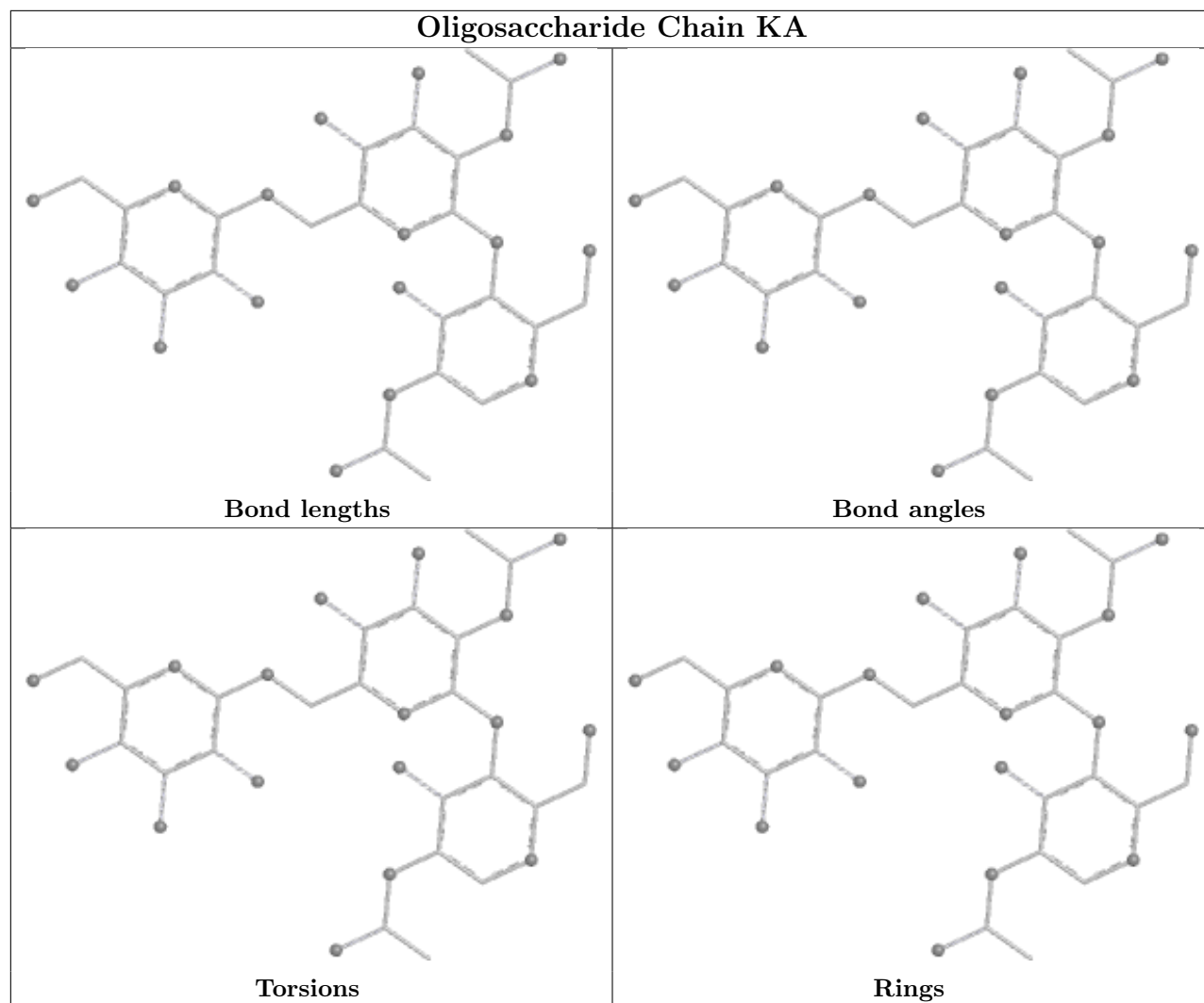
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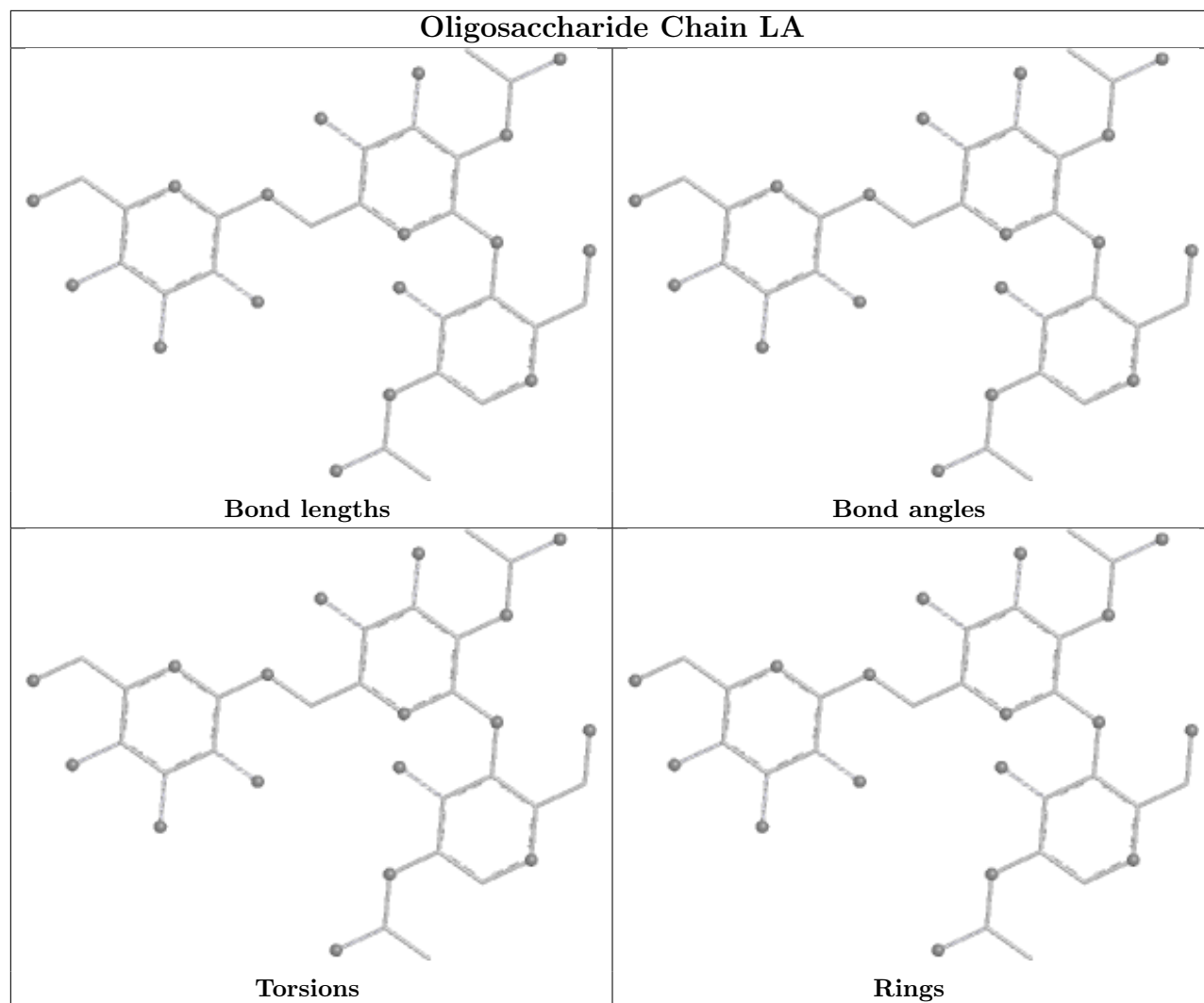
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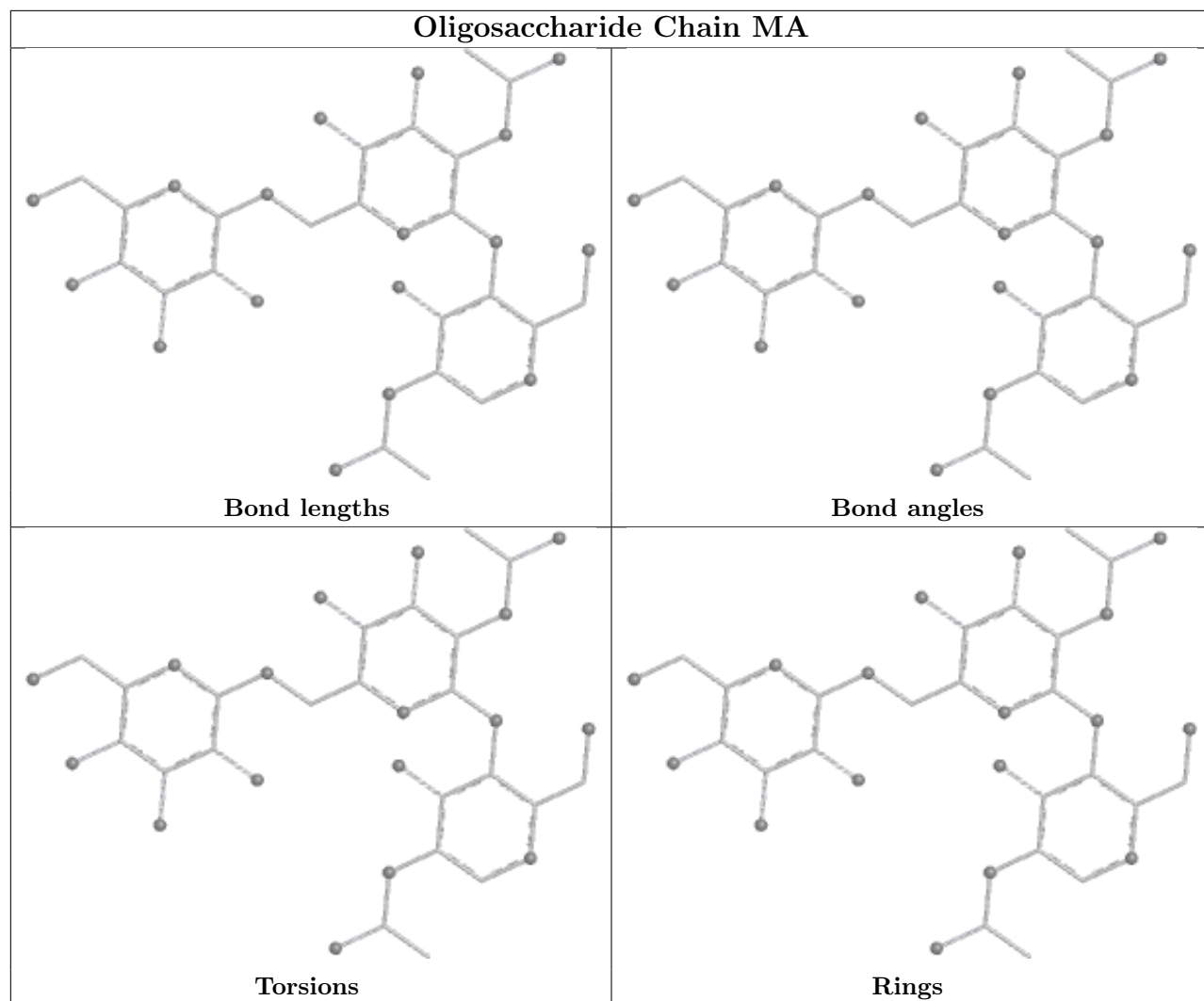
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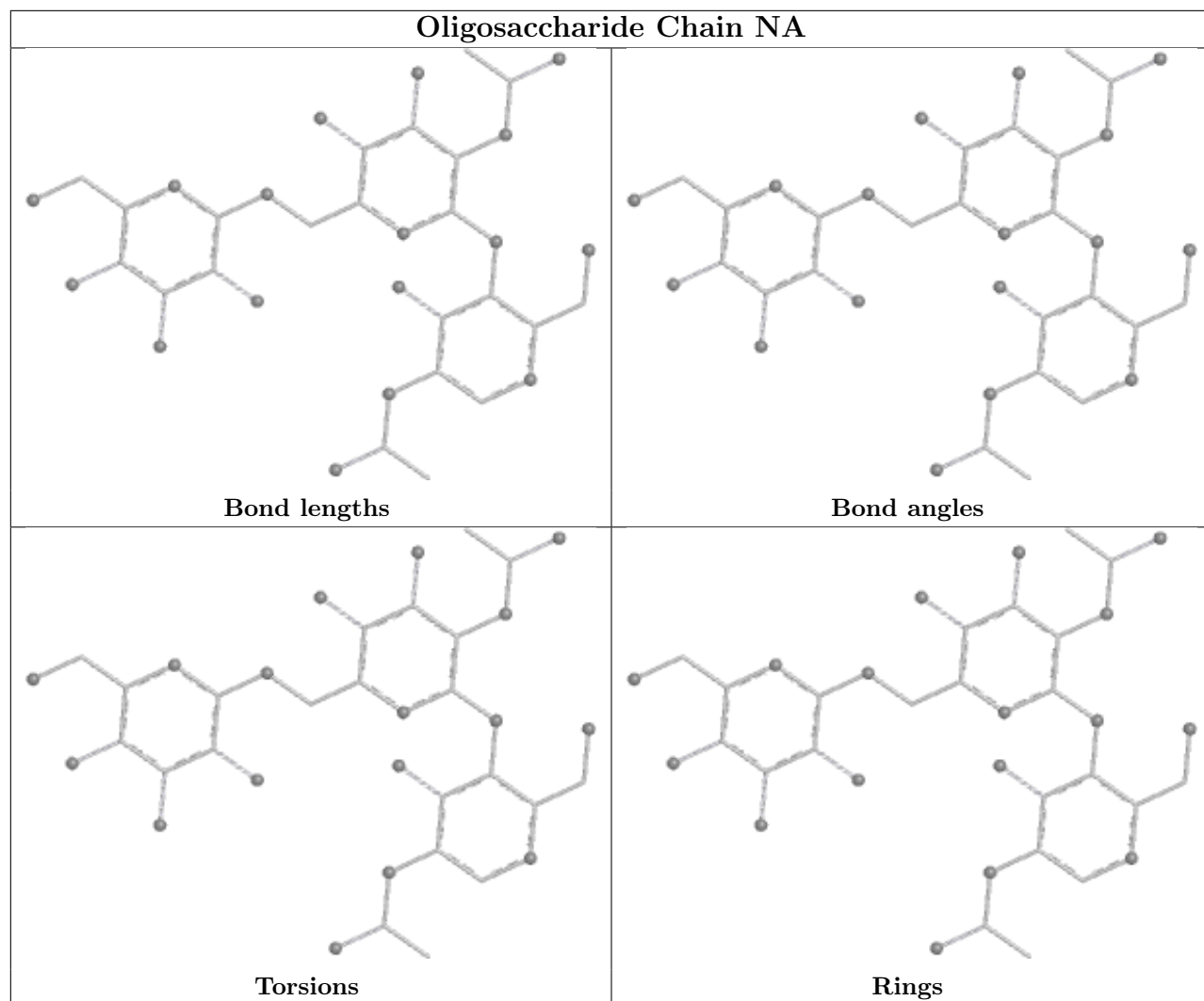


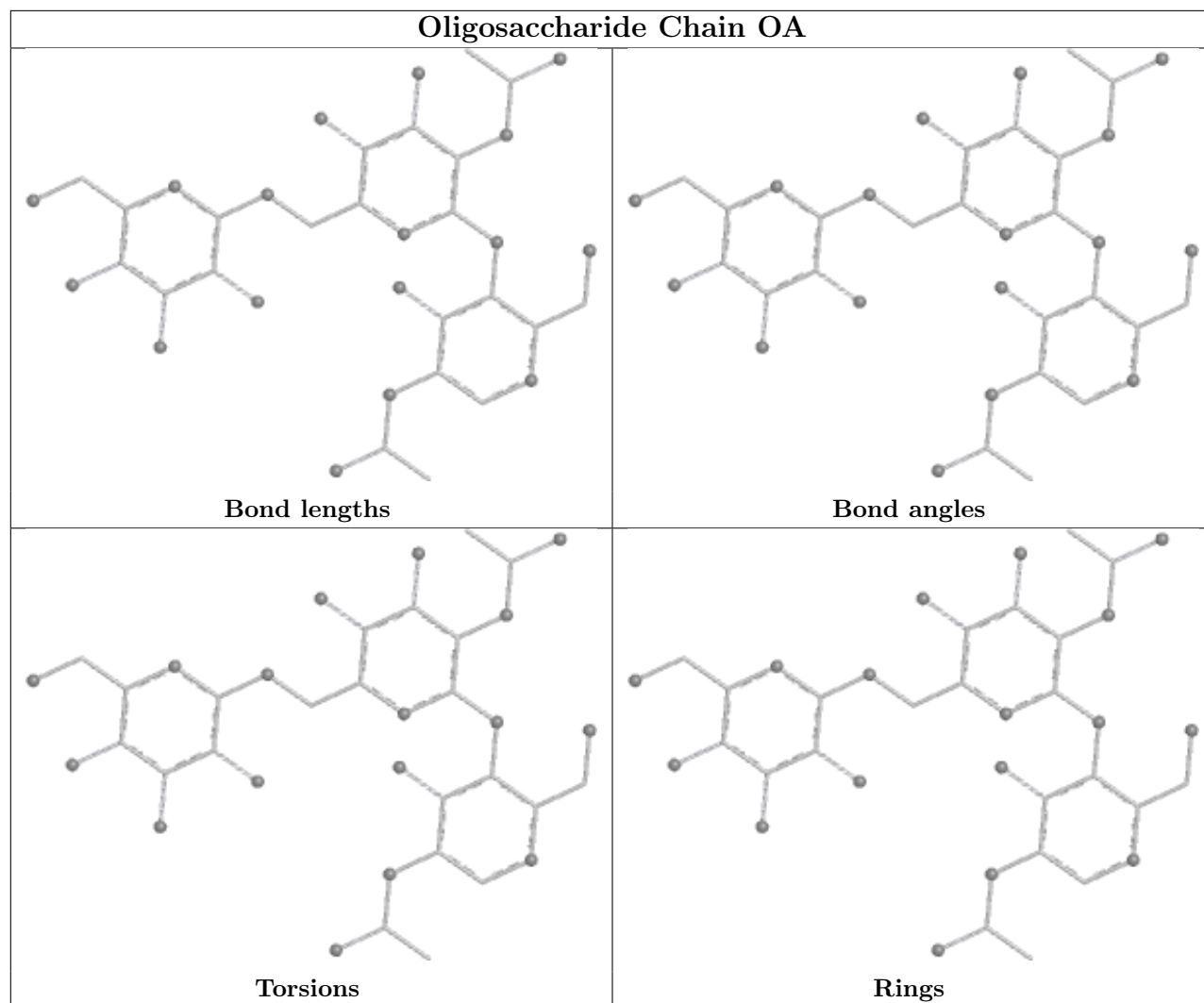
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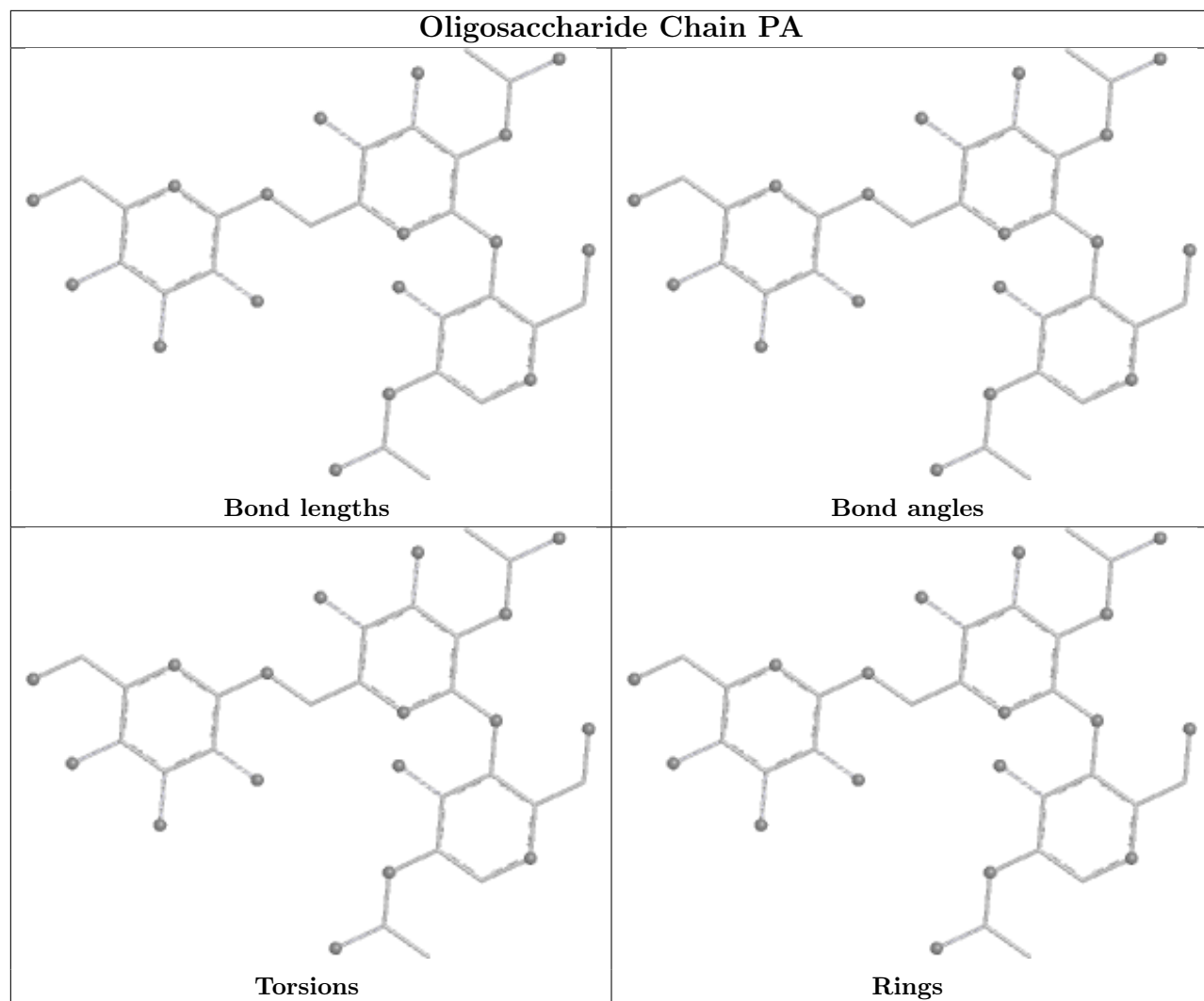
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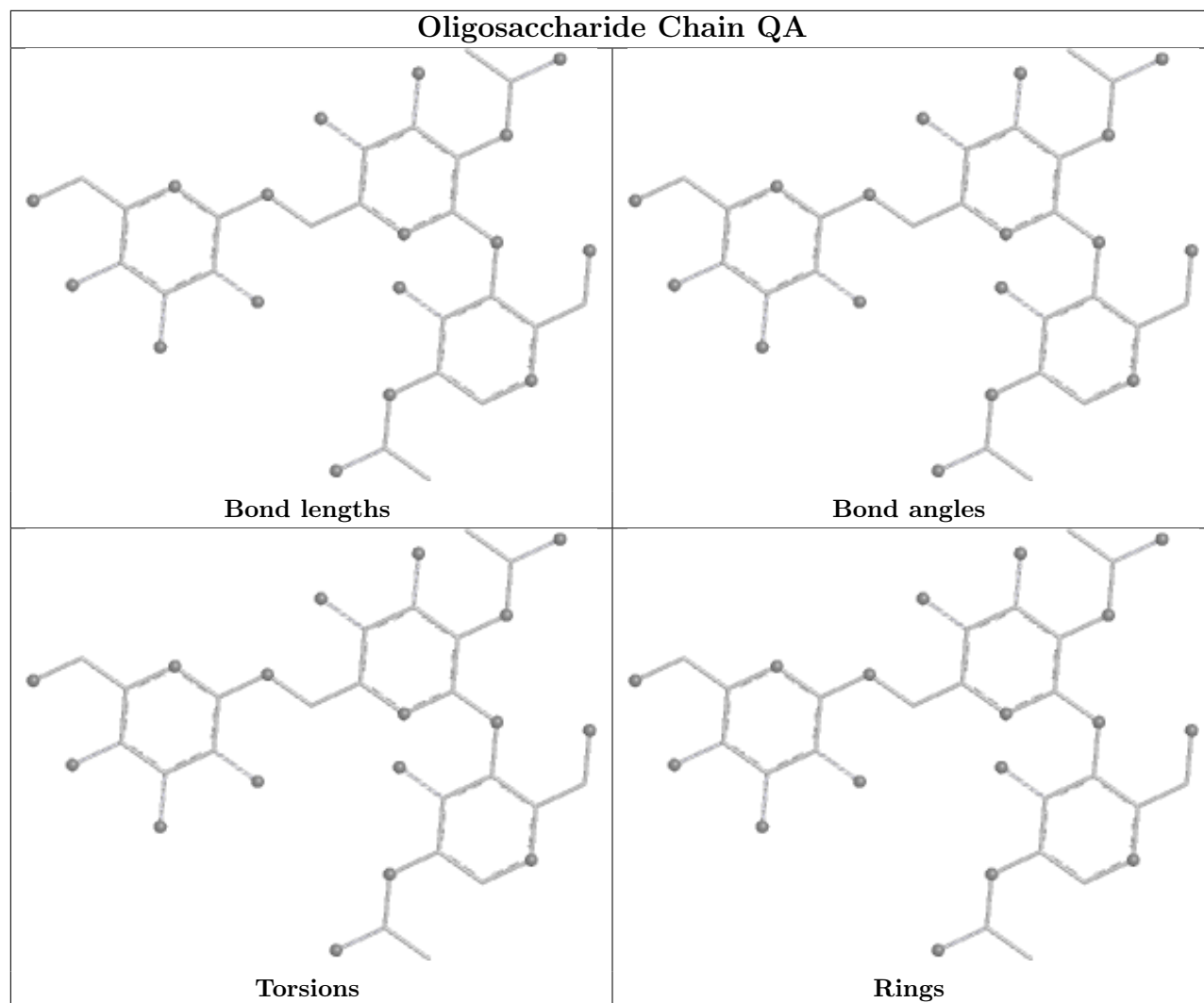
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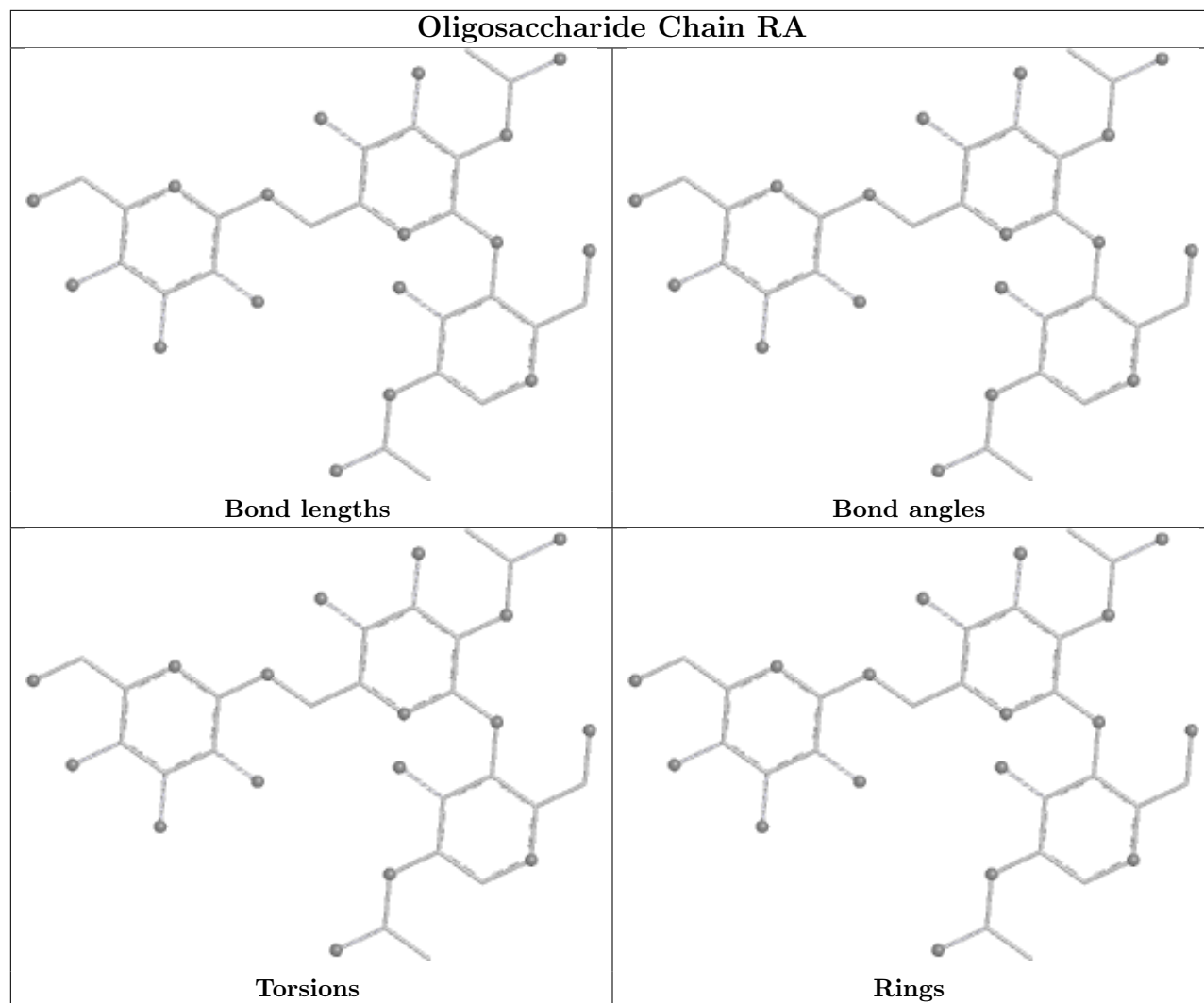
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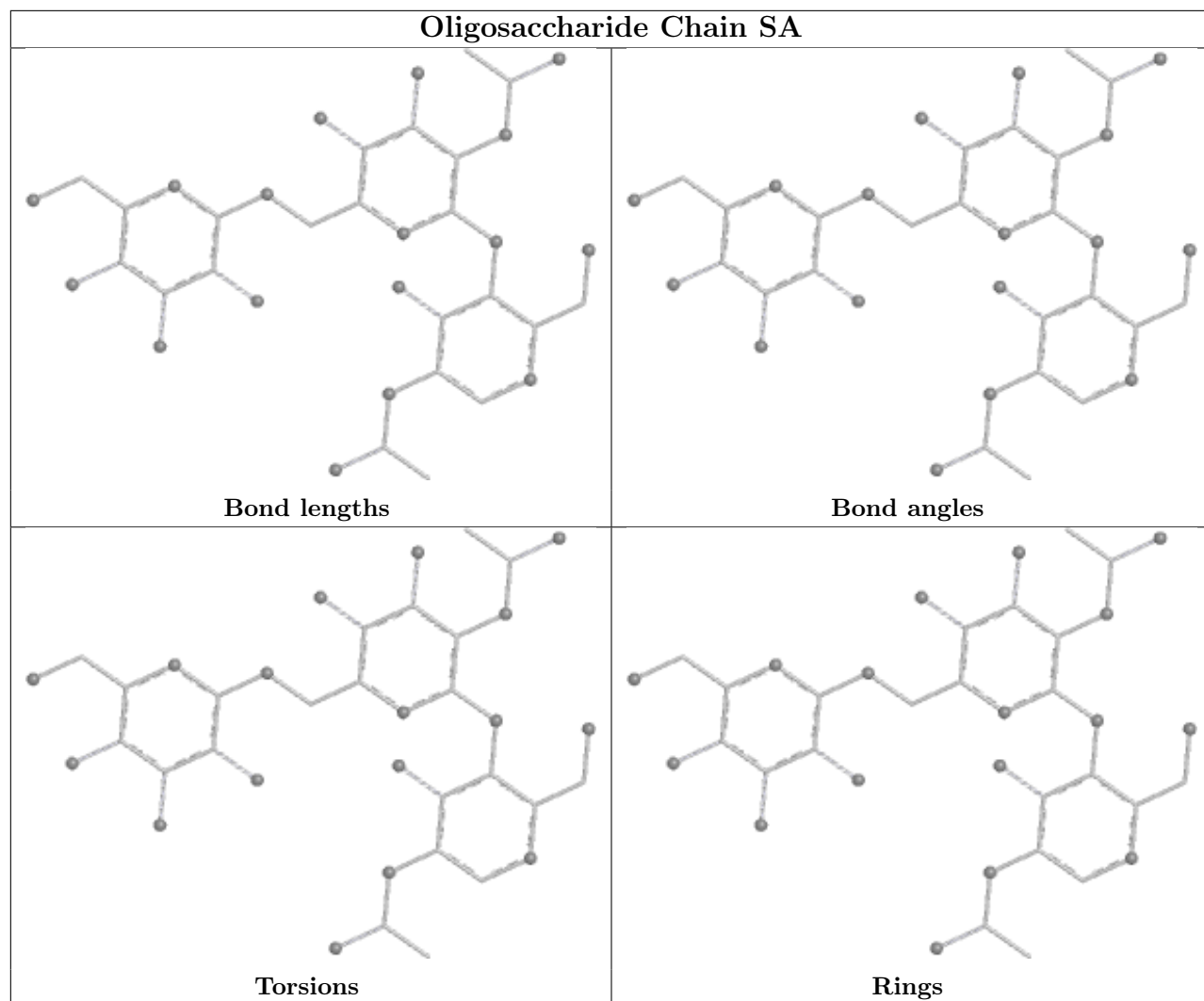
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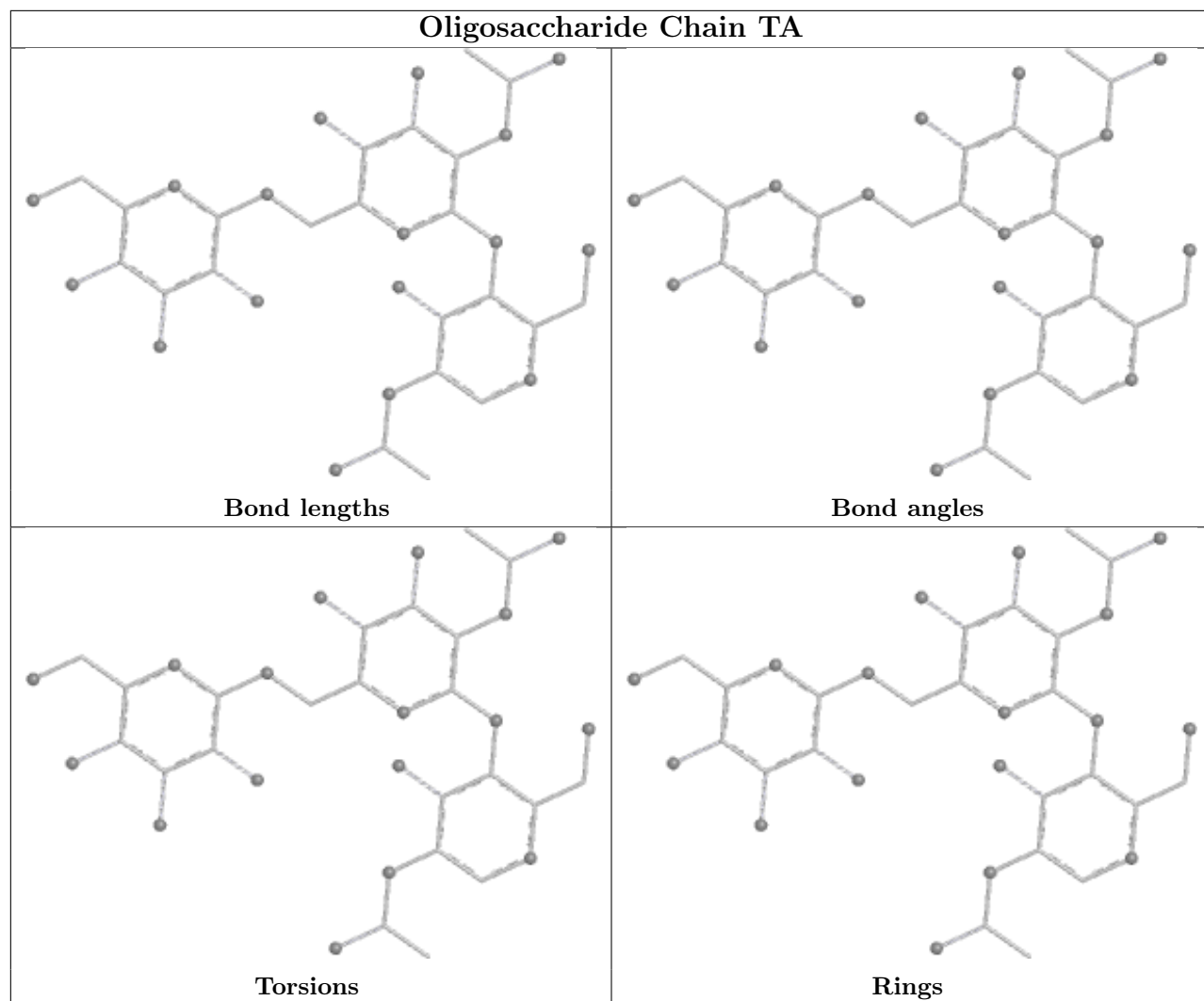
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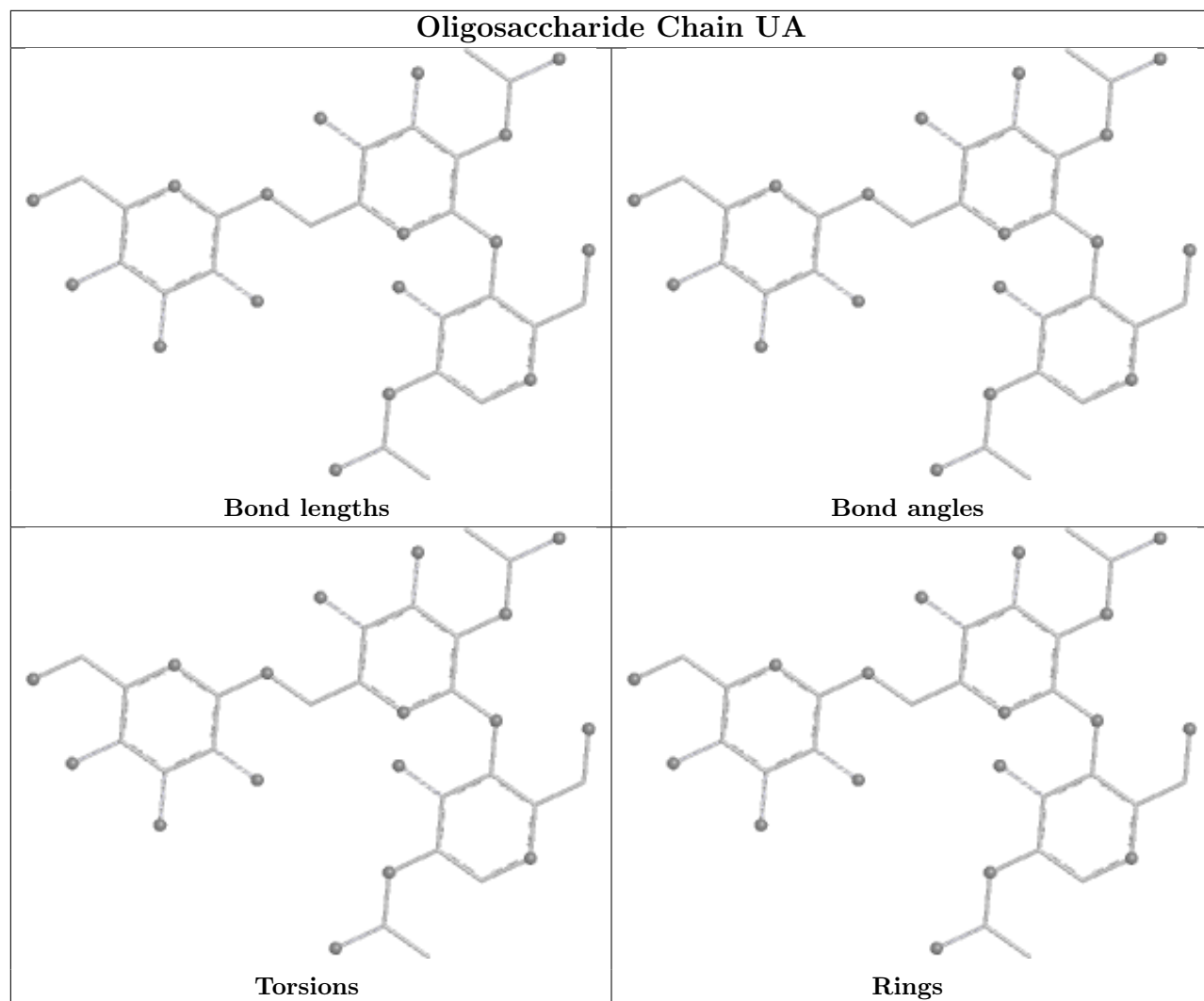
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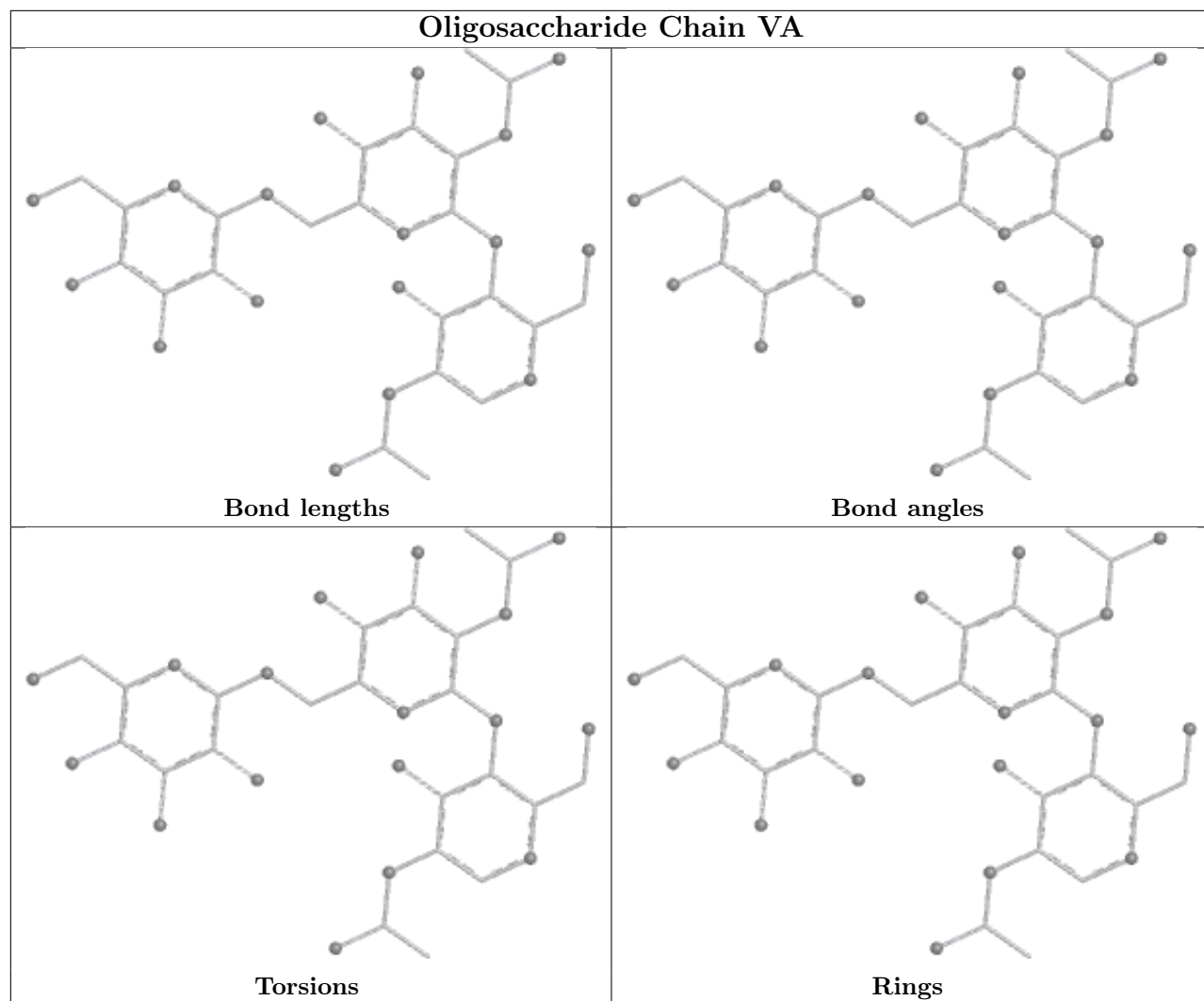
Oligosaccharide Chain QA

Oligosaccharide Chain RA

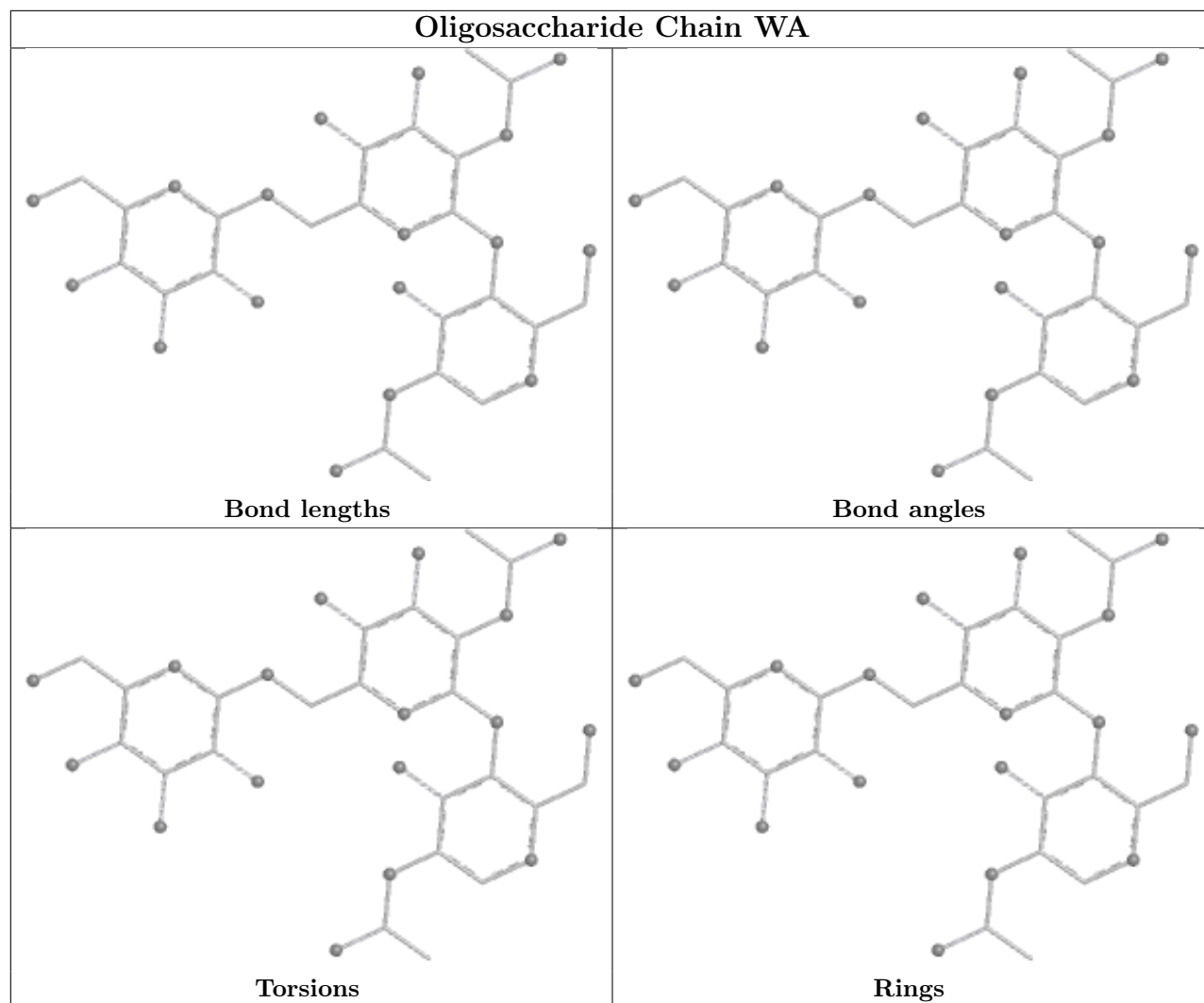
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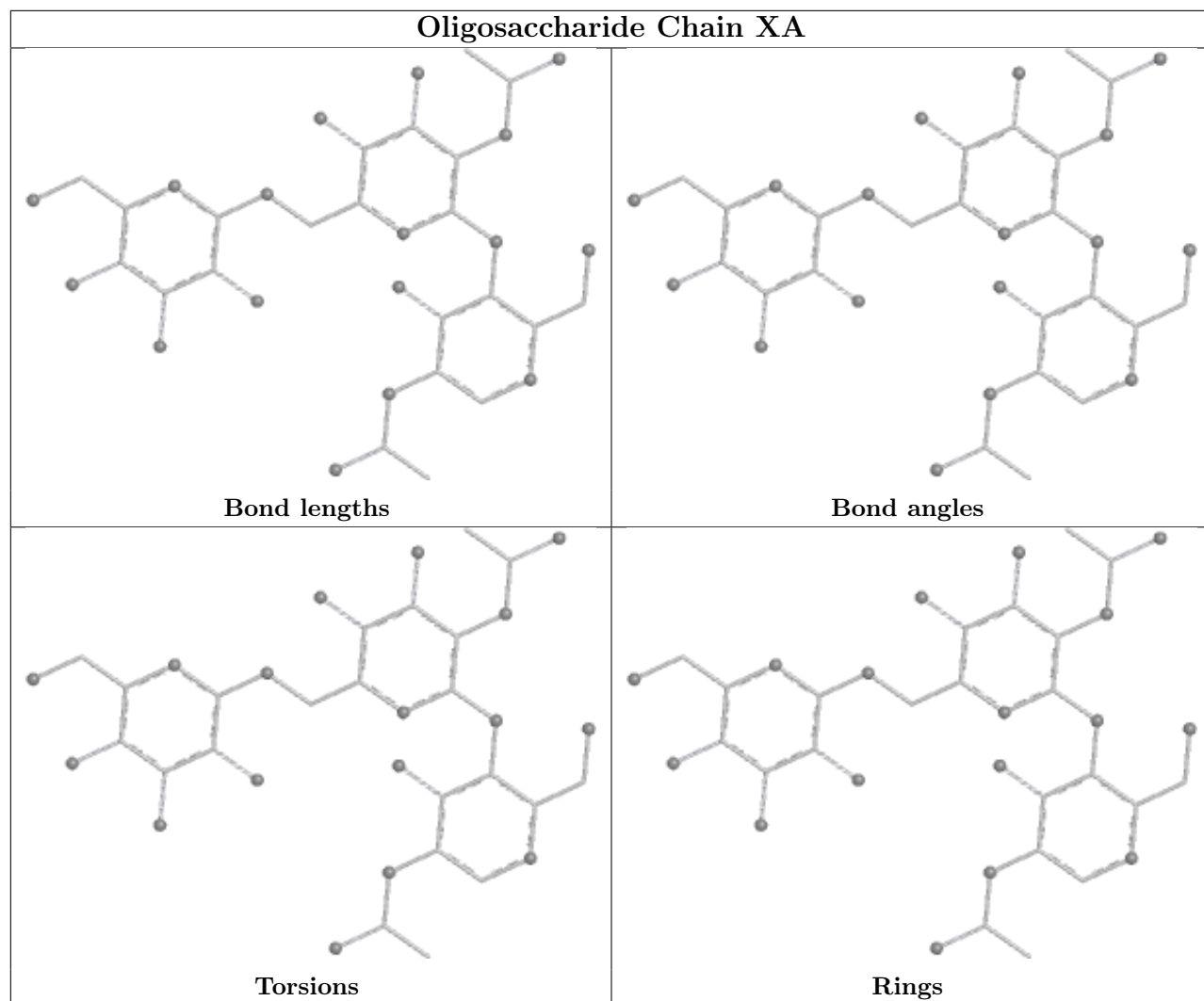
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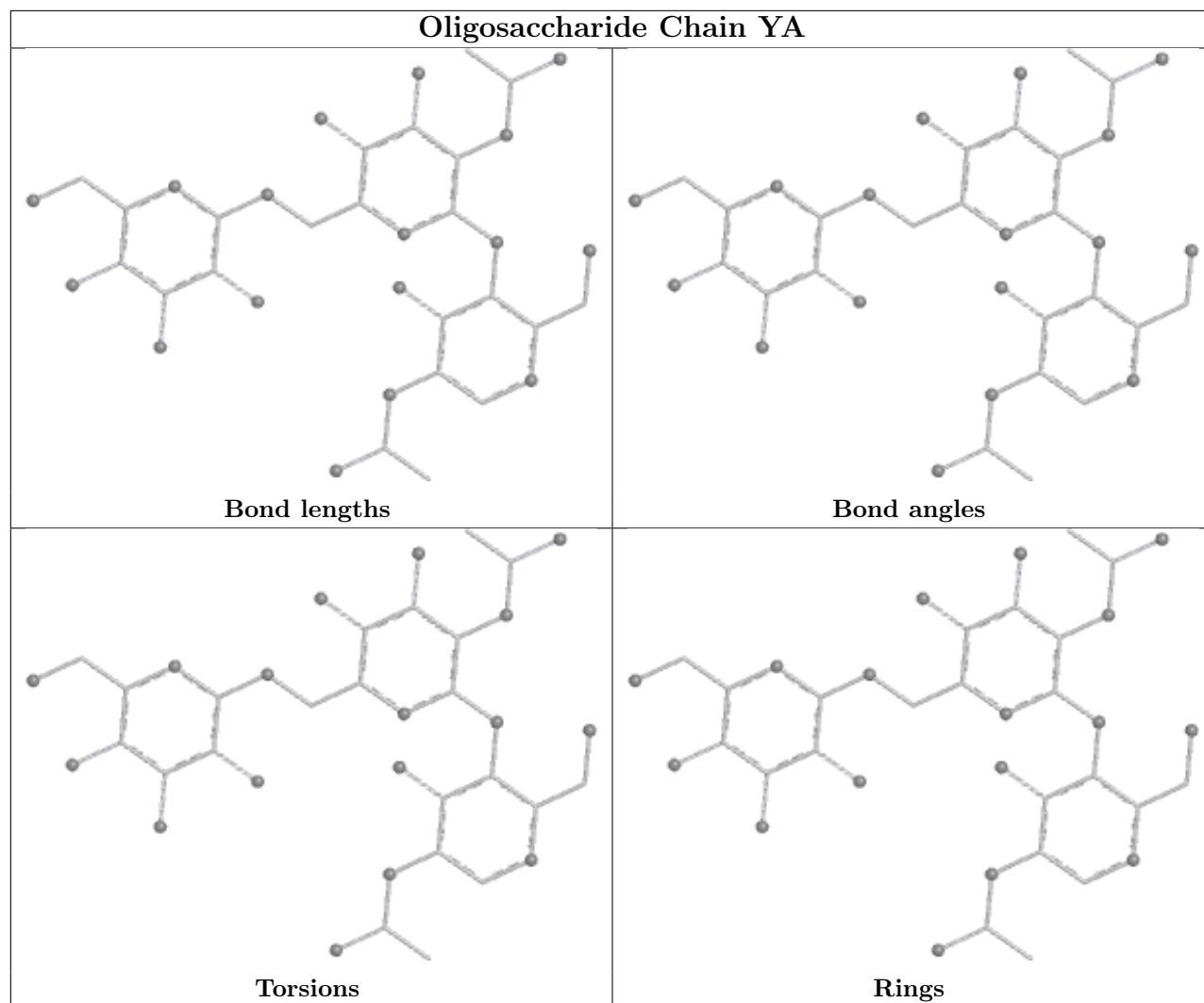
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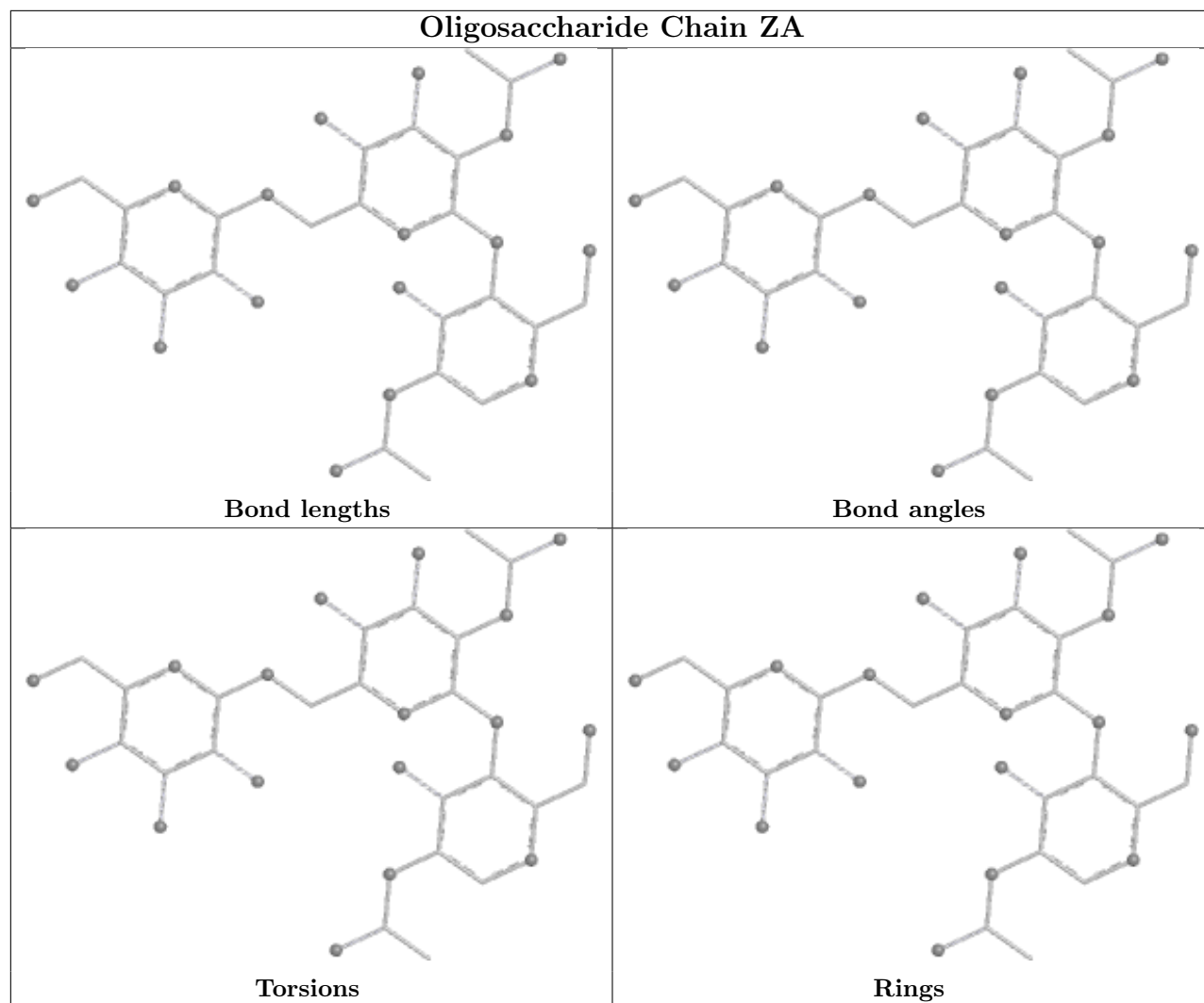
Oligosaccharide Chain VA

Oligosaccharide Chain WA

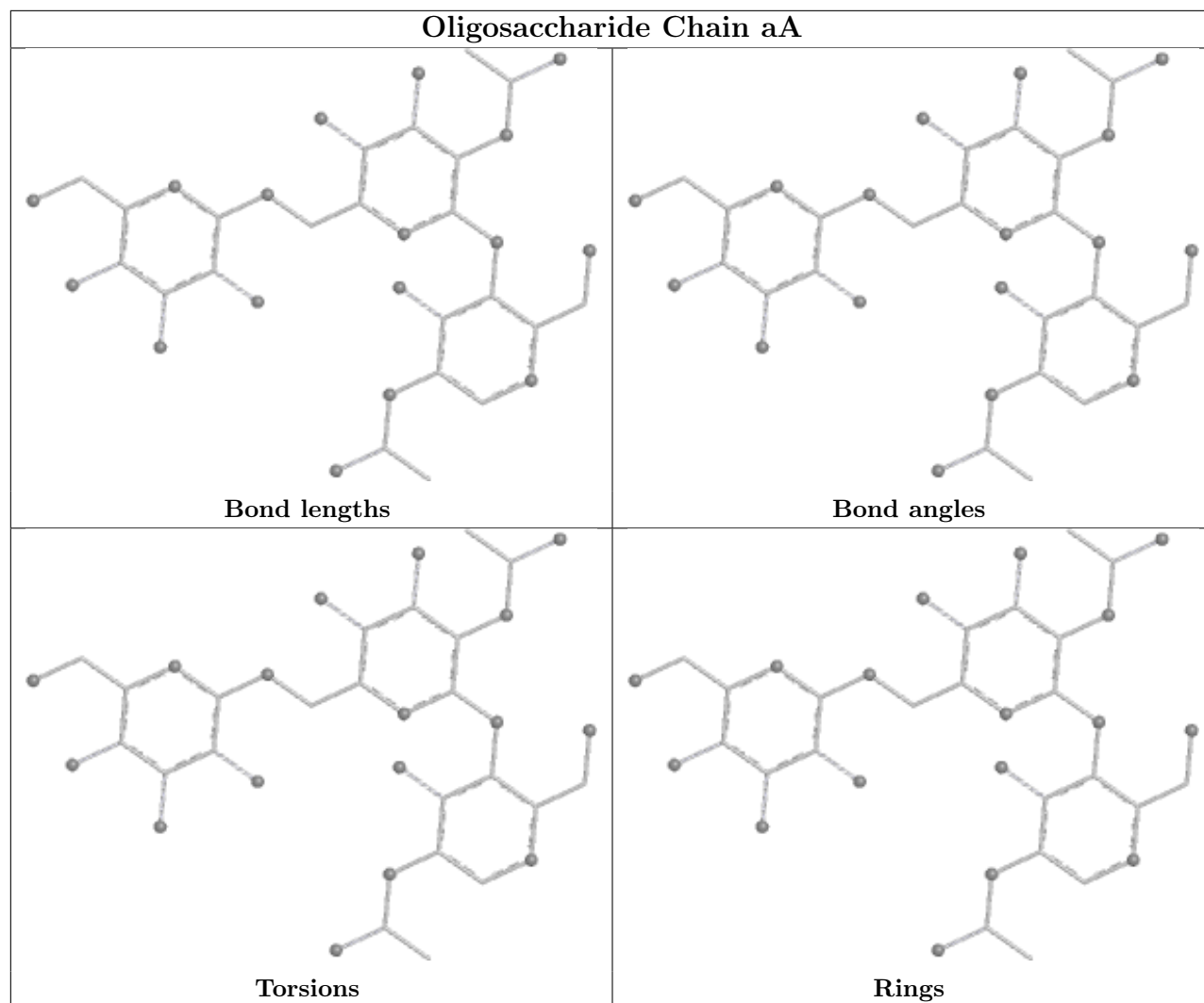


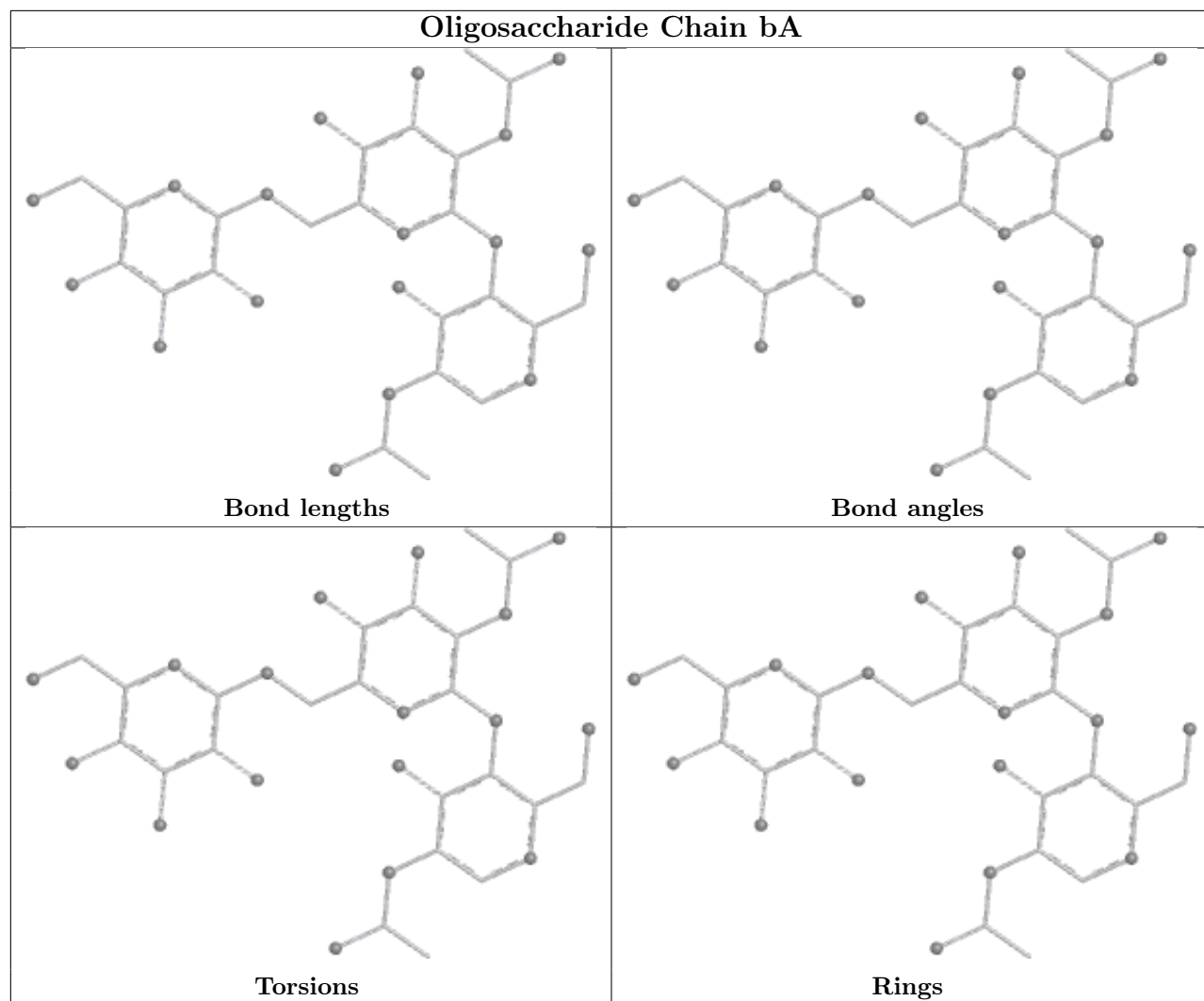
Oligosaccharide Chain XA

Oligosaccharide Chain YA

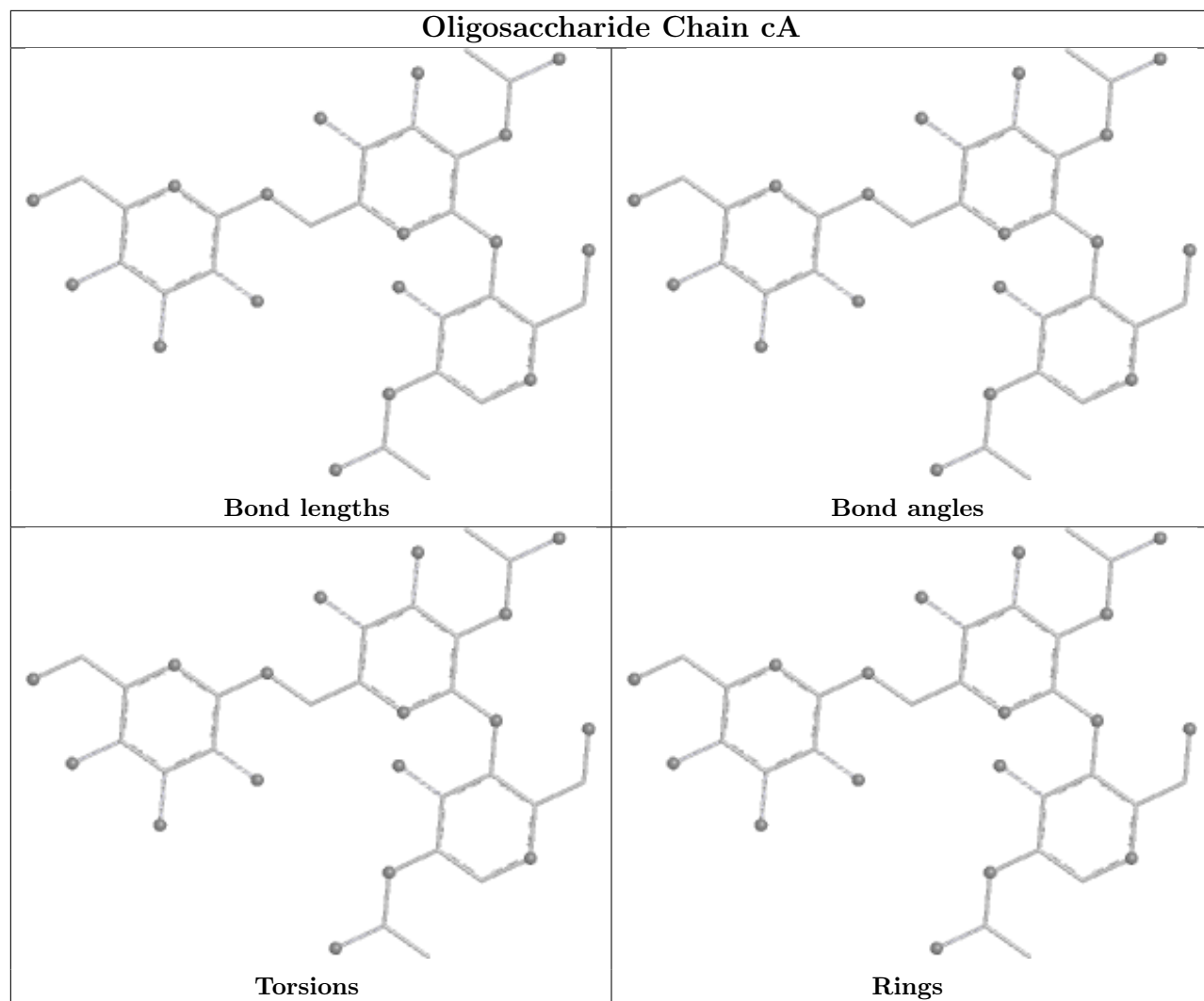
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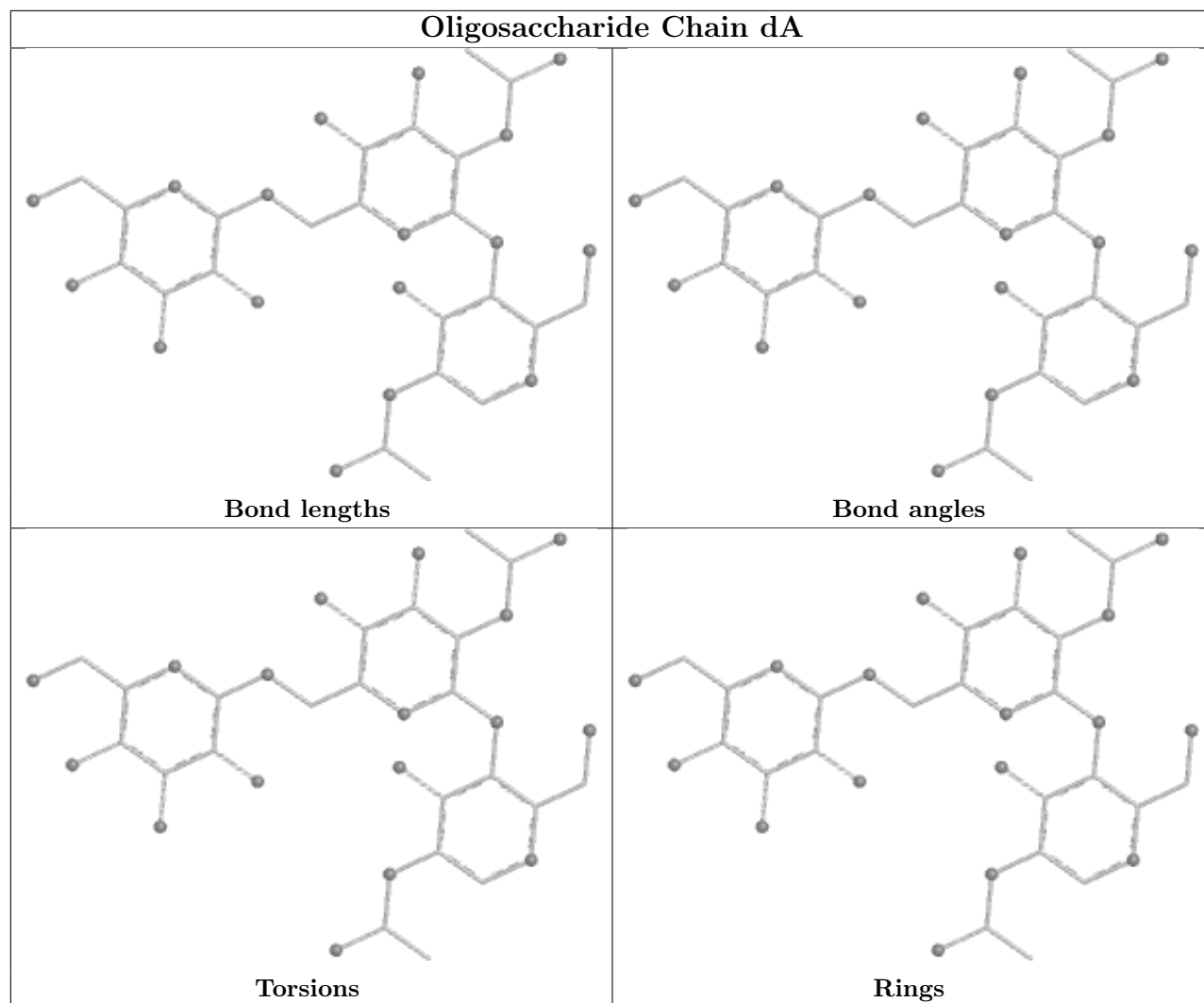
Oligosaccharide Chain aA



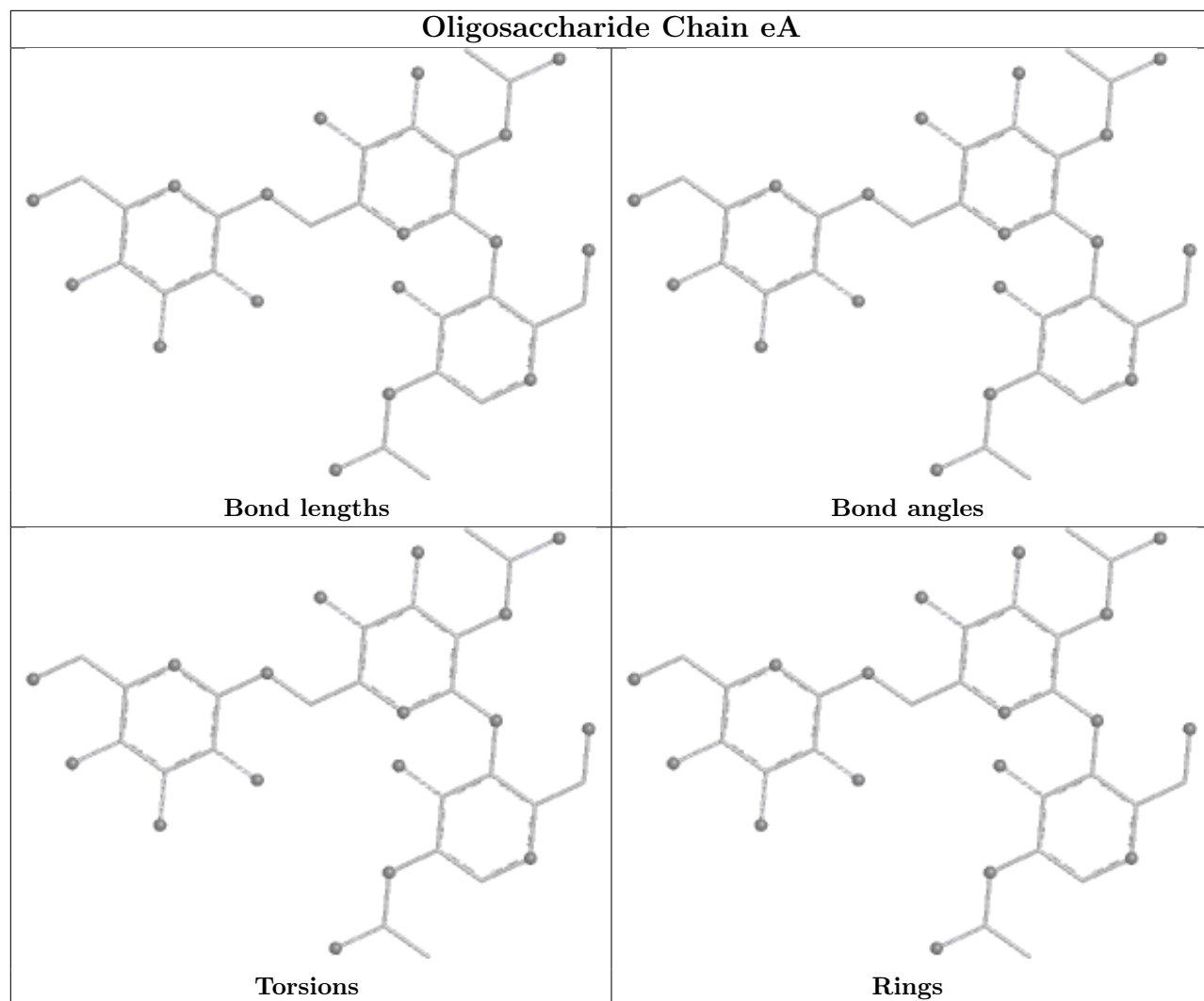
Oligosaccharide Chain bA

Oligosaccharide Chain cA

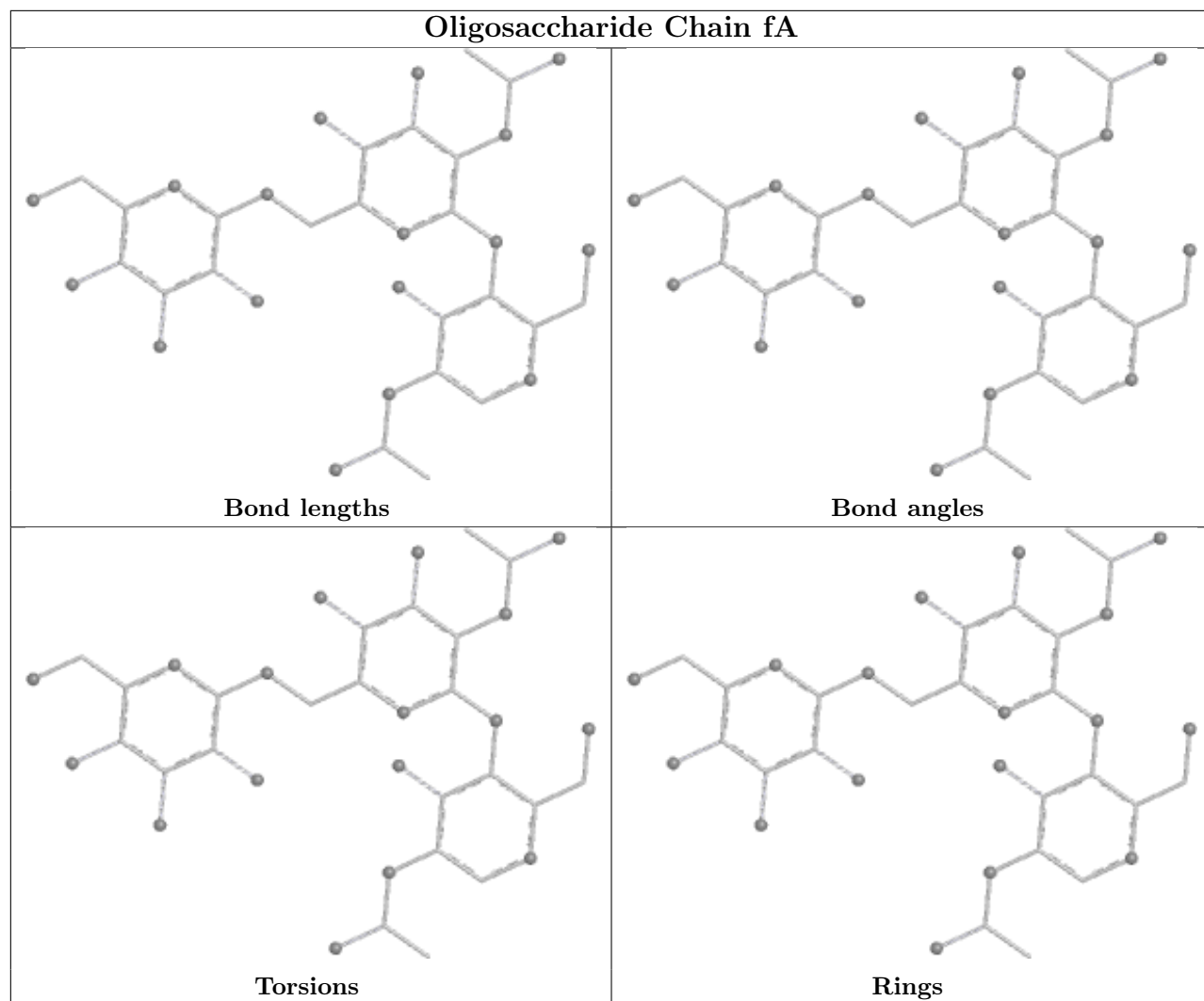


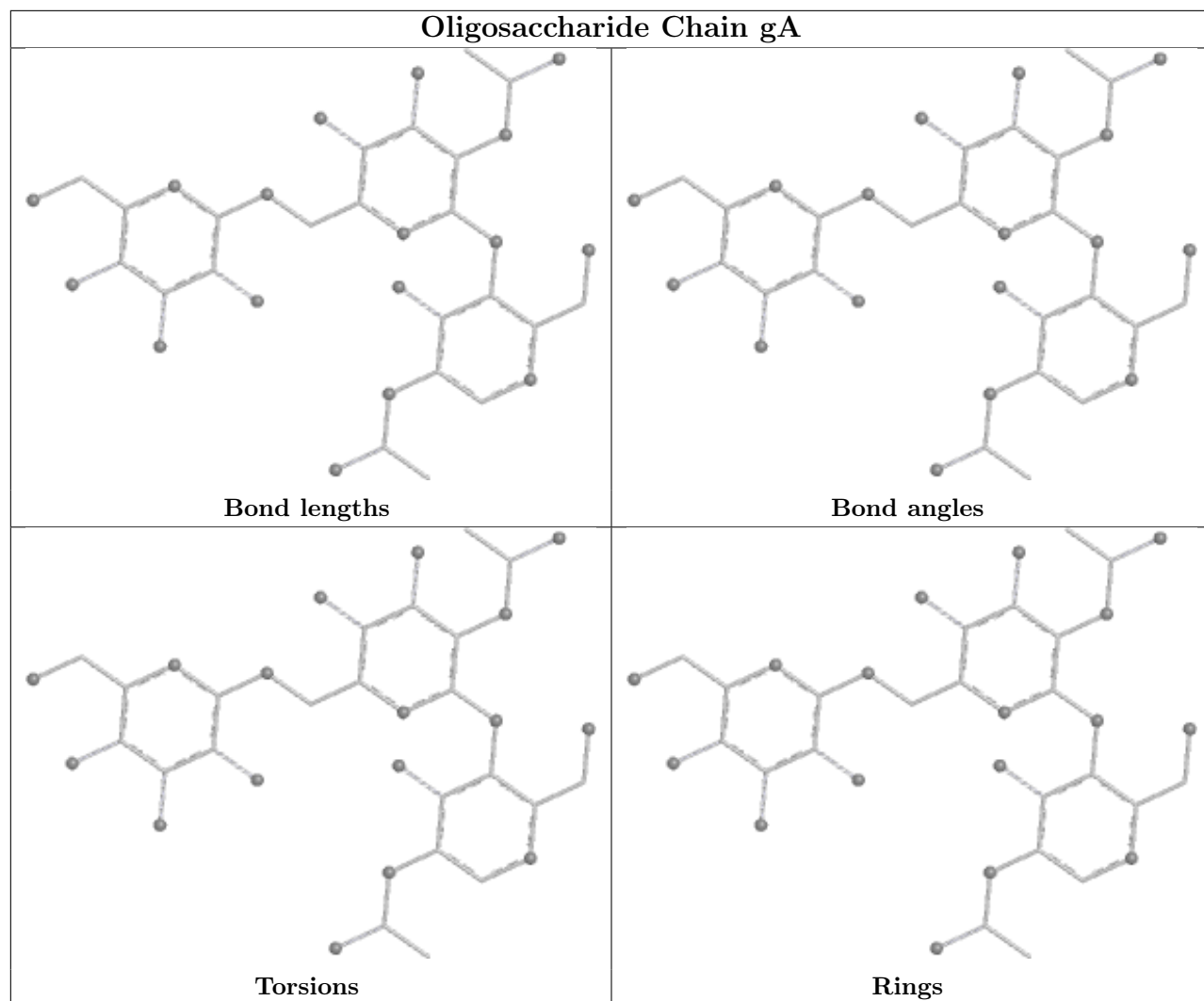
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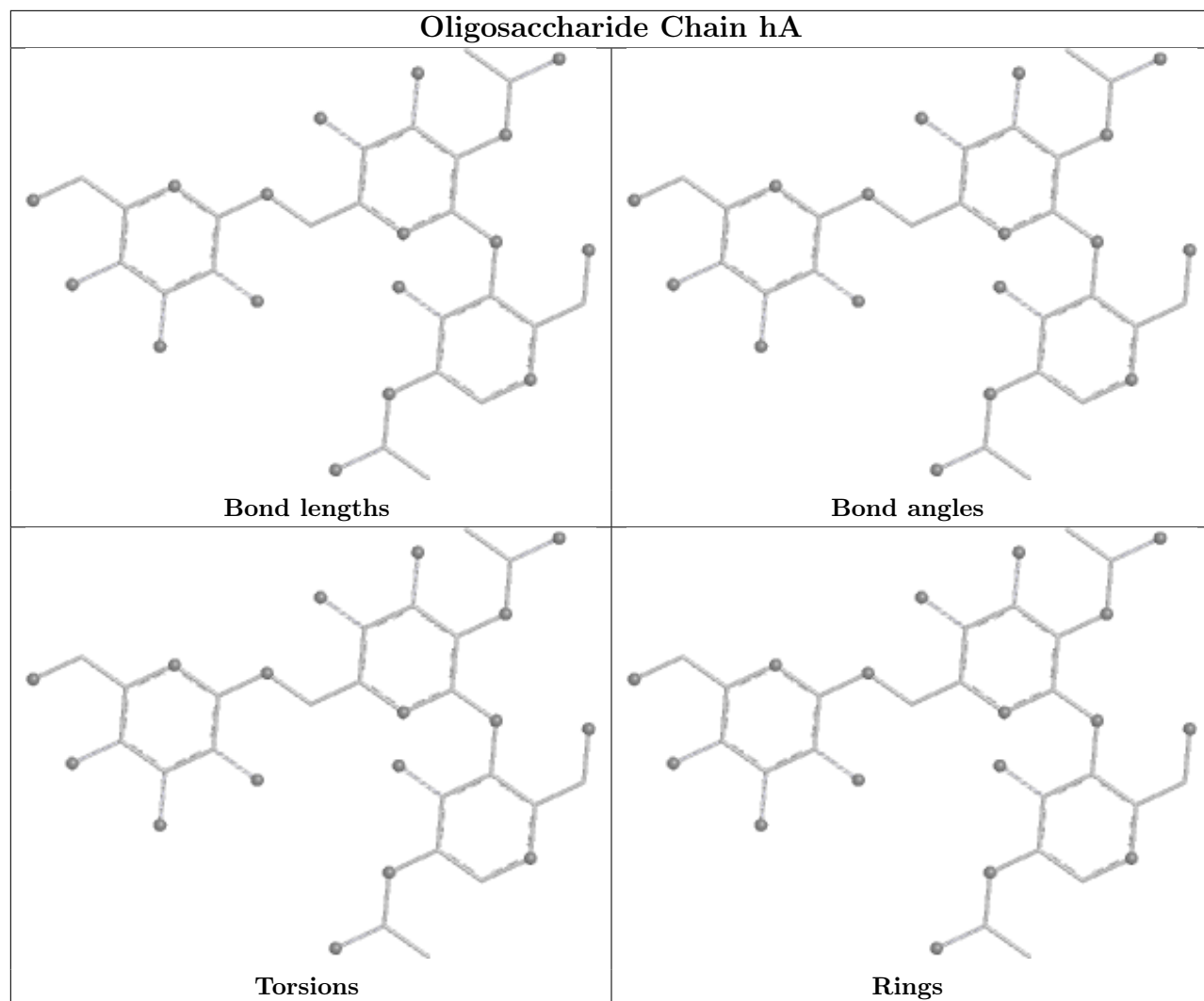
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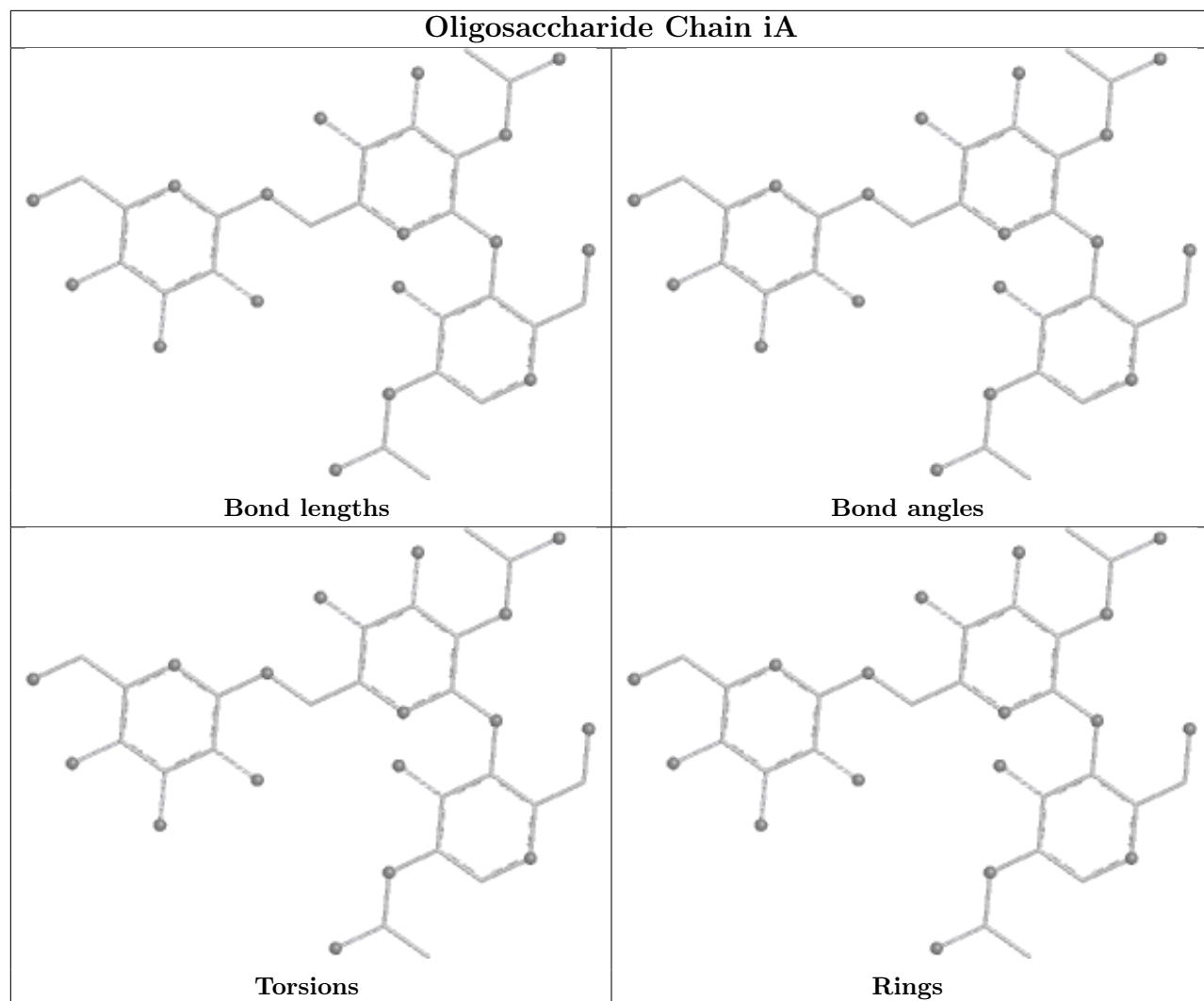
Oligosaccharide Chain fA



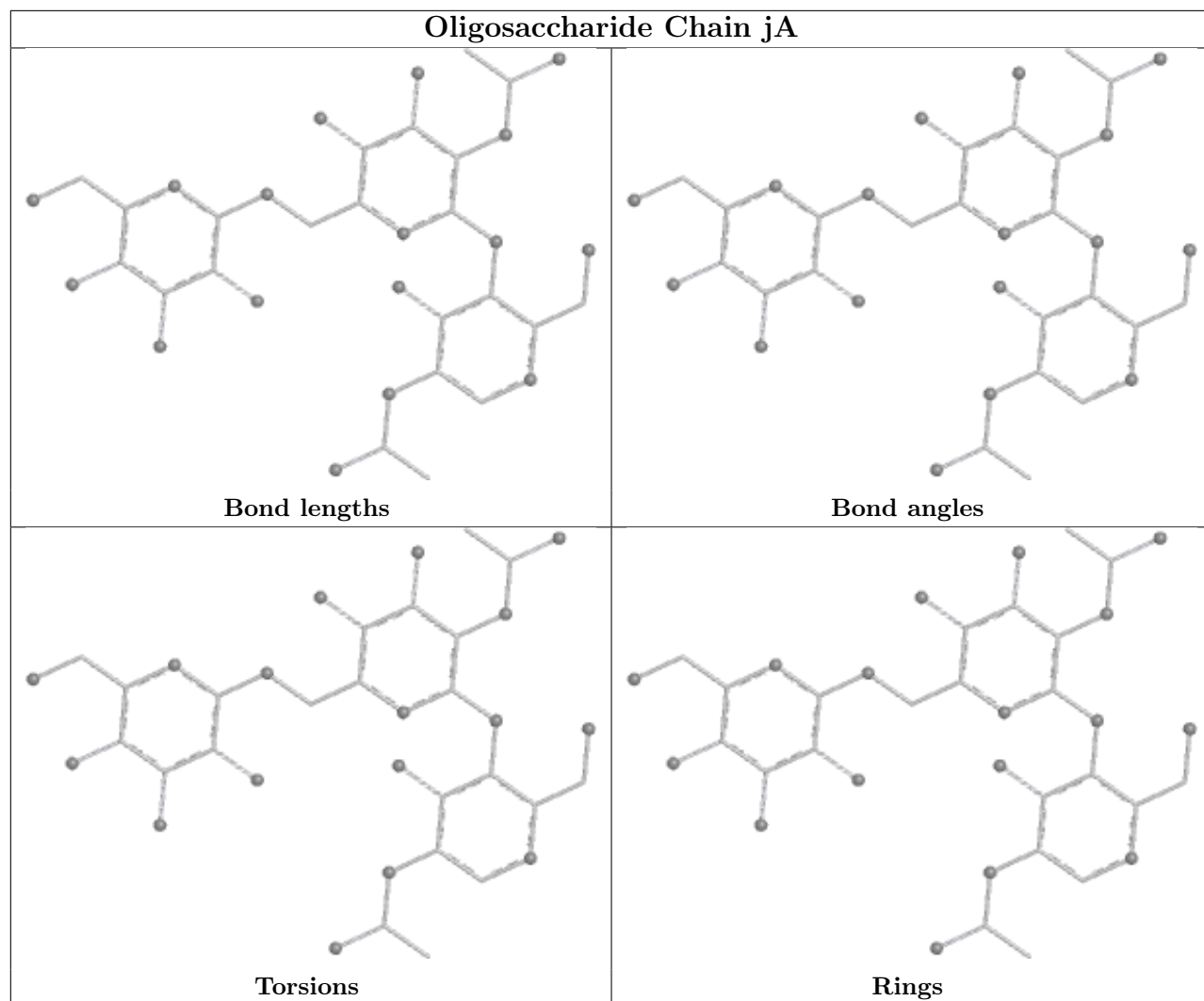
Oligosaccharide Chain gA

Oligosaccharide Chain hA

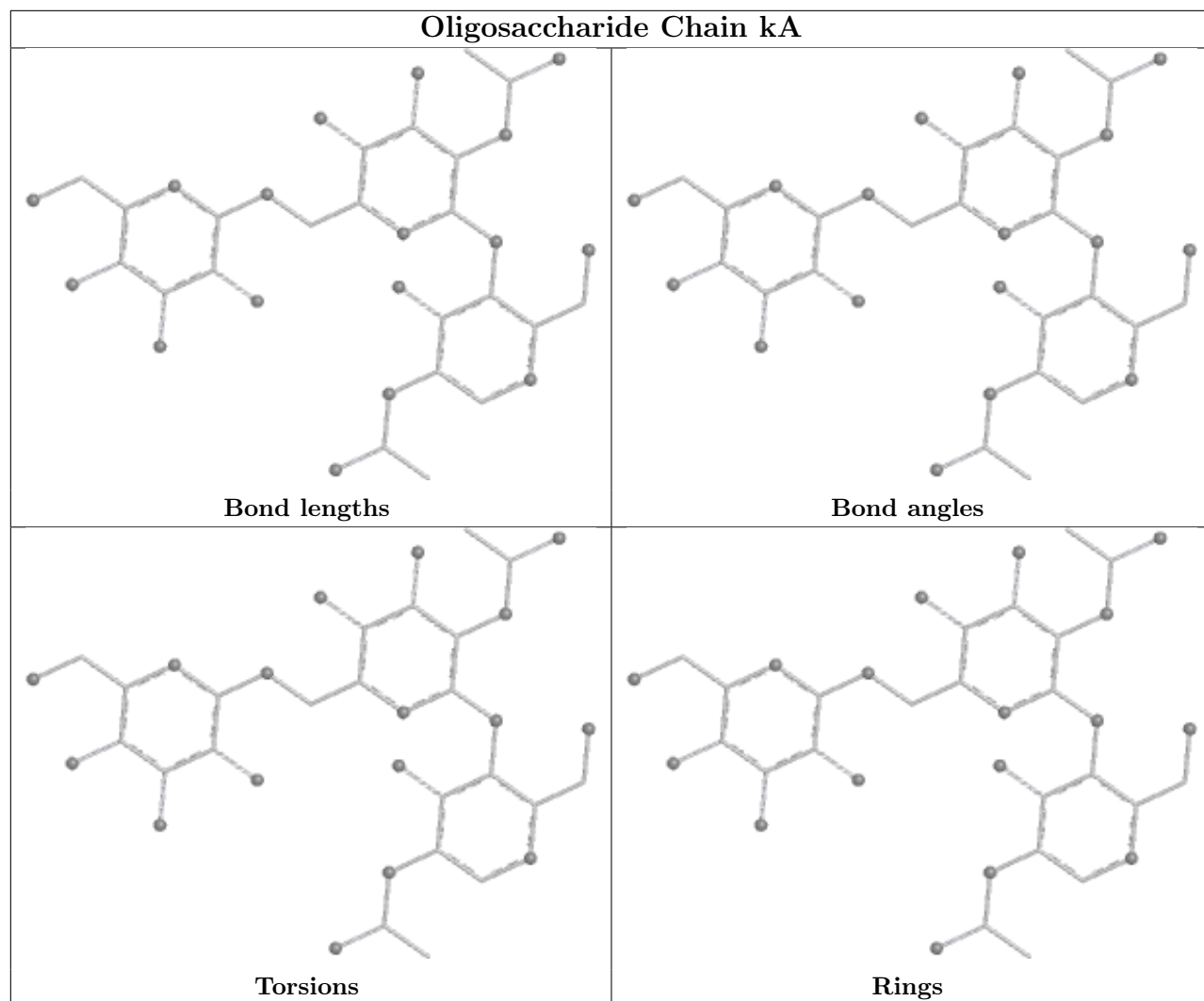
Oligosaccharide Chain iA

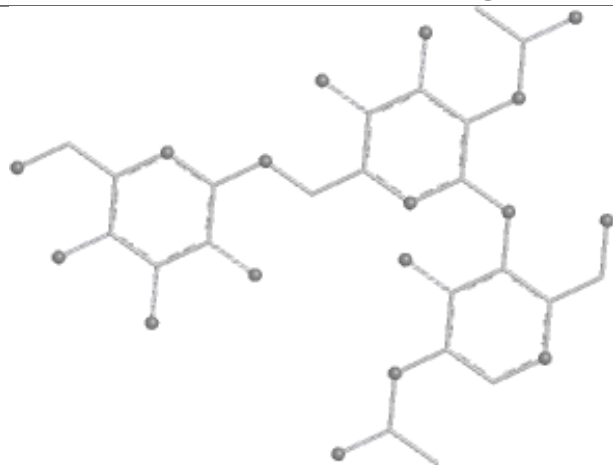
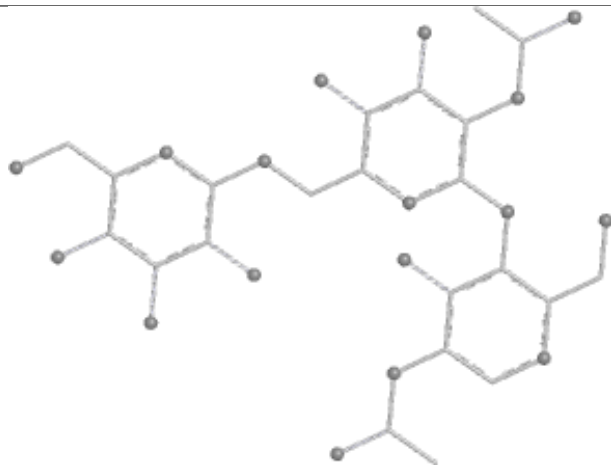
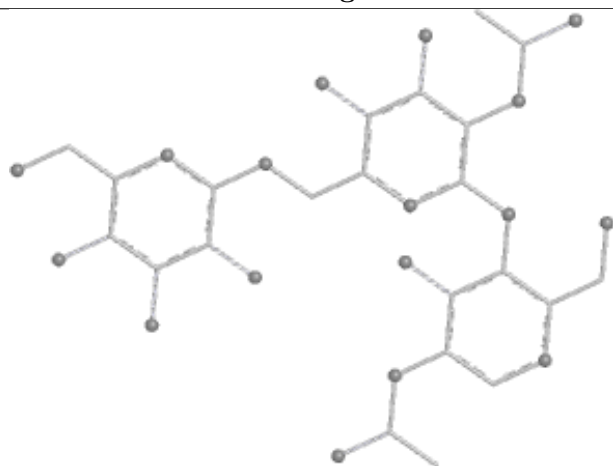
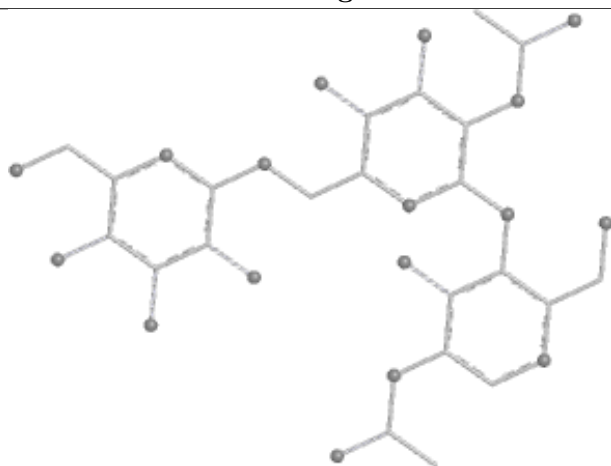


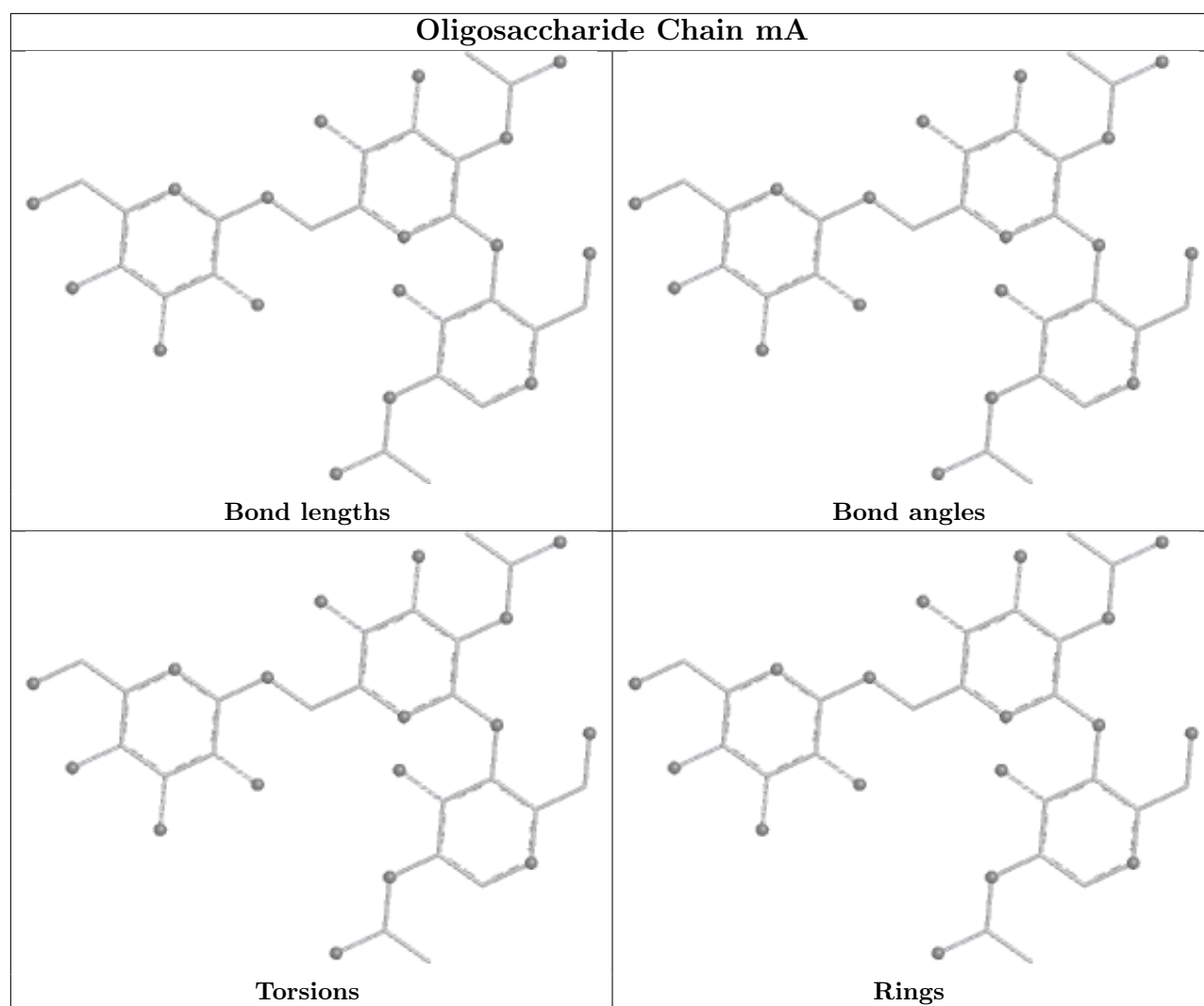
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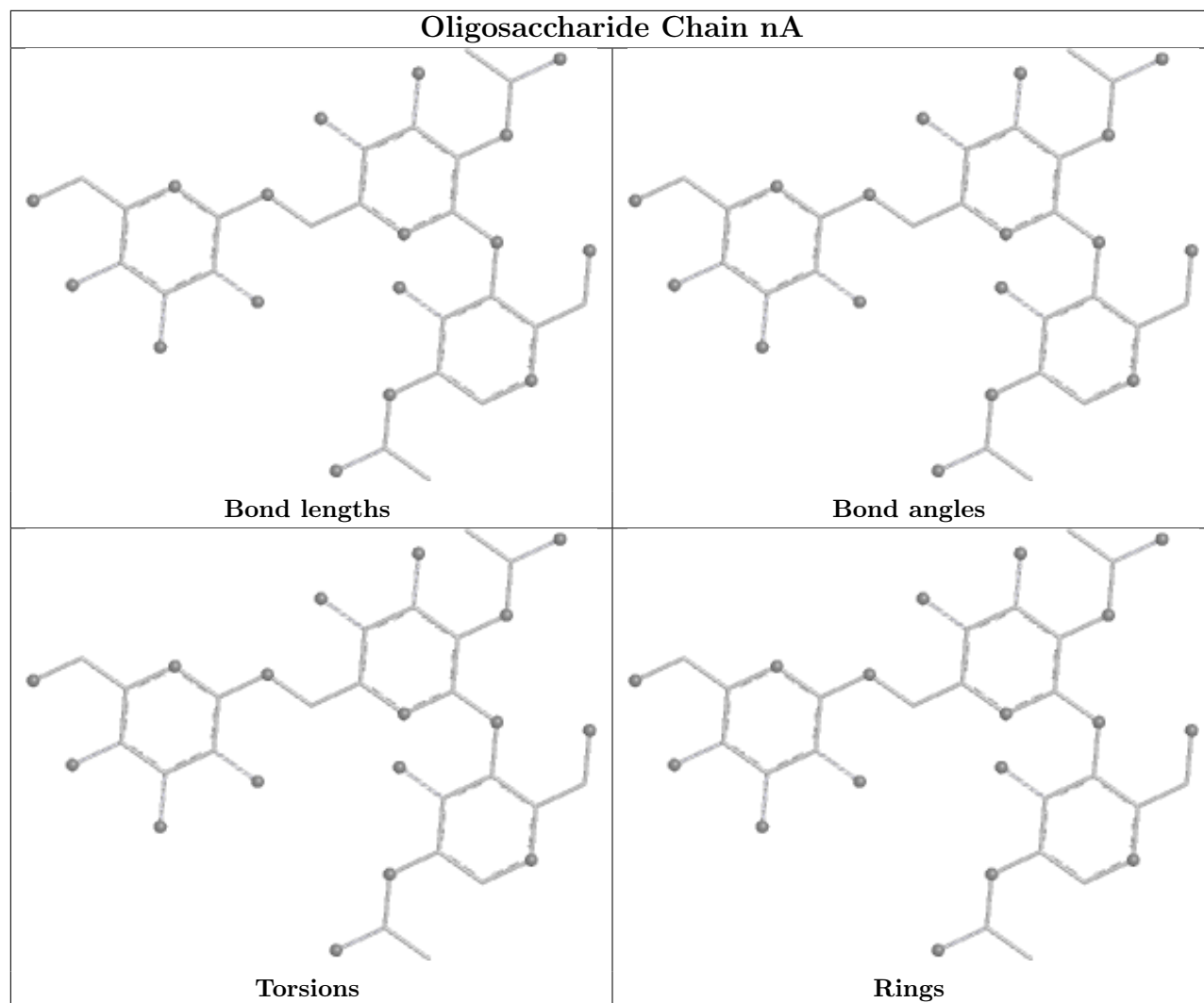


Oligosaccharide Chain kA

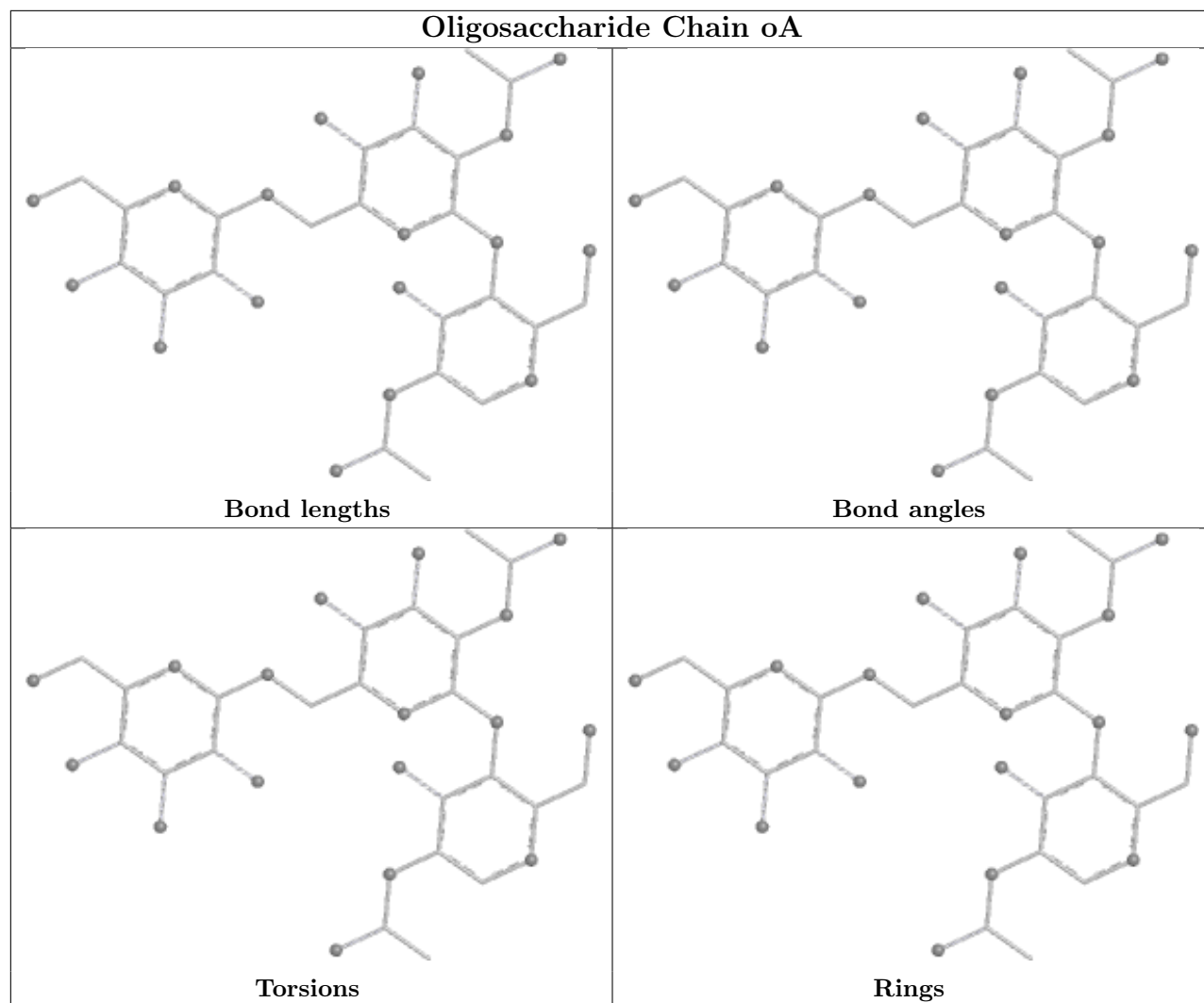


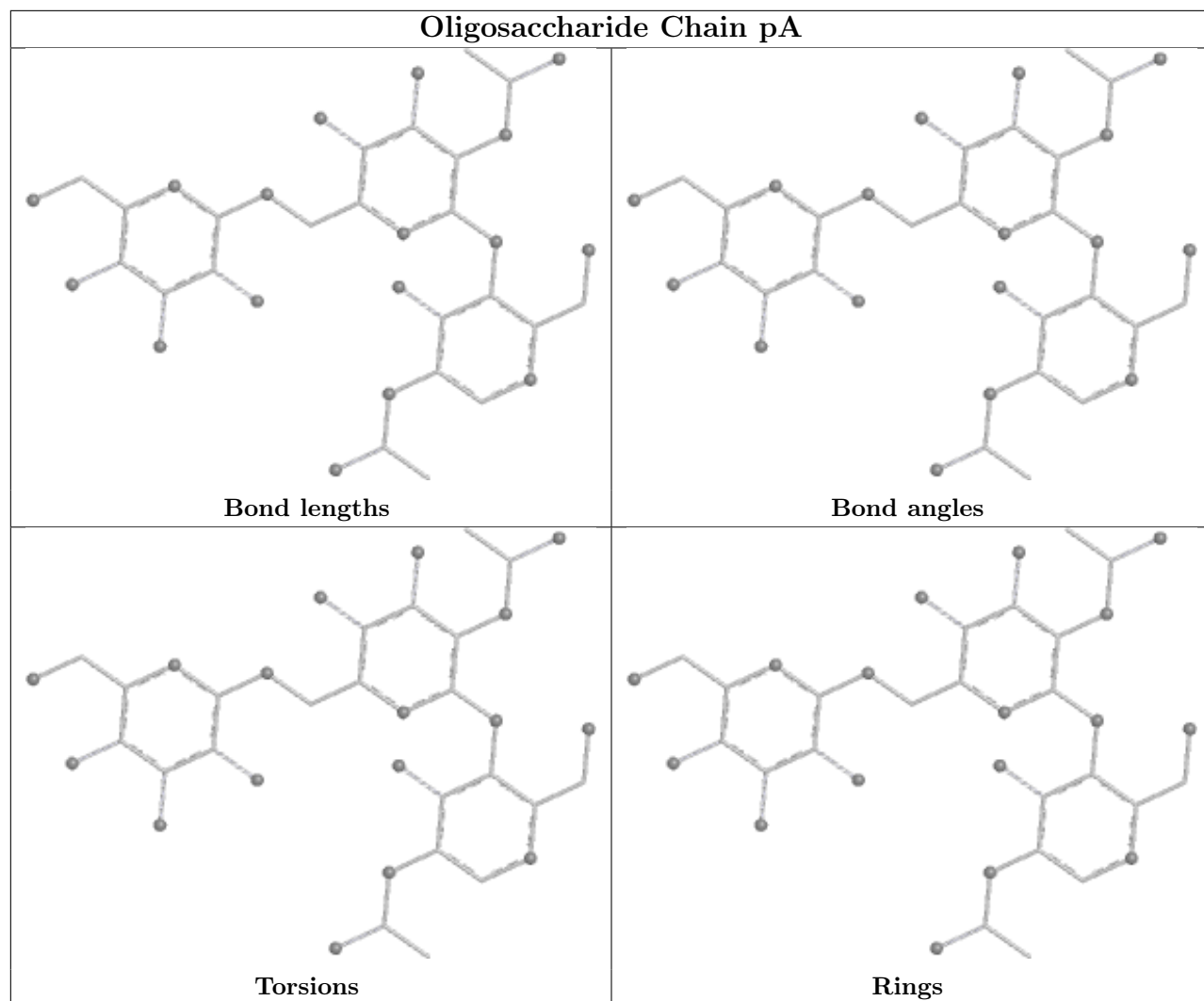
Oligosaccharide Chain 1A**Bond lengths****Bond angles****Torsions****Rings**

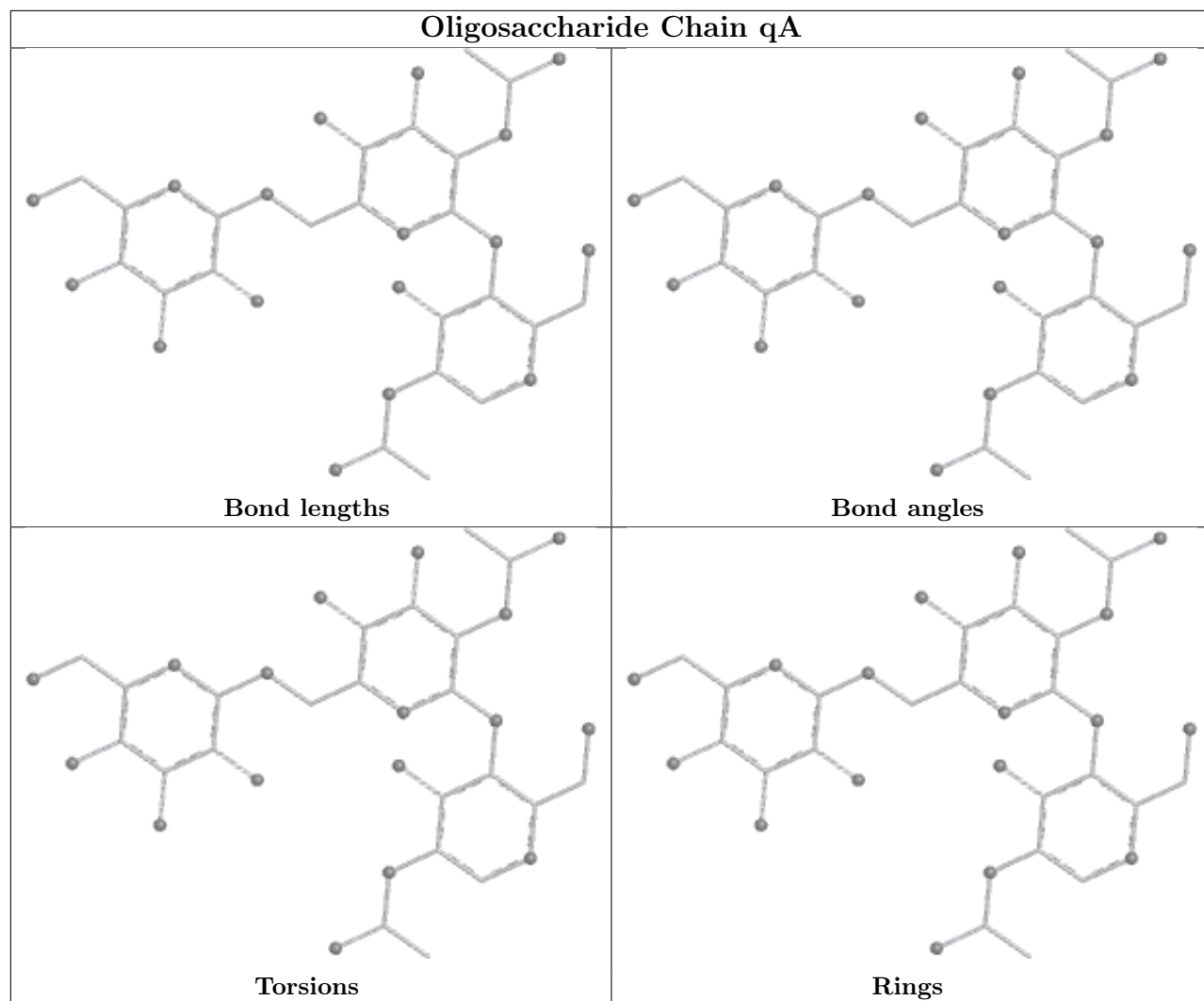


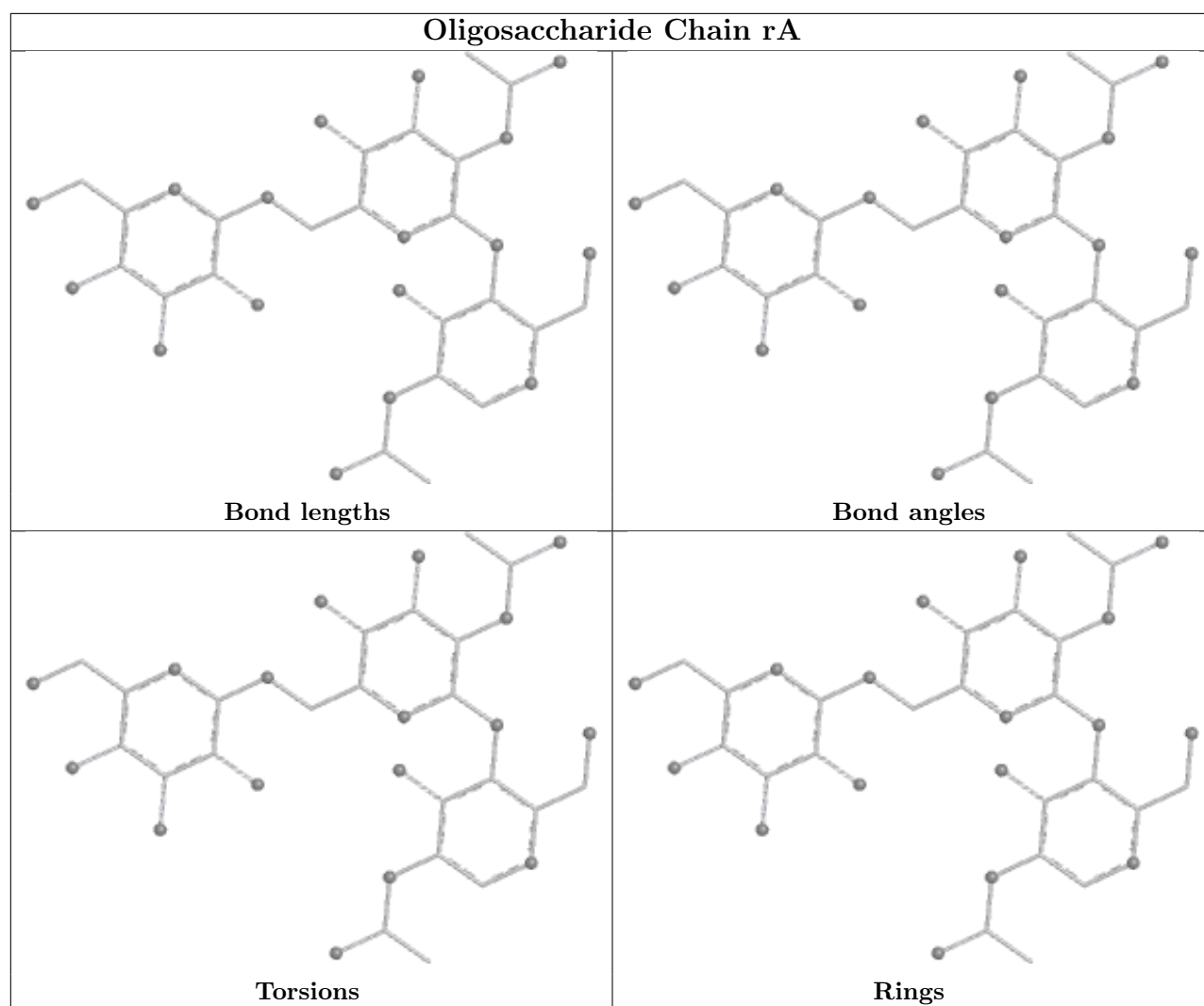


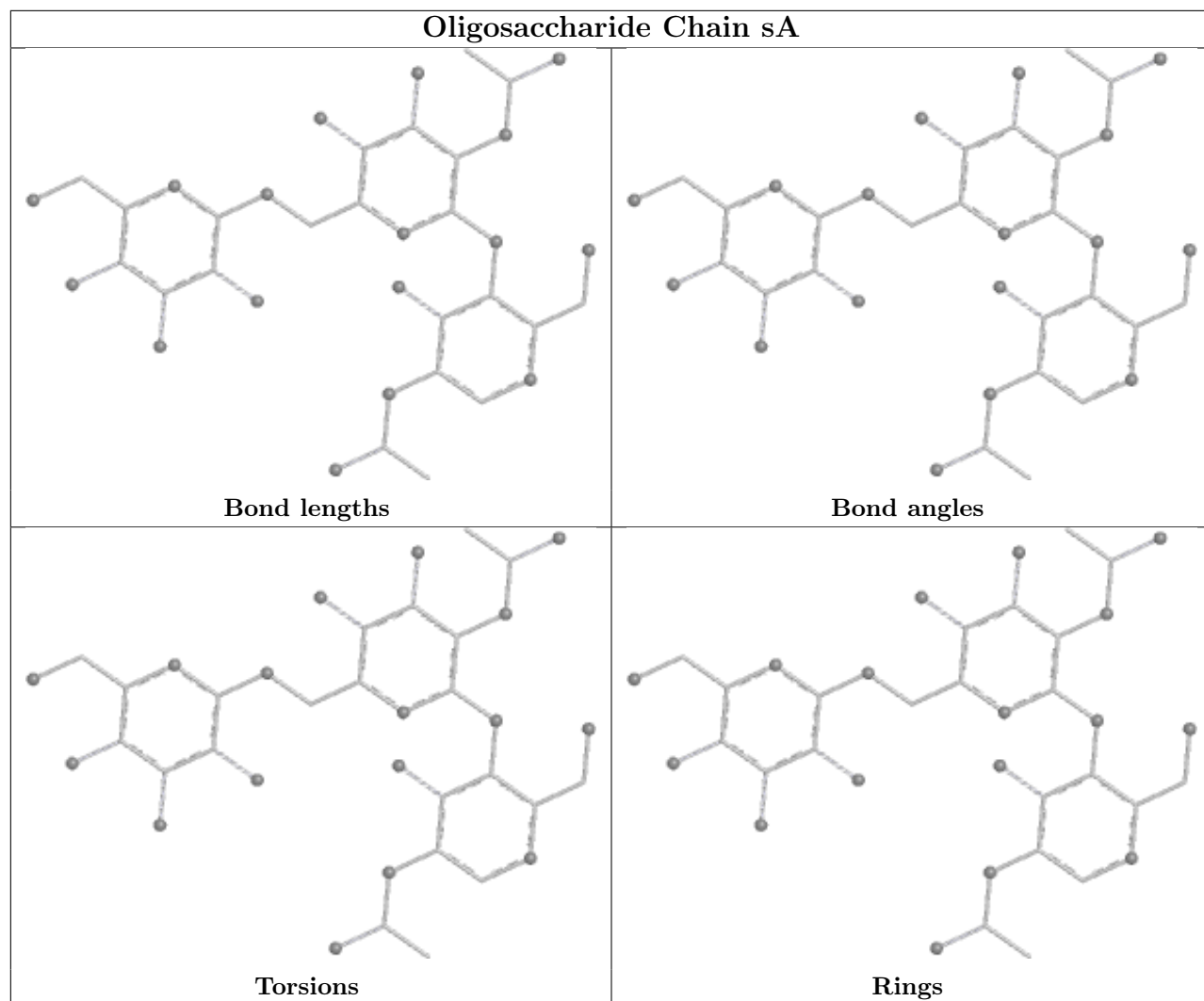
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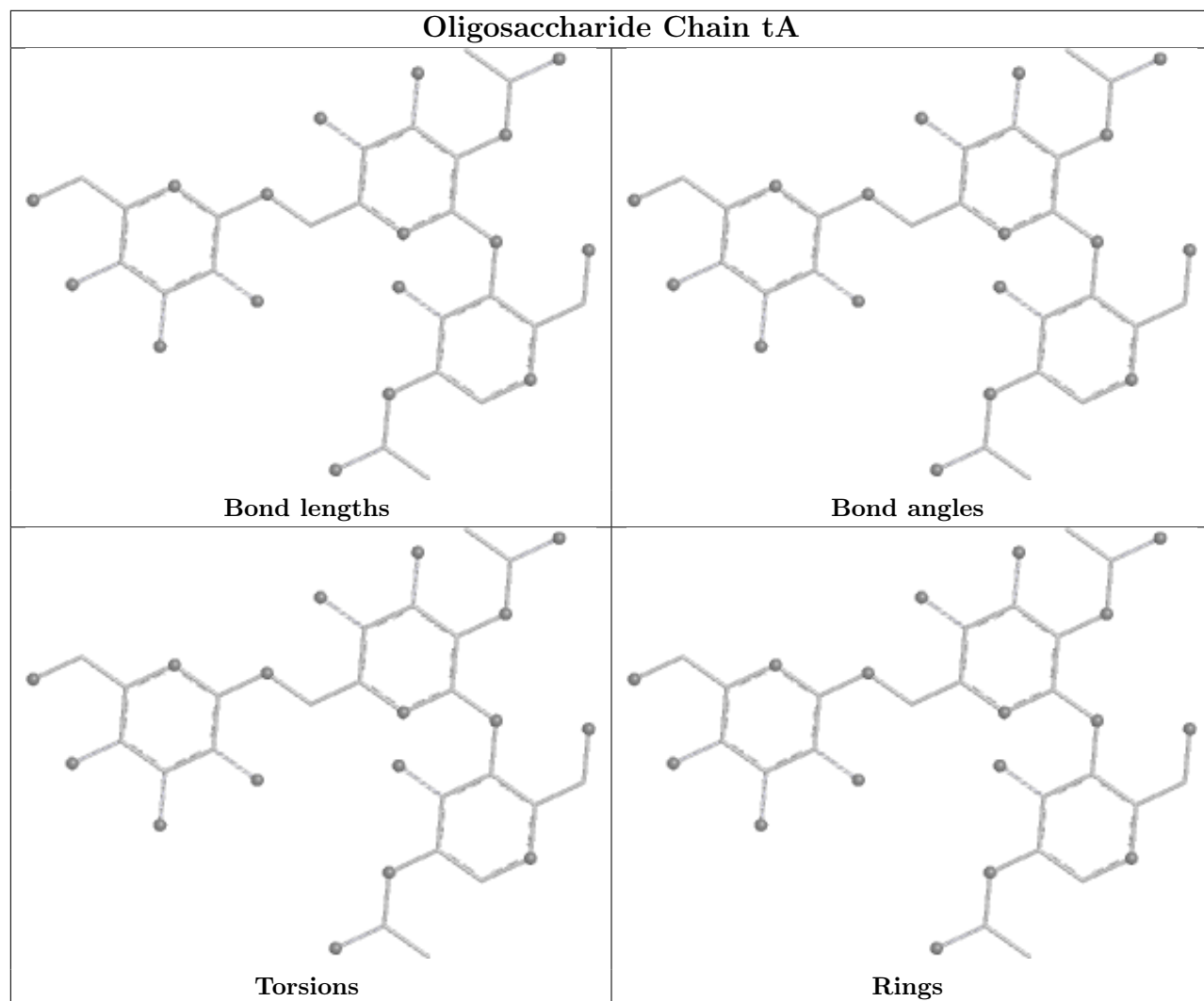
Oligosaccharide Chain pA

Oligosaccharide Chain qA

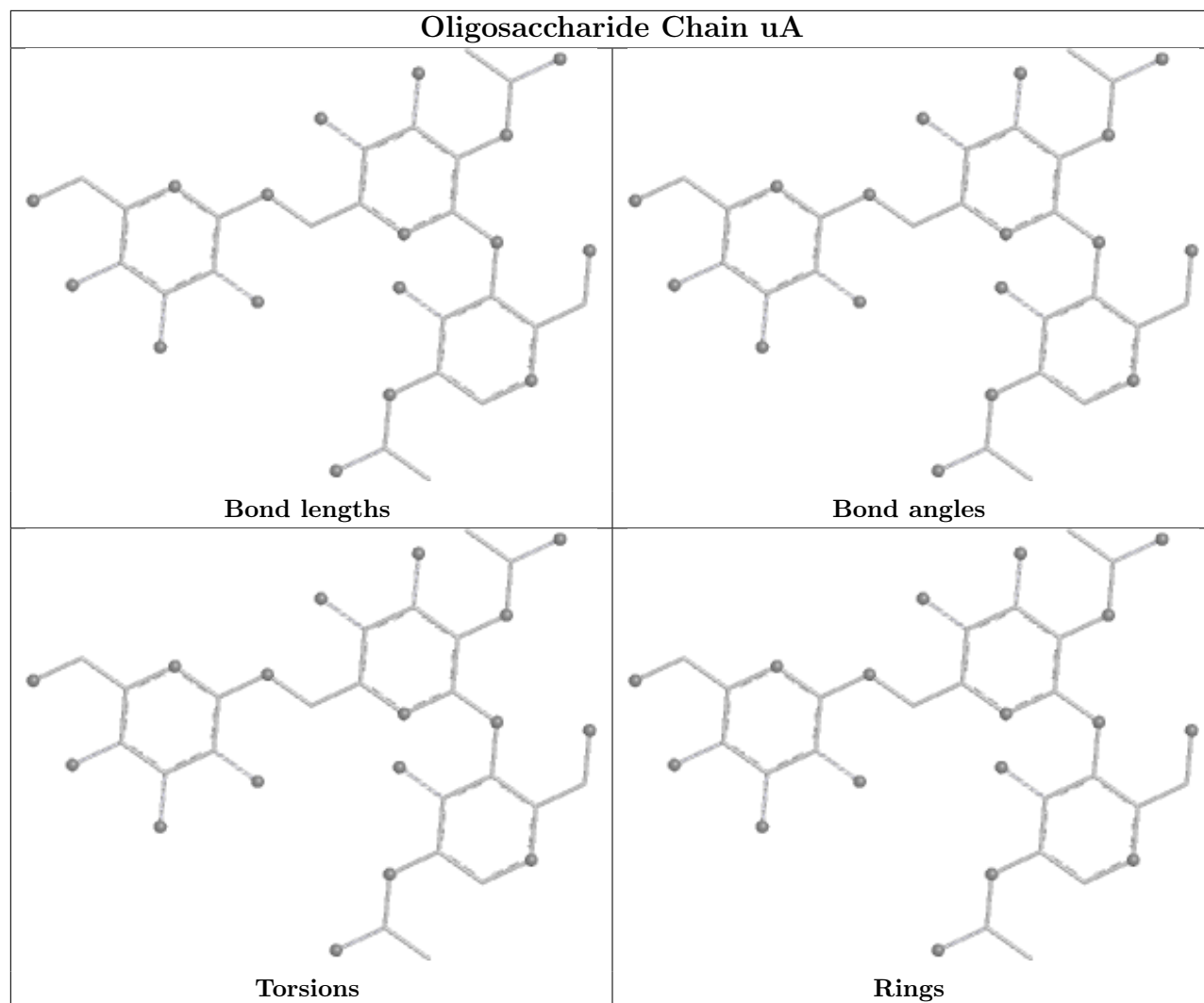


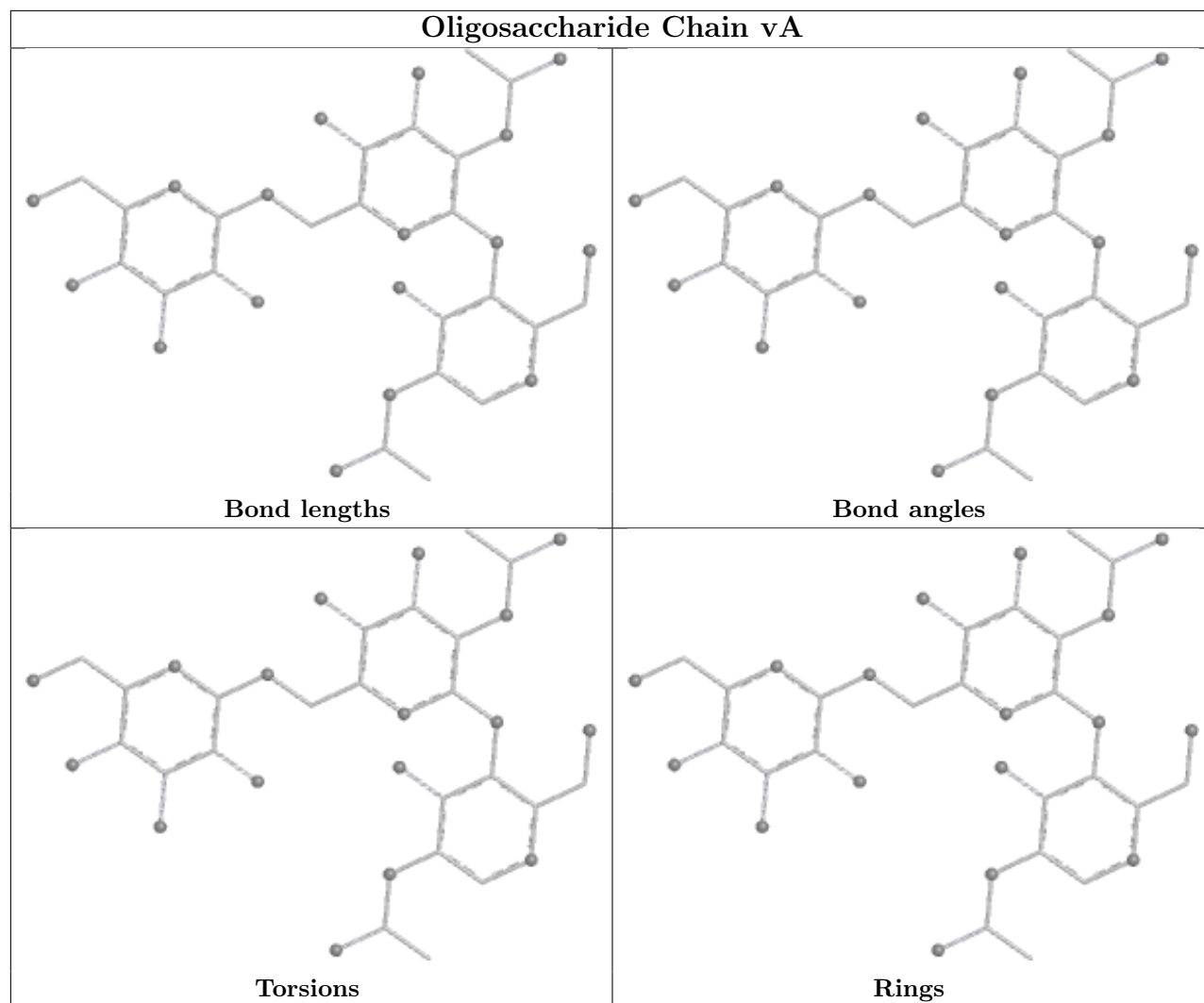


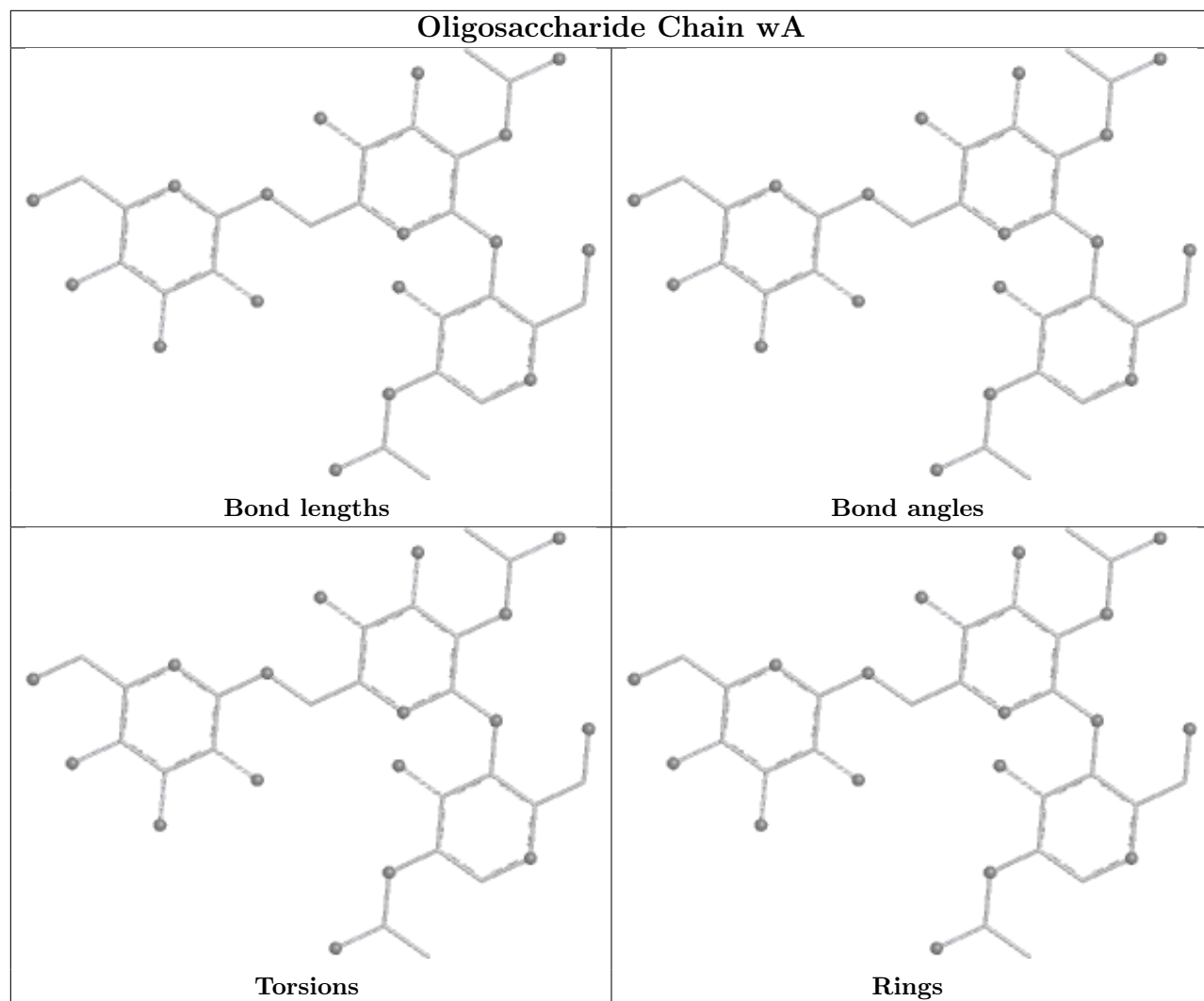
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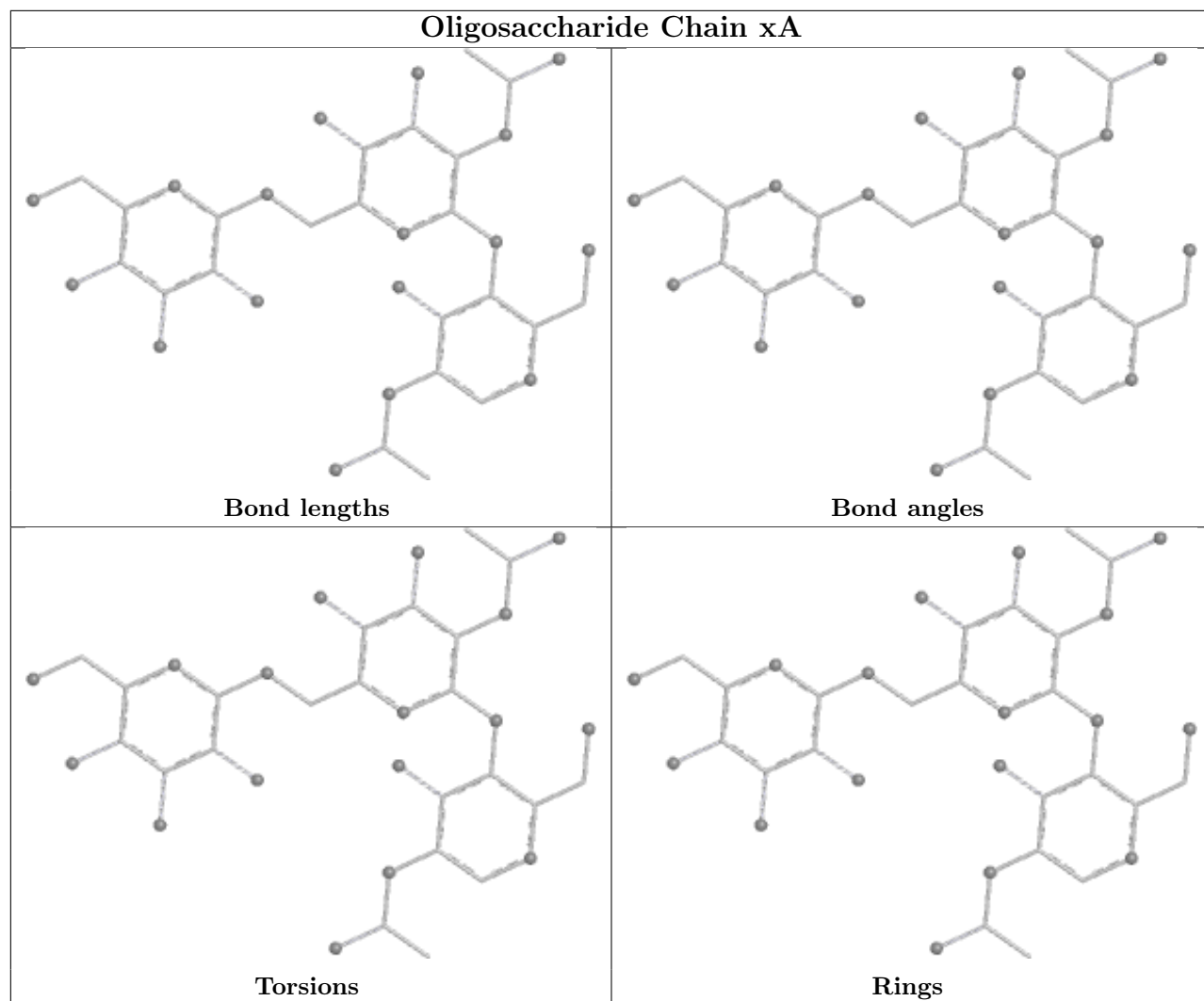


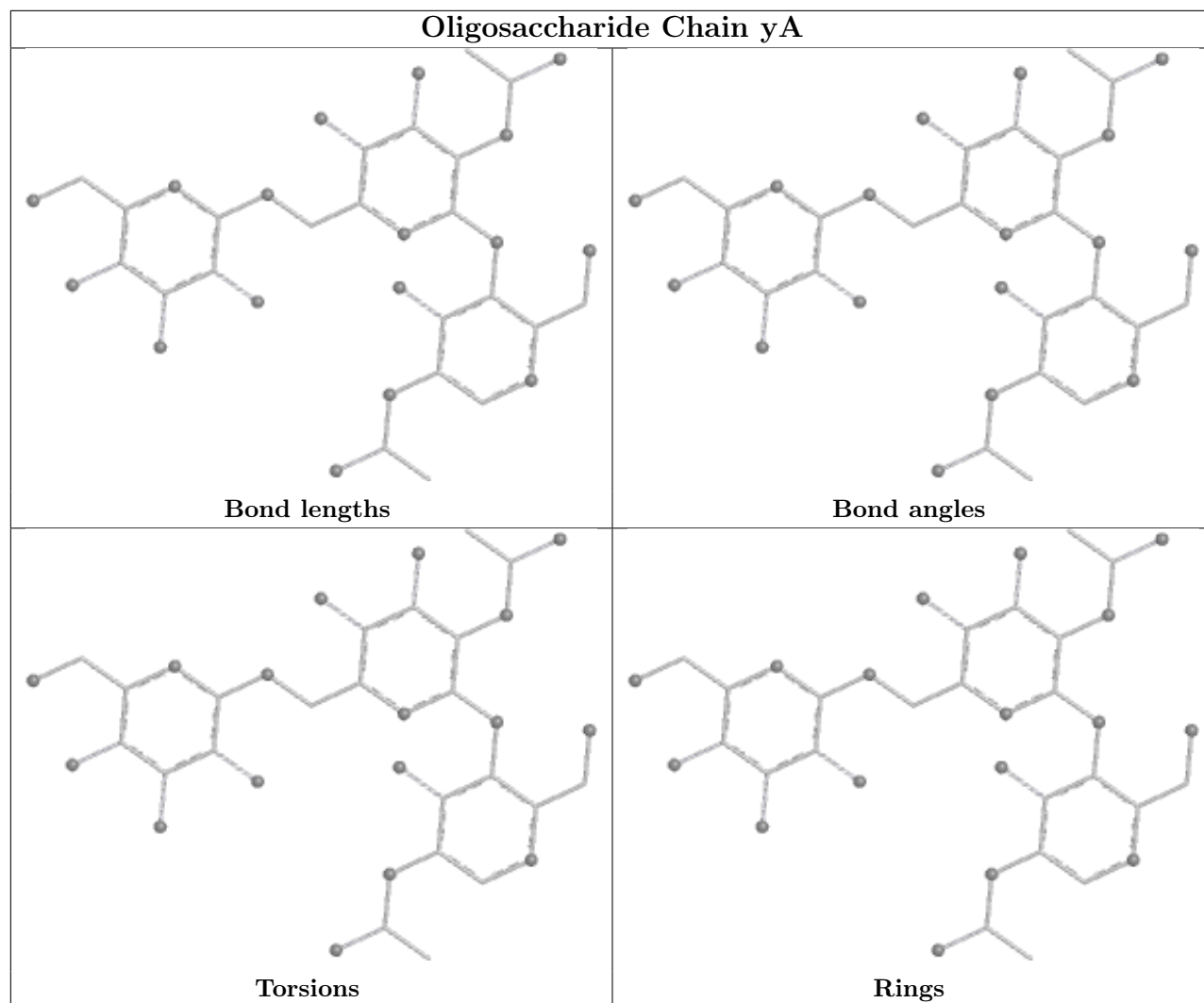
Oligosaccharide Chain uA



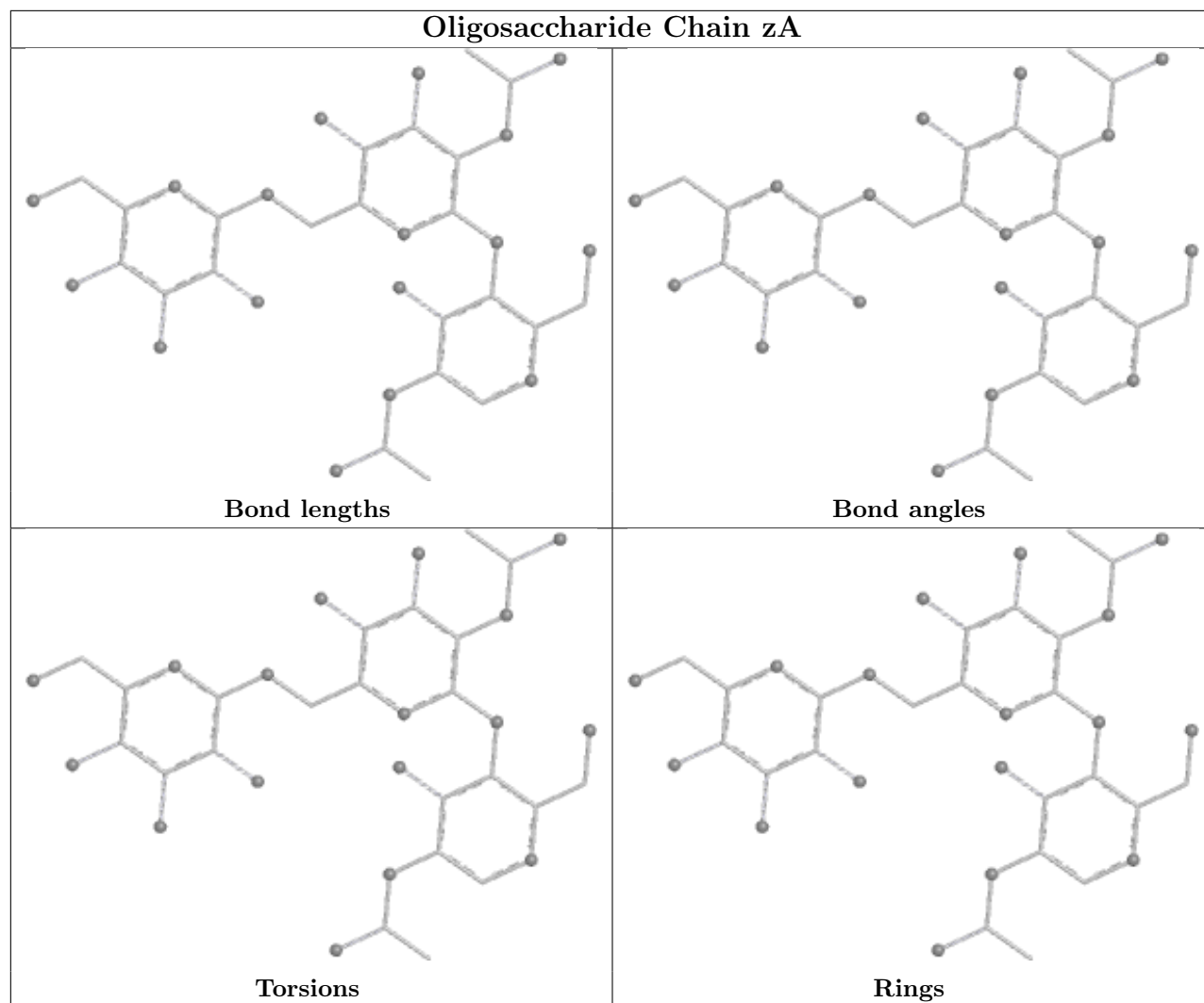
Oligosaccharide Chain vA

Oligosaccharide Chain wA

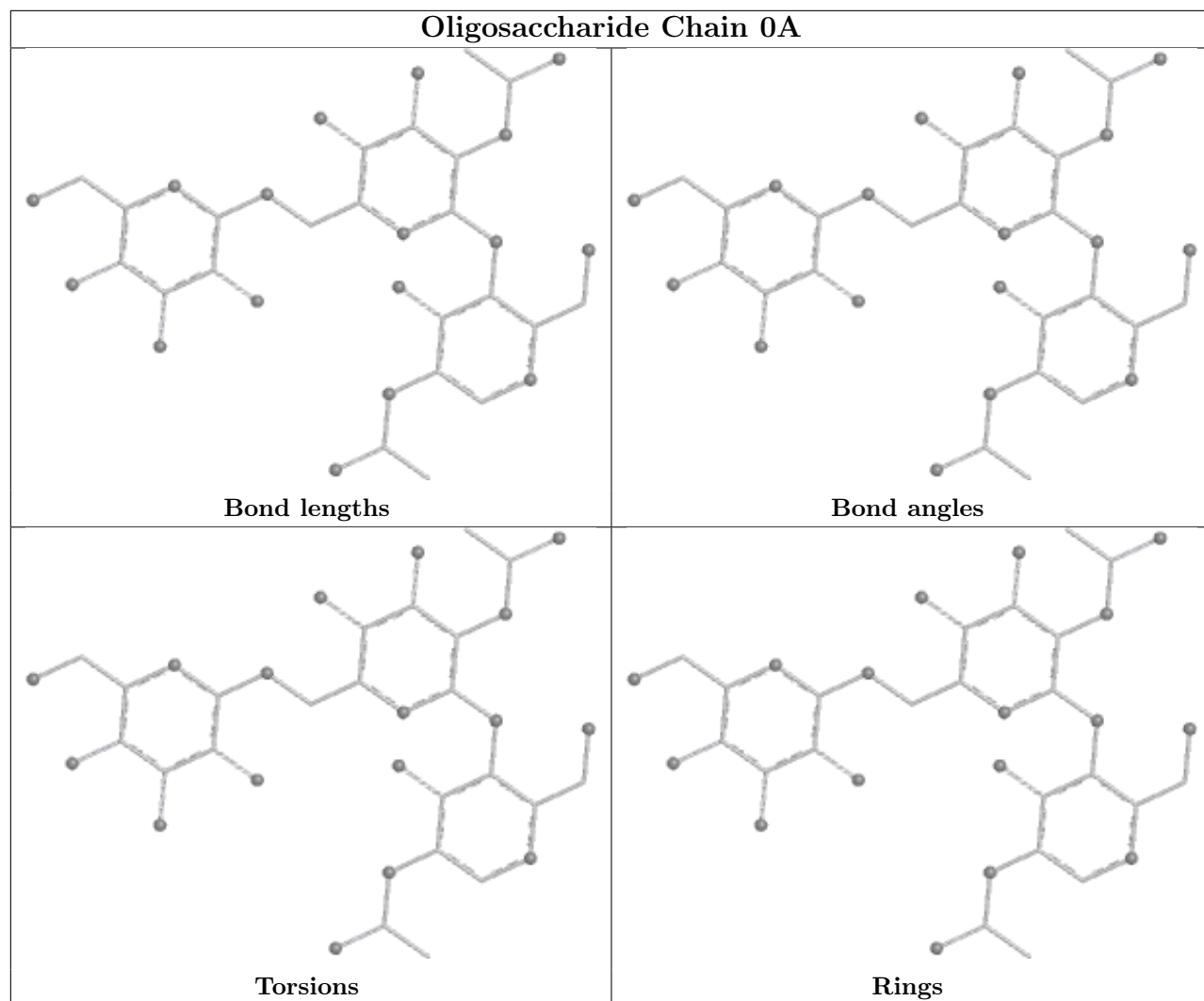


Oligosaccharide Chain yA

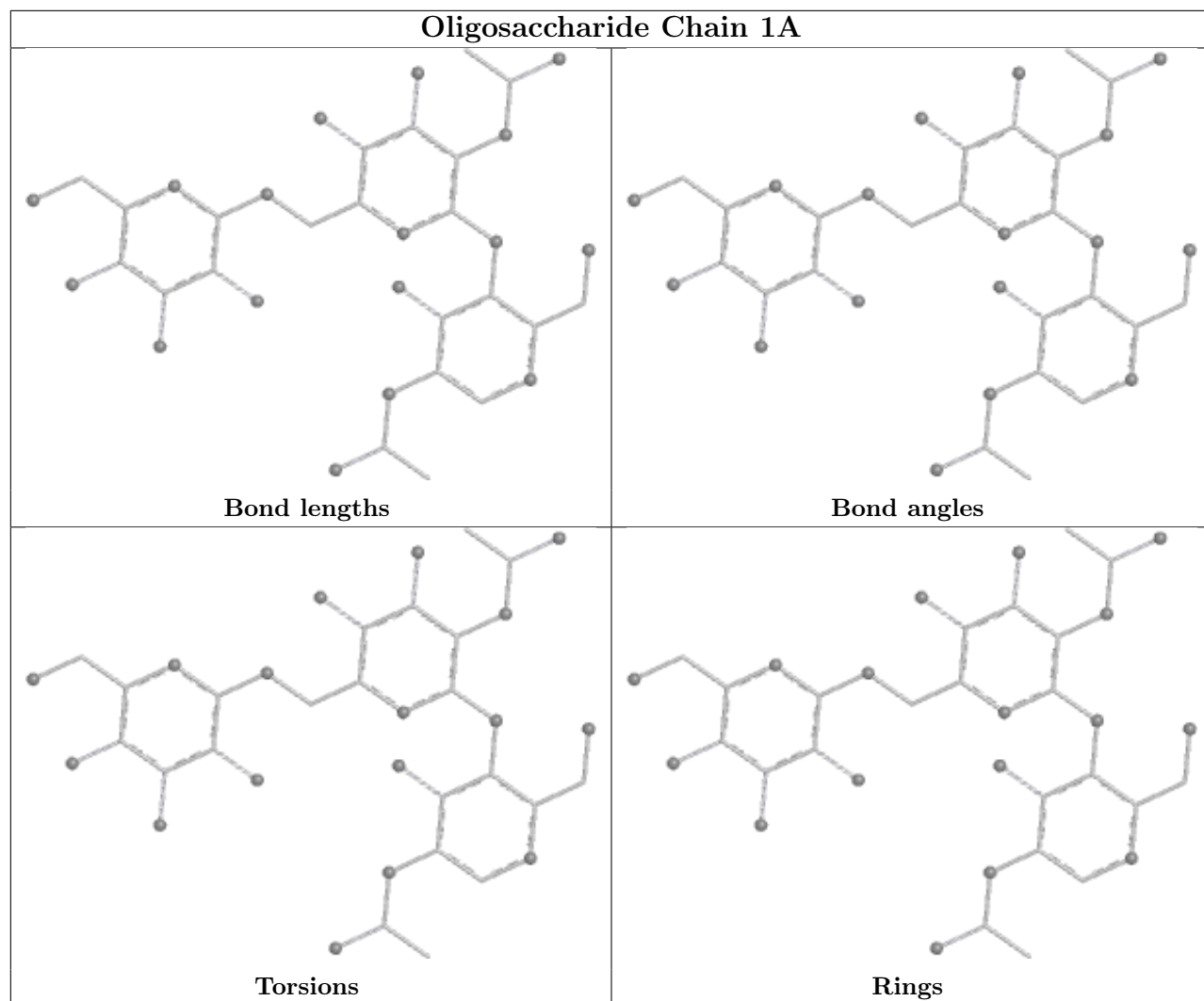
Oligosaccharide Chain zA



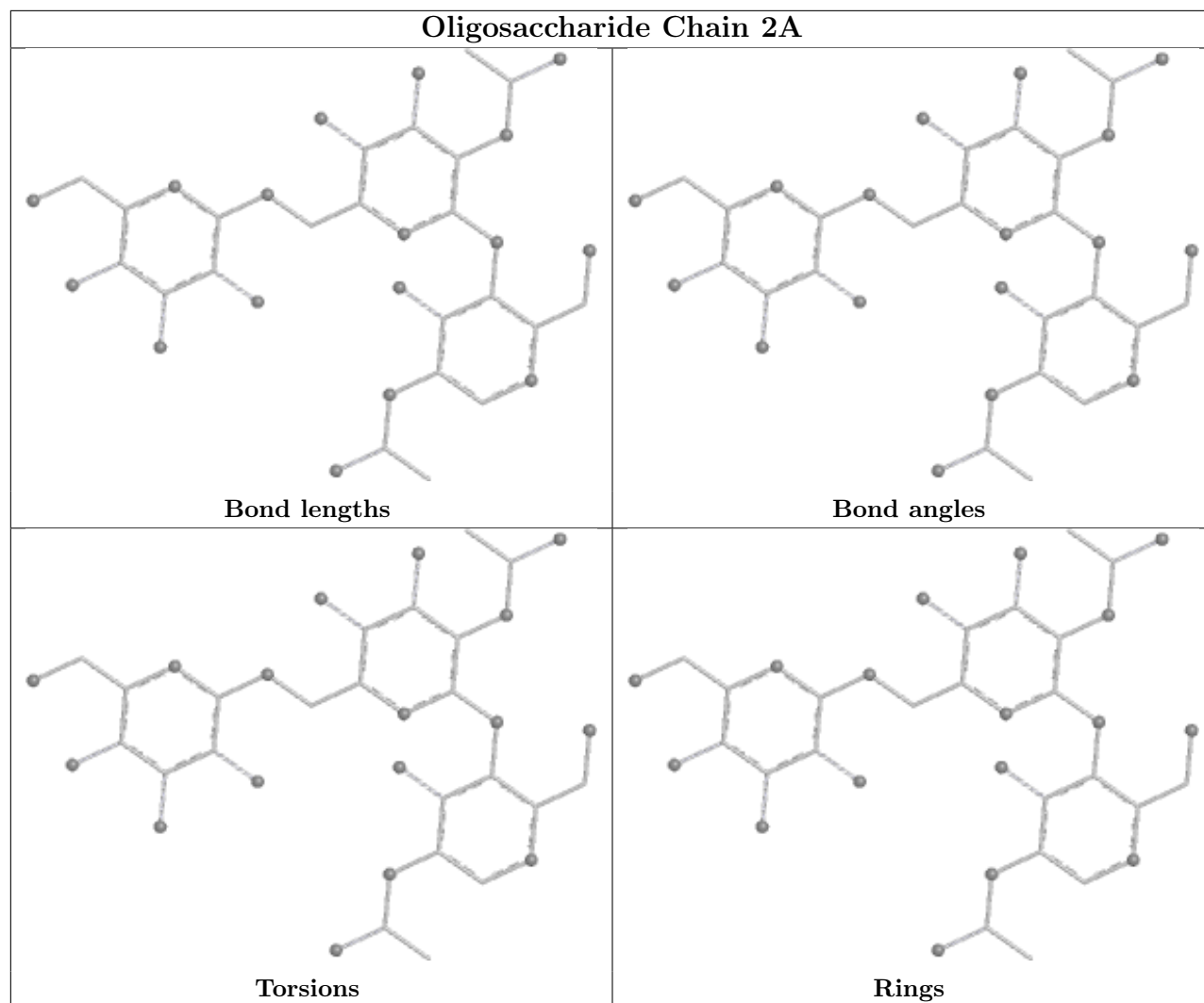
Oligosaccharide Chain 0A

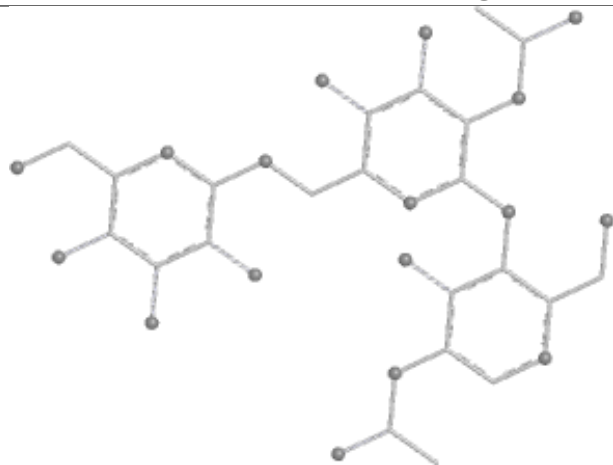
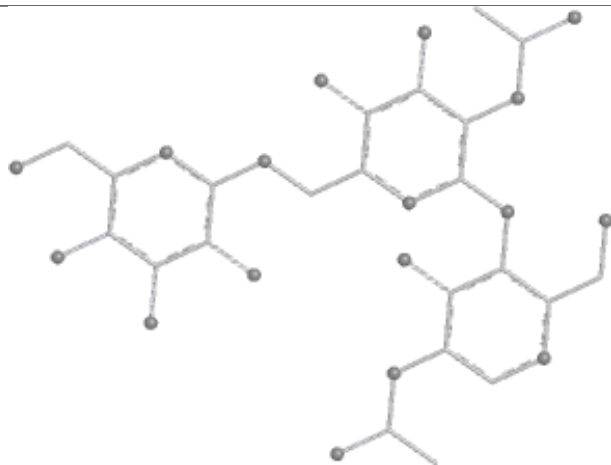
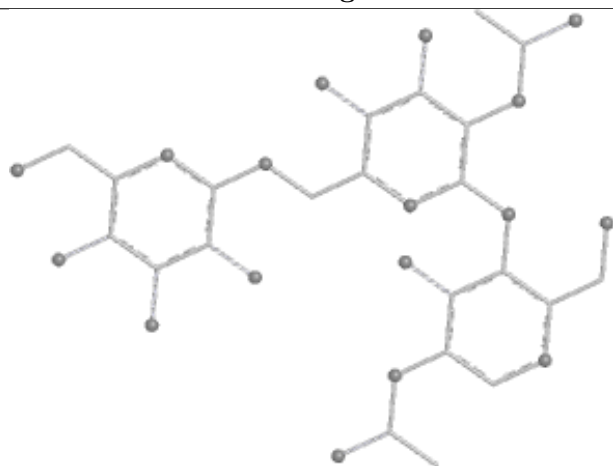
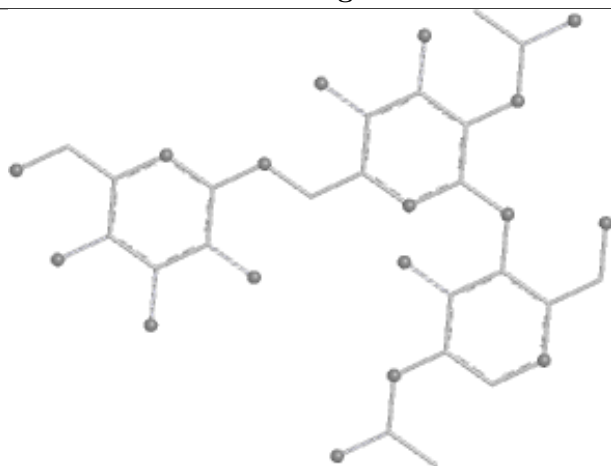


Oligosaccharide Chain 1A

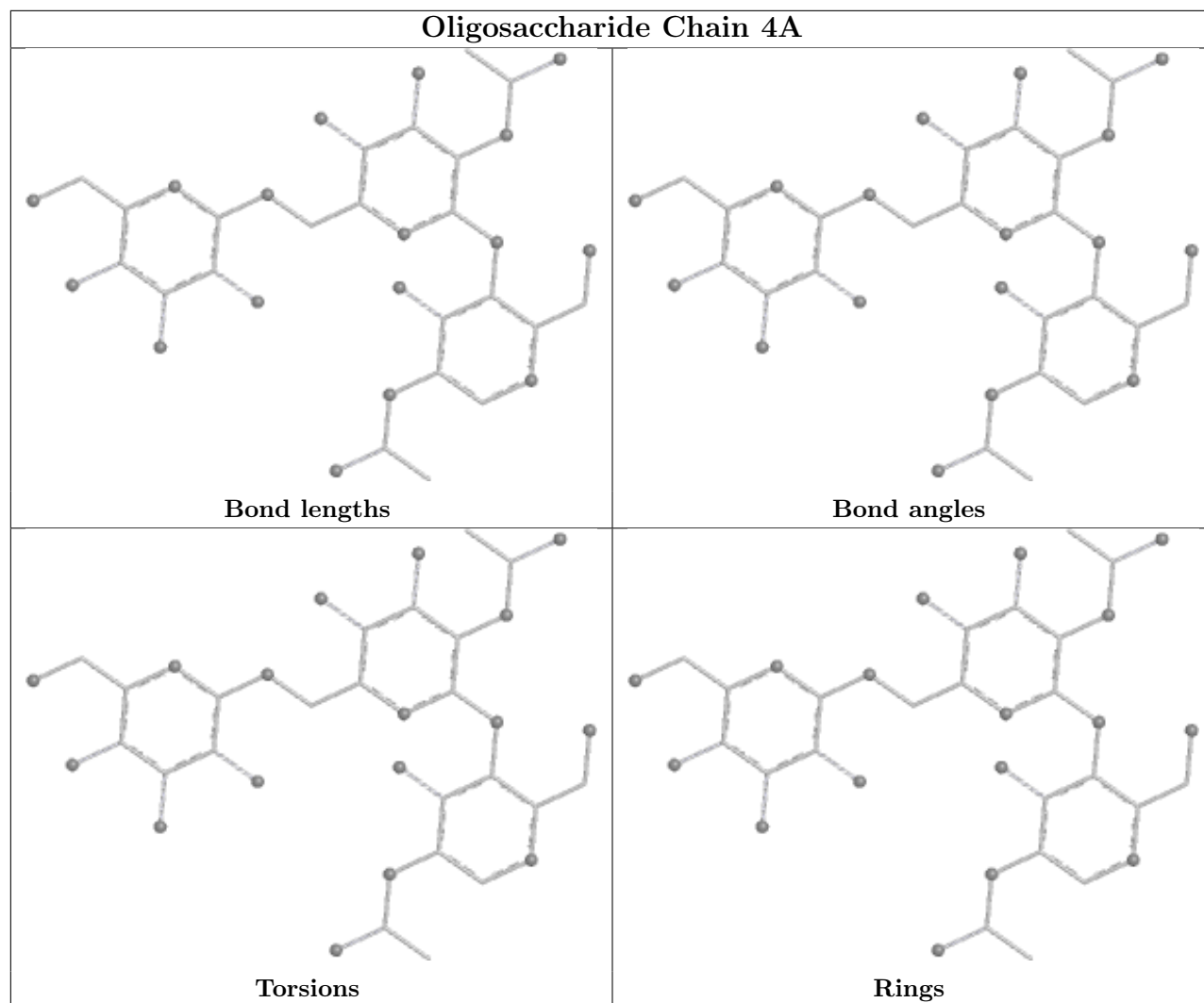


Oligosaccharide Chain 2A

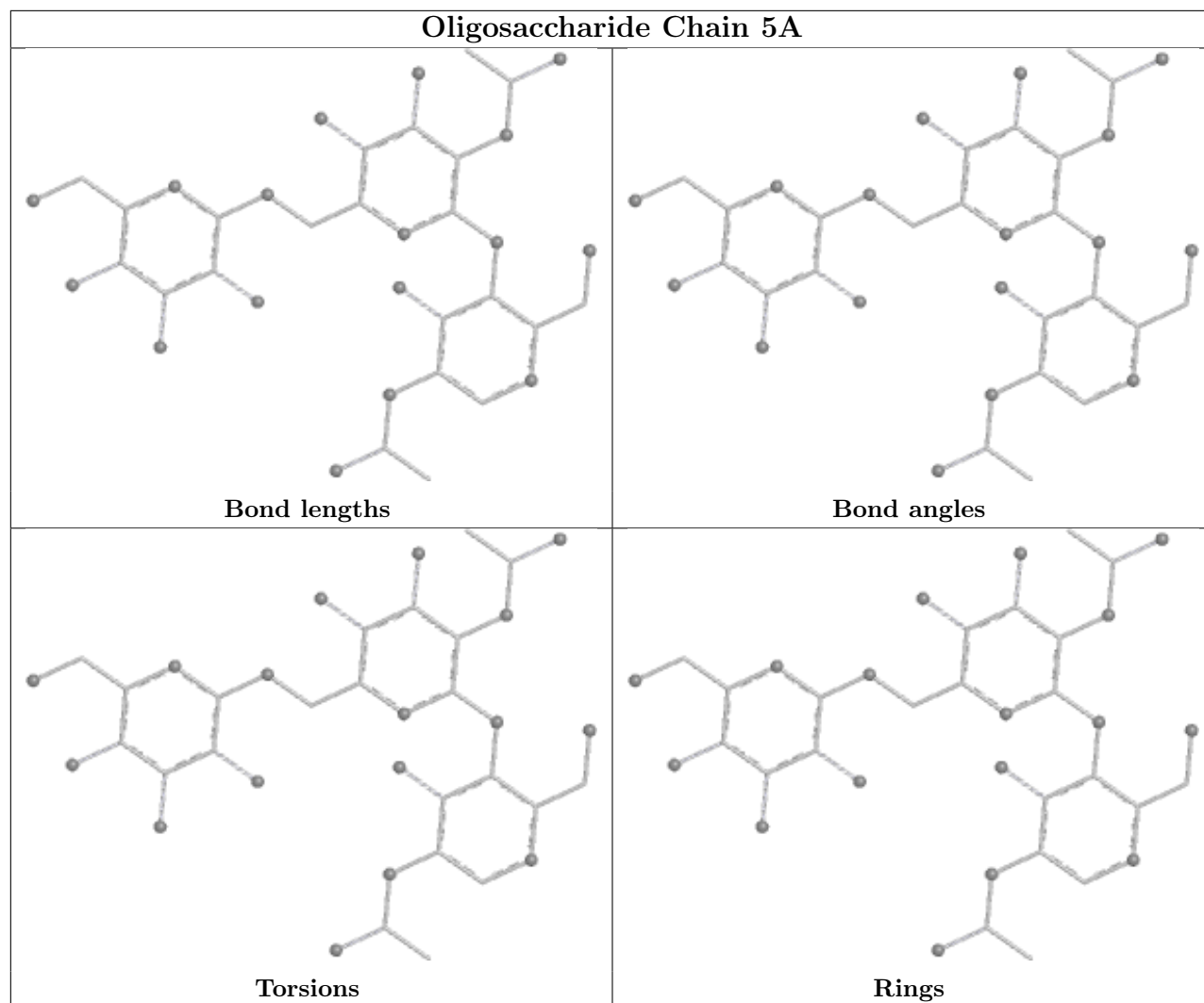


Oligosaccharide Chain 3A**Bond lengths****Bond angles****Torsions****Rings**

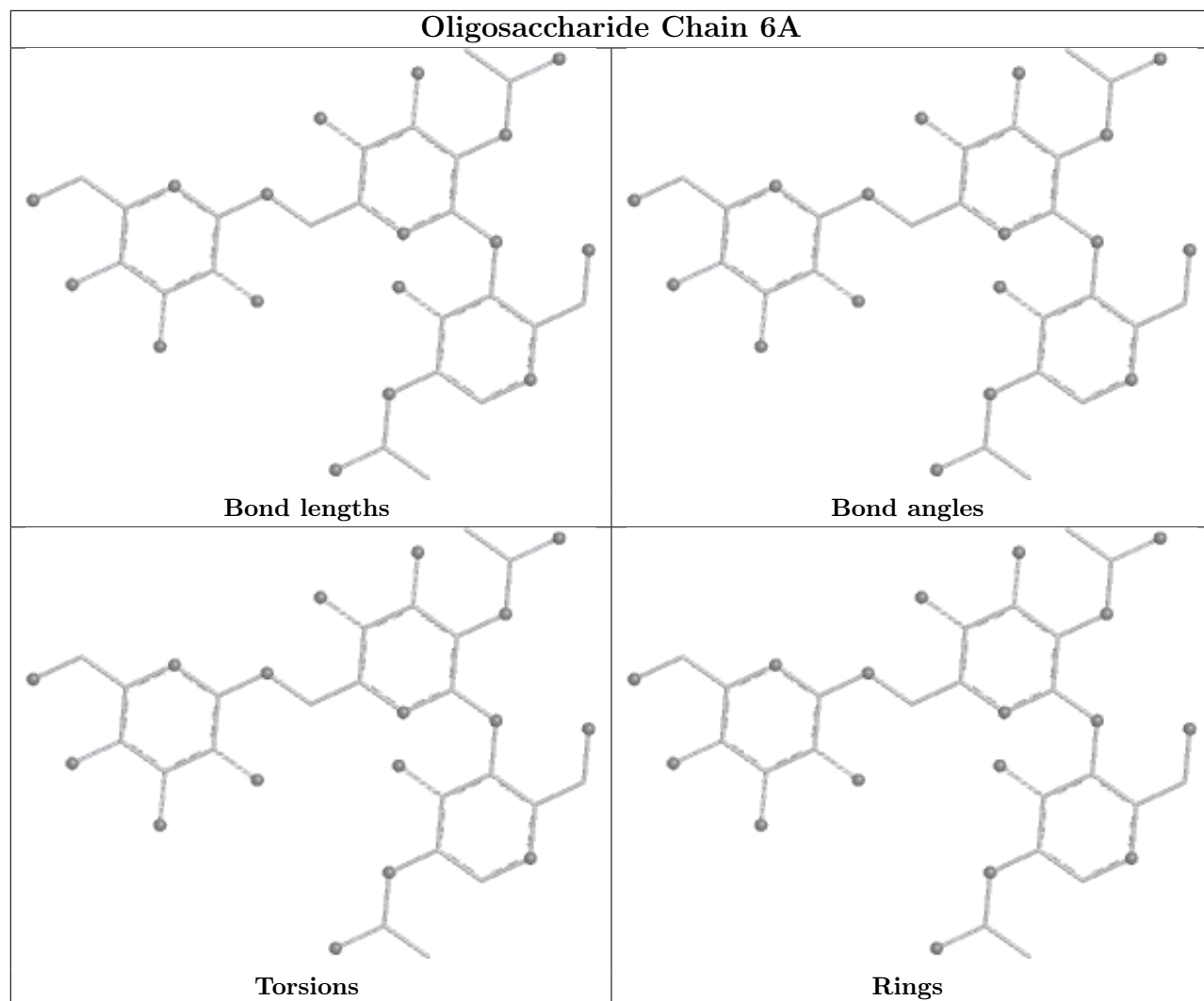
Oligosaccharide Chain 4A



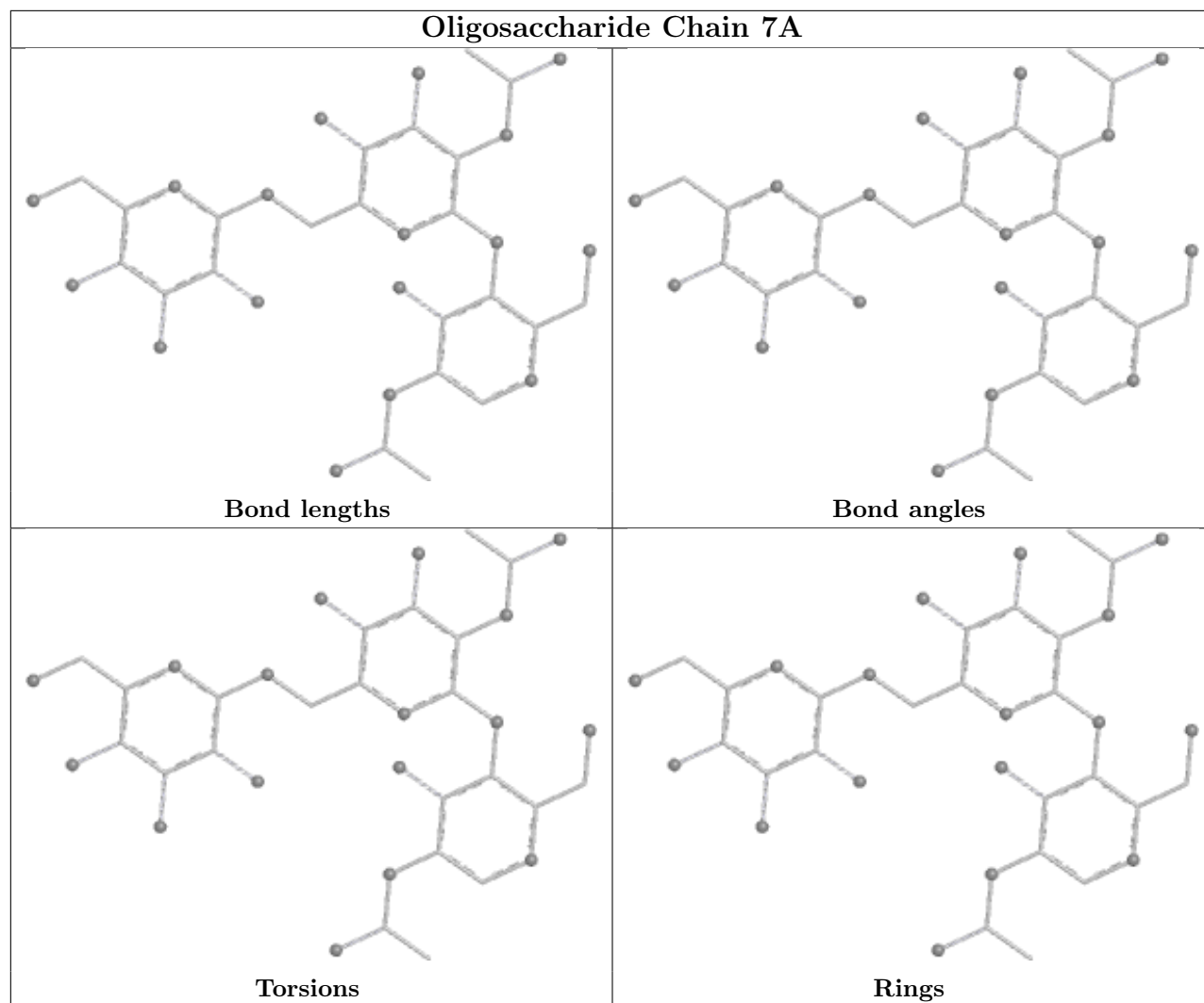
Oligosaccharide Chain 5A



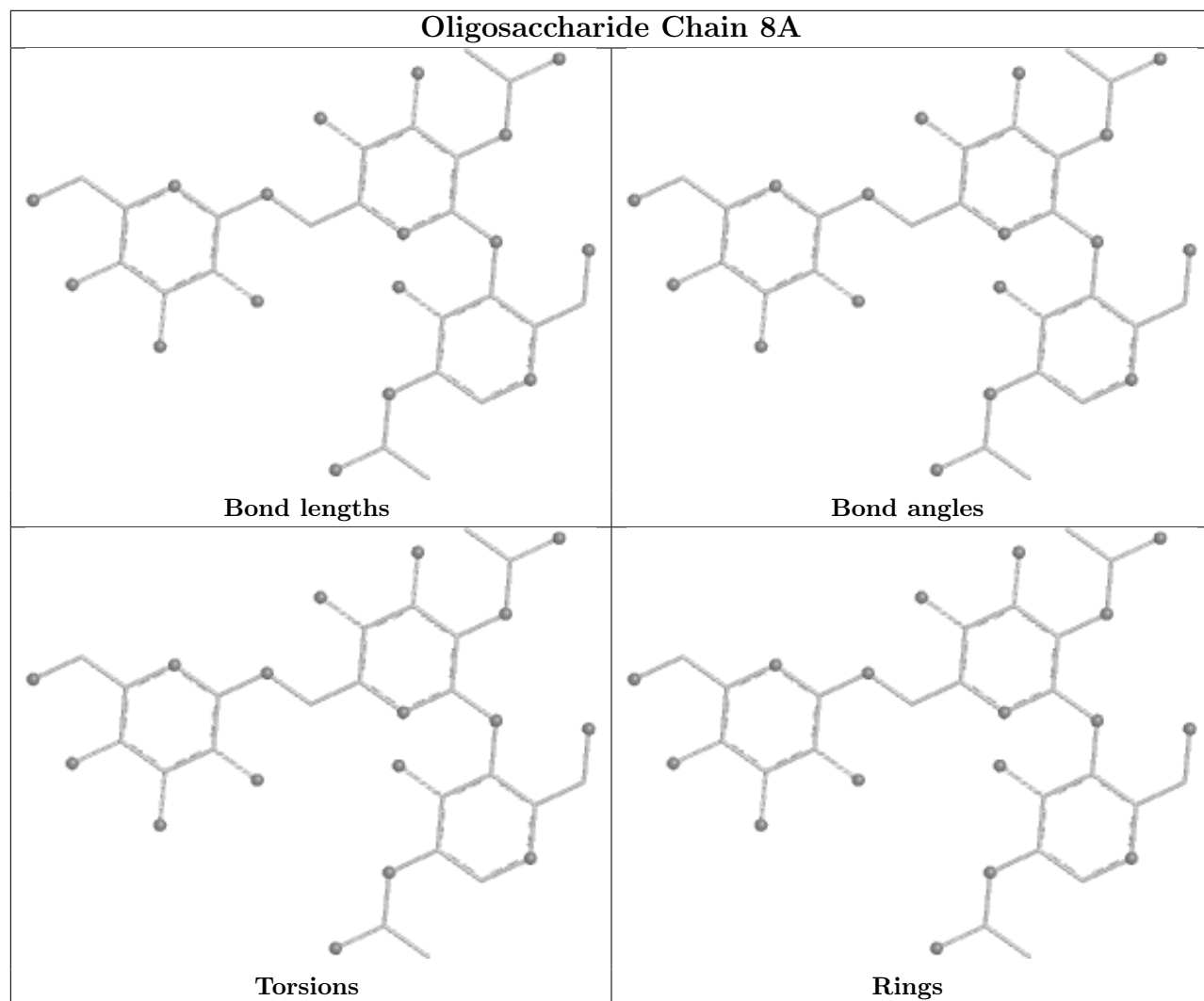
Oligosaccharide Chain 6A



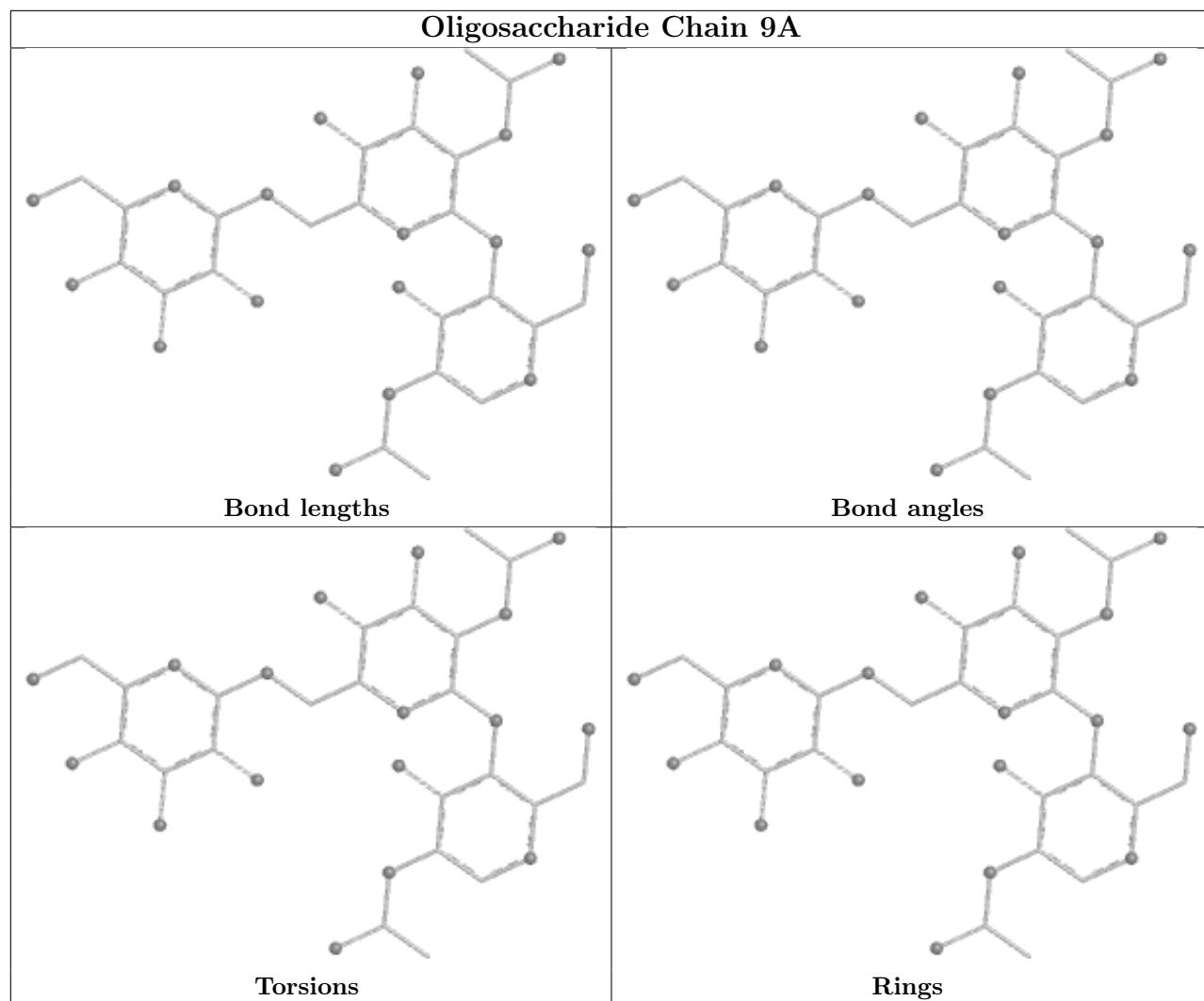
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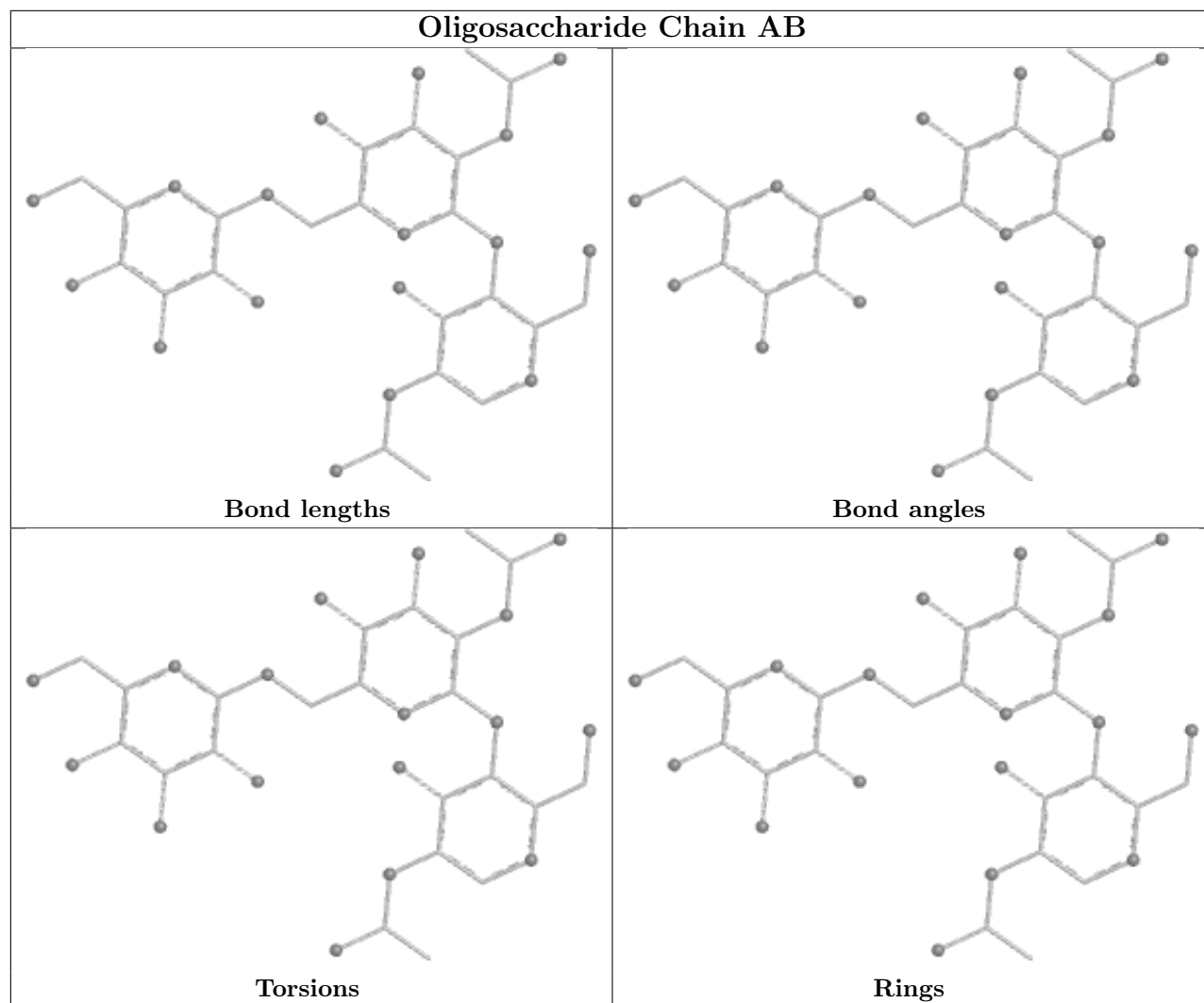


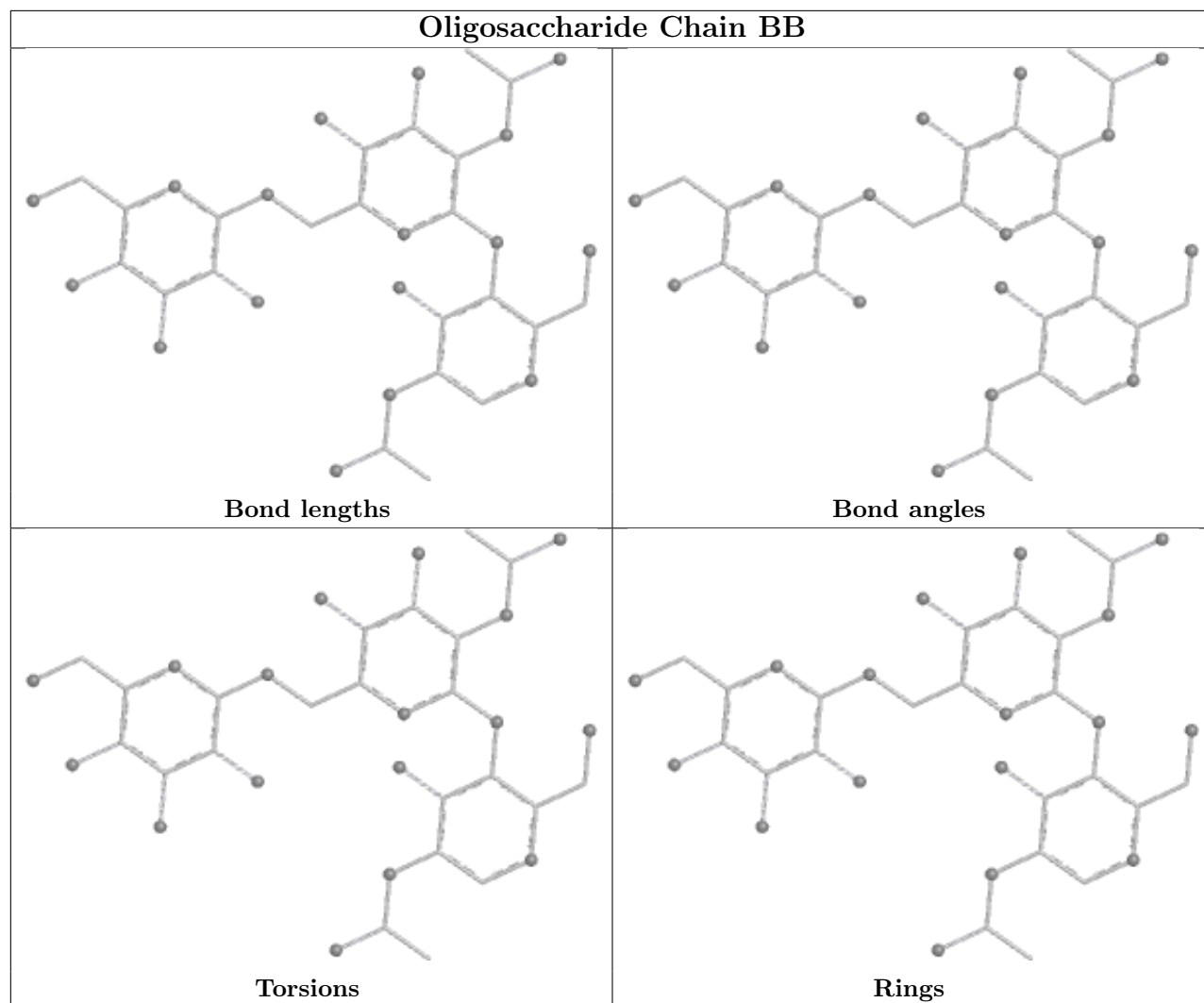
Oligosaccharide Chain 8A

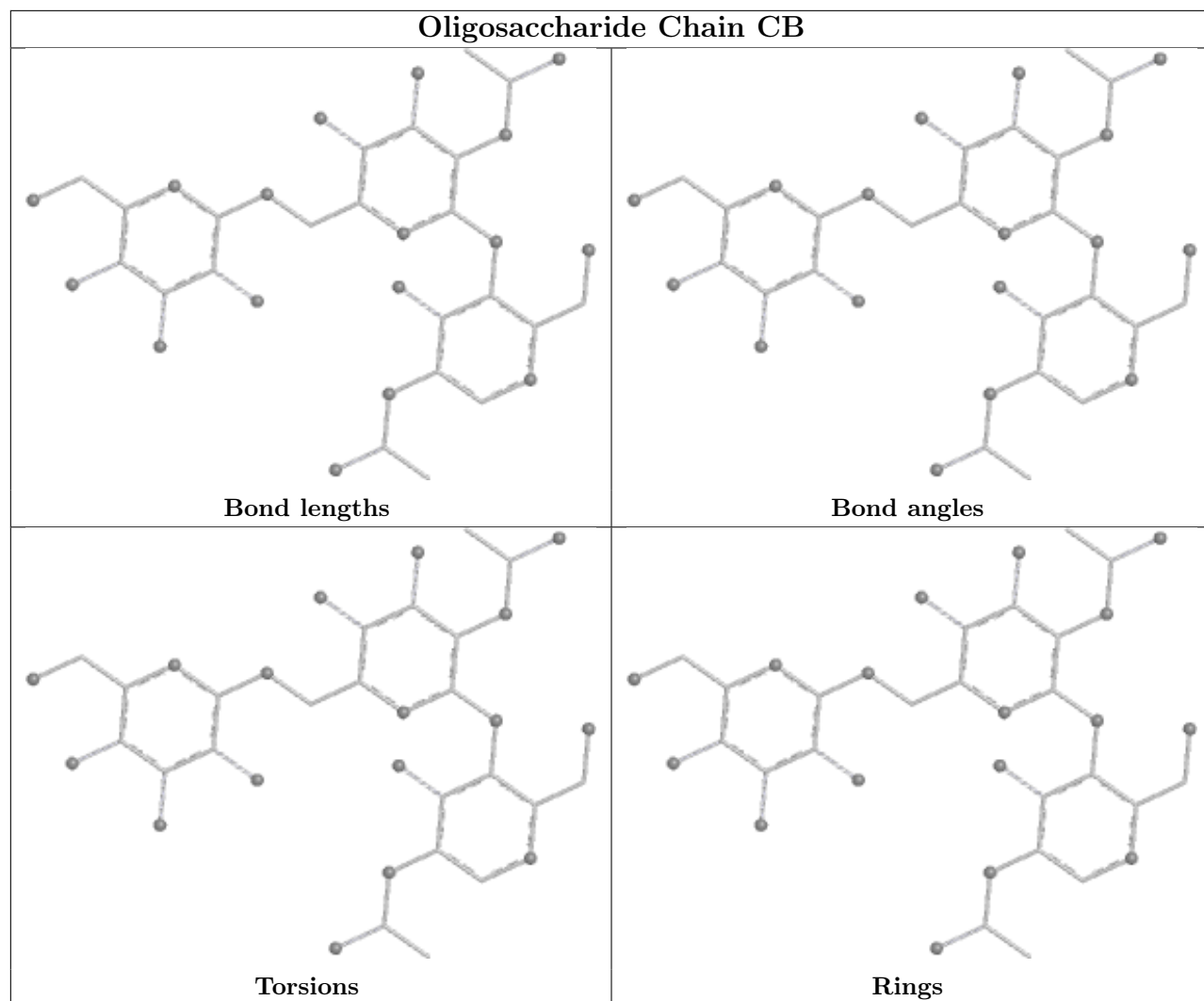


Oligosaccharide Chain 9A

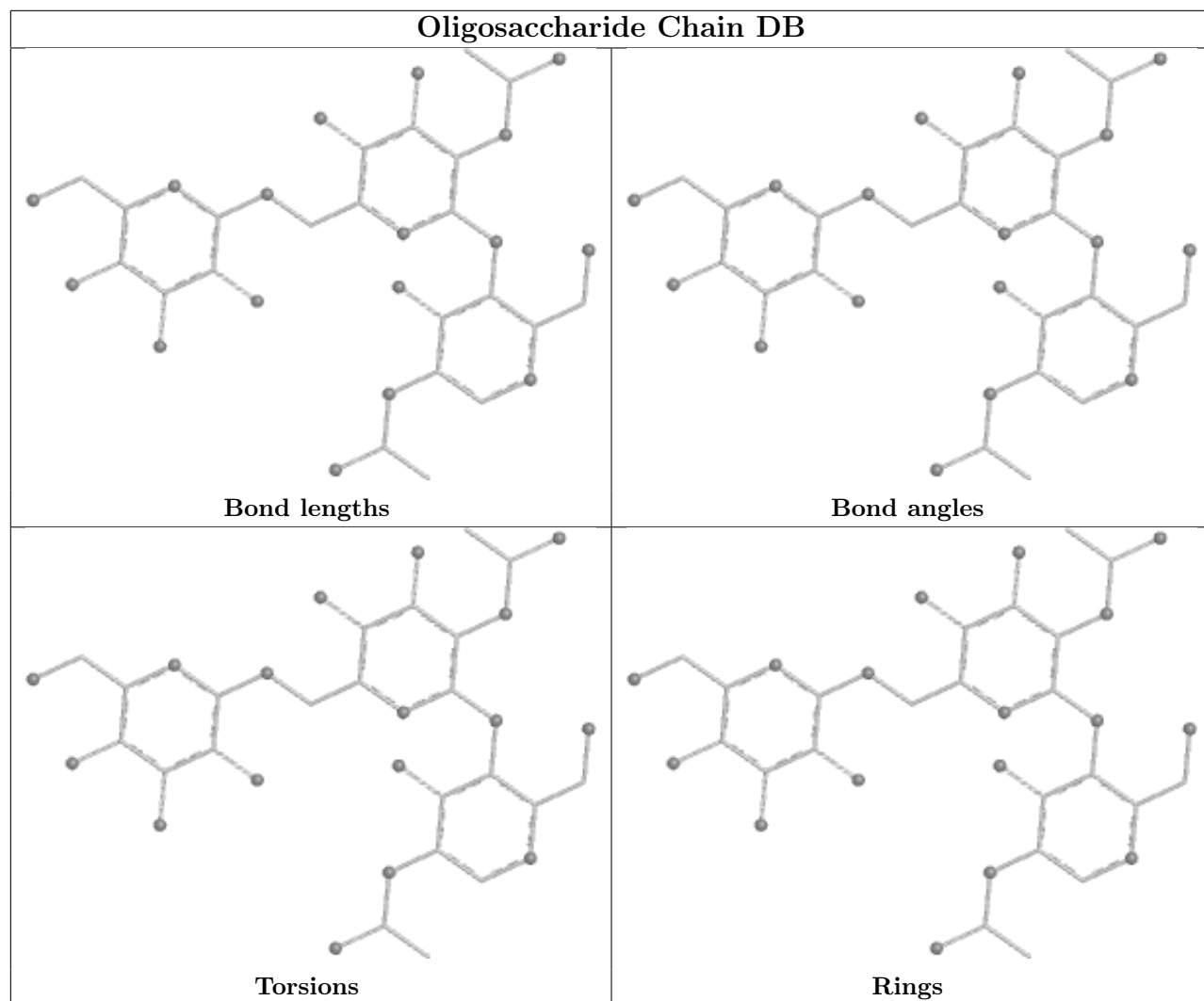


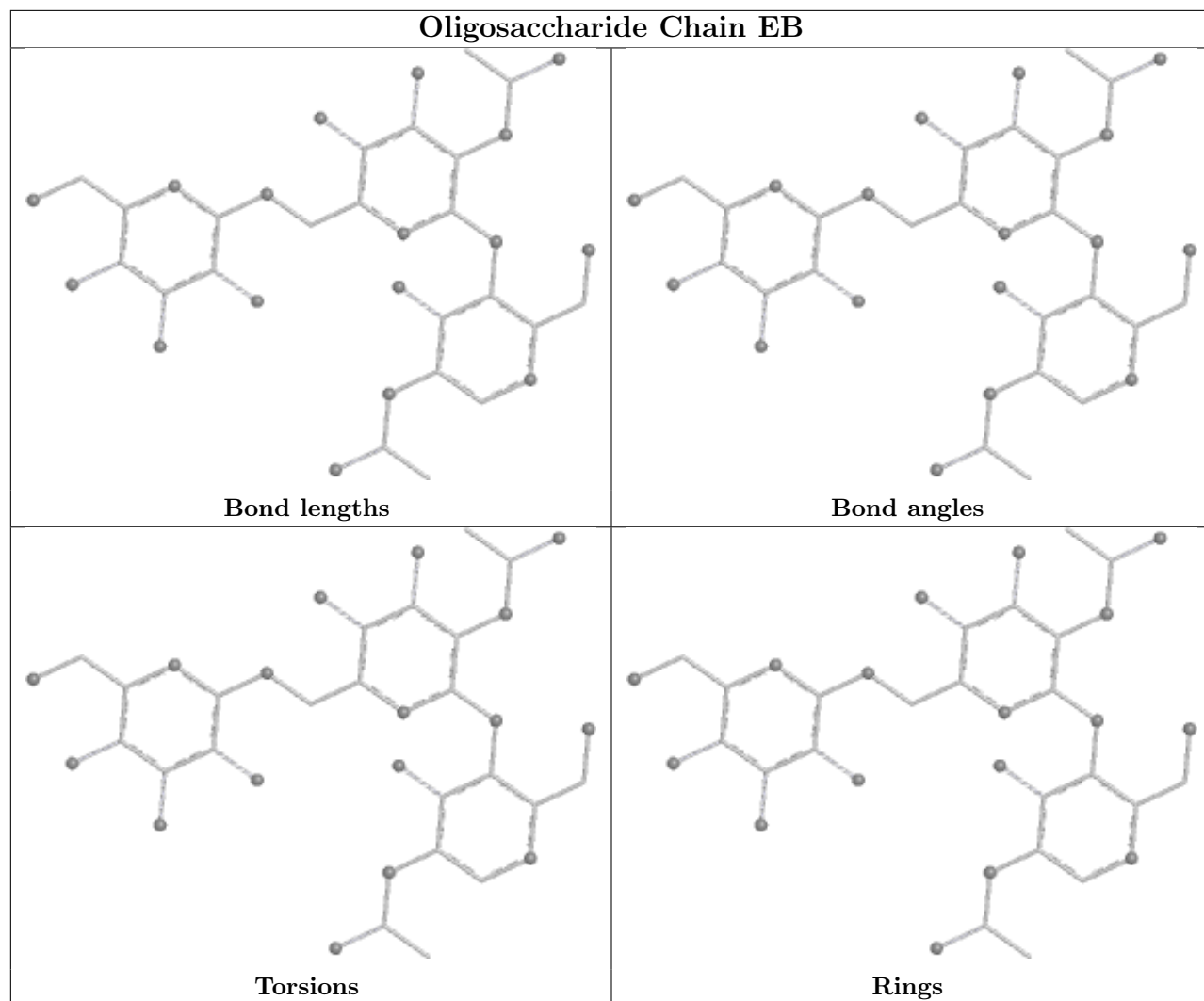
Oligosaccharide Chain AB

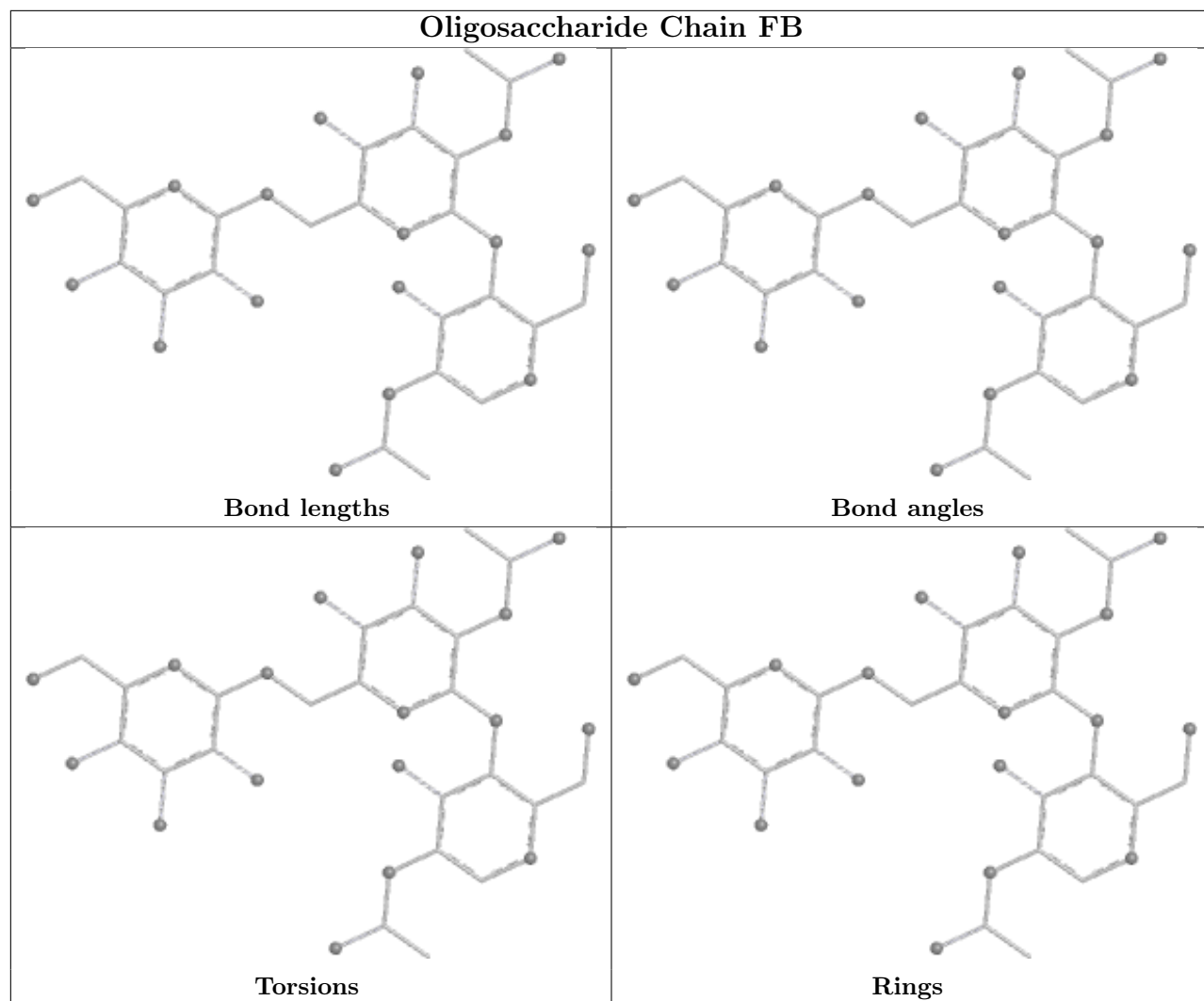
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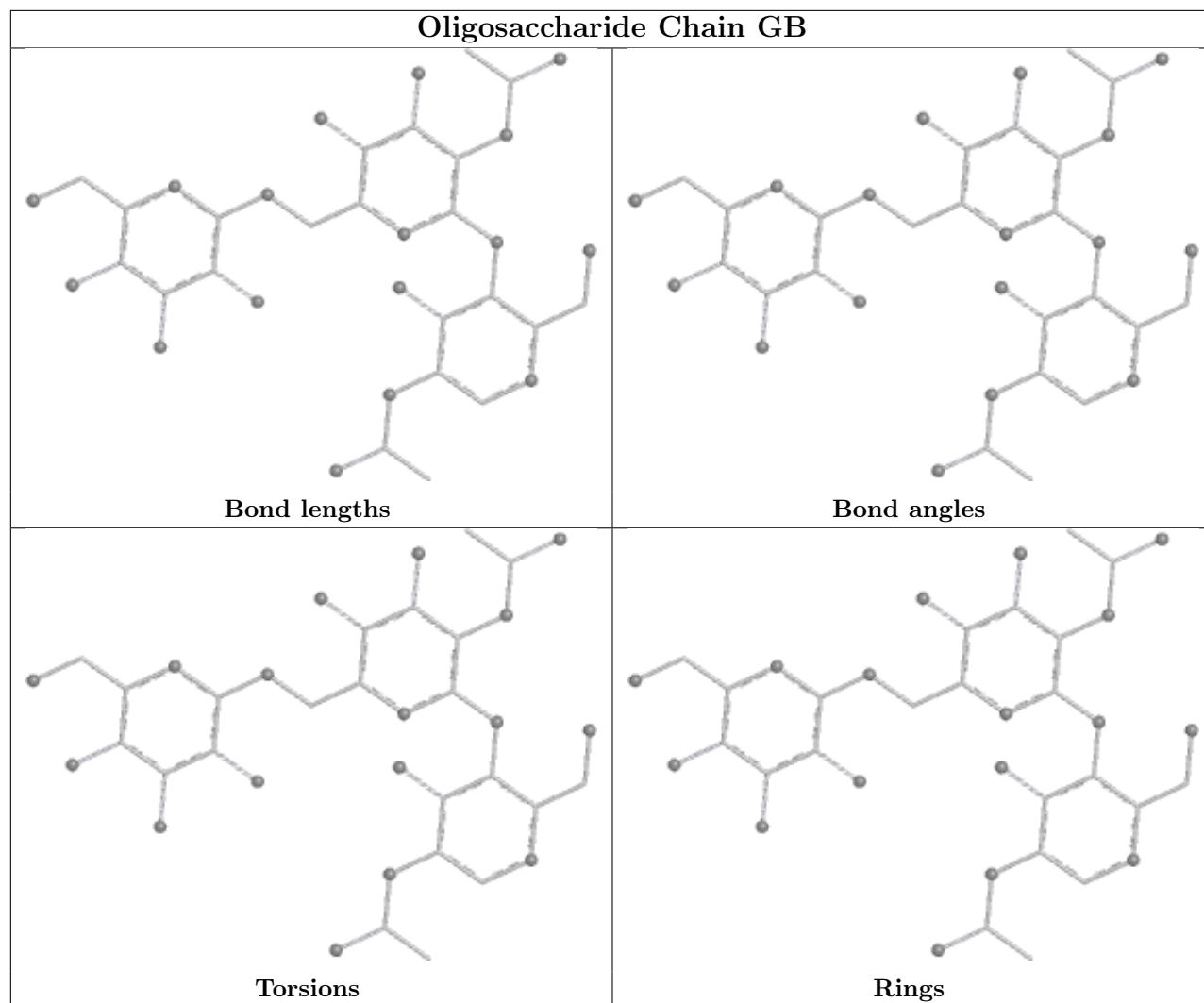
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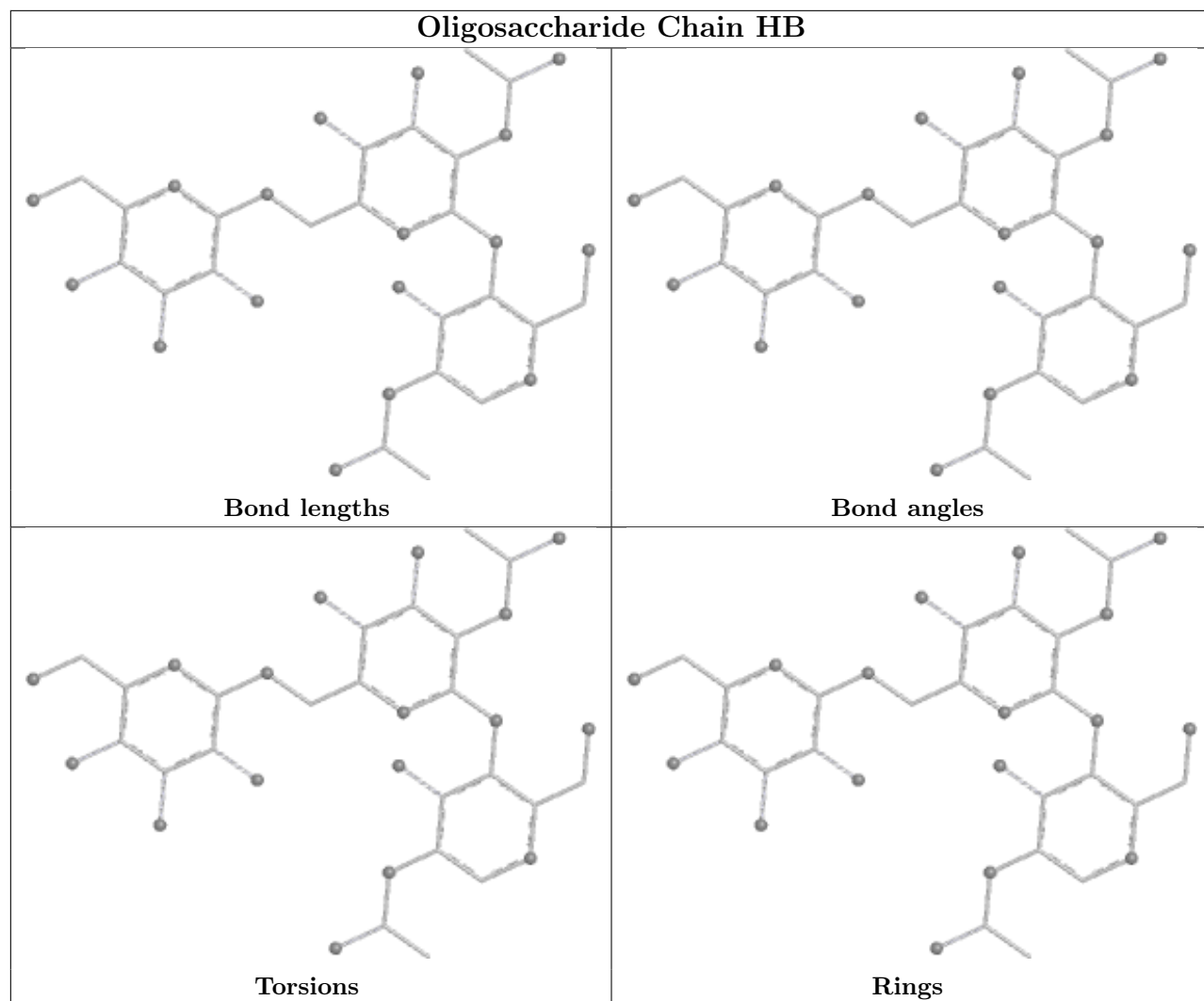
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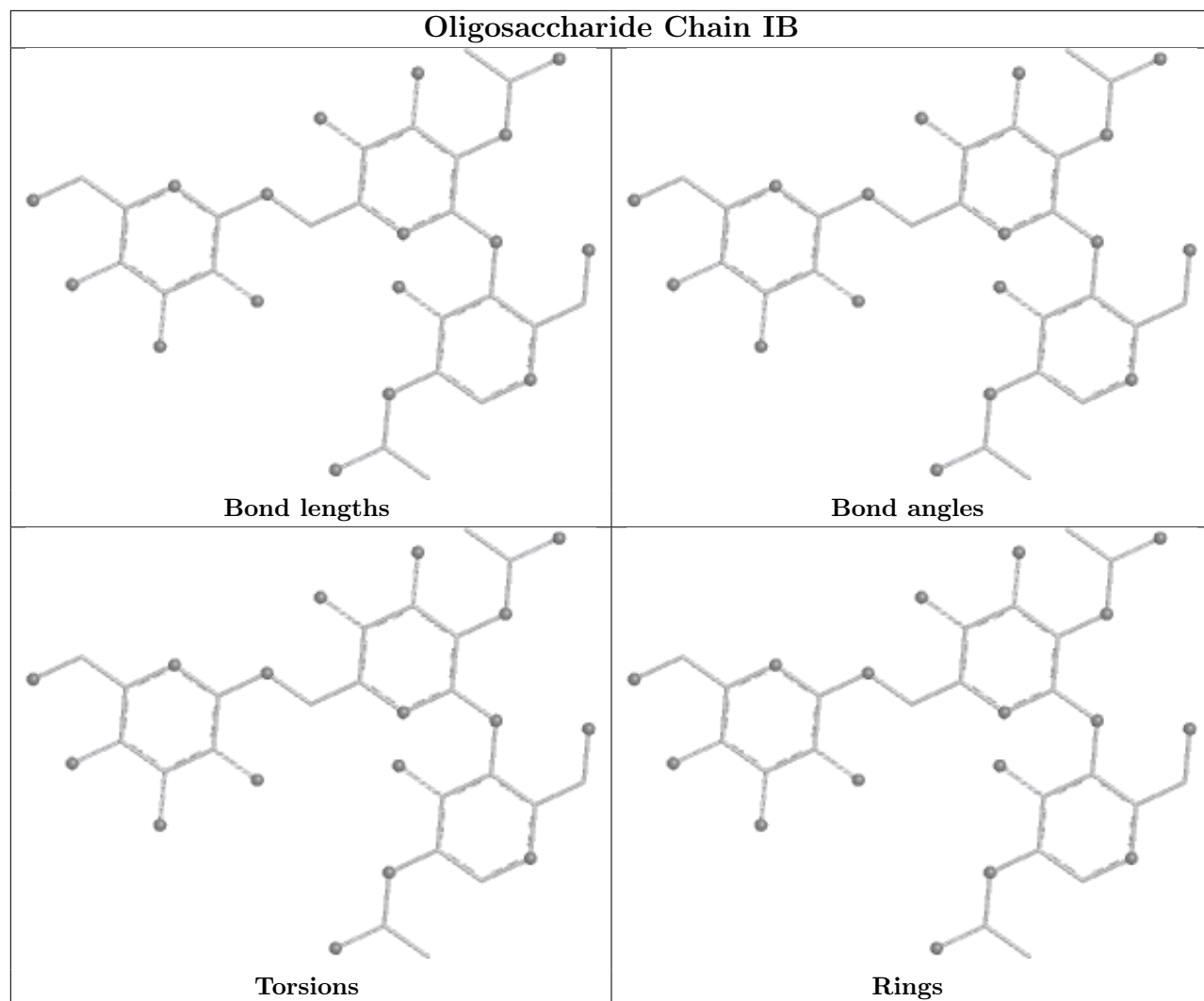


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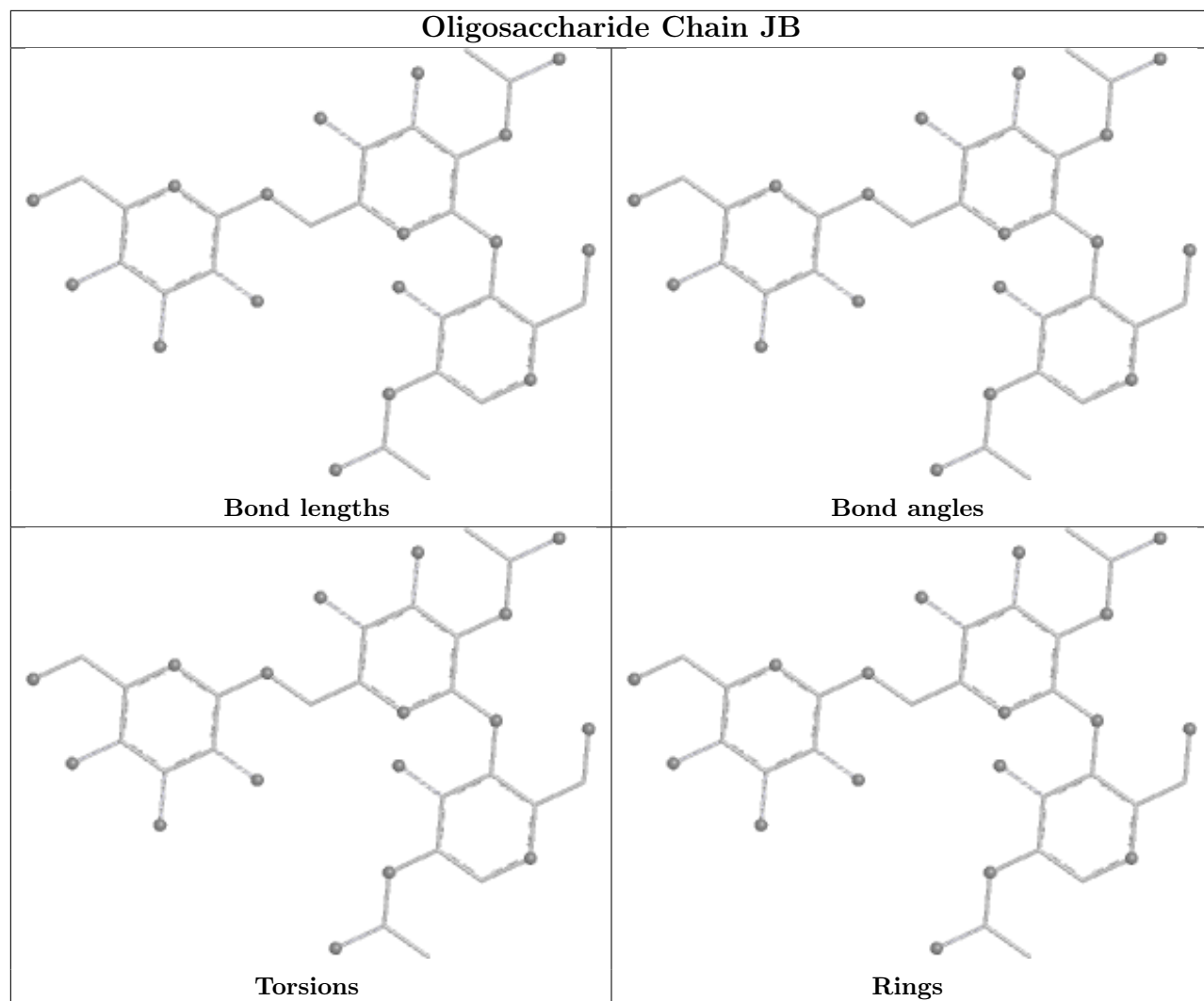
Oligosaccharide Chain FB

Oligosaccharide Chain GB

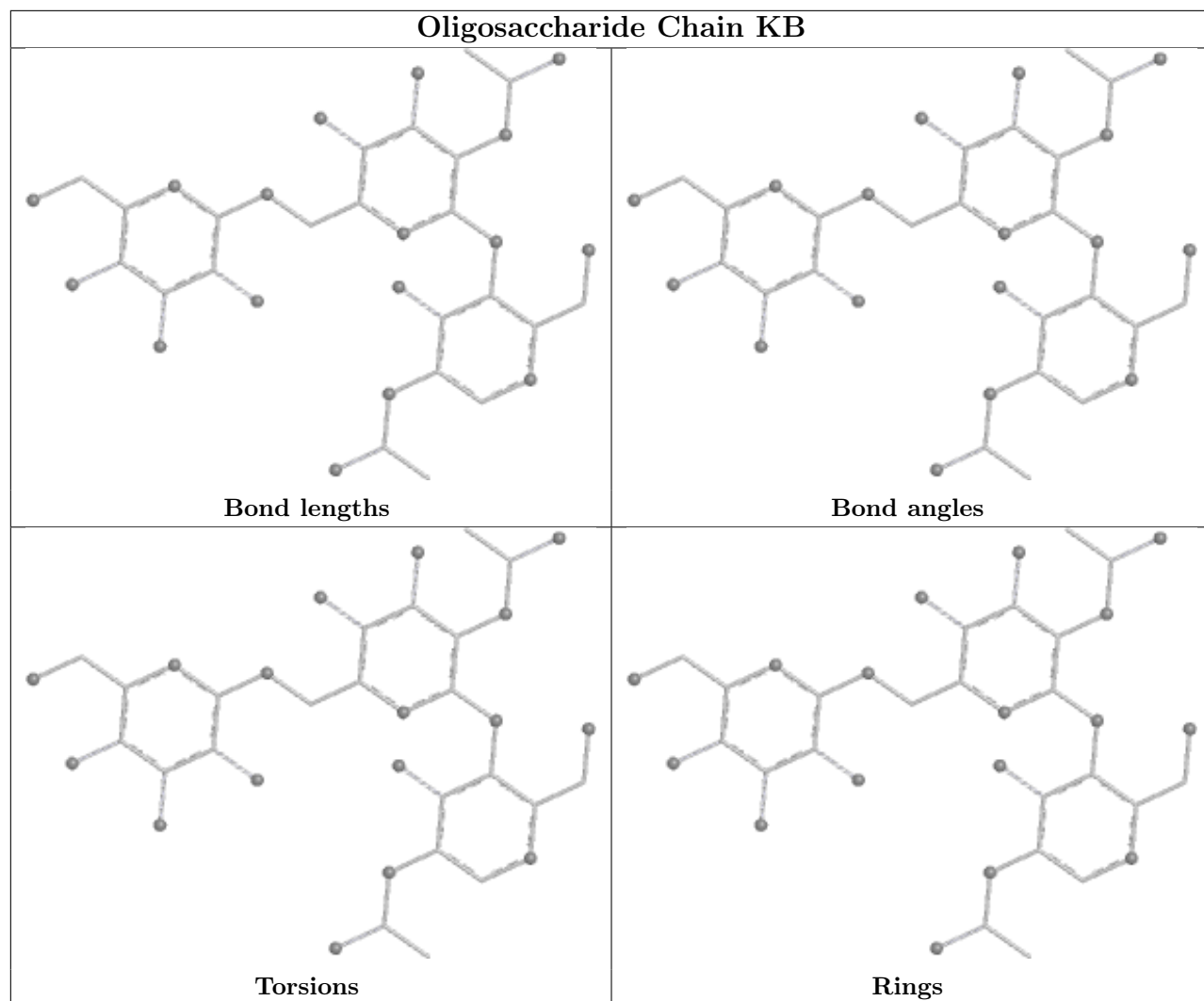
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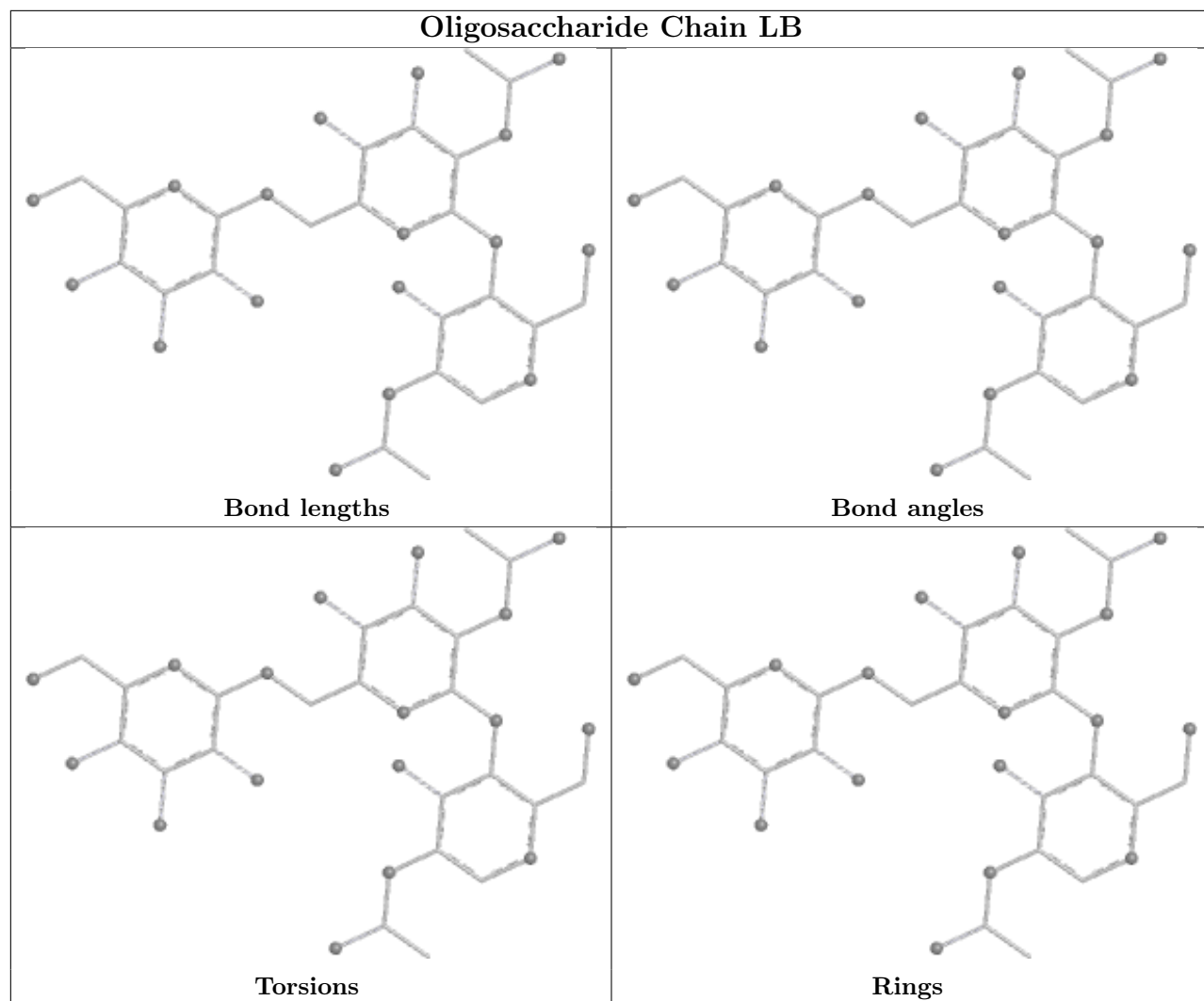
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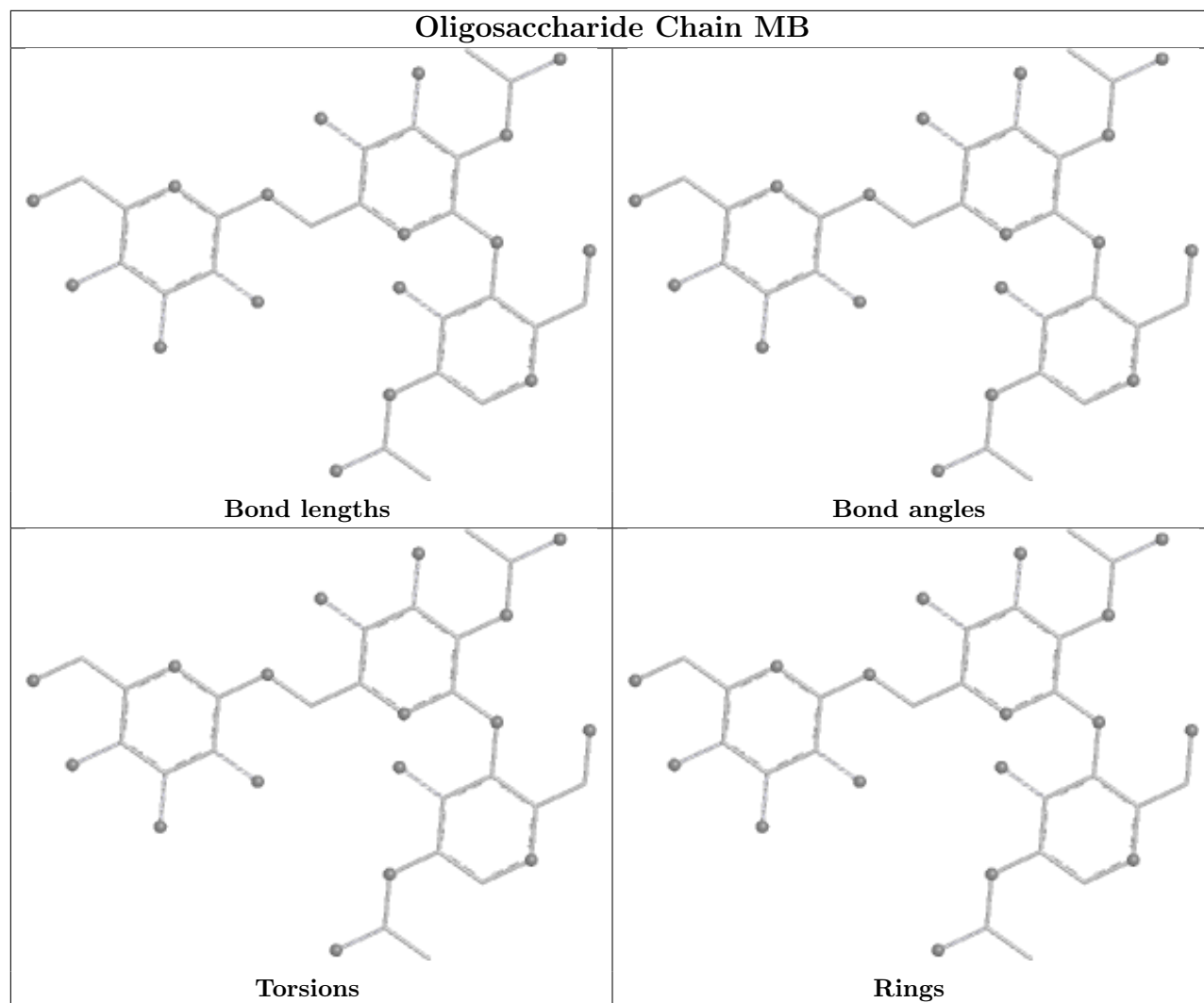
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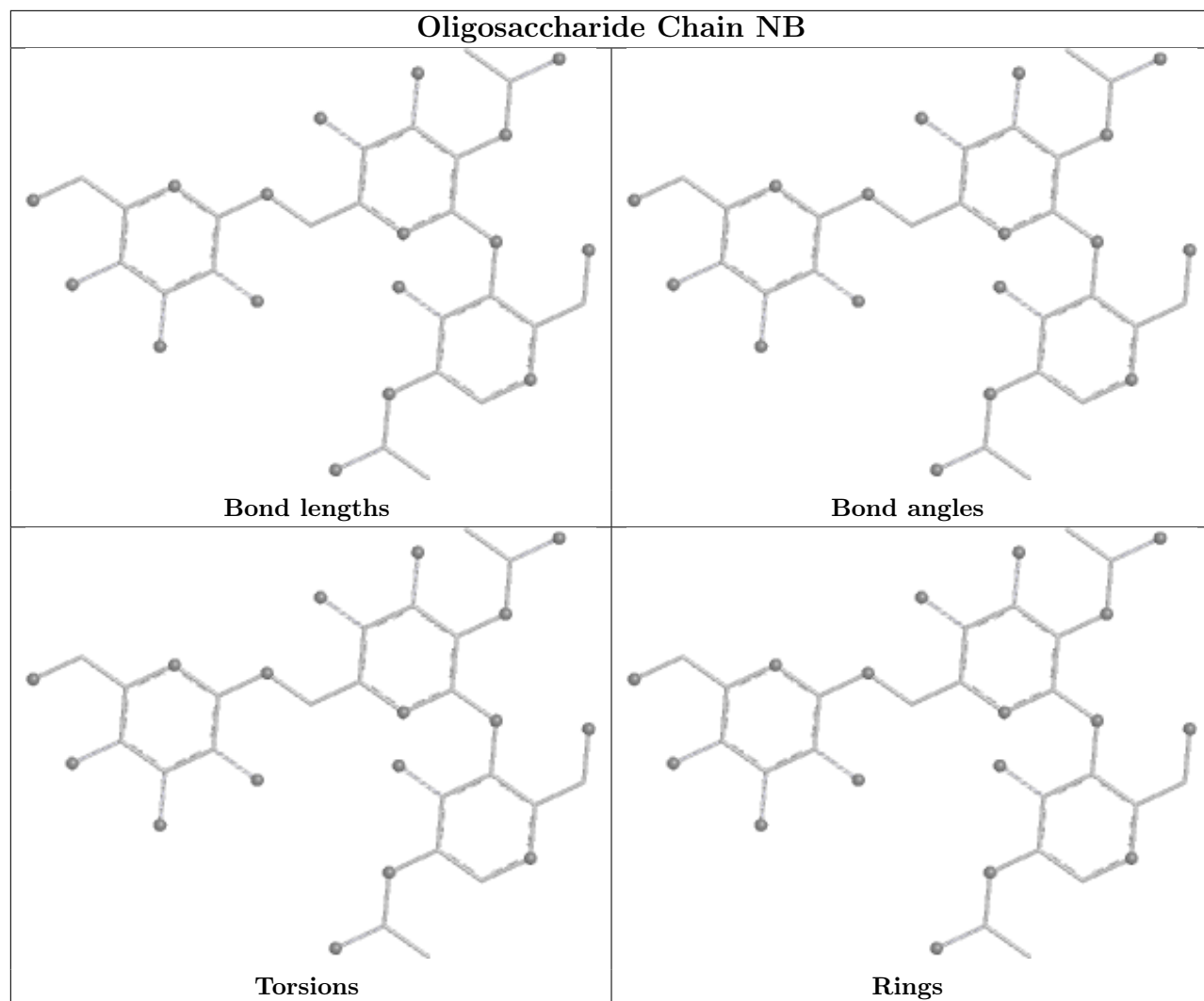


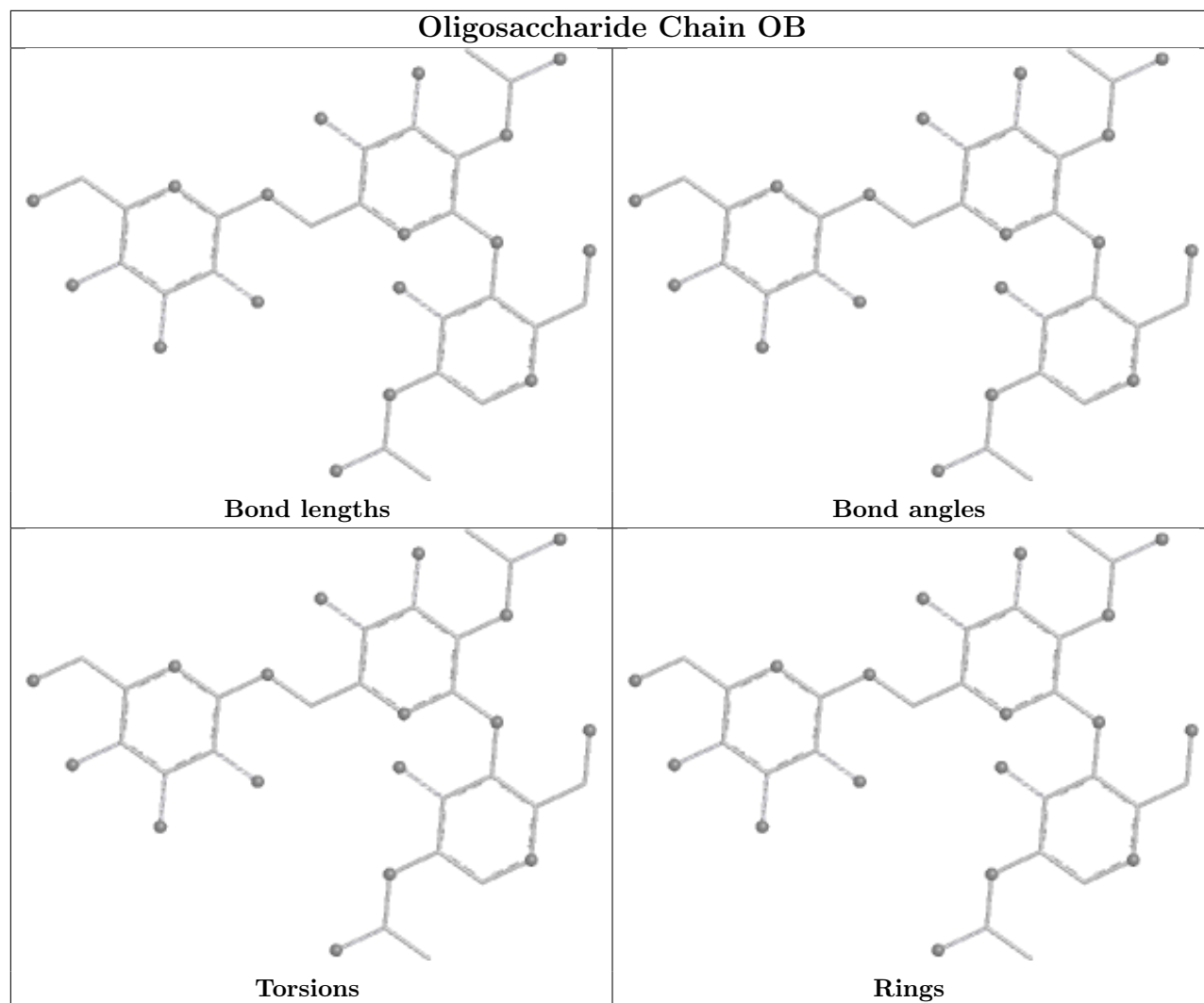
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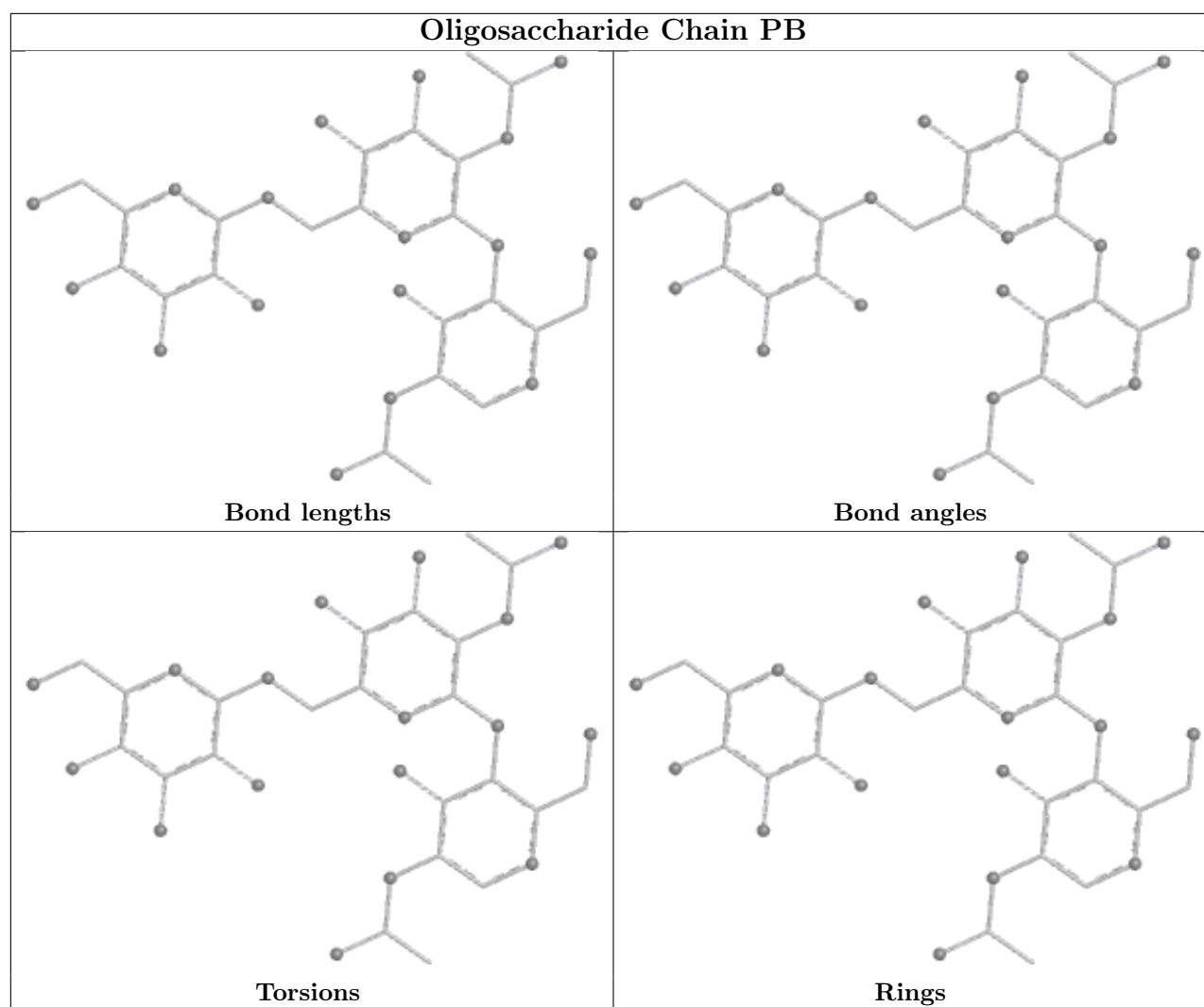


Oligosaccharide Chain LB

Oligosaccharide Chain MB

Oligosaccharide Chain NB

Oligosaccharide Chain OB



5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.

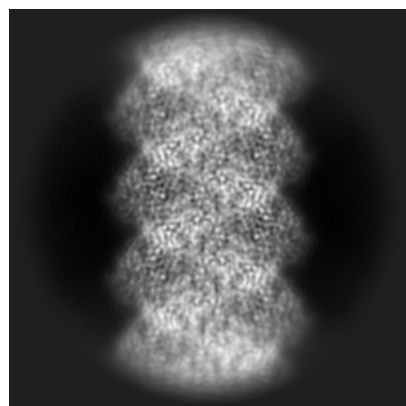
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19961. These allow visual inspection of the internal detail of the map and identification of artifacts.

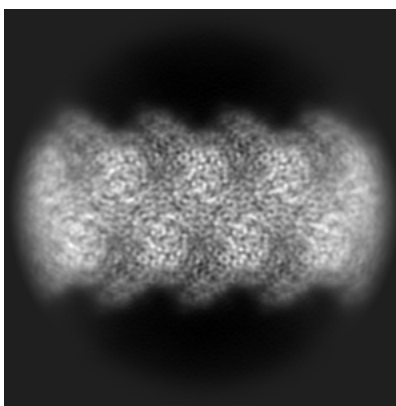
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

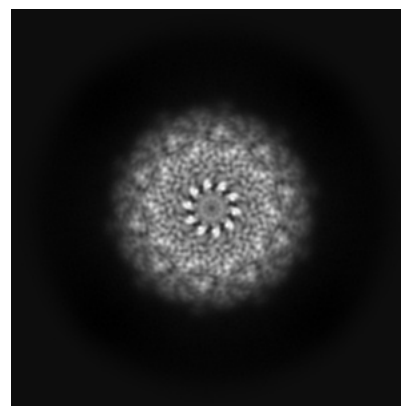
6.1.1 Primary map



X

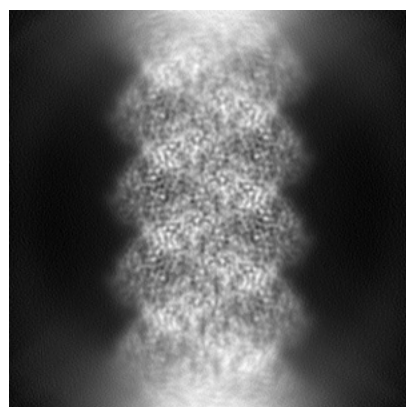


Y

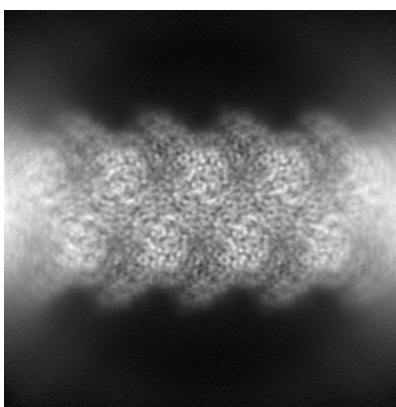


Z

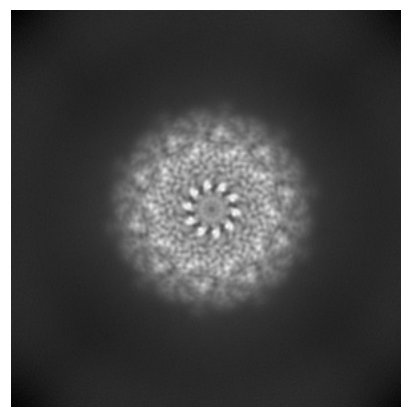
6.1.2 Raw map



X



Y

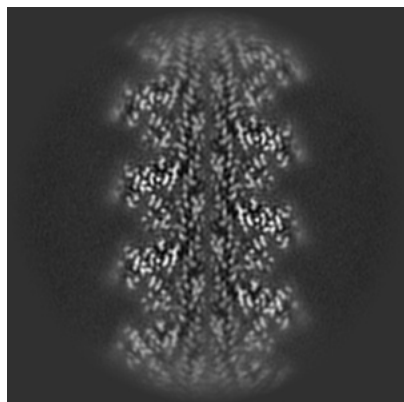


Z

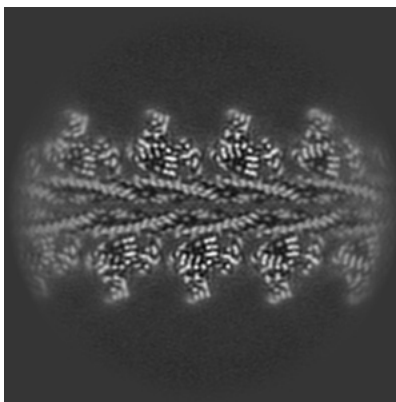
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

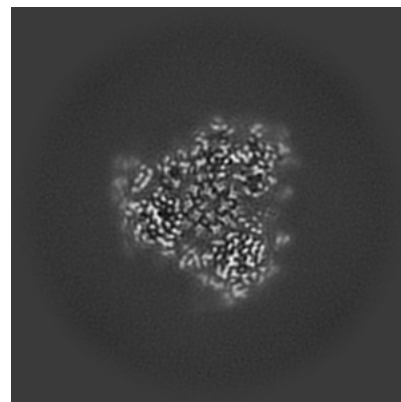
6.2.1 Primary map



X Index: 144

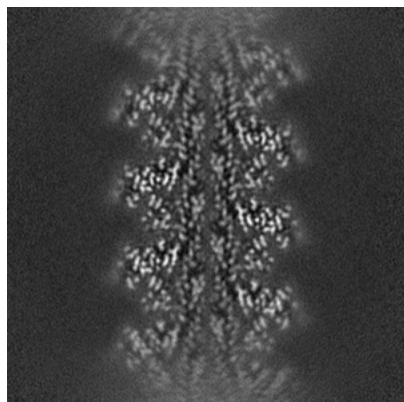


Y Index: 144

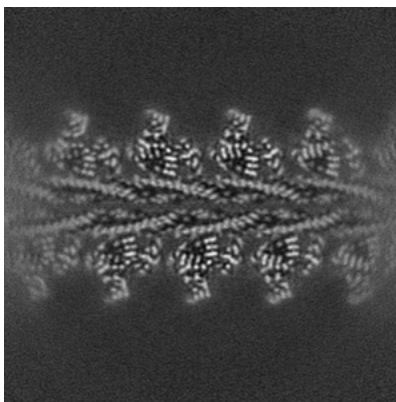


Z Index: 144

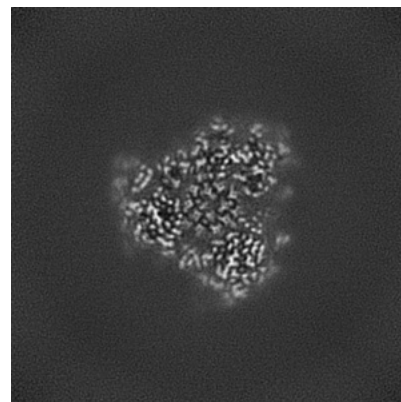
6.2.2 Raw map



X Index: 144



Y Index: 144

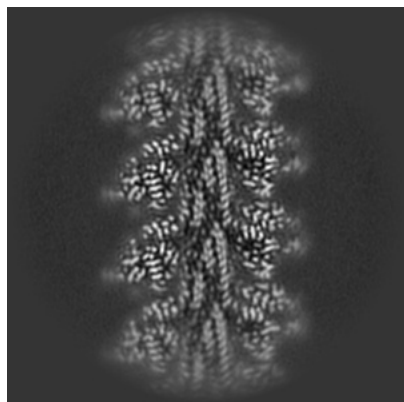


Z Index: 144

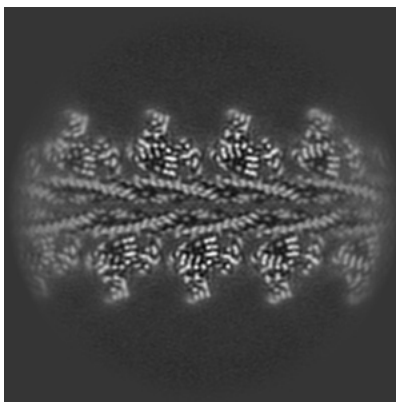
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

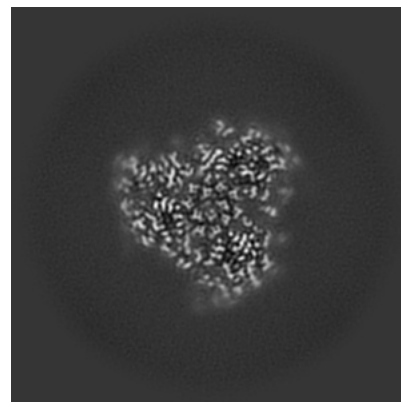
6.3.1 Primary map



X Index: 133

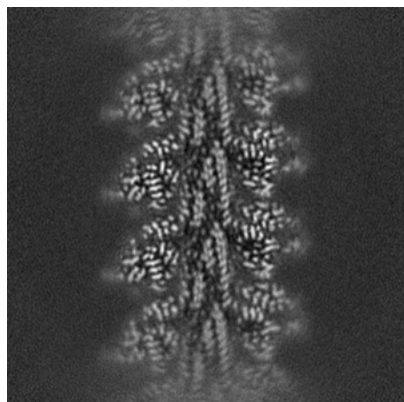


Y Index: 144

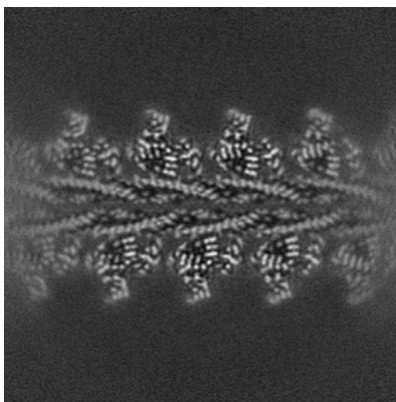


Z Index: 147

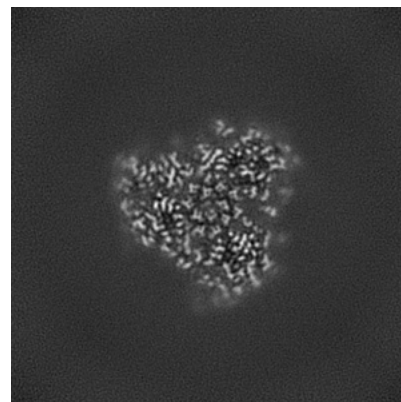
6.3.2 Raw map



X Index: 133



Y Index: 144

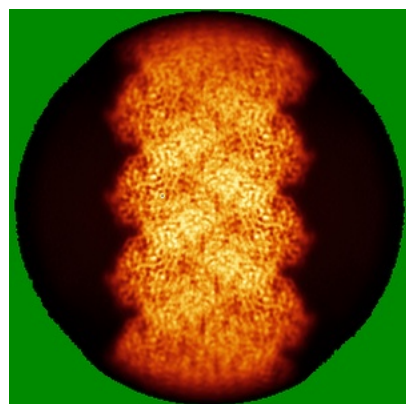


Z Index: 147

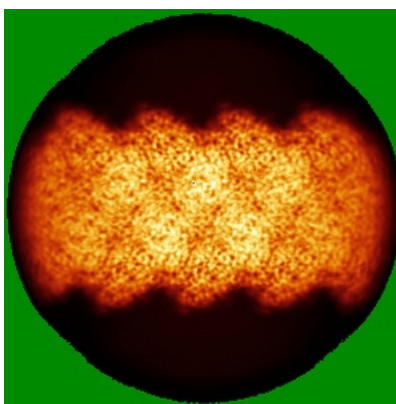
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

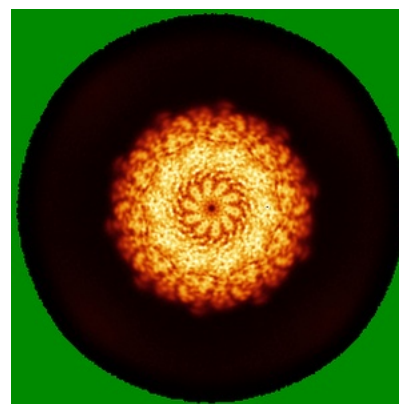
6.4.1 Primary map



X

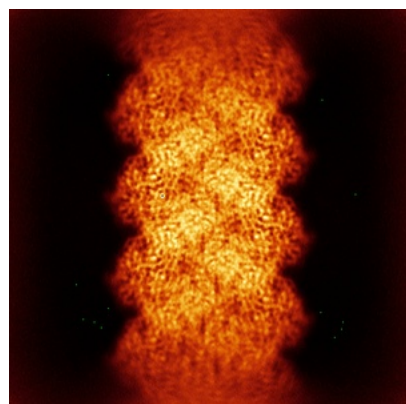


Y

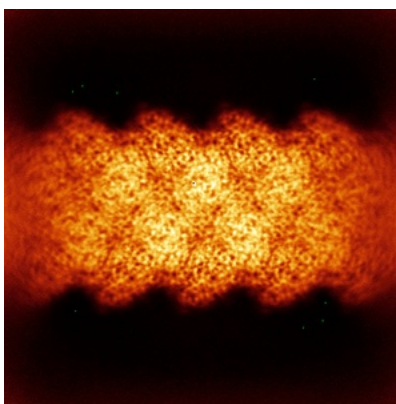


Z

6.4.2 Raw map



X



Y

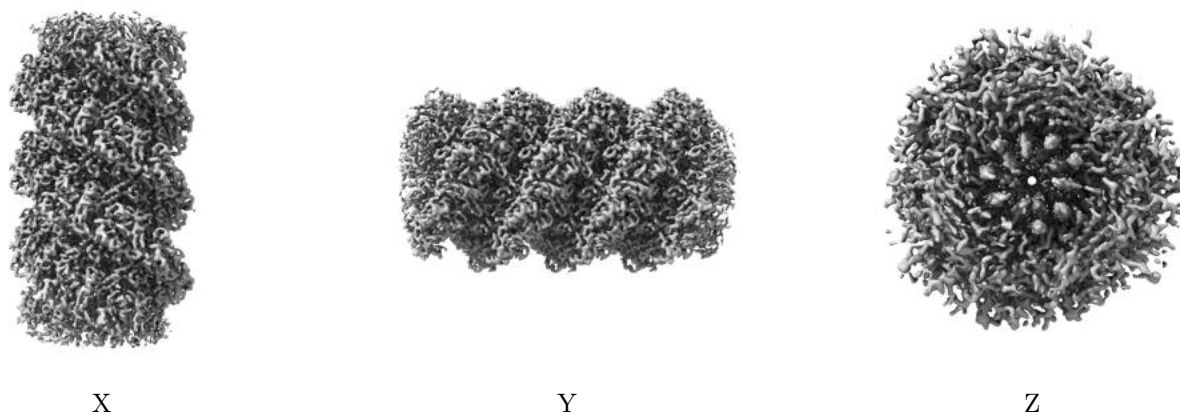


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

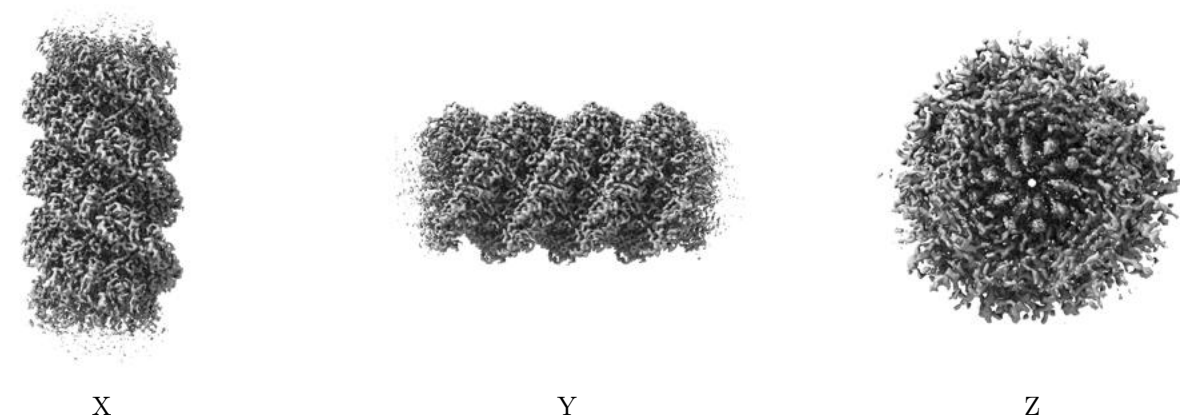
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.11. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

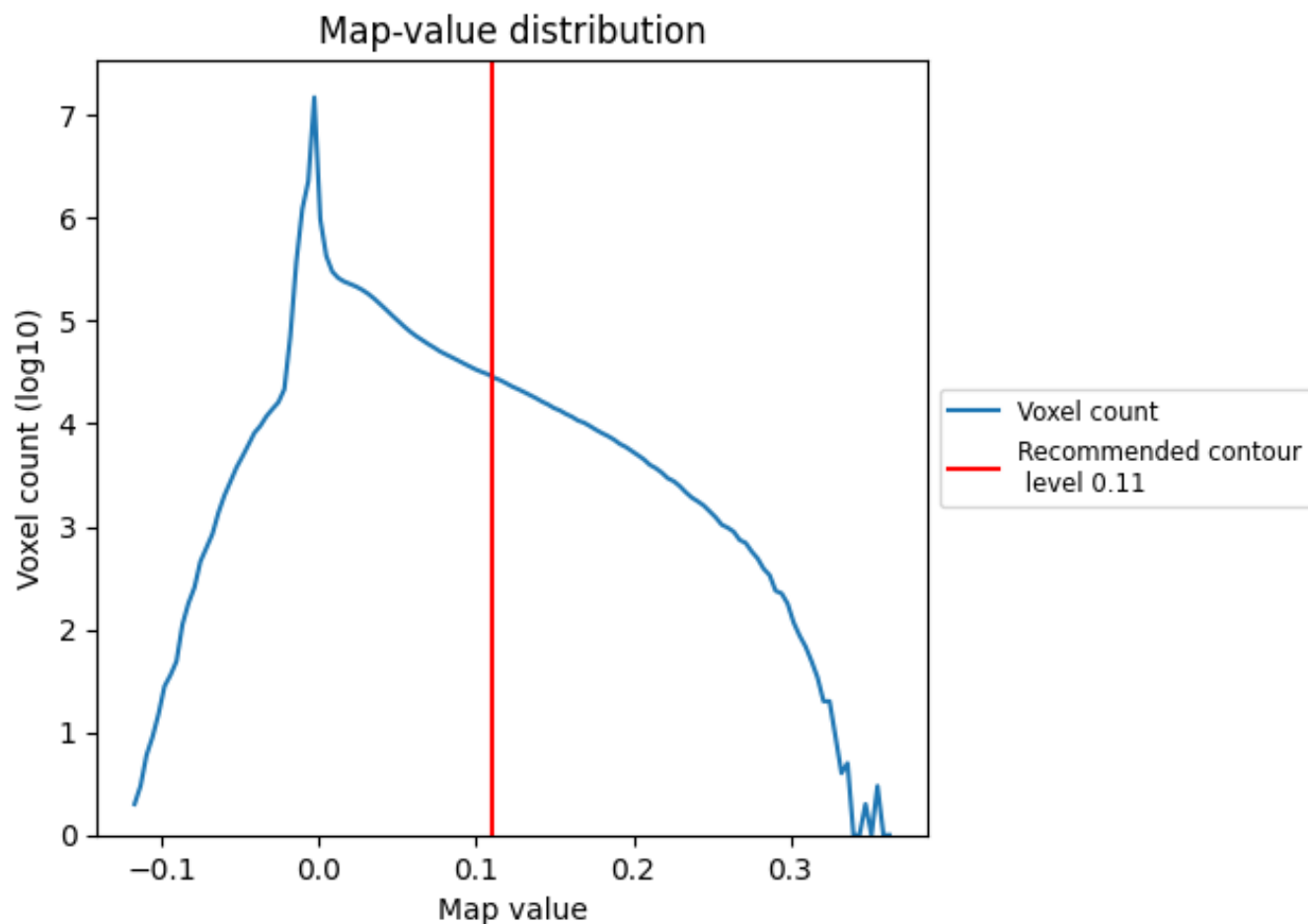
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

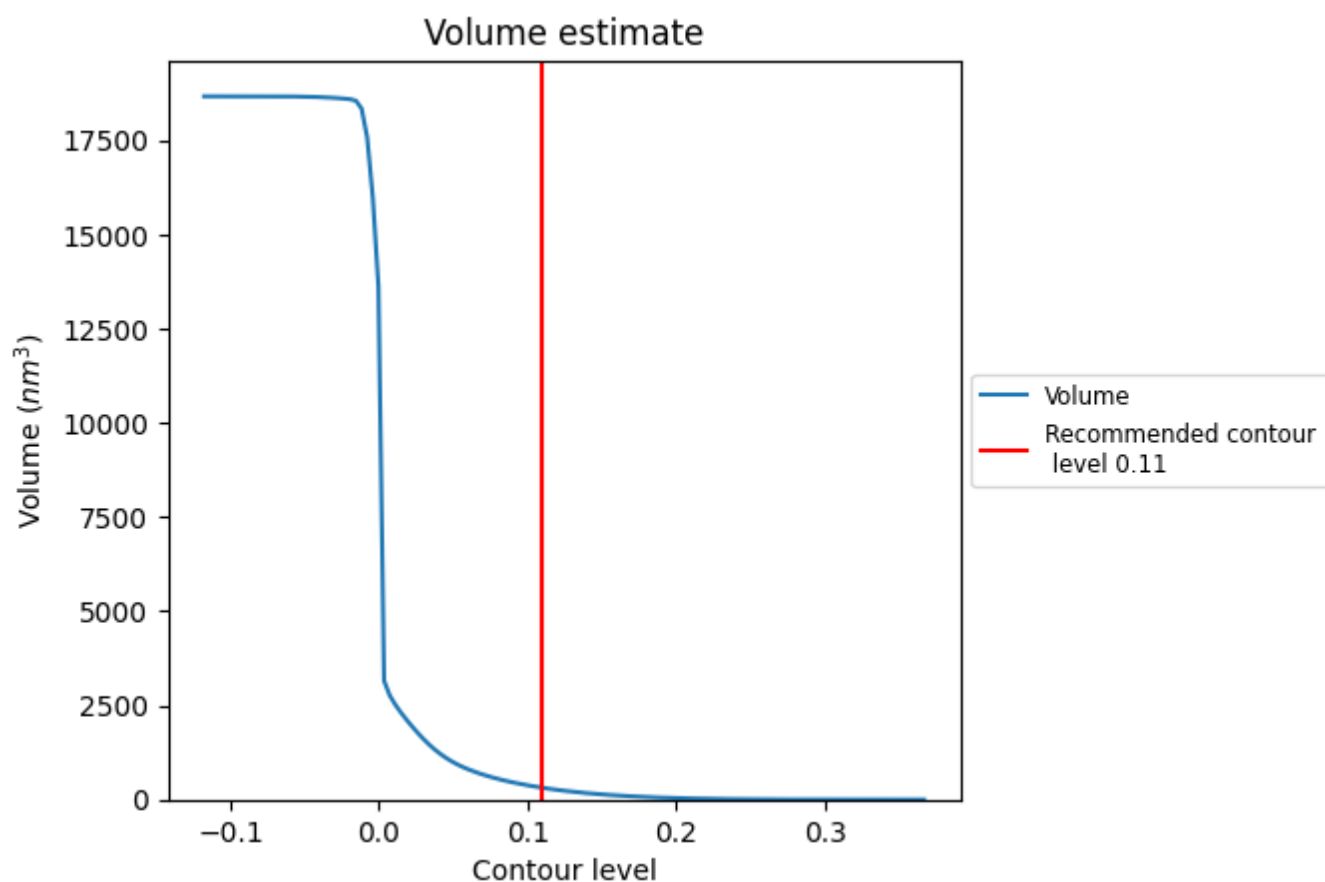
This section contains the results of statistical analysis of the map.

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.

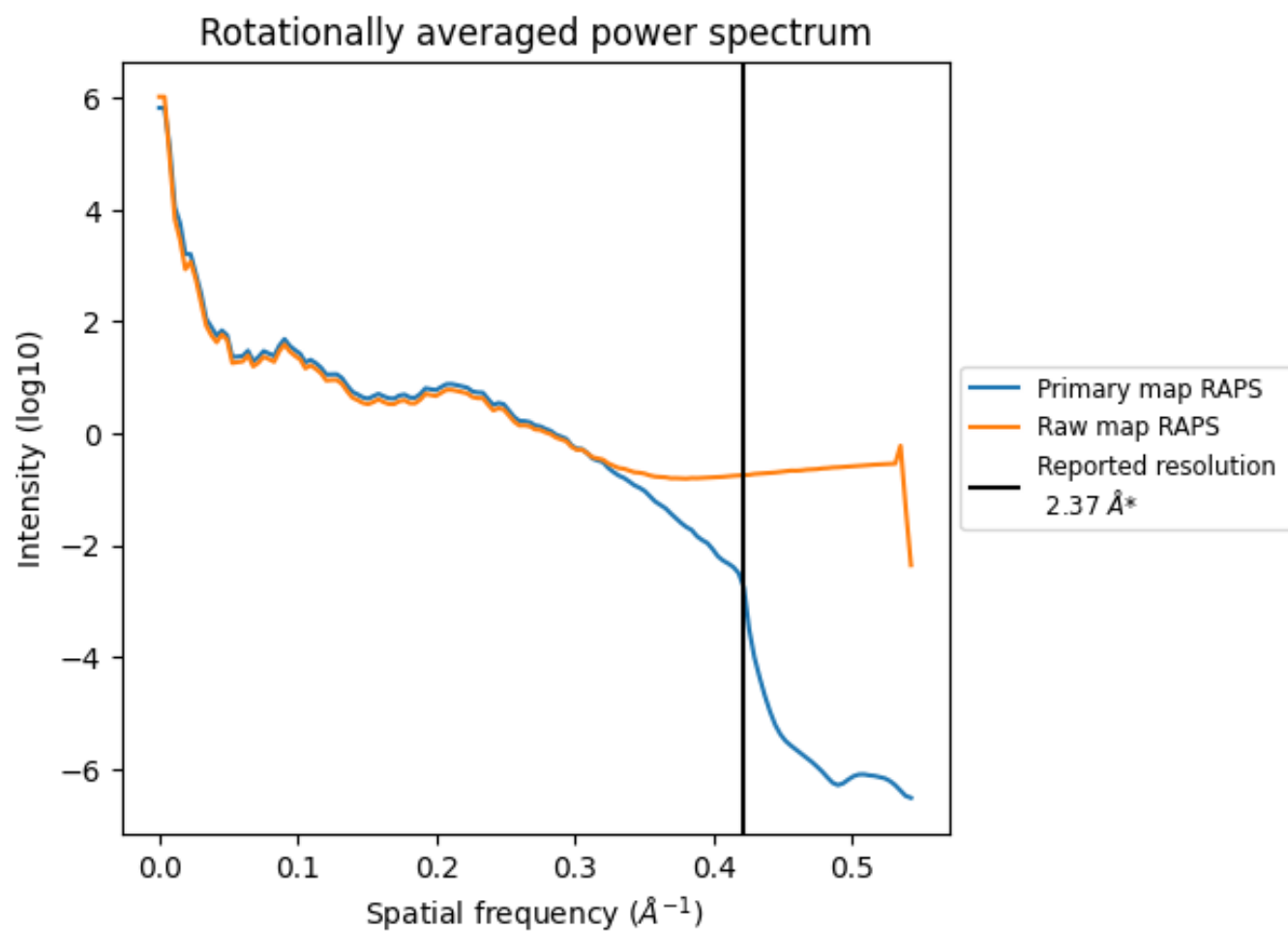
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 313 nm³; this corresponds to an approximate mass of 283 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 ⓘ

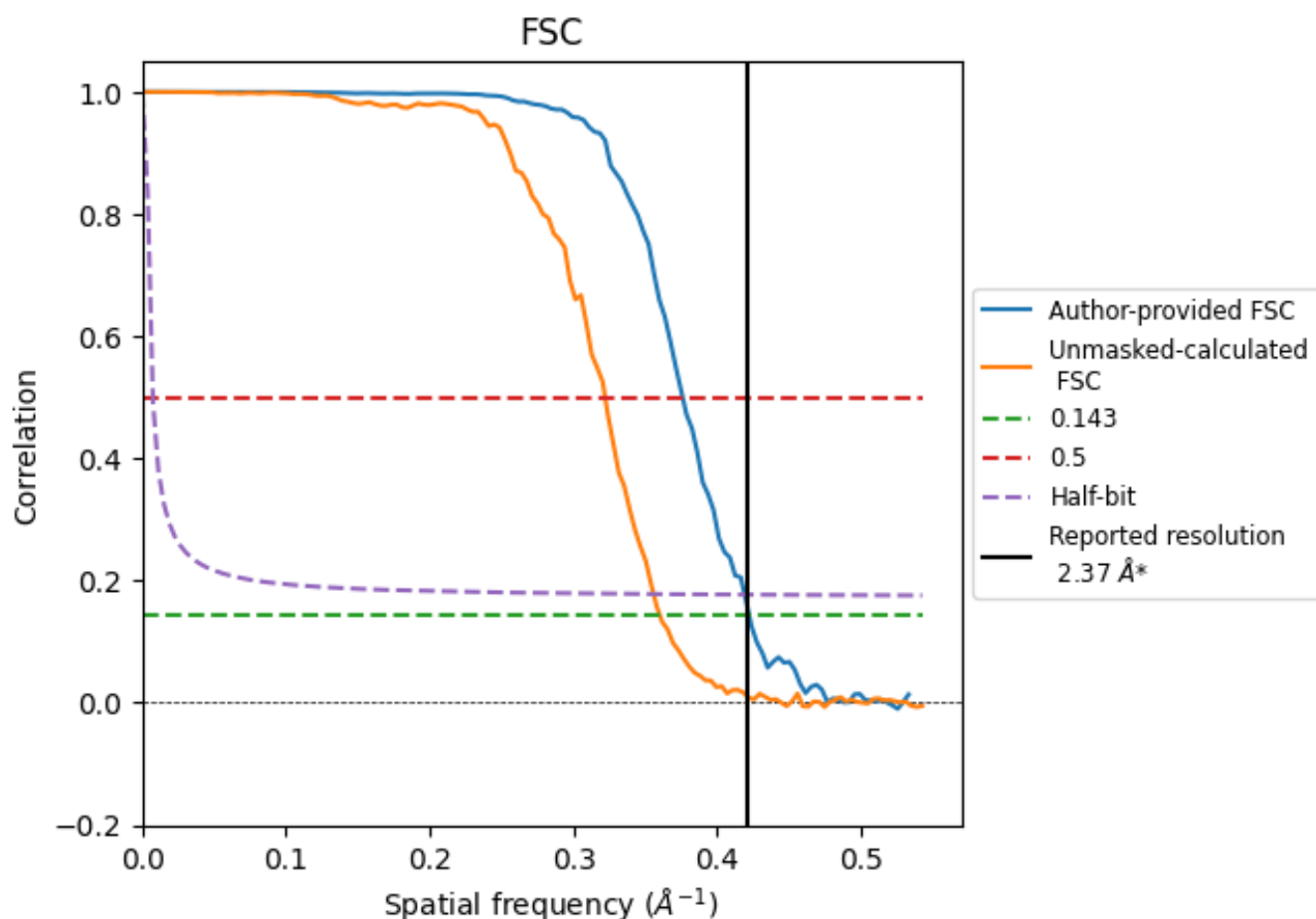


*Reported resolution corresponds to spatial frequency of 0.422 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.422 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

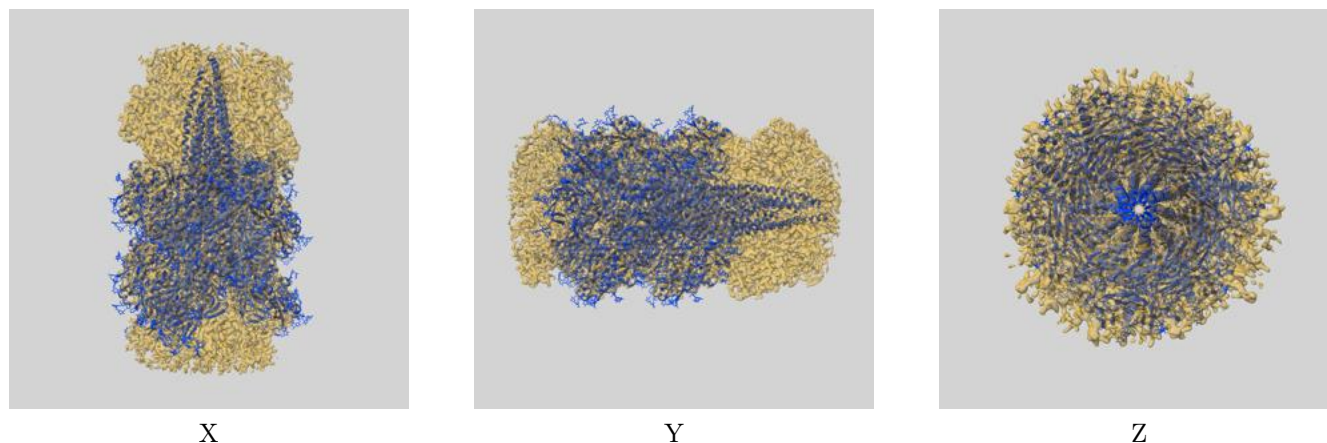
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.37	-	-
Author-provided FSC curve	2.37	2.66	2.38
Unmasked-calculated*	2.78	3.10	2.81

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.78 differs from the reported value 2.37 by more than 10 %

9 Map-model fit [i](#)

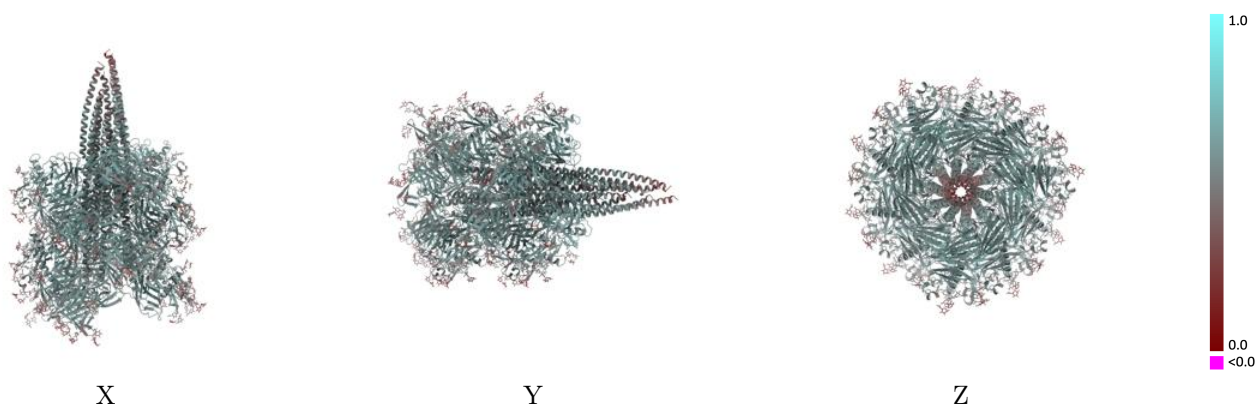
This section contains information regarding the fit between EMDB map EMD-19961 and PDB model 9ETT. Per-residue inclusion information can be found in section 3 on page 17.

9.1 Map-model overlay [i](#)



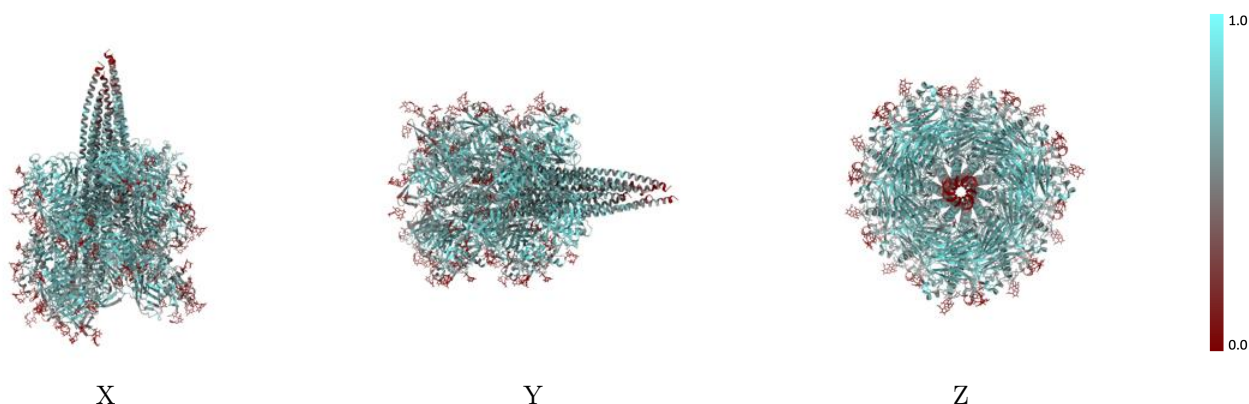
The images above show the 3D surface view of the map at the recommended contour level 0.11 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



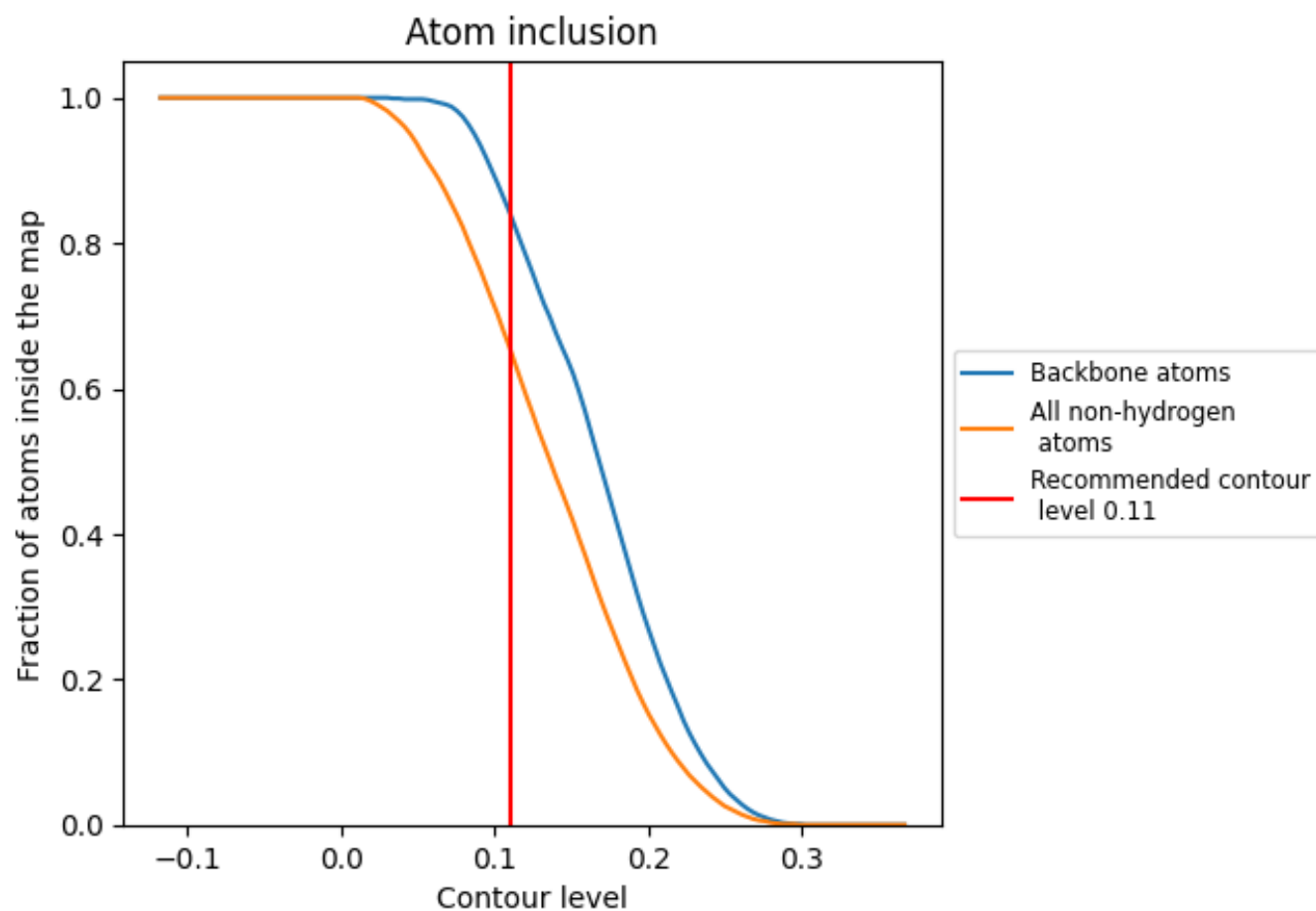
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.11).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 66% 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 (0.11) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6550	 0.5560
0	 0.0000	 0.2820
0A	 0.0510	 0.3580
1	 0.1030	 0.3430
1A	 0.6920	 0.4910
2	 0.0510	 0.3960
2A	 0.0000	 0.3280
3	 0.6920	 0.4990
3A	 0.4870	 0.5200
4	 0.0000	 0.3290
4A	 0.0000	 0.2650
5	 0.6150	 0.5420
5A	 0.0770	 0.3360
6	 0.0260	 0.2740
6A	 0.0510	 0.3710
7	 0.0770	 0.3530
7A	 0.6920	 0.4950
8	 0.0510	 0.4010
8A	 0.0000	 0.2830
9	 0.7180	 0.5110
9A	 0.3850	 0.5170
A	 0.7040	 0.5690
AA	 0.0000	 0.3340
AB	 0.0000	 0.2480
B	 0.7160	 0.5730
BA	 0.6150	 0.5420
BB	 0.0770	 0.3360
C	 0.7160	 0.5760
CA	 0.0000	 0.2840
CB	 0.0260	 0.3620
D	 0.7110	 0.5760
DA	 0.0770	 0.3430
DB	 0.6410	 0.4730
E	 0.7170	 0.5790
EA	 0.0510	 0.4010



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Chain	Atom inclusion	Q-score
EB	 0.0000	 0.2820
F	 0.7220	 0.5800
FA	 0.7180	 0.5270
FB	 0.3590	 0.5130
G	 0.7210	 0.5810
GA	 0.0000	 0.3510
GB	 0.0000	 0.2560
H	 0.7270	 0.5830
HA	 0.6150	 0.5360
HB	 0.0510	 0.3160
I	 0.7270	 0.5830
IA	 0.0000	 0.2650
IB	 0.0260	 0.3390
J	 0.7220	 0.5800
JA	 0.1030	 0.3540
JB	 0.6410	 0.4730
K	 0.7220	 0.5780
KA	 0.0510	 0.3720
KB	 0.0000	 0.2800
L	 0.7180	 0.5790
LA	 0.7180	 0.4970
LB	 0.3080	 0.5080
M	 0.7110	 0.5770
MA	 0.0000	 0.3540
MB	 0.0000	 0.2370
N	 0.7060	 0.5730
NA	 0.6150	 0.5380
NB	 0.0510	 0.3170
O	 0.6950	 0.5730
OA	 0.0000	 0.2610
OB	 0.0260	 0.3330
P	 0.6850	 0.5700
PA	 0.1030	 0.3470
PB	 0.6150	 0.4840
Q	 0.6710	 0.5640
QA	 0.0510	 0.3730
R	 0.6550	 0.5610
RA	 0.6920	 0.5070
S	 0.6350	 0.5570
SA	 0.0000	 0.3920
T	 0.6130	 0.5500
TA	 0.6150	 0.5310

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Chain	Atom inclusion	Q-score
U	 0.0000	 0.3380
UA	 0.0000	 0.2700
V	 0.6150	 0.5370
VA	 0.1280	 0.3290
W	 0.0000	 0.2790
WA	 0.0510	 0.3900
X	 0.0770	 0.3340
XA	 0.6920	 0.4950
Y	 0.0510	 0.3960
YA	 0.0000	 0.3550
Z	 0.7180	 0.5020
ZA	 0.6150	 0.5250
a	 0.0000	 0.3850
aA	 0.0000	 0.2500
b	 0.6410	 0.5530
bA	 0.1280	 0.3420
c	 0.0000	 0.2440
cA	 0.0510	 0.3690
d	 0.0510	 0.3230
dA	 0.6920	 0.4800
e	 0.1030	 0.4130
eA	 0.0000	 0.3690
f	 0.6920	 0.5130
fA	 0.6150	 0.5210
g	 0.0000	 0.3570
gA	 0.0000	 0.2770
h	 0.6410	 0.5330
hA	 0.1280	 0.3570
i	 0.0000	 0.2690
iA	 0.0510	 0.3620
j	 0.0510	 0.3400
jA	 0.6670	 0.4900
k	 0.1030	 0.3960
kA	 0.0000	 0.3800
l	 0.6920	 0.4960
lA	 0.6410	 0.5340
m	 0.0000	 0.3740
mA	 0.0000	 0.2700
n	 0.6410	 0.5360
nA	 0.1280	 0.3270
o	 0.0000	 0.2680
oA	 0.0510	 0.3680

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Chain	Atom inclusion	Q-score
p	 0.1030	 0.3710
pA	 0.6670	 0.4960
q	 0.1030	 0.4020
qA	 0.0000	 0.3430
r	 0.6920	 0.5040
rA	 0.6150	 0.5340
s	 0.0000	 0.3540
sA	 0.0000	 0.2510
t	 0.6150	 0.5430
tA	 0.1030	 0.3420
u	 0.0000	 0.2610
uA	 0.0510	 0.3710
v	 0.1030	 0.3390
vA	 0.6670	 0.4820
w	 0.0510	 0.3990
wA	 0.0000	 0.3320
x	 0.6920	 0.5110
xA	 0.5380	 0.5260
y	 0.0000	 0.3480
yA	 0.0000	 0.2490
z	 0.6150	 0.5410
zA	 0.1030	 0.3390