



# wwPDB EM Validation Summary Report ⓘ

Apr 2, 2024 – 03:27 PM JST

PDB ID : 8WA2  
EMDB ID : EMD-37389  
Title : cryo-EM structure of native mastigonemes isolated from *Chlamydomonas reinhardtii* at 3.0 angstrom resolution  
Authors : Huang, J.; Tao, H.; Chen, J.; Pan, J.; Yan, C.; Yan, N.  
Deposited on : 2023-09-06  
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

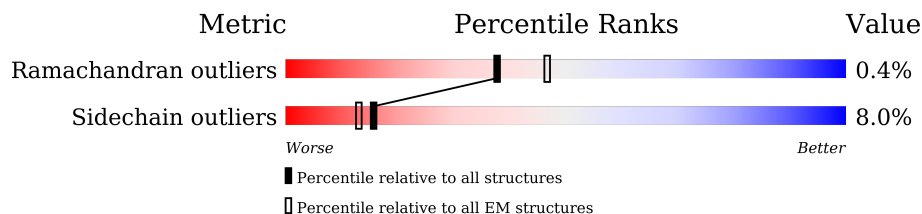
EMDB validation analysis : 0.0.1.dev70  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

# 1 Overall quality at a glance

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

The reported resolution of this entry is 3.00 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	1987	
1	B	1987	
1	C	1987	
1	D	1987	
1	E	1987	
1	F	1987	
2	G	64	
2	H	64	
2	I	64	

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Mol	Chain	Length	Quality of chain
3	0	3	67% 33%
3	0A	3	67% 33%
3	1	3	67% 33%
3	2	3	67% 33%
3	8C	3	100%
3	9C	3	33% 67%
3	BC	3	33% 67%
3	CC	3	33% 67%
3	DD	3	67% 33%
3	EB	3	100%
3	ED	3	67% 33%
3	FD	3	67% 33%
3	GC	3	67% 33%
3	HA	3	33% 67%
3	HC	3	67% 33%
3	IA	3	67% 33%
3	IC	3	67% 33%
3	ID	3	67% 33%
3	J	3	100%
3	K	3	100%
3	KD	3	67% 33%
3	LB	3	100%
3	LC	3	100%
3	MA	3	100%
3	NA	3	33% 67%




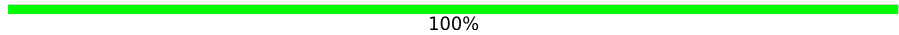
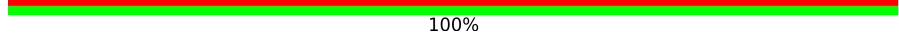

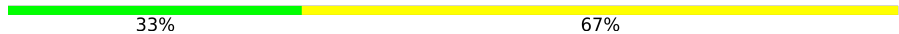
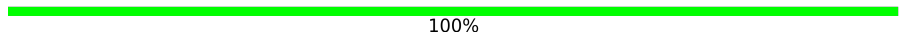
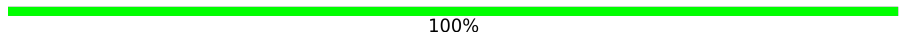
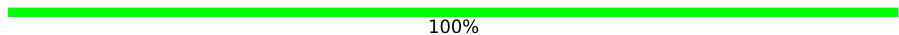

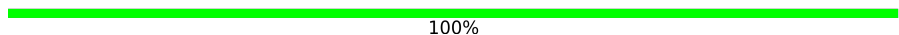

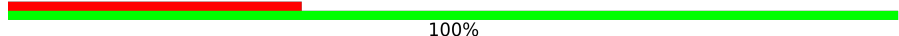

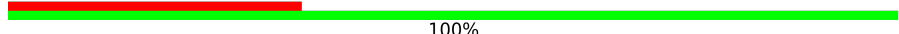



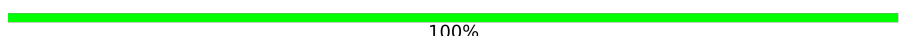

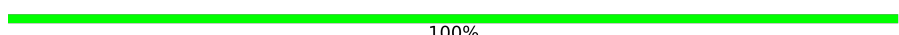



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Mol	Chain	Length	Quality of chain
3	NC	3	100%
3	O	3	67% 33%
3	OA	3	67% 33%
3	OB	3	100%
3	P	3	67% 33%
3	PB	3	33% 67% 33%
3	Q	3	67% 33%
3	QB	3	33% 67% 33%
3	QD	3	100%
3	RA	3	67% 33%
3	RB	3	67% 33% 67%
3	SB	3	100%
3	T	3	67% 33%
3	TA	3	33% 67%
3	TB	3	67% 33%
3	TC	3	100%
3	TD	3	100%
3	UB	3	67% 33%
3	V	3	67% 33%
3	WC	3	33% 67%
3	XA	3	33% 67% 33%
3	ZA	3	67% 33%
3	aD	3	33% 100%
3	b	3	67% 33%
3	bD	3	100%

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Mol	Chain	Length	Quality of chain
3	cA	3	 33% 67%
3	dC	3	 67% 33%
3	e	3	 67% 33%
3	eC	3	 100%
3	hB	3	 100%
3	iD	3	 67% 33%
3	jA	3	 33% 67%
3	kA	3	 100%
3	l	3	 100%
3	lC	3	 100%
3	lD	3	 67% 100%
3	m	3	 100%
3	mD	3	 33% 67% 33%
3	nD	3	 33% 100%
3	oB	3	 67% 33% 67%
3	oC	3	 33% 100%
3	oD	3	 33% 67% 33%
3	pC	3	 33% 67%
3	pD	3	 33% 67%
3	qC	3	 100%
3	qD	3	 67% 100%
3	rA	3	 100%
3	rB	3	 67% 33%
3	rC	3	 67% 33%
3	rD	3	 67% 33%

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Mol	Chain	Length	Quality of chain
3	sB	3	33% 100%
3	sC	3	100% 33% 67%
3	t	3	67% 33%
3	tB	3	33% 100%
3	tC	3	33% 67% 33%
3	uA	3	67% 33%
3	uB	3	67% 33%
3	uC	3	67% 67% 33%
3	vA	3	67% 33%
3	vB	3	33% 67% 33%
3	w	3	67% 33%
3	wA	3	67% 33%
3	wB	3	100%
3	x	3	33% 67%
3	xA	3	100%
3	xB	3	67% 33%
3	y	3	67% 33%
3	yA	3	67% 33%
3	z	3	67% 33%
3	zA	3	100%
4	AD	4	50% 50%
4	DC	4	50% 50%
4	JA	4	75% 25%
4	JB	4	50% 75% 25%
4	L	4	75% 25%

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Mol	Chain	Length	Quality of chain
4	LD	4	50% 50%
4	MD	4	100%
4	NB	4	50% 50%
4	OC	4	75% 25%
4	OD	4	50% 50%
4	PC	4	75% 25%
4	RC	4	75% 25%
4	RD	4	50% 50%
4	SD	4	50% 50%
4	UA	4	75% 25%
4	UC	4	100%
4	VA	4	75% 25%
4	VC	4	75% 25%
4	VD	4	50% 50%
4	W	4	75% 25%
4	X	4	75% 25%
4	YC	4	50% 50%
4	Z	4	25% 75%
4	ZD	4	25% 75% 25%
4	aA	4	100%
4	bA	4	100%
4	c	4	75% 25%
4	cC	4	50% 50%
4	d	4	25% 75%
4	eA	4	100%

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Mol	Chain	Length	Quality of chain
4	g	4	75% 25%
4	gD	4	25% 50% 50%
4	iA	4	50% 50%
4	jC	4	75% 25%
4	k	4	100%
4	kD	4	25% 100%
4	mB	4	75% 50% 50%
4	nC	4	25% 50% 50%
4	pA	4	100%
4	qB	4	25% 75%
4	r	4	100%
4	tA	4	50% 50%
4	v	4	75% 25%
5	BD	5	60% 40%
5	EC	5	40% 60%
5	KA	5	40% 60%
5	M	5	20% 80%
6	0B	3	33% 33% 33%
6	0C	3	33% 100% 67%
6	1C	3	67% 100% 33%
6	2C	3	33% 100% 67%
6	3A	3	67% 33%
6	3B	3	100%
6	3D	3	100%
6	4B	3	33% 67%

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Mol	Chain	Length	Quality of chain
6	5	3	67% 33%
6	5B	3	33% 67%
6	6A	3	33% 67%
6	6C	3	100% 100%
6	6D	3	100%
6	7A	3	33% 67%
6	7D	3	33% 67%
6	8	3	33% 67%
6	8A	3	100%
6	8D	3	100%
6	9	3	33% 67%
6	9B	3	33% 67%
6	AA	3	33% 67%
6	CB	3	33% 67%
6	CD	3	33% 33% 33%
6	EA	3	33% 67%
6	FC	3	100%
6	GD	3	33% 67%
6	JC	3	33% 67%
6	LA	3	33% 33% 33%
6	ME	3	67% 33%
6	N	3	33% 33% 33%
6	OE	3	67% 33%
6	PA	3	67% 33%
6	R	3	33% 67%

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Mol	Chain	Length	Quality of chain
6	XB	3	33% 33% 33%
6	ZE	3	33% 67%
6	aB	3	33% 67%
6	bB	3	100%
6	bE	3	67% 33%
6	cB	3	100%
6	gB	3	67% 33%
6	mE	3	33% 67%
6	nE	3	33% 67%
6	oE	3	33% 67%
6	uD	3	100% 33% 33% 33%
6	xC	3	100% 67% 33%
6	xD	3	100% 33% 67%
6	yD	3	100%
6	zD	3	100% 33% 67%
7	HD	4	50% 50%
7	KC	4	50% 50%
7	QA	4	50% 50%
7	S	4	25% 75%
7	UD	4	75% 25%
7	WD	4	75% 25%
7	XC	4	75% 25%
7	ZC	4	75% 25%
7	dA	4	50% 50%
7	f	4	25% 75%

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Mol	Chain	Length	Quality of chain
7	fA	4	100%
7	h	4	75% 25%
8	JD	5	80% 20%
8	MC	5	40% 60%
8	SA	5	80% 20%
8	U	5	40% 60%
9	ND	2	50% 50%
9	QC	2	100%
9	WA	2	100%
9	Y	2	100%
9	YD	2	100%
9	bC	2	100%
9	hA	2	50% 50%
9	j	2	50% 50%
10	1A	5	20% 80%
10	3	5	40% 60%
10	MB	5	80% 40% 60%
10	PD	5	60% 40%
10	SC	5	80% 20%
10	VB	5	20% 60% 40%
10	YA	5	80% 20%
10	a	5	20% 80%
10	jD	5	20% 60% 40%
10	mC	5	40% 40% 60%
10	pB	5	100% 60% 40%

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Mol	Chain	Length	Quality of chain
10	sA	5	
10	sD	5	
10	u	5	
10	vC	5	
10	yB	5	
11	XD	3	
11	aC	3	
11	gA	3	
11	i	3	
12	FB	5	
12	IB	5	
12	cD	5	
12	fC	5	
12	fD	5	
12	iB	5	
12	iC	5	
12	lA	5	
12	lB	5	
12	n	5	
12	oA	5	
12	q	5	
13	0D	4	
13	1B	4	
13	2A	4	
13	2B	4	

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Mol	Chain	Length	Quality of chain
13	3C	4	
13	4	4	
13	4A	4	
13	5A	4	
13	6	4	
13	6B	4	
13	7	4	
13	9A	4	
13	BA	4	
13	GB	4	
13	WB	4	
13	YB	4	
13	ZB	4	
13	dB	4	
13	dD	4	
13	gC	4	
13	jB	4	
13	mA	4	
13	o	4	
13	tD	4	
13	vD	4	
13	wC	4	
13	wD	4	
13	yC	4	
13	zB	4	

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Mol	Chain	Length	Quality of chain
13	zC	4	100% 25% 75%
14	HB	4	100% 50% 25% 25%
14	KB	4	100% 50% 25% 25%
14	eD	4	50% 25% 25%
14	hC	4	50% 25% 25%
14	hD	4	25% 50% 25%
14	kB	4	100% 25% 50% 25%
14	kC	4	50% 25% 25%
14	nA	4	75% 25%
14	nB	4	75% 25% 50% 25%
14	p	4	50% 25% 25%
14	qA	4	75% 25%
14	s	4	75% 25%
15	1D	5	100% 40% 60%
15	2D	5	100% 40% 60%
15	4C	5	100% 40% 60%
15	5C	5	100% 20% 80%
15	7B	5	60% 40%
15	8B	5	40% 60%
15	AB	5	20% 80%
15	BB	5	40% 60%
15	CA	5	40% 60%
15	DA	5	20% 80%
15	eB	5	40% 60%
15	fB	5	40% 60%

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Mol	Chain	Length	Quality of chain
16	4D	2	50% 
16	AC	2	100% 
16	FA	2	50% 
17	5D	6	50% 
17	7C	6	50% 
17	DB	6	17% 
17	GA	6	50% 
18	0E	5	60% 
18	9D	5	20% 
18	BE	5	20% 
18	DE	5	20% 
18	IE	5	20% 
18	JE	5	40% 
18	KE	5	60% 
18	PE	5	60% 
18	SE	5	60% 
18	cE	5	60% 
18	fE	5	40% 
18	pE	5	100% 
18	rE	5	20% 
18	tE	5	40% 
18	yE	5	20% 
18	zE	5	20% 
19	1E	4	50% 
19	AE	4	50% 

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Mol	Chain	Length	Quality of chain
19	LE	4	
19	NE	4	
19	aE	4	
19	qE	4	
20	CE	4	
20	EE	4	
20	HE	4	
20	TE	4	
20	UE	4	
20	WE	4	
20	gE	4	
20	hE	4	
20	jE	4	
20	sE	4	
20	uE	4	
20	xE	4	
21	FE	5	
21	kE	5	
21	vE	5	
22	GE	6	
22	QE	6	
22	RE	6	
22	VE	6	
22	dE	6	
22	eE	6	

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Mol	Chain	Length	Quality of chain
22	iE	6	
22	wE	6	
23	XE	6	
24	YE	6	
24	lE	6	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	AHR	1A	4	X	-	-	-
10	AHR	3	4	X	-	-	-
10	AHR	VB	4	X	-	-	-
10	AHR	sD	4	X	-	-	-
10	AHR	vC	4	X	-	-	-
10	AHR	yB	4	X	-	-	-
12	GZL	FB	3	X	-	-	-
12	GZL	IB	3	X	-	-	-
12	GZL	cD	3	X	-	-	-
12	GZL	fC	3	X	-	-	-
12	GZL	fD	3	X	-	-	-
12	GZL	iB	3	X	-	-	-
12	GZL	iC	3	X	-	-	-
12	GZL	lA	3	X	-	-	-
12	GZL	lB	3	X	-	-	-
12	GZL	n	3	X	-	-	-
12	GZL	oA	3	X	-	-	-
12	GZL	q	3	X	-	-	-
12	AHR	q	5	X	-	-	-
13	FUB	0D	2	X	-	-	-
13	GZL	1B	3	X	-	-	-
13	GZL	2A	3	X	-	-	-
13	GZL	2B	3	X	-	-	-
13	FUB	3C	2	X	-	-	-
13	GZL	4	3	X	X	-	-
13	GZL	4A	3	X	-	-	-
13	GZL	5A	3	X	-	-	-
13	GZL	6	3	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	FUB	6B	2	X	-	-	-
13	GZL	7	3	X	-	-	-
13	FUB	9A	2	X	-	-	-
13	FUB	BA	2	X	-	-	-
13	GZL	GB	3	X	-	-	-
13	GZL	WB	3	X	-	-	-
13	GZL	YB	3	X	-	-	-
13	GZL	ZB	3	X	-	-	-
13	FUB	dB	2	X	-	-	-
13	GZL	dD	3	X	-	-	-
13	GZL	gC	3	X	-	-	-
13	GZL	jB	3	X	-	-	-
13	GZL	mA	3	X	-	-	-
13	GZL	o	3	X	-	-	-
13	GZL	tD	3	X	-	-	-
13	GZL	vD	3	X	-	-	-
13	GZL	wC	3	X	-	-	-
13	GZL	wD	3	X	-	-	-
13	GZL	yC	3	X	-	-	-
13	GZL	zB	3	X	-	-	-
13	GZL	zC	3	X	-	-	-
14	GZL	HB	3	X	-	-	-
14	GZL	KB	3	X	-	-	-
14	GZL	eD	3	X	-	-	-
14	GZL	hC	3	X	-	-	-
14	GZL	hD	3	X	-	-	-
14	GZL	kB	3	X	-	-	-
14	GZL	kC	3	X	-	-	-
14	GZL	nA	3	X	-	-	-
14	GZL	nB	3	X	-	-	-
14	GZL	p	3	X	-	-	-
14	GZL	qA	3	X	-	-	-
14	GZL	s	3	X	-	-	-
15	GZL	1D	3	X	-	-	-
15	AHR	1D	5	X	-	-	-
15	GZL	2D	3	X	-	-	-
15	GZL	4C	3	X	-	-	-
15	AHR	4C	5	X	-	-	-
15	GZL	5C	3	X	-	-	-
15	GZL	7B	3	X	-	-	-
15	AHR	7B	5	X	-	-	-
15	GZL	8B	3	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	GZL	AB	3	X	-	-	-
15	AHR	AB	5	X	-	-	-
15	GZL	BB	3	X	-	-	-
15	GZL	CA	3	X	-	-	-
15	AHR	CA	5	X	-	-	-
15	GZL	DA	3	X	-	-	-
15	GZL	eB	3	X	-	-	-
15	AHR	eB	5	X	-	-	-
15	GZL	fB	3	X	-	-	-
17	MAN	5D	4	X	-	-	-
17	MAN	5D	6	X	-	-	-
17	MAN	7C	4	X	-	-	-
17	MAN	7C	6	X	-	-	-
17	MAN	DB	4	X	-	-	-
17	MAN	DB	6	X	-	-	-
17	MAN	GA	4	X	-	-	-
17	MAN	GA	6	X	-	-	-
18	GZL	0E	3	X	-	-	-
18	AHR	0E	4	X	-	-	-
18	AHR	0E	5	X	-	-	-
18	GZL	9D	3	X	-	-	-
18	AHR	9D	4	X	-	-	-
18	GZL	BE	3	X	-	-	-
18	AHR	BE	4	X	-	-	-
18	AHR	BE	5	X	-	-	-
18	GZL	DE	3	X	-	-	-
18	AHR	DE	5	X	-	-	-
18	GZL	IE	3	X	-	-	-
18	AHR	IE	4	X	-	-	-
18	GZL	JE	3	X	-	-	-
18	AHR	JE	5	X	-	-	-
18	GZL	KE	3	X	-	-	-
18	AHR	KE	4	X	-	-	-
18	AHR	KE	5	X	-	-	-
18	GZL	PE	3	X	-	-	-
18	AHR	PE	4	X	-	-	-
18	AHR	PE	5	X	-	-	-
18	FUB	SE	1	X	-	-	-
18	GZL	SE	3	X	-	-	-
18	AHR	SE	4	X	-	-	-
18	AHR	SE	5	X	-	-	-
18	GZL	cE	3	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	AHR	cE	4	X	-	-	-
18	AHR	cE	5	X	-	-	-
18	FUB	fE	1	X	-	-	-
18	GZL	fE	3	X	-	-	-
18	AHR	fE	4	X	-	-	-
18	AHR	fE	5	X	-	-	-
18	GZL	pE	3	X	-	-	-
18	AHR	pE	4	X	-	-	-
18	GZL	rE	3	X	-	-	-
18	AHR	rE	4	X	-	-	-
18	AHR	rE	5	X	-	-	-
18	GZL	tE	3	X	-	-	-
18	AHR	tE	5	X	-	-	-
18	GZL	yE	3	X	-	-	-
18	AHR	yE	4	X	-	-	-
18	GZL	zE	3	X	-	-	-
18	AHR	zE	5	X	-	-	-
19	GZL	1E	3	X	-	-	-
19	AHR	1E	4	X	-	-	-
19	GZL	AE	3	X	-	-	-
19	GZL	LE	3	X	-	-	-
19	AHR	LE	4	X	-	-	-
19	GZL	NE	3	X	-	-	-
19	AHR	NE	4	X	-	-	-
19	GZL	aE	3	X	-	-	-
19	AHR	aE	4	X	-	-	-
19	GZL	qE	3	X	-	-	-
2	HYP	G	23	X	-	-	-
2	HYP	G	26	X	-	-	-
2	HYP	I	23	X	-	-	-
2	HYP	I	26	X	-	-	-
20	GZL	CE	3	X	-	-	-
20	GZL	EE	3	X	-	-	-
20	GZL	HE	3	X	-	-	-
20	GZL	TE	3	X	-	-	-
20	AHR	TE	4	X	-	-	-
20	GZL	UE	3	X	-	-	-
20	GZL	WE	3	X	-	-	-
20	AHR	WE	4	X	-	-	-
20	GZL	gE	3	X	-	-	-
20	AHR	gE	4	X	-	-	-
20	GZL	hE	3	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	GZL	jE	3	X	-	-	-
20	AHR	jE	4	X	-	-	-
20	GZL	sE	3	X	-	-	-
20	GZL	uE	3	X	-	-	-
20	GZL	xE	3	X	-	-	-
21	GZL	FE	3	X	-	-	-
21	AHR	FE	4	X	-	-	-
21	AHR	FE	5	X	-	-	-
21	GZL	kE	3	X	-	-	-
21	AHR	kE	4	X	-	-	-
21	GZL	vE	3	X	-	-	-
21	AHR	vE	4	X	-	-	-
21	AHR	vE	5	X	-	-	-
22	GZL	GE	3	X	-	-	-
22	GZL	QE	3	X	-	-	-
22	AHR	QE	4	X	-	-	-
22	AHR	QE	6	X	-	-	-
22	GZL	RE	3	X	-	-	-
22	AHR	RE	4	X	-	-	-
22	GZL	VE	3	X	-	-	-
22	AHR	VE	4	X	-	-	-
22	GZL	dE	3	X	-	-	-
22	AHR	dE	4	X	-	-	-
22	AHR	dE	6	X	-	-	-
22	GZL	eE	3	X	-	-	-
22	AHR	eE	4	X	-	-	-
22	GZL	iE	3	X	-	-	-
22	AHR	iE	4	X	-	-	-
22	GZL	wE	3	X	-	-	-
23	GZL	XE	3	X	-	-	-
23	AHR	XE	4	X	-	-	-
23	AHR	XE	5	X	-	-	-
24	GZL	YE	3	X	-	-	-
24	AHR	YE	4	X	-	-	-
24	GZL	lE	3	X	-	-	-
24	AHR	lE	4	X	-	-	-
27	GLA	A	2007	X	-	-	-
27	GLA	B	2008	X	-	-	-
27	GLA	B	2014	X	-	-	-
27	GLA	E	2007	X	-	-	-
27	GLA	F	2009	X	-	-	-
3	FUB	XA	2	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	FUB	AD	1	X	-	-	-
4	FUB	DC	1	X	-	-	-
4	FUB	JA	1	X	-	-	-
4	FUB	L	1	X	-	-	-
4	FUB	OD	2	X	-	-	-
4	AHR	PC	4	X	-	-	-
4	FUB	RC	2	X	-	-	-
4	AHR	VA	4	X	-	-	-
4	FUB	Z	2	X	-	-	-
5	AHR	BD	5	X	-	-	-
6	GZL	0B	3	X	-	-	-
6	GZL	1C	3	X	-	-	-
6	FUB	2C	2	X	-	-	-
6	GZL	2C	3	X	-	-	-
6	GZL	3A	3	X	-	-	-
6	GZL	3D	3	X	-	-	-
6	GZL	4B	3	X	-	-	-
6	GZL	5	3	X	-	-	-
6	FUB	5B	2	X	-	-	-
6	GZL	5B	3	X	-	-	-
6	GZL	6C	3	X	-	-	-
6	GZL	6D	3	X	-	-	-
6	GZL	7A	3	X	-	-	-
6	GZL	7D	3	X	-	-	-
6	GZL	8	3	X	-	-	-
6	FUB	8A	2	X	-	-	-
6	GZL	8A	3	X	-	-	-
6	GZL	8D	3	X	-	-	-
6	GZL	9	3	X	-	-	-
6	GZL	9B	3	X	-	-	-
6	FUB	AA	2	X	-	-	-
6	GZL	AA	3	X	-	-	-
6	GZL	CB	3	X	-	-	-
6	GZL	CD	3	X	-	-	-
6	GZL	EA	3	X	-	-	-
6	GZL	FC	3	X	-	-	-
6	GZL	GD	3	X	-	-	-
6	GZL	JC	3	X	-	-	-
6	GZL	LA	3	X	-	-	-
6	GZL	ME	3	X	-	-	-
6	GZL	N	3	X	-	-	-
6	GZL	OE	3	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	GZL	PA	3	X	-	-	-
6	GZL	R	3	X	-	-	-
6	GZL	XB	3	X	-	-	-
6	GZL	ZE	3	X	-	-	-
6	GZL	bB	3	X	-	-	-
6	GZL	bE	3	X	-	-	-
6	FUB	cB	2	X	-	-	-
6	GZL	cB	3	X	-	-	-
6	GZL	gB	3	X	-	-	-
6	GZL	mE	3	X	-	-	-
6	GZL	nE	3	X	-	-	-
6	GZL	oE	3	X	-	-	-
6	GZL	uD	3	X	-	-	-
6	GZL	xC	3	X	-	-	-
6	GZL	yD	3	X	-	-	-
6	FUB	zD	2	X	-	-	-
6	GZL	zD	3	X	-	-	-

## 2 Entry composition [i](#)

There are 28 unique types of molecules in this entry. The entry contains 85288 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.

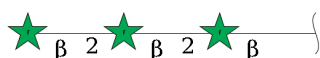
- Molecule 1 is a protein called Mst1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1907	13862	8723	2261	2797	81	0	0
1	B	1907	13862	8723	2261	2797	81	0	0
1	C	1494	10840	6862	1753	2179	46	0	0
1	D	1566	11377	7199	1841	2286	51	0	0
1	E	1449	10491	6595	1712	2105	79	0	0
1	F	1443	10455	6573	1705	2098	79	0	0

- Molecule 2 is a protein called Mstax.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	G	64	438	269	65	104	0	0
2	H	30	201	125	30	46	0	0
2	I	34	238	145	35	58	0	0

- Molecule 3 is an oligosaccharide called beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose.



Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
3	J	3	27	15	12	0	0

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Mol	Chain	Residues	Atoms			AltConf	Trace
3	K	3	Total	C	O	0	0
			27	15	12		
3	O	3	Total	C	O	0	0
			27	15	12		
3	P	3	Total	C	O	0	0
			27	15	12		
3	Q	3	Total	C	O	0	0
			27	15	12		
3	T	3	Total	C	O	0	0
			27	15	12		
3	V	3	Total	C	O	0	0
			27	15	12		
3	b	3	Total	C	O	0	0
			27	15	12		
3	e	3	Total	C	O	0	0
			27	15	12		
3	l	3	Total	C	O	0	0
			27	15	12		
3	m	3	Total	C	O	0	0
			27	15	12		
3	t	3	Total	C	O	0	0
			27	15	12		
3	w	3	Total	C	O	0	0
			27	15	12		
3	x	3	Total	C	O	0	0
			27	15	12		
3	y	3	Total	C	O	0	0
			27	15	12		
3	z	3	Total	C	O	0	0
			27	15	12		
3	0	3	Total	C	O	0	0
			27	15	12		
3	1	3	Total	C	O	0	0
			27	15	12		
3	2	3	Total	C	O	0	0
			27	15	12		
3	HA	3	Total	C	O	0	0
			27	15	12		
3	IA	3	Total	C	O	0	0
			27	15	12		
3	MA	3	Total	C	O	0	0
			27	15	12		

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Mol	Chain	Residues	Atoms			AltConf	Trace
3	NA	3	Total	C	O	0	0
			27	15	12		
3	OA	3	Total	C	O	0	0
			27	15	12		
3	RA	3	Total	C	O	0	0
			27	15	12		
3	TA	3	Total	C	O	0	0
			27	15	12		
3	XA	3	Total	C	O	0	0
			27	15	12		
3	ZA	3	Total	C	O	0	0
			27	15	12		
3	cA	3	Total	C	O	0	0
			27	15	12		
3	jA	3	Total	C	O	0	0
			27	15	12		
3	kA	3	Total	C	O	0	0
			27	15	12		
3	rA	3	Total	C	O	0	0
			27	15	12		
3	uA	3	Total	C	O	0	0
			27	15	12		
3	vA	3	Total	C	O	0	0
			27	15	12		
3	wA	3	Total	C	O	0	0
			27	15	12		
3	xA	3	Total	C	O	0	0
			27	15	12		
3	yA	3	Total	C	O	0	0
			27	15	12		
3	zA	3	Total	C	O	0	0
			27	15	12		
3	0A	3	Total	C	O	0	0
			27	15	12		
3	EB	3	Total	C	O	0	0
			27	15	12		
3	LB	3	Total	C	O	0	0
			27	15	12		
3	OB	3	Total	C	O	0	0
			27	15	12		
3	PB	3	Total	C	O	0	0
			27	15	12		

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Mol	Chain	Residues	Atoms			AltConf	Trace
3	QB	3	Total	C	O	0	0
			27	15	12		
3	RB	3	Total	C	O	0	0
			27	15	12		
3	SB	3	Total	C	O	0	0
			27	15	12		
3	TB	3	Total	C	O	0	0
			27	15	12		
3	UB	3	Total	C	O	0	0
			27	15	12		
3	hB	3	Total	C	O	0	0
			27	15	12		
3	oB	3	Total	C	O	0	0
			27	15	12		
3	rB	3	Total	C	O	0	0
			27	15	12		
3	sB	3	Total	C	O	0	0
			27	15	12		
3	tB	3	Total	C	O	0	0
			27	15	12		
3	uB	3	Total	C	O	0	0
			27	15	12		
3	vB	3	Total	C	O	0	0
			27	15	12		
3	wB	3	Total	C	O	0	0
			27	15	12		
3	xB	3	Total	C	O	0	0
			27	15	12		
3	BC	3	Total	C	O	0	0
			27	15	12		
3	CC	3	Total	C	O	0	0
			27	15	12		
3	GC	3	Total	C	O	0	0
			27	15	12		
3	HC	3	Total	C	O	0	0
			27	15	12		
3	IC	3	Total	C	O	0	0
			27	15	12		
3	LC	3	Total	C	O	0	0
			27	15	12		
3	NC	3	Total	C	O	0	0
			27	15	12		

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Mol	Chain	Residues	Atoms			AltConf	Trace
3	TC	3	Total	C	O	0	0
			27	15	12		
3	WC	3	Total	C	O	0	0
			27	15	12		
3	dC	3	Total	C	O	0	0
			27	15	12		
3	eC	3	Total	C	O	0	0
			27	15	12		
3	lC	3	Total	C	O	0	0
			27	15	12		
3	oC	3	Total	C	O	0	0
			27	15	12		
3	pC	3	Total	C	O	0	0
			27	15	12		
3	qC	3	Total	C	O	0	0
			27	15	12		
3	rC	3	Total	C	O	0	0
			27	15	12		
3	sC	3	Total	C	O	0	0
			27	15	12		
3	tC	3	Total	C	O	0	0
			27	15	12		
3	uC	3	Total	C	O	0	0
			27	15	12		
3	8C	3	Total	C	O	0	0
			27	15	12		
3	9C	3	Total	C	O	0	0
			27	15	12		
3	DD	3	Total	C	O	0	0
			27	15	12		
3	ED	3	Total	C	O	0	0
			27	15	12		
3	FD	3	Total	C	O	0	0
			27	15	12		
3	ID	3	Total	C	O	0	0
			27	15	12		
3	KD	3	Total	C	O	0	0
			27	15	12		
3	QD	3	Total	C	O	0	0
			27	15	12		
3	TD	3	Total	C	O	0	0
			27	15	12		

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Mol	Chain	Residues	Atoms			AltConf	Trace
3	aD	3	Total	C	O	0	0
			27	15	12		
3	bD	3	Total	C	O	0	0
			27	15	12		
3	iD	3	Total	C	O	0	0
			27	15	12		
3	lD	3	Total	C	O	0	0
			27	15	12		
3	mD	3	Total	C	O	0	0
			27	15	12		
3	nD	3	Total	C	O	0	0
			27	15	12		
3	oD	3	Total	C	O	0	0
			27	15	12		
3	pD	3	Total	C	O	0	0
			27	15	12		
3	qD	3	Total	C	O	0	0
			27	15	12		
3	rD	3	Total	C	O	0	0
			27	15	12		

- Molecule 4 is an oligosaccharide called alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose.



Mol	Chain	Residues	Atoms			AltConf	Trace
4	L	4	Total	C	O	0	0
			36	20	16		
4	W	4	Total	C	O	0	0
			36	20	16		
4	X	4	Total	C	O	0	0
			36	20	16		
4	Z	4	Total	C	O	0	0
			36	20	16		
4	c	4	Total	C	O	0	0
			36	20	16		
4	d	4	Total	C	O	0	0
			36	20	16		
4	g	4	Total	C	O	0	0
			36	20	16		

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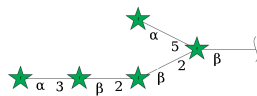
Mol	Chain	Residues	Atoms			AltConf	Trace
4	k	4	Total 36	C 20	O 16	0	0
4	r	4	Total 36	C 20	O 16	0	0
4	v	4	Total 36	C 20	O 16	0	0
4	JA	4	Total 36	C 20	O 16	0	0
4	UA	4	Total 36	C 20	O 16	0	0
4	VA	4	Total 36	C 20	O 16	0	0
4	aA	4	Total 36	C 20	O 16	0	0
4	bA	4	Total 36	C 20	O 16	0	0
4	eA	4	Total 36	C 20	O 16	0	0
4	iA	4	Total 36	C 20	O 16	0	0
4	pA	4	Total 36	C 20	O 16	0	0
4	tA	4	Total 36	C 20	O 16	0	0
4	JB	4	Total 36	C 20	O 16	0	0
4	NB	4	Total 36	C 20	O 16	0	0
4	mB	4	Total 36	C 20	O 16	0	0
4	qB	4	Total 36	C 20	O 16	0	0
4	DC	4	Total 36	C 20	O 16	0	0
4	OC	4	Total 36	C 20	O 16	0	0
4	PC	4	Total 36	C 20	O 16	0	0
4	RC	4	Total 36	C 20	O 16	0	0
4	UC	4	Total 36	C 20	O 16	0	0

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Mol	Chain	Residues	Atoms			AltConf	Trace
4	VC	4	Total	C	O	0	0
			36	20	16		
4	YC	4	Total	C	O	0	0
			36	20	16		
4	cC	4	Total	C	O	0	0
			36	20	16		
4	jC	4	Total	C	O	0	0
			36	20	16		
4	nC	4	Total	C	O	0	0
			36	20	16		
4	AD	4	Total	C	O	0	0
			36	20	16		
4	LD	4	Total	C	O	0	0
			36	20	16		
4	MD	4	Total	C	O	0	0
			36	20	16		
4	OD	4	Total	C	O	0	0
			36	20	16		
4	RD	4	Total	C	O	0	0
			36	20	16		
4	SD	4	Total	C	O	0	0
			36	20	16		
4	VD	4	Total	C	O	0	0
			36	20	16		
4	ZD	4	Total	C	O	0	0
			36	20	16		
4	gD	4	Total	C	O	0	0
			36	20	16		
4	kD	4	Total	C	O	0	0
			36	20	16		

- Molecule 5 is an oligosaccharide called alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose.



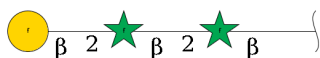
Mol	Chain	Residues	Atoms			AltConf	Trace
5	M	5	Total	C	O	0	0
			45	25	20		
5	KA	5	Total	C	O	0	0
			45	25	20		

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Mol	Chain	Residues	Atoms			AltConf	Trace
5	EC	5	Total	C	O	0	0
			45	25	20		
5	BD	5	Total	C	O	0	0
			45	25	20		

- Molecule 6 is an oligosaccharide called beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose.



Mol	Chain	Residues	Atoms			AltConf	Trace
6	N	3	Total	C	O	0	0
			29	16	13		
6	R	3	Total	C	O	0	0
			29	16	13		
6	5	3	Total	C	O	0	0
			29	16	13		
6	8	3	Total	C	O	0	0
			29	16	13		
6	9	3	Total	C	O	0	0
			29	16	13		
6	AA	3	Total	C	O	0	0
			29	16	13		
6	EA	3	Total	C	O	0	0
			29	16	13		
6	LA	3	Total	C	O	0	0
			29	16	13		
6	PA	3	Total	C	O	0	0
			29	16	13		
6	3A	3	Total	C	O	0	0
			29	16	13		
6	6A	3	Total	C	O	0	0
			29	16	13		
6	7A	3	Total	C	O	0	0
			29	16	13		
6	8A	3	Total	C	O	0	0
			29	16	13		
6	CB	3	Total	C	O	0	0
			29	16	13		
6	XB	3	Total	C	O	0	0
			29	16	13		

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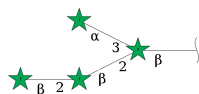
Mol	Chain	Residues	Atoms			AltConf	Trace
6	aB	3	Total	C	O	0	0
			29	16	13		
6	bB	3	Total	C	O	0	0
			29	16	13		
6	cB	3	Total	C	O	0	0
			29	16	13		
6	gB	3	Total	C	O	0	0
			29	16	13		
6	0B	3	Total	C	O	0	0
			29	16	13		
6	3B	3	Total	C	O	0	0
			29	16	13		
6	4B	3	Total	C	O	0	0
			29	16	13		
6	5B	3	Total	C	O	0	0
			29	16	13		
6	9B	3	Total	C	O	0	0
			29	16	13		
6	FC	3	Total	C	O	0	0
			29	16	13		
6	JC	3	Total	C	O	0	0
			29	16	13		
6	xC	3	Total	C	O	0	0
			29	16	13		
6	0C	3	Total	C	O	0	0
			29	16	13		
6	1C	3	Total	C	O	0	0
			29	16	13		
6	2C	3	Total	C	O	0	0
			29	16	13		
6	6C	3	Total	C	O	0	0
			29	16	13		
6	CD	3	Total	C	O	0	0
			29	16	13		
6	GD	3	Total	C	O	0	0
			29	16	13		
6	uD	3	Total	C	O	0	0
			29	16	13		
6	xD	3	Total	C	O	0	0
			29	16	13		
6	yD	3	Total	C	O	0	0
			29	16	13		

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Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
6	zD	3	29	16	13	0	0
6	3D	3	29	16	13	0	0
6	6D	3	29	16	13	0	0
6	7D	3	29	16	13	0	0
6	8D	3	29	16	13	0	0
6	ME	3	29	16	13	0	0
6	OE	3	29	16	13	0	0
6	ZE	3	29	16	13	0	0
6	bE	3	29	16	13	0	0
6	mE	3	29	16	13	0	0
6	nE	3	29	16	13	0	0
6	oE	3	29	16	13	0	0

- Molecule 7 is an oligosaccharide called beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose.



Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
7	S	4	36	20	16	0	0
7	f	4	36	20	16	0	0
7	h	4	36	20	16	0	0
7	QA	4	36	20	16	0	0
7	dA	4	36	20	16	0	0

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Mol	Chain	Residues	Atoms			AltConf	Trace
7	fA	4	Total	C	O	0	0
			36	20	16		
7	KC	4	Total	C	O	0	0
			36	20	16		
7	XC	4	Total	C	O	0	0
			36	20	16		
7	ZC	4	Total	C	O	0	0
			36	20	16		
7	HD	4	Total	C	O	0	0
			36	20	16		
7	UD	4	Total	C	O	0	0
			36	20	16		
7	WD	4	Total	C	O	0	0
			36	20	16		

- Molecule 8 is an oligosaccharide called alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose.



Mol	Chain	Residues	Atoms			AltConf	Trace
8	U	5	Total	C	O	0	0
			45	25	20		
8	SA	5	Total	C	O	0	0
			45	25	20		
8	MC	5	Total	C	O	0	0
			45	25	20		
8	JD	5	Total	C	O	0	0
			45	25	20		

- Molecule 9 is an oligosaccharide called beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose.



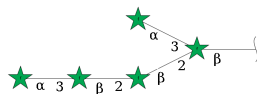
Mol	Chain	Residues	Atoms			AltConf	Trace
9	Y	2	Total	C	O	0	0
			18	10	8		

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Mol	Chain	Residues	Atoms			AltConf	Trace
9	j	2	Total	C	O	0	0
			18	10	8		
9	WA	2	Total	C	O	0	0
			18	10	8		
9	hA	2	Total	C	O	0	0
			18	10	8		
9	QC	2	Total	C	O	0	0
			18	10	8		
9	bC	2	Total	C	O	0	0
			18	10	8		
9	ND	2	Total	C	O	0	0
			18	10	8		
9	YD	2	Total	C	O	0	0
			18	10	8		

- Molecule 10 is an oligosaccharide called alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose.



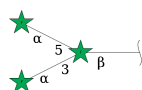
Mol	Chain	Residues	Atoms			AltConf	Trace
10	a	5	Total	C	O	0	0
			45	25	20		
10	u	5	Total	C	O	0	0
			45	25	20		
10	3	5	Total	C	O	0	0
			45	25	20		
10	YA	5	Total	C	O	0	0
			45	25	20		
10	sA	5	Total	C	O	0	0
			45	25	20		
10	1A	5	Total	C	O	0	0
			45	25	20		
10	MB	5	Total	C	O	0	0
			45	25	20		
10	VB	5	Total	C	O	0	0
			45	25	20		
10	pB	5	Total	C	O	0	0
			45	25	20		

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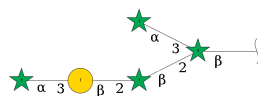
Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
10	yB	5	45	25	20	0	0
10	SC	5	45	25	20	0	0
10	mC	5	45	25	20	0	0
10	vC	5	45	25	20	0	0
10	PD	5	45	25	20	0	0
10	jD	5	45	25	20	0	0
10	sD	5	45	25	20	0	0

- Molecule 11 is an oligosaccharide called alpha-L-arabinofuranose-(1-3)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose.



Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
11	i	3	27	15	12	0	0
11	gA	3	27	15	12	0	0
11	aC	3	27	15	12	0	0
11	XD	3	27	15	12	0	0

- Molecule 12 is an oligosaccharide called alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose.



Mol	Chain	Residues	Atoms			AltConf	Trace
12	n	5	Total	C	O	0	0
			47	26	21		
12	q	5	Total	C	O	0	0
			47	26	21		
12	lA	5	Total	C	O	0	0
			47	26	21		
12	oA	5	Total	C	O	0	0
			47	26	21		
12	FB	5	Total	C	O	0	0
			47	26	21		
12	IB	5	Total	C	O	0	0
			47	26	21		
12	iB	5	Total	C	O	0	0
			47	26	21		
12	lB	5	Total	C	O	0	0
			47	26	21		
12	fC	5	Total	C	O	0	0
			47	26	21		
12	iC	5	Total	C	O	0	0
			47	26	21		
12	cD	5	Total	C	O	0	0
			47	26	21		
12	fD	5	Total	C	O	0	0
			47	26	21		

- Molecule 13 is an oligosaccharide called alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose.



Mol	Chain	Residues	Atoms			AltConf	Trace
13	o	4	Total	C	O	0	0
			38	21	17		
13	4	4	Total	C	O	0	0
			38	21	17		
13	6	4	Total	C	O	0	0
			38	21	17		
13	7	4	Total	C	O	0	0
			38	21	17		
13	BA	4	Total	C	O	0	0
			38	21	17		

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Mol	Chain	Residues	Atoms			AltConf	Trace
13	mA	4	Total 38	C 21	O 17	0	0
13	2A	4	Total 38	C 21	O 17	0	0
13	4A	4	Total 38	C 21	O 17	0	0
13	5A	4	Total 38	C 21	O 17	0	0
13	9A	4	Total 38	C 21	O 17	0	0
13	GB	4	Total 38	C 21	O 17	0	0
13	WB	4	Total 38	C 21	O 17	0	0
13	YB	4	Total 38	C 21	O 17	0	0
13	ZB	4	Total 38	C 21	O 17	0	0
13	dB	4	Total 38	C 21	O 17	0	0
13	jB	4	Total 38	C 21	O 17	0	0
13	zB	4	Total 38	C 21	O 17	0	0
13	1B	4	Total 38	C 21	O 17	0	0
13	2B	4	Total 38	C 21	O 17	0	0
13	6B	4	Total 38	C 21	O 17	0	0
13	gC	4	Total 38	C 21	O 17	0	0
13	wC	4	Total 38	C 21	O 17	0	0
13	yC	4	Total 38	C 21	O 17	0	0
13	zC	4	Total 38	C 21	O 17	0	0
13	3C	4	Total 38	C 21	O 17	0	0
13	dD	4	Total 38	C 21	O 17	0	0

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Mol	Chain	Residues	Atoms			AltConf	Trace
13	tD	4	Total	C	O	0	0
			38	21	17		
13	vD	4	Total	C	O	0	0
			38	21	17		
13	wD	4	Total	C	O	0	0
			38	21	17		
13	0D	4	Total	C	O	0	0
			38	21	17		

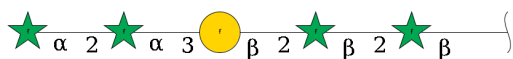
- Molecule 14 is an oligosaccharide called beta-L-arabinofuranose-(1-5)-beta-D-galactofuranos e-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose.



Mol	Chain	Residues	Atoms			AltConf	Trace
14	p	4	Total	C	O	0	0
			38	21	17		
14	s	4	Total	C	O	0	0
			38	21	17		
14	nA	4	Total	C	O	0	0
			38	21	17		
14	qA	4	Total	C	O	0	0
			38	21	17		
14	HB	4	Total	C	O	0	0
			38	21	17		
14	KB	4	Total	C	O	0	0
			38	21	17		
14	kB	4	Total	C	O	0	0
			38	21	17		
14	nB	4	Total	C	O	0	0
			38	21	17		
14	hC	4	Total	C	O	0	0
			38	21	17		
14	kC	4	Total	C	O	0	0
			38	21	17		
14	eD	4	Total	C	O	0	0
			38	21	17		
14	hD	4	Total	C	O	0	0
			38	21	17		



- Molecule 15 is an oligosaccharide called alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose.



Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
15	CA	5	47	26	21	0	0
15	DA	5	47	26	21	0	0
15	AB	5	47	26	21	0	0
15	BB	5	47	26	21	0	0
15	eB	5	47	26	21	0	0
15	fB	5	47	26	21	0	0
15	7B	5	47	26	21	0	0
15	8B	5	47	26	21	0	0
15	4C	5	47	26	21	0	0
15	5C	5	47	26	21	0	0
15	1D	5	47	26	21	0	0
15	2D	5	47	26	21	0	0

- Molecule 16 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



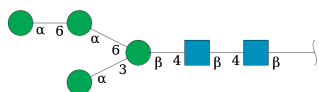
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
16	FA	2	28	16	2	10	0	0

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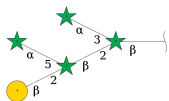
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
16	AC	2	28	16	2	10	0	0
16	4D	2	28	16	2	10	0	0

- Molecule 17 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
17	GA	6	72	40	2	30	0	0
17	DB	6	72	40	2	30	0	0
17	7C	6	72	40	2	30	0	0
17	5D	6	72	40	2	30	0	0

- Molecule 18 is an oligosaccharide called beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose.



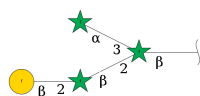
Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
18	9D	5	47	26	21	0	0
18	BE	5	47	26	21	0	0
18	DE	5	47	26	21	0	0
18	IE	5	47	26	21	0	0
18	JE	5	47	26	21	0	0

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Mol	Chain	Residues	Atoms			AltConf	Trace
18	KE	5	Total	C	O	0	0
			47	26	21		
18	PE	5	Total	C	O	0	0
			47	26	21		
18	SE	5	Total	C	O	0	0
			47	26	21		
18	cE	5	Total	C	O	0	0
			47	26	21		
18	fE	5	Total	C	O	0	0
			47	26	21		
18	pE	5	Total	C	O	0	0
			47	26	21		
18	rE	5	Total	C	O	0	0
			47	26	21		
18	tE	5	Total	C	O	0	0
			47	26	21		
18	yE	5	Total	C	O	0	0
			47	26	21		
18	zE	5	Total	C	O	0	0
			47	26	21		
18	0E	5	Total	C	O	0	0
			47	26	21		

- Molecule 19 is an oligosaccharide called beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose.



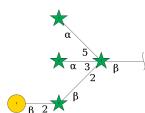
Mol	Chain	Residues	Atoms			AltConf	Trace
19	AE	4	Total	C	O	0	0
			38	21	17		
19	LE	4	Total	C	O	0	0
			38	21	17		
19	NE	4	Total	C	O	0	0
			38	21	17		
19	aE	4	Total	C	O	0	0
			38	21	17		
19	qE	4	Total	C	O	0	0
			38	21	17		
19	1E	4	Total	C	O	0	0
			38	21	17		

- Molecule 20 is an oligosaccharide called beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose.



Mol	Chain	Residues	Atoms			AltConf	Trace
20	CE	4	Total	C	O	0	0
			38	21	17		
20	EE	4	Total	C	O	0	0
			38	21	17		
20	HE	4	Total	C	O	0	0
			38	21	17		
20	TE	4	Total	C	O	0	0
			38	21	17		
20	UE	4	Total	C	O	0	0
			38	21	17		
20	WE	4	Total	C	O	0	0
			38	21	17		
20	gE	4	Total	C	O	0	0
			38	21	17		
20	hE	4	Total	C	O	0	0
			38	21	17		
20	jE	4	Total	C	O	0	0
			38	21	17		
20	sE	4	Total	C	O	0	0
			38	21	17		
20	uE	4	Total	C	O	0	0
			38	21	17		
20	xE	4	Total	C	O	0	0
			38	21	17		

- Molecule 21 is an oligosaccharide called beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)][alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose.



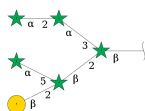
Mol	Chain	Residues	Atoms			AltConf	Trace
21	FE	5	Total	C	O	0	0
			47	26	21		

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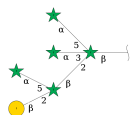
Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
21	kE	5	47	26	21	0	0
21	vE	5	47	26	21	0	0

- Molecule 22 is an oligosaccharide called beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose.



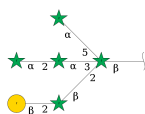
Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
22	GE	6	56	31	25	0	0
22	QE	6	56	31	25	0	0
22	RE	6	56	31	25	0	0
22	VE	6	56	31	25	0	0
22	dE	6	56	31	25	0	0
22	eE	6	56	31	25	0	0
22	iE	6	56	31	25	0	0
22	wE	6	56	31	25	0	0

- Molecule 23 is an oligosaccharide called beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)][alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose.



Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
23	XE	6	56	31	25	0	0

- Molecule 24 is an oligosaccharide called beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)][alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose.

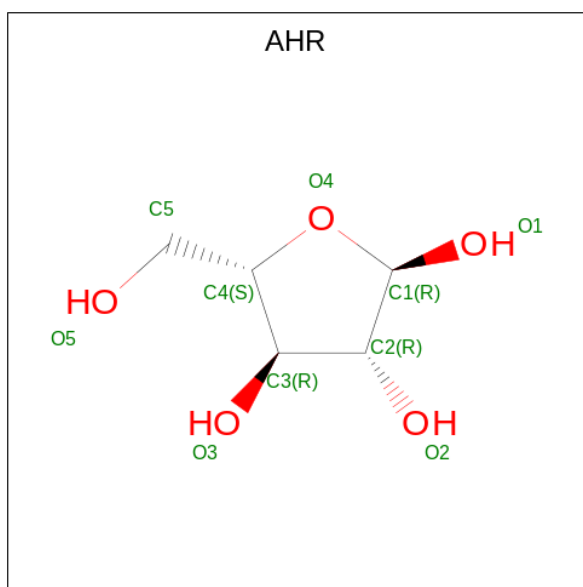


Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
24	YE	6	56	31	25	0	0
24	IE	6	56	31	25	0	0

- Molecule 25 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
			Total	Ca	
25	A	1	1	1	0
25	B	1	1	1	0
25	C	1	1	1	0
25	D	1	1	1	0
25	E	1	1	1	0
25	F	1	1	1	0

- Molecule 26 is alpha-L-arabinofuranose (three-letter code: AHR) (formula: C<sub>5</sub>H<sub>10</sub>O<sub>5</sub>) (labeled as "Ligand of Interest" by depositor).



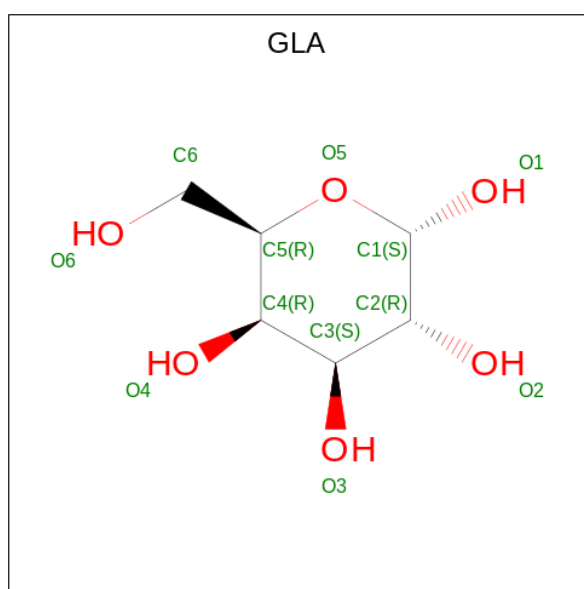
Mol	Chain	Residues	Atoms			AltConf
26	A	1	Total	C	O	0
			9	5	4	
26	A	1	Total	C	O	0
			9	5	4	
26	A	1	Total	C	O	0
			9	5	4	
26	A	1	Total	C	O	0
			9	5	4	
26	B	1	Total	C	O	0
			9	5	4	
26	B	1	Total	C	O	0
			9	5	4	
26	B	1	Total	C	O	0
			9	5	4	
26	B	1	Total	C	O	0
			9	5	4	
26	C	1	Total	C	O	0
			9	5	4	
26	C	1	Total	C	O	0
			9	5	4	
26	D	1	Total	C	O	0
			9	5	4	
26	D	1	Total	C	O	0
			9	5	4	
26	D	1	Total	C	O	0
			9	5	4	
26	E	1	Total	C	O	0
			9	5	4	

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Mol	Chain	Residues	Atoms			AltConf
26	E	1	Total	C	O	0
			9	5	4	
26	F	1	Total	C	O	0
			9	5	4	
26	F	1	Total	C	O	0
			9	5	4	
26	F	1	Total	C	O	0
			9	5	4	
26	F	1	Total	C	O	0
			9	5	4	

- Molecule 27 is alpha-D-galactopyranose (three-letter code: GLA) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
27	A	1	Total	C	O	0
			11	6	5	
27	A	1	Total	C	O	0
			11	6	5	
27	A	1	Total	C	O	0
			11	6	5	
27	A	1	Total	C	O	0
			11	6	5	
27	A	1	Total	C	O	0
			11	6	5	

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
27	A	1	11	6	5	0
27	A	1	11	6	5	0
27	A	1	11	6	5	0
27	A	1	11	6	5	0
27	A	1	11	6	5	0
27	A	1	11	6	5	0
27	A	1	11	6	5	0
27	A	1	11	6	5	0
27	B	1	11	6	5	0
27	B	1	11	6	5	0
27	B	1	11	6	5	0
27	B	1	11	6	5	0
27	B	1	11	6	5	0
27	B	1	11	6	5	0
27	B	1	11	6	5	0
27	B	1	11	6	5	0
27	B	1	11	6	5	0
27	B	1	11	6	5	0
27	B	1	11	6	5	0
27	B	1	11	6	5	0
27	B	1	11	6	5	0
27	B	1	11	6	5	0

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
27	C	1	11	6	5	0
27	C	1	11	6	5	0
27	C	1	11	6	5	0
27	C	1	11	6	5	0
27	C	1	11	6	5	0
27	D	1	11	6	5	0
27	D	1	11	6	5	0
27	D	1	11	6	5	0
27	D	1	11	6	5	0
27	D	1	11	6	5	0
27	D	1	11	6	5	0
27	E	1	11	6	5	0
27	E	1	11	6	5	0
27	E	1	11	6	5	0
27	E	1	11	6	5	0
27	E	1	11	6	5	0
27	E	1	11	6	5	0
27	E	1	11	6	5	0
27	E	1	11	6	5	0
27	E	1	11	6	5	0
27	E	1	11	6	5	0
27	E	1	11	6	5	0
27	E	1	11	6	5	0

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
27	E	1	11	6	5	0
27	E	1	11	6	5	0
27	F	1	11	6	5	0
27	F	1	11	6	5	0
27	F	1	11	6	5	0
27	F	1	11	6	5	0
27	F	1	11	6	5	0
27	F	1	11	6	5	0
27	F	1	11	6	5	0
27	F	1	11	6	5	0
27	F	1	11	6	5	0
27	F	1	11	6	5	0
27	F	1	11	6	5	0
27	F	1	11	6	5	0
27	F	1	11	6	5	0
27	F	1	11	6	5	0
27	F	1	11	6	5	0
27	F	1	11	6	5	0

- Molecule 28 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).

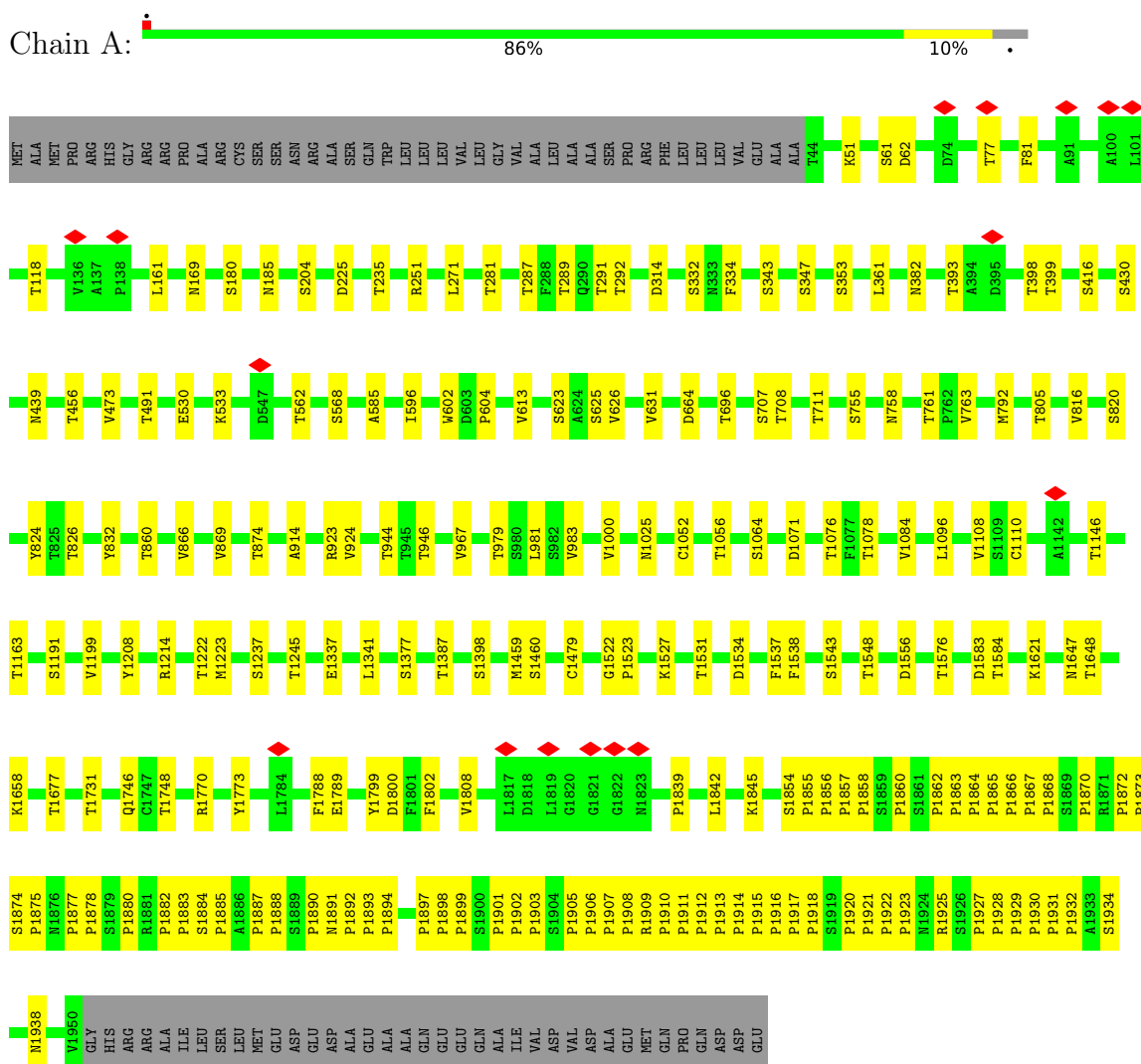


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
28	A	1	Total 14	C 8	N 1	O 5	0
28	B	1	Total 14	C 8	N 1	O 5	0
28	B	1	Total 14	C 8	N 1	O 5	0
28	C	1	Total 14	C 8	N 1	O 5	0
28	C	1	Total 14	C 8	N 1	O 5	0
28	D	1	Total 14	C 8	N 1	O 5	0
28	E	1	Total 14	C 8	N 1	O 5	0

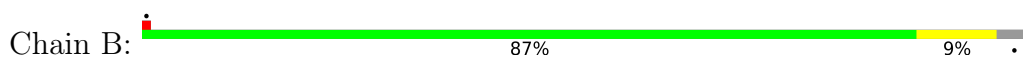
### 3 Residue-property plots

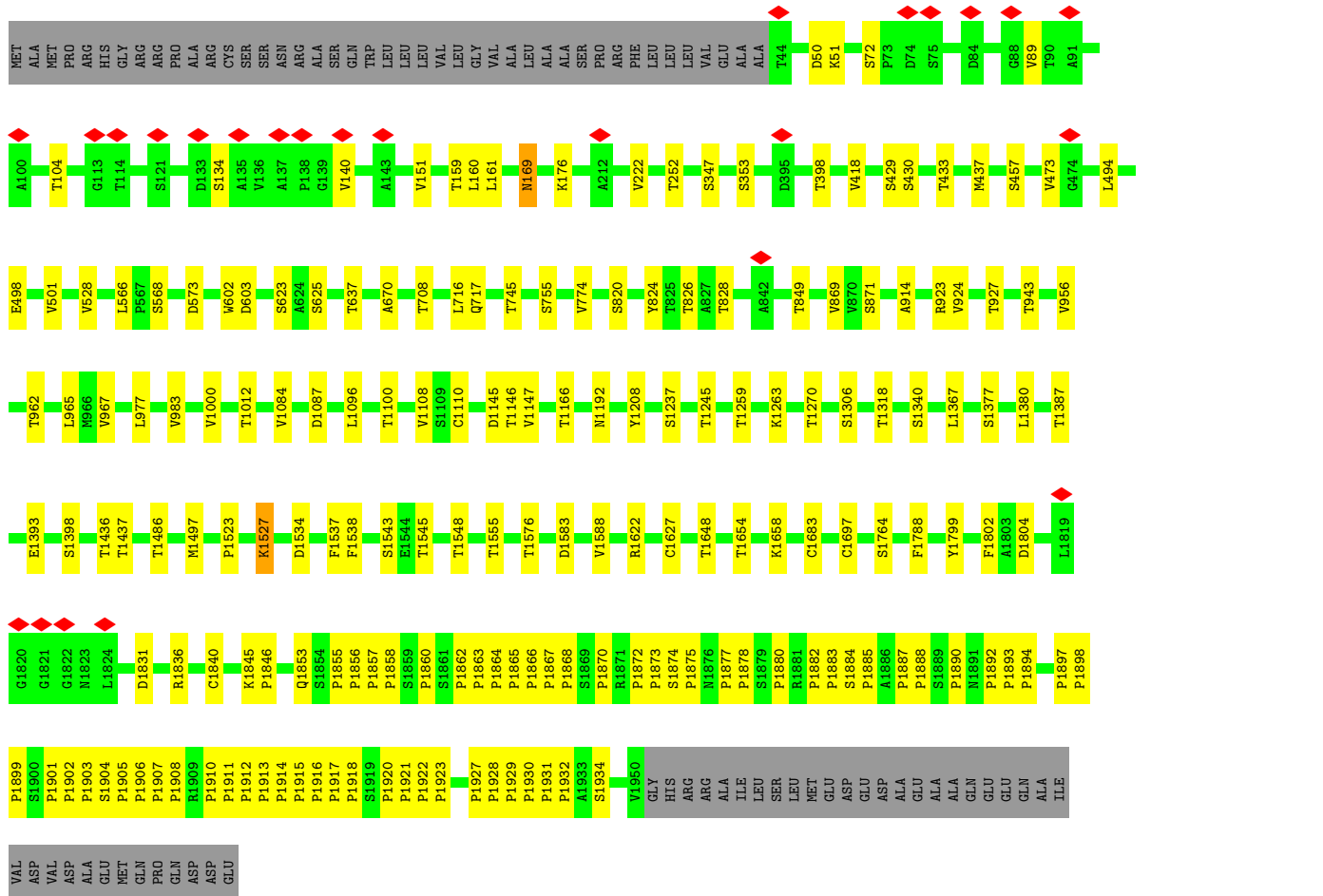
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

- Molecule 1: Mst1

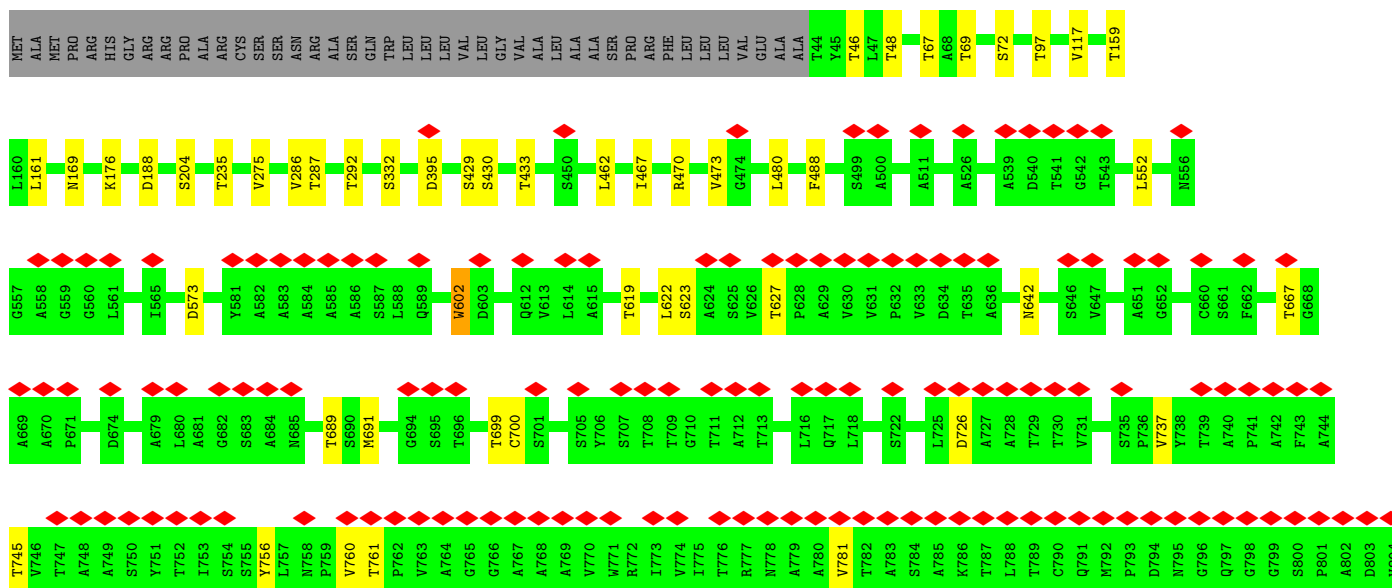


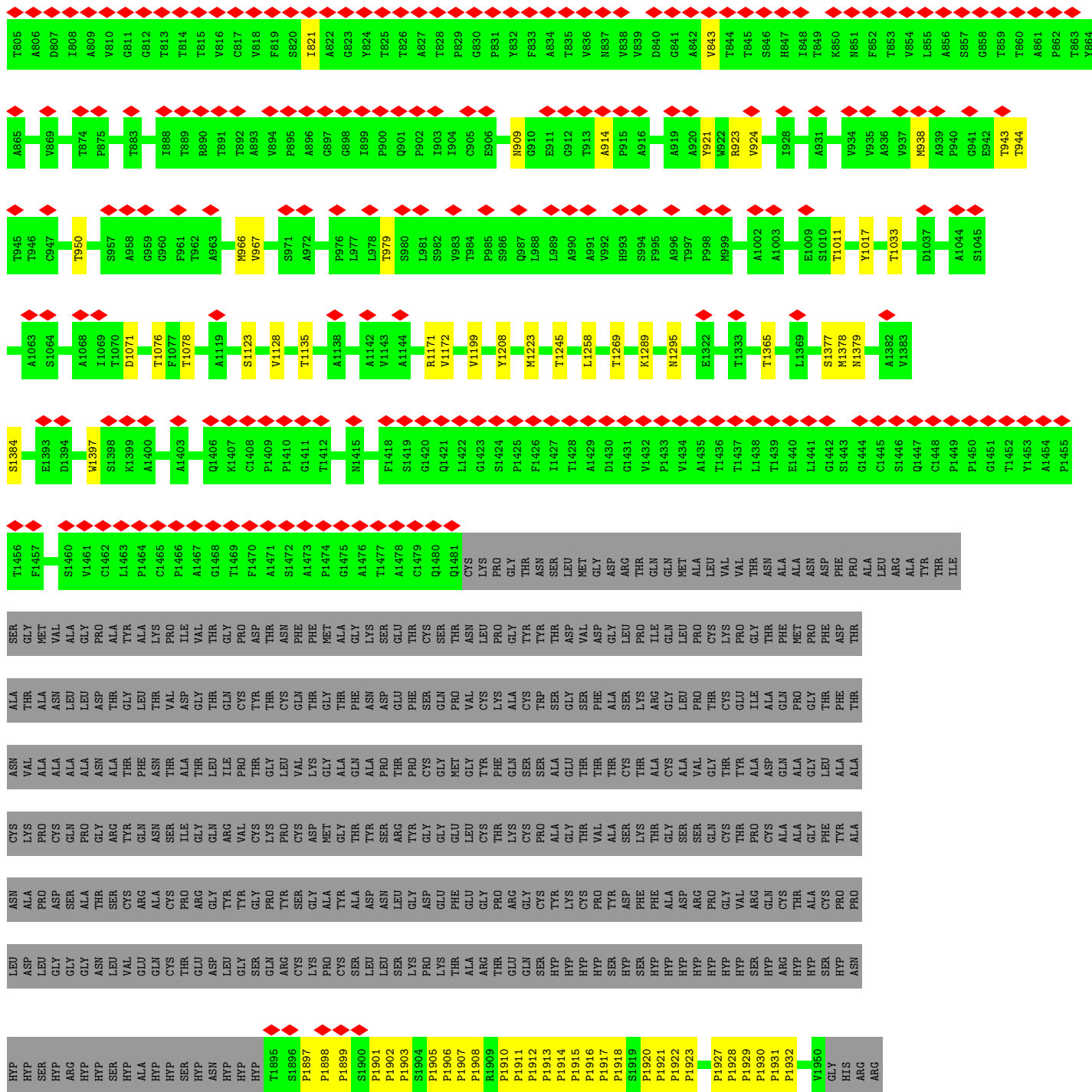
- Molecule 1: Mst1



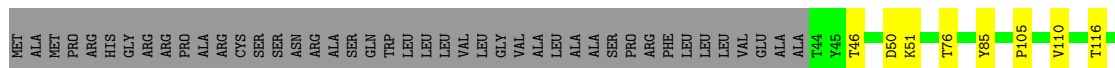


• Molecule 1: Mst1





• Molecule 1: Mst1



ALA	G1540	THR	A1540	G1420	M1192	T979	C905	F833	R772	P704	L614	A475	T159
GLN	G1541	PHE	G1541	Q1421	Y1208	S980	N909	A834	I773	S705	A615	L479	L160
ALA	K1542	ASN	K1542	L1422	G910	L981	G910	T835	V774	Y706	A616	T487	L161
PRO	S1543	THR	S1543	G1423	E911	S982	E911	V836	I775	S707	A617	T491	M169
THR	P1544	GLU	P1544	S1424	G912	V983	G912	M837	T776	T708	A618	T491	V179
CYS	T1545	PRO	T1545	P1425	T913	T984	T913	V838	R777	T709	P618	T491	S180
GLY	C1546	PRO	C1546	F1426	A914	P985	A914	V839	N778	G710	T619	A500	S181
LEU	S1547	VAL	S1547	T1427	P915	S986	P915	D940	G711	T711	T620	V501	S182
THR	M1548	CYS	M1548	T1428	A916	Q987	A916	G841	A712	T712	T621	E502	M185
ALA	N1549	ALA	N1549	T1429	S917	L988	S917	G842	A713	L716	L622	I507	S204
ALA	L1550	CYS	L1550	D1430	S918	L989	S918	V843	S784	Q717	S623	A508	I207
SER	P1551	TRP	P1551	G1431	A918	A990	A918	T844	S785	L718	S625	A509	I207
SER	D1552	GLY	D1552	V1432	A919	A991	A919	T845	A785	L718	S626	T509	I207
THR	Y1553	THR	Y1553	P1433	A920	V992	A920	S846	K786	I719	S627	V510	E231
THR	Y1554	ALA	Y1554	V1434	Y921	F995	Y921	H847	T787	T787	S628	A511	R251
ALA	T1555	ALA	T1555	V1435	K922	A996	K922	I848	L788	A724	S629	A512	R251
CYS	T1556	SER	T1556	T1436	R923	T997	R923	T849	L789	L725	V630	T524	T278
THR	D1557	LYS	D1557	T1437	V924	T998	V924	R850	C790	D726	V633	G527	S279
ALA	V1558	ALA	V1558	L1438	S925	P998	S925	R851	C791	A727	D634	G527	V280
CYS	D1559	LEU	D1559	L1439	T926	M999	T926	F852	M792	A728	T635	G531	V281
VAL	G1559	PRO	G1559	T1439	T927	V1000	T927	T853	P793	T729	T636	S531	T287
GLY	L1560	THR	L1560	E1440	I928	V1001	I928	V854	D794	T729	T637	C534	T289
THR	P1561	CYS	P1561	L1441	V934	A1002	V934	L855	N795	F733	L638	D540	F334
THR	I1562	ILE	I1562	G1442	V935	A1003	V935	L856	G796	L734	L639	D541	T352
ASP	Q1563	ALA	Q1563	S1443	V936	A1003	V936	S857	C797	S735	L639	D541	T352
GLN	L1564	GLN	L1564	G1444	A936	A1003	A936	S857	C797	S735	L639	D541	T352
ALA	P1565	PRO	P1565	C1445	V937	L1028	V937	S858	G798	P736	L639	D541	T352
GLY	L1566	GLY	L1566	S1446	V937	D1037	V937	S858	G798	P736	L639	D541	T352
CYS	P1566	GLY	P1566	T1446	V938	V1001	V938	S858	G798	P736	L639	D541	T352
LYS	D1507	THR	D1507	Q1447	A939	S1045	A939	S859	G799	A740	L639	D541	T352
THR	F1508	GLY	F1508	C1448	S1046	S1046	S1046	T860	S800	P741	L639	D541	T352
ALA	P1509	ALA	P1509	Q1449	M0659	S1064	M0659	T861	P801	A742	L639	D541	T352
VAL	A1510	VAL	A1510	P1450	T943	M0659	T943	T862	A802	A743	L639	D541	T352
ALA	L1511	MET	L1511	G1451	T944	T944	T944	T863	D803	F743	L639	D541	T352
ALA	A1512	PRO	A1512	T1452	T945	S1064	T945	T864	D803	A744	L639	D541	T352
ALA	R1512	PHE	R1512	G1453	T946	S1064	T946	T864	D803	A744	L639	D541	T352
ASN	A1513	ALA	A1513	Y1453	C947	S1067	C947	T867	T805	T745	L639	D541	T352
ASP	A1514	ASP	A1514	A1454	S1398	A1068	S1398	S868	A806	A748	L639	D541	T352
ALA	T1514	ALA	T1514	P1455	K1399	A1068	K1399	S868	A806	A748	L639	D541	T352
THR	T1515	THR	T1515	T1455	A1400	I1069	A1400	T869	D807	A749	L639	D541	T352
PHE	ILE	PHE	ILE	T1456	A1403	A1072	A1403	T869	I808	S750	L639	D541	T352
ASN	SER	ASN	SER	F1457	G1404	A1072	G1404	P872	A809	A809	L639	D541	T352
LEU	GLY	LEU	GLY	G1458	C1405	T1076	C1405	A873	V810	T752	L639	D541	T352
LEU	VAL	LEU	VAL	M1459	C1406	T1076	C1406	T874	G811	I753	L639	D541	T352
THR	ASP	THR	ASP	S1460	Q1406	L1096	Q1406	P875	G812	S754	L639	D541	T352
LEU	ALA	LEU	ALA	V1461	K1407	L1096	K1407	P876	T813	S755	L639	D541	T352
ILE	GLY	ILE	GLY	V1461	C1408	L1096	C1408	P876	T814	Y756	L639	D541	T352
LEU	PRO	LEU	PRO	L1463	C1408	L1096	C1408	F886	T815	L757	L639	D541	T352
VAL	VAL	VAL	VAL	L1463	P1409	T1100	P1409	T887	V816	L758	L639	D541	T352
CYS	ALA	CYS	ALA	L1463	P1410	T1100	P1410	T887	V816	L758	L639	D541	T352
VAL	ASP	VAL	ASP	L1465	G1411	G960	G1411	T888	C817	P759	L639	D541	T352
THR	GLY	THR	GLY	C1465	T1412	G960	T1412	T889	V818	V760	L639	D541	T352
GLY	THR	GLY	THR	P1466	Y1413	G960	Y1413	T889	F819	T761	L639	D541	T352
GLN	I1529	GLN	I1529	P1466	A1138	I1138	A1138	T891	S820	P762	L639	D541	T352
CYS	V1530	CYS	V1530	A1467	E970	T892	E970	T891	I821	V763	L639	D541	T352
THR	T1531	THR	T1531	G1468	S971	T892	S971	A893	A822	A764	L639	D541	T352
CYS	G1532	CYS	G1532	F1470	A972	A972	A972	V894	G823	G765	L639	D541	T352
GLN	P1533	GLN	P1533	A1471	T973	D1145	T973	A895	Y824	G766	L639	D541	T352
THR	D1534	THR	D1534	S1472	A974	D1145	A974	A896	Y825	A767	L639	D541	T352
GLY	T1535	GLY	T1535	A1473	A975	T1160	A975	G897	T826	A768	L639	D541	T352
GLY	M1536	GLY	M1536	P1474	L978	T1160	L978	G898	A827	A769	L639	D541	T352
GLY	F1537	GLY	F1537	G1475	L978	T1160	L978	G899	T828	V770	L639	D541	T352
GLY	M1539	GLY	M1539	T1477	L978	T1160	L978	G901	P829	A771	L639	D541	T352
GLY	C1479	GLY	C1479	C1479	L978	T1160	L978	P902	Y832	M771	L639	D541	T352





P1906	P1907	P1908	R1909	P1910	P1911	P1912	P1913	P1914	P1915	P1916	P1917	P1918	S1919	P1920	P1921	P1922	P1923	N1924	N1925	P1926	P1927	P1928	P1929	P1930	P1931	P1932	A1933	S1934	S1935	S1936	S1937	N1938	P1939	G1940	G1941	GLY	VAL	ASN	GLN	ASN	GLY	ASP	PRO	VAL	GLY	HIS	ARG	ARG	ALA	ALA	ILE	LEU	SER	SER	LEU	LEU	MET	GLU	ASP	GLU	ASP	ALA																									
T1229	L1832	S1841	S1844	P1855	P1856	P1857	P1858	S1859	P1860	S1861	P1862	P1863	P1864	P1865	P1866	P1867	P1868	S1869	P1870	R1871	P1872	P1873	S1874	P1875	M1876	P1877	P1878	S1879	P1880	R1881	P1882	P1883	S1884	P1885	P1887	P1888	S1889	P1890	M1891	P1892	P1893	P1894	T1895	S1896	P1897	P1898	P1899	S1900	P1901	P1902	P1903	S1904	P1905	T1416	S1460	C1479	D1507	R1512	T1515	P1523	K1527	D1534	M1539	T1548	V1558	T1648	T1677	T1678	T1721	Y1725	C1730	T1737	V1738	K1741	S1744	Y1773	D1786	E1787	F1788	Y1799	R1805	V1808	D1818	L1819	G1820	G1821	G1822
L1258	T1259	A1260	R1261	A1262	K1263	Y1264	S1265	T1266	D1267	P1268	T1269	L1270	Y1271	H1272	F1273	T1274	T1275	H1276	L1277	A1278	M1279	G1280	P1281	E1282	S1283	C1284	K1285	K1286	K1289	M1295	I1296	A1297	G1298	C1317	T1318	G1331	T1332	T1333	T1334	E1337	D1342	D1345	T1346	F1347	H1350	T1387	S1398	Y1413																																							
N1194	Y1195	T1196	N1197	G1198	P1199	R1200	Y1201	A1202	V1203	D1204	A1205	Y1206	P1207	Y1208	P1209	V1210	G1211	Q1212	C1213	R1214	K1215	C1216	P1217	G1218	G1219	T1220	A1221	T1222	M1223	D1224	G1225	Y1226	R1227	C1228	I1229	P1230	C1231	P1232	S1233	G1234	S1237	N1238	E1239	G1240	A1241	R1242	C1243	C1244	T1245	A1246	C1247	P1248	A1249	K1254	P1255	A1256	A1257																														
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● Molecule 1: Mst1



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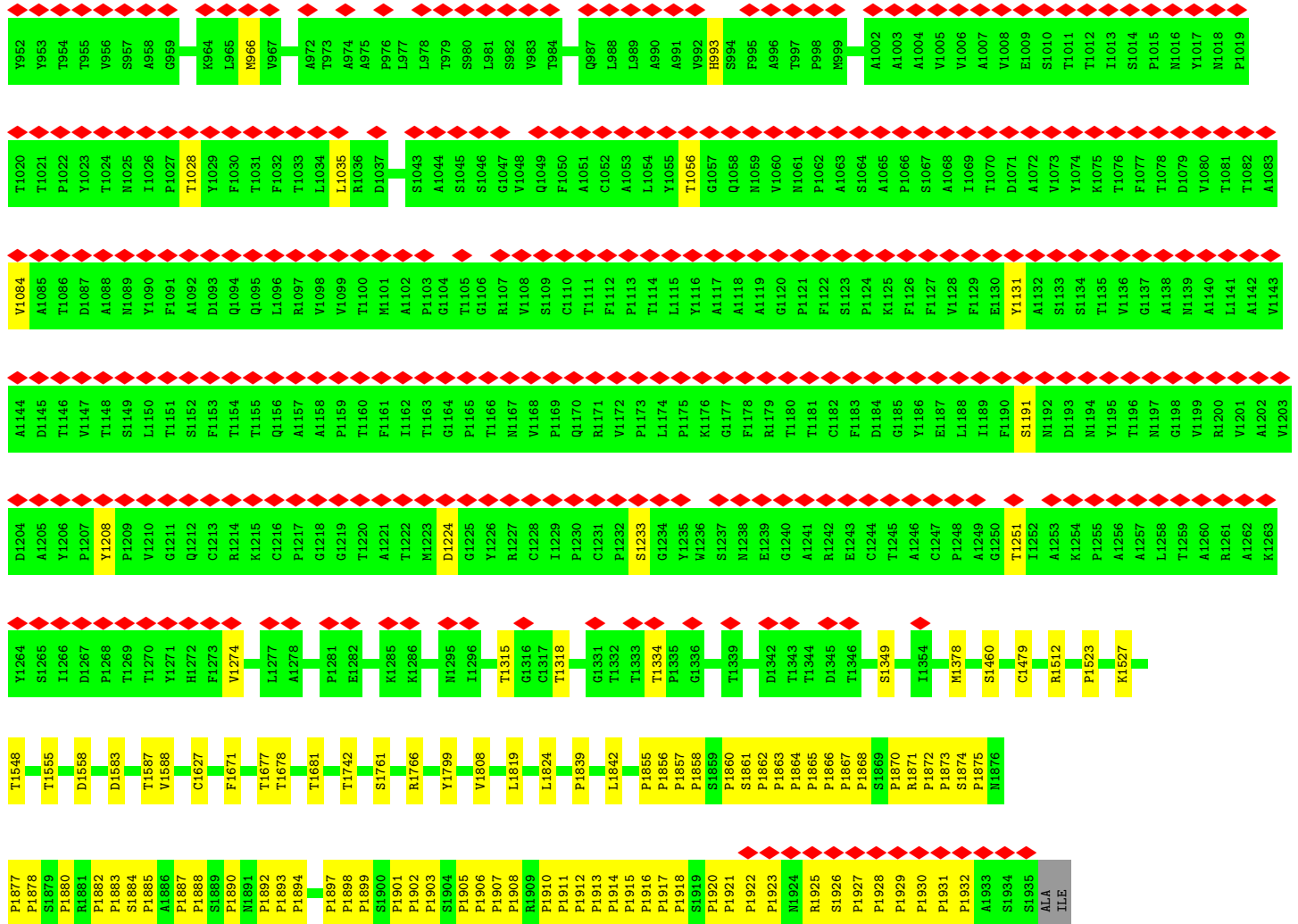
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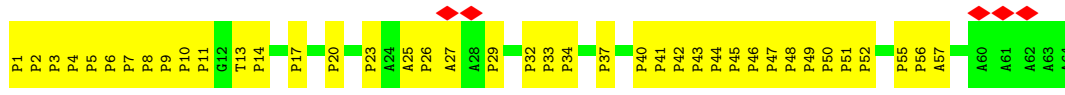
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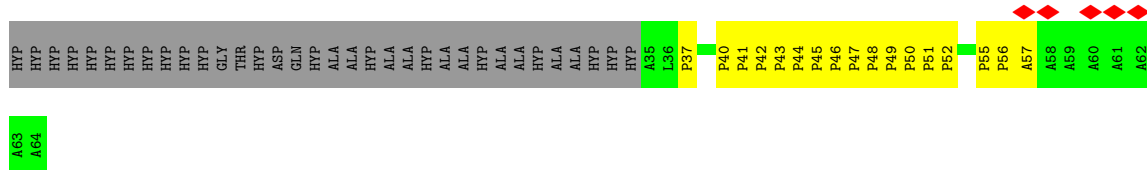
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L951



• Molecule 2: Mstax



• Molecule 2: Mstax



• Molecule 2: Mstax



• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranos e



• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranos e



• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranos e



• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranos e



• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranos e



• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranos e





- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain V: 67% 33%



- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain b: 67% 33%



- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain e: 67% 33%



- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain l: 100%



- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain m: 100%



- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain t: 67% 33%



- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain w:  67% 33%

FUB1  
FUB2  
FUB3

- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain x:  33% 67%

FUB1  
FUB2  
FUB3

- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain y:  67% 33%

FUB1  
FUB2  
FUB3

- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain z:  67% 33%

FUB1  
FUB2  
FUB3

- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 0:  67% 33%

FUB1  
FUB2  
FUB3

- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 1:  67% 33%

FUB1  
FUB2  
FUB3

- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 2:  67% 33%

FUB1  
FUB2  
FUB3

- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain HA:  33% 67%



- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain IA:  67% 33%



- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain MA:  100%



- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain NA:  33% 67%



- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain OA:  67% 33%

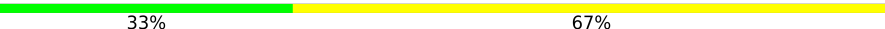


- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain RA:  67% 33%



- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain TA:  33% 67%





- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain uA:  67% 33%



- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain vA:  67% 33%



- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain wA:  67% 33%



- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain xA:  100%



- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain yA:  67% 33%



- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain zA:  100%



- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 0A:  67% 33%



- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose





- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose





- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

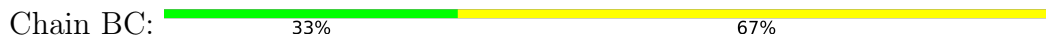


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- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain NC:  100%

FUB1  
FUB2  
FUB3

- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain TC:  100%

FUB1  
FUB2  
FUB3

- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain WC:  33% 67%

FUB1  
FUB2  
FUB3

- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain dC:  67% 33%

FUB1  
FUB2  
FUB3

- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain eC:  100%

FUB1  
FUB2  
FUB3

- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain IC:  100%


FUB1  
FUB2  
FUB3

- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain oC:  33% 100%

FUB1  
FUB2  
FUB3

- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain pC:  33% 67%



- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain qC:  100%



- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain rC:  100% 67% 33%



- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain sC:  100% 33% 67%



- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain tC:  33% 67% 33%



- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain uC:  67% 67% 33%






- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 8C:  100%

FUB1  
FUB2  
FUB3

- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 9C:  33% 67%

FUB1  
FUB2  
FUB3

- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain DD:  67% 33%

FUB1  
FUB2  
FUB3

- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain ED:  67% 33%

FUB1  
FUB2  
FUB3

- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain FD:  67% 33%

FUB1  
FUB2  
FUB3

- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain ID:  67% 33%

FUB1  
FUB2  
FUB3

- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain KD:  67% 33%



- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain QD: 100%



- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain TD: 100%



- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain aD: 33% 100%



- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain bD: 100%



- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain iD: 67% 33%



- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain lD: 67% 100%



- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose




- Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain L:  75% 25%




- Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain W:  75% 25%



- Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain X:  75% 25%



- Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain Z:  25% 75%

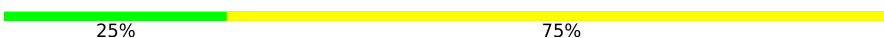


- Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain c:  75% 25%



- Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain d:  25% 75%



- Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain g:  75% 25%

FUB1  
FUB2  
FUB3  
AHR4

- Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain k:  100%

FUB1  
FUB2  
FUB3  
AHR4

- Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain r:  100%


FUB1  
FUB2  
FUB3  
AHR4

- Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain v:  75% 25%


FUB1  
FUB2  
FUB3  
AHR4

- Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain JA:  75% 25%


FUB1  
FUB2  
FUB3  
AHR4

- Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain UA:  75% 25%

FUB1  
FUB2  
FUB3  
AHR4

- Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain VA:  75% 25%



- Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain aA:  100%



- Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain bA:  100%



- Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain eA:  100%



- Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain iA:  50% 50%



- Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain pA:  100%



- Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain tA:  50% 50%



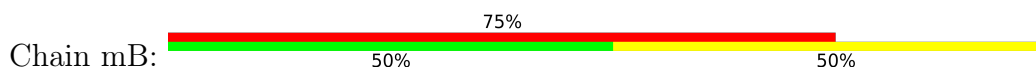
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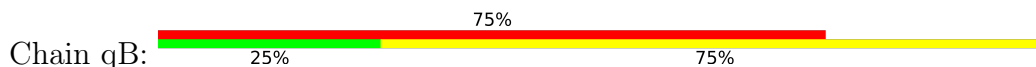
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- Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



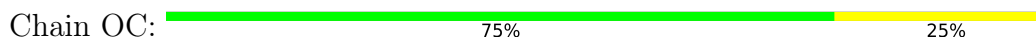
- Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose




- Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



- Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose




- Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain PC:  75% 25%



- Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain RC:  75% 25%




- Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain UC:  100%



- Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain VC:  75% 25%



- Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain YC:  50% 50%




- Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain cC:  50% 50%



- Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



Chain jC:  75% 25%



- Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain nC:  25% 50% 50%



- Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain AD:  50% 50%



- Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain LD:  50% 50%



- Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain MD:  100%



- Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain OD:  50% 50%



- Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain RD:  50% 50%



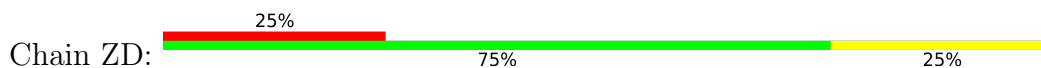
- Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



- Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



- Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



- Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



- Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



- Molecule 5: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose





- Molecule 5: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose



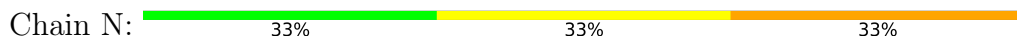
- Molecule 5: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose



- Molecule 5: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose



- Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



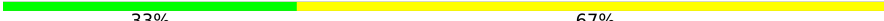
- Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



- Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



- Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 8:  33% 67%

FUB1  
FUB2  
GZL3

- Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranos e

Chain 9:  33% 67%

FUB1  
FUB2  
GZL3

- Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranos e

Chain AA:  33% 67%

FUB1  
FUB2  
GZL3

- Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranos e

Chain EA:  33% 67%

FUB1  
FUB2  
GZL3

- Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranos e

Chain LA:  33% 33% 33%

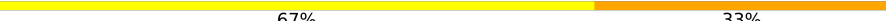
FUB1  
FUB2  
GZL3

- Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranos e

Chain PA:  67% 33%

FUB1  
FUB2  
GZL3

- Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranos e

Chain 3A:  67% 33%

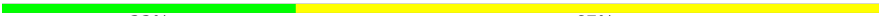
FUB1  
FUB2  
GZL3

- Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 6A:  33% 67%


  
FUB1  
FUB2  
GZL3

- Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 7A:  33% 67%

  
FUB1  
FUB2  
GZL3

- Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 8A:  100%

  
FUB1  
FUB2  
GZL3

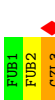
- Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain CB:  33% 67%


  
FUB1  
FUB2  
GZL3

- Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain XB:  33% 33% 33% 33%

  
FUB1  
FUB2  
GZL3

- Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain aB:  33% 67%


  
FUB1  
FUB2  
GZL3

- Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain bB:  100%

FUB1  
FUB2  
GZL3

- Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain cB:  100%

FUB1  
FUB2  
GZL3

- Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain gB:  67% 33%

FUB1  
FUB2  
GZL3

- Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 0B:  33% 33% 33%

FUB1  
FUB2  
GZL3

- Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 3B:  100%

FUB1  
FUB2  
GZL3

- Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 4B:  33% 67%

FUB1  
FUB2  
GZL3

- Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 5B:  33% 67%


FUB1  
FUB2  
GZL3

- Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 9B:  33% 67%


  
FUB1  
FUB2  
GZL3

- Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain FC:  100%

  
FUB1  
FUB2  
GZL3

- Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain JC:  33% 67%

  
FUB1  
FUB2  
GZL3

- Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain xC:  100%  
67% 33%

  
FUB1  
FUB2  
GZL3

- Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 0C:  100%  
33% 67%

  
FUB1  
FUB2  
GZL3

- Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 1C:  100%  
67% 33%

  
FUB1  
FUB2  
GZL3

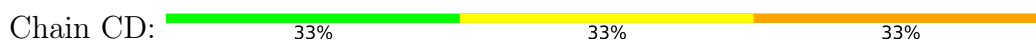
- Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



- Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



- Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



- Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



- Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



- Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



- Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose







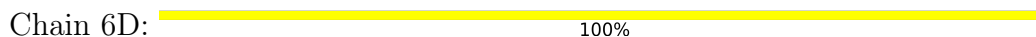
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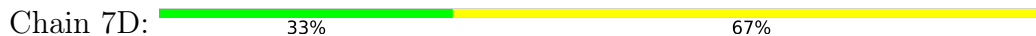
- Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



- Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



- Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



- Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



- Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

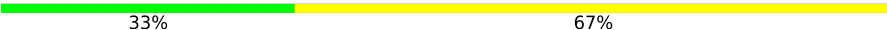


- Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain OE:  67% 33%

FUB1  
FUB2  
GZL3

- Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain ZE:  33% 67%

FUB1  
FUB2  
GZL3

- Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain bE:  67% 33%

FUB1  
FUB2  
GZL3

- Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain mE:  33% 67%


FUB1  
FUB2  
GZL3

- Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain nE:  33% 67%

FUB1  
FUB2  
GZL3

- Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain oE:  33% 67%

FUB1  
FUB2  
GZL3

- Molecule 7: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain S:  25% 75%



- Molecule 7: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranos e-(1-3)]beta-L-arabinofuranose

Chain f: 25% 75%



- Molecule 7: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranos e-(1-3)]beta-L-arabinofuranose

Chain h: 75% 25%



- Molecule 7: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranos e-(1-3)]beta-L-arabinofuranose

Chain QA: 50% 50%



- Molecule 7: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranos e-(1-3)]beta-L-arabinofuranose

Chain dA: 50% 50%



- Molecule 7: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranos e-(1-3)]beta-L-arabinofuranose

Chain fA: 100%



- Molecule 7: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranos e-(1-3)]beta-L-arabinofuranose

Chain KC: 50% 50%



- Molecule 7: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain XC:  75% 25%



- Molecule 7: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain ZC:  75% 25%




- Molecule 7: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain HD:  50% 50%




- Molecule 7: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain UD:  75% 25%

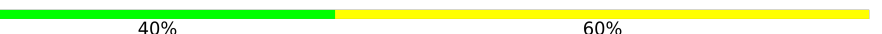


- Molecule 7: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain WD:  75% 25%




- Molecule 8: alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain U:  40% 60%



- Molecule 8: alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain SA:  80% 20%




- Molecule 8: alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain MC:  40% 60%



- Molecule 8: alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain JD:  80% 20%



- Molecule 9: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain Y:  100%



- Molecule 9: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain j:  50% 50%



- Molecule 9: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain WA:  100%



- Molecule 9: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain hA:  50% 50%



- Molecule 9: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain QC:  100%

FUB1  
FUB2

- Molecule 9: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain bC:  100%

FUB1  
FUB2

- Molecule 9: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain ND:  50% 50%

FUB1  
FUB2

- Molecule 9: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain YD:  100%

FUB1  
FUB2

- Molecule 10: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain a:  20% 80%

FUB1  
FUB2  
FUB3  
AHR4  
AHR5

- Molecule 10: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain u:  60% 40%


FUB1  
FUB2  
FUB3  
AHR4  
AHR5

- Molecule 10: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain 3:  40% 60%

FUB1  
FUB2  
FUB3  
AHR4  
AHR5

- Molecule 10: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain YA:  80% 20%



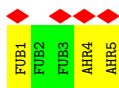
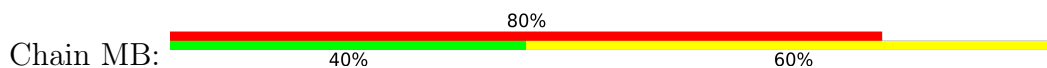
- Molecule 10: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose



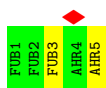
- Molecule 10: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose



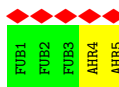
- Molecule 10: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose



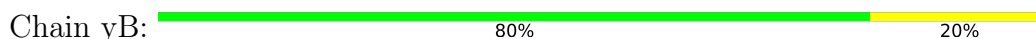
- Molecule 10: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose



- Molecule 10: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

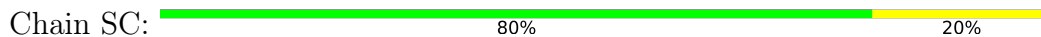


- Molecule 10: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

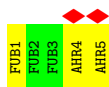




- Molecule 10: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose



- Molecule 10: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose



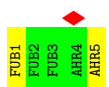
- Molecule 10: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose



- Molecule 10: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose



- Molecule 10: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose



- Molecule 10: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose







- Molecule 11: alpha-L-arabinofuranose-(1-3)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose

Chain i: 100%



- Molecule 11: alpha-L-arabinofuranose-(1-3)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose

Chain gA: 33% 67%



- Molecule 11: alpha-L-arabinofuranose-(1-3)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose

Chain aC: 33% 67%



- Molecule 11: alpha-L-arabinofuranose-(1-3)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose

Chain XD: 100%



- Molecule 12: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain n: 40% 40% 20%



- Molecule 12: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

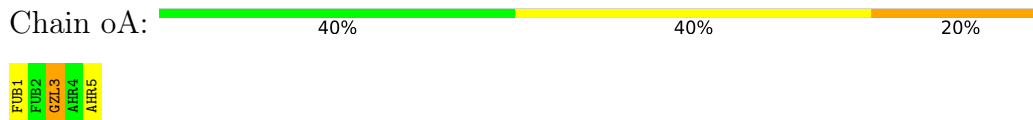
Chain q: 20% 60% 20%



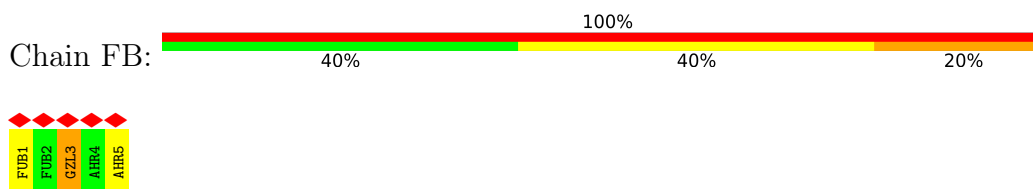
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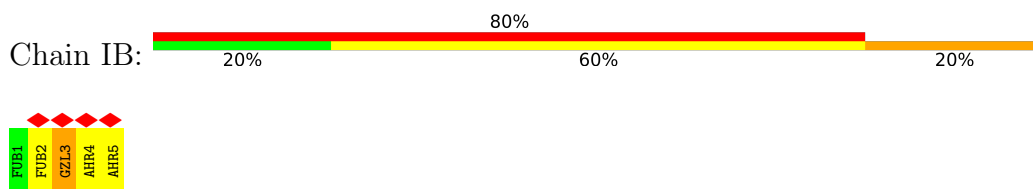
- Molecule 12: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose



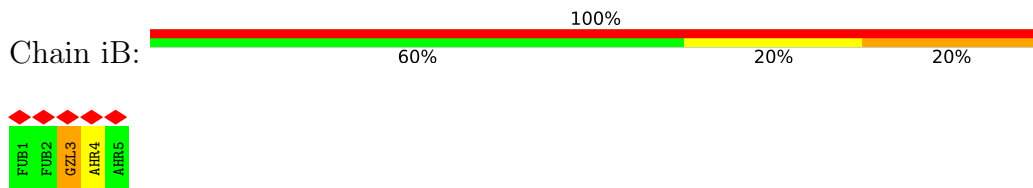
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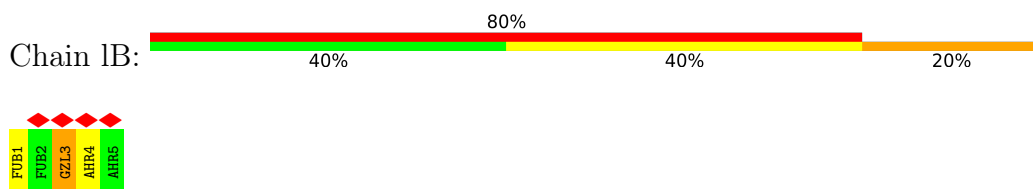
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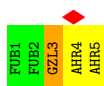
- Molecule 12: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose



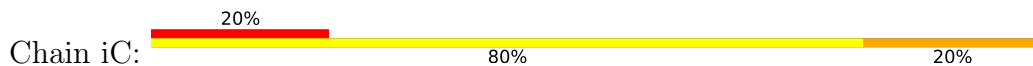
- Molecule 12: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose



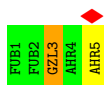
- Molecule 12: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose



- Molecule 12: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose



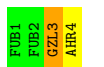
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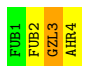
- Molecule 12: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose



- Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



- Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



- Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 6:  50% 50%



- Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 7:  50% 50%



- Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain BA:  50% 50%




- Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain mA:  50% 25% 25%



- Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 2A:  75% 25%



- Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 4A:  50% 50%



- Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 5A:  50% 50%




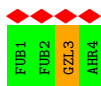
- Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranos e-(1-2)-beta-L-arabinofuranose

Chain 9A:  50% 50%



- Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranos e-(1-2)-beta-L-arabinofuranose

Chain GB:  100% 75% 25%



- Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranos e-(1-2)-beta-L-arabinofuranose

Chain WB:  25% 25% 50% 25%




- Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranos e-(1-2)-beta-L-arabinofuranose

Chain YB:  50% 50%



- Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranos e-(1-2)-beta-L-arabinofuranose

Chain ZB:  75% 25%

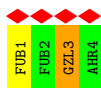


- Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranos e-(1-2)-beta-L-arabinofuranose

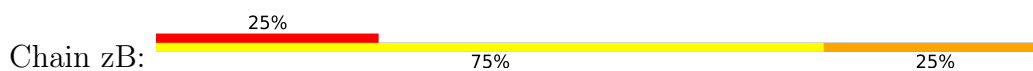
Chain dB:  50% 50%



- Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



- Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



- Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



- Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



- Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

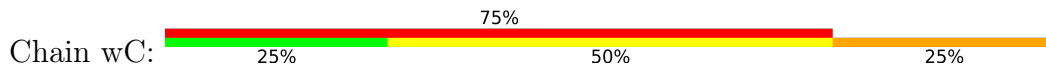


- Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose





- Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranos e-(1-2)-beta-L-arabinofuranose



- Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranos e-(1-2)-beta-L-arabinofuranose



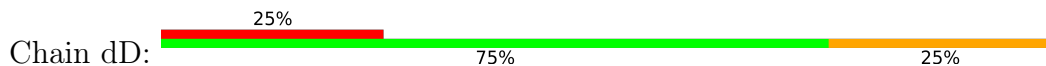
- Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranos e-(1-2)-beta-L-arabinofuranose



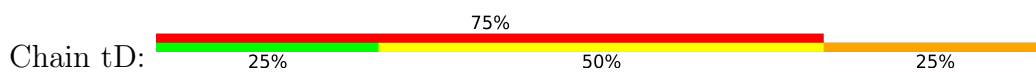
- Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranos e-(1-2)-beta-L-arabinofuranose



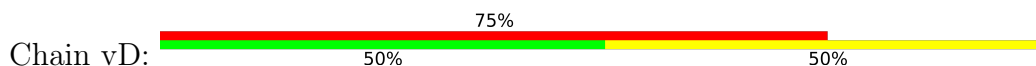
- Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranos e-(1-2)-beta-L-arabinofuranose



- Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranos e-(1-2)-beta-L-arabinofuranose



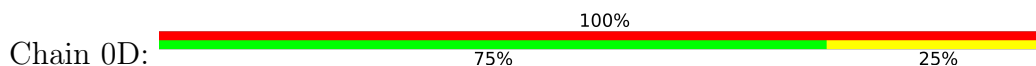
- Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



- Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



- Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



- Molecule 14: beta-L-arabinofuranose-(1-5)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose




- Molecule 14: beta-L-arabinofuranose-(1-5)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose




- Molecule 14: beta-L-arabinofuranose-(1-5)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



Chain nA:  75% 25%



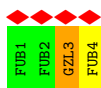
- Molecule 14: beta-L-arabinofuranose-(1-5)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain qA:  75% 25%



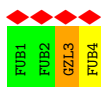
- Molecule 14: beta-L-arabinofuranose-(1-5)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain HB:  100% 50% 25% 25%



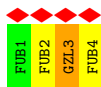
- Molecule 14: beta-L-arabinofuranose-(1-5)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain KB:  100% 50% 25% 25%

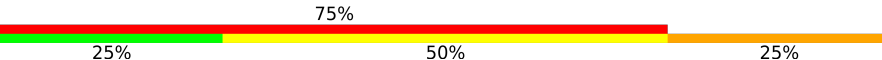


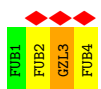
- Molecule 14: beta-L-arabinofuranose-(1-5)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain kB:  100% 25% 50% 25%



- Molecule 14: beta-L-arabinofuranose-(1-5)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain nB:  75% 25% 50% 25%



- Molecule 14: beta-L-arabinofuranose-(1-5)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain hC:  50% 25% 25%



- Molecule 14: beta-L-arabinofuranose-(1-5)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain kC:  50% 25% 25%



- Molecule 14: beta-L-arabinofuranose-(1-5)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain eD:  50% 25% 25%



- Molecule 14: beta-L-arabinofuranose-(1-5)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain hD:  25% 50% 25%

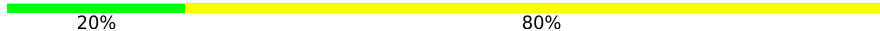


- Molecule 15: alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain CA:  40% 60%



- Molecule 15: alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain DA:  20% 80%



- Molecule 15: alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain AB:  20% 80%



- Molecule 15: alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain BB: 



- Molecule 15: alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain eB: 



- Molecule 15: alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain fB: 



- Molecule 15: alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 7B: 



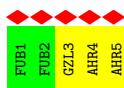
- Molecule 15: alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 8B: 

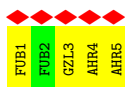


- Molecule 15: alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

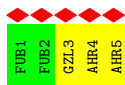
Chain 4C: 



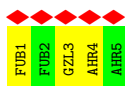
- Molecule 15: alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



- Molecule 15: alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



- Molecule 15: alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



- Molecule 16: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 16: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



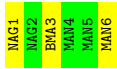
- Molecule 16: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



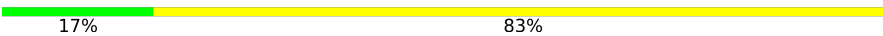
- Molecule 17: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-aceta

mido-2-deoxy-beta-D-glucopyranose

Chain GA:  50% 50%



- Molecule 17: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain DB:  17% 83%



- Molecule 17: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 7C:  50% 50%



- Molecule 17: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 5D:  50% 50%




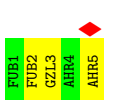
- Molecule 18: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain 9D:  20% 80%

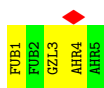


- Molecule 18: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain BE:  20% 40% 60%



- Molecule 18: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose



- Molecule 18: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose



- Molecule 18: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose



- Molecule 18: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose



- Molecule 18: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose



- Molecule 18: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose



- Molecule 18: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain cE:  60% 40%



- Molecule 18: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain fE:  40% 60%



- Molecule 18: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain pE:  100%



- Molecule 18: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain rE:  20% 40% 60%



- Molecule 18: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain tE:  40% 60%



- Molecule 18: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain yE:  20% 40% 60%



- Molecule 18: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

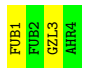
Chain zE:  20% 60% 40%



- Molecule 18: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose



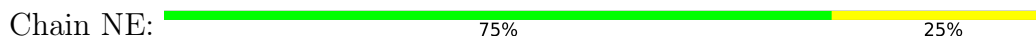
- Molecule 19: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose



- Molecule 19: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose



- Molecule 19: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose



- Molecule 19: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose



- Molecule 19: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose



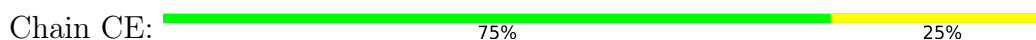




- Molecule 19: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose



- Molecule 20: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



- Molecule 20: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



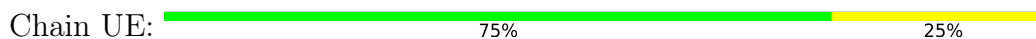
- Molecule 20: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



- Molecule 20: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



- Molecule 20: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



- Molecule 20: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain WE:  50% 50%




- Molecule 20: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain gE:  50% 50%




- Molecule 20: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain hE:  75% 25%



- Molecule 20: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain jE:  75% 25%



- Molecule 20: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain sE:  25% 75%



- Molecule 20: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain uE:  50% 50%



- Molecule 20: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain xE:  50% 50%

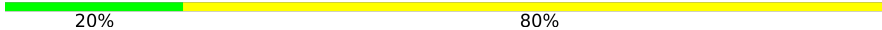
FUB1  
FUB2  
GZL3  
AHR4

- Molecule 21: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)][alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose

Chain FE:  20% 80%

FUB1  
FUB2  
GZL3  
AHR4  
AHR5

- Molecule 21: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)][alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose

Chain kE:  20% 80%

FUB1  
FUB2  
GZL3  
AHR4  
AHR5

- Molecule 21: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)][alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose

Chain vE:  40% 60%

FUB1  
FUB2  
GZL3  
AHR4  
AHR5

- Molecule 22: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain GE:  33% 67%

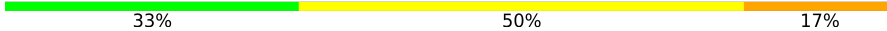
FUB1  
FUB2  
GZL3  
AHR4  
AHR5  
AHR6

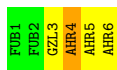
- Molecule 22: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain QE:  17% 33% 67%

FUB1  
FUB2  
GZL3  
AHR4  
AHR5  
AHR6

- Molecule 22: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain RE:  33% 50% 17%




- Molecule 22: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain VE:  33% 67%



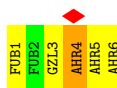
- Molecule 22: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain dE:  17% 83%



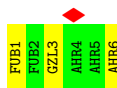
- Molecule 22: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain eE:  17% 17% 67% 17%



- Molecule 22: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain iE:  17% 50% 50%

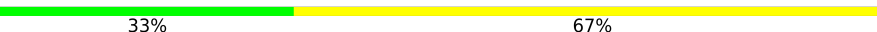


- Molecule 22: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain wE:  67% 33%

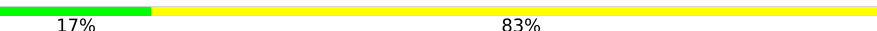


- Molecule 23: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)][alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose

Chain XE:  33% 67%

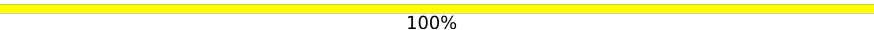
FUB1  
FUB2  
GZL3  
AHR4  
AHR5  
AHR6

- Molecule 24: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)][alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose

Chain YE:  17% 83%

FUB1  
FUB2  
GZL3  
AHR4  
AHR5  
AHR6

- Molecule 24: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)][alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose

Chain IE:  100%

FUB1  
FUB2  
GZL3  
AHR4  
AHR5  
AHR6

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	69065	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.527	Depositor
Minimum map value	-0.673	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.043	Depositor
Recommended contour level	0.23	Depositor
Map size ( $\text{\AA}$ )	554.24, 554.24, 554.24	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.0825, 1.0825, 1.0825	Depositor

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, FUB, AHR, MAN, CA, GLA, GZL, HYP, BMA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.29	0/13724	0.54	2/18848 (0.0%)
1	B	0.29	0/13724	0.54	3/18848 (0.0%)
1	C	0.27	0/10873	0.51	0/14984
1	D	0.27	0/11422	0.53	2/15734 (0.0%)
1	E	0.27	0/10283	0.51	0/14106
1	F	0.31	2/10246 (0.0%)	0.56	4/14055 (0.0%)
2	G	0.25	0/139	0.58	0/174
2	H	0.21	0/69	0.43	0/89
2	I	0.23	0/71	0.45	0/87
All	All	0.28	2/70551 (0.0%)	0.53	11/96925 (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	A	0	2
1	B	0	1
1	E	0	2
1	F	0	1
2	G	2	0
2	I	2	0
All	All	4	6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	632	PRO	CB-CG	-10.50	0.97	1.50
1	F	632	PRO	CG-CD	-9.54	1.19	1.50

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	632	PRO	N-CD-CG	-16.73	78.11	103.20
1	F	632	PRO	CB-CG-CD	14.79	164.20	106.50
1	F	632	PRO	CA-CB-CG	-13.73	77.91	104.00
1	B	1846	PRO	CA-N-CD	-12.21	94.40	111.50
1	A	1839	PRO	CA-N-CD	-11.07	96.00	111.50

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	G	23	HYP	CA
2	G	26	HYP	CA
2	I	23	HYP	CA
2	I	26	HYP	CA

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1522	GLY	Peptide
1	A	1527	LYS	Peptide
1	B	1527	LYS	Peptide
1	E	1527	LYS	Peptide
1	E	1725	TYR	Peptide

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

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

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1848/1987 (93%)	1690 (92%)	150 (8%)	8 (0%)	34 72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	1848/1987 (93%)	1691 (92%)	150 (8%)	7 (0%)	34	72
1	C	1461/1987 (74%)	1342 (92%)	115 (8%)	4 (0%)	41	76
1	D	1531/1987 (77%)	1411 (92%)	114 (7%)	6 (0%)	34	72
1	E	1390/1987 (70%)	1289 (93%)	97 (7%)	4 (0%)	41	76
1	F	1384/1987 (70%)	1273 (92%)	108 (8%)	3 (0%)	47	82
2	G	27/64 (42%)	17 (63%)	6 (22%)	4 (15%)	0	1
2	H	12/64 (19%)	11 (92%)	0	1 (8%)	1	4
2	I	14/64 (22%)	9 (64%)	3 (21%)	2 (14%)	0	1
All	All	9515/12114 (78%)	8733 (92%)	743 (8%)	39 (0%)	38	72

5 of 39 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	585	ALA
1	A	1523	PRO
1	B	1523	PRO
1	E	1523	PRO
1	F	1523	PRO

### 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	A	1451/1514 (96%)	1314 (91%)	137 (9%)	8	32
1	B	1451/1514 (96%)	1331 (92%)	120 (8%)	11	39
1	C	1149/1514 (76%)	1064 (93%)	85 (7%)	13	44
1	D	1209/1514 (80%)	1099 (91%)	110 (9%)	9	34
1	E	1081/1514 (71%)	1005 (93%)	76 (7%)	15	47
1	F	1078/1514 (71%)	1009 (94%)	69 (6%)	17	51
2	G	5/5 (100%)	5 (100%)	0	100	100
2	H	2/5 (40%)	2 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	I	3/5 (60%)	2 (67%)	1 (33%)	0	1
All	All	7429/9099 (82%)	6831 (92%)	598 (8%)	16	40

5 of 598 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	846	SER
1	F	1558	ASP
1	E	1078	THR
1	E	824	TYR
1	E	1844	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	1672	GLN
1	D	1212	GLN
1	B	1536	ASN
1	C	612	GLN
1	B	1293	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](#)

358 non-standard protein/DNA/RNA residues 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	HYP	I	17	2	6,8,9	0.43	0	5,10,12	1.20	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	HYP	A	1865	1	6,8,9	0.51	0	5,10,12	1.65	1 (20%)
2	HYP	I	20	2	6,8,9	0.49	0	5,10,12	1.27	1 (20%)
1	HYP	E	1858	1	6,8,9	0.51	0	5,10,12	1.67	1 (20%)
1	HYP	E	1860	1	6,8,9	0.55	0	5,10,12	1.86	3 (60%)
1	HYP	A	1930	1	6,8,9	0.52	0	5,10,12	1.66	1 (20%)
1	HYP	D	1899	1	6,8,9	0.46	0	5,10,12	1.70	2 (40%)
1	HYP	B	1905	1	6,8,9	0.39	0	5,10,12	1.19	1 (20%)
1	HYP	B	1912	1	6,8,9	0.38	0	5,10,12	1.24	1 (20%)
1	HYP	A	1929	1	6,8,9	0.40	0	5,10,12	1.24	1 (20%)
2	HYP	G	56	2	6,8,9	0.44	0	5,10,12	1.25	1 (20%)
2	HYP	G	4	2	6,8,9	0.52	0	5,10,12	1.38	1 (20%)
2	HYP	G	52	2	6,8,9	0.51	0	5,10,12	1.65	1 (20%)
1	HYP	A	1927	1	6,8,9	0.52	0	5,10,12	1.41	1 (20%)
1	HYP	D	1927	1	6,8,9	0.41	0	5,10,12	1.20	1 (20%)
1	HYP	F	1920	1	6,8,9	0.54	0	5,10,12	1.55	1 (20%)
1	HYP	A	1883	1	6,8,9	0.50	0	5,10,12	2.15	2 (40%)
1	HYP	E	1857	1	6,8,9	0.52	0	5,10,12	1.56	1 (20%)
2	HYP	H	51	2	6,8,9	0.50	0	5,10,12	1.62	1 (20%)
1	HYP	A	1863	1	6,8,9	0.48	0	5,10,12	1.36	1 (20%)
2	HYP	G	17	2	6,8,9	0.37	0	5,10,12	1.26	1 (20%)
1	HYP	D	1918	1	6,8,9	0.49	0	5,10,12	1.82	2 (40%)
2	HYP	G	47	2	6,8,9	0.39	0	5,10,12	1.27	1 (20%)
2	HYP	I	4	2	6,8,9	0.49	0	5,10,12	1.27	1 (20%)
1	HYP	A	1921	1	6,8,9	0.40	0	5,10,12	1.37	1 (20%)
2	HYP	G	14	2	6,8,9	0.39	0	5,10,12	1.32	1 (20%)
1	HYP	C	1899	1	6,8,9	0.37	0	5,10,12	1.28	1 (20%)
1	HYP	C	1906	1	6,8,9	0.40	0	5,10,12	1.16	1 (20%)
1	HYP	E	1911	1	6,8,9	0.41	0	5,10,12	1.22	1 (20%)
2	HYP	H	50	2	6,8,9	0.38	0	5,10,12	1.20	1 (20%)
1	HYP	A	1875	1	6,8,9	0.45	0	5,10,12	1.19	1 (20%)
1	HYP	A	1928	1	6,8,9	0.42	0	5,10,12	1.13	1 (20%)
1	HYP	A	1923	1	6,8,9	0.52	0	5,10,12	1.88	3 (60%)
1	HYP	B	1856	1	6,8,9	0.49	0	5,10,12	1.26	1 (20%)
1	HYP	E	1931	1	6,8,9	0.43	0	5,10,12	1.32	1 (20%)
2	HYP	I	7	2	6,8,9	0.50	0	5,10,12	1.63	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	HYP	A	1916	1	6,8,9	0.52	0	5,10,12	1.45	1 (20%)
1	HYP	E	1870	1	6,8,9	0.48	0	5,10,12	1.56	2 (40%)
1	HYP	A	1887	1	6,8,9	0.41	0	5,10,12	1.23	1 (20%)
1	HYP	D	1928	1	6,8,9	0.43	0	5,10,12	1.13	1 (20%)
1	HYP	E	1913	1	6,8,9	0.36	0	5,10,12	1.18	1 (20%)
1	HYP	B	1892	1	6,8,9	0.37	0	5,10,12	1.23	1 (20%)
1	HYP	A	1885	1	6,8,9	0.38	0	5,10,12	1.20	1 (20%)
1	HYP	F	1906	1	6,8,9	0.42	0	5,10,12	1.30	1 (20%)
1	HYP	B	1867	1	6,8,9	0.49	0	5,10,12	1.64	1 (20%)
1	HYP	E	1898	1	6,8,9	0.41	0	5,10,12	1.18	1 (20%)
1	HYP	A	1914	1	6,8,9	0.50	0	5,10,12	1.38	1 (20%)
1	HYP	E	1912	1	6,8,9	0.46	0	5,10,12	1.27	1 (20%)
1	HYP	B	1921	1	6,8,9	0.40	0	5,10,12	1.22	1 (20%)
1	HYP	B	1866	1	6,8,9	0.48	0	5,10,12	1.30	1 (20%)
1	HYP	E	1921	1	6,8,9	0.38	0	5,10,12	1.31	1 (20%)
1	HYP	A	1873	1	6,8,9	0.47	0	5,10,12	1.21	1 (20%)
2	HYP	I	34	2	6,8,9	0.50	0	5,10,12	1.61	1 (20%)
1	HYP	E	1899	1	6,8,9	0.37	0	5,10,12	1.29	1 (20%)
1	HYP	B	1893	1	6,8,9	0.40	0	5,10,12	1.23	1 (20%)
1	HYP	D	1910	1	6,8,9	0.43	0	5,10,12	1.14	1 (20%)
2	HYP	G	40	2	6,8,9	0.39	0	5,10,12	1.14	1 (20%)
1	HYP	C	1930	1	6,8,9	0.53	0	5,10,12	1.72	1 (20%)
1	HYP	B	1920	1	6,8,9	0.53	0	5,10,12	1.37	1 (20%)
2	HYP	G	42	2	6,8,9	0.37	0	5,10,12	1.25	1 (20%)
1	HYP	F	1868	1	6,8,9	0.52	0	5,10,12	2.02	3 (60%)
1	HYP	E	1894	1	6,8,9	0.38	0	5,10,12	1.25	1 (20%)
1	HYP	F	1903	1	6,8,9	0.55	0	5,10,12	1.70	2 (40%)
2	HYP	I	29	2	6,8,9	0.43	0	5,10,12	1.20	1 (20%)
1	HYP	E	1887	1	6,8,9	0.44	0	5,10,12	1.22	1 (20%)
2	HYP	H	56	2	6,8,9	0.44	0	5,10,12	1.24	1 (20%)
1	HYP	F	1865	1	6,8,9	0.55	0	5,10,12	1.64	1 (20%)
2	HYP	G	41	2	6,8,9	0.41	0	5,10,12	1.20	1 (20%)
1	HYP	B	1899	1	6,8,9	0.38	0	5,10,12	1.42	1 (20%)
1	HYP	F	1902	1	6,8,9	0.50	0	5,10,12	1.69	1 (20%)
1	HYP	F	1929	1	6,8,9	0.43	0	5,10,12	1.19	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	HYP	B	1914	1	6,8,9	0.47	0	5,10,12	1.52	1 (20%)
1	HYP	E	1872	1	6,8,9	0.52	0	5,10,12	1.27	1 (20%)
1	HYP	E	1914	1	6,8,9	0.50	0	5,10,12	1.25	1 (20%)
1	HYP	F	1928	1	6,8,9	0.44	0	5,10,12	1.25	1 (20%)
1	HYP	B	1890	1	6,8,9	0.45	0	5,10,12	1.19	1 (20%)
1	HYP	C	1910	1	6,8,9	0.46	0	5,10,12	1.17	1 (20%)
1	HYP	E	1862	1	6,8,9	0.53	0	5,10,12	1.47	1 (20%)
1	HYP	C	1923	1	6,8,9	0.53	0	5,10,12	1.93	2 (40%)
1	HYP	A	1910	1	6,8,9	0.39	0	5,10,12	1.15	1 (20%)
1	HYP	E	1928	1	6,8,9	0.43	0	5,10,12	1.22	1 (20%)
1	HYP	A	1898	1	6,8,9	0.42	0	5,10,12	1.21	1 (20%)
1	HYP	F	1931	1	6,8,9	0.41	0	5,10,12	1.35	1 (20%)
1	HYP	A	1920	1	6,8,9	0.53	0	5,10,12	1.55	1 (20%)
1	HYP	F	1870	1	6,8,9	0.50	0	5,10,12	1.57	1 (20%)
1	HYP	B	1917	1	6,8,9	0.54	0	5,10,12	1.65	1 (20%)
1	HYP	B	1888	1	6,8,9	0.54	0	5,10,12	1.68	2 (40%)
1	HYP	B	1931	1	6,8,9	0.46	0	5,10,12	1.41	1 (20%)
1	HYP	A	1862	1	6,8,9	0.53	0	5,10,12	1.43	1 (20%)
2	HYP	I	5	2	6,8,9	0.36	0	5,10,12	1.42	1 (20%)
1	HYP	C	1916	1	6,8,9	0.50	0	5,10,12	1.18	1 (20%)
1	HYP	F	1923	1	6,8,9	0.53	0	5,10,12	2.08	3 (60%)
2	HYP	G	11	2	6,8,9	0.48	0	5,10,12	1.93	2 (40%)
2	HYP	G	1	2	6,8,9	0.47	0	5,10,12	1.19	1 (20%)
1	HYP	A	1860	1	6,8,9	0.52	0	5,10,12	1.77	2 (40%)
1	HYP	E	1910	1	6,8,9	0.42	0	5,10,12	1.18	1 (20%)
1	HYP	B	1877	1	6,8,9	0.51	0	5,10,12	1.64	1 (20%)
1	HYP	E	1923	1	6,8,9	0.48	0	5,10,12	2.08	2 (40%)
1	HYP	F	1883	1	6,8,9	0.48	0	5,10,12	1.96	2 (40%)
2	HYP	G	37	2	6,8,9	0.45	0	5,10,12	0.96	1 (20%)
2	HYP	G	51	2	6,8,9	0.51	0	5,10,12	1.59	1 (20%)
1	HYP	E	1883	1	6,8,9	0.47	0	5,10,12	2.01	2 (40%)
1	HYP	B	1855	1	6,8,9	0.51	0	5,10,12	1.17	1 (20%)
1	HYP	F	1887	1	6,8,9	0.40	0	5,10,12	1.15	1 (20%)
1	HYP	F	1873	1	6,8,9	0.45	0	5,10,12	1.27	1 (20%)
1	HYP	F	1875	1	6,8,9	0.39	0	5,10,12	1.15	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	HYP	F	1882	1	6,8,9	0.42	0	5,10,12	1.17	1 (20%)
1	HYP	A	1902	1	6,8,9	0.54	0	5,10,12	1.60	1 (20%)
1	HYP	B	1911	1	6,8,9	0.39	0	5,10,12	1.18	1 (20%)
1	HYP	A	1931	1	6,8,9	0.49	0	5,10,12	1.41	1 (20%)
1	HYP	C	1911	1	6,8,9	0.42	0	5,10,12	1.20	1 (20%)
1	HYP	B	1932	1	6,8,9	0.51	0	5,10,12	1.55	1 (20%)
1	HYP	E	1877	1	6,8,9	0.51	0	5,10,12	1.76	2 (40%)
2	HYP	H	52	2	6,8,9	0.49	0	5,10,12	1.73	2 (40%)
1	HYP	C	1905	1	6,8,9	0.42	0	5,10,12	1.17	1 (20%)
1	HYP	B	1908	1	6,8,9	0.57	0	5,10,12	2.10	3 (60%)
2	HYP	G	49	2	6,8,9	0.51	0	5,10,12	1.48	1 (20%)
1	HYP	E	1873	1	6,8,9	0.46	0	5,10,12	1.32	1 (20%)
1	HYP	F	1864	1	6,8,9	0.51	0	5,10,12	1.43	1 (20%)
1	HYP	F	1858	1	6,8,9	0.54	0	5,10,12	1.69	1 (20%)
1	HYP	B	1880	1	6,8,9	0.42	0	5,10,12	1.34	1 (20%)
1	HYP	E	1918	1	6,8,9	0.48	0	5,10,12	1.70	2 (40%)
1	HYP	D	1908	1	6,8,9	0.54	0	5,10,12	1.70	2 (40%)
2	HYP	G	55	2	6,8,9	0.46	0	5,10,12	1.19	1 (20%)
1	HYP	C	1898	1	6,8,9	0.46	0	5,10,12	1.19	1 (20%)
1	HYP	E	1893	1	6,8,9	0.43	0	5,10,12	1.24	1 (20%)
1	HYP	D	1901	1	6,8,9	0.37	0	5,10,12	1.18	1 (20%)
2	HYP	H	44	2	6,8,9	0.50	0	5,10,12	1.63	1 (20%)
2	HYP	I	26	2	6,8,9	0.52	0	5,10,12	1.48	2 (40%)
1	HYP	C	1897	1	6,8,9	0.46	0	5,10,12	1.28	1 (20%)
1	HYP	E	1885	1	6,8,9	0.51	0	5,10,12	1.39	1 (20%)
1	HYP	B	1864	1	6,8,9	0.51	0	5,10,12	1.47	1 (20%)
1	HYP	C	1908	1	6,8,9	0.54	0	5,10,12	1.91	3 (60%)
1	HYP	E	1901	1	6,8,9	0.53	0	5,10,12	1.42	1 (20%)
1	HYP	A	1907	1	6,8,9	0.44	0	5,10,12	1.86	2 (40%)
1	HYP	A	1892	1	6,8,9	0.37	0	5,10,12	1.34	1 (20%)
1	HYP	A	1867	1	6,8,9	0.48	0	5,10,12	1.58	1 (20%)
1	HYP	D	1906	1	6,8,9	0.44	0	5,10,12	1.34	1 (20%)
2	HYP	H	46	2	6,8,9	0.48	0	5,10,12	1.60	1 (20%)
2	HYP	G	2	2	6,8,9	0.50	0	5,10,12	1.63	1 (20%)
1	HYP	C	1921	1	6,8,9	0.41	0	5,10,12	1.20	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	HYP	G	46	2	6,8,9	0.52	0	5,10,12	1.54	1 (20%)
1	HYP	C	1929	1	6,8,9	0.38	0	5,10,12	1.25	1 (20%)
2	HYP	I	6	2	6,8,9	0.35	0	5,10,12	1.29	1 (20%)
1	HYP	B	1868	1	6,8,9	0.49	0	5,10,12	1.97	2 (40%)
1	HYP	C	1902	1	6,8,9	0.54	0	5,10,12	1.77	2 (40%)
1	HYP	F	1912	1	6,8,9	0.41	0	5,10,12	1.15	1 (20%)
1	HYP	E	1908	1	6,8,9	0.54	0	5,10,12	2.07	3 (60%)
1	HYP	A	1918	1	6,8,9	0.51	0	5,10,12	1.60	1 (20%)
1	HYP	A	1858	1	6,8,9	0.38	0	5,10,12	1.22	1 (20%)
1	HYP	B	1929	1	6,8,9	0.41	0	5,10,12	1.36	1 (20%)
1	HYP	B	1913	1	6,8,9	0.38	0	5,10,12	1.31	1 (20%)
1	HYP	F	1862	1	6,8,9	0.49	0	5,10,12	1.35	1 (20%)
1	HYP	F	1927	1	6,8,9	0.39	0	5,10,12	1.14	1 (20%)
1	HYP	F	1894	1	6,8,9	0.48	0	5,10,12	1.93	2 (40%)
1	HYP	E	1927	1	6,8,9	0.40	0	5,10,12	1.19	1 (20%)
1	HYP	F	1901	1	6,8,9	0.38	0	5,10,12	1.14	1 (20%)
1	HYP	C	1931	1	6,8,9	0.44	0	5,10,12	1.38	1 (20%)
1	HYP	F	1872	1	6,8,9	0.48	0	5,10,12	1.23	1 (20%)
1	HYP	C	1917	1	6,8,9	0.53	0	5,10,12	1.46	1 (20%)
1	HYP	A	1856	1	6,8,9	0.52	0	5,10,12	1.33	1 (20%)
2	HYP	H	41	2	6,8,9	0.43	0	5,10,12	1.27	1 (20%)
1	HYP	E	1892	1	6,8,9	0.38	0	5,10,12	1.27	1 (20%)
2	HYP	G	50	2	6,8,9	0.41	0	5,10,12	1.18	1 (20%)
1	HYP	B	1897	1	6,8,9	0.43	0	5,10,12	1.14	1 (20%)
1	HYP	F	1857	1	6,8,9	0.52	0	5,10,12	1.58	1 (20%)
1	HYP	E	1867	1	6,8,9	0.53	0	5,10,12	1.78	1 (20%)
1	HYP	F	1890	1	6,8,9	0.39	0	5,10,12	1.15	1 (20%)
2	HYP	I	23	2	6,8,9	0.37	0	5,10,12	1.41	1 (20%)
2	HYP	G	29	2	6,8,9	0.41	0	5,10,12	1.21	1 (20%)
2	HYP	H	45	2	6,8,9	0.38	0	5,10,12	1.19	1 (20%)
1	HYP	A	1922	1	6,8,9	0.55	0	5,10,12	1.72	1 (20%)
1	HYP	B	1901	1	6,8,9	0.42	0	5,10,12	1.16	1 (20%)
1	HYP	C	1907	1	6,8,9	0.51	0	5,10,12	1.73	2 (40%)
1	HYP	A	1932	1	6,8,9	0.52	0	5,10,12	1.78	3 (60%)
2	HYP	H	55	2	6,8,9	0.44	0	5,10,12	1.19	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	HYP	A	1912	1	6,8,9	0.39	0	5,10,12	1.21	1 (20%)
2	HYP	G	33	2	6,8,9	0.51	0	5,10,12	1.61	1 (20%)
1	HYP	A	1908	1	6,8,9	0.53	0	5,10,12	2.18	3 (60%)
1	HYP	A	1866	1	6,8,9	0.51	0	5,10,12	1.46	1 (20%)
1	HYP	B	1873	1	6,8,9	0.48	0	5,10,12	1.35	1 (20%)
1	HYP	B	1906	1	6,8,9	0.39	0	5,10,12	1.16	1 (20%)
1	HYP	B	1882	1	6,8,9	0.39	0	5,10,12	1.21	1 (20%)
1	HYP	F	1910	1	6,8,9	0.40	0	5,10,12	1.13	1 (20%)
1	HYP	B	1928	1	6,8,9	0.53	0	5,10,12	1.52	1 (20%)
1	HYP	B	1857	1	6,8,9	0.55	0	5,10,12	1.60	1 (20%)
1	HYP	F	1913	1	6,8,9	0.38	0	5,10,12	1.24	1 (20%)
1	HYP	F	1930	1	6,8,9	0.49	0	5,10,12	1.52	1 (20%)
2	HYP	I	9	2	6,8,9	0.51	0	5,10,12	1.55	1 (20%)
2	HYP	H	37	2	6,8,9	0.49	0	5,10,12	1.15	1 (20%)
1	HYP	C	1901	1	6,8,9	0.37	0	5,10,12	1.16	1 (20%)
2	HYP	H	47	2	6,8,9	0.39	0	5,10,12	1.26	1 (20%)
2	HYP	G	8	2	6,8,9	0.50	0	5,10,12	1.59	1 (20%)
1	HYP	F	1922	1	6,8,9	0.54	0	5,10,12	1.57	1 (20%)
1	HYP	B	1865	1	6,8,9	0.49	0	5,10,12	1.68	1 (20%)
1	HYP	F	1899	1	6,8,9	0.37	0	5,10,12	1.29	1 (20%)
1	HYP	D	1905	1	6,8,9	0.39	0	5,10,12	1.18	1 (20%)
1	HYP	A	1880	1	6,8,9	0.41	0	5,10,12	1.38	1 (20%)
2	HYP	G	3	2	6,8,9	0.53	0	5,10,12	1.61	1 (20%)
1	HYP	C	1915	1	6,8,9	0.41	0	5,10,12	1.20	1 (20%)
1	HYP	B	1887	1	6,8,9	0.40	0	5,10,12	1.27	1 (20%)
1	HYP	F	1918	1	6,8,9	0.49	0	5,10,12	1.98	2 (40%)
1	HYP	E	1907	1	6,8,9	0.44	0	5,10,12	1.64	2 (40%)
1	HYP	B	1915	1	6,8,9	0.43	0	5,10,12	1.26	1 (20%)
1	HYP	E	1863	1	6,8,9	0.50	0	5,10,12	1.42	1 (20%)
1	HYP	F	1916	1	6,8,9	0.49	0	5,10,12	1.26	1 (20%)
2	HYP	G	5	2	6,8,9	0.36	0	5,10,12	1.17	1 (20%)
1	HYP	D	1922	1	6,8,9	0.50	0	5,10,12	1.40	1 (20%)
1	HYP	E	1880	1	6,8,9	0.48	0	5,10,12	1.44	1 (20%)
1	HYP	F	1915	1	6,8,9	0.41	0	5,10,12	1.20	1 (20%)
1	HYP	C	1912	1	6,8,9	0.38	0	5,10,12	1.18	1 (20%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	HYP	E	1888	1	6,8,9	0.44	0	5,10,12	1.82	2 (40%)
1	HYP	A	1890	1	6,8,9	0.48	0	5,10,12	1.23	1 (20%)
1	HYP	B	1923	1	6,8,9	0.54	0	5,10,12	1.96	3 (60%)
1	HYP	F	1885	1	6,8,9	0.45	0	5,10,12	1.22	1 (20%)
1	HYP	D	1929	1	6,8,9	0.38	0	5,10,12	1.20	1 (20%)
1	HYP	E	1916	1	6,8,9	0.51	0	5,10,12	1.33	1 (20%)
2	HYP	G	45	2	6,8,9	0.41	0	5,10,12	1.26	1 (20%)
1	HYP	E	1855	1	6,8,9	0.51	0	5,10,12	1.20	1 (20%)
1	HYP	C	1913	1	6,8,9	0.38	0	5,10,12	1.24	1 (20%)
1	HYP	F	1905	1	6,8,9	0.37	0	5,10,12	1.26	1 (20%)
1	HYP	A	1857	1	6,8,9	0.50	0	5,10,12	1.32	1 (20%)
1	HYP	D	1913	1	6,8,9	0.38	0	5,10,12	1.23	1 (20%)
1	HYP	A	1893	1	6,8,9	0.37	0	5,10,12	1.28	1 (20%)
1	HYP	B	1862	1	6,8,9	0.53	0	5,10,12	1.45	1 (20%)
1	HYP	E	1902	1	6,8,9	0.48	0	5,10,12	1.67	1 (20%)
1	HYP	E	1878	1	6,8,9	0.52	0	5,10,12	1.90	2 (40%)
1	HYP	C	1927	1	6,8,9	0.40	0	5,10,12	1.20	1 (20%)
1	HYP	C	1922	1	6,8,9	0.53	0	5,10,12	1.47	1 (20%)
2	HYP	I	32	2	6,8,9	0.42	0	5,10,12	1.15	1 (20%)
1	HYP	E	1932	1	6,8,9	0.52	0	5,10,12	1.45	1 (20%)
1	HYP	F	1866	1	6,8,9	0.52	0	5,10,12	1.35	1 (20%)
1	HYP	D	1897	1	6,8,9	0.42	0	5,10,12	1.23	1 (20%)
2	HYP	G	34	2	6,8,9	0.48	0	5,10,12	1.67	2 (40%)
1	HYP	C	1932	1	6,8,9	0.51	0	5,10,12	1.84	2 (40%)
2	HYP	I	8	2	6,8,9	0.51	0	5,10,12	1.50	1 (20%)
1	HYP	A	1877	1	6,8,9	0.47	0	5,10,12	1.32	1 (20%)
1	HYP	D	1915	1	6,8,9	0.39	0	5,10,12	1.23	1 (20%)
1	HYP	F	1856	1	6,8,9	0.52	0	5,10,12	1.35	1 (20%)
2	HYP	I	2	2	6,8,9	0.48	0	5,10,12	1.45	1 (20%)
1	HYP	C	1914	1	6,8,9	0.49	0	5,10,12	1.42	1 (20%)
1	HYP	F	1911	1	6,8,9	0.43	0	5,10,12	1.15	1 (20%)
1	HYP	A	1878	1	6,8,9	0.52	0	5,10,12	1.70	2 (40%)
1	HYP	B	1894	1	6,8,9	0.50	0	5,10,12	1.95	2 (40%)
1	HYP	D	1930	1	6,8,9	0.40	0	5,10,12	1.26	1 (20%)
1	HYP	F	1908	1	6,8,9	0.57	0	5,10,12	1.79	2 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	HYP	B	1870	1	6,8,9	0.52	0	5,10,12	1.54	1 (20%)
2	HYP	I	3	2	6,8,9	0.52	0	5,10,12	1.63	1 (20%)
1	HYP	B	1903	1	6,8,9	0.55	0	5,10,12	1.92	3 (60%)
1	HYP	B	1930	1	6,8,9	0.52	0	5,10,12	1.62	1 (20%)
1	HYP	B	1872	1	6,8,9	0.44	0	5,10,12	1.33	1 (20%)
1	HYP	F	1892	1	6,8,9	0.35	0	5,10,12	1.24	1 (20%)
2	HYP	H	43	2	6,8,9	0.49	0	5,10,12	1.48	1 (20%)
1	HYP	F	1914	1	6,8,9	0.51	0	5,10,12	1.45	1 (20%)
1	HYP	D	1914	1	6,8,9	0.46	0	5,10,12	1.10	1 (20%)
1	HYP	D	1898	1	6,8,9	0.41	0	5,10,12	1.23	1 (20%)
1	HYP	F	1863	1	6,8,9	0.51	0	5,10,12	1.39	1 (20%)
1	HYP	E	1866	1	6,8,9	0.54	0	5,10,12	1.41	1 (20%)
2	HYP	I	14	2	6,8,9	0.37	0	5,10,12	1.26	1 (20%)
1	HYP	A	1915	1	6,8,9	0.40	0	5,10,12	1.23	1 (20%)
1	HYP	B	1883	1	6,8,9	0.47	0	5,10,12	2.01	2 (40%)
1	HYP	D	1907	1	6,8,9	0.50	0	5,10,12	1.58	1 (20%)
1	HYP	E	1905	1	6,8,9	0.43	0	5,10,12	1.23	1 (20%)
2	HYP	G	26	2	6,8,9	0.38	0	5,10,12	1.15	1 (20%)
1	HYP	F	1921	1	6,8,9	0.37	0	5,10,12	1.34	1 (20%)
1	HYP	D	1921	1	6,8,9	0.43	0	5,10,12	1.22	1 (20%)
1	HYP	E	1856	1	6,8,9	0.51	0	5,10,12	1.30	1 (20%)
1	HYP	B	1898	1	6,8,9	0.40	0	5,10,12	1.25	1 (20%)
1	HYP	B	1878	1	6,8,9	0.51	0	5,10,12	1.84	2 (40%)
1	HYP	D	1917	1	6,8,9	0.51	0	5,10,12	1.51	1 (20%)
1	HYP	E	1868	1	6,8,9	0.52	0	5,10,12	1.79	2 (40%)
2	HYP	H	48	2	6,8,9	0.38	0	5,10,12	1.20	1 (20%)
1	HYP	F	1898	1	6,8,9	0.42	0	5,10,12	1.16	1 (20%)
1	HYP	B	1907	1	6,8,9	0.51	0	5,10,12	1.65	1 (20%)
2	HYP	G	44	2	6,8,9	0.52	0	5,10,12	1.52	1 (20%)
1	HYP	D	1916	1	6,8,9	0.51	0	5,10,12	1.39	1 (20%)
1	HYP	B	1922	1	6,8,9	0.53	0	5,10,12	1.61	1 (20%)
1	HYP	D	1932	1	6,8,9	0.53	0	5,10,12	1.81	3 (60%)
1	HYP	F	1867	1	6,8,9	0.50	0	5,10,12	1.64	1 (20%)
2	HYP	G	32	2	6,8,9	0.49	0	5,10,12	1.41	1 (20%)
1	HYP	F	1877	1	6,8,9	0.51	0	5,10,12	1.55	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	HYP	A	1870	1	6,8,9	0.50	0	5,10,12	1.57	2 (40%)
1	HYP	B	1927	1	6,8,9	0.41	0	5,10,12	1.20	1 (20%)
1	HYP	B	1916	1	6,8,9	0.52	0	5,10,12	1.45	1 (20%)
1	HYP	E	1897	1	6,8,9	0.45	0	5,10,12	1.19	1 (20%)
1	HYP	E	1922	1	6,8,9	0.55	0	5,10,12	1.52	1 (20%)
2	HYP	G	10	2	6,8,9	0.54	0	5,10,12	1.64	1 (20%)
1	HYP	B	1858	1	6,8,9	0.36	0	5,10,12	1.38	1 (20%)
1	HYP	E	1882	1	6,8,9	0.41	0	5,10,12	1.22	1 (20%)
1	HYP	B	1875	1	6,8,9	0.42	0	5,10,12	1.16	1 (20%)
1	HYP	E	1903	1	6,8,9	0.51	0	5,10,12	1.87	2 (40%)
1	HYP	C	1918	1	6,8,9	0.52	0	5,10,12	1.76	2 (40%)
1	HYP	E	1865	1	6,8,9	0.52	0	5,10,12	1.63	1 (20%)
1	HYP	C	1903	1	6,8,9	0.51	0	5,10,12	1.79	2 (40%)
1	HYP	D	1911	1	6,8,9	0.45	0	5,10,12	1.19	1 (20%)
1	HYP	A	1905	1	6,8,9	0.39	0	5,10,12	1.21	1 (20%)
2	HYP	I	10	2	6,8,9	0.52	0	5,10,12	1.70	1 (20%)
1	HYP	A	1913	1	6,8,9	0.38	0	5,10,12	1.27	1 (20%)
1	HYP	E	1929	1	6,8,9	0.36	0	5,10,12	1.23	1 (20%)
1	HYP	E	1906	1	6,8,9	0.37	0	5,10,12	1.22	1 (20%)
1	HYP	D	1923	1	6,8,9	0.50	0	5,10,12	1.82	3 (60%)
1	HYP	A	1917	1	6,8,9	0.51	0	5,10,12	1.59	1 (20%)
1	HYP	A	1868	1	6,8,9	0.50	0	5,10,12	1.92	3 (60%)
1	HYP	B	1918	1	6,8,9	0.56	0	5,10,12	1.59	1 (20%)
1	HYP	A	1903	1	6,8,9	0.55	0	5,10,12	1.77	2 (40%)
1	HYP	A	1872	1	6,8,9	0.47	0	5,10,12	1.31	1 (20%)
2	HYP	G	20	2	6,8,9	0.51	0	5,10,12	1.32	1 (20%)
1	HYP	F	1893	1	6,8,9	0.38	0	5,10,12	1.30	1 (20%)
1	HYP	D	1920	1	6,8,9	0.53	0	5,10,12	1.48	1 (20%)
1	HYP	A	1894	1	6,8,9	0.50	0	5,10,12	1.88	2 (40%)
1	HYP	A	1899	1	6,8,9	0.38	0	5,10,12	1.39	1 (20%)
1	HYP	F	1917	1	6,8,9	0.51	0	5,10,12	1.39	1 (20%)
1	HYP	E	1890	1	6,8,9	0.41	0	5,10,12	1.12	1 (20%)
2	HYP	G	23	2	6,8,9	0.39	0	5,10,12	1.46	1 (20%)
2	HYP	G	6	2	6,8,9	0.46	0	5,10,12	1.52	1 (20%)
1	HYP	B	1910	1	6,8,9	0.45	0	5,10,12	1.16	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	HYP	A	1911	1	6,8,9	0.39	0	5,10,12	1.20	1 (20%)
1	HYP	B	1885	1	6,8,9	0.42	0	5,10,12	1.16	1 (20%)
1	HYP	E	1915	1	6,8,9	0.37	0	5,10,12	1.14	1 (20%)
1	HYP	E	1920	1	6,8,9	0.53	0	5,10,12	1.45	1 (20%)
1	HYP	F	1897	1	6,8,9	0.45	0	5,10,12	1.28	1 (20%)
1	HYP	E	1930	1	6,8,9	0.36	0	5,10,12	1.21	1 (20%)
1	HYP	C	1928	1	6,8,9	0.39	0	5,10,12	1.26	1 (20%)
1	HYP	F	1860	1	6,8,9	0.57	0	5,10,12	1.56	1 (20%)
1	HYP	A	1888	1	6,8,9	0.52	0	5,10,12	1.52	1 (20%)
1	HYP	F	1907	1	6,8,9	0.52	0	5,10,12	1.74	2 (40%)
1	HYP	A	1855	1	6,8,9	0.49	0	5,10,12	1.16	1 (20%)
1	HYP	F	1880	1	6,8,9	0.42	0	5,10,12	1.42	1 (20%)
2	HYP	H	49	2	6,8,9	0.52	0	5,10,12	1.47	1 (20%)
1	HYP	A	1864	1	6,8,9	0.51	0	5,10,12	1.48	1 (20%)
1	HYP	E	1917	1	6,8,9	0.53	0	5,10,12	1.37	1 (20%)
2	HYP	G	43	2	6,8,9	0.49	0	5,10,12	1.47	1 (20%)
1	HYP	B	1860	1	6,8,9	0.51	0	5,10,12	1.71	2 (40%)
1	HYP	F	1888	1	6,8,9	0.44	0	5,10,12	1.85	2 (40%)
1	HYP	D	1903	1	6,8,9	0.55	0	5,10,12	1.74	2 (40%)
1	HYP	A	1906	1	6,8,9	0.39	0	5,10,12	1.35	1 (20%)
1	HYP	F	1855	1	6,8,9	0.56	0	5,10,12	1.43	1 (20%)
1	HYP	A	1897	1	6,8,9	0.43	0	5,10,12	1.26	1 (20%)
1	HYP	E	1875	1	6,8,9	0.45	0	5,10,12	1.17	1 (20%)
2	HYP	I	1	2	6,8,9	0.49	0	5,10,12	1.25	1 (20%)
1	HYP	A	1901	1	6,8,9	0.40	0	5,10,12	1.16	1 (20%)
1	HYP	D	1902	1	6,8,9	0.49	0	5,10,12	1.74	2 (40%)
1	HYP	F	1878	1	6,8,9	0.55	0	5,10,12	1.54	1 (20%)
2	HYP	G	7	2	6,8,9	0.38	0	5,10,12	1.36	1 (20%)
2	HYP	G	48	2	6,8,9	0.41	0	5,10,12	1.20	1 (20%)
1	HYP	D	1931	1	6,8,9	0.45	0	5,10,12	1.39	1 (20%)
2	HYP	H	40	2	6,8,9	0.39	0	5,10,12	1.12	1 (20%)
2	HYP	G	9	2	6,8,9	0.48	0	5,10,12	1.76	2 (40%)
1	HYP	B	1863	1	6,8,9	0.51	0	5,10,12	1.43	1 (20%)
2	HYP	I	33	2	6,8,9	0.47	0	5,10,12	1.25	1 (20%)
1	HYP	F	1932	1	6,8,9	0.49	0	5,10,12	1.71	2 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	HYP	I	11	2	6,8,9	0.48	0	5,10,12	1.79	2 (40%)
2	HYP	H	42	2	6,8,9	0.37	0	5,10,12	1.23	1 (20%)
1	HYP	D	1912	1	6,8,9	0.46	0	5,10,12	1.30	1 (20%)
1	HYP	B	1902	1	6,8,9	0.52	0	5,10,12	1.59	1 (20%)
1	HYP	C	1920	1	6,8,9	0.52	0	5,10,12	1.47	1 (20%)
1	HYP	A	1882	1	6,8,9	0.40	0	5,10,12	1.21	1 (20%)
1	HYP	E	1864	1	6,8,9	0.54	0	5,10,12	1.55	1 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HYP	I	17	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1865	1	-	0/0/11/13	0/1/1/1
2	HYP	I	20	2	-	0/0/11/13	0/1/1/1
1	HYP	E	1858	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1860	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1930	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1899	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1905	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1912	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1929	1	-	0/0/11/13	0/1/1/1
2	HYP	G	56	2	-	0/0/11/13	0/1/1/1
2	HYP	G	4	2	-	0/0/11/13	0/1/1/1
2	HYP	G	52	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1927	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1927	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1920	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1883	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1857	1	-	0/0/11/13	0/1/1/1
2	HYP	H	51	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1863	1	-	0/0/11/13	0/1/1/1
2	HYP	G	17	2	-	0/0/11/13	0/1/1/1
1	HYP	D	1918	1	-	0/0/11/13	0/1/1/1
2	HYP	G	47	2	-	0/0/11/13	0/1/1/1
2	HYP	I	4	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1921	1	-	0/0/11/13	0/1/1/1
2	HYP	G	14	2	-	0/0/11/13	0/1/1/1
1	HYP	C	1899	1	-	0/0/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	HYP	C	1906	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1911	1	-	0/0/11/13	0/1/1/1
2	HYP	H	50	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1875	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1928	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1923	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1856	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1931	1	-	0/0/11/13	0/1/1/1
2	HYP	I	7	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1916	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1870	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1887	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1928	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1913	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1892	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1885	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1906	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1867	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1898	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1914	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1912	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1921	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1866	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1921	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1873	1	-	0/0/11/13	0/1/1/1
2	HYP	I	34	2	-	0/0/11/13	0/1/1/1
1	HYP	E	1899	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1893	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1910	1	-	0/0/11/13	0/1/1/1
2	HYP	G	40	2	-	0/0/11/13	0/1/1/1
1	HYP	C	1930	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1920	1	-	0/0/11/13	0/1/1/1
2	HYP	G	42	2	-	0/0/11/13	0/1/1/1
1	HYP	F	1868	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1894	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1903	1	-	0/0/11/13	0/1/1/1
2	HYP	I	29	2	-	0/0/11/13	0/1/1/1
1	HYP	E	1887	1	-	0/0/11/13	0/1/1/1
2	HYP	H	56	2	-	0/0/11/13	0/1/1/1
1	HYP	F	1865	1	-	0/0/11/13	0/1/1/1
2	HYP	G	41	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1899	1	-	0/0/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	HYP	F	1902	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1929	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1914	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1872	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1914	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1928	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1890	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1910	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1862	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1923	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1910	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1928	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1898	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1931	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1920	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1870	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1917	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1888	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1931	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1862	1	-	0/0/11/13	0/1/1/1
2	HYP	I	5	2	-	0/0/11/13	0/1/1/1
1	HYP	C	1916	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1923	1	-	0/0/11/13	0/1/1/1
2	HYP	G	11	2	-	0/0/11/13	0/1/1/1
2	HYP	G	1	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1860	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1910	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1877	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1923	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1883	1	-	0/0/11/13	0/1/1/1
2	HYP	G	37	2	-	0/0/11/13	0/1/1/1
2	HYP	G	51	2	-	0/0/11/13	0/1/1/1
1	HYP	E	1883	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1855	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1887	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1873	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1875	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1882	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1902	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1911	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1931	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1911	1	-	0/0/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	HYP	B	1932	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1877	1	-	0/0/11/13	0/1/1/1
2	HYP	H	52	2	-	0/0/11/13	0/1/1/1
1	HYP	C	1905	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1908	1	-	0/0/11/13	0/1/1/1
2	HYP	G	49	2	-	0/0/11/13	0/1/1/1
1	HYP	E	1873	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1864	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1858	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1880	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1918	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1908	1	-	0/0/11/13	0/1/1/1
2	HYP	G	55	2	-	0/0/11/13	0/1/1/1
1	HYP	C	1898	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1893	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1901	1	-	0/0/11/13	0/1/1/1
2	HYP	H	44	2	-	0/0/11/13	0/1/1/1
2	HYP	I	26	2	1/1/2/4	0/0/11/13	0/1/1/1
1	HYP	C	1897	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1885	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1864	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1908	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1901	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1907	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1892	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1867	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1906	1	-	0/0/11/13	0/1/1/1
2	HYP	H	46	2	-	0/0/11/13	0/1/1/1
2	HYP	G	2	2	-	0/0/11/13	0/1/1/1
1	HYP	C	1921	1	-	0/0/11/13	0/1/1/1
2	HYP	G	46	2	-	0/0/11/13	0/1/1/1
1	HYP	C	1929	1	-	0/0/11/13	0/1/1/1
2	HYP	I	6	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1868	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1902	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1912	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1908	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1918	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1858	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1929	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1913	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1862	1	-	0/0/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	HYP	F	1927	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1894	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1927	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1901	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1931	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1872	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1917	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1856	1	-	0/0/11/13	0/1/1/1
2	HYP	H	41	2	-	0/0/11/13	0/1/1/1
1	HYP	E	1892	1	-	0/0/11/13	0/1/1/1
2	HYP	G	50	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1897	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1857	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1867	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1890	1	-	0/0/11/13	0/1/1/1
2	HYP	I	23	2	1/1/2/4	0/0/11/13	0/1/1/1
2	HYP	G	29	2	-	0/0/11/13	0/1/1/1
2	HYP	H	45	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1922	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1901	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1907	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1932	1	-	0/0/11/13	0/1/1/1
2	HYP	H	55	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1912	1	-	0/0/11/13	0/1/1/1
2	HYP	G	33	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1908	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1866	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1873	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1906	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1882	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1910	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1928	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1857	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1913	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1930	1	-	0/0/11/13	0/1/1/1
2	HYP	I	9	2	-	0/0/11/13	0/1/1/1
2	HYP	H	37	2	-	0/0/11/13	0/1/1/1
1	HYP	C	1901	1	-	0/0/11/13	0/1/1/1
2	HYP	H	47	2	-	0/0/11/13	0/1/1/1
2	HYP	G	8	2	-	0/0/11/13	0/1/1/1
1	HYP	F	1922	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1865	1	-	0/0/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	HYP	F	1899	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1905	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1880	1	-	0/0/11/13	0/1/1/1
2	HYP	G	3	2	-	0/0/11/13	0/1/1/1
1	HYP	C	1915	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1887	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1918	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1907	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1915	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1863	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1916	1	-	0/0/11/13	0/1/1/1
2	HYP	G	5	2	-	0/0/11/13	0/1/1/1
1	HYP	D	1922	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1880	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1915	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1912	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1888	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1890	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1923	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1885	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1929	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1916	1	-	0/0/11/13	0/1/1/1
2	HYP	G	45	2	-	0/0/11/13	0/1/1/1
1	HYP	E	1855	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1913	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1905	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1857	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1913	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1893	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1862	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1902	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1878	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1927	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1922	1	-	0/0/11/13	0/1/1/1
2	HYP	I	32	2	-	0/0/11/13	0/1/1/1
1	HYP	E	1932	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1866	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1897	1	-	0/0/11/13	0/1/1/1
2	HYP	G	34	2	-	0/0/11/13	0/1/1/1
1	HYP	C	1932	1	-	0/0/11/13	0/1/1/1
2	HYP	I	8	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1877	1	-	0/0/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	HYP	D	1915	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1856	1	-	0/0/11/13	0/1/1/1
2	HYP	I	2	2	-	0/0/11/13	0/1/1/1
1	HYP	C	1914	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1911	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1878	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1894	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1930	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1908	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1870	1	-	0/0/11/13	0/1/1/1
2	HYP	I	3	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1903	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1930	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1872	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1892	1	-	0/0/11/13	0/1/1/1
2	HYP	H	43	2	-	0/0/11/13	0/1/1/1
1	HYP	F	1914	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1914	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1898	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1863	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1866	1	-	0/0/11/13	0/1/1/1
2	HYP	I	14	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1915	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1883	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1907	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1905	1	-	0/0/11/13	0/1/1/1
2	HYP	G	26	2	1/1/2/4	0/0/11/13	0/1/1/1
1	HYP	F	1921	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1921	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1856	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1898	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1878	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1917	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1868	1	-	0/0/11/13	0/1/1/1
2	HYP	H	48	2	-	0/0/11/13	0/1/1/1
1	HYP	F	1898	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1907	1	-	0/0/11/13	0/1/1/1
2	HYP	G	44	2	-	0/0/11/13	0/1/1/1
1	HYP	D	1916	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1922	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1932	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1867	1	-	0/0/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HYP	G	32	2	-	0/0/11/13	0/1/1/1
1	HYP	F	1877	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1870	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1927	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1916	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1897	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1922	1	-	0/0/11/13	0/1/1/1
2	HYP	G	10	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1858	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1882	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1875	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1903	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1918	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1865	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1903	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1911	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1905	1	-	0/0/11/13	0/1/1/1
2	HYP	I	10	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1913	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1929	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1906	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1923	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1917	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1868	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1918	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1903	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1872	1	-	0/0/11/13	0/1/1/1
2	HYP	G	20	2	-	0/0/11/13	0/1/1/1
1	HYP	F	1893	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1920	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1894	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1899	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1917	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1890	1	-	0/0/11/13	0/1/1/1
2	HYP	G	23	2	1/1/2/4	0/0/11/13	0/1/1/1
2	HYP	G	6	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1910	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1911	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1885	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1915	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1920	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1897	1	-	0/0/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	HYP	E	1930	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1928	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1860	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1888	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1907	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1855	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1880	1	-	0/0/11/13	0/1/1/1
2	HYP	H	49	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1864	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1917	1	-	0/0/11/13	0/1/1/1
2	HYP	G	43	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1860	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1888	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1903	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1906	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1855	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1897	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1875	1	-	0/0/11/13	0/1/1/1
2	HYP	I	1	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1901	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1902	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1878	1	-	0/0/11/13	0/1/1/1
2	HYP	G	7	2	-	0/0/11/13	0/1/1/1
2	HYP	G	48	2	-	0/0/11/13	0/1/1/1
1	HYP	D	1931	1	-	0/0/11/13	0/1/1/1
2	HYP	H	40	2	-	0/0/11/13	0/1/1/1
2	HYP	G	9	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1863	1	-	0/0/11/13	0/1/1/1
2	HYP	I	33	2	-	0/0/11/13	0/1/1/1
1	HYP	F	1932	1	-	0/0/11/13	0/1/1/1
2	HYP	I	11	2	-	0/0/11/13	0/1/1/1
2	HYP	H	42	2	-	0/0/11/13	0/1/1/1
1	HYP	D	1912	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1902	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1920	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1882	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1864	1	-	0/0/11/13	0/1/1/1

There are no bond length outliers.

The worst 5 of 434 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	1883	HYP	CG-CB-CA	-3.50	99.55	103.96
1	A	1883	HYP	CG-CB-CA	-3.47	99.59	103.96
1	E	1923	HYP	CG-CB-CA	-3.37	99.71	103.96
1	F	1918	HYP	CG-CB-CA	-3.31	99.79	103.96
1	B	1883	HYP	CG-CB-CA	-3.27	99.84	103.96

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	G	23	HYP	CA
2	I	23	HYP	CA
2	G	26	HYP	CA
2	I	26	HYP	CA

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

1348 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	$\# Z  > 2$
3	FUB	0	1	3	9,9,10	0.58	0	10,12,14	1.12	1 (10%)
3	FUB	0	2	3	9,9,10	0.55	0	10,12,14	0.90	0
3	FUB	0	3	3	9,9,10	0.58	0	10,12,14	0.96	0
3	FUB	0A	1	3	9,9,10	0.57	0	10,12,14	0.98	1 (10%)
3	FUB	0A	2	3	9,9,10	0.54	0	10,12,14	0.78	0
3	FUB	0A	3	3	9,9,10	0.56	0	10,12,14	0.90	0
6	FUB	0B	1	6	9,9,10	0.57	0	10,12,14	1.01	0
6	FUB	0B	2	6	9,9,10	0.58	0	10,12,14	1.23	1 (10%)
6	GZL	0B	3	6	11,11,12	6.99	6 (54%)	14,15,17	3.96	4 (28%)
6	FUB	0C	1	6	9,9,10	0.59	0	10,12,14	0.82	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	FUB	0C	2	6	9,9,10	0.57	0	10,12,14	1.17	1 (10%)
6	GZL	0C	3	6	11,11,12	6.70	7 (63%)	14,15,17	1.49	2 (14%)
13	FUB	0D	1	13	9,9,10	0.59	0	10,12,14	0.88	0
13	FUB	0D	2	13	9,9,10	0.57	0	10,12,14	1.04	0
13	GZL	0D	3	13	11,11,12	6.70	7 (63%)	14,15,17	1.50	3 (21%)
13	AHR	0D	4	13	9,9,10	0.56	0	10,12,14	0.89	0
18	FUB	0E	1	18	9,9,10	0.59	0	10,12,14	0.99	0
18	FUB	0E	2	18	9,9,10	0.56	0	10,12,14	0.87	0
18	GZL	0E	3	18	11,11,12	6.73	7 (63%)	14,15,17	1.45	2 (14%)
18	AHR	0E	4	18	9,9,10	0.58	0	10,12,14	0.96	0
18	AHR	0E	5	18	9,9,10	0.58	0	10,12,14	1.08	1 (10%)
3	FUB	1	1	3	9,9,10	0.57	0	10,12,14	0.82	0
3	FUB	1	2	3	9,9,10	0.57	0	10,12,14	0.94	0
3	FUB	1	3	3	9,9,10	0.56	0	10,12,14	1.01	1 (10%)
10	FUB	1A	1	10	9,9,10	0.52	0	10,12,14	1.11	1 (10%)
10	FUB	1A	2	10	9,9,10	0.54	0	10,12,14	0.76	0
10	FUB	1A	3	10	9,9,10	0.57	0	10,12,14	1.10	1 (10%)
10	AHR	1A	4	10	9,9,10	0.58	0	10,12,14	0.85	1 (10%)
10	AHR	1A	5	10	9,9,10	0.57	0	10,12,14	0.96	1 (10%)
13	FUB	1B	1	13	9,9,10	0.55	0	10,12,14	0.86	0
13	FUB	1B	2	13	9,9,10	0.57	0	10,12,14	0.88	0
13	GZL	1B	3	13	11,11,12	6.77	7 (63%)	14,15,17	1.37	1 (7%)
13	AHR	1B	4	13	9,9,10	0.57	0	10,12,14	0.98	0
6	FUB	1C	1	6	9,9,10	0.55	0	10,12,14	0.70	0
6	FUB	1C	2	6	9,9,10	0.57	0	10,12,14	0.89	0
6	GZL	1C	3	6	11,11,12	6.72	7 (63%)	14,15,17	1.58	2 (14%)
15	FUB	1D	1	15	9,9,10	0.58	0	10,12,14	1.00	0
15	FUB	1D	2	15	9,9,10	0.59	0	10,12,14	0.97	0
15	GZL	1D	3	15	11,11,12	6.74	7 (63%)	14,15,17	1.30	1 (7%)
15	AHR	1D	4	15	9,9,10	0.56	0	10,12,14	1.03	1 (10%)
15	AHR	1D	5	15	9,9,10	0.57	0	10,12,14	1.10	1 (10%)
19	FUB	1E	1	19	9,9,10	0.56	0	10,12,14	1.12	1 (10%)
19	FUB	1E	2	19	9,9,10	0.58	0	10,12,14	1.01	1 (10%)
19	GZL	1E	3	19	11,11,12	6.72	7 (63%)	14,15,17	1.64	2 (14%)
19	AHR	1E	4	19	9,9,10	0.57	0	10,12,14	1.11	1 (10%)
3	FUB	2	1	3	9,9,10	0.56	0	10,12,14	0.98	0
3	FUB	2	2	3	9,9,10	0.54	0	10,12,14	0.74	0
3	FUB	2	3	3	9,9,10	0.57	0	10,12,14	1.01	1 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
13	FUB	2A	1	13	9,9,10	0.55	0	10,12,14	1.07	1 (10%)
13	FUB	2A	2	13	9,9,10	0.48	0	10,12,14	1.37	2 (20%)
13	GZL	2A	3	13	11,11,12	6.85	7 (63%)	14,15,17	0.98	0
13	AHR	2A	4	13	9,9,10	0.58	0	10,12,14	1.12	1 (10%)
13	FUB	2B	1	13	9,9,10	0.57	0	10,12,14	1.04	0
13	FUB	2B	2	13	9,9,10	0.57	0	10,12,14	0.89	0
13	GZL	2B	3	13	11,11,12	6.71	7 (63%)	14,15,17	1.52	2 (14%)
13	AHR	2B	4	13	9,9,10	0.58	0	10,12,14	1.01	1 (10%)
6	FUB	2C	1	6	9,9,10	0.59	0	10,12,14	0.93	0
6	FUB	2C	2	6	9,9,10	0.58	0	10,12,14	1.10	1 (10%)
6	GZL	2C	3	6	11,11,12	6.71	7 (63%)	14,15,17	1.57	2 (14%)
15	FUB	2D	1	15	9,9,10	0.58	0	10,12,14	1.03	1 (10%)
15	FUB	2D	2	15	9,9,10	0.59	0	10,12,14	0.91	0
15	GZL	2D	3	15	11,11,12	6.74	7 (63%)	14,15,17	1.49	2 (14%)
15	AHR	2D	4	15	9,9,10	0.56	0	10,12,14	1.06	1 (10%)
15	AHR	2D	5	15	9,9,10	0.59	0	10,12,14	0.98	0
10	FUB	3	1	10	9,9,10	0.55	0	10,12,14	1.10	1 (10%)
10	FUB	3	2	10	9,9,10	0.55	0	10,12,14	0.66	0
10	FUB	3	3	10	9,9,10	0.60	0	10,12,14	1.06	1 (10%)
10	AHR	3	4	10	9,9,10	0.57	0	10,12,14	0.95	0
10	AHR	3	5	10	9,9,10	0.58	0	10,12,14	0.88	1 (10%)
6	FUB	3A	1	6	9,9,10	0.56	0	10,12,14	1.02	1 (10%)
6	FUB	3A	2	6	9,9,10	0.54	0	10,12,14	1.17	1 (10%)
6	GZL	3A	3	6	11,11,12	6.88	6 (54%)	14,15,17	4.71	4 (28%)
6	FUB	3B	1	6	9,9,10	0.56	0	10,12,14	0.96	1 (10%)
6	FUB	3B	2	6	9,9,10	0.55	0	10,12,14	1.28	1 (10%)
6	GZL	3B	3	6	11,11,12	6.70	7 (63%)	14,15,17	1.60	2 (14%)
13	FUB	3C	1	13	9,9,10	0.58	0	10,12,14	0.97	0
13	FUB	3C	2	13	9,9,10	0.56	0	10,12,14	1.18	1 (10%)
13	GZL	3C	3	13	11,11,12	6.68	7 (63%)	14,15,17	1.51	2 (14%)
13	AHR	3C	4	13	9,9,10	0.59	0	10,12,14	0.85	0
6	FUB	3D	1	6	9,9,10	0.57	0	10,12,14	1.04	1 (10%)
6	FUB	3D	2	6	9,9,10	0.57	0	10,12,14	1.06	1 (10%)
6	GZL	3D	3	6	11,11,12	6.72	7 (63%)	14,15,17	1.43	2 (14%)
13	FUB	4	1	13	9,9,10	0.53	0	10,12,14	0.86	0
13	FUB	4	2	13	9,9,10	0.51	0	10,12,14	1.37	1 (10%)
13	GZL	4	3	13	11,11,12	6.84	7 (63%)	14,15,17	3.32	7 (50%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
13	AHR	4	4	13	9,9,10	0.58	0	10,12,14	1.01	1 (10%)
13	FUB	4A	1	13	9,9,10	0.53	0	10,12,14	0.89	0
13	FUB	4A	2	13	9,9,10	0.56	0	10,12,14	0.82	0
13	GZL	4A	3	13	11,11,12	6.78	7 (63%)	14,15,17	1.46	1 (7%)
13	AHR	4A	4	13	9,9,10	0.55	0	10,12,14	1.12	1 (10%)
6	FUB	4B	1	6	9,9,10	0.57	0	10,12,14	0.87	1 (10%)
6	FUB	4B	2	6	9,9,10	0.58	0	10,12,14	0.84	0
6	GZL	4B	3	6	11,11,12	6.72	7 (63%)	14,15,17	1.72	2 (14%)
15	FUB	4C	1	15	9,9,10	0.58	0	10,12,14	0.91	0
15	FUB	4C	2	15	9,9,10	0.58	0	10,12,14	0.98	0
15	GZL	4C	3	15	11,11,12	6.73	7 (63%)	14,15,17	1.43	1 (7%)
15	AHR	4C	4	15	9,9,10	0.57	0	10,12,14	1.07	1 (10%)
15	AHR	4C	5	15	9,9,10	0.57	0	10,12,14	1.07	1 (10%)
16	NAG	4D	1	16,1	14,14,15	0.34	0	17,19,21	0.55	0
16	NAG	4D	2	16	14,14,15	0.45	0	17,19,21	1.36	2 (11%)
6	FUB	5	1	6	9,9,10	0.55	0	10,12,14	0.97	1 (10%)
6	FUB	5	2	6	9,9,10	0.52	0	10,12,14	1.27	1 (10%)
6	GZL	5	3	6	11,11,12	6.73	6 (54%)	14,15,17	1.55	1 (7%)
13	FUB	5A	1	13	9,9,10	0.56	0	10,12,14	0.90	0
13	FUB	5A	2	13	9,9,10	0.55	0	10,12,14	0.78	0
13	GZL	5A	3	13	11,11,12	6.71	7 (63%)	14,15,17	1.31	1 (7%)
13	AHR	5A	4	13	9,9,10	0.58	0	10,12,14	1.07	1 (10%)
6	FUB	5B	1	6	9,9,10	0.55	0	10,12,14	0.80	0
6	FUB	5B	2	6	9,9,10	0.59	0	10,12,14	1.08	1 (10%)
6	GZL	5B	3	6	11,11,12	6.74	7 (63%)	14,15,17	1.38	1 (7%)
15	FUB	5C	1	15	9,9,10	0.56	0	10,12,14	1.09	1 (10%)
15	FUB	5C	2	15	9,9,10	0.58	0	10,12,14	0.97	0
15	GZL	5C	3	15	11,11,12	6.71	7 (63%)	14,15,17	1.64	2 (14%)
15	AHR	5C	4	15	9,9,10	0.58	0	10,12,14	1.00	1 (10%)
15	AHR	5C	5	15	9,9,10	0.57	0	10,12,14	1.08	1 (10%)
17	NAG	5D	1	17,1	14,14,15	0.33	0	17,19,21	0.98	1 (5%)
17	NAG	5D	2	17	14,14,15	0.30	0	17,19,21	0.76	0
17	BMA	5D	3	17	11,11,12	0.26	0	15,15,17	1.30	3 (20%)
17	MAN	5D	4	17	11,11,12	0.41	0	15,15,17	2.40	3 (20%)
17	MAN	5D	5	17	11,11,12	0.27	0	15,15,17	0.61	0
17	MAN	5D	6	17	11,11,12	0.30	0	15,15,17	0.85	0
13	FUB	6	1	13	9,9,10	0.54	0	10,12,14	0.77	0
13	FUB	6	2	13	9,9,10	0.58	0	10,12,14	0.82	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
13	GZL	6	3	13	11,11,12	6.78	6 (54%)	14,15,17	1.39	1 (7%)
13	AHR	6	4	13	9,9,10	0.58	0	10,12,14	1.09	1 (10%)
6	FUB	6A	1	6	9,9,10	0.56	0	10,12,14	0.88	0
6	FUB	6A	2	6	9,9,10	0.53	0	10,12,14	1.45	1 (10%)
6	GZL	6A	3	6	11,11,12	6.72	7 (63%)	14,15,17	1.48	1 (7%)
13	FUB	6B	1	13	9,9,10	0.56	0	10,12,14	0.89	0
13	FUB	6B	2	13	9,9,10	0.55	0	10,12,14	1.19	2 (20%)
13	GZL	6B	3	13	11,11,12	6.71	7 (63%)	14,15,17	1.84	4 (28%)
13	AHR	6B	4	13	9,9,10	0.55	0	10,12,14	0.97	0
6	FUB	6C	1	6	9,9,10	0.58	0	10,12,14	0.97	1 (10%)
6	FUB	6C	2	6	9,9,10	0.57	0	10,12,14	1.03	1 (10%)
6	GZL	6C	3	6	11,11,12	6.72	7 (63%)	14,15,17	1.48	1 (7%)
6	FUB	6D	1	6	9,9,10	0.58	0	10,12,14	1.07	1 (10%)
6	FUB	6D	2	6	9,9,10	0.57	0	10,12,14	1.15	1 (10%)
6	GZL	6D	3	6	11,11,12	6.68	7 (63%)	14,15,17	1.90	3 (21%)
13	FUB	7	1	13	9,9,10	0.58	0	10,12,14	0.98	0
13	FUB	7	2	13	9,9,10	0.57	0	10,12,14	0.77	0
13	GZL	7	3	13	11,11,12	6.73	7 (63%)	14,15,17	1.44	2 (14%)
13	AHR	7	4	13	9,9,10	0.56	0	10,12,14	1.15	1 (10%)
6	FUB	7A	1	6	9,9,10	0.56	0	10,12,14	0.98	1 (10%)
6	FUB	7A	2	6	9,9,10	0.58	0	10,12,14	0.96	0
6	GZL	7A	3	6	11,11,12	6.71	7 (63%)	14,15,17	1.43	1 (7%)
15	FUB	7B	1	15	9,9,10	0.51	0	10,12,14	0.96	0
15	FUB	7B	2	15	9,9,10	0.55	0	10,12,14	0.86	0
15	GZL	7B	3	15	11,11,12	6.75	7 (63%)	14,15,17	1.40	1 (7%)
15	AHR	7B	4	15	9,9,10	0.60	0	10,12,14	1.22	2 (20%)
15	AHR	7B	5	15	9,9,10	0.59	0	10,12,14	0.89	0
17	NAG	7C	1	17,1	14,14,15	0.32	0	17,19,21	0.84	1 (5%)
17	NAG	7C	2	17	14,14,15	0.35	0	17,19,21	0.99	0
17	BMA	7C	3	17	11,11,12	0.20	0	15,15,17	1.21	1 (6%)
17	MAN	7C	4	17	11,11,12	0.31	0	15,15,17	1.15	2 (13%)
17	MAN	7C	5	17	11,11,12	0.24	0	15,15,17	0.74	0
17	MAN	7C	6	17	11,11,12	0.29	0	15,15,17	0.98	0
6	FUB	7D	1	6	9,9,10	0.58	0	10,12,14	0.97	0
6	FUB	7D	2	6	9,9,10	0.56	0	10,12,14	1.02	1 (10%)
6	GZL	7D	3	6	11,11,12	6.72	7 (63%)	14,15,17	1.57	2 (14%)
6	FUB	8	1	6	9,9,10	0.56	0	10,12,14	0.99	1 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	FUB	8	2	6	9,9,10	0.55	0	10,12,14	0.81	0
6	GZL	8	3	6	11,11,12	6.72	7 (63%)	14,15,17	1.42	1 (7%)
6	FUB	8A	1	6	9,9,10	0.54	0	10,12,14	1.04	1 (10%)
6	FUB	8A	2	6	9,9,10	0.60	0	10,12,14	1.08	1 (10%)
6	GZL	8A	3	6	11,11,12	6.73	7 (63%)	14,15,17	1.52	1 (7%)
15	FUB	8B	1	15	9,9,10	0.58	0	10,12,14	0.95	0
15	FUB	8B	2	15	9,9,10	0.56	0	10,12,14	0.92	0
15	GZL	8B	3	15	11,11,12	6.74	7 (63%)	14,15,17	1.25	1 (7%)
15	AHR	8B	4	15	9,9,10	0.57	0	10,12,14	1.08	1 (10%)
15	AHR	8B	5	15	9,9,10	0.56	0	10,12,14	1.07	1 (10%)
3	FUB	8C	1	3	9,9,10	0.58	0	10,12,14	0.82	0
3	FUB	8C	2	3	9,9,10	0.55	0	10,12,14	0.81	0
3	FUB	8C	3	3	9,9,10	0.58	0	10,12,14	0.91	0
6	FUB	8D	1	6	9,9,10	0.56	0	10,12,14	0.91	1 (10%)
6	FUB	8D	2	6	9,9,10	0.57	0	10,12,14	0.92	1 (10%)
6	GZL	8D	3	6	11,11,12	6.74	7 (63%)	14,15,17	1.58	2 (14%)
6	FUB	9	1	6	9,9,10	0.54	0	10,12,14	0.88	1 (10%)
6	FUB	9	2	6	9,9,10	0.56	0	10,12,14	0.79	0
6	GZL	9	3	6	11,11,12	6.74	7 (63%)	14,15,17	1.33	1 (7%)
13	FUB	9A	1	13	9,9,10	0.56	0	10,12,14	0.89	0
13	FUB	9A	2	13	9,9,10	0.54	0	10,12,14	1.20	2 (20%)
13	GZL	9A	3	13	11,11,12	6.71	7 (63%)	14,15,17	1.93	4 (28%)
13	AHR	9A	4	13	9,9,10	0.56	0	10,12,14	1.01	0
6	FUB	9B	1	6	9,9,10	0.57	0	10,12,14	0.87	0
6	FUB	9B	2	6	9,9,10	0.56	0	10,12,14	1.04	1 (10%)
6	GZL	9B	3	6	11,11,12	6.69	7 (63%)	14,15,17	1.61	2 (14%)
3	FUB	9C	1	3	9,9,10	0.58	0	10,12,14	1.03	0
3	FUB	9C	2	3	9,9,10	0.58	0	10,12,14	1.06	1 (10%)
3	FUB	9C	3	3	9,9,10	0.57	0	10,12,14	0.89	1 (10%)
18	FUB	9D	1	18	9,9,10	0.59	0	10,12,14	2.72	5 (50%)
18	FUB	9D	2	18	9,9,10	0.56	0	10,12,14	0.91	0
18	GZL	9D	3	18	11,11,12	6.74	7 (63%)	14,15,17	1.42	2 (14%)
18	AHR	9D	4	18	9,9,10	0.57	0	10,12,14	1.10	1 (10%)
18	AHR	9D	5	18	9,9,10	0.59	0	10,12,14	1.26	1 (10%)
6	FUB	AA	1	6	9,9,10	0.53	0	10,12,14	0.77	0
6	FUB	AA	2	6	9,9,10	0.59	0	10,12,14	1.12	1 (10%)
6	GZL	AA	3	6	11,11,12	6.73	7 (63%)	14,15,17	1.27	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
15	FUB	AB	1	15	9,9,10	0.54	0	10,12,14	1.00	1 (10%)
15	FUB	AB	2	15	9,9,10	0.58	0	10,12,14	0.90	0
15	GZL	AB	3	15	11,11,12	6.73	7 (63%)	14,15,17	1.25	1 (7%)
15	AHR	AB	4	15	9,9,10	0.63	0	10,12,14	1.22	1 (10%)
15	AHR	AB	5	15	9,9,10	0.58	0	10,12,14	1.14	1 (10%)
16	NAG	AC	1	16,1	14,14,15	0.53	0	17,19,21	1.02	1 (5%)
16	NAG	AC	2	16	14,14,15	0.40	0	17,19,21	1.32	2 (11%)
4	FUB	AD	1	4	9,9,10	0.56	0	10,12,14	0.95	1 (10%)
4	FUB	AD	2	4	9,9,10	0.55	0	10,12,14	0.81	0
4	FUB	AD	3	4	9,9,10	0.55	0	10,12,14	0.77	0
4	AHR	AD	4	4	9,9,10	0.55	0	10,12,14	1.12	1 (10%)
19	FUB	AE	1	19	9,9,10	0.56	0	10,12,14	1.26	1 (10%)
19	FUB	AE	2	19	9,9,10	0.57	0	10,12,14	0.87	0
19	GZL	AE	3	19	11,11,12	6.75	7 (63%)	14,15,17	1.43	1 (7%)
19	AHR	AE	4	19	9,9,10	0.56	0	10,12,14	0.83	0
13	FUB	BA	1	13	9,9,10	0.56	0	10,12,14	0.75	0
13	FUB	BA	2	13	9,9,10	0.54	0	10,12,14	1.41	3 (30%)
13	GZL	BA	3	13	11,11,12	6.67	7 (63%)	14,15,17	1.91	4 (28%)
13	AHR	BA	4	13	9,9,10	0.55	0	10,12,14	0.85	0
15	FUB	BB	1	15	9,9,10	0.55	0	10,12,14	1.00	1 (10%)
15	FUB	BB	2	15	9,9,10	0.56	0	10,12,14	0.69	0
15	GZL	BB	3	15	11,11,12	6.75	7 (63%)	14,15,17	1.15	1 (7%)
15	AHR	BB	4	15	9,9,10	0.58	0	10,12,14	1.11	1 (10%)
15	AHR	BB	5	15	9,9,10	0.59	0	10,12,14	0.91	0
3	FUB	BC	1	3	9,9,10	0.56	0	10,12,14	1.00	1 (10%)
3	FUB	BC	2	3	9,9,10	0.55	0	10,12,14	0.93	1 (10%)
3	FUB	BC	3	3	9,9,10	0.56	0	10,12,14	0.87	0
5	FUB	BD	1	5	9,9,10	0.55	0	10,12,14	1.02	1 (10%)
5	FUB	BD	2	5	9,9,10	0.52	0	10,12,14	0.86	0
5	FUB	BD	3	5	9,9,10	0.57	0	10,12,14	0.93	0
5	AHR	BD	4	5	9,9,10	0.56	0	10,12,14	1.11	1 (10%)
5	AHR	BD	5	5	9,9,10	0.56	0	10,12,14	0.81	0
18	FUB	BE	1	18	9,9,10	0.60	0	10,12,14	0.91	0
18	FUB	BE	2	18	9,9,10	0.53	0	10,12,14	1.05	1 (10%)
18	GZL	BE	3	18	11,11,12	6.70	7 (63%)	14,15,17	1.55	2 (14%)
18	AHR	BE	4	18	9,9,10	0.56	0	10,12,14	0.80	0
18	AHR	BE	5	18	9,9,10	0.54	0	10,12,14	1.15	1 (10%)
15	FUB	CA	1	15	9,9,10	0.55	0	10,12,14	1.04	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
15	FUB	CA	2	15	9,9,10	0.54	0	10,12,14	0.83	0
15	GZL	CA	3	15	11,11,12	6.75	7 (63%)	14,15,17	1.18	1 (7%)
15	AHR	CA	4	15	9,9,10	0.60	0	10,12,14	1.27	2 (20%)
15	AHR	CA	5	15	9,9,10	0.58	0	10,12,14	1.07	1 (10%)
6	FUB	CB	1	6	9,9,10	0.56	0	10,12,14	1.02	1 (10%)
6	FUB	CB	2	6	9,9,10	0.56	0	10,12,14	0.87	0
6	GZL	CB	3	6	11,11,12	6.73	7 (63%)	14,15,17	1.48	3 (21%)
3	FUB	CC	1	3	9,9,10	0.57	0	10,12,14	0.95	1 (10%)
3	FUB	CC	2	3	9,9,10	0.55	0	10,12,14	0.91	1 (10%)
3	FUB	CC	3	3	9,9,10	0.56	0	10,12,14	0.79	0
6	FUB	CD	1	6	9,9,10	0.56	0	10,12,14	0.96	0
6	FUB	CD	2	6	9,9,10	0.50	0	10,12,14	1.12	1 (10%)
6	GZL	CD	3	6	11,11,12	7.12	7 (63%)	14,15,17	4.08	5 (35%)
20	FUB	CE	1	20	9,9,10	0.56	0	10,12,14	0.79	0
20	FUB	CE	2	20	9,9,10	0.51	0	10,12,14	0.84	0
20	GZL	CE	3	20	11,11,12	6.69	7 (63%)	14,15,17	1.62	2 (14%)
20	AHR	CE	4	20	9,9,10	0.59	0	10,12,14	0.86	0
15	FUB	DA	1	15	9,9,10	0.57	0	10,12,14	0.99	1 (10%)
15	FUB	DA	2	15	9,9,10	0.56	0	10,12,14	0.82	0
15	GZL	DA	3	15	11,11,12	6.74	6 (54%)	14,15,17	1.34	1 (7%)
15	AHR	DA	4	15	9,9,10	0.55	0	10,12,14	1.13	1 (10%)
15	AHR	DA	5	15	9,9,10	0.58	0	10,12,14	1.04	1 (10%)
17	NAG	DB	1	17,1	14,14,15	0.32	0	17,19,21	0.71	1 (5%)
17	NAG	DB	2	17	14,14,15	0.32	0	17,19,21	1.09	1 (5%)
17	BMA	DB	3	17	11,11,12	0.23	0	15,15,17	1.23	2 (13%)
17	MAN	DB	4	17	11,11,12	0.31	0	15,15,17	1.18	2 (13%)
17	MAN	DB	5	17	11,11,12	0.24	0	15,15,17	0.73	0
17	MAN	DB	6	17	11,11,12	0.40	0	15,15,17	1.52	2 (13%)
4	FUB	DC	1	4	9,9,10	0.56	0	10,12,14	1.08	1 (10%)
4	FUB	DC	2	4	9,9,10	0.56	0	10,12,14	0.83	0
4	FUB	DC	3	4	9,9,10	0.56	0	10,12,14	0.81	0
4	AHR	DC	4	4	9,9,10	0.57	0	10,12,14	1.01	1 (10%)
3	FUB	DD	1	3	9,9,10	0.57	0	10,12,14	1.10	1 (10%)
3	FUB	DD	2	3	9,9,10	0.57	0	10,12,14	0.80	0
3	FUB	DD	3	3	9,9,10	0.57	0	10,12,14	0.97	0
18	FUB	DE	1	18	9,9,10	0.52	0	10,12,14	1.09	1 (10%)
18	FUB	DE	2	18	9,9,10	0.51	0	10,12,14	0.81	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
18	GZL	DE	3	18	11,11,12	6.70	7 (63%)	14,15,17	1.66	2 (14%)
18	AHR	DE	4	18	9,9,10	0.57	0	10,12,14	1.02	1 (10%)
18	AHR	DE	5	18	9,9,10	0.58	0	10,12,14	0.92	0
6	FUB	EA	1	6	9,9,10	0.56	0	10,12,14	0.96	1 (10%)
6	FUB	EA	2	6	9,9,10	0.55	0	10,12,14	0.91	0
6	GZL	EA	3	6	11,11,12	6.74	7 (63%)	14,15,17	1.37	1 (7%)
3	FUB	EB	1	3	9,9,10	0.57	0	10,12,14	1.03	1 (10%)
3	FUB	EB	2	3	9,9,10	0.58	0	10,12,14	0.84	0
3	FUB	EB	3	3	9,9,10	0.57	0	10,12,14	0.98	0
5	FUB	EC	1	5	9,9,10	0.57	0	10,12,14	1.02	1 (10%)
5	FUB	EC	2	5	9,9,10	0.59	0	10,12,14	1.16	0
5	FUB	EC	3	5	9,9,10	0.58	0	10,12,14	1.08	1 (10%)
5	AHR	EC	4	5	9,9,10	0.57	0	10,12,14	1.01	1 (10%)
5	AHR	EC	5	5	9,9,10	0.56	0	10,12,14	0.80	0
3	FUB	ED	1	3	9,9,10	0.54	0	10,12,14	1.05	1 (10%)
3	FUB	ED	2	3	9,9,10	0.56	0	10,12,14	0.80	0
3	FUB	ED	3	3	9,9,10	0.58	0	10,12,14	0.80	0
20	FUB	EE	1	20	9,9,10	0.53	0	10,12,14	0.88	0
20	FUB	EE	2	20	9,9,10	0.55	0	10,12,14	1.10	1 (10%)
20	GZL	EE	3	20	11,11,12	6.73	7 (63%)	14,15,17	1.51	1 (7%)
20	AHR	EE	4	20	9,9,10	0.60	0	10,12,14	0.81	0
16	NAG	FA	1	16,1	14,14,15	0.42	0	17,19,21	0.59	0
16	NAG	FA	2	16	14,14,15	0.39	0	17,19,21	1.39	2 (11%)
12	FUB	FB	1	12	9,9,10	0.59	0	10,12,14	1.02	1 (10%)
12	FUB	FB	2	12	9,9,10	0.58	0	10,12,14	0.96	0
12	GZL	FB	3	12	11,11,12	6.67	7 (63%)	14,15,17	1.70	2 (14%)
12	AHR	FB	4	12	9,9,10	0.58	0	10,12,14	0.93	0
12	AHR	FB	5	12	9,9,10	0.58	0	10,12,14	1.04	1 (10%)
6	FUB	FC	1	6	9,9,10	0.56	0	10,12,14	1.29	2 (20%)
6	FUB	FC	2	6	9,9,10	0.60	0	10,12,14	1.20	1 (10%)
6	GZL	FC	3	6	11,11,12	6.60	7 (63%)	14,15,17	2.44	4 (28%)
3	FUB	FD	1	3	9,9,10	0.55	0	10,12,14	1.07	1 (10%)
3	FUB	FD	2	3	9,9,10	0.54	0	10,12,14	0.72	0
3	FUB	FD	3	3	9,9,10	0.58	0	10,12,14	0.90	0
21	FUB	FE	1	21	9,9,10	0.55	0	10,12,14	1.12	1 (10%)
21	FUB	FE	2	21	9,9,10	0.53	0	10,12,14	0.70	0
21	GZL	FE	3	21	11,11,12	6.75	6 (54%)	14,15,17	1.35	1 (7%)
21	AHR	FE	4	21	9,9,10	0.57	0	10,12,14	1.00	1 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
21	AHR	FE	5	21	9,9,10	0.60	0	10,12,14	1.02	1 (10%)
17	NAG	GA	1	17,1	14,14,15	0.35	0	17,19,21	0.79	1 (5%)
17	NAG	GA	2	17	14,14,15	0.33	0	17,19,21	0.94	0
17	BMA	GA	3	17	11,11,12	0.25	0	15,15,17	1.64	4 (26%)
17	MAN	GA	4	17	11,11,12	0.31	0	15,15,17	0.72	0
17	MAN	GA	5	17	11,11,12	0.24	0	15,15,17	0.62	0
17	MAN	GA	6	17	11,11,12	0.29	0	15,15,17	1.00	1 (6%)
13	FUB	GB	1	13	9,9,10	0.58	0	10,12,14	0.87	0
13	FUB	GB	2	13	9,9,10	0.59	0	10,12,14	0.92	0
13	GZL	GB	3	13	11,11,12	6.74	7 (63%)	14,15,17	1.29	1 (7%)
13	AHR	GB	4	13	9,9,10	0.56	0	10,12,14	0.99	0
3	FUB	GC	1	3	9,9,10	0.56	0	10,12,14	0.99	1 (10%)
3	FUB	GC	2	3	9,9,10	0.54	0	10,12,14	0.71	0
3	FUB	GC	3	3	9,9,10	0.58	0	10,12,14	0.87	0
6	FUB	GD	1	6	9,9,10	0.55	0	10,12,14	1.08	1 (10%)
6	FUB	GD	2	6	9,9,10	0.55	0	10,12,14	0.84	0
6	GZL	GD	3	6	11,11,12	6.71	7 (63%)	14,15,17	1.45	2 (14%)
22	FUB	GE	1	22	9,9,10	0.57	0	10,12,14	1.20	1 (10%)
22	FUB	GE	2	22	9,9,10	0.58	0	10,12,14	1.11	1 (10%)
22	GZL	GE	3	22	11,11,12	6.71	7 (63%)	14,15,17	1.46	2 (14%)
22	AHR	GE	4	22	9,9,10	0.56	0	10,12,14	0.76	0
22	AHR	GE	5	22	9,9,10	0.59	0	10,12,14	1.48	3 (30%)
22	AHR	GE	6	22	9,9,10	0.54	0	10,12,14	0.77	0
3	FUB	HA	1	3	9,9,10	0.55	0	10,12,14	0.93	1 (10%)
3	FUB	HA	2	3	9,9,10	0.58	0	10,12,14	0.79	0
3	FUB	HA	3	3	9,9,10	0.59	0	10,12,14	1.02	1 (10%)
14	FUB	HB	1	14	9,9,10	0.55	0	10,12,14	0.76	0
14	FUB	HB	2	14	9,9,10	0.56	0	10,12,14	0.87	0
14	GZL	HB	3	14	11,11,12	6.65	7 (63%)	14,15,17	1.76	3 (21%)
14	FUB	HB	4	14	9,9,10	0.59	0	10,12,14	1.08	1 (10%)
3	FUB	HC	1	3	9,9,10	0.55	0	10,12,14	1.13	1 (10%)
3	FUB	HC	2	3	9,9,10	0.56	0	10,12,14	0.74	0
3	FUB	HC	3	3	9,9,10	0.57	0	10,12,14	0.92	0
7	FUB	HD	1	7	9,9,10	0.58	0	10,12,14	1.16	1 (10%)
7	FUB	HD	2	7	9,9,10	0.56	0	10,12,14	0.86	0
7	FUB	HD	3	7	9,9,10	0.56	0	10,12,14	0.99	0
7	AHR	HD	4	7	9,9,10	0.56	0	10,12,14	0.96	1 (10%)
20	FUB	HE	1	20	9,9,10	0.59	0	10,12,14	1.15	1 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	FUB	HE	2	20	9,9,10	0.54	0	10,12,14	0.96	0
20	GZL	HE	3	20	11,11,12	6.72	7 (63%)	14,15,17	1.64	2 (14%)
20	AHR	HE	4	20	9,9,10	0.56	0	10,12,14	0.99	0
3	FUB	IA	1	3	9,9,10	0.54	0	10,12,14	0.74	0
3	FUB	IA	2	3	9,9,10	0.54	0	10,12,14	0.92	1 (10%)
3	FUB	IA	3	3	9,9,10	0.56	0	10,12,14	0.78	0
12	FUB	IB	1	12	9,9,10	0.58	0	10,12,14	0.92	0
12	FUB	IB	2	12	9,9,10	0.56	0	10,12,14	0.95	1 (10%)
12	GZL	IB	3	12	11,11,12	6.72	7 (63%)	14,15,17	1.43	1 (7%)
12	AHR	IB	4	12	9,9,10	0.56	0	10,12,14	1.06	1 (10%)
12	AHR	IB	5	12	9,9,10	0.56	0	10,12,14	1.11	1 (10%)
3	FUB	IC	1	3	9,9,10	0.58	0	10,12,14	1.06	1 (10%)
3	FUB	IC	2	3	9,9,10	0.52	0	10,12,14	0.80	0
3	FUB	IC	3	3	9,9,10	0.56	0	10,12,14	0.85	0
3	FUB	ID	1	3	9,9,10	0.57	0	10,12,14	1.05	1 (10%)
3	FUB	ID	2	3	9,9,10	0.54	0	10,12,14	0.80	0
3	FUB	ID	3	3	9,9,10	0.59	0	10,12,14	0.86	0
18	FUB	IE	1	18	9,9,10	0.58	0	10,12,14	1.10	1 (10%)
18	FUB	IE	2	18	9,9,10	0.52	0	10,12,14	0.89	0
18	GZL	IE	3	18	11,11,12	6.68	7 (63%)	14,15,17	1.71	3 (21%)
18	AHR	IE	4	18	9,9,10	0.55	0	10,12,14	1.12	1 (10%)
18	AHR	IE	5	18	9,9,10	0.56	0	10,12,14	1.17	1 (10%)
3	FUB	J	1	3	9,9,10	0.55	0	10,12,14	0.83	0
3	FUB	J	2	3	9,9,10	0.56	0	10,12,14	0.95	0
3	FUB	J	3	3	9,9,10	0.60	0	10,12,14	0.92	0
4	FUB	JA	1	4	9,9,10	0.58	0	10,12,14	0.86	0
4	FUB	JA	2	4	9,9,10	0.58	0	10,12,14	1.04	0
4	FUB	JA	3	4	9,9,10	0.57	0	10,12,14	0.94	0
4	AHR	JA	4	4	9,9,10	0.56	0	10,12,14	1.07	1 (10%)
4	FUB	JB	1	4	9,9,10	0.57	0	10,12,14	0.99	1 (10%)
4	FUB	JB	2	4	9,9,10	0.58	0	10,12,14	0.99	0
4	FUB	JB	3	4	9,9,10	0.58	0	10,12,14	0.88	0
4	AHR	JB	4	4	9,9,10	0.56	0	10,12,14	0.74	0
6	FUB	JC	1	6	9,9,10	0.57	0	10,12,14	1.10	1 (10%)
6	FUB	JC	2	6	9,9,10	0.56	0	10,12,14	0.83	0
6	GZL	JC	3	6	11,11,12	6.72	7 (63%)	14,15,17	1.44	1 (7%)
8	FUB	JD	1	8	9,9,10	0.56	0	10,12,14	0.81	0
8	FUB	JD	2	8	9,9,10	0.56	0	10,12,14	0.76	0
8	FUB	JD	3	8	9,9,10	0.59	0	10,12,14	0.77	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	AHR	JD	4	8	9,9,10	0.58	0	10,12,14	1.12	1 (10%)
8	AHR	JD	5	8	9,9,10	0.58	0	10,12,14	0.96	0
18	FUB	JE	1	18	9,9,10	0.58	0	10,12,14	1.10	1 (10%)
18	FUB	JE	2	18	9,9,10	0.57	0	10,12,14	0.90	0
18	GZL	JE	3	18	11,11,12	6.70	7 (63%)	14,15,17	1.59	2 (14%)
18	AHR	JE	4	18	9,9,10	0.58	0	10,12,14	0.80	0
18	AHR	JE	5	18	9,9,10	0.57	0	10,12,14	1.00	1 (10%)
3	FUB	K	1	3	9,9,10	0.56	0	10,12,14	0.63	0
3	FUB	K	2	3	9,9,10	0.54	0	10,12,14	0.81	0
3	FUB	K	3	3	9,9,10	0.55	0	10,12,14	0.76	0
5	FUB	KA	1	5	9,9,10	0.56	0	10,12,14	0.94	0
5	FUB	KA	2	5	9,9,10	0.59	0	10,12,14	0.96	0
5	FUB	KA	3	5	9,9,10	0.57	0	10,12,14	1.13	1 (10%)
5	AHR	KA	4	5	9,9,10	0.58	0	10,12,14	1.07	1 (10%)
5	AHR	KA	5	5	9,9,10	0.59	0	10,12,14	1.01	1 (10%)
14	FUB	KB	1	14	9,9,10	0.58	0	10,12,14	0.98	0
14	FUB	KB	2	14	9,9,10	0.59	0	10,12,14	0.99	0
14	GZL	KB	3	14	11,11,12	6.64	7 (63%)	14,15,17	1.85	2 (14%)
14	FUB	KB	4	14	9,9,10	0.58	0	10,12,14	1.04	1 (10%)
7	FUB	KC	1	7	9,9,10	0.57	0	10,12,14	1.14	1 (10%)
7	FUB	KC	2	7	9,9,10	0.56	0	10,12,14	0.77	0
7	FUB	KC	3	7	9,9,10	0.58	0	10,12,14	0.97	0
7	AHR	KC	4	7	9,9,10	0.56	0	10,12,14	1.00	1 (10%)
3	FUB	KD	1	3	9,9,10	0.57	0	10,12,14	0.98	1 (10%)
3	FUB	KD	2	3	9,9,10	0.56	0	10,12,14	0.92	0
3	FUB	KD	3	3	9,9,10	0.57	0	10,12,14	0.98	0
18	FUB	KE	1	18	9,9,10	0.59	0	10,12,14	1.10	0
18	FUB	KE	2	18	9,9,10	0.56	0	10,12,14	0.93	0
18	GZL	KE	3	18	11,11,12	6.68	7 (63%)	14,15,17	1.54	2 (14%)
18	AHR	KE	4	18	9,9,10	0.57	0	10,12,14	1.08	1 (10%)
18	AHR	KE	5	18	9,9,10	0.57	0	10,12,14	1.01	0
4	FUB	L	1	4	9,9,10	0.59	0	10,12,14	0.64	0
4	FUB	L	2	4	9,9,10	0.56	0	10,12,14	0.92	0
4	FUB	L	3	4	9,9,10	0.60	0	10,12,14	0.82	0
4	AHR	L	4	4	9,9,10	0.57	0	10,12,14	1.07	1 (10%)
6	FUB	LA	1	6	9,9,10	0.59	0	10,12,14	0.97	0
6	FUB	LA	2	6	9,9,10	0.56	0	10,12,14	1.26	1 (10%)
6	GZL	LA	3	6	11,11,12	7.12	7 (63%)	14,15,17	4.03	5 (35%)
3	FUB	LB	1	3	9,9,10	0.58	0	10,12,14	0.90	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	FUB	LB	2	3	9,9,10	0.57	0	10,12,14	0.85	0
3	FUB	LB	3	3	9,9,10	0.57	0	10,12,14	0.97	0
3	FUB	LC	1	3	9,9,10	0.58	0	10,12,14	1.02	0
3	FUB	LC	2	3	9,9,10	0.55	0	10,12,14	0.79	0
3	FUB	LC	3	3	9,9,10	0.58	0	10,12,14	0.84	0
4	FUB	LD	1	4	9,9,10	0.57	0	10,12,14	1.07	1 (10%)
4	FUB	LD	2	4	9,9,10	0.57	0	10,12,14	0.79	0
4	FUB	LD	3	4	9,9,10	0.58	0	10,12,14	0.80	0
4	AHR	LD	4	4	9,9,10	0.57	0	10,12,14	1.07	1 (10%)
19	FUB	LE	1	19	9,9,10	0.58	0	10,12,14	1.11	0
19	FUB	LE	2	19	9,9,10	0.56	0	10,12,14	1.07	1 (10%)
19	GZL	LE	3	19	11,11,12	6.74	7 (63%)	14,15,17	1.38	1 (7%)
19	AHR	LE	4	19	9,9,10	0.55	0	10,12,14	0.96	0
5	FUB	M	1	5	9,9,10	0.56	0	10,12,14	0.93	0
5	FUB	M	2	5	9,9,10	0.58	0	10,12,14	1.29	2 (20%)
5	FUB	M	3	5	9,9,10	0.56	0	10,12,14	1.12	1 (10%)
5	AHR	M	4	5	9,9,10	0.58	0	10,12,14	1.06	1 (10%)
5	AHR	M	5	5	9,9,10	0.56	0	10,12,14	1.17	1 (10%)
3	FUB	MA	1	3	9,9,10	0.56	0	10,12,14	0.84	0
3	FUB	MA	2	3	9,9,10	0.55	0	10,12,14	0.83	0
3	FUB	MA	3	3	9,9,10	0.58	0	10,12,14	0.87	0
10	FUB	MB	1	10	9,9,10	0.58	0	10,12,14	1.00	1 (10%)
10	FUB	MB	2	10	9,9,10	0.58	0	10,12,14	1.04	0
10	FUB	MB	3	10	9,9,10	0.58	0	10,12,14	0.83	0
10	AHR	MB	4	10	9,9,10	0.57	0	10,12,14	1.06	1 (10%)
10	AHR	MB	5	10	9,9,10	0.57	0	10,12,14	1.19	1 (10%)
8	FUB	MC	1	8	9,9,10	0.55	0	10,12,14	1.02	1 (10%)
8	FUB	MC	2	8	9,9,10	0.56	0	10,12,14	0.78	0
8	FUB	MC	3	8	9,9,10	0.56	0	10,12,14	0.83	0
8	AHR	MC	4	8	9,9,10	0.57	0	10,12,14	1.12	1 (10%)
8	AHR	MC	5	8	9,9,10	0.59	0	10,12,14	1.05	1 (10%)
4	FUB	MD	1	4	9,9,10	0.53	0	10,12,14	0.90	0
4	FUB	MD	2	4	9,9,10	0.55	0	10,12,14	0.84	0
4	FUB	MD	3	4	9,9,10	0.59	0	10,12,14	0.97	0
4	AHR	MD	4	4	9,9,10	0.56	0	10,12,14	0.79	0
6	FUB	ME	1	6	9,9,10	0.58	0	10,12,14	0.89	0
6	FUB	ME	2	6	9,9,10	0.57	0	10,12,14	0.80	0
6	GZL	ME	3	6	11,11,12	6.74	7 (63%)	14,15,17	1.47	1 (7%)
6	FUB	N	1	6	9,9,10	0.58	0	10,12,14	1.05	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	FUB	N	2	6	9,9,10	0.62	0	10,12,14	1.15	2 (20%)
6	GZL	N	3	6	11,11,12	6.64	7 (63%)	14,15,17	3.38	5 (35%)
3	FUB	NA	1	3	9,9,10	0.54	0	10,12,14	1.10	1 (10%)
3	FUB	NA	2	3	9,9,10	0.54	0	10,12,14	0.78	0
3	FUB	NA	3	3	9,9,10	0.57	0	10,12,14	1.02	1 (10%)
4	FUB	NB	1	4	9,9,10	0.58	0	10,12,14	1.04	1 (10%)
4	FUB	NB	2	4	9,9,10	0.58	0	10,12,14	0.95	0
4	FUB	NB	3	4	9,9,10	0.57	0	10,12,14	0.91	0
4	AHR	NB	4	4	9,9,10	0.56	0	10,12,14	1.00	1 (10%)
3	FUB	NC	1	3	9,9,10	0.58	0	10,12,14	0.91	0
3	FUB	NC	2	3	9,9,10	0.57	0	10,12,14	0.85	0
3	FUB	NC	3	3	9,9,10	0.56	0	10,12,14	0.98	0
9	FUB	ND	1	9	9,9,10	0.62	0	10,12,14	1.04	0
9	FUB	ND	2	9	9,9,10	0.58	0	10,12,14	1.09	1 (10%)
19	FUB	NE	1	19	9,9,10	0.58	0	10,12,14	0.92	0
19	FUB	NE	2	19	9,9,10	0.57	0	10,12,14	0.76	0
19	GZL	NE	3	19	11,11,12	6.71	7 (63%)	14,15,17	1.53	2 (14%)
19	AHR	NE	4	19	9,9,10	0.57	0	10,12,14	0.94	0
3	FUB	O	1	3	9,9,10	0.58	0	10,12,14	1.05	1 (10%)
3	FUB	O	2	3	9,9,10	0.56	0	10,12,14	0.83	0
3	FUB	O	3	3	9,9,10	0.59	0	10,12,14	0.98	0
3	FUB	OA	1	3	9,9,10	0.58	0	10,12,14	1.08	1 (10%)
3	FUB	OA	2	3	9,9,10	0.57	0	10,12,14	0.92	0
3	FUB	OA	3	3	9,9,10	0.57	0	10,12,14	0.94	0
3	FUB	OB	1	3	9,9,10	0.59	0	10,12,14	0.98	0
3	FUB	OB	2	3	9,9,10	0.59	0	10,12,14	0.90	0
3	FUB	OB	3	3	9,9,10	0.58	0	10,12,14	0.98	0
4	FUB	OC	1	4	9,9,10	0.53	0	10,12,14	0.89	0
4	FUB	OC	2	4	9,9,10	0.58	0	10,12,14	0.69	0
4	FUB	OC	3	4	9,9,10	0.56	0	10,12,14	0.82	0
4	AHR	OC	4	4	9,9,10	0.56	0	10,12,14	1.13	1 (10%)
4	FUB	OD	1	4	9,9,10	0.53	0	10,12,14	1.05	1 (10%)
4	FUB	OD	2	4	9,9,10	0.51	0	10,12,14	0.81	0
4	FUB	OD	3	4	9,9,10	0.58	0	10,12,14	0.86	0
4	AHR	OD	4	4	9,9,10	0.58	0	10,12,14	1.12	1 (10%)
6	FUB	OE	1	6	9,9,10	0.62	0	10,12,14	0.78	0
6	FUB	OE	2	6	9,9,10	0.58	0	10,12,14	0.90	0
6	GZL	OE	3	6	11,11,12	6.73	7 (63%)	14,15,17	1.60	2 (14%)
3	FUB	P	1	3	9,9,10	0.57	0	10,12,14	1.11	1 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	FUB	P	2	3	9,9,10	0.56	0	10,12,14	0.87	0
3	FUB	P	3	3	9,9,10	0.59	0	10,12,14	0.94	0
6	FUB	PA	1	6	9,9,10	0.58	0	10,12,14	1.00	0
6	FUB	PA	2	6	9,9,10	0.57	0	10,12,14	0.90	0
6	GZL	PA	3	6	11,11,12	6.73	7 (63%)	14,15,17	1.44	1 (7%)
3	FUB	PB	1	3	9,9,10	0.56	0	10,12,14	0.92	1 (10%)
3	FUB	PB	2	3	9,9,10	0.57	0	10,12,14	0.90	0
3	FUB	PB	3	3	9,9,10	0.56	0	10,12,14	0.88	0
4	FUB	PC	1	4	9,9,10	0.53	0	10,12,14	0.97	0
4	FUB	PC	2	4	9,9,10	0.54	0	10,12,14	0.82	0
4	FUB	PC	3	4	9,9,10	0.57	0	10,12,14	0.95	0
4	AHR	PC	4	4	9,9,10	0.64	0	10,12,14	1.23	2 (20%)
10	FUB	PD	1	10	9,9,10	0.54	0	10,12,14	1.06	1 (10%)
10	FUB	PD	2	10	9,9,10	0.59	0	10,12,14	0.94	0
10	FUB	PD	3	10	9,9,10	0.59	0	10,12,14	0.87	0
10	AHR	PD	4	10	9,9,10	0.57	0	10,12,14	1.13	1 (10%)
10	AHR	PD	5	10	9,9,10	0.58	0	10,12,14	1.00	0
18	FUB	PE	1	18	9,9,10	0.55	0	10,12,14	1.02	1 (10%)
18	FUB	PE	2	18	9,9,10	0.55	0	10,12,14	0.74	0
18	GZL	PE	3	18	11,11,12	6.75	7 (63%)	14,15,17	1.40	1 (7%)
18	AHR	PE	4	18	9,9,10	0.56	0	10,12,14	0.82	0
18	AHR	PE	5	18	9,9,10	0.57	0	10,12,14	1.03	0
3	FUB	Q	1	3	9,9,10	0.56	0	10,12,14	1.01	1 (10%)
3	FUB	Q	2	3	9,9,10	0.55	0	10,12,14	0.80	0
3	FUB	Q	3	3	9,9,10	0.56	0	10,12,14	0.80	0
7	FUB	QA	1	7	9,9,10	0.55	0	10,12,14	1.17	1 (10%)
7	FUB	QA	2	7	9,9,10	0.59	0	10,12,14	0.88	0
7	FUB	QA	3	7	9,9,10	0.59	0	10,12,14	1.04	1 (10%)
7	AHR	QA	4	7	9,9,10	0.55	0	10,12,14	0.87	0
3	FUB	QB	1	3	9,9,10	0.59	0	10,12,14	0.95	1 (10%)
3	FUB	QB	2	3	9,9,10	0.59	0	10,12,14	0.87	0
3	FUB	QB	3	3	9,9,10	0.54	0	10,12,14	0.80	0
9	FUB	QC	1	9	9,9,10	0.56	0	10,12,14	0.93	0
9	FUB	QC	2	9	9,9,10	0.57	0	10,12,14	0.94	0
3	FUB	QD	1	3	9,9,10	0.57	0	10,12,14	0.76	0
3	FUB	QD	2	3	9,9,10	0.59	0	10,12,14	0.96	0
3	FUB	QD	3	3	9,9,10	0.56	0	10,12,14	0.88	0
22	FUB	QE	1	22	9,9,10	0.56	0	10,12,14	0.86	1 (10%)
22	FUB	QE	2	22	9,9,10	0.57	0	10,12,14	0.95	0
22	GZL	QE	3	22	11,11,12	6.75	7 (63%)	14,15,17	1.43	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	AHR	QE	4	22	9,9,10	0.56	0	10,12,14	1.11	1 (10%)
22	AHR	QE	5	22	9,9,10	0.57	0	10,12,14	0.87	0
22	AHR	QE	6	22	9,9,10	0.56	0	10,12,14	1.11	1 (10%)
6	FUB	R	1	6	9,9,10	0.56	0	10,12,14	1.01	1 (10%)
6	FUB	R	2	6	9,9,10	0.57	0	10,12,14	0.91	0
6	GZL	R	3	6	11,11,12	6.73	7 (63%)	14,15,17	1.49	1 (7%)
3	FUB	RA	1	3	9,9,10	0.56	0	10,12,14	1.09	1 (10%)
3	FUB	RA	2	3	9,9,10	0.56	0	10,12,14	0.84	0
3	FUB	RA	3	3	9,9,10	0.58	0	10,12,14	0.94	0
3	FUB	RB	1	3	9,9,10	0.56	0	10,12,14	1.07	1 (10%)
3	FUB	RB	2	3	9,9,10	0.60	0	10,12,14	1.00	0
3	FUB	RB	3	3	9,9,10	0.57	0	10,12,14	1.07	1 (10%)
4	FUB	RC	1	4	9,9,10	0.55	0	10,12,14	0.94	0
4	FUB	RC	2	4	9,9,10	0.55	0	10,12,14	0.71	0
4	FUB	RC	3	4	9,9,10	0.59	0	10,12,14	0.94	0
4	AHR	RC	4	4	9,9,10	0.56	0	10,12,14	1.03	1 (10%)
4	FUB	RD	1	4	9,9,10	0.55	0	10,12,14	0.81	0
4	FUB	RD	2	4	9,9,10	0.58	0	10,12,14	0.97	1 (10%)
4	FUB	RD	3	4	9,9,10	0.59	0	10,12,14	0.95	0
4	AHR	RD	4	4	9,9,10	0.57	0	10,12,14	1.11	1 (10%)
22	FUB	RE	1	22	9,9,10	0.58	0	10,12,14	1.05	0
22	FUB	RE	2	22	9,9,10	0.56	0	10,12,14	0.90	0
22	GZL	RE	3	22	11,11,12	6.75	7 (63%)	14,15,17	1.36	1 (7%)
22	AHR	RE	4	22	9,9,10	0.57	0	10,12,14	1.05	1 (10%)
22	AHR	RE	5	22	9,9,10	0.55	0	10,12,14	1.19	2 (20%)
22	AHR	RE	6	22	9,9,10	0.62	0	10,12,14	1.23	1 (10%)
7	FUB	S	1	7	9,9,10	0.56	0	10,12,14	1.15	1 (10%)
7	FUB	S	2	7	9,9,10	0.56	0	10,12,14	0.81	0
7	FUB	S	3	7	9,9,10	0.55	0	10,12,14	1.04	1 (10%)
7	AHR	S	4	7	9,9,10	0.59	0	10,12,14	1.03	1 (10%)
8	FUB	SA	1	8	9,9,10	0.57	0	10,12,14	0.97	0
8	FUB	SA	2	8	9,9,10	0.57	0	10,12,14	0.85	0
8	FUB	SA	3	8	9,9,10	0.55	0	10,12,14	0.96	1 (10%)
8	AHR	SA	4	8	9,9,10	0.60	0	10,12,14	1.00	0
8	AHR	SA	5	8	9,9,10	0.58	0	10,12,14	0.85	0
3	FUB	SB	1	3	9,9,10	0.58	0	10,12,14	1.11	1 (10%)
3	FUB	SB	2	3	9,9,10	0.58	0	10,12,14	1.05	1 (10%)
3	FUB	SB	3	3	9,9,10	0.58	0	10,12,14	1.02	1 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
10	FUB	SC	1	10	9,9,10	0.57	0	10,12,14	0.93	0
10	FUB	SC	2	10	9,9,10	0.57	0	10,12,14	0.82	0
10	FUB	SC	3	10	9,9,10	0.60	0	10,12,14	0.89	0
10	AHR	SC	4	10	9,9,10	0.57	0	10,12,14	0.88	0
10	AHR	SC	5	10	9,9,10	0.59	0	10,12,14	1.05	1 (10%)
4	FUB	SD	1	4	9,9,10	0.57	0	10,12,14	1.01	0
4	FUB	SD	2	4	9,9,10	0.58	0	10,12,14	1.09	1 (10%)
4	FUB	SD	3	4	9,9,10	0.58	0	10,12,14	0.87	0
4	AHR	SD	4	4	9,9,10	0.57	0	10,12,14	1.07	1 (10%)
18	FUB	SE	1	18	9,9,10	0.56	0	10,12,14	1.16	1 (10%)
18	FUB	SE	2	18	9,9,10	0.53	0	10,12,14	0.86	0
18	GZL	SE	3	18	11,11,12	6.75	7 (63%)	14,15,17	1.40	1 (7%)
18	AHR	SE	4	18	9,9,10	0.57	0	10,12,14	0.99	0
18	AHR	SE	5	18	9,9,10	0.56	0	10,12,14	0.98	0
3	FUB	T	1	3	9,9,10	0.54	0	10,12,14	1.10	1 (10%)
3	FUB	T	2	3	9,9,10	0.56	0	10,12,14	0.82	0
3	FUB	T	3	3	9,9,10	0.58	0	10,12,14	0.96	0
3	FUB	TA	1	3	9,9,10	0.57	0	10,12,14	1.00	1 (10%)
3	FUB	TA	2	3	9,9,10	0.54	0	10,12,14	1.02	1 (10%)
3	FUB	TA	3	3	9,9,10	0.57	0	10,12,14	0.81	0
3	FUB	TB	1	3	9,9,10	0.55	0	10,12,14	0.74	0
3	FUB	TB	2	3	9,9,10	0.57	0	10,12,14	1.01	1 (10%)
3	FUB	TB	3	3	9,9,10	0.57	0	10,12,14	0.86	0
3	FUB	TC	1	3	9,9,10	0.59	0	10,12,14	1.13	1 (10%)
3	FUB	TC	2	3	9,9,10	0.58	0	10,12,14	1.04	1 (10%)
3	FUB	TC	3	3	9,9,10	0.57	0	10,12,14	1.09	1 (10%)
3	FUB	TD	1	3	9,9,10	0.56	0	10,12,14	0.79	0
3	FUB	TD	2	3	9,9,10	0.59	0	10,12,14	0.91	0
3	FUB	TD	3	3	9,9,10	0.57	0	10,12,14	0.90	0
20	FUB	TE	1	20	9,9,10	0.55	0	10,12,14	1.09	1 (10%)
20	FUB	TE	2	20	9,9,10	0.57	0	10,12,14	0.76	0
20	GZL	TE	3	20	11,11,12	6.74	7 (63%)	14,15,17	1.56	1 (7%)
20	AHR	TE	4	20	9,9,10	0.56	0	10,12,14	0.83	0
8	FUB	U	1	8	9,9,10	0.56	0	10,12,14	1.05	1 (10%)
8	FUB	U	2	8	9,9,10	0.57	0	10,12,14	1.00	1 (10%)
8	FUB	U	3	8	9,9,10	0.58	0	10,12,14	0.90	0
8	AHR	U	4	8	9,9,10	0.57	0	10,12,14	1.12	1 (10%)
8	AHR	U	5	8	9,9,10	0.59	0	10,12,14	0.92	0
4	FUB	UA	1	4	9,9,10	0.57	0	10,12,14	1.03	1 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	FUB	UA	2	4	9,9,10	0.57	0	10,12,14	0.83	0
4	FUB	UA	3	4	9,9,10	0.57	0	10,12,14	0.88	0
4	AHR	UA	4	4	9,9,10	0.58	0	10,12,14	0.89	0
3	FUB	UB	1	3	9,9,10	0.56	0	10,12,14	1.01	1 (10%)
3	FUB	UB	2	3	9,9,10	0.56	0	10,12,14	0.74	0
3	FUB	UB	3	3	9,9,10	0.57	0	10,12,14	0.96	0
4	FUB	UC	1	4	9,9,10	0.52	0	10,12,14	0.89	0
4	FUB	UC	2	4	9,9,10	0.56	0	10,12,14	0.93	0
4	FUB	UC	3	4	9,9,10	0.57	0	10,12,14	0.94	0
4	AHR	UC	4	4	9,9,10	0.59	0	10,12,14	0.93	0
7	FUB	UD	1	7	9,9,10	0.56	0	10,12,14	1.08	1 (10%)
7	FUB	UD	2	7	9,9,10	0.56	0	10,12,14	0.70	0
7	FUB	UD	3	7	9,9,10	0.57	0	10,12,14	0.84	0
7	AHR	UD	4	7	9,9,10	0.57	0	10,12,14	0.77	0
20	FUB	UE	1	20	9,9,10	0.54	0	10,12,14	0.87	0
20	FUB	UE	2	20	9,9,10	0.49	0	10,12,14	0.99	0
20	GZL	UE	3	20	11,11,12	6.75	7 (63%)	14,15,17	1.31	1 (7%)
20	AHR	UE	4	20	9,9,10	0.58	0	10,12,14	0.77	0
3	FUB	V	1	3	9,9,10	0.57	0	10,12,14	0.92	0
3	FUB	V	2	3	9,9,10	0.56	0	10,12,14	0.90	0
3	FUB	V	3	3	9,9,10	0.56	0	10,12,14	1.08	1 (10%)
4	FUB	VA	1	4	9,9,10	0.55	0	10,12,14	0.95	0
4	FUB	VA	2	4	9,9,10	0.57	0	10,12,14	0.90	0
4	FUB	VA	3	4	9,9,10	0.55	0	10,12,14	0.83	0
4	AHR	VA	4	4	9,9,10	0.60	0	10,12,14	0.76	0
10	FUB	VB	1	10	9,9,10	0.54	0	10,12,14	0.95	0
10	FUB	VB	2	10	9,9,10	0.56	0	10,12,14	0.81	0
10	FUB	VB	3	10	9,9,10	0.56	0	10,12,14	1.06	1 (10%)
10	AHR	VB	4	10	9,9,10	0.58	0	10,12,14	0.79	0
10	AHR	VB	5	10	9,9,10	0.58	0	10,12,14	1.05	1 (10%)
4	FUB	VC	1	4	9,9,10	0.55	0	10,12,14	0.85	0
4	FUB	VC	2	4	9,9,10	0.58	0	10,12,14	0.93	0
4	FUB	VC	3	4	9,9,10	0.58	0	10,12,14	0.85	0
4	AHR	VC	4	4	9,9,10	0.56	0	10,12,14	1.04	1 (10%)
4	FUB	VD	1	4	9,9,10	0.57	0	10,12,14	0.92	0
4	FUB	VD	2	4	9,9,10	0.58	0	10,12,14	0.99	1 (10%)
4	FUB	VD	3	4	9,9,10	0.58	0	10,12,14	0.86	0
4	AHR	VD	4	4	9,9,10	0.57	0	10,12,14	1.09	1 (10%)
22	FUB	VE	1	22	9,9,10	0.56	0	10,12,14	1.33	1 (10%)
22	FUB	VE	2	22	9,9,10	0.53	0	10,12,14	0.97	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	GZL	VE	3	22	11,11,12	6.73	7 (63%)	14,15,17	1.41	1 (7%)
22	AHR	VE	4	22	9,9,10	0.57	0	10,12,14	1.15	1 (10%)
22	AHR	VE	5	22	9,9,10	0.58	0	10,12,14	0.96	1 (10%)
22	AHR	VE	6	22	9,9,10	0.58	0	10,12,14	0.94	0
4	FUB	W	1	4	9,9,10	0.57	0	10,12,14	0.84	0
4	FUB	W	2	4	9,9,10	0.57	0	10,12,14	0.76	0
4	FUB	W	3	4	9,9,10	0.57	0	10,12,14	0.83	0
4	AHR	W	4	4	9,9,10	0.57	0	10,12,14	1.07	1 (10%)
9	FUB	WA	1	9	9,9,10	0.56	0	10,12,14	0.84	0
9	FUB	WA	2	9	9,9,10	0.58	0	10,12,14	0.95	0
13	FUB	WB	1	13	9,9,10	0.54	0	10,12,14	0.95	0
13	FUB	WB	2	13	9,9,10	0.55	0	10,12,14	1.07	1 (10%)
13	GZL	WB	3	13	11,11,12	6.80	7 (63%)	14,15,17	1.26	1 (7%)
13	AHR	WB	4	13	9,9,10	0.58	0	10,12,14	1.11	1 (10%)
3	FUB	WC	1	3	9,9,10	0.56	0	10,12,14	1.08	1 (10%)
3	FUB	WC	2	3	9,9,10	0.57	0	10,12,14	0.93	0
3	FUB	WC	3	3	9,9,10	0.57	0	10,12,14	1.03	1 (10%)
7	FUB	WD	1	7	9,9,10	0.60	0	10,12,14	0.93	0
7	FUB	WD	2	7	9,9,10	0.59	0	10,12,14	1.10	0
7	FUB	WD	3	7	9,9,10	0.58	0	10,12,14	0.95	0
7	AHR	WD	4	7	9,9,10	0.57	0	10,12,14	1.07	1 (10%)
20	FUB	WE	1	20	9,9,10	0.54	0	10,12,14	0.93	0
20	FUB	WE	2	20	9,9,10	0.56	0	10,12,14	0.81	0
20	GZL	WE	3	20	11,11,12	6.73	7 (63%)	14,15,17	1.36	1 (7%)
20	AHR	WE	4	20	9,9,10	0.57	0	10,12,14	1.11	1 (10%)
4	FUB	X	1	4	9,9,10	0.54	0	10,12,14	0.95	1 (10%)
4	FUB	X	2	4	9,9,10	0.55	0	10,12,14	0.79	0
4	FUB	X	3	4	9,9,10	0.57	0	10,12,14	0.83	0
4	AHR	X	4	4	9,9,10	0.58	0	10,12,14	0.98	0
3	FUB	XA	1	3	9,9,10	0.57	0	10,12,14	1.04	0
3	FUB	XA	2	3	9,9,10	0.53	0	10,12,14	0.65	0
3	FUB	XA	3	3	9,9,10	0.58	0	10,12,14	1.05	1 (10%)
6	FUB	XB	1	6	9,9,10	0.57	0	10,12,14	1.02	0
6	FUB	XB	2	6	9,9,10	0.58	0	10,12,14	1.07	1 (10%)
6	GZL	XB	3	6	11,11,12	7.02	6 (54%)	14,15,17	3.89	4 (28%)
7	FUB	XC	1	7	9,9,10	0.58	0	10,12,14	1.04	0
7	FUB	XC	2	7	9,9,10	0.53	0	10,12,14	0.99	1 (10%)
7	FUB	XC	3	7	9,9,10	0.59	0	10,12,14	0.87	0
7	AHR	XC	4	7	9,9,10	0.58	0	10,12,14	0.79	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
11	FUB	XD	1	11	9,9,10	0.66	0	10,12,14	1.19	1 (10%)
11	AHR	XD	2	11	9,9,10	0.58	0	10,12,14	1.00	1 (10%)
11	AHR	XD	3	11	9,9,10	0.56	0	10,12,14	1.09	1 (10%)
23	FUB	XE	1	23	9,9,10	0.56	0	10,12,14	1.20	1 (10%)
23	FUB	XE	2	23	9,9,10	0.56	0	10,12,14	0.71	0
23	GZL	XE	3	23	11,11,12	6.72	7 (63%)	14,15,17	1.41	1 (7%)
23	AHR	XE	4	23	9,9,10	0.56	0	10,12,14	0.88	1 (10%)
23	AHR	XE	5	23	9,9,10	0.57	0	10,12,14	0.92	0
23	AHR	XE	6	23	9,9,10	0.56	0	10,12,14	0.98	1 (10%)
9	FUB	Y	1	9	9,9,10	0.59	0	10,12,14	1.04	1 (10%)
9	FUB	Y	2	9	9,9,10	0.58	0	10,12,14	1.05	1 (10%)
10	FUB	YA	1	10	9,9,10	0.57	0	10,12,14	0.82	0
10	FUB	YA	2	10	9,9,10	0.58	0	10,12,14	0.85	0
10	FUB	YA	3	10	9,9,10	0.57	0	10,12,14	0.82	0
10	AHR	YA	4	10	9,9,10	0.58	0	10,12,14	0.99	0
10	AHR	YA	5	10	9,9,10	0.58	0	10,12,14	1.11	1 (10%)
13	FUB	YB	1	13	9,9,10	0.53	0	10,12,14	0.76	0
13	FUB	YB	2	13	9,9,10	0.57	0	10,12,14	0.75	0
13	GZL	YB	3	13	11,11,12	6.78	7 (63%)	14,15,17	1.14	1 (7%)
13	AHR	YB	4	13	9,9,10	0.56	0	10,12,14	1.12	1 (10%)
4	FUB	YC	1	4	9,9,10	0.57	0	10,12,14	0.87	0
4	FUB	YC	2	4	9,9,10	0.55	0	10,12,14	0.97	1 (10%)
4	FUB	YC	3	4	9,9,10	0.57	0	10,12,14	0.81	0
4	AHR	YC	4	4	9,9,10	0.57	0	10,12,14	1.10	1 (10%)
9	FUB	YD	1	9	9,9,10	0.55	0	10,12,14	0.60	0
9	FUB	YD	2	9	9,9,10	0.55	0	10,12,14	0.78	0
24	FUB	YE	1	24	9,9,10	0.54	0	10,12,14	1.47	1 (10%)
24	FUB	YE	2	24	9,9,10	0.55	0	10,12,14	0.80	0
24	GZL	YE	3	24	11,11,12	6.73	7 (63%)	14,15,17	1.39	1 (7%)
24	AHR	YE	4	24	9,9,10	0.59	0	10,12,14	1.10	2 (20%)
24	AHR	YE	5	24	9,9,10	0.58	0	10,12,14	1.18	1 (10%)
24	AHR	YE	6	24	9,9,10	0.59	0	10,12,14	1.00	1 (10%)
4	FUB	Z	1	4	9,9,10	0.55	0	10,12,14	1.13	1 (10%)
4	FUB	Z	2	4	9,9,10	0.55	0	10,12,14	0.96	1 (10%)
4	FUB	Z	3	4	9,9,10	0.56	0	10,12,14	0.81	0
4	AHR	Z	4	4	9,9,10	0.58	0	10,12,14	1.15	1 (10%)
3	FUB	ZA	1	3	9,9,10	0.57	0	10,12,14	1.11	1 (10%)
3	FUB	ZA	2	3	9,9,10	0.56	0	10,12,14	0.90	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	FUB	ZA	3	3	9,9,10	0.57	0	10,12,14	0.94	0
13	FUB	ZB	1	13	9,9,10	0.59	0	10,12,14	1.00	0
13	FUB	ZB	2	13	9,9,10	0.57	0	10,12,14	0.93	0
13	GZL	ZB	3	13	11,11,12	6.73	7 (63%)	14,15,17	1.57	3 (21%)
13	AHR	ZB	4	13	9,9,10	0.57	0	10,12,14	0.94	0
7	FUB	ZC	1	7	9,9,10	0.55	0	10,12,14	0.82	0
7	FUB	ZC	2	7	9,9,10	0.57	0	10,12,14	0.91	0
7	FUB	ZC	3	7	9,9,10	0.55	0	10,12,14	1.13	1 (10%)
7	AHR	ZC	4	7	9,9,10	0.57	0	10,12,14	1.01	0
4	FUB	ZD	1	4	9,9,10	0.57	0	10,12,14	0.99	1 (10%)
4	FUB	ZD	2	4	9,9,10	0.57	0	10,12,14	0.85	0
4	FUB	ZD	3	4	9,9,10	0.59	0	10,12,14	0.92	0
4	AHR	ZD	4	4	9,9,10	0.58	0	10,12,14	1.00	0
6	FUB	ZE	1	6	9,9,10	0.57	0	10,12,14	0.86	0
6	FUB	ZE	2	6	9,9,10	0.56	0	10,12,14	1.02	1 (10%)
6	GZL	ZE	3	6	11,11,12	6.70	7 (63%)	14,15,17	1.41	1 (7%)
10	FUB	a	1	10	9,9,10	0.56	0	10,12,14	1.08	1 (10%)
10	FUB	a	2	10	9,9,10	0.56	0	10,12,14	0.97	1 (10%)
10	FUB	a	3	10	9,9,10	0.57	0	10,12,14	0.82	0
10	AHR	a	4	10	9,9,10	0.55	0	10,12,14	1.18	1 (10%)
10	AHR	a	5	10	9,9,10	0.57	0	10,12,14	1.07	1 (10%)
4	FUB	aA	1	4	9,9,10	0.55	0	10,12,14	0.77	0
4	FUB	aA	2	4	9,9,10	0.58	0	10,12,14	0.92	0
4	FUB	aA	3	4	9,9,10	0.57	0	10,12,14	0.96	0
4	AHR	aA	4	4	9,9,10	0.57	0	10,12,14	0.98	0
6	FUB	aB	1	6	9,9,10	0.57	0	10,12,14	0.89	0
6	FUB	aB	2	6	9,9,10	0.54	0	10,12,14	1.25	2 (20%)
6	GZL	aB	3	6	11,11,12	6.71	7 (63%)	14,15,17	1.48	2 (14%)
11	FUB	aC	1	11	9,9,10	0.64	0	10,12,14	1.07	0
11	AHR	aC	2	11	9,9,10	0.57	0	10,12,14	1.03	1 (10%)
11	AHR	aC	3	11	9,9,10	0.58	0	10,12,14	1.00	1 (10%)
3	FUB	aD	1	3	9,9,10	0.57	0	10,12,14	0.92	0
3	FUB	aD	2	3	9,9,10	0.57	0	10,12,14	0.95	0
3	FUB	aD	3	3	9,9,10	0.58	0	10,12,14	0.89	0
19	FUB	aE	1	19	9,9,10	0.59	0	10,12,14	0.85	0
19	FUB	aE	2	19	9,9,10	0.57	0	10,12,14	0.98	0
19	GZL	aE	3	19	11,11,12	6.69	7 (63%)	14,15,17	1.69	3 (21%)
19	AHR	aE	4	19	9,9,10	0.57	0	10,12,14	1.08	1 (10%)
3	FUB	b	1	3	9,9,10	0.58	0	10,12,14	1.12	1 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	FUB	b	2	3	9,9,10	0.57	0	10,12,14	0.94	0
3	FUB	b	3	3	9,9,10	0.58	0	10,12,14	0.92	0
4	FUB	bA	1	4	9,9,10	0.55	0	10,12,14	0.88	0
4	FUB	bA	2	4	9,9,10	0.57	0	10,12,14	0.88	0
4	FUB	bA	3	4	9,9,10	0.57	0	10,12,14	0.98	0
4	AHR	bA	4	4	9,9,10	0.57	0	10,12,14	0.88	0
6	FUB	bB	1	6	9,9,10	0.55	0	10,12,14	1.05	1 (10%)
6	FUB	bB	2	6	9,9,10	0.59	0	10,12,14	0.96	1 (10%)
6	GZL	bB	3	6	11,11,12	6.73	7 (63%)	14,15,17	1.43	1 (7%)
9	FUB	bC	1	9	9,9,10	0.56	0	10,12,14	0.70	0
9	FUB	bC	2	9	9,9,10	0.54	0	10,12,14	0.82	0
3	FUB	bD	1	3	9,9,10	0.51	0	10,12,14	0.87	0
3	FUB	bD	2	3	9,9,10	0.58	0	10,12,14	0.87	0
3	FUB	bD	3	3	9,9,10	0.57	0	10,12,14	0.82	0
6	FUB	bE	1	6	9,9,10	0.61	0	10,12,14	1.01	0
6	FUB	bE	2	6	9,9,10	0.55	0	10,12,14	0.86	0
6	GZL	bE	3	6	11,11,12	6.77	7 (63%)	14,15,17	1.55	1 (7%)
4	FUB	c	1	4	9,9,10	0.56	0	10,12,14	0.79	0
4	FUB	c	2	4	9,9,10	0.58	0	10,12,14	0.89	0
4	FUB	c	3	4	9,9,10	0.55	0	10,12,14	0.92	0
4	AHR	c	4	4	9,9,10	0.56	0	10,12,14	1.02	1 (10%)
3	FUB	cA	1	3	9,9,10	0.56	0	10,12,14	0.83	0
3	FUB	cA	2	3	9,9,10	0.58	0	10,12,14	0.99	1 (10%)
3	FUB	cA	3	3	9,9,10	0.58	0	10,12,14	1.07	1 (10%)
6	FUB	cB	1	6	9,9,10	0.57	0	10,12,14	1.00	1 (10%)
6	FUB	cB	2	6	9,9,10	0.58	0	10,12,14	1.11	1 (10%)
6	GZL	cB	3	6	11,11,12	6.74	7 (63%)	14,15,17	1.59	2 (14%)
4	FUB	cC	1	4	9,9,10	0.56	0	10,12,14	1.19	1 (10%)
4	FUB	cC	2	4	9,9,10	0.57	0	10,12,14	0.85	0
4	FUB	cC	3	4	9,9,10	0.57	0	10,12,14	0.95	0
4	AHR	cC	4	4	9,9,10	0.57	0	10,12,14	1.06	1 (10%)
12	FUB	cD	1	12	9,9,10	0.57	0	10,12,14	0.80	0
12	FUB	cD	2	12	9,9,10	0.59	0	10,12,14	0.96	0
12	GZL	cD	3	12	11,11,12	6.72	7 (63%)	14,15,17	1.45	2 (14%)
12	AHR	cD	4	12	9,9,10	0.58	0	10,12,14	0.98	0
12	AHR	cD	5	12	9,9,10	0.59	0	10,12,14	1.02	1 (10%)
18	FUB	cE	1	18	9,9,10	0.55	0	10,12,14	1.05	1 (10%)
18	FUB	cE	2	18	9,9,10	0.59	0	10,12,14	0.88	0
18	GZL	cE	3	18	11,11,12	6.74	7 (63%)	14,15,17	1.66	2 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
18	AHR	cE	4	18	9,9,10	0.57	0	10,12,14	0.95	0
18	AHR	cE	5	18	9,9,10	0.57	0	10,12,14	0.87	0
4	FUB	d	1	4	9,9,10	0.55	0	10,12,14	0.97	1 (10%)
4	FUB	d	2	4	9,9,10	0.57	0	10,12,14	0.92	0
4	FUB	d	3	4	9,9,10	0.57	0	10,12,14	1.00	1 (10%)
4	AHR	d	4	4	9,9,10	0.56	0	10,12,14	1.15	1 (10%)
7	FUB	dA	1	7	9,9,10	0.56	0	10,12,14	1.11	1 (10%)
7	FUB	dA	2	7	9,9,10	0.54	0	10,12,14	1.07	1 (10%)
7	FUB	dA	3	7	9,9,10	0.56	0	10,12,14	0.88	0
7	AHR	dA	4	7	9,9,10	0.57	0	10,12,14	0.78	0
13	FUB	dB	1	13	9,9,10	0.58	0	10,12,14	0.74	0
13	FUB	dB	2	13	9,9,10	0.56	0	10,12,14	1.12	0
13	GZL	dB	3	13	11,11,12	6.75	7 (63%)	14,15,17	1.87	4 (28%)
13	AHR	dB	4	13	9,9,10	0.57	0	10,12,14	1.02	1 (10%)
3	FUB	dC	1	3	9,9,10	0.56	0	10,12,14	0.86	0
3	FUB	dC	2	3	9,9,10	0.58	0	10,12,14	0.86	0
3	FUB	dC	3	3	9,9,10	0.58	0	10,12,14	1.09	1 (10%)
13	FUB	dD	1	13	9,9,10	0.59	0	10,12,14	0.86	0
13	FUB	dD	2	13	9,9,10	0.56	0	10,12,14	0.84	0
13	GZL	dD	3	13	11,11,12	6.72	7 (63%)	14,15,17	1.27	1 (7%)
13	AHR	dD	4	13	9,9,10	0.56	0	10,12,14	0.93	0
22	FUB	dE	1	22	9,9,10	0.56	0	10,12,14	0.97	1 (10%)
22	FUB	dE	2	22	9,9,10	0.57	0	10,12,14	1.00	1 (10%)
22	GZL	dE	3	22	11,11,12	6.72	7 (63%)	14,15,17	1.53	1 (7%)
22	AHR	dE	4	22	9,9,10	0.55	0	10,12,14	1.14	1 (10%)
22	AHR	dE	5	22	9,9,10	0.58	0	10,12,14	1.10	0
22	AHR	dE	6	22	9,9,10	0.55	0	10,12,14	1.09	1 (10%)
3	FUB	e	1	3	9,9,10	0.59	0	10,12,14	0.83	0
3	FUB	e	2	3	9,9,10	0.58	0	10,12,14	0.93	0
3	FUB	e	3	3	9,9,10	0.57	0	10,12,14	1.11	1 (10%)
4	FUB	eA	1	4	9,9,10	0.58	0	10,12,14	0.98	0
4	FUB	eA	2	4	9,9,10	0.56	0	10,12,14	0.82	0
4	FUB	eA	3	4	9,9,10	0.58	0	10,12,14	0.99	0
4	AHR	eA	4	4	9,9,10	0.58	0	10,12,14	0.95	0
15	FUB	eB	1	15	9,9,10	0.55	0	10,12,14	1.00	1 (10%)
15	FUB	eB	2	15	9,9,10	0.57	0	10,12,14	0.92	0
15	GZL	eB	3	15	11,11,12	6.75	7 (63%)	14,15,17	1.49	2 (14%)
15	AHR	eB	4	15	9,9,10	0.61	0	10,12,14	1.21	1 (10%)
15	AHR	eB	5	15	9,9,10	0.59	0	10,12,14	0.95	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	FUB	eC	1	3	9,9,10	0.55	0	10,12,14	0.69	0
3	FUB	eC	2	3	9,9,10	0.58	0	10,12,14	0.89	0
3	FUB	eC	3	3	9,9,10	0.58	0	10,12,14	0.90	0
14	FUB	eD	1	14	9,9,10	0.56	0	10,12,14	0.90	0
14	FUB	eD	2	14	9,9,10	0.58	0	10,12,14	0.84	0
14	GZL	eD	3	14	11,11,12	6.70	7 (63%)	14,15,17	1.76	2 (14%)
14	FUB	eD	4	14	9,9,10	0.59	0	10,12,14	1.01	1 (10%)
22	FUB	eE	1	22	9,9,10	0.61	0	10,12,14	1.17	1 (10%)
22	FUB	eE	2	22	9,9,10	0.57	0	10,12,14	0.91	0
22	GZL	eE	3	22	11,11,12	6.74	6 (54%)	14,15,17	1.57	1 (7%)
22	AHR	eE	4	22	9,9,10	0.56	0	10,12,14	1.06	1 (10%)
22	AHR	eE	5	22	9,9,10	0.55	0	10,12,14	1.07	1 (10%)
22	AHR	eE	6	22	9,9,10	0.59	0	10,12,14	1.19	1 (10%)
7	FUB	f	1	7	9,9,10	0.56	0	10,12,14	1.03	1 (10%)
7	FUB	f	2	7	9,9,10	0.55	0	10,12,14	1.04	1 (10%)
7	FUB	f	3	7	9,9,10	0.56	0	10,12,14	1.01	1 (10%)
7	AHR	f	4	7	9,9,10	0.53	0	10,12,14	0.80	0
7	FUB	fA	1	7	9,9,10	0.57	0	10,12,14	0.99	0
7	FUB	fA	2	7	9,9,10	0.58	0	10,12,14	0.92	0
7	FUB	fA	3	7	9,9,10	0.58	0	10,12,14	0.96	0
7	AHR	fA	4	7	9,9,10	0.57	0	10,12,14	0.98	0
15	FUB	fB	1	15	9,9,10	0.57	0	10,12,14	1.01	0
15	FUB	fB	2	15	9,9,10	0.58	0	10,12,14	0.88	0
15	GZL	fB	3	15	11,11,12	6.74	7 (63%)	14,15,17	1.31	1 (7%)
15	AHR	fB	4	15	9,9,10	0.58	0	10,12,14	1.04	1 (10%)
15	AHR	fB	5	15	9,9,10	0.56	0	10,12,14	1.06	1 (10%)
12	FUB	fC	1	12	9,9,10	0.59	0	10,12,14	0.93	0
12	FUB	fC	2	12	9,9,10	0.56	0	10,12,14	0.87	0
12	GZL	fC	3	12	11,11,12	6.75	7 (63%)	14,15,17	1.31	1 (7%)
12	AHR	fC	4	12	9,9,10	0.57	0	10,12,14	1.10	1 (10%)
12	AHR	fC	5	12	9,9,10	0.59	0	10,12,14	1.03	1 (10%)
12	FUB	fD	1	12	9,9,10	0.56	0	10,12,14	1.03	1 (10%)
12	FUB	fD	2	12	9,9,10	0.57	0	10,12,14	1.01	1 (10%)
12	GZL	fD	3	12	11,11,12	6.70	7 (63%)	14,15,17	1.25	1 (7%)
12	AHR	fD	4	12	9,9,10	0.56	0	10,12,14	0.91	0
12	AHR	fD	5	12	9,9,10	0.58	0	10,12,14	1.07	1 (10%)
18	FUB	fE	1	18	9,9,10	0.54	0	10,12,14	1.14	1 (10%)
18	FUB	fE	2	18	9,9,10	0.54	0	10,12,14	0.93	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
18	GZL	fE	3	18	11,11,12	6.73	7 (63%)	14,15,17	1.34	1 (7%)
18	AHR	fE	4	18	9,9,10	0.56	0	10,12,14	1.03	1 (10%)
18	AHR	fE	5	18	9,9,10	0.58	0	10,12,14	0.85	0
4	FUB	g	1	4	9,9,10	0.56	0	10,12,14	1.03	0
4	FUB	g	2	4	9,9,10	0.58	0	10,12,14	0.89	0
4	FUB	g	3	4	9,9,10	0.57	0	10,12,14	0.90	0
4	AHR	g	4	4	9,9,10	0.58	0	10,12,14	1.06	1 (10%)
11	FUB	gA	1	11	9,9,10	0.66	0	10,12,14	1.36	1 (10%)
11	AHR	gA	2	11	9,9,10	0.57	0	10,12,14	0.94	0
11	AHR	gA	3	11	9,9,10	0.56	0	10,12,14	1.01	1 (10%)
6	FUB	gB	1	6	9,9,10	0.57	0	10,12,14	0.85	0
6	FUB	gB	2	6	9,9,10	0.56	0	10,12,14	0.90	0
6	GZL	gB	3	6	11,11,12	6.71	7 (63%)	14,15,17	1.54	2 (14%)
13	FUB	gC	1	13	9,9,10	0.58	0	10,12,14	0.85	0
13	FUB	gC	2	13	9,9,10	0.59	0	10,12,14	1.01	0
13	GZL	gC	3	13	11,11,12	6.75	7 (63%)	14,15,17	1.28	1 (7%)
13	AHR	gC	4	13	9,9,10	0.57	0	10,12,14	1.10	1 (10%)
4	FUB	gD	1	4	9,9,10	0.57	0	10,12,14	1.03	1 (10%)
4	FUB	gD	2	4	9,9,10	0.56	0	10,12,14	0.99	1 (10%)
4	FUB	gD	3	4	9,9,10	0.57	0	10,12,14	0.78	0
4	AHR	gD	4	4	9,9,10	0.57	0	10,12,14	0.79	0
20	FUB	gE	1	20	9,9,10	0.56	0	10,12,14	0.95	0
20	FUB	gE	2	20	9,9,10	0.59	0	10,12,14	1.03	1 (10%)
20	GZL	gE	3	20	11,11,12	6.74	7 (63%)	14,15,17	1.28	1 (7%)
20	AHR	gE	4	20	9,9,10	0.58	0	10,12,14	0.87	0
7	FUB	h	1	7	9,9,10	0.56	0	10,12,14	1.01	0
7	FUB	h	2	7	9,9,10	0.59	0	10,12,14	0.97	0
7	FUB	h	3	7	9,9,10	0.57	0	10,12,14	1.00	0
7	AHR	h	4	7	9,9,10	0.57	0	10,12,14	1.03	1 (10%)
9	FUB	hA	1	9	9,9,10	0.54	0	10,12,14	0.87	1 (10%)
9	FUB	hA	2	9	9,9,10	0.55	0	10,12,14	0.78	0
3	FUB	hB	1	3	9,9,10	0.58	0	10,12,14	0.81	0
3	FUB	hB	2	3	9,9,10	0.58	0	10,12,14	0.85	0
3	FUB	hB	3	3	9,9,10	0.59	0	10,12,14	0.94	0
14	FUB	hC	1	14	9,9,10	0.56	0	10,12,14	1.04	1 (10%)
14	FUB	hC	2	14	9,9,10	0.57	0	10,12,14	0.87	0
14	GZL	hC	3	14	11,11,12	6.72	7 (63%)	14,15,17	1.67	2 (14%)
14	FUB	hC	4	14	9,9,10	0.59	0	10,12,14	0.85	0
14	FUB	hD	1	14	9,9,10	0.57	0	10,12,14	0.98	1 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
14	FUB	hD	2	14	9,9,10	0.58	0	10,12,14	1.05	1 (10%)
14	GZL	hD	3	14	11,11,12	6.61	7 (63%)	14,15,17	1.61	2 (14%)
14	FUB	hD	4	14	9,9,10	0.57	0	10,12,14	0.94	0
20	FUB	hE	1	20	9,9,10	0.57	0	10,12,14	0.96	0
20	FUB	hE	2	20	9,9,10	0.56	0	10,12,14	0.83	0
20	GZL	hE	3	20	11,11,12	6.72	7 (63%)	14,15,17	1.44	1 (7%)
20	AHR	hE	4	20	9,9,10	0.56	0	10,12,14	0.88	0
11	FUB	i	1	11	9,9,10	0.65	0	10,12,14	1.31	1 (10%)
11	AHR	i	2	11	9,9,10	0.56	0	10,12,14	1.08	1 (10%)
11	AHR	i	3	11	9,9,10	0.55	0	10,12,14	1.07	1 (10%)
4	FUB	iA	1	4	9,9,10	0.56	0	10,12,14	1.11	1 (10%)
4	FUB	iA	2	4	9,9,10	0.57	0	10,12,14	0.97	0
4	FUB	iA	3	4	9,9,10	0.56	0	10,12,14	0.87	0
4	AHR	iA	4	4	9,9,10	0.57	0	10,12,14	1.18	1 (10%)
12	FUB	iB	1	12	9,9,10	0.60	0	10,12,14	0.94	0
12	FUB	iB	2	12	9,9,10	0.59	0	10,12,14	1.01	0
12	GZL	iB	3	12	11,11,12	6.71	7 (63%)	14,15,17	1.53	2 (14%)
12	AHR	iB	4	12	9,9,10	0.57	0	10,12,14	1.02	1 (10%)
12	AHR	iB	5	12	9,9,10	0.60	0	10,12,14	0.97	0
12	FUB	iC	1	12	9,9,10	0.57	0	10,12,14	1.12	1 (10%)
12	FUB	iC	2	12	9,9,10	0.58	0	10,12,14	0.99	1 (10%)
12	GZL	iC	3	12	11,11,12	6.68	7 (63%)	14,15,17	1.43	1 (7%)
12	AHR	iC	4	12	9,9,10	0.57	0	10,12,14	1.02	1 (10%)
12	AHR	iC	5	12	9,9,10	0.56	0	10,12,14	1.07	1 (10%)
3	FUB	iD	1	3	9,9,10	0.57	0	10,12,14	0.98	1 (10%)
3	FUB	iD	2	3	9,9,10	0.55	0	10,12,14	0.79	0
3	FUB	iD	3	3	9,9,10	0.57	0	10,12,14	0.92	0
22	FUB	iE	1	22	9,9,10	0.55	0	10,12,14	1.17	1 (10%)
22	FUB	iE	2	22	9,9,10	0.55	0	10,12,14	0.89	0
22	GZL	iE	3	22	11,11,12	6.75	7 (63%)	14,15,17	1.33	1 (7%)
22	AHR	iE	4	22	9,9,10	0.60	0	10,12,14	0.99	0
22	AHR	iE	5	22	9,9,10	0.56	0	10,12,14	0.64	0
22	AHR	iE	6	22	9,9,10	0.57	0	10,12,14	1.14	1 (10%)
9	FUB	j	1	9	9,9,10	0.57	0	10,12,14	1.02	1 (10%)
9	FUB	j	2	9	9,9,10	0.56	0	10,12,14	0.78	0
3	FUB	jA	1	3	9,9,10	0.57	0	10,12,14	1.00	1 (10%)
3	FUB	jA	2	3	9,9,10	0.58	0	10,12,14	0.90	0
3	FUB	jA	3	3	9,9,10	0.56	0	10,12,14	1.06	1 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
13	FUB	jB	1	13	9,9,10	0.56	0	10,12,14	1.05	1 (10%)
13	FUB	jB	2	13	9,9,10	0.56	0	10,12,14	0.89	0
13	GZL	jB	3	13	11,11,12	6.75	7 (63%)	14,15,17	1.33	1 (7%)
13	AHR	jB	4	13	9,9,10	0.59	0	10,12,14	0.98	0
4	FUB	jC	1	4	9,9,10	0.56	0	10,12,14	1.02	1 (10%)
4	FUB	jC	2	4	9,9,10	0.58	0	10,12,14	0.97	0
4	FUB	jC	3	4	9,9,10	0.57	0	10,12,14	0.99	0
4	AHR	jC	4	4	9,9,10	0.57	0	10,12,14	0.93	0
10	FUB	jD	1	10	9,9,10	0.55	0	10,12,14	1.20	1 (10%)
10	FUB	jD	2	10	9,9,10	0.59	0	10,12,14	0.98	0
10	FUB	jD	3	10	9,9,10	0.58	0	10,12,14	0.92	0
10	AHR	jD	4	10	9,9,10	0.58	0	10,12,14	0.96	0
10	AHR	jD	5	10	9,9,10	0.57	0	10,12,14	1.05	1 (10%)
20	FUB	jE	1	20	9,9,10	0.59	0	10,12,14	1.01	0
20	FUB	jE	2	20	9,9,10	0.57	0	10,12,14	0.91	0
20	GZL	jE	3	20	11,11,12	6.72	7 (63%)	14,15,17	1.58	2 (14%)
20	AHR	jE	4	20	9,9,10	0.57	0	10,12,14	0.89	0
4	FUB	k	1	4	9,9,10	0.58	0	10,12,14	0.83	0
4	FUB	k	2	4	9,9,10	0.58	0	10,12,14	0.96	0
4	FUB	k	3	4	9,9,10	0.55	0	10,12,14	0.94	0
4	AHR	k	4	4	9,9,10	0.58	0	10,12,14	0.96	0
3	FUB	kA	1	3	9,9,10	0.53	0	10,12,14	0.77	0
3	FUB	kA	2	3	9,9,10	0.55	0	10,12,14	0.80	0
3	FUB	kA	3	3	9,9,10	0.58	0	10,12,14	0.87	0
14	FUB	kB	1	14	9,9,10	0.59	0	10,12,14	0.90	0
14	FUB	kB	2	14	9,9,10	0.56	0	10,12,14	1.05	1 (10%)
14	GZL	kB	3	14	11,11,12	6.65	7 (63%)	14,15,17	1.63	3 (21%)
14	FUB	kB	4	14	9,9,10	0.57	0	10,12,14	1.07	1 (10%)
14	FUB	kC	1	14	9,9,10	0.57	0	10,12,14	0.97	1 (10%)
14	FUB	kC	2	14	9,9,10	0.58	0	10,12,14	0.99	0
14	GZL	kC	3	14	11,11,12	6.66	7 (63%)	14,15,17	1.91	2 (14%)
14	FUB	kC	4	14	9,9,10	0.60	0	10,12,14	0.85	0
4	FUB	kD	1	4	9,9,10	0.60	0	10,12,14	0.96	0
4	FUB	kD	2	4	9,9,10	0.58	0	10,12,14	0.85	0
4	FUB	kD	3	4	9,9,10	0.56	0	10,12,14	0.90	0
4	AHR	kD	4	4	9,9,10	0.57	0	10,12,14	0.93	0
21	FUB	kE	1	21	9,9,10	0.55	0	10,12,14	1.16	2 (20%)
21	FUB	kE	2	21	9,9,10	0.56	0	10,12,14	1.01	1 (10%)
21	GZL	kE	3	21	11,11,12	6.75	7 (63%)	14,15,17	1.24	1 (7%)
21	AHR	kE	4	21	9,9,10	0.58	0	10,12,14	0.98	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
21	AHR	kE	5	21	9,9,10	0.56	0	10,12,14	1.10	1 (10%)
3	FUB	l	1	3	9,9,10	0.58	0	10,12,14	0.92	0
3	FUB	l	2	3	9,9,10	0.53	0	10,12,14	0.82	0
3	FUB	l	3	3	9,9,10	0.57	0	10,12,14	0.88	0
12	FUB	lA	1	12	9,9,10	0.55	0	10,12,14	0.92	0
12	FUB	lA	2	12	9,9,10	0.58	0	10,12,14	0.94	0
12	GZL	lA	3	12	11,11,12	6.73	7 (63%)	14,15,17	1.24	1 (7%)
12	AHR	lA	4	12	9,9,10	0.57	0	10,12,14	1.12	1 (10%)
12	AHR	lA	5	12	9,9,10	0.58	0	10,12,14	1.12	1 (10%)
12	FUB	lB	1	12	9,9,10	0.54	0	10,12,14	1.16	1 (10%)
12	FUB	lB	2	12	9,9,10	0.57	0	10,12,14	0.94	0
12	GZL	lB	3	12	11,11,12	6.71	7 (63%)	14,15,17	1.36	1 (7%)
12	AHR	lB	4	12	9,9,10	0.57	0	10,12,14	1.01	1 (10%)
12	AHR	lB	5	12	9,9,10	0.58	0	10,12,14	0.97	0
3	FUB	lC	1	3	9,9,10	0.57	0	10,12,14	0.81	0
3	FUB	lC	2	3	9,9,10	0.56	0	10,12,14	0.87	0
3	FUB	lC	3	3	9,9,10	0.58	0	10,12,14	1.01	0
3	FUB	lD	1	3	9,9,10	0.59	0	10,12,14	0.87	0
3	FUB	lD	2	3	9,9,10	0.56	0	10,12,14	0.95	0
3	FUB	lD	3	3	9,9,10	0.59	0	10,12,14	0.86	0
24	FUB	lE	1	24	9,9,10	0.54	0	10,12,14	1.33	1 (10%)
24	FUB	lE	2	24	9,9,10	0.55	0	10,12,14	1.04	1 (10%)
24	GZL	lE	3	24	11,11,12	6.71	7 (63%)	14,15,17	1.48	1 (7%)
24	AHR	lE	4	24	9,9,10	0.59	0	10,12,14	1.15	2 (20%)
24	AHR	lE	5	24	9,9,10	0.55	0	10,12,14	1.10	1 (10%)
24	AHR	lE	6	24	9,9,10	0.57	0	10,12,14	1.13	1 (10%)
3	FUB	m	1	3	9,9,10	0.53	0	10,12,14	0.88	0
3	FUB	m	2	3	9,9,10	0.57	0	10,12,14	0.79	0
3	FUB	m	3	3	9,9,10	0.57	0	10,12,14	0.88	0
13	FUB	mA	1	13	9,9,10	0.56	0	10,12,14	0.83	0
13	FUB	mA	2	13	9,9,10	0.60	0	10,12,14	0.88	0
13	GZL	mA	3	13	11,11,12	6.76	7 (63%)	14,15,17	1.28	1 (7%)
13	AHR	mA	4	13	9,9,10	0.55	0	10,12,14	1.07	1 (10%)
4	FUB	mB	1	4	9,9,10	0.55	0	10,12,14	1.00	1 (10%)
4	FUB	mB	2	4	9,9,10	0.56	0	10,12,14	0.94	0
4	FUB	mB	3	4	9,9,10	0.57	0	10,12,14	1.02	0
4	AHR	mB	4	4	9,9,10	0.58	0	10,12,14	0.95	1 (10%)
10	FUB	mC	1	10	9,9,10	0.57	0	10,12,14	1.13	1 (10%)
10	FUB	mC	2	10	9,9,10	0.58	0	10,12,14	0.99	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
10	FUB	mC	3	10	9,9,10	0.57	0	10,12,14	0.82	0
10	AHR	mC	4	10	9,9,10	0.57	0	10,12,14	1.03	1 (10%)
10	AHR	mC	5	10	9,9,10	0.57	0	10,12,14	1.19	1 (10%)
3	FUB	mD	1	3	9,9,10	0.56	0	10,12,14	0.69	0
3	FUB	mD	2	3	9,9,10	0.58	0	10,12,14	0.99	0
3	FUB	mD	3	3	9,9,10	0.56	0	10,12,14	1.05	1 (10%)
6	FUB	mE	1	6	9,9,10	0.58	0	10,12,14	0.98	0
6	FUB	mE	2	6	9,9,10	0.58	0	10,12,14	0.97	1 (10%)
6	GZL	mE	3	6	11,11,12	6.72	7 (63%)	14,15,17	1.70	2 (14%)
12	FUB	n	1	12	9,9,10	0.55	0	10,12,14	0.87	0
12	FUB	n	2	12	9,9,10	0.58	0	10,12,14	0.84	0
12	GZL	n	3	12	11,11,12	6.73	7 (63%)	14,15,17	1.29	1 (7%)
12	AHR	n	4	12	9,9,10	0.55	0	10,12,14	1.14	1 (10%)
12	AHR	n	5	12	9,9,10	0.57	0	10,12,14	1.07	1 (10%)
14	FUB	nA	1	14	9,9,10	0.52	0	10,12,14	0.90	0
14	FUB	nA	2	14	9,9,10	0.59	0	10,12,14	0.86	0
14	GZL	nA	3	14	11,11,12	6.72	7 (63%)	14,15,17	1.90	4 (28%)
14	FUB	nA	4	14	9,9,10	0.59	0	10,12,14	1.07	0
14	FUB	nB	1	14	9,9,10	0.57	0	10,12,14	0.89	0
14	FUB	nB	2	14	9,9,10	0.58	0	10,12,14	1.01	1 (10%)
14	GZL	nB	3	14	11,11,12	6.67	7 (63%)	14,15,17	1.60	3 (21%)
14	FUB	nB	4	14	9,9,10	0.57	0	10,12,14	1.09	1 (10%)
4	FUB	nC	1	4	9,9,10	0.56	0	10,12,14	1.04	1 (10%)
4	FUB	nC	2	4	9,9,10	0.57	0	10,12,14	0.99	0
4	FUB	nC	3	4	9,9,10	0.58	0	10,12,14	0.97	0
4	AHR	nC	4	4	9,9,10	0.58	0	10,12,14	1.02	1 (10%)
3	FUB	nD	1	3	9,9,10	0.60	0	10,12,14	1.00	0
3	FUB	nD	2	3	9,9,10	0.58	0	10,12,14	0.95	0
3	FUB	nD	3	3	9,9,10	0.54	0	10,12,14	0.65	0
6	FUB	nE	1	6	9,9,10	0.57	0	10,12,14	1.11	1 (10%)
6	FUB	nE	2	6	9,9,10	0.57	0	10,12,14	0.97	0
6	GZL	nE	3	6	11,11,12	6.69	7 (63%)	14,15,17	1.64	2 (14%)
13	FUB	o	1	13	9,9,10	0.57	0	10,12,14	0.77	0
13	FUB	o	2	13	9,9,10	0.58	0	10,12,14	0.85	0
13	GZL	o	3	13	11,11,12	6.76	7 (63%)	14,15,17	1.26	1 (7%)
13	AHR	o	4	13	9,9,10	0.57	0	10,12,14	1.08	1 (10%)
12	FUB	oA	1	12	9,9,10	0.54	0	10,12,14	1.11	1 (10%)
12	FUB	oA	2	12	9,9,10	0.56	0	10,12,14	0.93	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
12	GZL	oA	3	12	11,11,12	6.75	7 (63%)	14,15,17	1.30	1 (7%)
12	AHR	oA	4	12	9,9,10	0.59	0	10,12,14	0.90	0
12	AHR	oA	5	12	9,9,10	0.59	0	10,12,14	1.04	1 (10%)
3	FUB	oB	1	3	9,9,10	0.57	0	10,12,14	1.07	1 (10%)
3	FUB	oB	2	3	9,9,10	0.56	0	10,12,14	0.82	0
3	FUB	oB	3	3	9,9,10	0.57	0	10,12,14	1.04	1 (10%)
3	FUB	oC	1	3	9,9,10	0.60	0	10,12,14	0.91	0
3	FUB	oC	2	3	9,9,10	0.57	0	10,12,14	0.92	0
3	FUB	oC	3	3	9,9,10	0.59	0	10,12,14	0.87	0
3	FUB	oD	1	3	9,9,10	0.59	0	10,12,14	0.96	0
3	FUB	oD	2	3	9,9,10	0.57	0	10,12,14	0.87	0
3	FUB	oD	3	3	9,9,10	0.58	0	10,12,14	1.04	1 (10%)
6	FUB	oE	1	6	9,9,10	0.57	0	10,12,14	0.86	0
6	FUB	oE	2	6	9,9,10	0.57	0	10,12,14	0.99	1 (10%)
6	GZL	oE	3	6	11,11,12	6.69	7 (63%)	14,15,17	1.67	2 (14%)
14	FUB	p	1	14	9,9,10	0.54	0	10,12,14	0.86	0
14	FUB	p	2	14	9,9,10	0.58	0	10,12,14	0.89	0
14	GZL	p	3	14	11,11,12	6.70	7 (63%)	14,15,17	1.69	4 (28%)
14	FUB	p	4	14	9,9,10	0.58	0	10,12,14	1.05	1 (10%)
4	FUB	pA	1	4	9,9,10	0.56	0	10,12,14	0.74	0
4	FUB	pA	2	4	9,9,10	0.57	0	10,12,14	0.84	0
4	FUB	pA	3	4	9,9,10	0.57	0	10,12,14	0.80	0
4	AHR	pA	4	4	9,9,10	0.56	0	10,12,14	0.92	0
10	FUB	pB	1	10	9,9,10	0.58	0	10,12,14	1.09	0
10	FUB	pB	2	10	9,9,10	0.58	0	10,12,14	1.05	0
10	FUB	pB	3	10	9,9,10	0.57	0	10,12,14	0.84	0
10	AHR	pB	4	10	9,9,10	0.58	0	10,12,14	1.06	1 (10%)
10	AHR	pB	5	10	9,9,10	0.58	0	10,12,14	1.17	1 (10%)
3	FUB	pC	1	3	9,9,10	0.58	0	10,12,14	1.07	1 (10%)
3	FUB	pC	2	3	9,9,10	0.58	0	10,12,14	1.02	1 (10%)
3	FUB	pC	3	3	9,9,10	0.58	0	10,12,14	0.90	0
3	FUB	pD	1	3	9,9,10	0.59	0	10,12,14	1.09	1 (10%)
3	FUB	pD	2	3	9,9,10	0.56	0	10,12,14	0.98	0
3	FUB	pD	3	3	9,9,10	0.56	0	10,12,14	1.05	1 (10%)
18	FUB	pE	1	18	9,9,10	0.55	0	10,12,14	2.39	5 (50%)
18	FUB	pE	2	18	9,9,10	0.57	0	10,12,14	1.00	1 (10%)
18	GZL	pE	3	18	11,11,12	6.71	7 (63%)	14,15,17	1.53	2 (14%)
18	AHR	pE	4	18	9,9,10	0.59	0	10,12,14	1.05	1 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
18	AHR	pE	5	18	9,9,10	0.61	0	10,12,14	1.20	1 (10%)
12	FUB	q	1	12	9,9,10	0.56	0	10,12,14	1.02	1 (10%)
12	FUB	q	2	12	9,9,10	0.57	0	10,12,14	0.94	0
12	GZL	q	3	12	11,11,12	6.72	7 (63%)	14,15,17	1.35	1 (7%)
12	AHR	q	4	12	9,9,10	0.58	0	10,12,14	0.97	1 (10%)
12	AHR	q	5	12	9,9,10	0.55	0	10,12,14	1.04	1 (10%)
14	FUB	qA	1	14	9,9,10	0.59	0	10,12,14	0.75	0
14	FUB	qA	2	14	9,9,10	0.59	0	10,12,14	0.90	0
14	GZL	qA	3	14	11,11,12	6.73	7 (63%)	14,15,17	1.72	2 (14%)
14	FUB	qA	4	14	9,9,10	0.58	0	10,12,14	1.02	0
4	FUB	qB	1	4	9,9,10	0.59	0	10,12,14	1.05	1 (10%)
4	FUB	qB	2	4	9,9,10	0.58	0	10,12,14	1.00	1 (10%)
4	FUB	qB	3	4	9,9,10	0.58	0	10,12,14	0.99	0
4	AHR	qB	4	4	9,9,10	0.57	0	10,12,14	1.08	1 (10%)
3	FUB	qC	1	3	9,9,10	0.57	0	10,12,14	0.98	0
3	FUB	qC	2	3	9,9,10	0.56	0	10,12,14	0.81	0
3	FUB	qC	3	3	9,9,10	0.54	0	10,12,14	0.63	0
3	FUB	qD	1	3	9,9,10	0.58	0	10,12,14	0.89	0
3	FUB	qD	2	3	9,9,10	0.58	0	10,12,14	0.93	0
3	FUB	qD	3	3	9,9,10	0.56	0	10,12,14	0.93	0
19	FUB	qE	1	19	9,9,10	0.57	0	10,12,14	1.27	1 (10%)
19	FUB	qE	2	19	9,9,10	0.58	0	10,12,14	0.88	0
19	GZL	qE	3	19	11,11,12	6.73	7 (63%)	14,15,17	1.54	2 (14%)
19	AHR	qE	4	19	9,9,10	0.59	0	10,12,14	0.80	0
4	FUB	r	1	4	9,9,10	0.55	0	10,12,14	0.78	0
4	FUB	r	2	4	9,9,10	0.57	0	10,12,14	0.87	0
4	FUB	r	3	4	9,9,10	0.57	0	10,12,14	0.90	0
4	AHR	r	4	4	9,9,10	0.58	0	10,12,14	0.83	0
3	FUB	rA	1	3	9,9,10	0.54	0	10,12,14	0.80	0
3	FUB	rA	2	3	9,9,10	0.55	0	10,12,14	0.81	0
3	FUB	rA	3	3	9,9,10	0.59	0	10,12,14	0.92	0
3	FUB	rB	1	3	9,9,10	0.56	0	10,12,14	0.95	1 (10%)
3	FUB	rB	2	3	9,9,10	0.57	0	10,12,14	0.83	0
3	FUB	rB	3	3	9,9,10	0.56	0	10,12,14	0.98	0
3	FUB	rC	1	3	9,9,10	0.57	0	10,12,14	1.06	1 (10%)
3	FUB	rC	2	3	9,9,10	0.57	0	10,12,14	0.92	0
3	FUB	rC	3	3	9,9,10	0.59	0	10,12,14	0.99	0
3	FUB	rD	1	3	9,9,10	0.56	0	10,12,14	1.05	1 (10%)
3	FUB	rD	2	3	9,9,10	0.58	0	10,12,14	0.89	0
3	FUB	rD	3	3	9,9,10	0.57	0	10,12,14	0.97	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
18	FUB	rE	1	18	9,9,10	0.61	0	10,12,14	1.03	0
18	FUB	rE	2	18	9,9,10	0.57	0	10,12,14	1.10	1 (10%)
18	GZL	rE	3	18	11,11,12	6.76	7 (63%)	14,15,17	1.46	2 (14%)
18	AHR	rE	4	18	9,9,10	0.55	0	10,12,14	0.77	0
18	AHR	rE	5	18	9,9,10	0.58	0	10,12,14	1.16	1 (10%)
14	FUB	s	1	14	9,9,10	0.55	0	10,12,14	0.86	0
14	FUB	s	2	14	9,9,10	0.59	0	10,12,14	0.94	0
14	GZL	s	3	14	11,11,12	6.70	7 (63%)	14,15,17	1.98	3 (21%)
14	FUB	s	4	14	9,9,10	0.60	0	10,12,14	0.88	0
10	FUB	sA	1	10	9,9,10	0.57	0	10,12,14	1.05	0
10	FUB	sA	2	10	9,9,10	0.57	0	10,12,14	0.85	0
10	FUB	sA	3	10	9,9,10	0.55	0	10,12,14	0.79	0
10	AHR	sA	4	10	9,9,10	0.58	0	10,12,14	1.13	1 (10%)
10	AHR	sA	5	10	9,9,10	0.57	0	10,12,14	1.16	1 (10%)
3	FUB	sB	1	3	9,9,10	0.60	0	10,12,14	0.93	0
3	FUB	sB	2	3	9,9,10	0.57	0	10,12,14	1.05	0
3	FUB	sB	3	3	9,9,10	0.58	0	10,12,14	0.83	0
3	FUB	sC	1	3	9,9,10	0.54	0	10,12,14	1.07	1 (10%)
3	FUB	sC	2	3	9,9,10	0.58	0	10,12,14	0.86	0
3	FUB	sC	3	3	9,9,10	0.57	0	10,12,14	1.01	1 (10%)
10	FUB	sD	1	10	9,9,10	0.56	0	10,12,14	1.07	1 (10%)
10	FUB	sD	2	10	9,9,10	0.57	0	10,12,14	0.82	0
10	FUB	sD	3	10	9,9,10	0.58	0	10,12,14	1.00	0
10	AHR	sD	4	10	9,9,10	0.57	0	10,12,14	0.90	0
10	AHR	sD	5	10	9,9,10	0.58	0	10,12,14	0.80	0
20	FUB	sE	1	20	9,9,10	0.56	0	10,12,14	1.05	1 (10%)
20	FUB	sE	2	20	9,9,10	0.57	0	10,12,14	1.00	0
20	GZL	sE	3	20	11,11,12	6.73	7 (63%)	14,15,17	1.59	2 (14%)
20	AHR	sE	4	20	9,9,10	0.58	0	10,12,14	1.04	1 (10%)
3	FUB	t	1	3	9,9,10	0.56	0	10,12,14	0.96	1 (10%)
3	FUB	t	2	3	9,9,10	0.56	0	10,12,14	0.77	0
3	FUB	t	3	3	9,9,10	0.57	0	10,12,14	0.97	0
4	FUB	tA	1	4	9,9,10	0.55	0	10,12,14	1.07	1 (10%)
4	FUB	tA	2	4	9,9,10	0.57	0	10,12,14	0.81	0
4	FUB	tA	3	4	9,9,10	0.56	0	10,12,14	0.79	0
4	AHR	tA	4	4	9,9,10	0.56	0	10,12,14	1.15	1 (10%)
3	FUB	tB	1	3	9,9,10	0.59	0	10,12,14	0.81	0
3	FUB	tB	2	3	9,9,10	0.56	0	10,12,14	0.84	0
3	FUB	tB	3	3	9,9,10	0.55	0	10,12,14	0.72	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	FUB	tC	1	3	9,9,10	0.59	0	10,12,14	1.01	0
3	FUB	tC	2	3	9,9,10	0.59	0	10,12,14	0.93	0
3	FUB	tC	3	3	9,9,10	0.59	0	10,12,14	1.08	1 (10%)
13	FUB	tD	1	13	9,9,10	0.57	0	10,12,14	1.06	0
13	FUB	tD	2	13	9,9,10	0.56	0	10,12,14	1.14	1 (10%)
13	GZL	tD	3	13	11,11,12	6.79	6 (54%)	14,15,17	1.14	2 (14%)
13	AHR	tD	4	13	9,9,10	0.59	0	10,12,14	1.18	1 (10%)
18	FUB	tE	1	18	9,9,10	0.54	0	10,12,14	0.93	1 (10%)
18	FUB	tE	2	18	9,9,10	0.53	0	10,12,14	0.76	0
18	GZL	tE	3	18	11,11,12	6.71	7 (63%)	14,15,17	1.59	2 (14%)
18	AHR	tE	4	18	9,9,10	0.59	0	10,12,14	1.04	1 (10%)
18	AHR	tE	5	18	9,9,10	0.59	0	10,12,14	0.98	0
10	FUB	u	1	10	9,9,10	0.57	0	10,12,14	1.09	1 (10%)
10	FUB	u	2	10	9,9,10	0.58	0	10,12,14	0.88	0
10	FUB	u	3	10	9,9,10	0.56	0	10,12,14	0.93	0
10	AHR	u	4	10	9,9,10	0.59	0	10,12,14	0.98	0
10	AHR	u	5	10	9,9,10	0.56	0	10,12,14	1.18	1 (10%)
3	FUB	uA	1	3	9,9,10	0.55	0	10,12,14	0.81	0
3	FUB	uA	2	3	9,9,10	0.58	0	10,12,14	0.82	0
3	FUB	uA	3	3	9,9,10	0.55	0	10,12,14	1.09	1 (10%)
3	FUB	uB	1	3	9,9,10	0.56	0	10,12,14	0.96	1 (10%)
3	FUB	uB	2	3	9,9,10	0.58	0	10,12,14	0.86	0
3	FUB	uB	3	3	9,9,10	0.58	0	10,12,14	0.89	0
3	FUB	uC	1	3	9,9,10	0.55	0	10,12,14	0.92	0
3	FUB	uC	2	3	9,9,10	0.57	0	10,12,14	0.97	0
3	FUB	uC	3	3	9,9,10	0.58	0	10,12,14	1.01	1 (10%)
6	FUB	uD	1	6	9,9,10	0.57	0	10,12,14	1.07	1 (10%)
6	FUB	uD	2	6	9,9,10	0.60	0	10,12,14	1.03	0
6	GZL	uD	3	6	11,11,12	7.02	6 (54%)	14,15,17	3.92	4 (28%)
20	FUB	uE	1	20	9,9,10	0.54	0	10,12,14	0.95	1 (10%)
20	FUB	uE	2	20	9,9,10	0.52	0	10,12,14	0.93	0
20	GZL	uE	3	20	11,11,12	6.71	7 (63%)	14,15,17	1.52	2 (14%)
20	AHR	uE	4	20	9,9,10	0.59	0	10,12,14	0.84	0
4	FUB	v	1	4	9,9,10	0.57	0	10,12,14	1.08	1 (10%)
4	FUB	v	2	4	9,9,10	0.56	0	10,12,14	0.88	0
4	FUB	v	3	4	9,9,10	0.56	0	10,12,14	0.90	0
4	AHR	v	4	4	9,9,10	0.58	0	10,12,14	1.01	0
3	FUB	vA	1	3	9,9,10	0.58	0	10,12,14	0.80	0
3	FUB	vA	2	3	9,9,10	0.57	0	10,12,14	0.88	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	FUB	vA	3	3	9,9,10	0.57	0	10,12,14	1.09	1 (10%)
3	FUB	vB	1	3	9,9,10	0.55	0	10,12,14	1.13	1 (10%)
3	FUB	vB	2	3	9,9,10	0.58	0	10,12,14	0.85	0
3	FUB	vB	3	3	9,9,10	0.59	0	10,12,14	0.90	0
10	FUB	vC	1	10	9,9,10	0.56	0	10,12,14	1.06	1 (10%)
10	FUB	vC	2	10	9,9,10	0.56	0	10,12,14	0.80	0
10	FUB	vC	3	10	9,9,10	0.58	0	10,12,14	0.99	1 (10%)
10	AHR	vC	4	10	9,9,10	0.61	0	10,12,14	0.87	0
10	AHR	vC	5	10	9,9,10	0.57	0	10,12,14	0.93	1 (10%)
13	FUB	vD	1	13	9,9,10	0.55	0	10,12,14	0.95	0
13	FUB	vD	2	13	9,9,10	0.58	0	10,12,14	0.94	0
13	GZL	vD	3	13	11,11,12	6.70	7 (63%)	14,15,17	1.54	2 (14%)
13	AHR	vD	4	13	9,9,10	0.57	0	10,12,14	1.13	1 (10%)
21	FUB	vE	1	21	9,9,10	0.53	0	10,12,14	1.01	1 (10%)
21	FUB	vE	2	21	9,9,10	0.56	0	10,12,14	0.82	0
21	GZL	vE	3	21	11,11,12	6.74	7 (63%)	14,15,17	1.37	1 (7%)
21	AHR	vE	4	21	9,9,10	0.58	0	10,12,14	1.00	0
21	AHR	vE	5	21	9,9,10	0.57	0	10,12,14	0.68	0
3	FUB	w	1	3	9,9,10	0.58	0	10,12,14	0.84	0
3	FUB	w	2	3	9,9,10	0.58	0	10,12,14	0.93	0
3	FUB	w	3	3	9,9,10	0.55	0	10,12,14	1.03	1 (10%)
3	FUB	wA	1	3	9,9,10	0.57	0	10,12,14	0.72	0
3	FUB	wA	2	3	9,9,10	0.57	0	10,12,14	0.81	0
3	FUB	wA	3	3	9,9,10	0.55	0	10,12,14	0.87	1 (10%)
3	FUB	wB	1	3	9,9,10	0.56	0	10,12,14	0.84	0
3	FUB	wB	2	3	9,9,10	0.56	0	10,12,14	0.84	0
3	FUB	wB	3	3	9,9,10	0.59	0	10,12,14	0.85	0
13	FUB	wC	1	13	9,9,10	0.56	0	10,12,14	0.97	0
13	FUB	wC	2	13	9,9,10	0.54	0	10,12,14	1.09	1 (10%)
13	GZL	wC	3	13	11,11,12	6.84	7 (63%)	14,15,17	1.25	2 (14%)
13	AHR	wC	4	13	9,9,10	0.60	0	10,12,14	1.19	1 (10%)
13	FUB	wD	1	13	9,9,10	0.56	0	10,12,14	0.99	1 (10%)
13	FUB	wD	2	13	9,9,10	0.57	0	10,12,14	0.81	0
13	GZL	wD	3	13	11,11,12	6.72	7 (63%)	14,15,17	1.55	3 (21%)
13	AHR	wD	4	13	9,9,10	0.56	0	10,12,14	1.06	1 (10%)
22	FUB	wE	1	22	9,9,10	0.59	0	10,12,14	1.05	0
22	FUB	wE	2	22	9,9,10	0.58	0	10,12,14	0.92	0
22	GZL	wE	3	22	11,11,12	6.75	7 (63%)	14,15,17	1.40	1 (7%)
22	AHR	wE	4	22	9,9,10	0.56	0	10,12,14	0.94	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	AHR	wE	5	22	9,9,10	0.59	0	10,12,14	1.53	3 (30%)
22	AHR	wE	6	22	9,9,10	0.55	0	10,12,14	0.75	0
3	FUB	x	1	3	9,9,10	0.57	0	10,12,14	0.76	0
3	FUB	x	2	3	9,9,10	0.59	0	10,12,14	0.98	1 (10%)
3	FUB	x	3	3	9,9,10	0.57	0	10,12,14	1.01	1 (10%)
3	FUB	xA	1	3	9,9,10	0.60	0	10,12,14	0.87	0
3	FUB	xA	2	3	9,9,10	0.58	0	10,12,14	0.89	0
3	FUB	xA	3	3	9,9,10	0.57	0	10,12,14	0.97	0
3	FUB	xB	1	3	9,9,10	0.55	0	10,12,14	1.07	1 (10%)
3	FUB	xB	2	3	9,9,10	0.55	0	10,12,14	0.79	0
3	FUB	xB	3	3	9,9,10	0.57	0	10,12,14	1.01	0
6	FUB	xC	1	6	9,9,10	0.55	0	10,12,14	1.09	1 (10%)
6	FUB	xC	2	6	9,9,10	0.59	0	10,12,14	1.05	1 (10%)
6	GZL	xC	3	6	11,11,12	7.01	6 (54%)	14,15,17	3.90	4 (28%)
6	FUB	xD	1	6	9,9,10	0.57	0	10,12,14	0.81	0
6	FUB	xD	2	6	9,9,10	0.58	0	10,12,14	1.21	2 (20%)
6	GZL	xD	3	6	11,11,12	6.65	7 (63%)	14,15,17	1.71	2 (14%)
20	FUB	xE	1	20	9,9,10	0.57	0	10,12,14	1.12	1 (10%)
20	FUB	xE	2	20	9,9,10	0.56	0	10,12,14	0.71	0
20	GZL	xE	3	20	11,11,12	6.69	7 (63%)	14,15,17	1.59	2 (14%)
20	AHR	xE	4	20	9,9,10	0.56	0	10,12,14	0.98	0
3	FUB	y	1	3	9,9,10	0.57	0	10,12,14	1.00	1 (10%)
3	FUB	y	2	3	9,9,10	0.58	0	10,12,14	0.91	0
3	FUB	y	3	3	9,9,10	0.54	0	10,12,14	0.86	0
3	FUB	yA	1	3	9,9,10	0.58	0	10,12,14	1.10	1 (10%)
3	FUB	yA	2	3	9,9,10	0.55	0	10,12,14	0.78	0
3	FUB	yA	3	3	9,9,10	0.58	0	10,12,14	0.86	0
10	FUB	yB	1	10	9,9,10	0.56	0	10,12,14	1.03	1 (10%)
10	FUB	yB	2	10	9,9,10	0.58	0	10,12,14	0.73	0
10	FUB	yB	3	10	9,9,10	0.59	0	10,12,14	1.09	0
10	AHR	yB	4	10	9,9,10	0.58	0	10,12,14	0.92	0
10	AHR	yB	5	10	9,9,10	0.57	0	10,12,14	0.79	0
13	FUB	yC	1	13	9,9,10	0.56	0	10,12,14	0.93	0
13	FUB	yC	2	13	9,9,10	0.56	0	10,12,14	1.00	1 (10%)
13	GZL	yC	3	13	11,11,12	6.70	7 (63%)	14,15,17	1.52	1 (7%)
13	AHR	yC	4	13	9,9,10	0.59	0	10,12,14	0.97	0
6	FUB	yD	1	6	9,9,10	0.54	0	10,12,14	0.91	1 (10%)
6	FUB	yD	2	6	9,9,10	0.56	0	10,12,14	1.08	1 (10%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	GZL	yD	3	6	11,11,12	6.74	7 (63%)	14,15,17	1.49	2 (14%)
18	FUB	yE	1	18	9,9,10	0.56	0	10,12,14	0.93	0
18	FUB	yE	2	18	9,9,10	0.52	0	10,12,14	0.91	0
18	GZL	yE	3	18	11,11,12	6.64	7 (63%)	14,15,17	1.79	3 (21%)
18	AHR	yE	4	18	9,9,10	0.57	0	10,12,14	1.11	1 (10%)
18	AHR	yE	5	18	9,9,10	0.56	0	10,12,14	1.13	1 (10%)
3	FUB	z	1	3	9,9,10	0.55	0	10,12,14	0.97	1 (10%)
3	FUB	z	2	3	9,9,10	0.56	0	10,12,14	0.90	0
3	FUB	z	3	3	9,9,10	0.57	0	10,12,14	0.84	0
3	FUB	zA	1	3	9,9,10	0.52	0	10,12,14	0.87	0
3	FUB	zA	2	3	9,9,10	0.59	0	10,12,14	0.87	0
3	FUB	zA	3	3	9,9,10	0.56	0	10,12,14	0.87	0
13	FUB	zB	1	13	9,9,10	0.54	0	10,12,14	1.03	1 (10%)
13	FUB	zB	2	13	9,9,10	0.54	0	10,12,14	1.06	1 (10%)
13	GZL	zB	3	13	11,11,12	6.77	7 (63%)	14,15,17	1.21	1 (7%)
13	AHR	zB	4	13	9,9,10	0.59	0	10,12,14	1.10	1 (10%)
13	FUB	zC	1	13	9,9,10	0.56	0	10,12,14	0.93	1 (10%)
13	FUB	zC	2	13	9,9,10	0.56	0	10,12,14	0.96	1 (10%)
13	GZL	zC	3	13	11,11,12	6.71	7 (63%)	14,15,17	1.53	3 (21%)
13	AHR	zC	4	13	9,9,10	0.57	0	10,12,14	0.99	0
6	FUB	zD	1	6	9,9,10	0.57	0	10,12,14	1.02	0
6	FUB	zD	2	6	9,9,10	0.57	0	10,12,14	1.00	1 (10%)
6	GZL	zD	3	6	11,11,12	6.73	7 (63%)	14,15,17	1.51	2 (14%)
18	FUB	zE	1	18	9,9,10	0.60	0	10,12,14	1.04	0
18	FUB	zE	2	18	9,9,10	0.59	0	10,12,14	1.07	1 (10%)
18	GZL	zE	3	18	11,11,12	6.66	7 (63%)	14,15,17	1.75	3 (21%)
18	AHR	zE	4	18	9,9,10	0.58	0	10,12,14	0.80	0
18	AHR	zE	5	18	9,9,10	0.58	0	10,12,14	0.95	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
3	FUB	0	1	3	-	0/2/15/18	0/1/1/1
3	FUB	0	2	3	-	0/2/15/18	0/1/1/1
3	FUB	0	3	3	-	0/2/15/18	0/1/1/1
3	FUB	0A	1	3	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FUB	0A	2	3	-	0/2/15/18	0/1/1/1
3	FUB	0A	3	3	-	0/2/15/18	0/1/1/1
6	FUB	0B	1	6	-	0/2/15/18	0/1/1/1
6	FUB	0B	2	6	-	0/2/15/18	0/1/1/1
6	GZL	0B	3	6	2/2/4/5	5/6/19/22	0/1/1/1
6	FUB	0C	1	6	-	0/2/15/18	0/1/1/1
6	FUB	0C	2	6	-	0/2/15/18	0/1/1/1
6	GZL	0C	3	6	-	2/6/19/22	0/1/1/1
13	FUB	0D	1	13	-	0/2/15/18	0/1/1/1
13	FUB	0D	2	13	1/1/3/4	0/2/15/18	0/1/1/1
13	GZL	0D	3	13	-	6/6/19/22	0/1/1/1
13	AHR	0D	4	13	-	0/2/15/18	0/1/1/1
18	FUB	0E	1	18	-	0/2/15/18	0/1/1/1
18	FUB	0E	2	18	-	0/2/15/18	0/1/1/1
18	GZL	0E	3	18	1/1/4/5	6/6/19/22	0/1/1/1
18	AHR	0E	4	18	1/1/3/4	0/2/15/18	0/1/1/1
18	AHR	0E	5	18	1/1/3/4	0/2/15/18	0/1/1/1
3	FUB	1	1	3	-	0/2/15/18	0/1/1/1
3	FUB	1	2	3	-	0/2/15/18	0/1/1/1
3	FUB	1	3	3	-	0/2/15/18	0/1/1/1
10	FUB	1A	1	10	-	0/2/15/18	0/1/1/1
10	FUB	1A	2	10	-	0/2/15/18	0/1/1/1
10	FUB	1A	3	10	-	0/2/15/18	0/1/1/1
10	AHR	1A	4	10	1/1/3/4	0/2/15/18	0/1/1/1
10	AHR	1A	5	10	-	0/2/15/18	0/1/1/1
13	FUB	1B	1	13	-	0/2/15/18	0/1/1/1
13	FUB	1B	2	13	-	0/2/15/18	0/1/1/1
13	GZL	1B	3	13	1/1/4/5	3/6/19/22	0/1/1/1
13	AHR	1B	4	13	-	0/2/15/18	0/1/1/1
6	FUB	1C	1	6	-	0/2/15/18	0/1/1/1
6	FUB	1C	2	6	-	0/2/15/18	0/1/1/1
6	GZL	1C	3	6	1/1/4/5	0/6/19/22	0/1/1/1
15	FUB	1D	1	15	-	0/2/15/18	0/1/1/1
15	FUB	1D	2	15	-	0/2/15/18	0/1/1/1
15	GZL	1D	3	15	1/1/4/5	4/6/19/22	0/1/1/1
15	AHR	1D	4	15	-	0/2/15/18	0/1/1/1
15	AHR	1D	5	15	1/1/3/4	0/2/15/18	0/1/1/1
19	FUB	1E	1	19	-	0/2/15/18	0/1/1/1
19	FUB	1E	2	19	-	0/2/15/18	0/1/1/1
19	GZL	1E	3	19	1/1/4/5	4/6/19/22	0/1/1/1
19	AHR	1E	4	19	1/1/3/4	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FUB	2	1	3	-	0/2/15/18	0/1/1/1
3	FUB	2	2	3	-	0/2/15/18	0/1/1/1
3	FUB	2	3	3	-	0/2/15/18	0/1/1/1
13	FUB	2A	1	13	-	0/2/15/18	0/1/1/1
13	FUB	2A	2	13	-	0/2/15/18	0/1/1/1
13	GZL	2A	3	13	3/3/4/5	2/6/19/22	0/1/1/1
13	AHR	2A	4	13	-	0/2/15/18	0/1/1/1
13	FUB	2B	1	13	-	0/2/15/18	0/1/1/1
13	FUB	2B	2	13	-	0/2/15/18	0/1/1/1
13	GZL	2B	3	13	1/1/4/5	0/6/19/22	0/1/1/1
13	AHR	2B	4	13	-	0/2/15/18	0/1/1/1
6	FUB	2C	1	6	-	0/2/15/18	0/1/1/1
6	FUB	2C	2	6	1/1/3/4	0/2/15/18	0/1/1/1
6	GZL	2C	3	6	1/1/4/5	4/6/19/22	0/1/1/1
15	FUB	2D	1	15	-	0/2/15/18	0/1/1/1
15	FUB	2D	2	15	-	0/2/15/18	0/1/1/1
15	GZL	2D	3	15	1/1/4/5	2/6/19/22	0/1/1/1
15	AHR	2D	4	15	-	0/2/15/18	0/1/1/1
15	AHR	2D	5	15	-	0/2/15/18	0/1/1/1
10	FUB	3	1	10	-	0/2/15/18	0/1/1/1
10	FUB	3	2	10	-	0/2/15/18	0/1/1/1
10	FUB	3	3	10	-	0/2/15/18	0/1/1/1
10	AHR	3	4	10	1/1/3/4	0/2/15/18	0/1/1/1
10	AHR	3	5	10	-	0/2/15/18	0/1/1/1
6	FUB	3A	1	6	-	0/2/15/18	0/1/1/1
6	FUB	3A	2	6	-	0/2/15/18	0/1/1/1
6	GZL	3A	3	6	2/2/4/5	4/6/19/22	0/1/1/1
6	FUB	3B	1	6	-	0/2/15/18	0/1/1/1
6	FUB	3B	2	6	-	0/2/15/18	0/1/1/1
6	GZL	3B	3	6	-	2/6/19/22	0/1/1/1
13	FUB	3C	1	13	-	0/2/15/18	0/1/1/1
13	FUB	3C	2	13	1/1/3/4	0/2/15/18	0/1/1/1
13	GZL	3C	3	13	-	4/6/19/22	0/1/1/1
13	AHR	3C	4	13	-	0/2/15/18	0/1/1/1
6	FUB	3D	1	6	-	0/2/15/18	0/1/1/1
6	FUB	3D	2	6	-	0/2/15/18	0/1/1/1
6	GZL	3D	3	6	1/1/4/5	0/6/19/22	0/1/1/1
13	FUB	4	1	13	-	0/2/15/18	0/1/1/1
13	FUB	4	2	13	-	0/2/15/18	0/1/1/1
13	GZL	4	3	13	2/2/4/5	5/6/19/22	0/1/1/1
13	AHR	4	4	13	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	FUB	4A	1	13	-	0/2/15/18	0/1/1/1
13	FUB	4A	2	13	-	0/2/15/18	0/1/1/1
13	GZL	4A	3	13	1/1/4/5	0/6/19/22	0/1/1/1
13	AHR	4A	4	13	-	0/2/15/18	0/1/1/1
6	FUB	4B	1	6	-	0/2/15/18	0/1/1/1
6	FUB	4B	2	6	-	0/2/15/18	0/1/1/1
6	GZL	4B	3	6	1/1/4/5	4/6/19/22	0/1/1/1
15	FUB	4C	1	15	-	0/2/15/18	0/1/1/1
15	FUB	4C	2	15	-	0/2/15/18	0/1/1/1
15	GZL	4C	3	15	1/1/4/5	2/6/19/22	0/1/1/1
15	AHR	4C	4	15	-	0/2/15/18	0/1/1/1
15	AHR	4C	5	15	1/1/3/4	0/2/15/18	0/1/1/1
16	NAG	4D	1	16,1	-	4/6/23/26	0/1/1/1
16	NAG	4D	2	16	-	0/6/23/26	0/1/1/1
6	FUB	5	1	6	-	0/2/15/18	0/1/1/1
6	FUB	5	2	6	-	0/2/15/18	0/1/1/1
6	GZL	5	3	6	3/3/4/5	2/6/19/22	0/1/1/1
13	FUB	5A	1	13	-	0/2/15/18	0/1/1/1
13	FUB	5A	2	13	-	0/2/15/18	0/1/1/1
13	GZL	5A	3	13	1/1/4/5	2/6/19/22	0/1/1/1
13	AHR	5A	4	13	-	0/2/15/18	0/1/1/1
6	FUB	5B	1	6	-	0/2/15/18	0/1/1/1
6	FUB	5B	2	6	1/1/3/4	0/2/15/18	0/1/1/1
6	GZL	5B	3	6	1/1/4/5	6/6/19/22	0/1/1/1
15	FUB	5C	1	15	-	0/2/15/18	0/1/1/1
15	FUB	5C	2	15	-	0/2/15/18	0/1/1/1
15	GZL	5C	3	15	1/1/4/5	0/6/19/22	0/1/1/1
15	AHR	5C	4	15	-	0/2/15/18	0/1/1/1
15	AHR	5C	5	15	-	0/2/15/18	0/1/1/1
17	NAG	5D	1	17,1	-	1/6/23/26	0/1/1/1
17	NAG	5D	2	17	-	2/6/23/26	0/1/1/1
17	BMA	5D	3	17	-	2/2/19/22	0/1/1/1
17	MAN	5D	4	17	1/1/4/5	2/2/19/22	0/1/1/1
17	MAN	5D	5	17	-	0/2/19/22	0/1/1/1
17	MAN	5D	6	17	1/1/4/5	2/2/19/22	0/1/1/1
13	FUB	6	1	13	-	0/2/15/18	0/1/1/1
13	FUB	6	2	13	-	0/2/15/18	0/1/1/1
13	GZL	6	3	13	1/1/4/5	3/6/19/22	0/1/1/1
13	AHR	6	4	13	-	0/2/15/18	0/1/1/1
6	FUB	6A	1	6	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	FUB	6A	2	6	-	0/2/15/18	0/1/1/1
6	GZL	6A	3	6	-	2/6/19/22	0/1/1/1
13	FUB	6B	1	13	-	0/2/15/18	0/1/1/1
13	FUB	6B	2	13	1/1/3/4	0/2/15/18	0/1/1/1
13	GZL	6B	3	13	-	4/6/19/22	0/1/1/1
13	AHR	6B	4	13	-	0/2/15/18	0/1/1/1
6	FUB	6C	1	6	-	0/2/15/18	0/1/1/1
6	FUB	6C	2	6	-	0/2/15/18	0/1/1/1
6	GZL	6C	3	6	1/1/4/5	2/6/19/22	0/1/1/1
6	FUB	6D	1	6	-	0/2/15/18	0/1/1/1
6	FUB	6D	2	6	-	0/2/15/18	0/1/1/1
6	GZL	6D	3	6	1/1/4/5	4/6/19/22	0/1/1/1
13	FUB	7	1	13	-	0/2/15/18	0/1/1/1
13	FUB	7	2	13	-	0/2/15/18	0/1/1/1
13	GZL	7	3	13	1/1/4/5	0/6/19/22	0/1/1/1
13	AHR	7	4	13	-	0/2/15/18	0/1/1/1
6	FUB	7A	1	6	-	0/2/15/18	0/1/1/1
6	FUB	7A	2	6	-	0/2/15/18	0/1/1/1
6	GZL	7A	3	6	1/1/4/5	2/6/19/22	0/1/1/1
15	FUB	7B	1	15	-	0/2/15/18	0/1/1/1
15	FUB	7B	2	15	-	0/2/15/18	0/1/1/1
15	GZL	7B	3	15	1/1/4/5	6/6/19/22	0/1/1/1
15	AHR	7B	4	15	-	0/2/15/18	0/1/1/1
15	AHR	7B	5	15	1/1/3/4	0/2/15/18	0/1/1/1
17	NAG	7C	1	17,1	-	1/6/23/26	0/1/1/1
17	NAG	7C	2	17	-	0/6/23/26	0/1/1/1
17	BMA	7C	3	17	-	2/2/19/22	0/1/1/1
17	MAN	7C	4	17	1/1/4/5	2/2/19/22	0/1/1/1
17	MAN	7C	5	17	-	2/2/19/22	0/1/1/1
17	MAN	7C	6	17	1/1/4/5	1/2/19/22	0/1/1/1
6	FUB	7D	1	6	-	0/2/15/18	0/1/1/1
6	FUB	7D	2	6	-	0/2/15/18	0/1/1/1
6	GZL	7D	3	6	1/1/4/5	6/6/19/22	0/1/1/1
6	FUB	8	1	6	-	0/2/15/18	0/1/1/1
6	FUB	8	2	6	-	0/2/15/18	0/1/1/1
6	GZL	8	3	6	1/1/4/5	0/6/19/22	0/1/1/1
6	FUB	8A	1	6	-	0/2/15/18	0/1/1/1
6	FUB	8A	2	6	1/1/3/4	0/2/15/18	0/1/1/1
6	GZL	8A	3	6	1/1/4/5	4/6/19/22	0/1/1/1
15	FUB	8B	1	15	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	FUB	8B	2	15	-	0/2/15/18	0/1/1/1
15	GZL	8B	3	15	1/1/4/5	2/6/19/22	0/1/1/1
15	AHR	8B	4	15	-	0/2/15/18	0/1/1/1
15	AHR	8B	5	15	-	0/2/15/18	0/1/1/1
3	FUB	8C	1	3	-	0/2/15/18	0/1/1/1
3	FUB	8C	2	3	-	0/2/15/18	0/1/1/1
3	FUB	8C	3	3	-	0/2/15/18	0/1/1/1
6	FUB	8D	1	6	-	0/2/15/18	0/1/1/1
6	FUB	8D	2	6	-	0/2/15/18	0/1/1/1
6	GZL	8D	3	6	1/1/4/5	2/6/19/22	0/1/1/1
6	FUB	9	1	6	-	0/2/15/18	0/1/1/1
6	FUB	9	2	6	-	0/2/15/18	0/1/1/1
6	GZL	9	3	6	1/1/4/5	1/6/19/22	0/1/1/1
13	FUB	9A	1	13	-	0/2/15/18	0/1/1/1
13	FUB	9A	2	13	1/1/3/4	0/2/15/18	0/1/1/1
13	GZL	9A	3	13	-	4/6/19/22	0/1/1/1
13	AHR	9A	4	13	-	0/2/15/18	0/1/1/1
6	FUB	9B	1	6	-	0/2/15/18	0/1/1/1
6	FUB	9B	2	6	-	0/2/15/18	0/1/1/1
6	GZL	9B	3	6	1/1/4/5	2/6/19/22	0/1/1/1
3	FUB	9C	1	3	-	0/2/15/18	0/1/1/1
3	FUB	9C	2	3	-	0/2/15/18	0/1/1/1
3	FUB	9C	3	3	-	0/2/15/18	0/1/1/1
18	FUB	9D	1	18	-	0/2/15/18	0/1/1/1
18	FUB	9D	2	18	-	0/2/15/18	0/1/1/1
18	GZL	9D	3	18	1/1/4/5	3/6/19/22	0/1/1/1
18	AHR	9D	4	18	1/1/3/4	0/2/15/18	0/1/1/1
18	AHR	9D	5	18	-	0/2/15/18	0/1/1/1
6	FUB	AA	1	6	-	0/2/15/18	0/1/1/1
6	FUB	AA	2	6	1/1/3/4	0/2/15/18	0/1/1/1
6	GZL	AA	3	6	1/1/4/5	6/6/19/22	0/1/1/1
15	FUB	AB	1	15	-	0/2/15/18	0/1/1/1
15	FUB	AB	2	15	-	0/2/15/18	0/1/1/1
15	GZL	AB	3	15	1/1/4/5	4/6/19/22	0/1/1/1
15	AHR	AB	4	15	-	0/2/15/18	0/1/1/1
15	AHR	AB	5	15	1/1/3/4	0/2/15/18	0/1/1/1
16	NAG	AC	1	16,1	-	3/6/23/26	0/1/1/1
16	NAG	AC	2	16	-	2/6/23/26	0/1/1/1
4	FUB	AD	1	4	1/1/3/4	0/2/15/18	0/1/1/1
4	FUB	AD	2	4	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FUB	AD	3	4	-	0/2/15/18	0/1/1/1
4	AHR	AD	4	4	-	0/2/15/18	0/1/1/1
19	FUB	AE	1	19	-	0/2/15/18	0/1/1/1
19	FUB	AE	2	19	-	0/2/15/18	0/1/1/1
19	GZL	AE	3	19	1/1/4/5	6/6/19/22	0/1/1/1
19	AHR	AE	4	19	-	0/2/15/18	0/1/1/1
13	FUB	BA	1	13	-	0/2/15/18	0/1/1/1
13	FUB	BA	2	13	1/1/3/4	0/2/15/18	0/1/1/1
13	GZL	BA	3	13	-	4/6/19/22	0/1/1/1
13	AHR	BA	4	13	-	0/2/15/18	0/1/1/1
15	FUB	BB	1	15	-	0/2/15/18	0/1/1/1
15	FUB	BB	2	15	-	0/2/15/18	0/1/1/1
15	GZL	BB	3	15	1/1/4/5	1/6/19/22	0/1/1/1
15	AHR	BB	4	15	-	0/2/15/18	0/1/1/1
15	AHR	BB	5	15	-	0/2/15/18	0/1/1/1
3	FUB	BC	1	3	-	0/2/15/18	0/1/1/1
3	FUB	BC	2	3	-	0/2/15/18	0/1/1/1
3	FUB	BC	3	3	-	0/2/15/18	0/1/1/1
5	FUB	BD	1	5	-	0/2/15/18	0/1/1/1
5	FUB	BD	2	5	-	0/2/15/18	0/1/1/1
5	FUB	BD	3	5	-	0/2/15/18	0/1/1/1
5	AHR	BD	4	5	-	0/2/15/18	0/1/1/1
5	AHR	BD	5	5	1/1/3/4	0/2/15/18	0/1/1/1
18	FUB	BE	1	18	-	0/2/15/18	0/1/1/1
18	FUB	BE	2	18	-	0/2/15/18	0/1/1/1
18	GZL	BE	3	18	1/1/4/5	4/6/19/22	0/1/1/1
18	AHR	BE	4	18	1/1/3/4	0/2/15/18	0/1/1/1
18	AHR	BE	5	18	1/1/3/4	0/2/15/18	0/1/1/1
15	FUB	CA	1	15	-	0/2/15/18	0/1/1/1
15	FUB	CA	2	15	-	0/2/15/18	0/1/1/1
15	GZL	CA	3	15	1/1/4/5	4/6/19/22	0/1/1/1
15	AHR	CA	4	15	-	0/2/15/18	0/1/1/1
15	AHR	CA	5	15	1/1/3/4	0/2/15/18	0/1/1/1
6	FUB	CB	1	6	-	0/2/15/18	0/1/1/1
6	FUB	CB	2	6	-	0/2/15/18	0/1/1/1
6	GZL	CB	3	6	1/1/4/5	2/6/19/22	0/1/1/1
3	FUB	CC	1	3	-	0/2/15/18	0/1/1/1
3	FUB	CC	2	3	-	0/2/15/18	0/1/1/1
3	FUB	CC	3	3	-	0/2/15/18	0/1/1/1
6	FUB	CD	1	6	-	0/2/15/18	0/1/1/1
6	FUB	CD	2	6	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GZL	CD	3	6	3/3/4/5	1/6/19/22	0/1/1/1
20	FUB	CE	1	20	-	0/2/15/18	0/1/1/1
20	FUB	CE	2	20	-	1/2/15/18	0/1/1/1
20	GZL	CE	3	20	1/1/4/5	6/6/19/22	0/1/1/1
20	AHR	CE	4	20	-	0/2/15/18	0/1/1/1
15	FUB	DA	1	15	-	0/2/15/18	0/1/1/1
15	FUB	DA	2	15	-	0/2/15/18	0/1/1/1
15	GZL	DA	3	15	1/1/4/5	2/6/19/22	0/1/1/1
15	AHR	DA	4	15	-	0/2/15/18	0/1/1/1
15	AHR	DA	5	15	-	0/2/15/18	0/1/1/1
17	NAG	DB	1	17,1	-	2/6/23/26	0/1/1/1
17	NAG	DB	2	17	-	2/6/23/26	0/1/1/1
17	BMA	DB	3	17	-	2/2/19/22	0/1/1/1
17	MAN	DB	4	17	1/1/4/5	2/2/19/22	0/1/1/1
17	MAN	DB	5	17	-	2/2/19/22	0/1/1/1
17	MAN	DB	6	17	1/1/4/5	1/2/19/22	0/1/1/1
4	FUB	DC	1	4	1/1/3/4	0/2/15/18	0/1/1/1
4	FUB	DC	2	4	-	0/2/15/18	0/1/1/1
4	FUB	DC	3	4	-	0/2/15/18	0/1/1/1
4	AHR	DC	4	4	-	0/2/15/18	0/1/1/1
3	FUB	DD	1	3	-	0/2/15/18	0/1/1/1
3	FUB	DD	2	3	-	0/2/15/18	0/1/1/1
3	FUB	DD	3	3	-	0/2/15/18	0/1/1/1
18	FUB	DE	1	18	-	0/2/15/18	0/1/1/1
18	FUB	DE	2	18	-	0/2/15/18	0/1/1/1
18	GZL	DE	3	18	1/1/4/5	2/6/19/22	0/1/1/1
18	AHR	DE	4	18	-	0/2/15/18	0/1/1/1
18	AHR	DE	5	18	1/1/3/4	0/2/15/18	0/1/1/1
6	FUB	EA	1	6	-	0/2/15/18	0/1/1/1
6	FUB	EA	2	6	-	0/2/15/18	0/1/1/1
6	GZL	EA	3	6	1/1/4/5	2/6/19/22	0/1/1/1
3	FUB	EB	1	3	-	0/2/15/18	0/1/1/1
3	FUB	EB	2	3	-	0/2/15/18	0/1/1/1
3	FUB	EB	3	3	-	0/2/15/18	0/1/1/1
5	FUB	EC	1	5	-	0/2/15/18	0/1/1/1
5	FUB	EC	2	5	-	0/2/15/18	0/1/1/1
5	FUB	EC	3	5	-	0/2/15/18	0/1/1/1
5	AHR	EC	4	5	-	0/2/15/18	0/1/1/1
5	AHR	EC	5	5	-	0/2/15/18	0/1/1/1
3	FUB	ED	1	3	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FUB	ED	2	3	-	0/2/15/18	0/1/1/1
3	FUB	ED	3	3	-	0/2/15/18	0/1/1/1
20	FUB	EE	1	20	-	0/2/15/18	0/1/1/1
20	FUB	EE	2	20	-	0/2/15/18	0/1/1/1
20	GZL	EE	3	20	1/1/4/5	0/6/19/22	0/1/1/1
20	AHR	EE	4	20	-	0/2/15/18	0/1/1/1
16	NAG	FA	1	16,1	-	4/6/23/26	0/1/1/1
16	NAG	FA	2	16	-	2/6/23/26	0/1/1/1
12	FUB	FB	1	12	-	0/2/15/18	0/1/1/1
12	FUB	FB	2	12	-	0/2/15/18	0/1/1/1
12	GZL	FB	3	12	2/2/4/5	3/6/19/22	0/1/1/1
12	AHR	FB	4	12	-	0/2/15/18	0/1/1/1
12	AHR	FB	5	12	-	0/2/15/18	0/1/1/1
6	FUB	FC	1	6	-	0/2/15/18	0/1/1/1
6	FUB	FC	2	6	-	0/2/15/18	0/1/1/1
6	GZL	FC	3	6	1/1/4/5	4/6/19/22	0/1/1/1
3	FUB	FD	1	3	-	0/2/15/18	0/1/1/1
3	FUB	FD	2	3	-	0/2/15/18	0/1/1/1
3	FUB	FD	3	3	-	0/2/15/18	0/1/1/1
21	FUB	FE	1	21	-	0/2/15/18	0/1/1/1
21	FUB	FE	2	21	-	0/2/15/18	0/1/1/1
21	GZL	FE	3	21	1/1/4/5	2/6/19/22	0/1/1/1
21	AHR	FE	4	21	1/1/3/4	0/2/15/18	0/1/1/1
21	AHR	FE	5	21	1/1/3/4	0/2/15/18	0/1/1/1
17	NAG	GA	1	17,1	-	1/6/23/26	0/1/1/1
17	NAG	GA	2	17	-	2/6/23/26	0/1/1/1
17	BMA	GA	3	17	-	2/2/19/22	0/1/1/1
17	MAN	GA	4	17	1/1/4/5	1/2/19/22	0/1/1/1
17	MAN	GA	5	17	-	1/2/19/22	0/1/1/1
17	MAN	GA	6	17	1/1/4/5	1/2/19/22	0/1/1/1
13	FUB	GB	1	13	-	0/2/15/18	0/1/1/1
13	FUB	GB	2	13	-	0/2/15/18	0/1/1/1
13	GZL	GB	3	13	2/2/4/5	3/6/19/22	0/1/1/1
13	AHR	GB	4	13	-	0/2/15/18	0/1/1/1
3	FUB	GC	1	3	-	0/2/15/18	0/1/1/1
3	FUB	GC	2	3	-	0/2/15/18	0/1/1/1
3	FUB	GC	3	3	-	0/2/15/18	0/1/1/1
6	FUB	GD	1	6	-	0/2/15/18	0/1/1/1
6	FUB	GD	2	6	-	0/2/15/18	0/1/1/1
6	GZL	GD	3	6	1/1/4/5	4/6/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	FUB	GE	1	22	-	0/2/15/18	0/1/1/1
22	FUB	GE	2	22	-	0/2/15/18	0/1/1/1
22	GZL	GE	3	22	1/1/4/5	6/6/19/22	0/1/1/1
22	AHR	GE	4	22	-	0/2/15/18	0/1/1/1
22	AHR	GE	5	22	-	0/2/15/18	0/1/1/1
22	AHR	GE	6	22	-	0/2/15/18	0/1/1/1
3	FUB	HA	1	3	-	0/2/15/18	0/1/1/1
3	FUB	HA	2	3	-	0/2/15/18	0/1/1/1
3	FUB	HA	3	3	-	0/2/15/18	0/1/1/1
14	FUB	HB	1	14	-	0/2/15/18	0/1/1/1
14	FUB	HB	2	14	-	0/2/15/18	0/1/1/1
14	GZL	HB	3	14	2/2/4/5	6/6/19/22	0/1/1/1
14	FUB	HB	4	14	-	0/2/15/18	0/1/1/1
3	FUB	HC	1	3	-	0/2/15/18	0/1/1/1
3	FUB	HC	2	3	-	0/2/15/18	0/1/1/1
3	FUB	HC	3	3	-	0/2/15/18	0/1/1/1
7	FUB	HD	1	7	-	0/2/15/18	0/1/1/1
7	FUB	HD	2	7	-	0/2/15/18	0/1/1/1
7	FUB	HD	3	7	-	0/2/15/18	0/1/1/1
7	AHR	HD	4	7	-	0/2/15/18	0/1/1/1
20	FUB	HE	1	20	-	0/2/15/18	0/1/1/1
20	FUB	HE	2	20	-	2/2/15/18	0/1/1/1
20	GZL	HE	3	20	1/1/4/5	6/6/19/22	0/1/1/1
20	AHR	HE	4	20	-	0/2/15/18	0/1/1/1
3	FUB	IA	1	3	-	0/2/15/18	0/1/1/1
3	FUB	IA	2	3	-	0/2/15/18	0/1/1/1
3	FUB	IA	3	3	-	0/2/15/18	0/1/1/1
12	FUB	IB	1	12	-	0/2/15/18	0/1/1/1
12	FUB	IB	2	12	-	0/2/15/18	0/1/1/1
12	GZL	IB	3	12	2/2/4/5	6/6/19/22	0/1/1/1
12	AHR	IB	4	12	-	0/2/15/18	0/1/1/1
12	AHR	IB	5	12	-	0/2/15/18	0/1/1/1
3	FUB	IC	1	3	-	0/2/15/18	0/1/1/1
3	FUB	IC	2	3	-	0/2/15/18	0/1/1/1
3	FUB	IC	3	3	-	0/2/15/18	0/1/1/1
3	FUB	ID	1	3	-	0/2/15/18	0/1/1/1
3	FUB	ID	2	3	-	0/2/15/18	0/1/1/1
3	FUB	ID	3	3	-	0/2/15/18	0/1/1/1
18	FUB	IE	1	18	-	0/2/15/18	0/1/1/1
18	FUB	IE	2	18	-	0/2/15/18	0/1/1/1
18	GZL	IE	3	18	1/1/4/5	6/6/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	AHR	IE	4	18	1/1/3/4	0/2/15/18	0/1/1/1
18	AHR	IE	5	18	-	0/2/15/18	0/1/1/1
3	FUB	J	1	3	-	0/2/15/18	0/1/1/1
3	FUB	J	2	3	-	0/2/15/18	0/1/1/1
3	FUB	J	3	3	-	0/2/15/18	0/1/1/1
4	FUB	JA	1	4	1/1/3/4	0/2/15/18	0/1/1/1
4	FUB	JA	2	4	-	0/2/15/18	0/1/1/1
4	FUB	JA	3	4	-	0/2/15/18	0/1/1/1
4	AHR	JA	4	4	-	0/2/15/18	0/1/1/1
4	FUB	JB	1	4	-	0/2/15/18	0/1/1/1
4	FUB	JB	2	4	-	0/2/15/18	0/1/1/1
4	FUB	JB	3	4	-	0/2/15/18	0/1/1/1
4	AHR	JB	4	4	-	0/2/15/18	0/1/1/1
6	FUB	JC	1	6	-	0/2/15/18	0/1/1/1
6	FUB	JC	2	6	-	0/2/15/18	0/1/1/1
6	GZL	JC	3	6	1/1/4/5	0/6/19/22	0/1/1/1
8	FUB	JD	1	8	-	0/2/15/18	0/1/1/1
8	FUB	JD	2	8	-	0/2/15/18	0/1/1/1
8	FUB	JD	3	8	-	0/2/15/18	0/1/1/1
8	AHR	JD	4	8	-	0/2/15/18	0/1/1/1
8	AHR	JD	5	8	-	0/2/15/18	0/1/1/1
18	FUB	JE	1	18	-	0/2/15/18	0/1/1/1
18	FUB	JE	2	18	-	0/2/15/18	0/1/1/1
18	GZL	JE	3	18	1/1/4/5	2/6/19/22	0/1/1/1
18	AHR	JE	4	18	-	0/2/15/18	0/1/1/1
18	AHR	JE	5	18	1/1/3/4	0/2/15/18	0/1/1/1
3	FUB	K	1	3	-	0/2/15/18	0/1/1/1
3	FUB	K	2	3	-	0/2/15/18	0/1/1/1
3	FUB	K	3	3	-	0/2/15/18	0/1/1/1
5	FUB	KA	1	5	-	0/2/15/18	0/1/1/1
5	FUB	KA	2	5	-	0/2/15/18	0/1/1/1
5	FUB	KA	3	5	-	0/2/15/18	0/1/1/1
5	AHR	KA	4	5	-	0/2/15/18	0/1/1/1
5	AHR	KA	5	5	-	0/2/15/18	0/1/1/1
14	FUB	KB	1	14	-	0/2/15/18	0/1/1/1
14	FUB	KB	2	14	-	0/2/15/18	0/1/1/1
14	GZL	KB	3	14	2/2/4/5	4/6/19/22	0/1/1/1
14	FUB	KB	4	14	-	0/2/15/18	0/1/1/1
7	FUB	KC	1	7	-	0/2/15/18	0/1/1/1
7	FUB	KC	2	7	-	0/2/15/18	0/1/1/1
7	FUB	KC	3	7	-	0/2/15/18	0/1/1/1
7	AHR	KC	4	7	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FUB	KD	1	3	-	0/2/15/18	0/1/1/1
3	FUB	KD	2	3	-	0/2/15/18	0/1/1/1
3	FUB	KD	3	3	-	0/2/15/18	0/1/1/1
18	FUB	KE	1	18	-	0/2/15/18	0/1/1/1
18	FUB	KE	2	18	-	0/2/15/18	0/1/1/1
18	GZL	KE	3	18	1/1/4/5	4/6/19/22	0/1/1/1
18	AHR	KE	4	18	1/1/3/4	0/2/15/18	0/1/1/1
18	AHR	KE	5	18	1/1/3/4	0/2/15/18	0/1/1/1
4	FUB	L	1	4	1/1/3/4	0/2/15/18	0/1/1/1
4	FUB	L	2	4	-	0/2/15/18	0/1/1/1
4	FUB	L	3	4	-	0/2/15/18	0/1/1/1
4	AHR	L	4	4	-	0/2/15/18	0/1/1/1
6	FUB	LA	1	6	-	0/2/15/18	0/1/1/1
6	FUB	LA	2	6	-	0/2/15/18	0/1/1/1
6	GZL	LA	3	6	2/2/4/5	2/6/19/22	0/1/1/1
3	FUB	LB	1	3	-	0/2/15/18	0/1/1/1
3	FUB	LB	2	3	-	0/2/15/18	0/1/1/1
3	FUB	LB	3	3	-	0/2/15/18	0/1/1/1
3	FUB	LC	1	3	-	0/2/15/18	0/1/1/1
3	FUB	LC	2	3	-	0/2/15/18	0/1/1/1
3	FUB	LC	3	3	-	0/2/15/18	0/1/1/1
4	FUB	LD	1	4	-	0/2/15/18	0/1/1/1
4	FUB	LD	2	4	-	0/2/15/18	0/1/1/1
4	FUB	LD	3	4	-	0/2/15/18	0/1/1/1
4	AHR	LD	4	4	-	0/2/15/18	0/1/1/1
19	FUB	LE	1	19	-	0/2/15/18	0/1/1/1
19	FUB	LE	2	19	-	0/2/15/18	0/1/1/1
19	GZL	LE	3	19	1/1/4/5	2/6/19/22	0/1/1/1
19	AHR	LE	4	19	1/1/3/4	0/2/15/18	0/1/1/1
5	FUB	M	1	5	-	0/2/15/18	0/1/1/1
5	FUB	M	2	5	-	0/2/15/18	0/1/1/1
5	FUB	M	3	5	-	0/2/15/18	0/1/1/1
5	AHR	M	4	5	-	0/2/15/18	0/1/1/1
5	AHR	M	5	5	-	0/2/15/18	0/1/1/1
3	FUB	MA	1	3	-	0/2/15/18	0/1/1/1
3	FUB	MA	2	3	-	0/2/15/18	0/1/1/1
3	FUB	MA	3	3	-	0/2/15/18	0/1/1/1
10	FUB	MB	1	10	-	0/2/15/18	0/1/1/1
10	FUB	MB	2	10	-	0/2/15/18	0/1/1/1
10	FUB	MB	3	10	-	0/2/15/18	0/1/1/1
10	AHR	MB	4	10	-	0/2/15/18	0/1/1/1
10	AHR	MB	5	10	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	FUB	MC	1	8	-	0/2/15/18	0/1/1/1
8	FUB	MC	2	8	-	0/2/15/18	0/1/1/1
8	FUB	MC	3	8	-	0/2/15/18	0/1/1/1
8	AHR	MC	4	8	-	0/2/15/18	0/1/1/1
8	AHR	MC	5	8	-	0/2/15/18	0/1/1/1
4	FUB	MD	1	4	-	0/2/15/18	0/1/1/1
4	FUB	MD	2	4	-	0/2/15/18	0/1/1/1
4	FUB	MD	3	4	-	0/2/15/18	0/1/1/1
4	AHR	MD	4	4	-	0/2/15/18	0/1/1/1
6	FUB	ME	1	6	-	0/2/15/18	0/1/1/1
6	FUB	ME	2	6	-	0/2/15/18	0/1/1/1
6	GZL	ME	3	6	1/1/4/5	4/6/19/22	0/1/1/1
6	FUB	N	1	6	-	0/2/15/18	0/1/1/1
6	FUB	N	2	6	-	0/2/15/18	0/1/1/1
6	GZL	N	3	6	2/2/4/5	2/6/19/22	0/1/1/1
3	FUB	NA	1	3	-	0/2/15/18	0/1/1/1
3	FUB	NA	2	3	-	0/2/15/18	0/1/1/1
3	FUB	NA	3	3	-	0/2/15/18	0/1/1/1
4	FUB	NB	1	4	-	0/2/15/18	0/1/1/1
4	FUB	NB	2	4	-	0/2/15/18	0/1/1/1
4	FUB	NB	3	4	-	0/2/15/18	0/1/1/1
4	AHR	NB	4	4	-	0/2/15/18	0/1/1/1
3	FUB	NC	1	3	-	0/2/15/18	0/1/1/1
3	FUB	NC	2	3	-	0/2/15/18	0/1/1/1
3	FUB	NC	3	3	-	0/2/15/18	0/1/1/1
9	FUB	ND	1	9	-	0/2/15/18	0/1/1/1
9	FUB	ND	2	9	-	0/2/15/18	0/1/1/1
19	FUB	NE	1	19	-	0/2/15/18	0/1/1/1
19	FUB	NE	2	19	-	0/2/15/18	0/1/1/1
19	GZL	NE	3	19	1/1/4/5	2/6/19/22	0/1/1/1
19	AHR	NE	4	19	1/1/3/4	0/2/15/18	0/1/1/1
3	FUB	O	1	3	-	0/2/15/18	0/1/1/1
3	FUB	O	2	3	-	0/2/15/18	0/1/1/1
3	FUB	O	3	3	-	0/2/15/18	0/1/1/1
3	FUB	OA	1	3	-	0/2/15/18	0/1/1/1
3	FUB	OA	2	3	-	0/2/15/18	0/1/1/1
3	FUB	OA	3	3	-	0/2/15/18	0/1/1/1
3	FUB	OB	1	3	-	0/2/15/18	0/1/1/1
3	FUB	OB	2	3	-	0/2/15/18	0/1/1/1
3	FUB	OB	3	3	-	0/2/15/18	0/1/1/1
4	FUB	OC	1	4	-	0/2/15/18	0/1/1/1
4	FUB	OC	2	4	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FUB	OC	3	4	-	0/2/15/18	0/1/1/1
4	AHR	OC	4	4	-	0/2/15/18	0/1/1/1
4	FUB	OD	1	4	-	0/2/15/18	0/1/1/1
4	FUB	OD	2	4	1/1/3/4	0/2/15/18	0/1/1/1
4	FUB	OD	3	4	-	0/2/15/18	0/1/1/1
4	AHR	OD	4	4	-	0/2/15/18	0/1/1/1
6	FUB	OE	1	6	-	0/2/15/18	0/1/1/1
6	FUB	OE	2	6	-	0/2/15/18	0/1/1/1
6	GZL	OE	3	6	1/1/4/5	4/6/19/22	0/1/1/1
3	FUB	P	1	3	-	0/2/15/18	0/1/1/1
3	FUB	P	2	3	-	0/2/15/18	0/1/1/1
3	FUB	P	3	3	-	0/2/15/18	0/1/1/1
6	FUB	PA	1	6	-	0/2/15/18	0/1/1/1
6	FUB	PA	2	6	-	0/2/15/18	0/1/1/1
6	GZL	PA	3	6	1/1/4/5	2/6/19/22	0/1/1/1
3	FUB	PB	1	3	-	0/2/15/18	0/1/1/1
3	FUB	PB	2	3	-	0/2/15/18	0/1/1/1
3	FUB	PB	3	3	-	0/2/15/18	0/1/1/1
4	FUB	PC	1	4	-	0/2/15/18	0/1/1/1
4	FUB	PC	2	4	-	0/2/15/18	0/1/1/1
4	FUB	PC	3	4	-	0/2/15/18	0/1/1/1
4	AHR	PC	4	4	1/1/3/4	0/2/15/18	0/1/1/1
10	FUB	PD	1	10	-	0/2/15/18	0/1/1/1
10	FUB	PD	2	10	-	0/2/15/18	0/1/1/1
10	FUB	PD	3	10	-	0/2/15/18	0/1/1/1
10	AHR	PD	4	10	-	0/2/15/18	0/1/1/1
10	AHR	PD	5	10	-	0/2/15/18	0/1/1/1
18	FUB	PE	1	18	-	0/2/15/18	0/1/1/1
18	FUB	PE	2	18	-	0/2/15/18	0/1/1/1
18	GZL	PE	3	18	1/1/4/5	2/6/19/22	0/1/1/1
18	AHR	PE	4	18	1/1/3/4	0/2/15/18	0/1/1/1
18	AHR	PE	5	18	1/1/3/4	0/2/15/18	0/1/1/1
3	FUB	Q	1	3	-	0/2/15/18	0/1/1/1
3	FUB	Q	2	3	-	0/2/15/18	0/1/1/1
3	FUB	Q	3	3	-	0/2/15/18	0/1/1/1
7	FUB	QA	1	7	-	0/2/15/18	0/1/1/1
7	FUB	QA	2	7	-	0/2/15/18	0/1/1/1
7	FUB	QA	3	7	-	0/2/15/18	0/1/1/1
7	AHR	QA	4	7	-	0/2/15/18	0/1/1/1
3	FUB	QB	1	3	-	0/2/15/18	0/1/1/1
3	FUB	QB	2	3	-	0/2/15/18	0/1/1/1
3	FUB	QB	3	3	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	FUB	QC	1	9	-	0/2/15/18	0/1/1/1
9	FUB	QC	2	9	-	0/2/15/18	0/1/1/1
3	FUB	QD	1	3	-	0/2/15/18	0/1/1/1
3	FUB	QD	2	3	-	0/2/15/18	0/1/1/1
3	FUB	QD	3	3	-	0/2/15/18	0/1/1/1
22	FUB	QE	1	22	-	0/2/15/18	0/1/1/1
22	FUB	QE	2	22	-	0/2/15/18	0/1/1/1
22	GZL	QE	3	22	1/1/4/5	2/6/19/22	0/1/1/1
22	AHR	QE	4	22	1/1/3/4	0/2/15/18	0/1/1/1
22	AHR	QE	5	22	-	0/2/15/18	0/1/1/1
22	AHR	QE	6	22	1/1/3/4	0/2/15/18	0/1/1/1
6	FUB	R	1	6	-	0/2/15/18	0/1/1/1
6	FUB	R	2	6	-	0/2/15/18	0/1/1/1
6	GZL	R	3	6	1/1/4/5	2/6/19/22	0/1/1/1
3	FUB	RA	1	3	-	0/2/15/18	0/1/1/1
3	FUB	RA	2	3	-	0/2/15/18	0/1/1/1
3	FUB	RA	3	3	-	0/2/15/18	0/1/1/1
3	FUB	RB	1	3	-	0/2/15/18	0/1/1/1
3	FUB	RB	2	3	-	0/2/15/18	0/1/1/1
3	FUB	RB	3	3	-	0/2/15/18	0/1/1/1
4	FUB	RC	1	4	-	0/2/15/18	0/1/1/1
4	FUB	RC	2	4	1/1/3/4	0/2/15/18	0/1/1/1
4	FUB	RC	3	4	-	0/2/15/18	0/1/1/1
4	AHR	RC	4	4	-	0/2/15/18	0/1/1/1
4	FUB	RD	1	4	-	0/2/15/18	0/1/1/1
4	FUB	RD	2	4	-	0/2/15/18	0/1/1/1
4	FUB	RD	3	4	-	0/2/15/18	0/1/1/1
4	AHR	RD	4	4	-	0/2/15/18	0/1/1/1
22	FUB	RE	1	22	-	0/2/15/18	0/1/1/1
22	FUB	RE	2	22	-	1/2/15/18	0/1/1/1
22	GZL	RE	3	22	1/1/4/5	3/6/19/22	0/1/1/1
22	AHR	RE	4	22	2/2/3/4	0/2/15/18	0/1/1/1
22	AHR	RE	5	22	-	0/2/15/18	0/1/1/1
22	AHR	RE	6	22	-	0/2/15/18	0/1/1/1
7	FUB	S	1	7	-	0/2/15/18	0/1/1/1
7	FUB	S	2	7	-	0/2/15/18	0/1/1/1
7	FUB	S	3	7	-	0/2/15/18	0/1/1/1
7	AHR	S	4	7	-	0/2/15/18	0/1/1/1
8	FUB	SA	1	8	-	0/2/15/18	0/1/1/1
8	FUB	SA	2	8	-	0/2/15/18	0/1/1/1
8	FUB	SA	3	8	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	AHR	SA	4	8	-	0/2/15/18	0/1/1/1
8	AHR	SA	5	8	-	0/2/15/18	0/1/1/1
3	FUB	SB	1	3	-	0/2/15/18	0/1/1/1
3	FUB	SB	2	3	-	0/2/15/18	0/1/1/1
3	FUB	SB	3	3	-	0/2/15/18	0/1/1/1
10	FUB	SC	1	10	-	0/2/15/18	0/1/1/1
10	FUB	SC	2	10	-	0/2/15/18	0/1/1/1
10	FUB	SC	3	10	-	0/2/15/18	0/1/1/1
10	AHR	SC	4	10	-	0/2/15/18	0/1/1/1
10	AHR	SC	5	10	-	0/2/15/18	0/1/1/1
4	FUB	SD	1	4	-	0/2/15/18	0/1/1/1
4	FUB	SD	2	4	-	0/2/15/18	0/1/1/1
4	FUB	SD	3	4	-	0/2/15/18	0/1/1/1
4	AHR	SD	4	4	-	0/2/15/18	0/1/1/1
18	FUB	SE	1	18	1/1/3/4	0/2/15/18	0/1/1/1
18	FUB	SE	2	18	-	0/2/15/18	0/1/1/1
18	GZL	SE	3	18	1/1/4/5	3/6/19/22	0/1/1/1
18	AHR	SE	4	18	1/1/3/4	0/2/15/18	0/1/1/1
18	AHR	SE	5	18	1/1/3/4	0/2/15/18	0/1/1/1
3	FUB	T	1	3	-	0/2/15/18	0/1/1/1
3	FUB	T	2	3	-	0/2/15/18	0/1/1/1
3	FUB	T	3	3	-	0/2/15/18	0/1/1/1
3	FUB	TA	1	3	-	0/2/15/18	0/1/1/1
3	FUB	TA	2	3	-	0/2/15/18	0/1/1/1
3	FUB	TA	3	3	-	0/2/15/18	0/1/1/1
3	FUB	TB	1	3	-	0/2/15/18	0/1/1/1
3	FUB	TB	2	3	-	0/2/15/18	0/1/1/1
3	FUB	TB	3	3	-	0/2/15/18	0/1/1/1
3	FUB	TC	1	3	-	0/2/15/18	0/1/1/1
3	FUB	TC	2	3	-	0/2/15/18	0/1/1/1
3	FUB	TC	3	3	-	0/2/15/18	0/1/1/1
3	FUB	TD	1	3	-	0/2/15/18	0/1/1/1
3	FUB	TD	2	3	-	0/2/15/18	0/1/1/1
3	FUB	TD	3	3	-	0/2/15/18	0/1/1/1
20	FUB	TE	1	20	-	0/2/15/18	0/1/1/1
20	FUB	TE	2	20	-	2/2/15/18	0/1/1/1
20	GZL	TE	3	20	1/1/4/5	4/6/19/22	0/1/1/1
20	AHR	TE	4	20	1/1/3/4	0/2/15/18	0/1/1/1
8	FUB	U	1	8	-	0/2/15/18	0/1/1/1
8	FUB	U	2	8	-	0/2/15/18	0/1/1/1
8	FUB	U	3	8	-	0/2/15/18	0/1/1/1
8	AHR	U	4	8	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	AHR	U	5	8	-	0/2/15/18	0/1/1/1
4	FUB	UA	1	4	-	0/2/15/18	0/1/1/1
4	FUB	UA	2	4	-	0/2/15/18	0/1/1/1
4	FUB	UA	3	4	-	0/2/15/18	0/1/1/1
4	AHR	UA	4	4	-	0/2/15/18	0/1/1/1
3	FUB	UB	1	3	-	0/2/15/18	0/1/1/1
3	FUB	UB	2	3	-	0/2/15/18	0/1/1/1
3	FUB	UB	3	3	-	0/2/15/18	0/1/1/1
4	FUB	UC	1	4	-	0/2/15/18	0/1/1/1
4	FUB	UC	2	4	-	0/2/15/18	0/1/1/1
4	FUB	UC	3	4	-	0/2/15/18	0/1/1/1
4	AHR	UC	4	4	-	0/2/15/18	0/1/1/1
7	FUB	UD	1	7	-	0/2/15/18	0/1/1/1
7	FUB	UD	2	7	-	0/2/15/18	0/1/1/1
7	FUB	UD	3	7	-	0/2/15/18	0/1/1/1
7	AHR	UD	4	7	-	0/2/15/18	0/1/1/1
20	FUB	UE	1	20	-	0/2/15/18	0/1/1/1
20	FUB	UE	2	20	-	0/2/15/18	0/1/1/1
20	GZL	UE	3	20	1/1/4/5	4/6/19/22	0/1/1/1
20	AHR	UE	4	20	-	0/2/15/18	0/1/1/1
3	FUB	V	1	3	-	0/2/15/18	0/1/1/1
3	FUB	V	2	3	-	0/2/15/18	0/1/1/1
3	FUB	V	3	3	-	0/2/15/18	0/1/1/1
4	FUB	VA	1	4	-	0/2/15/18	0/1/1/1
4	FUB	VA	2	4	-	0/2/15/18	0/1/1/1
4	FUB	VA	3	4	-	0/2/15/18	0/1/1/1
4	AHR	VA	4	4	2/2/3/4	0/2/15/18	0/1/1/1
10	FUB	VB	1	10	-	0/2/15/18	0/1/1/1
10	FUB	VB	2	10	-	0/2/15/18	0/1/1/1
10	FUB	VB	3	10	-	0/2/15/18	0/1/1/1
10	AHR	VB	4	10	1/1/3/4	0/2/15/18	0/1/1/1
10	AHR	VB	5	10	-	0/2/15/18	0/1/1/1
4	FUB	VC	1	4	-	0/2/15/18	0/1/1/1
4	FUB	VC	2	4	-	0/2/15/18	0/1/1/1
4	FUB	VC	3	4	-	0/2/15/18	0/1/1/1
4	AHR	VC	4	4	-	0/2/15/18	0/1/1/1
4	FUB	VD	1	4	-	0/2/15/18	0/1/1/1
4	FUB	VD	2	4	-	0/2/15/18	0/1/1/1
4	FUB	VD	3	4	-	0/2/15/18	0/1/1/1
4	AHR	VD	4	4	-	0/2/15/18	0/1/1/1
22	FUB	VE	1	22	-	0/2/15/18	0/1/1/1
22	FUB	VE	2	22	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	GZL	VE	3	22	1/1/4/5	2/6/19/22	0/1/1/1
22	AHR	VE	4	22	1/1/3/4	0/2/15/18	0/1/1/1
22	AHR	VE	5	22	-	0/2/15/18	0/1/1/1
22	AHR	VE	6	22	-	0/2/15/18	0/1/1/1
4	FUB	W	1	4	-	0/2/15/18	0/1/1/1
4	FUB	W	2	4	-	0/2/15/18	0/1/1/1
4	FUB	W	3	4	-	0/2/15/18	0/1/1/1
4	AHR	W	4	4	-	0/2/15/18	0/1/1/1
9	FUB	WA	1	9	-	0/2/15/18	0/1/1/1
9	FUB	WA	2	9	-	0/2/15/18	0/1/1/1
13	FUB	WB	1	13	-	0/2/15/18	0/1/1/1
13	FUB	WB	2	13	-	0/2/15/18	0/1/1/1
13	GZL	WB	3	13	3/3/4/5	1/6/19/22	0/1/1/1
13	AHR	WB	4	13	-	0/2/15/18	0/1/1/1
3	FUB	WC	1	3	-	0/2/15/18	0/1/1/1
3	FUB	WC	2	3	-	0/2/15/18	0/1/1/1
3	FUB	WC	3	3	-	0/2/15/18	0/1/1/1
7	FUB	WD	1	7	-	0/2/15/18	0/1/1/1
7	FUB	WD	2	7	-	0/2/15/18	0/1/1/1
7	FUB	WD	3	7	-	0/2/15/18	0/1/1/1
7	AHR	WD	4	7	-	0/2/15/18	0/1/1/1
20	FUB	WE	1	20	-	0/2/15/18	0/1/1/1
20	FUB	WE	2	20	-	0/2/15/18	0/1/1/1
20	GZL	WE	3	20	1/1/4/5	2/6/19/22	0/1/1/1
20	AHR	WE	4	20	1/1/3/4	0/2/15/18	0/1/1/1
4	FUB	X	1	4	-	0/2/15/18	0/1/1/1
4	FUB	X	2	4	-	0/2/15/18	0/1/1/1
4	FUB	X	3	4	-	0/2/15/18	0/1/1/1
4	AHR	X	4	4	-	0/2/15/18	0/1/1/1
3	FUB	XA	1	3	-	0/2/15/18	0/1/1/1
3	FUB	XA	2	3	1/1/3/4	0/2/15/18	0/1/1/1
3	FUB	XA	3	3	-	0/2/15/18	0/1/1/1
6	FUB	XB	1	6	-	0/2/15/18	0/1/1/1
6	FUB	XB	2	6	-	0/2/15/18	0/1/1/1
6	GZL	XB	3	6	2/2/4/5	5/6/19/22	0/1/1/1
7	FUB	XC	1	7	-	0/2/15/18	0/1/1/1
7	FUB	XC	2	7	-	0/2/15/18	0/1/1/1
7	FUB	XC	3	7	-	0/2/15/18	0/1/1/1
7	AHR	XC	4	7	-	0/2/15/18	0/1/1/1
11	FUB	XD	1	11	-	0/2/15/18	0/1/1/1
11	AHR	XD	2	11	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	AHR	XD	3	11	-	0/2/15/18	0/1/1/1
23	FUB	XE	1	23	-	0/2/15/18	0/1/1/1
23	FUB	XE	2	23	-	1/2/15/18	0/1/1/1
23	GZL	XE	3	23	1/1/4/5	2/6/19/22	0/1/1/1
23	AHR	XE	4	23	1/1/3/4	0/2/15/18	0/1/1/1
23	AHR	XE	5	23	1/1/3/4	0/2/15/18	0/1/1/1
23	AHR	XE	6	23	-	0/2/15/18	0/1/1/1
9	FUB	Y	1	9	-	0/2/15/18	0/1/1/1
9	FUB	Y	2	9	-	0/2/15/18	0/1/1/1
10	FUB	YA	1	10	-	0/2/15/18	0/1/1/1
10	FUB	YA	2	10	-	0/2/15/18	0/1/1/1
10	FUB	YA	3	10	-	0/2/15/18	0/1/1/1
10	AHR	YA	4	10	-	0/2/15/18	0/1/1/1
10	AHR	YA	5	10	-	0/2/15/18	0/1/1/1
13	FUB	YB	1	13	-	0/2/15/18	0/1/1/1
13	FUB	YB	2	13	-	0/2/15/18	0/1/1/1
13	GZL	YB	3	13	1/1/4/5	4/6/19/22	0/1/1/1
13	AHR	YB	4	13	-	0/2/15/18	0/1/1/1
4	FUB	YC	1	4	-	0/2/15/18	0/1/1/1
4	FUB	YC	2	4	-	0/2/15/18	0/1/1/1
4	FUB	YC	3	4	-	0/2/15/18	0/1/1/1
4	AHR	YC	4	4	-	0/2/15/18	0/1/1/1
9	FUB	YD	1	9	-	0/2/15/18	0/1/1/1
9	FUB	YD	2	9	-	0/2/15/18	0/1/1/1
24	FUB	YE	1	24	-	0/2/15/18	0/1/1/1
24	FUB	YE	2	24	-	0/2/15/18	0/1/1/1
24	GZL	YE	3	24	1/1/4/5	4/6/19/22	0/1/1/1
24	AHR	YE	4	24	1/1/3/4	0/2/15/18	0/1/1/1
24	AHR	YE	5	24	-	0/2/15/18	0/1/1/1
24	AHR	YE	6	24	-	0/2/15/18	0/1/1/1
4	FUB	Z	1	4	-	0/2/15/18	0/1/1/1
4	FUB	Z	2	4	1/1/3/4	0/2/15/18	0/1/1/1
4	FUB	Z	3	4	-	0/2/15/18	0/1/1/1
4	AHR	Z	4	4	-	0/2/15/18	0/1/1/1
3	FUB	ZA	1	3	-	0/2/15/18	0/1/1/1
3	FUB	ZA	2	3	-	0/2/15/18	0/1/1/1
3	FUB	ZA	3	3	-	0/2/15/18	0/1/1/1
13	FUB	ZB	1	13	-	0/2/15/18	0/1/1/1
13	FUB	ZB	2	13	-	0/2/15/18	0/1/1/1
13	GZL	ZB	3	13	1/1/4/5	2/6/19/22	0/1/1/1
13	AHR	ZB	4	13	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	FUB	ZC	1	7	-	0/2/15/18	0/1/1/1
7	FUB	ZC	2	7	-	0/2/15/18	0/1/1/1
7	FUB	ZC	3	7	-	0/2/15/18	0/1/1/1
7	AHR	ZC	4	7	-	0/2/15/18	0/1/1/1
4	FUB	ZD	1	4	-	0/2/15/18	0/1/1/1
4	FUB	ZD	2	4	-	0/2/15/18	0/1/1/1
4	FUB	ZD	3	4	-	0/2/15/18	0/1/1/1
4	AHR	ZD	4	4	-	0/2/15/18	0/1/1/1
6	FUB	ZE	1	6	-	0/2/15/18	0/1/1/1
6	FUB	ZE	2	6	-	0/2/15/18	0/1/1/1
6	GZL	ZE	3	6	1/1/4/5	2/6/19/22	0/1/1/1
10	FUB	a	1	10	-	0/2/15/18	0/1/1/1
10	FUB	a	2	10	-	0/2/15/18	0/1/1/1
10	FUB	a	3	10	-	0/2/15/18	0/1/1/1
10	AHR	a	4	10	-	0/2/15/18	0/1/1/1
10	AHR	a	5	10	-	0/2/15/18	0/1/1/1
4	FUB	aA	1	4	-	0/2/15/18	0/1/1/1
4	FUB	aA	2	4	-	0/2/15/18	0/1/1/1
4	FUB	aA	3	4	-	0/2/15/18	0/1/1/1
4	AHR	aA	4	4	-	0/2/15/18	0/1/1/1
6	FUB	aB	1	6	-	0/2/15/18	0/1/1/1
6	FUB	aB	2	6	-	0/2/15/18	0/1/1/1
6	GZL	aB	3	6	-	2/6/19/22	0/1/1/1
11	FUB	aC	1	11	-	0/2/15/18	0/1/1/1
11	AHR	aC	2	11	-	0/2/15/18	0/1/1/1
11	AHR	aC	3	11	-	0/2/15/18	0/1/1/1
3	FUB	aD	1	3	-	0/2/15/18	0/1/1/1
3	FUB	aD	2	3	-	0/2/15/18	0/1/1/1
3	FUB	aD	3	3	-	0/2/15/18	0/1/1/1
19	FUB	aE	1	19	-	0/2/15/18	0/1/1/1
19	FUB	aE	2	19	-	0/2/15/18	0/1/1/1
19	GZL	aE	3	19	1/1/4/5	2/6/19/22	0/1/1/1
19	AHR	aE	4	19	1/1/3/4	0/2/15/18	0/1/1/1
3	FUB	b	1	3	-	0/2/15/18	0/1/1/1
3	FUB	b	2	3	-	0/2/15/18	0/1/1/1
3	FUB	b	3	3	-	0/2/15/18	0/1/1/1
4	FUB	bA	1	4	-	0/2/15/18	0/1/1/1
4	FUB	bA	2	4	-	0/2/15/18	0/1/1/1
4	FUB	bA	3	4	-	0/2/15/18	0/1/1/1
4	AHR	bA	4	4	-	0/2/15/18	0/1/1/1
6	FUB	bB	1	6	-	0/2/15/18	0/1/1/1
6	FUB	bB	2	6	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GZL	bB	3	6	1/1/4/5	4/6/19/22	0/1/1/1
9	FUB	bC	1	9	-	0/2/15/18	0/1/1/1
9	FUB	bC	2	9	-	0/2/15/18	0/1/1/1
3	FUB	bD	1	3	-	0/2/15/18	0/1/1/1
3	FUB	bD	2	3	-	0/2/15/18	0/1/1/1
3	FUB	bD	3	3	-	0/2/15/18	0/1/1/1
6	FUB	bE	1	6	-	0/2/15/18	0/1/1/1
6	FUB	bE	2	6	-	0/2/15/18	0/1/1/1
6	GZL	bE	3	6	1/1/4/5	4/6/19/22	0/1/1/1
4	FUB	c	1	4	-	0/2/15/18	0/1/1/1
4	FUB	c	2	4	-	0/2/15/18	0/1/1/1
4	FUB	c	3	4	-	0/2/15/18	0/1/1/1
4	AHR	c	4	4	-	0/2/15/18	0/1/1/1
3	FUB	cA	1	3	-	0/2/15/18	0/1/1/1
3	FUB	cA	2	3	-	0/2/15/18	0/1/1/1
3	FUB	cA	3	3	-	0/2/15/18	0/1/1/1
6	FUB	cB	1	6	-	0/2/15/18	0/1/1/1
6	FUB	cB	2	6	1/1/3/4	0/2/15/18	0/1/1/1
6	GZL	cB	3	6	1/1/4/5	4/6/19/22	0/1/1/1
4	FUB	cC	1	4	-	0/2/15/18	0/1/1/1
4	FUB	cC	2	4	-	0/2/15/18	0/1/1/1
4	FUB	cC	3	4	-	0/2/15/18	0/1/1/1
4	AHR	cC	4	4	-	0/2/15/18	0/1/1/1
12	FUB	cD	1	12	-	0/2/15/18	0/1/1/1
12	FUB	cD	2	12	-	0/2/15/18	0/1/1/1
12	GZL	cD	3	12	2/2/4/5	2/6/19/22	0/1/1/1
12	AHR	cD	4	12	-	0/2/15/18	0/1/1/1
12	AHR	cD	5	12	-	0/2/15/18	0/1/1/1
18	FUB	cE	1	18	-	0/2/15/18	0/1/1/1
18	FUB	cE	2	18	-	0/2/15/18	0/1/1/1
18	GZL	cE	3	18	1/1/4/5	2/6/19/22	0/1/1/1
18	AHR	cE	4	18	1/1/3/4	0/2/15/18	0/1/1/1
18	AHR	cE	5	18	1/1/3/4	0/2/15/18	0/1/1/1
4	FUB	d	1	4	-	0/2/15/18	0/1/1/1
4	FUB	d	2	4	-	0/2/15/18	0/1/1/1
4	FUB	d	3	4	-	0/2/15/18	0/1/1/1
4	AHR	d	4	4	-	0/2/15/18	0/1/1/1
7	FUB	dA	1	7	-	0/2/15/18	0/1/1/1
7	FUB	dA	2	7	-	0/2/15/18	0/1/1/1
7	FUB	dA	3	7	-	0/2/15/18	0/1/1/1
7	AHR	dA	4	7	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	FUB	dB	1	13	-	0/2/15/18	0/1/1/1
13	FUB	dB	2	13	1/1/3/4	0/2/15/18	0/1/1/1
13	GZL	dB	3	13	-	4/6/19/22	0/1/1/1
13	AHR	dB	4	13	-	0/2/15/18	0/1/1/1
3	FUB	dC	1	3	-	0/2/15/18	0/1/1/1
3	FUB	dC	2	3	-	0/2/15/18	0/1/1/1
3	FUB	dC	3	3	-	0/2/15/18	0/1/1/1
13	FUB	dD	1	13	-	0/2/15/18	0/1/1/1
13	FUB	dD	2	13	-	0/2/15/18	0/1/1/1
13	GZL	dD	3	13	2/2/4/5	3/6/19/22	0/1/1/1
13	AHR	dD	4	13	-	0/2/15/18	0/1/1/1
22	FUB	dE	1	22	-	0/2/15/18	0/1/1/1
22	FUB	dE	2	22	-	0/2/15/18	0/1/1/1
22	GZL	dE	3	22	1/1/4/5	4/6/19/22	0/1/1/1
22	AHR	dE	4	22	1/1/3/4	0/2/15/18	0/1/1/1
22	AHR	dE	5	22	-	0/2/15/18	0/1/1/1
22	AHR	dE	6	22	1/1/3/4	0/2/15/18	0/1/1/1
3	FUB	e	1	3	-	0/2/15/18	0/1/1/1
3	FUB	e	2	3	-	0/2/15/18	0/1/1/1
3	FUB	e	3	3	-	0/2/15/18	0/1/1/1
4	FUB	eA	1	4	-	0/2/15/18	0/1/1/1
4	FUB	eA	2	4	-	0/2/15/18	0/1/1/1
4	FUB	eA	3	4	-	0/2/15/18	0/1/1/1
4	AHR	eA	4	4	-	0/2/15/18	0/1/1/1
15	FUB	eB	1	15	-	0/2/15/18	0/1/1/1
15	FUB	eB	2	15	-	0/2/15/18	0/1/1/1
15	GZL	eB	3	15	1/1/4/5	6/6/19/22	0/1/1/1
15	AHR	eB	4	15	-	0/2/15/18	0/1/1/1
15	AHR	eB	5	15	1/1/3/4	0/2/15/18	0/1/1/1
3	FUB	eC	1	3	-	0/2/15/18	0/1/1/1
3	FUB	eC	2	3	-	0/2/15/18	0/1/1/1
3	FUB	eC	3	3	-	0/2/15/18	0/1/1/1
14	FUB	eD	1	14	-	0/2/15/18	0/1/1/1
14	FUB	eD	2	14	-	0/2/15/18	0/1/1/1
14	GZL	eD	3	14	2/2/4/5	6/6/19/22	0/1/1/1
14	FUB	eD	4	14	-	0/2/15/18	0/1/1/1
22	FUB	eE	1	22	-	0/2/15/18	0/1/1/1
22	FUB	eE	2	22	-	0/2/15/18	0/1/1/1
22	GZL	eE	3	22	1/1/4/5	2/6/19/22	0/1/1/1
22	AHR	eE	4	22	2/2/3/4	0/2/15/18	0/1/1/1
22	AHR	eE	5	22	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	AHR	eE	6	22	-	0/2/15/18	0/1/1/1
7	FUB	f	1	7	-	0/2/15/18	0/1/1/1
7	FUB	f	2	7	-	0/2/15/18	0/1/1/1
7	FUB	f	3	7	-	0/2/15/18	0/1/1/1
7	AHR	f	4	7	-	0/2/15/18	0/1/1/1
7	FUB	fA	1	7	-	0/2/15/18	0/1/1/1
7	FUB	fA	2	7	-	0/2/15/18	0/1/1/1
7	FUB	fA	3	7	-	0/2/15/18	0/1/1/1
7	AHR	fA	4	7	-	0/2/15/18	0/1/1/1
15	FUB	fB	1	15	-	0/2/15/18	0/1/1/1
15	FUB	fB	2	15	-	0/2/15/18	0/1/1/1
15	GZL	fB	3	15	1/1/4/5	0/6/19/22	0/1/1/1
15	AHR	fB	4	15	-	0/2/15/18	0/1/1/1
15	AHR	fB	5	15	-	0/2/15/18	0/1/1/1
12	FUB	fC	1	12	-	0/2/15/18	0/1/1/1
12	FUB	fC	2	12	-	0/2/15/18	0/1/1/1
12	GZL	fC	3	12	2/2/4/5	6/6/19/22	0/1/1/1
12	AHR	fC	4	12	-	0/2/15/18	0/1/1/1
12	AHR	fC	5	12	-	0/2/15/18	0/1/1/1
12	FUB	fD	1	12	-	0/2/15/18	0/1/1/1
12	FUB	fD	2	12	-	0/2/15/18	0/1/1/1
12	GZL	fD	3	12	2/2/4/5	2/6/19/22	0/1/1/1
12	AHR	fD	4	12	-	0/2/15/18	0/1/1/1
12	AHR	fD	5	12	-	0/2/15/18	0/1/1/1
18	FUB	fE	1	18	1/1/3/4	0/2/15/18	0/1/1/1
18	FUB	fE	2	18	-	0/2/15/18	0/1/1/1
18	GZL	fE	3	18	1/1/4/5	6/6/19/22	0/1/1/1
18	AHR	fE	4	18	1/1/3/4	0/2/15/18	0/1/1/1
18	AHR	fE	5	18	1/1/3/4	0/2/15/18	0/1/1/1
4	FUB	g	1	4	-	0/2/15/18	0/1/1/1
4	FUB	g	2	4	-	0/2/15/18	0/1/1/1
4	FUB	g	3	4	-	0/2/15/18	0/1/1/1
4	AHR	g	4	4	-	0/2/15/18	0/1/1/1
11	FUB	gA	1	11	-	1/2/15/18	0/1/1/1
11	AHR	gA	2	11	-	0/2/15/18	0/1/1/1
11	AHR	gA	3	11	-	0/2/15/18	0/1/1/1
6	FUB	gB	1	6	-	0/2/15/18	0/1/1/1
6	FUB	gB	2	6	-	0/2/15/18	0/1/1/1
6	GZL	gB	3	6	1/1/4/5	6/6/19/22	0/1/1/1
13	FUB	gC	1	13	-	0/2/15/18	0/1/1/1
13	FUB	gC	2	13	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	GZL	gC	3	13	2/2/4/5	2/6/19/22	0/1/1/1
13	AHR	gC	4	13	-	0/2/15/18	0/1/1/1
4	FUB	gD	1	4	-	0/2/15/18	0/1/1/1
4	FUB	gD	2	4	-	0/2/15/18	0/1/1/1
4	FUB	gD	3	4	-	0/2/15/18	0/1/1/1
4	AHR	gD	4	4	-	0/2/15/18	0/1/1/1
20	FUB	gE	1	20	-	0/2/15/18	0/1/1/1
20	FUB	gE	2	20	-	0/2/15/18	0/1/1/1
20	GZL	gE	3	20	1/1/4/5	2/6/19/22	0/1/1/1
20	AHR	gE	4	20	1/1/3/4	0/2/15/18	0/1/1/1
7	FUB	h	1	7	-	0/2/15/18	0/1/1/1
7	FUB	h	2	7	-	0/2/15/18	0/1/1/1
7	FUB	h	3	7	-	0/2/15/18	0/1/1/1
7	AHR	h	4	7	-	0/2/15/18	0/1/1/1
9	FUB	hA	1	9	-	0/2/15/18	0/1/1/1
9	FUB	hA	2	9	-	0/2/15/18	0/1/1/1
3	FUB	hB	1	3	-	0/2/15/18	0/1/1/1
3	FUB	hB	2	3	-	0/2/15/18	0/1/1/1
3	FUB	hB	3	3	-	0/2/15/18	0/1/1/1
14	FUB	hC	1	14	-	0/2/15/18	0/1/1/1
14	FUB	hC	2	14	-	0/2/15/18	0/1/1/1
14	GZL	hC	3	14	2/2/4/5	3/6/19/22	0/1/1/1
14	FUB	hC	4	14	-	0/2/15/18	0/1/1/1
14	FUB	hD	1	14	-	0/2/15/18	0/1/1/1
14	FUB	hD	2	14	-	0/2/15/18	0/1/1/1
14	GZL	hD	3	14	2/2/4/5	4/6/19/22	0/1/1/1
14	FUB	hD	4	14	-	0/2/15/18	0/1/1/1
20	FUB	hE	1	20	-	0/2/15/18	0/1/1/1
20	FUB	hE	2	20	-	2/2/15/18	0/1/1/1
20	GZL	hE	3	20	1/1/4/5	3/6/19/22	0/1/1/1
20	AHR	hE	4	20	-	0/2/15/18	0/1/1/1
11	FUB	i	1	11	-	0/2/15/18	0/1/1/1
11	AHR	i	2	11	-	0/2/15/18	0/1/1/1
11	AHR	i	3	11	-	0/2/15/18	0/1/1/1
4	FUB	iA	1	4	-	0/2/15/18	0/1/1/1
4	FUB	iA	2	4	-	0/2/15/18	0/1/1/1
4	FUB	iA	3	4	-	0/2/15/18	0/1/1/1
4	AHR	iA	4	4	-	0/2/15/18	0/1/1/1
12	FUB	iB	1	12	-	0/2/15/18	0/1/1/1
12	FUB	iB	2	12	-	0/2/15/18	0/1/1/1
12	GZL	iB	3	12	2/2/4/5	6/6/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	AHR	iB	4	12	-	0/2/15/18	0/1/1/1
12	AHR	iB	5	12	-	0/2/15/18	0/1/1/1
12	FUB	iC	1	12	-	0/2/15/18	0/1/1/1
12	FUB	iC	2	12	-	0/2/15/18	0/1/1/1
12	GZL	iC	3	12	2/2/4/5	6/6/19/22	0/1/1/1
12	AHR	iC	4	12	-	0/2/15/18	0/1/1/1
12	AHR	iC	5	12	-	0/2/15/18	0/1/1/1
3	FUB	iD	1	3	-	0/2/15/18	0/1/1/1
3	FUB	iD	2	3	-	0/2/15/18	0/1/1/1
3	FUB	iD	3	3	-	0/2/15/18	0/1/1/1
22	FUB	iE	1	22	-	0/2/15/18	0/1/1/1
22	FUB	iE	2	22	-	0/2/15/18	0/1/1/1
22	GZL	iE	3	22	1/1/4/5	2/6/19/22	0/1/1/1
22	AHR	iE	4	22	1/1/3/4	0/2/15/18	0/1/1/1
22	AHR	iE	5	22	-	0/2/15/18	0/1/1/1
22	AHR	iE	6	22	-	0/2/15/18	0/1/1/1
9	FUB	j	1	9	-	0/2/15/18	0/1/1/1
9	FUB	j	2	9	-	0/2/15/18	0/1/1/1
3	FUB	jA	1	3	-	0/2/15/18	0/1/1/1
3	FUB	jA	2	3	-	0/2/15/18	0/1/1/1
3	FUB	jA	3	3	-	0/2/15/18	0/1/1/1
13	FUB	jB	1	13	-	0/2/15/18	0/1/1/1
13	FUB	jB	2	13	-	0/2/15/18	0/1/1/1
13	GZL	jB	3	13	2/2/4/5	3/6/19/22	0/1/1/1
13	AHR	jB	4	13	-	0/2/15/18	0/1/1/1
4	FUB	jC	1	4	-	0/2/15/18	0/1/1/1
4	FUB	jC	2	4	-	0/2/15/18	0/1/1/1
4	FUB	jC	3	4	-	0/2/15/18	0/1/1/1
4	AHR	jC	4	4	-	0/2/15/18	0/1/1/1
10	FUB	jD	1	10	-	0/2/15/18	0/1/1/1
10	FUB	jD	2	10	-	0/2/15/18	0/1/1/1
10	FUB	jD	3	10	-	0/2/15/18	0/1/1/1
10	AHR	jD	4	10	-	0/2/15/18	0/1/1/1
10	AHR	jD	5	10	-	0/2/15/18	0/1/1/1
20	FUB	jE	1	20	-	0/2/15/18	0/1/1/1
20	FUB	jE	2	20	-	0/2/15/18	0/1/1/1
20	GZL	jE	3	20	1/1/4/5	4/6/19/22	0/1/1/1
20	AHR	jE	4	20	1/1/3/4	0/2/15/18	0/1/1/1
4	FUB	k	1	4	-	0/2/15/18	0/1/1/1
4	FUB	k	2	4	-	0/2/15/18	0/1/1/1
4	FUB	k	3	4	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	AHR	k	4	4	-	0/2/15/18	0/1/1/1
3	FUB	kA	1	3	-	0/2/15/18	0/1/1/1
3	FUB	kA	2	3	-	0/2/15/18	0/1/1/1
3	FUB	kA	3	3	-	0/2/15/18	0/1/1/1
14	FUB	kB	1	14	-	0/2/15/18	0/1/1/1
14	FUB	kB	2	14	-	0/2/15/18	0/1/1/1
14	GZL	kB	3	14	2/2/4/5	6/6/19/22	0/1/1/1
14	FUB	kB	4	14	-	0/2/15/18	0/1/1/1
14	FUB	kC	1	14	-	0/2/15/18	0/1/1/1
14	FUB	kC	2	14	-	0/2/15/18	0/1/1/1
14	GZL	kC	3	14	2/2/4/5	6/6/19/22	0/1/1/1
14	FUB	kC	4	14	-	0/2/15/18	0/1/1/1
4	FUB	kD	1	4	-	0/2/15/18	0/1/1/1
4	FUB	kD	2	4	-	0/2/15/18	0/1/1/1
4	FUB	kD	3	4	-	0/2/15/18	0/1/1/1
4	AHR	kD	4	4	-	0/2/15/18	0/1/1/1
21	FUB	kE	1	21	-	0/2/15/18	0/1/1/1
21	FUB	kE	2	21	-	0/2/15/18	0/1/1/1
21	GZL	kE	3	21	1/1/4/5	0/6/19/22	0/1/1/1
21	AHR	kE	4	21	1/1/3/4	0/2/15/18	0/1/1/1
21	AHR	kE	5	21	-	0/2/15/18	0/1/1/1
3	FUB	l	1	3	-	0/2/15/18	0/1/1/1
3	FUB	l	2	3	-	0/2/15/18	0/1/1/1
3	FUB	l	3	3	-	0/2/15/18	0/1/1/1
12	FUB	lA	1	12	-	0/2/15/18	0/1/1/1
12	FUB	lA	2	12	-	0/2/15/18	0/1/1/1
12	GZL	lA	3	12	2/2/4/5	2/6/19/22	0/1/1/1
12	AHR	lA	4	12	-	0/2/15/18	0/1/1/1
12	AHR	lA	5	12	-	0/2/15/18	0/1/1/1
12	FUB	lB	1	12	-	0/2/15/18	0/1/1/1
12	FUB	lB	2	12	-	0/2/15/18	0/1/1/1
12	GZL	lB	3	12	2/2/4/5	6/6/19/22	0/1/1/1
12	AHR	lB	4	12	-	0/2/15/18	0/1/1/1
12	AHR	lB	5	12	-	0/2/15/18	0/1/1/1
3	FUB	lC	1	3	-	0/2/15/18	0/1/1/1
3	FUB	lC	2	3	-	0/2/15/18	0/1/1/1
3	FUB	lC	3	3	-	0/2/15/18	0/1/1/1
3	FUB	lD	1	3	-	0/2/15/18	0/1/1/1
3	FUB	lD	2	3	-	0/2/15/18	0/1/1/1
3	FUB	lD	3	3	-	0/2/15/18	0/1/1/1
24	FUB	lE	1	24	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	FUB	lE	2	24	-	0/2/15/18	0/1/1/1
24	GZL	lE	3	24	1/1/4/5	5/6/19/22	0/1/1/1
24	AHR	lE	4	24	1/1/3/4	0/2/15/18	0/1/1/1
24	AHR	lE	5	24	-	0/2/15/18	0/1/1/1
24	AHR	lE	6	24	-	0/2/15/18	0/1/1/1
3	FUB	m	1	3	-	0/2/15/18	0/1/1/1
3	FUB	m	2	3	-	0/2/15/18	0/1/1/1
3	FUB	m	3	3	-	0/2/15/18	0/1/1/1
13	FUB	mA	1	13	-	0/2/15/18	0/1/1/1
13	FUB	mA	2	13	-	0/2/15/18	0/1/1/1
13	GZL	mA	3	13	2/2/4/5	4/6/19/22	0/1/1/1
13	AHR	mA	4	13	-	0/2/15/18	0/1/1/1
4	FUB	mB	1	4	-	0/2/15/18	0/1/1/1
4	FUB	mB	2	4	-	0/2/15/18	0/1/1/1
4	FUB	mB	3	4	-	0/2/15/18	0/1/1/1
4	AHR	mB	4	4	-	0/2/15/18	0/1/1/1
10	FUB	mC	1	10	-	0/2/15/18	0/1/1/1
10	FUB	mC	2	10	-	0/2/15/18	0/1/1/1
10	FUB	mC	3	10	-	0/2/15/18	0/1/1/1
10	AHR	mC	4	10	-	0/2/15/18	0/1/1/1
10	AHR	mC	5	10	-	0/2/15/18	0/1/1/1
3	FUB	mD	1	3	-	0/2/15/18	0/1/1/1
3	FUB	mD	2	3	-	0/2/15/18	0/1/1/1
3	FUB	mD	3	3	-	0/2/15/18	0/1/1/1
6	FUB	mE	1	6	-	0/2/15/18	0/1/1/1
6	FUB	mE	2	6	-	0/2/15/18	0/1/1/1
6	GZL	mE	3	6	1/1/4/5	4/6/19/22	0/1/1/1
12	FUB	n	1	12	-	0/2/15/18	0/1/1/1
12	FUB	n	2	12	-	0/2/15/18	0/1/1/1
12	GZL	n	3	12	2/2/4/5	2/6/19/22	0/1/1/1
12	AHR	n	4	12	-	0/2/15/18	0/1/1/1
12	AHR	n	5	12	-	0/2/15/18	0/1/1/1
14	FUB	nA	1	14	-	0/2/15/18	0/1/1/1
14	FUB	nA	2	14	-	0/2/15/18	0/1/1/1
14	GZL	nA	3	14	2/2/4/5	6/6/19/22	0/1/1/1
14	FUB	nA	4	14	-	0/2/15/18	0/1/1/1
14	FUB	nB	1	14	-	0/2/15/18	0/1/1/1
14	FUB	nB	2	14	-	0/2/15/18	0/1/1/1
14	GZL	nB	3	14	2/2/4/5	6/6/19/22	0/1/1/1
14	FUB	nB	4	14	-	0/2/15/18	0/1/1/1
4	FUB	nC	1	4	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FUB	nC	2	4	-	0/2/15/18	0/1/1/1
4	FUB	nC	3	4	-	0/2/15/18	0/1/1/1
4	AHR	nC	4	4	-	0/2/15/18	0/1/1/1
3	FUB	nD	1	3	-	0/2/15/18	0/1/1/1
3	FUB	nD	2	3	-	0/2/15/18	0/1/1/1
3	FUB	nD	3	3	-	0/2/15/18	0/1/1/1
6	FUB	nE	1	6	-	0/2/15/18	0/1/1/1
6	FUB	nE	2	6	-	0/2/15/18	0/1/1/1
6	GZL	nE	3	6	1/1/4/5	6/6/19/22	0/1/1/1
13	FUB	o	1	13	-	0/2/15/18	0/1/1/1
13	FUB	o	2	13	-	0/2/15/18	0/1/1/1
13	GZL	o	3	13	2/2/4/5	2/6/19/22	0/1/1/1
13	AHR	o	4	13	-	0/2/15/18	0/1/1/1
12	FUB	oA	1	12	-	0/2/15/18	0/1/1/1
12	FUB	oA	2	12	-	0/2/15/18	0/1/1/1
12	GZL	oA	3	12	2/2/4/5	2/6/19/22	0/1/1/1
12	AHR	oA	4	12	-	0/2/15/18	0/1/1/1
12	AHR	oA	5	12	-	0/2/15/18	0/1/1/1
3	FUB	oB	1	3	-	0/2/15/18	0/1/1/1
3	FUB	oB	2	3	-	0/2/15/18	0/1/1/1
3	FUB	oB	3	3	-	0/2/15/18	0/1/1/1
3	FUB	oC	1	3	-	0/2/15/18	0/1/1/1
3	FUB	oC	2	3	-	0/2/15/18	0/1/1/1
3	FUB	oC	3	3	-	0/2/15/18	0/1/1/1
3	FUB	oD	1	3	-	0/2/15/18	0/1/1/1
3	FUB	oD	2	3	-	0/2/15/18	0/1/1/1
3	FUB	oD	3	3	-	0/2/15/18	0/1/1/1
6	FUB	oE	1	6	-	0/2/15/18	0/1/1/1
6	FUB	oE	2	6	-	0/2/15/18	0/1/1/1
6	GZL	oE	3	6	1/1/4/5	4/6/19/22	0/1/1/1
14	FUB	p	1	14	-	0/2/15/18	0/1/1/1
14	FUB	p	2	14	-	0/2/15/18	0/1/1/1
14	GZL	p	3	14	2/2/4/5	6/6/19/22	0/1/1/1
14	FUB	p	4	14	-	0/2/15/18	0/1/1/1
4	FUB	pA	1	4	-	0/2/15/18	0/1/1/1
4	FUB	pA	2	4	-	0/2/15/18	0/1/1/1
4	FUB	pA	3	4	-	0/2/15/18	0/1/1/1
4	AHR	pA	4	4	-	0/2/15/18	0/1/1/1
10	FUB	pB	1	10	-	0/2/15/18	0/1/1/1
10	FUB	pB	2	10	-	0/2/15/18	0/1/1/1
10	FUB	pB	3	10	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	AHR	pB	4	10	-	0/2/15/18	0/1/1/1
10	AHR	pB	5	10	-	0/2/15/18	0/1/1/1
3	FUB	pC	1	3	-	0/2/15/18	0/1/1/1
3	FUB	pC	2	3	-	0/2/15/18	0/1/1/1
3	FUB	pC	3	3	-	0/2/15/18	0/1/1/1
3	FUB	pD	1	3	-	0/2/15/18	0/1/1/1
3	FUB	pD	2	3	-	0/2/15/18	0/1/1/1
3	FUB	pD	3	3	-	0/2/15/18	0/1/1/1
18	FUB	pE	1	18	-	0/2/15/18	0/1/1/1
18	FUB	pE	2	18	-	0/2/15/18	0/1/1/1
18	GZL	pE	3	18	1/1/4/5	4/6/19/22	0/1/1/1
18	AHR	pE	4	18	1/1/3/4	0/2/15/18	0/1/1/1
18	AHR	pE	5	18	-	0/2/15/18	0/1/1/1
12	FUB	q	1	12	-	0/2/15/18	0/1/1/1
12	FUB	q	2	12	-	0/2/15/18	0/1/1/1
12	GZL	q	3	12	2/2/4/5	0/6/19/22	0/1/1/1
12	AHR	q	4	12	-	0/2/15/18	0/1/1/1
12	AHR	q	5	12	1/1/3/4	0/2/15/18	0/1/1/1
14	FUB	qA	1	14	-	0/2/15/18	0/1/1/1
14	FUB	qA	2	14	-	0/2/15/18	0/1/1/1
14	GZL	qA	3	14	2/2/4/5	4/6/19/22	0/1/1/1
14	FUB	qA	4	14	-	0/2/15/18	0/1/1/1
4	FUB	qB	1	4	-	0/2/15/18	0/1/1/1
4	FUB	qB	2	4	-	0/2/15/18	0/1/1/1
4	FUB	qB	3	4	-	0/2/15/18	0/1/1/1
4	AHR	qB	4	4	-	0/2/15/18	0/1/1/1
3	FUB	qC	1	3	-	0/2/15/18	0/1/1/1
3	FUB	qC	2	3	-	0/2/15/18	0/1/1/1
3	FUB	qC	3	3	-	0/2/15/18	0/1/1/1
3	FUB	qD	1	3	-	0/2/15/18	0/1/1/1
3	FUB	qD	2	3	-	0/2/15/18	0/1/1/1
3	FUB	qD	3	3	-	0/2/15/18	0/1/1/1
19	FUB	qE	1	19	-	0/2/15/18	0/1/1/1
19	FUB	qE	2	19	-	0/2/15/18	0/1/1/1
19	GZL	qE	3	19	1/1/4/5	4/6/19/22	0/1/1/1
19	AHR	qE	4	19	-	0/2/15/18	0/1/1/1
4	FUB	r	1	4	-	0/2/15/18	0/1/1/1
4	FUB	r	2	4	-	0/2/15/18	0/1/1/1
4	FUB	r	3	4	-	0/2/15/18	0/1/1/1
4	AHR	r	4	4	-	0/2/15/18	0/1/1/1
3	FUB	rA	1	3	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FUB	rA	2	3	-	0/2/15/18	0/1/1/1
3	FUB	rA	3	3	-	0/2/15/18	0/1/1/1
3	FUB	rB	1	3	-	0/2/15/18	0/1/1/1
3	FUB	rB	2	3	-	0/2/15/18	0/1/1/1
3	FUB	rB	3	3	-	0/2/15/18	0/1/1/1
3	FUB	rC	1	3	-	0/2/15/18	0/1/1/1
3	FUB	rC	2	3	-	0/2/15/18	0/1/1/1
3	FUB	rC	3	3	-	0/2/15/18	0/1/1/1
3	FUB	rD	1	3	-	0/2/15/18	0/1/1/1
3	FUB	rD	2	3	-	0/2/15/18	0/1/1/1
3	FUB	rD	3	3	-	0/2/15/18	0/1/1/1
18	FUB	rE	1	18	-	0/2/15/18	0/1/1/1
18	FUB	rE	2	18	-	0/2/15/18	0/1/1/1
18	GZL	rE	3	18	1/1/4/5	3/6/19/22	0/1/1/1
18	AHR	rE	4	18	1/1/3/4	0/2/15/18	0/1/1/1
18	AHR	rE	5	18	1/1/3/4	0/2/15/18	0/1/1/1
14	FUB	s	1	14	-	0/2/15/18	0/1/1/1
14	FUB	s	2	14	-	0/2/15/18	0/1/1/1
14	GZL	s	3	14	2/2/4/5	4/6/19/22	0/1/1/1
14	FUB	s	4	14	-	0/2/15/18	0/1/1/1
10	FUB	sA	1	10	-	0/2/15/18	0/1/1/1
10	FUB	sA	2	10	-	0/2/15/18	0/1/1/1
10	FUB	sA	3	10	-	0/2/15/18	0/1/1/1
10	AHR	sA	4	10	-	0/2/15/18	0/1/1/1
10	AHR	sA	5	10	-	0/2/15/18	0/1/1/1
3	FUB	sB	1	3	-	0/2/15/18	0/1/1/1
3	FUB	sB	2	3	-	0/2/15/18	0/1/1/1
3	FUB	sB	3	3	-	0/2/15/18	0/1/1/1
3	FUB	sC	1	3	-	0/2/15/18	0/1/1/1
3	FUB	sC	2	3	-	0/2/15/18	0/1/1/1
3	FUB	sC	3	3	-	0/2/15/18	0/1/1/1
10	FUB	sD	1	10	-	0/2/15/18	0/1/1/1
10	FUB	sD	2	10	-	0/2/15/18	0/1/1/1
10	FUB	sD	3	10	-	0/2/15/18	0/1/1/1
10	AHR	sD	4	10	1/1/3/4	0/2/15/18	0/1/1/1
10	AHR	sD	5	10	-	0/2/15/18	0/1/1/1
20	FUB	sE	1	20	-	0/2/15/18	0/1/1/1
20	FUB	sE	2	20	-	0/2/15/18	0/1/1/1
20	GZL	sE	3	20	1/1/4/5	6/6/19/22	0/1/1/1
20	AHR	sE	4	20	-	0/2/15/18	0/1/1/1
3	FUB	t	1	3	-	0/2/15/18	0/1/1/1
3	FUB	t	2	3	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FUB	t	3	3	-	0/2/15/18	0/1/1/1
4	FUB	tA	1	4	-	0/2/15/18	0/1/1/1
4	FUB	tA	2	4	-	0/2/15/18	0/1/1/1
4	FUB	tA	3	4	-	0/2/15/18	0/1/1/1
4	AHR	tA	4	4	-	0/2/15/18	0/1/1/1
3	FUB	tB	1	3	-	0/2/15/18	0/1/1/1
3	FUB	tB	2	3	-	0/2/15/18	0/1/1/1
3	FUB	tB	3	3	-	0/2/15/18	0/1/1/1
3	FUB	tC	1	3	-	0/2/15/18	0/1/1/1
3	FUB	tC	2	3	-	0/2/15/18	0/1/1/1
3	FUB	tC	3	3	-	0/2/15/18	0/1/1/1
13	FUB	tD	1	13	-	0/2/15/18	0/1/1/1
13	FUB	tD	2	13	-	0/2/15/18	0/1/1/1
13	GZL	tD	3	13	3/3/4/5	0/6/19/22	0/1/1/1
13	AHR	tD	4	13	-	0/2/15/18	0/1/1/1
18	FUB	tE	1	18	-	0/2/15/18	0/1/1/1
18	FUB	tE	2	18	-	0/2/15/18	0/1/1/1
18	GZL	tE	3	18	1/1/4/5	2/6/19/22	0/1/1/1
18	AHR	tE	4	18	-	0/2/15/18	0/1/1/1
18	AHR	tE	5	18	1/1/3/4	0/2/15/18	0/1/1/1
10	FUB	u	1	10	-	0/2/15/18	0/1/1/1
10	FUB	u	2	10	-	0/2/15/18	0/1/1/1
10	FUB	u	3	10	-	0/2/15/18	0/1/1/1
10	AHR	u	4	10	-	0/2/15/18	0/1/1/1
10	AHR	u	5	10	-	0/2/15/18	0/1/1/1
3	FUB	uA	1	3	-	0/2/15/18	0/1/1/1
3	FUB	uA	2	3	-	0/2/15/18	0/1/1/1
3	FUB	uA	3	3	-	0/2/15/18	0/1/1/1
3	FUB	uB	1	3	-	0/2/15/18	0/1/1/1
3	FUB	uB	2	3	-	0/2/15/18	0/1/1/1
3	FUB	uB	3	3	-	0/2/15/18	0/1/1/1
3	FUB	uC	1	3	-	0/2/15/18	0/1/1/1
3	FUB	uC	2	3	-	0/2/15/18	0/1/1/1
3	FUB	uC	3	3	-	0/2/15/18	0/1/1/1
6	FUB	uD	1	6	-	0/2/15/18	0/1/1/1
6	FUB	uD	2	6	-	0/2/15/18	0/1/1/1
6	GZL	uD	3	6	2/2/4/5	6/6/19/22	0/1/1/1
20	FUB	uE	1	20	-	0/2/15/18	0/1/1/1
20	FUB	uE	2	20	-	0/2/15/18	0/1/1/1
20	GZL	uE	3	20	1/1/4/5	4/6/19/22	0/1/1/1
20	AHR	uE	4	20	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FUB	v	1	4	-	0/2/15/18	0/1/1/1
4	FUB	v	2	4	-	0/2/15/18	0/1/1/1
4	FUB	v	3	4	-	0/2/15/18	0/1/1/1
4	AHR	v	4	4	-	0/2/15/18	0/1/1/1
3	FUB	vA	1	3	-	0/2/15/18	0/1/1/1
3	FUB	vA	2	3	-	0/2/15/18	0/1/1/1
3	FUB	vA	3	3	-	0/2/15/18	0/1/1/1
3	FUB	vB	1	3	-	0/2/15/18	0/1/1/1
3	FUB	vB	2	3	-	0/2/15/18	0/1/1/1
3	FUB	vB	3	3	-	0/2/15/18	0/1/1/1
10	FUB	vC	1	10	-	0/2/15/18	0/1/1/1
10	FUB	vC	2	10	-	0/2/15/18	0/1/1/1
10	FUB	vC	3	10	-	0/2/15/18	0/1/1/1
10	AHR	vC	4	10	1/1/3/4	0/2/15/18	0/1/1/1
10	AHR	vC	5	10	-	0/2/15/18	0/1/1/1
13	FUB	vD	1	13	-	0/2/15/18	0/1/1/1
13	FUB	vD	2	13	-	0/2/15/18	0/1/1/1
13	GZL	vD	3	13	1/1/4/5	4/6/19/22	0/1/1/1
13	AHR	vD	4	13	-	0/2/15/18	0/1/1/1
21	FUB	vE	1	21	-	0/2/15/18	0/1/1/1
21	FUB	vE	2	21	-	0/2/15/18	0/1/1/1
21	GZL	vE	3	21	1/1/4/5	4/6/19/22	0/1/1/1
21	AHR	vE	4	21	1/1/3/4	0/2/15/18	0/1/1/1
21	AHR	vE	5	21	2/2/3/4	0/2/15/18	0/1/1/1
3	FUB	w	1	3	-	0/2/15/18	0/1/1/1
3	FUB	w	2	3	-	0/2/15/18	0/1/1/1
3	FUB	w	3	3	-	0/2/15/18	0/1/1/1
3	FUB	wA	1	3	-	0/2/15/18	0/1/1/1
3	FUB	wA	2	3	-	0/2/15/18	0/1/1/1
3	FUB	wA	3	3	-	0/2/15/18	0/1/1/1
3	FUB	wB	1	3	-	0/2/15/18	0/1/1/1
3	FUB	wB	2	3	-	0/2/15/18	0/1/1/1
3	FUB	wB	3	3	-	0/2/15/18	0/1/1/1
13	FUB	wC	1	13	-	0/2/15/18	0/1/1/1
13	FUB	wC	2	13	-	0/2/15/18	0/1/1/1
13	GZL	wC	3	13	3/3/4/5	1/6/19/22	0/1/1/1
13	AHR	wC	4	13	-	0/2/15/18	0/1/1/1
13	FUB	wD	1	13	-	0/2/15/18	0/1/1/1
13	FUB	wD	2	13	-	0/2/15/18	0/1/1/1
13	GZL	wD	3	13	1/1/4/5	6/6/19/22	0/1/1/1
13	AHR	wD	4	13	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	FUB	wE	1	22	-	0/2/15/18	0/1/1/1
22	FUB	wE	2	22	-	0/2/15/18	0/1/1/1
22	GZL	wE	3	22	1/1/4/5	2/6/19/22	0/1/1/1
22	AHR	wE	4	22	-	0/2/15/18	0/1/1/1
22	AHR	wE	5	22	-	0/2/15/18	0/1/1/1
22	AHR	wE	6	22	-	0/2/15/18	0/1/1/1
3	FUB	x	1	3	-	0/2/15/18	0/1/1/1
3	FUB	x	2	3	-	0/2/15/18	0/1/1/1
3	FUB	x	3	3	-	0/2/15/18	0/1/1/1
3	FUB	xA	1	3	-	0/2/15/18	0/1/1/1
3	FUB	xA	2	3	-	0/2/15/18	0/1/1/1
3	FUB	xA	3	3	-	0/2/15/18	0/1/1/1
3	FUB	xB	1	3	-	0/2/15/18	0/1/1/1
3	FUB	xB	2	3	-	0/2/15/18	0/1/1/1
3	FUB	xB	3	3	-	0/2/15/18	0/1/1/1
6	FUB	xC	1	6	-	0/2/15/18	0/1/1/1
6	FUB	xC	2	6	-	0/2/15/18	0/1/1/1
6	GZL	xC	3	6	2/2/4/5	5/6/19/22	0/1/1/1
6	FUB	xD	1	6	-	0/2/15/18	0/1/1/1
6	FUB	xD	2	6	-	0/2/15/18	0/1/1/1
6	GZL	xD	3	6	-	6/6/19/22	0/1/1/1
20	FUB	xE	1	20	-	0/2/15/18	0/1/1/1
20	FUB	xE	2	20	-	2/2/15/18	0/1/1/1
20	GZL	xE	3	20	1/1/4/5	6/6/19/22	0/1/1/1
20	AHR	xE	4	20	-	0/2/15/18	0/1/1/1
3	FUB	y	1	3	-	0/2/15/18	0/1/1/1
3	FUB	y	2	3	-	0/2/15/18	0/1/1/1
3	FUB	y	3	3	-	0/2/15/18	0/1/1/1
3	FUB	yA	1	3	-	0/2/15/18	0/1/1/1
3	FUB	yA	2	3	-	0/2/15/18	0/1/1/1
3	FUB	yA	3	3	-	0/2/15/18	0/1/1/1
10	FUB	yB	1	10	-	0/2/15/18	0/1/1/1
10	FUB	yB	2	10	-	0/2/15/18	0/1/1/1
10	FUB	yB	3	10	-	0/2/15/18	0/1/1/1
10	AHR	yB	4	10	1/1/3/4	0/2/15/18	0/1/1/1
10	AHR	yB	5	10	-	0/2/15/18	0/1/1/1
13	FUB	yC	1	13	-	0/2/15/18	0/1/1/1
13	FUB	yC	2	13	-	0/2/15/18	0/1/1/1
13	GZL	yC	3	13	1/1/4/5	2/6/19/22	0/1/1/1
13	AHR	yC	4	13	-	0/2/15/18	0/1/1/1
6	FUB	yD	1	6	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	FUB	yD	2	6	-	0/2/15/18	0/1/1/1
6	GZL	yD	3	6	1/1/4/5	2/6/19/22	0/1/1/1
18	FUB	yE	1	18	-	0/2/15/18	0/1/1/1
18	FUB	yE	2	18	-	0/2/15/18	0/1/1/1
18	GZL	yE	3	18	1/1/4/5	6/6/19/22	0/1/1/1
18	AHR	yE	4	18	1/1/3/4	0/2/15/18	0/1/1/1
18	AHR	yE	5	18	-	0/2/15/18	0/1/1/1
3	FUB	z	1	3	-	0/2/15/18	0/1/1/1
3	FUB	z	2	3	-	0/2/15/18	0/1/1/1
3	FUB	z	3	3	-	0/2/15/18	0/1/1/1
3	FUB	zA	1	3	-	0/2/15/18	0/1/1/1
3	FUB	zA	2	3	-	0/2/15/18	0/1/1/1
3	FUB	zA	3	3	-	0/2/15/18	0/1/1/1
13	FUB	zB	1	13	-	0/2/15/18	0/1/1/1
13	FUB	zB	2	13	-	0/2/15/18	0/1/1/1
13	GZL	zB	3	13	3/3/4/5	2/6/19/22	0/1/1/1
13	AHR	zB	4	13	-	0/2/15/18	0/1/1/1
13	FUB	zC	1	13	-	0/2/15/18	0/1/1/1
13	FUB	zC	2	13	-	0/2/15/18	0/1/1/1
13	GZL	zC	3	13	1/1/4/5	6/6/19/22	0/1/1/1
13	AHR	zC	4	13	-	0/2/15/18	0/1/1/1
6	FUB	zD	1	6	-	0/2/15/18	0/1/1/1
6	FUB	zD	2	6	1/1/3/4	0/2/15/18	0/1/1/1
6	GZL	zD	3	6	1/1/4/5	2/6/19/22	0/1/1/1
18	FUB	zE	1	18	-	0/2/15/18	0/1/1/1
18	FUB	zE	2	18	-	0/2/15/18	0/1/1/1
18	GZL	zE	3	18	1/1/4/5	6/6/19/22	0/1/1/1
18	AHR	zE	4	18	-	0/2/15/18	0/1/1/1
18	AHR	zE	5	18	1/1/3/4	0/2/15/18	0/1/1/1

The worst 5 of 1123 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	CD	3	GZL	C2-C3	-19.62	1.22	1.53
6	LA	3	GZL	C2-C3	-19.56	1.22	1.53
6	uD	3	GZL	C2-C3	-19.38	1.22	1.53
6	xC	3	GZL	C2-C3	-19.37	1.22	1.53
6	XB	3	GZL	C2-C3	-19.34	1.22	1.53

The worst 5 of 834 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	3A	3	GZL	C1-O4-C4	-12.65	82.02	107.84
6	N	3	GZL	C5-C4-C3	-9.92	102.60	115.86
6	CD	3	GZL	C1-O4-C4	-9.73	87.98	107.84
6	0B	3	GZL	C1-O4-C4	-9.43	88.59	107.84
6	LA	3	GZL	C1-O4-C4	-9.36	88.73	107.84

5 of 302 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	XA	2	FUB	C1
4	L	1	FUB	C4
4	Z	2	FUB	C1
4	JA	1	FUB	C4
4	VA	4	AHR	C1

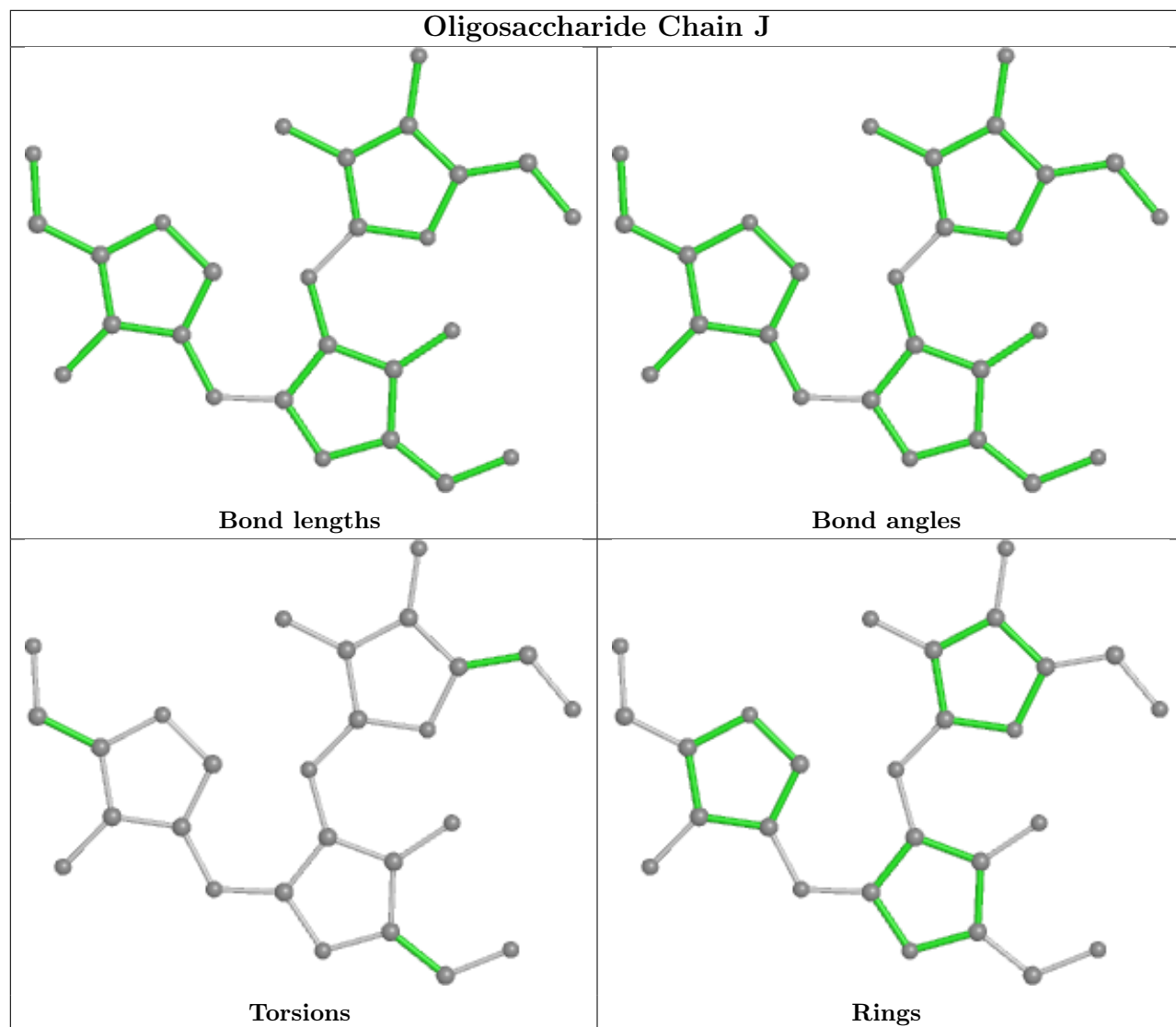
5 of 605 torsion outliers are listed below:

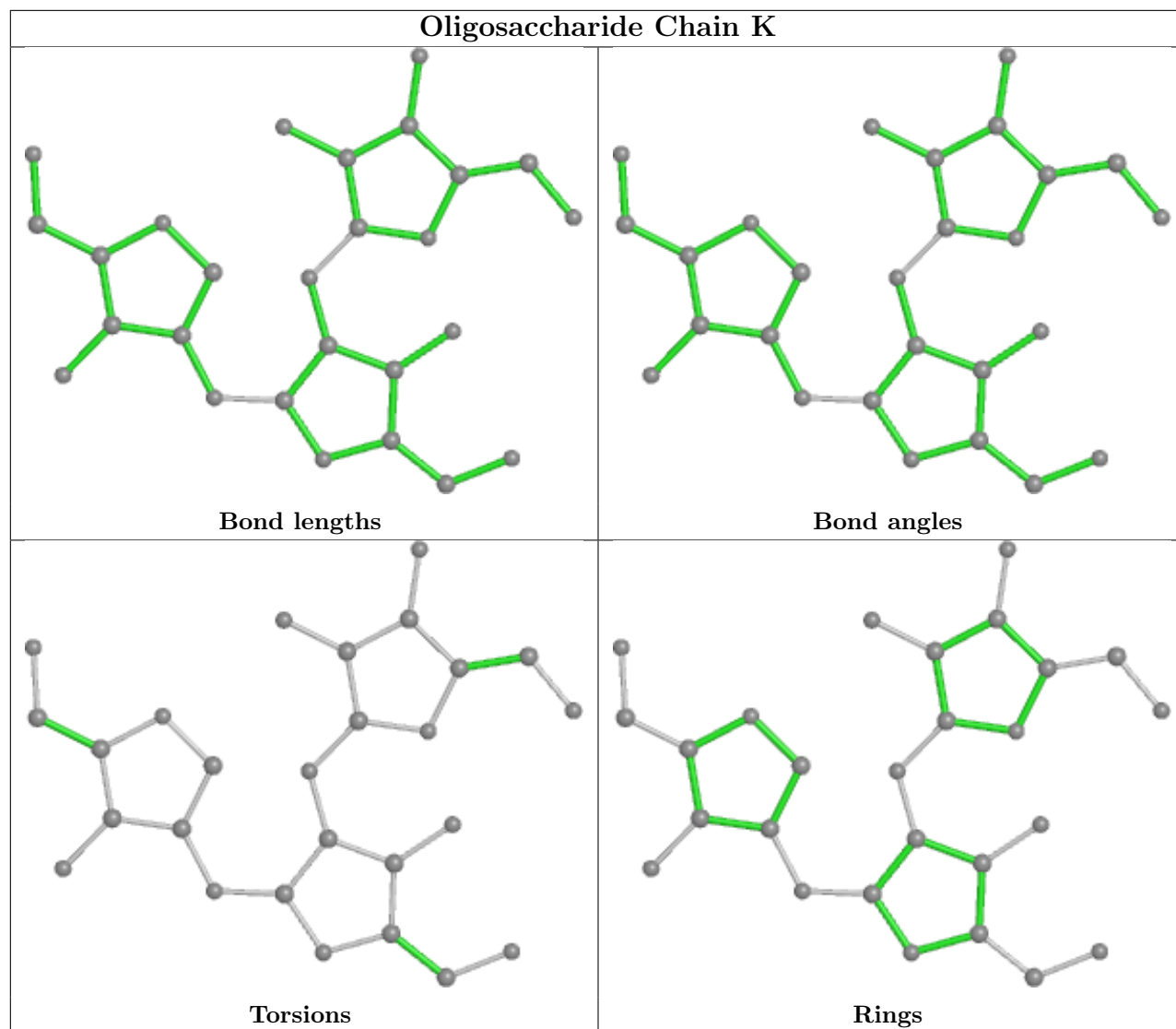
Mol	Chain	Res	Type	Atoms
6	N	3	GZL	C4-C5-C6-O6
6	N	3	GZL	O5-C5-C6-O6
6	5	3	GZL	O5-C5-C6-O6
6	AA	3	GZL	C3-C4-C5-C6
6	AA	3	GZL	O4-C4-C5-C6

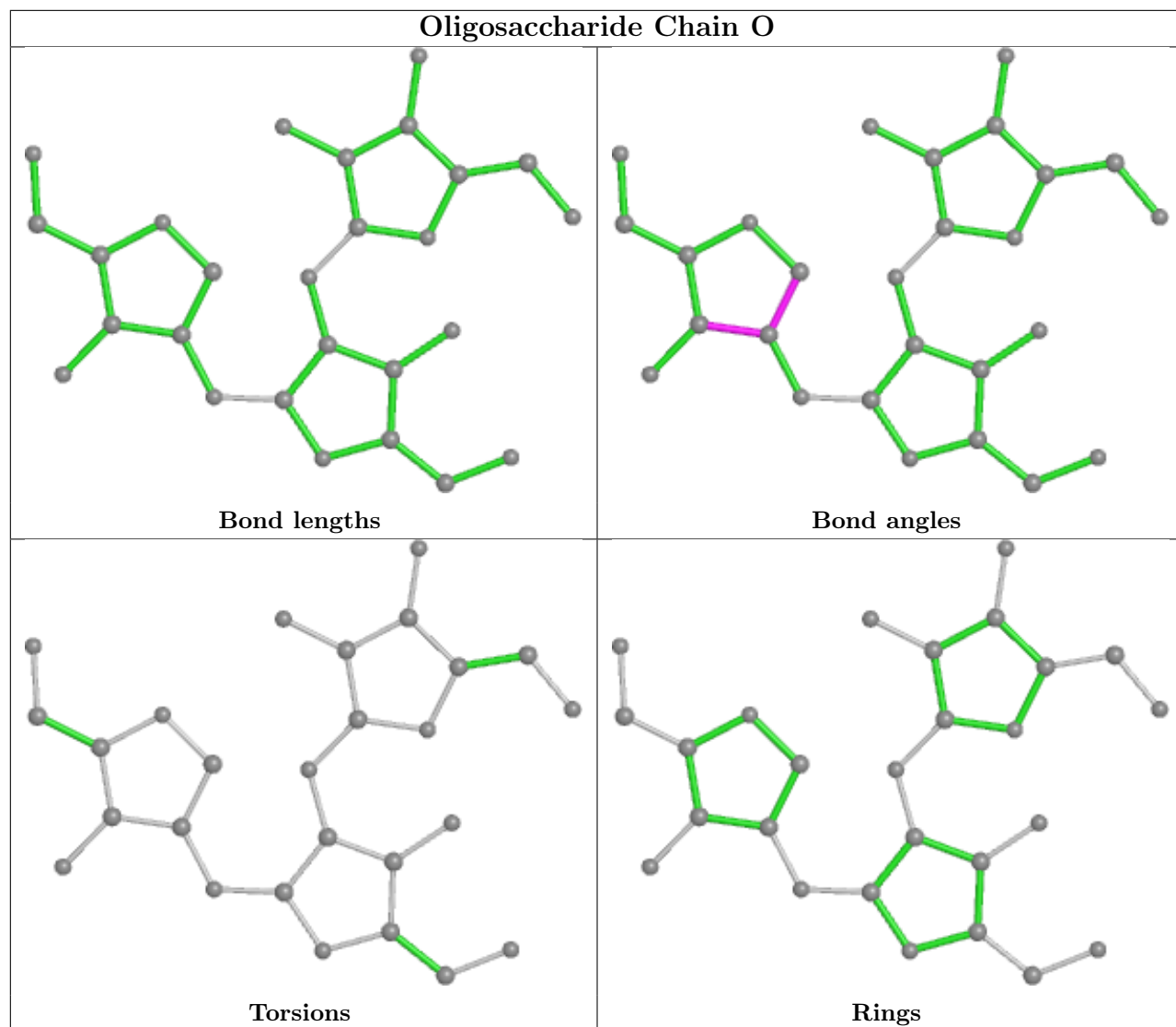
There are no ring outliers.

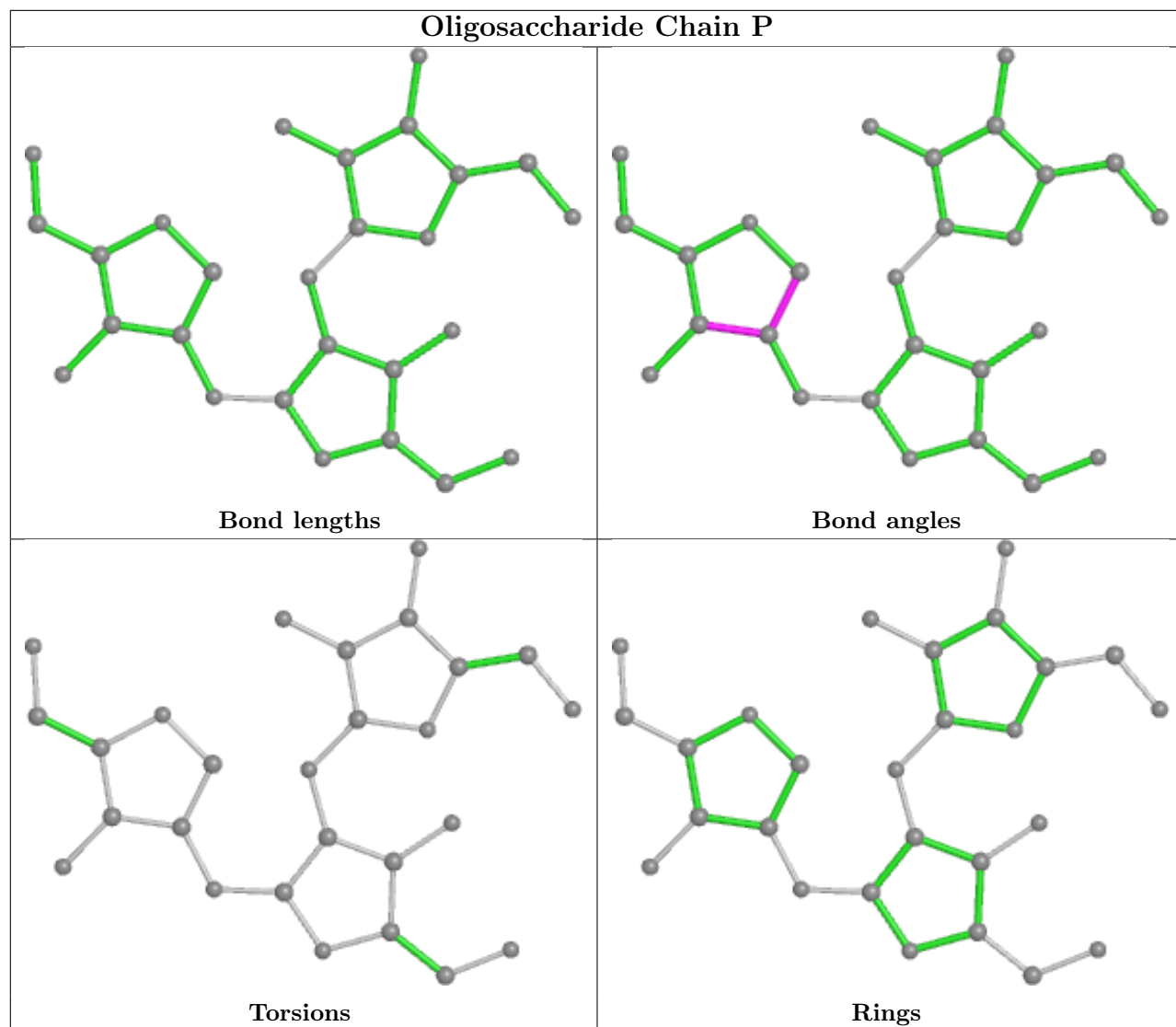
No monomer is involved in short contacts.

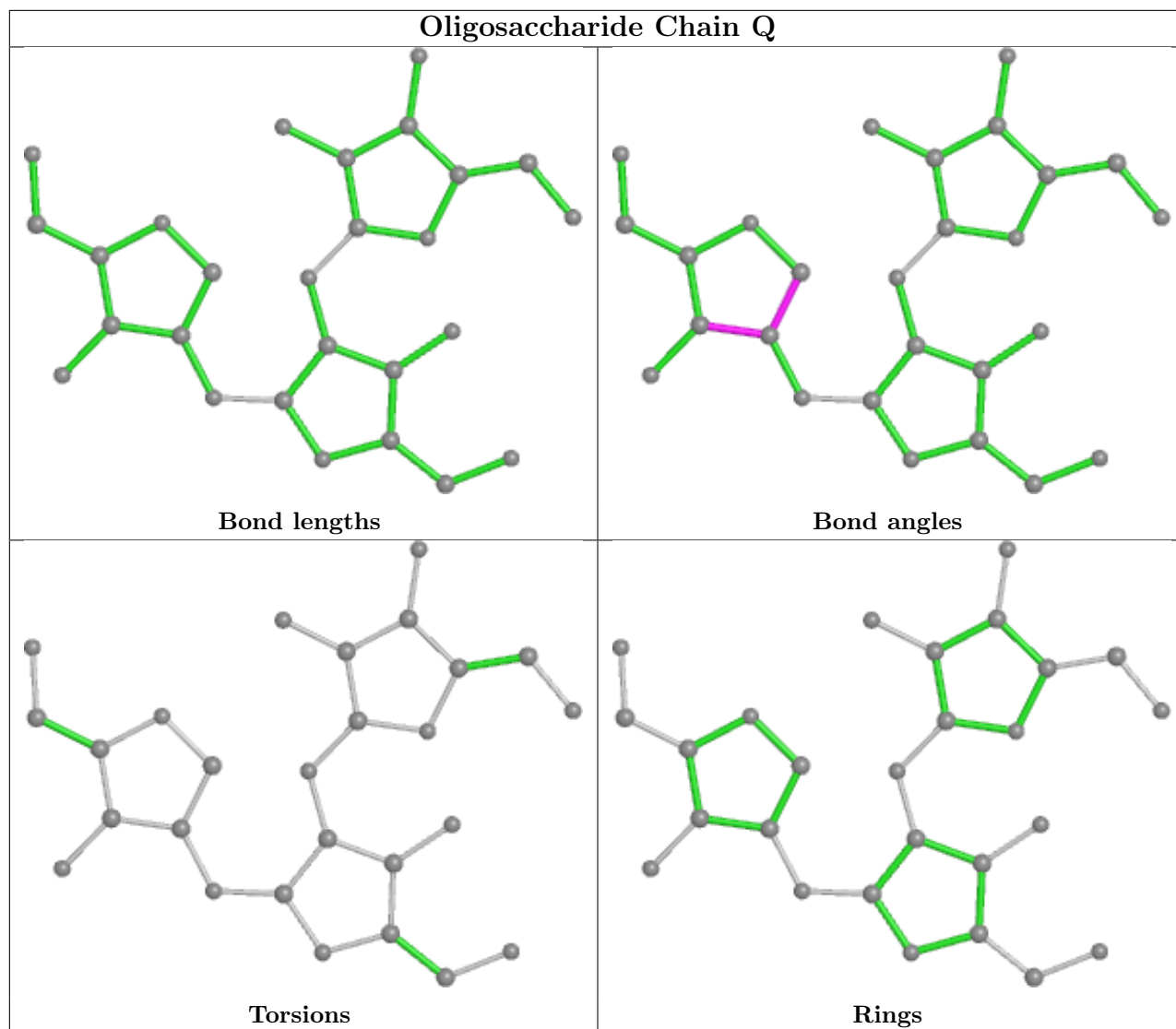
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



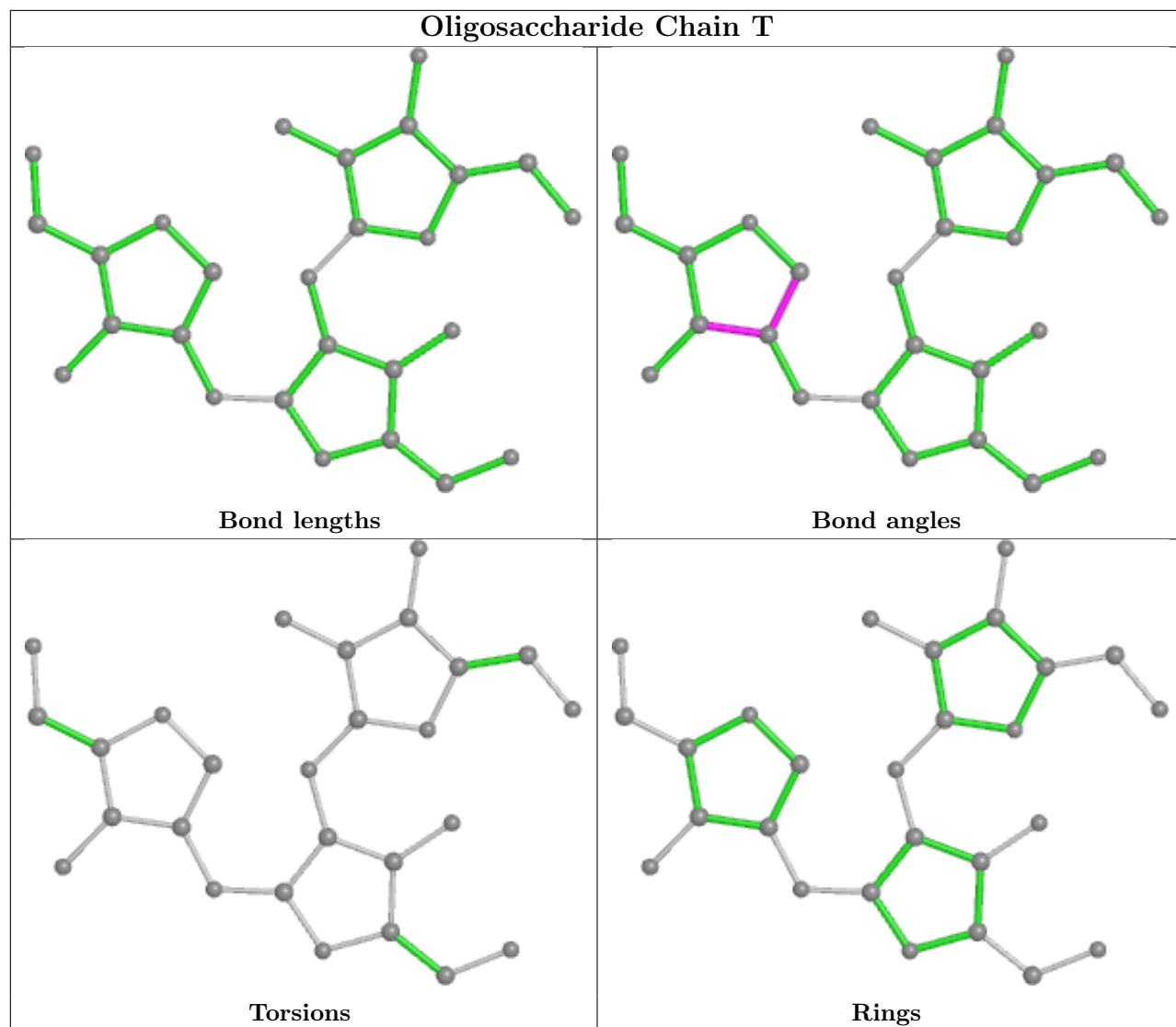


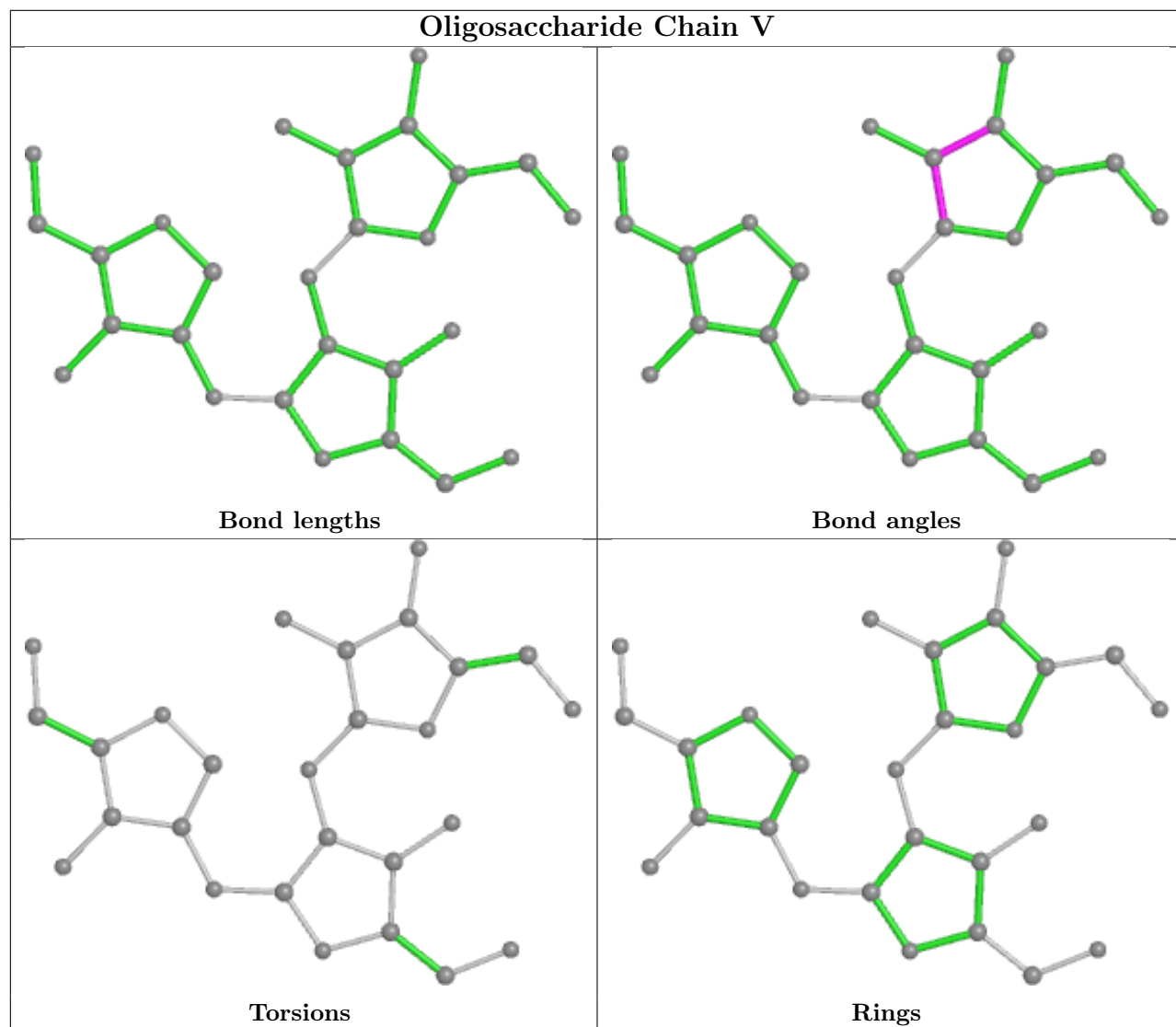


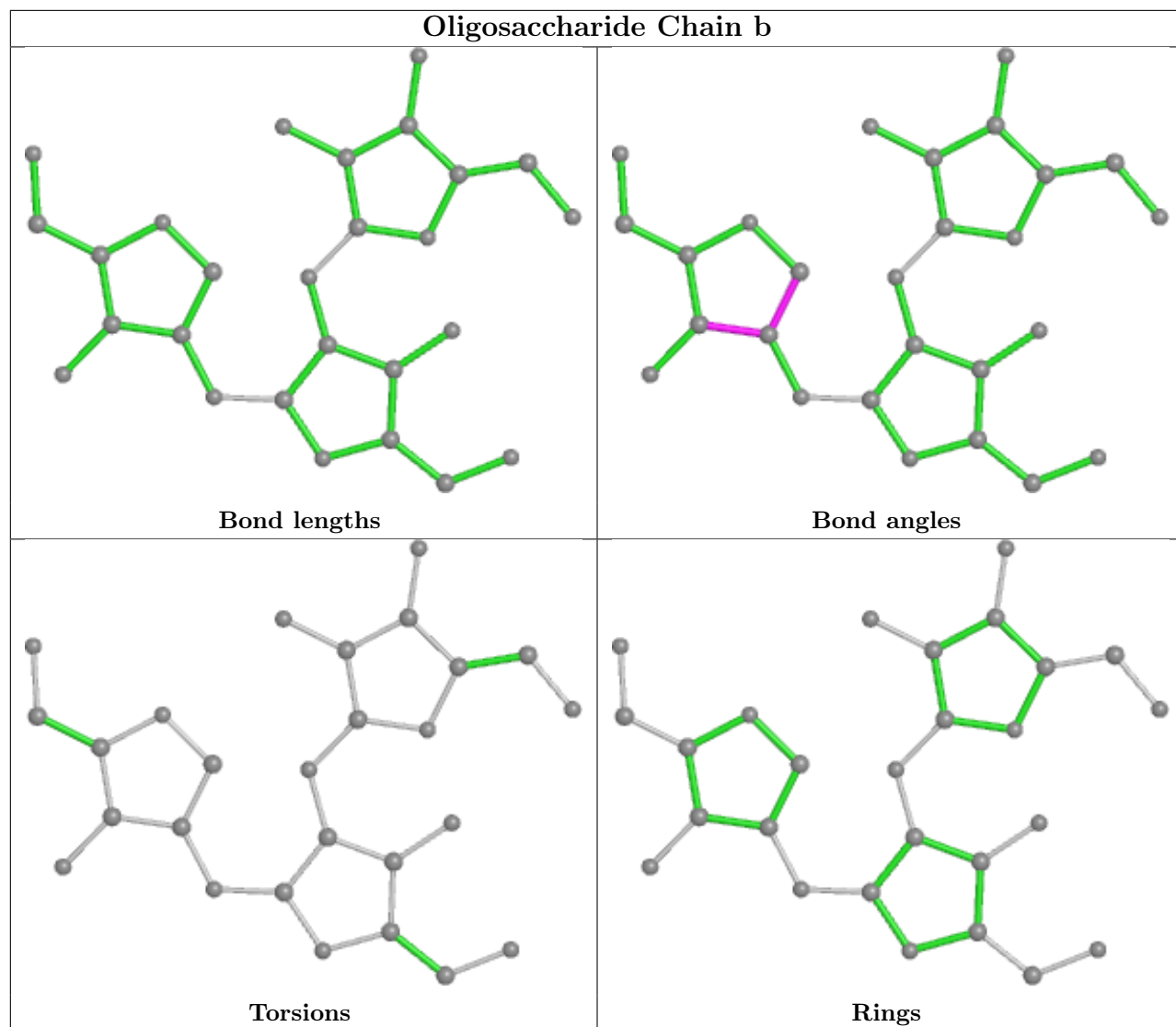


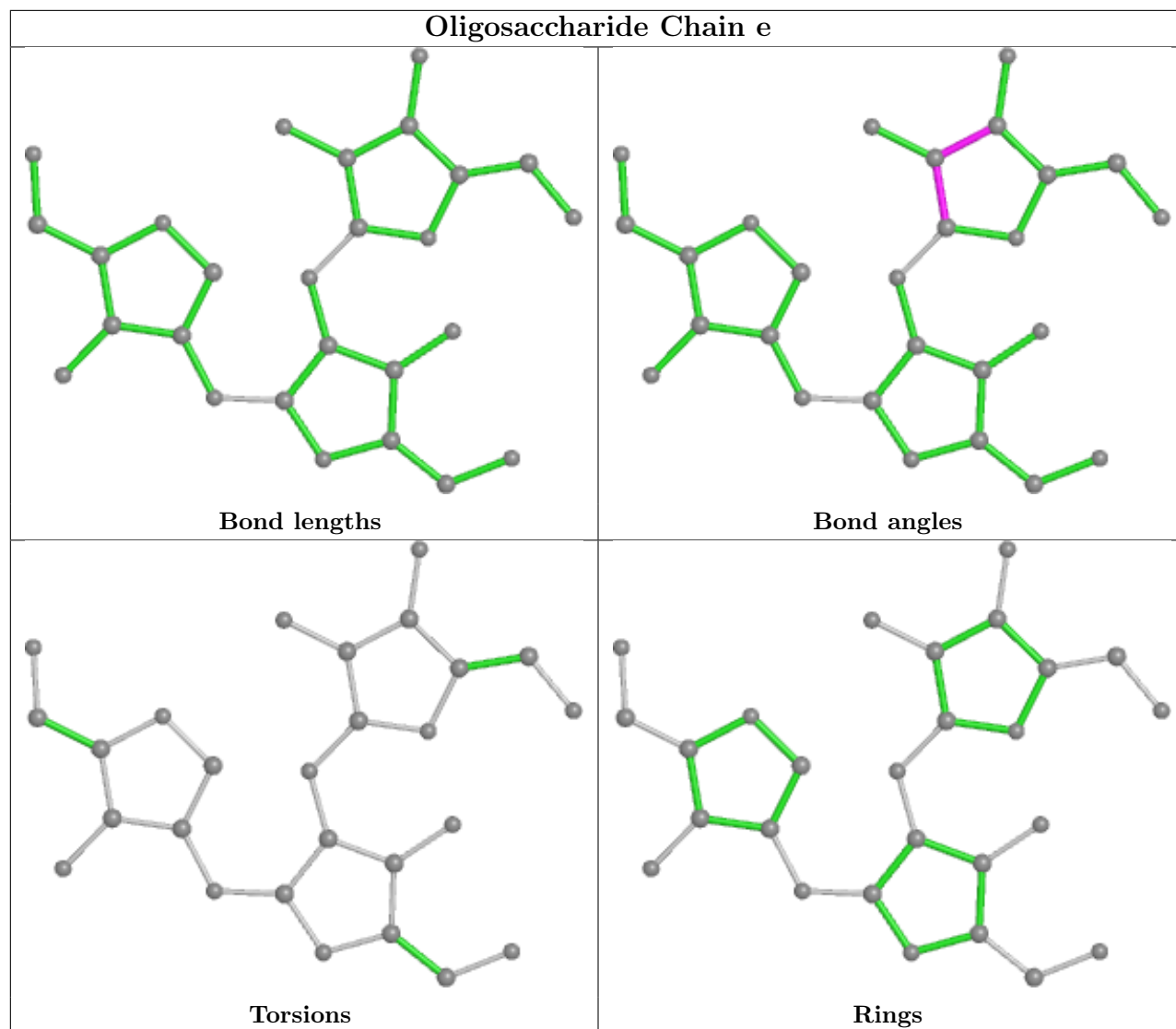


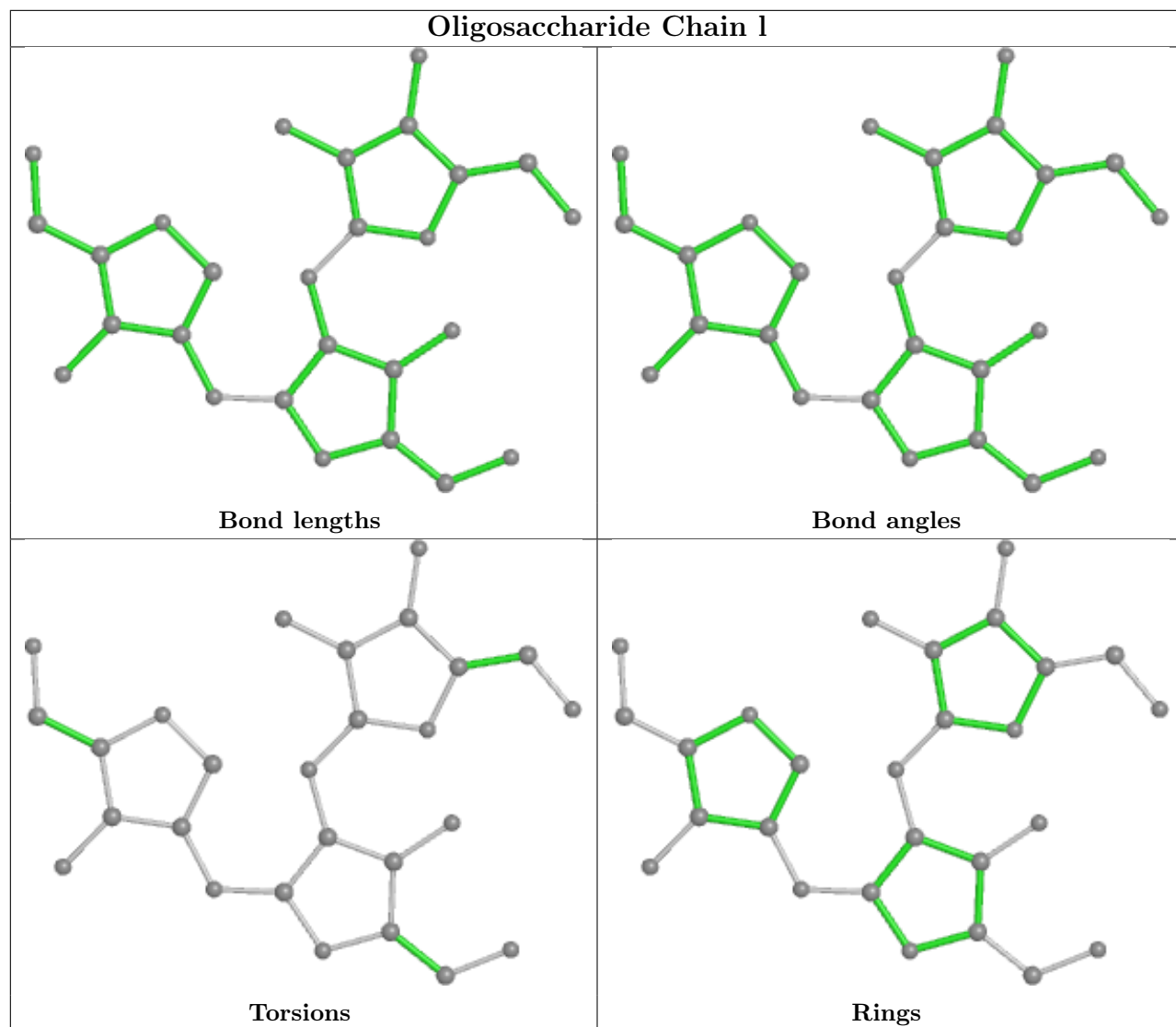


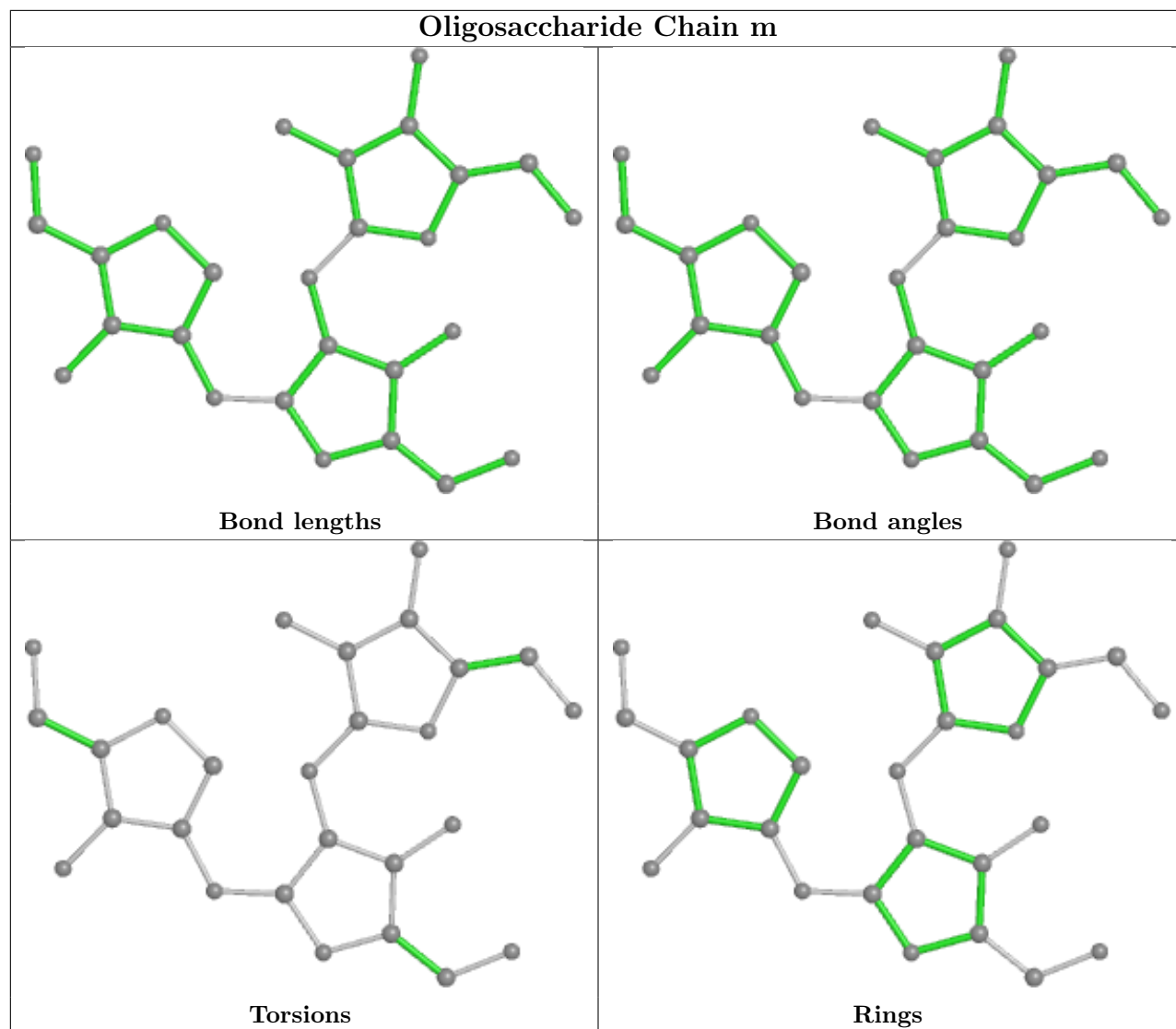


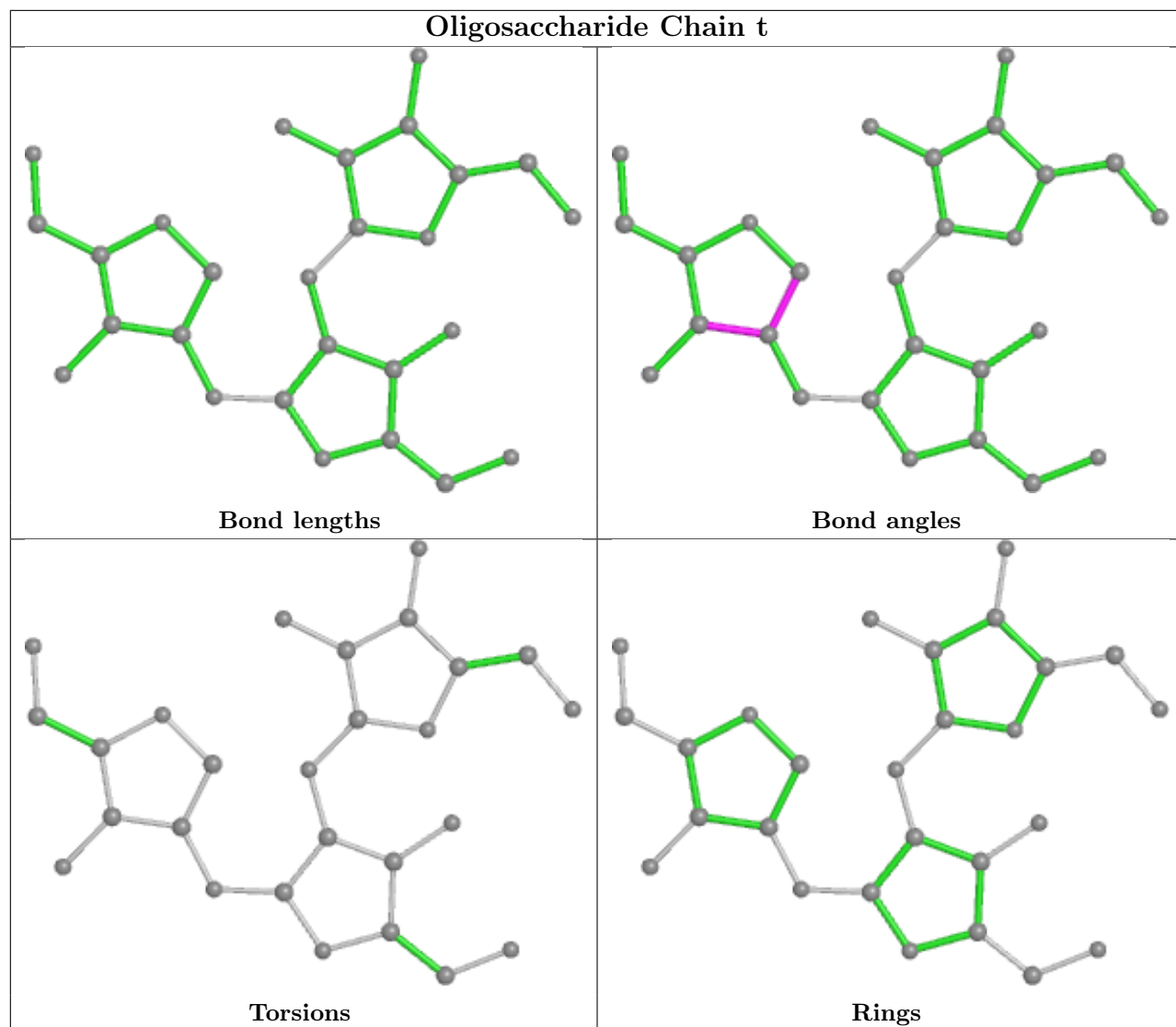


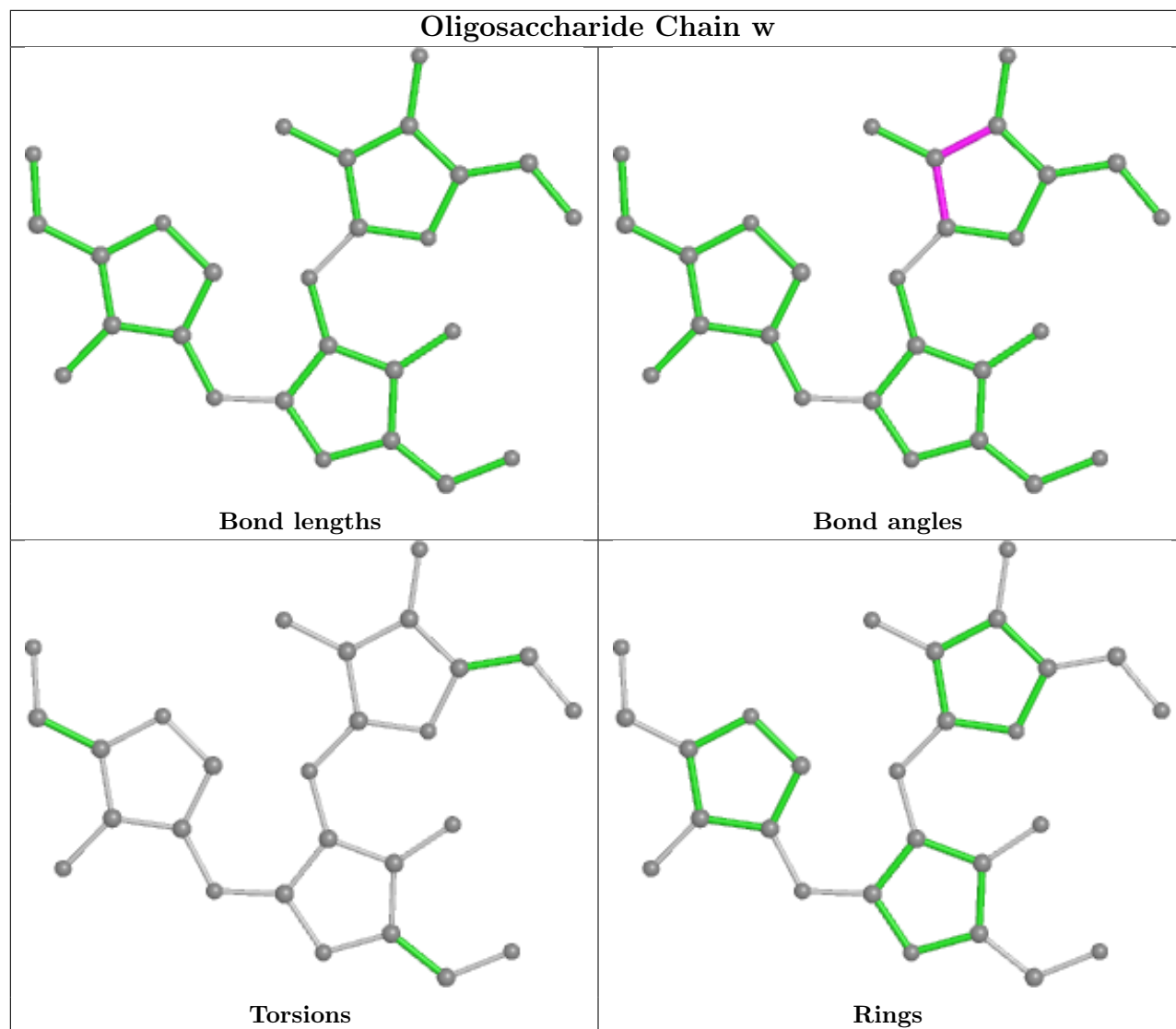




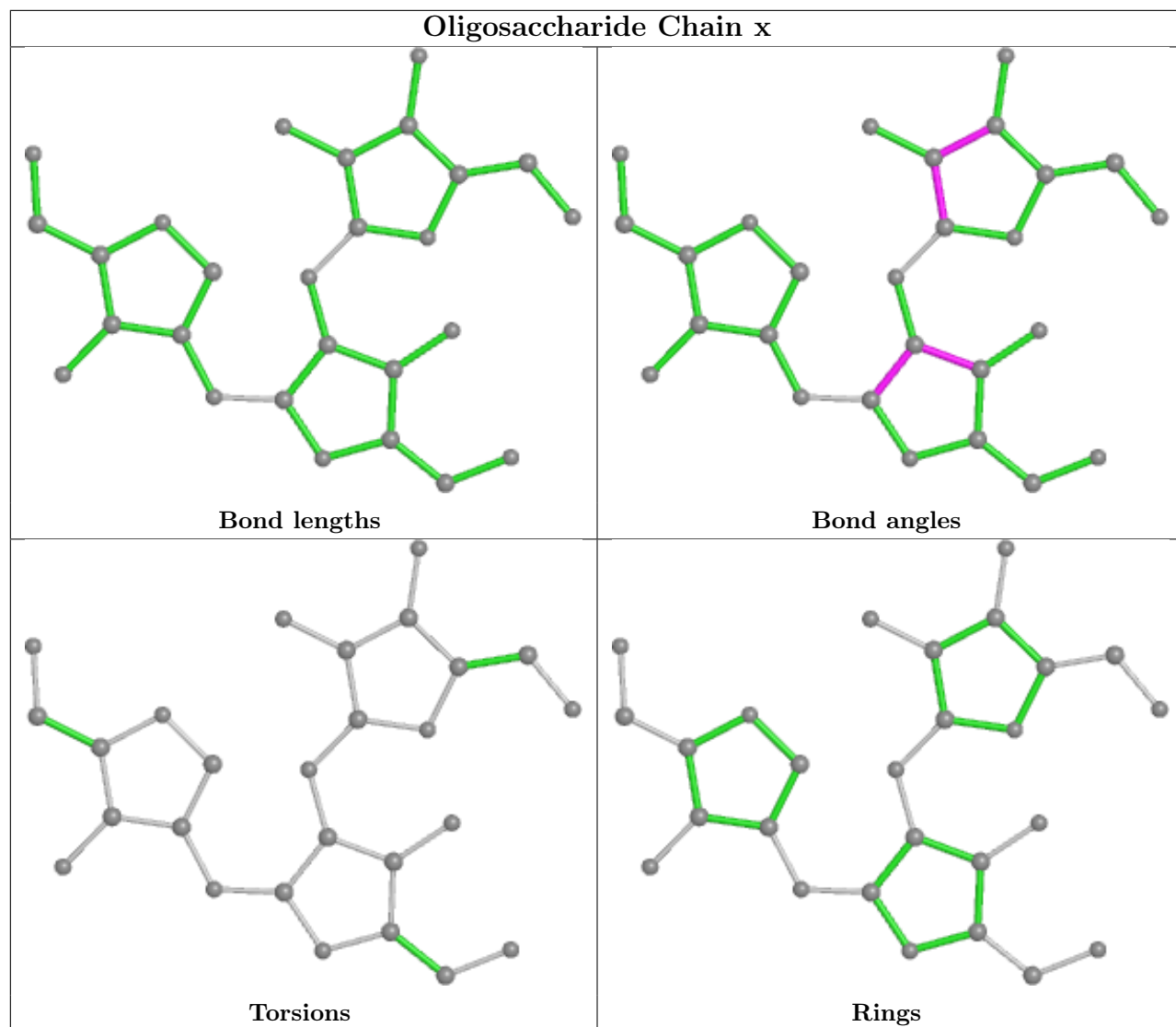


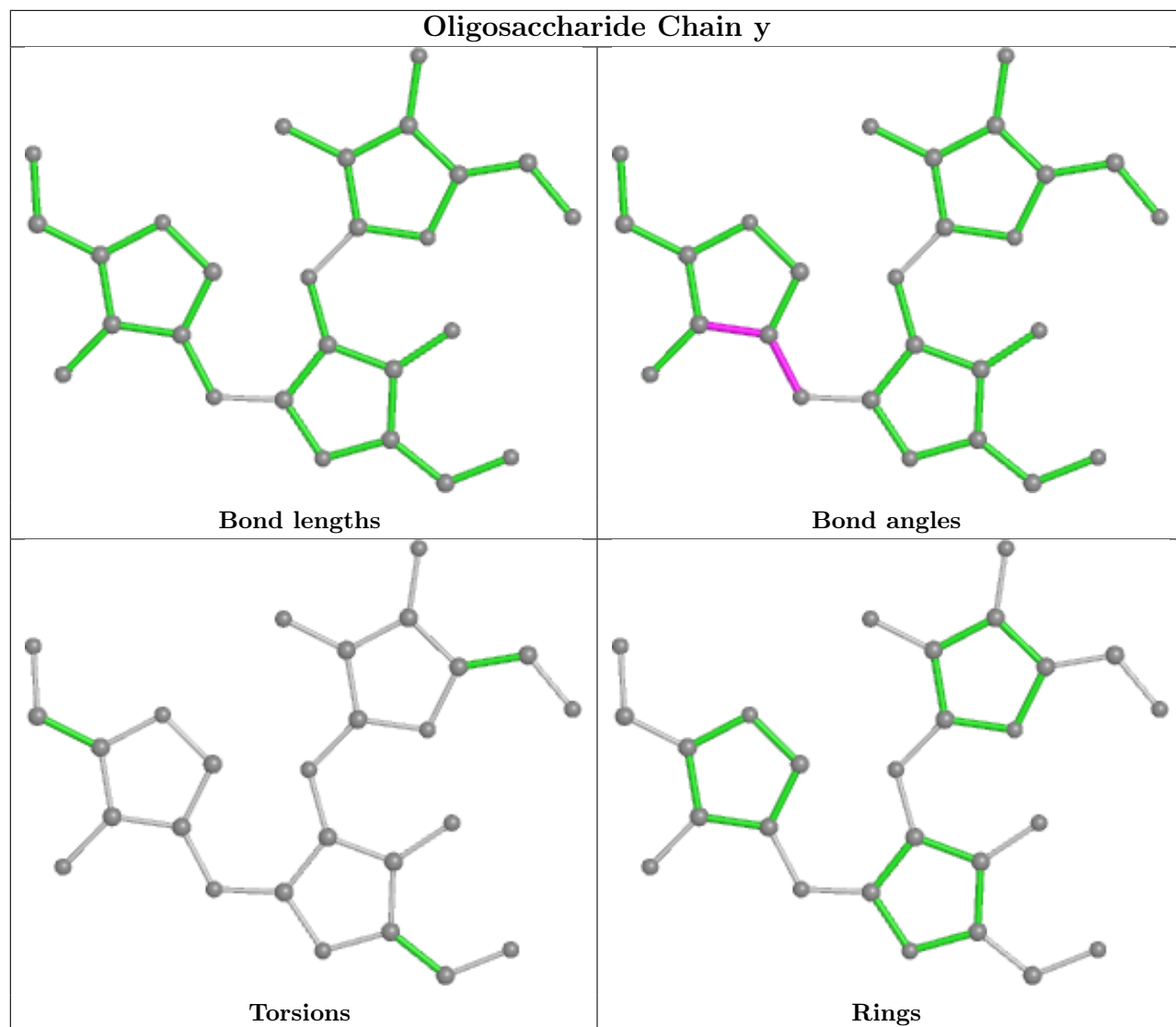


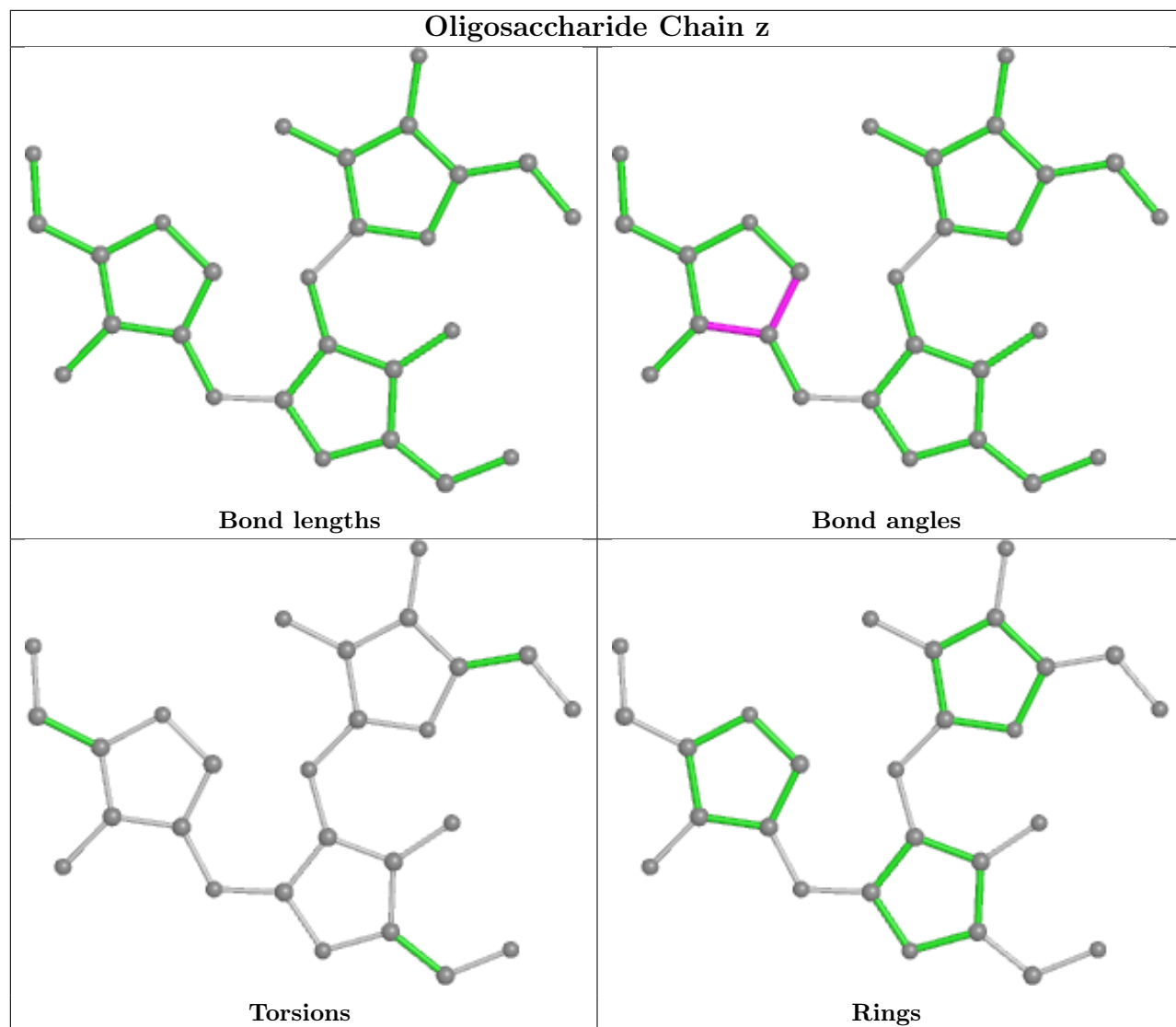


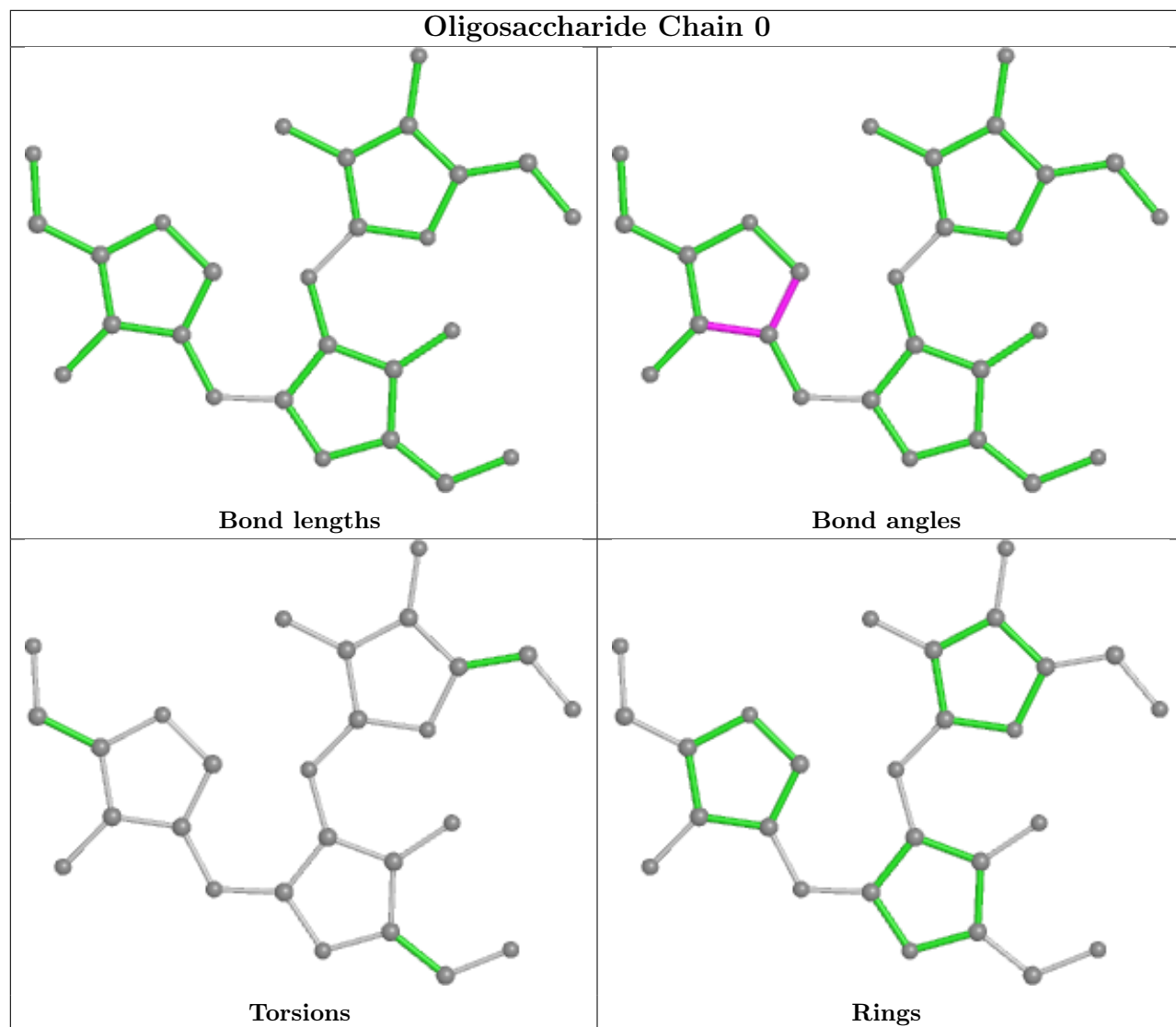


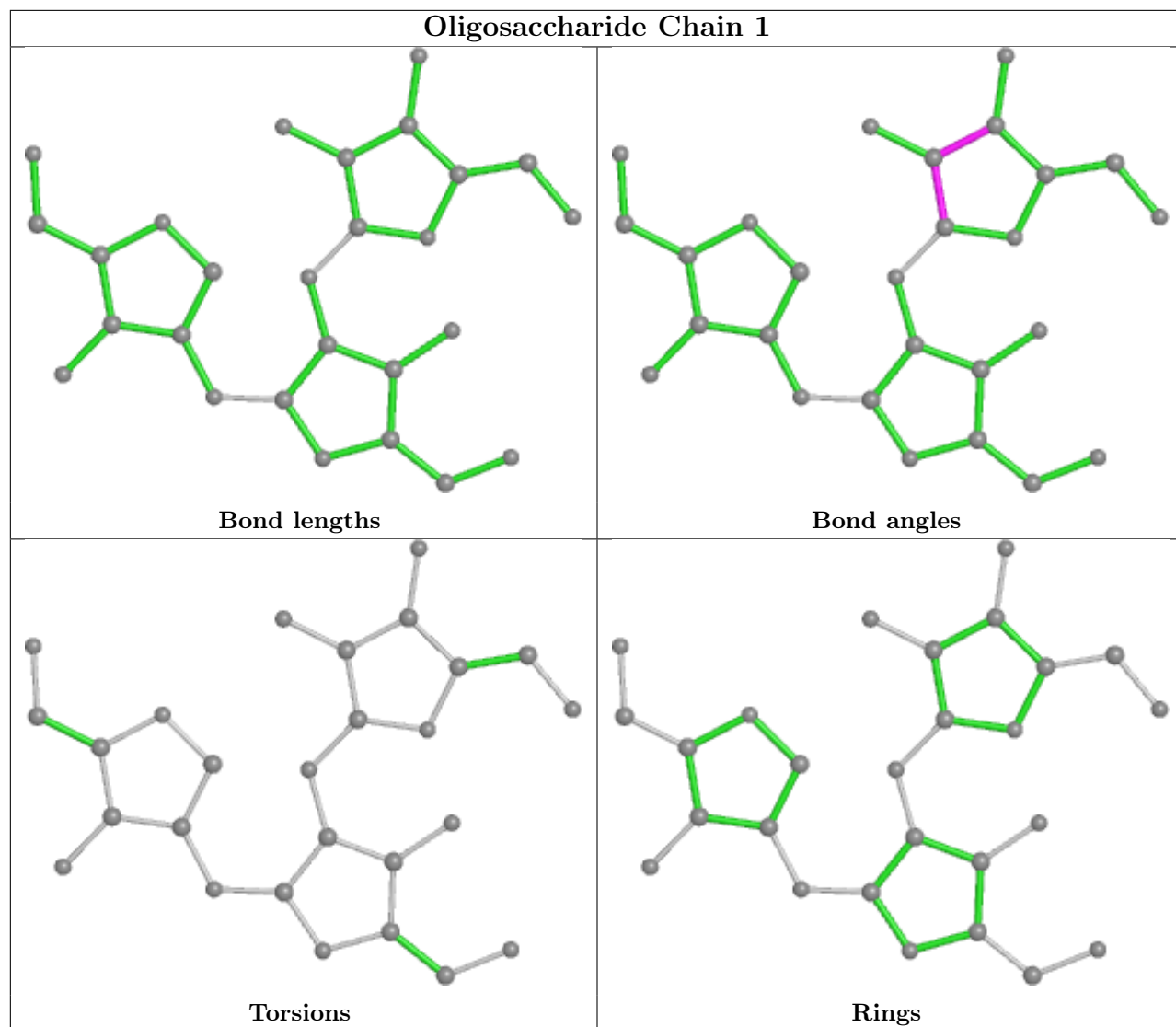


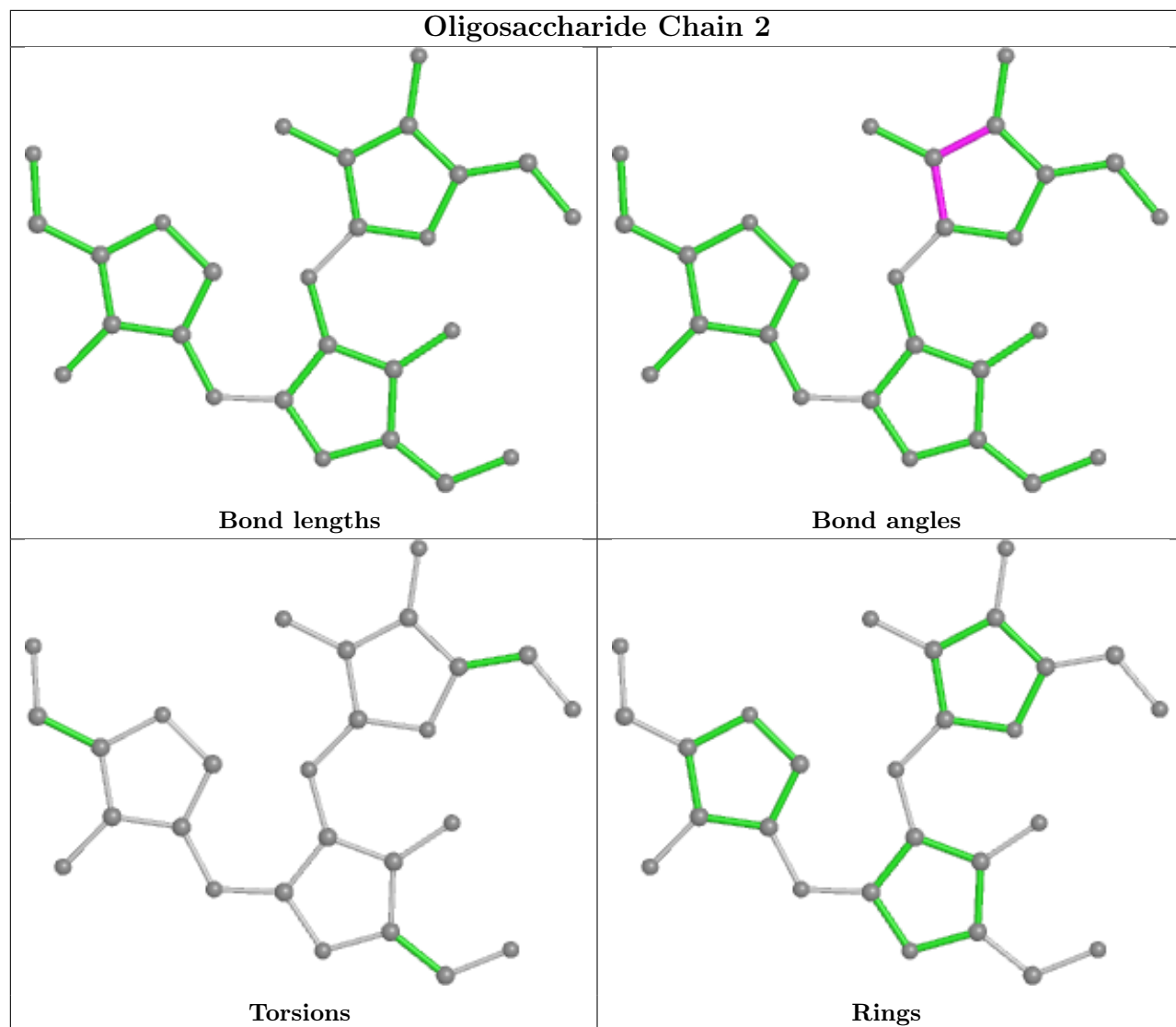


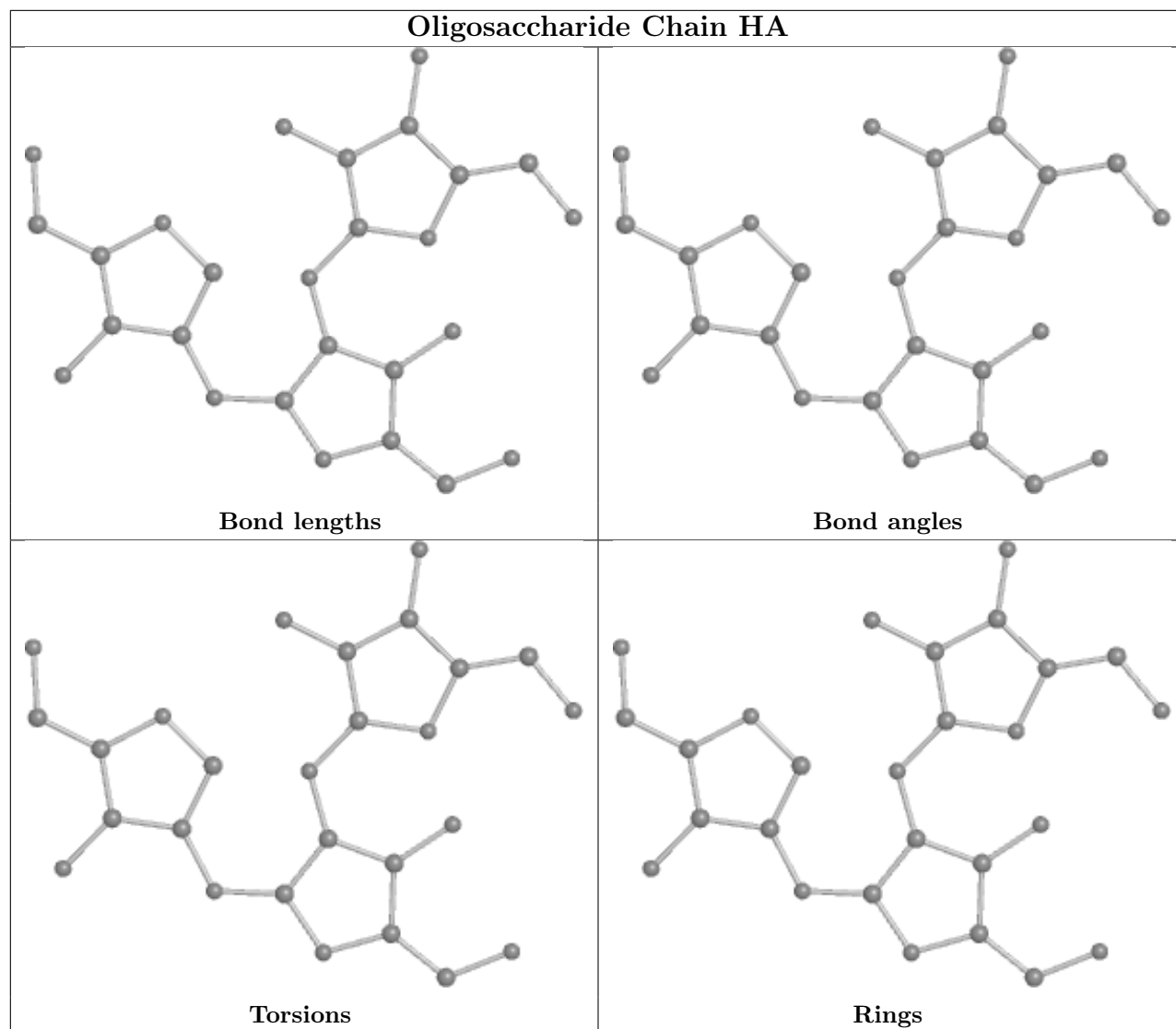


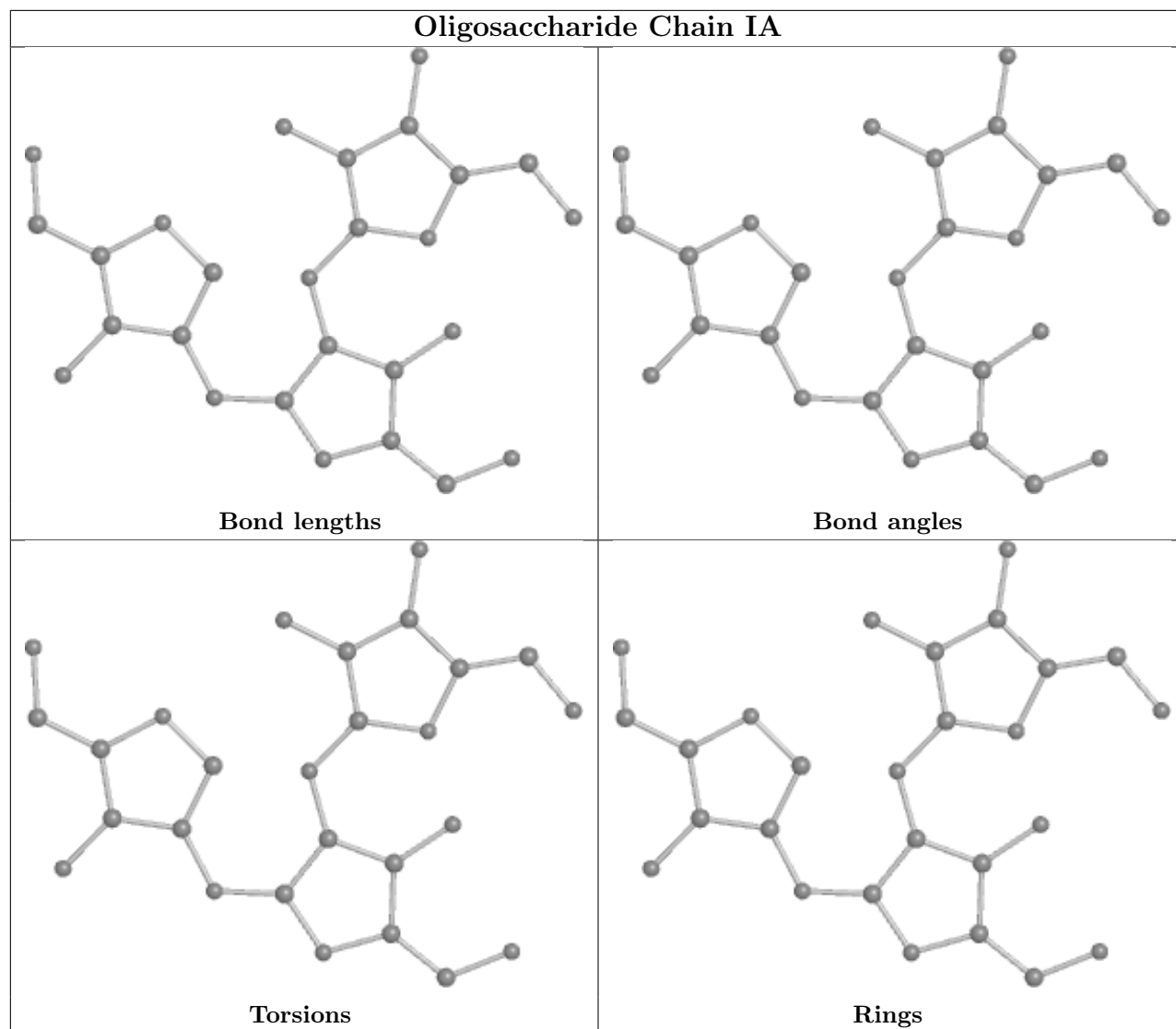




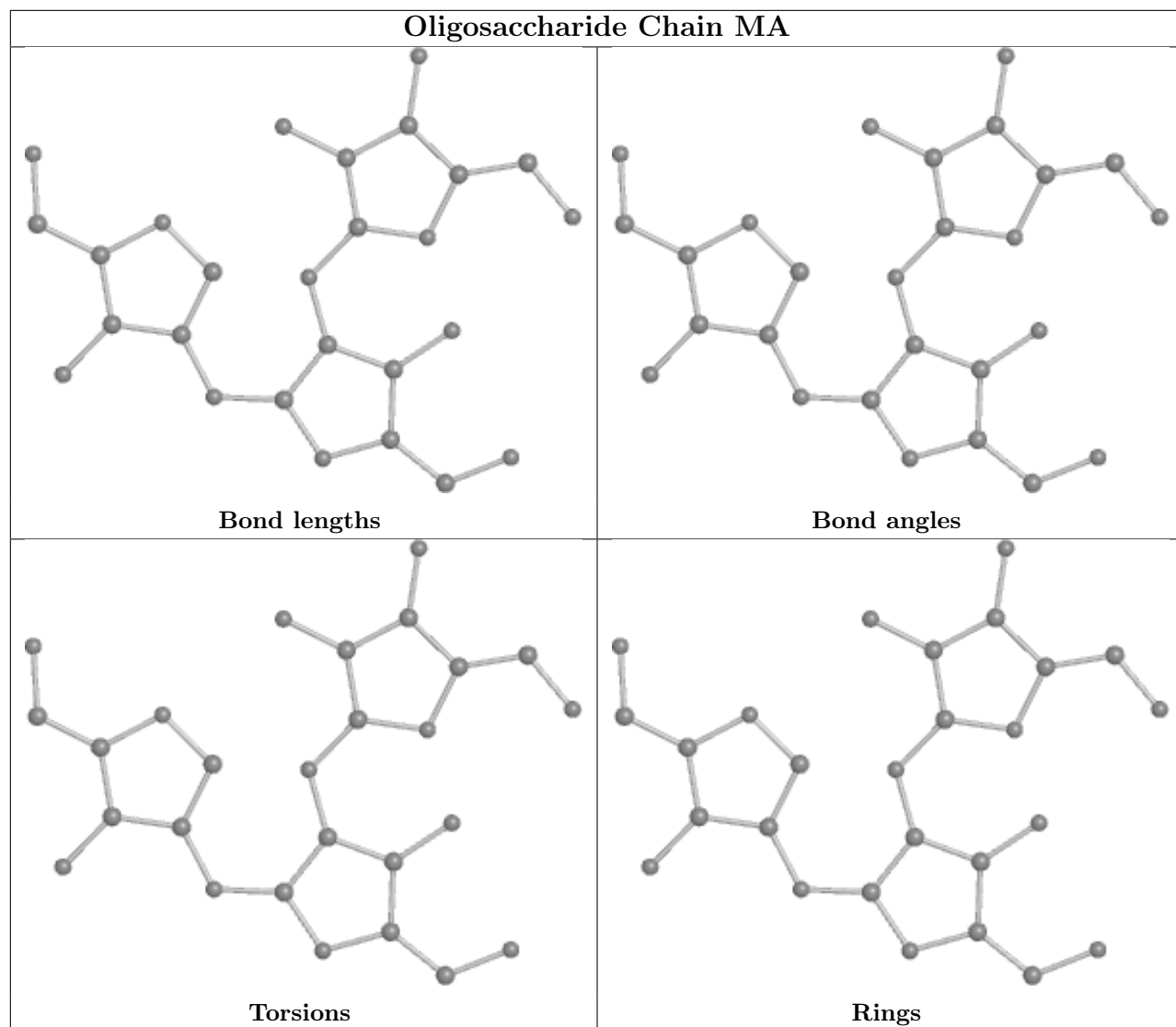


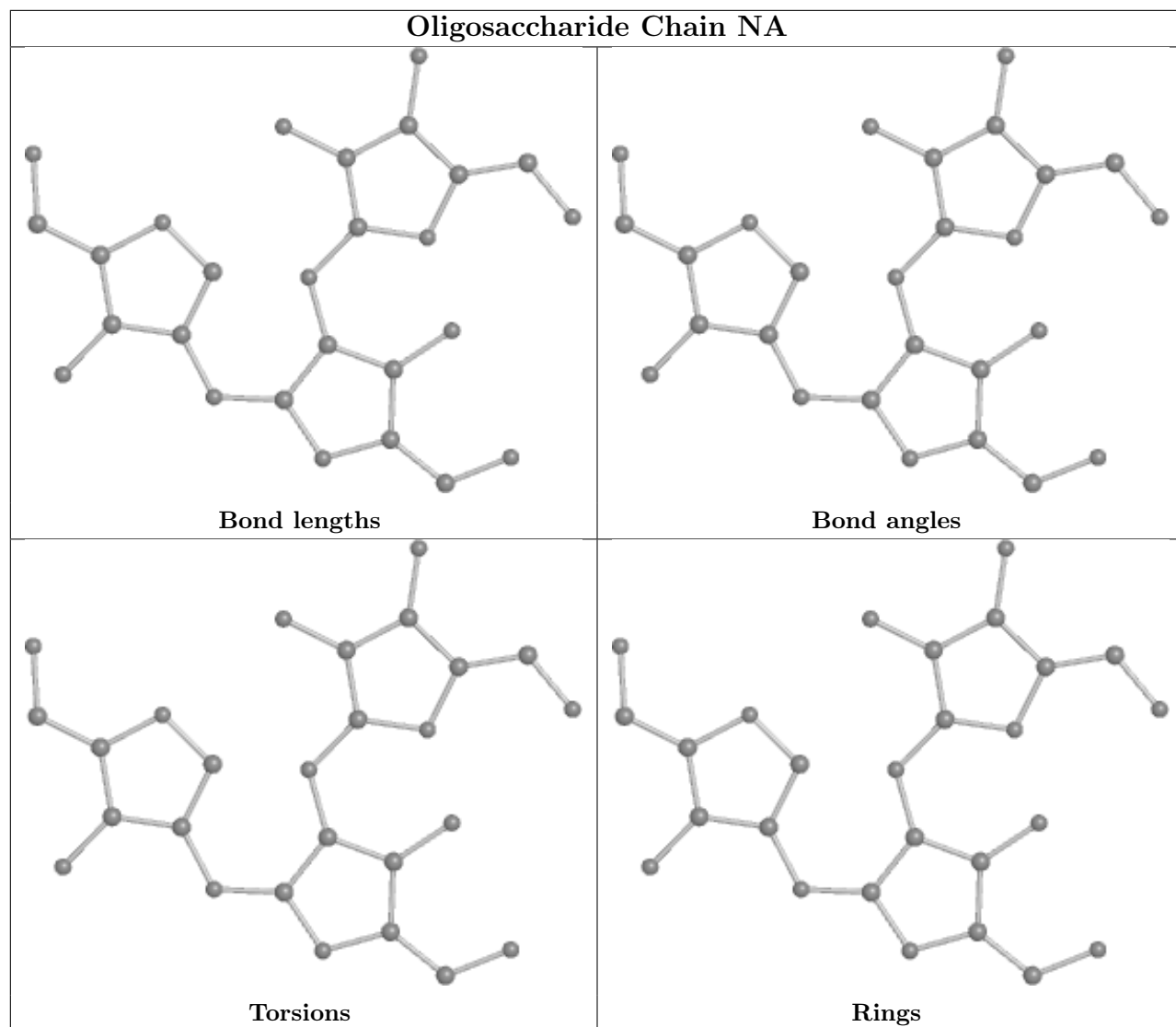


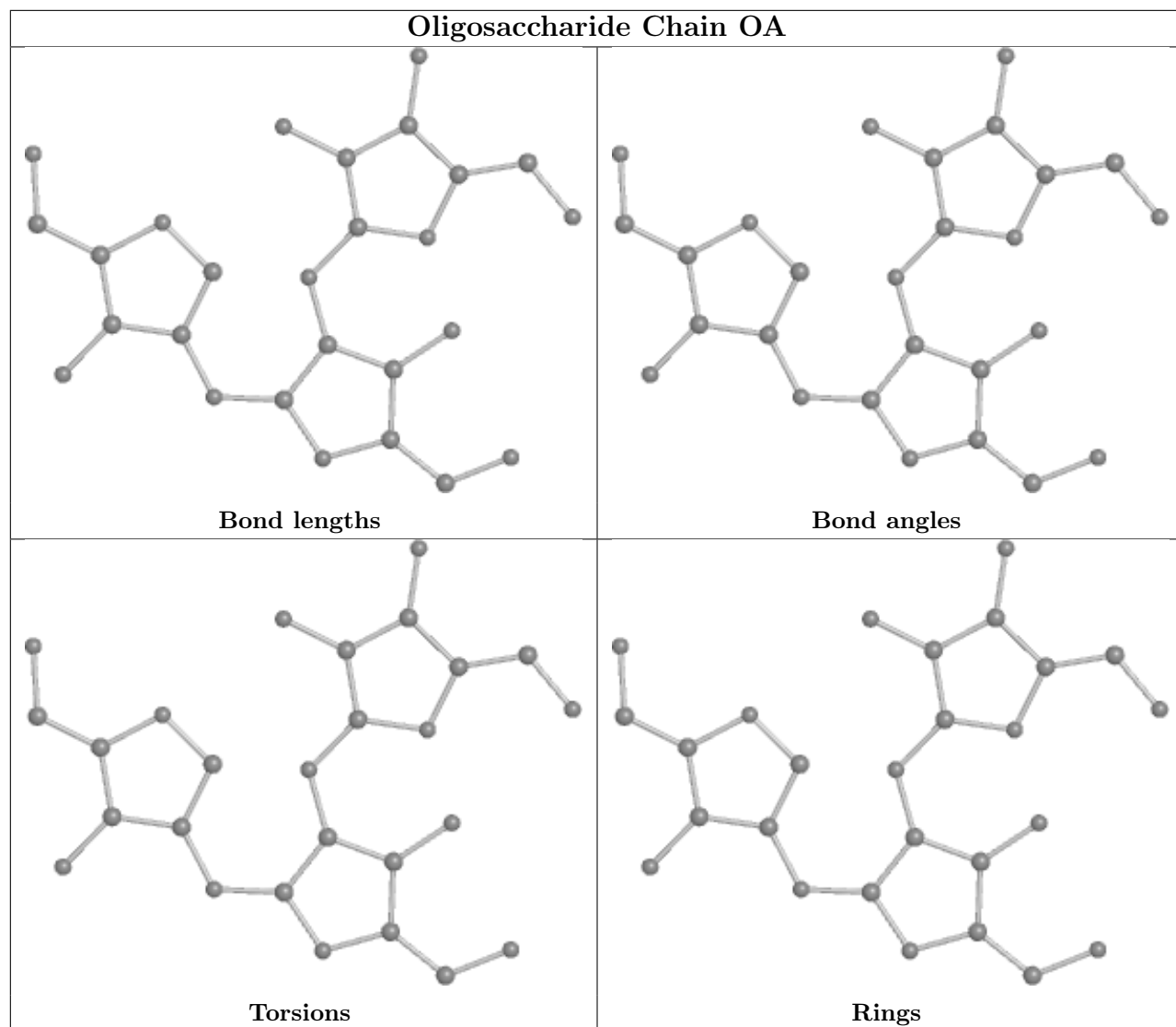


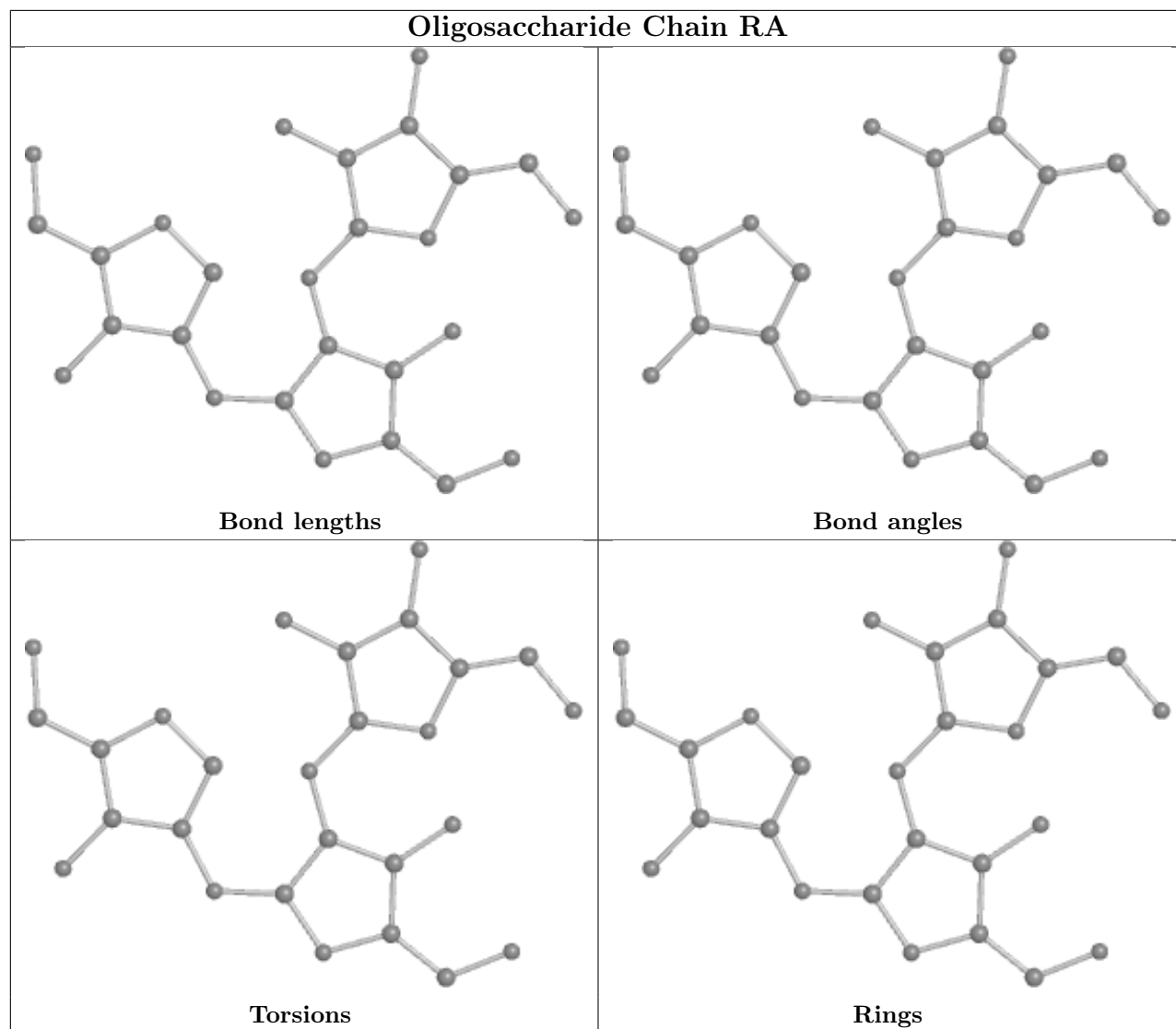


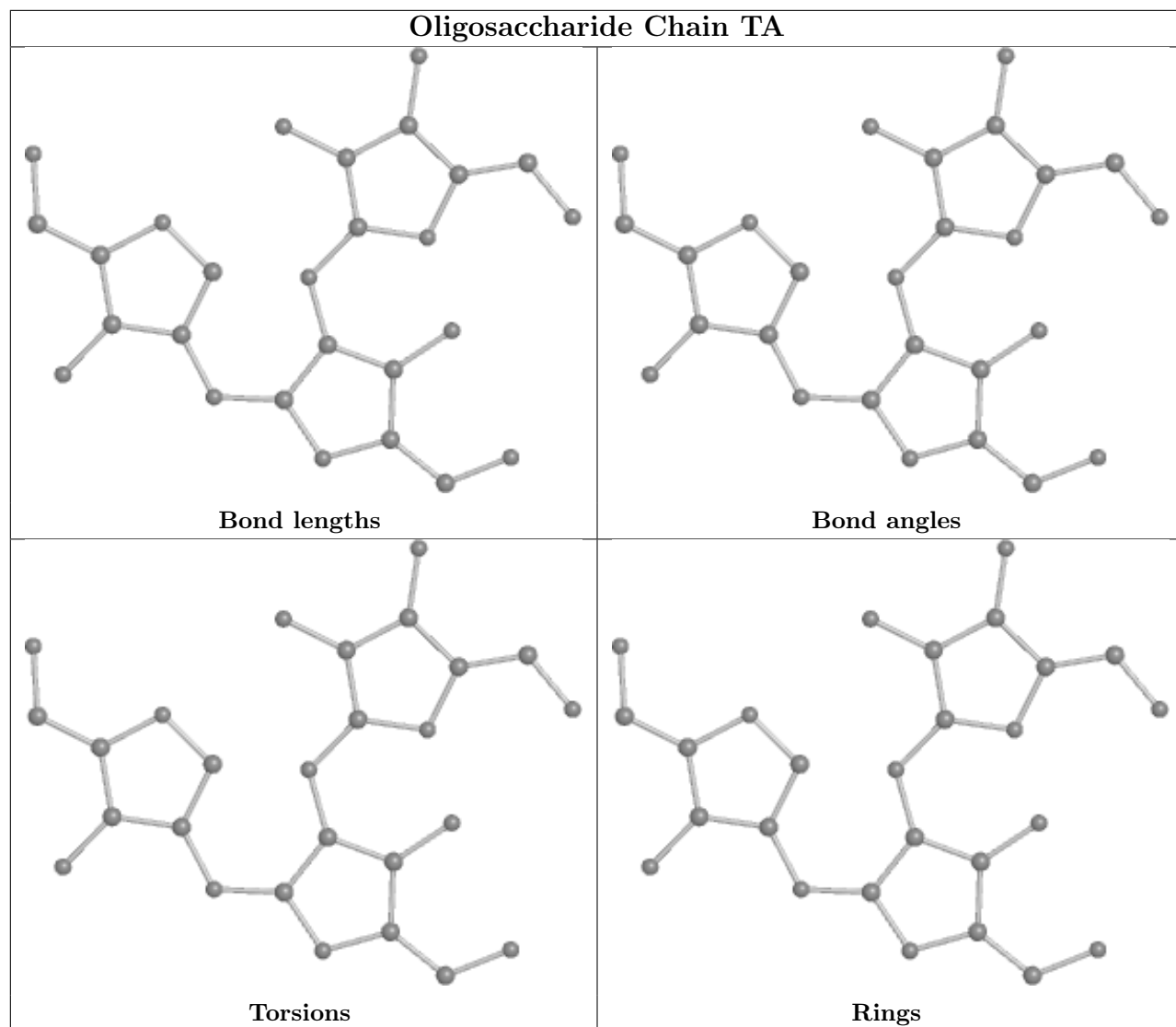


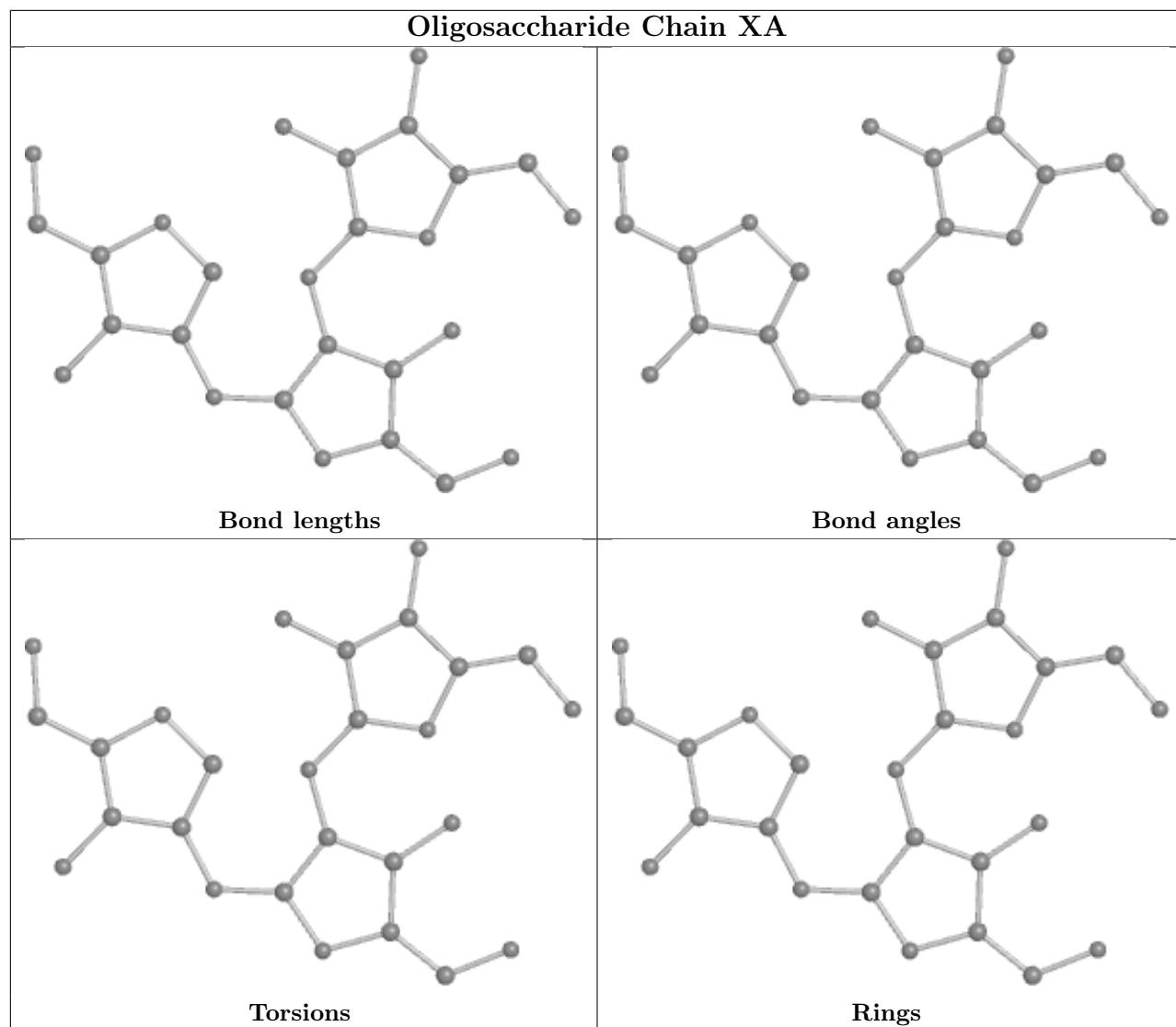


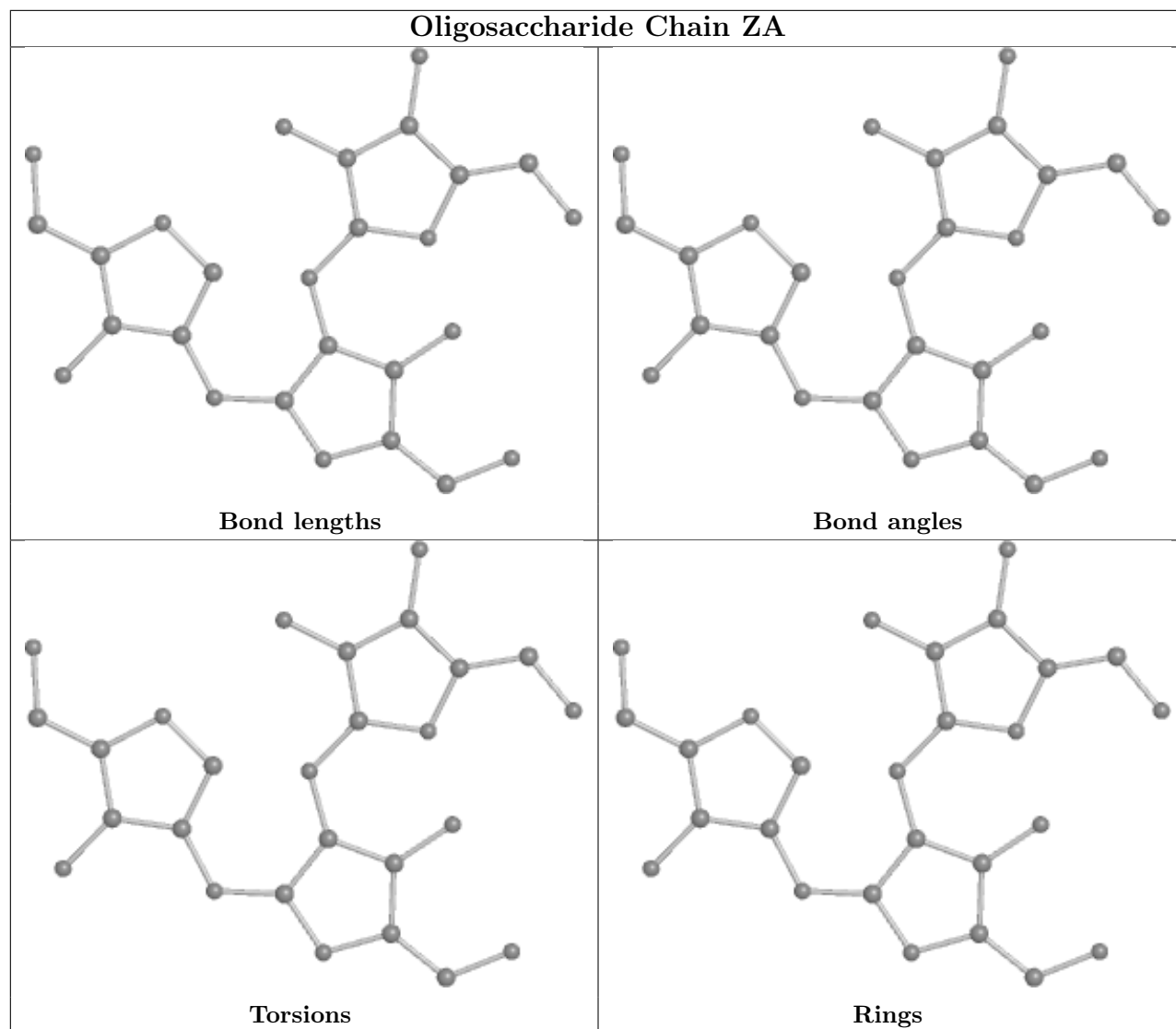


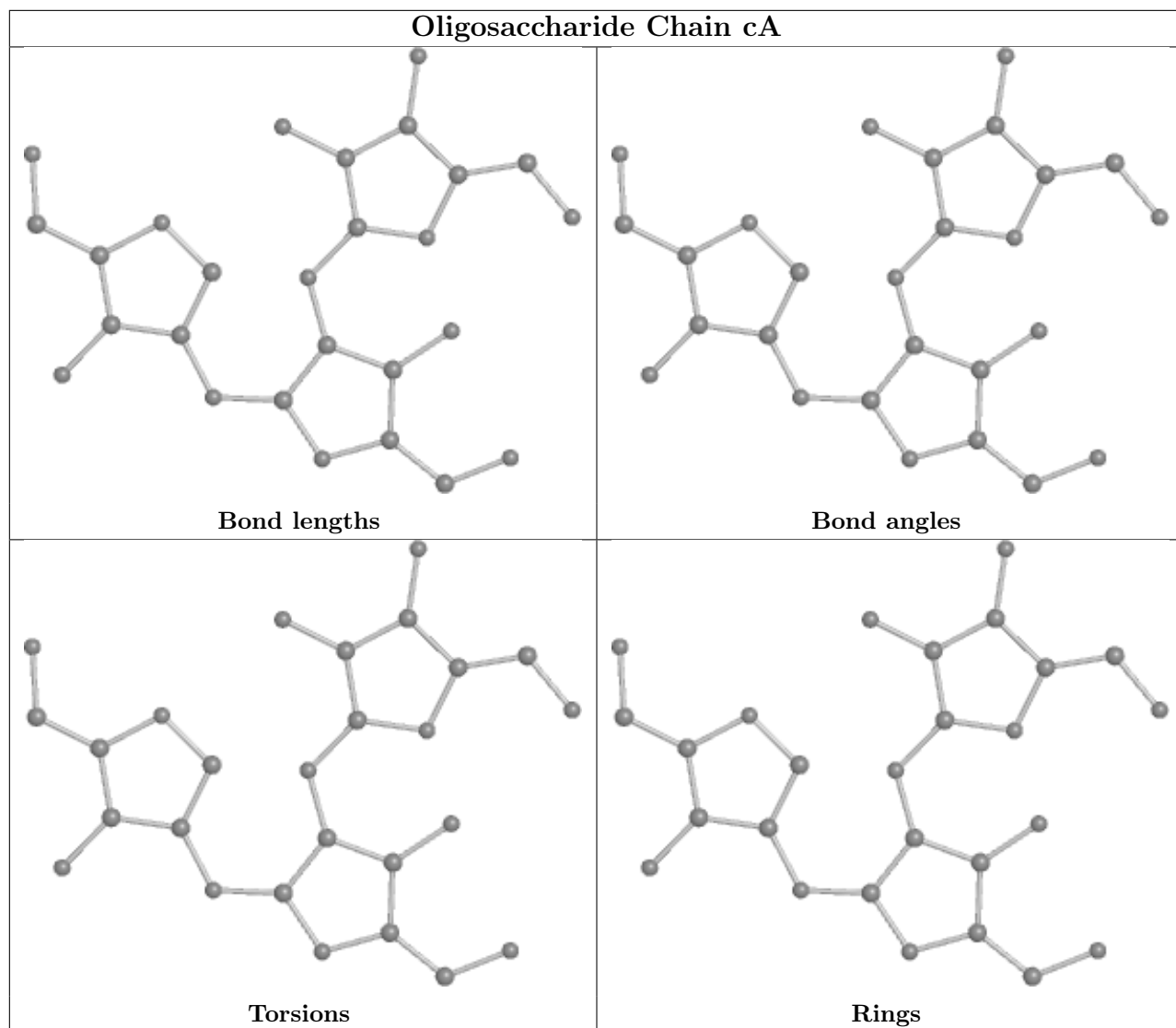




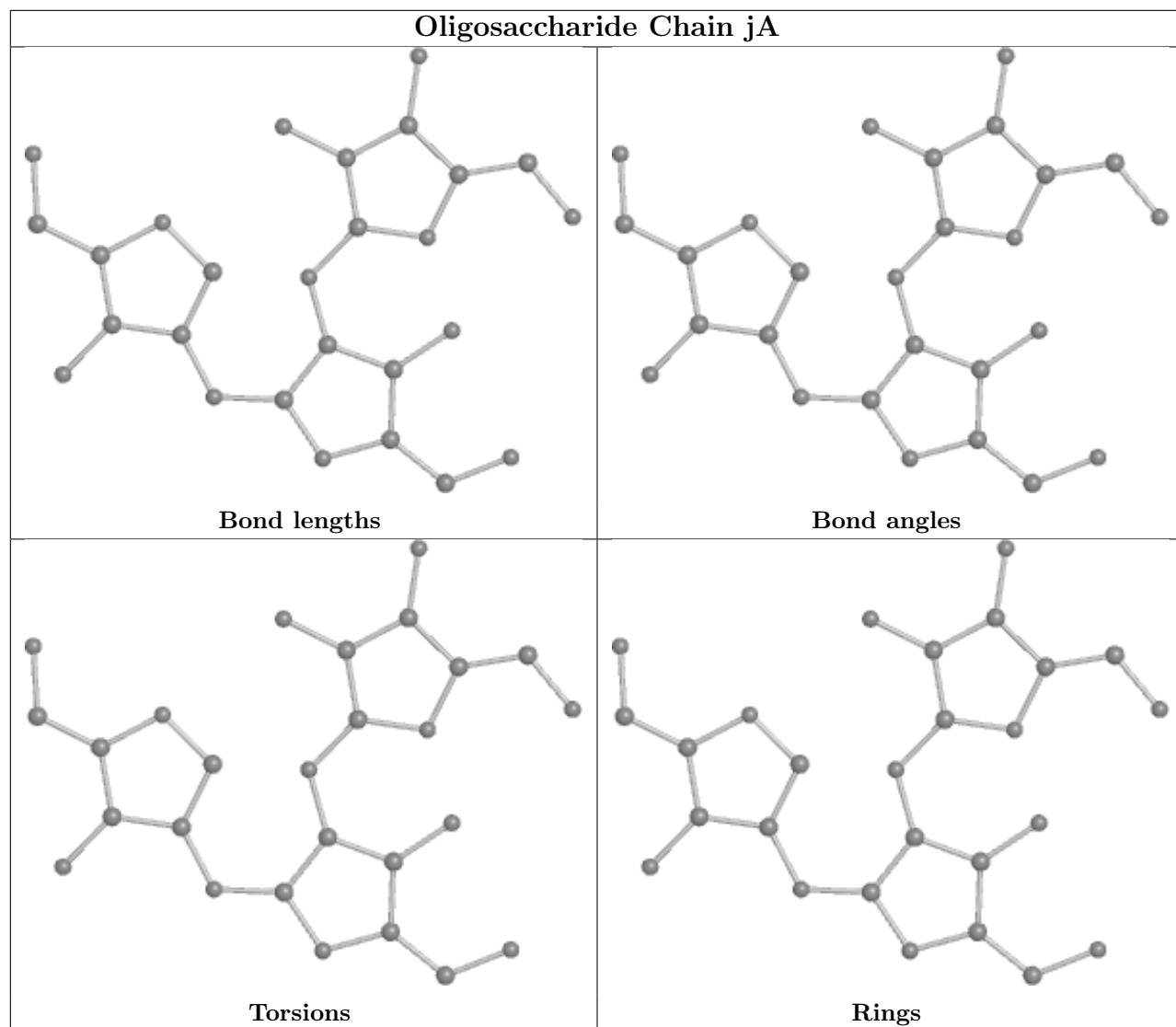


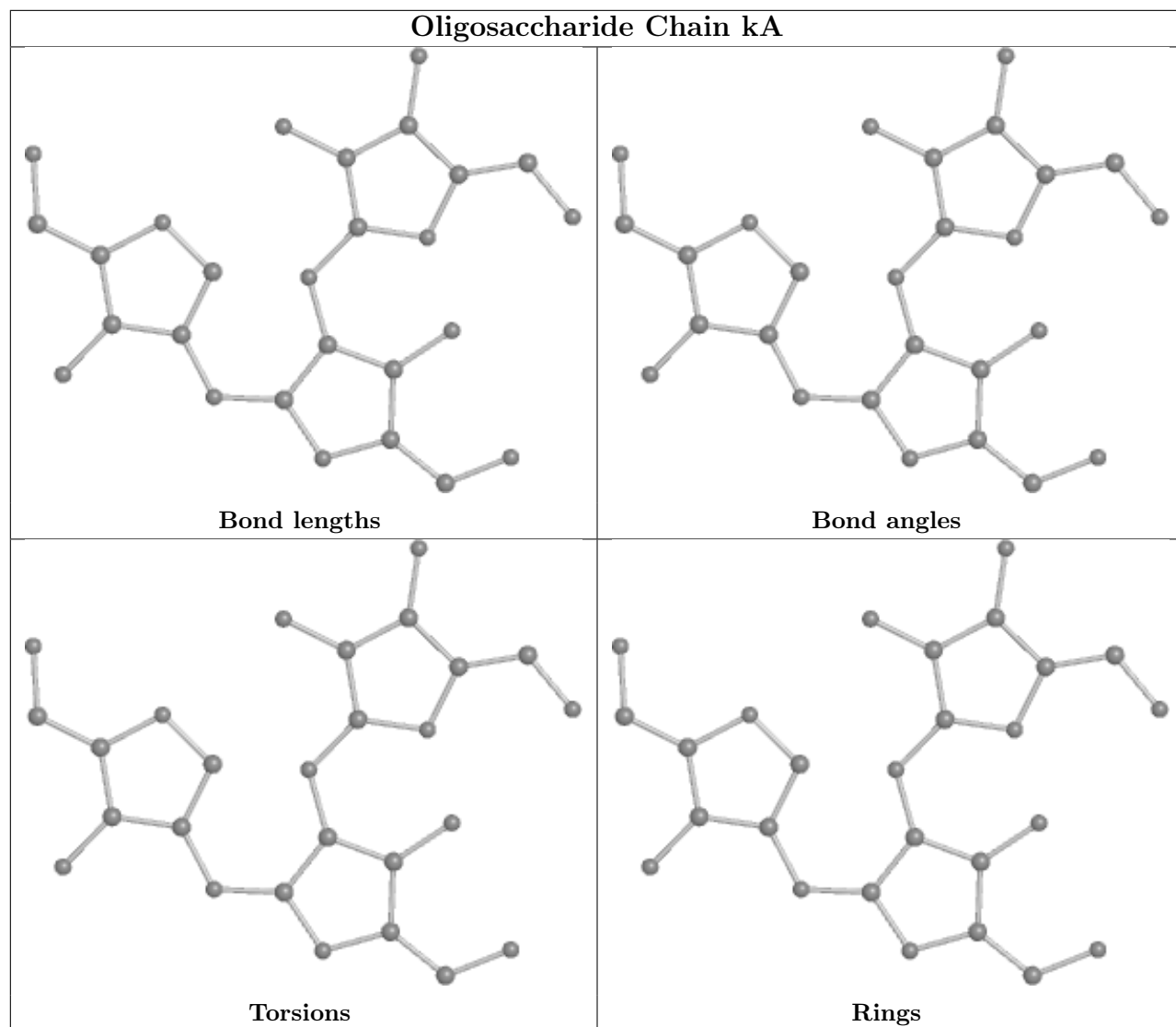


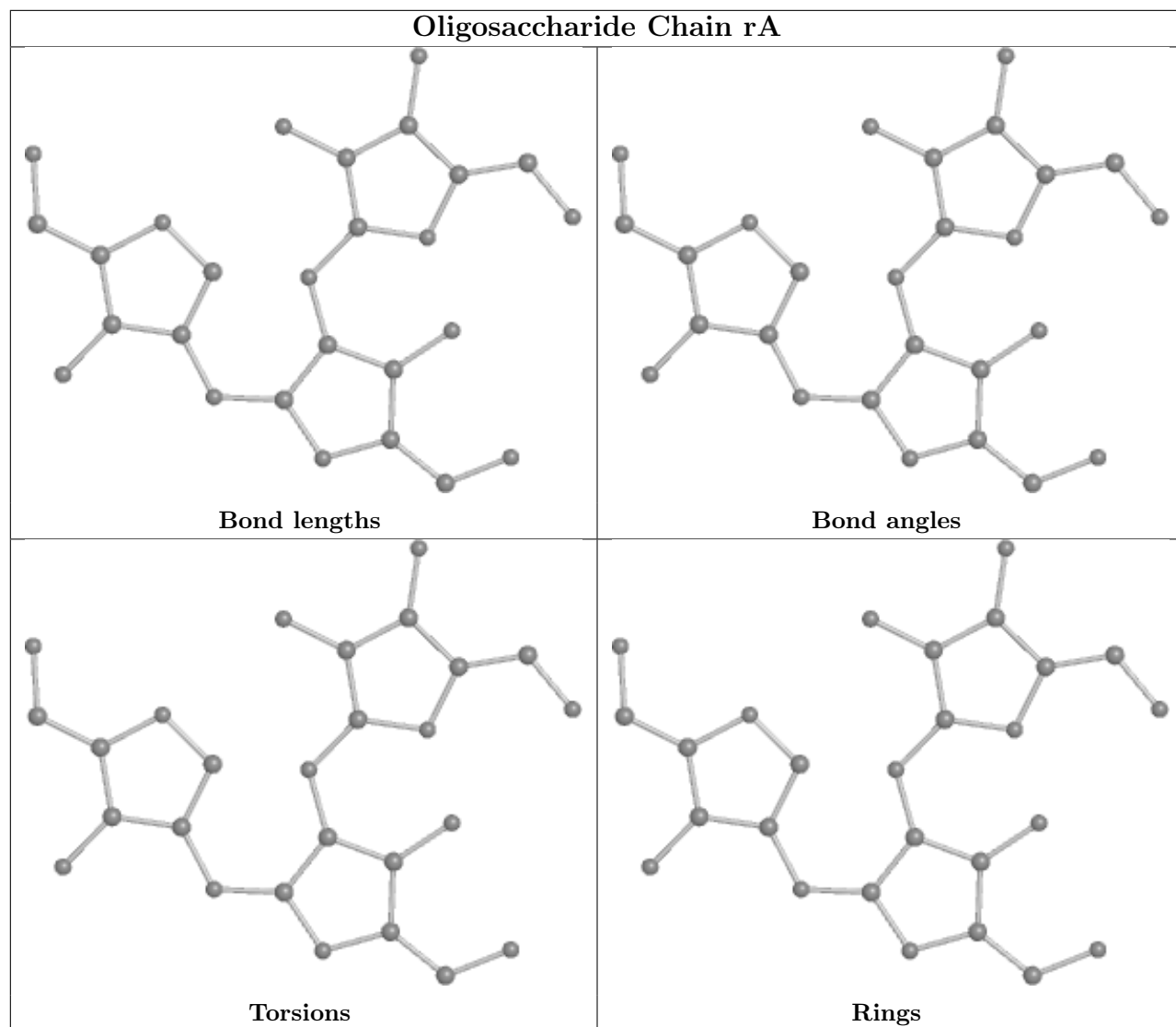


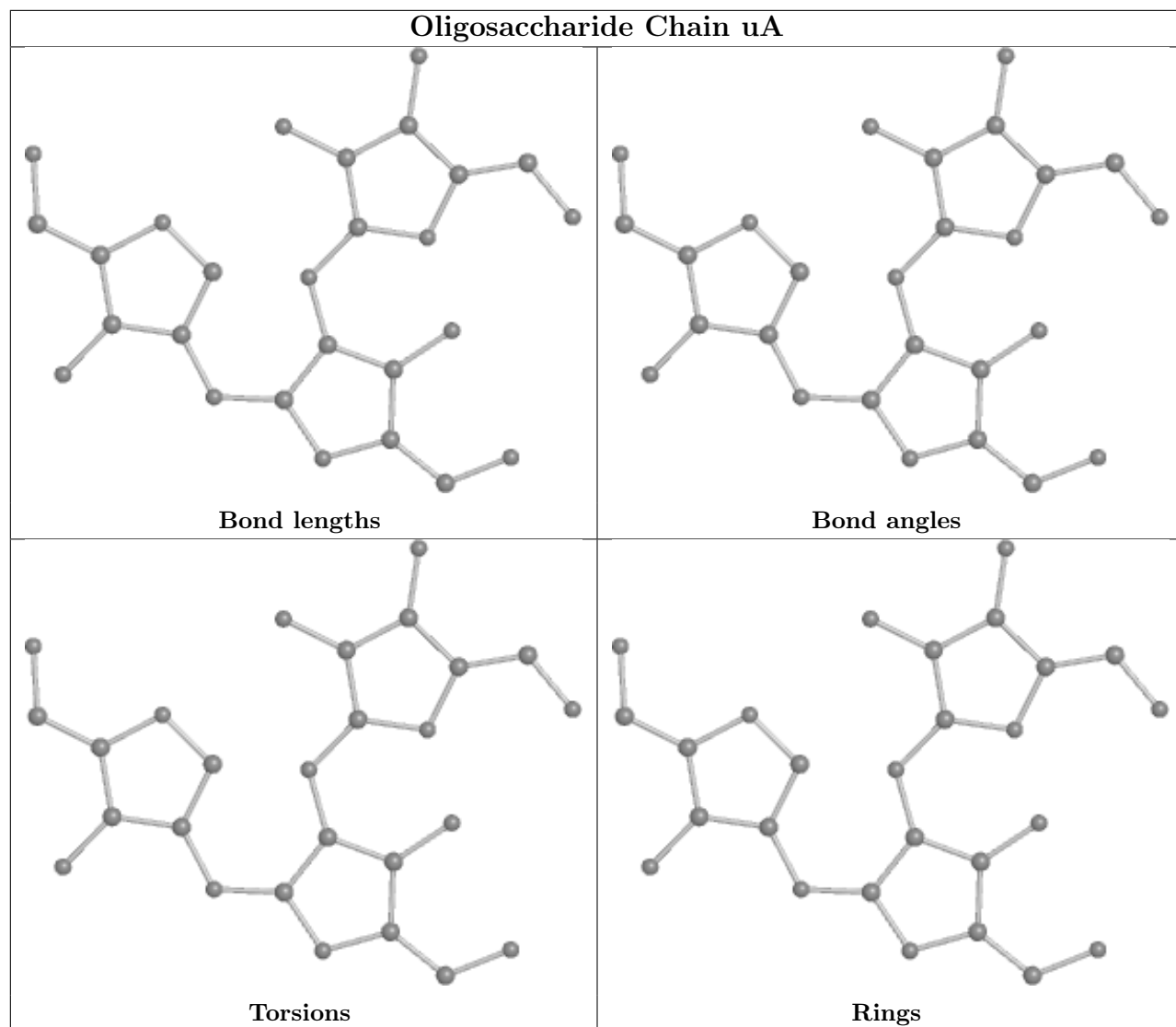


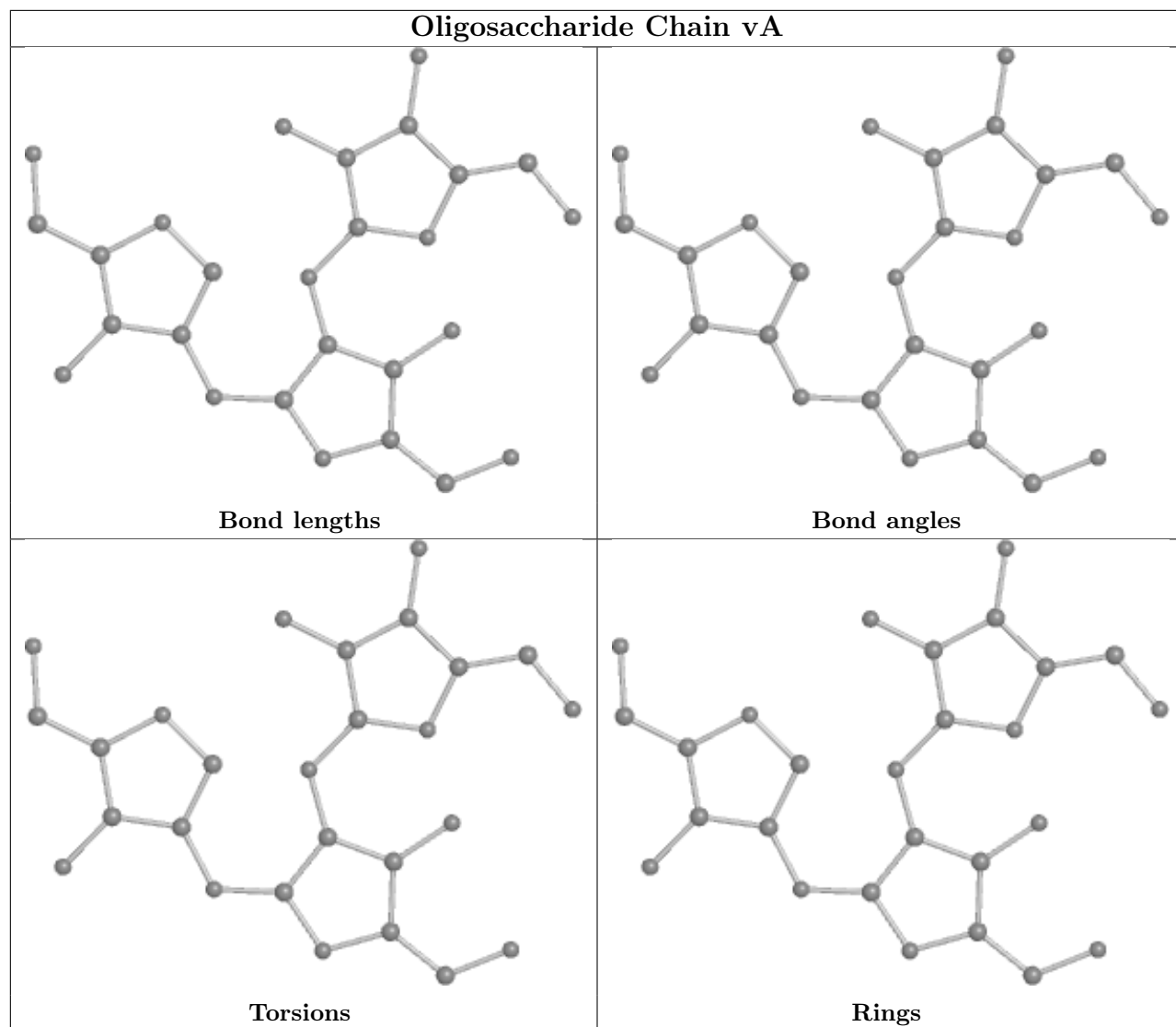


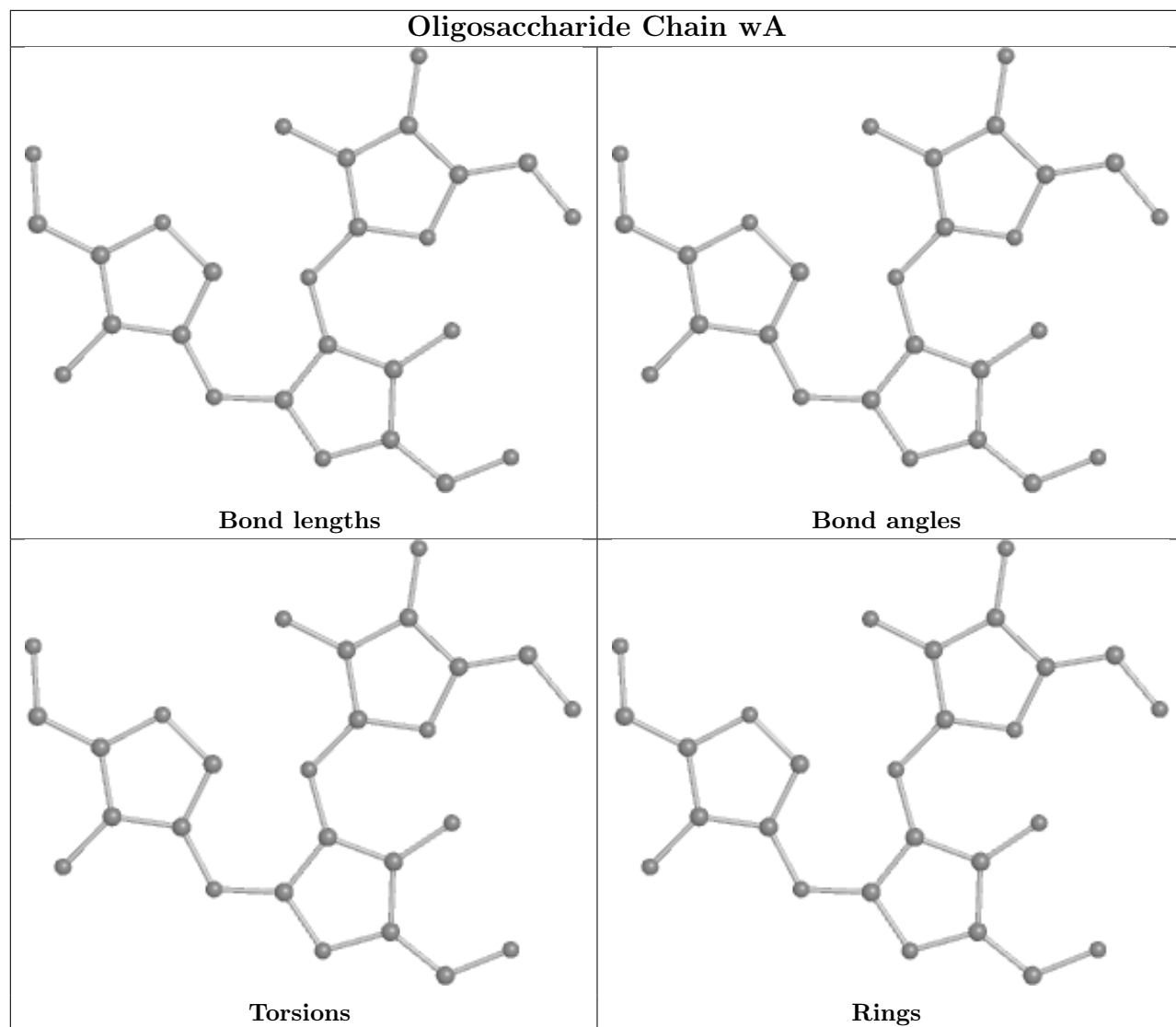


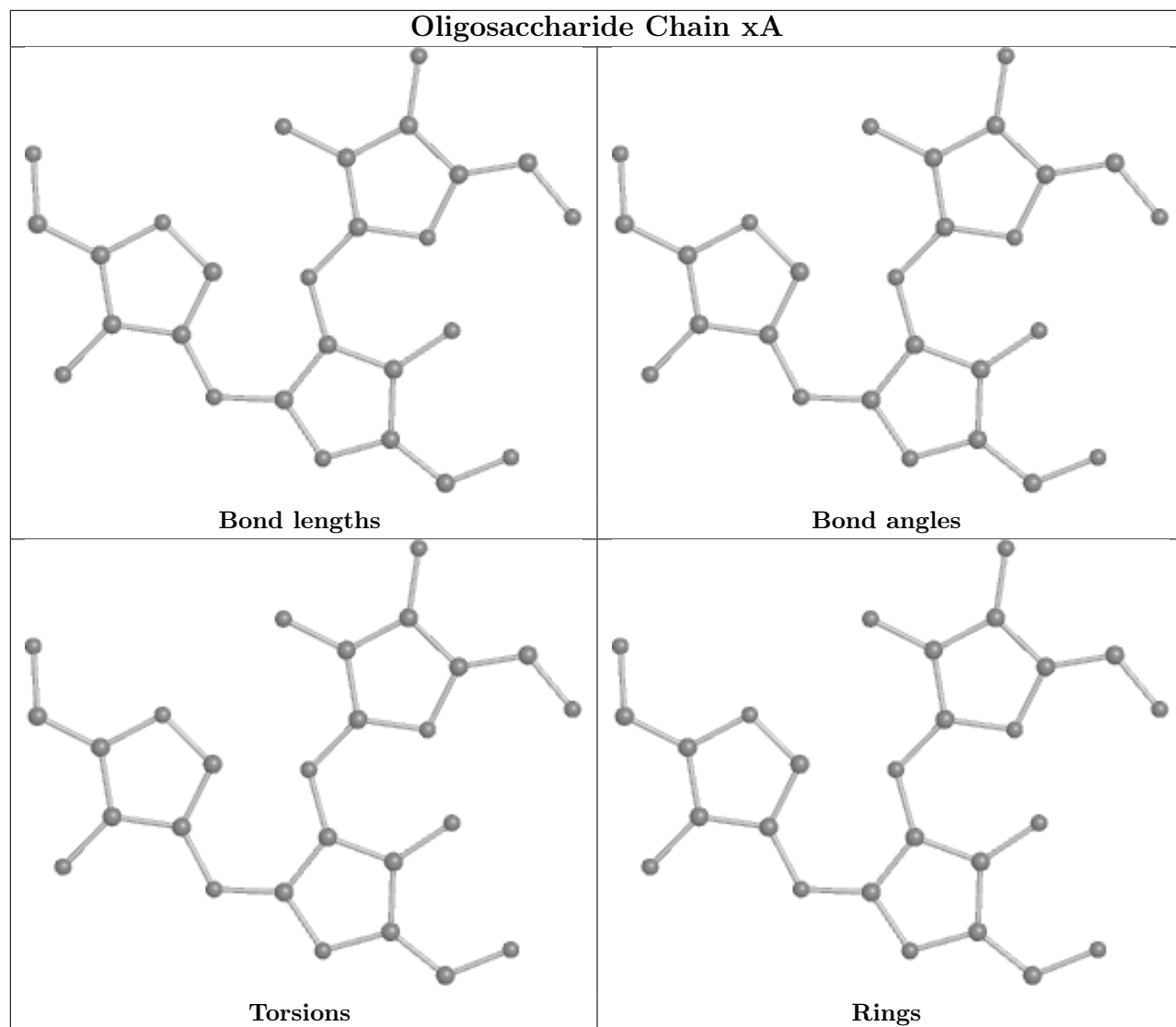


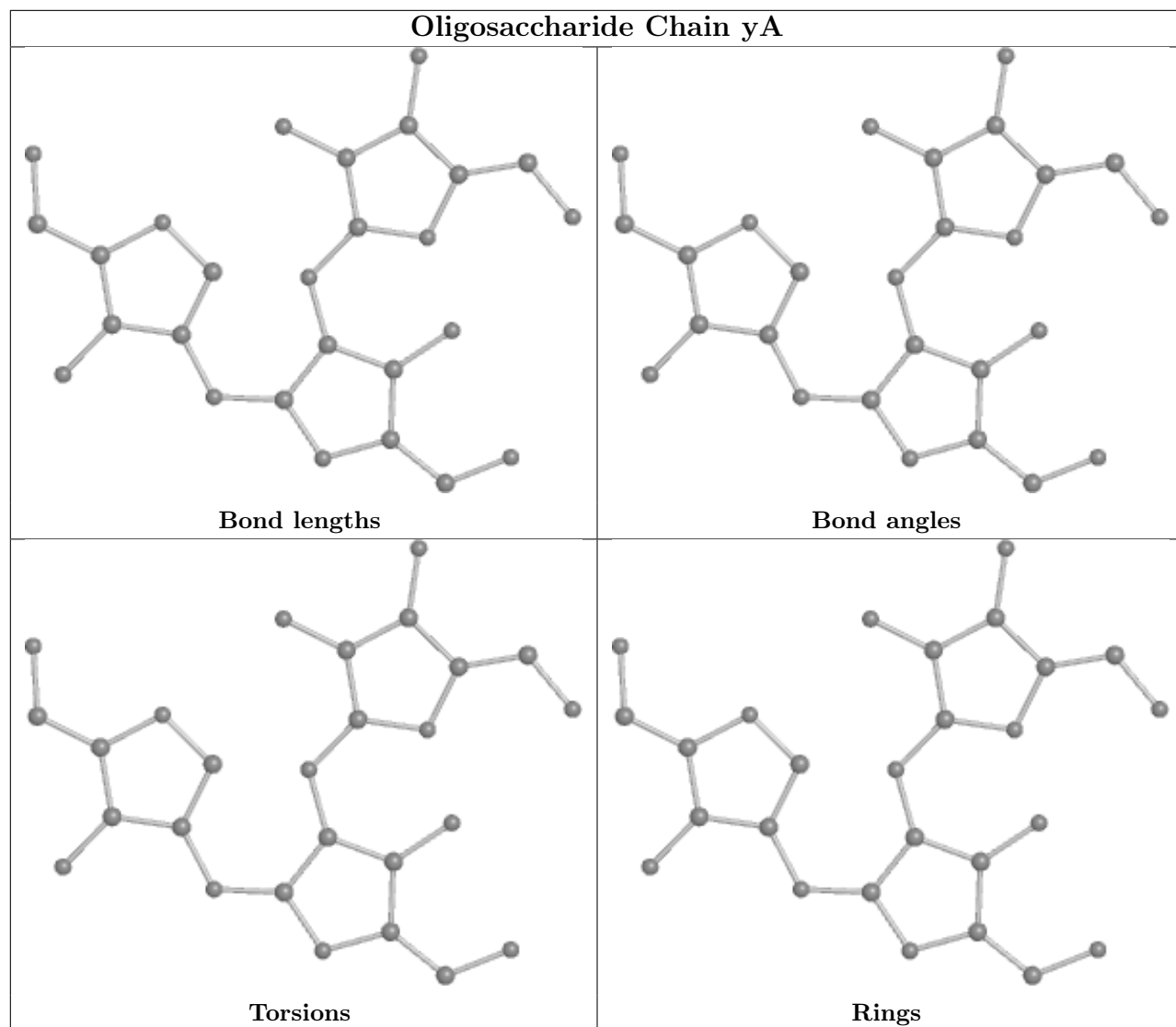




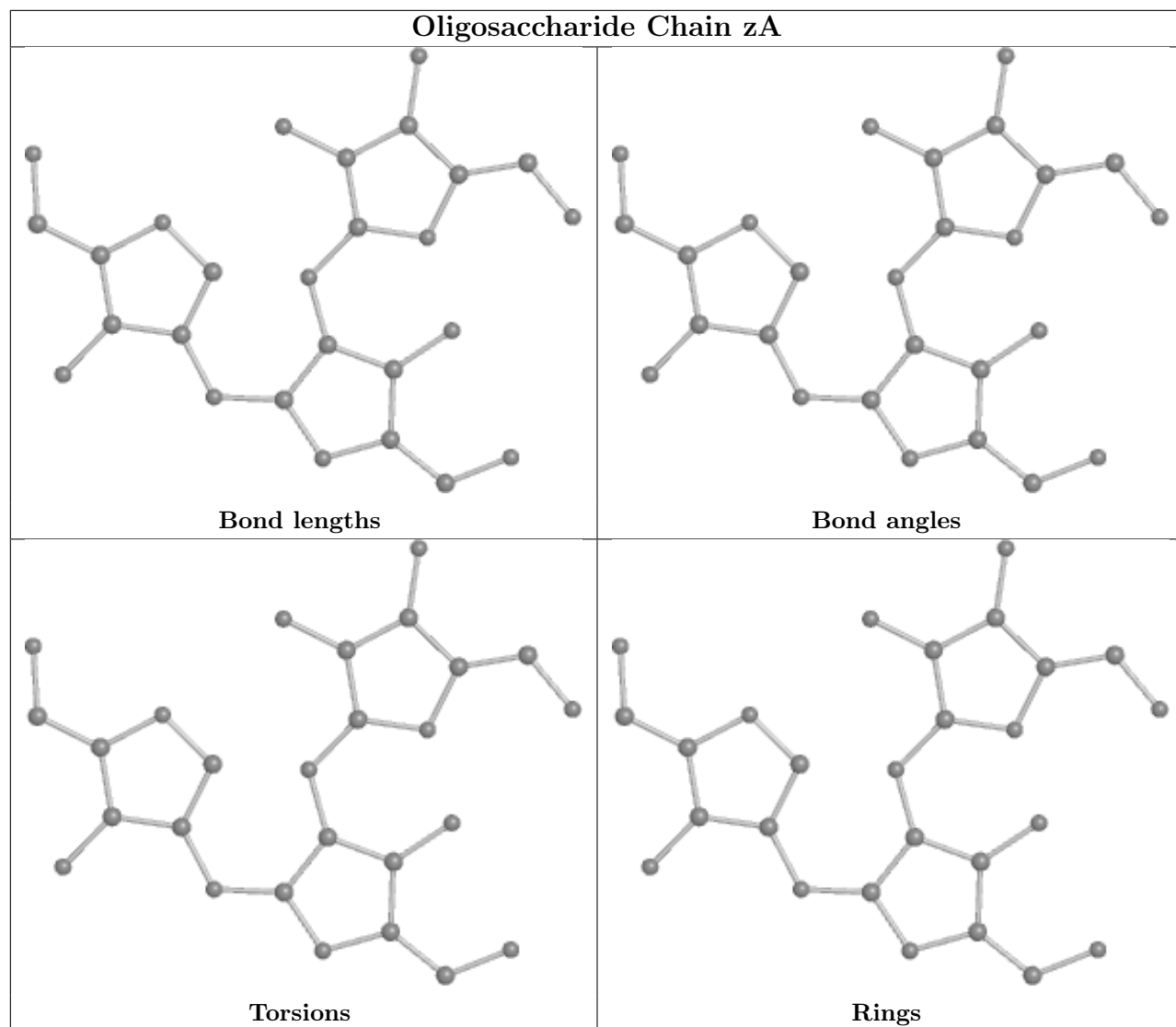


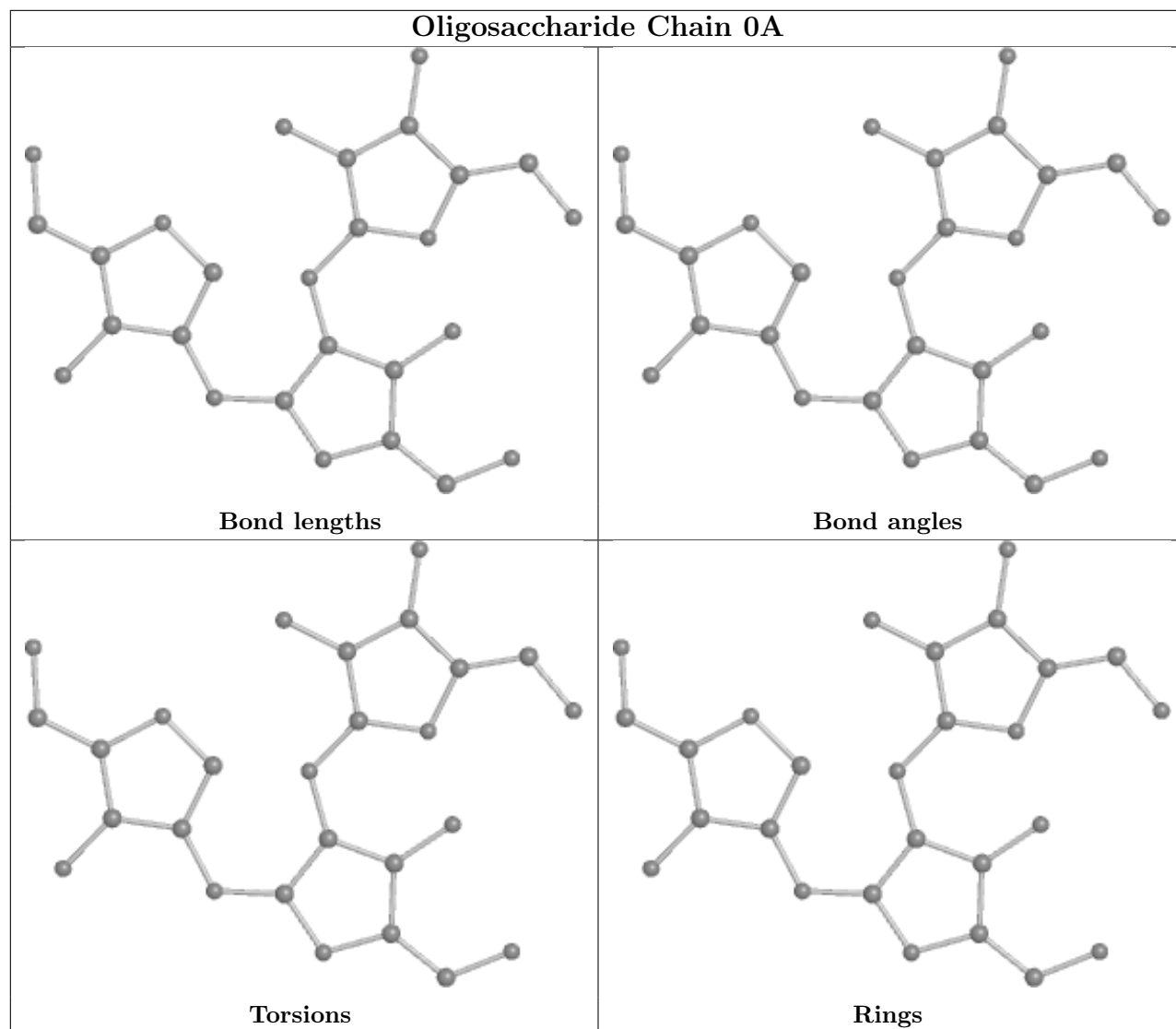


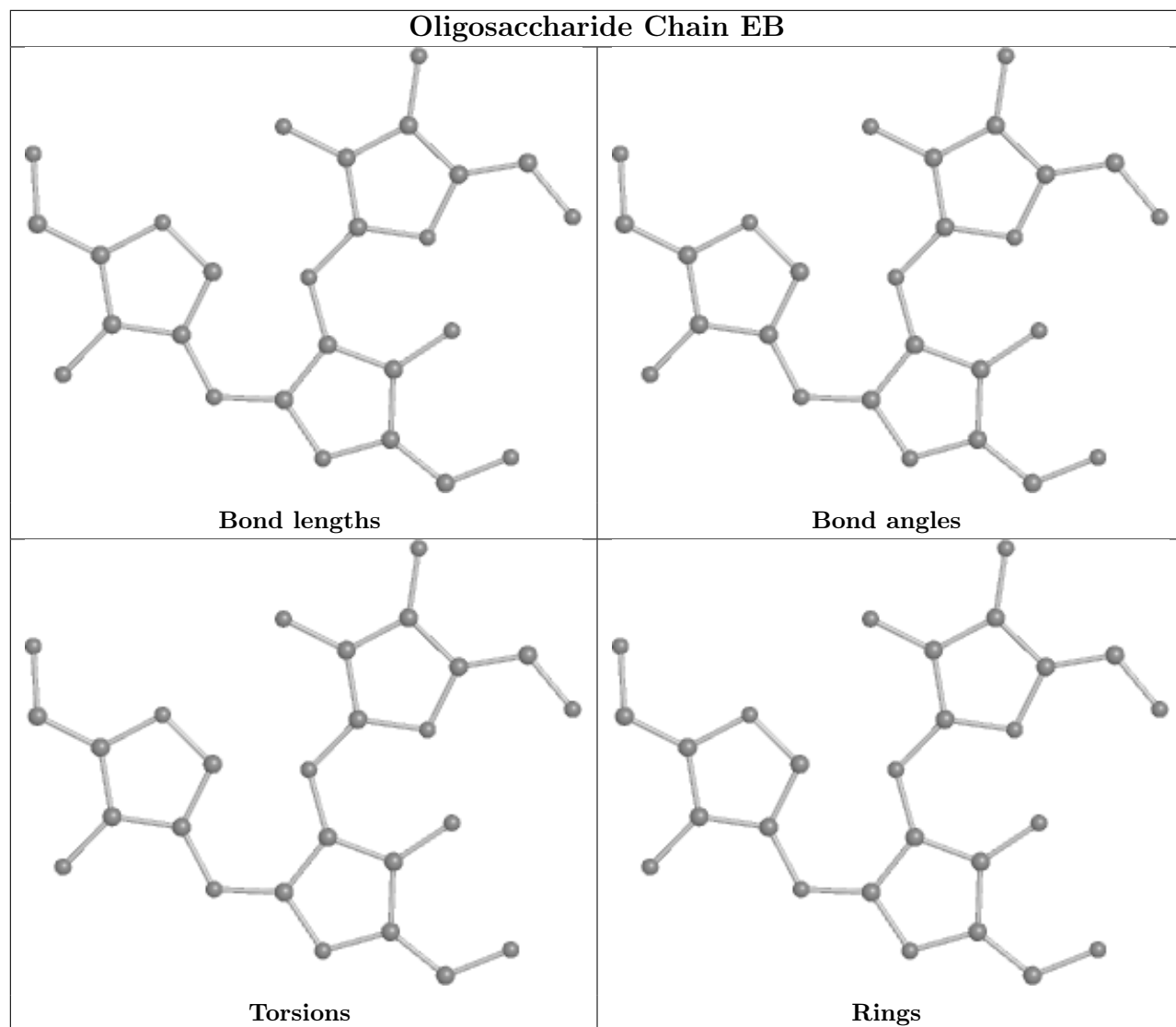


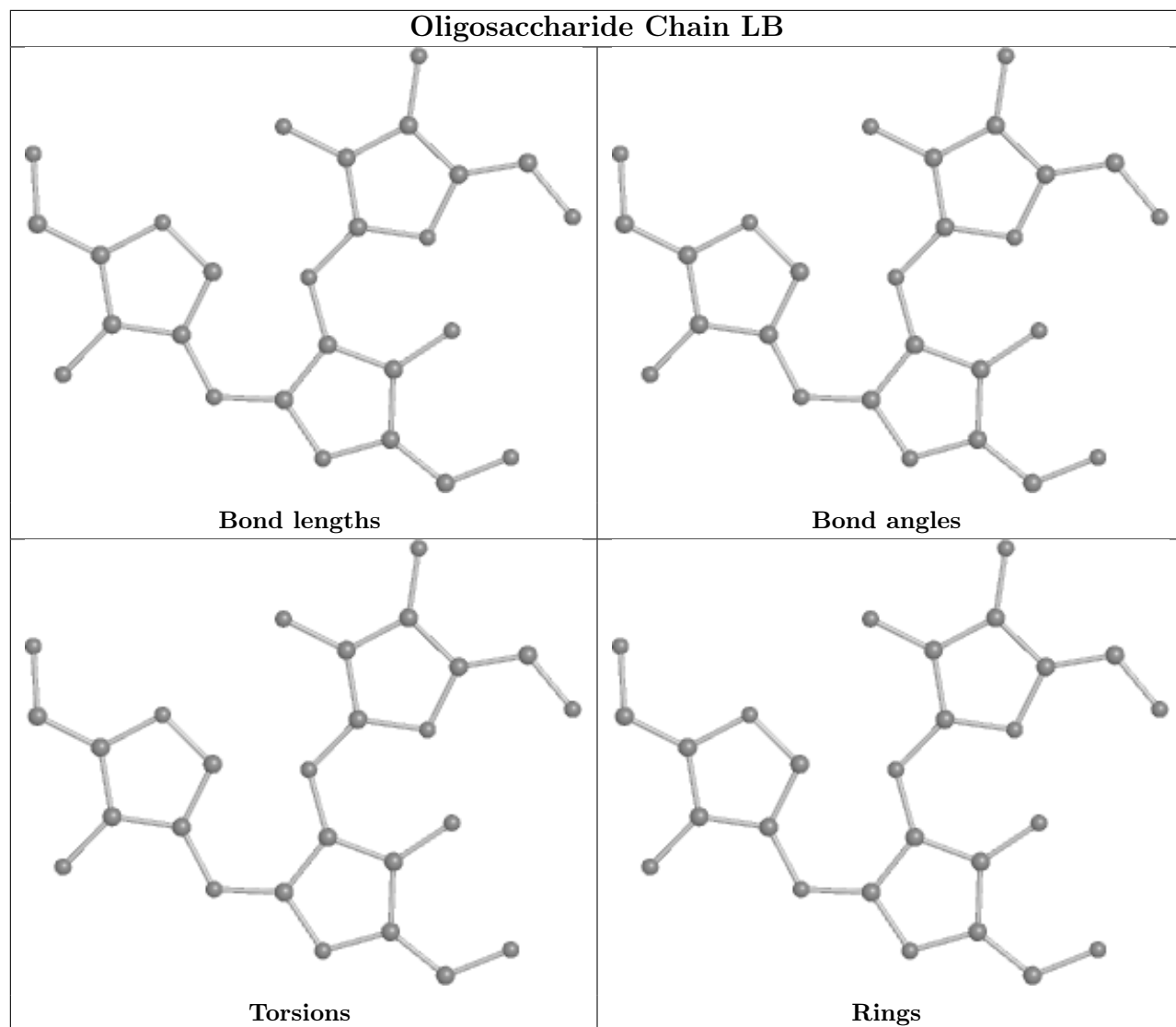


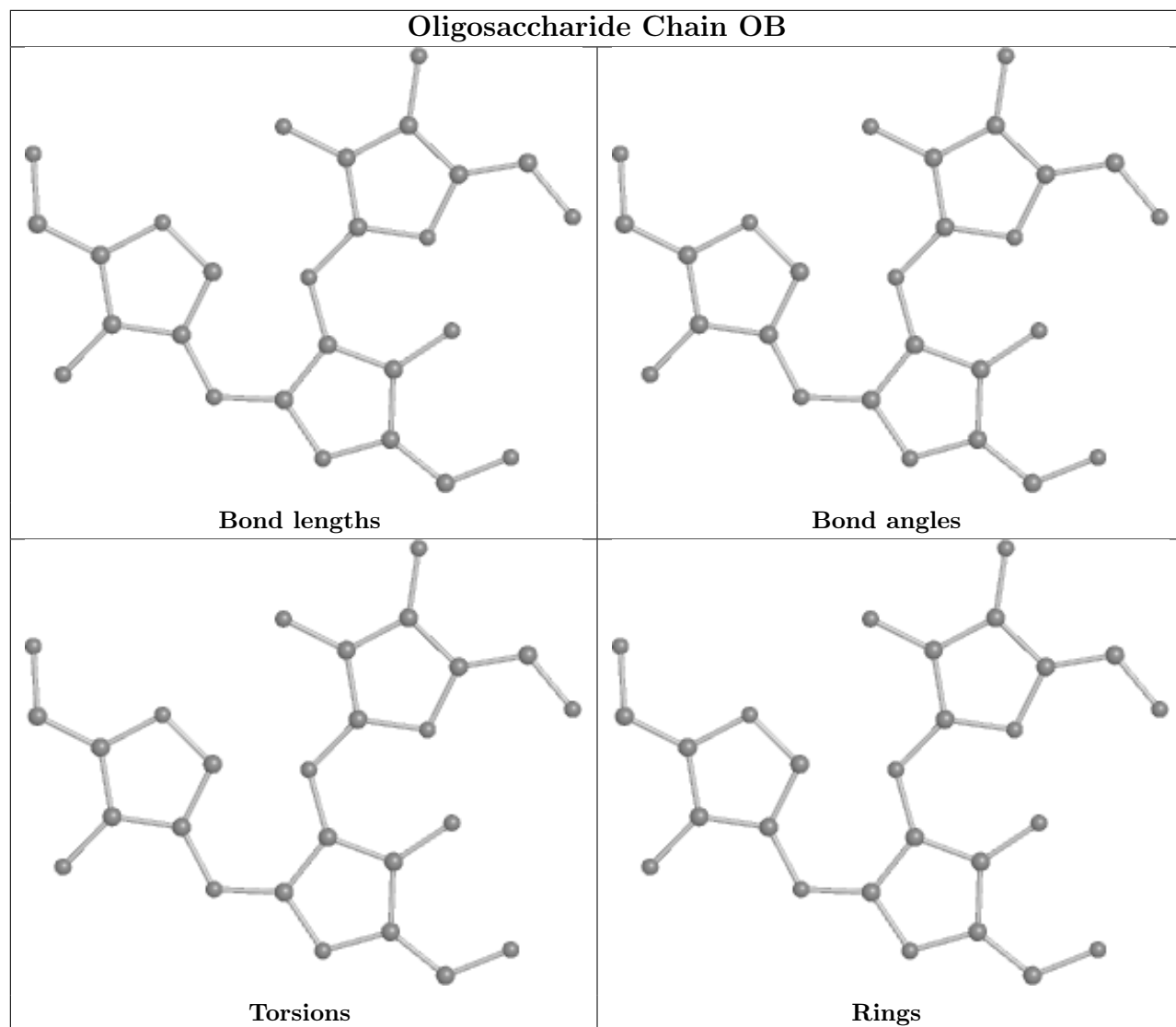


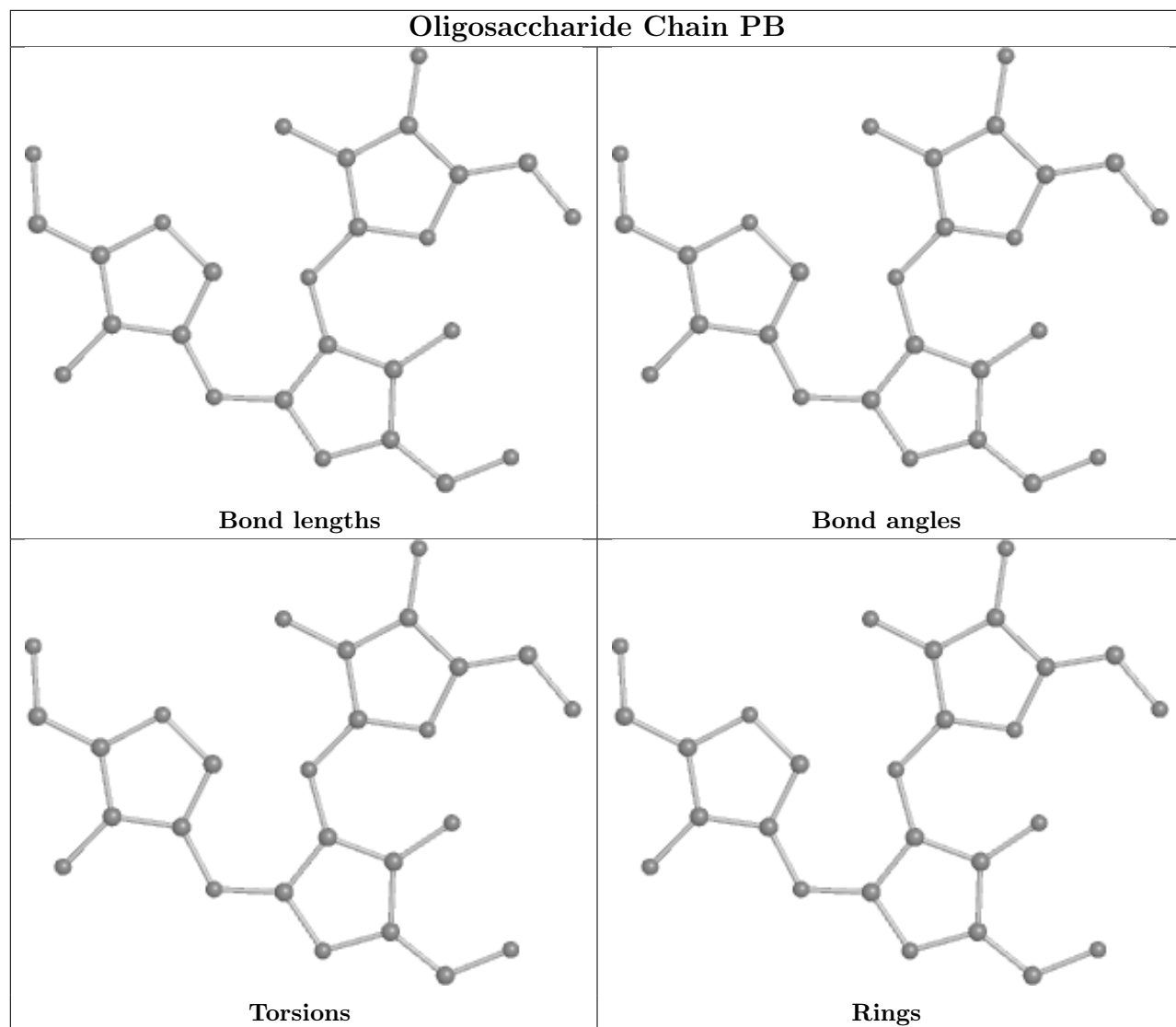


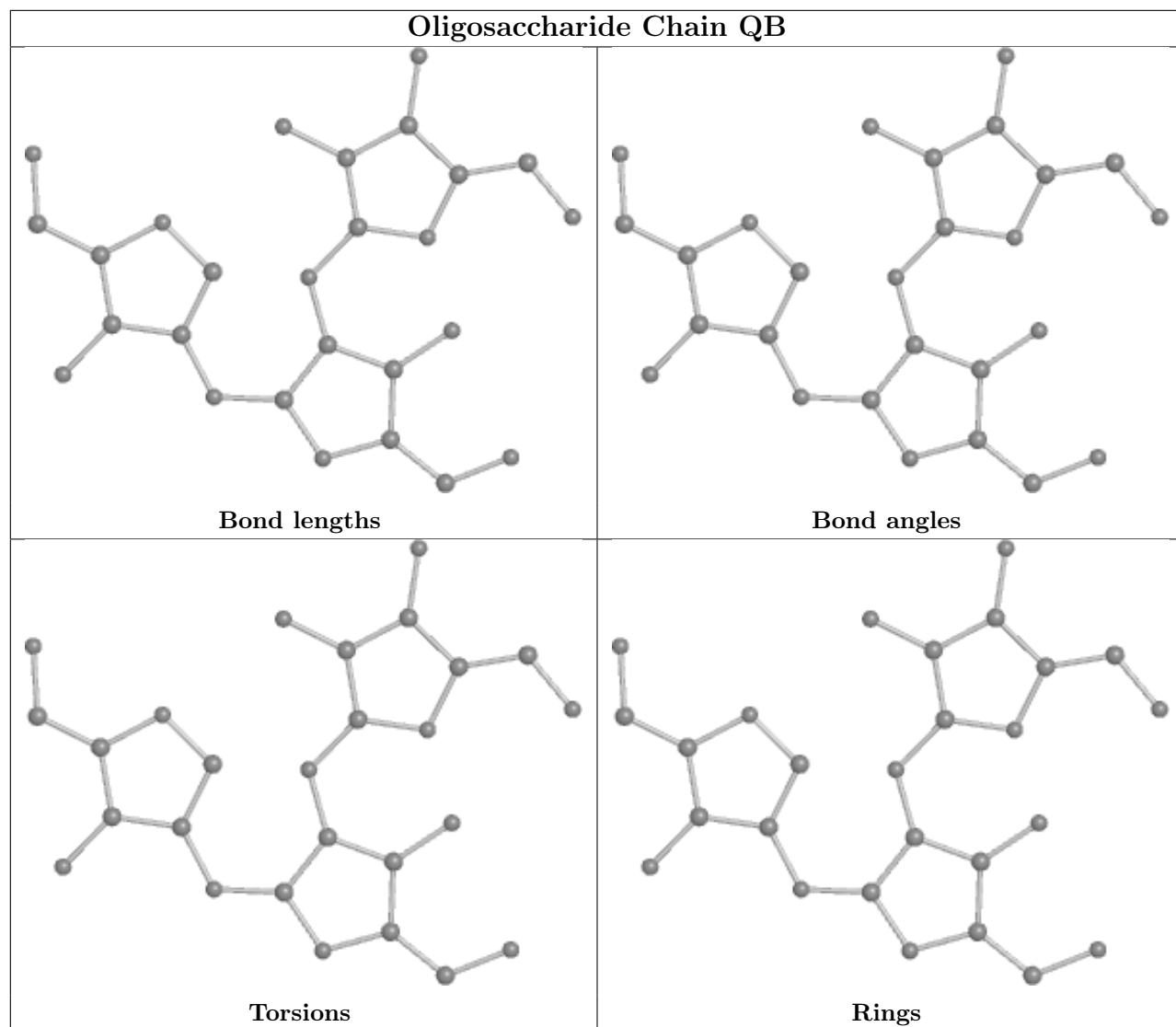


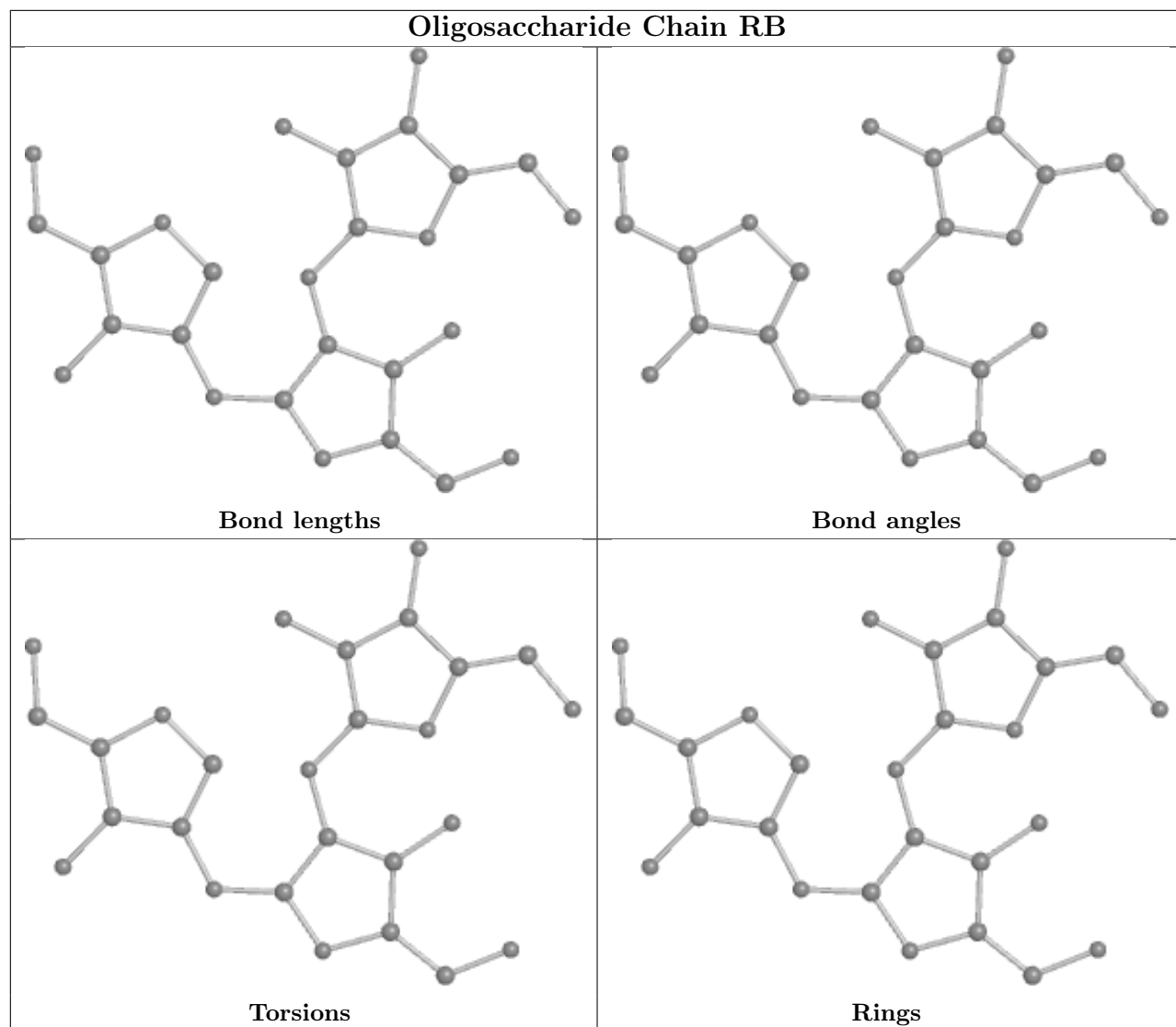




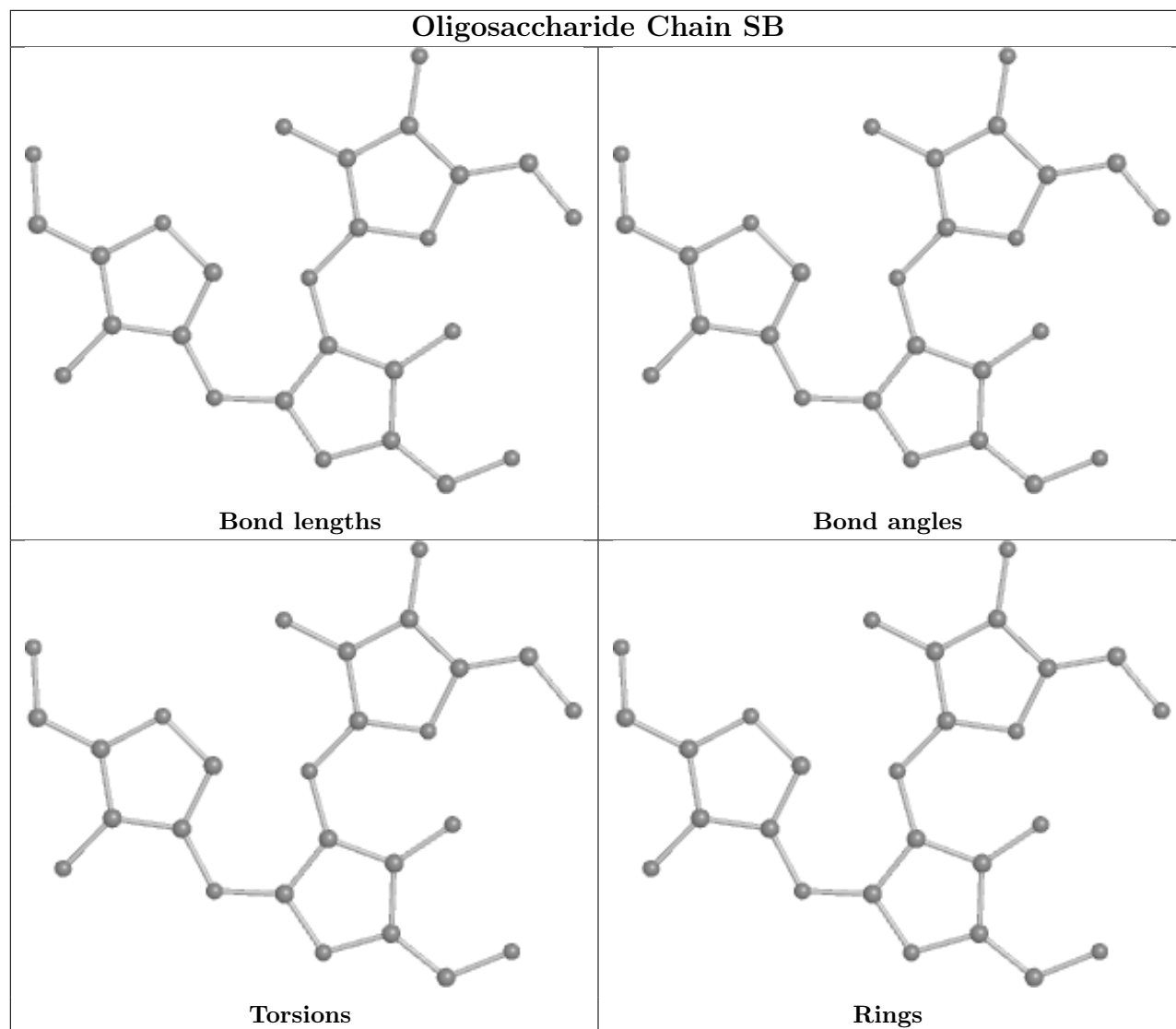


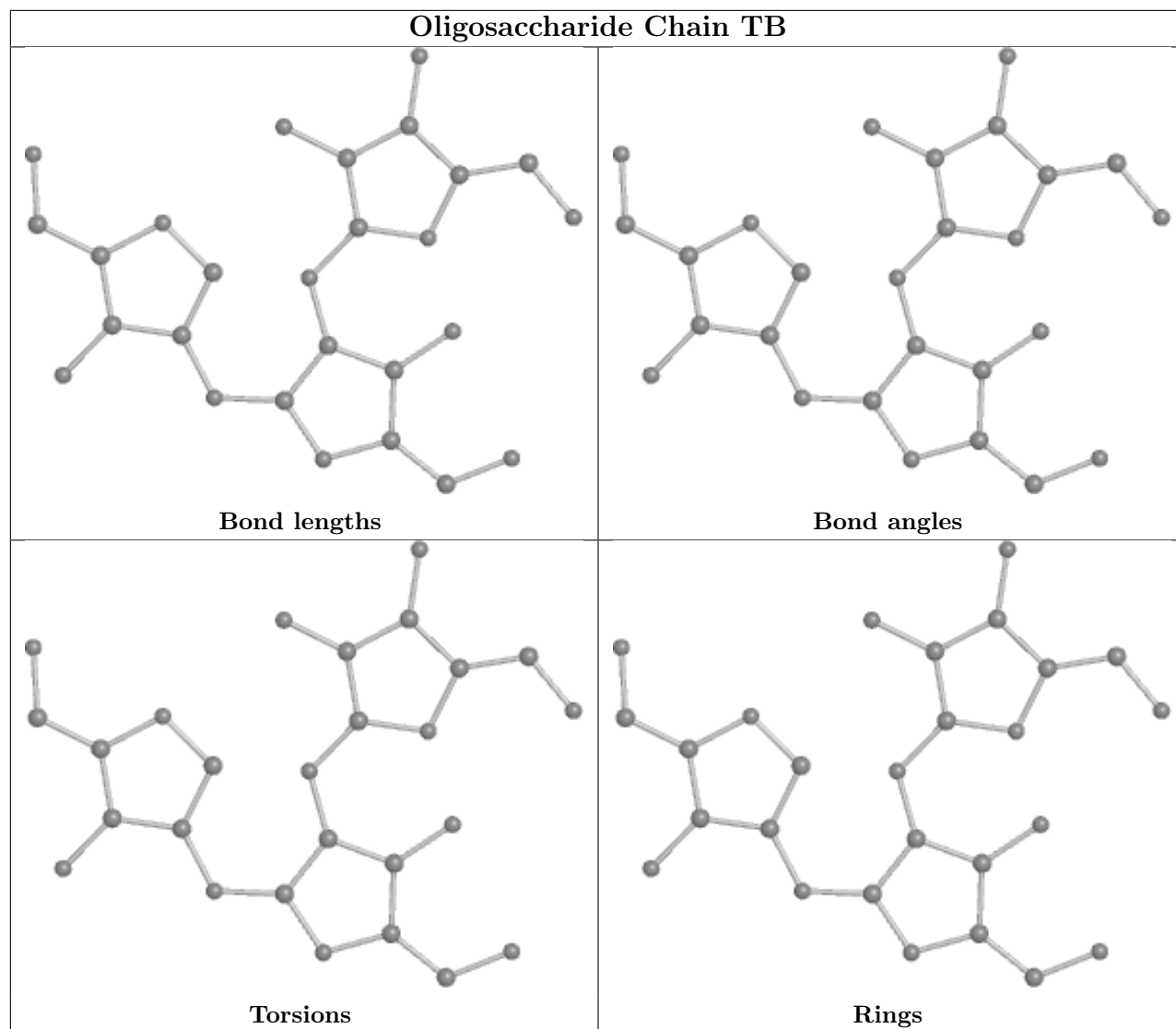


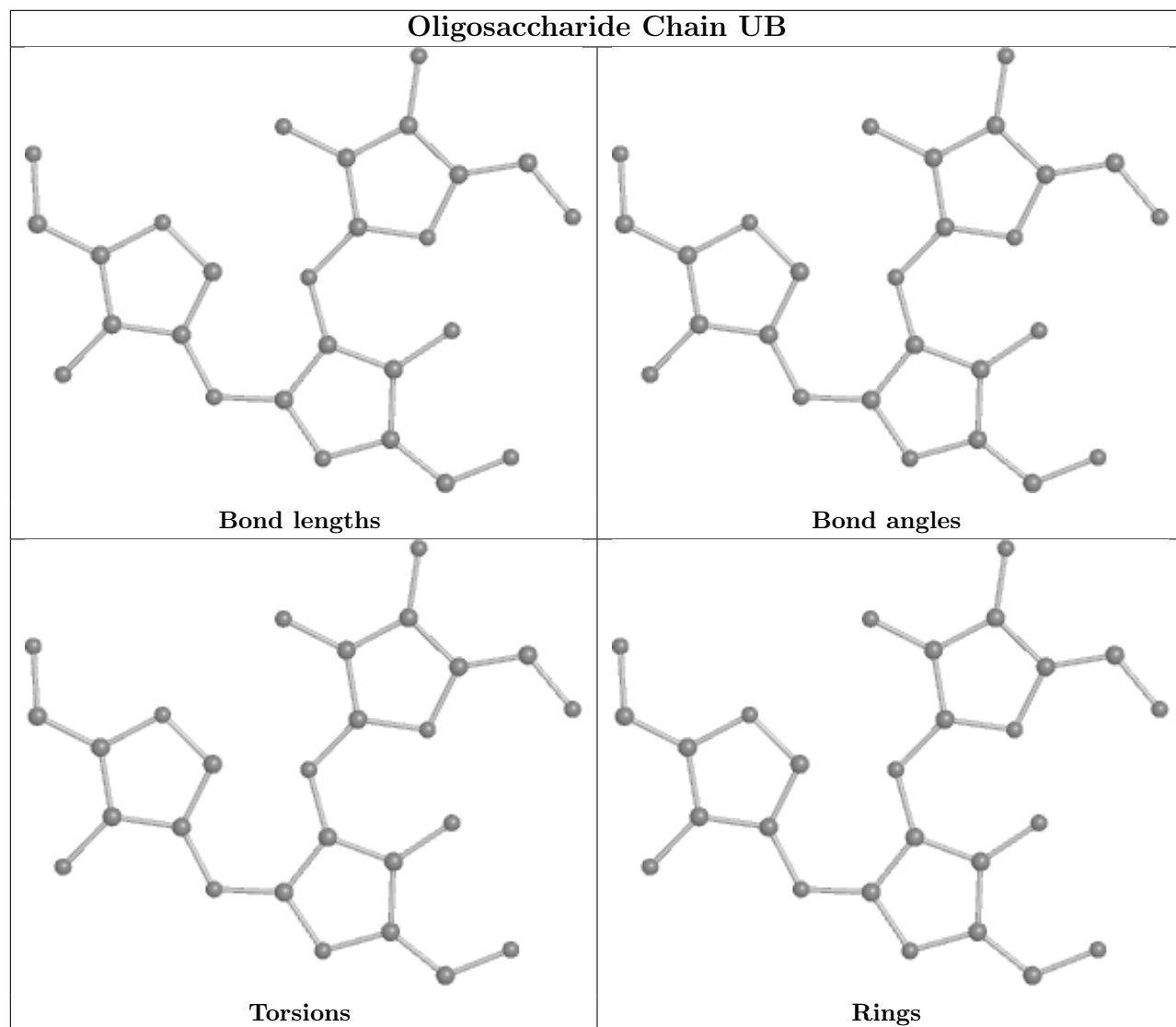


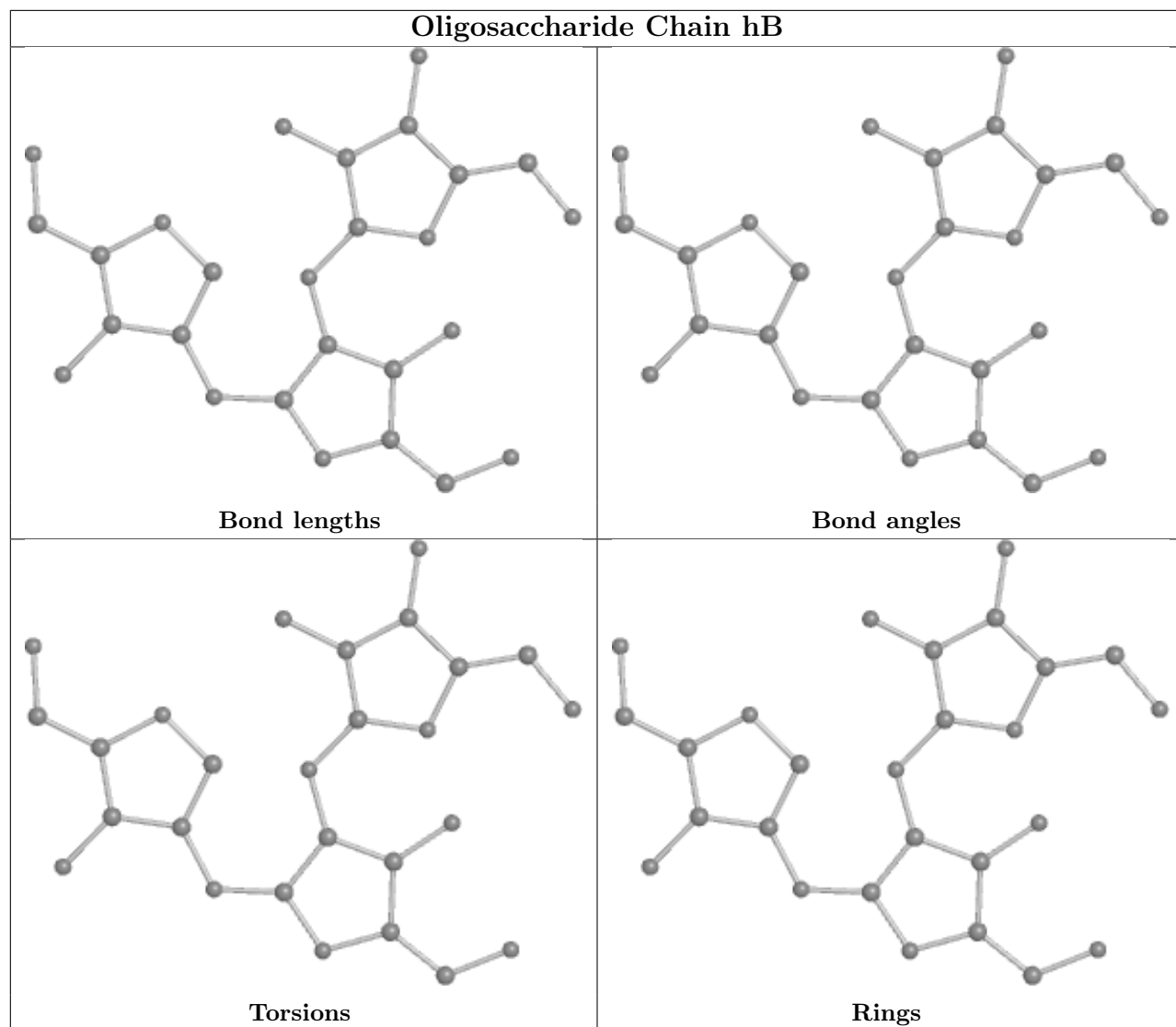


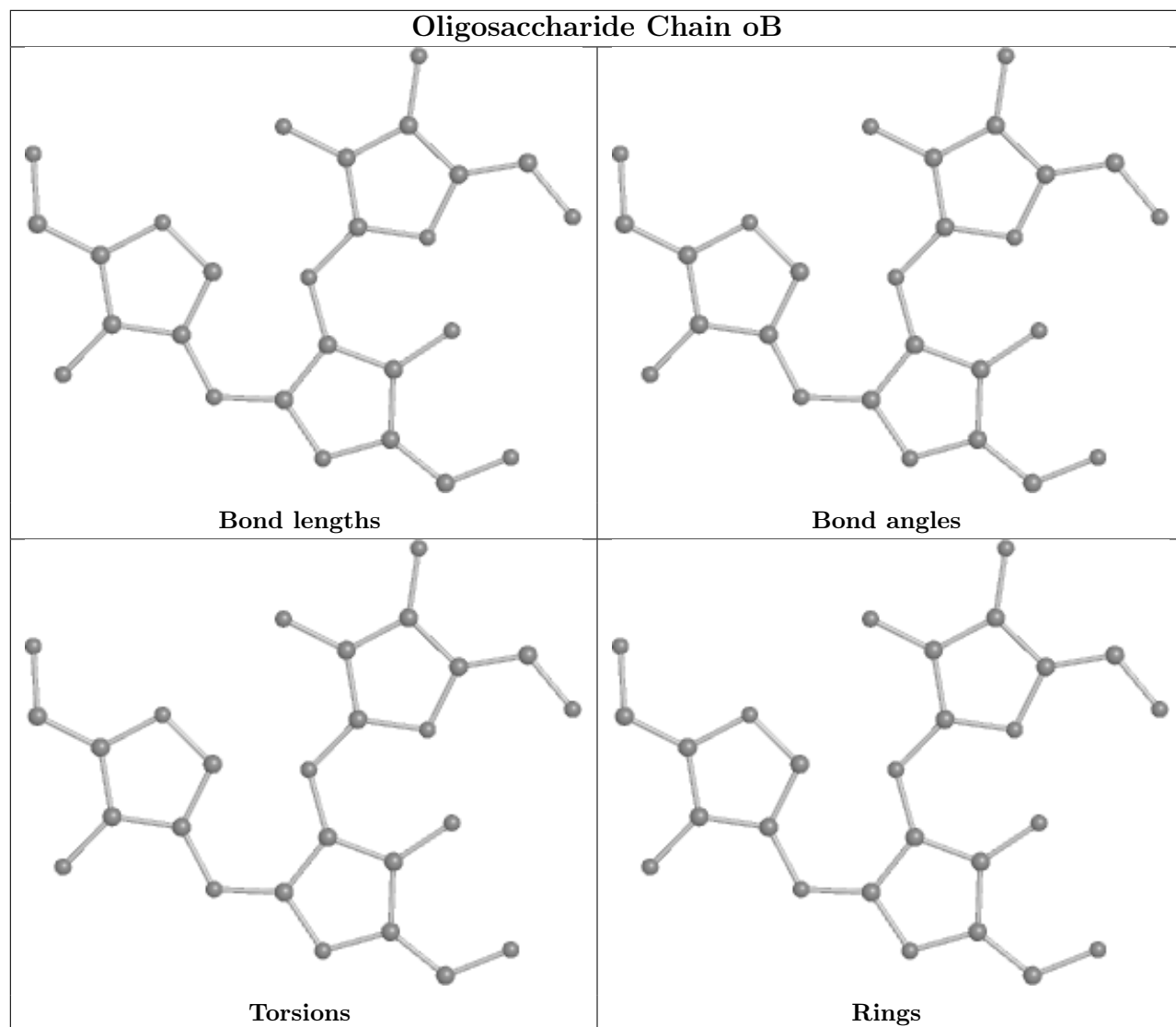


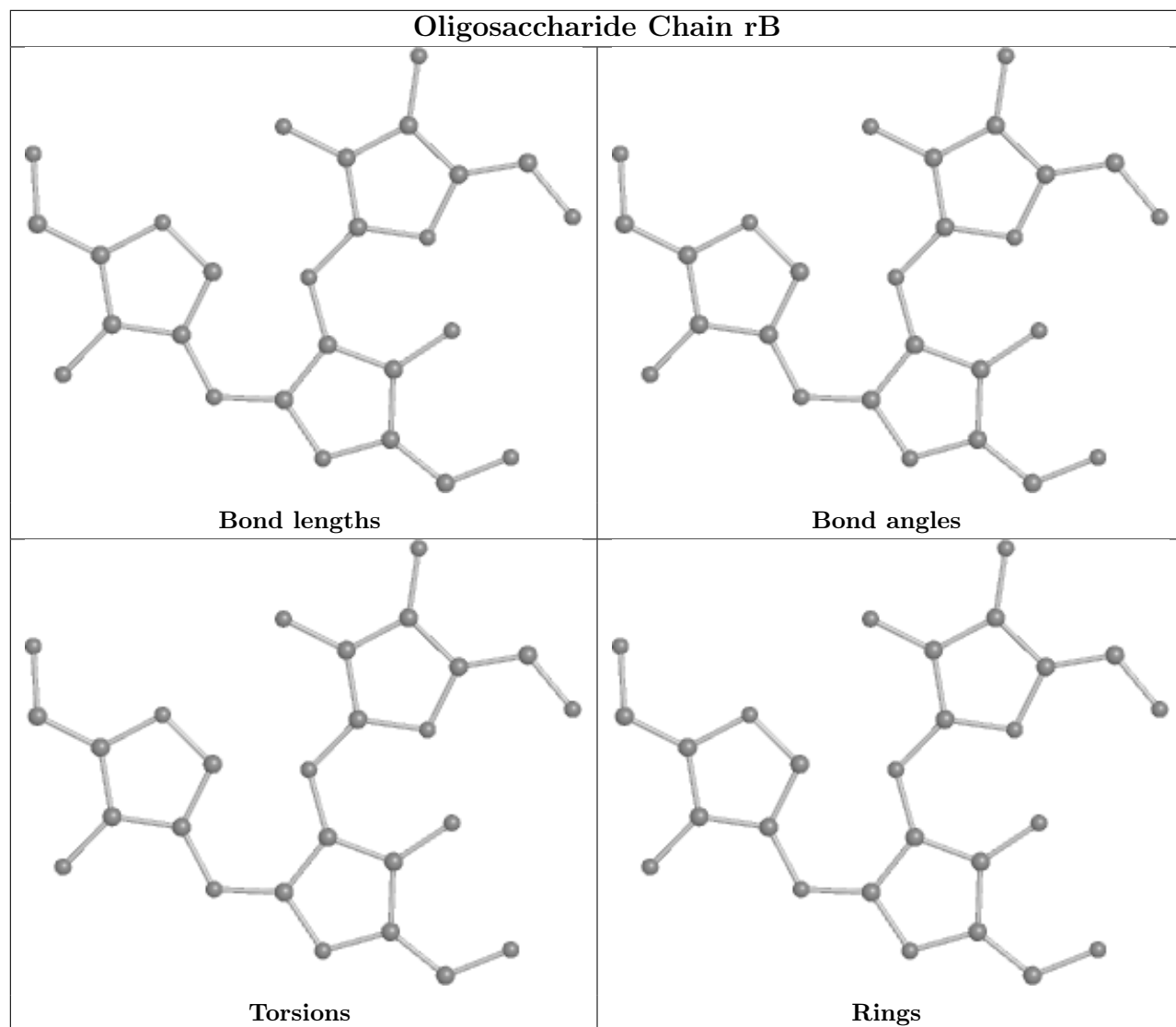


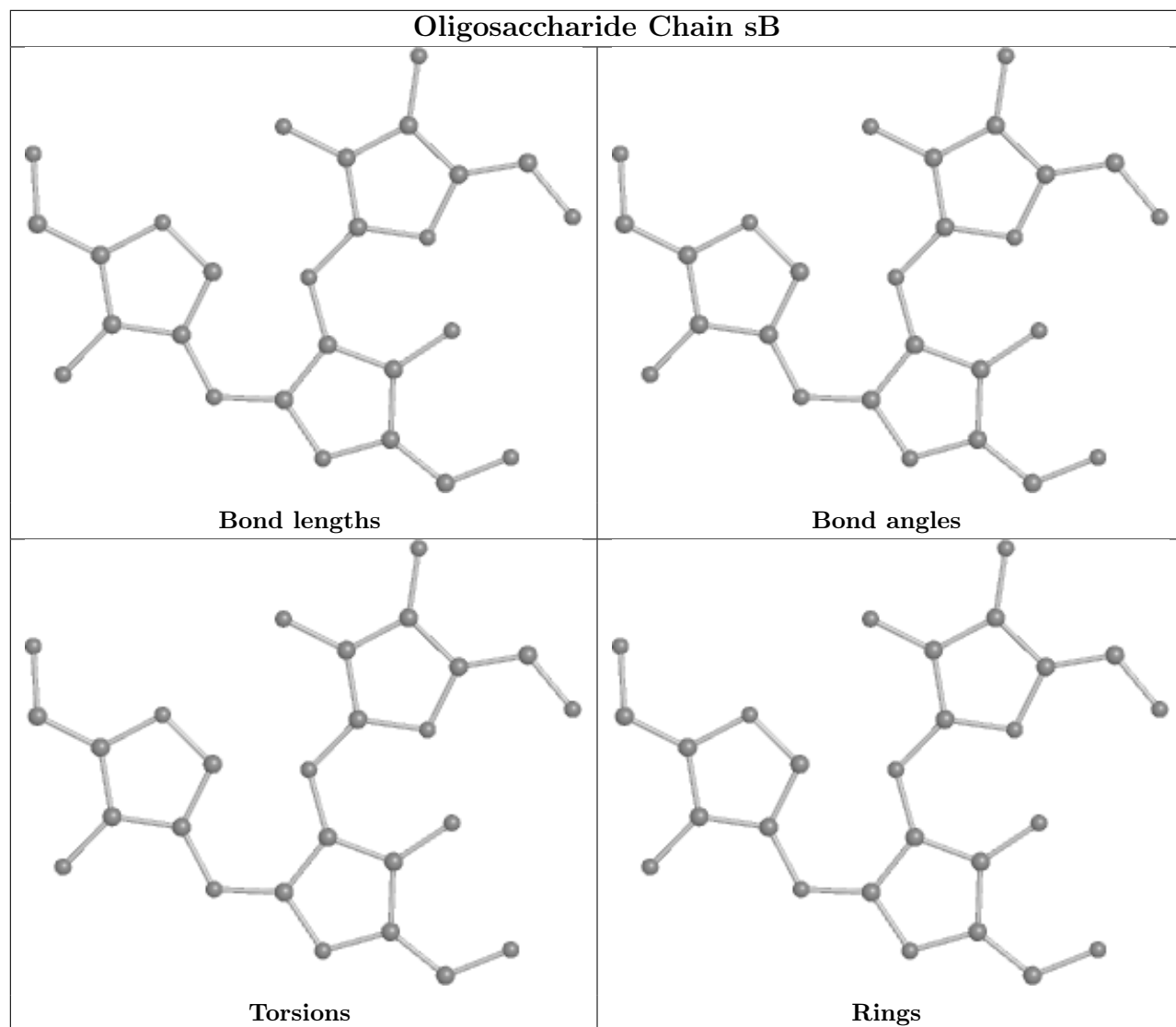


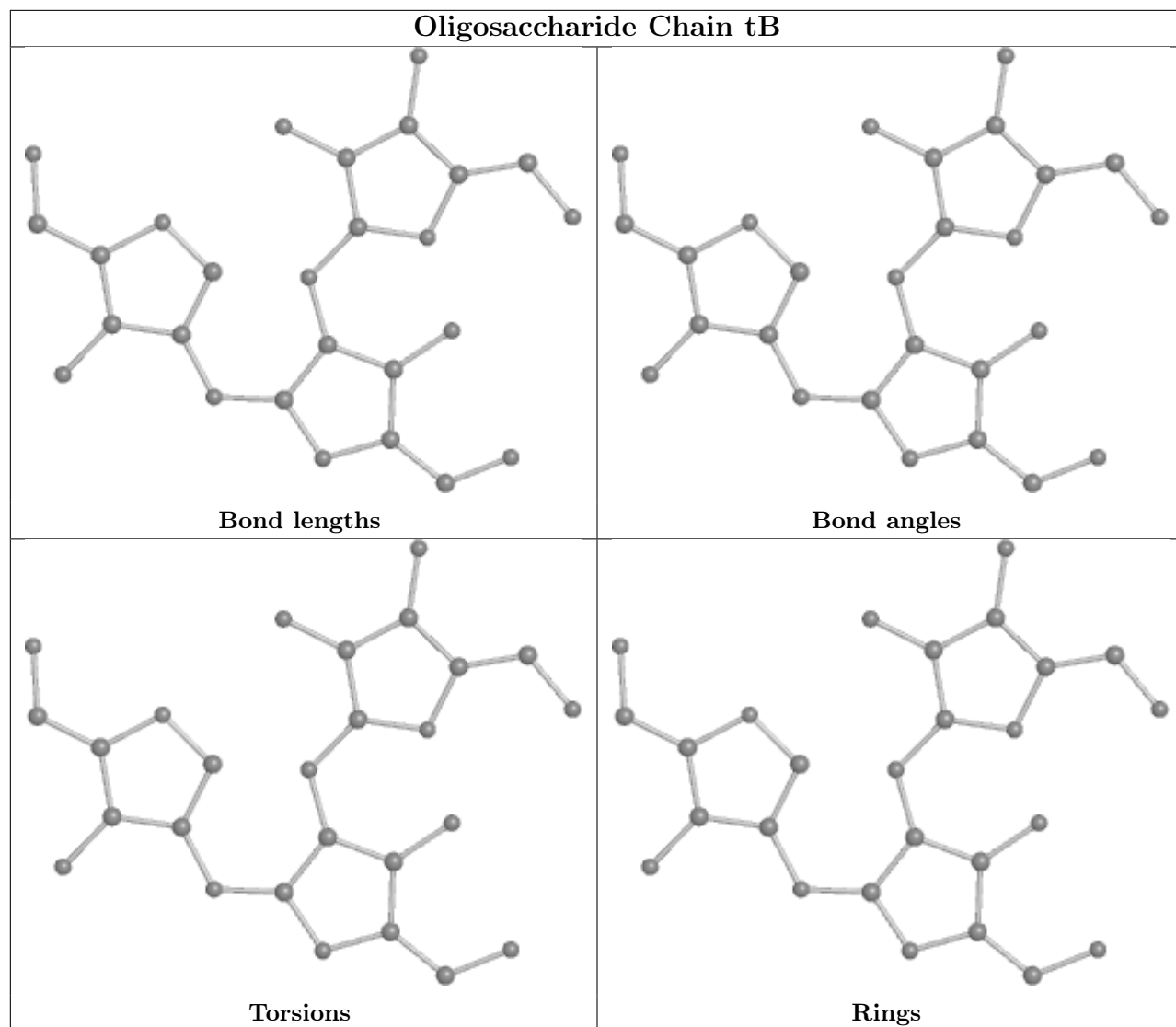




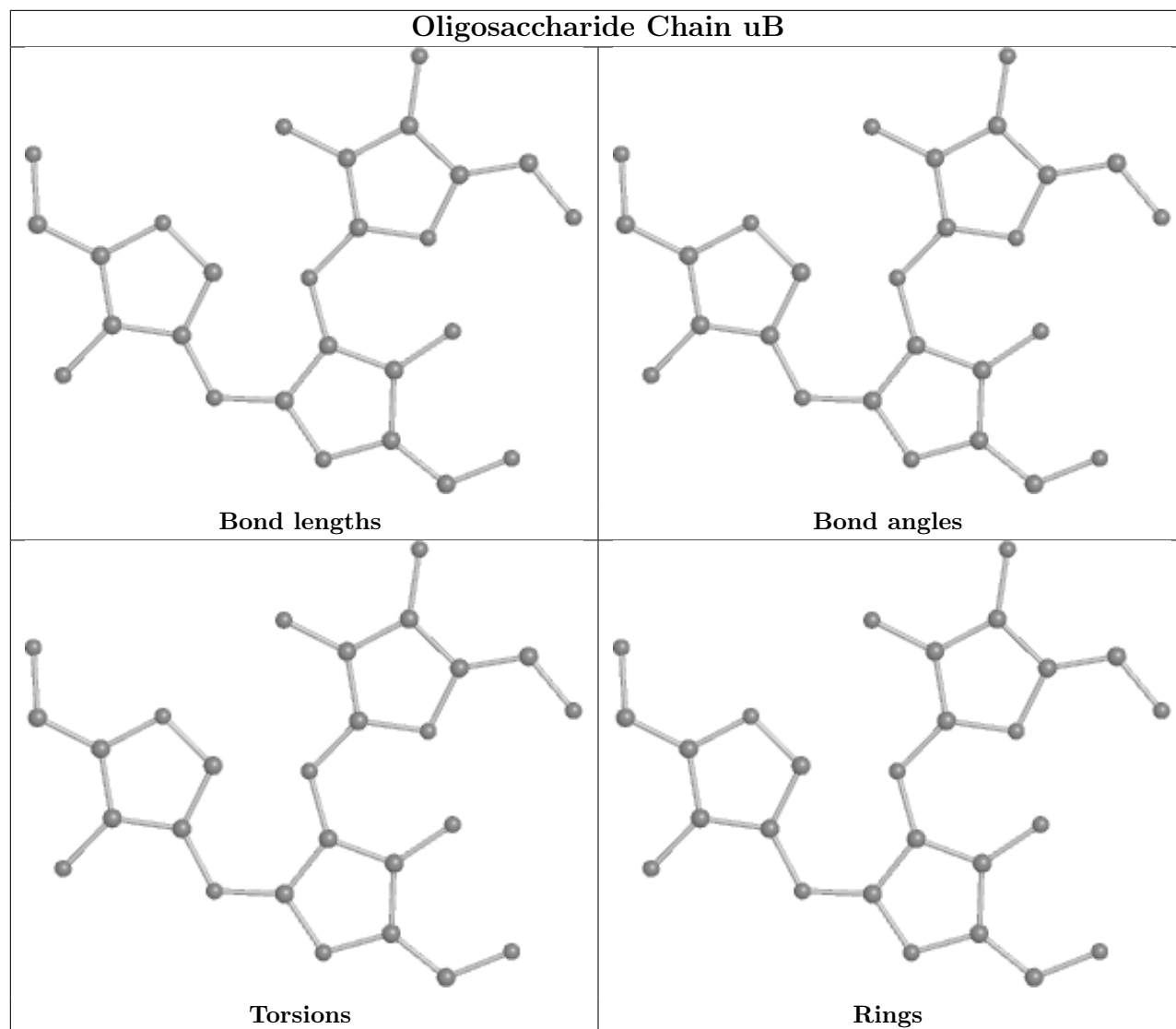


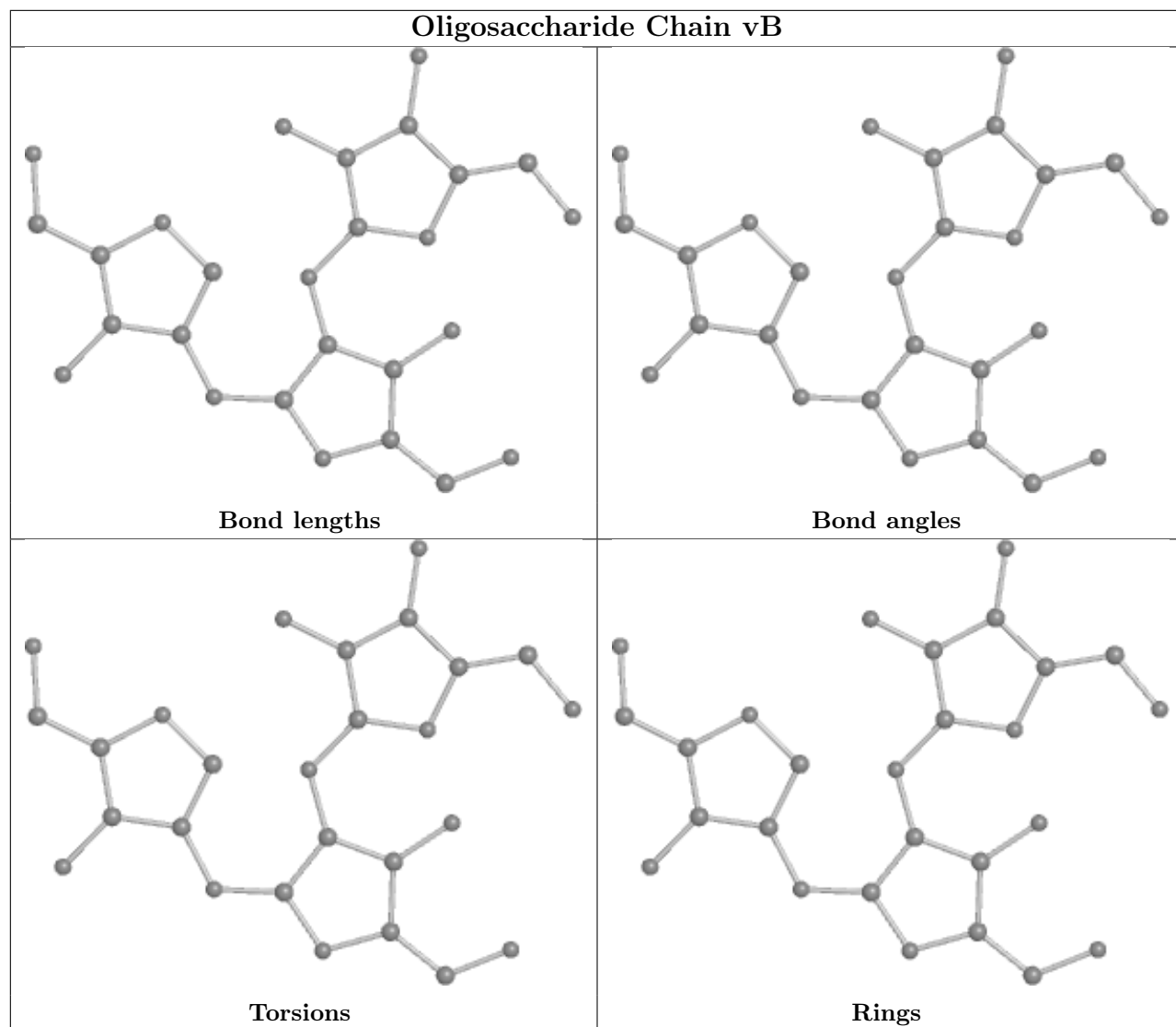


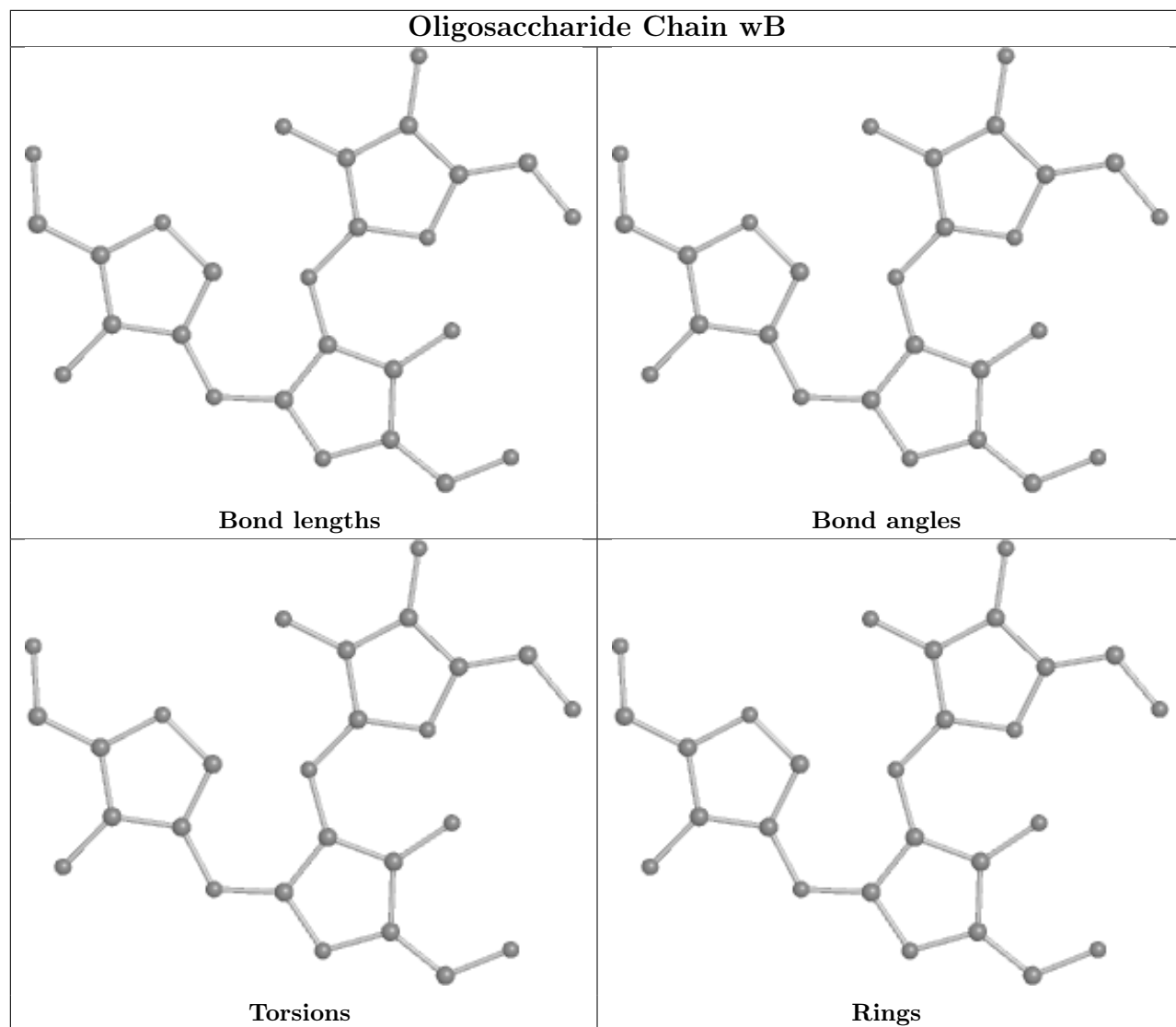


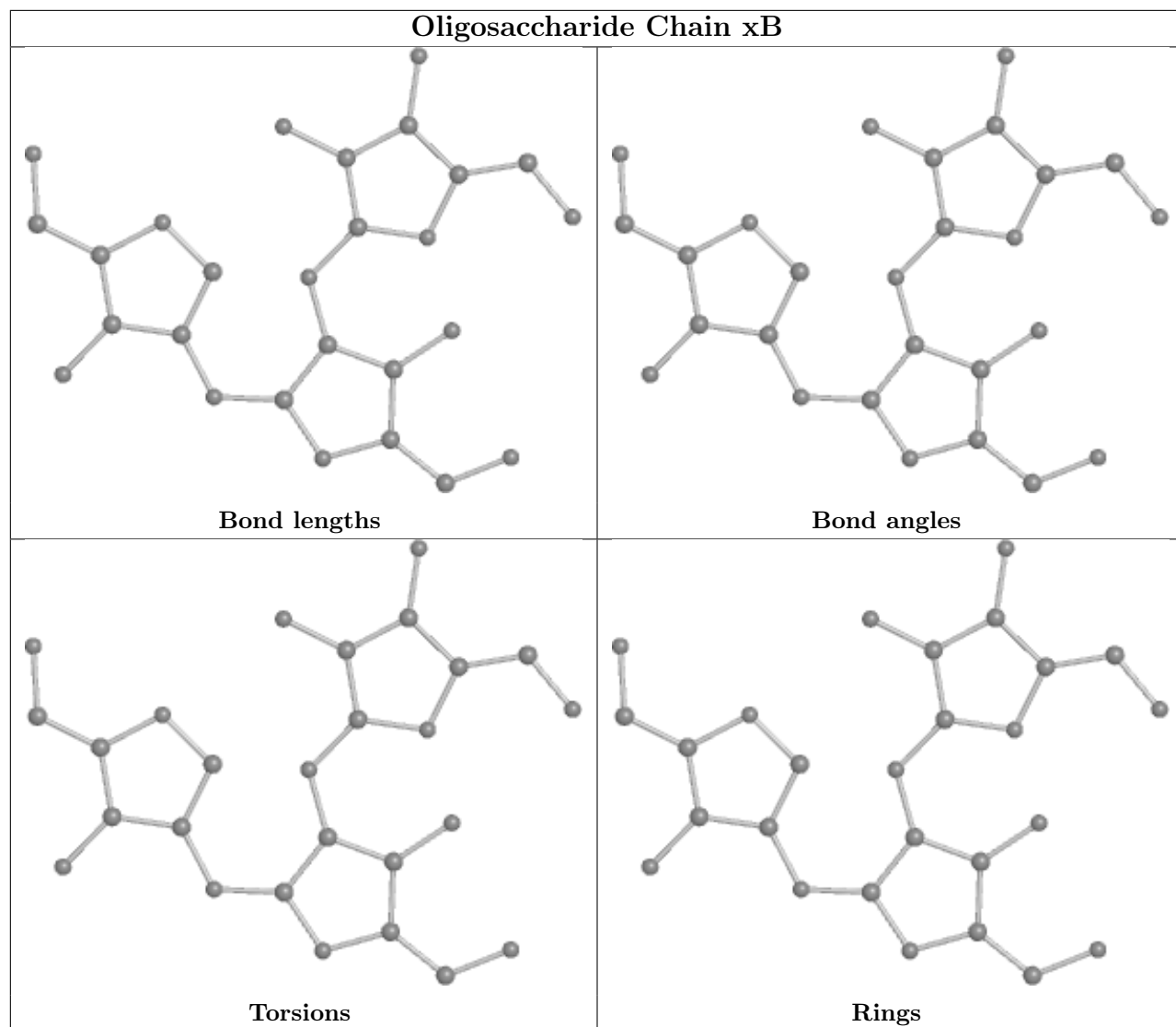


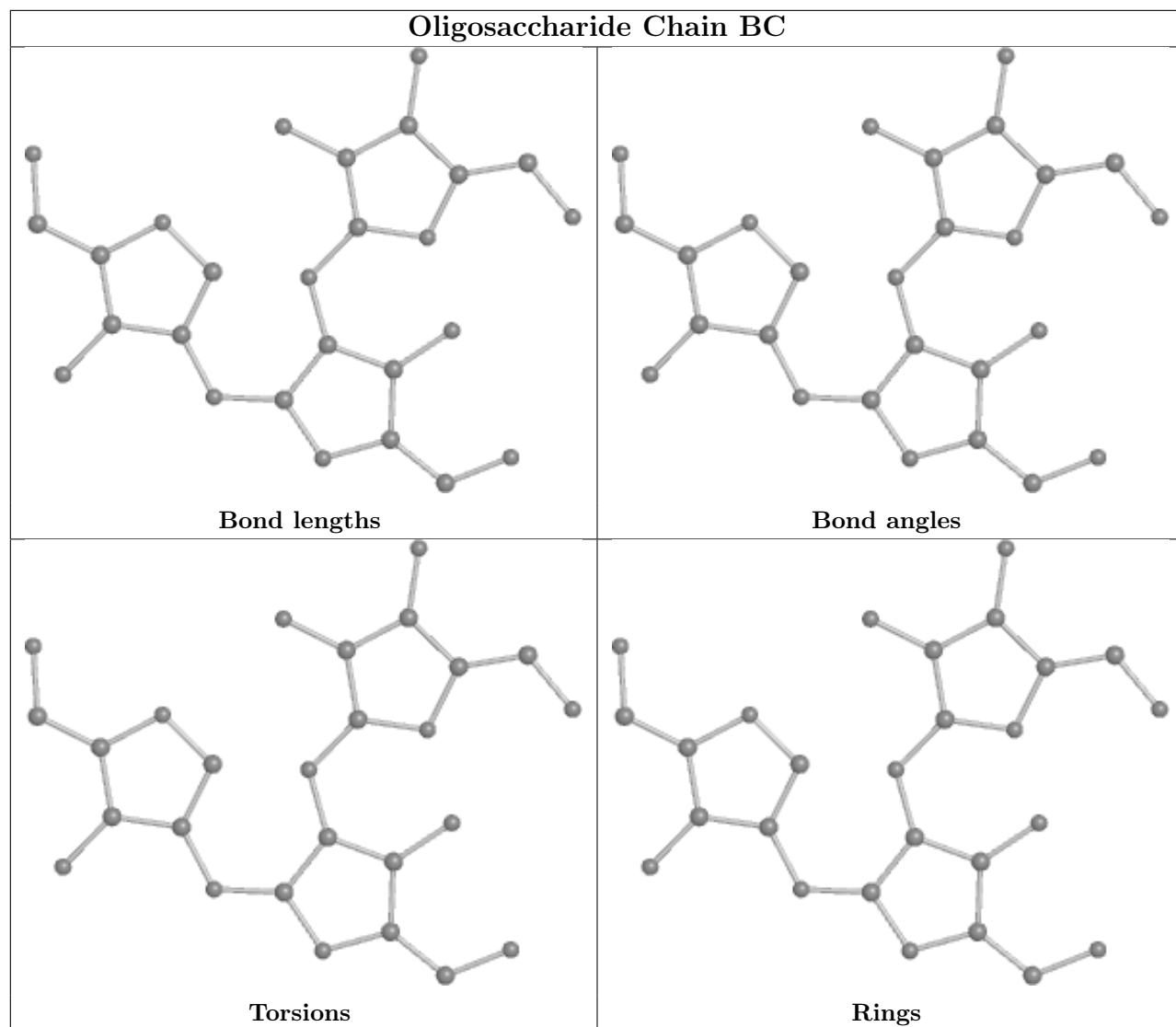


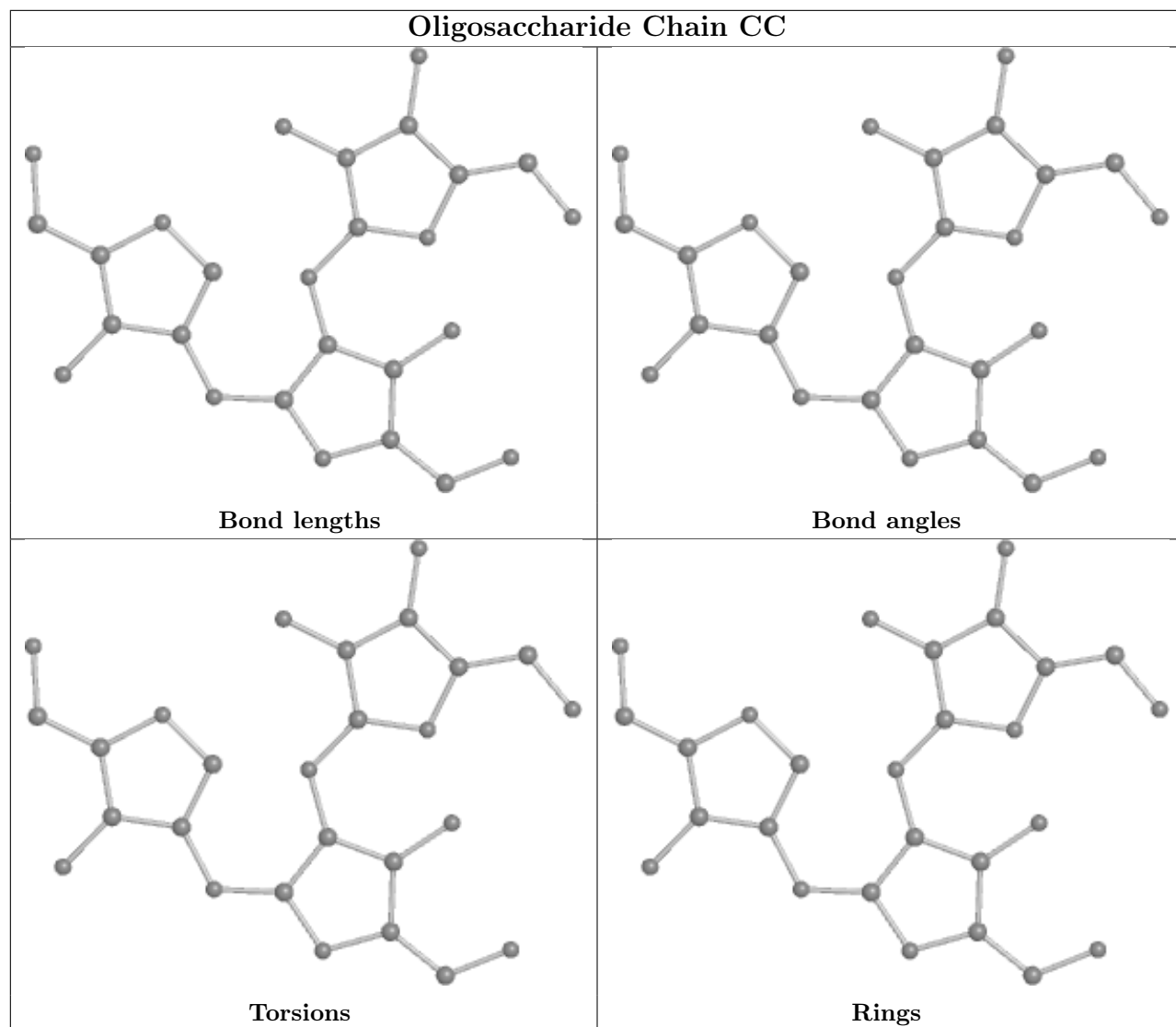


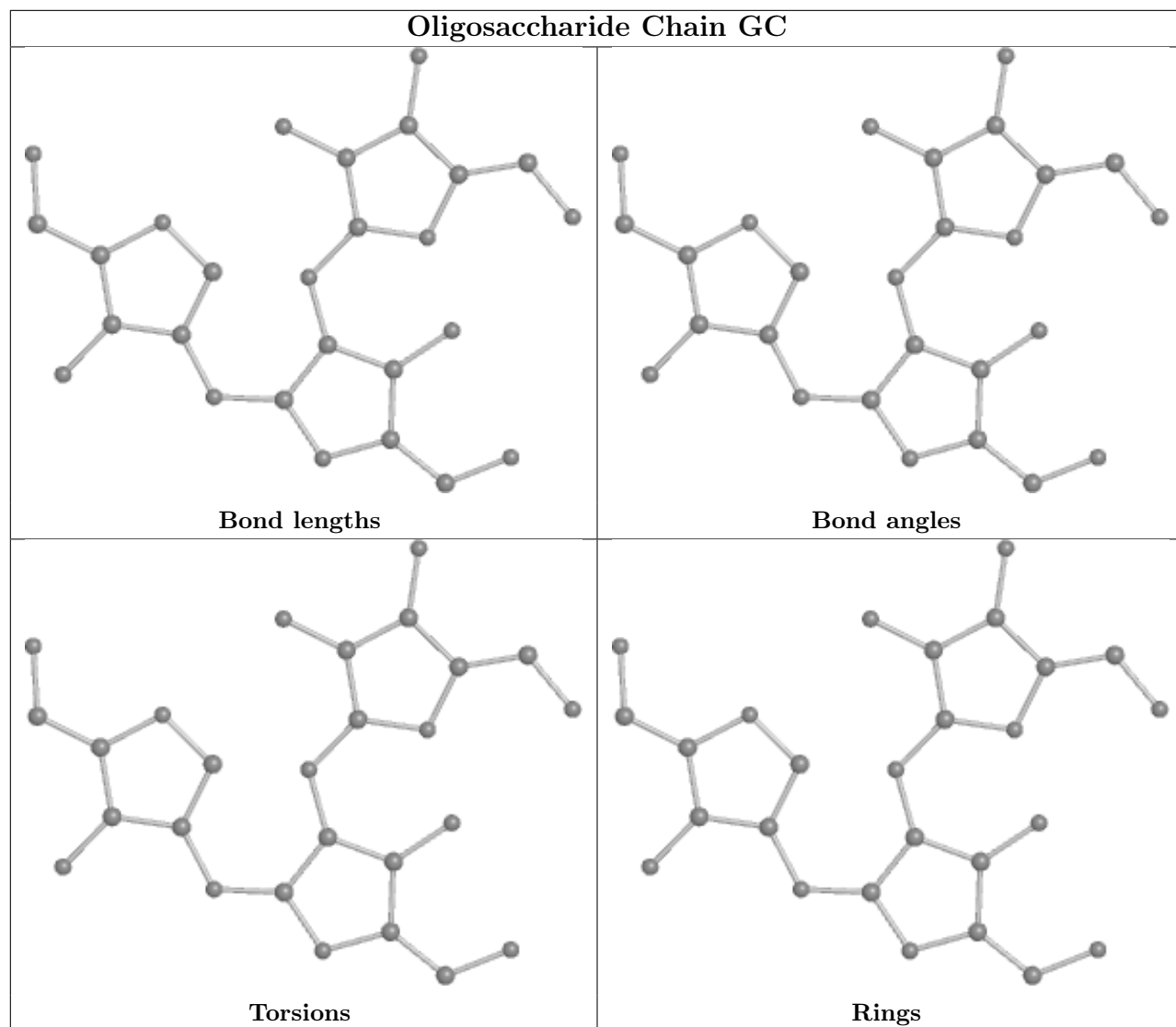


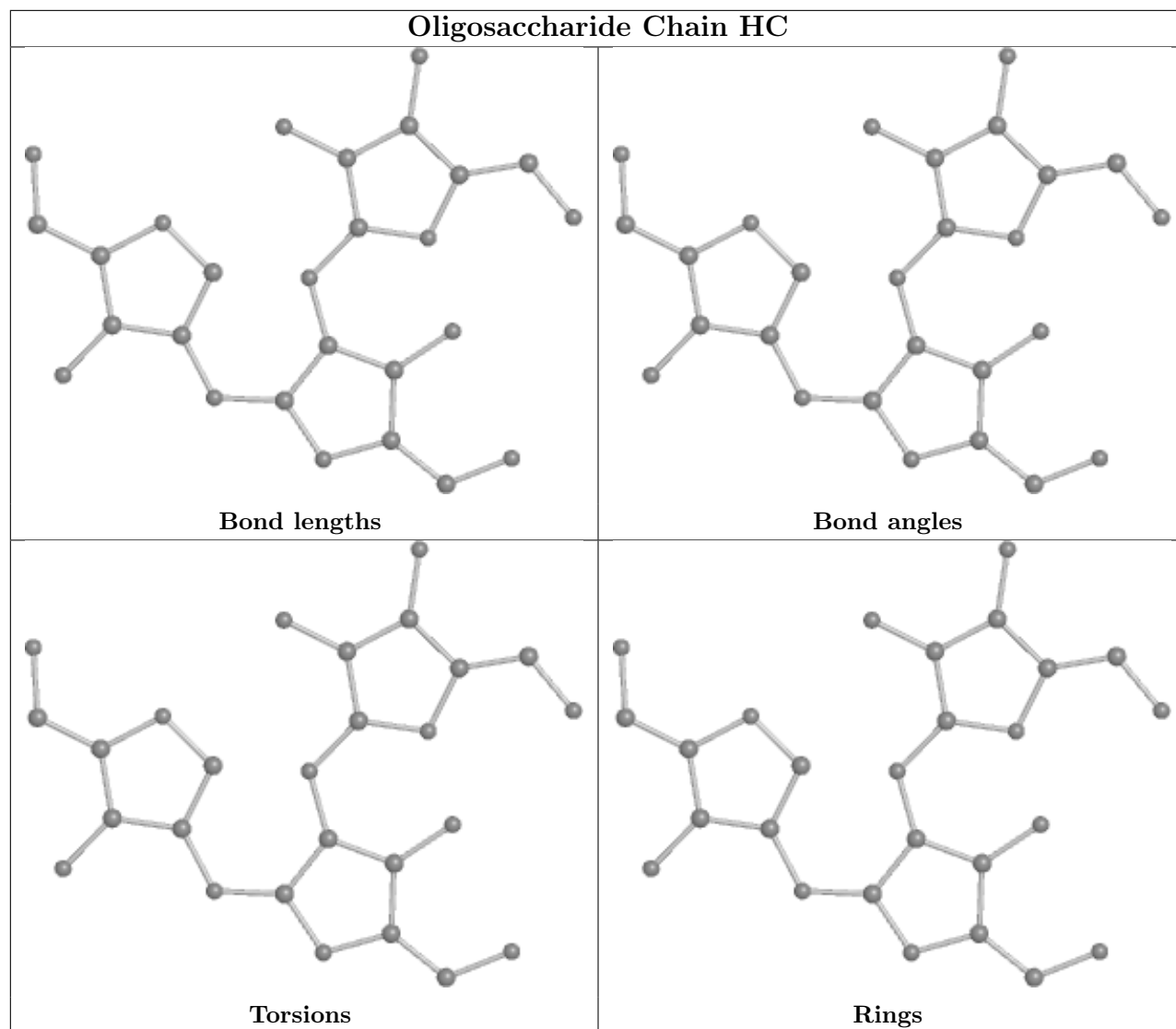




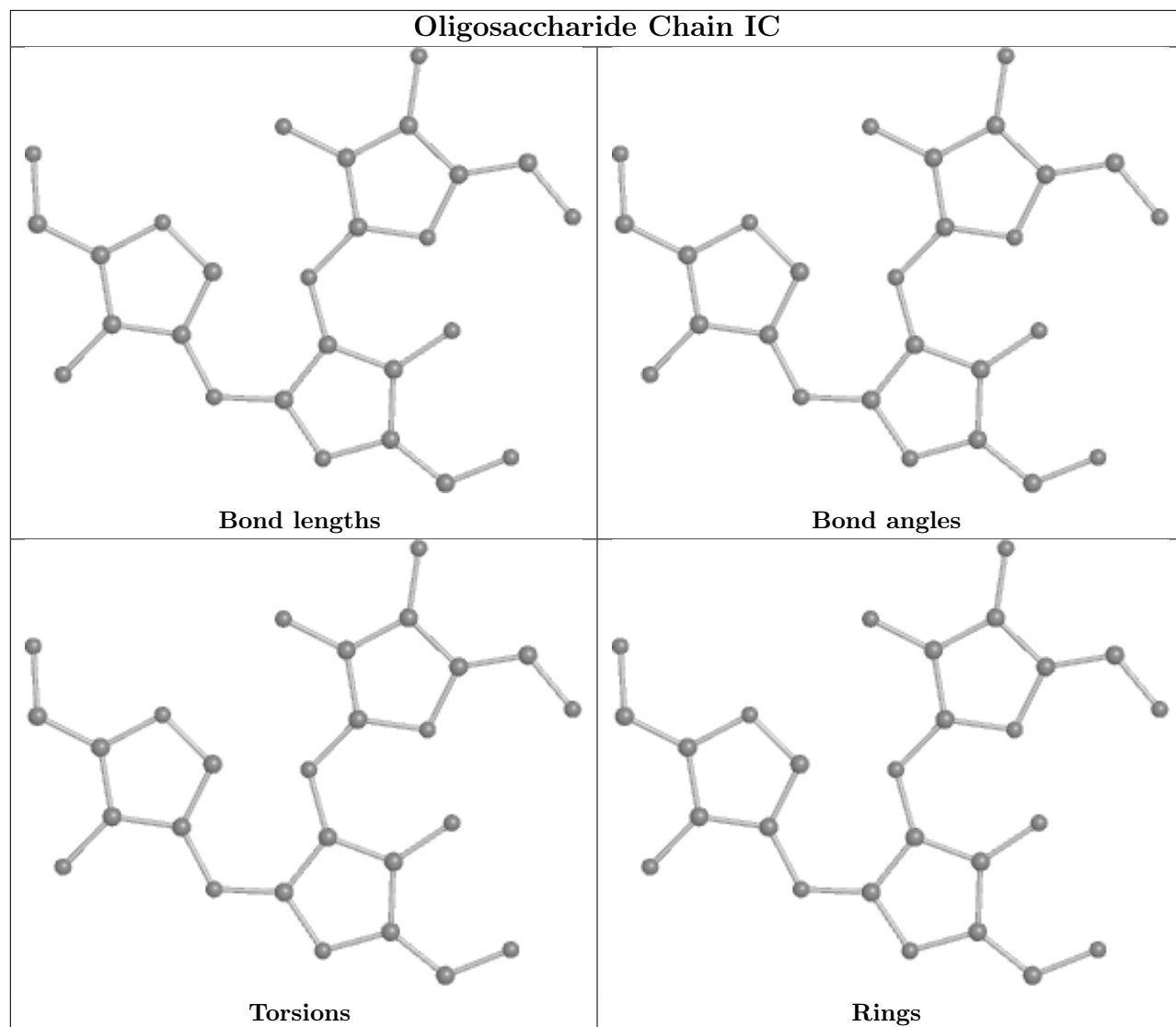


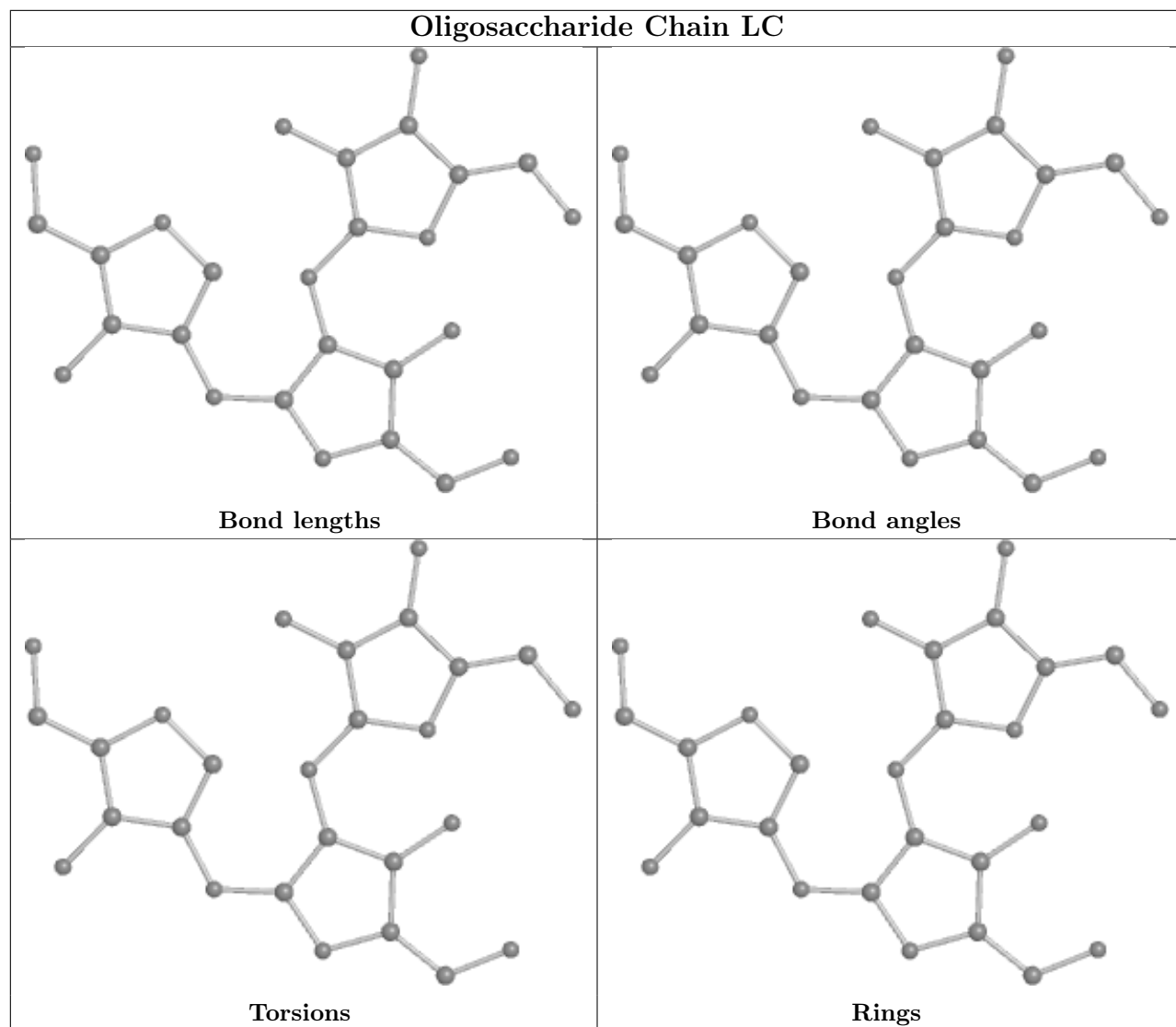


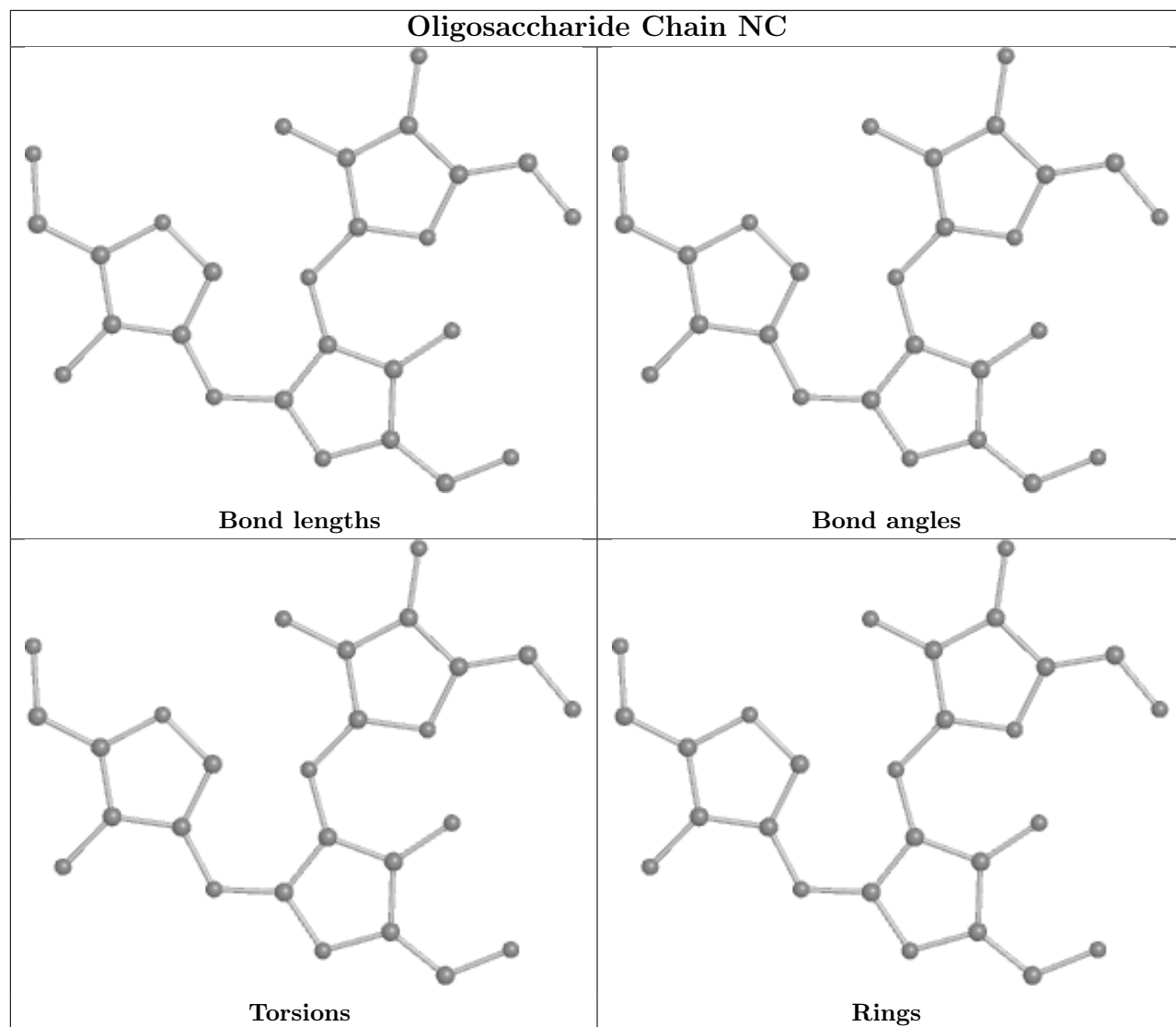


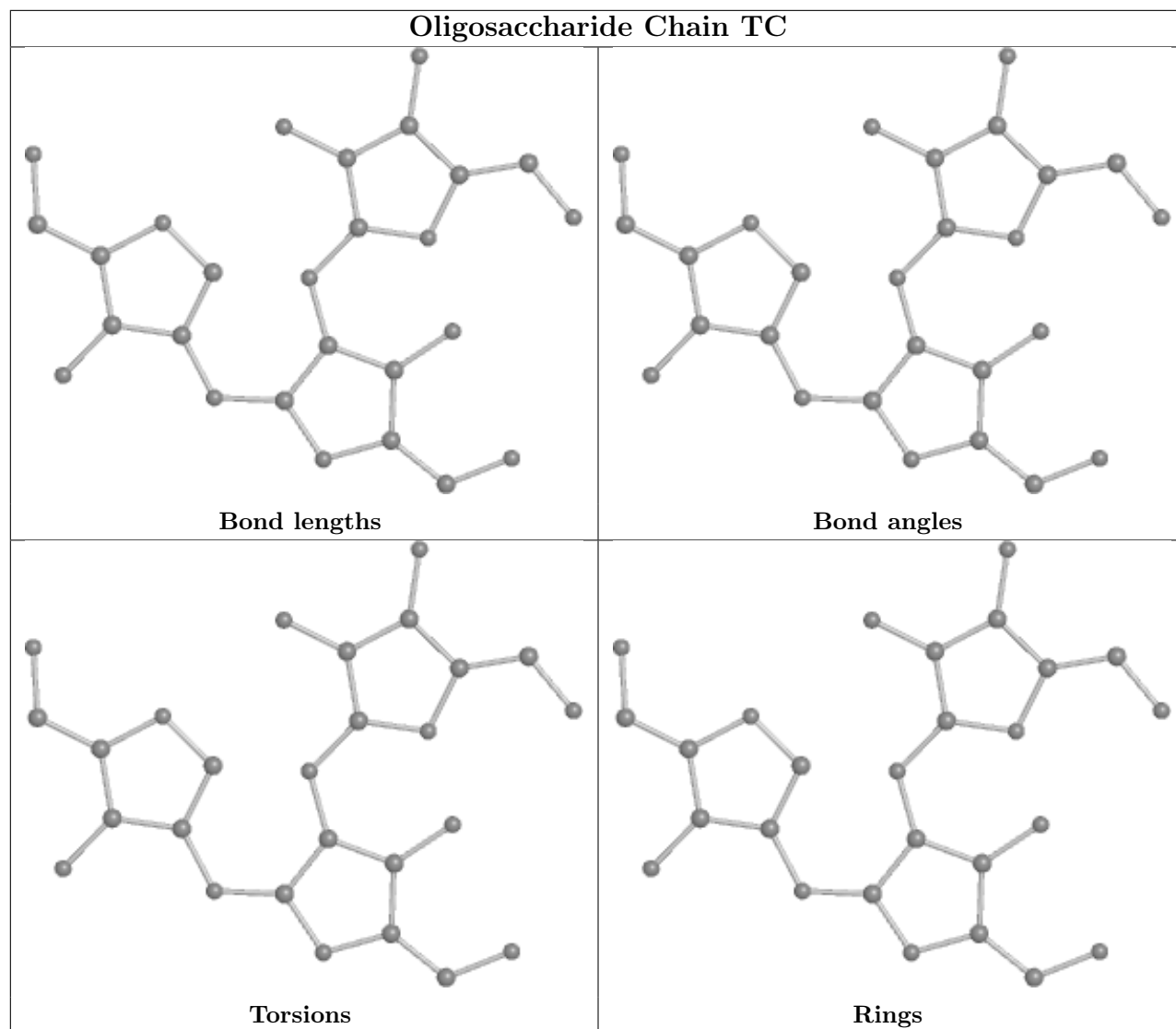


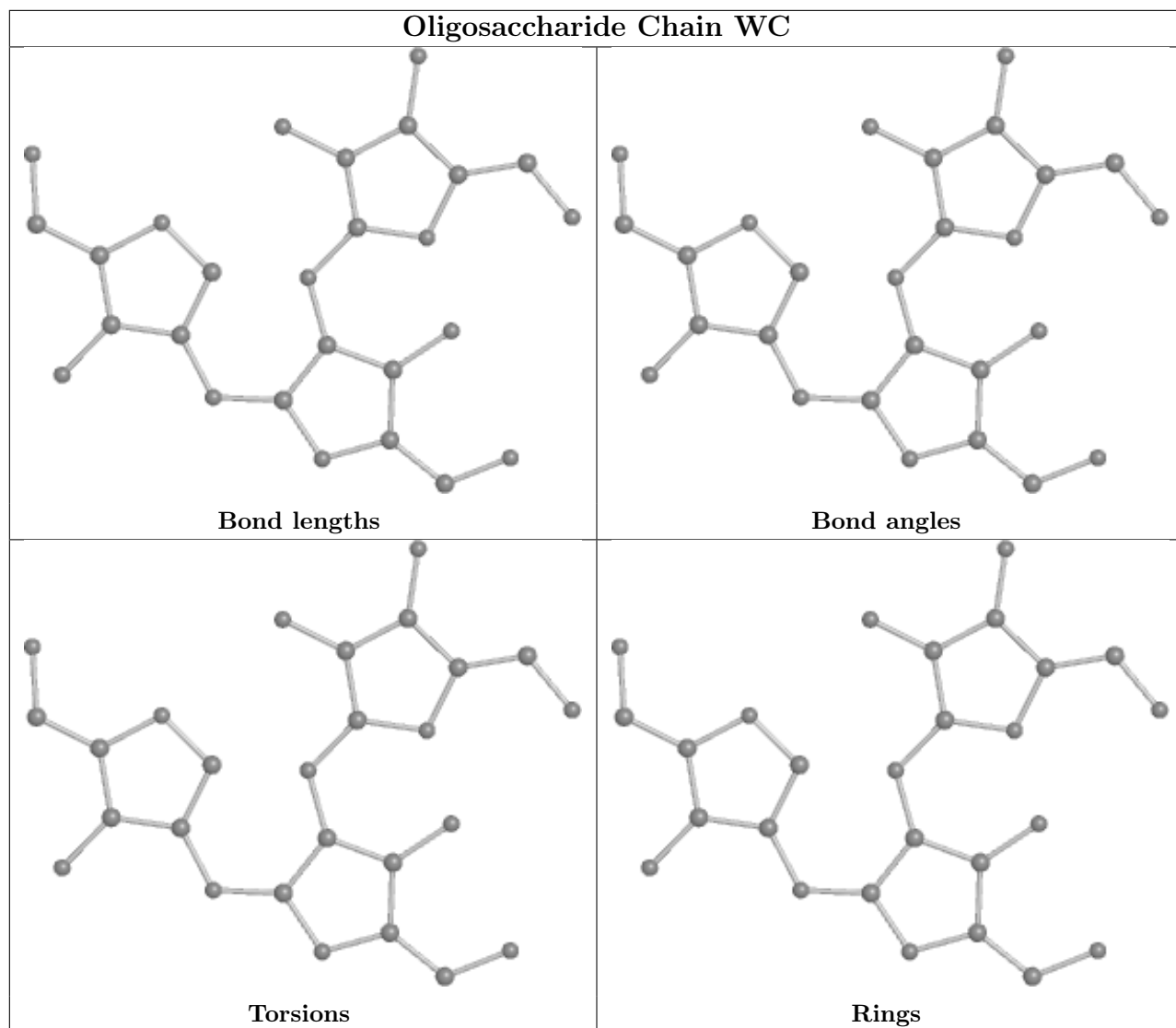


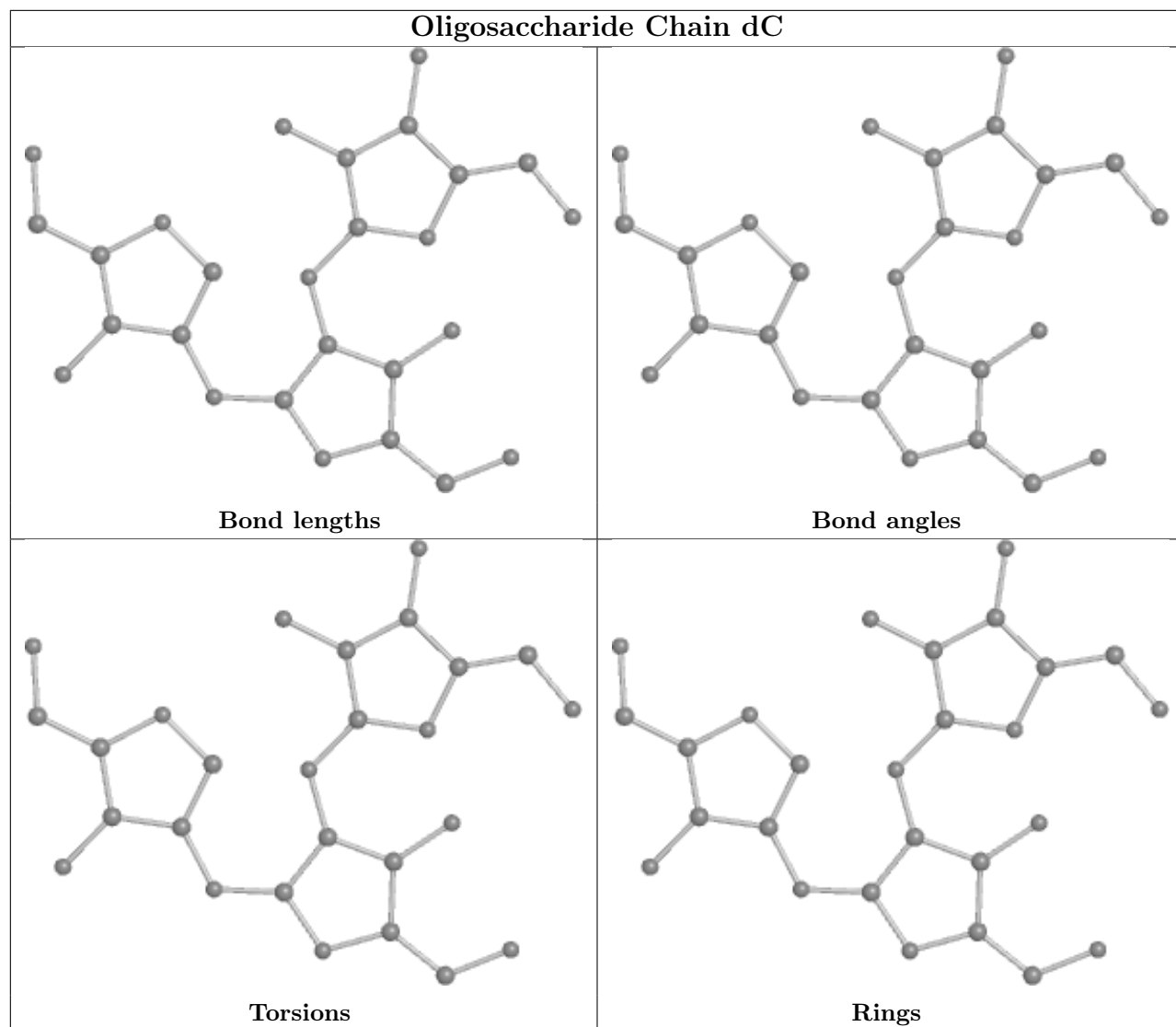


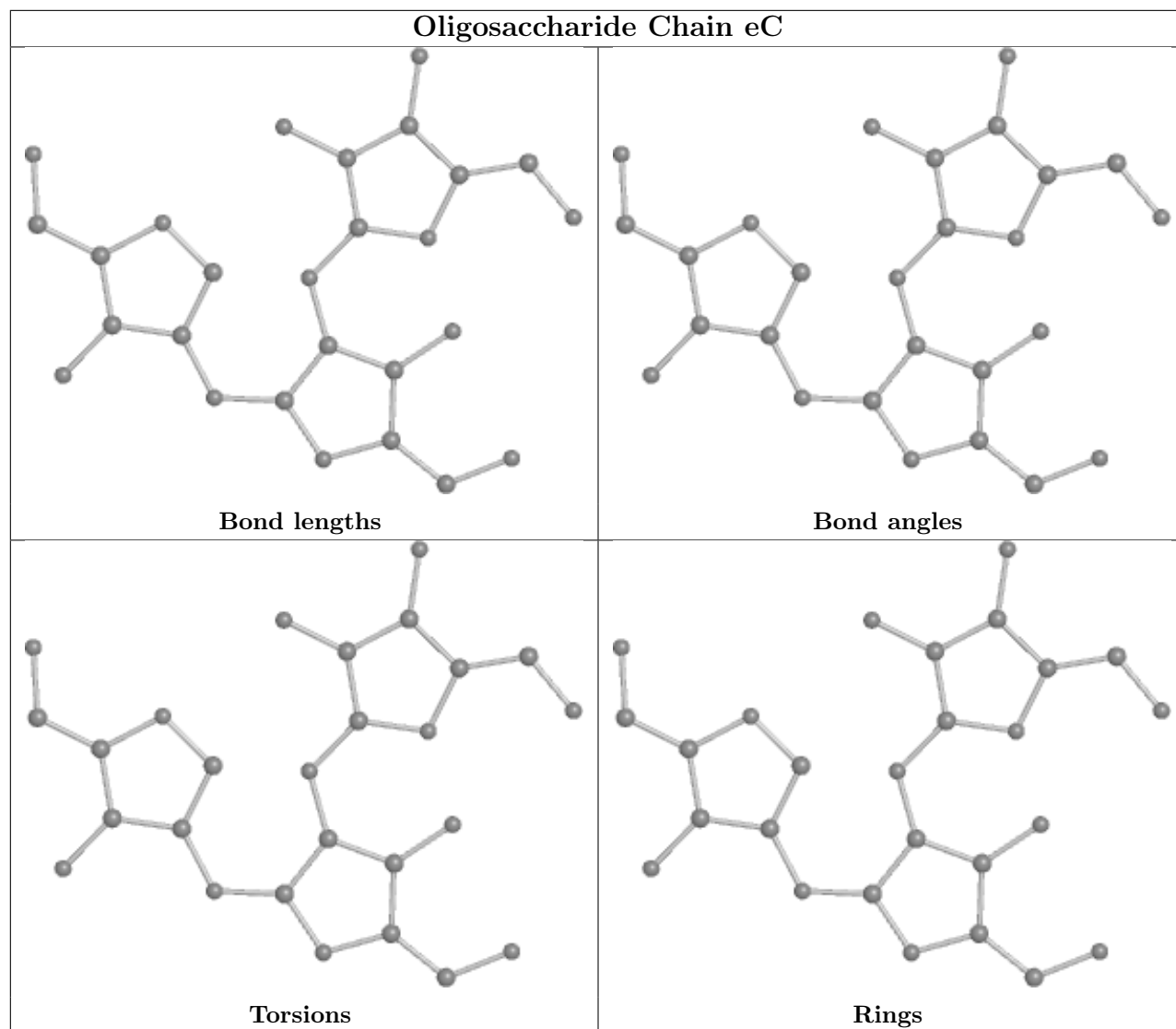


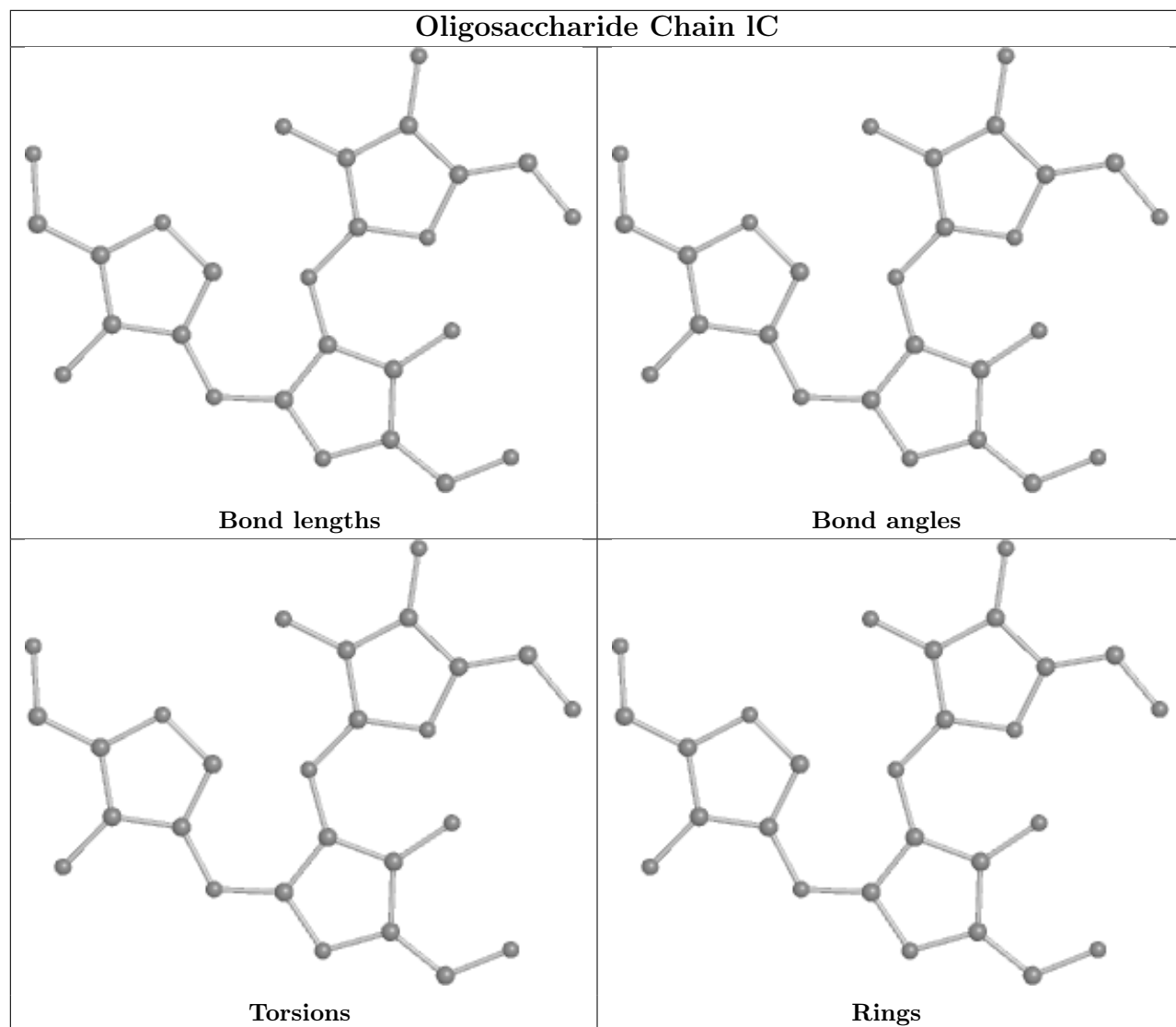




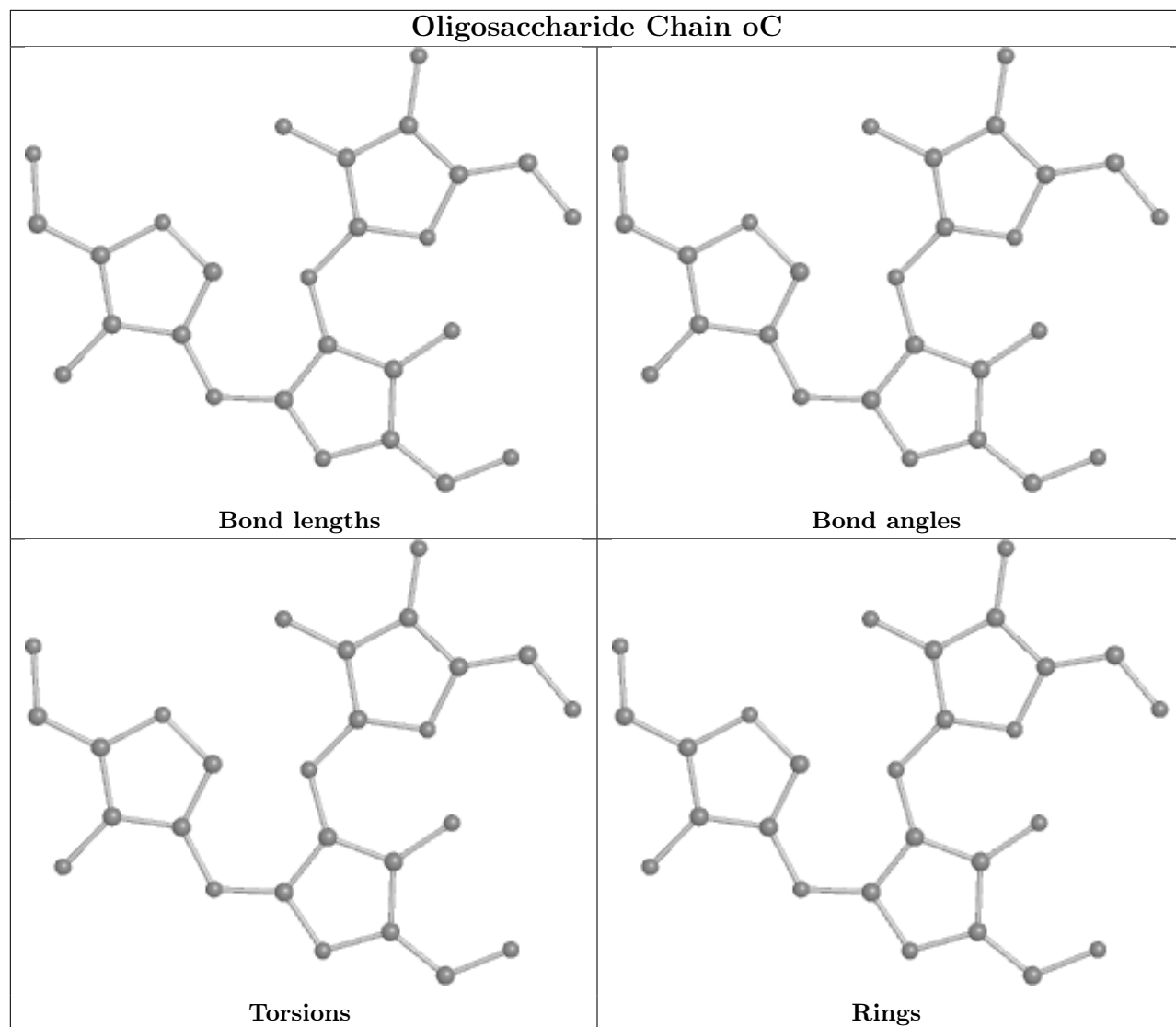


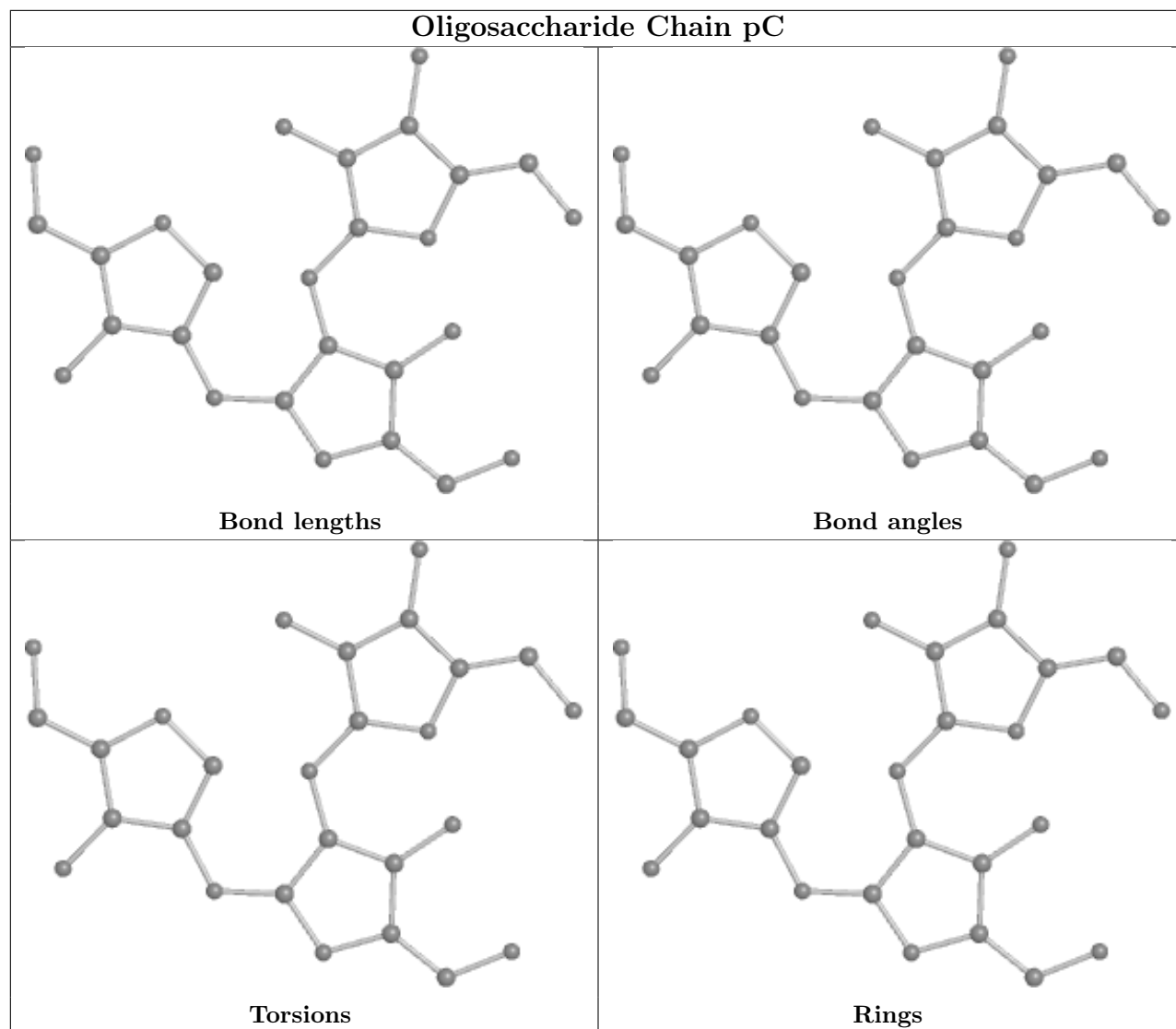


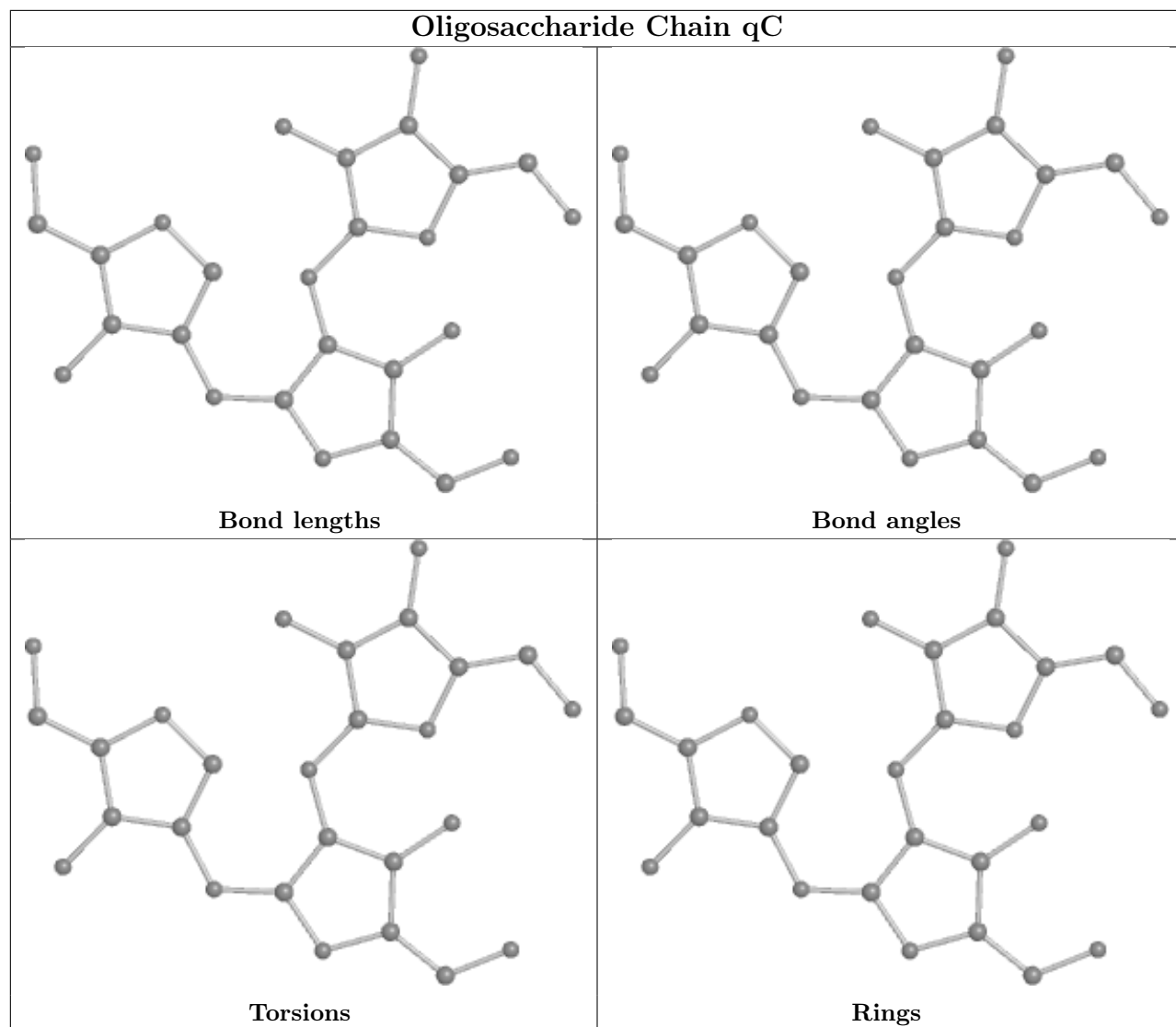


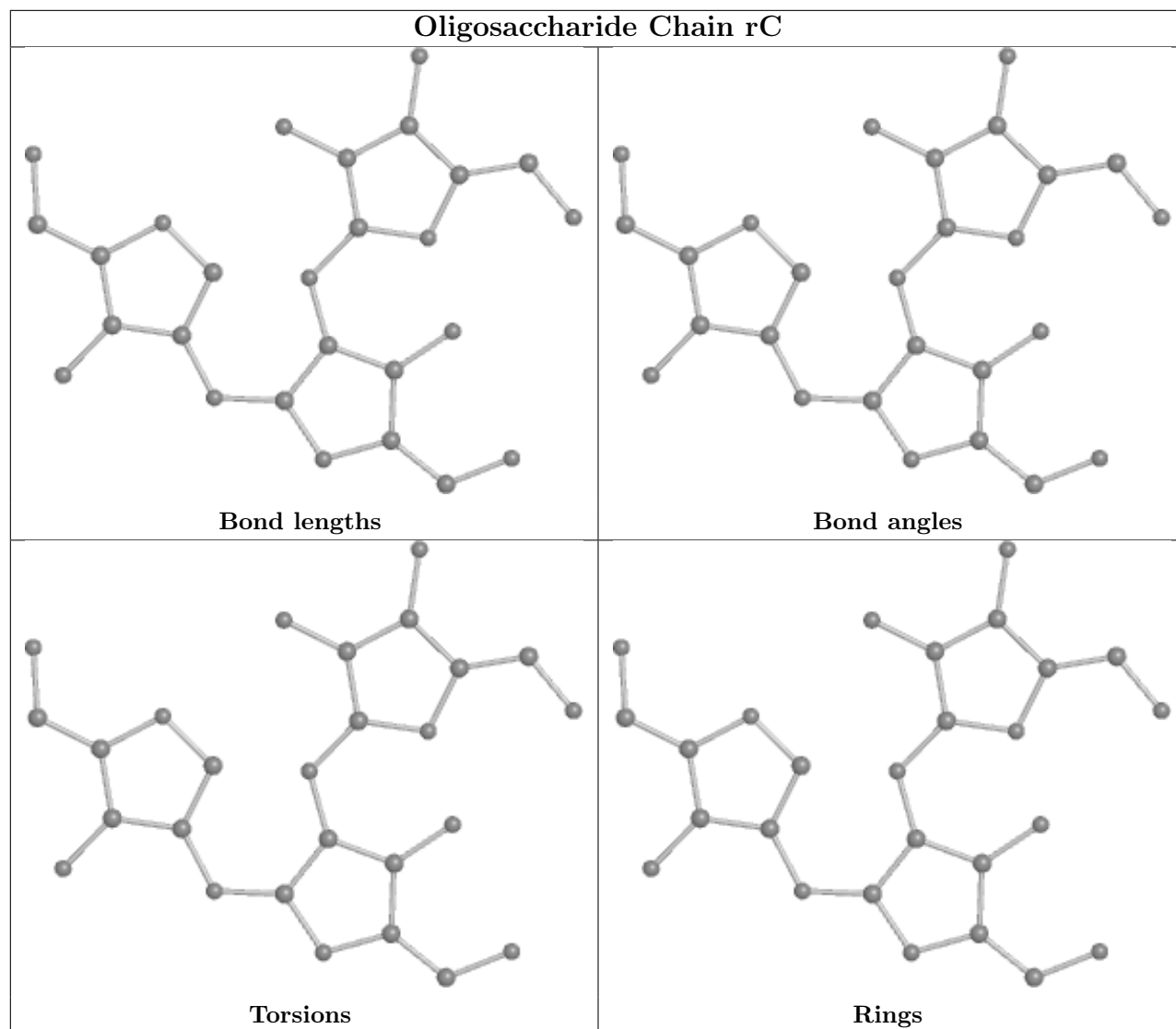


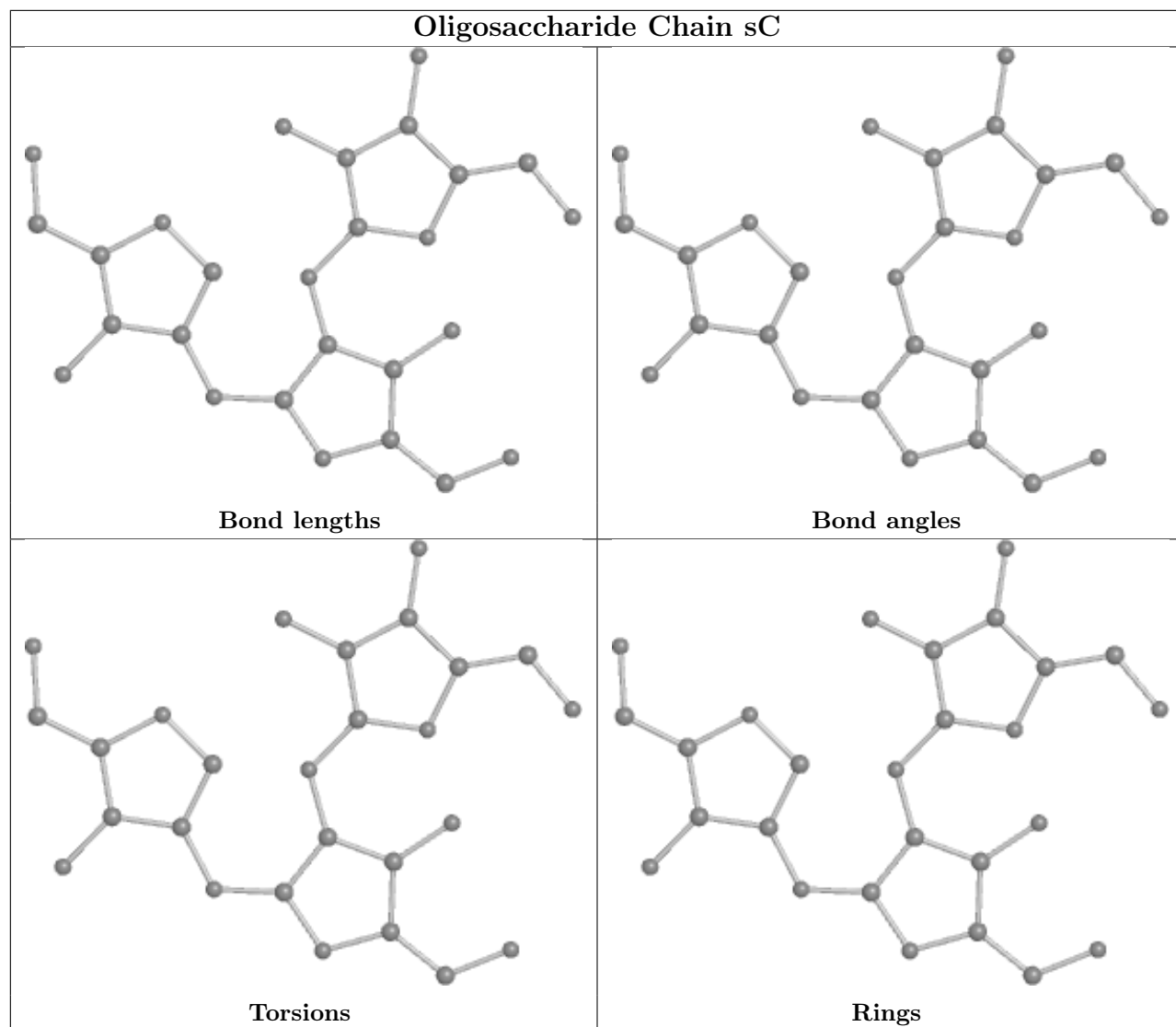


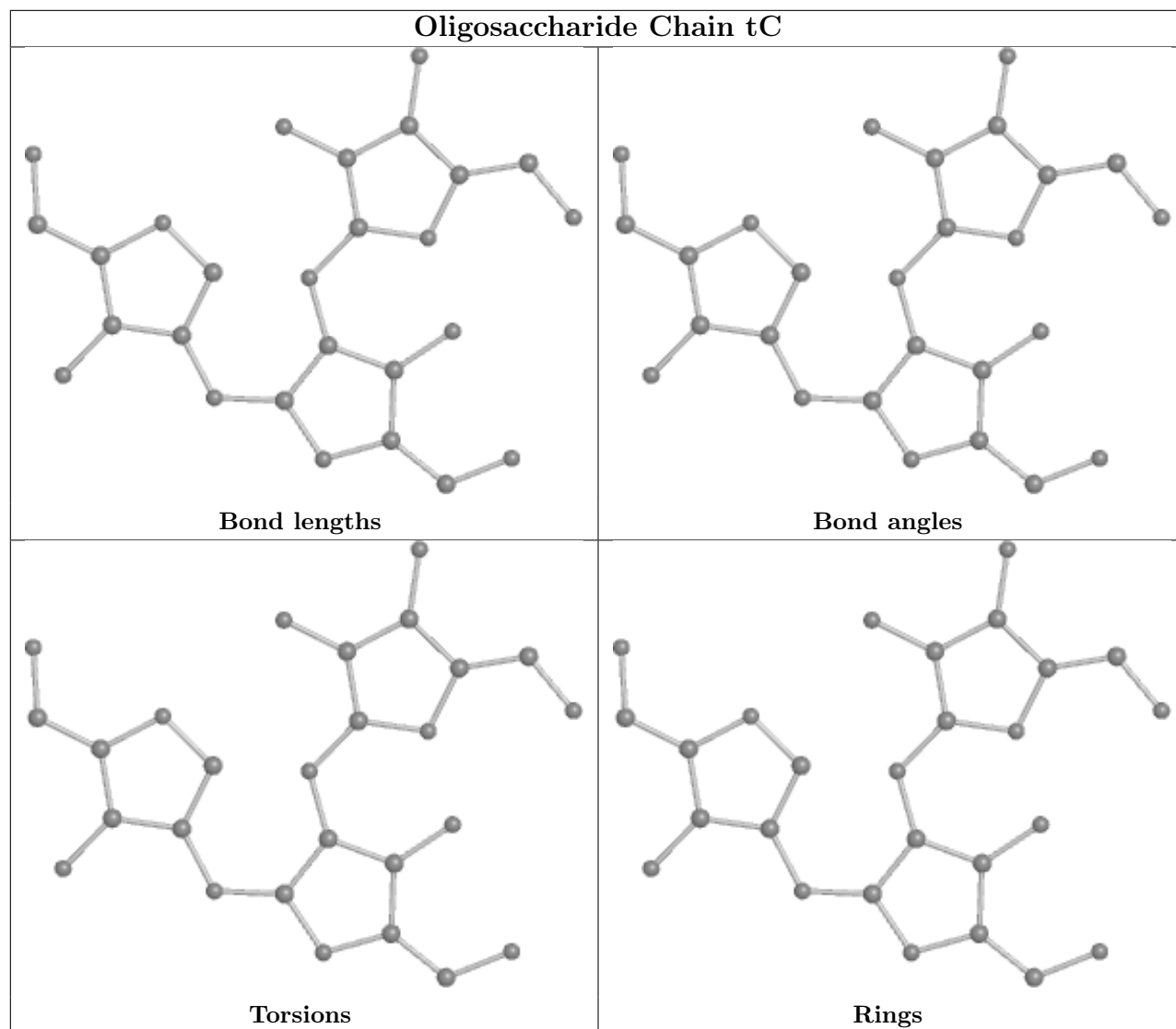


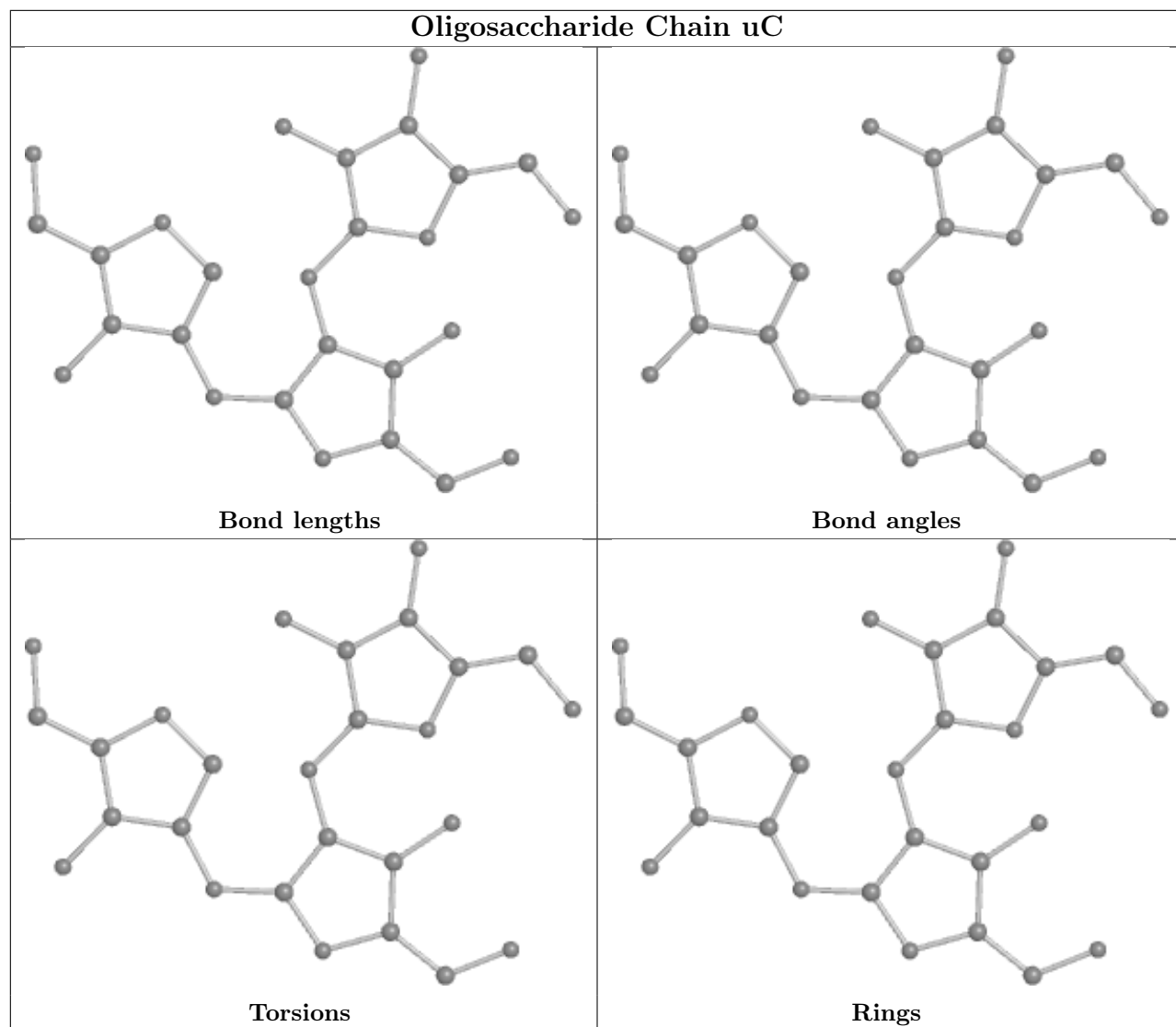


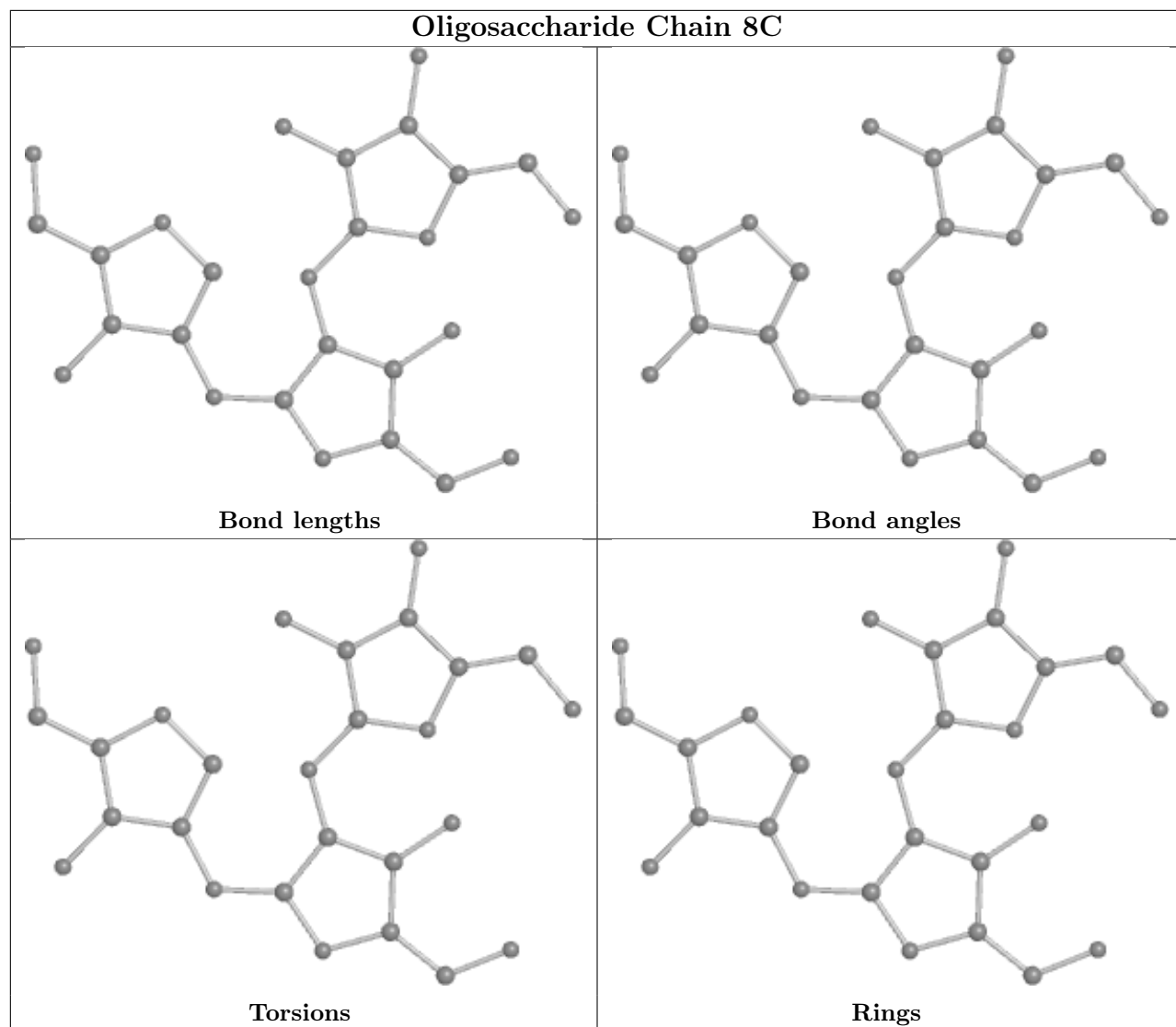




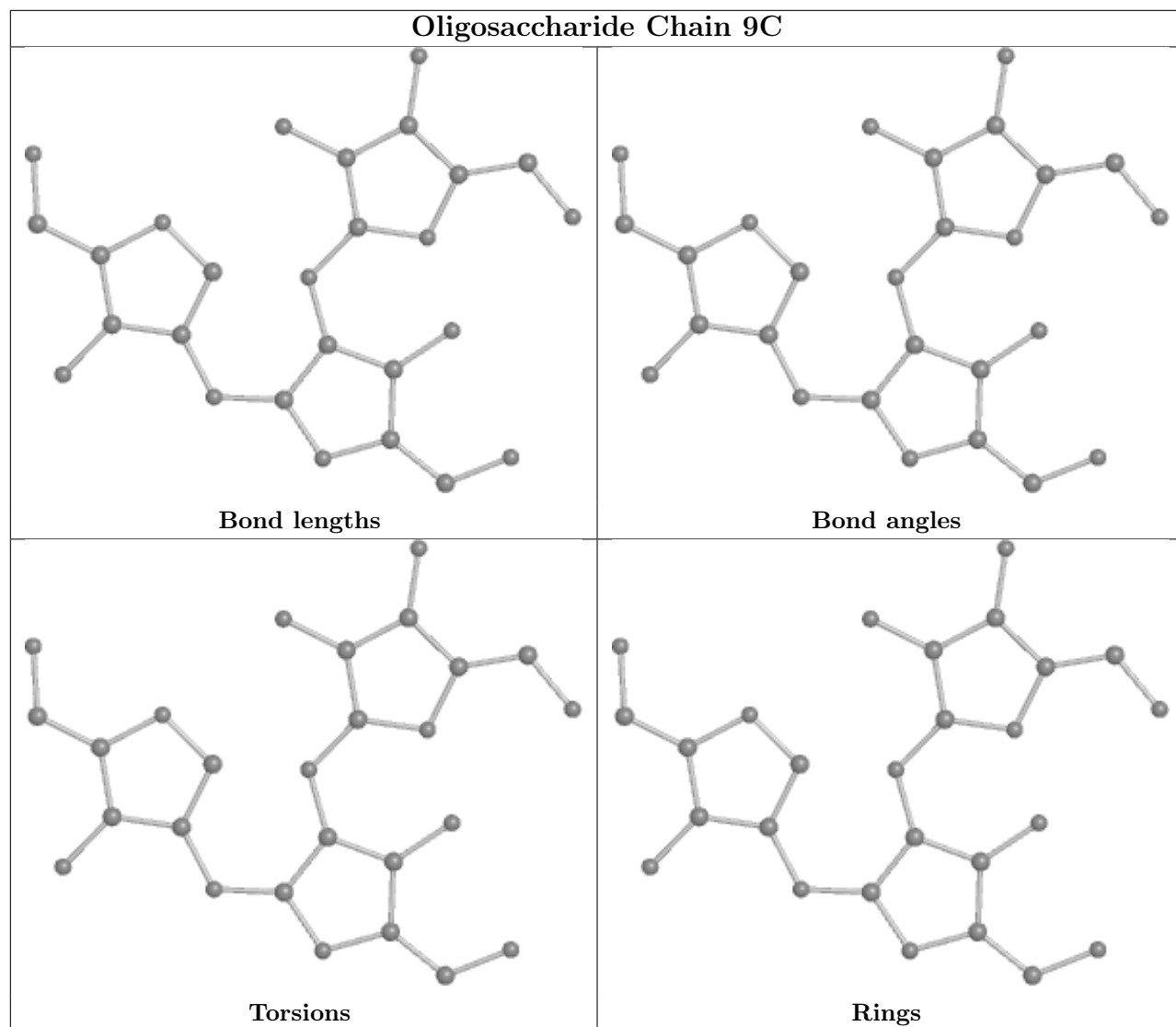


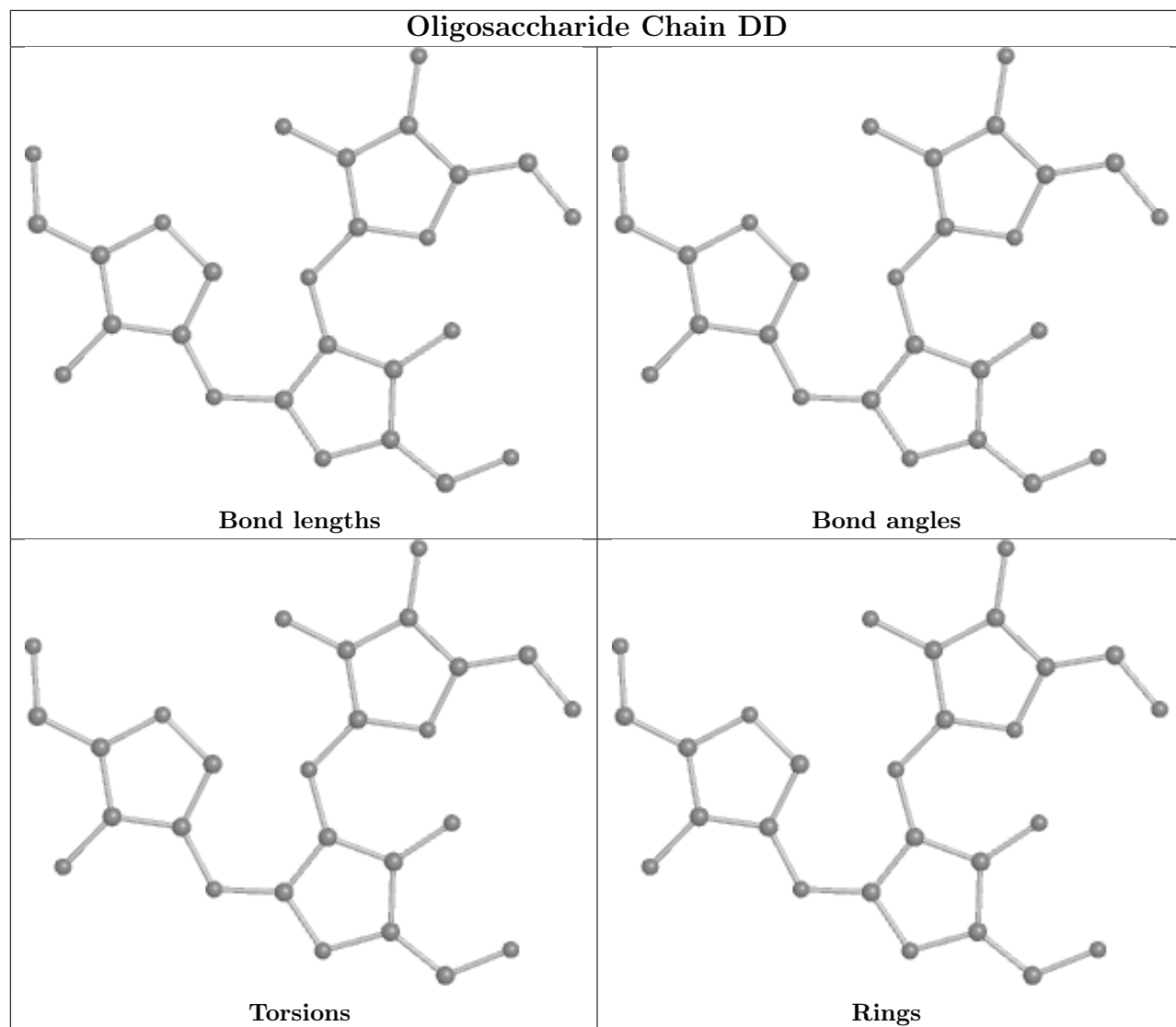


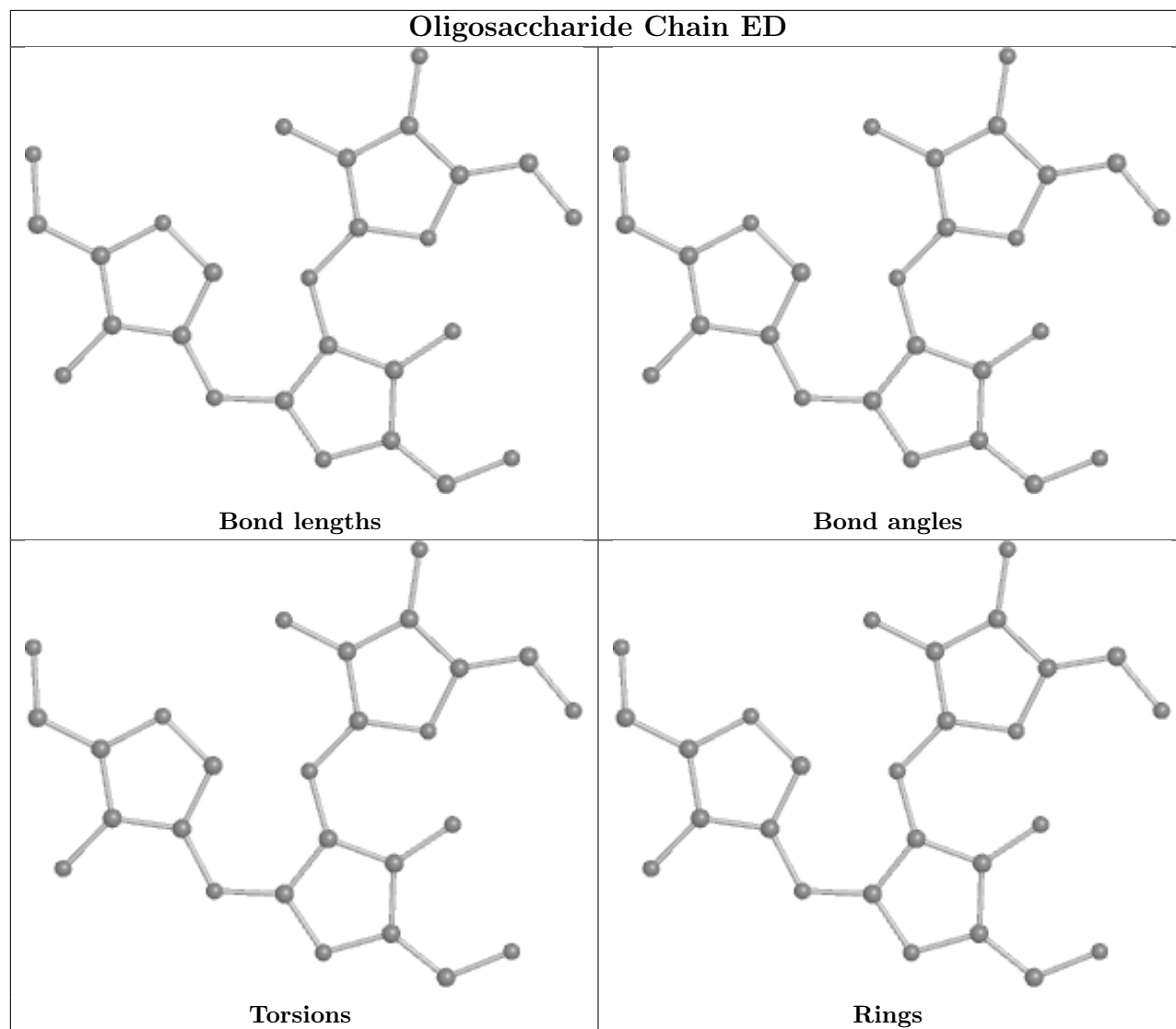


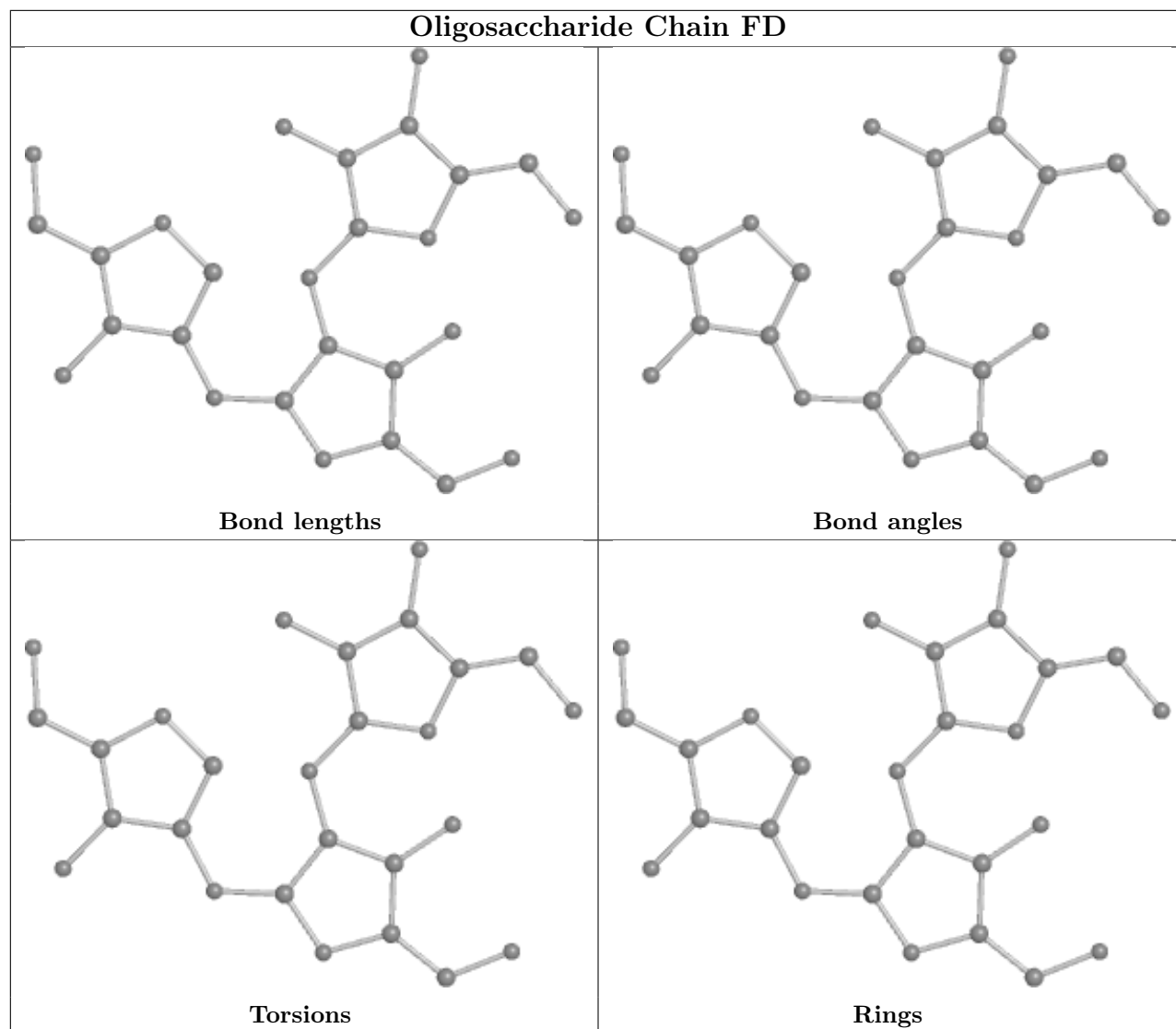


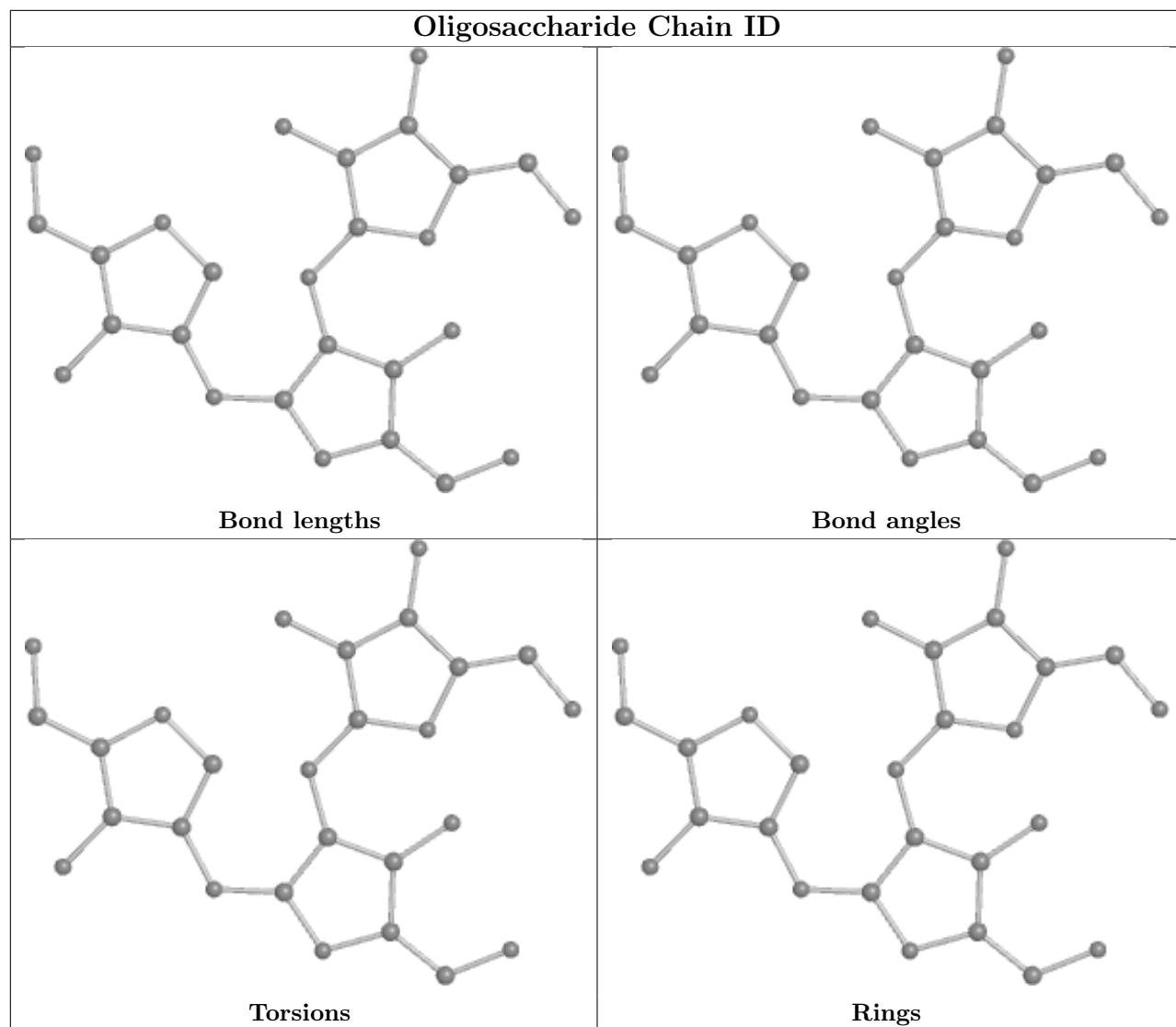


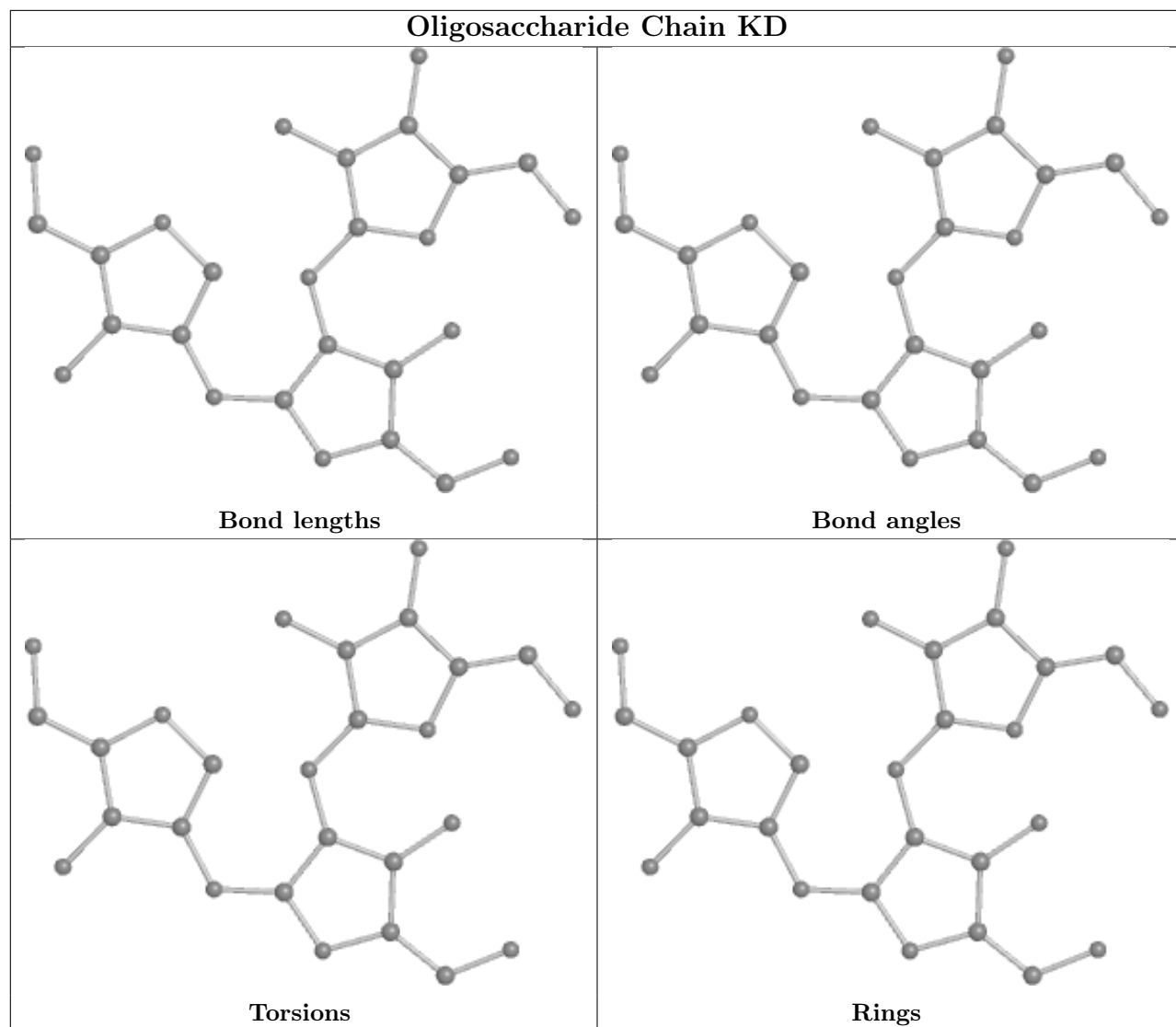


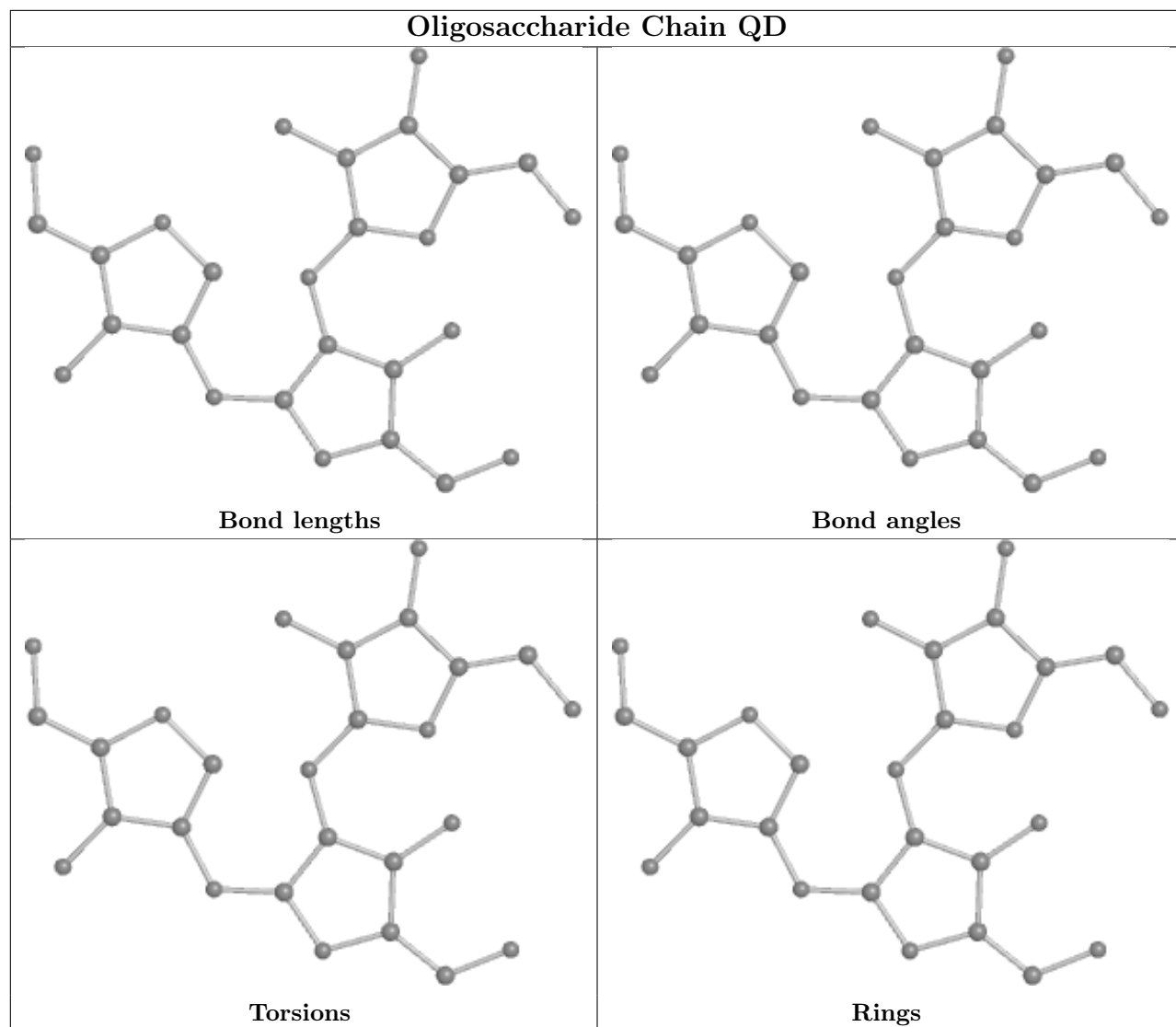


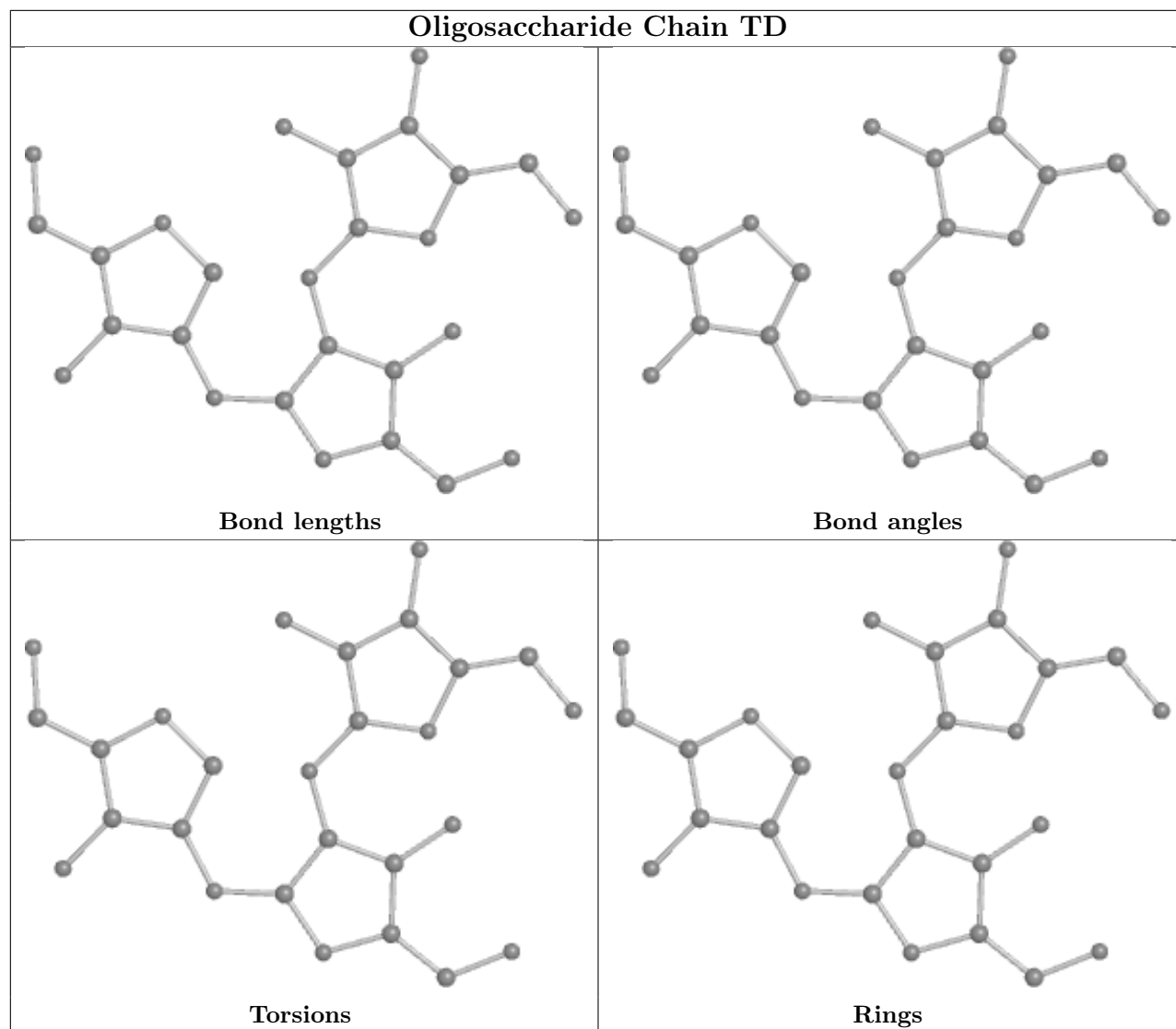




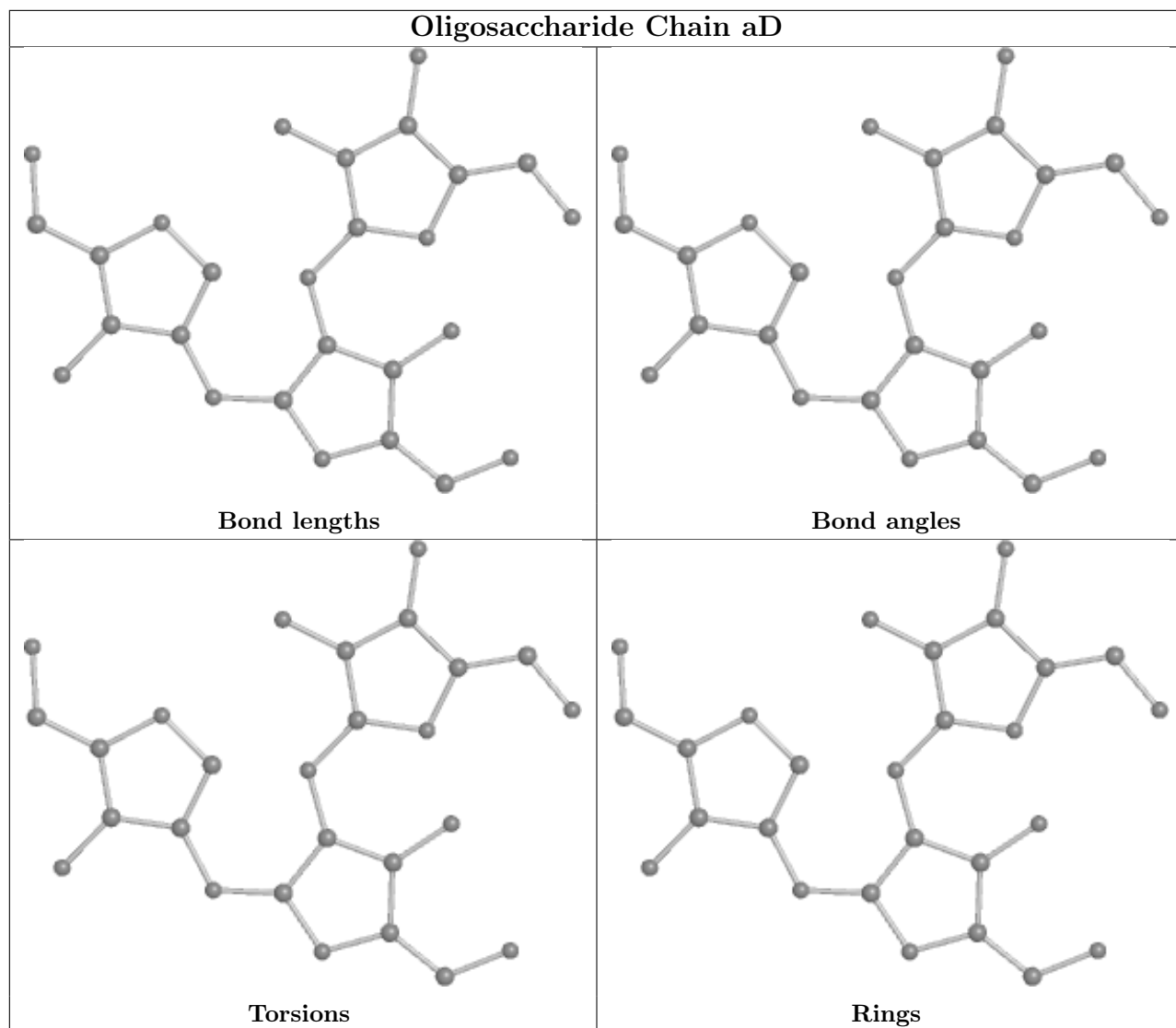


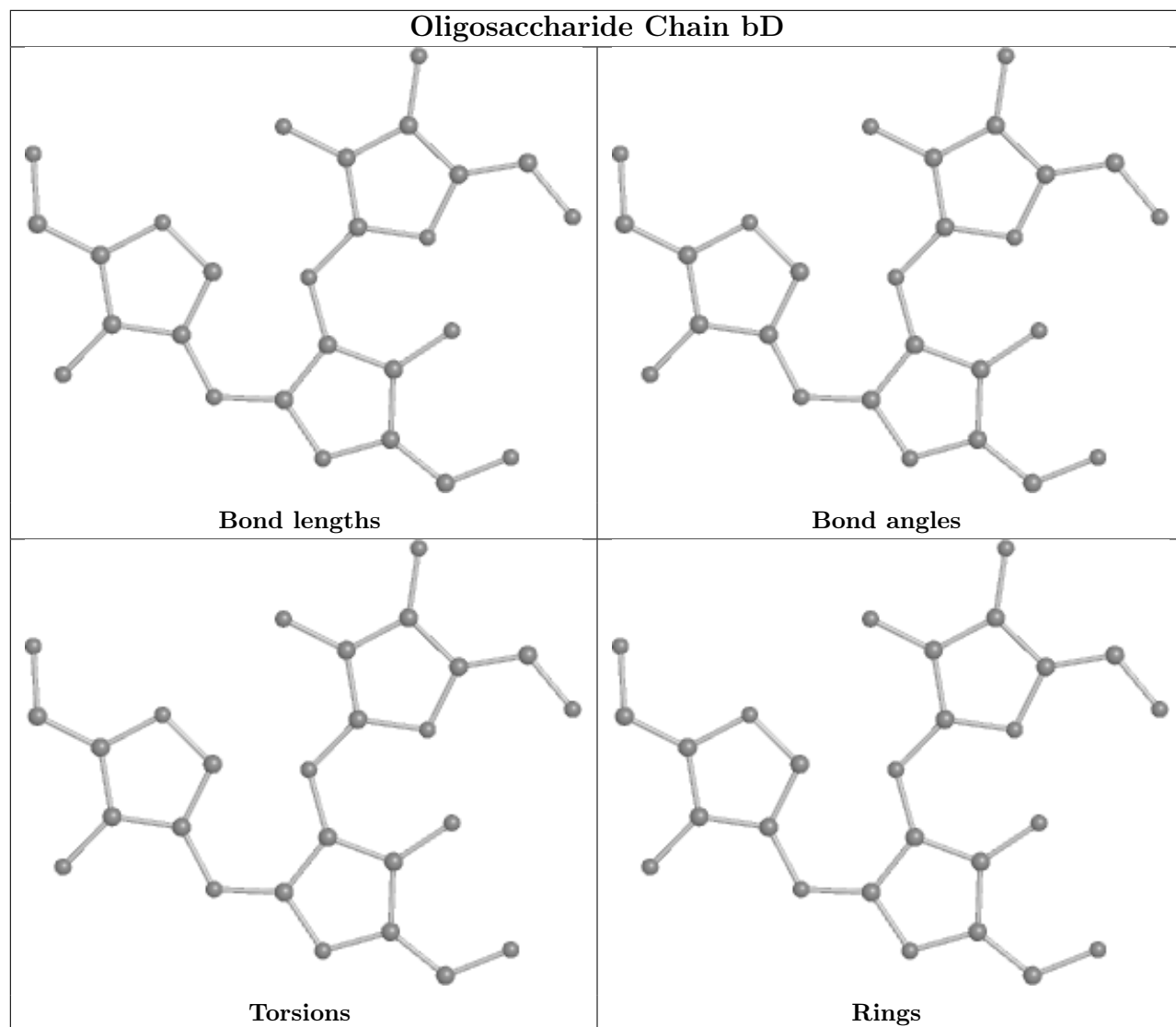


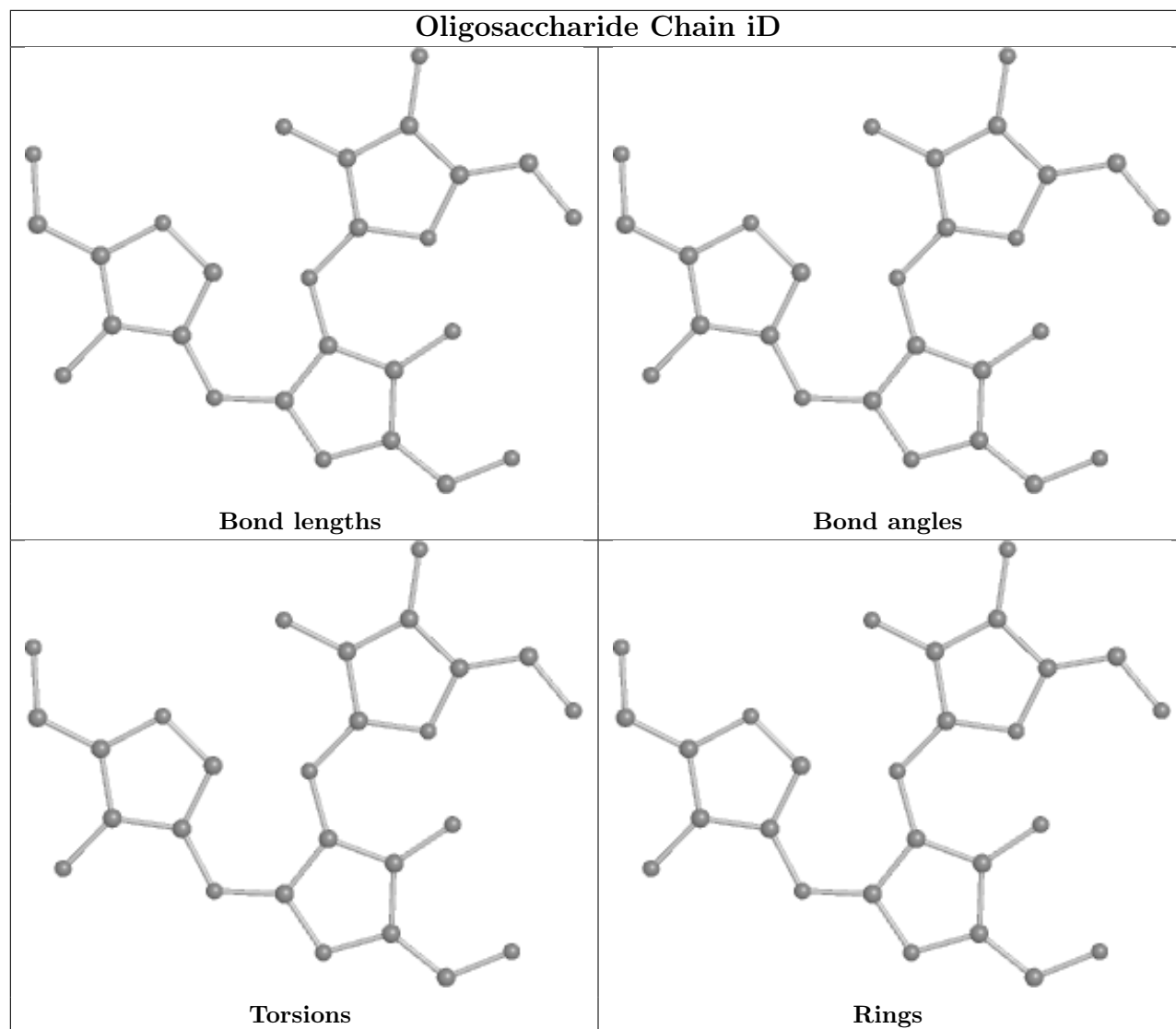


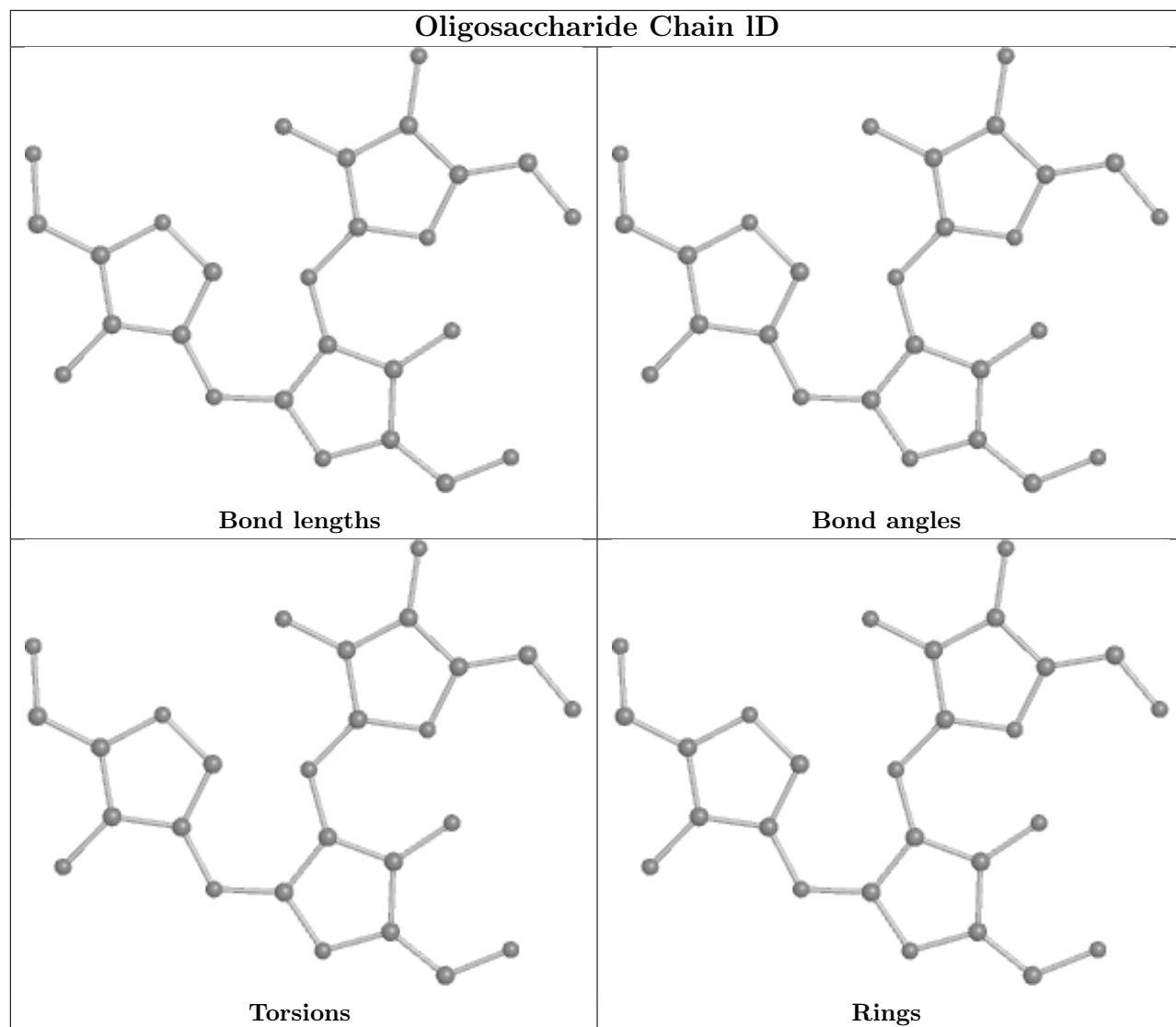


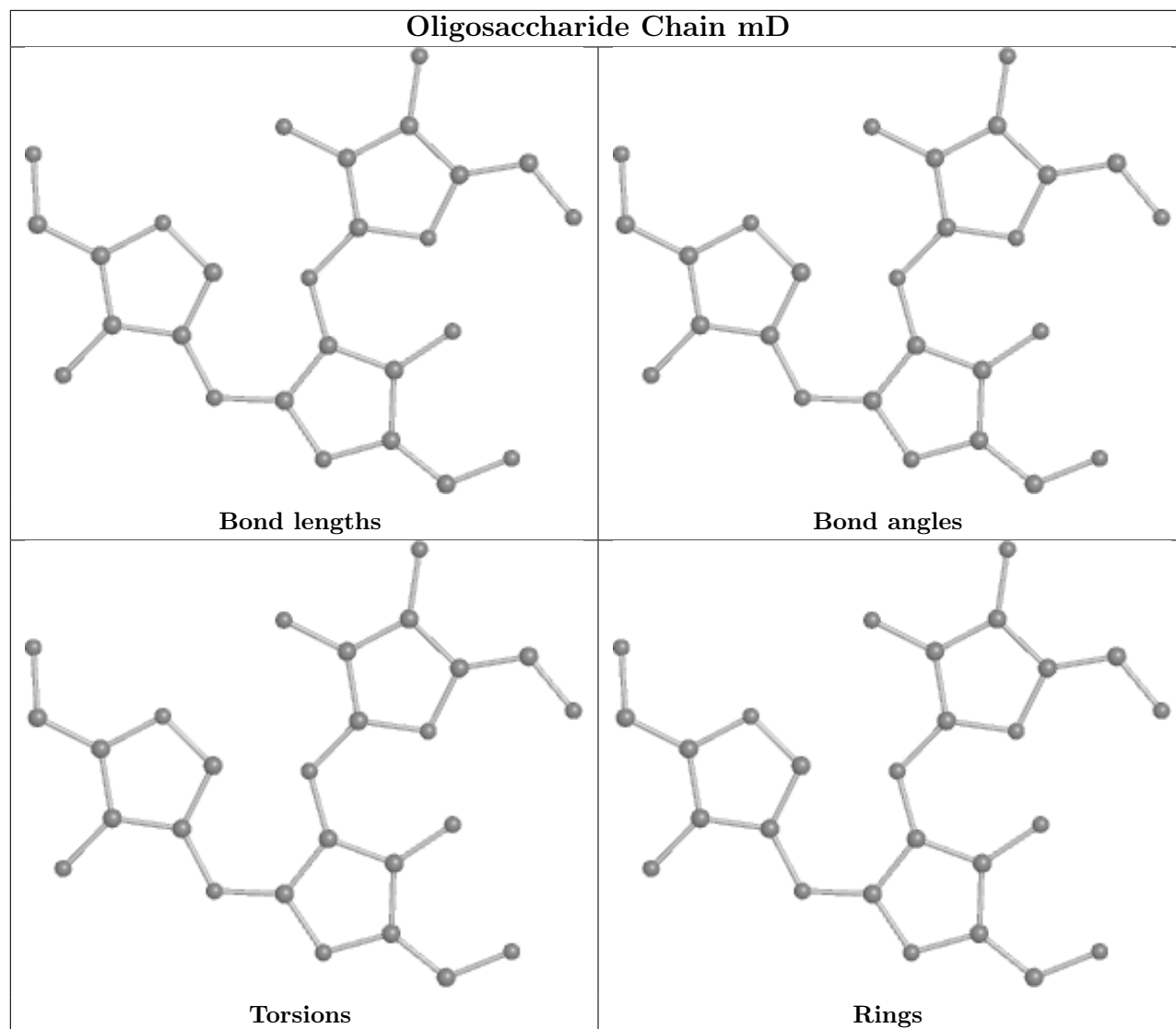


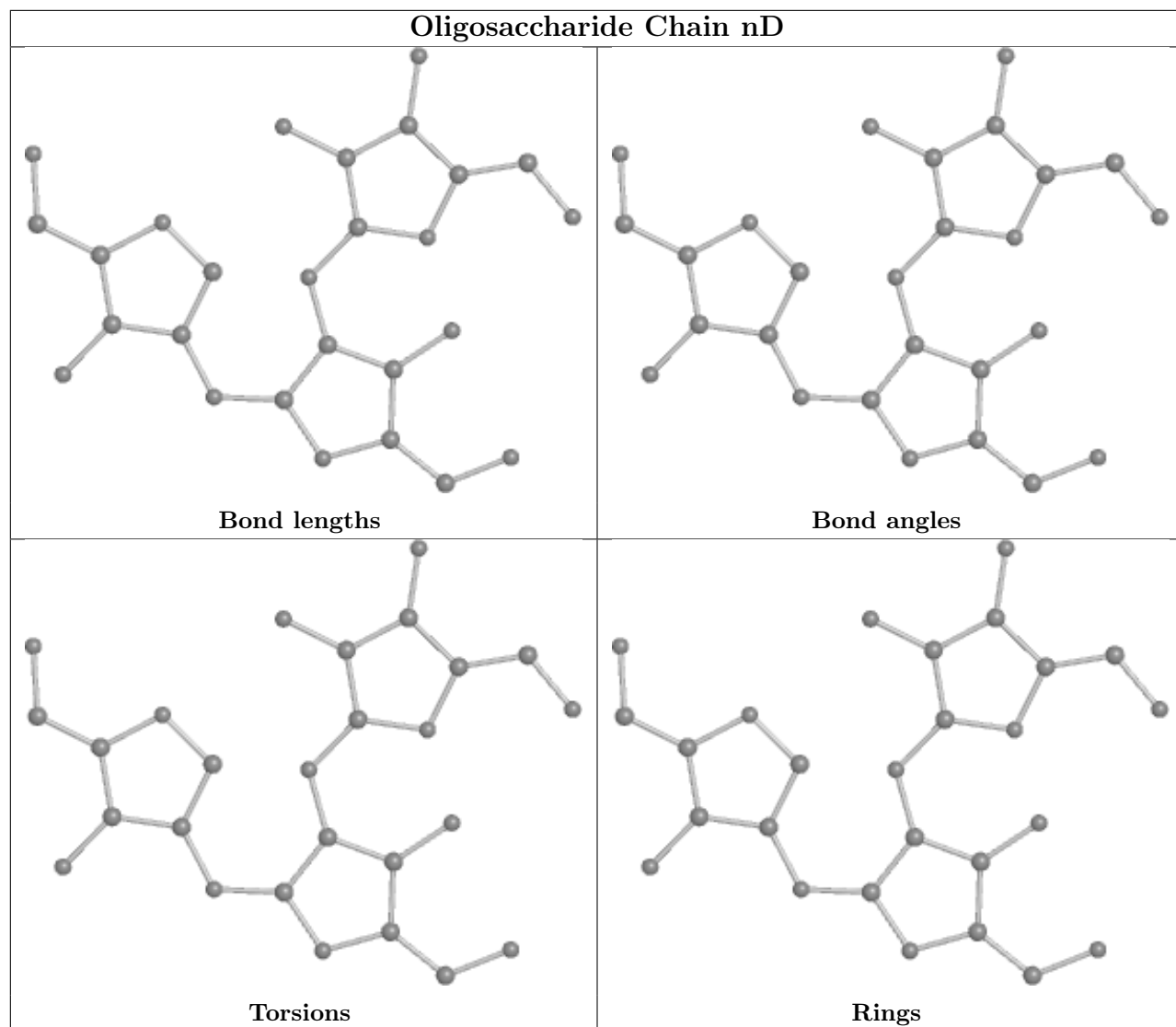


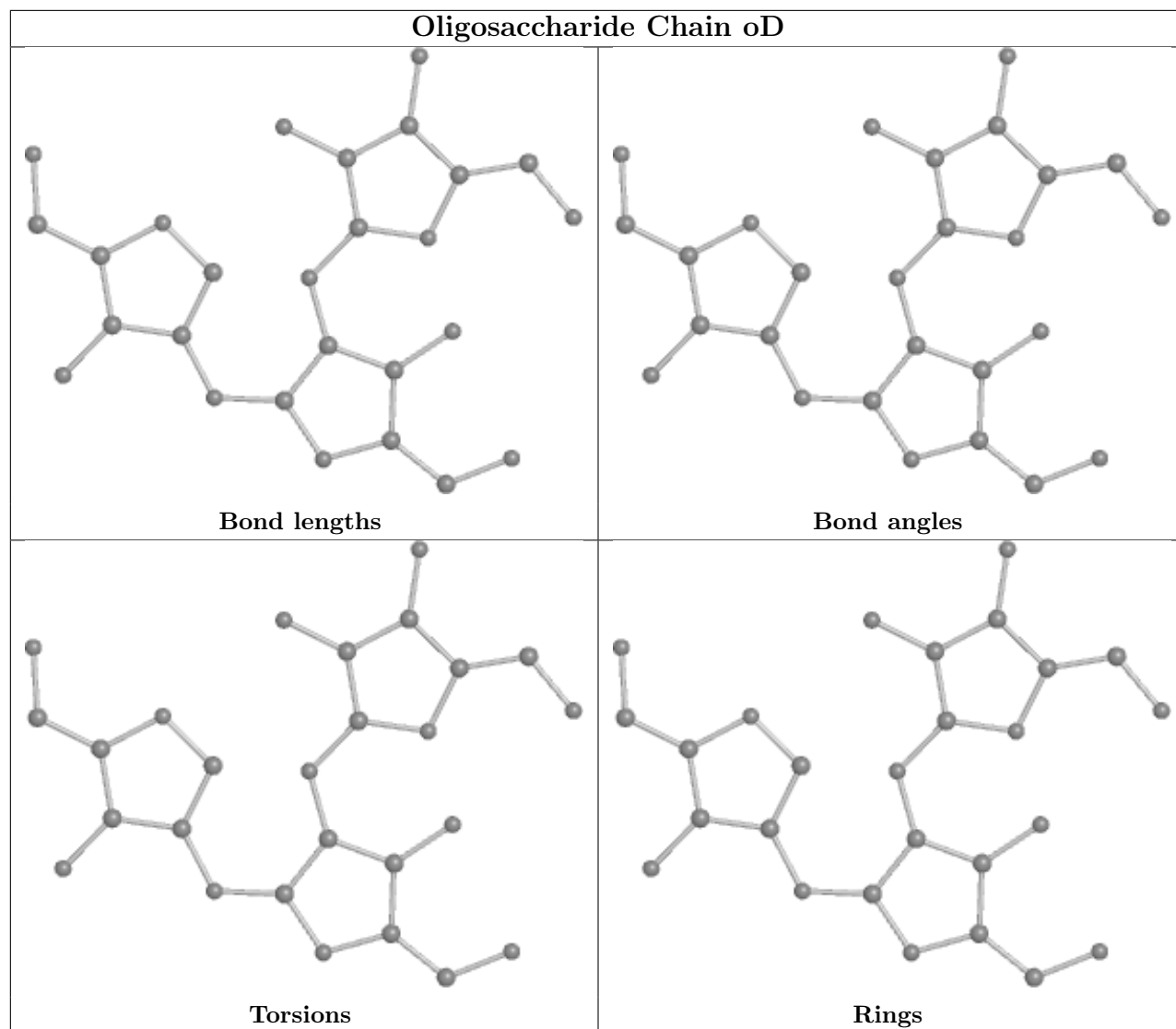


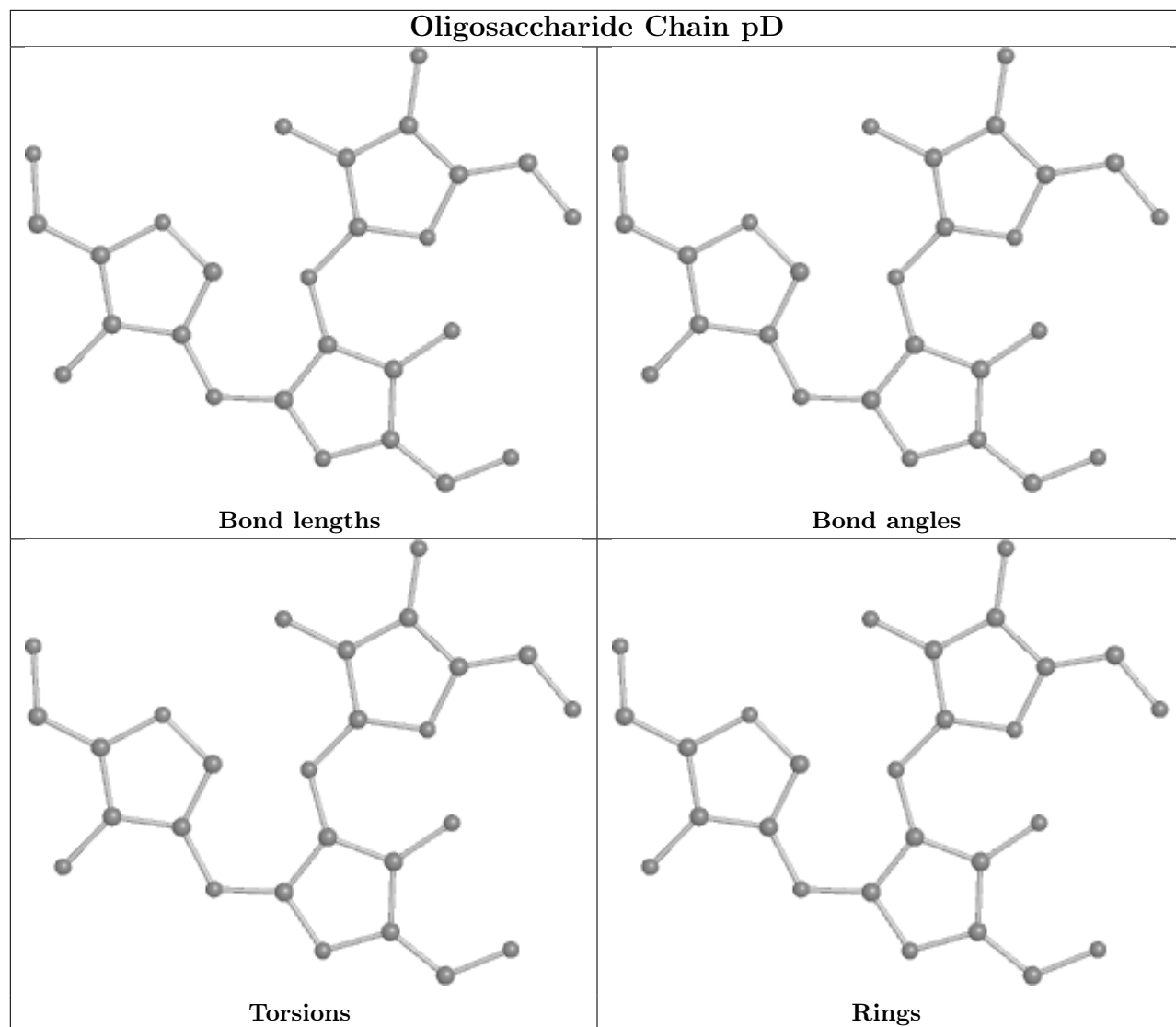




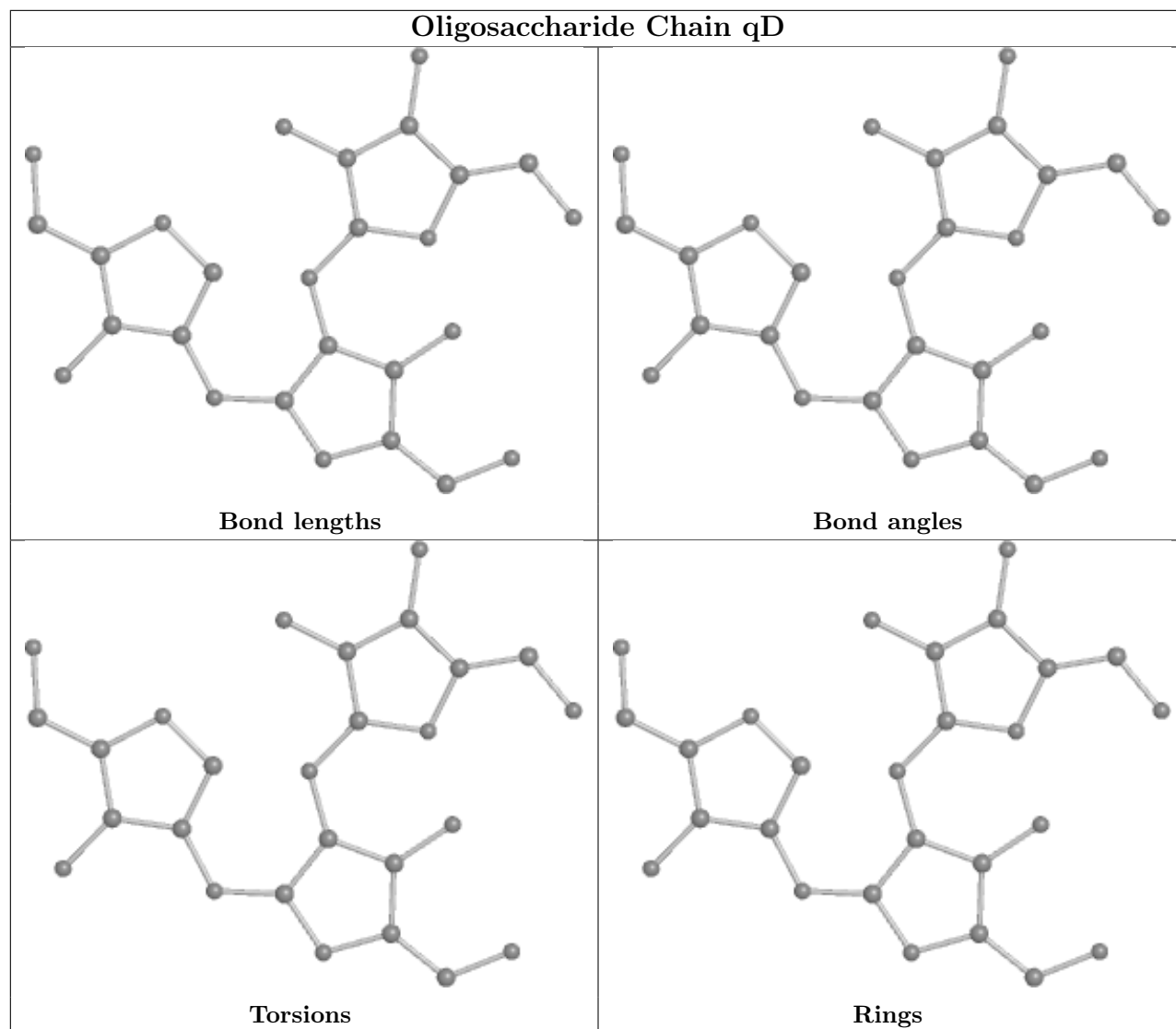


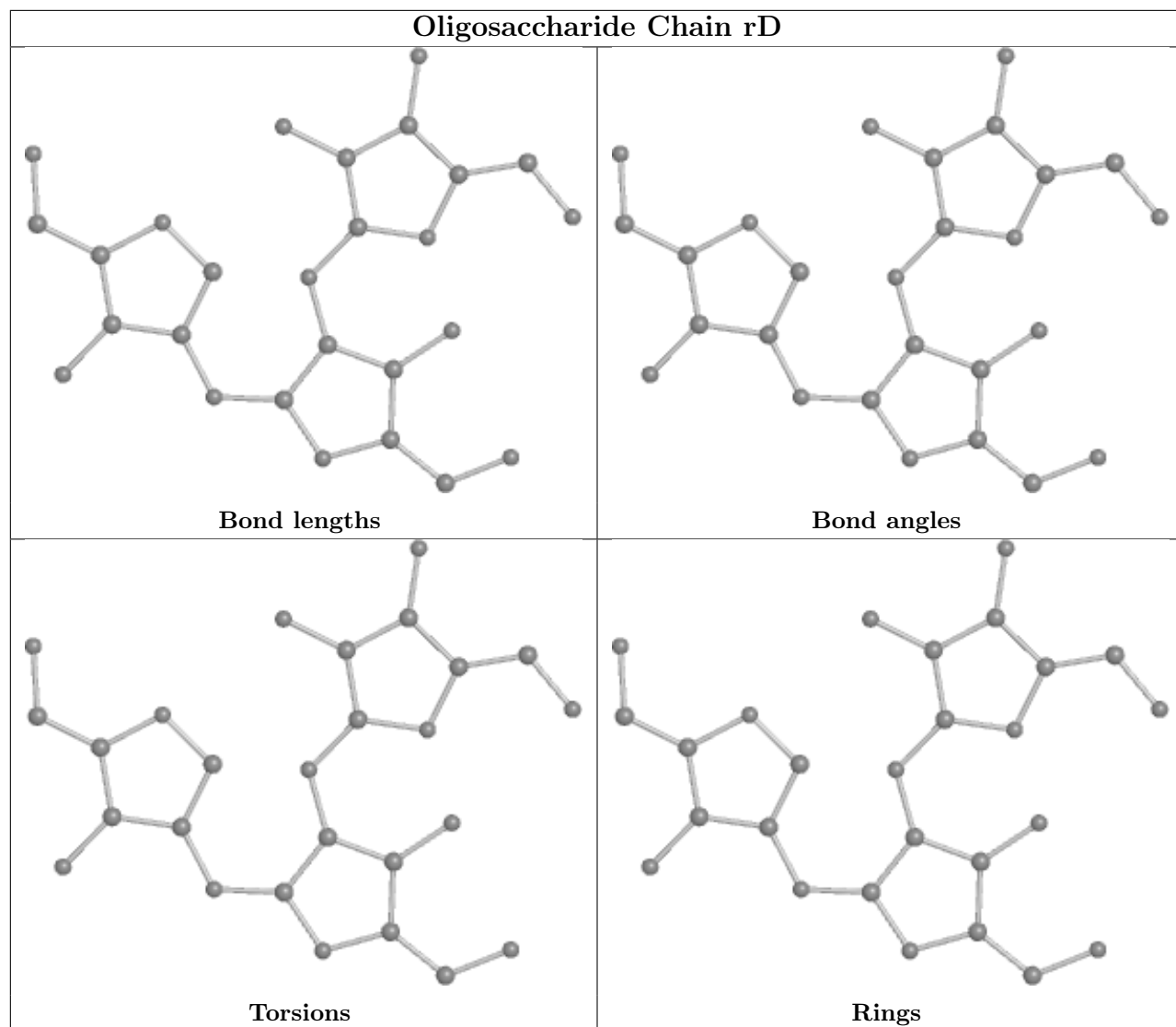


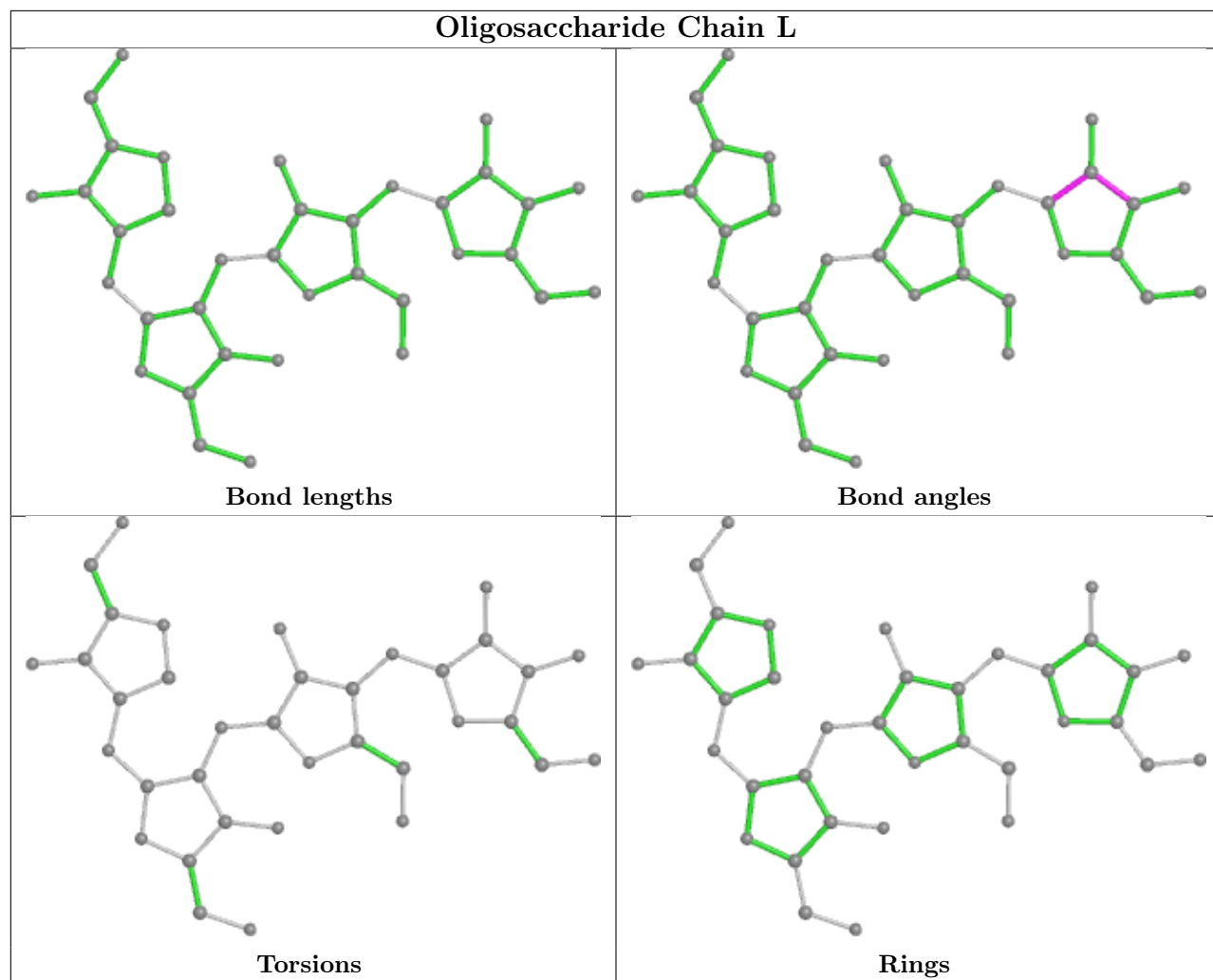


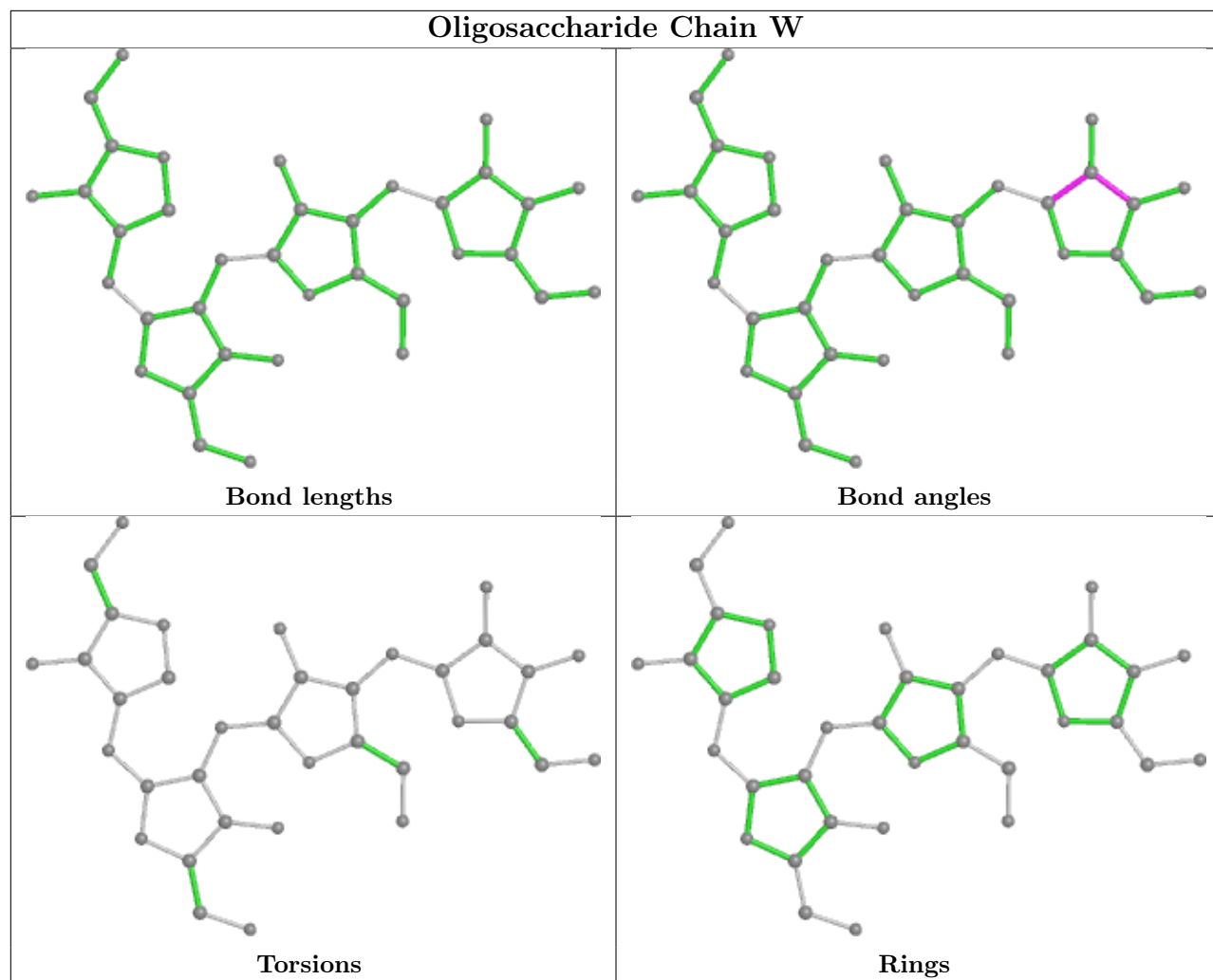


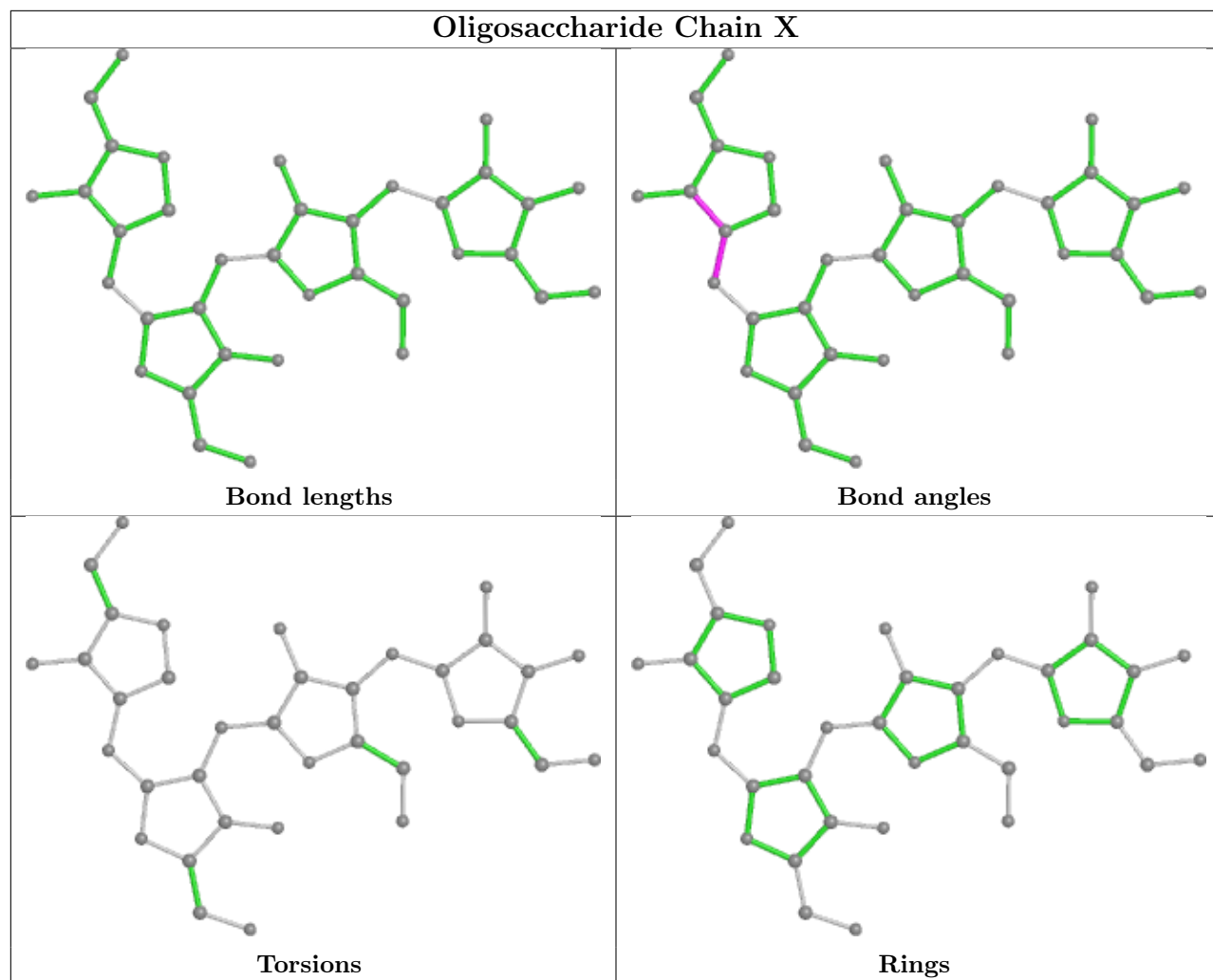


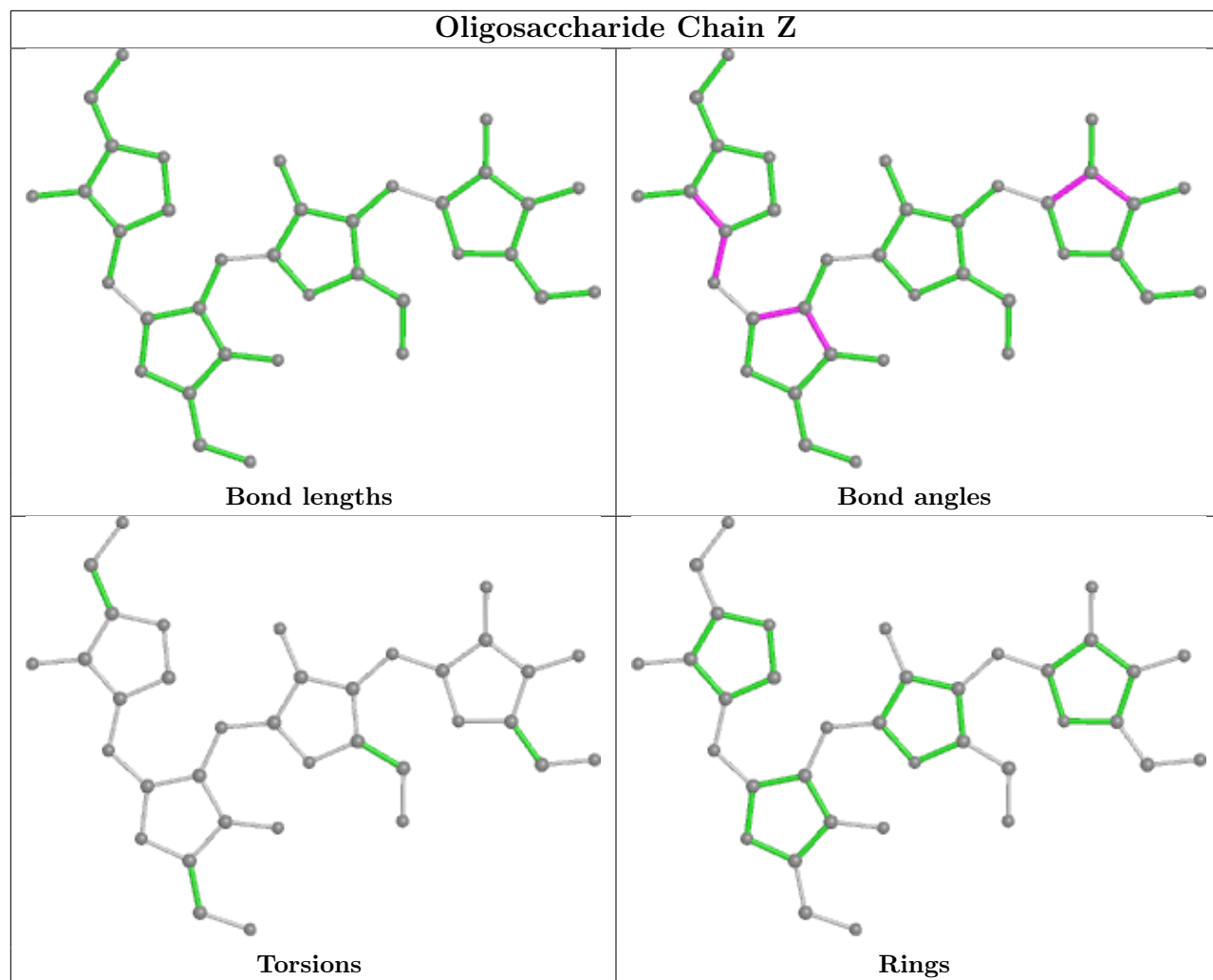


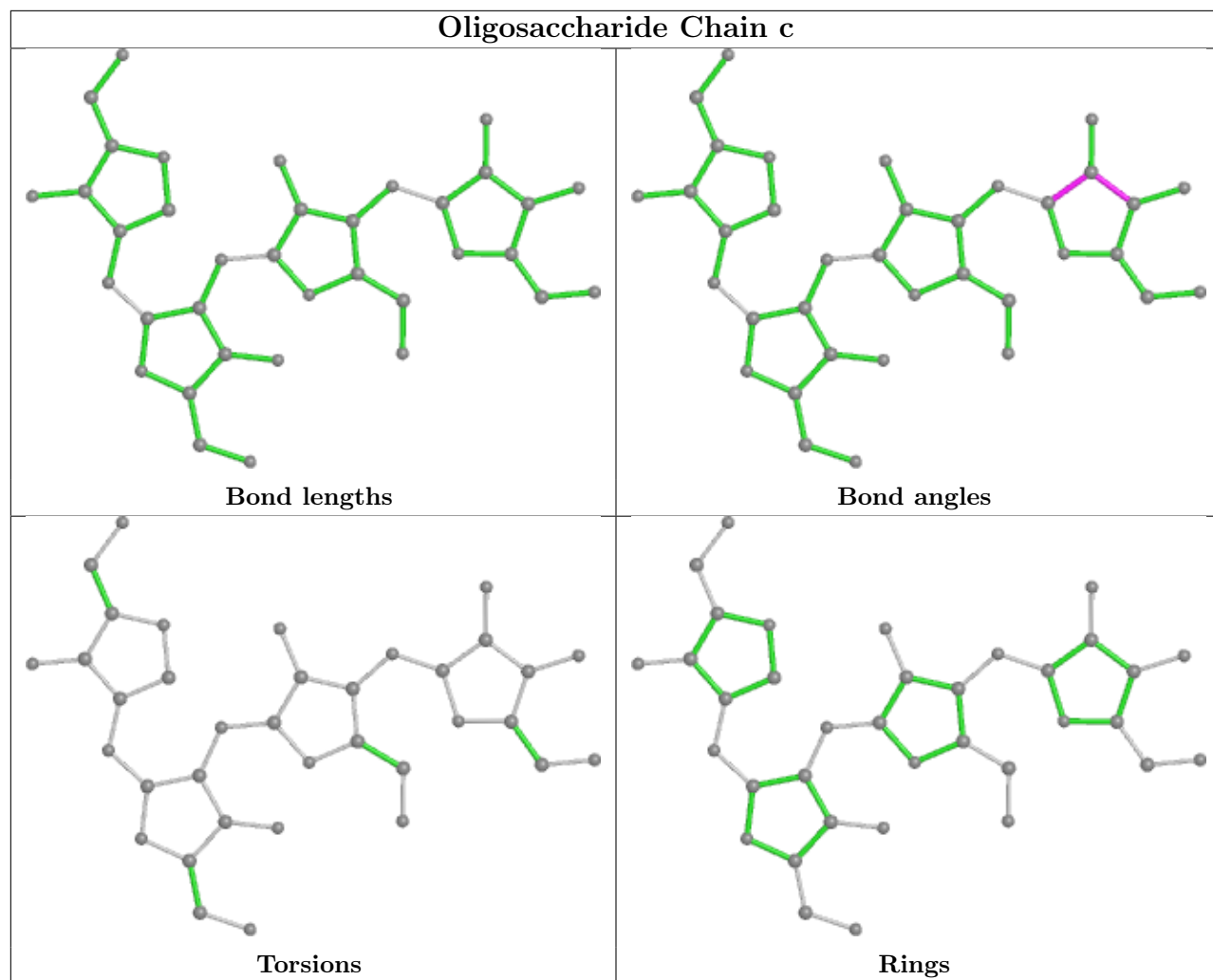


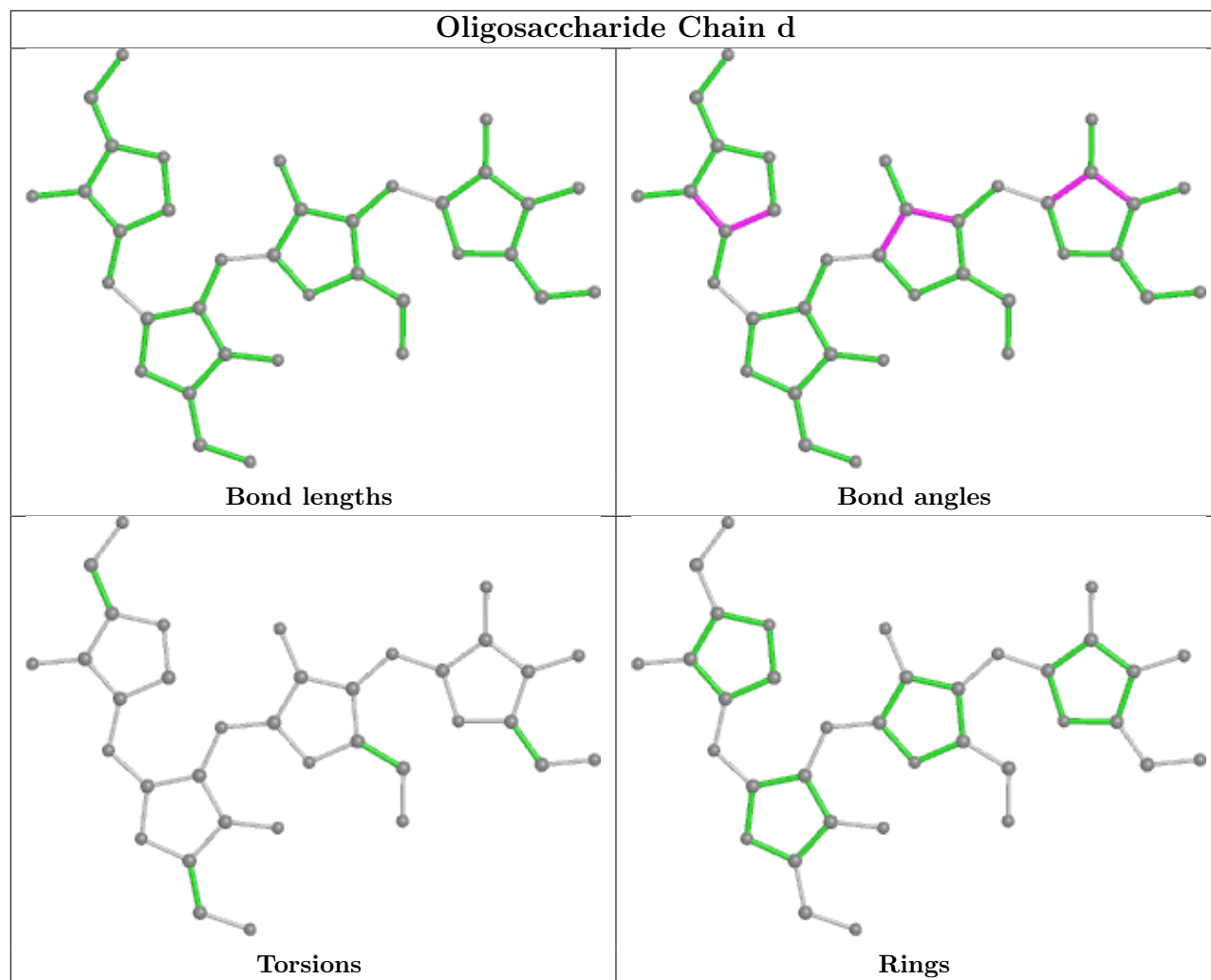




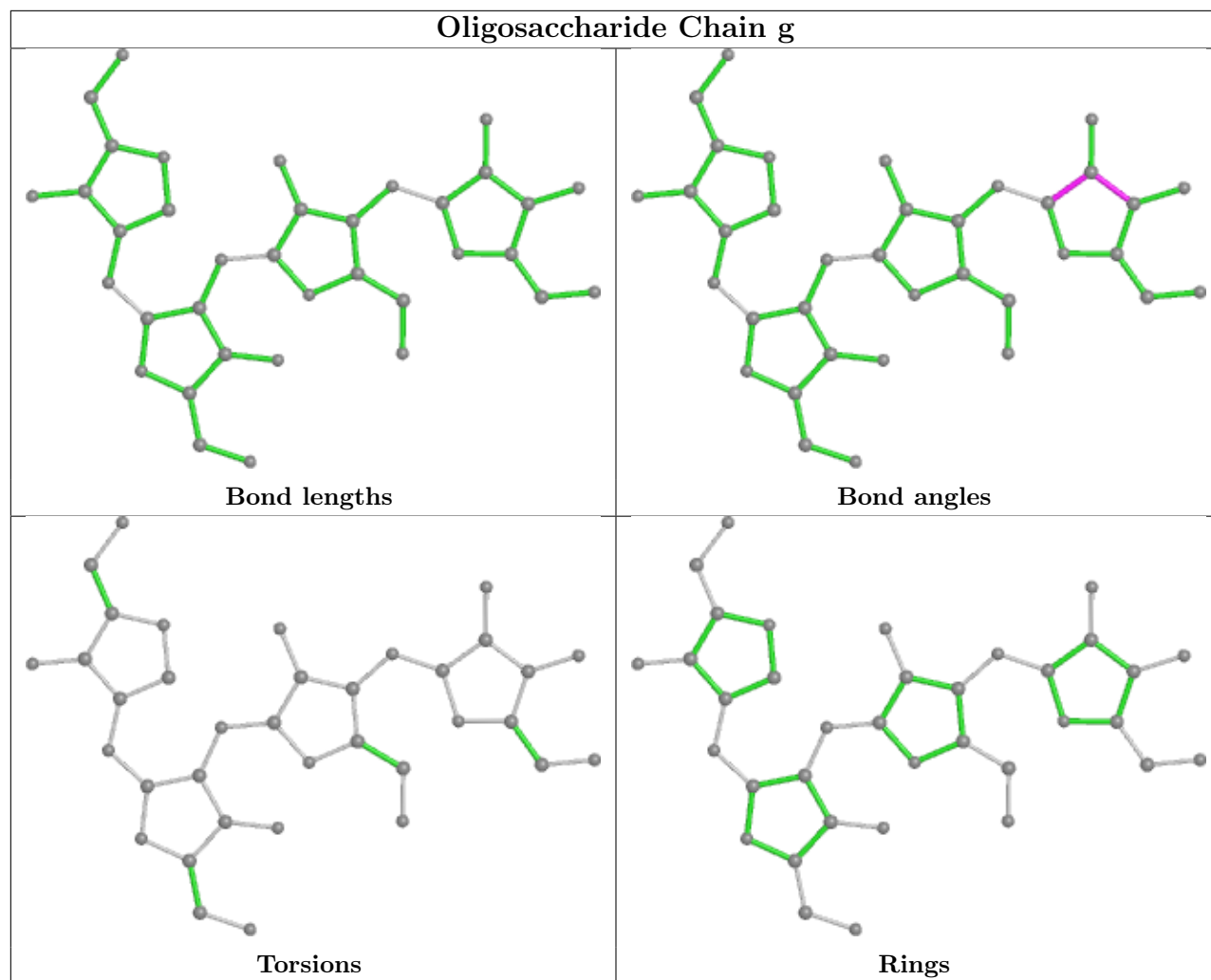


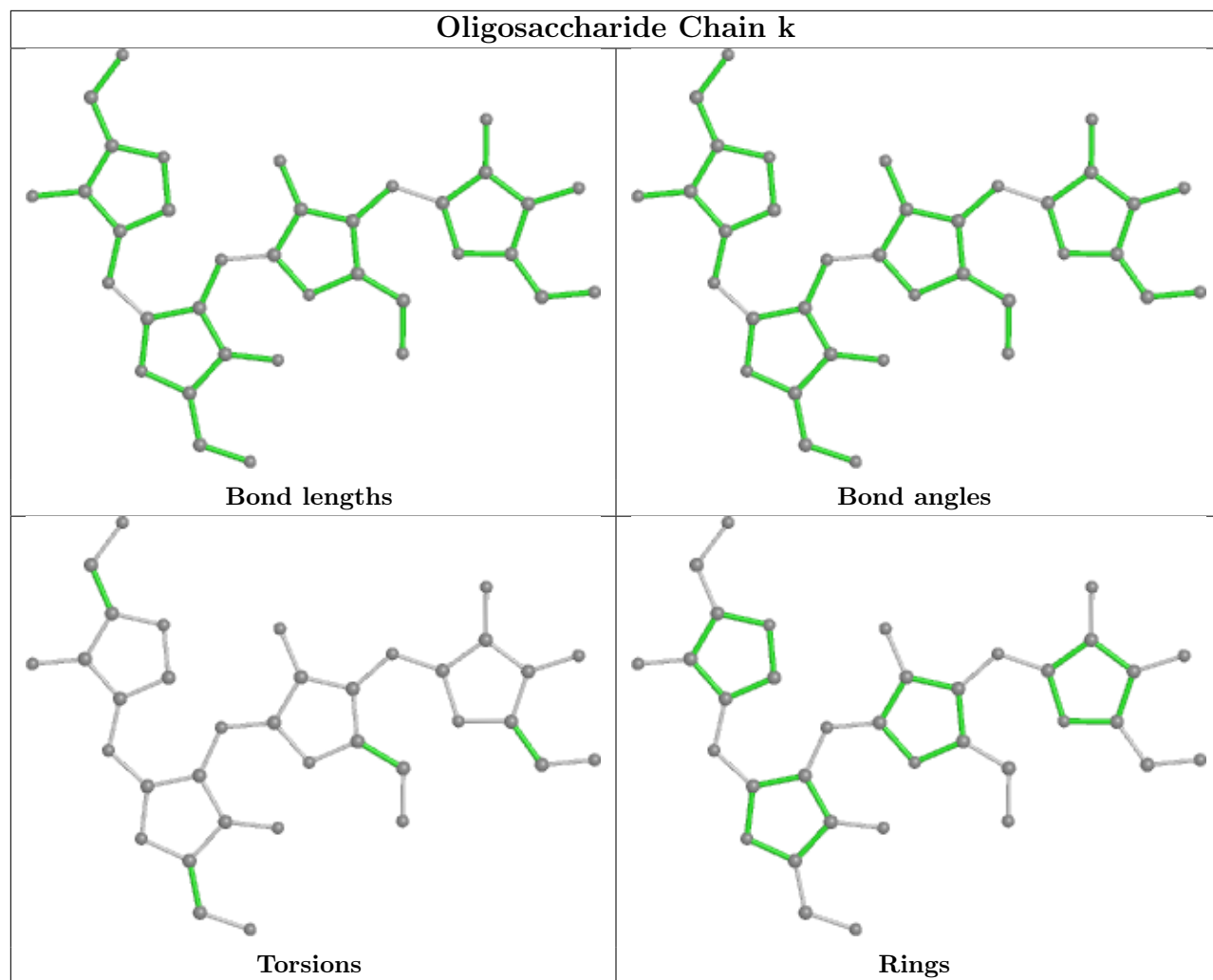


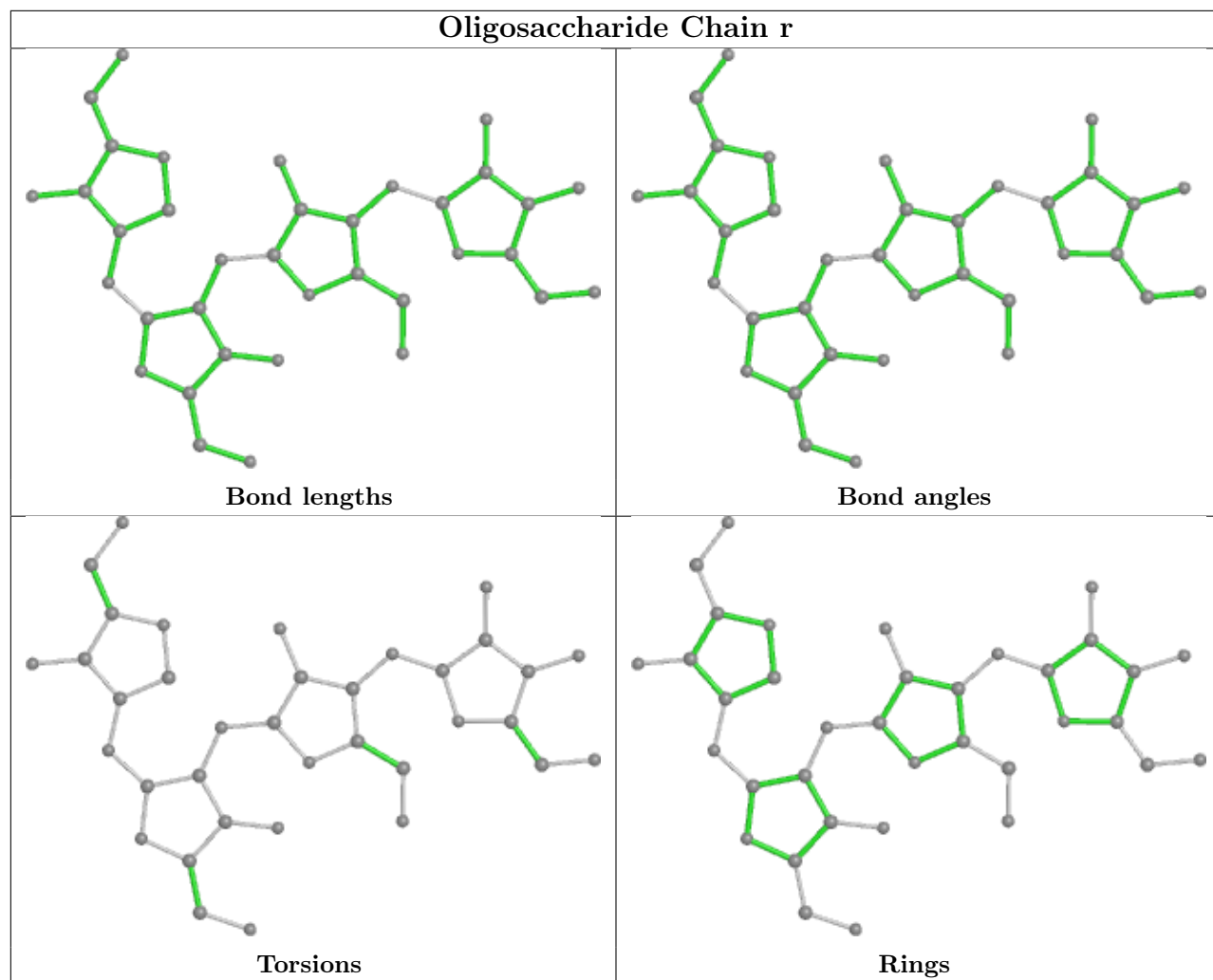


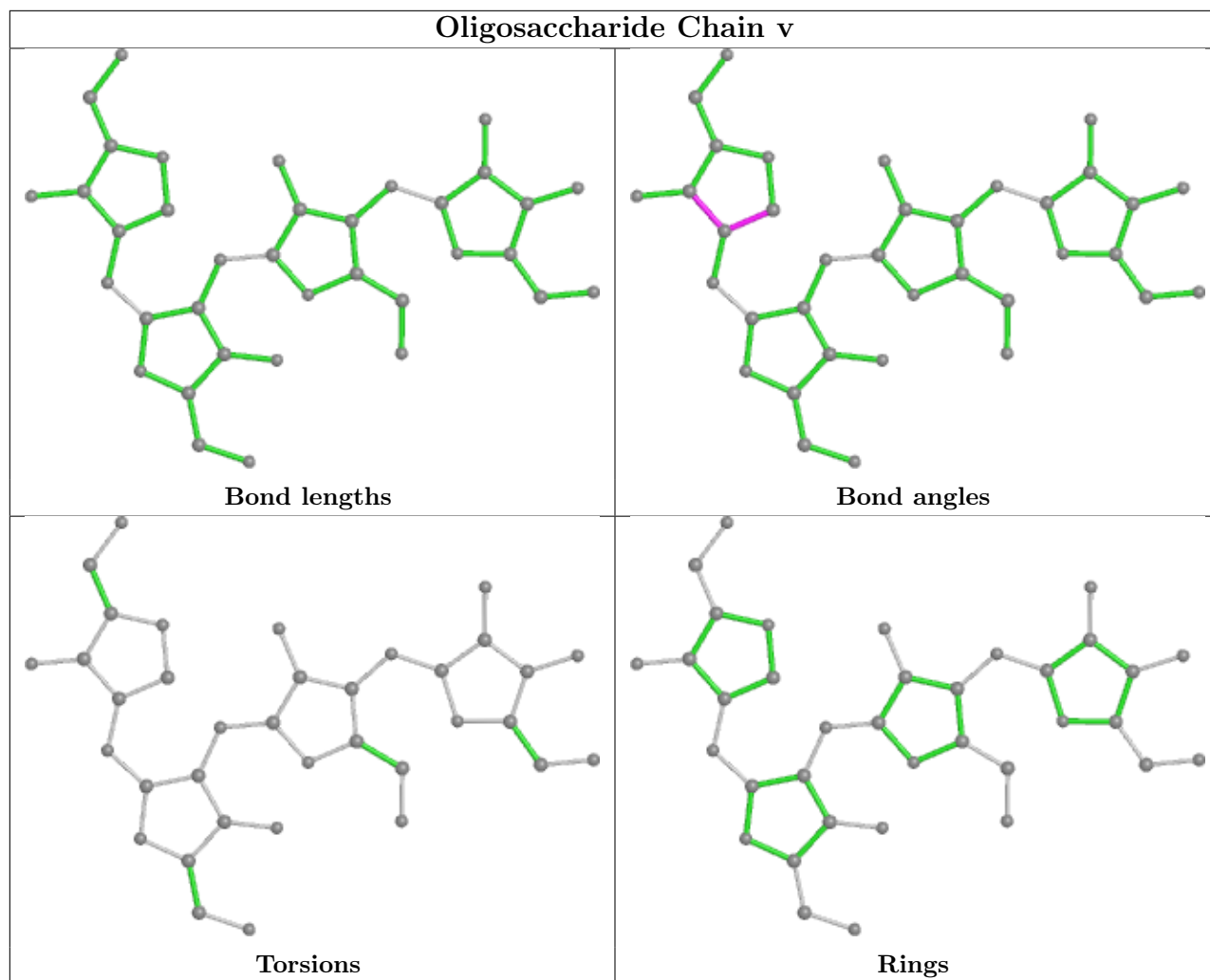


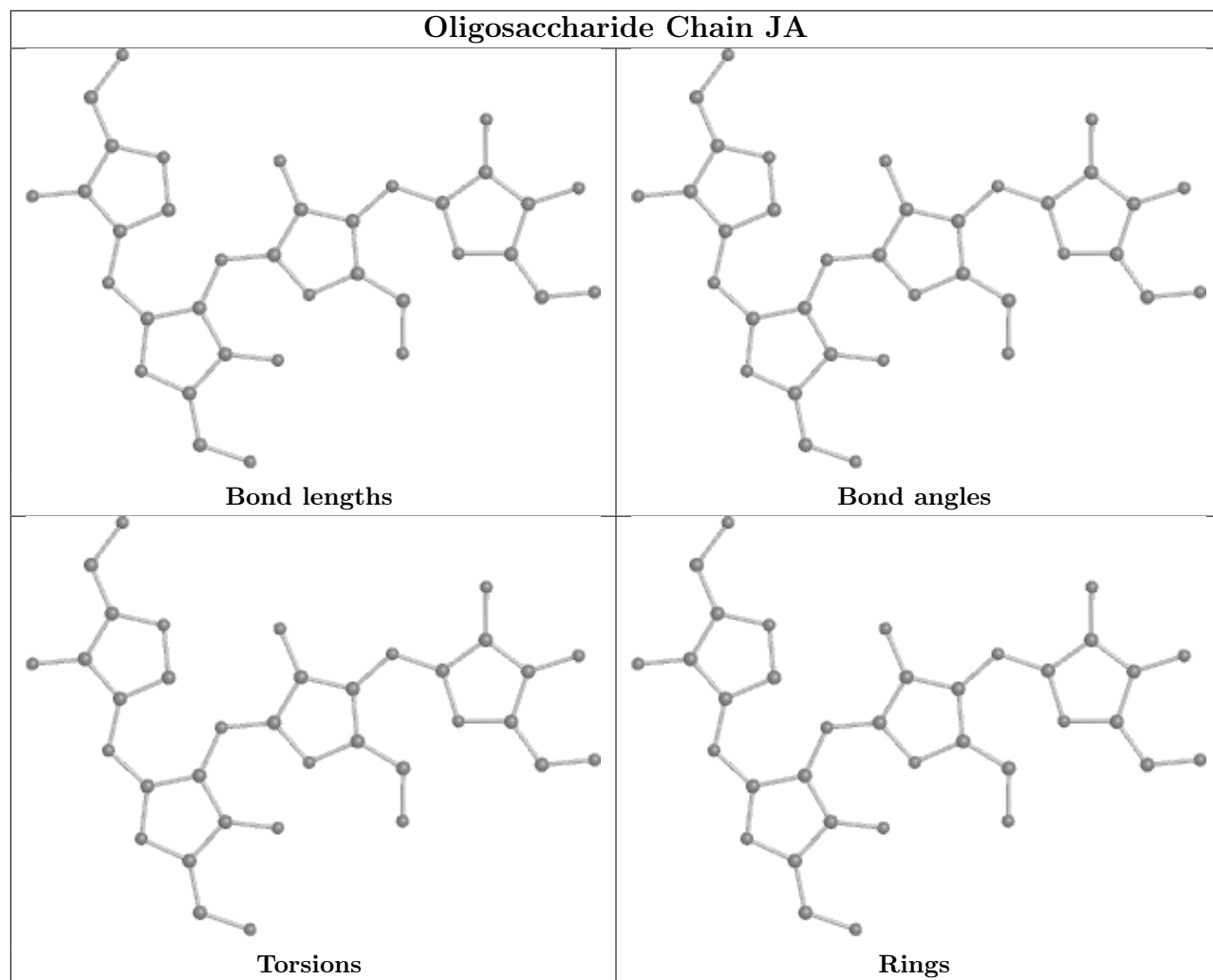


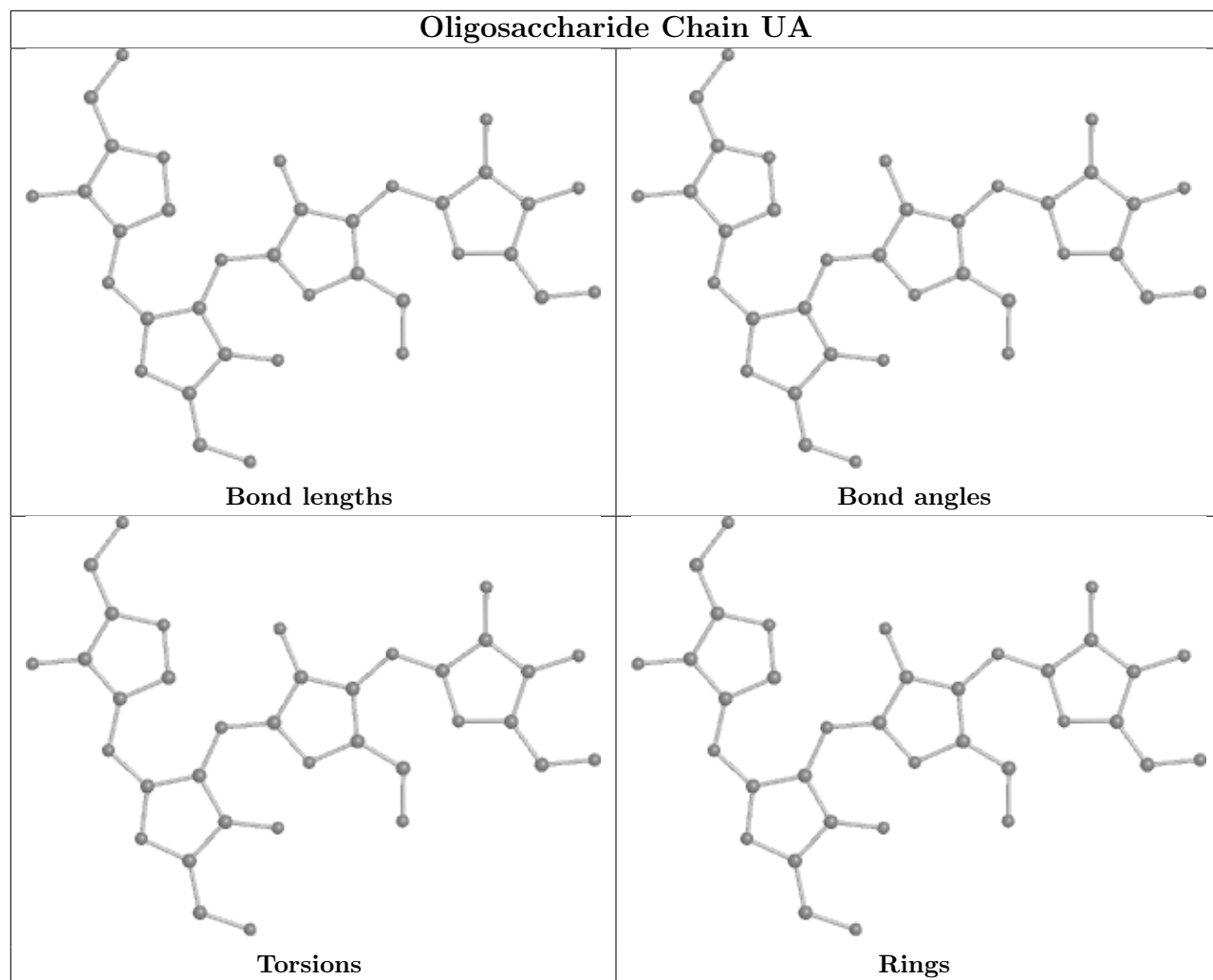


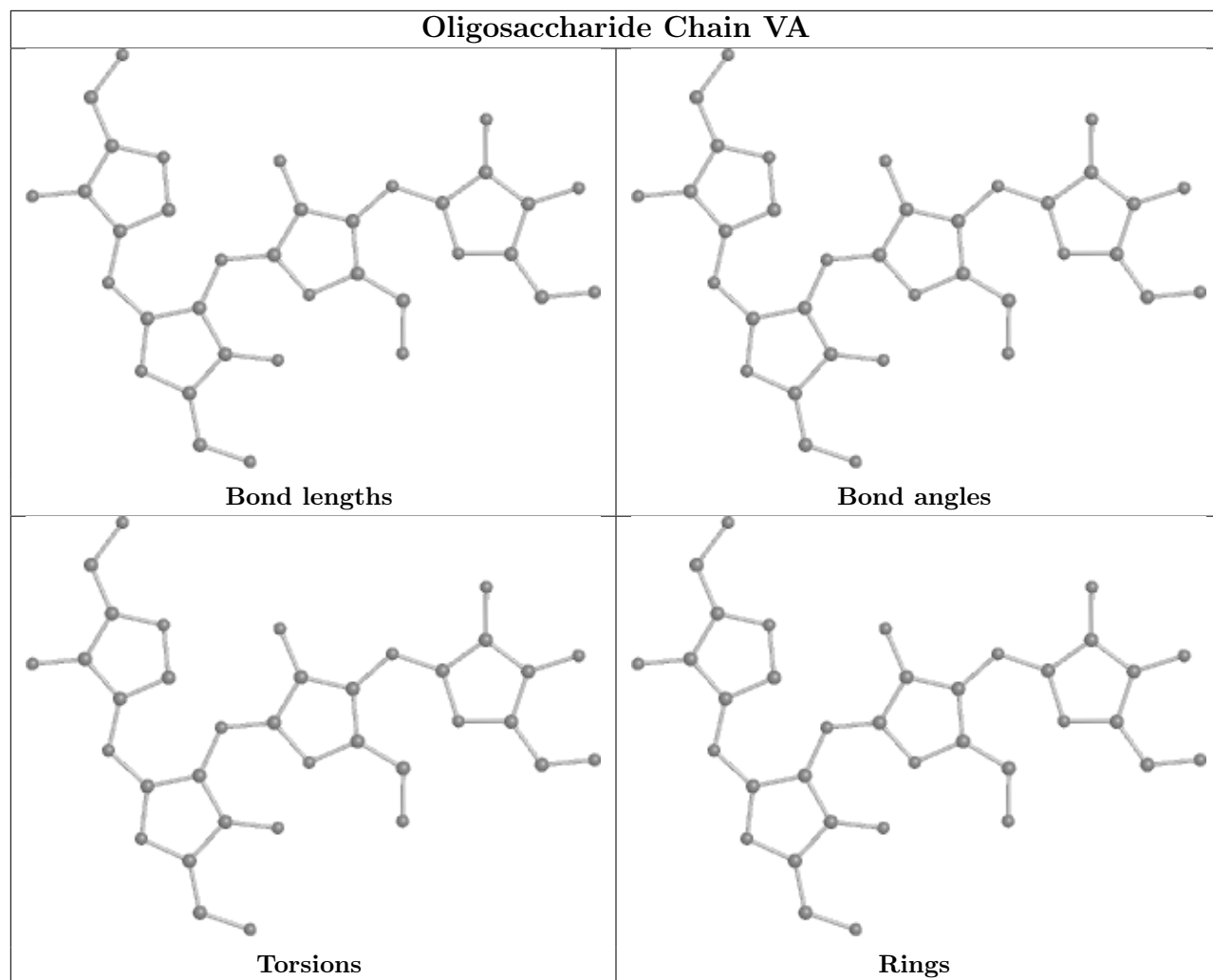


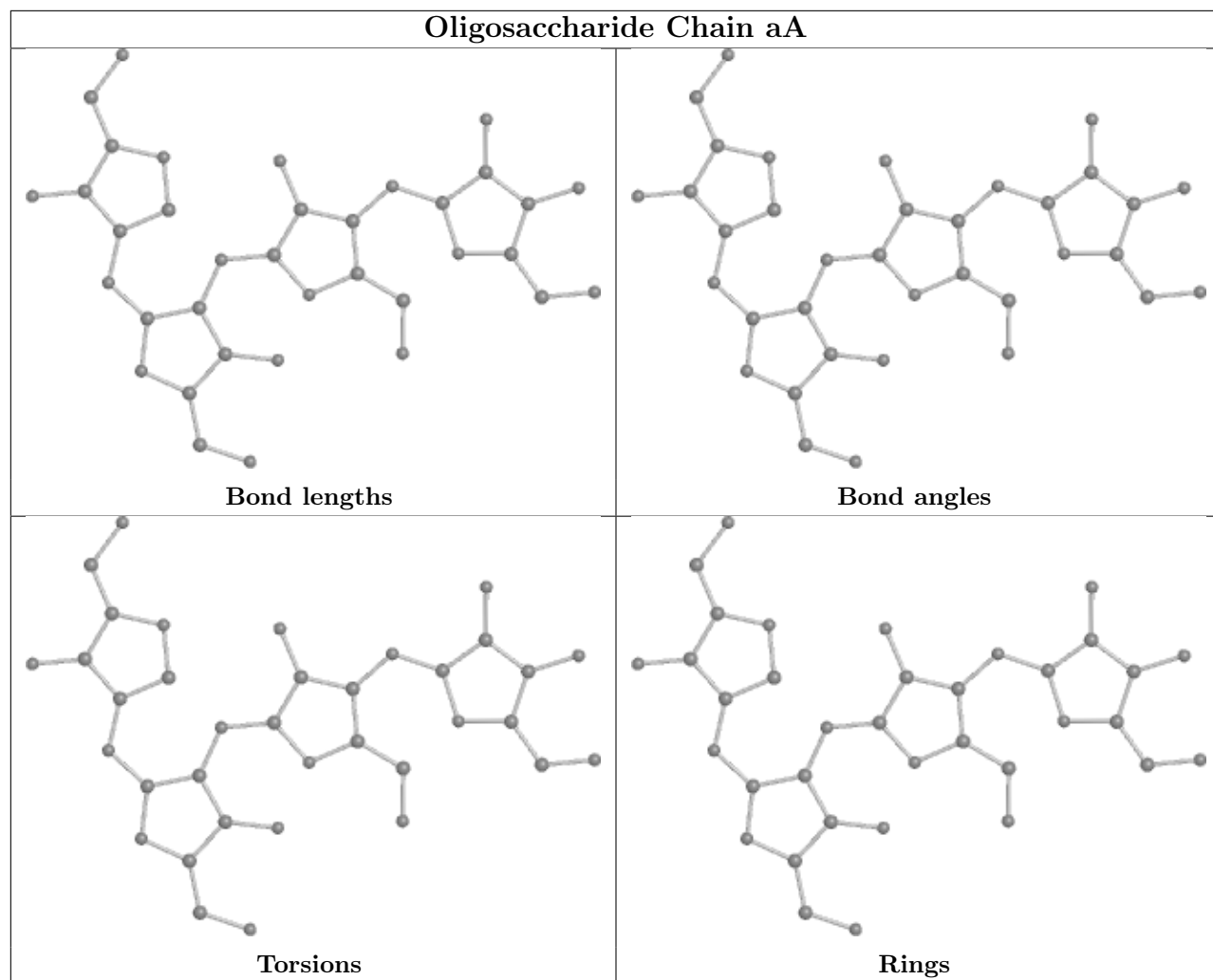




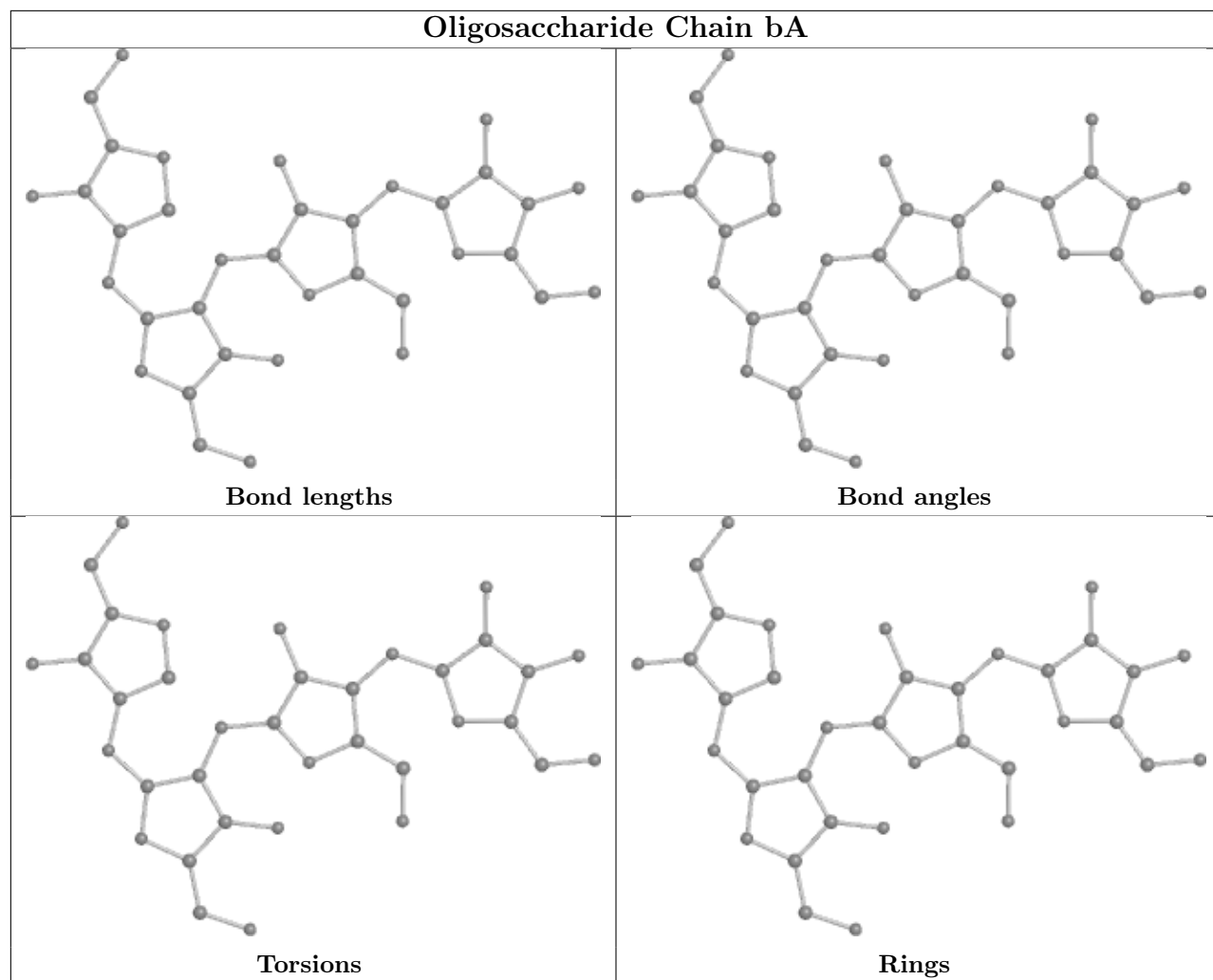


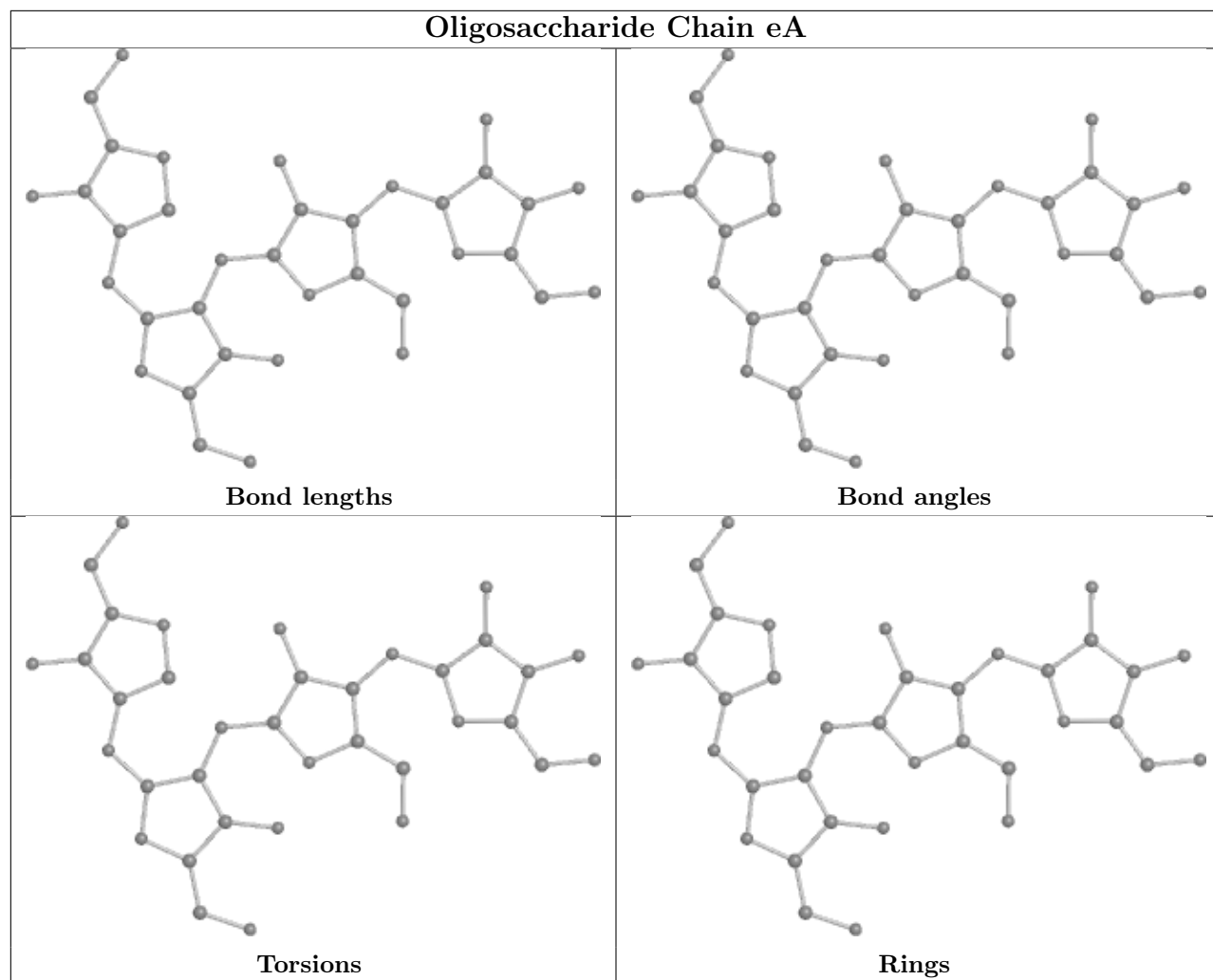


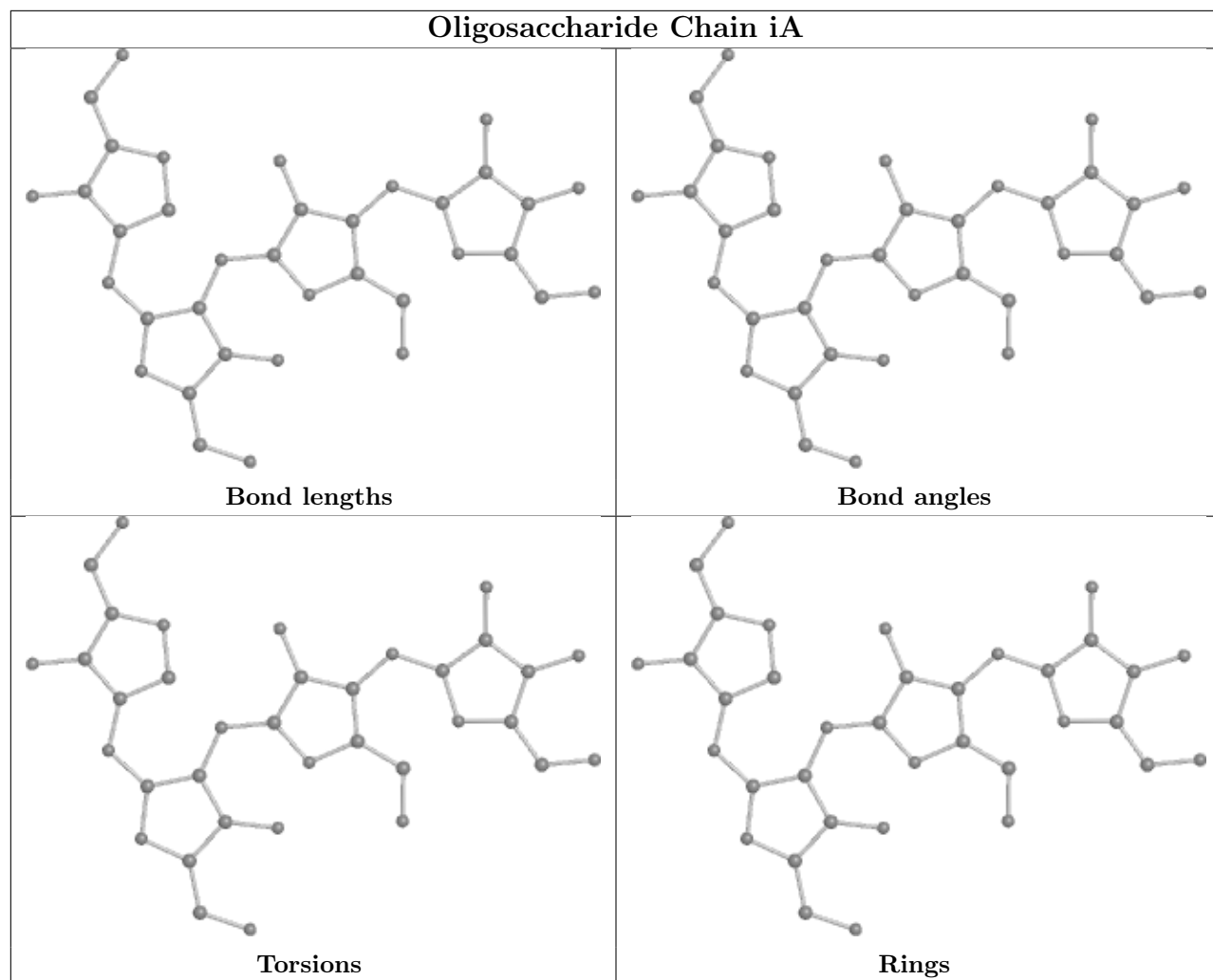


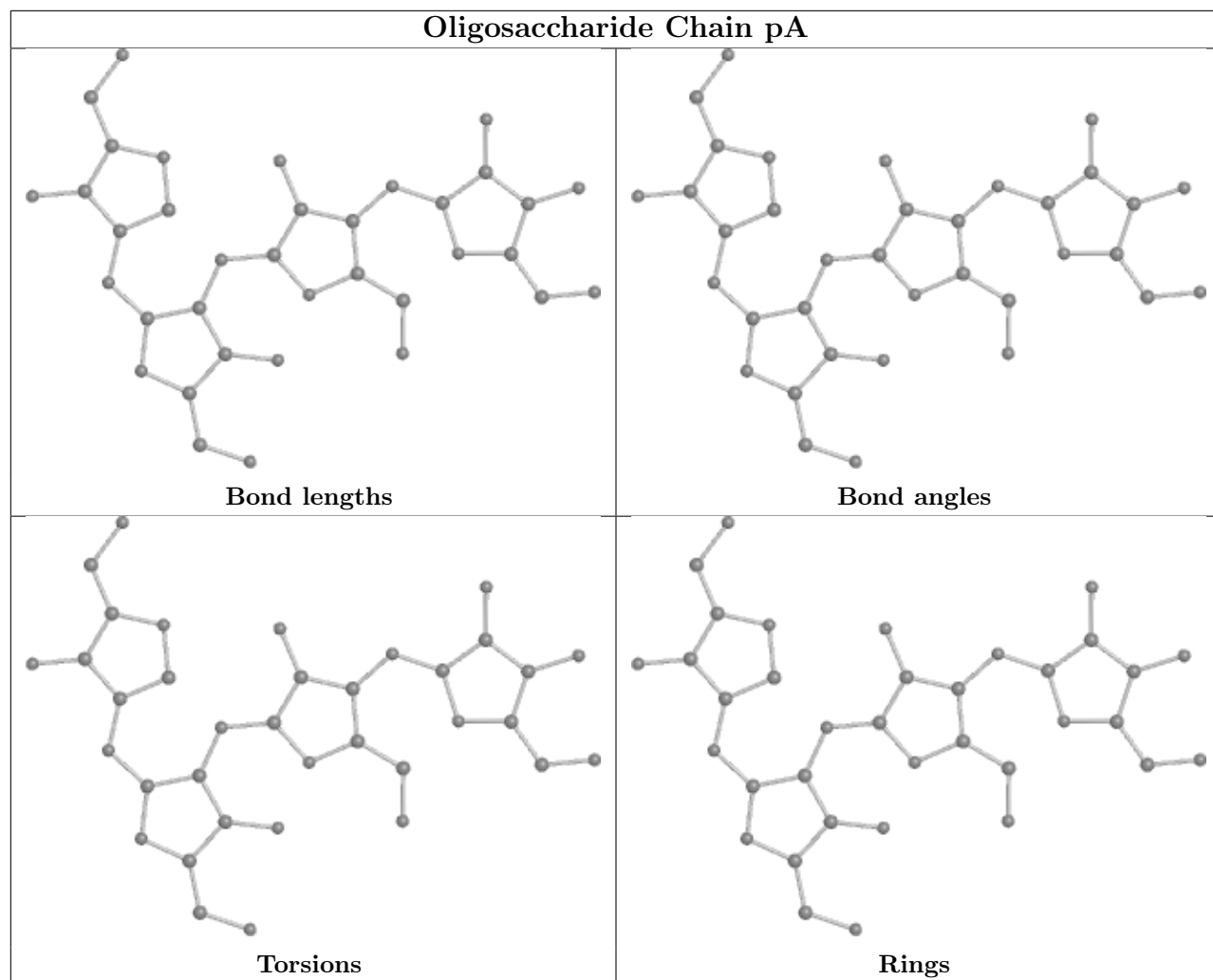


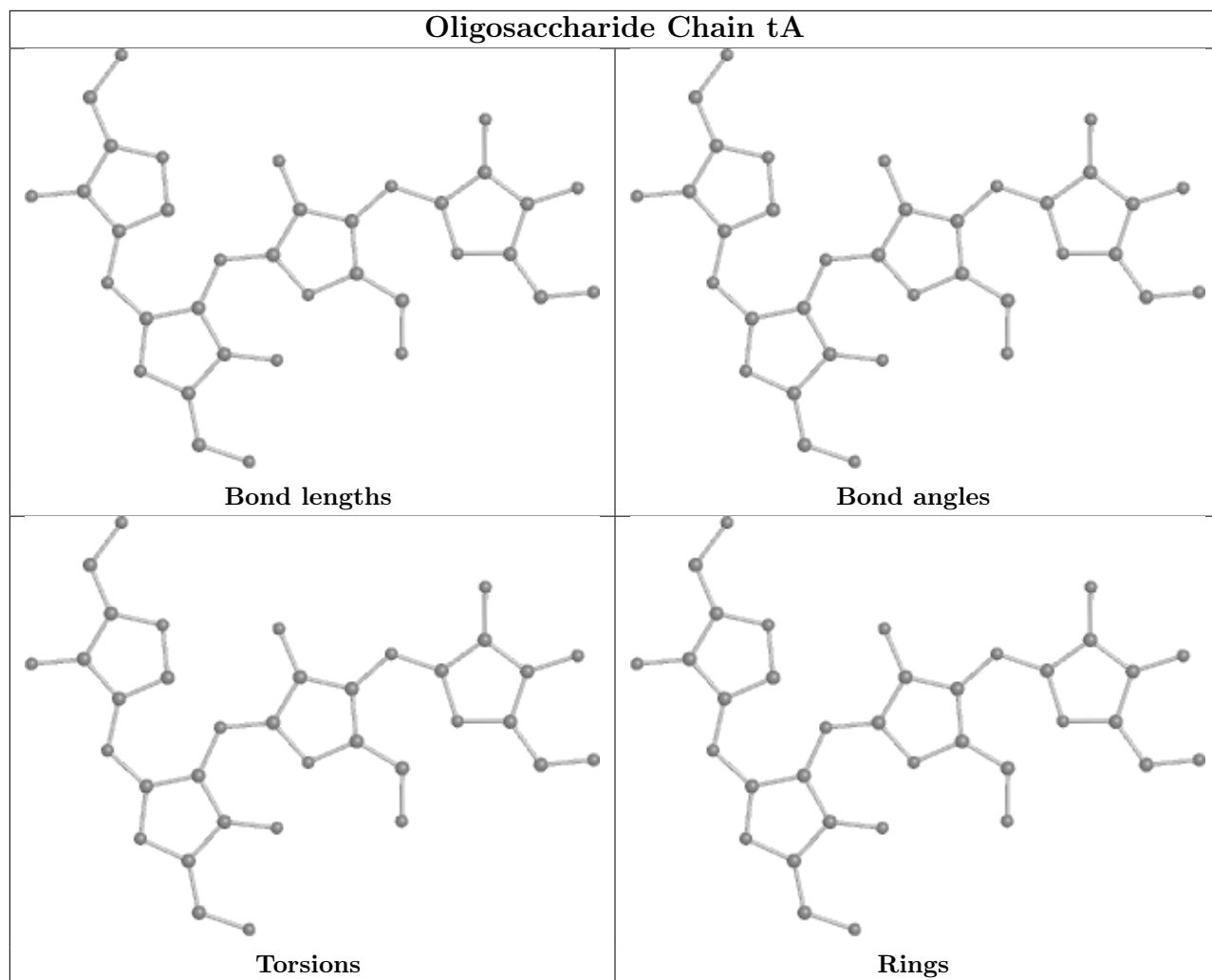


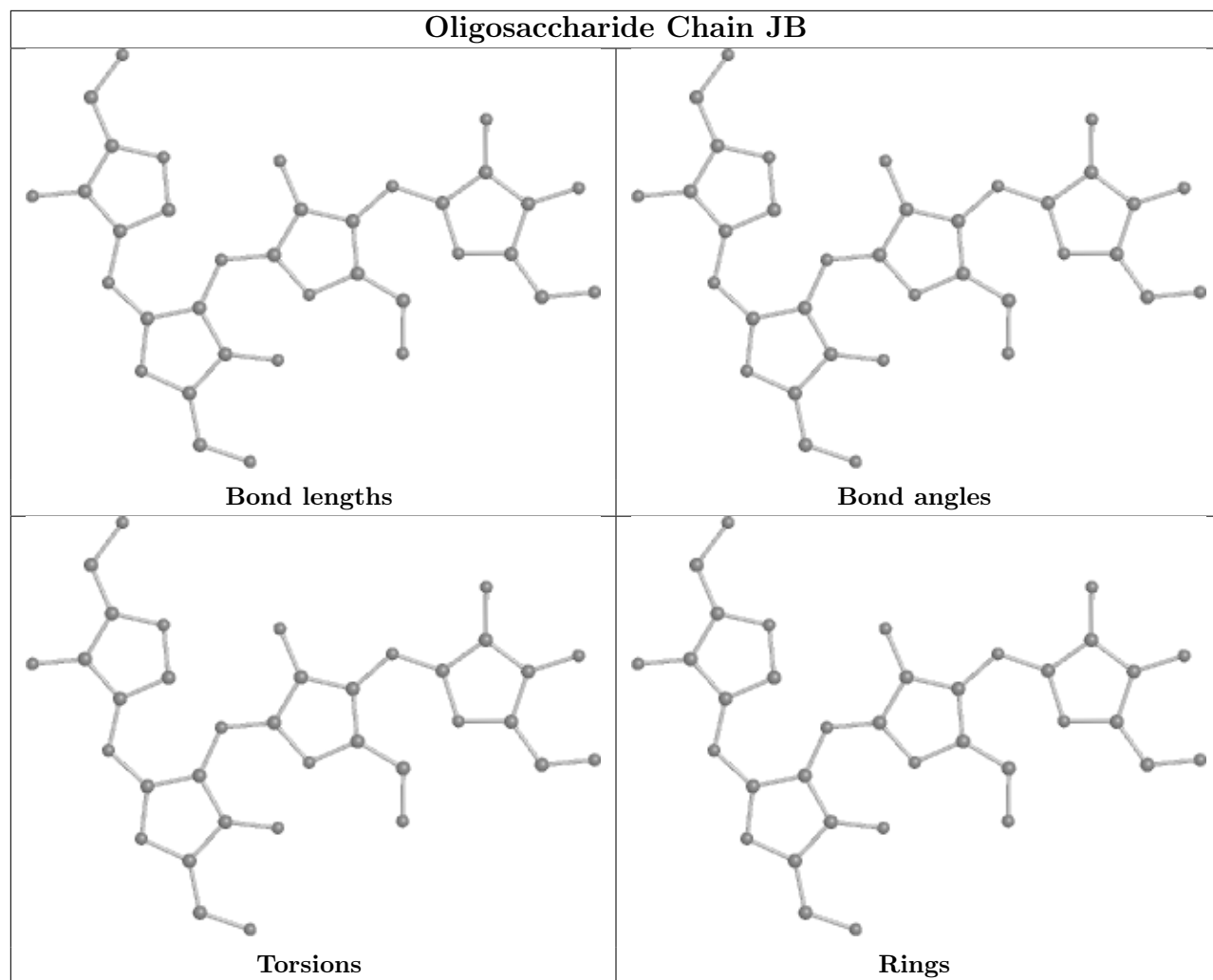


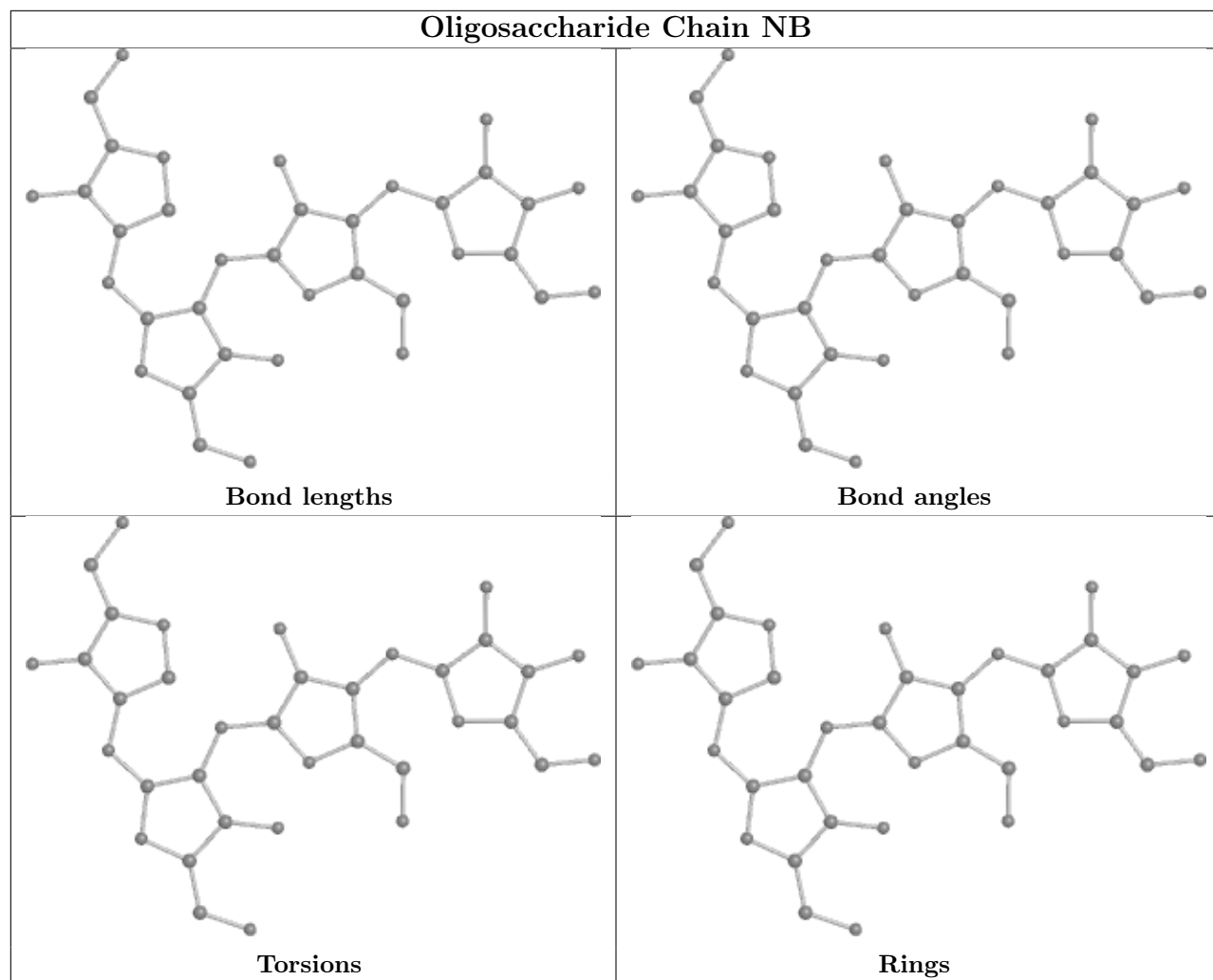


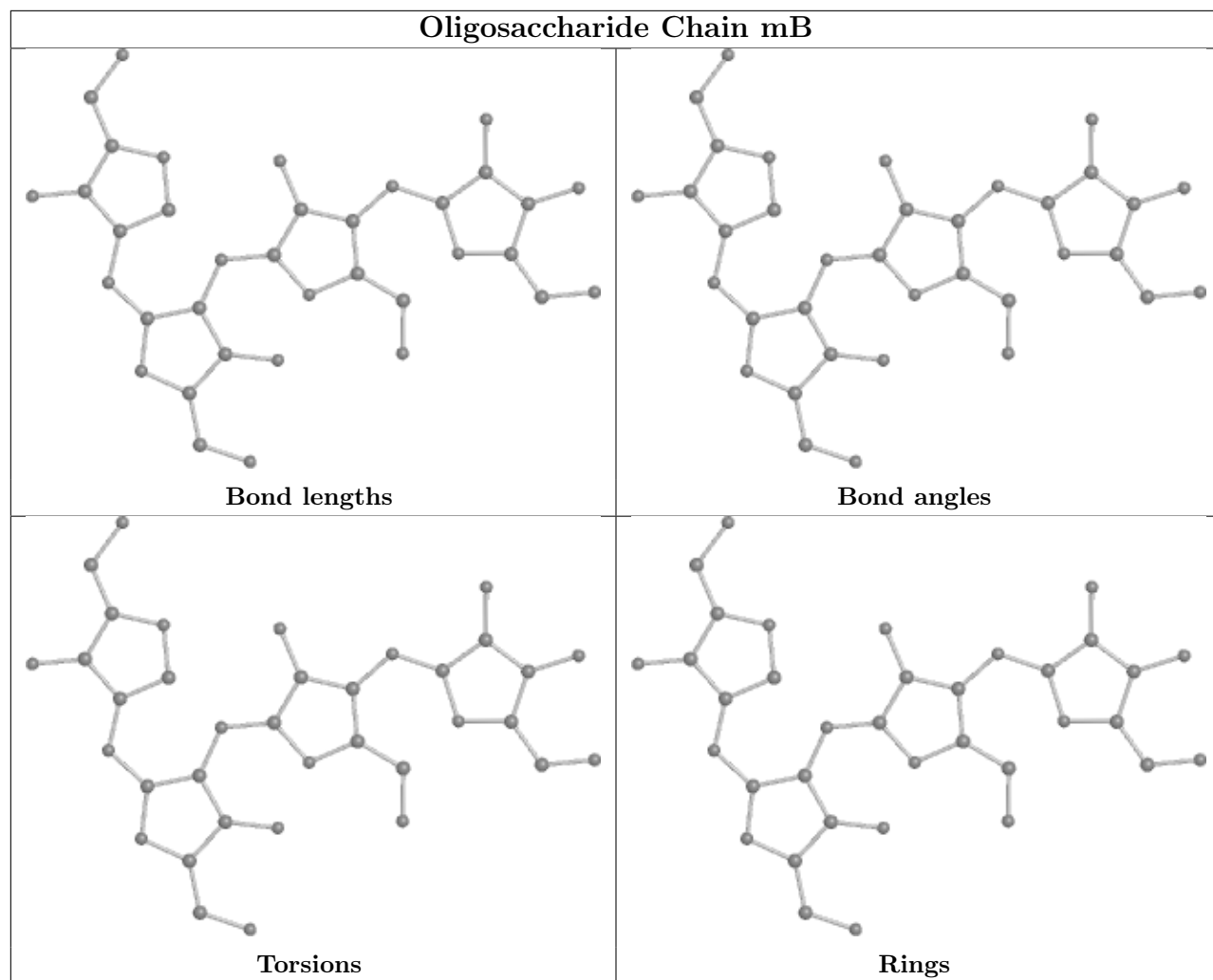




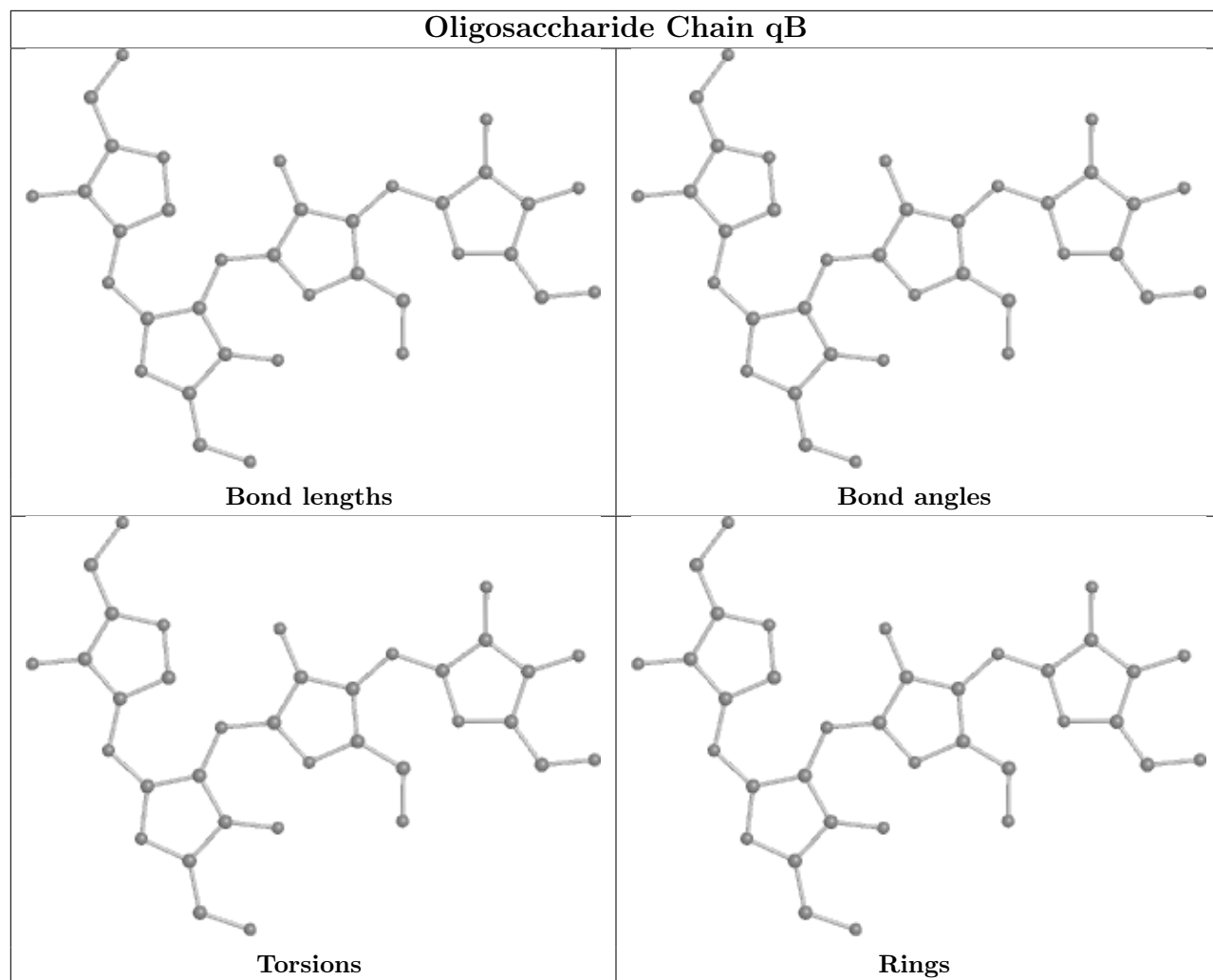


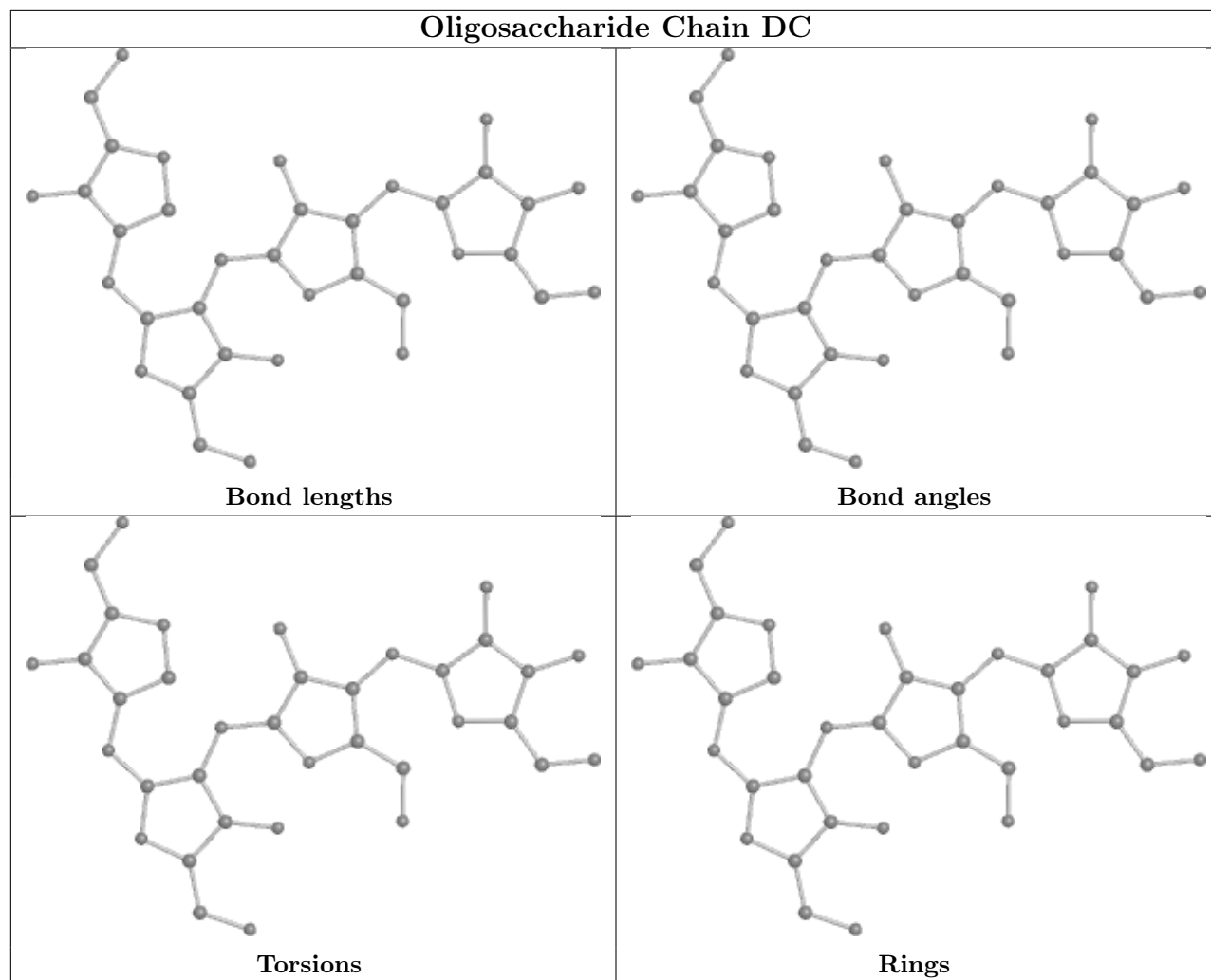


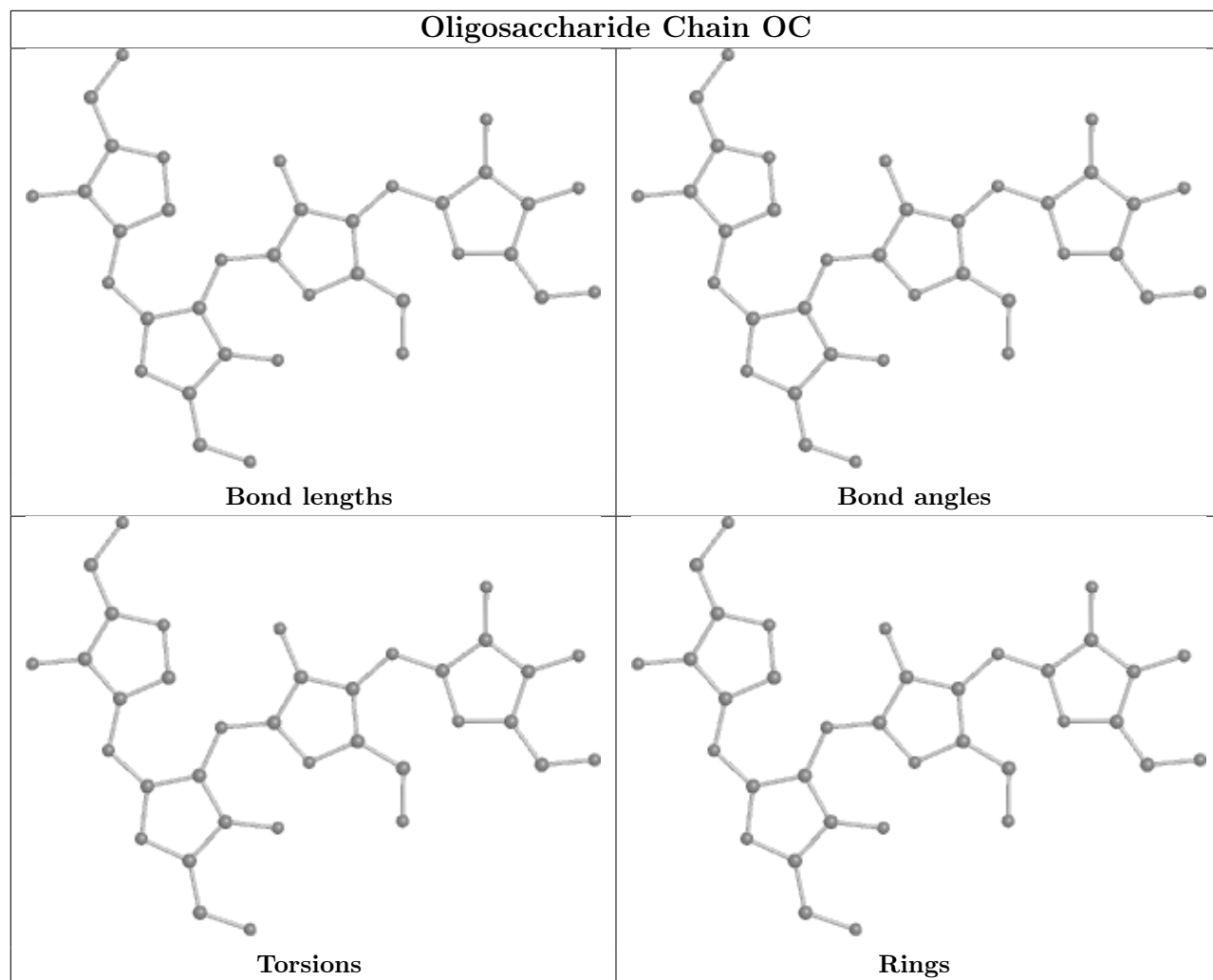


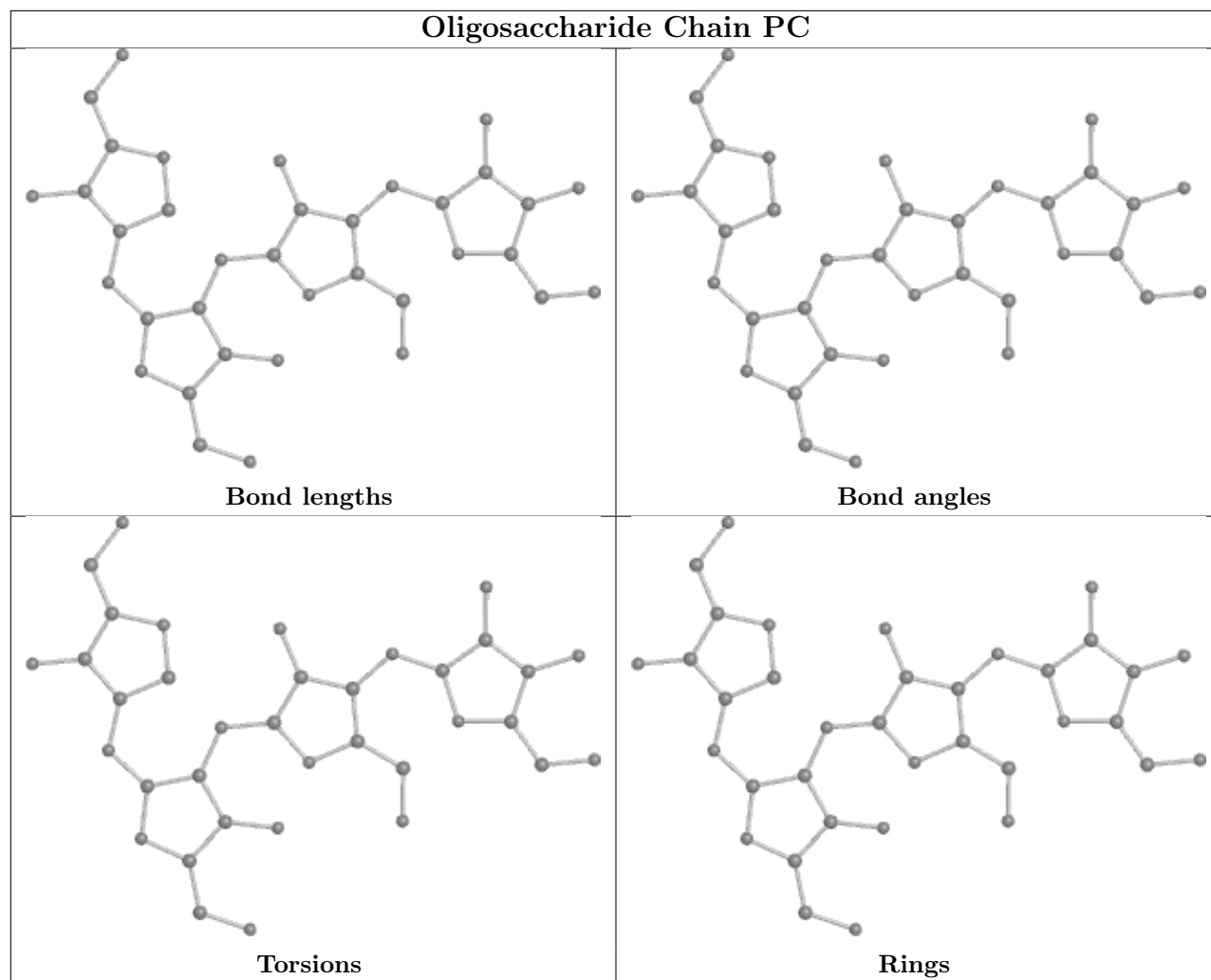


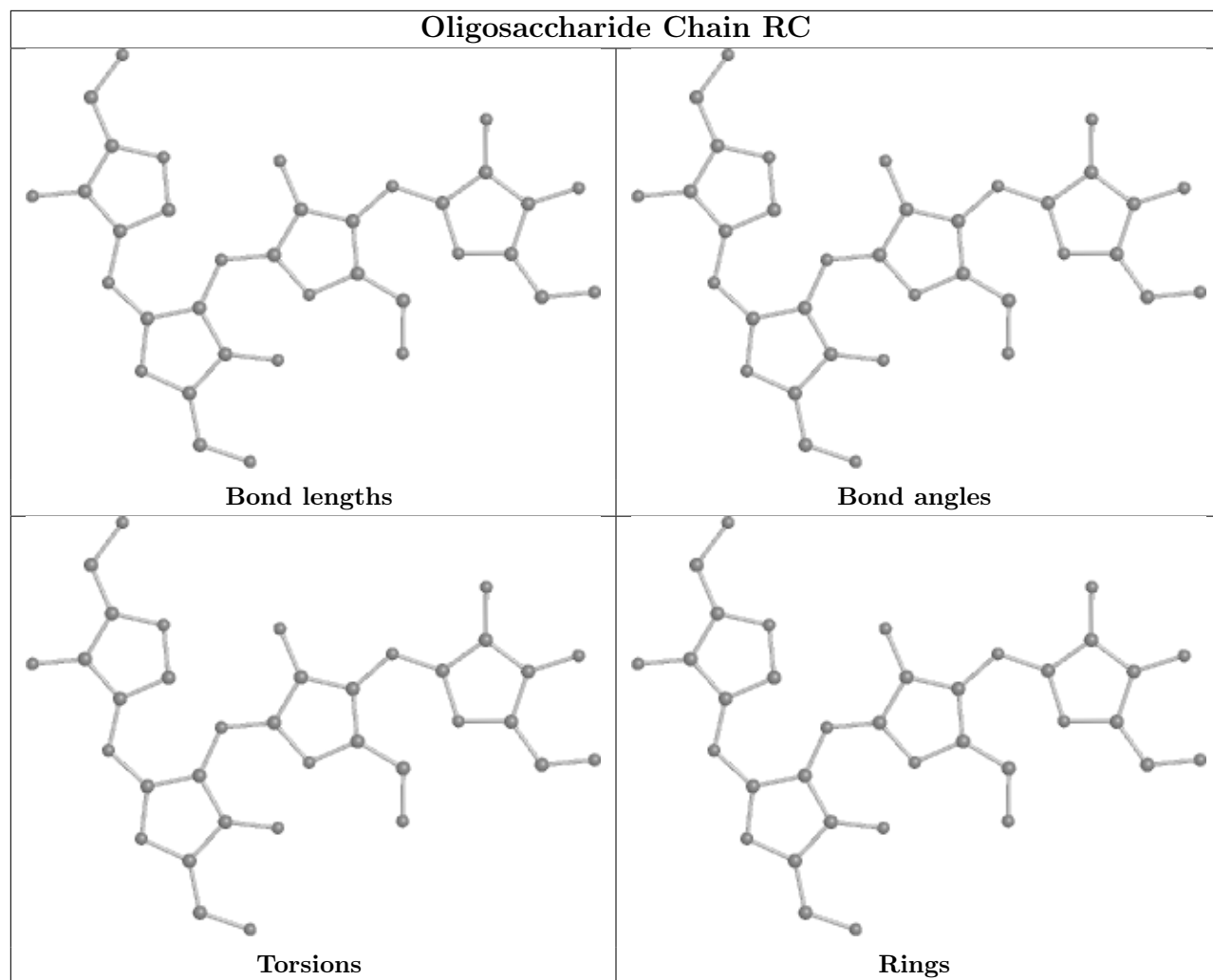


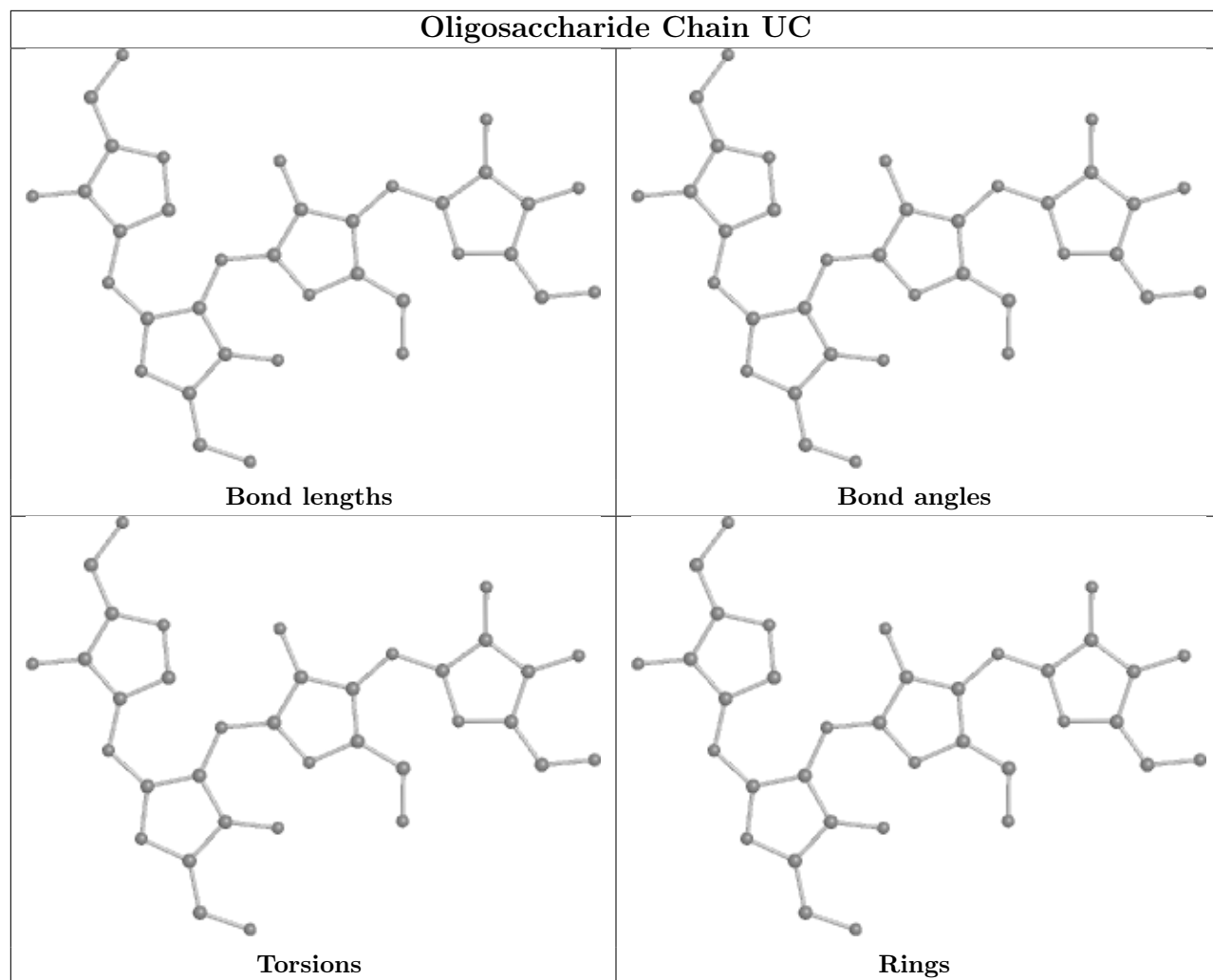


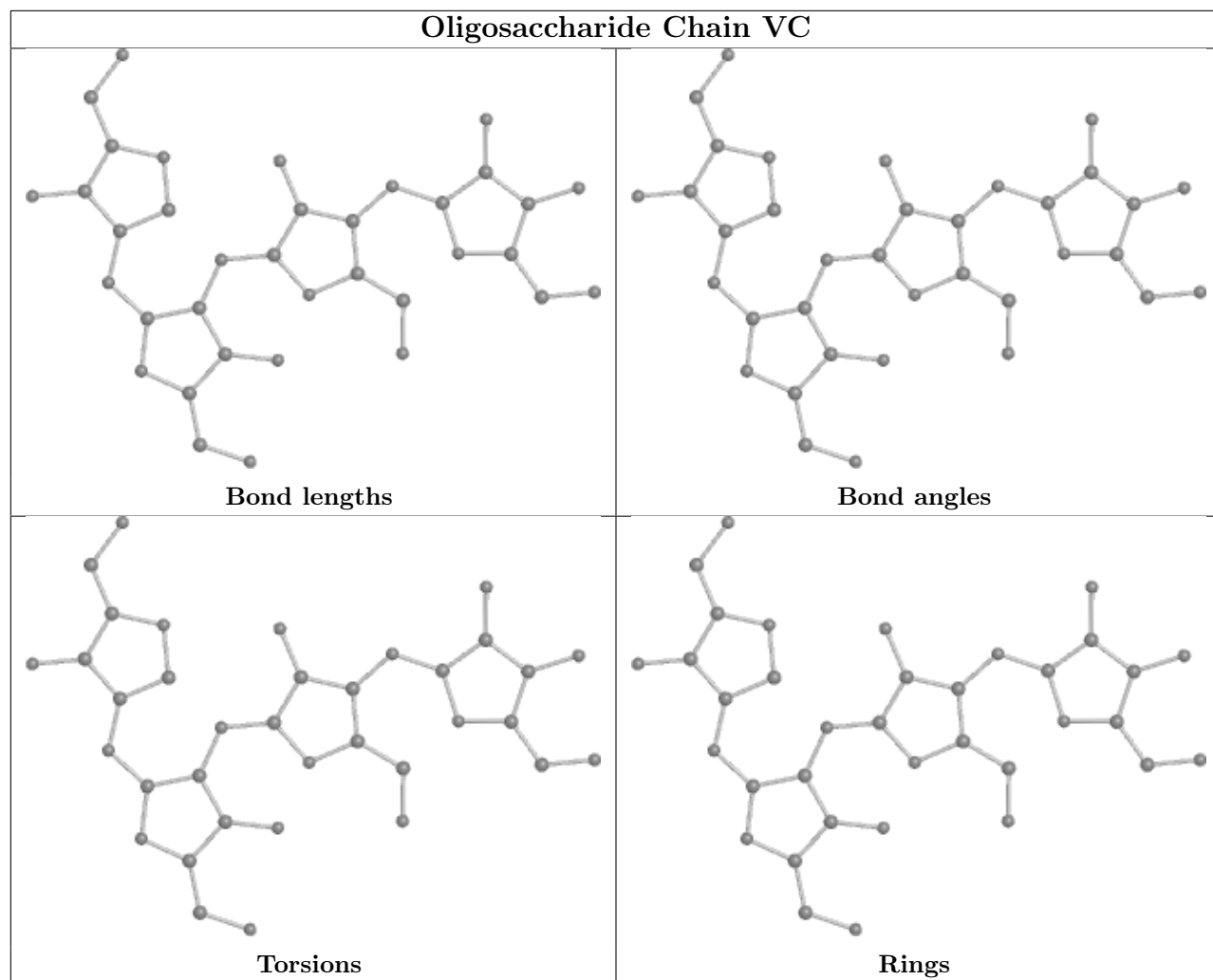


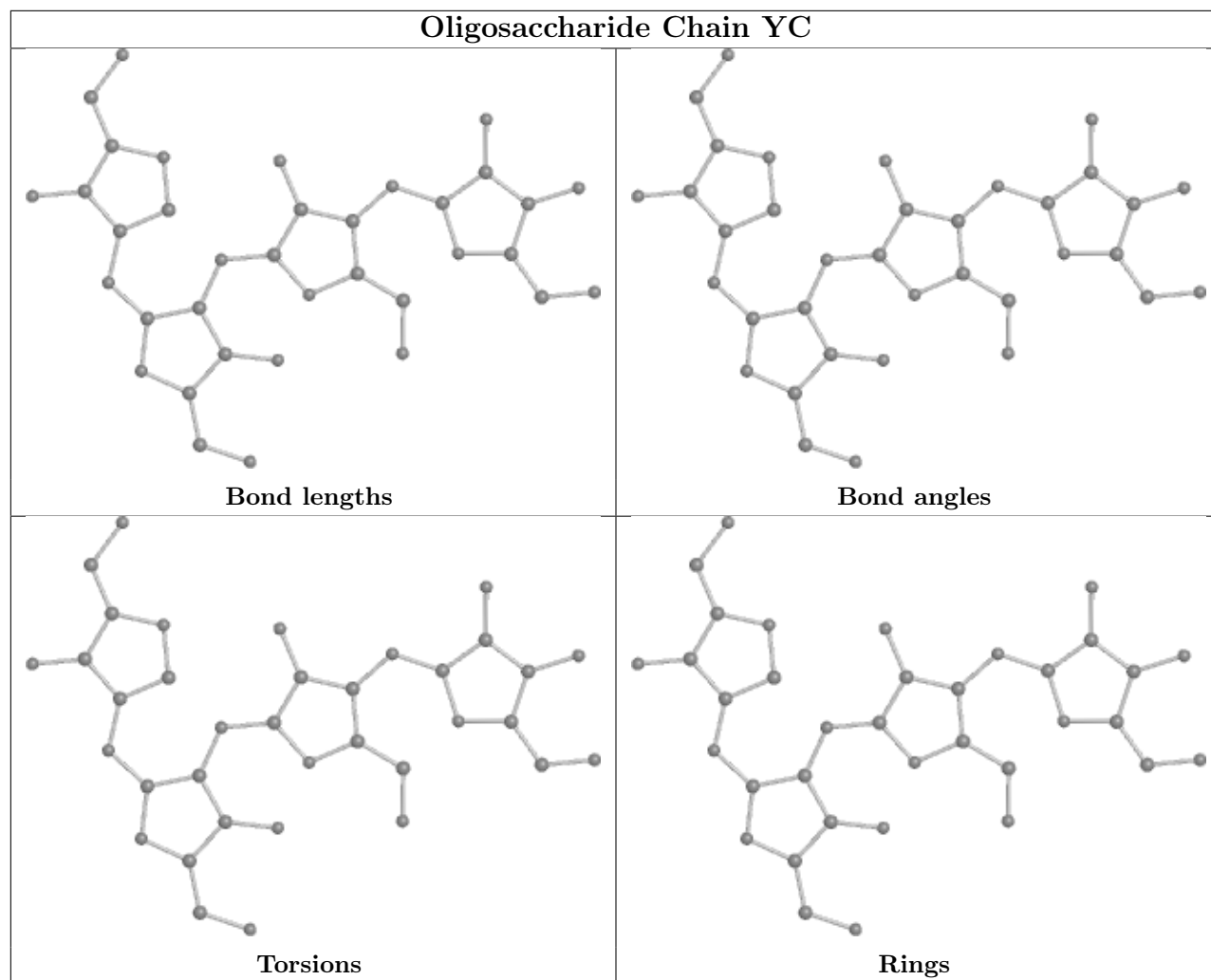




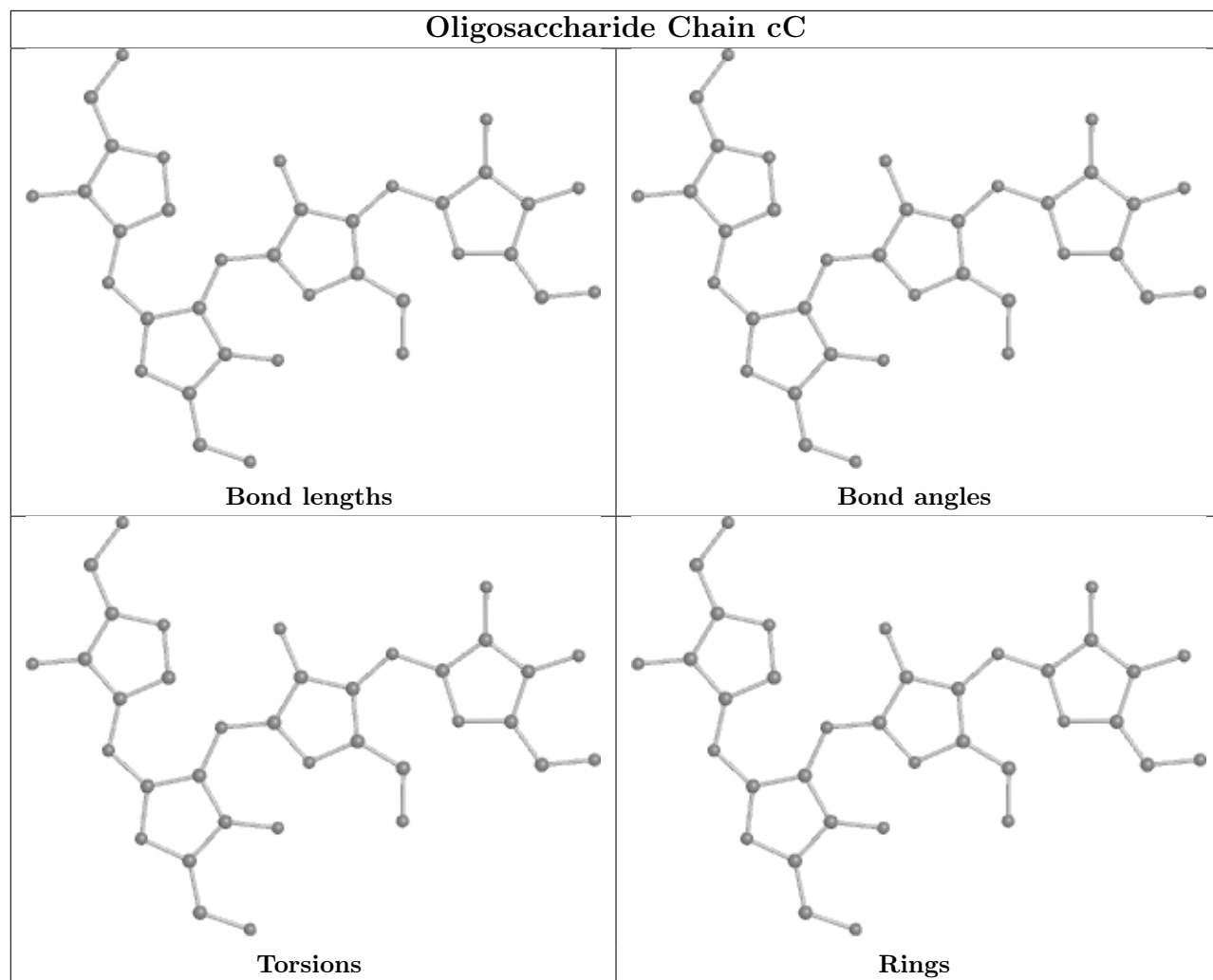


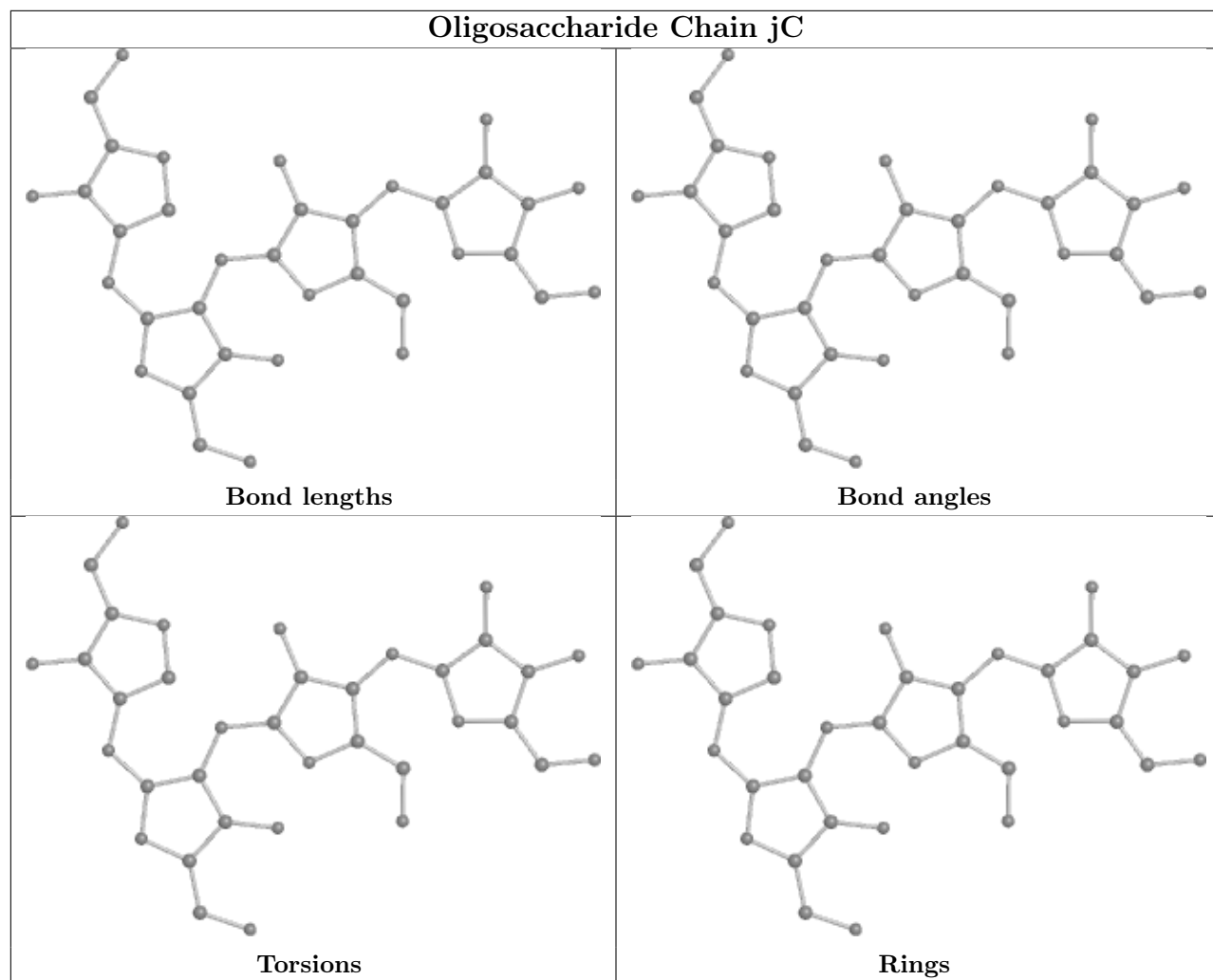


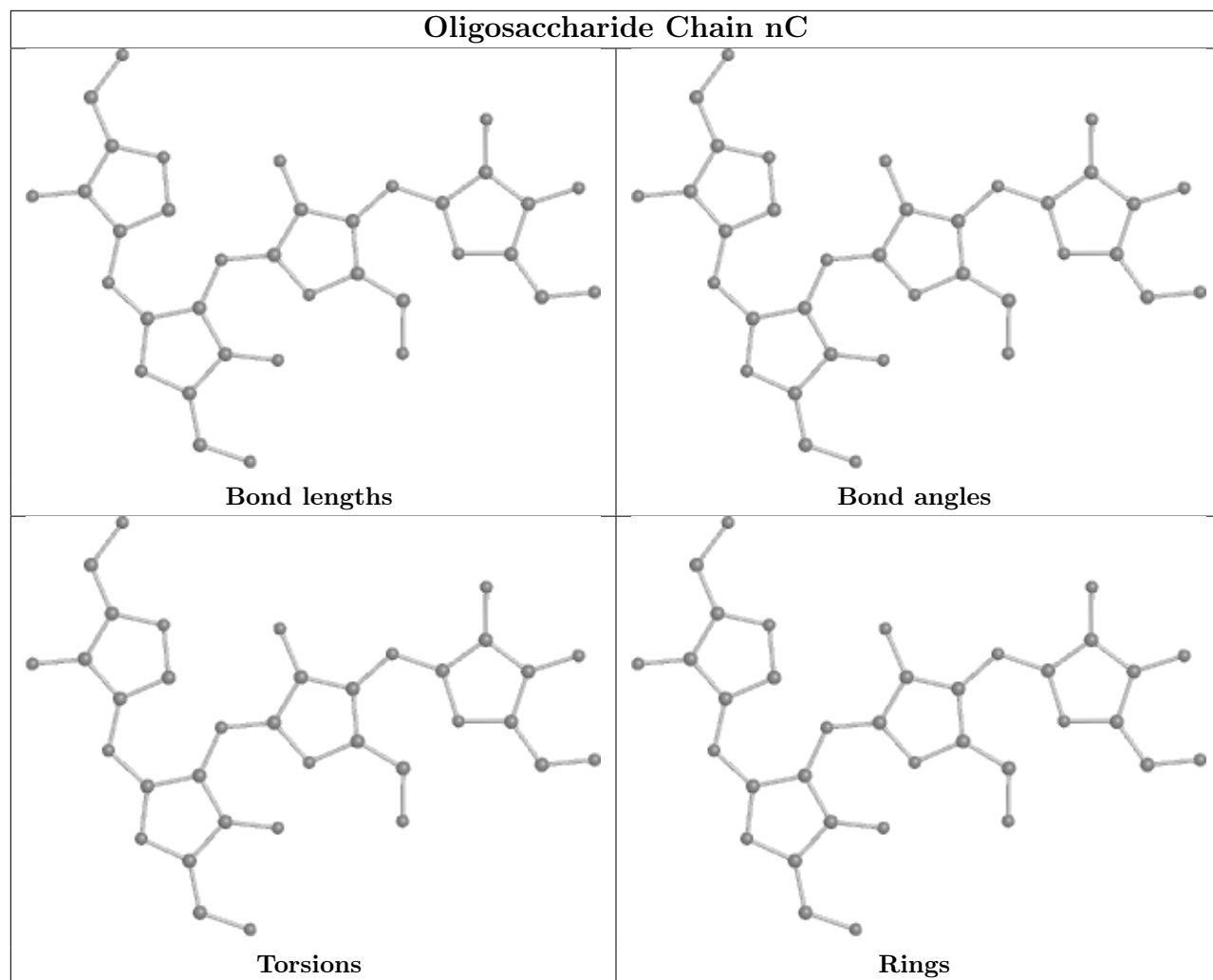


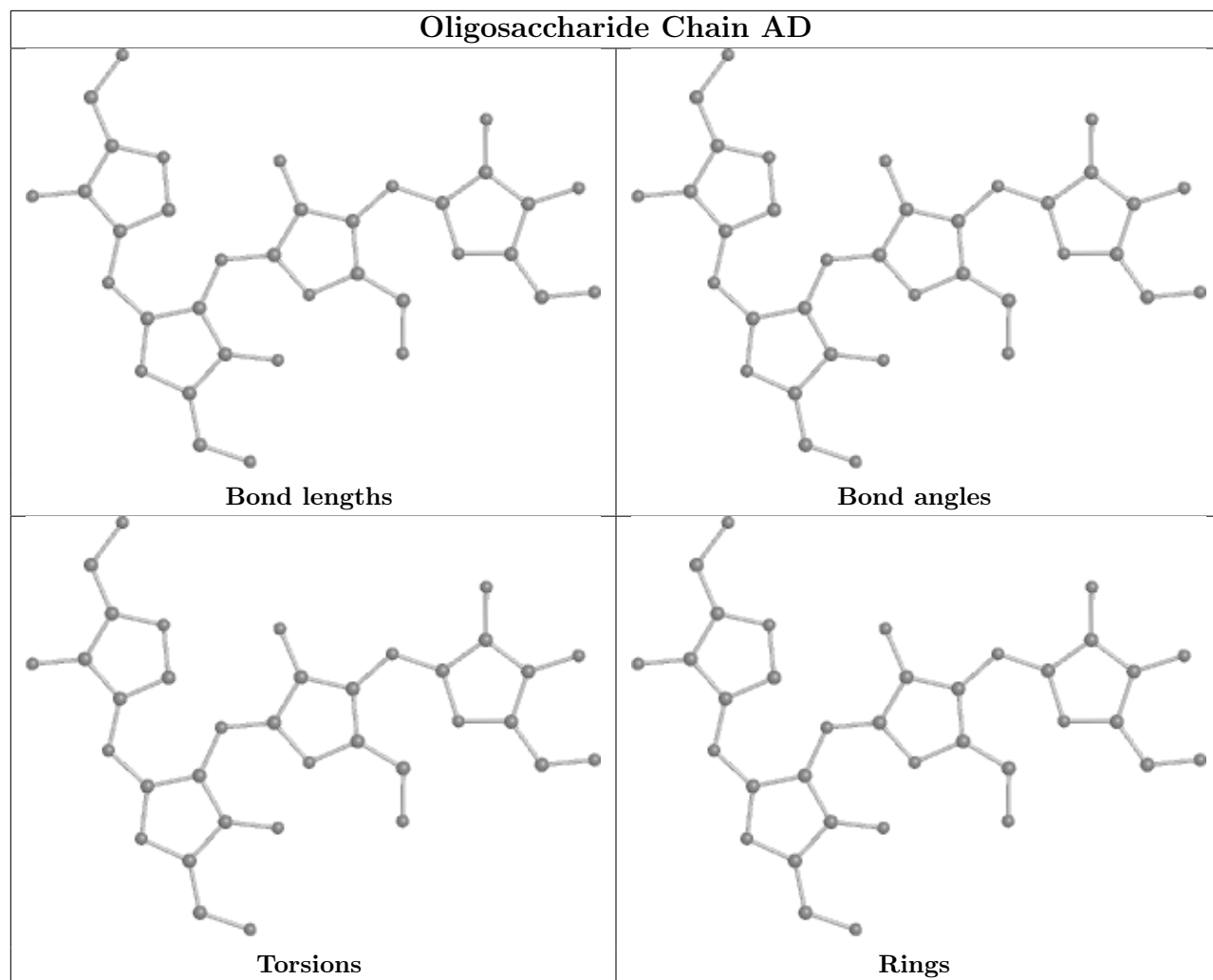


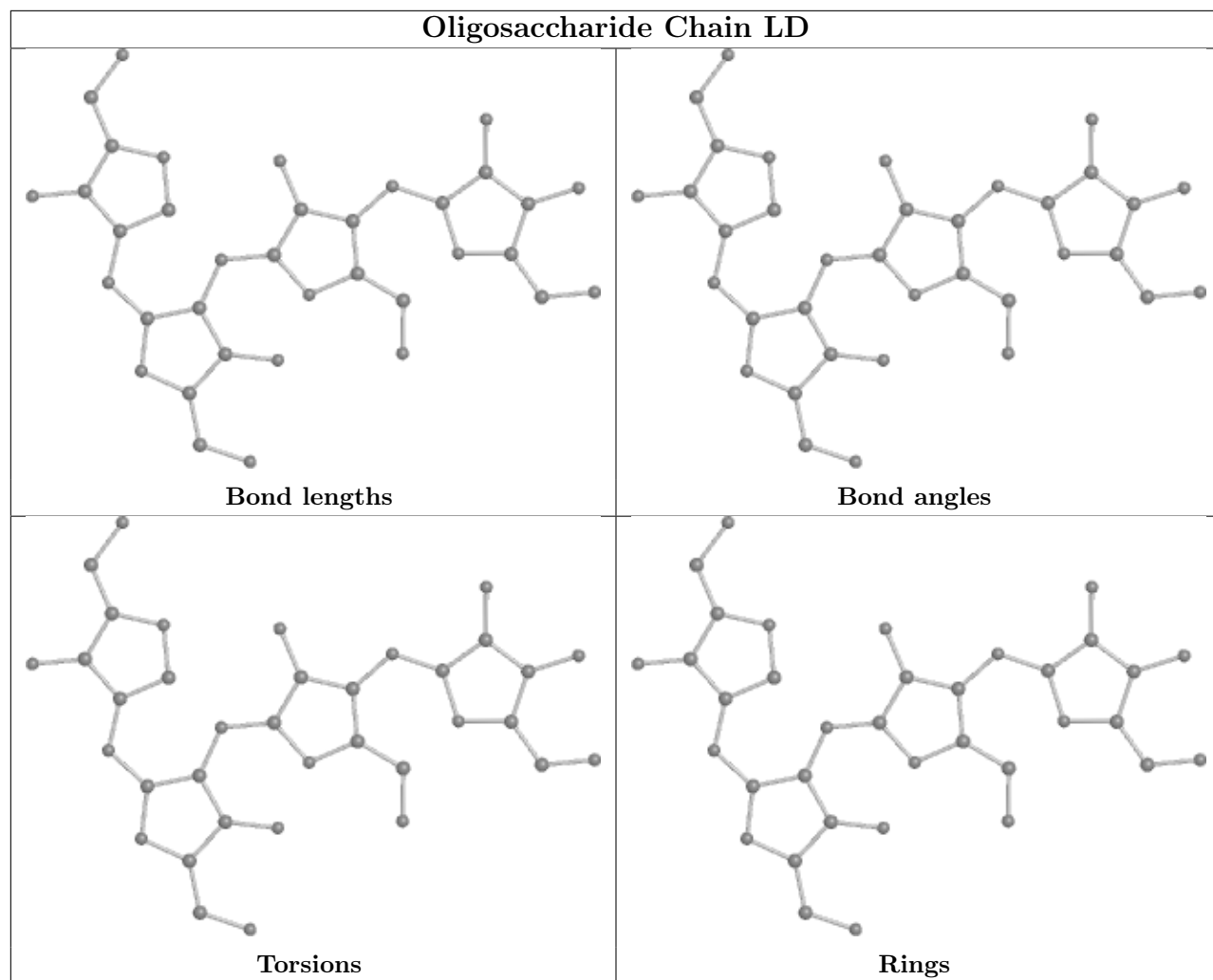


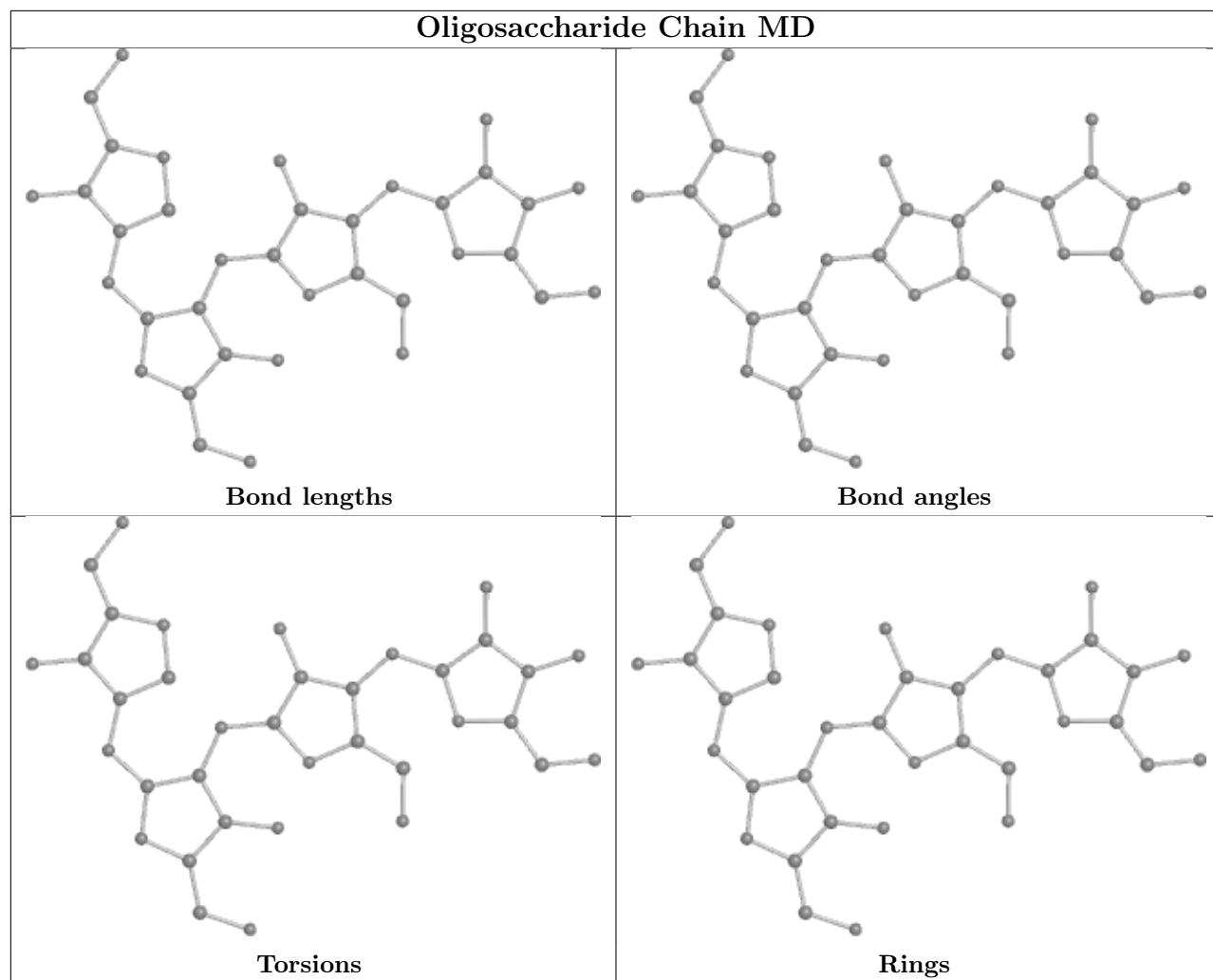


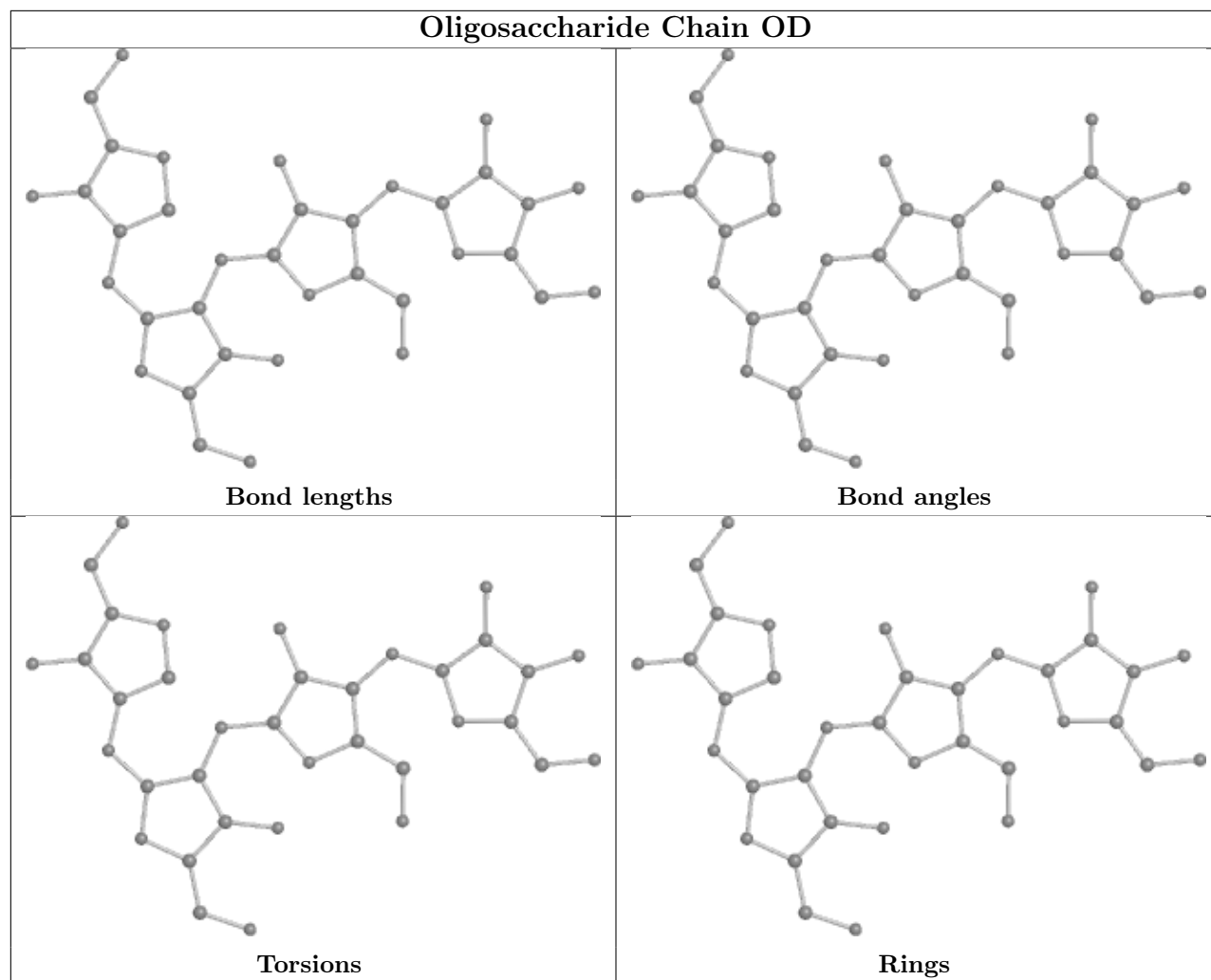


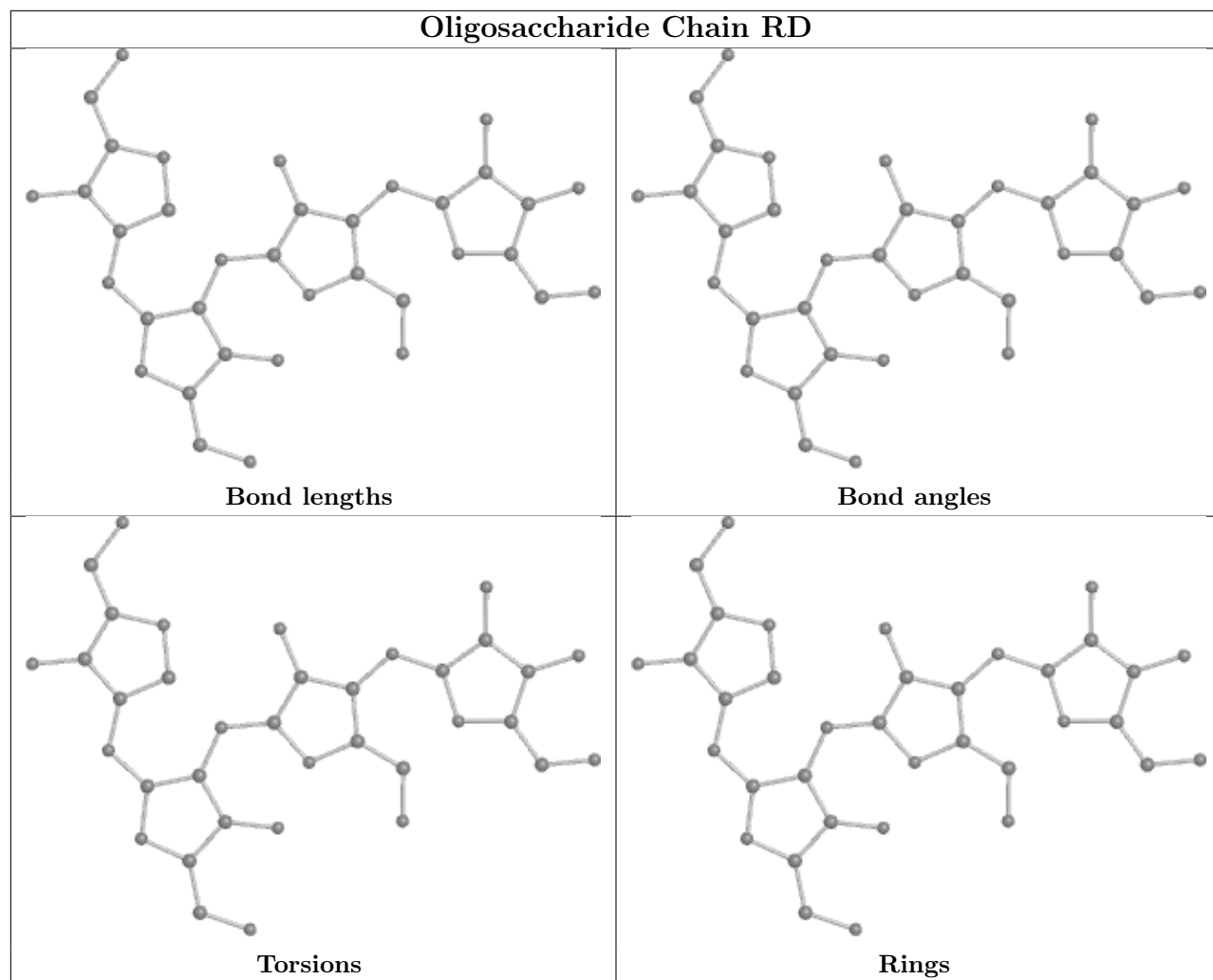




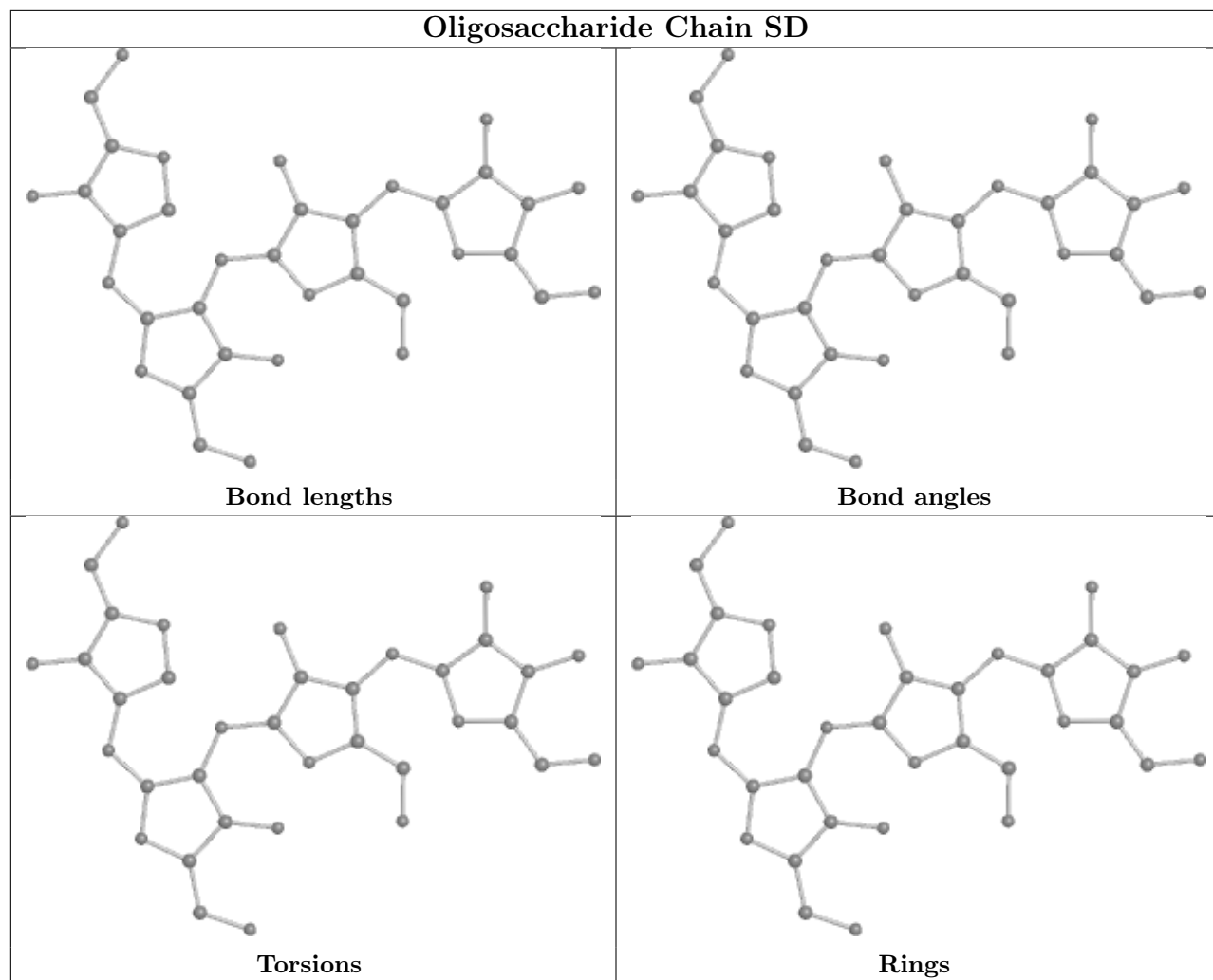


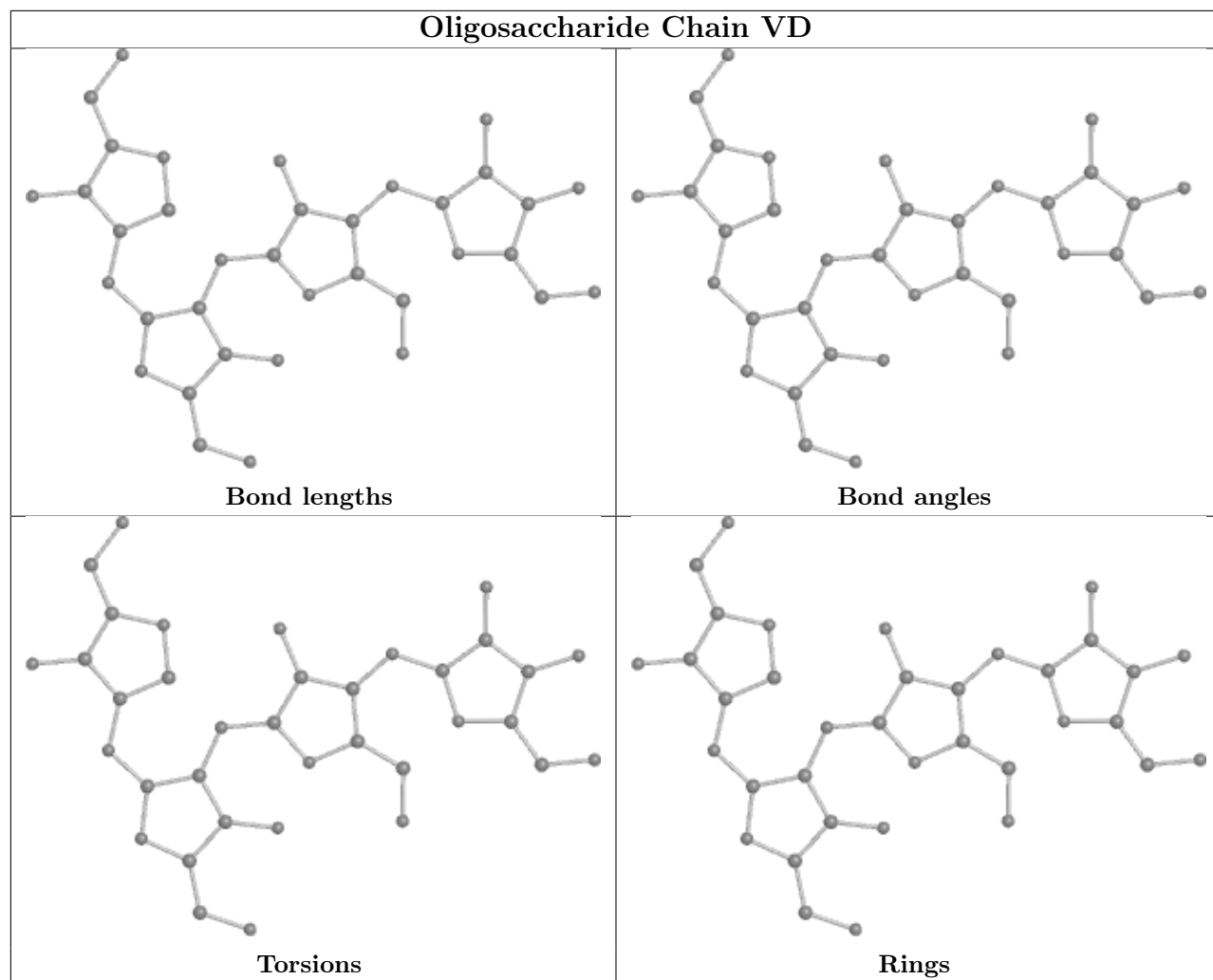


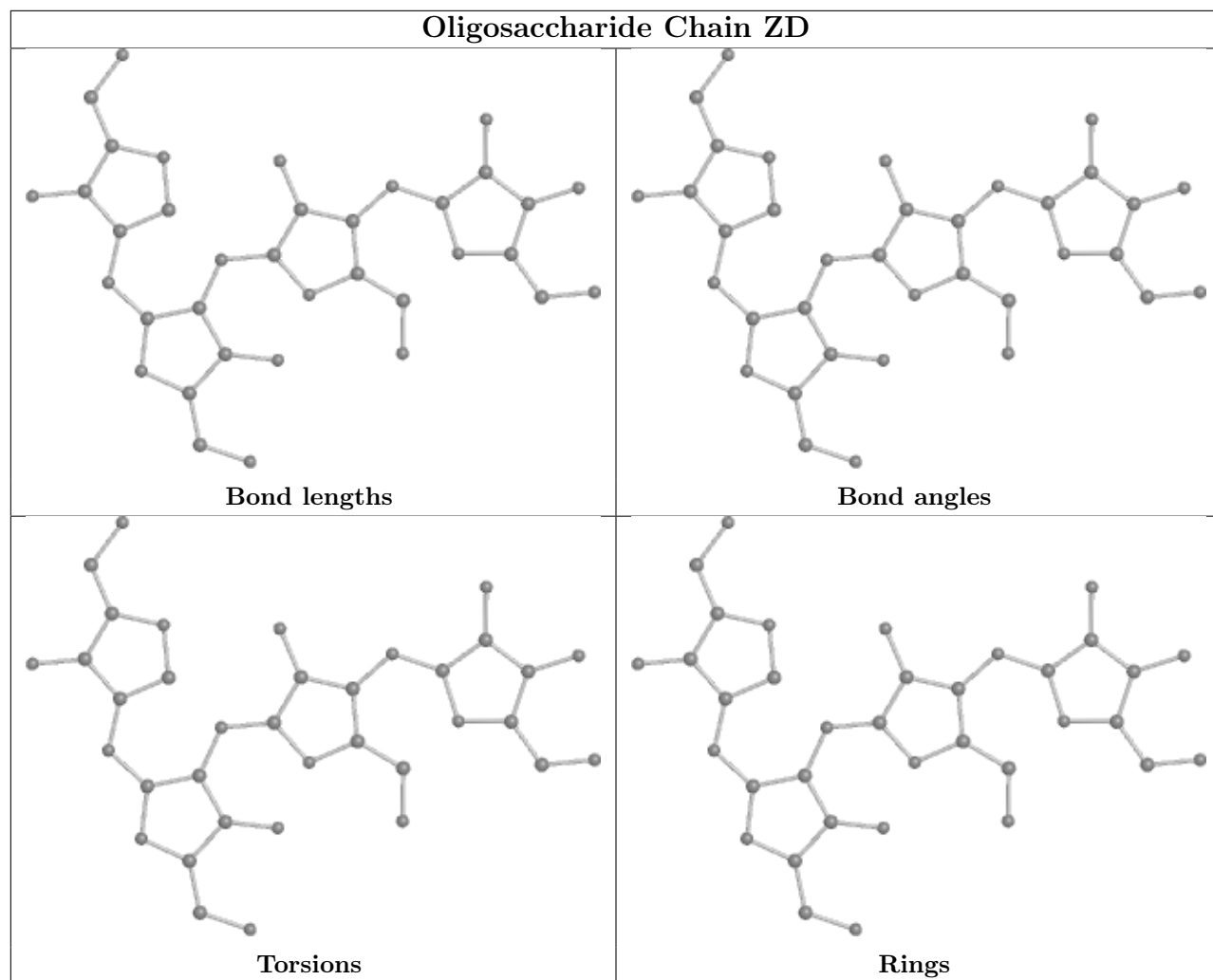


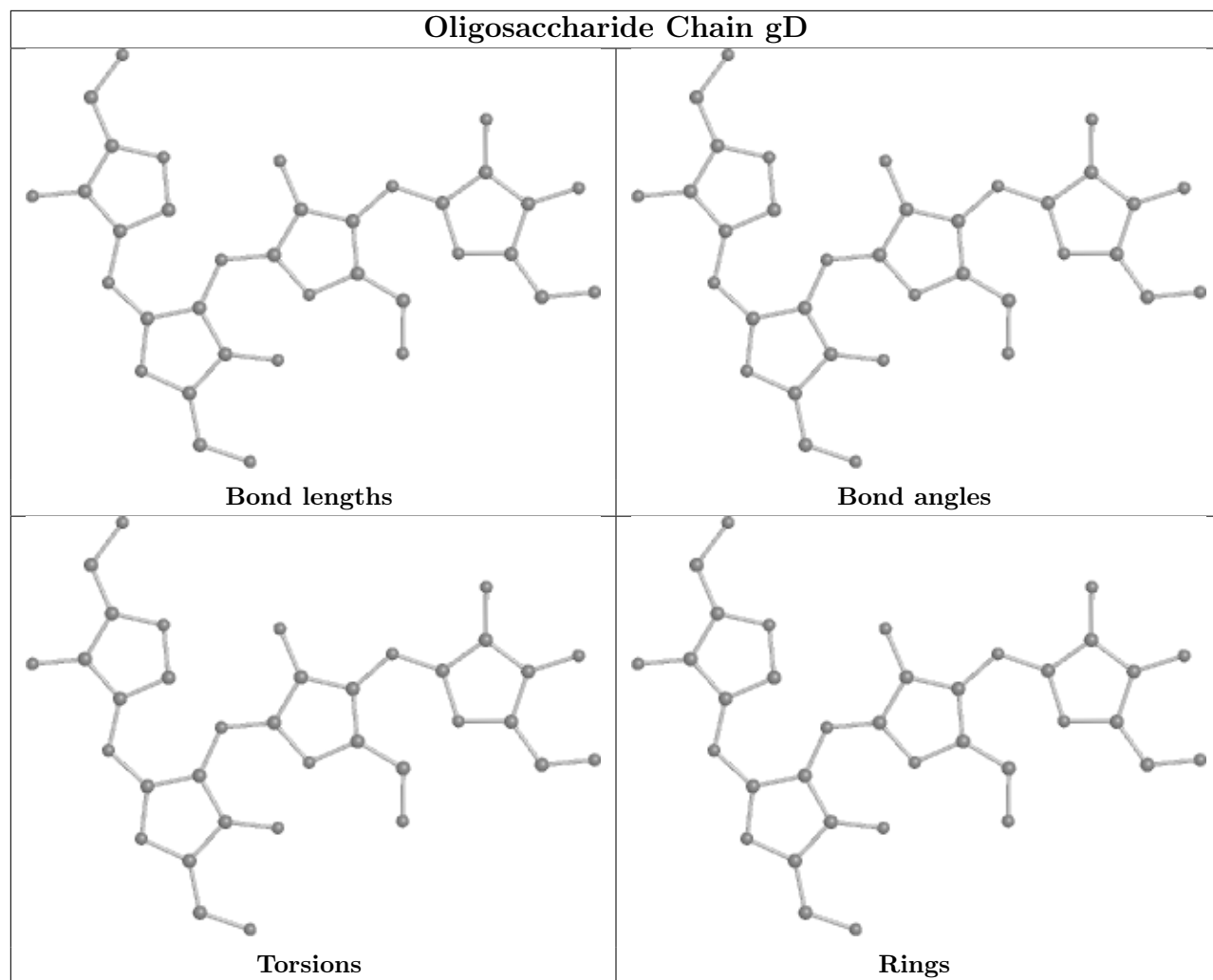


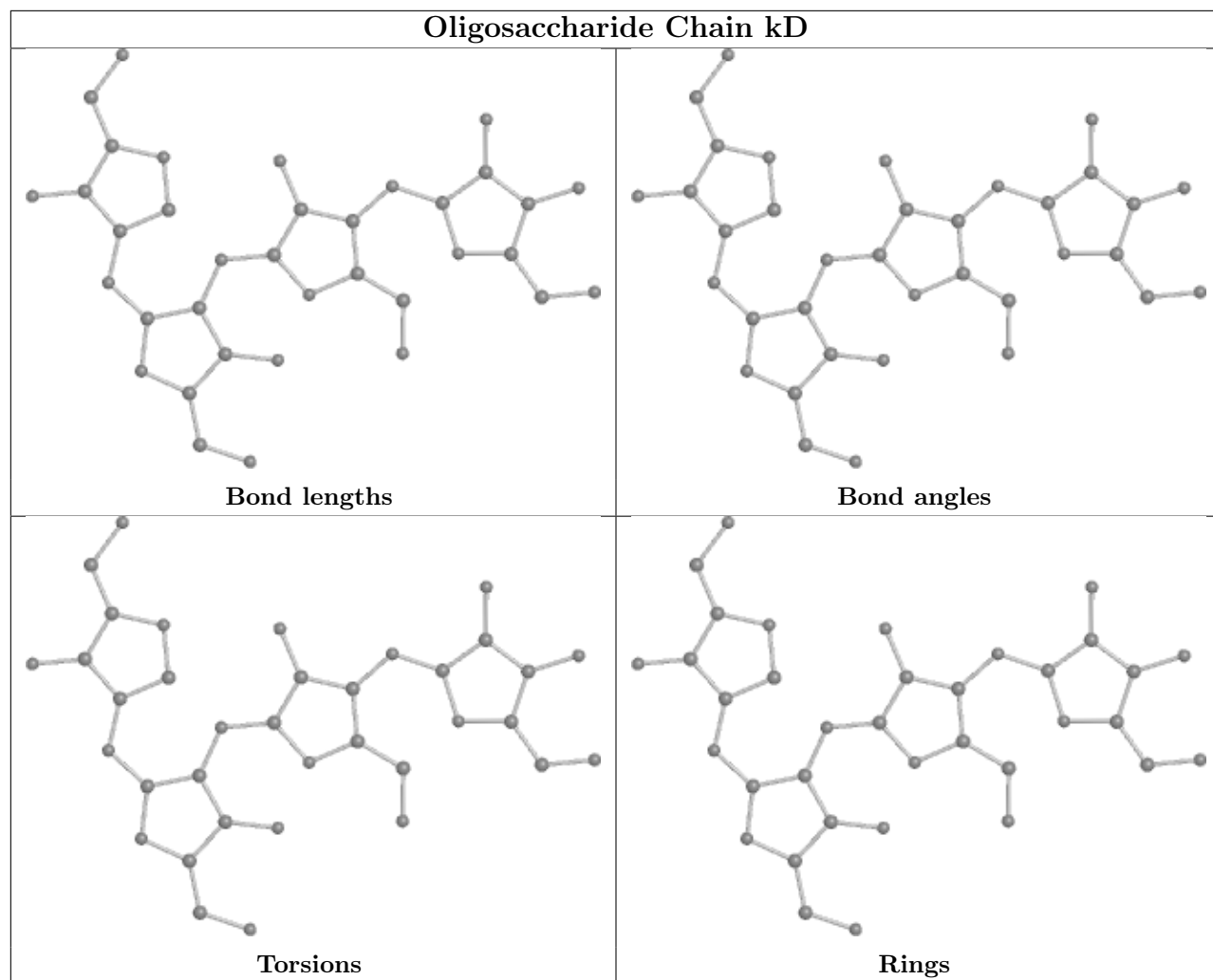


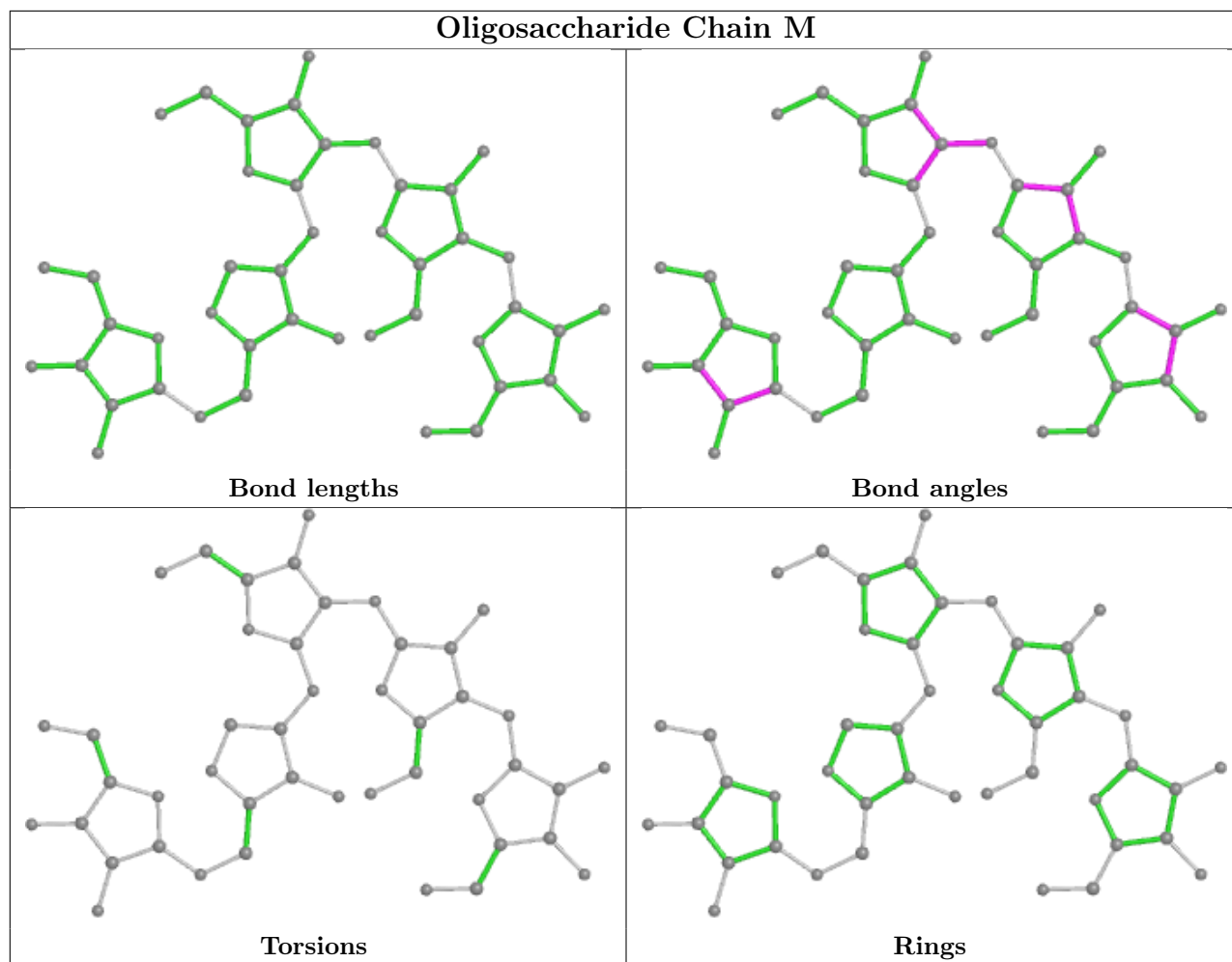


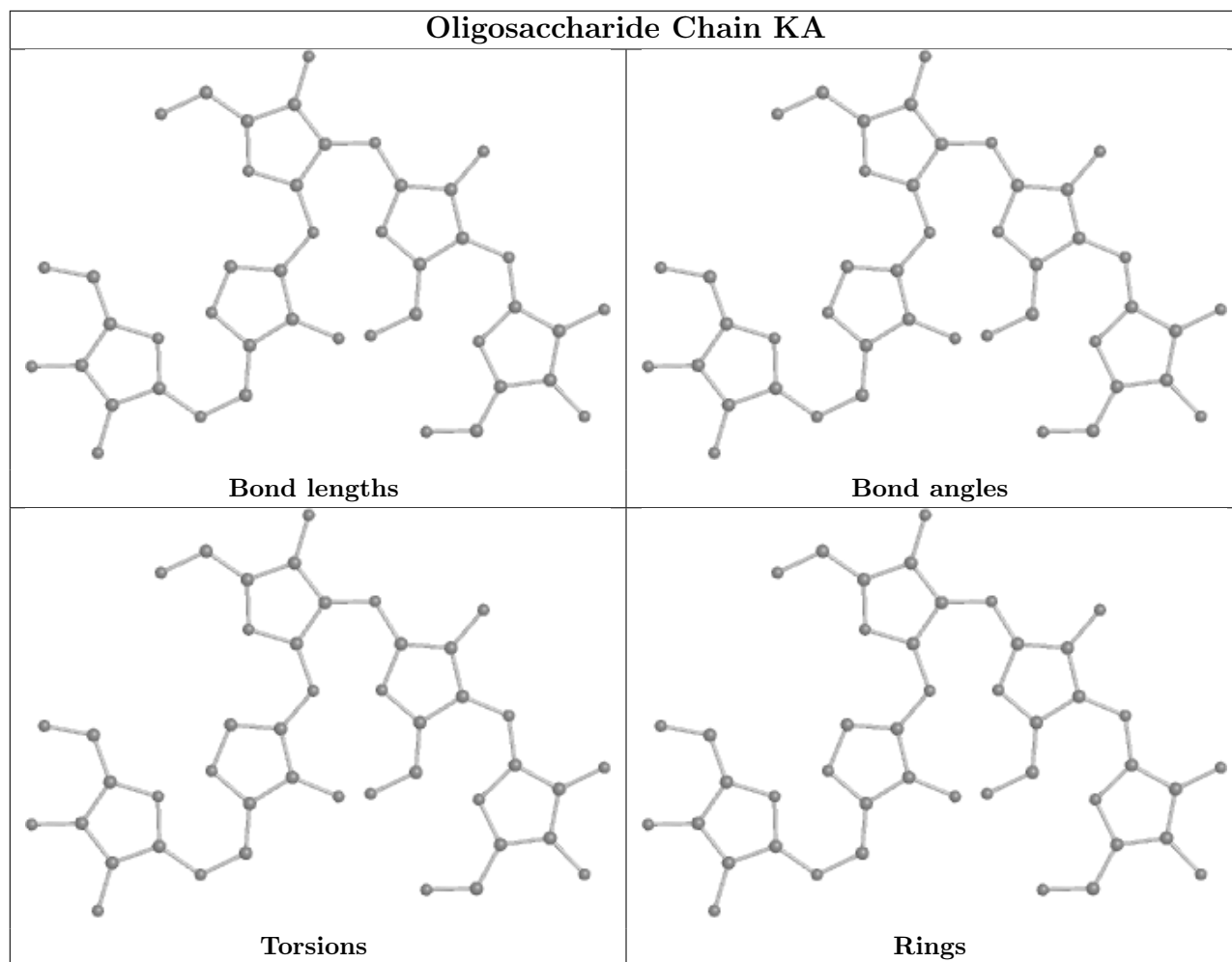


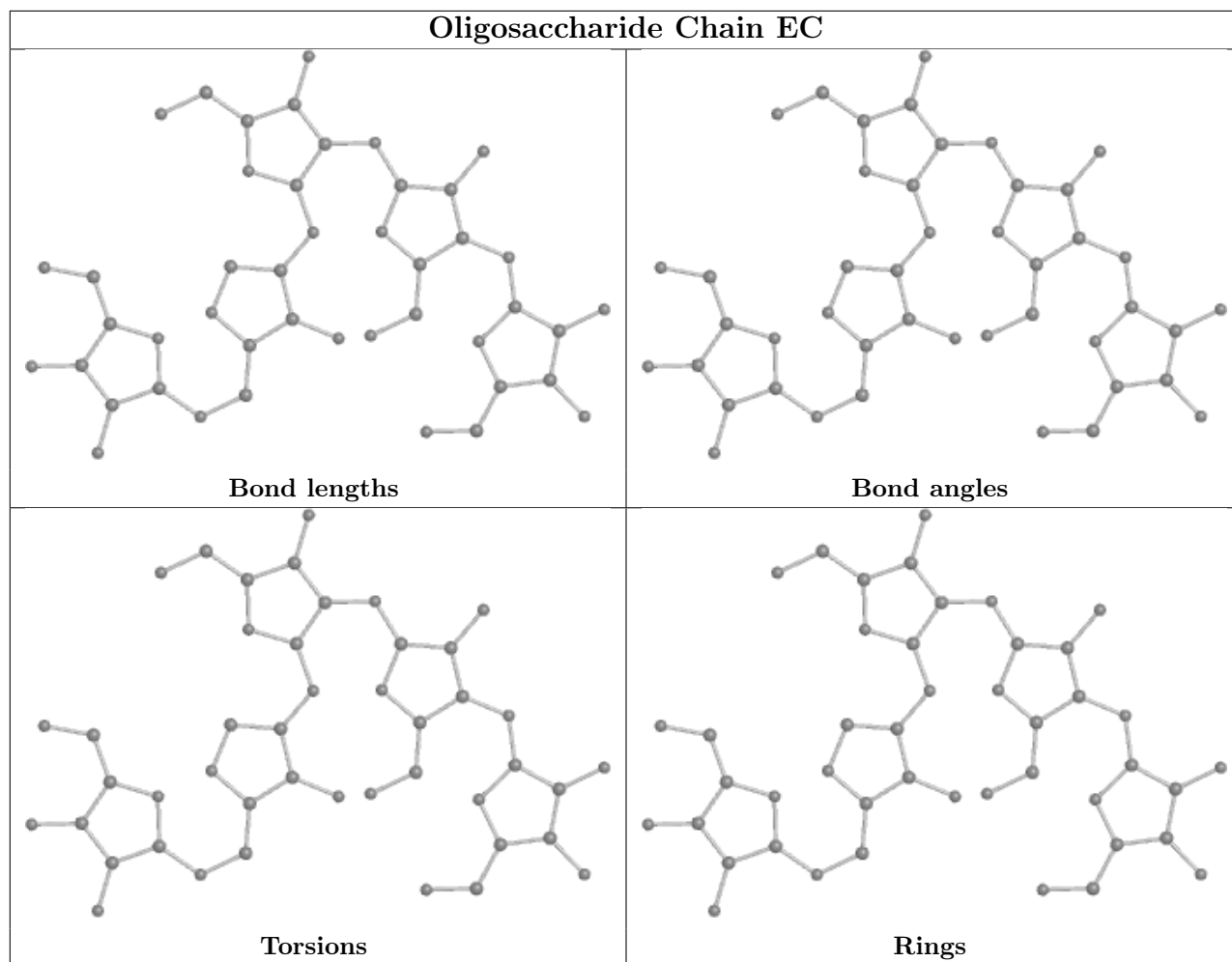




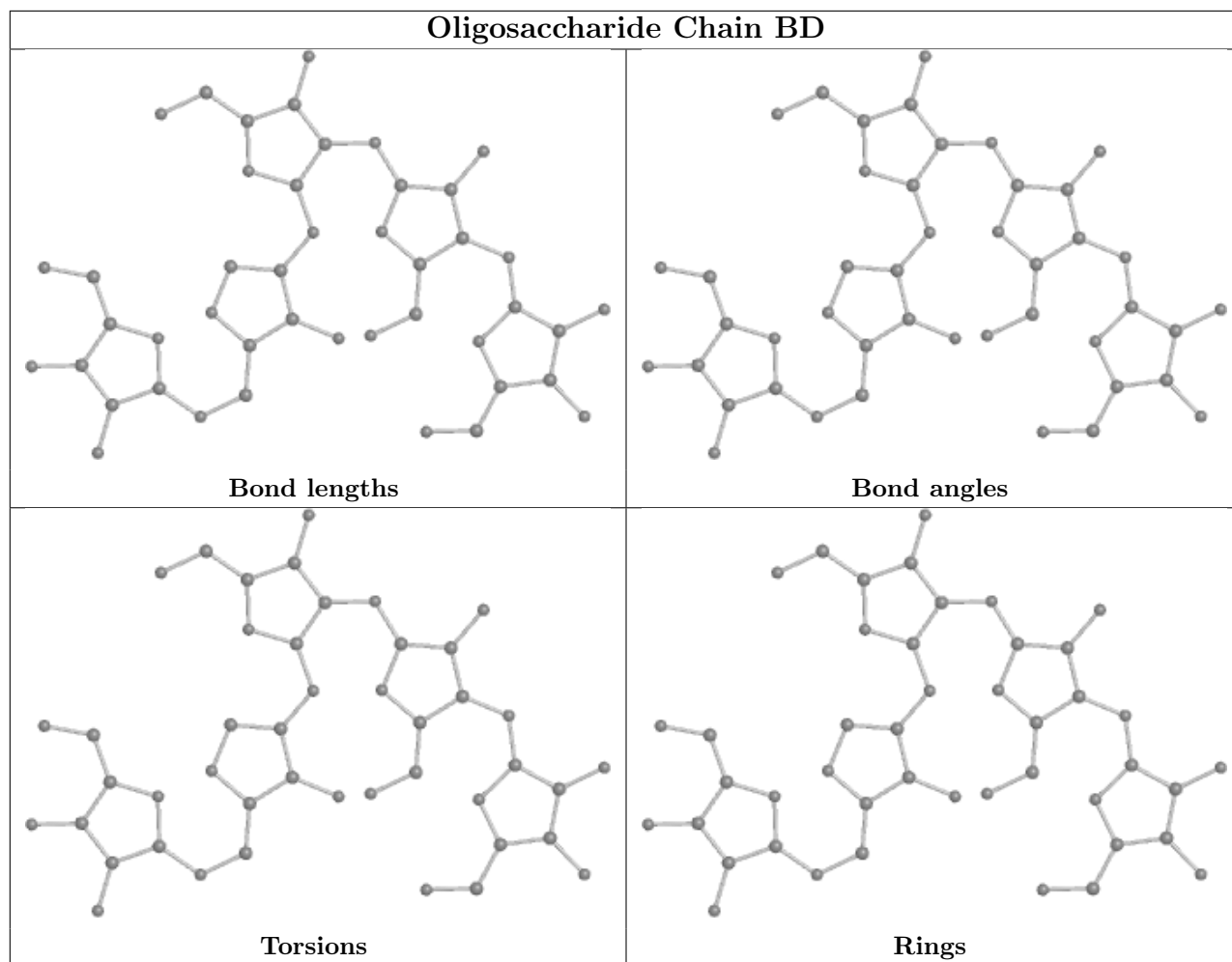


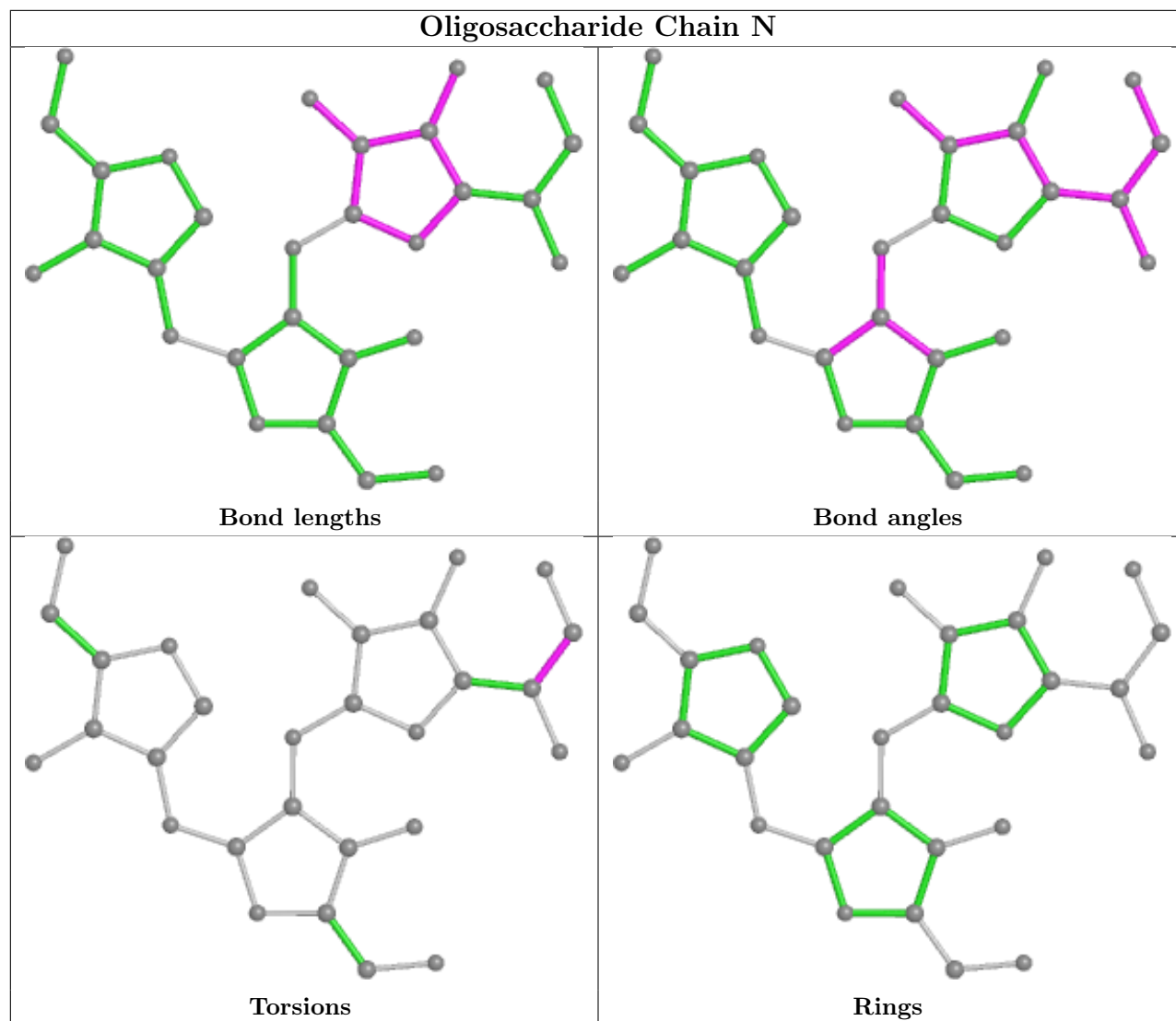


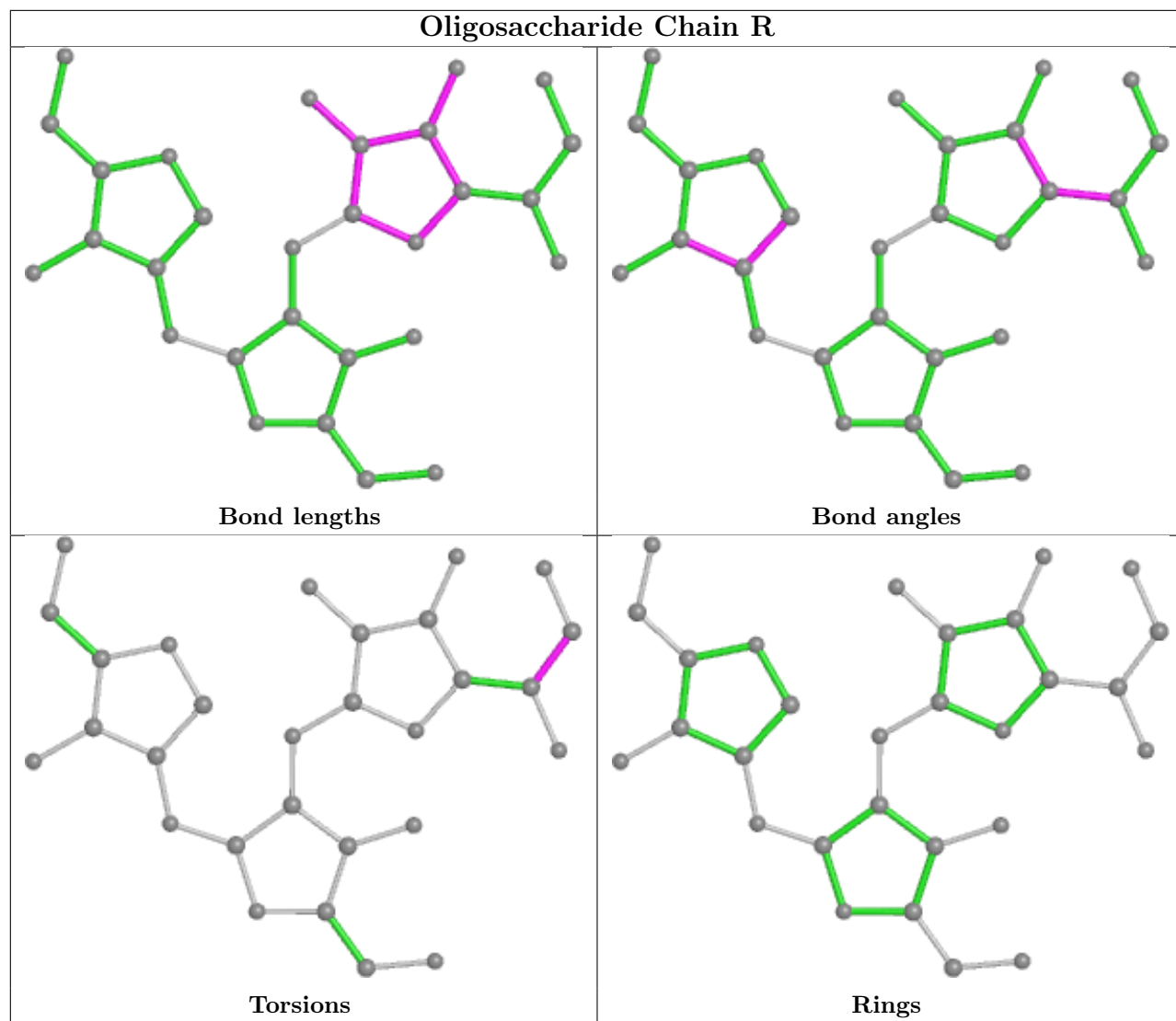


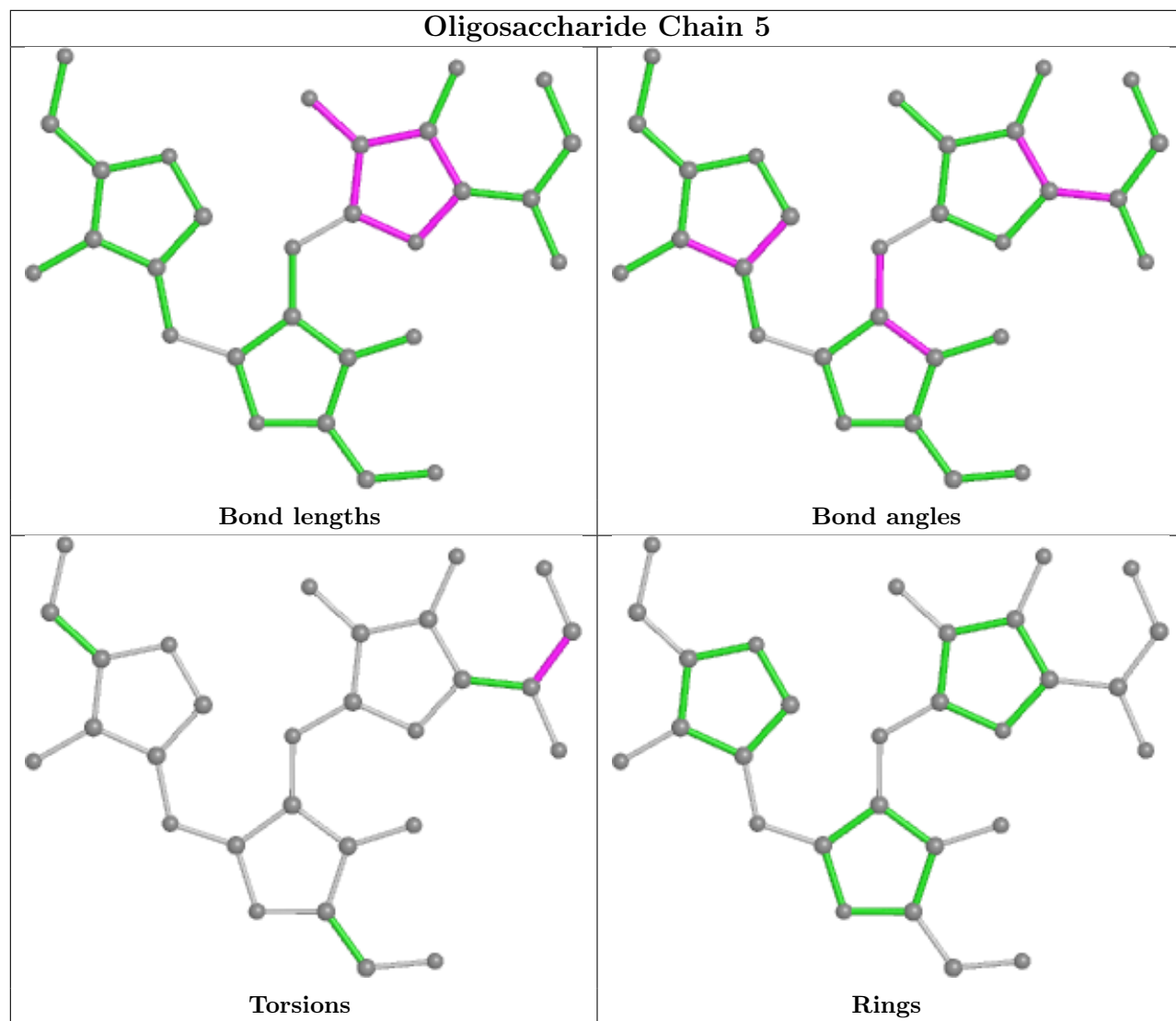


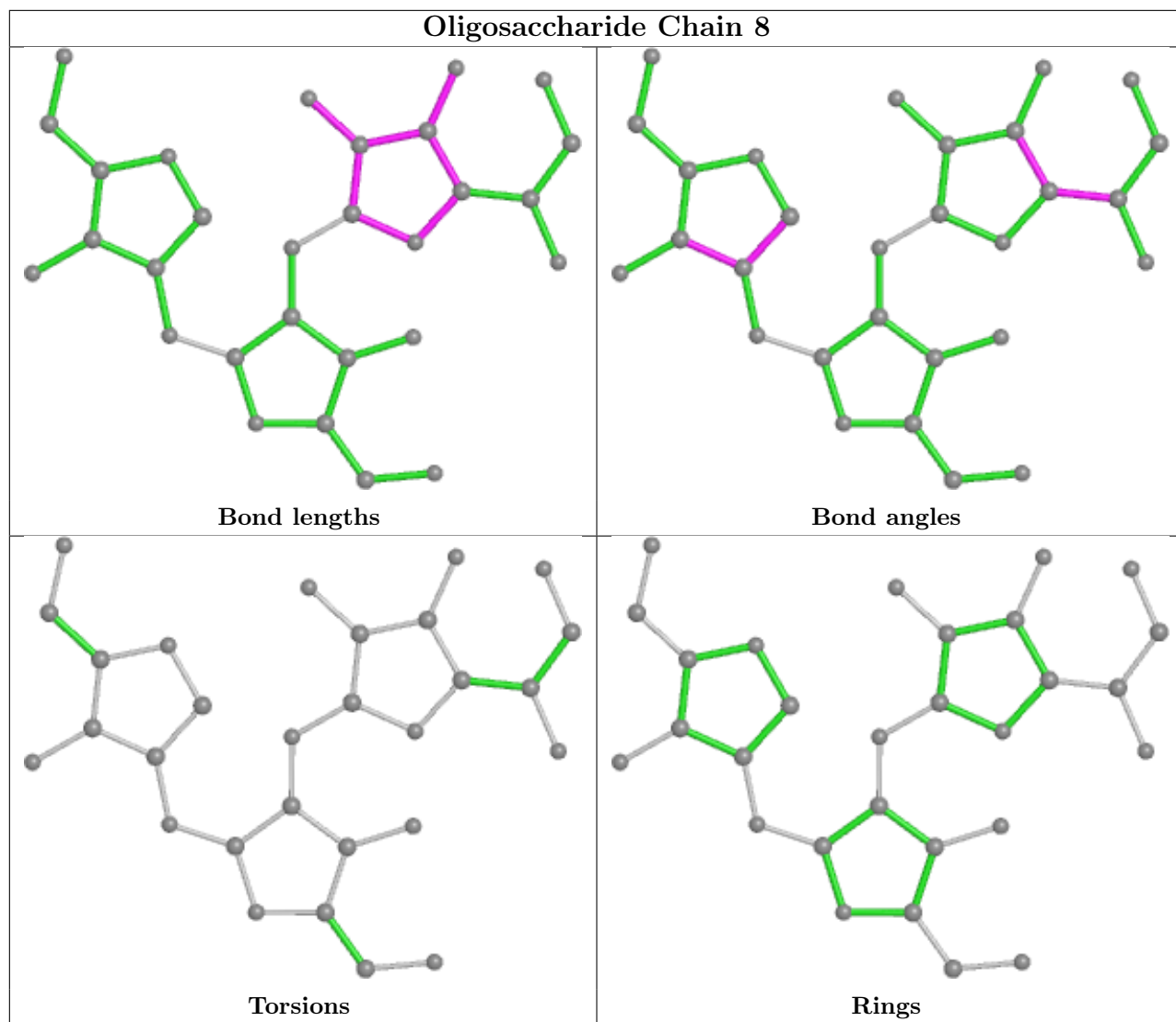


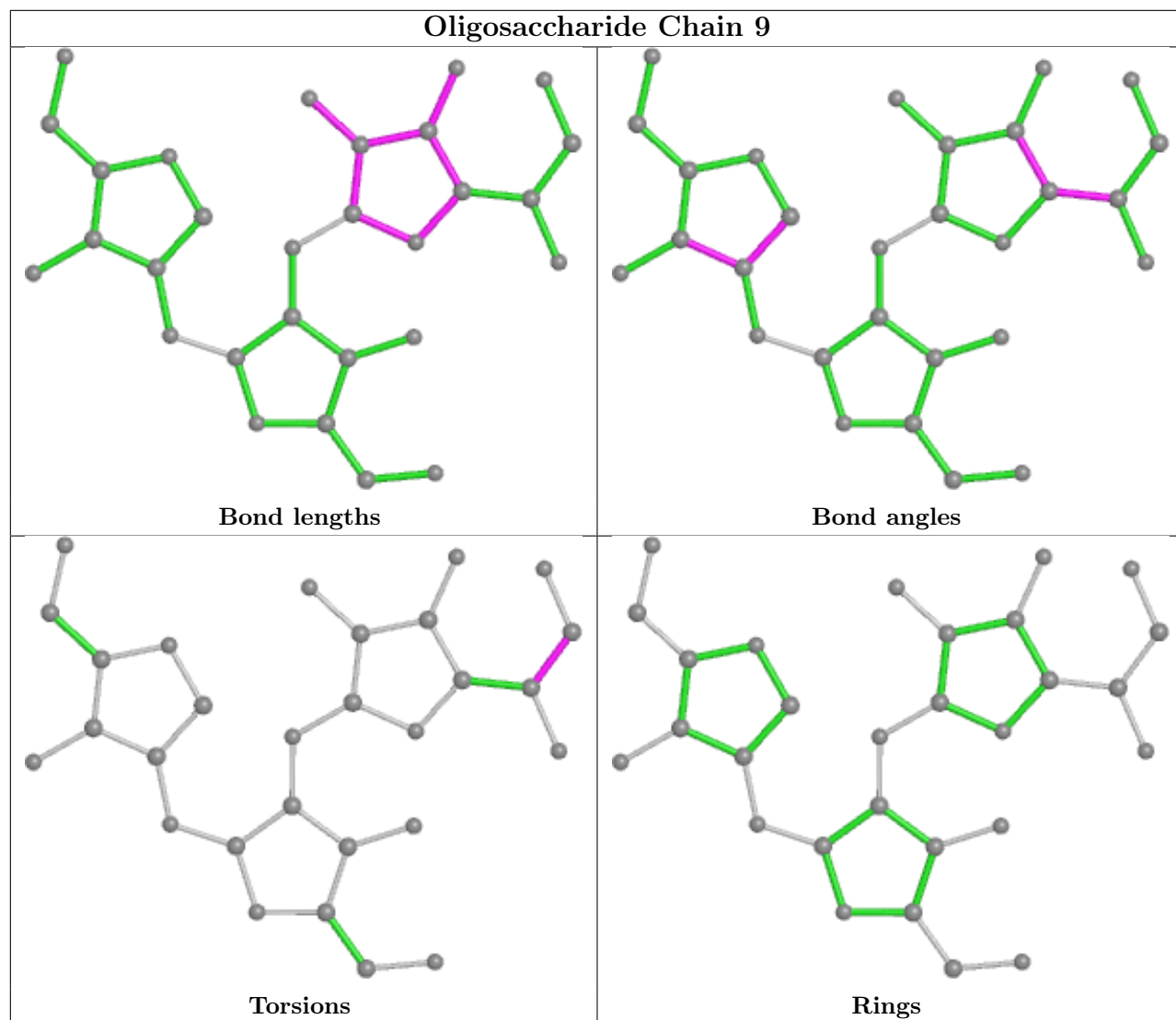


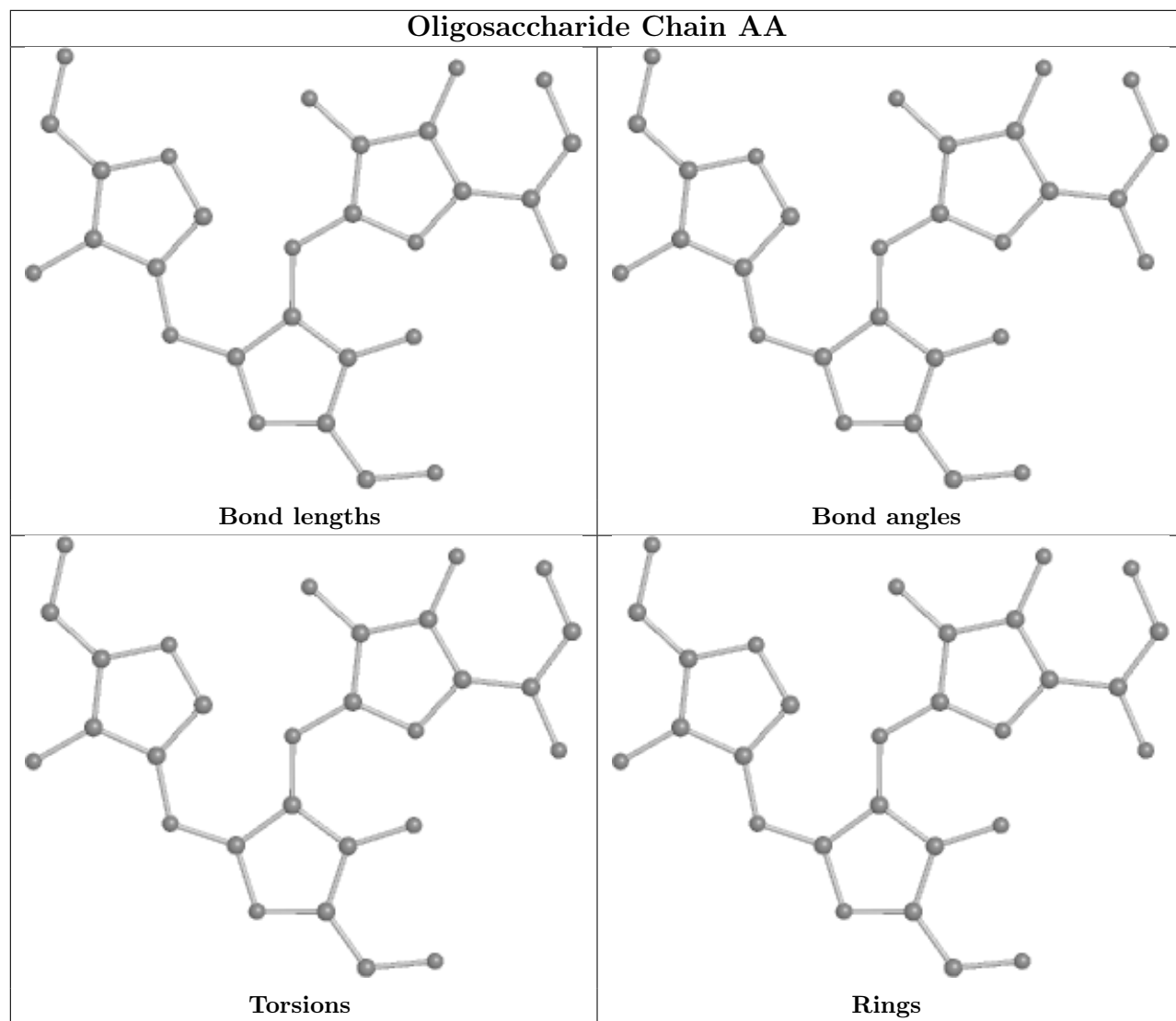


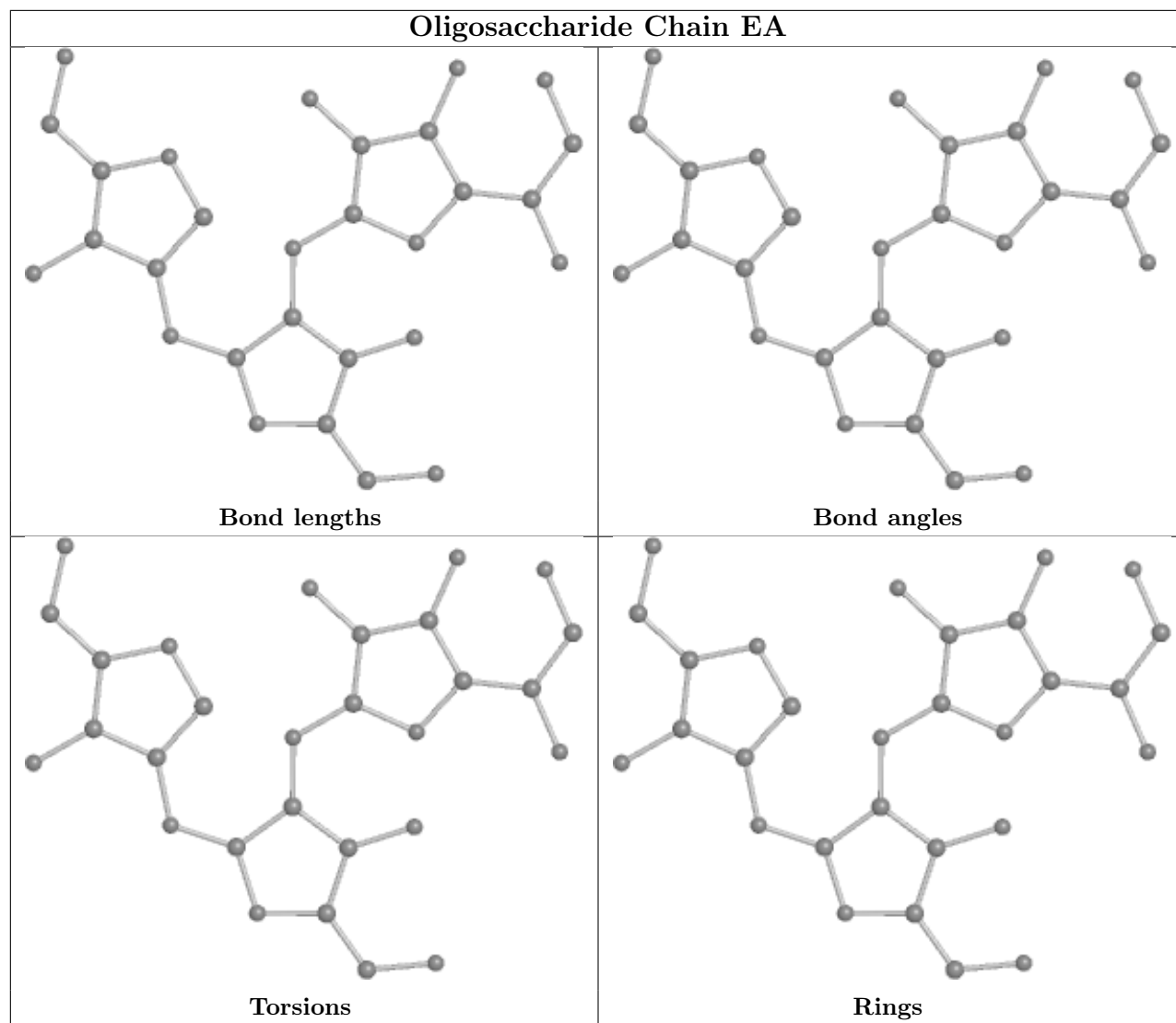




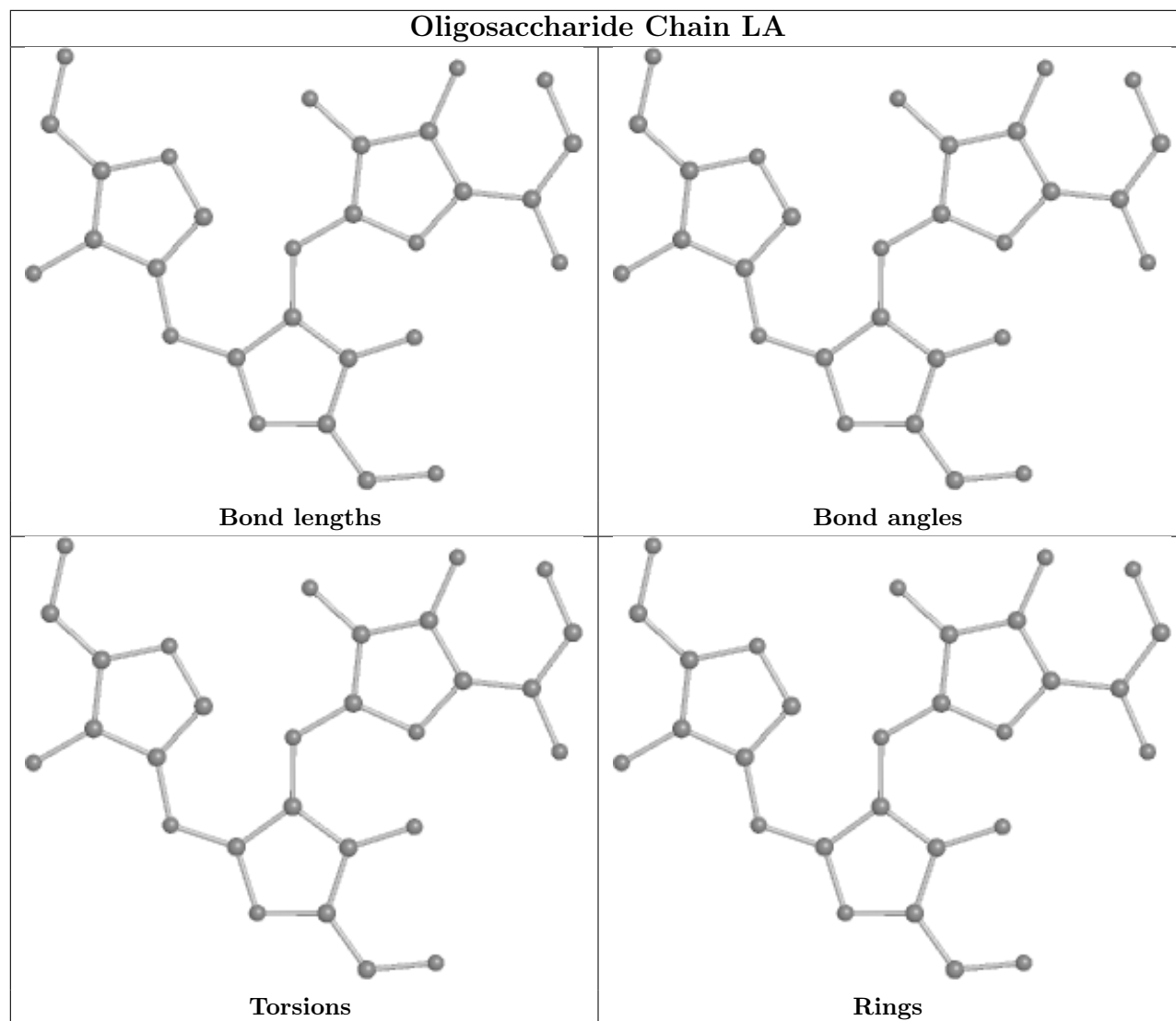


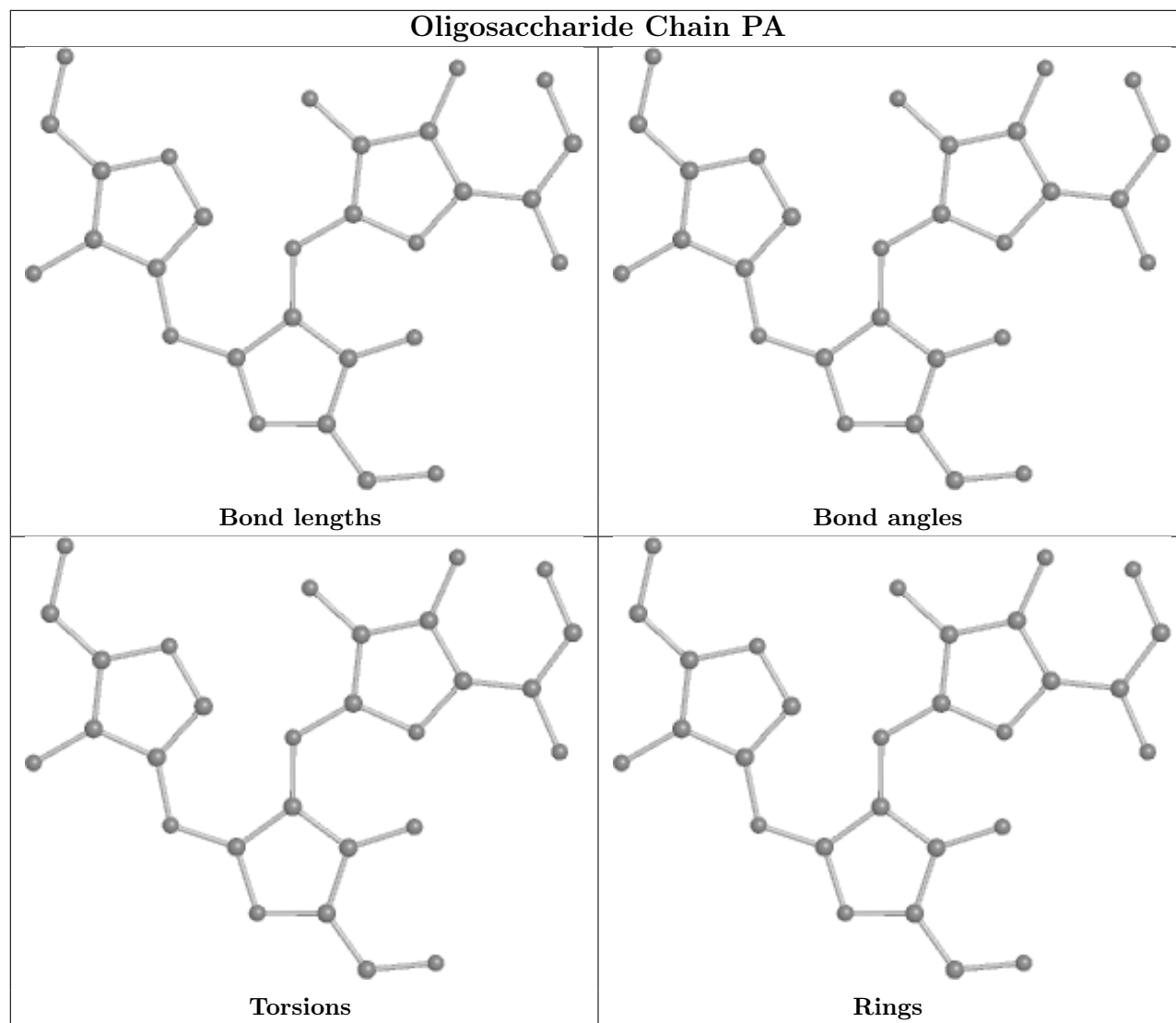


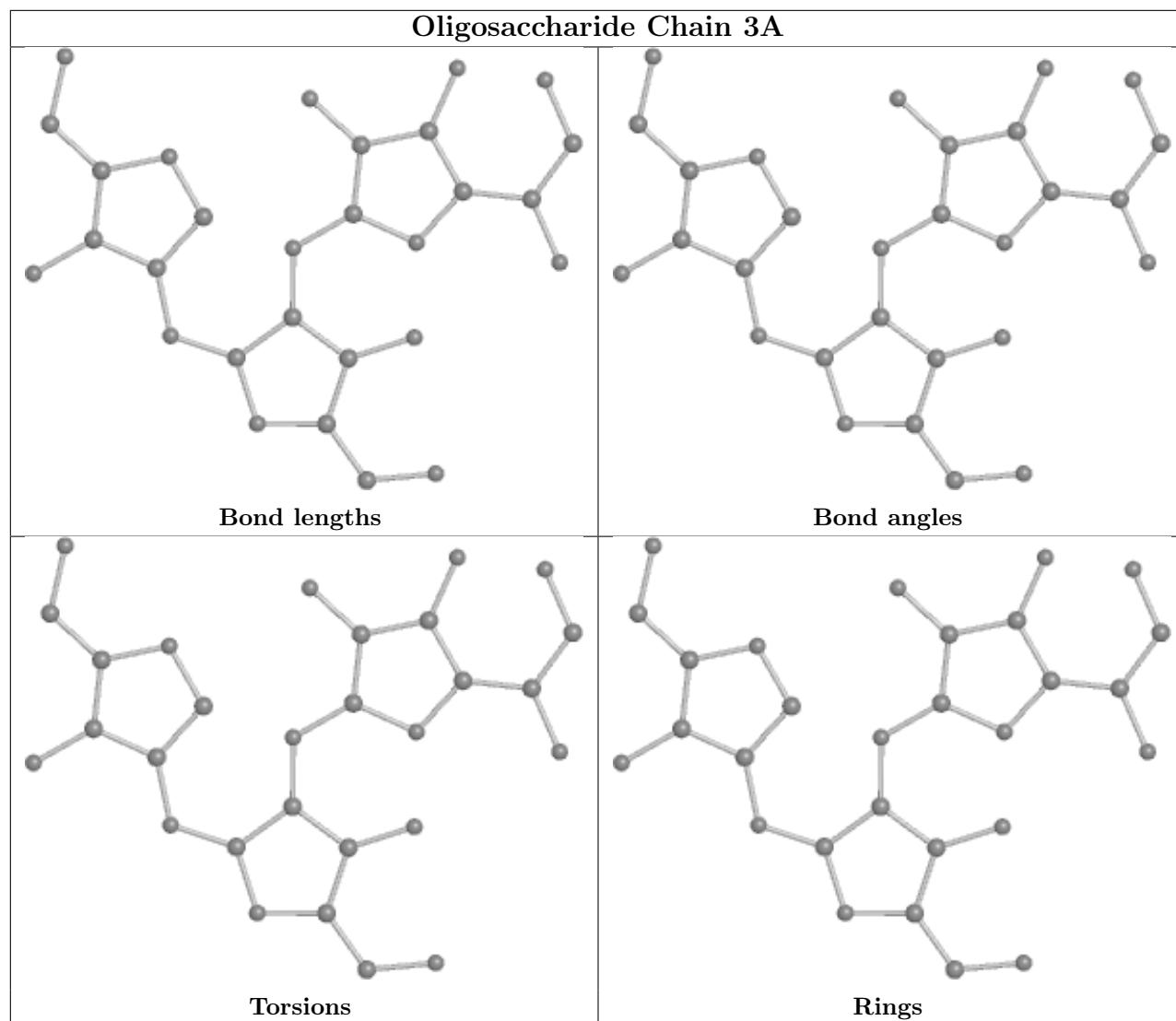


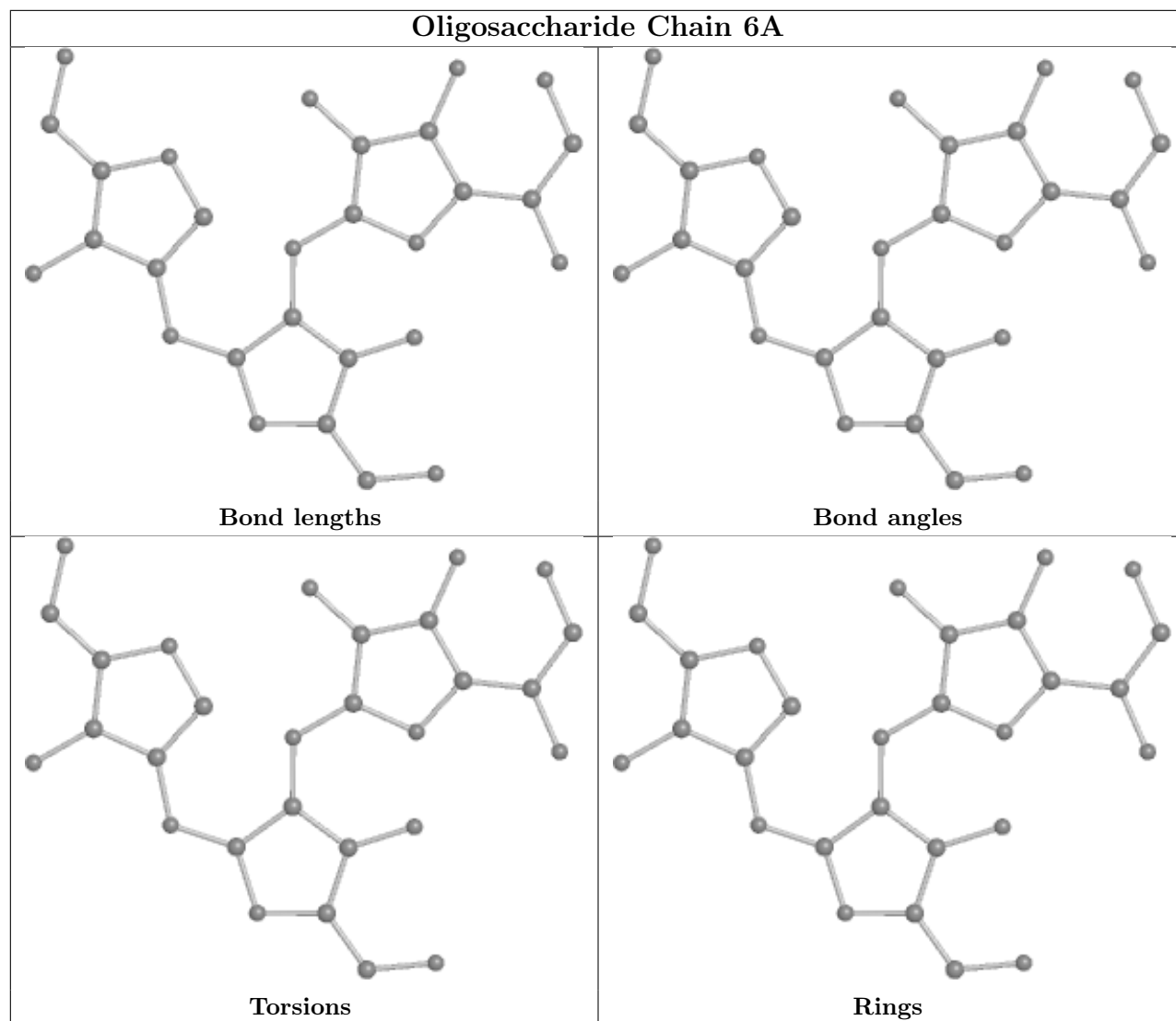


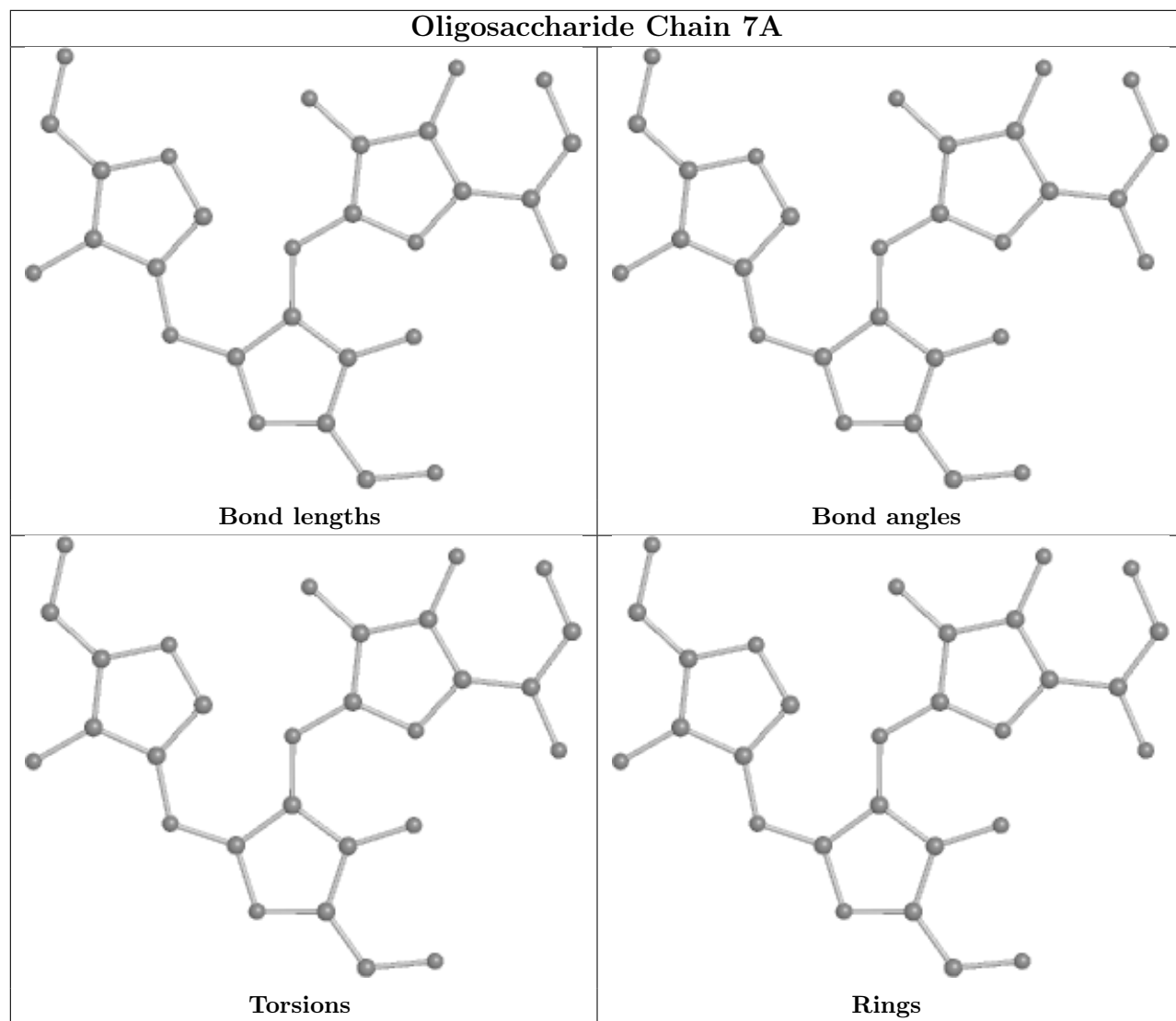


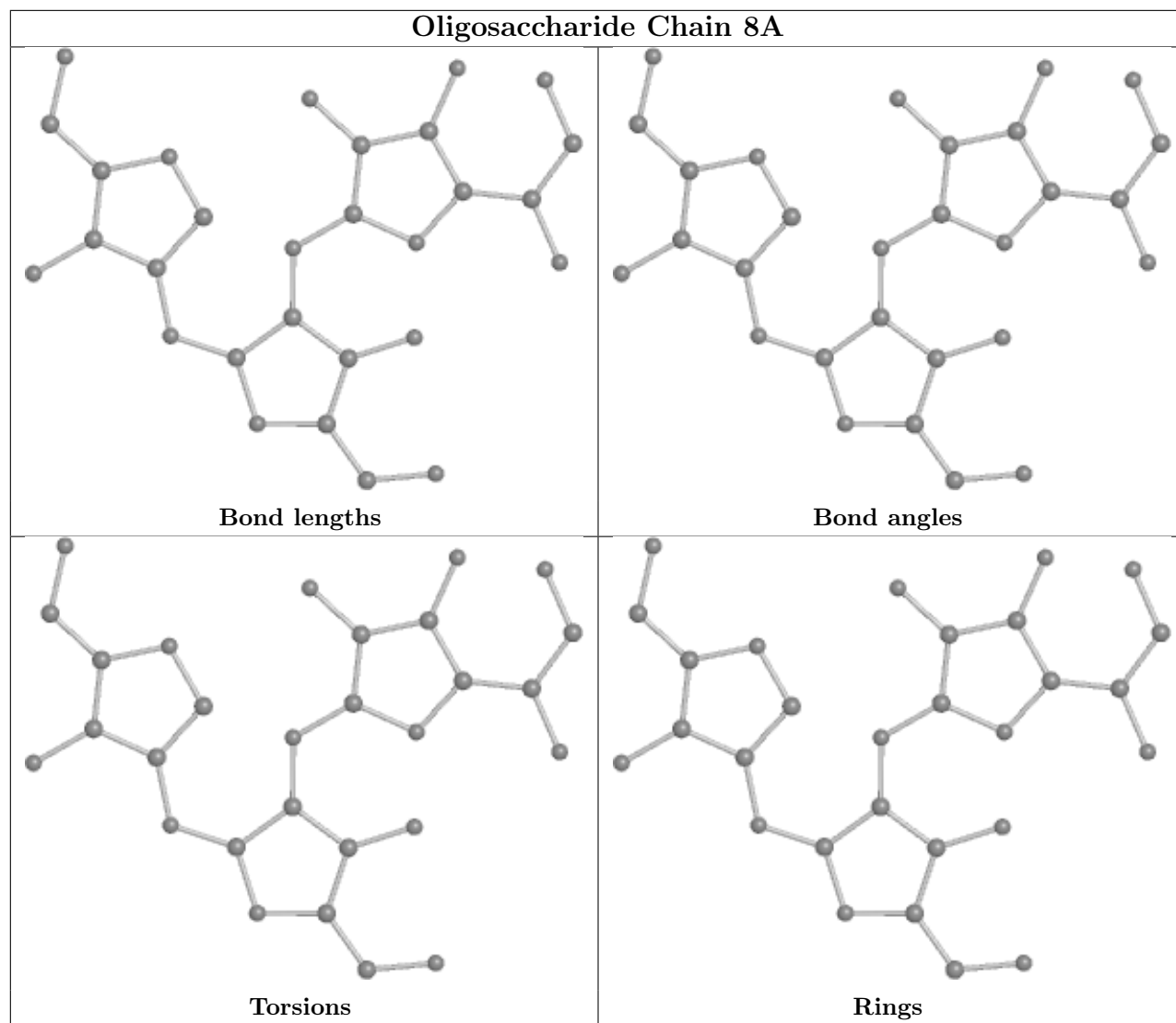


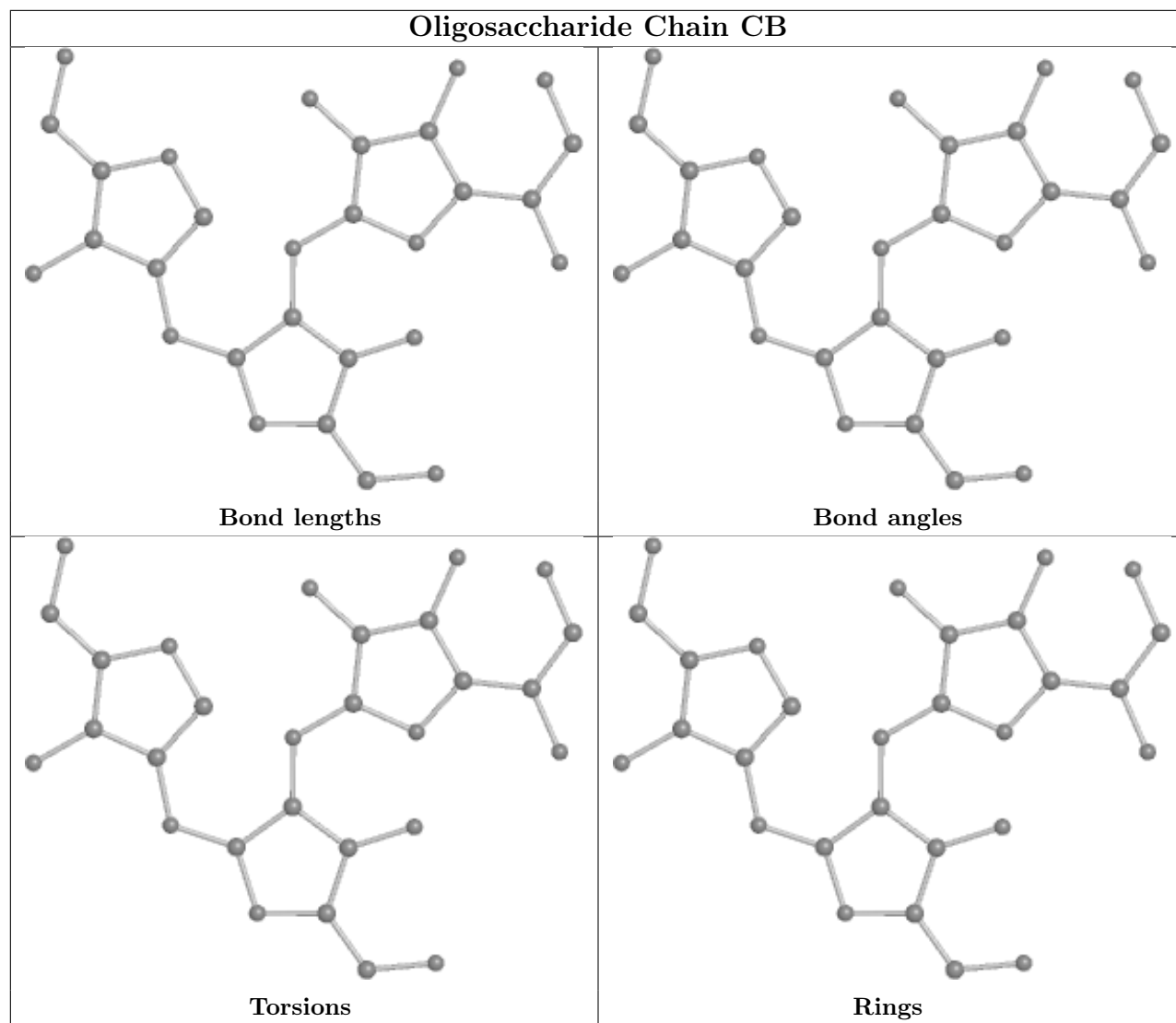


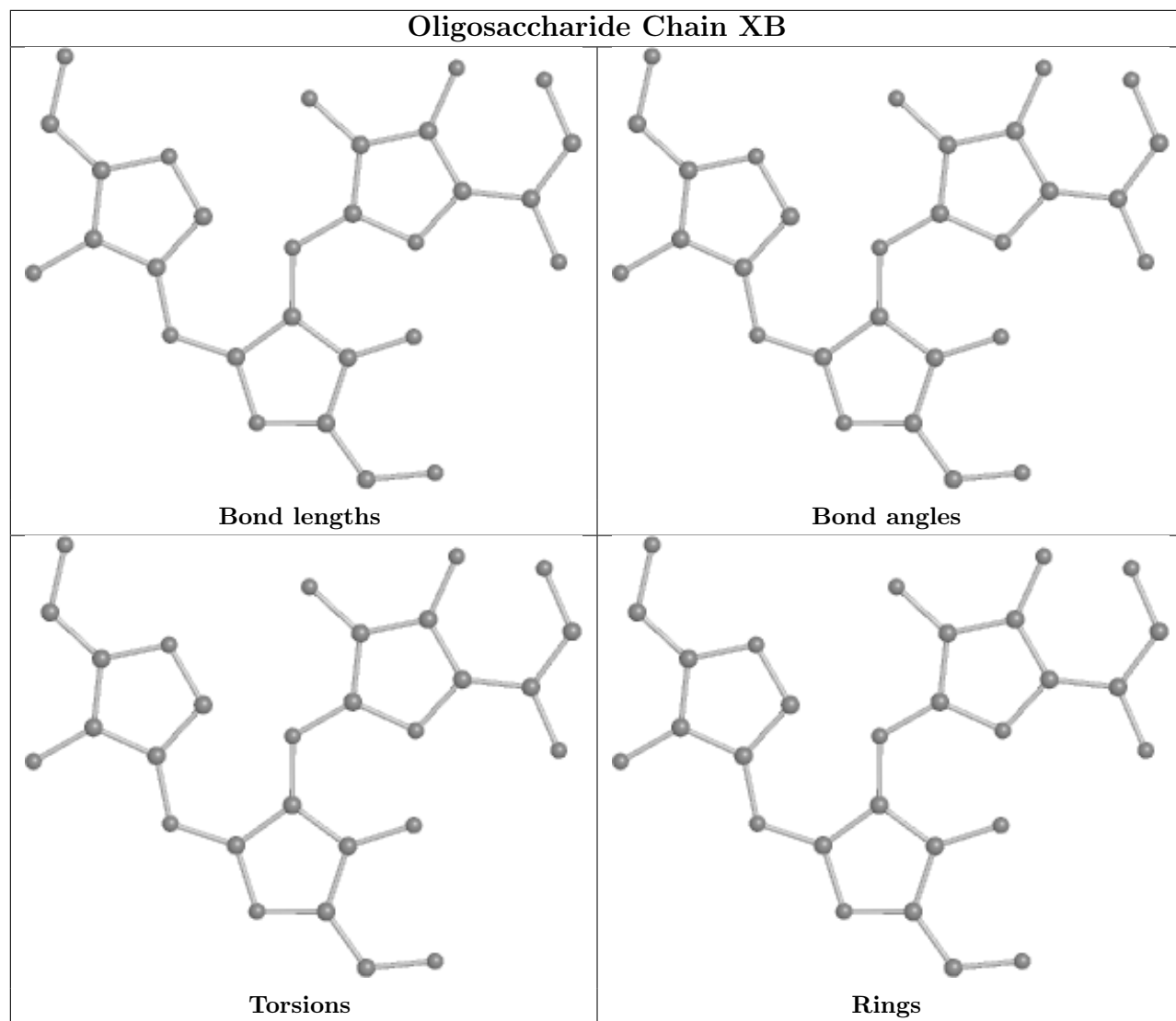




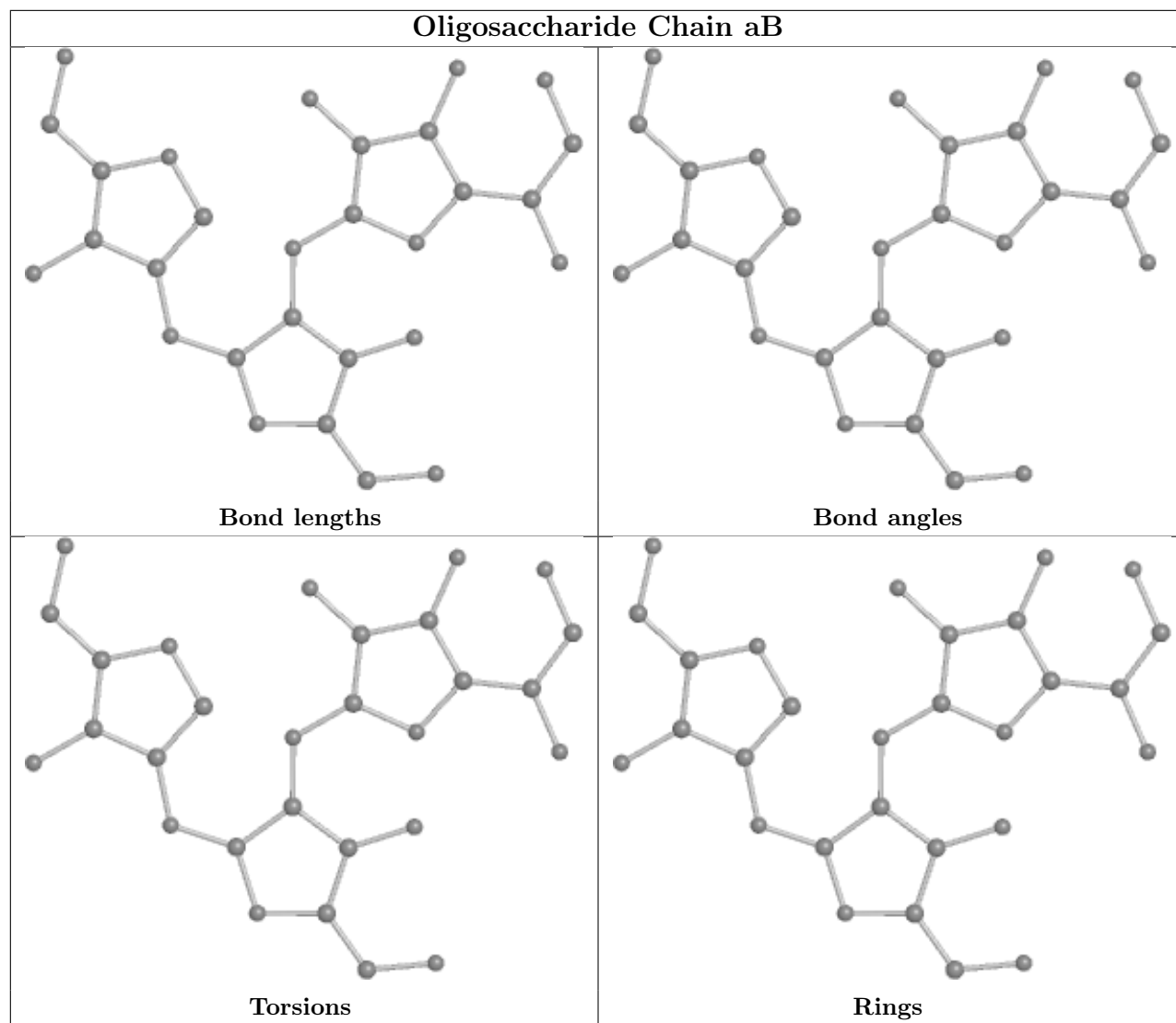


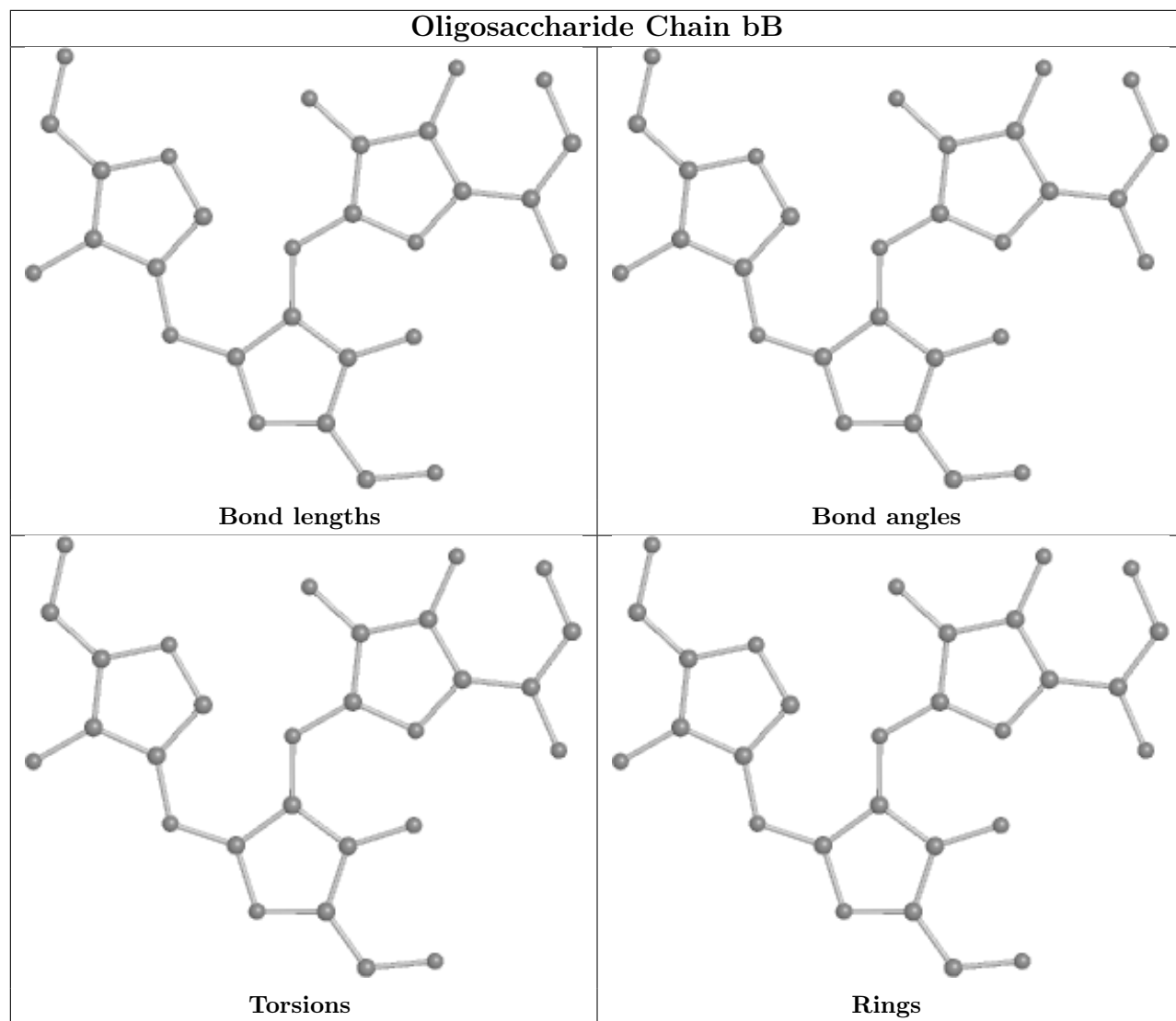


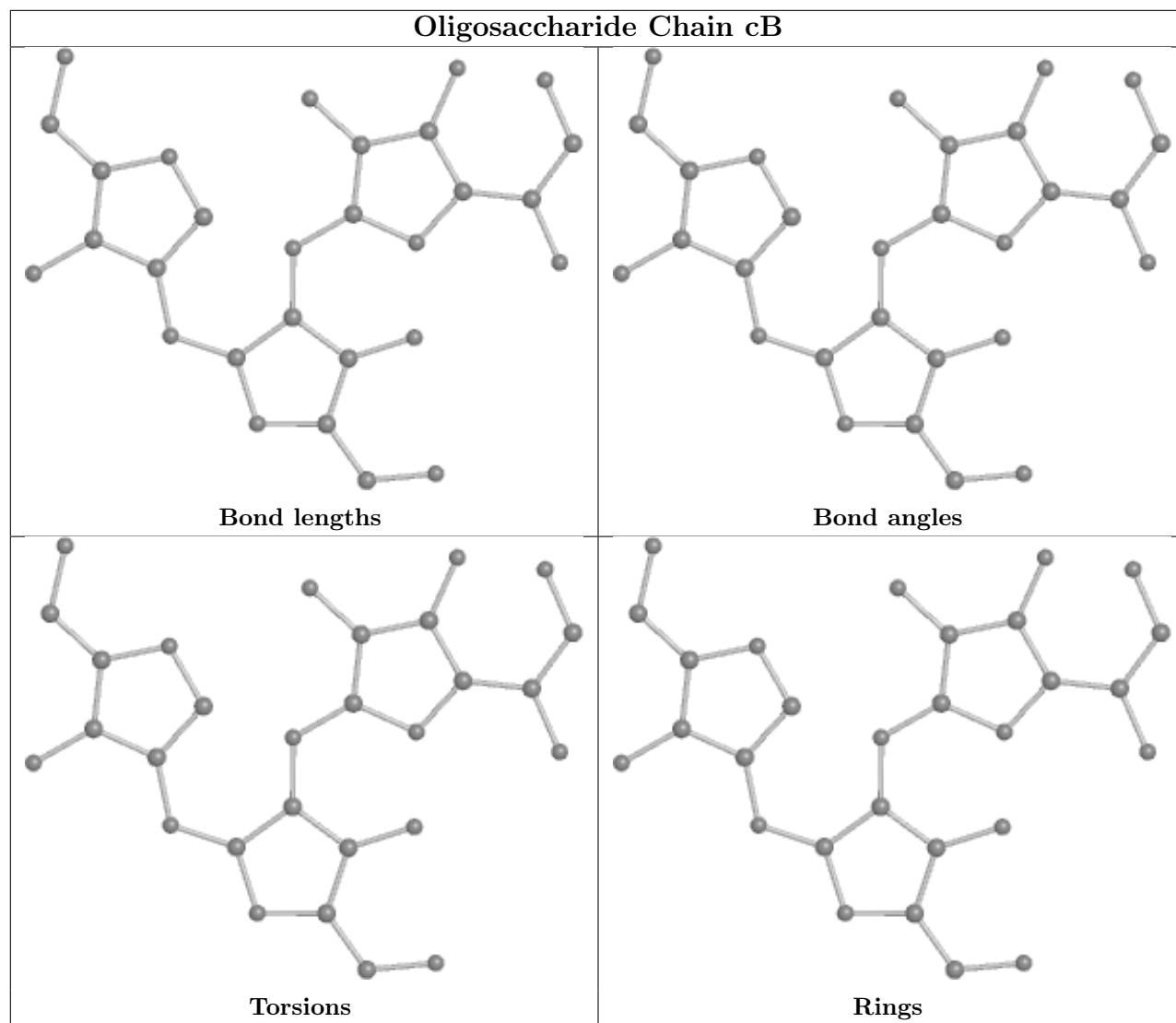


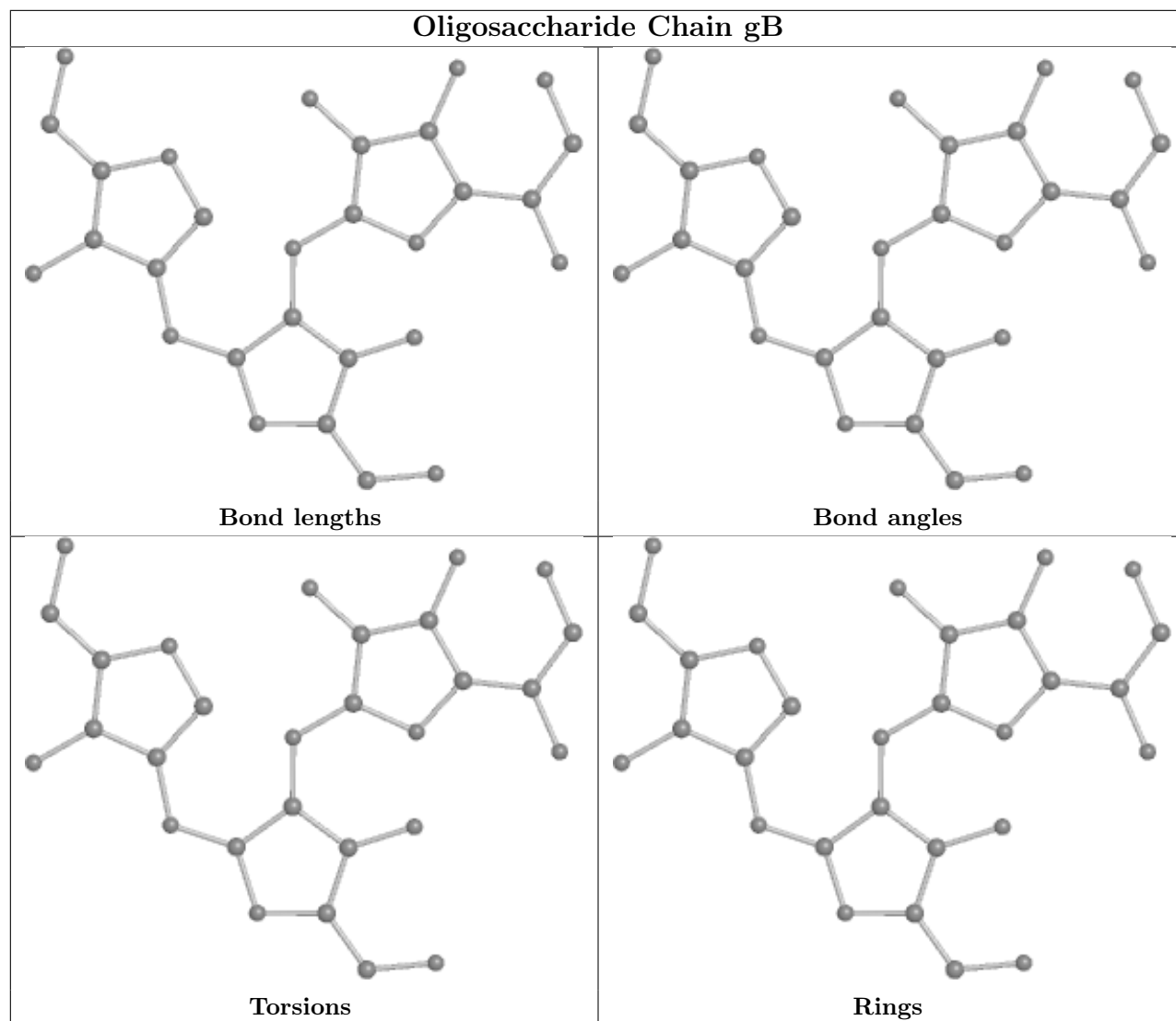


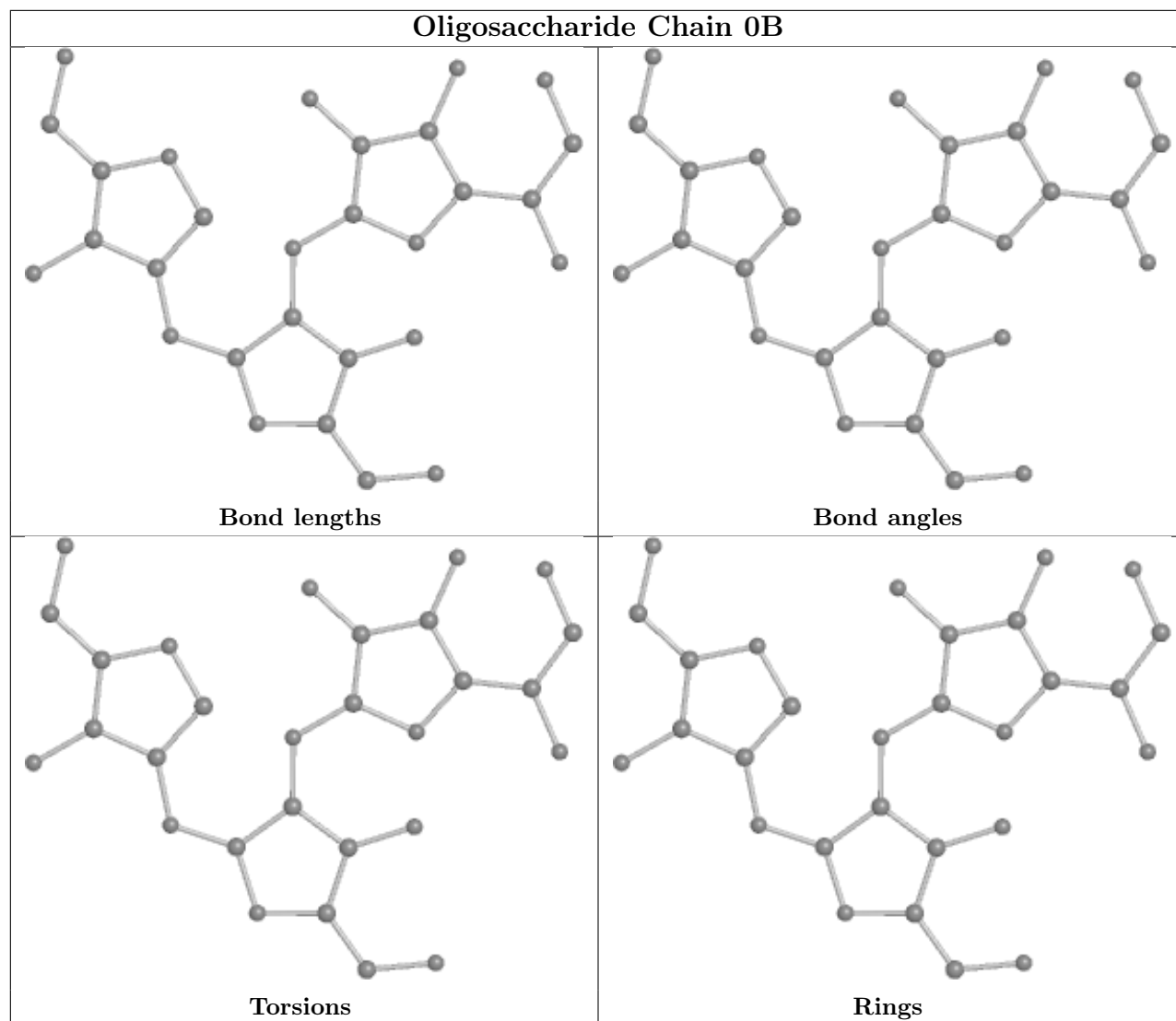


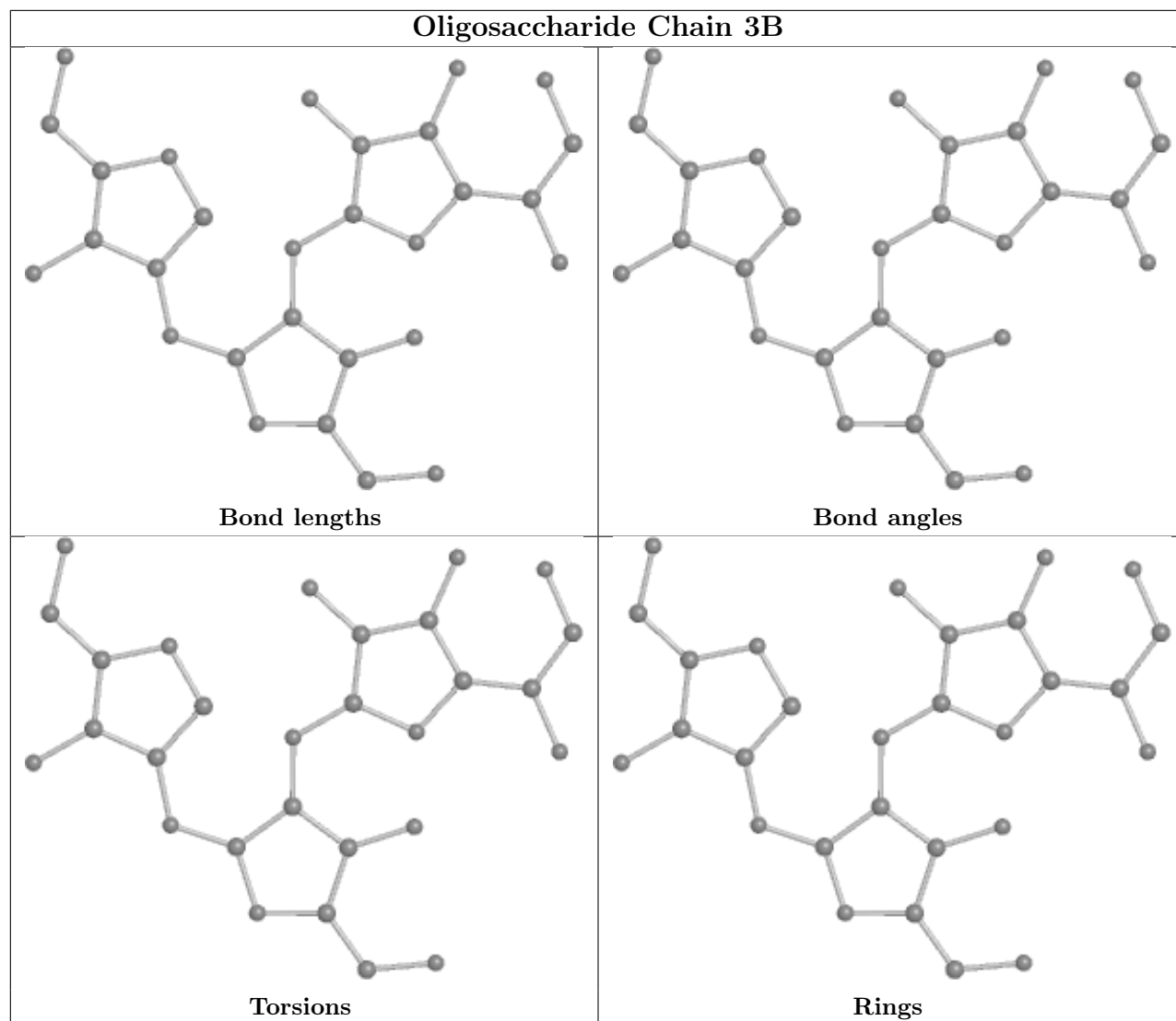


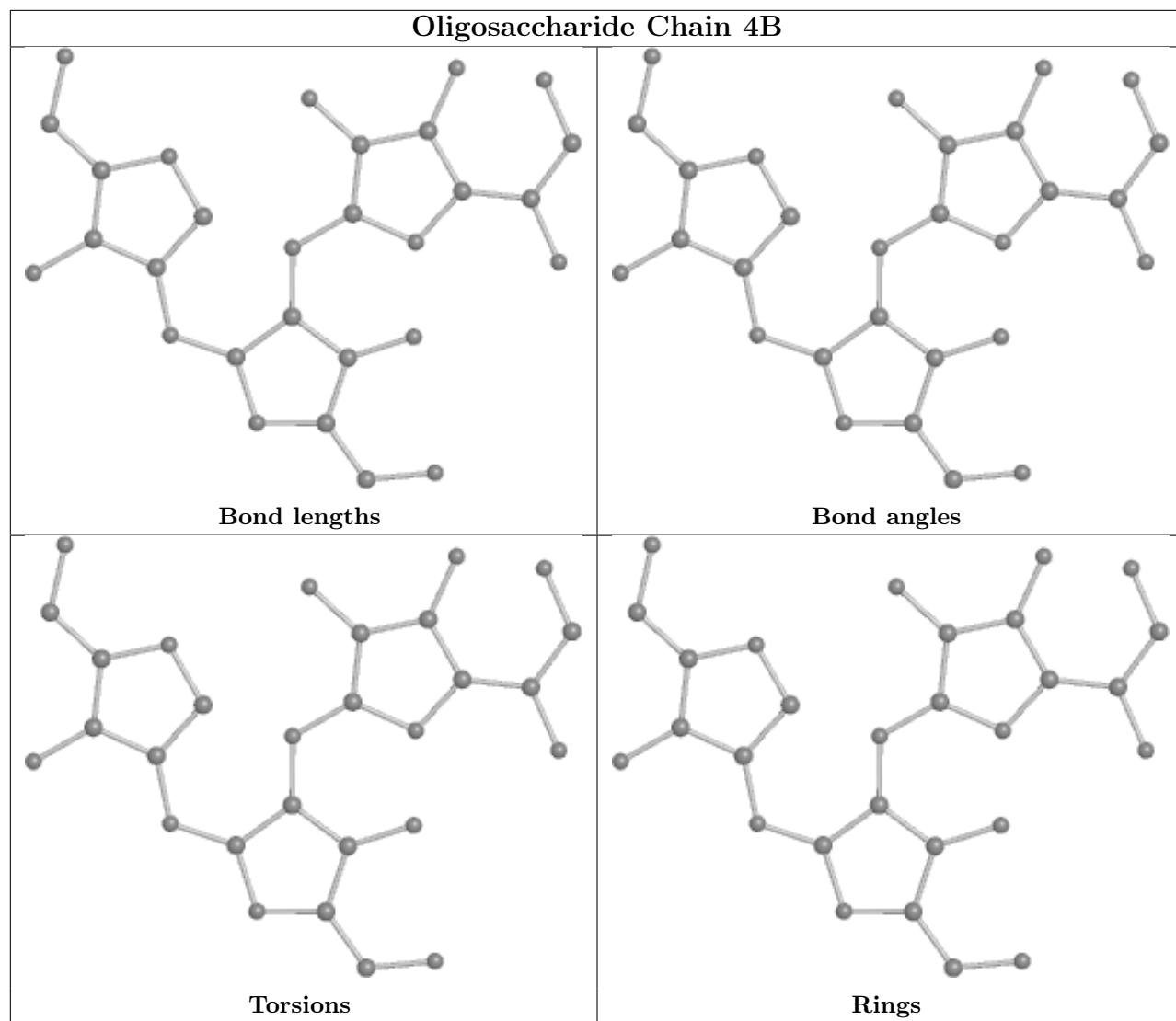


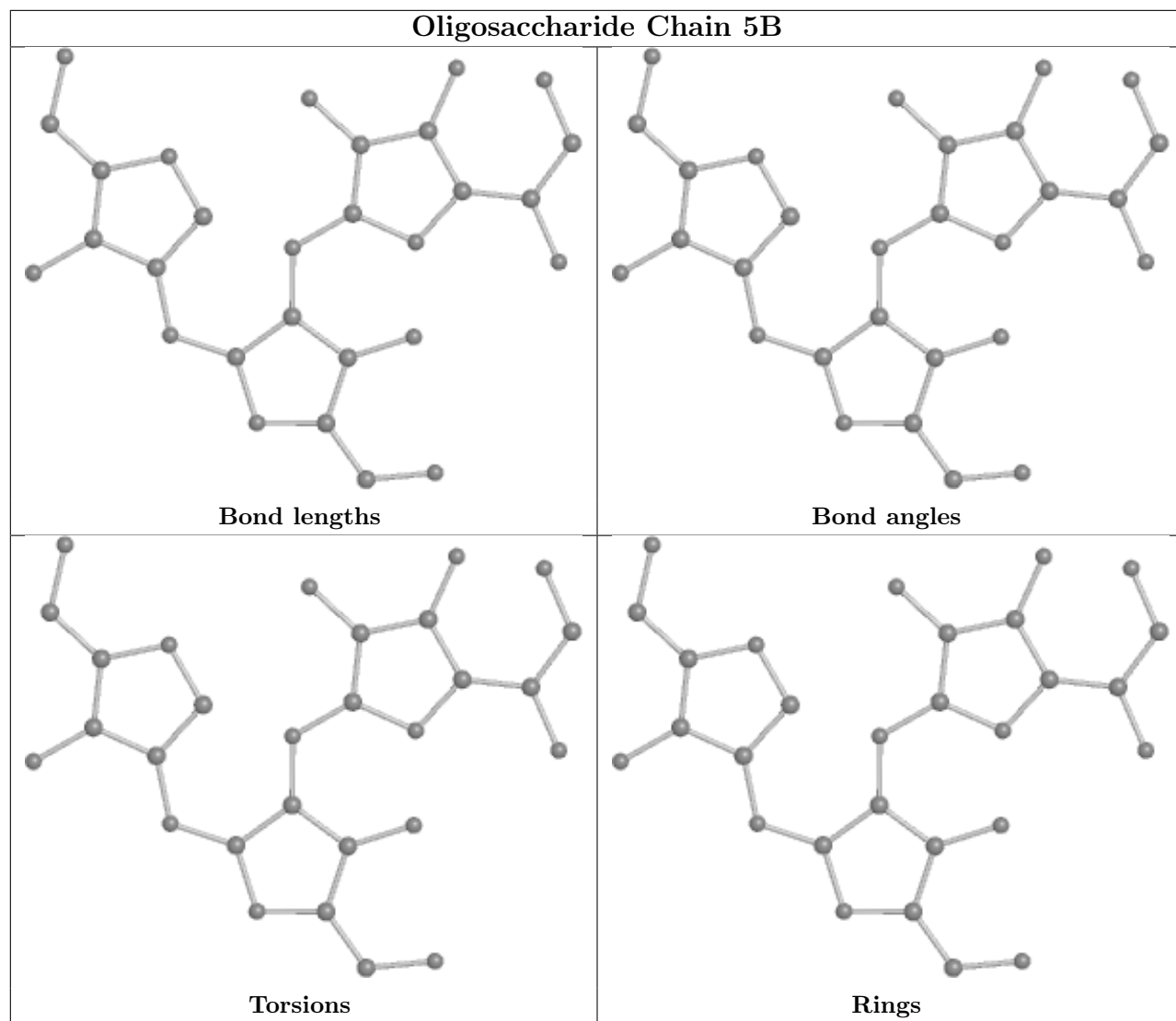




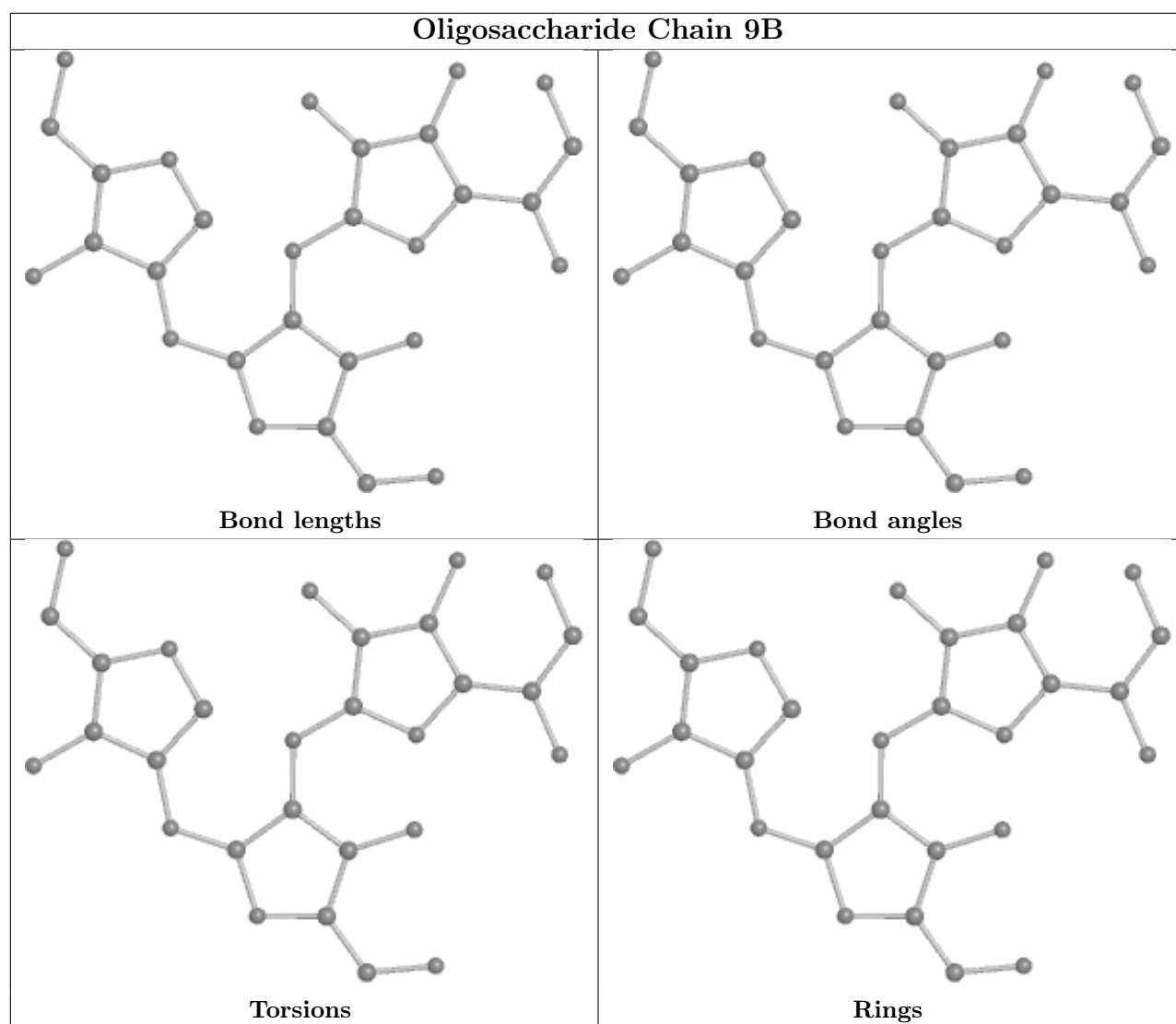


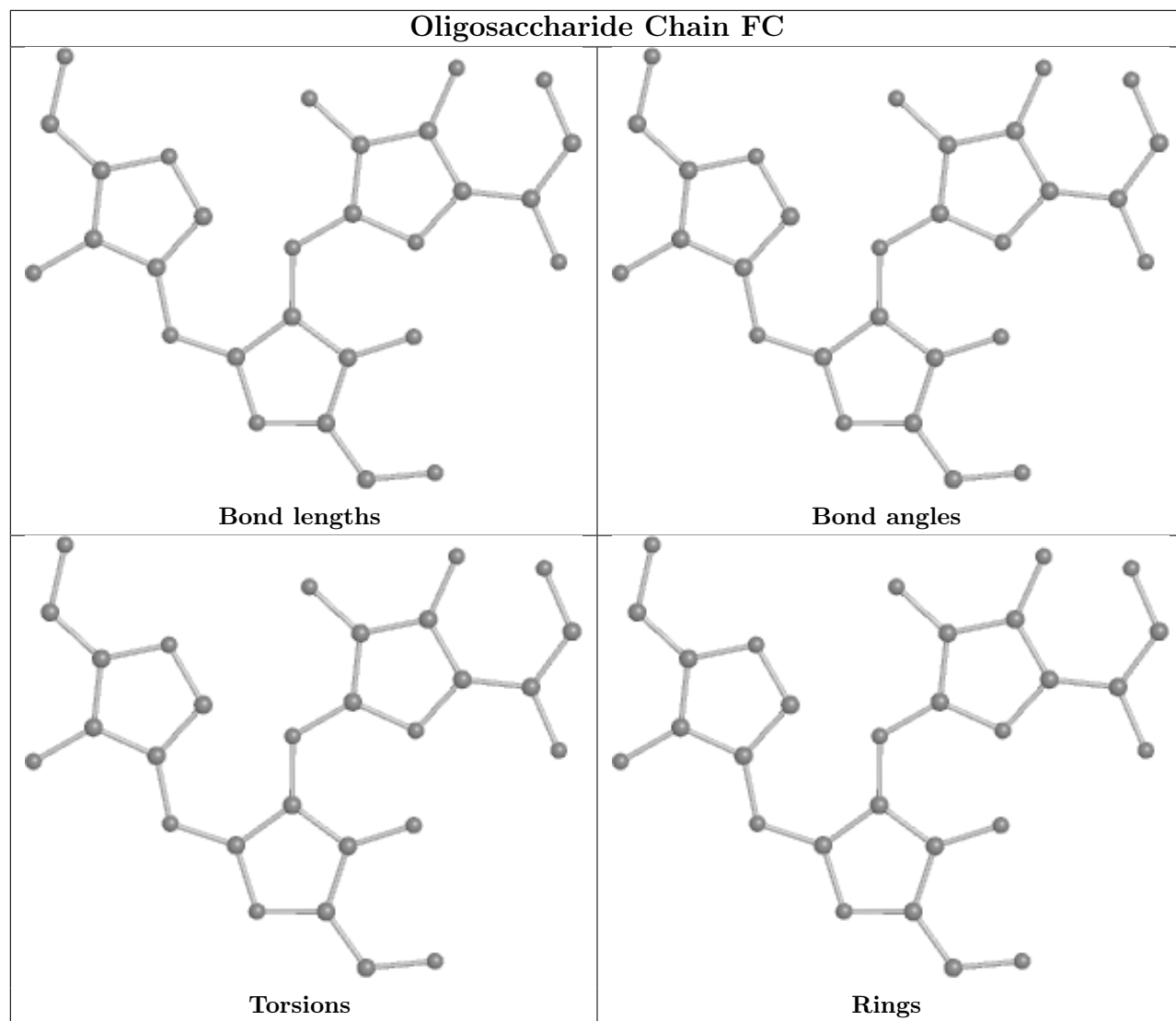


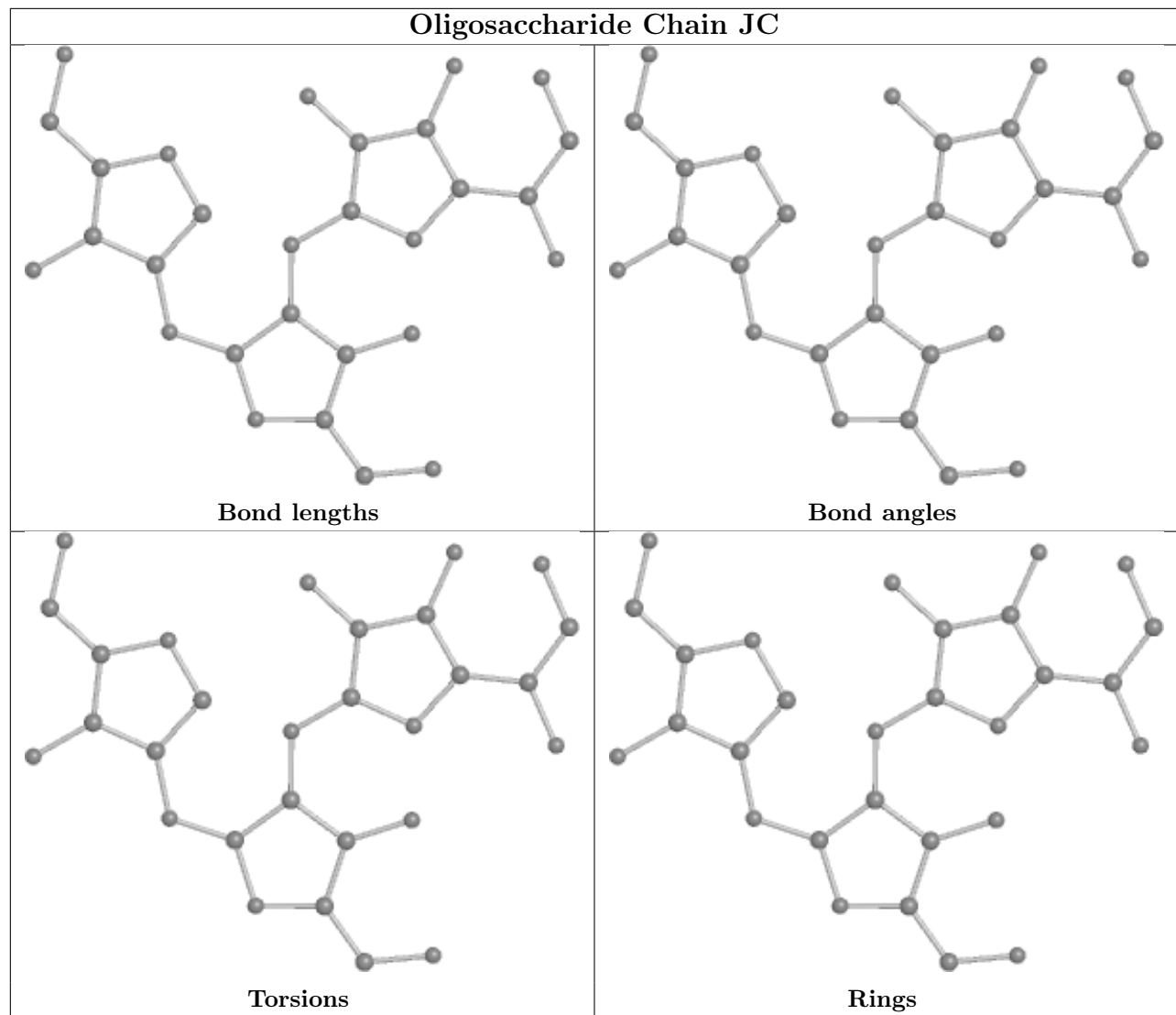


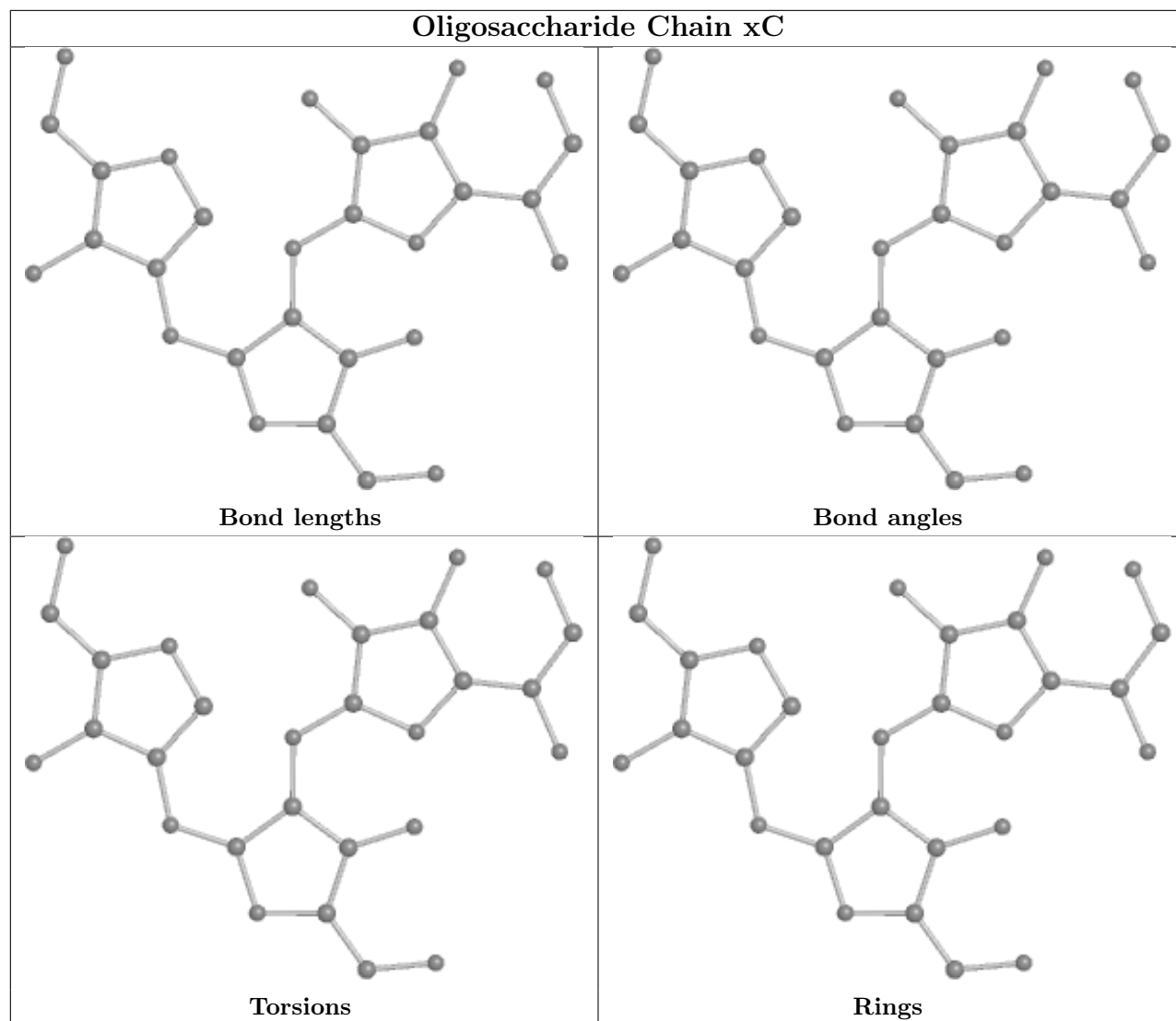


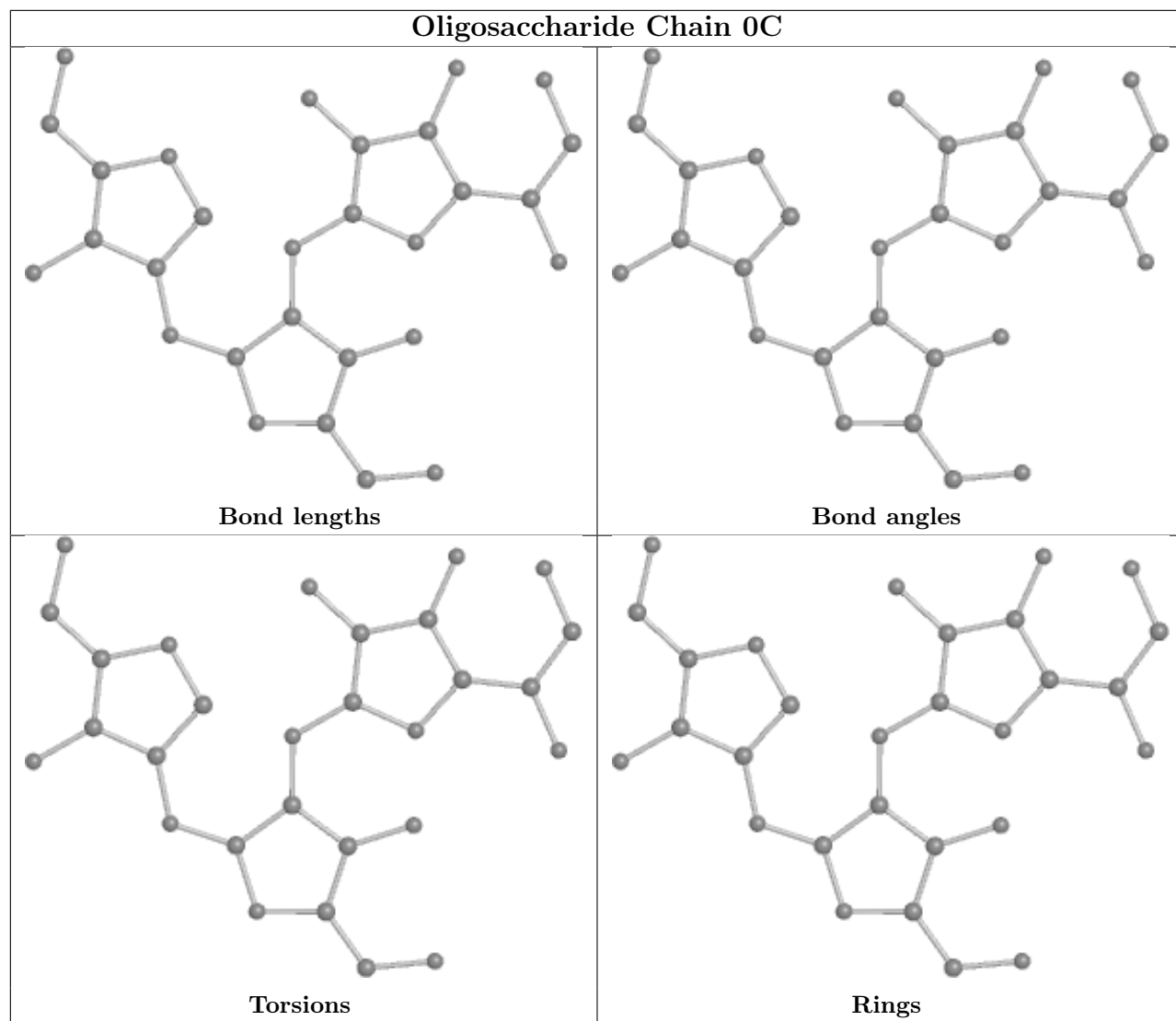


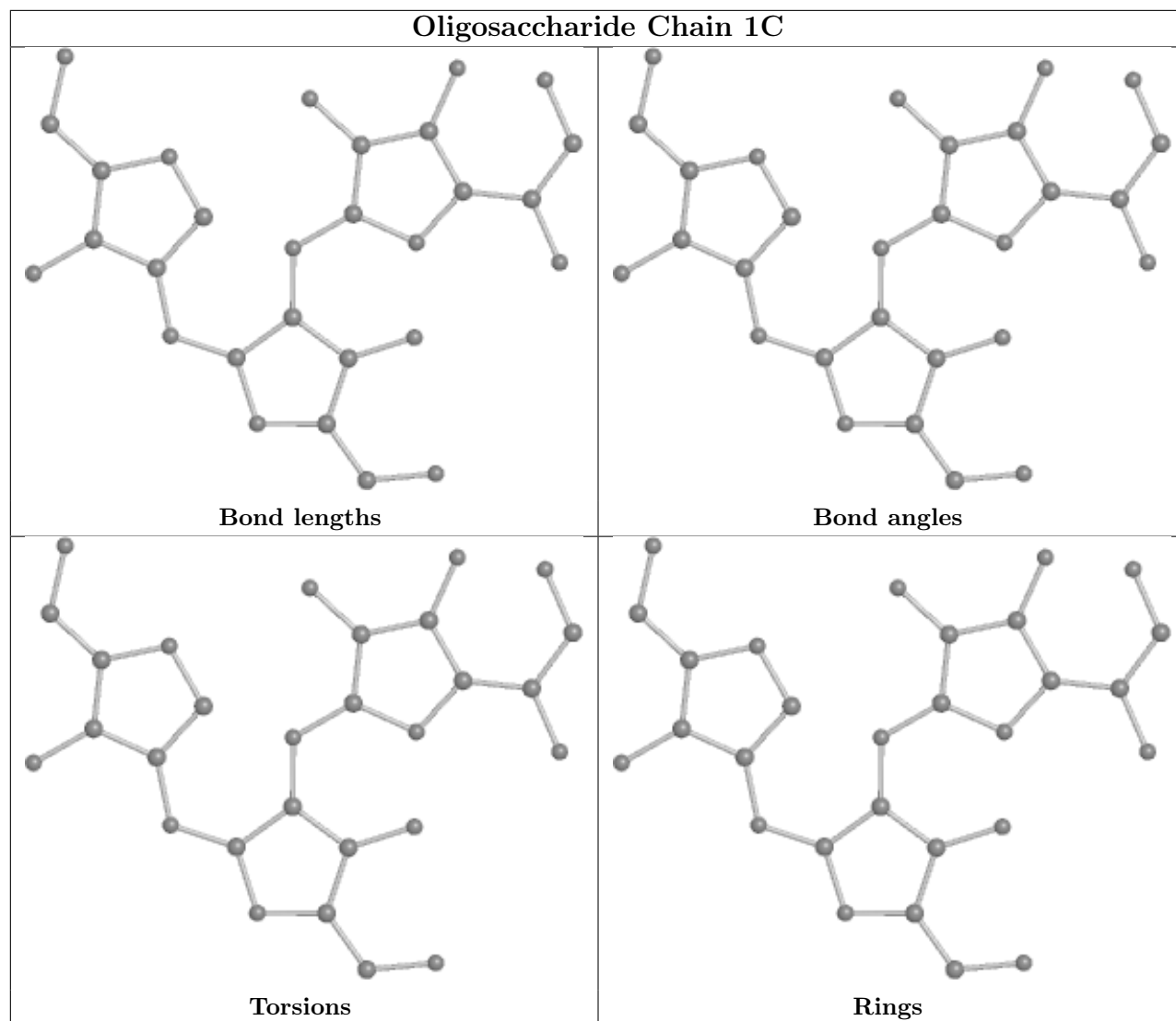


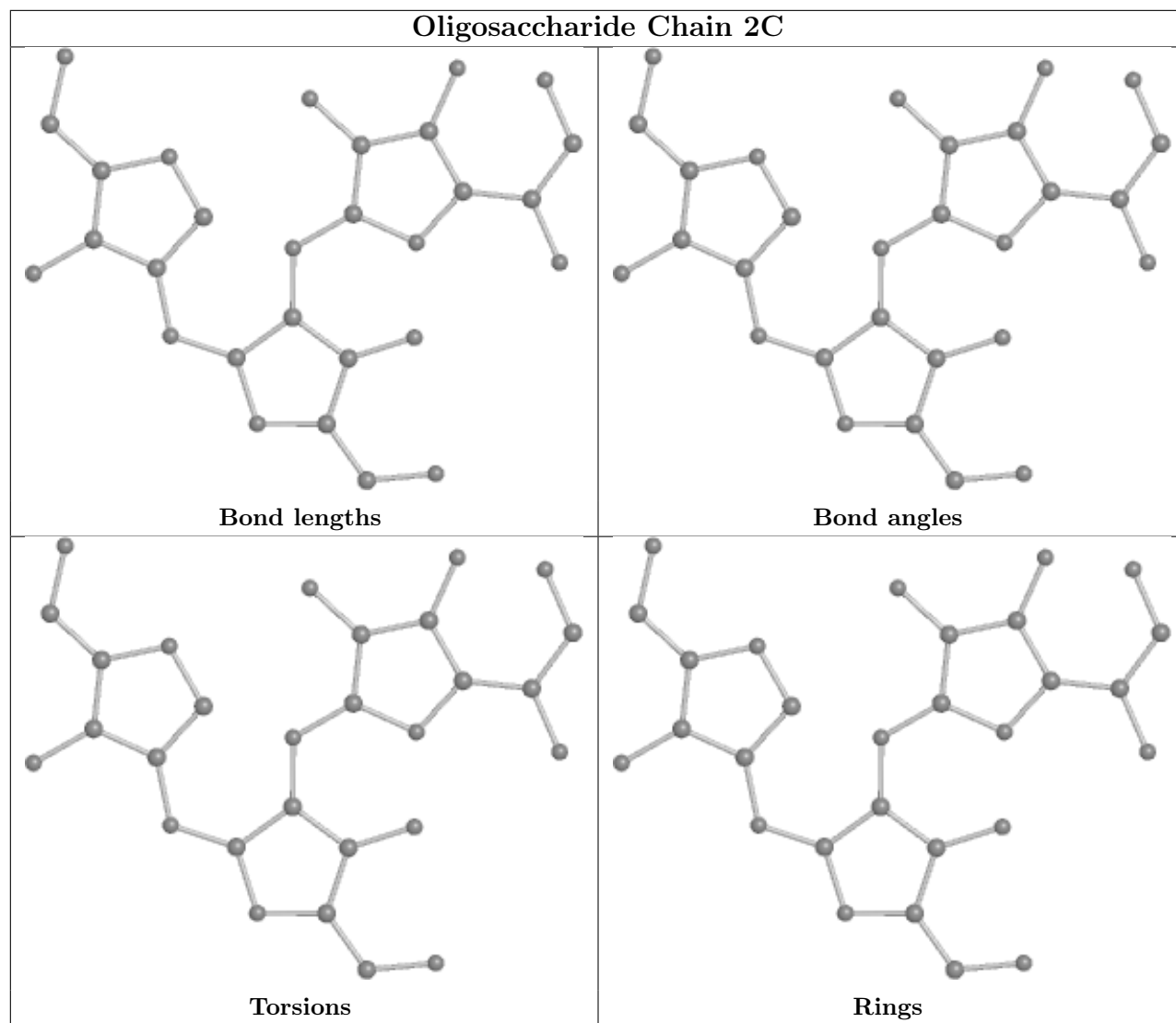


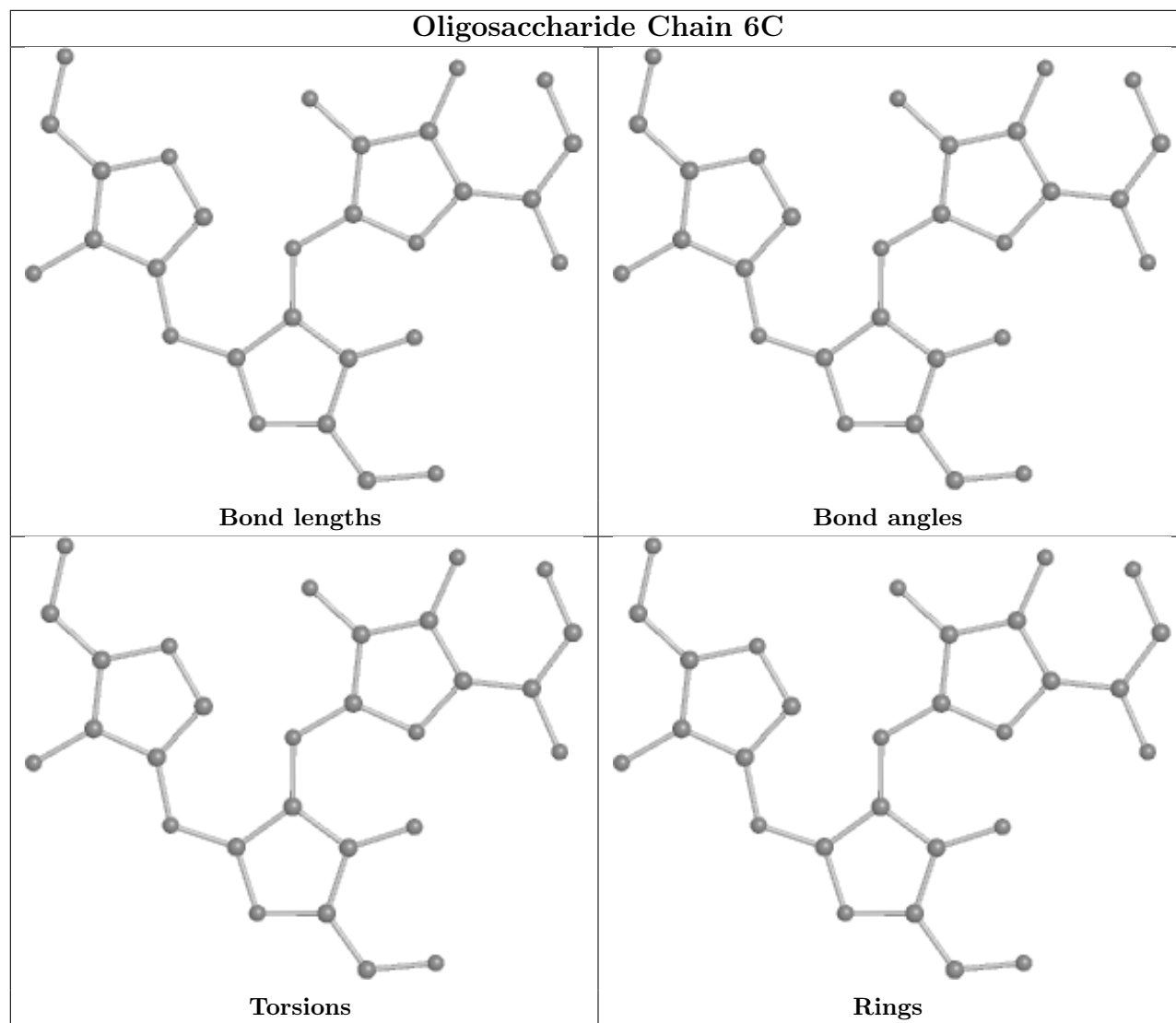




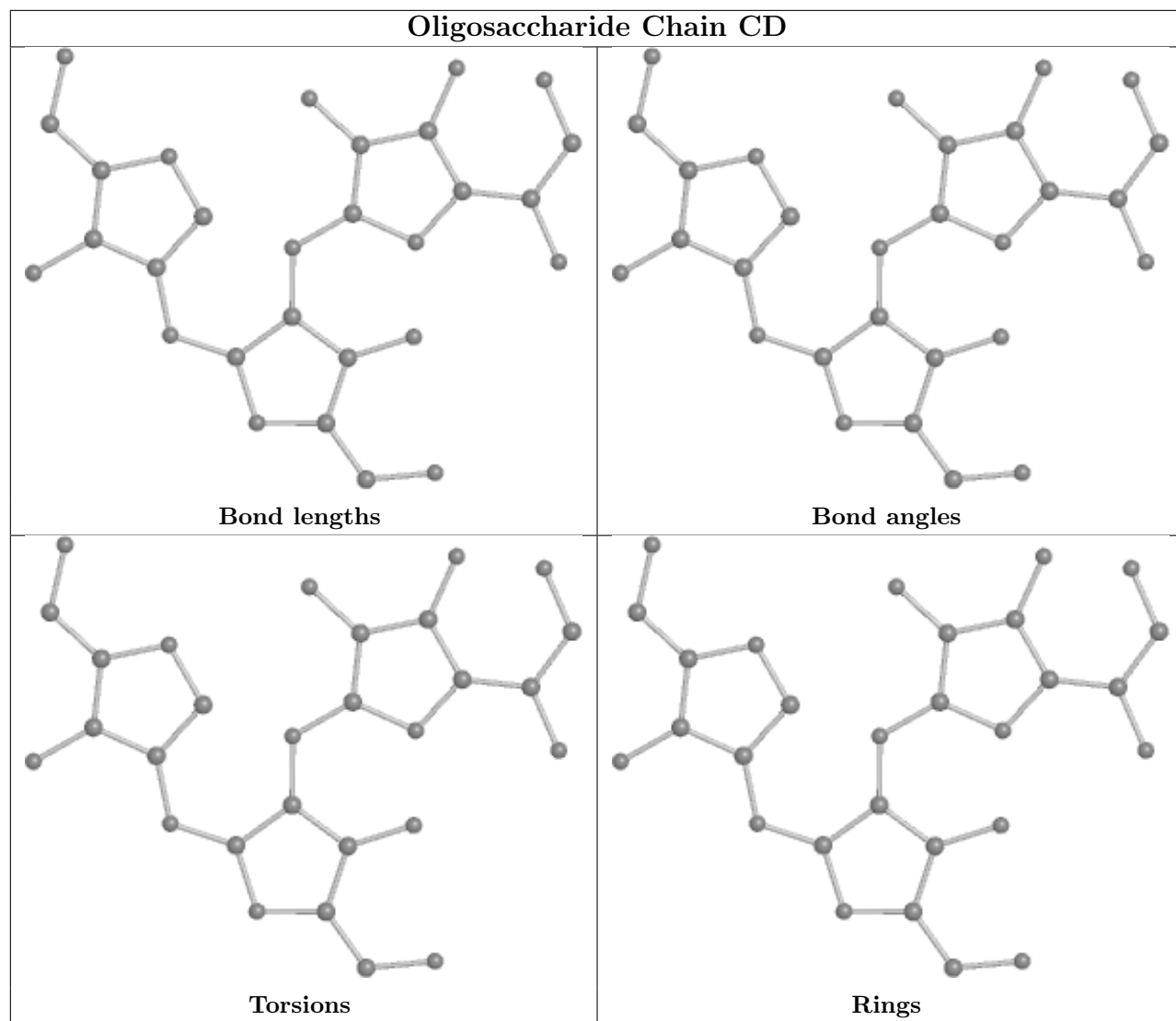


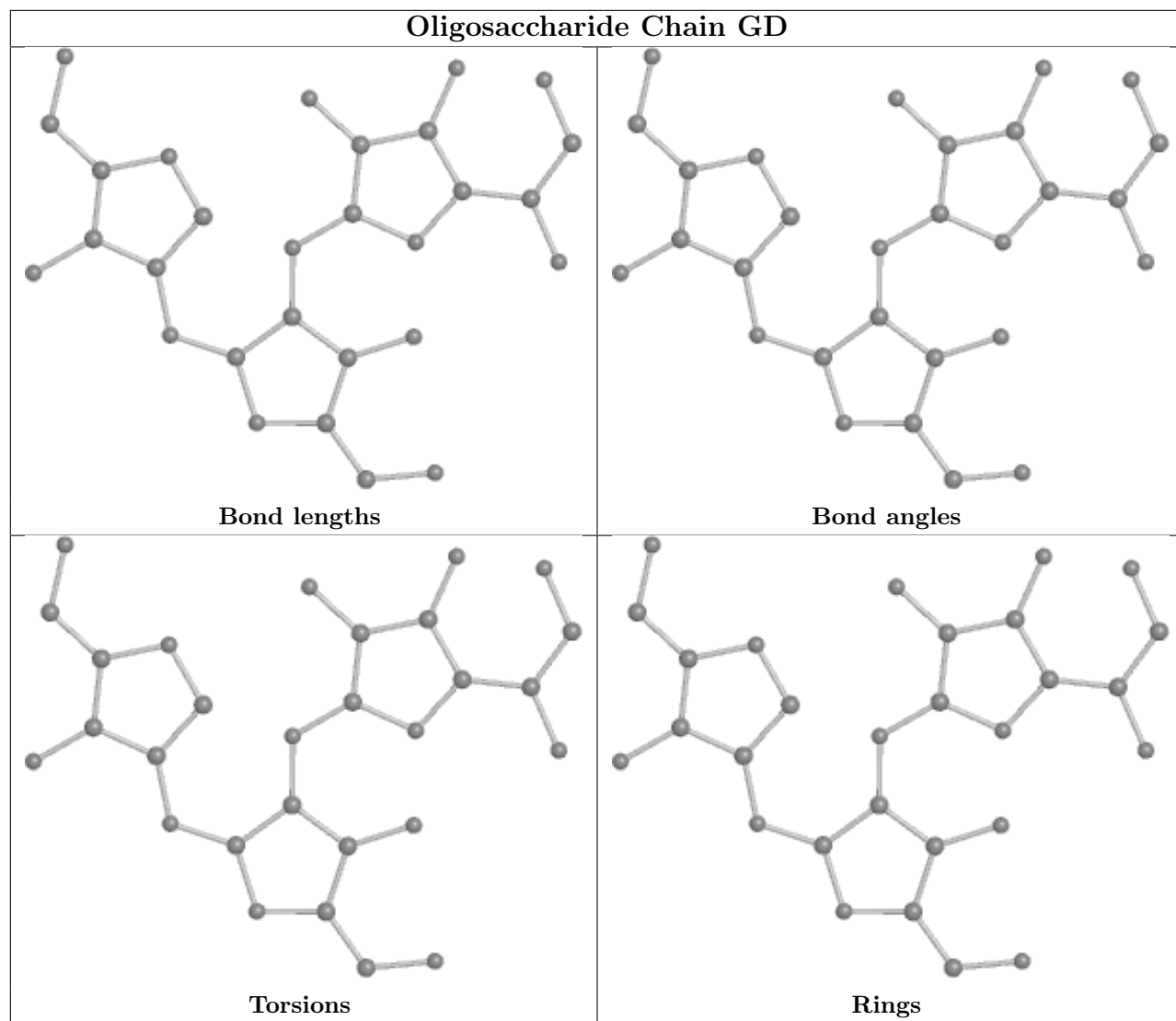


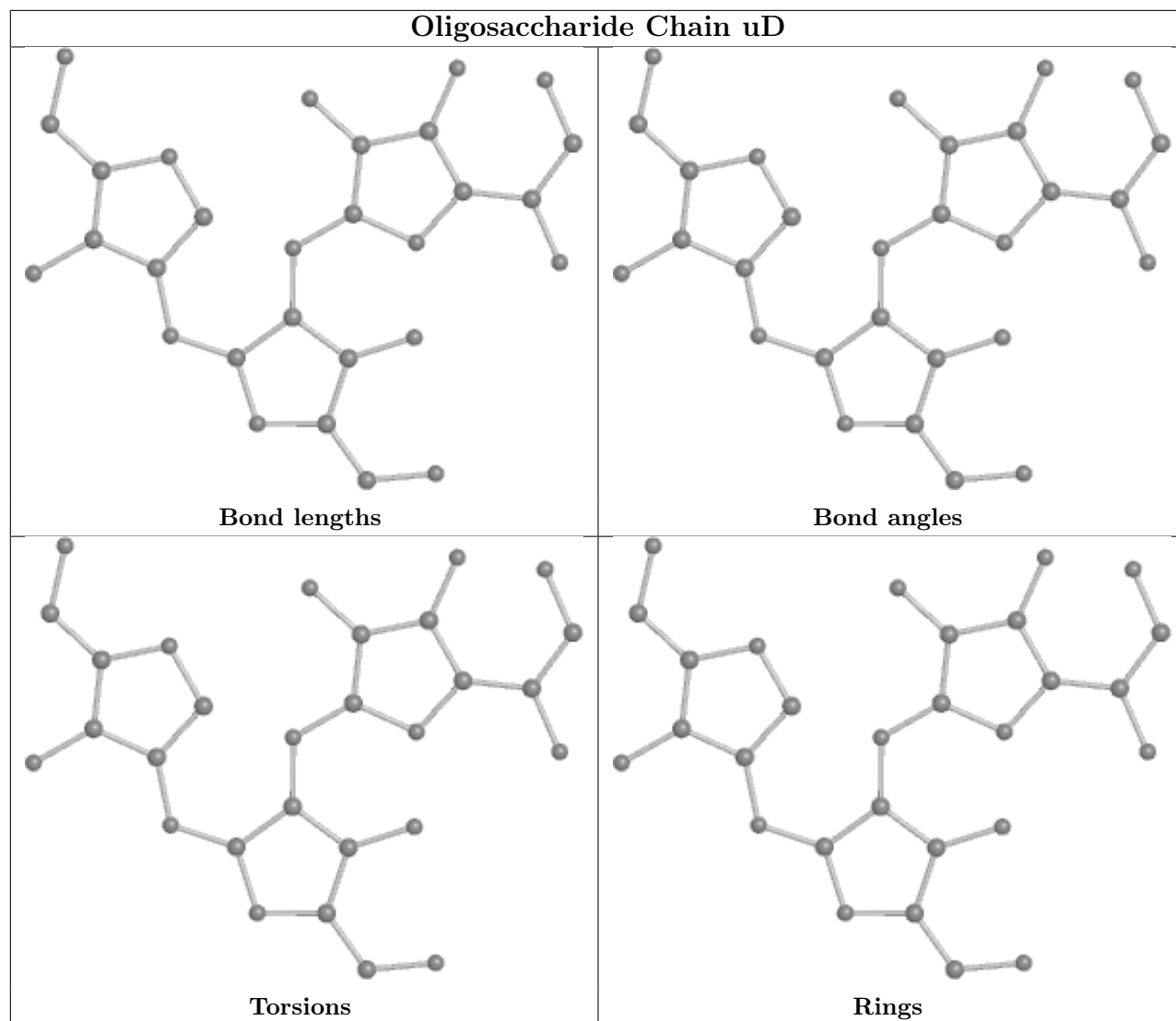


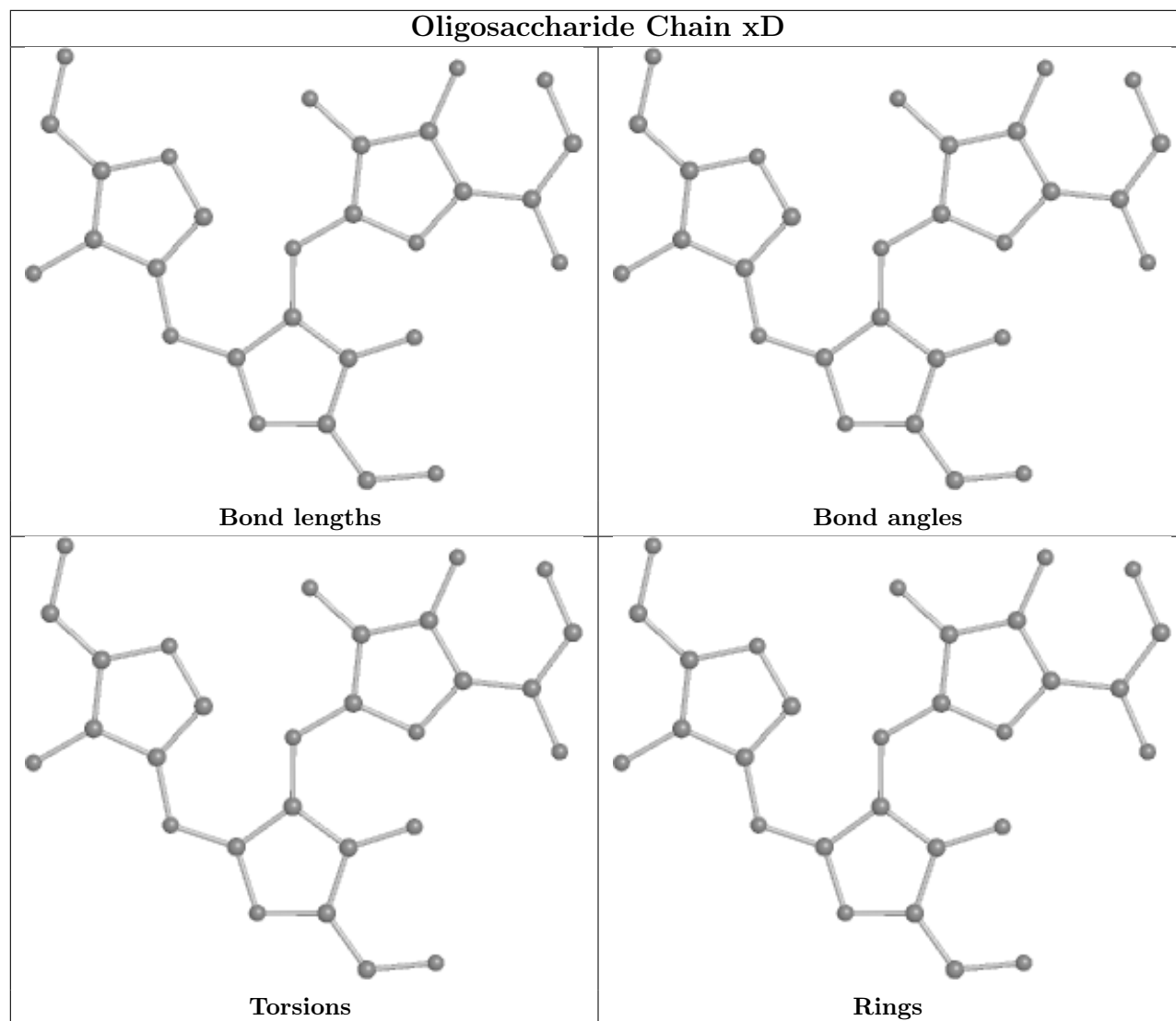


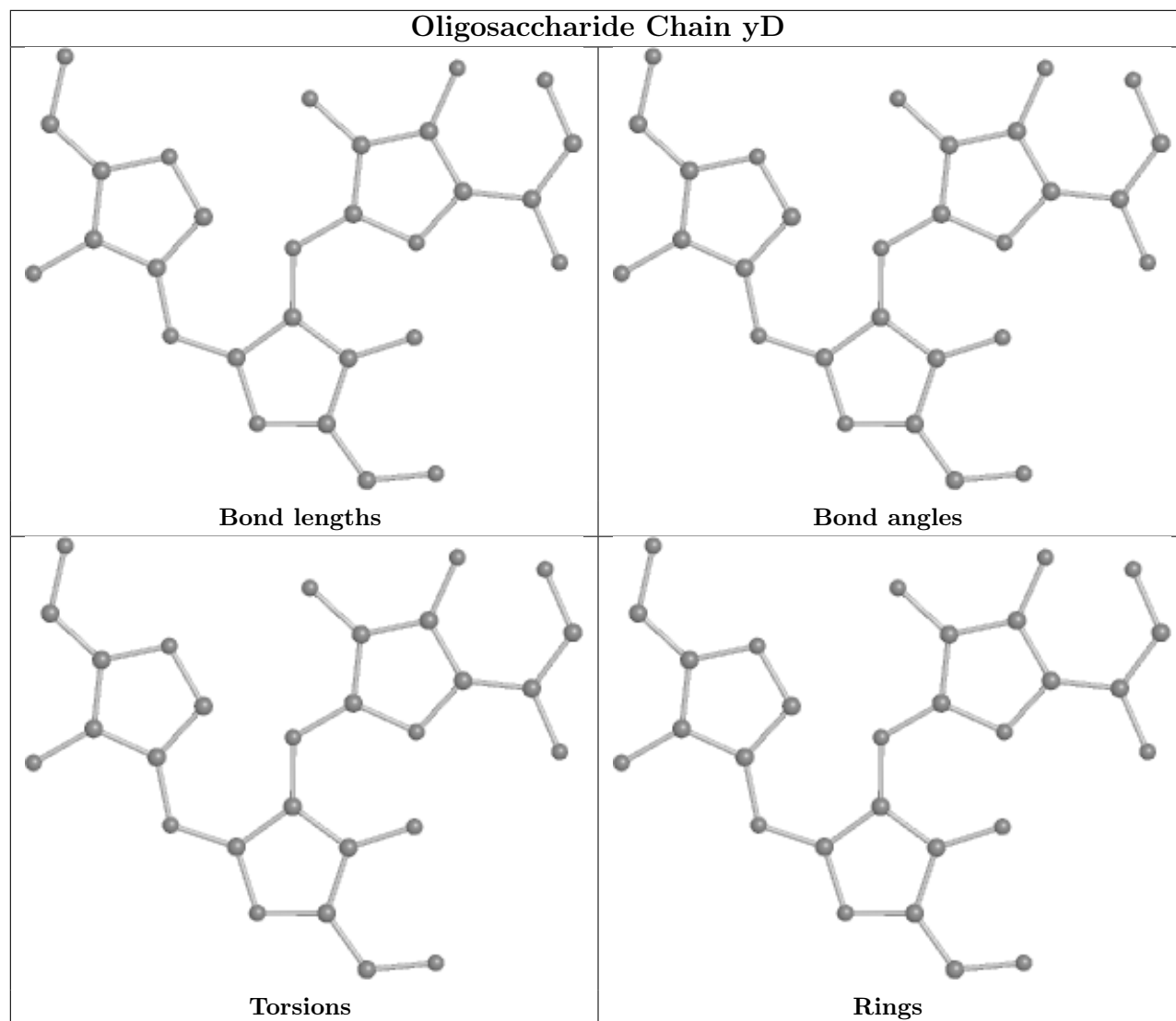


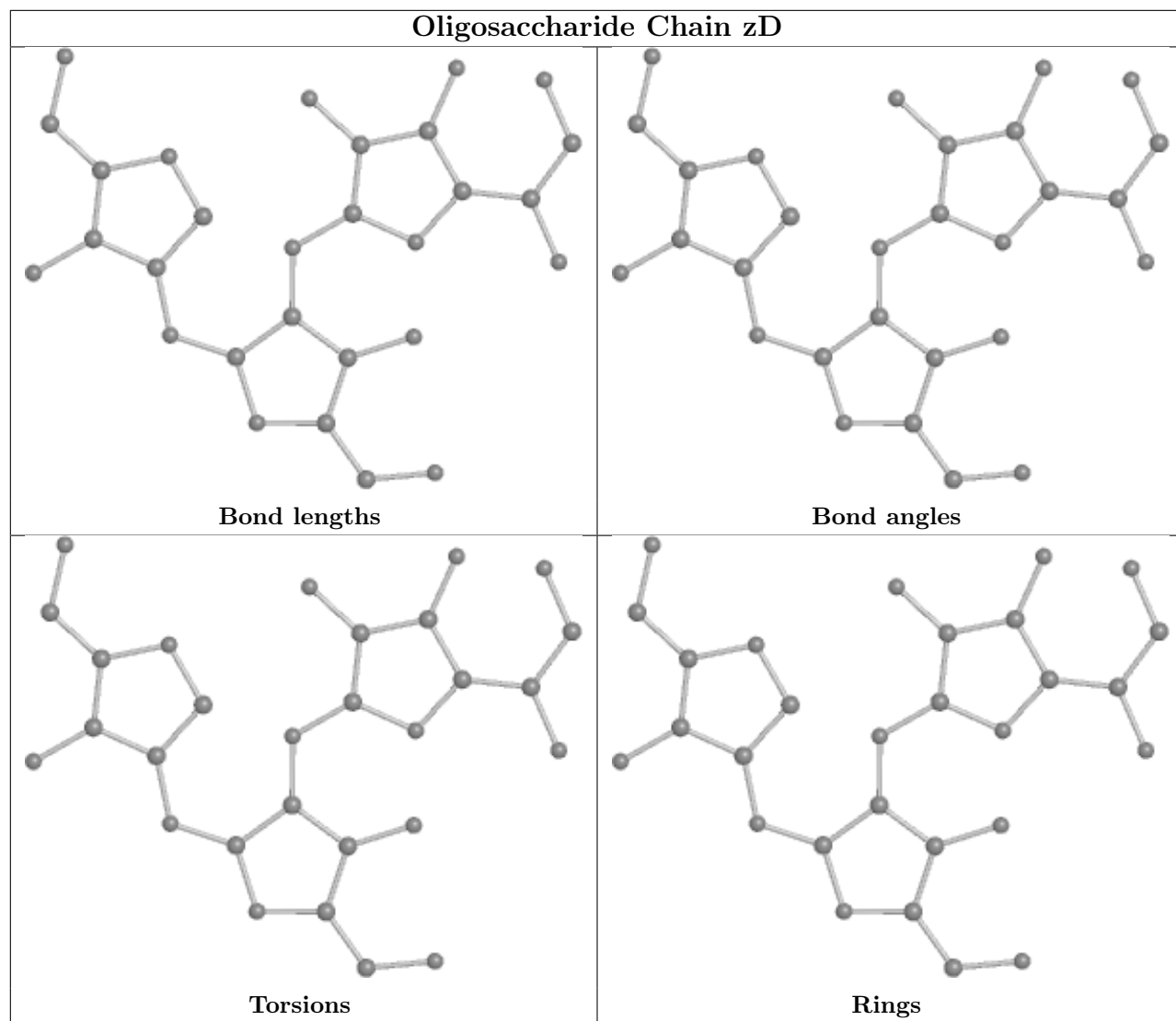


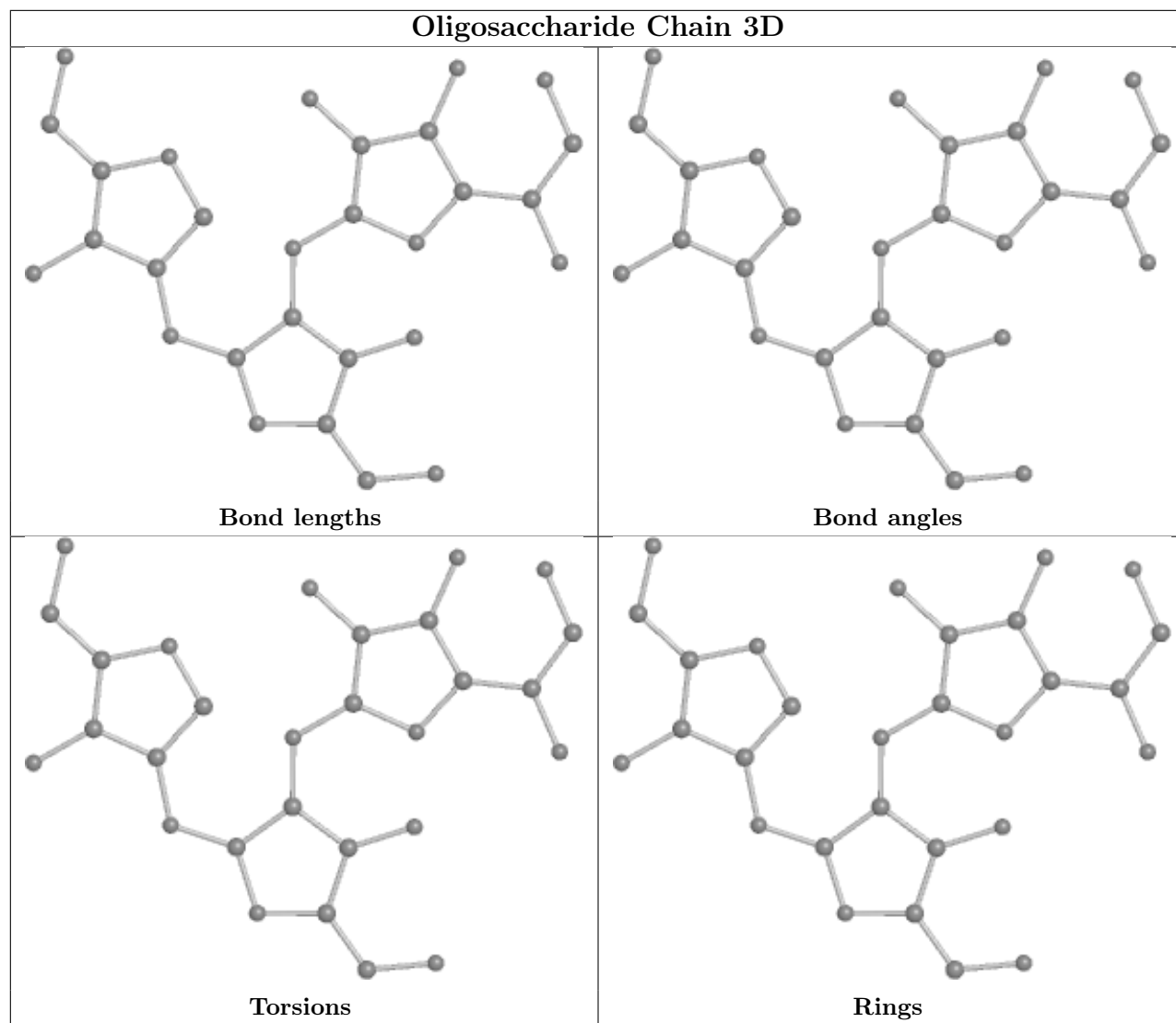


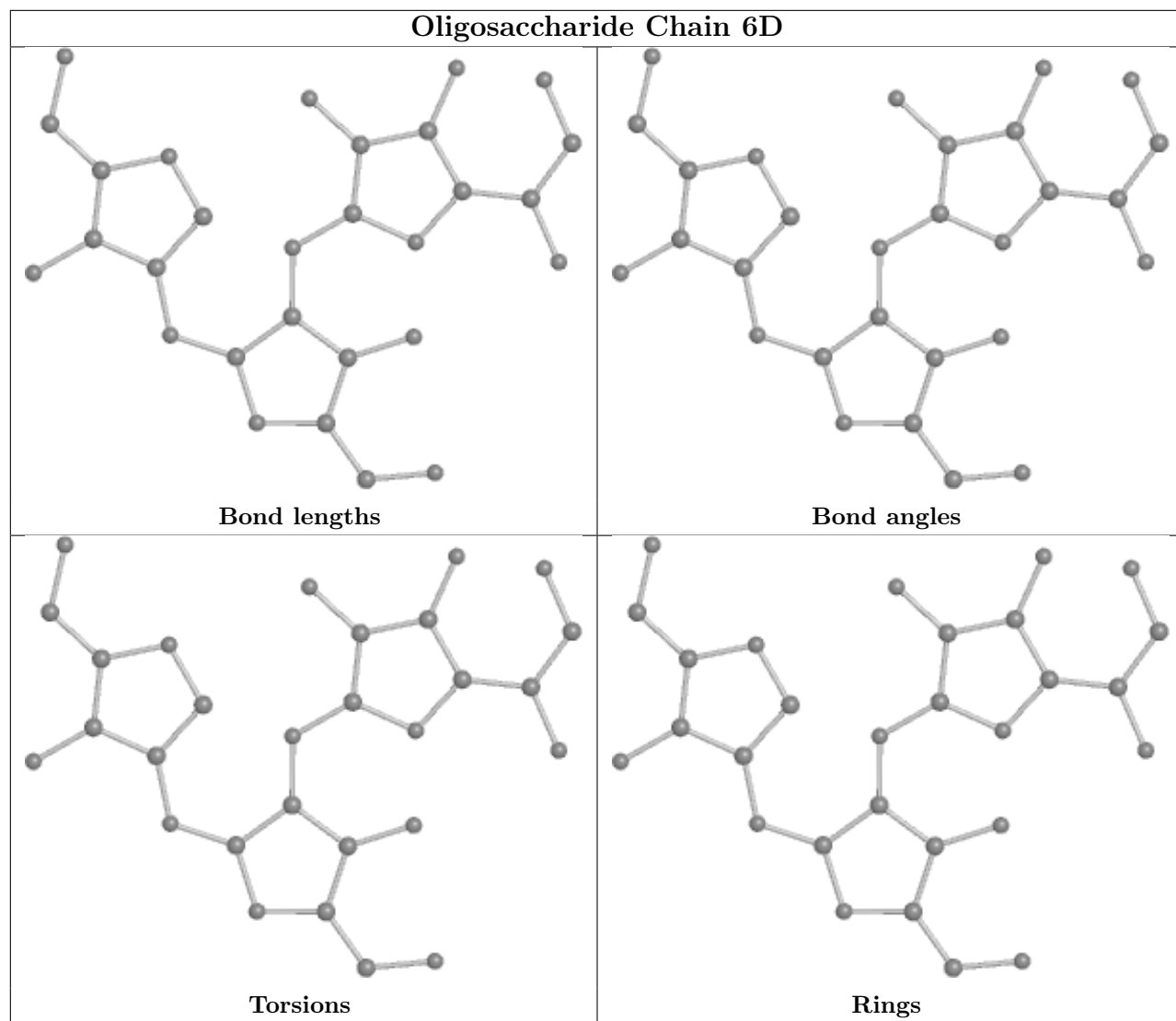




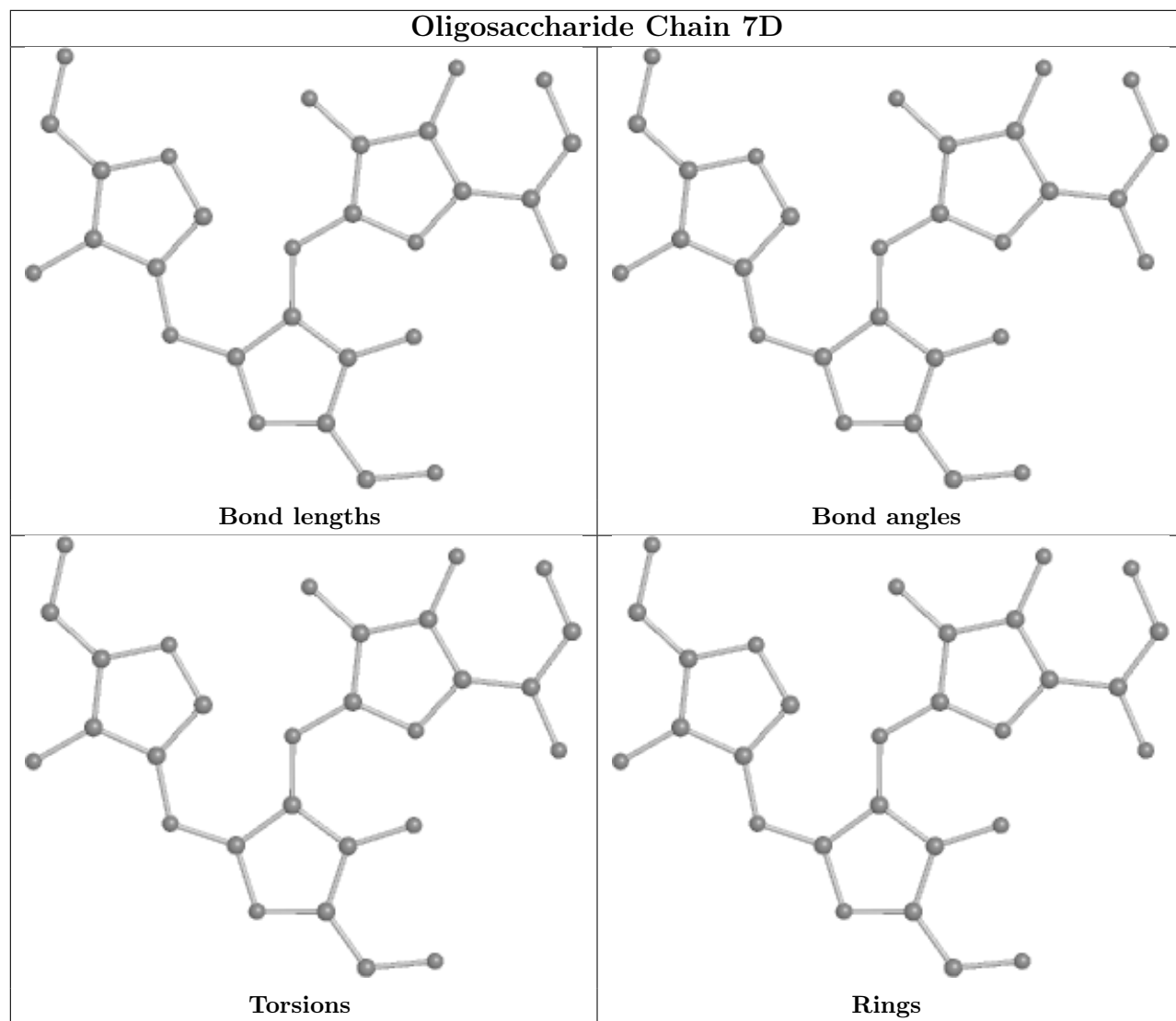


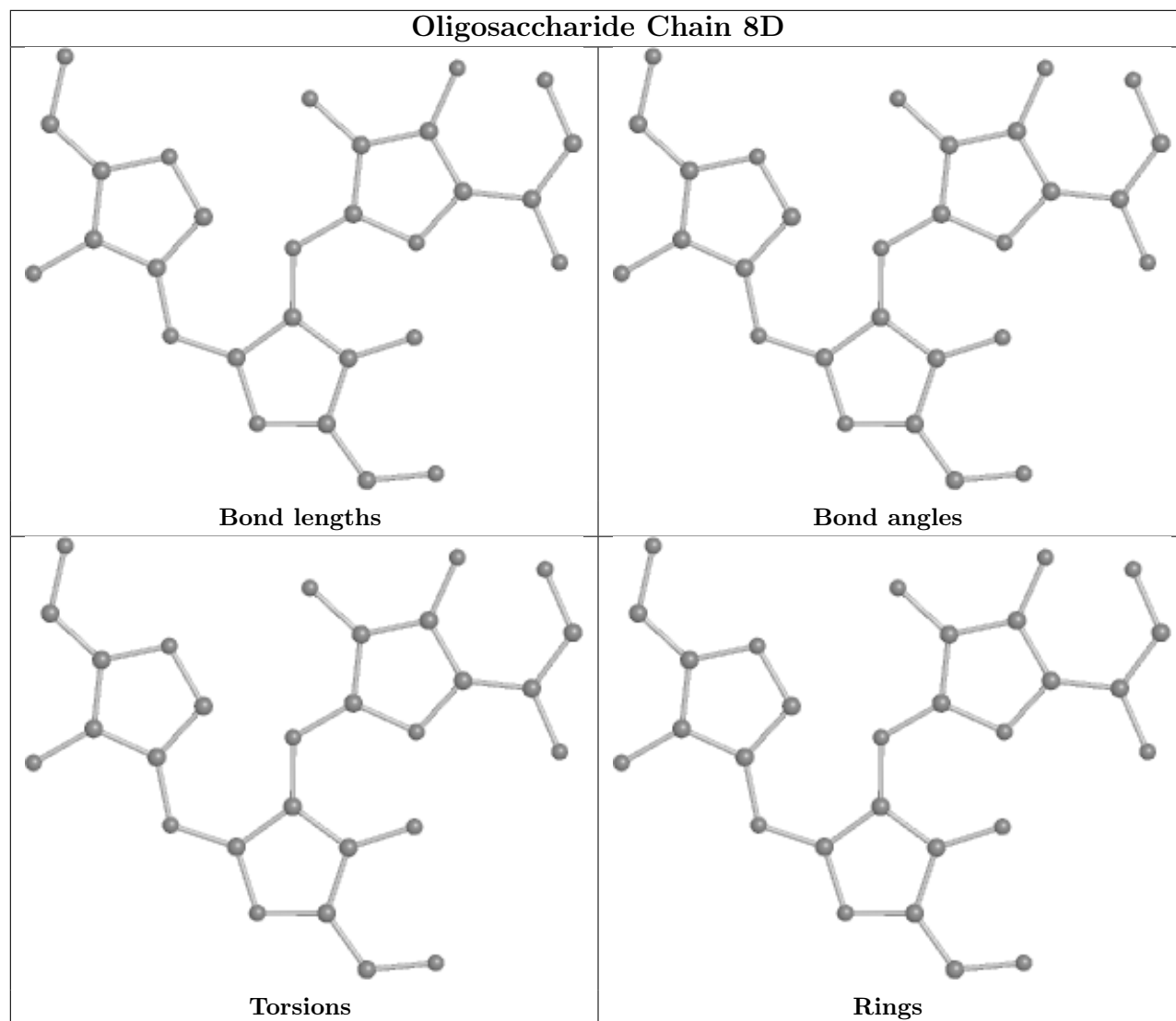


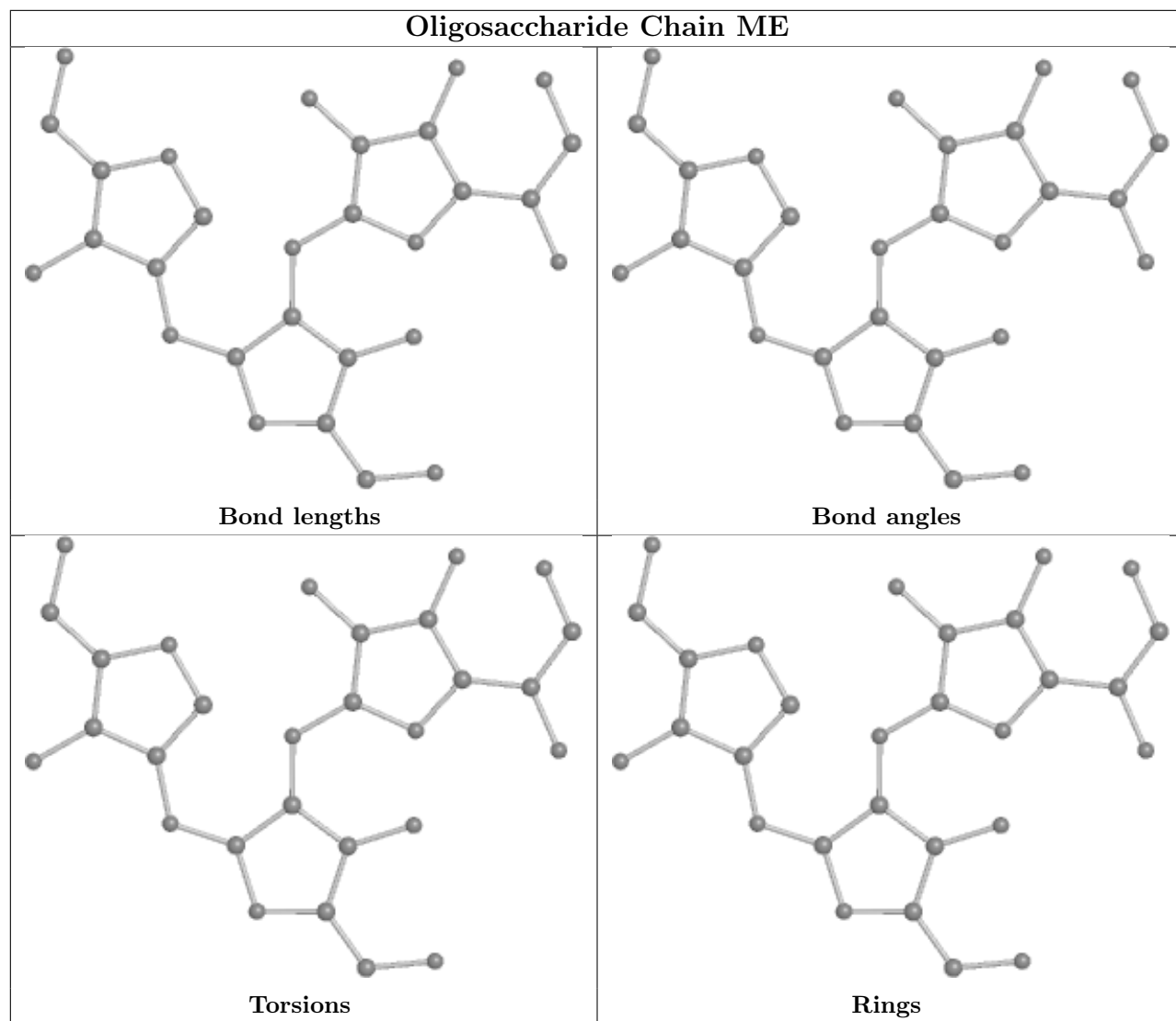


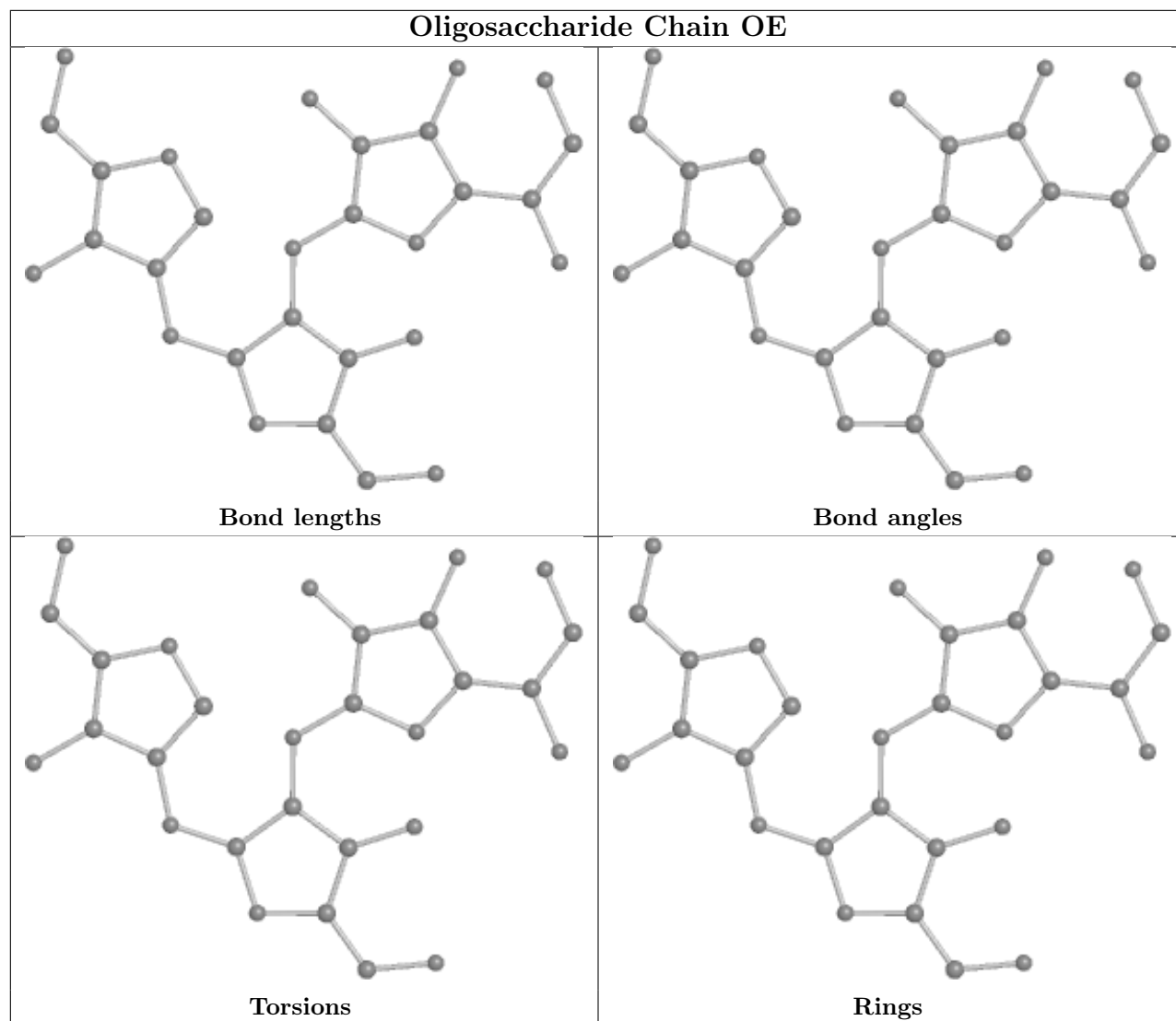


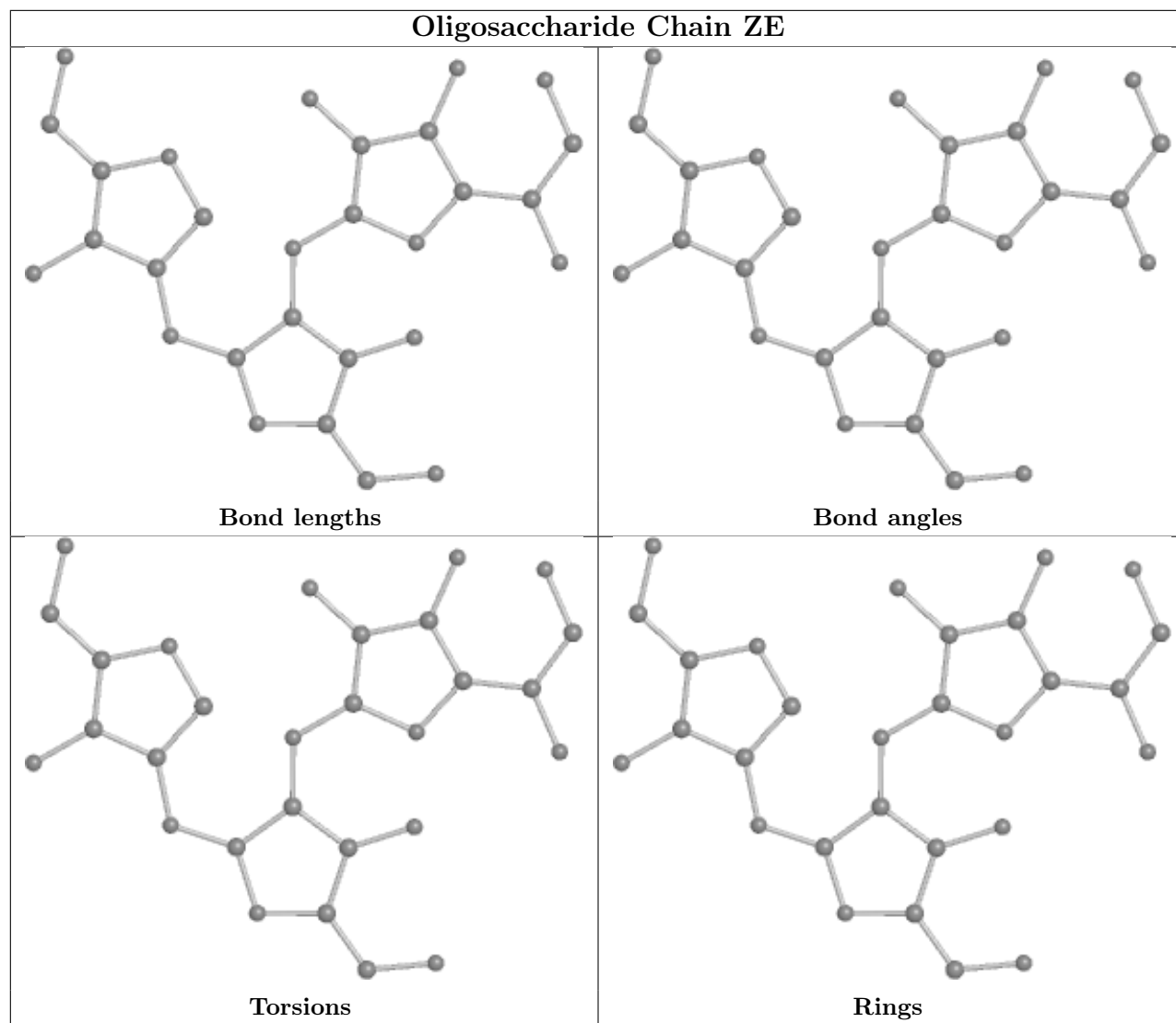


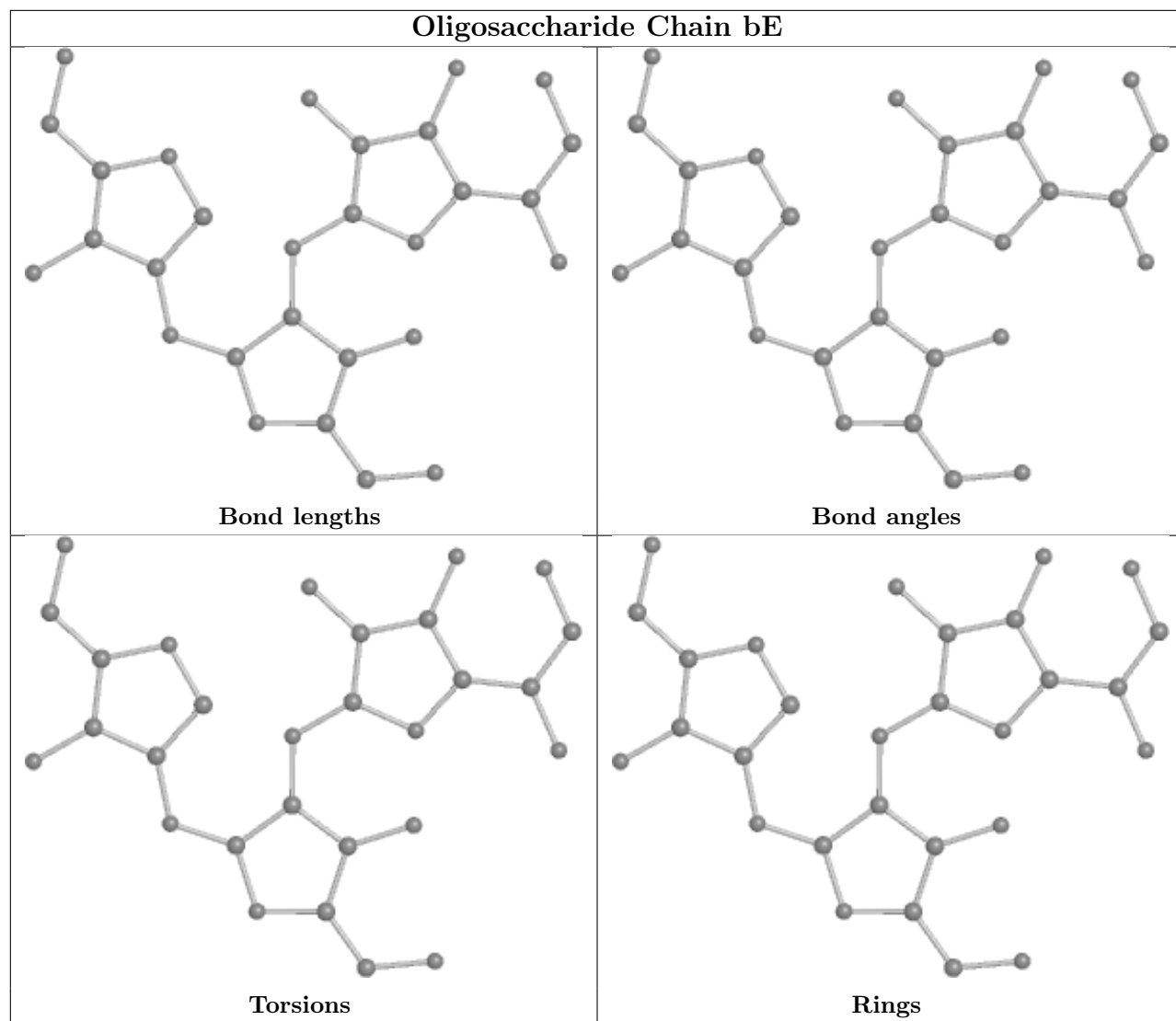


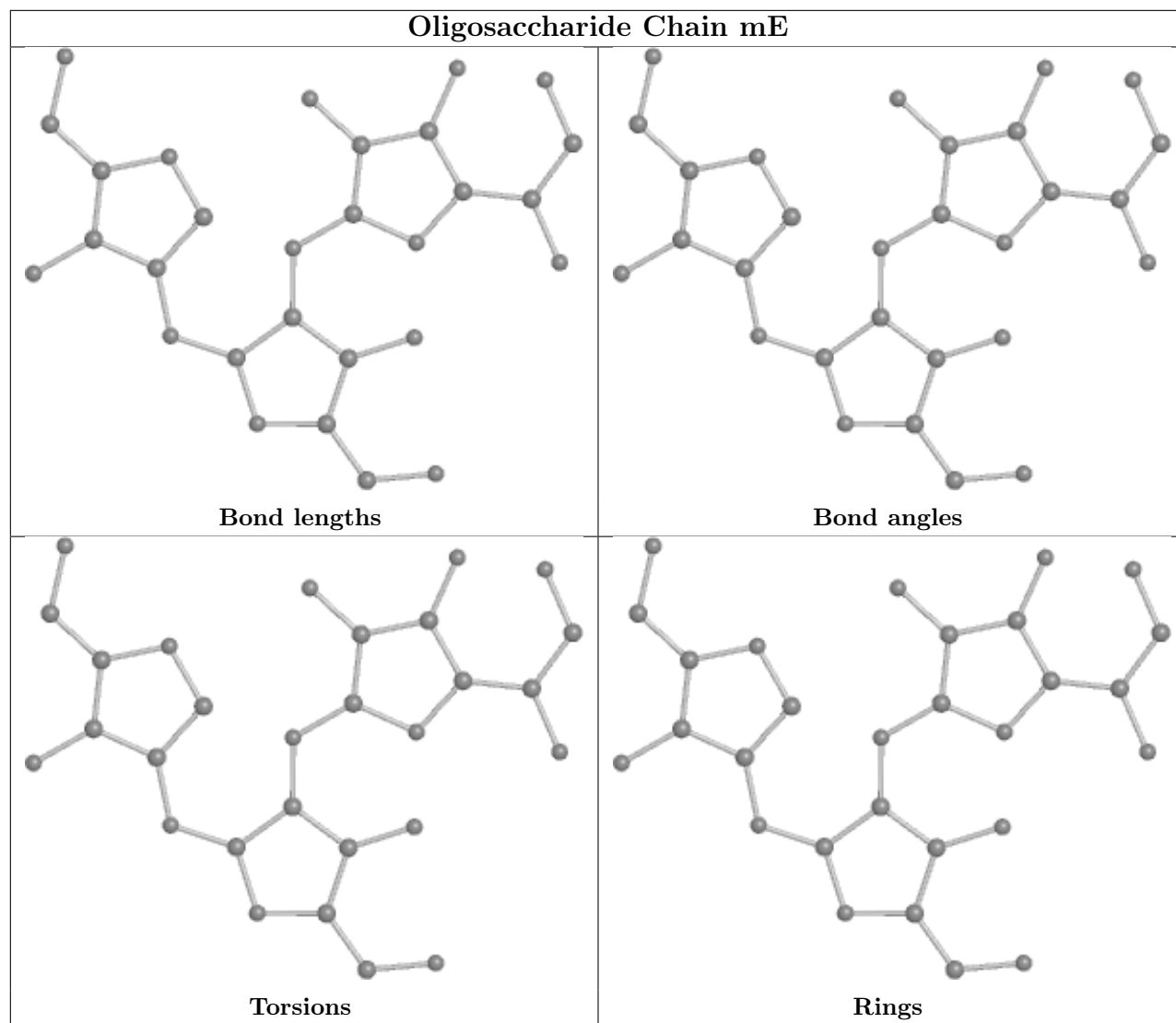


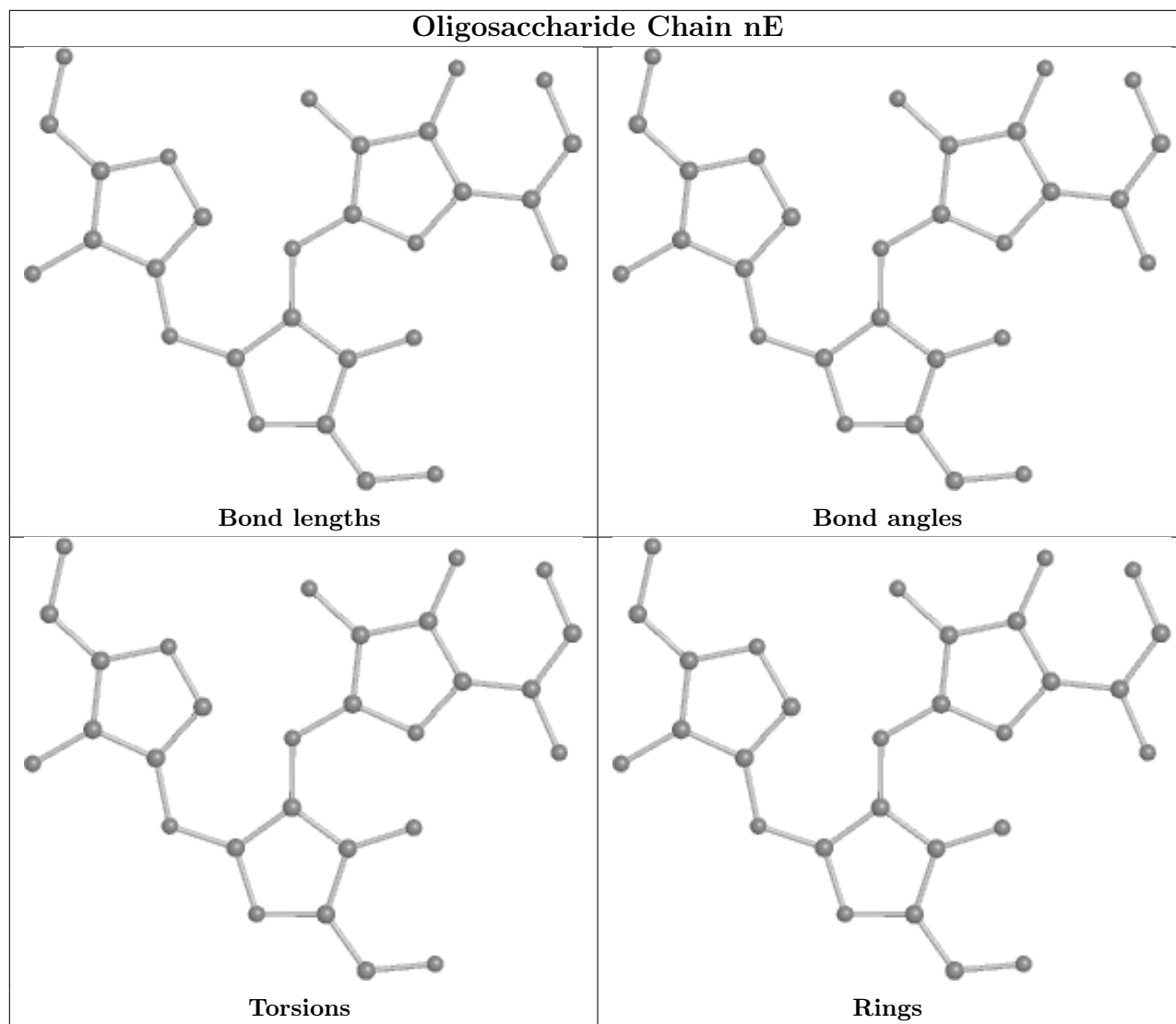




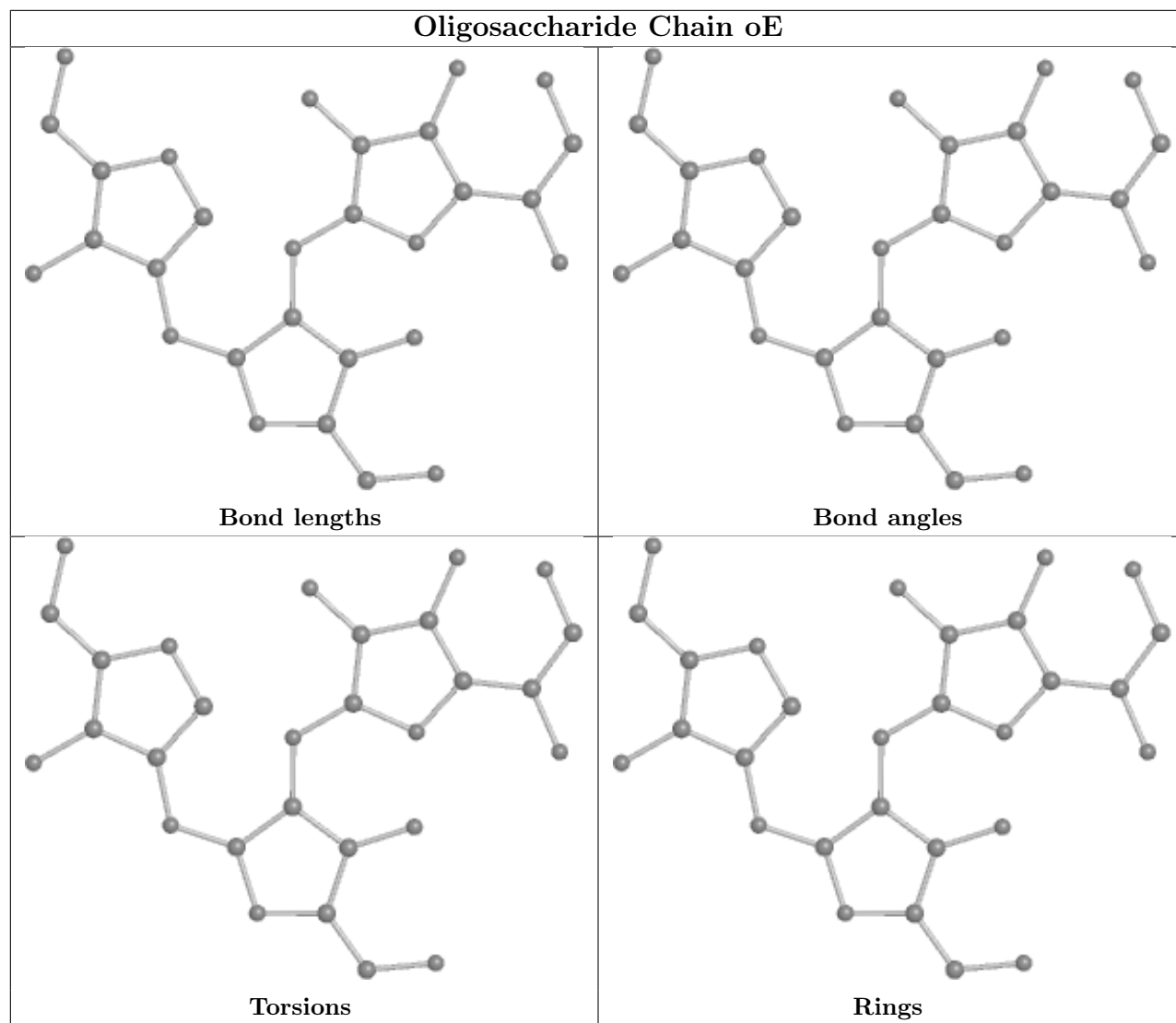


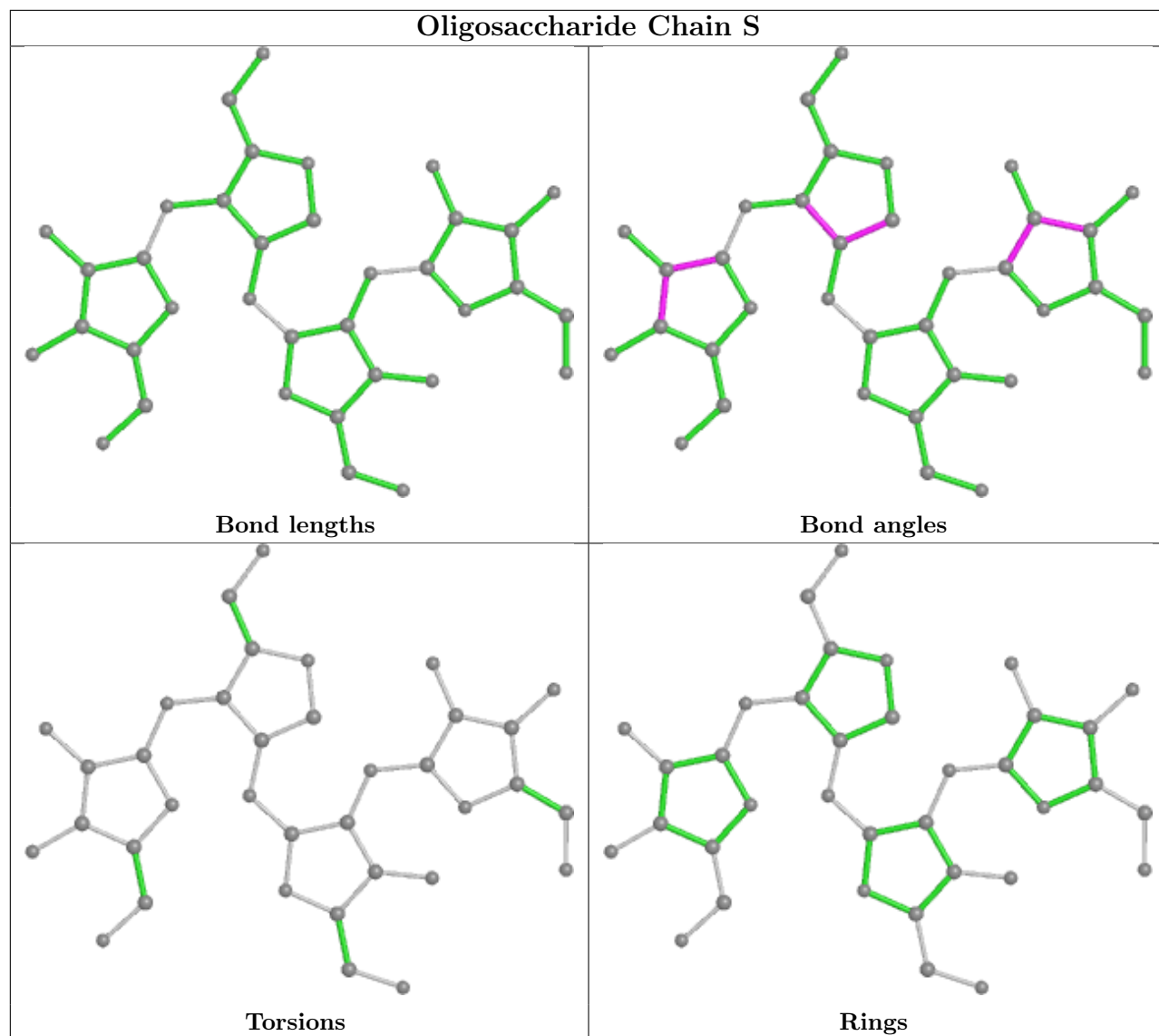


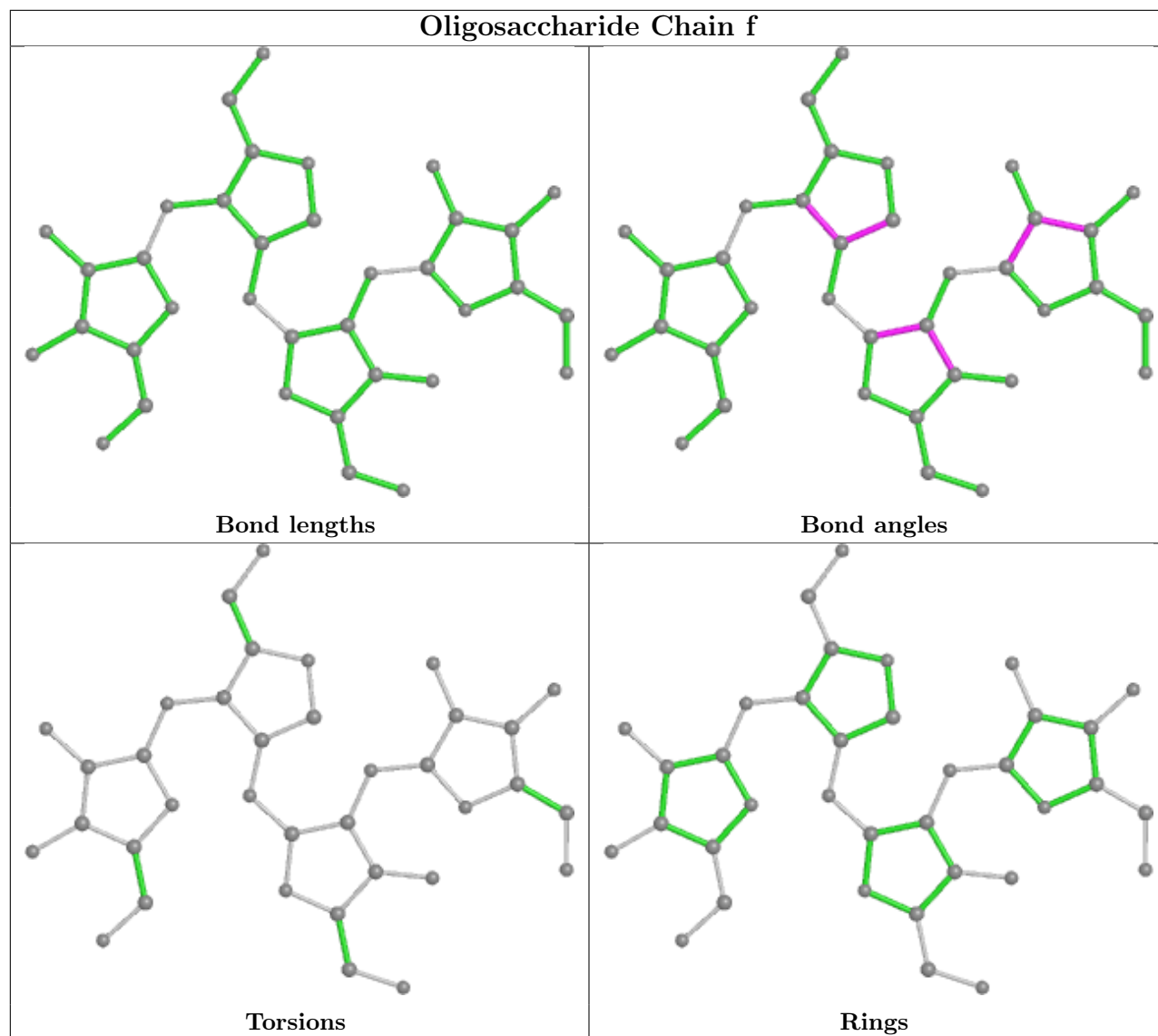


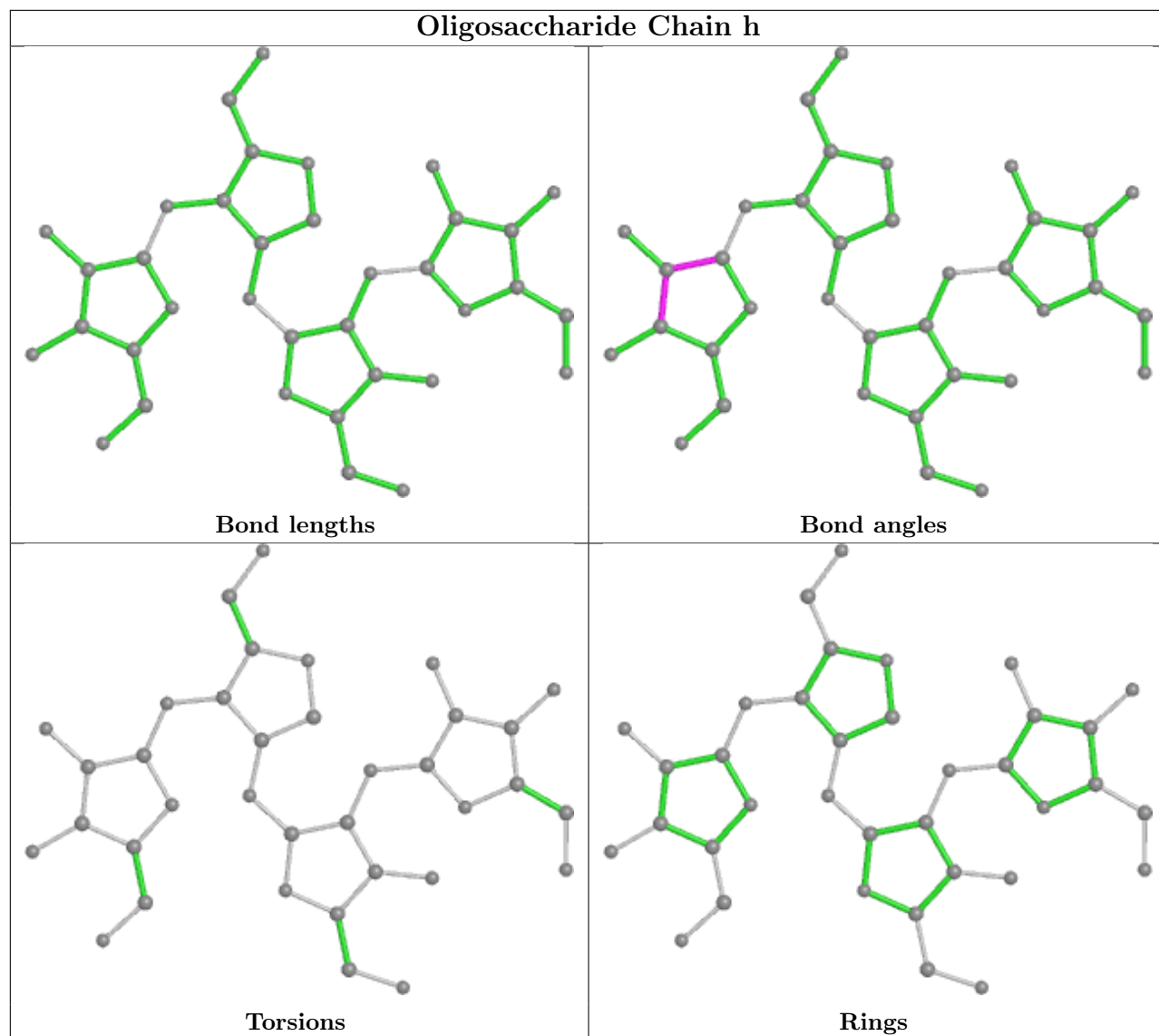


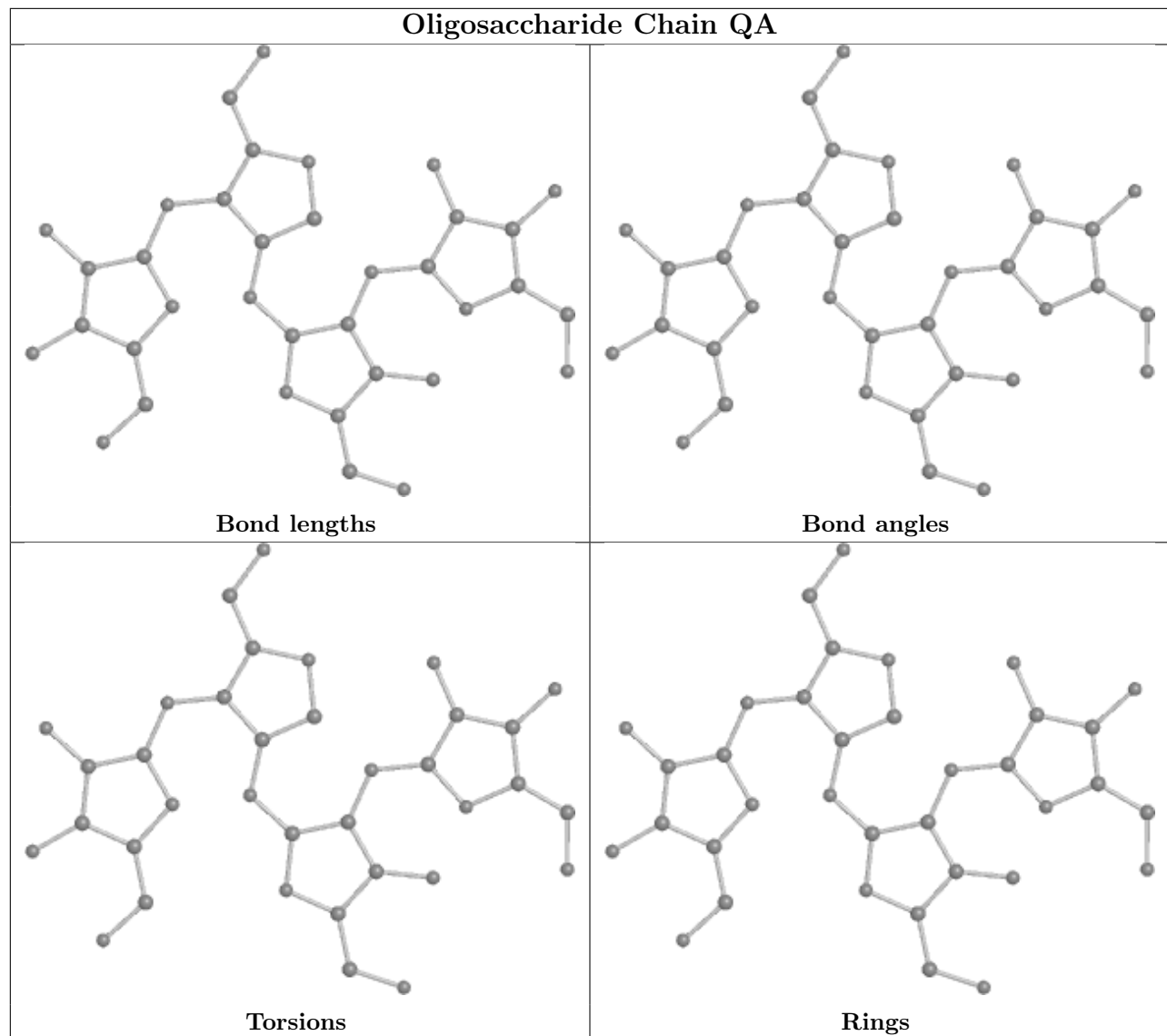


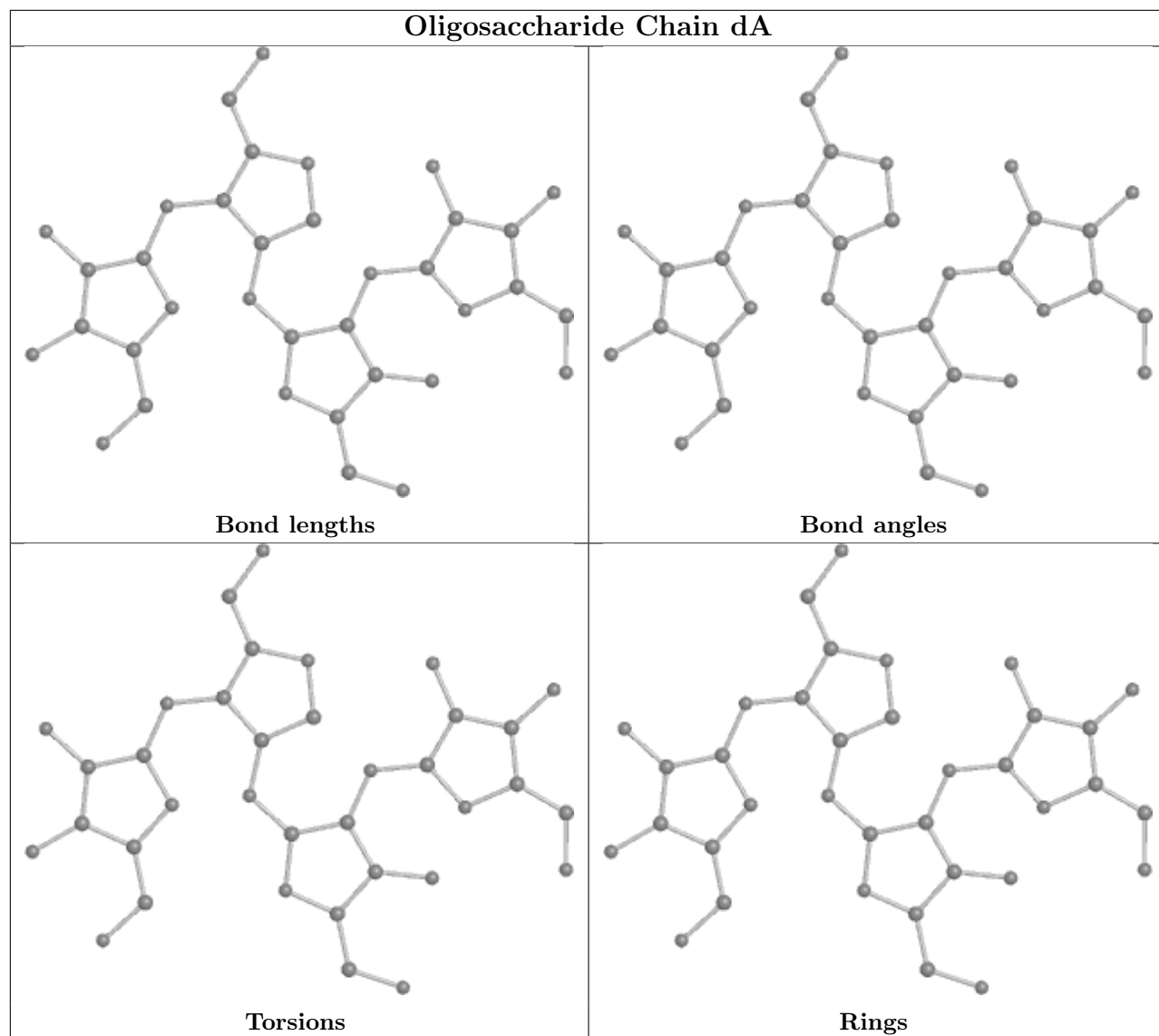


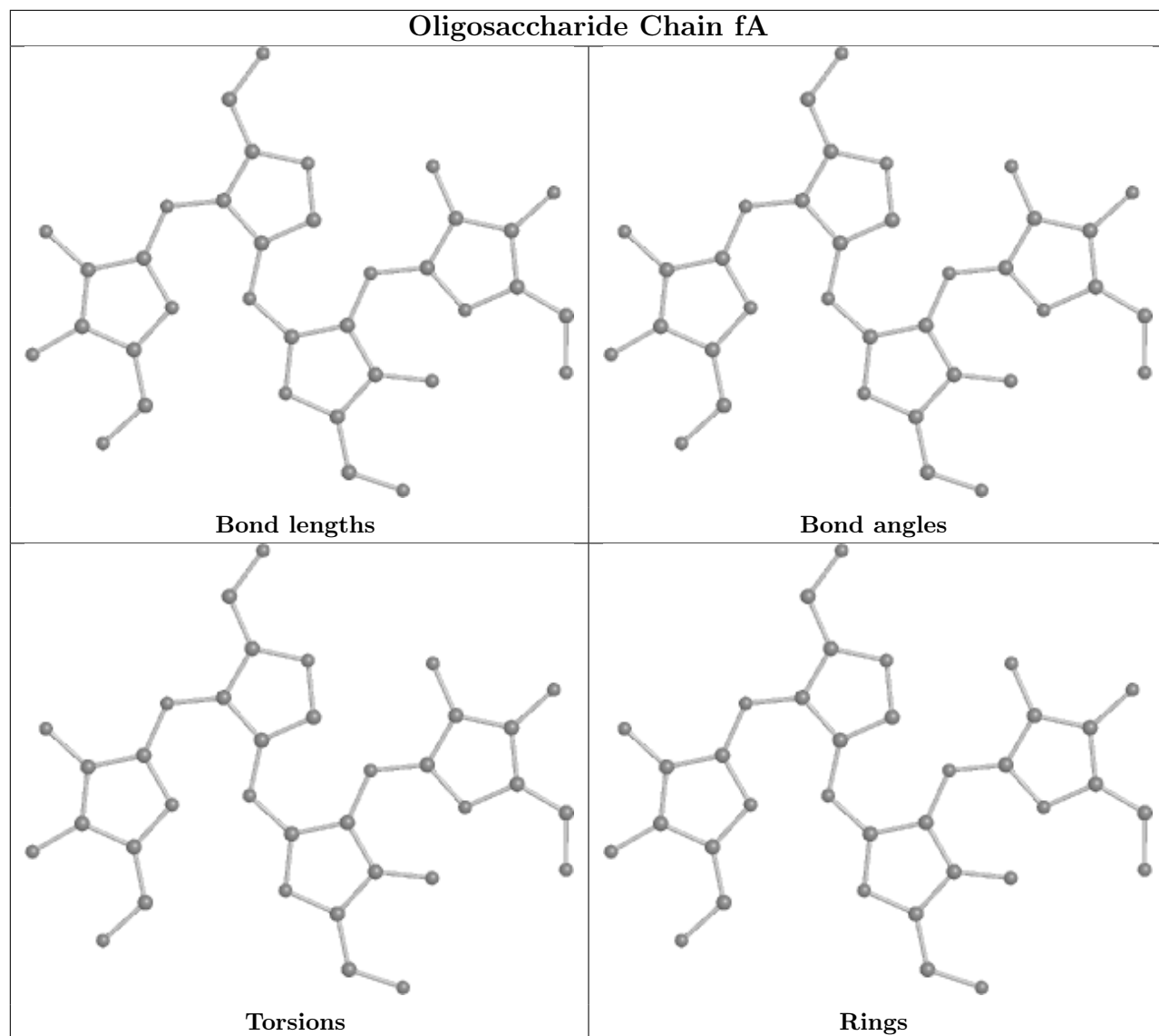


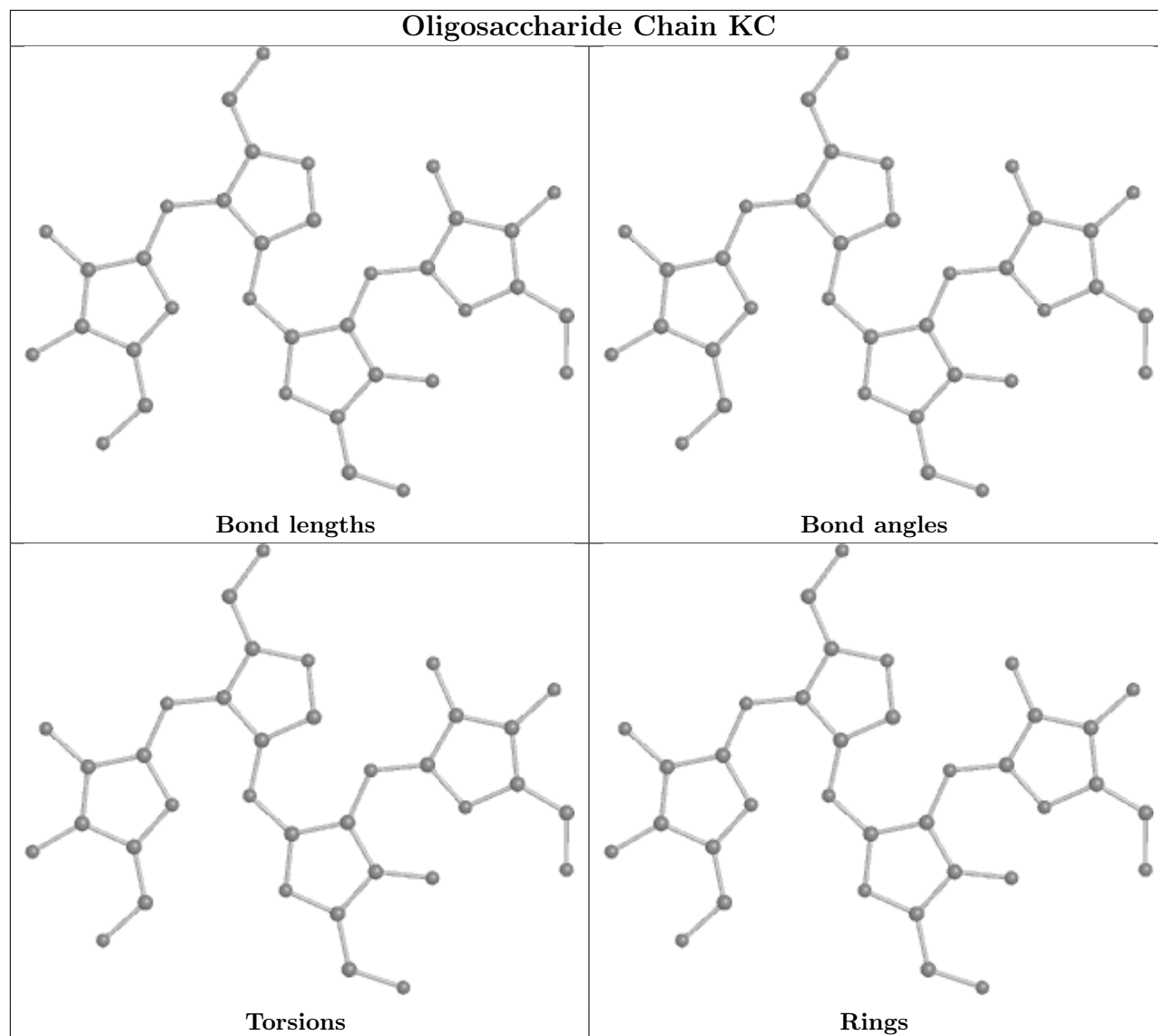




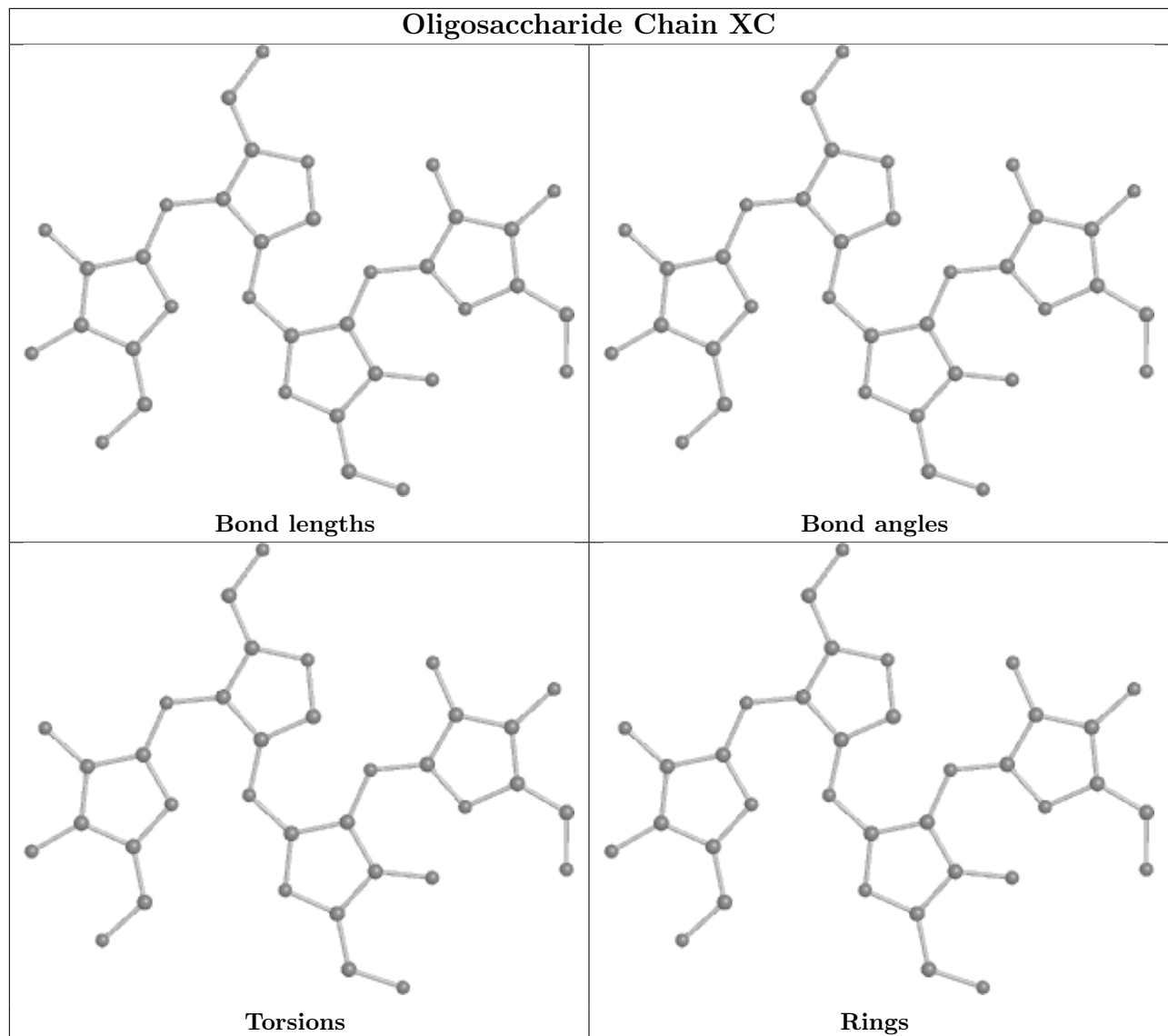


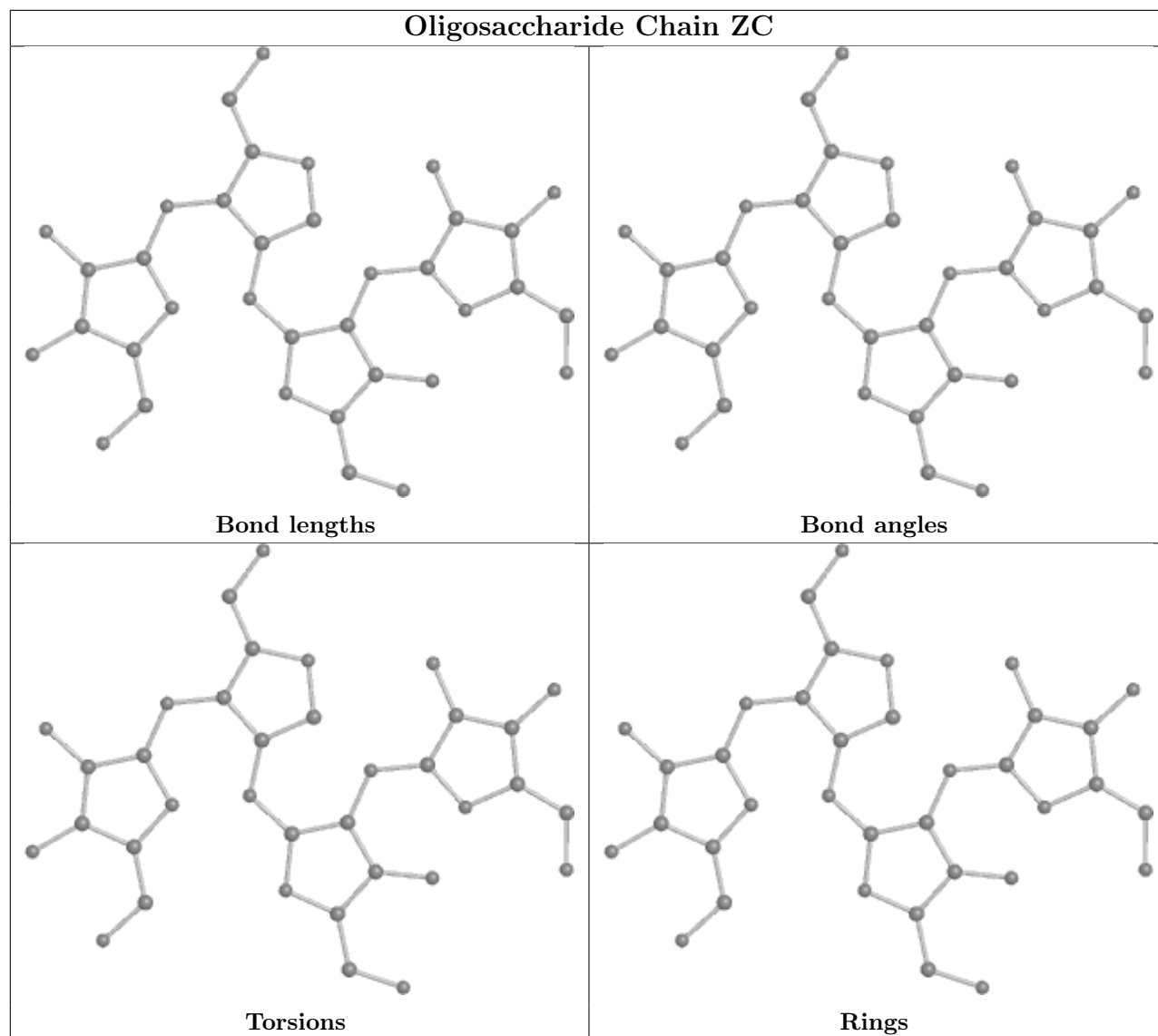


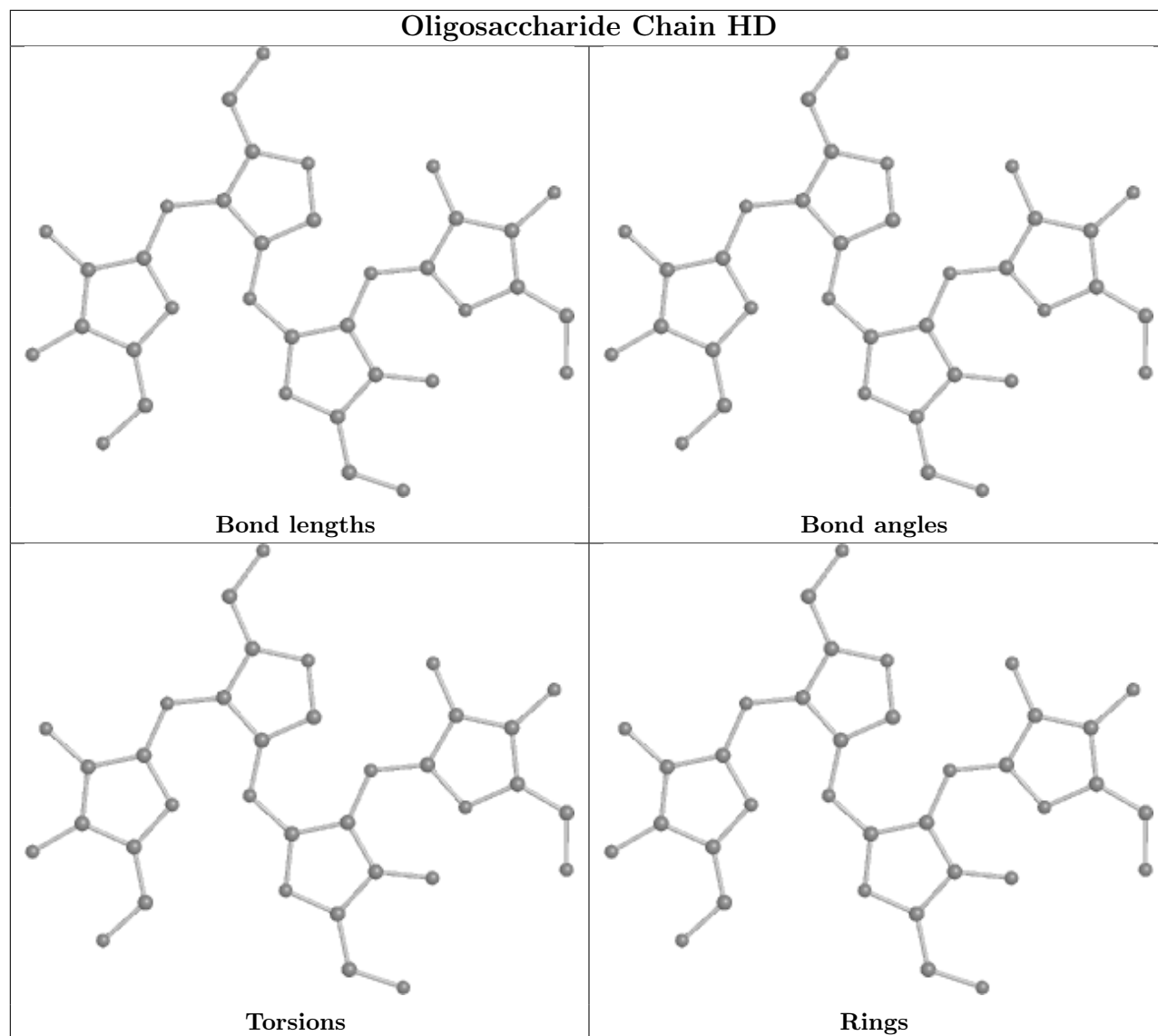


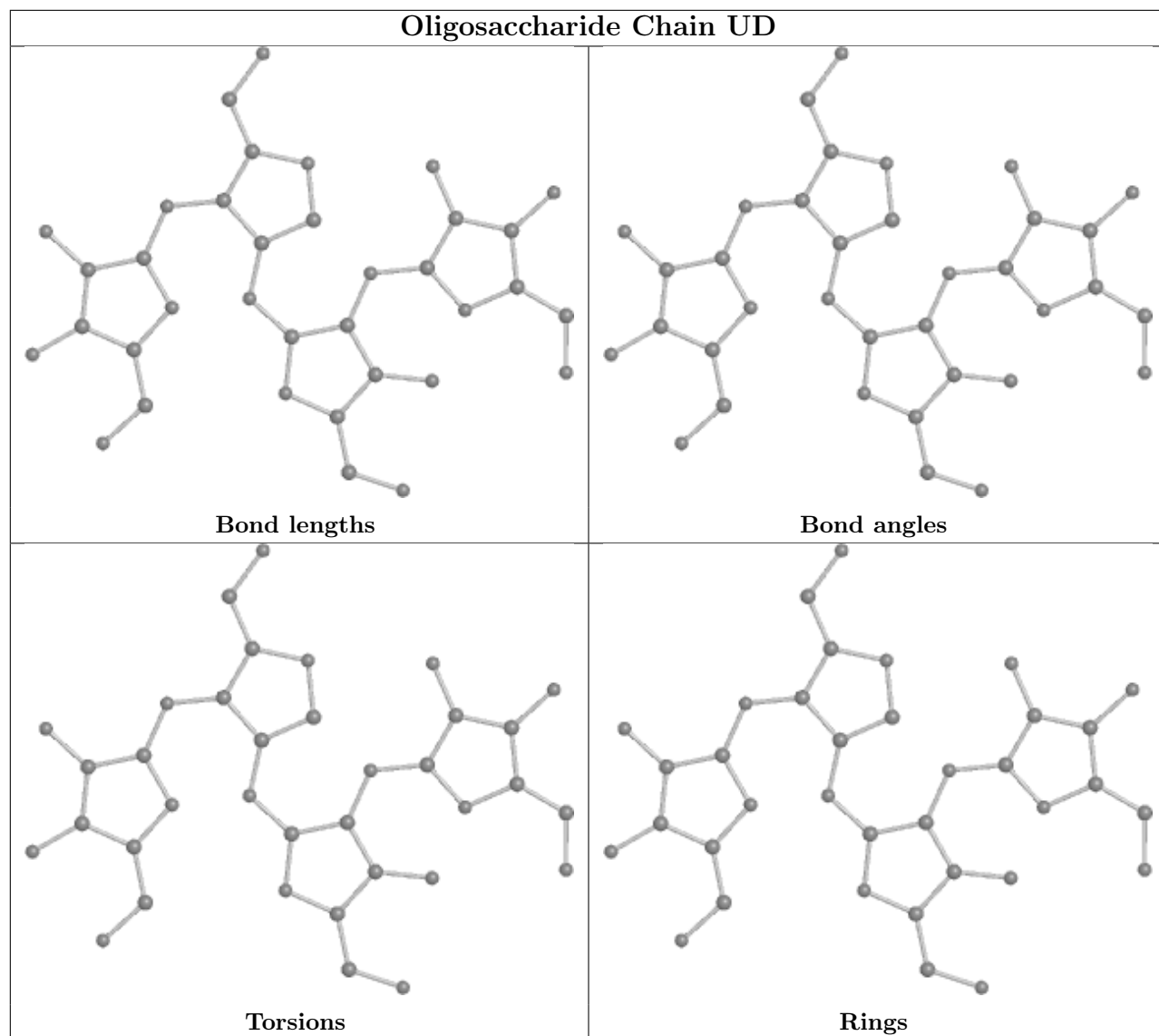


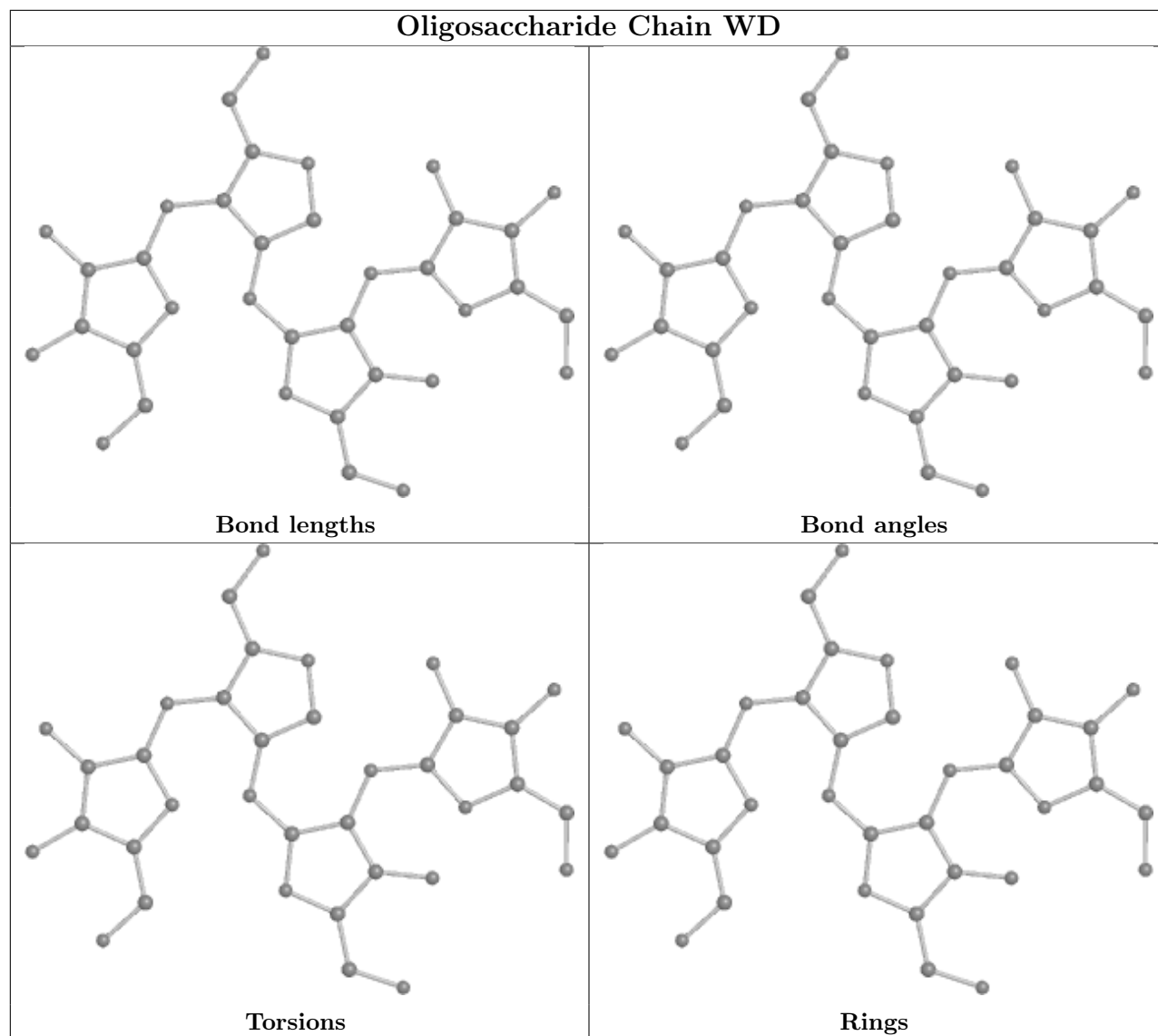


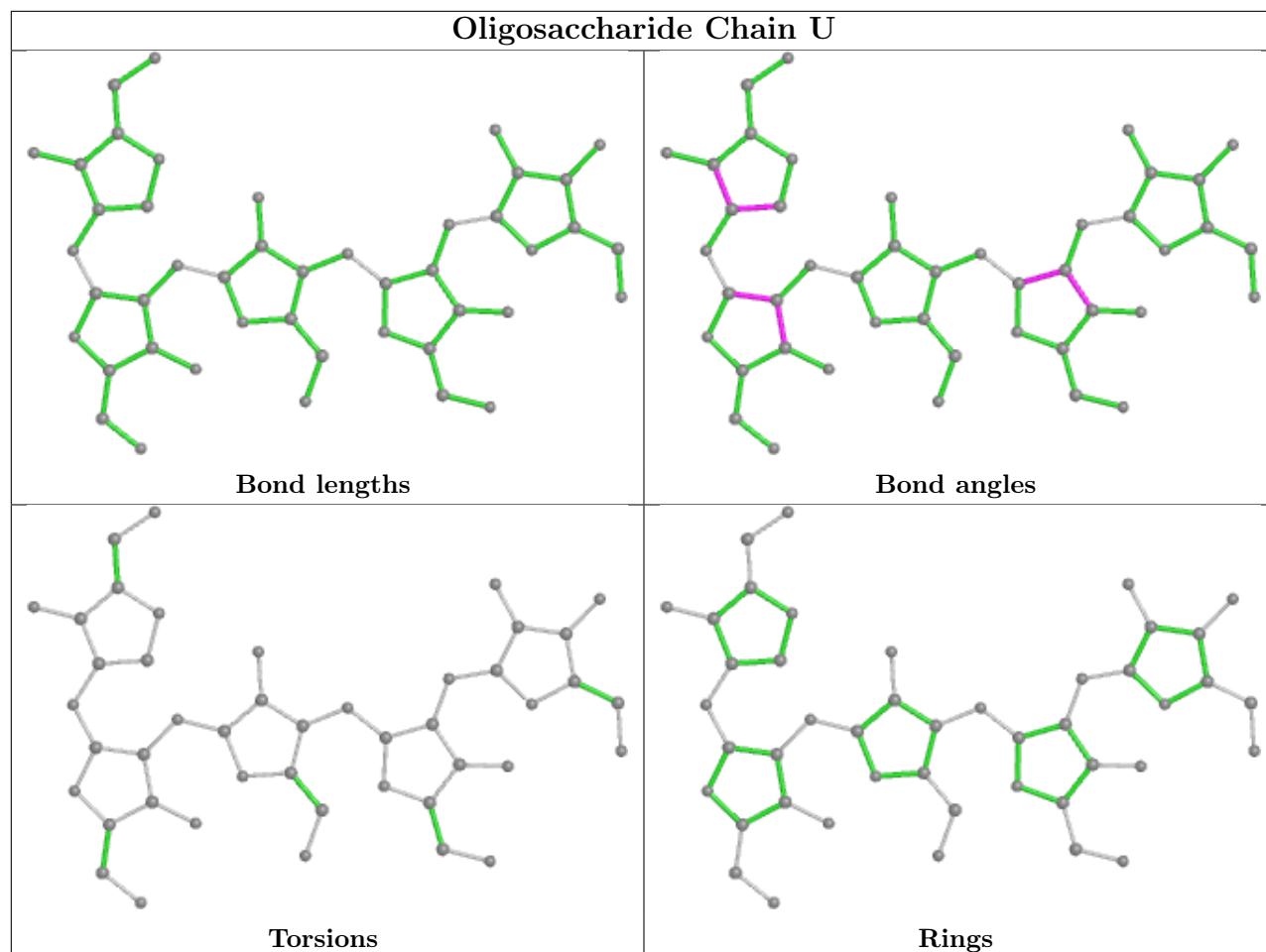


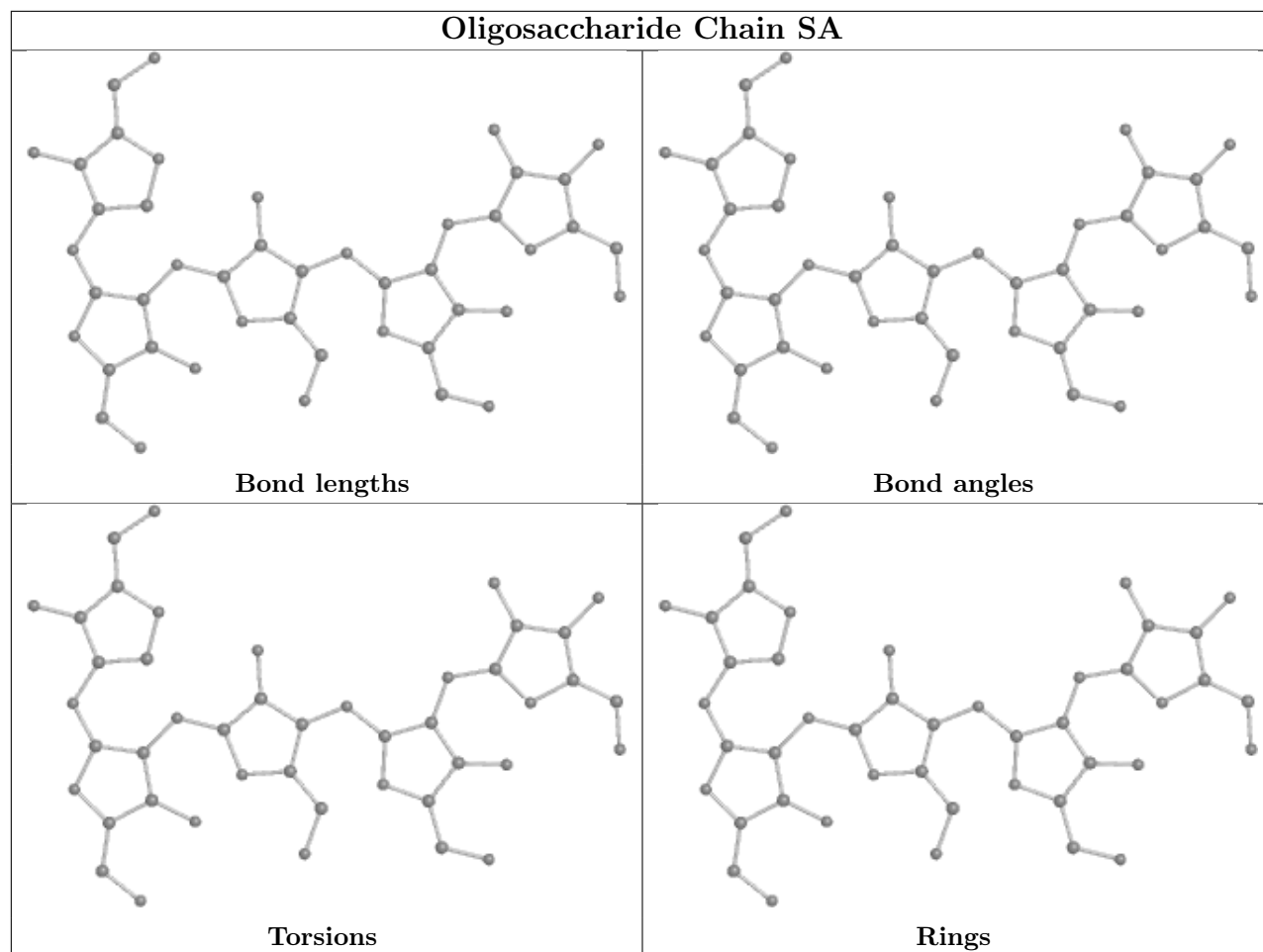


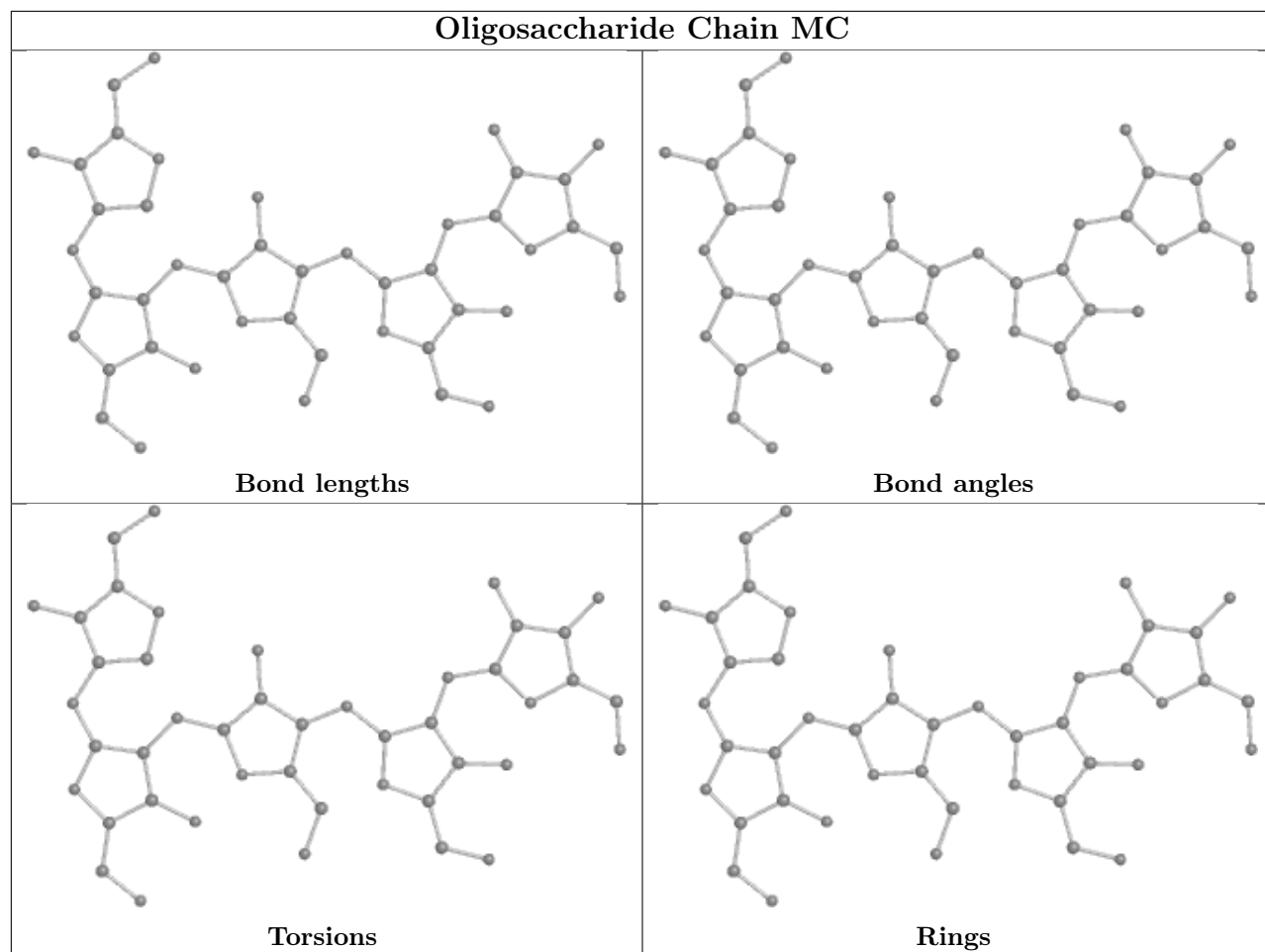




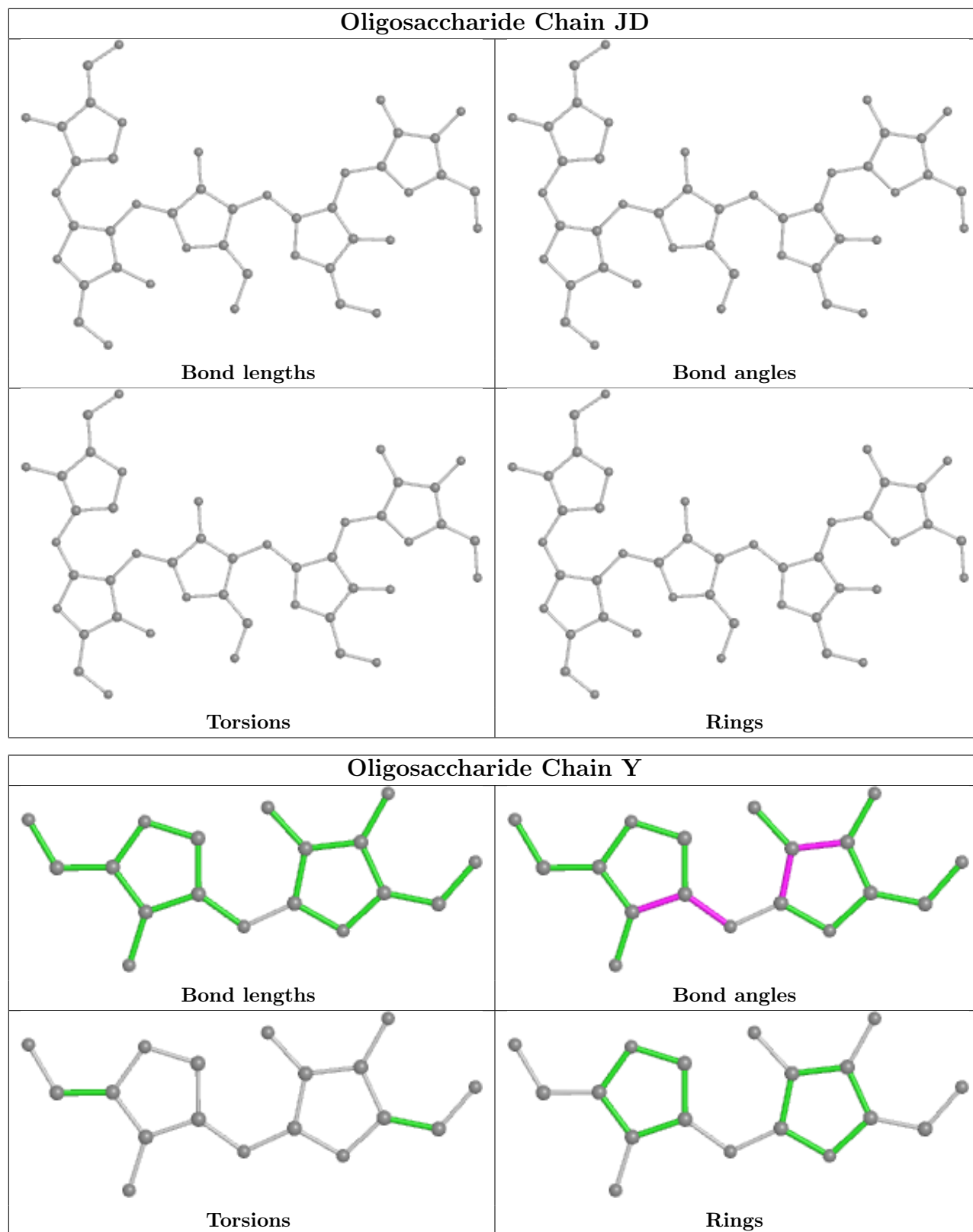


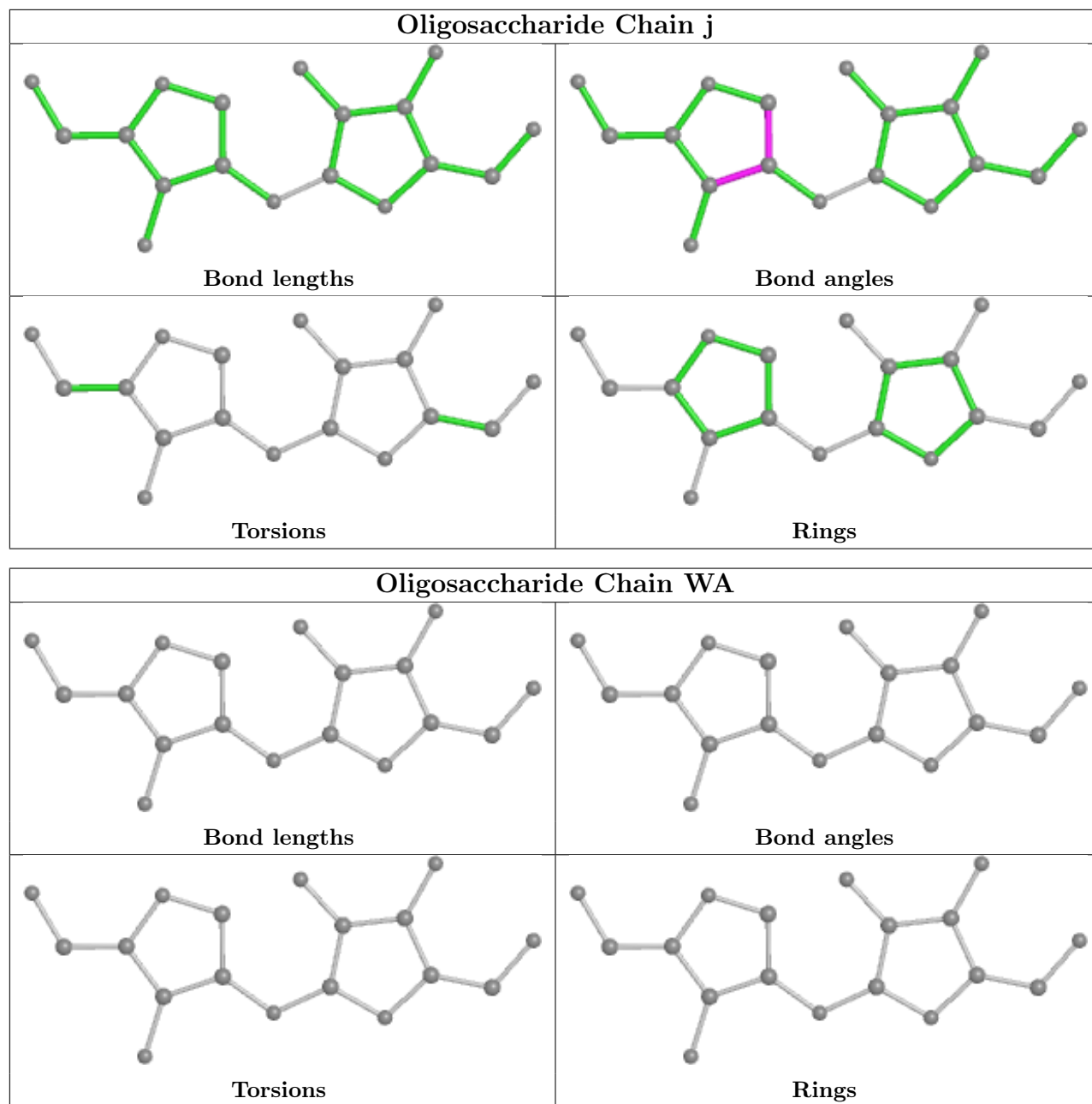


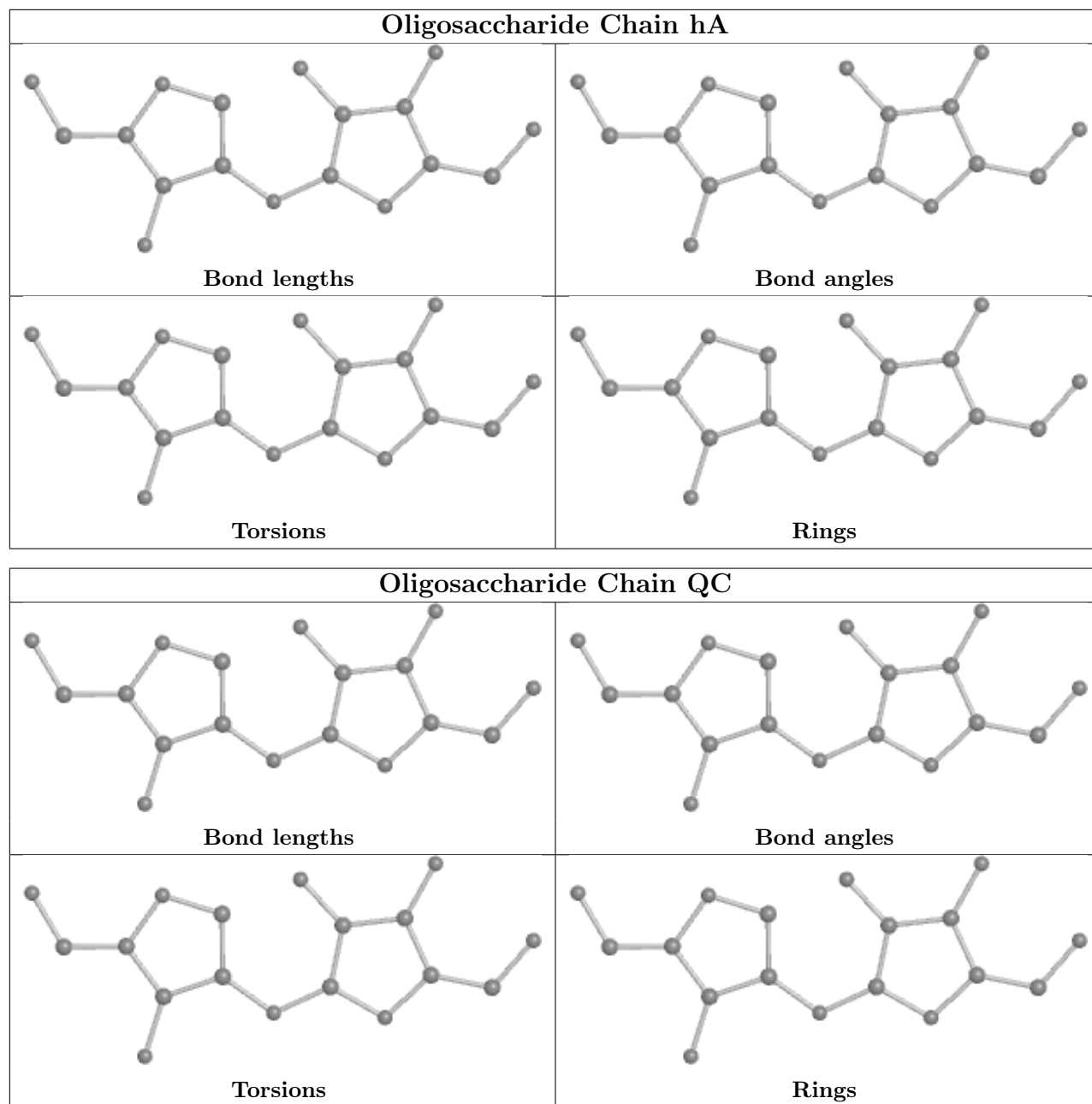


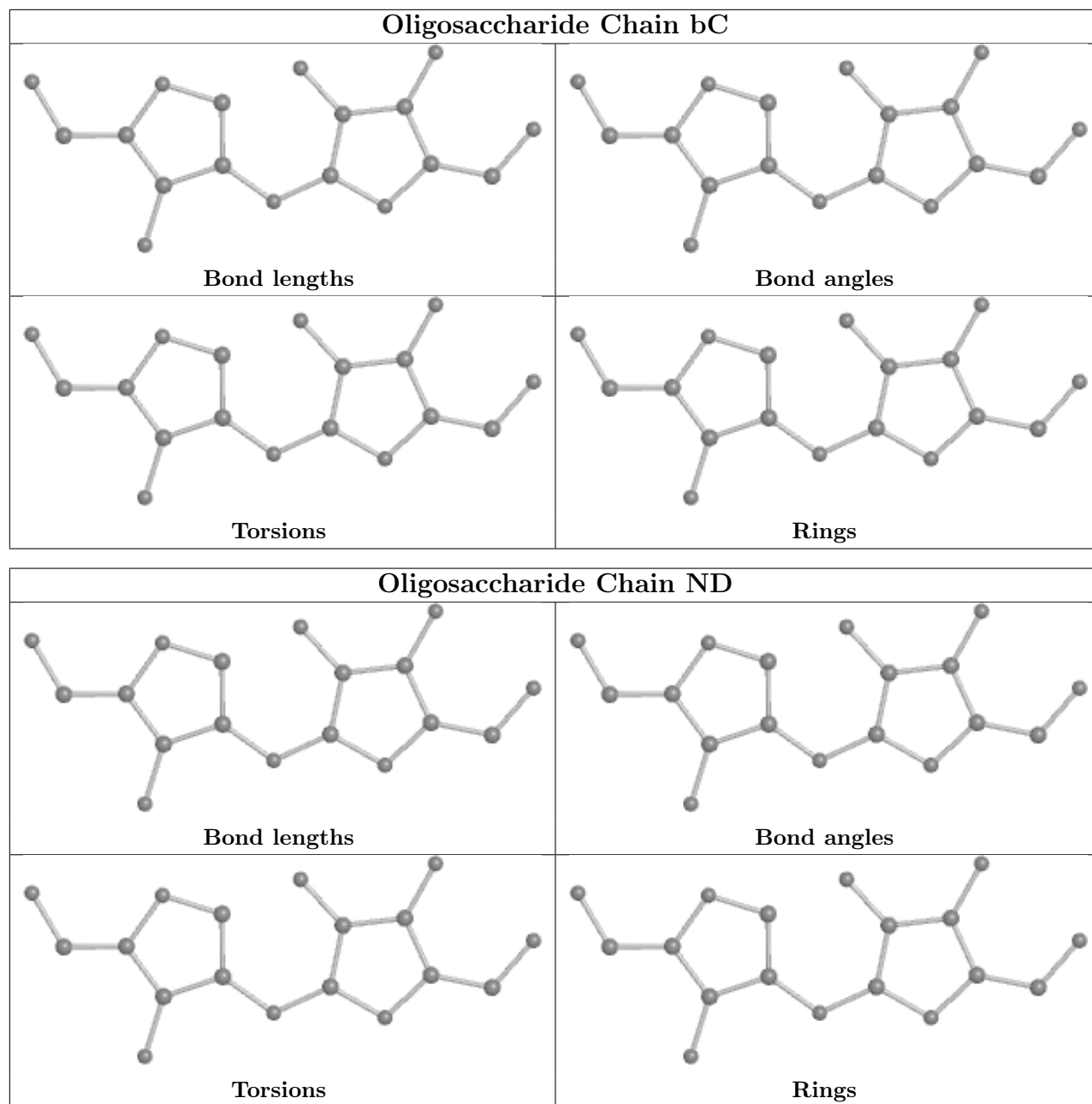


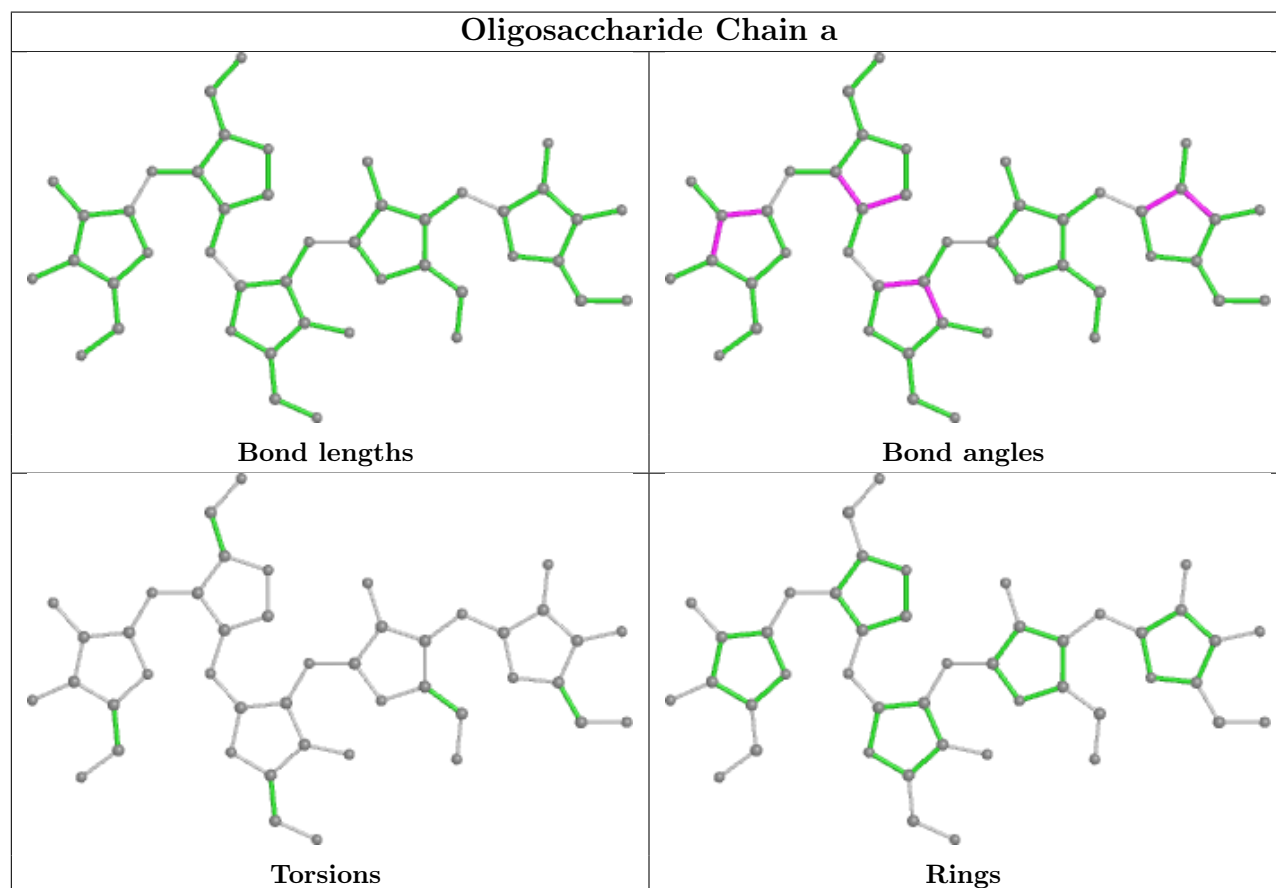
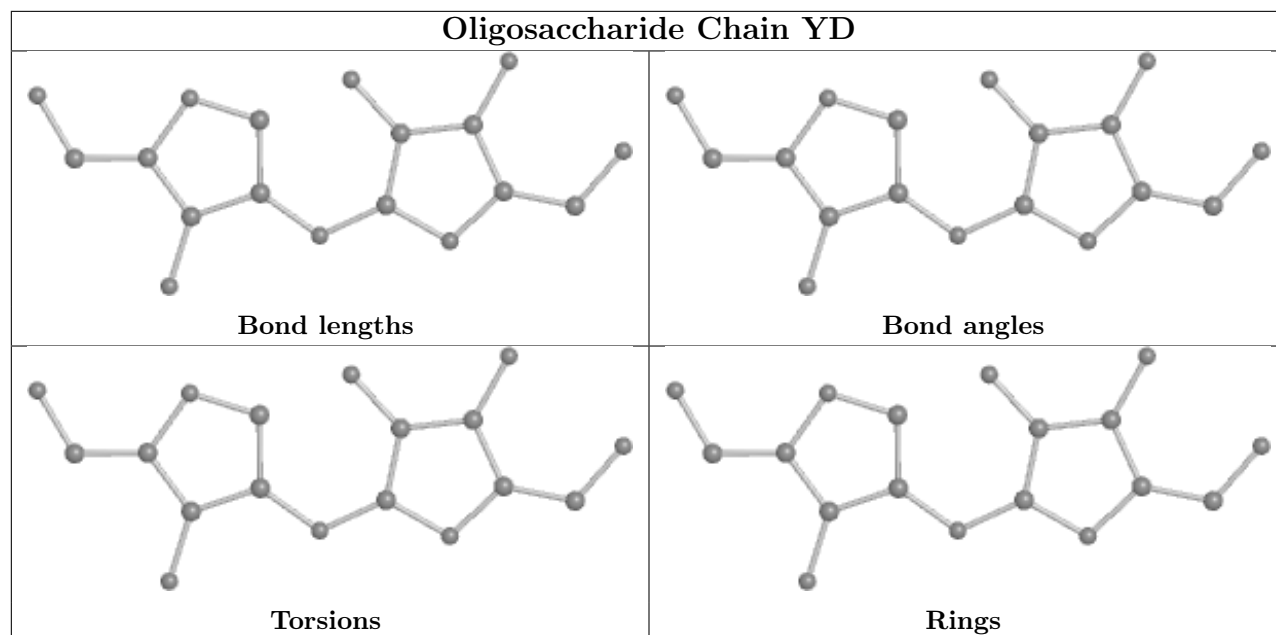


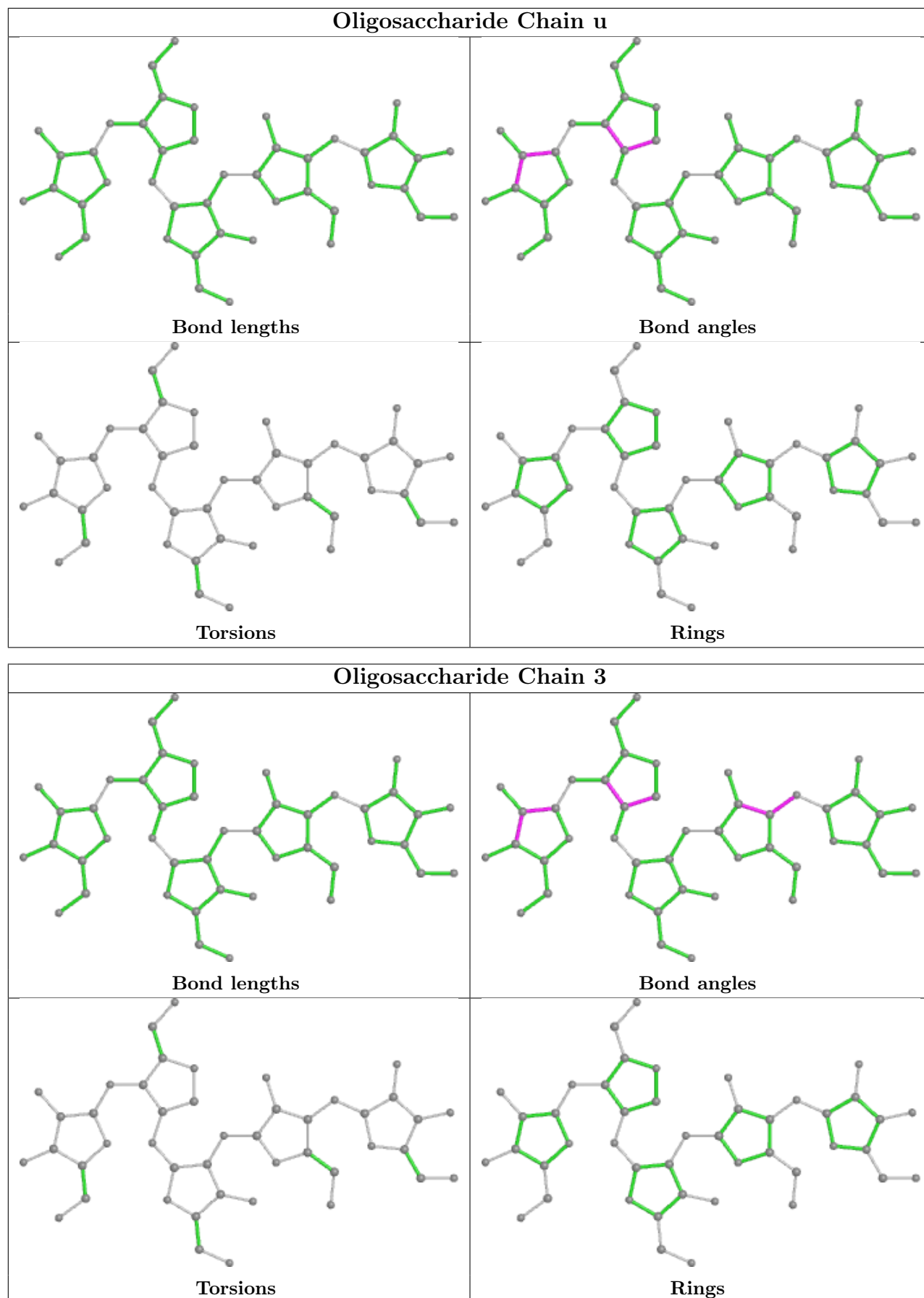


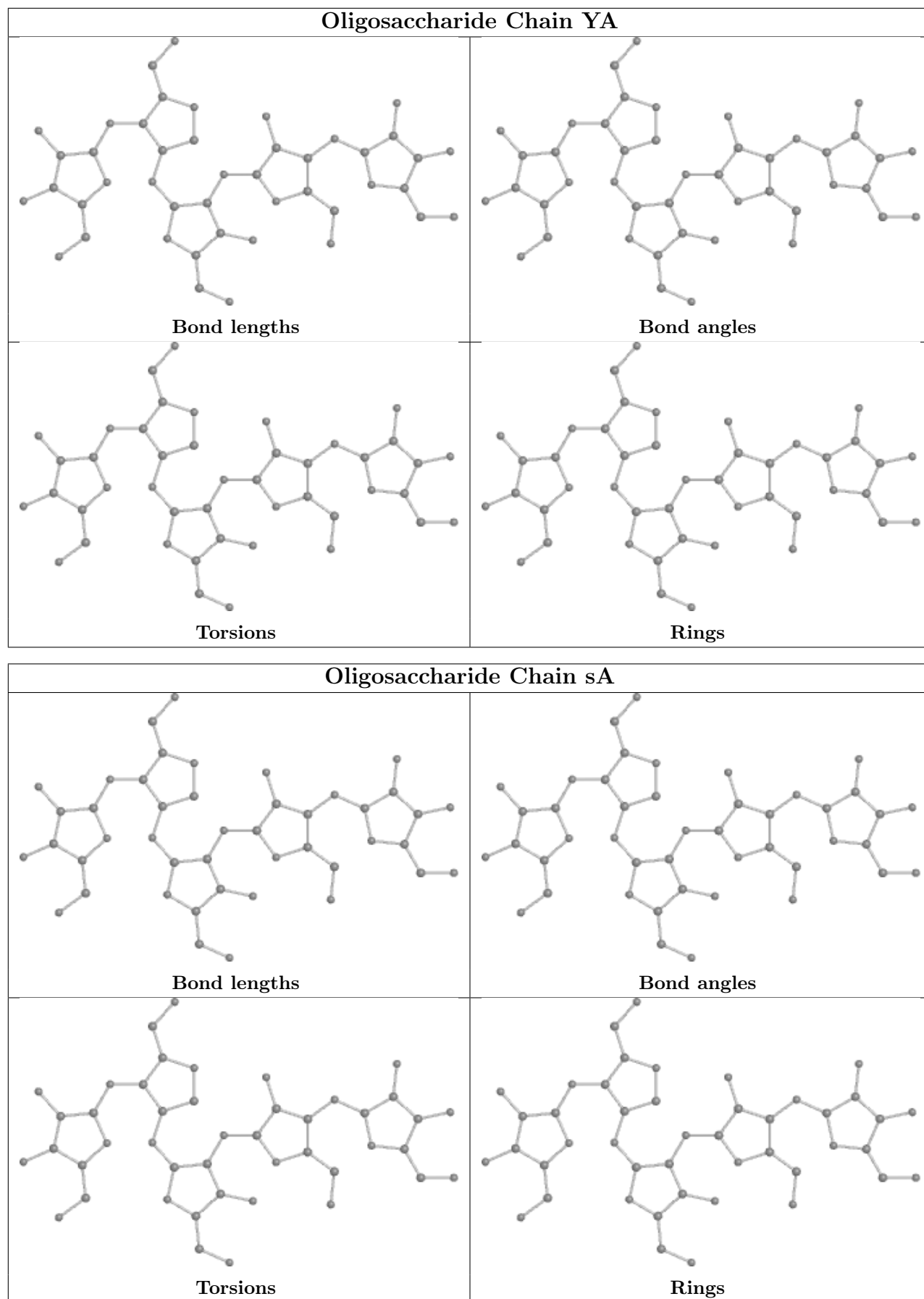


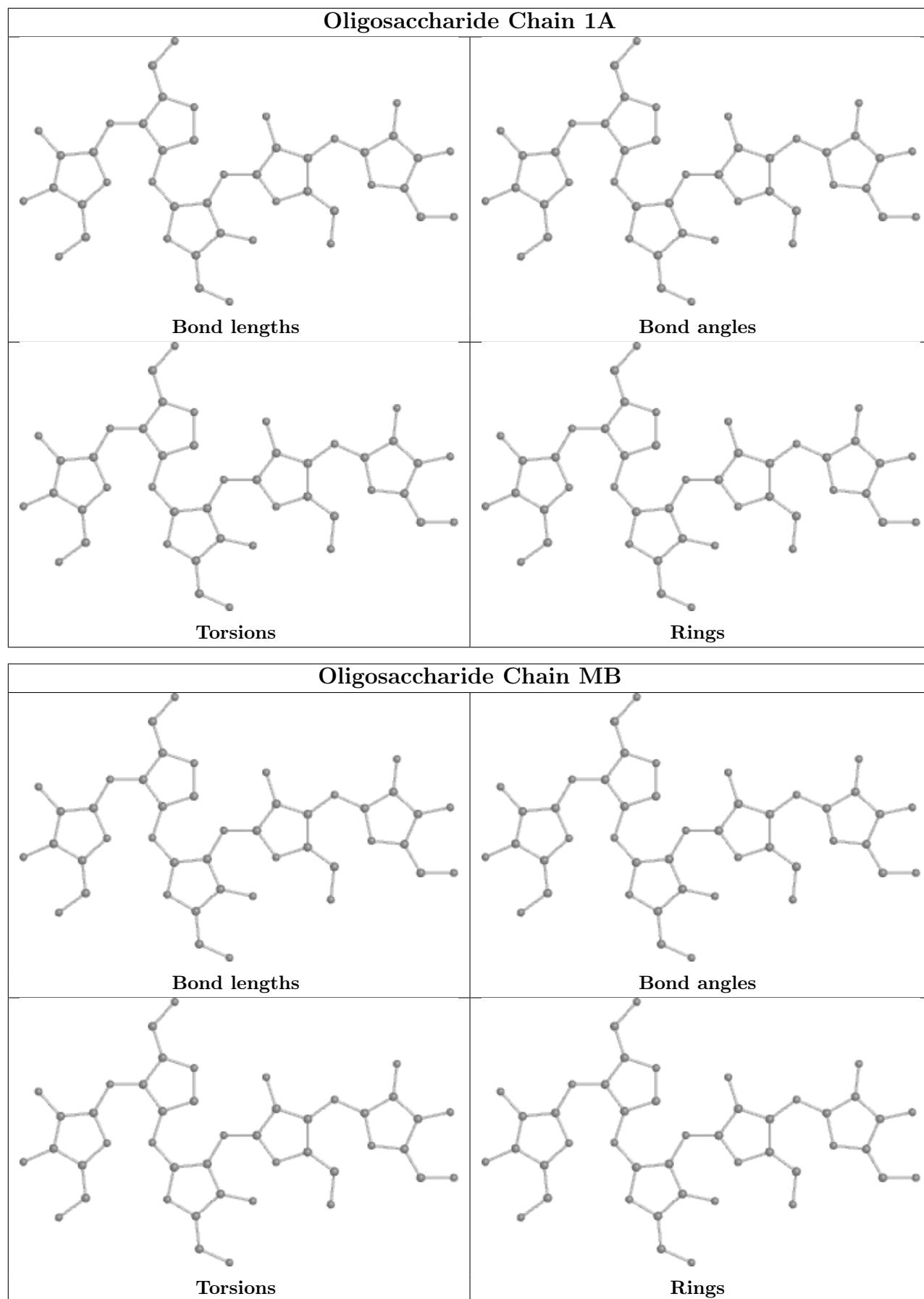




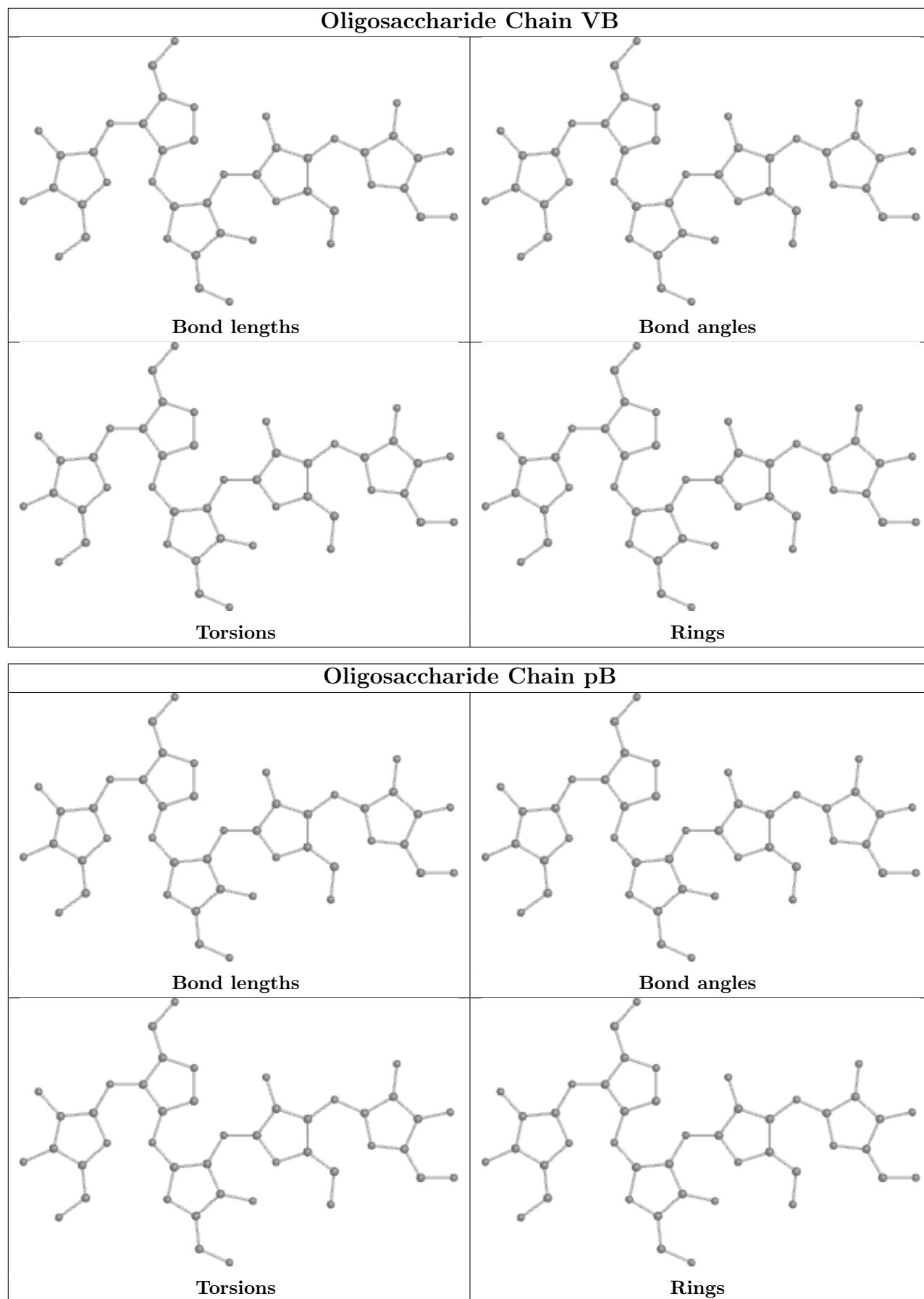


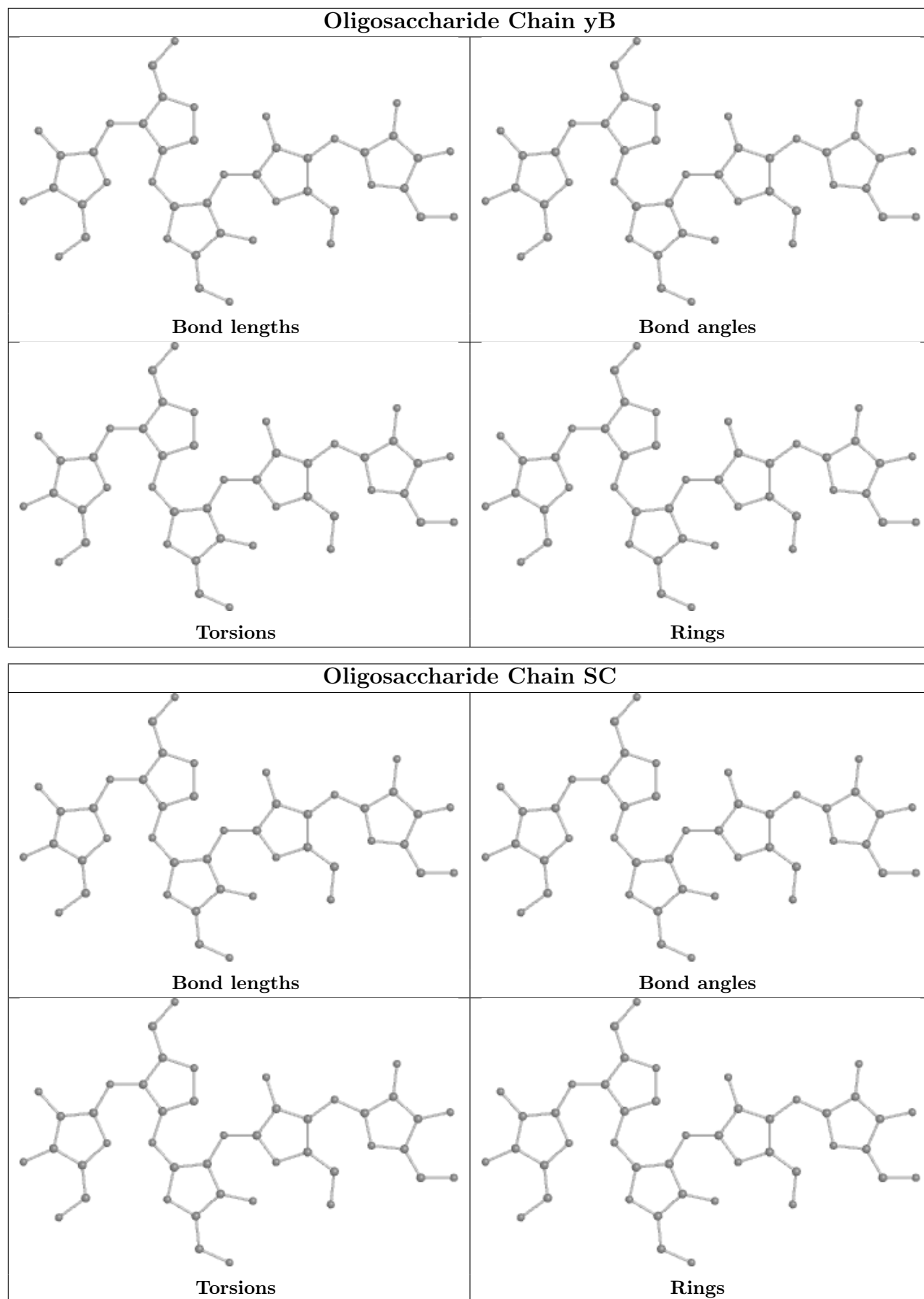


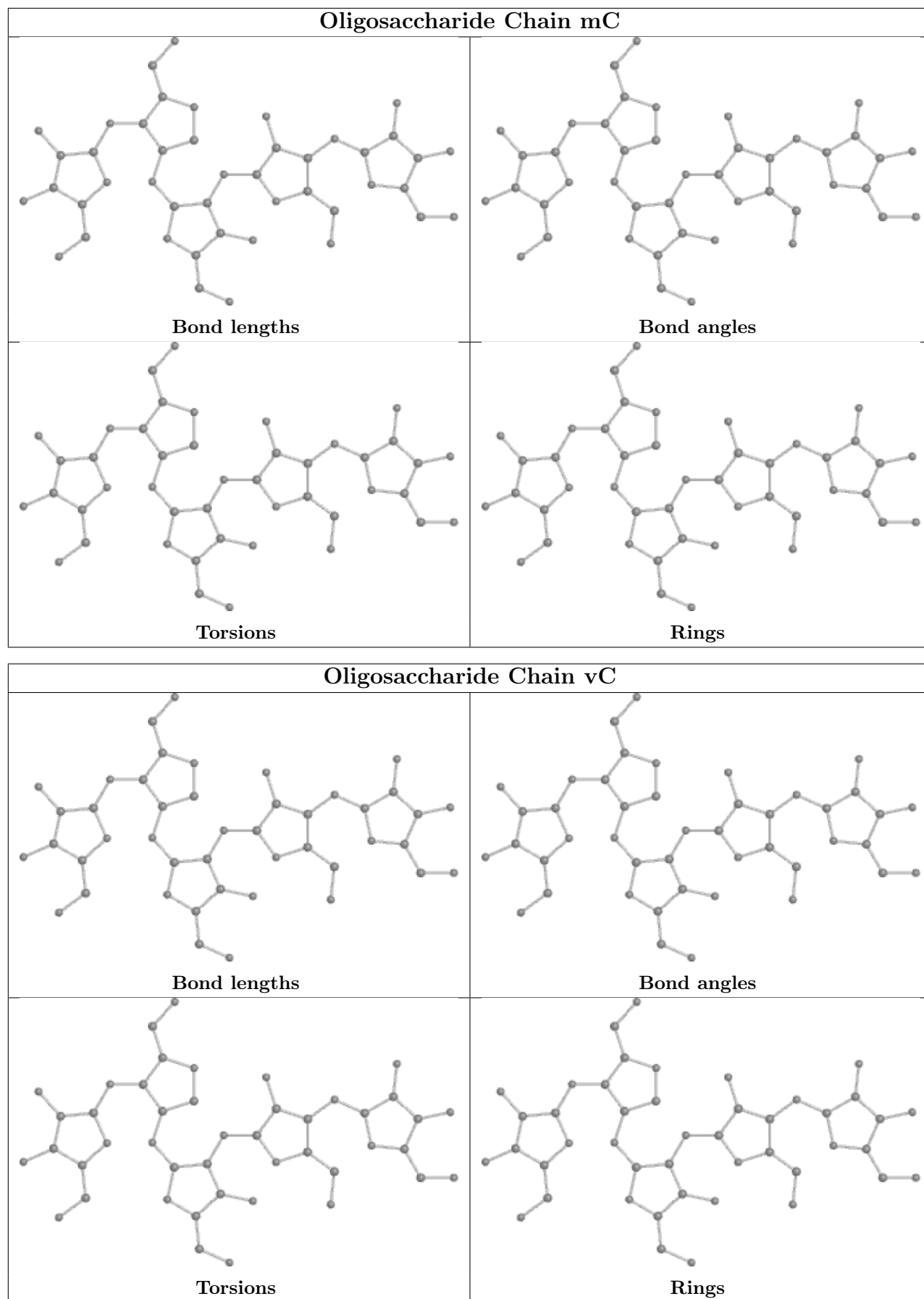


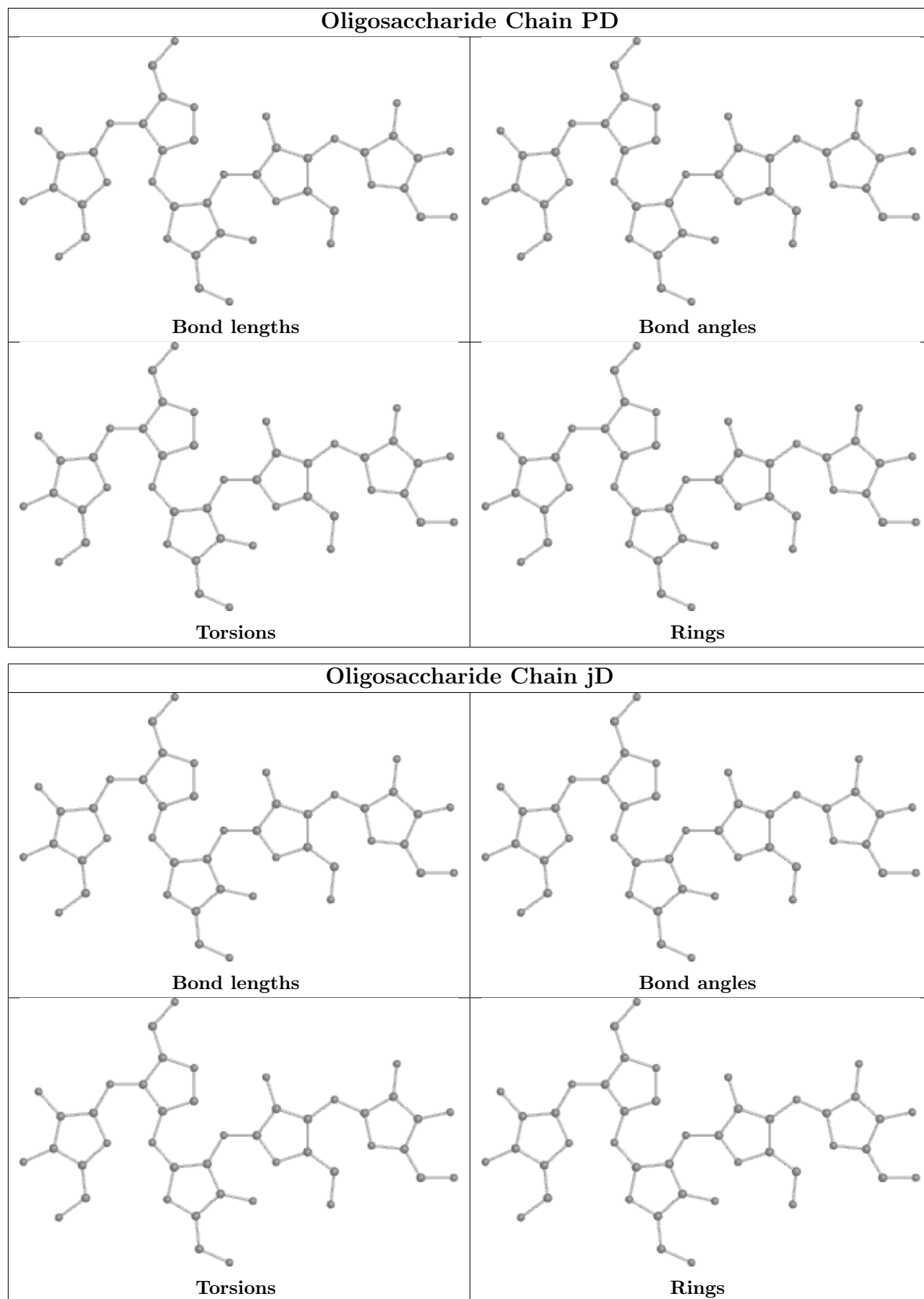


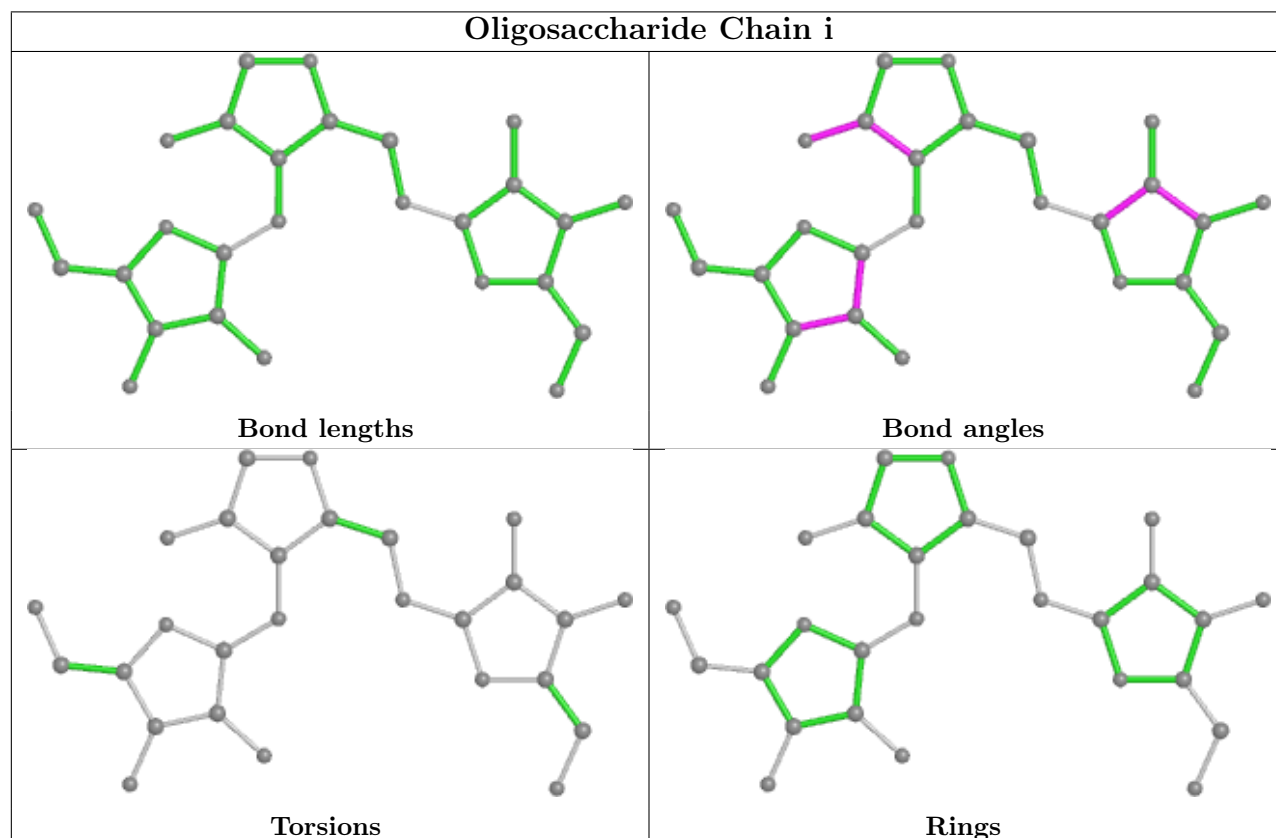
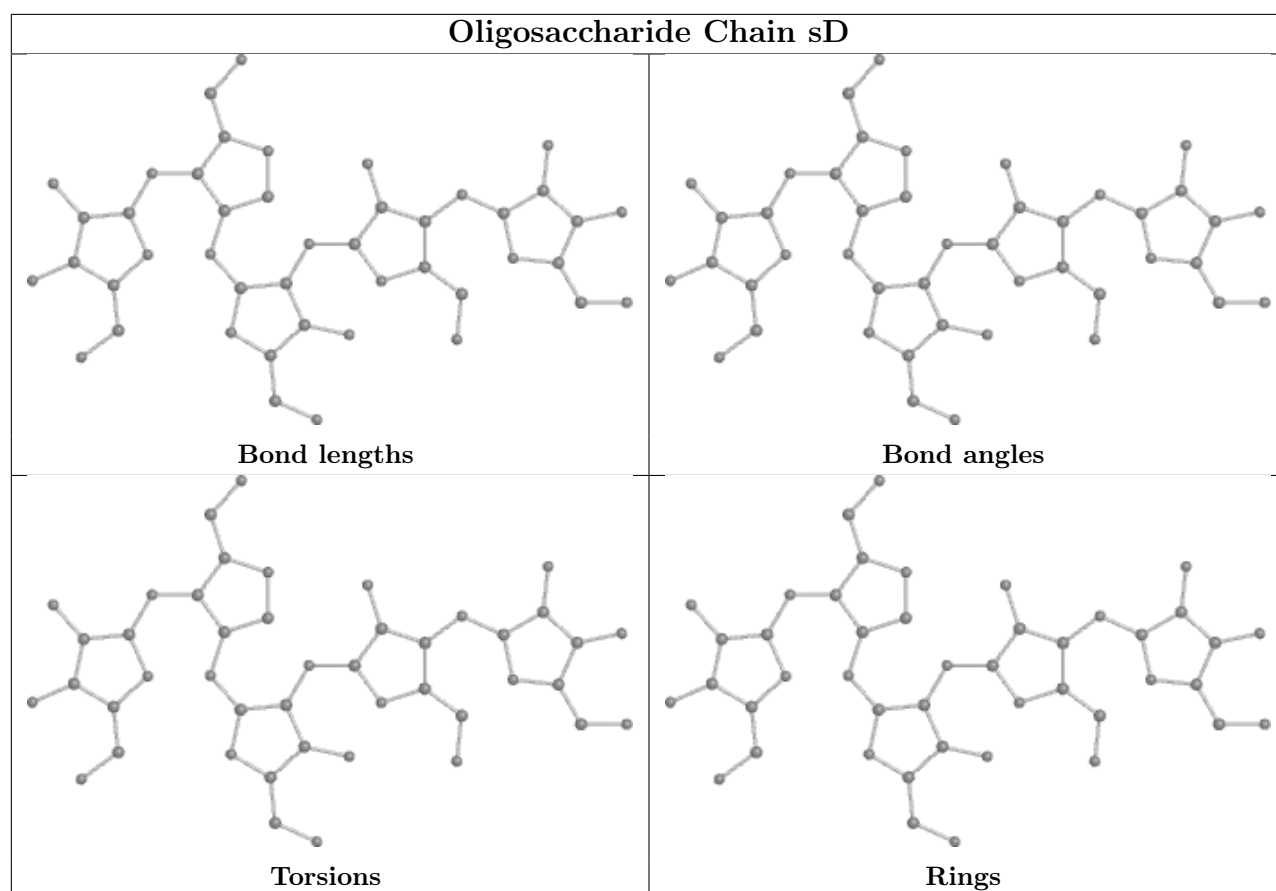


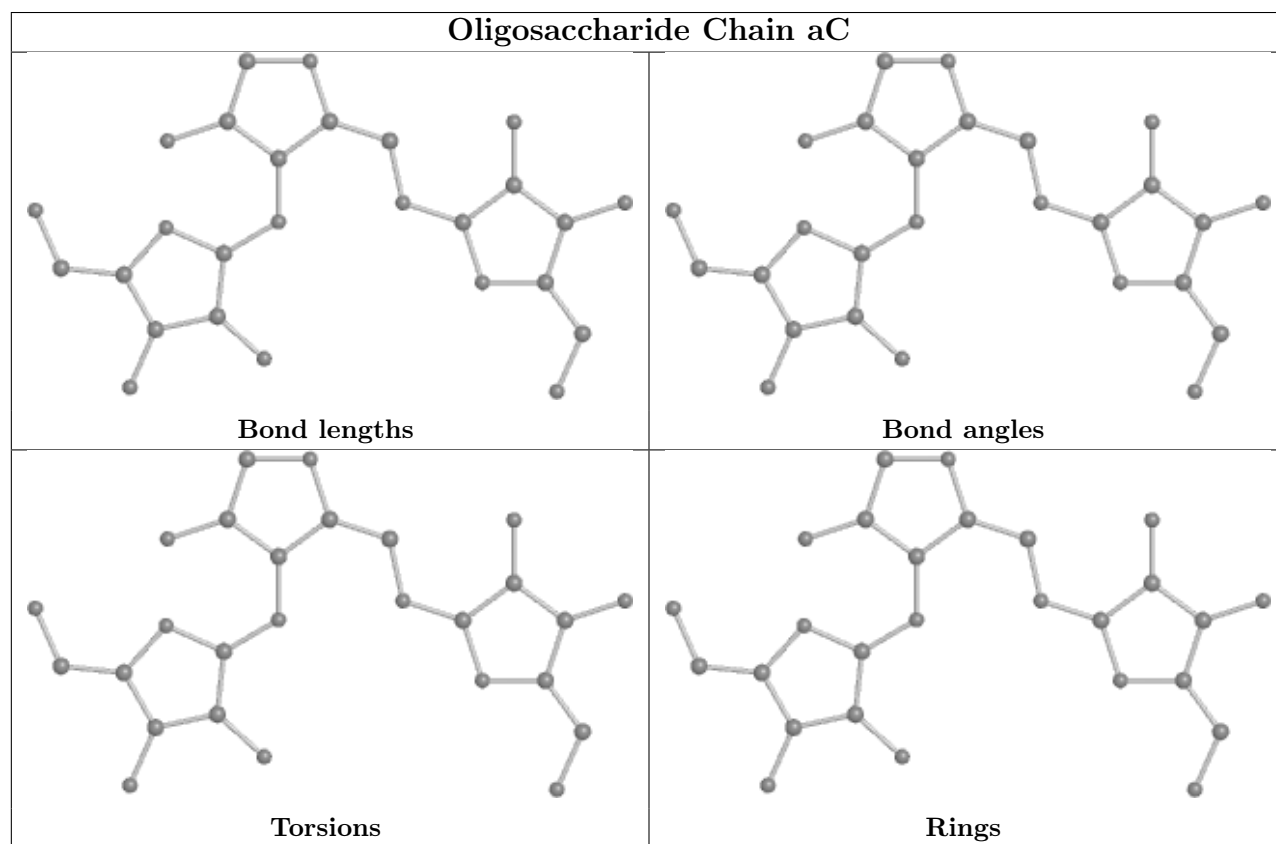
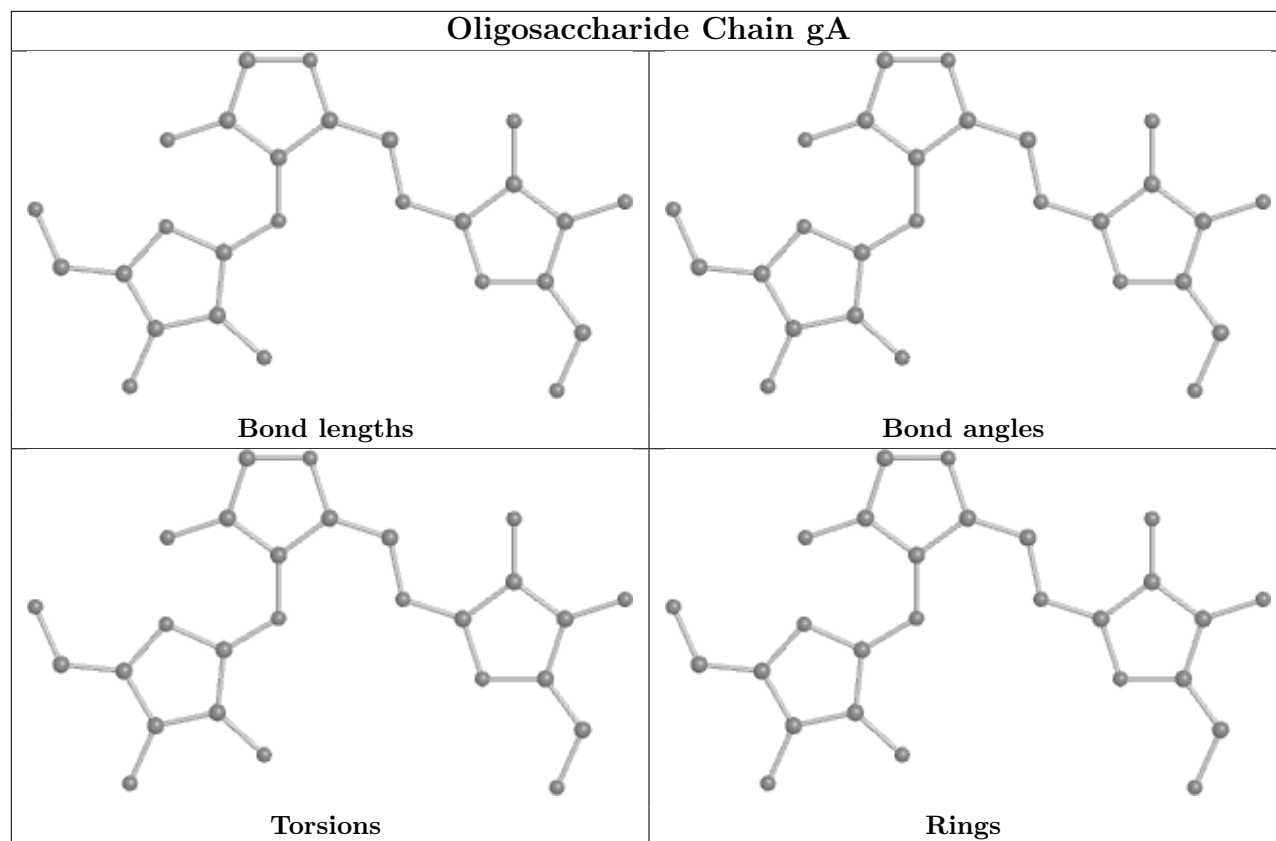


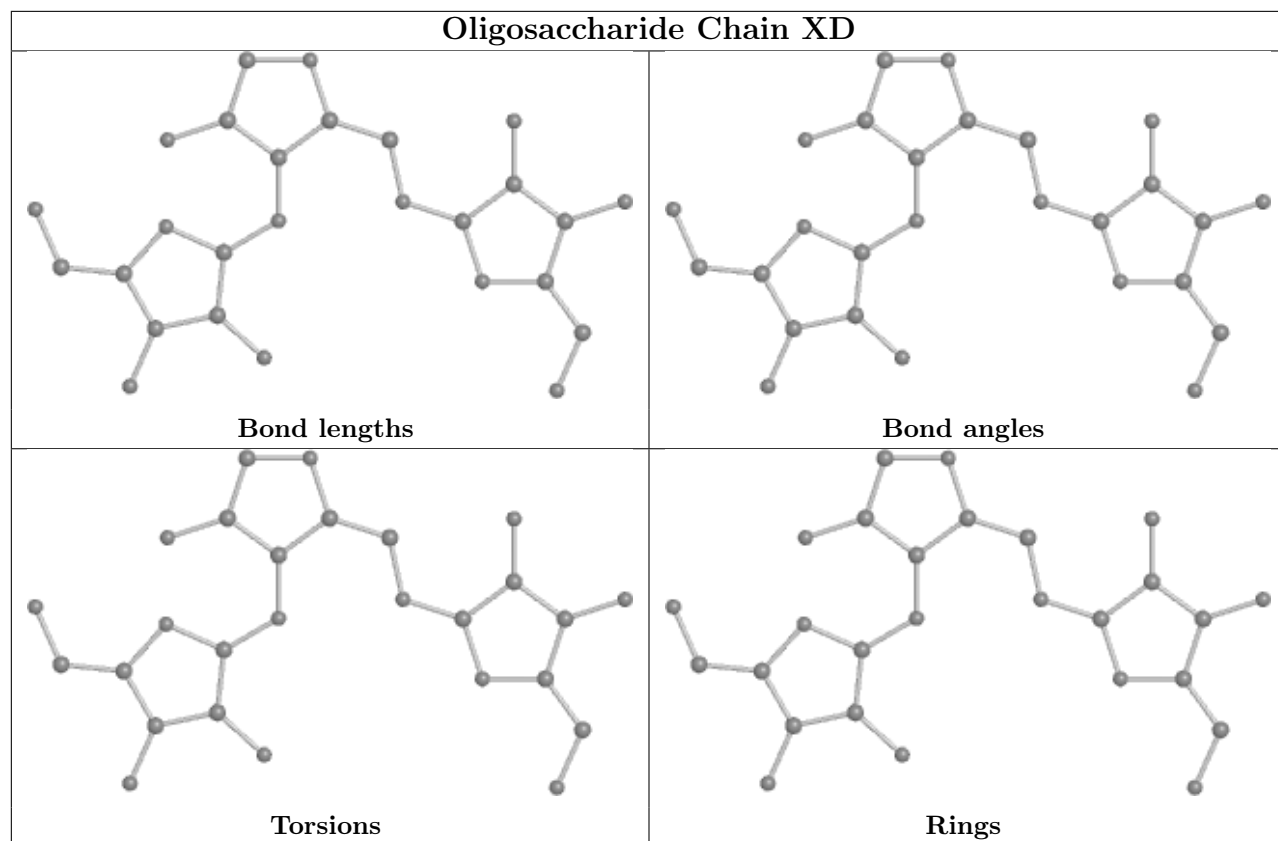


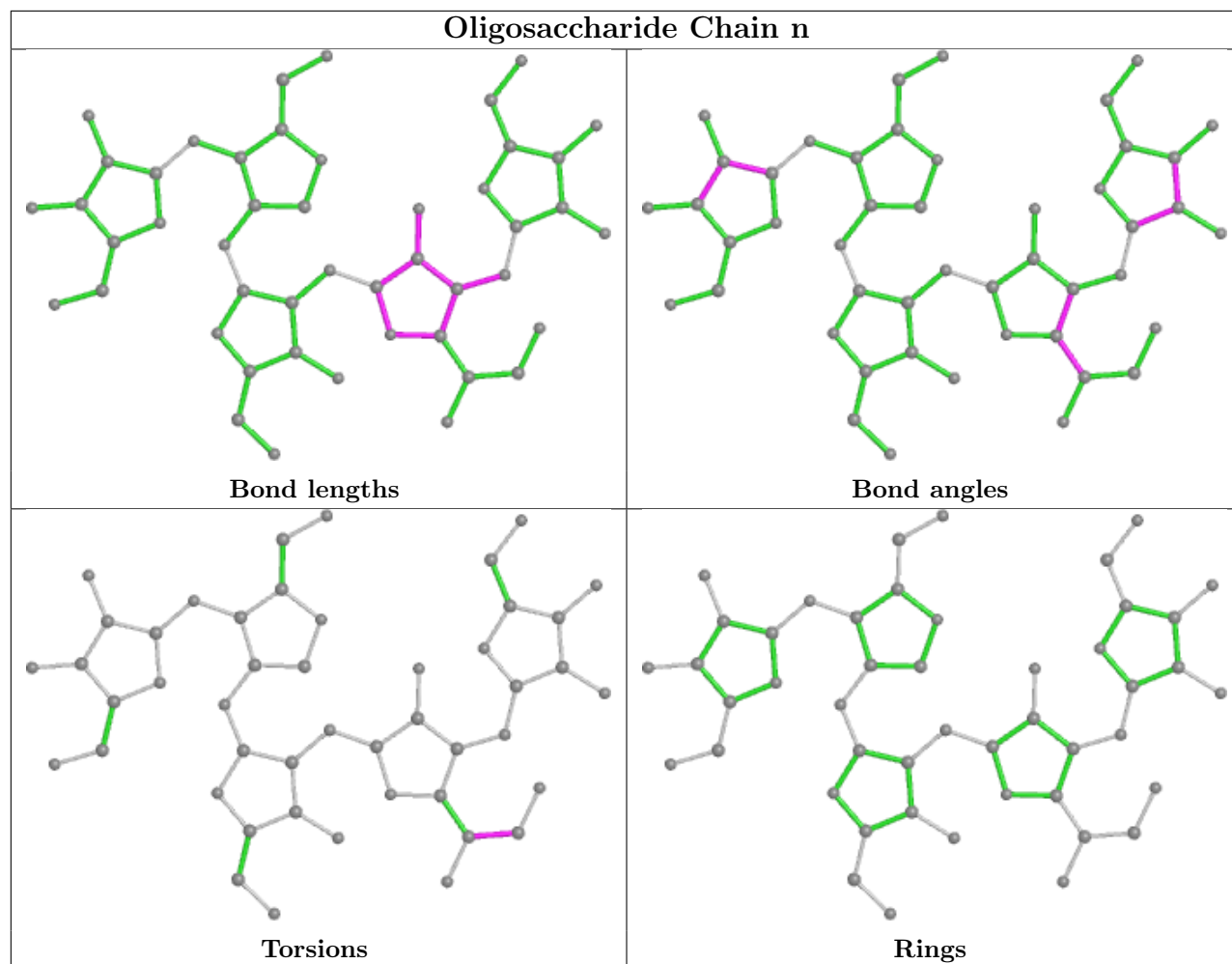




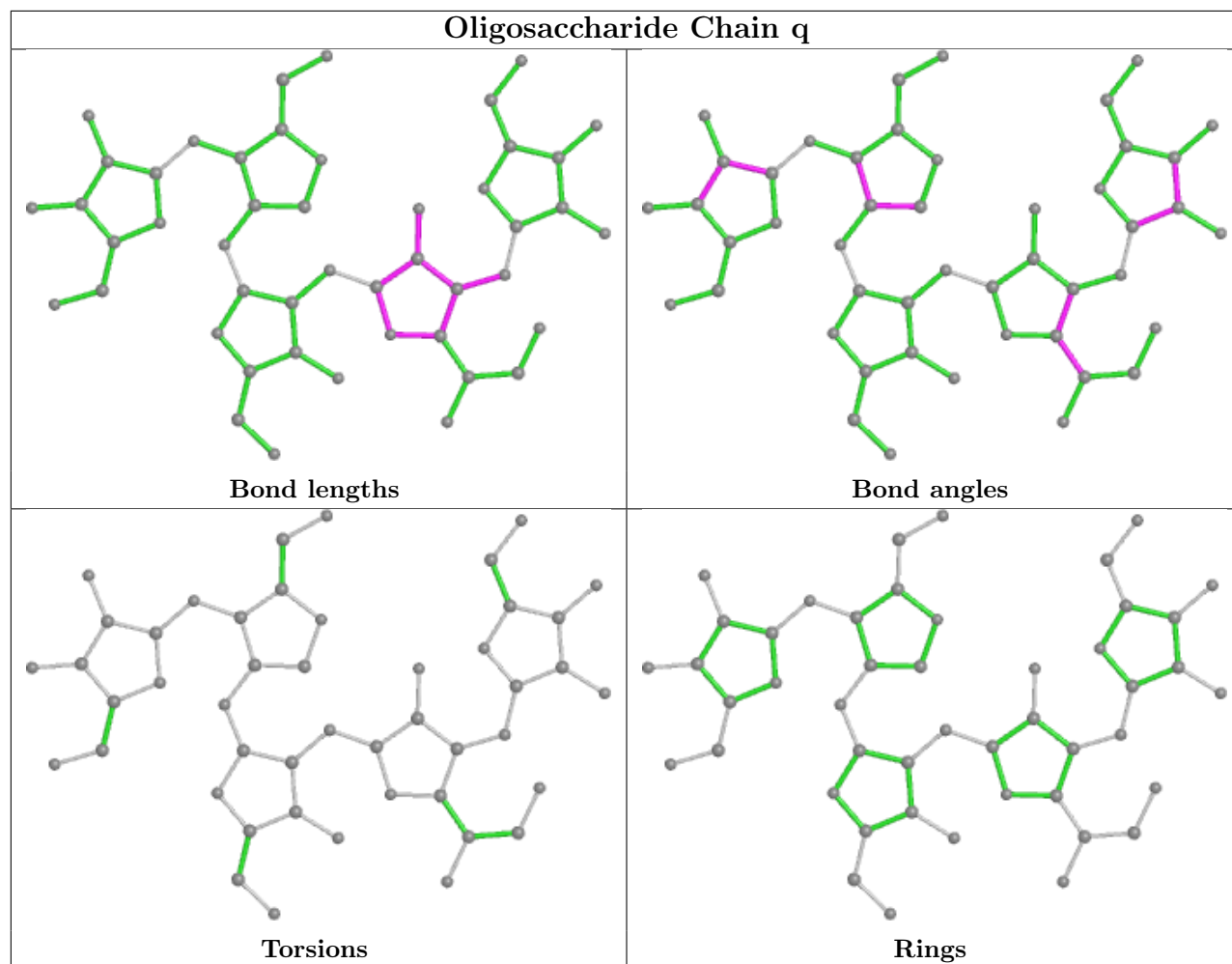


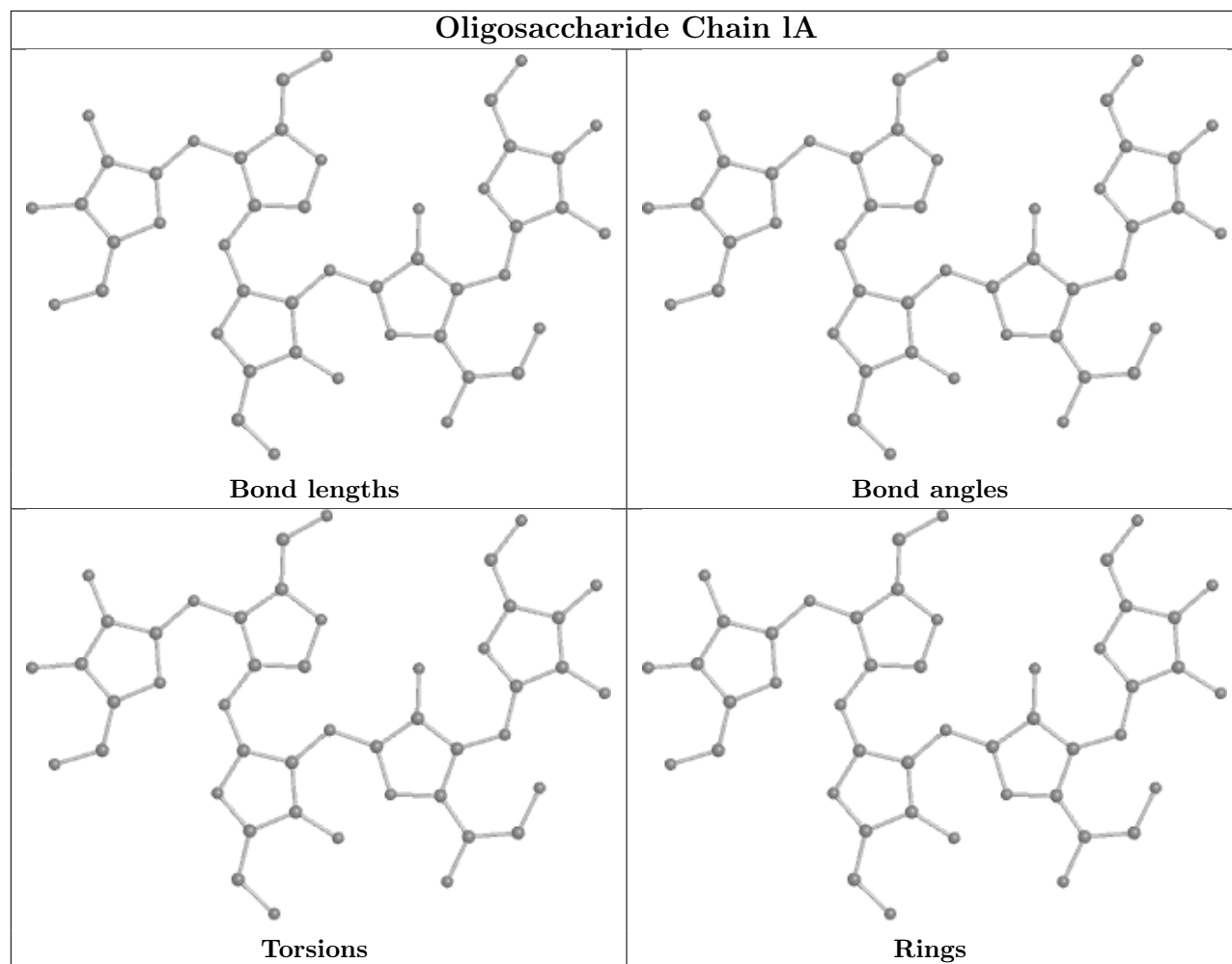


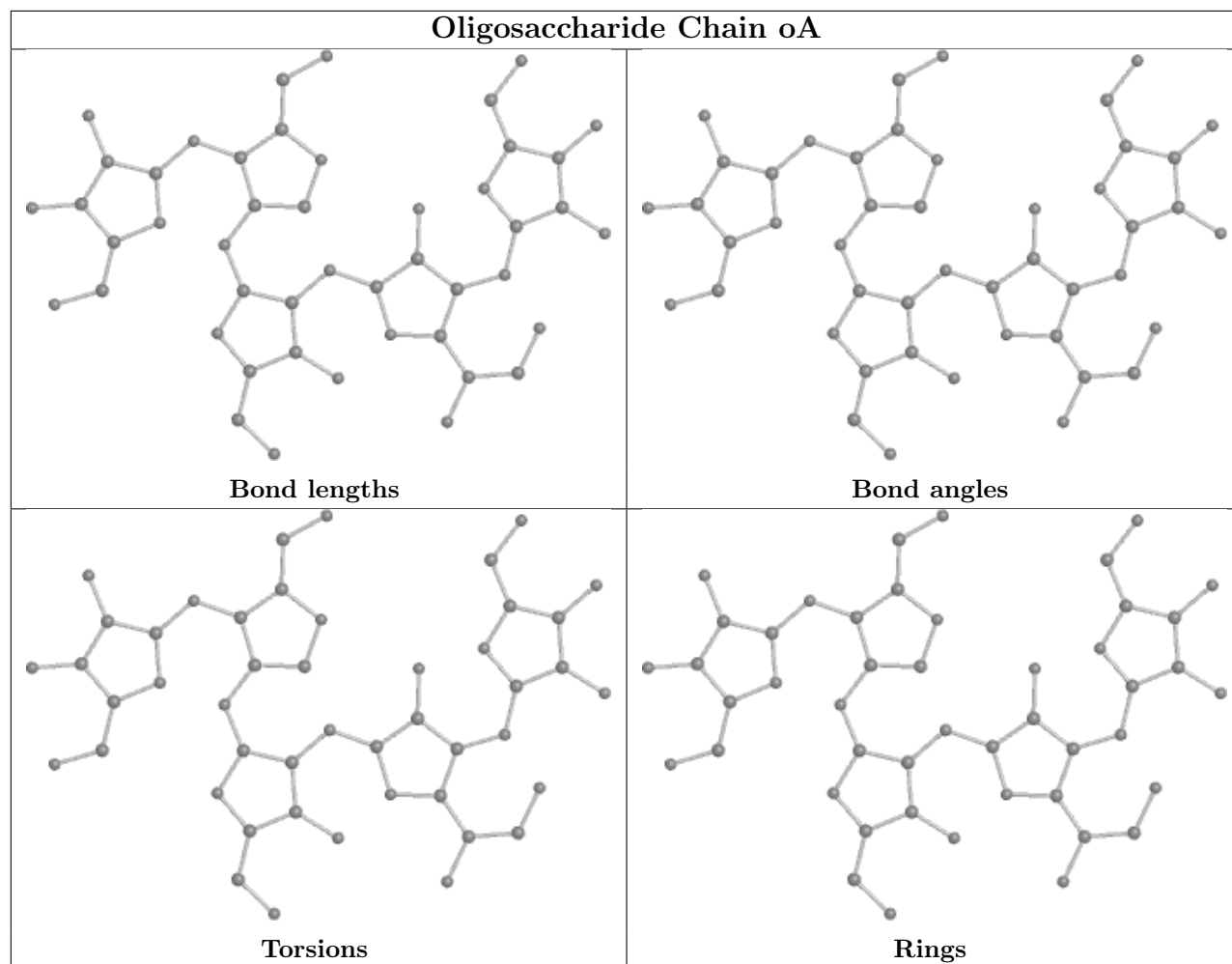


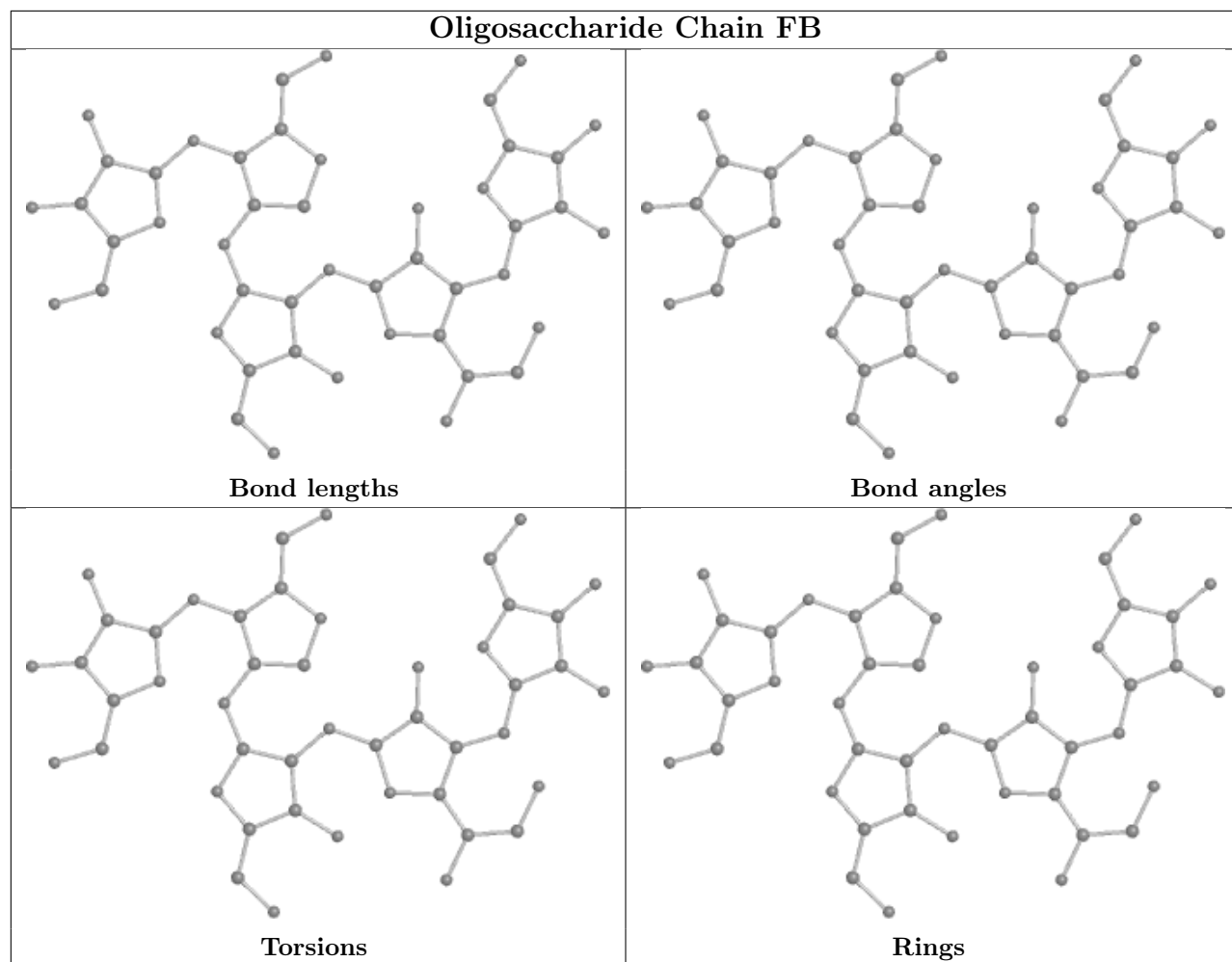


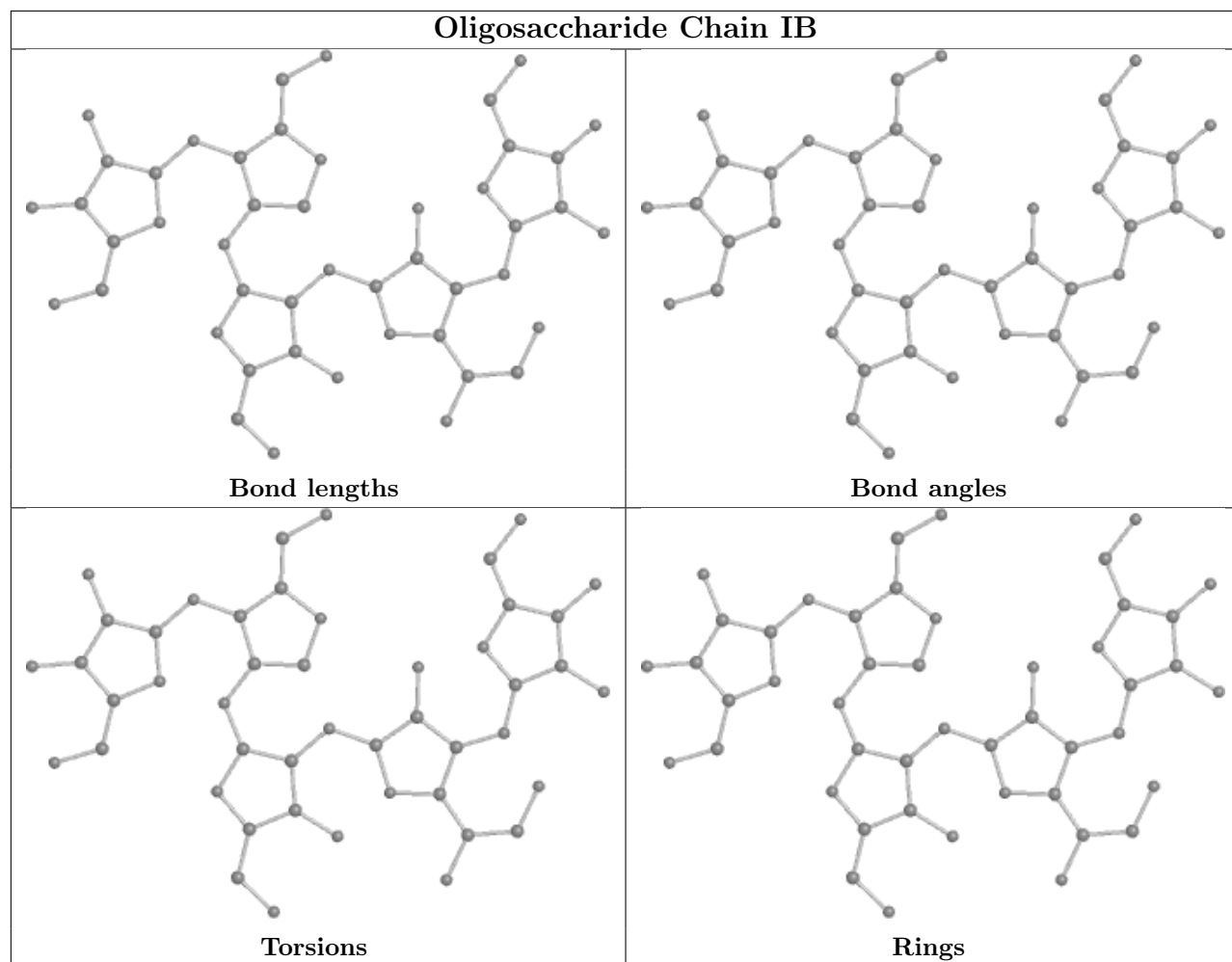


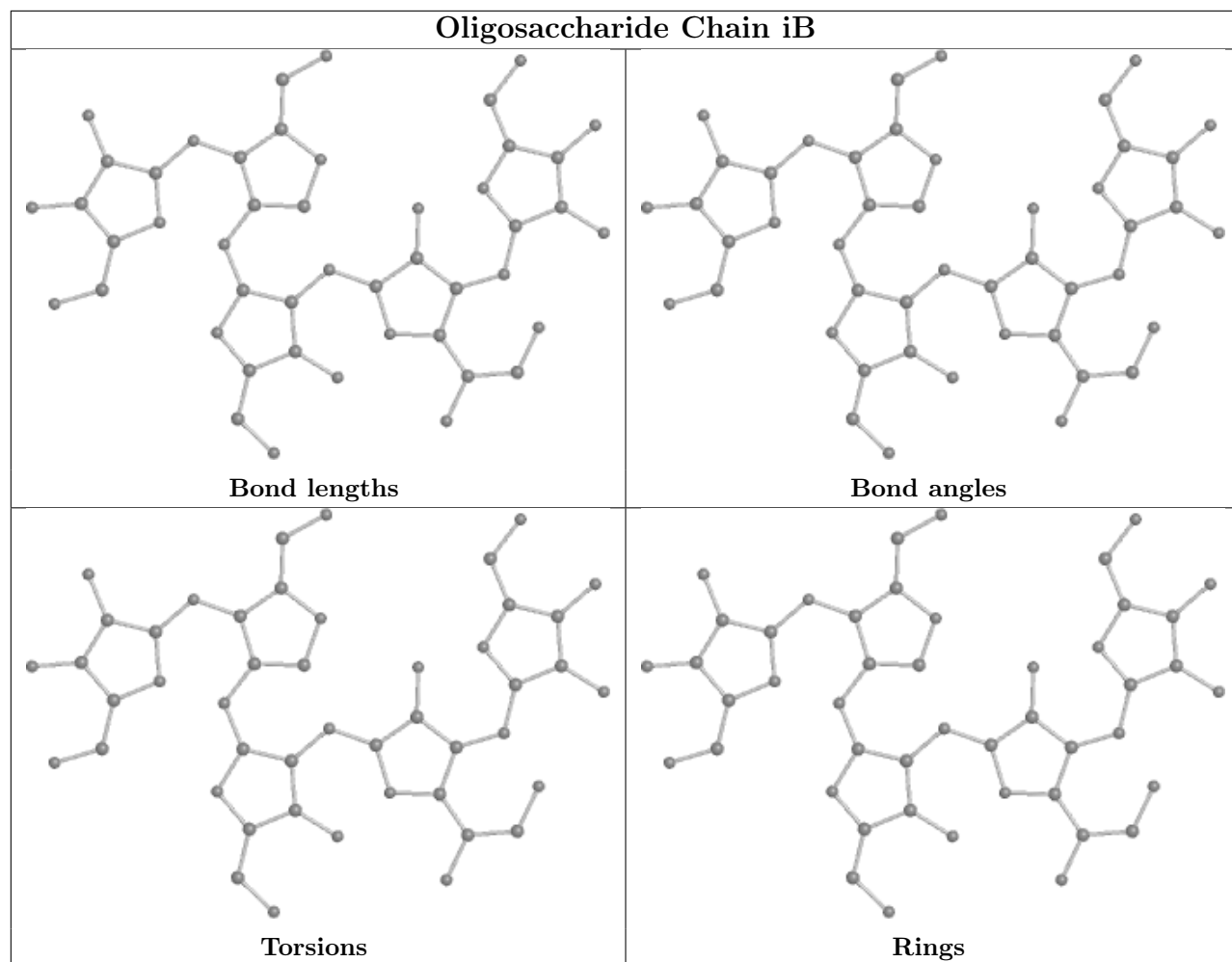


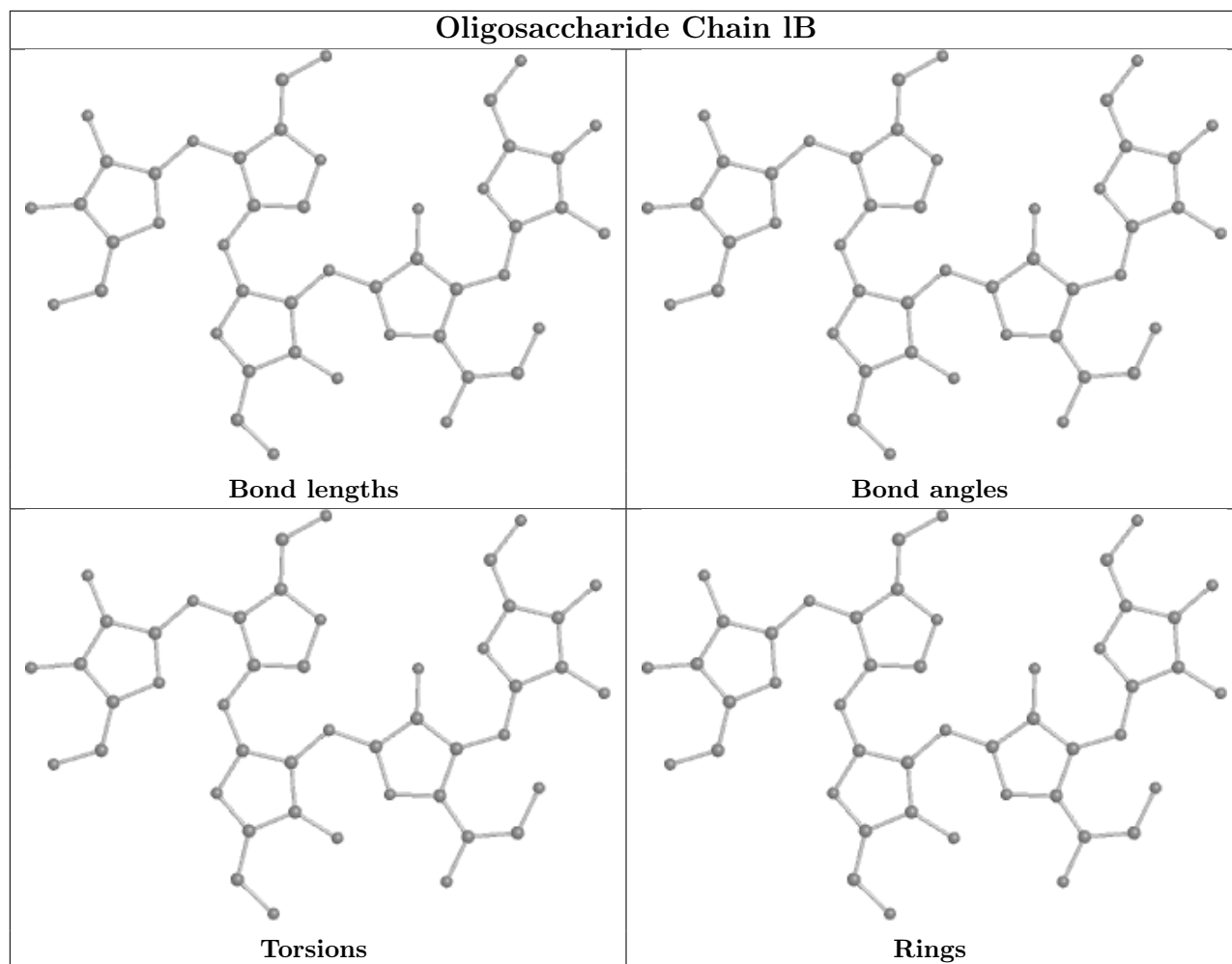


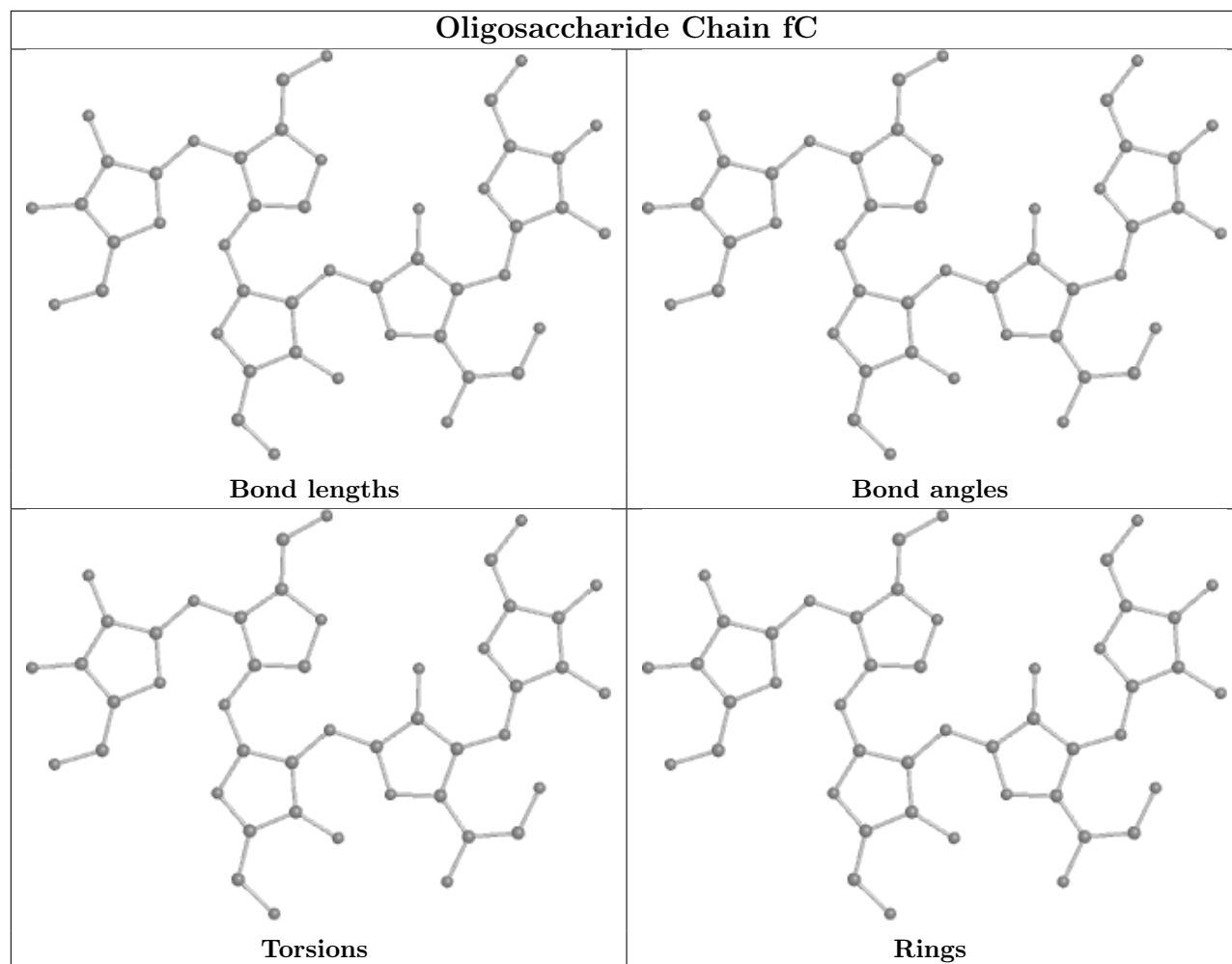




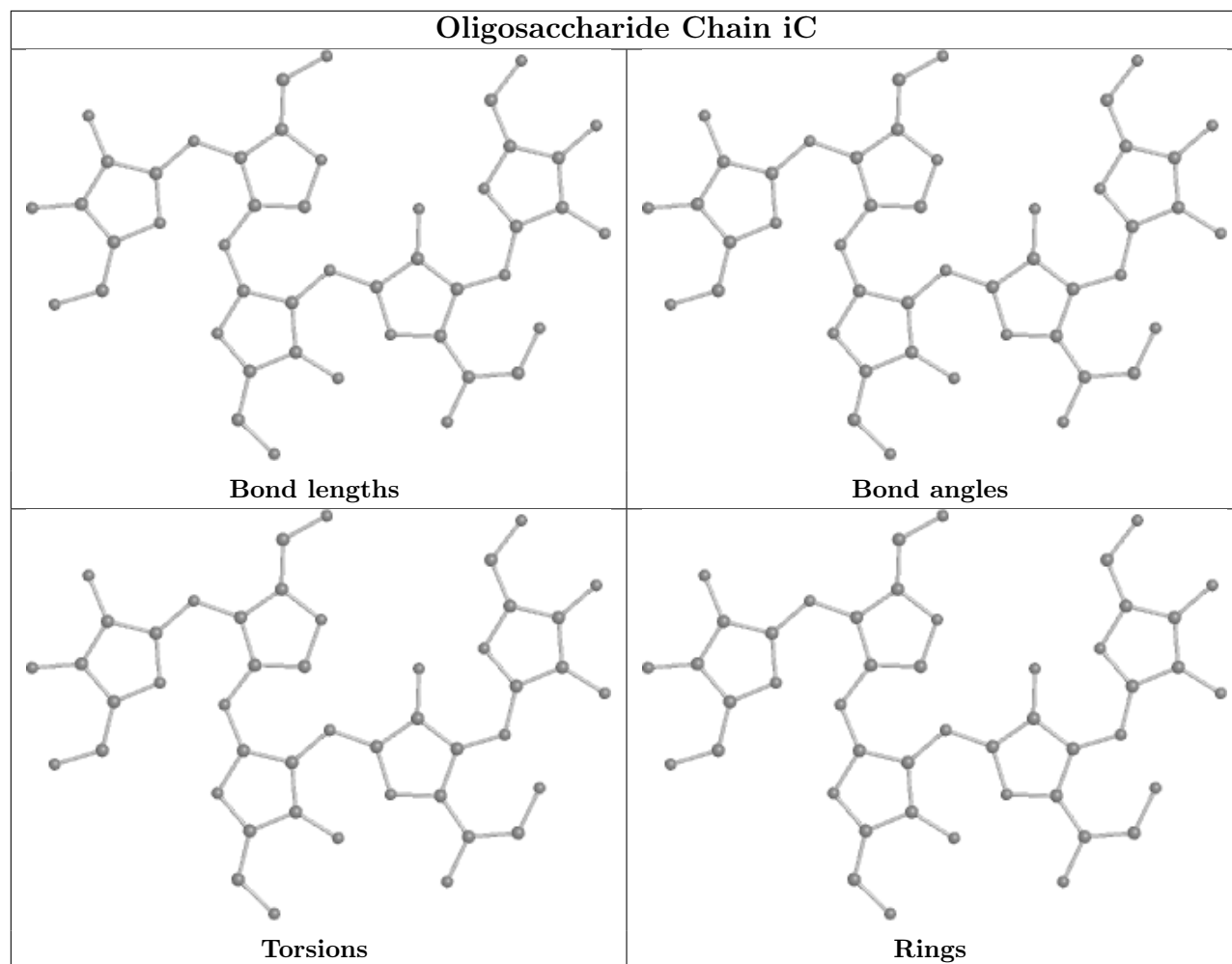


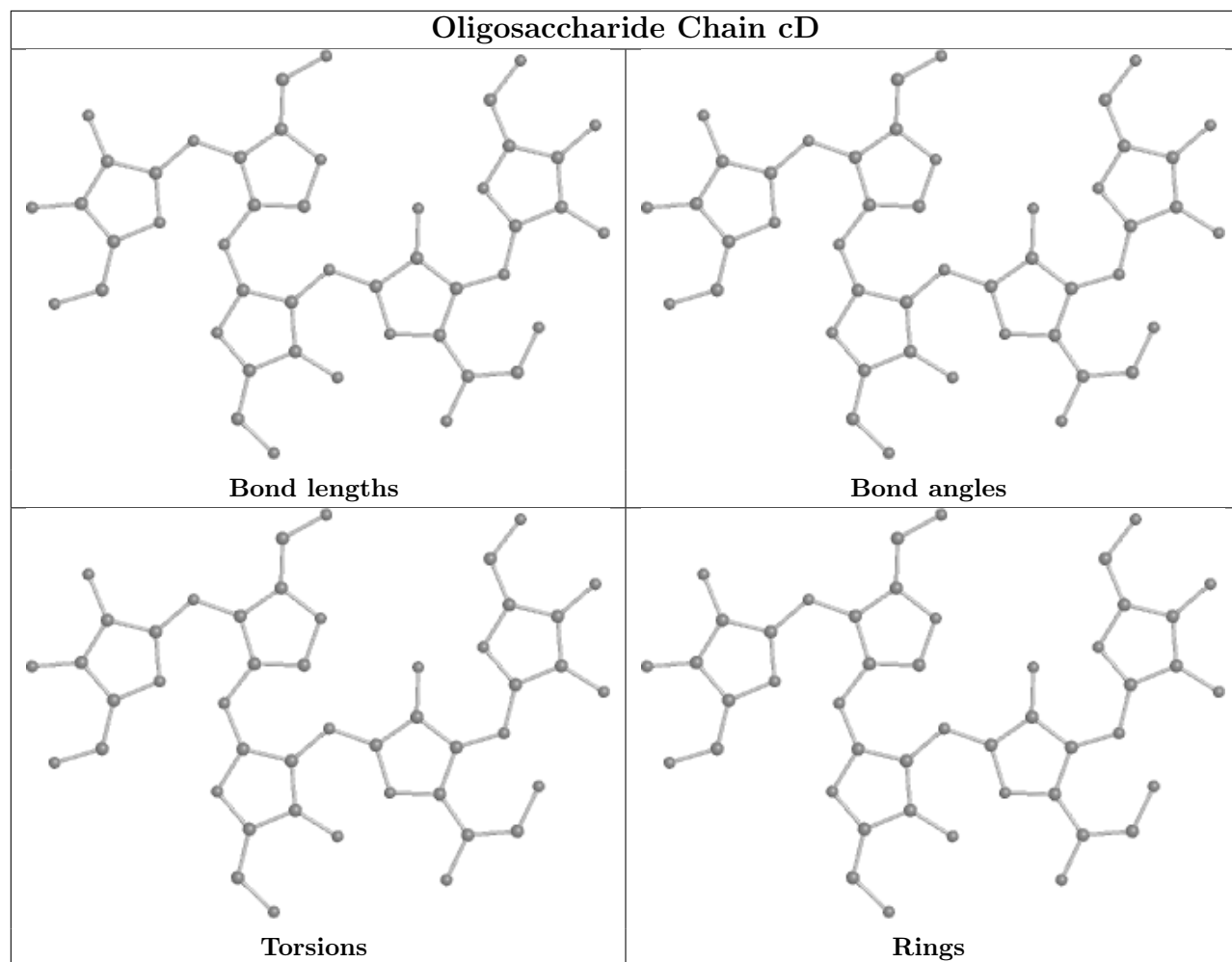


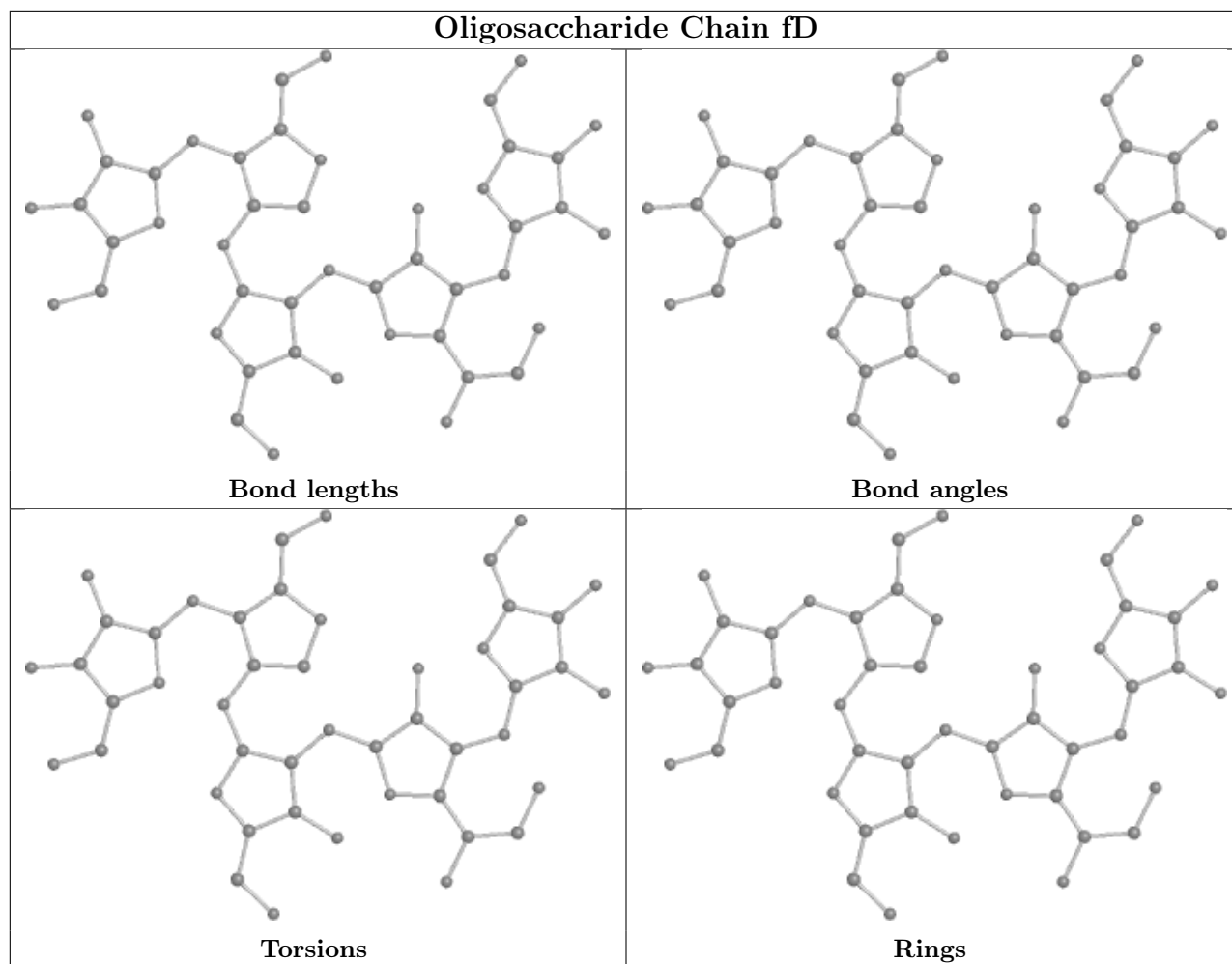


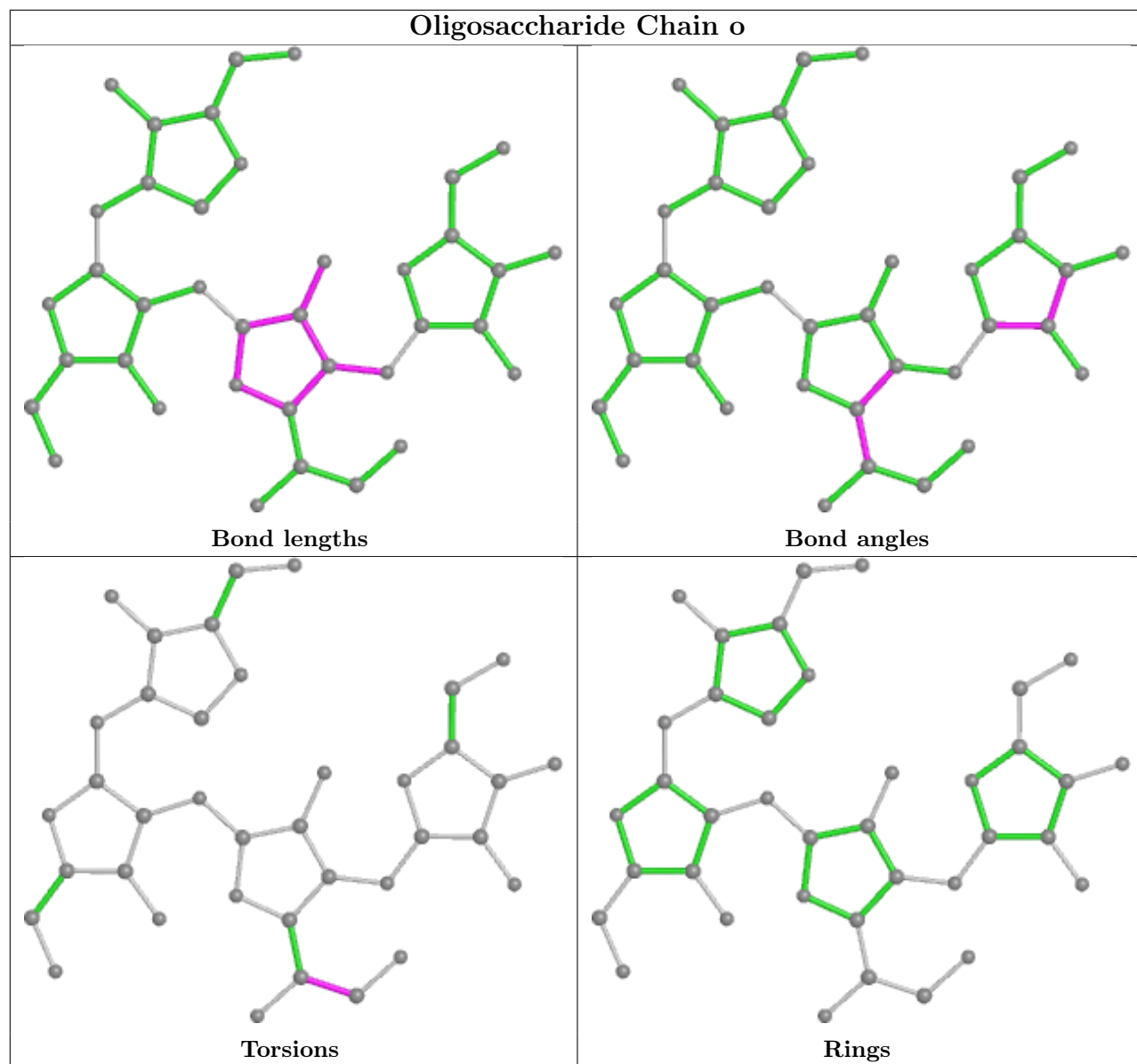


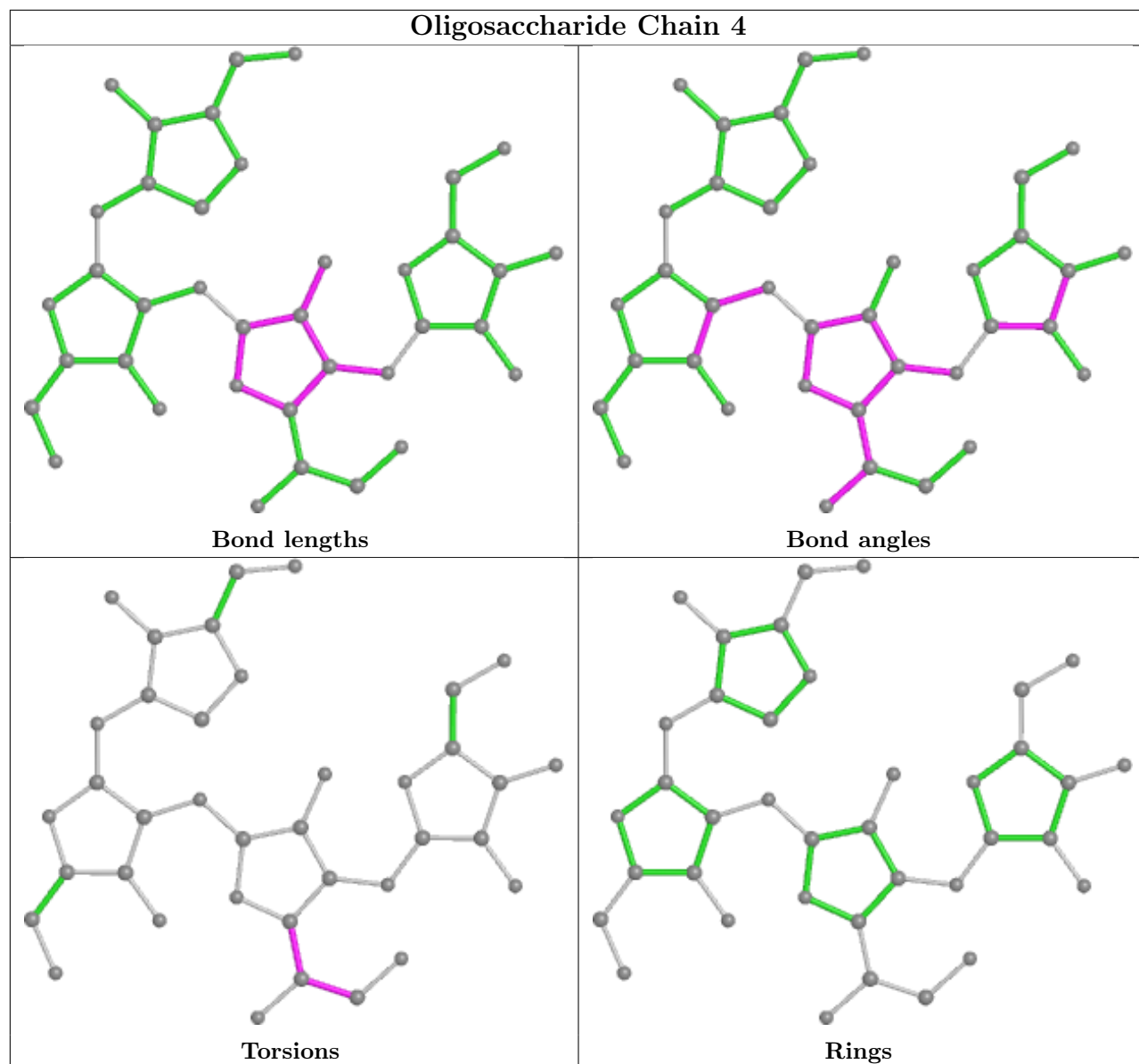


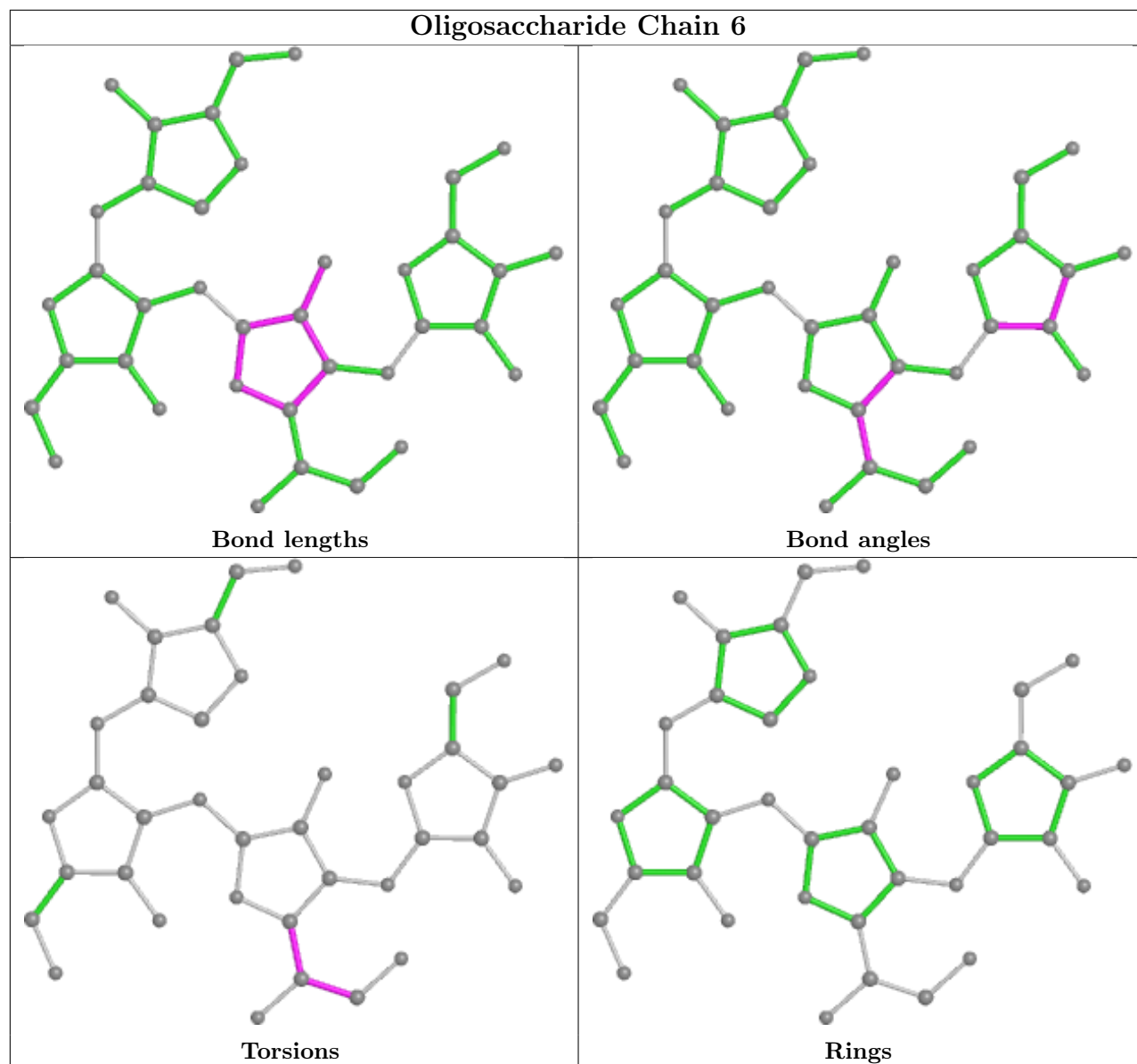


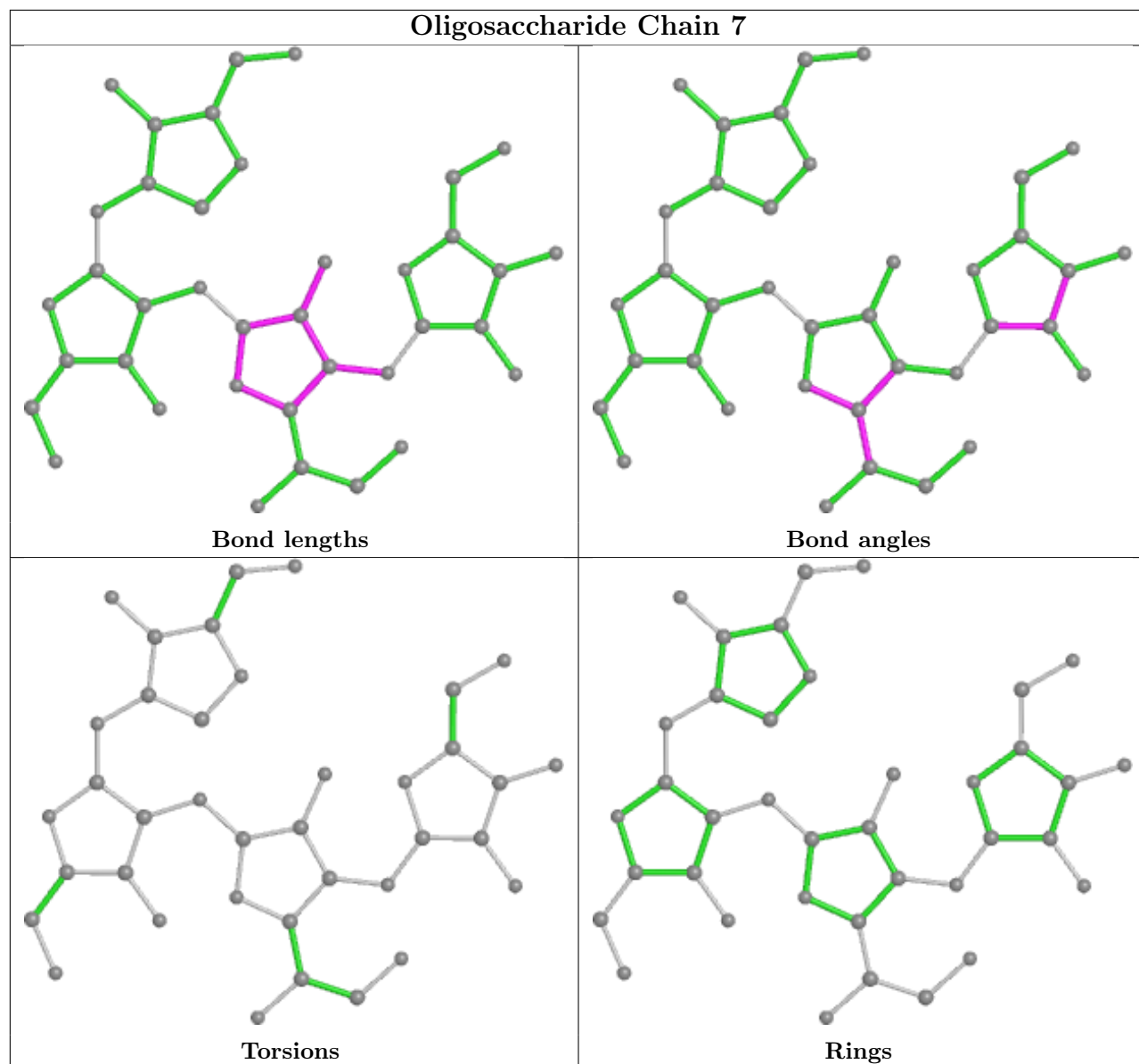


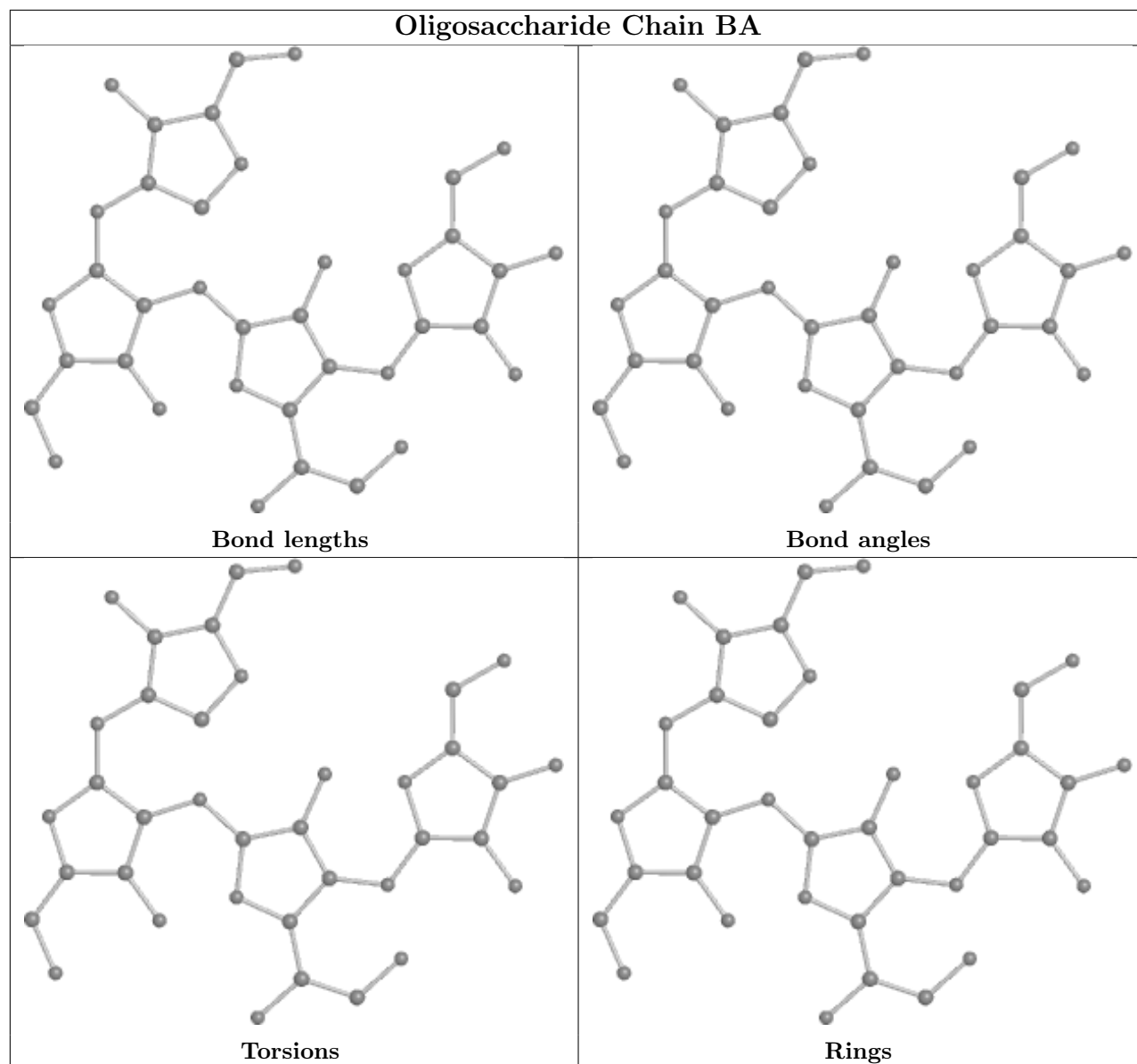




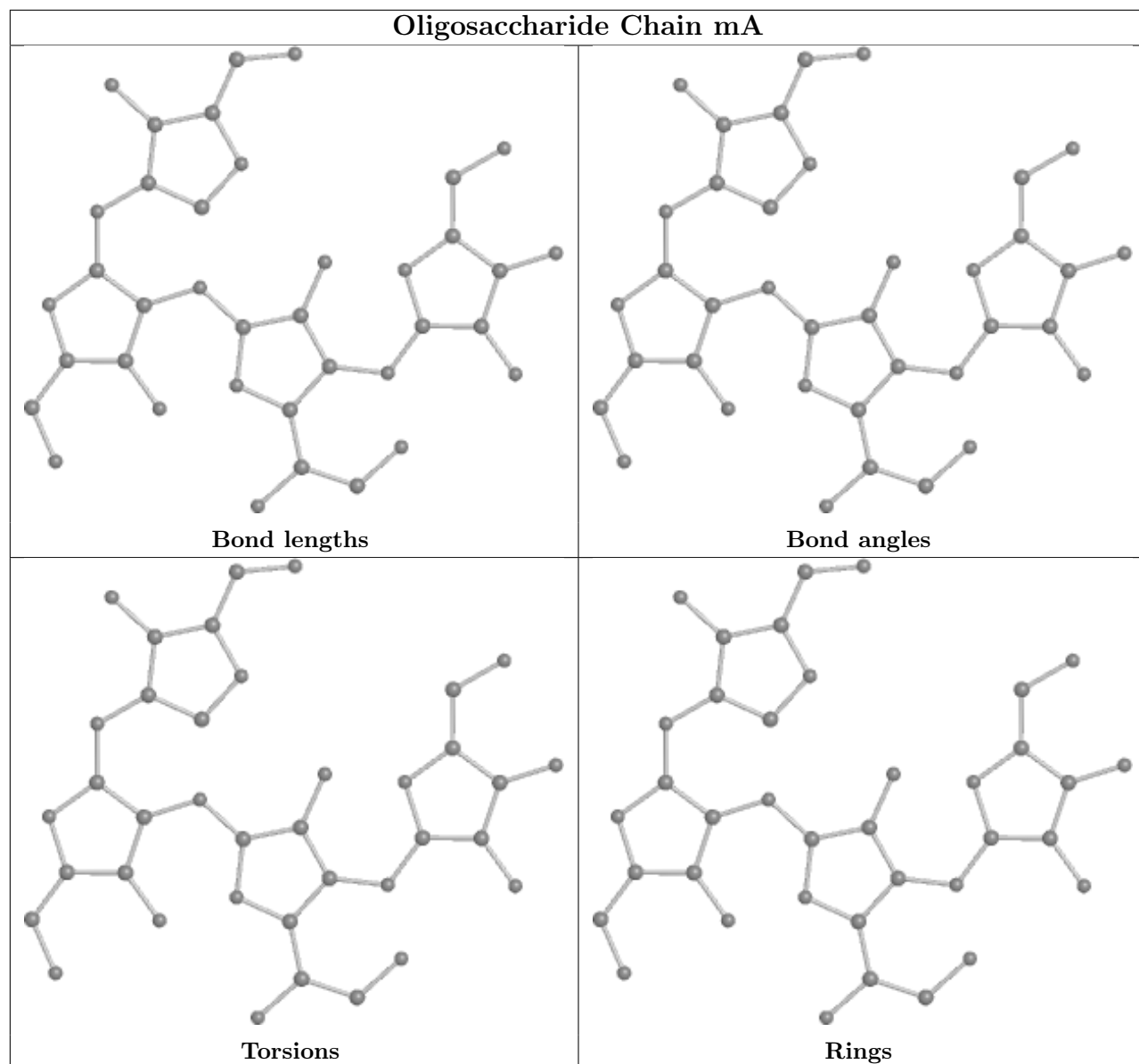


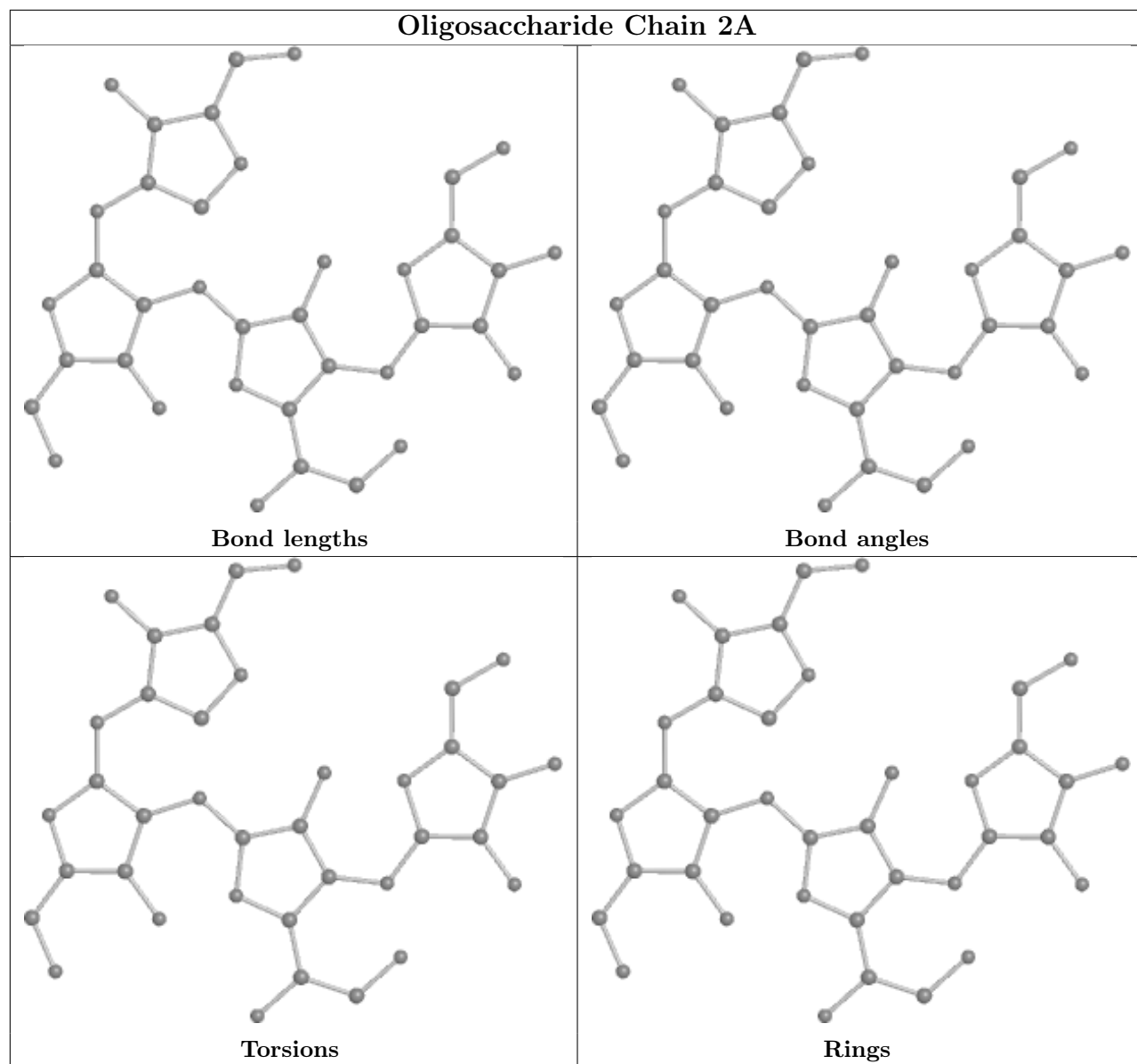


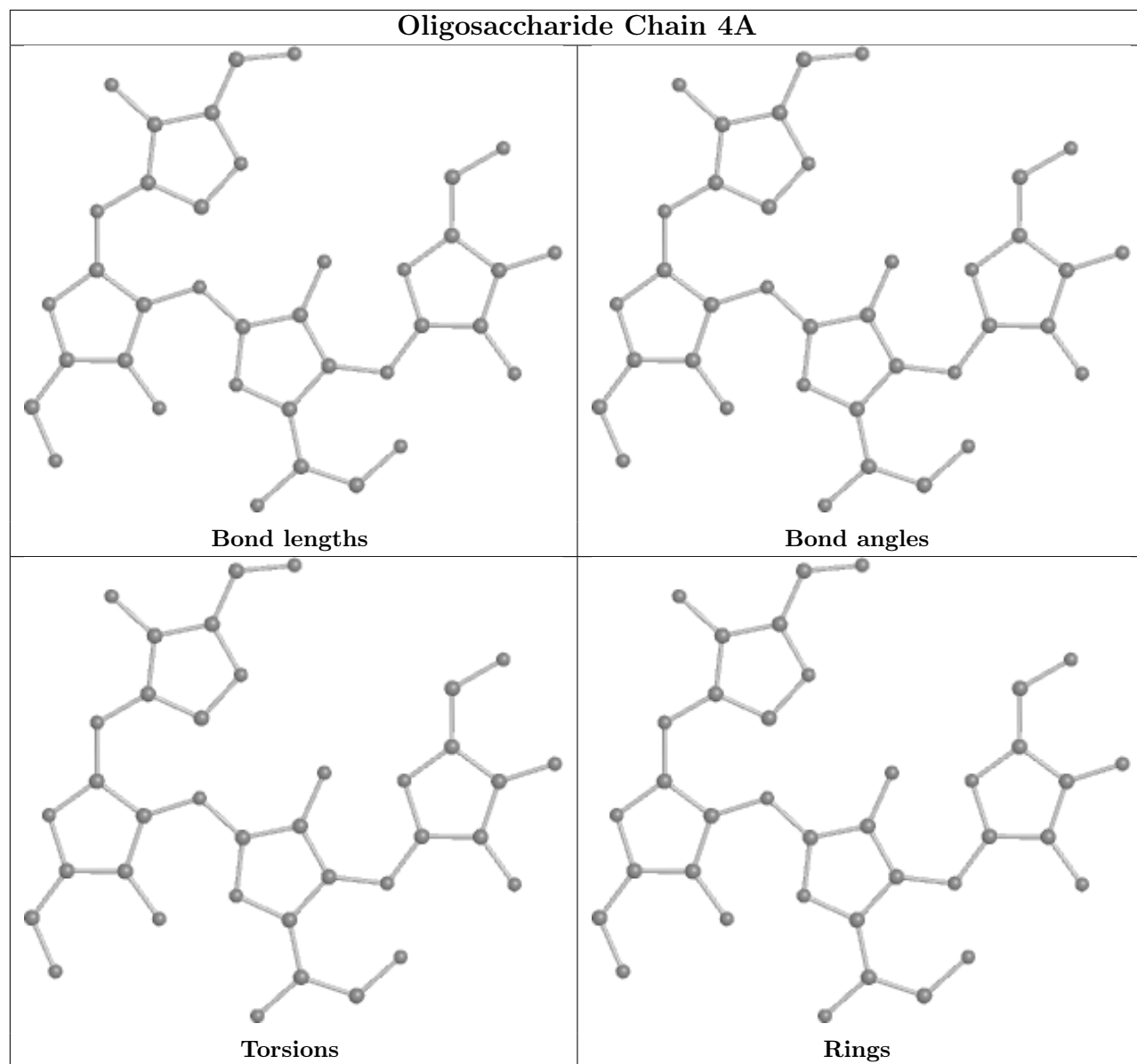


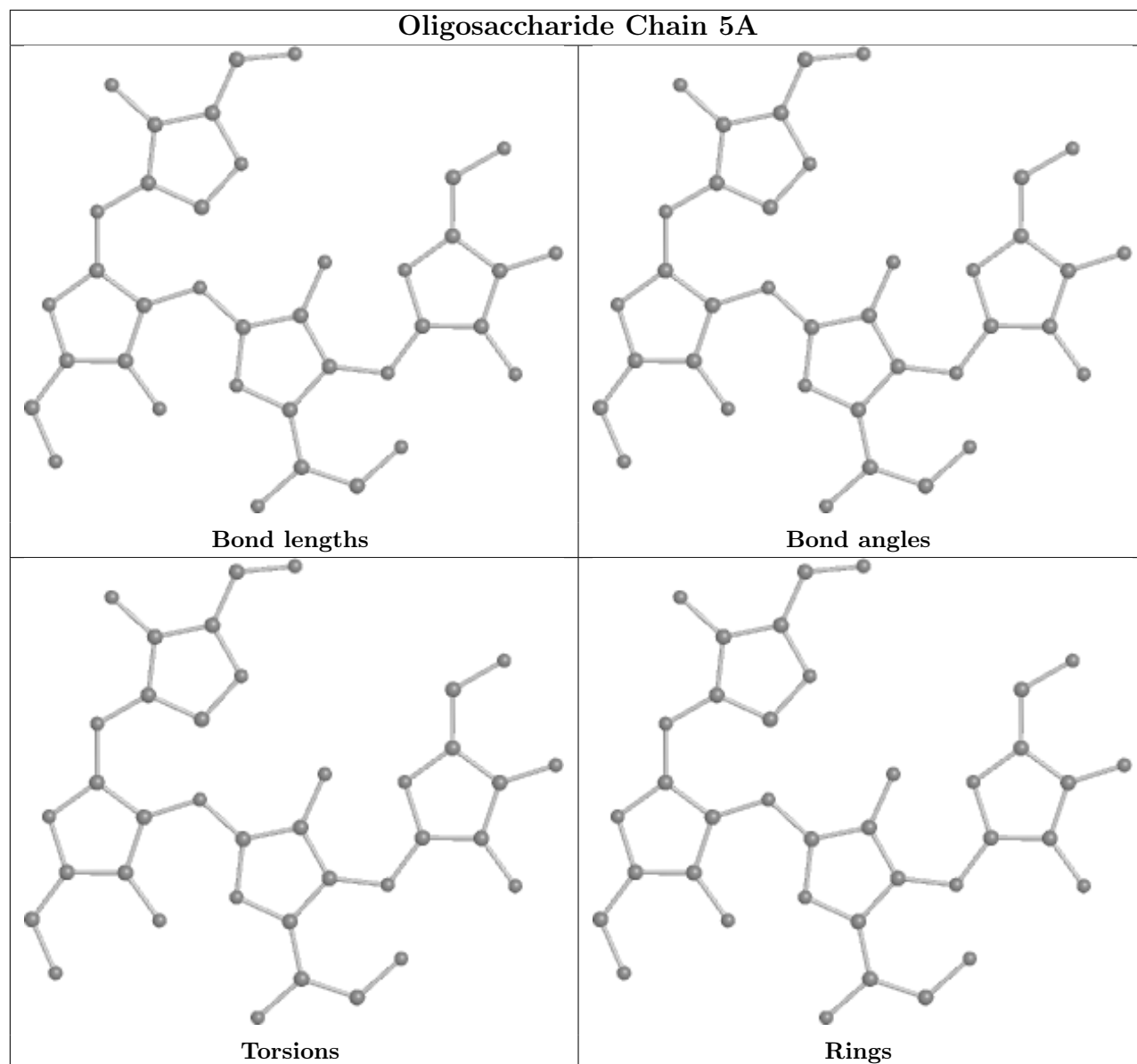


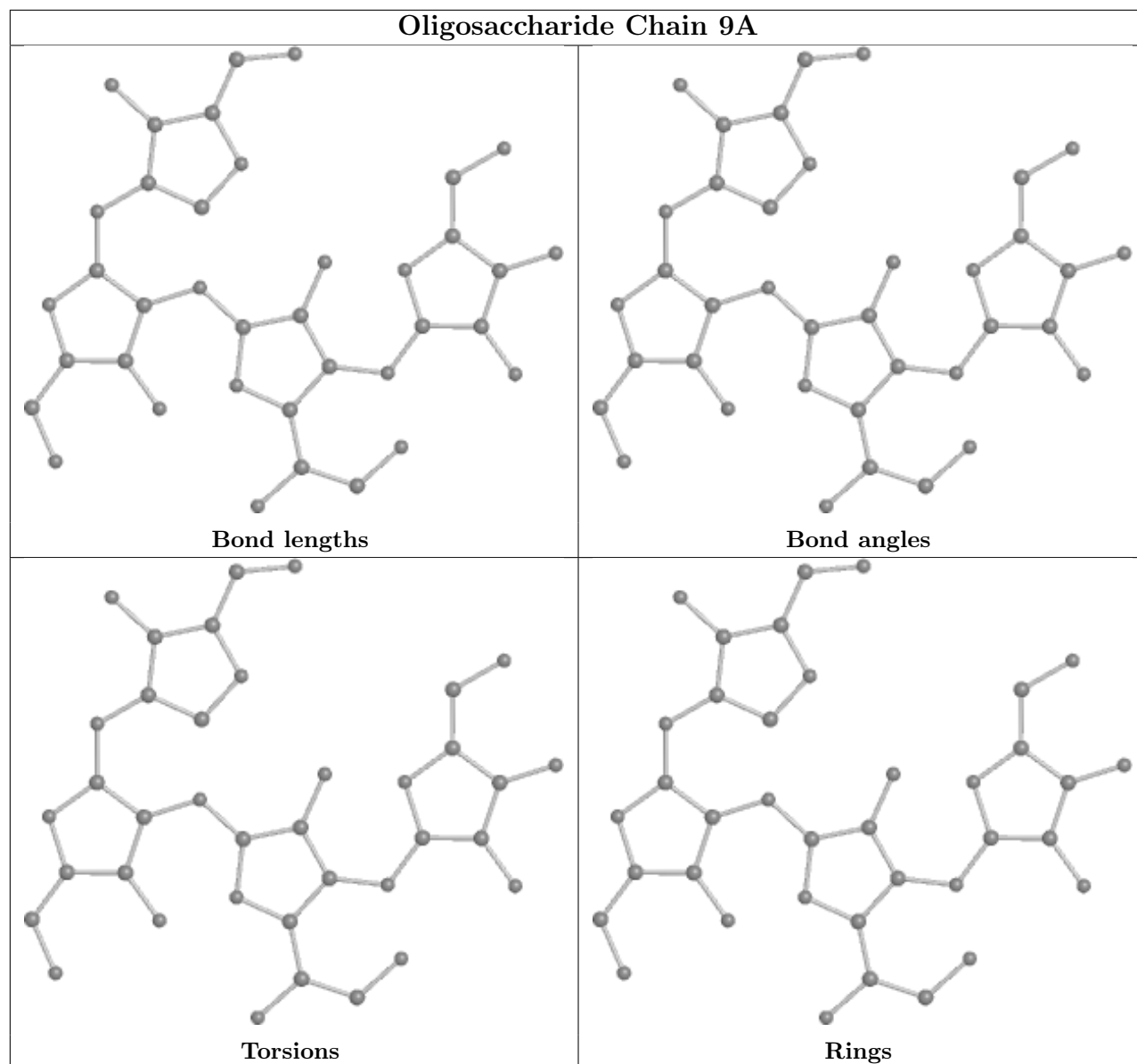


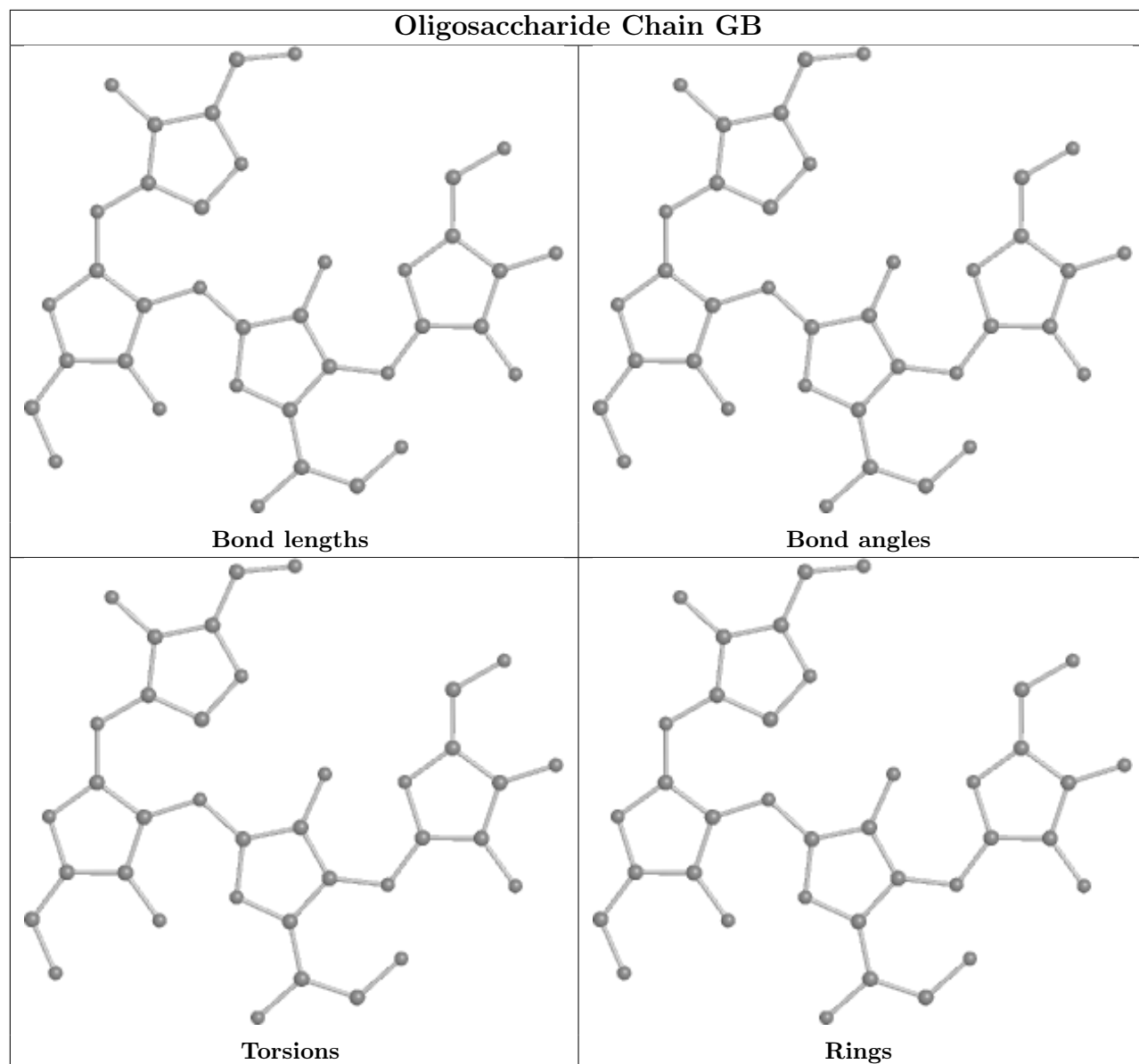


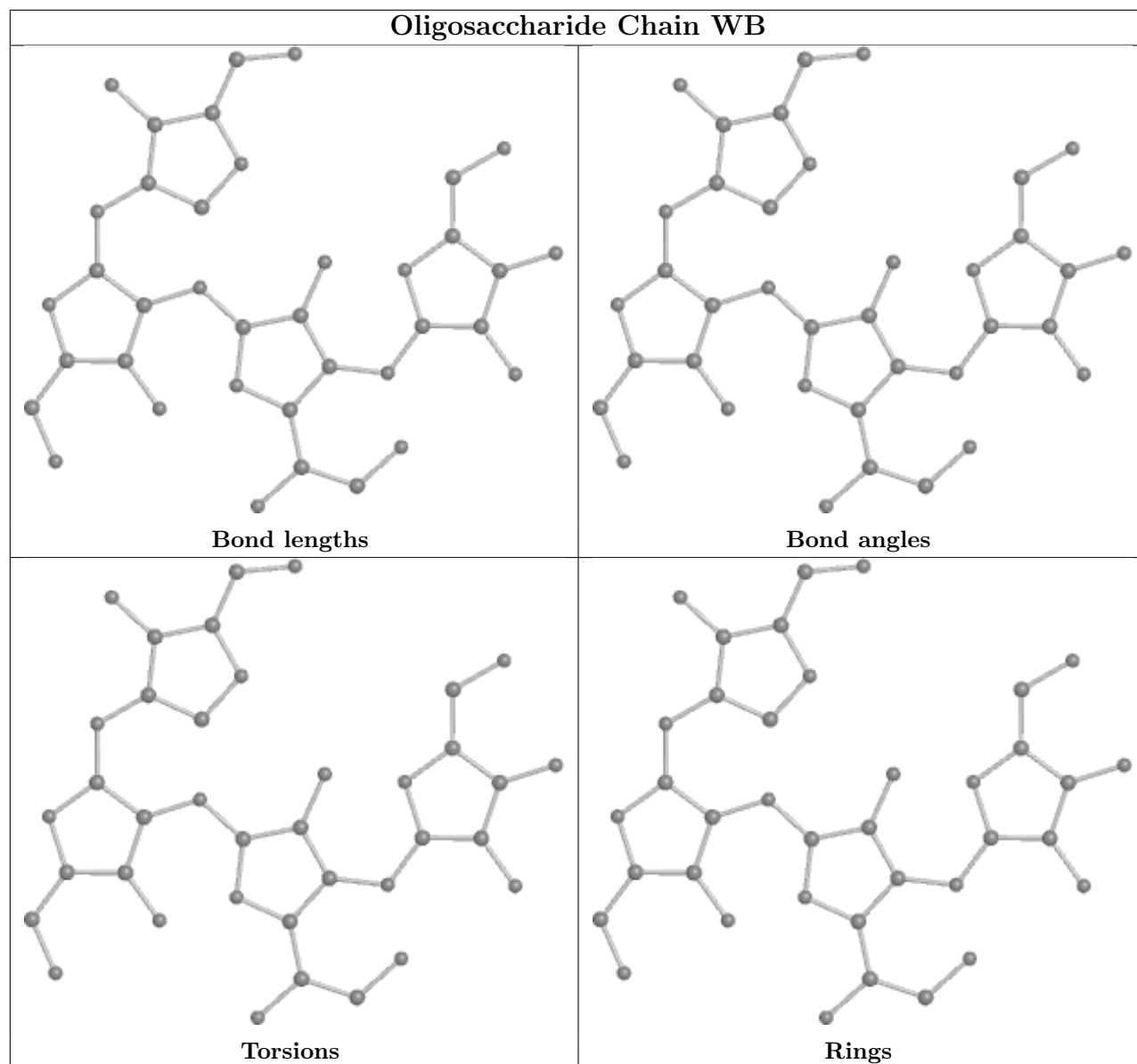


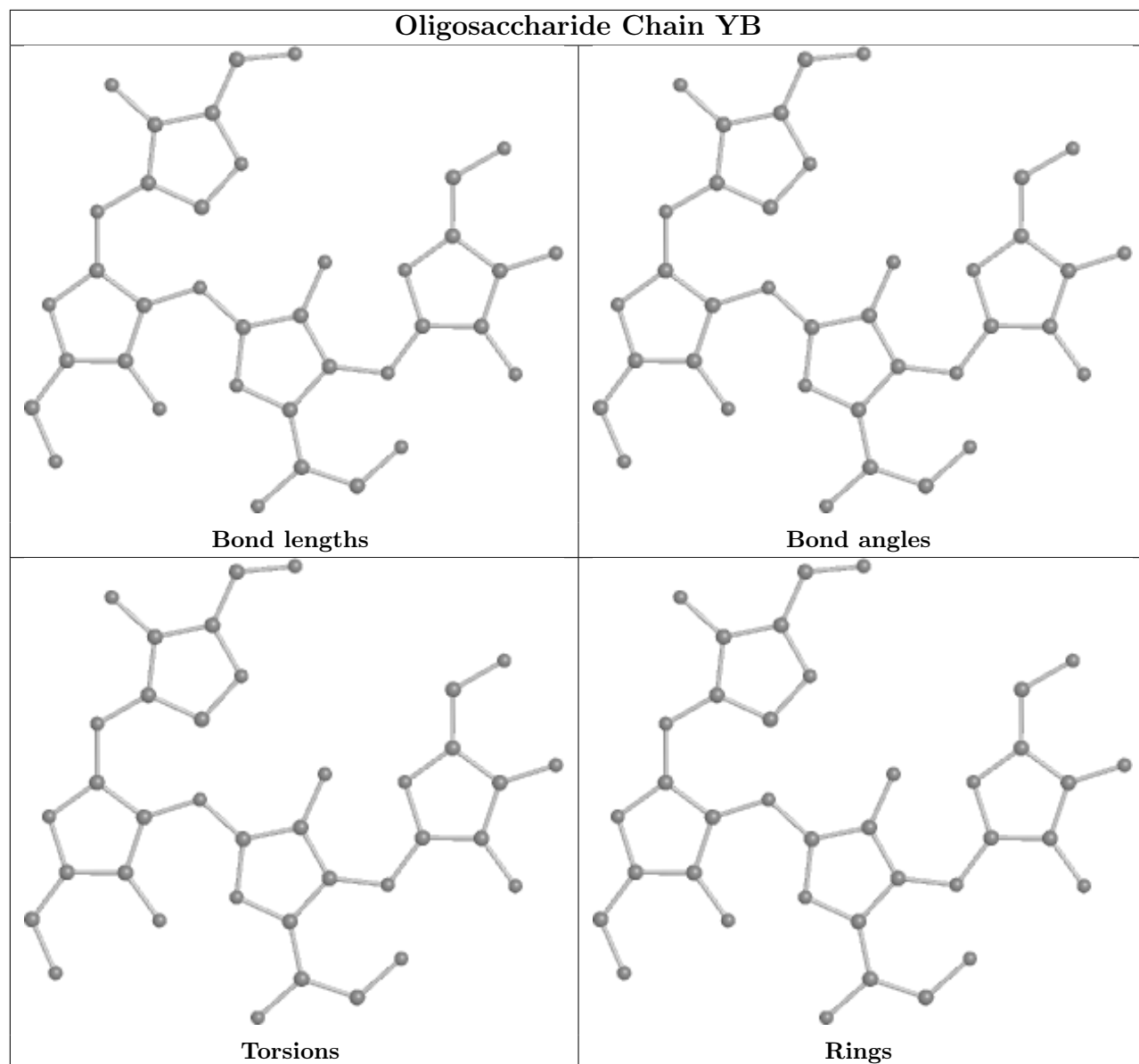




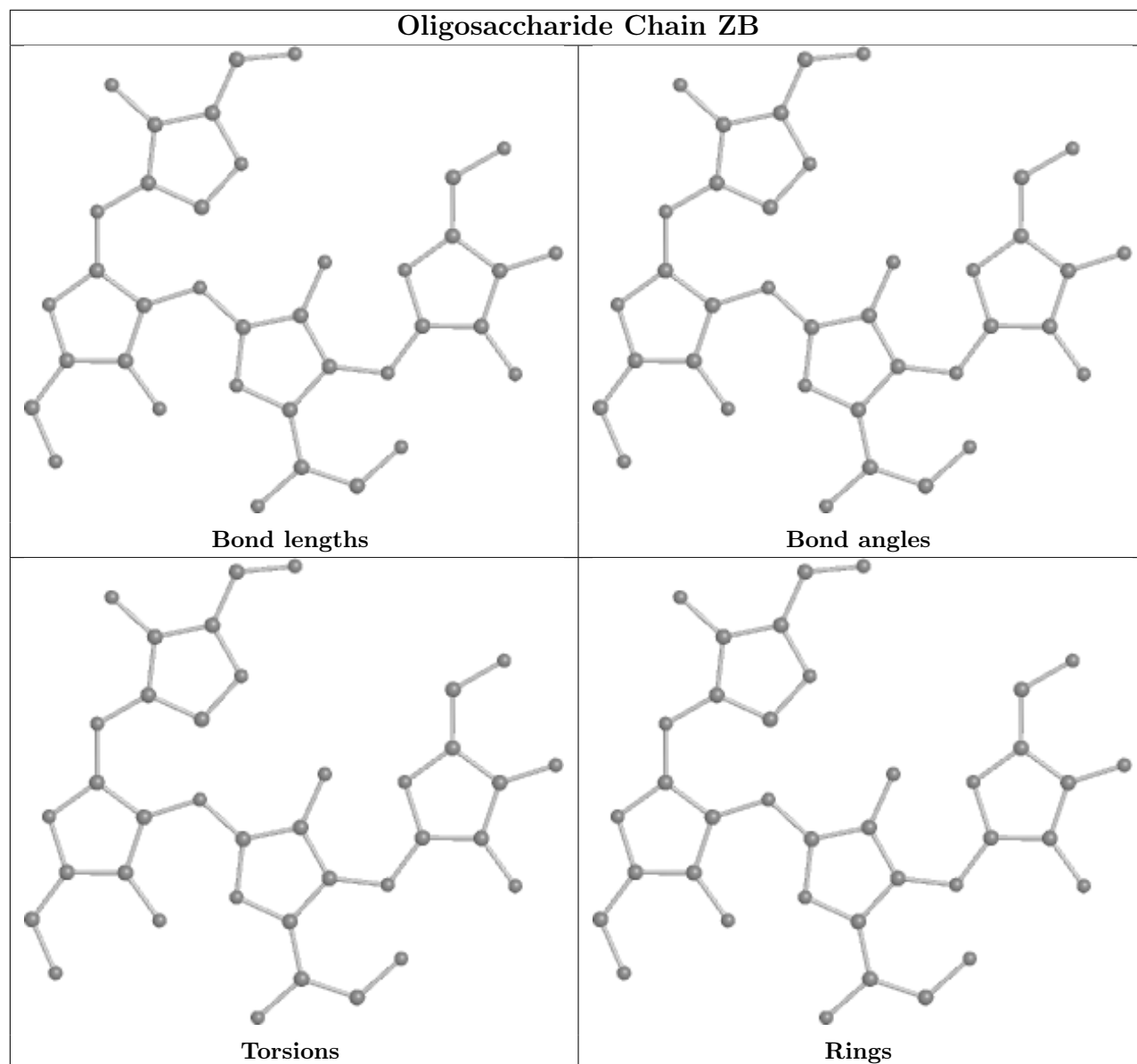


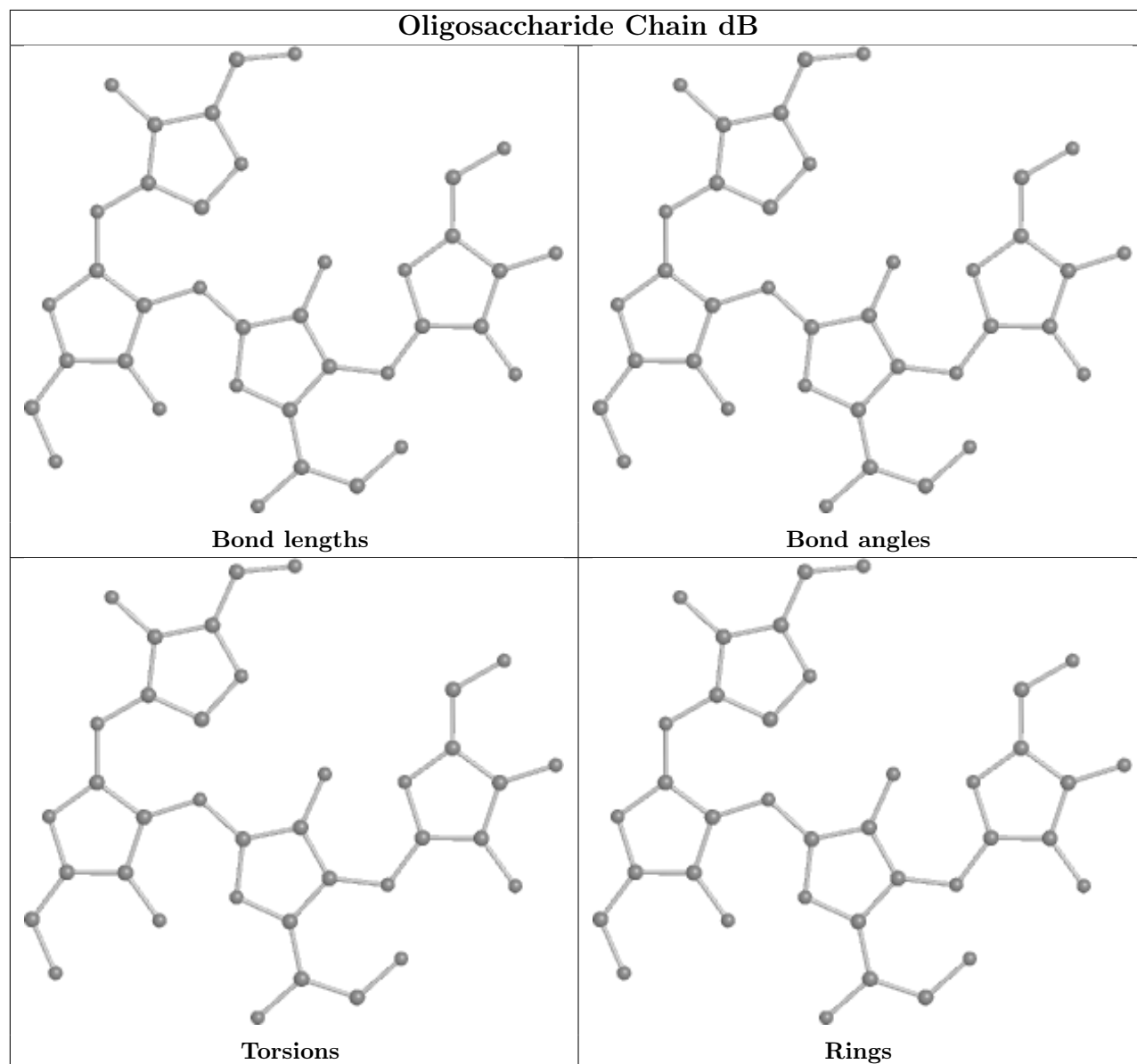


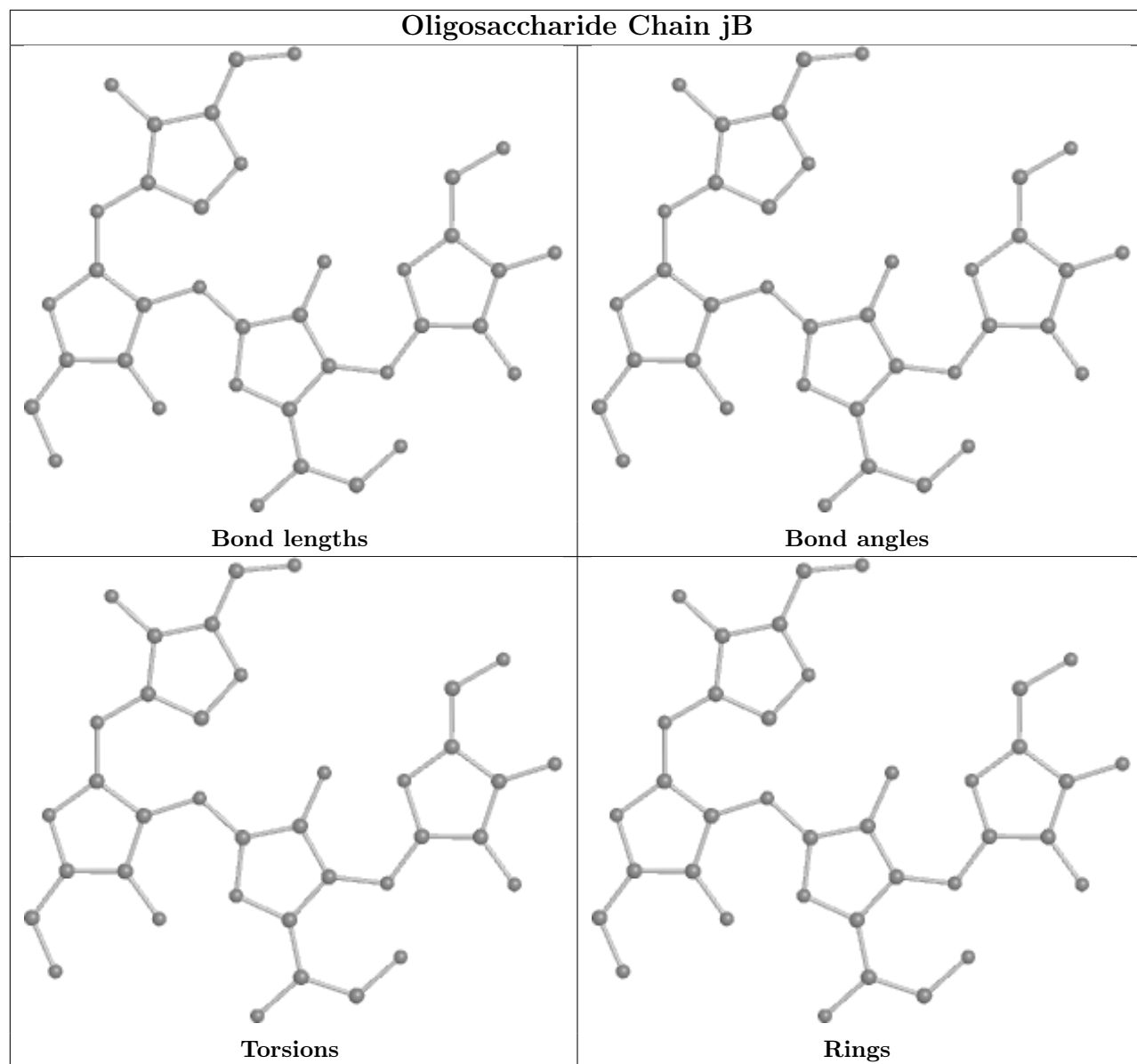


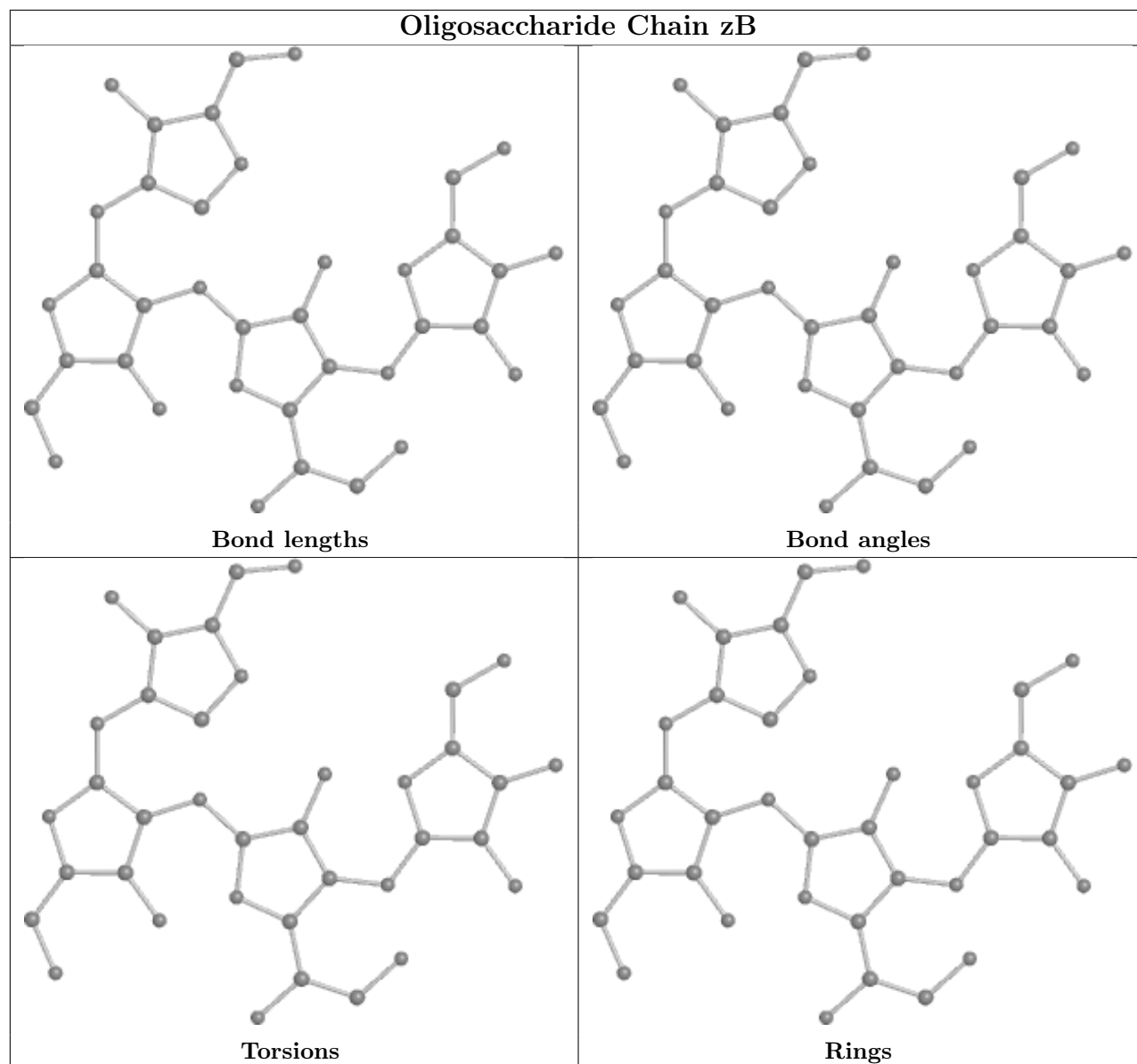


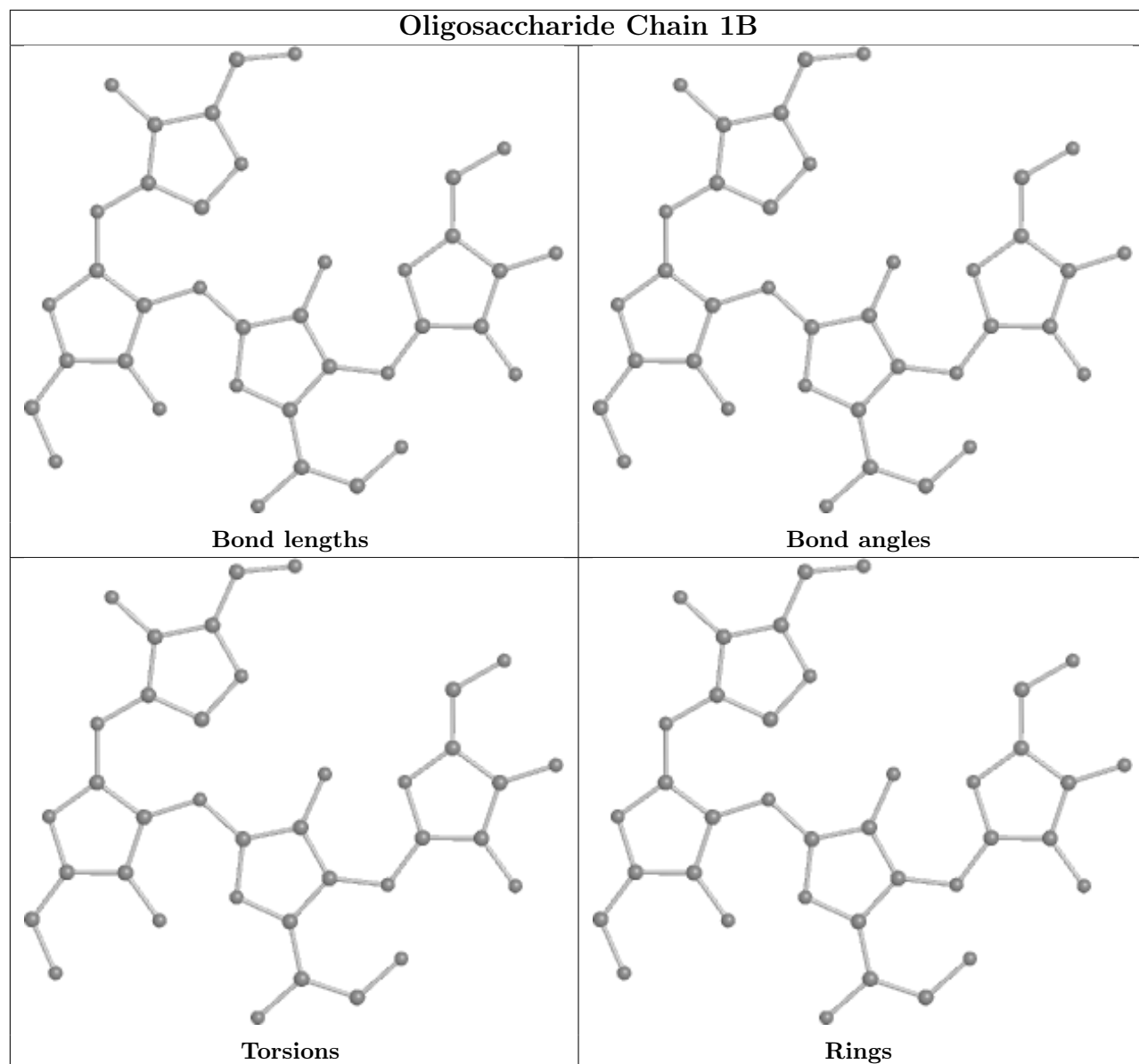


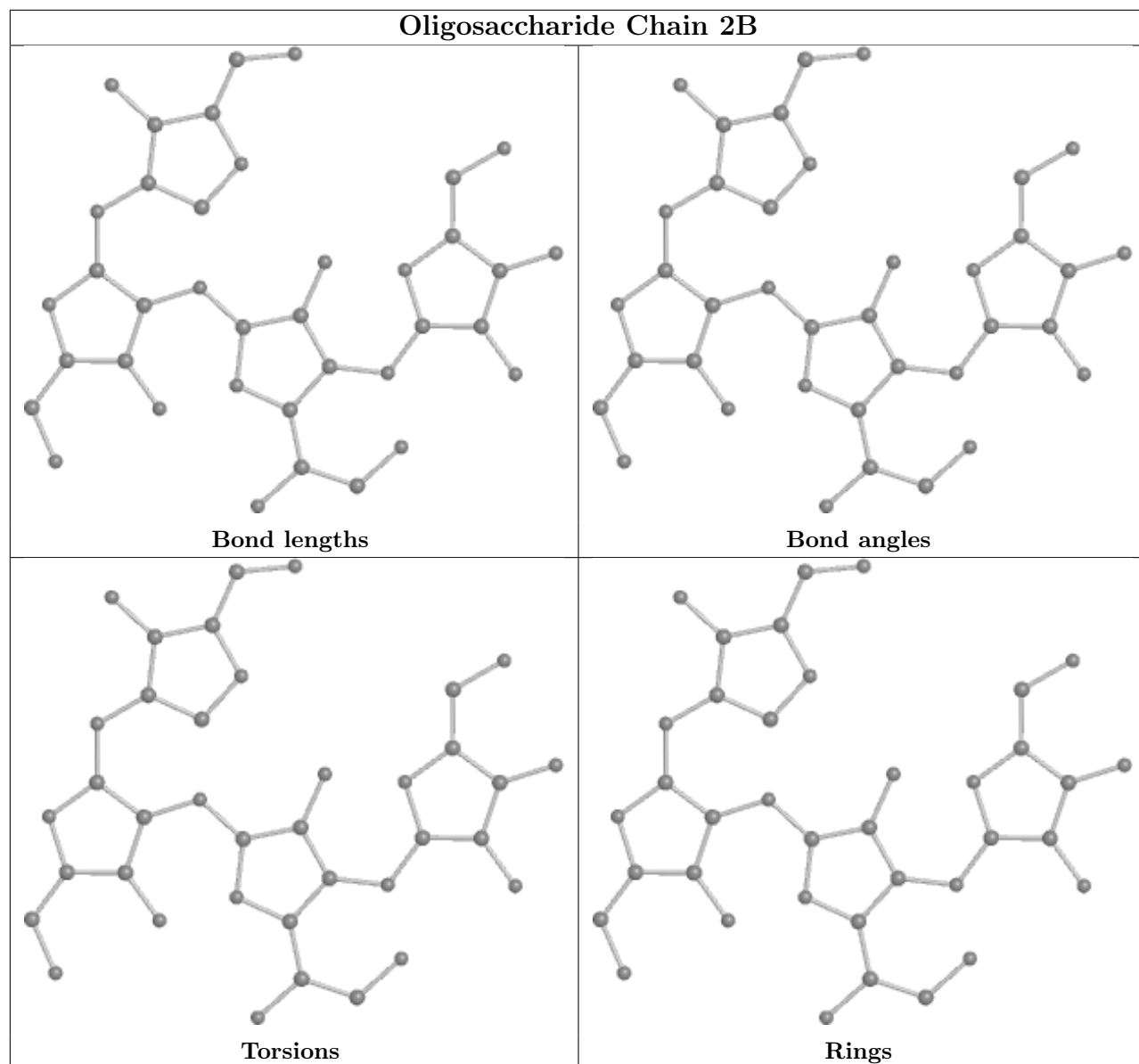


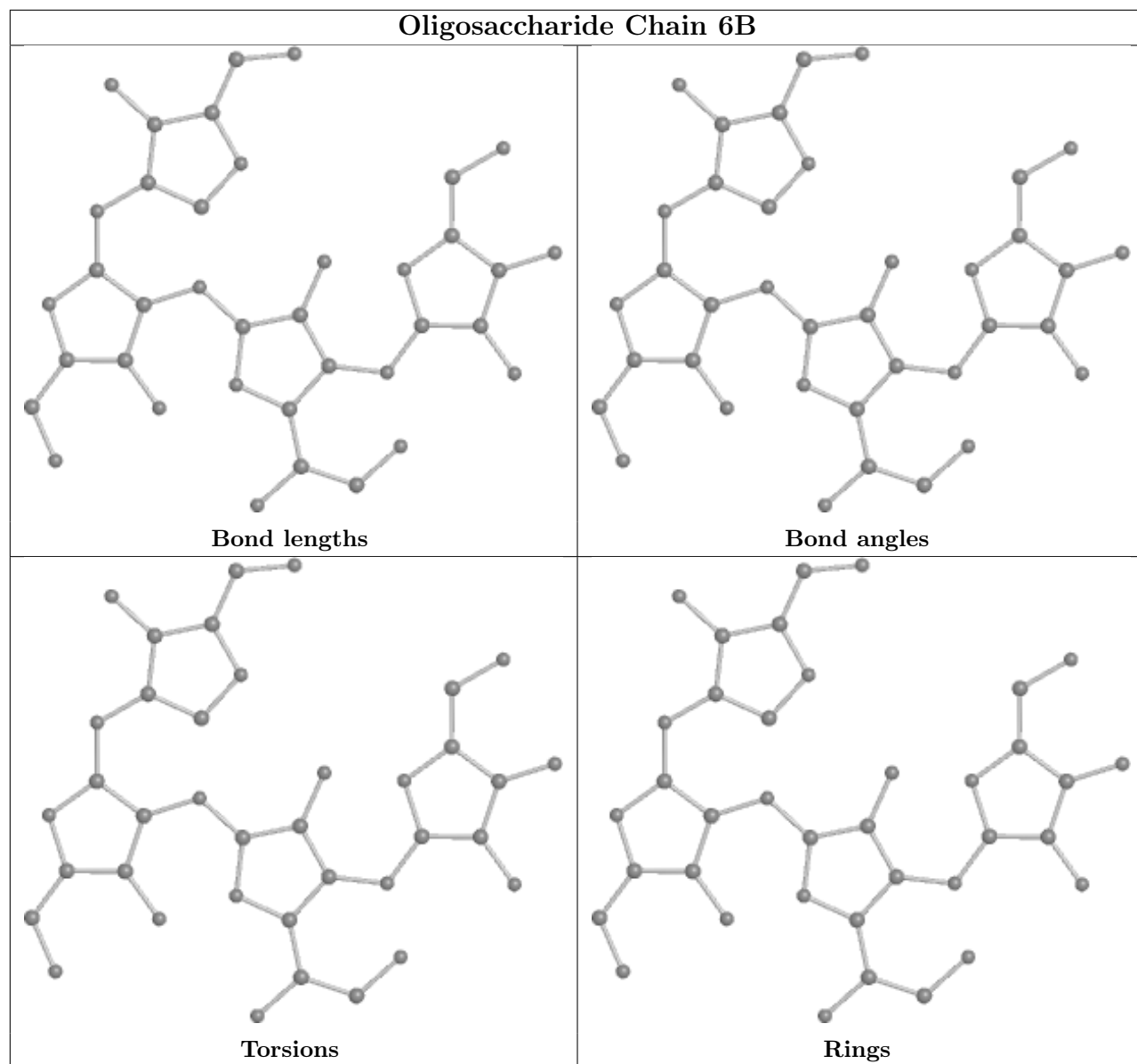


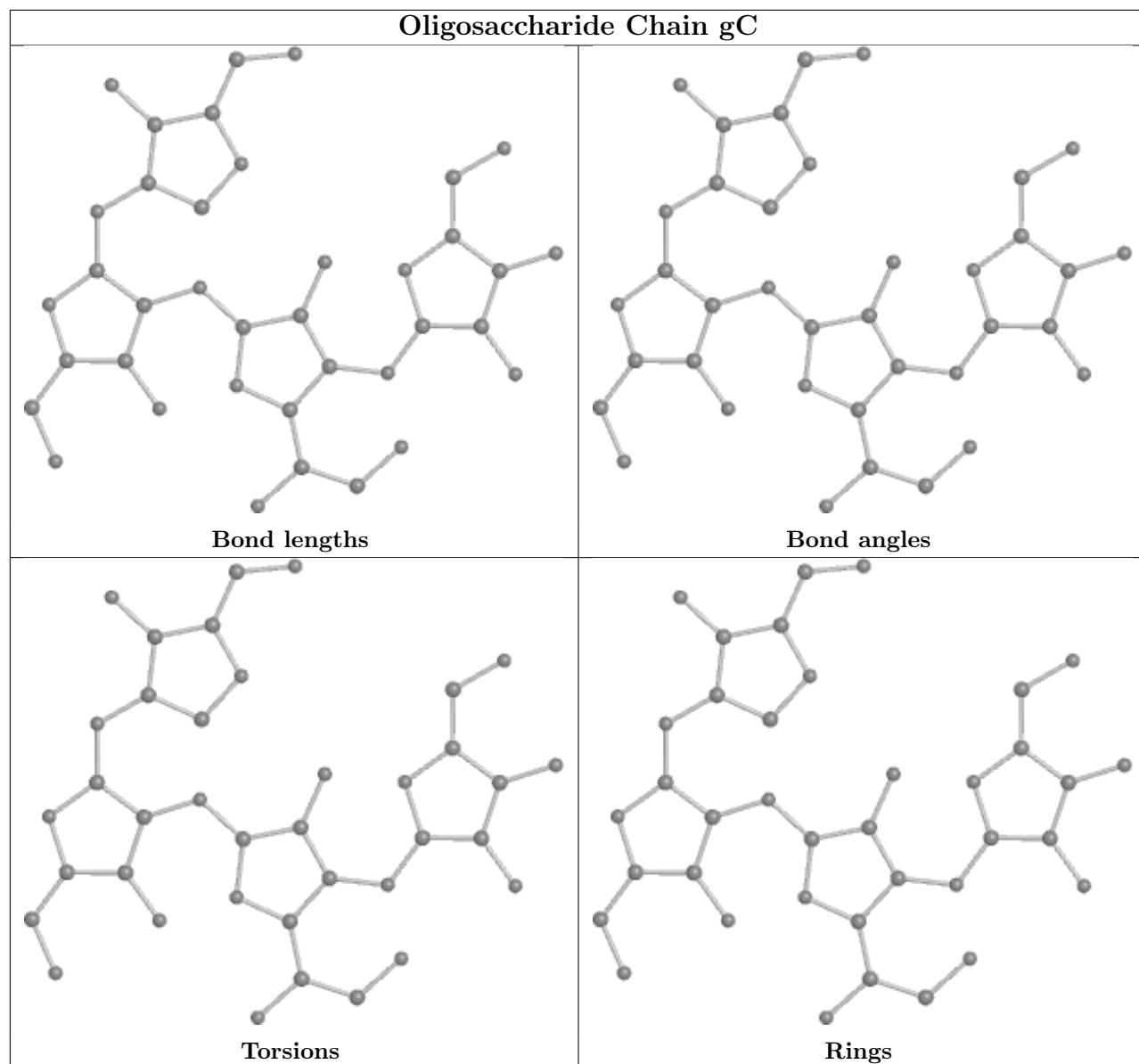




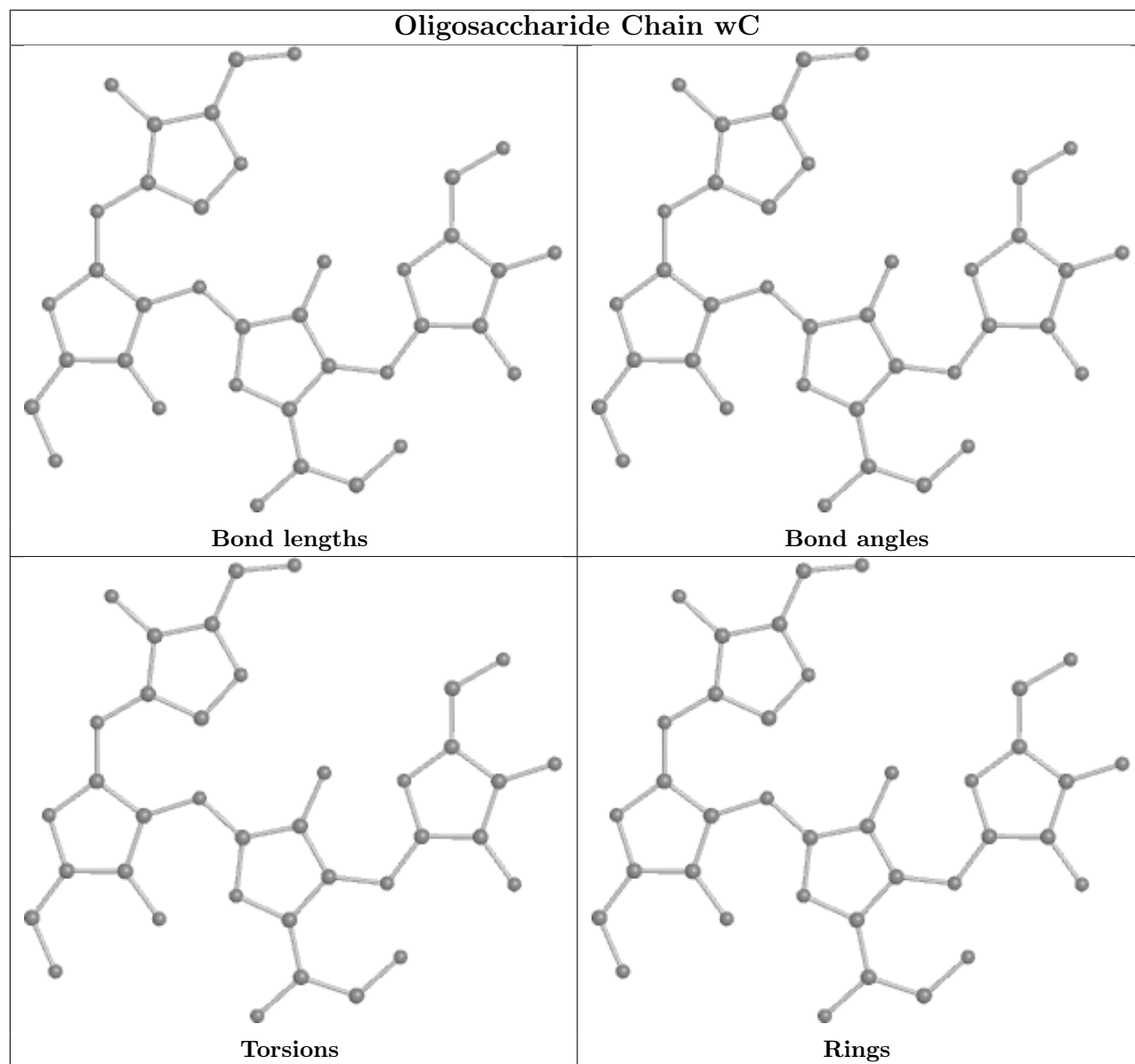


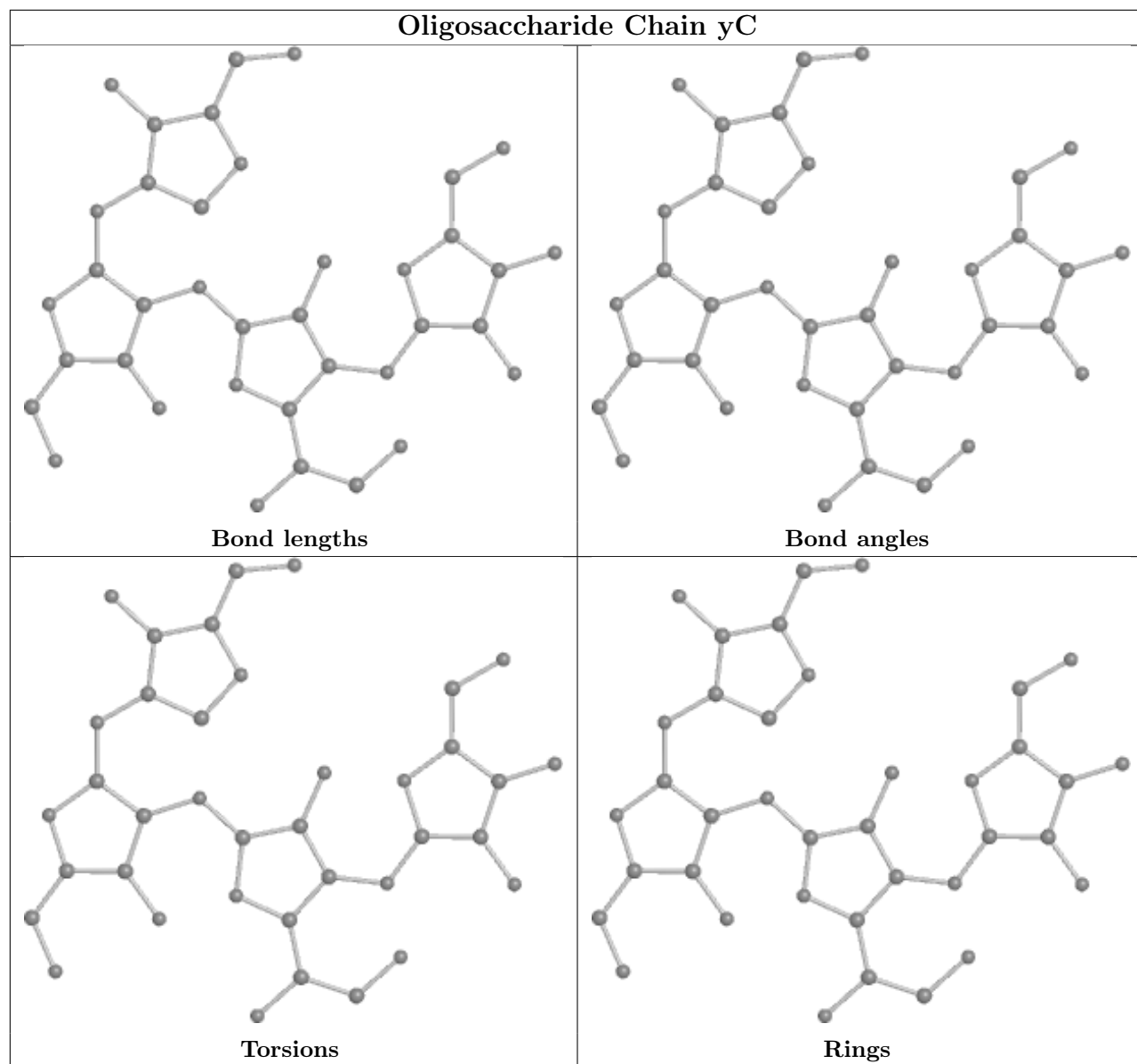


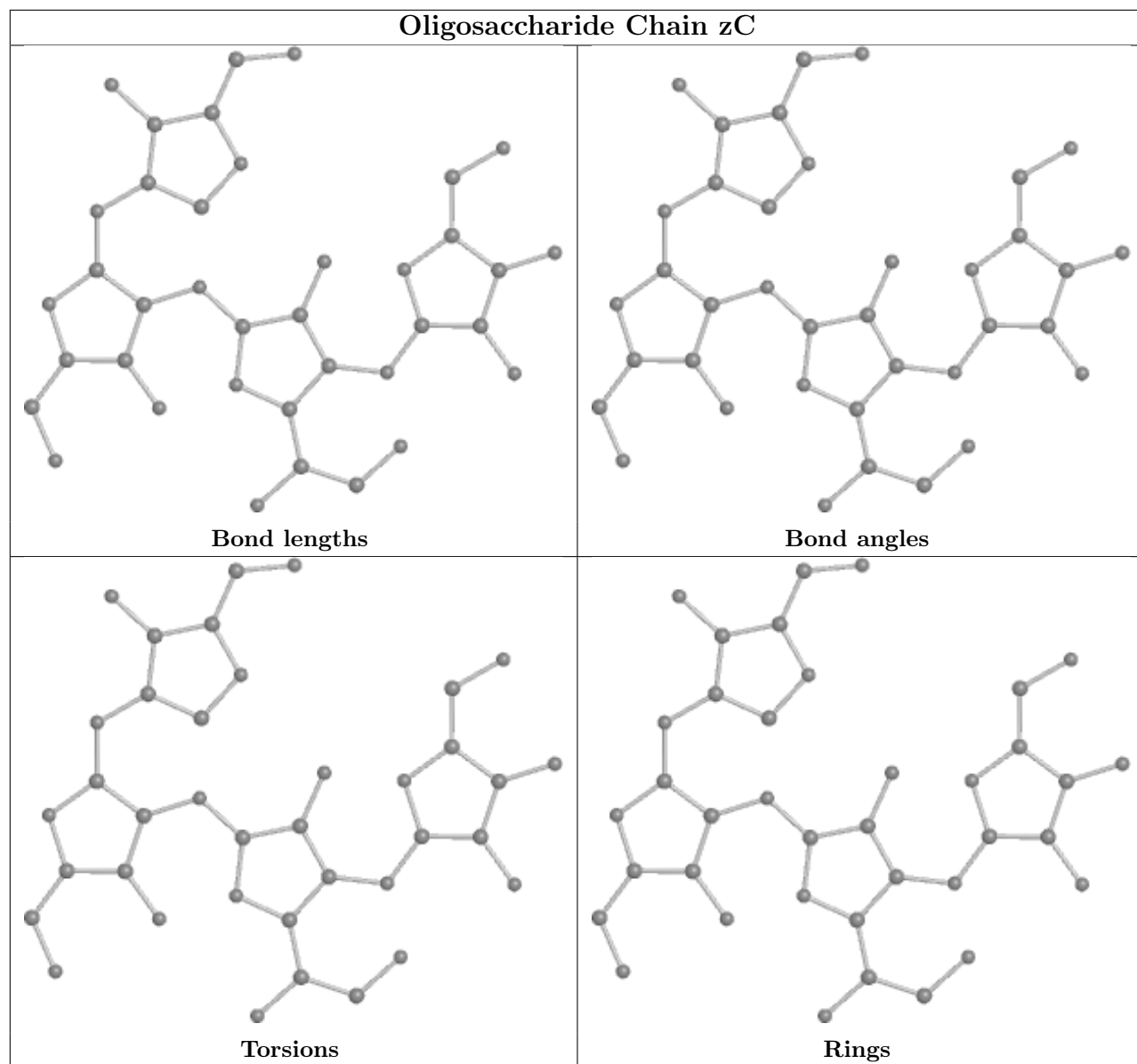


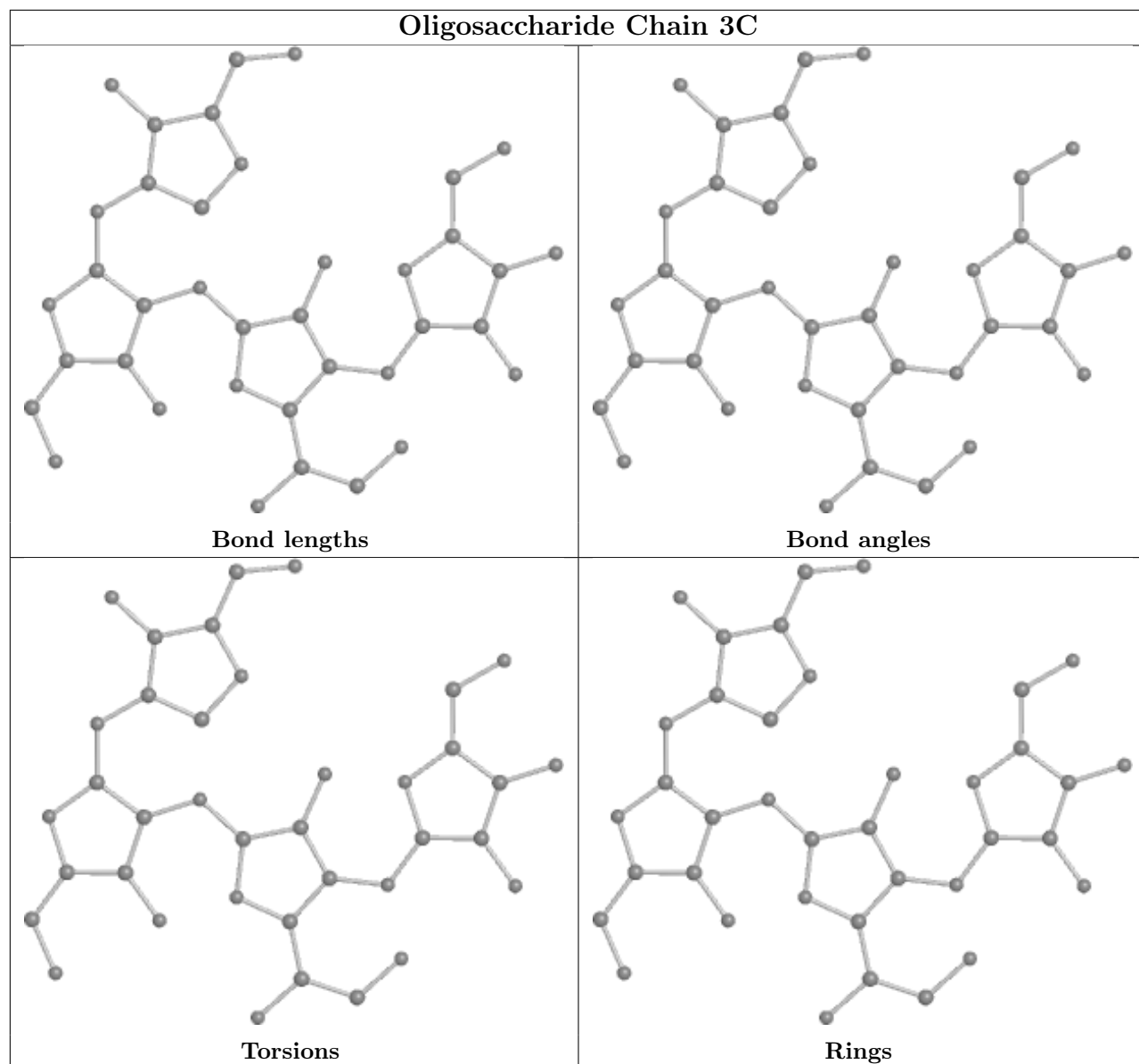


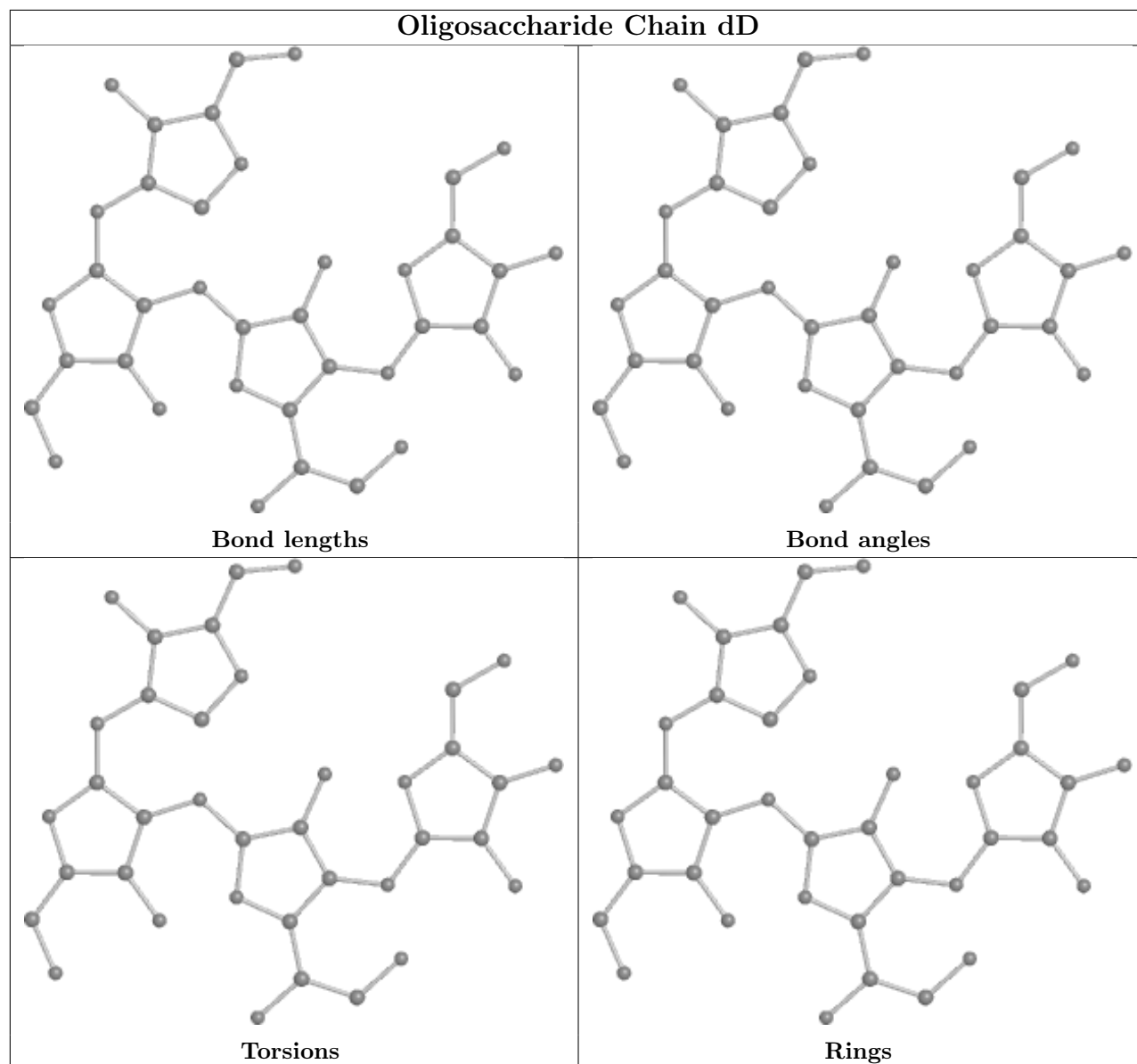


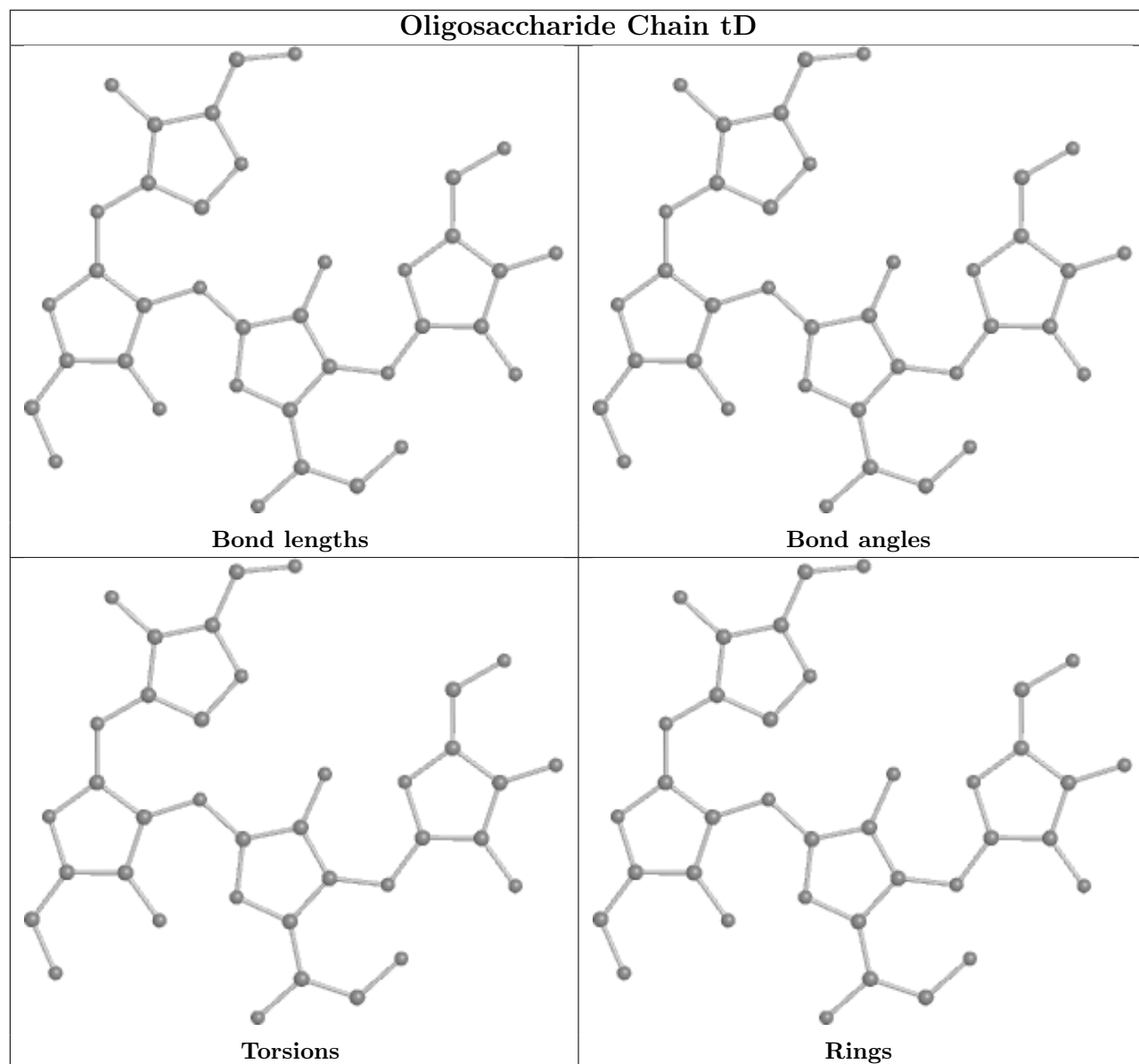


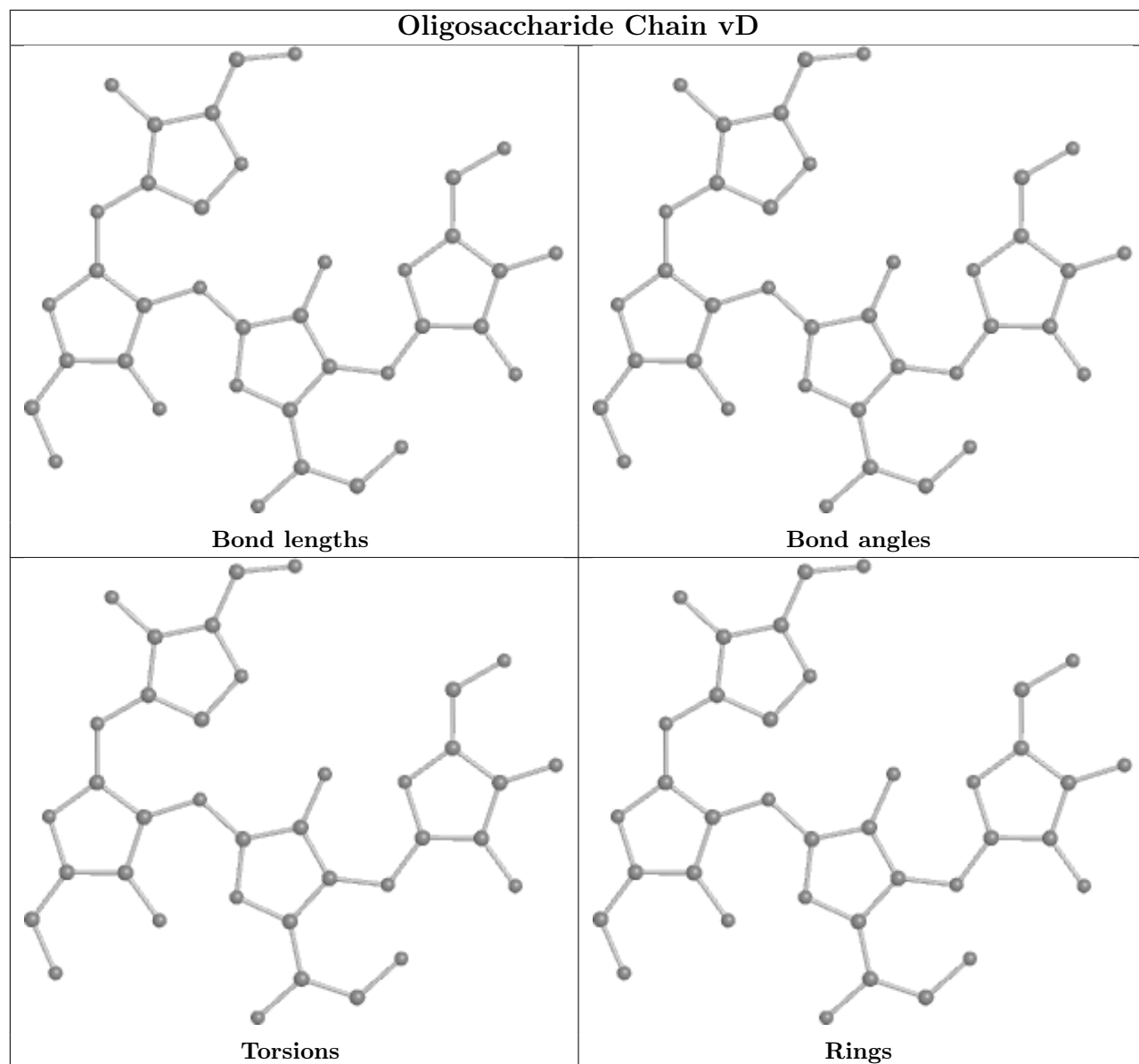


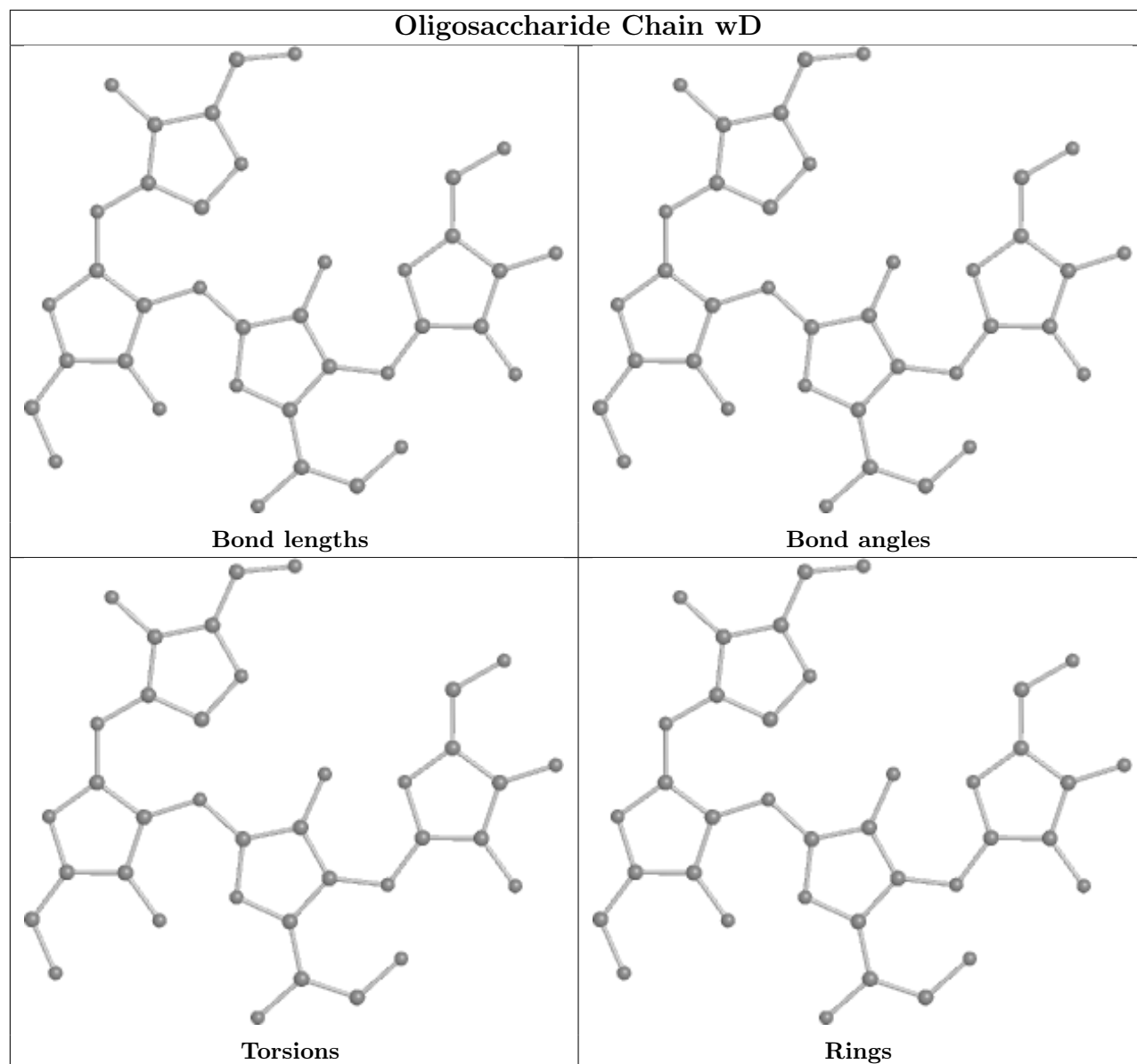




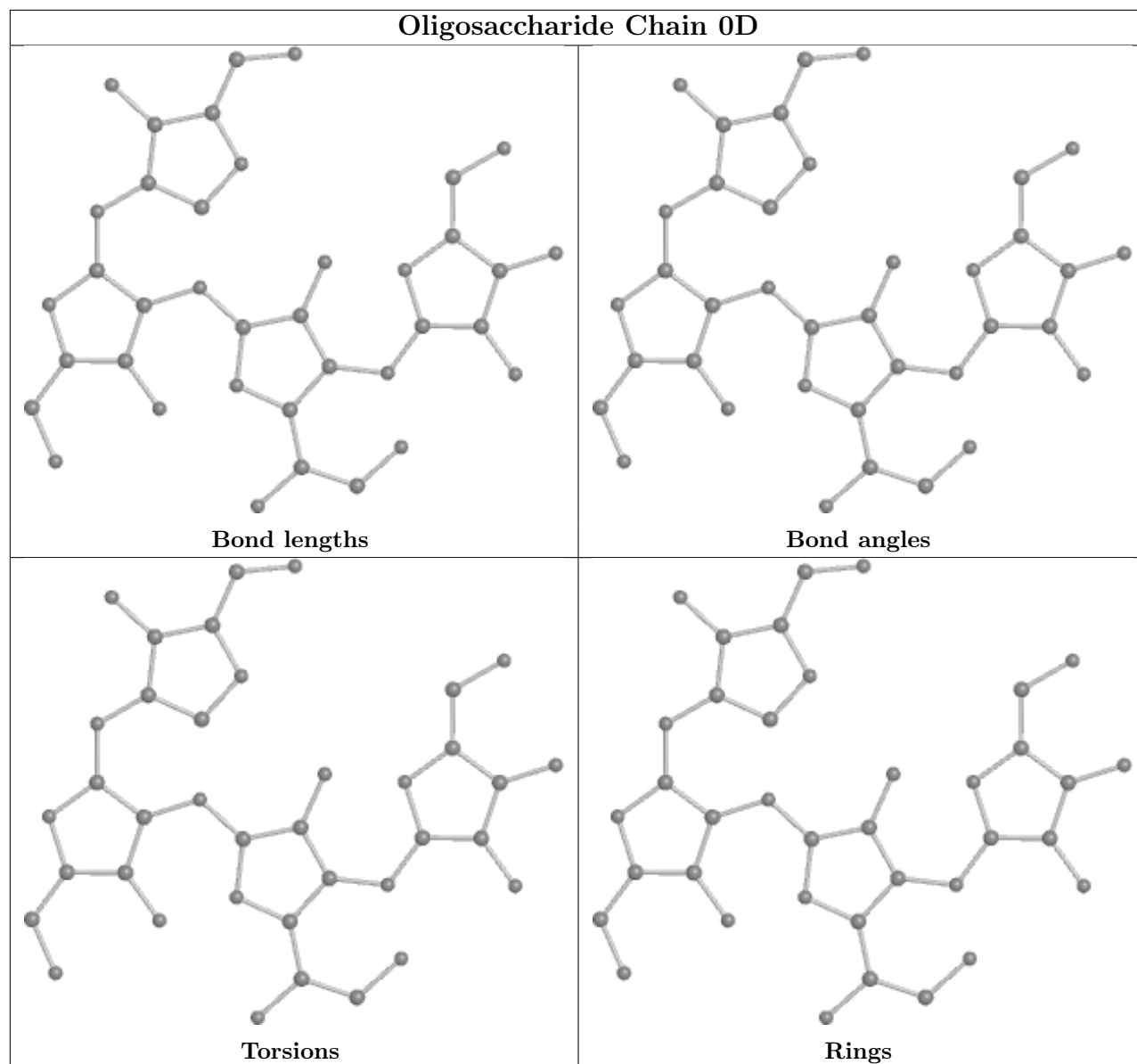


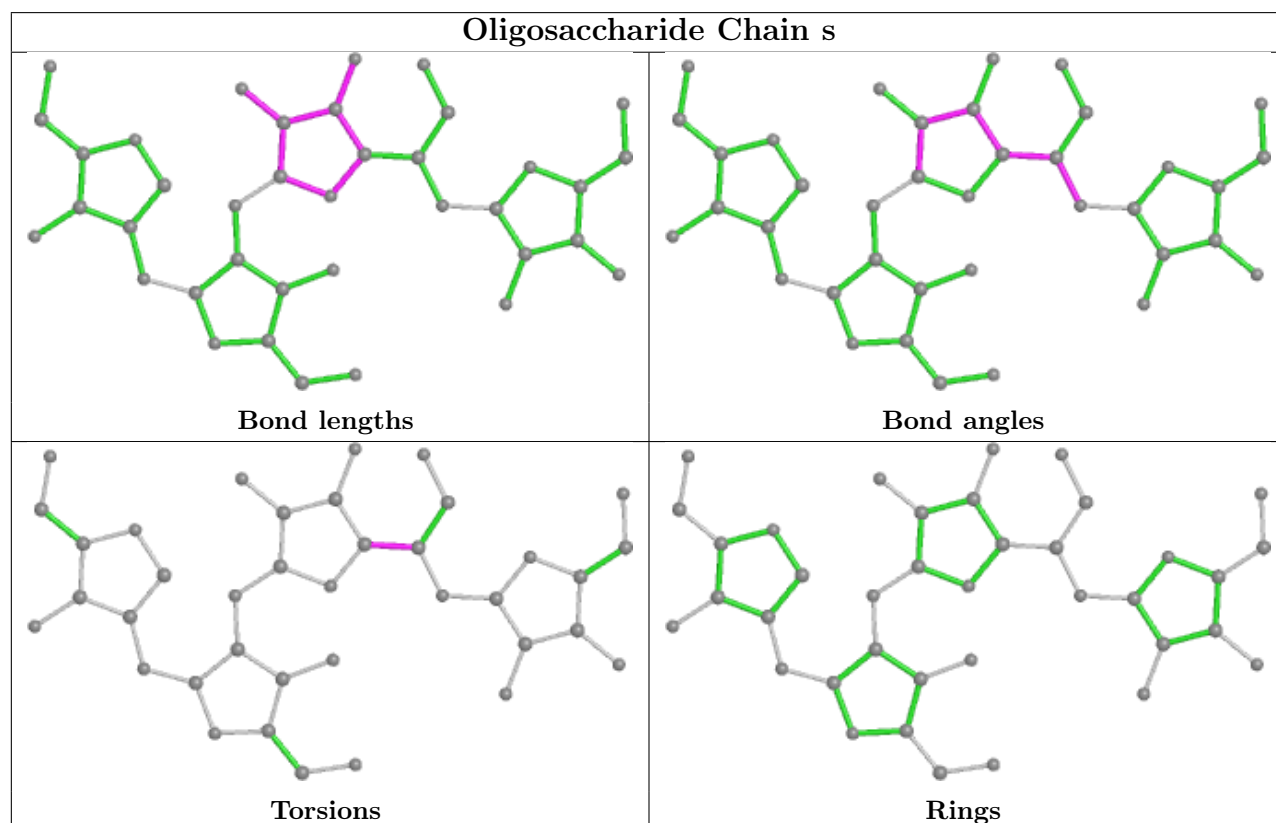
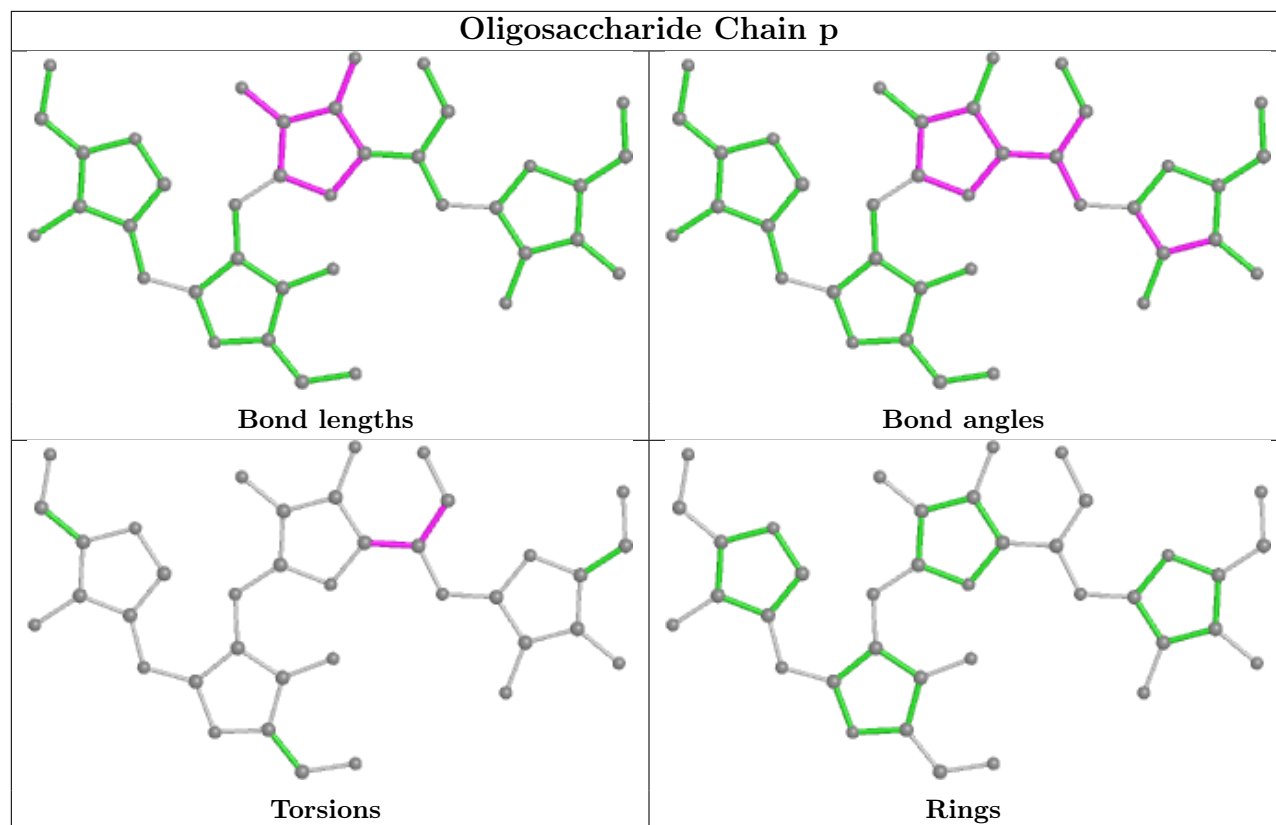


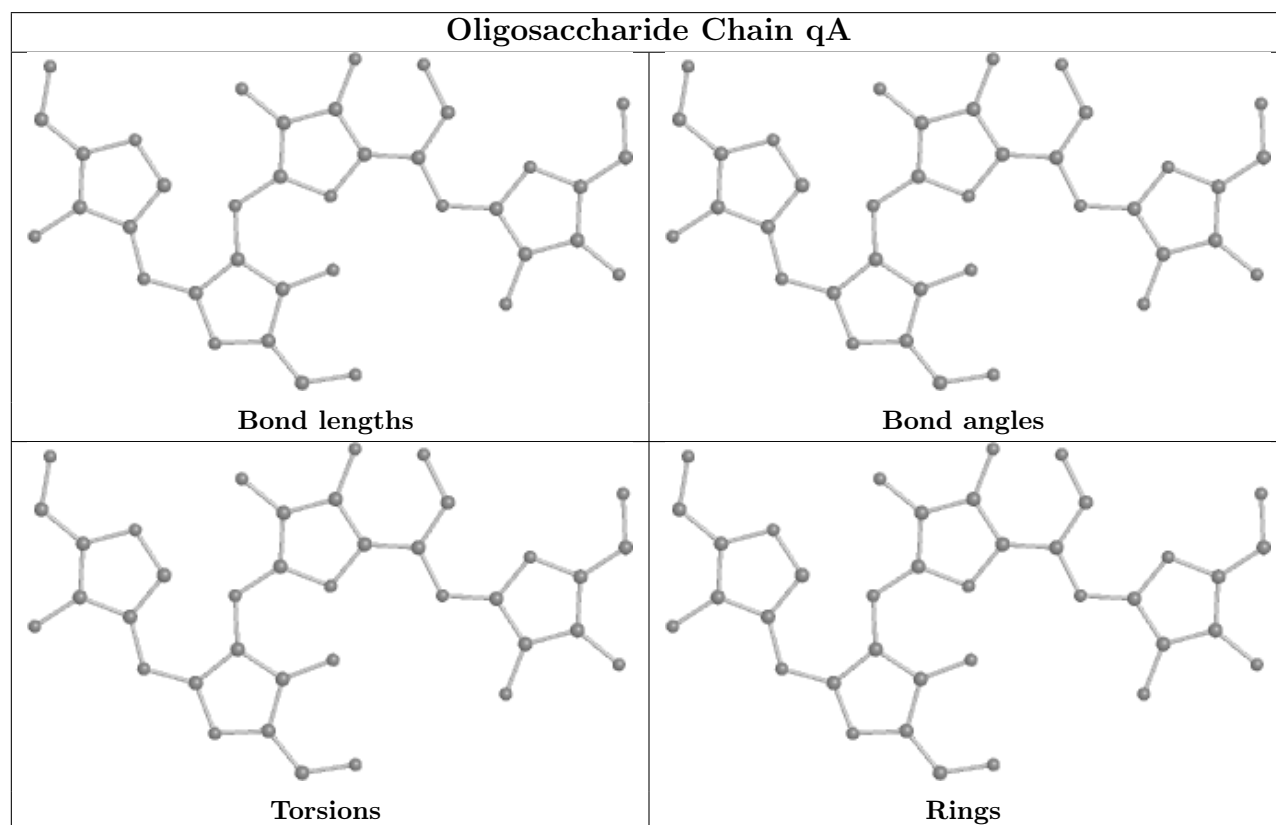
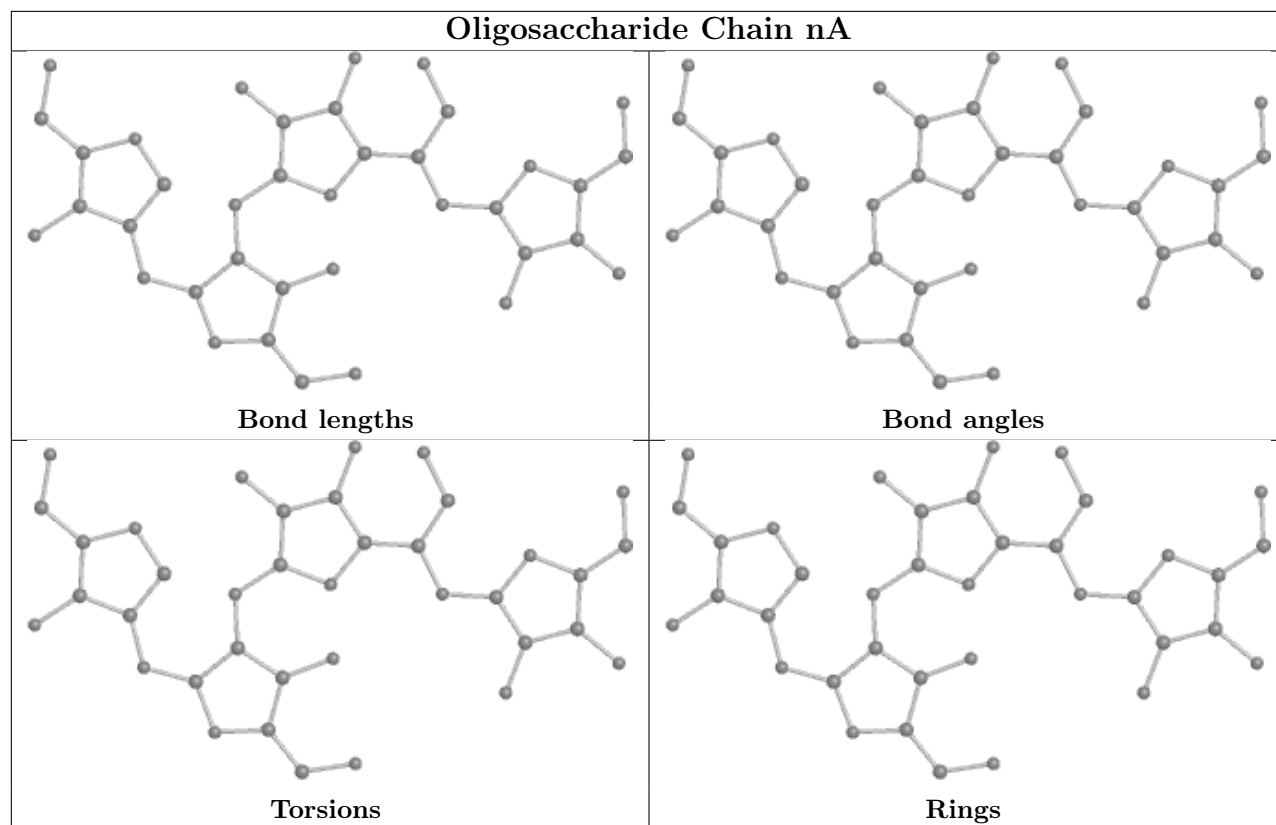


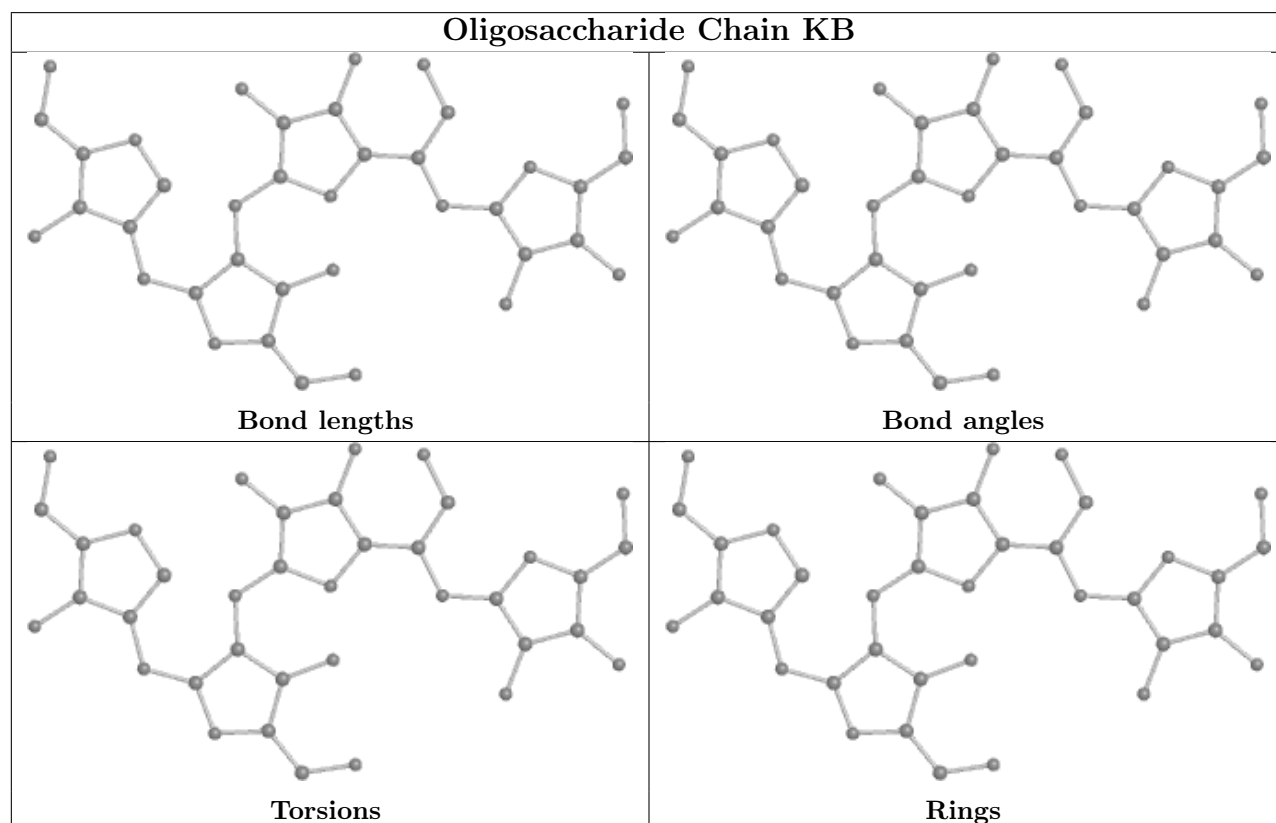
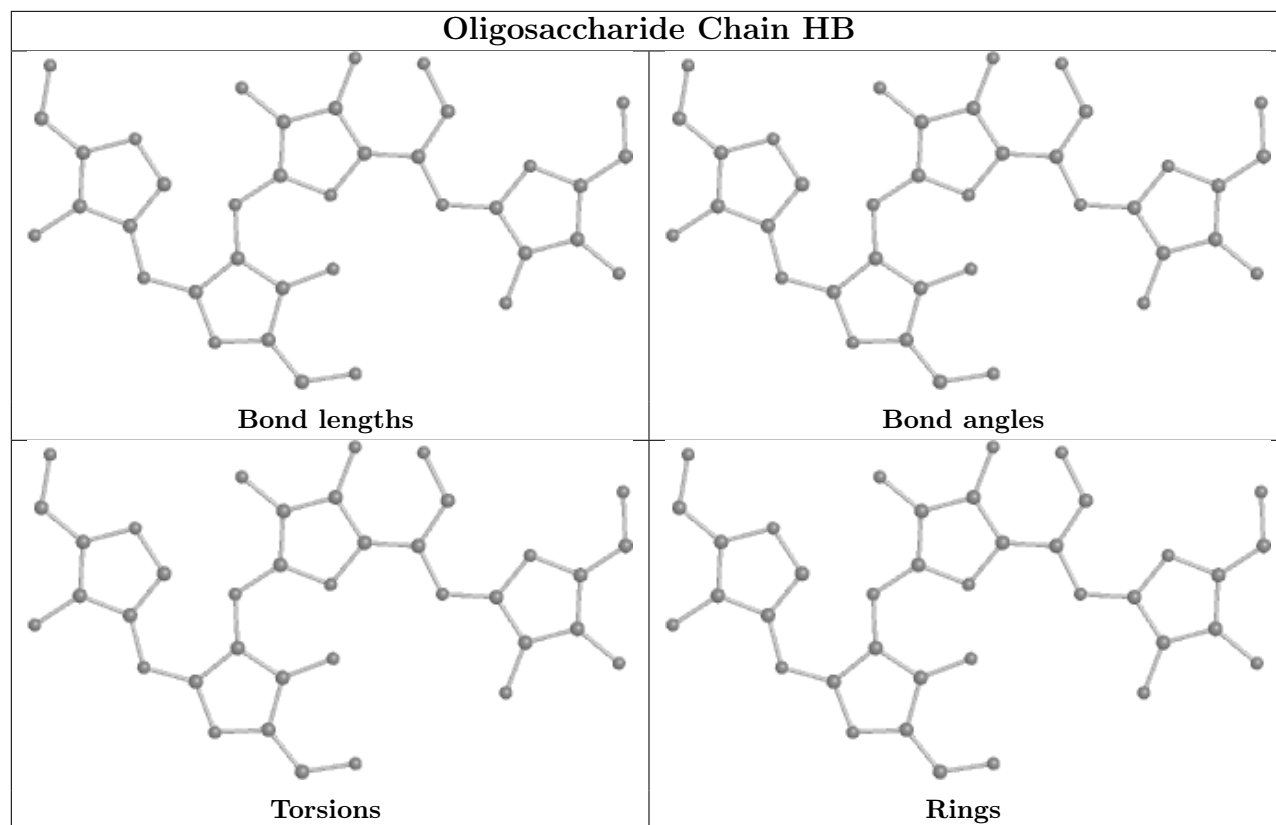


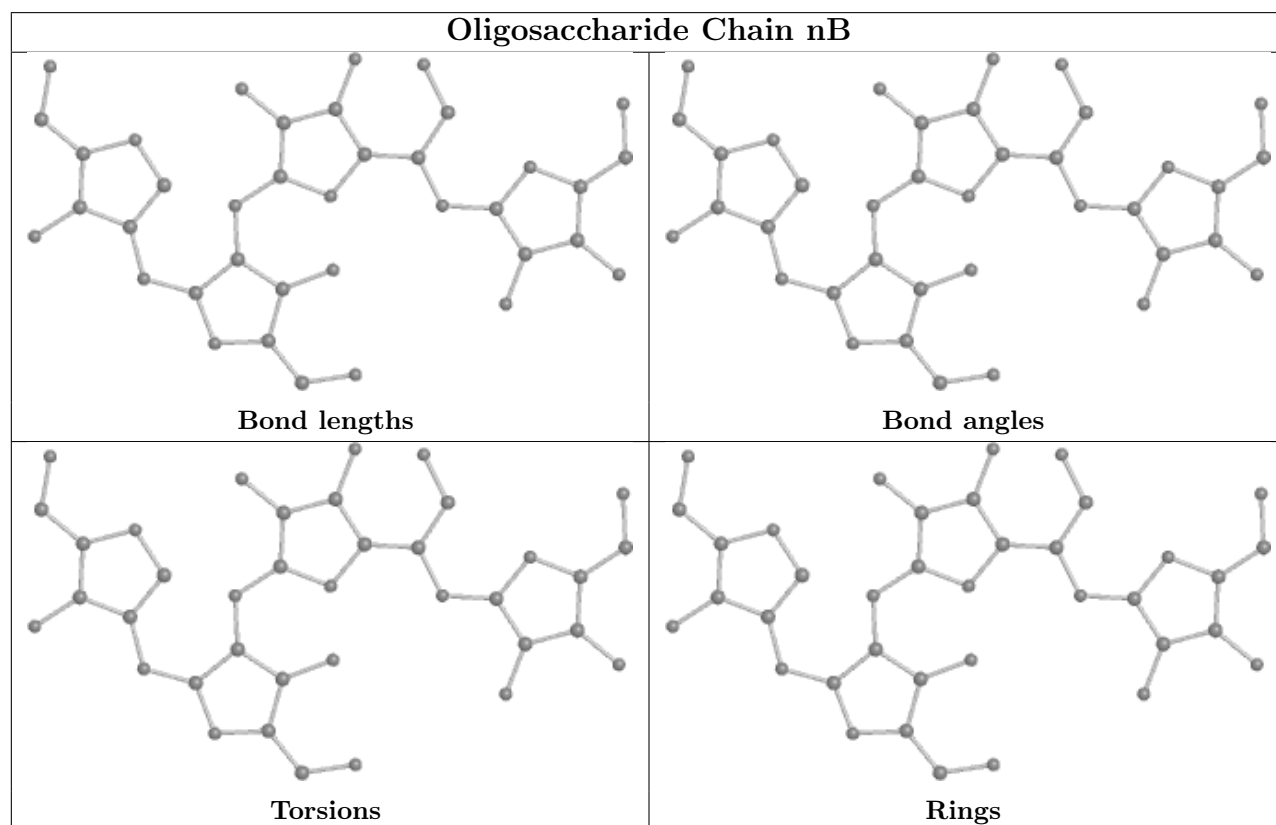
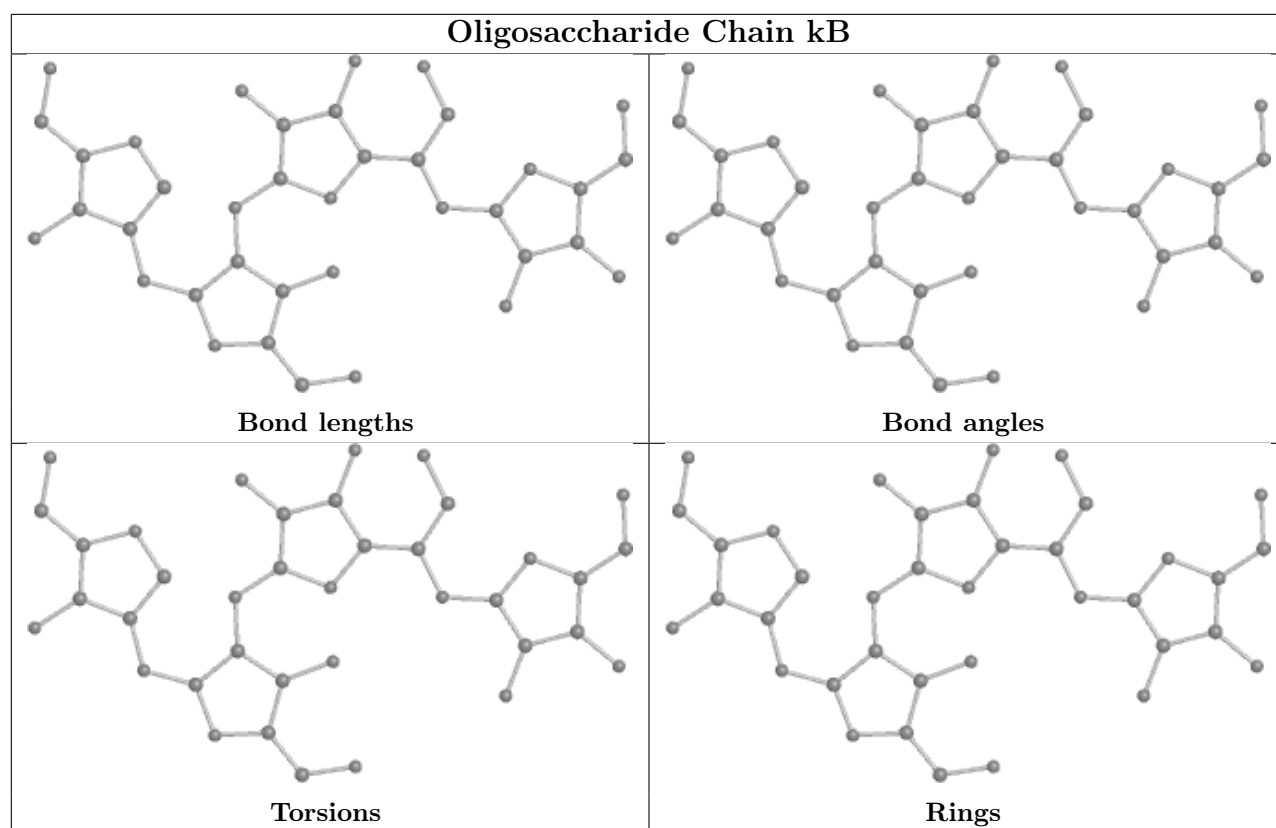


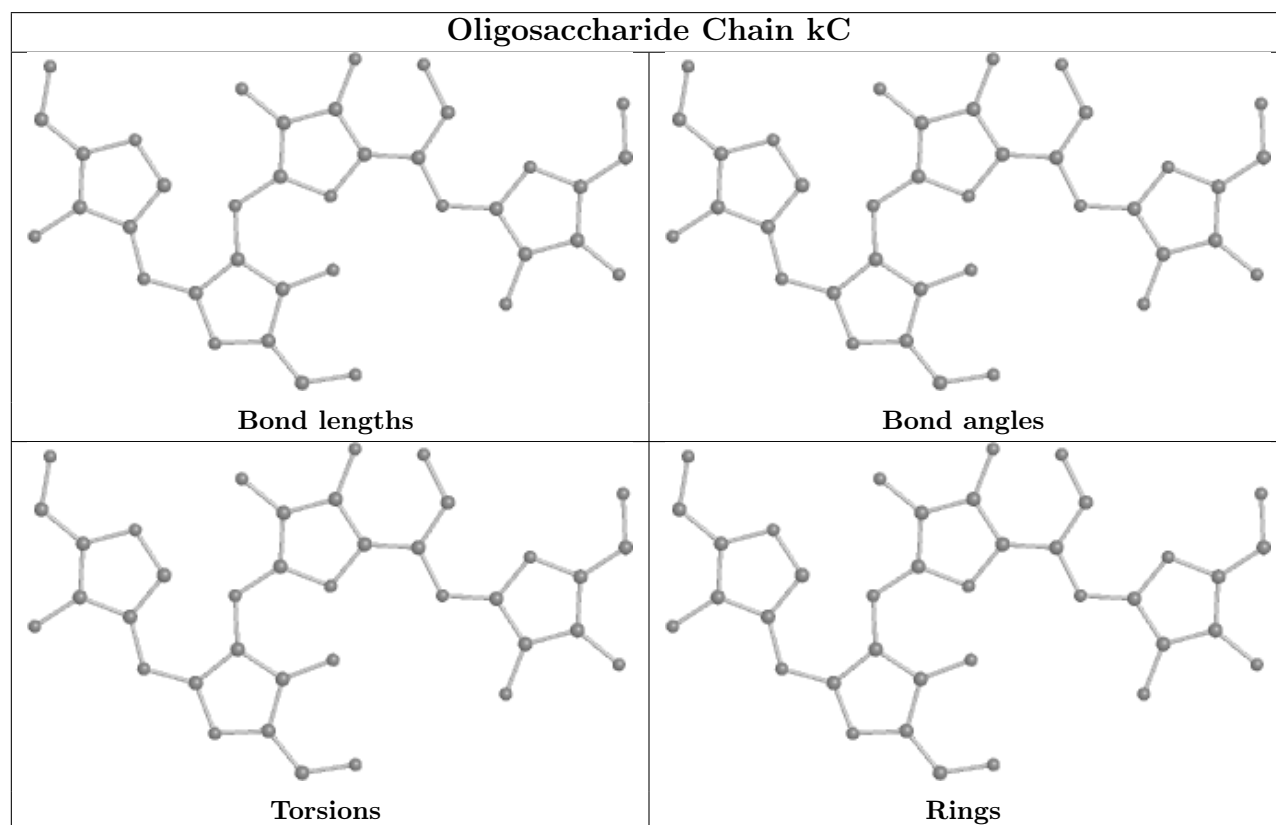
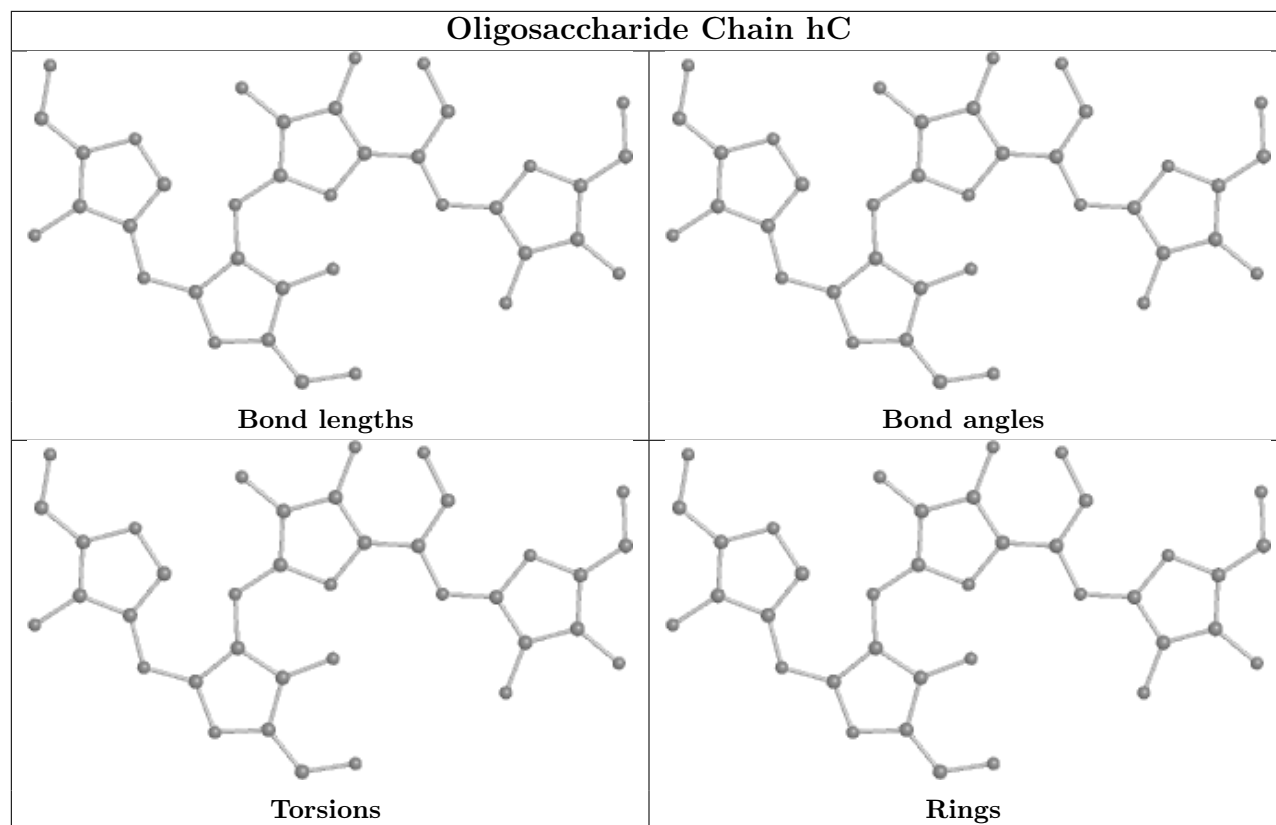


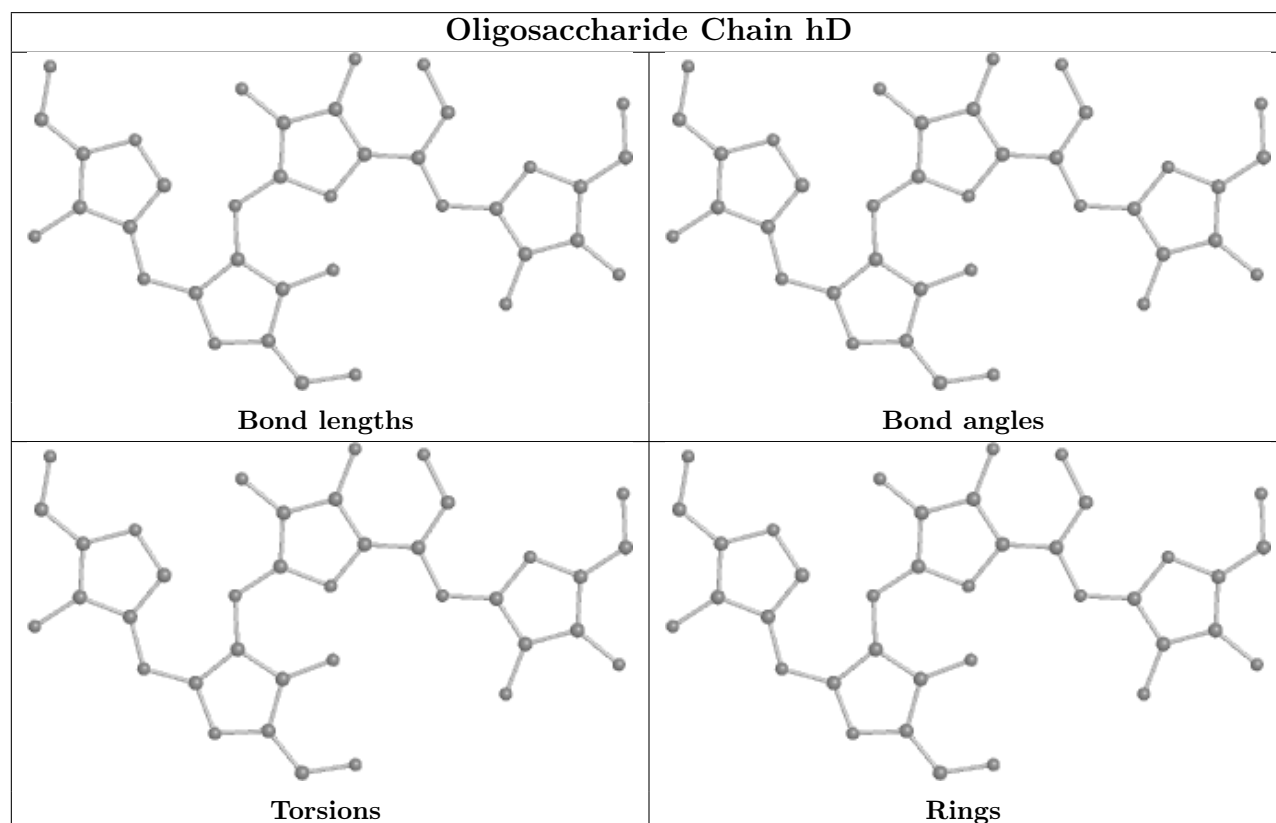
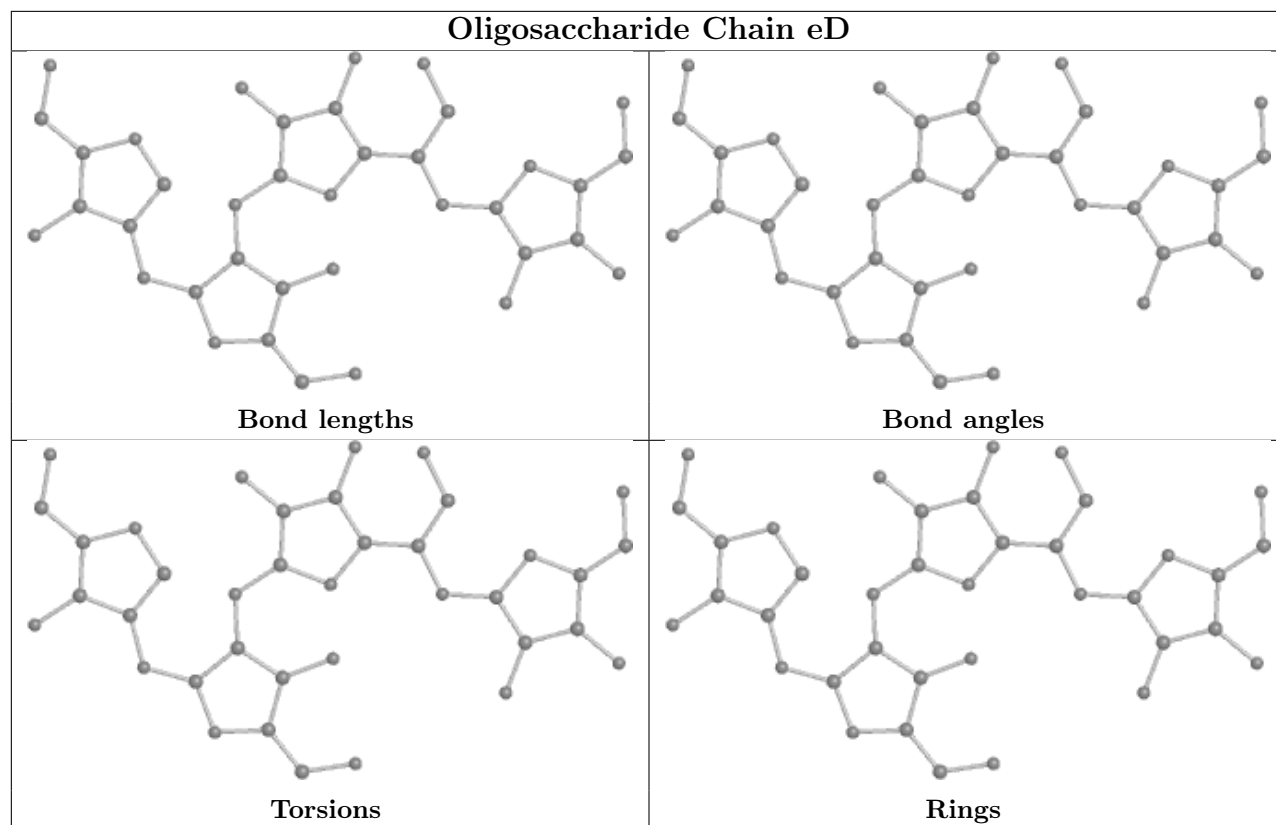


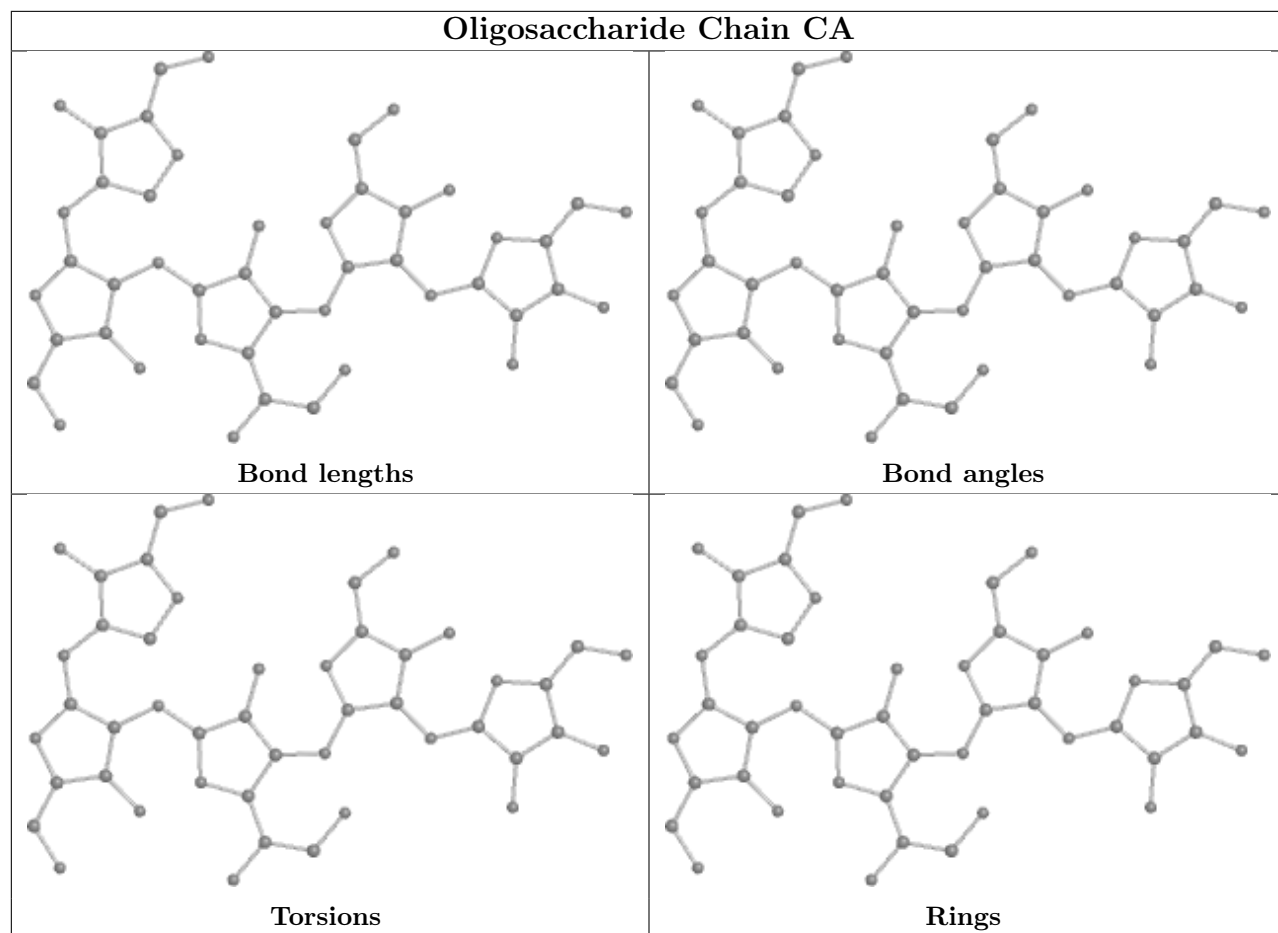




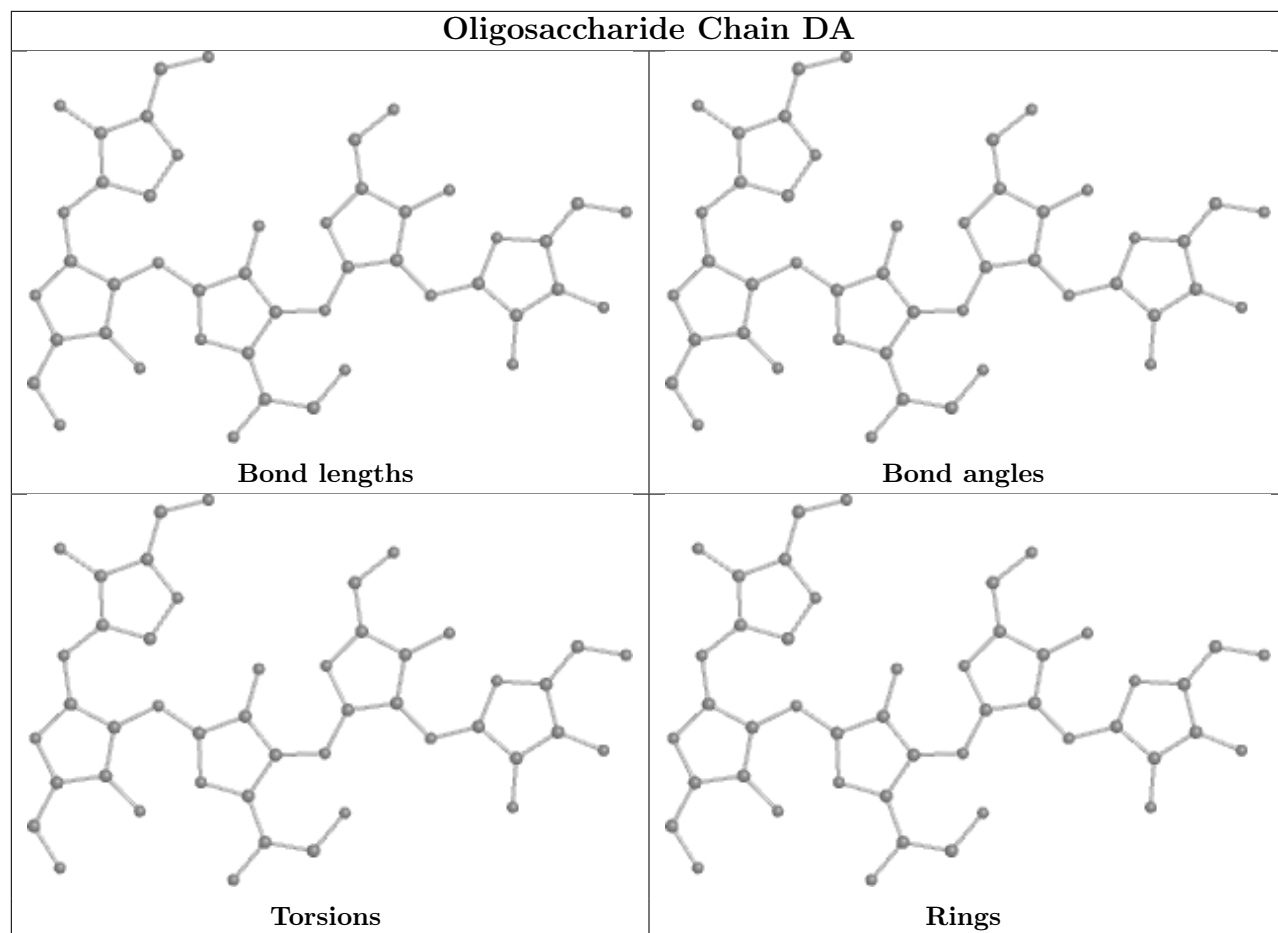


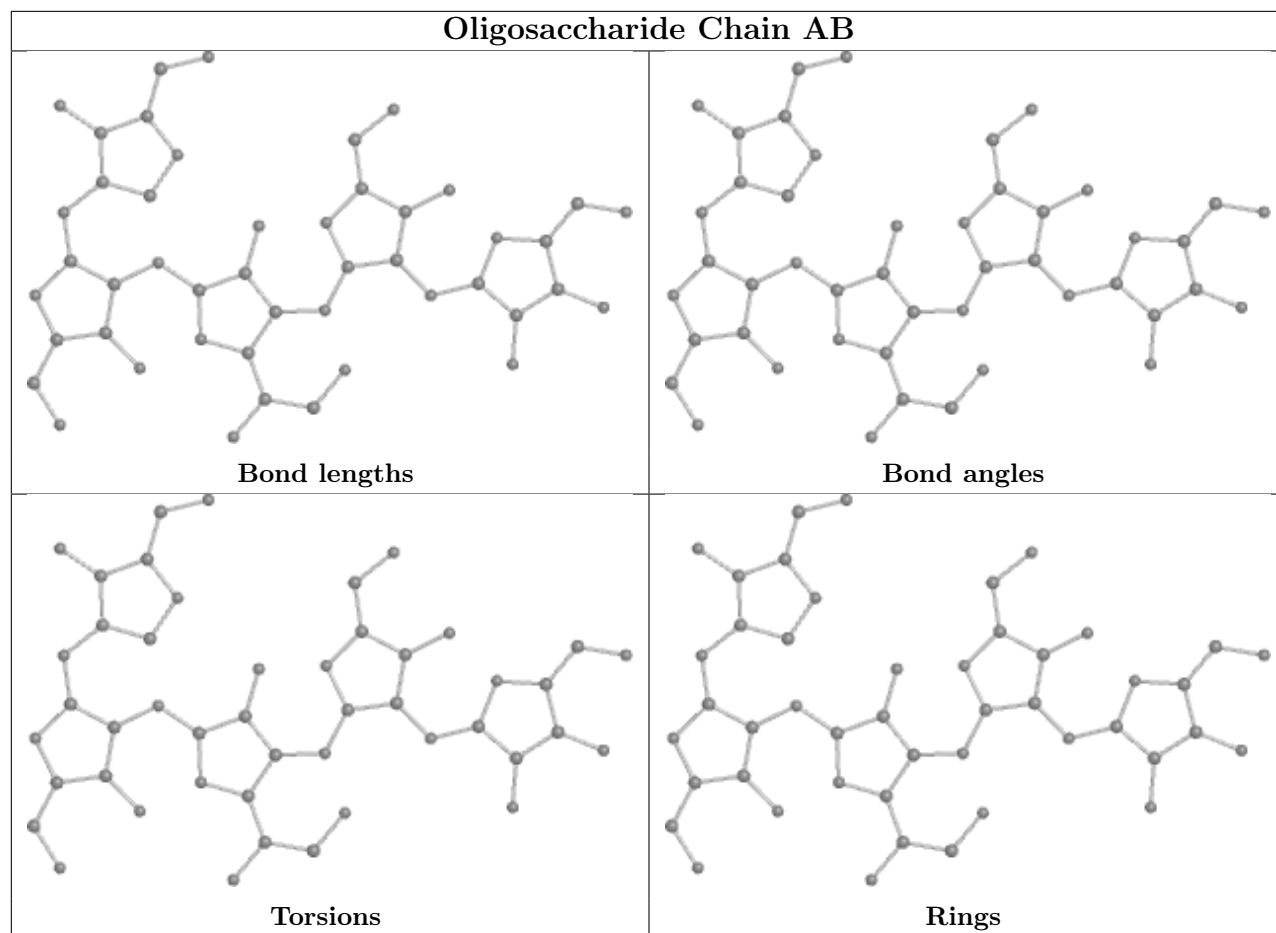


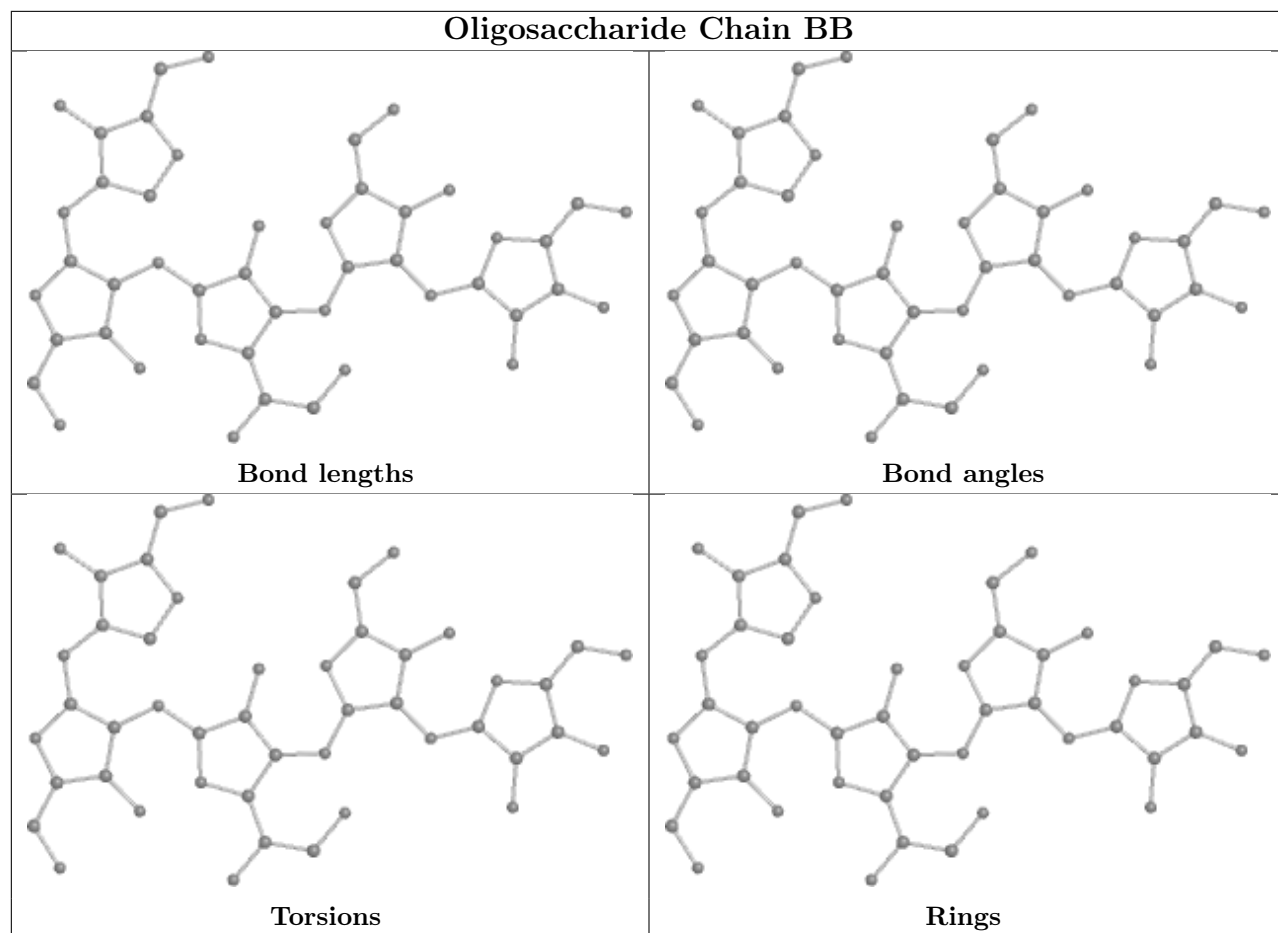


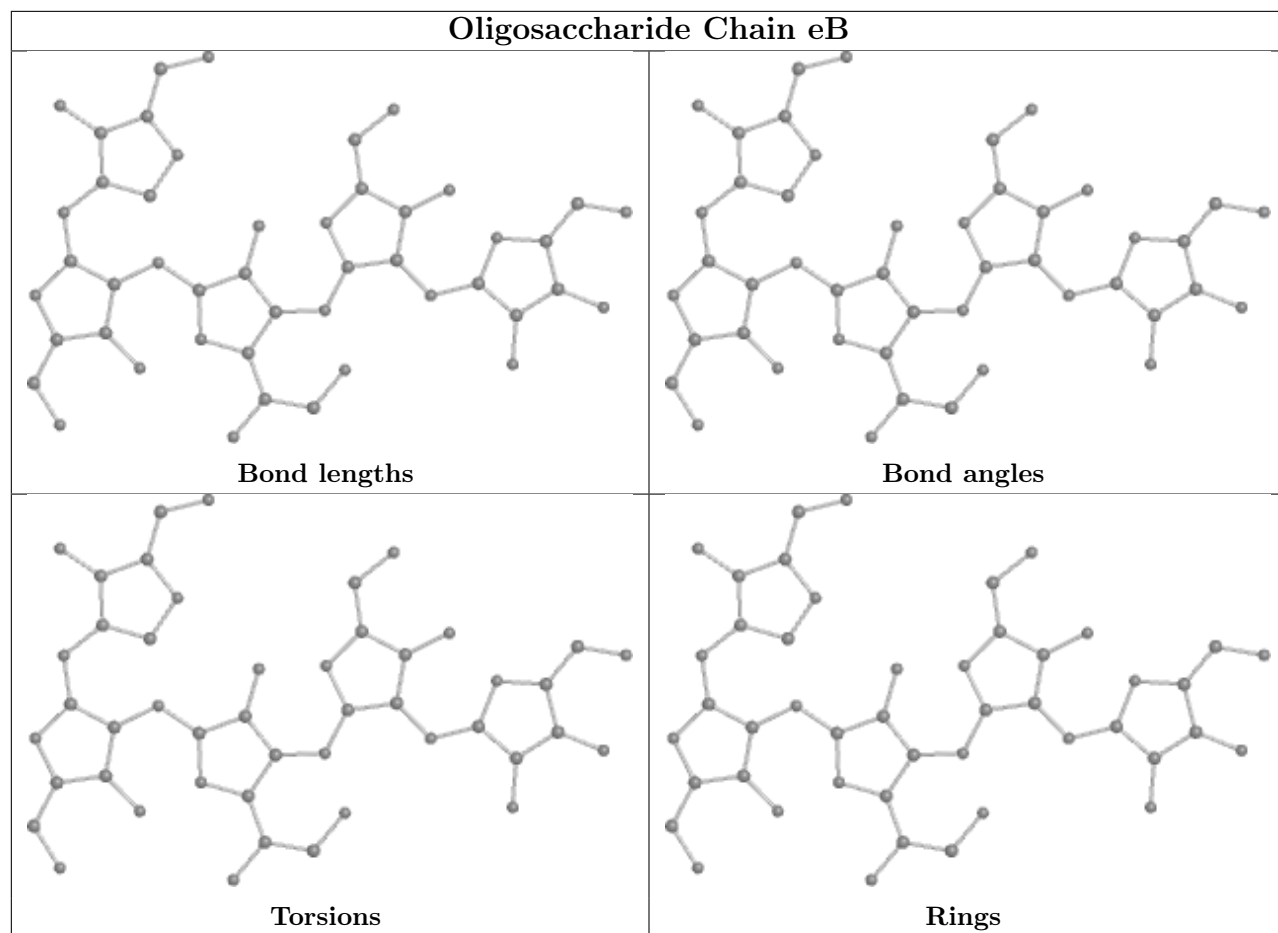


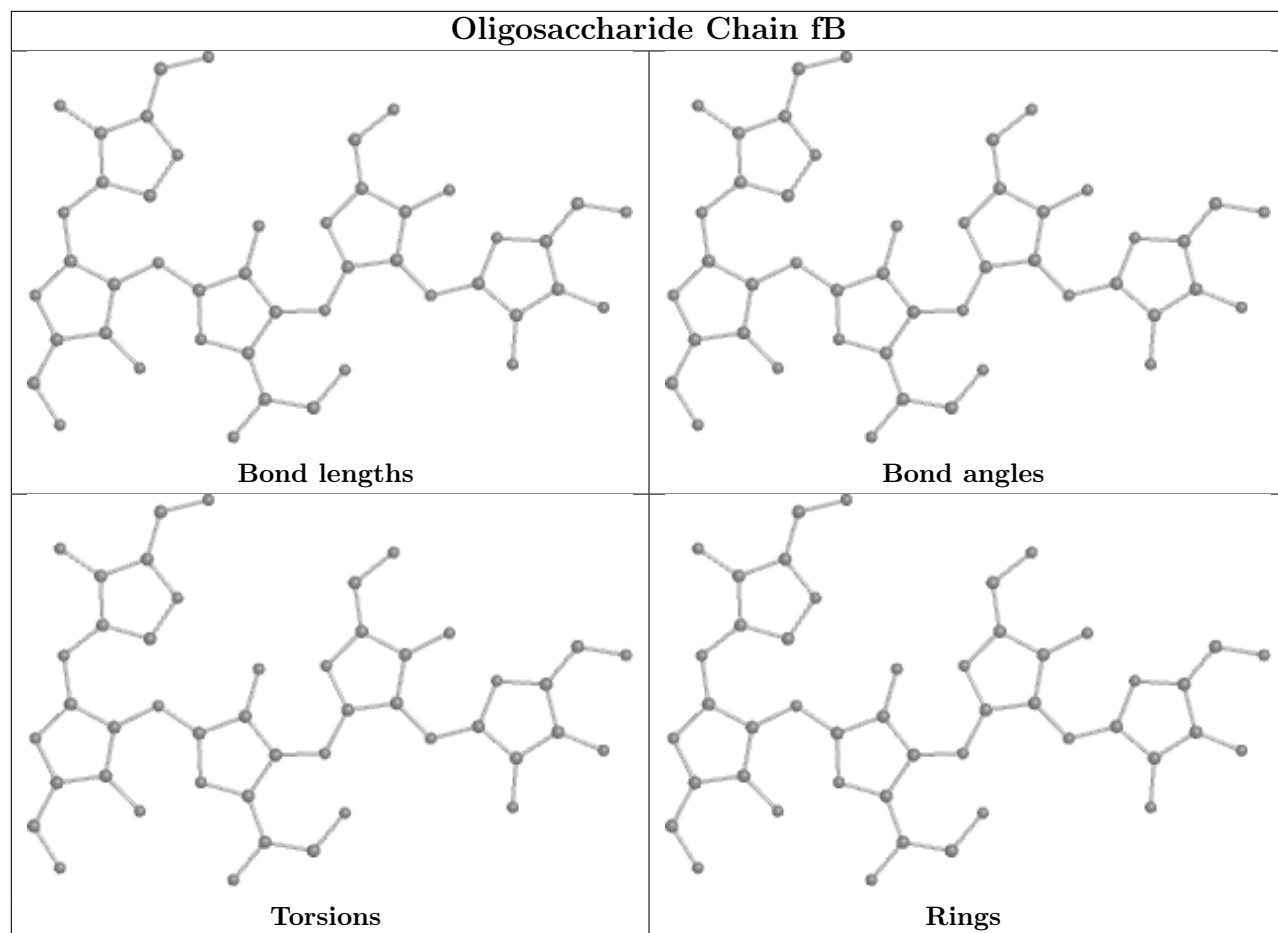


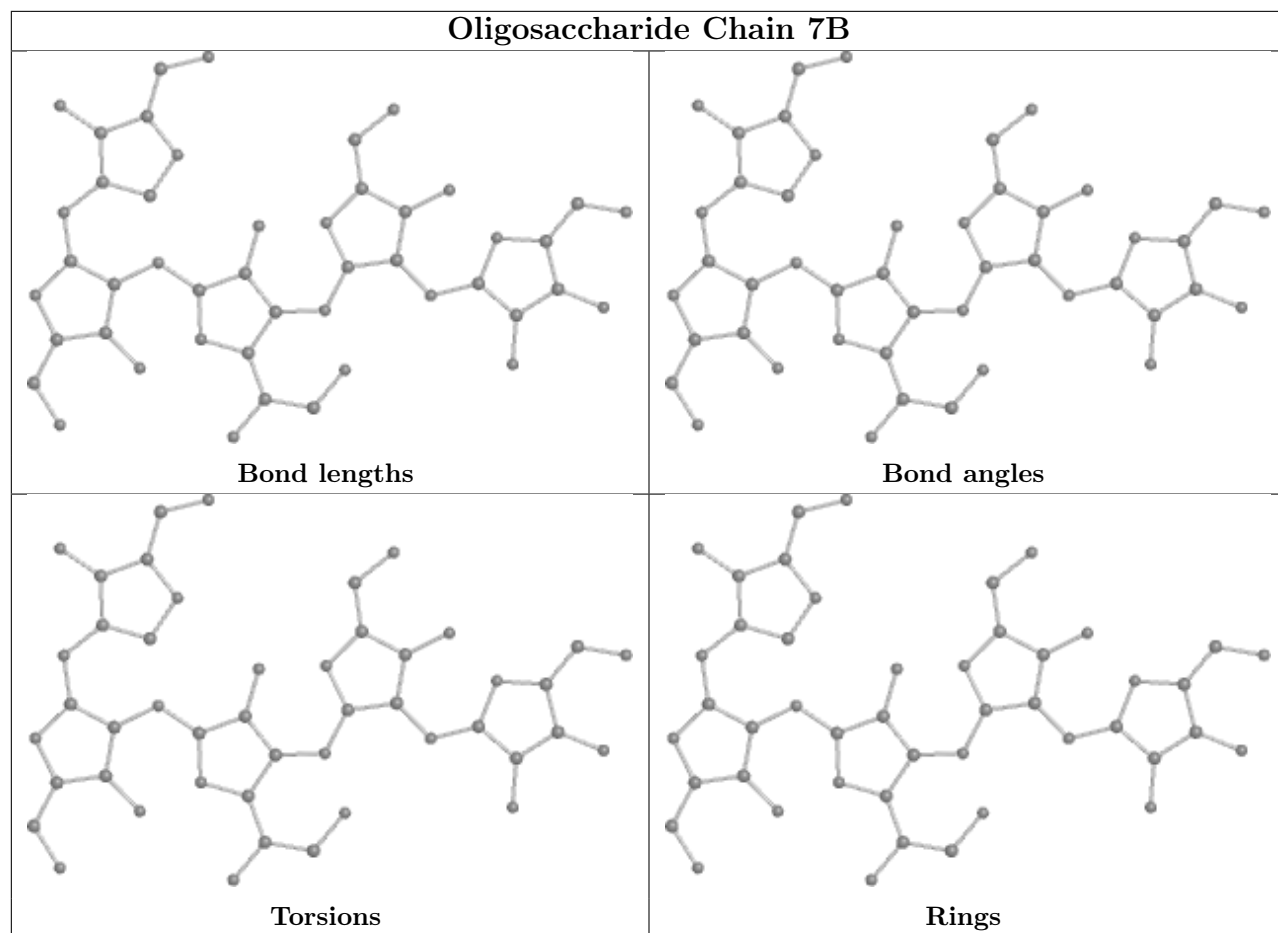


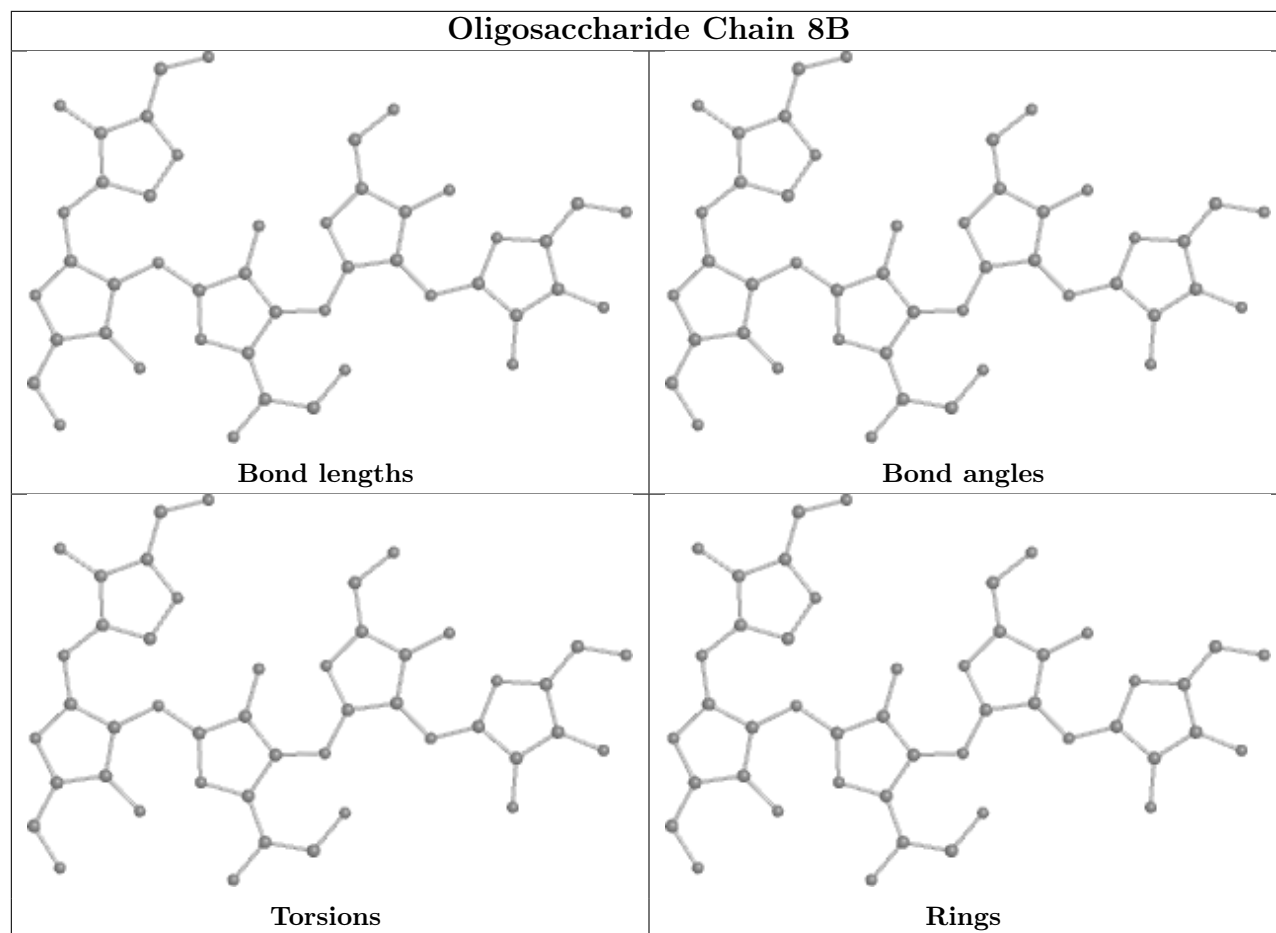


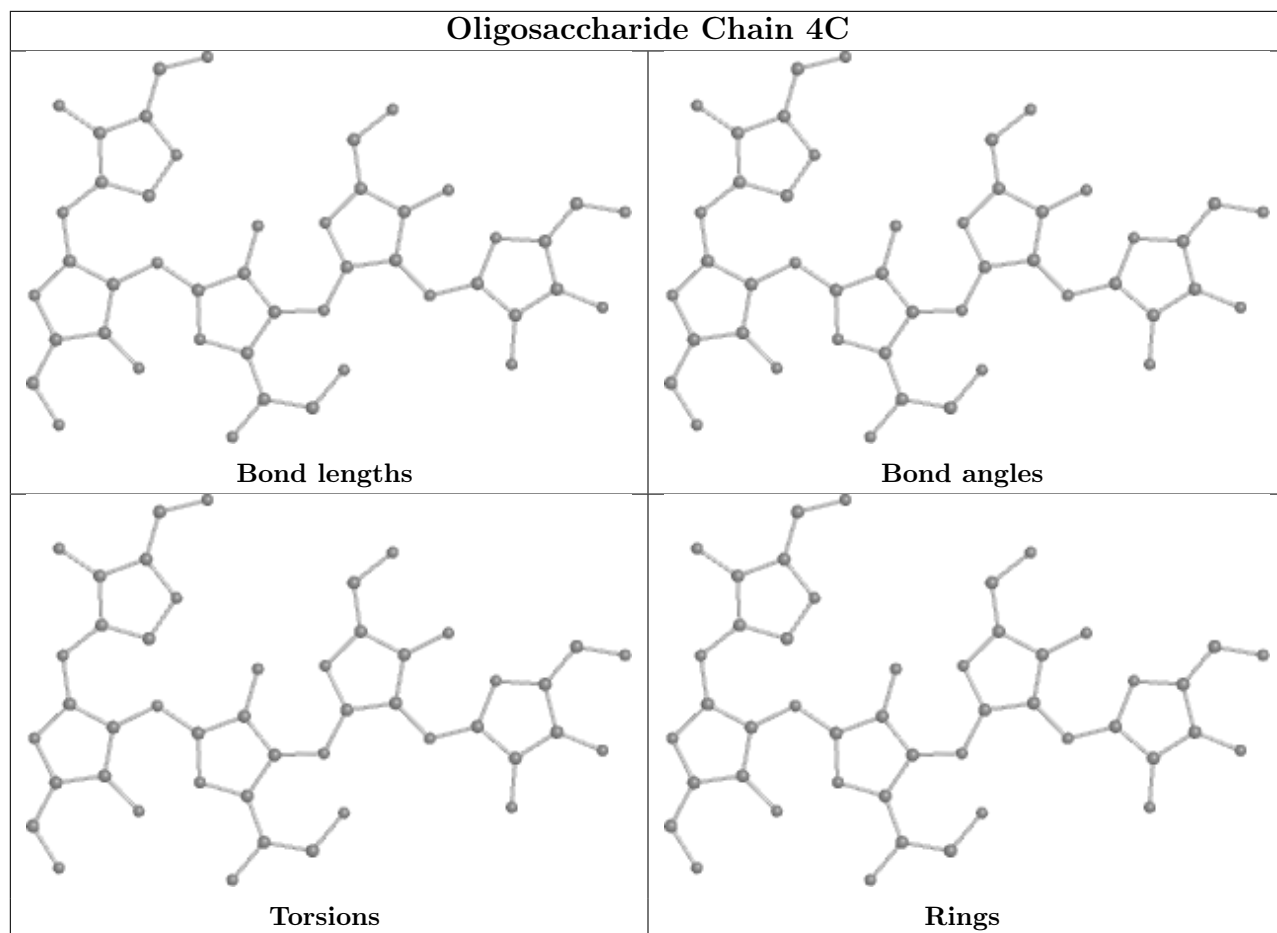




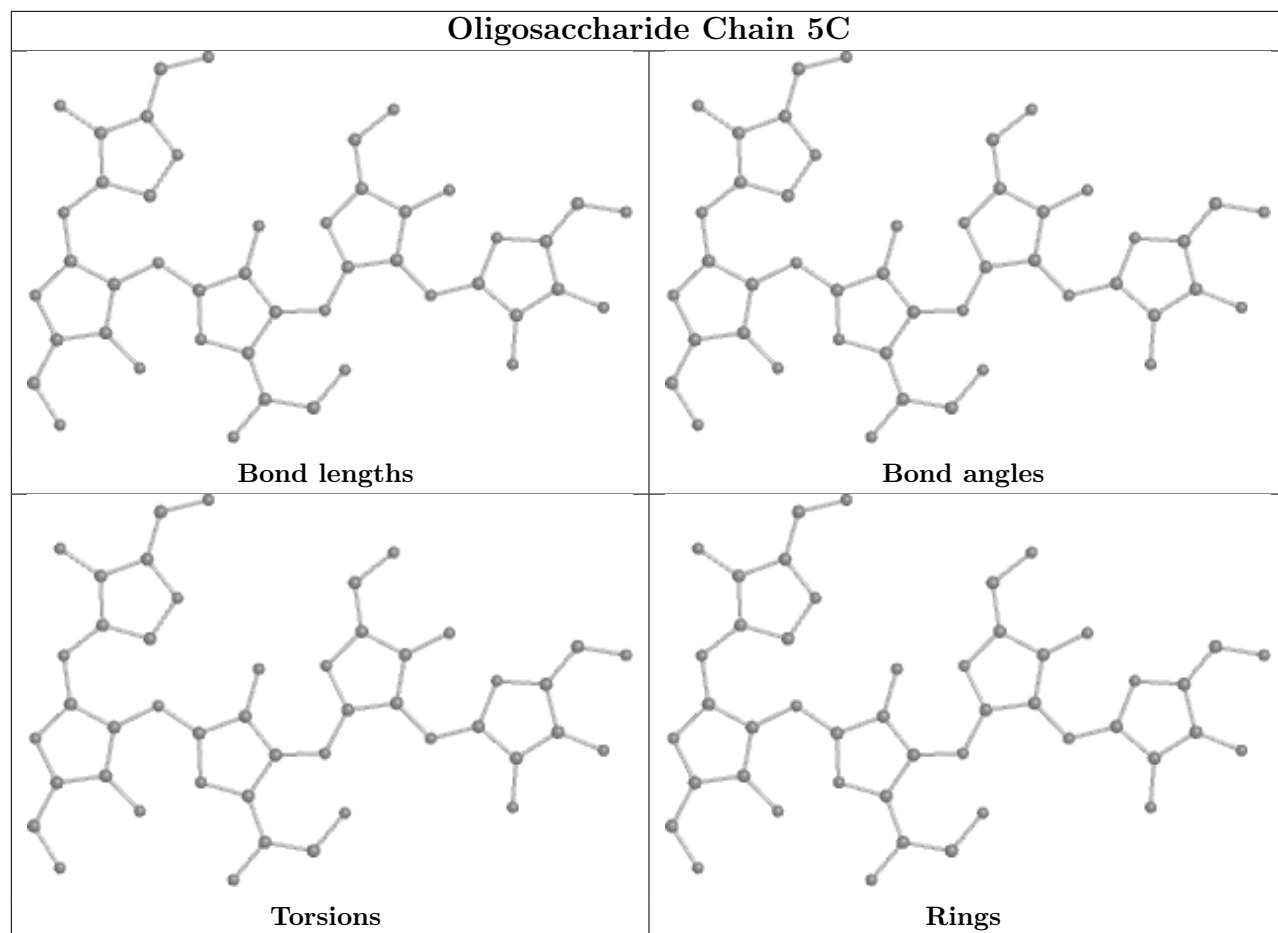


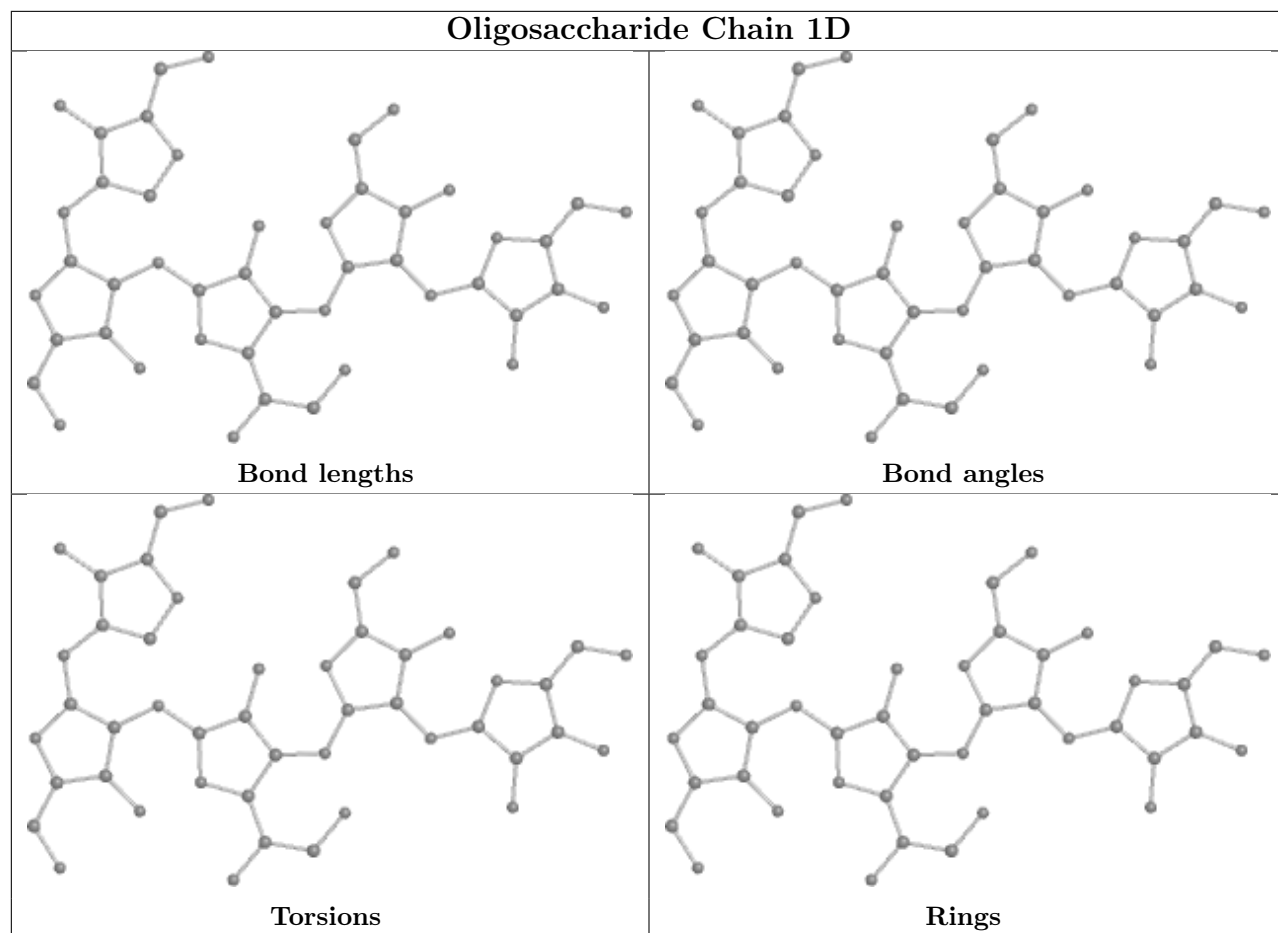


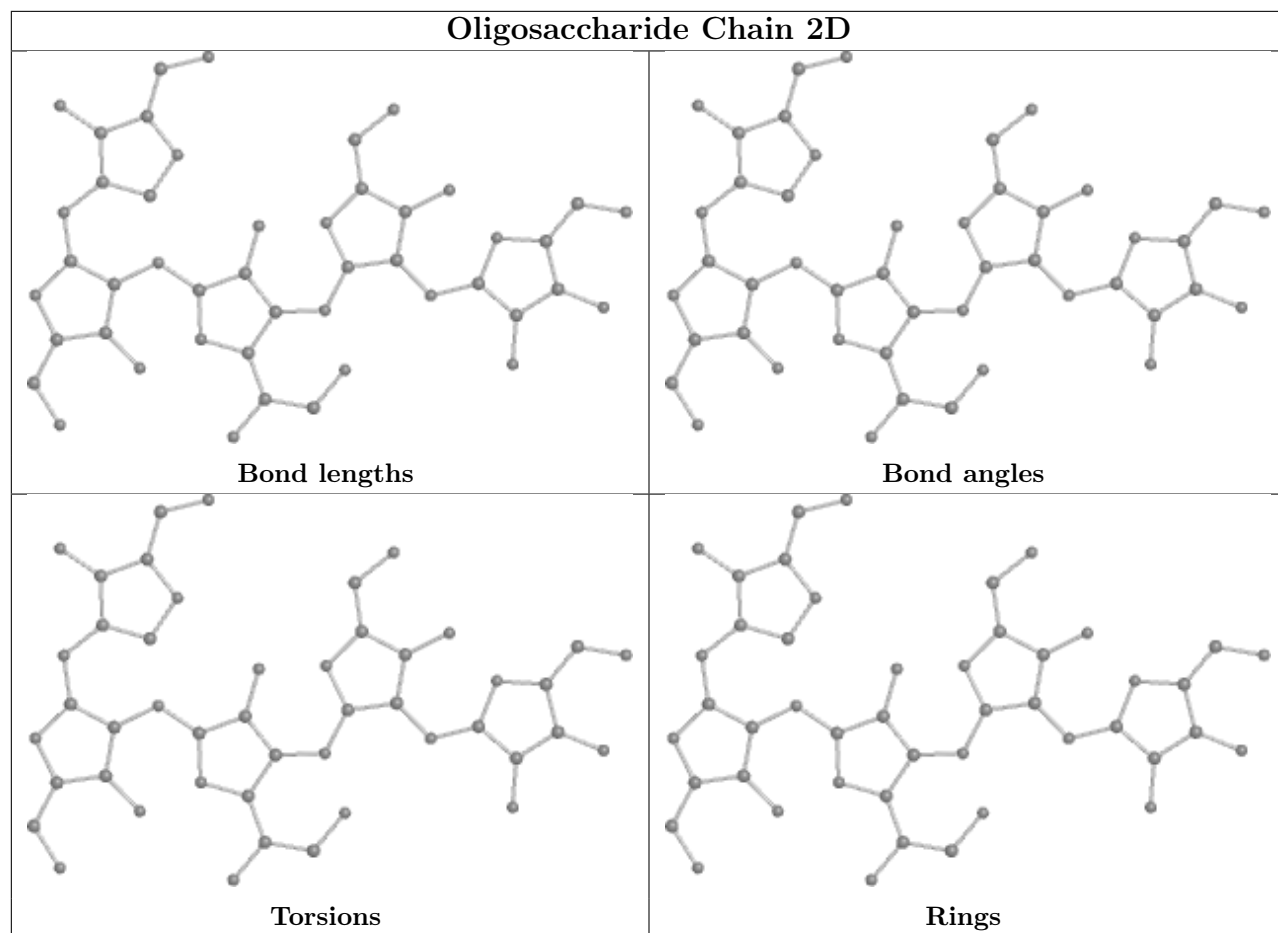


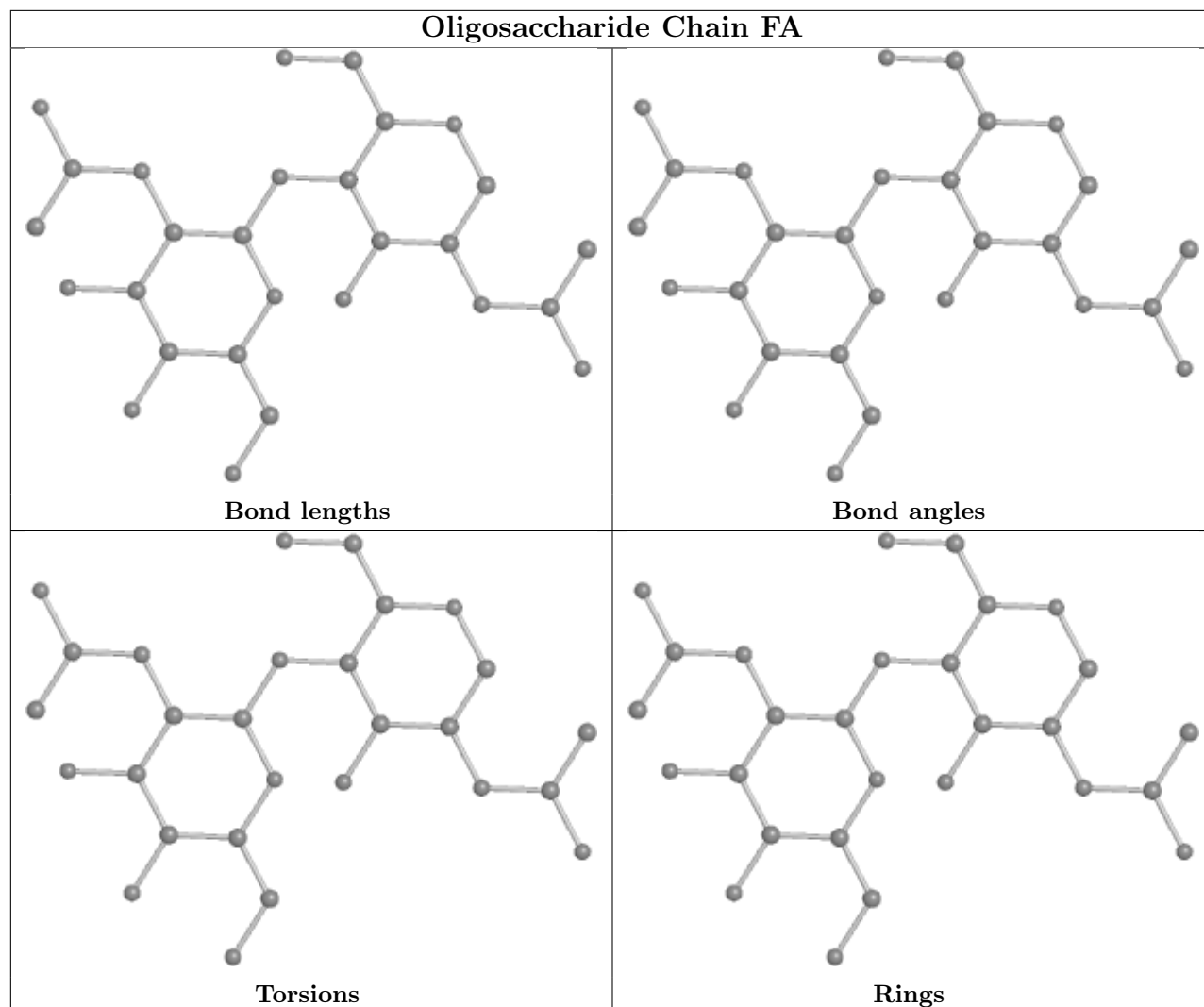


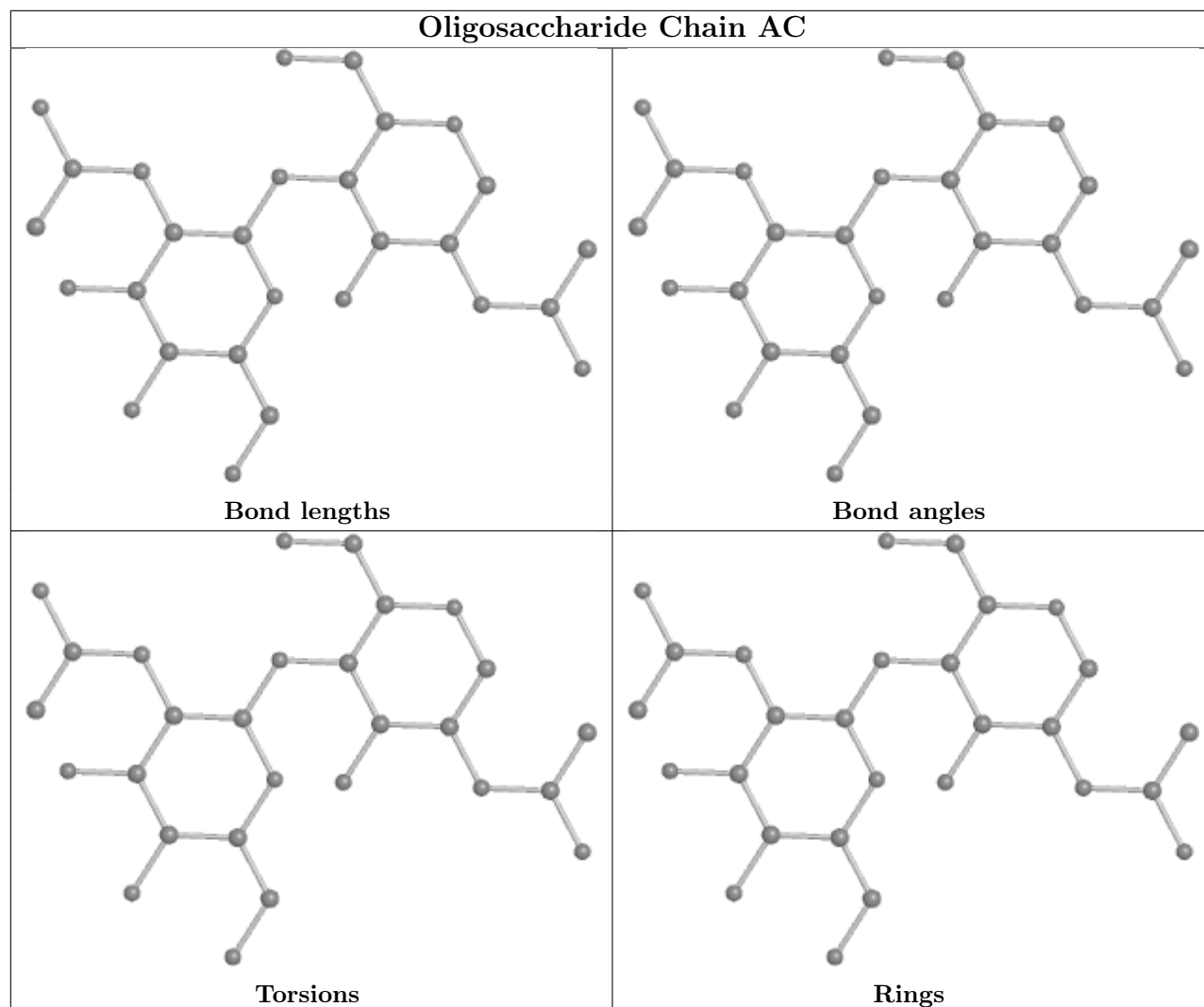


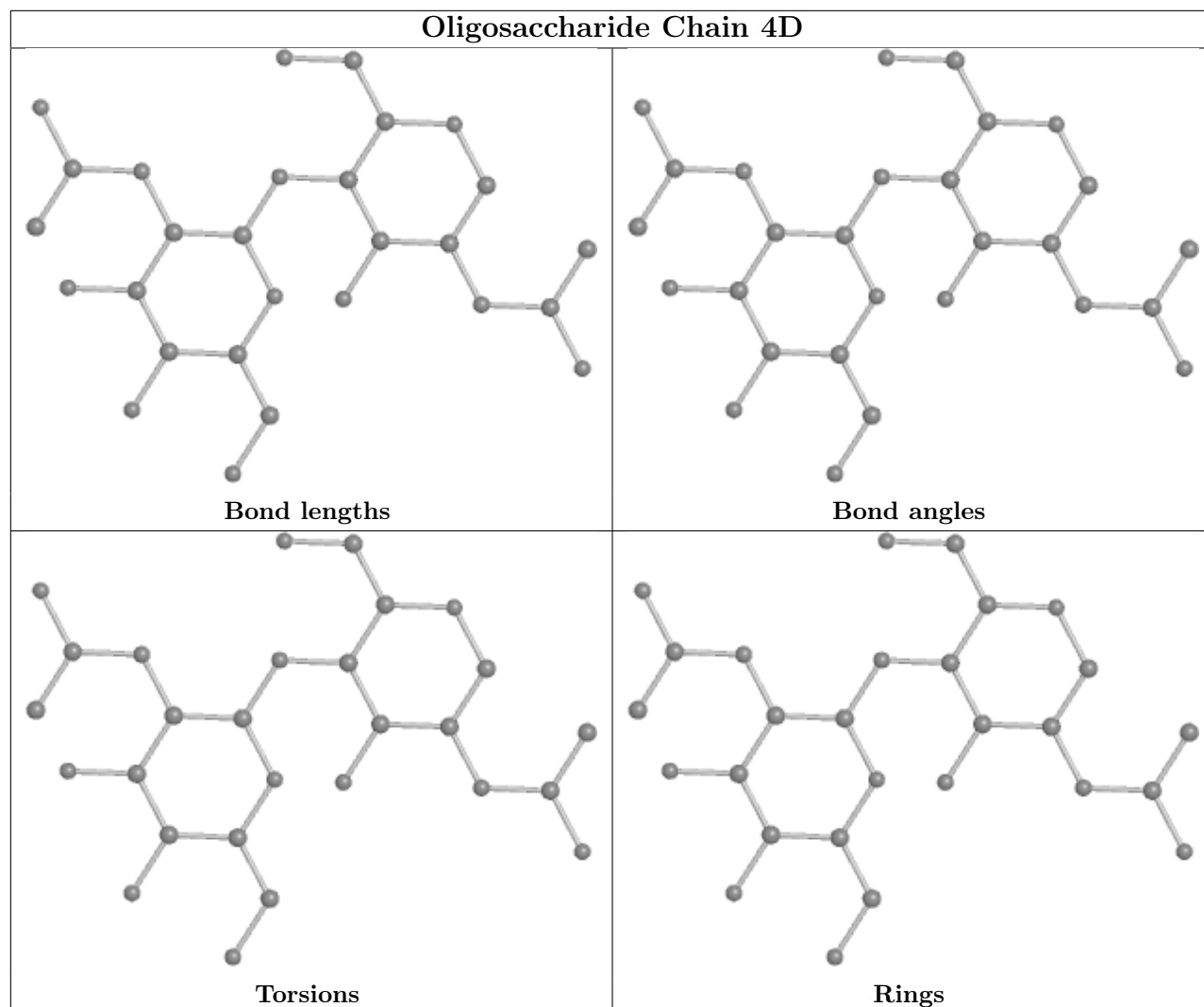


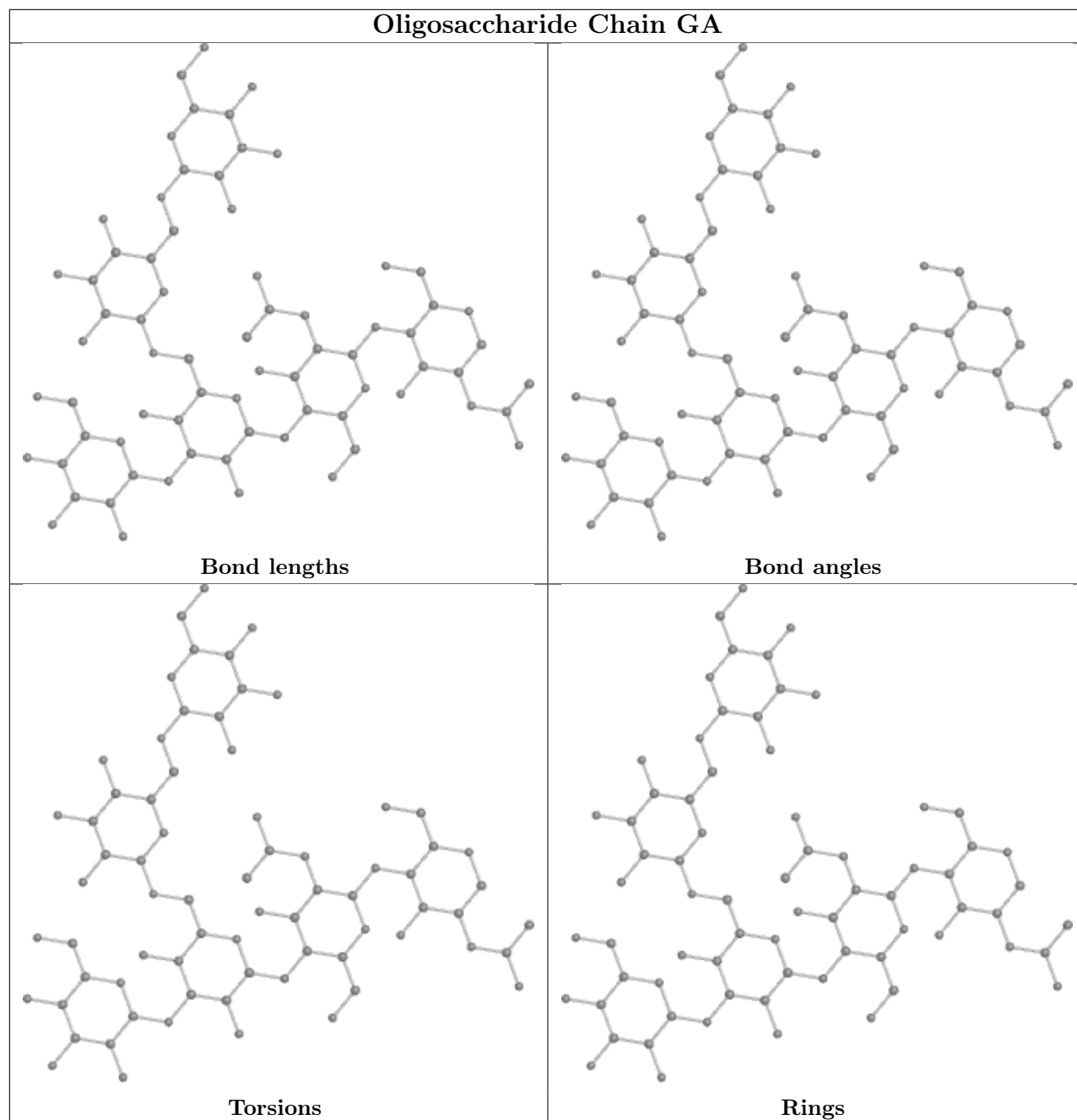


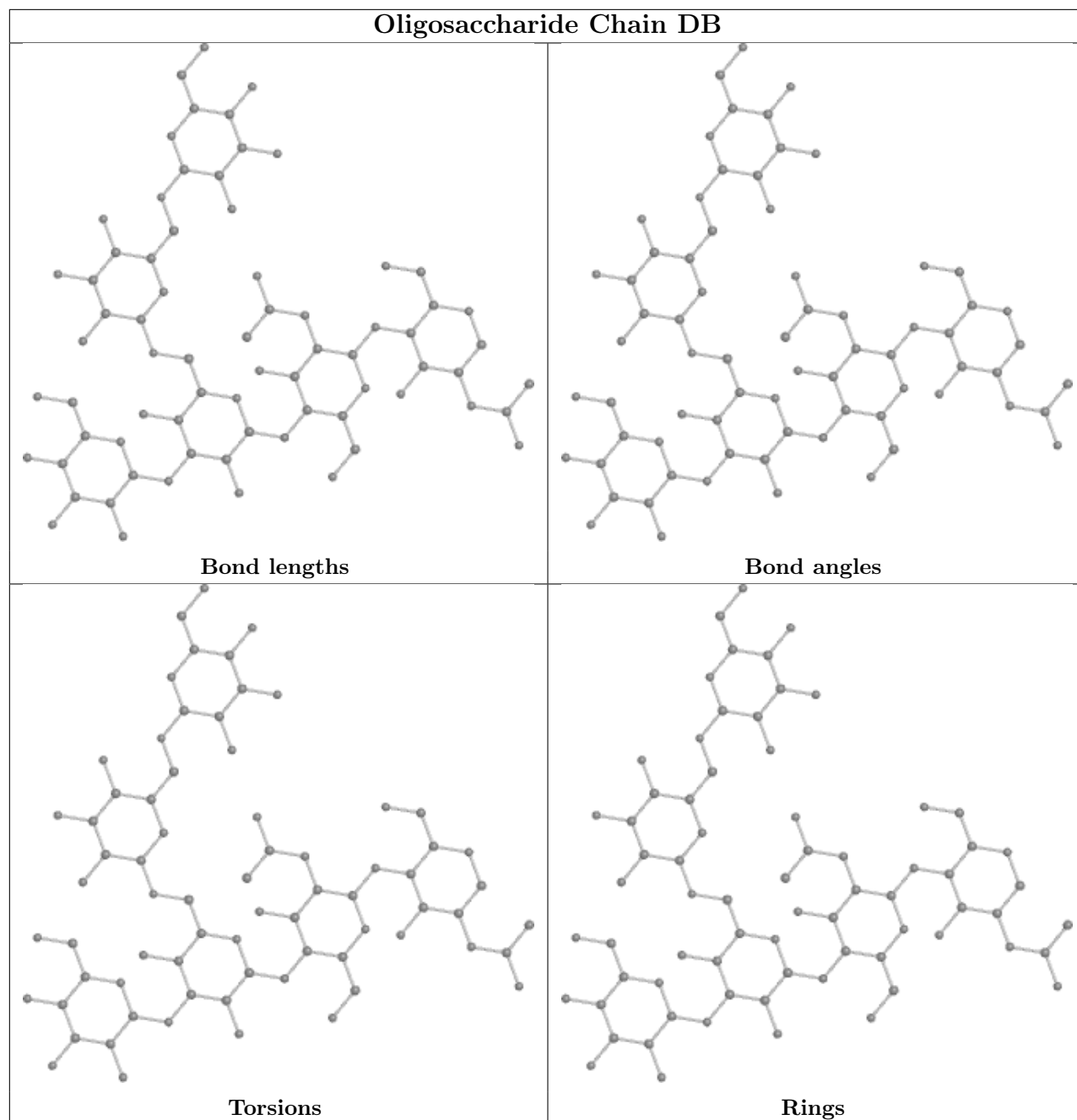




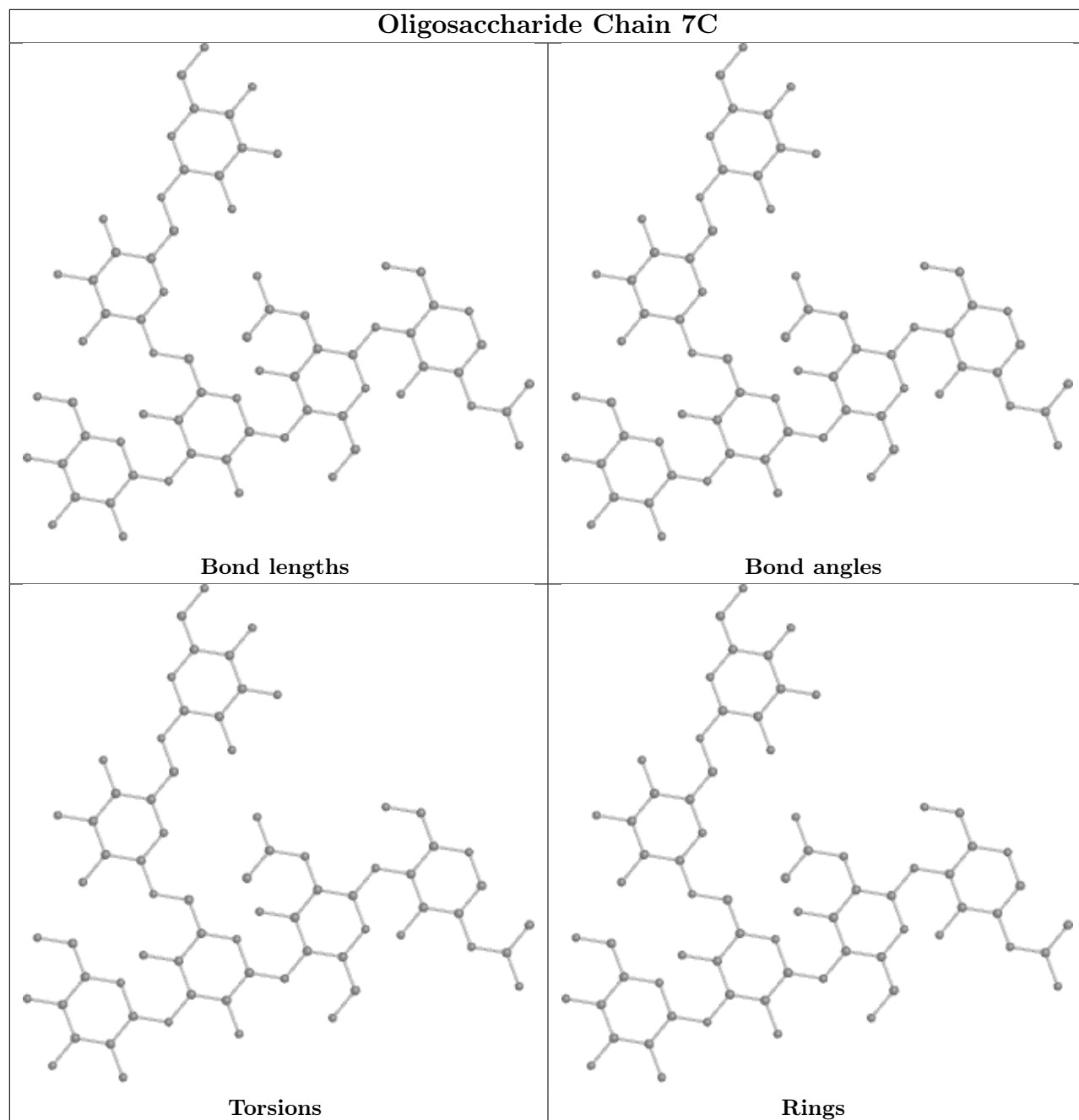


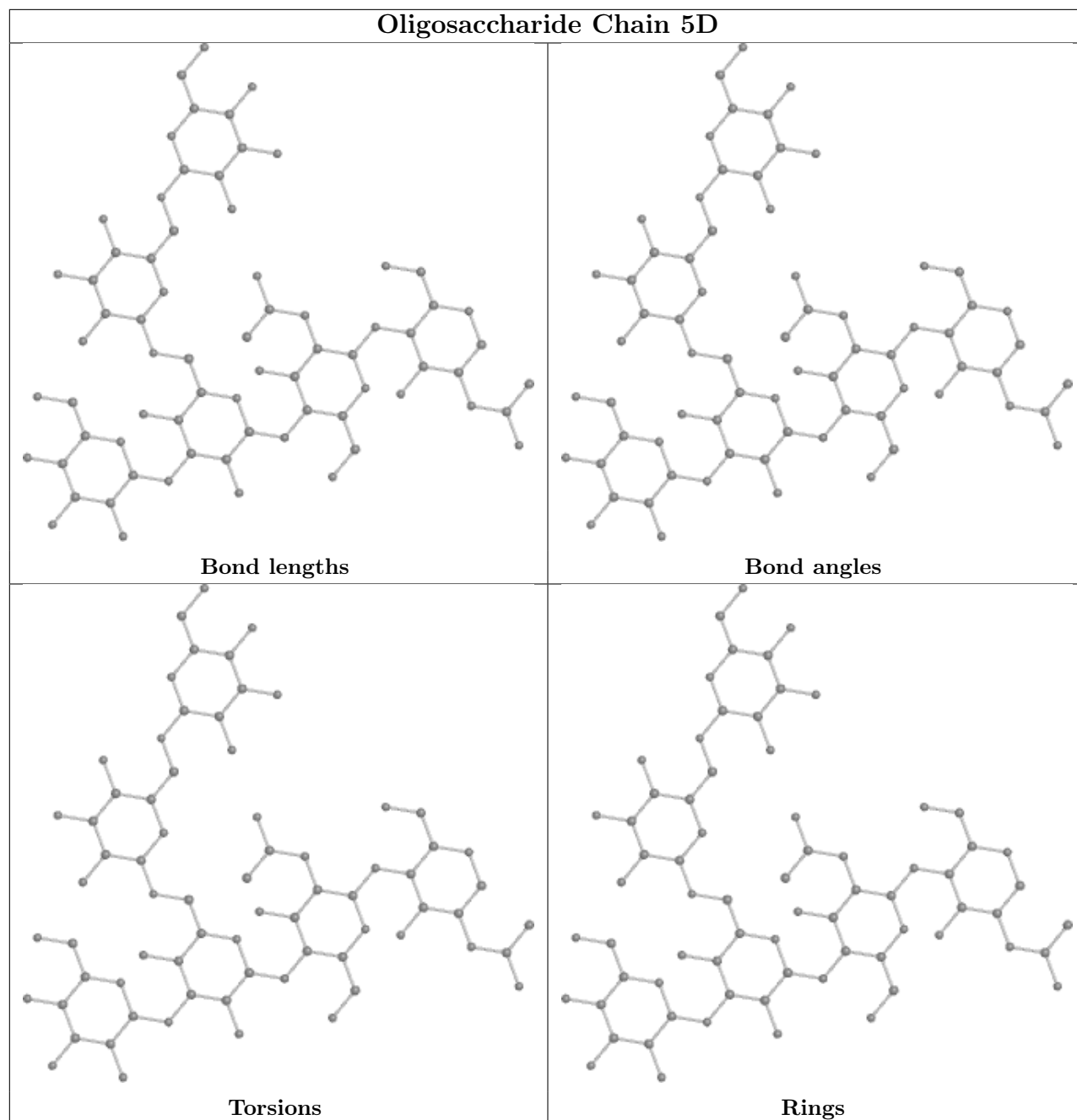


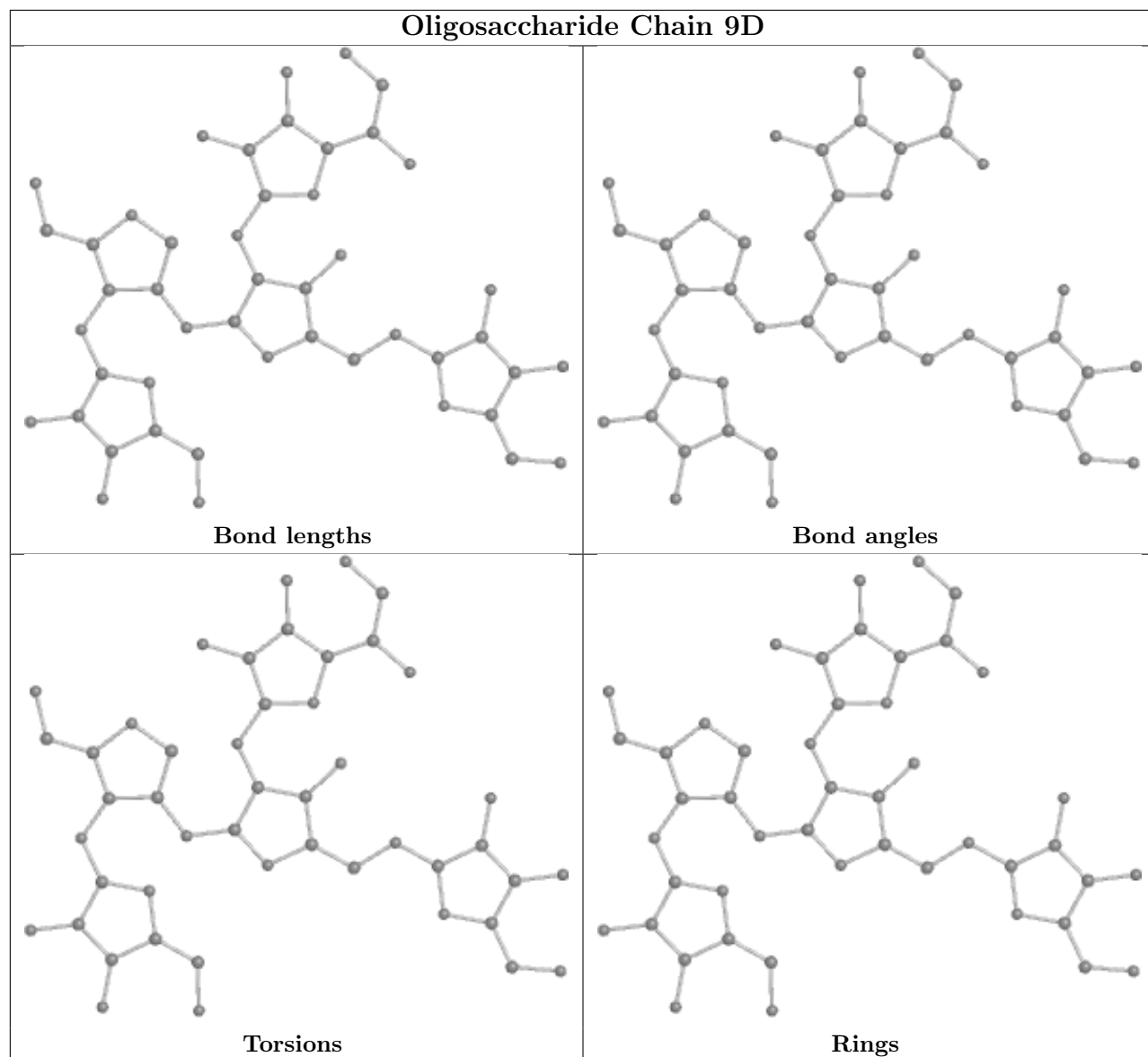


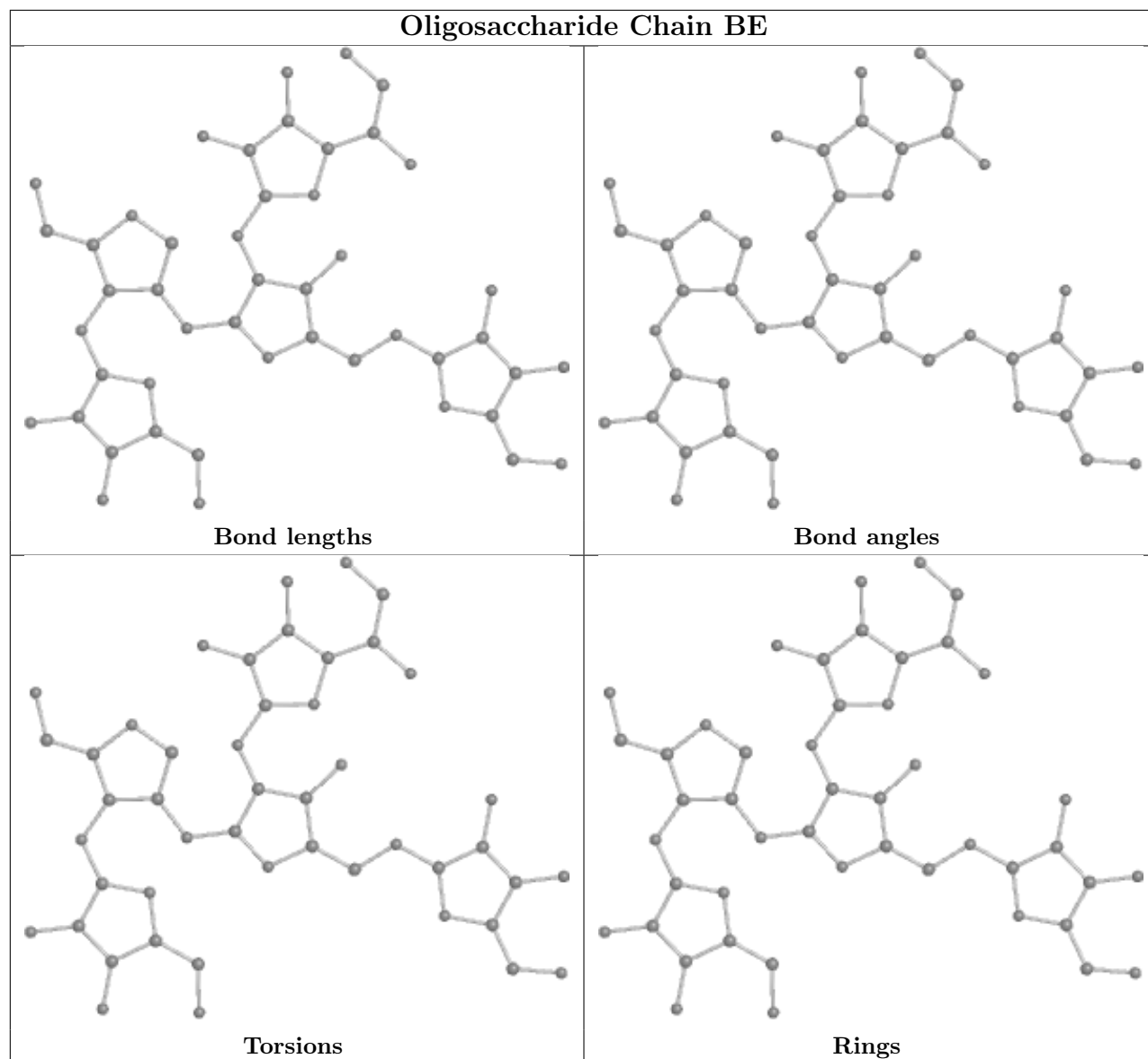


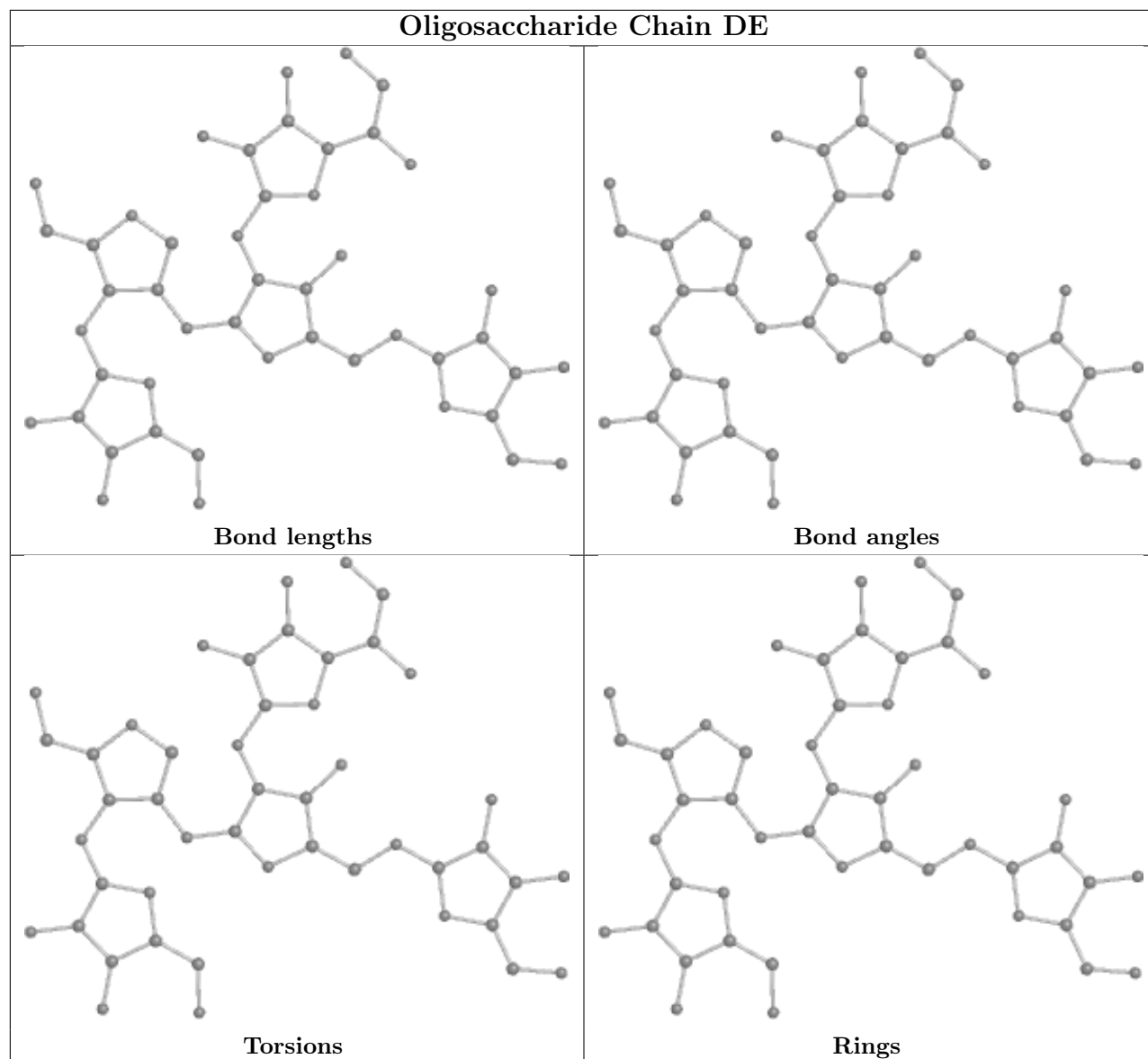


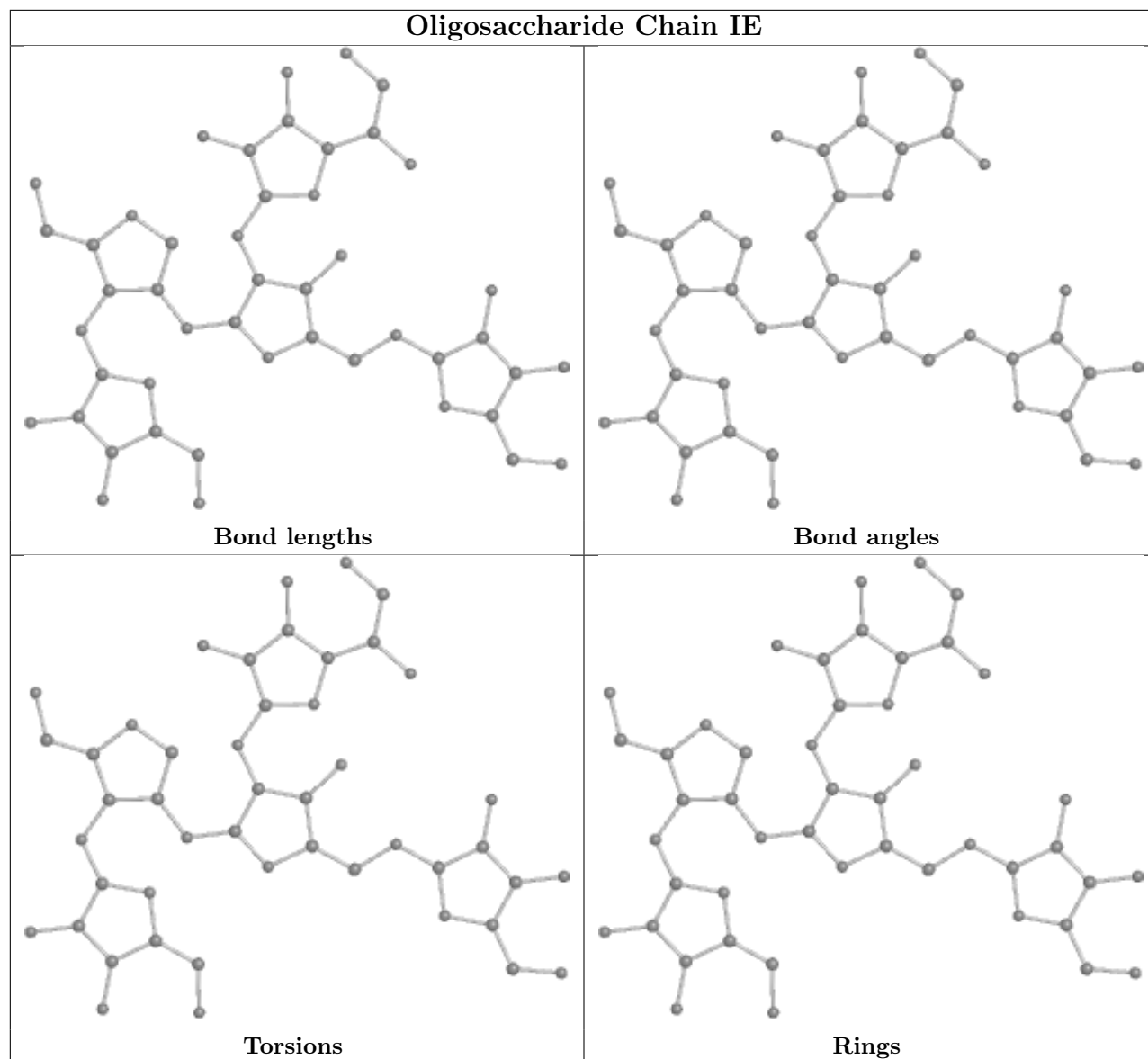


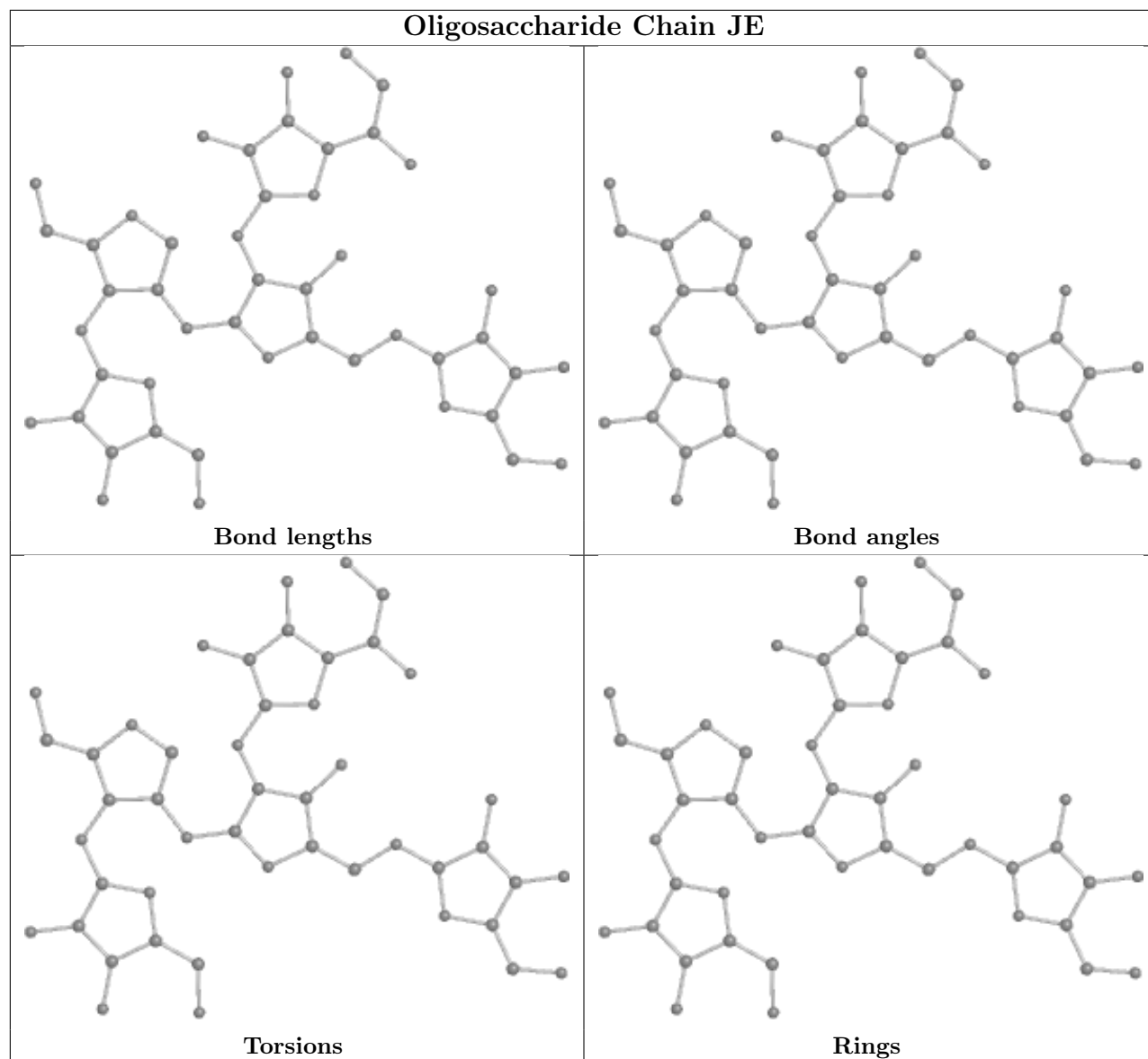


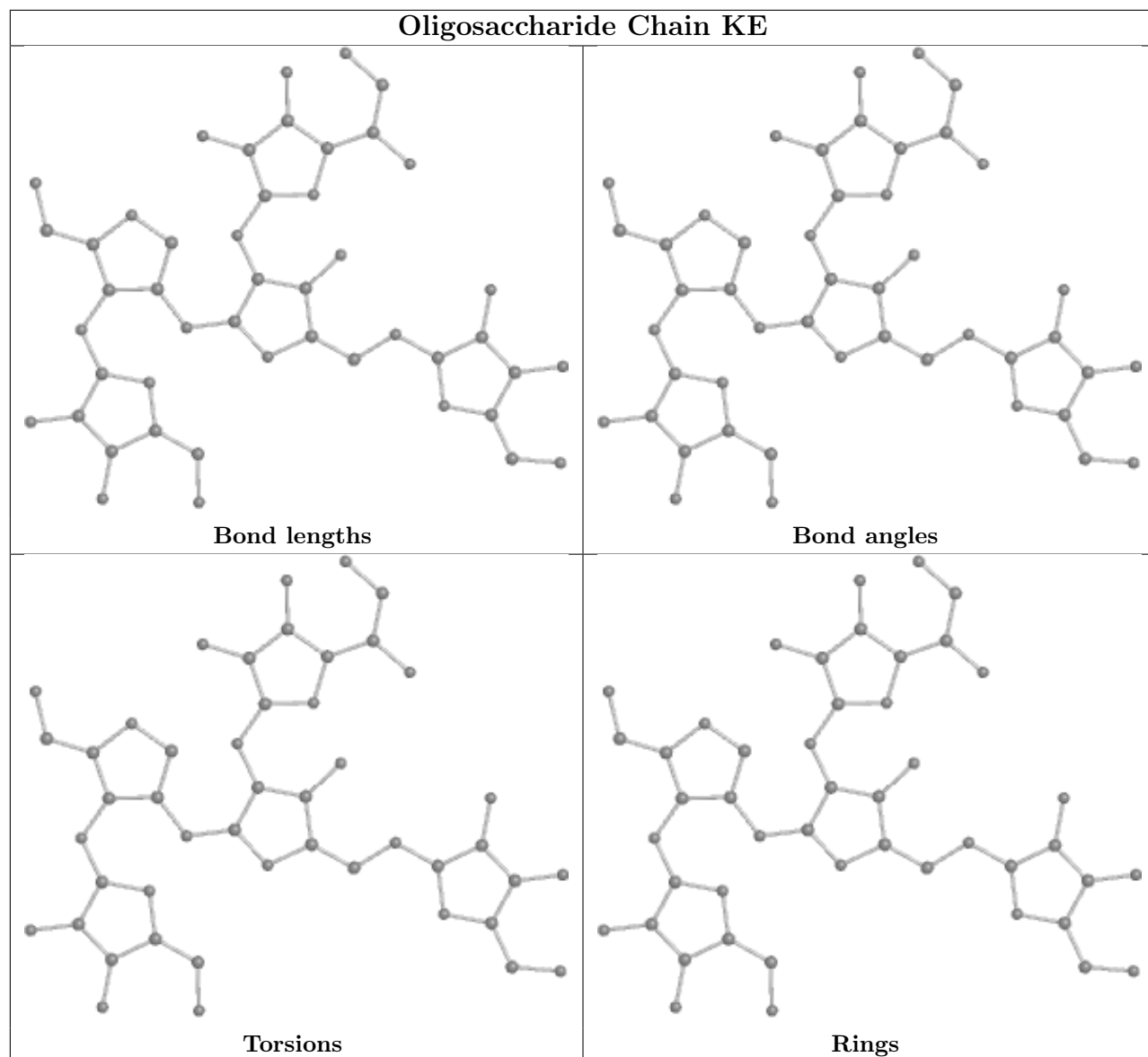




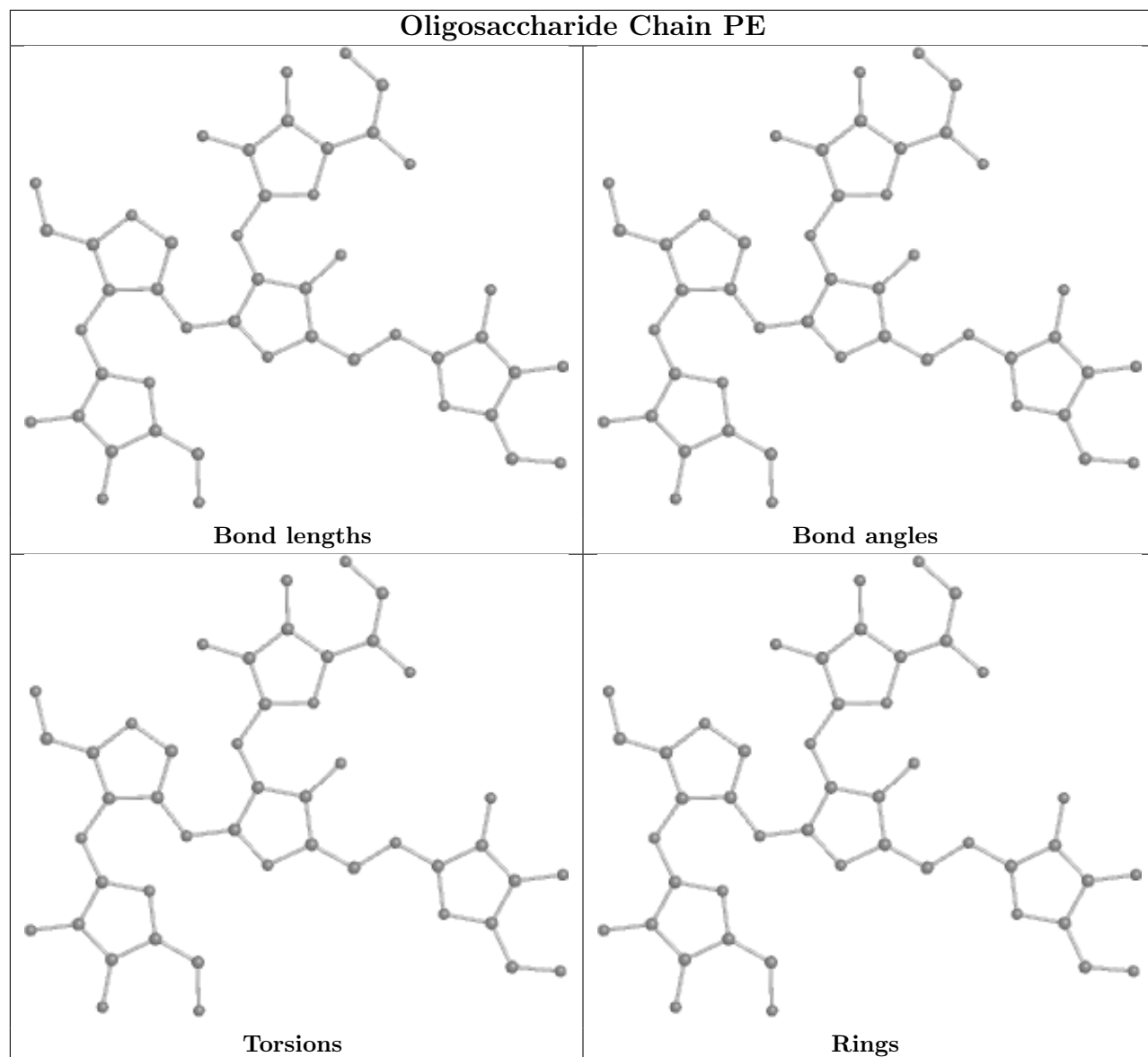


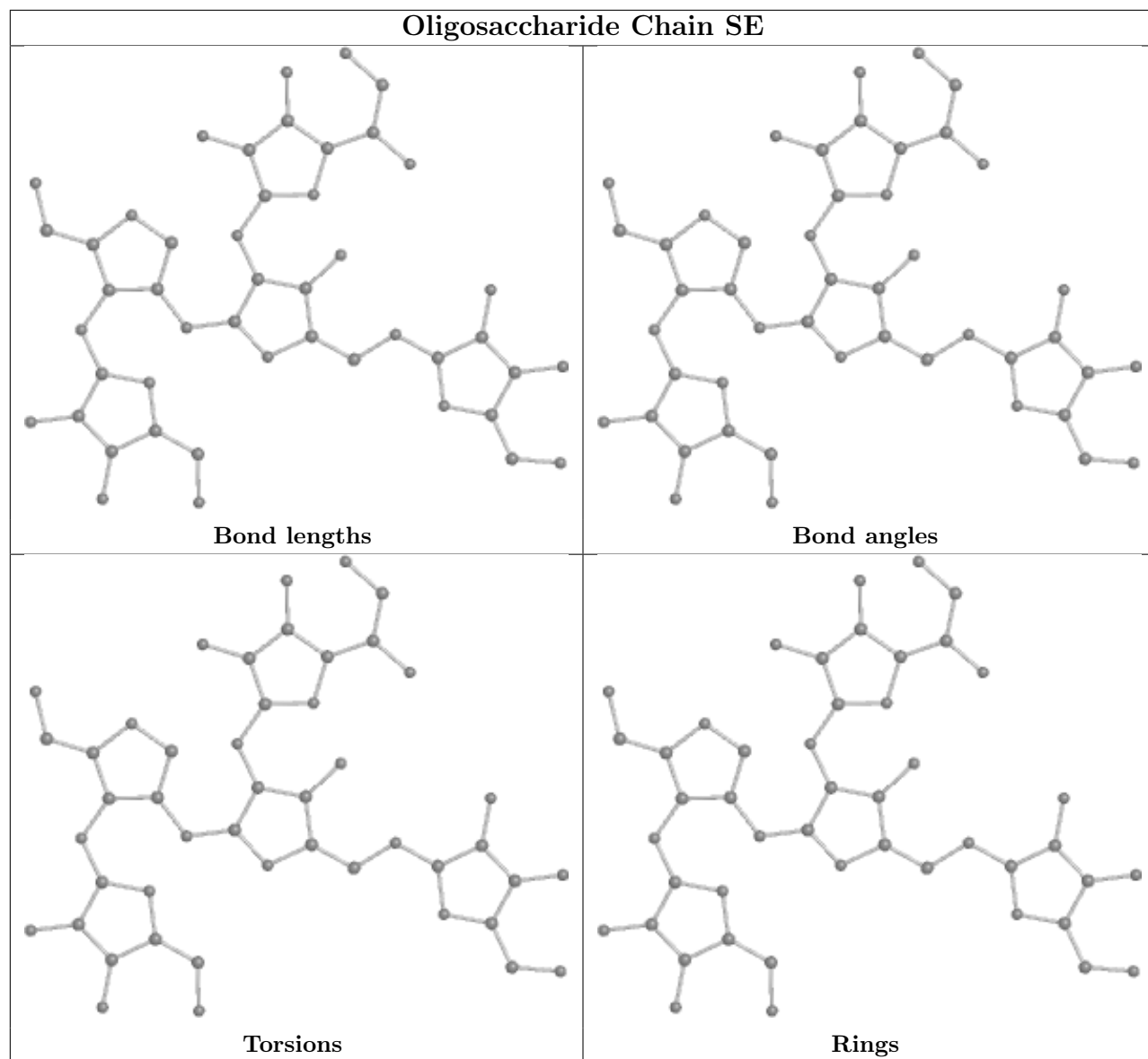


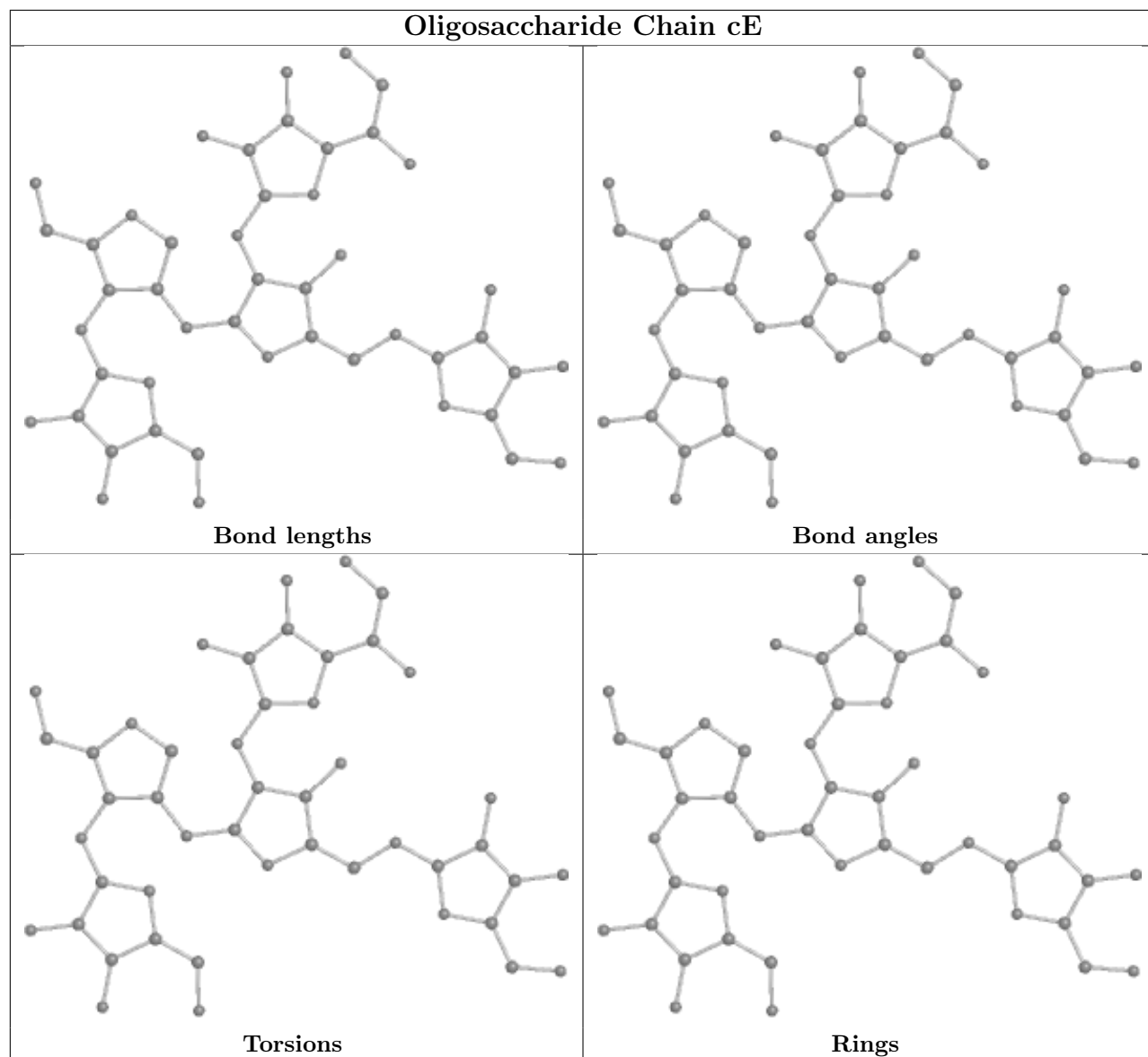


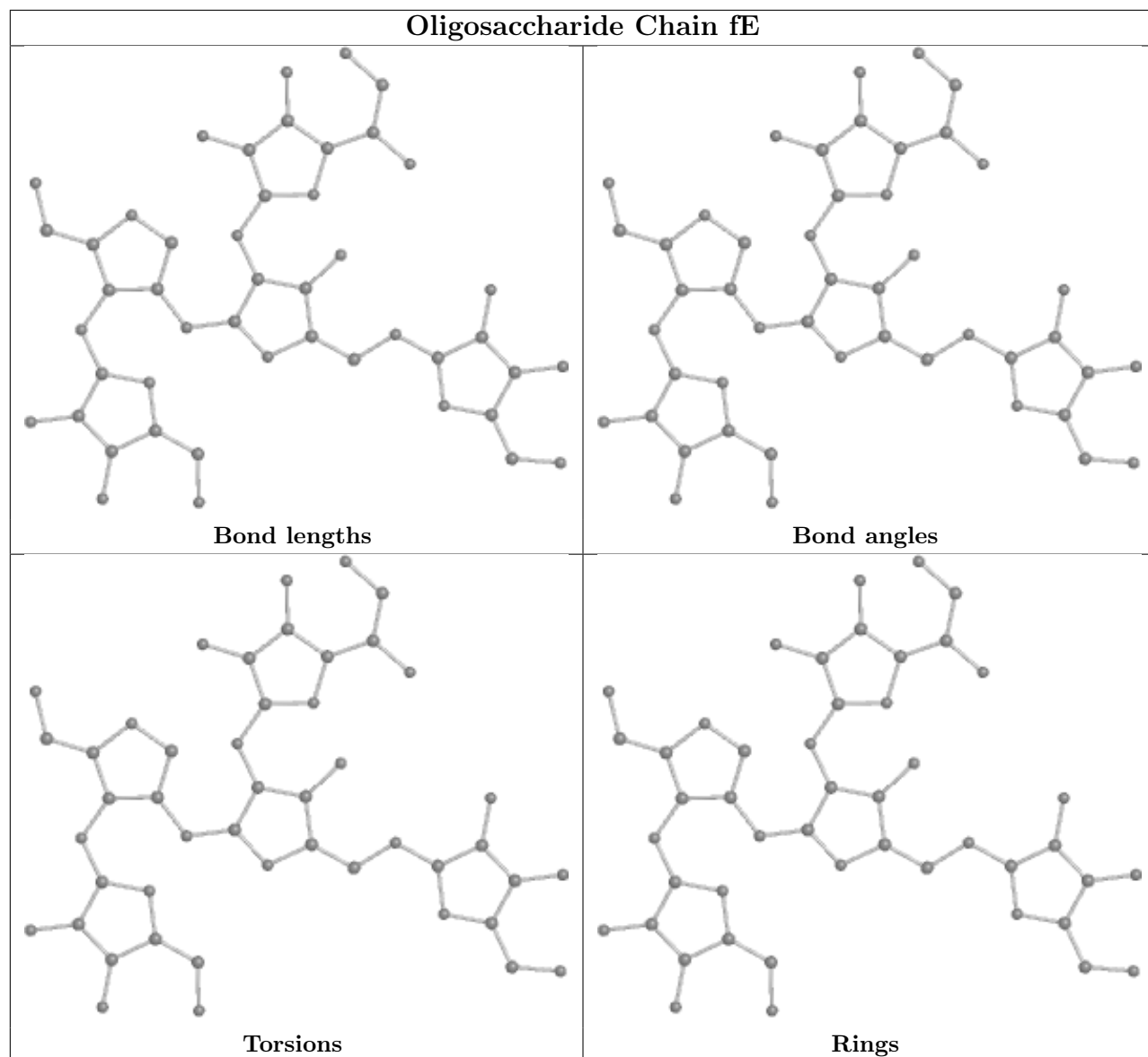


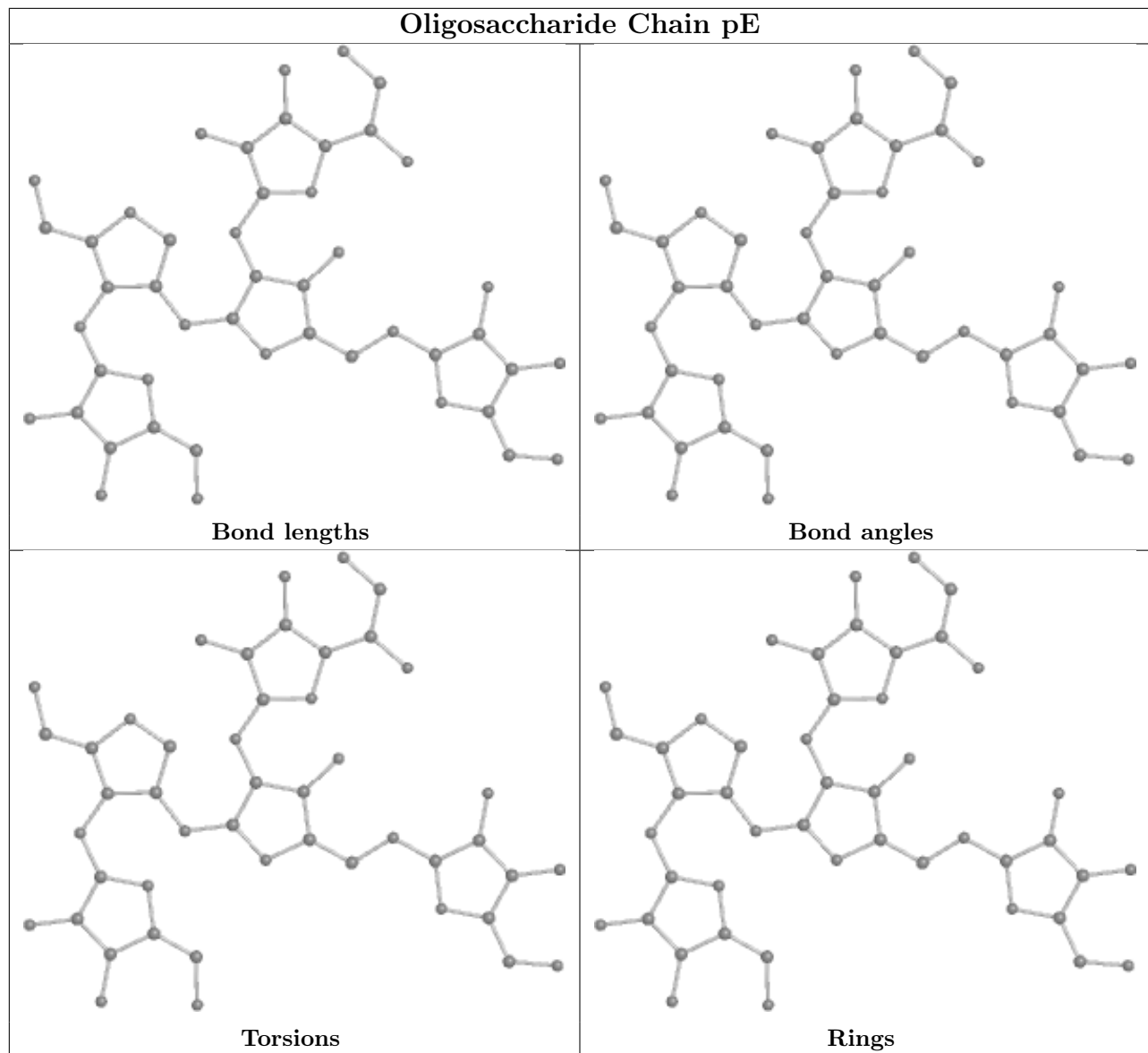


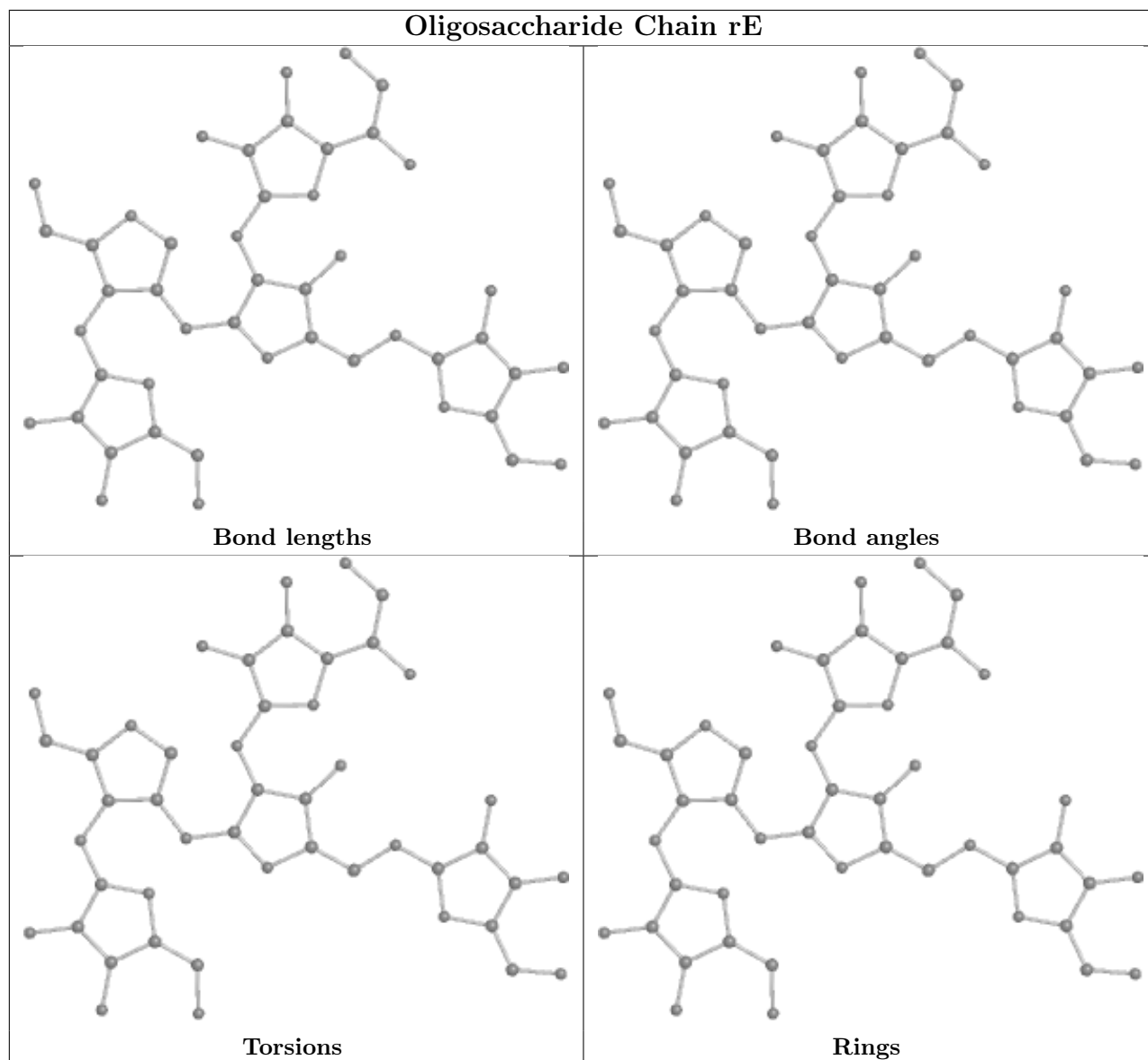


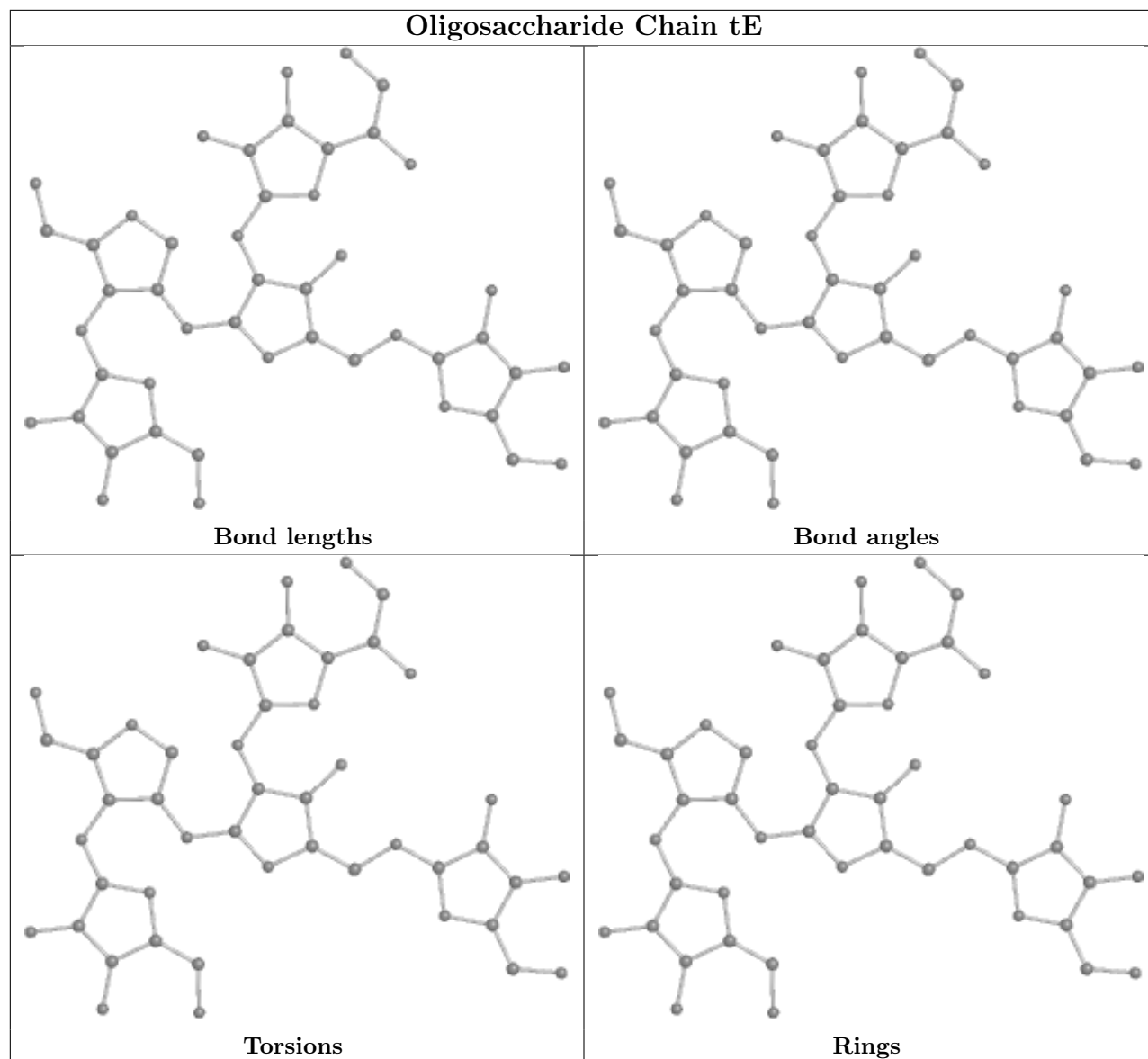


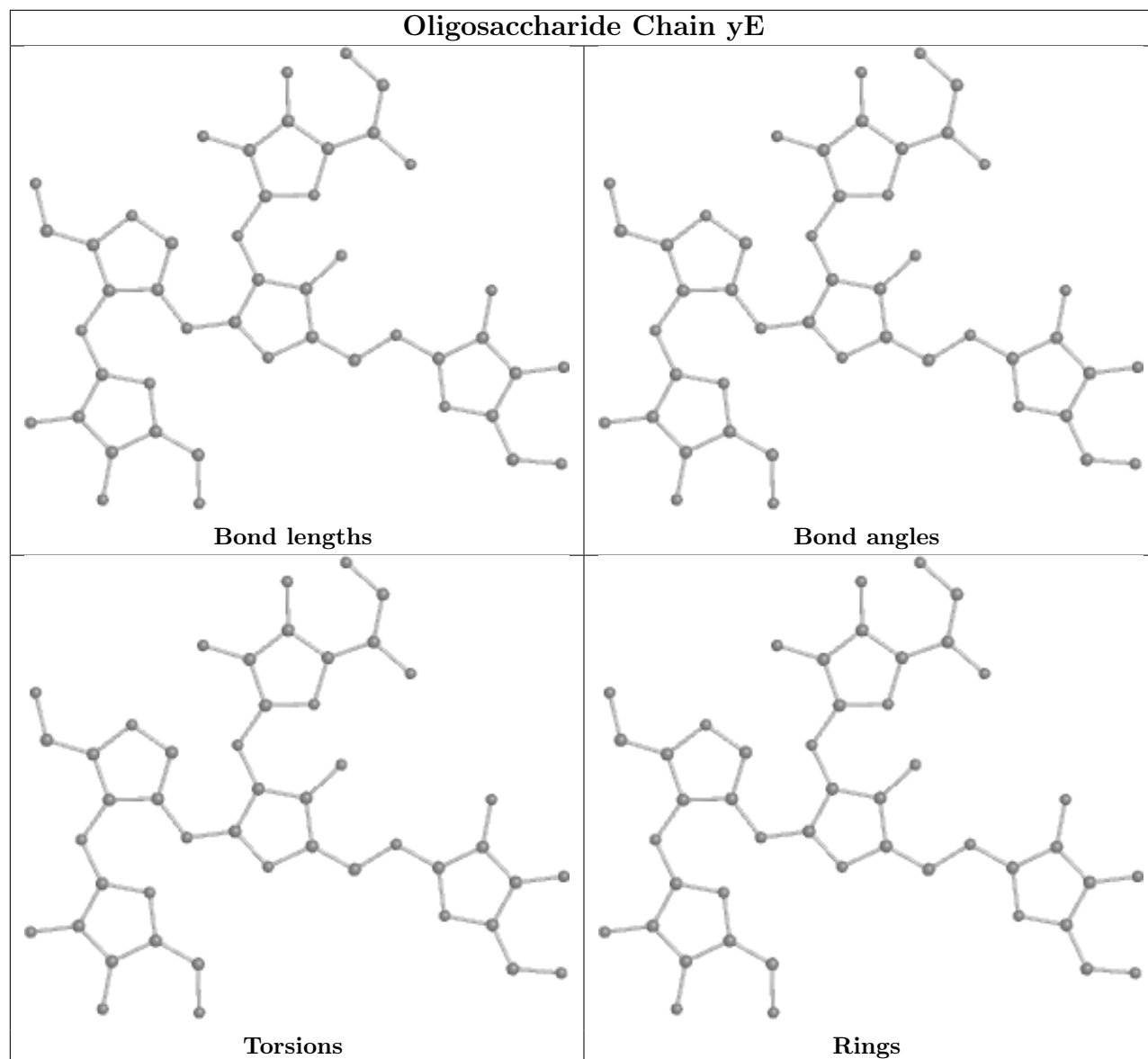




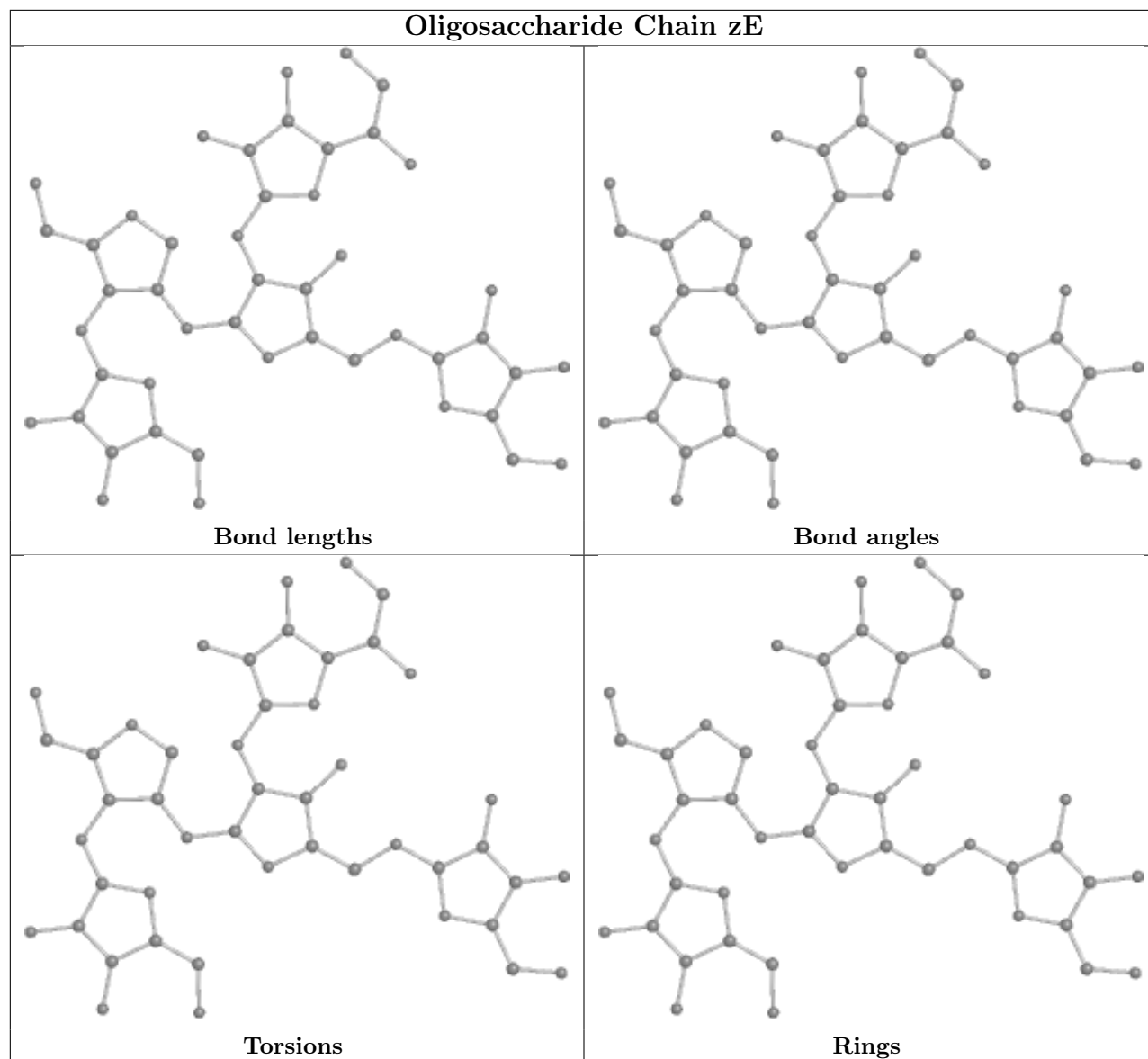


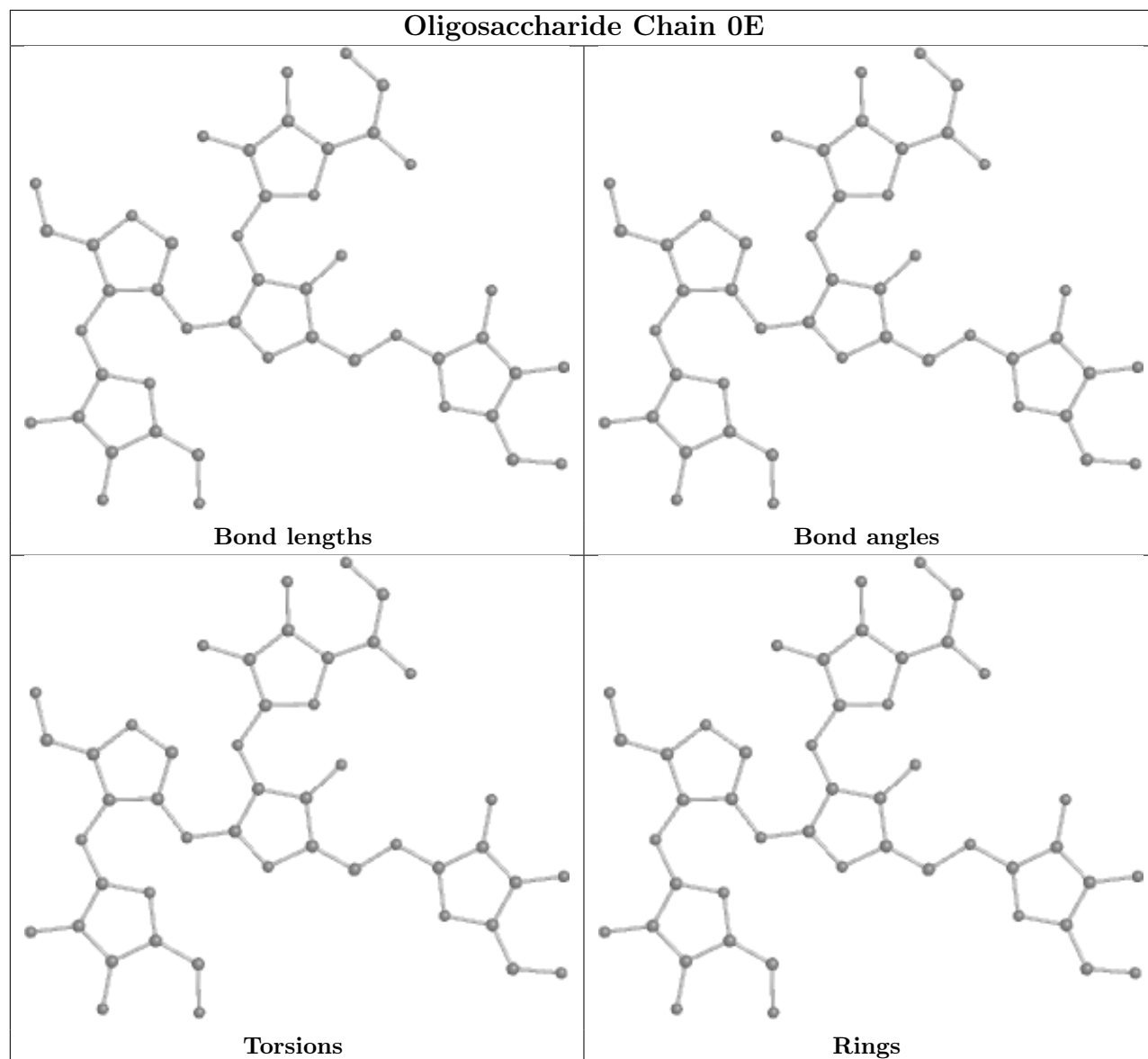


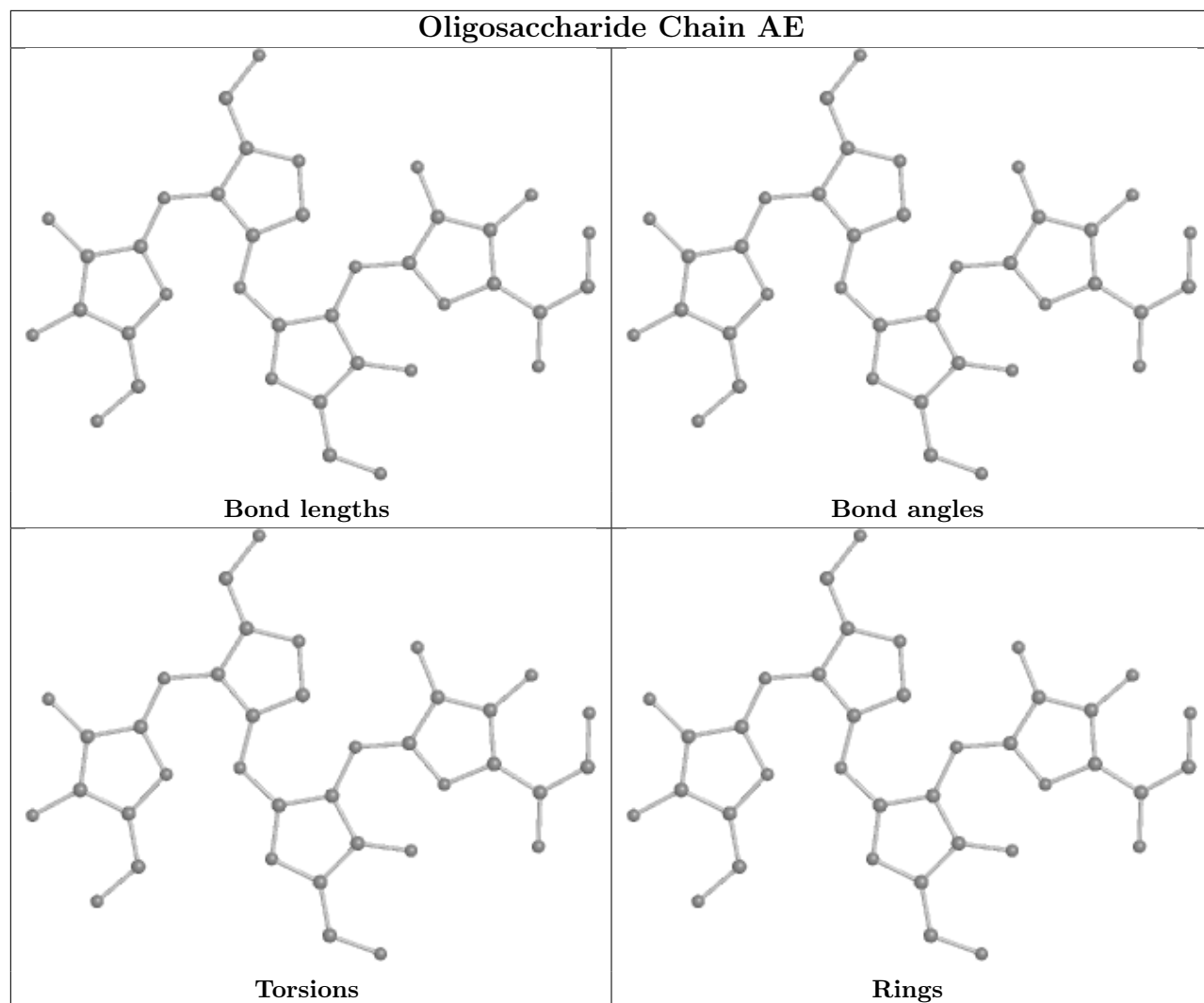


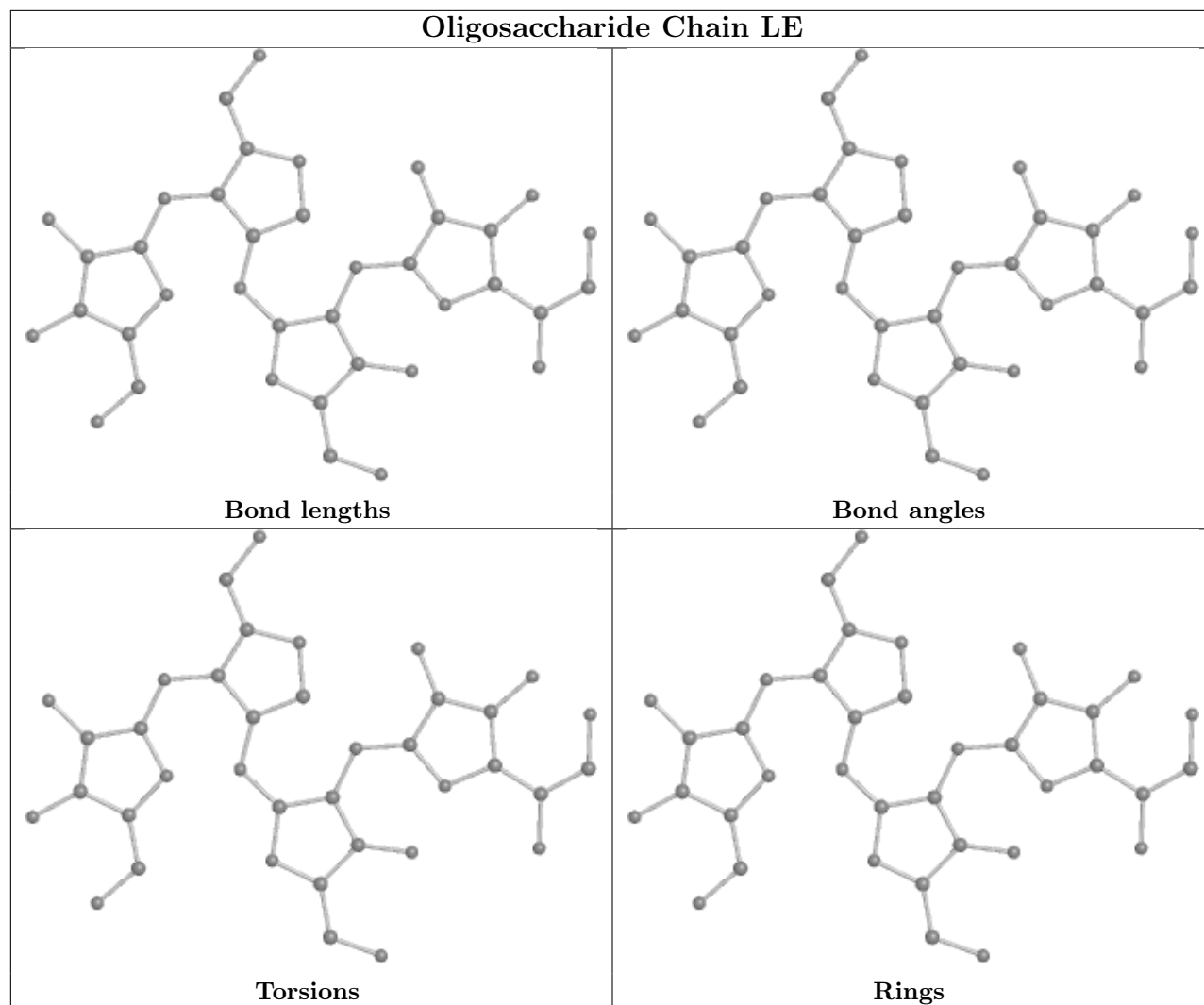


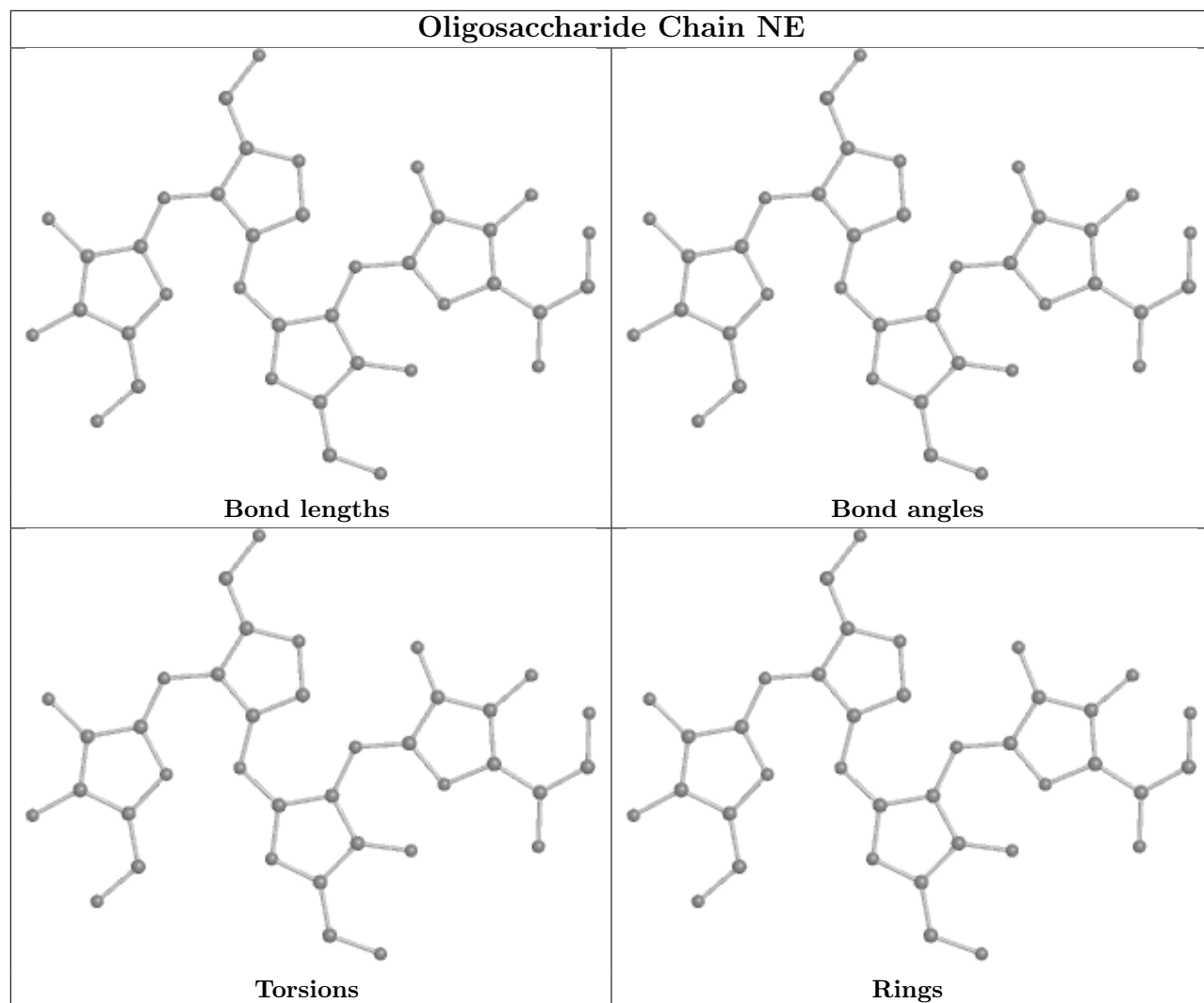


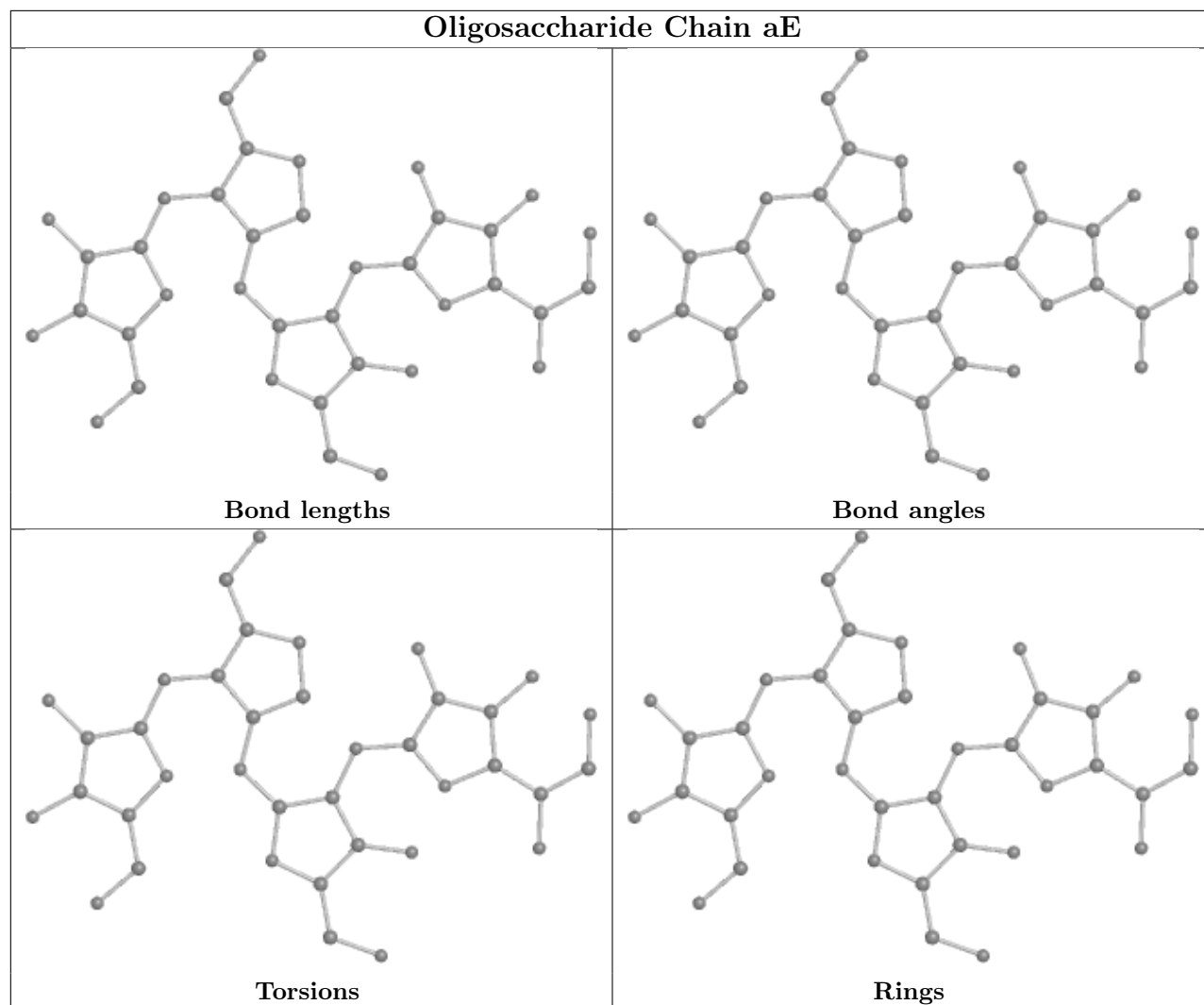


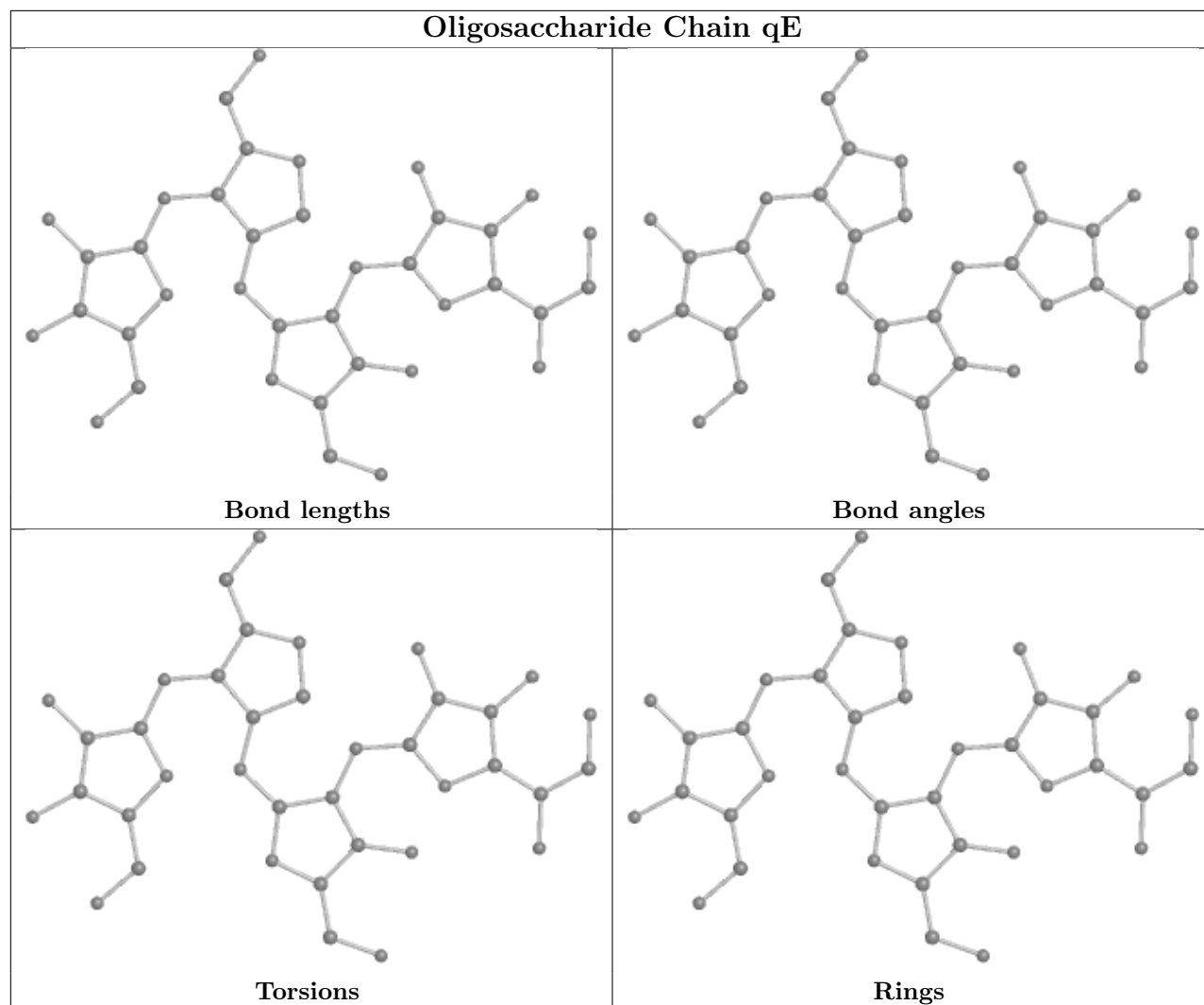


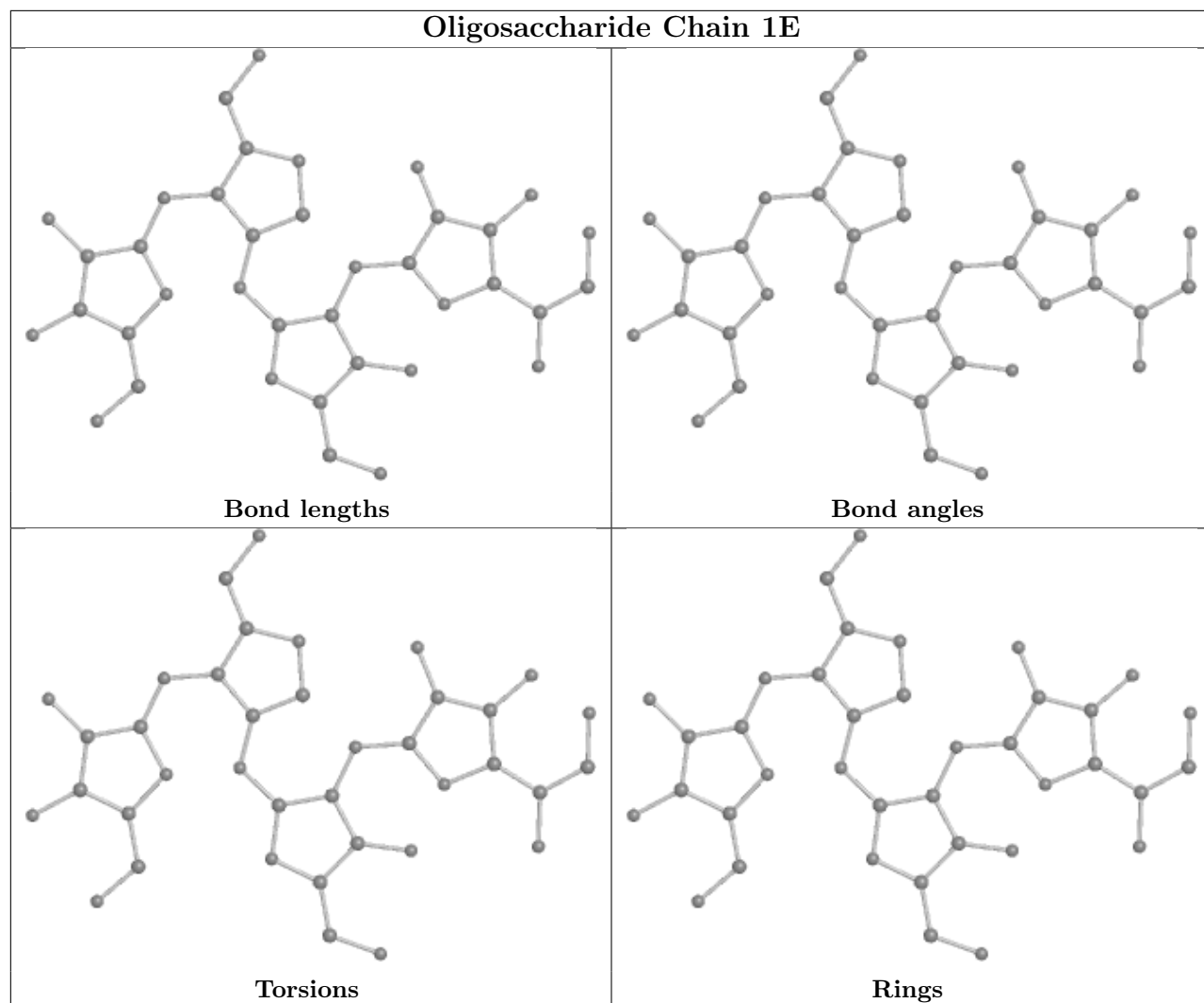




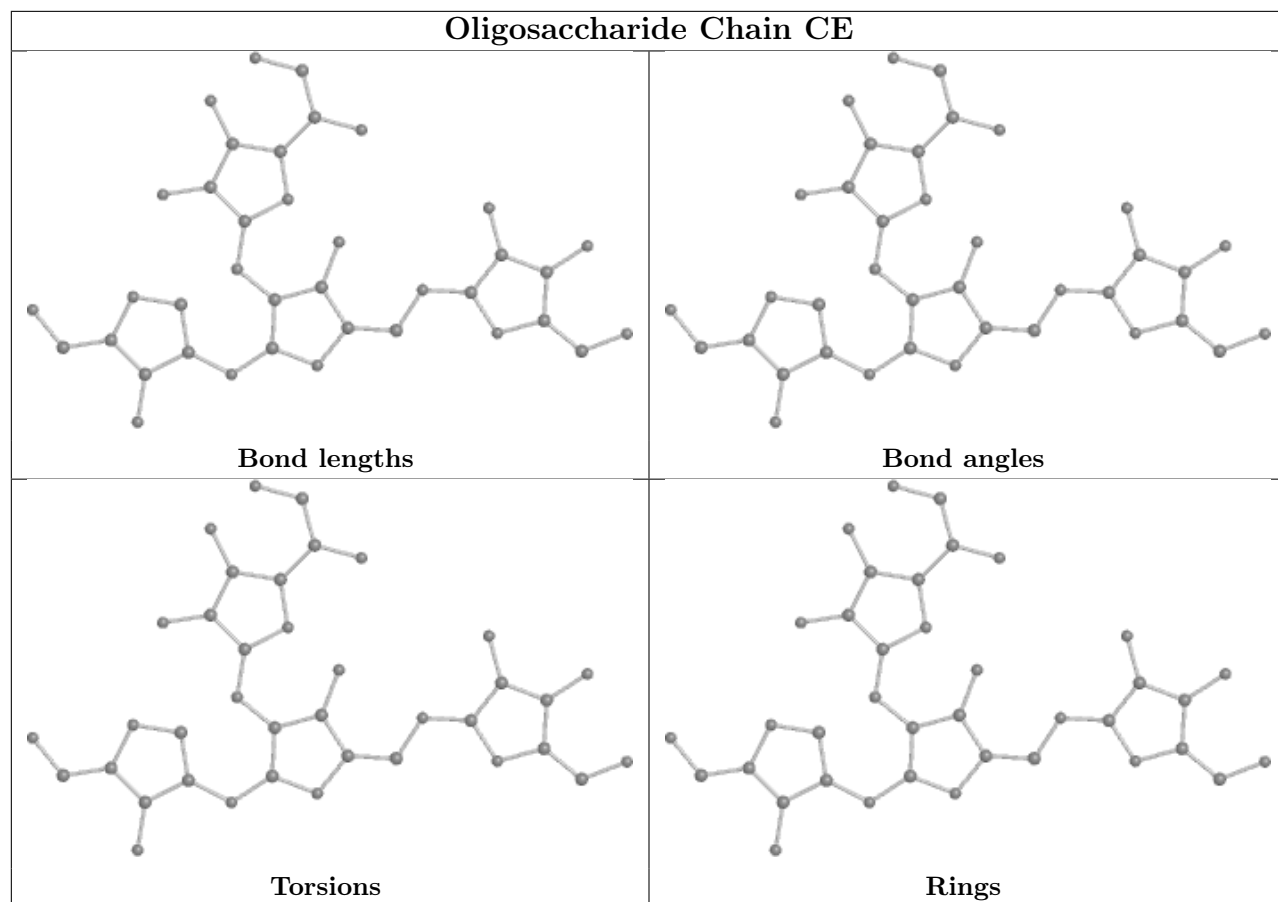


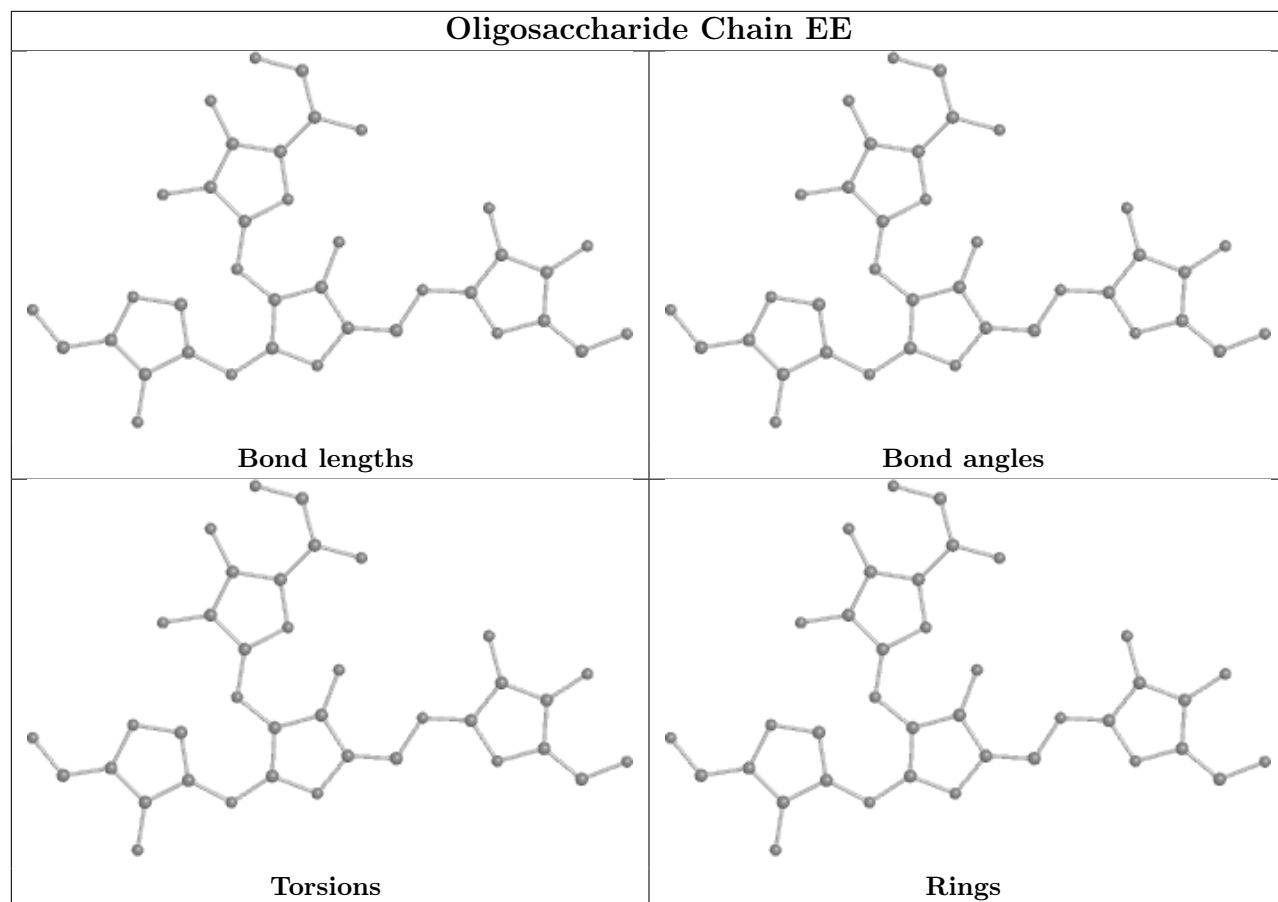


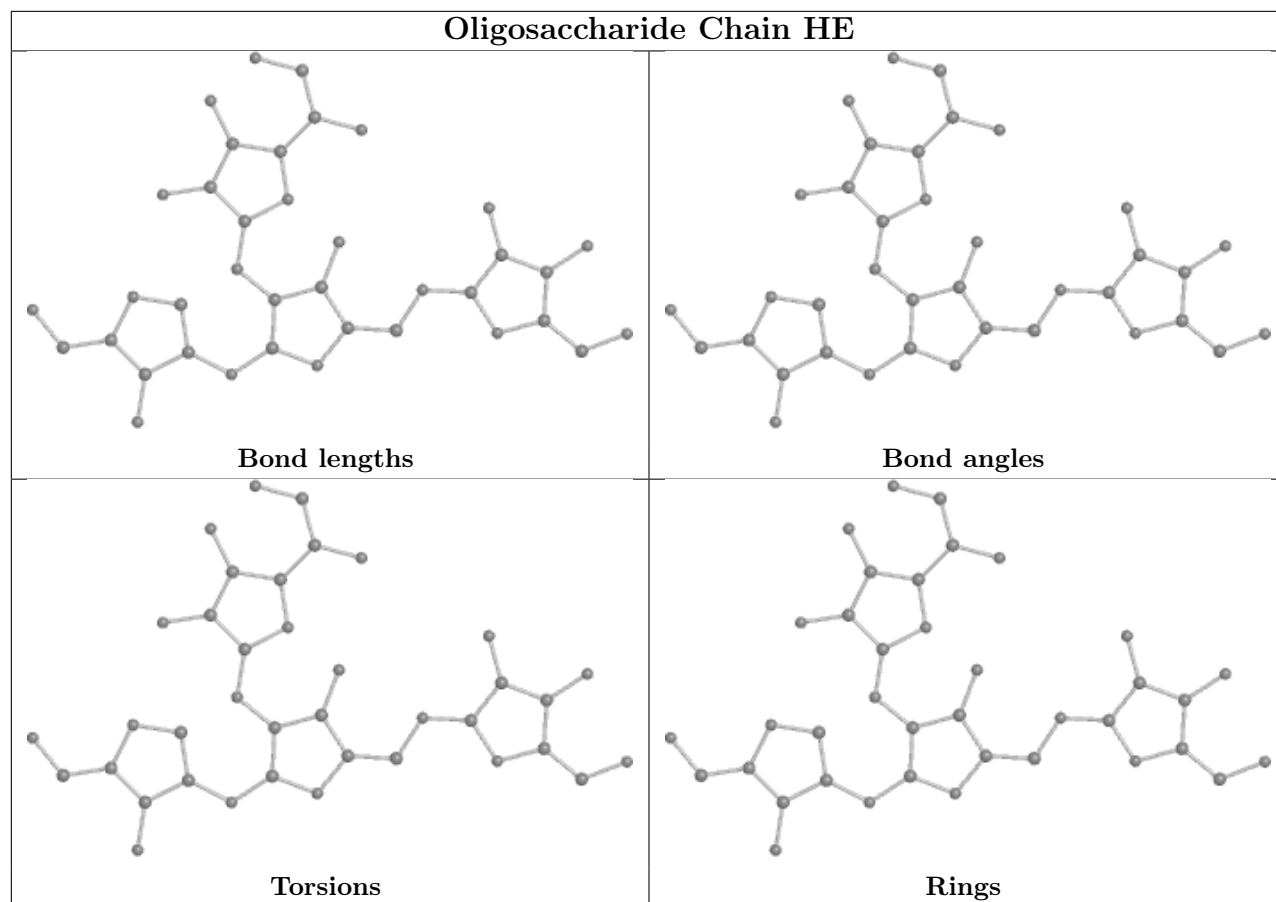


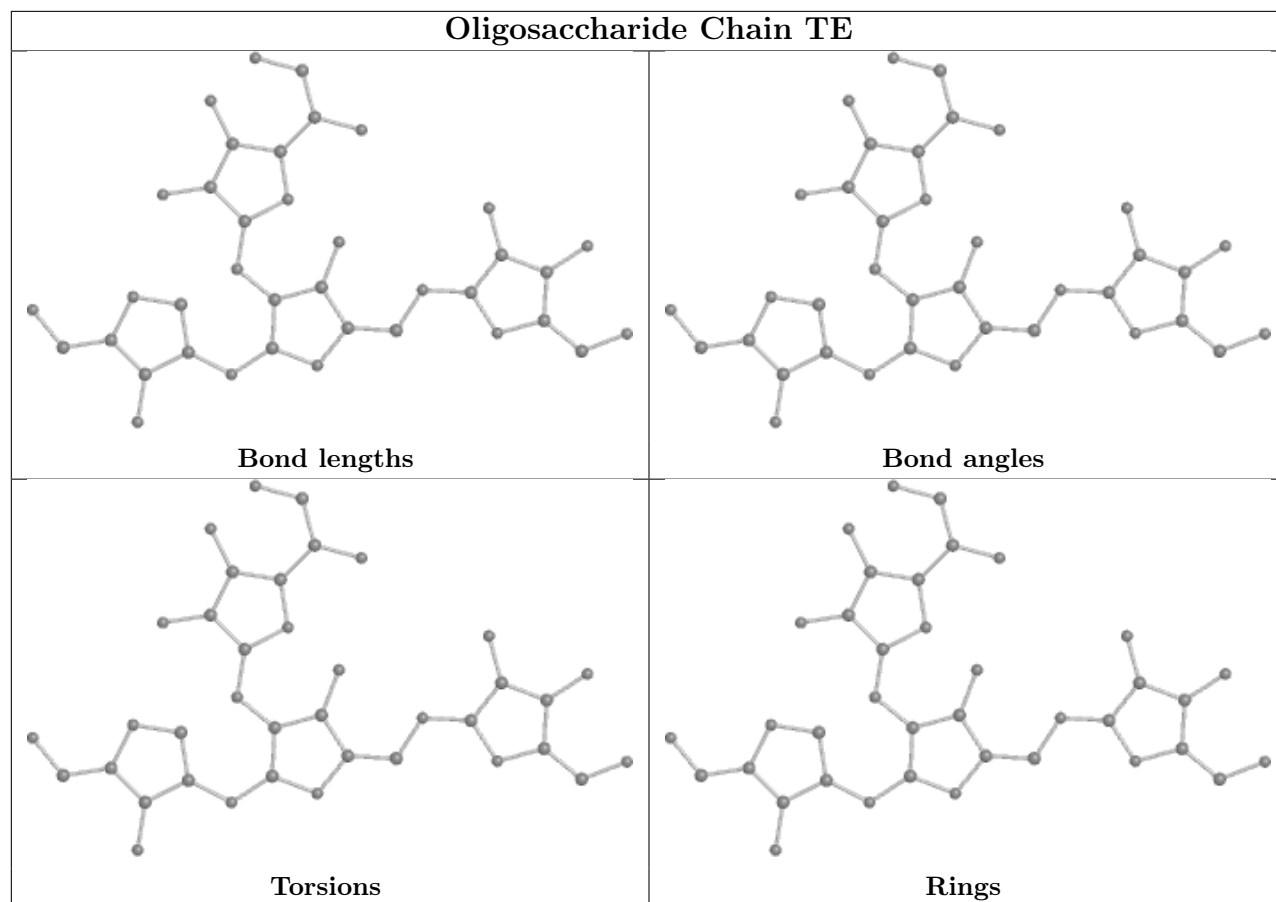


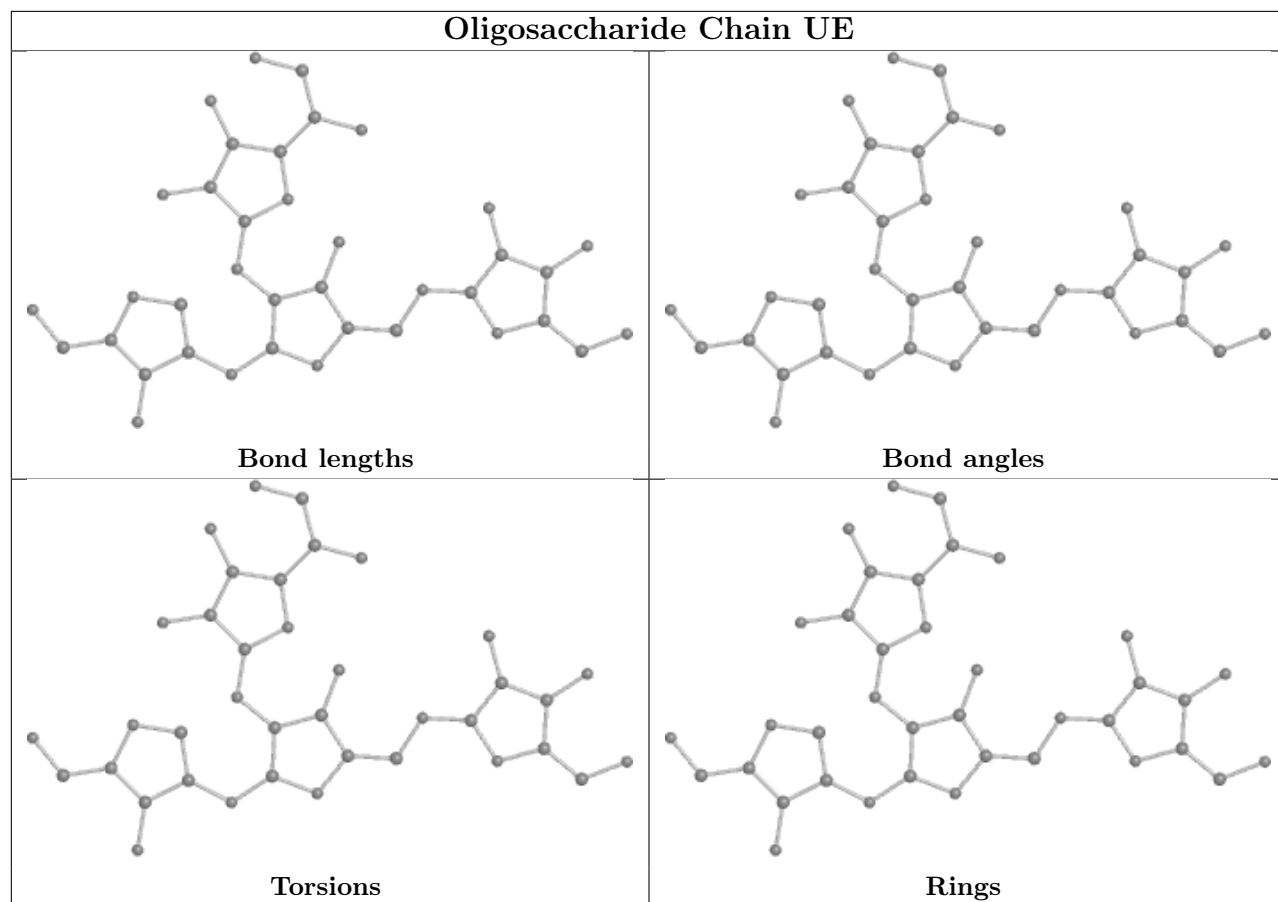


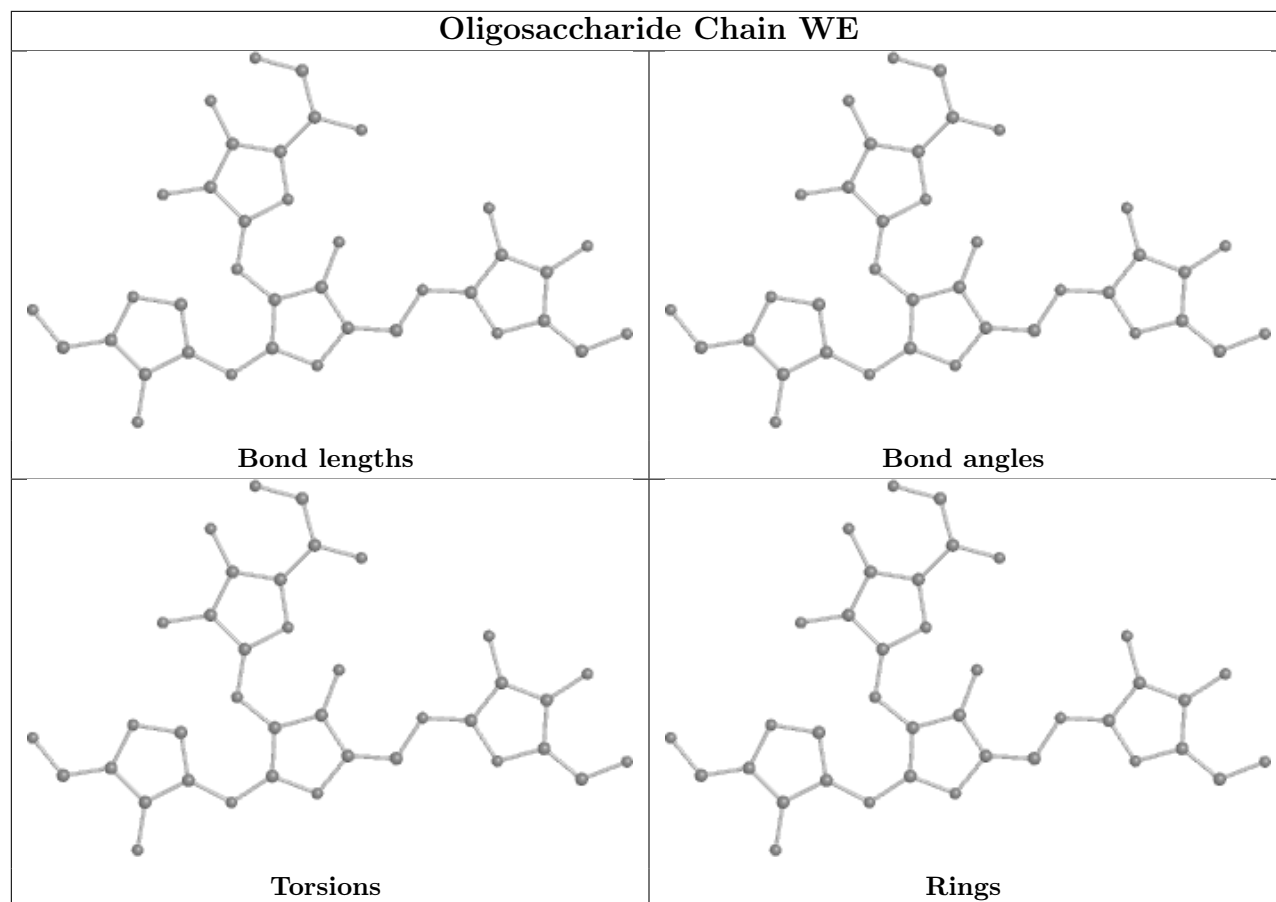


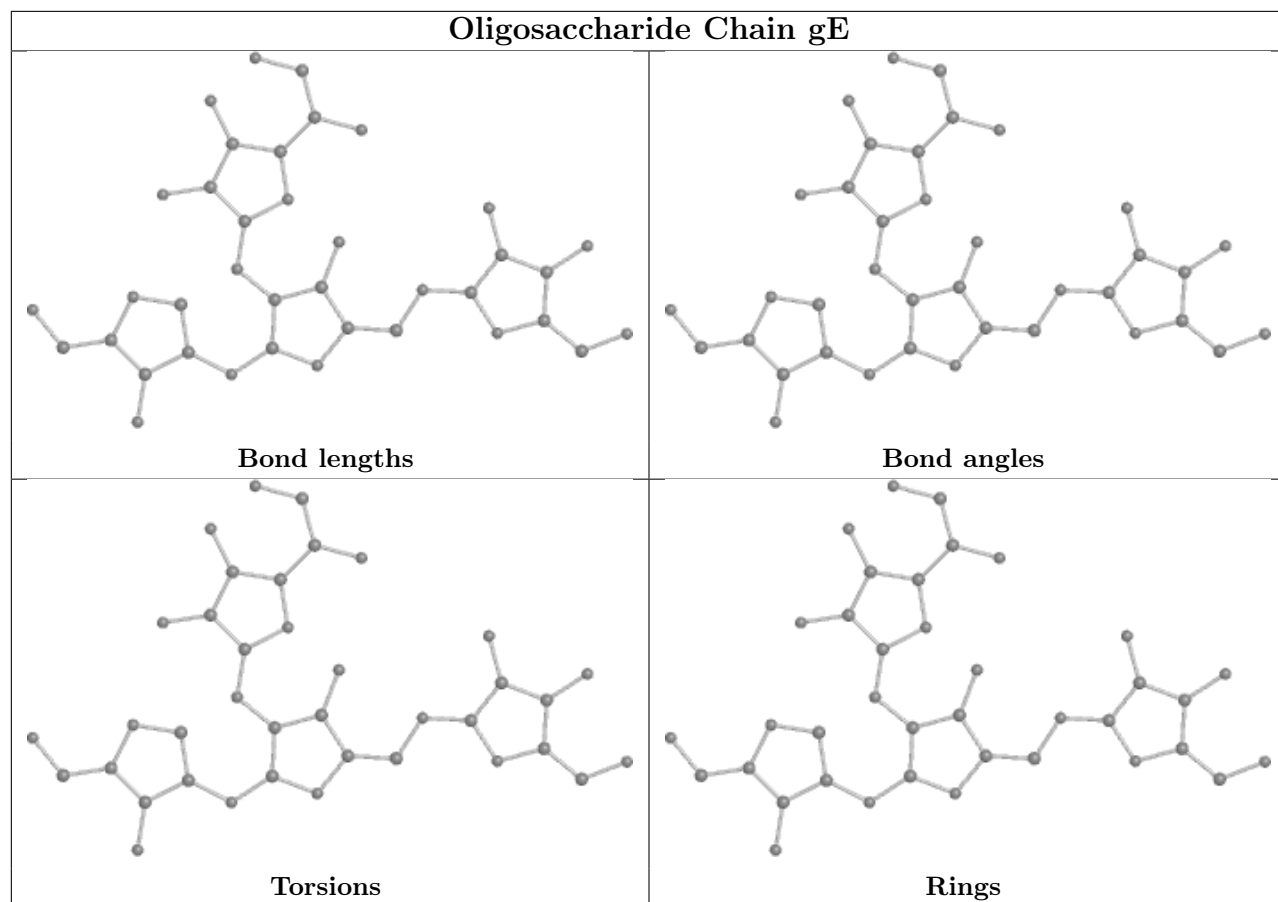


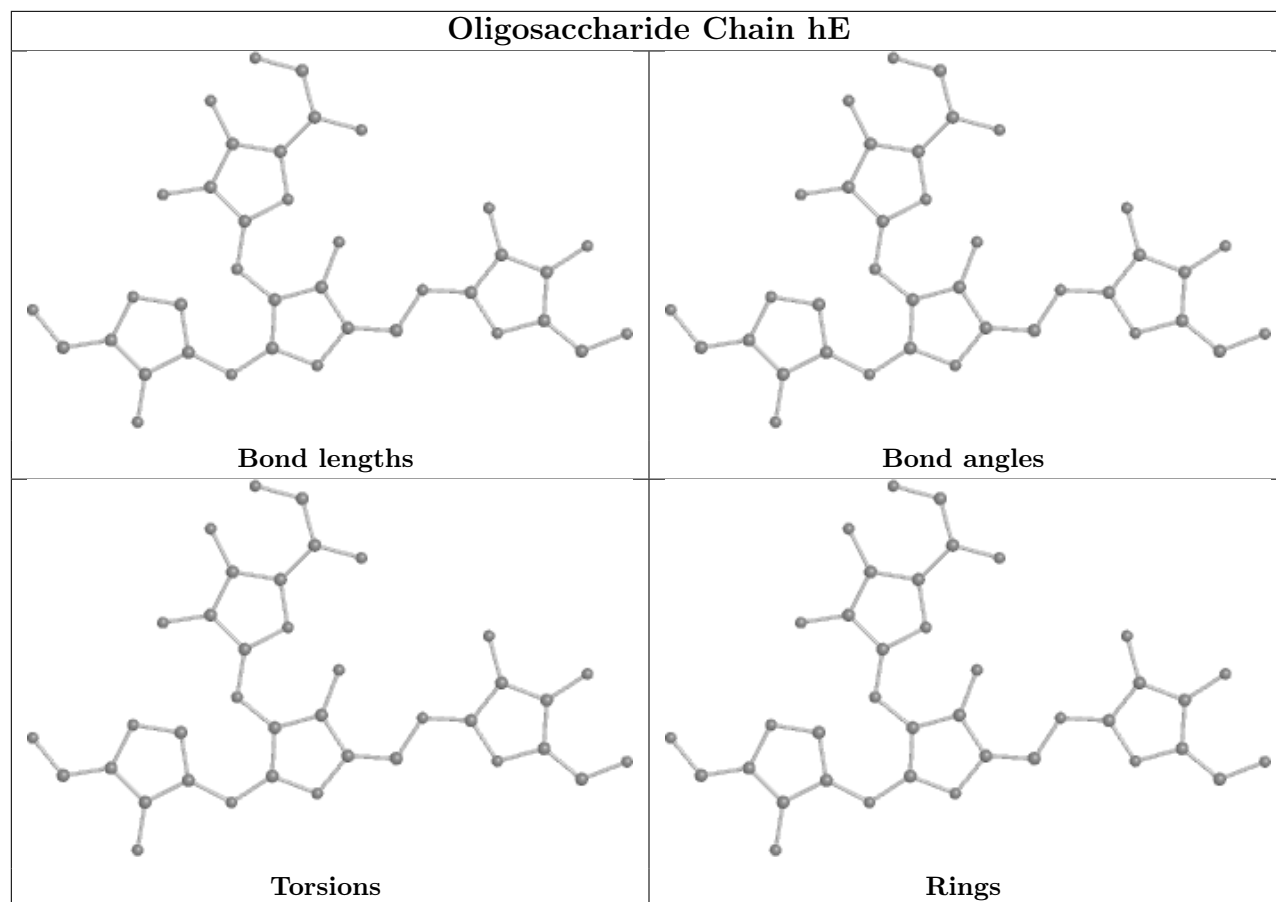




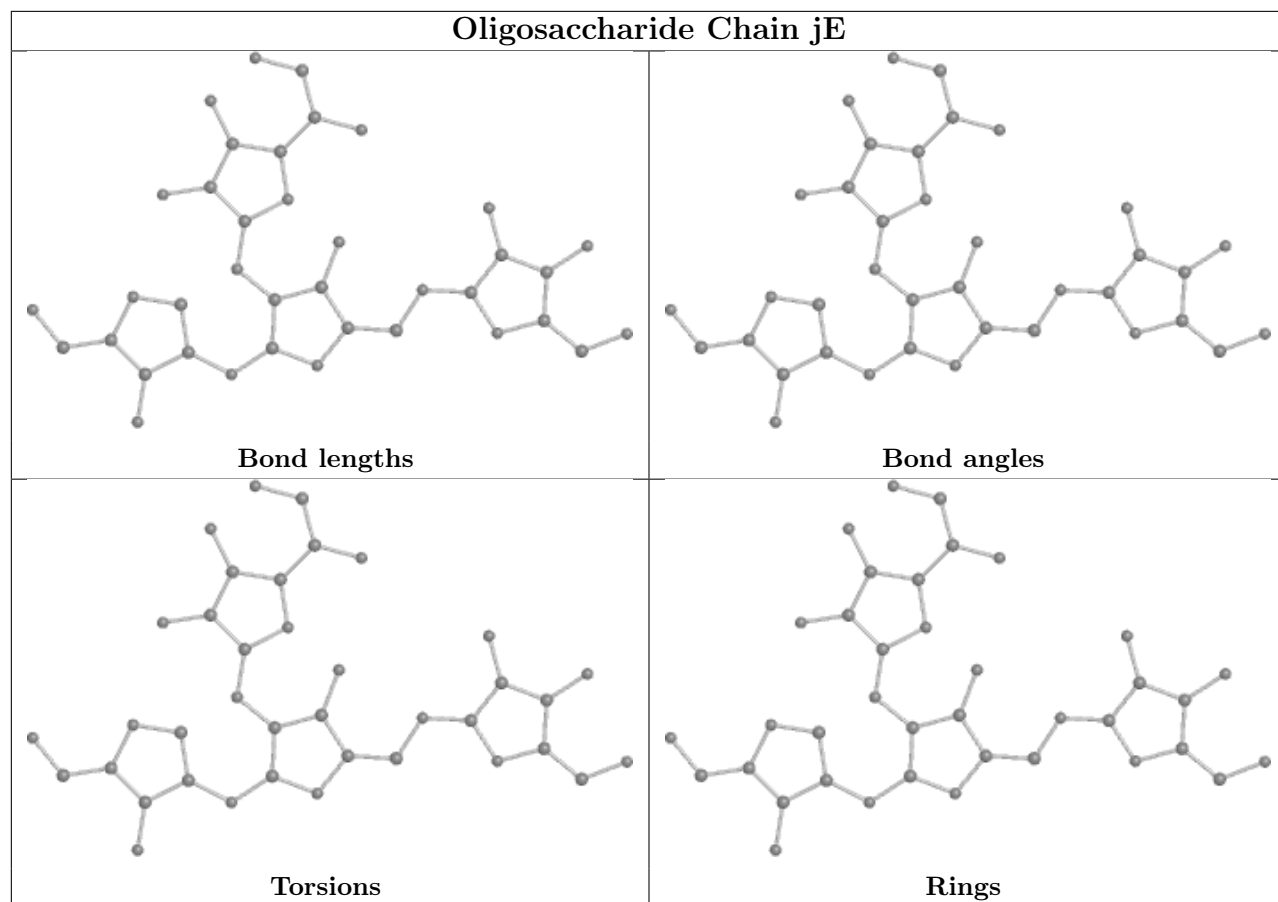


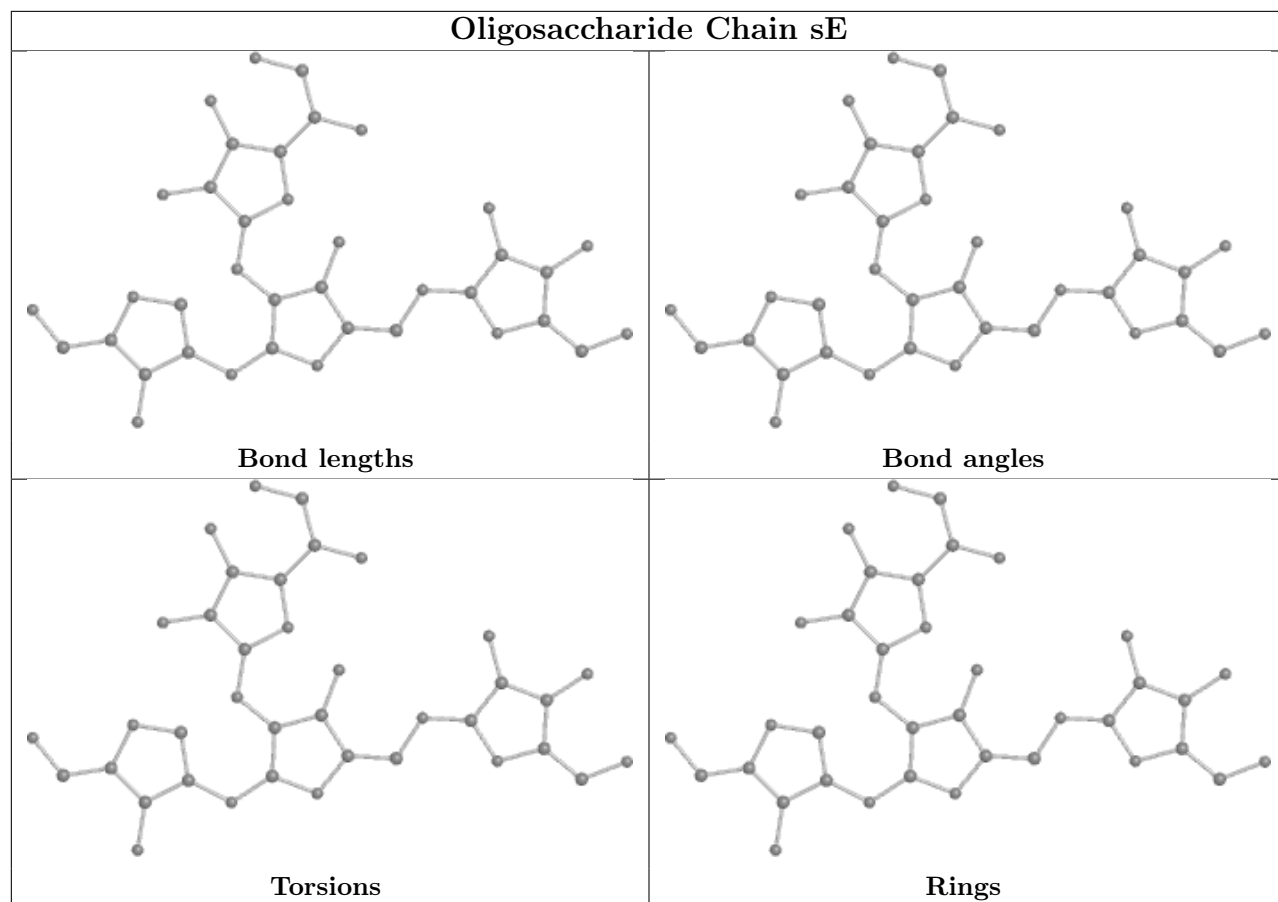


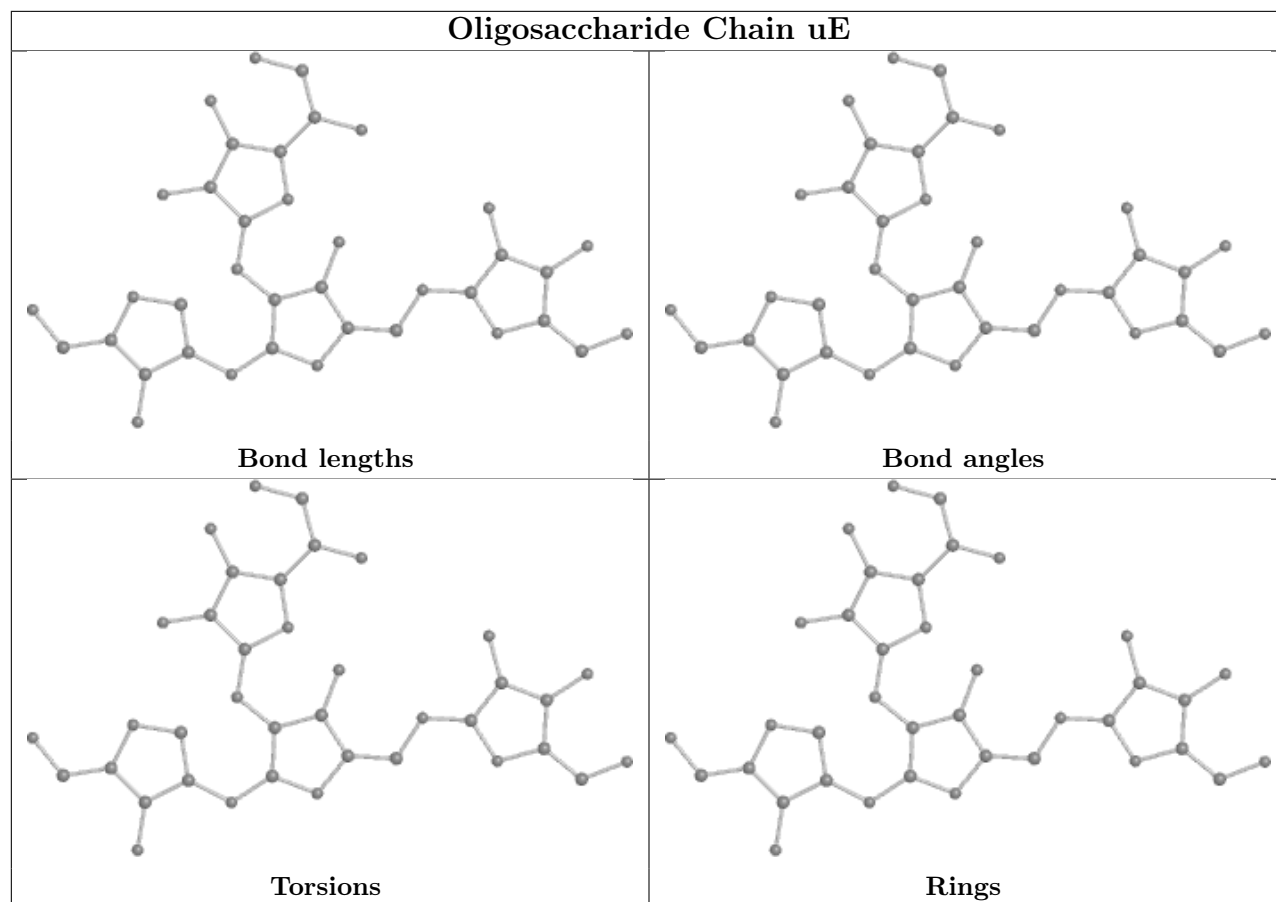


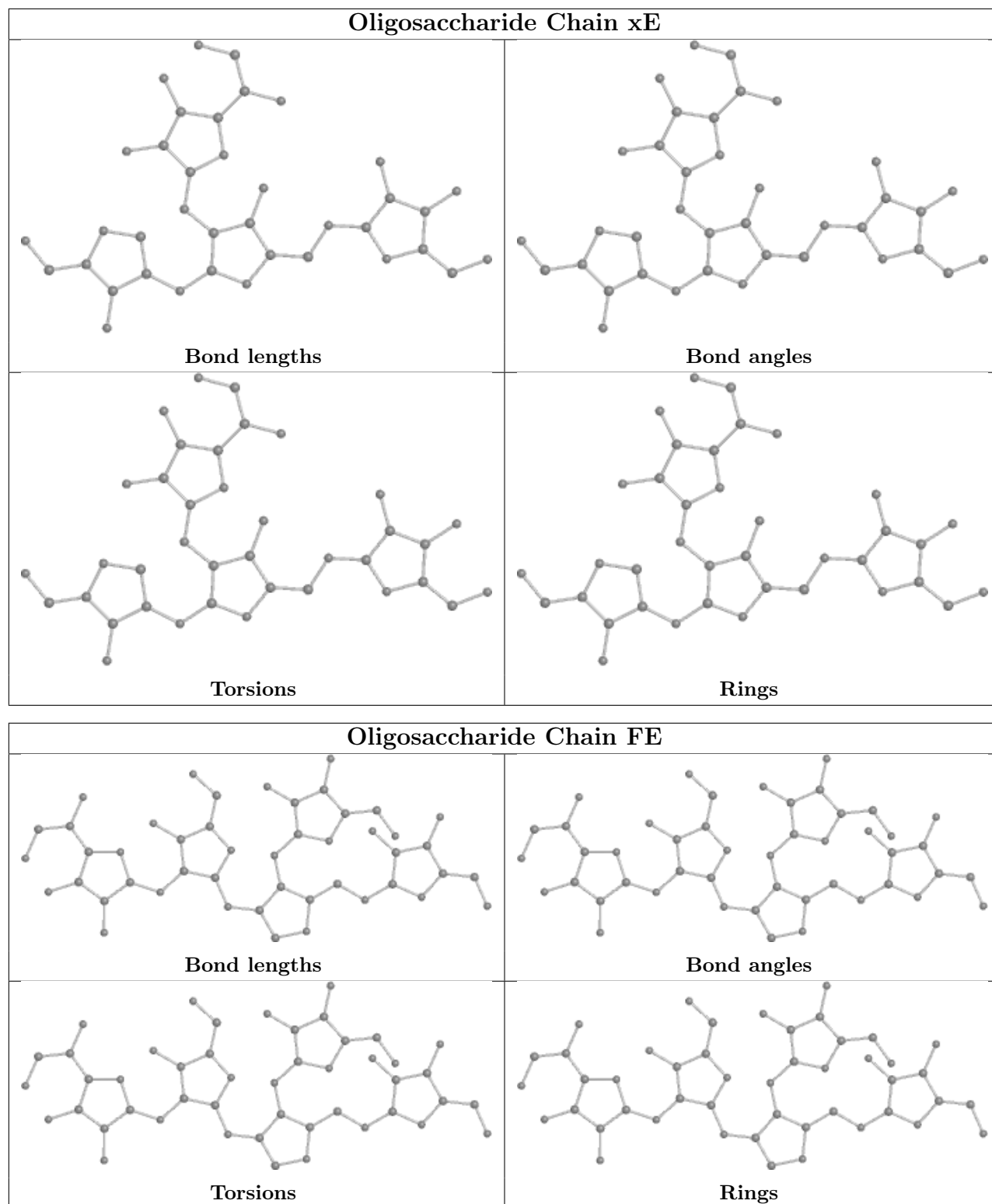


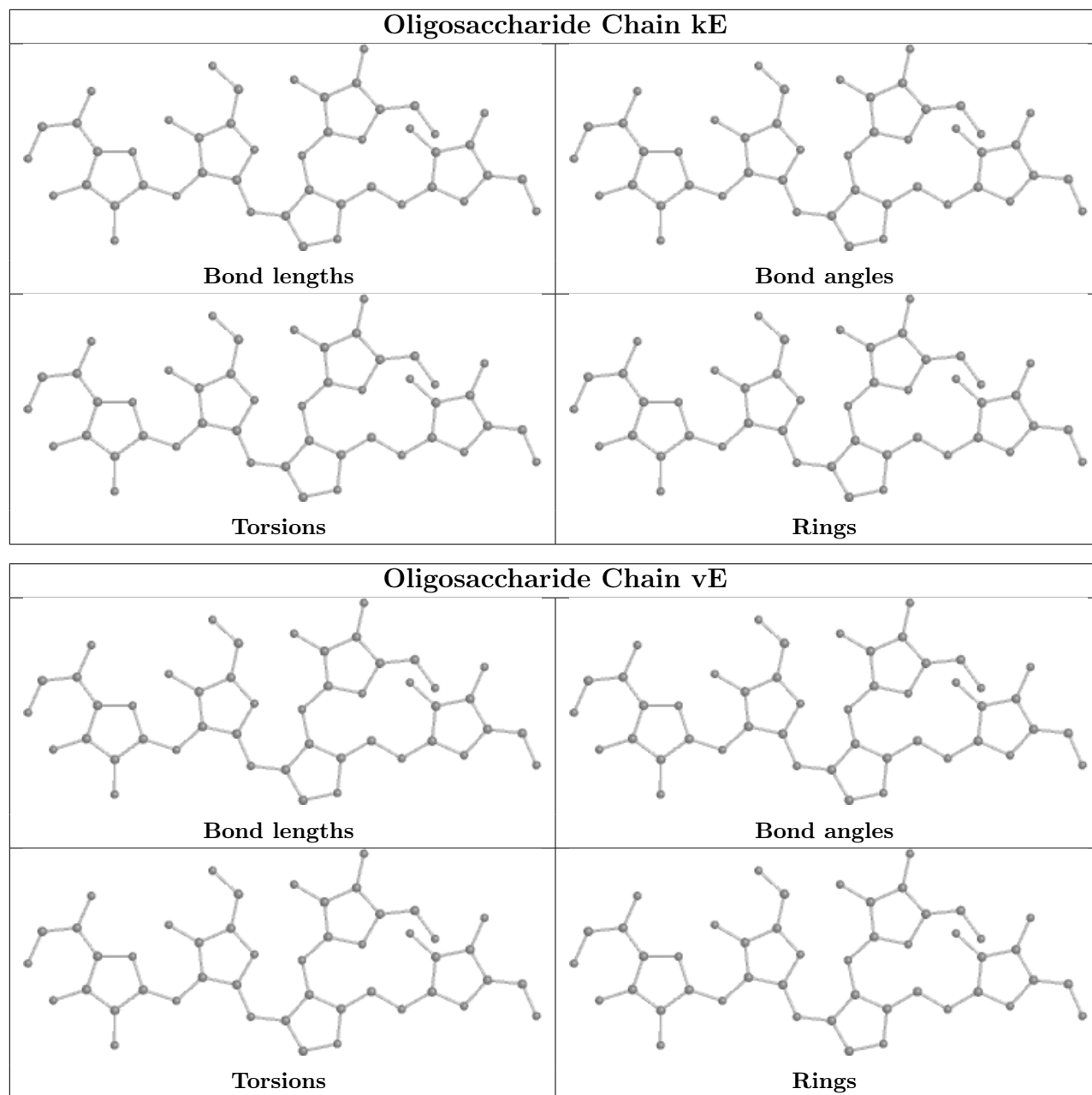


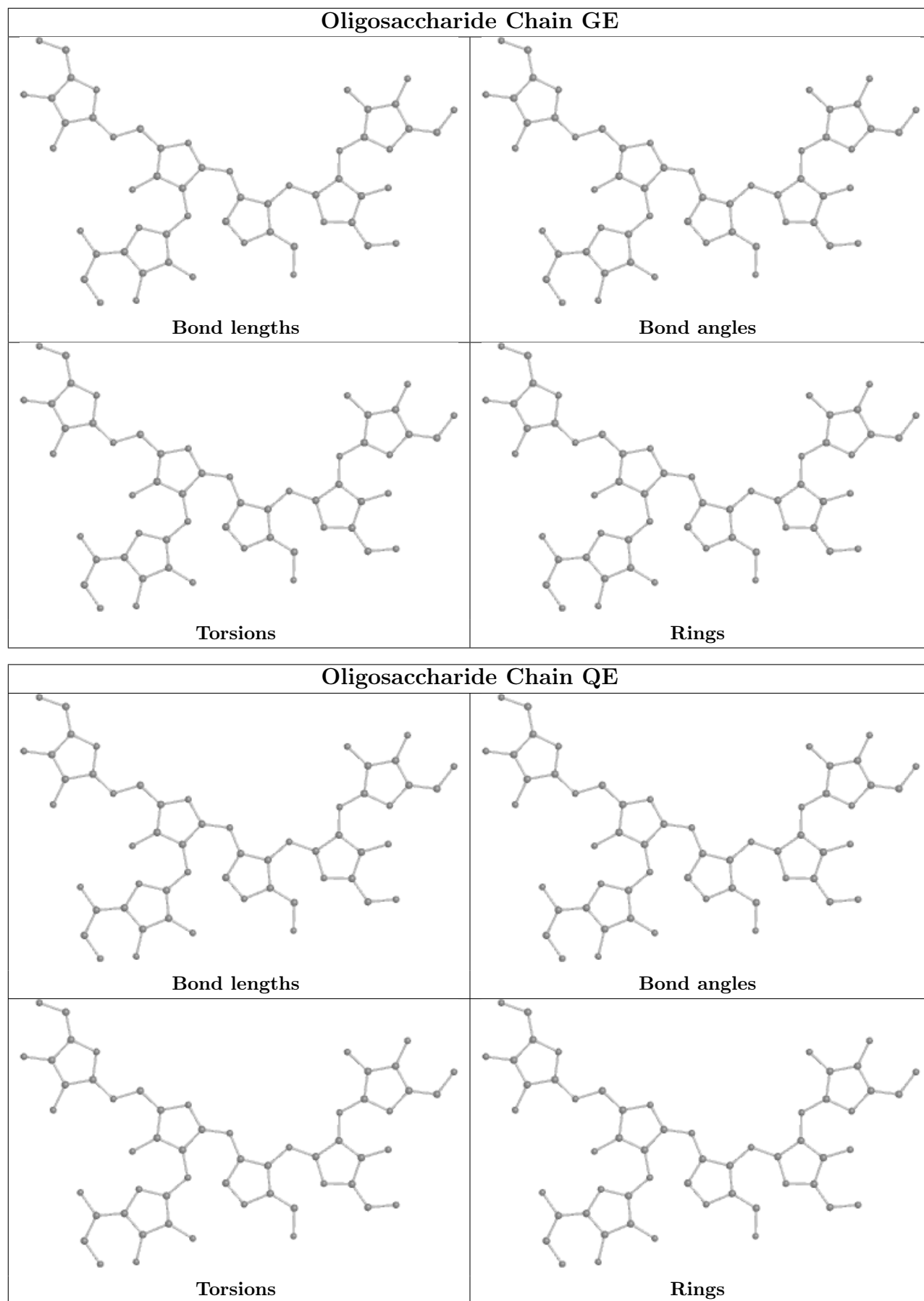


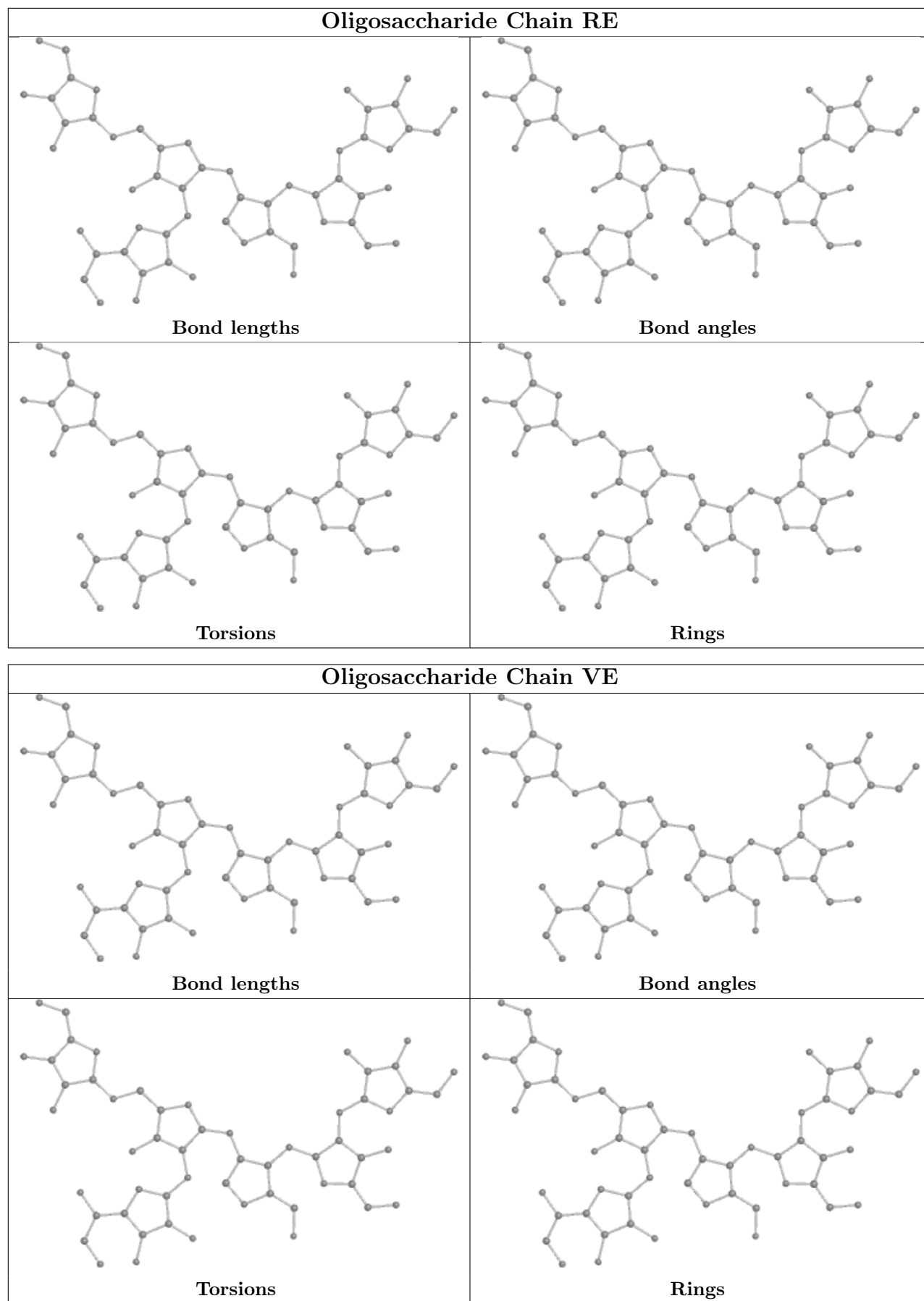


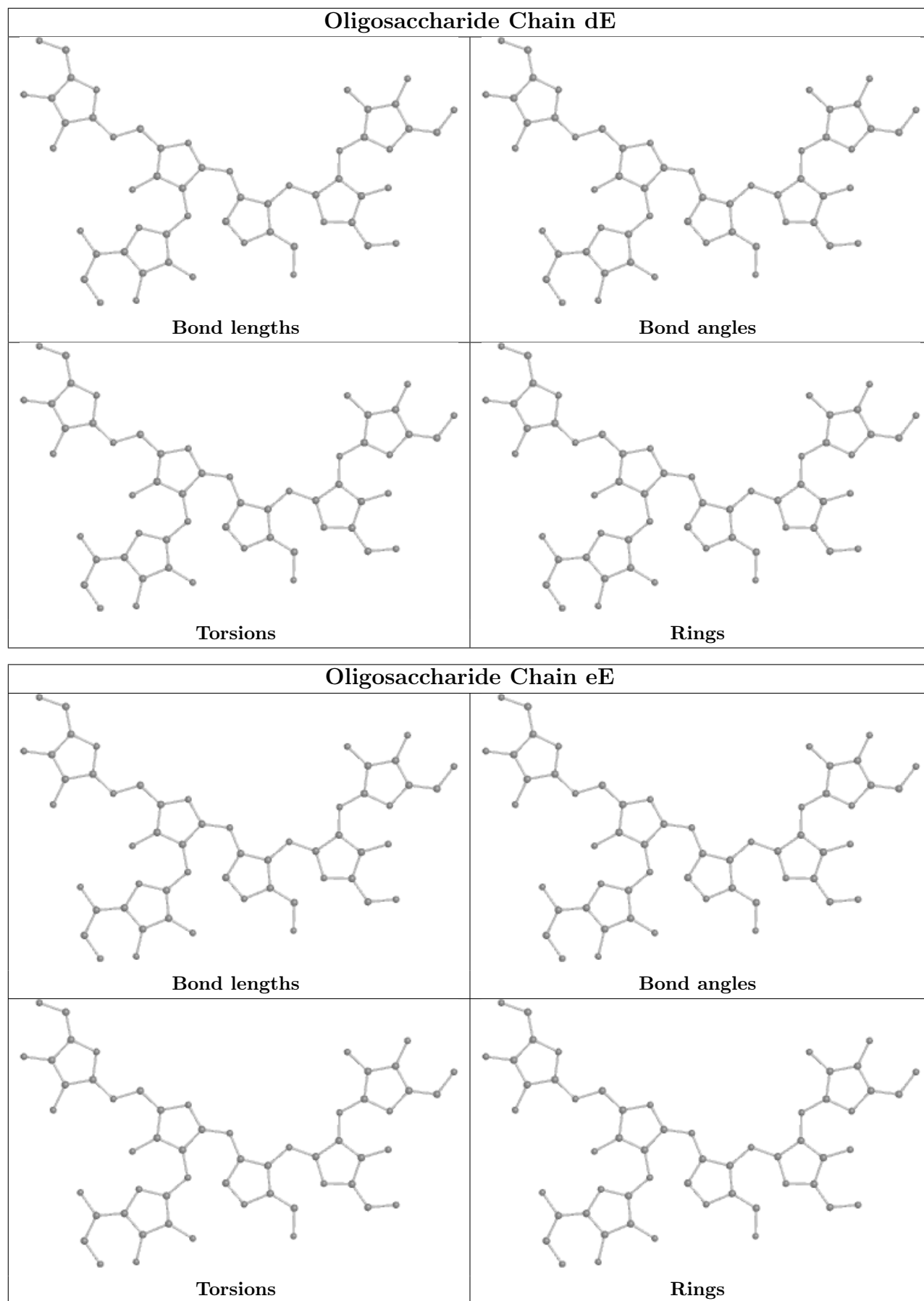




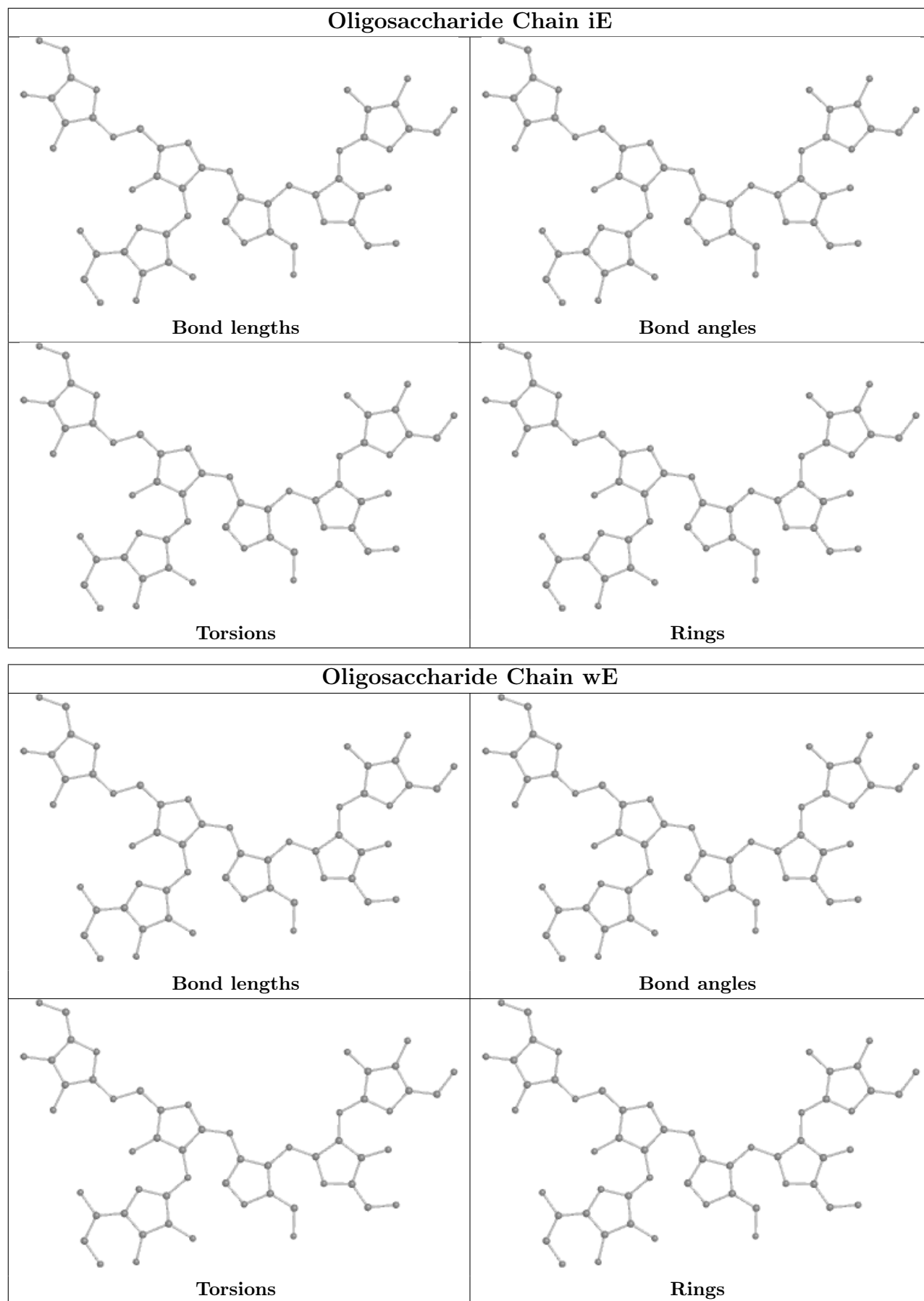


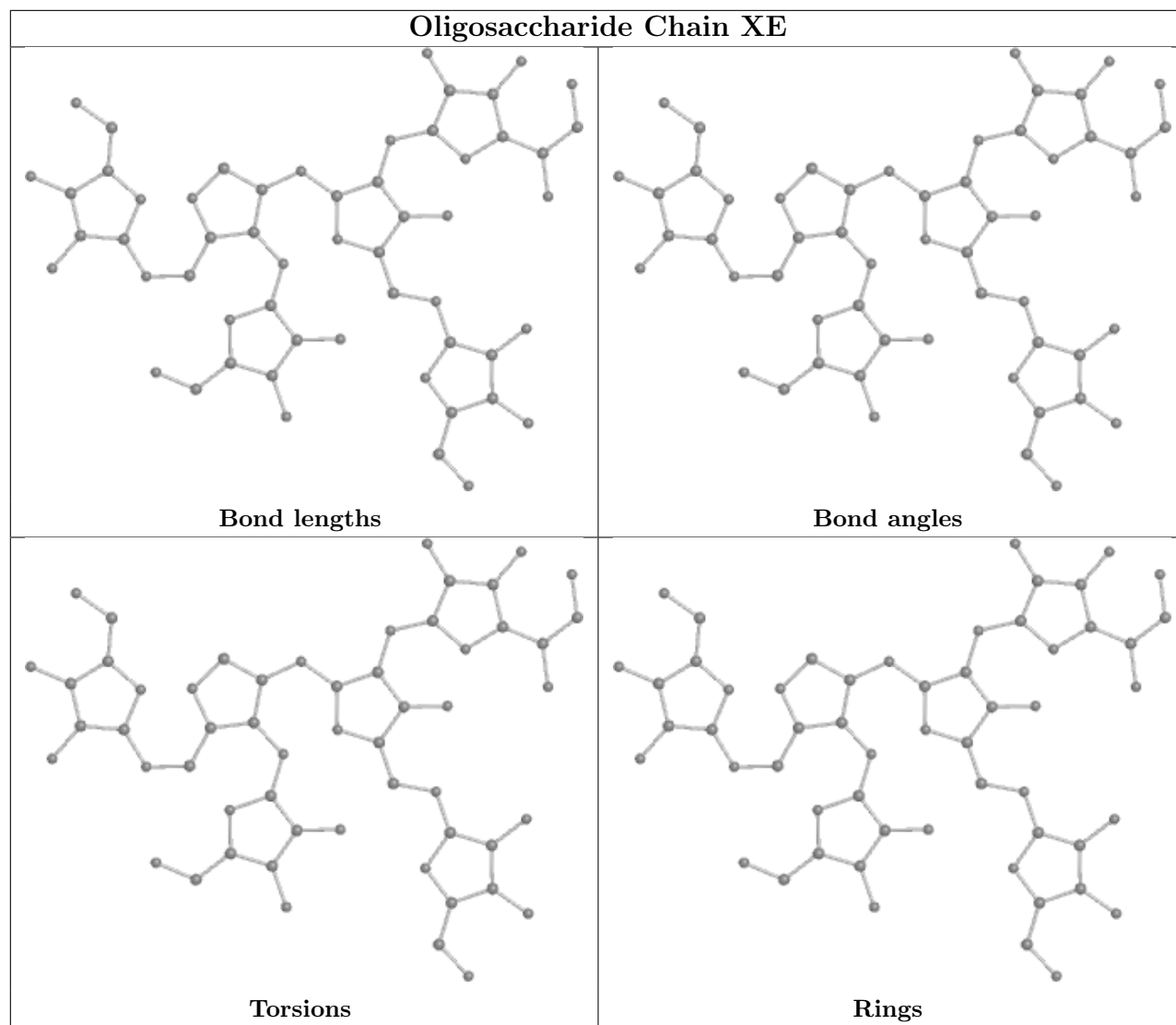


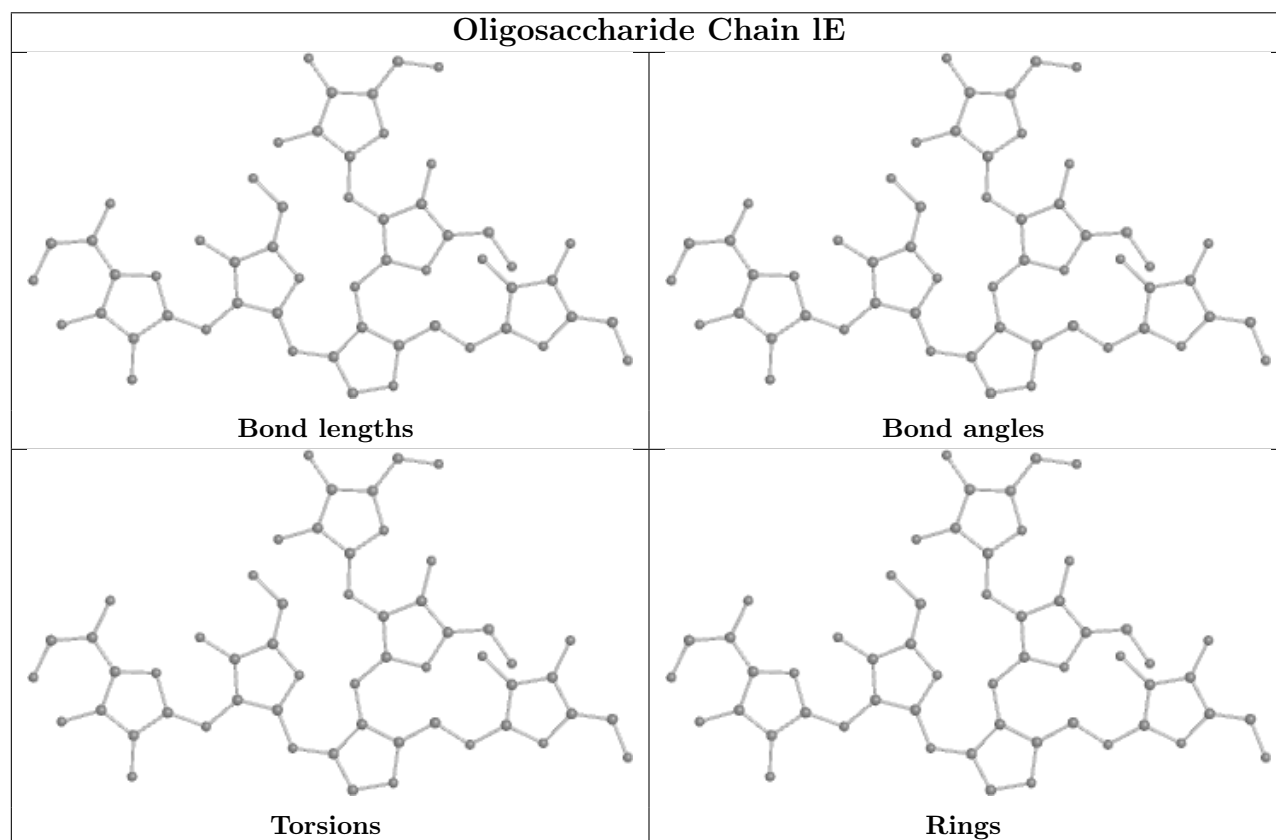
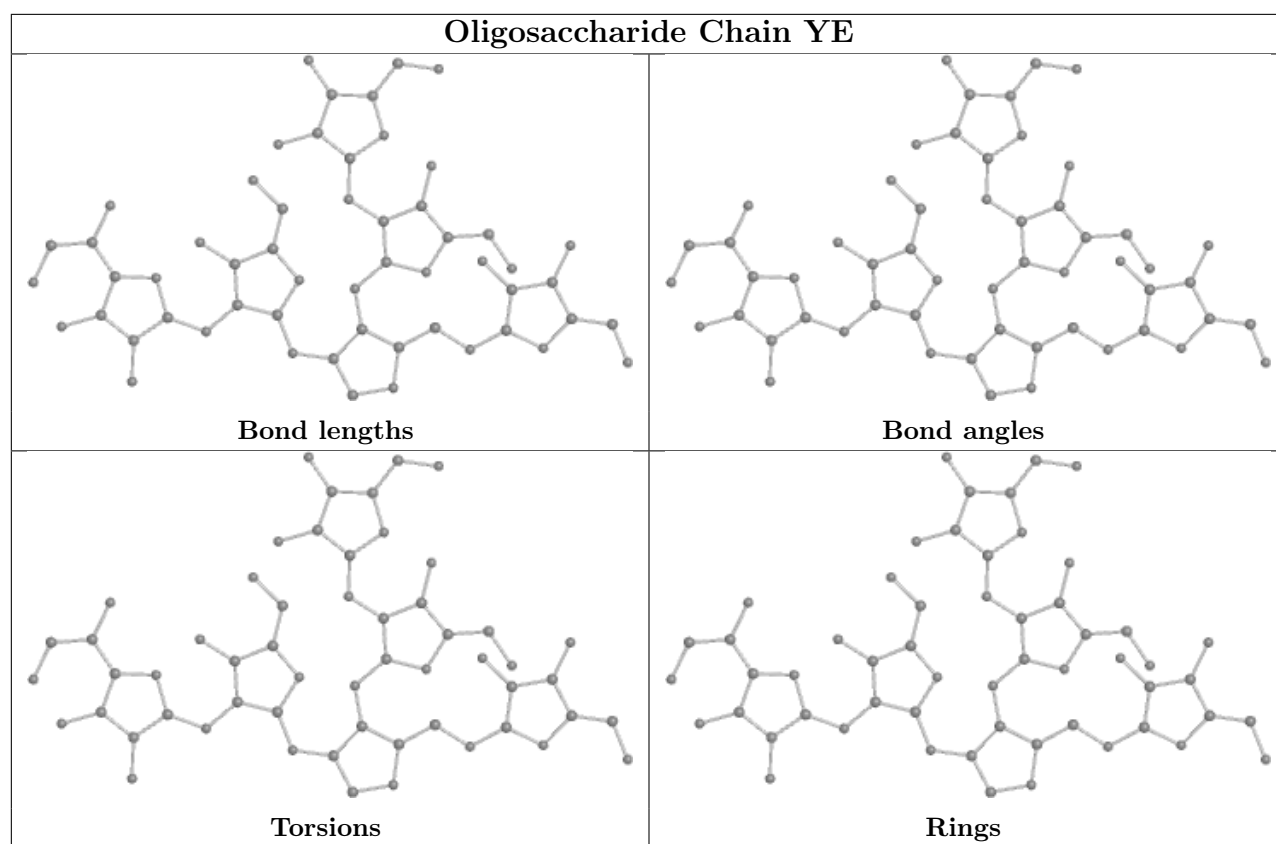












## 5.6 Ligand geometry

Of 95 ligands modelled in this entry, 6 are monoatomic - leaving 89 for Mogul analysis.

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
27	GLA	F	2011	1	11,11,12	1.78	3 (27%)	15,15,17	0.91	0
27	GLA	E	2005	1	11,11,12	1.77	3 (27%)	15,15,17	0.95	1 (6%)
27	GLA	B	2005	1	11,11,12	1.88	3 (27%)	15,15,17	1.86	4 (26%)
26	AHR	C	2003	-	9,9,10	0.82	0	10,12,14	1.58	2 (20%)
27	GLA	A	2011	1	11,11,12	1.79	3 (27%)	15,15,17	0.94	1 (6%)
28	NAG	C	2009	1	14,14,15	0.36	0	17,19,21	0.78	0
27	GLA	F	2009	1	11,11,12	1.68	2 (18%)	15,15,17	0.89	1 (6%)
26	AHR	E	2003	-	9,9,10	0.67	0	10,12,14	1.58	3 (30%)
27	GLA	B	2013	1	11,11,12	1.73	2 (18%)	15,15,17	0.99	1 (6%)
27	GLA	C	2005	1	11,11,12	1.70	2 (18%)	15,15,17	0.99	1 (6%)
27	GLA	E	2011	1	11,11,12	1.74	3 (27%)	15,15,17	0.91	0
26	AHR	F	2004	-	9,9,10	0.67	0	10,12,14	1.59	3 (30%)
26	AHR	A	2003	-	9,9,10	0.79	1 (11%)	10,12,14	1.57	2 (20%)
27	GLA	F	2016	1	11,11,12	1.70	2 (18%)	15,15,17	0.97	1 (6%)
26	AHR	F	2001	-	9,9,10	0.68	0	10,12,14	1.57	3 (30%)
26	AHR	F	2003	-	9,9,10	0.57	0	10,12,14	1.59	1 (10%)
28	NAG	D	2010	1	14,14,15	0.31	0	17,19,21	0.74	0
27	GLA	F	2006	1	11,11,12	1.83	3 (27%)	15,15,17	2.17	4 (26%)
27	GLA	A	2012	1	11,11,12	1.76	3 (27%)	15,15,17	0.94	1 (6%)
27	GLA	B	2007	1	11,11,12	1.81	3 (27%)	15,15,17	0.90	0
27	GLA	B	2010	1	11,11,12	1.78	3 (27%)	15,15,17	0.86	0
27	GLA	E	2009	1	11,11,12	1.73	3 (27%)	15,15,17	1.13	1 (6%)
27	GLA	B	2011	1	11,11,12	1.72	3 (27%)	15,15,17	1.04	2 (13%)
28	NAG	A	2017	1	14,14,15	0.32	0	17,19,21	0.66	0
27	GLA	D	2005	1	11,11,12	1.79	3 (27%)	15,15,17	0.95	0
27	GLA	A	2015	1	11,11,12	1.81	3 (27%)	15,15,17	0.84	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	GLA	B	2015	1	11,11,12	1.77	2 (18%)	15,15,17	0.86	0
27	GLA	A	2009	1	11,11,12	1.73	3 (27%)	15,15,17	1.12	1 (6%)
27	GLA	A	2004	1	11,11,12	1.89	3 (27%)	15,15,17	1.92	4 (26%)
27	GLA	A	2013	1	11,11,12	1.78	3 (27%)	15,15,17	0.69	0
27	GLA	E	2004	1	11,11,12	1.89	3 (27%)	15,15,17	2.03	4 (26%)
27	GLA	B	2012	1	11,11,12	1.81	3 (27%)	15,15,17	0.77	0
27	GLA	C	2004	1	11,11,12	1.77	3 (27%)	15,15,17	0.81	0
27	GLA	A	2010	1	11,11,12	1.74	3 (27%)	15,15,17	0.92	1 (6%)
27	GLA	B	2016	1	11,11,12	1.85	3 (27%)	15,15,17	0.84	0
27	GLA	F	2017	1	11,11,12	1.75	3 (27%)	15,15,17	1.18	1 (6%)
27	GLA	A	2007	1	11,11,12	1.77	3 (27%)	15,15,17	0.67	0
27	GLA	F	2013	1	11,11,12	1.78	2 (18%)	15,15,17	1.02	1 (6%)
27	GLA	A	2005	1	11,11,12	1.72	2 (18%)	15,15,17	0.93	1 (6%)
26	AHR	A	2018	-	9,9,10	0.56	0	10,12,14	1.09	1 (10%)
27	GLA	E	2014	1	11,11,12	1.75	2 (18%)	15,15,17	0.98	0
27	GLA	E	2008	-	11,11,12	1.76	3 (27%)	15,15,17	1.12	1 (6%)
27	GLA	D	2006	1	11,11,12	1.70	2 (18%)	15,15,17	1.06	1 (6%)
27	GLA	B	2017	1	11,11,12	1.67	2 (18%)	15,15,17	1.55	2 (13%)
27	GLA	F	2018	1	11,11,12	1.78	3 (27%)	15,15,17	0.69	0
27	GLA	D	2009	1	11,11,12	1.82	3 (27%)	15,15,17	0.84	1 (6%)
27	GLA	F	2012	1	11,11,12	1.75	3 (27%)	15,15,17	0.90	1 (6%)
28	NAG	E	2017	1	14,14,15	0.32	0	17,19,21	1.00	2 (11%)
27	GLA	E	2010	1	11,11,12	1.70	2 (18%)	15,15,17	1.43	1 (6%)
27	GLA	E	2006	1	11,11,12	1.79	3 (27%)	15,15,17	0.82	0
26	AHR	A	2002	-	9,9,10	0.87	1 (11%)	10,12,14	1.47	2 (20%)
27	GLA	E	2013	1	11,11,12	1.82	3 (27%)	15,15,17	0.84	0
28	NAG	B	2019	1	14,14,15	0.35	0	17,19,21	0.98	1 (5%)
27	GLA	A	2016	1	11,11,12	1.77	2 (18%)	15,15,17	1.10	1 (6%)
27	GLA	F	2007	1	11,11,12	1.70	3 (27%)	15,15,17	1.09	1 (6%)
27	GLA	E	2007	1	11,11,12	1.82	3 (27%)	15,15,17	1.47	3 (20%)
27	GLA	B	2009	-	11,11,12	1.78	2 (18%)	15,15,17	1.72	2 (13%)
27	GLA	F	2014	1	11,11,12	1.79	3 (27%)	15,15,17	0.88	0
26	AHR	B	2004	-	9,9,10	0.80	0	10,12,14	1.79	4 (40%)
26	AHR	B	2003	-	9,9,10	0.91	0	10,12,14	1.83	4 (40%)
27	GLA	C	2008	1	11,11,12	1.80	3 (27%)	15,15,17	1.01	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	GLA	B	2006	1	11,11,12	1.77	3 (27%)	15,15,17	0.75	0
27	GLA	F	2008	1	11,11,12	1.76	3 (27%)	15,15,17	1.04	2 (13%)
26	AHR	D	2003	-	9,9,10	0.84	0	10,12,14	1.56	2 (20%)
27	GLA	E	2012	1	11,11,12	1.66	2 (18%)	15,15,17	1.32	1 (6%)
27	GLA	B	2014	1	11,11,12	1.68	2 (18%)	15,15,17	0.86	1 (6%)
26	AHR	A	2019	-	9,9,10	0.56	0	10,12,14	0.89	0
27	GLA	F	2010	-	11,11,12	1.80	3 (27%)	15,15,17	0.90	0
27	GLA	A	2008	-	11,11,12	1.79	2 (18%)	15,15,17	1.59	2 (13%)
26	AHR	C	2001	-	9,9,10	0.55	0	10,12,14	1.61	1 (10%)
27	GLA	D	2008	1	11,11,12	1.77	3 (27%)	15,15,17	0.78	0
26	AHR	F	2005	-	9,9,10	0.67	0	10,12,14	1.57	3 (30%)
26	AHR	F	2019	-	9,9,10	0.56	0	10,12,14	0.63	0
28	NAG	C	2010	1	14,14,15	0.32	0	17,19,21	0.91	1 (5%)
26	AHR	B	2002	-	9,9,10	0.56	0	10,12,14	1.16	1 (10%)
28	NAG	B	2018	1	14,14,15	0.35	0	17,19,21	0.81	0
27	GLA	F	2015	1	11,11,12	1.78	3 (27%)	15,15,17	0.70	0
27	GLA	C	2007	1	11,11,12	1.80	3 (27%)	15,15,17	0.89	0
26	AHR	D	2001	-	9,9,10	0.68	0	10,12,14	1.55	2 (20%)
27	GLA	B	2008	1	11,11,12	1.76	2 (18%)	15,15,17	0.81	0
26	AHR	D	2004	-	9,9,10	0.69	0	10,12,14	1.59	3 (30%)
27	GLA	C	2006	1	11,11,12	1.71	2 (18%)	15,15,17	0.84	0
27	GLA	E	2015	1	11,11,12	1.71	2 (18%)	15,15,17	1.36	1 (6%)
26	AHR	B	2020	-	9,9,10	0.90	0	10,12,14	1.02	1 (10%)
27	GLA	D	2007	1	11,11,12	1.73	2 (18%)	15,15,17	0.93	0
26	AHR	E	2002	-	9,9,10	0.82	1 (11%)	10,12,14	1.59	2 (20%)
27	GLA	E	2016	1	11,11,12	1.85	3 (27%)	15,15,17	0.85	0
27	GLA	A	2006	1	11,11,12	1.81	3 (27%)	15,15,17	1.02	1 (6%)
27	GLA	A	2014	1	11,11,12	1.80	2 (18%)	15,15,17	0.93	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. <sup>1,2</sup> means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	GLA	F	2011	1	-	1/2/19/22	0/1/1/1
27	GLA	E	2005	1	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	GLA	B	2005	1	-	0/2/19/22	0/1/1/1
26	AHR	C	2003	-	-	2/2/15/18	0/1/1/1
27	GLA	A	2011	1	-	2/2/19/22	0/1/1/1
28	NAG	C	2009	1	-	4/6/23/26	0/1/1/1
27	GLA	F	2009	1	1/1/4/5	2/2/19/22	0/1/1/1
26	AHR	E	2003	-	-	2/2/15/18	0/1/1/1
27	GLA	B	2013	1	-	1/2/19/22	0/1/1/1
27	GLA	C	2005	1	-	2/2/19/22	0/1/1/1
27	GLA	E	2011	1	-	2/2/19/22	0/1/1/1
26	AHR	F	2004	-	-	2/2/15/18	0/1/1/1
26	AHR	A	2003	-	-	2/2/15/18	0/1/1/1
27	GLA	F	2016	1	-	2/2/19/22	0/1/1/1
26	AHR	F	2001	-	-	2/2/15/18	0/1/1/1
26	AHR	F	2003	-	-	1/2/15/18	0/1/1/1
28	NAG	D	2010	1	-	0/6/23/26	0/1/1/1
27	GLA	F	2006	1	-	0/2/19/22	0/1/1/1
27	GLA	A	2012	1	-	2/2/19/22	0/1/1/1
27	GLA	B	2007	1	-	2/2/19/22	0/1/1/1
27	GLA	B	2010	1	-	2/2/19/22	0/1/1/1
27	GLA	E	2009	1	-	0/2/19/22	0/1/1/1
27	GLA	B	2011	1	-	1/2/19/22	0/1/1/1
28	NAG	A	2017	1	-	2/6/23/26	0/1/1/1
27	GLA	D	2005	1	-	2/2/19/22	0/1/1/1
27	GLA	A	2015	1	-	2/2/19/22	0/1/1/1
27	GLA	B	2015	1	-	2/2/19/22	0/1/1/1
27	GLA	A	2009	1	-	1/2/19/22	0/1/1/1
27	GLA	A	2004	1	-	0/2/19/22	0/1/1/1
27	GLA	A	2013	1	-	0/2/19/22	0/1/1/1
27	GLA	E	2004	1	-	0/2/19/22	0/1/1/1
27	GLA	B	2012	1	-	1/2/19/22	0/1/1/1
27	GLA	C	2004	1	-	2/2/19/22	0/1/1/1
27	GLA	A	2010	1	-	2/2/19/22	0/1/1/1
27	GLA	B	2016	1	-	2/2/19/22	0/1/1/1
27	GLA	F	2017	1	-	2/2/19/22	0/1/1/1
27	GLA	A	2007	1	1/1/4/5	2/2/19/22	0/1/1/1
27	GLA	F	2013	1	-	0/2/19/22	0/1/1/1
27	GLA	A	2005	1	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	AHR	A	2018	-	-	0/2/15/18	0/1/1/1
27	GLA	E	2014	1	-	2/2/19/22	0/1/1/1
27	GLA	E	2008	-	-	2/2/19/22	0/1/1/1
27	GLA	D	2006	1	-	0/2/19/22	0/1/1/1
27	GLA	B	2017	1	-	2/2/19/22	0/1/1/1
27	GLA	F	2018	1	-	2/2/19/22	0/1/1/1
27	GLA	D	2009	1	-	2/2/19/22	0/1/1/1
27	GLA	F	2012	1	-	2/2/19/22	0/1/1/1
28	NAG	E	2017	1	-	4/6/23/26	0/1/1/1
27	GLA	E	2010	1	-	1/2/19/22	0/1/1/1
27	GLA	E	2006	1	-	2/2/19/22	0/1/1/1
26	AHR	A	2002	-	-	2/2/15/18	0/1/1/1
27	GLA	E	2013	1	-	2/2/19/22	0/1/1/1
28	NAG	B	2019	1	-	2/6/23/26	0/1/1/1
27	GLA	A	2016	1	-	1/2/19/22	0/1/1/1
27	GLA	F	2007	1	-	2/2/19/22	0/1/1/1
27	GLA	E	2007	1	1/1/4/5	2/2/19/22	0/1/1/1
27	GLA	B	2009	-	-	2/2/19/22	0/1/1/1
27	GLA	F	2014	1	-	2/2/19/22	0/1/1/1
26	AHR	B	2004	-	-	2/2/15/18	0/1/1/1
26	AHR	B	2003	-	-	2/2/15/18	0/1/1/1
27	GLA	C	2008	1	-	2/2/19/22	0/1/1/1
27	GLA	B	2006	1	-	0/2/19/22	0/1/1/1
27	GLA	F	2008	1	-	1/2/19/22	0/1/1/1
26	AHR	D	2003	-	-	2/2/15/18	0/1/1/1
27	GLA	E	2012	1	-	1/2/19/22	0/1/1/1
27	GLA	B	2014	1	1/1/4/5	0/2/19/22	0/1/1/1
26	AHR	A	2019	-	-	0/2/15/18	0/1/1/1
27	GLA	F	2010	-	-	2/2/19/22	0/1/1/1
27	GLA	A	2008	-	-	2/2/19/22	0/1/1/1
26	AHR	C	2001	-	-	2/2/15/18	0/1/1/1
27	GLA	D	2008	1	-	2/2/19/22	0/1/1/1
26	AHR	F	2005	-	-	2/2/15/18	0/1/1/1
26	AHR	F	2019	-	-	0/2/15/18	0/1/1/1
28	NAG	C	2010	1	-	4/6/23/26	0/1/1/1
26	AHR	B	2002	-	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	NAG	B	2018	1	-	4/6/23/26	0/1/1/1
27	GLA	F	2015	1	-	0/2/19/22	0/1/1/1
27	GLA	C	2007	1	-	2/2/19/22	0/1/1/1
26	AHR	D	2001	-	-	1/2/15/18	0/1/1/1
27	GLA	B	2008	1	1/1/4/5	2/2/19/22	0/1/1/1
26	AHR	D	2004	-	-	2/2/15/18	0/1/1/1
27	GLA	C	2006	1	-	0/2/19/22	0/1/1/1
27	GLA	E	2015	1	-	0/2/19/22	0/1/1/1
26	AHR	B	2020	-	-	1/2/15/18	0/1/1/1
27	GLA	D	2007	1	-	2/2/19/22	0/1/1/1
26	AHR	E	2002	-	-	2/2/15/18	0/1/1/1
27	GLA	E	2016	1	-	2/2/19/22	0/1/1/1
27	GLA	A	2006	1	-	1/2/19/22	0/1/1/1
27	GLA	A	2014	1	-	2/2/19/22	0/1/1/1

The worst 5 of 168 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	2004	GLA	O5-C1	4.89	1.51	1.43
27	B	2005	GLA	O5-C1	4.86	1.51	1.43
27	B	2009	GLA	O5-C1	4.77	1.51	1.43
27	E	2004	GLA	O5-C1	4.73	1.51	1.43
27	A	2008	GLA	O5-C1	4.73	1.51	1.43

The worst 5 of 98 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	F	2006	GLA	O5-C1-C2	5.56	119.35	110.77
27	B	2009	GLA	C1-C2-C3	4.96	115.76	109.67
27	E	2004	GLA	O5-C1-C2	4.71	118.04	110.77
27	B	2005	GLA	O5-C1-C2	4.65	117.95	110.77
27	A	2004	GLA	O5-C1-C2	4.47	117.67	110.77

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
27	A	2007	GLA	C1
27	B	2008	GLA	C1
27	B	2014	GLA	C1
27	E	2007	GLA	C1

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Mol	Chain	Res	Type	Atom
27	F	2009	GLA	C1

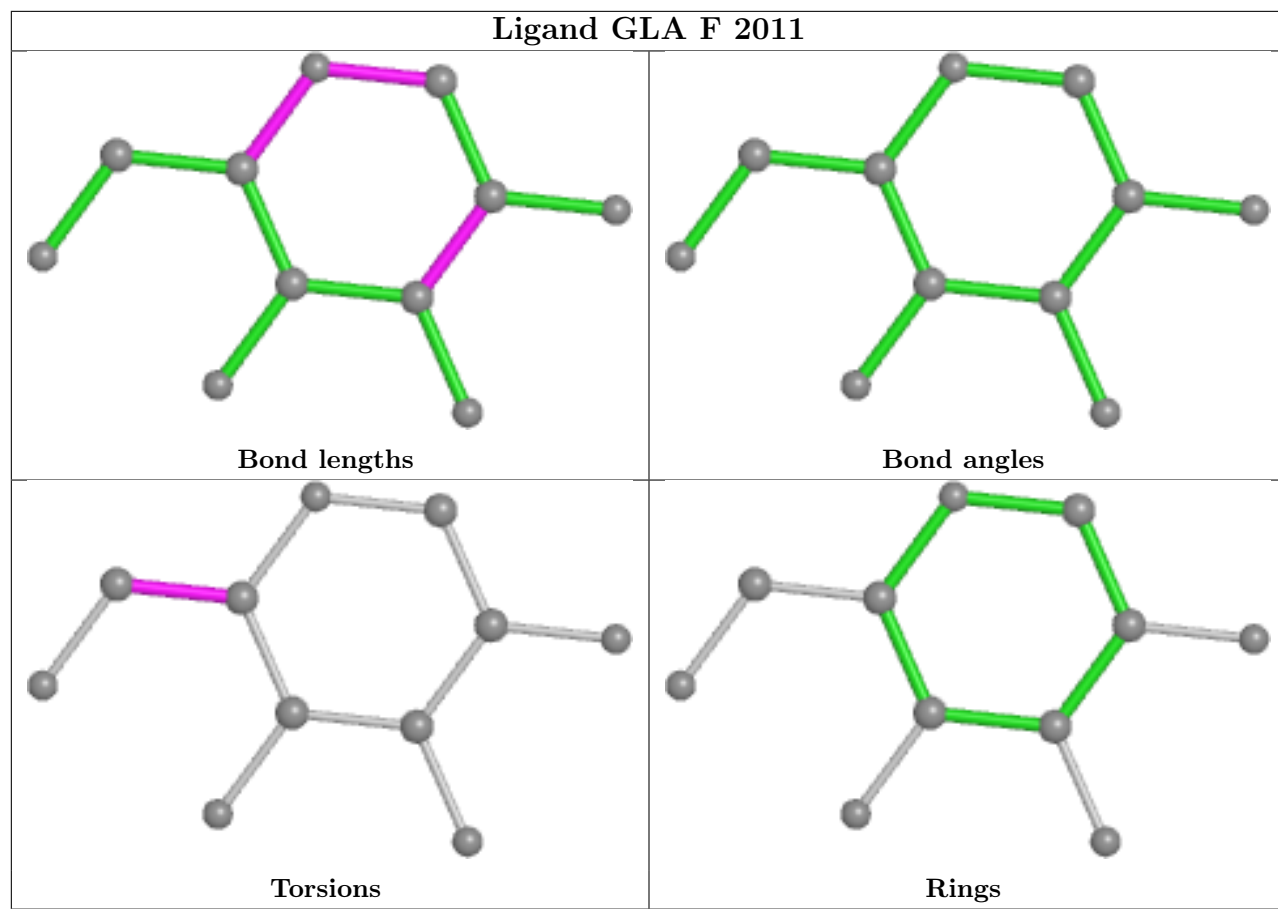
5 of 135 torsion outliers are listed below:

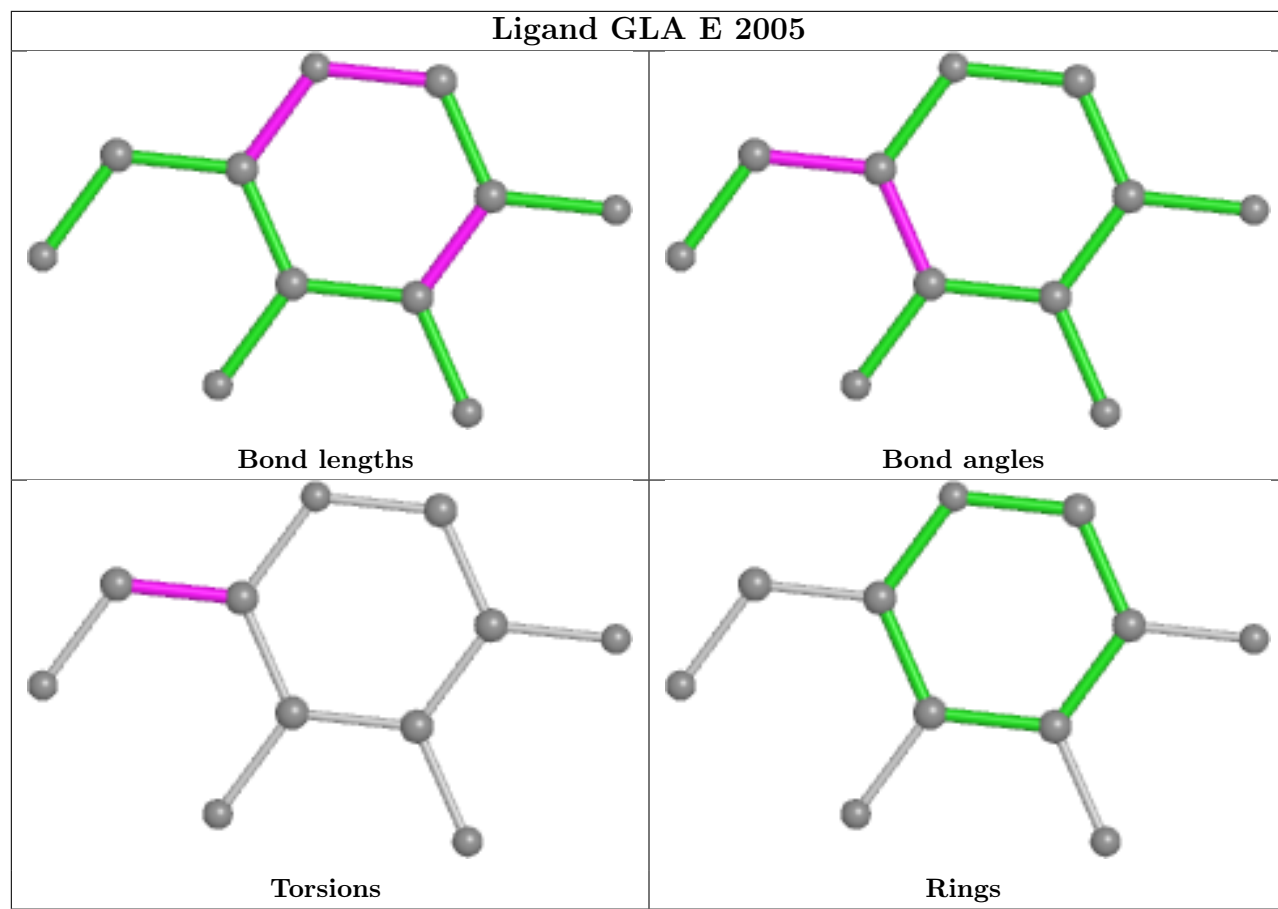
Mol	Chain	Res	Type	Atoms
28	B	2018	NAG	C3-C2-N2-C7
28	B	2018	NAG	C8-C7-N2-C2
28	B	2018	NAG	O7-C7-N2-C2
28	C	2009	NAG	C3-C2-N2-C7
28	C	2009	NAG	C8-C7-N2-C2

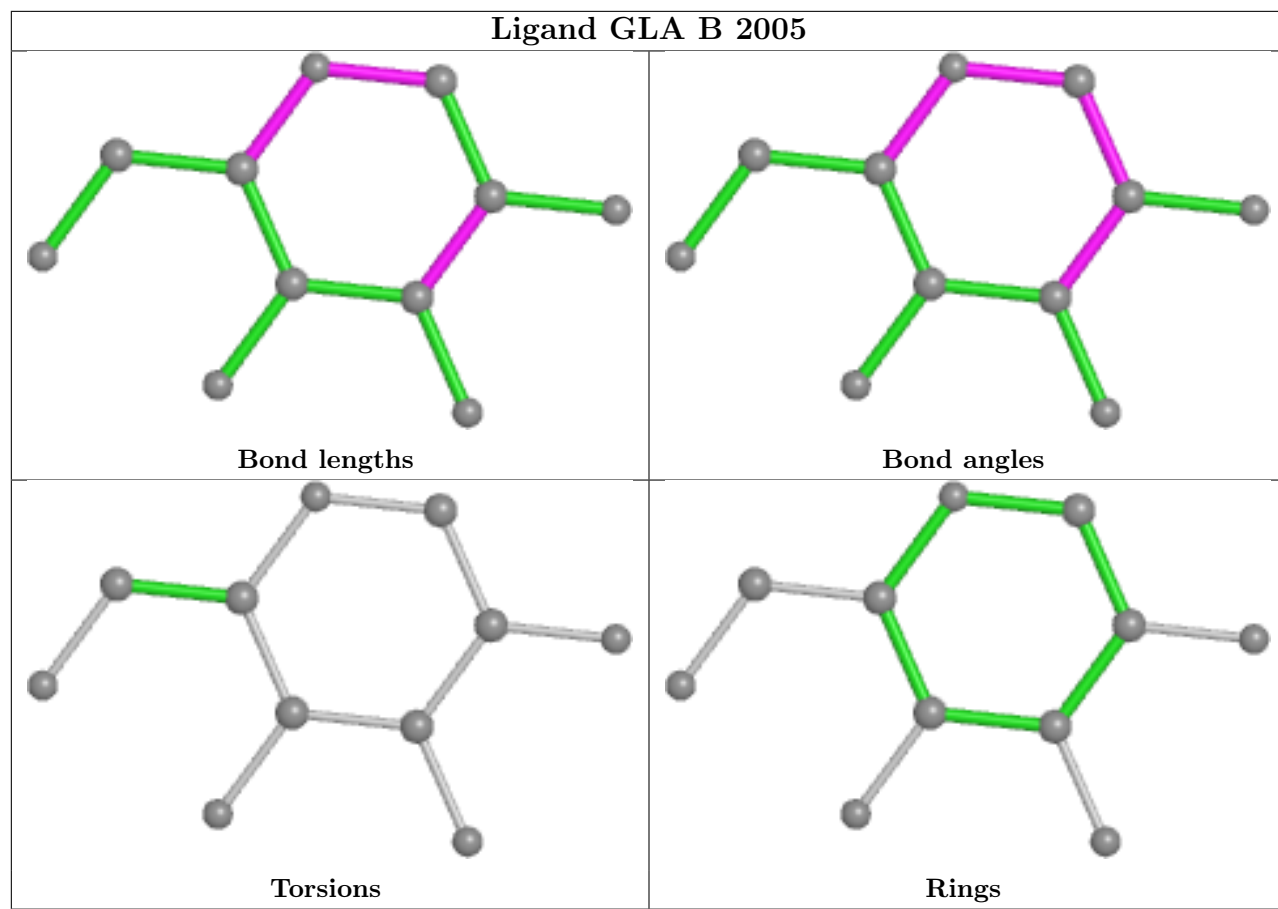
There are no ring outliers.

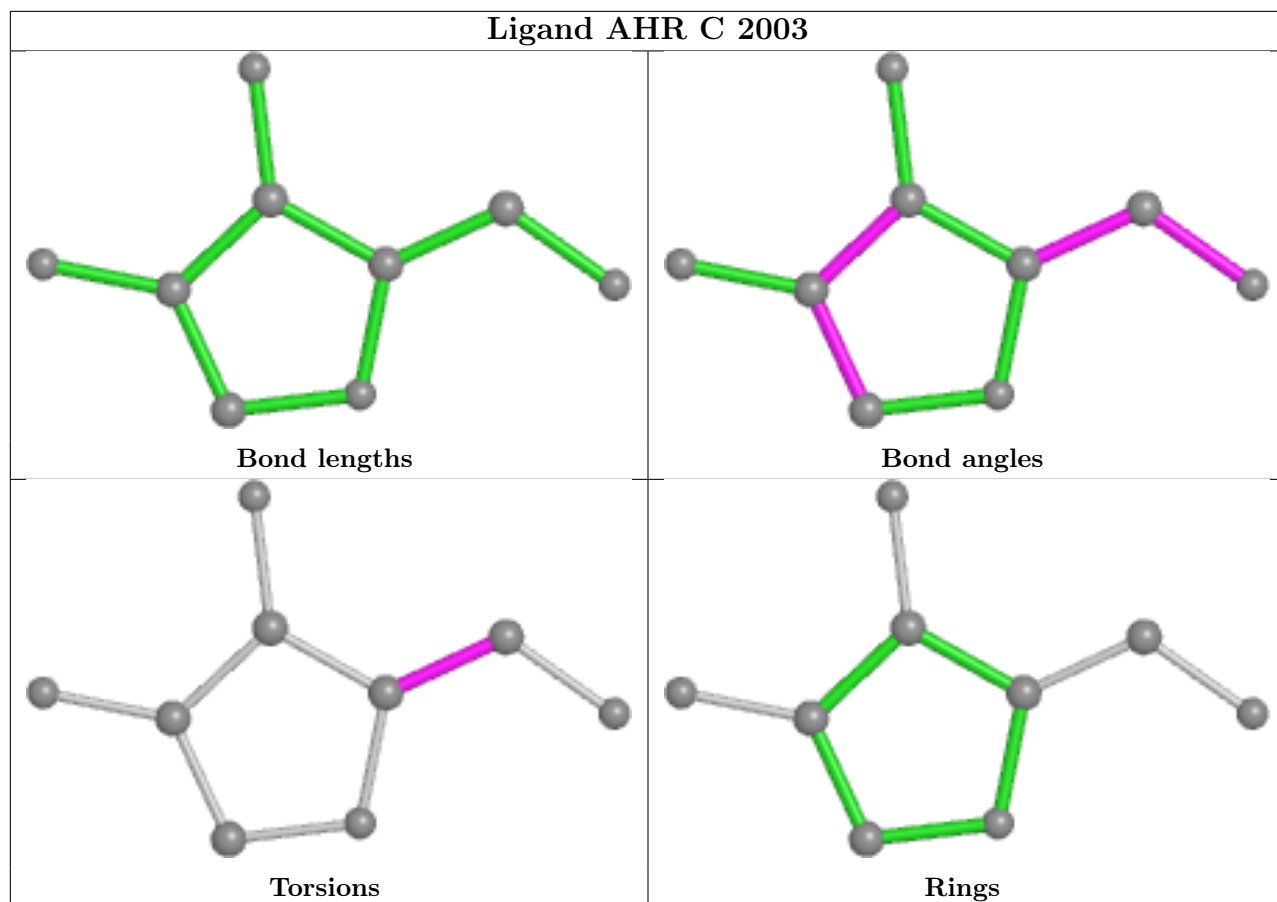
No monomer is involved in short contacts.

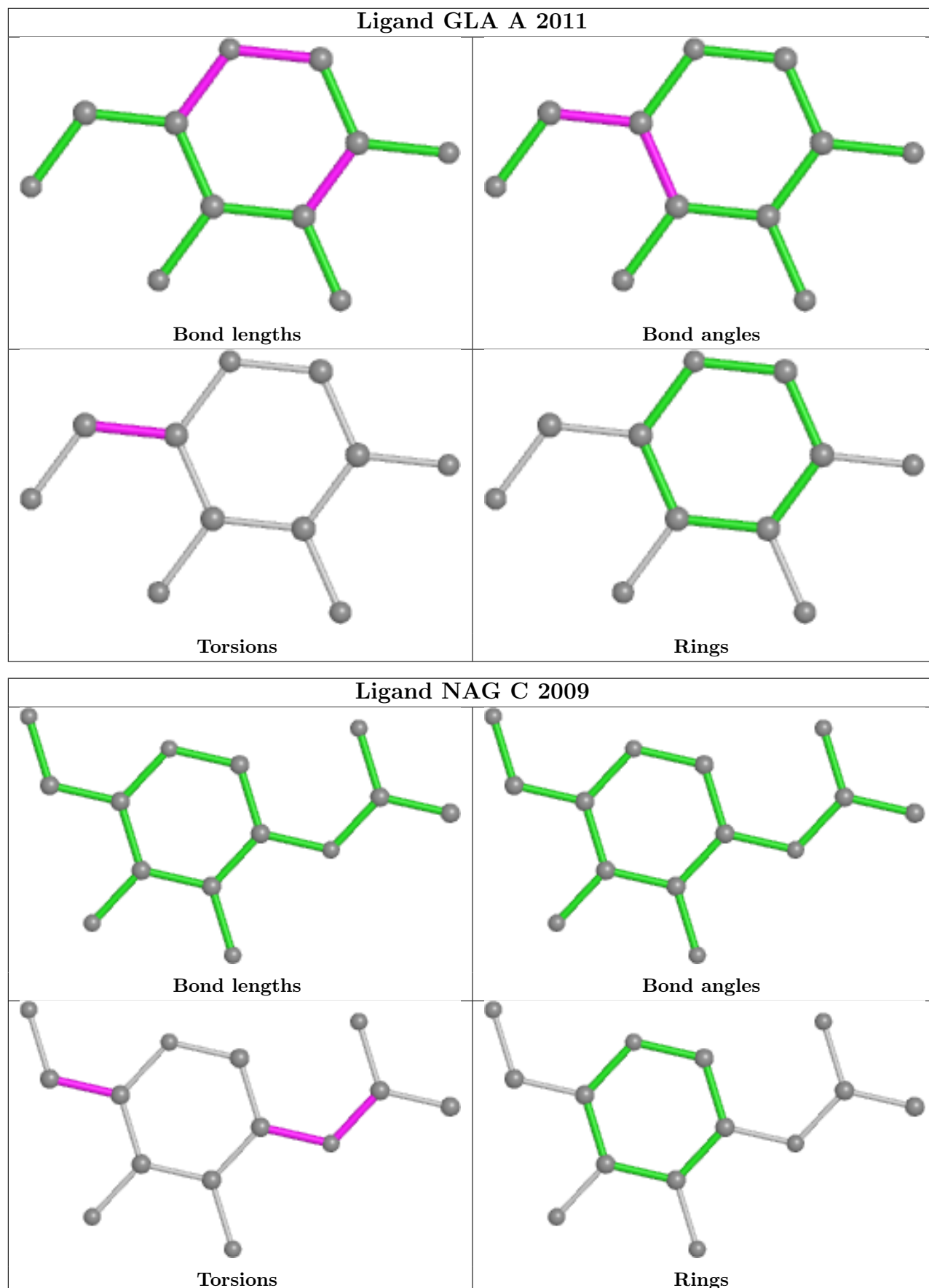
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

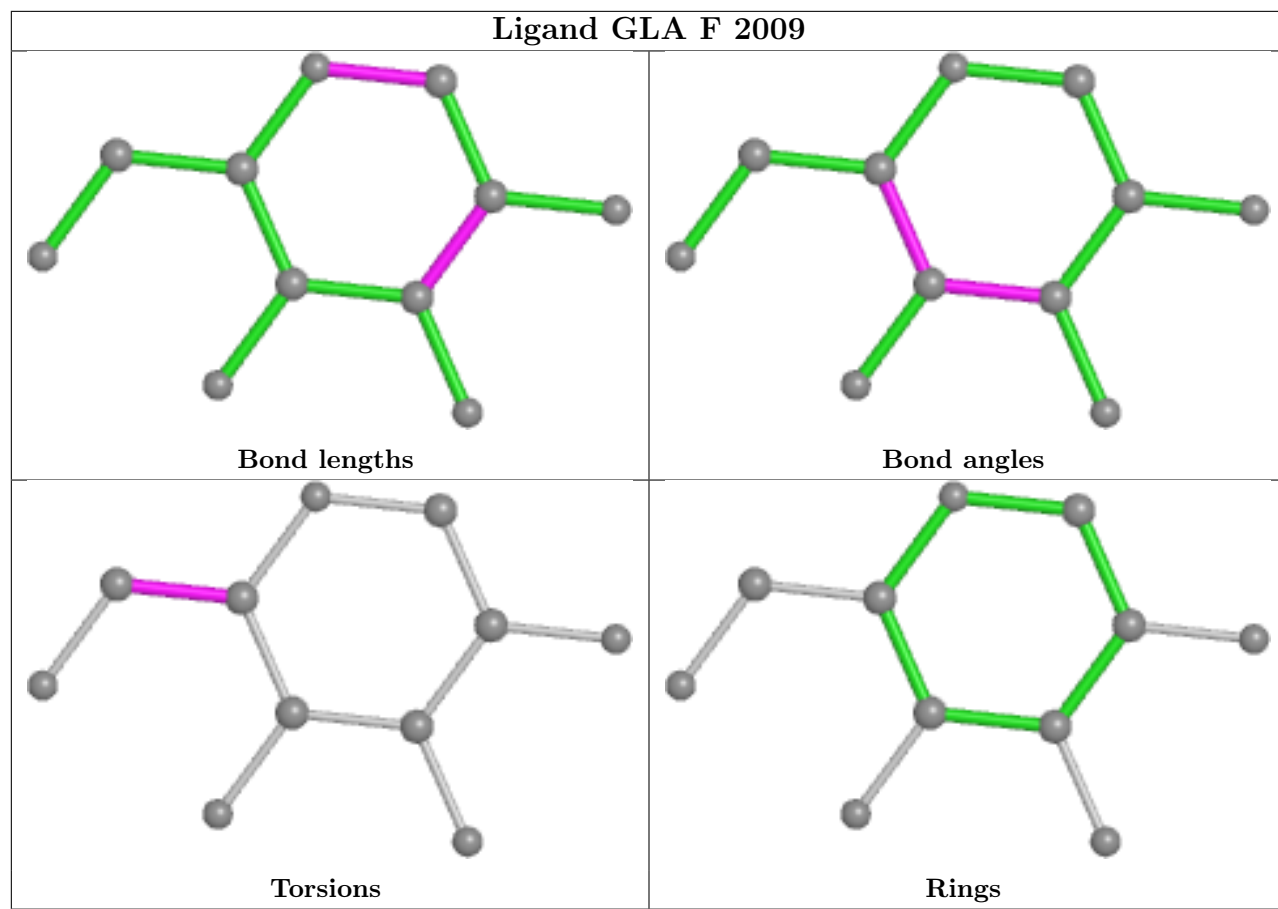




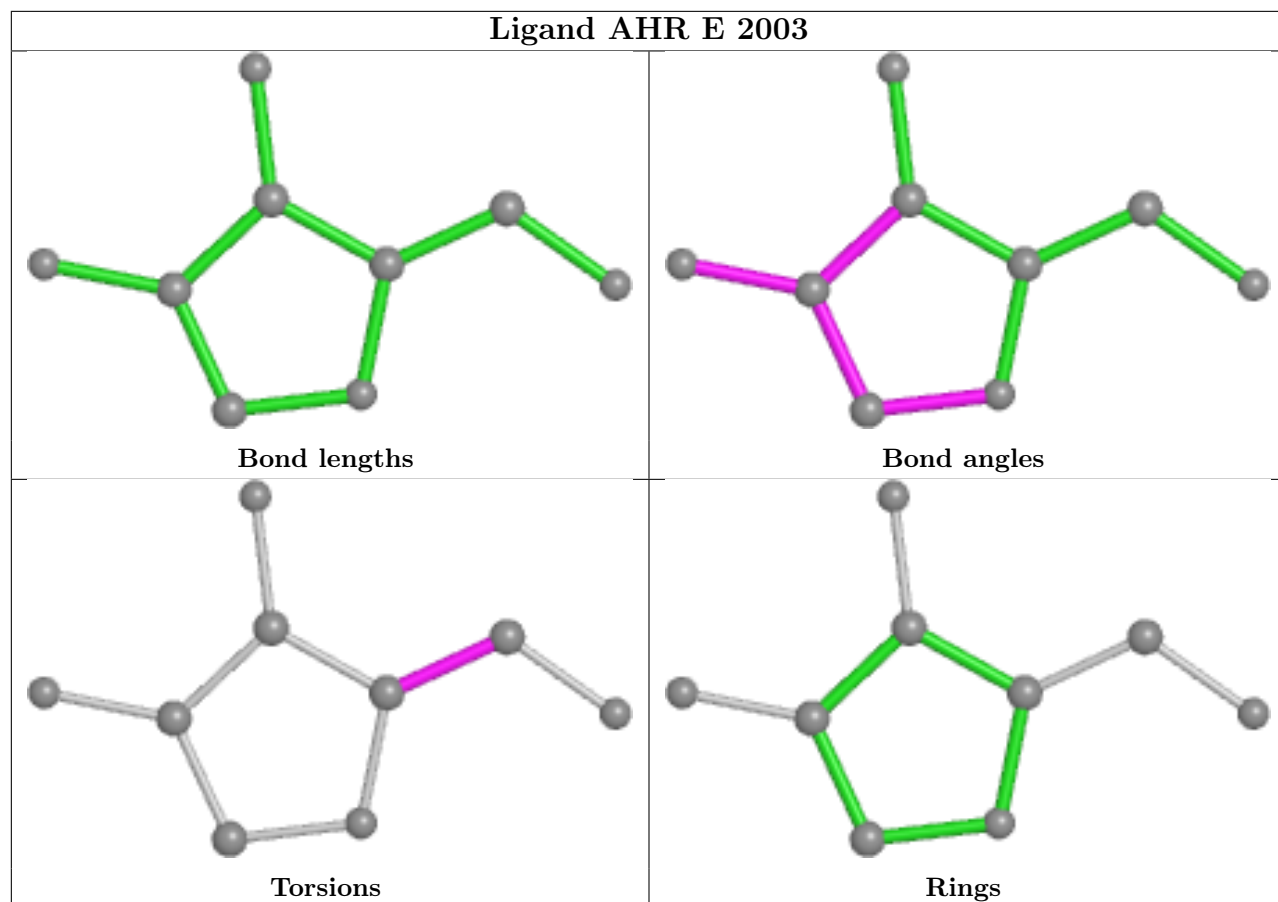


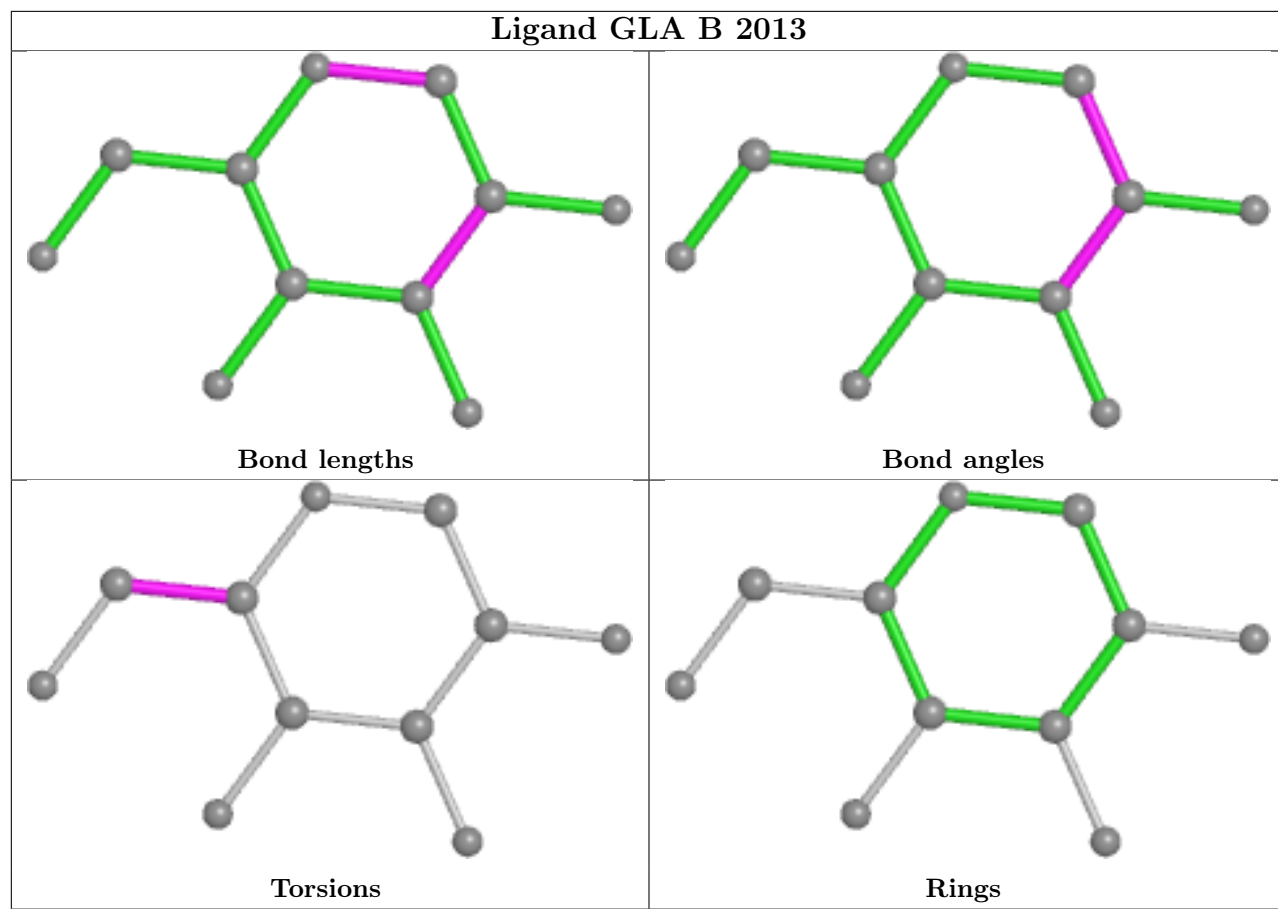


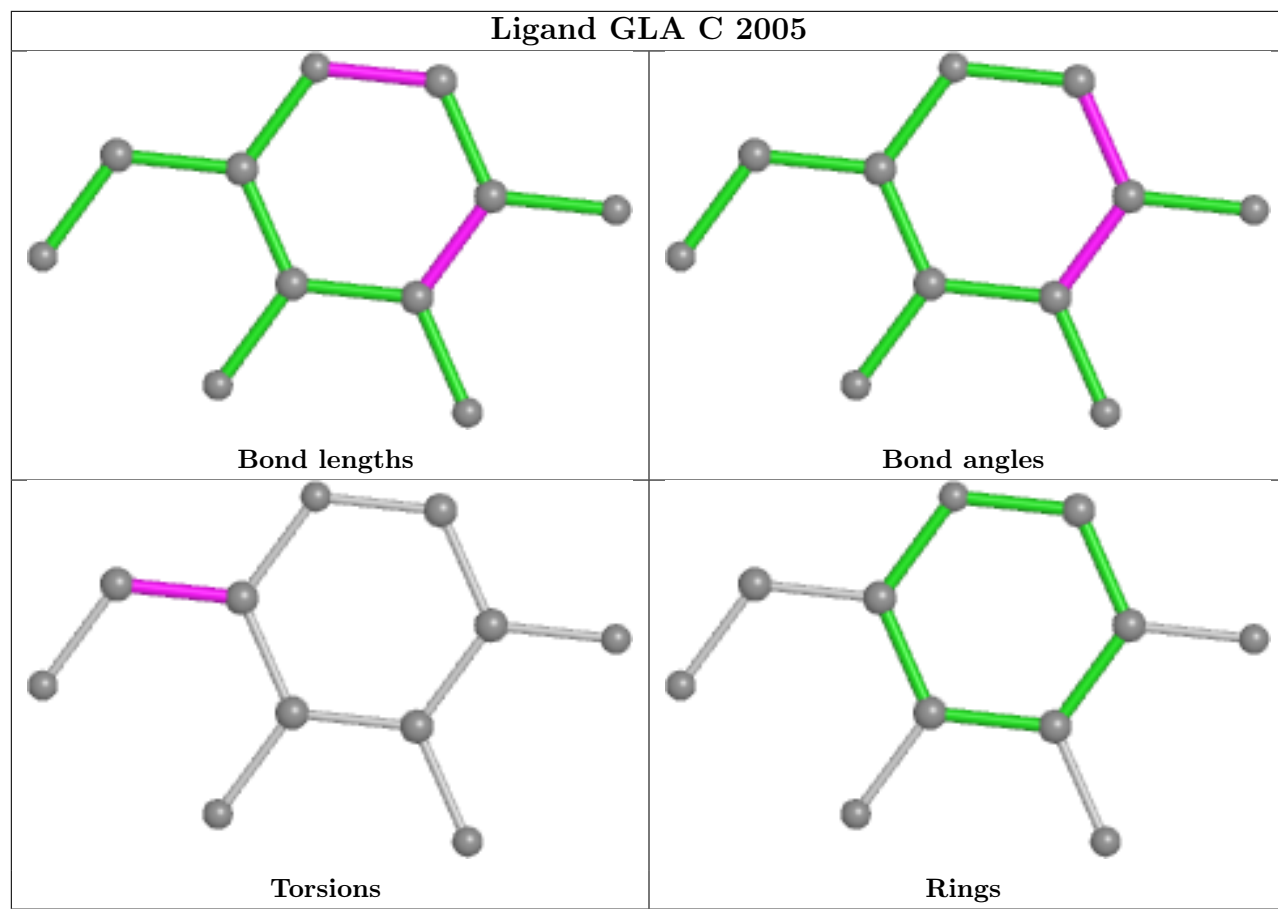


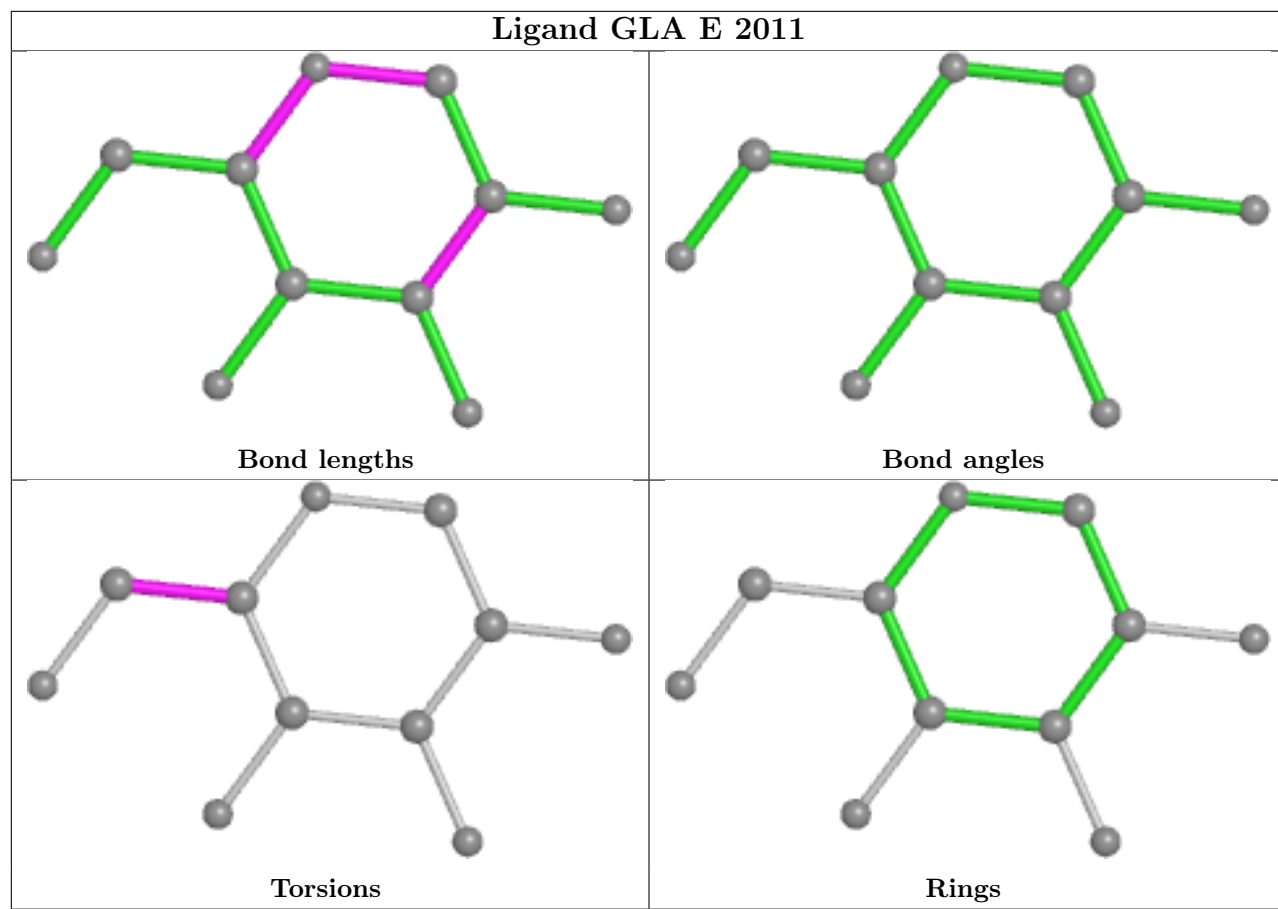


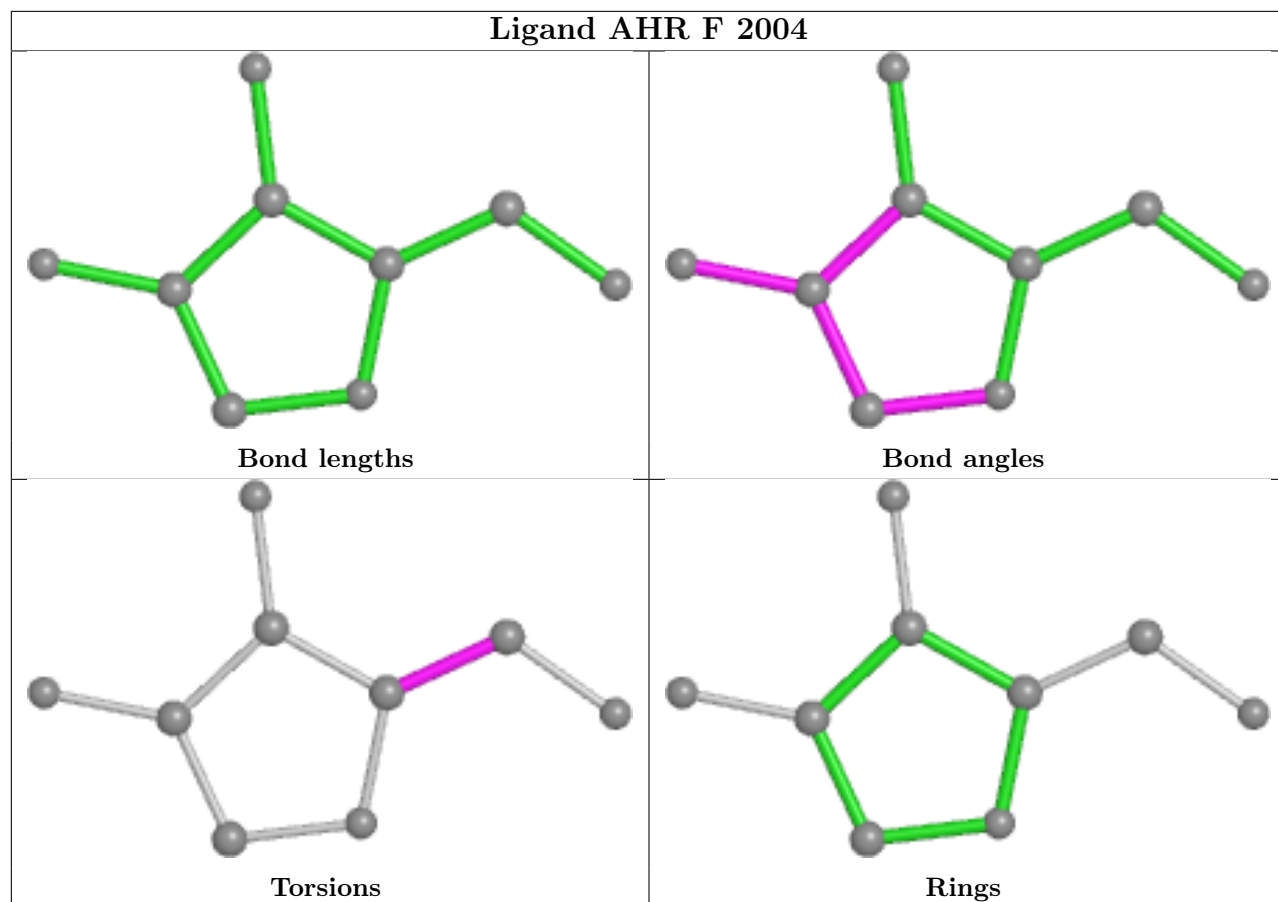


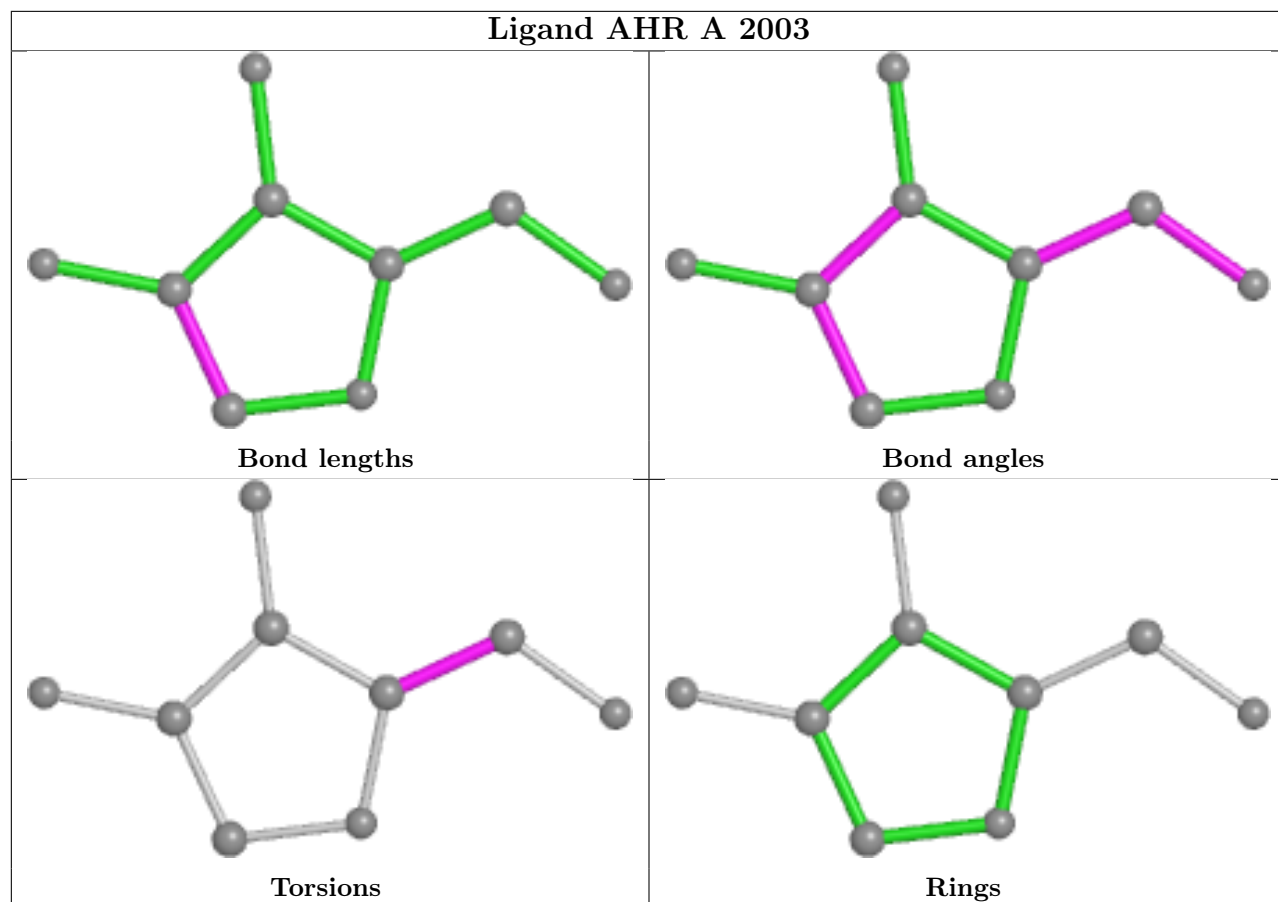


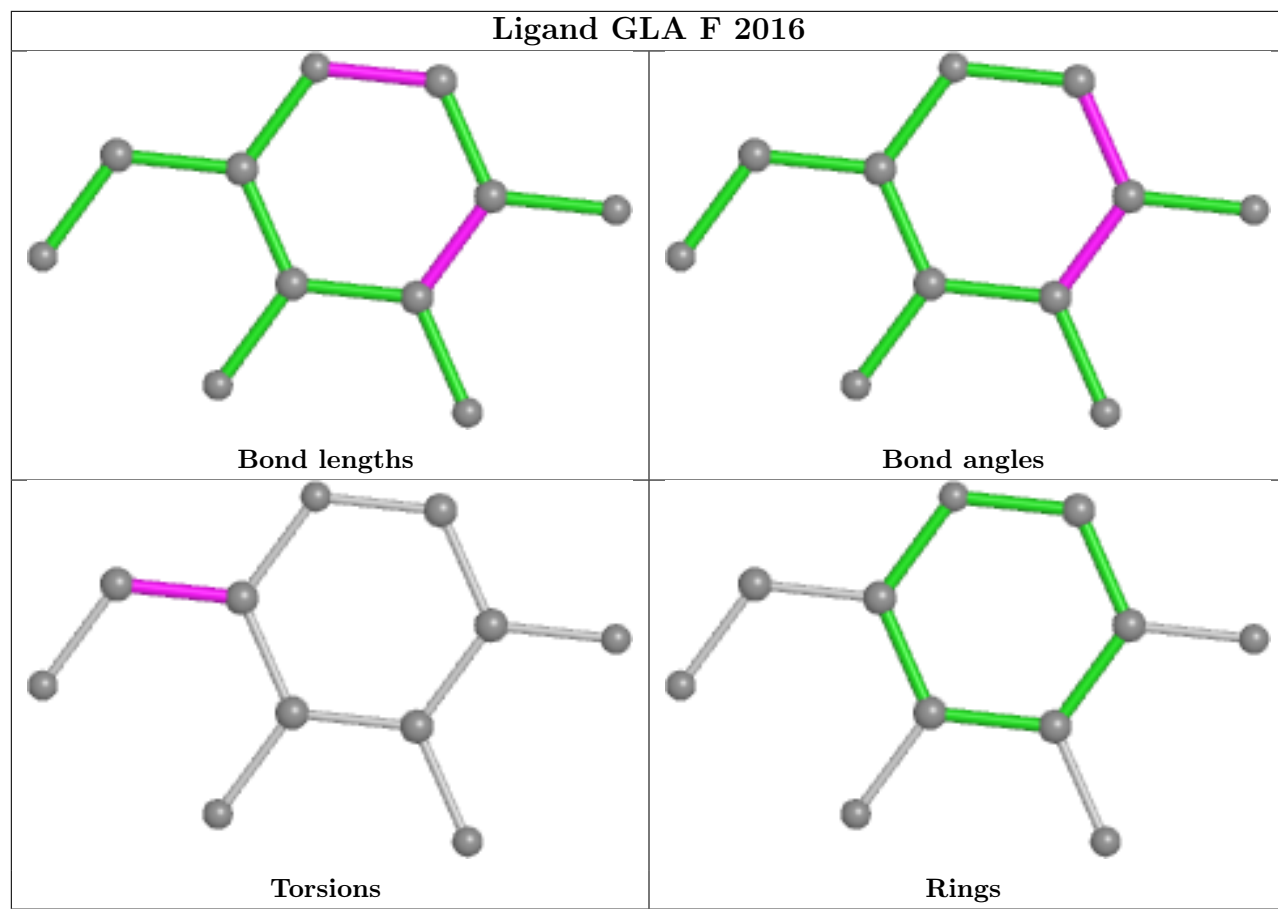


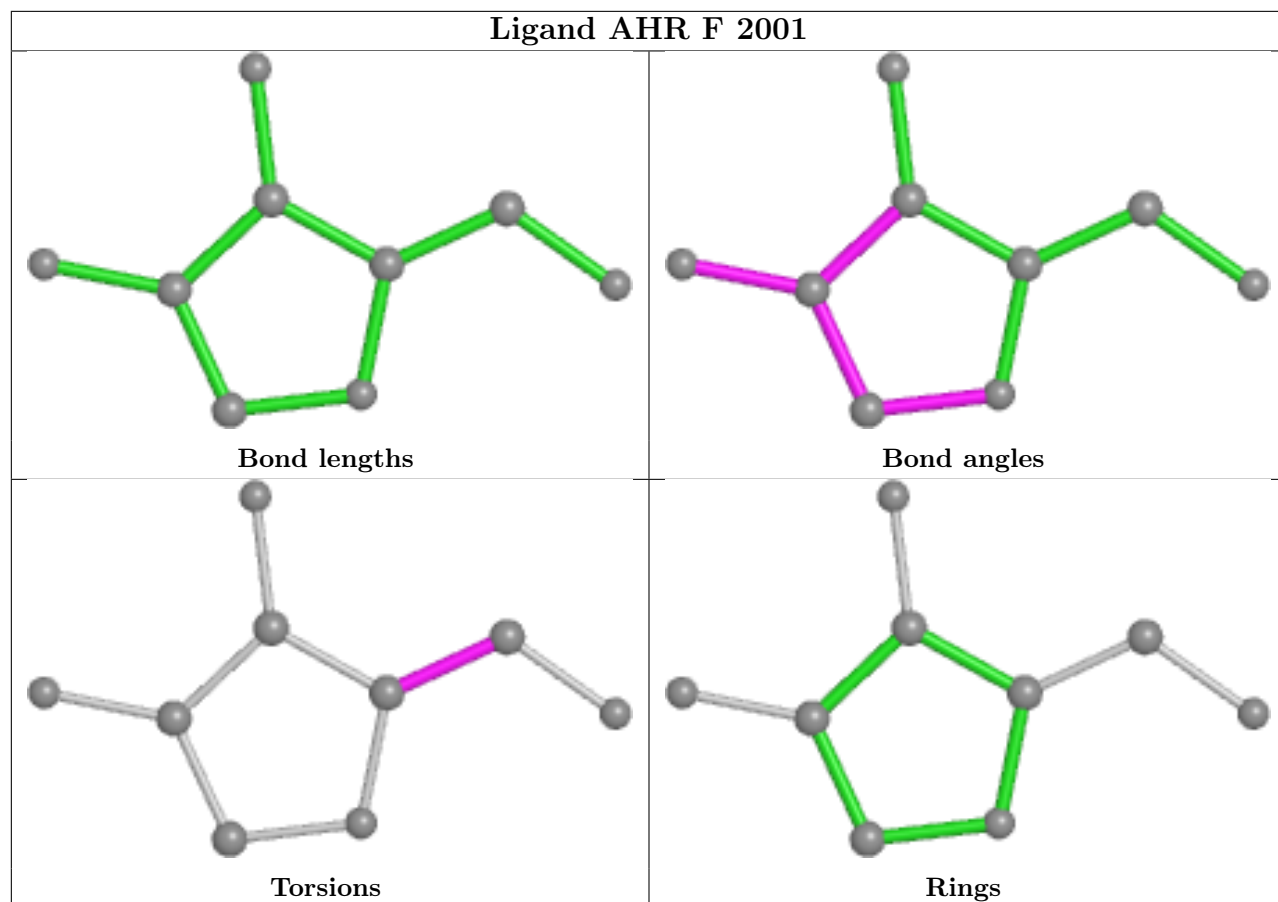




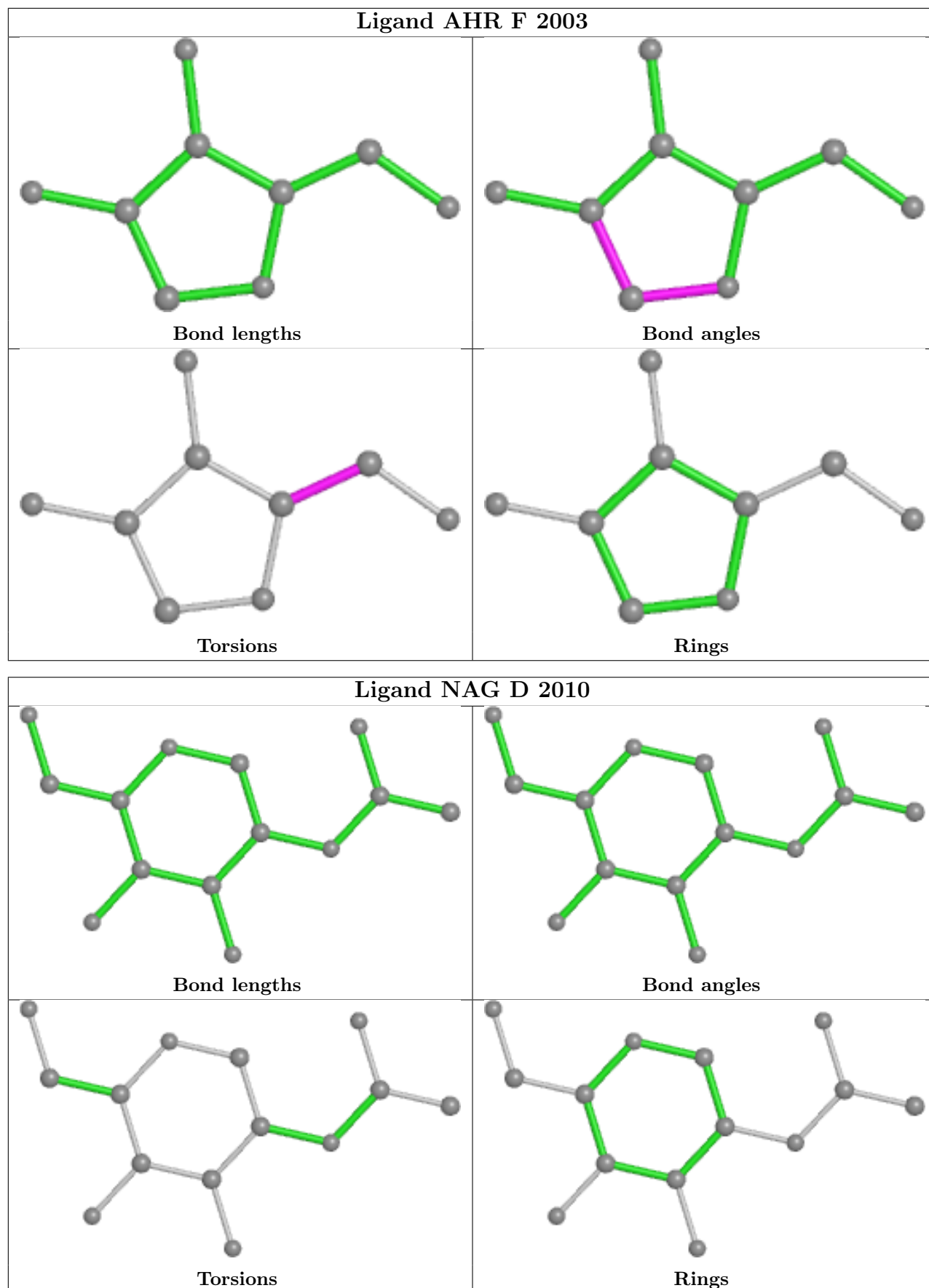


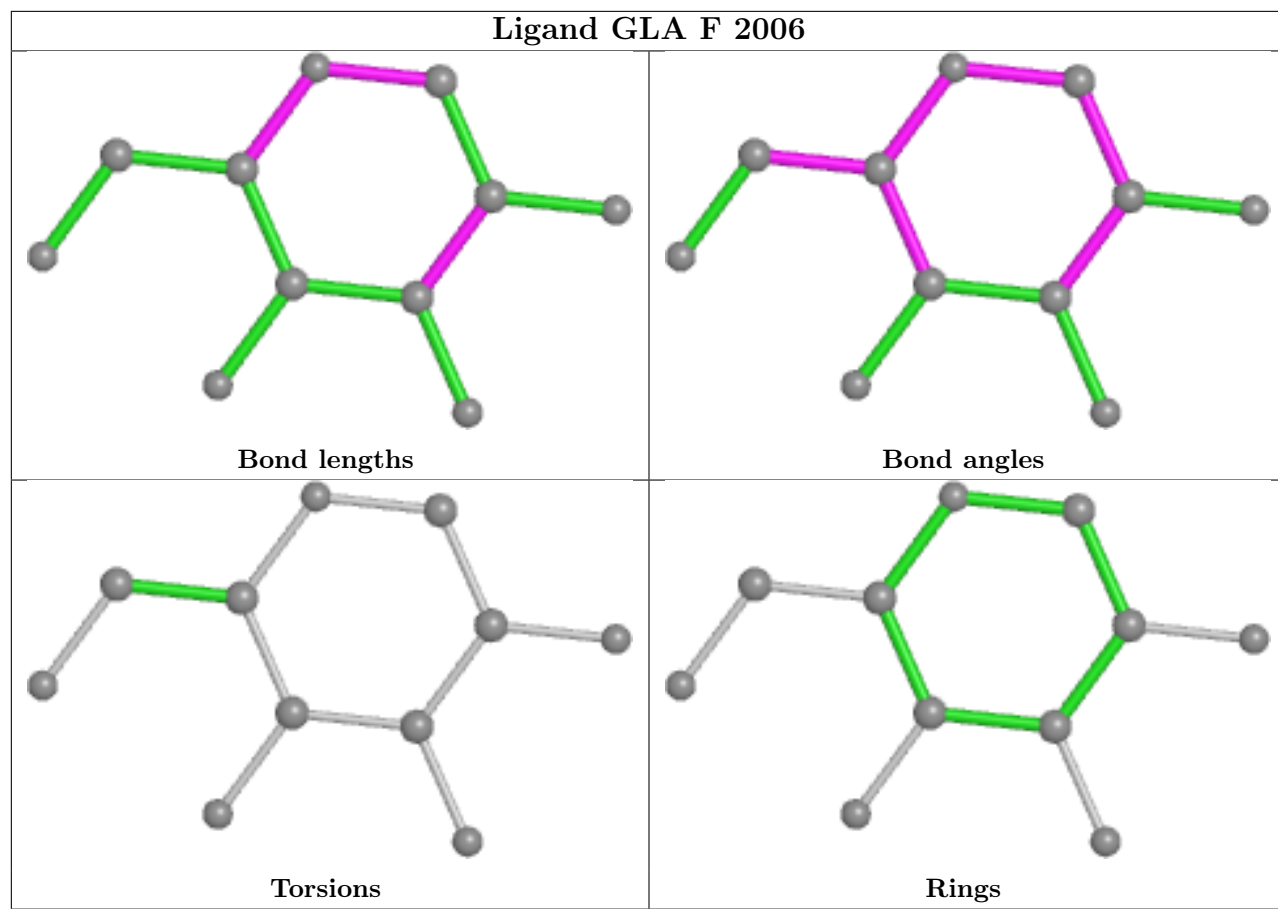


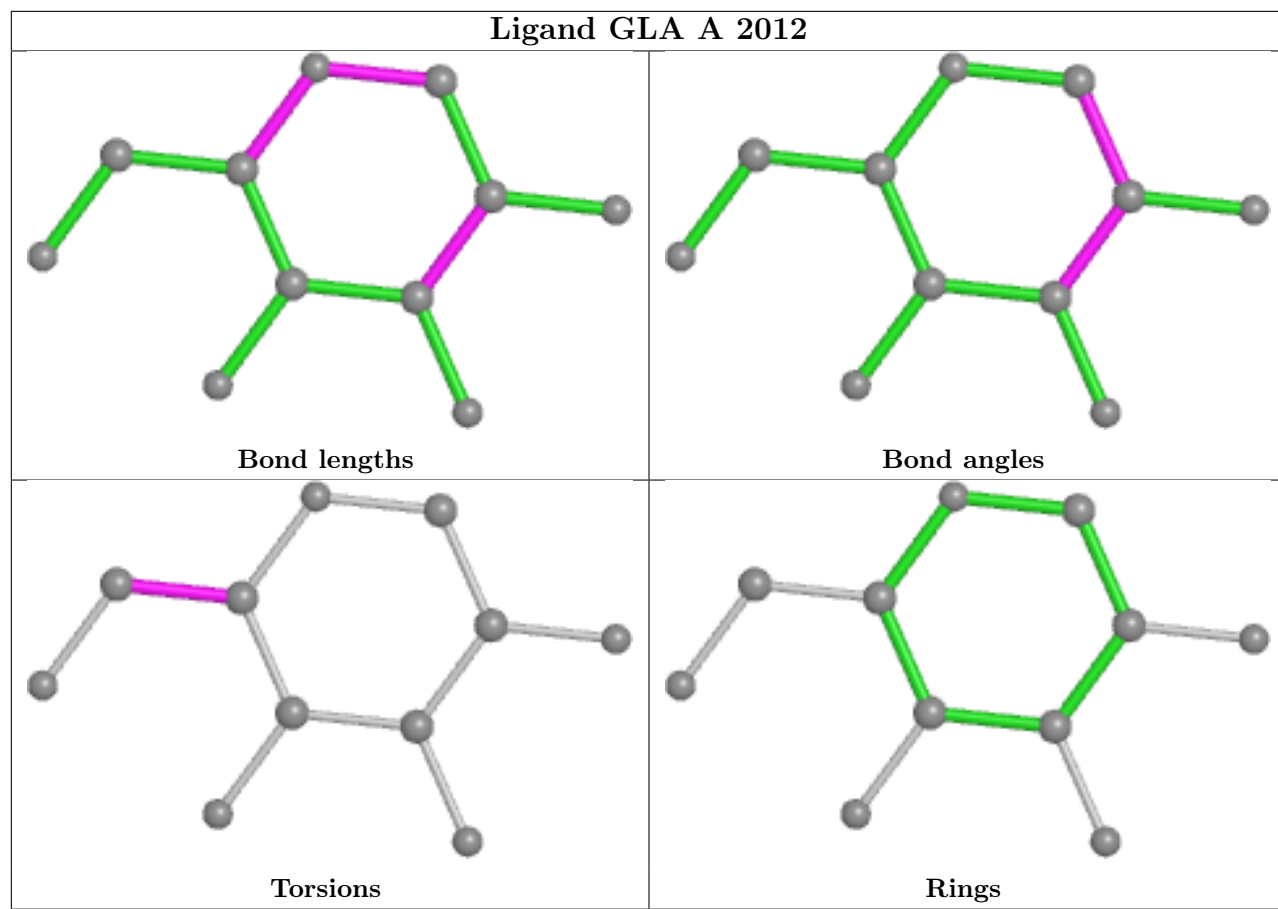


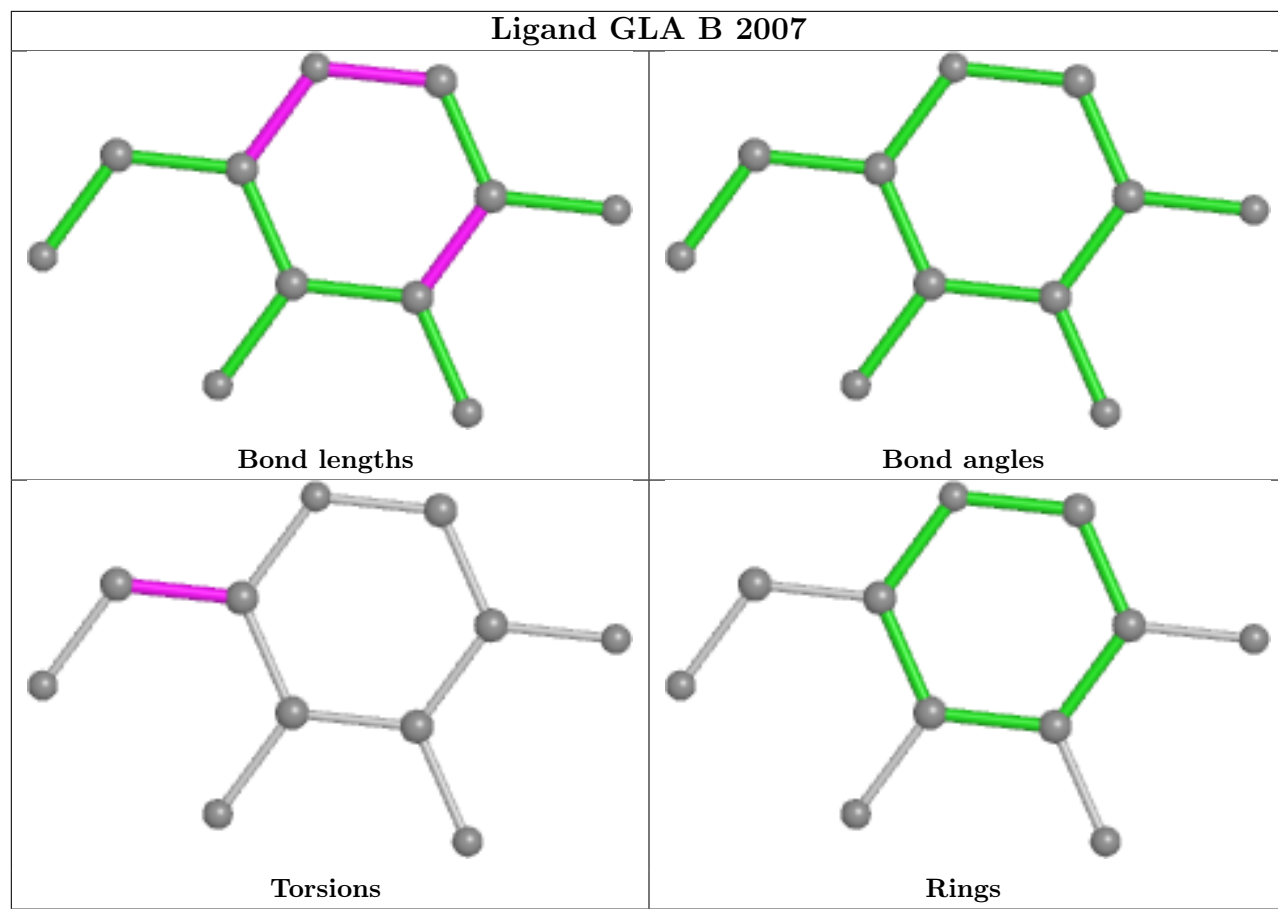


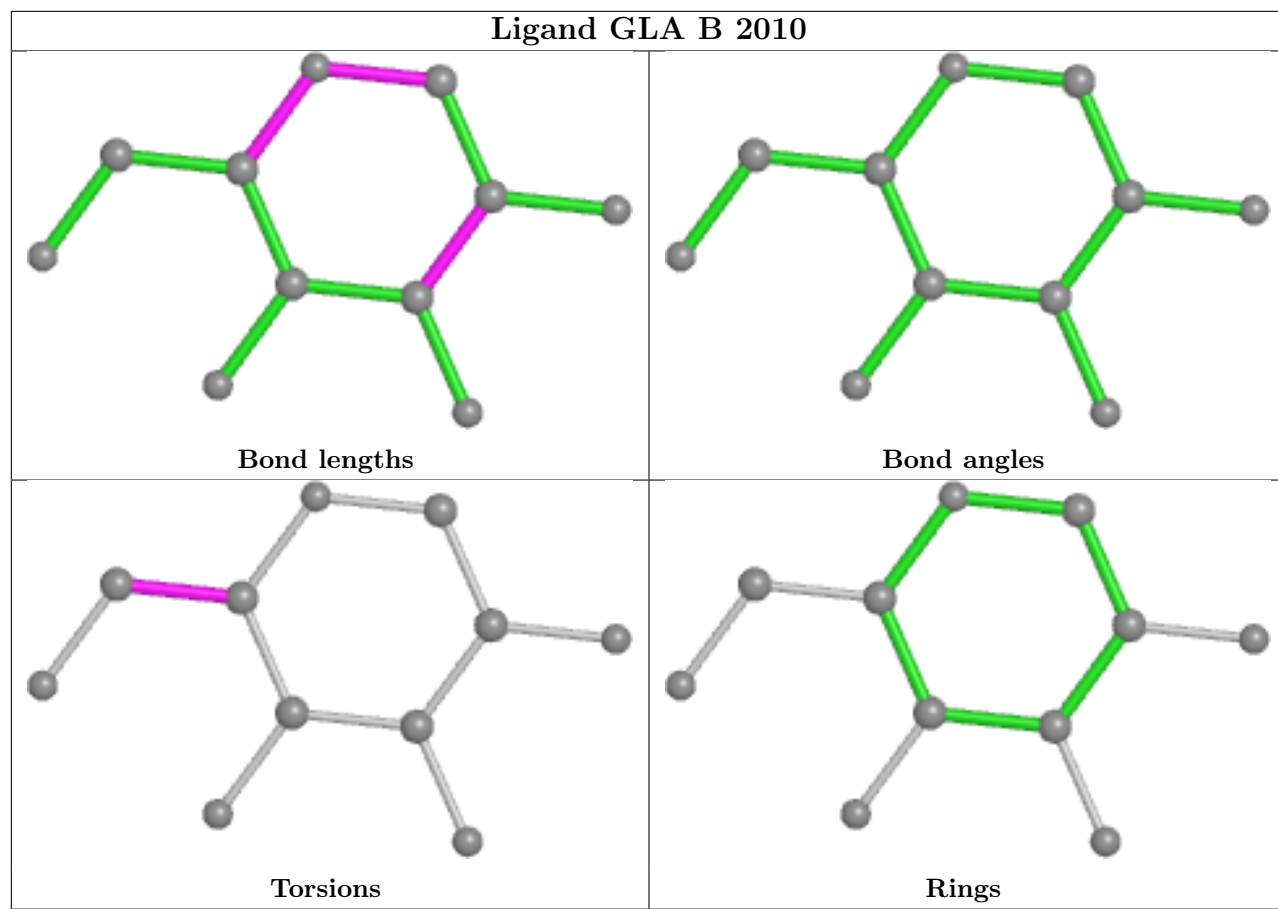


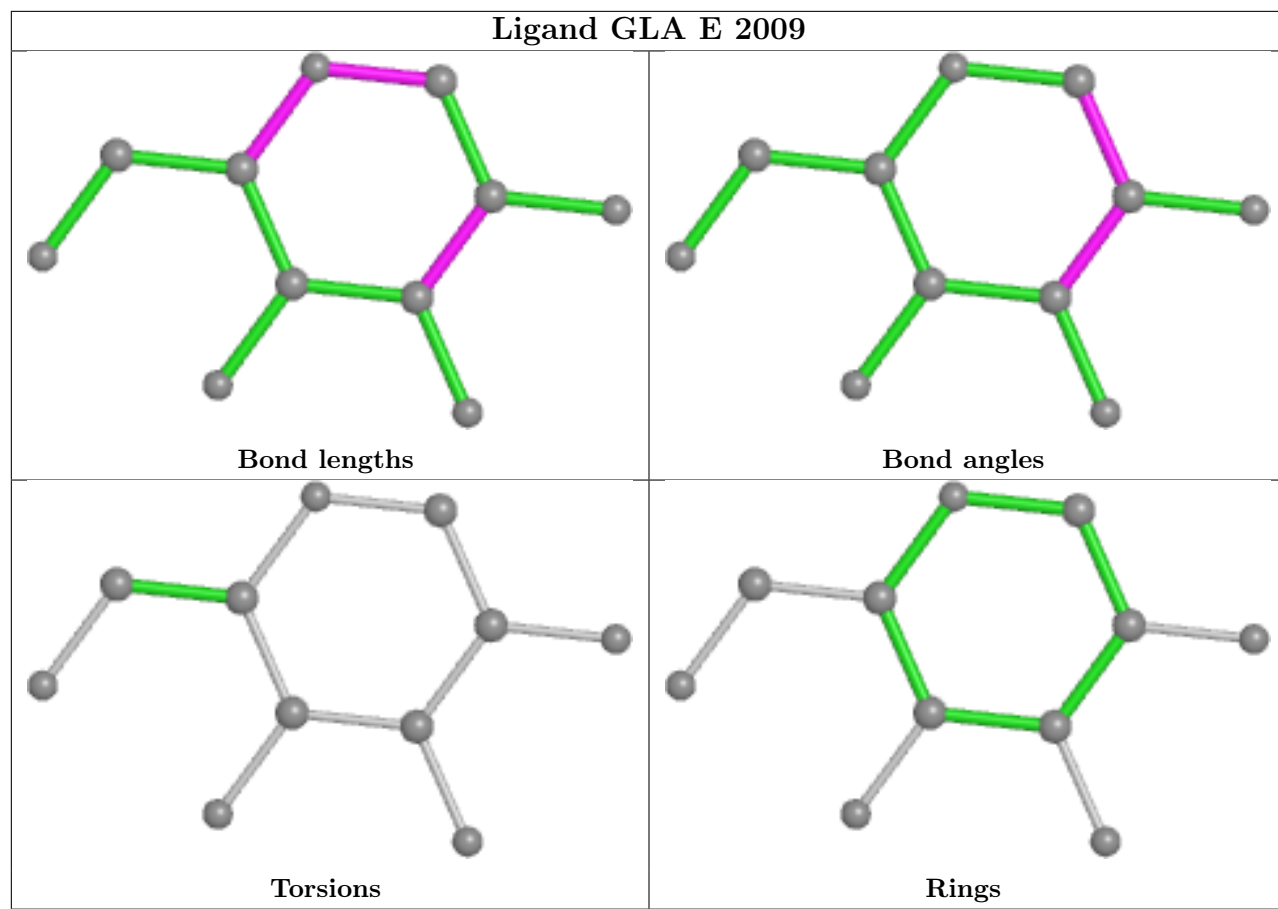


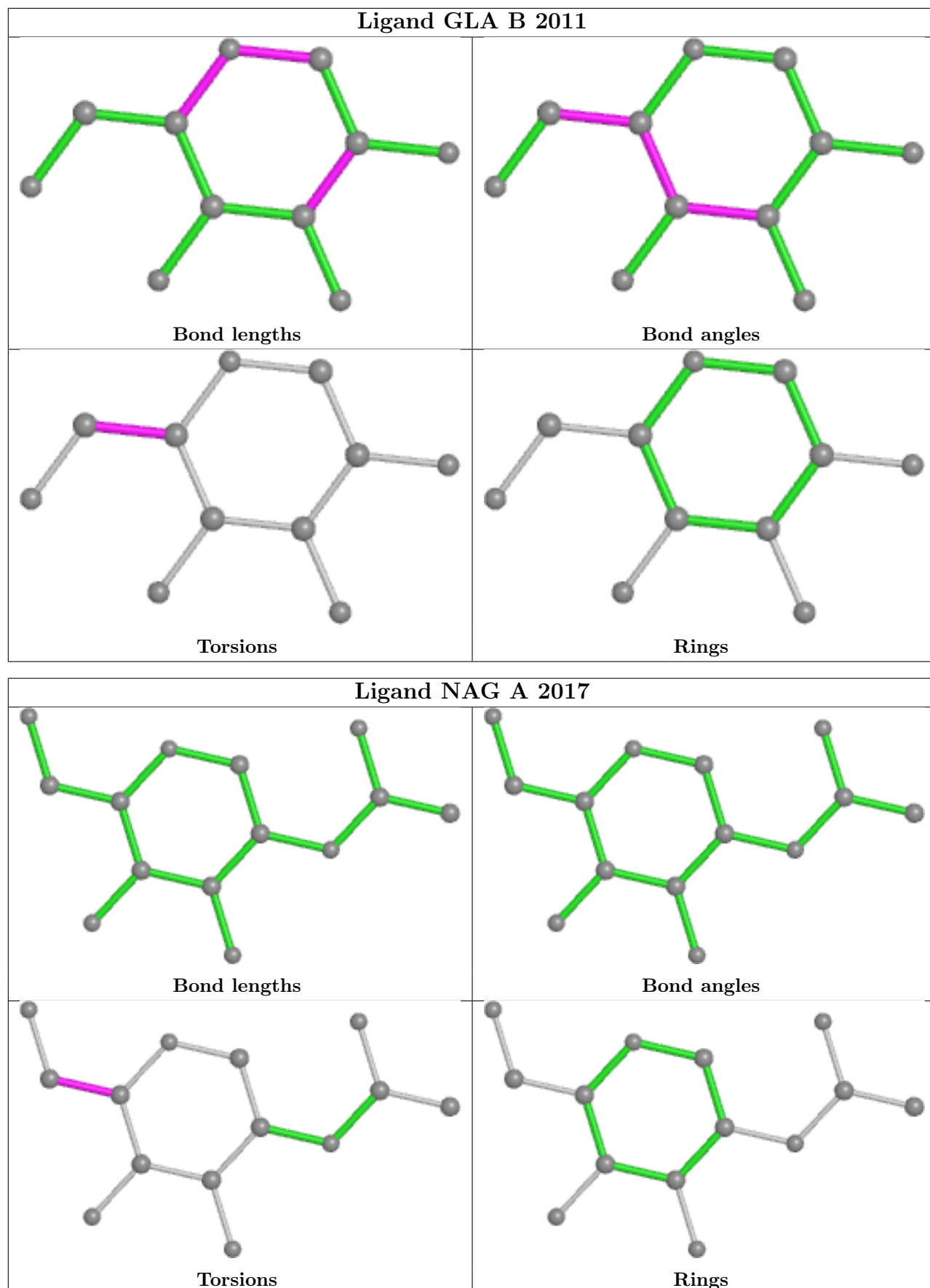


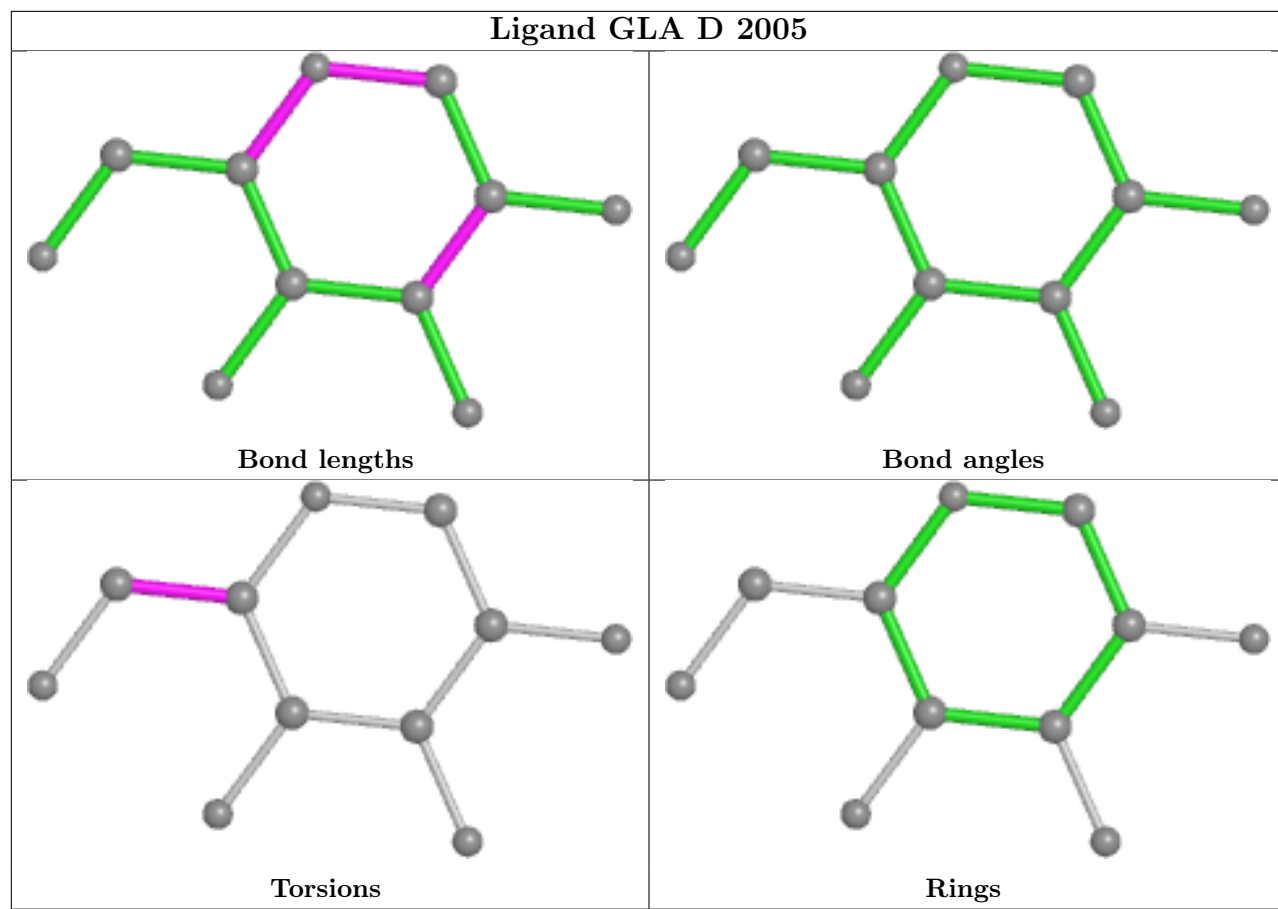




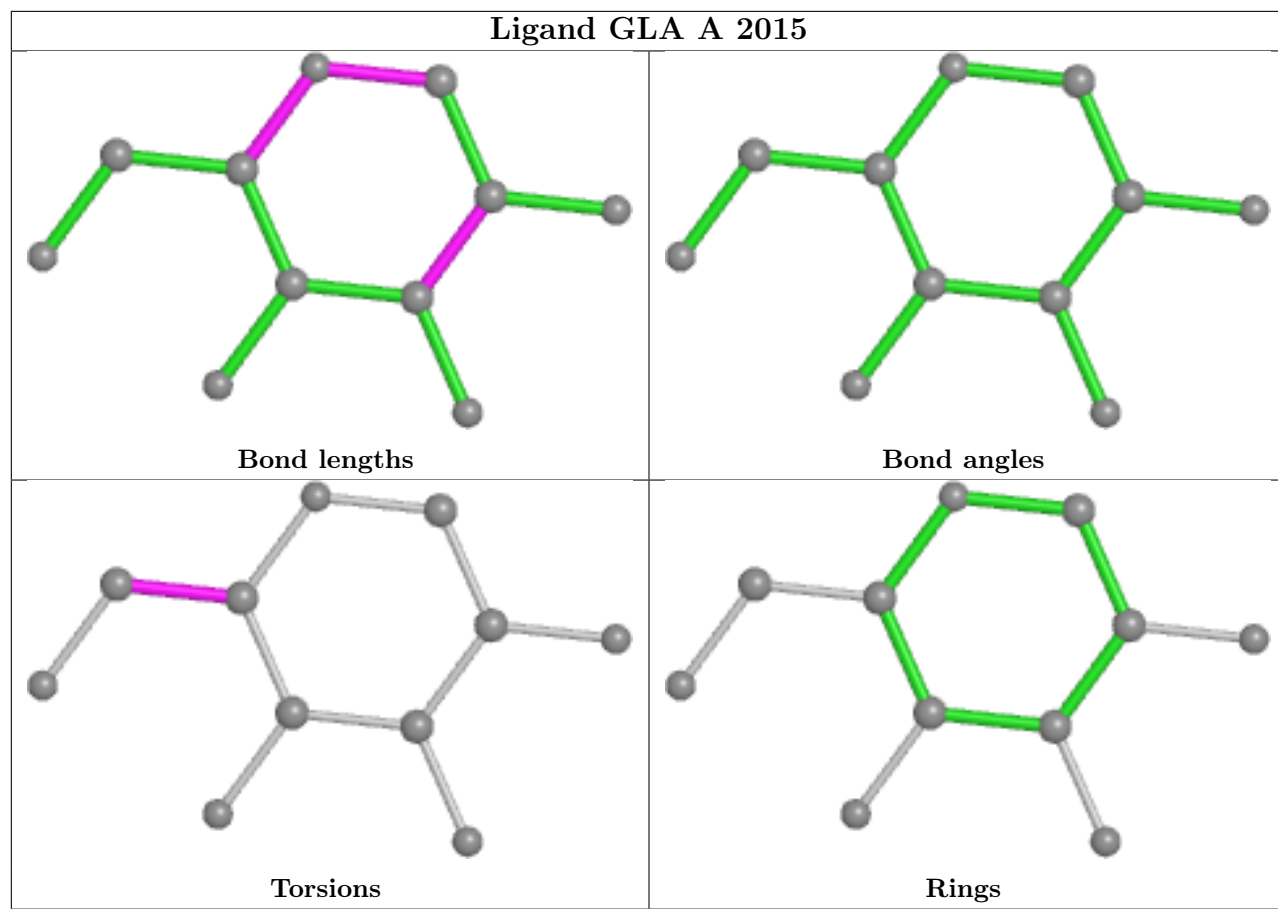


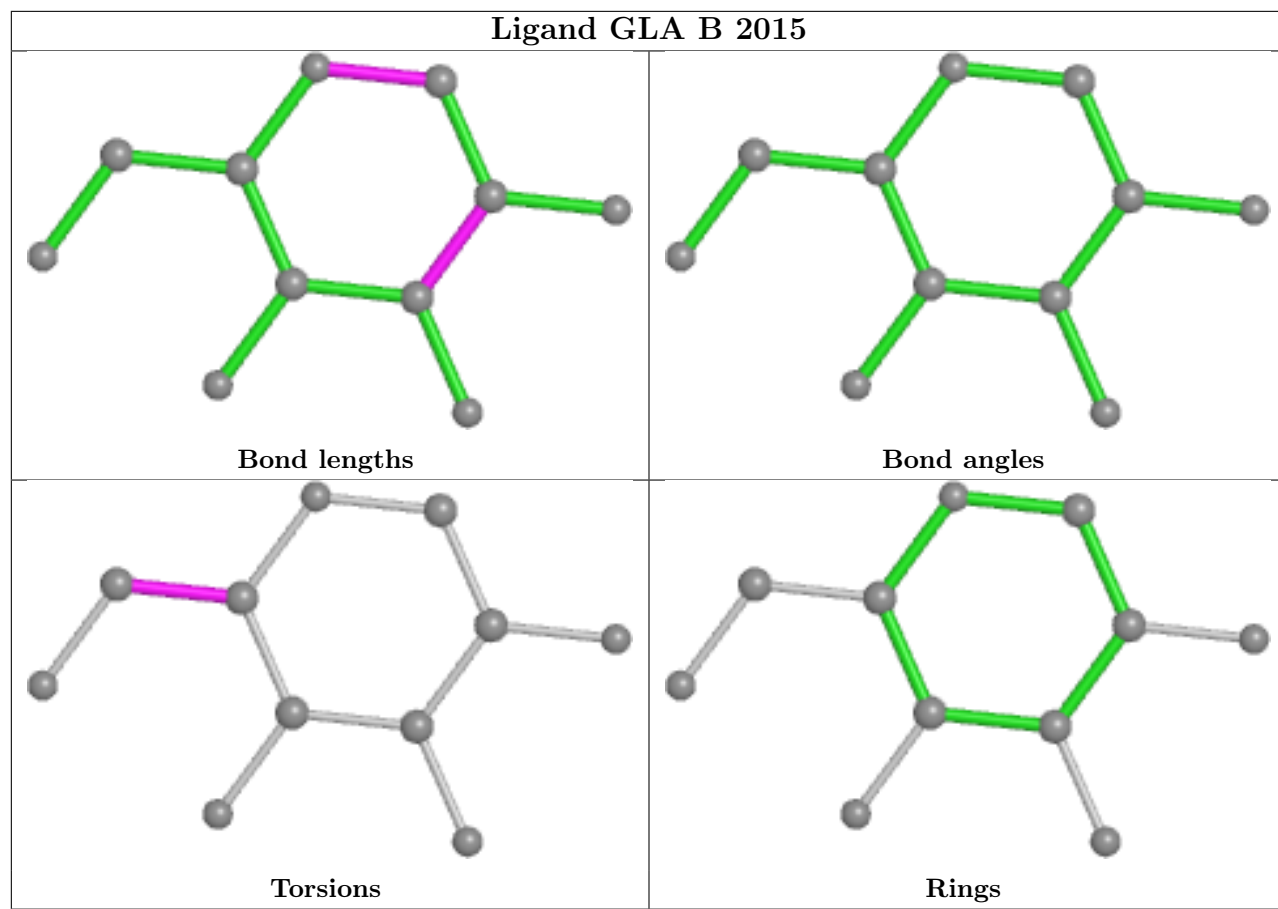


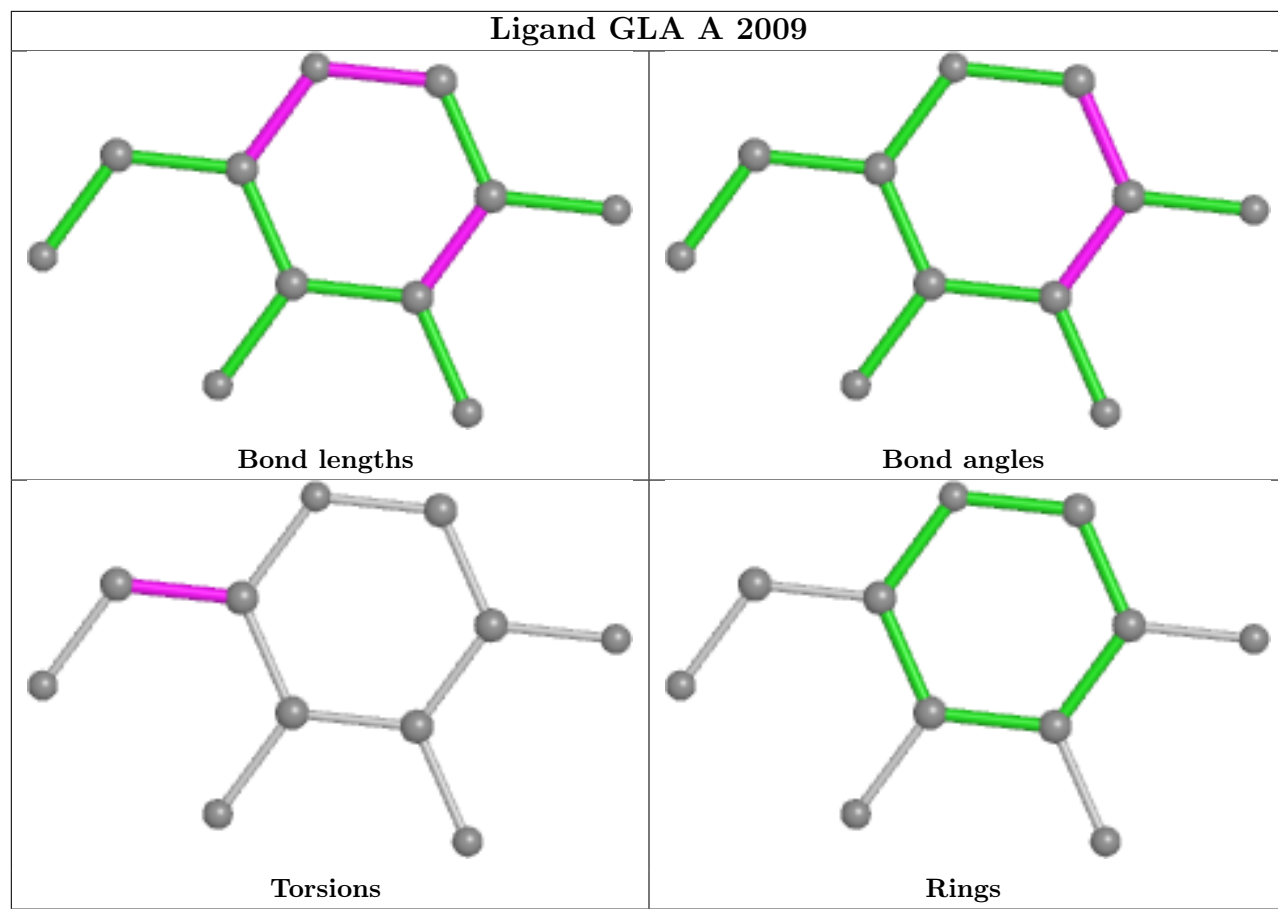


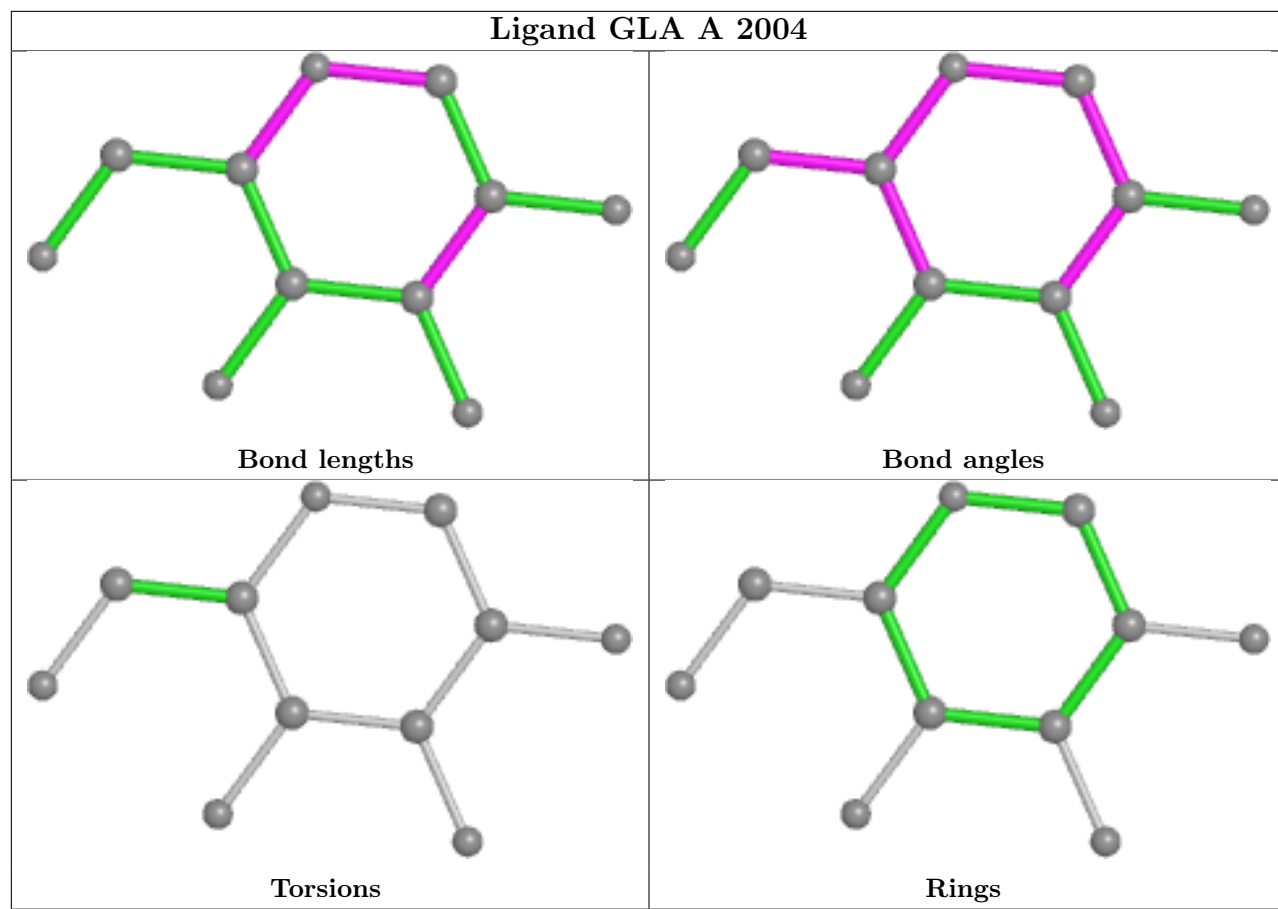


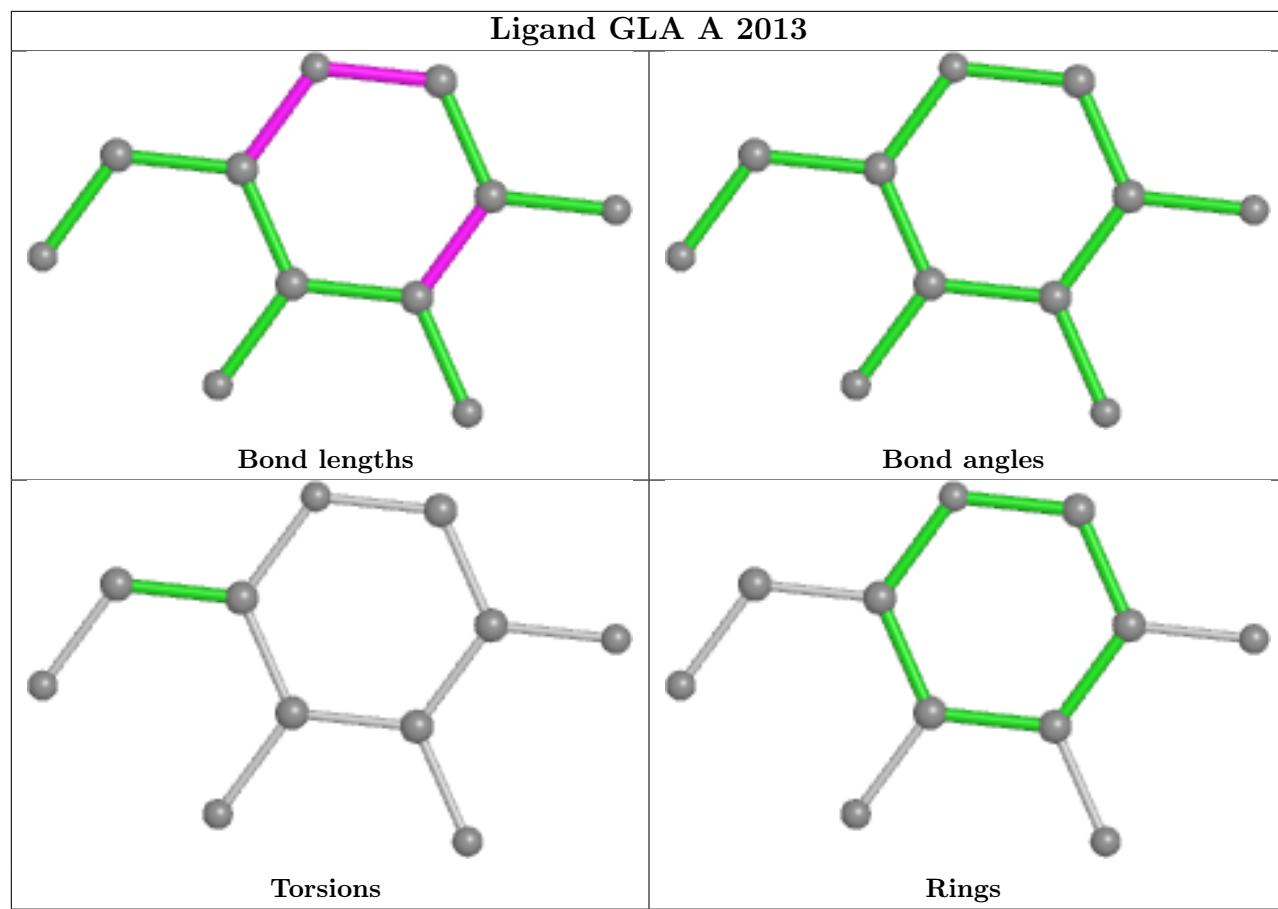


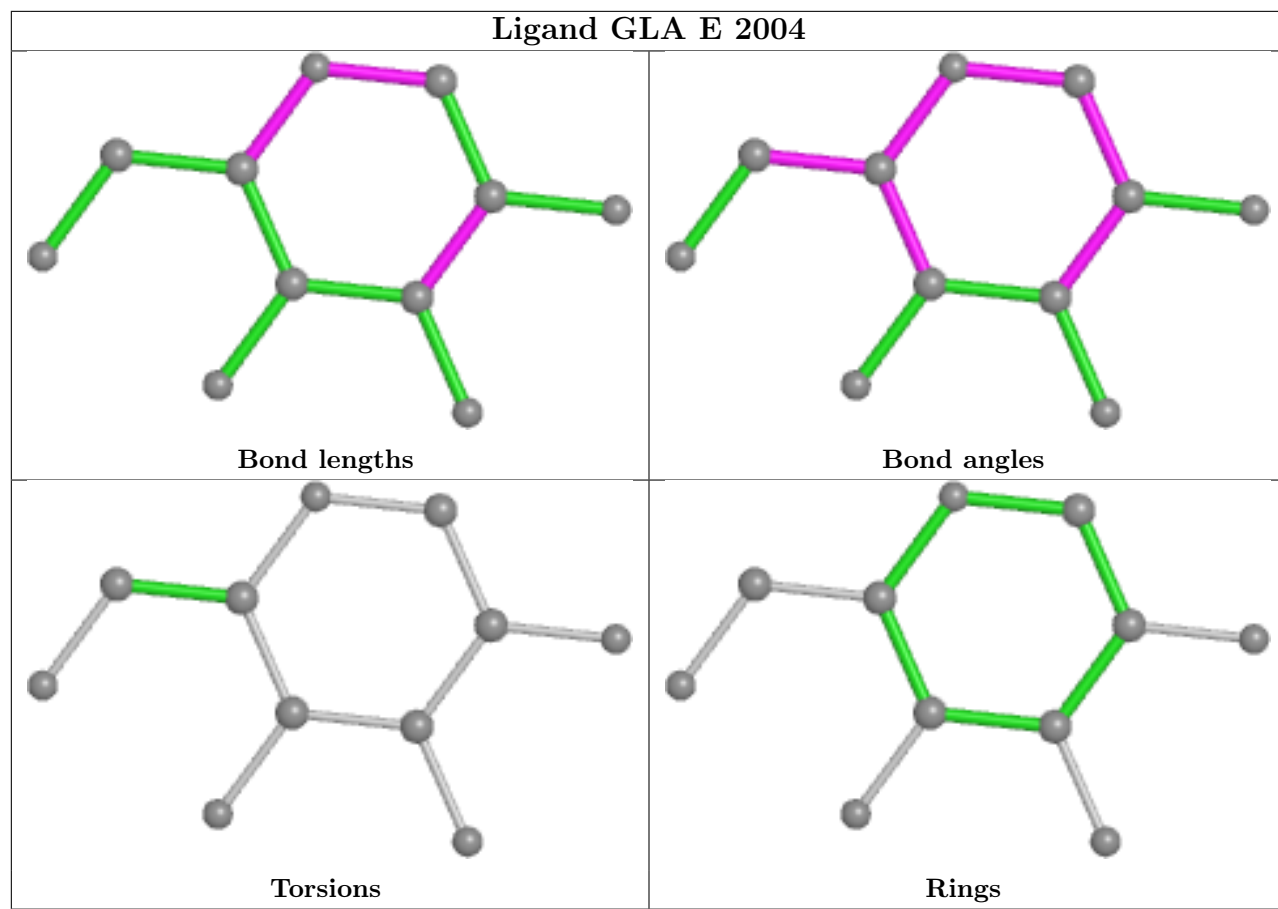


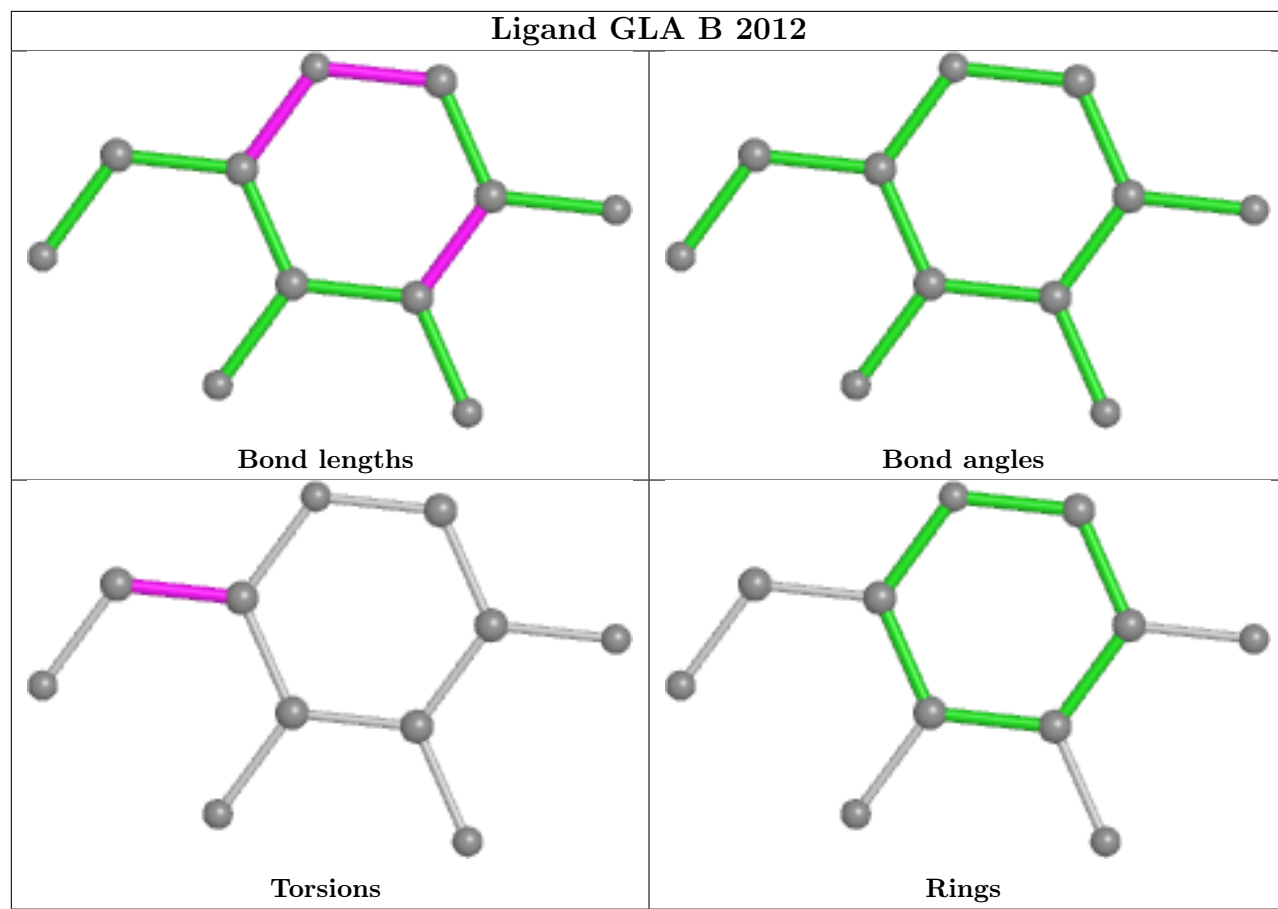


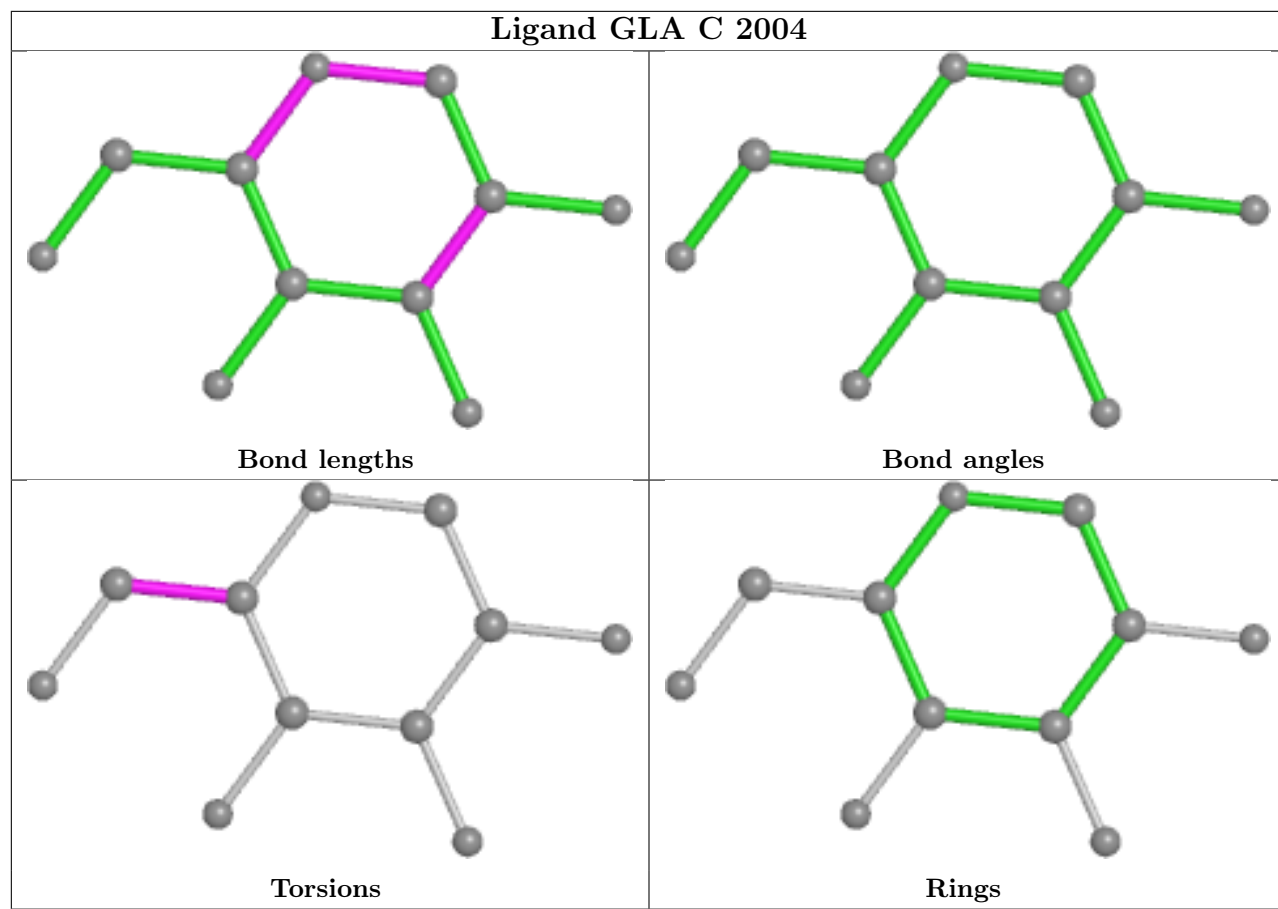




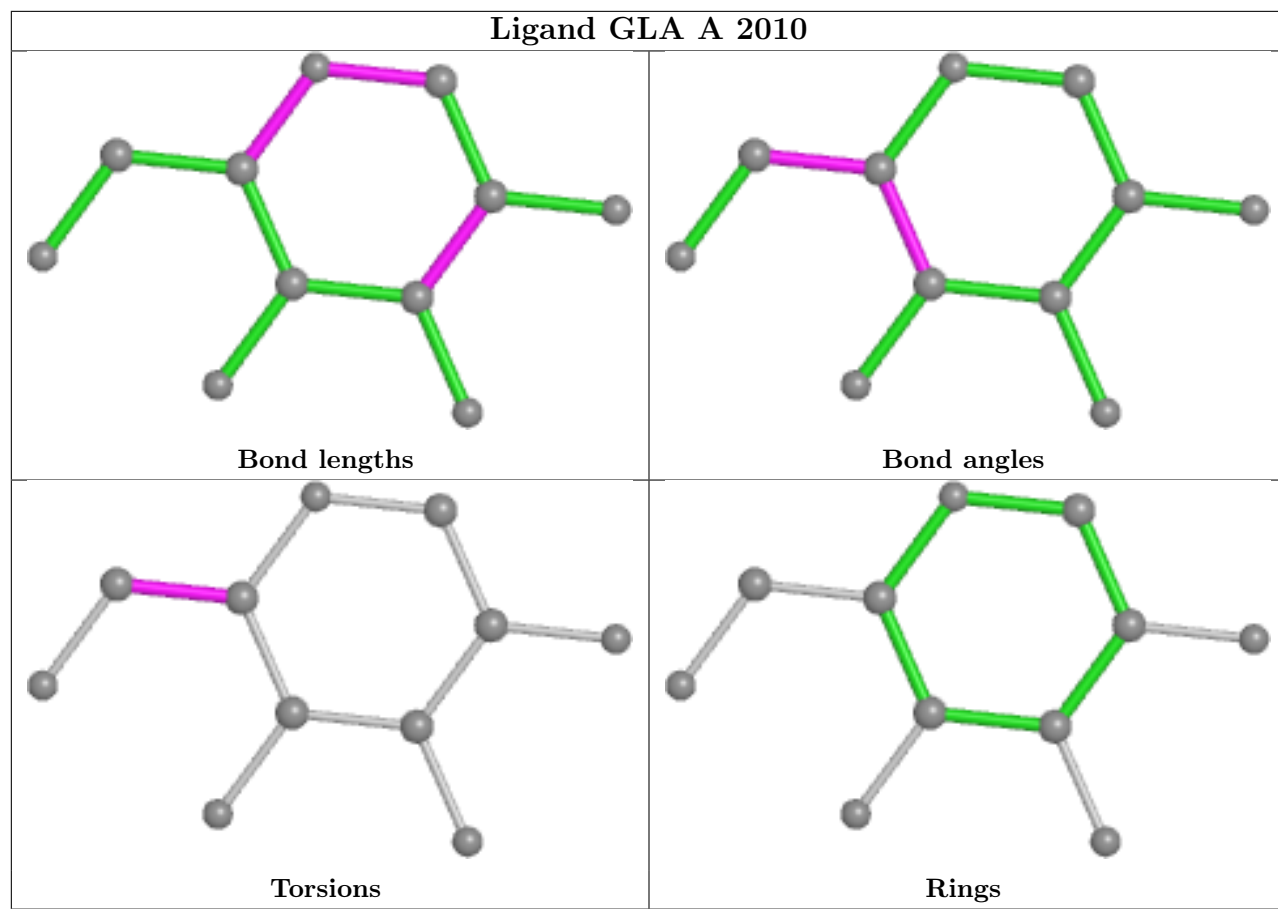


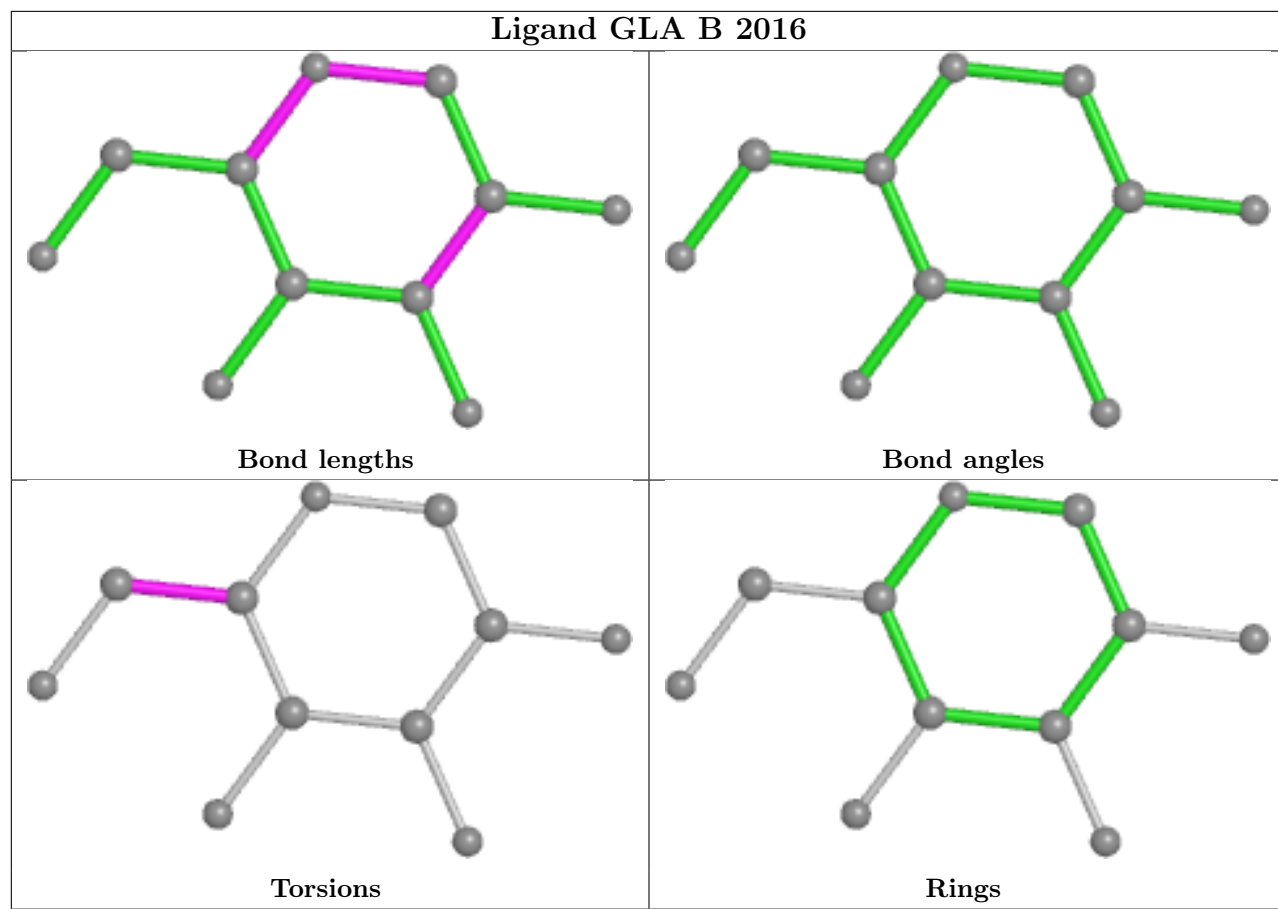


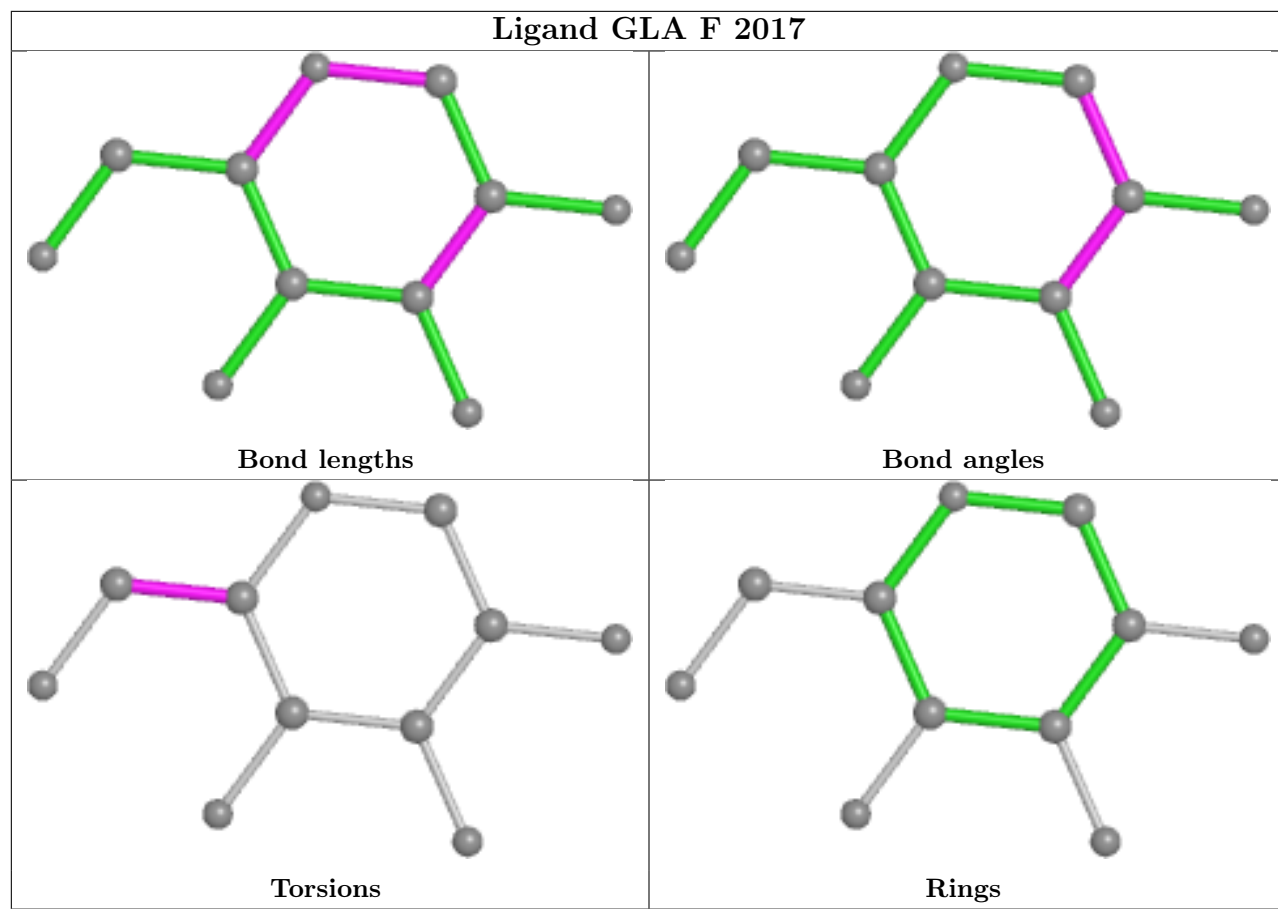


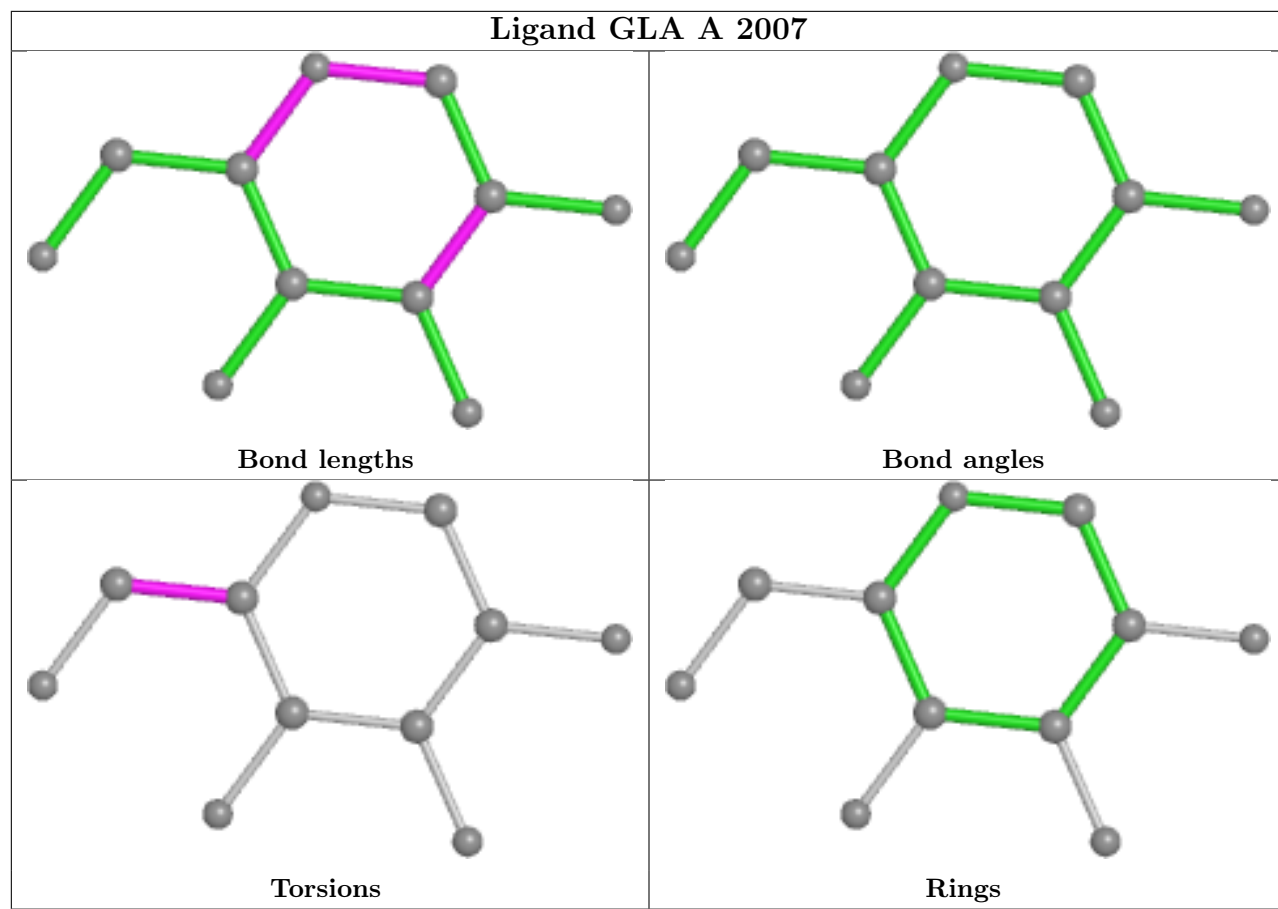


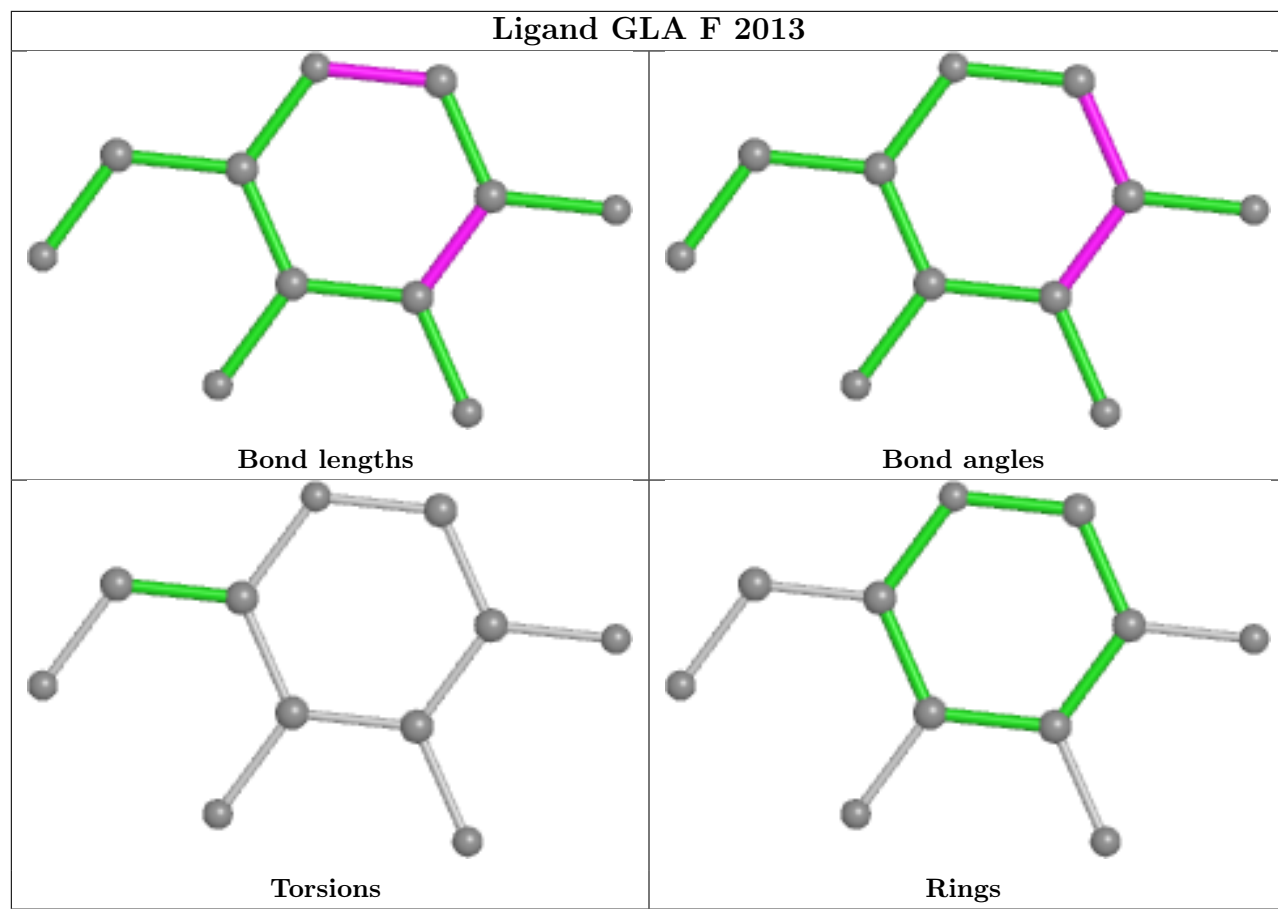


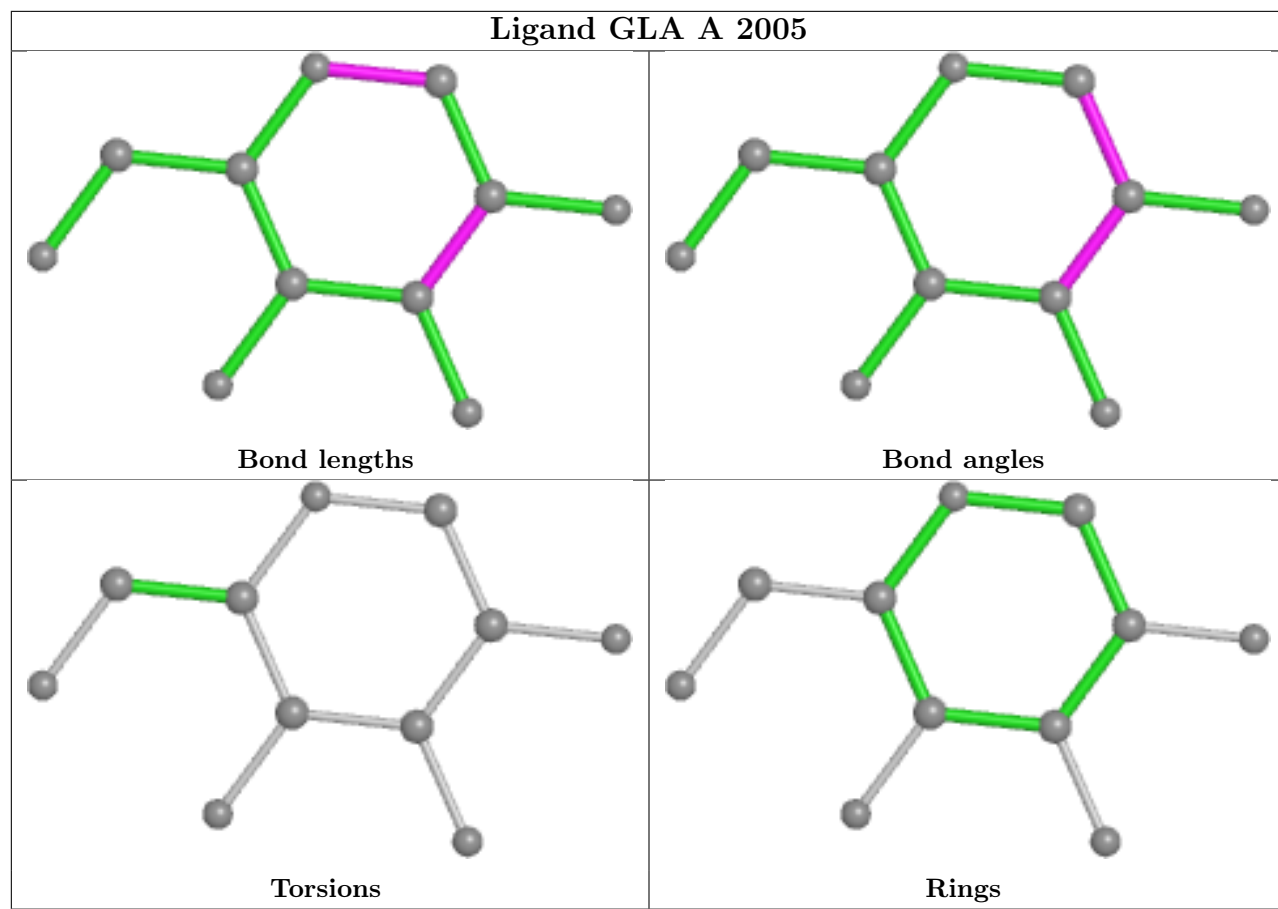


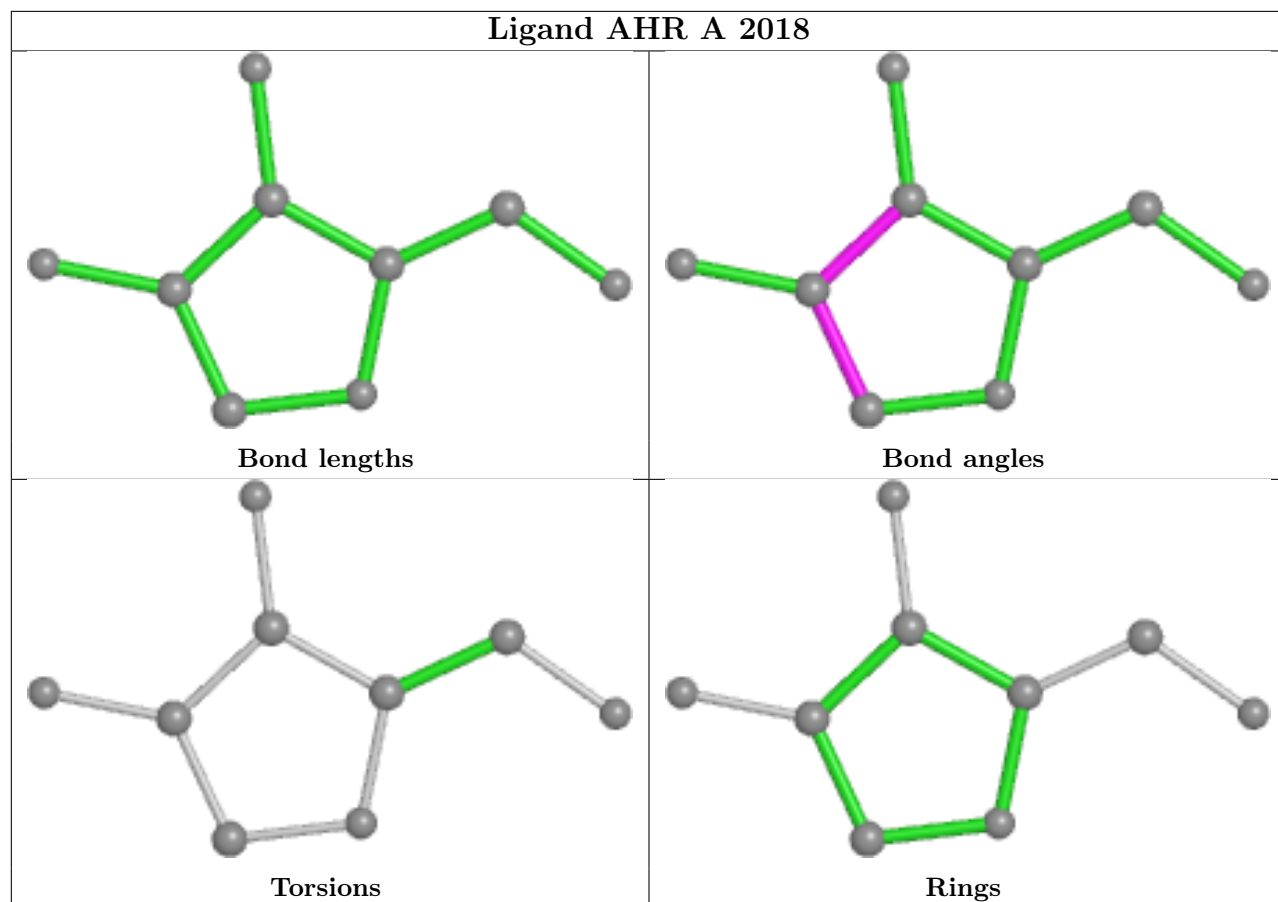


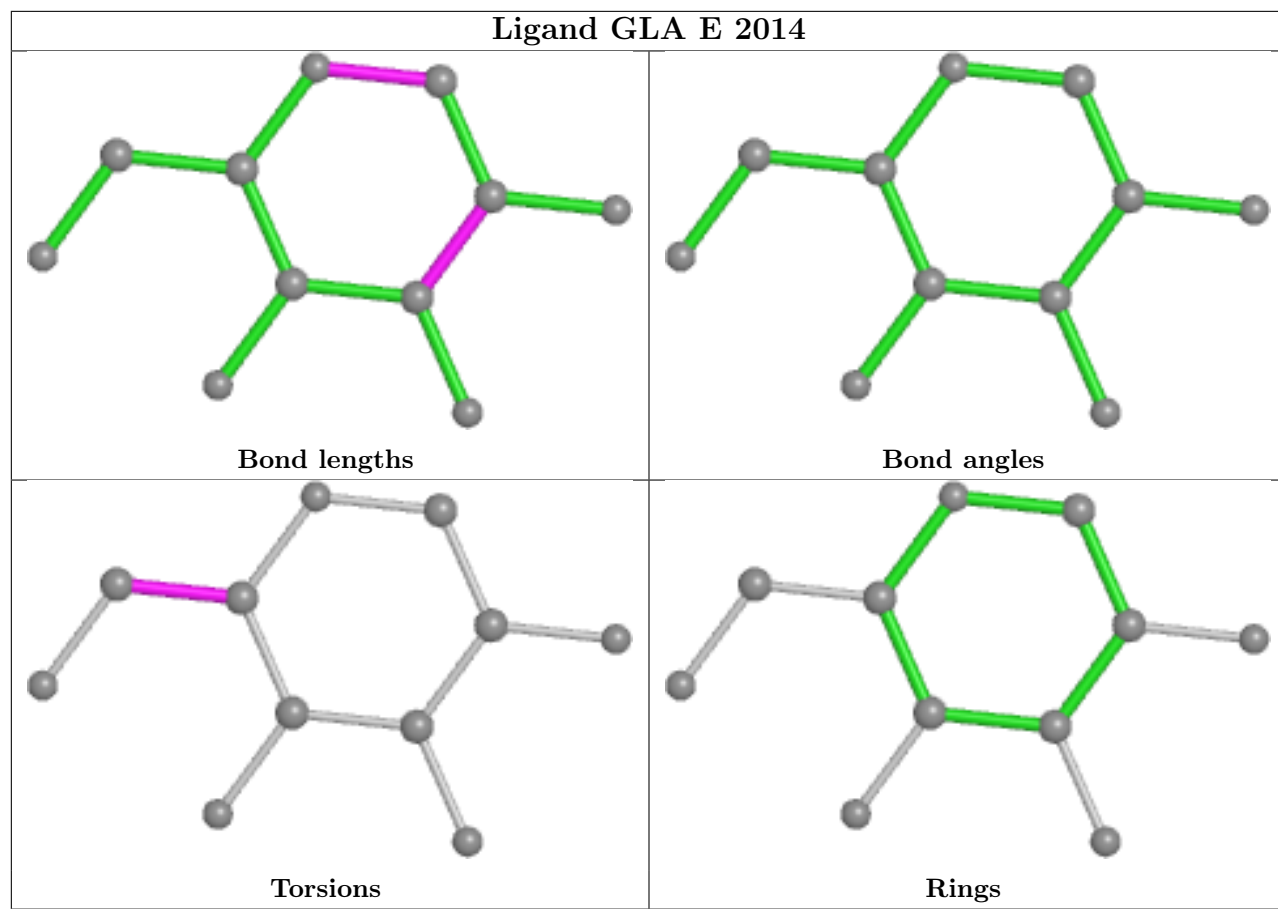




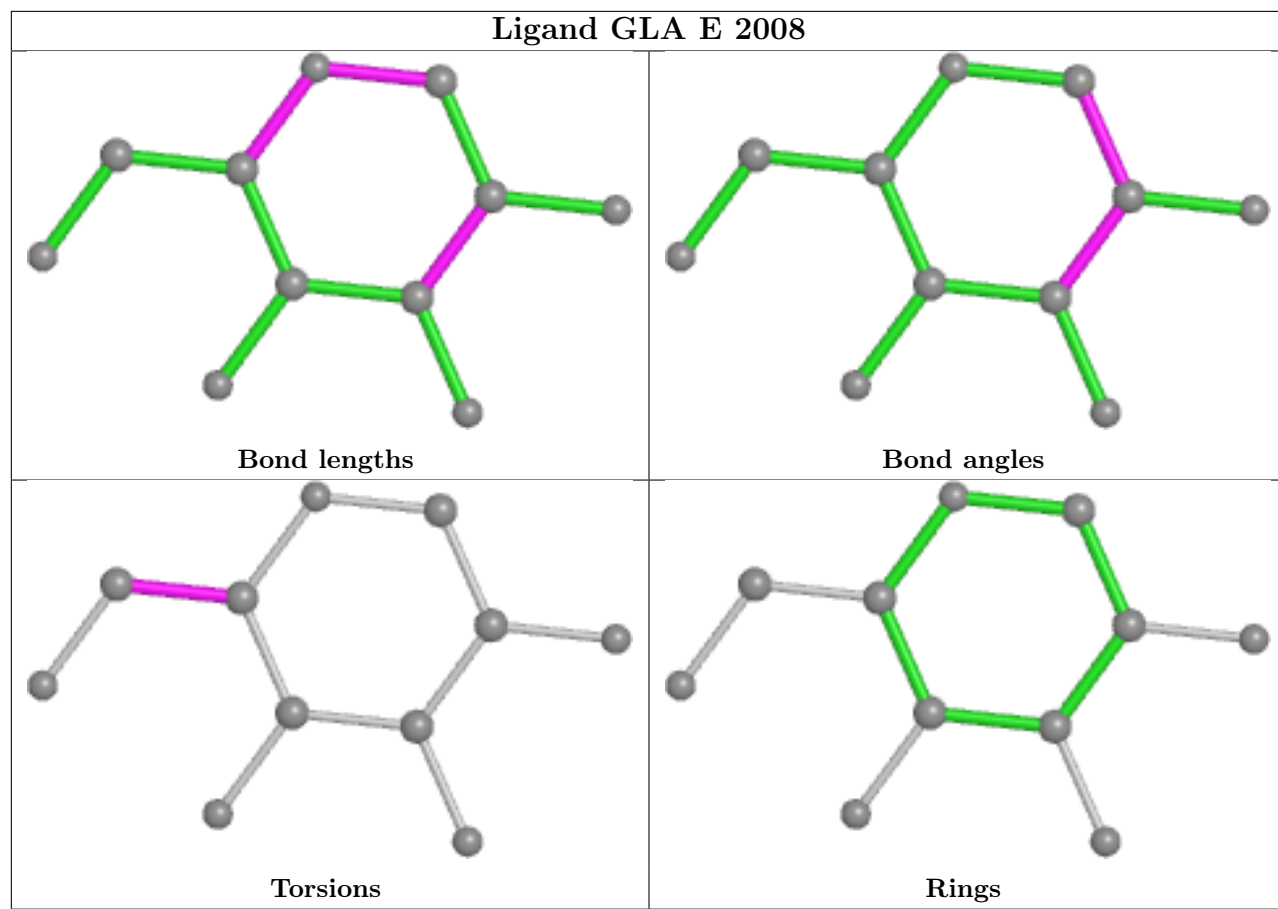


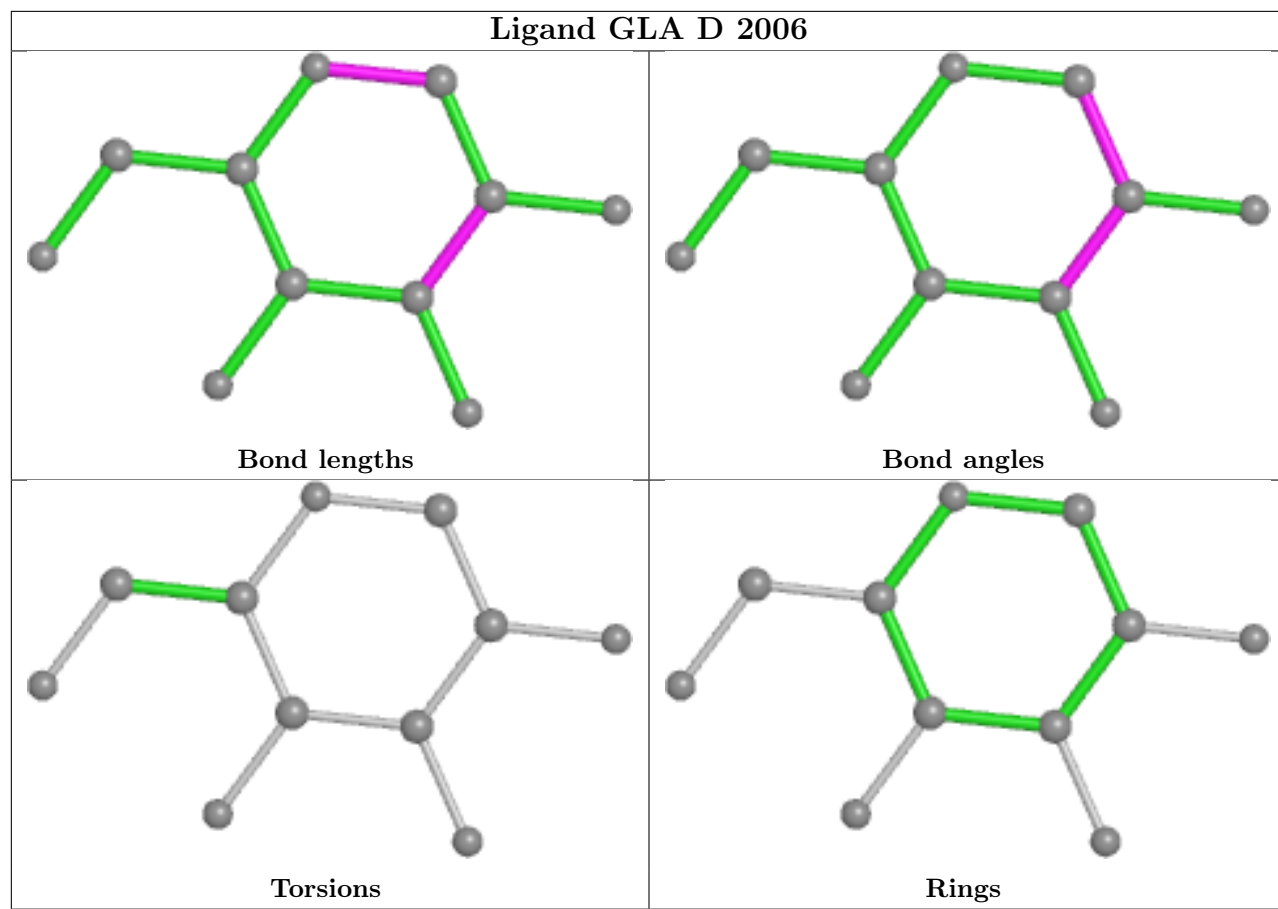


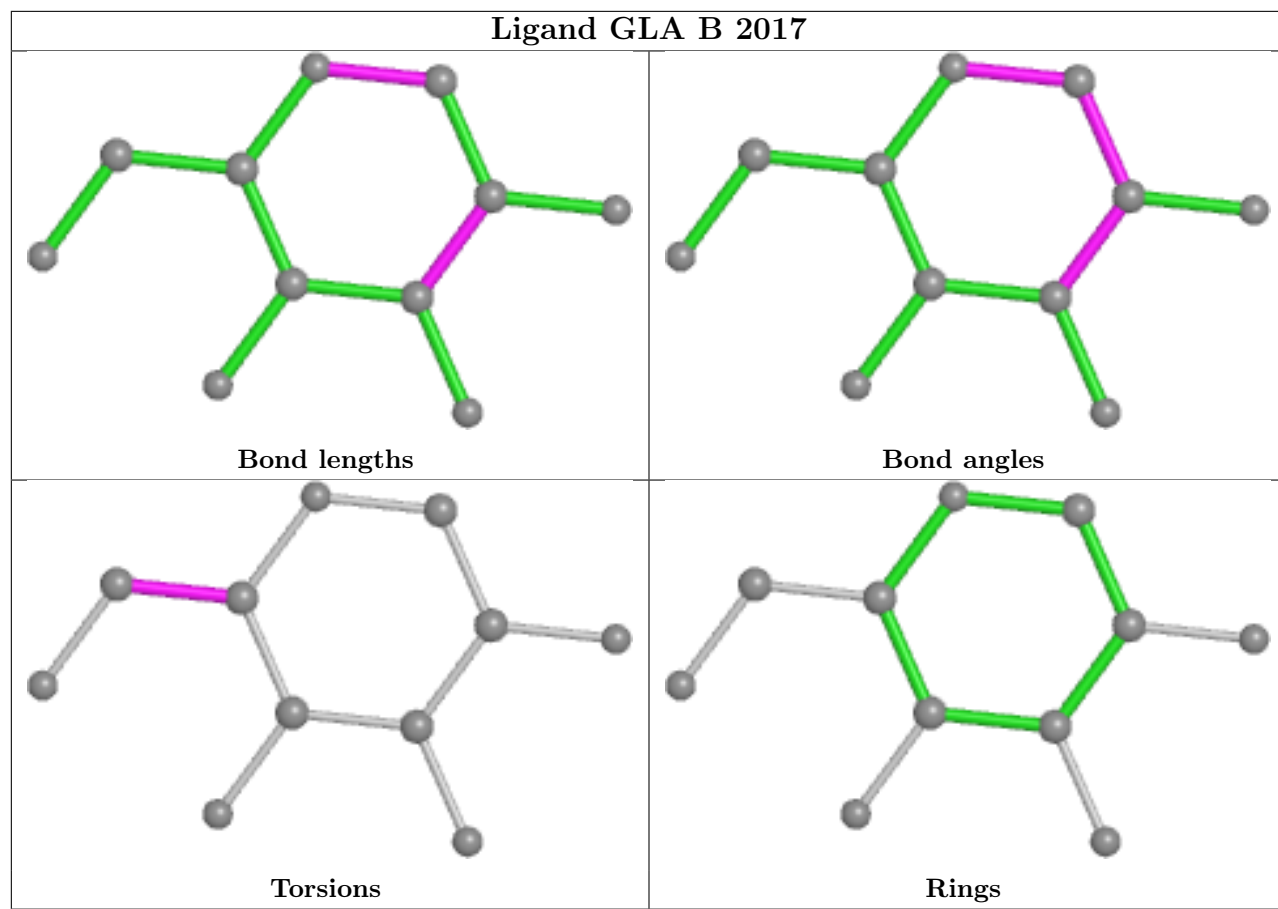


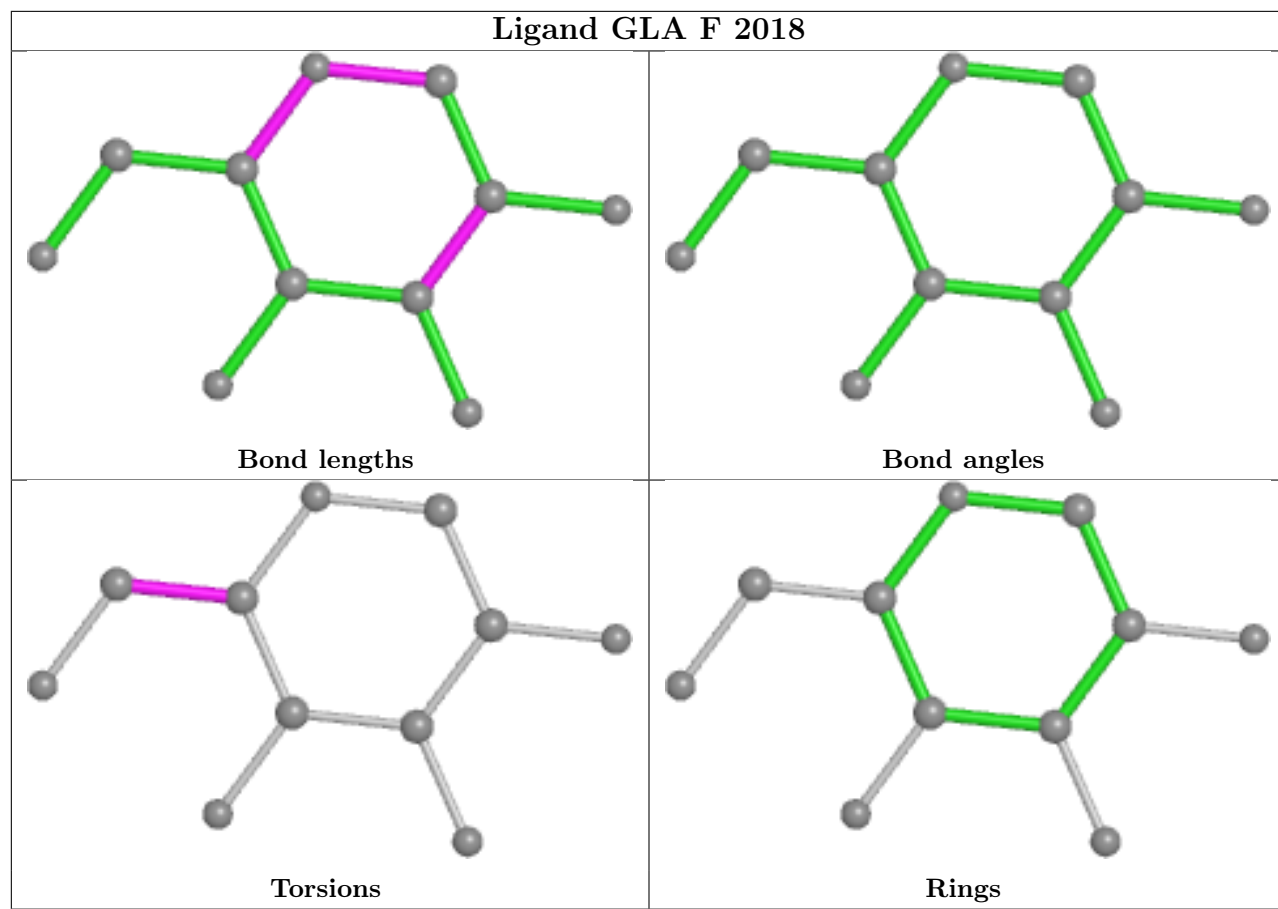


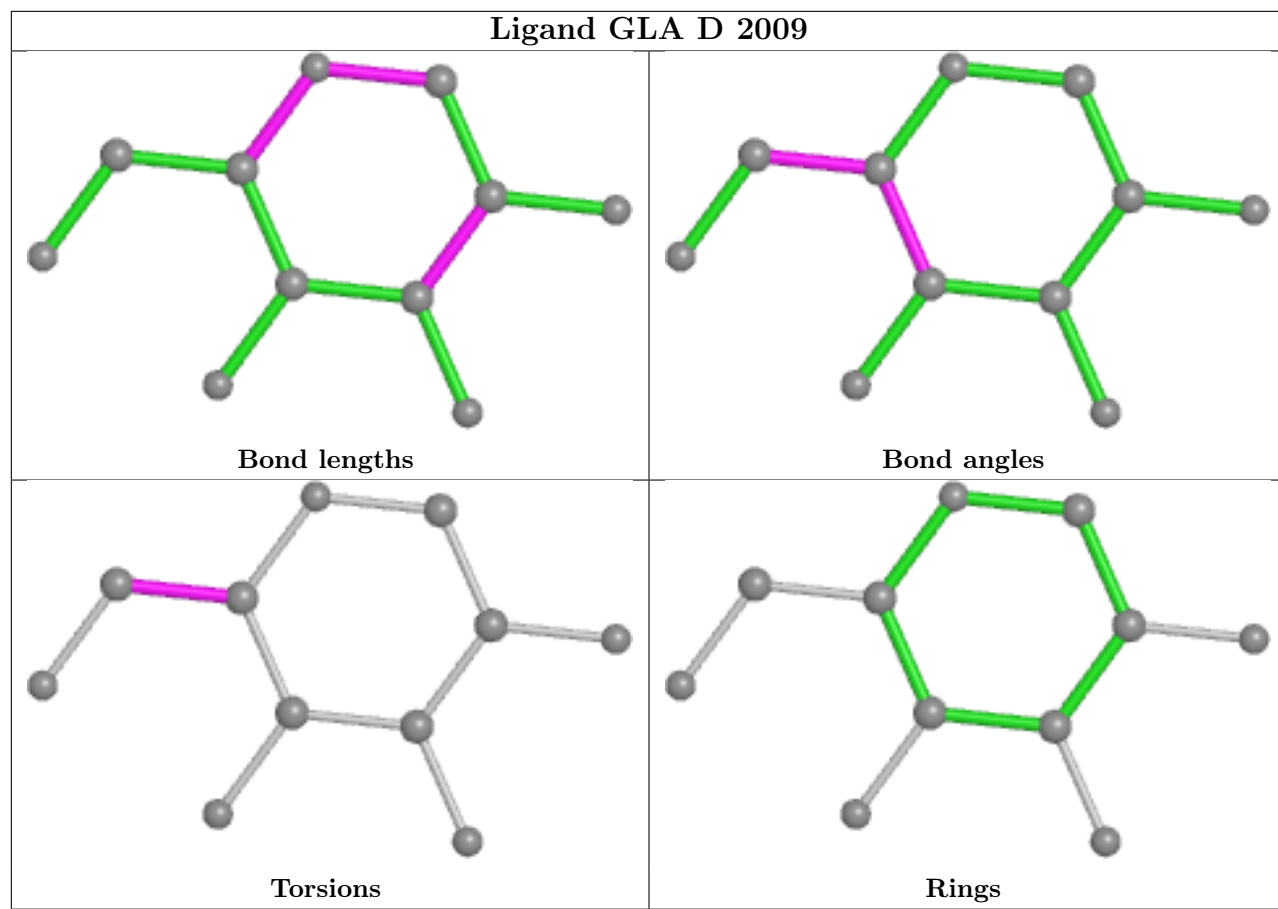


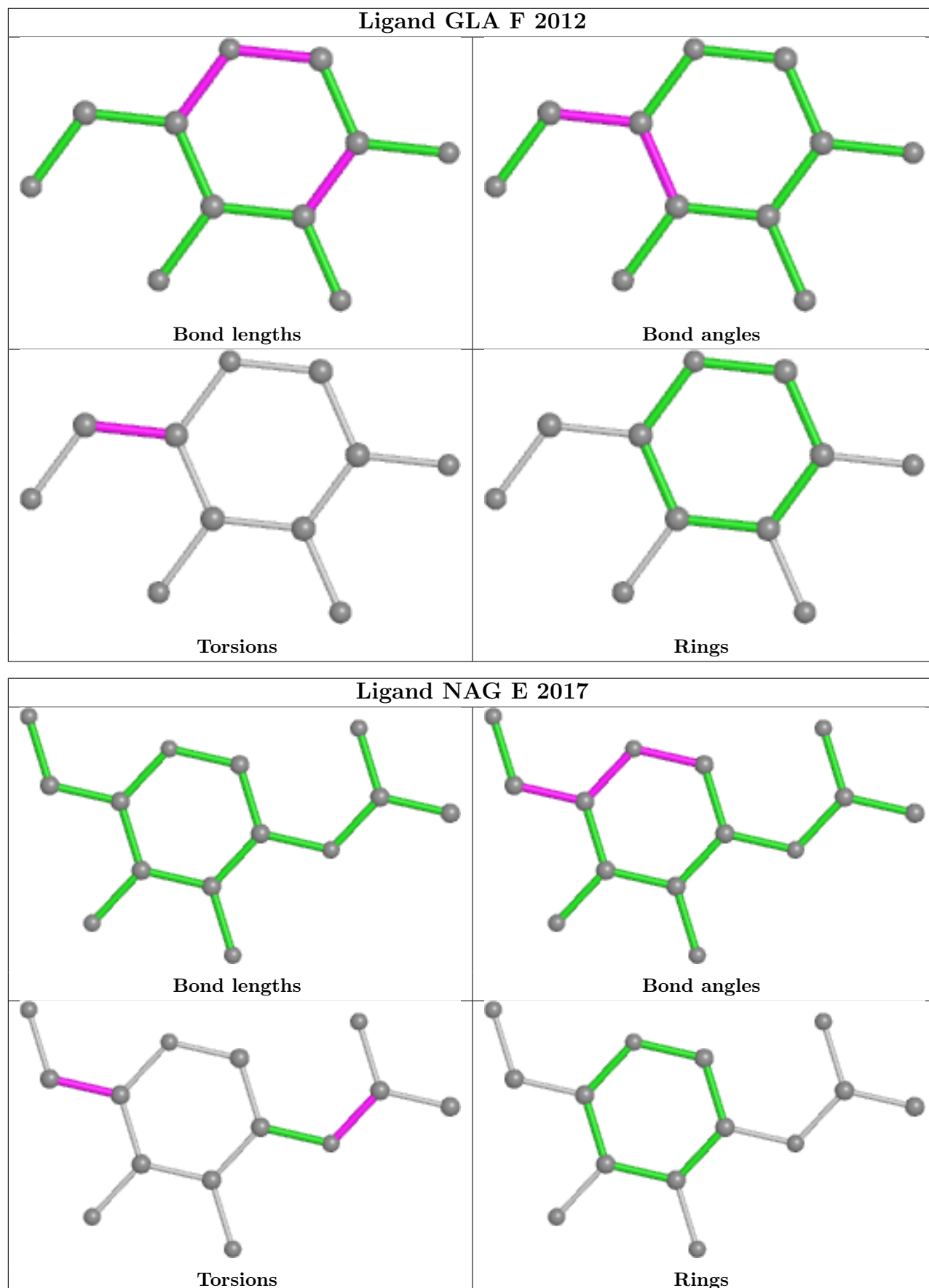


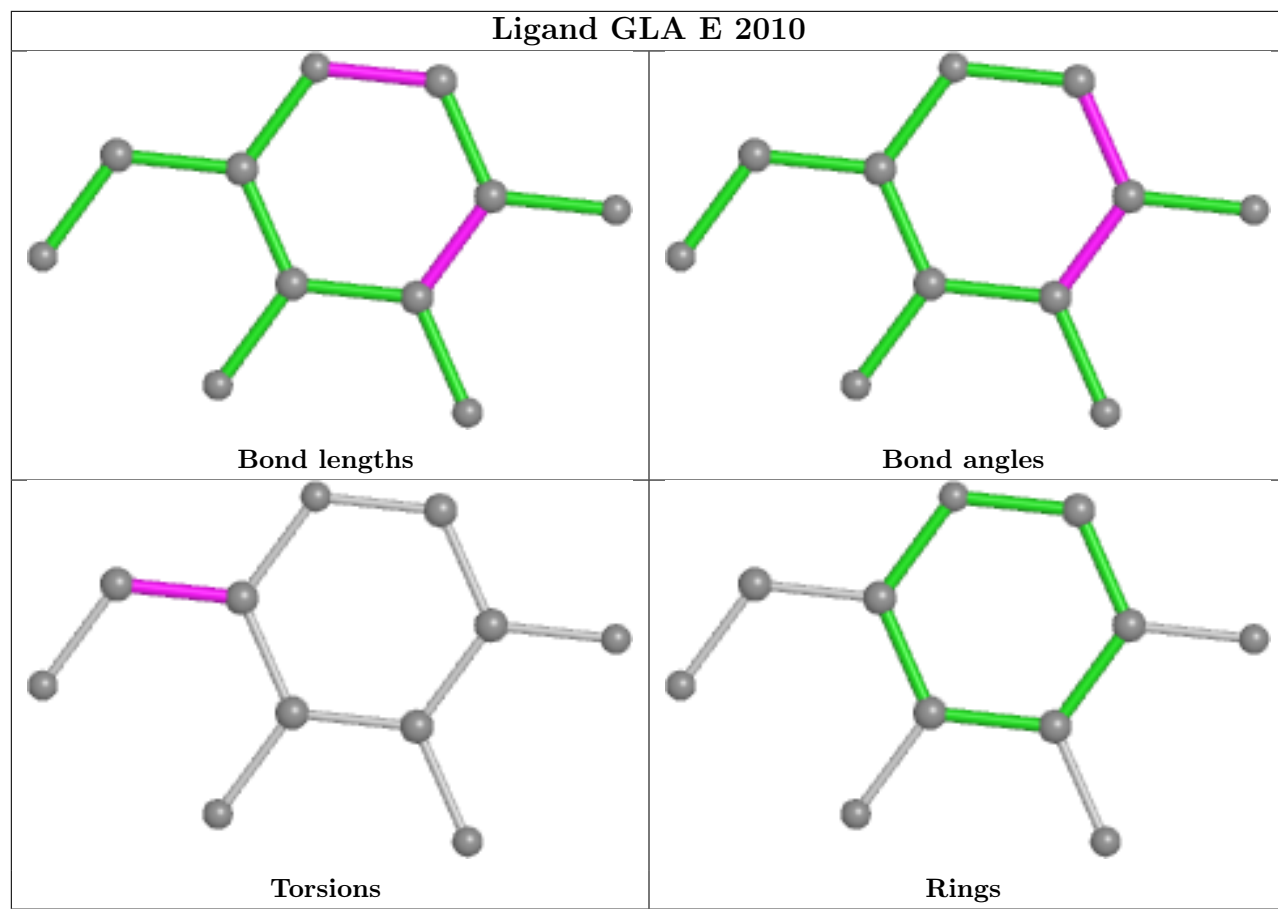


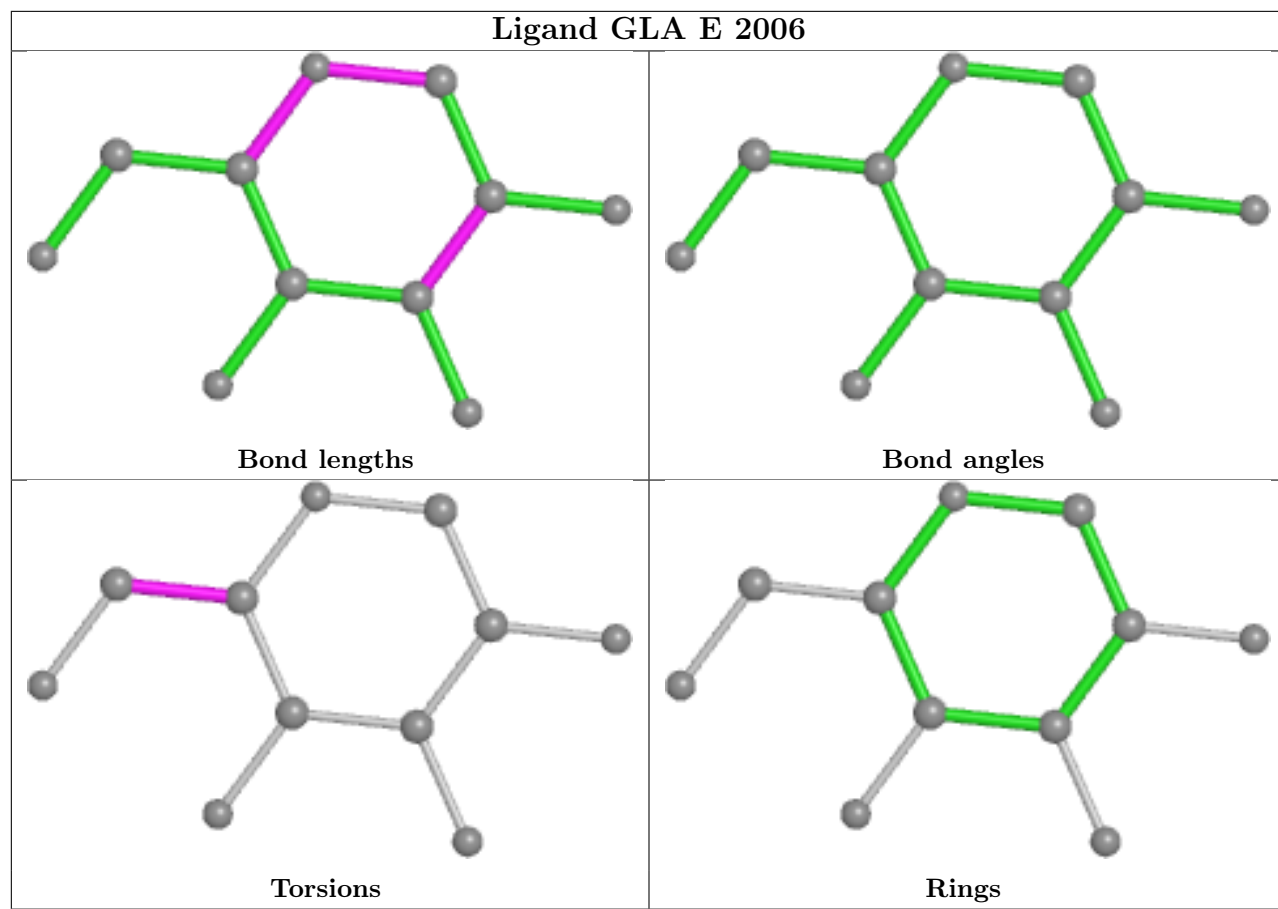




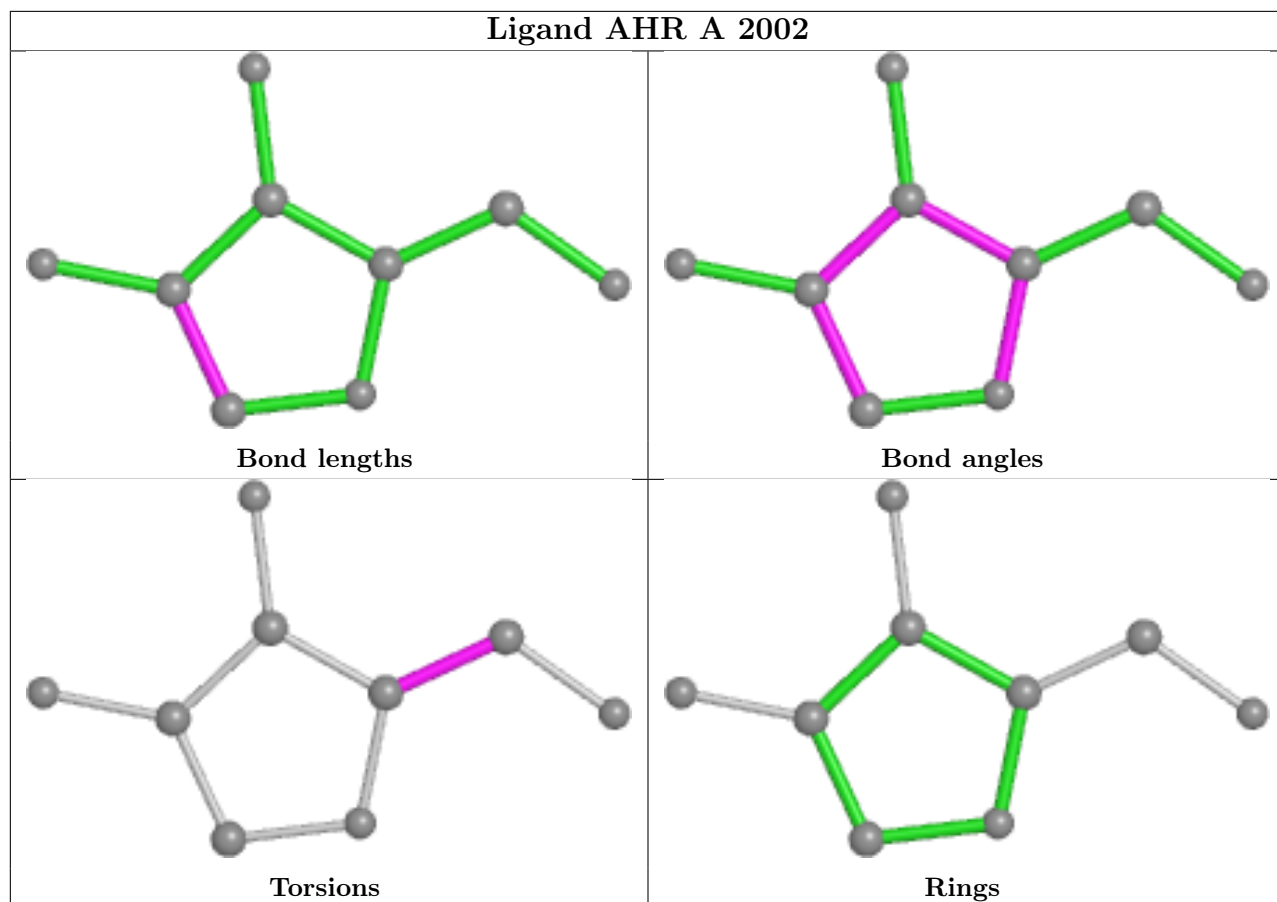


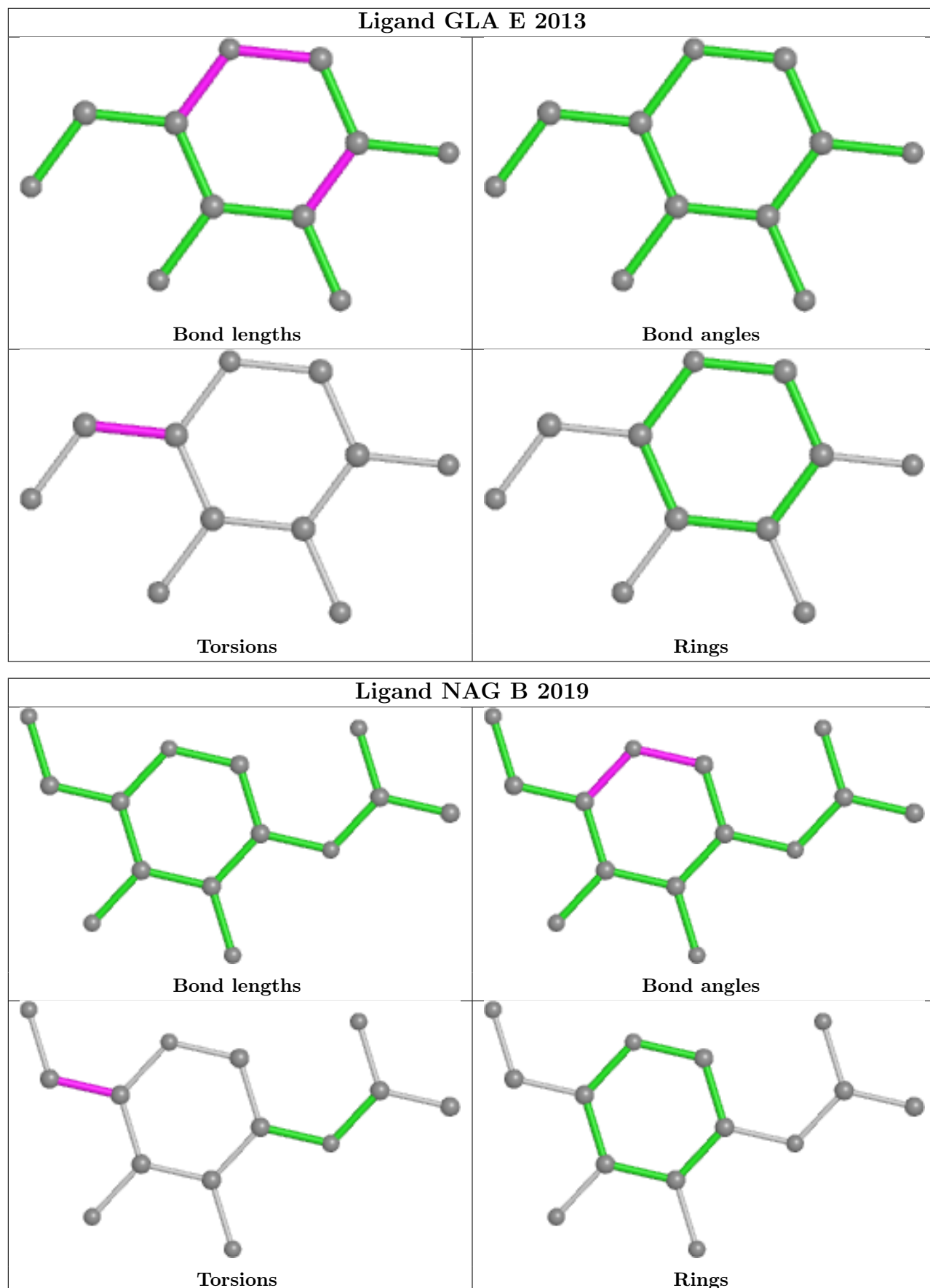


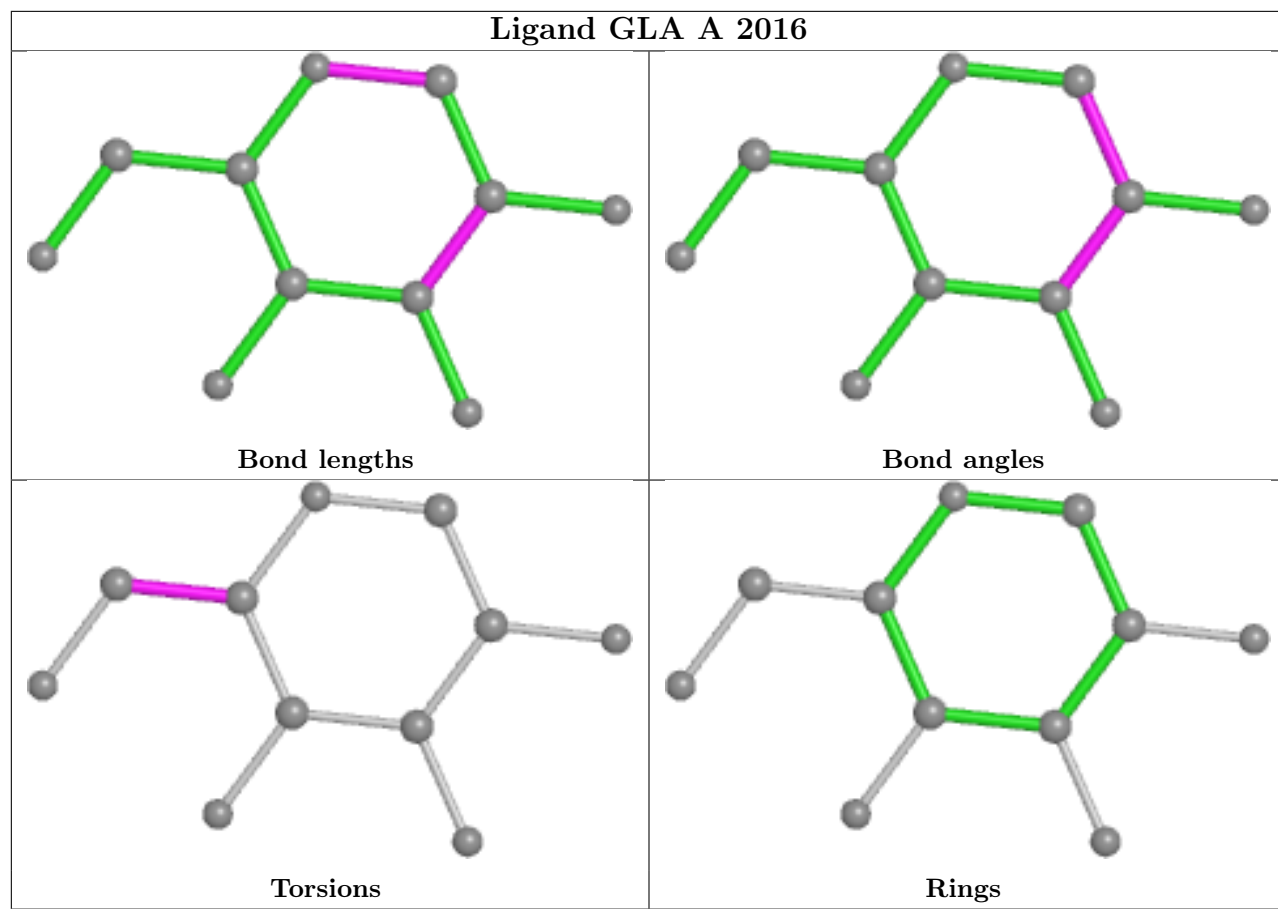


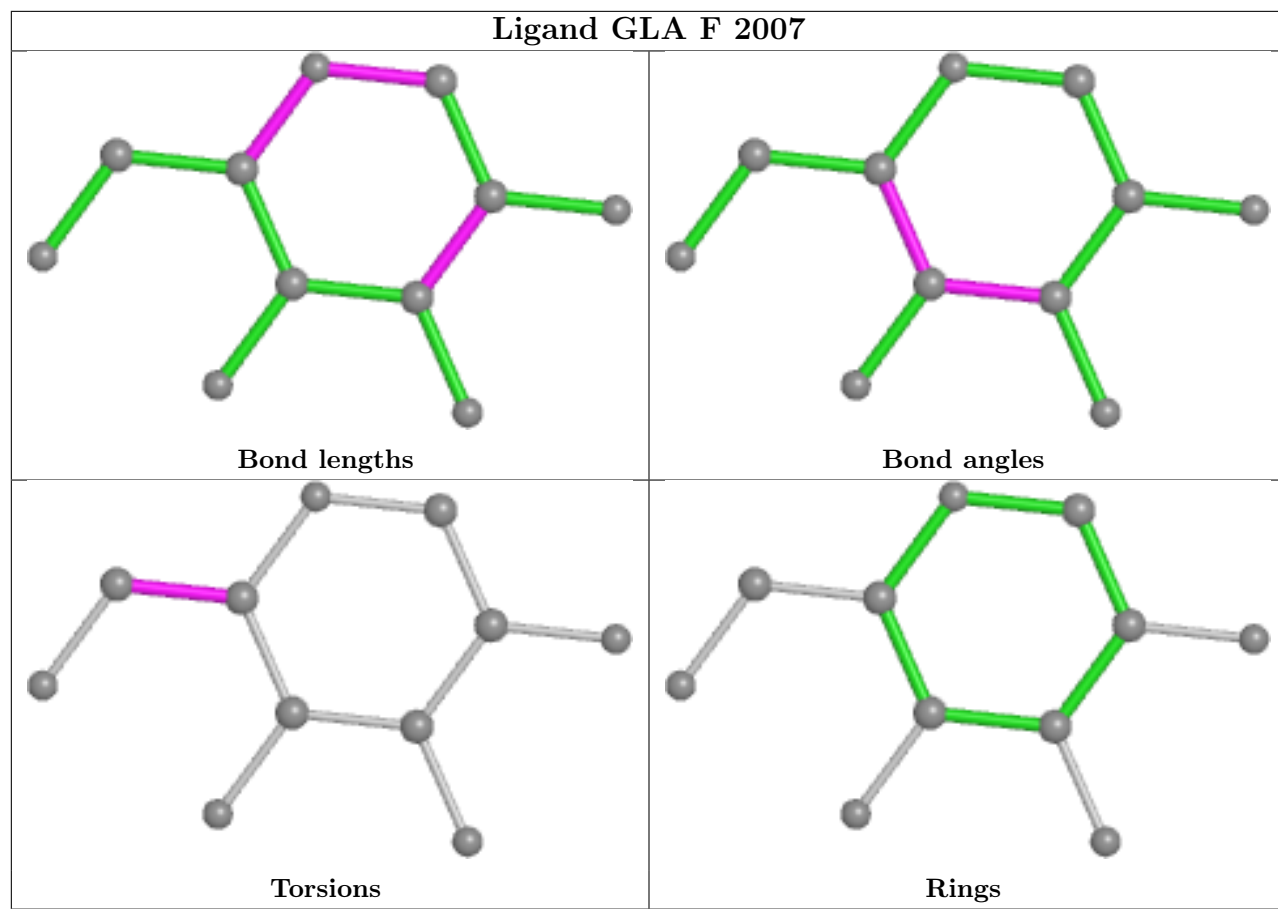


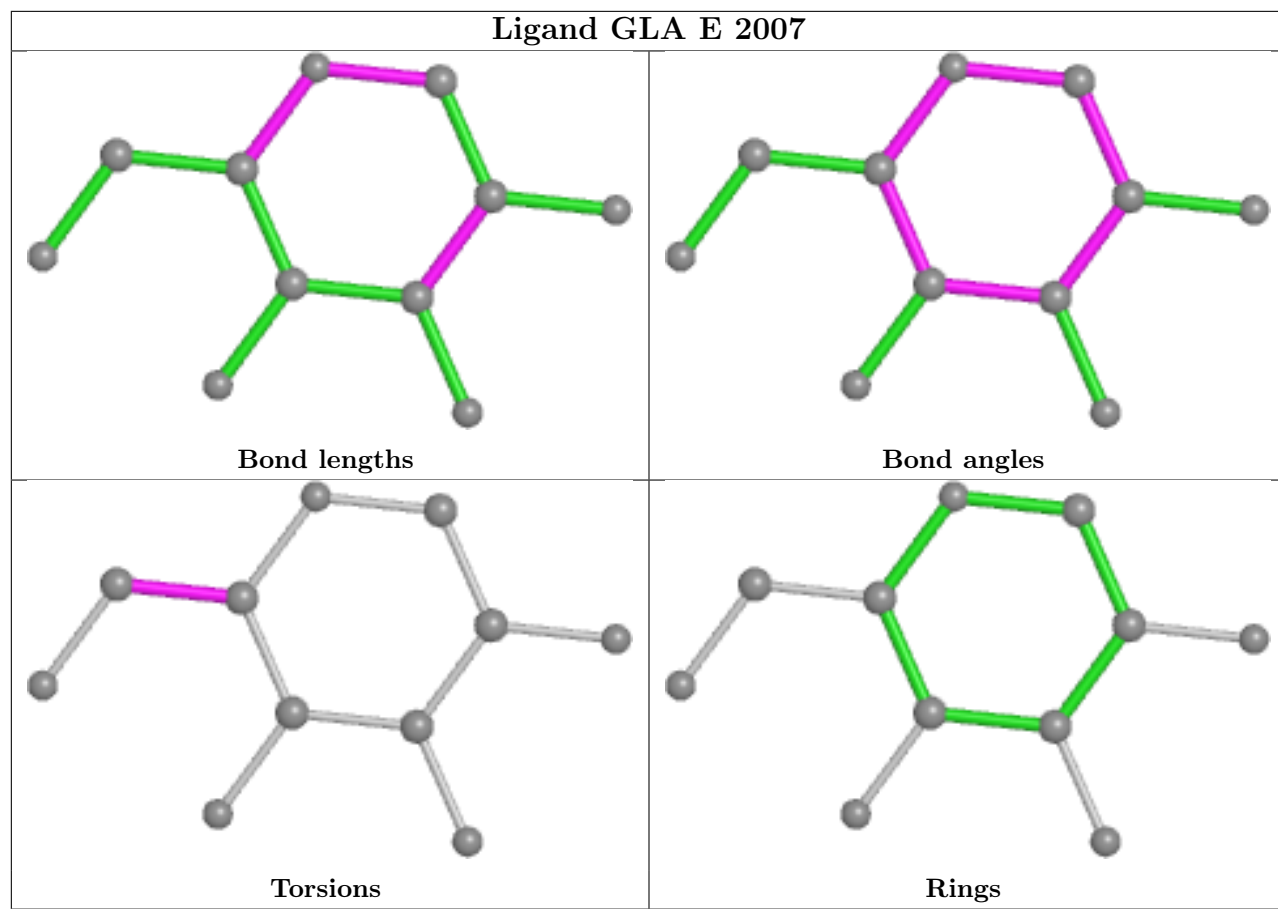


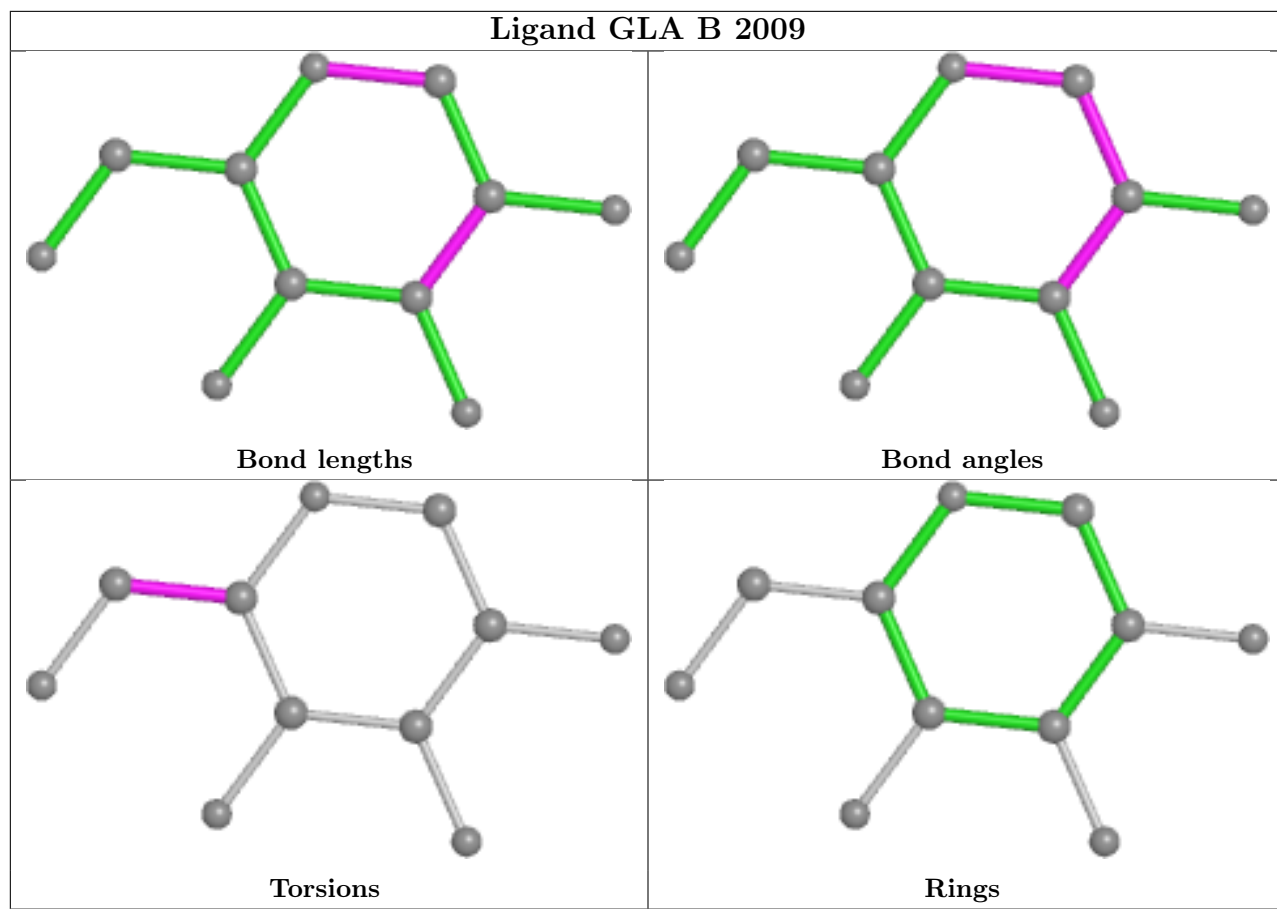


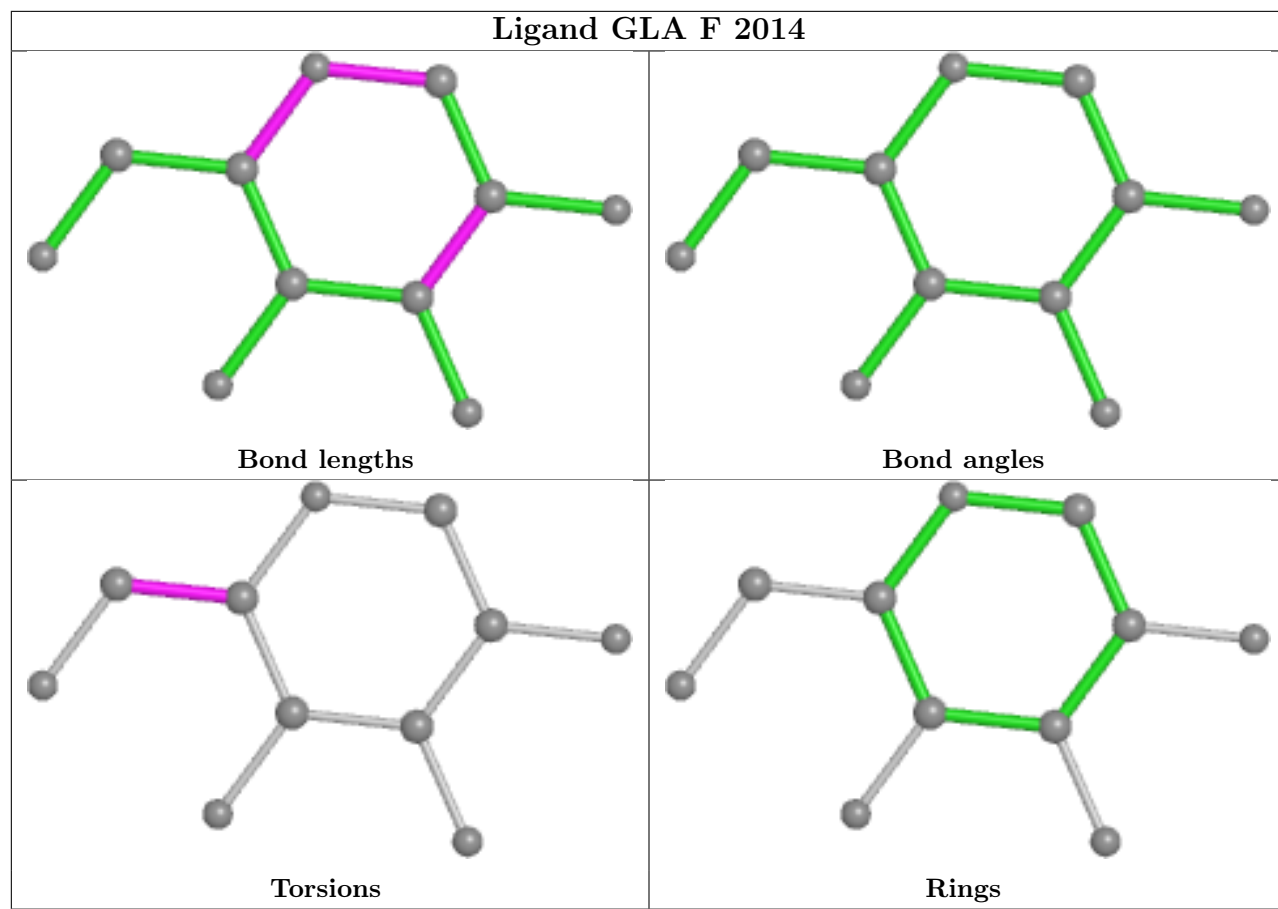


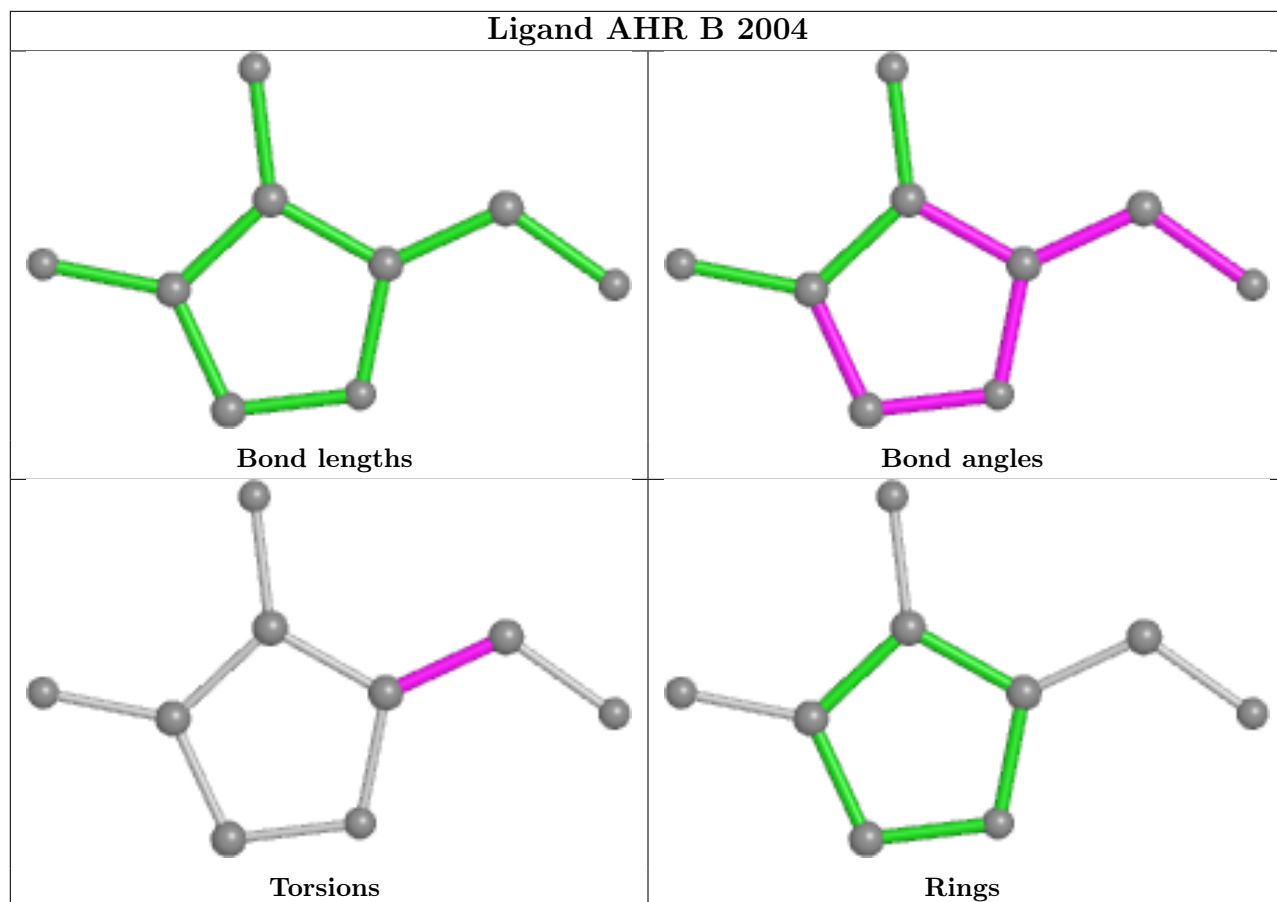




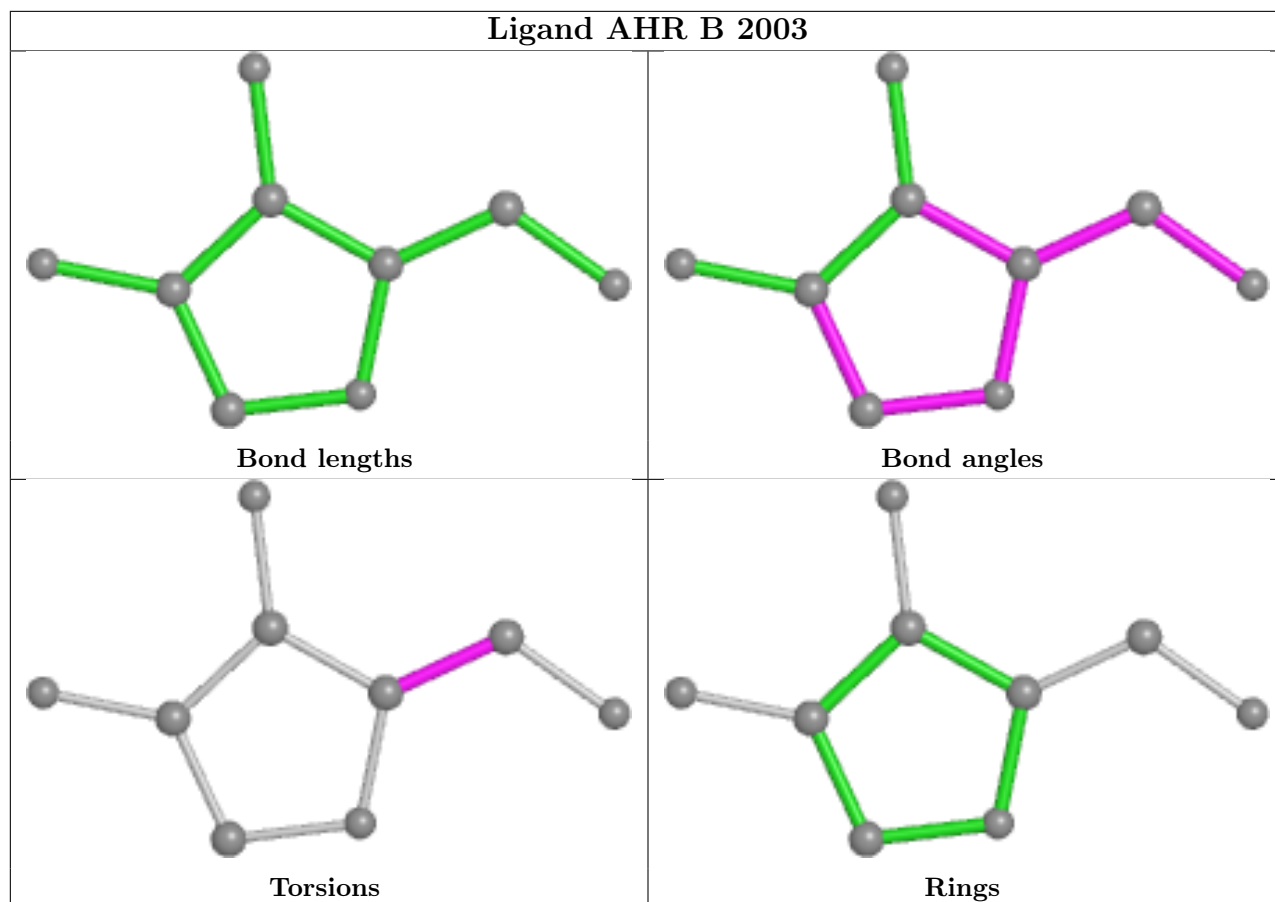


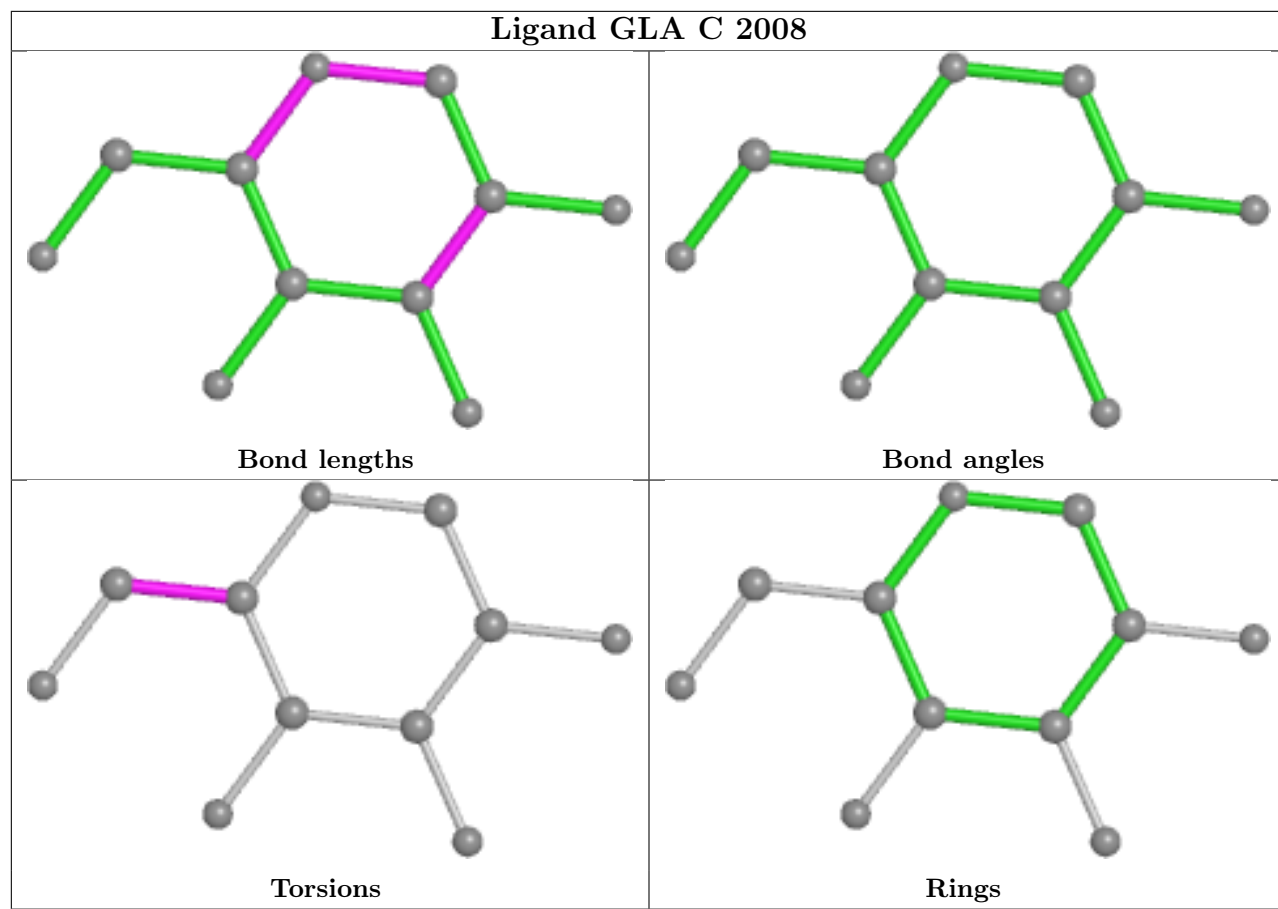


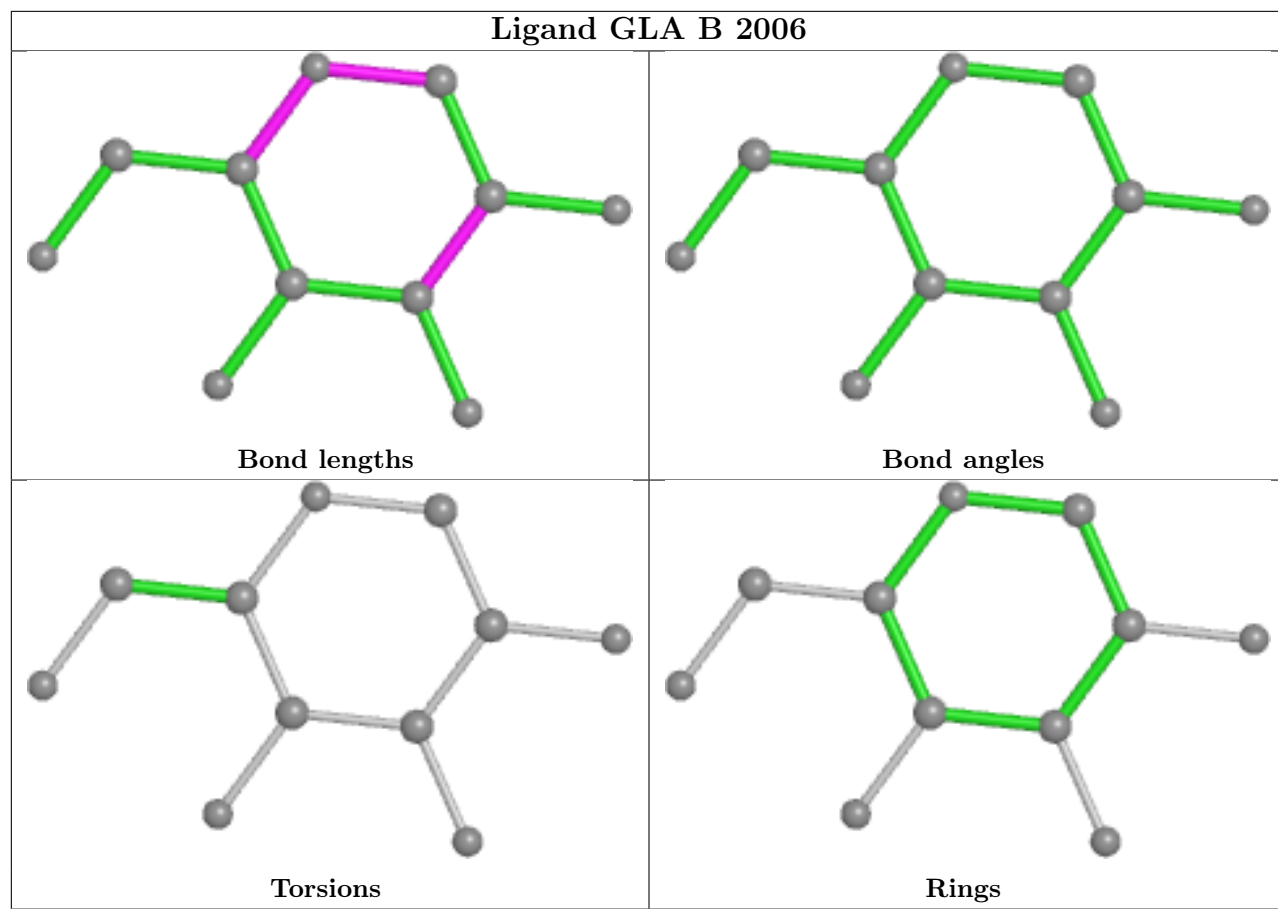


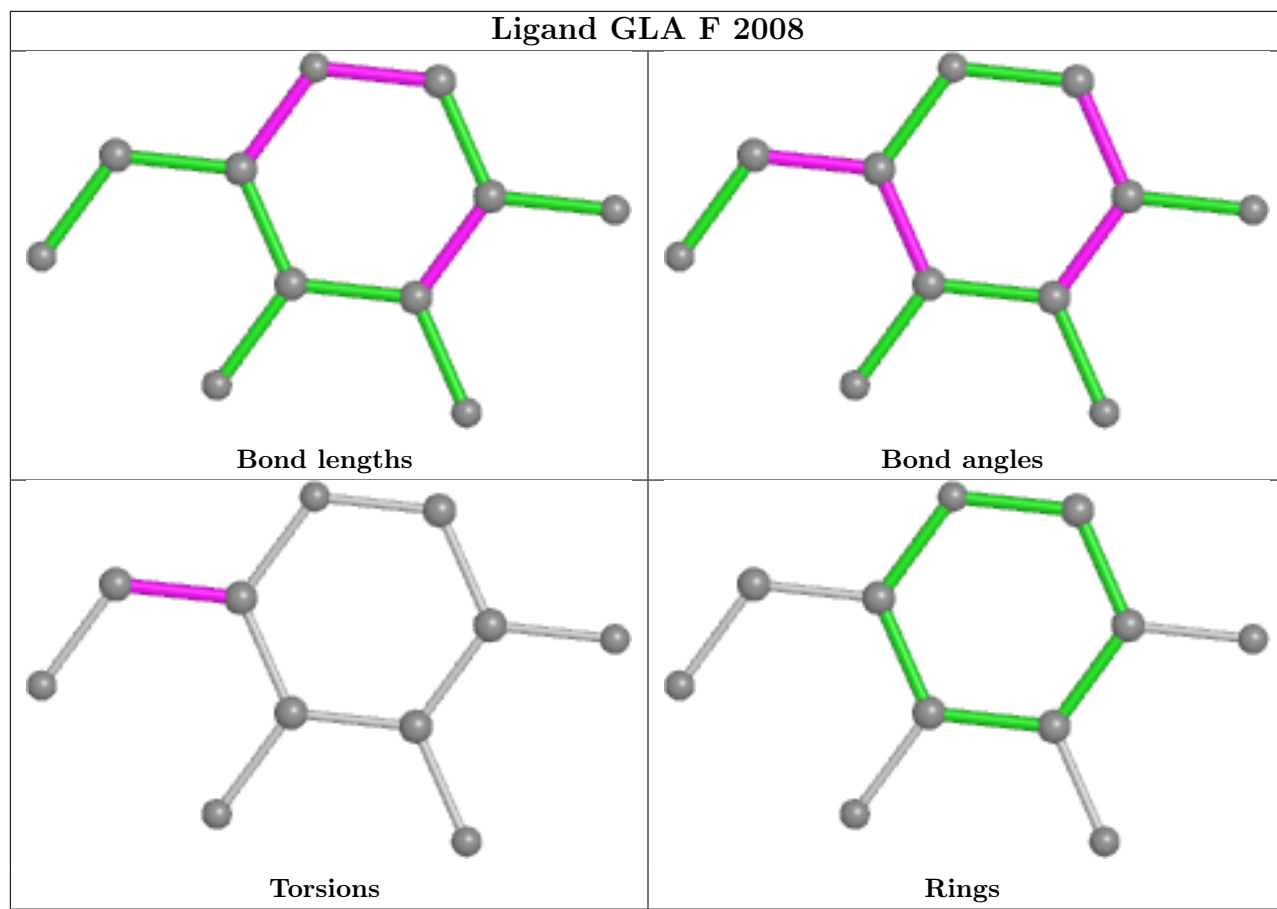


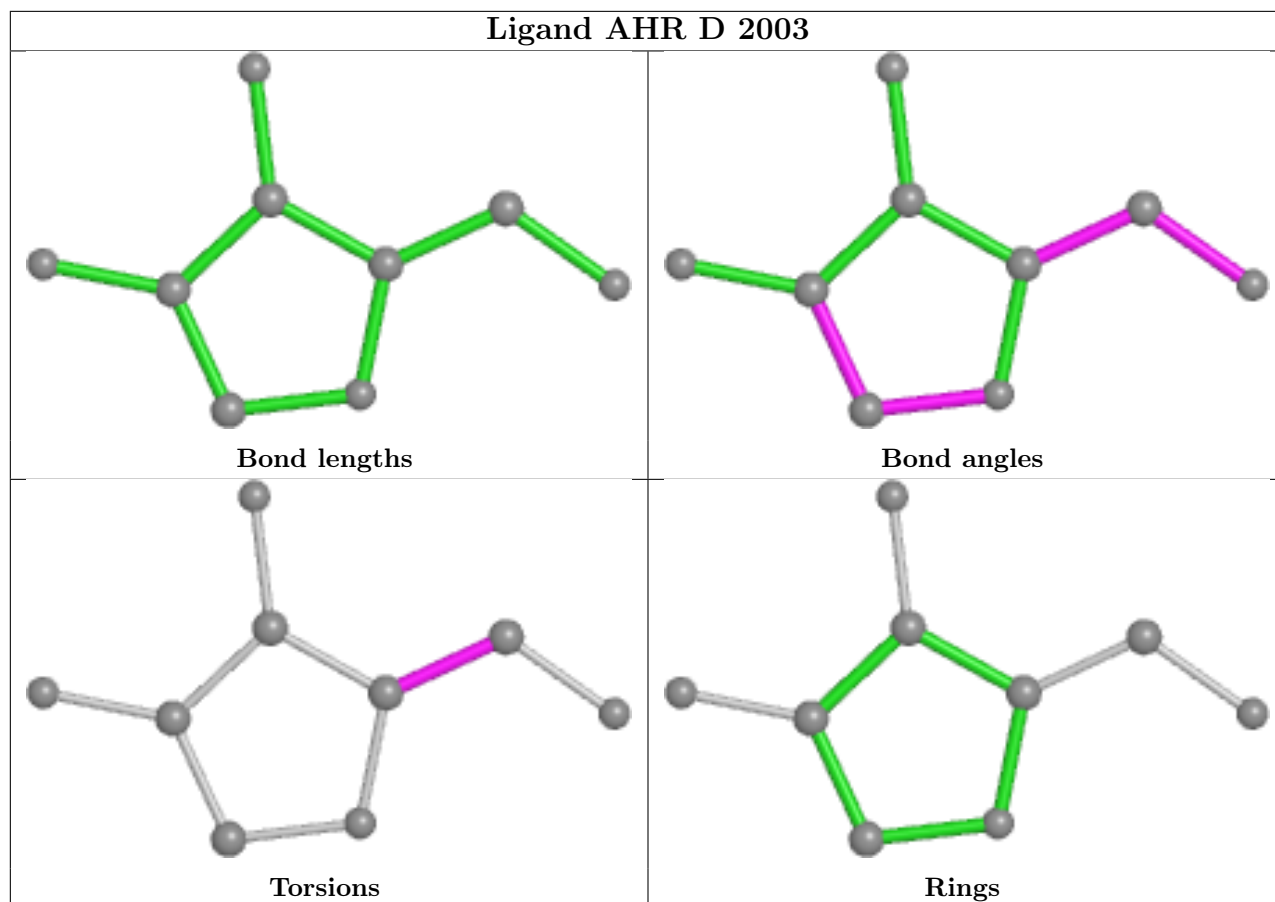


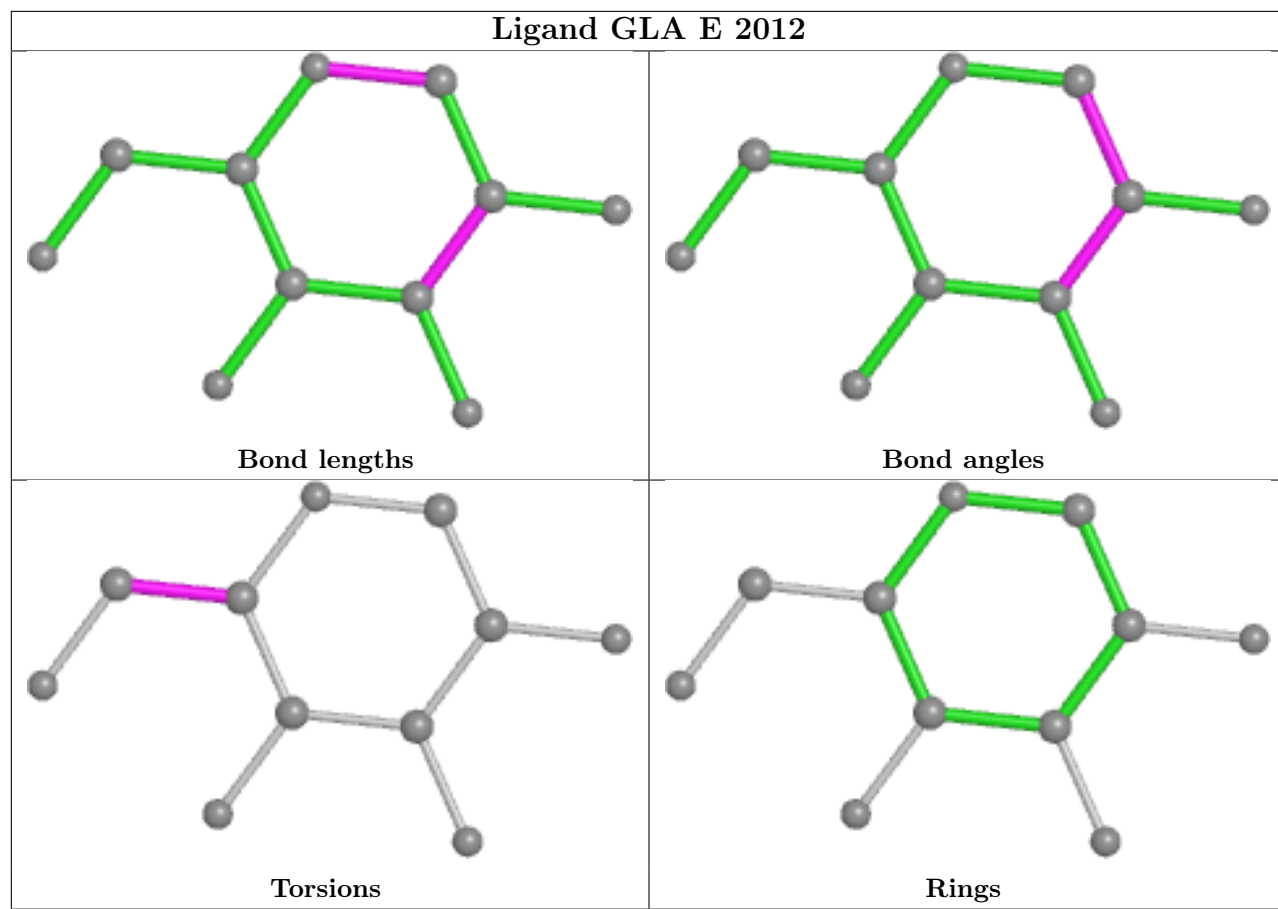


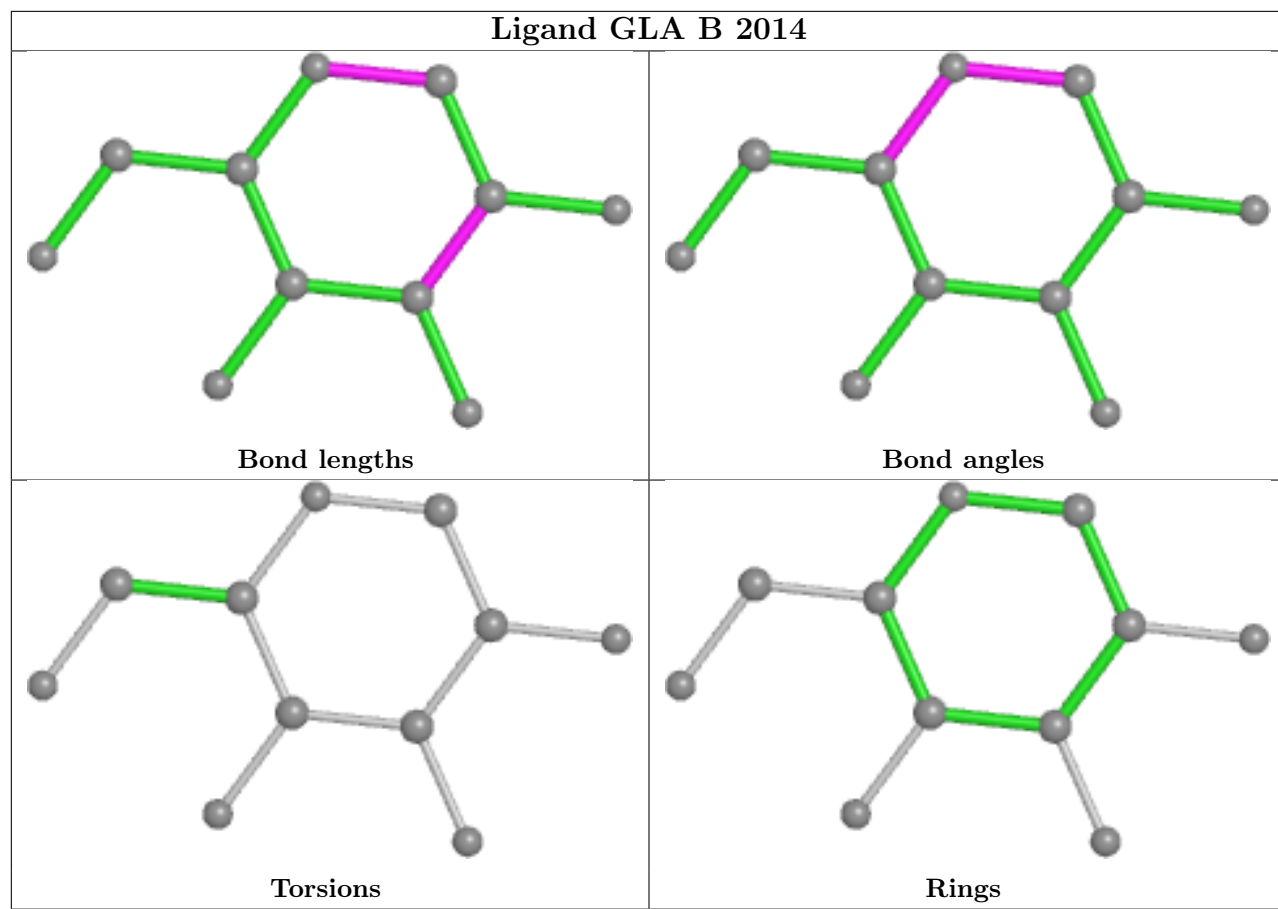


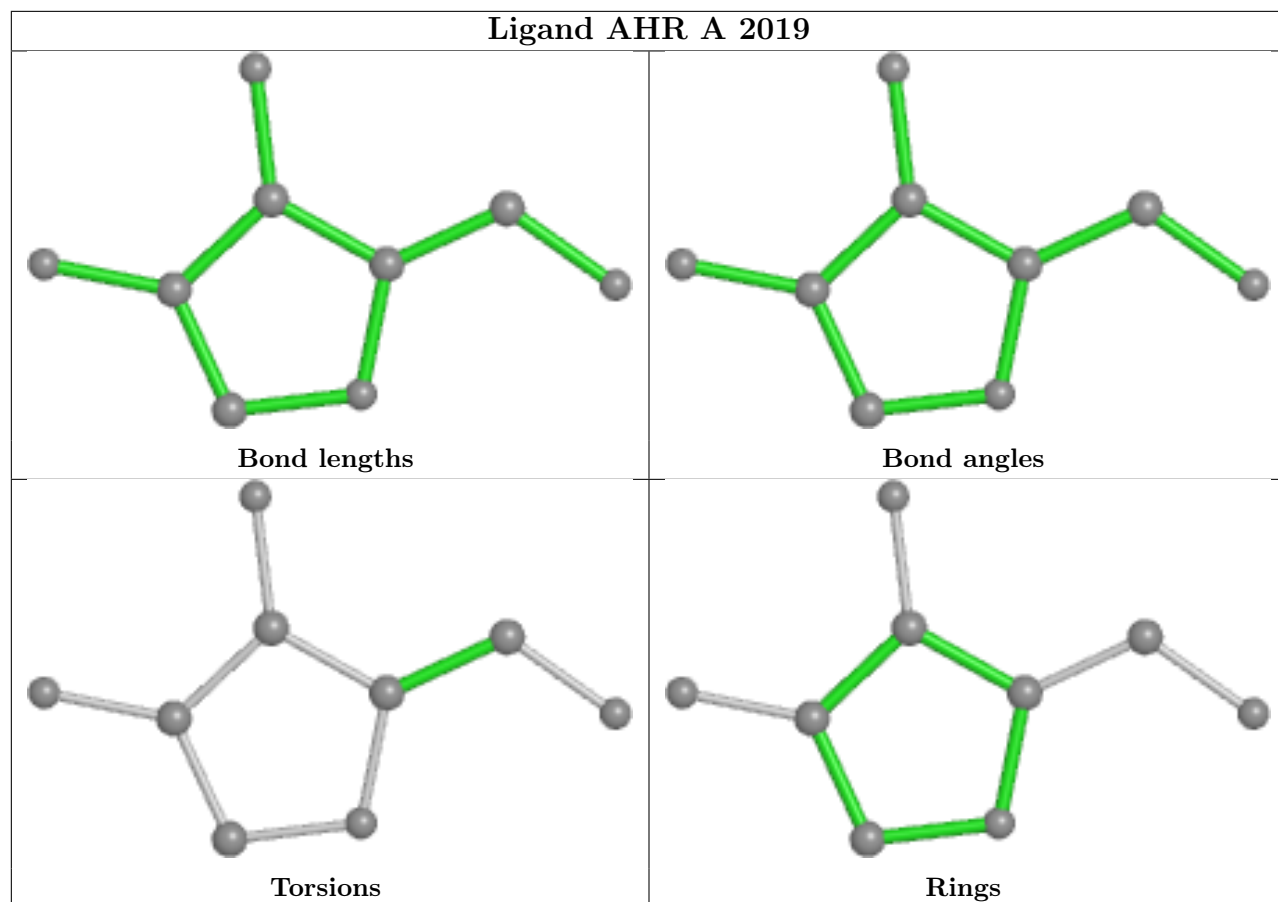




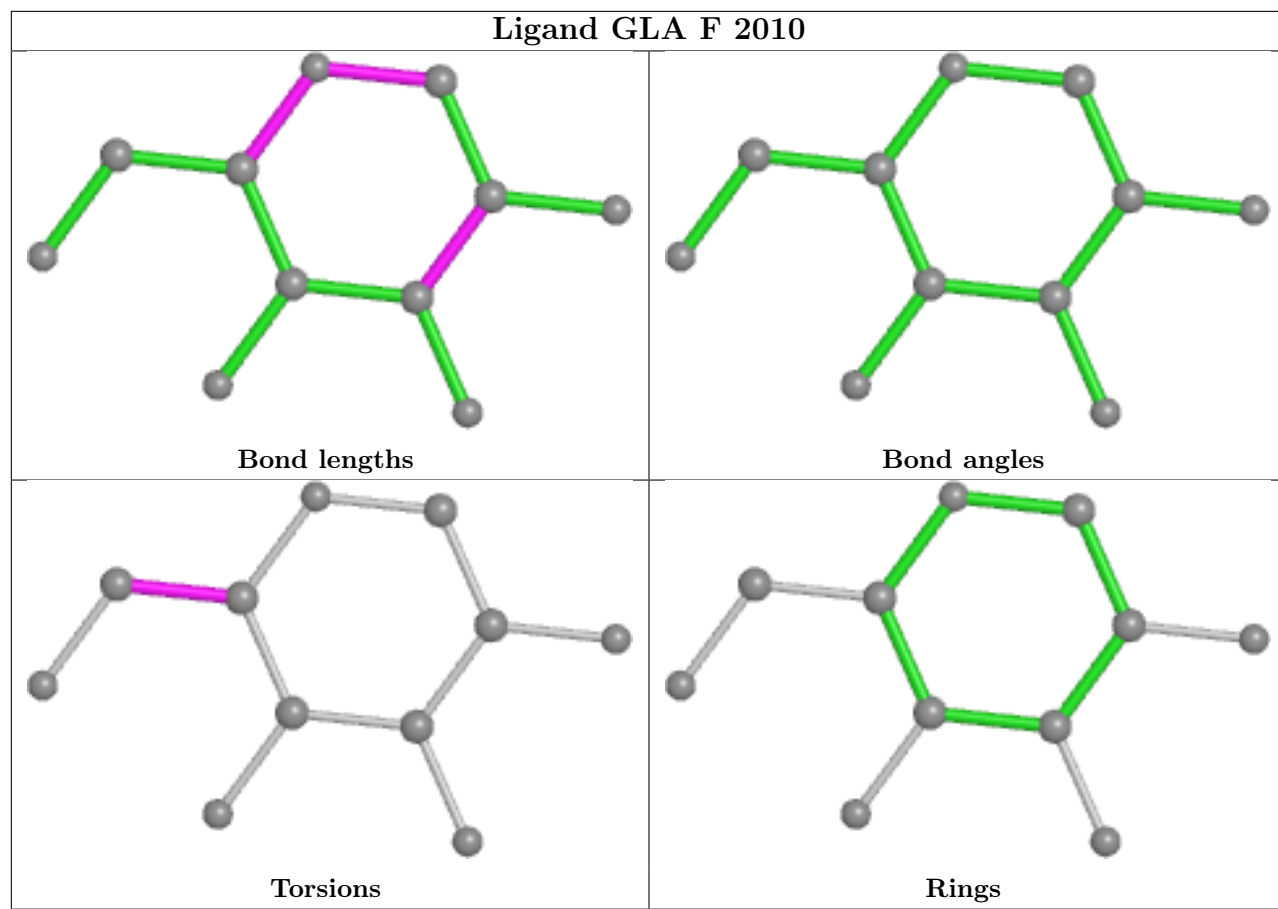


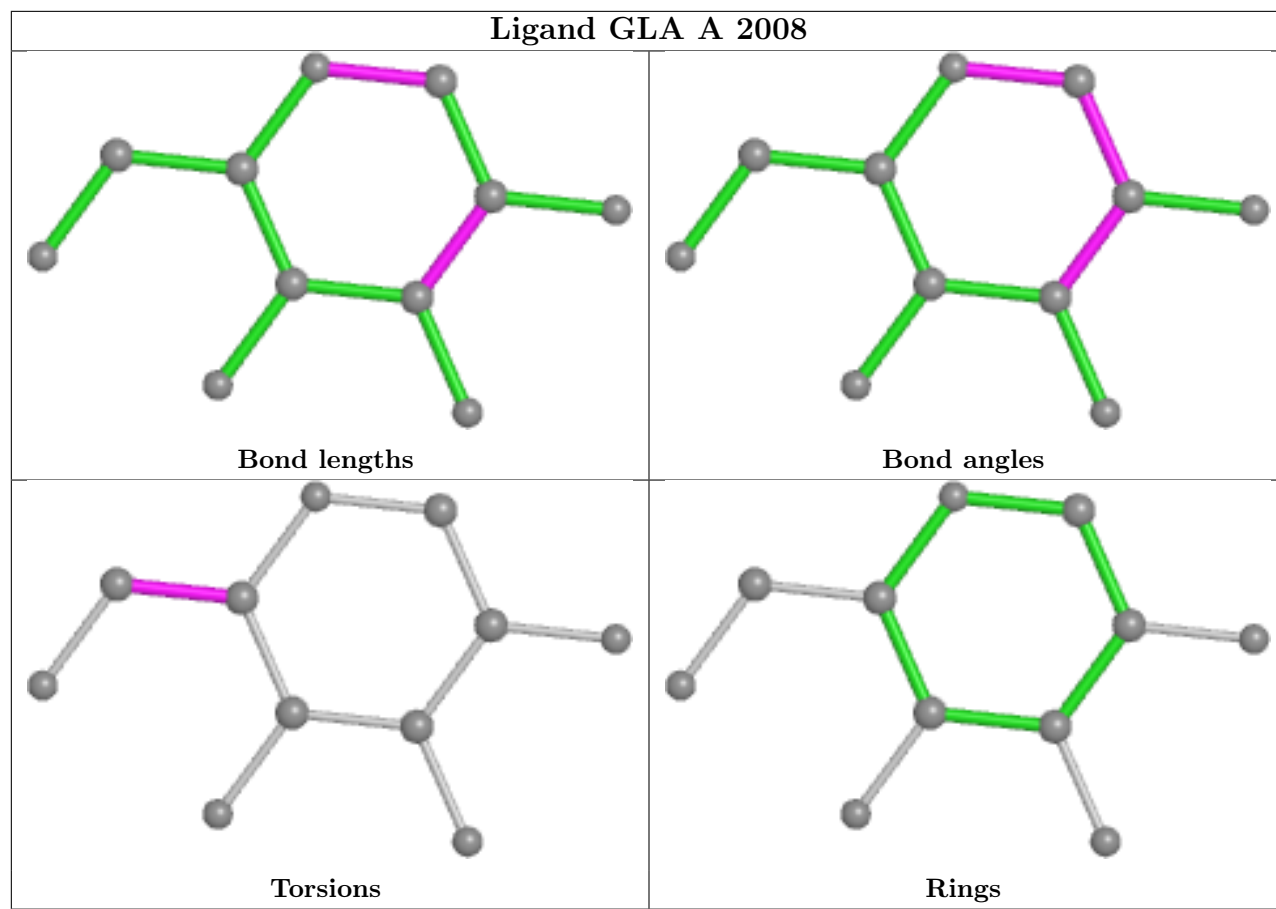


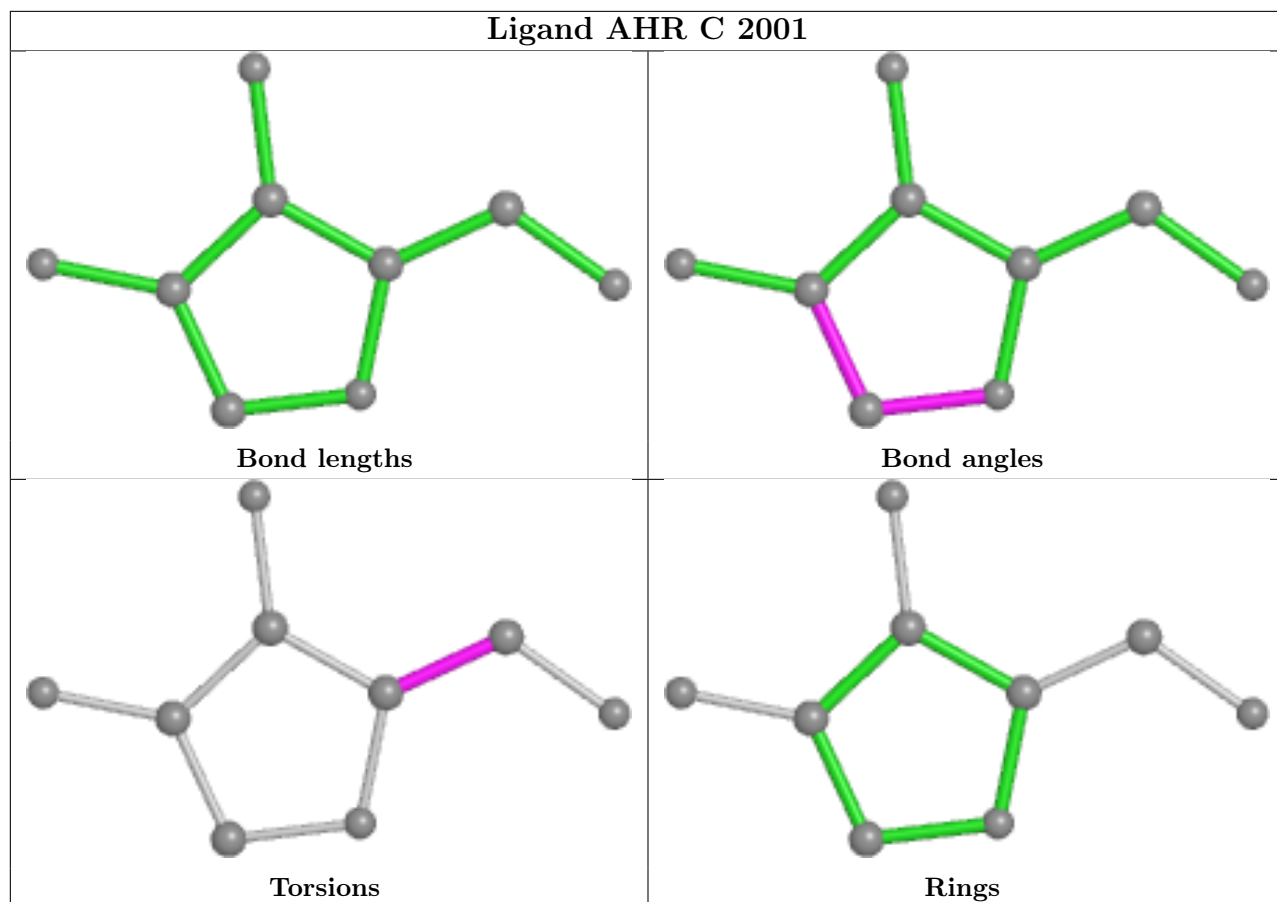


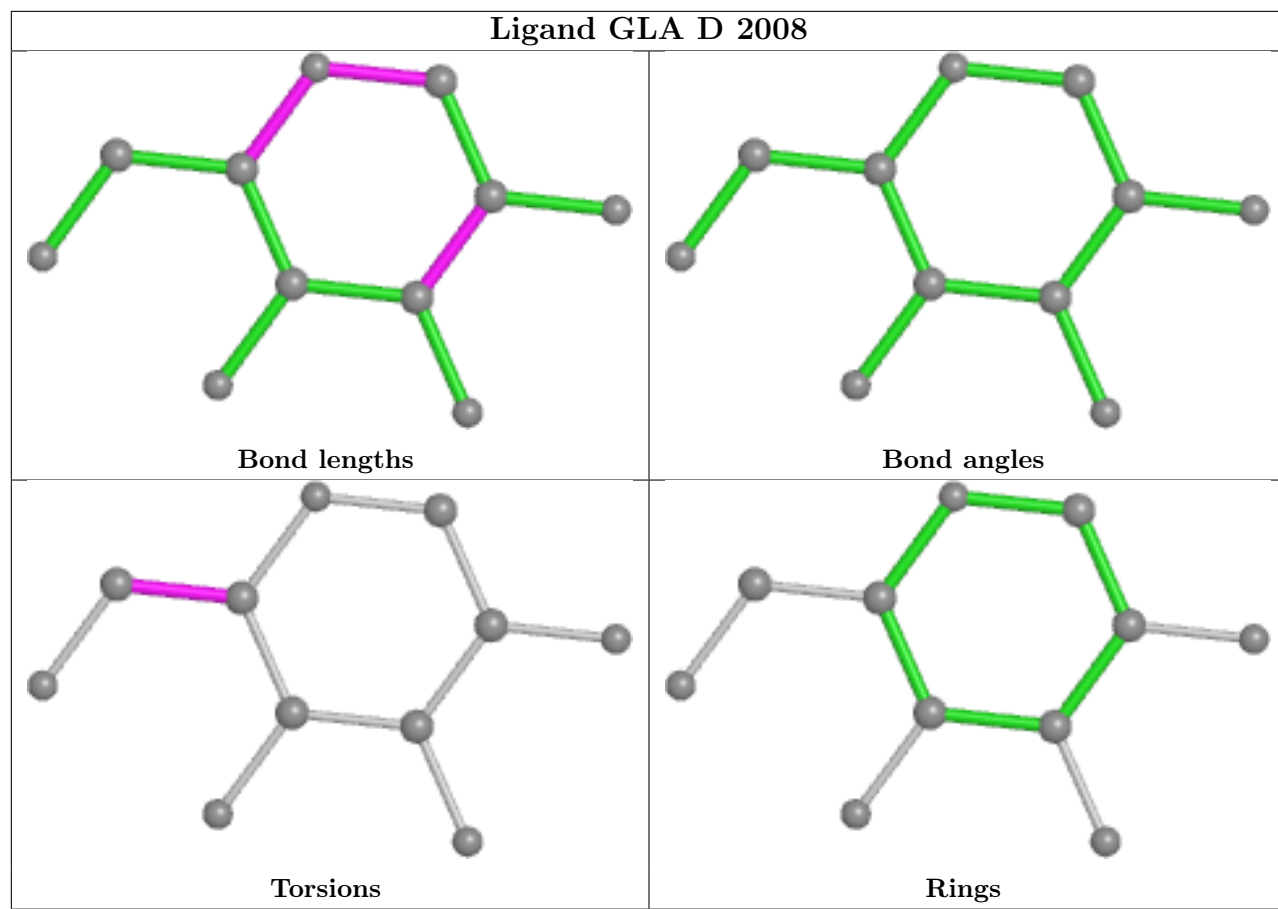


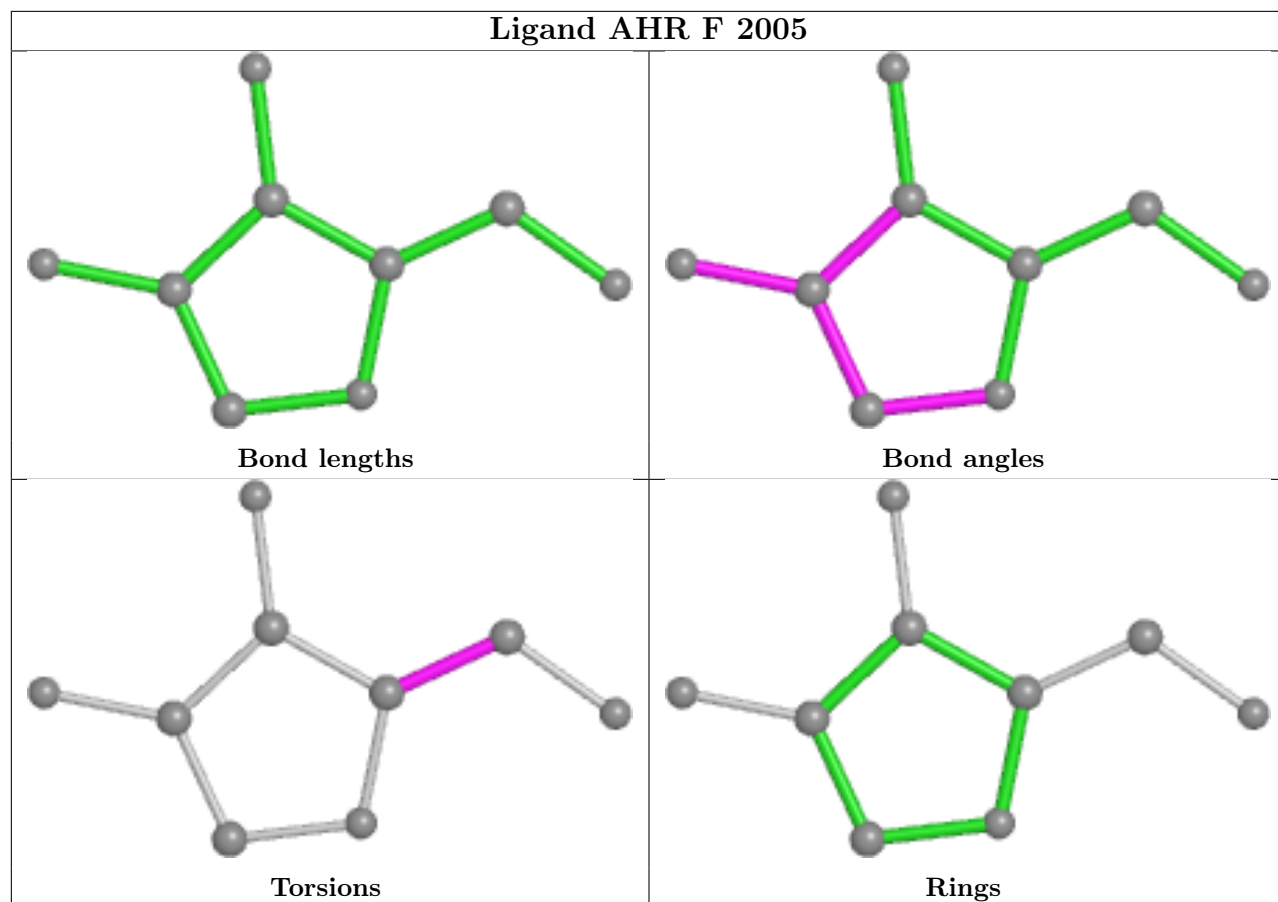


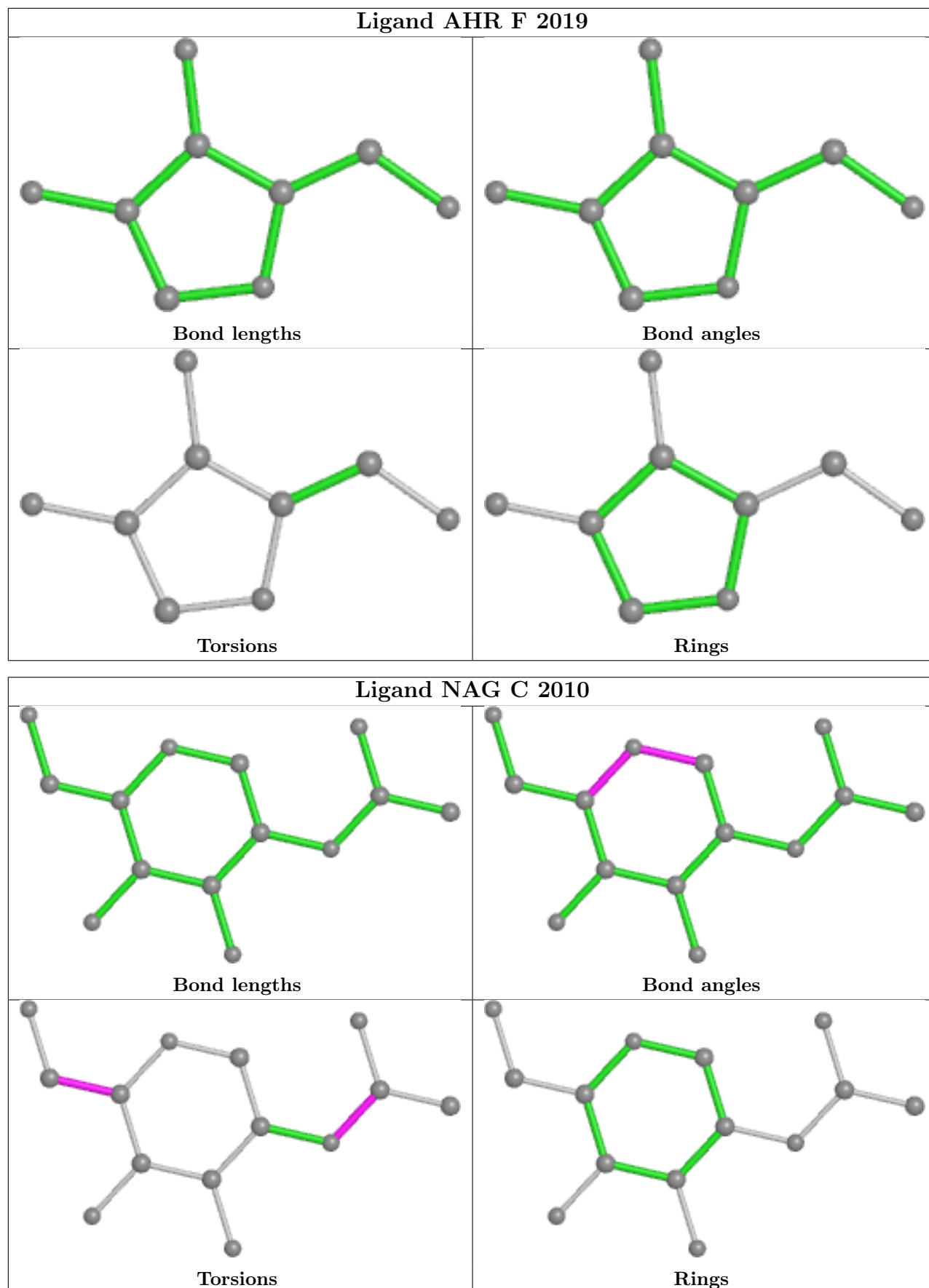


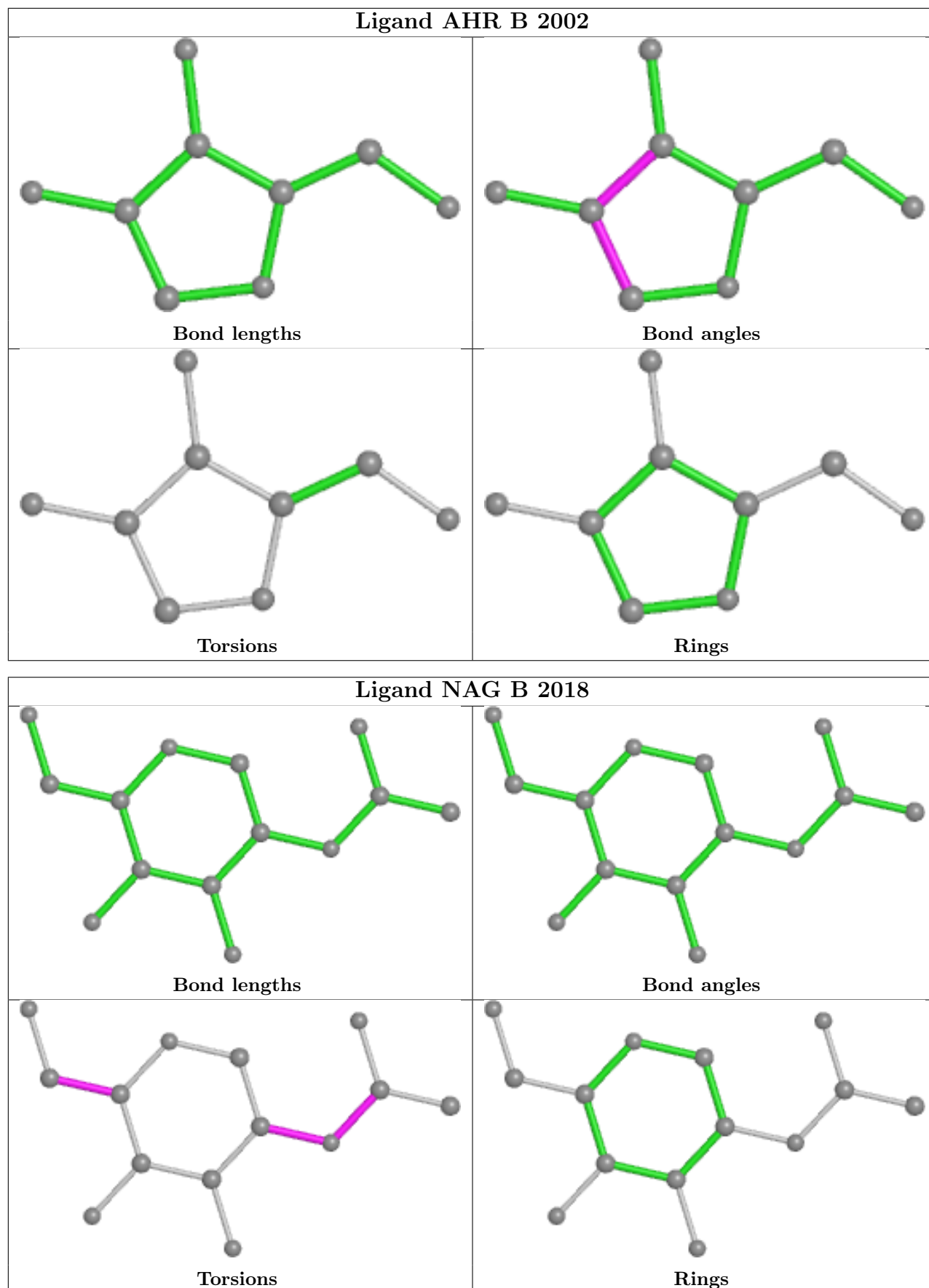


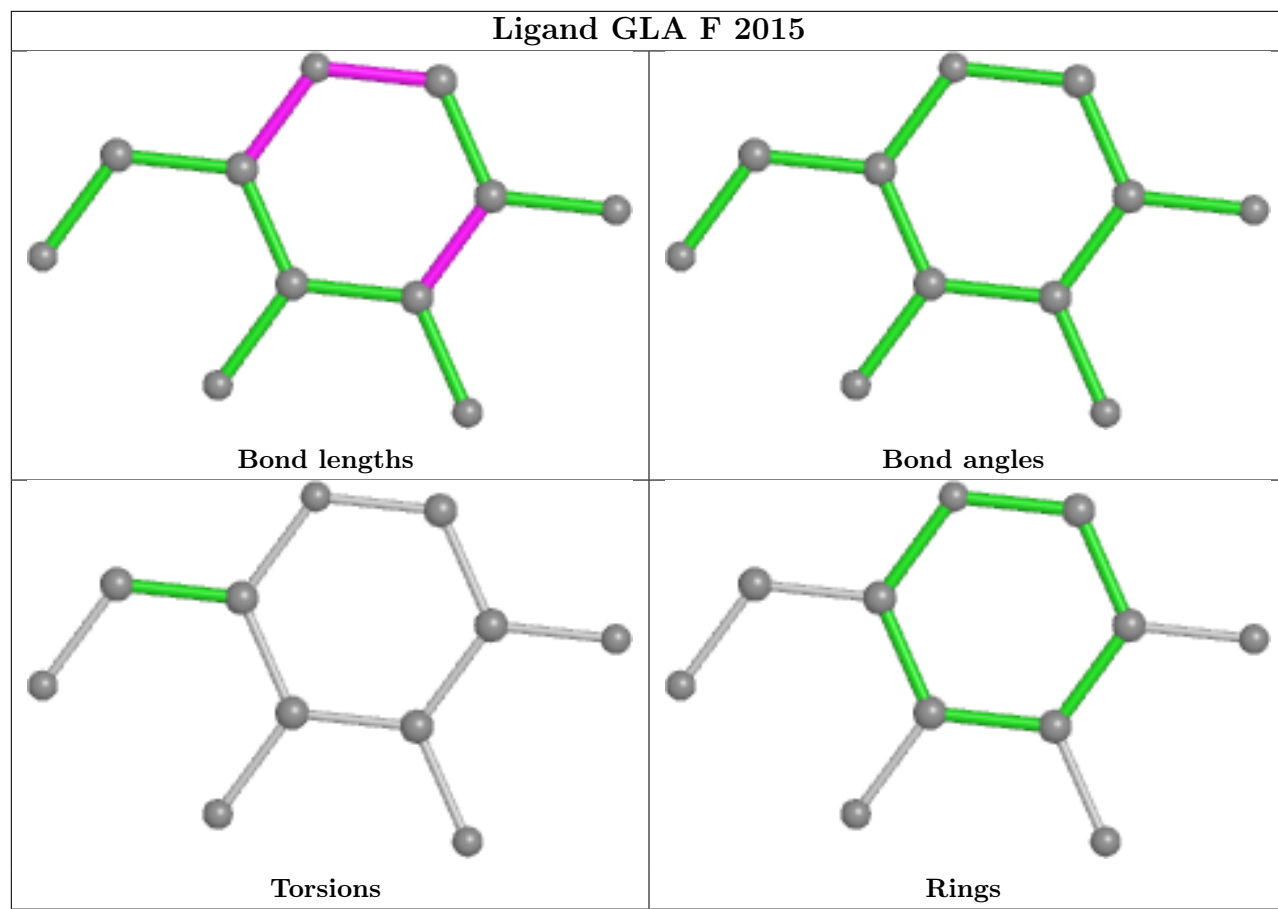




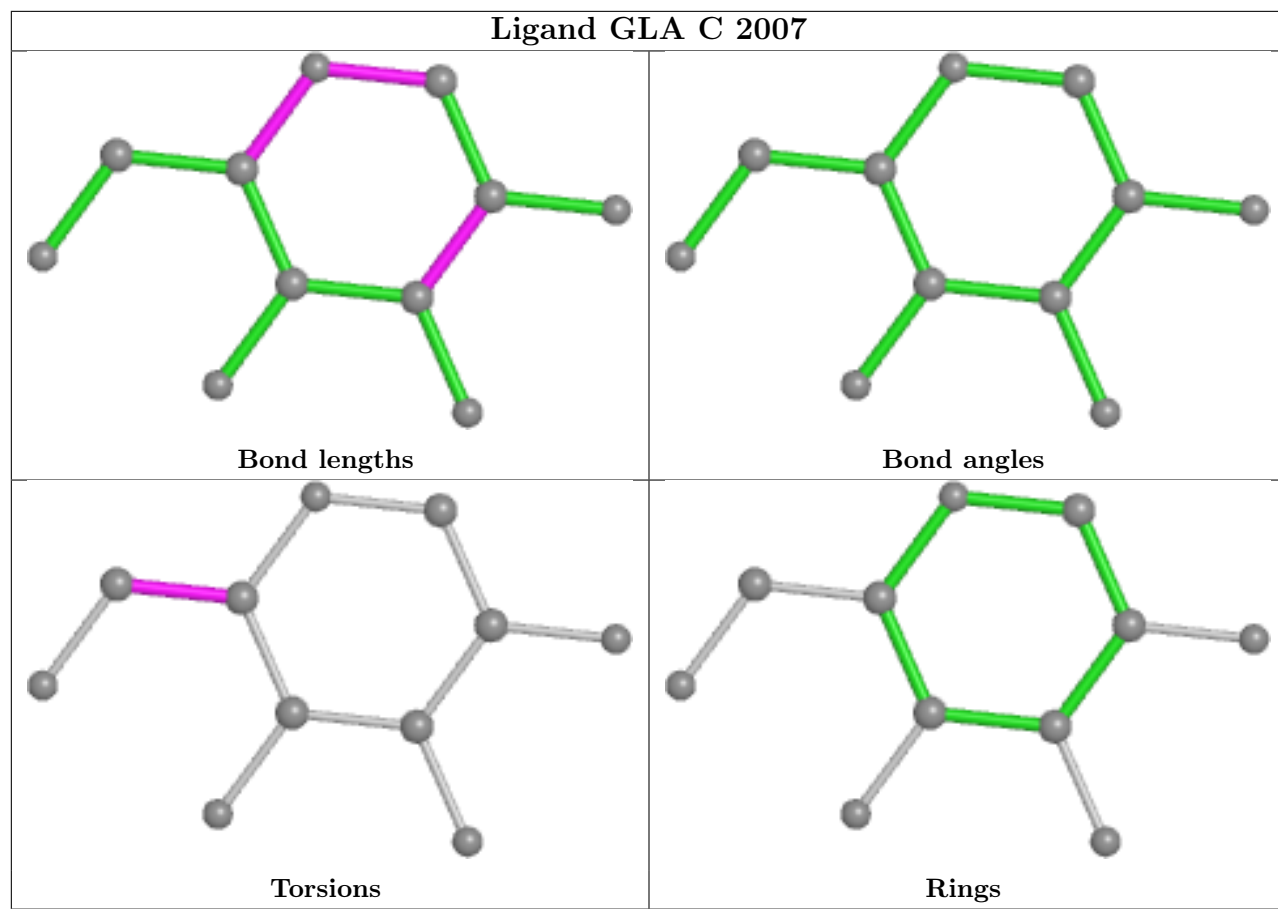


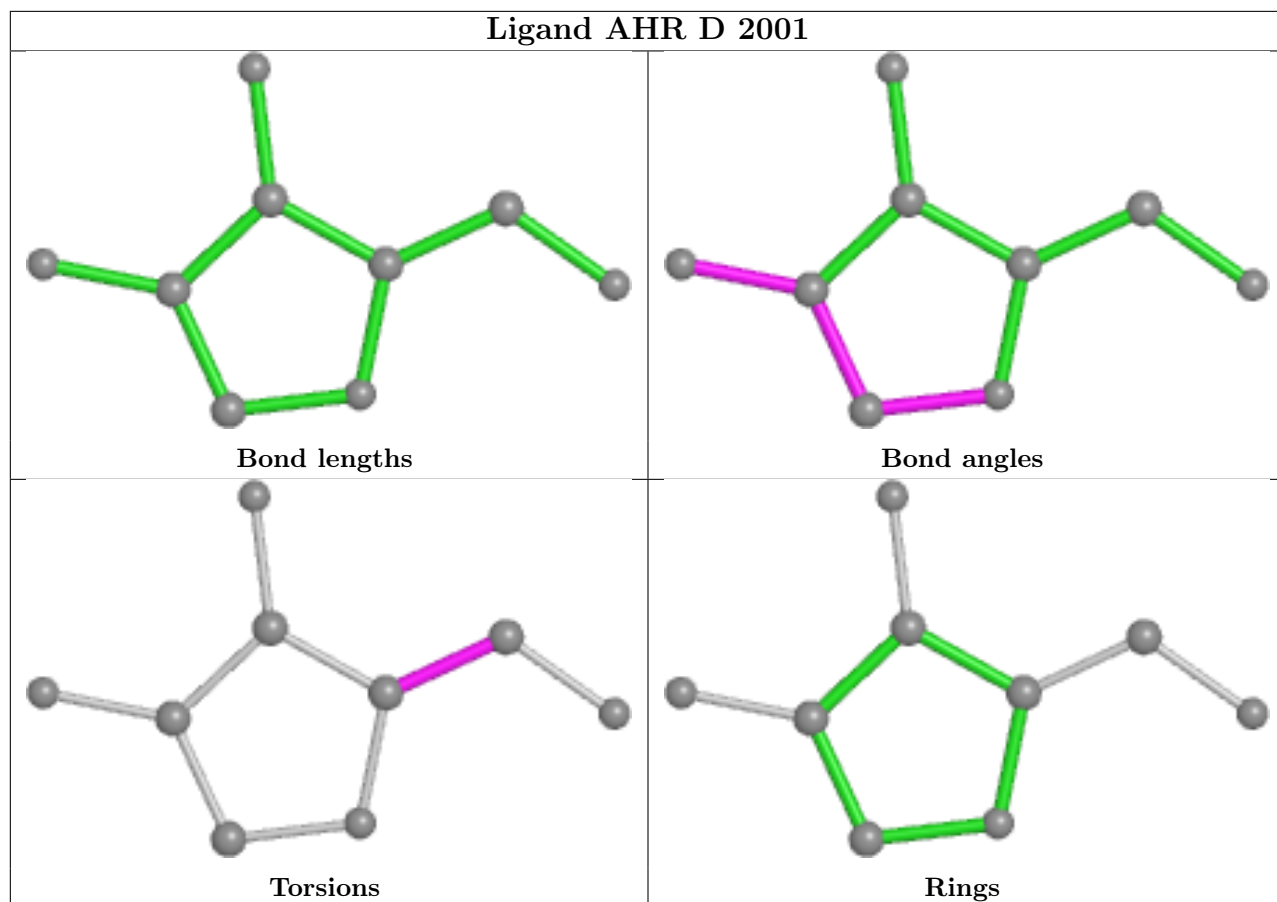


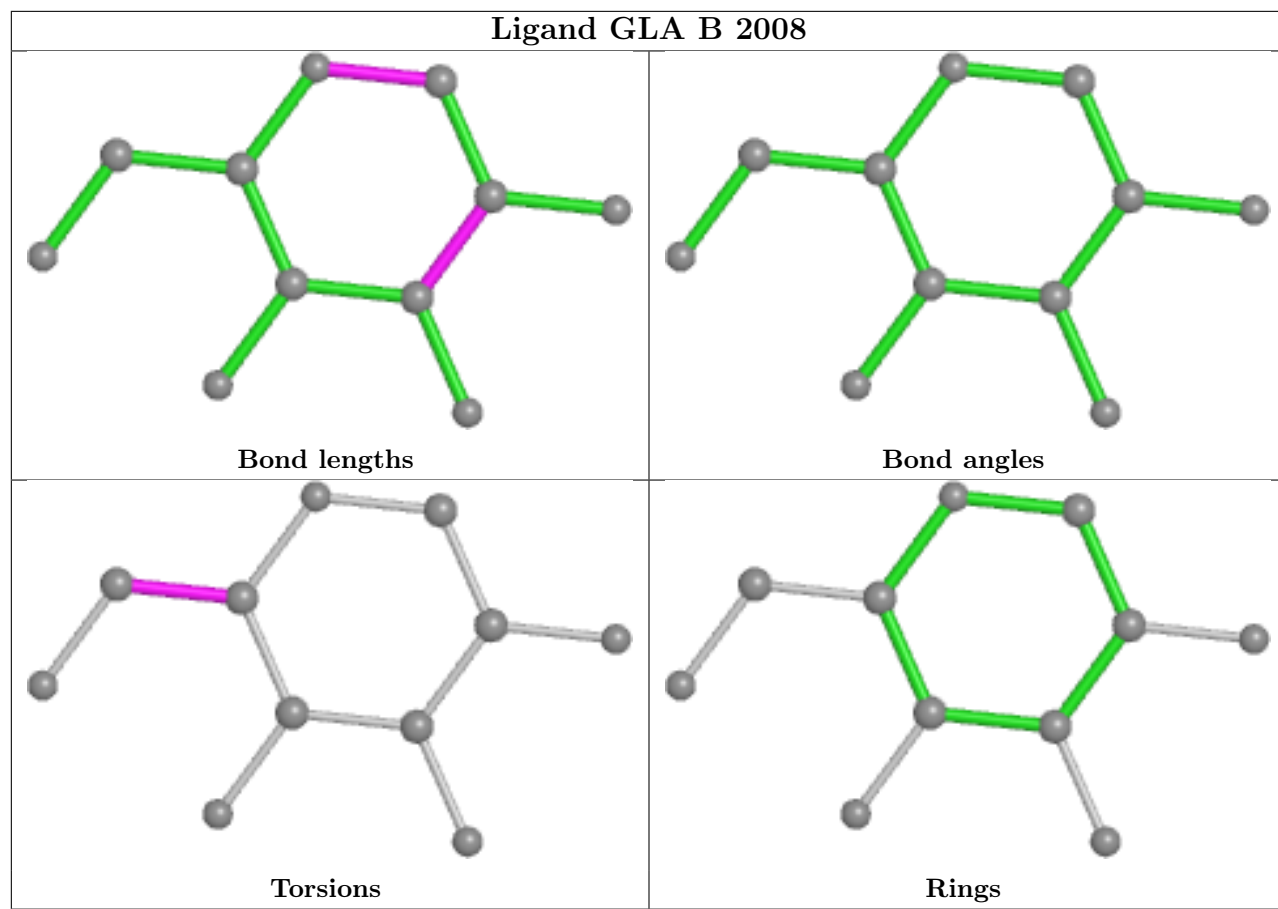


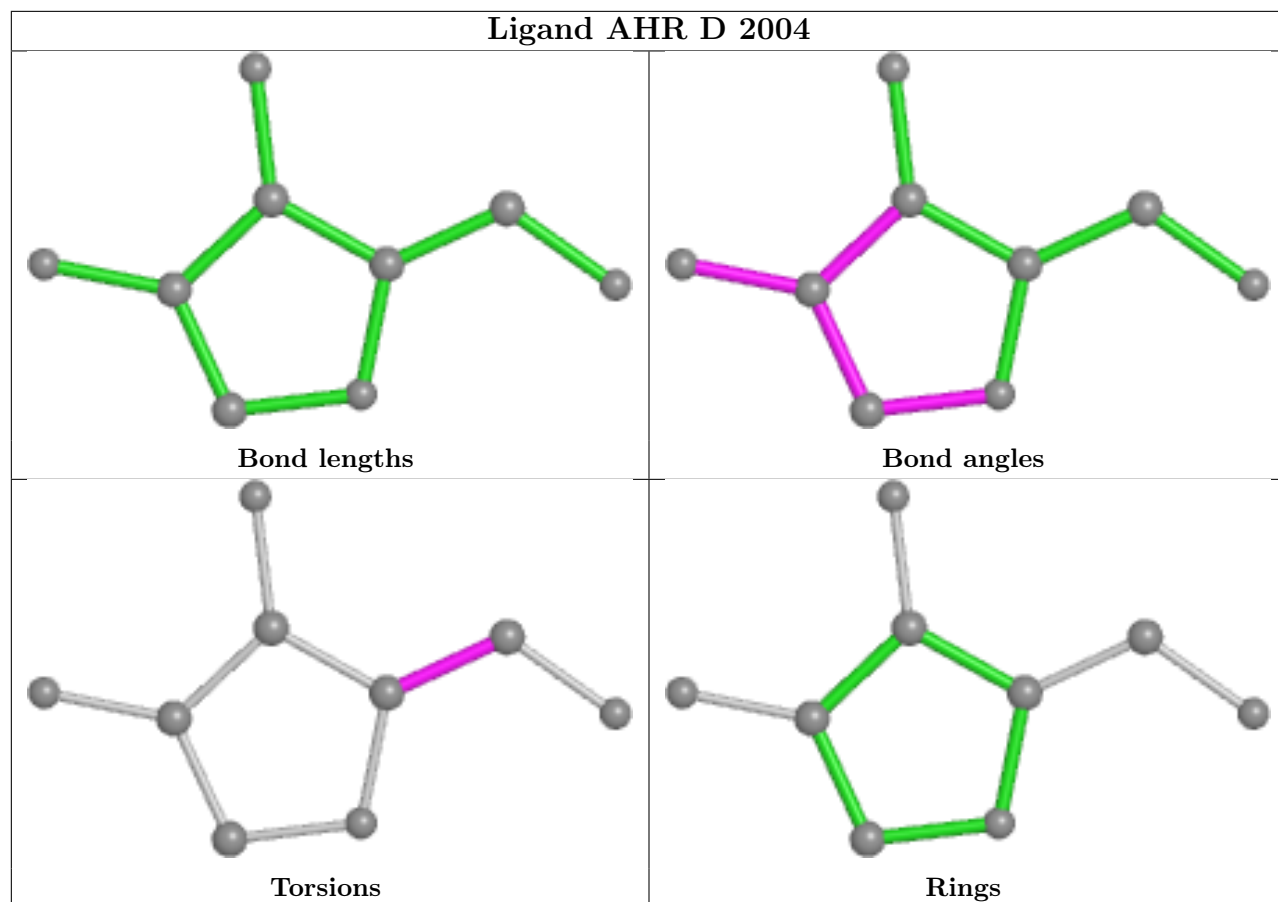


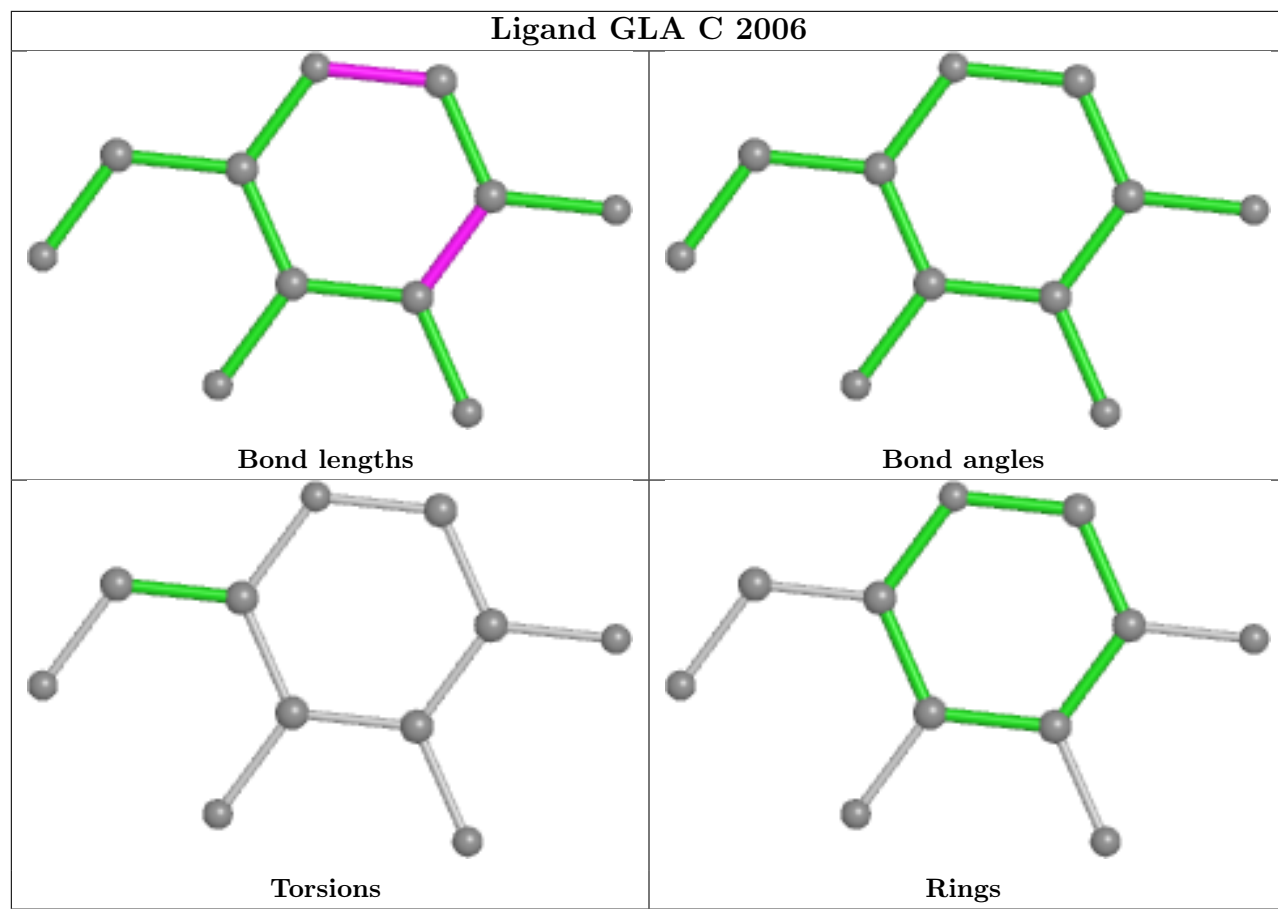


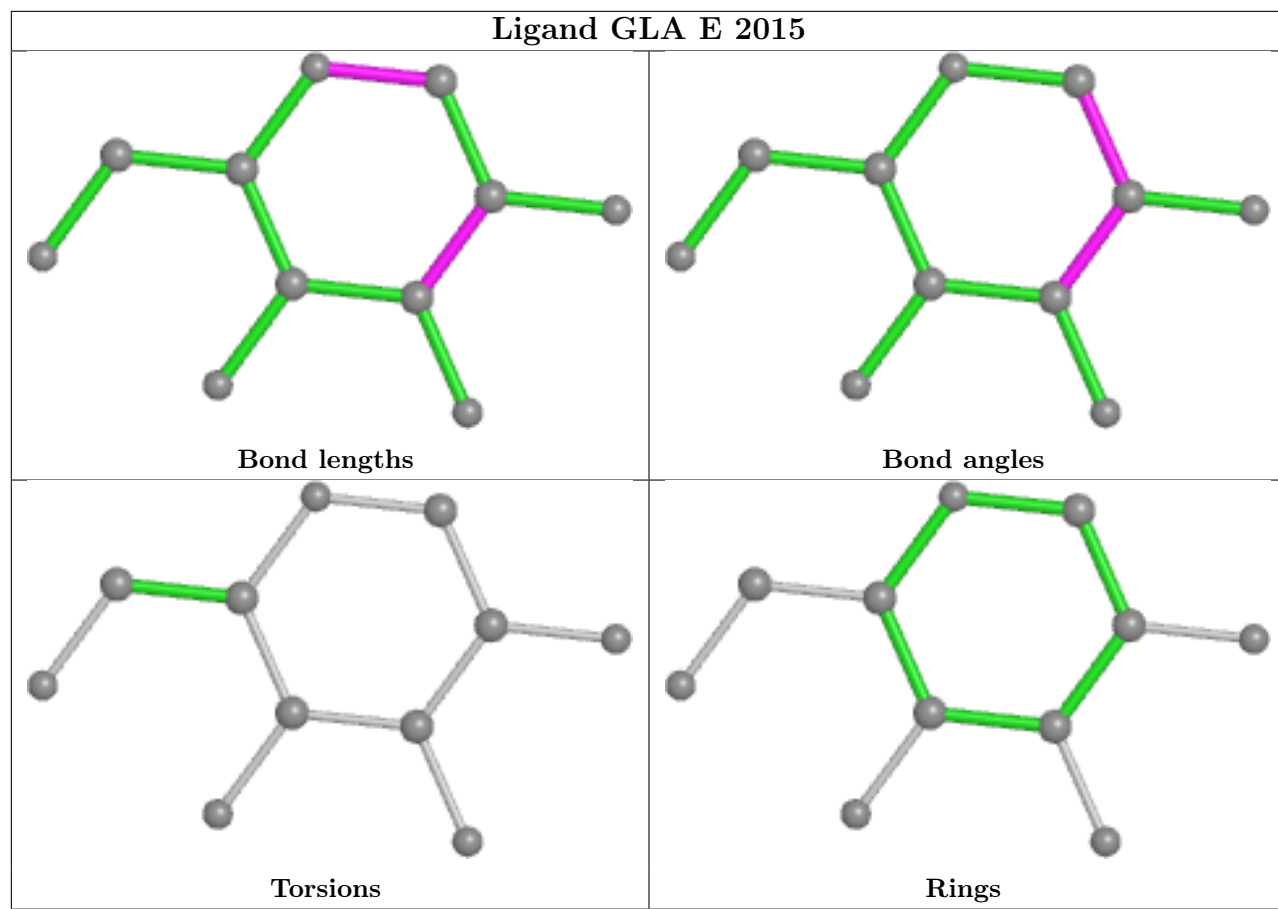


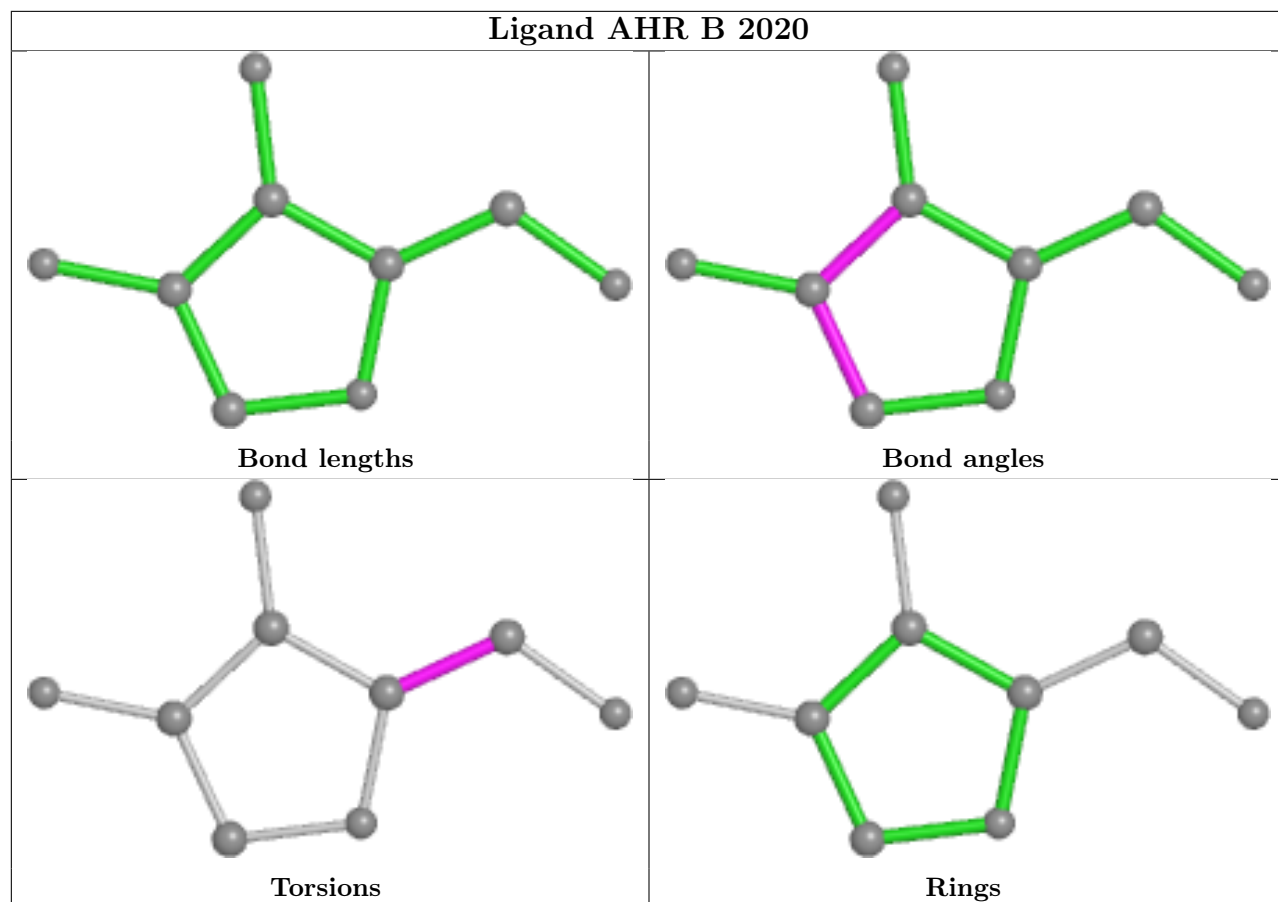


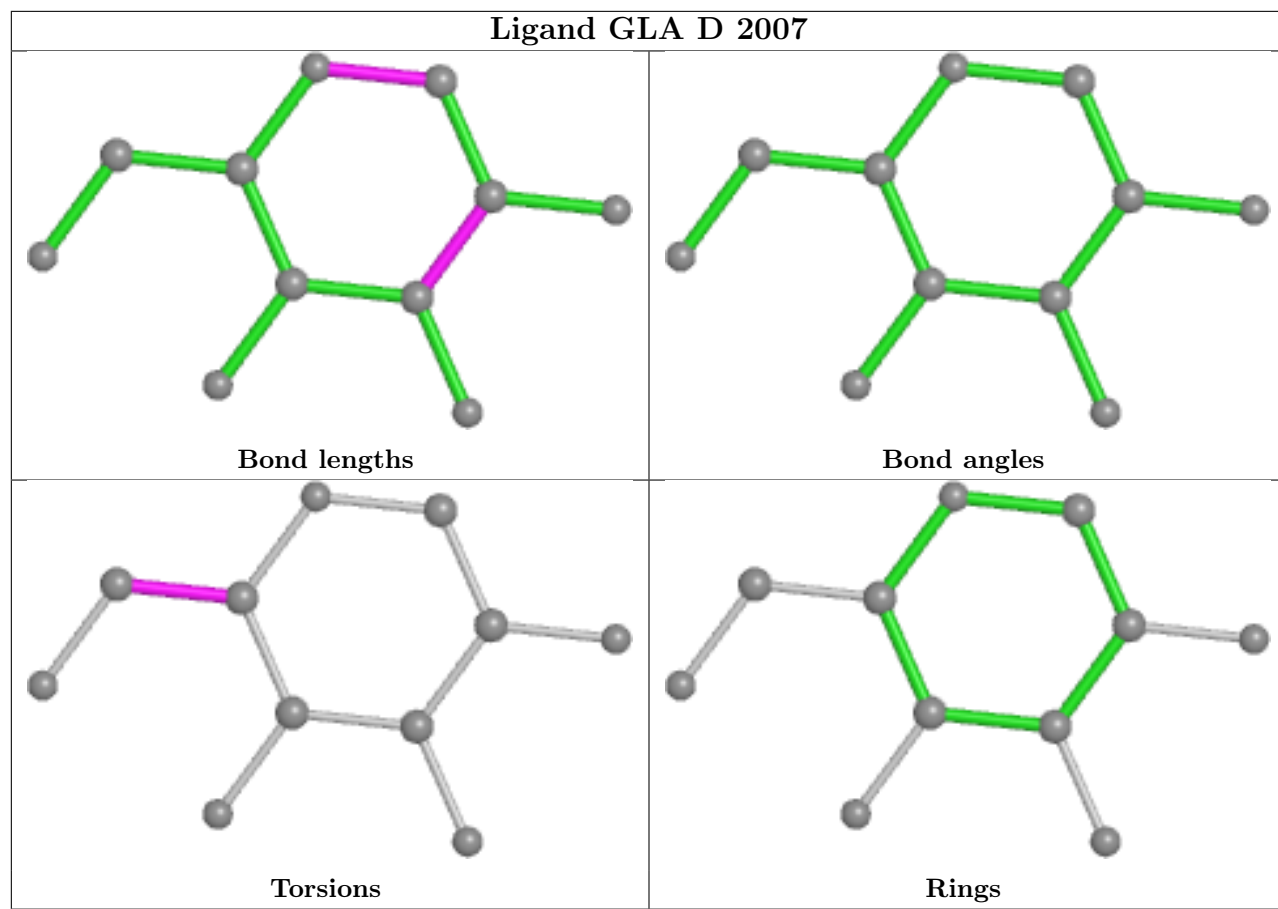




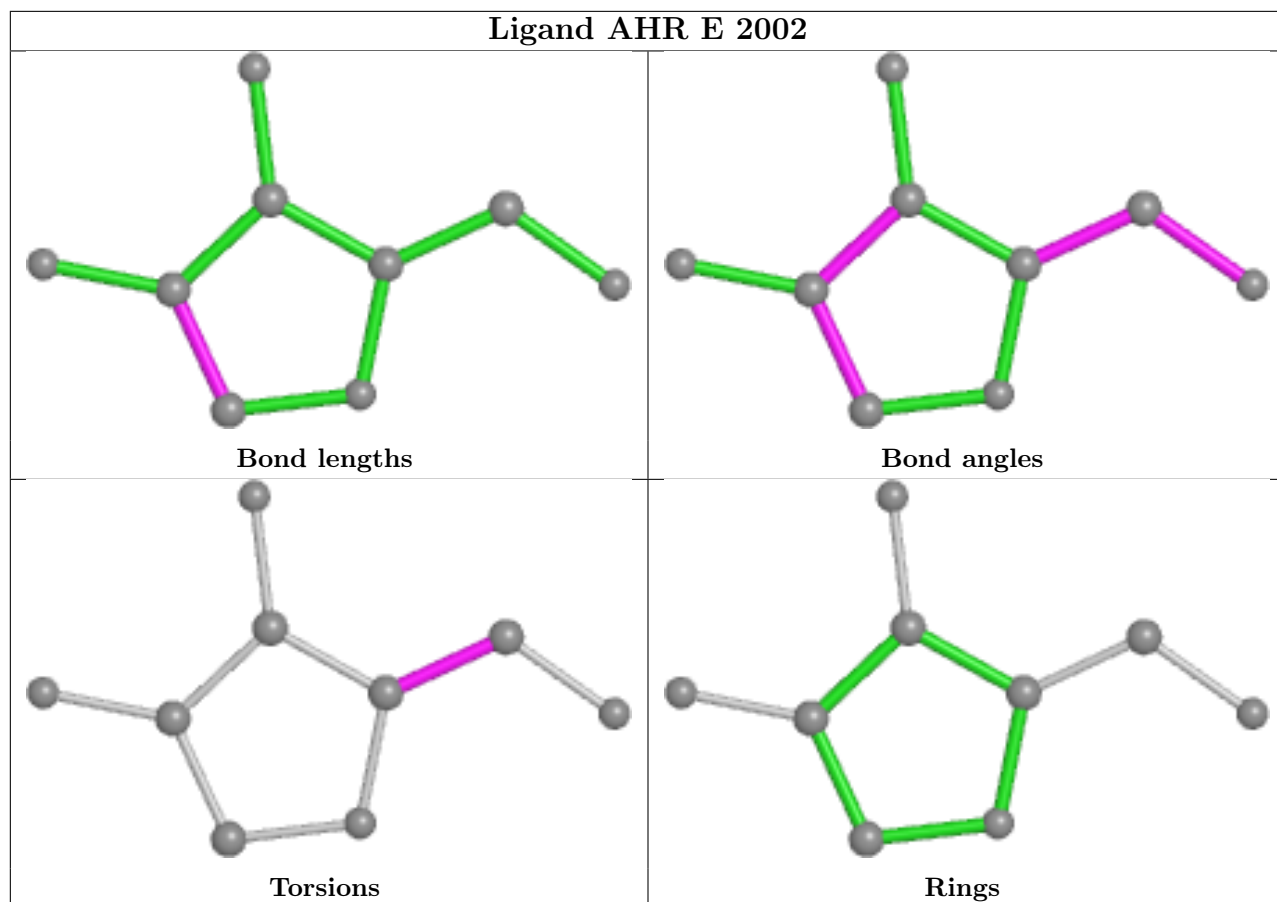


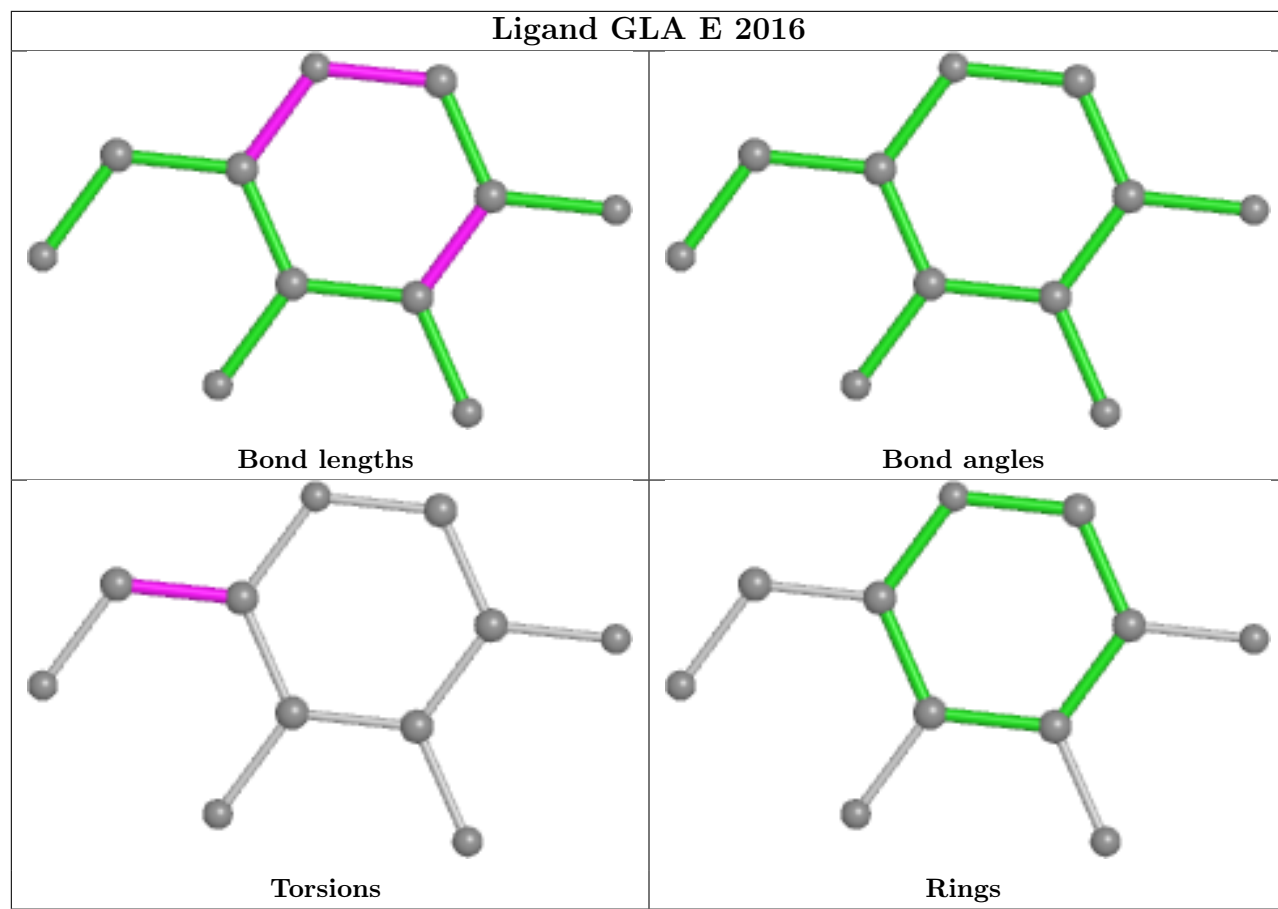


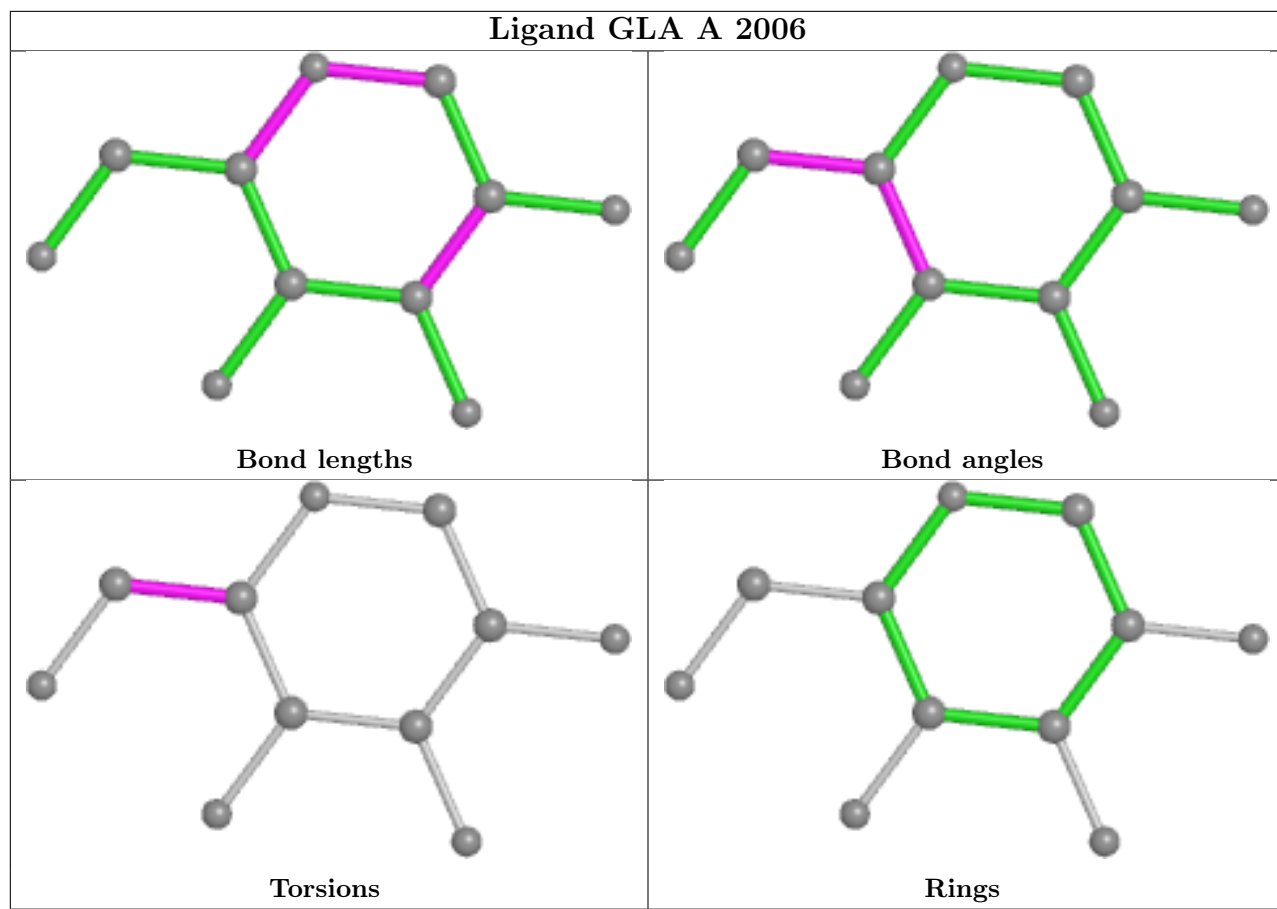


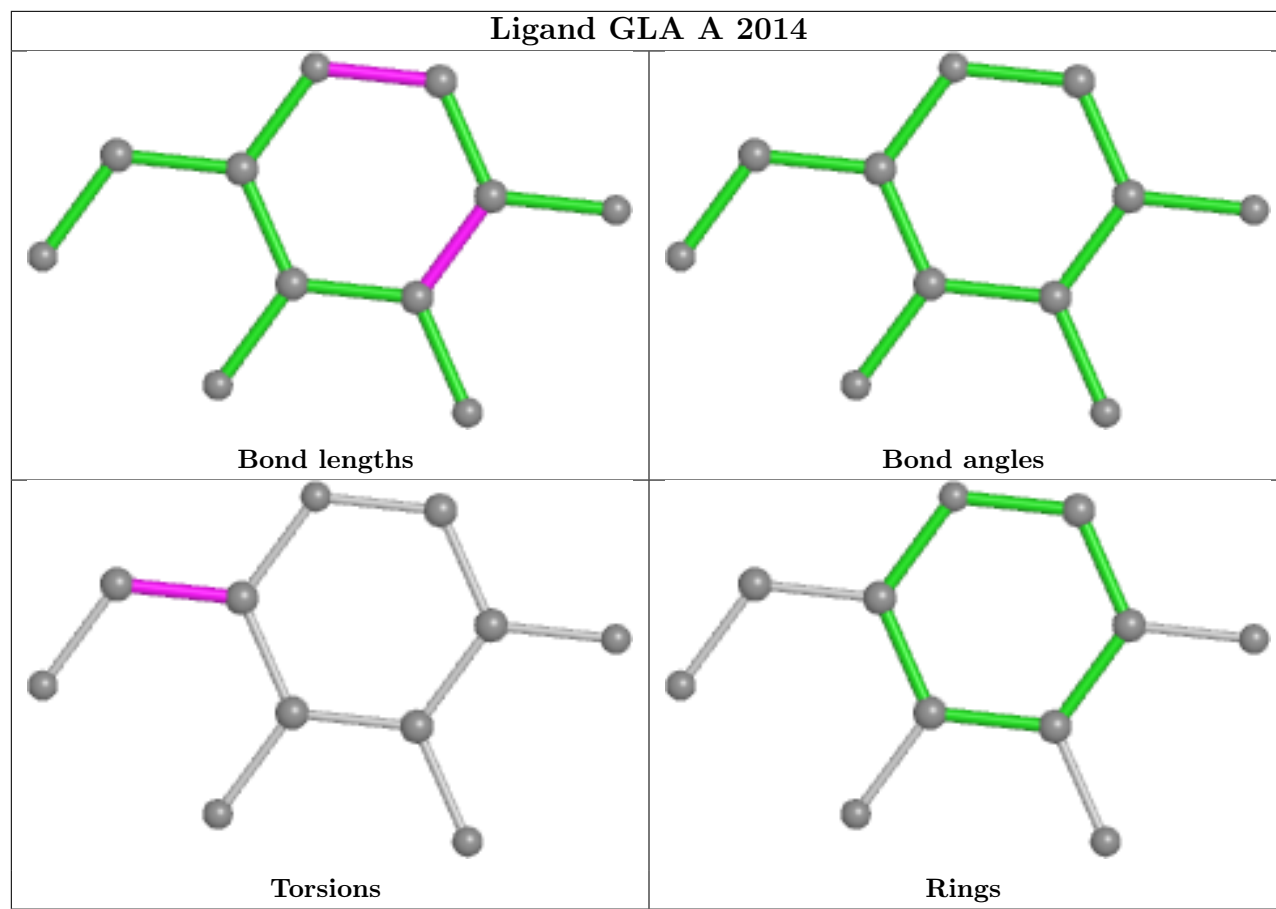












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

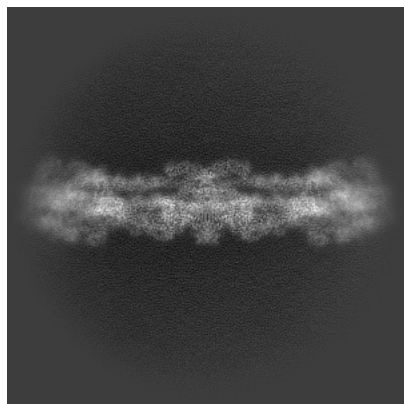
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37389. These allow visual inspection of the internal detail of the map and identification of artifacts.

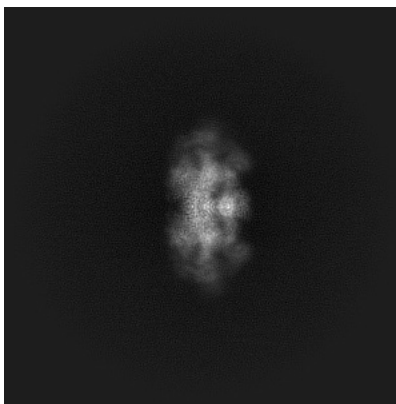
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

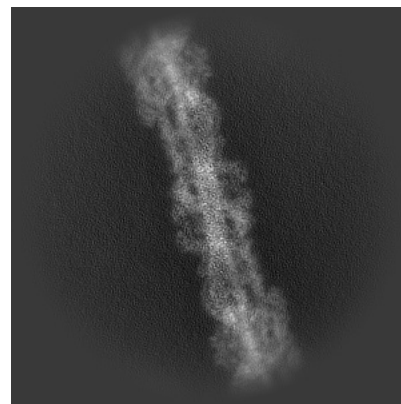
#### 6.1.1 Primary map



X

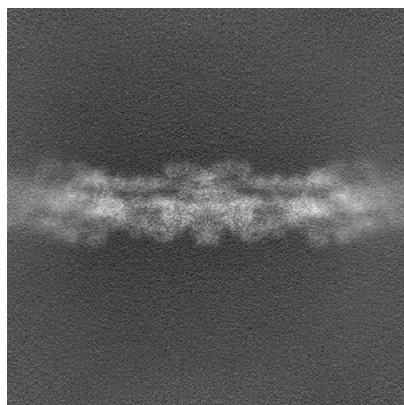


Y

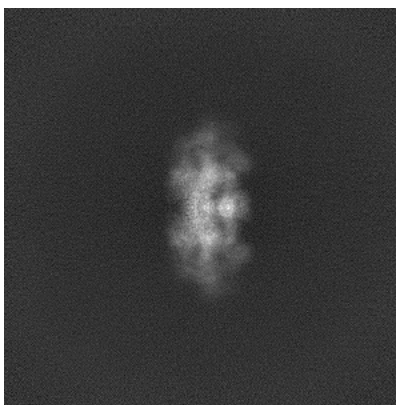


Z

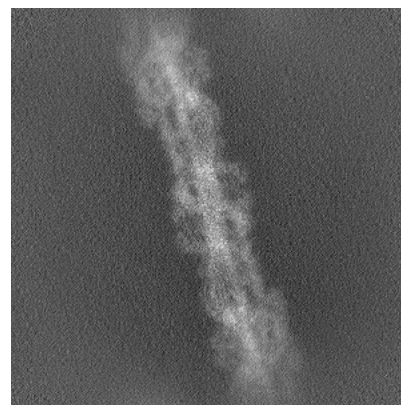
#### 6.1.2 Raw map



X



Y

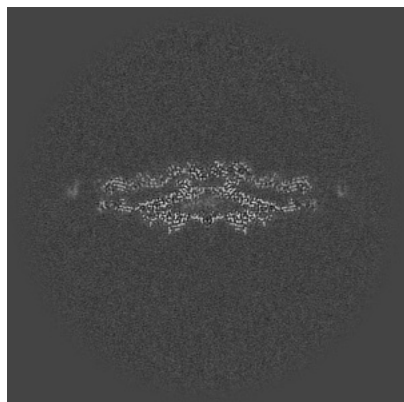


Z

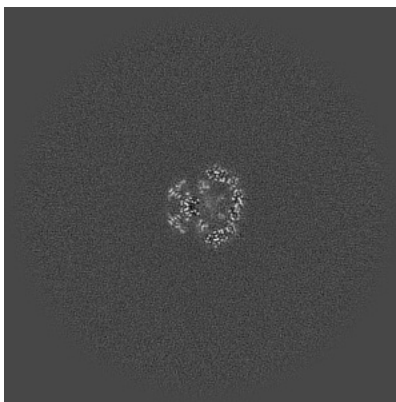
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

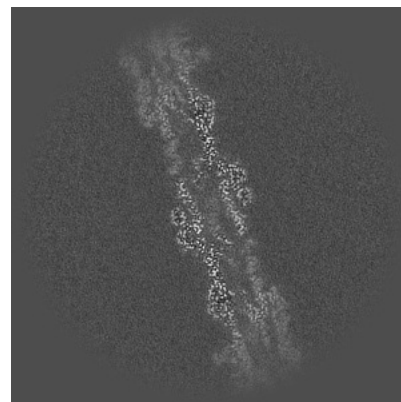
### 6.2.1 Primary map



X Index: 256

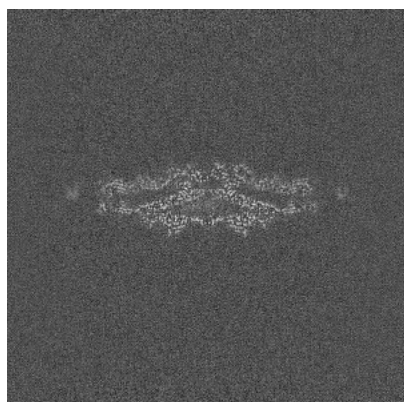


Y Index: 256

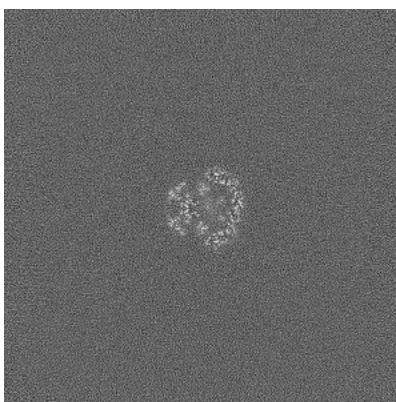


Z Index: 256

### 6.2.2 Raw map



X Index: 256



Y Index: 256

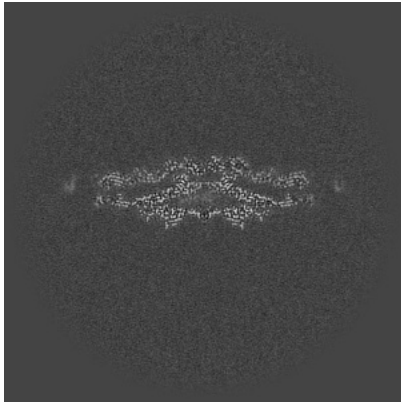


Z Index: 256

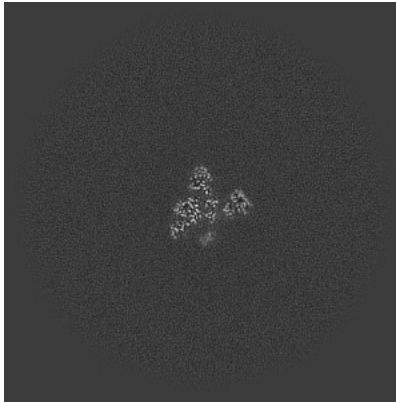
The images above show central slices of the map in three orthogonal directions.

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

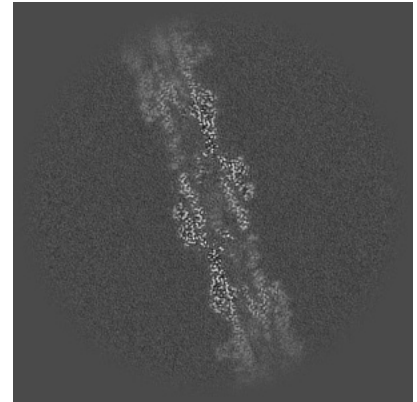
### 6.3.1 Primary map



X Index: 256

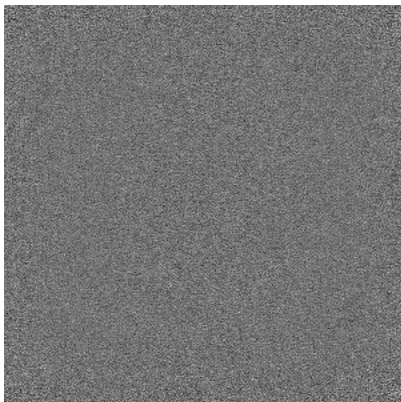


Y Index: 302

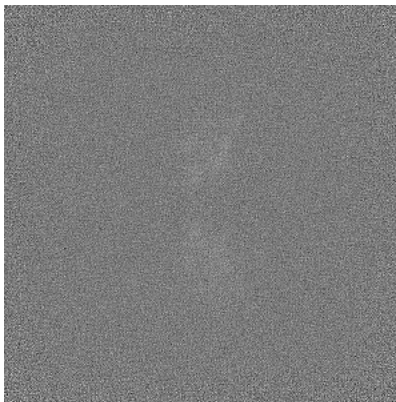


Z Index: 255

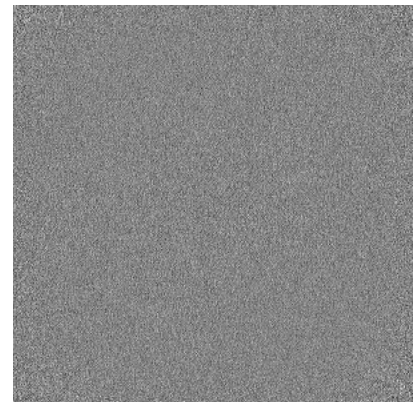
### 6.3.2 Raw map



X Index: 0



Y Index: 0

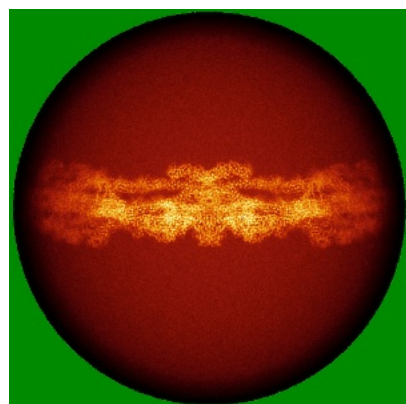


Z Index: 0

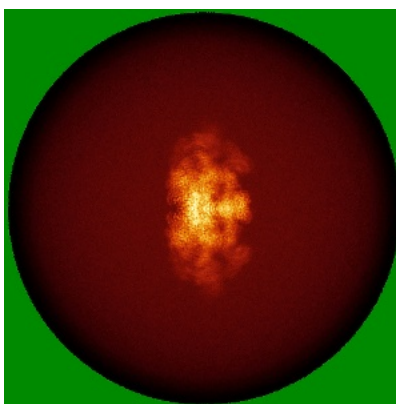
The images above show the largest variance slices of the map in three orthogonal directions.

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

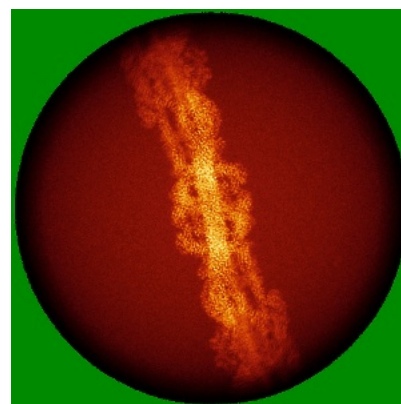
### 6.4.1 Primary map



X

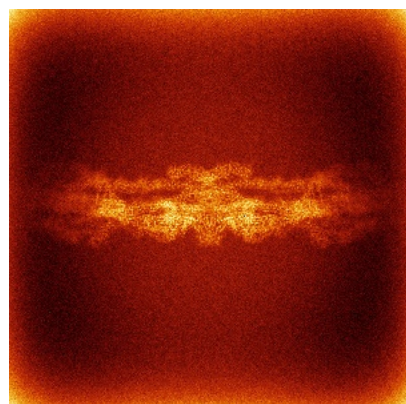


Y

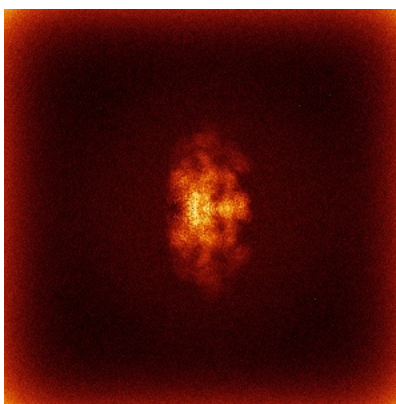


Z

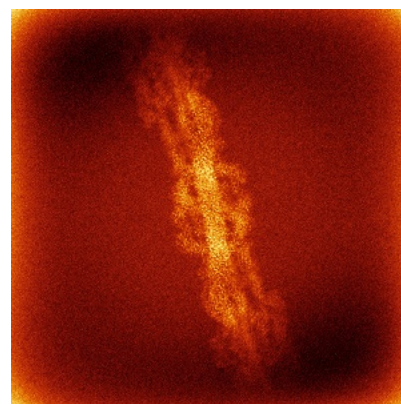
### 6.4.2 Raw map



X



Y



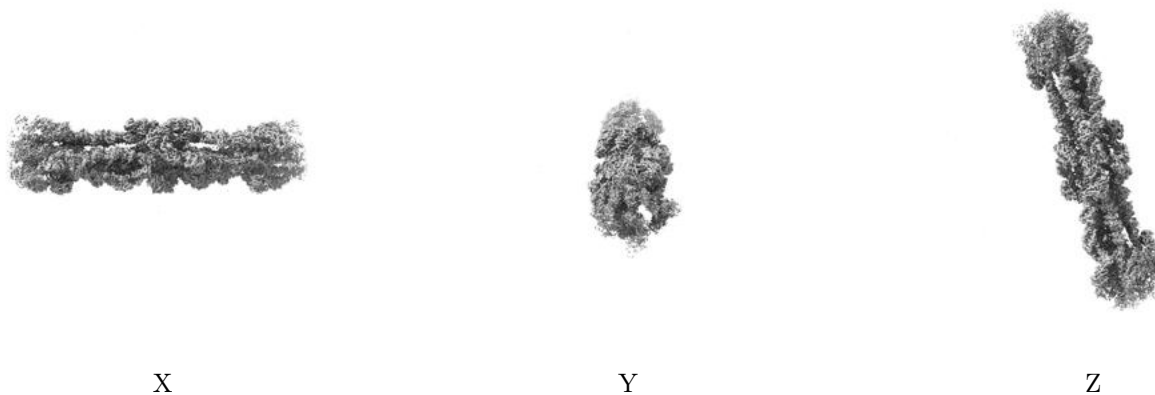
Z

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



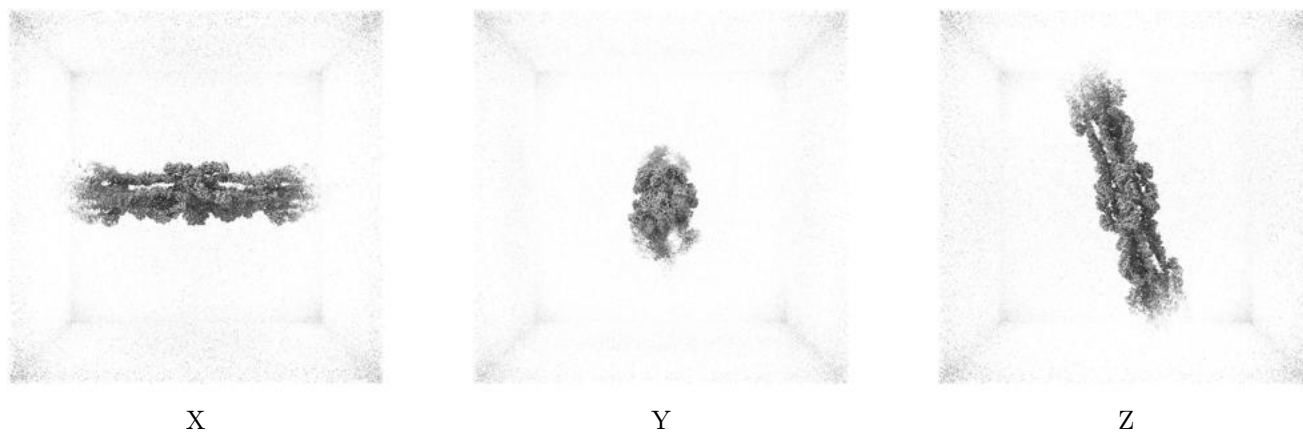
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.23. 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.

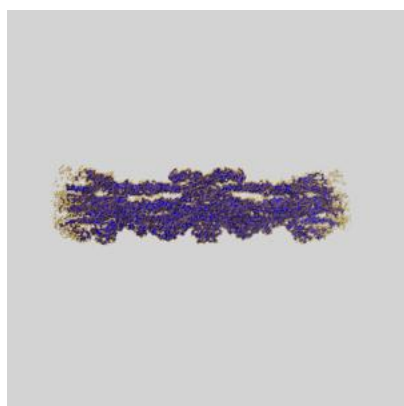
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

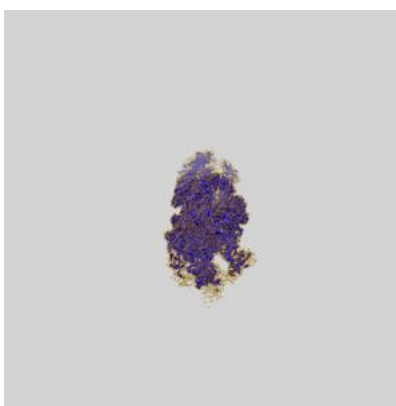
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

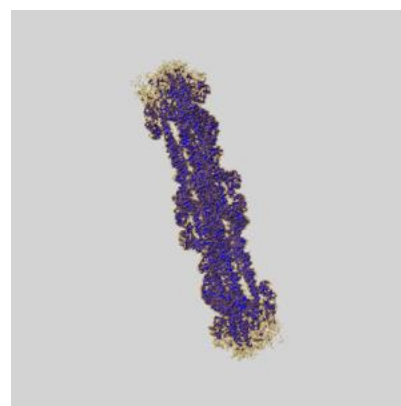
### 6.6.1 emd\_37389\_msk\_1.map [i](#)



X



Y

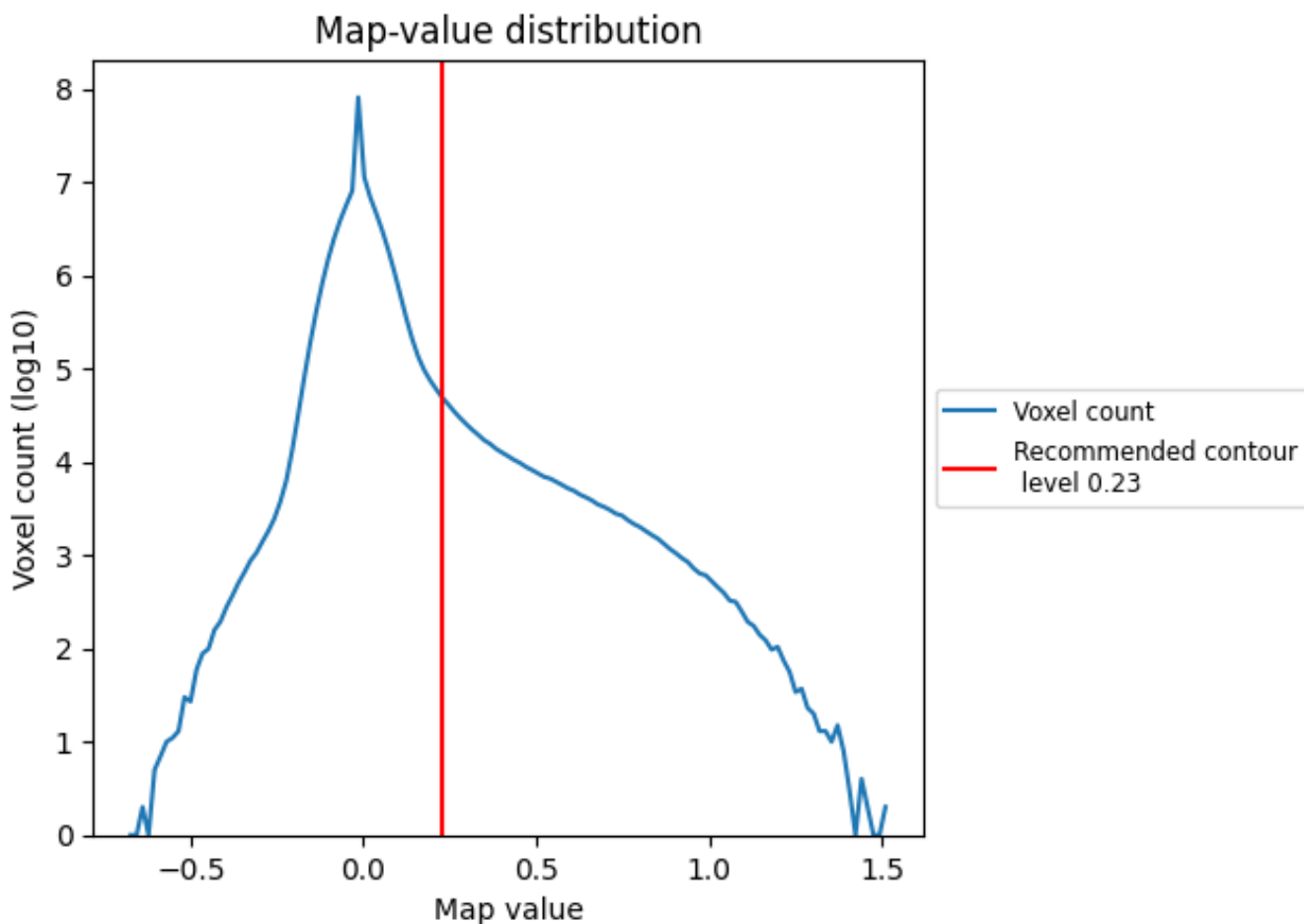


Z

## 7 Map analysis [i](#)

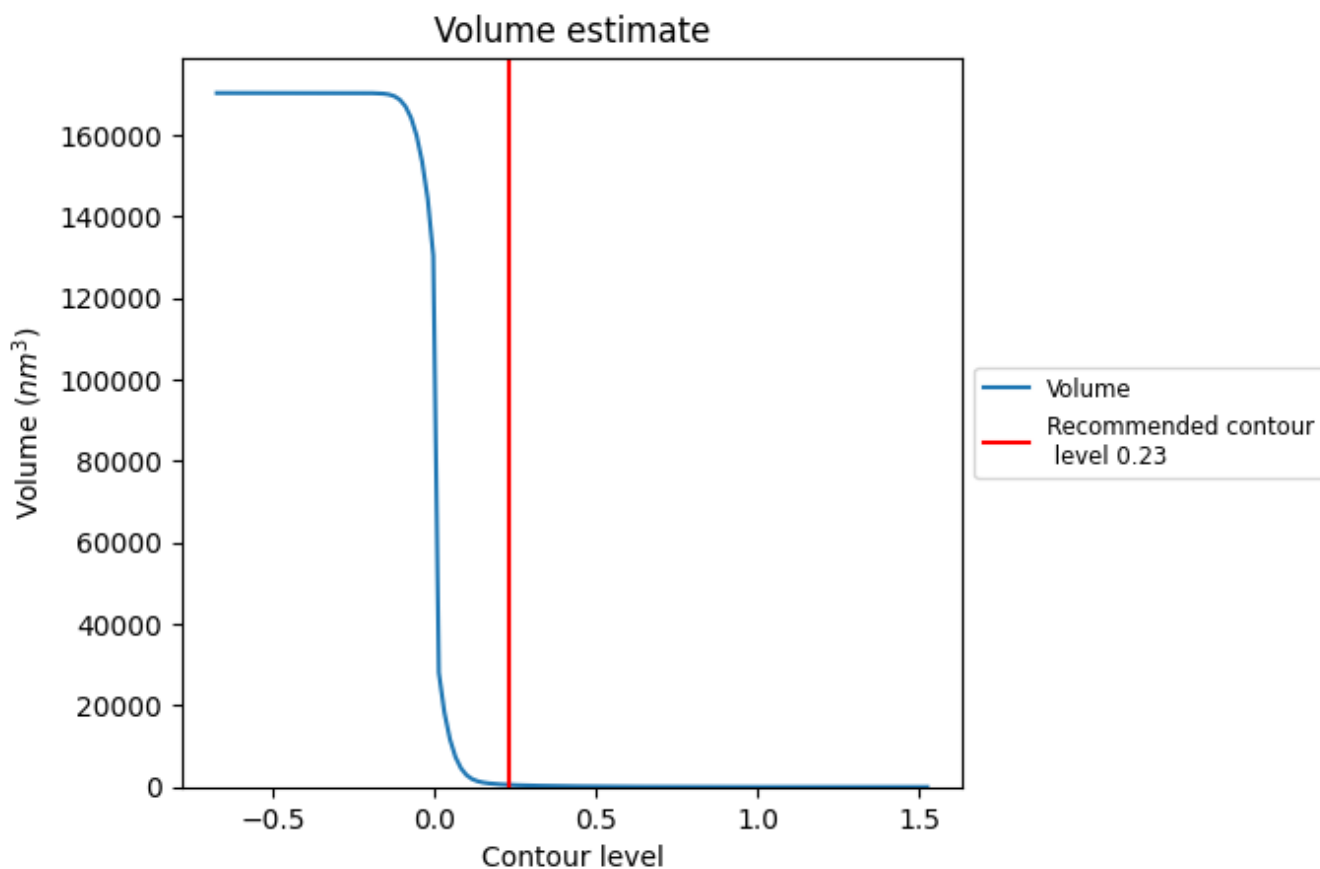
This section contains the results of statistical analysis of the map.

### 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.

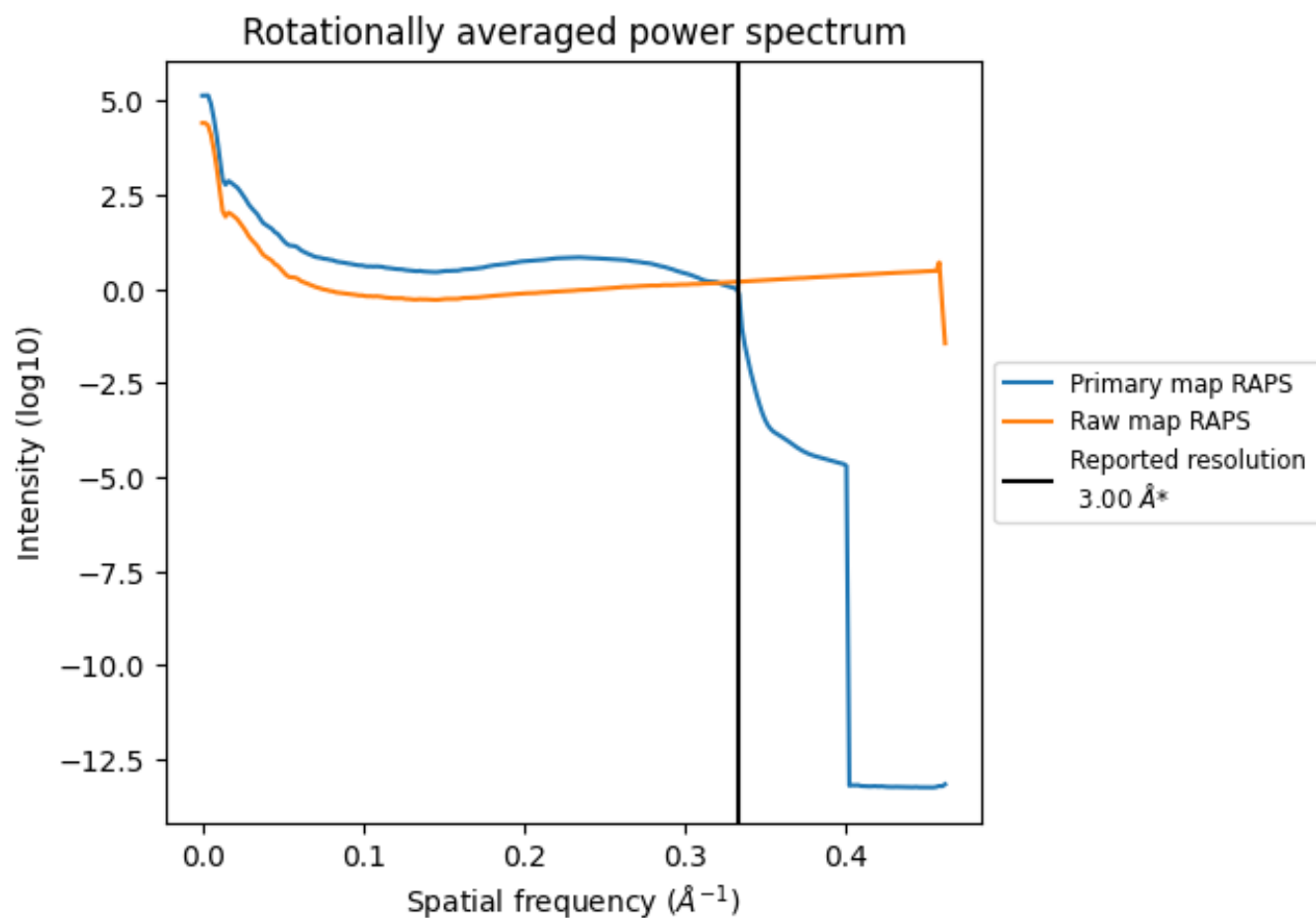
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is  $527 \text{ nm}^3$ ; this corresponds to an approximate mass of 476 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](#)

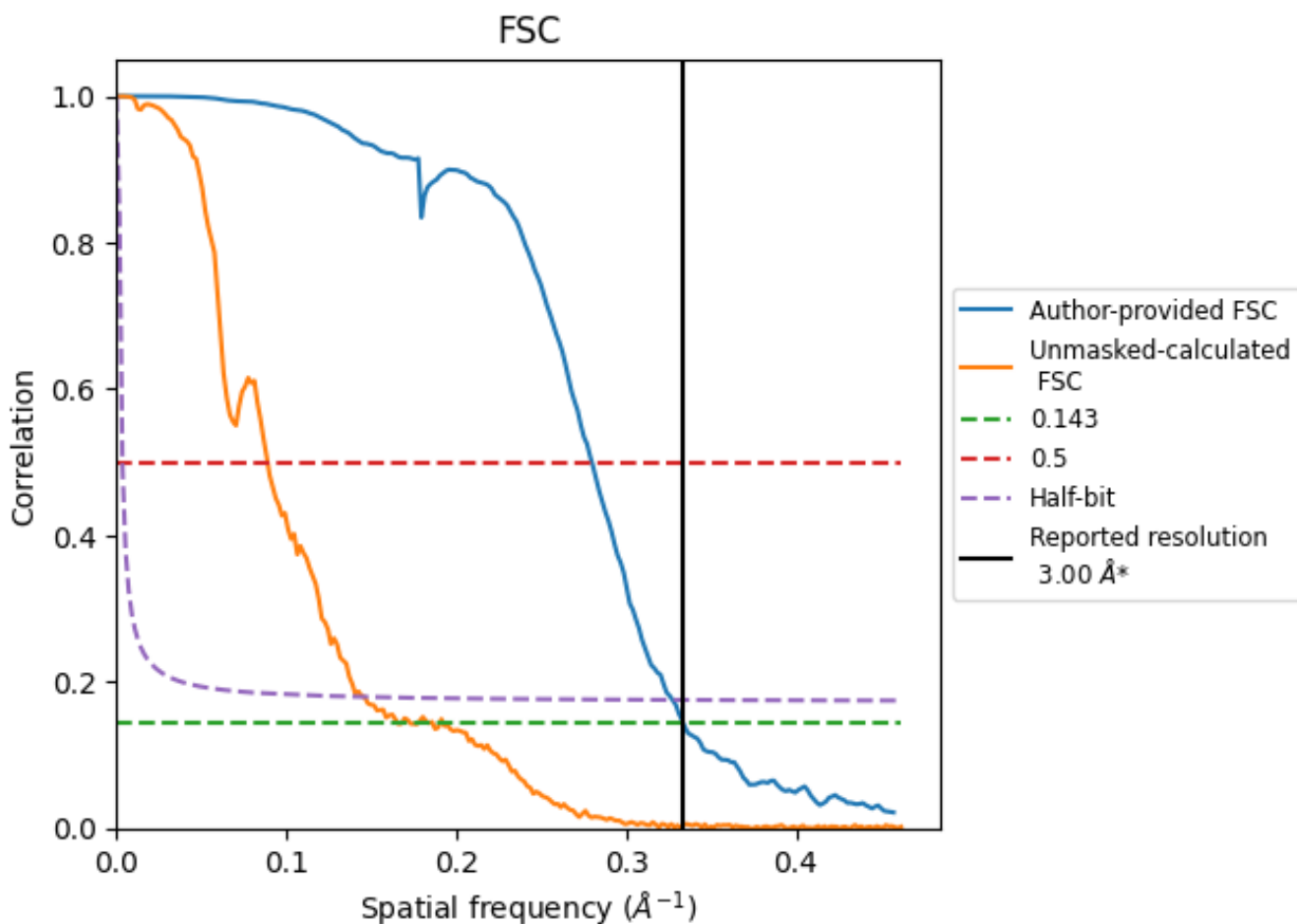


\*Reported resolution corresponds to spatial frequency of 0.333 Å<sup>-1</sup>

## 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 0.333 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

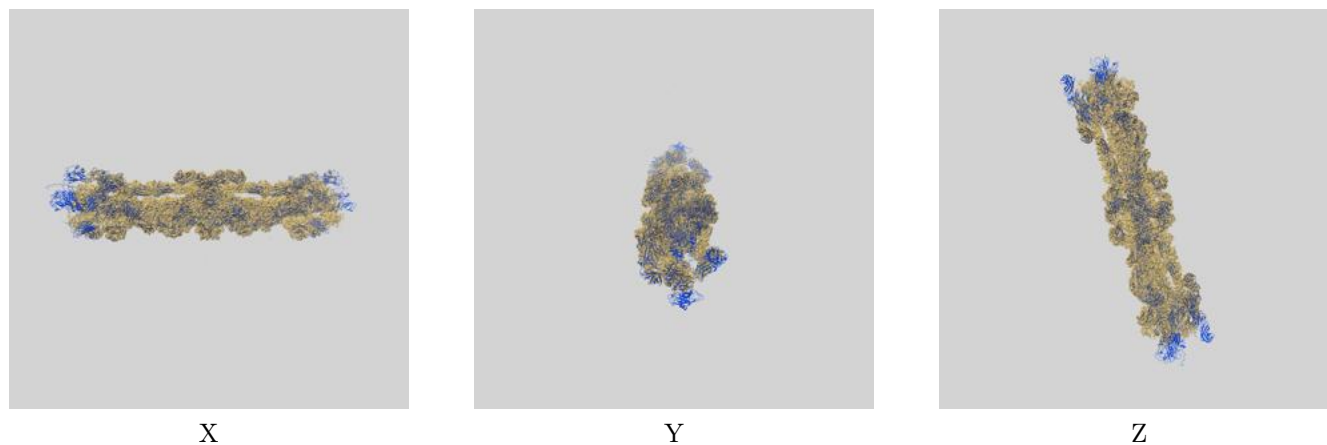
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.00	3.57	3.06
Unmasked-calculated*	6.04	11.24	6.84

\*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 6.04 differs from the reported value 3.0 by more than 10 %

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

This section contains information regarding the fit between EMDB map EMD-37389 and PDB model 8WA2. Per-residue inclusion information can be found in section 3 on page 53.

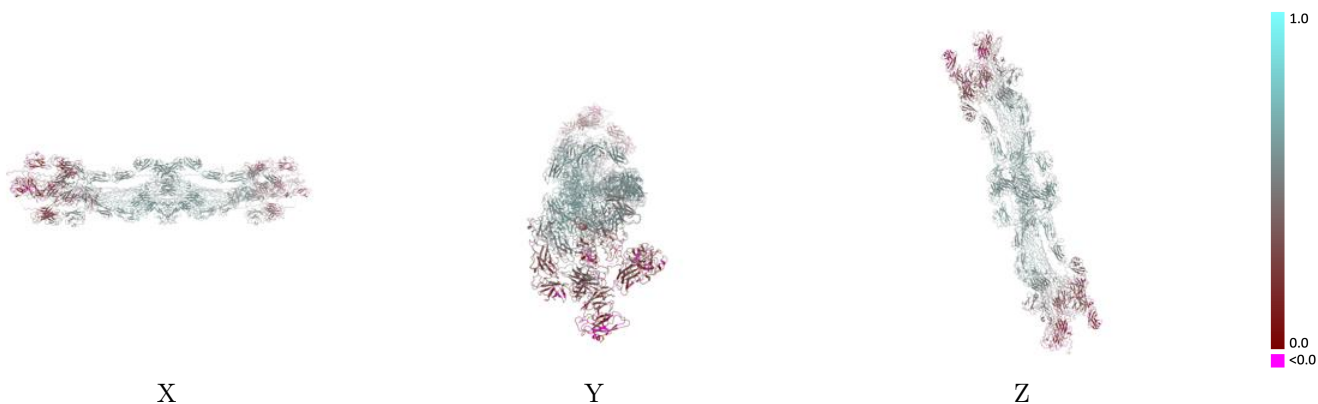
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.23 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.

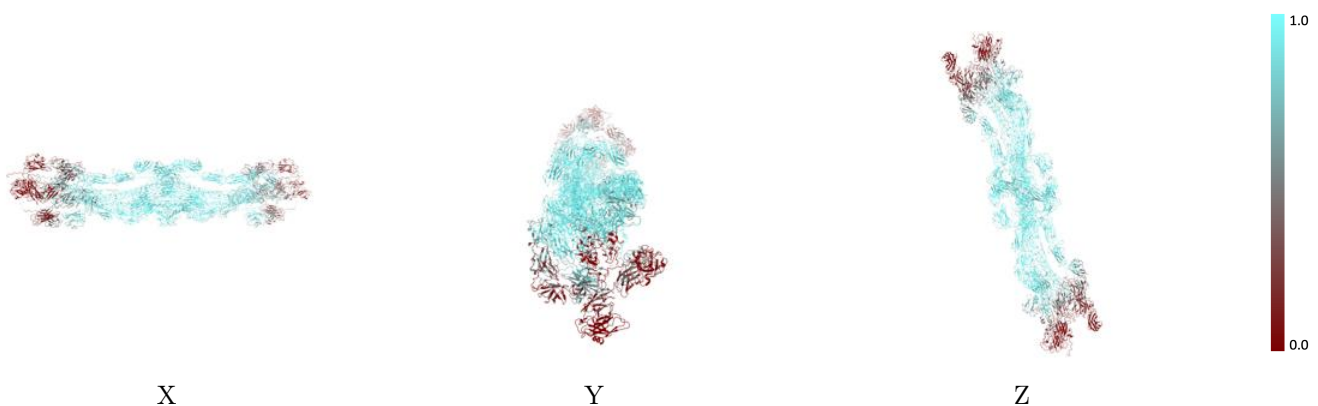


## 9.2 Q-score mapped to coordinate model [\(i\)](#)



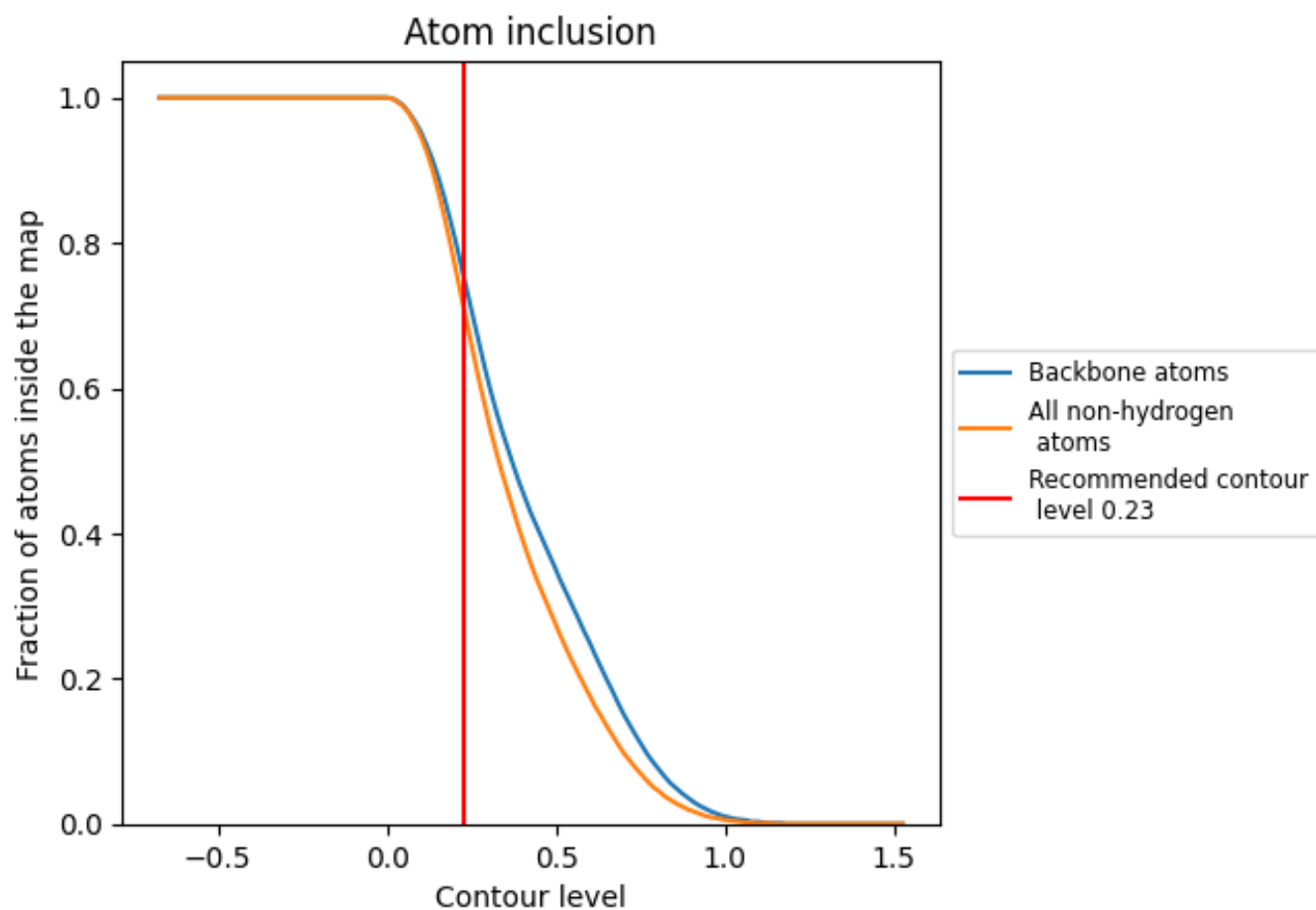
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.23).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 70% 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 (0.23) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7030	 0.4570
0	 0.7780	 0.5390
0A	 0.9630	 0.5780
0B	 0.5170	 0.3330
0C	 0.1030	 0.2620
0D	 0.0000	 0.1240
0E	 0.7020	 0.3580
1	 0.8520	 0.5260
1A	 0.8440	 0.5240
1B	 0.8680	 0.5140
1C	 0.0000	 0.2620
1D	 0.0000	 0.2680
1E	 0.3680	 0.3570
2	 0.9260	 0.5380
2A	 0.7110	 0.4020
2B	 0.6840	 0.4460
2C	 0.0000	 0.0900
2D	 0.0000	 0.0530
3	 0.9110	 0.4940
3A	 0.6900	 0.3980
3B	 0.7240	 0.4480
3C	 0.0000	 0.2000
3D	 0.0000	 0.1280
4	 0.8160	 0.4770
4A	 0.9470	 0.5720
4B	 0.8280	 0.5020
4C	 0.0000	 0.1630
4D	 0.5360	 0.4130
5	 0.7240	 0.4800
5A	 0.8420	 0.5660
5B	 0.8620	 0.5280
5C	 0.0000	 0.1930
5D	 0.9170	 0.5420
6	 0.9470	 0.5720
6A	 0.9310	 0.5780



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Chain	Atom inclusion	Q-score
6B	0.8160	0.5310
6C	0.0000	0.1720
6D	0.6550	0.4610
7	0.8680	0.5540
7A	0.8620	0.5180
7B	0.9360	0.5350
7C	0.8750	0.5120
7D	0.7590	0.4250
8	0.8970	0.5490
8A	1.0000	0.6020
8B	0.7870	0.5060
8C	0.9260	0.5860
8D	0.7590	0.5330
9	0.8970	0.5620
9A	0.8680	0.5550
9B	0.9310	0.5480
9C	0.7780	0.5220
9D	0.7450	0.4270
A	0.9040	0.5460
AA	0.8970	0.5580
AB	0.9790	0.5770
AC	0.1070	0.1330
AD	0.9170	0.5680
AE	0.9470	0.5010
B	0.9040	0.5440
BA	0.8950	0.5540
BB	0.8940	0.5440
BC	0.9630	0.5780
BD	0.9330	0.5860
BE	0.7450	0.4390
C	0.6800	0.4450
CA	0.9790	0.5780
CB	0.9310	0.5860
CC	0.7780	0.4690
CD	0.7930	0.4910
CE	0.8420	0.5000
D	0.6430	0.4310
DA	0.8720	0.5340
DB	0.8470	0.5200
DC	0.8890	0.5450
DD	0.9260	0.5220
DE	0.8080	0.5160





















































































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Chain	Atom inclusion	Q-score
E	0.4780	0.3750
EA	0.9310	0.5840
EB	0.0000	0.1940
EC	0.9560	0.5550
ED	0.8890	0.5400
EE	0.9210	0.5520
F	0.4870	0.3680
FA	0.7860	0.4320
FB	0.0000	0.2820
FC	0.7930	0.4170
FD	0.9260	0.5590
FE	0.9570	0.5680
G	0.8520	0.4770
GA	0.9030	0.5140
GB	0.0530	0.1760
GC	1.0000	0.5770
GD	0.8970	0.5680
GE	0.8390	0.5100
H	0.8010	0.4250
HA	0.7410	0.4240
HB	0.1050	0.3060
HC	0.9260	0.5570
HD	0.8610	0.5370
HE	0.8420	0.4860
I	0.7730	0.4450
IA	0.7410	0.4510
IB	0.2340	0.3620
IC	0.9260	0.5610
ID	0.9260	0.5270
IE	0.8940	0.5000
J	0.7780	0.3940
JA	0.7780	0.3850
JB	0.2500	0.3280
JC	0.8970	0.5550
JD	0.8440	0.4440
JE	0.8720	0.5120
K	0.7410	0.4130
KA	0.8440	0.4740
KB	0.1840	0.3940
KC	0.8890	0.5240
KD	0.8890	0.5280
KE	0.8080	0.4650





















































































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Chain	Atom inclusion	Q-score
L	 0.7780	 0.4480
LA	 0.6900	 0.3950
LB	 0.4810	 0.3960
LC	 0.8890	 0.5170
LD	 0.8890	 0.5310
LE	 0.5790	 0.4390
M	 0.8220	 0.4470
MA	 0.8520	 0.4740
MB	 0.2440	 0.3120
MC	 0.8440	 0.5570
MD	 0.8610	 0.4970
ME	 0.8970	 0.5040
N	 0.6210	 0.2840
NA	 0.8520	 0.4270
NB	 0.3330	 0.3090
NC	 0.8150	 0.4630
ND	 0.7220	 0.4700
NE	 0.7890	 0.4830
O	 0.7780	 0.4630
OA	 0.8520	 0.5060
OB	 0.1850	 0.1930
OC	 0.8060	 0.4770
OD	 0.6940	 0.3100
OE	 0.9310	 0.5220
P	 0.7780	 0.4600
PA	 0.8280	 0.5150
PB	 0.5180	 0.4800
PC	 0.8060	 0.4790
PD	 0.8670	 0.4610
PE	 0.8510	 0.4710
Q	 0.8520	 0.4620
QA	 0.7780	 0.4610
QB	 0.4810	 0.2860
QC	 0.8330	 0.5180
QD	 0.8890	 0.5130
QE	 0.7500	 0.4370
R	 0.9310	 0.5370
RA	 0.8150	 0.4940
RB	 0.4440	 0.2560
RC	 0.8060	 0.3840
RD	 0.7780	 0.3870
RE	 0.9110	 0.5200





















































































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Chain	Atom inclusion	Q-score
S	 0.7780	 0.4730
SA	 0.7110	 0.4530
SB	 0.7410	 0.4440
SC	 0.8440	 0.4550
SD	 0.8060	 0.3980
SE	 0.9150	 0.5260
T	 0.8150	 0.4580
TA	 0.7410	 0.4780
TB	 0.6300	 0.3990
TC	 0.8150	 0.4830
TD	 0.8150	 0.4730
TE	 0.8420	 0.4880
U	 0.8000	 0.4630
UA	 0.8890	 0.4630
UB	 0.7040	 0.4000
UC	 0.7780	 0.3260
UD	 0.8610	 0.3960
UE	 0.8160	 0.5000
V	 0.7780	 0.4470
VA	 0.9170	 0.4570
VB	 0.6440	 0.4450
VC	 0.8890	 0.4570
VD	 0.8060	 0.4110
VE	 0.8750	 0.5190
W	 0.8330	 0.4910
WA	 0.7780	 0.4080
WB	 0.5530	 0.3180
WC	 0.7780	 0.4970
WD	 0.7780	 0.4540
WE	 0.7890	 0.5130
X	 0.8610	 0.4700
XA	 0.7780	 0.3600
XB	 0.4480	 0.2390
XC	 0.8610	 0.4050
XD	 0.8150	 0.3350
XE	 0.8040	 0.5410
Y	 0.8330	 0.4590
YA	 0.8000	 0.3910
YB	 0.7630	 0.4680
YC	 0.8890	 0.4860
YD	 0.7780	 0.2770
YE	 0.8930	 0.5300

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Chain	Atom inclusion	Q-score
Z	 0.8610	 0.4340
ZA	 0.7410	 0.4490
ZB	 0.7630	 0.4570
ZC	 0.6670	 0.4550
ZD	 0.6390	 0.4140
ZE	 0.7930	 0.3920
a	 0.8440	 0.4410
aA	 0.8330	 0.4450
aB	 0.7930	 0.4980
aC	 0.8520	 0.4480
aD	 0.5180	 0.3540
aE	 0.6050	 0.3810
b	 0.7780	 0.4510
bA	 0.8330	 0.4410
bB	 0.8280	 0.5180
bC	 0.5000	 0.2290
bD	 0.7780	 0.4130
bE	 0.7590	 0.4020
c	 0.8060	 0.4370
cA	 0.7780	 0.4530
cB	 0.8970	 0.5360
cC	 0.5280	 0.3360
cD	 0.6810	 0.4300
cE	 0.7660	 0.3640
d	 0.7780	 0.4580
dA	 0.8610	 0.3890
dB	 0.8420	 0.4970
dC	 0.6300	 0.3600
dD	 0.6580	 0.4100
dE	 0.7140	 0.4370
e	 0.8150	 0.4870
eA	 0.9170	 0.4630
eB	 0.9150	 0.5530
eC	 0.6300	 0.4180
eD	 0.7630	 0.3990
eE	 0.7860	 0.4490
f	 0.9440	 0.5040
fA	 0.6940	 0.4290
fB	 0.7870	 0.5330
fC	 0.5750	 0.3830
fD	 0.7230	 0.4490
fE	 0.8720	 0.4850

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





























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Chain	Atom inclusion	Q-score
g	 0.8330	 0.4840
gA	 0.8150	 0.4250
gB	 0.8280	 0.5060
gC	 0.6580	 0.4490
gD	 0.6390	 0.4450
gE	 0.8160	 0.4100
h	 0.7500	 0.4980
hA	 0.8330	 0.4740
hB	 0.0000	 0.1560
hC	 0.7890	 0.4280
hD	 0.6320	 0.3890
hE	 0.8420	 0.5460
i	 0.8520	 0.4700
iA	 0.7780	 0.4720
iB	 0.0000	 0.2310
iC	 0.6170	 0.4160
iD	 0.6670	 0.4500
iE	 0.7680	 0.4430
j	 0.8890	 0.4050
jA	 0.8150	 0.4760
jB	 0.0260	 0.2520
jC	 0.7220	 0.4740
jD	 0.6670	 0.3890
jE	 0.6580	 0.4430
k	 0.6670	 0.4760
kA	 0.7780	 0.4850
kB	 0.0790	 0.3290
kC	 0.6050	 0.4680
kD	 0.5000	 0.3100
kE	 0.7870	 0.5230
l	 0.8520	 0.5100
lA	 0.7450	 0.5000
lB	 0.1280	 0.2920
lC	 0.7410	 0.4410
lD	 0.4070	 0.3160
lE	 0.7140	 0.4250
m	 0.8150	 0.5080
mA	 0.7630	 0.4890
mB	 0.1940	 0.3010
mC	 0.4890	 0.3020
mD	 0.4440	 0.3290
mE	 0.6900	 0.3890









































































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Chain	Atom inclusion	Q-score
n	 0.8080	 0.5140
nA	 0.8950	 0.5250
nB	 0.1840	 0.3300
nC	 0.5280	 0.3920
nD	 0.5560	 0.3220
nE	 0.6550	 0.3630
o	 0.7630	 0.5030
oA	 0.8510	 0.5520
oB	 0.3330	 0.3180
oC	 0.5180	 0.3730
oD	 0.4440	 0.2630
oE	 0.7590	 0.4430
p	 0.8680	 0.5220
pA	 0.8330	 0.5440
pB	 0.2220	 0.2920
pC	 0.6300	 0.4570
pD	 0.3330	 0.2780
pE	 0.7230	 0.4180
q	 0.8720	 0.5400
qA	 0.7890	 0.5110
qB	 0.3330	 0.3340
qC	 0.6300	 0.4800
qD	 0.4440	 0.3680
qE	 0.9470	 0.4750
r	 0.8890	 0.5240
rA	 0.8520	 0.5530
rB	 0.2220	 0.3440
rC	 0.2220	 0.2050
rD	 0.4440	 0.3570
rE	 0.6170	 0.3780
s	 0.8680	 0.5100
sA	 0.8220	 0.5170
sB	 0.5180	 0.4020
sC	 0.2960	 0.1860
sD	 0.3560	 0.2430
sE	 0.7630	 0.4880
t	 0.8890	 0.5320
tA	 0.8060	 0.5160
tB	 0.4810	 0.3170
tC	 0.5180	 0.3590
tD	 0.2630	 0.1910
tE	 0.8300	 0.4560

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Chain	Atom inclusion	Q-score
u	 0.8000	 0.4770
uA	 0.8150	 0.5290
uB	 0.5180	 0.3210
uC	 0.2960	 0.4020
uD	 0.1380	 0.3240
uE	 0.8420	 0.4630
v	 0.8060	 0.5020
vA	 0.8150	 0.5300
vB	 0.4810	 0.3010
vC	 0.4220	 0.3310
vD	 0.3160	 0.3560
vE	 0.8300	 0.5180
w	 0.7780	 0.4950
wA	 0.8520	 0.5070
wB	 0.7040	 0.4330
wC	 0.3420	 0.1360
wD	 0.3420	 0.3580
wE	 0.8210	 0.4240
x	 0.7040	 0.4250
xA	 0.8520	 0.5250
xB	 0.8520	 0.5470
xC	 0.1380	 0.2600
xD	 0.1030	 0.2690
xE	 0.7630	 0.4430
y	 0.8520	 0.5030
yA	 0.8520	 0.5570
yB	 0.7110	 0.4230
yC	 0.3420	 0.2610
yD	 0.0000	 0.2070
yE	 0.7660	 0.4270
z	 0.7780	 0.4980
zA	 0.8890	 0.5340
zB	 0.6320	 0.3580
zC	 0.1050	 0.2530
zD	 0.0000	 0.1780
zE	 0.6810	 0.4300