



## Full wwPDB EM Validation Report ⓘ

Feb 29, 2024 – 04:45 pm GMT

PDB ID : 8Q30  
EMDB ID : EMD-18119  
Title : Sulfolobus acidocaldarius AAP filament.  
Authors : Isupov, M.N.; Gaines, M.; Daum, B.; McLaren, M.  
Deposited on : 2023-08-03  
Resolution : 3.22 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

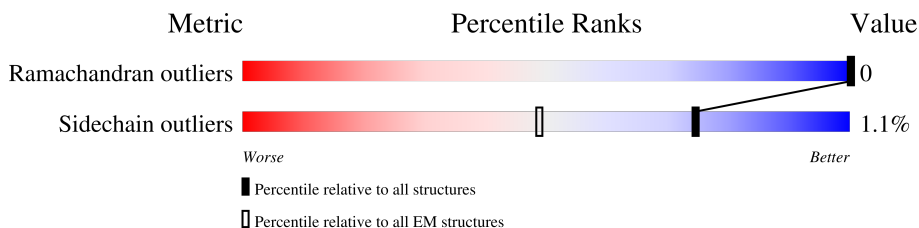
EMDB validation analysis : 0.0.1.dev70  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

# 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 3.22 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	0	141	13% (red), 99% (green), . (grey)
1	1	141	16% (red), 99% (green), . (grey)
1	2	141	12% (red), 99% (green), . (grey)
1	3	141	13% (red), 100% (green)
1	4	141	16% (red), 99% (green), . (grey)
1	5	141	12% (red), 99% (green), . (grey)
1	6	141	13% (red), 100% (green)
1	7	141	15% (red), 99% (green), . (grey)
1	8	141	13% (red), 99% (green), . (grey)

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Mol	Chain	Length	Quality of chain
1	9	141	14% 100%
1	A	141	14% 99%
1	B	141	17% 99%
1	C	141	12% 99%
1	D	141	13% 99%
1	E	141	16% 99%
1	F	141	12% 99%
1	G	141	13% 100%
1	H	141	13% 99%
1	I	141	12% 99%
1	J	141	14% 100%
1	K	141	16% 100%
1	L	141	12% 98%
1	LA	141	12% 99%
1	LB	141	13% 100%
1	LC	141	17% 99%
1	LD	141	12% 99%
1	LE	141	14% 100%
1	LF	141	16% 99%
1	LG	141	11% 99%
1	LH	141	12% 99%
1	LI	141	16% 99%
1	LJ	141	12% 99%
1	M	141	13% 100%
1	N	141	15% 98%

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Mol	Chain	Length	Quality of chain
1	O	141	12% 99%
1	P	141	13% 99%
1	Q	141	14% 99%
1	R	141	12% 97%
1	S	141	15% 100%
1	T	141	14% 100%
1	U	141	12% 98%
1	V	141	15% 99%
1	W	141	16% 98%
1	X	141	12% 99%
1	Y	141	13% 99%
1	Z	141	15% 99%
1	a	141	13% 99%
1	b	141	14% 99%
1	c	141	14% 99%
1	d	141	12% 97%
1	e	141	15% 99%
1	f	141	16% 99%
1	g	141	12% 99%
1	h	141	13% 100%
1	i	141	15% 99%
1	j	141	12% 99%
1	k	141	13% 100%
1	l	141	16% 100%
1	m	141	12% 98%

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Mol	Chain	Length	Quality of chain
1	n	141	14% 100%
1	o	141	16% 100%
1	p	141	12% 98%
1	q	141	14% 99%
1	r	141	15% 99%
1	s	141	12% 98%
1	t	141	14% 100%
1	u	141	14% 99%
1	v	141	12% 99%
1	w	141	13% 99%
1	x	141	15% 99%
1	y	141	12% 99%
1	z	141	14% 100%
2	0A	2	100% 50% 50%
2	1B	2	100%
2	2A	2	100%
2	2B	2	100%
2	3A	2	100%
2	3B	2	100% 50% 50%
2	4A	2	100% 50% 50%
2	5B	2	100% 50% 50%
2	6A	2	100% 50% 50%
2	7B	2	100%
2	8A	2	100%
2	8B	2	100%

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Mol	Chain	Length	Quality of chain
2	9A	2	100% 
2	9B	2	100% 
2	AA	2	100% 
2	AB	2	100% 
2	BA	2	100% 
2	BC	2	100% 
2	CB	2	100% 
2	DA	2	100% 
2	DC	2	100% 
2	EB	2	100% 
2	EC	2	100% 
2	FA	2	100% 
2	FB	2	100% 
2	FC	2	100% 
2	GA	2	100% 
2	GB	2	100% 
2	HA	2	100% 
2	HC	2	100% 
2	IB	2	100% 
2	JA	2	100% 
2	JC	2	100% 
2	KB	2	100% 
2	KC	2	100% 
2	MA	2	100% 
2	MB	2	100% 

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Mol	Chain	Length	Quality of chain
2	MC	2	100% 50% 50%
2	NA	2	100%
2	NB	2	100% 50% 50%
2	OA	2	100% 50% 50%
2	OC	2	100% 50% 50%
2	PB	2	100% 50% 50%
2	QA	2	100% 50% 50%
2	QC	2	100%
2	RB	2	100%
2	RC	2	100%
2	SA	2	100%
2	SB	2	100%
2	SC	2	100% 50% 50%
2	TA	2	100%
2	TB	2	100% 50% 50%
2	UA	2	100% 50% 50%
2	UC	2	100% 50% 50%
2	VB	2	100% 50% 50%
2	WA	2	100% 50% 50%
2	WC	2	100%
2	XB	2	100%
2	YA	2	50% 100%
2	YB	2	100%
2	ZA	2	100%
2	ZB	2	100% 50% 50%

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Mol	Chain	Length	Quality of chain
2	aA	2	100%  50% 50%
2	bB	2	100%  50% 50%
2	cA	2	100%  50% 50%
2	dB	2	100%  100%
2	eA	2	100%  100%
2	eB	2	100%  100%
2	fA	2	100%  100%
2	fB	2	100%  50% 50%
2	gA	2	100%  50% 50%
2	hB	2	100%  50% 50%
2	iA	2	100%  50% 50%
2	jB	2	100%  100%
2	kA	2	100%  100%
2	kB	2	100%  100%
2	lA	2	100%  100%
2	lB	2	100%  50% 50%
2	mA	2	100%  50% 50%
2	nB	2	100%  50% 50%
2	oA	2	100%  50% 50%
2	pB	2	100%  100%
2	qA	2	100%  100%
2	qB	2	100%  50% 50%
2	rA	2	100%  100%
2	rB	2	100%  50% 50%
2	sA	2	100%  50% 50%

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Mol	Chain	Length	Quality of chain
2	tB	2	100% 50% 50%
2	uA	2	100% 50% 50%
2	vB	2	100%
2	wA	2	100%
2	wB	2	100%
2	xA	2	100% 50% 50%
2	xB	2	100% 50% 50%
2	yA	2	100% 50% 50%
2	zB	2	100% 50% 50%
3	0B	3	67% 67% 33%
3	1A	3	100% 67% 33%
3	4B	3	100% 67% 33%
3	5A	3	100% 67% 33%
3	6B	3	67% 67% 33%
3	7A	3	67% 67% 33%
3	AC	3	100% 67% 33%
3	BB	3	100% 67% 33%
3	CA	3	100% 67% 33%
3	CC	3	67% 67% 33%
3	DB	3	100% 67% 33%
3	EA	3	67% 67% 33%
3	GC	3	100% 67% 33%
3	HB	3	100% 67% 33%
3	IA	3	100% 67% 33%
3	IC	3	67% 67% 33%

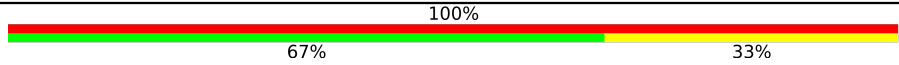
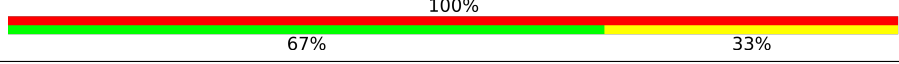
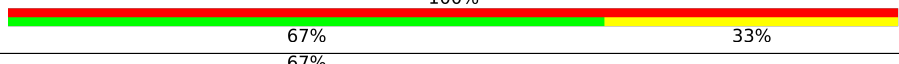
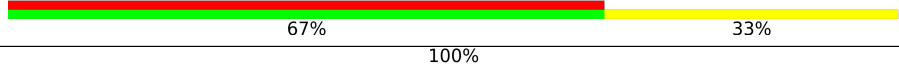
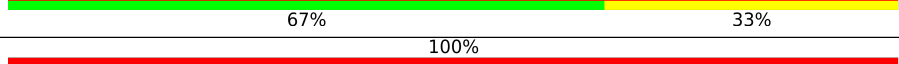
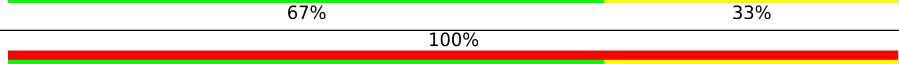
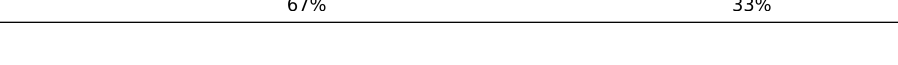
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Mol	Chain	Length	Quality of chain	
3	JB	3	100%	33%
3	KA	3	67%	33%
3	NC	3	100%	33%
3	OB	3	100%	33%
3	PA	3	100%	33%
3	PC	3	100%	33%
3	QB	3	67%	33%
3	RA	3	67%	33%
3	TC	3	100%	33%
3	UB	3	100%	33%
3	VA	3	100%	33%
3	VC	3	100%	33%
3	WB	3	67%	33%
3	XA	3	100%	33%
3	aB	3	100%	33%
3	bA	3	100%	33%
3	cB	3	100%	33%
3	dA	3	100%	33%
3	gB	3	100%	33%
3	hA	3	100%	33%
3	iB	3	67%	33%
3	jA	3	100%	33%
3	mB	3	100%	33%
3	nA	3	100%	33%
3	oB	3	67%	33%

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Mol	Chain	Length	Quality of chain
3	pA	3	 100% 67% 33%
3	sB	3	 100% 67% 33%
3	tA	3	 100% 67% 33%
3	uB	3	 100% 67% 33%
3	vA	3	 100% 67% 33%
3	yB	3	 100% 67% 33%
3	zA	3	 100% 67% 33%

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 77784 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 DUF4352 domain-containing protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	A	141	1001	639	165	197	0	0
1	B	141	1001	639	165	197	0	0
1	C	141	1001	639	165	197	0	0
1	D	141	1001	639	165	197	0	0
1	E	141	1001	639	165	197	0	0
1	F	141	1001	639	165	197	0	0
1	G	141	1001	639	165	197	0	0
1	H	141	1001	639	165	197	0	0
1	I	141	1001	639	165	197	0	0
1	J	141	1001	639	165	197	0	0
1	K	141	1001	639	165	197	0	0
1	L	141	1001	639	165	197	0	0
1	M	141	1001	639	165	197	0	0
1	N	141	1001	639	165	197	0	0
1	O	141	1001	639	165	197	0	0
1	P	141	1001	639	165	197	0	0
1	Q	141	1001	639	165	197	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
1	R	141	Total 1001	C 639	N 165	O 197	0	0
1	S	141	Total 1001	C 639	N 165	O 197	0	0
1	T	141	Total 1001	C 639	N 165	O 197	0	0
1	U	141	Total 1001	C 639	N 165	O 197	0	0
1	V	141	Total 1001	C 639	N 165	O 197	0	0
1	W	141	Total 1001	C 639	N 165	O 197	0	0
1	X	141	Total 1001	C 639	N 165	O 197	0	0
1	Y	141	Total 1001	C 639	N 165	O 197	0	0
1	Z	141	Total 1001	C 639	N 165	O 197	0	0
1	a	141	Total 1001	C 639	N 165	O 197	0	0
1	b	141	Total 1001	C 639	N 165	O 197	0	0
1	c	141	Total 1001	C 639	N 165	O 197	0	0
1	d	141	Total 1001	C 639	N 165	O 197	0	0
1	e	141	Total 1001	C 639	N 165	O 197	0	0
1	f	141	Total 1001	C 639	N 165	O 197	0	0
1	g	141	Total 1001	C 639	N 165	O 197	0	0
1	h	141	Total 1001	C 639	N 165	O 197	0	0
1	i	141	Total 1001	C 639	N 165	O 197	0	0
1	j	141	Total 1001	C 639	N 165	O 197	0	0
1	k	141	Total 1001	C 639	N 165	O 197	0	0
1	l	141	Total 1001	C 639	N 165	O 197	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
1	m	141	Total 1001	C 639	N 165	O 197	0	0
1	n	141	Total 1001	C 639	N 165	O 197	0	0
1	o	141	Total 1001	C 639	N 165	O 197	0	0
1	p	141	Total 1001	C 639	N 165	O 197	0	0
1	q	141	Total 1001	C 639	N 165	O 197	0	0
1	r	141	Total 1001	C 639	N 165	O 197	0	0
1	s	141	Total 1001	C 639	N 165	O 197	0	0
1	t	141	Total 1001	C 639	N 165	O 197	0	0
1	u	141	Total 1001	C 639	N 165	O 197	0	0
1	v	141	Total 1001	C 639	N 165	O 197	0	0
1	w	141	Total 1001	C 639	N 165	O 197	0	0
1	x	141	Total 1001	C 639	N 165	O 197	0	0
1	y	141	Total 1001	C 639	N 165	O 197	0	0
1	z	141	Total 1001	C 639	N 165	O 197	0	0
1	1	141	Total 1001	C 639	N 165	O 197	0	0
1	2	141	Total 1001	C 639	N 165	O 197	0	0
1	3	141	Total 1001	C 639	N 165	O 197	0	0
1	4	141	Total 1001	C 639	N 165	O 197	0	0
1	5	141	Total 1001	C 639	N 165	O 197	0	0
1	6	141	Total 1001	C 639	N 165	O 197	0	0
1	7	141	Total 1001	C 639	N 165	O 197	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
1	8	141	Total	C	N	O	0	0
			1001	639	165	197		
1	9	141	Total	C	N	O	0	0
			1001	639	165	197		
1	0	141	Total	C	N	O	0	0
			1001	639	165	197		
1	LA	141	Total	C	N	O	0	0
			1001	639	165	197		
1	LB	141	Total	C	N	O	0	0
			1001	639	165	197		
1	LC	141	Total	C	N	O	0	0
			1001	639	165	197		
1	LD	141	Total	C	N	O	0	0
			1001	639	165	197		
1	LE	141	Total	C	N	O	0	0
			1001	639	165	197		
1	LF	141	Total	C	N	O	0	0
			1001	639	165	197		
1	LG	141	Total	C	N	O	0	0
			1001	639	165	197		
1	LH	141	Total	C	N	O	0	0
			1001	639	165	197		
1	LI	141	Total	C	N	O	0	0
			1001	639	165	197		
1	LJ	141	Total	C	N	O	0	0
			1001	639	165	197		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
2	AA	2	Total	C	N	O	0	0
			28	16	2	10		
2	BA	2	Total	C	N	O	0	0
			28	16	2	10		
2	DA	2	Total	C	N	O	0	0
			28	16	2	10		
2	FA	2	Total	C	N	O	0	0
			28	16	2	10		

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	GA	2	28	16	2	10	0	0
2	HA	2	28	16	2	10	0	0
2	JA	2	28	16	2	10	0	0
2	MA	2	28	16	2	10	0	0
2	NA	2	28	16	2	10	0	0
2	OA	2	28	16	2	10	0	0
2	QA	2	28	16	2	10	0	0
2	SA	2	28	16	2	10	0	0
2	TA	2	28	16	2	10	0	0
2	UA	2	28	16	2	10	0	0
2	WA	2	28	16	2	10	0	0
2	YA	2	28	16	2	10	0	0
2	ZA	2	28	16	2	10	0	0
2	aA	2	28	16	2	10	0	0
2	cA	2	28	16	2	10	0	0
2	eA	2	28	16	2	10	0	0
2	fA	2	28	16	2	10	0	0
2	gA	2	28	16	2	10	0	0
2	iA	2	28	16	2	10	0	0
2	kA	2	28	16	2	10	0	0
2	lA	2	28	16	2	10	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	mA	2	Total 28	C 16	N 2	O 10	0	0
2	oA	2	Total 28	C 16	N 2	O 10	0	0
2	qA	2	Total 28	C 16	N 2	O 10	0	0
2	rA	2	Total 28	C 16	N 2	O 10	0	0
2	sA	2	Total 28	C 16	N 2	O 10	0	0
2	uA	2	Total 28	C 16	N 2	O 10	0	0
2	wA	2	Total 28	C 16	N 2	O 10	0	0
2	xA	2	Total 28	C 16	N 2	O 10	0	0
2	yA	2	Total 28	C 16	N 2	O 10	0	0
2	0A	2	Total 28	C 16	N 2	O 10	0	0
2	2A	2	Total 28	C 16	N 2	O 10	0	0
2	3A	2	Total 28	C 16	N 2	O 10	0	0
2	4A	2	Total 28	C 16	N 2	O 10	0	0
2	6A	2	Total 28	C 16	N 2	O 10	0	0
2	8A	2	Total 28	C 16	N 2	O 10	0	0
2	9A	2	Total 28	C 16	N 2	O 10	0	0
2	AB	2	Total 28	C 16	N 2	O 10	0	0
2	CB	2	Total 28	C 16	N 2	O 10	0	0
2	EB	2	Total 28	C 16	N 2	O 10	0	0
2	FB	2	Total 28	C 16	N 2	O 10	0	0
2	GB	2	Total 28	C 16	N 2	O 10	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	IB	2	Total 28	C 16	N 2	O 10	0	0
2	KB	2	Total 28	C 16	N 2	O 10	0	0
2	MB	2	Total 28	C 16	N 2	O 10	0	0
2	NB	2	Total 28	C 16	N 2	O 10	0	0
2	PB	2	Total 28	C 16	N 2	O 10	0	0
2	RB	2	Total 28	C 16	N 2	O 10	0	0
2	SB	2	Total 28	C 16	N 2	O 10	0	0
2	TB	2	Total 28	C 16	N 2	O 10	0	0
2	VB	2	Total 28	C 16	N 2	O 10	0	0
2	XB	2	Total 28	C 16	N 2	O 10	0	0
2	YB	2	Total 28	C 16	N 2	O 10	0	0
2	ZB	2	Total 28	C 16	N 2	O 10	0	0
2	bB	2	Total 28	C 16	N 2	O 10	0	0
2	dB	2	Total 28	C 16	N 2	O 10	0	0
2	eB	2	Total 28	C 16	N 2	O 10	0	0
2	fB	2	Total 28	C 16	N 2	O 10	0	0
2	hB	2	Total 28	C 16	N 2	O 10	0	0
2	jB	2	Total 28	C 16	N 2	O 10	0	0
2	kB	2	Total 28	C 16	N 2	O 10	0	0
2	lB	2	Total 28	C 16	N 2	O 10	0	0
2	nB	2	Total 28	C 16	N 2	O 10	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	pB	2	28	16	2	10	0	0
2	qB	2	28	16	2	10	0	0
2	rB	2	28	16	2	10	0	0
2	tB	2	28	16	2	10	0	0
2	vB	2	28	16	2	10	0	0
2	wB	2	28	16	2	10	0	0
2	xB	2	28	16	2	10	0	0
2	zB	2	28	16	2	10	0	0
2	1B	2	28	16	2	10	0	0
2	2B	2	28	16	2	10	0	0
2	3B	2	28	16	2	10	0	0
2	5B	2	28	16	2	10	0	0
2	7B	2	28	16	2	10	0	0
2	8B	2	28	16	2	10	0	0
2	9B	2	28	16	2	10	0	0
2	BC	2	28	16	2	10	0	0
2	DC	2	28	16	2	10	0	0
2	EC	2	28	16	2	10	0	0
2	FC	2	28	16	2	10	0	0
2	HC	2	28	16	2	10	0	0
2	JC	2	28	16	2	10	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	KC	2	28	16	2	10	0	0
2	MC	2	28	16	2	10	0	0
2	OC	2	28	16	2	10	0	0
2	QC	2	28	16	2	10	0	0
2	RC	2	28	16	2	10	0	0
2	SC	2	28	16	2	10	0	0
2	UC	2	28	16	2	10	0	0
2	WC	2	28	16	2	10	0	0

- Molecule 3 is an oligosaccharide called 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	CA	3	42	22	2	17	1	0	0
3	EA	3	42	22	2	17	1	0	0
3	IA	3	42	22	2	17	1	0	0
3	KA	3	42	22	2	17	1	0	0
3	PA	3	42	22	2	17	1	0	0
3	RA	3	42	22	2	17	1	0	0
3	VA	3	42	22	2	17	1	0	0
3	XA	3	42	22	2	17	1	0	0
3	bA	3	42	22	2	17	1	0	0
3	dA	3	42	22	2	17	1	0	0
3	hA	3	42	22	2	17	1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	jA	3	Total 42	C 22	N 2	O 17	S 1	0	0
3	nA	3	Total 42	C 22	N 2	O 17	S 1	0	0
3	pA	3	Total 42	C 22	N 2	O 17	S 1	0	0
3	tA	3	Total 42	C 22	N 2	O 17	S 1	0	0
3	vA	3	Total 42	C 22	N 2	O 17	S 1	0	0
3	zA	3	Total 42	C 22	N 2	O 17	S 1	0	0
3	1A	3	Total 42	C 22	N 2	O 17	S 1	0	0
3	5A	3	Total 42	C 22	N 2	O 17	S 1	0	0
3	7A	3	Total 42	C 22	N 2	O 17	S 1	0	0
3	BB	3	Total 42	C 22	N 2	O 17	S 1	0	0
3	DB	3	Total 42	C 22	N 2	O 17	S 1	0	0
3	HB	3	Total 42	C 22	N 2	O 17	S 1	0	0
3	JB	3	Total 42	C 22	N 2	O 17	S 1	0	0
3	OB	3	Total 42	C 22	N 2	O 17	S 1	0	0
3	QB	3	Total 42	C 22	N 2	O 17	S 1	0	0
3	UB	3	Total 42	C 22	N 2	O 17	S 1	0	0
3	WB	3	Total 42	C 22	N 2	O 17	S 1	0	0
3	aB	3	Total 42	C 22	N 2	O 17	S 1	0	0
3	cB	3	Total 42	C 22	N 2	O 17	S 1	0	0
3	gB	3	Total 42	C 22	N 2	O 17	S 1	0	0
3	iB	3	Total 42	C 22	N 2	O 17	S 1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	mB	3	Total 42	C 22	N 2	O 17	S 1	0	0
3	oB	3	Total 42	C 22	N 2	O 17	S 1	0	0
3	sB	3	Total 42	C 22	N 2	O 17	S 1	0	0
3	uB	3	Total 42	C 22	N 2	O 17	S 1	0	0
3	yB	3	Total 42	C 22	N 2	O 17	S 1	0	0
3	0B	3	Total 42	C 22	N 2	O 17	S 1	0	0
3	4B	3	Total 42	C 22	N 2	O 17	S 1	0	0
3	6B	3	Total 42	C 22	N 2	O 17	S 1	0	0
3	AC	3	Total 42	C 22	N 2	O 17	S 1	0	0
3	CC	3	Total 42	C 22	N 2	O 17	S 1	0	0
3	GC	3	Total 42	C 22	N 2	O 17	S 1	0	0
3	IC	3	Total 42	C 22	N 2	O 17	S 1	0	0
3	NC	3	Total 42	C 22	N 2	O 17	S 1	0	0
3	PC	3	Total 42	C 22	N 2	O 17	S 1	0	0
3	TC	3	Total 42	C 22	N 2	O 17	S 1	0	0
3	VC	3	Total 42	C 22	N 2	O 17	S 1	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
4	A	1	Total 14	8	1	5	0
4	B	1	Total 14	8	1	5	0
4	C	1	Total 14	8	1	5	0
4	D	1	Total 14	8	1	5	0
4	E	1	Total 14	8	1	5	0
4	F	1	Total 14	8	1	5	0
4	G	1	Total 14	8	1	5	0
4	H	1	Total 14	8	1	5	0
4	I	1	Total 14	8	1	5	0
4	J	1	Total 14	8	1	5	0
4	K	1	Total 14	8	1	5	0
4	L	1	Total 14	8	1	5	0
4	M	1	Total 14	8	1	5	0
4	N	1	Total 14	8	1	5	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
4	O	1	Total 14	8	1	5	0
4	P	1	Total 14	8	1	5	0
4	Q	1	Total 14	8	1	5	0
4	R	1	Total 14	8	1	5	0
4	S	1	Total 14	8	1	5	0
4	T	1	Total 14	8	1	5	0
4	U	1	Total 14	8	1	5	0
4	V	1	Total 14	8	1	5	0
4	W	1	Total 14	8	1	5	0
4	X	1	Total 14	8	1	5	0
4	Y	1	Total 14	8	1	5	0
4	Z	1	Total 14	8	1	5	0
4	a	1	Total 14	8	1	5	0
4	b	1	Total 14	8	1	5	0
4	c	1	Total 14	8	1	5	0
4	d	1	Total 14	8	1	5	0
4	e	1	Total 14	8	1	5	0
4	f	1	Total 14	8	1	5	0
4	g	1	Total 14	8	1	5	0
4	h	1	Total 14	8	1	5	0
4	i	1	Total 14	8	1	5	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
4	j	1	Total 14	8	1	5	0
4	k	1	Total 14	8	1	5	0
4	l	1	Total 14	8	1	5	0
4	m	1	Total 14	8	1	5	0
4	n	1	Total 14	8	1	5	0
4	o	1	Total 14	8	1	5	0
4	p	1	Total 14	8	1	5	0
4	q	1	Total 14	8	1	5	0
4	r	1	Total 14	8	1	5	0
4	s	1	Total 14	8	1	5	0
4	t	1	Total 14	8	1	5	0
4	u	1	Total 14	8	1	5	0
4	v	1	Total 14	8	1	5	0
4	w	1	Total 14	8	1	5	0
4	x	1	Total 14	8	1	5	0
4	y	1	Total 14	8	1	5	0
4	z	1	Total 14	8	1	5	0
4	1	1	Total 14	8	1	5	0
4	2	1	Total 14	8	1	5	0
4	3	1	Total 14	8	1	5	0
4	4	1	Total 14	8	1	5	0

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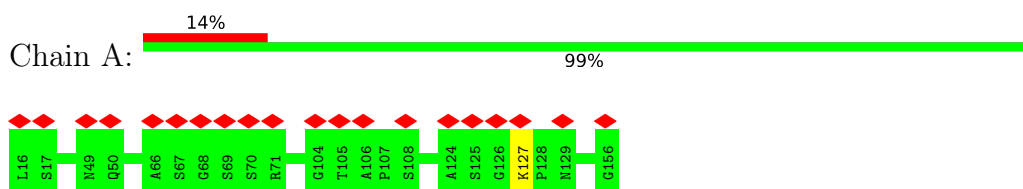
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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
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4	6	1	Total 14	8	1	5	0
4	7	1	Total 14	8	1	5	0
4	8	1	Total 14	8	1	5	0
4	9	1	Total 14	8	1	5	0
4	0	1	Total 14	8	1	5	0
4	LA	1	Total 14	8	1	5	0
4	LB	1	Total 14	8	1	5	0
4	LC	1	Total 14	8	1	5	0
4	LD	1	Total 14	8	1	5	0
4	LE	1	Total 14	8	1	5	0
4	LF	1	Total 14	8	1	5	0
4	LG	1	Total 14	8	1	5	0
4	LH	1	Total 14	8	1	5	0
4	LI	1	Total 14	8	1	5	0
4	LJ	1	Total 14	8	1	5	0

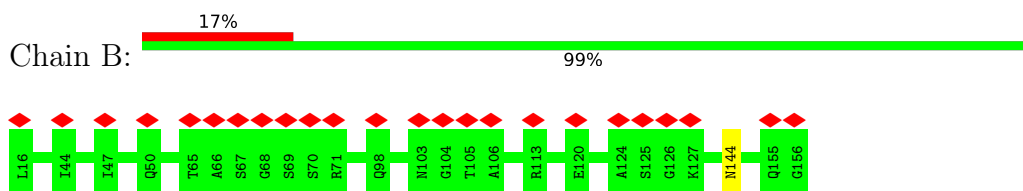
### 3 Residue-property plots [i](#)

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.

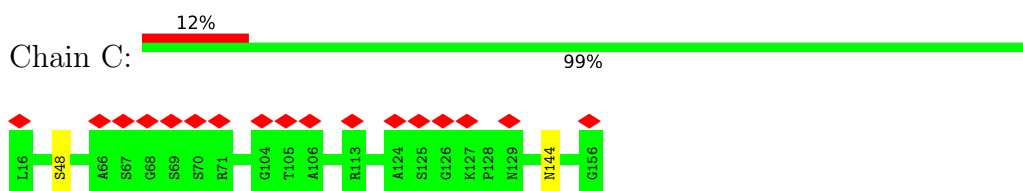
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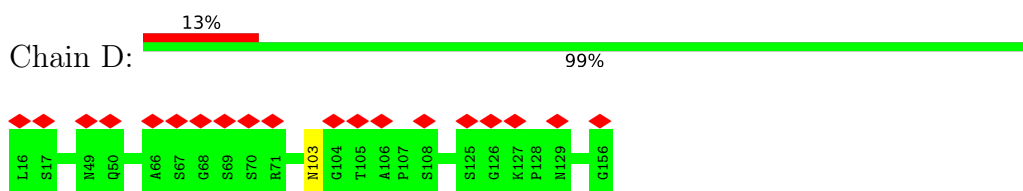
- Molecule 1: DUF4352 domain-containing protein



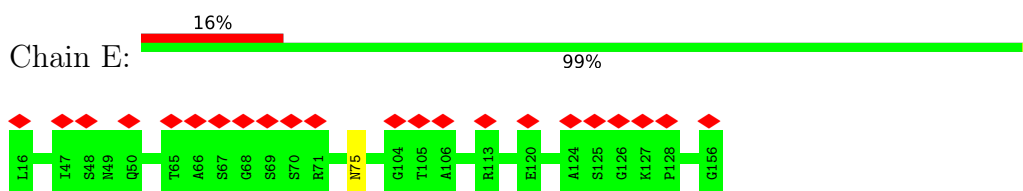
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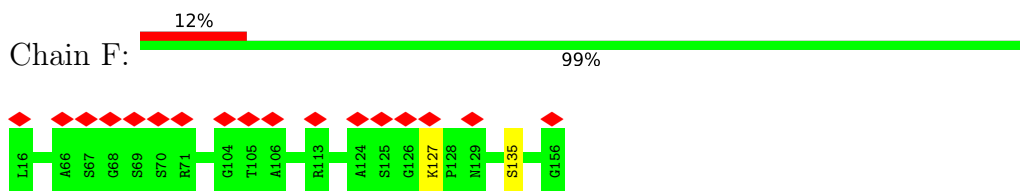
- Molecule 1: DUF4352 domain-containing protein



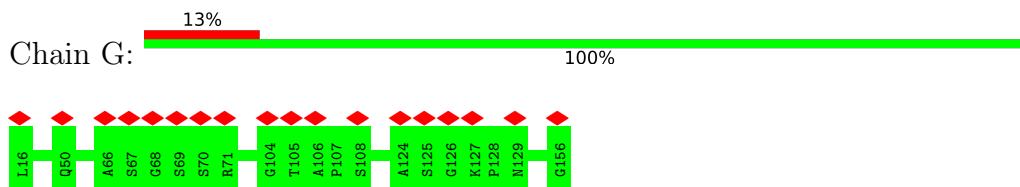
- Molecule 1: DUF4352 domain-containing protein



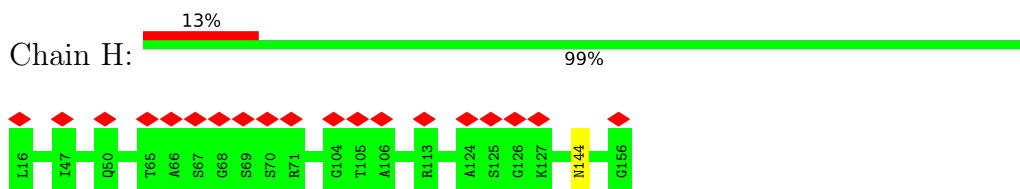
- Molecule 1: DUF4352 domain-containing protein



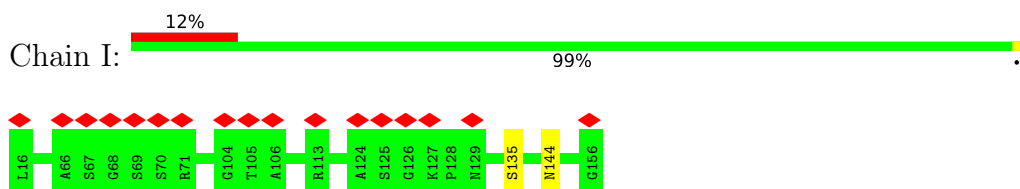
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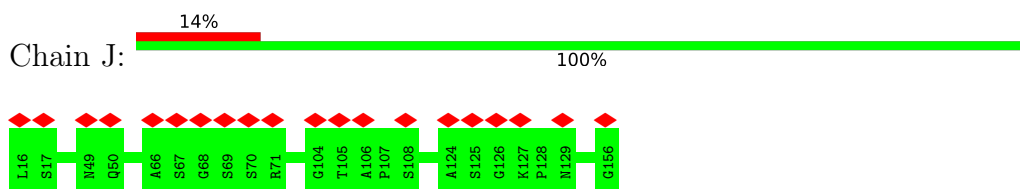
- Molecule 1: DUF4352 domain-containing protein



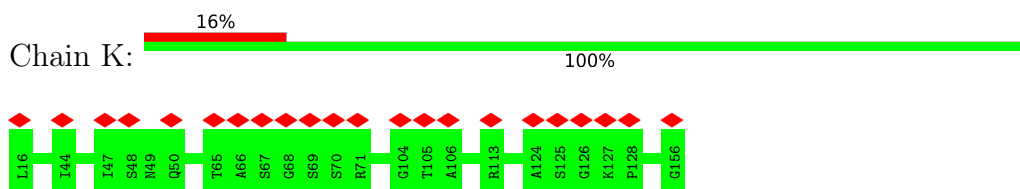
- Molecule 1: DUF4352 domain-containing protein



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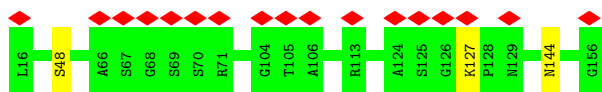


- Molecule 1: DUF4352 domain-containing protein

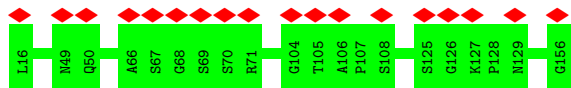


- Molecule 1: DUF4352 domain-containing protein

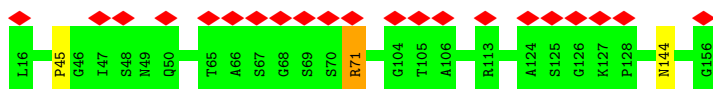




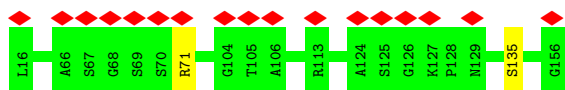
- Molecule 1: DUF4352 domain-containing protein



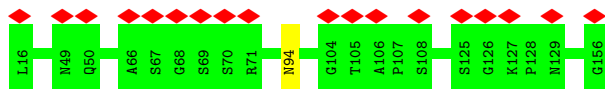
- Molecule 1: DUF4352 domain-containing protein



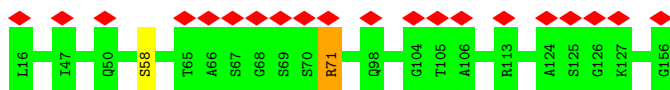
- Molecule 1: DUF4352 domain-containing protein



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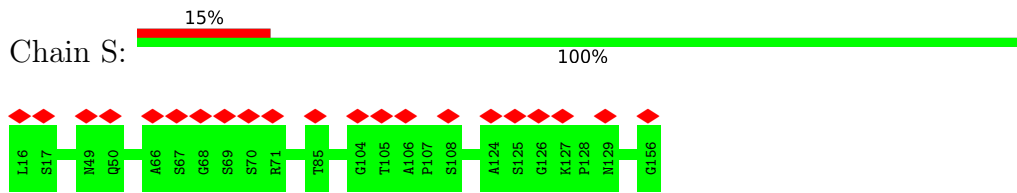
- Molecule 1: DUF4352 domain-containing protein



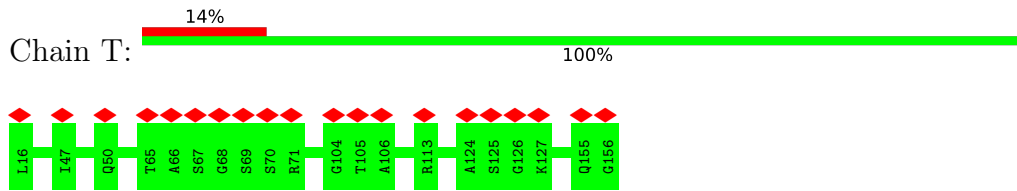
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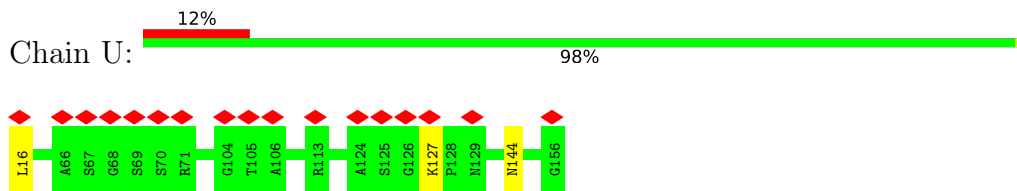
- Molecule 1: DUF4352 domain-containing protein



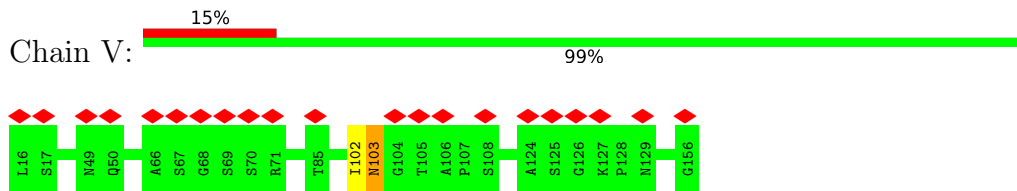
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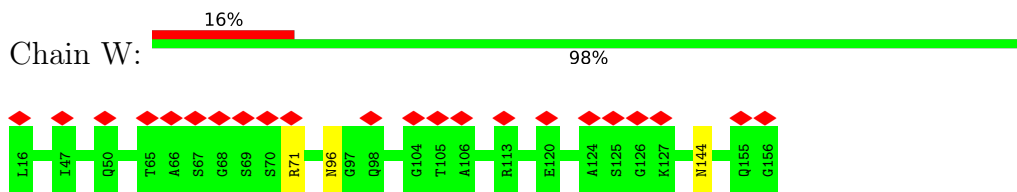
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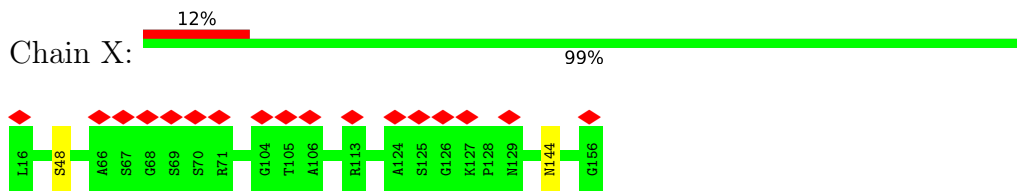
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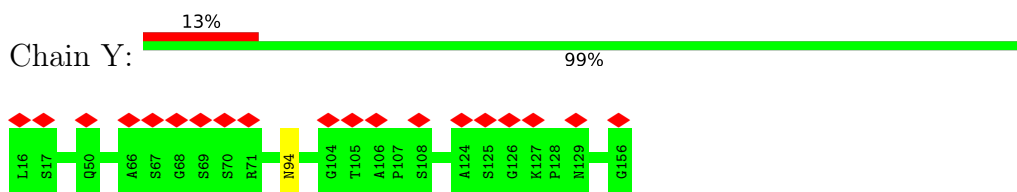
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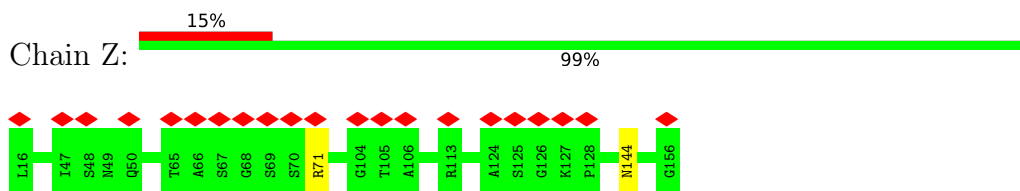
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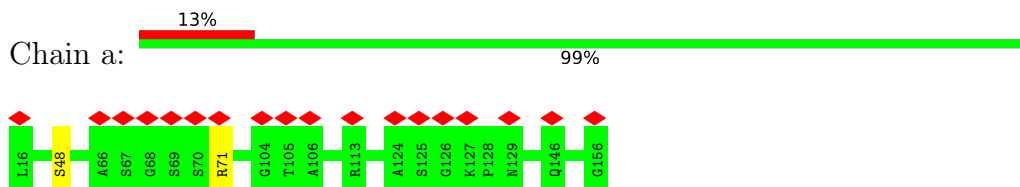
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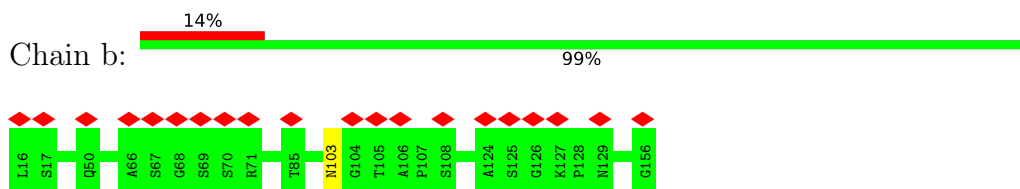
- Molecule 1: DUF4352 domain-containing protein



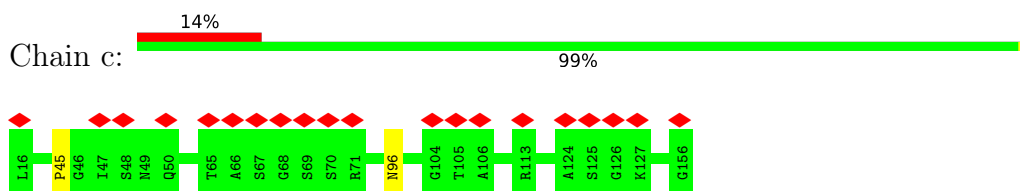
- Molecule 1: DUF4352 domain-containing protein



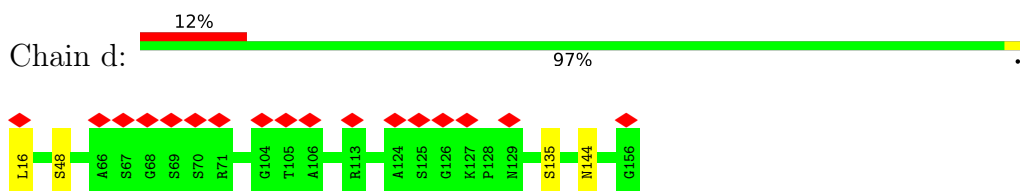
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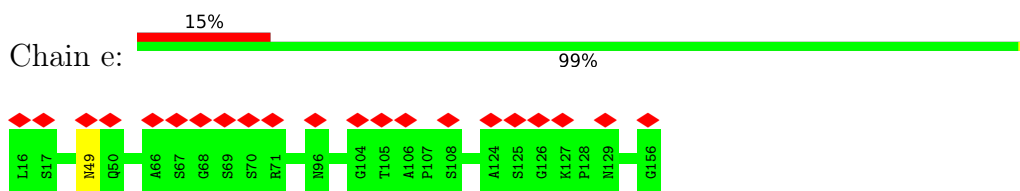
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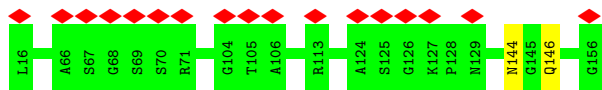


- Molecule 1: DUF4352 domain-containing protein

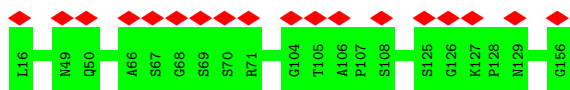




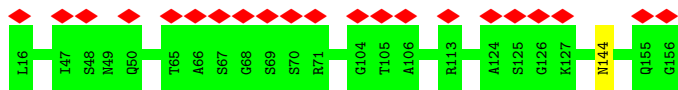
- Molecule 1: DUF4352 domain-containing protein



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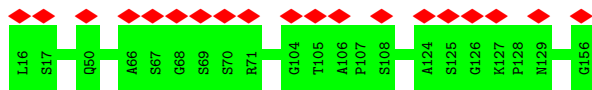
- Molecule 1: DUF4352 domain-containing protein



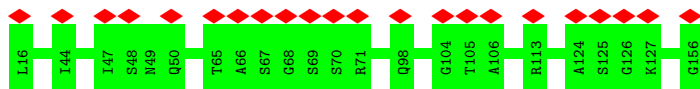
- Molecule 1: DUF4352 domain-containing protein



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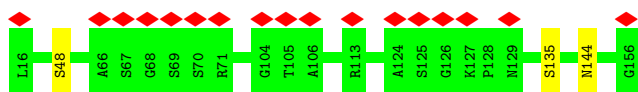


- Molecule 1: DUF4352 domain-containing protein

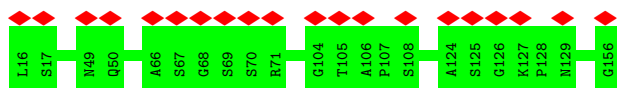


- Molecule 1: DUF4352 domain-containing protein

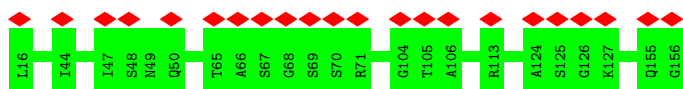




- Molecule 1: DUF4352 domain-containing protein



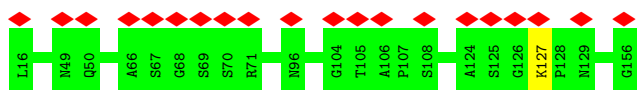
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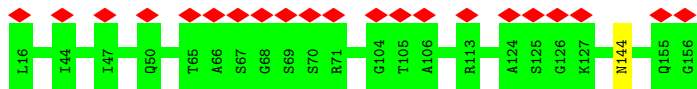
- Molecule 1: DUF4352 domain-containing protein



- Molecule 1: DUF4352 domain-containing protein

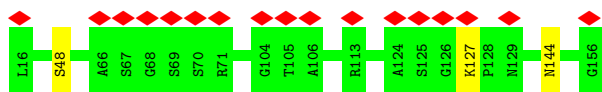


- Molecule 1: DUF4352 domain-containing protein

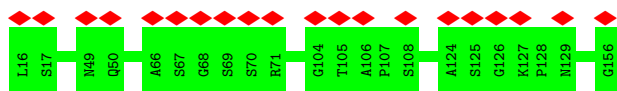


- Molecule 1: DUF4352 domain-containing protein

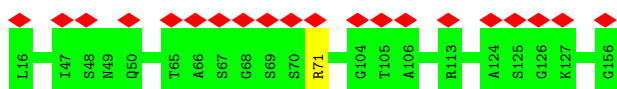




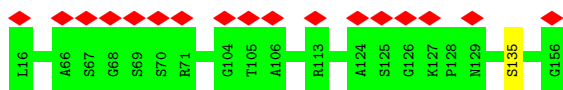
- Molecule 1: DUF4352 domain-containing protein



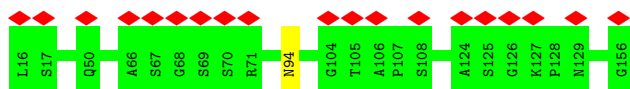
- Molecule 1: DUF4352 domain-containing protein



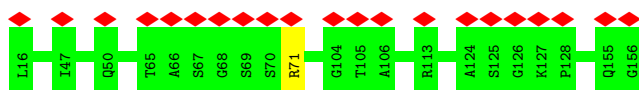
- Molecule 1: DUF4352 domain-containing protein



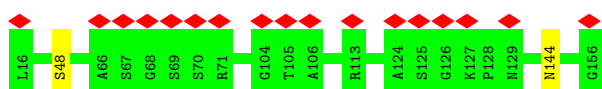
- Molecule 1: DUF4352 domain-containing protein



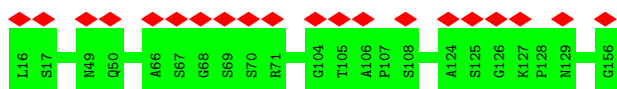
- Molecule 1: DUF4352 domain-containing protein



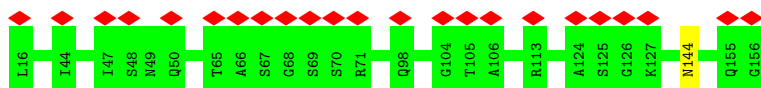
- Molecule 1: DUF4352 domain-containing protein



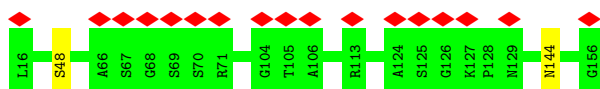
- Molecule 1: DUF4352 domain-containing protein



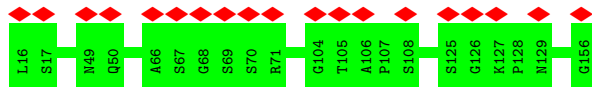
- Molecule 1: DUF4352 domain-containing protein



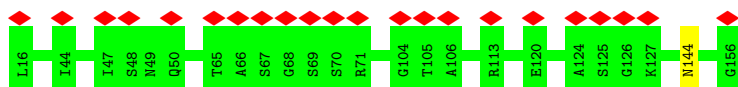
- Molecule 1: DUF4352 domain-containing protein



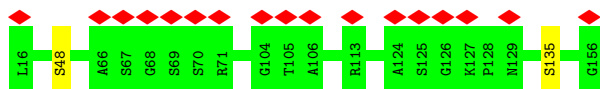
- Molecule 1: DUF4352 domain-containing protein



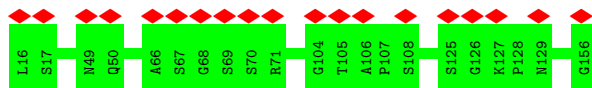
- Molecule 1: DUF4352 domain-containing protein



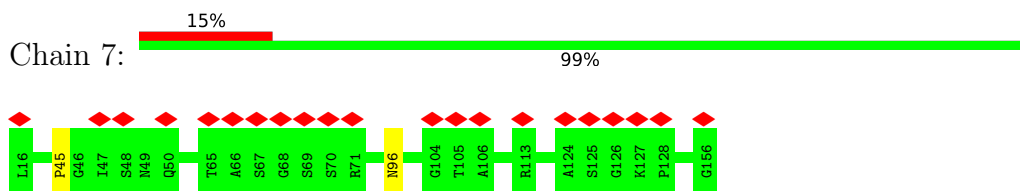
- Molecule 1: DUF4352 domain-containing protein



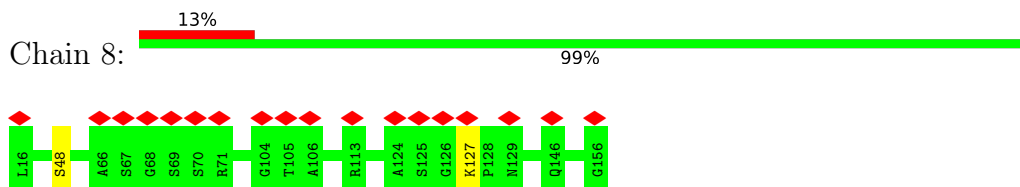
- Molecule 1: DUF4352 domain-containing protein



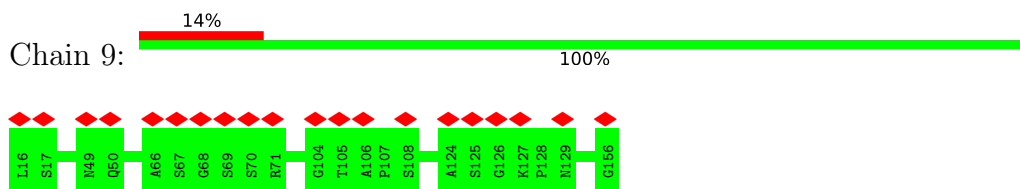
- Molecule 1: DUF4352 domain-containing protein



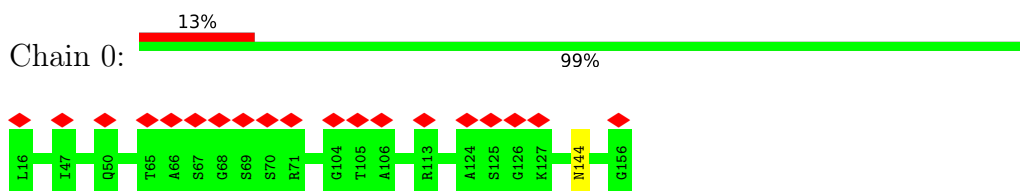
- Molecule 1: DUF4352 domain-containing protein



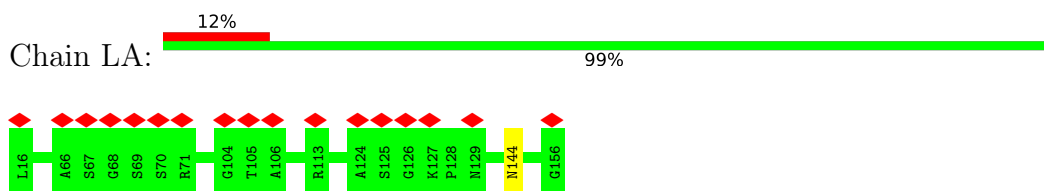
- Molecule 1: DUF4352 domain-containing protein



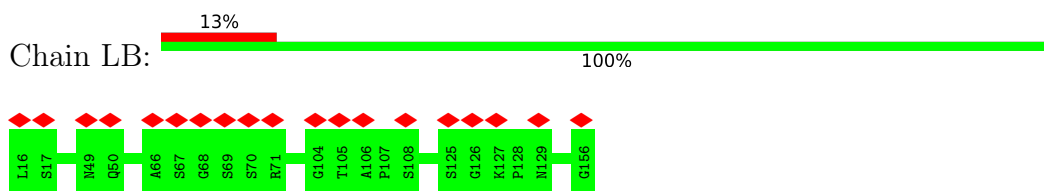
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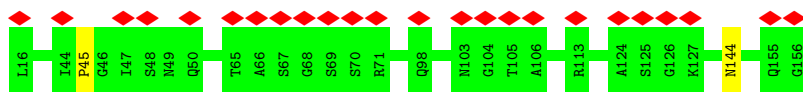


- Molecule 1: DUF4352 domain-containing protein

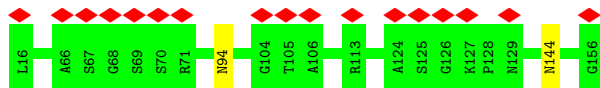


- Molecule 1: DUF4352 domain-containing protein

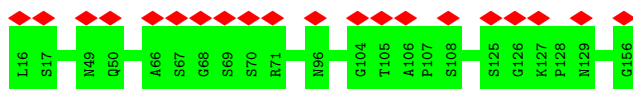




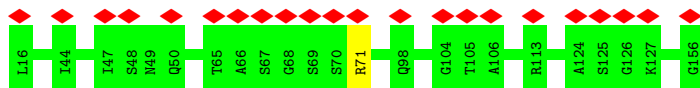
- Molecule 1: DUF4352 domain-containing protein



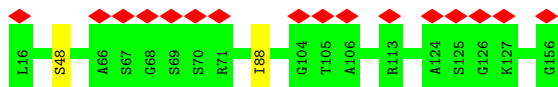
- Molecule 1: DUF4352 domain-containing protein



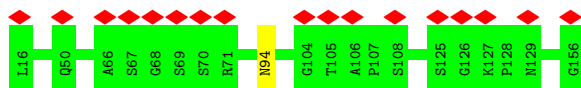
- Molecule 1: DUF4352 domain-containing protein



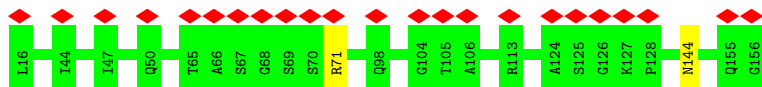
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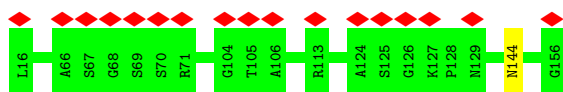


- Molecule 1: DUF4352 domain-containing protein



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Chain LJ: 



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

Chain AA: 



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

Chain BA: 



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

Chain DA: 



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

Chain FA: 



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

Chain GA: 



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



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



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

Chain YB:  100%  
100%



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

Chain ZB:  100%  
50% 50%



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

Chain bB:  100%  
50% 50%



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

Chain dB:  100%  
100%



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

Chain eB:  100%  
100%



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

Chain fB:  100%  
50% 50%





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



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



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

Chain EC:  100%  
100%



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

Chain FC:  100%  
50% 50%



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

Chain HC:  100%  
50% 50%



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

Chain JC:  100%  
100%



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

Chain KC:  100%  
100%



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

Chain MC:  100%  
50% 50%



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



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



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





- Molecule 3: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 3: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 3: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 3: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



## 4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-39.879°, rise=15.403 Å, axial sym=C1	Depositor
Number of segments used	947729	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 ( $e^-/\text{Å}^2$ )	42.33	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.875	Depositor
Minimum map value	-0.800	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.050	Depositor
Recommended contour level	0.59	Depositor
Map size (Å)	536.064, 536.064, 536.064	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.047, 1.047, 1.047	Depositor



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: YZT, 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	0	0.29	0/1019	0.51	0/1396
1	1	0.29	0/1019	0.50	0/1396
1	2	0.28	0/1019	0.49	0/1396
1	3	0.30	0/1019	0.50	0/1396
1	4	0.30	0/1019	0.52	0/1396
1	5	0.29	0/1019	0.48	0/1396
1	6	0.29	0/1019	0.50	0/1396
1	7	0.29	0/1019	0.54	1/1396 (0.1%)
1	8	0.30	0/1019	0.50	0/1396
1	9	0.31	0/1019	0.52	0/1396
1	A	0.28	0/1019	0.49	0/1396
1	B	0.29	0/1019	0.50	0/1396
1	C	0.32	0/1019	0.49	0/1396
1	D	0.32	0/1019	1.07	3/1396 (0.2%)
1	E	0.30	0/1019	0.52	0/1396
1	F	0.29	0/1019	0.50	0/1396
1	G	0.29	0/1019	0.51	0/1396
1	H	0.30	0/1019	0.52	0/1396
1	I	0.29	0/1019	0.49	0/1396
1	J	0.29	0/1019	0.51	0/1396
1	K	0.30	0/1019	0.51	0/1396
1	L	0.29	0/1019	0.48	0/1396
1	LA	0.32	0/1019	0.50	0/1396
1	LB	0.31	0/1019	0.53	0/1396
1	LC	0.29	0/1019	0.54	1/1396 (0.1%)
1	LD	0.31	0/1019	0.49	0/1396
1	LE	0.28	0/1019	0.49	0/1396
1	LF	0.30	0/1019	0.53	0/1396
1	LG	0.29	0/1019	0.51	1/1396 (0.1%)
1	LH	0.28	0/1019	0.51	0/1396
1	LI	0.30	0/1019	0.56	0/1396
1	LJ	0.30	0/1019	0.49	0/1396

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	M	0.30	0/1019	0.51	0/1396
1	N	0.30	0/1019	0.55	1/1396 (0.1%)
1	O	0.29	0/1019	0.49	0/1396
1	P	0.30	0/1019	0.50	0/1396
1	Q	0.29	0/1019	0.52	0/1396
1	R	0.29	0/1019	0.50	0/1396
1	S	0.29	0/1019	0.53	0/1396
1	T	0.30	0/1019	0.51	0/1396
1	U	0.28	0/1019	0.48	0/1396
1	V	0.38	1/1019 (0.1%)	0.54	0/1396
1	W	0.30	0/1019	0.52	0/1396
1	X	0.30	0/1019	0.49	0/1396
1	Y	0.29	0/1019	0.49	0/1396
1	Z	0.31	0/1019	0.56	0/1396
1	a	0.29	0/1019	0.48	0/1396
1	b	0.34	1/1019 (0.1%)	0.53	0/1396
1	c	0.30	0/1019	0.54	1/1396 (0.1%)
1	d	0.33	0/1019	0.49	0/1396
1	e	0.30	0/1019	0.50	0/1396
1	f	0.30	0/1019	0.52	0/1396
1	g	0.30	0/1019	0.50	0/1396
1	h	0.30	0/1019	0.51	0/1396
1	i	0.29	0/1019	0.51	0/1396
1	j	0.31	0/1019	0.48	0/1396
1	k	0.29	0/1019	0.51	0/1396
1	l	0.29	0/1019	0.51	0/1396
1	m	0.29	0/1019	0.50	0/1396
1	n	0.29	0/1019	0.51	0/1396
1	o	0.29	0/1019	0.51	0/1396
1	p	0.30	0/1019	0.49	0/1396
1	q	0.29	0/1019	0.50	0/1396
1	r	0.30	0/1019	0.51	0/1396
1	s	0.29	0/1019	0.49	0/1396
1	t	0.29	0/1019	0.49	0/1396
1	u	0.30	0/1019	0.52	0/1396
1	v	0.29	0/1019	0.49	0/1396
1	w	0.30	0/1019	0.51	0/1396
1	x	0.29	0/1019	0.51	0/1396
1	y	0.31	0/1019	0.50	0/1396
1	z	0.30	0/1019	0.52	0/1396
All	All	0.30	2/73368 (0.0%)	0.52	8/100512 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	N	0	1
1	Q	0	1
1	V	0	2
1	W	0	1
1	x	0	1
All	All	0	6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	V	103	ASN	CG-ND2	6.37	1.48	1.32
1	b	103	ASN	CG-ND2	5.04	1.45	1.32

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	103	ASN	CB-CG-OD1	29.16	179.93	121.60
1	D	103	ASN	CB-CG-ND2	-17.54	74.60	116.70
1	D	103	ASN	OD1-CG-ND2	-7.17	105.42	121.90
1	LC	45	PRO	CA-N-CD	-5.35	104.01	111.50
1	N	45	PRO	CA-N-CD	-5.30	104.08	111.50
1	c	45	PRO	CA-N-CD	-5.24	104.17	111.50
1	LG	88	ILE	CG1-CB-CG2	-5.17	100.02	111.40
1	7	45	PRO	CA-N-CD	-5.14	104.31	111.50

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	N	71	ARG	Sidechain
1	Q	71	ARG	Sidechain
1	V	102	ILE	Peptide
1	V	103	ASN	Sidechain
1	W	71	ARG	Sidechain
1	x	71	ARG	Sidechain

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

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

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	139/141 (99%)	137 (99%)	2 (1%)	0	100	100
1	1	139/141 (99%)	136 (98%)	3 (2%)	0	100	100
1	2	139/141 (99%)	139 (100%)	0	0	100	100
1	3	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
1	4	139/141 (99%)	136 (98%)	3 (2%)	0	100	100
1	5	139/141 (99%)	139 (100%)	0	0	100	100
1	6	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
1	7	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
1	8	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
1	9	139/141 (99%)	137 (99%)	2 (1%)	0	100	100
1	A	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
1	B	139/141 (99%)	137 (99%)	2 (1%)	0	100	100
1	C	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
1	D	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
1	E	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
1	F	139/141 (99%)	139 (100%)	0	0	100	100
1	G	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
1	H	139/141 (99%)	137 (99%)	2 (1%)	0	100	100
1	I	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
1	J	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
1	K	139/141 (99%)	138 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	139/141 (99%)	139 (100%)	0	0	100	100
1	LA	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
1	LB	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
1	LC	139/141 (99%)	136 (98%)	3 (2%)	0	100	100
1	LD	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
1	LE	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
1	LF	139/141 (99%)	136 (98%)	3 (2%)	0	100	100
1	LG	139/141 (99%)	139 (100%)	0	0	100	100
1	LH	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
1	LI	139/141 (99%)	136 (98%)	3 (2%)	0	100	100
1	LJ	139/141 (99%)	139 (100%)	0	0	100	100
1	M	139/141 (99%)	139 (100%)	0	0	100	100
1	N	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
1	O	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
1	P	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
1	Q	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
1	R	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
1	S	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
1	T	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
1	U	139/141 (99%)	139 (100%)	0	0	100	100
1	V	139/141 (99%)	136 (98%)	3 (2%)	0	100	100
1	W	139/141 (99%)	137 (99%)	2 (1%)	0	100	100
1	X	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
1	Y	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
1	Z	139/141 (99%)	137 (99%)	2 (1%)	0	100	100
1	a	139/141 (99%)	139 (100%)	0	0	100	100
1	b	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
1	c	139/141 (99%)	137 (99%)	2 (1%)	0	100	100
1	d	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
1	e	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
1	f	139/141 (99%)	138 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	g	139/141 (99%)	139 (100%)	0	0	100	100
1	h	139/141 (99%)	137 (99%)	2 (1%)	0	100	100
1	i	139/141 (99%)	137 (99%)	2 (1%)	0	100	100
1	j	139/141 (99%)	139 (100%)	0	0	100	100
1	k	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
1	l	139/141 (99%)	136 (98%)	3 (2%)	0	100	100
1	m	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
1	n	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
1	o	139/141 (99%)	136 (98%)	3 (2%)	0	100	100
1	p	139/141 (99%)	139 (100%)	0	0	100	100
1	q	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
1	r	139/141 (99%)	137 (99%)	2 (1%)	0	100	100
1	s	139/141 (99%)	139 (100%)	0	0	100	100
1	t	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
1	u	139/141 (99%)	137 (99%)	2 (1%)	0	100	100
1	v	139/141 (99%)	139 (100%)	0	0	100	100
1	w	139/141 (99%)	137 (99%)	2 (1%)	0	100	100
1	x	139/141 (99%)	137 (99%)	2 (1%)	0	100	100
1	y	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
1	z	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
All	All	10008/10152 (99%)	9921 (99%)	87 (1%)	0	100	100

There are no Ramachandran outliers to report.

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	110/110 (100%)	109 (99%)	1 (1%)	78	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	110/110 (100%)	109 (99%)	1 (1%)	78	90
1	2	110/110 (100%)	108 (98%)	2 (2%)	59	81
1	3	110/110 (100%)	110 (100%)	0	100	100
1	4	110/110 (100%)	109 (99%)	1 (1%)	78	90
1	5	110/110 (100%)	108 (98%)	2 (2%)	59	81
1	6	110/110 (100%)	110 (100%)	0	100	100
1	7	110/110 (100%)	109 (99%)	1 (1%)	78	90
1	8	110/110 (100%)	108 (98%)	2 (2%)	59	81
1	9	110/110 (100%)	110 (100%)	0	100	100
1	A	110/110 (100%)	109 (99%)	1 (1%)	78	90
1	B	110/110 (100%)	109 (99%)	1 (1%)	78	90
1	C	110/110 (100%)	108 (98%)	2 (2%)	59	81
1	D	110/110 (100%)	110 (100%)	0	100	100
1	E	110/110 (100%)	109 (99%)	1 (1%)	78	90
1	F	110/110 (100%)	108 (98%)	2 (2%)	59	81
1	G	110/110 (100%)	110 (100%)	0	100	100
1	H	110/110 (100%)	109 (99%)	1 (1%)	78	90
1	I	110/110 (100%)	108 (98%)	2 (2%)	59	81
1	J	110/110 (100%)	110 (100%)	0	100	100
1	K	110/110 (100%)	110 (100%)	0	100	100
1	L	110/110 (100%)	107 (97%)	3 (3%)	44	74
1	LA	110/110 (100%)	109 (99%)	1 (1%)	78	90
1	LB	110/110 (100%)	110 (100%)	0	100	100
1	LC	110/110 (100%)	109 (99%)	1 (1%)	78	90
1	LD	110/110 (100%)	108 (98%)	2 (2%)	59	81
1	LE	110/110 (100%)	110 (100%)	0	100	100
1	LF	110/110 (100%)	109 (99%)	1 (1%)	78	90
1	LG	110/110 (100%)	109 (99%)	1 (1%)	78	90
1	LH	110/110 (100%)	109 (99%)	1 (1%)	78	90
1	LI	110/110 (100%)	108 (98%)	2 (2%)	59	81
1	LJ	110/110 (100%)	109 (99%)	1 (1%)	78	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	M	110/110 (100%)	110 (100%)	0	100	100
1	N	110/110 (100%)	108 (98%)	2 (2%)	59	81
1	O	110/110 (100%)	108 (98%)	2 (2%)	59	81
1	P	110/110 (100%)	109 (99%)	1 (1%)	78	90
1	Q	110/110 (100%)	108 (98%)	2 (2%)	59	81
1	R	110/110 (100%)	106 (96%)	4 (4%)	35	68
1	S	110/110 (100%)	110 (100%)	0	100	100
1	T	110/110 (100%)	110 (100%)	0	100	100
1	U	110/110 (100%)	107 (97%)	3 (3%)	44	74
1	V	110/110 (100%)	110 (100%)	0	100	100
1	W	110/110 (100%)	108 (98%)	2 (2%)	59	81
1	X	110/110 (100%)	108 (98%)	2 (2%)	59	81
1	Y	110/110 (100%)	109 (99%)	1 (1%)	78	90
1	Z	110/110 (100%)	108 (98%)	2 (2%)	59	81
1	a	110/110 (100%)	108 (98%)	2 (2%)	59	81
1	b	110/110 (100%)	110 (100%)	0	100	100
1	c	110/110 (100%)	109 (99%)	1 (1%)	78	90
1	d	110/110 (100%)	106 (96%)	4 (4%)	35	68
1	e	110/110 (100%)	109 (99%)	1 (1%)	78	90
1	f	110/110 (100%)	108 (98%)	2 (2%)	59	81
1	g	110/110 (100%)	108 (98%)	2 (2%)	59	81
1	h	110/110 (100%)	110 (100%)	0	100	100
1	i	110/110 (100%)	109 (99%)	1 (1%)	78	90
1	j	110/110 (100%)	108 (98%)	2 (2%)	59	81
1	k	110/110 (100%)	110 (100%)	0	100	100
1	l	110/110 (100%)	110 (100%)	0	100	100
1	m	110/110 (100%)	107 (97%)	3 (3%)	44	74
1	n	110/110 (100%)	110 (100%)	0	100	100
1	o	110/110 (100%)	110 (100%)	0	100	100
1	p	110/110 (100%)	107 (97%)	3 (3%)	44	74
1	q	110/110 (100%)	109 (99%)	1 (1%)	78	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	r	110/110 (100%)	109 (99%)	1 (1%)	78	90
1	s	110/110 (100%)	107 (97%)	3 (3%)	44	74
1	t	110/110 (100%)	110 (100%)	0	100	100
1	u	110/110 (100%)	109 (99%)	1 (1%)	78	90
1	v	110/110 (100%)	109 (99%)	1 (1%)	78	90
1	w	110/110 (100%)	109 (99%)	1 (1%)	78	90
1	x	110/110 (100%)	110 (100%)	0	100	100
1	y	110/110 (100%)	108 (98%)	2 (2%)	59	81
1	z	110/110 (100%)	110 (100%)	0	100	100
All	All	7920/7920 (100%)	7835 (99%)	85 (1%)	74	88

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	127	LYS
1	B	144	ASN
1	C	48	SER
1	C	144	ASN
1	E	75	ASN
1	F	127	LYS
1	F	135	SER
1	H	144	ASN
1	I	135	SER
1	I	144	ASN
1	L	48	SER
1	L	127	LYS
1	L	144	ASN
1	N	71	ARG
1	N	144	ASN
1	O	71	ARG
1	O	135	SER
1	P	94	ASN
1	Q	58	SER
1	Q	71	ARG
1	R	48	SER
1	R	127	LYS
1	R	135	SER
1	R	144	ASN
1	U	16	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	U	127	LYS
1	U	144	ASN
1	W	96	ASN
1	W	144	ASN
1	X	48	SER
1	X	144	ASN
1	Y	94	ASN
1	Z	71	ARG
1	Z	144	ASN
1	a	48	SER
1	a	71	ARG
1	c	96	ASN
1	d	16	LEU
1	d	48	SER
1	d	135	SER
1	d	144	ASN
1	e	49	ASN
1	f	71	ARG
1	f	144	ASN
1	g	144	ASN
1	g	146	GLN
1	i	144	ASN
1	j	135	SER
1	j	144	ASN
1	m	48	SER
1	m	135	SER
1	m	144	ASN
1	p	48	SER
1	p	144	ASN
1	p	146	GLN
1	q	127	LYS
1	r	144	ASN
1	s	48	SER
1	s	127	LYS
1	s	144	ASN
1	u	71	ARG
1	v	135	SER
1	w	94	ASN
1	y	48	SER
1	y	144	ASN
1	1	144	ASN
1	2	48	SER

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Mol	Chain	Res	Type
1	2	144	ASN
1	4	144	ASN
1	5	48	SER
1	5	135	SER
1	7	96	ASN
1	8	48	SER
1	8	127	LYS
1	0	144	ASN
1	LA	144	ASN
1	LC	144	ASN
1	LD	94	ASN
1	LD	144	ASN
1	LF	71	ARG
1	LG	48	SER
1	LH	94	ASN
1	LI	71	ARG
1	LI	144	ASN
1	LJ	144	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (145) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	ASN
1	A	54	GLN
1	A	94	ASN
1	A	129	ASN
1	A	155	GLN
1	C	50	GLN
1	C	115	GLN
1	C	144	ASN
1	D	54	GLN
1	E	49	ASN
1	F	115	GLN
1	G	54	GLN
1	H	54	GLN
1	H	115	GLN
1	I	115	GLN
1	I	146	GLN
1	J	49	ASN
1	J	50	GLN
1	J	155	GLN
1	K	49	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	K	101	ASN
1	L	115	GLN
1	L	144	ASN
1	M	94	ASN
1	N	49	ASN
1	N	115	GLN
1	O	115	GLN
1	O	155	GLN
1	P	49	ASN
1	P	50	GLN
1	P	54	GLN
1	P	115	GLN
1	P	155	GLN
1	Q	49	ASN
1	R	115	GLN
1	R	155	GLN
1	S	54	GLN
1	S	129	ASN
1	T	49	ASN
1	T	54	GLN
1	T	115	GLN
1	U	50	GLN
1	U	115	GLN
1	U	144	ASN
1	U	146	GLN
1	V	94	ASN
1	V	129	ASN
1	W	49	ASN
1	X	144	ASN
1	X	146	GLN
1	Y	54	GLN
1	Z	49	ASN
1	Z	96	ASN
1	Z	98	GLN
1	Z	144	ASN
1	c	49	ASN
1	c	54	GLN
1	c	155	GLN
1	d	50	GLN
1	d	115	GLN
1	d	146	GLN
1	e	54	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	e	155	GLN
1	f	49	ASN
1	f	115	GLN
1	f	144	ASN
1	g	50	GLN
1	g	115	GLN
1	g	146	GLN
1	h	54	GLN
1	i	49	ASN
1	k	49	ASN
1	k	54	GLN
1	l	115	GLN
1	l	144	ASN
1	m	155	GLN
1	o	54	GLN
1	p	144	ASN
1	p	146	GLN
1	q	49	ASN
1	q	54	GLN
1	q	115	GLN
1	r	49	ASN
1	r	54	GLN
1	r	155	GLN
1	s	155	GLN
1	t	54	GLN
1	t	115	GLN
1	u	49	ASN
1	u	98	GLN
1	v	50	GLN
1	w	49	ASN
1	w	54	GLN
1	w	98	GLN
1	w	115	GLN
1	x	49	ASN
1	y	115	GLN
1	z	115	GLN
1	z	155	GLN
1	1	49	ASN
1	1	115	GLN
1	2	115	GLN
1	2	144	ASN
1	2	155	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	3	49	ASN
1	3	115	GLN
1	4	49	ASN
1	4	115	GLN
1	5	115	GLN
1	6	54	GLN
1	7	115	GLN
1	8	50	GLN
1	8	146	GLN
1	8	155	GLN
1	9	129	ASN
1	9	155	GLN
1	0	49	ASN
1	0	115	GLN
1	LA	115	GLN
1	LA	146	GLN
1	LB	54	GLN
1	LB	94	ASN
1	LB	96	ASN
1	LB	115	GLN
1	LB	155	GLN
1	LC	49	ASN
1	LC	54	GLN
1	LC	155	GLN
1	LD	115	GLN
1	LE	49	ASN
1	LE	54	GLN
1	LE	115	GLN
1	LE	155	GLN
1	LF	49	ASN
1	LF	54	GLN
1	LF	115	GLN
1	LG	50	GLN
1	LH	54	GLN
1	LH	115	GLN
1	LI	49	ASN
1	LI	96	ASN
1	LI	101	ASN
1	LI	115	GLN
1	LJ	144	ASN
1	LJ	146	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

336 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	0A	1	2,1	14,14,15	0.55	0	17,19,21	1.53	3 (17%)
2	NAG	0A	2	2	14,14,15	0.14	0	17,19,21	0.42	0
3	NAG	0B	1	3,1	14,14,15	0.26	0	17,19,21	0.67	0
3	NAG	0B	2	3	14,14,15	0.21	0	17,19,21	0.51	0
3	YZT	0B	3	3	13,14,15	1.05	1 (7%)	18,21,23	1.36	2 (11%)
3	NAG	1A	1	3,1	14,14,15	0.25	0	17,19,21	0.66	0
3	NAG	1A	2	3	14,14,15	0.21	0	17,19,21	0.51	0
3	YZT	1A	3	3	13,14,15	1.05	1 (7%)	18,21,23	1.36	2 (11%)
2	NAG	1B	1	2,1	14,14,15	0.52	0	17,19,21	0.59	0
2	NAG	1B	2	2	14,14,15	0.19	0	17,19,21	0.38	0
2	NAG	2A	1	2,1	14,14,15	0.50	0	17,19,21	0.57	0
2	NAG	2A	2	2	14,14,15	0.17	0	17,19,21	0.36	0
2	NAG	2B	1	2,1	14,14,15	0.53	0	17,19,21	0.62	0
2	NAG	2B	2	2	14,14,15	0.29	0	17,19,21	0.46	0
2	NAG	3A	1	2,1	14,14,15	0.54	0	17,19,21	0.62	0
2	NAG	3A	2	2	14,14,15	0.29	0	17,19,21	0.47	0
2	NAG	3B	1	2,1	14,14,15	0.81	1 (7%)	17,19,21	0.67	0
2	NAG	3B	2	2	14,14,15	0.19	0	17,19,21	0.62	0
2	NAG	4A	1	2,1	14,14,15	0.85	1 (7%)	17,19,21	0.68	0
2	NAG	4A	2	2	14,14,15	0.19	0	17,19,21	0.62	0
3	NAG	4B	1	3,1	14,14,15	0.48	0	17,19,21	0.92	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	4B	2	3	14,14,15	0.28	0	17,19,21	0.60	0
3	YZT	4B	3	3	13,14,15	1.05	1 (7%)	18,21,23	1.35	2 (11%)
3	NAG	5A	1	3,1	14,14,15	0.47	0	17,19,21	0.92	0
3	NAG	5A	2	3	14,14,15	0.27	0	17,19,21	0.60	0
3	YZT	5A	3	3	13,14,15	1.05	1 (7%)	18,21,23	1.36	2 (11%)
2	NAG	5B	1	2,1	14,14,15	0.50	0	17,19,21	1.49	2 (11%)
2	NAG	5B	2	2	14,14,15	0.14	0	17,19,21	0.41	0
2	NAG	6A	1	2,1	14,14,15	0.48	0	17,19,21	1.49	2 (11%)
2	NAG	6A	2	2	14,14,15	0.15	0	17,19,21	0.43	0
3	NAG	6B	1	3,1	14,14,15	0.23	0	17,19,21	0.66	0
3	NAG	6B	2	3	14,14,15	0.22	0	17,19,21	0.51	0
3	YZT	6B	3	3	13,14,15	1.06	1 (7%)	18,21,23	1.36	2 (11%)
3	NAG	7A	1	3,1	14,14,15	0.25	0	17,19,21	0.66	0
3	NAG	7A	2	3	14,14,15	0.21	0	17,19,21	0.52	0
3	YZT	7A	3	3	13,14,15	1.05	1 (7%)	18,21,23	1.35	2 (11%)
2	NAG	7B	1	2,1	14,14,15	0.44	0	17,19,21	0.53	0
2	NAG	7B	2	2	14,14,15	0.21	0	17,19,21	0.37	0
2	NAG	8A	1	2,1	14,14,15	0.51	0	17,19,21	0.63	0
2	NAG	8A	2	2	14,14,15	0.19	0	17,19,21	0.39	0
2	NAG	8B	1	2,1	14,14,15	0.55	0	17,19,21	0.62	0
2	NAG	8B	2	2	14,14,15	0.30	0	17,19,21	0.46	0
2	NAG	9A	1	2,1	14,14,15	0.56	0	17,19,21	0.63	0
2	NAG	9A	2	2	14,14,15	0.29	0	17,19,21	0.47	0
2	NAG	9B	1	2,1	14,14,15	0.82	1 (7%)	17,19,21	0.66	0
2	NAG	9B	2	2	14,14,15	0.19	0	17,19,21	0.63	0
2	NAG	AA	1	2,1	14,14,15	0.54	0	17,19,21	0.62	0
2	NAG	AA	2	2	14,14,15	0.29	0	17,19,21	0.46	0
2	NAG	AB	1	2,1	14,14,15	0.82	1 (7%)	17,19,21	0.69	0
2	NAG	AB	2	2	14,14,15	0.20	0	17,19,21	0.63	0
3	NAG	AC	1	3,1	14,14,15	0.49	0	17,19,21	0.93	0
3	NAG	AC	2	3	14,14,15	0.28	0	17,19,21	0.61	0
3	YZT	AC	3	3	13,14,15	1.05	1 (7%)	18,21,23	1.36	2 (11%)
2	NAG	BA	1	2,1	14,14,15	0.82	1 (7%)	17,19,21	0.68	0
2	NAG	BA	2	2	14,14,15	0.19	0	17,19,21	0.63	0
3	NAG	BB	1	3,1	14,14,15	0.48	0	17,19,21	0.92	0
3	NAG	BB	2	3	14,14,15	0.28	0	17,19,21	0.59	0
3	YZT	BB	3	3	13,14,15	1.06	1 (7%)	18,21,23	1.36	2 (11%)
2	NAG	BC	1	2,1	14,14,15	0.47	0	17,19,21	1.48	2 (11%)
2	NAG	BC	2	2	14,14,15	0.14	0	17,19,21	0.42	0
3	NAG	CA	1	3,1	14,14,15	0.46	0	17,19,21	0.91	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	CA	2	3	14,14,15	0.28	0	17,19,21	0.59	0
3	YZT	CA	3	3	13,14,15	1.05	1 (7%)	18,21,23	1.35	2 (11%)
2	NAG	CB	1	2,1	14,14,15	0.52	0	17,19,21	1.50	2 (11%)
2	NAG	CB	2	2	14,14,15	0.14	0	17,19,21	0.41	0
3	NAG	CC	1	3,1	14,14,15	0.25	0	17,19,21	0.65	0
3	NAG	CC	2	3	14,14,15	0.21	0	17,19,21	0.52	0
3	YZT	CC	3	3	13,14,15	1.05	1 (7%)	18,21,23	1.37	2 (11%)
2	NAG	DA	1	2,1	14,14,15	0.47	0	17,19,21	1.47	2 (11%)
2	NAG	DA	2	2	14,14,15	0.14	0	17,19,21	0.41	0
3	NAG	DB	1	3,1	14,14,15	0.24	0	17,19,21	0.66	0
3	NAG	DB	2	3	14,14,15	0.21	0	17,19,21	0.51	0
3	YZT	DB	3	3	13,14,15	1.05	1 (7%)	18,21,23	1.36	2 (11%)
2	NAG	DC	1	2,1	14,14,15	0.51	0	17,19,21	0.57	0
2	NAG	DC	2	2	14,14,15	0.17	0	17,19,21	0.36	0
3	NAG	EA	1	3,1	14,14,15	0.26	0	17,19,21	0.67	0
3	NAG	EA	2	3	14,14,15	0.20	0	17,19,21	0.50	0
3	YZT	EA	3	3	13,14,15	1.05	1 (7%)	18,21,23	1.35	2 (11%)
2	NAG	EB	1	2,1	14,14,15	0.43	0	17,19,21	0.53	0
2	NAG	EB	2	2	14,14,15	0.21	0	17,19,21	0.36	0
2	NAG	EC	1	2,1	14,14,15	0.54	0	17,19,21	0.62	0
2	NAG	EC	2	2	14,14,15	0.29	0	17,19,21	0.46	0
2	NAG	FA	1	2,1	14,14,15	0.51	0	17,19,21	0.57	0
2	NAG	FA	2	2	14,14,15	0.19	0	17,19,21	0.37	0
2	NAG	FB	1	2,1	14,14,15	0.54	0	17,19,21	0.62	0
2	NAG	FB	2	2	14,14,15	0.30	0	17,19,21	0.46	0
2	NAG	FC	1	2,1	14,14,15	0.78	1 (7%)	17,19,21	0.67	0
2	NAG	FC	2	2	14,14,15	0.20	0	17,19,21	0.62	0
2	NAG	GA	1	2,1	14,14,15	0.56	0	17,19,21	0.63	0
2	NAG	GA	2	2	14,14,15	0.29	0	17,19,21	0.46	0
2	NAG	GB	1	2,1	14,14,15	0.83	1 (7%)	17,19,21	0.69	0
2	NAG	GB	2	2	14,14,15	0.20	0	17,19,21	0.62	0
3	NAG	GC	1	3,1	14,14,15	0.49	0	17,19,21	0.92	0
3	NAG	GC	2	3	14,14,15	0.26	0	17,19,21	0.59	0
3	YZT	GC	3	3	13,14,15	1.06	1 (7%)	18,21,23	1.36	2 (11%)
2	NAG	HA	1	2,1	14,14,15	0.85	1 (7%)	17,19,21	0.71	0
2	NAG	HA	2	2	14,14,15	0.19	0	17,19,21	0.62	0
3	NAG	HB	1	3,1	14,14,15	0.47	0	17,19,21	0.92	0
3	NAG	HB	2	3	14,14,15	0.27	0	17,19,21	0.60	0
3	YZT	HB	3	3	13,14,15	1.05	1 (7%)	18,21,23	1.34	2 (11%)
2	NAG	HC	1	2,1	14,14,15	0.48	0	17,19,21	1.52	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	HC	2	2	14,14,15	0.17	0	17,19,21	0.45	0
3	NAG	IA	1	3,1	14,14,15	0.47	0	17,19,21	0.91	0
3	NAG	IA	2	3	14,14,15	0.27	0	17,19,21	0.60	0
3	YZT	IA	3	3	13,14,15	1.05	1 (7%)	18,21,23	1.36	2 (11%)
2	NAG	IB	1	2,1	14,14,15	0.41	0	17,19,21	1.48	2 (11%)
2	NAG	IB	2	2	14,14,15	0.14	0	17,19,21	0.41	0
3	NAG	IC	1	3,1	14,14,15	0.25	0	17,19,21	0.65	0
3	NAG	IC	2	3	14,14,15	0.21	0	17,19,21	0.50	0
3	YZT	IC	3	3	13,14,15	1.05	1 (7%)	18,21,23	1.36	2 (11%)
2	NAG	JA	1	2,1	14,14,15	0.53	0	17,19,21	1.33	2 (11%)
2	NAG	JA	2	2	14,14,15	0.33	0	17,19,21	0.44	0
3	NAG	JB	1	3,1	14,14,15	0.26	0	17,19,21	0.65	0
3	NAG	JB	2	3	14,14,15	0.20	0	17,19,21	0.52	0
3	YZT	JB	3	3	13,14,15	1.06	1 (7%)	18,21,23	1.37	2 (11%)
2	NAG	JC	1	2,1	14,14,15	0.44	0	17,19,21	0.54	0
2	NAG	JC	2	2	14,14,15	0.17	0	17,19,21	0.37	0
3	NAG	KA	1	3,1	14,14,15	0.24	0	17,19,21	0.65	0
3	NAG	KA	2	3	14,14,15	0.21	0	17,19,21	0.51	0
3	YZT	KA	3	3	13,14,15	1.05	1 (7%)	18,21,23	1.36	2 (11%)
2	NAG	KB	1	2,1	14,14,15	0.51	0	17,19,21	0.58	0
2	NAG	KB	2	2	14,14,15	0.17	0	17,19,21	0.37	0
2	NAG	KC	1	2,1	14,14,15	0.55	0	17,19,21	0.62	0
2	NAG	KC	2	2	14,14,15	0.29	0	17,19,21	0.47	0
2	NAG	MA	1	2,1	14,14,15	0.42	0	17,19,21	0.51	0
2	NAG	MA	2	2	14,14,15	0.20	0	17,19,21	0.37	0
2	NAG	MB	1	2,1	14,14,15	0.57	0	17,19,21	0.63	0
2	NAG	MB	2	2	14,14,15	0.29	0	17,19,21	0.46	0
2	NAG	MC	1	2,1	14,14,15	0.78	1 (7%)	17,19,21	0.65	0
2	NAG	MC	2	2	14,14,15	0.19	0	17,19,21	0.62	0
2	NAG	NA	1	2,1	14,14,15	0.54	0	17,19,21	0.62	0
2	NAG	NA	2	2	14,14,15	0.30	0	17,19,21	0.47	0
2	NAG	NB	1	2,1	14,14,15	0.84	1 (7%)	17,19,21	0.70	0
2	NAG	NB	2	2	14,14,15	0.20	0	17,19,21	0.62	0
3	NAG	NC	1	3,1	14,14,15	0.46	0	17,19,21	0.91	0
3	NAG	NC	2	3	14,14,15	0.27	0	17,19,21	0.60	0
3	YZT	NC	3	3	13,14,15	1.05	1 (7%)	18,21,23	1.35	2 (11%)
2	NAG	OA	1	2,1	14,14,15	0.83	1 (7%)	17,19,21	0.69	0
2	NAG	OA	2	2	14,14,15	0.19	0	17,19,21	0.62	0
3	NAG	OB	1	3,1	14,14,15	0.49	0	17,19,21	0.91	0
3	NAG	OB	2	3	14,14,15	0.28	0	17,19,21	0.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	YZT	OB	3	3	13,14,15	1.06	1 (7%)	18,21,23	1.35	2 (11%)
2	NAG	OC	1	2,1	14,14,15	0.54	0	17,19,21	1.51	3 (17%)
2	NAG	OC	2	2	14,14,15	0.14	0	17,19,21	0.43	0
3	NAG	PA	1	3,1	14,14,15	0.47	0	17,19,21	0.92	0
3	NAG	PA	2	3	14,14,15	0.27	0	17,19,21	0.61	0
3	YZT	PA	3	3	13,14,15	1.05	1 (7%)	18,21,23	1.34	2 (11%)
2	NAG	PB	1	2,1	14,14,15	0.36	0	17,19,21	1.53	4 (23%)
2	NAG	PB	2	2	14,14,15	0.16	0	17,19,21	0.46	0
3	NAG	PC	1	3,1	14,14,15	0.24	0	17,19,21	0.66	0
3	NAG	PC	2	3	14,14,15	0.22	0	17,19,21	0.51	0
3	YZT	PC	3	3	13,14,15	1.05	1 (7%)	18,21,23	1.36	2 (11%)
2	NAG	QA	1	2,1	14,14,15	0.33	0	17,19,21	1.48	2 (11%)
2	NAG	QA	2	2	14,14,15	0.17	0	17,19,21	0.44	0
3	NAG	QB	1	3,1	14,14,15	0.24	0	17,19,21	0.67	0
3	NAG	QB	2	3	14,14,15	0.20	0	17,19,21	0.51	0
3	YZT	QB	3	3	13,14,15	1.05	1 (7%)	18,21,23	1.35	2 (11%)
2	NAG	QC	1	2,1	14,14,15	0.48	0	17,19,21	0.58	0
2	NAG	QC	2	2	14,14,15	0.16	0	17,19,21	0.36	0
3	NAG	RA	1	3,1	14,14,15	0.24	0	17,19,21	0.67	0
3	NAG	RA	2	3	14,14,15	0.21	0	17,19,21	0.50	0
3	YZT	RA	3	3	13,14,15	1.05	1 (7%)	18,21,23	1.37	2 (11%)
2	NAG	RB	1	2,1	14,14,15	0.43	0	17,19,21	0.51	0
2	NAG	RB	2	2	14,14,15	0.19	0	17,19,21	0.38	0
2	NAG	RC	1	2,1	14,14,15	0.53	0	17,19,21	0.62	0
2	NAG	RC	2	2	14,14,15	0.29	0	17,19,21	0.47	0
2	NAG	SA	1	2,1	14,14,15	0.49	0	17,19,21	0.56	0
2	NAG	SA	2	2	14,14,15	0.17	0	17,19,21	0.38	0
2	NAG	SB	1	2,1	14,14,15	0.53	0	17,19,21	0.63	0
2	NAG	SB	2	2	14,14,15	0.30	0	17,19,21	0.47	0
2	NAG	SC	1	2,1	14,14,15	0.80	1 (7%)	17,19,21	0.66	0
2	NAG	SC	2	2	14,14,15	0.20	0	17,19,21	0.61	0
2	NAG	TA	1	2,1	14,14,15	0.55	0	17,19,21	0.61	0
2	NAG	TA	2	2	14,14,15	0.28	0	17,19,21	0.46	0
2	NAG	TB	1	2,1	14,14,15	0.84	1 (7%)	17,19,21	0.68	0
2	NAG	TB	2	2	14,14,15	0.20	0	17,19,21	0.63	0
3	NAG	TC	1	3,1	14,14,15	0.49	0	17,19,21	0.93	0
3	NAG	TC	2	3	14,14,15	0.27	0	17,19,21	0.60	0
3	YZT	TC	3	3	13,14,15	1.06	1 (7%)	18,21,23	1.36	2 (11%)
2	NAG	UA	1	2,1	14,14,15	0.83	1 (7%)	17,19,21	0.69	0
2	NAG	UA	2	2	14,14,15	0.19	0	17,19,21	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	UB	1	3,1	14,14,15	0.47	0	17,19,21	0.92	0
3	NAG	UB	2	3	14,14,15	0.28	0	17,19,21	0.61	0
3	YZT	UB	3	3	13,14,15	1.05	1 (7%)	18,21,23	1.36	2 (11%)
2	NAG	UC	1	2,1	14,14,15	0.36	0	17,19,21	1.54	3 (17%)
2	NAG	UC	2	2	14,14,15	0.15	0	17,19,21	0.44	0
3	NAG	VA	1	3,1	14,14,15	0.46	0	17,19,21	0.91	0
3	NAG	VA	2	3	14,14,15	0.26	0	17,19,21	0.60	0
3	YZT	VA	3	3	13,14,15	1.05	1 (7%)	18,21,23	1.35	2 (11%)
2	NAG	VB	1	2,1	14,14,15	0.54	0	17,19,21	1.54	3 (17%)
2	NAG	VB	2	2	14,14,15	0.15	0	17,19,21	0.43	0
3	NAG	VC	1	3,1	14,14,15	0.25	0	17,19,21	0.66	0
3	NAG	VC	2	3	14,14,15	0.21	0	17,19,21	0.51	0
3	YZT	VC	3	3	13,14,15	1.05	1 (7%)	18,21,23	1.37	2 (11%)
2	NAG	WA	1	2,1	14,14,15	0.35	0	17,19,21	1.39	2 (11%)
2	NAG	WA	2	2	14,14,15	0.28	0	17,19,21	0.42	0
3	NAG	WB	1	3,1	14,14,15	0.26	0	17,19,21	0.66	0
3	NAG	WB	2	3	14,14,15	0.21	0	17,19,21	0.51	0
3	YZT	WB	3	3	13,14,15	1.05	1 (7%)	18,21,23	1.36	2 (11%)
2	NAG	WC	1	2,1	14,14,15	0.49	0	17,19,21	0.59	0
2	NAG	WC	2	2	14,14,15	0.20	0	17,19,21	0.38	0
3	NAG	XA	1	3,1	14,14,15	0.24	0	17,19,21	0.65	0
3	NAG	XA	2	3	14,14,15	0.21	0	17,19,21	0.50	0
3	YZT	XA	3	3	13,14,15	1.05	1 (7%)	18,21,23	1.36	2 (11%)
2	NAG	XB	1	2,1	14,14,15	0.47	0	17,19,21	0.55	0
2	NAG	XB	2	2	14,14,15	0.19	0	17,19,21	0.36	0
2	NAG	YA	1	2,1	14,14,15	0.41	0	17,19,21	0.51	0
2	NAG	YA	2	2	14,14,15	0.18	0	17,19,21	0.36	0
2	NAG	YB	1	2,1	14,14,15	0.52	0	17,19,21	0.61	0
2	NAG	YB	2	2	14,14,15	0.28	0	17,19,21	0.46	0
2	NAG	ZA	1	2,1	14,14,15	0.55	0	17,19,21	0.62	0
2	NAG	ZA	2	2	14,14,15	0.30	0	17,19,21	0.46	0
2	NAG	ZB	1	2,1	14,14,15	0.79	1 (7%)	17,19,21	0.66	0
2	NAG	ZB	2	2	14,14,15	0.20	0	17,19,21	0.62	0
2	NAG	aA	1	2,1	14,14,15	0.82	1 (7%)	17,19,21	0.67	0
2	NAG	aA	2	2	14,14,15	0.19	0	17,19,21	0.63	0
3	NAG	aB	1	3,1	14,14,15	0.47	0	17,19,21	0.92	0
3	NAG	aB	2	3	14,14,15	0.27	0	17,19,21	0.61	0
3	YZT	aB	3	3	13,14,15	1.05	1 (7%)	18,21,23	1.36	2 (11%)
3	NAG	bA	1	3,1	14,14,15	0.47	0	17,19,21	0.90	0
3	NAG	bA	2	3	14,14,15	0.28	0	17,19,21	0.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	YZT	bA	3	3	13,14,15	1.05	1 (7%)	18,21,23	1.35	2 (11%)
2	NAG	bB	1	2,1	14,14,15	0.80	1 (7%)	17,19,21	1.50	2 (11%)
2	NAG	bB	2	2	14,14,15	0.20	0	17,19,21	0.43	0
2	NAG	cA	1	2,1	14,14,15	0.56	0	17,19,21	1.52	3 (17%)
2	NAG	cA	2	2	14,14,15	0.15	0	17,19,21	0.42	0
3	NAG	cB	1	3,1	14,14,15	0.24	0	17,19,21	0.66	0
3	NAG	cB	2	3	14,14,15	0.21	0	17,19,21	0.51	0
3	YZT	cB	3	3	13,14,15	1.06	1 (7%)	18,21,23	1.37	2 (11%)
3	NAG	dA	1	3,1	14,14,15	0.25	0	17,19,21	0.66	0
3	NAG	dA	2	3	14,14,15	0.21	0	17,19,21	0.51	0
3	YZT	dA	3	3	13,14,15	1.04	1 (7%)	18,21,23	1.36	2 (11%)
2	NAG	dB	1	2,1	14,14,15	0.49	0	17,19,21	0.57	0
2	NAG	dB	2	2	14,14,15	0.19	0	17,19,21	0.39	0
2	NAG	eA	1	2,1	14,14,15	0.48	0	17,19,21	0.55	0
2	NAG	eA	2	2	14,14,15	0.18	0	17,19,21	0.37	0
2	NAG	eB	1	2,1	14,14,15	0.55	0	17,19,21	0.62	0
2	NAG	eB	2	2	14,14,15	0.30	0	17,19,21	0.47	0
2	NAG	fA	1	2,1	14,14,15	0.54	0	17,19,21	0.63	0
2	NAG	fA	2	2	14,14,15	0.28	0	17,19,21	0.46	0
2	NAG	fB	1	2,1	14,14,15	0.82	1 (7%)	17,19,21	0.68	0
2	NAG	fB	2	2	14,14,15	0.20	0	17,19,21	0.62	0
2	NAG	gA	1	2,1	14,14,15	0.84	1 (7%)	17,19,21	0.67	0
2	NAG	gA	2	2	14,14,15	0.19	0	17,19,21	0.62	0
3	NAG	gB	1	3,1	14,14,15	0.46	0	17,19,21	0.91	0
3	NAG	gB	2	3	14,14,15	0.28	0	17,19,21	0.60	0
3	YZT	gB	3	3	13,14,15	1.06	1 (7%)	18,21,23	1.35	2 (11%)
3	NAG	hA	1	3,1	14,14,15	0.47	0	17,19,21	0.92	0
3	NAG	hA	2	3	14,14,15	0.27	0	17,19,21	0.60	0
3	YZT	hA	3	3	13,14,15	1.05	1 (7%)	18,21,23	1.35	2 (11%)
2	NAG	hB	1	2,1	14,14,15	0.56	0	17,19,21	1.52	3 (17%)
2	NAG	hB	2	2	14,14,15	0.15	0	17,19,21	0.42	0
2	NAG	iA	1	2,1	14,14,15	0.54	0	17,19,21	1.49	2 (11%)
2	NAG	iA	2	2	14,14,15	0.15	0	17,19,21	0.44	0
3	NAG	iB	1	3,1	14,14,15	0.26	0	17,19,21	0.66	0
3	NAG	iB	2	3	14,14,15	0.21	0	17,19,21	0.52	0
3	YZT	iB	3	3	13,14,15	1.05	1 (7%)	18,21,23	1.36	2 (11%)
3	NAG	jA	1	3,1	14,14,15	0.25	0	17,19,21	0.65	0
3	NAG	jA	2	3	14,14,15	0.22	0	17,19,21	0.51	0
3	YZT	jA	3	3	13,14,15	1.05	1 (7%)	18,21,23	1.35	2 (11%)
2	NAG	jB	1	2,1	14,14,15	0.52	0	17,19,21	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	jB	2	2	14,14,15	0.18	0	17,19,21	0.37	0
2	NAG	kA	1	2,1	14,14,15	0.49	0	17,19,21	0.57	0
2	NAG	kA	2	2	14,14,15	0.20	0	17,19,21	0.38	0
2	NAG	kB	1	2,1	14,14,15	0.56	0	17,19,21	0.62	0
2	NAG	kB	2	2	14,14,15	0.27	0	17,19,21	0.46	0
2	NAG	lA	1	2,1	14,14,15	0.56	0	17,19,21	0.62	0
2	NAG	lA	2	2	14,14,15	0.28	0	17,19,21	0.47	0
2	NAG	lB	1	2,1	14,14,15	0.80	1 (7%)	17,19,21	0.65	0
2	NAG	lB	2	2	14,14,15	0.18	0	17,19,21	0.62	0
2	NAG	mA	1	2,1	14,14,15	0.81	1 (7%)	17,19,21	0.68	0
2	NAG	mA	2	2	14,14,15	0.18	0	17,19,21	0.62	0
3	NAG	mB	1	3,1	14,14,15	0.47	0	17,19,21	0.91	0
3	NAG	mB	2	3	14,14,15	0.27	0	17,19,21	0.60	0
3	YZT	mB	3	3	13,14,15	1.06	1 (7%)	18,21,23	1.36	2 (11%)
3	NAG	nA	1	3,1	14,14,15	0.47	0	17,19,21	0.91	0
3	NAG	nA	2	3	14,14,15	0.27	0	17,19,21	0.61	0
3	YZT	nA	3	3	13,14,15	1.06	1 (7%)	18,21,23	1.36	2 (11%)
2	NAG	nB	1	2,1	14,14,15	0.41	0	17,19,21	1.53	2 (11%)
2	NAG	nB	2	2	14,14,15	0.19	0	17,19,21	0.51	0
2	NAG	oA	1	2,1	14,14,15	0.53	0	17,19,21	1.56	3 (17%)
2	NAG	oA	2	2	14,14,15	0.21	0	17,19,21	0.44	0
3	NAG	oB	1	3,1	14,14,15	0.25	0	17,19,21	0.66	0
3	NAG	oB	2	3	14,14,15	0.21	0	17,19,21	0.50	0
3	YZT	oB	3	3	13,14,15	1.05	1 (7%)	18,21,23	1.35	2 (11%)
3	NAG	pA	1	3,1	14,14,15	0.25	0	17,19,21	0.65	0
3	NAG	pA	2	3	14,14,15	0.21	0	17,19,21	0.51	0
3	YZT	pA	3	3	13,14,15	1.05	1 (7%)	18,21,23	1.36	2 (11%)
2	NAG	pB	1	2,1	14,14,15	0.51	0	17,19,21	0.58	0
2	NAG	pB	2	2	14,14,15	0.17	0	17,19,21	0.38	0
2	NAG	qA	1	2,1	14,14,15	0.49	0	17,19,21	0.58	0
2	NAG	qA	2	2	14,14,15	0.16	0	17,19,21	0.36	0
2	NAG	qB	1	2,1	14,14,15	0.57	1 (7%)	17,19,21	0.62	0
2	NAG	qB	2	2	14,14,15	0.29	0	17,19,21	0.46	0
2	NAG	rA	1	2,1	14,14,15	0.54	0	17,19,21	0.62	0
2	NAG	rA	2	2	14,14,15	0.28	0	17,19,21	0.47	0
2	NAG	rB	1	2,1	14,14,15	0.76	1 (7%)	17,19,21	0.63	0
2	NAG	rB	2	2	14,14,15	0.20	0	17,19,21	0.63	0
2	NAG	sA	1	2,1	14,14,15	0.78	1 (7%)	17,19,21	0.65	0
2	NAG	sA	2	2	14,14,15	0.21	0	17,19,21	0.62	0
3	NAG	sB	1	3,1	14,14,15	0.49	0	17,19,21	0.92	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	sB	2	3	14,14,15	0.28	0	17,19,21	0.61	0
3	YZT	sB	3	3	13,14,15	1.05	1 (7%)	18,21,23	1.35	2 (11%)
3	NAG	tA	1	3,1	14,14,15	0.47	0	17,19,21	0.91	0
3	NAG	tA	2	3	14,14,15	0.28	0	17,19,21	0.60	0
3	YZT	tA	3	3	13,14,15	1.05	1 (7%)	18,21,23	1.35	2 (11%)
2	NAG	tB	1	2,1	14,14,15	0.53	0	17,19,21	1.50	3 (17%)
2	NAG	tB	2	2	14,14,15	0.15	0	17,19,21	0.43	0
2	NAG	uA	1	2,1	14,14,15	0.71	1 (7%)	17,19,21	1.46	2 (11%)
2	NAG	uA	2	2	14,14,15	0.22	0	17,19,21	0.42	0
3	NAG	uB	1	3,1	14,14,15	0.25	0	17,19,21	0.66	0
3	NAG	uB	2	3	14,14,15	0.21	0	17,19,21	0.50	0
3	YZT	uB	3	3	13,14,15	1.05	1 (7%)	18,21,23	1.36	2 (11%)
3	NAG	vA	1	3,1	14,14,15	0.26	0	17,19,21	0.65	0
3	NAG	vA	2	3	14,14,15	0.21	0	17,19,21	0.51	0
3	YZT	vA	3	3	13,14,15	1.05	1 (7%)	18,21,23	1.36	2 (11%)
2	NAG	vB	1	2,1	14,14,15	0.50	0	17,19,21	0.57	0
2	NAG	vB	2	2	14,14,15	0.17	0	17,19,21	0.36	0
2	NAG	wA	1	2,1	14,14,15	0.49	0	17,19,21	0.57	0
2	NAG	wA	2	2	14,14,15	0.17	0	17,19,21	0.38	0
2	NAG	wB	1	2,1	14,14,15	0.54	0	17,19,21	0.62	0
2	NAG	wB	2	2	14,14,15	0.29	0	17,19,21	0.47	0
2	NAG	xA	1	2,1	14,14,15	0.59	1 (7%)	17,19,21	0.65	0
2	NAG	xA	2	2	14,14,15	0.30	0	17,19,21	0.47	0
2	NAG	xB	1	2,1	14,14,15	0.79	1 (7%)	17,19,21	0.65	0
2	NAG	xB	2	2	14,14,15	0.19	0	17,19,21	0.62	0
2	NAG	yA	1	2,1	14,14,15	0.82	1 (7%)	17,19,21	0.66	0
2	NAG	yA	2	2	14,14,15	0.19	0	17,19,21	0.62	0
3	NAG	yB	1	3,1	14,14,15	0.48	0	17,19,21	0.92	0
3	NAG	yB	2	3	14,14,15	0.27	0	17,19,21	0.60	0
3	YZT	yB	3	3	13,14,15	1.06	1 (7%)	18,21,23	1.36	2 (11%)
3	NAG	zA	1	3,1	14,14,15	0.47	0	17,19,21	0.91	0
3	NAG	zA	2	3	14,14,15	0.28	0	17,19,21	0.60	0
3	YZT	zA	3	3	13,14,15	1.06	1 (7%)	18,21,23	1.35	2 (11%)
2	NAG	zB	1	2,1	14,14,15	0.74	1 (7%)	17,19,21	1.43	2 (11%)
2	NAG	zB	2	2	14,14,15	0.21	0	17,19,21	0.43	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	0A	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	0A	2	2	-	1/6/23/26	0/1/1/1
3	NAG	0B	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	0B	2	3	-	1/6/23/26	0/1/1/1
3	YZT	0B	3	3	-	0/5/22/25	0/1/1/1
3	NAG	1A	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	1A	2	3	-	1/6/23/26	0/1/1/1
3	YZT	1A	3	3	-	0/5/22/25	0/1/1/1
2	NAG	1B	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	1B	2	2	-	0/6/23/26	0/1/1/1
2	NAG	2A	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	2A	2	2	-	0/6/23/26	0/1/1/1
2	NAG	2B	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	2B	2	2	-	0/6/23/26	0/1/1/1
2	NAG	3A	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	3A	2	2	-	0/6/23/26	0/1/1/1
2	NAG	3B	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	3B	2	2	-	2/6/23/26	0/1/1/1
2	NAG	4A	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	4A	2	2	-	2/6/23/26	0/1/1/1
3	NAG	4B	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	4B	2	3	-	2/6/23/26	0/1/1/1
3	YZT	4B	3	3	-	0/5/22/25	0/1/1/1
3	NAG	5A	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	5A	2	3	-	2/6/23/26	0/1/1/1
3	YZT	5A	3	3	-	0/5/22/25	0/1/1/1
2	NAG	5B	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	5B	2	2	-	1/6/23/26	0/1/1/1
2	NAG	6A	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	6A	2	2	-	1/6/23/26	0/1/1/1
3	NAG	6B	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	6B	2	3	-	1/6/23/26	0/1/1/1
3	YZT	6B	3	3	-	0/5/22/25	0/1/1/1
3	NAG	7A	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	7A	2	3	-	1/6/23/26	0/1/1/1
3	YZT	7A	3	3	-	0/5/22/25	0/1/1/1
2	NAG	7B	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	7B	2	2	-	0/6/23/26	0/1/1/1
2	NAG	8A	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	8A	2	2	-	0/6/23/26	0/1/1/1
2	NAG	8B	1	2,1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	8B	2	2	-	0/6/23/26	0/1/1/1
2	NAG	9A	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	9A	2	2	-	0/6/23/26	0/1/1/1
2	NAG	9B	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	9B	2	2	-	2/6/23/26	0/1/1/1
2	NAG	AA	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	AA	2	2	-	0/6/23/26	0/1/1/1
2	NAG	AB	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	AB	2	2	-	2/6/23/26	0/1/1/1
3	NAG	AC	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	AC	2	3	-	2/6/23/26	0/1/1/1
3	YZT	AC	3	3	-	0/5/22/25	0/1/1/1
2	NAG	BA	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	BA	2	2	-	2/6/23/26	0/1/1/1
3	NAG	BB	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	BB	2	3	-	2/6/23/26	0/1/1/1
3	YZT	BB	3	3	-	0/5/22/25	0/1/1/1
2	NAG	BC	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	BC	2	2	-	1/6/23/26	0/1/1/1
3	NAG	CA	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	CA	2	3	-	2/6/23/26	0/1/1/1
3	YZT	CA	3	3	-	0/5/22/25	0/1/1/1
2	NAG	CB	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	CB	2	2	-	1/6/23/26	0/1/1/1
3	NAG	CC	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	CC	2	3	-	1/6/23/26	0/1/1/1
3	YZT	CC	3	3	-	0/5/22/25	0/1/1/1
2	NAG	DA	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	DA	2	2	-	0/6/23/26	0/1/1/1
3	NAG	DB	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	DB	2	3	-	1/6/23/26	0/1/1/1
3	YZT	DB	3	3	-	0/5/22/25	0/1/1/1
2	NAG	DC	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	DC	2	2	-	0/6/23/26	0/1/1/1
3	NAG	EA	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	EA	2	3	-	1/6/23/26	0/1/1/1
3	YZT	EA	3	3	-	0/5/22/25	0/1/1/1
2	NAG	EB	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	EB	2	2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	EC	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	EC	2	2	-	0/6/23/26	0/1/1/1
2	NAG	FA	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	FA	2	2	-	0/6/23/26	0/1/1/1
2	NAG	FB	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	FB	2	2	-	0/6/23/26	0/1/1/1
2	NAG	FC	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	FC	2	2	-	2/6/23/26	0/1/1/1
2	NAG	GA	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	GA	2	2	-	0/6/23/26	0/1/1/1
2	NAG	GB	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	GB	2	2	-	2/6/23/26	0/1/1/1
3	NAG	GC	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	GC	2	3	-	2/6/23/26	0/1/1/1
3	YZT	GC	3	3	-	0/5/22/25	0/1/1/1
2	NAG	HA	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	HA	2	2	-	2/6/23/26	0/1/1/1
3	NAG	HB	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	HB	2	3	-	2/6/23/26	0/1/1/1
3	YZT	HB	3	3	-	0/5/22/25	0/1/1/1
2	NAG	HC	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	HC	2	2	-	1/6/23/26	0/1/1/1
3	NAG	IA	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	IA	2	3	-	2/6/23/26	0/1/1/1
3	YZT	IA	3	3	-	0/5/22/25	0/1/1/1
2	NAG	IB	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	IB	2	2	-	1/6/23/26	0/1/1/1
3	NAG	IC	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	IC	2	3	-	1/6/23/26	0/1/1/1
3	YZT	IC	3	3	-	0/5/22/25	0/1/1/1
2	NAG	JA	1	2,1	-	5/6/23/26	0/1/1/1
2	NAG	JA	2	2	-	1/6/23/26	0/1/1/1
3	NAG	JB	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	JB	2	3	-	1/6/23/26	0/1/1/1
3	YZT	JB	3	3	-	0/5/22/25	0/1/1/1
2	NAG	JC	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	JC	2	2	-	0/6/23/26	0/1/1/1
3	NAG	KA	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	KA	2	3	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	YZT	KA	3	3	-	0/5/22/25	0/1/1/1
2	NAG	KB	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	KB	2	2	-	0/6/23/26	0/1/1/1
2	NAG	KC	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	KC	2	2	-	0/6/23/26	0/1/1/1
2	NAG	MA	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	MA	2	2	-	0/6/23/26	0/1/1/1
2	NAG	MB	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	MB	2	2	-	0/6/23/26	0/1/1/1
2	NAG	MC	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	MC	2	2	-	2/6/23/26	0/1/1/1
2	NAG	NA	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	NA	2	2	-	0/6/23/26	0/1/1/1
2	NAG	NB	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	NB	2	2	-	2/6/23/26	0/1/1/1
3	NAG	NC	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	NC	2	3	-	2/6/23/26	0/1/1/1
3	YZT	NC	3	3	-	0/5/22/25	0/1/1/1
2	NAG	OA	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	OA	2	2	-	2/6/23/26	0/1/1/1
3	NAG	OB	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	OB	2	3	-	2/6/23/26	0/1/1/1
3	YZT	OB	3	3	-	0/5/22/25	0/1/1/1
2	NAG	OC	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	OC	2	2	-	1/6/23/26	0/1/1/1
3	NAG	PA	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	PA	2	3	-	2/6/23/26	0/1/1/1
3	YZT	PA	3	3	-	0/5/22/25	0/1/1/1
2	NAG	PB	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	PB	2	2	-	1/6/23/26	0/1/1/1
3	NAG	PC	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	PC	2	3	-	1/6/23/26	0/1/1/1
3	YZT	PC	3	3	-	0/5/22/25	0/1/1/1
2	NAG	QA	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	QA	2	2	-	1/6/23/26	0/1/1/1
3	NAG	QB	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	QB	2	3	-	1/6/23/26	0/1/1/1
3	YZT	QB	3	3	-	0/5/22/25	0/1/1/1
2	NAG	QC	1	2,1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	QC	2	2	-	0/6/23/26	0/1/1/1
3	NAG	RA	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	RA	2	3	-	1/6/23/26	0/1/1/1
3	YZT	RA	3	3	-	0/5/22/25	0/1/1/1
2	NAG	RB	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	RB	2	2	-	0/6/23/26	0/1/1/1
2	NAG	RC	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	RC	2	2	-	0/6/23/26	0/1/1/1
2	NAG	SA	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	SA	2	2	-	0/6/23/26	0/1/1/1
2	NAG	SB	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	SB	2	2	-	0/6/23/26	0/1/1/1
2	NAG	SC	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	SC	2	2	-	2/6/23/26	0/1/1/1
2	NAG	TA	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	TA	2	2	-	0/6/23/26	0/1/1/1
2	NAG	TB	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	TB	2	2	-	2/6/23/26	0/1/1/1
3	NAG	TC	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	TC	2	3	-	2/6/23/26	0/1/1/1
3	YZT	TC	3	3	-	0/5/22/25	0/1/1/1
2	NAG	UA	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	UA	2	2	-	2/6/23/26	0/1/1/1
3	NAG	UB	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	UB	2	3	-	2/6/23/26	0/1/1/1
3	YZT	UB	3	3	-	0/5/22/25	0/1/1/1
2	NAG	UC	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	UC	2	2	-	1/6/23/26	0/1/1/1
3	NAG	VA	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	VA	2	3	-	2/6/23/26	0/1/1/1
3	YZT	VA	3	3	-	0/5/22/25	0/1/1/1
2	NAG	VB	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	VB	2	2	-	1/6/23/26	0/1/1/1
3	NAG	VC	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	VC	2	3	-	1/6/23/26	0/1/1/1
3	YZT	VC	3	3	-	0/5/22/25	0/1/1/1
2	NAG	WA	1	2,1	-	5/6/23/26	0/1/1/1
2	NAG	WA	2	2	-	1/6/23/26	0/1/1/1
3	NAG	WB	1	3,1	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	WB	2	3	-	1/6/23/26	0/1/1/1
3	YZT	WB	3	3	-	0/5/22/25	0/1/1/1
2	NAG	WC	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	WC	2	2	-	0/6/23/26	0/1/1/1
3	NAG	XA	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	XA	2	3	-	1/6/23/26	0/1/1/1
3	YZT	XA	3	3	-	0/5/22/25	0/1/1/1
2	NAG	XB	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	XB	2	2	-	0/6/23/26	0/1/1/1
2	NAG	YA	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	YA	2	2	-	0/6/23/26	0/1/1/1
2	NAG	YB	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	YB	2	2	-	0/6/23/26	0/1/1/1
2	NAG	ZA	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	ZA	2	2	-	0/6/23/26	0/1/1/1
2	NAG	ZB	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	ZB	2	2	-	2/6/23/26	0/1/1/1
2	NAG	aA	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	aA	2	2	-	2/6/23/26	0/1/1/1
3	NAG	aB	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	aB	2	3	-	2/6/23/26	0/1/1/1
3	YZT	aB	3	3	-	0/5/22/25	0/1/1/1
3	NAG	bA	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	bA	2	3	-	2/6/23/26	0/1/1/1
3	YZT	bA	3	3	-	0/5/22/25	0/1/1/1
2	NAG	bB	1	2,1	-	5/6/23/26	0/1/1/1
2	NAG	bB	2	2	-	1/6/23/26	0/1/1/1
2	NAG	cA	1	2,1	-	5/6/23/26	0/1/1/1
2	NAG	cA	2	2	-	1/6/23/26	0/1/1/1
3	NAG	cB	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	cB	2	3	-	1/6/23/26	0/1/1/1
3	YZT	cB	3	3	-	0/5/22/25	0/1/1/1
3	NAG	dA	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	dA	2	3	-	1/6/23/26	0/1/1/1
3	YZT	dA	3	3	-	0/5/22/25	0/1/1/1
2	NAG	dB	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	dB	2	2	-	0/6/23/26	0/1/1/1
2	NAG	eA	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	eA	2	2	-	0/6/23/26	0/1/1/1
2	NAG	eB	1	2,1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	eB	2	2	-	0/6/23/26	0/1/1/1
2	NAG	fA	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	fA	2	2	-	0/6/23/26	0/1/1/1
2	NAG	fB	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	fB	2	2	-	2/6/23/26	0/1/1/1
2	NAG	gA	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	gA	2	2	-	2/6/23/26	0/1/1/1
3	NAG	gB	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	gB	2	3	-	2/6/23/26	0/1/1/1
3	YZT	gB	3	3	-	0/5/22/25	0/1/1/1
3	NAG	hA	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	hA	2	3	-	2/6/23/26	0/1/1/1
3	YZT	hA	3	3	-	0/5/22/25	0/1/1/1
2	NAG	hB	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	hB	2	2	-	1/6/23/26	0/1/1/1
2	NAG	iA	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	iA	2	2	-	1/6/23/26	0/1/1/1
3	NAG	iB	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	iB	2	3	-	1/6/23/26	0/1/1/1
3	YZT	iB	3	3	-	0/5/22/25	0/1/1/1
3	NAG	jA	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	jA	2	3	-	1/6/23/26	0/1/1/1
3	YZT	jA	3	3	-	0/5/22/25	0/1/1/1
2	NAG	jB	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	jB	2	2	-	0/6/23/26	0/1/1/1
2	NAG	kA	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	kA	2	2	-	0/6/23/26	0/1/1/1
2	NAG	kB	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	kB	2	2	-	0/6/23/26	0/1/1/1
2	NAG	lA	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	lA	2	2	-	0/6/23/26	0/1/1/1
2	NAG	lB	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	lB	2	2	-	2/6/23/26	0/1/1/1
2	NAG	mA	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	mA	2	2	-	2/6/23/26	0/1/1/1
3	NAG	mB	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	mB	2	3	-	2/6/23/26	0/1/1/1
3	YZT	mB	3	3	-	0/5/22/25	0/1/1/1
3	NAG	nA	1	3,1	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	nA	2	3	-	2/6/23/26	0/1/1/1
3	YZT	nA	3	3	-	0/5/22/25	0/1/1/1
2	NAG	nB	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	nB	2	2	-	1/6/23/26	0/1/1/1
2	NAG	oA	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	oA	2	2	-	1/6/23/26	0/1/1/1
3	NAG	oB	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	oB	2	3	-	1/6/23/26	0/1/1/1
3	YZT	oB	3	3	-	0/5/22/25	0/1/1/1
3	NAG	pA	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	pA	2	3	-	1/6/23/26	0/1/1/1
3	YZT	pA	3	3	-	0/5/22/25	0/1/1/1
2	NAG	pB	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	pB	2	2	-	0/6/23/26	0/1/1/1
2	NAG	qA	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	qA	2	2	-	0/6/23/26	0/1/1/1
2	NAG	qB	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	qB	2	2	-	0/6/23/26	0/1/1/1
2	NAG	rA	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	rA	2	2	-	0/6/23/26	0/1/1/1
2	NAG	rB	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	rB	2	2	-	2/6/23/26	0/1/1/1
2	NAG	sA	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	sA	2	2	-	2/6/23/26	0/1/1/1
3	NAG	sB	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	sB	2	3	-	2/6/23/26	0/1/1/1
3	YZT	sB	3	3	-	0/5/22/25	0/1/1/1
3	NAG	tA	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	tA	2	3	-	2/6/23/26	0/1/1/1
3	YZT	tA	3	3	-	0/5/22/25	0/1/1/1
2	NAG	tB	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	tB	2	2	-	1/6/23/26	0/1/1/1
2	NAG	uA	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	uA	2	2	-	1/6/23/26	0/1/1/1
3	NAG	uB	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	uB	2	3	-	1/6/23/26	0/1/1/1
3	YZT	uB	3	3	-	0/5/22/25	0/1/1/1
3	NAG	vA	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	vA	2	3	-	1/6/23/26	0/1/1/1
3	YZT	vA	3	3	-	0/5/22/25	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	vB	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	vB	2	2	-	0/6/23/26	0/1/1/1
2	NAG	wA	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	wA	2	2	-	0/6/23/26	0/1/1/1
2	NAG	wB	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	wB	2	2	-	0/6/23/26	0/1/1/1
2	NAG	xA	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	xA	2	2	-	0/6/23/26	0/1/1/1
2	NAG	xB	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	xB	2	2	-	2/6/23/26	0/1/1/1
2	NAG	yA	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	yA	2	2	-	2/6/23/26	0/1/1/1
3	NAG	yB	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	yB	2	3	-	2/6/23/26	0/1/1/1
3	YZT	yB	3	3	-	0/5/22/25	0/1/1/1
3	NAG	zA	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	zA	2	3	-	2/6/23/26	0/1/1/1
3	YZT	zA	3	3	-	0/5/22/25	0/1/1/1
2	NAG	zB	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	zB	2	2	-	1/6/23/26	0/1/1/1

All (77) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	nA	3	YZT	O2S6-S6	3.48	1.55	1.45
3	cB	3	YZT	O2S6-S6	3.47	1.55	1.45
3	BB	3	YZT	O2S6-S6	3.47	1.55	1.45
3	OB	3	YZT	O2S6-S6	3.47	1.55	1.45
3	6B	3	YZT	O2S6-S6	3.47	1.55	1.45
3	JB	3	YZT	O2S6-S6	3.47	1.55	1.45
3	GC	3	YZT	O2S6-S6	3.47	1.55	1.45
3	uB	3	YZT	O2S6-S6	3.46	1.55	1.45
3	mB	3	YZT	O2S6-S6	3.46	1.55	1.45
3	7A	3	YZT	O2S6-S6	3.46	1.55	1.45
3	zA	3	YZT	O2S6-S6	3.46	1.55	1.45
3	WB	3	YZT	O2S6-S6	3.46	1.55	1.45
3	CC	3	YZT	O2S6-S6	3.46	1.55	1.45
3	gB	3	YZT	O2S6-S6	3.46	1.55	1.45
3	VA	3	YZT	O2S6-S6	3.45	1.55	1.45
3	TC	3	YZT	O2S6-S6	3.45	1.55	1.45
3	IA	3	YZT	O2S6-S6	3.45	1.55	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	RA	3	YZT	O2S6-S6	3.45	1.55	1.45
3	VC	3	YZT	O2S6-S6	3.45	1.55	1.45
3	tA	3	YZT	O2S6-S6	3.45	1.55	1.45
3	DB	3	YZT	O2S6-S6	3.45	1.55	1.45
3	XA	3	YZT	O2S6-S6	3.45	1.55	1.45
3	AC	3	YZT	O2S6-S6	3.45	1.55	1.45
3	EA	3	YZT	O2S6-S6	3.45	1.55	1.45
3	pA	3	YZT	O2S6-S6	3.45	1.55	1.45
3	yB	3	YZT	O2S6-S6	3.45	1.55	1.45
3	0B	3	YZT	O2S6-S6	3.45	1.55	1.45
3	IC	3	YZT	O2S6-S6	3.45	1.55	1.45
3	UB	3	YZT	O2S6-S6	3.45	1.55	1.45
3	5A	3	YZT	O2S6-S6	3.45	1.55	1.45
3	NC	3	YZT	O2S6-S6	3.45	1.55	1.45
3	vA	3	YZT	O2S6-S6	3.45	1.55	1.45
3	HB	3	YZT	O2S6-S6	3.45	1.55	1.45
3	1A	3	YZT	O2S6-S6	3.44	1.55	1.45
3	iB	3	YZT	O2S6-S6	3.44	1.55	1.45
3	hA	3	YZT	O2S6-S6	3.44	1.55	1.45
3	jA	3	YZT	O2S6-S6	3.44	1.55	1.45
3	PC	3	YZT	O2S6-S6	3.44	1.55	1.45
3	aB	3	YZT	O2S6-S6	3.44	1.55	1.45
3	QB	3	YZT	O2S6-S6	3.44	1.55	1.45
3	oB	3	YZT	O2S6-S6	3.43	1.55	1.45
3	bA	3	YZT	O2S6-S6	3.43	1.55	1.45
3	PA	3	YZT	O2S6-S6	3.43	1.55	1.45
3	KA	3	YZT	O2S6-S6	3.43	1.55	1.45
3	sB	3	YZT	O2S6-S6	3.43	1.55	1.45
3	CA	3	YZT	O2S6-S6	3.42	1.55	1.45
3	dA	3	YZT	O2S6-S6	3.42	1.55	1.45
3	4B	3	YZT	O2S6-S6	3.42	1.55	1.45
2	HA	1	NAG	O5-C1	-3.07	1.38	1.43
2	gA	1	NAG	O5-C1	-3.06	1.38	1.43
2	4A	1	NAG	O5-C1	-3.06	1.38	1.43
2	NB	1	NAG	O5-C1	-3.04	1.38	1.43
2	TB	1	NAG	O5-C1	-3.03	1.38	1.43
2	UA	1	NAG	O5-C1	-3.02	1.38	1.43
2	OA	1	NAG	O5-C1	-3.01	1.38	1.43
2	BA	1	NAG	O5-C1	-2.99	1.38	1.43
2	GB	1	NAG	O5-C1	-2.98	1.39	1.43
2	fB	1	NAG	O5-C1	-2.98	1.39	1.43
2	yA	1	NAG	O5-C1	-2.96	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	9B	1	NAG	O5-C1	-2.96	1.39	1.43
2	AB	1	NAG	O5-C1	-2.95	1.39	1.43
2	aA	1	NAG	O5-C1	-2.94	1.39	1.43
2	3B	1	NAG	O5-C1	-2.93	1.39	1.43
2	mA	1	NAG	O5-C1	-2.92	1.39	1.43
2	lB	1	NAG	O5-C1	-2.91	1.39	1.43
2	SC	1	NAG	O5-C1	-2.88	1.39	1.43
2	ZB	1	NAG	O5-C1	-2.85	1.39	1.43
2	xB	1	NAG	O5-C1	-2.85	1.39	1.43
2	sA	1	NAG	O5-C1	-2.83	1.39	1.43
2	FC	1	NAG	O5-C1	-2.82	1.39	1.43
2	MC	1	NAG	O5-C1	-2.82	1.39	1.43
2	bB	1	NAG	O5-C1	-2.76	1.39	1.43
2	rB	1	NAG	O5-C1	-2.73	1.39	1.43
2	zB	1	NAG	O5-C1	-2.52	1.39	1.43
2	uA	1	NAG	O5-C1	-2.41	1.39	1.43
2	xA	1	NAG	O5-C1	-2.07	1.40	1.43
2	qB	1	NAG	O5-C1	-2.01	1.40	1.43

All (154) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	lB	1	NAG	C2-N2-C7	4.56	129.40	122.90
2	oA	1	NAG	C2-N2-C7	4.55	129.38	122.90
2	0A	1	NAG	C2-N2-C7	4.54	129.37	122.90
2	6A	1	NAG	C2-N2-C7	4.53	129.35	122.90
2	nB	1	NAG	C2-N2-C7	4.53	129.35	122.90
2	hB	1	NAG	C2-N2-C7	4.52	129.34	122.90
2	WA	1	NAG	C2-N2-C7	4.52	129.34	122.90
2	cA	1	NAG	C2-N2-C7	4.51	129.33	122.90
2	UC	1	NAG	C2-N2-C7	4.51	129.33	122.90
2	VB	1	NAG	C2-N2-C7	4.51	129.32	122.90
2	DA	1	NAG	C2-N2-C7	4.51	129.32	122.90
2	HC	1	NAG	C2-N2-C7	4.50	129.32	122.90
2	iA	1	NAG	C2-N2-C7	4.50	129.31	122.90
2	5B	1	NAG	C2-N2-C7	4.50	129.31	122.90
2	OC	1	NAG	C2-N2-C7	4.50	129.31	122.90
2	CB	1	NAG	C2-N2-C7	4.49	129.30	122.90
2	BC	1	NAG	C2-N2-C7	4.49	129.30	122.90
2	QA	1	NAG	C2-N2-C7	4.49	129.30	122.90
2	PB	1	NAG	C2-N2-C7	4.48	129.29	122.90
2	tB	1	NAG	C2-N2-C7	4.46	129.25	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	JA	1	NAG	C2-N2-C7	4.45	129.25	122.90
2	uA	1	NAG	C2-N2-C7	4.45	129.24	122.90
2	bB	1	NAG	C2-N2-C7	4.42	129.19	122.90
2	zB	1	NAG	C2-N2-C7	4.39	129.15	122.90
3	JB	3	YZT	O2S6-S6-C6	-4.17	101.98	106.94
3	CC	3	YZT	O2S6-S6-C6	-4.17	101.98	106.94
3	RA	3	YZT	O2S6-S6-C6	-4.16	101.99	106.94
3	pA	3	YZT	O2S6-S6-C6	-4.16	102.00	106.94
3	dA	3	YZT	O2S6-S6-C6	-4.15	102.00	106.94
3	VC	3	YZT	O2S6-S6-C6	-4.15	102.01	106.94
3	1A	3	YZT	O2S6-S6-C6	-4.15	102.01	106.94
3	iB	3	YZT	O2S6-S6-C6	-4.15	102.01	106.94
3	KA	3	YZT	O2S6-S6-C6	-4.15	102.01	106.94
3	WB	3	YZT	O2S6-S6-C6	-4.15	102.01	106.94
3	uB	3	YZT	O2S6-S6-C6	-4.14	102.02	106.94
3	IC	3	YZT	O2S6-S6-C6	-4.14	102.02	106.94
3	vA	3	YZT	O2S6-S6-C6	-4.14	102.02	106.94
3	cB	3	YZT	O2S6-S6-C6	-4.14	102.02	106.94
3	DB	3	YZT	O2S6-S6-C6	-4.13	102.03	106.94
3	6B	3	YZT	O2S6-S6-C6	-4.13	102.03	106.94
3	XA	3	YZT	O2S6-S6-C6	-4.13	102.03	106.94
3	0B	3	YZT	O2S6-S6-C6	-4.12	102.04	106.94
3	jA	3	YZT	O2S6-S6-C6	-4.12	102.05	106.94
3	7A	3	YZT	O2S6-S6-C6	-4.12	102.05	106.94
3	PC	3	YZT	O2S6-S6-C6	-4.12	102.05	106.94
3	EA	3	YZT	O2S6-S6-C6	-4.11	102.06	106.94
3	QB	3	YZT	O2S6-S6-C6	-4.10	102.07	106.94
3	oB	3	YZT	O2S6-S6-C6	-4.09	102.07	106.94
3	BB	3	YZT	O2S6-S6-C6	-4.03	102.15	106.94
3	yB	3	YZT	O2S6-S6-C6	-4.03	102.15	106.94
3	AC	3	YZT	O2S6-S6-C6	-4.02	102.16	106.94
3	UB	3	YZT	O2S6-S6-C6	-4.02	102.16	106.94
3	mB	3	YZT	O2S6-S6-C6	-4.02	102.17	106.94
3	TC	3	YZT	O2S6-S6-C6	-4.01	102.17	106.94
3	5A	3	YZT	O2S6-S6-C6	-4.01	102.17	106.94
3	nA	3	YZT	O2S6-S6-C6	-4.01	102.17	106.94
3	aB	3	YZT	O2S6-S6-C6	-4.01	102.18	106.94
3	IA	3	YZT	O2S6-S6-C6	-4.01	102.18	106.94
3	OB	3	YZT	O2S6-S6-C6	-4.01	102.18	106.94
3	zA	3	YZT	O2S6-S6-C6	-4.00	102.18	106.94
3	GC	3	YZT	O2S6-S6-C6	-4.00	102.18	106.94
3	bA	3	YZT	O2S6-S6-C6	-4.00	102.18	106.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	hA	3	YZT	O2S6-S6-C6	-4.00	102.19	106.94
3	NC	3	YZT	O2S6-S6-C6	-4.00	102.19	106.94
3	VA	3	YZT	O2S6-S6-C6	-4.00	102.19	106.94
3	gB	3	YZT	O2S6-S6-C6	-4.00	102.19	106.94
3	4B	3	YZT	O2S6-S6-C6	-3.99	102.19	106.94
3	sB	3	YZT	O2S6-S6-C6	-3.99	102.20	106.94
3	CA	3	YZT	O2S6-S6-C6	-3.97	102.22	106.94
3	HB	3	YZT	O2S6-S6-C6	-3.96	102.23	106.94
3	PA	3	YZT	O2S6-S6-C6	-3.95	102.24	106.94
3	tA	3	YZT	O2S6-S6-C6	-3.95	102.24	106.94
3	mB	3	YZT	O1S6-S6-O3S6	2.95	118.47	111.27
3	5A	3	YZT	O1S6-S6-O3S6	2.94	118.47	111.27
3	TC	3	YZT	O1S6-S6-O3S6	2.94	118.45	111.27
3	BB	3	YZT	O1S6-S6-O3S6	2.93	118.44	111.27
3	hA	3	YZT	O1S6-S6-O3S6	2.93	118.44	111.27
3	IA	3	YZT	O1S6-S6-O3S6	2.93	118.42	111.27
3	nA	3	YZT	O1S6-S6-O3S6	2.93	118.42	111.27
3	aB	3	YZT	O1S6-S6-O3S6	2.93	118.42	111.27
3	yB	3	YZT	O1S6-S6-O3S6	2.93	118.42	111.27
3	OB	3	YZT	O1S6-S6-O3S6	2.92	118.42	111.27
3	VA	3	YZT	O1S6-S6-O3S6	2.92	118.42	111.27
3	GC	3	YZT	O1S6-S6-O3S6	2.92	118.41	111.27
3	CA	3	YZT	O1S6-S6-O3S6	2.92	118.41	111.27
3	AC	3	YZT	O1S6-S6-O3S6	2.92	118.41	111.27
3	sB	3	YZT	O1S6-S6-O3S6	2.92	118.40	111.27
3	gB	3	YZT	O1S6-S6-O3S6	2.91	118.39	111.27
3	bA	3	YZT	O1S6-S6-O3S6	2.91	118.39	111.27
3	NC	3	YZT	O1S6-S6-O3S6	2.91	118.39	111.27
3	4B	3	YZT	O1S6-S6-O3S6	2.91	118.39	111.27
3	CC	3	YZT	O1S6-S6-O3S6	2.91	118.39	111.27
3	UB	3	YZT	O1S6-S6-O3S6	2.91	118.39	111.27
3	IC	3	YZT	O1S6-S6-O3S6	2.91	118.38	111.27
3	zA	3	YZT	O1S6-S6-O3S6	2.91	118.37	111.27
3	tA	3	YZT	O1S6-S6-O3S6	2.90	118.37	111.27
3	vA	3	YZT	O1S6-S6-O3S6	2.90	118.37	111.27
3	HB	3	YZT	O1S6-S6-O3S6	2.90	118.36	111.27
3	RA	3	YZT	O1S6-S6-O3S6	2.90	118.36	111.27
3	cB	3	YZT	O1S6-S6-O3S6	2.90	118.36	111.27
3	VC	3	YZT	O1S6-S6-O3S6	2.90	118.35	111.27
3	KA	3	YZT	O1S6-S6-O3S6	2.89	118.34	111.27
3	PC	3	YZT	O1S6-S6-O3S6	2.89	118.34	111.27
3	1A	3	YZT	O1S6-S6-O3S6	2.89	118.33	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	uB	3	YZT	O1S6-S6-O3S6	2.89	118.33	111.27
3	JB	3	YZT	O1S6-S6-O3S6	2.89	118.33	111.27
3	PA	3	YZT	O1S6-S6-O3S6	2.89	118.33	111.27
3	XA	3	YZT	O1S6-S6-O3S6	2.89	118.33	111.27
3	QB	3	YZT	O1S6-S6-O3S6	2.89	118.33	111.27
3	dA	3	YZT	O1S6-S6-O3S6	2.89	118.33	111.27
3	WB	3	YZT	O1S6-S6-O3S6	2.88	118.32	111.27
3	0B	3	YZT	O1S6-S6-O3S6	2.88	118.32	111.27
3	pA	3	YZT	O1S6-S6-O3S6	2.88	118.32	111.27
3	iB	3	YZT	O1S6-S6-O3S6	2.88	118.32	111.27
3	jA	3	YZT	O1S6-S6-O3S6	2.88	118.31	111.27
3	6B	3	YZT	O1S6-S6-O3S6	2.88	118.31	111.27
3	DB	3	YZT	O1S6-S6-O3S6	2.88	118.31	111.27
3	oB	3	YZT	O1S6-S6-O3S6	2.87	118.29	111.27
3	7A	3	YZT	O1S6-S6-O3S6	2.87	118.28	111.27
3	EA	3	YZT	O1S6-S6-O3S6	2.87	118.28	111.27
2	DA	1	NAG	C1-C2-N2	2.61	114.95	110.49
2	IB	1	NAG	C1-C2-N2	2.53	114.81	110.49
2	oA	1	NAG	C1-C2-N2	2.50	114.76	110.49
2	CB	1	NAG	C1-C2-N2	2.49	114.74	110.49
2	6A	1	NAG	C1-C2-N2	2.46	114.69	110.49
2	nB	1	NAG	C1-C2-N2	2.46	114.69	110.49
2	BC	1	NAG	C1-C2-N2	2.46	114.68	110.49
2	iA	1	NAG	C1-C2-N2	2.45	114.68	110.49
2	hB	1	NAG	C1-C2-N2	2.43	114.65	110.49
2	cA	1	NAG	C1-C2-N2	2.43	114.64	110.49
2	VB	1	NAG	C1-C2-N2	2.43	114.64	110.49
2	0A	1	NAG	C1-C2-N2	2.42	114.62	110.49
2	5B	1	NAG	C1-C2-N2	2.41	114.61	110.49
2	HC	1	NAG	C1-C2-N2	2.41	114.60	110.49
2	OC	1	NAG	C1-C2-N2	2.40	114.59	110.49
2	tB	1	NAG	C1-C2-N2	2.38	114.56	110.49
2	uA	1	NAG	C1-C2-N2	2.29	114.40	110.49
2	zB	1	NAG	C1-C2-N2	2.28	114.39	110.49
2	WA	1	NAG	C1-C2-N2	2.28	114.38	110.49
2	bB	1	NAG	C1-C2-N2	2.27	114.37	110.49
2	QA	1	NAG	C1-C2-N2	2.23	114.29	110.49
2	0A	1	NAG	C3-C4-C5	2.21	114.18	110.24
2	UC	1	NAG	C1-C2-N2	2.15	114.16	110.49
2	PB	1	NAG	C1-C2-N2	2.14	114.15	110.49
2	OC	1	NAG	C3-C4-C5	2.13	114.04	110.24
2	hB	1	NAG	C3-C4-C5	2.11	114.01	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	UC	1	NAG	C1-O5-C5	2.10	115.04	112.19
2	JA	1	NAG	C1-C2-N2	2.08	114.03	110.49
2	cA	1	NAG	C3-C4-C5	2.07	113.93	110.24
2	VB	1	NAG	C3-C4-C5	2.06	113.92	110.24
2	oA	1	NAG	C3-C4-C5	2.05	113.90	110.24
2	PB	1	NAG	C1-O5-C5	2.04	114.95	112.19
2	tB	1	NAG	C3-C4-C5	2.02	113.85	110.24
2	PB	1	NAG	C3-C4-C5	2.02	113.85	110.24

There are no chirality outliers.

All (331) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	IA	2	NAG	O5-C5-C6-O6
3	VA	2	NAG	O5-C5-C6-O6
3	bA	2	NAG	O5-C5-C6-O6
3	tA	2	NAG	O5-C5-C6-O6
3	HB	2	NAG	O5-C5-C6-O6
3	gB	2	NAG	O5-C5-C6-O6
3	4B	2	NAG	O5-C5-C6-O6
3	AC	2	NAG	O5-C5-C6-O6
3	GC	2	NAG	O5-C5-C6-O6
3	PA	2	NAG	O5-C5-C6-O6
3	BB	2	NAG	O5-C5-C6-O6
3	aB	2	NAG	O5-C5-C6-O6
3	mB	2	NAG	O5-C5-C6-O6
3	sB	2	NAG	O5-C5-C6-O6
3	yB	2	NAG	O5-C5-C6-O6
3	CA	2	NAG	O5-C5-C6-O6
3	hA	2	NAG	O5-C5-C6-O6
3	nA	2	NAG	O5-C5-C6-O6
3	zA	2	NAG	O5-C5-C6-O6
3	5A	2	NAG	O5-C5-C6-O6
3	OB	2	NAG	O5-C5-C6-O6
3	UB	2	NAG	O5-C5-C6-O6
3	NC	2	NAG	O5-C5-C6-O6
3	TC	2	NAG	O5-C5-C6-O6
3	NC	2	NAG	C4-C5-C6-O6
3	UB	2	NAG	C4-C5-C6-O6
3	TC	2	NAG	C4-C5-C6-O6
3	PA	2	NAG	C4-C5-C6-O6
3	VA	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	hA	2	NAG	C4-C5-C6-O6
3	tA	2	NAG	C4-C5-C6-O6
3	OB	2	NAG	C4-C5-C6-O6
3	aB	2	NAG	C4-C5-C6-O6
3	mB	2	NAG	C4-C5-C6-O6
3	GC	2	NAG	C4-C5-C6-O6
3	CA	2	NAG	C4-C5-C6-O6
3	IA	2	NAG	C4-C5-C6-O6
3	bA	2	NAG	C4-C5-C6-O6
3	BB	2	NAG	C4-C5-C6-O6
3	HB	2	NAG	C4-C5-C6-O6
3	gB	2	NAG	C4-C5-C6-O6
3	sB	2	NAG	C4-C5-C6-O6
3	yB	2	NAG	C4-C5-C6-O6
3	4B	2	NAG	C4-C5-C6-O6
3	AC	2	NAG	C4-C5-C6-O6
2	DA	1	NAG	C8-C7-N2-C2
2	DA	1	NAG	O7-C7-N2-C2
2	JA	1	NAG	C8-C7-N2-C2
2	JA	1	NAG	O7-C7-N2-C2
2	QA	1	NAG	C8-C7-N2-C2
2	QA	1	NAG	O7-C7-N2-C2
2	WA	1	NAG	C8-C7-N2-C2
2	WA	1	NAG	O7-C7-N2-C2
2	cA	1	NAG	C8-C7-N2-C2
2	cA	1	NAG	O7-C7-N2-C2
2	iA	1	NAG	C8-C7-N2-C2
2	iA	1	NAG	O7-C7-N2-C2
2	oA	1	NAG	C8-C7-N2-C2
2	oA	1	NAG	O7-C7-N2-C2
2	uA	1	NAG	C8-C7-N2-C2
2	uA	1	NAG	O7-C7-N2-C2
2	0A	1	NAG	C8-C7-N2-C2
2	0A	1	NAG	O7-C7-N2-C2
2	6A	1	NAG	C8-C7-N2-C2
2	6A	1	NAG	O7-C7-N2-C2
2	CB	1	NAG	C8-C7-N2-C2
2	CB	1	NAG	O7-C7-N2-C2
2	IB	1	NAG	C8-C7-N2-C2
2	IB	1	NAG	O7-C7-N2-C2
2	PB	1	NAG	C8-C7-N2-C2
2	PB	1	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
2	VB	1	NAG	C8-C7-N2-C2
2	VB	1	NAG	O7-C7-N2-C2
2	bB	1	NAG	C8-C7-N2-C2
2	bB	1	NAG	O7-C7-N2-C2
2	hB	1	NAG	C8-C7-N2-C2
2	hB	1	NAG	O7-C7-N2-C2
2	nB	1	NAG	C8-C7-N2-C2
2	nB	1	NAG	O7-C7-N2-C2
2	tB	1	NAG	C8-C7-N2-C2
2	tB	1	NAG	O7-C7-N2-C2
2	zB	1	NAG	C8-C7-N2-C2
2	zB	1	NAG	O7-C7-N2-C2
2	5B	1	NAG	C8-C7-N2-C2
2	5B	1	NAG	O7-C7-N2-C2
2	BC	1	NAG	C8-C7-N2-C2
2	BC	1	NAG	O7-C7-N2-C2
2	HC	1	NAG	C8-C7-N2-C2
2	HC	1	NAG	O7-C7-N2-C2
2	OC	1	NAG	C8-C7-N2-C2
2	OC	1	NAG	O7-C7-N2-C2
2	UC	1	NAG	C8-C7-N2-C2
2	UC	1	NAG	O7-C7-N2-C2
3	nA	2	NAG	C4-C5-C6-O6
3	zA	2	NAG	C4-C5-C6-O6
3	5A	2	NAG	C4-C5-C6-O6
2	fB	1	NAG	O5-C5-C6-O6
2	rB	1	NAG	O5-C5-C6-O6
2	yA	1	NAG	O5-C5-C6-O6
2	ZB	1	NAG	O5-C5-C6-O6
2	lB	1	NAG	O5-C5-C6-O6
2	BA	1	NAG	O5-C5-C6-O6
2	HA	1	NAG	O5-C5-C6-O6
2	aA	1	NAG	O5-C5-C6-O6
2	gA	1	NAG	O5-C5-C6-O6
2	mA	1	NAG	O5-C5-C6-O6
2	sA	1	NAG	O5-C5-C6-O6
2	4A	1	NAG	O5-C5-C6-O6
2	AB	1	NAG	O5-C5-C6-O6
2	TB	1	NAG	O5-C5-C6-O6
2	3B	1	NAG	O5-C5-C6-O6
2	9B	1	NAG	O5-C5-C6-O6
2	FC	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	MC	1	NAG	O5-C5-C6-O6
2	SC	1	NAG	O5-C5-C6-O6
2	bB	1	NAG	C4-C5-C6-O6
2	OA	1	NAG	O5-C5-C6-O6
2	UA	1	NAG	O5-C5-C6-O6
2	GB	1	NAG	O5-C5-C6-O6
2	NB	1	NAG	O5-C5-C6-O6
2	xB	1	NAG	O5-C5-C6-O6
2	WA	1	NAG	C4-C5-C6-O6
2	cA	1	NAG	C4-C5-C6-O6
2	fB	1	NAG	C4-C5-C6-O6
2	rB	1	NAG	C4-C5-C6-O6
2	lB	1	NAG	C4-C5-C6-O6
2	yA	1	NAG	C4-C5-C6-O6
2	ZB	1	NAG	C4-C5-C6-O6
2	JA	1	NAG	C4-C5-C6-O6
2	SC	1	NAG	C4-C5-C6-O6
2	HA	1	NAG	C4-C5-C6-O6
2	BA	1	NAG	C4-C5-C6-O6
2	gA	1	NAG	C4-C5-C6-O6
2	mA	1	NAG	C4-C5-C6-O6
2	sA	1	NAG	C4-C5-C6-O6
2	0A	1	NAG	C4-C5-C6-O6
2	4A	1	NAG	C4-C5-C6-O6
2	AB	1	NAG	C4-C5-C6-O6
2	3B	1	NAG	C4-C5-C6-O6
2	9B	1	NAG	C4-C5-C6-O6
2	FC	1	NAG	C4-C5-C6-O6
2	MC	1	NAG	C4-C5-C6-O6
2	TB	1	NAG	C4-C5-C6-O6
2	OA	1	NAG	C4-C5-C6-O6
2	aA	1	NAG	C4-C5-C6-O6
2	uA	1	NAG	C4-C5-C6-O6
2	GB	1	NAG	C4-C5-C6-O6
2	xB	1	NAG	C4-C5-C6-O6
2	OC	1	NAG	C4-C5-C6-O6
2	CB	1	NAG	C4-C5-C6-O6
2	UA	1	NAG	C4-C5-C6-O6
2	NB	1	NAG	C4-C5-C6-O6
2	hB	1	NAG	C4-C5-C6-O6
2	bB	1	NAG	O5-C5-C6-O6
2	UC	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	VB	2	NAG	O5-C5-C6-O6
2	zB	1	NAG	C4-C5-C6-O6
2	PB	2	NAG	O5-C5-C6-O6
2	tB	1	NAG	C4-C5-C6-O6
2	HC	2	NAG	O5-C5-C6-O6
2	WA	1	NAG	O5-C5-C6-O6
2	oA	2	NAG	O5-C5-C6-O6
2	tB	2	NAG	O5-C5-C6-O6
2	WA	2	NAG	O5-C5-C6-O6
2	0A	2	NAG	O5-C5-C6-O6
3	QB	2	NAG	O5-C5-C6-O6
2	hB	2	NAG	O5-C5-C6-O6
2	bB	2	NAG	O5-C5-C6-O6
2	OC	2	NAG	O5-C5-C6-O6
3	JB	2	NAG	O5-C5-C6-O6
2	iA	2	NAG	O5-C5-C6-O6
2	5B	2	NAG	O5-C5-C6-O6
3	DB	2	NAG	O5-C5-C6-O6
2	cA	2	NAG	O5-C5-C6-O6
3	pA	2	NAG	O5-C5-C6-O6
3	CC	2	NAG	O5-C5-C6-O6
3	dA	2	NAG	O5-C5-C6-O6
3	vA	2	NAG	O5-C5-C6-O6
3	1A	2	NAG	O5-C5-C6-O6
3	7A	2	NAG	O5-C5-C6-O6
2	nB	2	NAG	O5-C5-C6-O6
2	BC	2	NAG	O5-C5-C6-O6
3	XA	2	NAG	O5-C5-C6-O6
3	jA	2	NAG	O5-C5-C6-O6
3	iB	2	NAG	O5-C5-C6-O6
3	6B	2	NAG	O5-C5-C6-O6
2	6A	2	NAG	O5-C5-C6-O6
3	WB	2	NAG	O5-C5-C6-O6
2	CB	2	NAG	O5-C5-C6-O6
3	KA	2	NAG	O5-C5-C6-O6
2	5B	1	NAG	C4-C5-C6-O6
3	cB	2	NAG	O5-C5-C6-O6
3	IC	2	NAG	O5-C5-C6-O6
3	uB	2	NAG	O5-C5-C6-O6
2	QA	2	NAG	O5-C5-C6-O6
3	RA	2	NAG	O5-C5-C6-O6
2	BA	2	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
2	DA	1	NAG	C3-C2-N2-C7
2	HA	2	NAG	C3-C2-N2-C7
2	JA	1	NAG	C3-C2-N2-C7
2	OA	2	NAG	C3-C2-N2-C7
2	UA	2	NAG	C3-C2-N2-C7
2	WA	1	NAG	C3-C2-N2-C7
2	aA	2	NAG	C3-C2-N2-C7
2	gA	2	NAG	C3-C2-N2-C7
2	mA	2	NAG	C3-C2-N2-C7
2	sA	2	NAG	C3-C2-N2-C7
2	uA	1	NAG	C3-C2-N2-C7
2	yA	2	NAG	C3-C2-N2-C7
2	4A	2	NAG	C3-C2-N2-C7
2	AB	2	NAG	C3-C2-N2-C7
2	GB	2	NAG	C3-C2-N2-C7
2	NB	2	NAG	C3-C2-N2-C7
2	PB	1	NAG	C3-C2-N2-C7
2	TB	2	NAG	C3-C2-N2-C7
2	ZB	2	NAG	C3-C2-N2-C7
2	bB	1	NAG	C3-C2-N2-C7
2	fB	2	NAG	C3-C2-N2-C7
2	lB	2	NAG	C3-C2-N2-C7
2	rB	2	NAG	C3-C2-N2-C7
2	xB	2	NAG	C3-C2-N2-C7
2	zB	1	NAG	C3-C2-N2-C7
2	3B	2	NAG	C3-C2-N2-C7
2	9B	2	NAG	C3-C2-N2-C7
2	FC	2	NAG	C3-C2-N2-C7
2	MC	2	NAG	C3-C2-N2-C7
2	UC	1	NAG	C3-C2-N2-C7
3	CA	1	NAG	C3-C2-N2-C7
3	EA	1	NAG	C3-C2-N2-C7
3	IA	1	NAG	C3-C2-N2-C7
3	KA	1	NAG	C3-C2-N2-C7
3	PA	1	NAG	C3-C2-N2-C7
3	RA	1	NAG	C3-C2-N2-C7
3	VA	1	NAG	C3-C2-N2-C7
3	XA	1	NAG	C3-C2-N2-C7
3	bA	1	NAG	C3-C2-N2-C7
3	dA	1	NAG	C3-C2-N2-C7
3	hA	1	NAG	C3-C2-N2-C7
3	jA	1	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
3	nA	1	NAG	C3-C2-N2-C7
3	pA	1	NAG	C3-C2-N2-C7
3	tA	1	NAG	C3-C2-N2-C7
3	vA	1	NAG	C3-C2-N2-C7
3	zA	1	NAG	C3-C2-N2-C7
3	1A	1	NAG	C3-C2-N2-C7
3	5A	1	NAG	C3-C2-N2-C7
3	7A	1	NAG	C3-C2-N2-C7
3	BB	1	NAG	C3-C2-N2-C7
3	DB	1	NAG	C3-C2-N2-C7
3	HB	1	NAG	C3-C2-N2-C7
3	JB	1	NAG	C3-C2-N2-C7
3	OB	1	NAG	C3-C2-N2-C7
3	QB	1	NAG	C3-C2-N2-C7
3	UB	1	NAG	C3-C2-N2-C7
3	WB	1	NAG	C3-C2-N2-C7
3	aB	1	NAG	C3-C2-N2-C7
3	cB	1	NAG	C3-C2-N2-C7
3	gB	1	NAG	C3-C2-N2-C7
3	iB	1	NAG	C3-C2-N2-C7
3	mB	1	NAG	C3-C2-N2-C7
3	oB	1	NAG	C3-C2-N2-C7
3	sB	1	NAG	C3-C2-N2-C7
3	uB	1	NAG	C3-C2-N2-C7
3	yB	1	NAG	C3-C2-N2-C7
3	0B	1	NAG	C3-C2-N2-C7
3	4B	1	NAG	C3-C2-N2-C7
3	6B	1	NAG	C3-C2-N2-C7
3	AC	1	NAG	C3-C2-N2-C7
3	CC	1	NAG	C3-C2-N2-C7
3	GC	1	NAG	C3-C2-N2-C7
3	IC	1	NAG	C3-C2-N2-C7
3	NC	1	NAG	C3-C2-N2-C7
3	PC	1	NAG	C3-C2-N2-C7
3	TC	1	NAG	C3-C2-N2-C7
3	VC	1	NAG	C3-C2-N2-C7
3	oB	2	NAG	O5-C5-C6-O6
3	0B	2	NAG	O5-C5-C6-O6
2	JA	2	NAG	O5-C5-C6-O6
3	PC	2	NAG	O5-C5-C6-O6
3	EA	2	NAG	O5-C5-C6-O6
3	VC	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	uA	2	NAG	O5-C5-C6-O6
2	BA	2	NAG	C1-C2-N2-C7
2	HA	2	NAG	C1-C2-N2-C7
2	OA	2	NAG	C1-C2-N2-C7
2	UA	2	NAG	C1-C2-N2-C7
2	aA	2	NAG	C1-C2-N2-C7
2	gA	2	NAG	C1-C2-N2-C7
2	mA	2	NAG	C1-C2-N2-C7
2	sA	2	NAG	C1-C2-N2-C7
2	yA	2	NAG	C1-C2-N2-C7
2	4A	2	NAG	C1-C2-N2-C7
2	AB	2	NAG	C1-C2-N2-C7
2	GB	2	NAG	C1-C2-N2-C7
2	NB	2	NAG	C1-C2-N2-C7
2	TB	2	NAG	C1-C2-N2-C7
2	ZB	2	NAG	C1-C2-N2-C7
2	fB	2	NAG	C1-C2-N2-C7
2	lB	2	NAG	C1-C2-N2-C7
2	rB	2	NAG	C1-C2-N2-C7
2	xB	2	NAG	C1-C2-N2-C7
2	3B	2	NAG	C1-C2-N2-C7
2	9B	2	NAG	C1-C2-N2-C7
2	FC	2	NAG	C1-C2-N2-C7
2	MC	2	NAG	C1-C2-N2-C7
2	SC	2	NAG	C1-C2-N2-C7
2	iA	1	NAG	C4-C5-C6-O6
2	JA	1	NAG	O5-C5-C6-O6
2	cA	1	NAG	O5-C5-C6-O6
2	DA	1	NAG	C4-C5-C6-O6
2	QA	1	NAG	C3-C2-N2-C7
2	cA	1	NAG	C3-C2-N2-C7
2	iA	1	NAG	C3-C2-N2-C7
2	oA	1	NAG	C3-C2-N2-C7
2	0A	1	NAG	C3-C2-N2-C7
2	6A	1	NAG	C3-C2-N2-C7
2	CB	1	NAG	C3-C2-N2-C7
2	IB	1	NAG	C3-C2-N2-C7
2	VB	1	NAG	C3-C2-N2-C7
2	hB	1	NAG	C3-C2-N2-C7
2	nB	1	NAG	C3-C2-N2-C7
2	tB	1	NAG	C3-C2-N2-C7
2	5B	1	NAG	C3-C2-N2-C7

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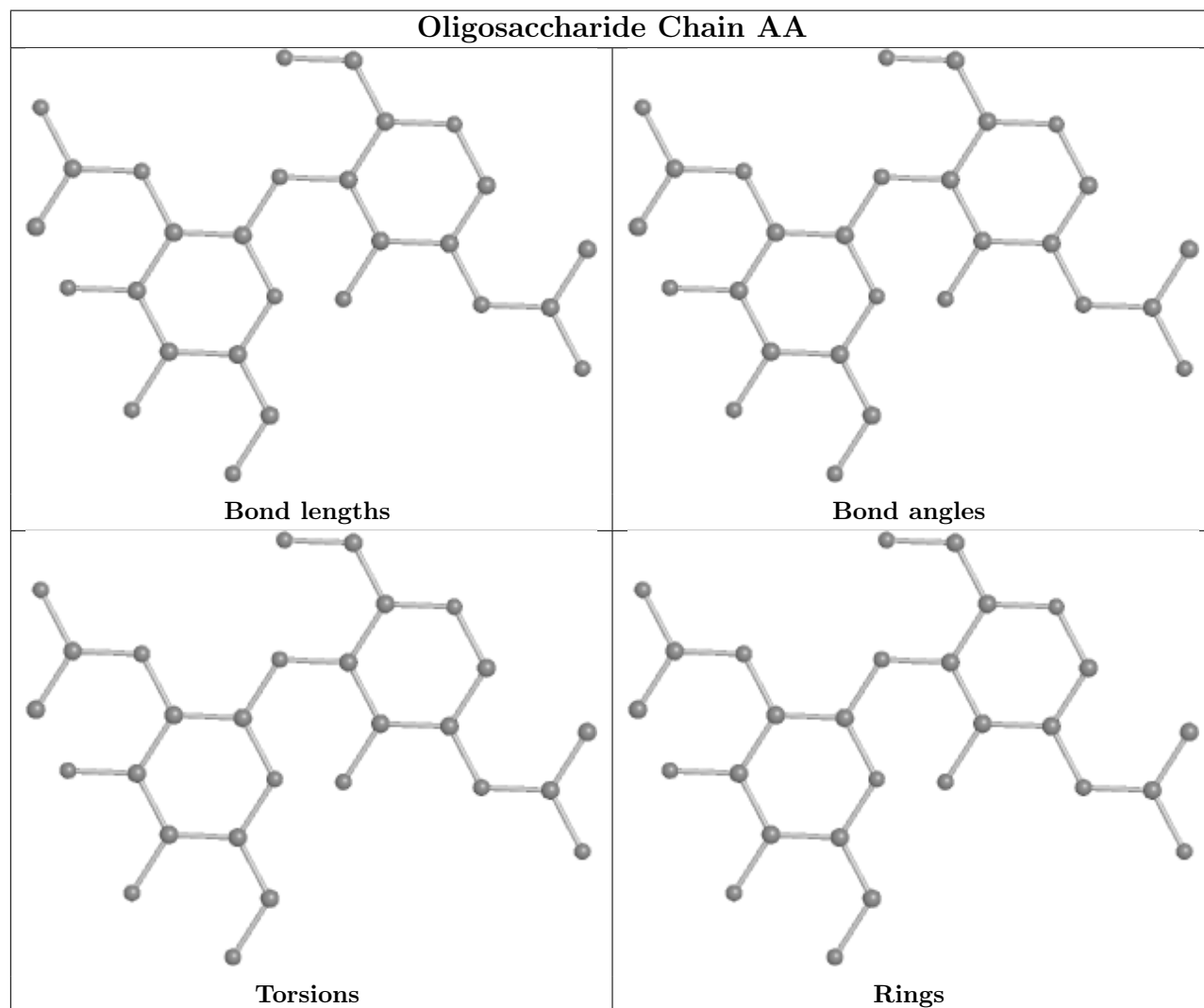
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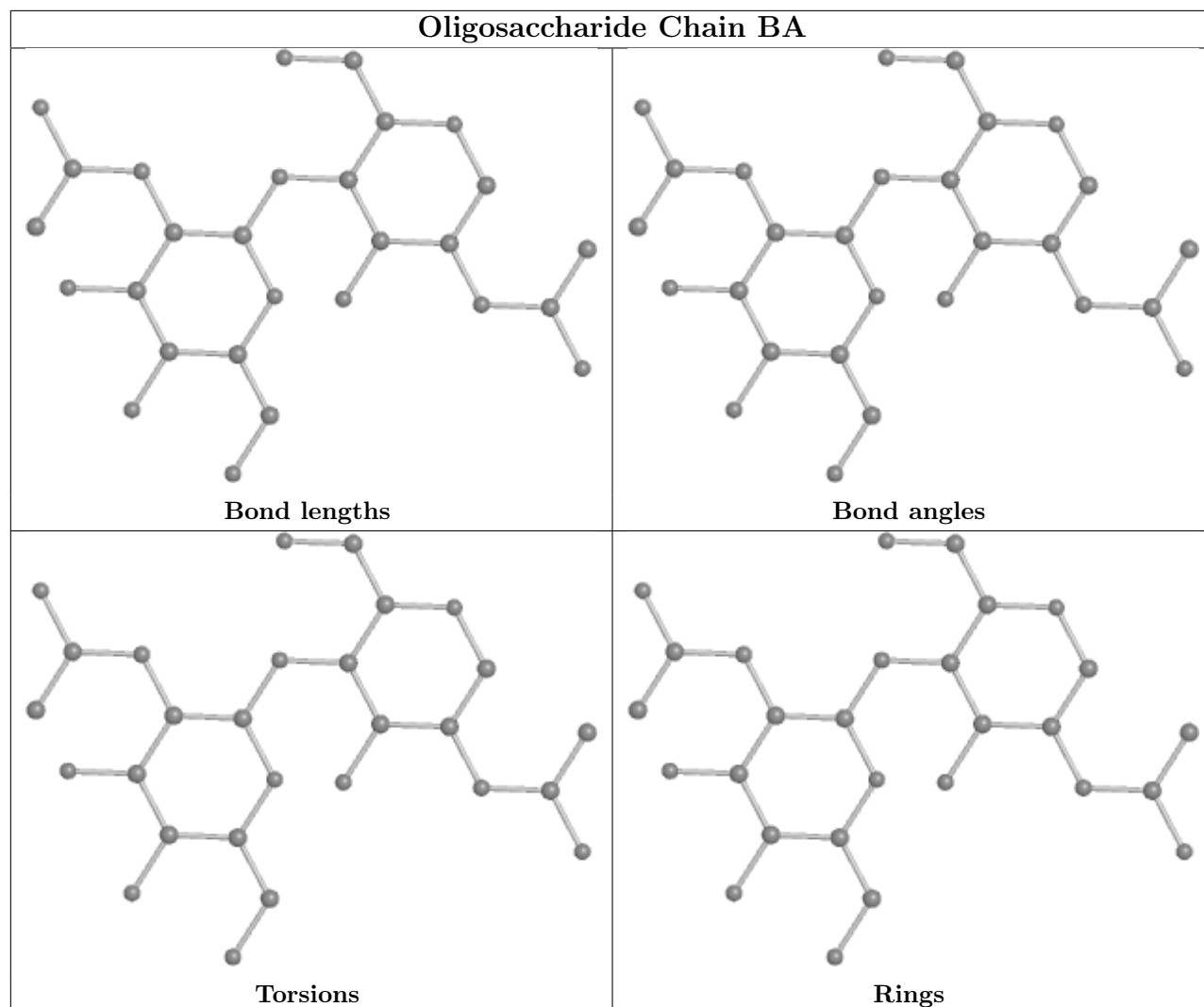
Mol	Chain	Res	Type	Atoms
2	BC	1	NAG	C3-C2-N2-C7
2	HC	1	NAG	C3-C2-N2-C7
2	OC	1	NAG	C3-C2-N2-C7
2	SC	2	NAG	C3-C2-N2-C7
2	IB	2	NAG	O5-C5-C6-O6
2	zB	2	NAG	O5-C5-C6-O6
2	oA	1	NAG	C4-C5-C6-O6
2	jB	1	NAG	O5-C5-C6-O6

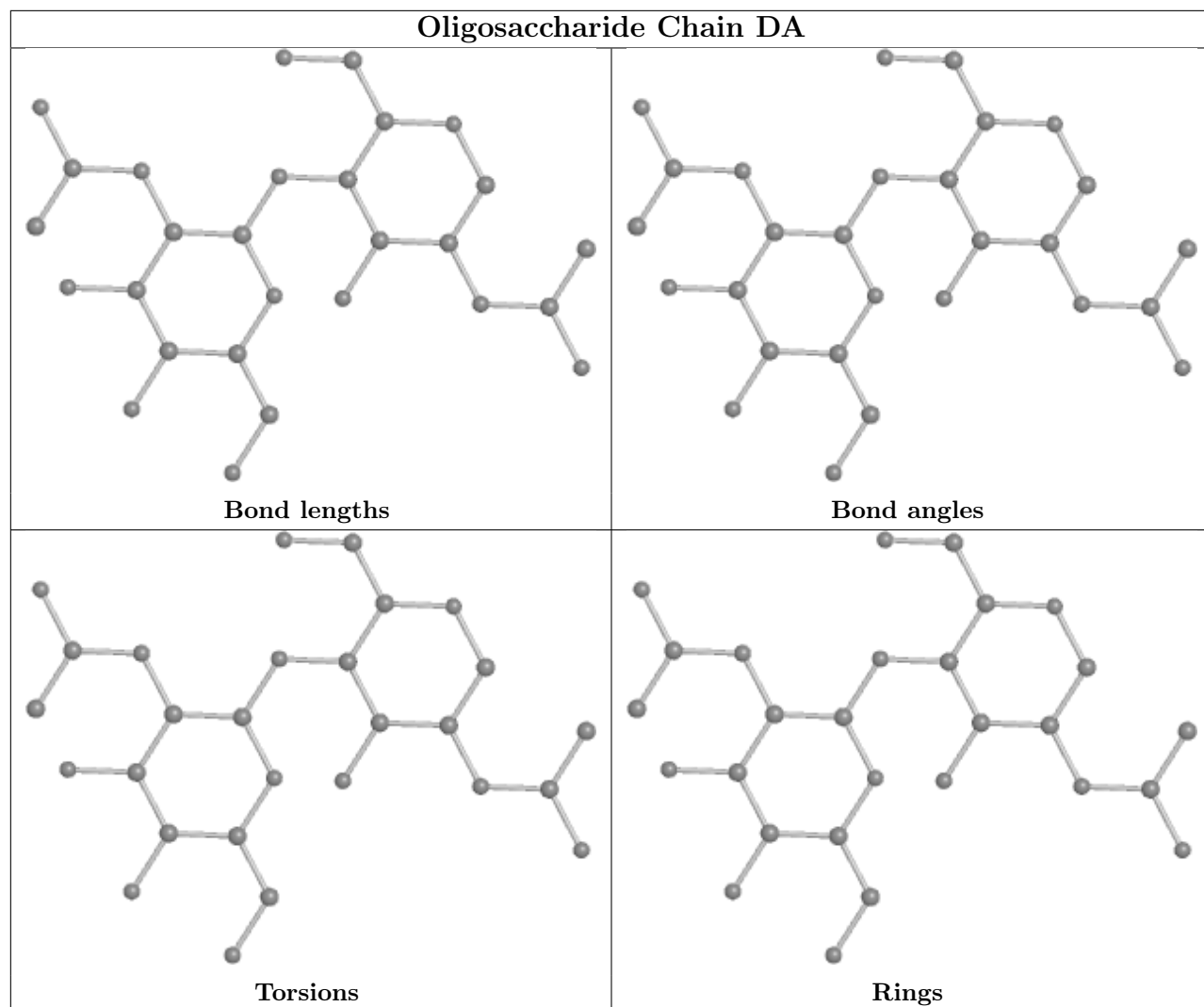
There are no ring outliers.

No monomer is involved in short contacts.

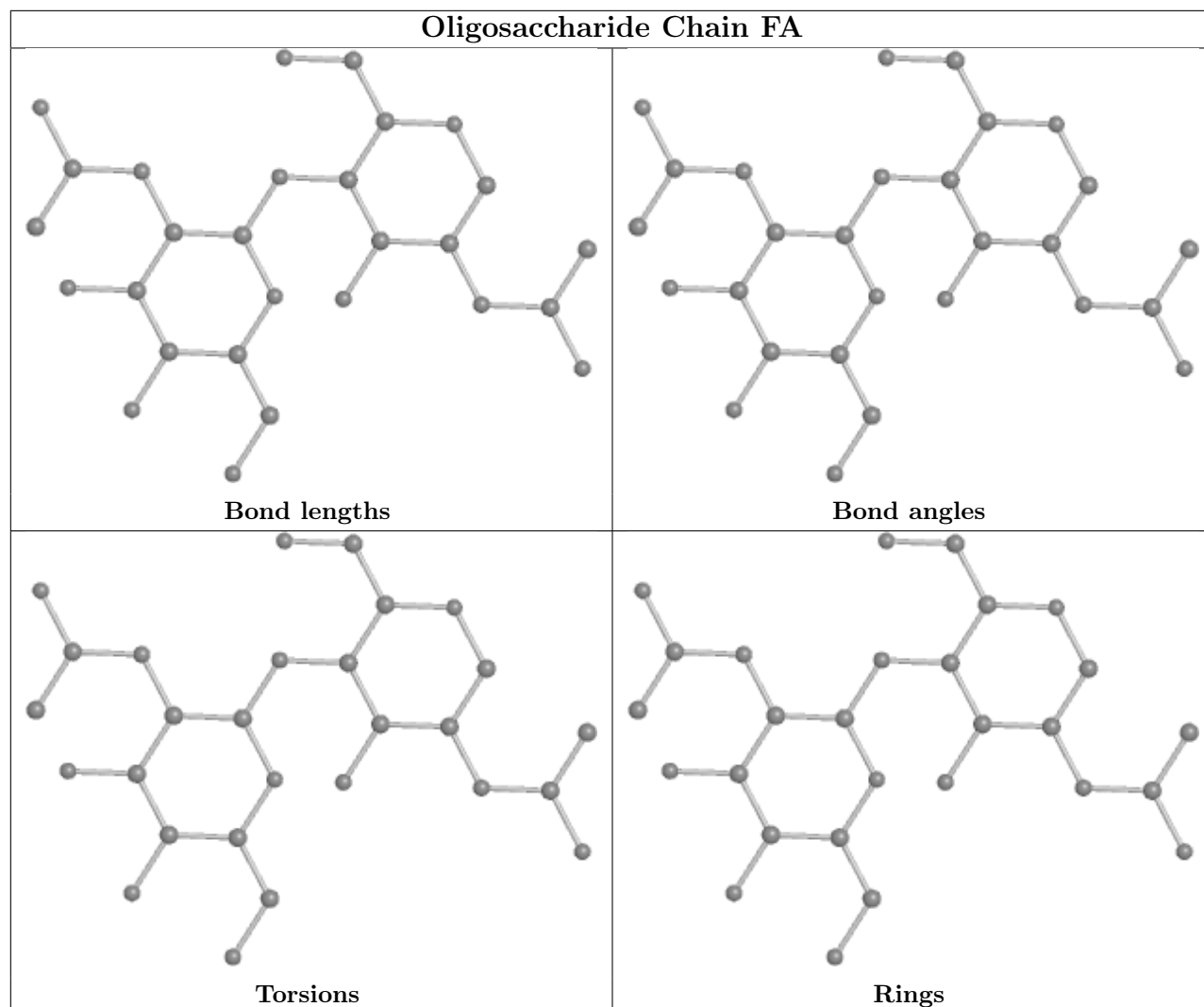
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

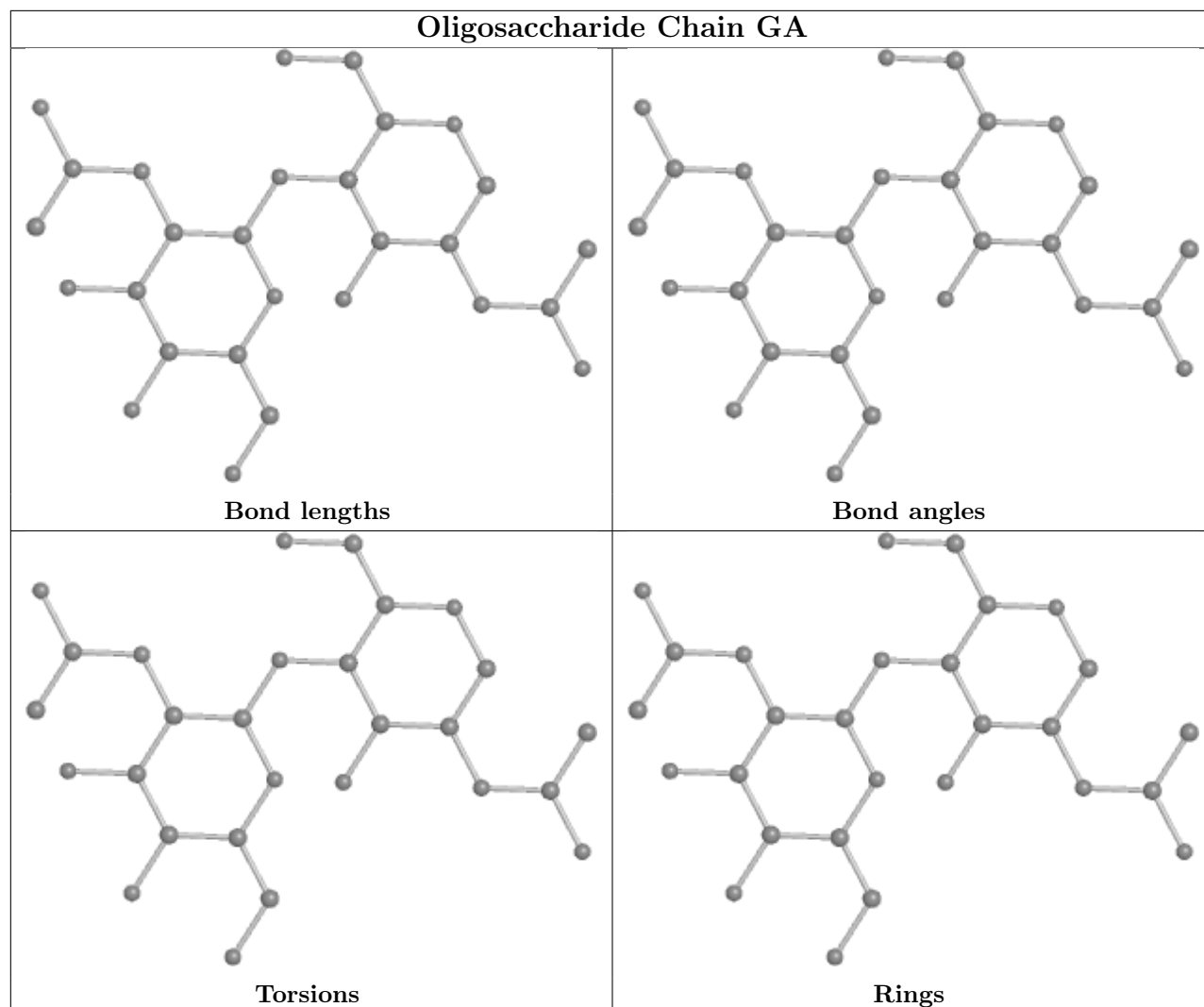


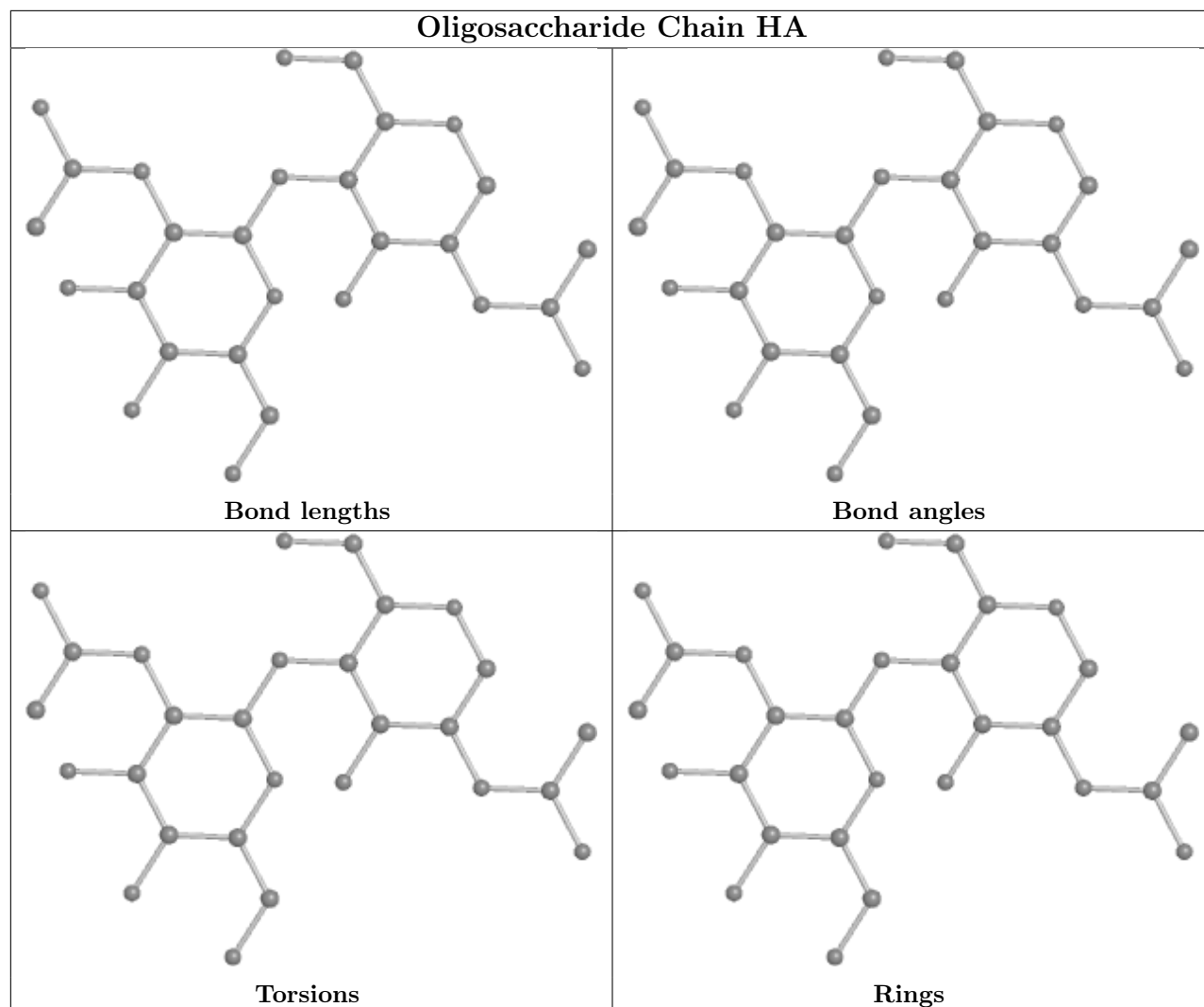


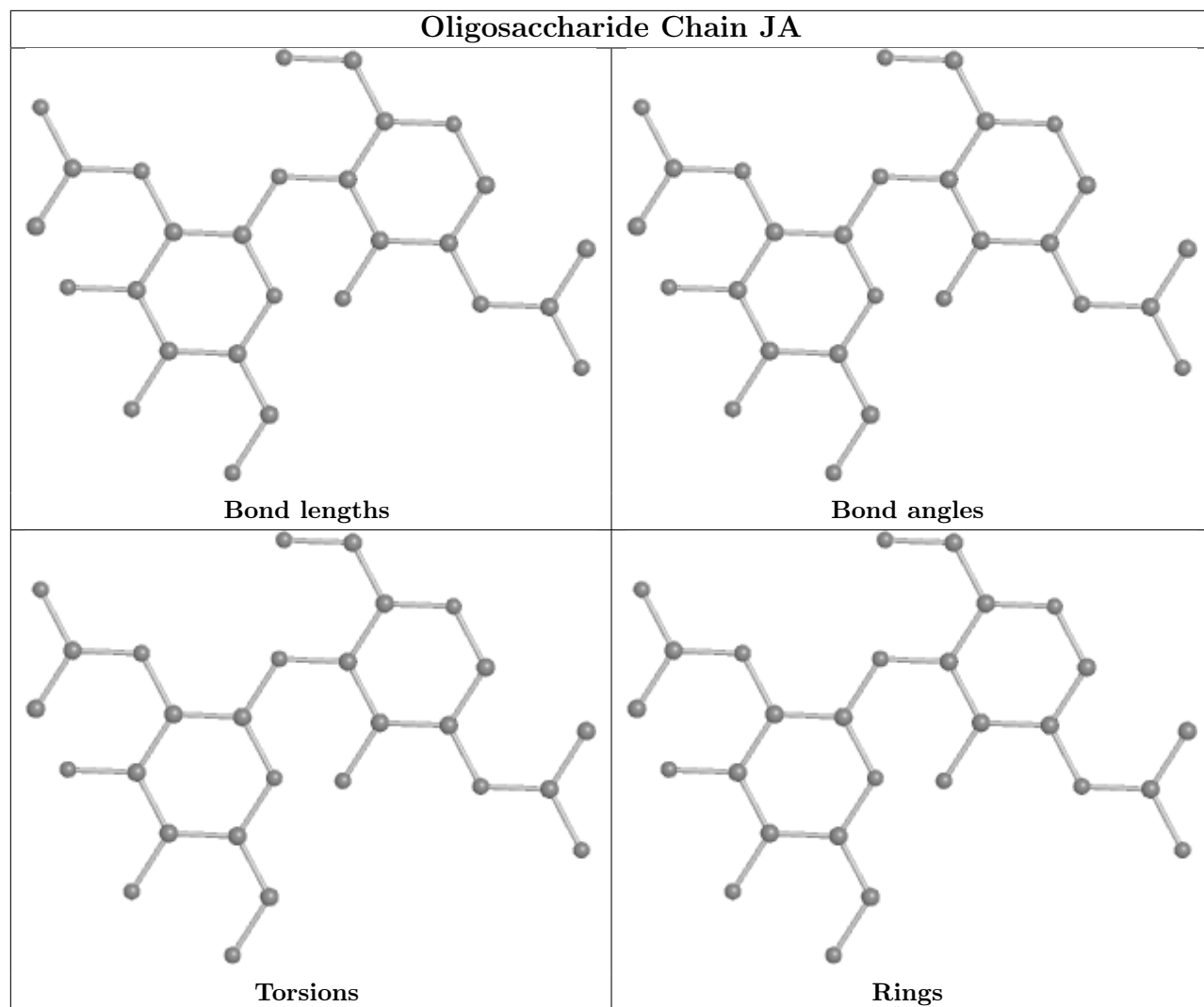


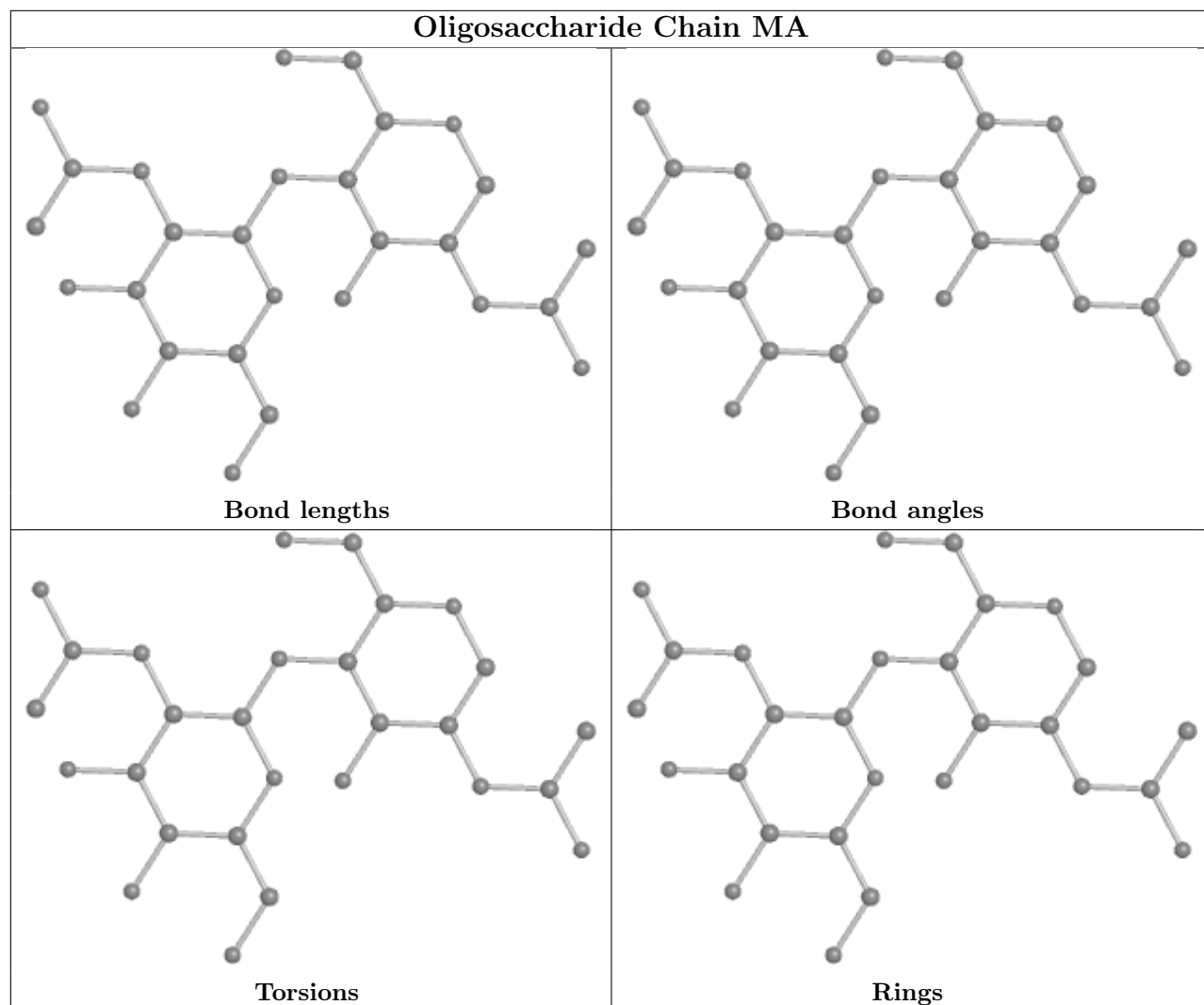


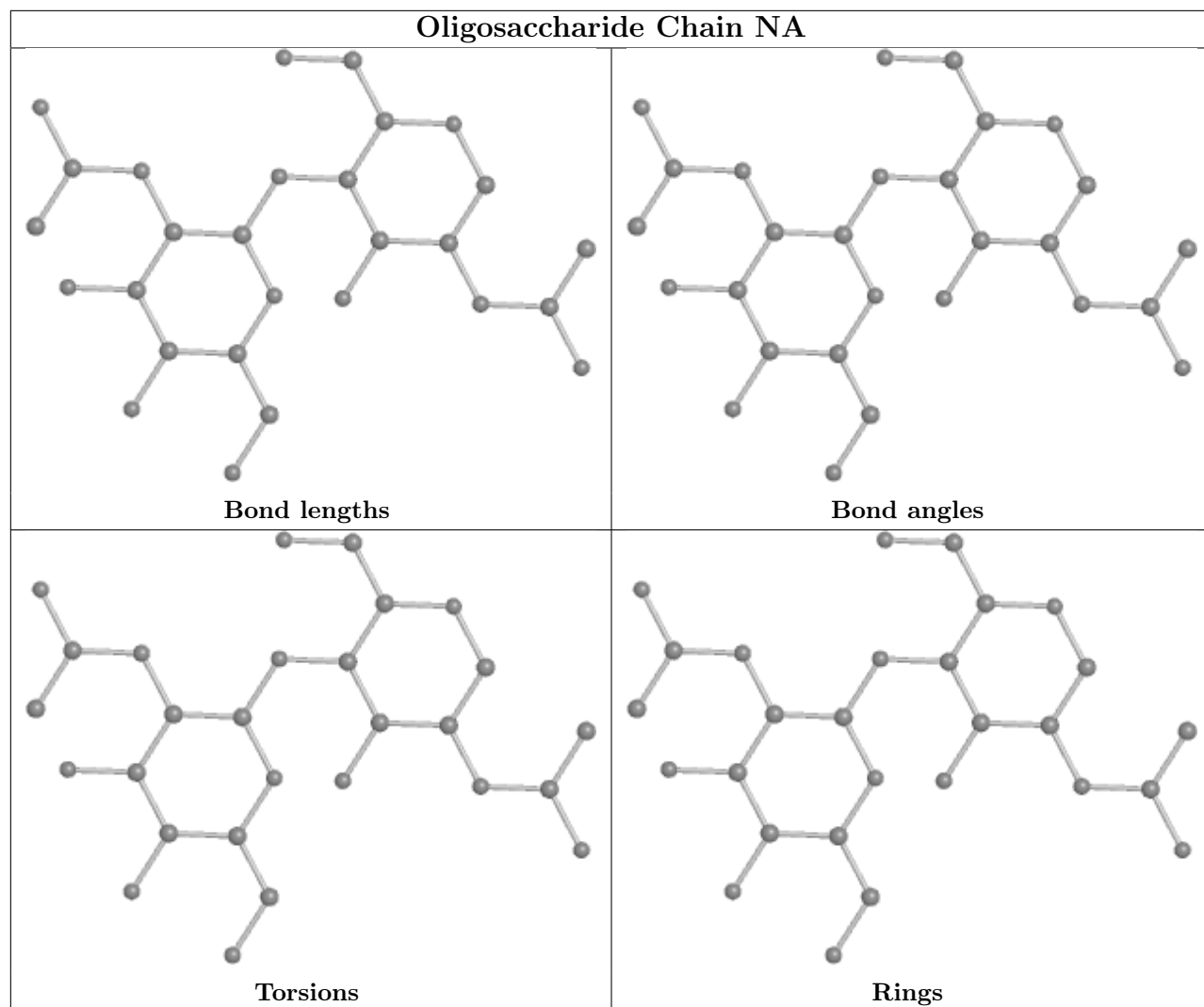


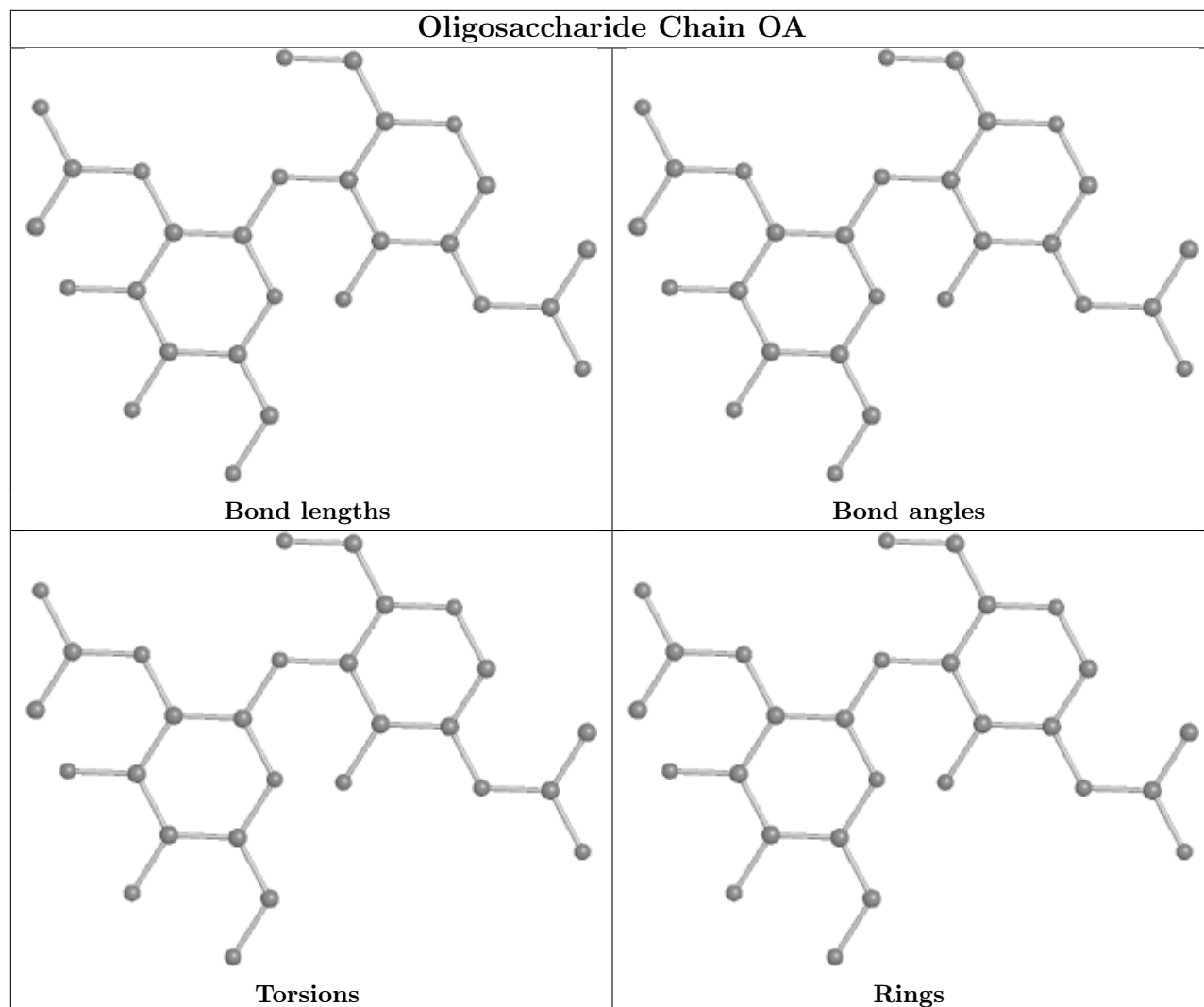


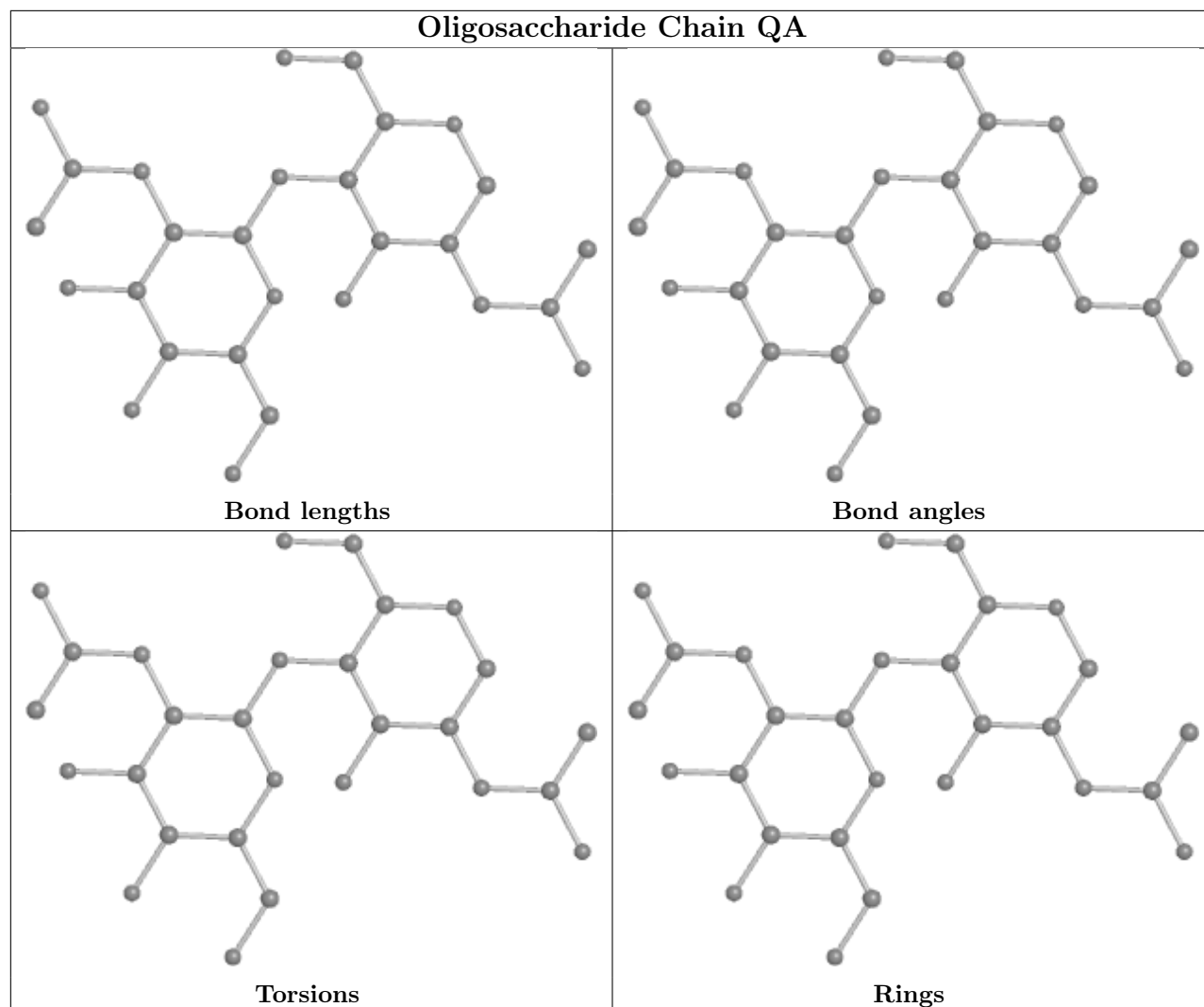




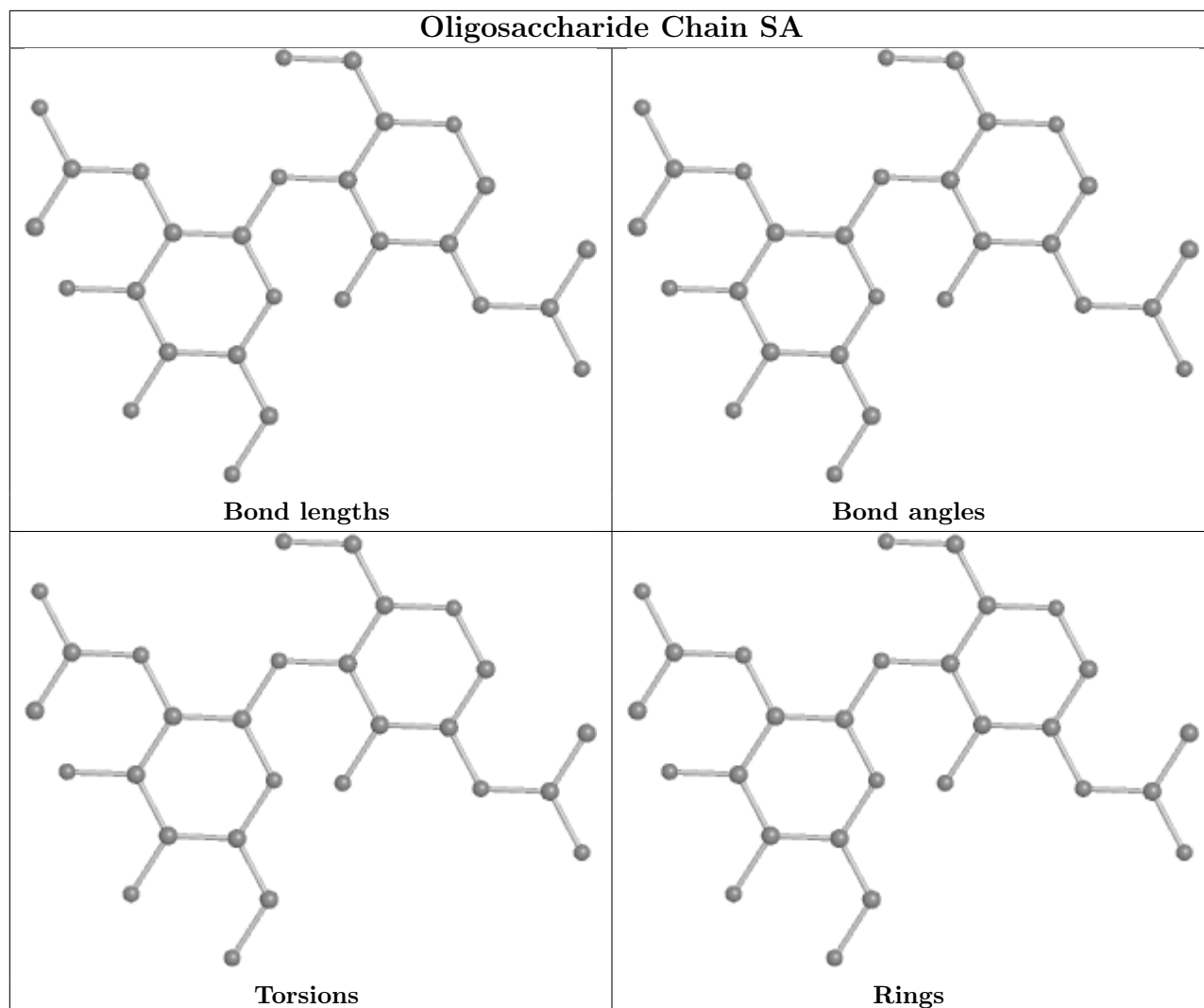


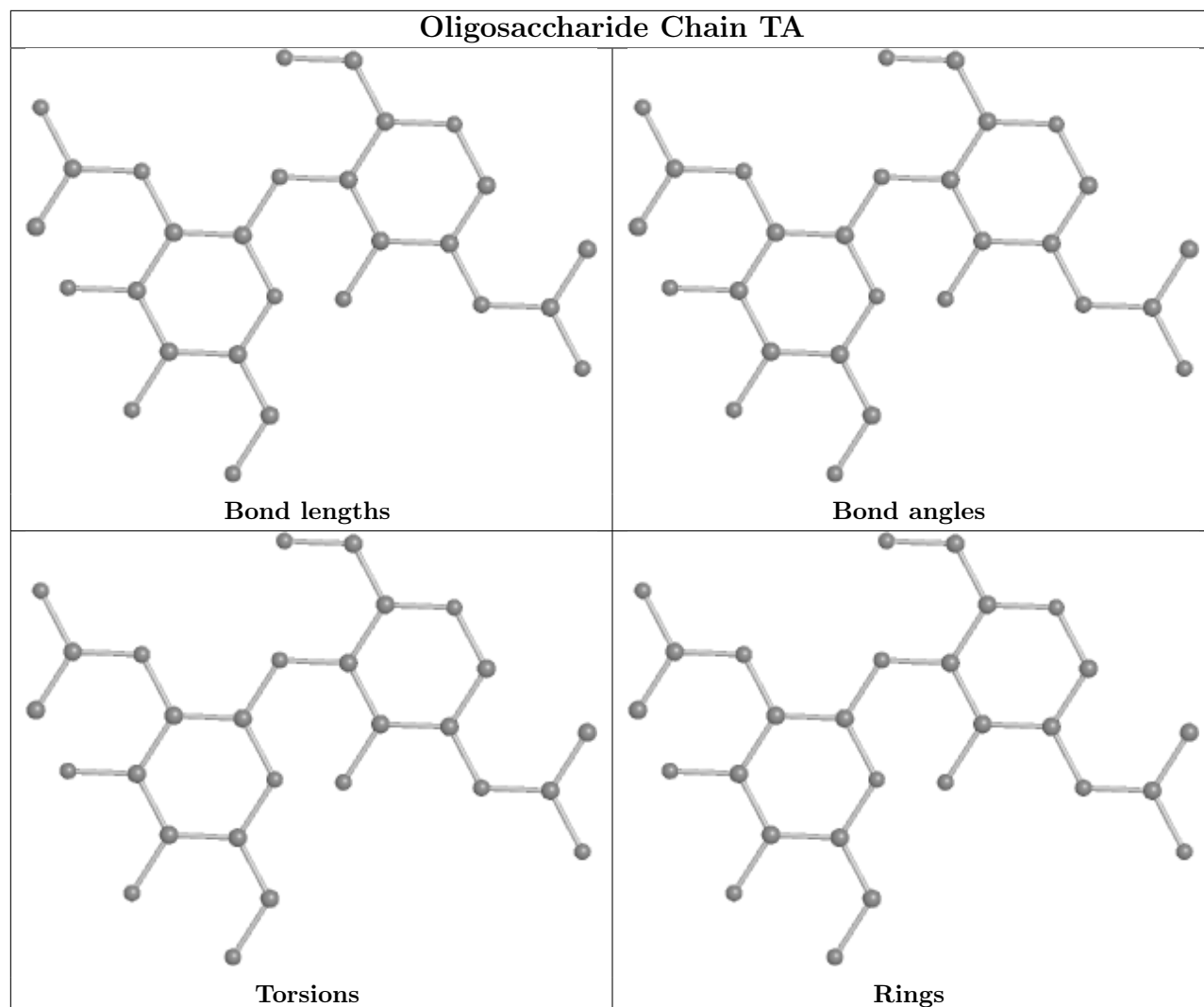


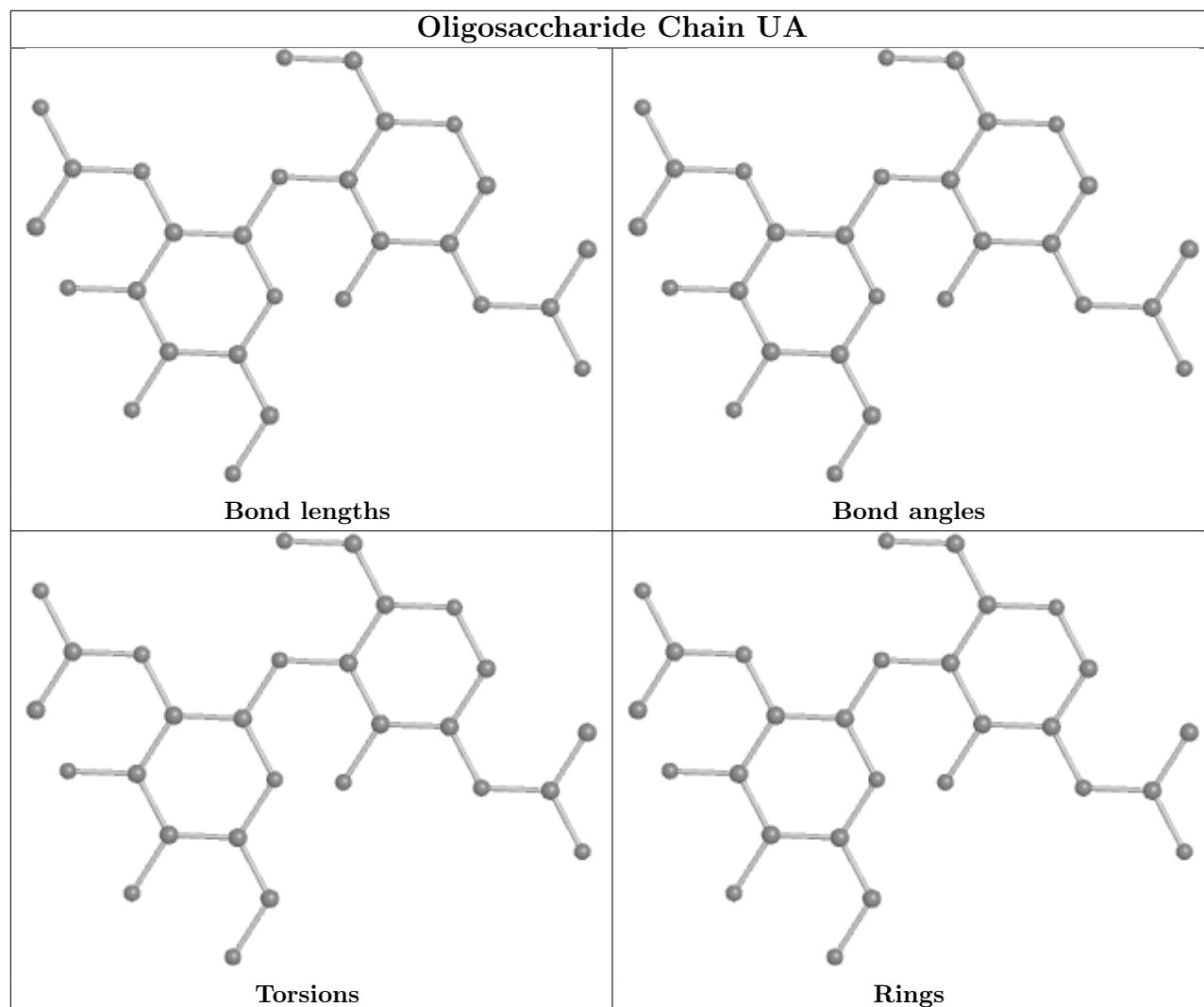


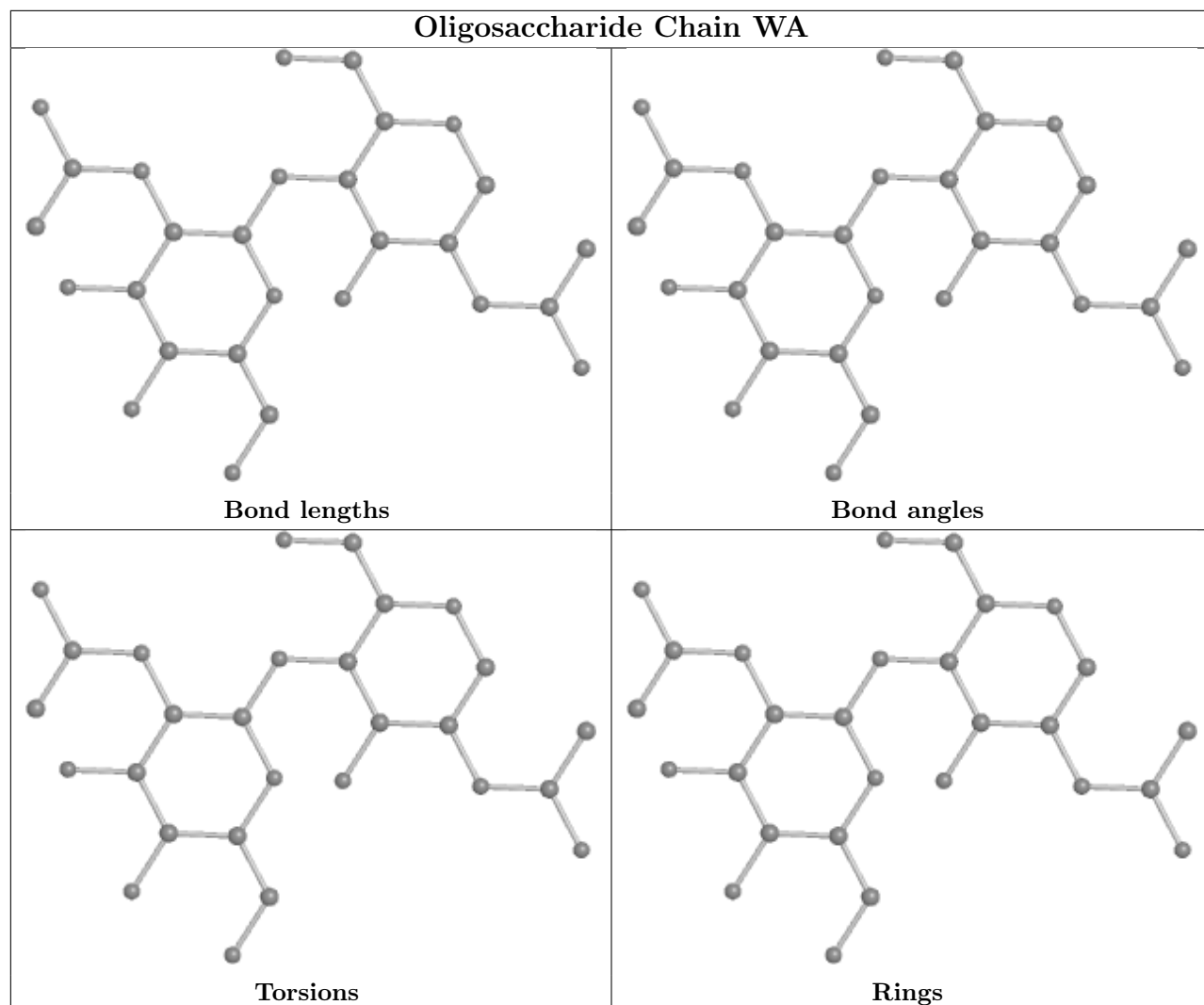


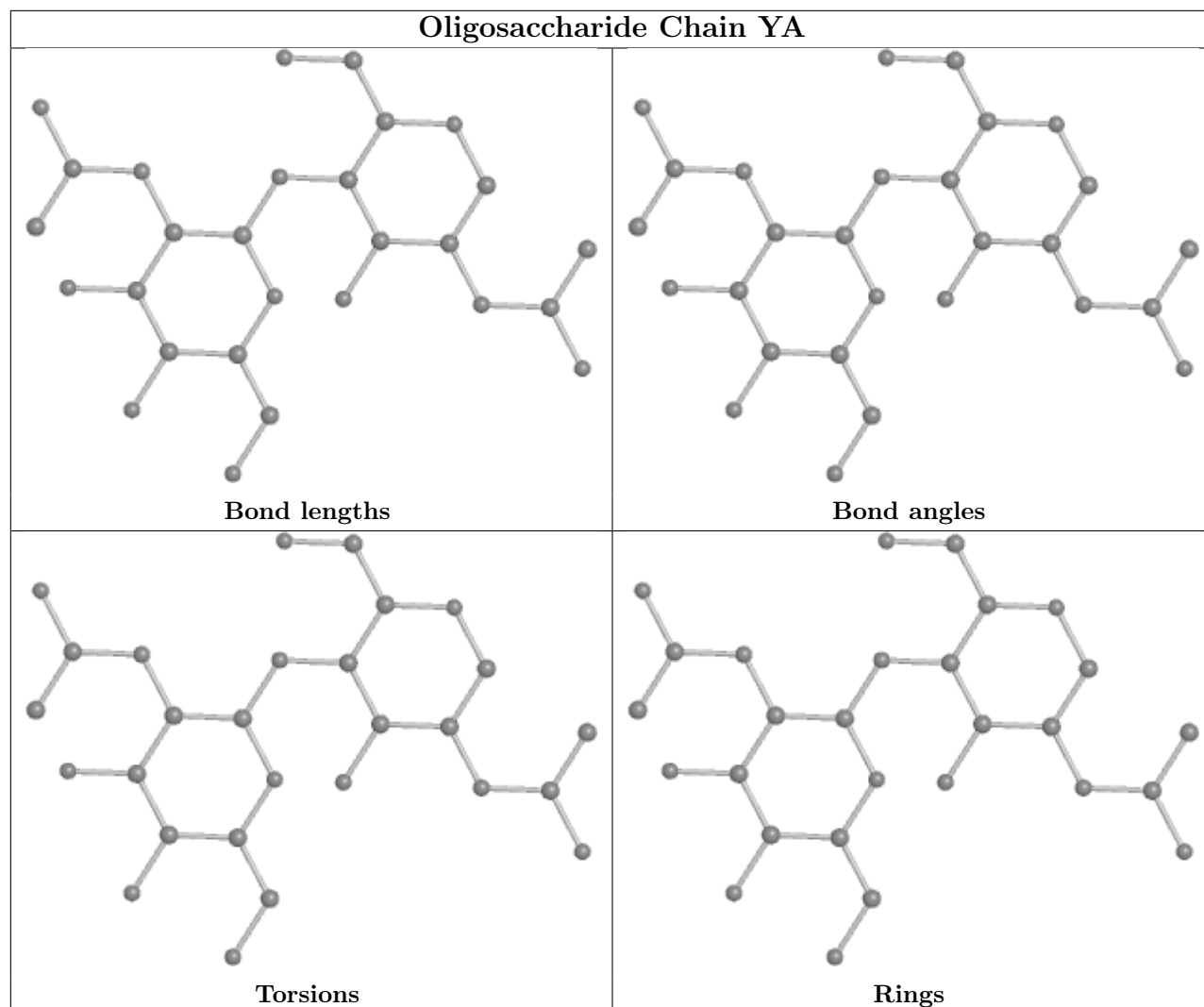


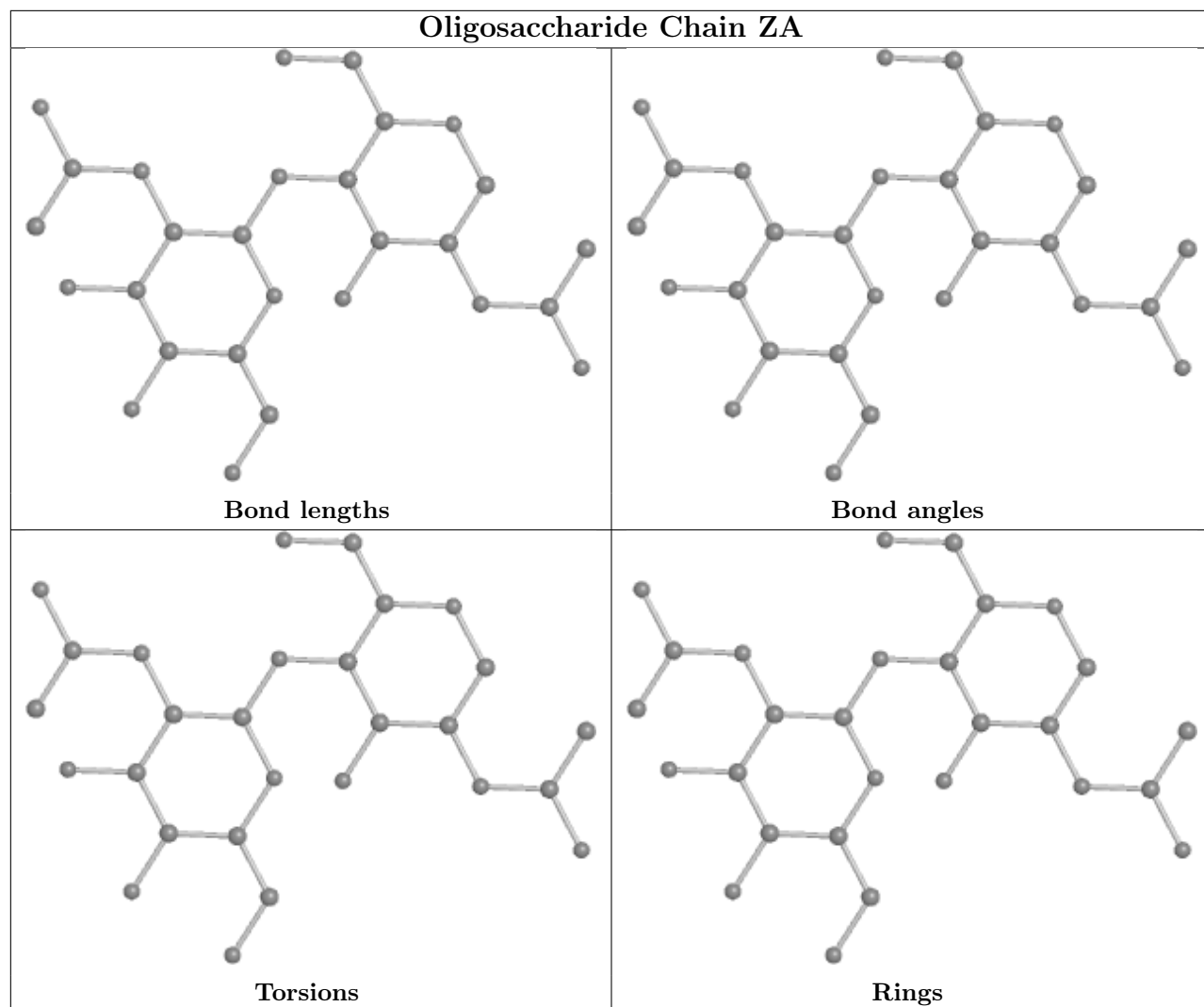


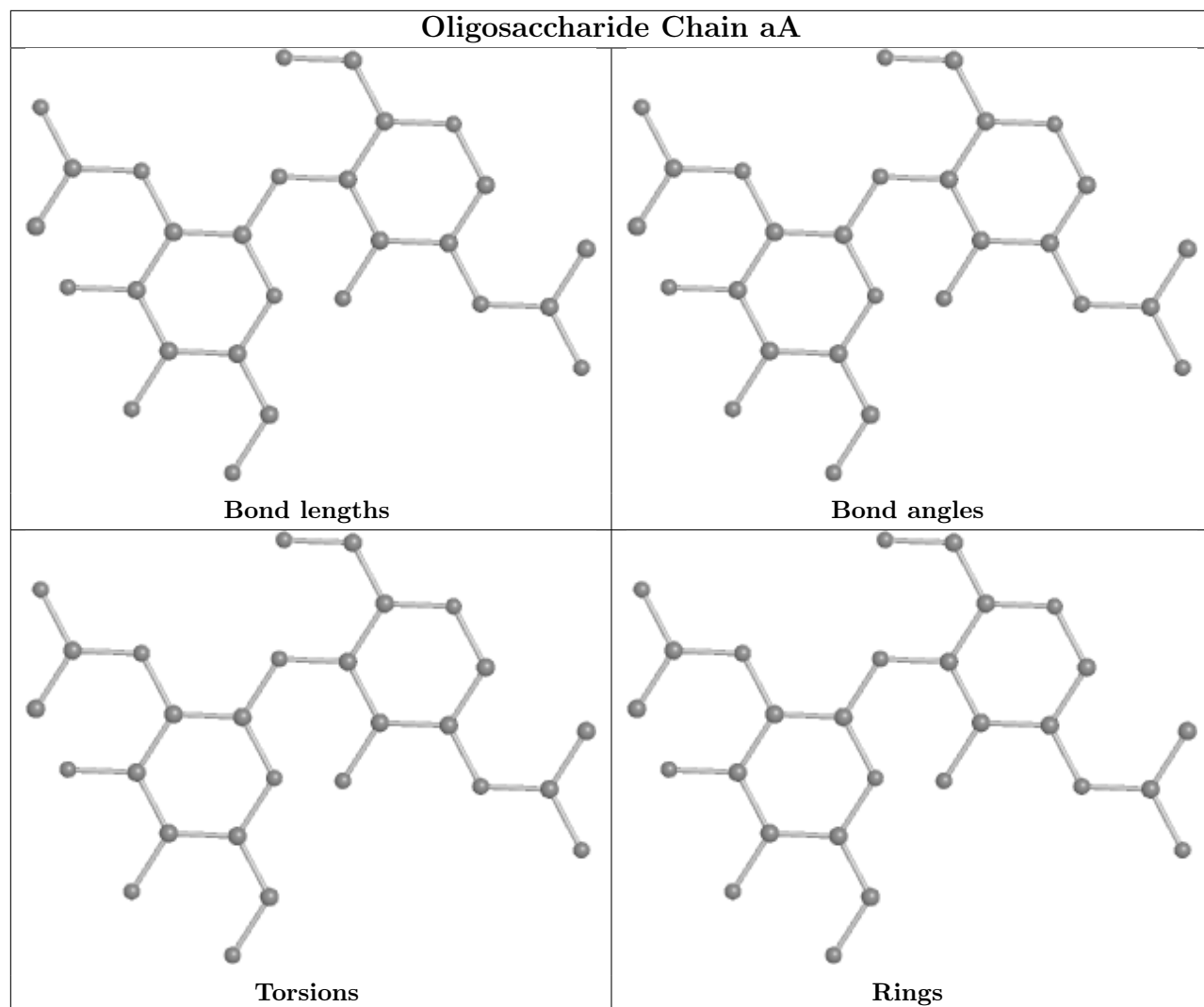


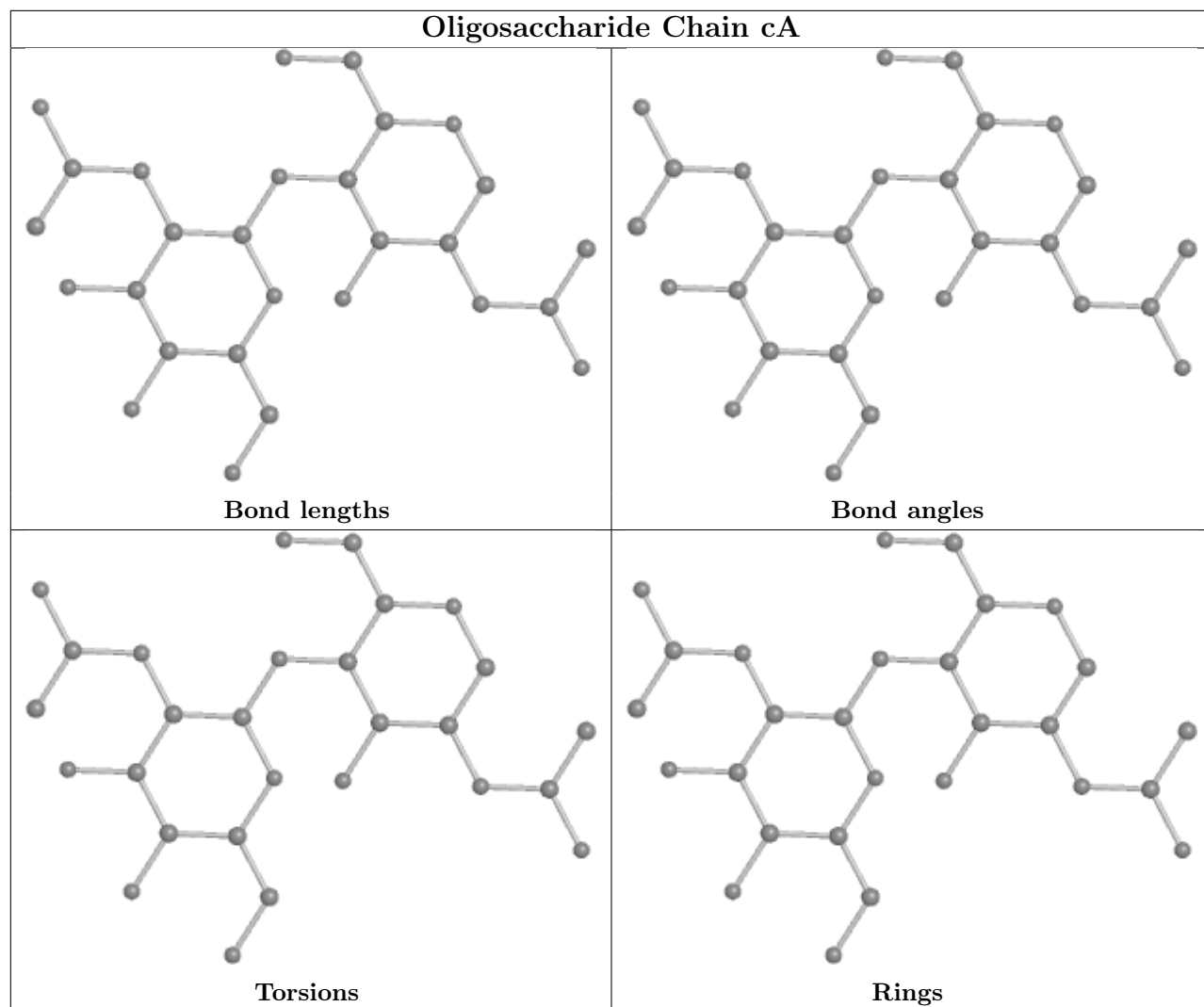




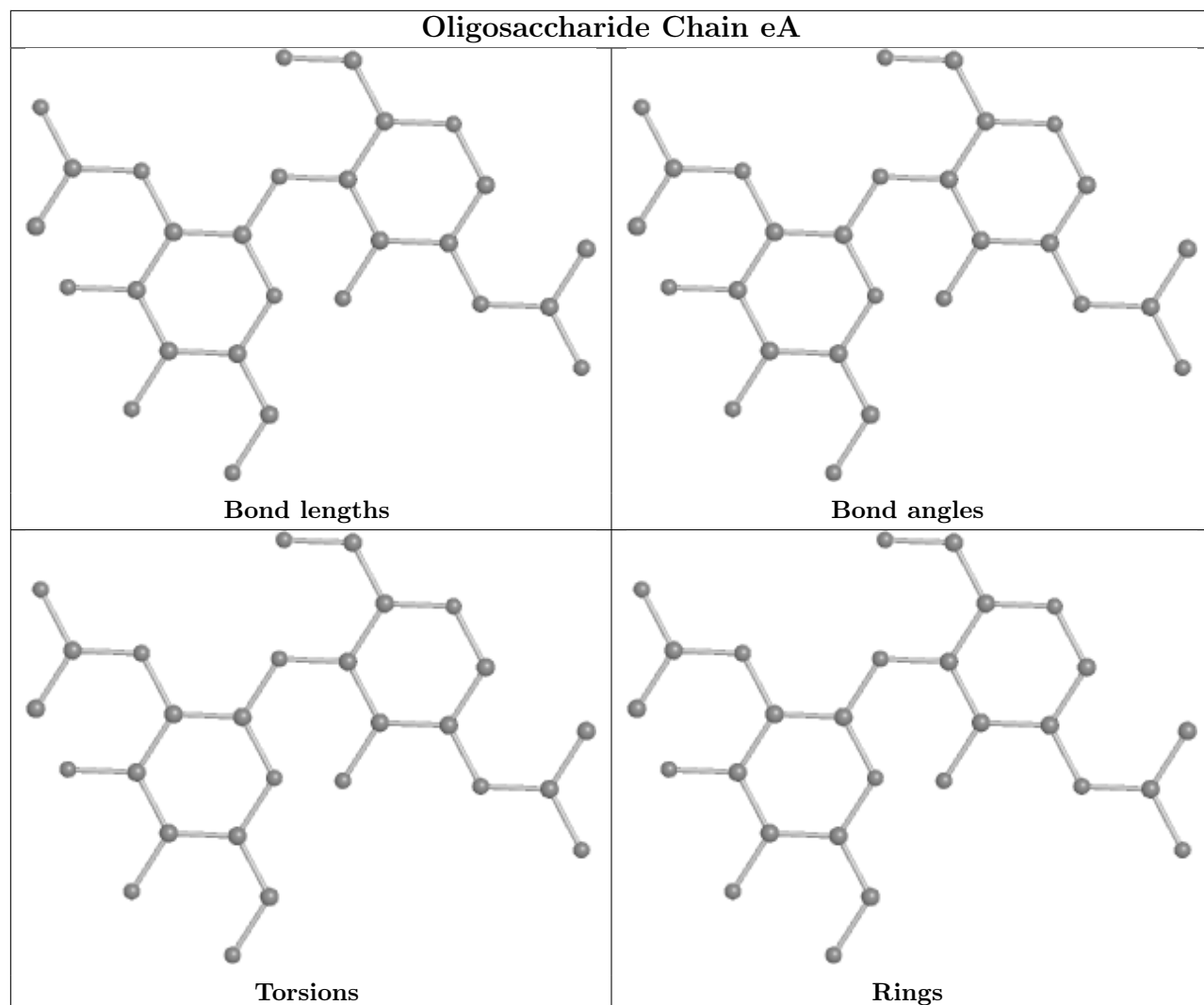


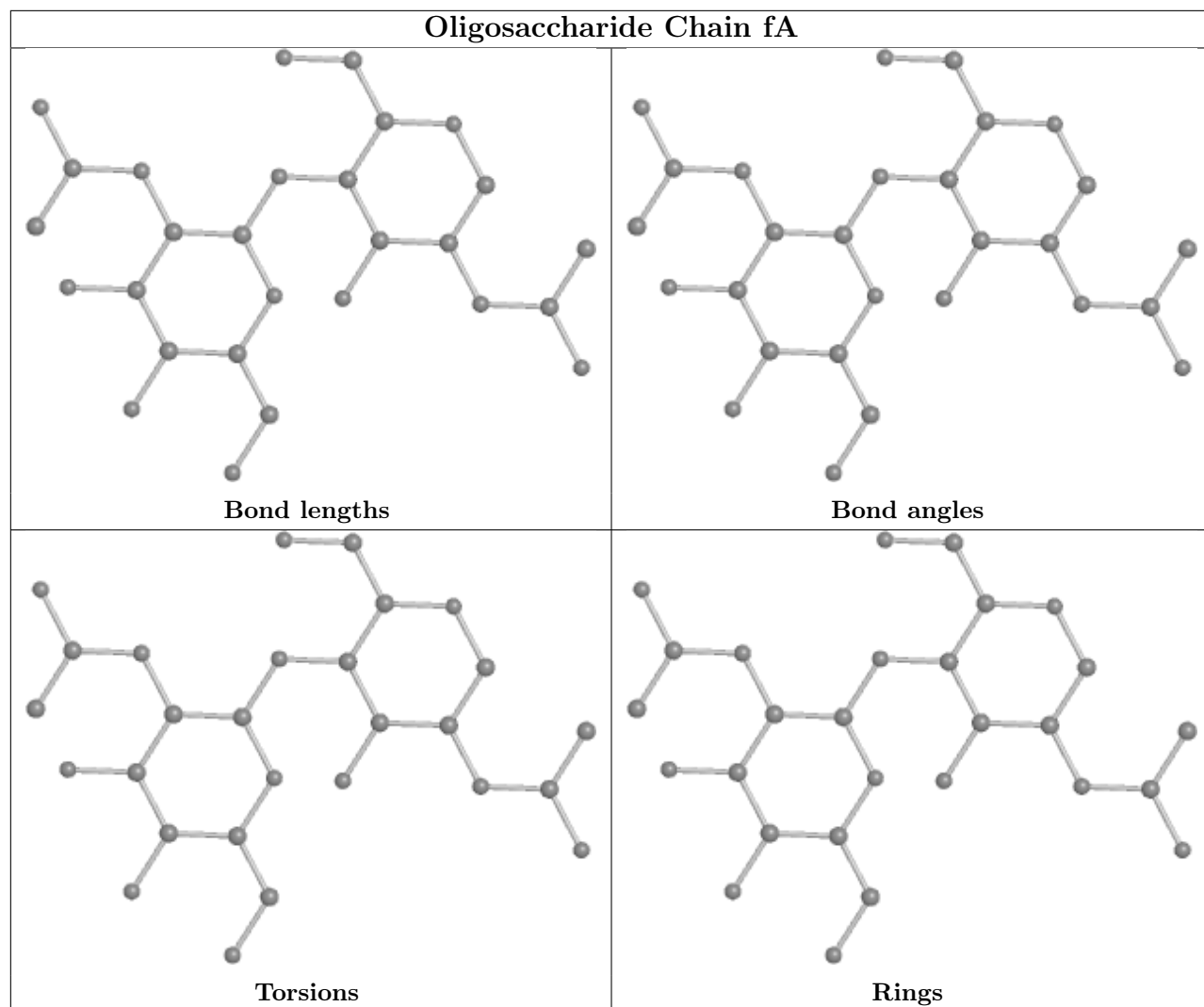


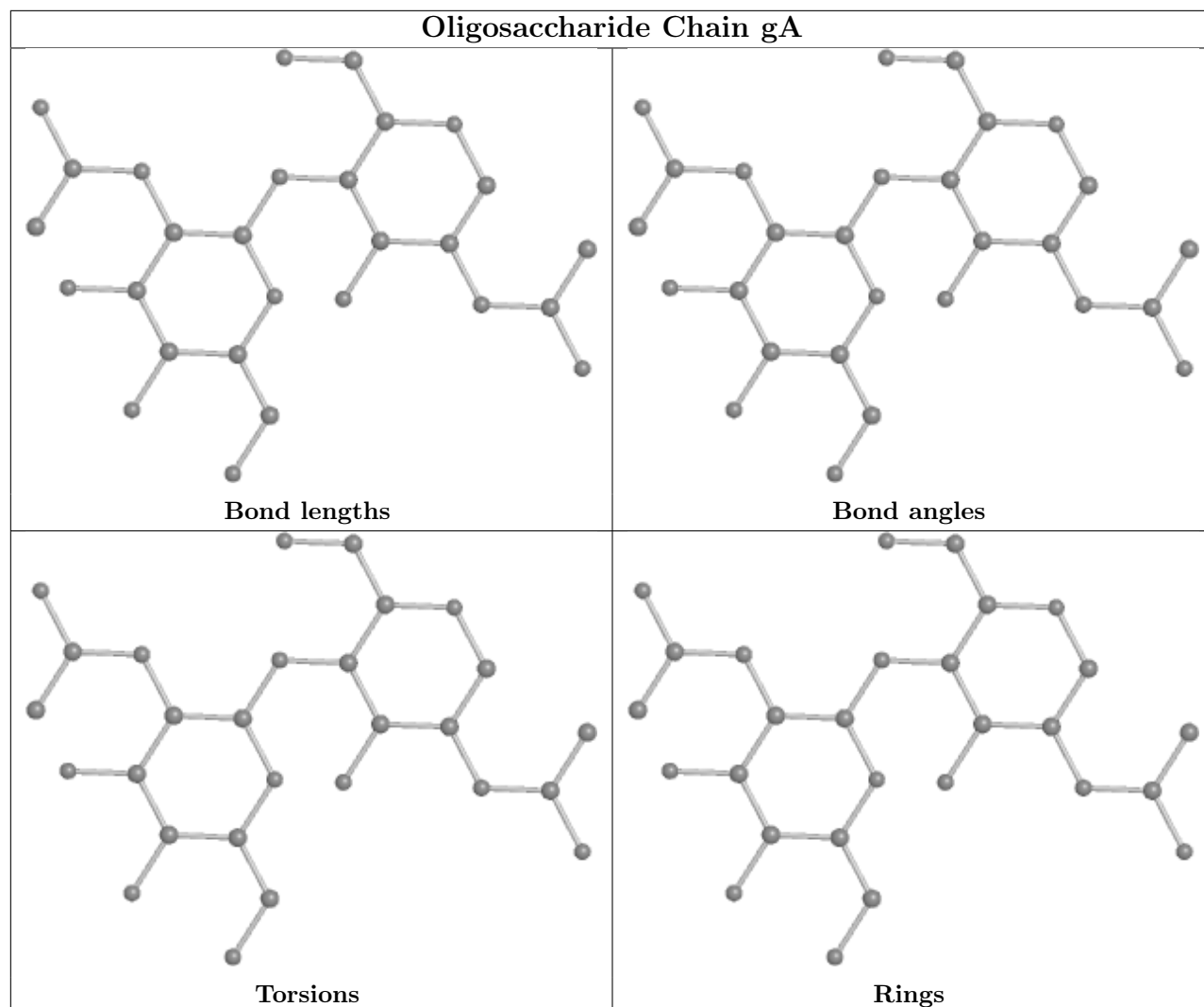


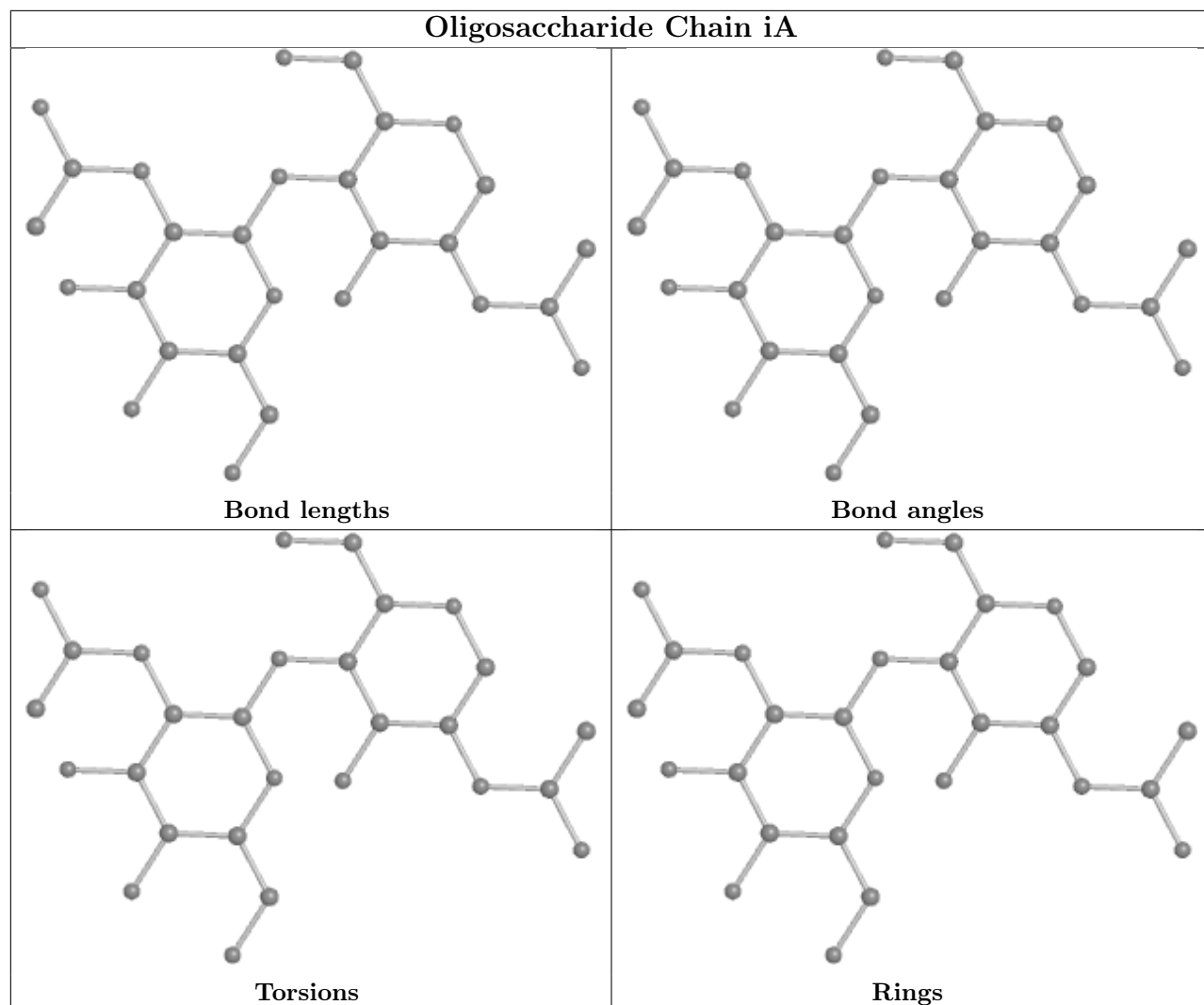


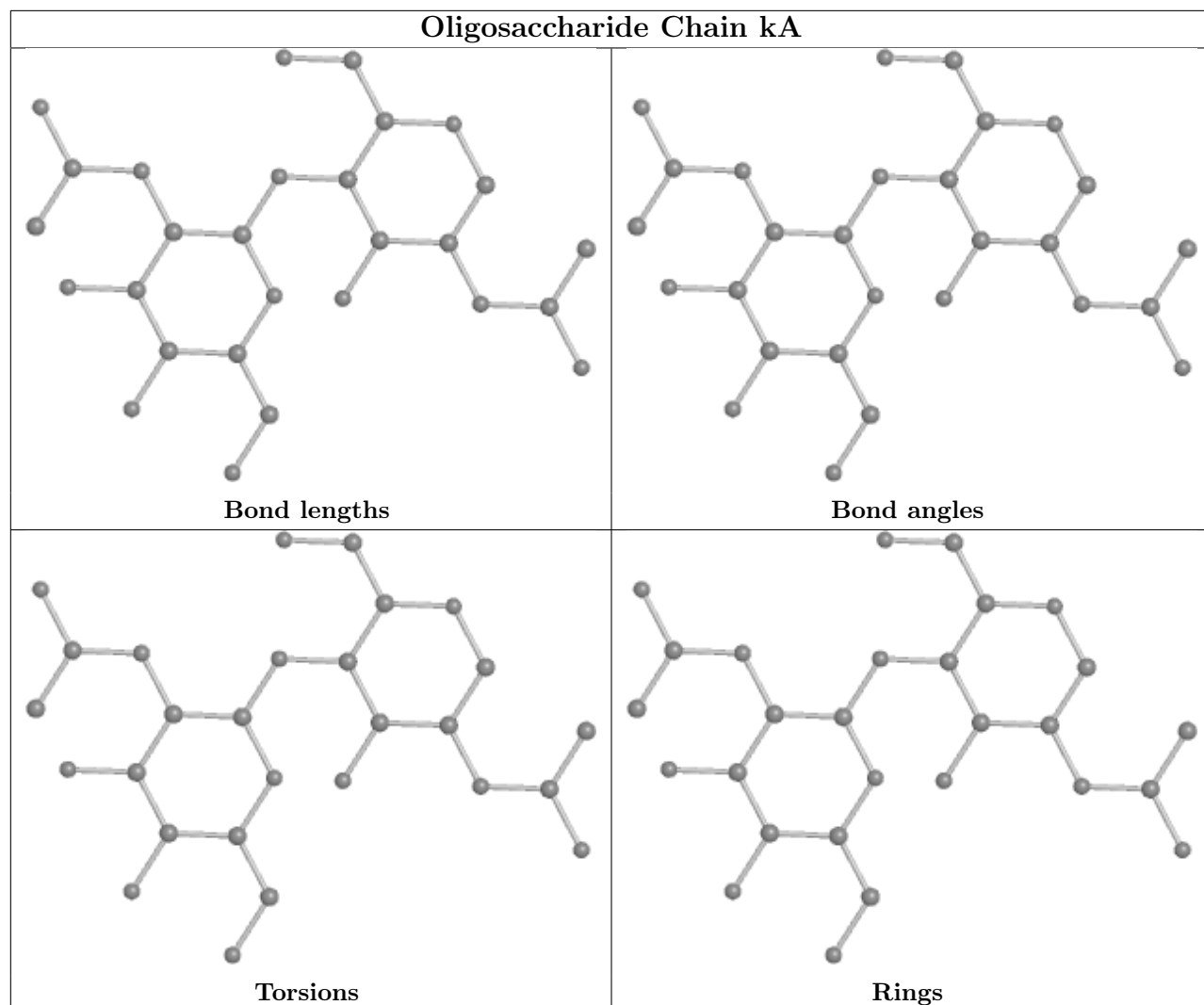


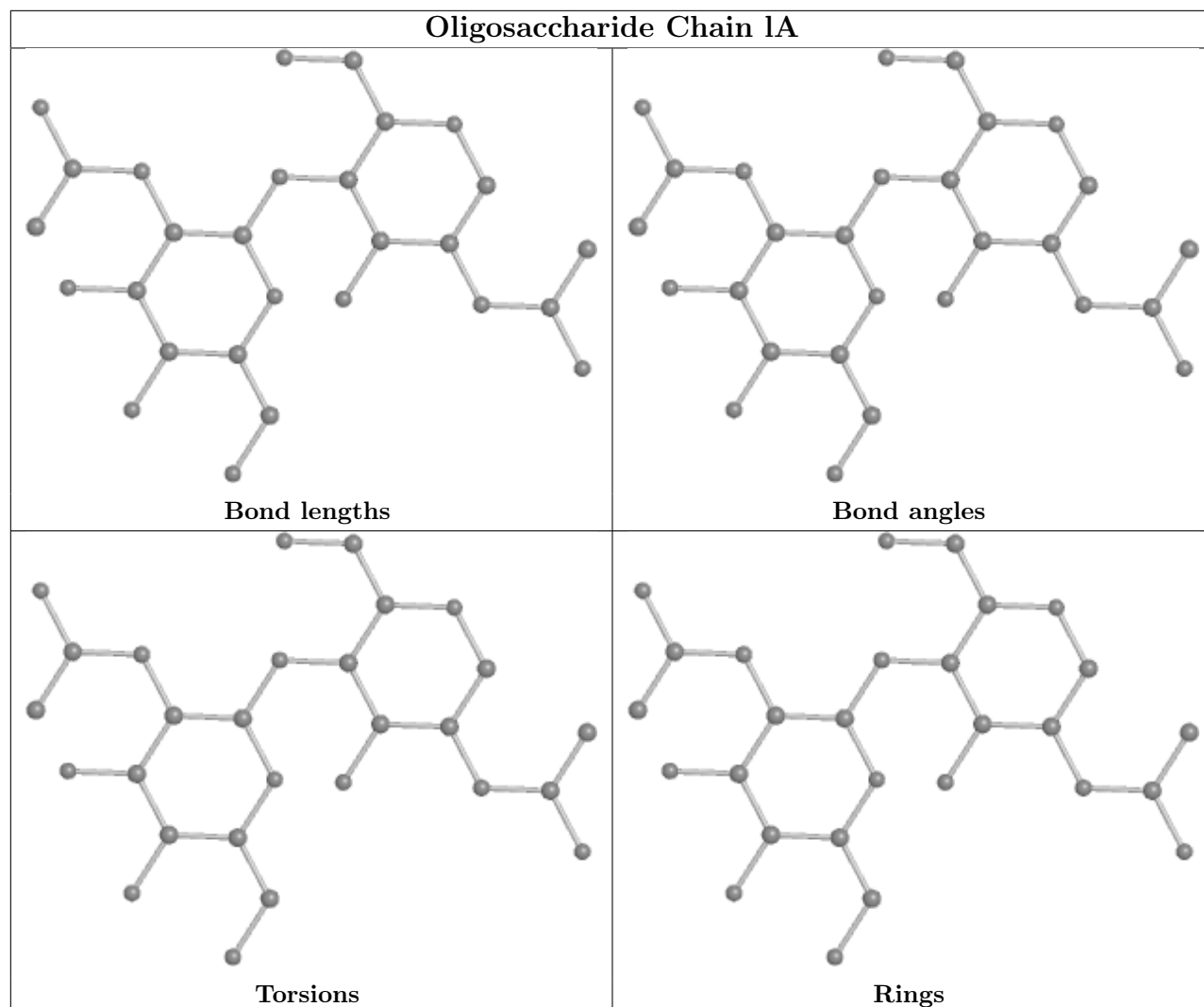


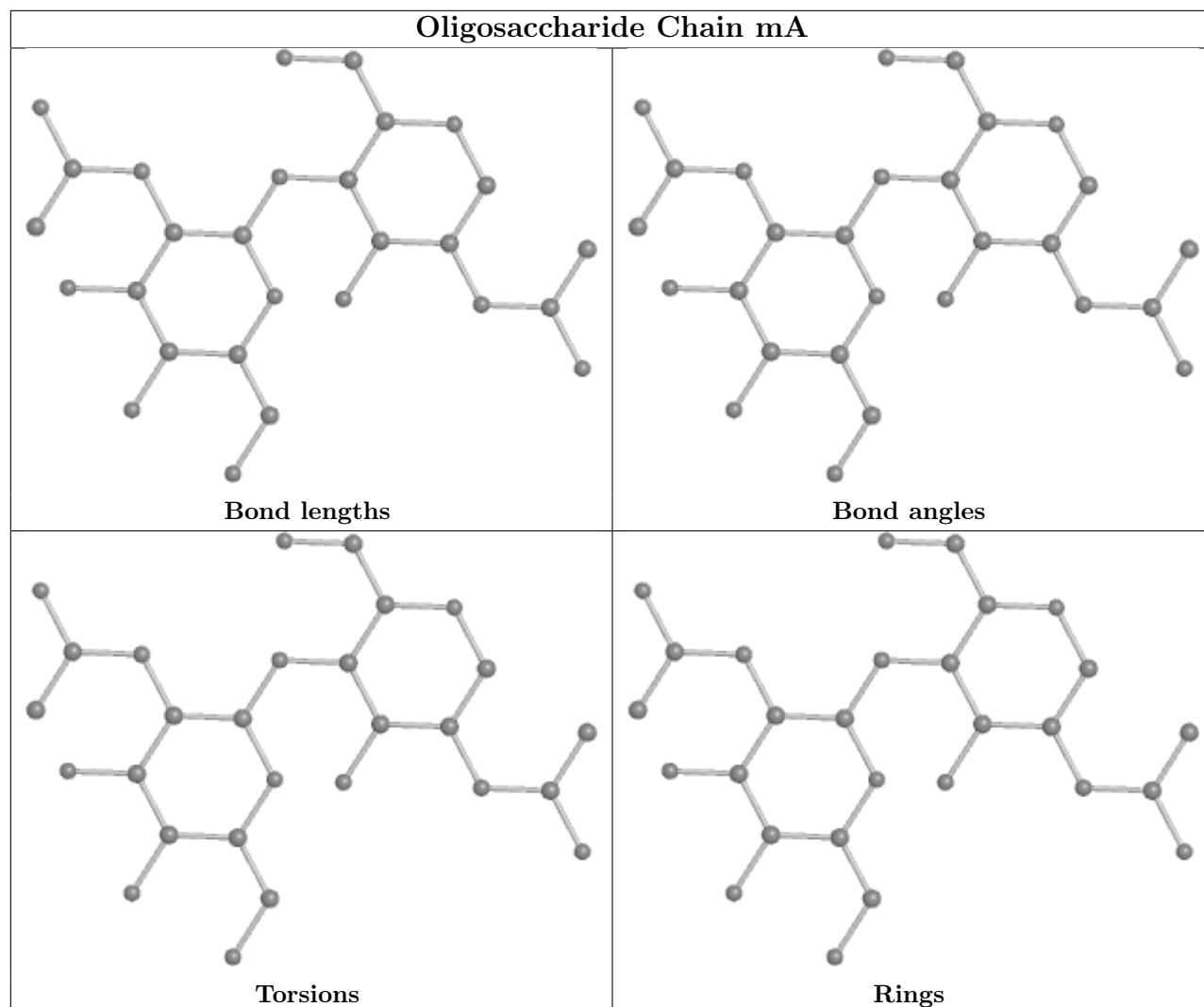


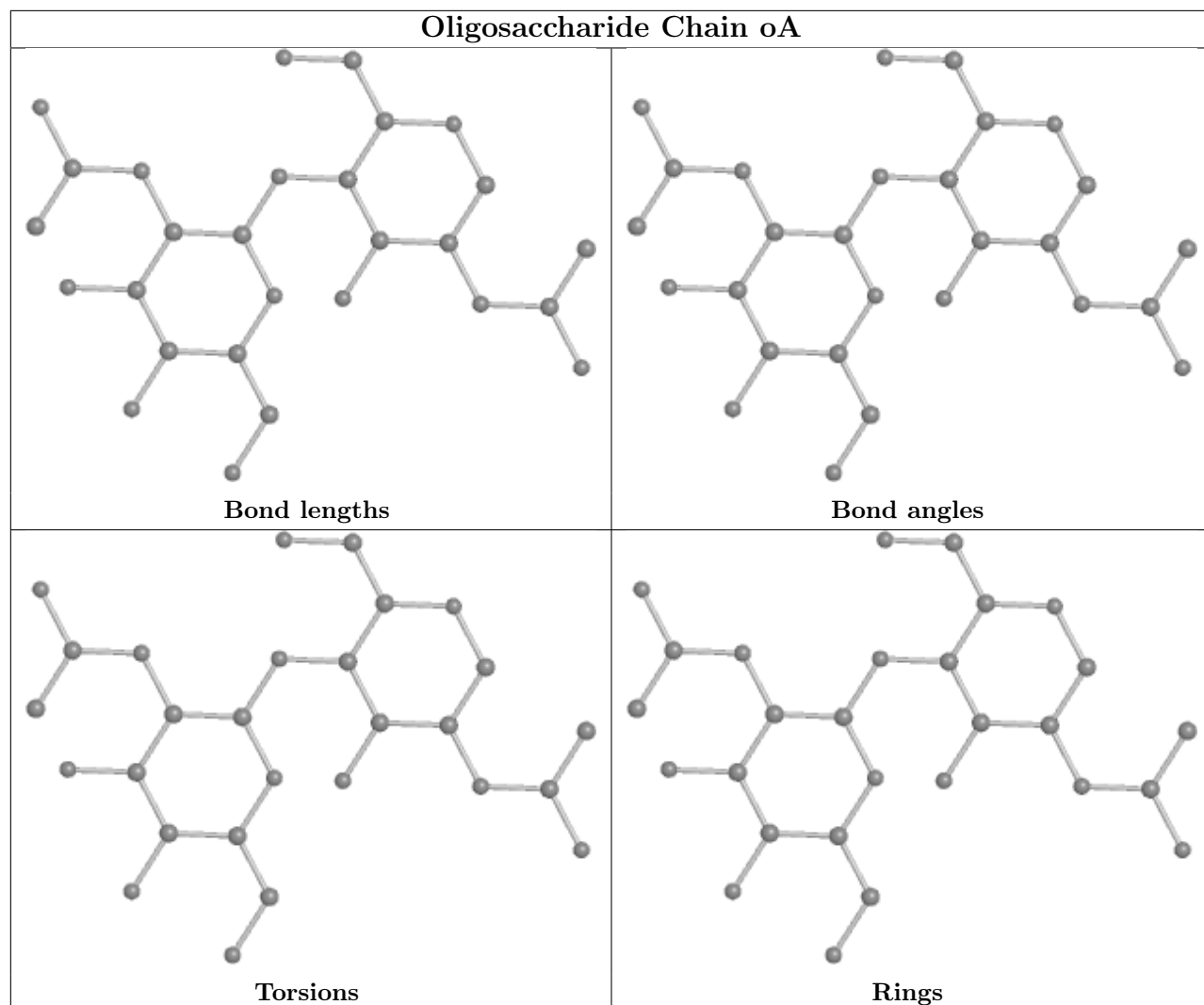




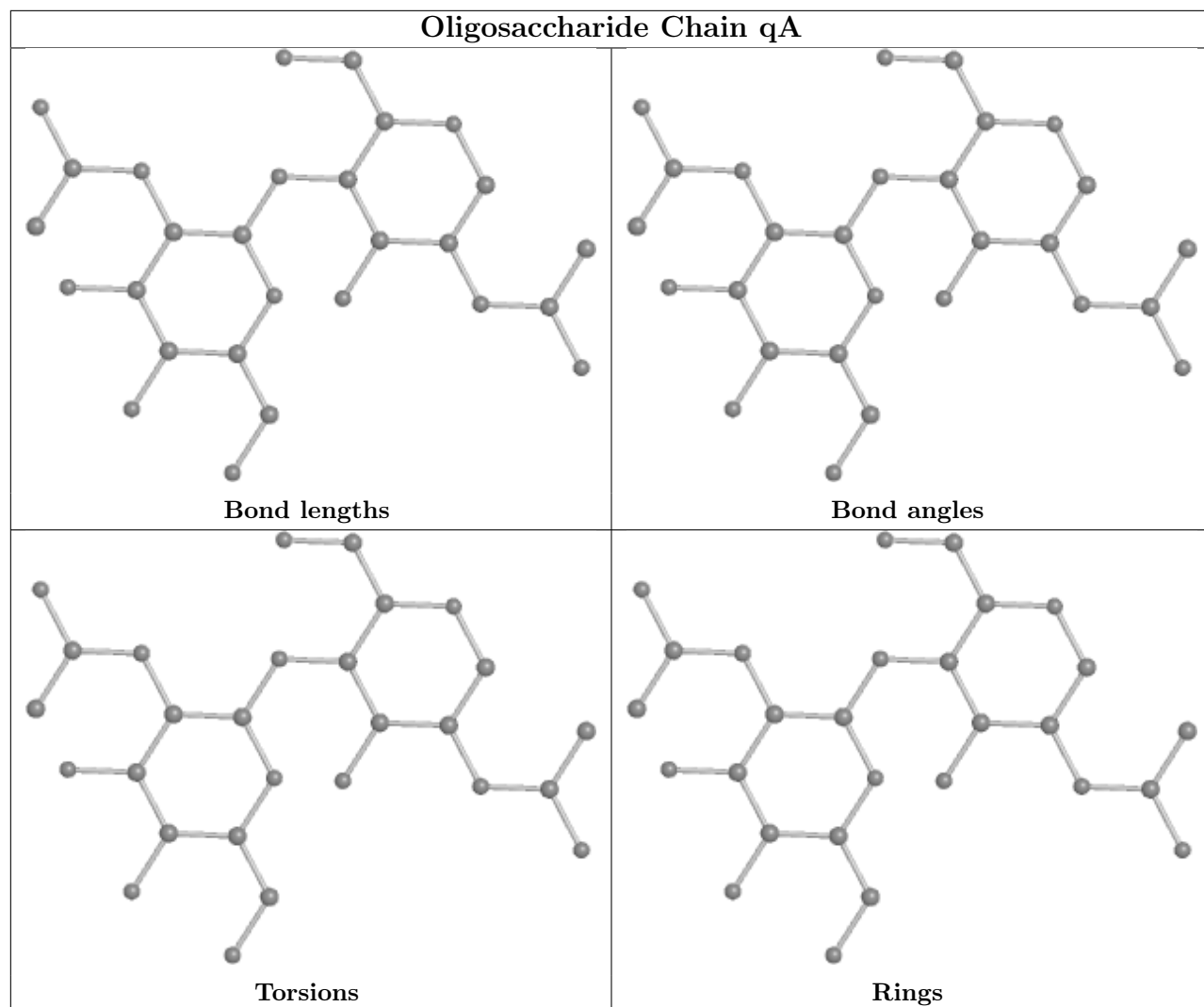


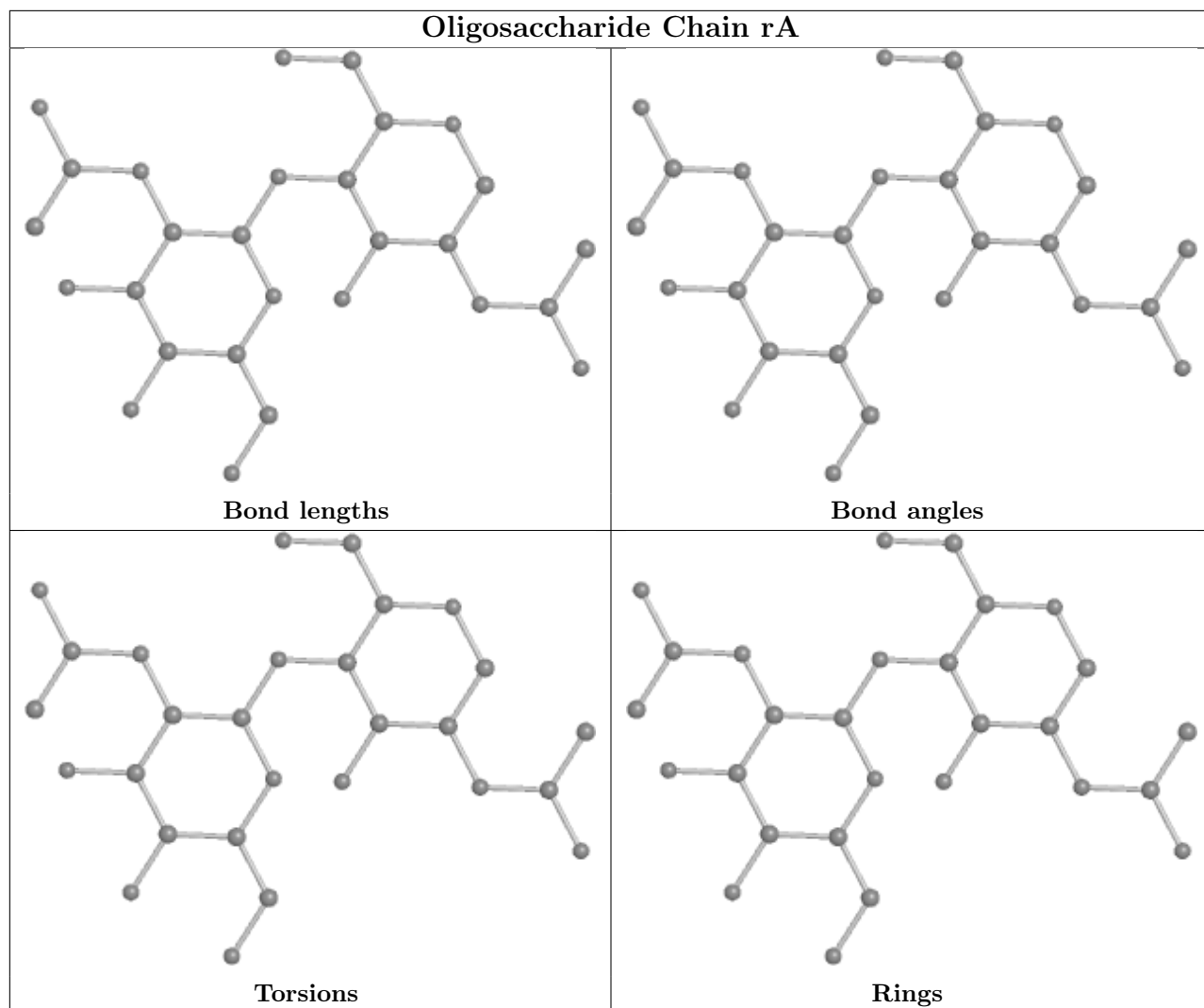


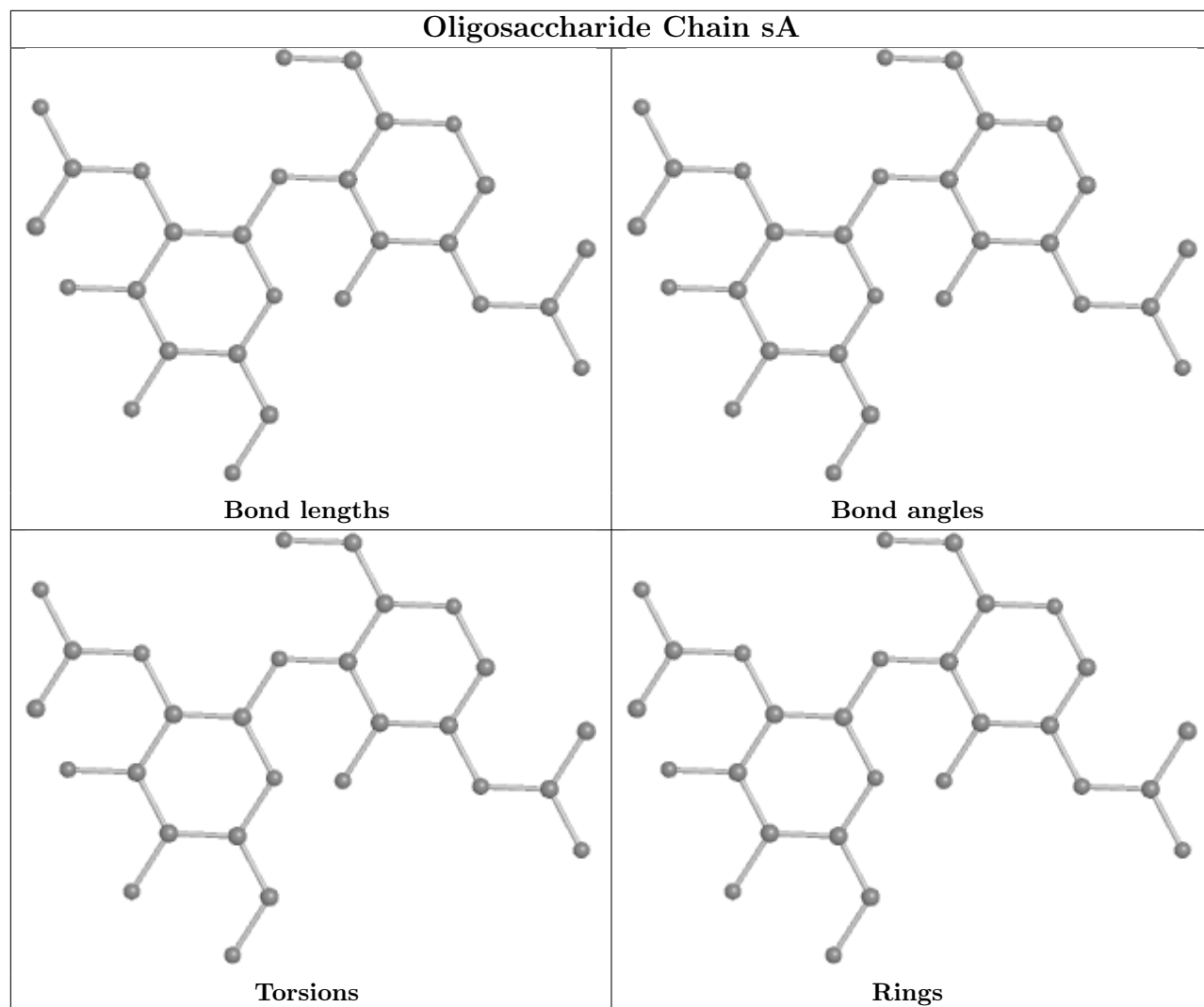


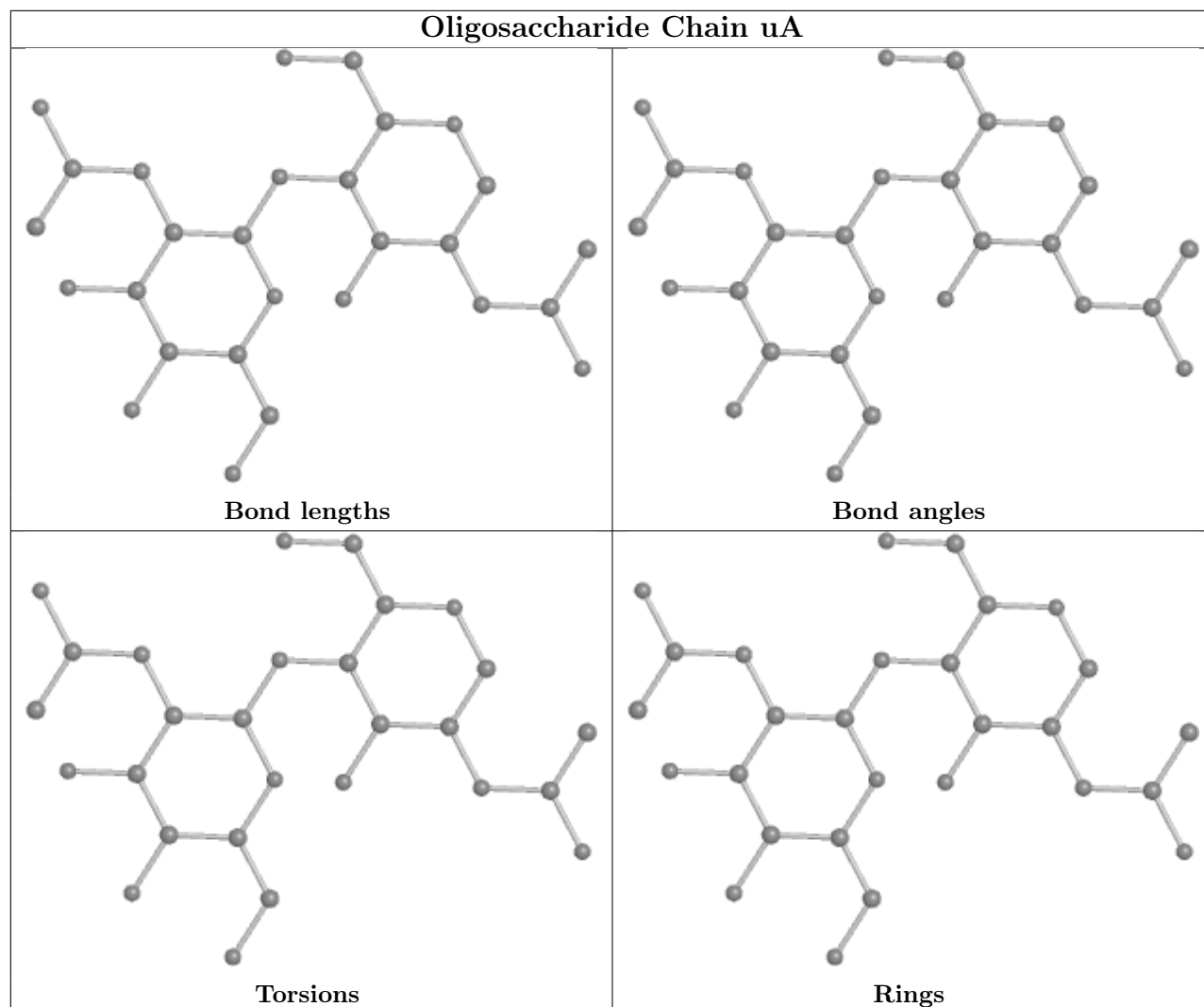


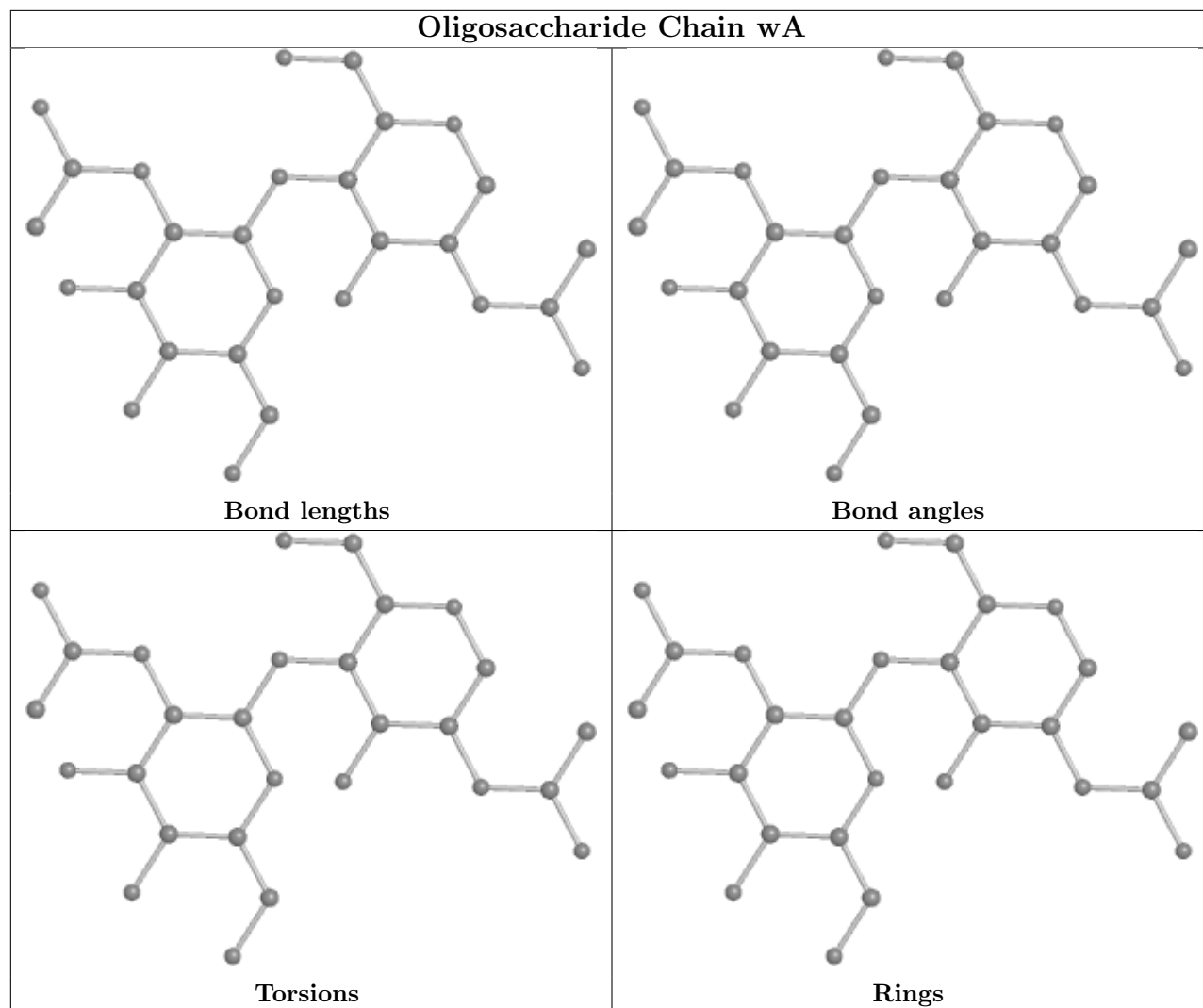


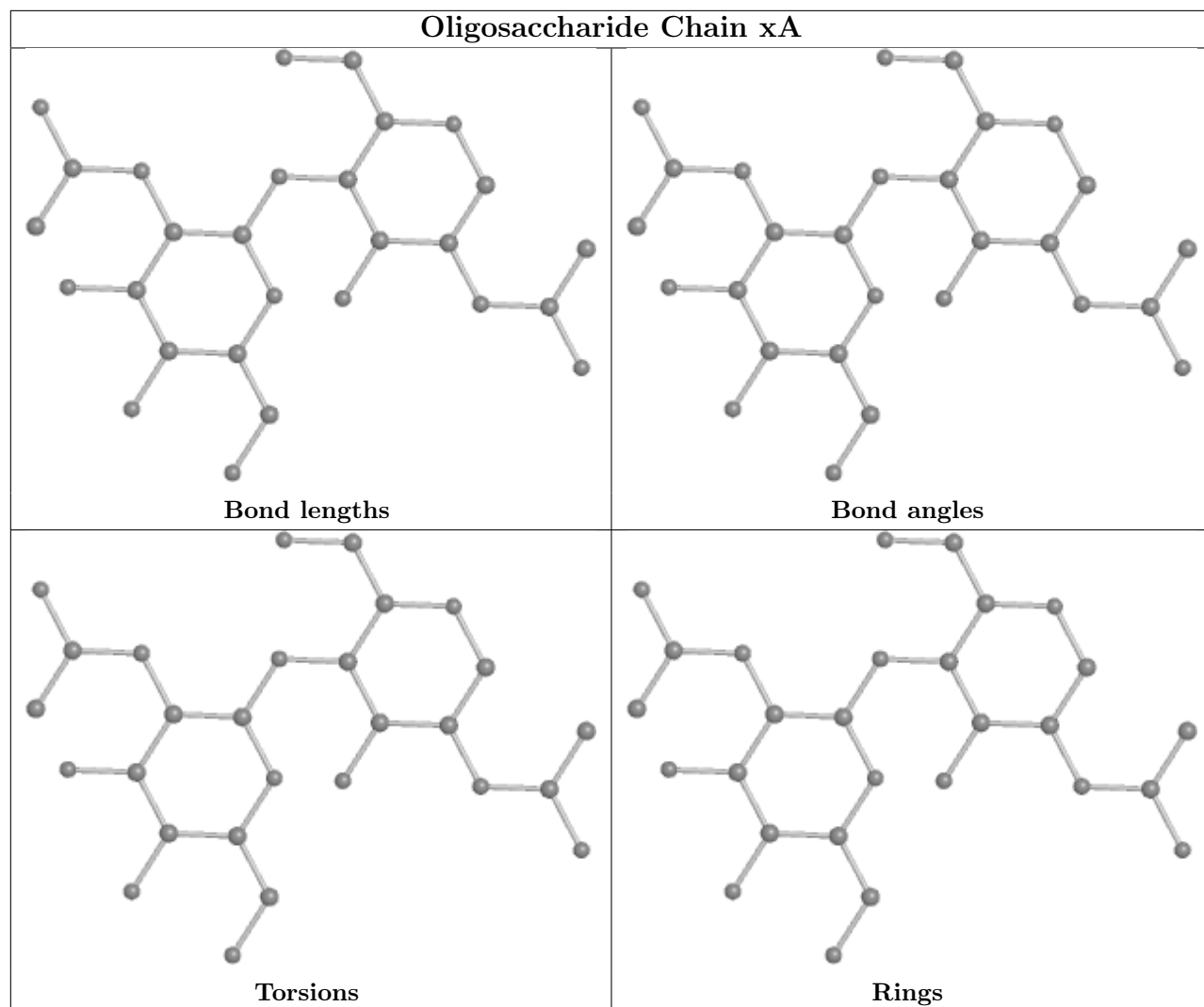


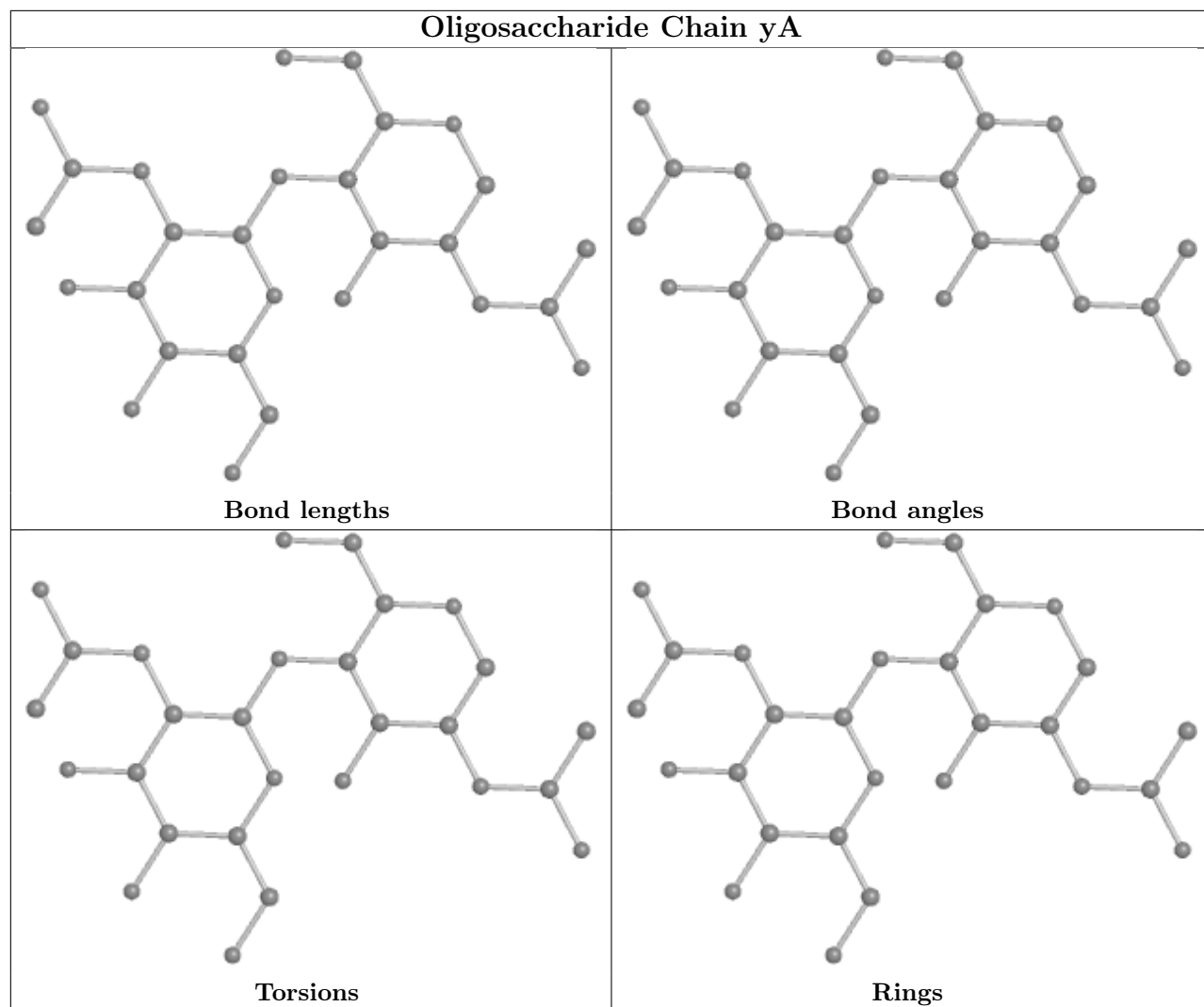


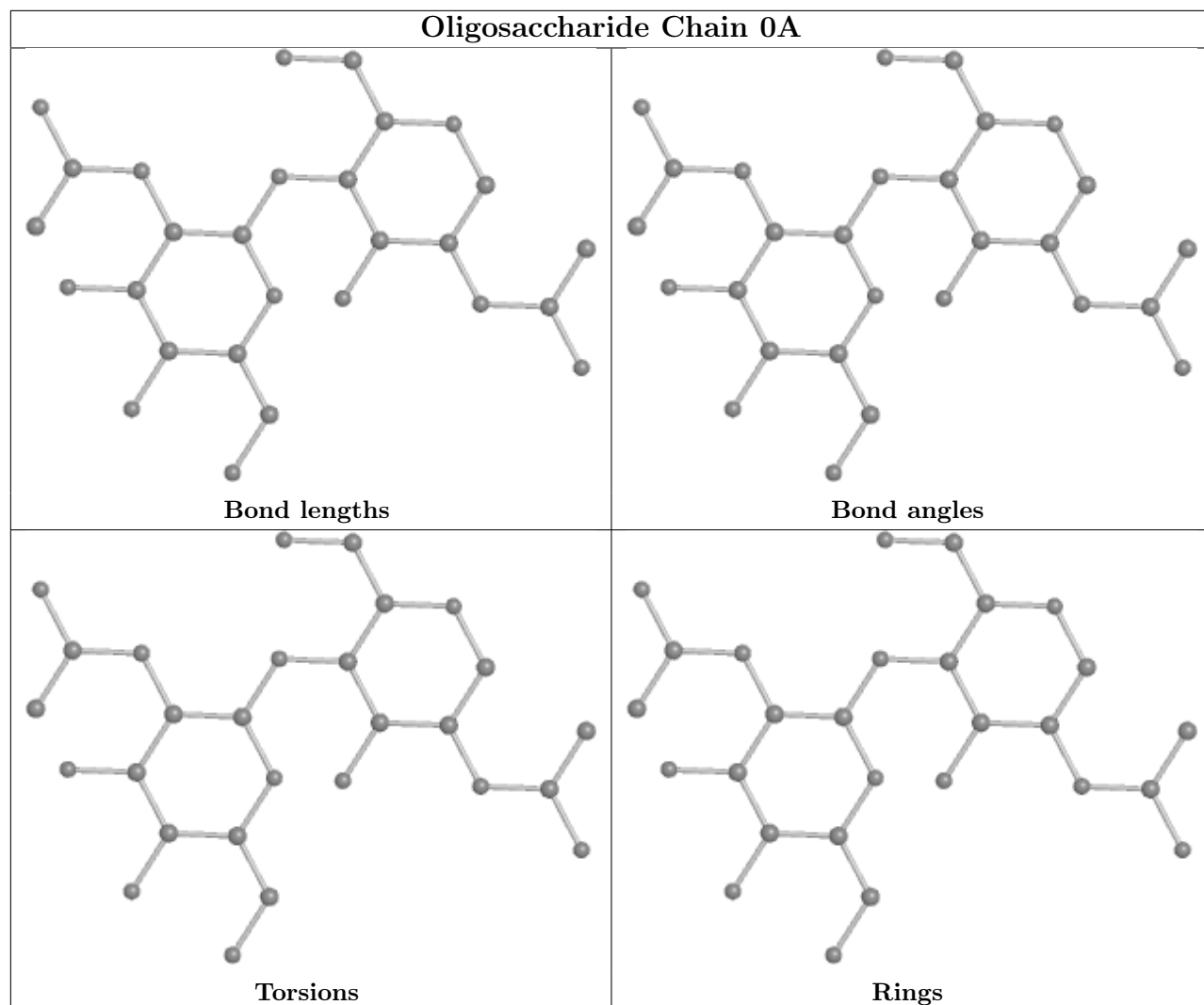




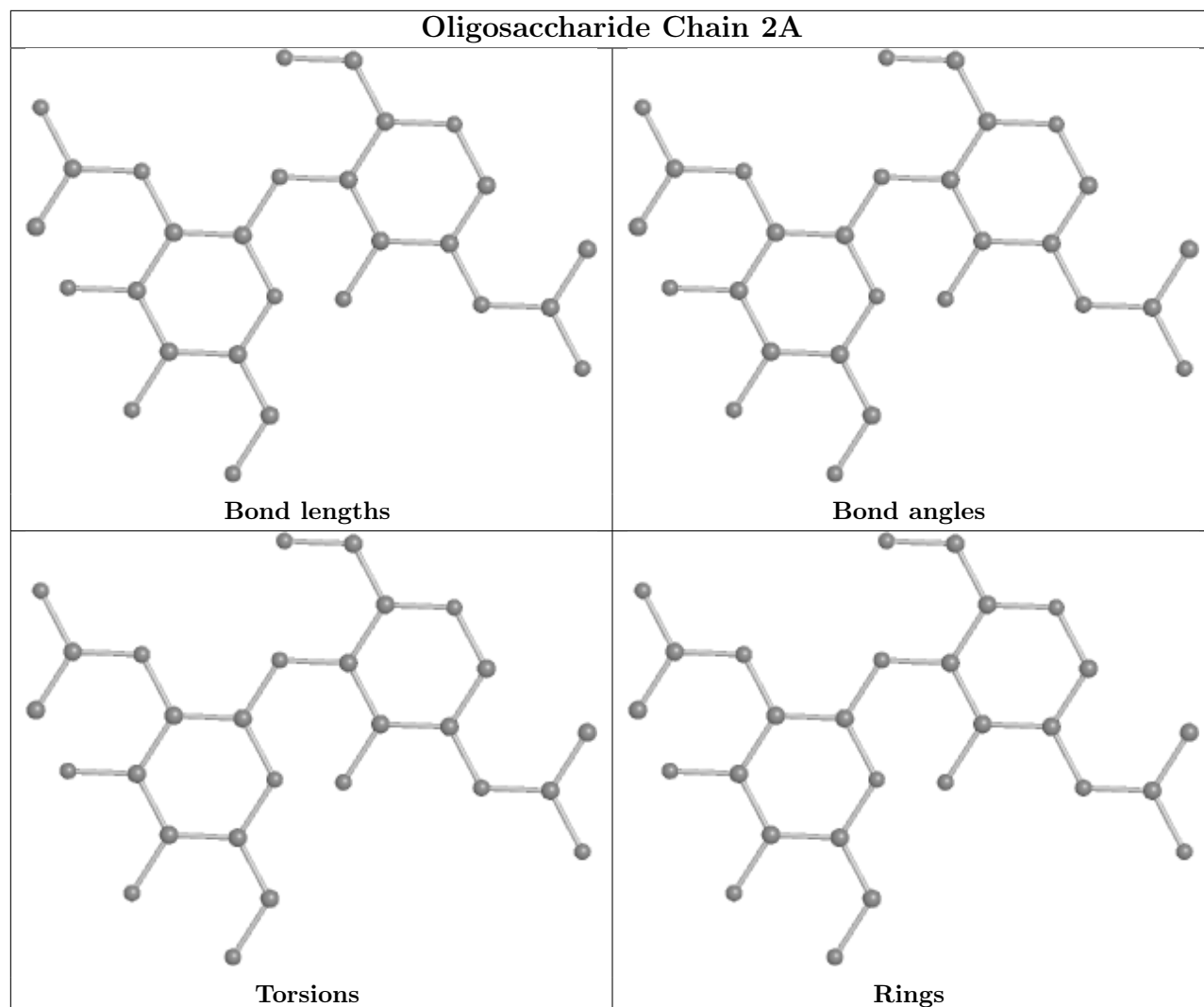


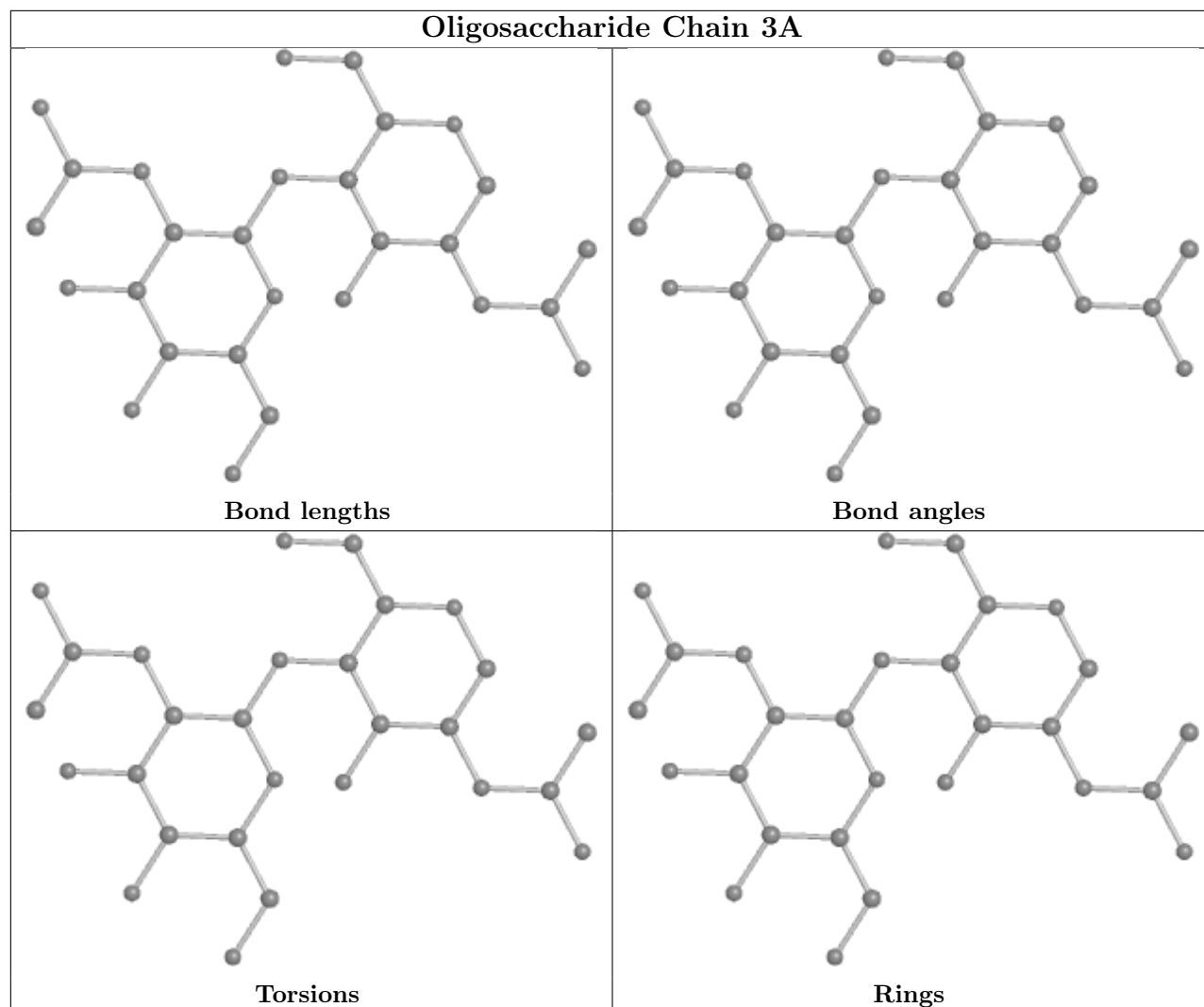


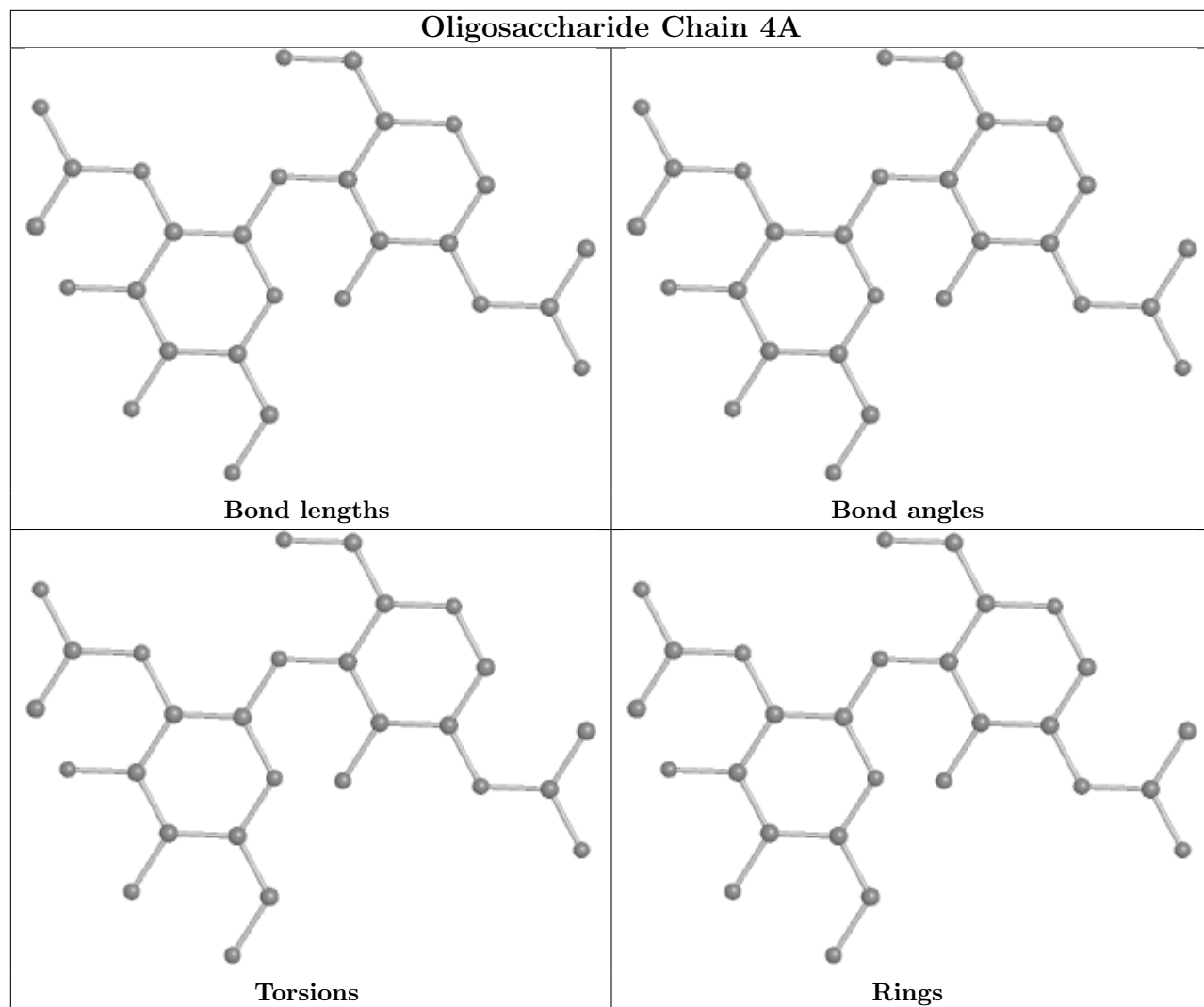


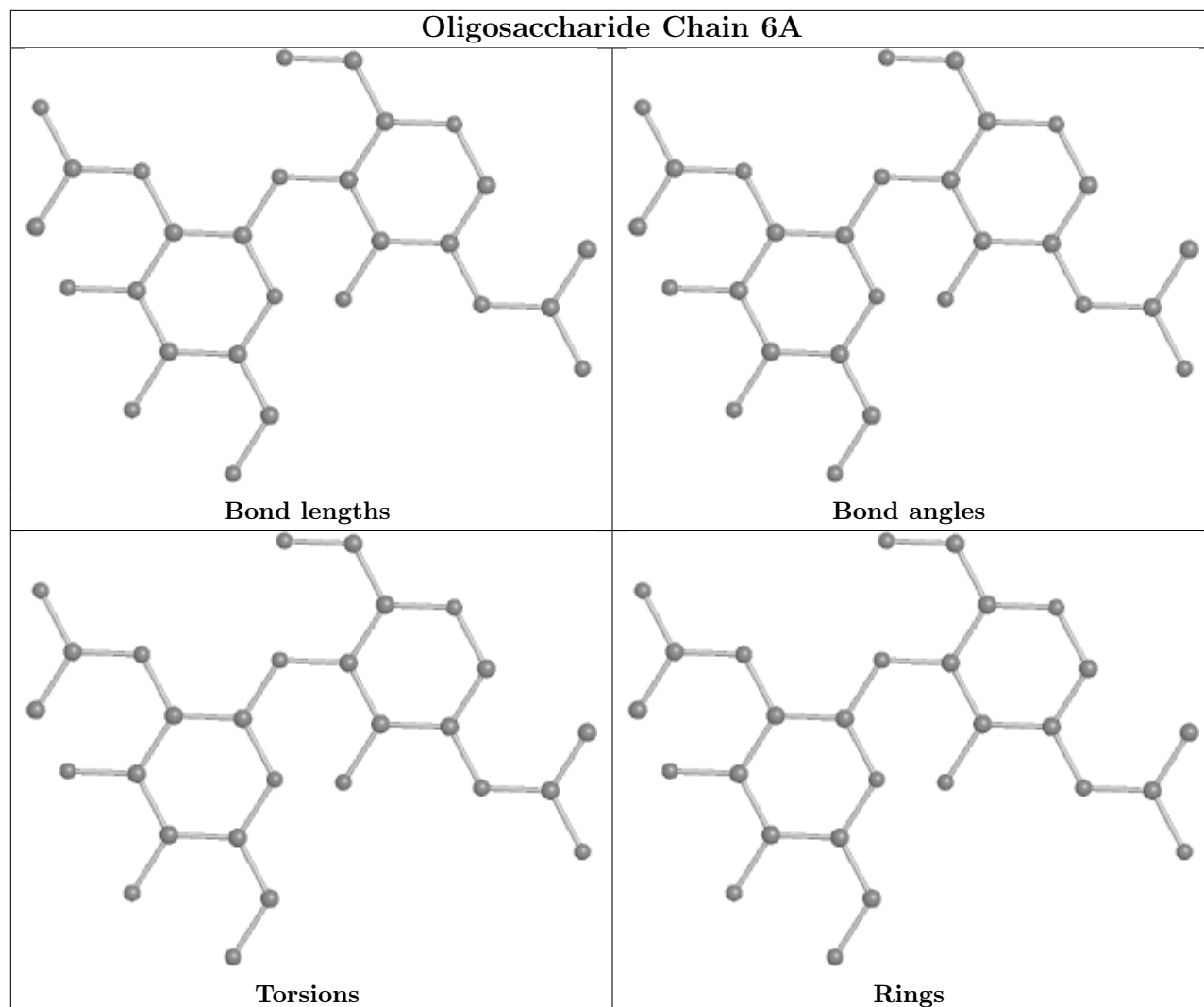


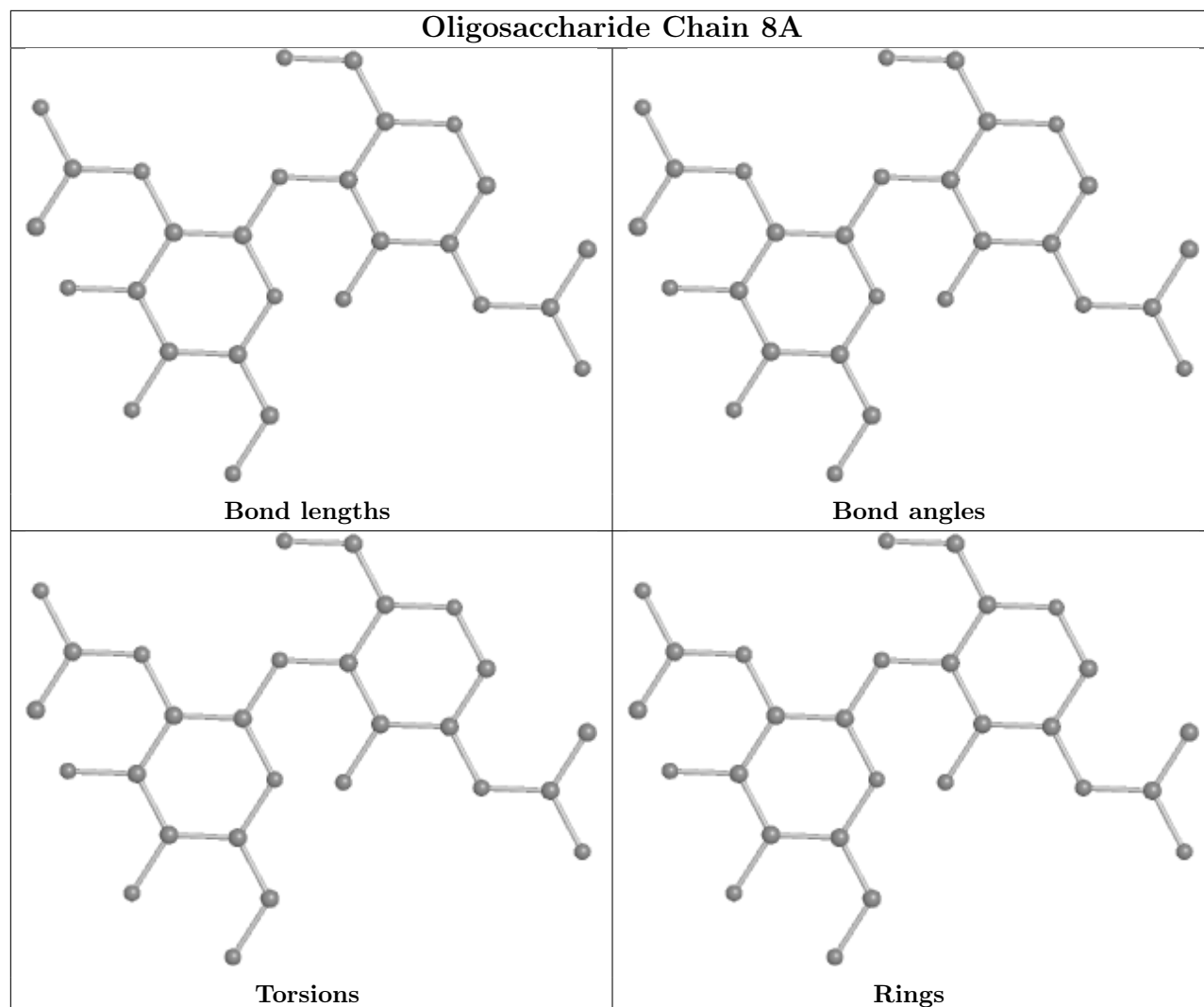


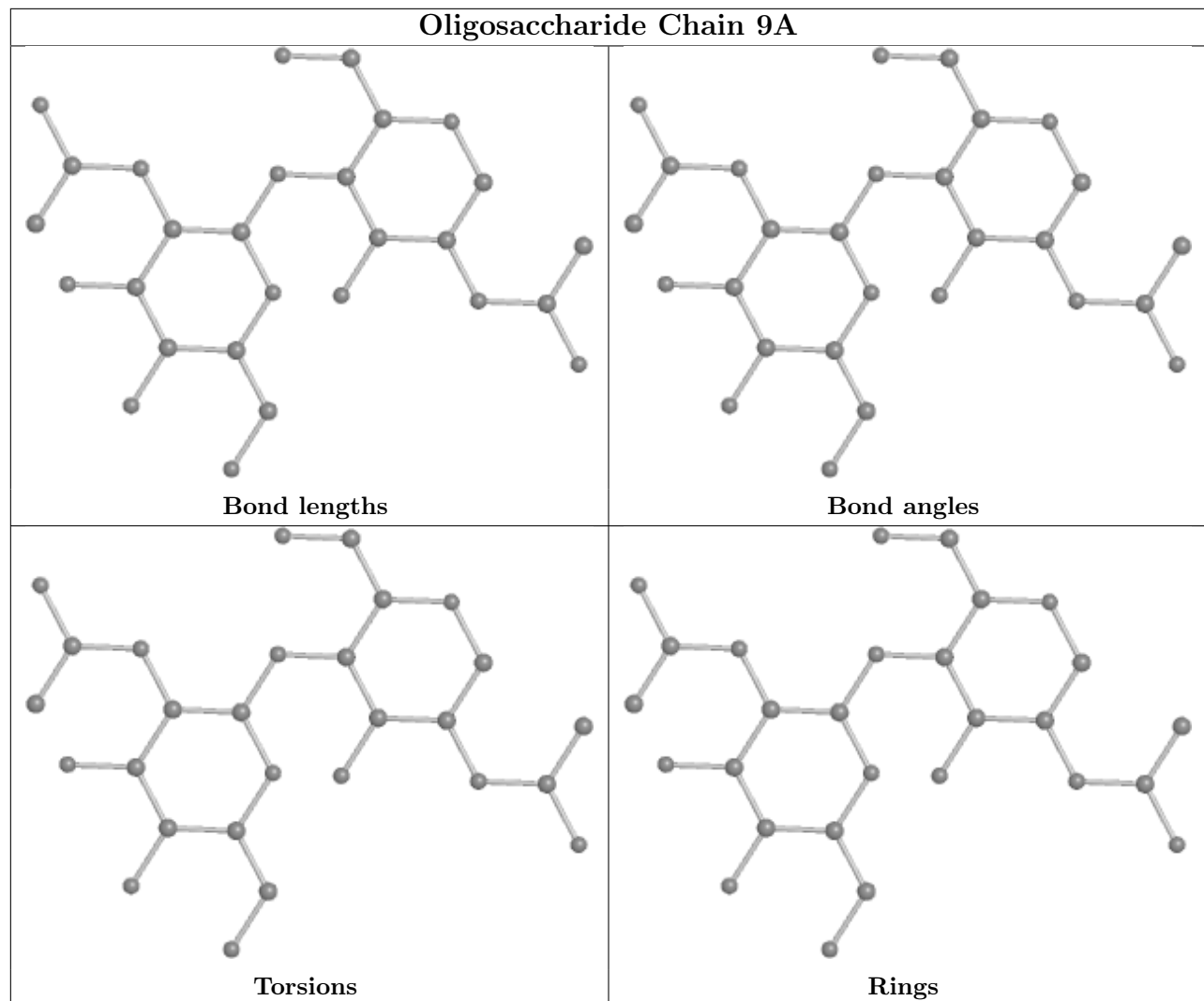


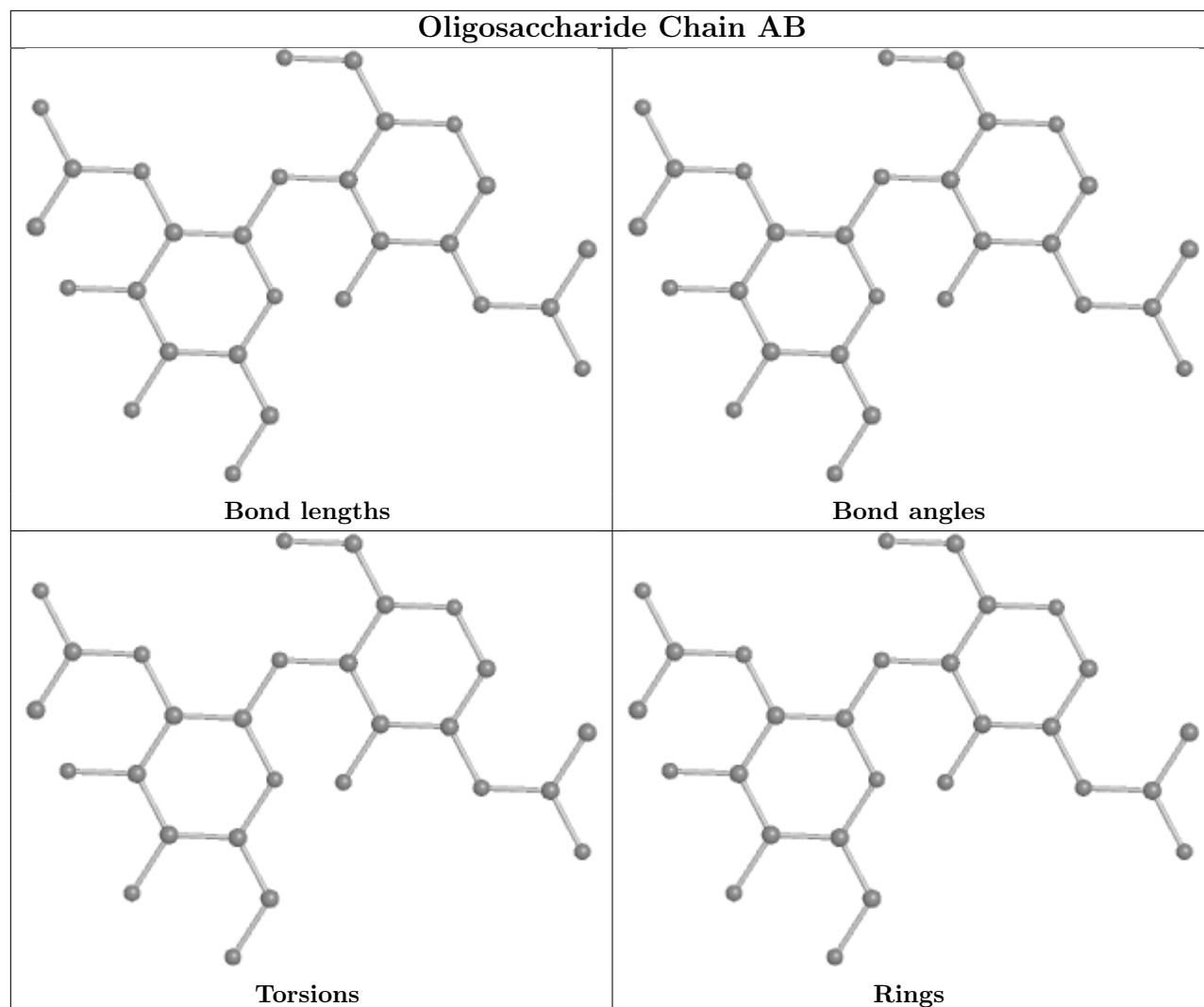


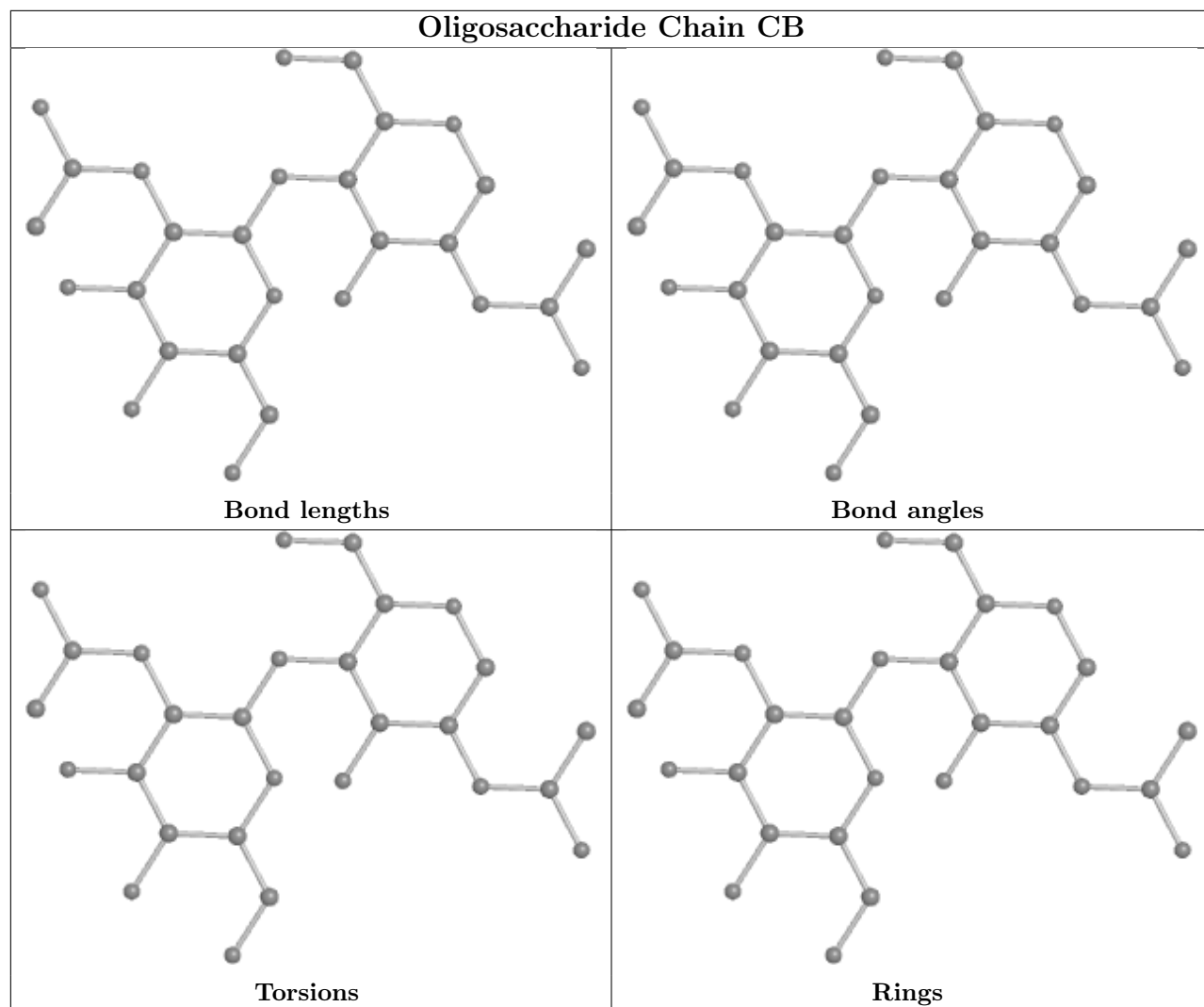




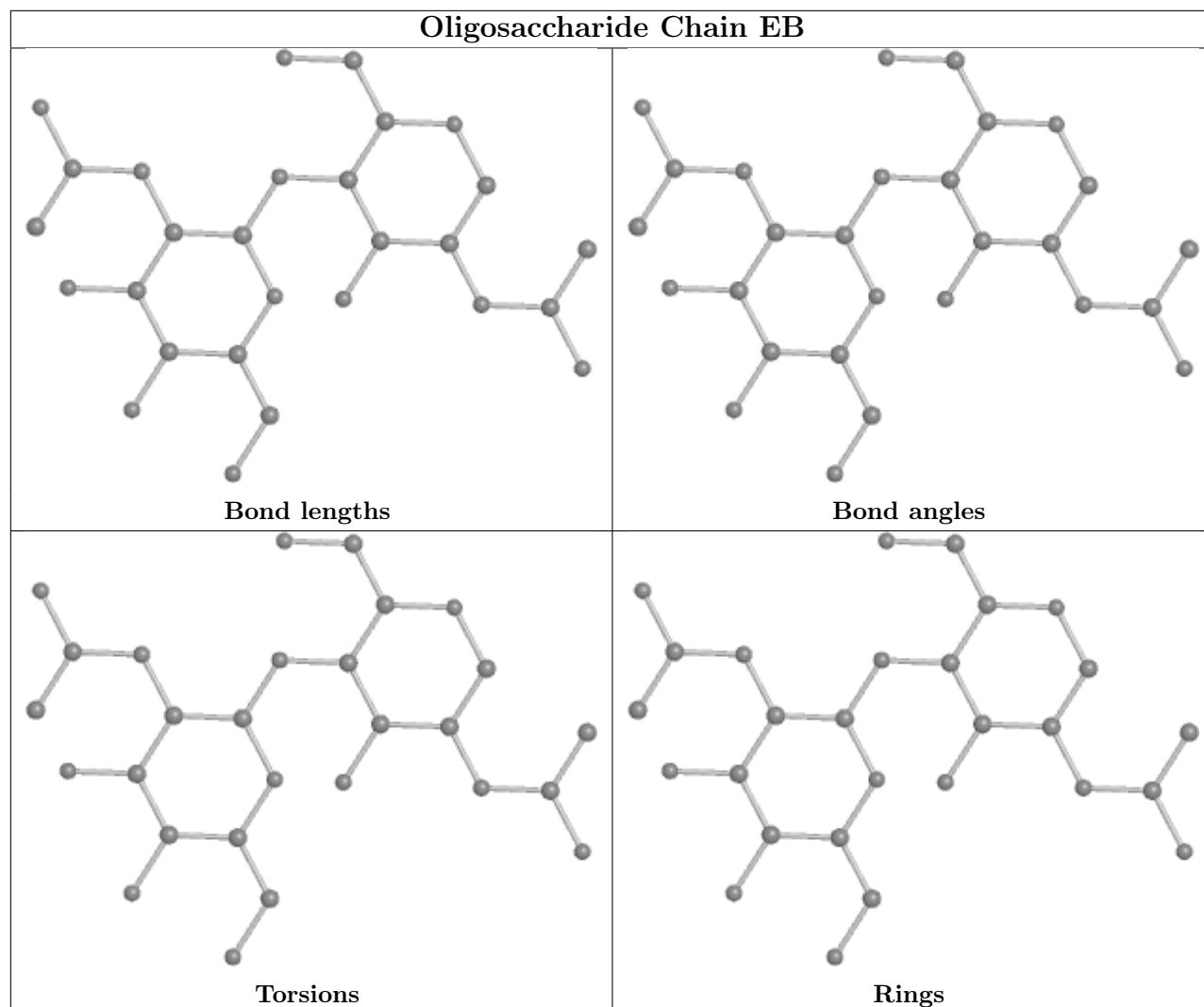


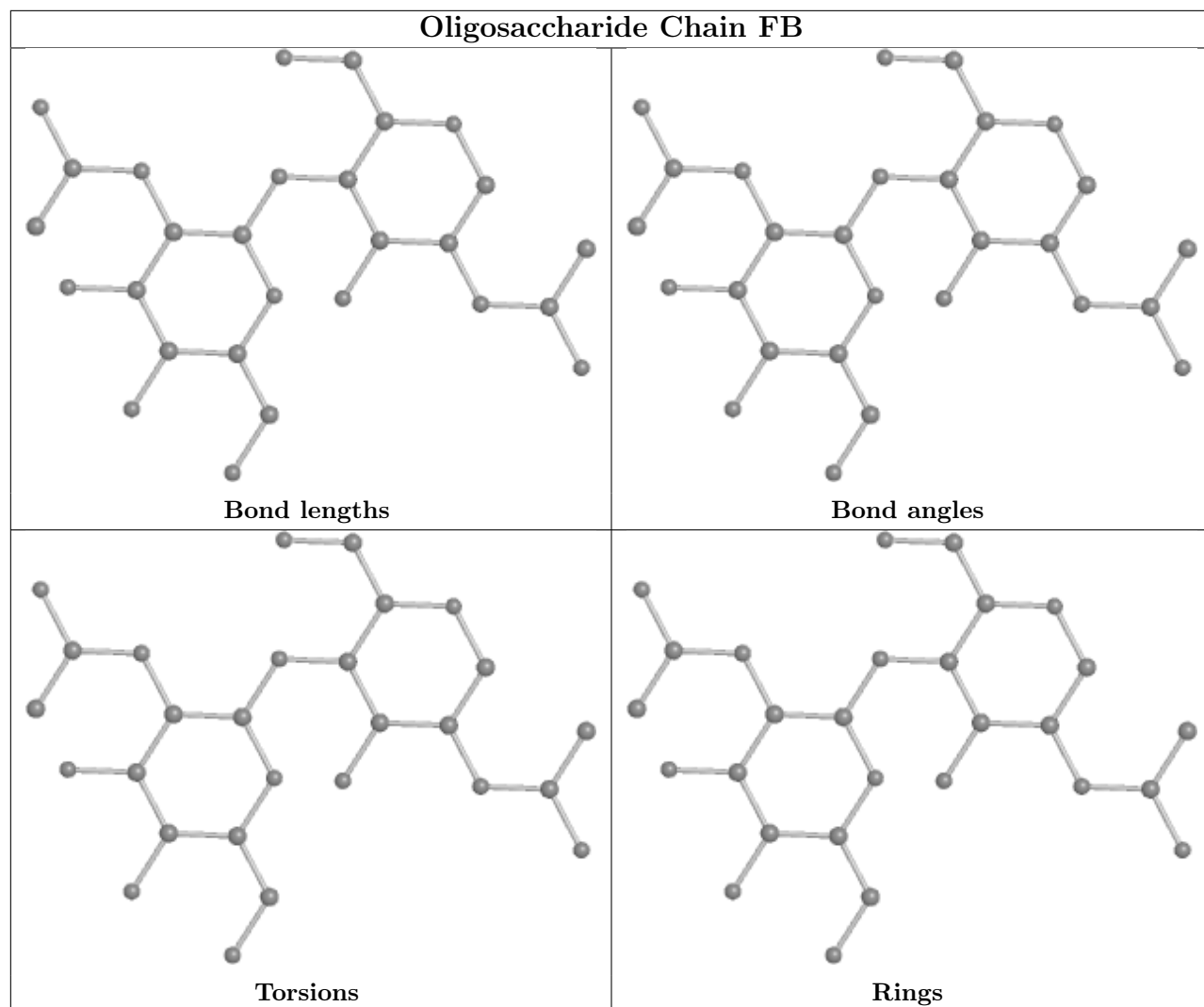


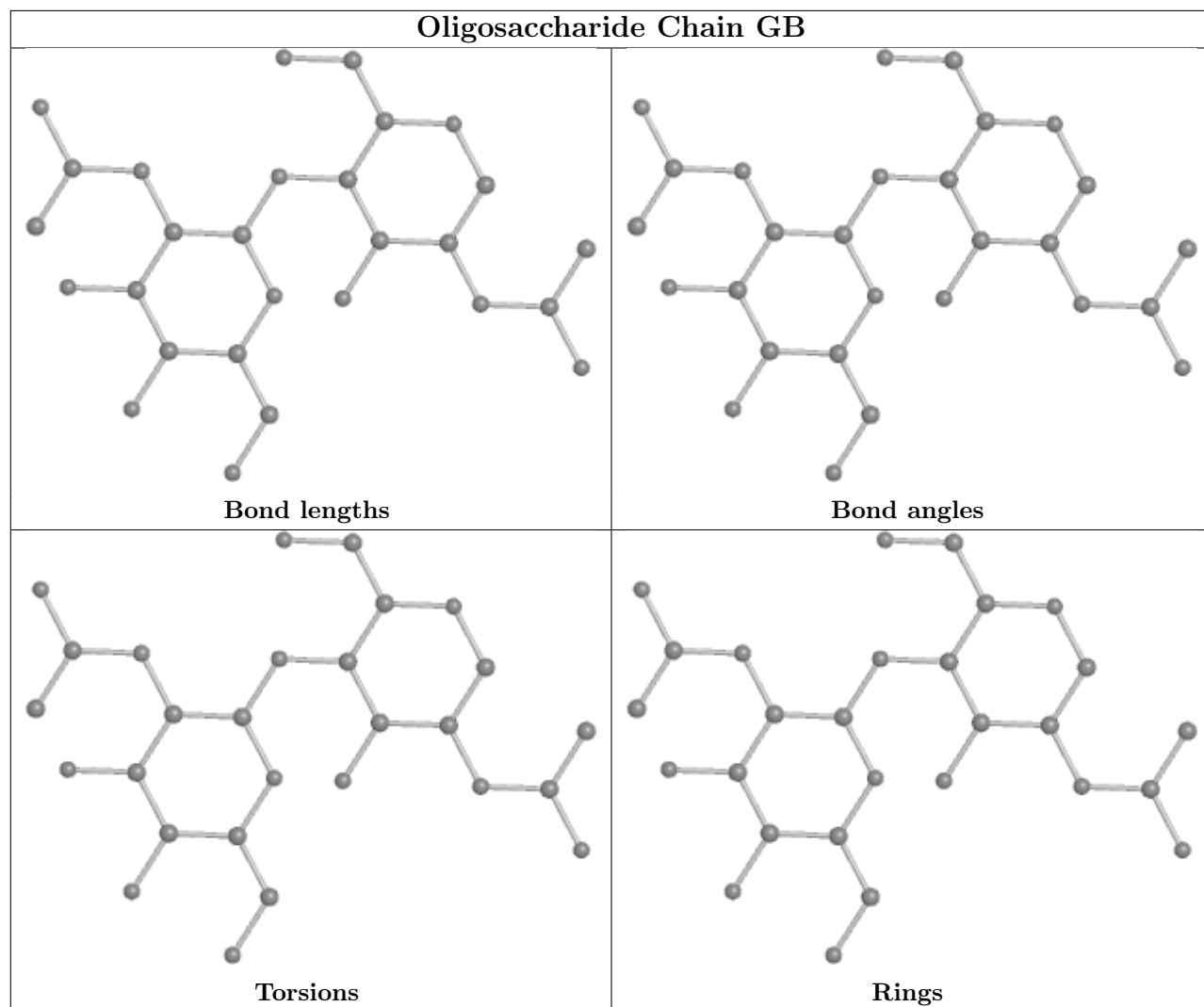


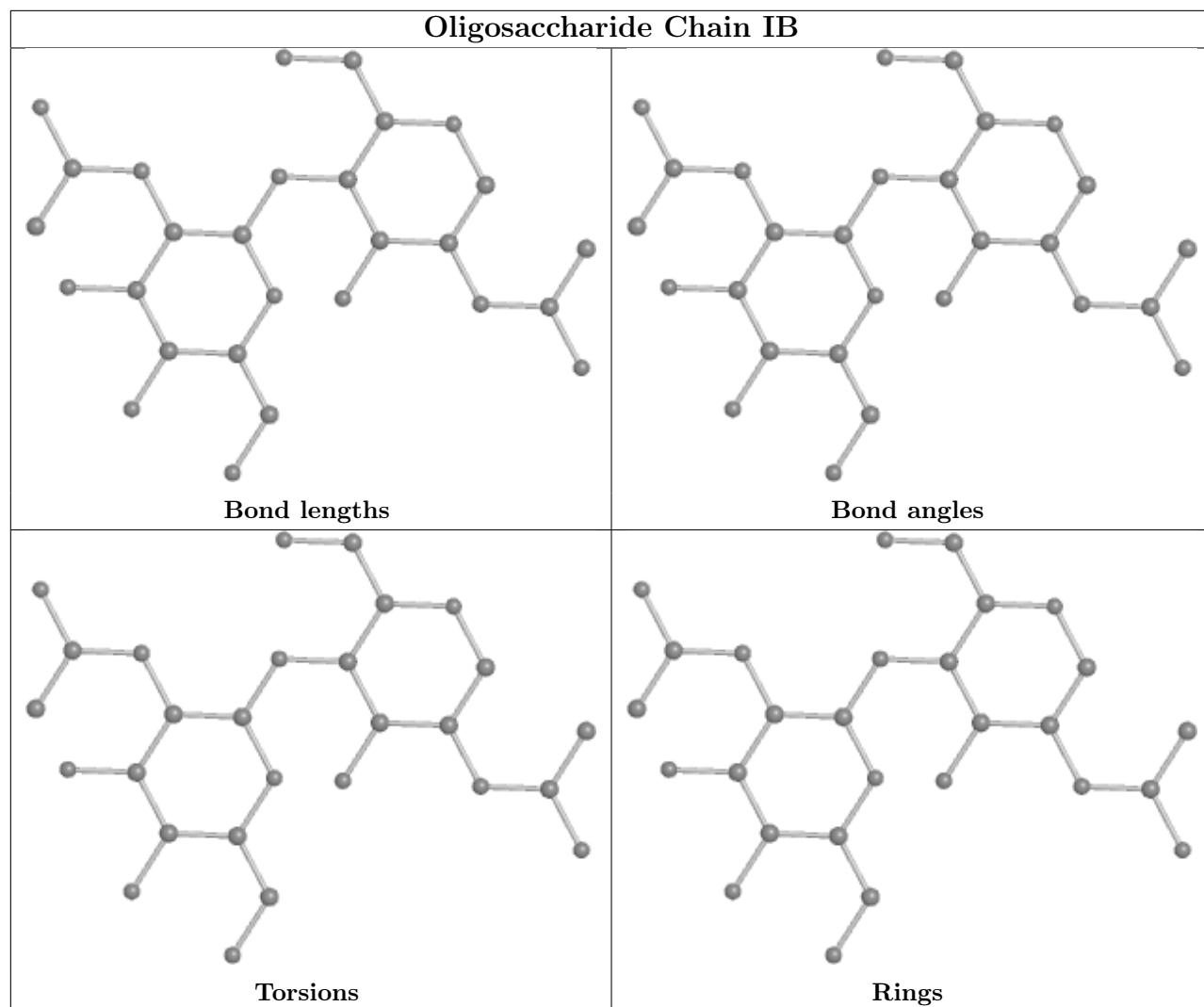


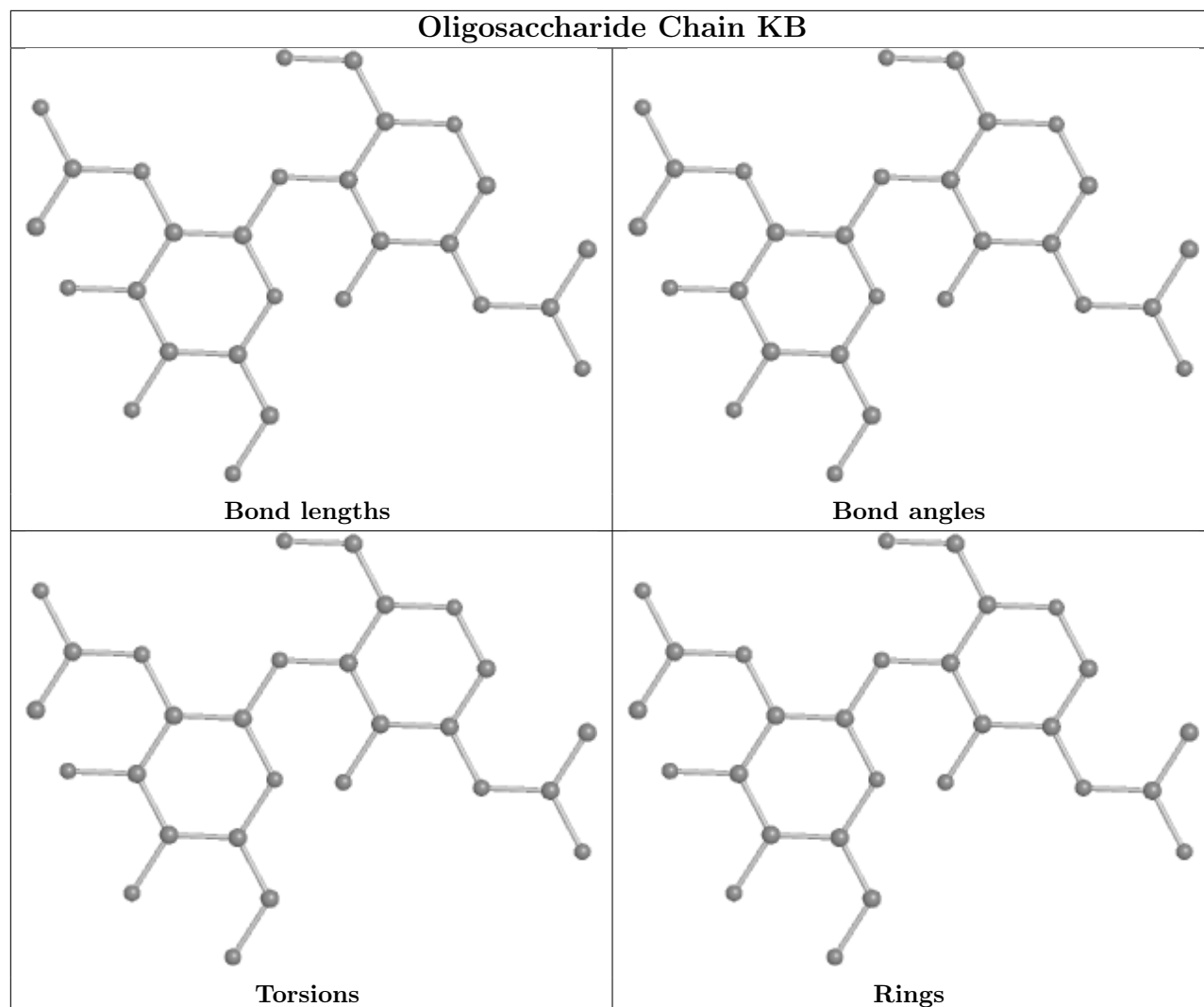


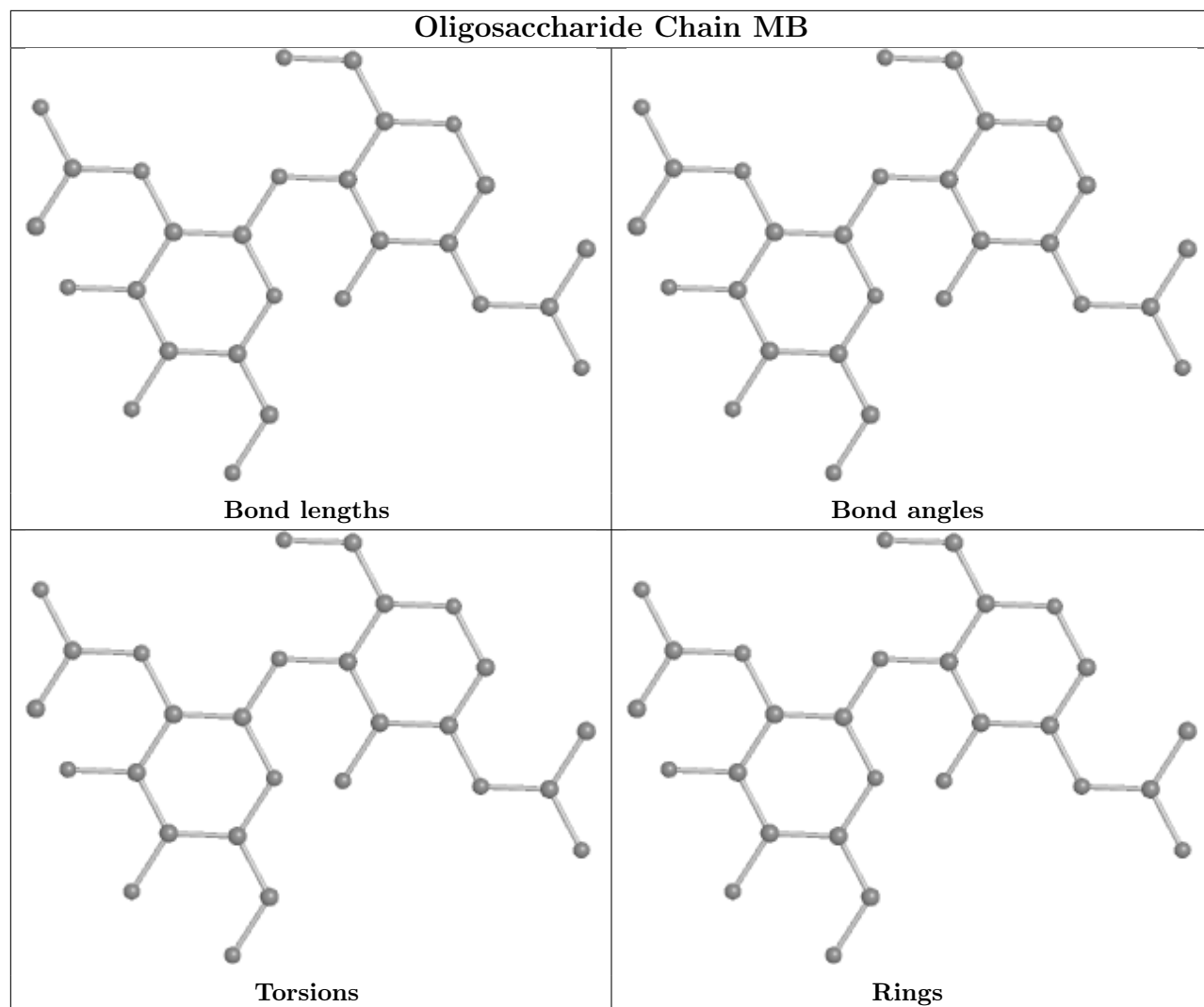


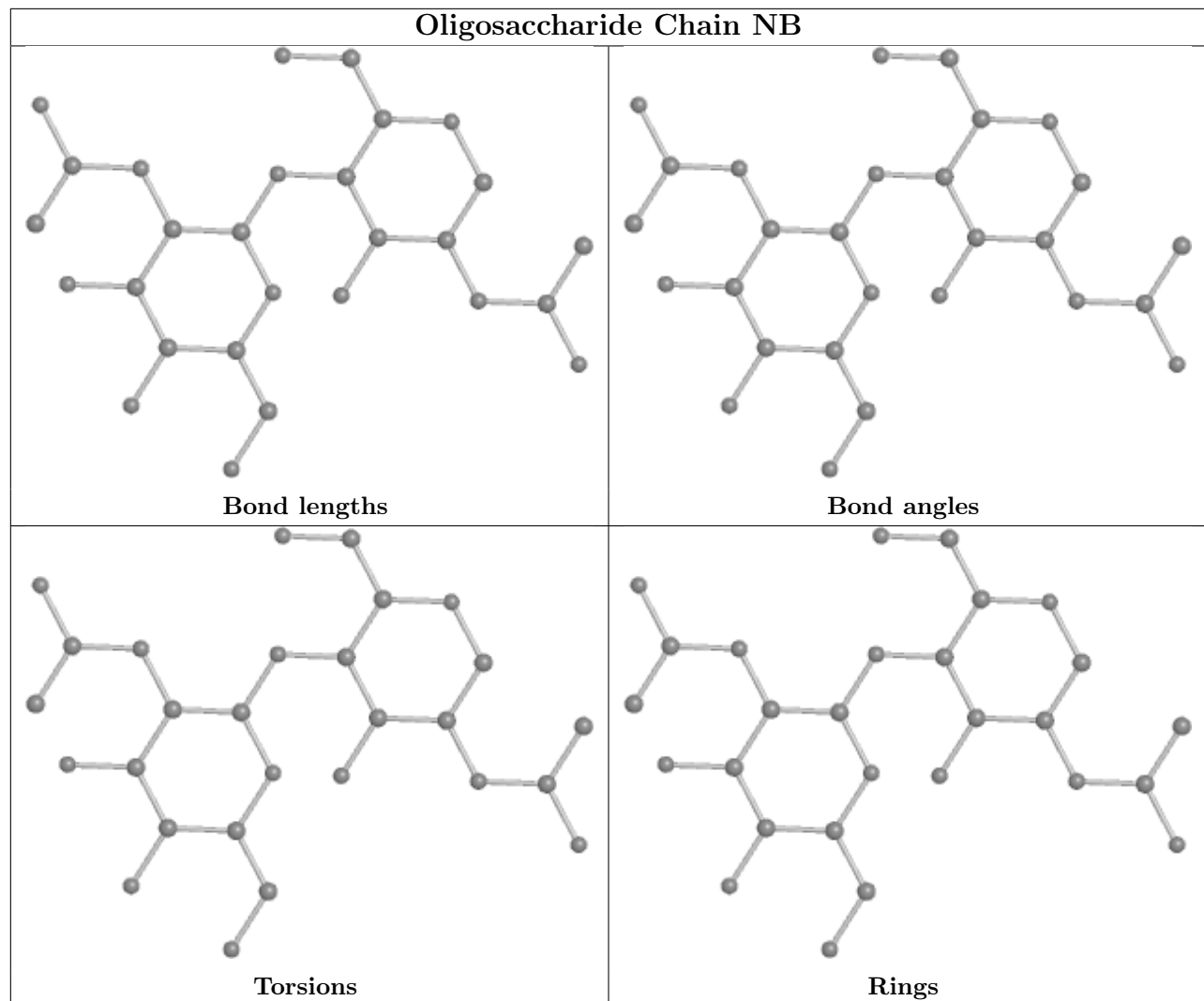


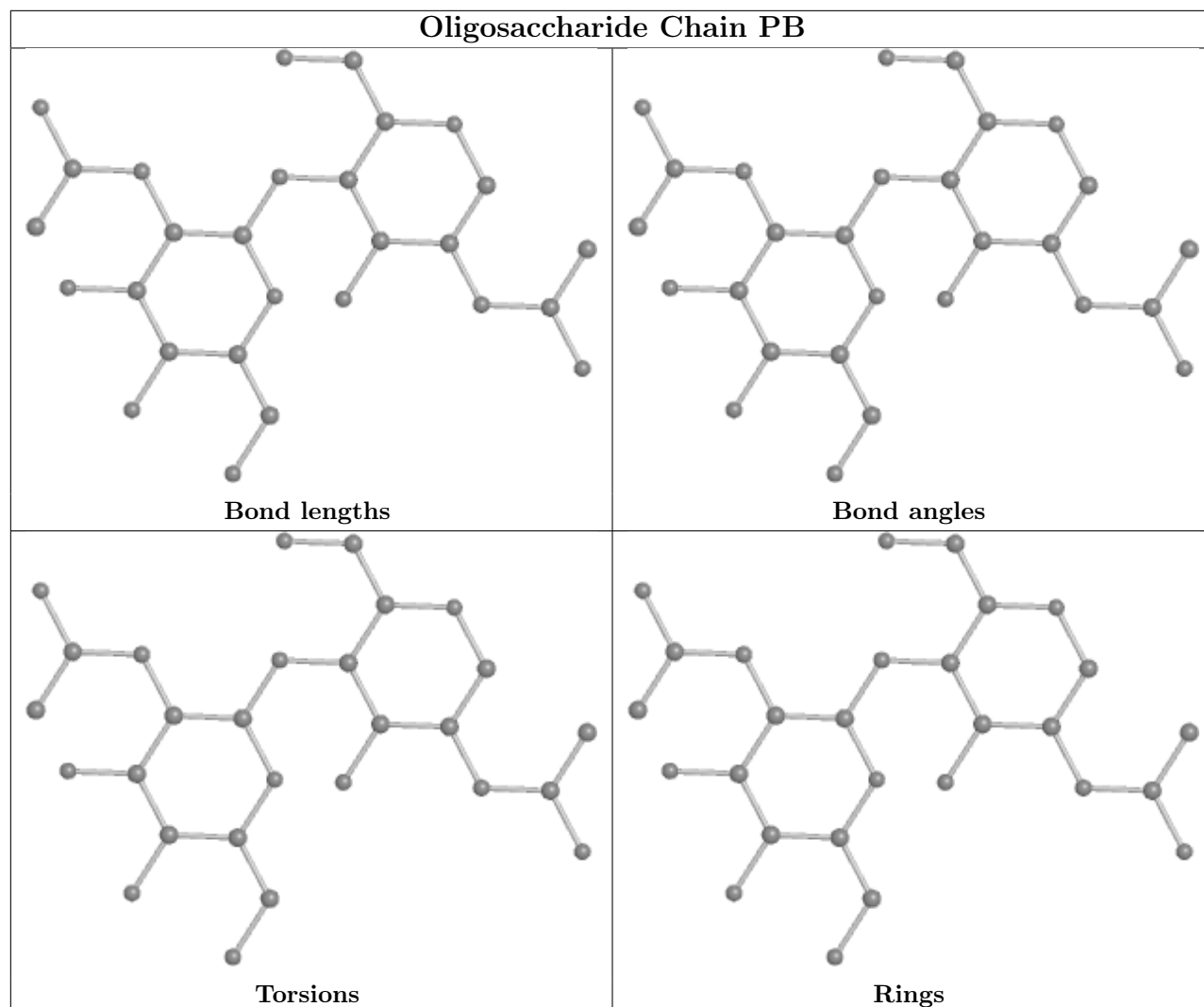




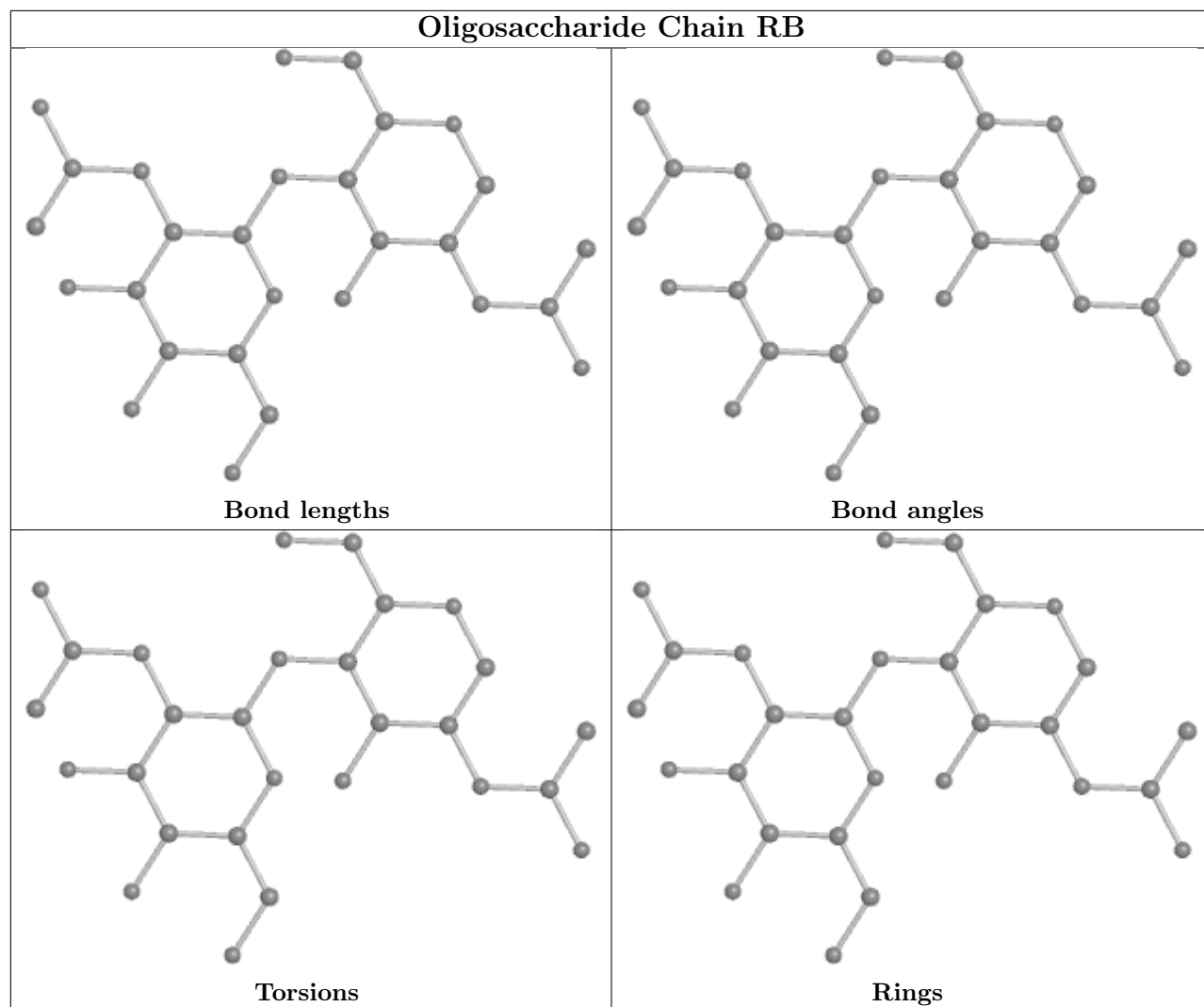


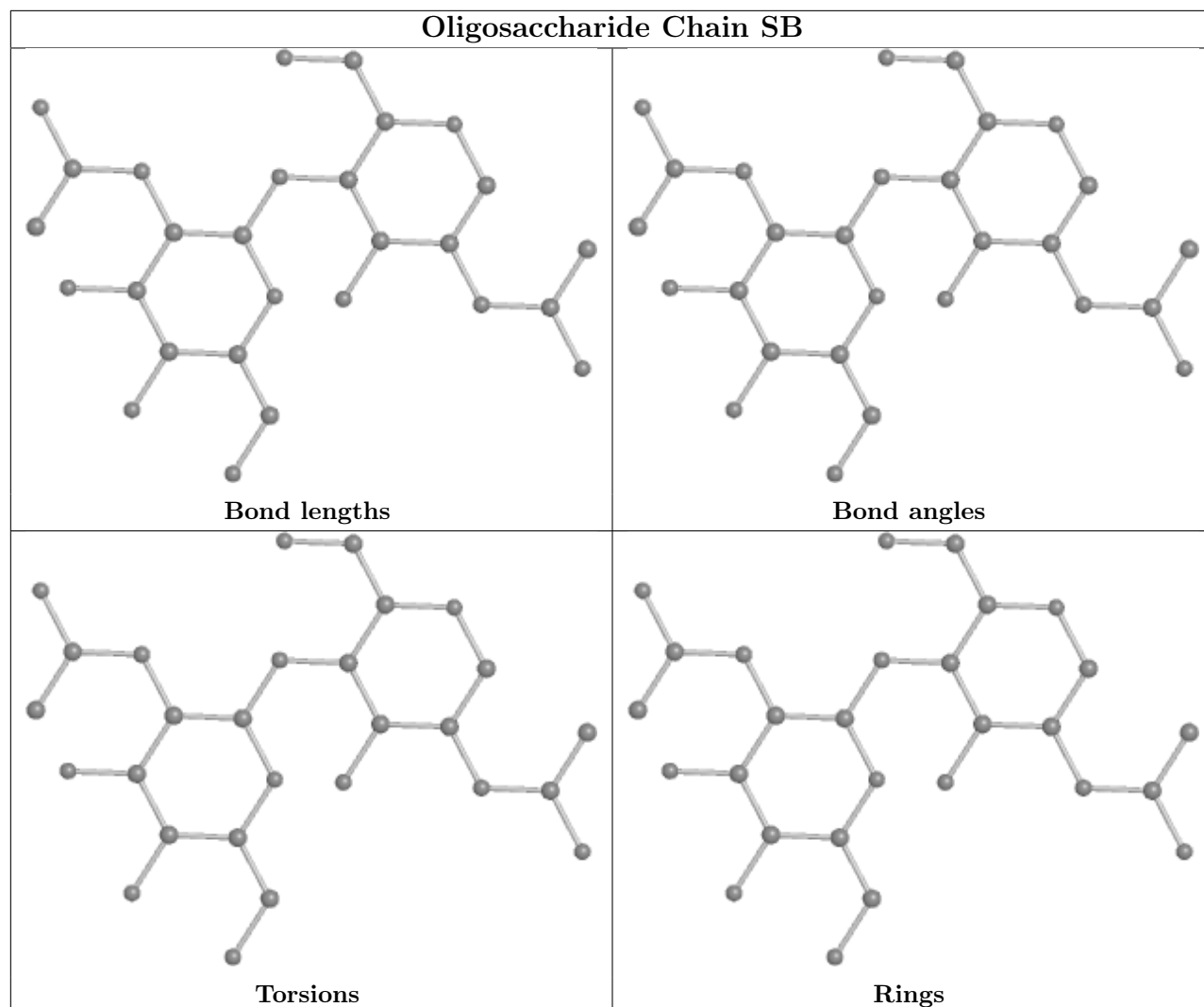


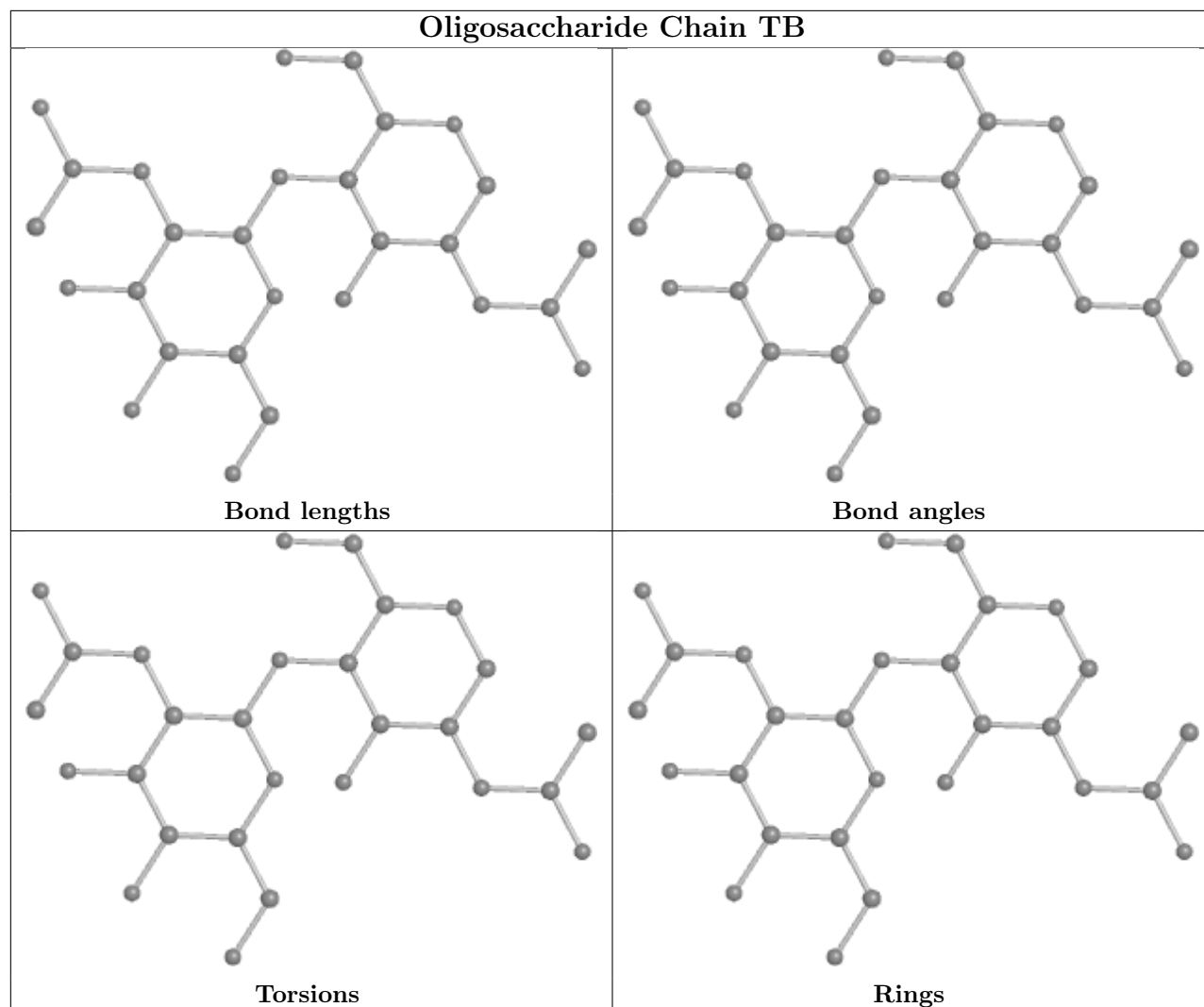


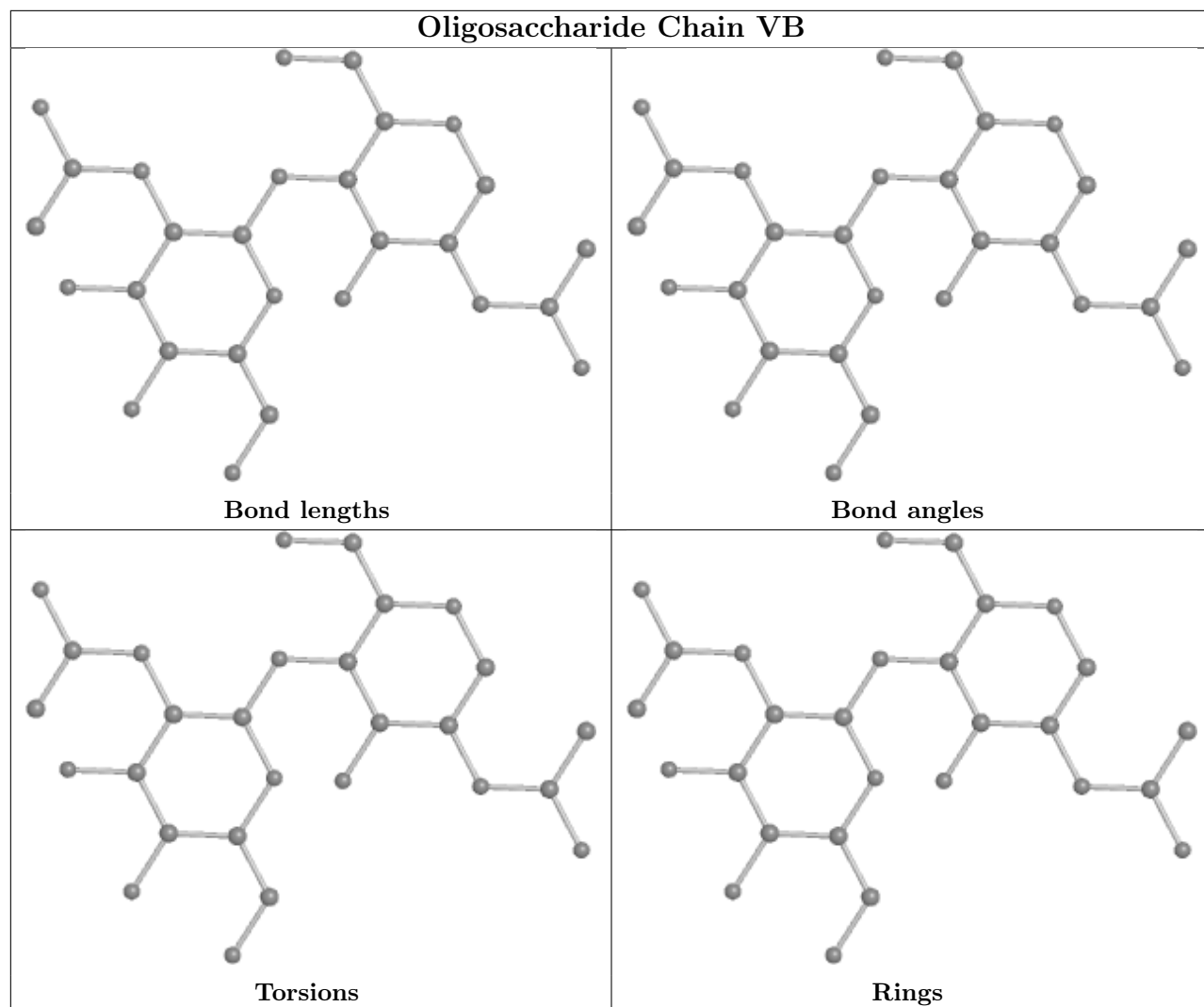


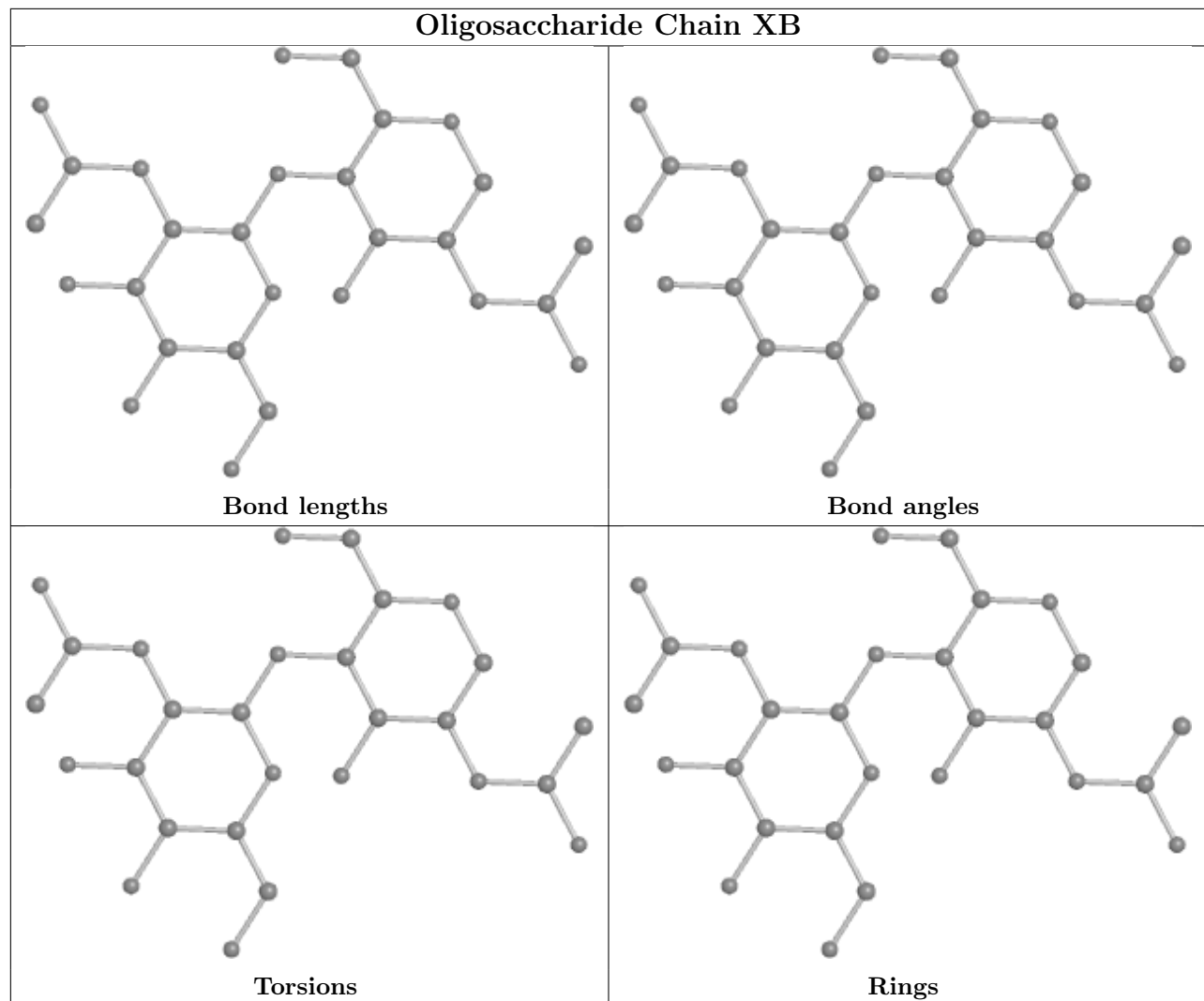


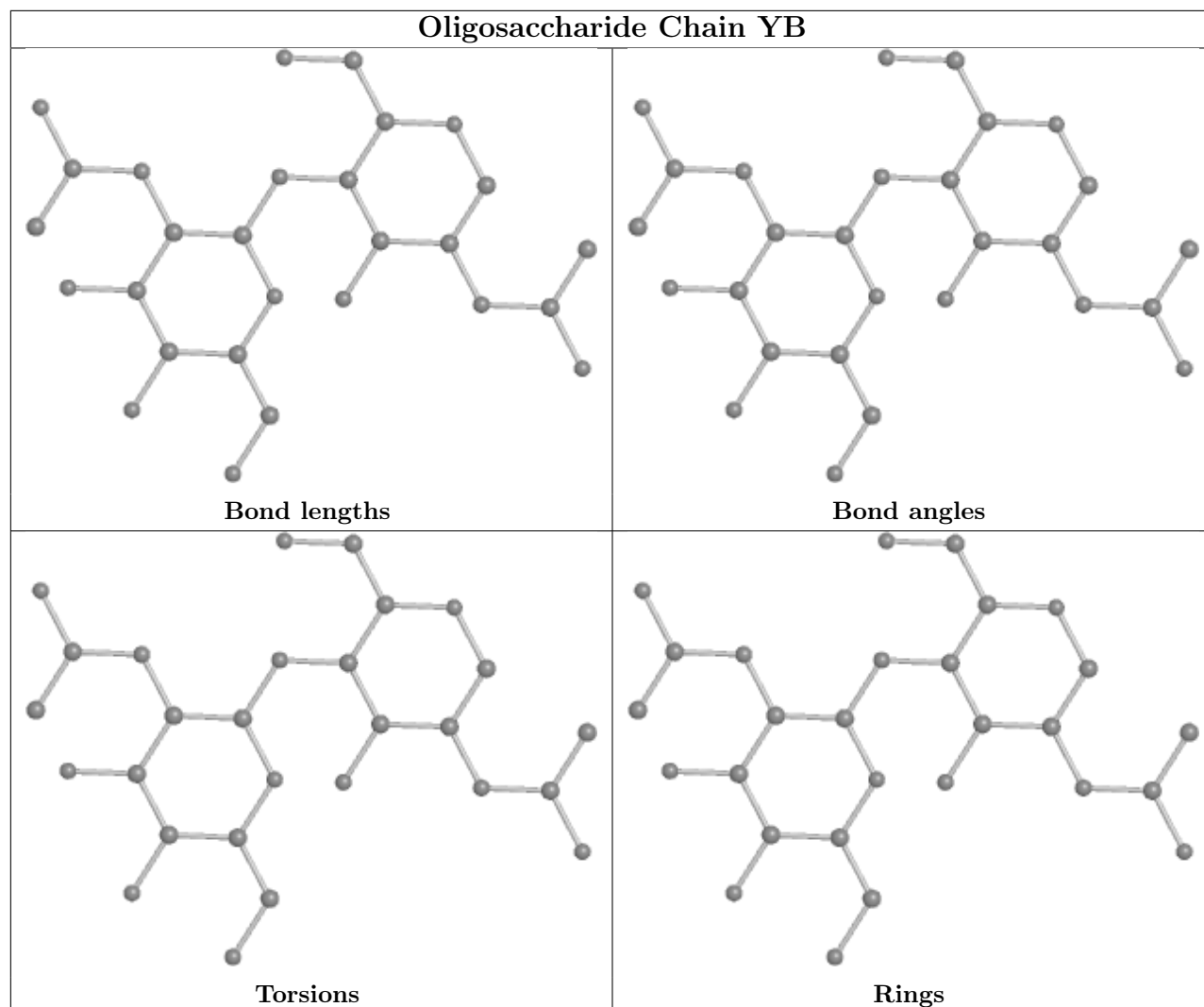


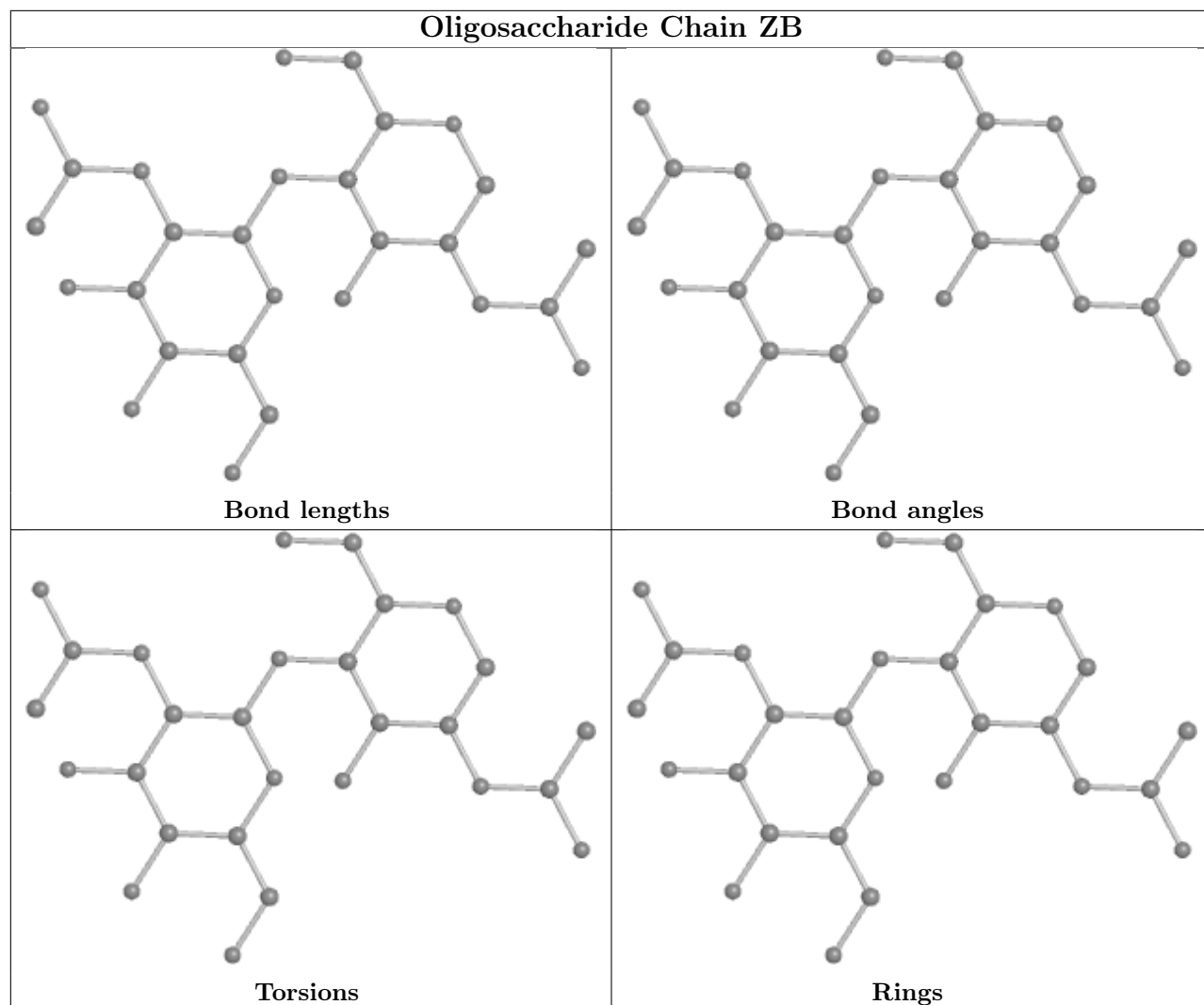


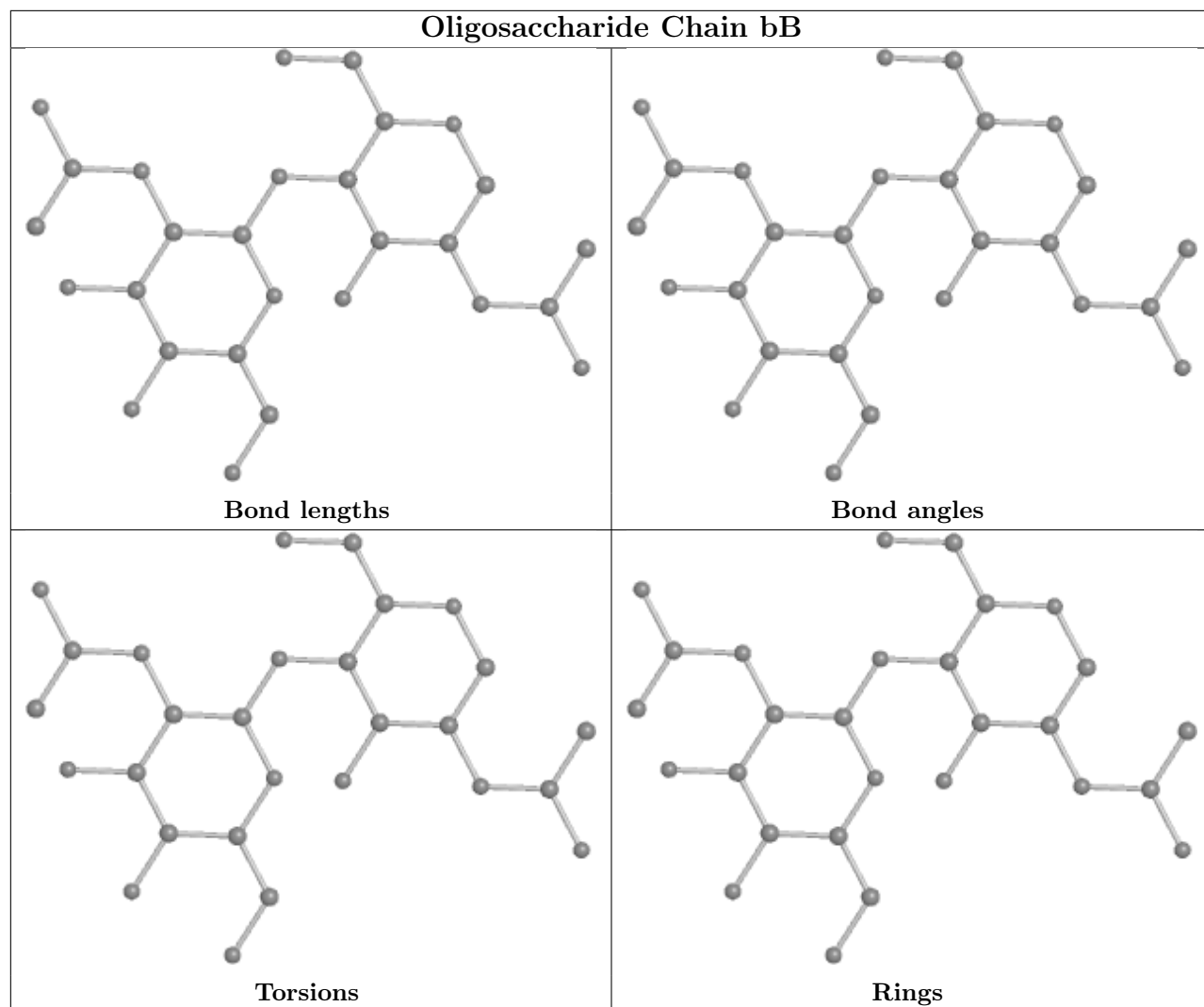




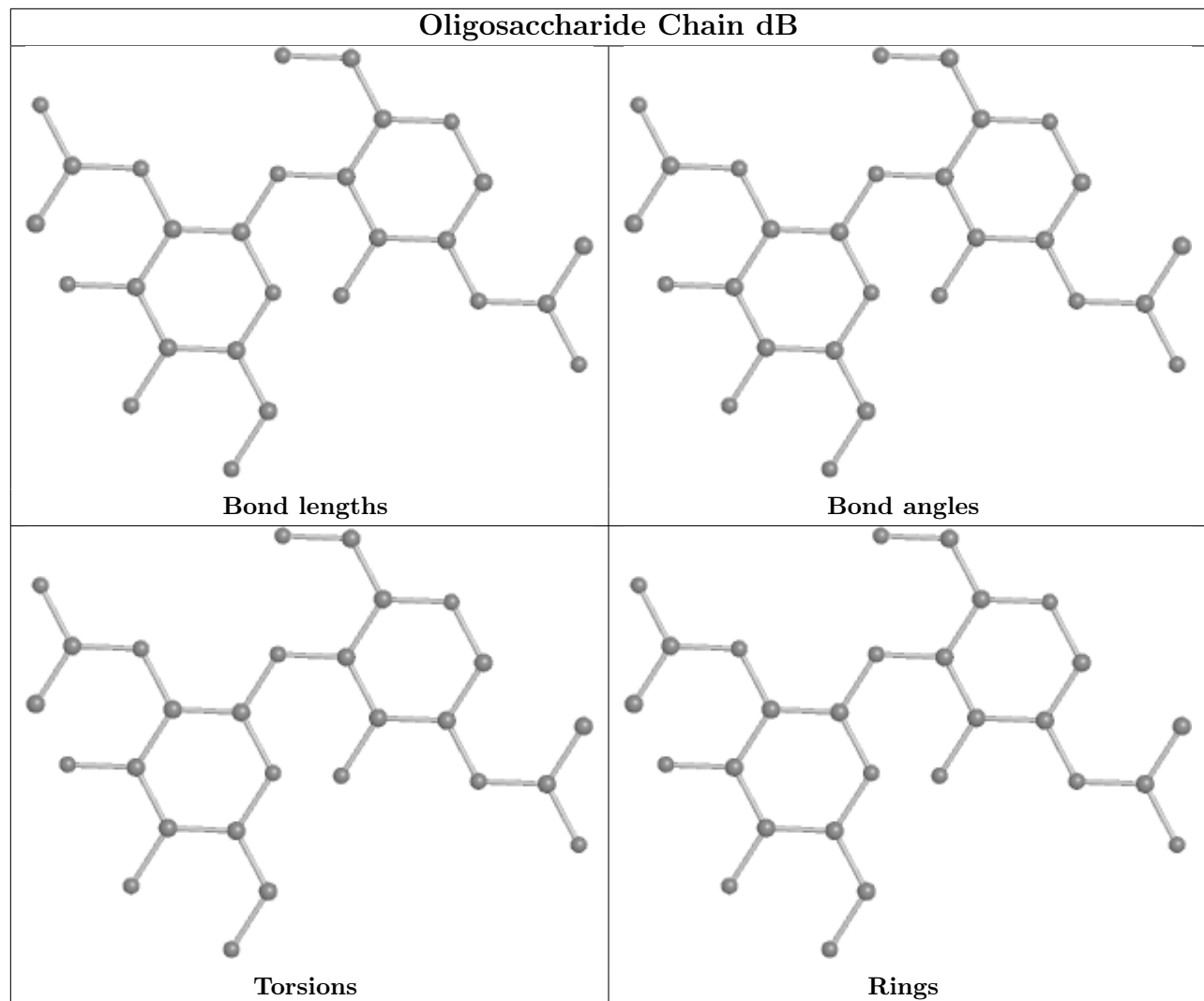


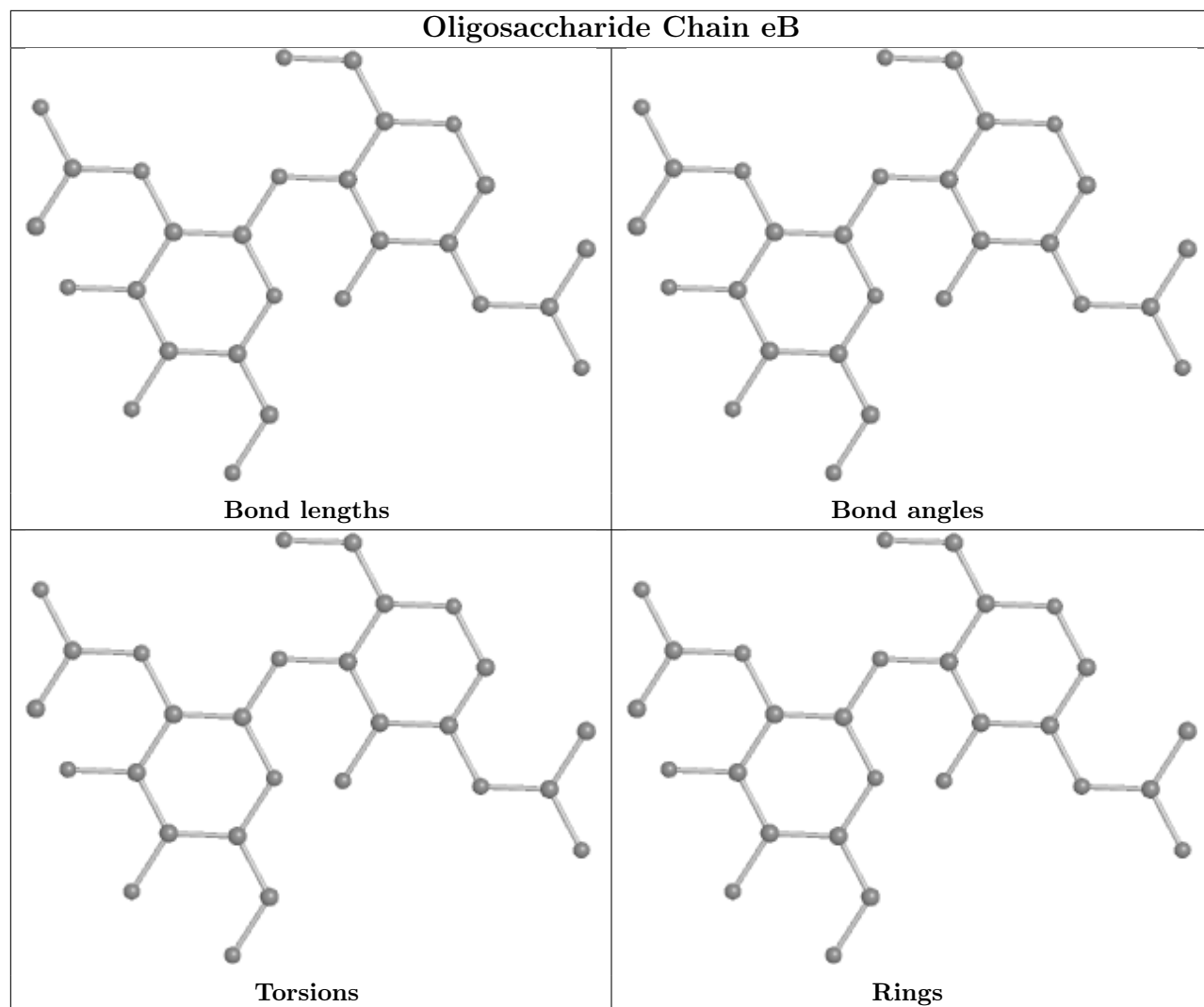


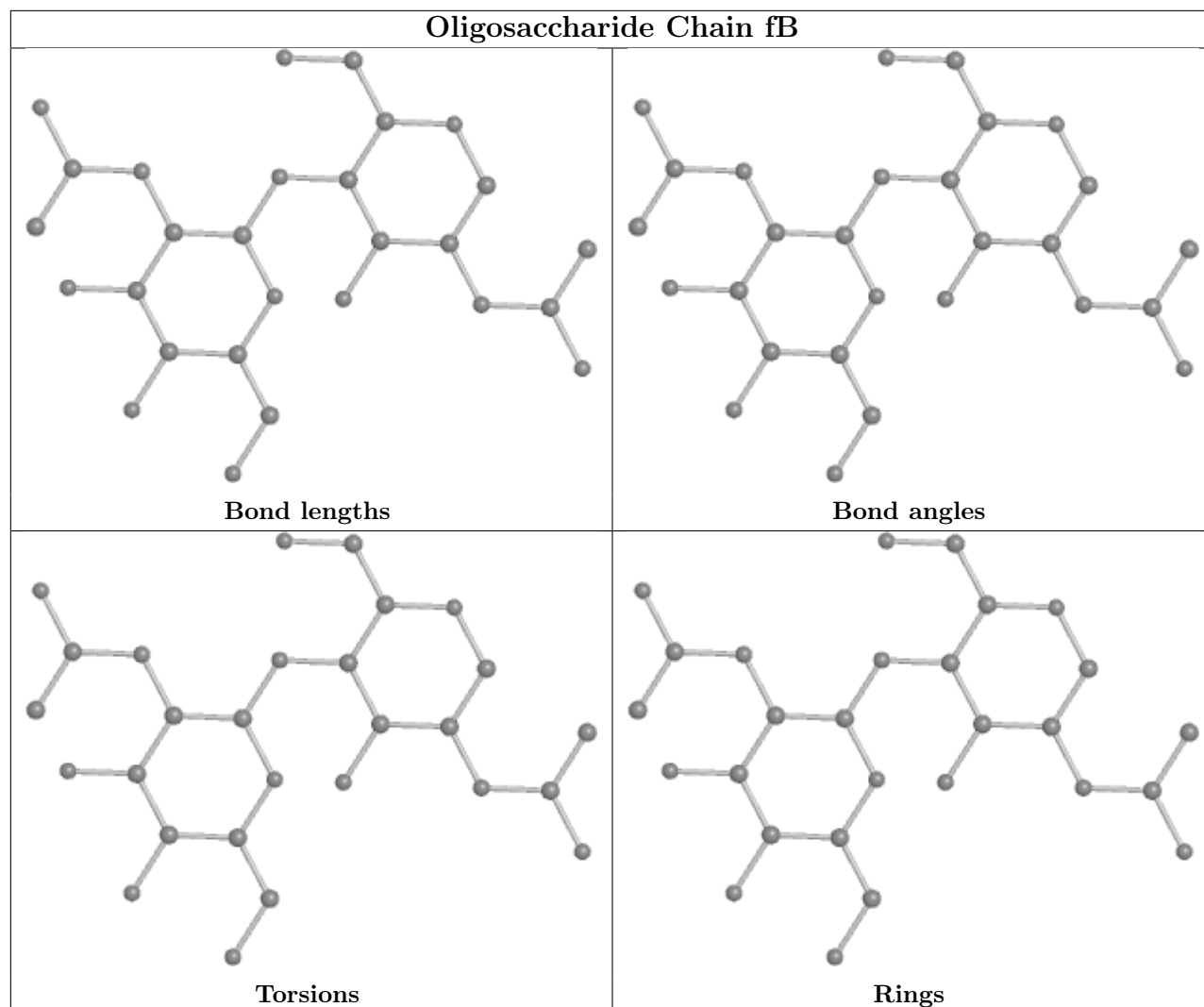


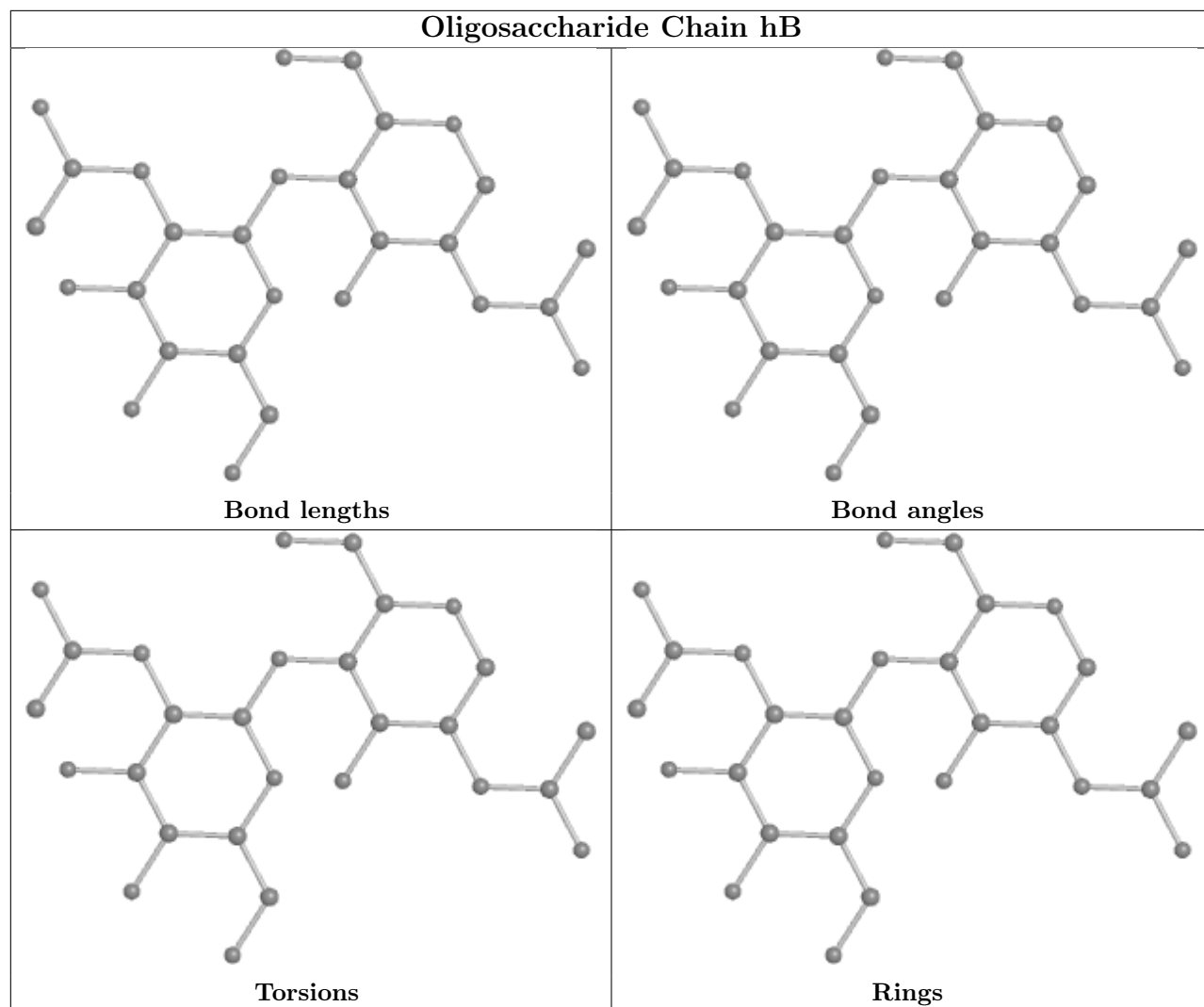


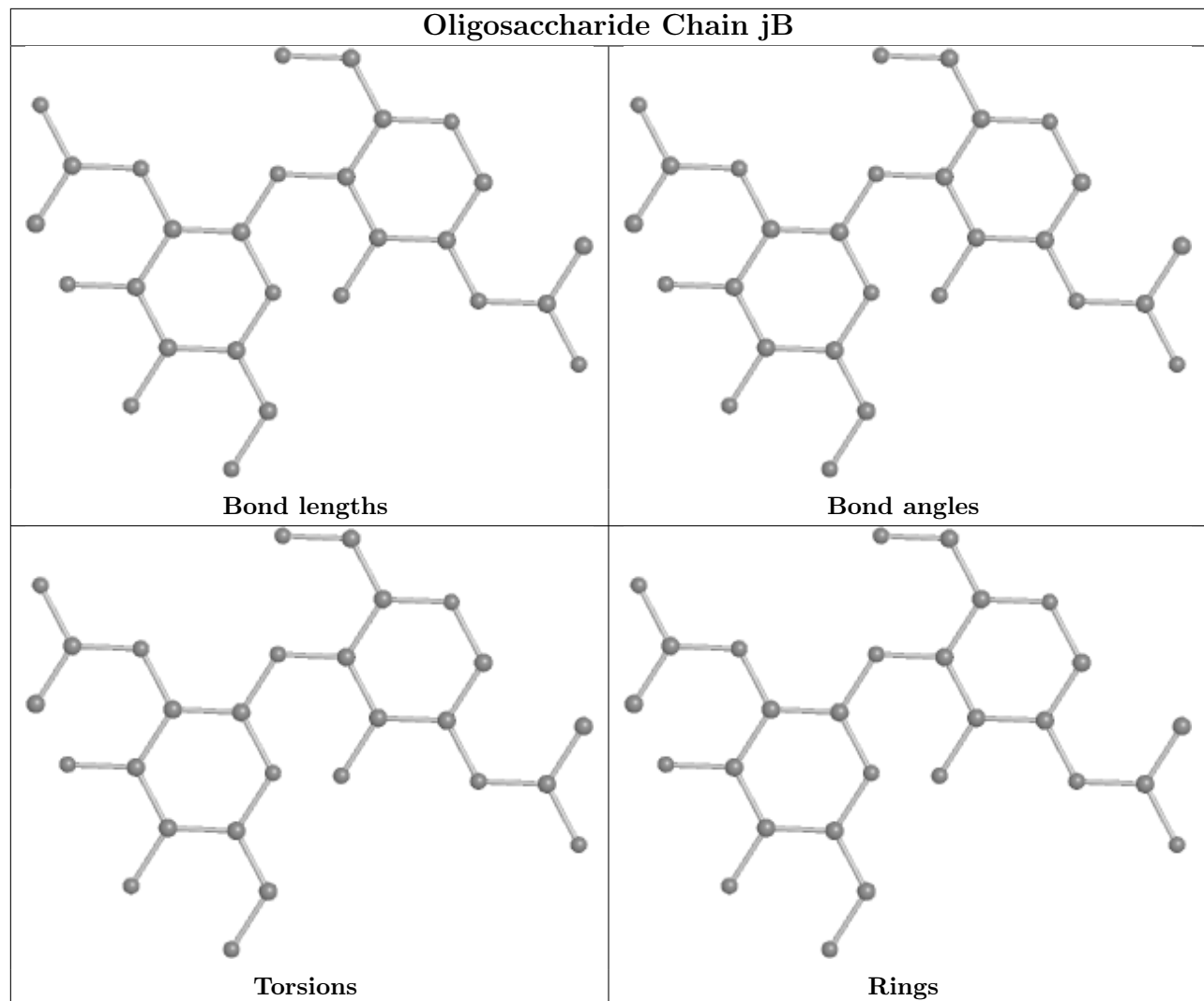


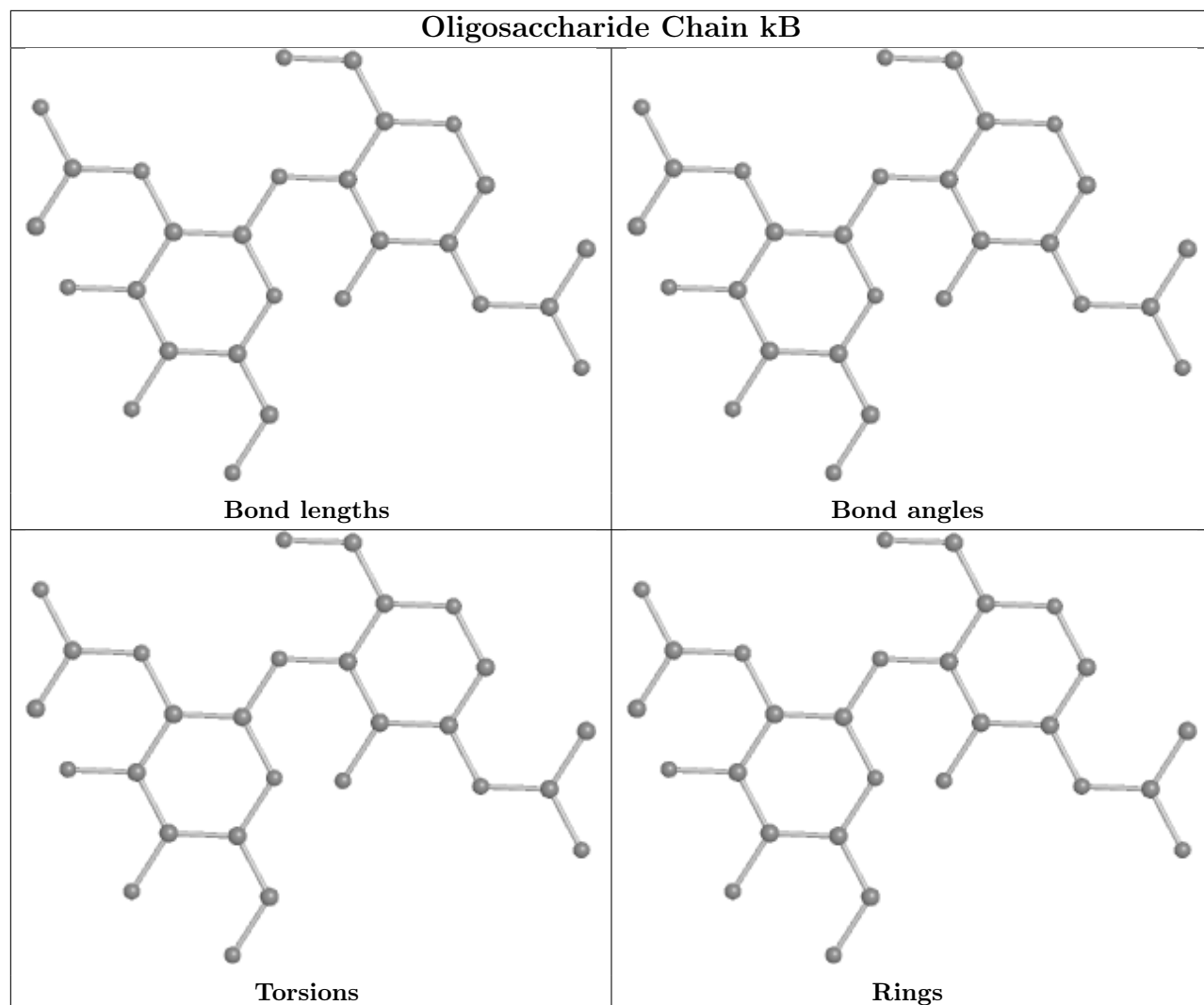


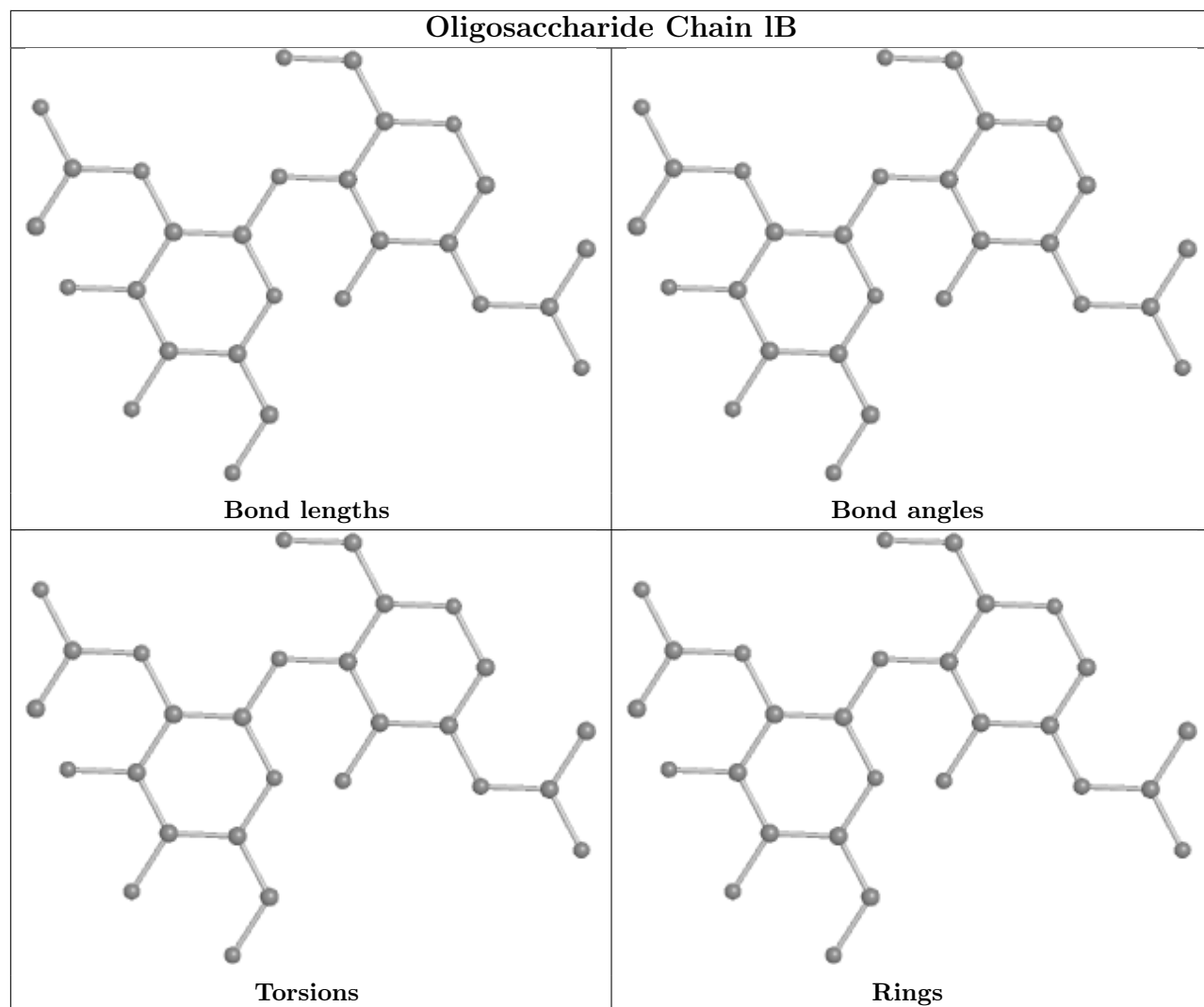


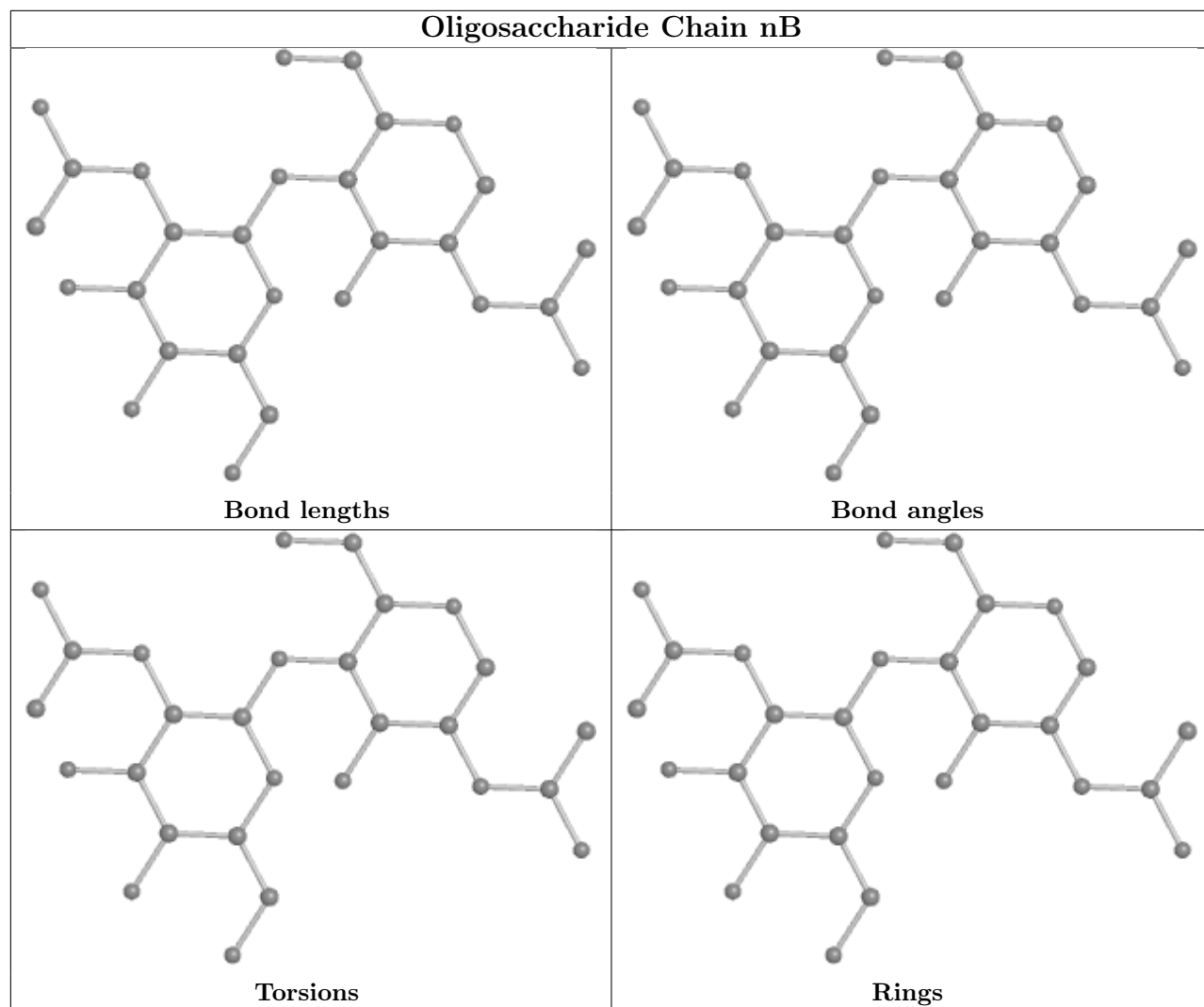




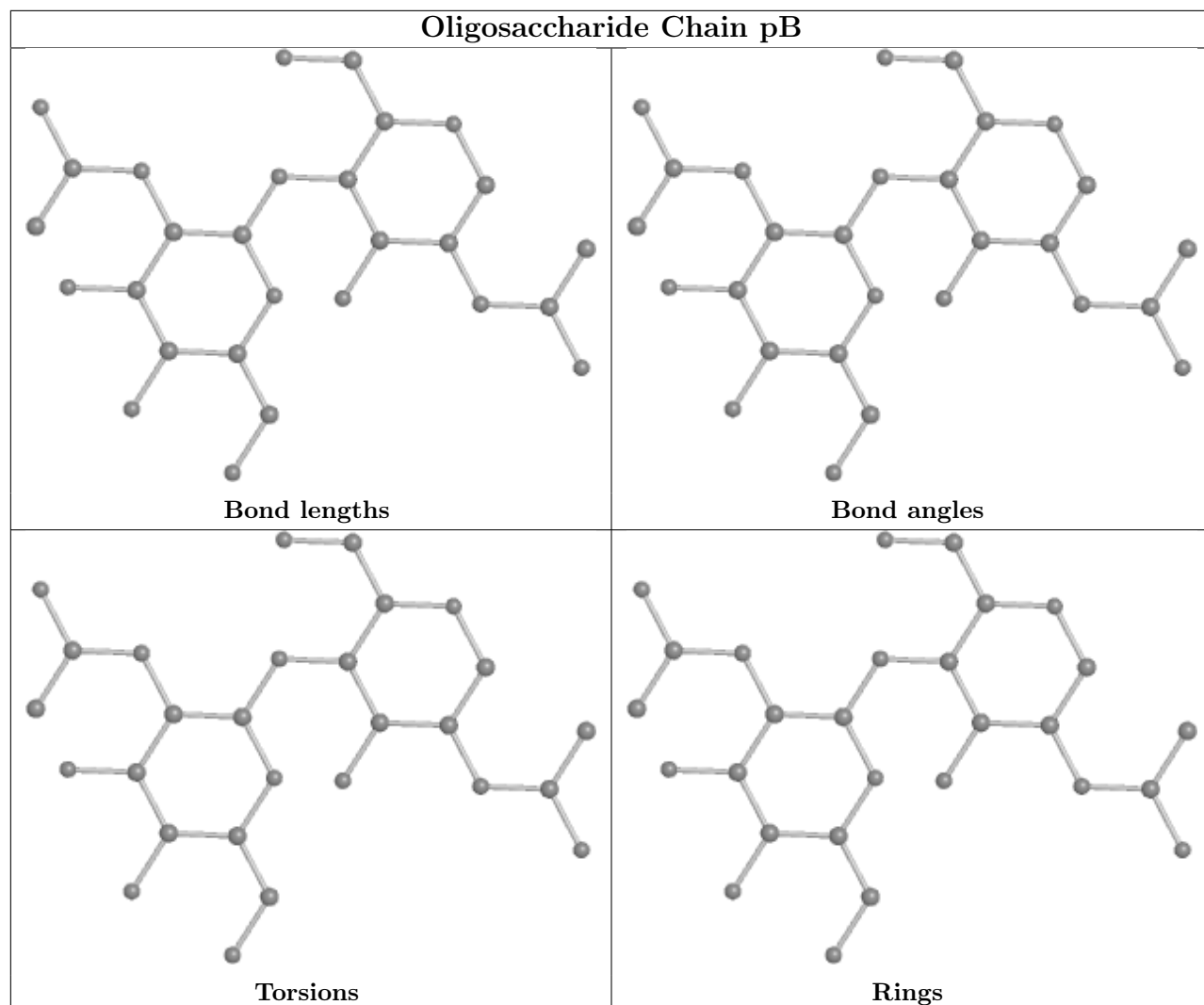


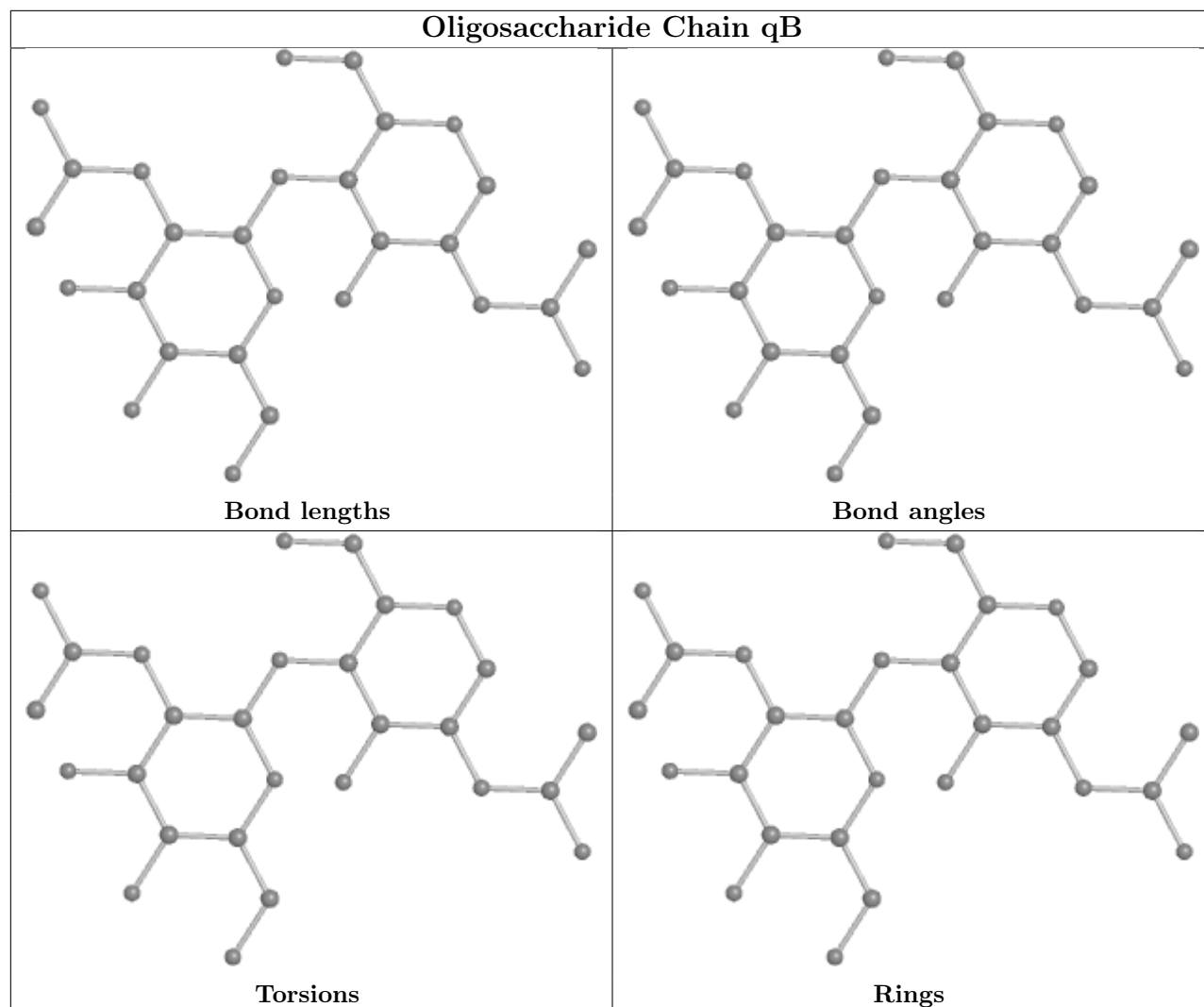


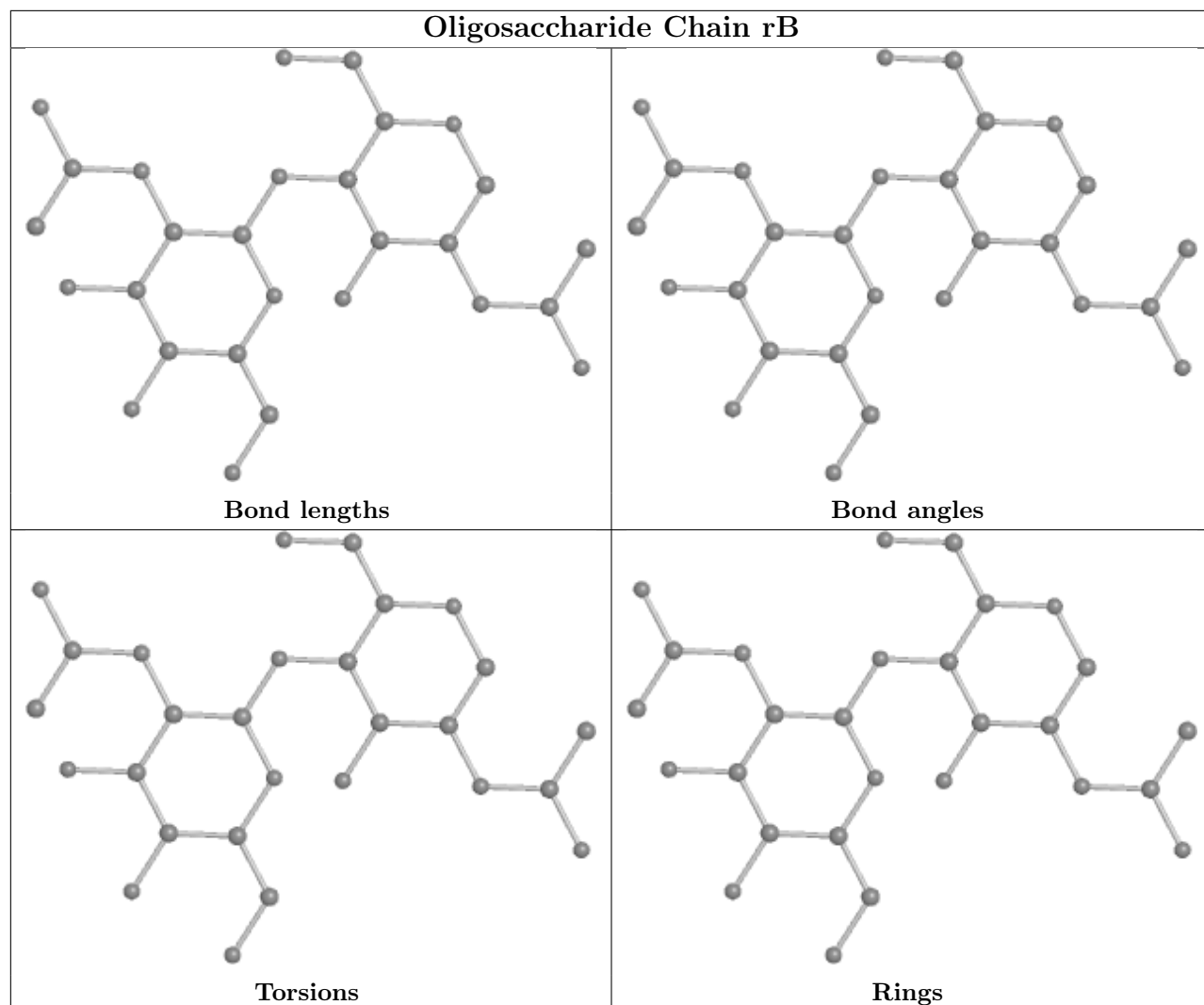


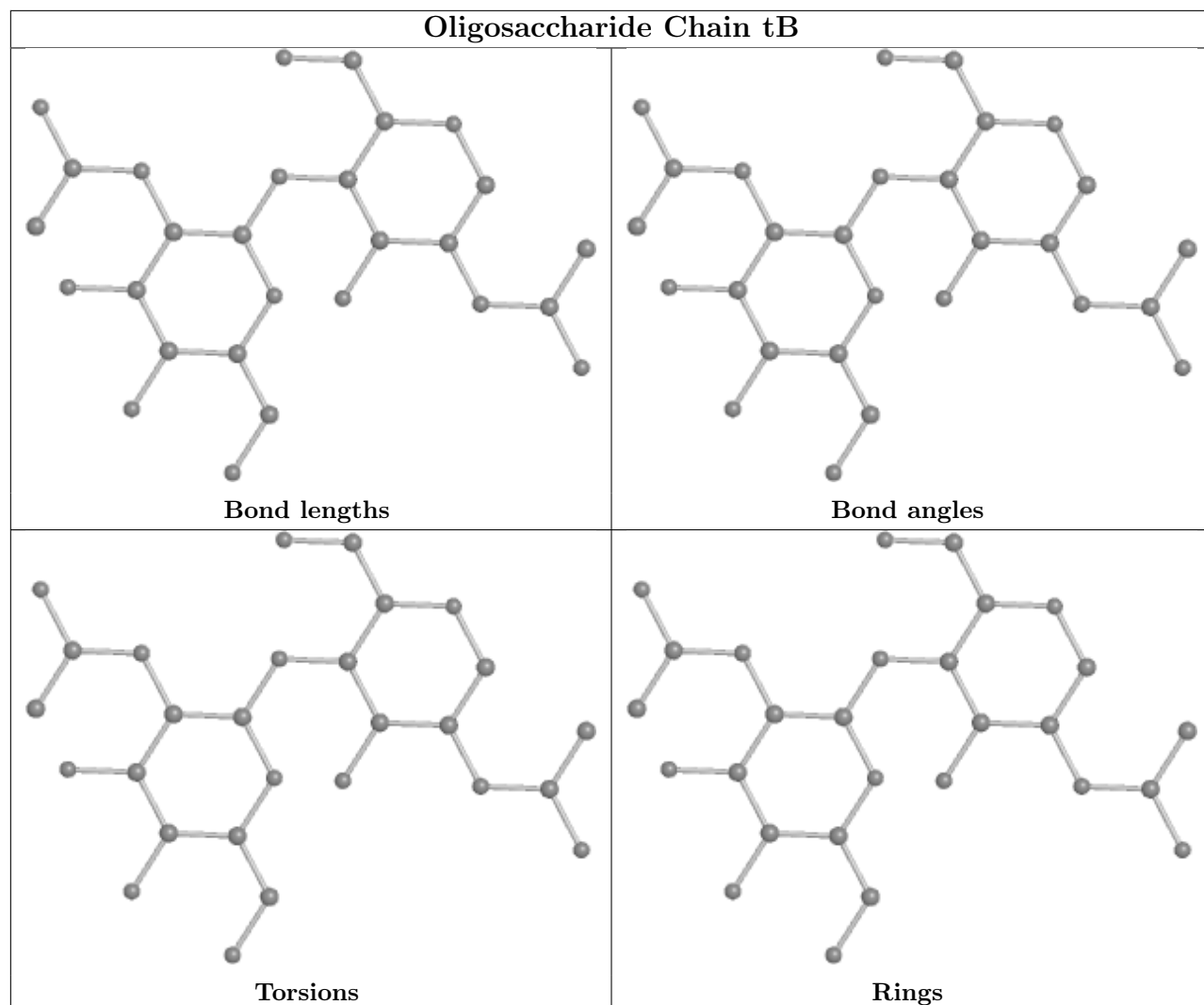


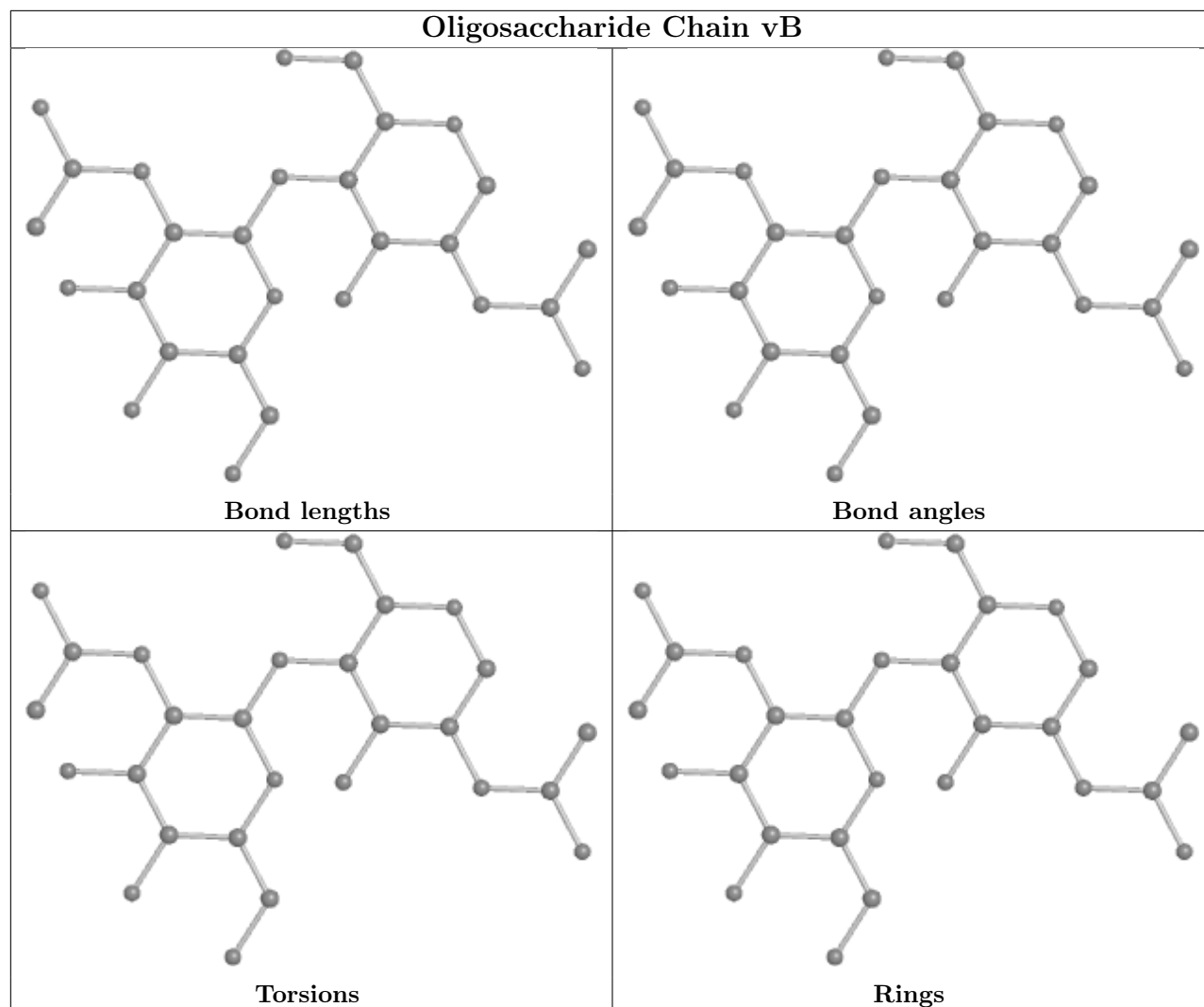


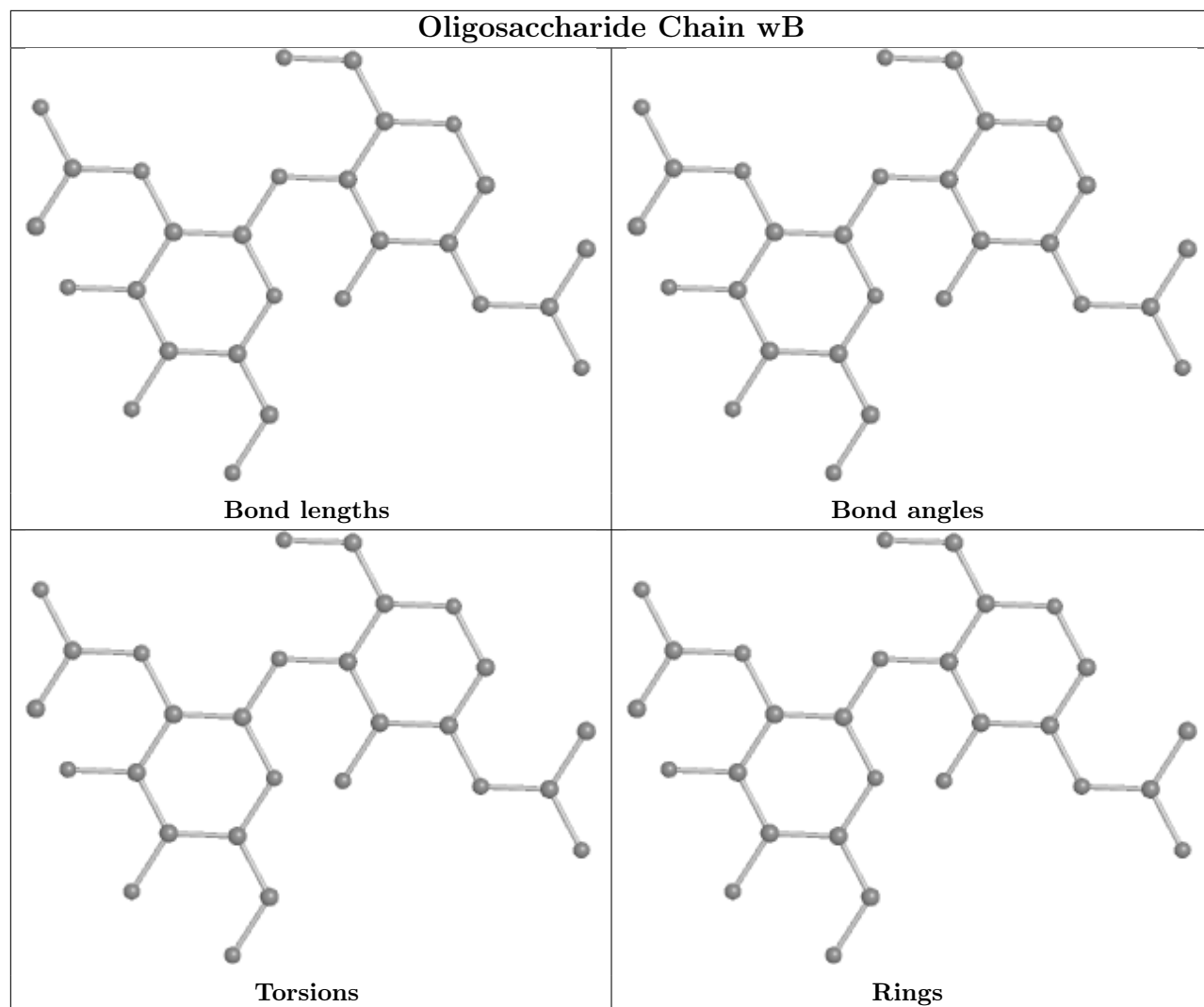


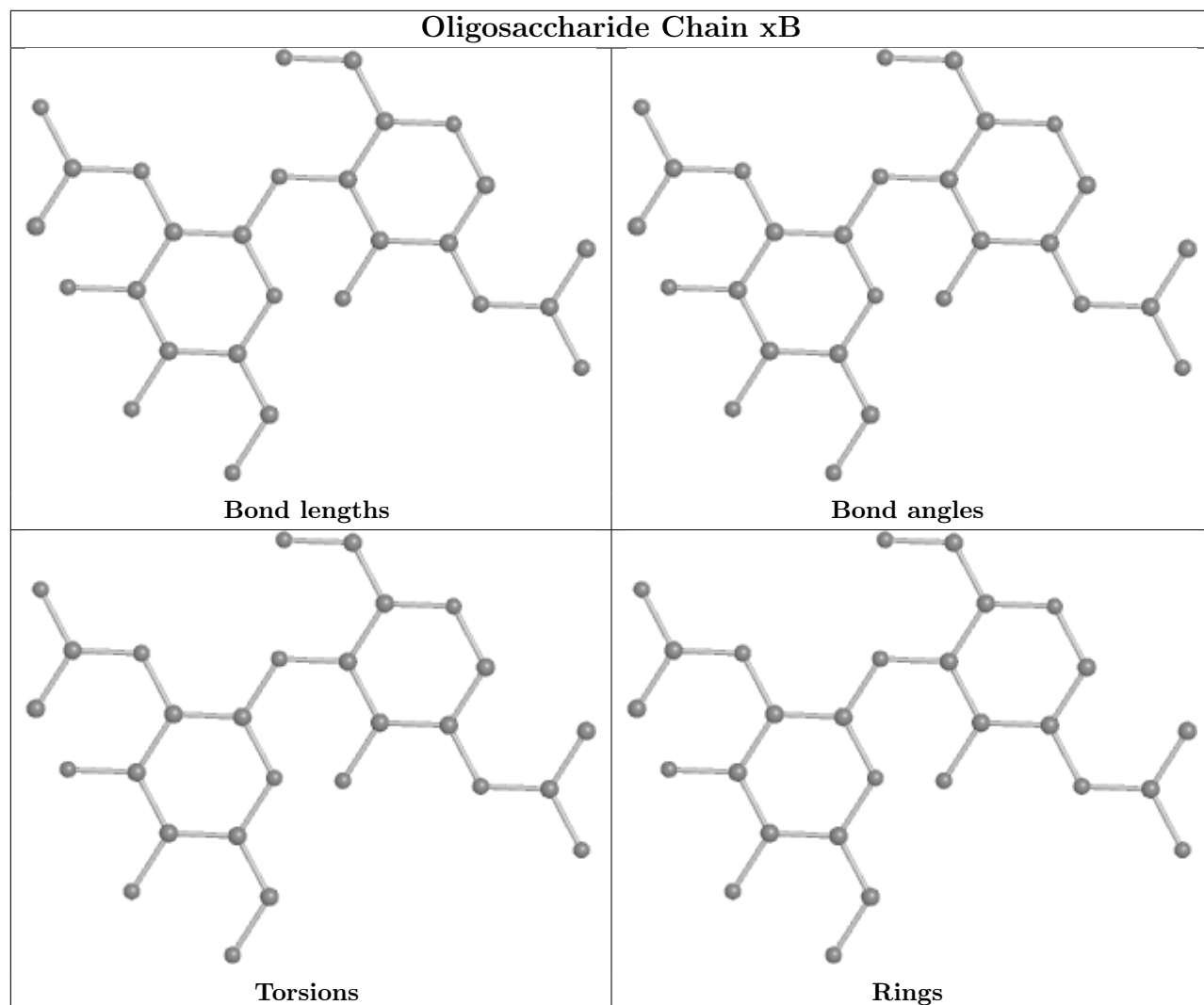


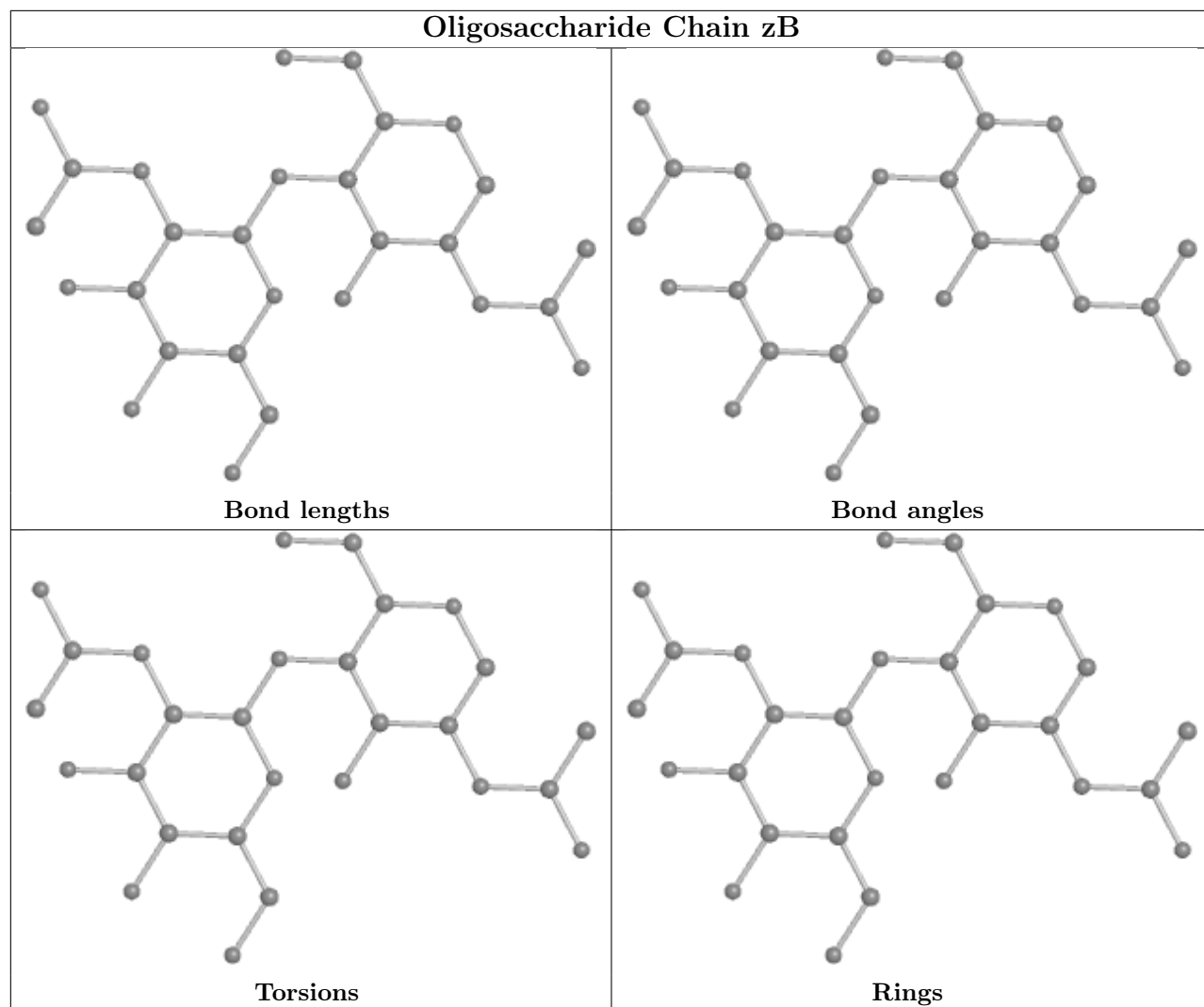




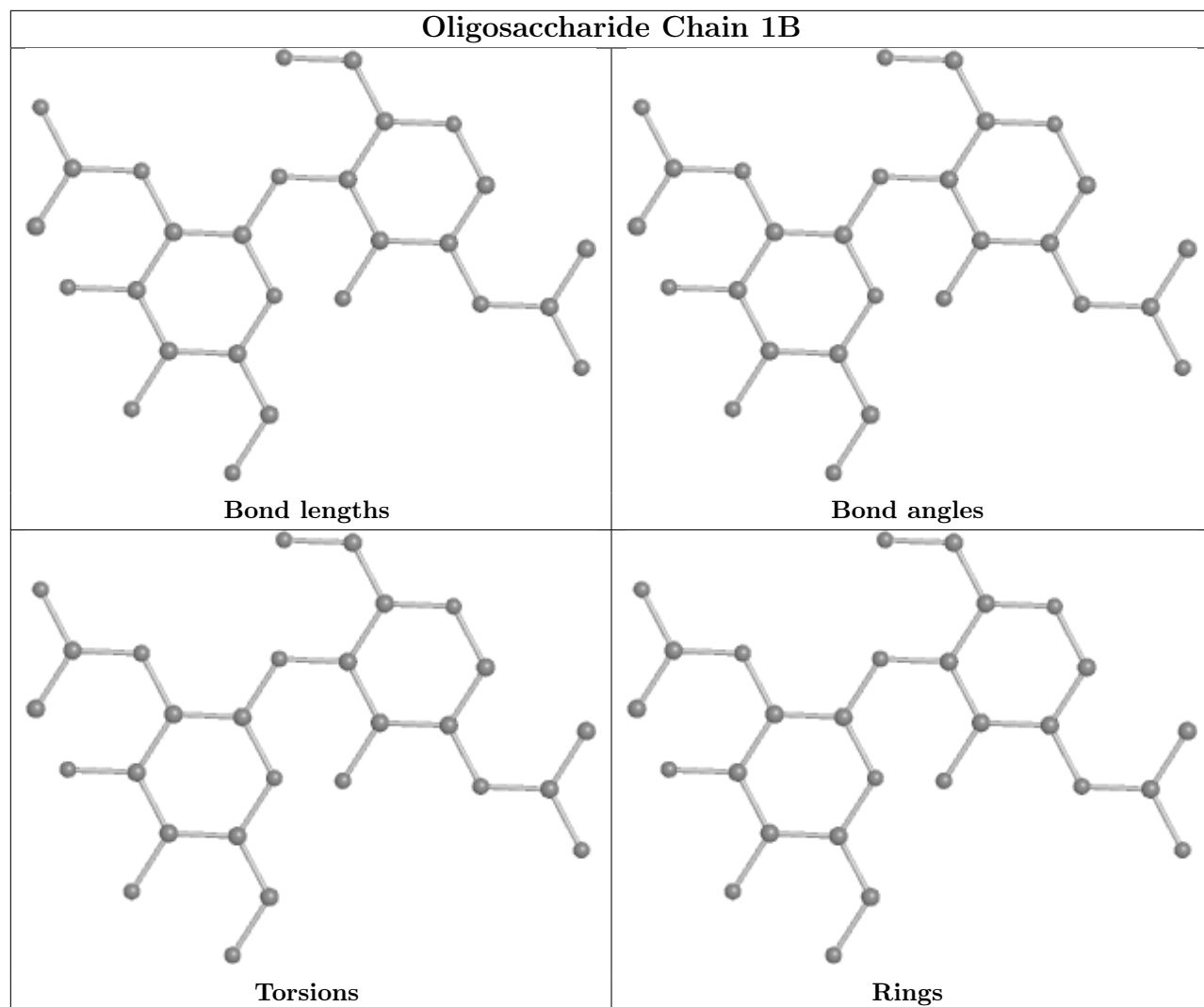


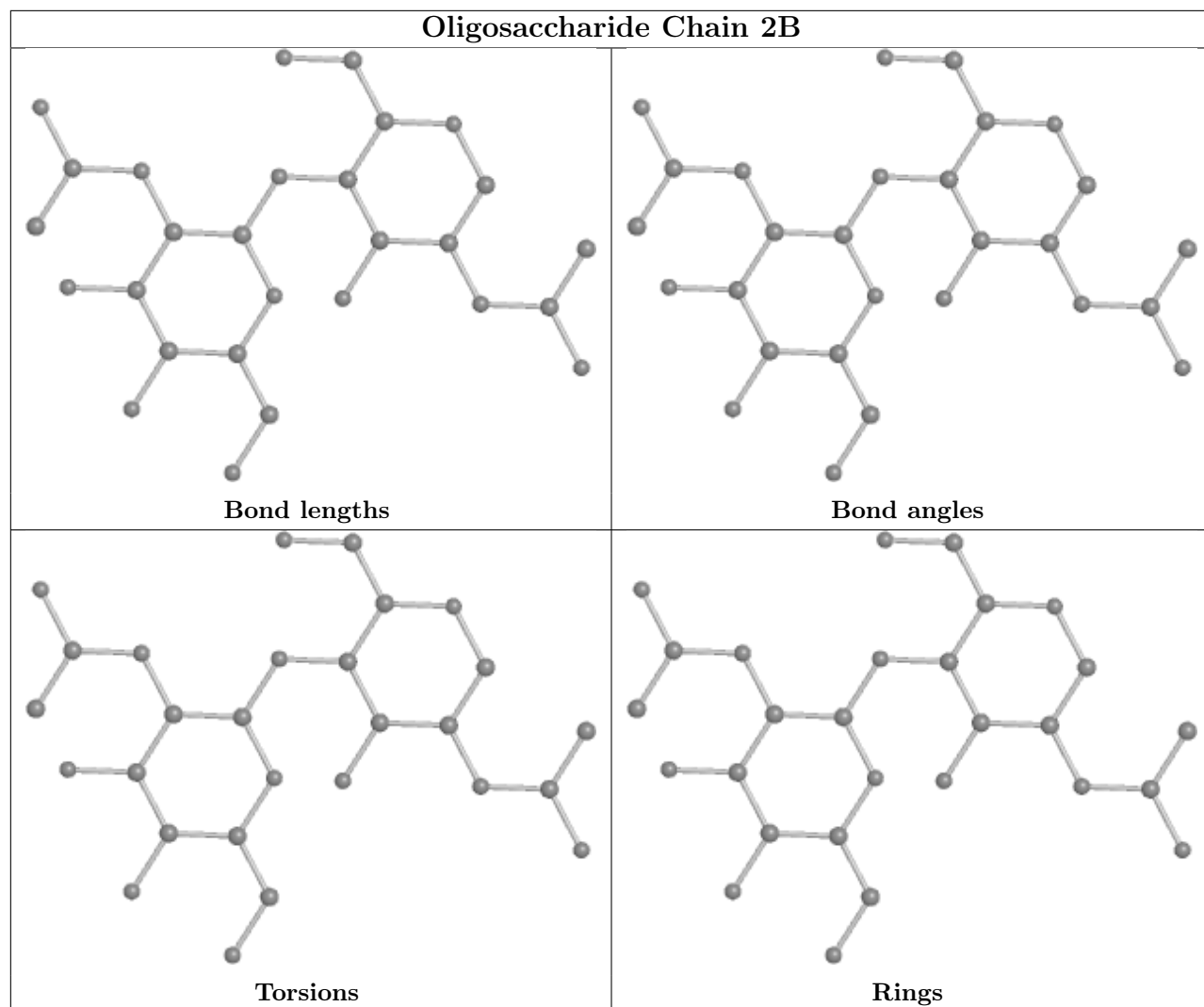


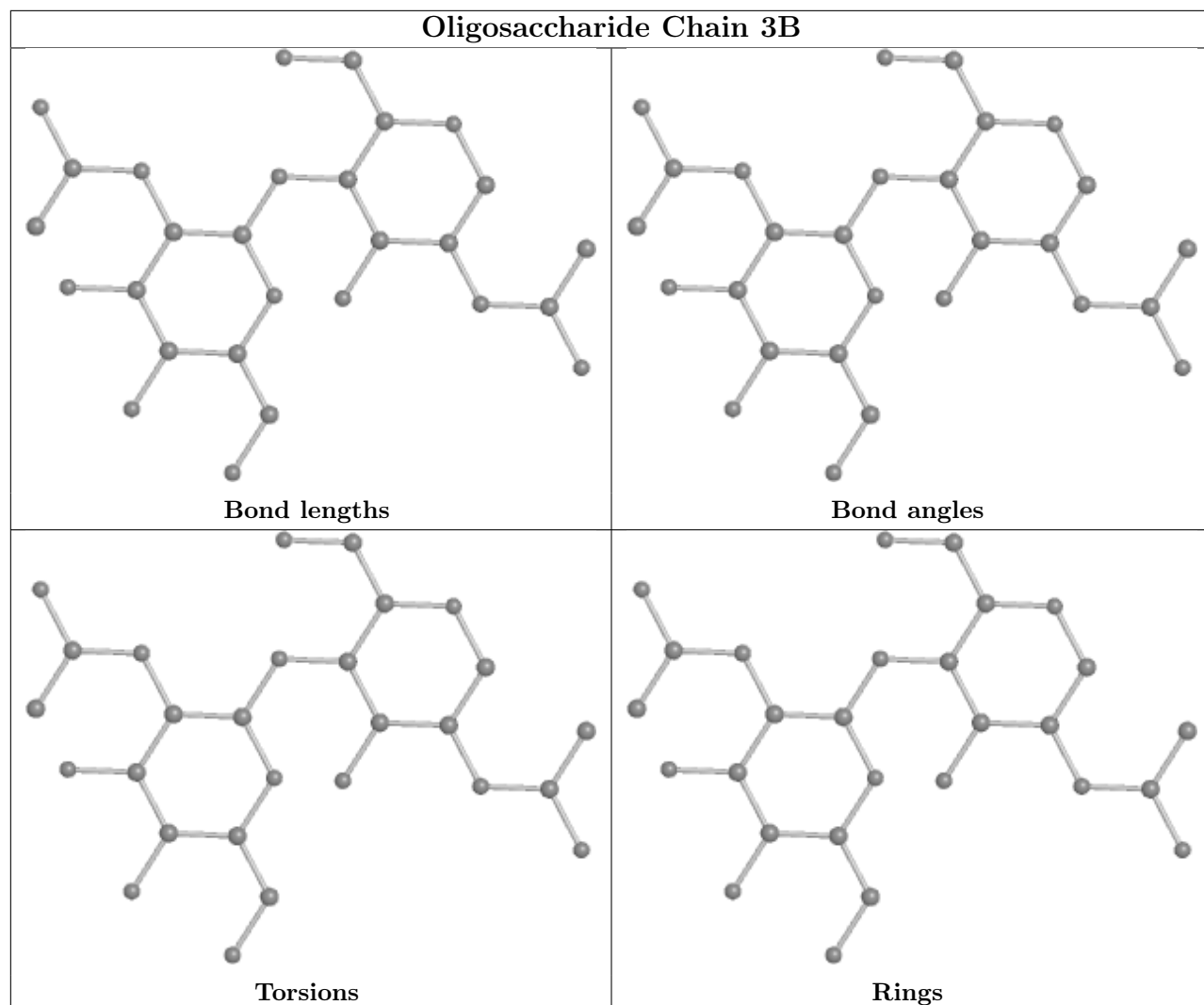


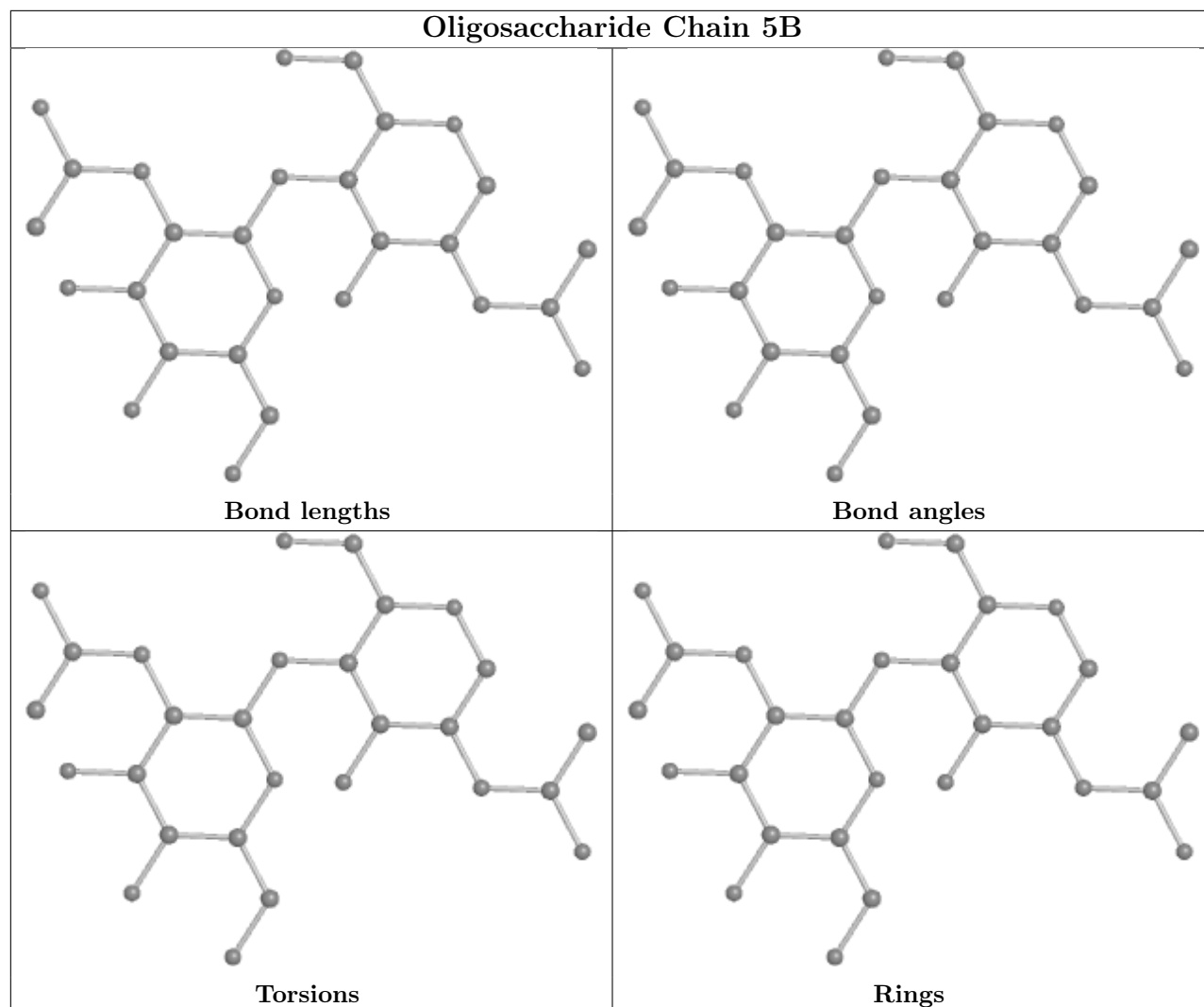


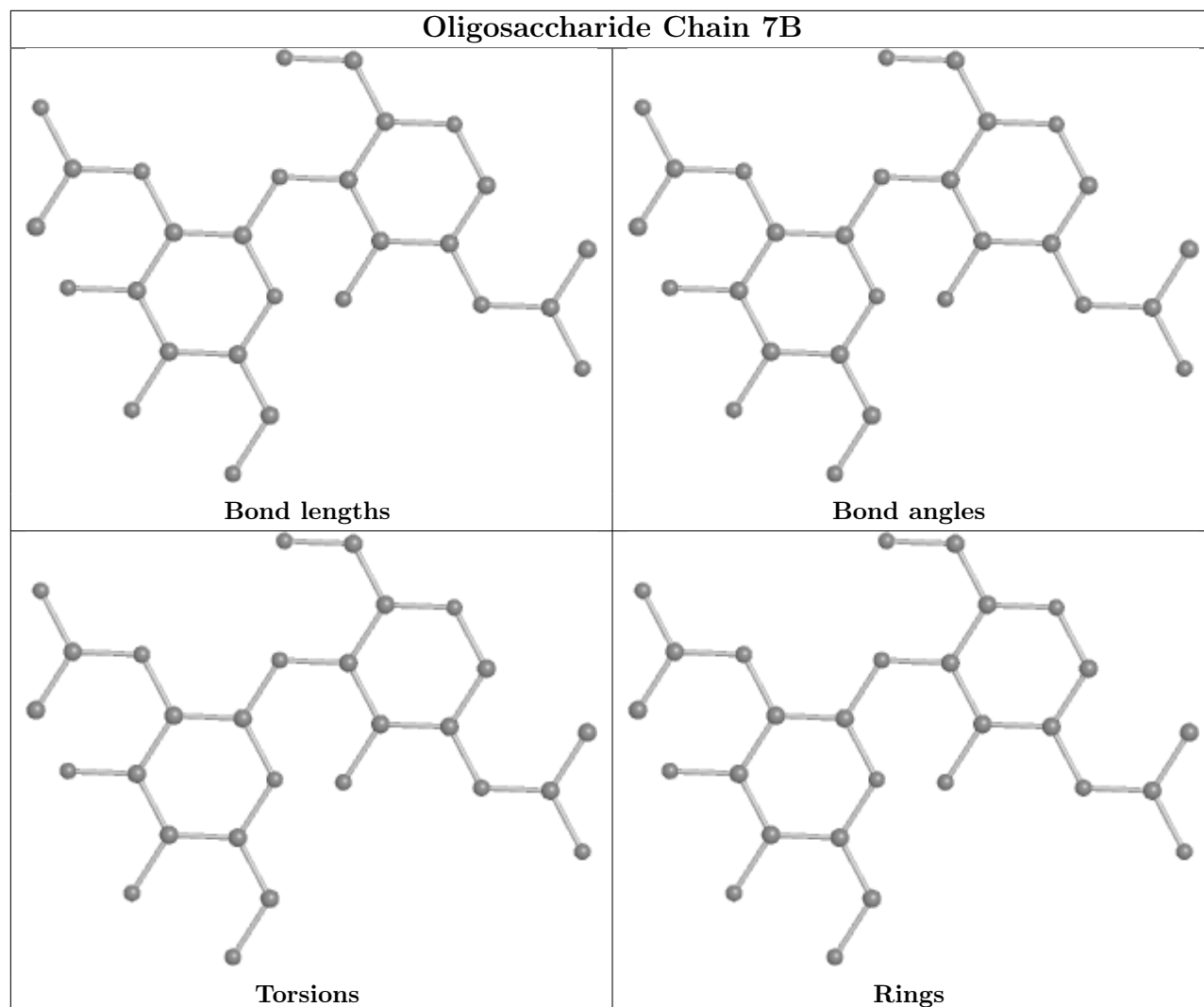


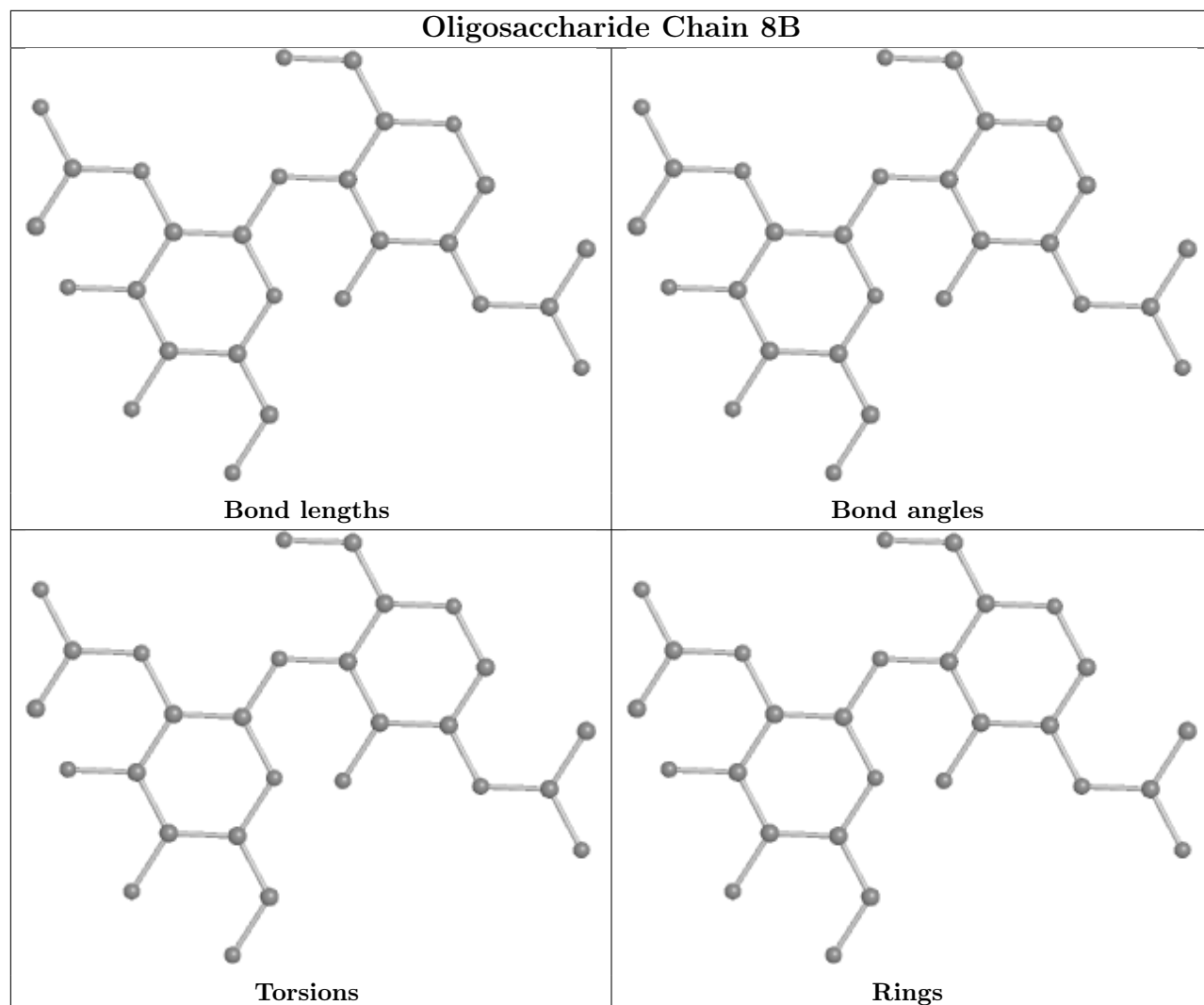


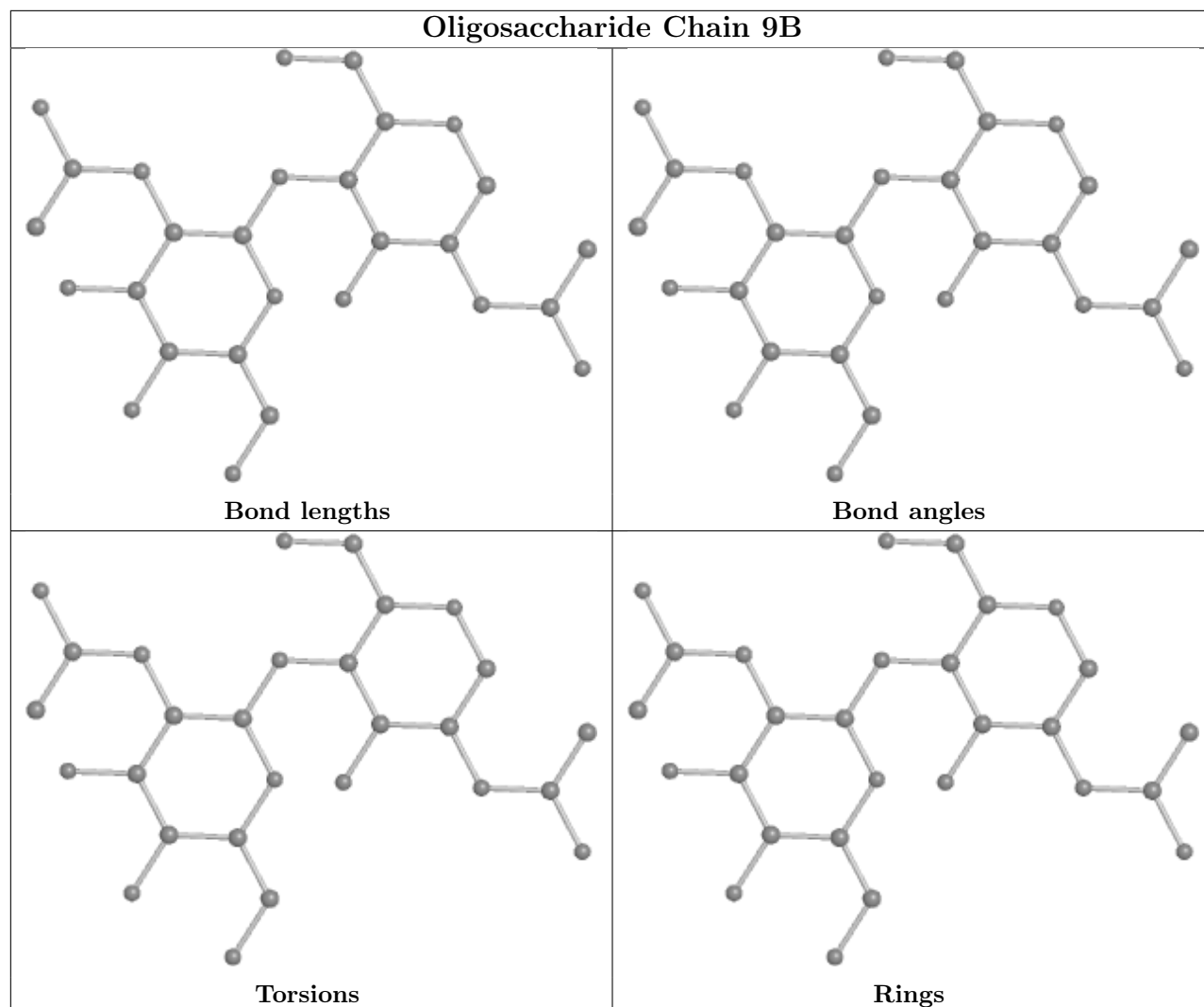


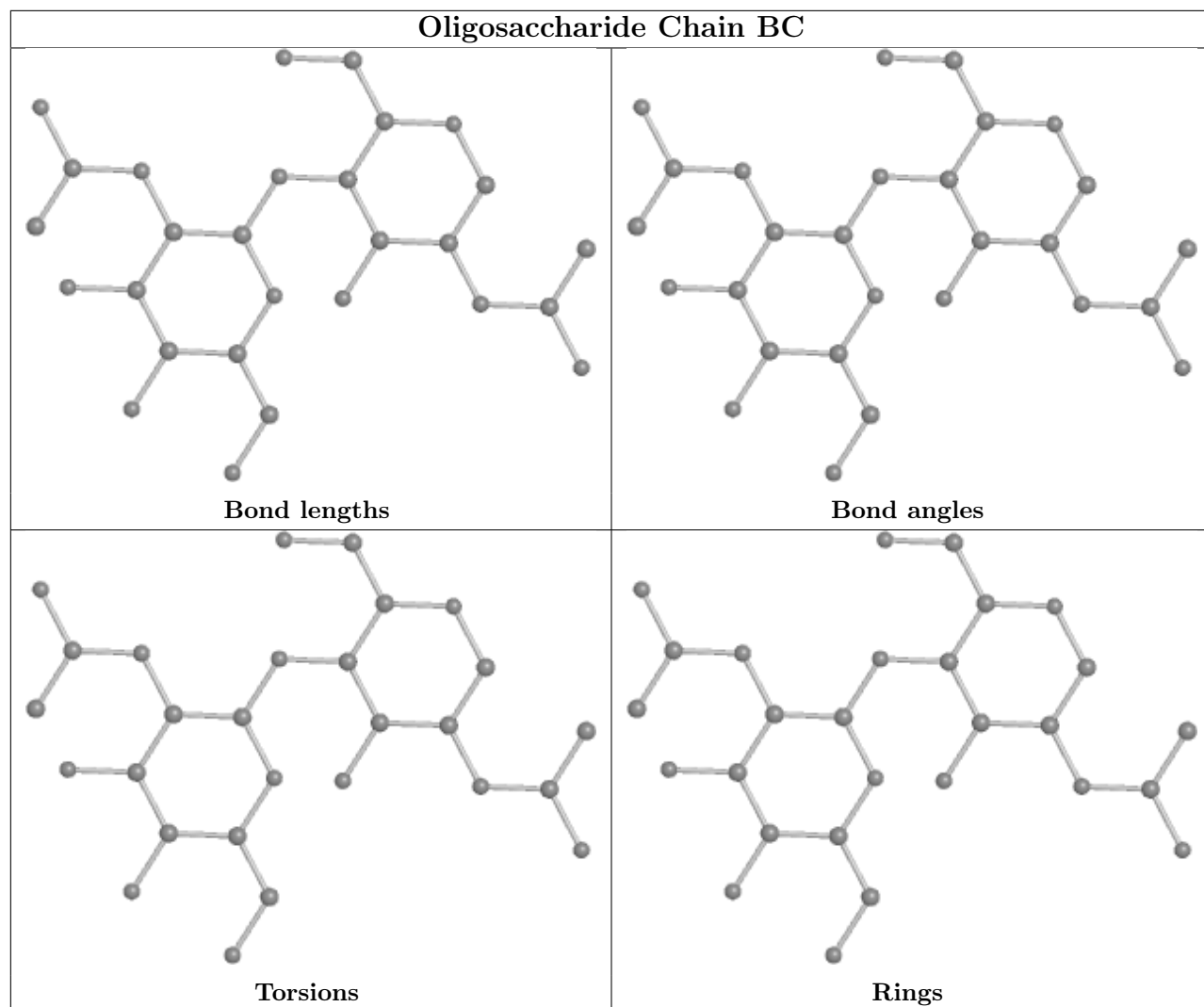




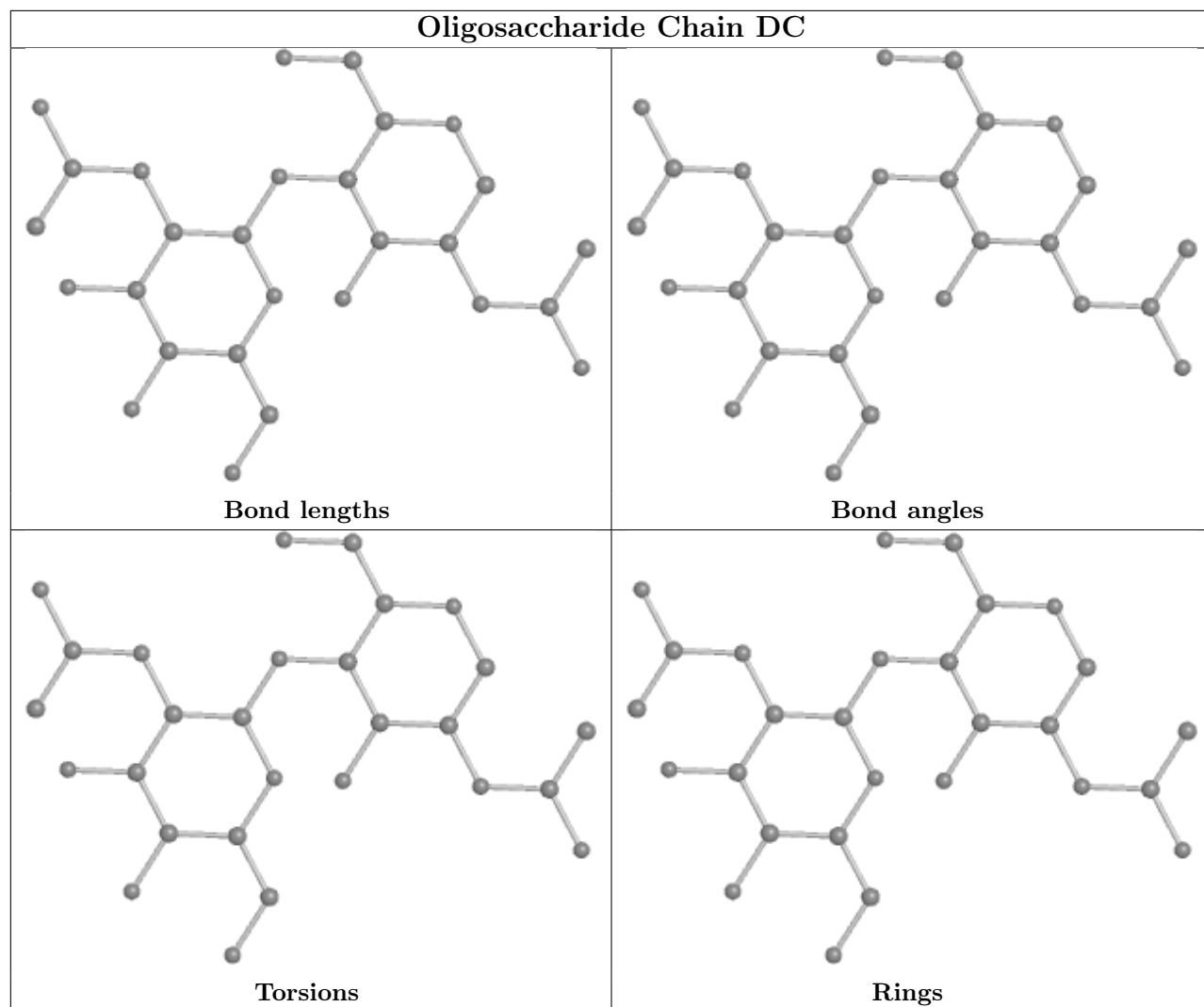


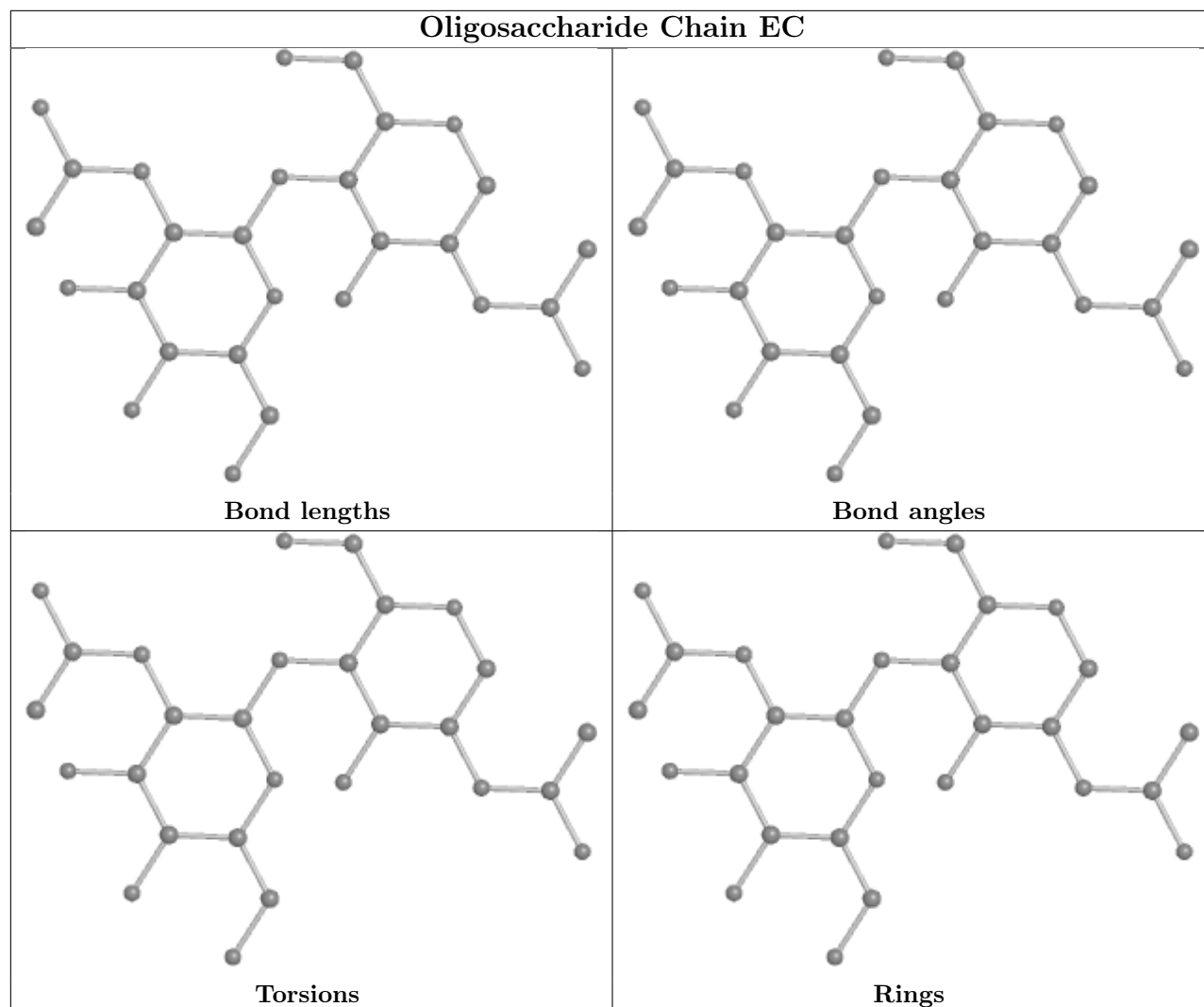


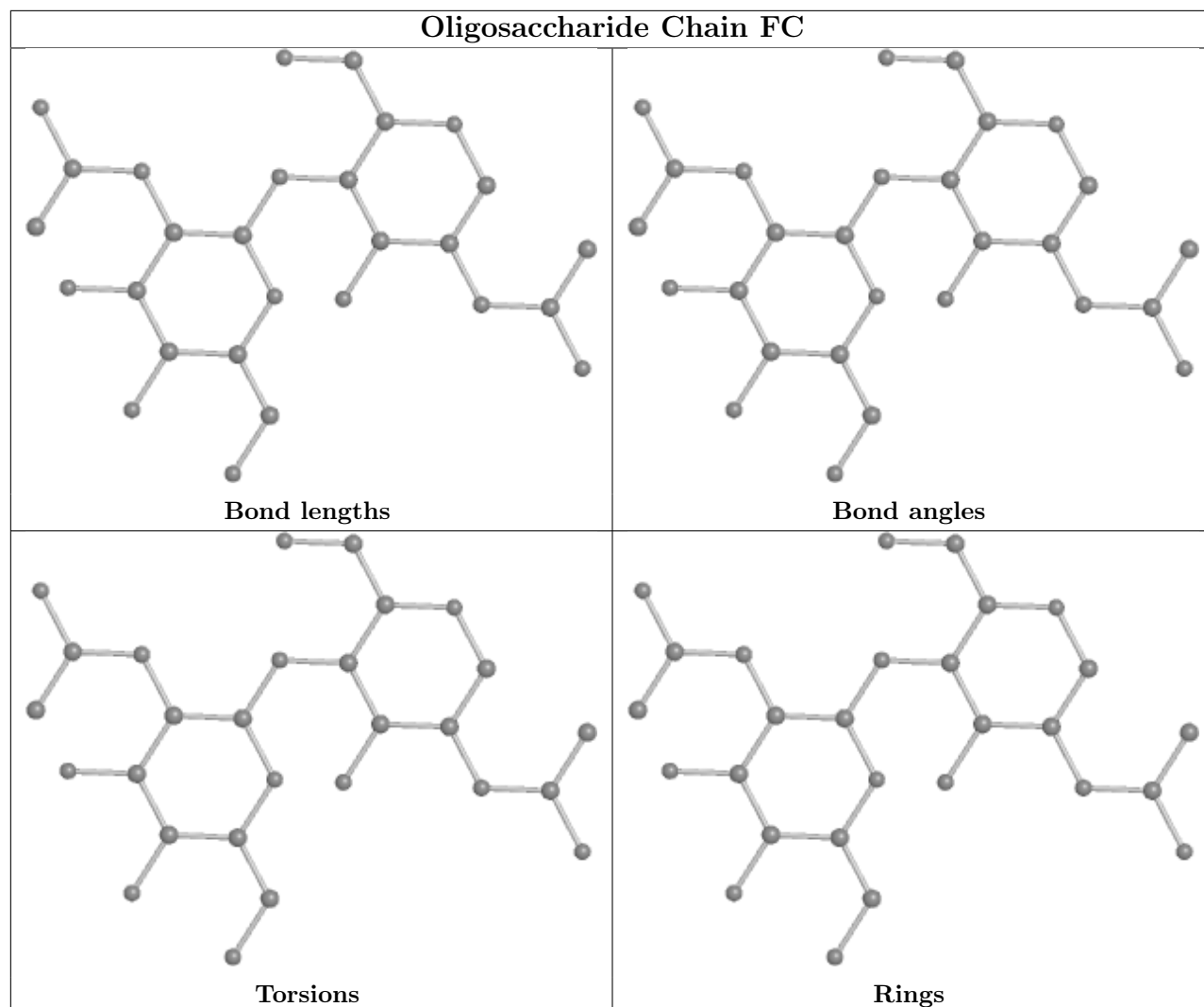


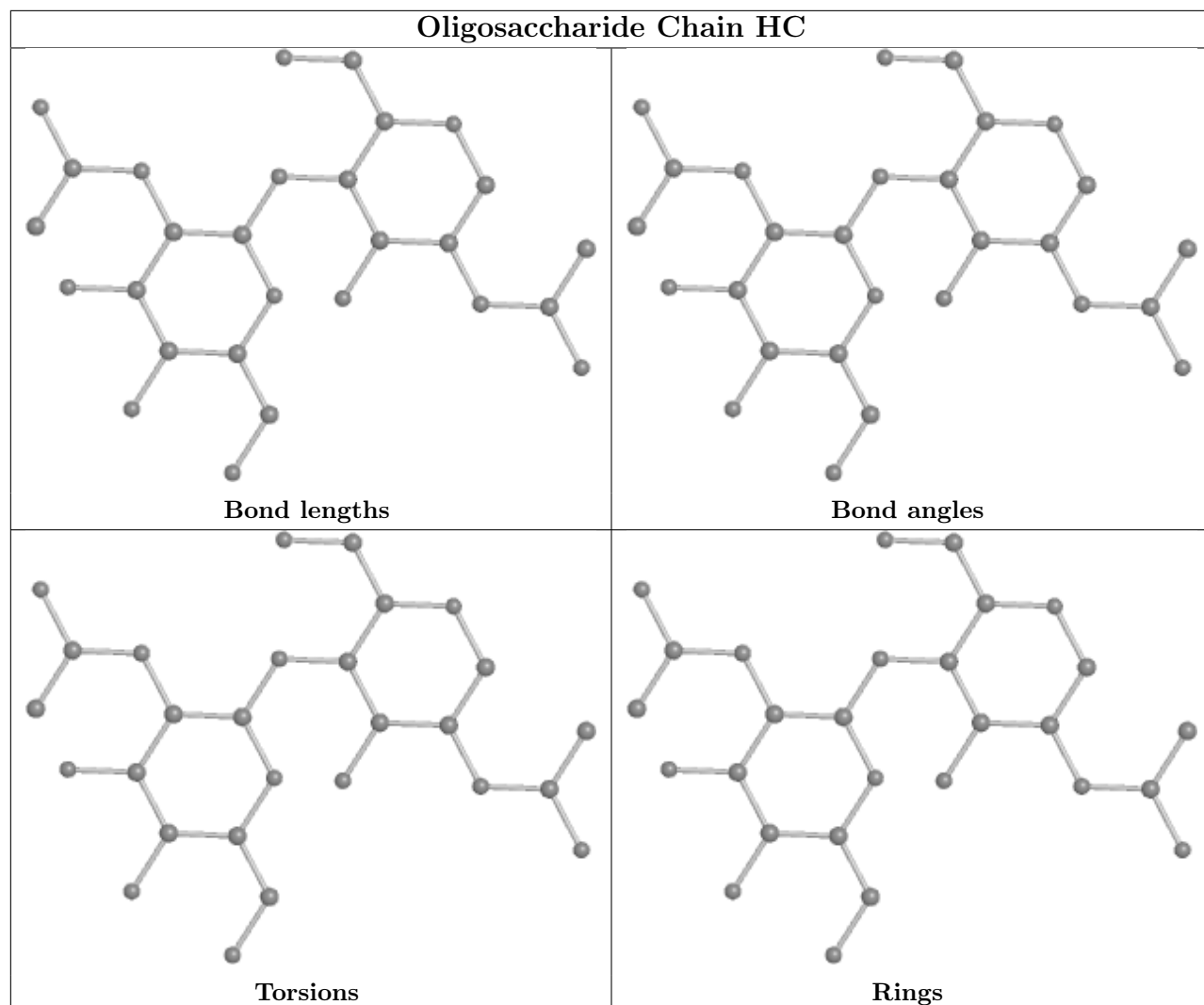


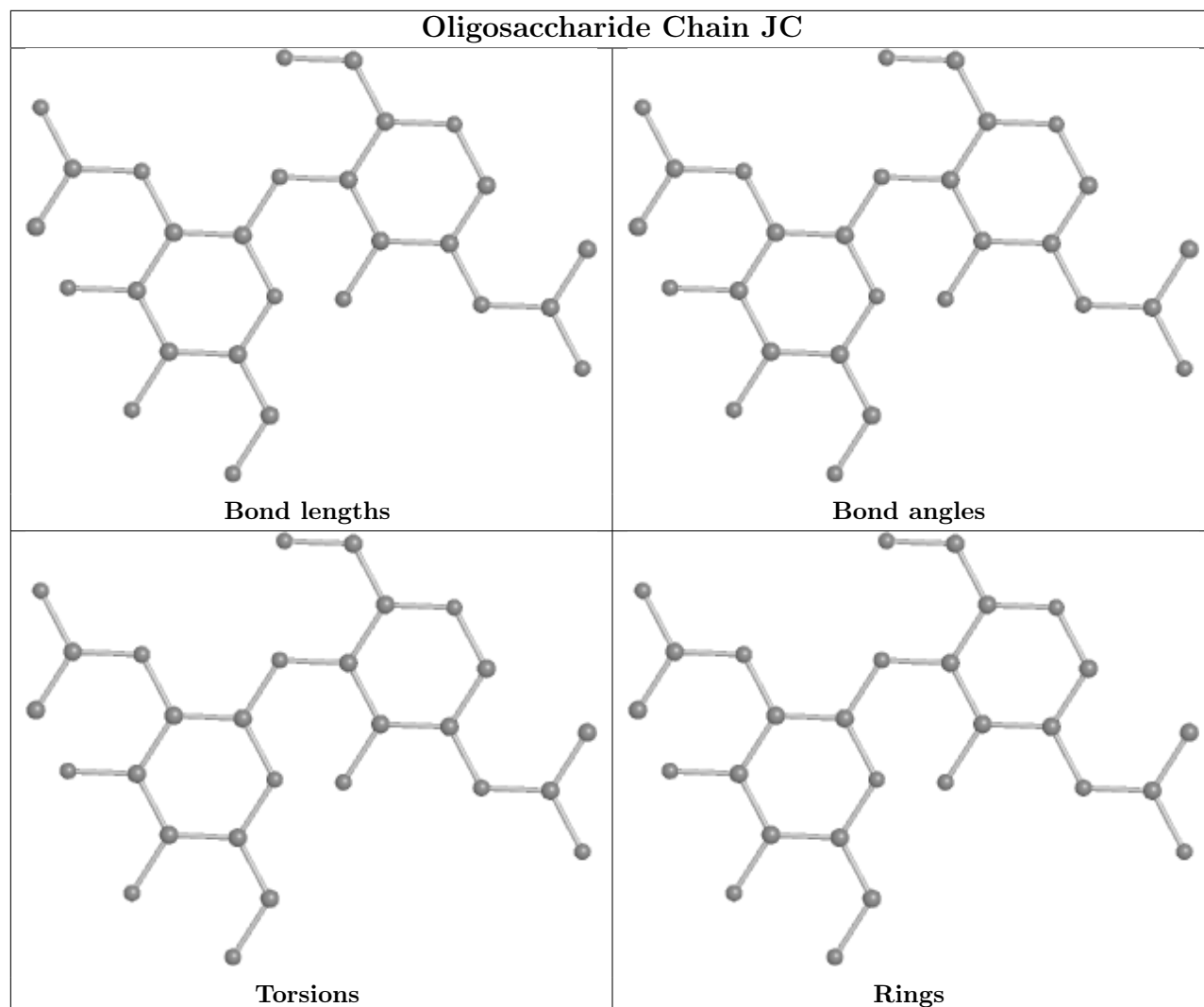


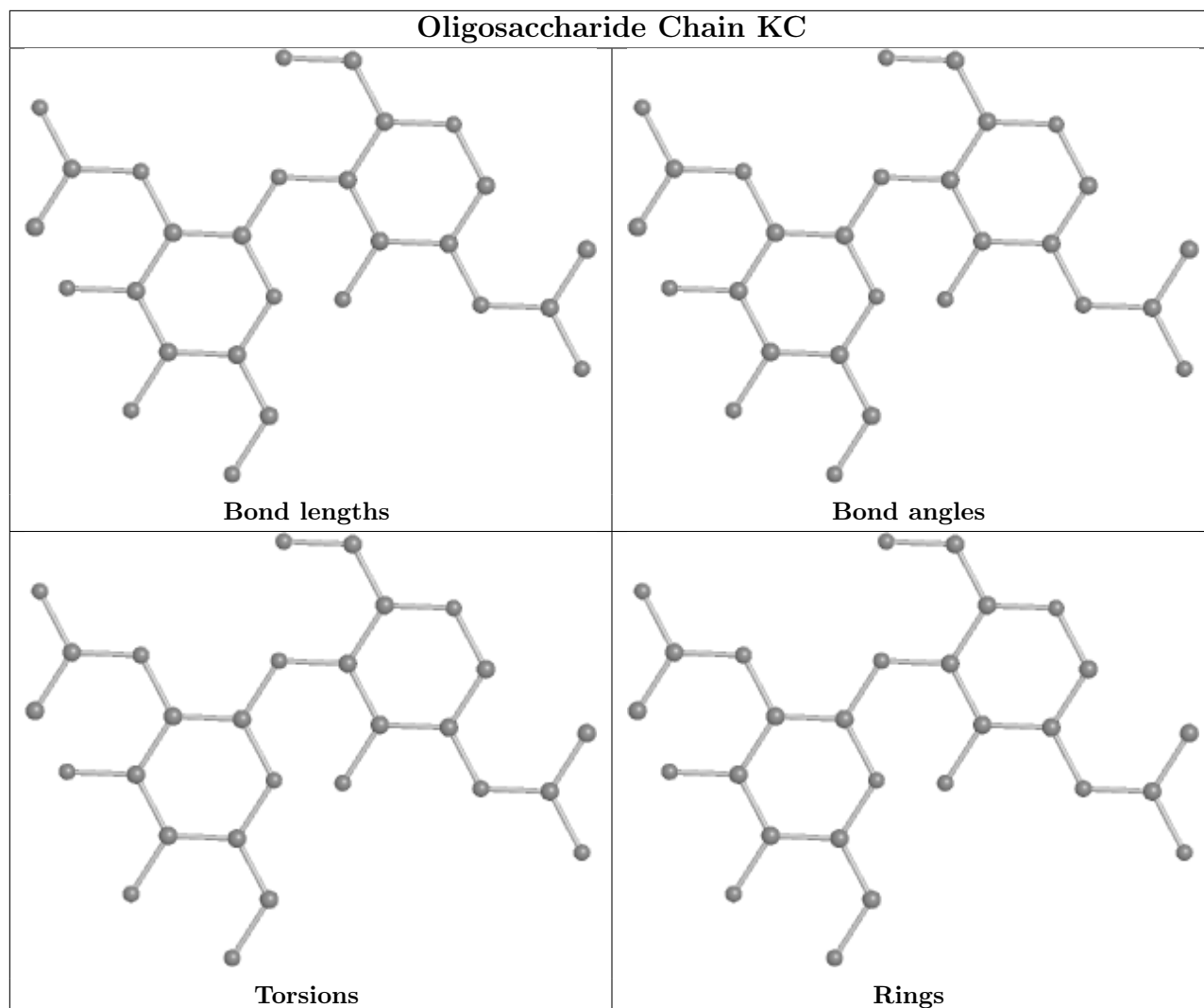


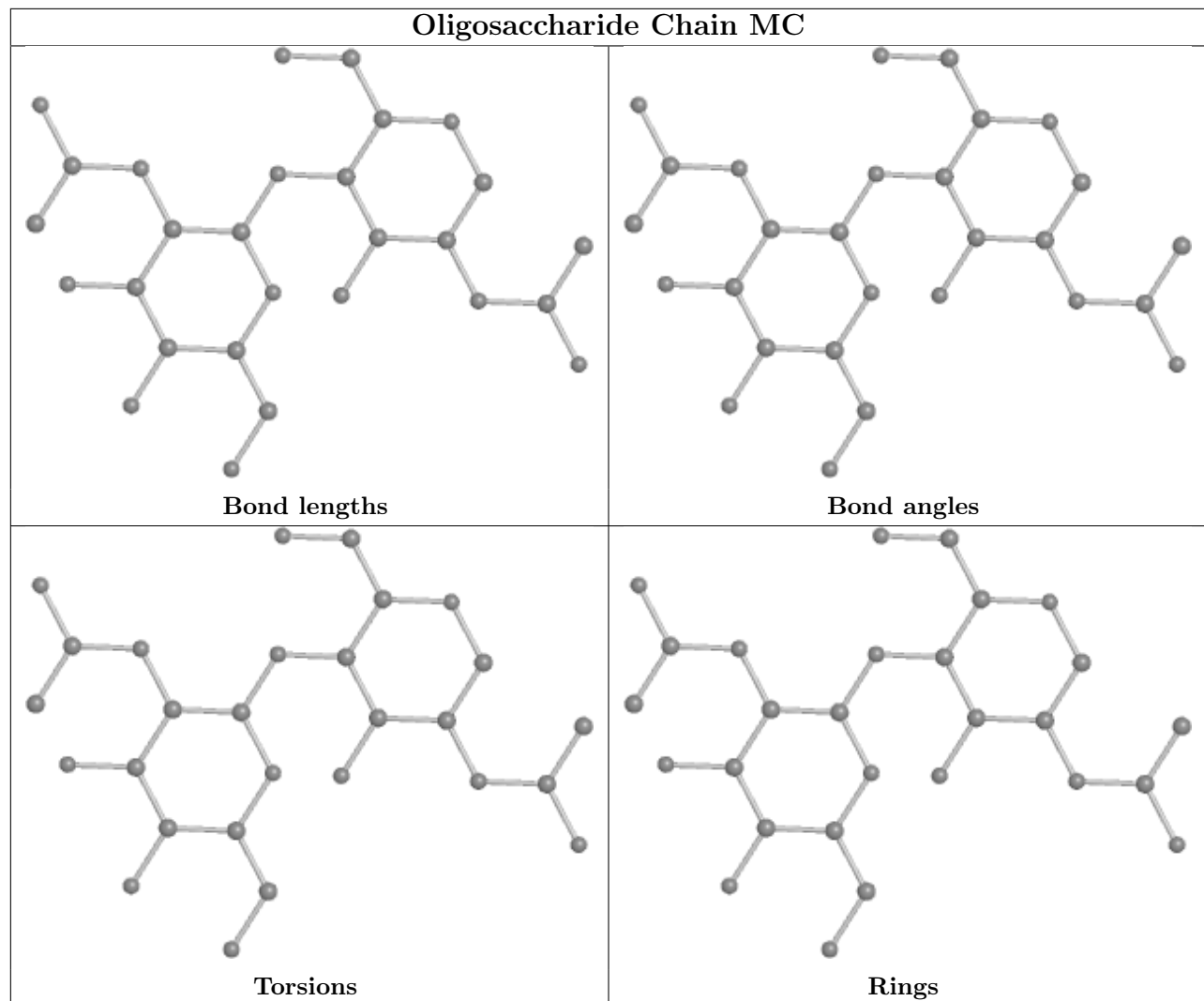


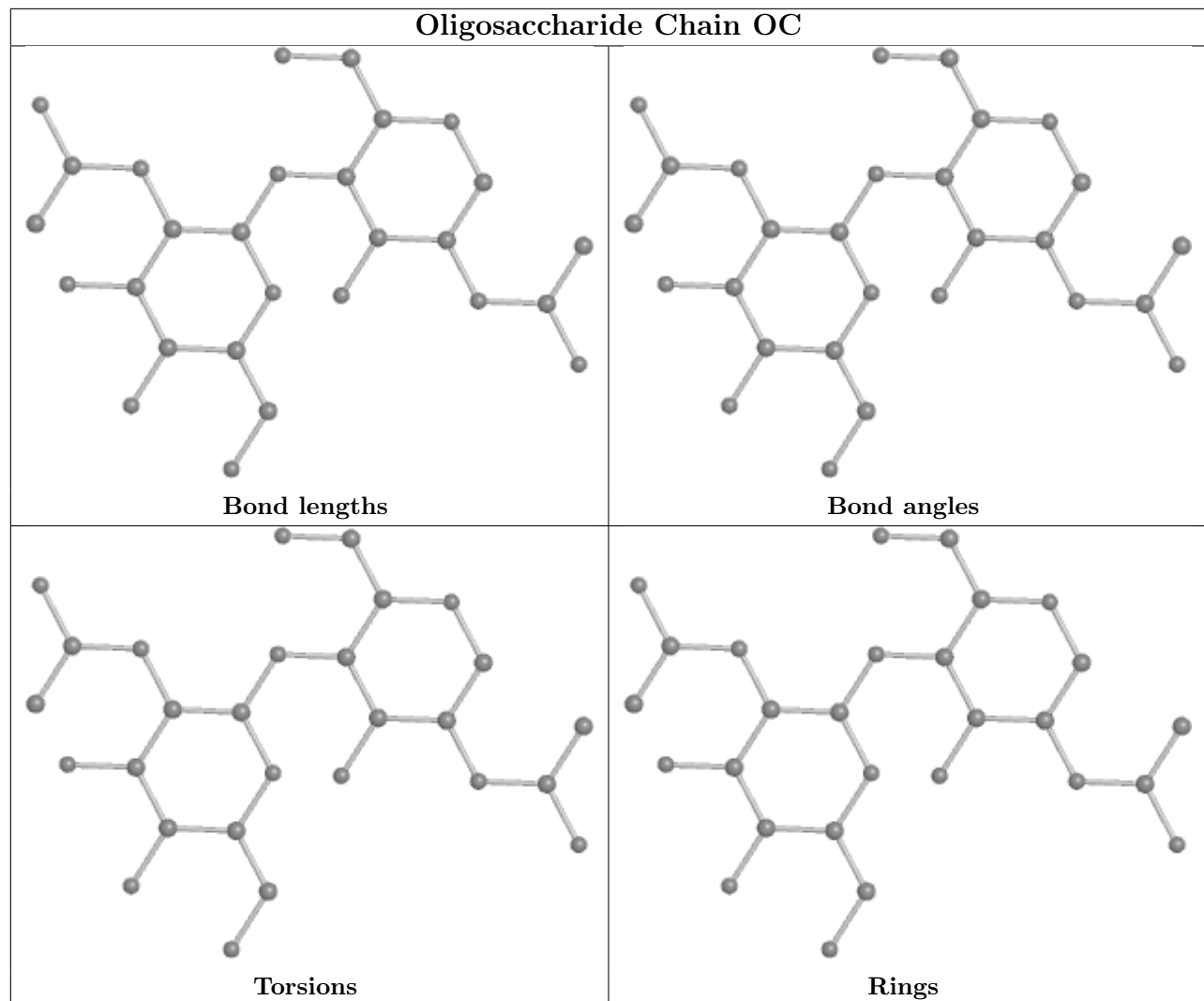




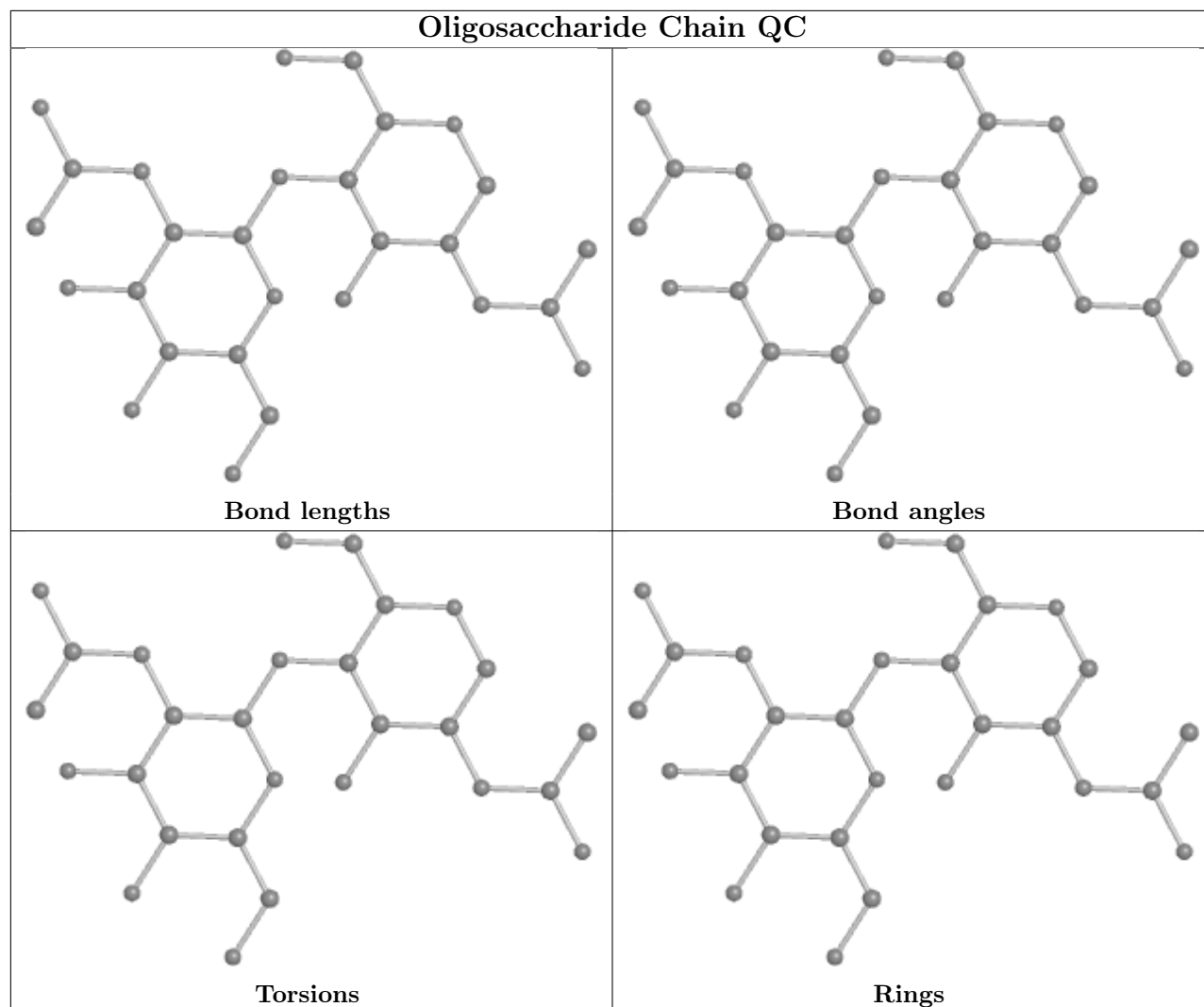


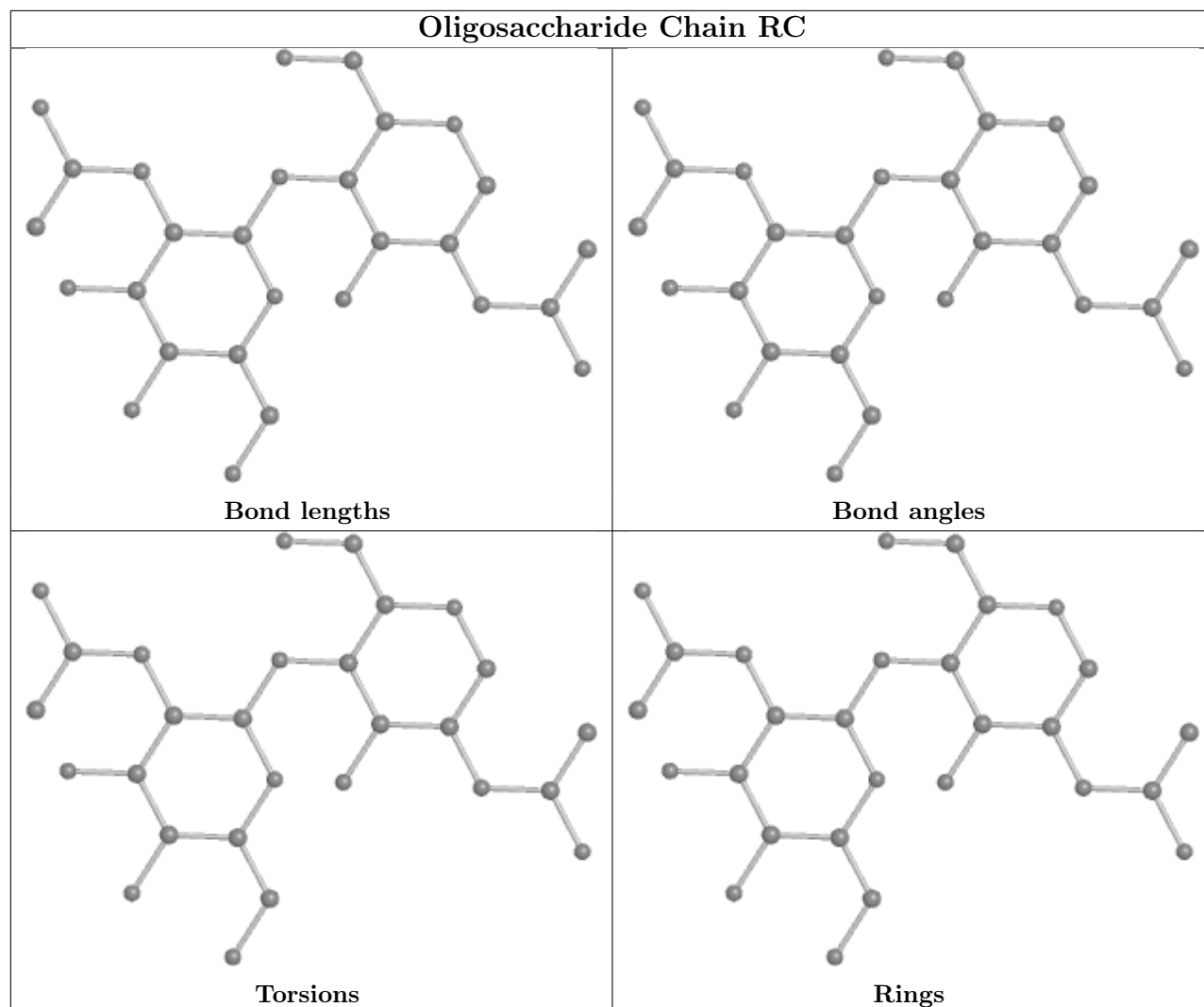


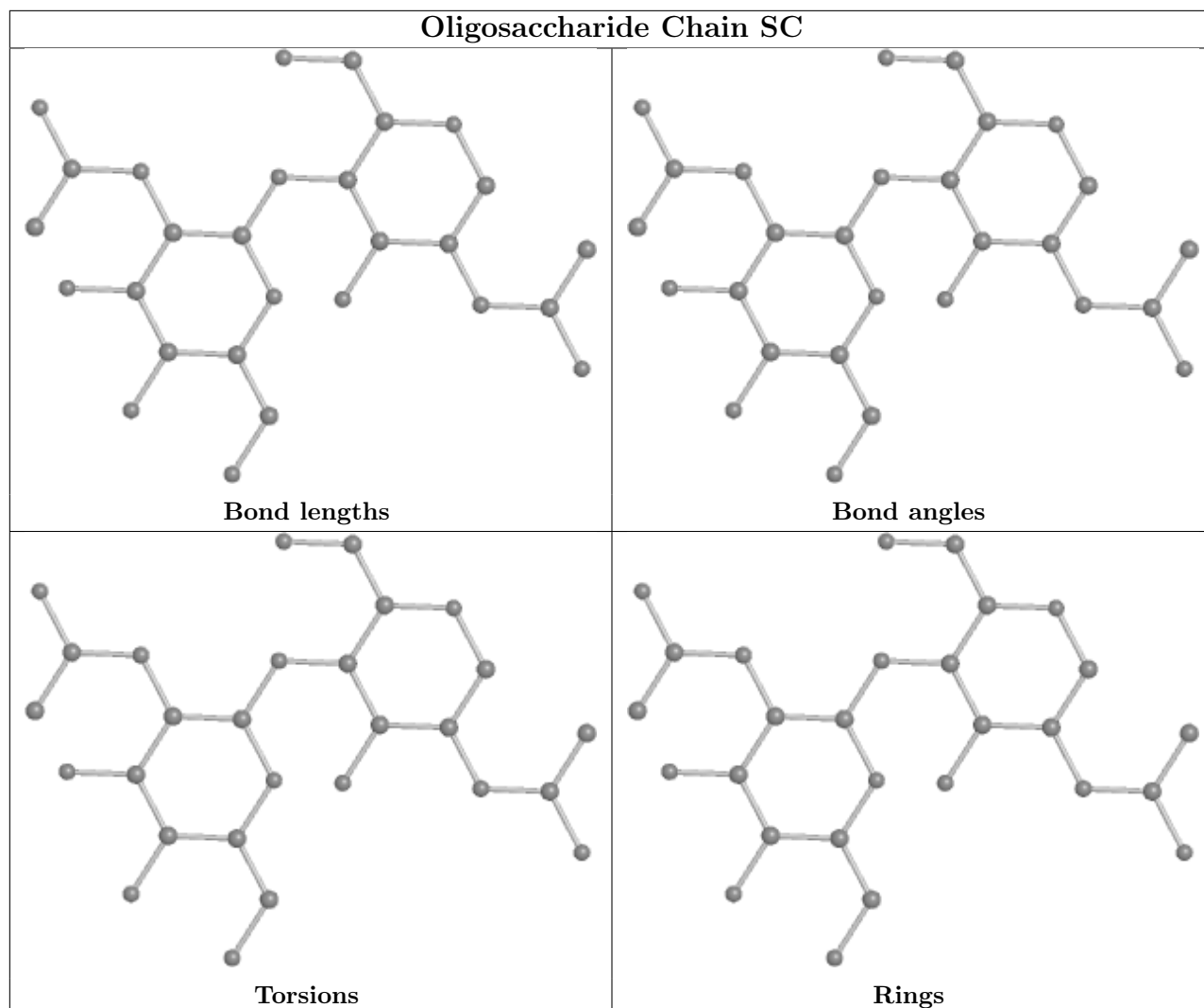


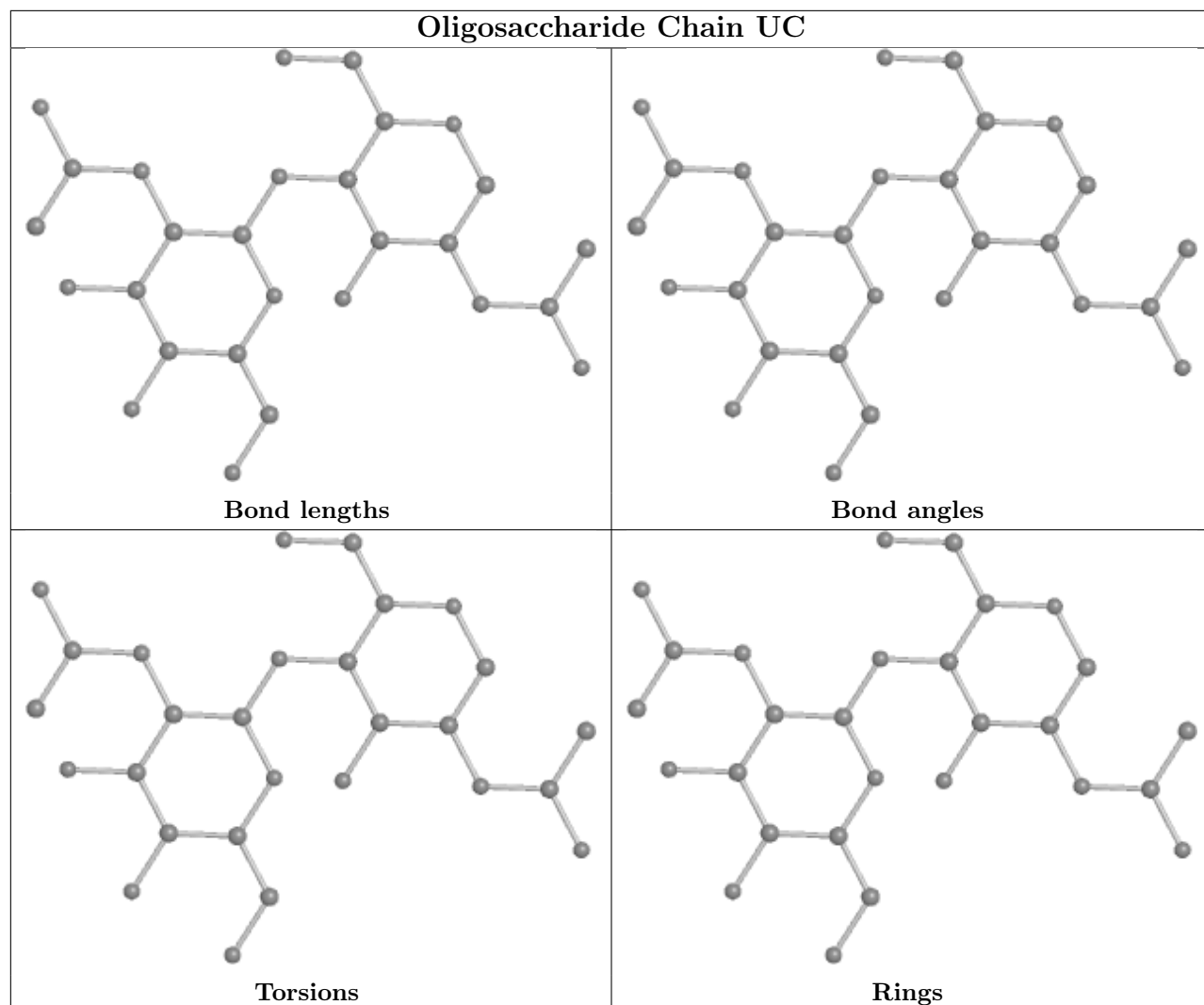


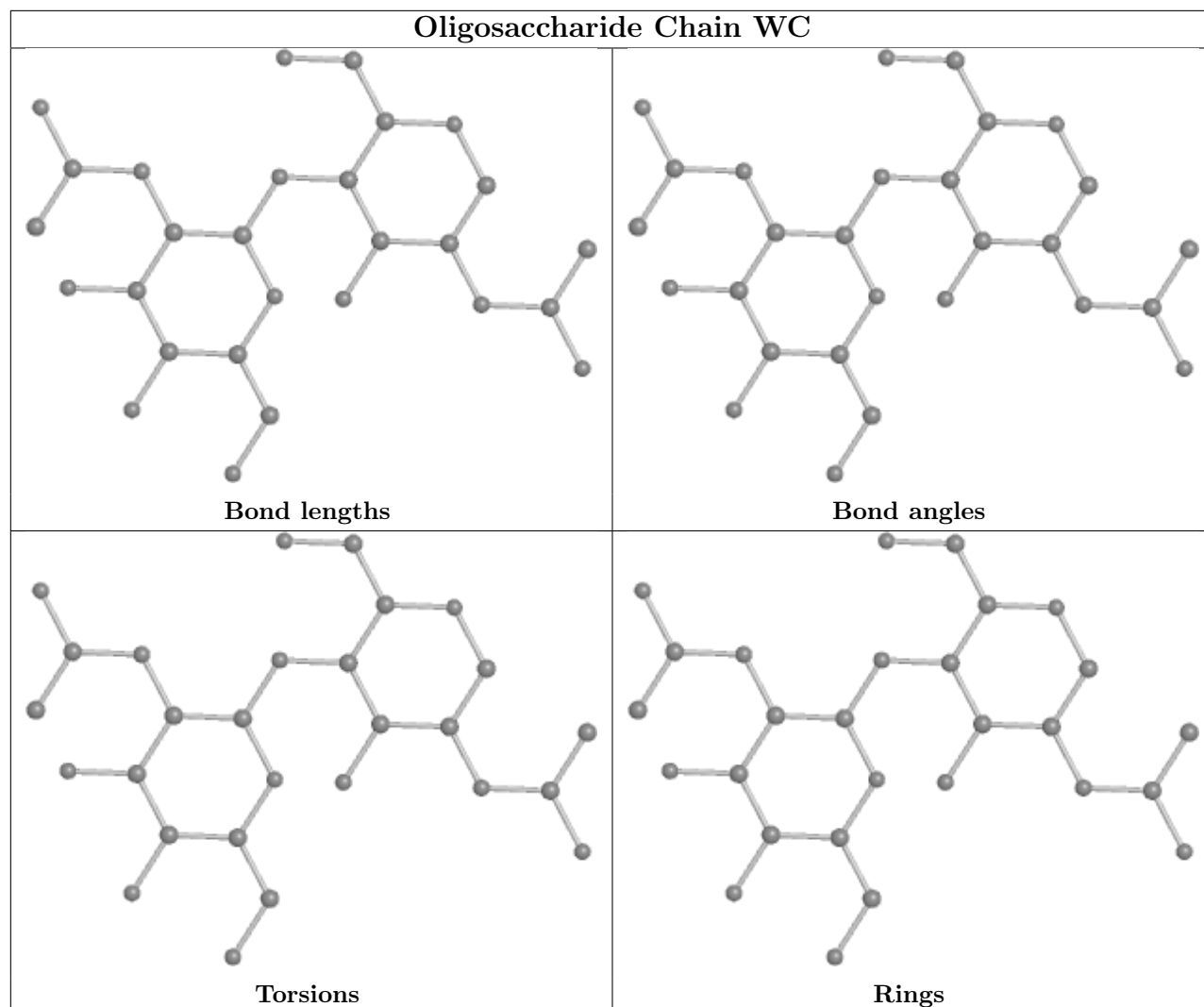


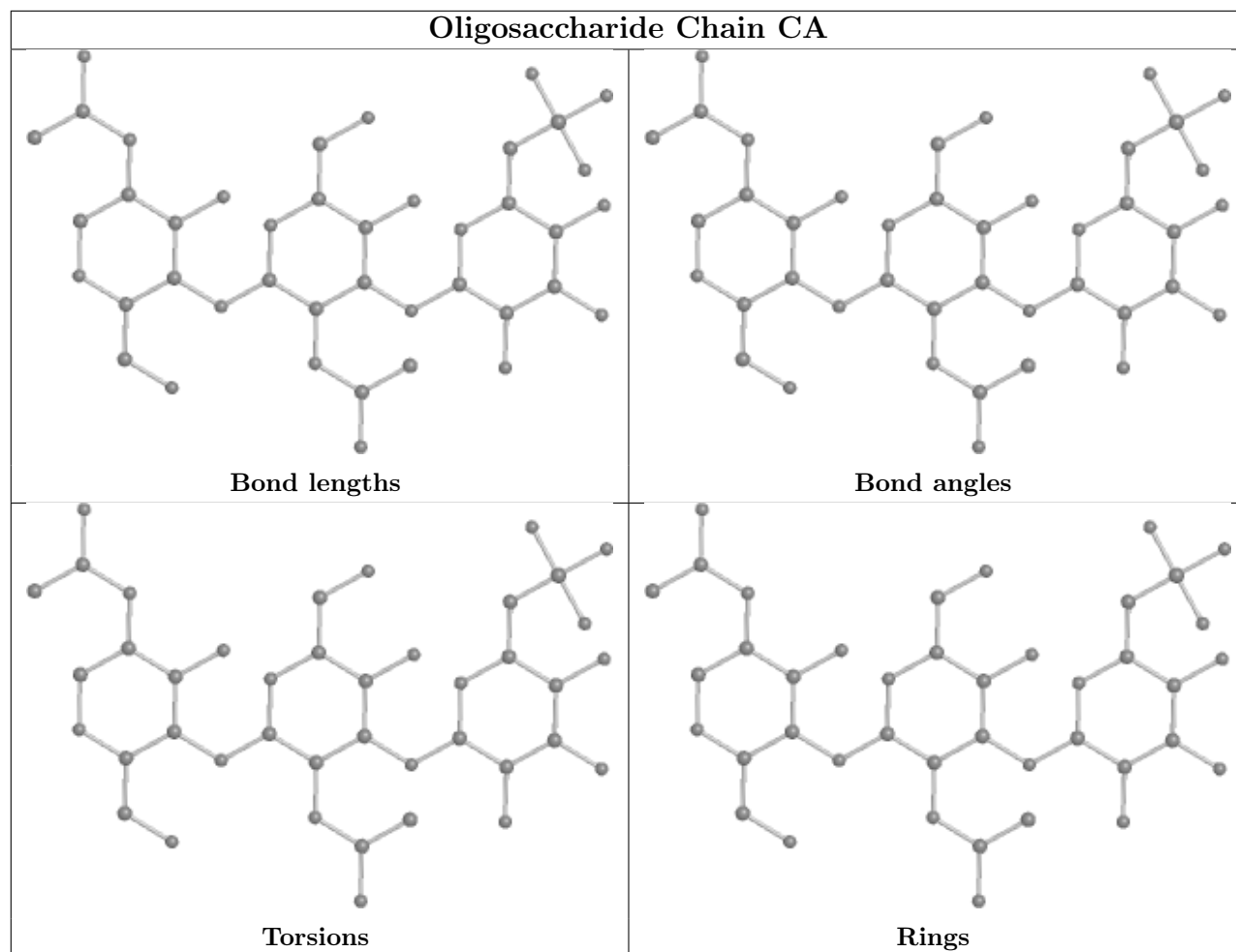


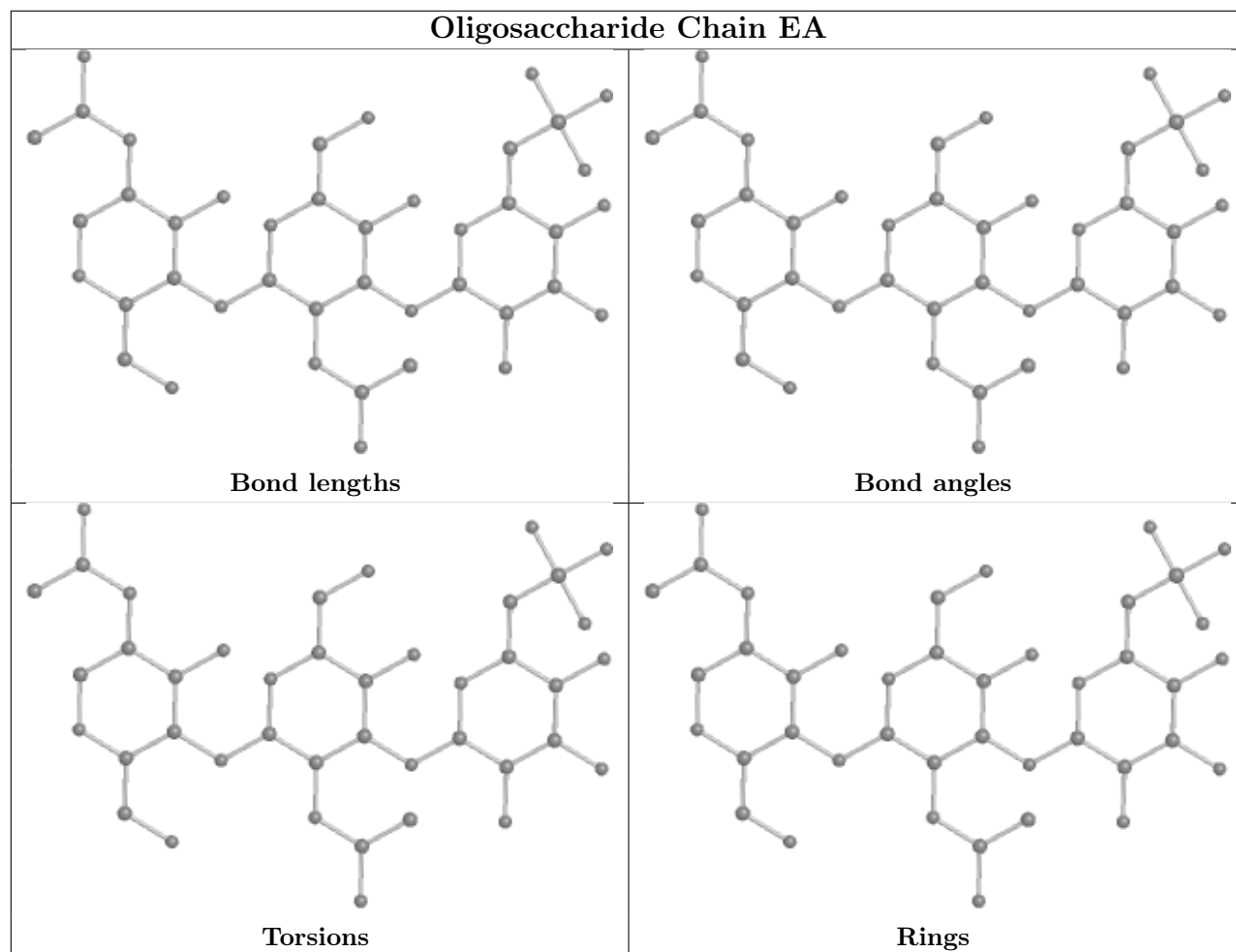


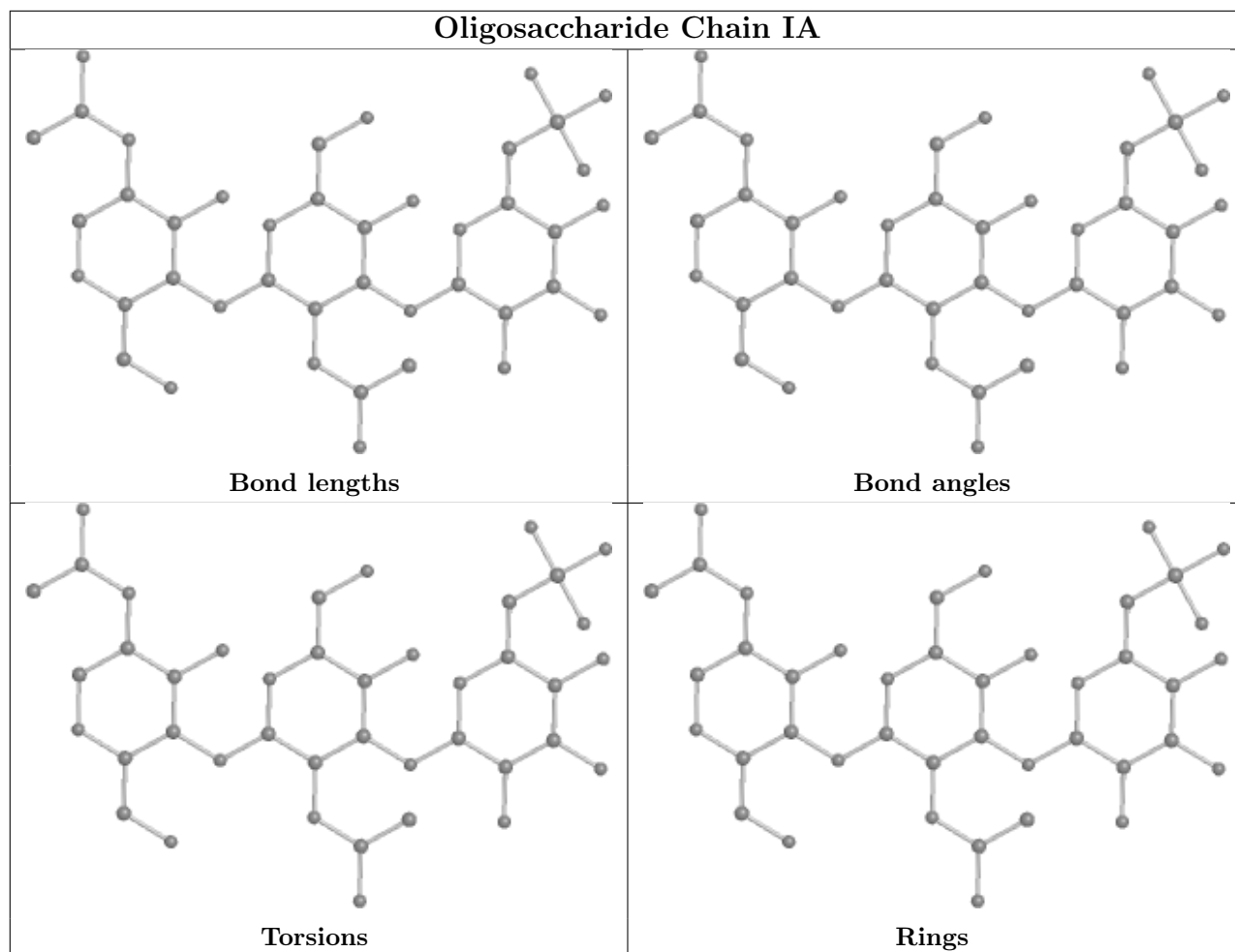




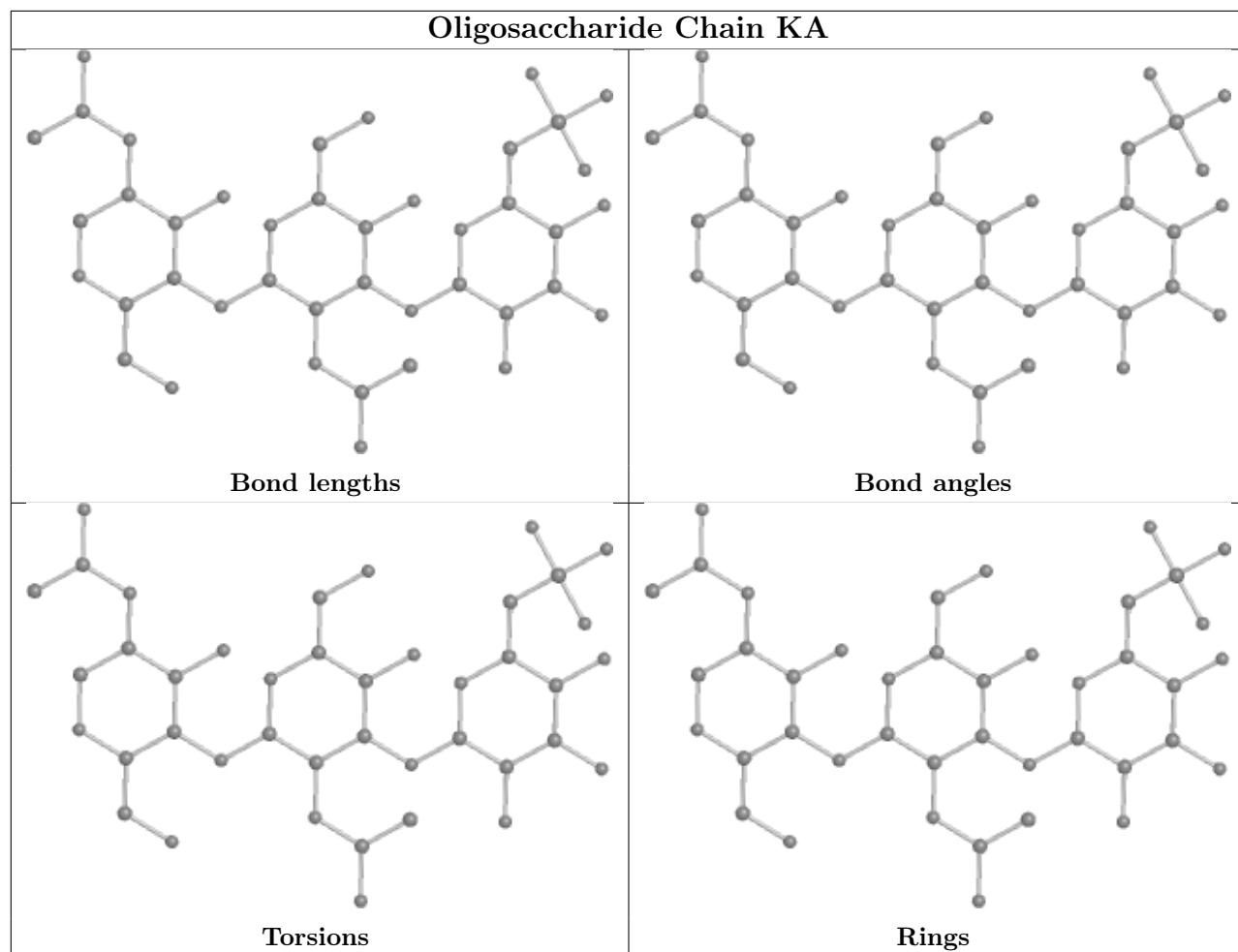


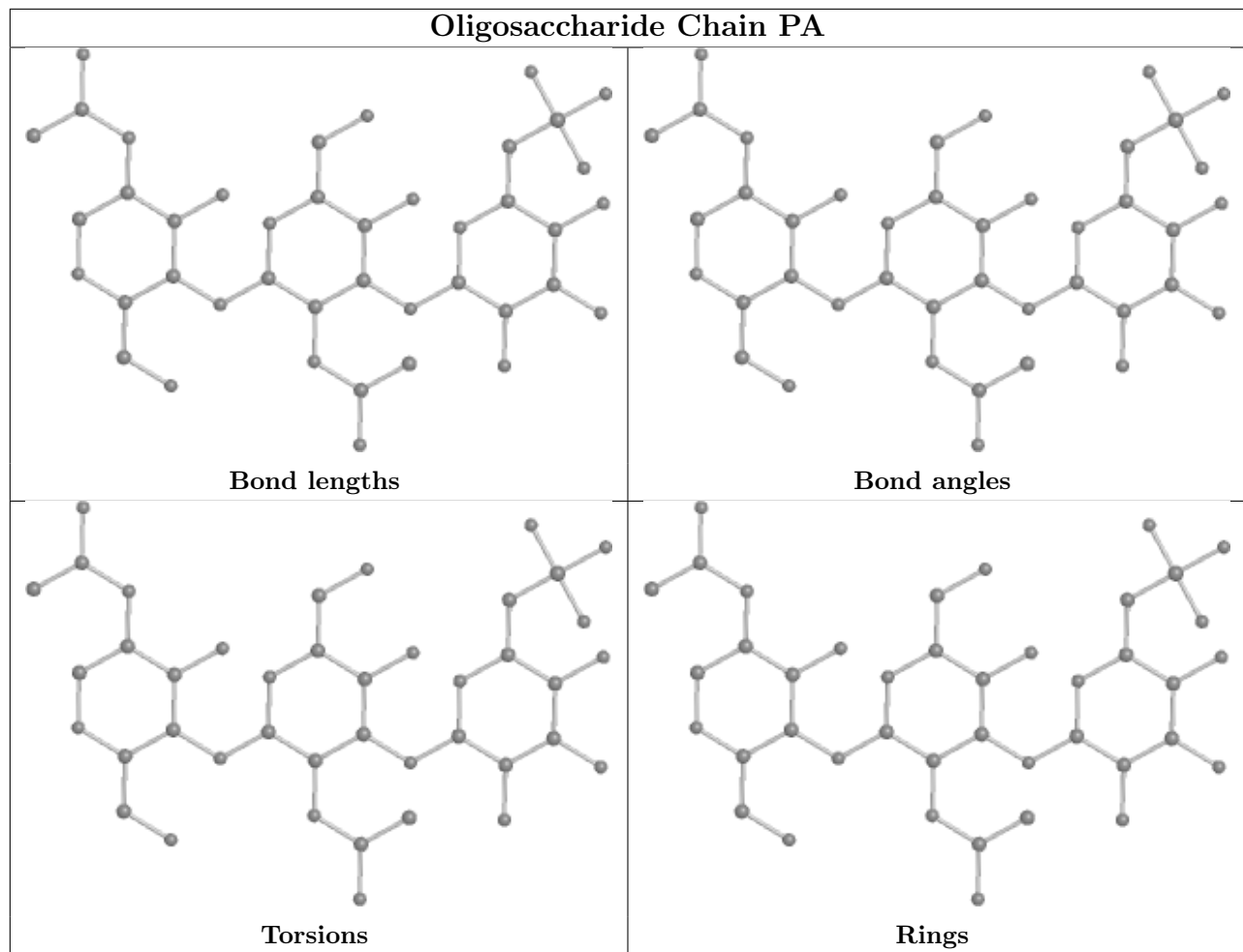


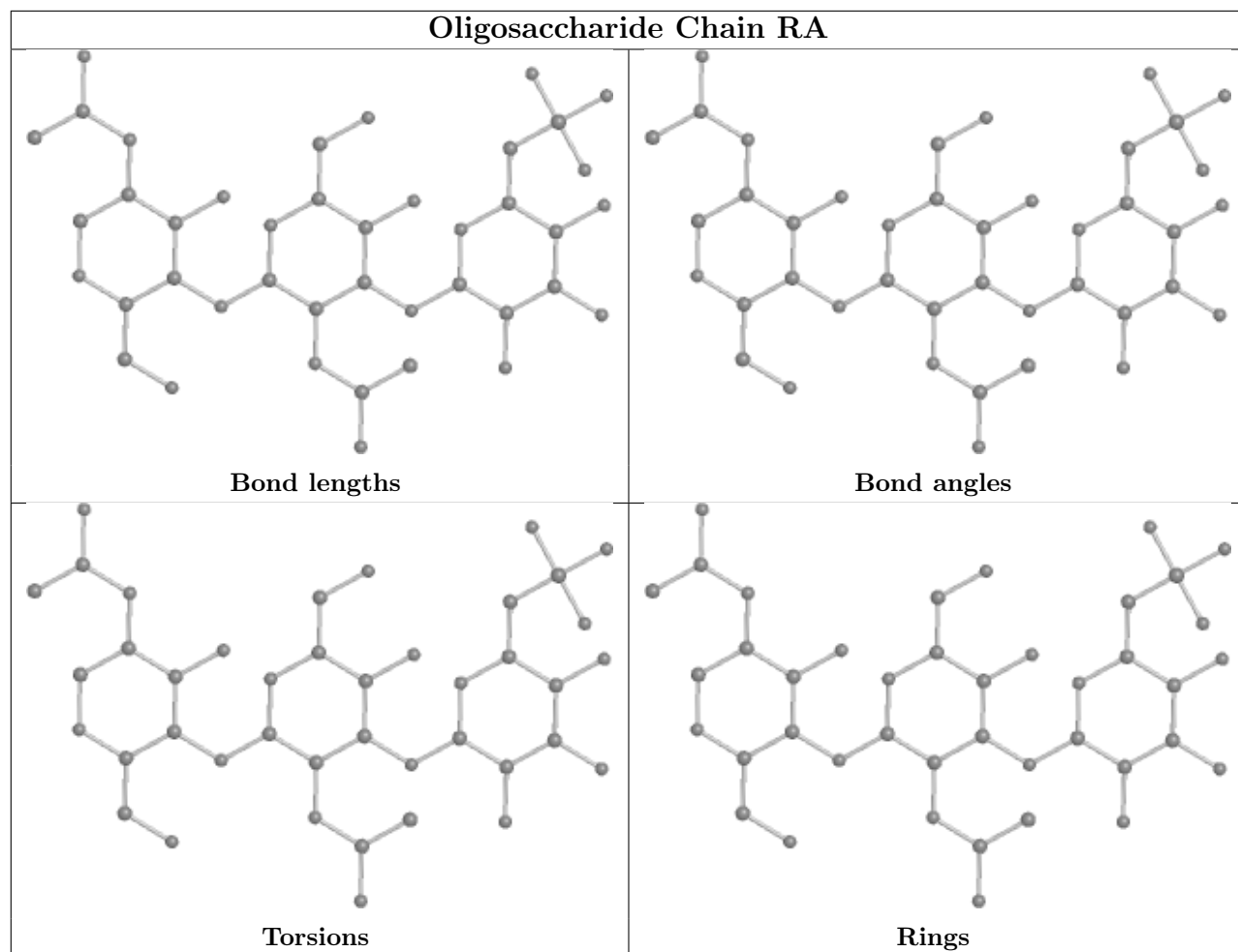


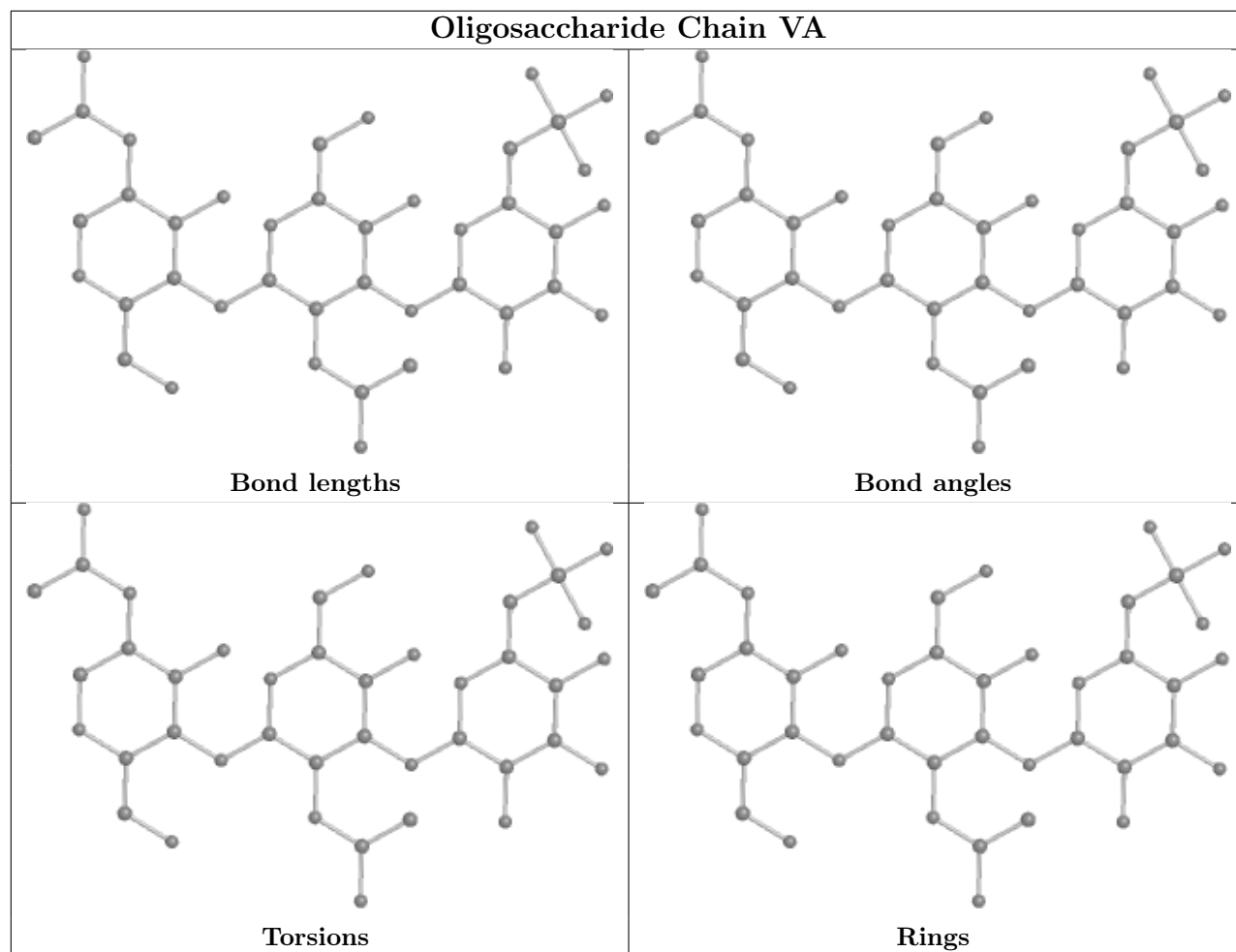


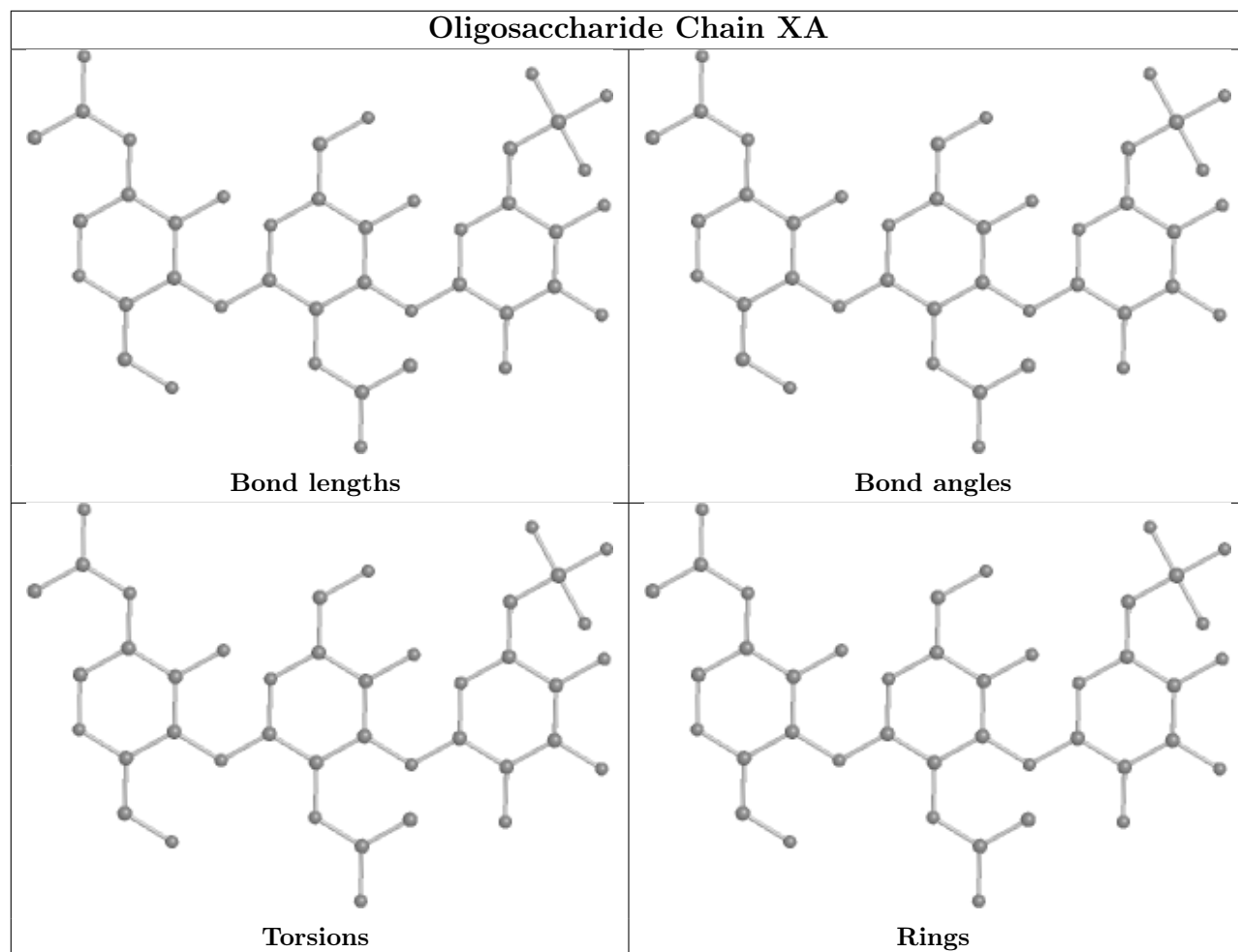


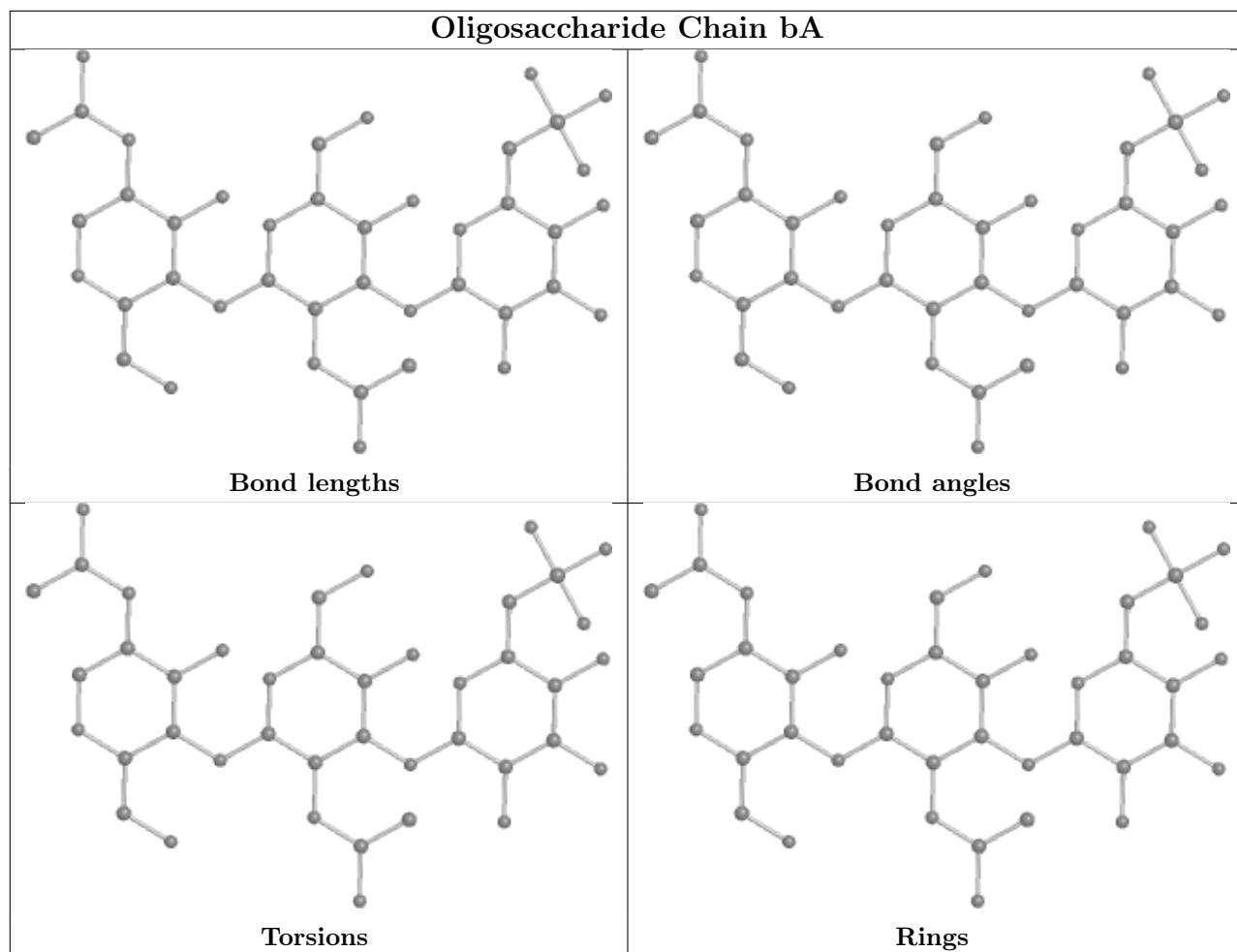


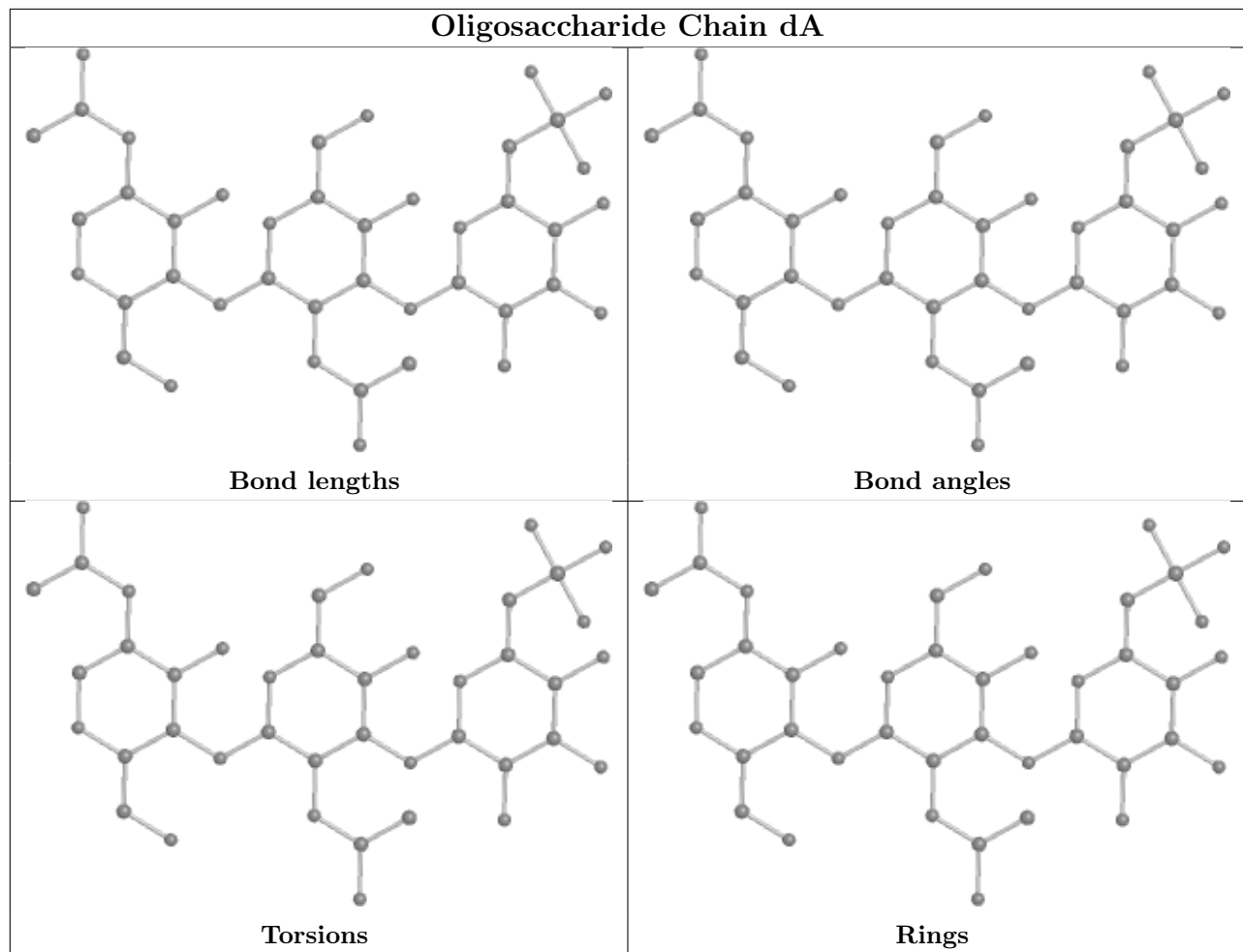


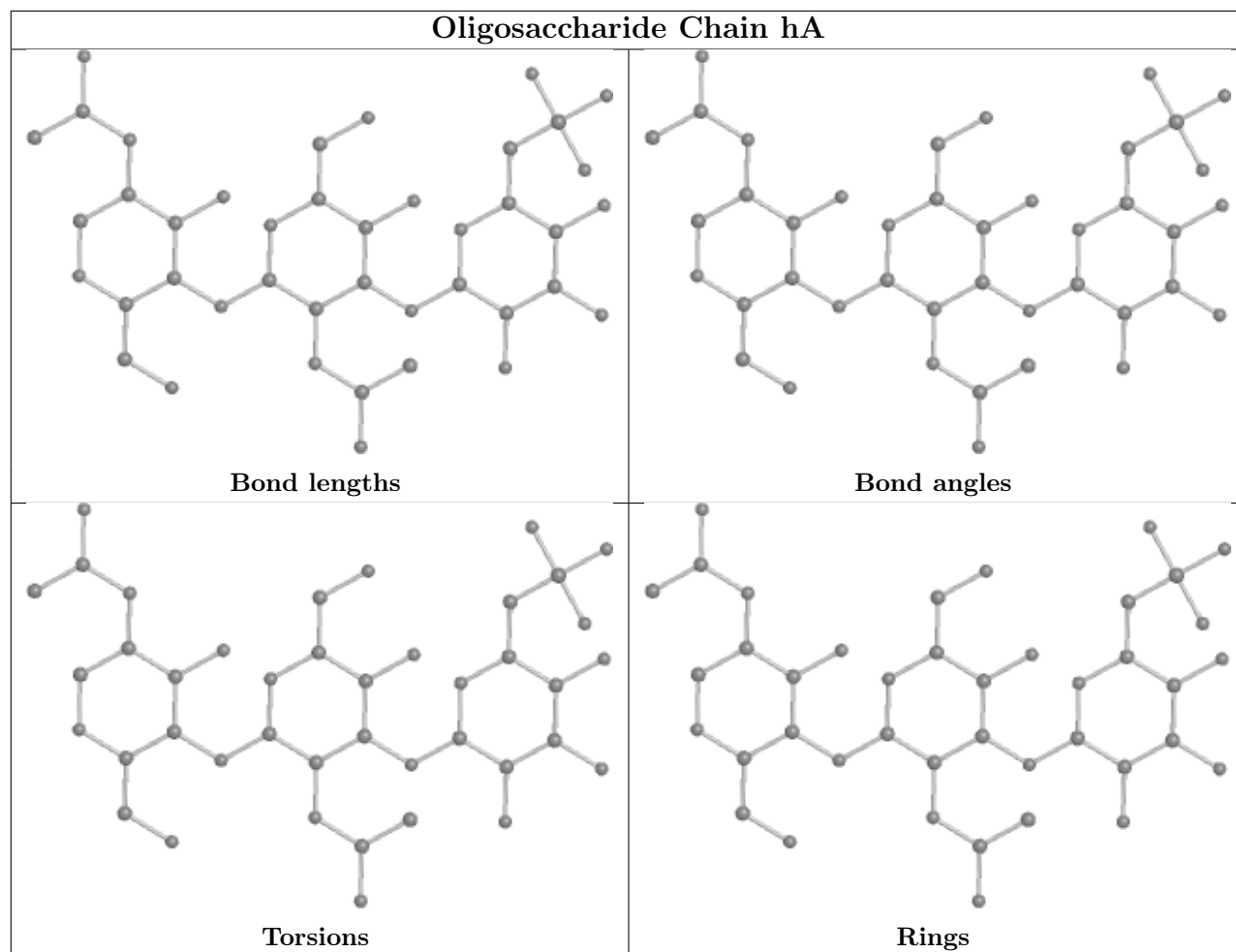




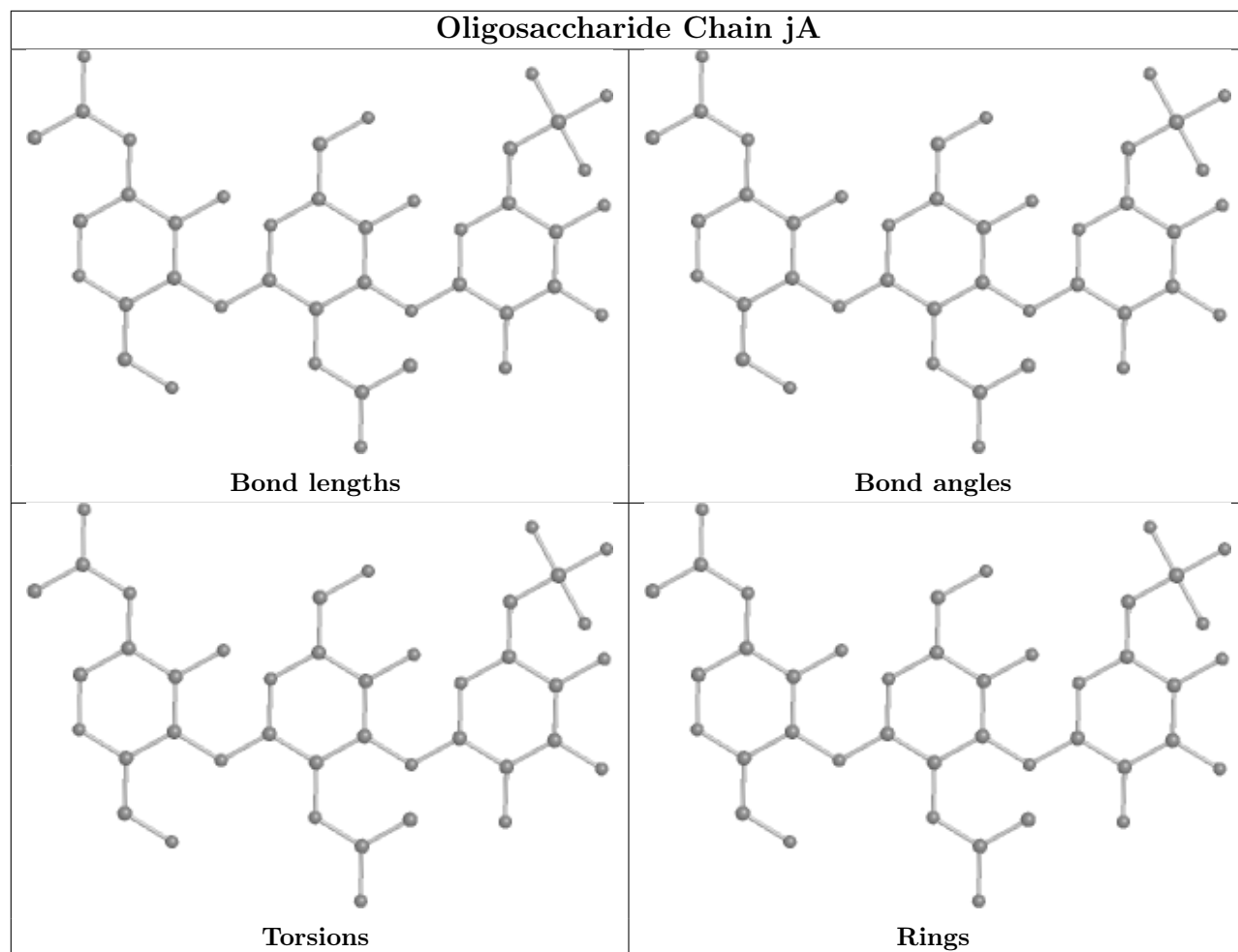


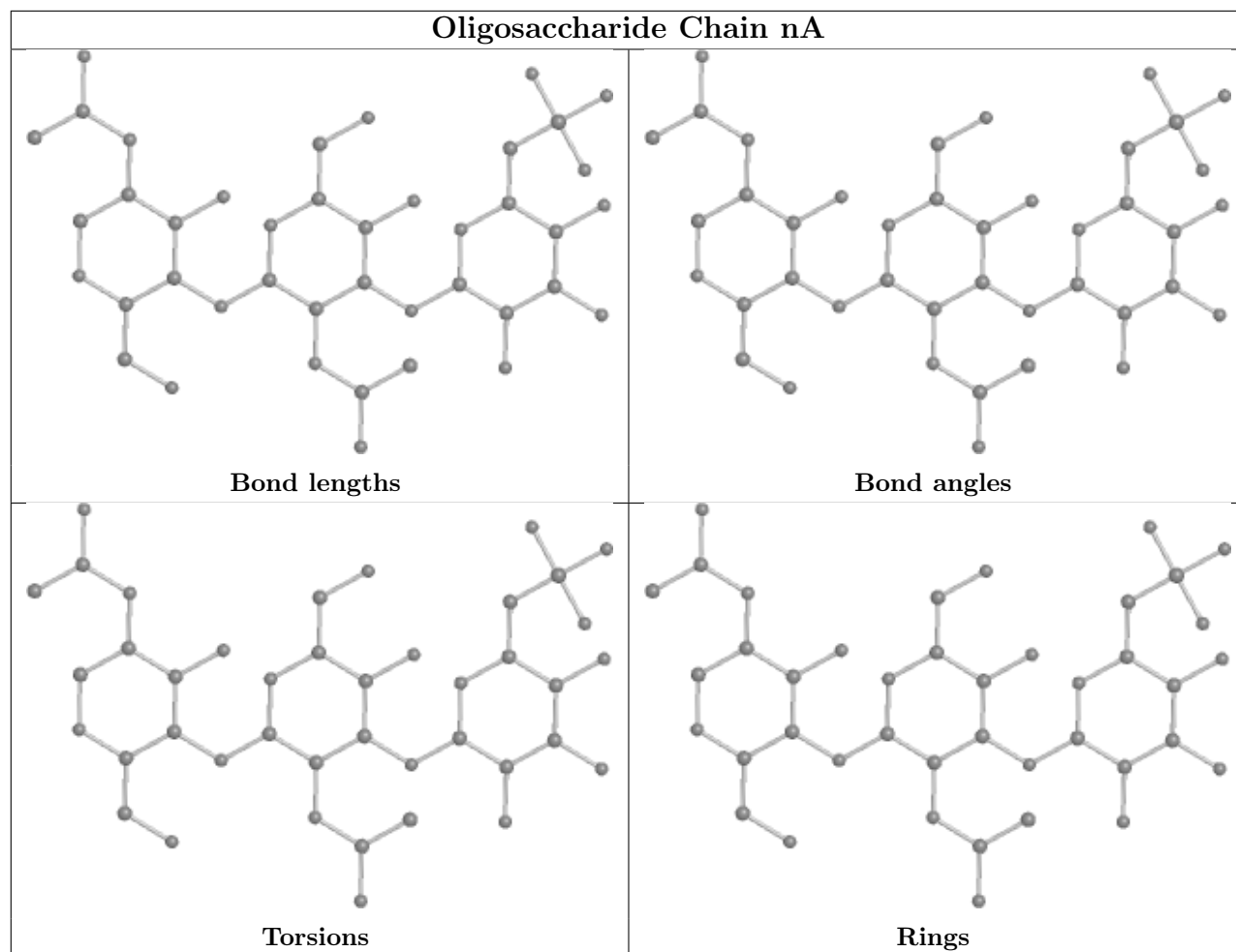


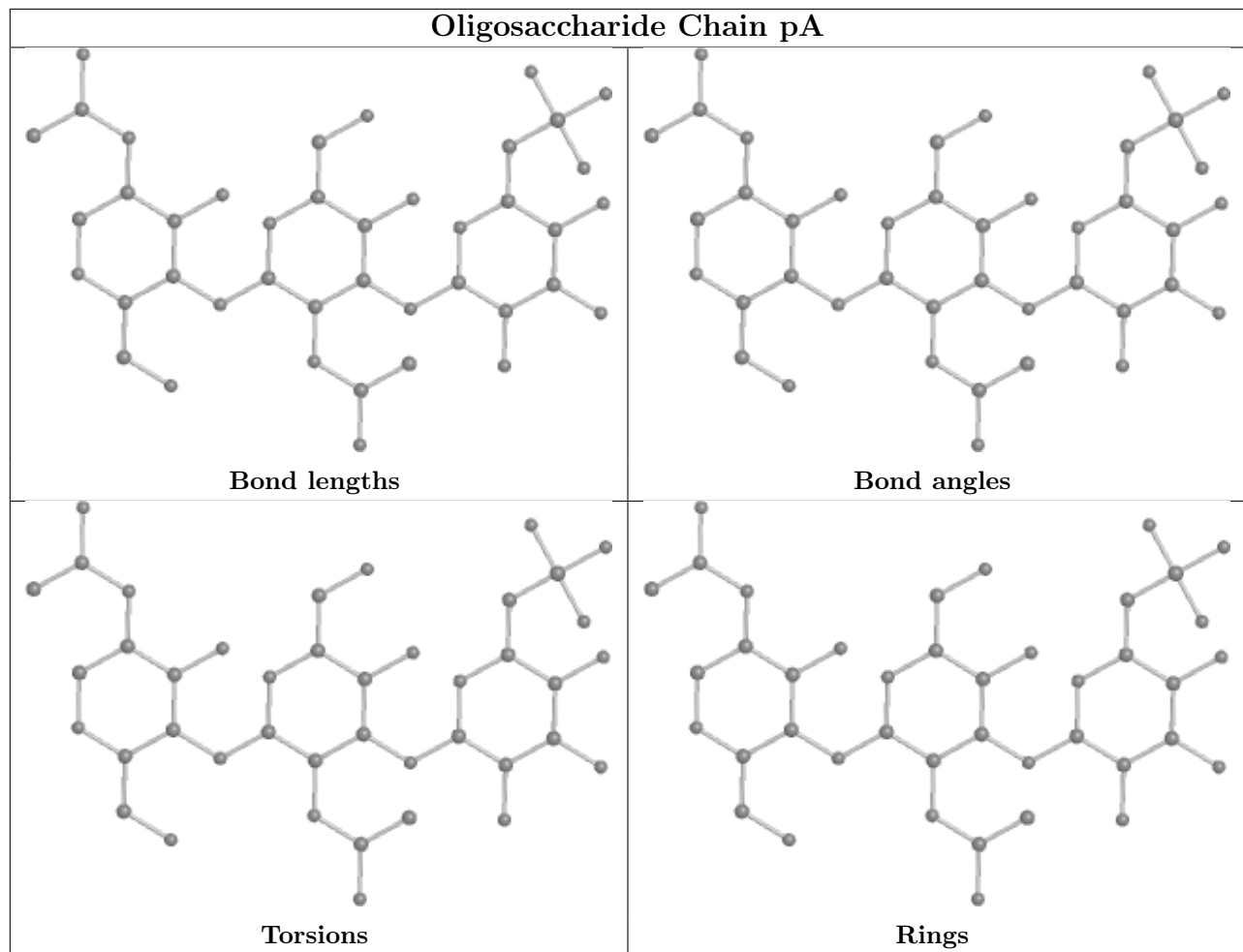


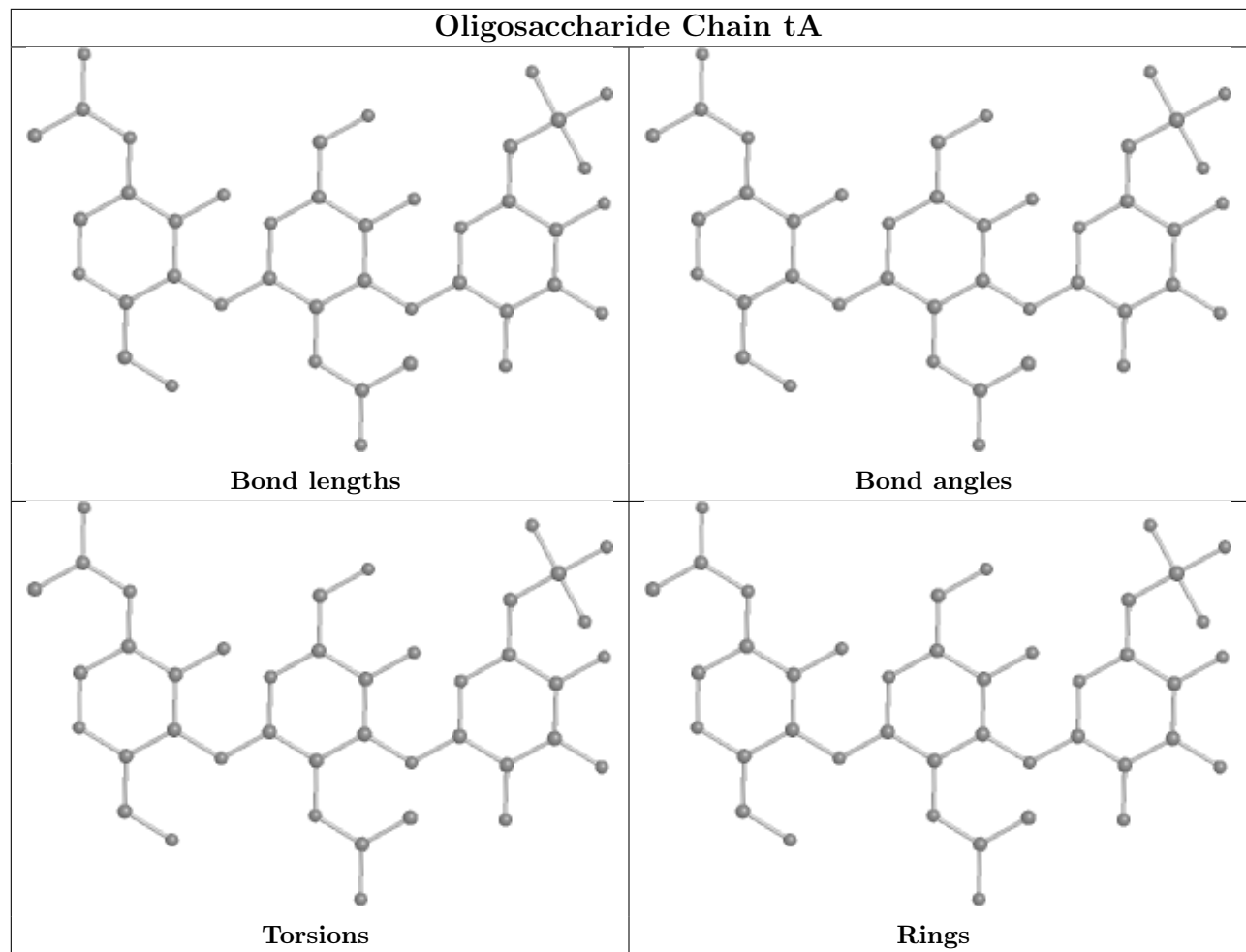


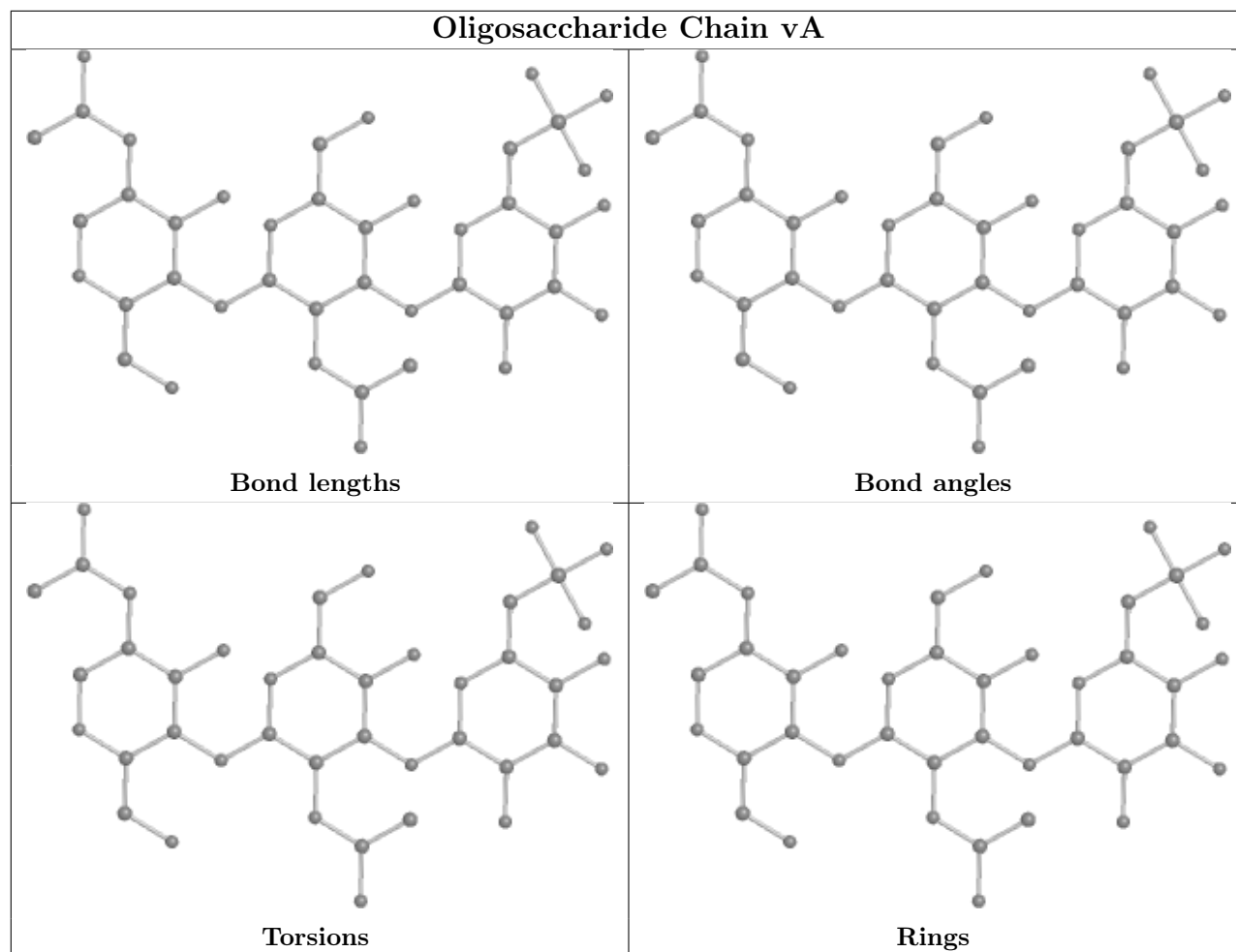


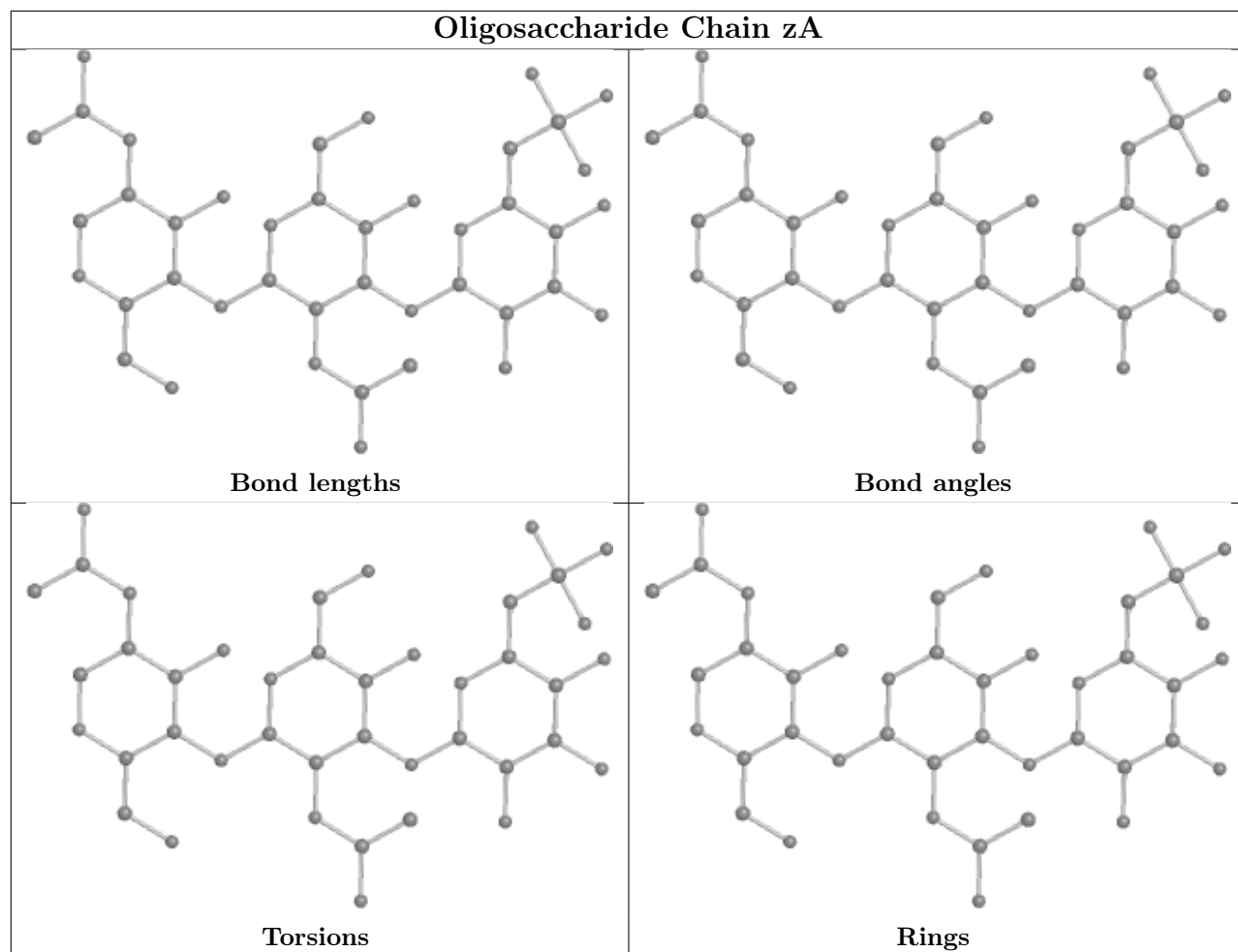


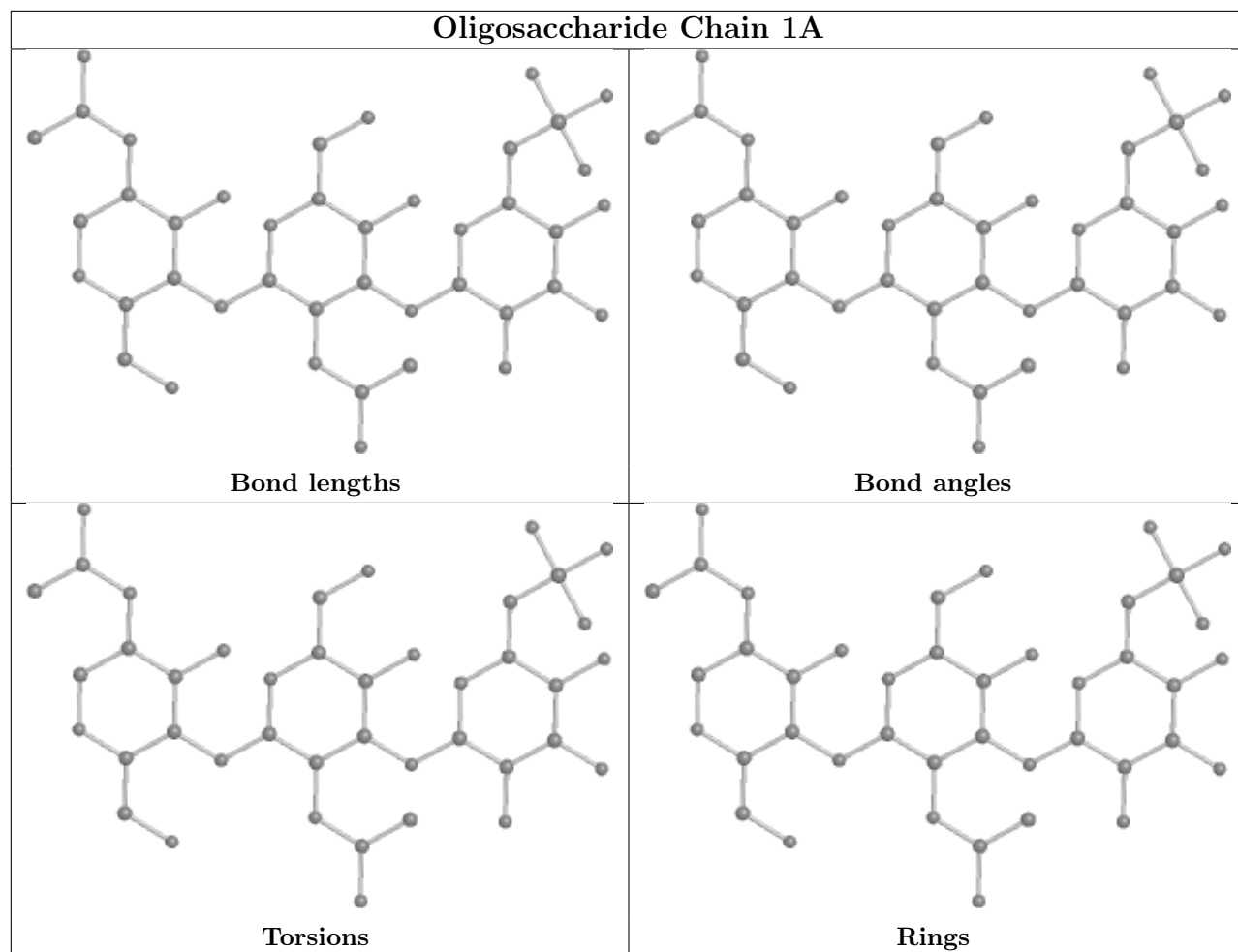


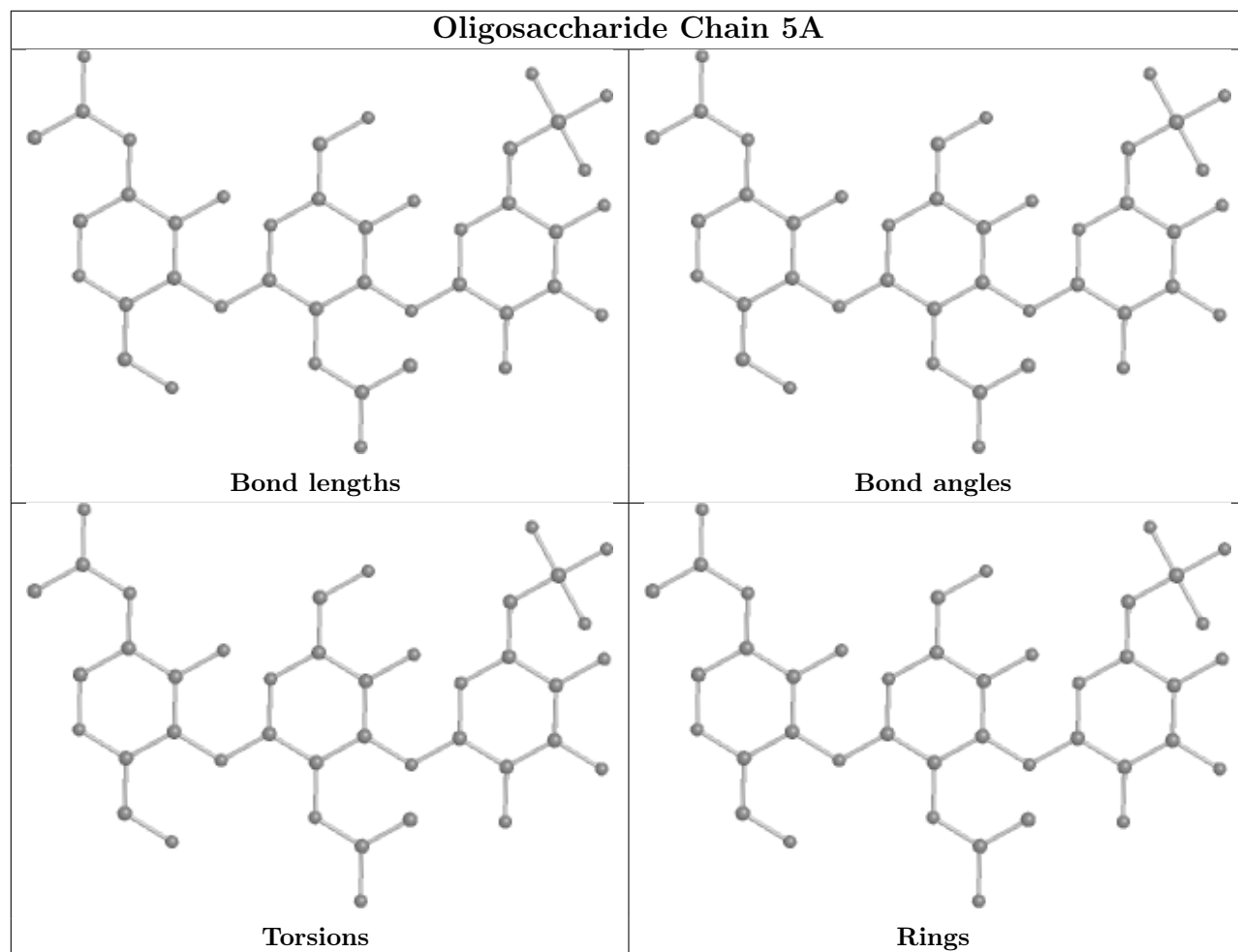




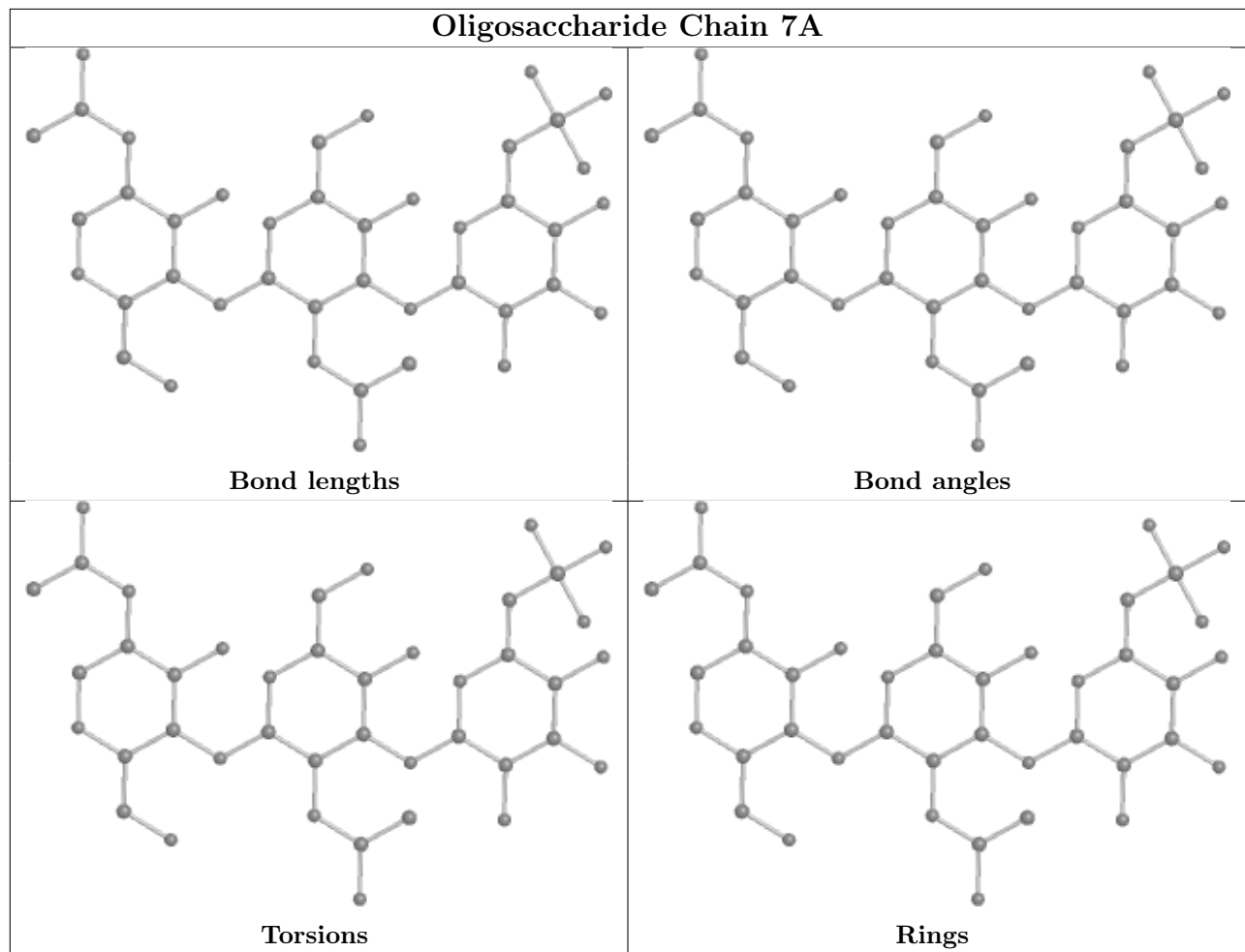


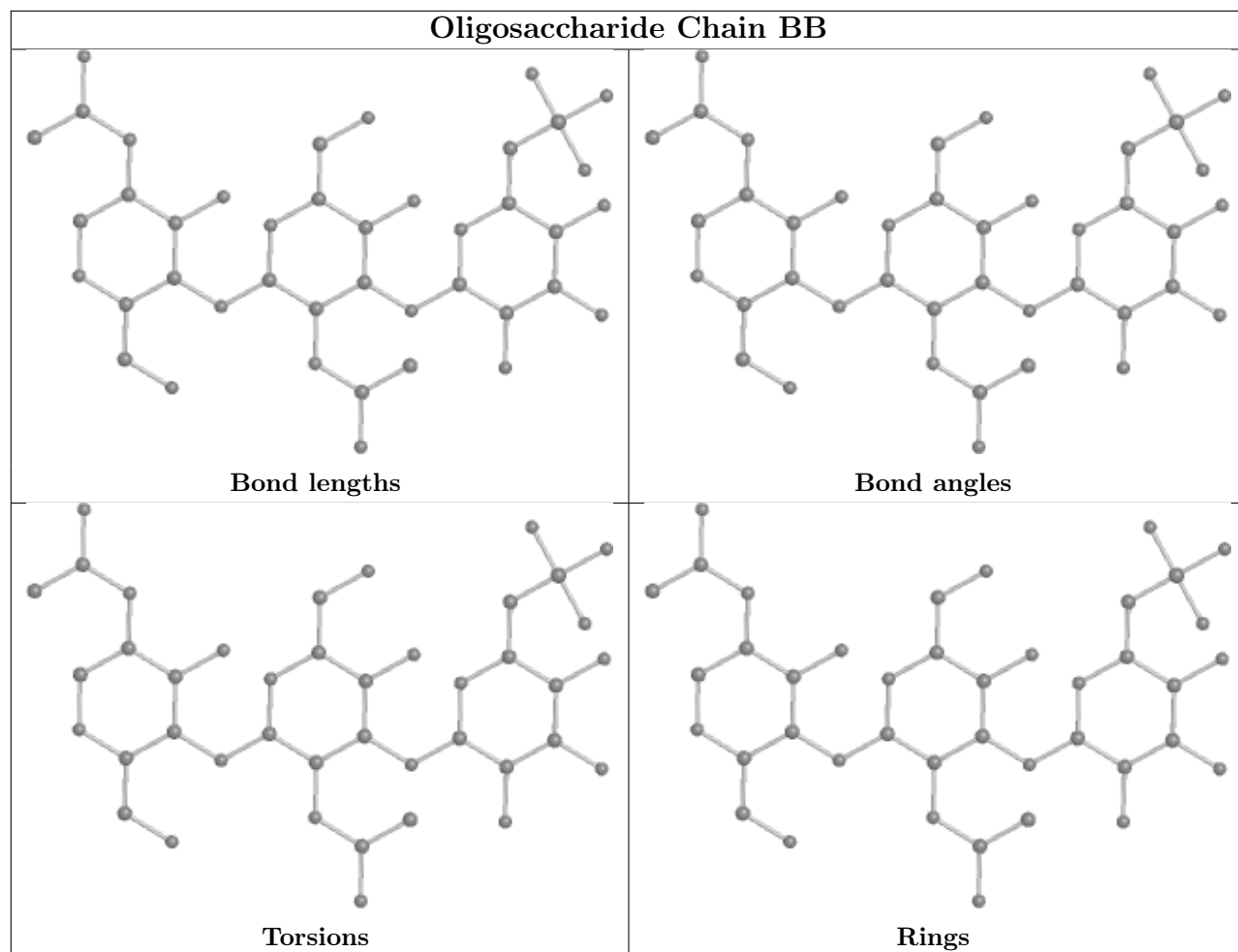


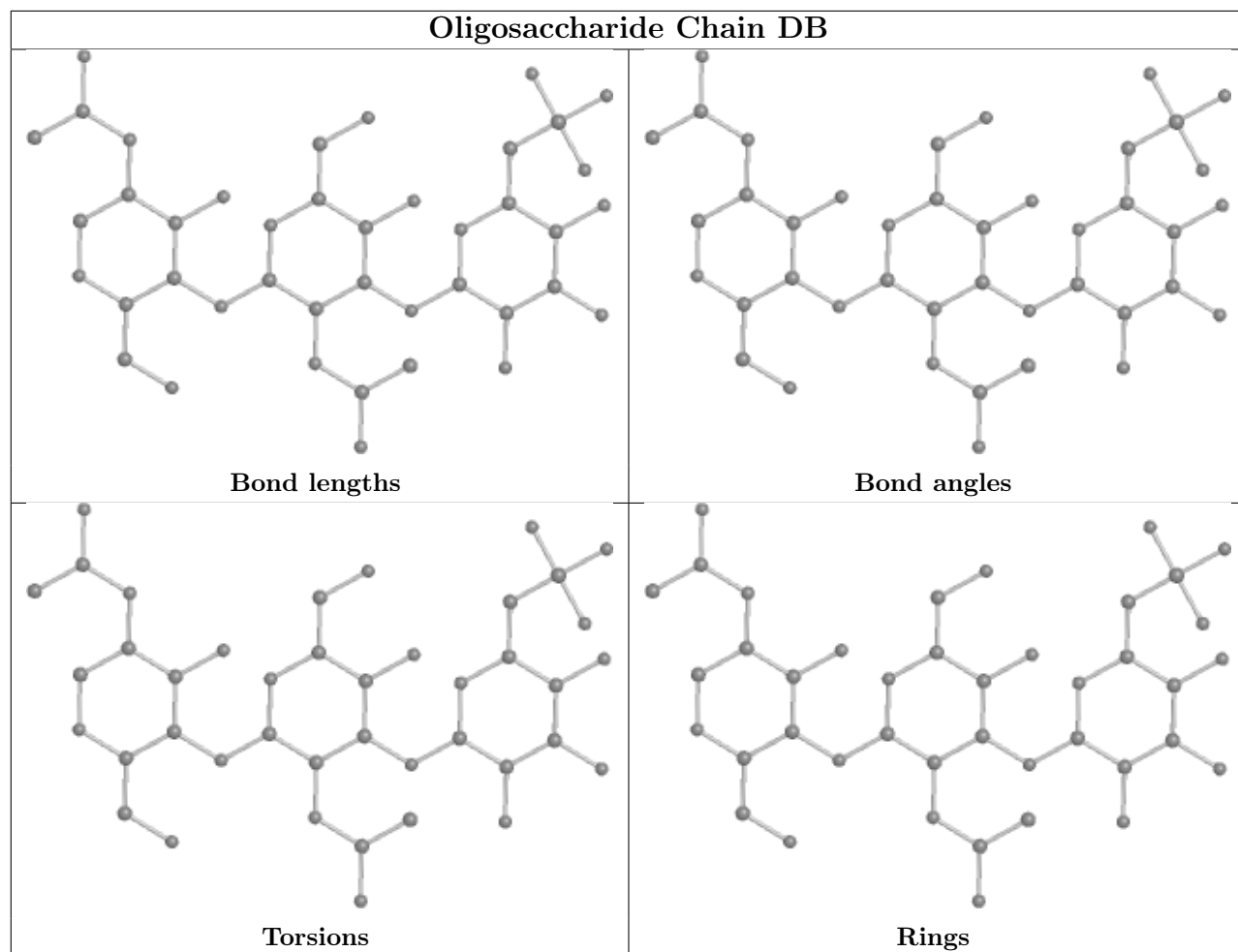


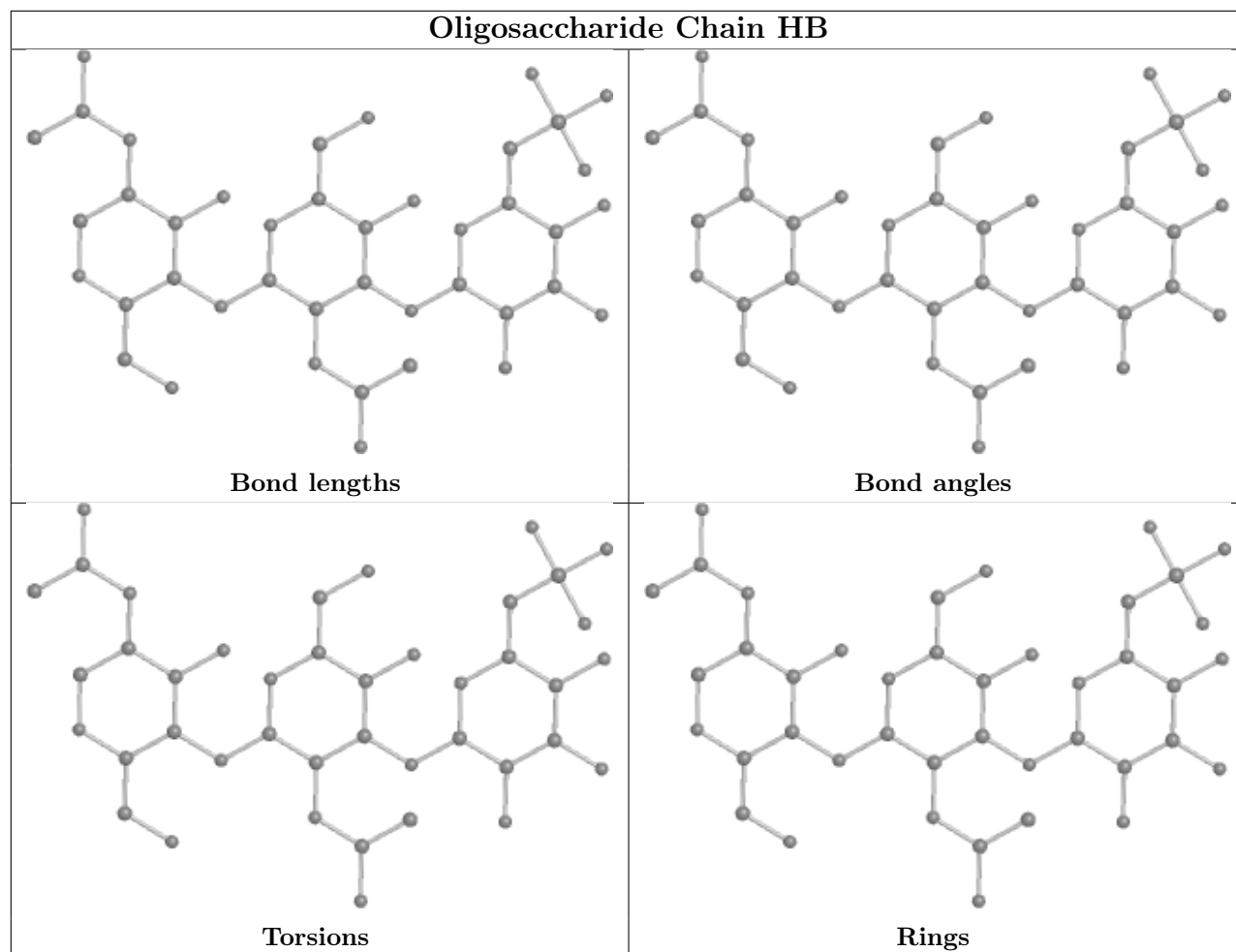


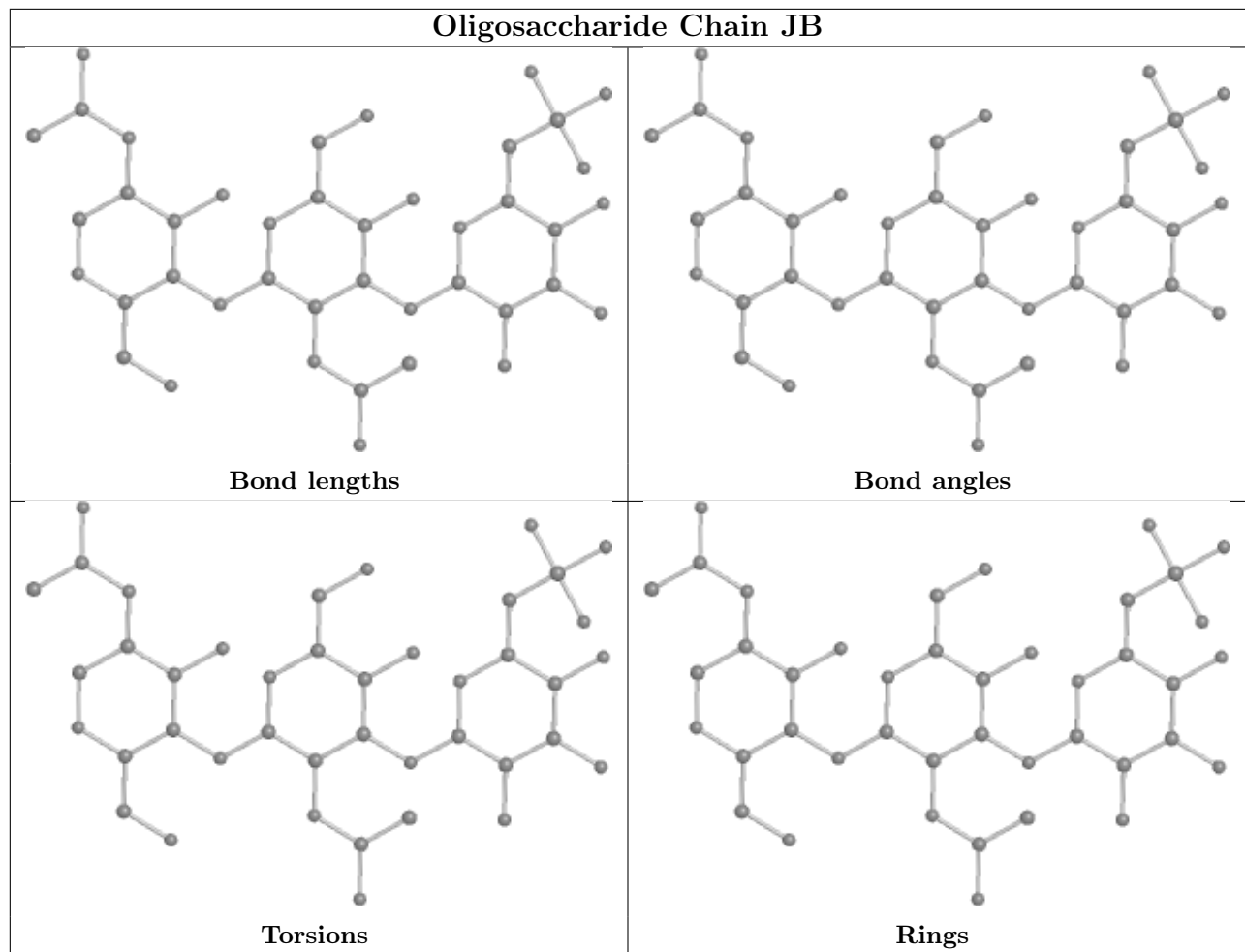


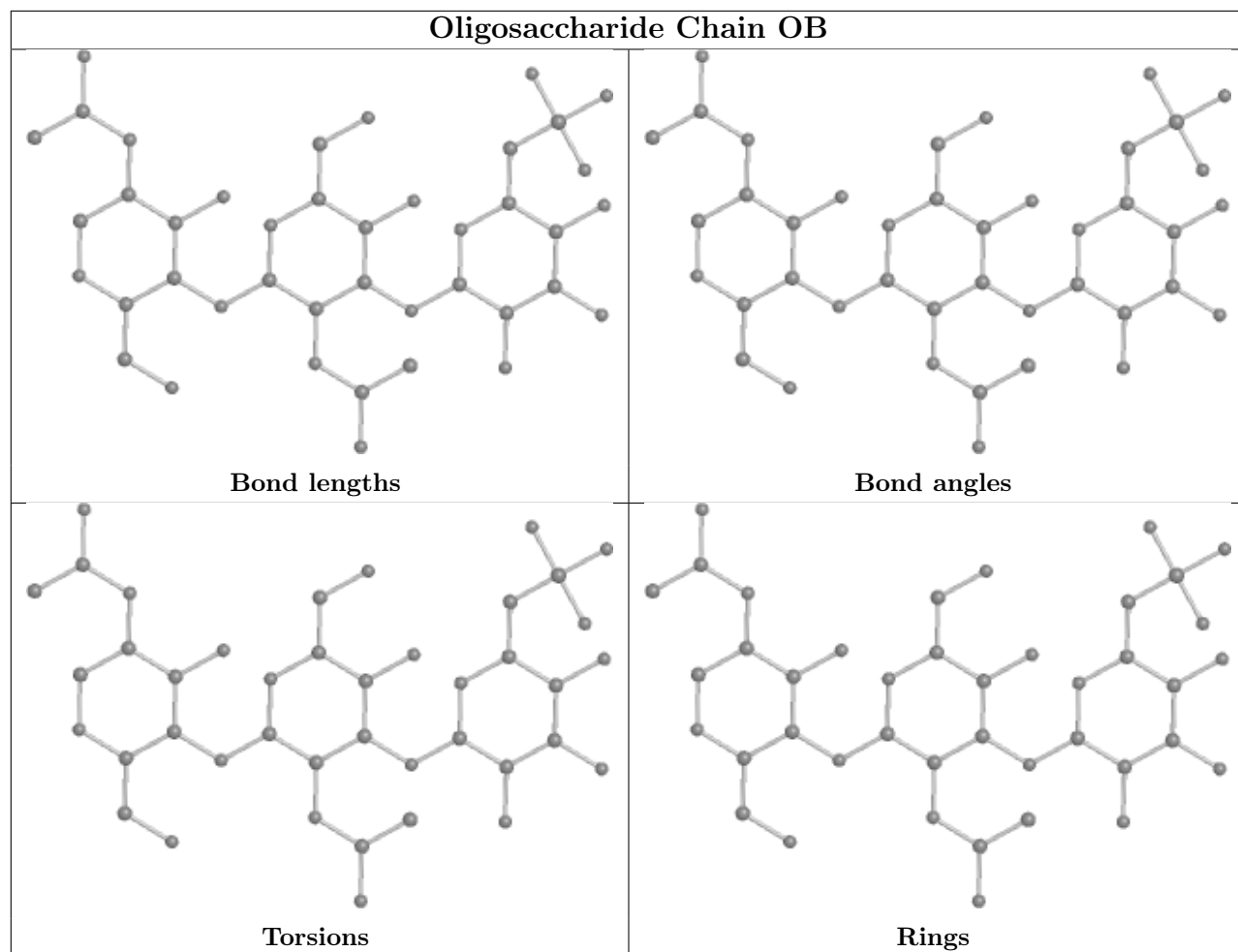


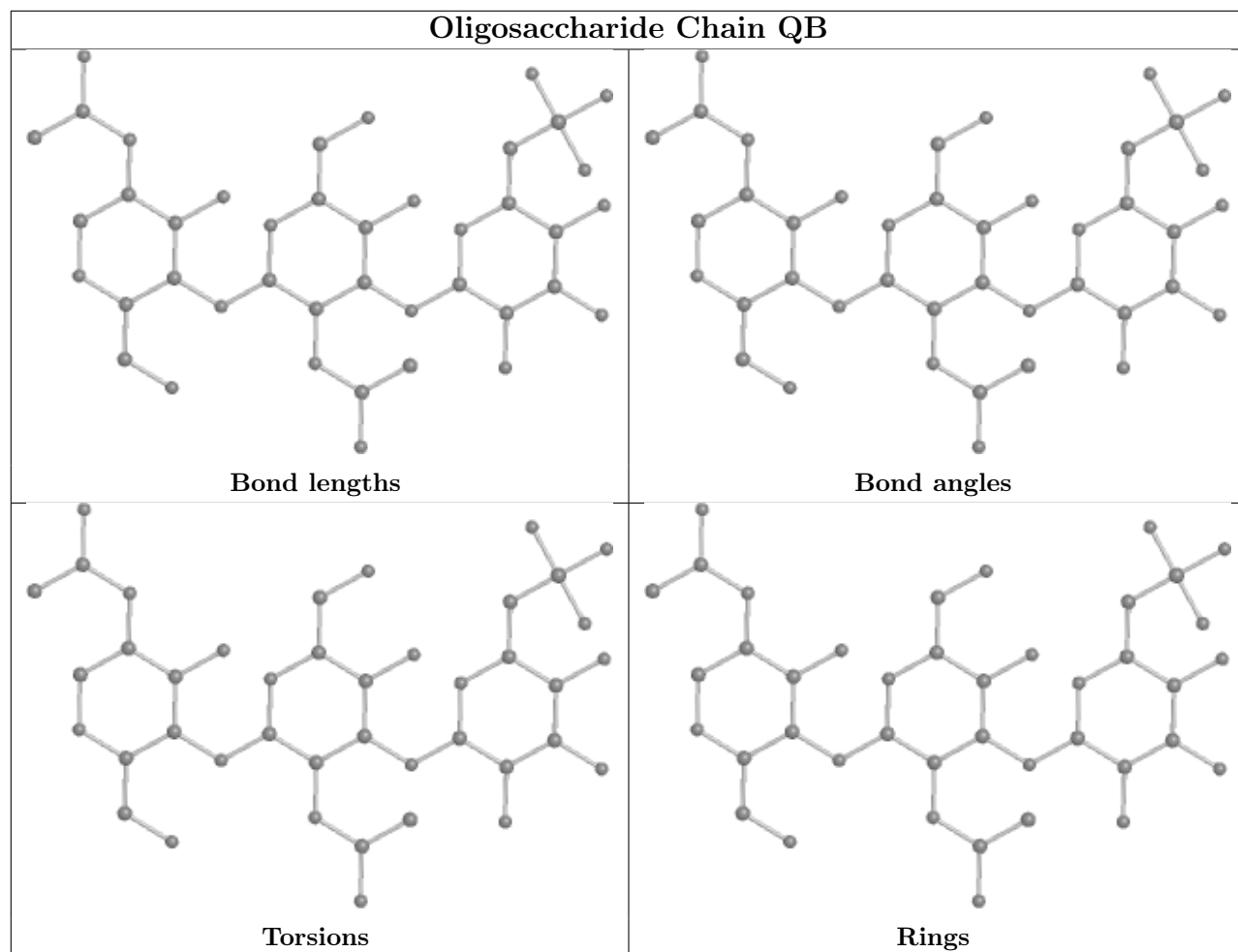


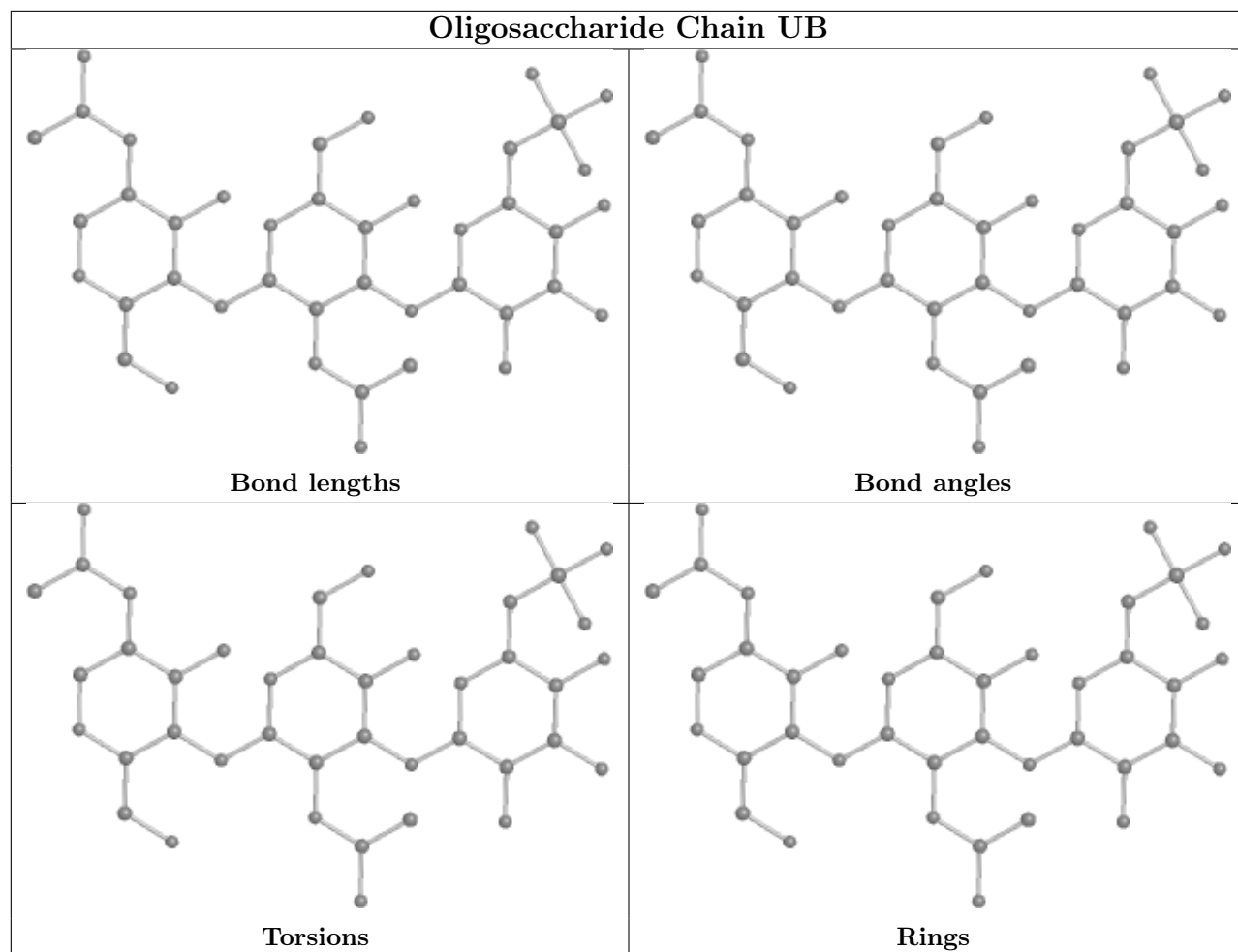




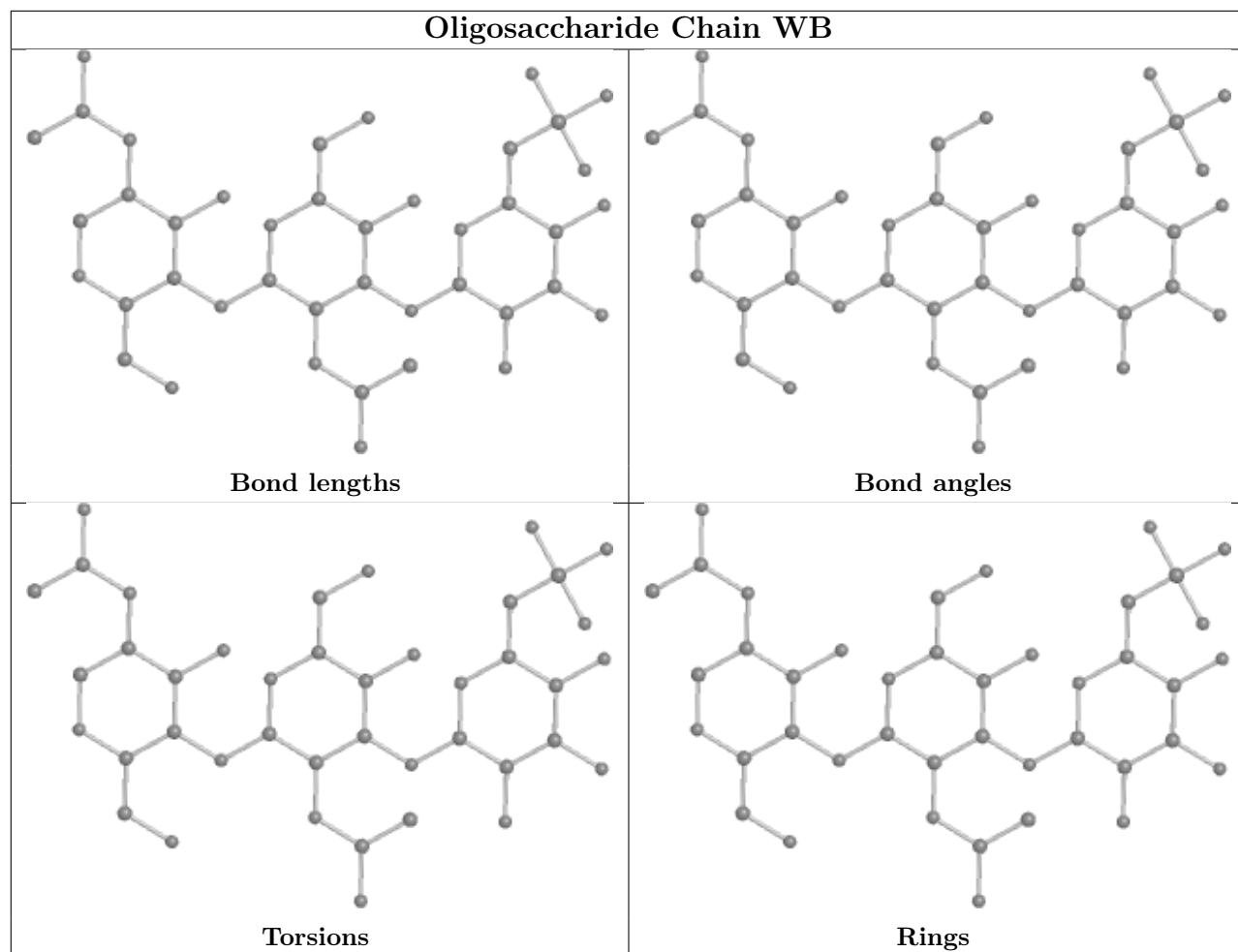


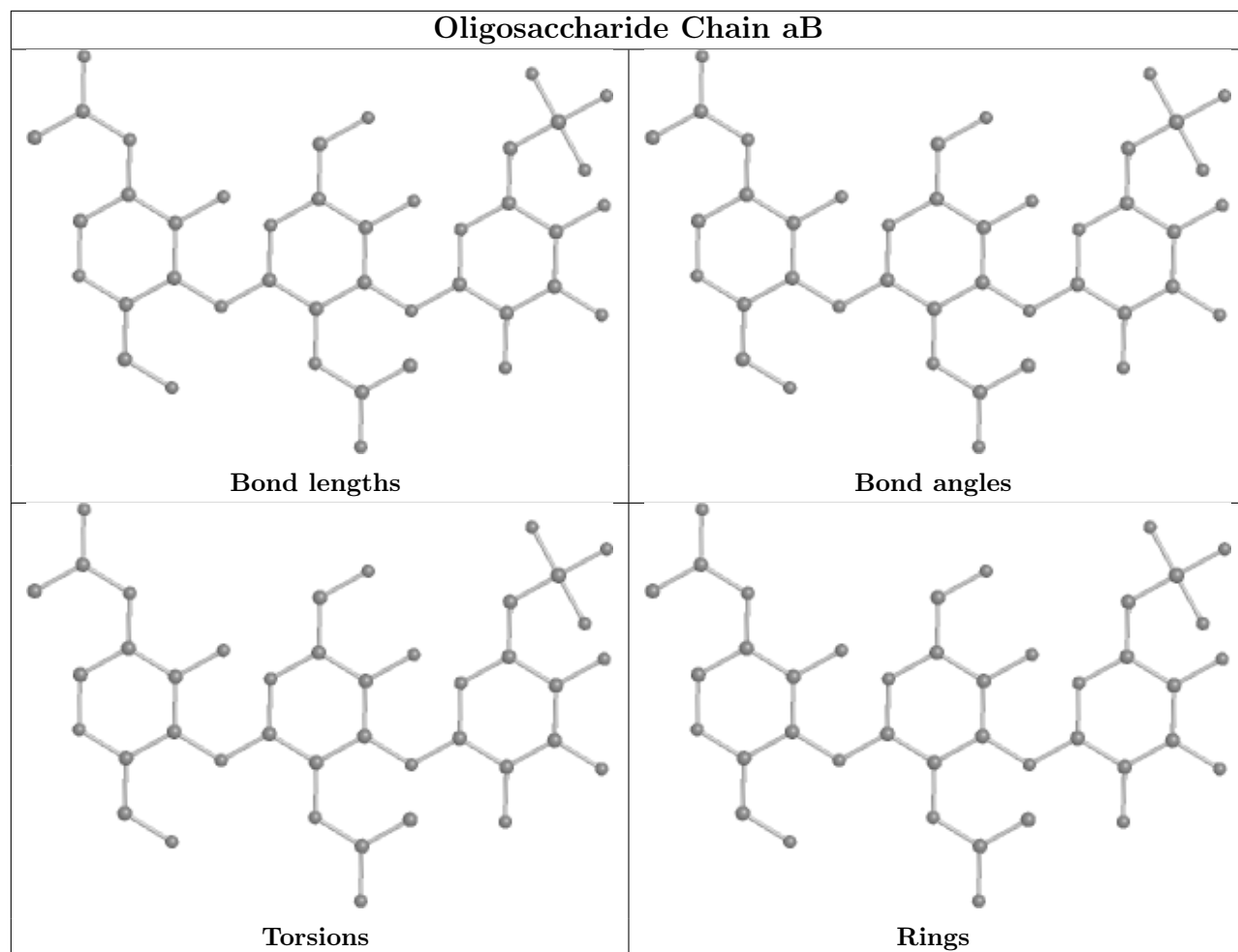


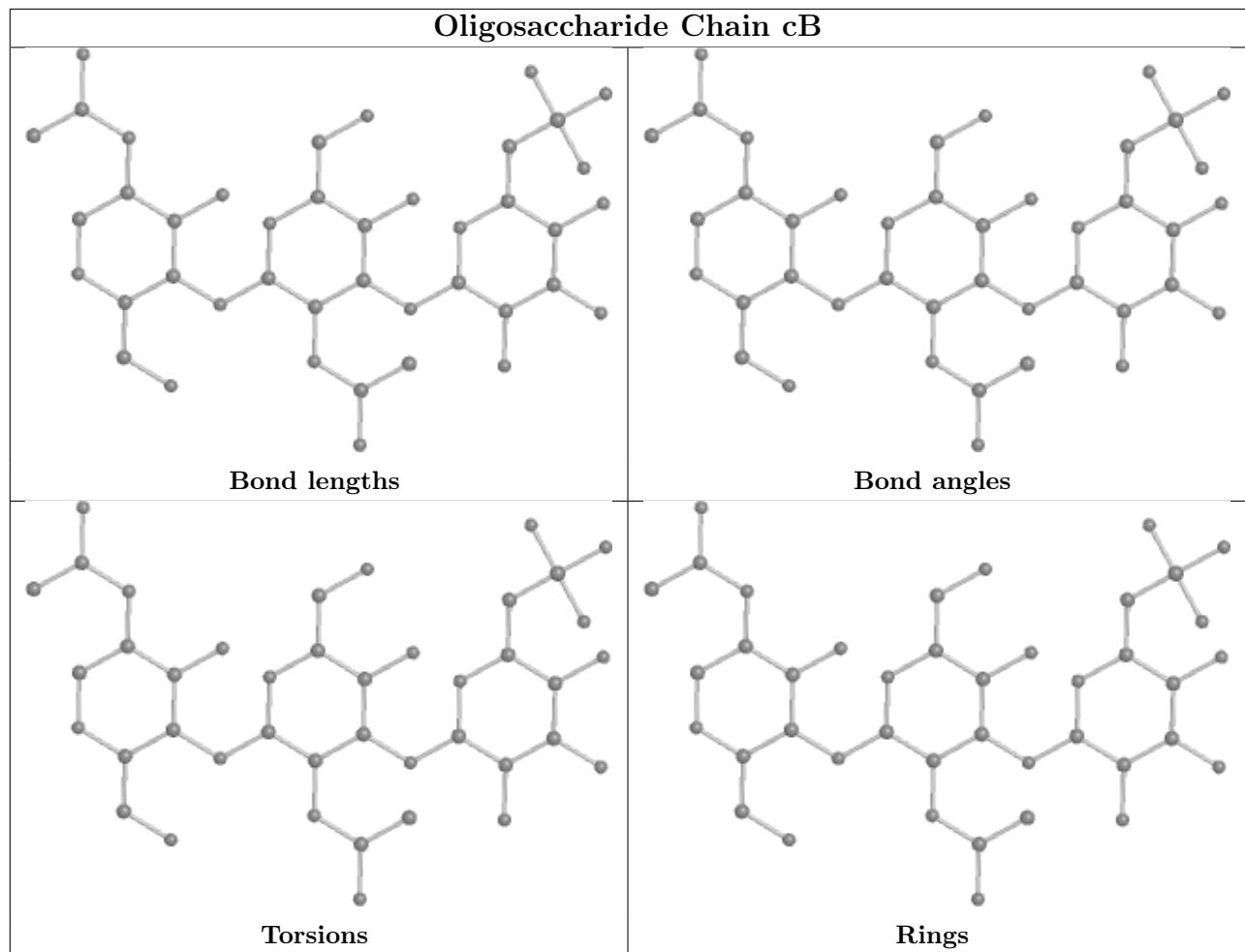


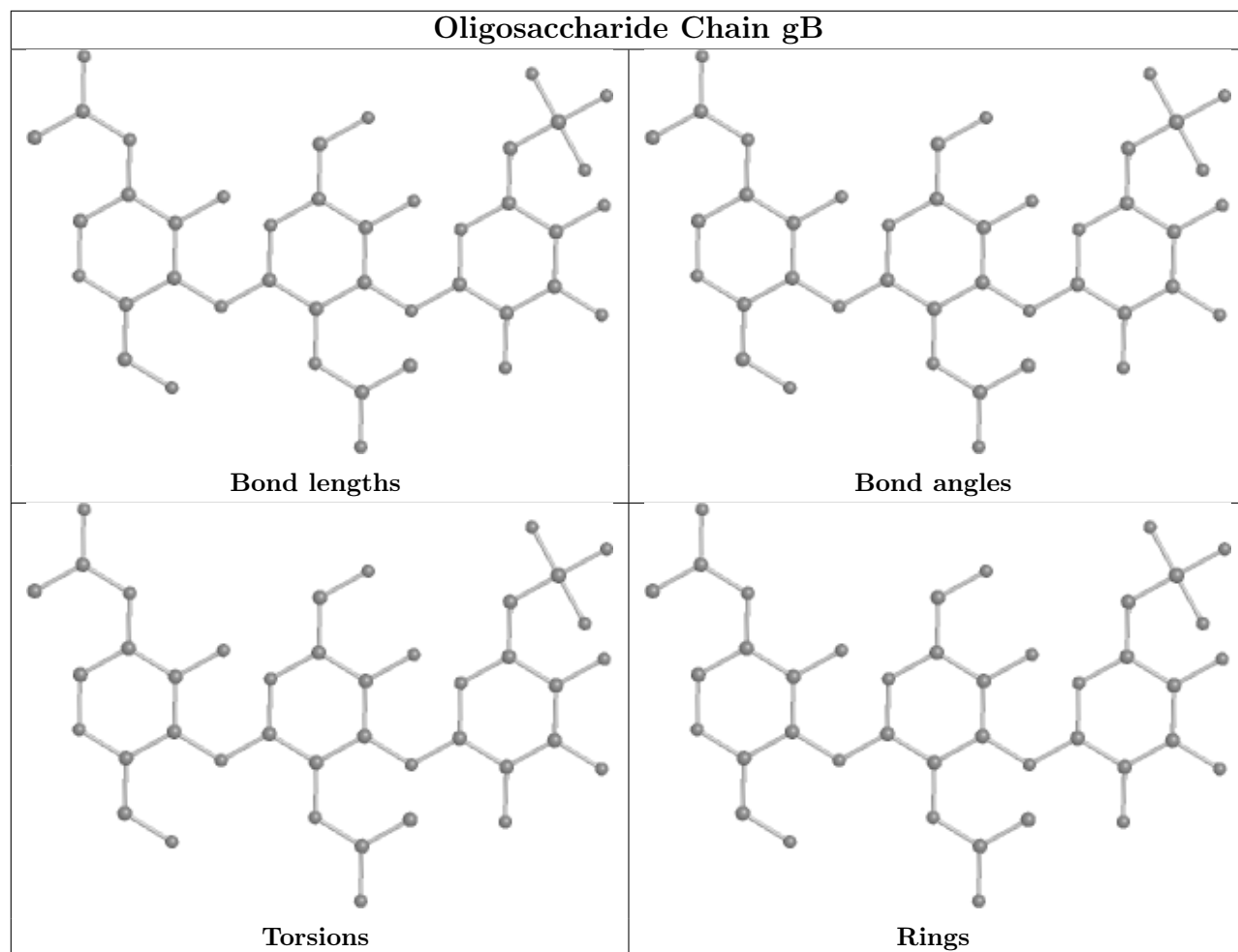


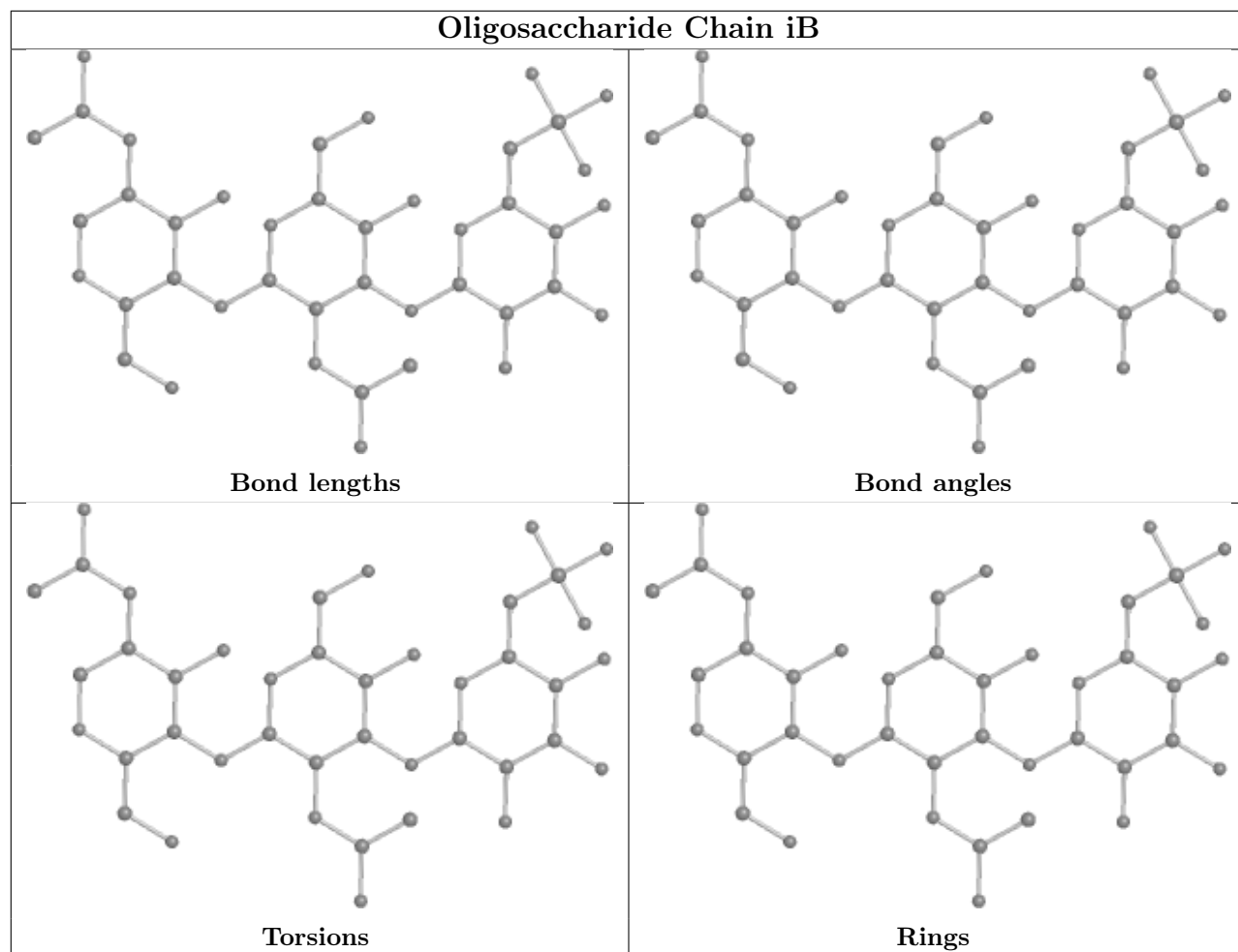


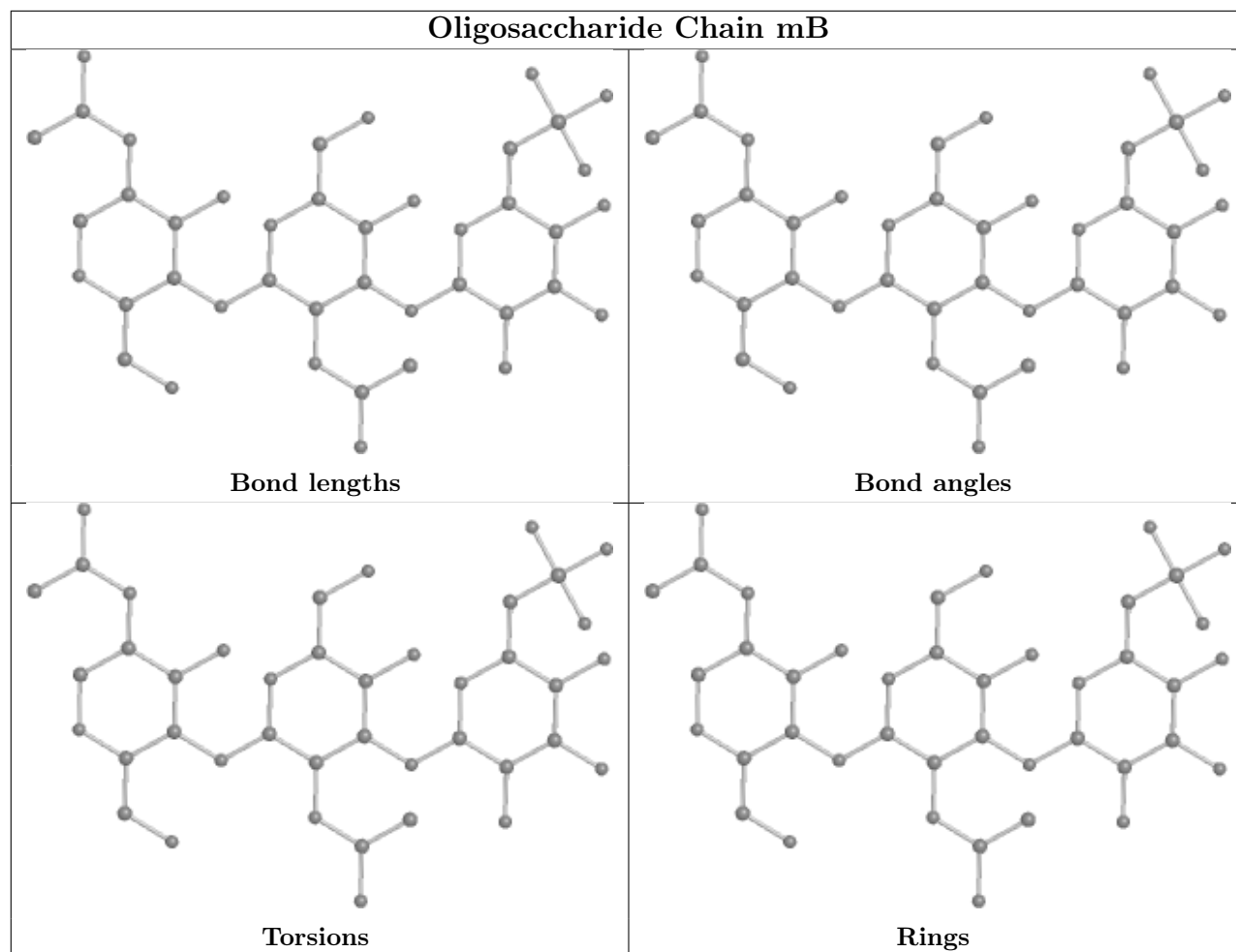


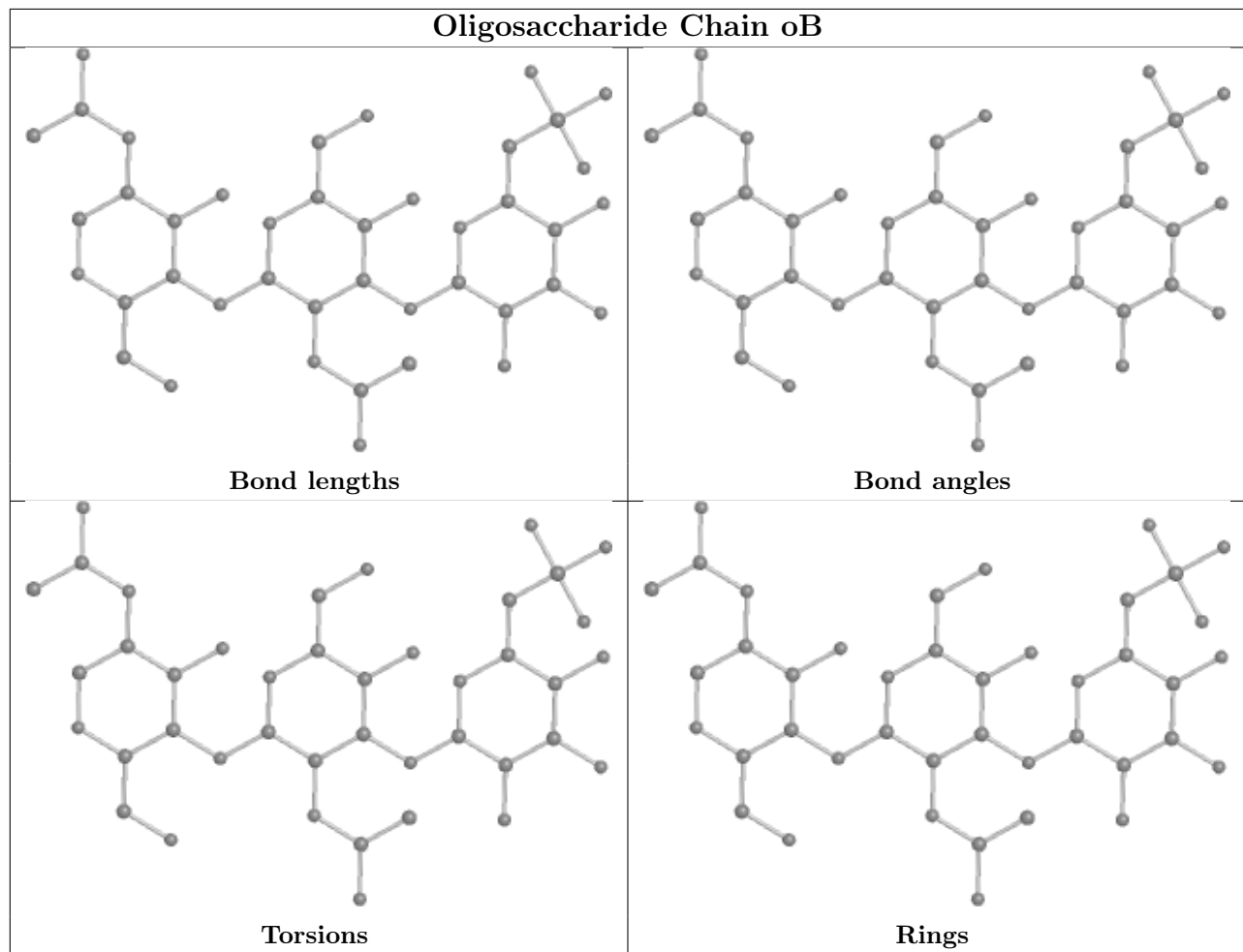


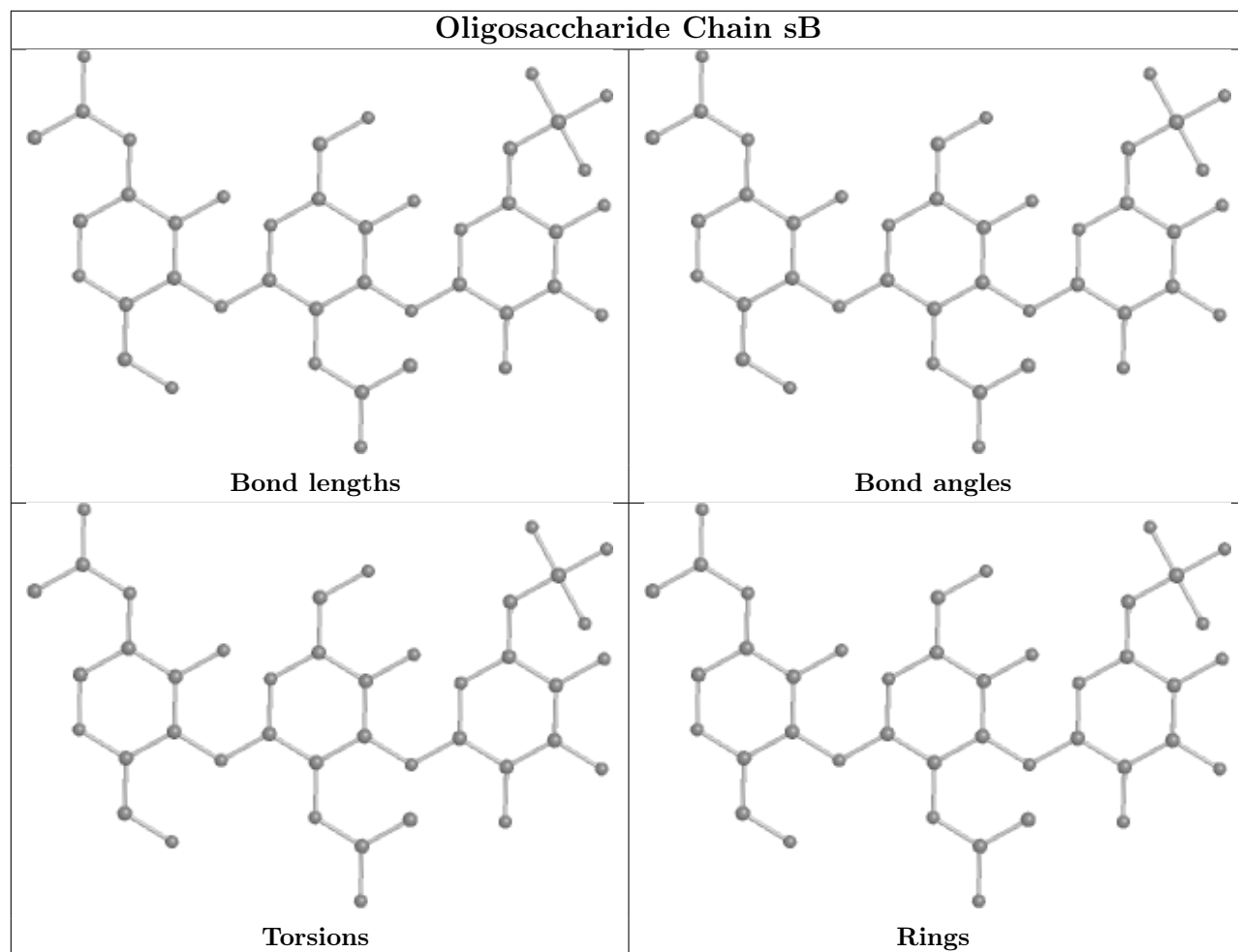




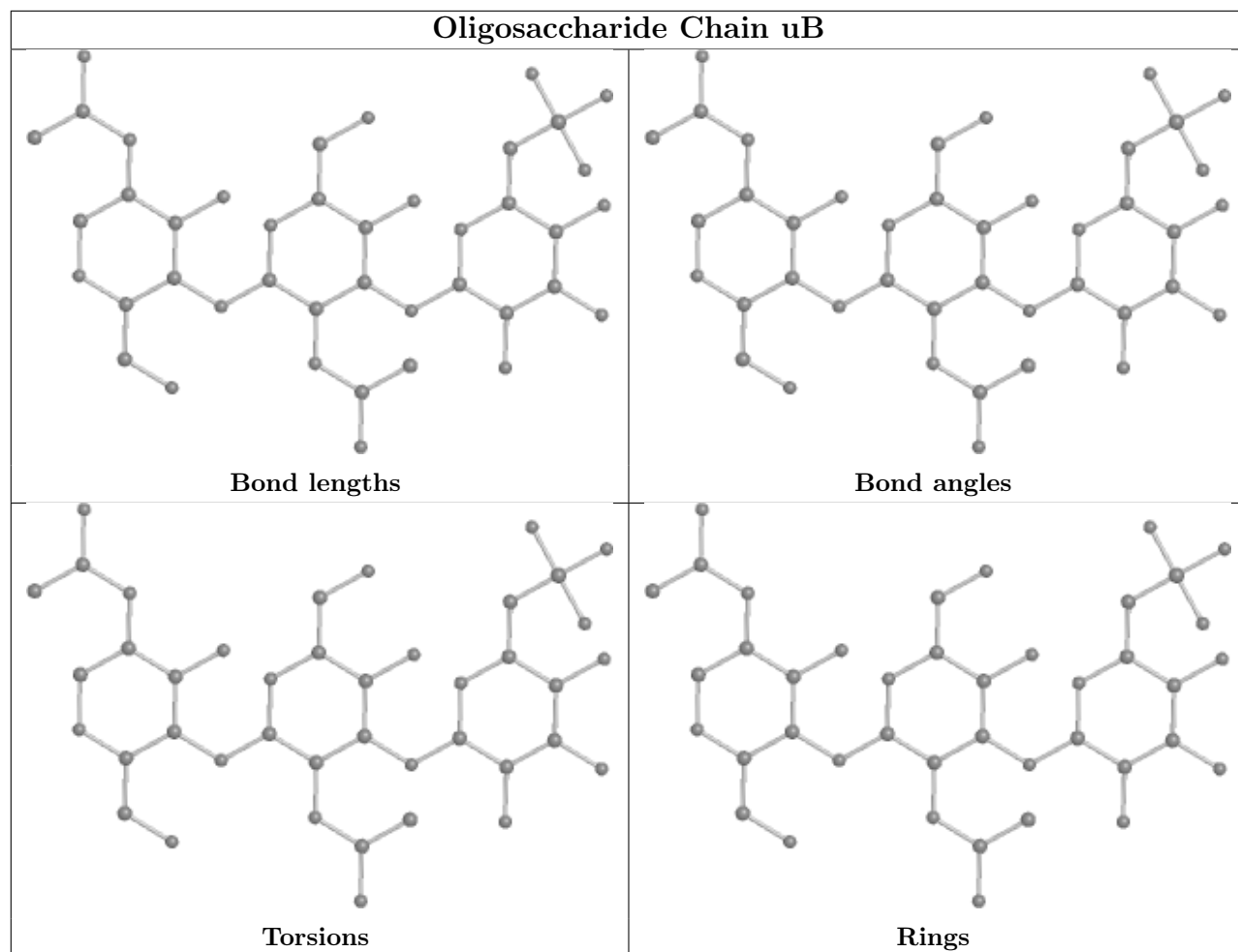


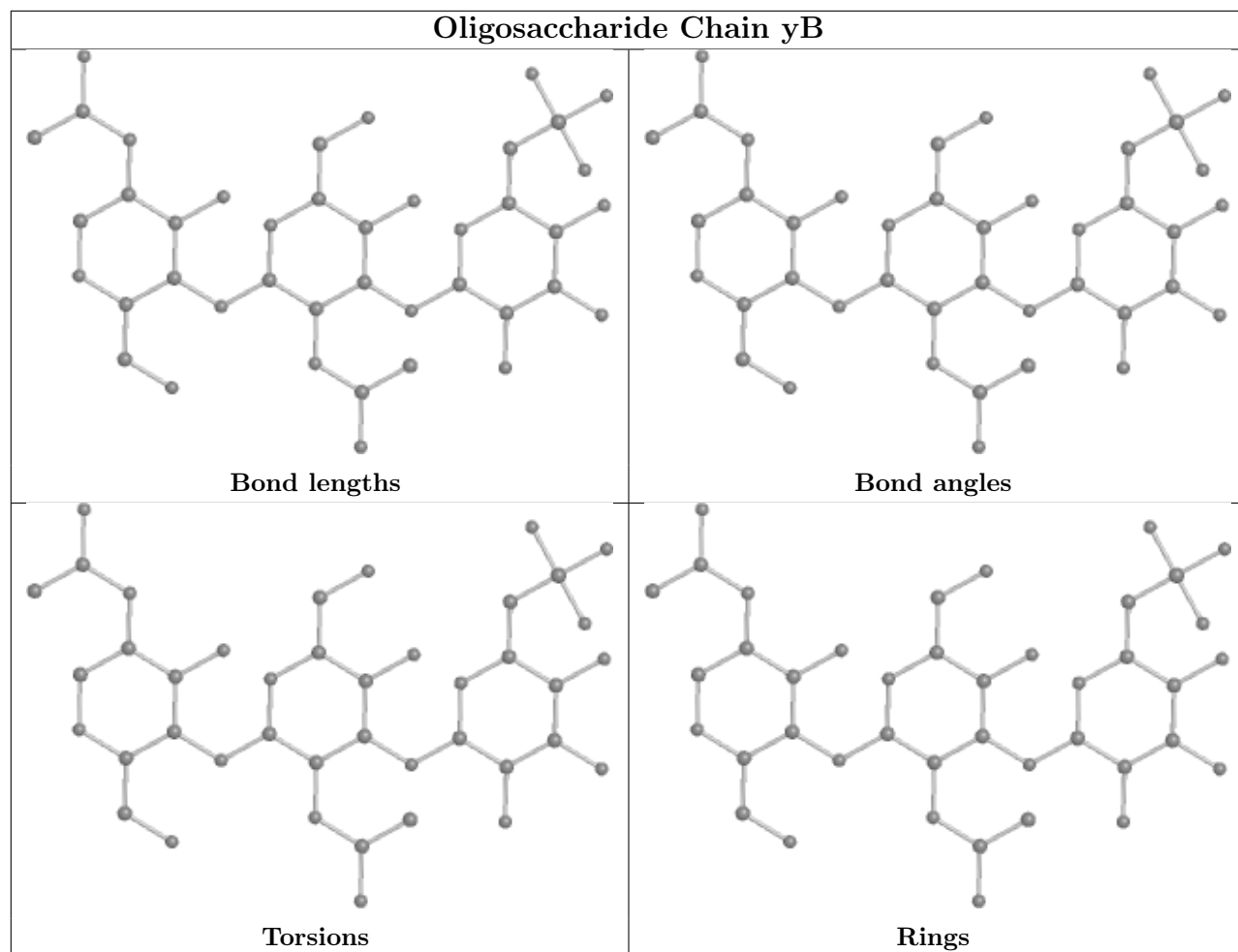


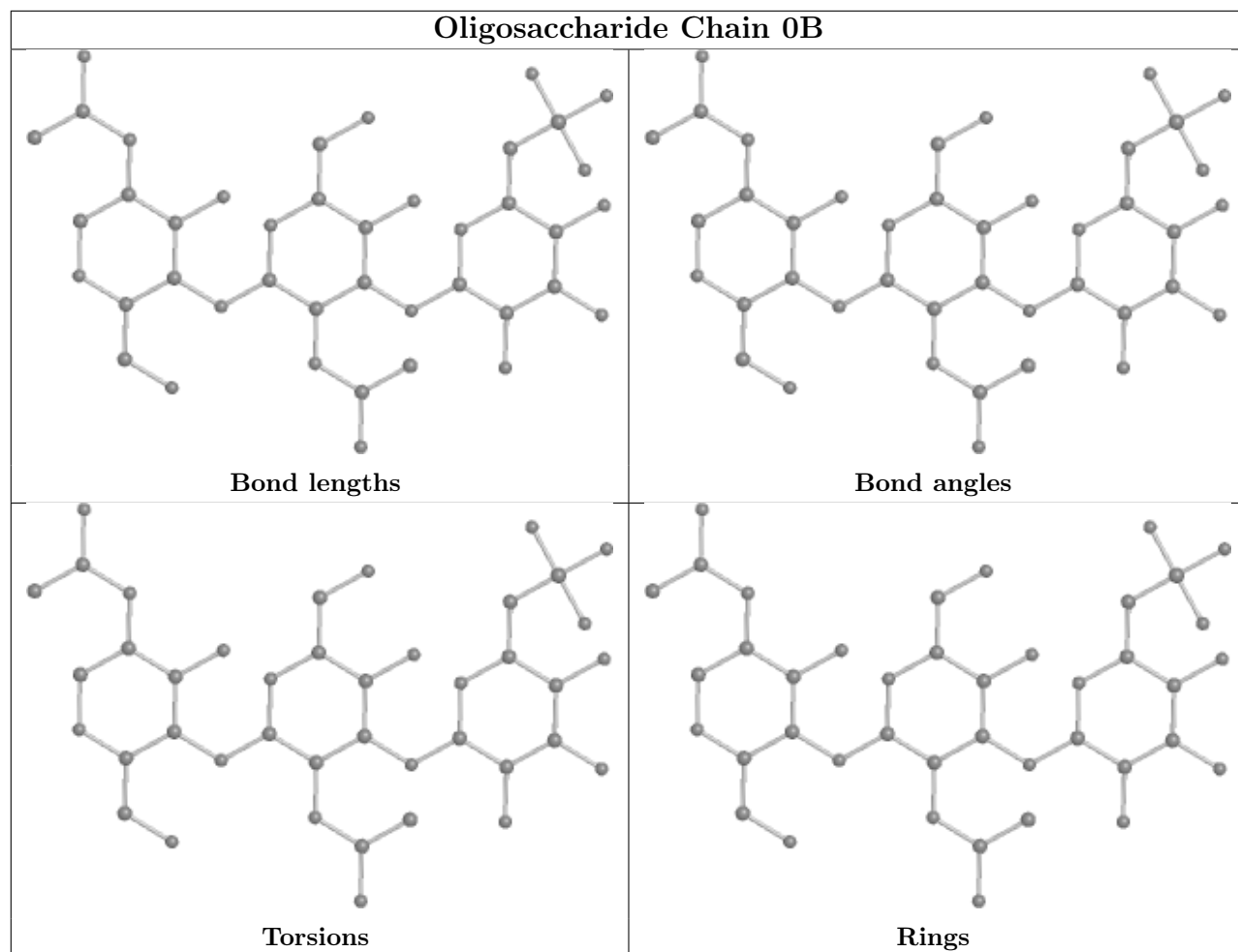


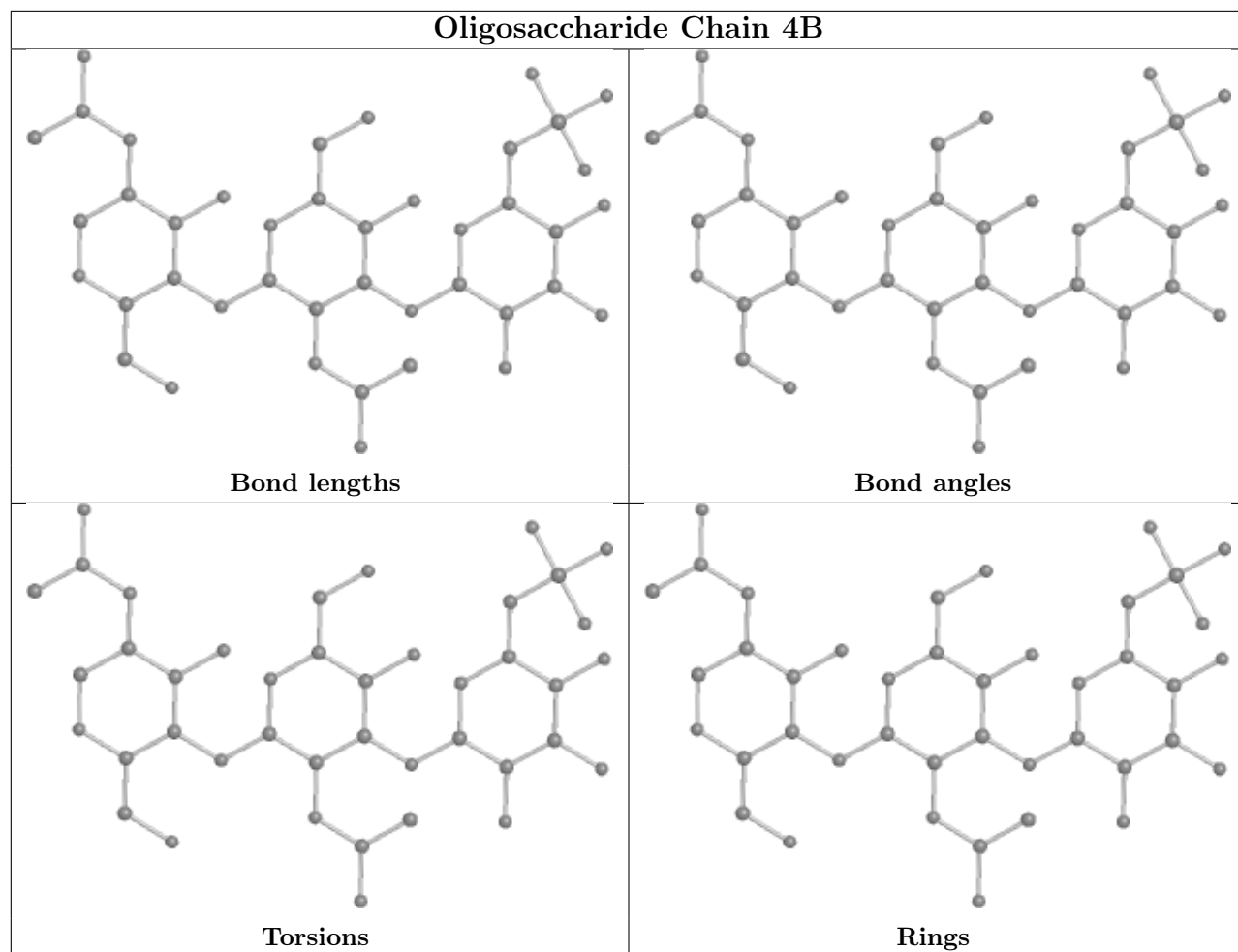


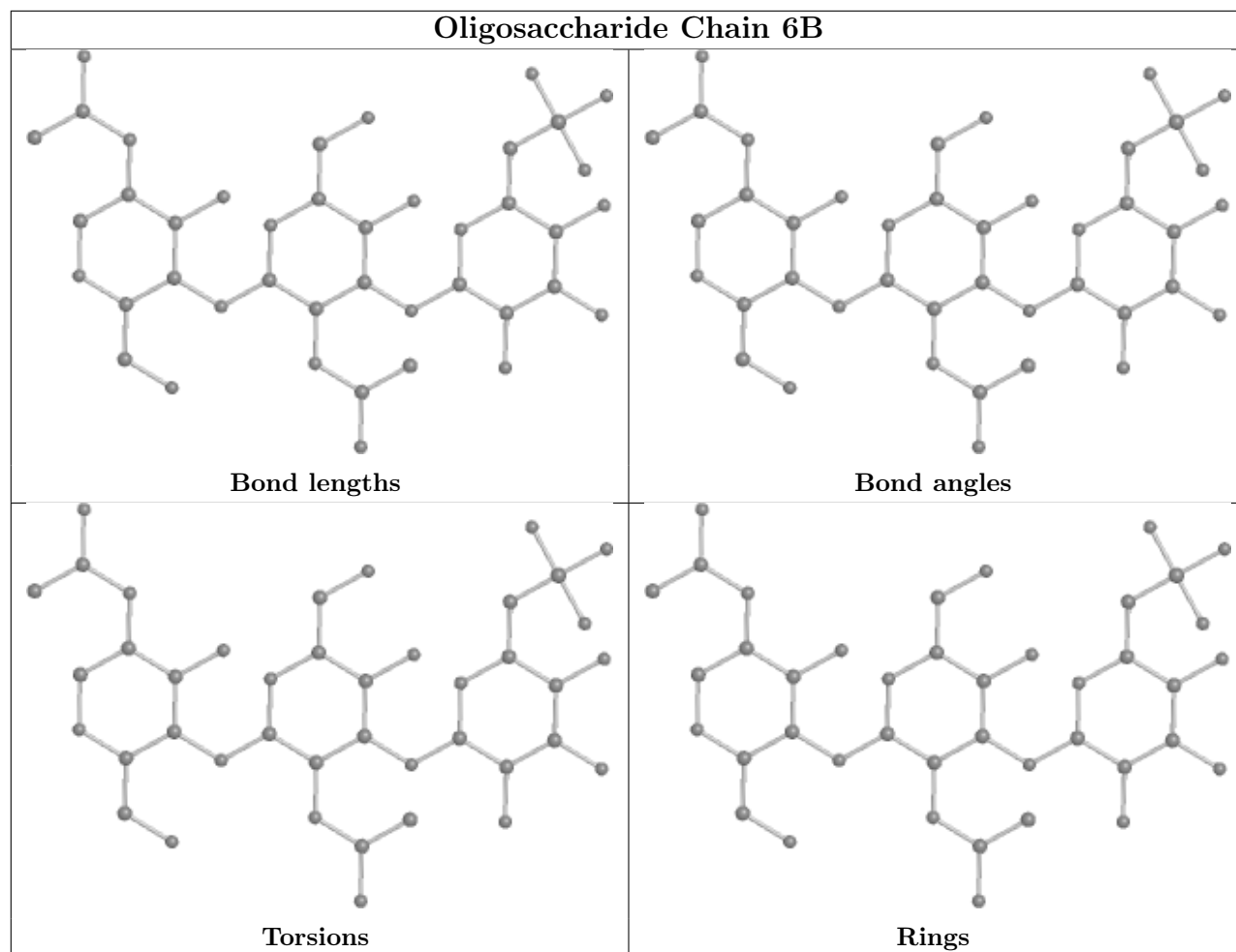


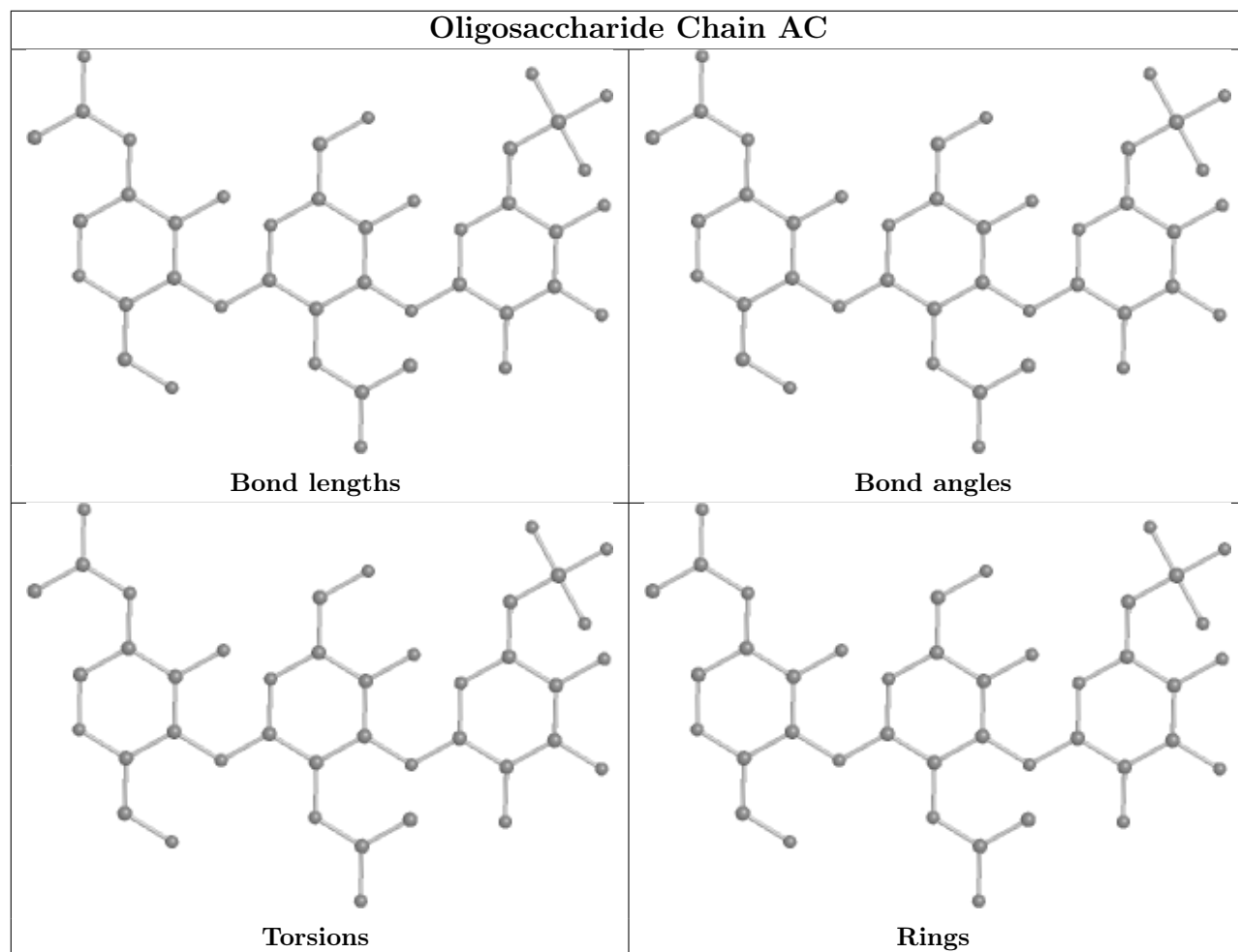


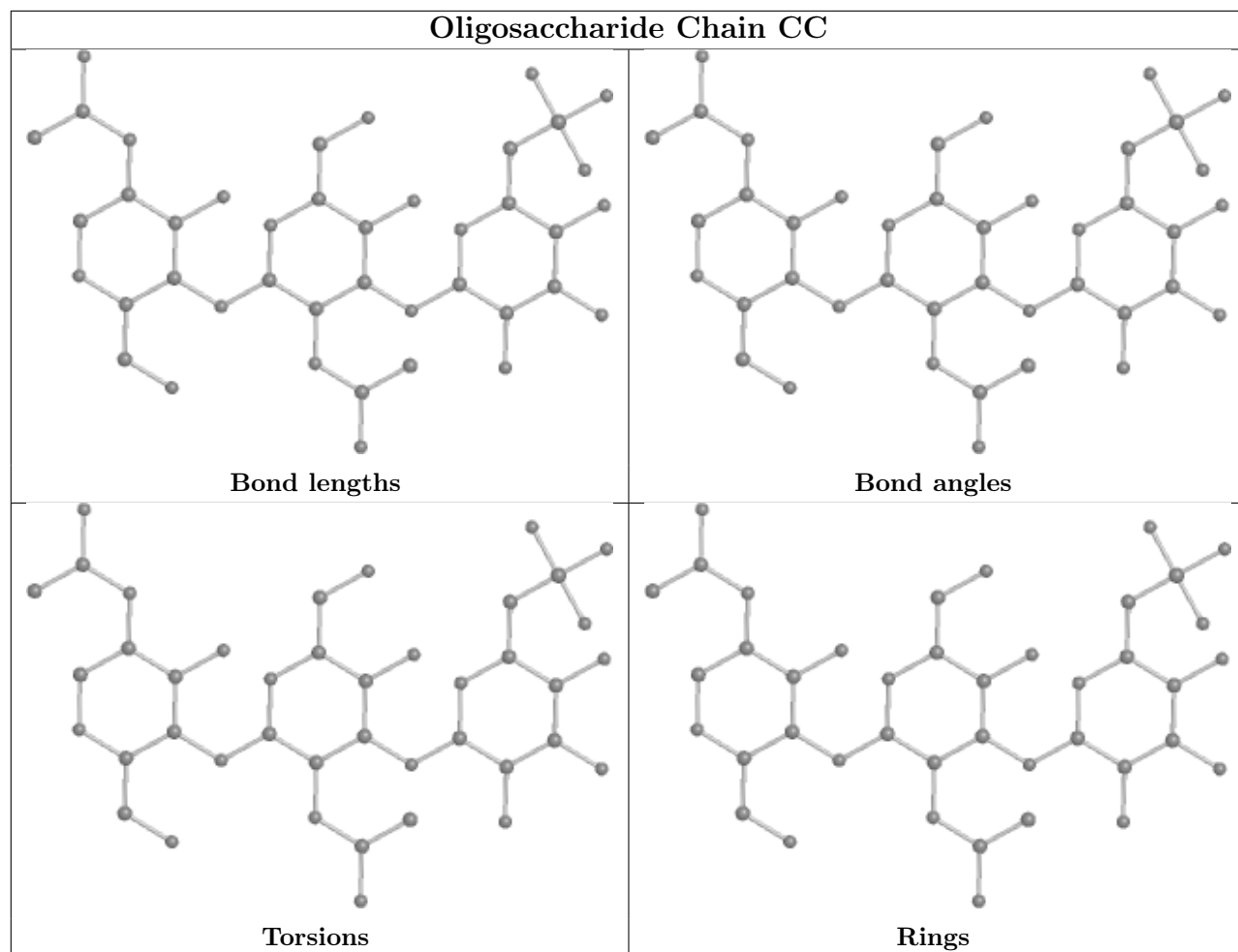


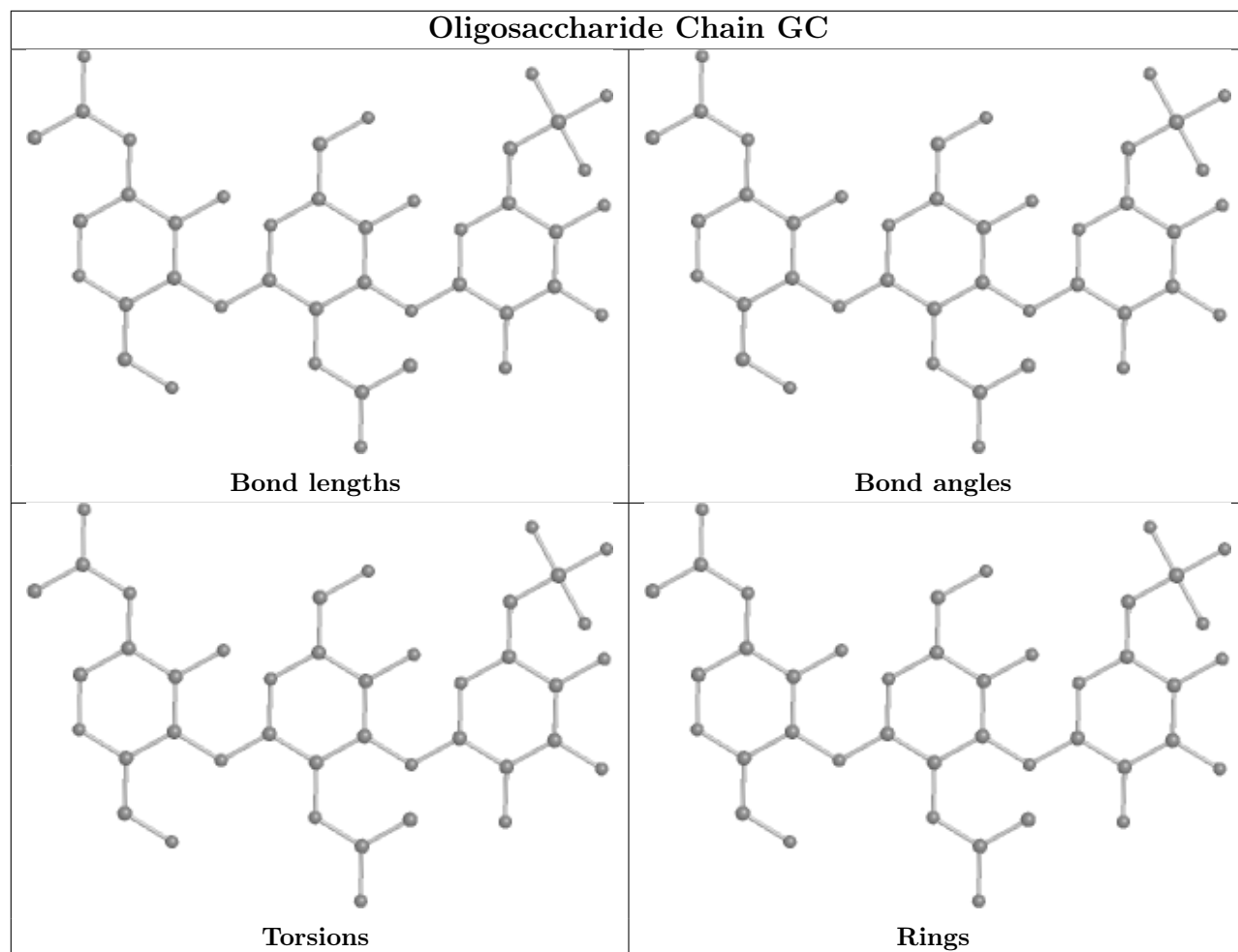




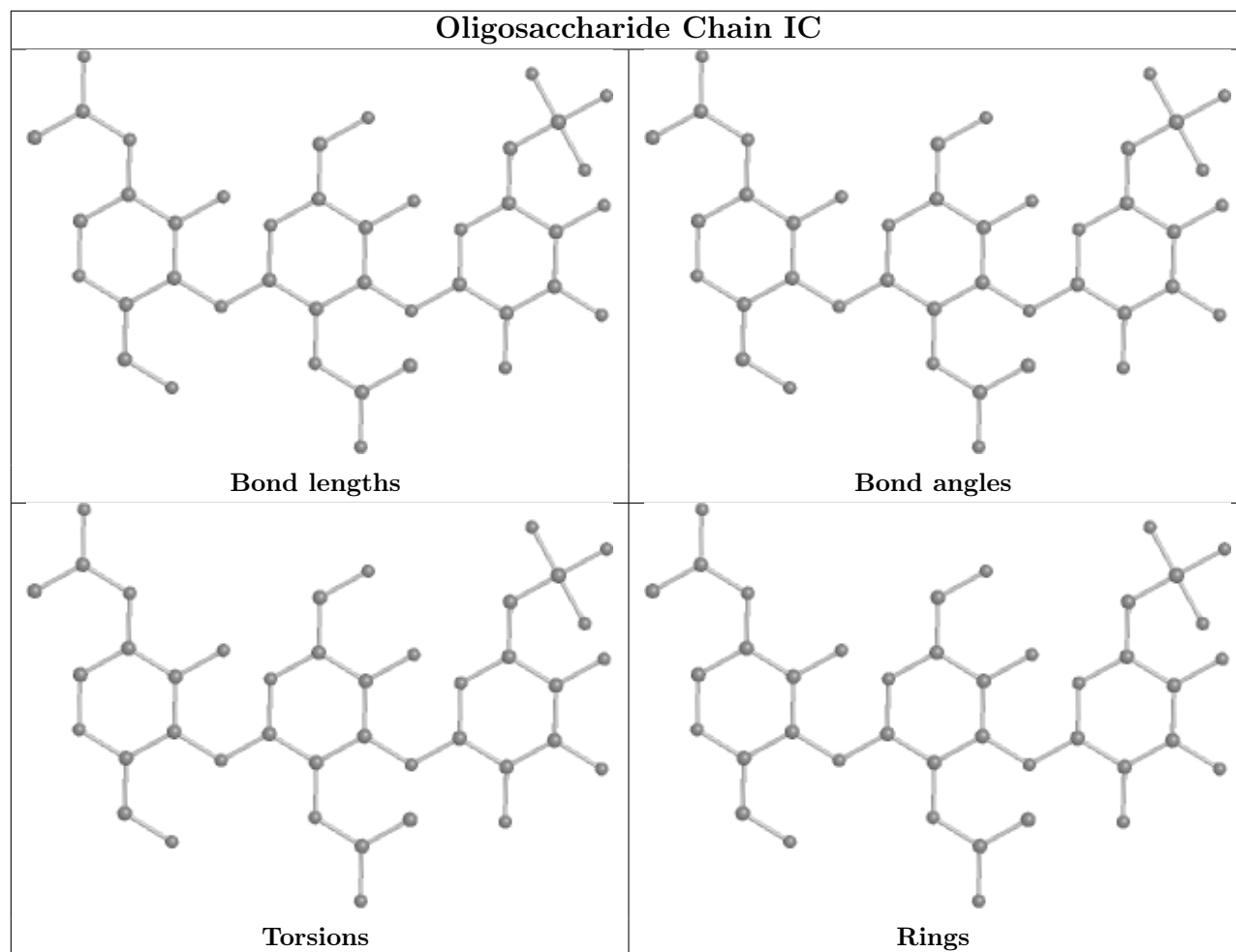


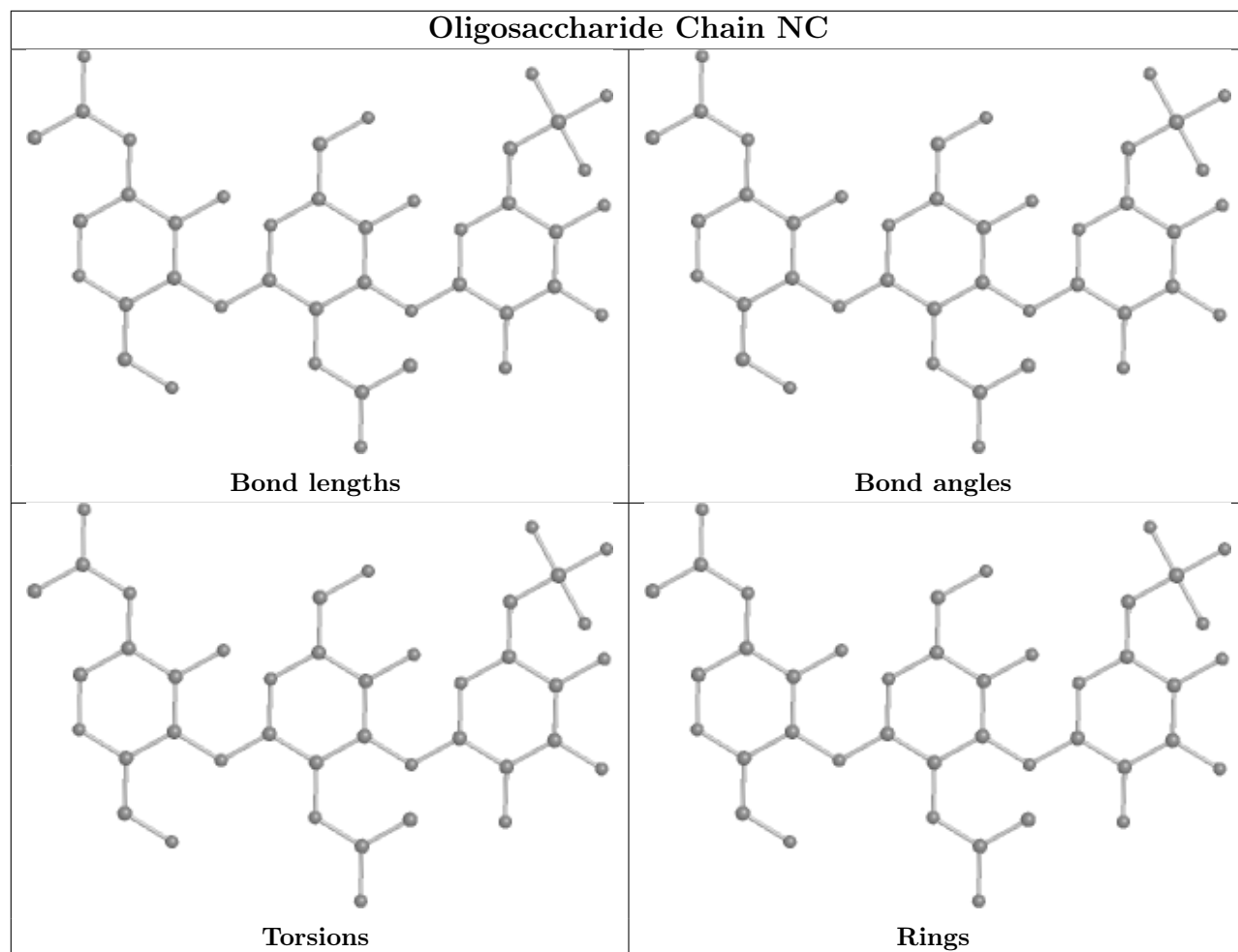


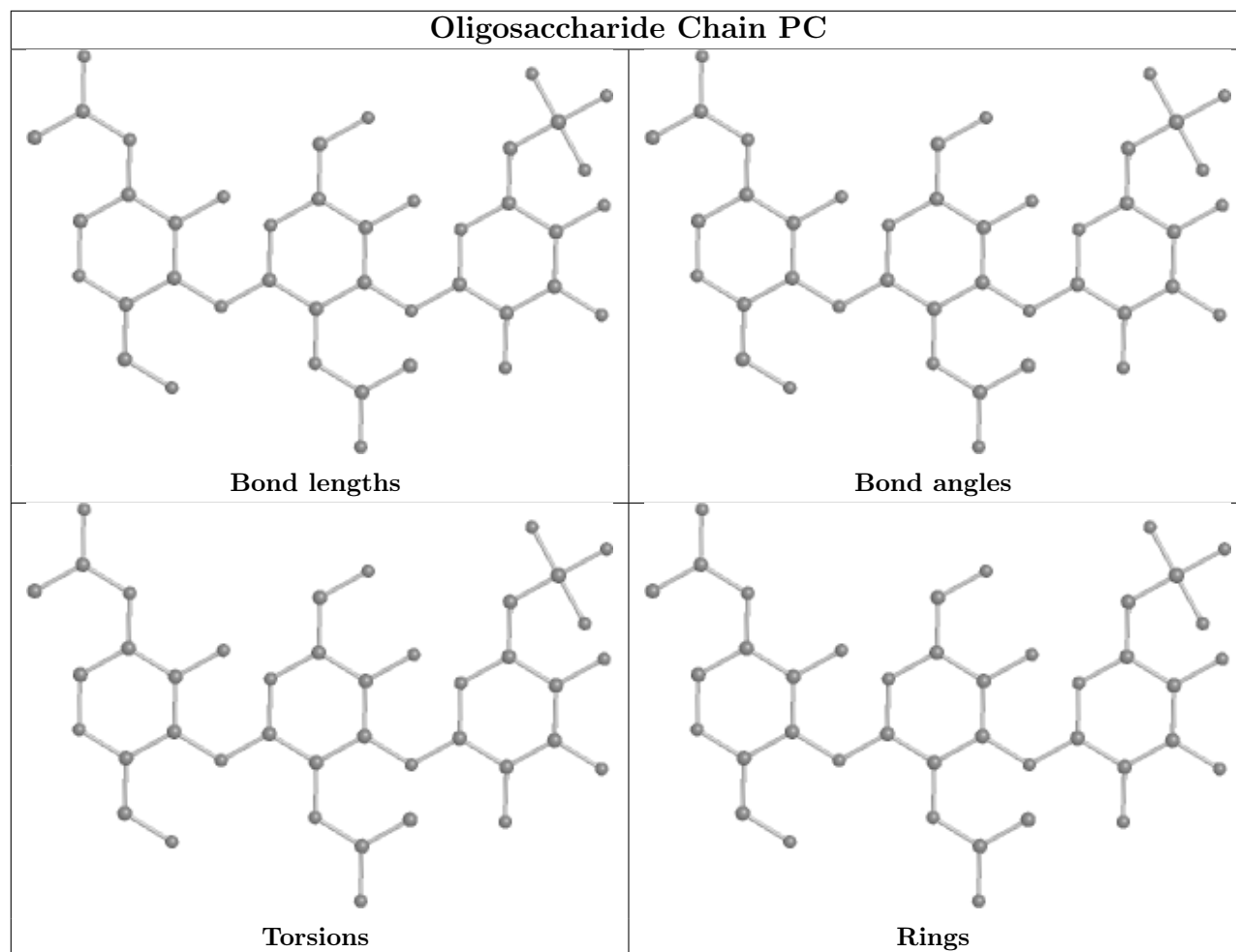


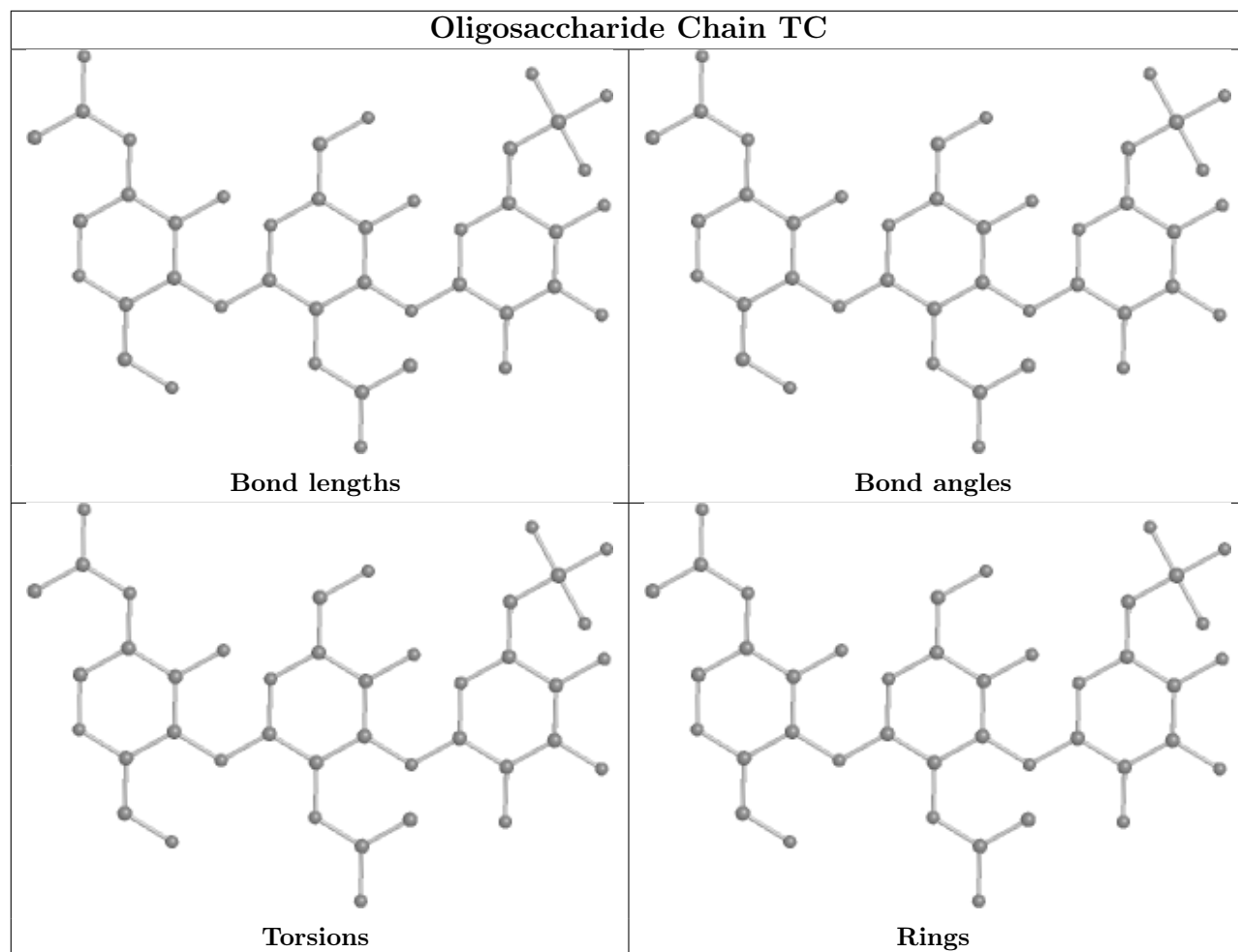


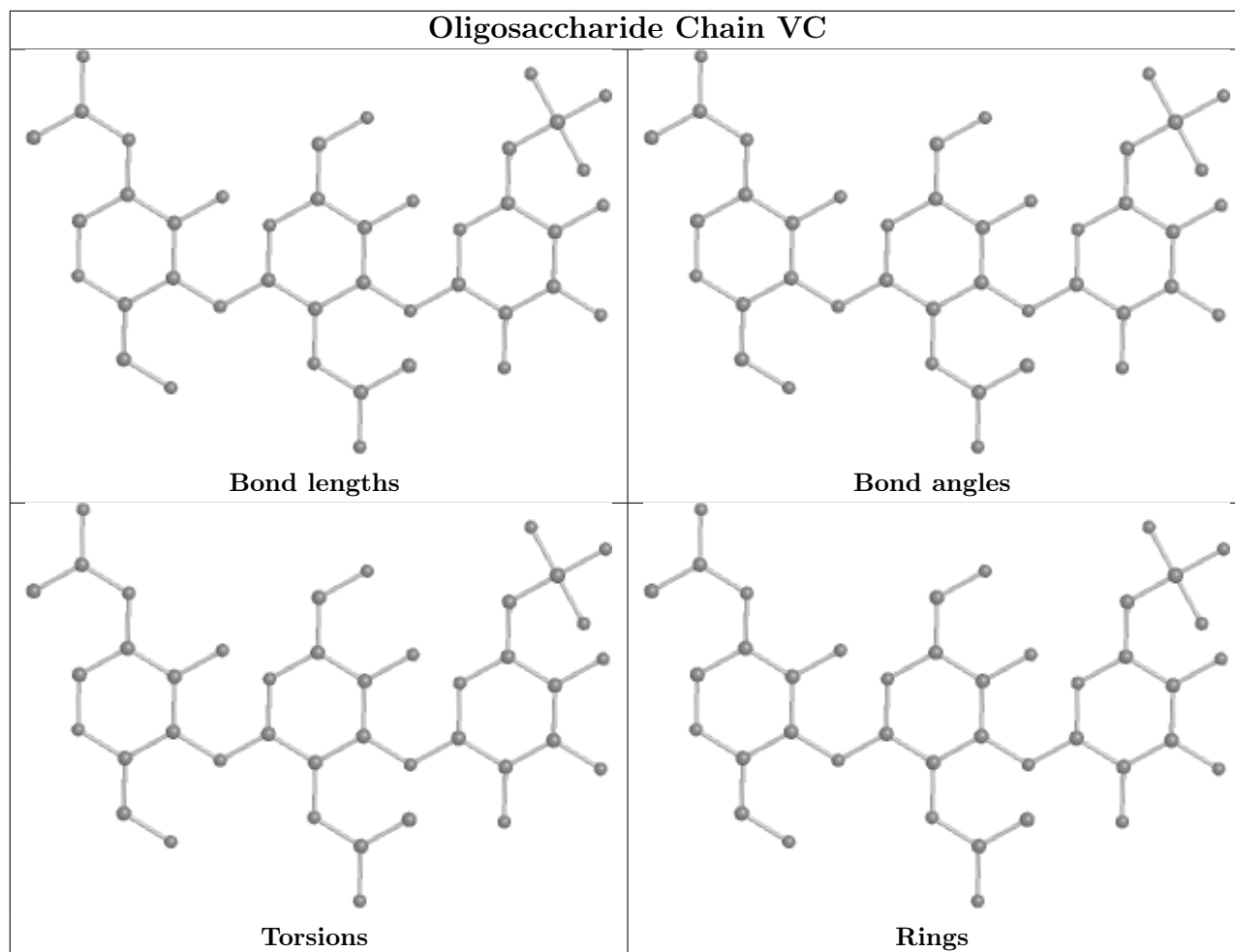












## 5.6 Ligand geometry [i](#)

72 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	NAG	J	400	1	14,14,15	0.49	0	17,19,21	0.54	0
4	NAG	7	202	1	14,14,15	0.62	0	17,19,21	0.85	1 (5%)
4	NAG	0	202	1	14,14,15	0.58	0	17,19,21	0.84	1 (5%)
4	NAG	8	202	1	14,14,15	0.31	0	17,19,21	0.66	0
4	NAG	LG	202	1	14,14,15	0.29	0	17,19,21	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	6	400	1	14,14,15	0.75	1 (7%)	17,19,21	0.37	0
4	NAG	l	202	1	14,14,15	0.62	0	17,19,21	0.84	1 (5%)
4	NAG	T	202	1	14,14,15	0.67	0	17,19,21	0.77	1 (5%)
4	NAG	LI	202	1	14,14,15	0.55	0	17,19,21	0.82	1 (5%)
4	NAG	V	400	1	14,14,15	1.56	1 (7%)	17,19,21	1.41	3 (17%)
4	NAG	H	202	1	14,14,15	0.62	0	17,19,21	0.81	1 (5%)
4	NAG	B	202	1	14,14,15	0.58	0	17,19,21	0.78	1 (5%)
4	NAG	K	202	1	14,14,15	0.56	0	17,19,21	0.82	1 (5%)
4	NAG	j	202	1	14,14,15	0.31	0	17,19,21	0.55	0
4	NAG	p	202	1	14,14,15	0.32	0	17,19,21	0.54	0
4	NAG	o	202	1	14,14,15	0.53	0	17,19,21	0.78	1 (5%)
4	NAG	D	400	1	14,14,15	0.83	0	17,19,21	2.01	3 (17%)
4	NAG	LC	202	1	14,14,15	0.63	0	17,19,21	0.88	1 (5%)
4	NAG	Z	202	1	14,14,15	0.60	0	17,19,21	0.84	1 (5%)
4	NAG	E	202	1	14,14,15	0.66	0	17,19,21	0.89	1 (5%)
4	NAG	4	202	1	14,14,15	0.63	0	17,19,21	0.81	1 (5%)
4	NAG	G	400	1	14,14,15	0.40	0	17,19,21	0.38	0
4	NAG	Y	400	1	14,14,15	0.48	0	17,19,21	0.54	0
4	NAG	c	202	1	14,14,15	0.58	0	17,19,21	0.84	1 (5%)
4	NAG	LE	400	1	14,14,15	0.39	0	17,19,21	0.38	0
4	NAG	S	400	1	14,14,15	0.42	0	17,19,21	0.40	0
4	NAG	r	202	1	14,14,15	0.56	0	17,19,21	0.82	1 (5%)
4	NAG	R	202	1	14,14,15	0.33	0	17,19,21	0.53	0
4	NAG	s	202	1	14,14,15	0.32	0	17,19,21	0.54	0
4	NAG	u	202	1	14,14,15	0.59	0	17,19,21	0.78	1 (5%)
4	NAG	n	400	1	14,14,15	0.38	0	17,19,21	0.38	0
4	NAG	A	400	1	14,14,15	0.36	0	17,19,21	0.39	0
4	NAG	g	202	1	14,14,15	0.28	0	17,19,21	0.56	0
4	NAG	q	400	1	14,14,15	0.45	0	17,19,21	0.53	0
4	NAG	z	400	1	14,14,15	0.68	1 (7%)	17,19,21	0.98	1 (5%)
4	NAG	9	400	1	14,14,15	0.46	0	17,19,21	0.55	0
4	NAG	m	202	1	14,14,15	0.34	0	17,19,21	0.55	0
4	NAG	x	202	1	14,14,15	0.61	0	17,19,21	0.82	1 (5%)
4	NAG	LF	202	1	14,14,15	0.59	0	17,19,21	0.83	1 (5%)
4	NAG	C	202	1	14,14,15	0.27	0	17,19,21	0.51	0
4	NAG	l	202	1	14,14,15	0.61	0	17,19,21	0.80	1 (5%)
4	NAG	P	400	1	14,14,15	0.45	0	17,19,21	0.54	0
4	NAG	b	400	1	14,14,15	2.06	2 (14%)	17,19,21	0.97	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	O	202	1	14,14,15	0.20	0	17,19,21	0.50	0
4	NAG	v	202	1	14,14,15	0.30	0	17,19,21	0.55	0
4	NAG	LA	202	1	14,14,15	0.32	0	17,19,21	0.54	0
4	NAG	3	400	1	14,14,15	0.37	0	17,19,21	0.36	0
4	NAG	w	400	1	14,14,15	0.76	1 (7%)	17,19,21	0.44	0
4	NAG	L	202	1	14,14,15	0.36	0	17,19,21	0.63	0
4	NAG	M	400	1	14,14,15	1.06	1 (7%)	17,19,21	0.55	0
4	NAG	U	202	1	14,14,15	0.31	0	17,19,21	0.58	0
4	NAG	N	202	1	14,14,15	0.59	0	17,19,21	0.81	1 (5%)
4	NAG	W	202	1	14,14,15	0.60	0	17,19,21	0.82	1 (5%)
4	NAG	2	202	1	14,14,15	0.30	0	17,19,21	0.57	0
4	NAG	f	202	1	14,14,15	0.64	0	17,19,21	0.95	1 (5%)
4	NAG	k	400	1	14,14,15	0.41	0	17,19,21	0.39	0
4	NAG	Q	202	1	14,14,15	0.61	0	17,19,21	0.83	1 (5%)
4	NAG	d	202	1	14,14,15	0.41	0	17,19,21	0.60	0
4	NAG	LH	400	1	14,14,15	0.42	0	17,19,21	0.36	0
4	NAG	t	400	1	14,14,15	0.61	1 (7%)	17,19,21	0.63	0
4	NAG	y	202	1	14,14,15	0.33	0	17,19,21	0.50	0
4	NAG	i	202	1	14,14,15	0.61	0	17,19,21	0.82	1 (5%)
4	NAG	5	202	1	14,14,15	0.28	0	17,19,21	0.52	0
4	NAG	a	202	1	14,14,15	0.26	0	17,19,21	0.46	0
4	NAG	LJ	202	1	14,14,15	0.29	0	17,19,21	0.51	0
4	NAG	h	400	1	14,14,15	0.47	0	17,19,21	0.54	0
4	NAG	LD	202	1	14,14,15	0.31	0	17,19,21	0.57	0
4	NAG	F	202	1	14,14,15	0.28	0	17,19,21	0.56	0
4	NAG	X	202	1	14,14,15	0.33	0	17,19,21	0.57	0
4	NAG	I	202	1	14,14,15	0.22	0	17,19,21	0.50	0
4	NAG	e	400	1	14,14,15	0.66	0	17,19,21	0.98	1 (5%)
4	NAG	LB	400	1	14,14,15	0.82	1 (7%)	17,19,21	0.99	1 (5%)

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
4	NAG	J	400	1	-	2/6/23/26	0/1/1/1
4	NAG	7	202	1	-	1/6/23/26	0/1/1/1
4	NAG	0	202	1	-	1/6/23/26	0/1/1/1
4	NAG	8	202	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	LG	202	1	-	2/6/23/26	0/1/1/1
4	NAG	6	400	1	-	4/6/23/26	0/1/1/1
4	NAG	l	202	1	-	1/6/23/26	0/1/1/1
4	NAG	T	202	1	-	1/6/23/26	0/1/1/1
4	NAG	LI	202	1	-	1/6/23/26	0/1/1/1
4	NAG	V	400	1	-	4/6/23/26	0/1/1/1
4	NAG	H	202	1	-	1/6/23/26	0/1/1/1
4	NAG	B	202	1	-	1/6/23/26	0/1/1/1
4	NAG	K	202	1	-	1/6/23/26	0/1/1/1
4	NAG	j	202	1	-	2/6/23/26	0/1/1/1
4	NAG	p	202	1	-	2/6/23/26	0/1/1/1
4	NAG	o	202	1	-	1/6/23/26	0/1/1/1
4	NAG	D	400	1	-	2/6/23/26	0/1/1/1
4	NAG	LC	202	1	-	1/6/23/26	0/1/1/1
4	NAG	Z	202	1	-	1/6/23/26	0/1/1/1
4	NAG	E	202	1	-	1/6/23/26	0/1/1/1
4	NAG	4	202	1	-	1/6/23/26	0/1/1/1
4	NAG	G	400	1	-	4/6/23/26	0/1/1/1
4	NAG	Y	400	1	-	3/6/23/26	0/1/1/1
4	NAG	c	202	1	-	1/6/23/26	0/1/1/1
4	NAG	LE	400	1	-	4/6/23/26	0/1/1/1
4	NAG	S	400	1	-	4/6/23/26	0/1/1/1
4	NAG	r	202	1	-	1/6/23/26	0/1/1/1
4	NAG	R	202	1	-	2/6/23/26	0/1/1/1
4	NAG	s	202	1	-	2/6/23/26	0/1/1/1
4	NAG	u	202	1	-	1/6/23/26	0/1/1/1
4	NAG	n	400	1	-	4/6/23/26	0/1/1/1
4	NAG	A	400	1	-	4/6/23/26	0/1/1/1
4	NAG	g	202	1	-	2/6/23/26	0/1/1/1
4	NAG	q	400	1	-	4/6/23/26	0/1/1/1
4	NAG	z	400	1	-	2/6/23/26	0/1/1/1
4	NAG	9	400	1	-	4/6/23/26	0/1/1/1
4	NAG	m	202	1	-	2/6/23/26	0/1/1/1
4	NAG	x	202	1	-	1/6/23/26	0/1/1/1
4	NAG	LF	202	1	-	1/6/23/26	0/1/1/1
4	NAG	C	202	1	-	2/6/23/26	0/1/1/1
4	NAG	l	202	1	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	P	400	1	-	2/6/23/26	0/1/1/1
4	NAG	b	400	1	-	2/6/23/26	0/1/1/1
4	NAG	O	202	1	-	2/6/23/26	0/1/1/1
4	NAG	v	202	1	-	2/6/23/26	0/1/1/1
4	NAG	LA	202	1	-	2/6/23/26	0/1/1/1
4	NAG	3	400	1	-	4/6/23/26	0/1/1/1
4	NAG	w	400	1	-	4/6/23/26	0/1/1/1
4	NAG	L	202	1	-	2/6/23/26	0/1/1/1
4	NAG	M	400	1	-	4/6/23/26	0/1/1/1
4	NAG	U	202	1	-	2/6/23/26	0/1/1/1
4	NAG	N	202	1	-	1/6/23/26	0/1/1/1
4	NAG	W	202	1	-	1/6/23/26	0/1/1/1
4	NAG	2	202	1	-	2/6/23/26	0/1/1/1
4	NAG	f	202	1	-	1/6/23/26	0/1/1/1
4	NAG	k	400	1	-	4/6/23/26	0/1/1/1
4	NAG	Q	202	1	-	1/6/23/26	0/1/1/1
4	NAG	d	202	1	-	0/6/23/26	0/1/1/1
4	NAG	LH	400	1	-	4/6/23/26	0/1/1/1
4	NAG	t	400	1	-	4/6/23/26	0/1/1/1
4	NAG	y	202	1	-	2/6/23/26	0/1/1/1
4	NAG	i	202	1	-	1/6/23/26	0/1/1/1
4	NAG	5	202	1	-	2/6/23/26	0/1/1/1
4	NAG	a	202	1	-	2/6/23/26	0/1/1/1
4	NAG	LJ	202	1	-	2/6/23/26	0/1/1/1
4	NAG	h	400	1	-	4/6/23/26	0/1/1/1
4	NAG	LD	202	1	-	2/6/23/26	0/1/1/1
4	NAG	F	202	1	-	2/6/23/26	0/1/1/1
4	NAG	X	202	1	-	2/6/23/26	0/1/1/1
4	NAG	I	202	1	-	2/6/23/26	0/1/1/1
4	NAG	e	400	1	-	2/6/23/26	0/1/1/1
4	NAG	LB	400	1	-	2/6/23/26	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	b	400	NAG	C1-C2	-5.78	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	V	400	NAG	O5-C1	5.19	1.52	1.43
4	b	400	NAG	O5-C1	4.62	1.51	1.43
4	M	400	NAG	O5-C1	3.49	1.49	1.43
4	LB	400	NAG	C1-C2	3.03	1.56	1.52
4	6	400	NAG	O5-C1	2.40	1.47	1.43
4	w	400	NAG	O5-C1	2.30	1.47	1.43
4	t	400	NAG	C1-C2	2.13	1.55	1.52
4	z	400	NAG	C1-C2	2.04	1.55	1.52

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	400	NAG	C1-O5-C5	5.58	119.76	112.19
4	V	400	NAG	C1-O5-C5	3.27	116.63	112.19
4	D	400	NAG	O5-C5-C4	-3.12	103.23	110.83
4	f	202	NAG	C1-O5-C5	3.08	116.36	112.19
4	LB	400	NAG	C1-O5-C5	2.99	116.24	112.19
4	D	400	NAG	C1-C2-N2	2.98	115.57	110.49
4	e	400	NAG	C1-O5-C5	2.83	116.02	112.19
4	z	400	NAG	C1-O5-C5	2.78	115.96	112.19
4	E	202	NAG	C1-O5-C5	2.75	115.92	112.19
4	V	400	NAG	O4-C4-C3	-2.71	104.08	110.35
4	LC	202	NAG	C1-O5-C5	2.71	115.86	112.19
4	7	202	NAG	C1-O5-C5	2.61	115.72	112.19
4	0	202	NAG	C1-O5-C5	2.58	115.69	112.19
4	c	202	NAG	C1-O5-C5	2.57	115.67	112.19
4	Z	202	NAG	C1-O5-C5	2.56	115.66	112.19
4	r	202	NAG	C1-O5-C5	2.56	115.66	112.19
4	l	202	NAG	C1-O5-C5	2.55	115.65	112.19
4	LF	202	NAG	C1-O5-C5	2.54	115.63	112.19
4	i	202	NAG	C1-O5-C5	2.54	115.63	112.19
4	Q	202	NAG	C1-O5-C5	2.52	115.61	112.19
4	N	202	NAG	C1-O5-C5	2.50	115.58	112.19
4	K	202	NAG	C1-O5-C5	2.50	115.57	112.19
4	x	202	NAG	C1-O5-C5	2.49	115.57	112.19
4	H	202	NAG	C1-O5-C5	2.49	115.56	112.19
4	W	202	NAG	C1-O5-C5	2.49	115.56	112.19
4	LI	202	NAG	C1-O5-C5	2.44	115.50	112.19
4	V	400	NAG	C4-C3-C2	-2.44	107.44	111.02
4	B	202	NAG	C1-O5-C5	2.44	115.50	112.19
4	4	202	NAG	C1-O5-C5	2.42	115.47	112.19
4	o	202	NAG	C1-O5-C5	2.39	115.44	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	l	202	NAG	C1-O5-C5	2.38	115.42	112.19
4	u	202	NAG	C1-O5-C5	2.27	115.27	112.19
4	T	202	NAG	C1-O5-C5	2.22	115.19	112.19
4	b	400	NAG	C3-C4-C5	-2.04	106.59	110.24

There are no chirality outliers.

All (151) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	400	NAG	C1-C2-N2-C7
4	V	400	NAG	C1-C2-N2-C7
4	e	400	NAG	C1-C2-N2-C7
4	z	400	NAG	C1-C2-N2-C7
4	LB	400	NAG	C1-C2-N2-C7
4	b	400	NAG	C1-C2-N2-C7
4	3	400	NAG	C4-C5-C6-O6
4	m	202	NAG	C4-C5-C6-O6
4	s	202	NAG	C4-C5-C6-O6
4	LH	400	NAG	C4-C5-C6-O6
4	a	202	NAG	C4-C5-C6-O6
4	p	202	NAG	C4-C5-C6-O6
4	9	400	NAG	C4-C5-C6-O6
4	C	202	NAG	C4-C5-C6-O6
4	R	202	NAG	C4-C5-C6-O6
4	X	202	NAG	C4-C5-C6-O6
4	g	202	NAG	C4-C5-C6-O6
4	j	202	NAG	C4-C5-C6-O6
4	5	202	NAG	C4-C5-C6-O6
4	LA	202	NAG	C4-C5-C6-O6
4	s	202	NAG	O5-C5-C6-O6
4	F	202	NAG	C4-C5-C6-O6
4	2	202	NAG	C4-C5-C6-O6
4	I	202	NAG	C4-C5-C6-O6
4	O	202	NAG	C4-C5-C6-O6
4	k	400	NAG	C4-C5-C6-O6
4	v	202	NAG	C4-C5-C6-O6
4	A	400	NAG	C4-C5-C6-O6
4	G	400	NAG	C4-C5-C6-O6
4	C	202	NAG	O5-C5-C6-O6
4	X	202	NAG	O5-C5-C6-O6
4	a	202	NAG	O5-C5-C6-O6
4	j	202	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	m	202	NAG	O5-C5-C6-O6
4	p	202	NAG	O5-C5-C6-O6
4	5	202	NAG	O5-C5-C6-O6
4	LA	202	NAG	O5-C5-C6-O6
4	F	202	NAG	O5-C5-C6-O6
4	R	202	NAG	O5-C5-C6-O6
4	g	202	NAG	O5-C5-C6-O6
4	2	202	NAG	O5-C5-C6-O6
4	w	400	NAG	C4-C5-C6-O6
4	I	202	NAG	O5-C5-C6-O6
4	O	202	NAG	O5-C5-C6-O6
4	V	400	NAG	C4-C5-C6-O6
4	LE	400	NAG	C4-C5-C6-O6
4	3	400	NAG	O5-C5-C6-O6
4	v	202	NAG	O5-C5-C6-O6
4	LH	400	NAG	O5-C5-C6-O6
4	6	400	NAG	C4-C5-C6-O6
4	y	202	NAG	C4-C5-C6-O6
4	M	400	NAG	C1-C2-N2-C7
4	P	400	NAG	C1-C2-N2-C7
4	Y	400	NAG	C1-C2-N2-C7
4	h	400	NAG	C1-C2-N2-C7
4	t	400	NAG	C1-C2-N2-C7
4	LG	202	NAG	C4-C5-C6-O6
4	LJ	202	NAG	C4-C5-C6-O6
4	A	400	NAG	O5-C5-C6-O6
4	9	400	NAG	O5-C5-C6-O6
4	k	400	NAG	O5-C5-C6-O6
4	M	400	NAG	C4-C5-C6-O6
4	A	400	NAG	C1-C2-N2-C7
4	J	400	NAG	C1-C2-N2-C7
4	S	400	NAG	C1-C2-N2-C7
4	k	400	NAG	C1-C2-N2-C7
4	n	400	NAG	C1-C2-N2-C7
4	q	400	NAG	C1-C2-N2-C7
4	w	400	NAG	C1-C2-N2-C7
4	9	400	NAG	C1-C2-N2-C7
4	LE	400	NAG	C1-C2-N2-C7
4	U	202	NAG	C4-C5-C6-O6
4	G	400	NAG	O5-C5-C6-O6
4	V	400	NAG	O5-C5-C6-O6
4	G	400	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
4	6	400	NAG	C1-C2-N2-C7
4	w	400	NAG	O5-C5-C6-O6
4	LD	202	NAG	C4-C5-C6-O6
4	LE	400	NAG	O5-C5-C6-O6
4	8	202	NAG	C4-C5-C6-O6
4	3	400	NAG	C1-C2-N2-C7
4	LH	400	NAG	C1-C2-N2-C7
4	6	400	NAG	O5-C5-C6-O6
4	L	202	NAG	C4-C5-C6-O6
4	y	202	NAG	O5-C5-C6-O6
4	LG	202	NAG	O5-C5-C6-O6
4	f	202	NAG	C3-C2-N2-C7
4	LJ	202	NAG	O5-C5-C6-O6
4	n	400	NAG	O5-C5-C6-O6
4	n	400	NAG	C4-C5-C6-O6
4	U	202	NAG	O5-C5-C6-O6
4	M	400	NAG	O5-C5-C6-O6
4	t	400	NAG	O5-C5-C6-O6
4	LD	202	NAG	O5-C5-C6-O6
4	S	400	NAG	O5-C5-C6-O6
4	8	202	NAG	O5-C5-C6-O6
4	S	400	NAG	C4-C5-C6-O6
4	t	400	NAG	C4-C5-C6-O6
4	B	202	NAG	C3-C2-N2-C7
4	D	400	NAG	C3-C2-N2-C7
4	E	202	NAG	C3-C2-N2-C7
4	H	202	NAG	C3-C2-N2-C7
4	J	400	NAG	C3-C2-N2-C7
4	K	202	NAG	C3-C2-N2-C7
4	M	400	NAG	C3-C2-N2-C7
4	N	202	NAG	C3-C2-N2-C7
4	P	400	NAG	C3-C2-N2-C7
4	Q	202	NAG	C3-C2-N2-C7
4	T	202	NAG	C3-C2-N2-C7
4	V	400	NAG	C3-C2-N2-C7
4	W	202	NAG	C3-C2-N2-C7
4	Z	202	NAG	C3-C2-N2-C7
4	b	400	NAG	C3-C2-N2-C7
4	c	202	NAG	C3-C2-N2-C7
4	e	400	NAG	C3-C2-N2-C7
4	h	400	NAG	C3-C2-N2-C7
4	i	202	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
4	l	202	NAG	C3-C2-N2-C7
4	n	400	NAG	C3-C2-N2-C7
4	o	202	NAG	C3-C2-N2-C7
4	q	400	NAG	C3-C2-N2-C7
4	r	202	NAG	C3-C2-N2-C7
4	t	400	NAG	C3-C2-N2-C7
4	u	202	NAG	C3-C2-N2-C7
4	x	202	NAG	C3-C2-N2-C7
4	z	400	NAG	C3-C2-N2-C7
4	1	202	NAG	C3-C2-N2-C7
4	4	202	NAG	C3-C2-N2-C7
4	7	202	NAG	C3-C2-N2-C7
4	0	202	NAG	C3-C2-N2-C7
4	LB	400	NAG	C3-C2-N2-C7
4	LC	202	NAG	C3-C2-N2-C7
4	LF	202	NAG	C3-C2-N2-C7
4	LI	202	NAG	C3-C2-N2-C7
4	h	400	NAG	O5-C5-C6-O6
4	L	202	NAG	O5-C5-C6-O6
4	h	400	NAG	C4-C5-C6-O6
4	q	400	NAG	O5-C5-C6-O6
4	A	400	NAG	C3-C2-N2-C7
4	G	400	NAG	C3-C2-N2-C7
4	S	400	NAG	C3-C2-N2-C7
4	Y	400	NAG	C3-C2-N2-C7
4	k	400	NAG	C3-C2-N2-C7
4	w	400	NAG	C3-C2-N2-C7
4	3	400	NAG	C3-C2-N2-C7
4	6	400	NAG	C3-C2-N2-C7
4	9	400	NAG	C3-C2-N2-C7
4	LE	400	NAG	C3-C2-N2-C7
4	LH	400	NAG	C3-C2-N2-C7
4	q	400	NAG	C4-C5-C6-O6
4	Y	400	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

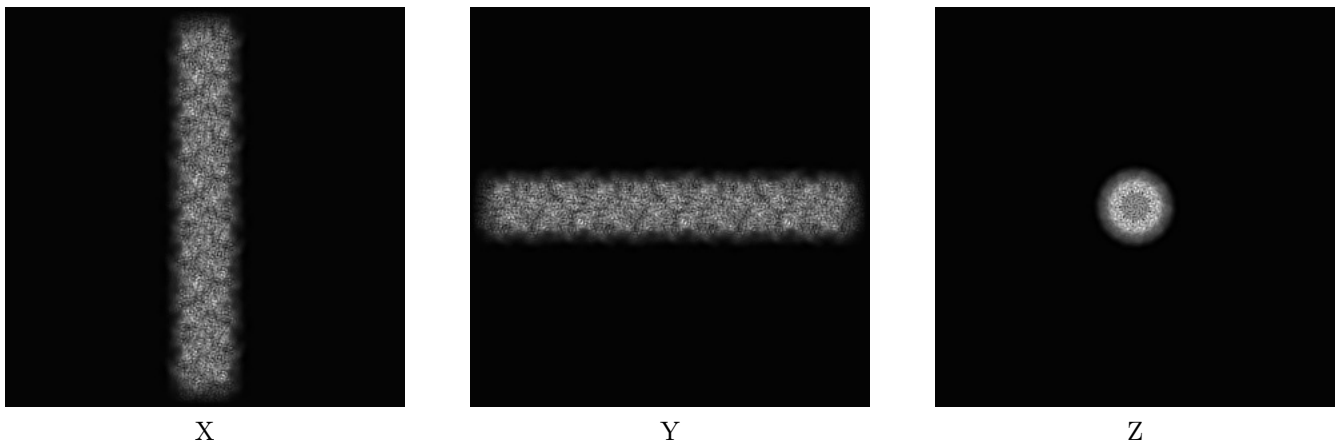
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18119. These allow visual inspection of the internal detail of the map and identification of artifacts.

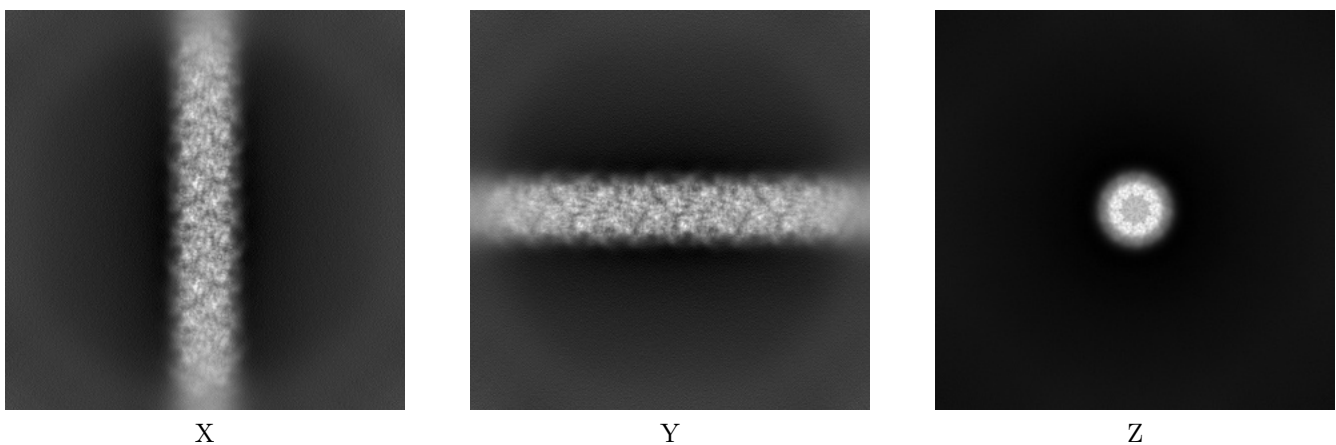
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

#### 6.1.1 Primary map



#### 6.1.2 Raw map

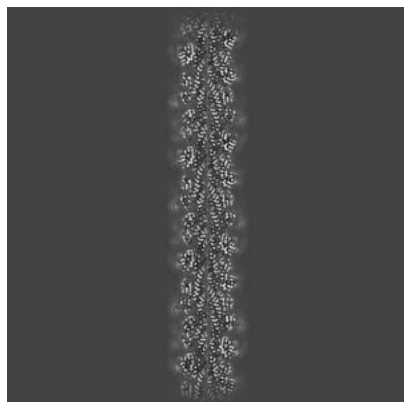


The images above show the map projected in three orthogonal directions.

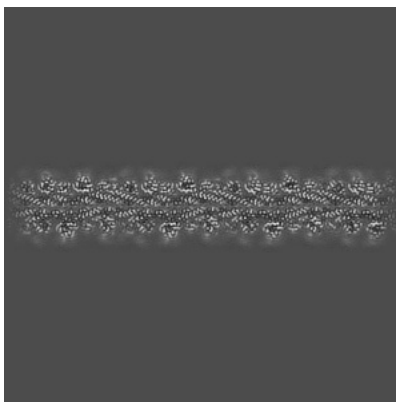


## 6.2 Central slices [i](#)

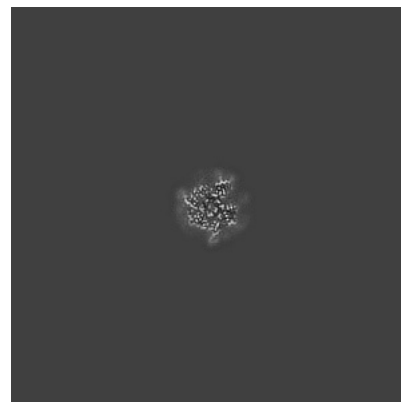
### 6.2.1 Primary map



X Index: 256

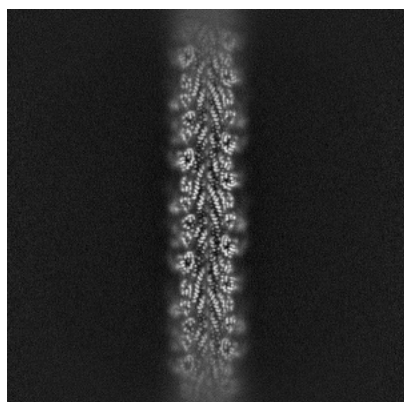


Y Index: 256

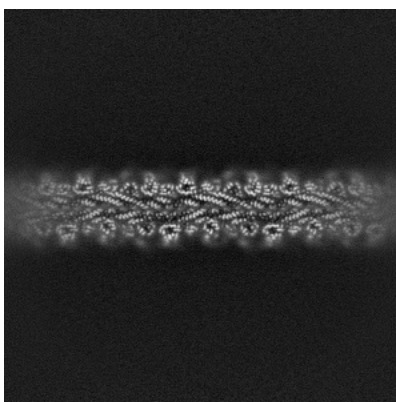


Z Index: 256

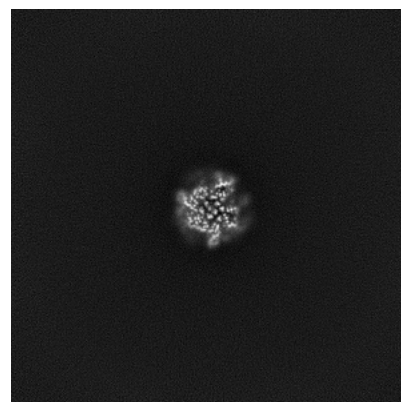
### 6.2.2 Raw map



X Index: 256



Y Index: 256

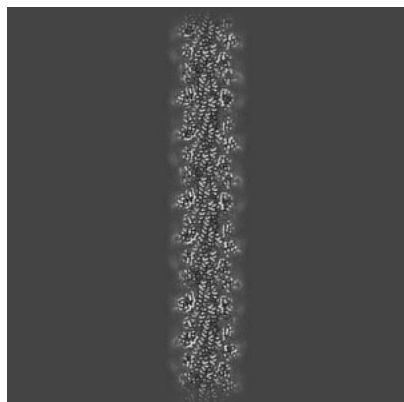


Z Index: 256

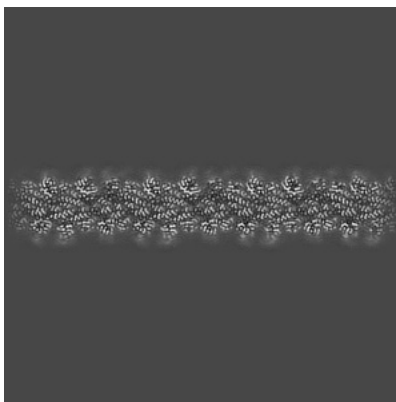
The images above show central slices of the map in three orthogonal directions.

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

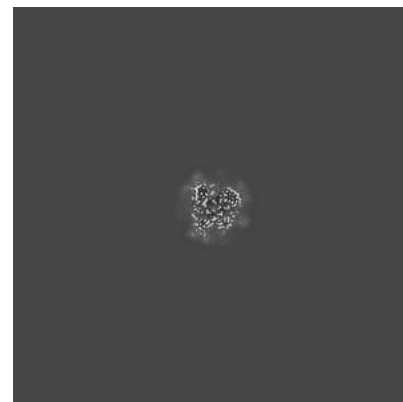
### 6.3.1 Primary map



X Index: 263

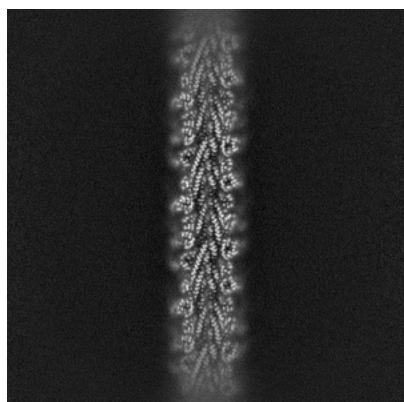


Y Index: 260

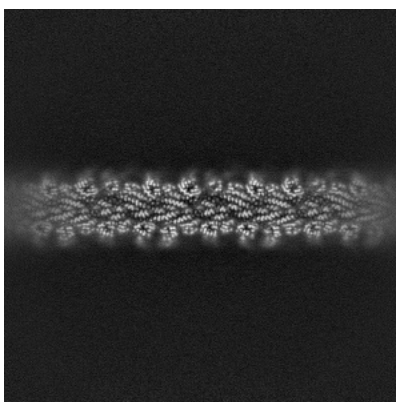


Z Index: 275

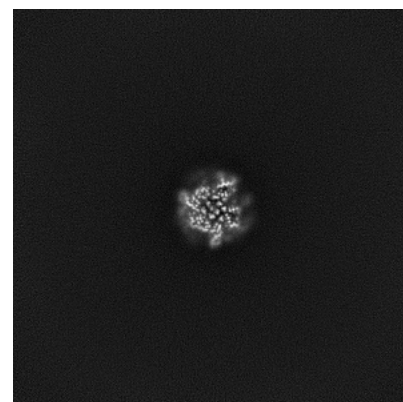
### 6.3.2 Raw map



X Index: 259



Y Index: 260

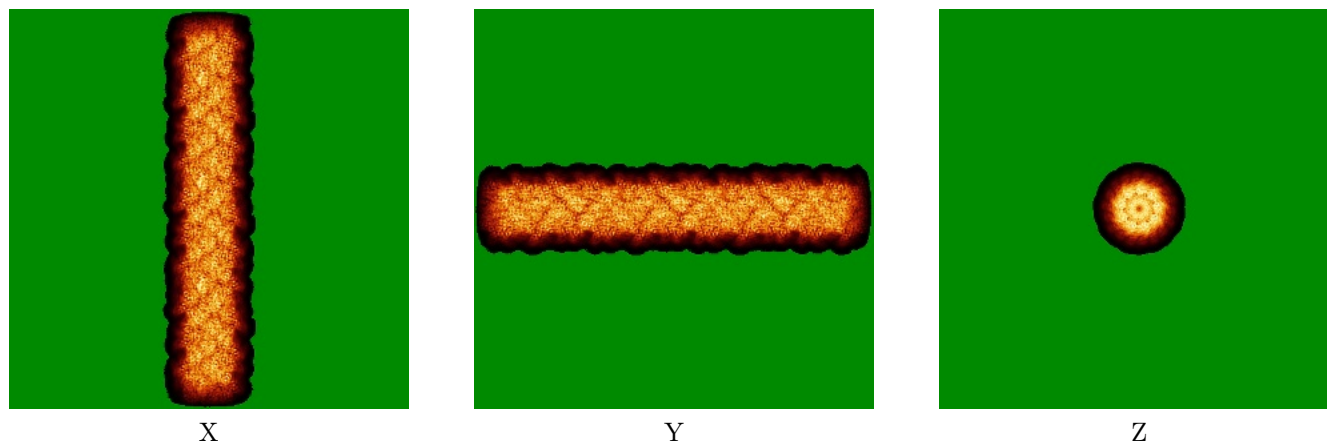


Z Index: 256

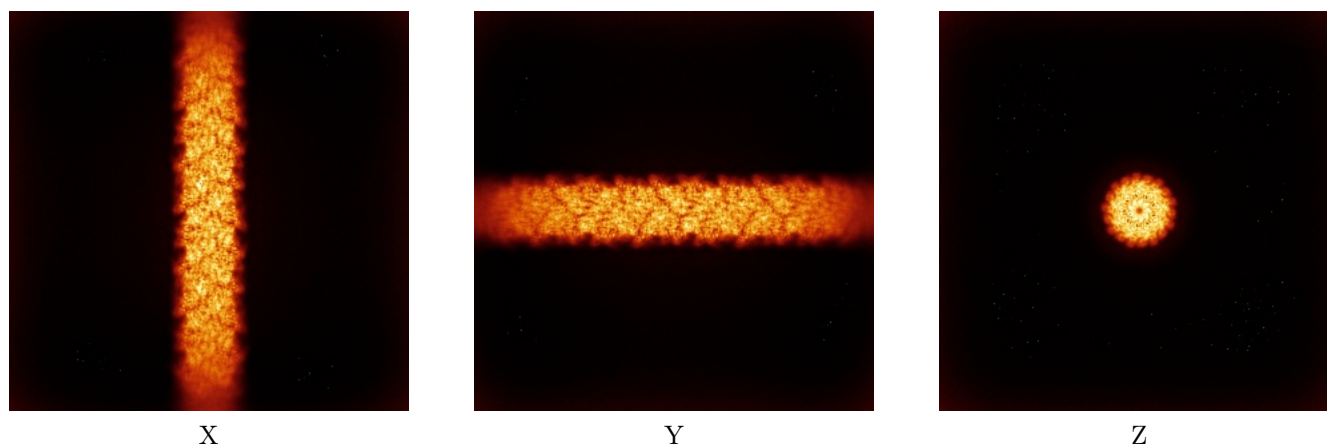
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



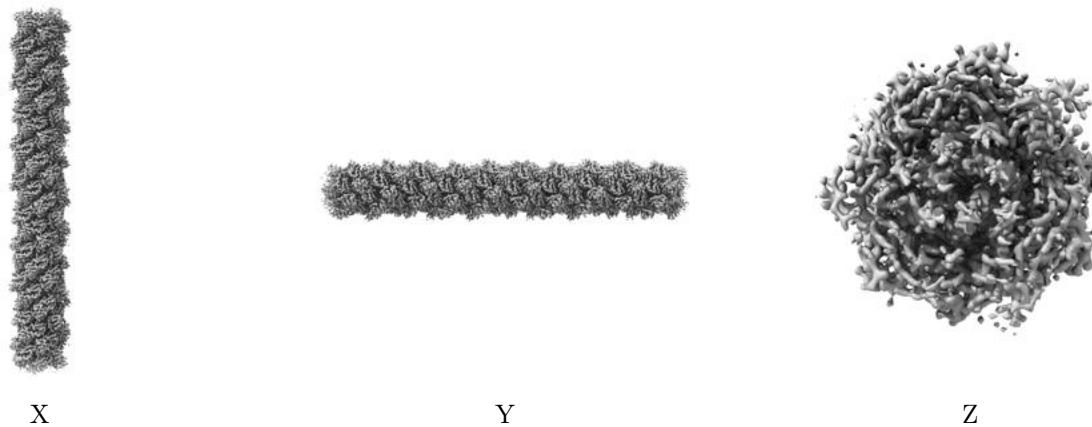
### 6.4.2 Raw map



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.

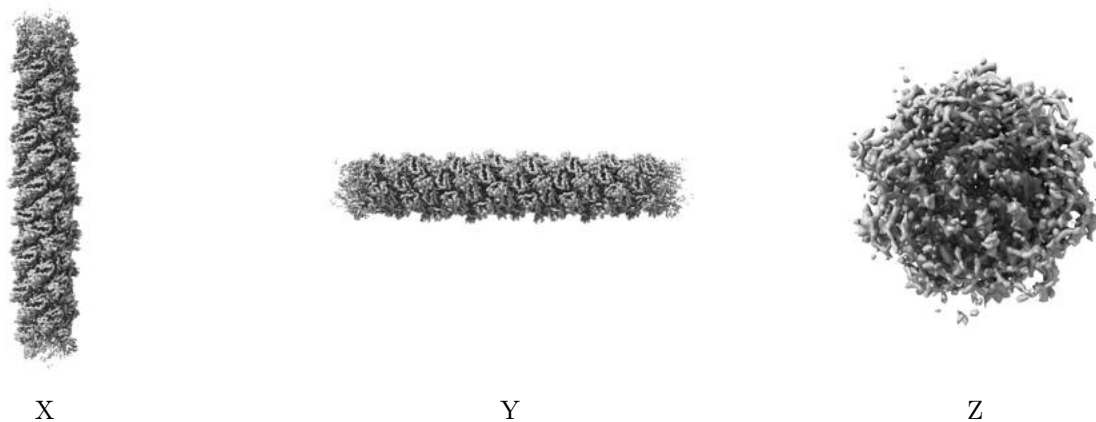
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.59. 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.

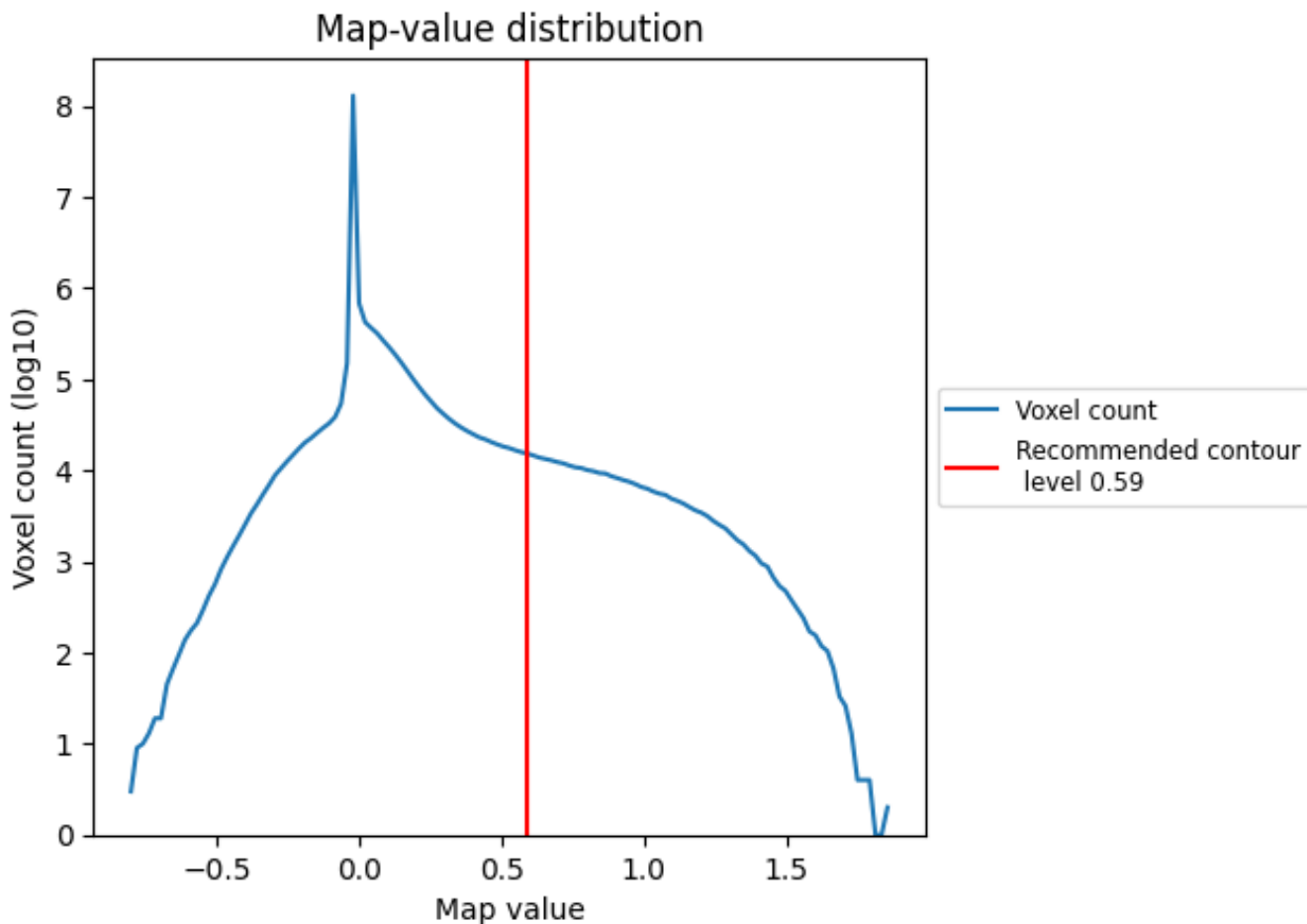
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

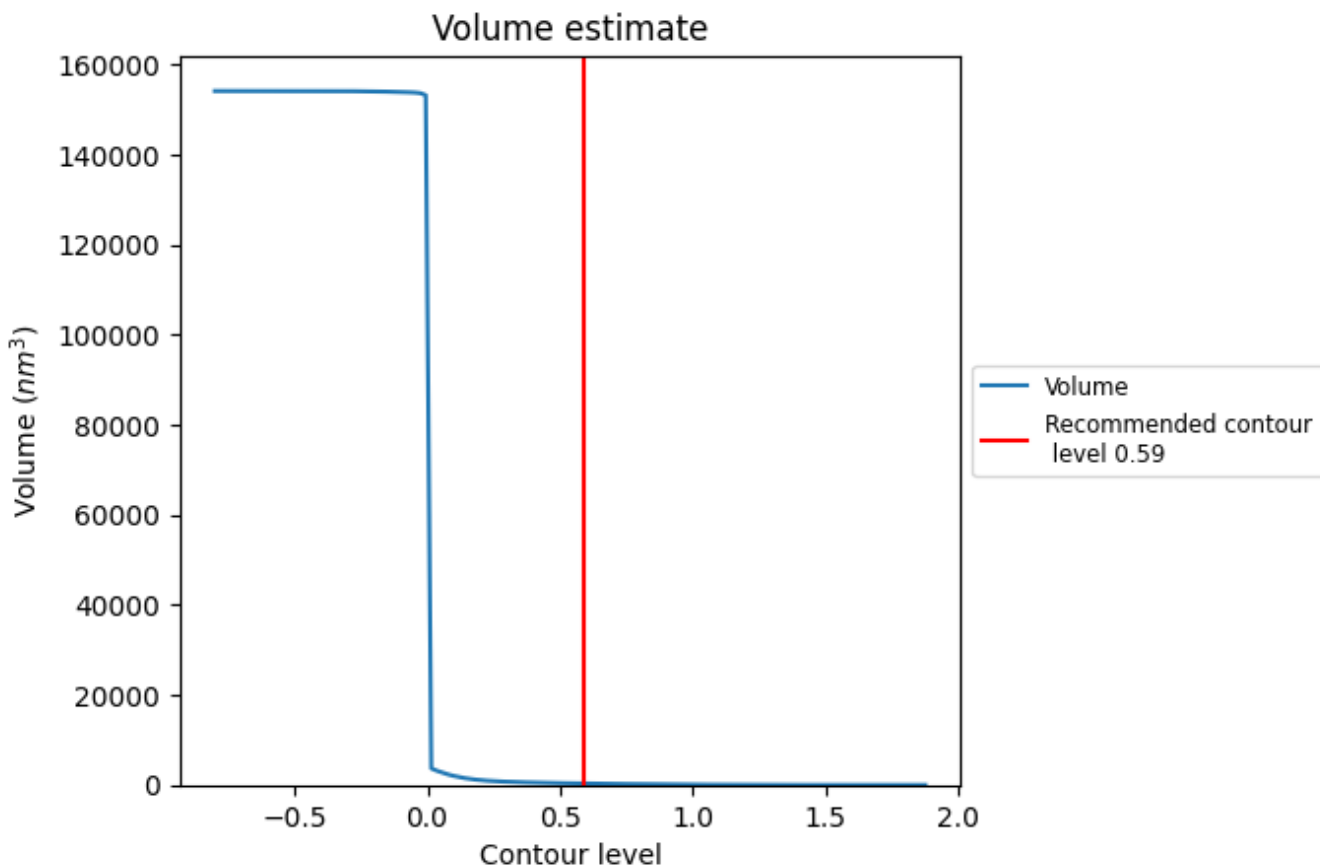
This section contains the results of statistical analysis of the map.

### 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.

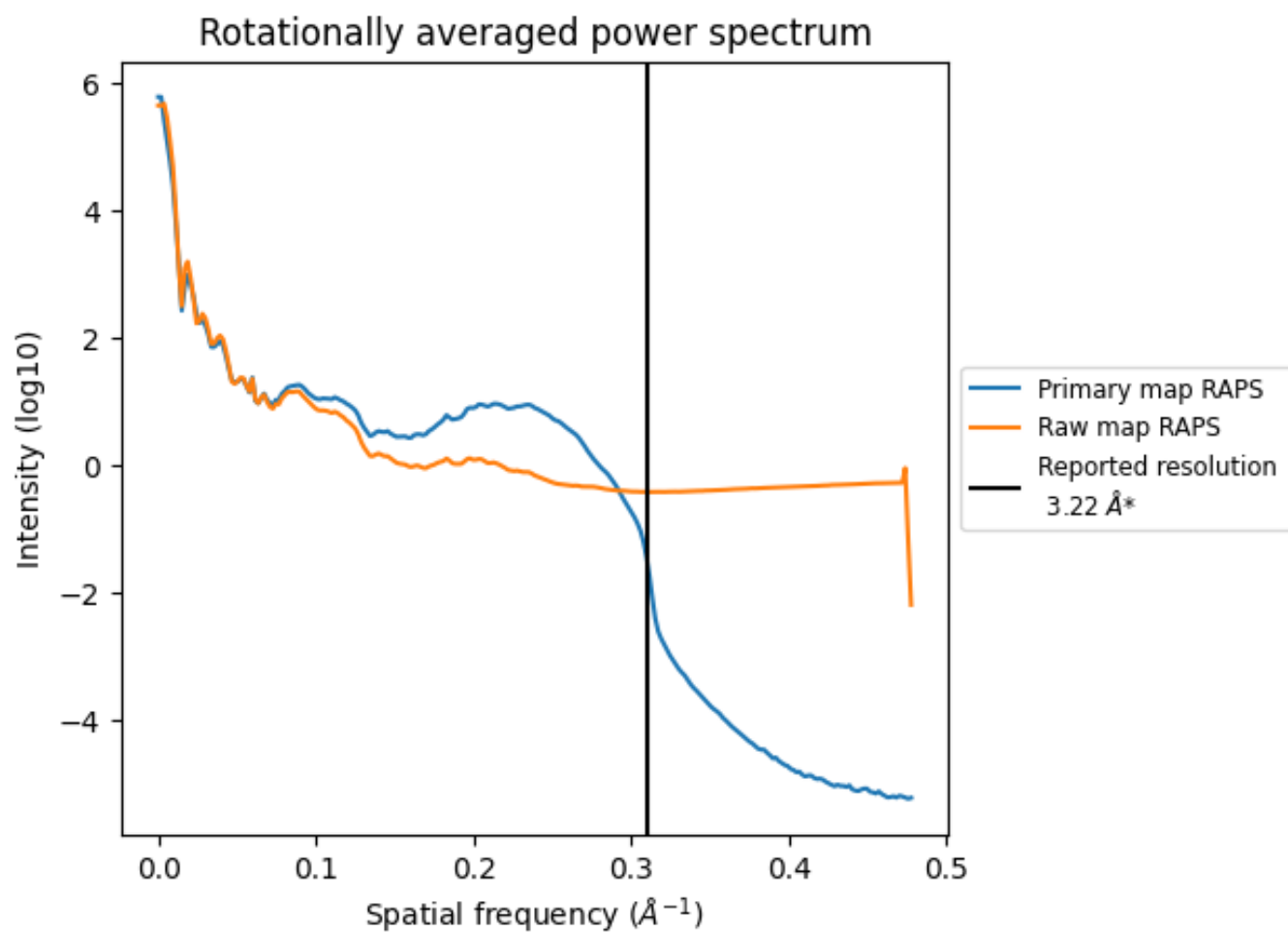
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 325 nm<sup>3</sup>; this corresponds to an approximate mass of 294 kDa.

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

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

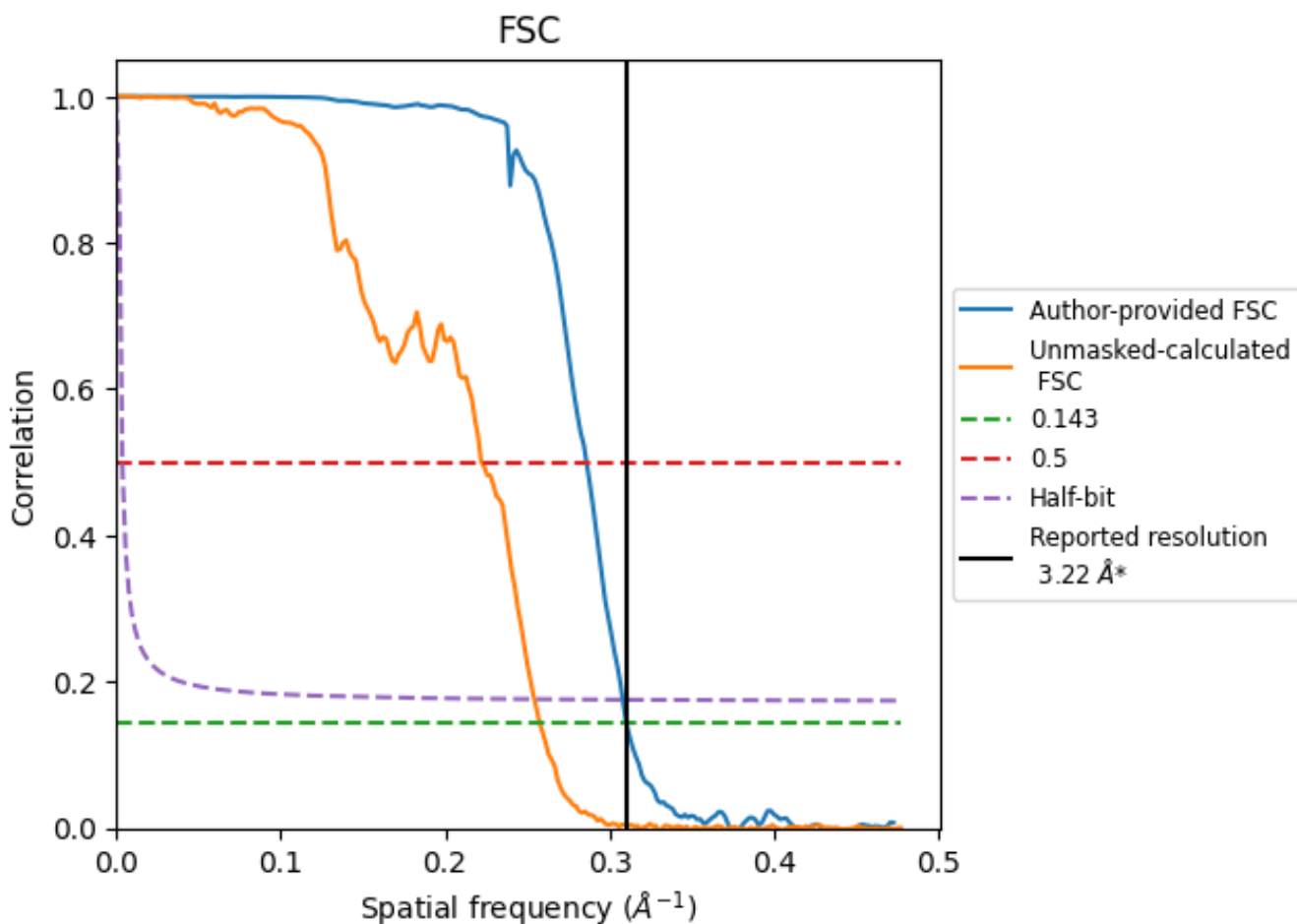


\*Reported resolution corresponds to spatial frequency of 0.311 Å<sup>-1</sup>

## 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  $0.311 \text{\AA}^{-1}$



## 8.2 Resolution estimates [i](#)

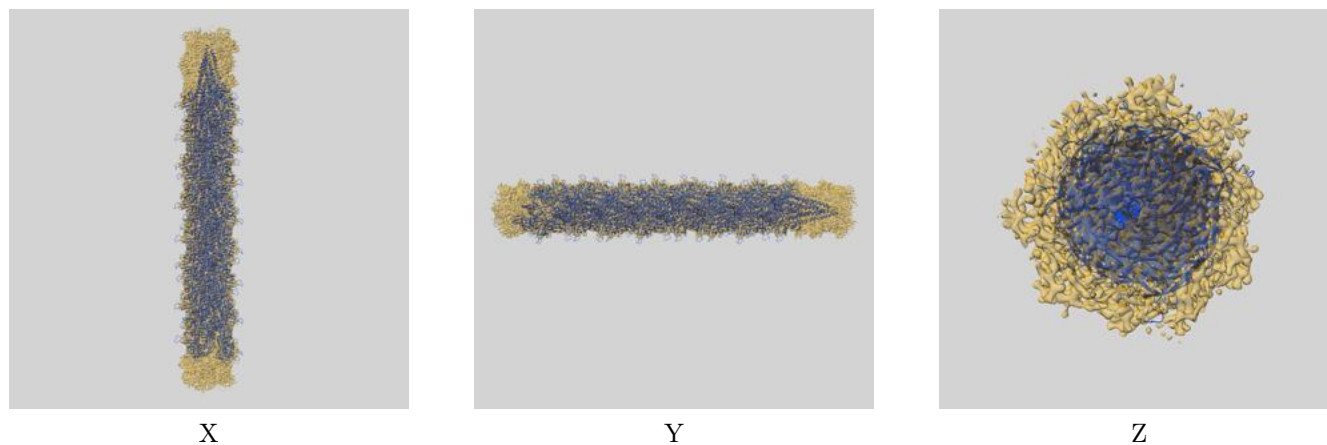
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.22	-	-
Author-provided FSC curve	3.22	3.49	3.24
Unmasked-calculated*	3.88	4.50	3.93

\*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 3.88 differs from the reported value 3.22 by more than 10 %

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

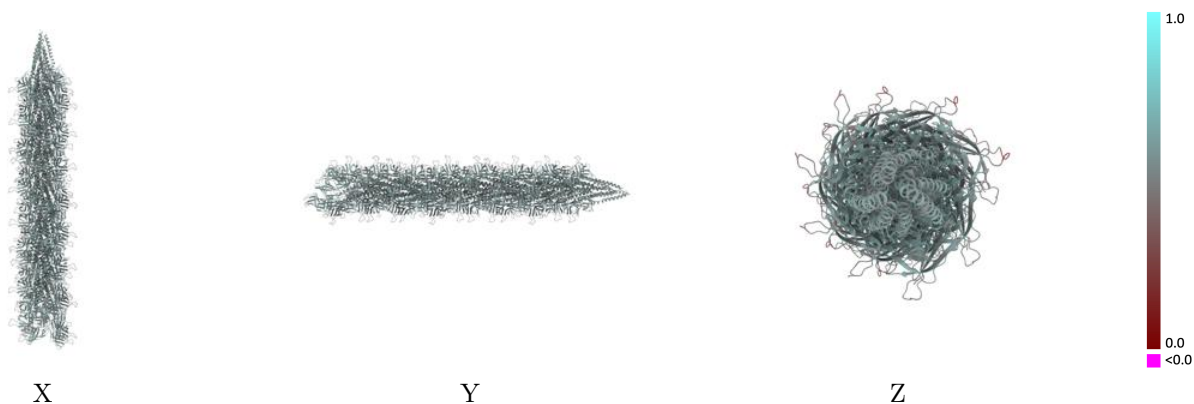
This section contains information regarding the fit between EMDB map EMD-18119 and PDB model 8Q30. Per-residue inclusion information can be found in section 3 on page 27.

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



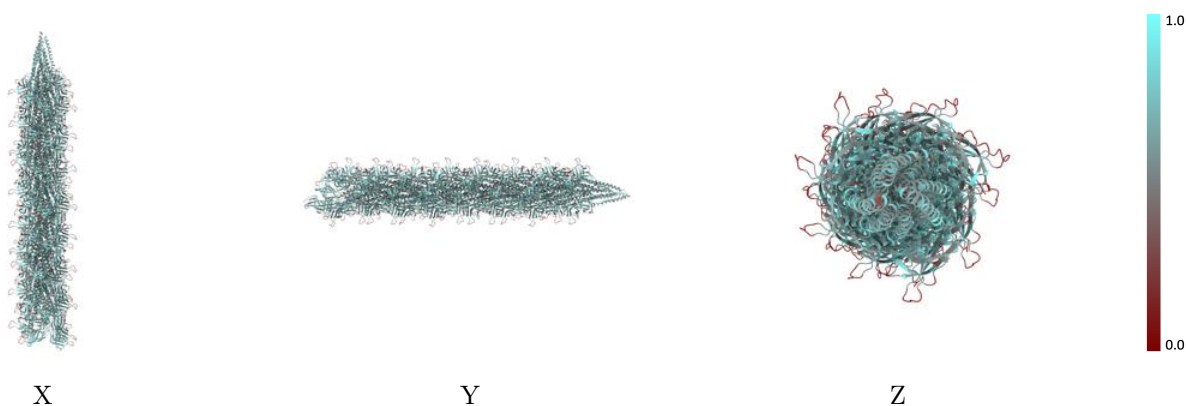
The images above show the 3D surface view of the map at the recommended contour level 0.59 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



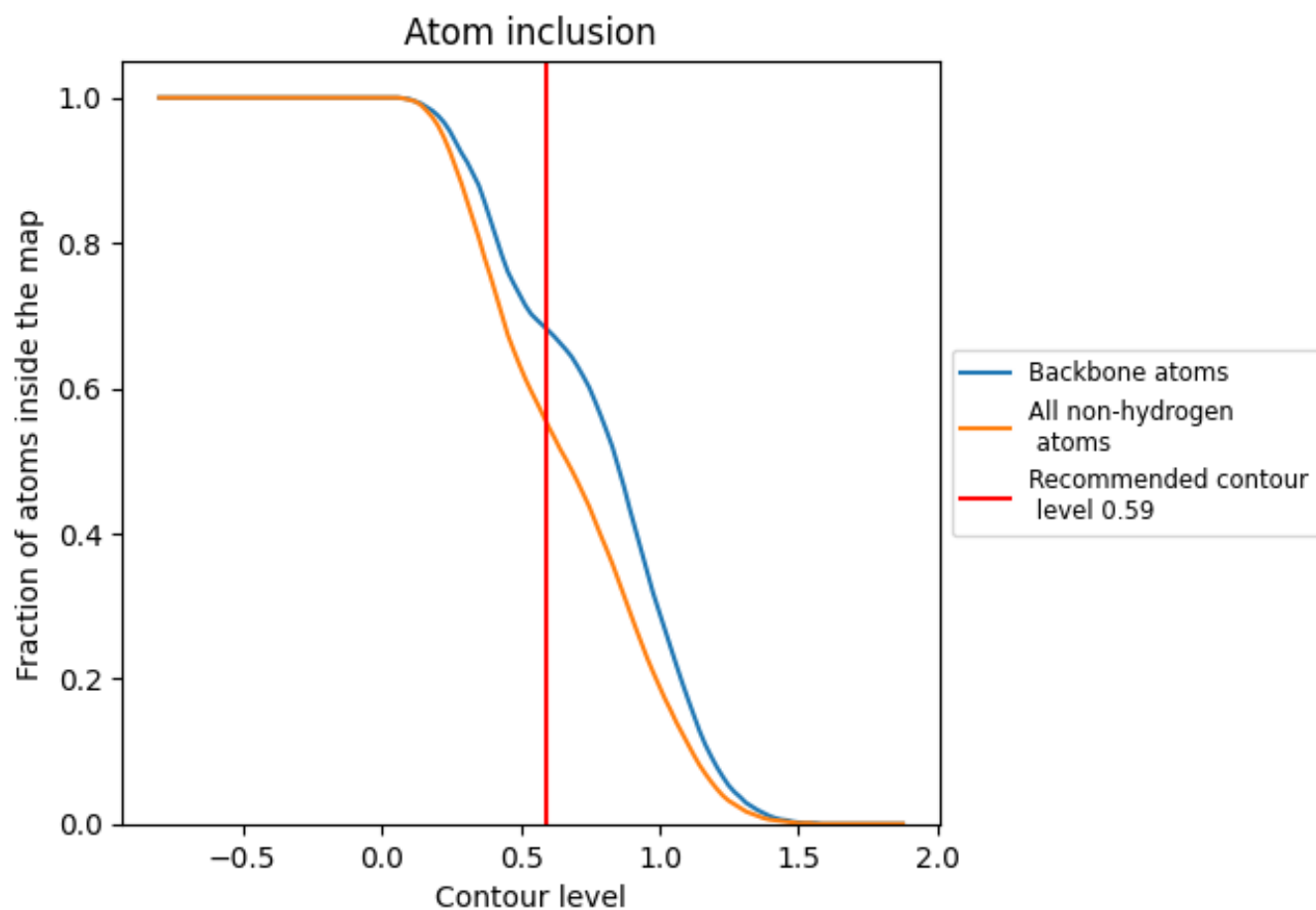
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.59).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 68% of all backbone atoms, 56% 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 (0.59) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5550	 0.5300
0	 0.5690	 0.5290
0A	 0.0000	 0.3380
0B	 0.1670	 0.4650
1	 0.5630	 0.5300
1A	 0.1430	 0.4580
1B	 0.0710	 0.2540
2	 0.5980	 0.5450
2A	 0.1070	 0.2630
2B	 0.0710	 0.4590
3	 0.5950	 0.5410
3A	 0.0710	 0.4520
3B	 0.0710	 0.4320
4	 0.5710	 0.5250
4A	 0.0710	 0.4190
4B	 0.0000	 0.4110
5	 0.5980	 0.5450
5A	 0.0000	 0.4100
5B	 0.0360	 0.3490
6	 0.5950	 0.5410
6A	 0.0360	 0.3550
6B	 0.1430	 0.4560
7	 0.5650	 0.5270
7A	 0.1670	 0.4620
7B	 0.1790	 0.2840
8	 0.6010	 0.5480
8A	 0.0710	 0.2370
8B	 0.1070	 0.4700
9	 0.5860	 0.5420
9A	 0.1070	 0.4700
9B	 0.0710	 0.4310
A	 0.5860	 0.5400
AA	 0.1070	 0.4710
AB	 0.0710	 0.4410
AC	 0.0000	 0.4120























































































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Chain	Atom inclusion	Q-score
B	 0.5620	 0.5280
BA	 0.0710	 0.4290
BB	 0.0240	 0.4090
BC	 0.0360	 0.3470
C	 0.5940	 0.5430
CA	 0.0240	 0.4060
CB	 0.0360	 0.3450
CC	 0.1670	 0.4660
D	 0.5940	 0.5420
DA	 0.0360	 0.3580
DB	 0.1430	 0.4680
DC	 0.1430	 0.2450
E	 0.5650	 0.5280
EA	 0.1670	 0.4720
EB	 0.1790	 0.2790
EC	 0.1070	 0.4760
F	 0.6030	 0.5460
FA	 0.1070	 0.2710
FB	 0.1070	 0.4780
FC	 0.1070	 0.4400
G	 0.5910	 0.5410
GA	 0.1070	 0.4630
GB	 0.0710	 0.4300
GC	 0.0240	 0.4090
H	 0.5670	 0.5260
HA	 0.0710	 0.4430
HB	 0.0000	 0.4060
HC	 0.0000	 0.3510
I	 0.5990	 0.5470
IA	 0.0000	 0.4060
IB	 0.0360	 0.3620
IC	 0.1430	 0.4700
J	 0.5900	 0.5390
JA	 0.0000	 0.3470
JB	 0.1190	 0.4700
JC	 0.1430	 0.2810
K	 0.5630	 0.5270
KA	 0.1670	 0.4600
KB	 0.1430	 0.2510
KC	 0.0710	 0.4550
L	 0.5980	 0.5440
LA	 0.5980	 0.5470

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Chain	Atom inclusion	Q-score
LB	 0.5950	 0.5440
LC	 0.5650	 0.5290
LD	 0.5980	 0.5450
LE	 0.5940	 0.5430
LF	 0.5680	 0.5270
LG	 0.5980	 0.5470
LH	 0.5900	 0.5380
LI	 0.5650	 0.5280
LJ	 0.5980	 0.5450
M	 0.5970	 0.5410
MA	 0.1790	 0.2910
MB	 0.0710	 0.4660
MC	 0.0710	 0.4310
N	 0.5710	 0.5290
NA	 0.0710	 0.4690
NB	 0.0710	 0.4300
NC	 0.0000	 0.4010
O	 0.5960	 0.5440
OA	 0.0710	 0.4320
OB	 0.0000	 0.3950
OC	 0.0360	 0.3130
P	 0.6010	 0.5390
PA	 0.0000	 0.4070
PB	 0.0360	 0.3560
PC	 0.1430	 0.4550
Q	 0.5630	 0.5250
QA	 0.0360	 0.3600
QB	 0.1670	 0.4670
QC	 0.0710	 0.2210
R	 0.6010	 0.5430
RA	 0.1430	 0.4650
RB	 0.1790	 0.2860
RC	 0.0710	 0.4500
S	 0.5930	 0.5370
SA	 0.1430	 0.2610
SB	 0.1070	 0.4530
SC	 0.1070	 0.4150
T	 0.5670	 0.5270
TA	 0.1070	 0.4670
TB	 0.0710	 0.4270
TC	 0.0000	 0.4030
U	 0.6010	 0.5450

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























































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Chain	Atom inclusion	Q-score
UA	0.0710	0.4310
UB	0.0000	0.4030
UC	0.0360	0.3370
V	0.5910	0.5380
VA	0.0240	0.4040
VB	0.0360	0.3350
VC	0.1430	0.4610
W	0.5640	0.5280
WA	0.0000	0.3290
WB	0.1430	0.4600
WC	0.0710	0.2420
X	0.5940	0.5460
XA	0.1430	0.4690
XB	0.1430	0.2440
Y	0.5960	0.5410
YA	0.2140	0.3100
YB	0.1070	0.4670
Z	0.5690	0.5260
ZA	0.1070	0.4600
ZB	0.0710	0.4230
a	0.5970	0.5430
aA	0.0710	0.4360
aB	0.0240	0.3950
b	0.5910	0.5410
bA	0.0240	0.3960
bB	0.0360	0.3350
c	0.5680	0.5280
cA	0.0000	0.3430
cB	0.1430	0.4710
d	0.6020	0.5450
dA	0.0950	0.4700
dB	0.1790	0.2580
e	0.5940	0.5420
eA	0.1430	0.2630
eB	0.1070	0.4580
f	0.5650	0.5300
fA	0.1070	0.4590
fB	0.0710	0.4190
g	0.6030	0.5460
gA	0.0710	0.4110
gB	0.0000	0.4100
h	0.5980	0.5400

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Chain	Atom inclusion	Q-score
hA	 0.0000	 0.3940
hB	 0.0360	 0.3360
i	 0.5680	 0.5270
iA	 0.0360	 0.3510
iB	 0.1670	 0.4670
j	 0.6020	 0.5470
jA	 0.1190	 0.4600
jB	 0.0710	 0.2410
k	 0.5960	 0.5410
kA	 0.1790	 0.2630
kB	 0.0710	 0.4590
l	 0.5670	 0.5270
lA	 0.1070	 0.4550
lB	 0.0710	 0.4240
m	 0.6050	 0.5460
mA	 0.0710	 0.4250
mB	 0.0000	 0.4040
n	 0.5920	 0.5380
nA	 0.0240	 0.4110
nB	 0.0360	 0.3550
o	 0.5700	 0.5290
oA	 0.0360	 0.3500
oB	 0.1670	 0.4620
p	 0.6010	 0.5460
pA	 0.1190	 0.4710
pB	 0.0710	 0.2630
q	 0.5910	 0.5360
qA	 0.1430	 0.2510
qB	 0.1070	 0.4670
r	 0.5680	 0.5300
rA	 0.1070	 0.4720
rB	 0.1070	 0.4320
s	 0.6010	 0.5440
sA	 0.0710	 0.4230
sB	 0.0240	 0.4090
t	 0.5900	 0.5410
tA	 0.0240	 0.3980
tB	 0.0000	 0.3280
u	 0.5680	 0.5270
uA	 0.0360	 0.3590
uB	 0.1910	 0.4550
v	 0.6080	 0.5460

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Chain	Atom inclusion	Q-score
vA	 0.1190	 0.4730
vB	 0.1070	 0.2570
w	 0.5920	 0.5420
wA	 0.1430	 0.2640
wB	 0.1070	 0.4660
x	 0.5700	 0.5280
xA	 0.1070	 0.4610
xB	 0.0710	 0.4260
y	 0.5970	 0.5500
yA	 0.0710	 0.4290
yB	 0.0000	 0.4090
z	 0.5890	 0.5430
zA	 0.0000	 0.4030
zB	 0.0360	 0.3550