



wwPDB EM Validation Summary Report ⓘ

Jan 1, 2025 – 06:11 PM EST

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

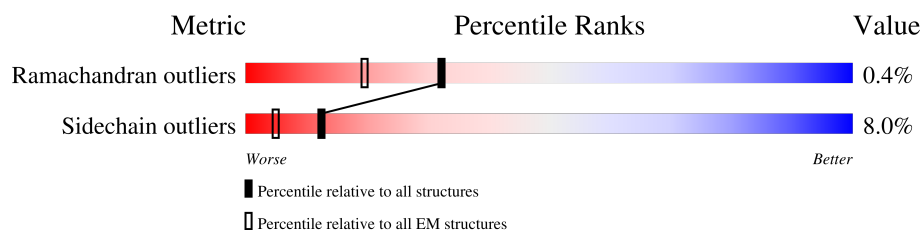
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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.






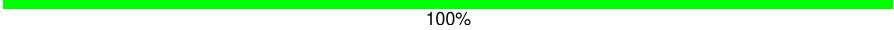
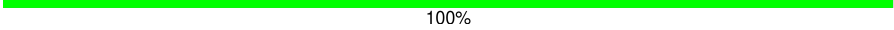






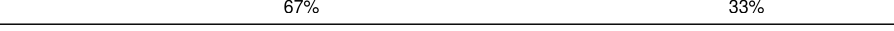



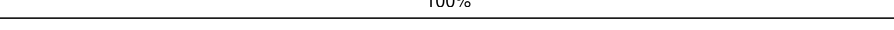


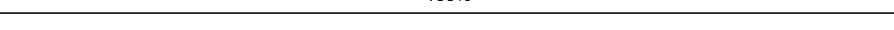
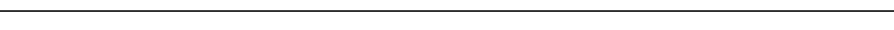

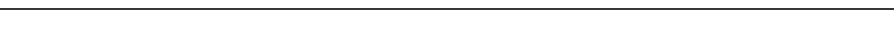
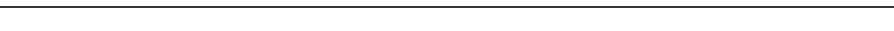


Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	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	 100%
3	8C	3	 100%
3	9C	3	 33% 67%
3	BC	3	 67% 33%
3	CC	3	 33% 67%
3	DD	3	 67% 33%
3	EB	3	 100% 67% 33%
3	ED	3	 67% 33%
3	FD	3	 67% 33%
3	GC	3	 67% 33%
3	HA	3	 67% 33%
3	HC	3	 67% 33%
3	IA	3	 100%
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%




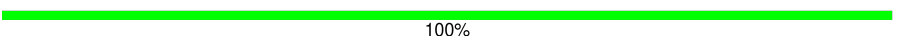
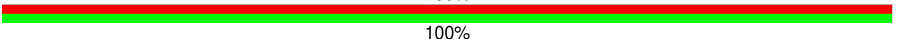
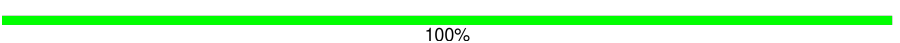
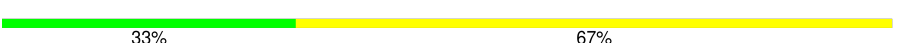

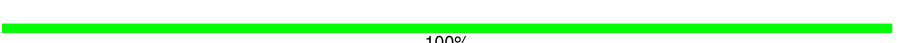
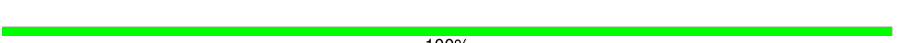

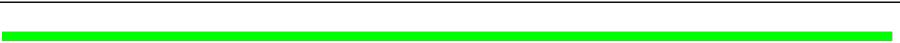




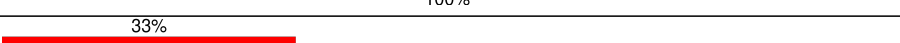
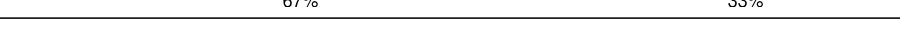


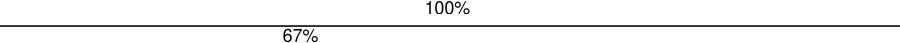
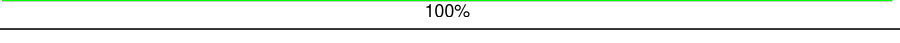
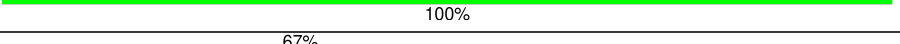
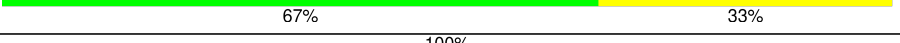

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Mol	Chain	Length	Quality of chain
3	NC	3	100%
3	O	3	67% 33%
3	OA	3	67% 33%
3	OB	3	100% 100%
3	P	3	67% 33%
3	PB	3	33% 100%
3	Q	3	67% 33%
3	QB	3	33% 67% 33%
3	QD	3	100%
3	RA	3	67% 33%
3	RB	3	67% 67% 33%
3	SB	3	33% 67%
3	T	3	67% 33%
3	TA	3	33% 67%
3	TB	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	
3	dC	3	
3	e	3	
3	eC	3	
3	hB	3	
3	iD	3	
3	jA	3	
3	kA	3	
3	l	3	
3	lC	3	
3	lD	3	
3	m	3	
3	mD	3	
3	nD	3	
3	oB	3	
3	oC	3	
3	oD	3	
3	pC	3	
3	pD	3	
3	qC	3	
3	qD	3	
3	rA	3	
3	rB	3	
3	rC	3	
3	rD	3	

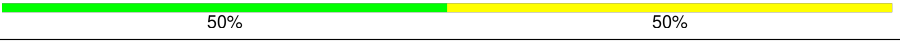
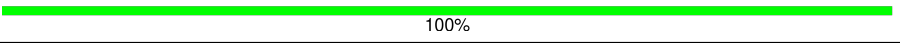









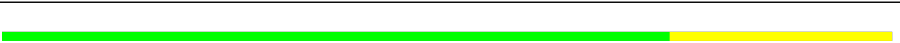




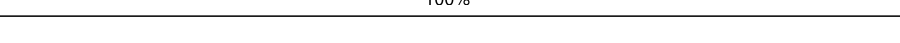
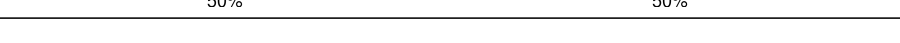


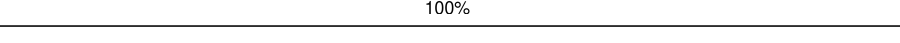
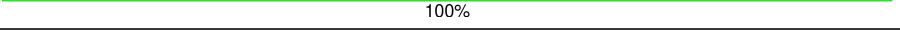



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Mol	Chain	Length	Quality of chain
3	sB	3	
3	sC	3	
3	t	3	
3	tB	3	
3	tC	3	
3	uA	3	
3	uB	3	
3	uC	3	
3	vA	3	
3	vB	3	
3	w	3	
3	wA	3	
3	wB	3	
3	x	3	
3	xA	3	
3	xB	3	
3	y	3	
3	yA	3	
3	z	3	
3	zA	3	
4	AD	4	
4	DC	4	
4	JA	4	
4	JB	4	
4	L	4	

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Mol	Chain	Length	Quality of chain
4	LD	4	 50%50%
4	MD	4	 100%
4	NB	4	 50%50%50%
4	OC	4	 75%25%
4	OD	4	 75%25%
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	 100%
4	YC	4	 50%50%
4	Z	4	 50%50%
4	ZD	4	 25%75%25%
4	aA	4	 100%
4	bA	4	 100%
4	c	4	 75%25%
4	cC	4	 50%50%50%
4	d	4	 50%50%
4	eA	4	 100%


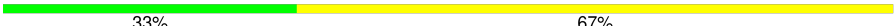






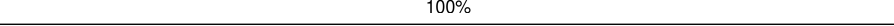





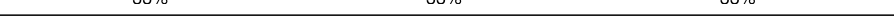

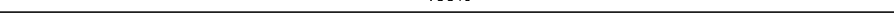








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Mol	Chain	Length	Quality of chain
4	g	4	
4	gD	4	
4	iA	4	
4	jC	4	
4	k	4	
4	kD	4	
4	mB	4	
4	nC	4	
4	pA	4	
4	qB	4	
4	r	4	
4	tA	4	
4	v	4	
5	BD	5	
5	EC	5	
5	KA	5	
5	M	5	
6	0B	3	
6	0C	3	
6	1C	3	
6	2C	3	
6	3A	3	
6	3B	3	
6	3D	3	
6	4B	3	

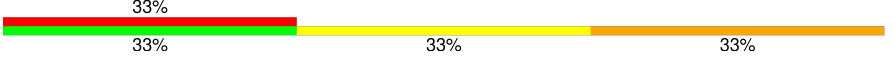
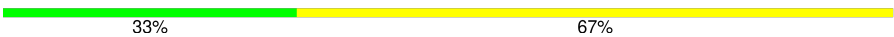



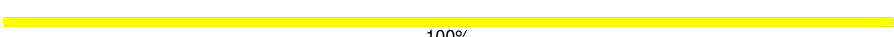


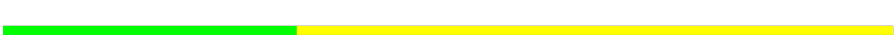

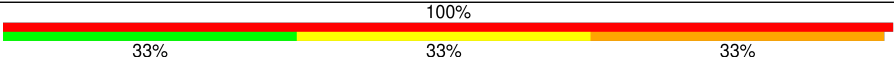
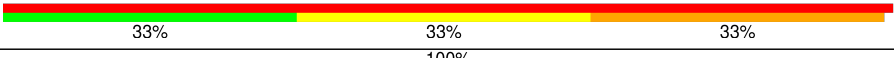
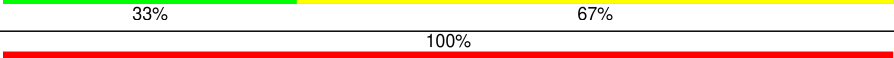
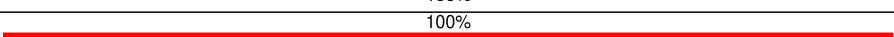



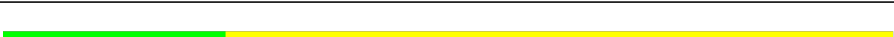







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Mol	Chain	Length	Quality of chain
6	5	3	 67% 33%
6	5B	3	 33% 67%
6	6A	3	 33% 67%
6	6C	3	 33% 67% 100%
6	6D	3	 33% 67%
6	7A	3	 33% 67%
6	7D	3	 33% 67%
6	8	3	 33% 67%
6	8A	3	 100%
6	8D	3	 67% 33%
6	9	3	 33% 67%
6	9B	3	 33% 67%
6	AA	3	 33% 67%
6	CB	3	 33% 67%
6	CD	3	 33% 33% 33%
6	EA	3	 67% 33%
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	
6	ZE	3	
6	aB	3	
6	bB	3	
6	bE	3	
6	cB	3	
6	gB	3	
6	mE	3	
6	nE	3	
6	oE	3	
6	uD	3	
6	xC	3	
6	xD	3	
6	yD	3	
6	zD	3	
7	HD	4	
7	KC	4	
7	QA	4	
7	S	4	
7	UD	4	
7	WD	4	
7	XC	4	
7	ZC	4	
7	dA	4	
7	f	4	

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

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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	
14	HB	4	
14	KB	4	
14	eD	4	
14	hC	4	
14	hD	4	
14	kB	4	
14	kC	4	
14	nA	4	
14	nB	4	
14	p	4	
14	qA	4	
14	s	4	
15	1D	5	
15	2D	5	
15	4C	5	
15	5C	5	
15	7B	5	
15	8B	5	
15	AB	5	
15	BB	5	
15	CA	5	
15	DA	5	
15	eB	5	
15	fB	5	




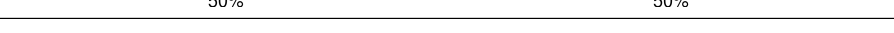
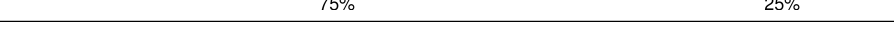
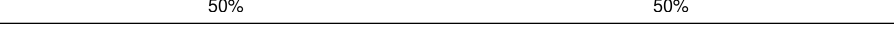
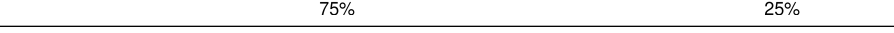






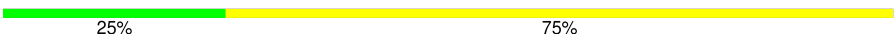


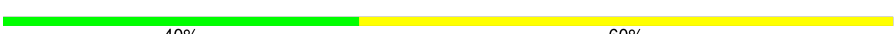
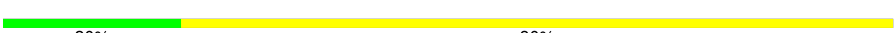



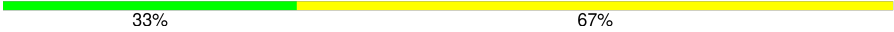
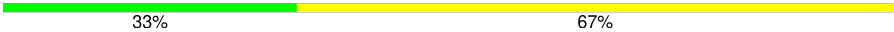
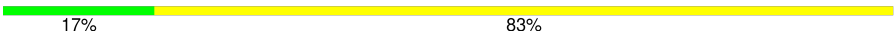
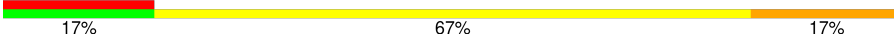
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Mol	Chain	Length	Quality of chain
16	4D	2	<div> <div>50%</div> <div>50%</div> </div>
16	AC	2	<div> <div>100%</div> <div>100%</div> </div>
16	FA	2	<div> <div>50%</div> <div>50%</div> </div>
17	5D	6	<div> <div>50%</div> <div>50%</div> </div>
17	7C	6	<div> <div>50%</div> <div>50%</div> </div>
17	DB	6	<div> <div>17%</div> <div>83%</div> </div>
17	GA	6	<div> <div>67%</div> <div>33%</div> </div>
18	0E	5	<div> <div>60%</div> <div>40%</div> </div>
18	9D	5	<div> <div>20%</div> <div>80%</div> </div>
18	BE	5	<div> <div>20%</div> <div>40%</div> <div>60%</div> </div>
18	DE	5	<div> <div>20%</div> <div>40%</div> <div>60%</div> </div>
18	IE	5	<div> <div>20%</div> <div>80%</div> </div>
18	JE	5	<div> <div>60%</div> <div>40%</div> </div>
18	KE	5	<div> <div>60%</div> <div>40%</div> </div>
18	PE	5	<div> <div>60%</div> <div>40%</div> </div>
18	SE	5	<div> <div>60%</div> <div>40%</div> </div>
18	cE	5	<div> <div>60%</div> <div>40%</div> </div>
18	fE	5	<div> <div>60%</div> <div>40%</div> </div>
18	pE	5	<div> <div>40%</div> <div>60%</div> </div>
18	rE	5	<div> <div>20%</div> <div>40%</div> <div>60%</div> </div>
18	tE	5	<div> <div>40%</div> <div>60%</div> </div>
18	yE	5	<div> <div>20%</div> <div>40%</div> <div>60%</div> </div>
18	zE	5	<div> <div>20%</div> <div>60%</div> <div>40%</div> </div>
19	1E	4	<div> <div>50%</div> <div>100%</div> </div>
19	AE	4	<div> <div>50%</div> <div>50%</div> </div>




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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	-	-	-
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.

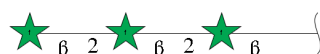
- Molecule 1 is a protein called Mst1.

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

- Molecule 2 is a protein called Mstax.

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

- 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
3	J	3	Total	C	O	0	0
			27	15	12		

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

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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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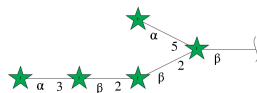
Mol	Chain	Residues	Atoms			AltConf	Trace
4	k	4	Total 36	C 20	O 16	0	0
4	r	4	Total 36	C 20	O 16	0	0
4	v	4	Total 36	C 20	O 16	0	0
4	JA	4	Total 36	C 20	O 16	0	0
4	UA	4	Total 36	C 20	O 16	0	0
4	VA	4	Total 36	C 20	O 16	0	0
4	aA	4	Total 36	C 20	O 16	0	0
4	bA	4	Total 36	C 20	O 16	0	0
4	eA	4	Total 36	C 20	O 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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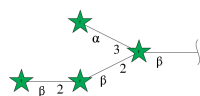
Mol	Chain	Residues	Atoms			AltConf	Trace
6	aB	3	Total	C	O	0	0
			29	16	13		
6	bB	3	Total	C	O	0	0
			29	16	13		
6	cB	3	Total	C	O	0	0
			29	16	13		
6	gB	3	Total	C	O	0	0
			29	16	13		
6	0B	3	Total	C	O	0	0
			29	16	13		
6	3B	3	Total	C	O	0	0
			29	16	13		
6	4B	3	Total	C	O	0	0
			29	16	13		
6	5B	3	Total	C	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
6	zD	3	Total	C	O	0	0
			29	16	13		
6	3D	3	Total	C	O	0	0
			29	16	13		
6	6D	3	Total	C	O	0	0
			29	16	13		
6	7D	3	Total	C	O	0	0
			29	16	13		
6	8D	3	Total	C	O	0	0
			29	16	13		
6	ME	3	Total	C	O	0	0
			29	16	13		
6	OE	3	Total	C	O	0	0
			29	16	13		
6	ZE	3	Total	C	O	0	0
			29	16	13		
6	bE	3	Total	C	O	0	0
			29	16	13		
6	mE	3	Total	C	O	0	0
			29	16	13		
6	nE	3	Total	C	O	0	0
			29	16	13		
6	oE	3	Total	C	O	0	0
			29	16	13		

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



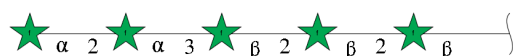
Mol	Chain	Residues	Atoms			AltConf	Trace
7	S	4	Total	C	O	0	0
			36	20	16		
7	f	4	Total	C	O	0	0
			36	20	16		
7	h	4	Total	C	O	0	0
			36	20	16		
7	QA	4	Total	C	O	0	0
			36	20	16		
7	dA	4	Total	C	O	0	0
			36	20	16		

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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.



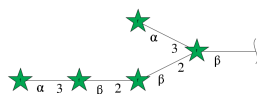
Mol	Chain	Residues	Atoms			AltConf	Trace
9	Y	2	Total	C	O	0	0
			18	10	8		

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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.



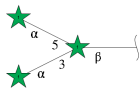
Mol	Chain	Residues	Atoms			AltConf	Trace
10	a	5	Total	C	O	0	0
			45	25	20		
10	u	5	Total	C	O	0	0
			45	25	20		
10	3	5	Total	C	O	0	0
			45	25	20		
10	YA	5	Total	C	O	0	0
			45	25	20		
10	sA	5	Total	C	O	0	0
			45	25	20		
10	1A	5	Total	C	O	0	0
			45	25	20		
10	MB	5	Total	C	O	0	0
			45	25	20		
10	VB	5	Total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

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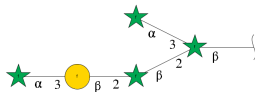
Mol	Chain	Residues	Atoms			AltConf	Trace
10	yB	5	Total	C	O	0	0
			45	25	20		
10	SC	5	Total	C	O	0	0
			45	25	20		
10	mC	5	Total	C	O	0	0
			45	25	20		
10	vC	5	Total	C	O	0	0
			45	25	20		
10	PD	5	Total	C	O	0	0
			45	25	20		
10	jD	5	Total	C	O	0	0
			45	25	20		
10	sD	5	Total	C	O	0	0
			45	25	20		

- 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
11	i	3	Total	C	O	0	0
			27	15	12		
11	gA	3	Total	C	O	0	0
			27	15	12		
11	aC	3	Total	C	O	0	0
			27	15	12		
11	XD	3	Total	C	O	0	0
			27	15	12		

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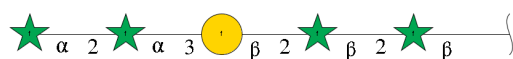
Mol	Chain	Residues	Atoms			AltConf	Trace
13	tD	4	Total	C	O	0	0
			38	21	17		
13	vD	4	Total	C	O	0	0
			38	21	17		
13	wD	4	Total	C	O	0	0
			38	21	17		
13	0D	4	Total	C	O	0	0
			38	21	17		

- Molecule 14 is an oligosaccharide called beta-L-arabinofuranose-(1-5)-beta-D-galactofuranose-(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
15	CA	5	Total	C	O	0	0
			47	26	21		
15	DA	5	Total	C	O	0	0
			47	26	21		
15	AB	5	Total	C	O	0	0
			47	26	21		
15	BB	5	Total	C	O	0	0
			47	26	21		
15	eB	5	Total	C	O	0	0
			47	26	21		
15	fB	5	Total	C	O	0	0
			47	26	21		
15	7B	5	Total	C	O	0	0
			47	26	21		
15	8B	5	Total	C	O	0	0
			47	26	21		
15	4C	5	Total	C	O	0	0
			47	26	21		
15	5C	5	Total	C	O	0	0
			47	26	21		
15	1D	5	Total	C	O	0	0
			47	26	21		
15	2D	5	Total	C	O	0	0
			47	26	21		

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



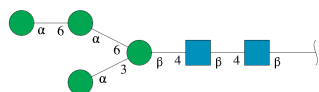
Mol	Chain	Residues	Atoms				AltConf	Trace
16	FA	2	Total	C	N	O	0	0
			28	16	2	10		

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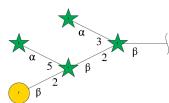
Mol	Chain	Residues	Atoms				AltConf	Trace
16	AC	2	Total	C	N	O	0	0
			28	16	2	10		
16	4D	2	Total	C	N	O	0	0
			28	16	2	10		

- 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
17	GA	6	Total	C	N	O	0	0
			72	40	2	30		
17	DB	6	Total	C	N	O	0	0
			72	40	2	30		
17	7C	6	Total	C	N	O	0	0
			72	40	2	30		
17	5D	6	Total	C	N	O	0	0
			72	40	2	30		

- 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.



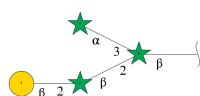
Mol	Chain	Residues	Atoms			AltConf	Trace
18	9D	5	Total	C	O	0	0
			47	26	21		
18	BE	5	Total	C	O	0	0
			47	26	21		
18	DE	5	Total	C	O	0	0
			47	26	21		
18	IE	5	Total	C	O	0	0
			47	26	21		
18	JE	5	Total	C	O	0	0
			47	26	21		

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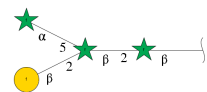
Mol	Chain	Residues	Atoms			AltConf	Trace
18	KE	5	Total	C	O	0	0
			47	26	21		
18	PE	5	Total	C	O	0	0
			47	26	21		
18	SE	5	Total	C	O	0	0
			47	26	21		
18	cE	5	Total	C	O	0	0
			47	26	21		
18	fE	5	Total	C	O	0	0
			47	26	21		
18	pE	5	Total	C	O	0	0
			47	26	21		
18	rE	5	Total	C	O	0	0
			47	26	21		
18	tE	5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



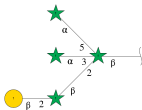
Mol	Chain	Residues	Atoms			AltConf	Trace
19	AE	4	Total	C	O	0	0
			38	21	17		
19	LE	4	Total	C	O	0	0
			38	21	17		
19	NE	4	Total	C	O	0	0
			38	21	17		
19	aE	4	Total	C	O	0	0
			38	21	17		
19	qE	4	Total	C	O	0	0
			38	21	17		
19	1E	4	Total	C	O	0	0
			38	21	17		

- 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.



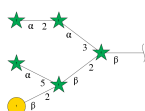
Mol	Chain	Residues	Atoms			AltConf	Trace
21	FE	5	Total	C	O	0	0
			47	26	21		

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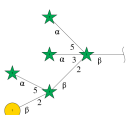
Mol	Chain	Residues	Atoms			AltConf	Trace
21	kE	5	Total	C	O	0	0
			47	26	21		
21	vE	5	Total	C	O	0	0
			47	26	21		

- 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.



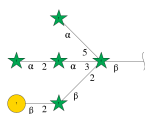
Mol	Chain	Residues	Atoms			AltConf	Trace
22	GE	6	Total	C	O	0	0
			56	31	25		
22	QE	6	Total	C	O	0	0
			56	31	25		
22	RE	6	Total	C	O	0	0
			56	31	25		
22	VE	6	Total	C	O	0	0
			56	31	25		
22	dE	6	Total	C	O	0	0
			56	31	25		
22	eE	6	Total	C	O	0	0
			56	31	25		
22	iE	6	Total	C	O	0	0
			56	31	25		
22	wE	6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

- 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
23	XE	6	Total	C	O	0	0
			56	31	25		

- 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.

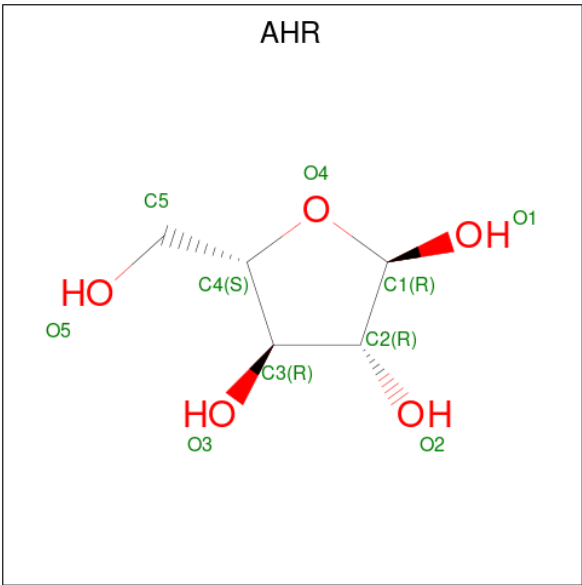


Mol	Chain	Residues	Atoms			AltConf	Trace
24	YE	6	Total	C	O	0	0
			56	31	25		
24	IE	6	Total	C	O	0	0
			56	31	25		

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

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

- Molecule 26 is alpha-L-arabinofuranose (three-letter code: AHR) (formula: C₅H₁₀O₅) (labeled as "Ligand of Interest" by depositor).



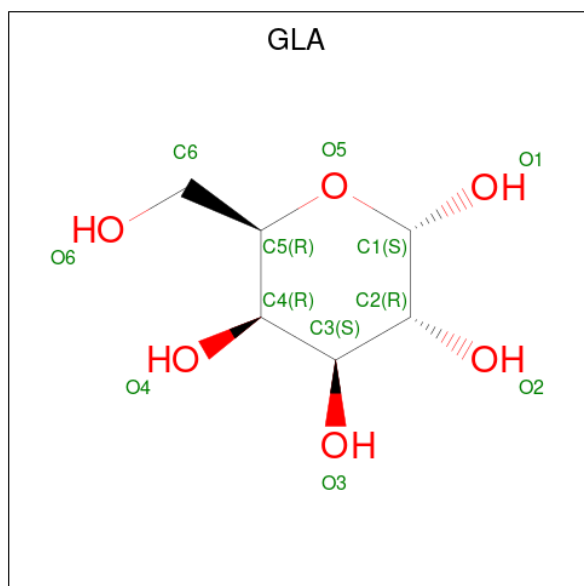
Mol	Chain	Residues	Atoms			AltConf
26	A	1	Total	C	O	0
			9	5	4	
26	A	1	Total	C	O	0
			9	5	4	
26	A	1	Total	C	O	0
			9	5	4	
26	A	1	Total	C	O	0
			9	5	4	
26	B	1	Total	C	O	0
			9	5	4	
26	B	1	Total	C	O	0
			9	5	4	
26	B	1	Total	C	O	0
			9	5	4	
26	B	1	Total	C	O	0
			9	5	4	
26	C	1	Total	C	O	0
			9	5	4	
26	C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

- Molecule 27 is alpha-D-galactopyranose (three-letter code: GLA) (formula: C₆H₁₂O₆) (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
27	B	1	11	6	5	0

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

- Molecule 28 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).

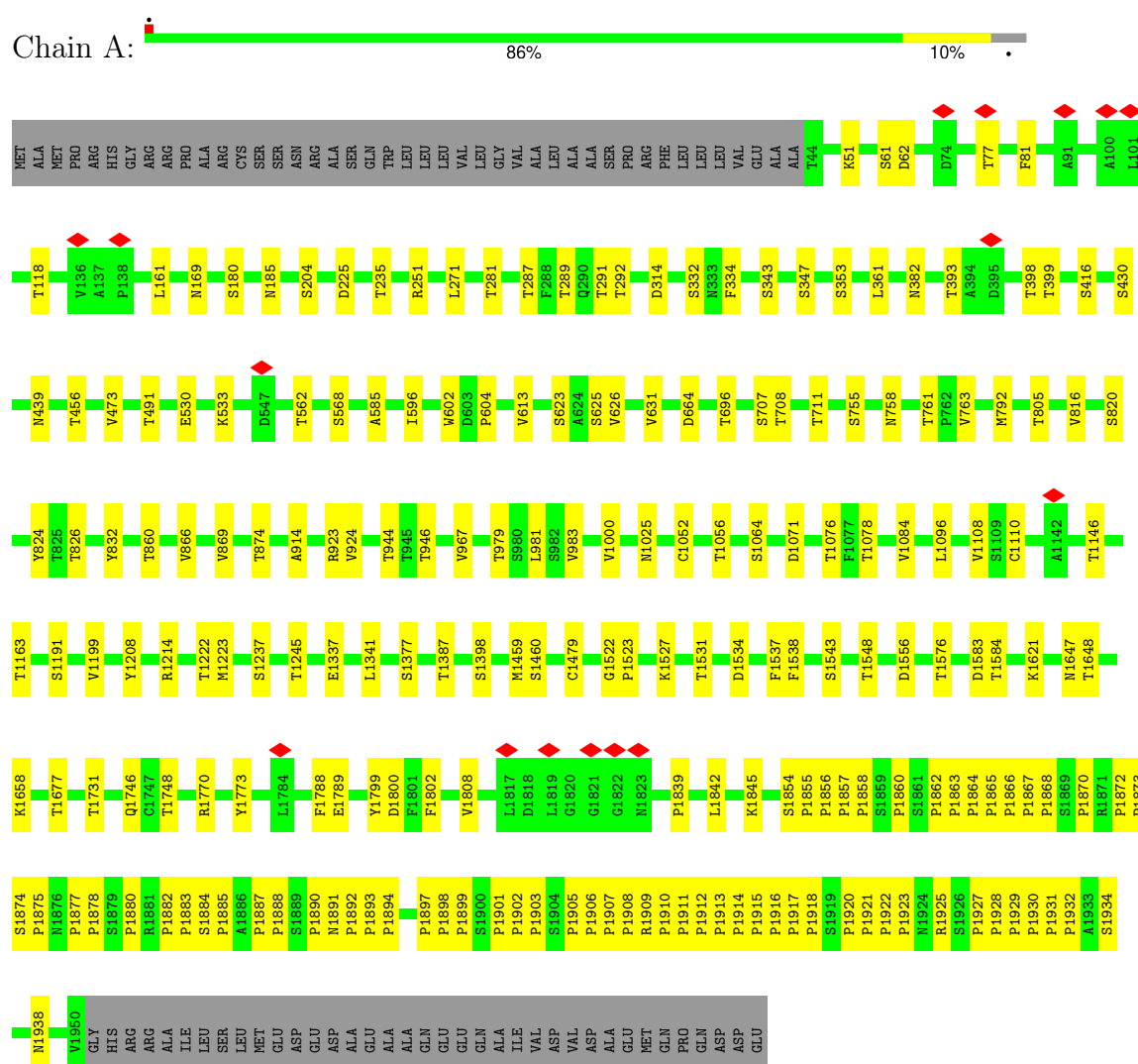


Mol	Chain	Residues	Atoms				AltConf
28	A	1	Total	C	N	O	0
			14	8	1	5	
28	B	1	Total	C	N	O	0
			14	8	1	5	
28	B	1	Total	C	N	O	0
			14	8	1	5	
28	C	1	Total	C	N	O	0
			14	8	1	5	
28	C	1	Total	C	N	O	0
			14	8	1	5	
28	D	1	Total	C	N	O	0
			14	8	1	5	
28	E	1	Total	C	N	O	0
			14	8	1	5	

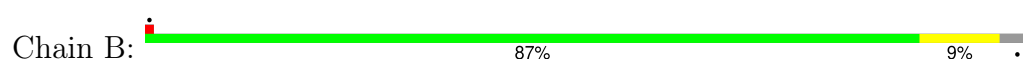
3 Residue-property plots

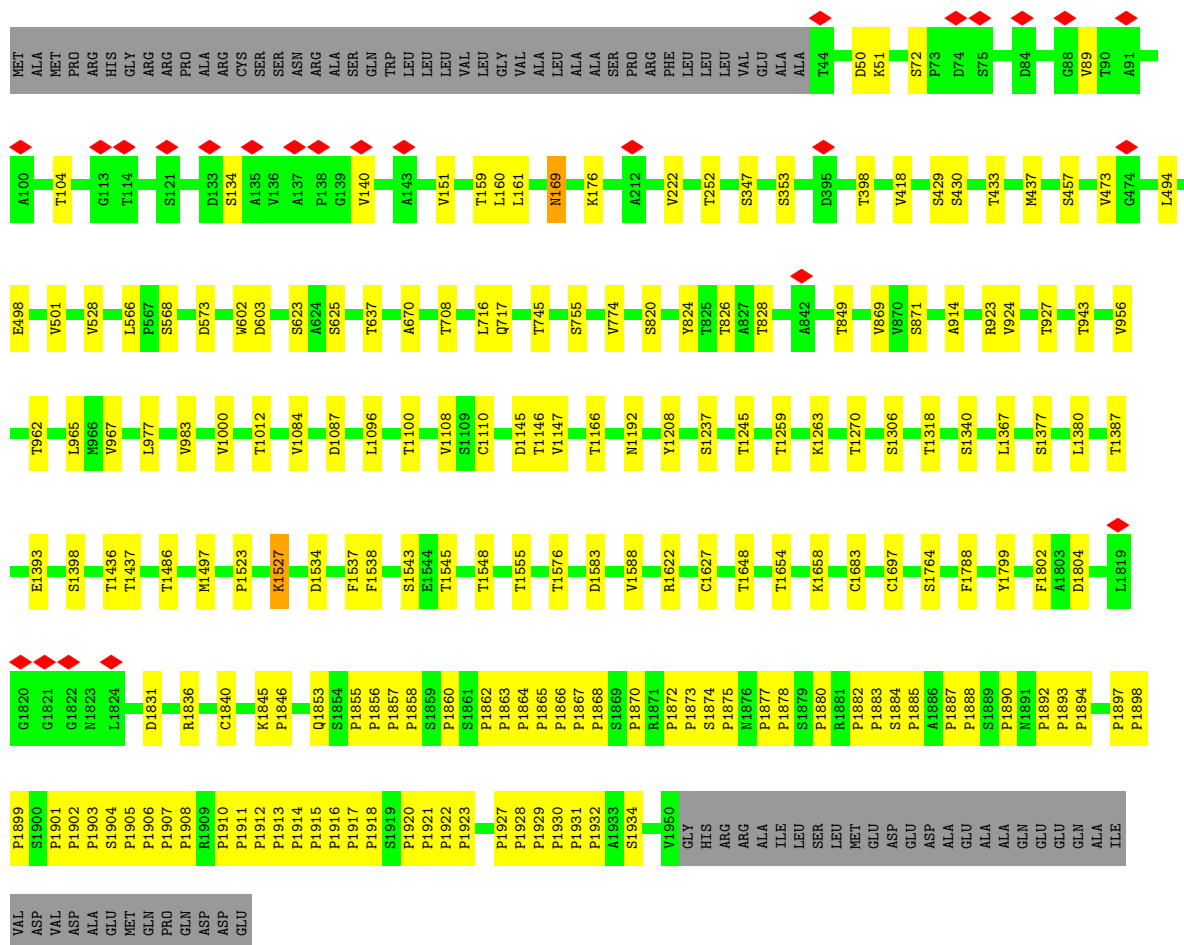
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

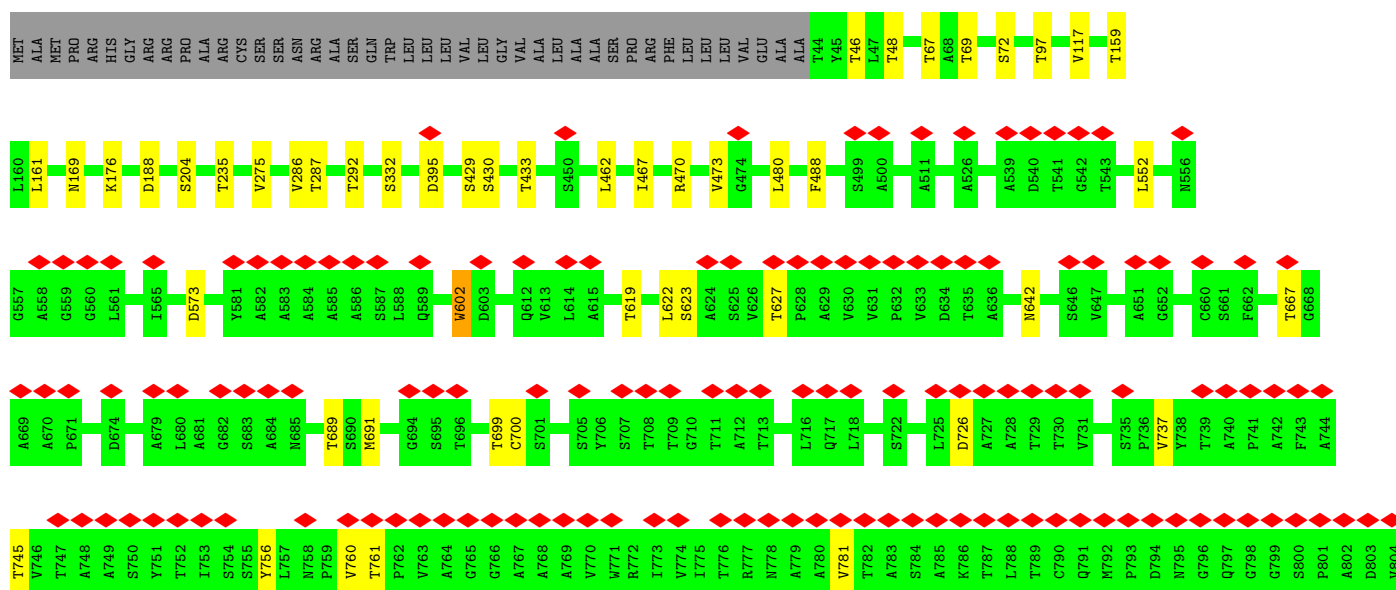


• Molecule 1: Mst1





• Molecule 1: Mst1





ALA	GLN	ALA	THR	A1540	Q1480	G1420	M1192	T979	C905	F833	R772	P704	L614	A475	T159
GLN	ASN	ALA	PHE	G1541	Q1481	Q1421	Y1208	S980	C905	A834	I773	S705	L614	A475	L160
PRO	GLU	ALA	ASP	K1542	Q1482	L1422	Y1208	L981	N909	A835	V774	Y706	A615	L479	L161
PRO	THR	GLU	GLU	S1543	K1483	G1423	M1223	S982	G910	V836	I775	S707	A616	T487	N169
CYS	SER	ALA	PHE	E1544	P1484	S1424	Y1229	V983	E911	N837	T776	T708	A617	T491	V179
GLY	SER	GLN	SER	T1545	G1485	P1425	I1229	T984	G912	V838	R777	T709	P618	T491	S190
MET	THR	PRO	VAL	T1546	T1486	F1426	R1242	S985	G912	V839	R777	T709	P618	T491	S181
TYR	GLY	VAL	VAL	S1547	N1487	I1427	R1242	T984	G912	V838	R777	T709	P618	T491	S182
PHE	CYS	THR	CYS	T1548	N1488	T1428	K1286	S986	A914	D840	N778	T711	T619	A500	S190
GLN	ALA	ALA	ALA	N1549	L1489	T1428	K1286	S986	A914	D840	N778	T711	T619	A500	S182
SER	SER	ALA	ALA	L1550	M1490	A1429	T1299	S987	P915	G841	N781	T712	T620	E502	N185
THR	THR	THR	THR	P1551	G1491	G1431	T1333	Q987	P915	G841	N781	T712	T620	E502	S204
GLY	GLY	GLY	GLY	G1552	D1492	V1432	T1333	Q987	P915	G841	N781	T712	T620	E502	I207
THR	SER	ALA	SER	Y1553	R1493	P1433	E1337	S988	A916	V843	A783	L716	A824	I507	E231
THR	THR	ALA	PHE	Y1554	T1494	V1434	T1339	L988	S917	V843	A783	L716	A824	I507	R251
CYS	SER	ALA	ALA	T1555	Q1495	A1435	T1339	A990	A918	T844	A785	L717	S825	T509	T278
THR	THR	LYS	SER	D1556	Q1496	T1436	P1362	T997	A918	T844	A785	L717	S825	T509	T289
ALA	ALA	ARG	ARG	V1557	M1497	T1437	P1362	T997	A919	T845	K786	P828	T627	V510	T287
CYS	CYS	GLY	GLY	D1558	A1498	L1438	A1363	N999	A919	T845	K786	P828	T627	V510	T287
VAL	VAL	LEU	LEU	V1559	L1499	T1439	A1363	N999	A919	T845	K786	P828	T627	V510	T287
GLY	GLY	THR	THR	L1560	V1500	E1440	Y1366	V1000	A920	S846	T787	I719	T627	V510	T287
THR	CYS	GLY	CYS	P1561	R1370	L1441	Y1366	V1000	A920	S846	T787	I719	T627	V510	T287
ALA	ILE	ALA	GLU	I1562	T1502	G1442	S1377	A1002	R921	H847	T787	I719	T627	V510	T287
ASP	ALA	ALA	ILE	Q1563	T1503	S1443	S1377	A1003	R921	H847	T787	I719	T627	V510	T287
GLN	GLN	GLN	GLN	L1564	M1504	G1444	M1378	T1028	R922	I848	A788	L725	V830	A512	T278
ALA	PRO	ALA	PRO	P1565	A1505	C1445	M1378	T1028	R922	I848	A788	L725	V830	A512	T278
GLY	GLY	GLY	GLY	CYS	A1506	S1446	L1380	D1037	S925	K850	C790	D726	V633	T524	T278
LEU	LEU	THR	THR	LVS	M1507	Q1447	A1381	D1037	S925	K850	C790	D726	V633	T524	T278
ALA	ALA	PHE	PHE	PRO	D1507	Q1448	A1382	S1045	R922	I848	A788	L725	V830	T524	T278
ALA	ALA	THR	THR	GLY	F1508	C1448	A1382	S1046	R922	I848	A788	L725	V830	T524	T278
CYS	CYS	ASN	ASN	THR	P1509	P1449	E1393	M1059	E942	T860	P801	A740	A651	G527	S279
PRO	PRO	ALA	VAL	PHE	A1510	P1450	D1394	M1059	E942	T860	P801	A740	A651	G527	S279
CYS	CYS	ALA	ALA	MET	L1511	G1451	G1395	S1064	T943	P862	D803	F743	T541	G542	T280
GLN	GLN	ALA	ALA	PHE	R1512	T1452	G1395	S1064	T943	P862	D803	F743	T541	G542	T280
ASP	GLY	ALA	ASN	ASP	A1513	Y1453	G1395	S1064	T943	P862	D803	F743	T541	G542	T280
ARG	ARG	ALA	THR	THR	Y1514	A1454	K1399	A1068	T946	T867	D807	A749	A670	G560	T281
TYR	THR	ALA	THR	THR	T1515	P1455	A1400	I1069	C947	T867	D807	A749	A670	G560	T281
GLN	PHE	ALA	PHE	ALA	T1456	T1456	A1403	I1072	Y853	P872	A809	Y751	T672	D573	S429
ASN	ASN	ASN	ASN	ASN	F1457	F1457	A1403	I1072	Y853	P872	A809	Y751	T672	D573	S430
SER	SER	GLY	THR	GLY	SER	G1458	G1404	T1076	V956	P872	A809	Y751	T672	D573	S430
ILE	ILE	ALA	LEU	LEU	MET	G1458	C1405	T1076	S957	T874	G811	T752	A675	F577	T433
GLY	THR	THR	THR	THR	VAL	M1459	C1405	T1076	S957	T874	G811	T752	A675	F577	T433
ARG	GLN	LEU	LEU	ASP	ALA	S1460	Q1407	L1096	G959	V876	T813	S755	Y581	Y581	M437
THR	ILE	THR	ILE	THR	ALA	V1461	K1407	L1096	G959	V876	T813	S755	Y581	Y581	M437
VAL	VAL	PRO	PRO	GLY	PRO	C1462	C1408	T1100	G960	T814	T815	Y756	L580	A582	A442
CYS	THR	THR	THR	GLY	ALA	C1462	C1408	T1100	G960	T814	T815	Y756	L580	A582	A442
LYS	GLY	THR	GLY	THR	TYR	L1463	P1409	V1128	T962	F886	V816	N758	G882	A584	R466
ASP	ALA	ASP	VAL	ASP	ALA	P1464	P1410	V1128	T962	F886	V816	N758	G882	A584	R466
PRO	PRO	LEU	LEU	THR	ALA	C1465	G1411	S1133	K964	T889	V818	P759	A585	A586	R470
GLY	GLY	THR	GLY	GLY	THR	P1466	T1412	S1133	K964	T889	V818	P759	A585	A586	R470
GLN	GLN	GLN	GLN	GLN	P1528	P1467	Y1413	A1138	M966	T889	V818	P759	A585	A586	R470
CYS	CYS	CYS	CYS	CYS	I1529	A1467	R1414	A1138	M966	T889	V818	P759	A585	A586	R470
THR	THR	THR	THR	THR	V1530	G1468	N1415	A1142	E970	A893	G823	A764	M691	W602	V473
THR	THR	THR	THR	THR	T1531	T1469	T1416	V1143	S971	A893	G823	A764	M691	W602	V473
CYS	CYS	CYS	CYS	CYS	G1532	F1470	T1417	A1144	S971	A893	G823	A764	M691	W602	V473
GLN	GLN	GLN	GLN	GLN	P1533	A1471	F1418	D1145	A972	T973	Y824	G766	T696	D603	V473
THR	THR	THR	THR	THR	D1534	S1472	S1419	T1160	A974	T973	Y824	G766	T696	D603	V473
GLY	GLY	GLY	GLY	GLY	T1535	A1473	T1475	L978	A975	G897	T826	A767	T697	T608	G474
					M1536	P1474				G897	T826	A767	T697	T608	G474
					F1537	G1475				G897	T826	A767	T697	T608	G474
					F1538	T1477				G897	T826	A767	T697	T608	G474
					M1539	C1479				G897	T826	A767	T697	T608	G474

- Molecule 1: Mst1

[illegible]

P1906	P1907	P1908	P1909	P1910	P1911	P1912	P1913	P1914	P1915	P1916	P1917	P1918	P1919	P1920	P1921	P1922	P1923	P1924	P1925	P1926	P1927	P1928	P1929	P1930	P1931	P1932	P1933	P1934	P1935	P1936	P1937	P1938	P1939	P1940	G1941	GLY	VAL	ASN	GLN	ASN	GLY	ASP	PRO	VAL	GLY	HIS	ARG	ARG	ALA	ILE	LEU	SER	LEU	MET	GLU	ASP	GLU	ASP	ALA																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
T1229	T1416	L1832	S1460	G1479	D1507	R1552	T1515	P1523	P1860	S1861	P1862	P1863	P1864	P1865	P1866	P1867	P1868	S1869	P1870	R1871	P1872	P1873	P1874	P1875	P1876	P1877	P1878	P1879	P1880	P1881	P1882	P1883	P1884	P1885	P1886	P1887	P1888	P1889	P1890	M1891	P1892	P1893	P1894	T1895	S1896	P1897	P1898	P1899	S1900	P1901	P1902	P1903	S1904	P1905																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
L1258	T1259	A1260	R1261	A1262	K1263	Y1264	S1265	I1266	D1267	P1268	T1269	Y1270	H1271	F1272	F1273	V1274	T1275	H1276	L1277	M1278	M1279	G1280	E1281	S1282	C1283	K1284	K1285	K1286	K1287	M1288	M1289	M1290	M1291	M1292	M1293	M1294	M1295	I1296	A1297	G1298	C1299	E1299	F1299	T1300	T1301	T1302	T1303	T1304	T1305	T1306	T1307	T1308	T1309	T1310	T1311	T1312	T1313	T1314	T1315	T1316	T1317	T1318	T1319	T1320	T1321	T1322	T1323	T1324	T1325	T1326	T1327	T1328	T1329	T1330	T1331	T1332	T1333	T1334	T1335	T1336	T1337	T1338	T1339	T1340	T1341	T1342	T1343	T1344	T1345	T1346	T1347	T1348	T1349	T1350	T1351	T1352	T1353	T1354	T1355	T1356	T1357	T1358	T1359	T1360	T1361	T1362	T1363	T1364	T1365	T1366	T1367	T1368	T1369	T1370	T1371	T1372	T1373	T1374	T1375	T1376	T1377	T1378	T1379	T1380	T1381	T1382	T1383	T1384	T1385	T1386	T1387	T1388	T1389	T1390	T1391	T1392	T1393	T1394	T1395	T1396	T1397	T1398	T1399	T1400	T1401	T1402	T1403	T1404	T1405	T1406	T1407	T1408	T1409	T1410	T1411	T1412	T1413	T1414	T1415	T1416	T1417	T1418	T1419	T1420	T1421	T1422	T1423	T1424	T1425	T1426	T1427	T1428	T1429	T1430	T1431	T1432	T1433	T1434	T1435	T1436	T1437	T1438	T1439	T1440	T1441	T1442	T1443	T1444	T1445	T1446	T1447	T1448	T1449	T1450	T1451	T1452	T1453	T1454	T1455	T1456	T1457	T1458	T1459	T1460	T1461	T1462	T1463	T1464	T1465	T1466	T1467	T1468	T1469	T1470	T1471	T1472	T1473	T1474	T1475	T1476	T1477	T1478	T1479	T1480	T1481	T1482	T1483	T1484	T1485	T1486	T1487	T1488	T1489	T1490	T1491	T1492	T1493	T1494	T1495	T1496	T1497	T1498	T1499	T1500	T1501	T1502	T1503	T1504	T1505	T1506	T1507	T1508	T1509	T1510	T1511	T1512	T1513	T1514	T1515	T1516	T1517	T1518	T1519	T1520	T1521	T1522	T1523	T1524	T1525	T1526	T1527	T1528	T1529	T1530	T1531	T1532	T1533	T1534	T1535	T1536	T1537	T1538	T1539	T1540	T1541	T1542	T1543	T1544	T1545	T1546	T1547	T1548	T1549	T1550	T1551	T1552	T1553	T1554	T1555	T1556	T1557	T1558	T1559	T1560	T1561	T1562	T1563	T1564	T1565	T1566	T1567	T1568	T1569	T1570	T1571	T1572	T1573	T1574	T1575	T1576	T1577	T1578	T1579	T1580	T1581	T1582	T1583	T1584	T1585	T1586	T1587	T1588	T1589	T1590	T1591	T1592	T1593	T1594	T1595	T1596	T1597	T1598	T1599	T1600	T1601	T1602	T1603	T1604	T1605	T1606	T1607	T1608	T1609	T1610	T1611	T1612	T1613	T1614	T1615	T1616	T1617	T1618	T1619	T1620	T1621	T1622	T1623	T1624	T1625	T1626	T1627	T1628	T1629	T1630	T1631	T1632	T1633	T1634	T1635	T1636	T1637	T1638	T1639	T1640	T1641	T1642	T1643	T1644	T1645	T1646	T1647	T1648	T1649	T1650	T1651	T1652	T1653	T1654	T1655	T1656	T1657	T1658	T1659	T1660	T1661	T1662	T1663	T1664	T1665	T1666	T1667	T1668	T1669	T1670	T1671	T1672	T1673	T1674	T1675	T1676	T1677	T1678	T1679	T1680	T1681	T1682	T1683	T1684	T1685	T1686	T1687	T1688	T1689	T1690	T1691	T1692	T1693	T1694	T1695	T1696	T1697	T1698	T1699	T1700	T1701	T1702	T1703	T1704	T1705	T1706	T1707	T1708	T1709	T1710	T1711	T1712	T1713	T1714	T1715	T1716	T1717	T1718	T1719	T1720	T1721	T1722	T1723	T1724	T1725	T1726	T1727	T1728	T1729	T1730	T1731	T1732	T1733	T1734	T1735	T1736	T1737	T1738	T1739	T1740	T1741	T1742	T1743	T1744	T1745	T1746	T1747	T1748	T1749	T1750	T1751	T1752	T1753	T1754	T1755	T1756	T1757	T1758	T1759	T1760	T1761	T1762	T1763	T1764	T1765	T1766	T1767	T1768	T1769	T1770	T1771	T1772	T1773	T1774	T1775	T1776	T1777	T1778	T1779	T1780	T1781	T1782	T1783	T1784	T1785	T1786	T1787	T1788	T1789	T1790	T1791	T1792	T1793	T1794	T1795	T1796	T1797	T1798	T1799	T1800	T1801	T1802	T1803	T1804	T1805	T1806	T1807	T1808	T1809	T1810	T1811	T1812	T1813	T1814	T1815	T1816	T1817	T1818	T1819	T1820	T1821	T1822	T1823	T1824	T1825	T1826	T1827	T1828	T1829	T1830	T1831	T1832	T1833	T1834	T1835	T1836	T1837	T1838	T1839	T1840	T1841	T1842	T1843	T1844	T1845	T1846	T1847	T1848	T1849	T1850	T1851	T1852	T1853	T1854	T1855	T1856	T1857	T1858	T1859	T1860	T1861	T1862	T1863	T1864	T1865	T1866	T1867	T1868	T1869	T1870	T1871	T1872	T1873	T1874	T1875	T1876	T1877	T1878	T1879	T1880	T1881	T1882	T1883	T1884	T1885	T1886	T1887	T1888	T1889	T1890	T1891	T1892	T1893	T1894	T1895	T1896	T1897	T1898	T1899	T1900	T1901	T1902	T1903	T1904	T1905	T1906	T1907	T1908	T1909	T1910	T1911	T1912	T1913	T1914	T1915	T1916	T1917	T1918	T1919	T1920	T1921	T1922	T1923	T1924	T1925	T1926	T1927	T1928	T1929	T1930	T1931	T1932	T1933	T1934	T1935	T1936	T1937	T1938	T1939	T1940	T1941	T1942	T1943	T1944	T1945	T1946	T1947	T1948	T1949	T1950	T1951	T1952	T1953	T1954	T1955	T1956	T1957	T1958	T1959	T1960	T1961	T1962	T1963	T1964	T1965	T1966	T1967	T1968	T1969	T1970	T1971	T1972	T1973	T1974	T1975	T1976	T1977	T1978	T1979	T1980	T1981	T1982	T1983	T1984	T1985	T1986	T1987	T1988	T1989	T1990	T1991	T1992	T1993	T1994	T1995	T1996	T1997	T1998	T1999	T2000	T2001	T2002	T2003	T2004	T2005	T2006	T2007	T2008	T2009	T2010	T2011	T2012	T2013	T2014	T2015	T2016	T2017	T2018	T2019	T2020	T2021	T2022	T2023	T2024	T2025	T2026	T2027	T2028	T2029	T2030	T2031	T2032	T2033	T2034	T2035	T2036	T2037	T2038	T2039	T2040	T2041	T2042	T2043	T2044	T2045	T2046	T2047	T2048	T2049	T2050	T2051	T2052	T2053	T2054	T2055	T2056	T2057	T2058	T2059	T2060	T2061	T2062	T2063	T2064	T2065	T2066	T2067	T2068	T2069	T2070	T2071	T2072	T2073	T2074	T2075	T2076	T2077	T2078	T2079	T2080	T2081	T2082	T2083	T2084	T2085	T2086	T2087	T2088	T2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- Chain T:  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

Chain w:  67% 33%

FUB1
FUB2
FUB3

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

Chain x:  67% 33%

FUB1
FUB2
FUB3

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

Chain y:  100%

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:  100%

FUB1
FUB2
FUB3

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

Chain HA:  67% 33%



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

Chain IA:  100%



- 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



- 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

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 lC:  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:  67% 33%



- 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% 67% 33%



- 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:  100%



- 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:  100%



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

Chain Z:  50% 50%



- 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:  50% 50%



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

Chain g:  75% 25%



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

Chain k:  100%



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

Chain r:  100%




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

Chain v:  75% 25%




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

Chain JA:  75% 25%




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

Chain UA:  75% 25%



- 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%



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

Chain JB: 




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

Chain NB: 




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

Chain mB: 



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

Chain qB: 



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

Chain DC: 




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

Chain OC: 




- 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% 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:  75% 25%



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

Chain RD:  50% 50%



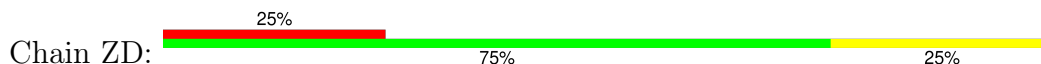
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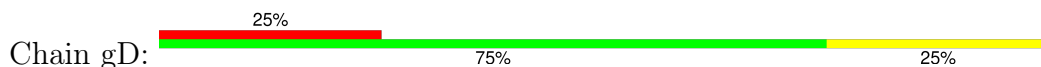
- Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



- 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 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



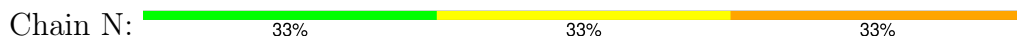
- Molecule 5: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose



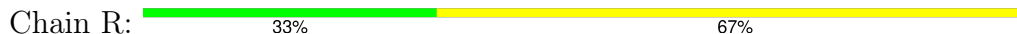
- Molecule 5: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose



- 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-arabinofuranose

Chain 9:  33% 67%

FUB1
FUB2
GZL3

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

Chain AA:  33% 67%

FUB1
FUB2
GZL3

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

Chain EA:  67% 33%

FUB1
FUB2
GZL3

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

Chain LA:  33% 33% 33%

FUB1
FUB2
GZL3

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

Chain PA:  67% 33%

FUB1
FUB2
GZL3

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

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%



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

Chain 7A:  33% 67%



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

Chain 8A:  100%



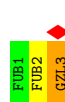
- Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain CB:  33% 67%




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

Chain XB:  33% 33% 33% 33%



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

Chain aB:  33% 67%



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

Chain bB:  33% 67%



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

Chain cB:  100%



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

Chain gB:  67% 33%



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

Chain 0B:  33% 33% 33%



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

Chain 3B:  33% 67%



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

Chain 4B:  33% 67%



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

Chain 5B:  33% 67%



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

Chain 9B:  33% 67%



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

Chain FC:  100%



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

Chain JC:  33% 67%



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

Chain xC:  33% 100% 33% 33%



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

Chain 0C:  33% 100% 67%



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

Chain 1C:  100% 67% 33%



- 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





- 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

Chain OE:  67% 33%



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

Chain ZE:  33% 67%



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

Chain bE:  67% 33%



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

Chain mE:  67% 33%



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

Chain nE:  33% 67%




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

Chain oE:  33% 67%



- 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-arabinofuranose-(1-3)]beta-L-arabinofuranose



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



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



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




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



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




- 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:  60% 40%



- 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:  100%


FUB1
FUB2
FUB3
AHR4
AHR5

- 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%

FUB1
FUB2
FUB3
AHR4
AHR5

- 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%

FUB1
FUB2
FUB3
AHR4
AHR5

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

Chain Y:  50% 50%

FUB1
FUB2

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

Chain j:  50% 50%

FUB1
FUB2

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

Chain WA:  100%

FUB1
FUB2

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

Chain hA:  50% 50%

FUB1
FUB2

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

Chain QC:  100%



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

Chain bC:  100%



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

Chain ND:  50% 50%



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

Chain YD:  100%



- 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:  40% 60%



- 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%




- 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%



- 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%



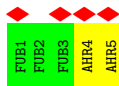
- Molecule 10: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose



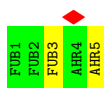
- Molecule 10: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose



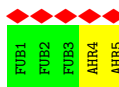
- Molecule 10: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose



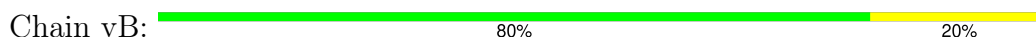
- Molecule 10: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose



- 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





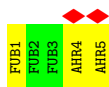
- Molecule 10: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain SC:



- 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 mC:



- 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 vC:



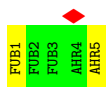
- Molecule 10: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain PD:



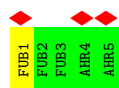
- Molecule 10: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain jD:



- 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 sD:



- 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:  67% 33%



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

Chain XD:  33% 67%



- 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%



- 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 1A: 



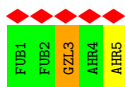
- Molecule 12: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain oA: 

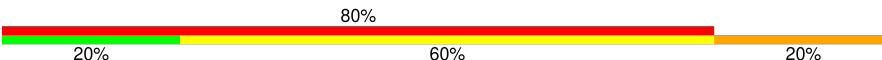


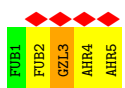
- Molecule 12: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain FB: 




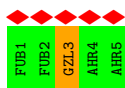
- Molecule 12: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain IB: 




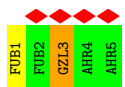
- Molecule 12: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain iB: 

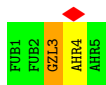


- Molecule 12: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

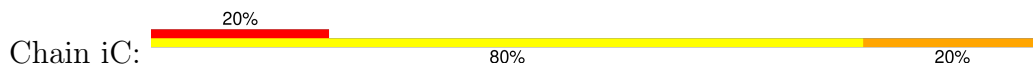
Chain lB: 



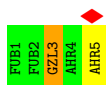
- Molecule 12: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose



- 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



- 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%



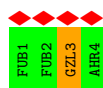
- Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranos e-(1-2)-beta-L-arabinofuranose

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% 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%

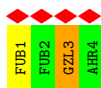


- Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranos e-(1-2)-beta-L-arabinofuranose

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

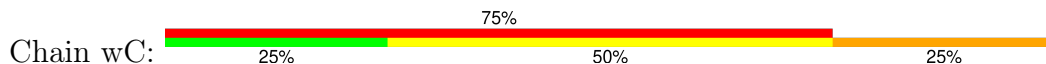


- Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose





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



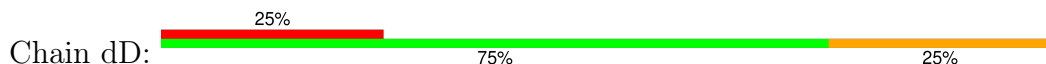
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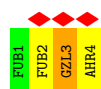
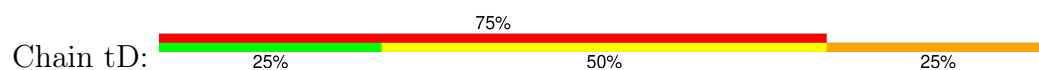
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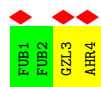
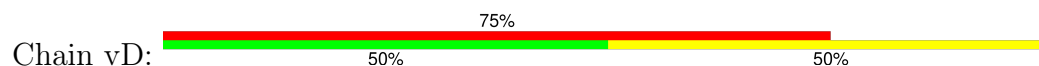
- Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



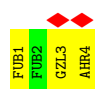
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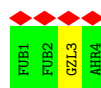
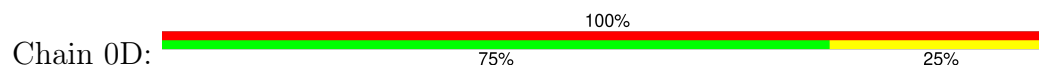
- Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



- 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%



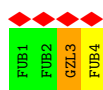
- Molecule 14: beta-L-arabinofuranose-(1-5)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain qA:  75% 25%



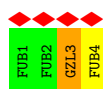
- Molecule 14: beta-L-arabinofuranose-(1-5)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain HB:  50% 25% 25%



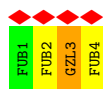
- Molecule 14: beta-L-arabinofuranose-(1-5)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain KB:  50% 25% 25%




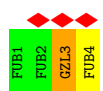
- Molecule 14: beta-L-arabinofuranose-(1-5)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain kB:  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:  50% 25% 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:  75% 25%




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

Chain eD:  75% 25%



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

Chain hD:  75% 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:  60% 40%



- 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:  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 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: 



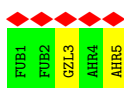
- Molecule 15: alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 8B: 

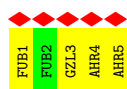


- Molecule 15: alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

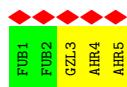
Chain 4C: 



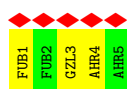
- Molecule 15: alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



- 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



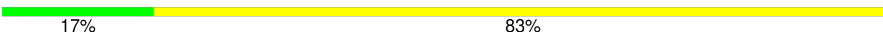
- Molecule 17: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

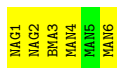
mido-2-deoxy-beta-D-glucopyranose

Chain GA:  67% 33%



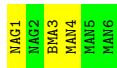
- Molecule 17: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain DB:  17% 83%



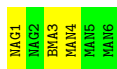
- Molecule 17: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 7C:  50% 50%

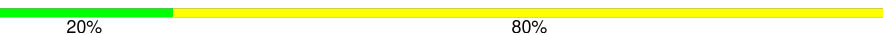


- Molecule 17: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 5D:  50% 50%




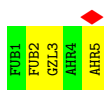
- Molecule 18: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain 9D:  20% 80%



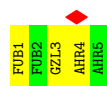
- Molecule 18: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

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

Chain DE: 



- 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 IE: 



- 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 JE: 



- 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 KE: 



- 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: 



- 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 SE: 



- 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%



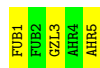
- Molecule 18: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain fE:  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 pE:  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 rE:  20% 40% 60%



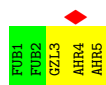
- Molecule 18: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

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

Chain 0E: 60% 40%



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

Chain AE: 50% 50%



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

Chain LE: 25% 50% 50%



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

Chain NE: 75% 25%



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

Chain aE: 25% 50% 50%



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

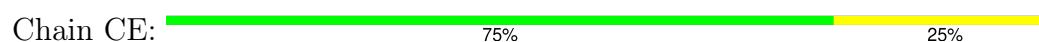
Chain qE: 50% 50%



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



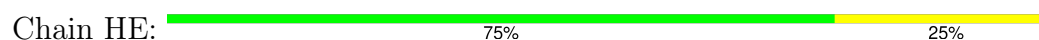
- Molecule 20: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



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



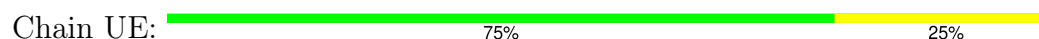
- Molecule 20: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



- 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:  75% 25%



- 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%



- 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:  40% 60%



- 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%



- 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%



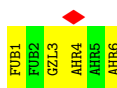
- Molecule 22: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain GE:  33% 67%



- 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%



- 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% 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 VE:  33% 67%



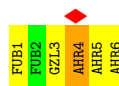
- Molecule 22: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain dE:  17% 83%



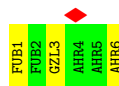
- Molecule 22: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

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%

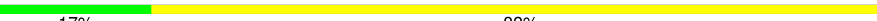


- Molecule 23: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)][alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose

Chain XE:  50% 50%

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 (\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 (\AA)	1.0825, 1.0825, 1.0825	Depositor

5 Model quality

5.1 Standard geometry

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

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%)	30 66

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	1848/1987 (93%)	1691 (92%)	150 (8%)	7 (0%)	30	66
1	C	1461/1987 (74%)	1342 (92%)	115 (8%)	4 (0%)	37	70
1	D	1531/1987 (77%)	1411 (92%)	114 (7%)	6 (0%)	30	66
1	E	1390/1987 (70%)	1289 (93%)	97 (7%)	4 (0%)	37	70
1	F	1384/1987 (70%)	1273 (92%)	108 (8%)	3 (0%)	44	77
2	G	27/64 (42%)	17 (63%)	6 (22%)	4 (15%)	0	0
2	H	12/64 (19%)	11 (92%)	0	1 (8%)	0	3
2	I	14/64 (22%)	9 (64%)	3 (21%)	2 (14%)	0	1
All	All	9515/12114 (78%)	8733 (92%)	743 (8%)	39 (0%)	32	66

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 ⓘ

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%)	7	28
1	B	1451/1514 (96%)	1331 (92%)	120 (8%)	9	34
1	C	1149/1514 (76%)	1064 (93%)	85 (7%)	11	38
1	D	1209/1514 (80%)	1099 (91%)	110 (9%)	7	30
1	E	1081/1514 (71%)	1005 (93%)	76 (7%)	12	41
1	F	1078/1514 (71%)	1009 (94%)	69 (6%)	14	44
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%)	12	35

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 ⓘ

There are no RNA molecules in this entry.

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

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
1	HYP	C	1906	1	7,8,9	0.56	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	1866	1	7,8,9	0.56	0	5,10,12	1.48	1 (20%)
1	HYP	F	1894	1	7,8,9	0.51	0	5,10,12	1.98	2 (40%)
1	HYP	E	1880	1	7,8,9	0.53	0	5,10,12	1.45	1 (20%)
2	HYP	G	9	2	7,8,9	0.55	0	5,10,12	1.80	2 (40%)
1	HYP	A	1878	1	7,8,9	0.52	0	5,10,12	1.75	2 (40%)
1	HYP	E	1914	1	7,8,9	0.56	0	5,10,12	1.26	1 (20%)
1	HYP	E	1911	1	7,8,9	0.56	0	5,10,12	1.25	1 (20%)
1	HYP	D	1914	1	7,8,9	0.53	0	5,10,12	1.11	1 (20%)
1	HYP	C	1897	1	7,8,9	0.53	0	5,10,12	1.30	1 (20%)
2	HYP	G	33	2	7,8,9	0.51	0	5,10,12	1.65	1 (20%)
1	HYP	A	1894	1	7,8,9	0.55	0	5,10,12	1.93	2 (40%)
1	HYP	E	1898	1	7,8,9	0.57	0	5,10,12	1.22	1 (20%)
1	HYP	C	1903	1	7,8,9	0.54	0	5,10,12	1.84	3 (60%)
1	HYP	E	1912	1	7,8,9	0.57	0	5,10,12	1.29	1 (20%)
1	HYP	D	1932	1	7,8,9	0.56	0	5,10,12	1.87	3 (60%)
1	HYP	E	1865	1	7,8,9	0.55	0	5,10,12	1.66	1 (20%)
1	HYP	D	1918	1	7,8,9	0.55	0	5,10,12	1.86	2 (40%)
1	HYP	B	1873	1	7,8,9	0.49	0	5,10,12	1.37	1 (20%)
1	HYP	A	1870	1	7,8,9	0.50	0	5,10,12	1.60	2 (40%)
2	HYP	G	56	2	7,8,9	0.53	0	5,10,12	1.28	1 (20%)
2	HYP	G	46	2	7,8,9	0.57	0	5,10,12	1.57	1 (20%)
1	HYP	A	1887	1	7,8,9	0.55	0	5,10,12	1.27	1 (20%)
1	HYP	E	1893	1	7,8,9	0.58	0	5,10,12	1.26	1 (20%)
1	HYP	F	1898	1	7,8,9	0.58	0	5,10,12	1.19	1 (20%)
1	HYP	B	1917	1	7,8,9	0.60	0	5,10,12	1.68	1 (20%)
2	HYP	G	32	2	7,8,9	0.52	0	5,10,12	1.43	1 (20%)
1	HYP	A	1883	1	7,8,9	0.55	0	5,10,12	2.22	2 (40%)
1	HYP	A	1882	1	7,8,9	0.55	0	5,10,12	1.25	1 (20%)
1	HYP	E	1902	1	7,8,9	0.52	0	5,10,12	1.70	1 (20%)
1	HYP	B	1894	1	7,8,9	0.55	0	5,10,12	2.01	2 (40%)
1	HYP	C	1899	1	7,8,9	0.59	0	5,10,12	1.32	1 (20%)
1	HYP	F	1917	1	7,8,9	0.54	0	5,10,12	1.41	1 (20%)
1	HYP	B	1907	1	7,8,9	0.56	0	5,10,12	1.68	1 (20%)
1	HYP	E	1916	1	7,8,9	0.59	0	5,10,12	1.34	1 (20%)
1	HYP	F	1914	1	7,8,9	0.54	0	5,10,12	1.48	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	HYP	F	1899	1	7,8,9	0.61	0	5,10,12	1.33	1 (20%)
1	HYP	B	1908	1	7,8,9	0.56	0	5,10,12	2.17	3 (60%)
1	HYP	E	1888	1	7,8,9	0.50	0	5,10,12	1.86	2 (40%)
1	HYP	B	1875	1	7,8,9	0.56	0	5,10,12	1.20	1 (20%)
1	HYP	B	1888	1	7,8,9	0.54	0	5,10,12	1.72	2 (40%)
1	HYP	E	1929	1	7,8,9	0.59	0	5,10,12	1.27	1 (20%)
2	HYP	G	1	2	7,8,9	0.53	0	5,10,12	1.21	1 (20%)
1	HYP	E	1899	1	7,8,9	0.59	0	5,10,12	1.34	1 (20%)
1	HYP	F	1877	1	7,8,9	0.54	0	5,10,12	1.58	1 (20%)
1	HYP	E	1855	1	7,8,9	0.60	0	5,10,12	1.22	1 (20%)
1	HYP	C	1927	1	7,8,9	0.57	0	5,10,12	1.23	1 (20%)
1	HYP	F	1929	1	7,8,9	0.57	0	5,10,12	1.22	1 (20%)
1	HYP	F	1865	1	7,8,9	0.57	0	5,10,12	1.68	2 (40%)
1	HYP	D	1921	1	7,8,9	0.59	0	5,10,12	1.25	1 (20%)
1	HYP	A	1903	1	7,8,9	0.58	0	5,10,12	1.81	2 (40%)
1	HYP	B	1929	1	7,8,9	0.68	0	5,10,12	1.40	1 (20%)
1	HYP	B	1887	1	7,8,9	0.58	0	5,10,12	1.30	1 (20%)
1	HYP	D	1923	1	7,8,9	0.53	0	5,10,12	1.86	3 (60%)
1	HYP	B	1910	1	7,8,9	0.54	0	5,10,12	1.18	1 (20%)
1	HYP	A	1910	1	7,8,9	0.55	0	5,10,12	1.19	1 (20%)
1	HYP	F	1905	1	7,8,9	0.59	0	5,10,12	1.30	1 (20%)
1	HYP	A	1918	1	7,8,9	0.57	0	5,10,12	1.62	1 (20%)
1	HYP	B	1866	1	7,8,9	0.51	0	5,10,12	1.32	1 (20%)
1	HYP	F	1893	1	7,8,9	0.57	0	5,10,12	1.34	1 (20%)
1	HYP	B	1928	1	7,8,9	0.56	0	5,10,12	1.54	1 (20%)
1	HYP	B	1897	1	7,8,9	0.57	0	5,10,12	1.17	1 (20%)
1	HYP	E	1877	1	7,8,9	0.54	0	5,10,12	1.80	2 (40%)
1	HYP	E	1892	1	7,8,9	0.52	0	5,10,12	1.32	1 (20%)
1	HYP	A	1890	1	7,8,9	0.59	0	5,10,12	1.25	1 (20%)
1	HYP	E	1908	1	7,8,9	0.54	0	5,10,12	2.14	3 (60%)
2	HYP	I	2	2	7,8,9	0.48	0	5,10,12	1.48	1 (20%)
1	HYP	A	1916	1	7,8,9	0.58	0	5,10,12	1.47	1 (20%)
1	HYP	F	1890	1	7,8,9	0.57	0	5,10,12	1.18	1 (20%)
1	HYP	E	1862	1	7,8,9	0.54	0	5,10,12	1.49	1 (20%)
1	HYP	E	1858	1	7,8,9	0.54	0	5,10,12	1.70	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	HYP	F	1916	1	7,8,9	0.54	0	5,10,12	1.28	1 (20%)
1	HYP	F	1928	1	7,8,9	0.56	0	5,10,12	1.28	1 (20%)
1	HYP	B	1877	1	7,8,9	0.51	0	5,10,12	1.68	1 (20%)
1	HYP	B	1892	1	7,8,9	0.51	0	5,10,12	1.27	1 (20%)
1	HYP	F	1855	1	7,8,9	0.62	0	5,10,12	1.46	1 (20%)
2	HYP	G	41	2	7,8,9	0.58	0	5,10,12	1.23	1 (20%)
1	HYP	C	1911	1	7,8,9	0.54	0	5,10,12	1.23	1 (20%)
1	HYP	D	1897	1	7,8,9	0.51	0	5,10,12	1.27	1 (20%)
1	HYP	F	1885	1	7,8,9	0.54	0	5,10,12	1.24	1 (20%)
2	HYP	G	5	2	7,8,9	0.47	0	5,10,12	1.20	1 (20%)
2	HYP	G	17	2	7,8,9	0.56	0	5,10,12	1.31	1 (20%)
1	HYP	B	1870	1	7,8,9	0.56	0	5,10,12	1.57	1 (20%)
1	HYP	C	1913	1	7,8,9	0.57	0	5,10,12	1.27	1 (20%)
1	HYP	B	1858	1	7,8,9	0.56	0	5,10,12	1.43	1 (20%)
1	HYP	A	1885	1	7,8,9	0.57	0	5,10,12	1.23	1 (20%)
1	HYP	B	1901	1	7,8,9	0.57	0	5,10,12	1.20	1 (20%)
1	HYP	A	1911	1	7,8,9	0.56	0	5,10,12	1.24	1 (20%)
2	HYP	H	48	2	7,8,9	0.62	0	5,10,12	1.23	1 (20%)
1	HYP	A	1867	1	7,8,9	0.51	0	5,10,12	1.61	1 (20%)
1	HYP	C	1901	1	7,8,9	0.56	0	5,10,12	1.20	1 (20%)
1	HYP	D	1911	1	7,8,9	0.57	0	5,10,12	1.22	1 (20%)
1	HYP	A	1856	1	7,8,9	0.56	0	5,10,12	1.34	1 (20%)
1	HYP	C	1905	1	7,8,9	0.58	0	5,10,12	1.20	1 (20%)
1	HYP	E	1870	1	7,8,9	0.50	0	5,10,12	1.59	2 (40%)
1	HYP	A	1912	1	7,8,9	0.60	0	5,10,12	1.24	1 (20%)
1	HYP	F	1930	1	7,8,9	0.53	0	5,10,12	1.54	1 (20%)
1	HYP	A	1913	1	7,8,9	0.62	0	5,10,12	1.30	1 (20%)
2	HYP	G	8	2	7,8,9	0.59	0	5,10,12	1.62	1 (20%)
2	HYP	G	43	2	7,8,9	0.54	0	5,10,12	1.49	1 (20%)
2	HYP	I	7	2	7,8,9	0.52	0	5,10,12	1.67	1 (20%)
1	HYP	B	1890	1	7,8,9	0.59	0	5,10,12	1.21	1 (20%)
1	HYP	F	1872	1	7,8,9	0.56	0	5,10,12	1.25	1 (20%)
1	HYP	D	1908	1	7,8,9	0.54	0	5,10,12	1.74	2 (40%)
1	HYP	F	1915	1	7,8,9	0.52	0	5,10,12	1.24	1 (20%)
1	HYP	D	1907	1	7,8,9	0.50	0	5,10,12	1.61	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	HYP	D	1905	1	7,8,9	0.55	0	5,10,12	1.22	1 (20%)
1	HYP	A	1917	1	7,8,9	0.55	0	5,10,12	1.62	1 (20%)
1	HYP	A	1915	1	7,8,9	0.57	0	5,10,12	1.27	1 (20%)
1	HYP	B	1864	1	7,8,9	0.53	0	5,10,12	1.49	1 (20%)
1	HYP	F	1863	1	7,8,9	0.54	0	5,10,12	1.41	1 (20%)
1	HYP	F	1862	1	7,8,9	0.50	0	5,10,12	1.37	1 (20%)
1	HYP	A	1880	1	7,8,9	0.53	0	5,10,12	1.41	1 (20%)
1	HYP	E	1864	1	7,8,9	0.58	0	5,10,12	1.58	1 (20%)
2	HYP	G	49	2	7,8,9	0.57	0	5,10,12	1.51	1 (20%)
1	HYP	A	1914	1	7,8,9	0.57	0	5,10,12	1.40	1 (20%)
1	HYP	D	1920	1	7,8,9	0.57	0	5,10,12	1.51	1 (20%)
1	HYP	C	1917	1	7,8,9	0.57	0	5,10,12	1.48	1 (20%)
1	HYP	A	1898	1	7,8,9	0.64	0	5,10,12	1.23	1 (20%)
1	HYP	B	1927	1	7,8,9	0.58	0	5,10,12	1.23	1 (20%)
2	HYP	G	29	2	7,8,9	0.53	0	5,10,12	1.24	1 (20%)
1	HYP	B	1857	1	7,8,9	0.57	0	5,10,12	1.63	2 (40%)
2	HYP	G	47	2	7,8,9	0.61	0	5,10,12	1.31	1 (20%)
2	HYP	G	45	2	7,8,9	0.59	0	5,10,12	1.29	1 (20%)
1	HYP	D	1910	1	7,8,9	0.50	0	5,10,12	1.17	1 (20%)
1	HYP	F	1870	1	7,8,9	0.52	0	5,10,12	1.60	1 (20%)
1	HYP	A	1929	1	7,8,9	0.62	0	5,10,12	1.27	1 (20%)
1	HYP	E	1863	1	7,8,9	0.54	0	5,10,12	1.44	1 (20%)
1	HYP	C	1912	1	7,8,9	0.56	0	5,10,12	1.21	1 (20%)
1	HYP	A	1928	1	7,8,9	0.56	0	5,10,12	1.16	1 (20%)
1	HYP	F	1868	1	7,8,9	0.58	0	5,10,12	2.08	3 (60%)
1	HYP	E	1932	1	7,8,9	0.54	0	5,10,12	1.48	1 (20%)
1	HYP	E	1910	1	7,8,9	0.52	0	5,10,12	1.22	1 (20%)
1	HYP	A	1921	1	7,8,9	0.66	0	5,10,12	1.42	1 (20%)
1	HYP	E	1918	1	7,8,9	0.54	0	5,10,12	1.73	2 (40%)
1	HYP	A	1893	1	7,8,9	0.61	0	5,10,12	1.32	1 (20%)
1	HYP	B	1867	1	7,8,9	0.51	0	5,10,12	1.67	1 (20%)
1	HYP	C	1910	1	7,8,9	0.55	0	5,10,12	1.20	1 (20%)
1	HYP	D	1922	1	7,8,9	0.56	0	5,10,12	1.42	1 (20%)
2	HYP	I	4	2	7,8,9	0.54	0	5,10,12	1.29	1 (20%)
1	HYP	F	1902	1	7,8,9	0.57	0	5,10,12	1.72	2 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	HYP	B	1856	1	7,8,9	0.50	0	5,10,12	1.28	1 (20%)
1	HYP	D	1931	1	7,8,9	0.54	0	5,10,12	1.41	1 (20%)
2	HYP	H	52	2	7,8,9	0.52	0	5,10,12	1.77	2 (40%)
1	HYP	F	1910	1	7,8,9	0.52	0	5,10,12	1.16	1 (20%)
2	HYP	G	50	2	7,8,9	0.58	0	5,10,12	1.21	1 (20%)
1	HYP	F	1882	1	7,8,9	0.53	0	5,10,12	1.20	1 (20%)
2	HYP	H	40	2	7,8,9	0.51	0	5,10,12	1.15	1 (20%)
2	HYP	I	23	2	7,8,9	0.42	0	5,10,12	1.45	1 (20%)
1	HYP	B	1905	1	7,8,9	0.59	0	5,10,12	1.23	1 (20%)
1	HYP	C	1931	1	7,8,9	0.56	0	5,10,12	1.40	1 (20%)
1	HYP	B	1898	1	7,8,9	0.64	0	5,10,12	1.29	1 (20%)
2	HYP	H	56	2	7,8,9	0.53	0	5,10,12	1.26	1 (20%)
1	HYP	E	1887	1	7,8,9	0.53	0	5,10,12	1.25	1 (20%)
1	HYP	A	1892	1	7,8,9	0.56	0	5,10,12	1.39	1 (20%)
1	HYP	A	1899	1	7,8,9	0.65	0	5,10,12	1.44	1 (20%)
1	HYP	C	1916	1	7,8,9	0.56	0	5,10,12	1.19	1 (20%)
1	HYP	F	1883	1	7,8,9	0.53	0	5,10,12	2.03	2 (40%)
1	HYP	F	1921	1	7,8,9	0.61	0	5,10,12	1.38	1 (20%)
2	HYP	G	11	2	7,8,9	0.51	0	5,10,12	1.98	2 (40%)
2	HYP	I	3	2	7,8,9	0.54	0	5,10,12	1.66	2 (40%)
1	HYP	B	1911	1	7,8,9	0.57	0	5,10,12	1.21	1 (20%)
1	HYP	A	1858	1	7,8,9	0.56	0	5,10,12	1.26	1 (20%)
2	HYP	I	20	2	7,8,9	0.55	0	5,10,12	1.28	1 (20%)
2	HYP	G	26	2	7,8,9	0.55	0	5,10,12	1.19	1 (20%)
1	HYP	F	1912	1	7,8,9	0.57	0	5,10,12	1.17	1 (20%)
1	HYP	E	1882	1	7,8,9	0.53	0	5,10,12	1.26	1 (20%)
1	HYP	E	1873	1	7,8,9	0.47	0	5,10,12	1.34	1 (20%)
2	HYP	I	10	2	7,8,9	0.57	0	5,10,12	1.73	1 (20%)
1	HYP	B	1914	1	7,8,9	0.53	0	5,10,12	1.55	1 (20%)
1	HYP	E	1906	1	7,8,9	0.56	0	5,10,12	1.26	1 (20%)
1	HYP	B	1913	1	7,8,9	0.62	0	5,10,12	1.34	1 (20%)
1	HYP	B	1931	1	7,8,9	0.56	0	5,10,12	1.43	1 (20%)
1	HYP	E	1860	1	7,8,9	0.57	0	5,10,12	1.92	3 (60%)
1	HYP	E	1867	1	7,8,9	0.58	0	5,10,12	1.82	2 (40%)
1	HYP	E	1922	1	7,8,9	0.62	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
2	HYP	G	48	2	7,8,9	0.59	0	5,10,12	1.23	1 (20%)
2	HYP	G	20	2	7,8,9	0.54	0	5,10,12	1.33	1 (20%)
1	HYP	C	1918	1	7,8,9	0.56	0	5,10,12	1.81	2 (40%)
1	HYP	E	1856	1	7,8,9	0.54	0	5,10,12	1.32	1 (20%)
1	HYP	F	1892	1	7,8,9	0.57	0	5,10,12	1.28	1 (20%)
1	HYP	F	1923	1	7,8,9	0.56	0	5,10,12	2.15	3 (60%)
2	HYP	G	52	2	7,8,9	0.55	0	5,10,12	1.68	2 (40%)
1	HYP	F	1888	1	7,8,9	0.50	0	5,10,12	1.90	2 (40%)
1	HYP	F	1932	1	7,8,9	0.50	0	5,10,12	1.75	2 (40%)
1	HYP	E	1921	1	7,8,9	0.60	0	5,10,12	1.35	1 (20%)
1	HYP	A	1877	1	7,8,9	0.50	0	5,10,12	1.34	1 (20%)
1	HYP	D	1917	1	7,8,9	0.57	0	5,10,12	1.53	1 (20%)
1	HYP	B	1915	1	7,8,9	0.57	0	5,10,12	1.29	1 (20%)
1	HYP	F	1918	1	7,8,9	0.53	0	5,10,12	2.04	2 (40%)
1	HYP	A	1865	1	7,8,9	0.56	0	5,10,12	1.68	1 (20%)
1	HYP	E	1920	1	7,8,9	0.56	0	5,10,12	1.47	1 (20%)
1	HYP	E	1923	1	7,8,9	0.53	0	5,10,12	2.15	2 (40%)
1	HYP	B	1860	1	7,8,9	0.51	0	5,10,12	1.75	3 (60%)
1	HYP	A	1862	1	7,8,9	0.54	0	5,10,12	1.45	1 (20%)
2	HYP	H	50	2	7,8,9	0.57	0	5,10,12	1.23	1 (20%)
1	HYP	E	1915	1	7,8,9	0.52	0	5,10,12	1.17	1 (20%)
1	HYP	A	1931	1	7,8,9	0.58	0	5,10,12	1.43	1 (20%)
1	HYP	A	1868	1	7,8,9	0.56	0	5,10,12	1.98	3 (60%)
1	HYP	E	1930	1	7,8,9	0.59	0	5,10,12	1.24	1 (20%)
1	HYP	F	1927	1	7,8,9	0.53	0	5,10,12	1.18	1 (20%)
1	HYP	F	1887	1	7,8,9	0.54	0	5,10,12	1.19	1 (20%)
1	HYP	B	1921	1	7,8,9	0.61	0	5,10,12	1.25	1 (20%)
1	HYP	F	1857	1	7,8,9	0.56	0	5,10,12	1.61	1 (20%)
1	HYP	D	1916	1	7,8,9	0.57	0	5,10,12	1.40	1 (20%)
2	HYP	I	26	2	7,8,9	0.54	0	5,10,12	1.51	2 (40%)
2	HYP	I	17	2	7,8,9	0.56	0	5,10,12	1.24	1 (20%)
1	HYP	A	1857	1	7,8,9	0.57	0	5,10,12	1.34	1 (20%)
2	HYP	I	33	2	7,8,9	0.51	0	5,10,12	1.27	1 (20%)
1	HYP	A	1902	1	7,8,9	0.61	0	5,10,12	1.63	1 (20%)
1	HYP	F	1873	1	7,8,9	0.46	0	5,10,12	1.29	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	HYP	A	1906	1	7,8,9	0.59	0	5,10,12	1.39	1 (20%)
2	HYP	G	2	2	7,8,9	0.55	0	5,10,12	1.66	2 (40%)
2	HYP	I	29	2	7,8,9	0.54	0	5,10,12	1.22	1 (20%)
1	HYP	B	1855	1	7,8,9	0.54	0	5,10,12	1.20	1 (20%)
1	HYP	B	1930	1	7,8,9	0.60	0	5,10,12	1.65	1 (20%)
2	HYP	I	1	2	7,8,9	0.50	0	5,10,12	1.27	1 (20%)
2	HYP	H	42	2	7,8,9	0.56	0	5,10,12	1.26	1 (20%)
1	HYP	F	1906	1	7,8,9	0.55	0	5,10,12	1.33	1 (20%)
1	HYP	C	1898	1	7,8,9	0.56	0	5,10,12	1.22	1 (20%)
1	HYP	E	1907	1	7,8,9	0.54	0	5,10,12	1.67	2 (40%)
2	HYP	G	6	2	7,8,9	0.49	0	5,10,12	1.54	1 (20%)
1	HYP	C	1915	1	7,8,9	0.57	0	5,10,12	1.23	1 (20%)
1	HYP	E	1901	1	7,8,9	0.55	0	5,10,12	1.44	1 (20%)
1	HYP	B	1920	1	7,8,9	0.57	0	5,10,12	1.39	1 (20%)
1	HYP	B	1885	1	7,8,9	0.58	0	5,10,12	1.19	1 (20%)
1	HYP	B	1899	1	7,8,9	0.64	0	5,10,12	1.47	1 (20%)
1	HYP	B	1918	1	7,8,9	0.61	0	5,10,12	1.62	1 (20%)
1	HYP	A	1872	1	7,8,9	0.53	0	5,10,12	1.33	1 (20%)
1	HYP	E	1927	1	7,8,9	0.55	0	5,10,12	1.22	1 (20%)
2	HYP	G	37	2	7,8,9	0.55	0	5,10,12	0.98	1 (20%)
1	HYP	E	1875	1	7,8,9	0.55	0	5,10,12	1.20	1 (20%)
1	HYP	C	1922	1	7,8,9	0.57	0	5,10,12	1.49	1 (20%)
1	HYP	C	1914	1	7,8,9	0.53	0	5,10,12	1.44	1 (20%)
1	HYP	B	1882	1	7,8,9	0.53	0	5,10,12	1.24	1 (20%)
1	HYP	A	1930	1	7,8,9	0.58	0	5,10,12	1.69	1 (20%)
1	HYP	E	1866	1	7,8,9	0.59	0	5,10,12	1.43	1 (20%)
1	HYP	B	1902	1	7,8,9	0.59	0	5,10,12	1.62	1 (20%)
1	HYP	F	1875	1	7,8,9	0.55	0	5,10,12	1.18	1 (20%)
1	HYP	E	1905	1	7,8,9	0.55	0	5,10,12	1.26	1 (20%)
2	HYP	G	51	2	7,8,9	0.57	0	5,10,12	1.62	1 (20%)
1	HYP	A	1908	1	7,8,9	0.52	0	5,10,12	2.25	3 (60%)
1	HYP	F	1878	1	7,8,9	0.57	0	5,10,12	1.57	2 (40%)
1	HYP	B	1893	1	7,8,9	0.56	0	5,10,12	1.26	1 (20%)
1	HYP	C	1929	1	7,8,9	0.63	0	5,10,12	1.30	1 (20%)
1	HYP	C	1928	1	7,8,9	0.61	0	5,10,12	1.30	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	HYP	D	1898	1	7,8,9	0.56	0	5,10,12	1.26	1 (20%)
1	HYP	F	1866	1	7,8,9	0.57	0	5,10,12	1.37	1 (20%)
1	HYP	C	1921	1	7,8,9	0.57	0	5,10,12	1.23	1 (20%)
2	HYP	H	37	2	7,8,9	0.56	0	5,10,12	1.16	1 (20%)
1	HYP	D	1912	1	7,8,9	0.56	0	5,10,12	1.33	1 (20%)
1	HYP	A	1888	1	7,8,9	0.54	0	5,10,12	1.55	1 (20%)
2	HYP	I	6	2	7,8,9	0.53	0	5,10,12	1.32	1 (20%)
1	HYP	D	1915	1	7,8,9	0.56	0	5,10,12	1.26	1 (20%)
1	HYP	A	1932	1	7,8,9	0.54	0	5,10,12	1.82	3 (60%)
1	HYP	D	1929	1	7,8,9	0.59	0	5,10,12	1.24	1 (20%)
1	HYP	F	1897	1	7,8,9	0.55	0	5,10,12	1.30	1 (20%)
2	HYP	H	51	2	7,8,9	0.53	0	5,10,12	1.64	1 (20%)
1	HYP	D	1899	1	7,8,9	0.52	0	5,10,12	1.73	2 (40%)
1	HYP	E	1878	1	7,8,9	0.51	0	5,10,12	1.96	2 (40%)
1	HYP	A	1897	1	7,8,9	0.55	0	5,10,12	1.29	1 (20%)
1	HYP	A	1922	1	7,8,9	0.61	0	5,10,12	1.76	1 (20%)
1	HYP	A	1875	1	7,8,9	0.58	0	5,10,12	1.21	1 (20%)
1	HYP	E	1894	1	7,8,9	0.59	0	5,10,12	1.29	1 (20%)
1	HYP	B	1862	1	7,8,9	0.53	0	5,10,12	1.48	1 (20%)
2	HYP	I	8	2	7,8,9	0.55	0	5,10,12	1.52	1 (20%)
2	HYP	G	10	2	7,8,9	0.62	0	5,10,12	1.67	1 (20%)
1	HYP	F	1911	1	7,8,9	0.54	0	5,10,12	1.18	1 (20%)
2	HYP	G	7	2	7,8,9	0.63	0	5,10,12	1.41	1 (20%)
1	HYP	C	1932	1	7,8,9	0.55	0	5,10,12	1.89	2 (40%)
1	HYP	B	1868	1	7,8,9	0.52	0	5,10,12	2.03	3 (60%)
1	HYP	B	1916	1	7,8,9	0.58	0	5,10,12	1.47	1 (20%)
2	HYP	H	45	2	7,8,9	0.55	0	5,10,12	1.22	1 (20%)
1	HYP	D	1903	1	7,8,9	0.57	0	5,10,12	1.78	2 (40%)
2	HYP	G	3	2	7,8,9	0.56	0	5,10,12	1.64	2 (40%)
1	HYP	E	1931	1	7,8,9	0.55	0	5,10,12	1.35	1 (20%)
2	HYP	I	34	2	7,8,9	0.52	0	5,10,12	1.63	1 (20%)
1	HYP	B	1912	1	7,8,9	0.59	0	5,10,12	1.28	1 (20%)
1	HYP	E	1928	1	7,8,9	0.54	0	5,10,12	1.25	1 (20%)
1	HYP	D	1928	1	7,8,9	0.57	0	5,10,12	1.16	1 (20%)
1	HYP	F	1931	1	7,8,9	0.54	0	5,10,12	1.39	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	HYP	E	1857	1	7,8,9	0.54	0	5,10,12	1.59	1 (20%)
2	HYP	I	9	2	7,8,9	0.52	0	5,10,12	1.58	1 (20%)
1	HYP	A	1855	1	7,8,9	0.61	0	5,10,12	1.20	1 (20%)
1	HYP	E	1890	1	7,8,9	0.55	0	5,10,12	1.15	1 (20%)
1	HYP	A	1873	1	7,8,9	0.50	0	5,10,12	1.23	1 (20%)
1	HYP	C	1902	1	7,8,9	0.57	0	5,10,12	1.81	2 (40%)
2	HYP	H	49	2	7,8,9	0.59	0	5,10,12	1.49	1 (20%)
1	HYP	A	1860	1	7,8,9	0.53	0	5,10,12	1.82	3 (60%)
1	HYP	C	1923	1	7,8,9	0.57	0	5,10,12	1.99	3 (60%)
2	HYP	I	32	2	7,8,9	0.50	0	5,10,12	1.18	1 (20%)
2	HYP	H	46	2	7,8,9	0.51	0	5,10,12	1.63	1 (20%)
2	HYP	H	44	2	7,8,9	0.54	0	5,10,12	1.67	1 (20%)
1	HYP	B	1863	1	7,8,9	0.54	0	5,10,12	1.45	1 (20%)
1	HYP	B	1880	1	7,8,9	0.54	0	5,10,12	1.38	1 (20%)
2	HYP	G	14	2	7,8,9	0.57	0	5,10,12	1.37	1 (20%)
2	HYP	H	47	2	7,8,9	0.59	0	5,10,12	1.30	1 (20%)
1	HYP	B	1878	1	7,8,9	0.54	0	5,10,12	1.88	2 (40%)
1	HYP	F	1864	1	7,8,9	0.55	0	5,10,12	1.45	1 (20%)
1	HYP	B	1923	1	7,8,9	0.57	0	5,10,12	2.02	3 (60%)
1	HYP	A	1923	1	7,8,9	0.55	0	5,10,12	1.93	3 (60%)
2	HYP	G	55	2	7,8,9	0.53	0	5,10,12	1.21	1 (20%)
1	HYP	B	1922	1	7,8,9	0.60	0	5,10,12	1.64	1 (20%)
1	HYP	E	1903	1	7,8,9	0.54	0	5,10,12	1.92	3 (60%)
1	HYP	B	1932	1	7,8,9	0.54	0	5,10,12	1.57	1 (20%)
1	HYP	F	1922	1	7,8,9	0.60	0	5,10,12	1.60	1 (20%)
1	HYP	A	1863	1	7,8,9	0.49	0	5,10,12	1.38	1 (20%)
1	HYP	A	1927	1	7,8,9	0.55	0	5,10,12	1.43	1 (20%)
1	HYP	F	1880	1	7,8,9	0.53	0	5,10,12	1.44	1 (20%)
1	HYP	D	1927	1	7,8,9	0.55	0	5,10,12	1.23	1 (20%)
1	HYP	E	1872	1	7,8,9	0.59	0	5,10,12	1.29	1 (20%)
2	HYP	G	44	2	7,8,9	0.56	0	5,10,12	1.55	1 (20%)
1	HYP	D	1913	1	7,8,9	0.56	0	5,10,12	1.26	1 (20%)
2	HYP	G	42	2	7,8,9	0.61	0	5,10,12	1.29	1 (20%)
1	HYP	D	1902	1	7,8,9	0.52	0	5,10,12	1.77	2 (40%)
1	HYP	C	1908	1	7,8,9	0.54	0	5,10,12	1.96	3 (60%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	HYP	F	1901	1	7,8,9	0.53	0	5,10,12	1.18	1 (20%)
1	HYP	F	1908	1	7,8,9	0.57	0	5,10,12	1.84	2 (40%)
2	HYP	I	11	2	7,8,9	0.50	0	5,10,12	1.84	2 (40%)
1	HYP	C	1920	1	7,8,9	0.56	0	5,10,12	1.49	1 (20%)
1	HYP	F	1860	1	7,8,9	0.59	0	5,10,12	1.59	2 (40%)
1	HYP	F	1867	1	7,8,9	0.54	0	5,10,12	1.67	1 (20%)
1	HYP	A	1907	1	7,8,9	0.53	0	5,10,12	1.91	2 (40%)
1	HYP	D	1906	1	7,8,9	0.54	0	5,10,12	1.37	1 (20%)
1	HYP	A	1901	1	7,8,9	0.58	0	5,10,12	1.19	1 (20%)
1	HYP	F	1856	1	7,8,9	0.56	0	5,10,12	1.37	1 (20%)
2	HYP	I	14	2	7,8,9	0.57	0	5,10,12	1.31	1 (20%)
1	HYP	D	1901	1	7,8,9	0.56	0	5,10,12	1.22	1 (20%)
1	HYP	F	1858	1	7,8,9	0.57	0	5,10,12	1.72	2 (40%)
1	HYP	C	1930	1	7,8,9	0.60	0	5,10,12	1.76	2 (40%)
1	HYP	E	1897	1	7,8,9	0.52	0	5,10,12	1.22	1 (20%)
2	HYP	H	55	2	7,8,9	0.52	0	5,10,12	1.22	1 (20%)
1	HYP	F	1903	1	7,8,9	0.57	0	5,10,12	1.74	2 (40%)
1	HYP	C	1907	1	7,8,9	0.55	0	5,10,12	1.77	2 (40%)
1	HYP	B	1883	1	7,8,9	0.54	0	5,10,12	2.07	2 (40%)
2	HYP	H	41	2	7,8,9	0.54	0	5,10,12	1.30	1 (20%)
1	HYP	E	1885	1	7,8,9	0.53	0	5,10,12	1.41	1 (20%)
1	HYP	A	1864	1	7,8,9	0.54	0	5,10,12	1.50	1 (20%)
2	HYP	G	4	2	7,8,9	0.59	0	5,10,12	1.40	1 (20%)
1	HYP	A	1905	1	7,8,9	0.60	0	5,10,12	1.24	1 (20%)
1	HYP	B	1872	1	7,8,9	0.49	0	5,10,12	1.35	1 (20%)
1	HYP	E	1913	1	7,8,9	0.56	0	5,10,12	1.22	1 (20%)
1	HYP	F	1907	1	7,8,9	0.55	0	5,10,12	1.78	3 (60%)
1	HYP	D	1930	1	7,8,9	0.63	0	5,10,12	1.30	1 (20%)
2	HYP	G	40	2	7,8,9	0.50	0	5,10,12	1.18	1 (20%)
1	HYP	F	1920	1	7,8,9	0.56	0	5,10,12	1.58	2 (40%)
1	HYP	B	1906	1	7,8,9	0.59	0	5,10,12	1.20	1 (20%)
2	HYP	H	43	2	7,8,9	0.55	0	5,10,12	1.50	1 (20%)
1	HYP	B	1865	1	7,8,9	0.53	0	5,10,12	1.71	1 (20%)
1	HYP	F	1913	1	7,8,9	0.55	0	5,10,12	1.28	1 (20%)
2	HYP	G	23	2	7,8,9	0.44	0	5,10,12	1.51	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	HYP	A	1920	1	7,8,9	0.55	0	5,10,12	1.58	1 (20%)
1	HYP	E	1917	1	7,8,9	0.56	0	5,10,12	1.40	1 (20%)
1	HYP	E	1883	1	7,8,9	0.55	0	5,10,12	2.08	2 (40%)
2	HYP	I	5	2	7,8,9	0.55	0	5,10,12	1.47	1 (20%)
2	HYP	G	34	2	7,8,9	0.51	0	5,10,12	1.70	2 (40%)
1	HYP	E	1868	1	7,8,9	0.57	0	5,10,12	1.83	2 (40%)
1	HYP	B	1903	1	7,8,9	0.57	0	5,10,12	1.97	3 (60%)

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
1	HYP	C	1906	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1866	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	1880	1	-	0/0/11/13	0/1/1/1
2	HYP	G	9	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1878	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1914	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1911	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1914	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1897	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	1894	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1898	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1903	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1912	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1932	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1865	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1918	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1873	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1870	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	46	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1887	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1893	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1898	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1917	1	-	0/0/11/13	0/1/1/1
2	HYP	G	32	2	-	0/0/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	HYP	A	1883	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	1902	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1894	1	-	0/0/11/13	0/1/1/1
1	HYP	C	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	B	1907	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1916	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1914	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1899	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1908	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1888	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1875	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1888	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1929	1	-	0/0/11/13	0/1/1/1
2	HYP	G	1	2	-	0/0/11/13	0/1/1/1
1	HYP	E	1899	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1877	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1855	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1927	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1929	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1865	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1921	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1903	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	1887	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1923	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1910	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1910	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	1918	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1866	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1893	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	1897	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1877	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1892	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1890	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1908	1	-	0/0/11/13	0/1/1/1
2	HYP	I	2	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1916	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1890	1	-	0/0/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	HYP	E	1862	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1858	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1916	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	1877	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1892	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1855	1	-	0/0/11/13	0/1/1/1
2	HYP	G	41	2	-	0/0/11/13	0/1/1/1
1	HYP	C	1911	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1897	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1885	1	-	0/0/11/13	0/1/1/1
2	HYP	G	5	2	-	0/0/11/13	0/1/1/1
2	HYP	G	17	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1870	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1913	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1858	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1885	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1901	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1911	1	-	0/0/11/13	0/1/1/1
2	HYP	H	48	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1867	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1901	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	1856	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1905	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	1912	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1930	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1913	1	-	0/0/11/13	0/1/1/1
2	HYP	G	8	2	-	0/0/11/13	0/1/1/1
2	HYP	G	43	2	-	0/0/11/13	0/1/1/1
2	HYP	I	7	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1890	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1872	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1908	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1915	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1907	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	1917	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1915	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1864	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1863	1	-	0/0/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	HYP	F	1862	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1880	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1864	1	-	0/0/11/13	0/1/1/1
2	HYP	G	49	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1914	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1920	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	1898	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1927	1	-	0/0/11/13	0/1/1/1
2	HYP	G	29	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1857	1	-	0/0/11/13	0/1/1/1
2	HYP	G	47	2	-	0/0/11/13	0/1/1/1
2	HYP	G	45	2	-	0/0/11/13	0/1/1/1
1	HYP	D	1910	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1870	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1929	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1863	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1912	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1928	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1868	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1932	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1910	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1921	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1918	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	1867	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1910	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1922	1	-	0/0/11/13	0/1/1/1
2	HYP	I	4	2	-	0/0/11/13	0/1/1/1
1	HYP	F	1902	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1856	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1931	1	-	0/0/11/13	0/1/1/1
2	HYP	H	52	2	-	0/0/11/13	0/1/1/1
1	HYP	F	1910	1	-	0/0/11/13	0/1/1/1
2	HYP	G	50	2	-	0/0/11/13	0/1/1/1
1	HYP	F	1882	1	-	0/0/11/13	0/1/1/1
2	HYP	H	40	2	-	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
1	HYP	B	1905	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1931	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1898	1	-	0/0/11/13	0/1/1/1
2	HYP	H	56	2	-	0/0/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	HYP	E	1887	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	1899	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1916	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1883	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1921	1	-	0/0/11/13	0/1/1/1
2	HYP	G	11	2	-	0/0/11/13	0/1/1/1
2	HYP	I	3	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1911	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1858	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
2	HYP	I	20	2	-	0/0/11/13	0/1/1/1
1	HYP	F	1912	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1882	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1873	1	-	0/0/11/13	0/1/1/1
2	HYP	I	10	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1914	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1906	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1913	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1931	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1860	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1867	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	48	2	-	0/0/11/13	0/1/1/1
2	HYP	G	20	2	-	0/0/11/13	0/1/1/1
1	HYP	C	1918	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1856	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1892	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	52	2	-	0/0/11/13	0/1/1/1
1	HYP	F	1888	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1932	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	1877	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1917	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1915	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1918	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1865	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1920	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1923	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1860	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1862	1	-	0/0/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HYP	H	50	2	-	0/0/11/13	0/1/1/1
1	HYP	E	1915	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1931	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1868	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1930	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1927	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1887	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1921	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1857	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1916	1	-	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
2	HYP	I	17	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1857	1	-	0/0/11/13	0/1/1/1
2	HYP	I	33	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1902	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1873	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1906	1	-	0/0/11/13	0/1/1/1
2	HYP	G	2	2	-	0/0/11/13	0/1/1/1
2	HYP	I	29	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1855	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1930	1	-	0/0/11/13	0/1/1/1
2	HYP	I	1	2	-	0/0/11/13	0/1/1/1
2	HYP	H	42	2	-	0/0/11/13	0/1/1/1
1	HYP	F	1906	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1898	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1907	1	-	0/0/11/13	0/1/1/1
2	HYP	G	6	2	-	0/0/11/13	0/1/1/1
1	HYP	C	1915	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1901	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1920	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1885	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1899	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	1872	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1927	1	-	0/0/11/13	0/1/1/1
2	HYP	G	37	2	-	0/0/11/13	0/1/1/1
1	HYP	E	1875	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1922	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1914	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1882	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1930	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1866	1	-	0/0/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	HYP	B	1902	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1875	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	51	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1908	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1878	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1893	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1929	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1928	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	1866	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1921	1	-	0/0/11/13	0/1/1/1
2	HYP	H	37	2	-	0/0/11/13	0/1/1/1
1	HYP	D	1912	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1888	1	-	0/0/11/13	0/1/1/1
2	HYP	I	6	2	-	0/0/11/13	0/1/1/1
1	HYP	D	1915	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1932	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1929	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1897	1	-	0/0/11/13	0/1/1/1
2	HYP	H	51	2	-	0/0/11/13	0/1/1/1
1	HYP	D	1899	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1878	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1897	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1922	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1875	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1894	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1862	1	-	0/0/11/13	0/1/1/1
2	HYP	I	8	2	-	0/0/11/13	0/1/1/1
2	HYP	G	10	2	-	0/0/11/13	0/1/1/1
1	HYP	F	1911	1	-	0/0/11/13	0/1/1/1
2	HYP	G	7	2	-	0/0/11/13	0/1/1/1
1	HYP	C	1932	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1868	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1916	1	-	0/0/11/13	0/1/1/1
2	HYP	H	45	2	-	0/0/11/13	0/1/1/1
1	HYP	D	1903	1	-	0/0/11/13	0/1/1/1
2	HYP	G	3	2	-	0/0/11/13	0/1/1/1
1	HYP	E	1931	1	-	0/0/11/13	0/1/1/1
2	HYP	I	34	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1912	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1928	1	-	0/0/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	HYP	D	1928	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1931	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1857	1	-	0/0/11/13	0/1/1/1
2	HYP	I	9	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1855	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1890	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1873	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1902	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	1860	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1923	1	-	0/0/11/13	0/1/1/1
2	HYP	I	32	2	-	0/0/11/13	0/1/1/1
2	HYP	H	46	2	-	0/0/11/13	0/1/1/1
2	HYP	H	44	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1863	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1880	1	-	0/0/11/13	0/1/1/1
2	HYP	G	14	2	-	0/0/11/13	0/1/1/1
2	HYP	H	47	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1878	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1864	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1923	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1923	1	-	0/0/11/13	0/1/1/1
2	HYP	G	55	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1922	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1903	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1932	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1922	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1863	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1927	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1880	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1927	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1872	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	1913	1	-	0/0/11/13	0/1/1/1
2	HYP	G	42	2	-	0/0/11/13	0/1/1/1
1	HYP	D	1902	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1908	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1901	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1908	1	-	0/0/11/13	0/1/1/1
2	HYP	I	11	2	-	0/0/11/13	0/1/1/1
1	HYP	C	1920	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1860	1	-	0/0/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	HYP	F	1867	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1907	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1906	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1901	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	14	2	-	0/0/11/13	0/1/1/1
1	HYP	D	1901	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1858	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1930	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1897	1	-	0/0/11/13	0/1/1/1
2	HYP	H	55	2	-	0/0/11/13	0/1/1/1
1	HYP	F	1903	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1907	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1883	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	1885	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1864	1	-	0/0/11/13	0/1/1/1
2	HYP	G	4	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1905	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1872	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1913	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1907	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1930	1	-	0/0/11/13	0/1/1/1
2	HYP	G	40	2	-	0/0/11/13	0/1/1/1
1	HYP	F	1920	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1906	1	-	0/0/11/13	0/1/1/1
2	HYP	H	43	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1865	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1913	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
1	HYP	A	1920	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1917	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1883	1	-	0/0/11/13	0/1/1/1
2	HYP	I	5	2	-	0/0/11/13	0/1/1/1
2	HYP	G	34	2	-	0/0/11/13	0/1/1/1
1	HYP	E	1868	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1903	1	-	0/0/11/13	0/1/1/1

There are no bond length outliers.

The worst 5 of 454 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	1883	HYP	CG-CB-CA	-3.64	99.55	103.75
1	A	1883	HYP	CG-CB-CA	-3.60	99.59	103.75
1	E	1923	HYP	CG-CB-CA	-3.50	99.71	103.75
1	F	1918	HYP	CG-CB-CA	-3.43	99.79	103.75
1	B	1883	HYP	CG-CB-CA	-3.39	99.84	103.75

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	0.55	0	11,12,14	1.13	1 (9%)
3	FUB	0	2	3	9,9,10	0.52	0	11,12,14	0.88	0
3	FUB	0	3	3	9,9,10	0.55	0	11,12,14	0.93	0
3	FUB	0A	1	3	9,9,10	0.54	0	11,12,14	0.95	1 (9%)
3	FUB	0A	2	3	9,9,10	0.52	0	11,12,14	0.77	0
3	FUB	0A	3	3	9,9,10	0.53	0	11,12,14	0.88	0
6	FUB	0B	1	6	9,9,10	0.54	0	11,12,14	0.99	0
6	FUB	0B	2	6	9,9,10	0.55	0	11,12,14	1.20	2 (18%)
6	GZL	0B	3	6	11,11,12	6.84	6 (54%)	13,15,17	4.19	4 (30%)
6	FUB	0C	1	6	9,9,10	0.56	0	11,12,14	0.83	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	0.54	0	11,12,14	1.11	1 (9%)
6	GZL	0C	3	6	11,11,12	6.56	7 (63%)	13,15,17	1.46	2 (15%)
13	FUB	0D	1	13	9,9,10	0.56	0	11,12,14	0.86	0
13	FUB	0D	2	13	9,9,10	0.54	0	11,12,14	1.03	0
13	GZL	0D	3	13	11,11,12	6.56	7 (63%)	13,15,17	1.43	2 (15%)
13	AHR	0D	4	13	9,9,10	0.54	0	11,12,14	0.88	0
18	FUB	0E	1	18	9,9,10	0.57	0	11,12,14	0.98	0
18	FUB	0E	2	18	9,9,10	0.54	0	11,12,14	0.87	0
18	GZL	0E	3	18	11,11,12	6.59	7 (63%)	13,15,17	1.33	1 (7%)
18	AHR	0E	4	18	9,9,10	0.56	0	11,12,14	0.95	0
18	AHR	0E	5	18	9,9,10	0.55	0	11,12,14	1.04	1 (9%)
3	FUB	1	1	3	9,9,10	0.55	0	11,12,14	0.83	0
3	FUB	1	2	3	9,9,10	0.54	0	11,12,14	0.92	0
3	FUB	1	3	3	9,9,10	0.53	0	11,12,14	0.97	1 (9%)
10	FUB	1A	1	10	9,9,10	0.50	0	11,12,14	1.05	1 (9%)
10	FUB	1A	2	10	9,9,10	0.52	0	11,12,14	0.76	0
10	FUB	1A	3	10	9,9,10	0.54	0	11,12,14	1.08	1 (9%)
10	AHR	1A	4	10	9,9,10	0.55	0	11,12,14	0.84	1 (9%)
10	AHR	1A	5	10	9,9,10	0.55	0	11,12,14	0.87	1 (9%)
13	FUB	1B	1	13	9,9,10	0.53	0	11,12,14	0.84	0
13	FUB	1B	2	13	9,9,10	0.55	0	11,12,14	0.88	0
13	GZL	1B	3	13	11,11,12	6.63	7 (63%)	13,15,17	1.36	1 (7%)
13	AHR	1B	4	13	9,9,10	0.55	0	11,12,14	0.96	0
6	FUB	1C	1	6	9,9,10	0.53	0	11,12,14	0.71	0
6	FUB	1C	2	6	9,9,10	0.55	0	11,12,14	0.88	0
6	GZL	1C	3	6	11,11,12	6.58	7 (63%)	13,15,17	1.46	1 (7%)
15	FUB	1D	1	15	9,9,10	0.55	0	11,12,14	0.97	0
15	FUB	1D	2	15	9,9,10	0.56	0	11,12,14	0.95	0
15	GZL	1D	3	15	11,11,12	6.60	7 (63%)	13,15,17	1.29	1 (7%)
15	AHR	1D	4	15	9,9,10	0.54	0	11,12,14	0.99	1 (9%)
15	AHR	1D	5	15	9,9,10	0.54	0	11,12,14	1.07	1 (9%)
19	FUB	1E	1	19	9,9,10	0.53	0	11,12,14	1.06	1 (9%)
19	FUB	1E	2	19	9,9,10	0.55	0	11,12,14	0.98	1 (9%)
19	GZL	1E	3	19	11,11,12	6.58	7 (63%)	13,15,17	1.47	1 (7%)
19	AHR	1E	4	19	9,9,10	0.54	0	11,12,14	1.07	1 (9%)
3	FUB	2	1	3	9,9,10	0.53	0	11,12,14	0.95	0
3	FUB	2	2	3	9,9,10	0.51	0	11,12,14	0.74	0
3	FUB	2	3	3	9,9,10	0.54	0	11,12,14	0.97	0

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	0.53	0	11,12,14	1.04	1 (9%)
13	FUB	2A	2	13	9,9,10	0.45	0	11,12,14	1.30	2 (18%)
13	GZL	2A	3	13	11,11,12	6.71	6 (54%)	13,15,17	1.01	0
13	AHR	2A	4	13	9,9,10	0.56	0	11,12,14	1.06	1 (9%)
13	FUB	2B	1	13	9,9,10	0.54	0	11,12,14	1.01	0
13	FUB	2B	2	13	9,9,10	0.54	0	11,12,14	0.87	0
13	GZL	2B	3	13	11,11,12	6.57	7 (63%)	13,15,17	1.48	2 (15%)
13	AHR	2B	4	13	9,9,10	0.55	0	11,12,14	0.98	1 (9%)
6	FUB	2C	1	6	9,9,10	0.57	0	11,12,14	0.91	0
6	FUB	2C	2	6	9,9,10	0.56	0	11,12,14	1.05	1 (9%)
6	GZL	2C	3	6	11,11,12	6.57	7 (63%)	13,15,17	1.42	1 (7%)
15	FUB	2D	1	15	9,9,10	0.55	0	11,12,14	1.01	1 (9%)
15	FUB	2D	2	15	9,9,10	0.56	0	11,12,14	0.89	0
15	GZL	2D	3	15	11,11,12	6.60	7 (63%)	13,15,17	1.36	1 (7%)
15	AHR	2D	4	15	9,9,10	0.53	0	11,12,14	1.02	1 (9%)
15	AHR	2D	5	15	9,9,10	0.56	0	11,12,14	0.96	0
10	FUB	3	1	10	9,9,10	0.53	0	11,12,14	1.05	1 (9%)
10	FUB	3	2	10	9,9,10	0.52	0	11,12,14	0.68	0
10	FUB	3	3	10	9,9,10	0.58	0	11,12,14	1.06	1 (9%)
10	AHR	3	4	10	9,9,10	0.54	0	11,12,14	0.92	0
10	AHR	3	5	10	9,9,10	0.55	0	11,12,14	0.80	1 (9%)
6	FUB	3A	1	6	9,9,10	0.53	0	11,12,14	1.01	1 (9%)
6	FUB	3A	2	6	9,9,10	0.51	0	11,12,14	1.13	2 (18%)
6	GZL	3A	3	6	11,11,12	6.73	6 (54%)	13,15,17	4.98	4 (30%)
6	FUB	3B	1	6	9,9,10	0.53	0	11,12,14	0.94	0
6	FUB	3B	2	6	9,9,10	0.52	0	11,12,14	1.21	1 (9%)
6	GZL	3B	3	6	11,11,12	6.57	7 (63%)	13,15,17	1.55	2 (15%)
13	FUB	3C	1	13	9,9,10	0.56	0	11,12,14	0.95	0
13	FUB	3C	2	13	9,9,10	0.53	0	11,12,14	1.13	1 (9%)
13	GZL	3C	3	13	11,11,12	6.54	7 (63%)	13,15,17	1.42	2 (15%)
13	AHR	3C	4	13	9,9,10	0.56	0	11,12,14	0.86	0
6	FUB	3D	1	6	9,9,10	0.54	0	11,12,14	1.01	1 (9%)
6	FUB	3D	2	6	9,9,10	0.54	0	11,12,14	1.02	1 (9%)
6	GZL	3D	3	6	11,11,12	6.58	7 (63%)	13,15,17	1.36	1 (7%)
13	FUB	4	1	13	9,9,10	0.51	0	11,12,14	0.85	0
13	FUB	4	2	13	9,9,10	0.49	0	11,12,14	1.29	1 (9%)
13	GZL	4	3	13	11,11,12	6.68	7 (63%)	13,15,17	3.35	6 (46%)

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	0.55	0	11,12,14	0.91	1 (9%)
13	FUB	4A	1	13	9,9,10	0.51	0	11,12,14	0.86	0
13	FUB	4A	2	13	9,9,10	0.54	0	11,12,14	0.82	0
13	GZL	4A	3	13	11,11,12	6.63	6 (54%)	13,15,17	1.41	1 (7%)
13	AHR	4A	4	13	9,9,10	0.52	0	11,12,14	1.07	1 (9%)
6	FUB	4B	1	6	9,9,10	0.55	0	11,12,14	0.87	1 (9%)
6	FUB	4B	2	6	9,9,10	0.56	0	11,12,14	0.83	0
6	GZL	4B	3	6	11,11,12	6.58	7 (63%)	13,15,17	1.63	2 (15%)
15	FUB	4C	1	15	9,9,10	0.56	0	11,12,14	0.90	0
15	FUB	4C	2	15	9,9,10	0.55	0	11,12,14	0.96	0
15	GZL	4C	3	15	11,11,12	6.59	7 (63%)	13,15,17	1.34	1 (7%)
15	AHR	4C	4	15	9,9,10	0.54	0	11,12,14	1.03	0
15	AHR	4C	5	15	9,9,10	0.55	0	11,12,14	1.05	1 (9%)
16	NAG	4D	1	1,16	14,14,15	0.34	0	17,19,21	0.53	0
16	NAG	4D	2	16	14,14,15	0.48	0	17,19,21	1.34	2 (11%)
6	FUB	5	1	6	9,9,10	0.52	0	11,12,14	0.97	1 (9%)
6	FUB	5	2	6	9,9,10	0.50	0	11,12,14	1.22	2 (18%)
6	GZL	5	3	6	11,11,12	6.58	6 (54%)	13,15,17	1.55	1 (7%)
13	FUB	5A	1	13	9,9,10	0.53	0	11,12,14	0.88	0
13	FUB	5A	2	13	9,9,10	0.52	0	11,12,14	0.77	0
13	GZL	5A	3	13	11,11,12	6.57	7 (63%)	13,15,17	1.22	1 (7%)
13	AHR	5A	4	13	9,9,10	0.55	0	11,12,14	1.02	1 (9%)
6	FUB	5B	1	6	9,9,10	0.52	0	11,12,14	0.79	0
6	FUB	5B	2	6	9,9,10	0.56	0	11,12,14	1.03	1 (9%)
6	GZL	5B	3	6	11,11,12	6.59	7 (63%)	13,15,17	1.28	1 (7%)
15	FUB	5C	1	15	9,9,10	0.53	0	11,12,14	1.04	1 (9%)
15	FUB	5C	2	15	9,9,10	0.56	0	11,12,14	0.95	0
15	GZL	5C	3	15	11,11,12	6.57	7 (63%)	13,15,17	1.49	1 (7%)
15	AHR	5C	4	15	9,9,10	0.55	0	11,12,14	0.97	1 (9%)
15	AHR	5C	5	15	9,9,10	0.54	0	11,12,14	1.04	1 (9%)
17	NAG	5D	1	1,17	14,14,15	0.32	0	17,19,21	0.99	1 (5%)
17	NAG	5D	2	17	14,14,15	0.30	0	17,19,21	0.70	0
17	BMA	5D	3	17	11,11,12	0.25	0	15,15,17	1.22	3 (20%)
17	MAN	5D	4	17	11,11,12	0.40	0	15,15,17	2.06	3 (20%)
17	MAN	5D	5	17	11,11,12	0.26	0	15,15,17	0.52	0
17	MAN	5D	6	17	11,11,12	0.29	0	15,15,17	0.77	0
13	FUB	6	1	13	9,9,10	0.52	0	11,12,14	0.76	0
13	FUB	6	2	13	9,9,10	0.56	0	11,12,14	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	6.64	6 (54%)	13,15,17	1.37	1 (7%)
13	AHR	6	4	13	9,9,10	0.55	0	11,12,14	1.04	1 (9%)
6	FUB	6A	1	6	9,9,10	0.53	0	11,12,14	0.86	0
6	FUB	6A	2	6	9,9,10	0.50	0	11,12,14	1.35	1 (9%)
6	GZL	6A	3	6	11,11,12	6.58	6 (54%)	13,15,17	1.38	1 (7%)
13	FUB	6B	1	13	9,9,10	0.54	0	11,12,14	0.89	0
13	FUB	6B	2	13	9,9,10	0.52	0	11,12,14	1.15	2 (18%)
13	GZL	6B	3	13	11,11,12	6.57	7 (63%)	13,15,17	1.85	4 (30%)
13	AHR	6B	4	13	9,9,10	0.52	0	11,12,14	0.92	0
6	FUB	6C	1	6	9,9,10	0.55	0	11,12,14	0.95	0
6	FUB	6C	2	6	9,9,10	0.54	0	11,12,14	1.00	1 (9%)
6	GZL	6C	3	6	11,11,12	6.58	7 (63%)	13,15,17	1.39	1 (7%)
6	FUB	6D	1	6	9,9,10	0.56	0	11,12,14	1.03	0
6	FUB	6D	2	6	9,9,10	0.55	0	11,12,14	1.11	1 (9%)
6	GZL	6D	3	6	11,11,12	6.54	6 (54%)	13,15,17	1.75	2 (15%)
13	FUB	7	1	13	9,9,10	0.55	0	11,12,14	0.95	0
13	FUB	7	2	13	9,9,10	0.54	0	11,12,14	0.75	0
13	GZL	7	3	13	11,11,12	6.59	7 (63%)	13,15,17	1.32	1 (7%)
13	AHR	7	4	13	9,9,10	0.53	0	11,12,14	1.10	1 (9%)
6	FUB	7A	1	6	9,9,10	0.53	0	11,12,14	0.95	1 (9%)
6	FUB	7A	2	6	9,9,10	0.55	0	11,12,14	0.93	0
6	GZL	7A	3	6	11,11,12	6.57	6 (54%)	13,15,17	1.41	1 (7%)
15	FUB	7B	1	15	9,9,10	0.50	0	11,12,14	0.92	0
15	FUB	7B	2	15	9,9,10	0.53	0	11,12,14	0.85	0
15	GZL	7B	3	15	11,11,12	6.61	6 (54%)	13,15,17	1.39	1 (7%)
15	AHR	7B	4	15	9,9,10	0.57	0	11,12,14	1.17	1 (9%)
15	AHR	7B	5	15	9,9,10	0.56	0	11,12,14	0.89	0
17	NAG	7C	1	1,17	14,14,15	0.32	0	17,19,21	0.86	1 (5%)
17	NAG	7C	2	17	14,14,15	0.35	0	17,19,21	0.98	0
17	BMA	7C	3	17	11,11,12	0.20	0	15,15,17	1.11	1 (6%)
17	MAN	7C	4	17	11,11,12	0.31	0	15,15,17	1.08	1 (6%)
17	MAN	7C	5	17	11,11,12	0.23	0	15,15,17	0.63	0
17	MAN	7C	6	17	11,11,12	0.28	0	15,15,17	0.85	0
6	FUB	7D	1	6	9,9,10	0.55	0	11,12,14	0.96	0
6	FUB	7D	2	6	9,9,10	0.54	0	11,12,14	0.98	1 (9%)
6	GZL	7D	3	6	11,11,12	6.58	6 (54%)	13,15,17	1.52	2 (15%)
6	FUB	8	1	6	9,9,10	0.53	0	11,12,14	0.96	1 (9%)
6	FUB	8	2	6	9,9,10	0.53	0	11,12,14	0.80	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	GZL	8	3	6	11,11,12	6.58	6 (54%)	13,15,17	1.35	1 (7%)
6	FUB	8A	1	6	9,9,10	0.51	0	11,12,14	0.99	1 (9%)
6	FUB	8A	2	6	9,9,10	0.58	0	11,12,14	1.04	1 (9%)
6	GZL	8A	3	6	11,11,12	6.59	7 (63%)	13,15,17	1.45	1 (7%)
15	FUB	8B	1	15	9,9,10	0.56	0	11,12,14	0.92	0
15	FUB	8B	2	15	9,9,10	0.53	0	11,12,14	0.90	0
15	GZL	8B	3	15	11,11,12	6.60	7 (63%)	13,15,17	1.17	1 (7%)
15	AHR	8B	4	15	9,9,10	0.54	0	11,12,14	1.05	1 (9%)
15	AHR	8B	5	15	9,9,10	0.53	0	11,12,14	1.04	1 (9%)
3	FUB	8C	1	3	9,9,10	0.55	0	11,12,14	0.83	0
3	FUB	8C	2	3	9,9,10	0.53	0	11,12,14	0.80	0
3	FUB	8C	3	3	9,9,10	0.56	0	11,12,14	0.88	0
6	FUB	8D	1	6	9,9,10	0.54	0	11,12,14	0.83	0
6	FUB	8D	2	6	9,9,10	0.54	0	11,12,14	0.91	0
6	GZL	8D	3	6	11,11,12	6.60	6 (54%)	13,15,17	1.54	2 (15%)
6	FUB	9	1	6	9,9,10	0.52	0	11,12,14	0.87	1 (9%)
6	FUB	9	2	6	9,9,10	0.54	0	11,12,14	0.79	0
6	GZL	9	3	6	11,11,12	6.60	6 (54%)	13,15,17	1.29	1 (7%)
13	FUB	9A	1	13	9,9,10	0.53	0	11,12,14	0.89	0
13	FUB	9A	2	13	9,9,10	0.51	0	11,12,14	1.15	2 (18%)
13	GZL	9A	3	13	11,11,12	6.58	7 (63%)	13,15,17	1.94	4 (30%)
13	AHR	9A	4	13	9,9,10	0.53	0	11,12,14	0.96	0
6	FUB	9B	1	6	9,9,10	0.54	0	11,12,14	0.86	0
6	FUB	9B	2	6	9,9,10	0.54	0	11,12,14	1.00	1 (9%)
6	GZL	9B	3	6	11,11,12	6.56	7 (63%)	13,15,17	1.58	2 (15%)
3	FUB	9C	1	3	9,9,10	0.55	0	11,12,14	0.99	0
3	FUB	9C	2	3	9,9,10	0.56	0	11,12,14	1.01	1 (9%)
3	FUB	9C	3	3	9,9,10	0.54	0	11,12,14	0.82	1 (9%)
18	FUB	9D	1	18	9,9,10	0.57	0	11,12,14	2.51	5 (45%)
18	FUB	9D	2	18	9,9,10	0.54	0	11,12,14	0.87	0
18	GZL	9D	3	18	11,11,12	6.60	7 (63%)	13,15,17	1.29	1 (7%)
18	AHR	9D	4	18	9,9,10	0.55	0	11,12,14	1.05	1 (9%)
18	AHR	9D	5	18	9,9,10	0.56	0	11,12,14	1.21	1 (9%)
6	FUB	AA	1	6	9,9,10	0.51	0	11,12,14	0.77	0
6	FUB	AA	2	6	9,9,10	0.58	0	11,12,14	1.07	1 (9%)
6	GZL	AA	3	6	11,11,12	6.59	7 (63%)	13,15,17	1.22	1 (7%)
15	FUB	AB	1	15	9,9,10	0.52	0	11,12,14	0.97	1 (9%)
15	FUB	AB	2	15	9,9,10	0.55	0	11,12,14	0.88	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	GZL	AB	3	15	11,11,12	6.59	6 (54%)	13,15,17	1.26	1 (7%)
15	AHR	AB	4	15	9,9,10	0.60	0	11,12,14	1.18	1 (9%)
15	AHR	AB	5	15	9,9,10	0.55	0	11,12,14	1.10	1 (9%)
16	NAG	AC	1	1,16	14,14,15	0.55	0	17,19,21	0.97	1 (5%)
16	NAG	AC	2	16	14,14,15	0.41	0	17,19,21	1.30	2 (11%)
4	FUB	AD	1	4	9,9,10	0.54	0	11,12,14	0.91	1 (9%)
4	FUB	AD	2	4	9,9,10	0.52	0	11,12,14	0.80	0
4	FUB	AD	3	4	9,9,10	0.53	0	11,12,14	0.76	0
4	AHR	AD	4	4	9,9,10	0.53	0	11,12,14	1.07	1 (9%)
19	FUB	AE	1	19	9,9,10	0.55	0	11,12,14	1.18	1 (9%)
19	FUB	AE	2	19	9,9,10	0.54	0	11,12,14	0.85	0
19	GZL	AE	3	19	11,11,12	6.61	6 (54%)	13,15,17	1.40	1 (7%)
19	AHR	AE	4	19	9,9,10	0.54	0	11,12,14	0.85	0
13	FUB	BA	1	13	9,9,10	0.54	0	11,12,14	0.77	0
13	FUB	BA	2	13	9,9,10	0.52	0	11,12,14	1.33	3 (27%)
13	GZL	BA	3	13	11,11,12	6.53	7 (63%)	13,15,17	1.93	4 (30%)
13	AHR	BA	4	13	9,9,10	0.52	0	11,12,14	0.83	0
15	FUB	BB	1	15	9,9,10	0.52	0	11,12,14	0.96	1 (9%)
15	FUB	BB	2	15	9,9,10	0.54	0	11,12,14	0.70	0
15	GZL	BB	3	15	11,11,12	6.61	6 (54%)	13,15,17	1.13	1 (7%)
15	AHR	BB	4	15	9,9,10	0.55	0	11,12,14	1.06	1 (9%)
15	AHR	BB	5	15	9,9,10	0.56	0	11,12,14	0.90	0
3	FUB	BC	1	3	9,9,10	0.53	0	11,12,14	0.97	1 (9%)
3	FUB	BC	2	3	9,9,10	0.52	0	11,12,14	0.89	0
3	FUB	BC	3	3	9,9,10	0.54	0	11,12,14	0.86	0
5	FUB	BD	1	5	9,9,10	0.52	0	11,12,14	0.97	1 (9%)
5	FUB	BD	2	5	9,9,10	0.51	0	11,12,14	0.84	0
5	FUB	BD	3	5	9,9,10	0.55	0	11,12,14	0.89	0
5	AHR	BD	4	5	9,9,10	0.53	0	11,12,14	1.06	1 (9%)
5	AHR	BD	5	5	9,9,10	0.54	0	11,12,14	0.81	0
18	FUB	BE	1	18	9,9,10	0.58	0	11,12,14	0.92	0
18	FUB	BE	2	18	9,9,10	0.51	0	11,12,14	1.00	1 (9%)
18	GZL	BE	3	18	11,11,12	6.56	7 (63%)	13,15,17	1.50	2 (15%)
18	AHR	BE	4	18	9,9,10	0.54	0	11,12,14	0.82	0
18	AHR	BE	5	18	9,9,10	0.52	0	11,12,14	1.10	1 (9%)
15	FUB	CA	1	15	9,9,10	0.52	0	11,12,14	0.99	0
15	FUB	CA	2	15	9,9,10	0.51	0	11,12,14	0.82	0
15	GZL	CA	3	15	11,11,12	6.61	7 (63%)	13,15,17	1.17	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	AHR	CA	4	15	9,9,10	0.56	0	11,12,14	1.22	2 (18%)
15	AHR	CA	5	15	9,9,10	0.56	0	11,12,14	1.04	0
6	FUB	CB	1	6	9,9,10	0.54	0	11,12,14	0.98	1 (9%)
6	FUB	CB	2	6	9,9,10	0.53	0	11,12,14	0.84	0
6	GZL	CB	3	6	11,11,12	6.59	7 (63%)	13,15,17	1.49	3 (23%)
3	FUB	CC	1	3	9,9,10	0.54	0	11,12,14	0.92	1 (9%)
3	FUB	CC	2	3	9,9,10	0.53	0	11,12,14	0.89	1 (9%)
3	FUB	CC	3	3	9,9,10	0.54	0	11,12,14	0.79	0
6	FUB	CD	1	6	9,9,10	0.53	0	11,12,14	0.95	0
6	FUB	CD	2	6	9,9,10	0.48	0	11,12,14	1.08	2 (18%)
6	GZL	CD	3	6	11,11,12	6.96	6 (54%)	13,15,17	4.33	5 (38%)
20	FUB	CE	1	20	9,9,10	0.53	0	11,12,14	0.80	0
20	FUB	CE	2	20	9,9,10	0.50	0	11,12,14	0.80	0
20	GZL	CE	3	20	11,11,12	6.55	6 (54%)	13,15,17	1.48	1 (7%)
20	AHR	CE	4	20	9,9,10	0.56	0	11,12,14	0.86	0
15	FUB	DA	1	15	9,9,10	0.54	0	11,12,14	0.94	0
15	FUB	DA	2	15	9,9,10	0.53	0	11,12,14	0.81	0
15	GZL	DA	3	15	11,11,12	6.60	6 (54%)	13,15,17	1.30	1 (7%)
15	AHR	DA	4	15	9,9,10	0.53	0	11,12,14	1.08	1 (9%)
15	AHR	DA	5	15	9,9,10	0.55	0	11,12,14	1.01	1 (9%)
17	NAG	DB	1	1,17	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	1.06	1 (5%)
17	BMA	DB	3	17	11,11,12	0.22	0	15,15,17	1.13	1 (6%)
17	MAN	DB	4	17	11,11,12	0.31	0	15,15,17	1.06	2 (13%)
17	MAN	DB	5	17	11,11,12	0.23	0	15,15,17	0.62	0
17	MAN	DB	6	17	11,11,12	0.39	0	15,15,17	1.31	2 (13%)
4	FUB	DC	1	4	9,9,10	0.54	0	11,12,14	1.02	1 (9%)
4	FUB	DC	2	4	9,9,10	0.54	0	11,12,14	0.82	0
4	FUB	DC	3	4	9,9,10	0.53	0	11,12,14	0.81	0
4	AHR	DC	4	4	9,9,10	0.54	0	11,12,14	0.97	1 (9%)
3	FUB	DD	1	3	9,9,10	0.54	0	11,12,14	1.08	1 (9%)
3	FUB	DD	2	3	9,9,10	0.55	0	11,12,14	0.80	0
3	FUB	DD	3	3	9,9,10	0.54	0	11,12,14	0.95	0
18	FUB	DE	1	18	9,9,10	0.50	0	11,12,14	1.02	1 (9%)
18	FUB	DE	2	18	9,9,10	0.49	0	11,12,14	0.76	0
18	GZL	DE	3	18	11,11,12	6.56	7 (63%)	13,15,17	1.53	1 (7%)
18	AHR	DE	4	18	9,9,10	0.55	0	11,12,14	0.99	1 (9%)
18	AHR	DE	5	18	9,9,10	0.56	0	11,12,14	0.90	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	FUB	EA	1	6	9,9,10	0.54	0	11,12,14	0.93	0
6	FUB	EA	2	6	9,9,10	0.52	0	11,12,14	0.88	0
6	GZL	EA	3	6	11,11,12	6.60	6 (54%)	13,15,17	1.37	1 (7%)
3	FUB	EB	1	3	9,9,10	0.54	0	11,12,14	0.99	1 (9%)
3	FUB	EB	2	3	9,9,10	0.55	0	11,12,14	0.83	0
3	FUB	EB	3	3	9,9,10	0.55	0	11,12,14	0.97	0
5	FUB	EC	1	5	9,9,10	0.55	0	11,12,14	0.97	0
5	FUB	EC	2	5	9,9,10	0.56	0	11,12,14	1.07	0
5	FUB	EC	3	5	9,9,10	0.55	0	11,12,14	1.02	1 (9%)
5	AHR	EC	4	5	9,9,10	0.54	0	11,12,14	0.98	1 (9%)
5	AHR	EC	5	5	9,9,10	0.54	0	11,12,14	0.83	0
3	FUB	ED	1	3	9,9,10	0.51	0	11,12,14	1.04	1 (9%)
3	FUB	ED	2	3	9,9,10	0.54	0	11,12,14	0.79	0
3	FUB	ED	3	3	9,9,10	0.55	0	11,12,14	0.81	0
20	FUB	EE	1	20	9,9,10	0.51	0	11,12,14	0.81	0
20	FUB	EE	2	20	9,9,10	0.55	0	11,12,14	1.04	1 (9%)
20	GZL	EE	3	20	11,11,12	6.59	7 (63%)	13,15,17	1.43	1 (7%)
20	AHR	EE	4	20	9,9,10	0.57	0	11,12,14	0.83	0
16	NAG	FA	1	1,16	14,14,15	0.42	0	17,19,21	0.58	0
16	NAG	FA	2	16	14,14,15	0.40	0	17,19,21	1.40	2 (11%)
12	FUB	FB	1	12	9,9,10	0.56	0	11,12,14	0.99	0
12	FUB	FB	2	12	9,9,10	0.56	0	11,12,14	0.94	0
12	GZL	FB	3	12	11,11,12	6.53	7 (63%)	13,15,17	1.64	2 (15%)
12	AHR	FB	4	12	9,9,10	0.55	0	11,12,14	0.92	0
12	AHR	FB	5	12	9,9,10	0.56	0	11,12,14	1.00	1 (9%)
6	FUB	FC	1	6	9,9,10	0.53	0	11,12,14	1.23	2 (18%)
6	FUB	FC	2	6	9,9,10	0.58	0	11,12,14	1.15	1 (9%)
6	GZL	FC	3	6	11,11,12	6.45	6 (54%)	13,15,17	2.37	3 (23%)
3	FUB	FD	1	3	9,9,10	0.52	0	11,12,14	1.04	1 (9%)
3	FUB	FD	2	3	9,9,10	0.52	0	11,12,14	0.73	0
3	FUB	FD	3	3	9,9,10	0.55	0	11,12,14	0.87	0
21	FUB	FE	1	21	9,9,10	0.53	0	11,12,14	1.04	1 (9%)
21	FUB	FE	2	21	9,9,10	0.51	0	11,12,14	0.70	0
21	GZL	FE	3	21	11,11,12	6.61	6 (54%)	13,15,17	1.30	1 (7%)
21	AHR	FE	4	21	9,9,10	0.54	0	11,12,14	0.98	0
21	AHR	FE	5	21	9,9,10	0.59	0	11,12,14	0.95	1 (9%)
17	NAG	GA	1	1,17	14,14,15	0.34	0	17,19,21	0.80	1 (5%)
17	NAG	GA	2	17	14,14,15	0.33	0	17,19,21	0.92	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	BMA	GA	3	17	11,11,12	0.23	0	15,15,17	1.59	3 (20%)
17	MAN	GA	4	17	11,11,12	0.30	0	15,15,17	0.70	0
17	MAN	GA	5	17	11,11,12	0.24	0	15,15,17	0.55	0
17	MAN	GA	6	17	11,11,12	0.28	0	15,15,17	0.91	0
13	FUB	GB	1	13	9,9,10	0.55	0	11,12,14	0.87	0
13	FUB	GB	2	13	9,9,10	0.56	0	11,12,14	0.91	0
13	GZL	GB	3	13	11,11,12	6.60	7 (63%)	13,15,17	1.22	1 (7%)
13	AHR	GB	4	13	9,9,10	0.53	0	11,12,14	0.97	0
3	FUB	GC	1	3	9,9,10	0.53	0	11,12,14	0.98	1 (9%)
3	FUB	GC	2	3	9,9,10	0.52	0	11,12,14	0.71	0
3	FUB	GC	3	3	9,9,10	0.55	0	11,12,14	0.85	0
6	FUB	GD	1	6	9,9,10	0.53	0	11,12,14	1.03	1 (9%)
6	FUB	GD	2	6	9,9,10	0.53	0	11,12,14	0.82	0
6	GZL	GD	3	6	11,11,12	6.57	7 (63%)	13,15,17	1.33	1 (7%)
22	FUB	GE	1	22	9,9,10	0.55	0	11,12,14	1.12	1 (9%)
22	FUB	GE	2	22	9,9,10	0.56	0	11,12,14	1.11	1 (9%)
22	GZL	GE	3	22	11,11,12	6.57	7 (63%)	13,15,17	1.34	1 (7%)
22	AHR	GE	4	22	9,9,10	0.53	0	11,12,14	0.78	0
22	AHR	GE	5	22	9,9,10	0.57	0	11,12,14	1.40	3 (27%)
22	AHR	GE	6	22	9,9,10	0.52	0	11,12,14	0.80	0
3	FUB	HA	1	3	9,9,10	0.52	0	11,12,14	0.85	0
3	FUB	HA	2	3	9,9,10	0.55	0	11,12,14	0.80	0
3	FUB	HA	3	3	9,9,10	0.56	0	11,12,14	0.99	1 (9%)
14	FUB	HB	1	14	9,9,10	0.53	0	11,12,14	0.77	0
14	FUB	HB	2	14	9,9,10	0.54	0	11,12,14	0.86	0
14	GZL	HB	3	14	11,11,12	6.52	7 (63%)	13,15,17	1.71	3 (23%)
14	FUB	HB	4	14	9,9,10	0.56	0	11,12,14	1.04	1 (9%)
3	FUB	HC	1	3	9,9,10	0.52	0	11,12,14	1.12	1 (9%)
3	FUB	HC	2	3	9,9,10	0.53	0	11,12,14	0.75	0
3	FUB	HC	3	3	9,9,10	0.54	0	11,12,14	0.90	0
7	FUB	HD	1	7	9,9,10	0.56	0	11,12,14	1.10	1 (9%)
7	FUB	HD	2	7	9,9,10	0.54	0	11,12,14	0.84	0
7	FUB	HD	3	7	9,9,10	0.54	0	11,12,14	0.96	0
7	AHR	HD	4	7	9,9,10	0.53	0	11,12,14	0.94	1 (9%)
20	FUB	HE	1	20	9,9,10	0.56	0	11,12,14	1.14	0
20	FUB	HE	2	20	9,9,10	0.53	0	11,12,14	0.92	0
20	GZL	HE	3	20	11,11,12	6.58	7 (63%)	13,15,17	1.49	1 (7%)
20	AHR	HE	4	20	9,9,10	0.54	0	11,12,14	0.97	0
3	FUB	IA	1	3	9,9,10	0.52	0	11,12,14	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	FUB	IA	2	3	9,9,10	0.53	0	11,12,14	0.88	0
3	FUB	IA	3	3	9,9,10	0.53	0	11,12,14	0.78	0
12	FUB	IB	1	12	9,9,10	0.55	0	11,12,14	0.91	0
12	FUB	IB	2	12	9,9,10	0.54	0	11,12,14	0.93	1 (9%)
12	GZL	IB	3	12	11,11,12	6.58	7 (63%)	13,15,17	1.33	1 (7%)
12	AHR	IB	4	12	9,9,10	0.53	0	11,12,14	1.02	1 (9%)
12	AHR	IB	5	12	9,9,10	0.54	0	11,12,14	1.05	1 (9%)
3	FUB	IC	1	3	9,9,10	0.55	0	11,12,14	1.05	1 (9%)
3	FUB	IC	2	3	9,9,10	0.49	0	11,12,14	0.80	0
3	FUB	IC	3	3	9,9,10	0.53	0	11,12,14	0.84	0
3	FUB	ID	1	3	9,9,10	0.54	0	11,12,14	1.04	1 (9%)
3	FUB	ID	2	3	9,9,10	0.52	0	11,12,14	0.78	0
3	FUB	ID	3	3	9,9,10	0.56	0	11,12,14	0.85	0
18	FUB	IE	1	18	9,9,10	0.55	0	11,12,14	1.06	1 (9%)
18	FUB	IE	2	18	9,9,10	0.50	0	11,12,14	0.84	0
18	GZL	IE	3	18	11,11,12	6.54	7 (63%)	13,15,17	1.55	1 (7%)
18	AHR	IE	4	18	9,9,10	0.53	0	11,12,14	1.11	1 (9%)
18	AHR	IE	5	18	9,9,10	0.54	0	11,12,14	1.11	1 (9%)
3	FUB	J	1	3	9,9,10	0.53	0	11,12,14	0.76	0
3	FUB	J	2	3	9,9,10	0.53	0	11,12,14	0.94	0
3	FUB	J	3	3	9,9,10	0.57	0	11,12,14	0.92	0
4	FUB	JA	1	4	9,9,10	0.55	0	11,12,14	0.83	0
4	FUB	JA	2	4	9,9,10	0.55	0	11,12,14	1.00	0
4	FUB	JA	3	4	9,9,10	0.55	0	11,12,14	0.92	0
4	AHR	JA	4	4	9,9,10	0.53	0	11,12,14	1.04	1 (9%)
4	FUB	JB	1	4	9,9,10	0.54	0	11,12,14	0.96	0
4	FUB	JB	2	4	9,9,10	0.56	0	11,12,14	0.98	0
4	FUB	JB	3	4	9,9,10	0.56	0	11,12,14	0.87	0
4	AHR	JB	4	4	9,9,10	0.54	0	11,12,14	0.68	0
6	FUB	JC	1	6	9,9,10	0.54	0	11,12,14	1.06	1 (9%)
6	FUB	JC	2	6	9,9,10	0.53	0	11,12,14	0.82	0
6	GZL	JC	3	6	11,11,12	6.58	6 (54%)	13,15,17	1.34	1 (7%)
8	FUB	JD	1	8	9,9,10	0.53	0	11,12,14	0.81	0
8	FUB	JD	2	8	9,9,10	0.54	0	11,12,14	0.77	0
8	FUB	JD	3	8	9,9,10	0.56	0	11,12,14	0.76	0
8	AHR	JD	4	8	9,9,10	0.55	0	11,12,14	1.09	1 (9%)
8	AHR	JD	5	8	9,9,10	0.55	0	11,12,14	0.94	0
18	FUB	JE	1	18	9,9,10	0.56	0	11,12,14	1.05	1 (9%)
18	FUB	JE	2	18	9,9,10	0.54	0	11,12,14	0.89	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	GZL	JE	3	18	11,11,12	6.56	7 (63%)	13,15,17	1.43	1 (7%)
18	AHR	JE	4	18	9,9,10	0.55	0	11,12,14	0.82	0
18	AHR	JE	5	18	9,9,10	0.54	0	11,12,14	0.98	0
3	FUB	K	1	3	9,9,10	0.54	0	11,12,14	0.64	0
3	FUB	K	2	3	9,9,10	0.52	0	11,12,14	0.78	0
3	FUB	K	3	3	9,9,10	0.53	0	11,12,14	0.76	0
5	FUB	KA	1	5	9,9,10	0.54	0	11,12,14	0.92	0
5	FUB	KA	2	5	9,9,10	0.56	0	11,12,14	0.87	0
5	FUB	KA	3	5	9,9,10	0.54	0	11,12,14	1.08	1 (9%)
5	AHR	KA	4	5	9,9,10	0.55	0	11,12,14	1.04	1 (9%)
5	AHR	KA	5	5	9,9,10	0.56	0	11,12,14	0.98	1 (9%)
14	FUB	KB	1	14	9,9,10	0.56	0	11,12,14	0.96	0
14	FUB	KB	2	14	9,9,10	0.56	0	11,12,14	0.97	0
14	GZL	KB	3	14	11,11,12	6.50	7 (63%)	13,15,17	1.80	2 (15%)
14	FUB	KB	4	14	9,9,10	0.55	0	11,12,14	1.00	1 (9%)
7	FUB	KC	1	7	9,9,10	0.54	0	11,12,14	1.06	1 (9%)
7	FUB	KC	2	7	9,9,10	0.53	0	11,12,14	0.75	0
7	FUB	KC	3	7	9,9,10	0.55	0	11,12,14	0.94	0
7	AHR	KC	4	7	9,9,10	0.53	0	11,12,14	0.97	1 (9%)
3	FUB	KD	1	3	9,9,10	0.54	0	11,12,14	0.95	1 (9%)
3	FUB	KD	2	3	9,9,10	0.53	0	11,12,14	0.89	0
3	FUB	KD	3	3	9,9,10	0.54	0	11,12,14	0.95	0
18	FUB	KE	1	18	9,9,10	0.57	0	11,12,14	1.09	0
18	FUB	KE	2	18	9,9,10	0.54	0	11,12,14	0.92	0
18	GZL	KE	3	18	11,11,12	6.54	7 (63%)	13,15,17	1.39	1 (7%)
18	AHR	KE	4	18	9,9,10	0.55	0	11,12,14	1.05	1 (9%)
18	AHR	KE	5	18	9,9,10	0.55	0	11,12,14	0.99	0
4	FUB	L	1	4	9,9,10	0.56	0	11,12,14	0.67	0
4	FUB	L	2	4	9,9,10	0.54	0	11,12,14	0.89	0
4	FUB	L	3	4	9,9,10	0.57	0	11,12,14	0.83	0
4	AHR	L	4	4	9,9,10	0.54	0	11,12,14	1.03	1 (9%)
6	FUB	LA	1	6	9,9,10	0.56	0	11,12,14	0.96	0
6	FUB	LA	2	6	9,9,10	0.54	0	11,12,14	1.15	1 (9%)
6	GZL	LA	3	6	11,11,12	6.97	6 (54%)	13,15,17	4.26	5 (38%)
3	FUB	LB	1	3	9,9,10	0.55	0	11,12,14	0.89	0
3	FUB	LB	2	3	9,9,10	0.54	0	11,12,14	0.84	0
3	FUB	LB	3	3	9,9,10	0.54	0	11,12,14	0.94	0
3	FUB	LC	1	3	9,9,10	0.55	0	11,12,14	1.00	0
3	FUB	LC	2	3	9,9,10	0.52	0	11,12,14	0.77	0
3	FUB	LC	3	3	9,9,10	0.55	0	11,12,14	0.83	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	FUB	LD	1	4	9,9,10	0.55	0	11,12,14	1.03	1 (9%)
4	FUB	LD	2	4	9,9,10	0.54	0	11,12,14	0.80	0
4	FUB	LD	3	4	9,9,10	0.55	0	11,12,14	0.80	0
4	AHR	LD	4	4	9,9,10	0.55	0	11,12,14	1.02	1 (9%)
19	FUB	LE	1	19	9,9,10	0.55	0	11,12,14	1.08	0
19	FUB	LE	2	19	9,9,10	0.54	0	11,12,14	1.02	1 (9%)
19	GZL	LE	3	19	11,11,12	6.60	7 (63%)	13,15,17	1.34	1 (7%)
19	AHR	LE	4	19	9,9,10	0.53	0	11,12,14	0.93	0
5	FUB	M	1	5	9,9,10	0.53	0	11,12,14	0.89	0
5	FUB	M	2	5	9,9,10	0.55	0	11,12,14	1.19	2 (18%)
5	FUB	M	3	5	9,9,10	0.54	0	11,12,14	1.07	1 (9%)
5	AHR	M	4	5	9,9,10	0.55	0	11,12,14	1.01	1 (9%)
5	AHR	M	5	5	9,9,10	0.54	0	11,12,14	1.12	1 (9%)
3	FUB	MA	1	3	9,9,10	0.53	0	11,12,14	0.84	0
3	FUB	MA	2	3	9,9,10	0.53	0	11,12,14	0.82	0
3	FUB	MA	3	3	9,9,10	0.55	0	11,12,14	0.86	0
10	FUB	MB	1	10	9,9,10	0.55	0	11,12,14	0.97	0
10	FUB	MB	2	10	9,9,10	0.55	0	11,12,14	1.01	0
10	FUB	MB	3	10	9,9,10	0.55	0	11,12,14	0.83	0
10	AHR	MB	4	10	9,9,10	0.54	0	11,12,14	1.02	1 (9%)
10	AHR	MB	5	10	9,9,10	0.54	0	11,12,14	1.13	1 (9%)
8	FUB	MC	1	8	9,9,10	0.53	0	11,12,14	0.98	1 (9%)
8	FUB	MC	2	8	9,9,10	0.54	0	11,12,14	0.78	0
8	FUB	MC	3	8	9,9,10	0.54	0	11,12,14	0.82	0
8	AHR	MC	4	8	9,9,10	0.55	0	11,12,14	1.07	1 (9%)
8	AHR	MC	5	8	9,9,10	0.56	0	11,12,14	1.01	1 (9%)
4	FUB	MD	1	4	9,9,10	0.51	0	11,12,14	0.88	0
4	FUB	MD	2	4	9,9,10	0.52	0	11,12,14	0.83	0
4	FUB	MD	3	4	9,9,10	0.56	0	11,12,14	0.95	0
4	AHR	MD	4	4	9,9,10	0.54	0	11,12,14	0.81	0
6	FUB	ME	1	6	9,9,10	0.55	0	11,12,14	0.81	0
6	FUB	ME	2	6	9,9,10	0.55	0	11,12,14	0.81	0
6	GZL	ME	3	6	11,11,12	6.59	6 (54%)	13,15,17	1.40	1 (7%)
6	FUB	N	1	6	9,9,10	0.55	0	11,12,14	1.02	0
6	FUB	N	2	6	9,9,10	0.59	0	11,12,14	1.11	1 (9%)
6	GZL	N	3	6	11,11,12	6.50	7 (63%)	13,15,17	3.34	5 (38%)
3	FUB	NA	1	3	9,9,10	0.52	0	11,12,14	1.06	1 (9%)
3	FUB	NA	2	3	9,9,10	0.52	0	11,12,14	0.79	0
3	FUB	NA	3	3	9,9,10	0.55	0	11,12,14	0.98	1 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	FUB	NB	1	4	9,9,10	0.56	0	11,12,14	1.01	1 (9%)
4	FUB	NB	2	4	9,9,10	0.56	0	11,12,14	0.93	0
4	FUB	NB	3	4	9,9,10	0.54	0	11,12,14	0.90	0
4	AHR	NB	4	4	9,9,10	0.53	0	11,12,14	0.97	1 (9%)
3	FUB	NC	1	3	9,9,10	0.55	0	11,12,14	0.91	0
3	FUB	NC	2	3	9,9,10	0.54	0	11,12,14	0.84	0
3	FUB	NC	3	3	9,9,10	0.54	0	11,12,14	0.95	0
9	FUB	ND	1	9	9,9,10	0.59	0	11,12,14	1.02	0
9	FUB	ND	2	9	9,9,10	0.56	0	11,12,14	1.05	1 (9%)
19	FUB	NE	1	19	9,9,10	0.56	0	11,12,14	0.93	0
19	FUB	NE	2	19	9,9,10	0.54	0	11,12,14	0.76	0
19	GZL	NE	3	19	11,11,12	6.57	7 (63%)	13,15,17	1.40	1 (7%)
19	AHR	NE	4	19	9,9,10	0.55	0	11,12,14	0.92	0
3	FUB	O	1	3	9,9,10	0.55	0	11,12,14	1.03	1 (9%)
3	FUB	O	2	3	9,9,10	0.54	0	11,12,14	0.83	0
3	FUB	O	3	3	9,9,10	0.56	0	11,12,14	0.95	0
3	FUB	OA	1	3	9,9,10	0.55	0	11,12,14	1.06	1 (9%)
3	FUB	OA	2	3	9,9,10	0.55	0	11,12,14	0.90	0
3	FUB	OA	3	3	9,9,10	0.55	0	11,12,14	0.92	0
3	FUB	OB	1	3	9,9,10	0.56	0	11,12,14	0.97	0
3	FUB	OB	2	3	9,9,10	0.56	0	11,12,14	0.87	0
3	FUB	OB	3	3	9,9,10	0.56	0	11,12,14	0.95	0
4	FUB	OC	1	4	9,9,10	0.51	0	11,12,14	0.87	0
4	FUB	OC	2	4	9,9,10	0.56	0	11,12,14	0.71	0
4	FUB	OC	3	4	9,9,10	0.54	0	11,12,14	0.82	0
4	AHR	OC	4	4	9,9,10	0.53	0	11,12,14	1.08	1 (9%)
4	FUB	OD	1	4	9,9,10	0.51	0	11,12,14	1.02	0
4	FUB	OD	2	4	9,9,10	0.49	0	11,12,14	0.77	0
4	FUB	OD	3	4	9,9,10	0.55	0	11,12,14	0.85	0
4	AHR	OD	4	4	9,9,10	0.55	0	11,12,14	1.07	1 (9%)
6	FUB	OE	1	6	9,9,10	0.60	0	11,12,14	0.85	0
6	FUB	OE	2	6	9,9,10	0.56	0	11,12,14	0.89	0
6	GZL	OE	3	6	11,11,12	6.59	6 (54%)	13,15,17	1.46	1 (7%)
3	FUB	P	1	3	9,9,10	0.55	0	11,12,14	1.07	1 (9%)
3	FUB	P	2	3	9,9,10	0.54	0	11,12,14	0.86	0
3	FUB	P	3	3	9,9,10	0.56	0	11,12,14	0.92	0
6	FUB	PA	1	6	9,9,10	0.56	0	11,12,14	0.98	0
6	FUB	PA	2	6	9,9,10	0.54	0	11,12,14	0.88	0
6	GZL	PA	3	6	11,11,12	6.59	6 (54%)	13,15,17	1.42	1 (7%)
3	FUB	PB	1	3	9,9,10	0.54	0	11,12,14	0.91	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	FUB	PB	2	3	9,9,10	0.54	0	11,12,14	0.90	0
3	FUB	PB	3	3	9,9,10	0.53	0	11,12,14	0.86	0
4	FUB	PC	1	4	9,9,10	0.51	0	11,12,14	0.92	0
4	FUB	PC	2	4	9,9,10	0.52	0	11,12,14	0.81	0
4	FUB	PC	3	4	9,9,10	0.55	0	11,12,14	0.91	0
4	AHR	PC	4	4	9,9,10	0.61	0	11,12,14	1.18	1 (9%)
10	FUB	PD	1	10	9,9,10	0.52	0	11,12,14	1.01	1 (9%)
10	FUB	PD	2	10	9,9,10	0.57	0	11,12,14	0.92	0
10	FUB	PD	3	10	9,9,10	0.56	0	11,12,14	0.87	0
10	AHR	PD	4	10	9,9,10	0.55	0	11,12,14	1.08	1 (9%)
10	AHR	PD	5	10	9,9,10	0.55	0	11,12,14	0.98	0
18	FUB	PE	1	18	9,9,10	0.53	0	11,12,14	0.96	1 (9%)
18	FUB	PE	2	18	9,9,10	0.52	0	11,12,14	0.76	0
18	GZL	PE	3	18	11,11,12	6.60	6 (54%)	13,15,17	1.36	1 (7%)
18	AHR	PE	4	18	9,9,10	0.54	0	11,12,14	0.80	0
18	AHR	PE	5	18	9,9,10	0.54	0	11,12,14	0.98	0
3	FUB	Q	1	3	9,9,10	0.54	0	11,12,14	0.99	1 (9%)
3	FUB	Q	2	3	9,9,10	0.52	0	11,12,14	0.80	0
3	FUB	Q	3	3	9,9,10	0.54	0	11,12,14	0.79	0
7	FUB	QA	1	7	9,9,10	0.53	0	11,12,14	1.11	1 (9%)
7	FUB	QA	2	7	9,9,10	0.56	0	11,12,14	0.87	0
7	FUB	QA	3	7	9,9,10	0.57	0	11,12,14	1.01	1 (9%)
7	AHR	QA	4	7	9,9,10	0.53	0	11,12,14	0.88	0
3	FUB	QB	1	3	9,9,10	0.56	0	11,12,14	0.94	1 (9%)
3	FUB	QB	2	3	9,9,10	0.56	0	11,12,14	0.88	0
3	FUB	QB	3	3	9,9,10	0.52	0	11,12,14	0.80	0
9	FUB	QC	1	9	9,9,10	0.54	0	11,12,14	0.91	0
9	FUB	QC	2	9	9,9,10	0.54	0	11,12,14	0.91	0
3	FUB	QD	1	3	9,9,10	0.55	0	11,12,14	0.77	0
3	FUB	QD	2	3	9,9,10	0.56	0	11,12,14	0.95	0
3	FUB	QD	3	3	9,9,10	0.54	0	11,12,14	0.87	0
22	FUB	QE	1	22	9,9,10	0.54	0	11,12,14	0.79	1 (9%)
22	FUB	QE	2	22	9,9,10	0.54	0	11,12,14	0.93	0
22	GZL	QE	3	22	11,11,12	6.60	6 (54%)	13,15,17	1.37	1 (7%)
22	AHR	QE	4	22	9,9,10	0.54	0	11,12,14	1.08	1 (9%)
22	AHR	QE	5	22	9,9,10	0.55	0	11,12,14	0.87	0
22	AHR	QE	6	22	9,9,10	0.54	0	11,12,14	1.05	1 (9%)
6	FUB	R	1	6	9,9,10	0.53	0	11,12,14	1.00	1 (9%)
6	FUB	R	2	6	9,9,10	0.54	0	11,12,14	0.89	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	GZL	R	3	6	11,11,12	6.59	7 (63%)	13,15,17	1.39	1 (7%)
3	FUB	RA	1	3	9,9,10	0.53	0	11,12,14	1.06	1 (9%)
3	FUB	RA	2	3	9,9,10	0.54	0	11,12,14	0.83	0
3	FUB	RA	3	3	9,9,10	0.55	0	11,12,14	0.91	0
3	FUB	RB	1	3	9,9,10	0.53	0	11,12,14	1.04	0
3	FUB	RB	2	3	9,9,10	0.58	0	11,12,14	0.98	0
3	FUB	RB	3	3	9,9,10	0.55	0	11,12,14	1.03	1 (9%)
4	FUB	RC	1	4	9,9,10	0.53	0	11,12,14	0.93	0
4	FUB	RC	2	4	9,9,10	0.54	0	11,12,14	0.68	0
4	FUB	RC	3	4	9,9,10	0.57	0	11,12,14	0.93	0
4	AHR	RC	4	4	9,9,10	0.54	0	11,12,14	1.00	1 (9%)
4	FUB	RD	1	4	9,9,10	0.52	0	11,12,14	0.81	0
4	FUB	RD	2	4	9,9,10	0.55	0	11,12,14	0.94	1 (9%)
4	FUB	RD	3	4	9,9,10	0.57	0	11,12,14	0.95	0
4	AHR	RD	4	4	9,9,10	0.54	0	11,12,14	1.06	1 (9%)
22	FUB	RE	1	22	9,9,10	0.57	0	11,12,14	1.01	0
22	FUB	RE	2	22	9,9,10	0.54	0	11,12,14	0.87	0
22	GZL	RE	3	22	11,11,12	6.60	6 (54%)	13,15,17	1.35	1 (7%)
22	AHR	RE	4	22	9,9,10	0.54	0	11,12,14	0.95	0
22	AHR	RE	5	22	9,9,10	0.53	0	11,12,14	1.13	1 (9%)
22	AHR	RE	6	22	9,9,10	0.60	0	11,12,14	1.16	1 (9%)
7	FUB	S	1	7	9,9,10	0.54	0	11,12,14	1.09	1 (9%)
7	FUB	S	2	7	9,9,10	0.53	0	11,12,14	0.81	0
7	FUB	S	3	7	9,9,10	0.53	0	11,12,14	1.01	1 (9%)
7	AHR	S	4	7	9,9,10	0.56	0	11,12,14	1.00	1 (9%)
8	FUB	SA	1	8	9,9,10	0.55	0	11,12,14	0.94	0
8	FUB	SA	2	8	9,9,10	0.54	0	11,12,14	0.84	0
8	FUB	SA	3	8	9,9,10	0.53	0	11,12,14	0.92	0
8	AHR	SA	4	8	9,9,10	0.57	0	11,12,14	0.99	0
8	AHR	SA	5	8	9,9,10	0.56	0	11,12,14	0.85	0
3	FUB	SB	1	3	9,9,10	0.56	0	11,12,14	1.08	1 (9%)
3	FUB	SB	2	3	9,9,10	0.55	0	11,12,14	1.01	1 (9%)
3	FUB	SB	3	3	9,9,10	0.55	0	11,12,14	0.99	0
10	FUB	SC	1	10	9,9,10	0.54	0	11,12,14	0.90	0
10	FUB	SC	2	10	9,9,10	0.55	0	11,12,14	0.82	0
10	FUB	SC	3	10	9,9,10	0.58	0	11,12,14	0.90	0
10	AHR	SC	4	10	9,9,10	0.54	0	11,12,14	0.87	0
10	AHR	SC	5	10	9,9,10	0.56	0	11,12,14	1.02	1 (9%)
4	FUB	SD	1	4	9,9,10	0.55	0	11,12,14	0.97	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	FUB	SD	2	4	9,9,10	0.55	0	11,12,14	1.05	1 (9%)
4	FUB	SD	3	4	9,9,10	0.55	0	11,12,14	0.88	0
4	AHR	SD	4	4	9,9,10	0.55	0	11,12,14	1.03	1 (9%)
18	FUB	SE	1	18	9,9,10	0.54	0	11,12,14	1.06	1 (9%)
18	FUB	SE	2	18	9,9,10	0.51	0	11,12,14	0.82	0
18	GZL	SE	3	18	11,11,12	6.61	6 (54%)	13,15,17	1.36	1 (7%)
18	AHR	SE	4	18	9,9,10	0.54	0	11,12,14	0.97	0
18	AHR	SE	5	18	9,9,10	0.54	0	11,12,14	0.96	0
3	FUB	T	1	3	9,9,10	0.51	0	11,12,14	1.08	1 (9%)
3	FUB	T	2	3	9,9,10	0.53	0	11,12,14	0.81	0
3	FUB	T	3	3	9,9,10	0.56	0	11,12,14	0.93	0
3	FUB	TA	1	3	9,9,10	0.54	0	11,12,14	0.99	1 (9%)
3	FUB	TA	2	3	9,9,10	0.51	0	11,12,14	0.98	1 (9%)
3	FUB	TA	3	3	9,9,10	0.54	0	11,12,14	0.81	0
3	FUB	TB	1	3	9,9,10	0.53	0	11,12,14	0.75	0
3	FUB	TB	2	3	9,9,10	0.55	0	11,12,14	0.98	1 (9%)
3	FUB	TB	3	3	9,9,10	0.54	0	11,12,14	0.85	0
3	FUB	TC	1	3	9,9,10	0.56	0	11,12,14	1.07	1 (9%)
3	FUB	TC	2	3	9,9,10	0.55	0	11,12,14	1.03	1 (9%)
3	FUB	TC	3	3	9,9,10	0.55	0	11,12,14	1.04	1 (9%)
3	FUB	TD	1	3	9,9,10	0.53	0	11,12,14	0.80	0
3	FUB	TD	2	3	9,9,10	0.57	0	11,12,14	0.91	0
3	FUB	TD	3	3	9,9,10	0.54	0	11,12,14	0.89	0
20	FUB	TE	1	20	9,9,10	0.53	0	11,12,14	0.99	1 (9%)
20	FUB	TE	2	20	9,9,10	0.54	0	11,12,14	0.80	0
20	GZL	TE	3	20	11,11,12	6.60	7 (63%)	13,15,17	1.55	1 (7%)
20	AHR	TE	4	20	9,9,10	0.53	0	11,12,14	0.80	0
8	FUB	U	1	8	9,9,10	0.53	0	11,12,14	1.01	0
8	FUB	U	2	8	9,9,10	0.54	0	11,12,14	0.96	1 (9%)
8	FUB	U	3	8	9,9,10	0.56	0	11,12,14	0.88	0
8	AHR	U	4	8	9,9,10	0.54	0	11,12,14	1.08	1 (9%)
8	AHR	U	5	8	9,9,10	0.57	0	11,12,14	0.92	0
4	FUB	UA	1	4	9,9,10	0.55	0	11,12,14	1.02	1 (9%)
4	FUB	UA	2	4	9,9,10	0.54	0	11,12,14	0.84	0
4	FUB	UA	3	4	9,9,10	0.54	0	11,12,14	0.88	0
4	AHR	UA	4	4	9,9,10	0.55	0	11,12,14	0.89	0
3	FUB	UB	1	3	9,9,10	0.54	0	11,12,14	0.98	1 (9%)
3	FUB	UB	2	3	9,9,10	0.54	0	11,12,14	0.75	0
3	FUB	UB	3	3	9,9,10	0.55	0	11,12,14	0.94	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	FUB	UC	1	4	9,9,10	0.50	0	11,12,14	0.88	0
4	FUB	UC	2	4	9,9,10	0.53	0	11,12,14	0.91	0
4	FUB	UC	3	4	9,9,10	0.54	0	11,12,14	0.93	0
4	AHR	UC	4	4	9,9,10	0.56	0	11,12,14	0.93	0
7	FUB	UD	1	7	9,9,10	0.53	0	11,12,14	1.02	1 (9%)
7	FUB	UD	2	7	9,9,10	0.53	0	11,12,14	0.71	0
7	FUB	UD	3	7	9,9,10	0.55	0	11,12,14	0.84	0
7	AHR	UD	4	7	9,9,10	0.55	0	11,12,14	0.79	0
20	FUB	UE	1	20	9,9,10	0.52	0	11,12,14	0.87	0
20	FUB	UE	2	20	9,9,10	0.48	0	11,12,14	0.99	0
20	GZL	UE	3	20	11,11,12	6.61	6 (54%)	13,15,17	1.29	1 (7%)
20	AHR	UE	4	20	9,9,10	0.56	0	11,12,14	0.81	0
3	FUB	V	1	3	9,9,10	0.55	0	11,12,14	0.90	0
3	FUB	V	2	3	9,9,10	0.54	0	11,12,14	0.88	0
3	FUB	V	3	3	9,9,10	0.53	0	11,12,14	1.04	1 (9%)
4	FUB	VA	1	4	9,9,10	0.53	0	11,12,14	0.92	0
4	FUB	VA	2	4	9,9,10	0.54	0	11,12,14	0.89	0
4	FUB	VA	3	4	9,9,10	0.53	0	11,12,14	0.83	0
4	AHR	VA	4	4	9,9,10	0.58	0	11,12,14	0.77	0
10	FUB	VB	1	10	9,9,10	0.52	0	11,12,14	0.91	0
10	FUB	VB	2	10	9,9,10	0.53	0	11,12,14	0.80	0
10	FUB	VB	3	10	9,9,10	0.54	0	11,12,14	1.06	1 (9%)
10	AHR	VB	4	10	9,9,10	0.56	0	11,12,14	0.80	0
10	AHR	VB	5	10	9,9,10	0.56	0	11,12,14	0.95	1 (9%)
4	FUB	VC	1	4	9,9,10	0.53	0	11,12,14	0.85	0
4	FUB	VC	2	4	9,9,10	0.56	0	11,12,14	0.91	0
4	FUB	VC	3	4	9,9,10	0.56	0	11,12,14	0.85	0
4	AHR	VC	4	4	9,9,10	0.54	0	11,12,14	1.01	1 (9%)
4	FUB	VD	1	4	9,9,10	0.55	0	11,12,14	0.92	0
4	FUB	VD	2	4	9,9,10	0.55	0	11,12,14	0.97	1 (9%)
4	FUB	VD	3	4	9,9,10	0.55	0	11,12,14	0.87	0
4	AHR	VD	4	4	9,9,10	0.55	0	11,12,14	1.05	1 (9%)
22	FUB	VE	1	22	9,9,10	0.53	0	11,12,14	1.24	1 (9%)
22	FUB	VE	2	22	9,9,10	0.52	0	11,12,14	0.92	0
22	GZL	VE	3	22	11,11,12	6.59	6 (54%)	13,15,17	1.38	1 (7%)
22	AHR	VE	4	22	9,9,10	0.54	0	11,12,14	1.11	1 (9%)
22	AHR	VE	5	22	9,9,10	0.55	0	11,12,14	0.87	1 (9%)
22	AHR	VE	6	22	9,9,10	0.56	0	11,12,14	0.92	0
4	FUB	W	1	4	9,9,10	0.55	0	11,12,14	0.84	0
4	FUB	W	2	4	9,9,10	0.55	0	11,12,14	0.78	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	FUB	W	3	4	9,9,10	0.55	0	11,12,14	0.84	0
4	AHR	W	4	4	9,9,10	0.54	0	11,12,14	1.02	1 (9%)
9	FUB	WA	1	9	9,9,10	0.54	0	11,12,14	0.84	0
9	FUB	WA	2	9	9,9,10	0.55	0	11,12,14	0.92	0
13	FUB	WB	1	13	9,9,10	0.51	0	11,12,14	0.93	0
13	FUB	WB	2	13	9,9,10	0.52	0	11,12,14	1.03	1 (9%)
13	GZL	WB	3	13	11,11,12	6.66	7 (63%)	13,15,17	1.24	1 (7%)
13	AHR	WB	4	13	9,9,10	0.55	0	11,12,14	1.06	1 (9%)
3	FUB	WC	1	3	9,9,10	0.53	0	11,12,14	1.03	1 (9%)
3	FUB	WC	2	3	9,9,10	0.55	0	11,12,14	0.89	0
3	FUB	WC	3	3	9,9,10	0.54	0	11,12,14	1.00	1 (9%)
7	FUB	WD	1	7	9,9,10	0.58	0	11,12,14	0.92	0
7	FUB	WD	2	7	9,9,10	0.56	0	11,12,14	1.06	0
7	FUB	WD	3	7	9,9,10	0.55	0	11,12,14	0.93	0
7	AHR	WD	4	7	9,9,10	0.54	0	11,12,14	1.04	1 (9%)
20	FUB	WE	1	20	9,9,10	0.52	0	11,12,14	0.90	0
20	FUB	WE	2	20	9,9,10	0.54	0	11,12,14	0.81	0
20	GZL	WE	3	20	11,11,12	6.59	7 (63%)	13,15,17	1.32	1 (7%)
20	AHR	WE	4	20	9,9,10	0.54	0	11,12,14	1.07	1 (9%)
4	FUB	X	1	4	9,9,10	0.51	0	11,12,14	0.92	0
4	FUB	X	2	4	9,9,10	0.52	0	11,12,14	0.79	0
4	FUB	X	3	4	9,9,10	0.55	0	11,12,14	0.84	0
4	AHR	X	4	4	9,9,10	0.56	0	11,12,14	0.96	0
3	FUB	XA	1	3	9,9,10	0.54	0	11,12,14	1.00	0
3	FUB	XA	2	3	9,9,10	0.52	0	11,12,14	0.63	0
3	FUB	XA	3	3	9,9,10	0.55	0	11,12,14	1.01	1 (9%)
6	FUB	XB	1	6	9,9,10	0.55	0	11,12,14	1.00	0
6	FUB	XB	2	6	9,9,10	0.56	0	11,12,14	1.03	1 (9%)
6	GZL	XB	3	6	11,11,12	6.86	6 (54%)	13,15,17	4.11	4 (30%)
7	FUB	XC	1	7	9,9,10	0.56	0	11,12,14	1.03	0
7	FUB	XC	2	7	9,9,10	0.52	0	11,12,14	0.94	1 (9%)
7	FUB	XC	3	7	9,9,10	0.57	0	11,12,14	0.87	0
7	AHR	XC	4	7	9,9,10	0.55	0	11,12,14	0.81	0
11	FUB	XD	1	11	9,9,10	0.63	0	11,12,14	1.21	1 (9%)
11	AHR	XD	2	11	9,9,10	0.55	0	11,12,14	0.98	0
11	AHR	XD	3	11	9,9,10	0.53	0	11,12,14	1.05	1 (9%)
23	FUB	XE	1	23	9,9,10	0.56	0	11,12,14	1.14	1 (9%)
23	FUB	XE	2	23	9,9,10	0.53	0	11,12,14	0.74	0
23	GZL	XE	3	23	11,11,12	6.58	6 (54%)	13,15,17	1.38	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	AHR	XE	4	23	9,9,10	0.56	0	11,12,14	0.85	1 (9%)
23	AHR	XE	5	23	9,9,10	0.55	0	11,12,14	0.91	0
23	AHR	XE	6	23	9,9,10	0.53	0	11,12,14	0.96	0
9	FUB	Y	1	9	9,9,10	0.56	0	11,12,14	1.00	1 (9%)
9	FUB	Y	2	9	9,9,10	0.55	0	11,12,14	0.99	0
10	FUB	YA	1	10	9,9,10	0.54	0	11,12,14	0.80	0
10	FUB	YA	2	10	9,9,10	0.55	0	11,12,14	0.84	0
10	FUB	YA	3	10	9,9,10	0.55	0	11,12,14	0.81	0
10	AHR	YA	4	10	9,9,10	0.55	0	11,12,14	0.97	0
10	AHR	YA	5	10	9,9,10	0.55	0	11,12,14	1.07	1 (9%)
13	FUB	YB	1	13	9,9,10	0.51	0	11,12,14	0.76	0
13	FUB	YB	2	13	9,9,10	0.55	0	11,12,14	0.76	0
13	GZL	YB	3	13	11,11,12	6.63	6 (54%)	13,15,17	1.16	1 (7%)
13	AHR	YB	4	13	9,9,10	0.54	0	11,12,14	1.07	1 (9%)
4	FUB	YC	1	4	9,9,10	0.55	0	11,12,14	0.87	0
4	FUB	YC	2	4	9,9,10	0.53	0	11,12,14	0.94	1 (9%)
4	FUB	YC	3	4	9,9,10	0.54	0	11,12,14	0.81	0
4	AHR	YC	4	4	9,9,10	0.54	0	11,12,14	1.05	1 (9%)
9	FUB	YD	1	9	9,9,10	0.52	0	11,12,14	0.63	0
9	FUB	YD	2	9	9,9,10	0.53	0	11,12,14	0.79	0
24	FUB	YE	1	24	9,9,10	0.52	0	11,12,14	1.35	1 (9%)
24	FUB	YE	2	24	9,9,10	0.53	0	11,12,14	0.79	0
24	GZL	YE	3	24	11,11,12	6.59	7 (63%)	13,15,17	1.35	1 (7%)
24	AHR	YE	4	24	9,9,10	0.56	0	11,12,14	1.06	2 (18%)
24	AHR	YE	5	24	9,9,10	0.55	0	11,12,14	1.12	1 (9%)
24	AHR	YE	6	24	9,9,10	0.56	0	11,12,14	0.98	1 (9%)
4	FUB	Z	1	4	9,9,10	0.53	0	11,12,14	1.09	1 (9%)
4	FUB	Z	2	4	9,9,10	0.54	0	11,12,14	0.91	0
4	FUB	Z	3	4	9,9,10	0.53	0	11,12,14	0.81	0
4	AHR	Z	4	4	9,9,10	0.55	0	11,12,14	1.10	1 (9%)
3	FUB	ZA	1	3	9,9,10	0.55	0	11,12,14	1.08	1 (9%)
3	FUB	ZA	2	3	9,9,10	0.54	0	11,12,14	0.88	0
3	FUB	ZA	3	3	9,9,10	0.54	0	11,12,14	0.91	0
13	FUB	ZB	1	13	9,9,10	0.56	0	11,12,14	0.97	0
13	FUB	ZB	2	13	9,9,10	0.54	0	11,12,14	0.90	0
13	GZL	ZB	3	13	11,11,12	6.59	7 (63%)	13,15,17	1.43	2 (15%)
13	AHR	ZB	4	13	9,9,10	0.54	0	11,12,14	0.92	0
7	FUB	ZC	1	7	9,9,10	0.53	0	11,12,14	0.82	0
7	FUB	ZC	2	7	9,9,10	0.54	0	11,12,14	0.90	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	FUB	ZC	3	7	9,9,10	0.52	0	11,12,14	1.09	1 (9%)
7	AHR	ZC	4	7	9,9,10	0.55	0	11,12,14	0.99	0
4	FUB	ZD	1	4	9,9,10	0.54	0	11,12,14	0.96	1 (9%)
4	FUB	ZD	2	4	9,9,10	0.55	0	11,12,14	0.84	0
4	FUB	ZD	3	4	9,9,10	0.56	0	11,12,14	0.91	0
4	AHR	ZD	4	4	9,9,10	0.55	0	11,12,14	0.97	0
6	FUB	ZE	1	6	9,9,10	0.54	0	11,12,14	0.79	0
6	FUB	ZE	2	6	9,9,10	0.54	0	11,12,14	0.99	1 (9%)
6	GZL	ZE	3	6	11,11,12	6.57	7 (63%)	13,15,17	1.40	1 (7%)
10	FUB	a	1	10	9,9,10	0.53	0	11,12,14	1.02	1 (9%)
10	FUB	a	2	10	9,9,10	0.54	0	11,12,14	0.95	0
10	FUB	a	3	10	9,9,10	0.55	0	11,12,14	0.83	0
10	AHR	a	4	10	9,9,10	0.53	0	11,12,14	1.12	1 (9%)
10	AHR	a	5	10	9,9,10	0.54	0	11,12,14	1.03	1 (9%)
4	FUB	aA	1	4	9,9,10	0.53	0	11,12,14	0.78	0
4	FUB	aA	2	4	9,9,10	0.56	0	11,12,14	0.90	0
4	FUB	aA	3	4	9,9,10	0.54	0	11,12,14	0.95	0
4	AHR	aA	4	4	9,9,10	0.54	0	11,12,14	0.96	0
6	FUB	aB	1	6	9,9,10	0.54	0	11,12,14	0.88	0
6	FUB	aB	2	6	9,9,10	0.51	0	11,12,14	1.18	2 (18%)
6	GZL	aB	3	6	11,11,12	6.57	7 (63%)	13,15,17	1.34	1 (7%)
11	FUB	aC	1	11	9,9,10	0.61	0	11,12,14	1.10	0
11	AHR	aC	2	11	9,9,10	0.54	0	11,12,14	1.00	1 (9%)
11	AHR	aC	3	11	9,9,10	0.56	0	11,12,14	0.98	0
3	FUB	aD	1	3	9,9,10	0.55	0	11,12,14	0.91	0
3	FUB	aD	2	3	9,9,10	0.55	0	11,12,14	0.93	0
3	FUB	aD	3	3	9,9,10	0.55	0	11,12,14	0.87	0
19	FUB	aE	1	19	9,9,10	0.56	0	11,12,14	0.87	0
19	FUB	aE	2	19	9,9,10	0.54	0	11,12,14	0.96	0
19	GZL	aE	3	19	11,11,12	6.55	7 (63%)	13,15,17	1.49	2 (15%)
19	AHR	aE	4	19	9,9,10	0.55	0	11,12,14	1.03	1 (9%)
3	FUB	b	1	3	9,9,10	0.55	0	11,12,14	1.08	1 (9%)
3	FUB	b	2	3	9,9,10	0.54	0	11,12,14	0.93	0
3	FUB	b	3	3	9,9,10	0.56	0	11,12,14	0.89	0
4	FUB	bA	1	4	9,9,10	0.52	0	11,12,14	0.87	0
4	FUB	bA	2	4	9,9,10	0.55	0	11,12,14	0.86	0
4	FUB	bA	3	4	9,9,10	0.54	0	11,12,14	0.95	0
4	AHR	bA	4	4	9,9,10	0.55	0	11,12,14	0.88	0
6	FUB	bB	1	6	9,9,10	0.53	0	11,12,14	1.01	1 (9%)
6	FUB	bB	2	6	9,9,10	0.57	0	11,12,14	0.94	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	GZL	bB	3	6	11,11,12	6.59	7 (63%)	13,15,17	1.35	1 (7%)
9	FUB	bC	1	9	9,9,10	0.54	0	11,12,14	0.72	0
9	FUB	bC	2	9	9,9,10	0.52	0	11,12,14	0.83	0
3	FUB	bD	1	3	9,9,10	0.49	0	11,12,14	0.85	0
3	FUB	bD	2	3	9,9,10	0.55	0	11,12,14	0.86	0
3	FUB	bD	3	3	9,9,10	0.55	0	11,12,14	0.82	0
6	FUB	bE	1	6	9,9,10	0.59	0	11,12,14	1.02	0
6	FUB	bE	2	6	9,9,10	0.53	0	11,12,14	0.83	0
6	GZL	bE	3	6	11,11,12	6.62	7 (63%)	13,15,17	1.46	1 (7%)
4	FUB	c	1	4	9,9,10	0.54	0	11,12,14	0.79	0
4	FUB	c	2	4	9,9,10	0.55	0	11,12,14	0.88	0
4	FUB	c	3	4	9,9,10	0.52	0	11,12,14	0.90	0
4	AHR	c	4	4	9,9,10	0.53	0	11,12,14	0.98	1 (9%)
3	FUB	cA	1	3	9,9,10	0.53	0	11,12,14	0.84	0
3	FUB	cA	2	3	9,9,10	0.56	0	11,12,14	0.96	1 (9%)
3	FUB	cA	3	3	9,9,10	0.56	0	11,12,14	1.03	1 (9%)
6	FUB	cB	1	6	9,9,10	0.54	0	11,12,14	0.95	1 (9%)
6	FUB	cB	2	6	9,9,10	0.56	0	11,12,14	1.06	1 (9%)
6	GZL	cB	3	6	11,11,12	6.60	6 (54%)	13,15,17	1.52	2 (15%)
4	FUB	cC	1	4	9,9,10	0.54	0	11,12,14	1.15	1 (9%)
4	FUB	cC	2	4	9,9,10	0.54	0	11,12,14	0.84	0
4	FUB	cC	3	4	9,9,10	0.54	0	11,12,14	0.93	0
4	AHR	cC	4	4	9,9,10	0.55	0	11,12,14	1.03	1 (9%)
12	FUB	cD	1	12	9,9,10	0.54	0	11,12,14	0.80	0
12	FUB	cD	2	12	9,9,10	0.56	0	11,12,14	0.94	0
12	GZL	cD	3	12	11,11,12	6.58	7 (63%)	13,15,17	1.29	1 (7%)
12	AHR	cD	4	12	9,9,10	0.55	0	11,12,14	0.96	0
12	AHR	cD	5	12	9,9,10	0.57	0	11,12,14	0.98	1 (9%)
18	FUB	cE	1	18	9,9,10	0.52	0	11,12,14	0.97	1 (9%)
18	FUB	cE	2	18	9,9,10	0.56	0	11,12,14	0.88	0
18	GZL	cE	3	18	11,11,12	6.59	7 (63%)	13,15,17	1.50	1 (7%)
18	AHR	cE	4	18	9,9,10	0.55	0	11,12,14	0.93	0
18	AHR	cE	5	18	9,9,10	0.55	0	11,12,14	0.85	0
4	FUB	d	1	4	9,9,10	0.53	0	11,12,14	0.94	1 (9%)
4	FUB	d	2	4	9,9,10	0.54	0	11,12,14	0.89	0
4	FUB	d	3	4	9,9,10	0.55	0	11,12,14	0.98	0
4	AHR	d	4	4	9,9,10	0.54	0	11,12,14	1.09	1 (9%)
7	FUB	dA	1	7	9,9,10	0.53	0	11,12,14	1.06	1 (9%)
7	FUB	dA	2	7	9,9,10	0.52	0	11,12,14	1.03	1 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	FUB	dA	3	7	9,9,10	0.53	0	11,12,14	0.86	0
7	AHR	dA	4	7	9,9,10	0.55	0	11,12,14	0.81	0
13	FUB	dB	1	13	9,9,10	0.55	0	11,12,14	0.77	0
13	FUB	dB	2	13	9,9,10	0.53	0	11,12,14	1.09	1 (9%)
13	GZL	dB	3	13	11,11,12	6.61	7 (63%)	13,15,17	1.89	4 (30%)
13	AHR	dB	4	13	9,9,10	0.54	0	11,12,14	0.98	0
3	FUB	dC	1	3	9,9,10	0.53	0	11,12,14	0.85	0
3	FUB	dC	2	3	9,9,10	0.55	0	11,12,14	0.86	0
3	FUB	dC	3	3	9,9,10	0.55	0	11,12,14	1.06	1 (9%)
13	FUB	dD	1	13	9,9,10	0.57	0	11,12,14	0.87	0
13	FUB	dD	2	13	9,9,10	0.53	0	11,12,14	0.84	0
13	GZL	dD	3	13	11,11,12	6.58	7 (63%)	13,15,17	1.22	1 (7%)
13	AHR	dD	4	13	9,9,10	0.53	0	11,12,14	0.91	0
22	FUB	dE	1	22	9,9,10	0.54	0	11,12,14	0.88	1 (9%)
22	FUB	dE	2	22	9,9,10	0.55	0	11,12,14	0.97	1 (9%)
22	GZL	dE	3	22	11,11,12	6.58	7 (63%)	13,15,17	1.45	1 (7%)
22	AHR	dE	4	22	9,9,10	0.53	0	11,12,14	1.10	1 (9%)
22	AHR	dE	5	22	9,9,10	0.55	0	11,12,14	1.05	0
22	AHR	dE	6	22	9,9,10	0.53	0	11,12,14	1.05	1 (9%)
3	FUB	e	1	3	9,9,10	0.56	0	11,12,14	0.83	0
3	FUB	e	2	3	9,9,10	0.56	0	11,12,14	0.91	0
3	FUB	e	3	3	9,9,10	0.55	0	11,12,14	1.06	1 (9%)
4	FUB	eA	1	4	9,9,10	0.55	0	11,12,14	0.96	0
4	FUB	eA	2	4	9,9,10	0.54	0	11,12,14	0.82	0
4	FUB	eA	3	4	9,9,10	0.56	0	11,12,14	0.99	0
4	AHR	eA	4	4	9,9,10	0.56	0	11,12,14	0.93	0
15	FUB	eB	1	15	9,9,10	0.52	0	11,12,14	0.96	1 (9%)
15	FUB	eB	2	15	9,9,10	0.54	0	11,12,14	0.89	0
15	GZL	eB	3	15	11,11,12	6.61	6 (54%)	13,15,17	1.38	1 (7%)
15	AHR	eB	4	15	9,9,10	0.58	0	11,12,14	1.18	1 (9%)
15	AHR	eB	5	15	9,9,10	0.56	0	11,12,14	0.95	0
3	FUB	eC	1	3	9,9,10	0.53	0	11,12,14	0.72	0
3	FUB	eC	2	3	9,9,10	0.55	0	11,12,14	0.88	0
3	FUB	eC	3	3	9,9,10	0.56	0	11,12,14	0.89	0
14	FUB	eD	1	14	9,9,10	0.54	0	11,12,14	0.89	0
14	FUB	eD	2	14	9,9,10	0.55	0	11,12,14	0.83	0
14	GZL	eD	3	14	11,11,12	6.56	7 (63%)	13,15,17	1.73	2 (15%)
14	FUB	eD	4	14	9,9,10	0.57	0	11,12,14	0.99	0
22	FUB	eE	1	22	9,9,10	0.58	0	11,12,14	1.15	1 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	FUB	eE	2	22	9,9,10	0.55	0	11,12,14	0.88	0
22	GZL	eE	3	22	11,11,12	6.60	6 (54%)	13,15,17	1.47	1 (7%)
22	AHR	eE	4	22	9,9,10	0.54	0	11,12,14	0.96	1 (9%)
22	AHR	eE	5	22	9,9,10	0.53	0	11,12,14	1.04	1 (9%)
22	AHR	eE	6	22	9,9,10	0.56	0	11,12,14	1.12	1 (9%)
7	FUB	f	1	7	9,9,10	0.53	0	11,12,14	0.97	0
7	FUB	f	2	7	9,9,10	0.52	0	11,12,14	1.01	1 (9%)
7	FUB	f	3	7	9,9,10	0.53	0	11,12,14	0.98	1 (9%)
7	AHR	f	4	7	9,9,10	0.51	0	11,12,14	0.82	0
7	FUB	fA	1	7	9,9,10	0.55	0	11,12,14	0.96	0
7	FUB	fA	2	7	9,9,10	0.55	0	11,12,14	0.90	0
7	FUB	fA	3	7	9,9,10	0.56	0	11,12,14	0.94	0
7	AHR	fA	4	7	9,9,10	0.54	0	11,12,14	0.96	0
15	FUB	fB	1	15	9,9,10	0.54	0	11,12,14	0.97	0
15	FUB	fB	2	15	9,9,10	0.55	0	11,12,14	0.86	0
15	GZL	fB	3	15	11,11,12	6.60	6 (54%)	13,15,17	1.26	1 (7%)
15	AHR	fB	4	15	9,9,10	0.55	0	11,12,14	1.00	1 (9%)
15	AHR	fB	5	15	9,9,10	0.54	0	11,12,14	1.02	1 (9%)
12	FUB	fC	1	12	9,9,10	0.56	0	11,12,14	0.92	0
12	FUB	fC	2	12	9,9,10	0.54	0	11,12,14	0.85	0
12	GZL	fC	3	12	11,11,12	6.60	6 (54%)	13,15,17	1.26	1 (7%)
12	AHR	fC	4	12	9,9,10	0.54	0	11,12,14	1.05	1 (9%)
12	AHR	fC	5	12	9,9,10	0.56	0	11,12,14	1.00	0
12	FUB	fD	1	12	9,9,10	0.54	0	11,12,14	1.00	1 (9%)
12	FUB	fD	2	12	9,9,10	0.55	0	11,12,14	0.98	1 (9%)
12	GZL	fD	3	12	11,11,12	6.56	7 (63%)	13,15,17	1.14	1 (7%)
12	AHR	fD	4	12	9,9,10	0.53	0	11,12,14	0.91	0
12	AHR	fD	5	12	9,9,10	0.55	0	11,12,14	1.03	1 (9%)
18	FUB	fE	1	18	9,9,10	0.51	0	11,12,14	1.04	1 (9%)
18	FUB	fE	2	18	9,9,10	0.52	0	11,12,14	0.87	0
18	GZL	fE	3	18	11,11,12	6.58	6 (54%)	13,15,17	1.28	1 (7%)
18	AHR	fE	4	18	9,9,10	0.54	0	11,12,14	1.00	0
18	AHR	fE	5	18	9,9,10	0.55	0	11,12,14	0.85	0
4	FUB	g	1	4	9,9,10	0.53	0	11,12,14	0.99	0
4	FUB	g	2	4	9,9,10	0.56	0	11,12,14	0.88	0
4	FUB	g	3	4	9,9,10	0.54	0	11,12,14	0.90	0
4	AHR	g	4	4	9,9,10	0.55	0	11,12,14	1.01	1 (9%)
11	FUB	gA	1	11	9,9,10	0.63	0	11,12,14	1.38	1 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	AHR	gA	2	11	9,9,10	0.55	0	11,12,14	0.93	0
11	AHR	gA	3	11	9,9,10	0.53	0	11,12,14	0.97	1 (9%)
6	FUB	gB	1	6	9,9,10	0.55	0	11,12,14	0.83	0
6	FUB	gB	2	6	9,9,10	0.53	0	11,12,14	0.88	0
6	GZL	gB	3	6	11,11,12	6.57	7 (63%)	13,15,17	1.50	2 (15%)
13	FUB	gC	1	13	9,9,10	0.56	0	11,12,14	0.85	0
13	FUB	gC	2	13	9,9,10	0.56	0	11,12,14	0.99	0
13	GZL	gC	3	13	11,11,12	6.61	7 (63%)	13,15,17	1.25	1 (7%)
13	AHR	gC	4	13	9,9,10	0.54	0	11,12,14	1.06	1 (9%)
4	FUB	gD	1	4	9,9,10	0.54	0	11,12,14	0.98	1 (9%)
4	FUB	gD	2	4	9,9,10	0.54	0	11,12,14	0.97	0
4	FUB	gD	3	4	9,9,10	0.54	0	11,12,14	0.78	0
4	AHR	gD	4	4	9,9,10	0.54	0	11,12,14	0.72	0
20	FUB	gE	1	20	9,9,10	0.53	0	11,12,14	0.87	0
20	FUB	gE	2	20	9,9,10	0.56	0	11,12,14	1.00	0
20	GZL	gE	3	20	11,11,12	6.60	7 (63%)	13,15,17	1.26	1 (7%)
20	AHR	gE	4	20	9,9,10	0.55	0	11,12,14	0.84	0
7	FUB	h	1	7	9,9,10	0.54	0	11,12,14	0.96	0
7	FUB	h	2	7	9,9,10	0.57	0	11,12,14	0.94	0
7	FUB	h	3	7	9,9,10	0.55	0	11,12,14	0.97	0
7	AHR	h	4	7	9,9,10	0.54	0	11,12,14	0.99	1 (9%)
9	FUB	hA	1	9	9,9,10	0.52	0	11,12,14	0.87	1 (9%)
9	FUB	hA	2	9	9,9,10	0.53	0	11,12,14	0.80	0
3	FUB	hB	1	3	9,9,10	0.55	0	11,12,14	0.81	0
3	FUB	hB	2	3	9,9,10	0.55	0	11,12,14	0.85	0
3	FUB	hB	3	3	9,9,10	0.56	0	11,12,14	0.92	0
14	FUB	hC	1	14	9,9,10	0.53	0	11,12,14	1.00	1 (9%)
14	FUB	hC	2	14	9,9,10	0.54	0	11,12,14	0.86	0
14	GZL	hC	3	14	11,11,12	6.58	7 (63%)	13,15,17	1.62	2 (15%)
14	FUB	hC	4	14	9,9,10	0.57	0	11,12,14	0.85	0
14	FUB	hD	1	14	9,9,10	0.54	0	11,12,14	0.95	0
14	FUB	hD	2	14	9,9,10	0.55	0	11,12,14	1.02	0
14	GZL	hD	3	14	11,11,12	6.48	7 (63%)	13,15,17	1.57	2 (15%)
14	FUB	hD	4	14	9,9,10	0.54	0	11,12,14	0.91	0
20	FUB	hE	1	20	9,9,10	0.54	0	11,12,14	0.95	0
20	FUB	hE	2	20	9,9,10	0.54	0	11,12,14	0.83	0
20	GZL	hE	3	20	11,11,12	6.58	7 (63%)	13,15,17	1.38	1 (7%)
20	AHR	hE	4	20	9,9,10	0.54	0	11,12,14	0.87	0
11	FUB	i	1	11	9,9,10	0.62	0	11,12,14	1.29	1 (9%)
11	AHR	i	2	11	9,9,10	0.54	0	11,12,14	1.04	1 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	AHR	i	3	11	9,9,10	0.52	0	11,12,14	1.04	1 (9%)
4	FUB	iA	1	4	9,9,10	0.54	0	11,12,14	1.07	1 (9%)
4	FUB	iA	2	4	9,9,10	0.54	0	11,12,14	0.94	0
4	FUB	iA	3	4	9,9,10	0.54	0	11,12,14	0.85	0
4	AHR	iA	4	4	9,9,10	0.54	0	11,12,14	1.13	1 (9%)
12	FUB	iB	1	12	9,9,10	0.57	0	11,12,14	0.92	0
12	FUB	iB	2	12	9,9,10	0.56	0	11,12,14	0.98	0
12	GZL	iB	3	12	11,11,12	6.57	7 (63%)	13,15,17	1.50	2 (15%)
12	AHR	iB	4	12	9,9,10	0.55	0	11,12,14	0.99	0
12	AHR	iB	5	12	9,9,10	0.57	0	11,12,14	0.95	0
12	FUB	iC	1	12	9,9,10	0.54	0	11,12,14	1.07	1 (9%)
12	FUB	iC	2	12	9,9,10	0.55	0	11,12,14	0.95	1 (9%)
12	GZL	iC	3	12	11,11,12	6.54	7 (63%)	13,15,17	1.33	1 (7%)
12	AHR	iC	4	12	9,9,10	0.54	0	11,12,14	0.98	1 (9%)
12	AHR	iC	5	12	9,9,10	0.53	0	11,12,14	1.04	1 (9%)
3	FUB	iD	1	3	9,9,10	0.54	0	11,12,14	0.96	0
3	FUB	iD	2	3	9,9,10	0.53	0	11,12,14	0.80	0
3	FUB	iD	3	3	9,9,10	0.54	0	11,12,14	0.91	0
22	FUB	iE	1	22	9,9,10	0.52	0	11,12,14	1.10	1 (9%)
22	FUB	iE	2	22	9,9,10	0.53	0	11,12,14	0.86	0
22	GZL	iE	3	22	11,11,12	6.61	6 (54%)	13,15,17	1.28	1 (7%)
22	AHR	iE	4	22	9,9,10	0.57	0	11,12,14	0.98	0
22	AHR	iE	5	22	9,9,10	0.54	0	11,12,14	0.60	0
22	AHR	iE	6	22	9,9,10	0.55	0	11,12,14	1.08	1 (9%)
9	FUB	j	1	9	9,9,10	0.55	0	11,12,14	1.01	1 (9%)
9	FUB	j	2	9	9,9,10	0.54	0	11,12,14	0.77	0
3	FUB	jA	1	3	9,9,10	0.54	0	11,12,14	0.98	1 (9%)
3	FUB	jA	2	3	9,9,10	0.56	0	11,12,14	0.88	0
3	FUB	jA	3	3	9,9,10	0.54	0	11,12,14	1.02	1 (9%)
13	FUB	jB	1	13	9,9,10	0.54	0	11,12,14	1.02	1 (9%)
13	FUB	jB	2	13	9,9,10	0.54	0	11,12,14	0.88	0
13	GZL	jB	3	13	11,11,12	6.61	7 (63%)	13,15,17	1.33	1 (7%)
13	AHR	jB	4	13	9,9,10	0.56	0	11,12,14	0.96	0
4	FUB	jC	1	4	9,9,10	0.53	0	11,12,14	0.97	1 (9%)
4	FUB	jC	2	4	9,9,10	0.55	0	11,12,14	0.94	0
4	FUB	jC	3	4	9,9,10	0.54	0	11,12,14	0.96	0
4	AHR	jC	4	4	9,9,10	0.54	0	11,12,14	0.85	0
10	FUB	jD	1	10	9,9,10	0.52	0	11,12,14	1.11	1 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	FUB	jD	2	10	9,9,10	0.56	0	11,12,14	0.95	0
10	FUB	jD	3	10	9,9,10	0.55	0	11,12,14	0.91	0
10	AHR	jD	4	10	9,9,10	0.56	0	11,12,14	0.95	0
10	AHR	jD	5	10	9,9,10	0.55	0	11,12,14	1.02	1 (9%)
20	FUB	jE	1	20	9,9,10	0.56	0	11,12,14	0.99	0
20	FUB	jE	2	20	9,9,10	0.54	0	11,12,14	0.90	0
20	GZL	jE	3	20	11,11,12	6.58	6 (54%)	13,15,17	1.51	2 (15%)
20	AHR	jE	4	20	9,9,10	0.55	0	11,12,14	0.88	0
4	FUB	k	1	4	9,9,10	0.56	0	11,12,14	0.83	0
4	FUB	k	2	4	9,9,10	0.56	0	11,12,14	0.94	0
4	FUB	k	3	4	9,9,10	0.53	0	11,12,14	0.90	0
4	AHR	k	4	4	9,9,10	0.55	0	11,12,14	0.95	0
3	FUB	kA	1	3	9,9,10	0.51	0	11,12,14	0.76	0
3	FUB	kA	2	3	9,9,10	0.53	0	11,12,14	0.80	0
3	FUB	kA	3	3	9,9,10	0.55	0	11,12,14	0.86	0
14	FUB	kB	1	14	9,9,10	0.56	0	11,12,14	0.89	0
14	FUB	kB	2	14	9,9,10	0.53	0	11,12,14	1.02	1 (9%)
14	GZL	kB	3	14	11,11,12	6.51	7 (63%)	13,15,17	1.61	3 (23%)
14	FUB	kB	4	14	9,9,10	0.54	0	11,12,14	1.04	1 (9%)
14	FUB	kC	1	14	9,9,10	0.55	0	11,12,14	0.95	0
14	FUB	kC	2	14	9,9,10	0.56	0	11,12,14	0.95	0
14	GZL	kC	3	14	11,11,12	6.52	7 (63%)	13,15,17	1.89	2 (15%)
14	FUB	kC	4	14	9,9,10	0.58	0	11,12,14	0.87	0
4	FUB	kD	1	4	9,9,10	0.57	0	11,12,14	0.94	0
4	FUB	kD	2	4	9,9,10	0.55	0	11,12,14	0.85	0
4	FUB	kD	3	4	9,9,10	0.53	0	11,12,14	0.89	0
4	AHR	kD	4	4	9,9,10	0.54	0	11,12,14	0.92	0
21	FUB	kE	1	21	9,9,10	0.54	0	11,12,14	1.09	1 (9%)
21	FUB	kE	2	21	9,9,10	0.54	0	11,12,14	0.99	1 (9%)
21	GZL	kE	3	21	11,11,12	6.60	6 (54%)	13,15,17	1.23	1 (7%)
21	AHR	kE	4	21	9,9,10	0.56	0	11,12,14	0.96	0
21	AHR	kE	5	21	9,9,10	0.54	0	11,12,14	1.06	1 (9%)
3	FUB	l	1	3	9,9,10	0.55	0	11,12,14	0.90	0
3	FUB	l	2	3	9,9,10	0.51	0	11,12,14	0.82	0
3	FUB	l	3	3	9,9,10	0.54	0	11,12,14	0.87	0
12	FUB	lA	1	12	9,9,10	0.52	0	11,12,14	0.90	0
12	FUB	lA	2	12	9,9,10	0.56	0	11,12,14	0.92	0
12	GZL	lA	3	12	11,11,12	6.59	7 (63%)	13,15,17	1.22	1 (7%)
12	AHR	lA	4	12	9,9,10	0.55	0	11,12,14	1.08	1 (9%)
12	AHR	lA	5	12	9,9,10	0.55	0	11,12,14	1.07	1 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	FUB	lB	1	12	9,9,10	0.52	0	11,12,14	1.10	1 (9%)
12	FUB	lB	2	12	9,9,10	0.55	0	11,12,14	0.93	0
12	GZL	lB	3	12	11,11,12	6.57	7 (63%)	13,15,17	1.25	1 (7%)
12	AHR	lB	4	12	9,9,10	0.54	0	11,12,14	0.98	0
12	AHR	lB	5	12	9,9,10	0.55	0	11,12,14	0.95	0
3	FUB	lC	1	3	9,9,10	0.54	0	11,12,14	0.81	0
3	FUB	lC	2	3	9,9,10	0.54	0	11,12,14	0.86	0
3	FUB	lC	3	3	9,9,10	0.56	0	11,12,14	0.97	0
3	FUB	lD	1	3	9,9,10	0.56	0	11,12,14	0.87	0
3	FUB	lD	2	3	9,9,10	0.54	0	11,12,14	0.92	0
3	FUB	lD	3	3	9,9,10	0.56	0	11,12,14	0.85	0
24	FUB	lE	1	24	9,9,10	0.52	0	11,12,14	1.22	1 (9%)
24	FUB	lE	2	24	9,9,10	0.53	0	11,12,14	1.00	1 (9%)
24	GZL	lE	3	24	11,11,12	6.57	7 (63%)	13,15,17	1.43	1 (7%)
24	AHR	lE	4	24	9,9,10	0.57	0	11,12,14	1.11	2 (18%)
24	AHR	lE	5	24	9,9,10	0.53	0	11,12,14	1.05	1 (9%)
24	AHR	lE	6	24	9,9,10	0.54	0	11,12,14	1.08	1 (9%)
3	FUB	m	1	3	9,9,10	0.51	0	11,12,14	0.86	0
3	FUB	m	2	3	9,9,10	0.54	0	11,12,14	0.80	0
3	FUB	m	3	3	9,9,10	0.55	0	11,12,14	0.86	0
13	FUB	mA	1	13	9,9,10	0.54	0	11,12,14	0.83	0
13	FUB	mA	2	13	9,9,10	0.57	0	11,12,14	0.88	0
13	GZL	mA	3	13	11,11,12	6.61	6 (54%)	13,15,17	1.26	1 (7%)
13	AHR	mA	4	13	9,9,10	0.52	0	11,12,14	1.03	1 (9%)
4	FUB	mB	1	4	9,9,10	0.53	0	11,12,14	0.96	1 (9%)
4	FUB	mB	2	4	9,9,10	0.53	0	11,12,14	0.92	0
4	FUB	mB	3	4	9,9,10	0.55	0	11,12,14	1.00	0
4	AHR	mB	4	4	9,9,10	0.55	0	11,12,14	0.87	1 (9%)
10	FUB	mC	1	10	9,9,10	0.55	0	11,12,14	1.09	1 (9%)
10	FUB	mC	2	10	9,9,10	0.56	0	11,12,14	0.97	0
10	FUB	mC	3	10	9,9,10	0.55	0	11,12,14	0.82	0
10	AHR	mC	4	10	9,9,10	0.54	0	11,12,14	0.99	1 (9%)
10	AHR	mC	5	10	9,9,10	0.54	0	11,12,14	1.13	1 (9%)
3	FUB	mD	1	3	9,9,10	0.54	0	11,12,14	0.71	0
3	FUB	mD	2	3	9,9,10	0.55	0	11,12,14	0.96	0
3	FUB	mD	3	3	9,9,10	0.53	0	11,12,14	1.01	1 (9%)
6	FUB	mE	1	6	9,9,10	0.56	0	11,12,14	0.96	0
6	FUB	mE	2	6	9,9,10	0.55	0	11,12,14	0.95	0
6	GZL	mE	3	6	11,11,12	6.58	6 (54%)	13,15,17	1.64	2 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	FUB	n	1	12	9,9,10	0.53	0	11,12,14	0.84	0
12	FUB	n	2	12	9,9,10	0.55	0	11,12,14	0.82	0
12	GZL	n	3	12	11,11,12	6.58	7 (63%)	13,15,17	1.28	1 (7%)
12	AHR	n	4	12	9,9,10	0.53	0	11,12,14	1.09	1 (9%)
12	AHR	n	5	12	9,9,10	0.55	0	11,12,14	1.03	1 (9%)
14	FUB	nA	1	14	9,9,10	0.50	0	11,12,14	0.88	0
14	FUB	nA	2	14	9,9,10	0.56	0	11,12,14	0.85	0
14	GZL	nA	3	14	11,11,12	6.58	6 (54%)	13,15,17	1.92	4 (30%)
14	FUB	nA	4	14	9,9,10	0.56	0	11,12,14	1.05	0
14	FUB	nB	1	14	9,9,10	0.55	0	11,12,14	0.89	0
14	FUB	nB	2	14	9,9,10	0.55	0	11,12,14	0.99	0
14	GZL	nB	3	14	11,11,12	6.53	7 (63%)	13,15,17	1.61	3 (23%)
14	FUB	nB	4	14	9,9,10	0.55	0	11,12,14	1.05	1 (9%)
4	FUB	nC	1	4	9,9,10	0.54	0	11,12,14	1.02	1 (9%)
4	FUB	nC	2	4	9,9,10	0.54	0	11,12,14	0.96	0
4	FUB	nC	3	4	9,9,10	0.55	0	11,12,14	0.94	0
4	AHR	nC	4	4	9,9,10	0.56	0	11,12,14	1.00	1 (9%)
3	FUB	nD	1	3	9,9,10	0.57	0	11,12,14	0.98	0
3	FUB	nD	2	3	9,9,10	0.56	0	11,12,14	0.93	0
3	FUB	nD	3	3	9,9,10	0.52	0	11,12,14	0.65	0
6	FUB	nE	1	6	9,9,10	0.55	0	11,12,14	1.08	1 (9%)
6	FUB	nE	2	6	9,9,10	0.55	0	11,12,14	0.95	0
6	GZL	nE	3	6	11,11,12	6.55	7 (63%)	13,15,17	1.49	1 (7%)
13	FUB	o	1	13	9,9,10	0.55	0	11,12,14	0.78	0
13	FUB	o	2	13	9,9,10	0.56	0	11,12,14	0.85	0
13	GZL	o	3	13	11,11,12	6.62	7 (63%)	13,15,17	1.26	1 (7%)
13	AHR	o	4	13	9,9,10	0.54	0	11,12,14	1.04	1 (9%)
12	FUB	oA	1	12	9,9,10	0.52	0	11,12,14	1.06	1 (9%)
12	FUB	oA	2	12	9,9,10	0.54	0	11,12,14	0.91	0
12	GZL	oA	3	12	11,11,12	6.60	6 (54%)	13,15,17	1.27	1 (7%)
12	AHR	oA	4	12	9,9,10	0.57	0	11,12,14	0.91	0
12	AHR	oA	5	12	9,9,10	0.57	0	11,12,14	1.02	0
3	FUB	oB	1	3	9,9,10	0.54	0	11,12,14	1.04	1 (9%)
3	FUB	oB	2	3	9,9,10	0.54	0	11,12,14	0.82	0
3	FUB	oB	3	3	9,9,10	0.54	0	11,12,14	1.01	1 (9%)
3	FUB	oC	1	3	9,9,10	0.57	0	11,12,14	0.91	0
3	FUB	oC	2	3	9,9,10	0.54	0	11,12,14	0.90	0
3	FUB	oC	3	3	9,9,10	0.57	0	11,12,14	0.88	0
3	FUB	oD	1	3	9,9,10	0.56	0	11,12,14	0.96	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	FUB	oD	2	3	9,9,10	0.55	0	11,12,14	0.86	0
3	FUB	oD	3	3	9,9,10	0.55	0	11,12,14	1.02	1 (9%)
6	FUB	oE	1	6	9,9,10	0.55	0	11,12,14	0.78	0
6	FUB	oE	2	6	9,9,10	0.54	0	11,12,14	0.96	1 (9%)
6	GZL	oE	3	6	11,11,12	6.55	7 (63%)	13,15,17	1.65	2 (15%)
14	FUB	p	1	14	9,9,10	0.52	0	11,12,14	0.85	0
14	FUB	p	2	14	9,9,10	0.55	0	11,12,14	0.88	0
14	GZL	p	3	14	11,11,12	6.56	6 (54%)	13,15,17	1.72	4 (30%)
14	FUB	p	4	14	9,9,10	0.55	0	11,12,14	1.04	1 (9%)
4	FUB	pA	1	4	9,9,10	0.54	0	11,12,14	0.74	0
4	FUB	pA	2	4	9,9,10	0.54	0	11,12,14	0.83	0
4	FUB	pA	3	4	9,9,10	0.55	0	11,12,14	0.80	0
4	AHR	pA	4	4	9,9,10	0.53	0	11,12,14	0.83	0
10	FUB	pB	1	10	9,9,10	0.56	0	11,12,14	1.05	0
10	FUB	pB	2	10	9,9,10	0.55	0	11,12,14	1.02	0
10	FUB	pB	3	10	9,9,10	0.55	0	11,12,14	0.83	0
10	AHR	pB	4	10	9,9,10	0.55	0	11,12,14	1.02	1 (9%)
10	AHR	pB	5	10	9,9,10	0.55	0	11,12,14	1.11	1 (9%)
3	FUB	pC	1	3	9,9,10	0.55	0	11,12,14	1.04	1 (9%)
3	FUB	pC	2	3	9,9,10	0.55	0	11,12,14	1.01	0
3	FUB	pC	3	3	9,9,10	0.55	0	11,12,14	0.88	0
3	FUB	pD	1	3	9,9,10	0.56	0	11,12,14	1.07	0
3	FUB	pD	2	3	9,9,10	0.53	0	11,12,14	0.95	0
3	FUB	pD	3	3	9,9,10	0.53	0	11,12,14	1.01	1 (9%)
18	FUB	pE	1	18	9,9,10	0.53	0	11,12,14	2.22	5 (45%)
18	FUB	pE	2	18	9,9,10	0.55	0	11,12,14	0.95	0
18	GZL	pE	3	18	11,11,12	6.57	7 (63%)	13,15,17	1.42	1 (7%)
18	AHR	pE	4	18	9,9,10	0.56	0	11,12,14	1.01	0
18	AHR	pE	5	18	9,9,10	0.58	0	11,12,14	1.15	1 (9%)
12	FUB	q	1	12	9,9,10	0.53	0	11,12,14	0.99	1 (9%)
12	FUB	q	2	12	9,9,10	0.54	0	11,12,14	0.91	0
12	GZL	q	3	12	11,11,12	6.58	7 (63%)	13,15,17	1.30	1 (7%)
12	AHR	q	4	12	9,9,10	0.55	0	11,12,14	0.95	1 (9%)
12	AHR	q	5	12	9,9,10	0.53	0	11,12,14	1.01	1 (9%)
14	FUB	qA	1	14	9,9,10	0.57	0	11,12,14	0.78	0
14	FUB	qA	2	14	9,9,10	0.56	0	11,12,14	0.89	0
14	GZL	qA	3	14	11,11,12	6.59	6 (54%)	13,15,17	1.72	2 (15%)
14	FUB	qA	4	14	9,9,10	0.56	0	11,12,14	0.99	0
4	FUB	qB	1	4	9,9,10	0.56	0	11,12,14	1.02	1 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	FUB	qB	2	4	9,9,10	0.55	0	11,12,14	0.97	1 (9%)
4	FUB	qB	3	4	9,9,10	0.55	0	11,12,14	0.96	0
4	AHR	qB	4	4	9,9,10	0.54	0	11,12,14	1.04	1 (9%)
3	FUB	qC	1	3	9,9,10	0.54	0	11,12,14	0.95	0
3	FUB	qC	2	3	9,9,10	0.54	0	11,12,14	0.81	0
3	FUB	qC	3	3	9,9,10	0.52	0	11,12,14	0.63	0
3	FUB	qD	1	3	9,9,10	0.56	0	11,12,14	0.88	0
3	FUB	qD	2	3	9,9,10	0.55	0	11,12,14	0.91	0
3	FUB	qD	3	3	9,9,10	0.53	0	11,12,14	0.91	0
19	FUB	qE	1	19	9,9,10	0.55	0	11,12,14	1.16	1 (9%)
19	FUB	qE	2	19	9,9,10	0.56	0	11,12,14	0.86	0
19	GZL	qE	3	19	11,11,12	6.59	6 (54%)	13,15,17	1.49	2 (15%)
19	AHR	qE	4	19	9,9,10	0.56	0	11,12,14	0.83	0
4	FUB	r	1	4	9,9,10	0.53	0	11,12,14	0.77	0
4	FUB	r	2	4	9,9,10	0.54	0	11,12,14	0.85	0
4	FUB	r	3	4	9,9,10	0.55	0	11,12,14	0.88	0
4	AHR	r	4	4	9,9,10	0.55	0	11,12,14	0.76	0
3	FUB	rA	1	3	9,9,10	0.52	0	11,12,14	0.80	0
3	FUB	rA	2	3	9,9,10	0.53	0	11,12,14	0.78	0
3	FUB	rA	3	3	9,9,10	0.56	0	11,12,14	0.90	0
3	FUB	rB	1	3	9,9,10	0.54	0	11,12,14	0.93	1 (9%)
3	FUB	rB	2	3	9,9,10	0.54	0	11,12,14	0.83	0
3	FUB	rB	3	3	9,9,10	0.54	0	11,12,14	0.96	0
3	FUB	rC	1	3	9,9,10	0.55	0	11,12,14	1.04	1 (9%)
3	FUB	rC	2	3	9,9,10	0.55	0	11,12,14	0.90	0
3	FUB	rC	3	3	9,9,10	0.56	0	11,12,14	0.96	0
3	FUB	rD	1	3	9,9,10	0.53	0	11,12,14	1.02	1 (9%)
3	FUB	rD	2	3	9,9,10	0.56	0	11,12,14	0.88	0
3	FUB	rD	3	3	9,9,10	0.54	0	11,12,14	0.95	0
18	FUB	rE	1	18	9,9,10	0.58	0	11,12,14	1.02	0
18	FUB	rE	2	18	9,9,10	0.54	0	11,12,14	1.06	1 (9%)
18	GZL	rE	3	18	11,11,12	6.61	7 (63%)	13,15,17	1.35	1 (7%)
18	AHR	rE	4	18	9,9,10	0.53	0	11,12,14	0.78	0
18	AHR	rE	5	18	9,9,10	0.55	0	11,12,14	1.10	1 (9%)
14	FUB	s	1	14	9,9,10	0.52	0	11,12,14	0.86	0
14	FUB	s	2	14	9,9,10	0.56	0	11,12,14	0.92	0
14	GZL	s	3	14	11,11,12	6.56	7 (63%)	13,15,17	1.95	3 (23%)
14	FUB	s	4	14	9,9,10	0.57	0	11,12,14	0.88	0
10	FUB	sA	1	10	9,9,10	0.55	0	11,12,14	0.98	0
10	FUB	sA	2	10	9,9,10	0.54	0	11,12,14	0.84	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	FUB	sA	3	10	9,9,10	0.53	0	11,12,14	0.79	0
10	AHR	sA	4	10	9,9,10	0.55	0	11,12,14	1.07	1 (9%)
10	AHR	sA	5	10	9,9,10	0.54	0	11,12,14	1.12	1 (9%)
3	FUB	sB	1	3	9,9,10	0.58	0	11,12,14	0.92	0
3	FUB	sB	2	3	9,9,10	0.55	0	11,12,14	1.01	0
3	FUB	sB	3	3	9,9,10	0.55	0	11,12,14	0.82	0
3	FUB	sC	1	3	9,9,10	0.52	0	11,12,14	1.04	1 (9%)
3	FUB	sC	2	3	9,9,10	0.55	0	11,12,14	0.86	0
3	FUB	sC	3	3	9,9,10	0.55	0	11,12,14	0.99	0
10	FUB	sD	1	10	9,9,10	0.54	0	11,12,14	1.04	1 (9%)
10	FUB	sD	2	10	9,9,10	0.55	0	11,12,14	0.82	0
10	FUB	sD	3	10	9,9,10	0.55	0	11,12,14	0.98	0
10	AHR	sD	4	10	9,9,10	0.55	0	11,12,14	0.89	0
10	AHR	sD	5	10	9,9,10	0.55	0	11,12,14	0.73	0
20	FUB	sE	1	20	9,9,10	0.53	0	11,12,14	1.02	1 (9%)
20	FUB	sE	2	20	9,9,10	0.55	0	11,12,14	0.99	0
20	GZL	sE	3	20	11,11,12	6.59	6 (54%)	13,15,17	1.45	1 (7%)
20	AHR	sE	4	20	9,9,10	0.55	0	11,12,14	1.02	1 (9%)
3	FUB	t	1	3	9,9,10	0.54	0	11,12,14	0.94	0
3	FUB	t	2	3	9,9,10	0.54	0	11,12,14	0.77	0
3	FUB	t	3	3	9,9,10	0.55	0	11,12,14	0.95	0
4	FUB	tA	1	4	9,9,10	0.52	0	11,12,14	1.05	1 (9%)
4	FUB	tA	2	4	9,9,10	0.55	0	11,12,14	0.80	0
4	FUB	tA	3	4	9,9,10	0.54	0	11,12,14	0.78	0
4	AHR	tA	4	4	9,9,10	0.54	0	11,12,14	1.10	1 (9%)
3	FUB	tB	1	3	9,9,10	0.56	0	11,12,14	0.82	0
3	FUB	tB	2	3	9,9,10	0.54	0	11,12,14	0.83	0
3	FUB	tB	3	3	9,9,10	0.53	0	11,12,14	0.73	0
3	FUB	tC	1	3	9,9,10	0.56	0	11,12,14	0.98	0
3	FUB	tC	2	3	9,9,10	0.56	0	11,12,14	0.91	0
3	FUB	tC	3	3	9,9,10	0.56	0	11,12,14	1.04	1 (9%)
13	FUB	tD	1	13	9,9,10	0.55	0	11,12,14	1.02	0
13	FUB	tD	2	13	9,9,10	0.53	0	11,12,14	1.11	1 (9%)
13	GZL	tD	3	13	11,11,12	6.65	6 (54%)	13,15,17	1.12	2 (15%)
13	AHR	tD	4	13	9,9,10	0.56	0	11,12,14	1.14	1 (9%)
18	FUB	tE	1	18	9,9,10	0.51	0	11,12,14	0.88	1 (9%)
18	FUB	tE	2	18	9,9,10	0.51	0	11,12,14	0.71	0
18	GZL	tE	3	18	11,11,12	6.57	7 (63%)	13,15,17	1.46	1 (7%)
18	AHR	tE	4	18	9,9,10	0.56	0	11,12,14	1.00	1 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	AHR	tE	5	18	9,9,10	0.56	0	11,12,14	0.94	0
10	FUB	u	1	10	9,9,10	0.55	0	11,12,14	1.03	1 (9%)
10	FUB	u	2	10	9,9,10	0.55	0	11,12,14	0.86	0
10	FUB	u	3	10	9,9,10	0.53	0	11,12,14	0.91	0
10	AHR	u	4	10	9,9,10	0.56	0	11,12,14	0.96	0
10	AHR	u	5	10	9,9,10	0.54	0	11,12,14	1.14	1 (9%)
3	FUB	uA	1	3	9,9,10	0.53	0	11,12,14	0.82	0
3	FUB	uA	2	3	9,9,10	0.55	0	11,12,14	0.82	0
3	FUB	uA	3	3	9,9,10	0.53	0	11,12,14	1.04	1 (9%)
3	FUB	uB	1	3	9,9,10	0.54	0	11,12,14	0.95	0
3	FUB	uB	2	3	9,9,10	0.55	0	11,12,14	0.86	0
3	FUB	uB	3	3	9,9,10	0.55	0	11,12,14	0.88	0
3	FUB	uC	1	3	9,9,10	0.52	0	11,12,14	0.89	0
3	FUB	uC	2	3	9,9,10	0.54	0	11,12,14	0.94	0
3	FUB	uC	3	3	9,9,10	0.56	0	11,12,14	0.98	1 (9%)
6	FUB	uD	1	6	9,9,10	0.54	0	11,12,14	1.04	1 (9%)
6	FUB	uD	2	6	9,9,10	0.57	0	11,12,14	1.00	0
6	GZL	uD	3	6	11,11,12	6.87	6 (54%)	13,15,17	4.15	4 (30%)
20	FUB	uE	1	20	9,9,10	0.52	0	11,12,14	0.87	1 (9%)
20	FUB	uE	2	20	9,9,10	0.50	0	11,12,14	0.88	0
20	GZL	uE	3	20	11,11,12	6.57	7 (63%)	13,15,17	1.39	1 (7%)
20	AHR	uE	4	20	9,9,10	0.56	0	11,12,14	0.85	0
4	FUB	v	1	4	9,9,10	0.54	0	11,12,14	1.05	1 (9%)
4	FUB	v	2	4	9,9,10	0.54	0	11,12,14	0.87	0
4	FUB	v	3	4	9,9,10	0.54	0	11,12,14	0.88	0
4	AHR	v	4	4	9,9,10	0.55	0	11,12,14	0.98	0
3	FUB	vA	1	3	9,9,10	0.55	0	11,12,14	0.81	0
3	FUB	vA	2	3	9,9,10	0.55	0	11,12,14	0.87	0
3	FUB	vA	3	3	9,9,10	0.55	0	11,12,14	1.05	1 (9%)
3	FUB	vB	1	3	9,9,10	0.52	0	11,12,14	1.12	1 (9%)
3	FUB	vB	2	3	9,9,10	0.56	0	11,12,14	0.85	0
3	FUB	vB	3	3	9,9,10	0.56	0	11,12,14	0.90	0
10	FUB	vC	1	10	9,9,10	0.53	0	11,12,14	1.02	1 (9%)
10	FUB	vC	2	10	9,9,10	0.54	0	11,12,14	0.79	0
10	FUB	vC	3	10	9,9,10	0.56	0	11,12,14	0.98	1 (9%)
10	AHR	vC	4	10	9,9,10	0.58	0	11,12,14	0.87	0
10	AHR	vC	5	10	9,9,10	0.54	0	11,12,14	0.84	1 (9%)
13	FUB	vD	1	13	9,9,10	0.53	0	11,12,14	0.93	0
13	FUB	vD	2	13	9,9,10	0.56	0	11,12,14	0.93	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	GZL	vD	3	13	11,11,12	6.56	7 (63%)	13,15,17	1.38	1 (7%)
13	AHR	vD	4	13	9,9,10	0.54	0	11,12,14	1.08	1 (9%)
21	FUB	vE	1	21	9,9,10	0.51	0	11,12,14	0.93	1 (9%)
21	FUB	vE	2	21	9,9,10	0.54	0	11,12,14	0.79	0
21	GZL	vE	3	21	11,11,12	6.60	6 (54%)	13,15,17	1.37	1 (7%)
21	AHR	vE	4	21	9,9,10	0.55	0	11,12,14	0.98	0
21	AHR	vE	5	21	9,9,10	0.54	0	11,12,14	0.70	0
3	FUB	w	1	3	9,9,10	0.55	0	11,12,14	0.85	0
3	FUB	w	2	3	9,9,10	0.56	0	11,12,14	0.91	0
3	FUB	w	3	3	9,9,10	0.53	0	11,12,14	1.00	1 (9%)
3	FUB	wA	1	3	9,9,10	0.55	0	11,12,14	0.74	0
3	FUB	wA	2	3	9,9,10	0.55	0	11,12,14	0.83	0
3	FUB	wA	3	3	9,9,10	0.55	0	11,12,14	0.85	1 (9%)
3	FUB	wB	1	3	9,9,10	0.54	0	11,12,14	0.83	0
3	FUB	wB	2	3	9,9,10	0.54	0	11,12,14	0.84	0
3	FUB	wB	3	3	9,9,10	0.56	0	11,12,14	0.84	0
13	FUB	wC	1	13	9,9,10	0.53	0	11,12,14	0.94	0
13	FUB	wC	2	13	9,9,10	0.51	0	11,12,14	1.05	1 (9%)
13	GZL	wC	3	13	11,11,12	6.69	7 (63%)	13,15,17	1.25	3 (23%)
13	AHR	wC	4	13	9,9,10	0.57	0	11,12,14	1.16	1 (9%)
13	FUB	wD	1	13	9,9,10	0.53	0	11,12,14	0.96	1 (9%)
13	FUB	wD	2	13	9,9,10	0.55	0	11,12,14	0.80	0
13	GZL	wD	3	13	11,11,12	6.58	7 (63%)	13,15,17	1.43	2 (15%)
13	AHR	wD	4	13	9,9,10	0.53	0	11,12,14	1.03	1 (9%)
22	FUB	wE	1	22	9,9,10	0.56	0	11,12,14	1.01	0
22	FUB	wE	2	22	9,9,10	0.56	0	11,12,14	0.93	0
22	GZL	wE	3	22	11,11,12	6.61	7 (63%)	13,15,17	1.33	1 (7%)
22	AHR	wE	4	22	9,9,10	0.53	0	11,12,14	0.93	0
22	AHR	wE	5	22	9,9,10	0.56	0	11,12,14	1.44	3 (27%)
22	AHR	wE	6	22	9,9,10	0.53	0	11,12,14	0.79	0
3	FUB	x	1	3	9,9,10	0.55	0	11,12,14	0.80	0
3	FUB	x	2	3	9,9,10	0.56	0	11,12,14	0.96	0
3	FUB	x	3	3	9,9,10	0.54	0	11,12,14	0.99	1 (9%)
3	FUB	xA	1	3	9,9,10	0.57	0	11,12,14	0.90	0
3	FUB	xA	2	3	9,9,10	0.56	0	11,12,14	0.88	0
3	FUB	xA	3	3	9,9,10	0.55	0	11,12,14	0.95	0
3	FUB	xB	1	3	9,9,10	0.52	0	11,12,14	1.04	1 (9%)
3	FUB	xB	2	3	9,9,10	0.53	0	11,12,14	0.80	0
3	FUB	xB	3	3	9,9,10	0.54	0	11,12,14	0.97	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	FUB	xC	1	6	9,9,10	0.52	0	11,12,14	1.05	1 (9%)
6	FUB	xC	2	6	9,9,10	0.56	0	11,12,14	1.02	0
6	GZL	xC	3	6	11,11,12	6.86	6 (54%)	13,15,17	4.12	4 (30%)
6	FUB	xD	1	6	9,9,10	0.55	0	11,12,14	0.82	0
6	FUB	xD	2	6	9,9,10	0.55	0	11,12,14	1.15	2 (18%)
6	GZL	xD	3	6	11,11,12	6.52	7 (63%)	13,15,17	1.63	2 (15%)
20	FUB	xE	1	20	9,9,10	0.55	0	11,12,14	1.11	1 (9%)
20	FUB	xE	2	20	9,9,10	0.54	0	11,12,14	0.70	0
20	GZL	xE	3	20	11,11,12	6.55	7 (63%)	13,15,17	1.44	1 (7%)
20	AHR	xE	4	20	9,9,10	0.53	0	11,12,14	0.96	0
3	FUB	y	1	3	9,9,10	0.54	0	11,12,14	0.99	0
3	FUB	y	2	3	9,9,10	0.55	0	11,12,14	0.90	0
3	FUB	y	3	3	9,9,10	0.53	0	11,12,14	0.83	0
3	FUB	yA	1	3	9,9,10	0.55	0	11,12,14	1.10	1 (9%)
3	FUB	yA	2	3	9,9,10	0.52	0	11,12,14	0.78	0
3	FUB	yA	3	3	9,9,10	0.55	0	11,12,14	0.84	0
10	FUB	yB	1	10	9,9,10	0.53	0	11,12,14	1.00	1 (9%)
10	FUB	yB	2	10	9,9,10	0.55	0	11,12,14	0.74	0
10	FUB	yB	3	10	9,9,10	0.56	0	11,12,14	1.08	0
10	AHR	yB	4	10	9,9,10	0.55	0	11,12,14	0.91	0
10	AHR	yB	5	10	9,9,10	0.55	0	11,12,14	0.73	0
13	FUB	yC	1	13	9,9,10	0.54	0	11,12,14	0.90	0
13	FUB	yC	2	13	9,9,10	0.53	0	11,12,14	0.98	1 (9%)
13	GZL	yC	3	13	11,11,12	6.56	7 (63%)	13,15,17	1.41	1 (7%)
13	AHR	yC	4	13	9,9,10	0.56	0	11,12,14	0.95	0
6	FUB	yD	1	6	9,9,10	0.52	0	11,12,14	0.89	1 (9%)
6	FUB	yD	2	6	9,9,10	0.53	0	11,12,14	1.03	1 (9%)
6	GZL	yD	3	6	11,11,12	6.60	7 (63%)	13,15,17	1.38	1 (7%)
18	FUB	yE	1	18	9,9,10	0.53	0	11,12,14	0.90	0
18	FUB	yE	2	18	9,9,10	0.50	0	11,12,14	0.86	0
18	GZL	yE	3	18	11,11,12	6.50	7 (63%)	13,15,17	1.62	2 (15%)
18	AHR	yE	4	18	9,9,10	0.55	0	11,12,14	1.09	1 (9%)
18	AHR	yE	5	18	9,9,10	0.53	0	11,12,14	1.08	1 (9%)
3	FUB	z	1	3	9,9,10	0.53	0	11,12,14	0.95	1 (9%)
3	FUB	z	2	3	9,9,10	0.54	0	11,12,14	0.88	0
3	FUB	z	3	3	9,9,10	0.54	0	11,12,14	0.83	0
3	FUB	zA	1	3	9,9,10	0.50	0	11,12,14	0.85	0
3	FUB	zA	2	3	9,9,10	0.56	0	11,12,14	0.85	0
3	FUB	zA	3	3	9,9,10	0.54	0	11,12,14	0.85	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	FUB	zB	1	13	9,9,10	0.52	0	11,12,14	1.00	0
13	FUB	zB	2	13	9,9,10	0.51	0	11,12,14	1.03	1 (9%)
13	GZL	zB	3	13	11,11,12	6.62	7 (63%)	13,15,17	1.17	1 (7%)
13	AHR	zB	4	13	9,9,10	0.56	0	11,12,14	1.08	1 (9%)
13	FUB	zC	1	13	9,9,10	0.54	0	11,12,14	0.91	0
13	FUB	zC	2	13	9,9,10	0.53	0	11,12,14	0.94	1 (9%)
13	GZL	zC	3	13	11,11,12	6.57	7 (63%)	13,15,17	1.41	2 (15%)
13	AHR	zC	4	13	9,9,10	0.54	0	11,12,14	0.97	0
6	FUB	zD	1	6	9,9,10	0.55	0	11,12,14	1.00	0
6	FUB	zD	2	6	9,9,10	0.55	0	11,12,14	0.96	1 (9%)
6	GZL	zD	3	6	11,11,12	6.59	7 (63%)	13,15,17	1.37	1 (7%)
18	FUB	zE	1	18	9,9,10	0.57	0	11,12,14	1.00	0
18	FUB	zE	2	18	9,9,10	0.56	0	11,12,14	1.05	1 (9%)
18	GZL	zE	3	18	11,11,12	6.53	7 (63%)	13,15,17	1.57	2 (15%)
18	AHR	zE	4	18	9,9,10	0.56	0	11,12,14	0.80	0
18	AHR	zE	5	18	9,9,10	0.55	0	11,12,14	0.94	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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	2/6/19/22	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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	NAG	4D	1	1,16	-	3/6/23/26	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	1,17	-	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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	1,17	-	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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	FUB	9	2	6	-	0/2/15/18	0/1/1/1
6	GZL	9	3	6	1/1/4/5	2/6/19/22	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	1,16	-	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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	FUB	BB	2	15	-	0/2/15/18	0/1/1/1
15	GZL	BB	3	15	1/1/4/5	2/6/19/22	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	5/6/19/22	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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	NAG	DB	1	1,17	-	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
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	1,16	-	3/6/23/26	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	1,17	-	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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	1/6/19/22	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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	5/6/19/22	0/1/1/1
20	AHR	uE	4	20	-	0/2/15/18	0/1/1/1
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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 1076 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	CD	3	GZL	C2-C3	-18.93	1.22	1.53
6	LA	3	GZL	C2-C3	-18.87	1.22	1.53
6	uD	3	GZL	C2-C3	-18.70	1.22	1.53
6	xC	3	GZL	C2-C3	-18.69	1.22	1.53
6	XB	3	GZL	C2-C3	-18.66	1.22	1.53

The worst 5 of 723 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	3A	3	GZL	C1-O4-C4	-12.94	82.02	107.84
6	CD	3	GZL	C1-O4-C4	-9.95	87.98	107.84
6	0B	3	GZL	C1-O4-C4	-9.64	88.59	107.84
6	LA	3	GZL	C1-O4-C4	-9.57	88.73	107.84
6	uD	3	GZL	C1-O4-C4	-9.30	89.28	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	C2

5 of 607 torsion outliers are listed below:

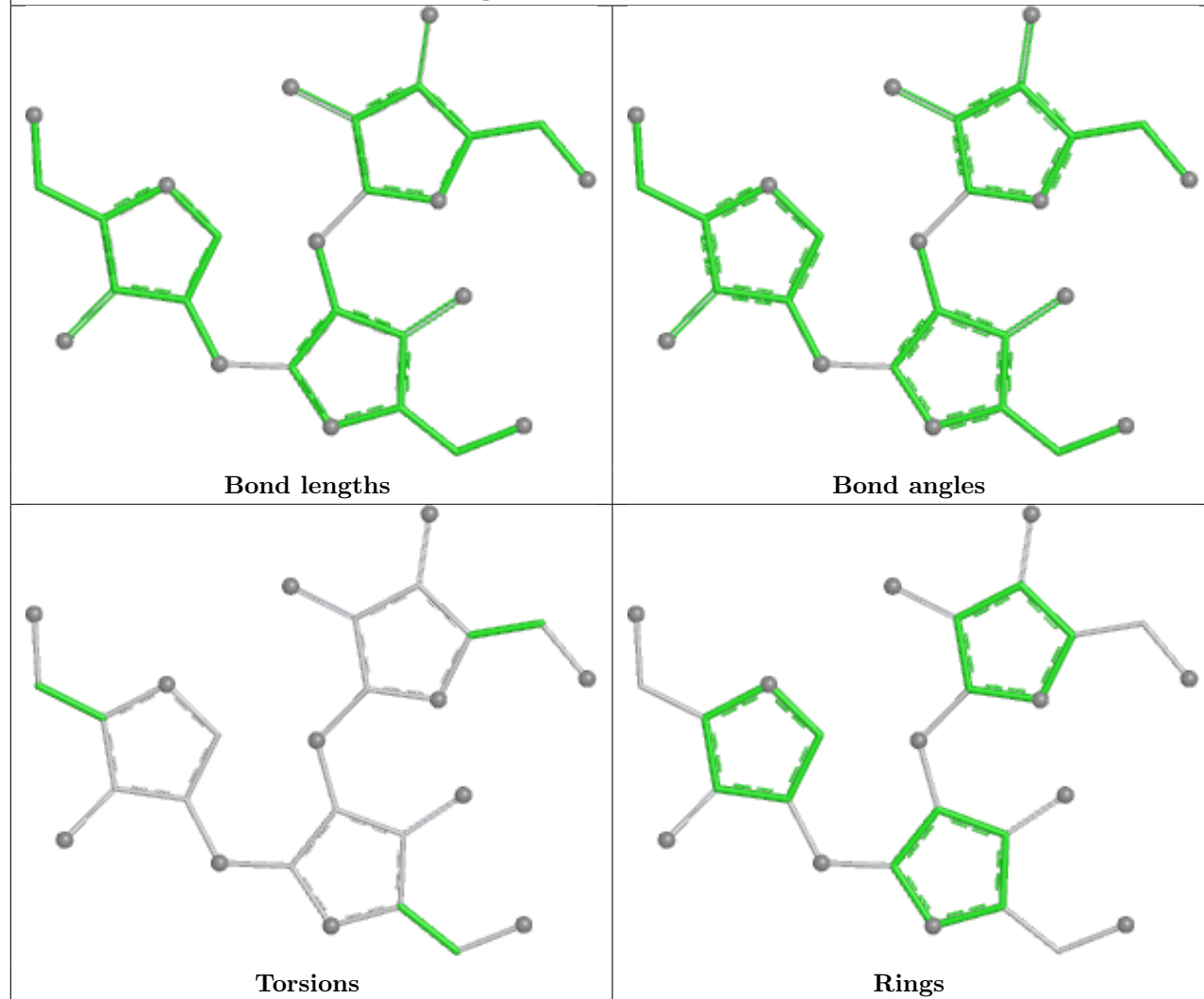
Mol	Chain	Res	Type	Atoms
6	N	3	GZL	C4-C5-C6-O6
6	N	3	GZL	O5-C5-C6-O6
6	5	3	GZL	O5-C5-C6-O6
6	AA	3	GZL	C3-C4-C5-C6
6	AA	3	GZL	O4-C4-C5-C6

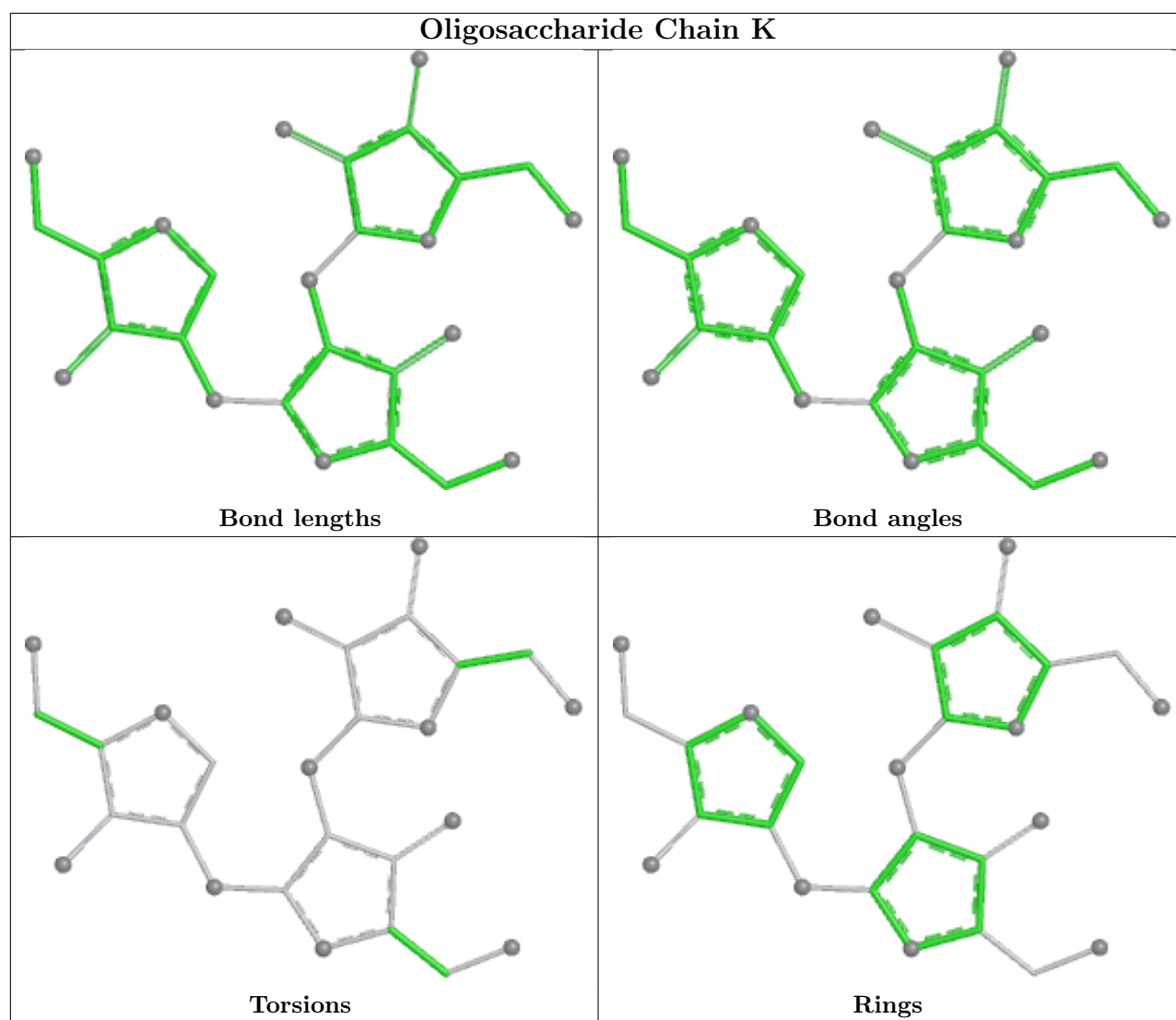
There are no ring outliers.

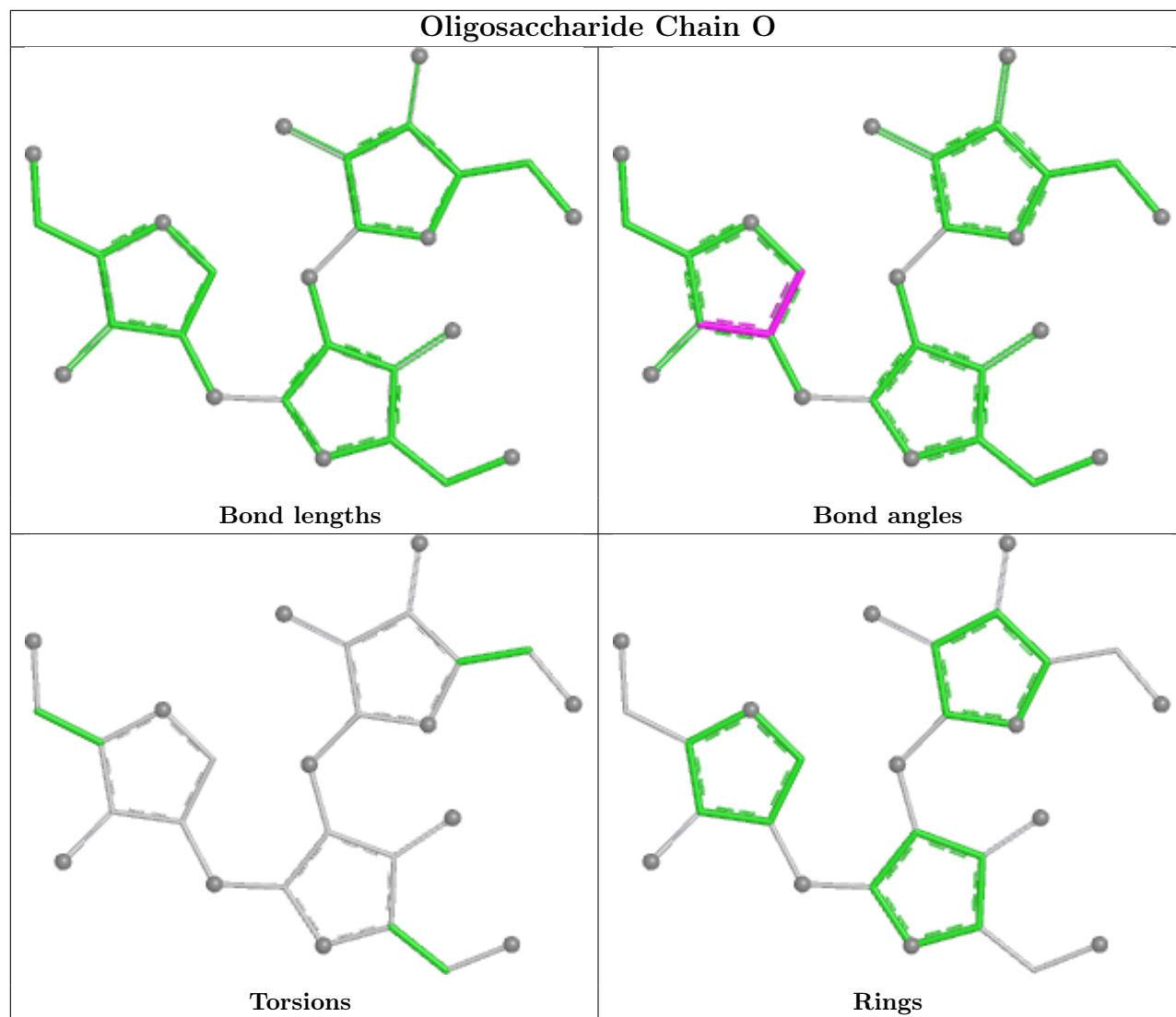
No monomer is involved in short contacts.

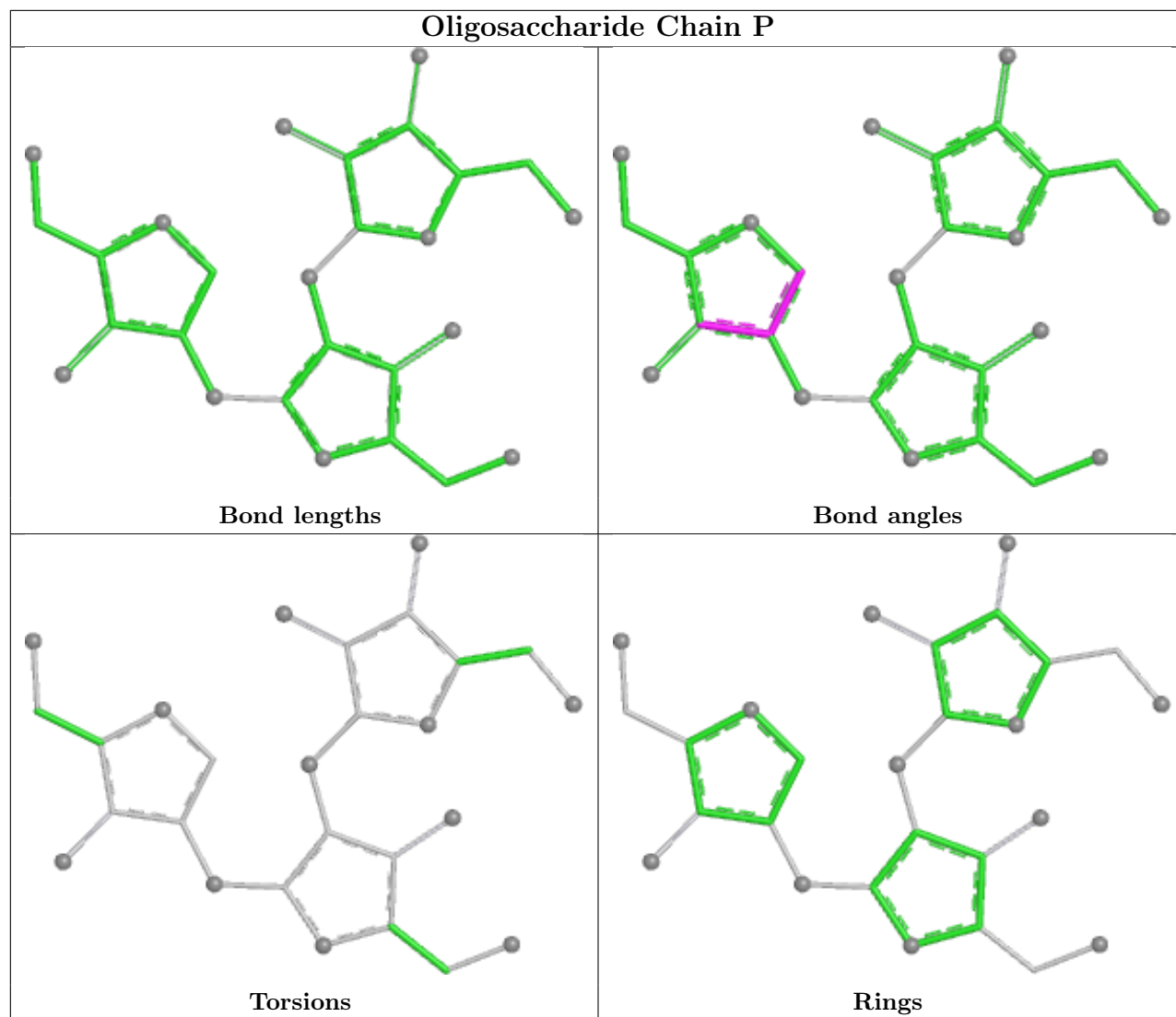
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

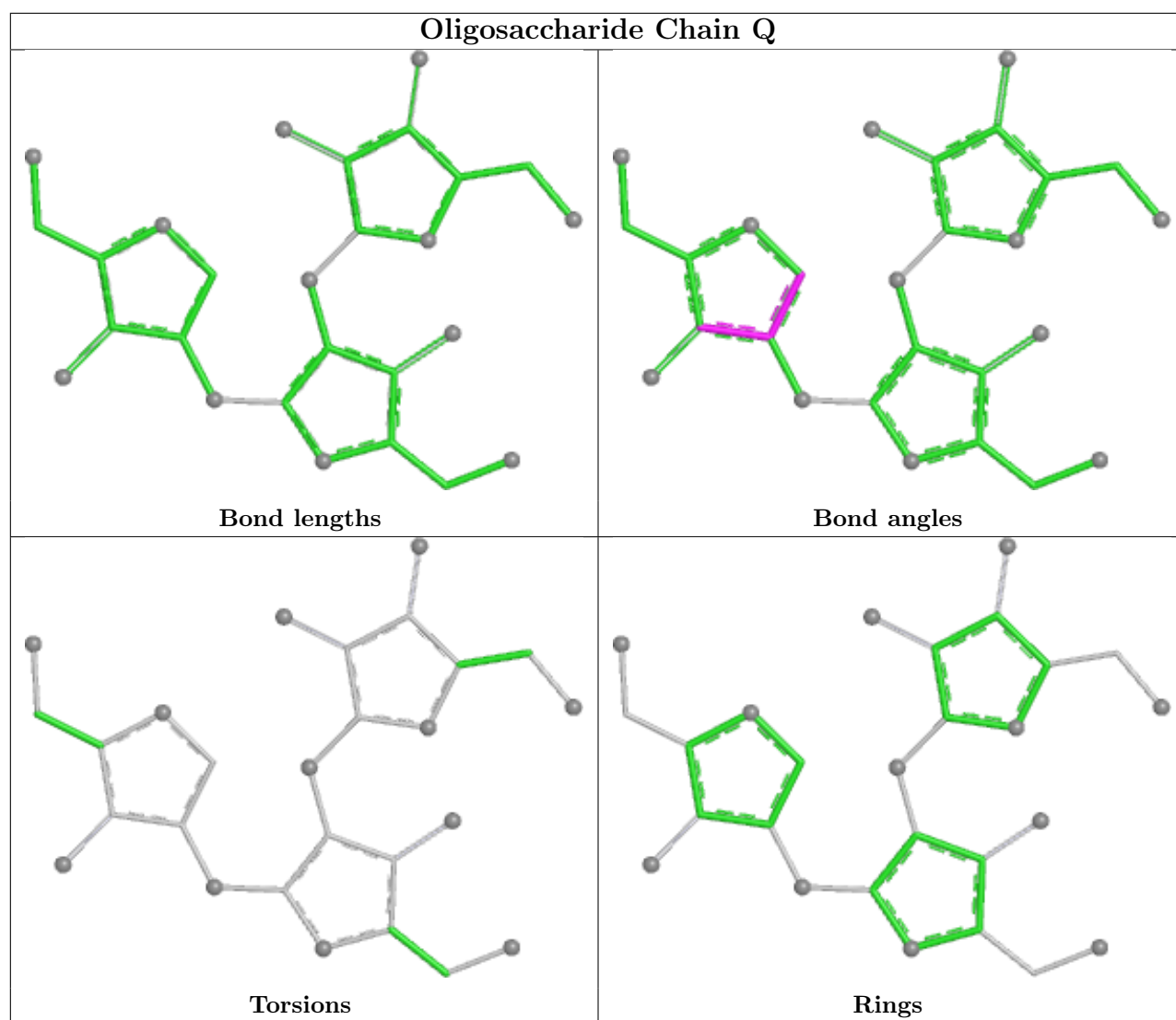
Oligosaccharide Chain J

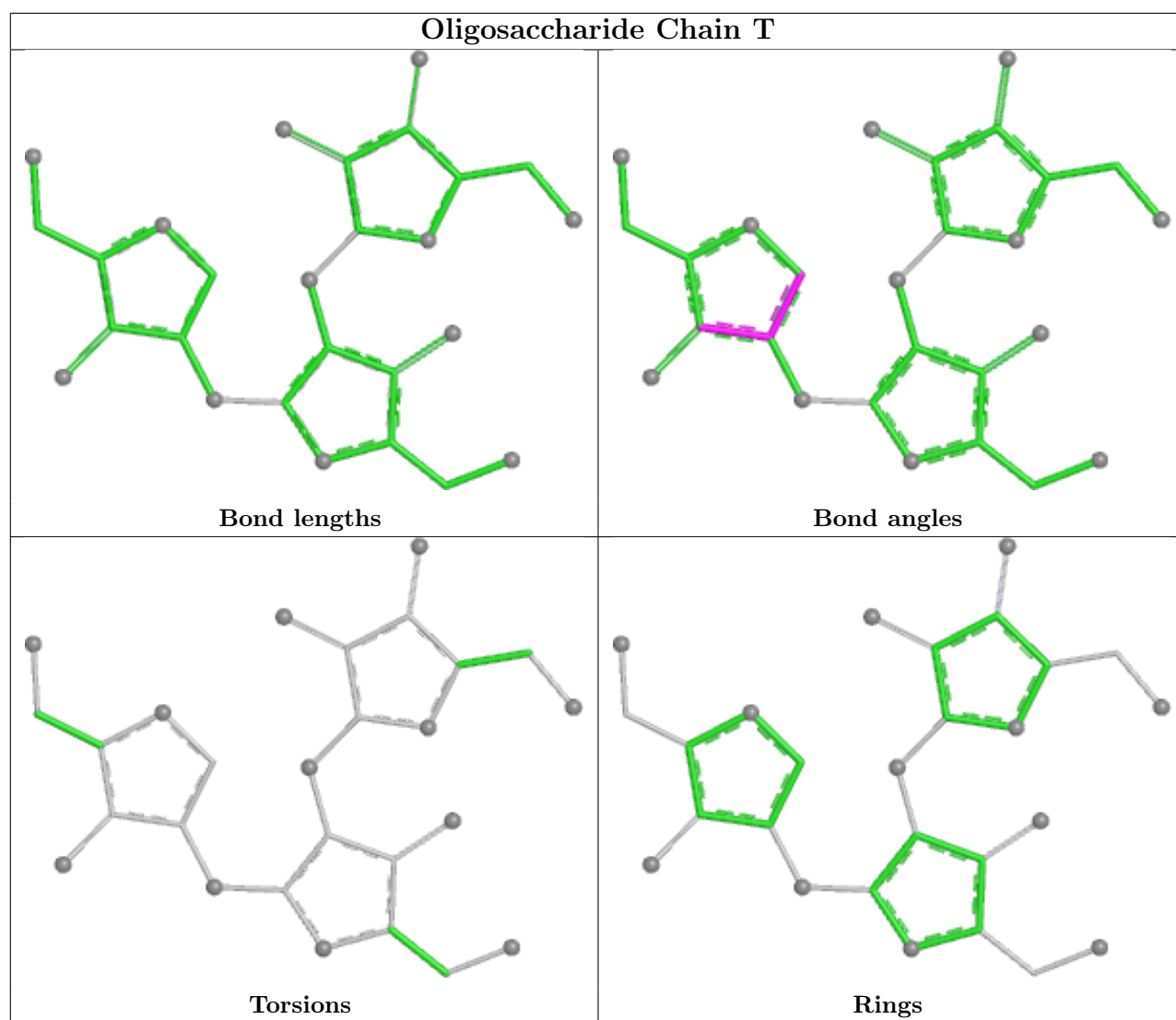


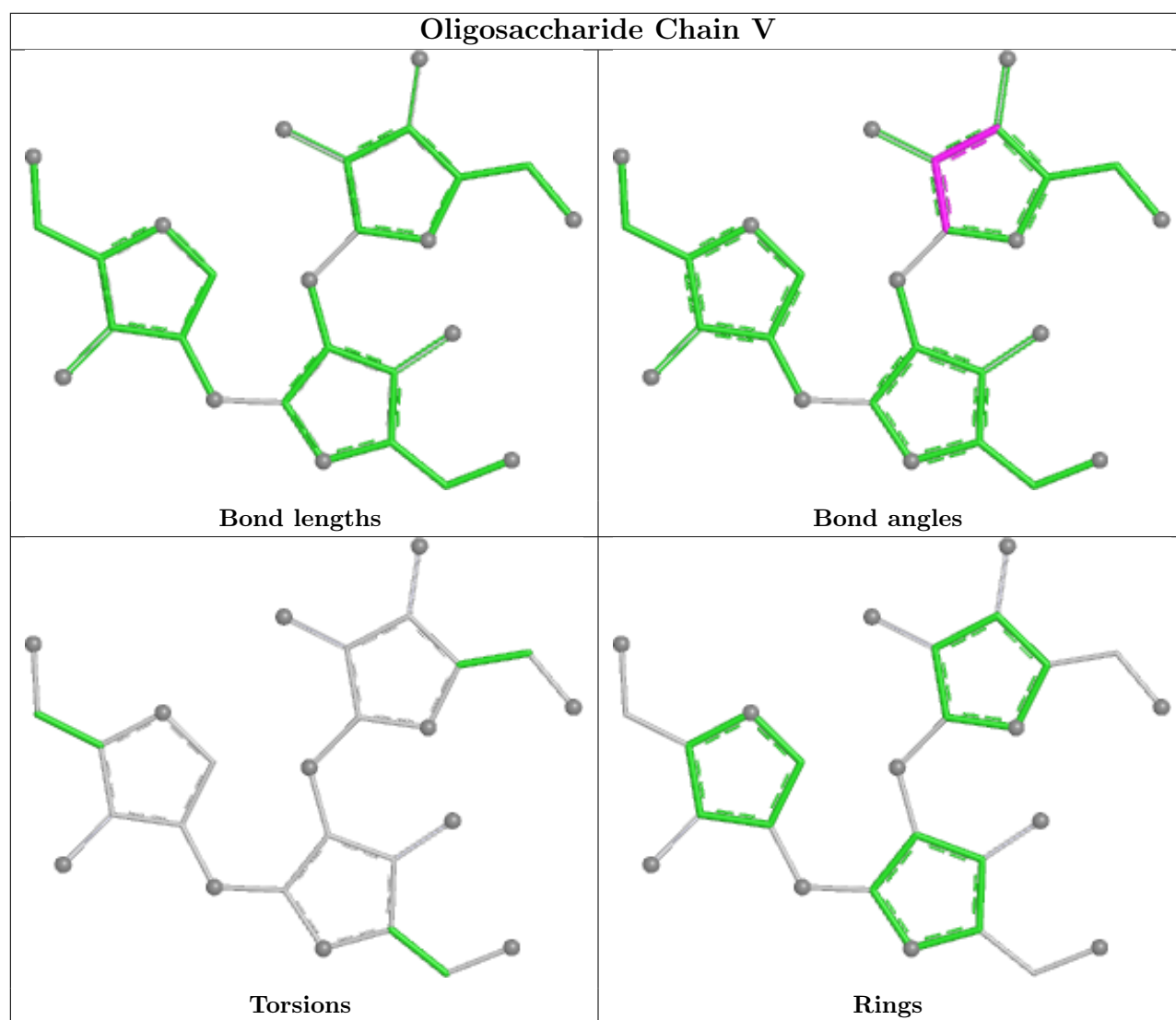


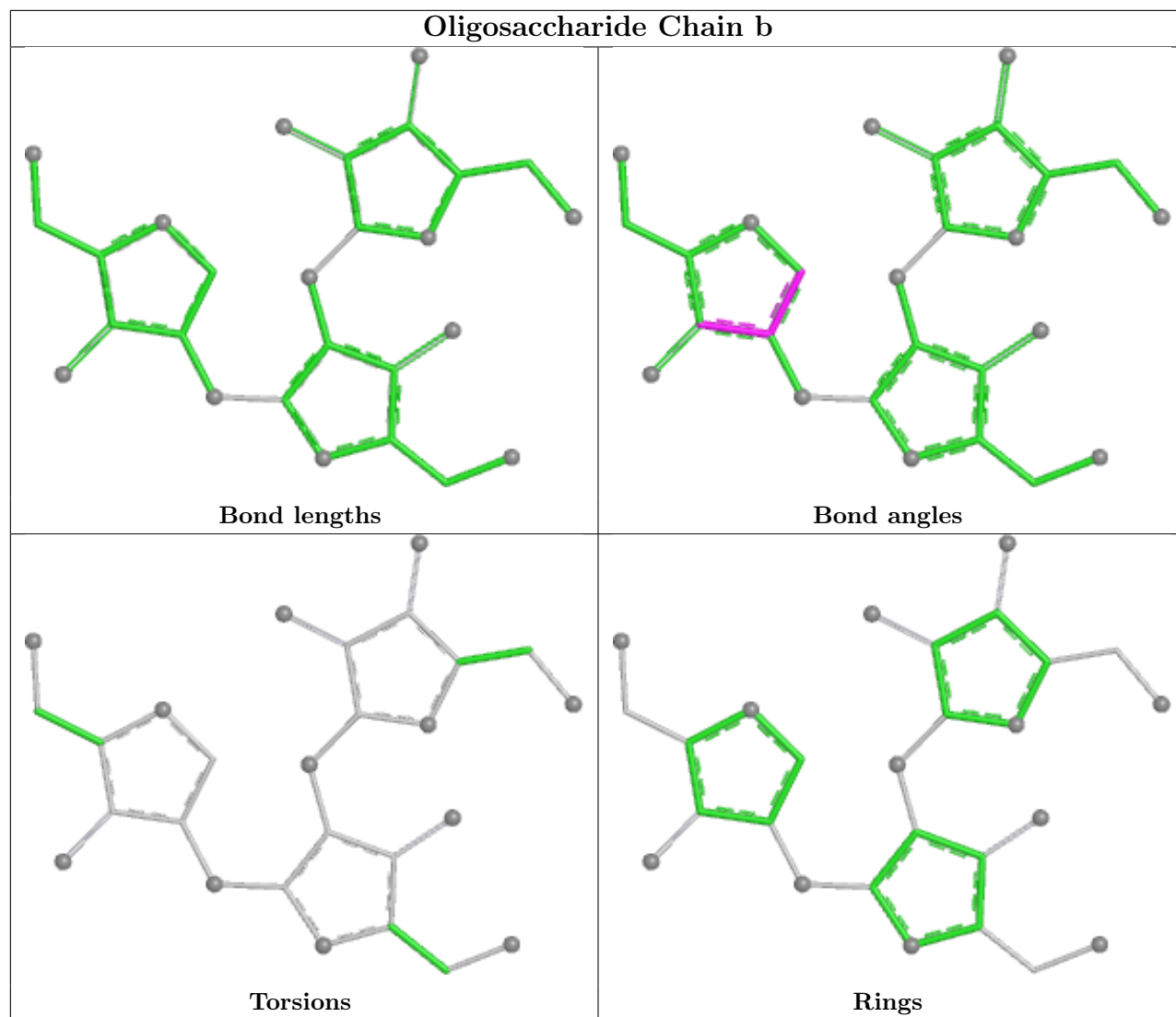


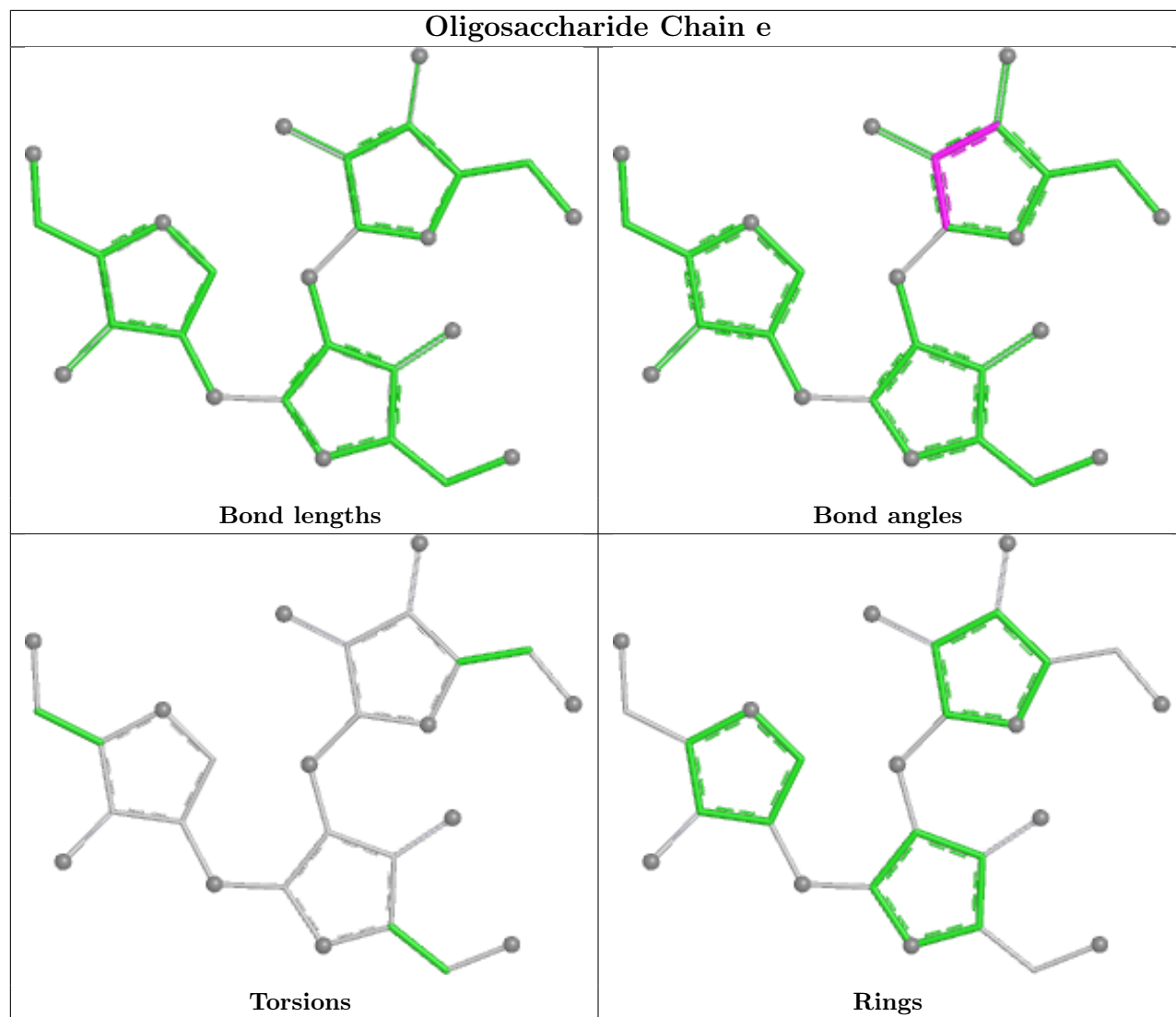


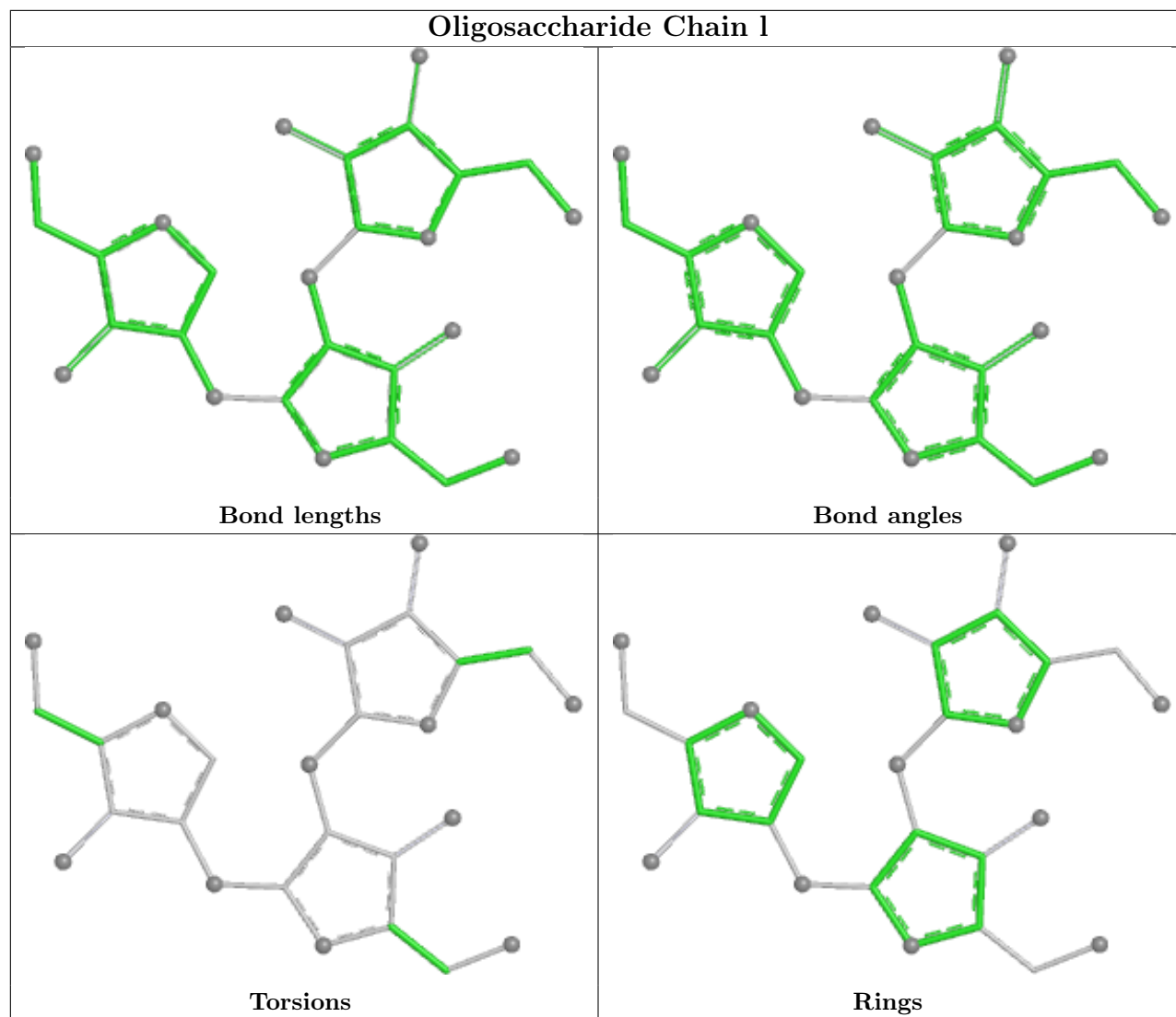


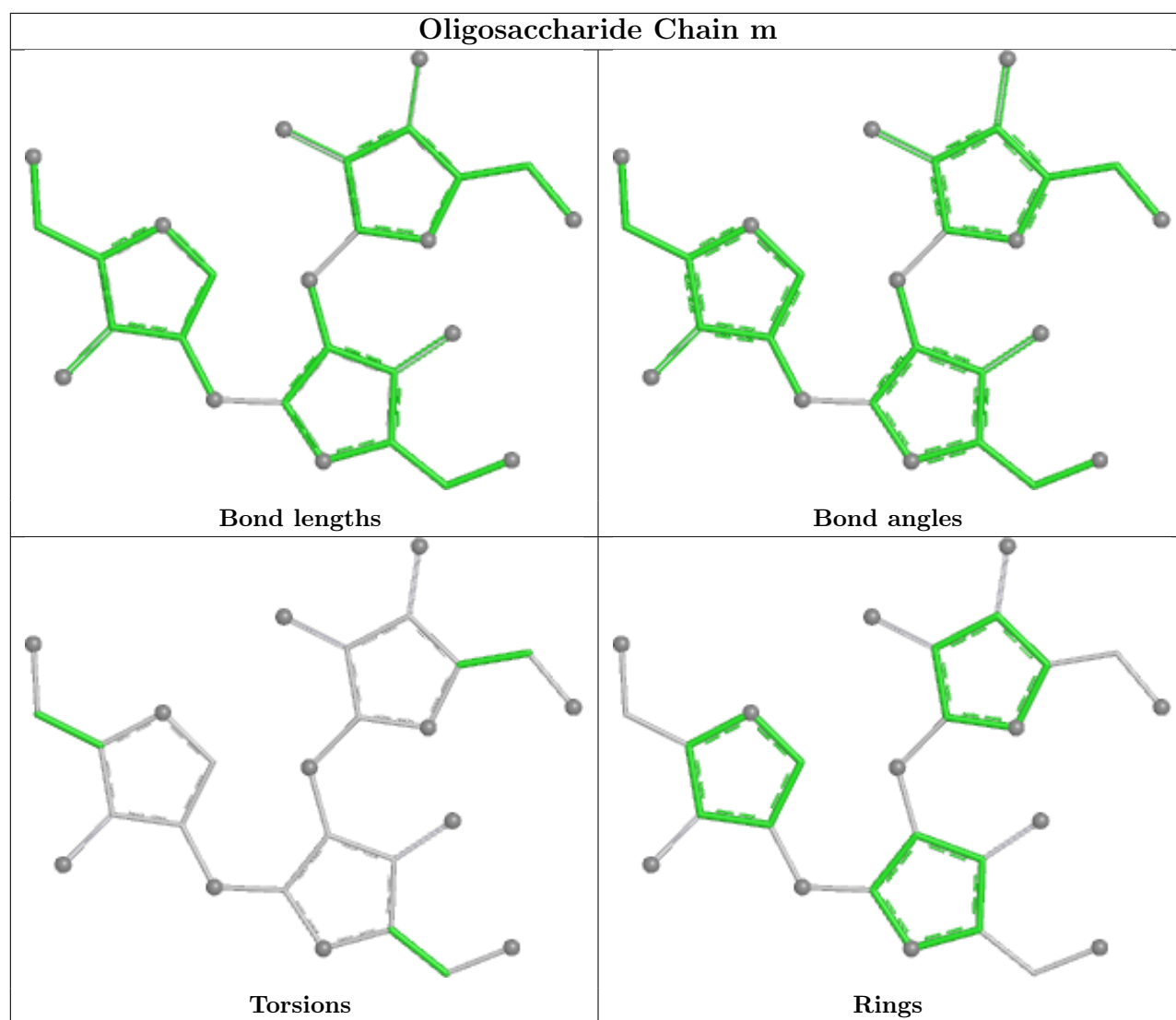


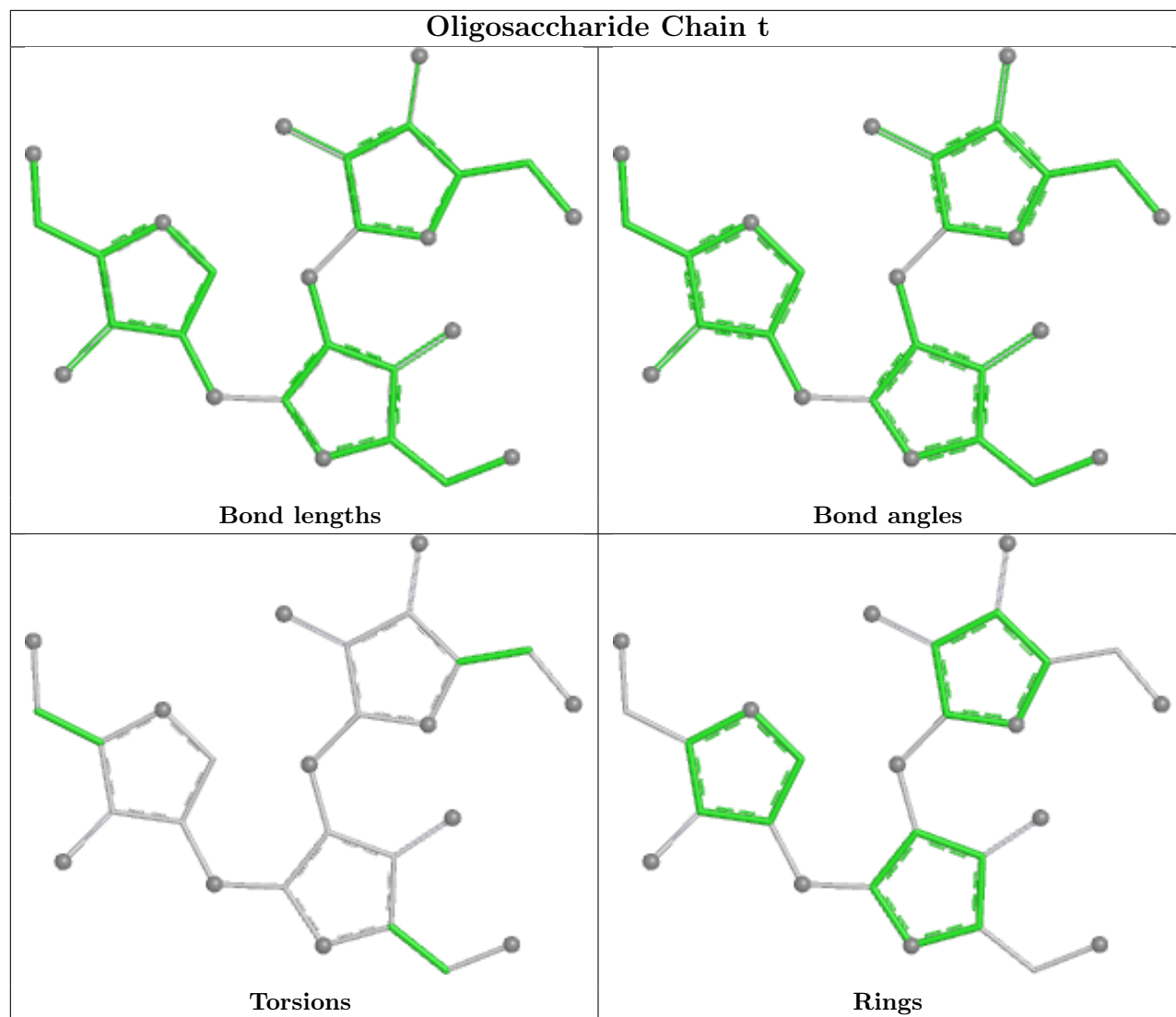


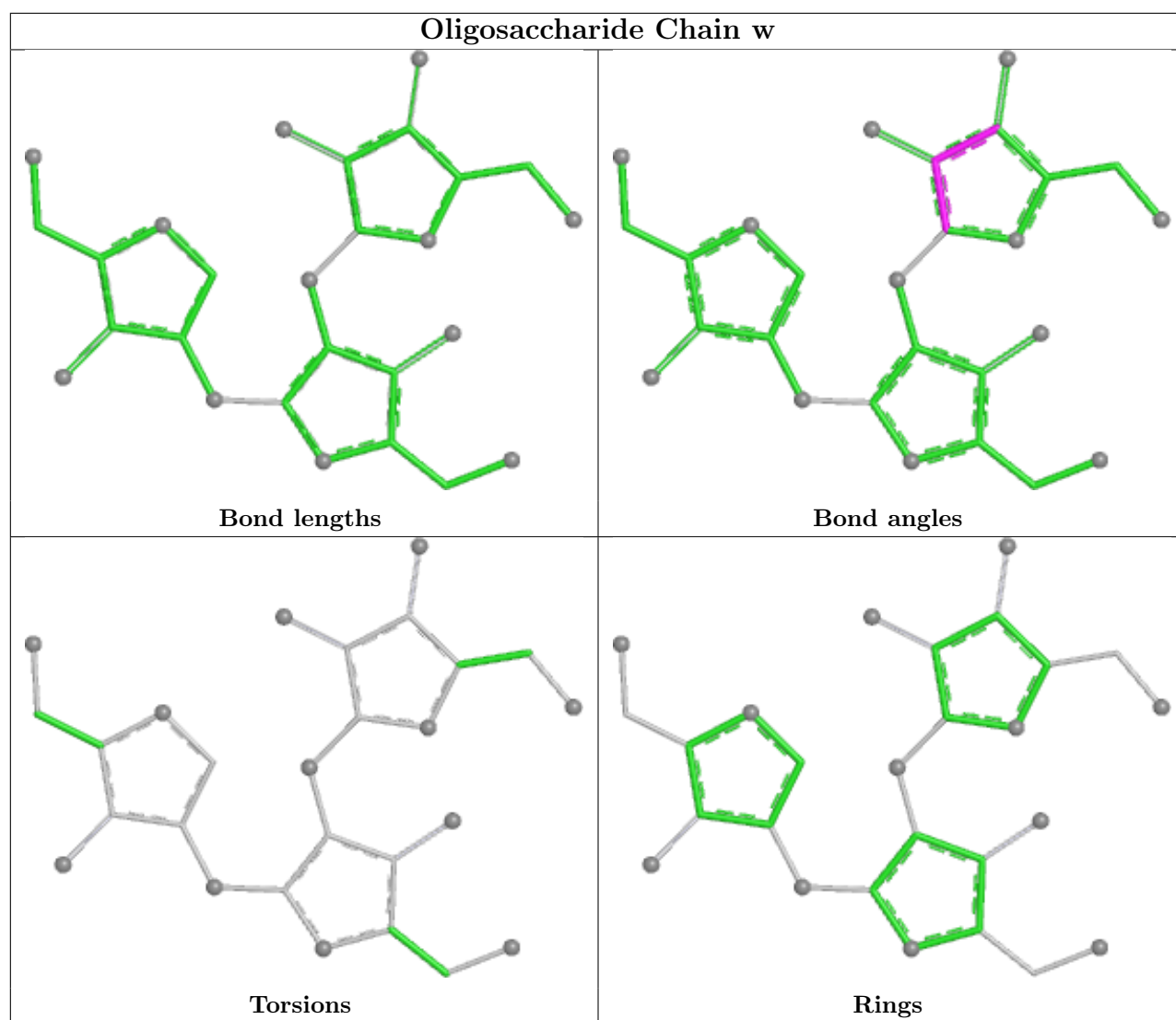


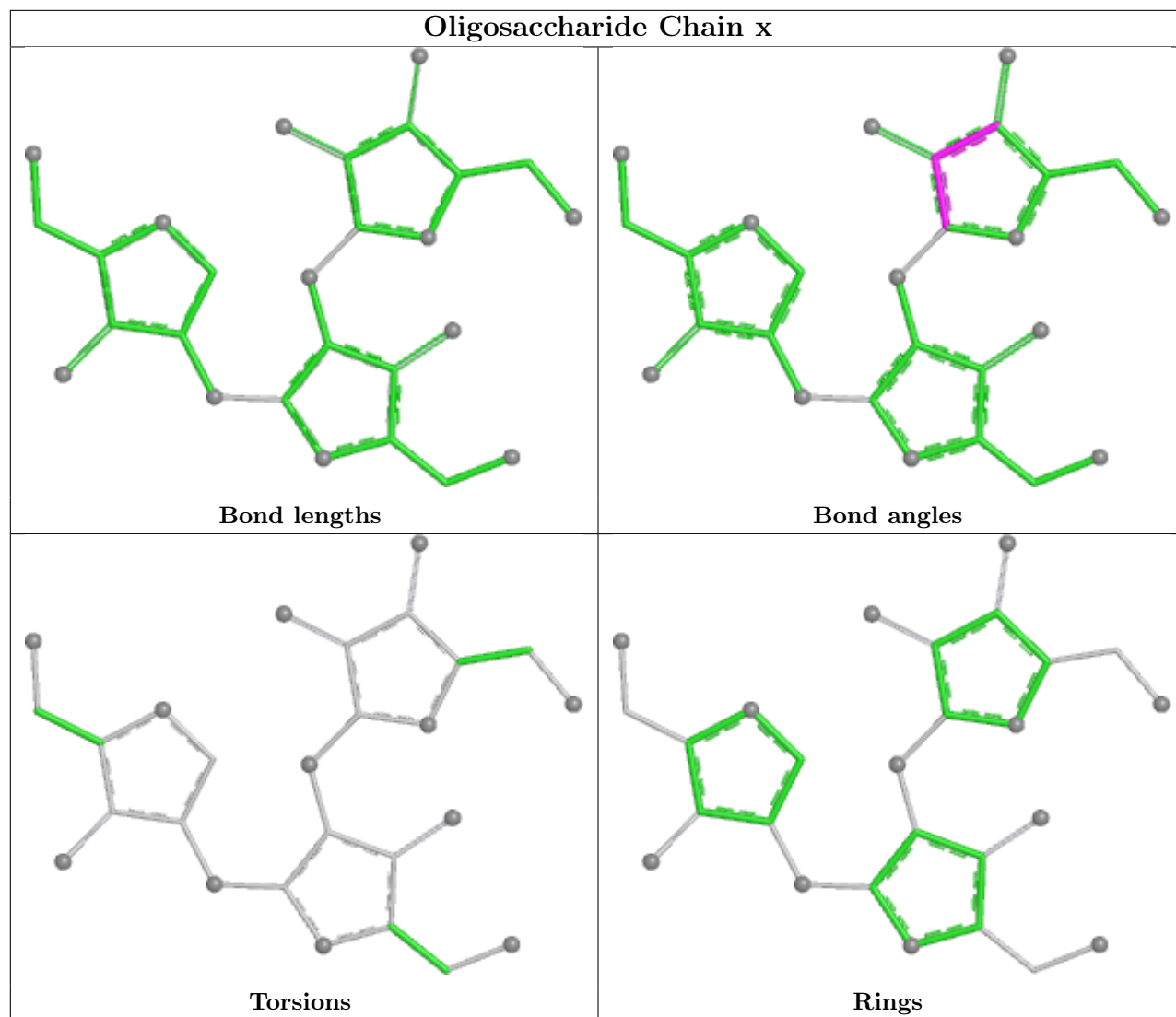


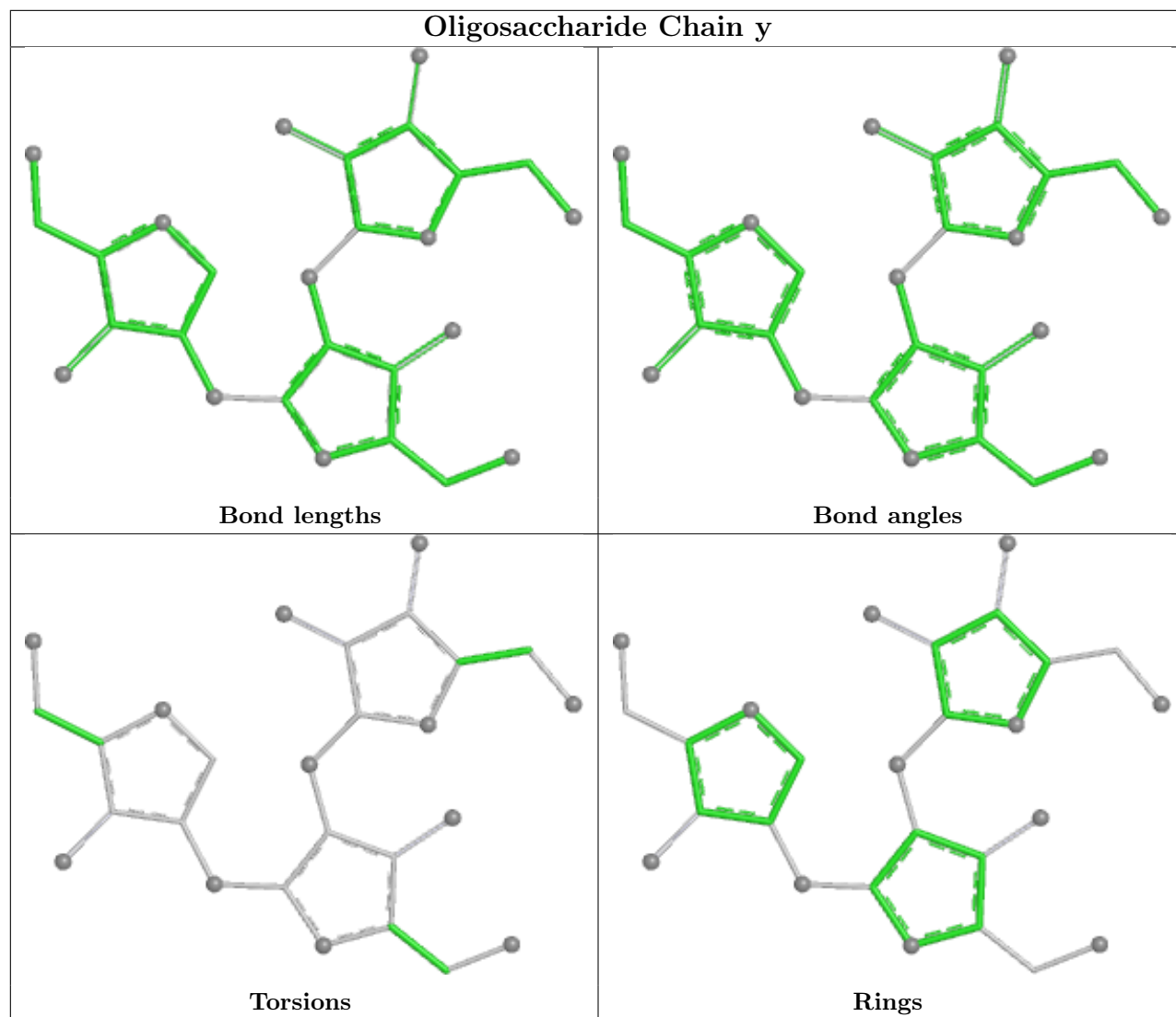


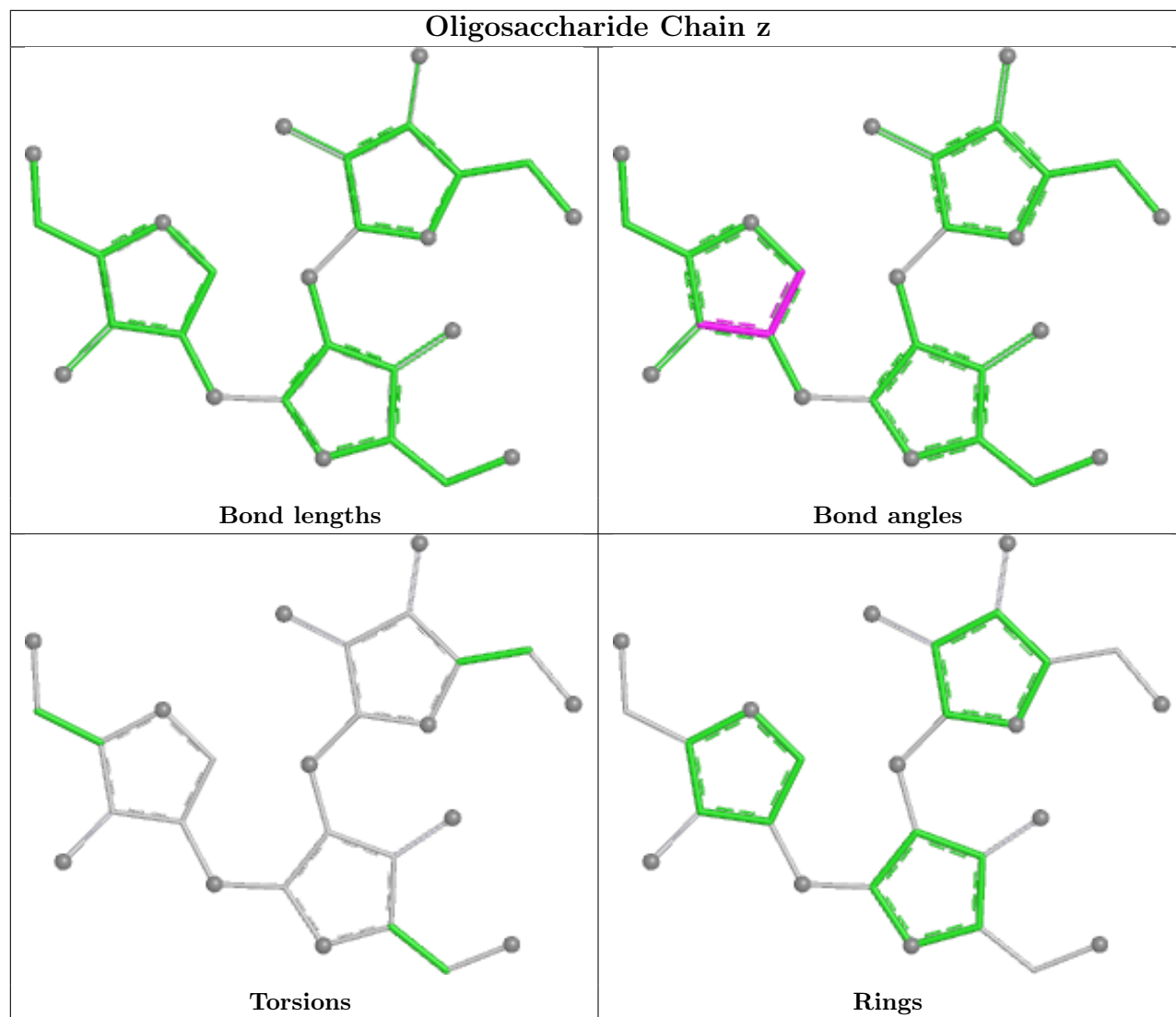


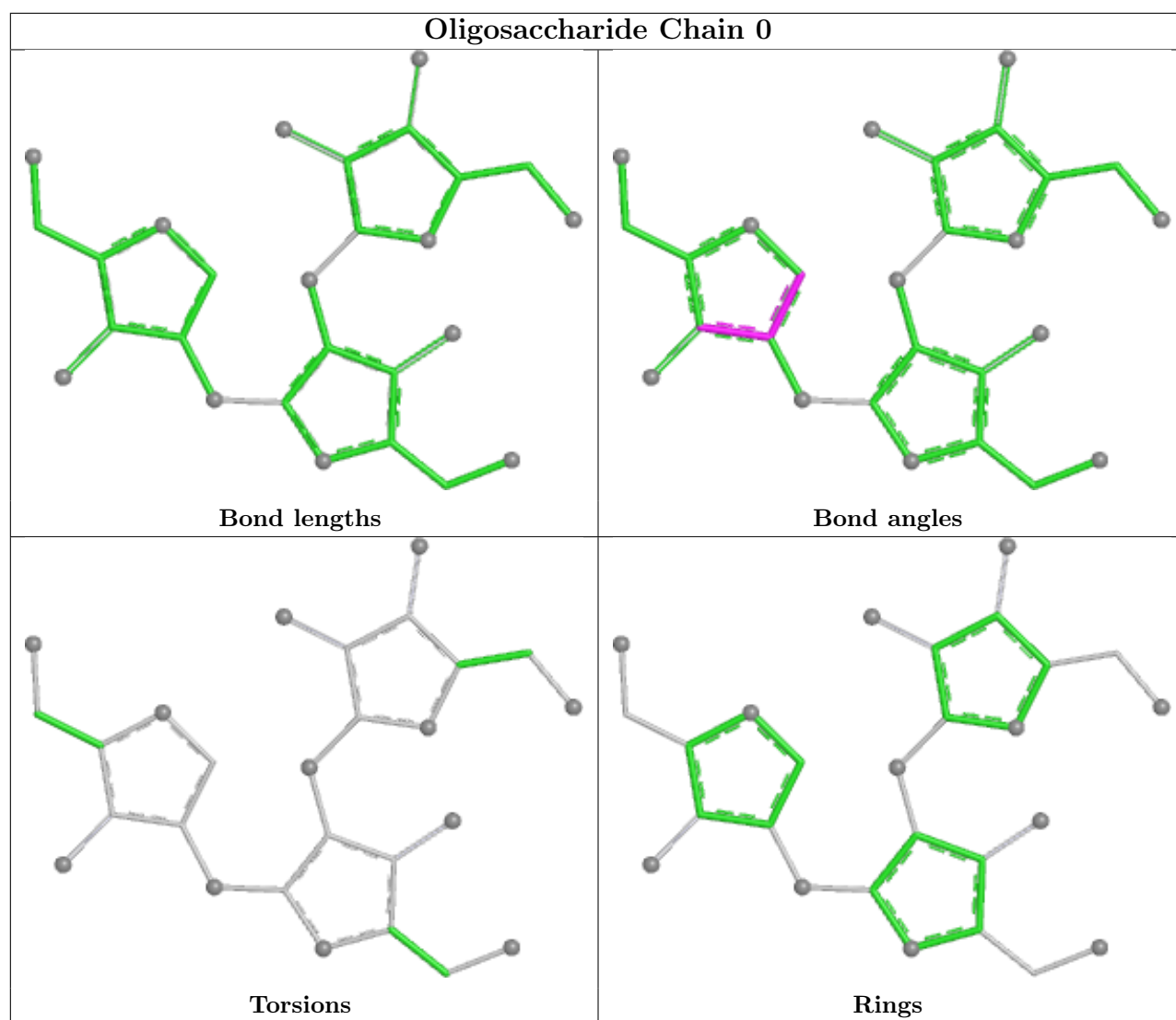


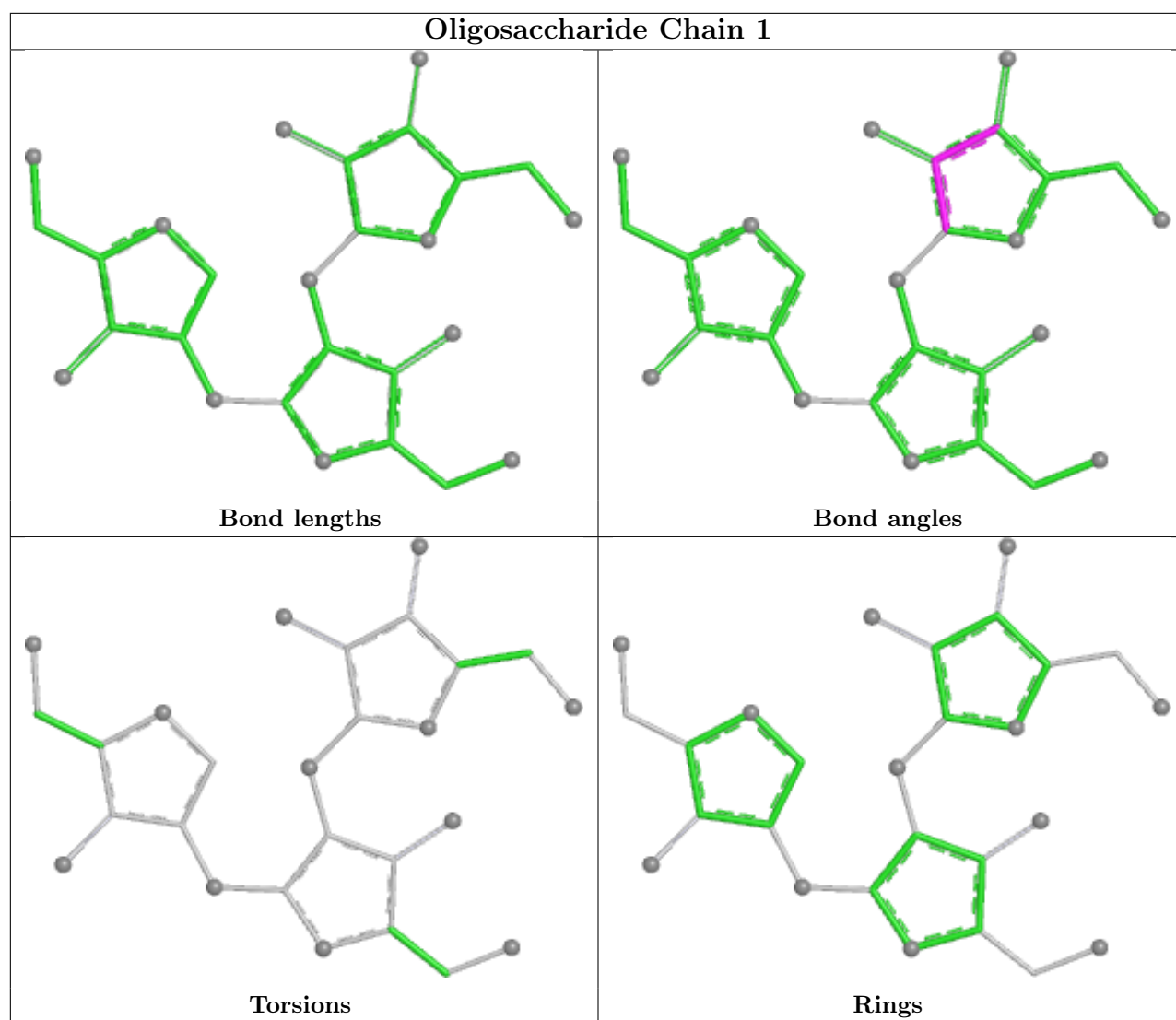


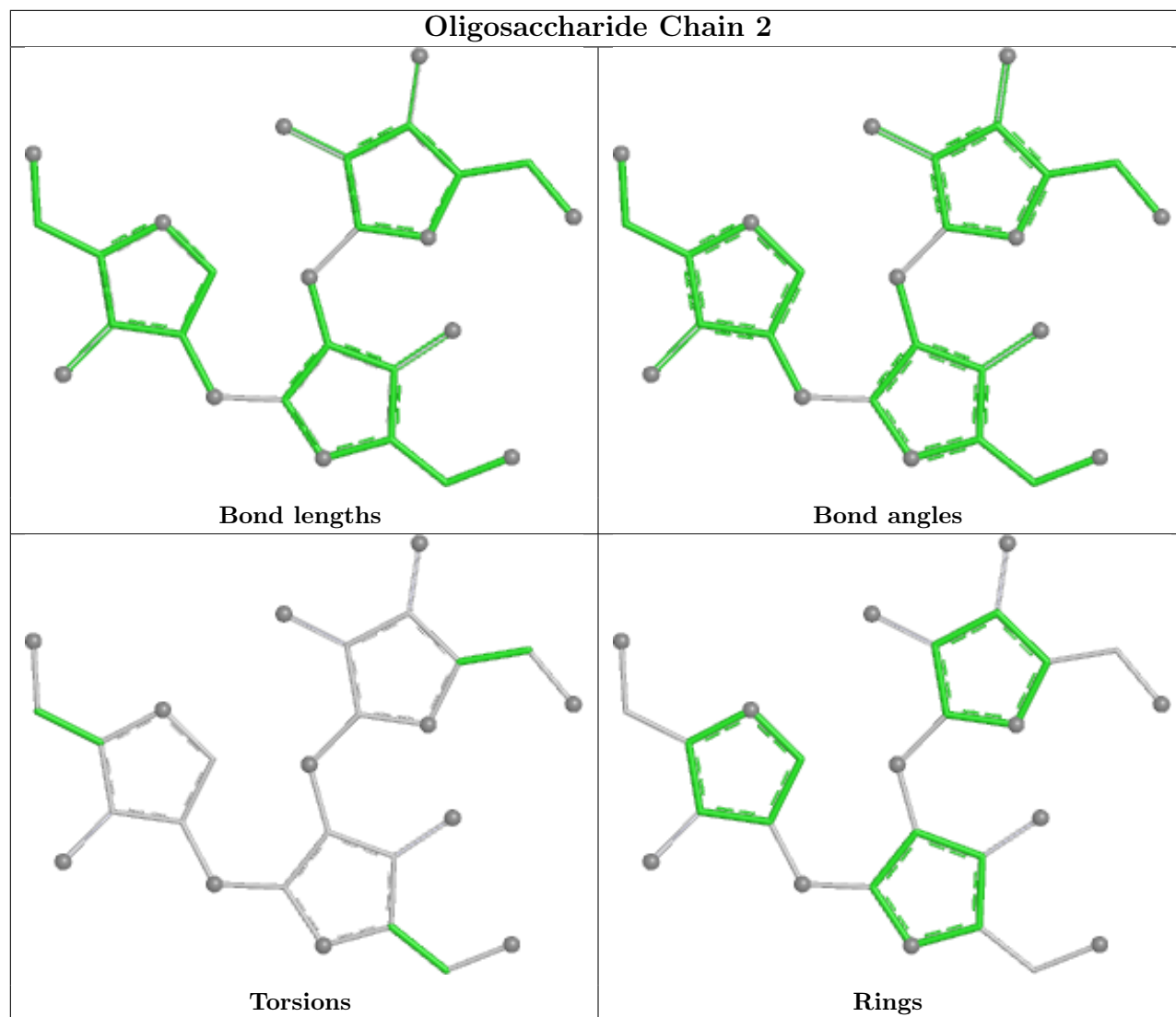


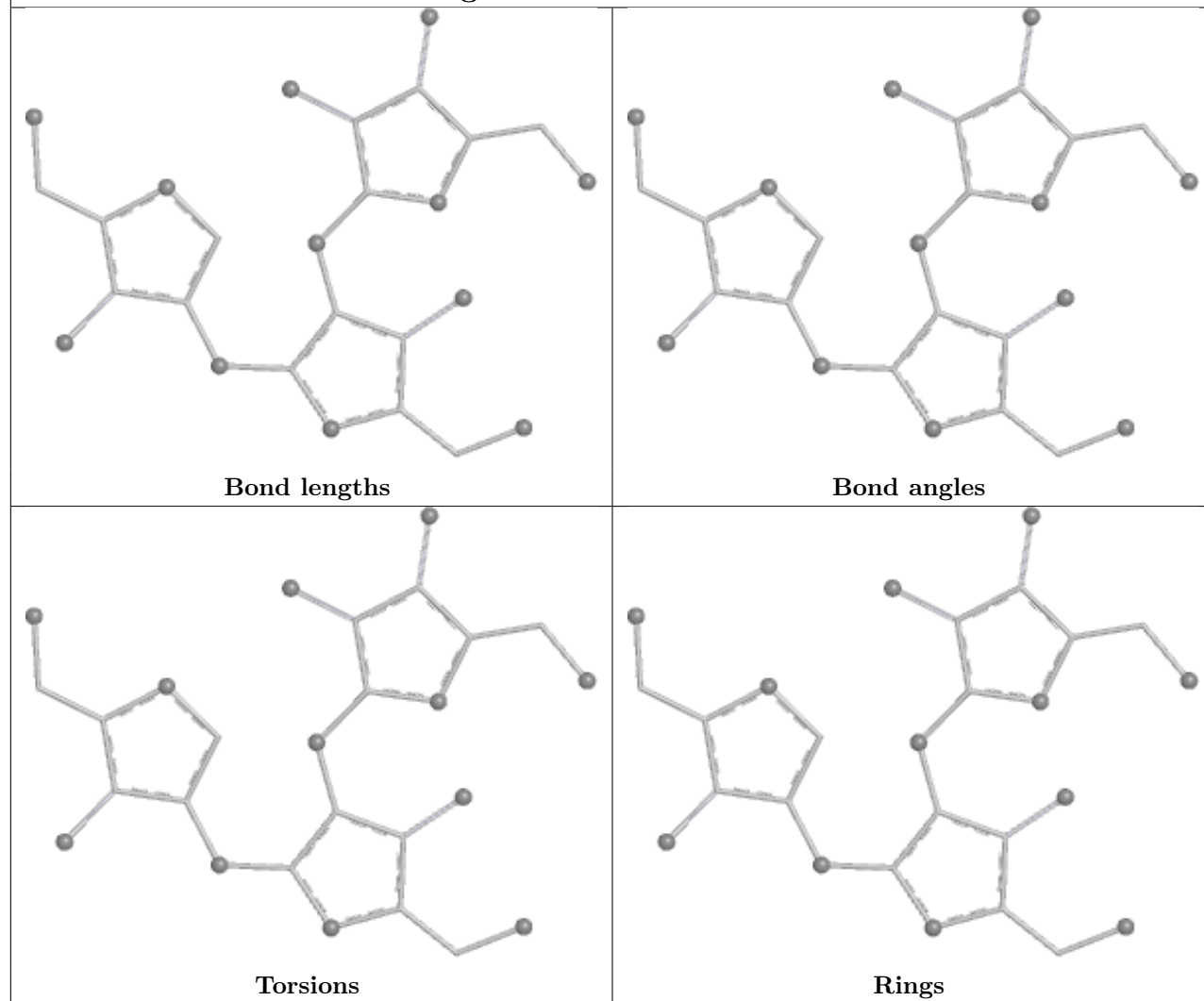


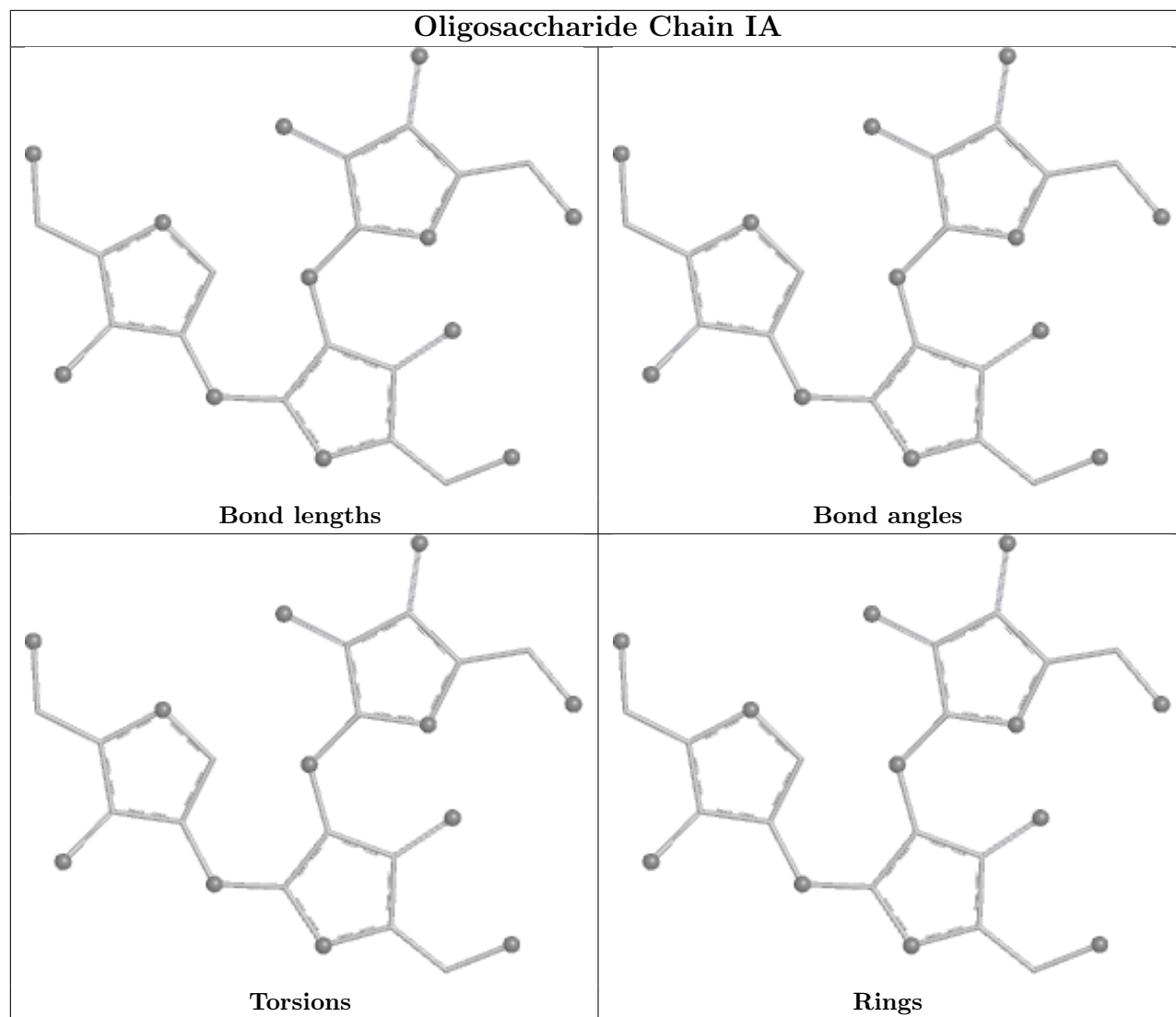




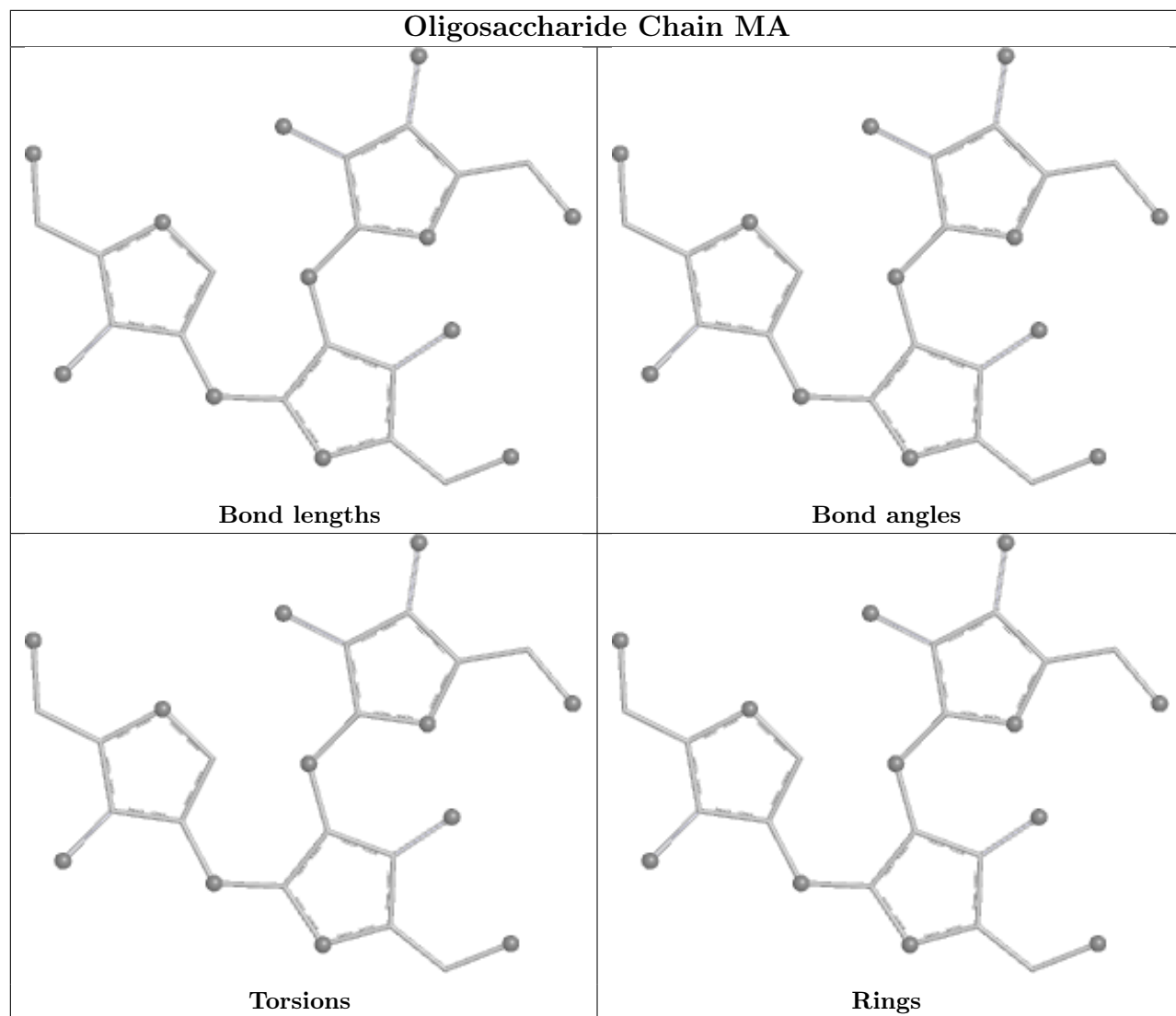


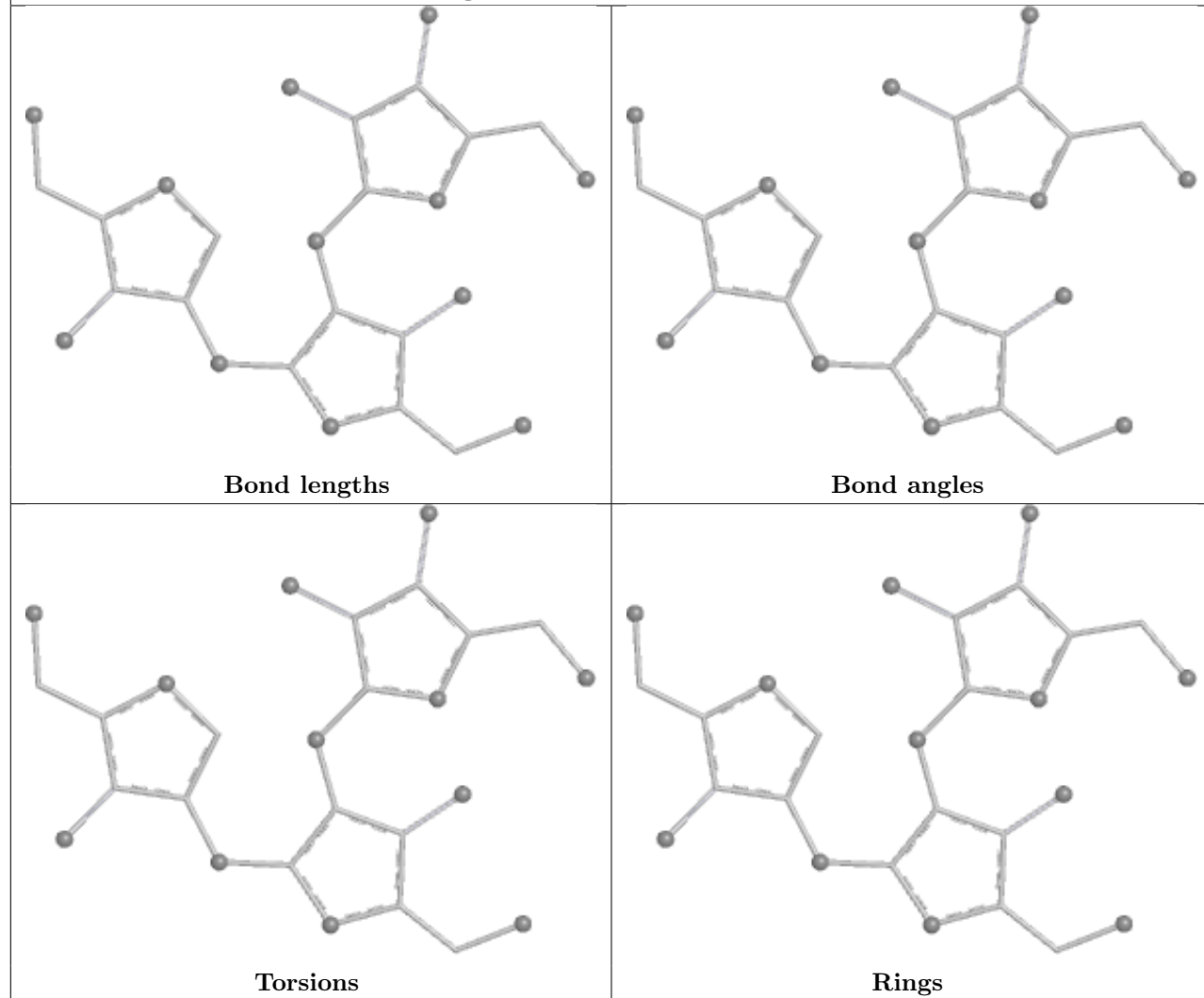


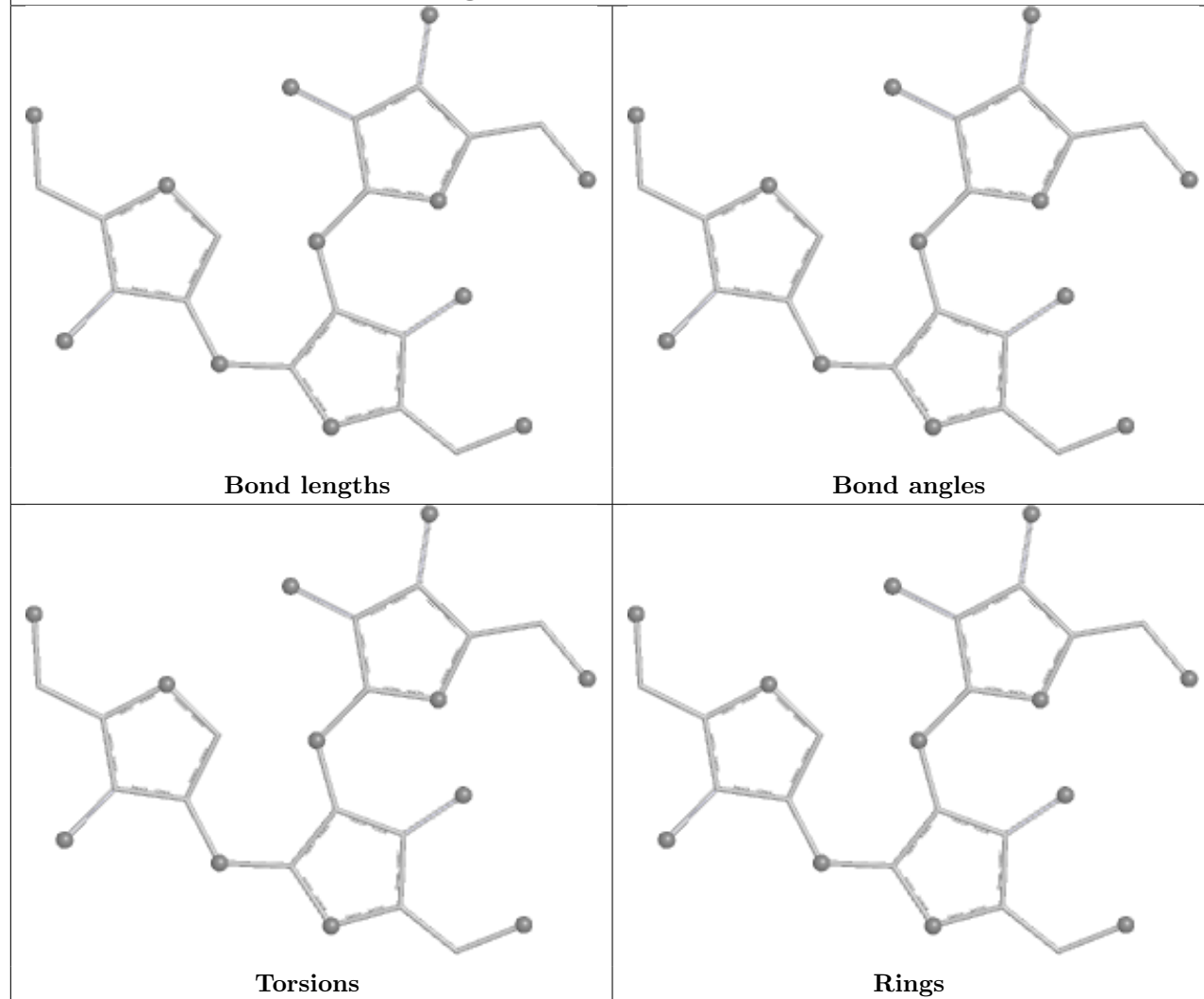
Oligosaccharide Chain HA

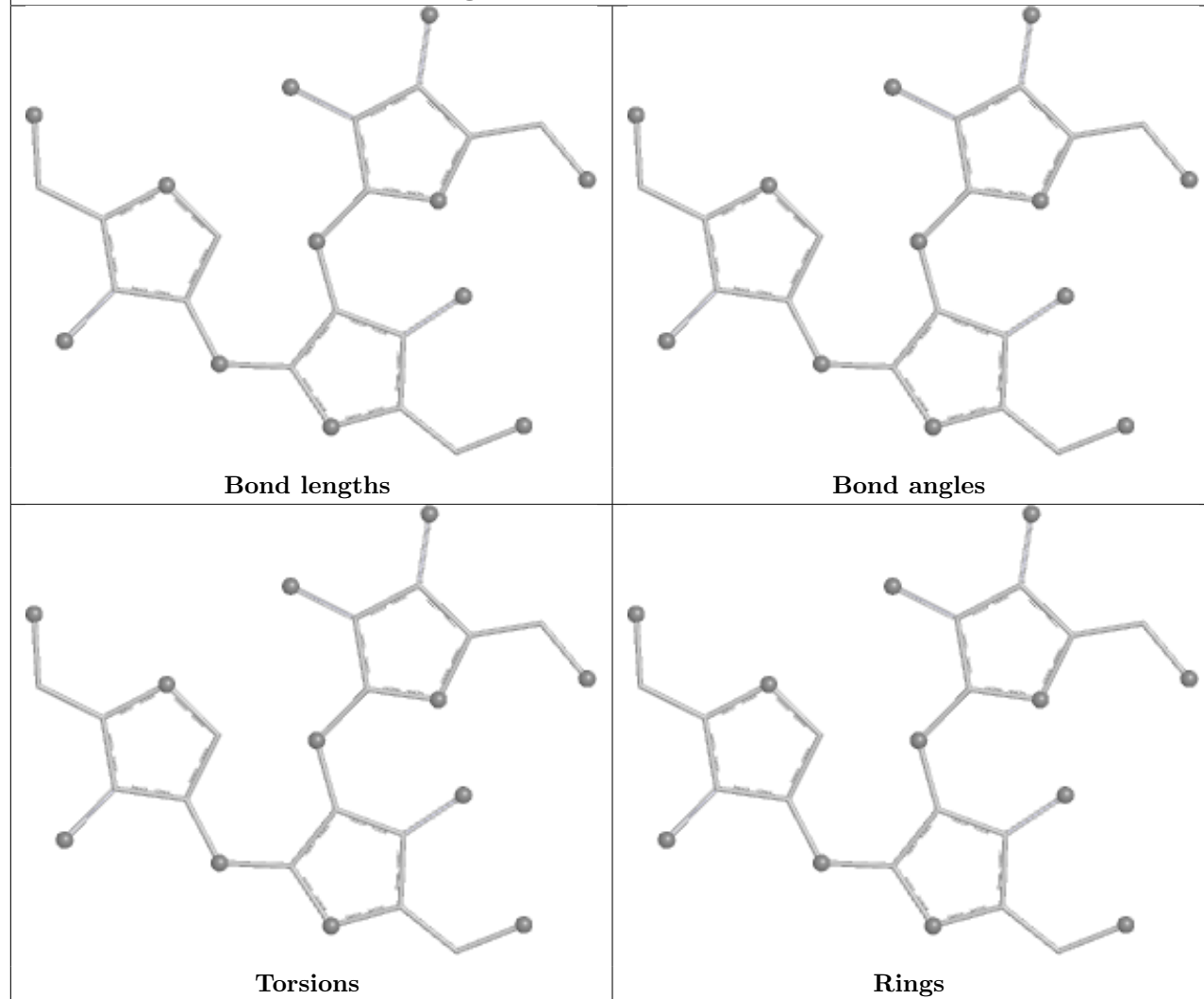


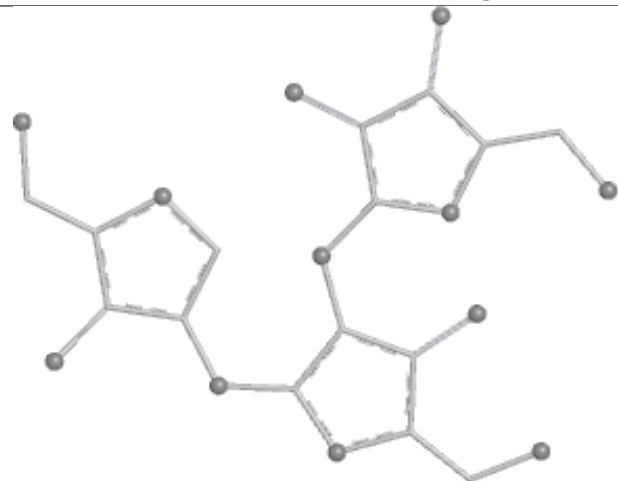
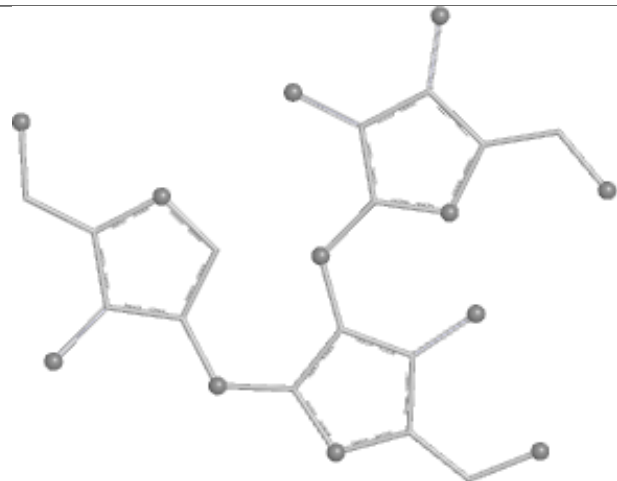
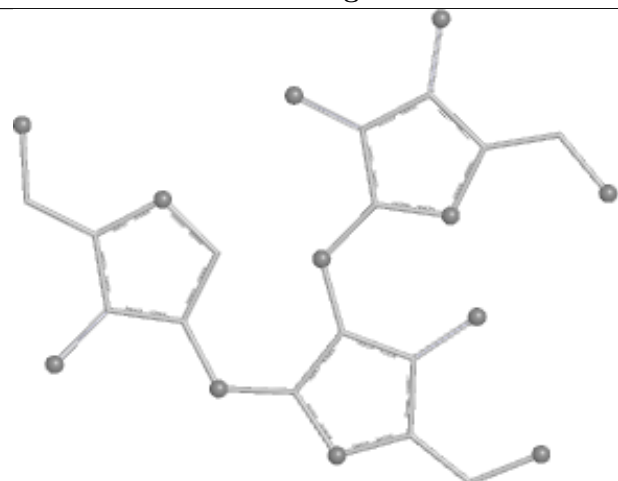
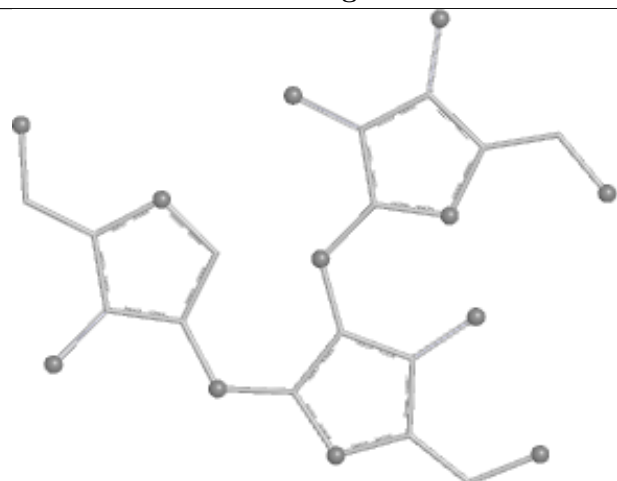
Oligosaccharide Chain MA

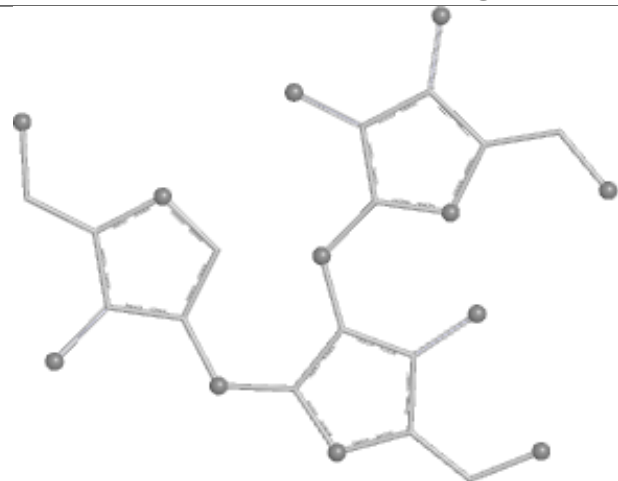
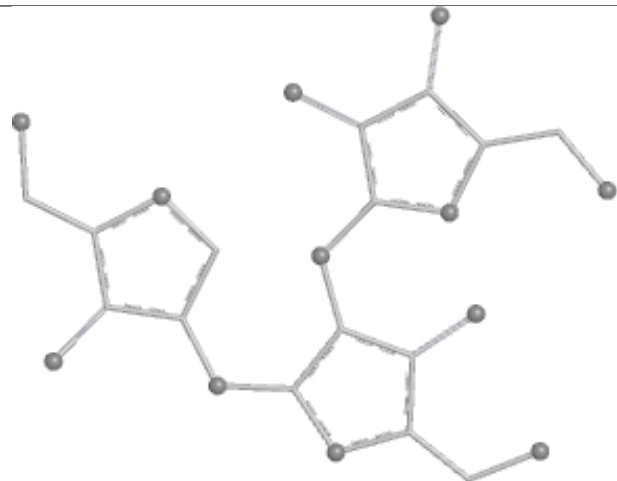
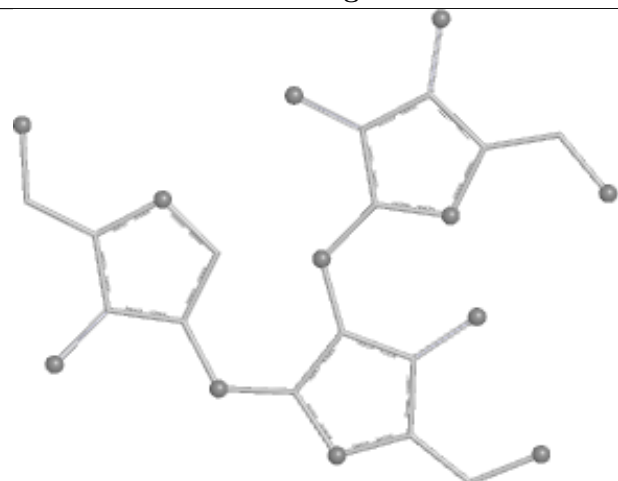
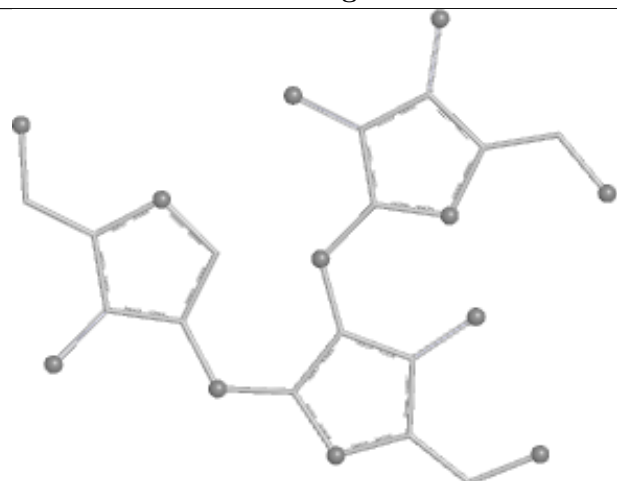


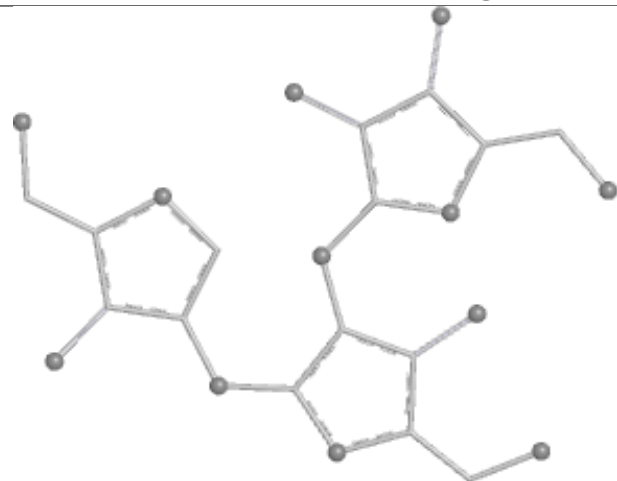
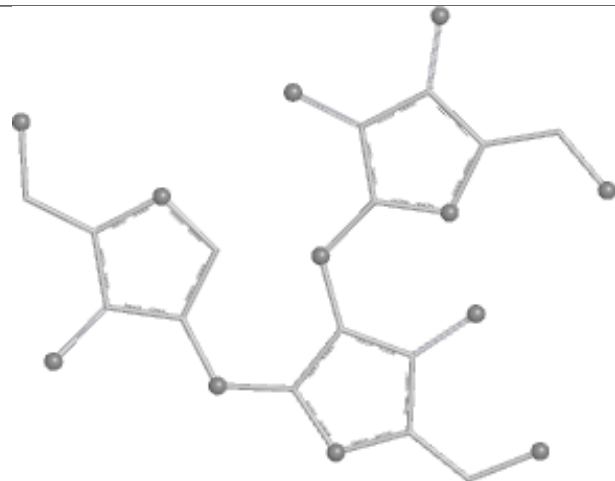
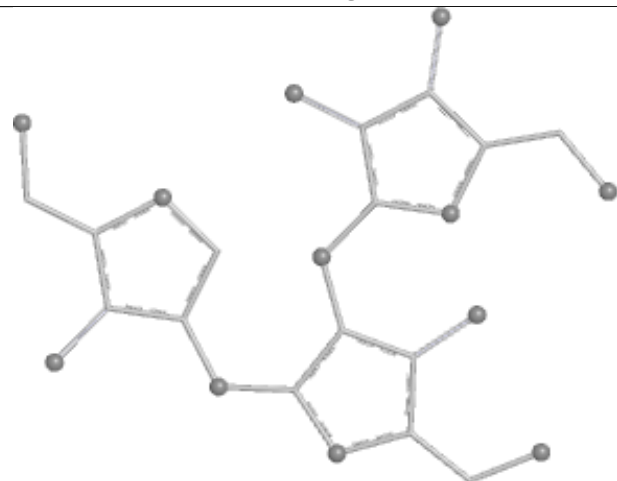
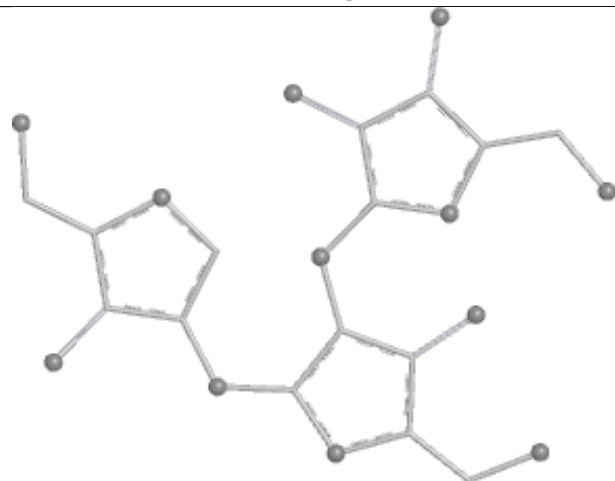
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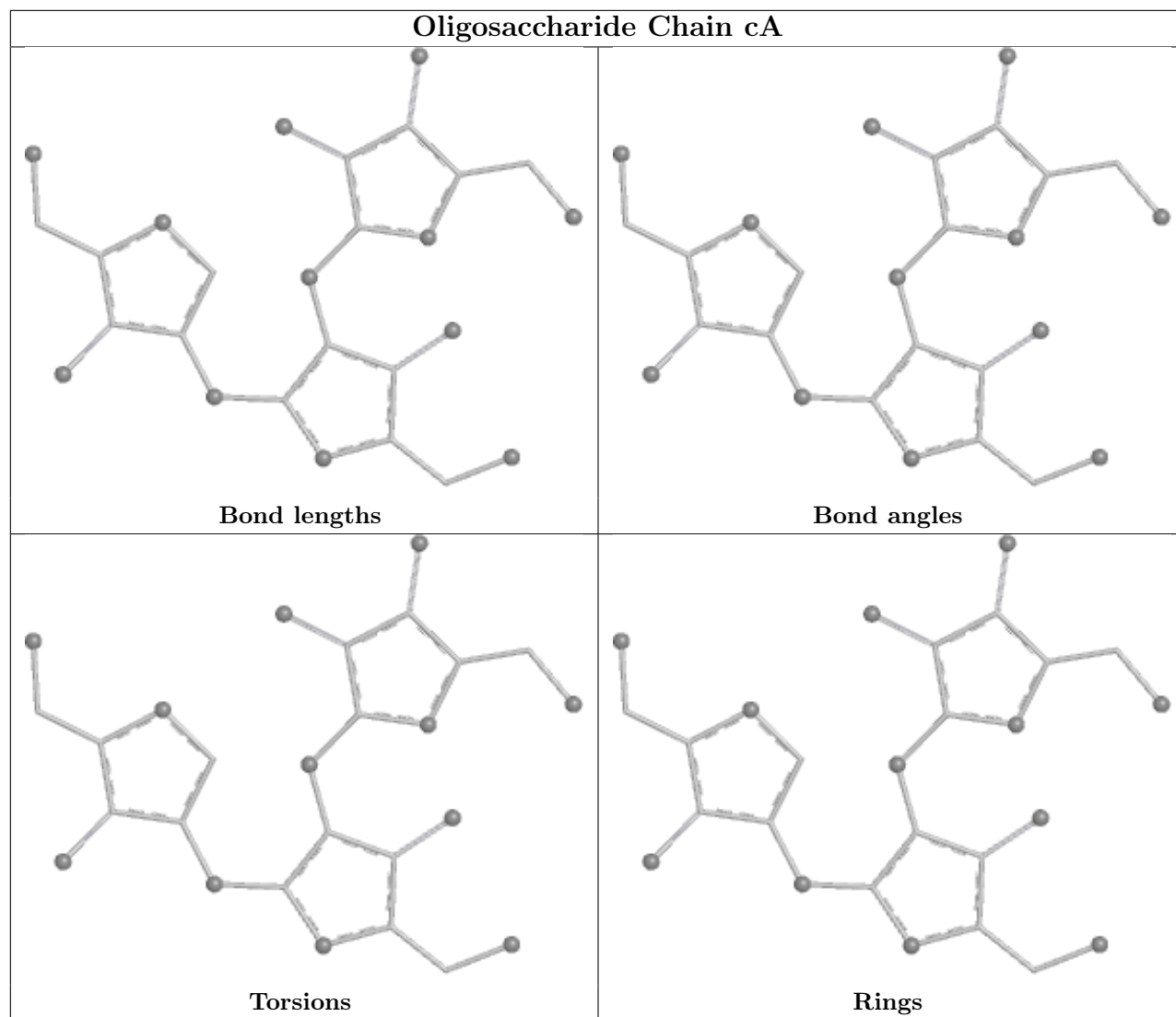
Oligosaccharide Chain OA

Oligosaccharide Chain RA

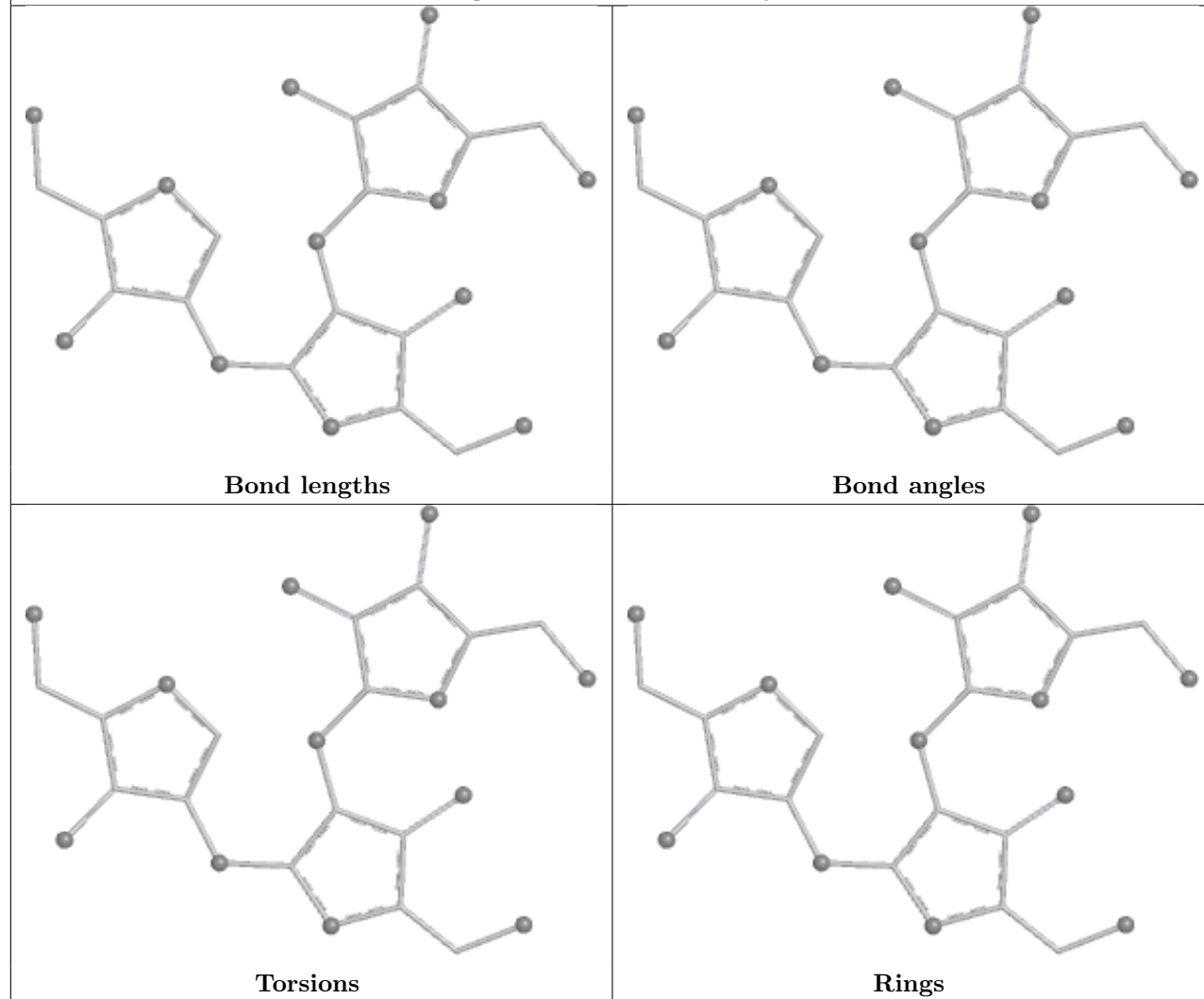
Oligosaccharide Chain TA**Bond lengths****Bond angles****Torsions****Rings**

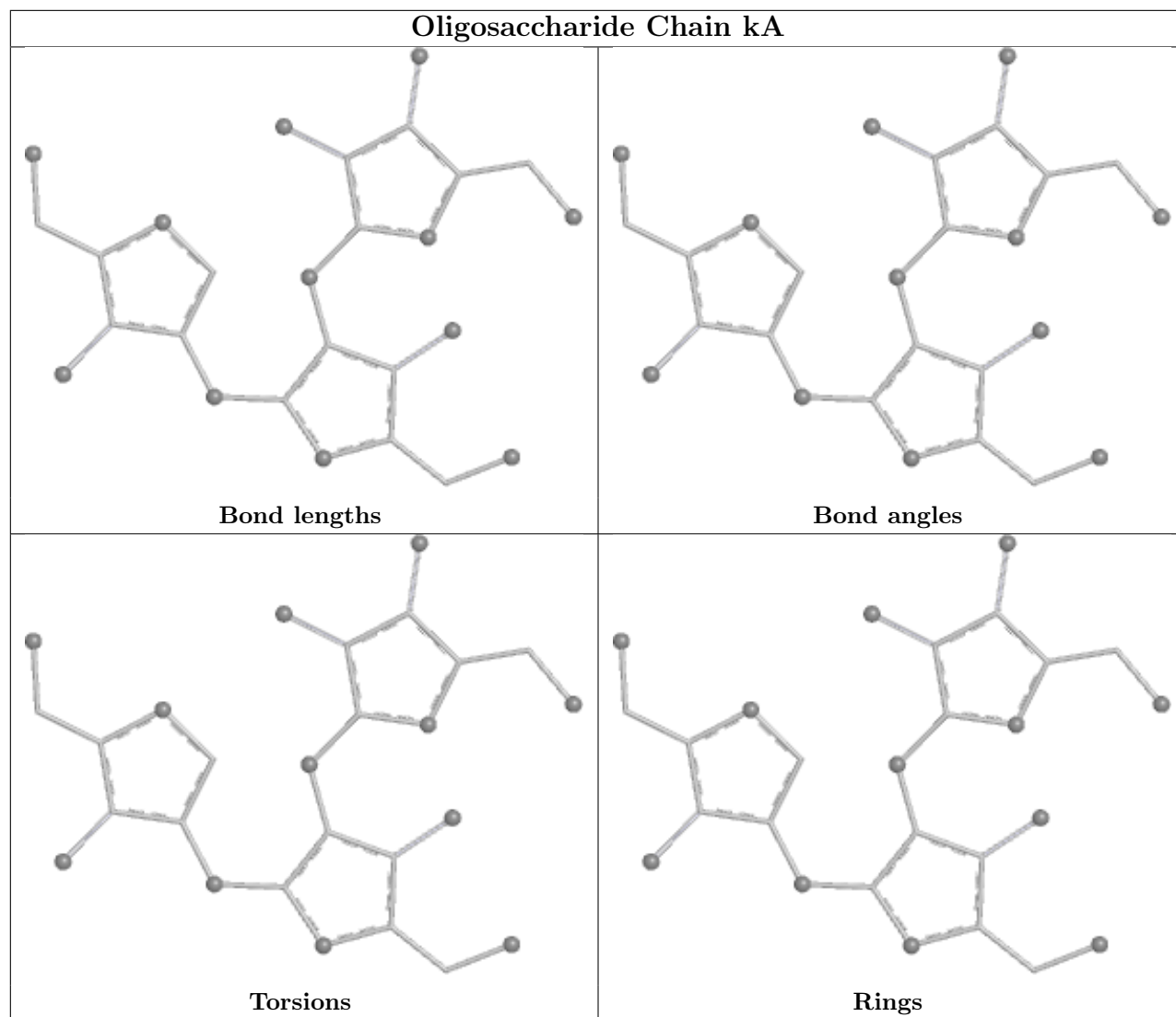
Oligosaccharide Chain XA**Bond lengths****Bond angles****Torsions****Rings**

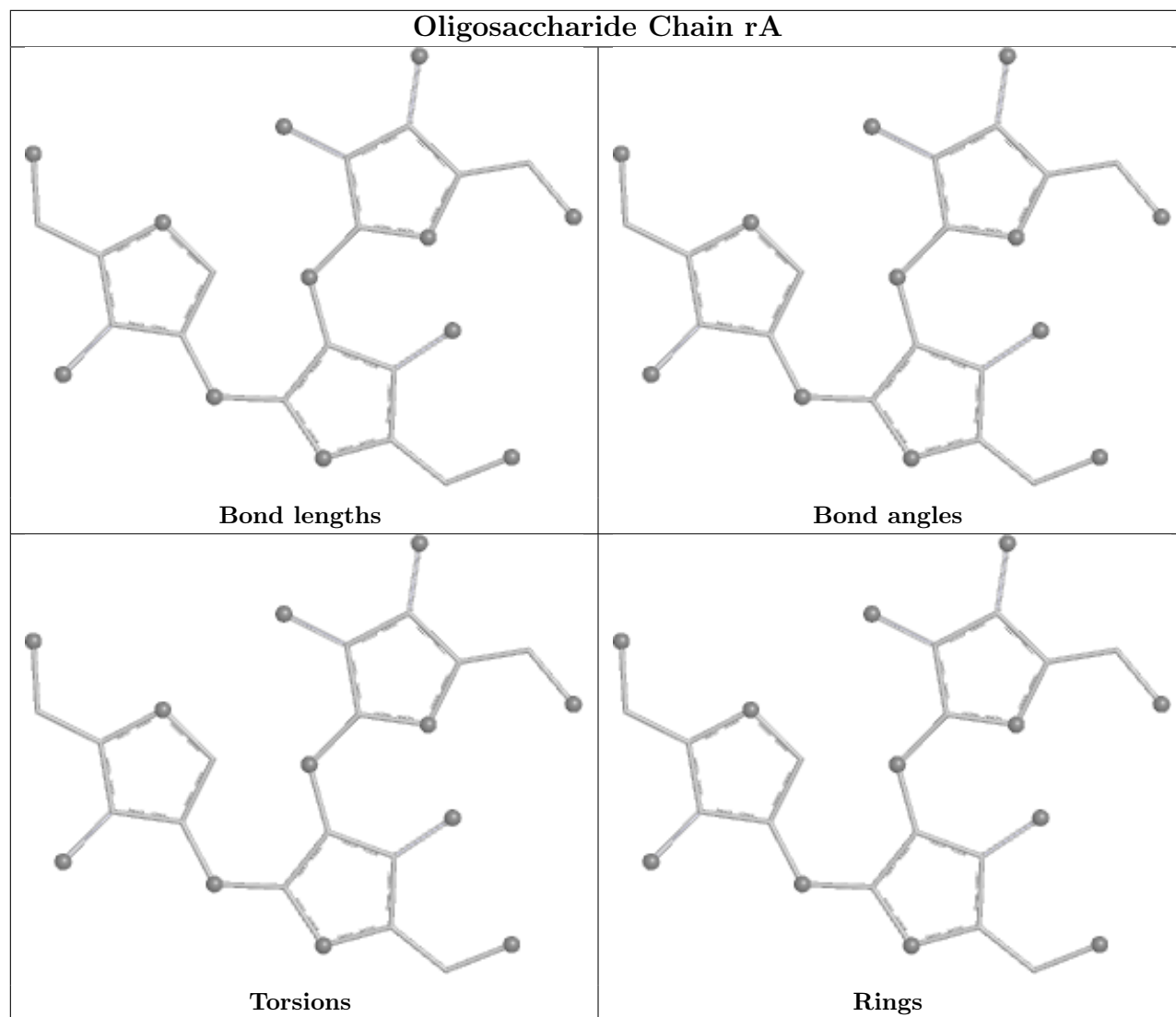
Oligosaccharide Chain ZA**Bond lengths****Bond angles****Torsions****Rings**

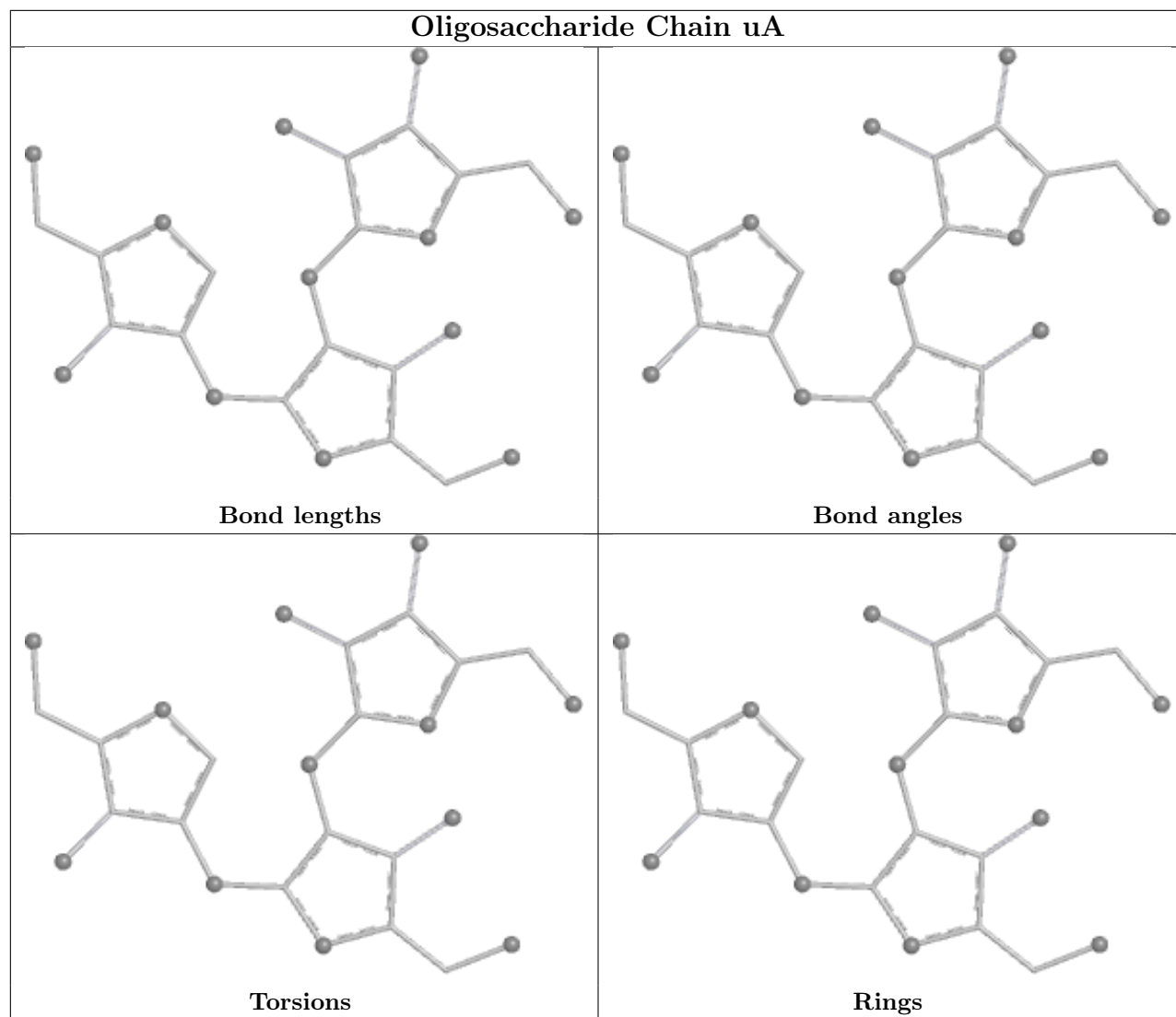


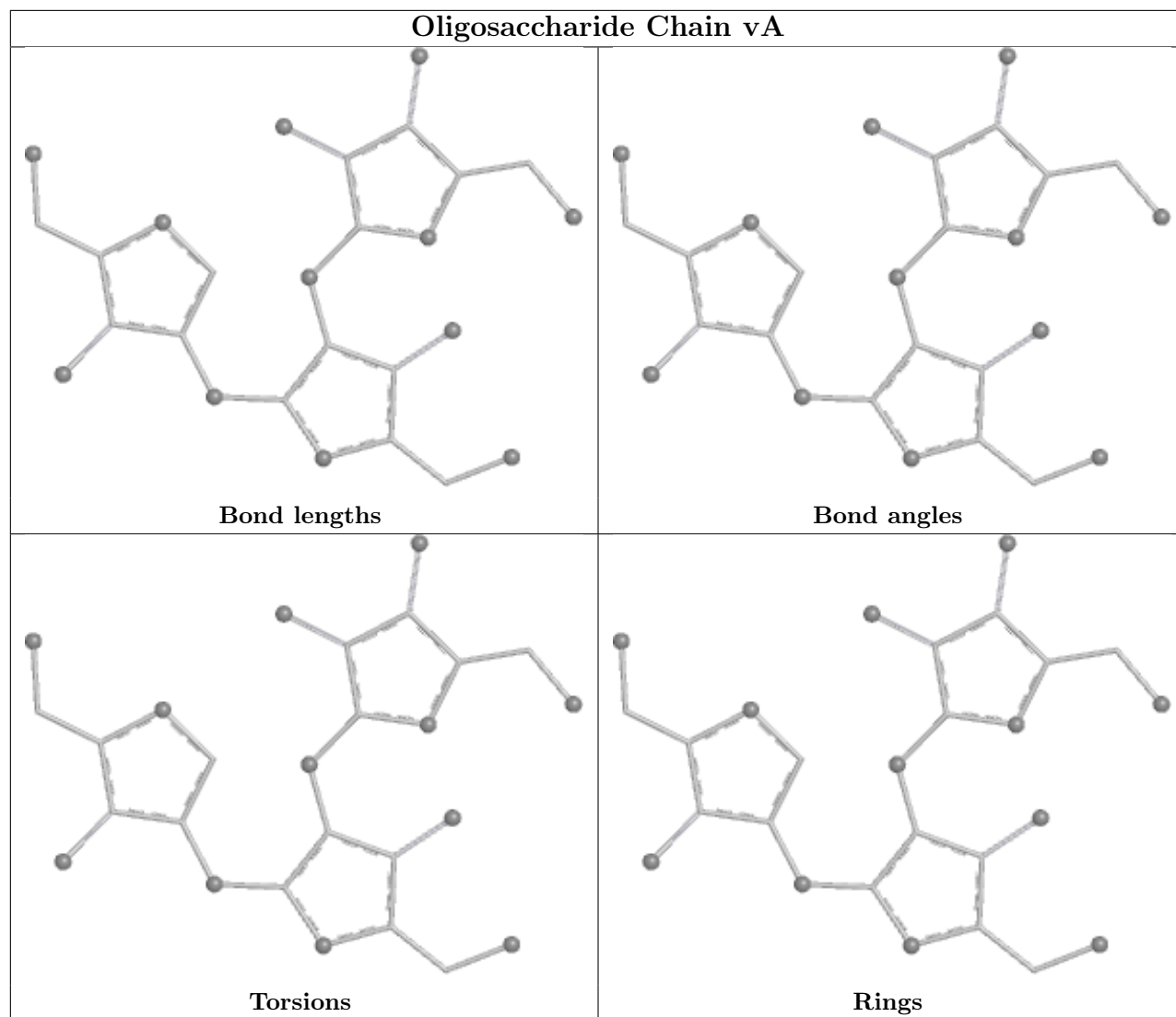
Oligosaccharide Chain jA

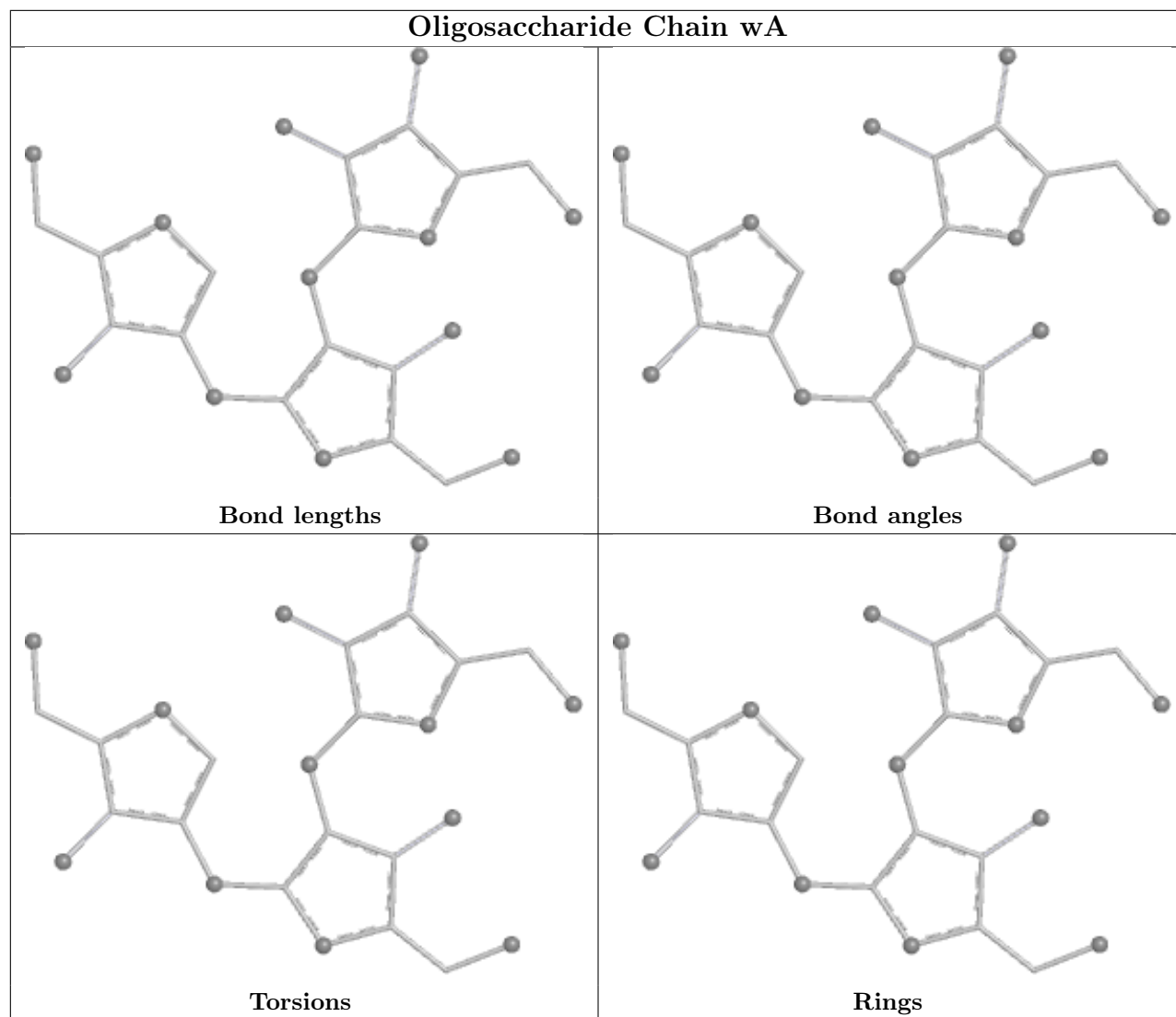


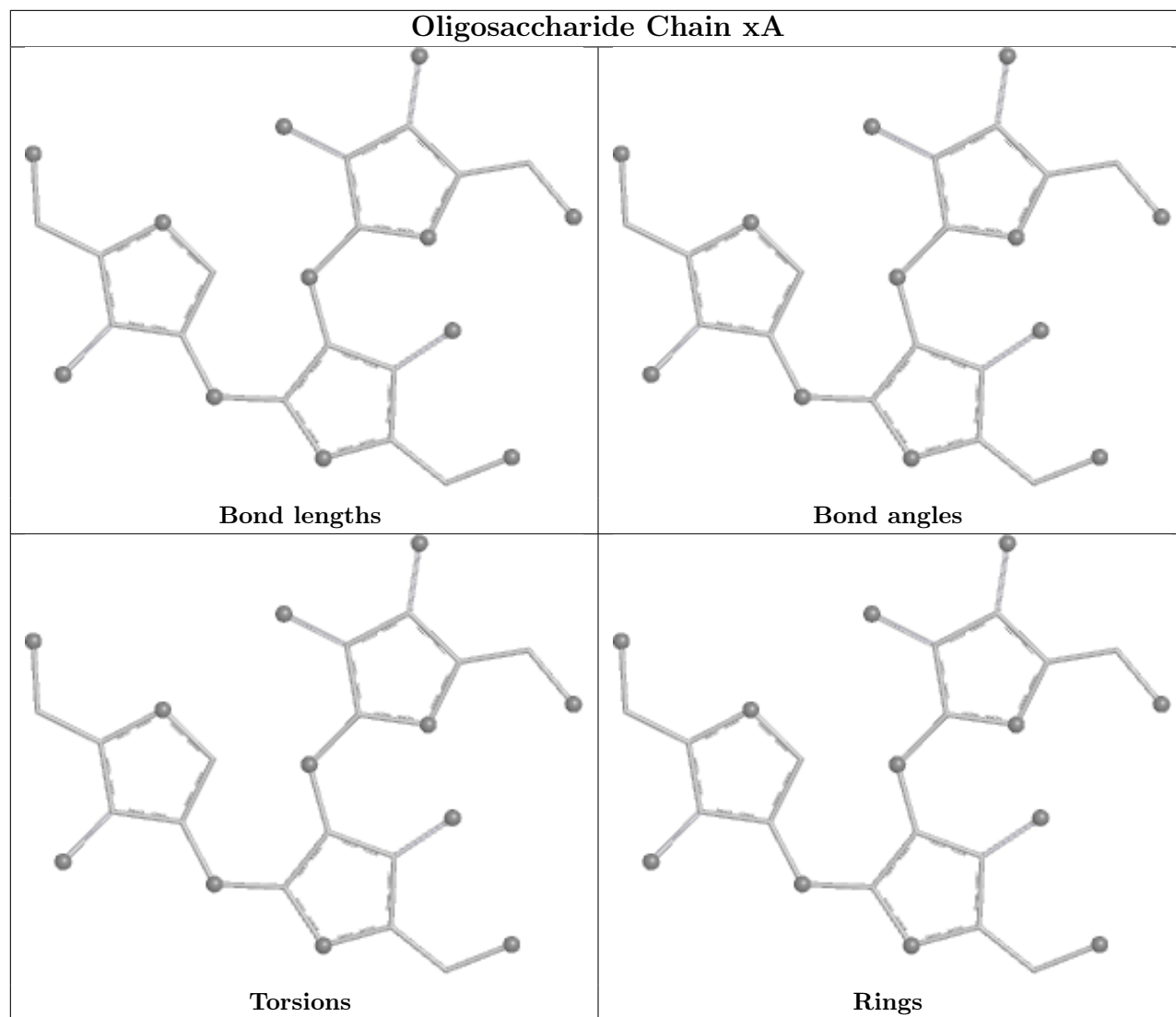


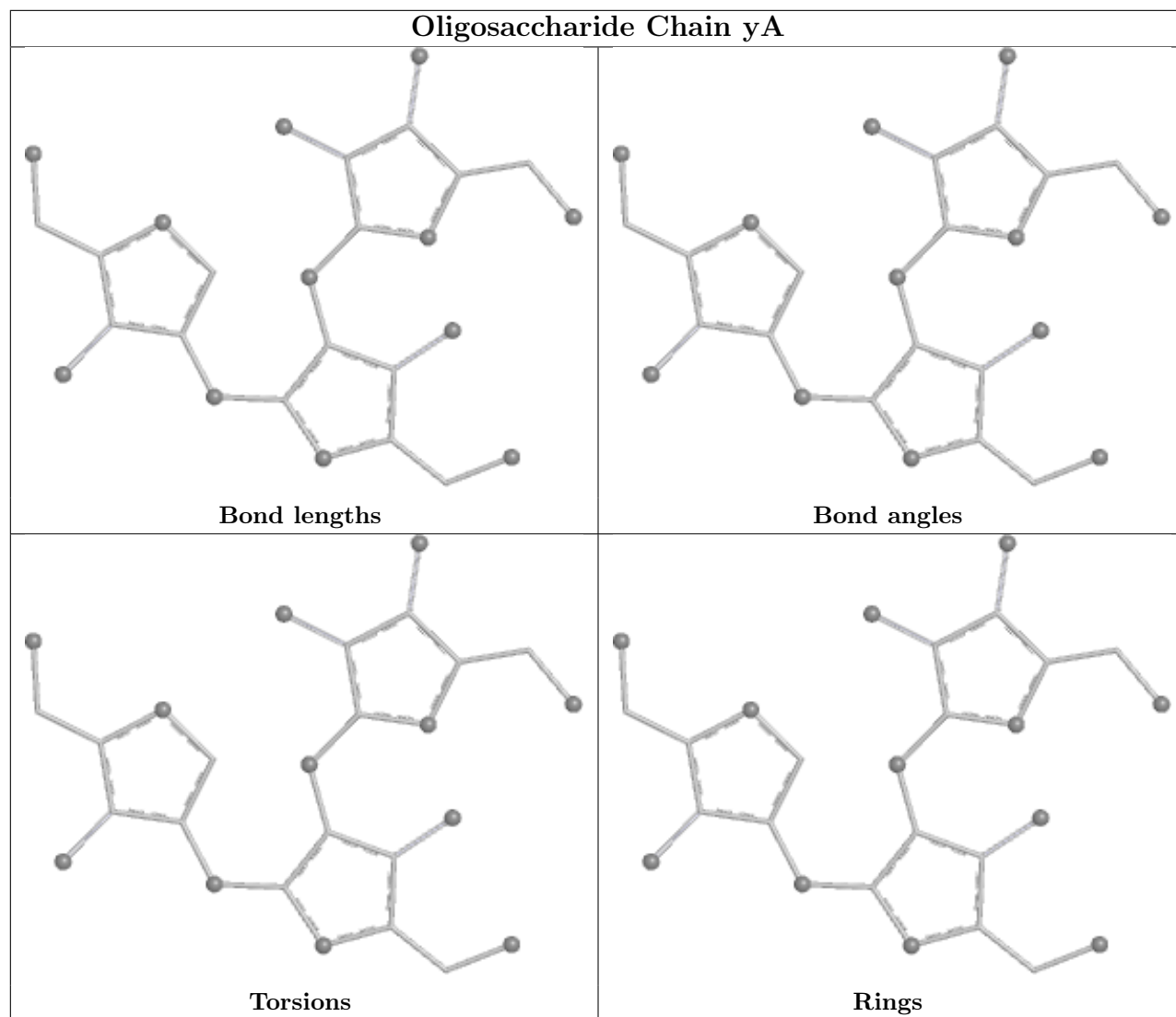


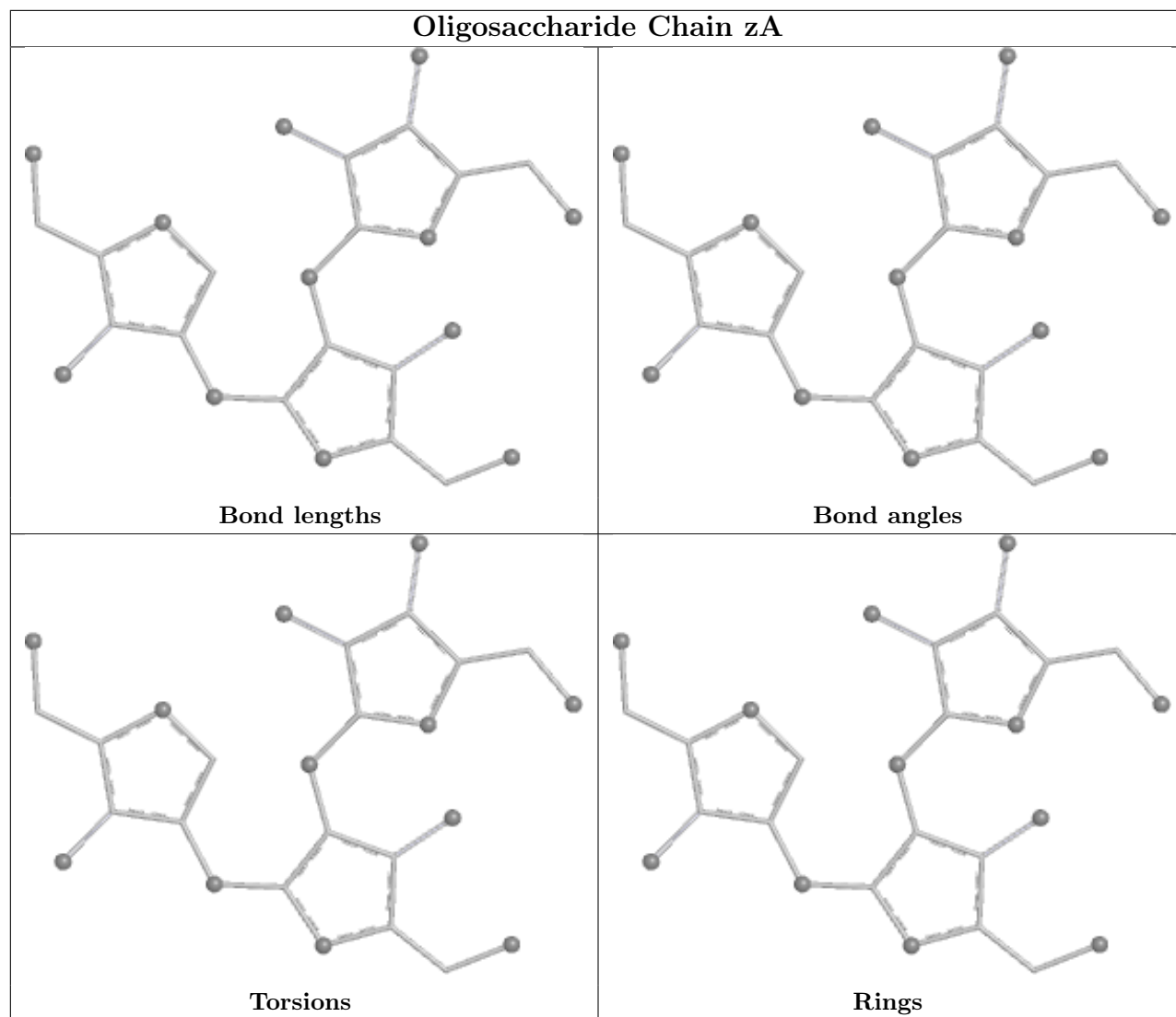


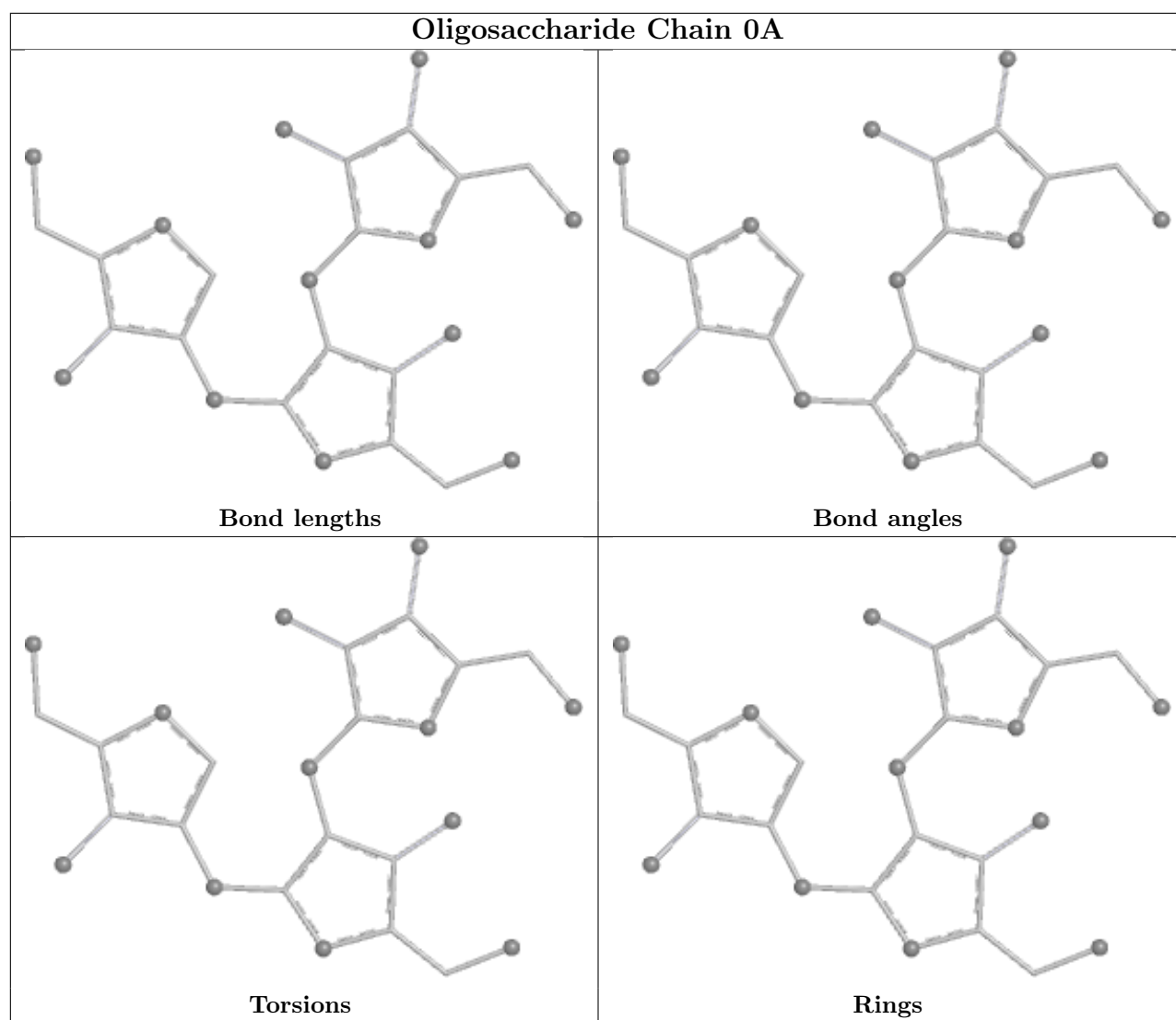


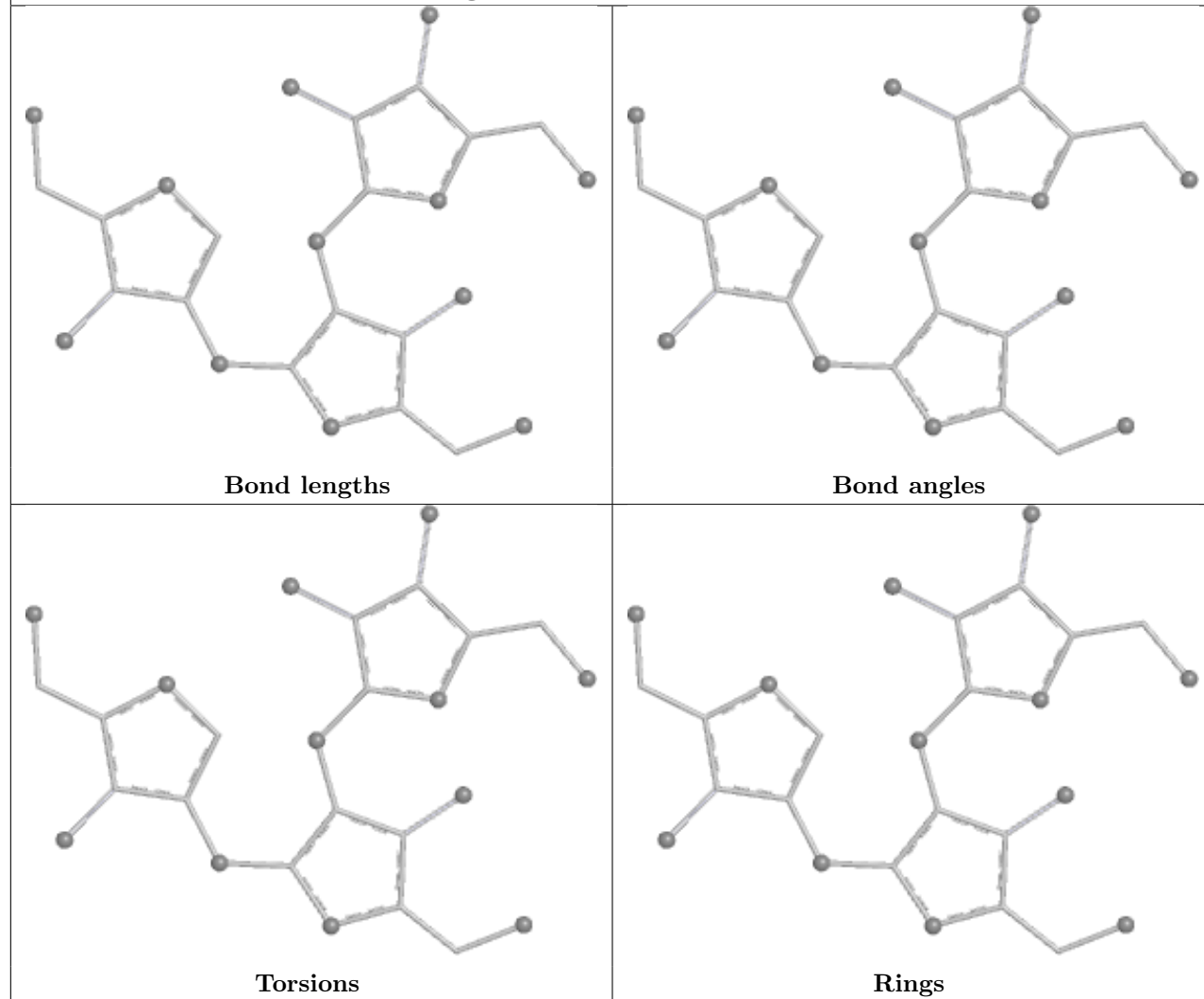


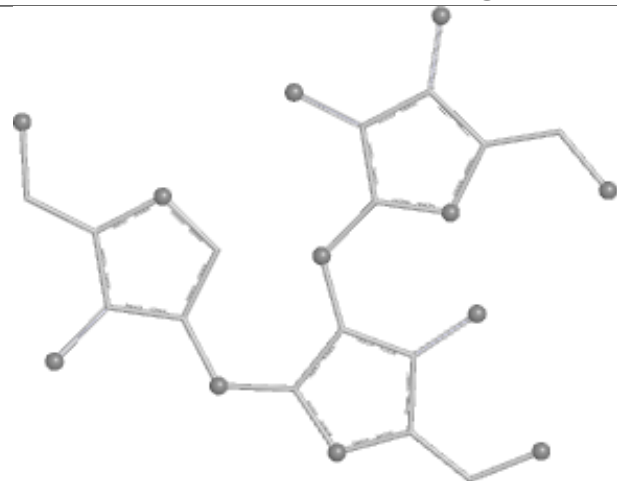
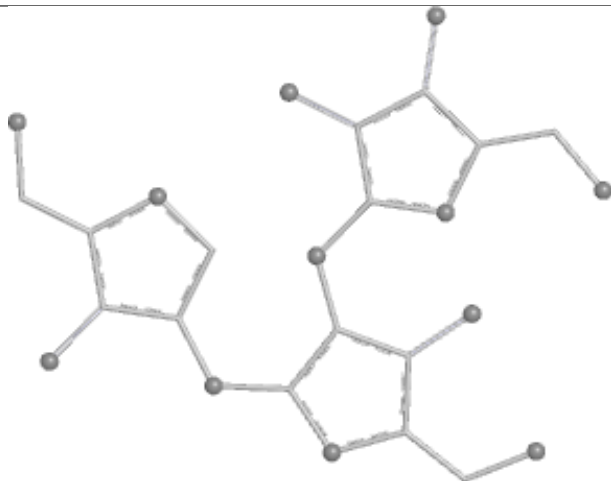
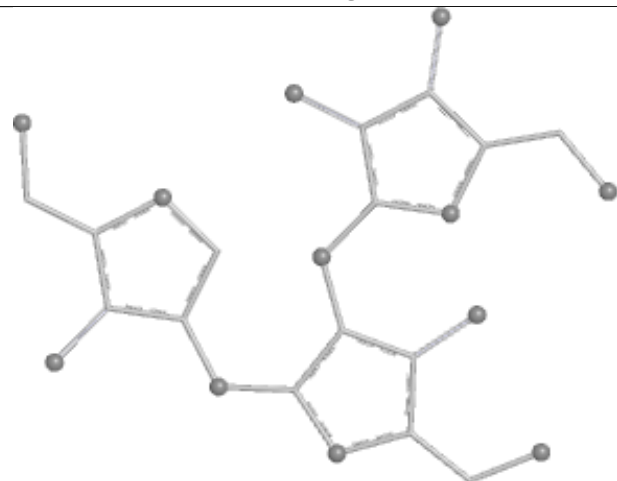
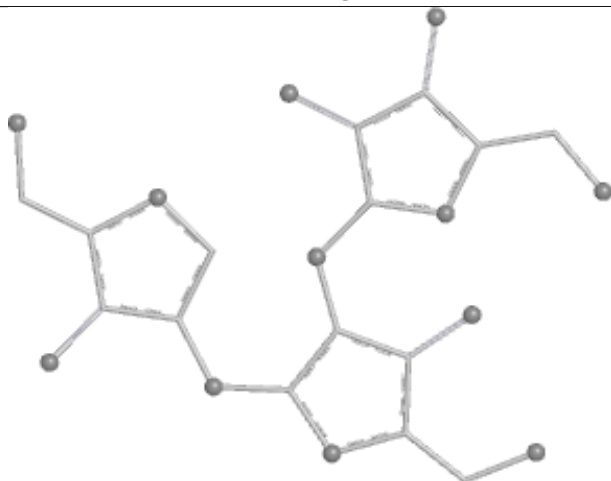


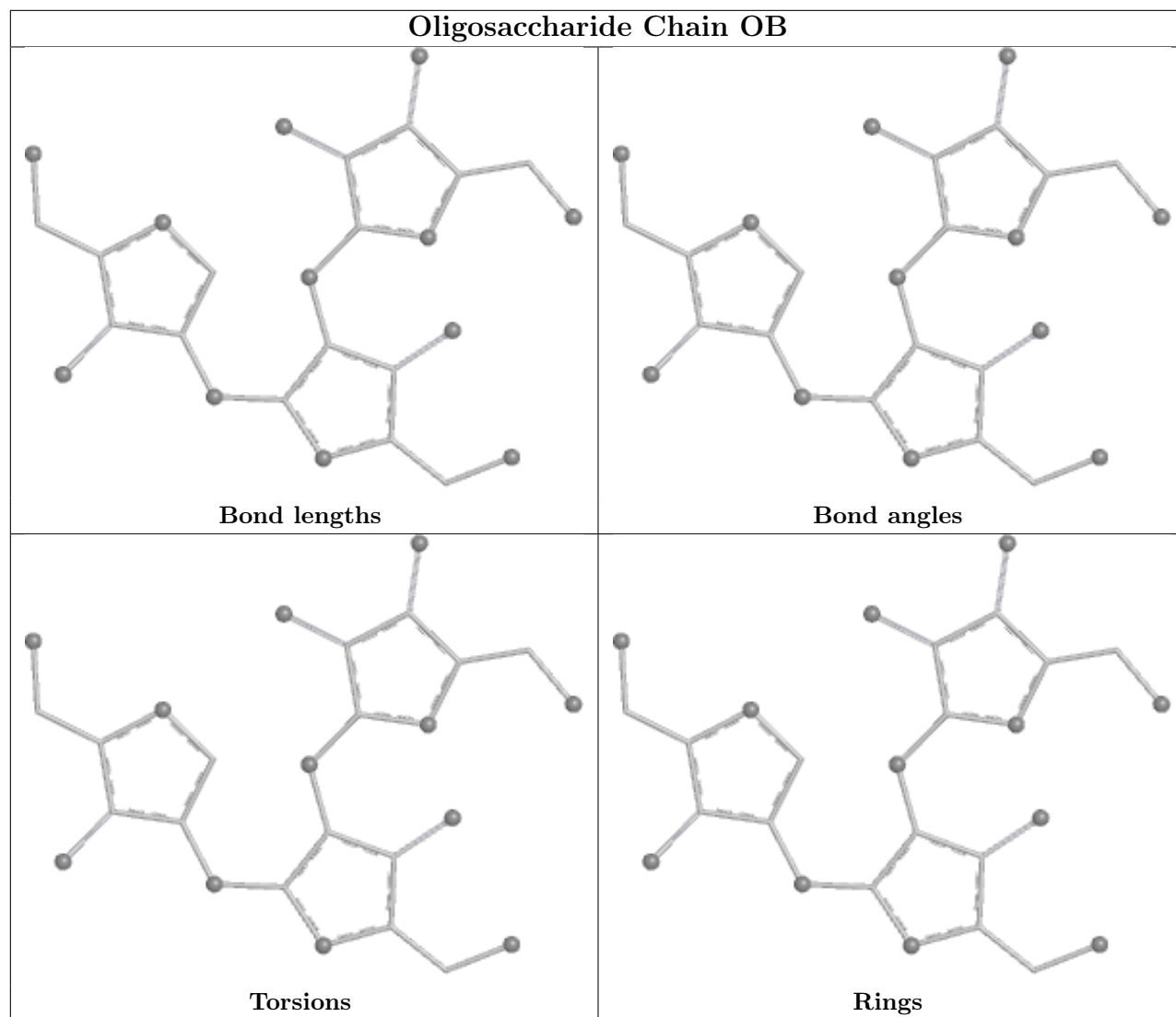


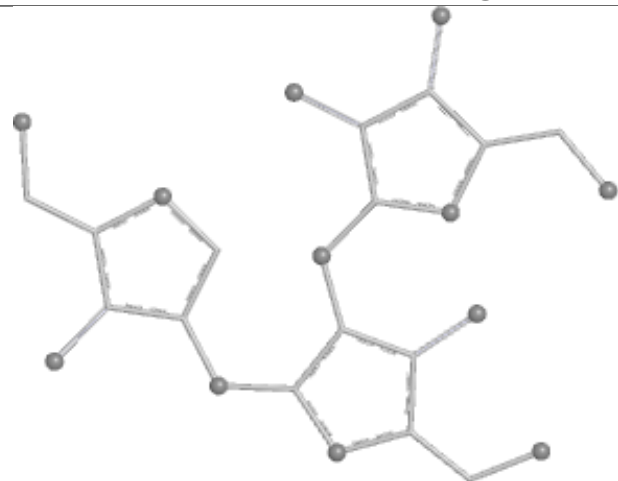
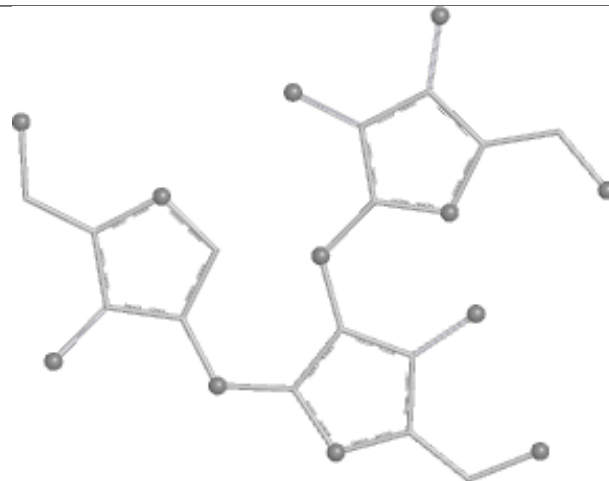
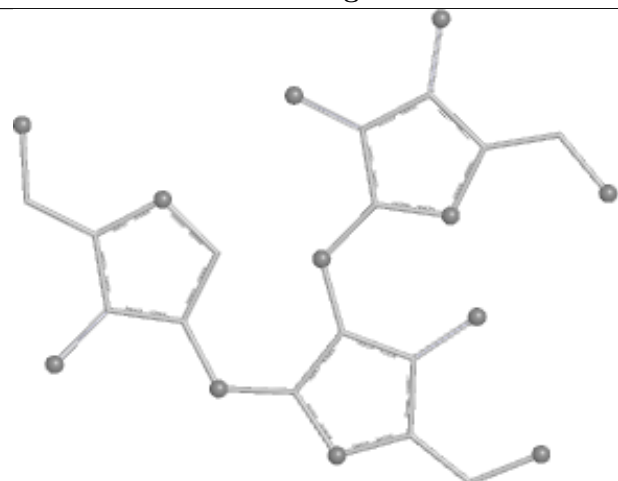
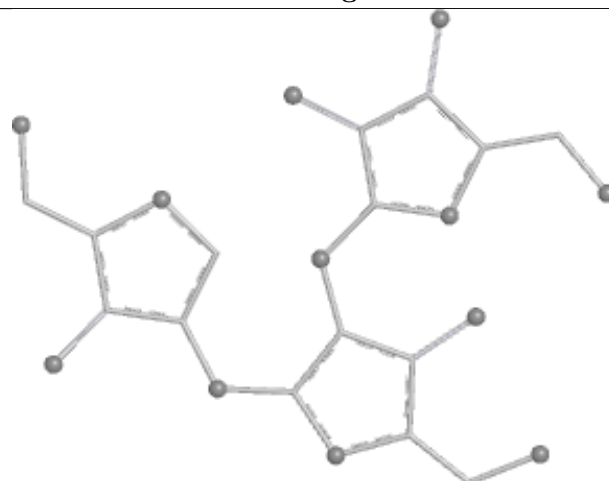


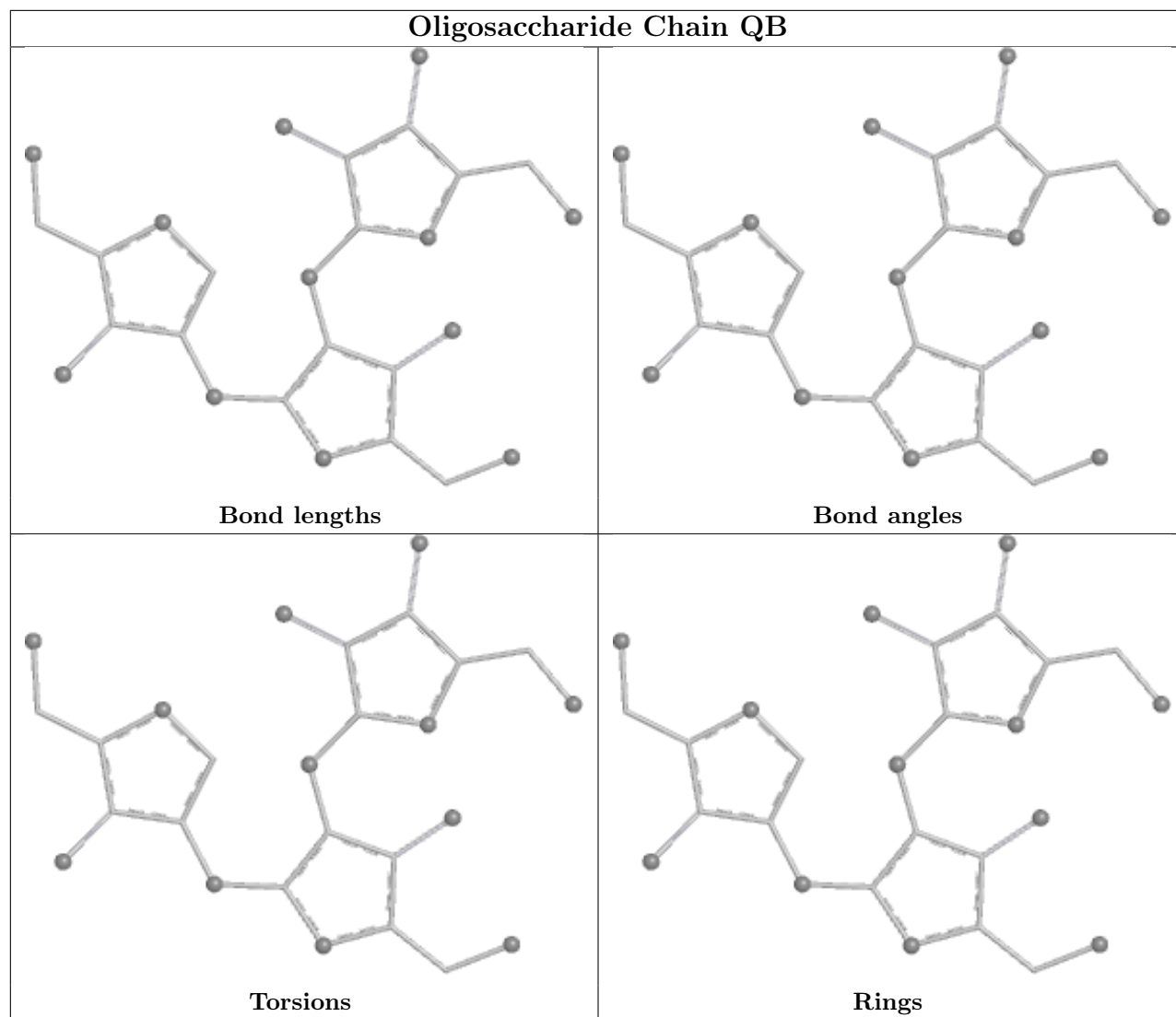


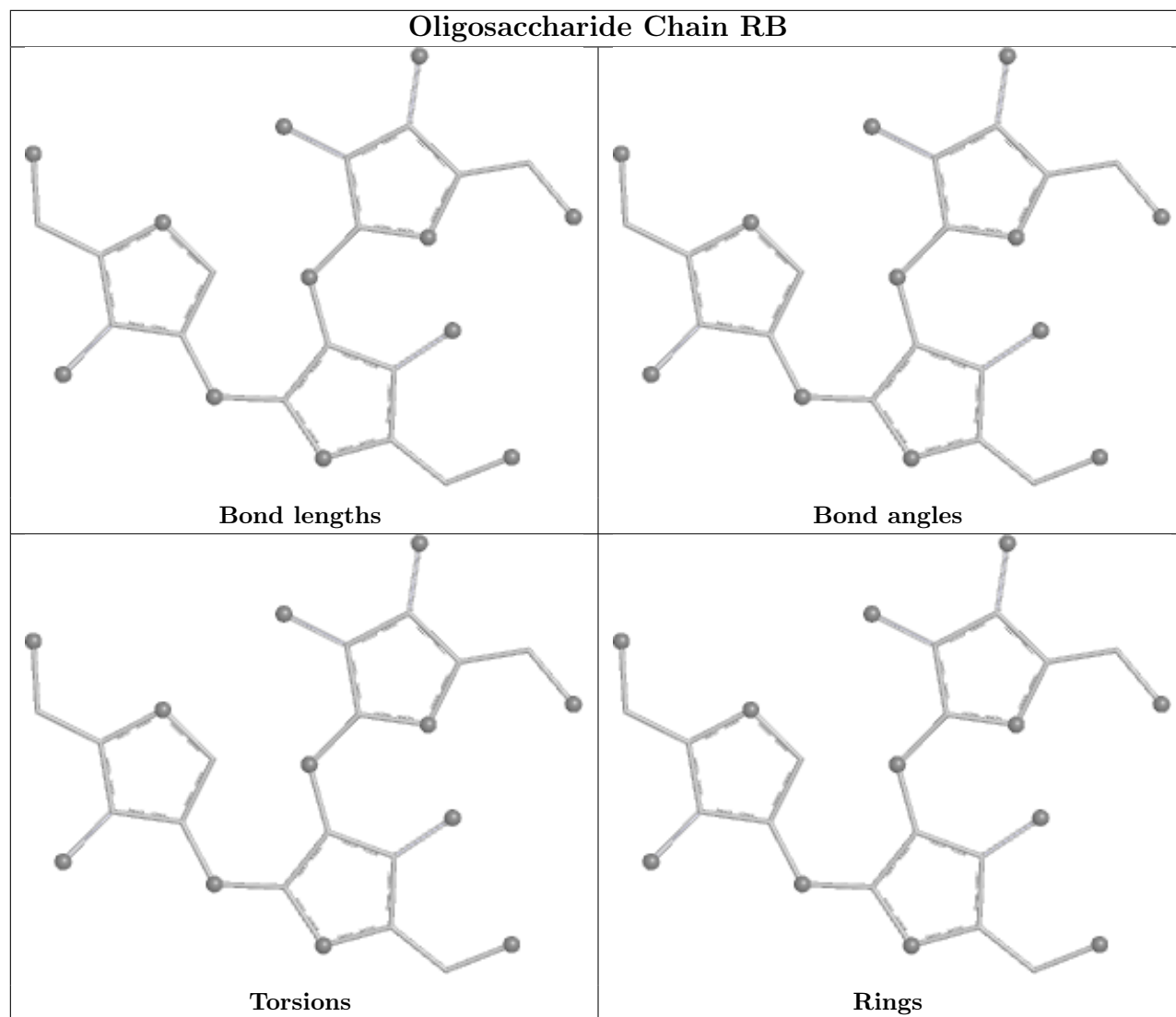
Oligosaccharide Chain EB

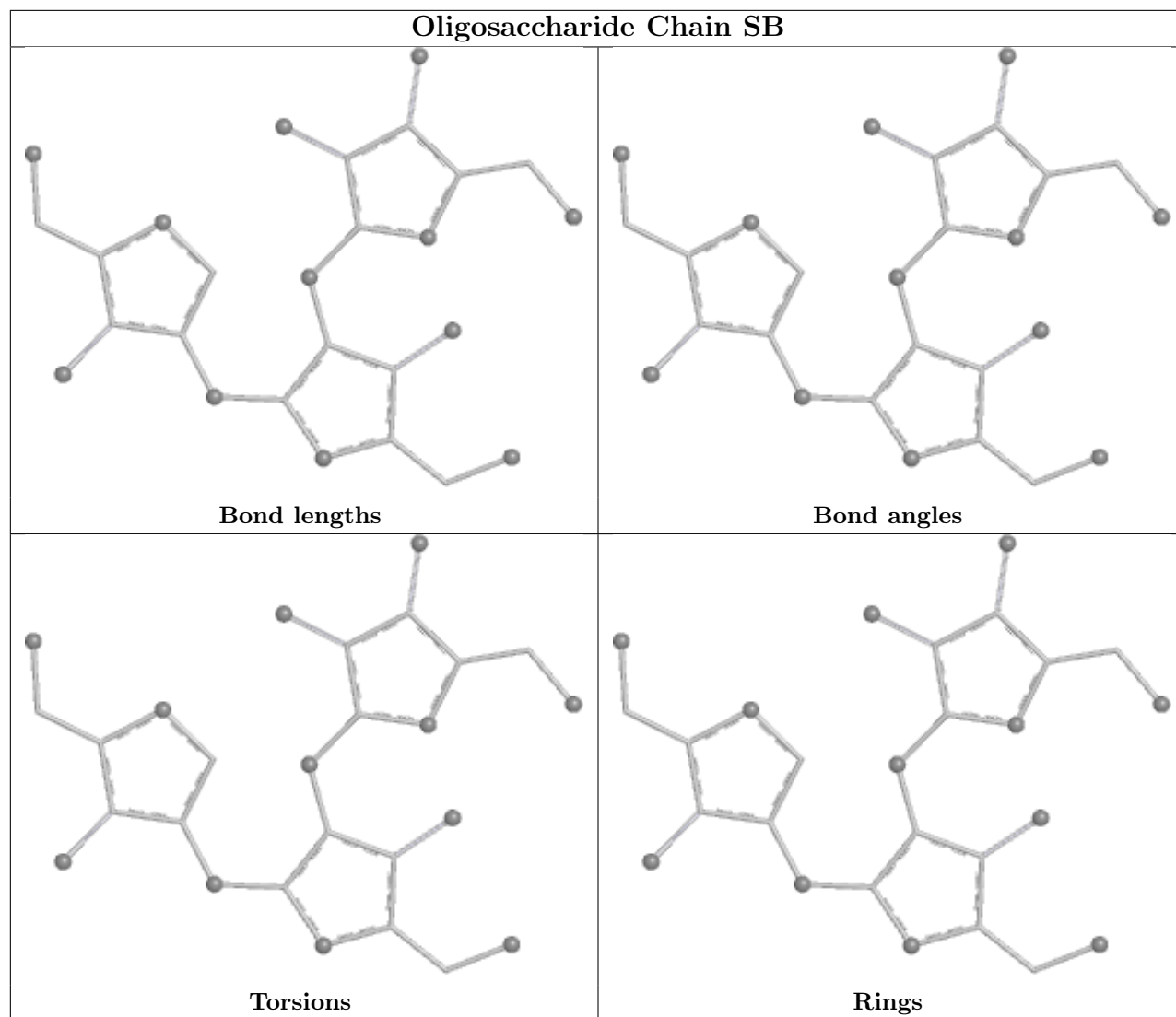
Oligosaccharide Chain LB**Bond lengths****Bond angles****Torsions****Rings**

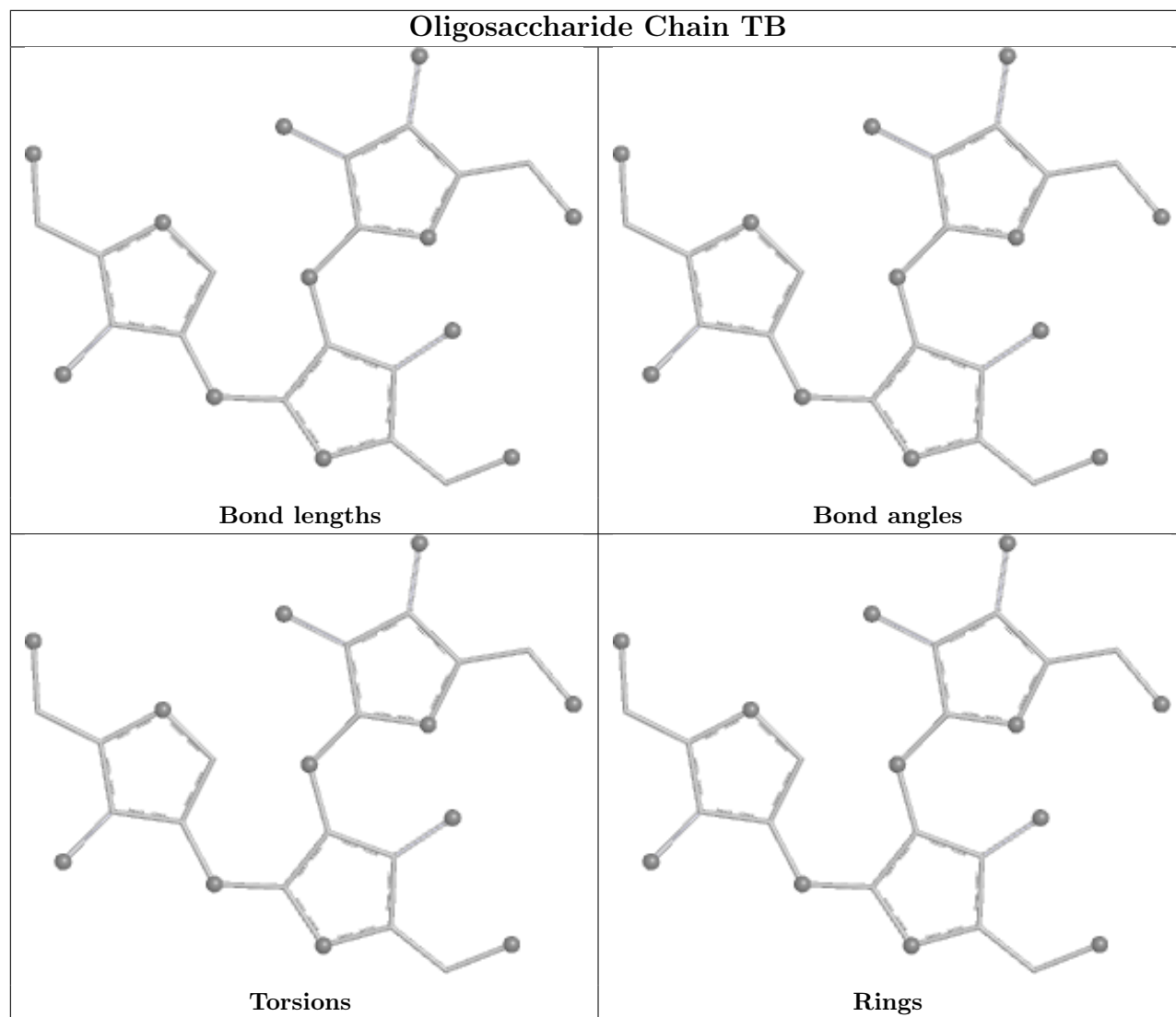


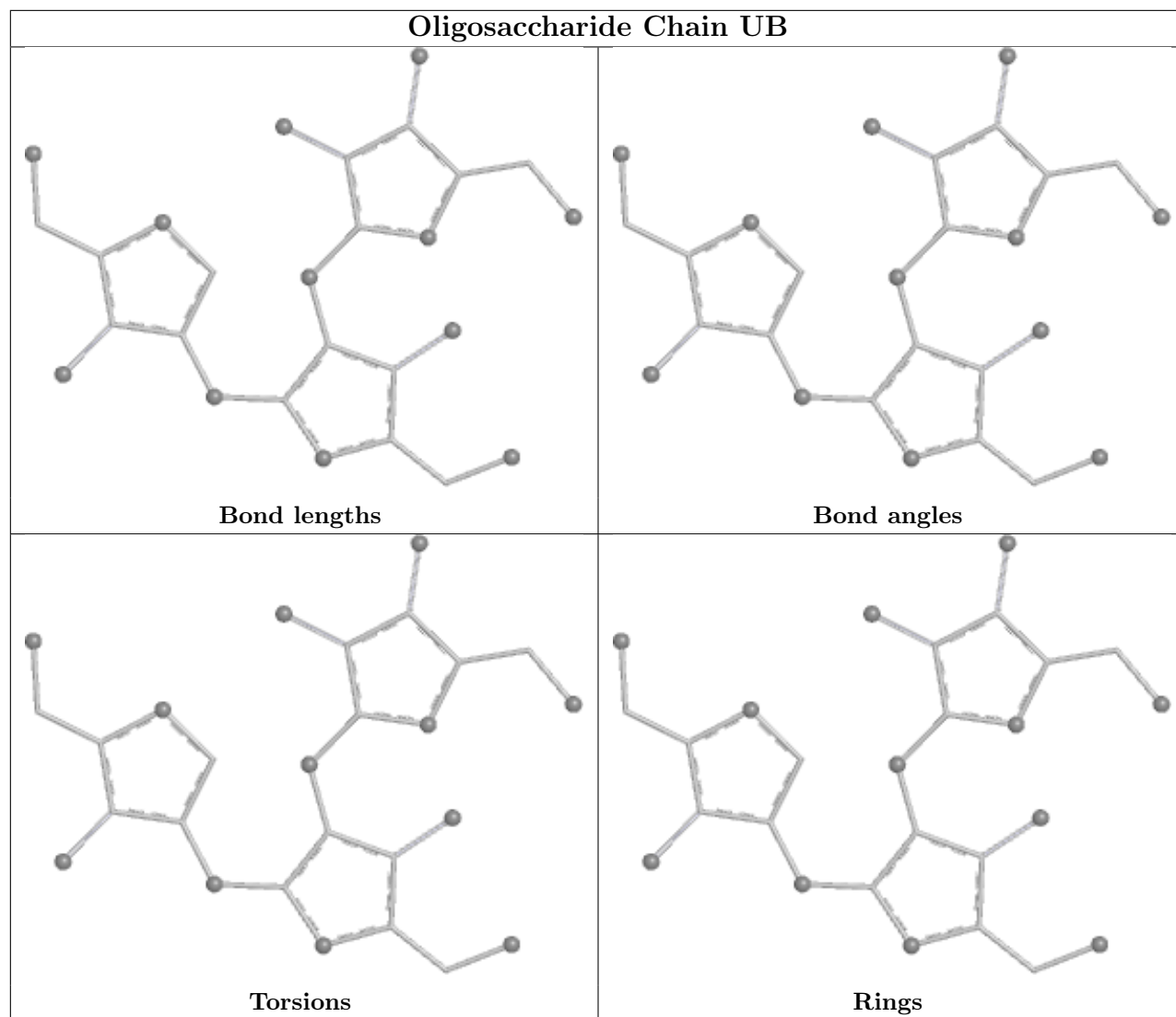
Oligosaccharide Chain PB**Bond lengths****Bond angles****Torsions****Rings**

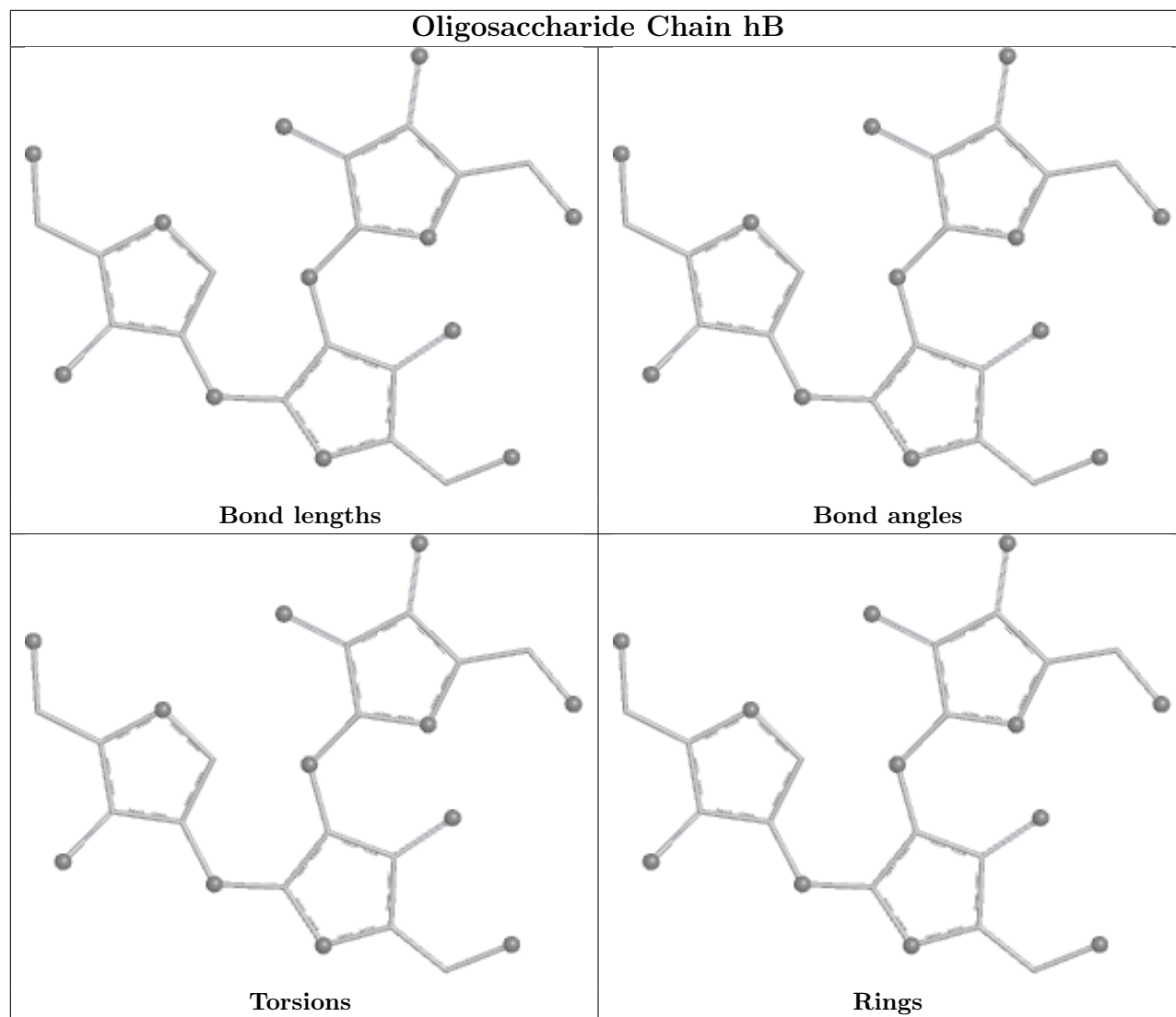


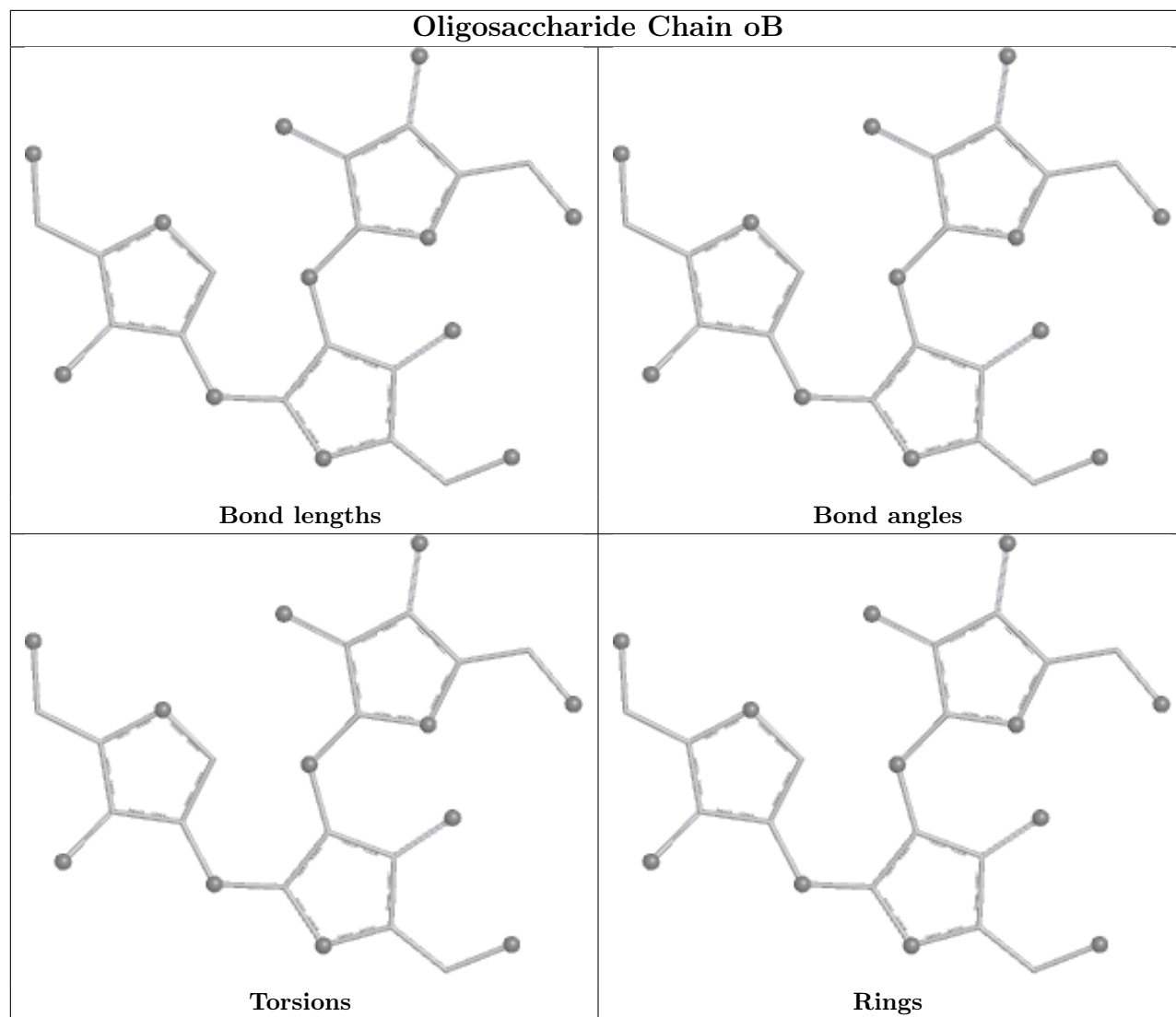


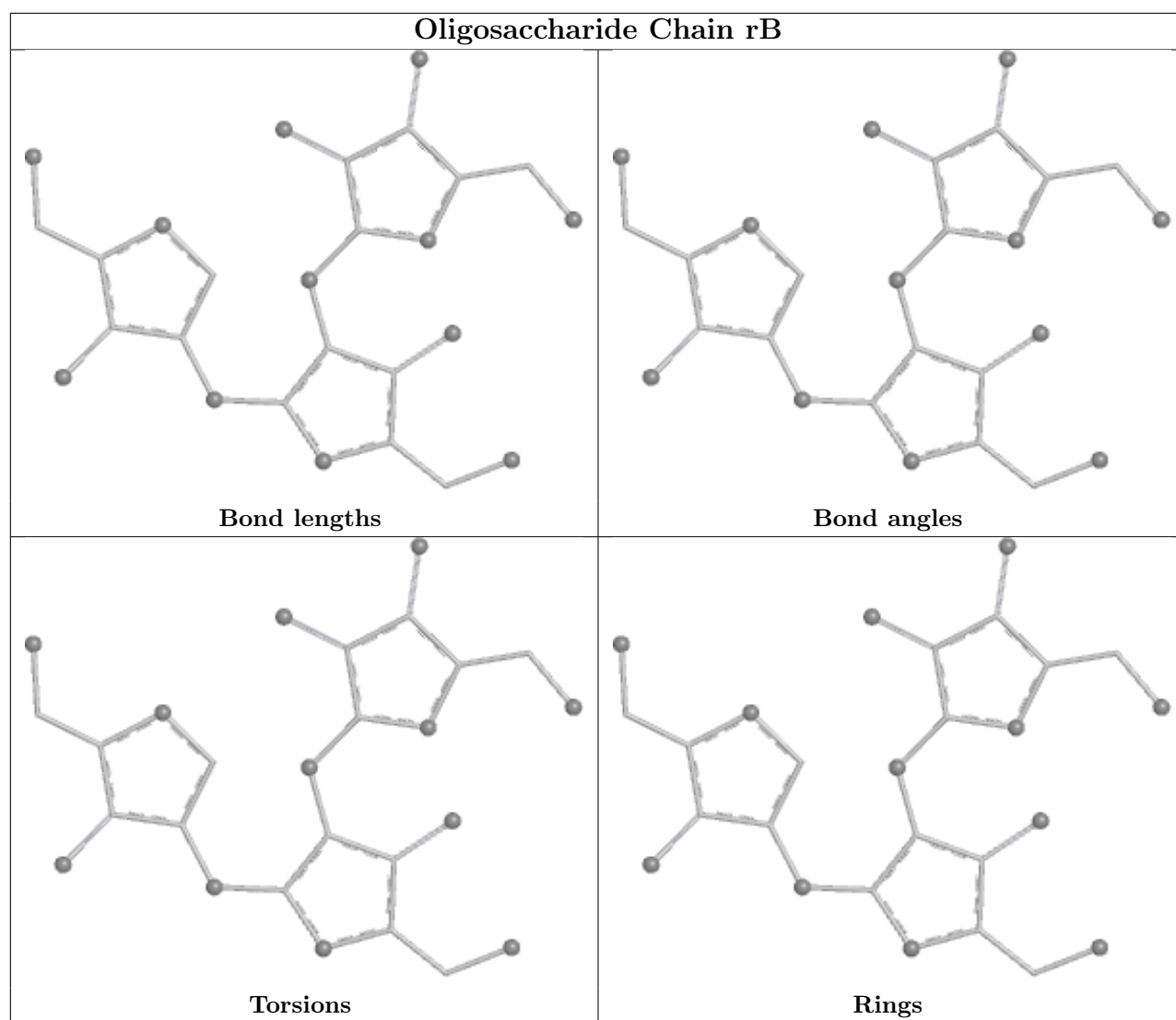


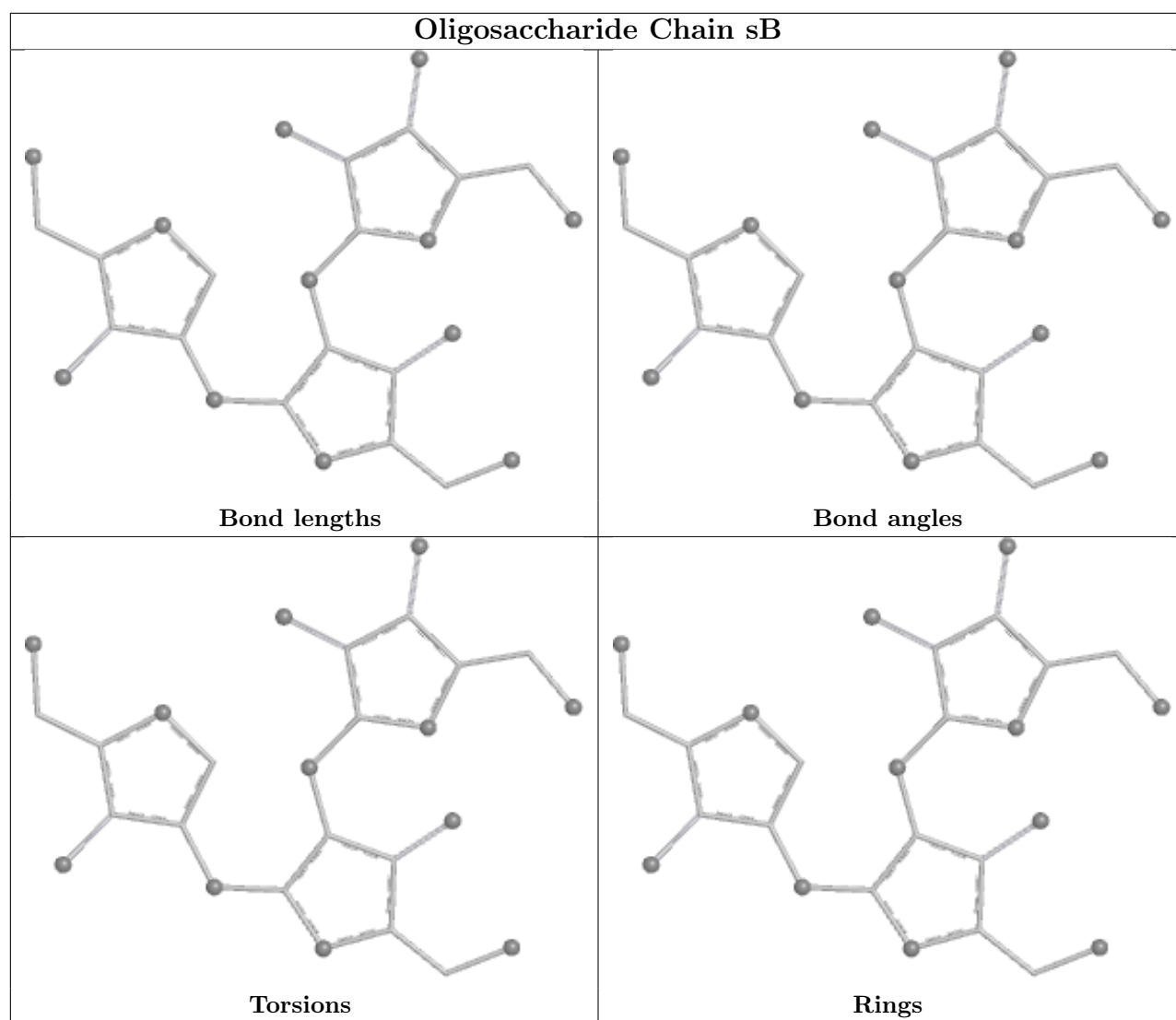


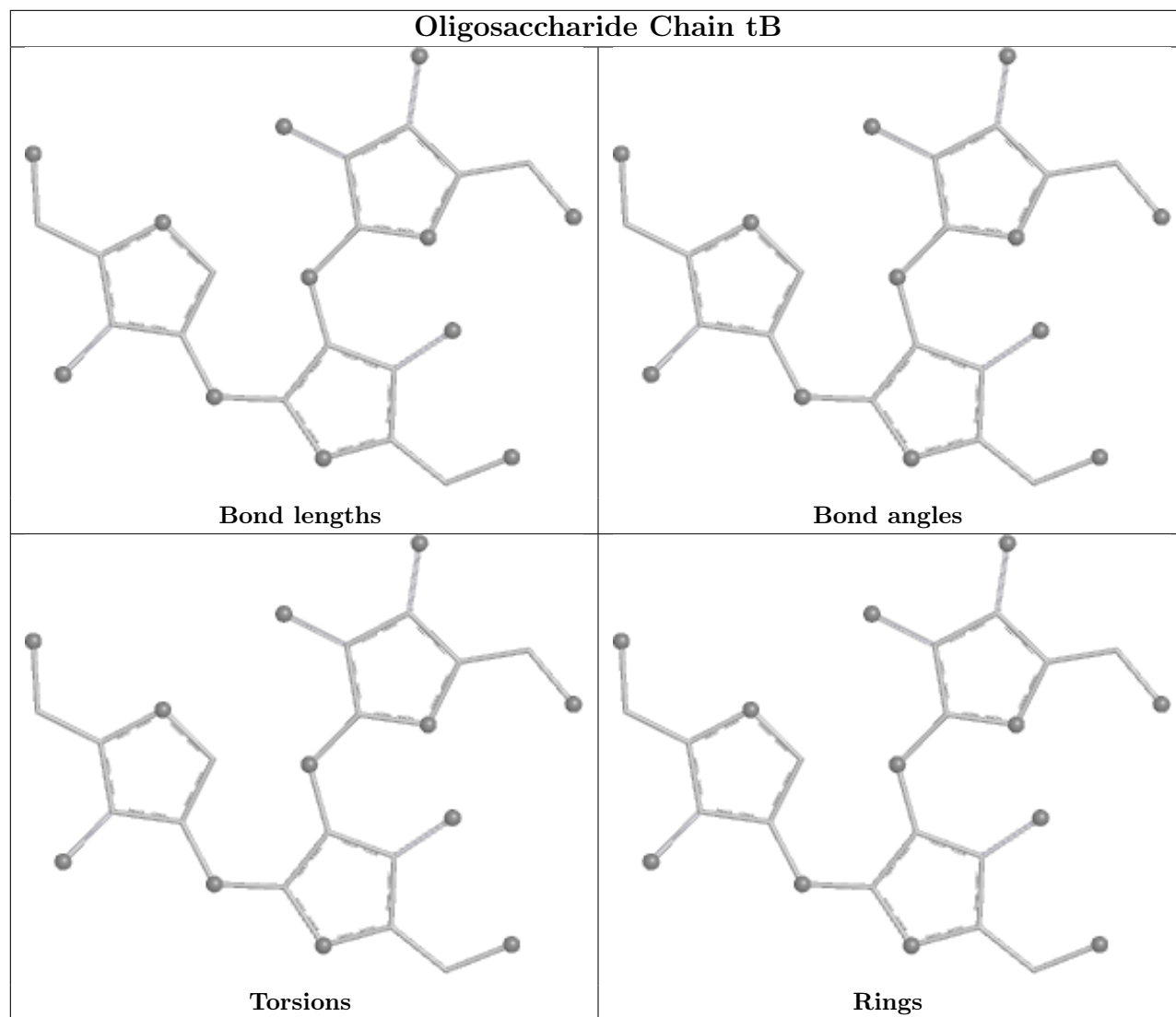


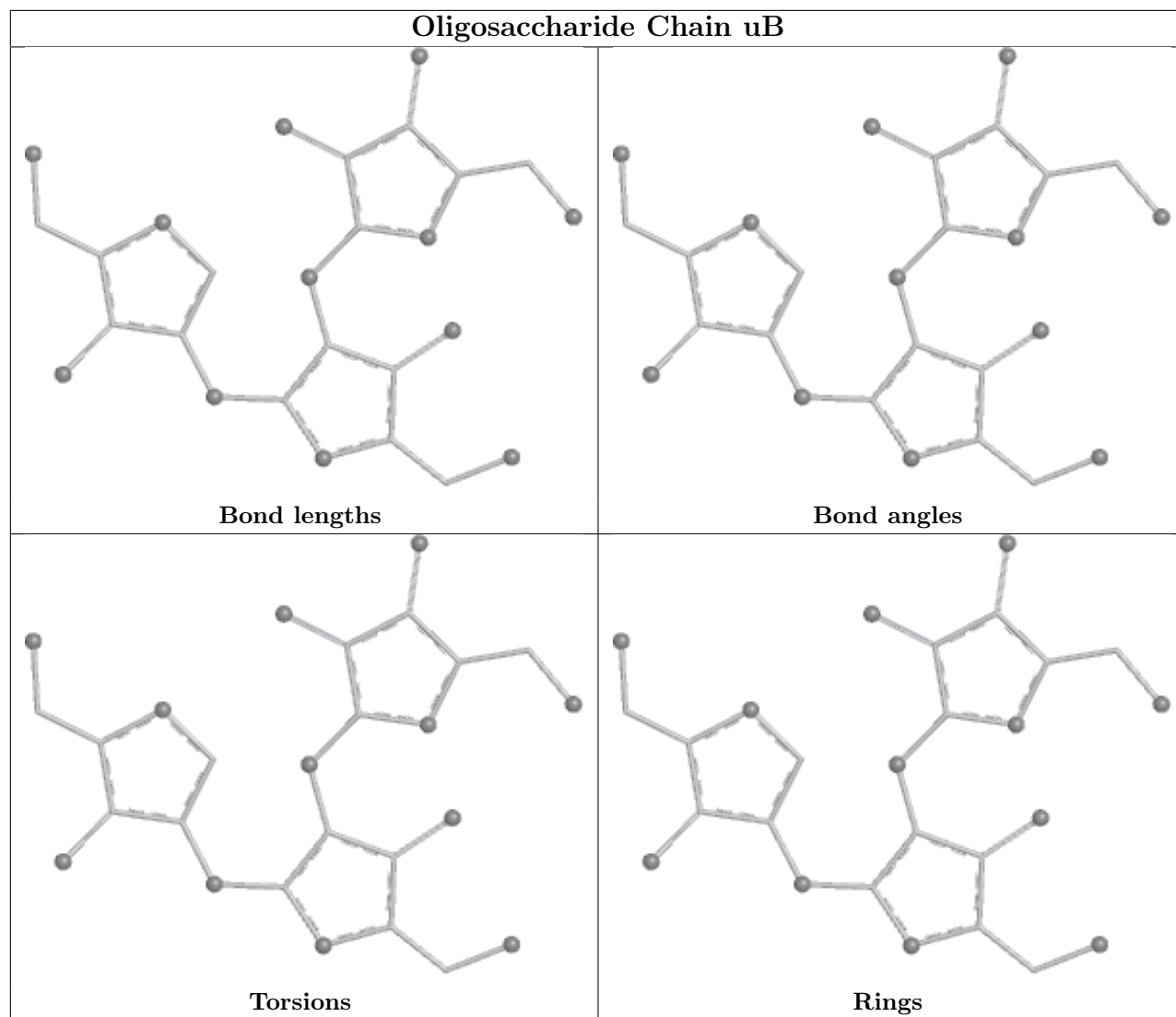


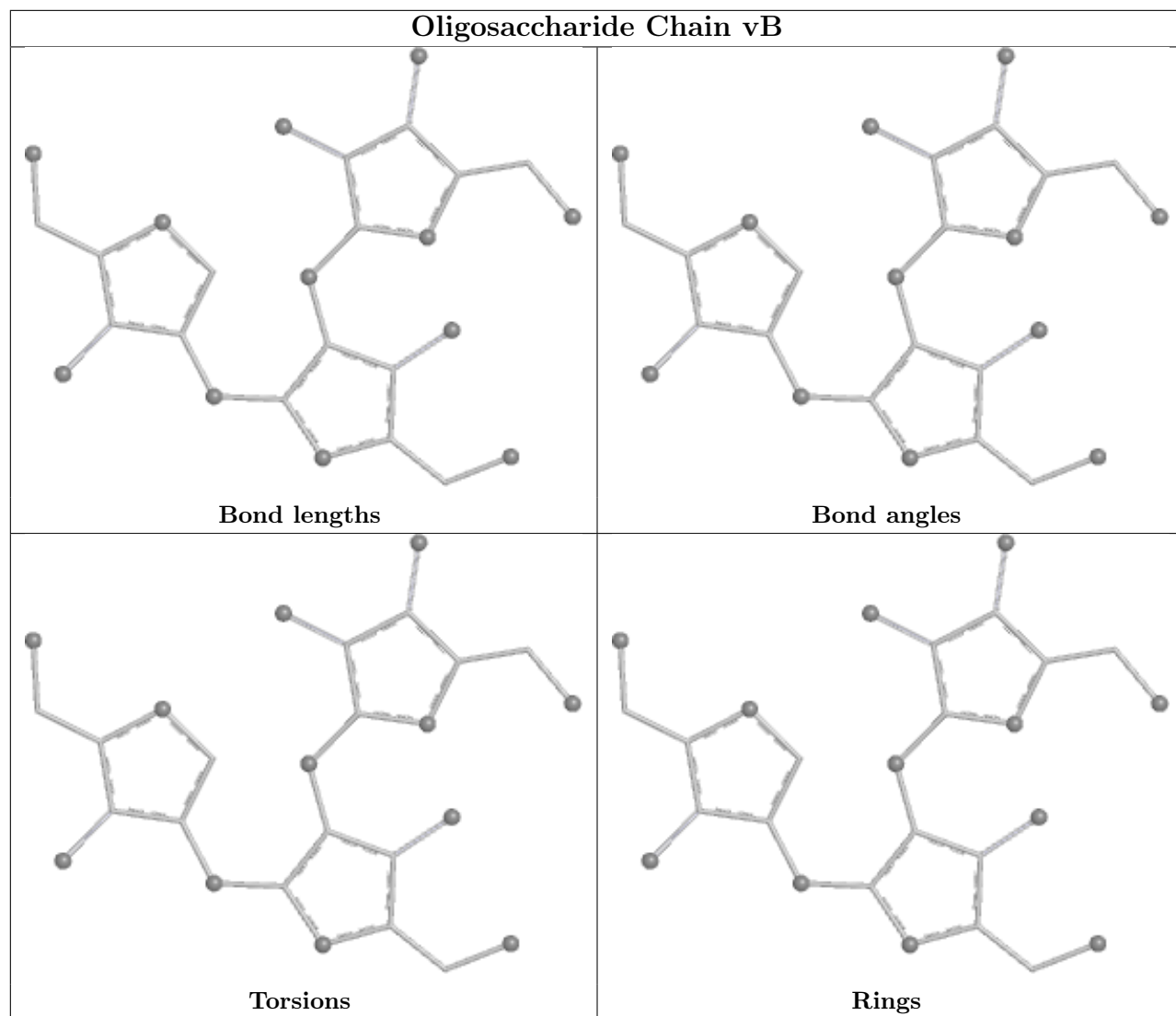


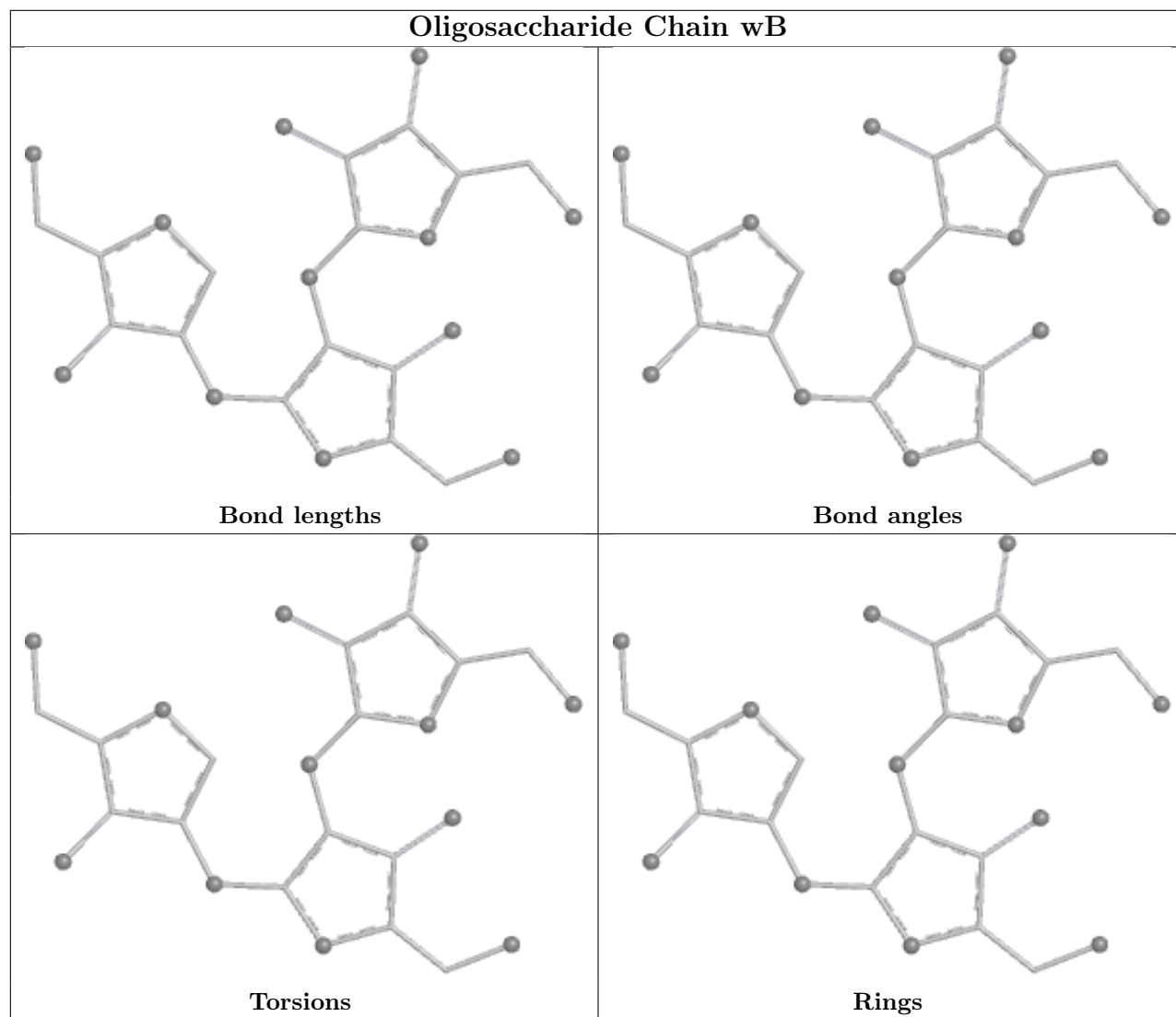


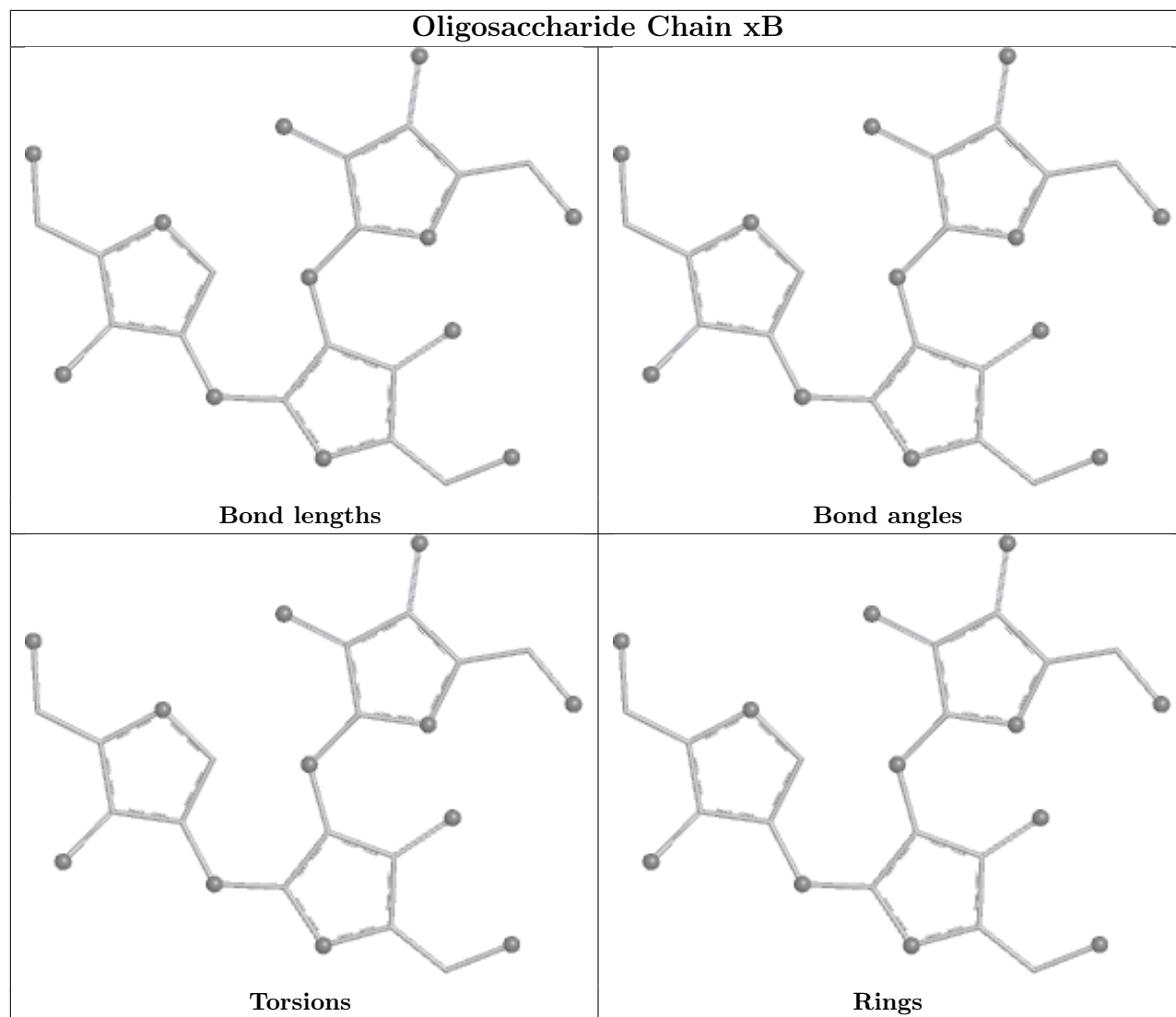


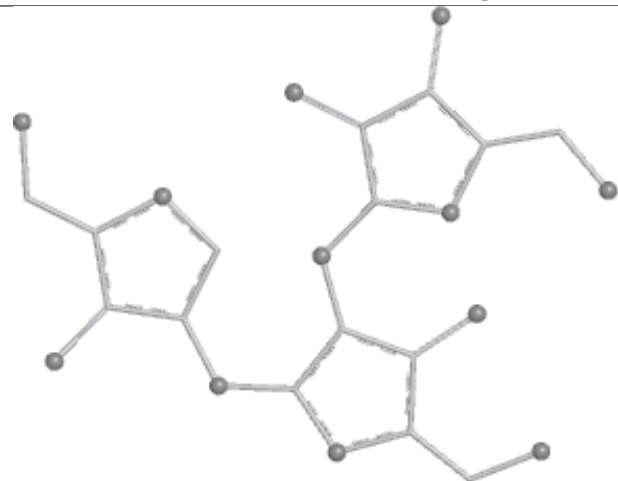
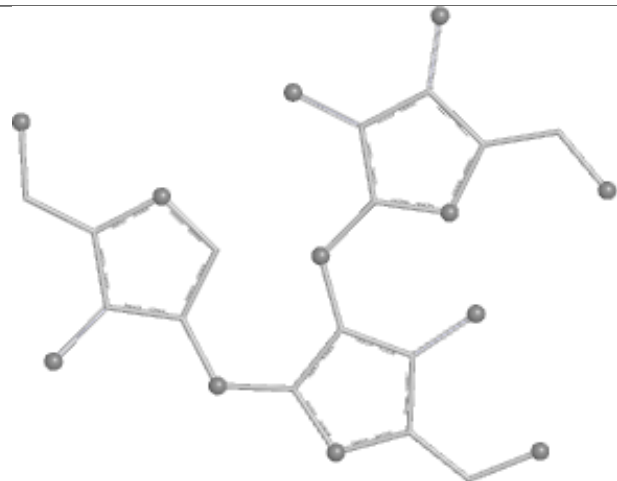
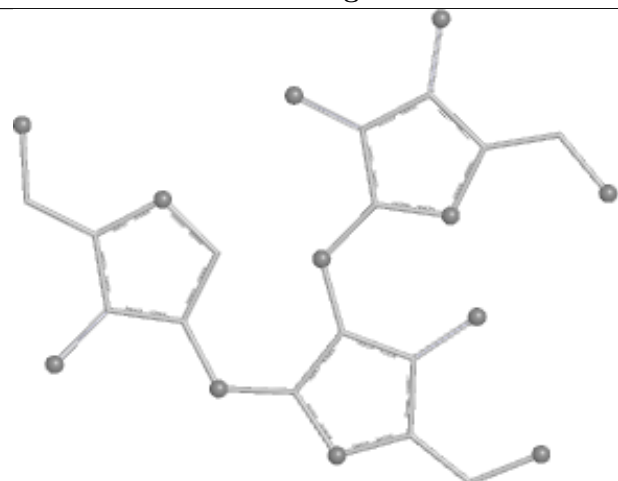
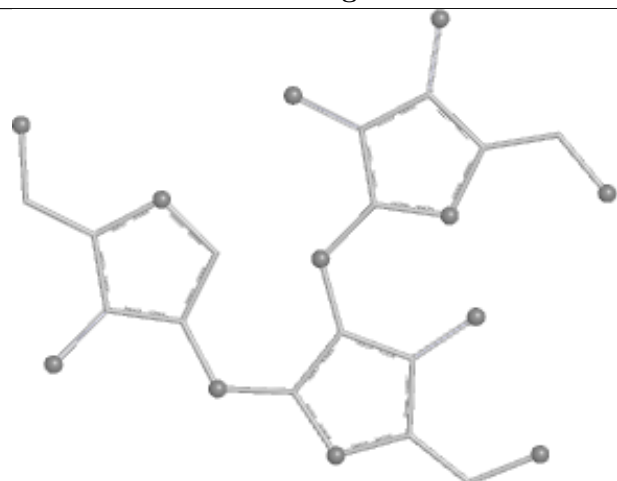




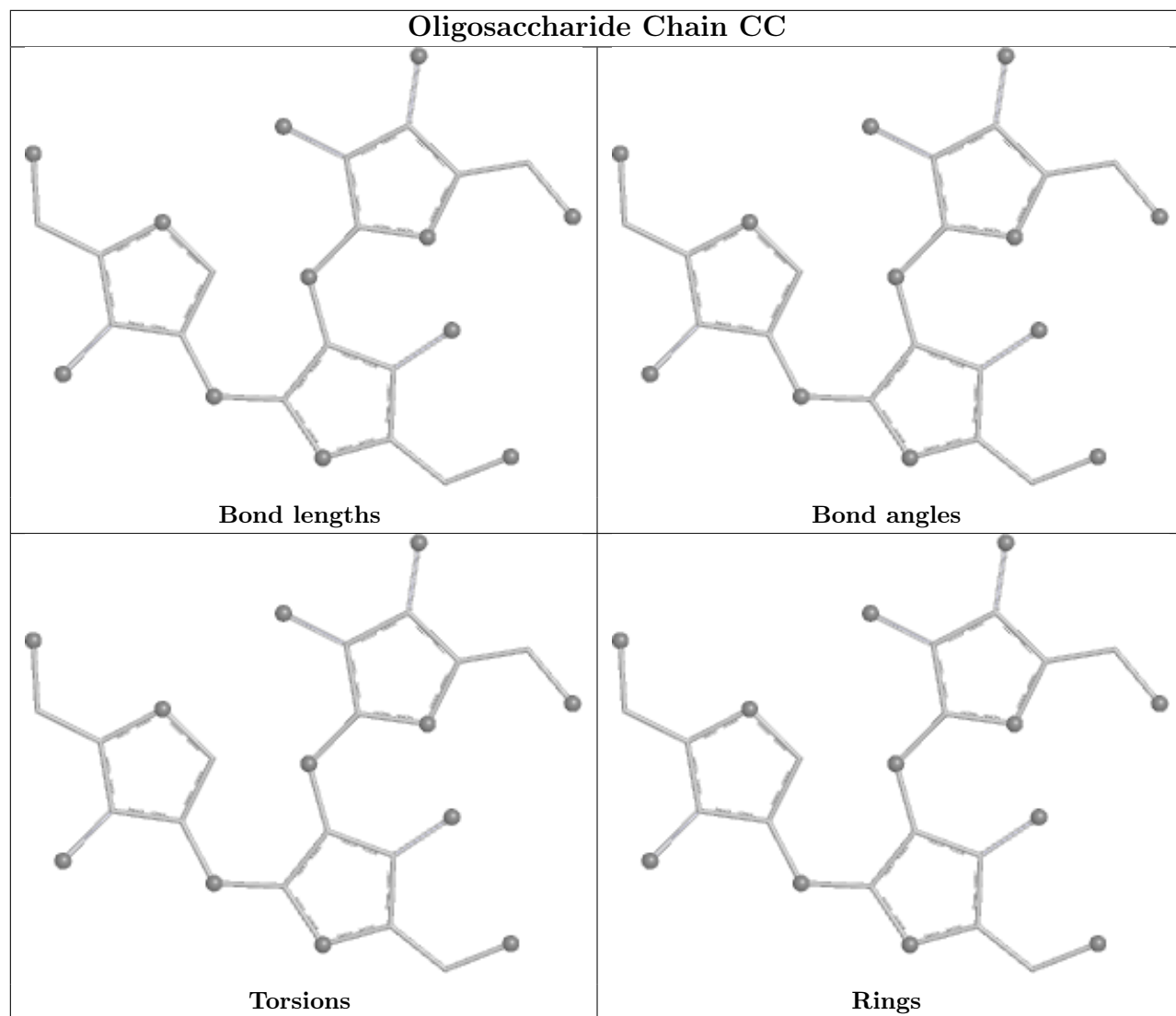


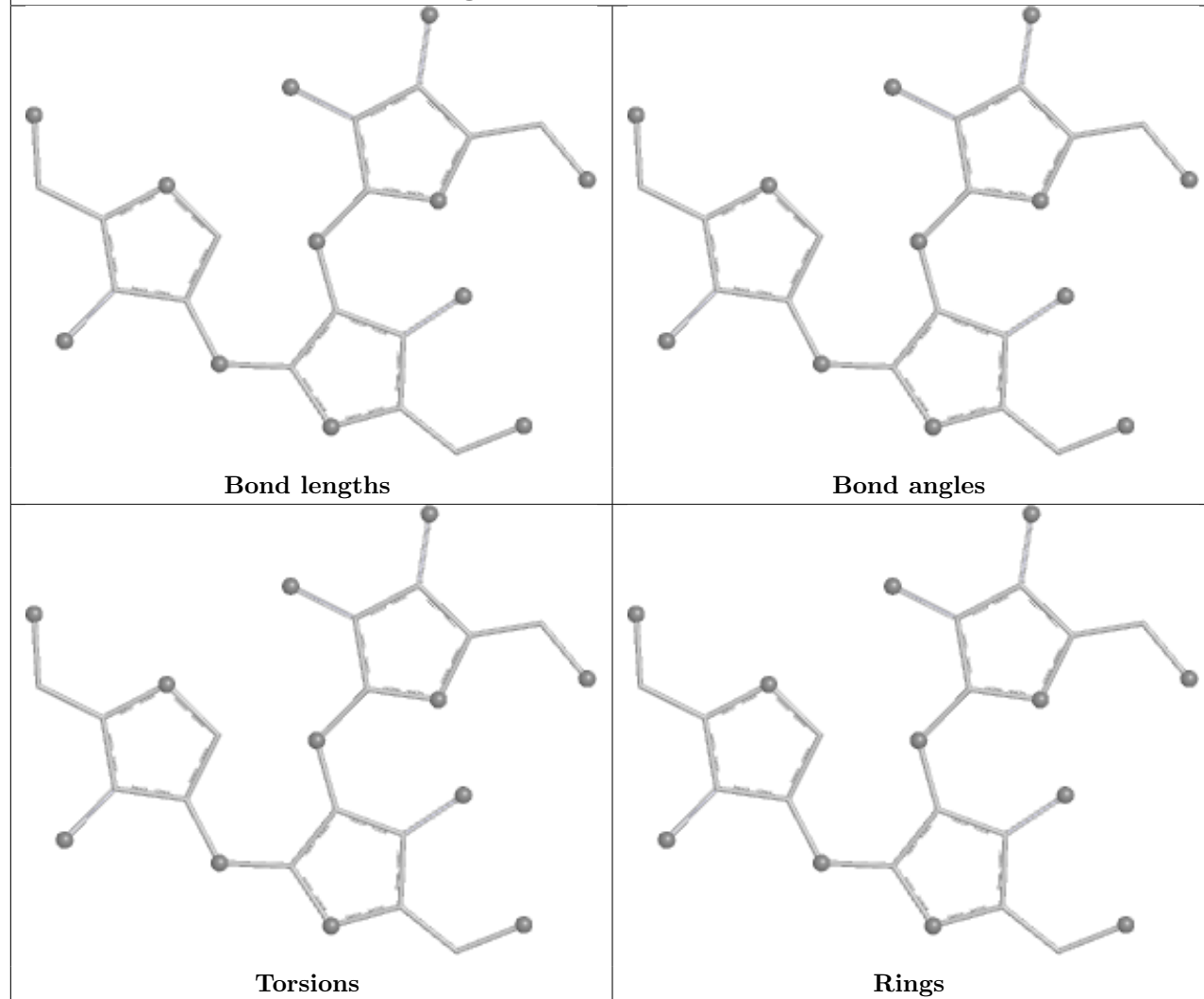


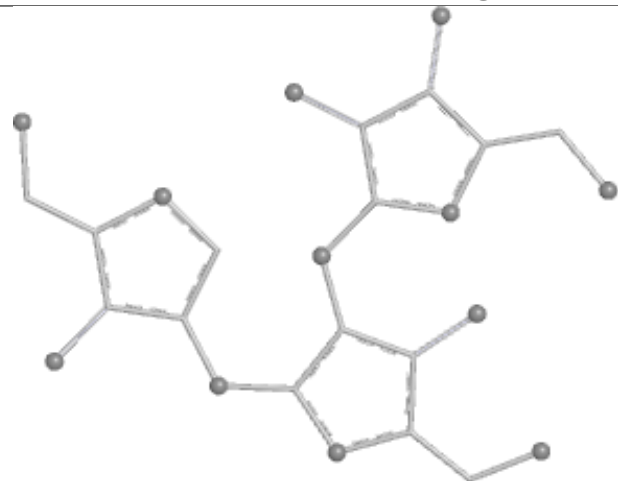
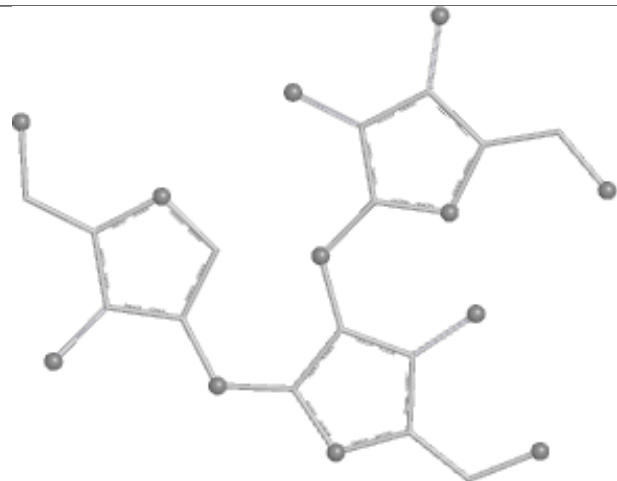
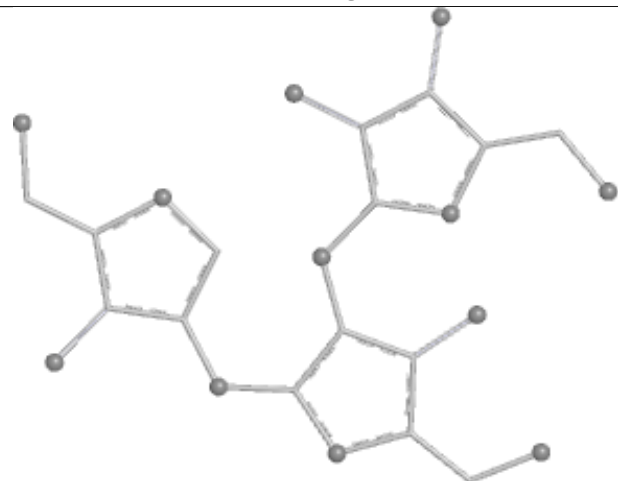
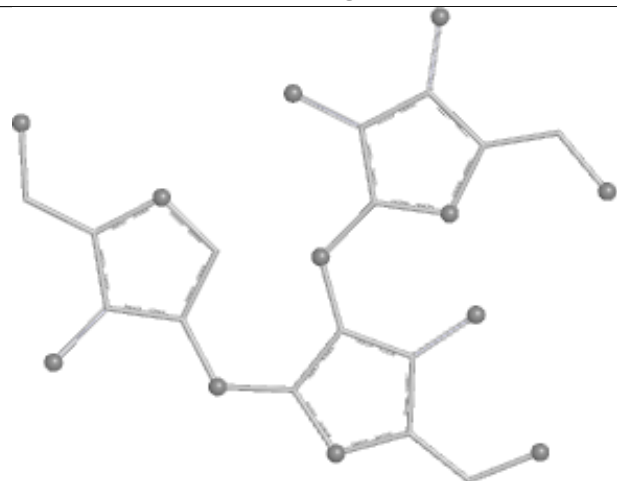


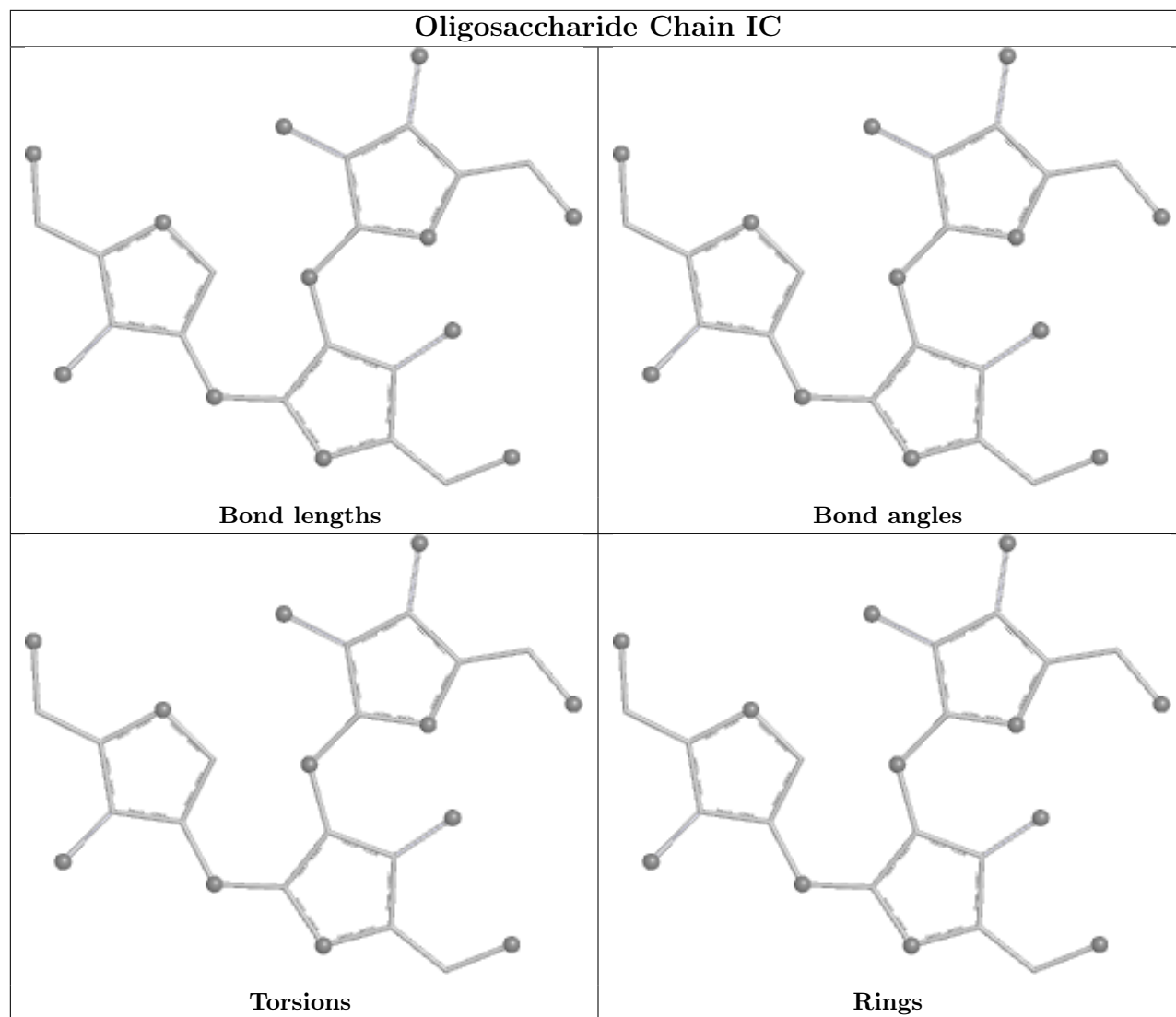
Oligosaccharide Chain BC**Bond lengths****Bond angles****Torsions****Rings**

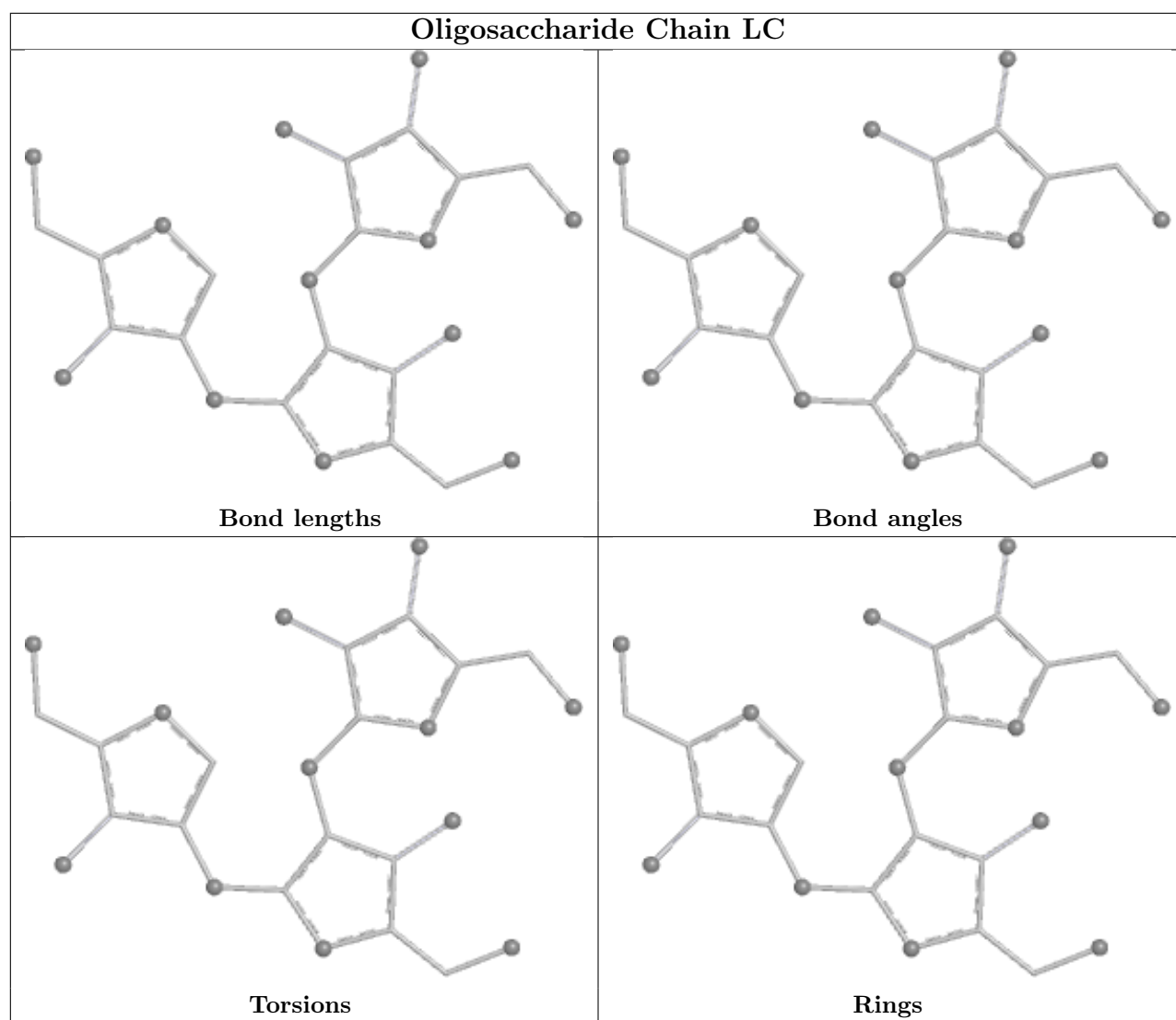
Oligosaccharide Chain CC



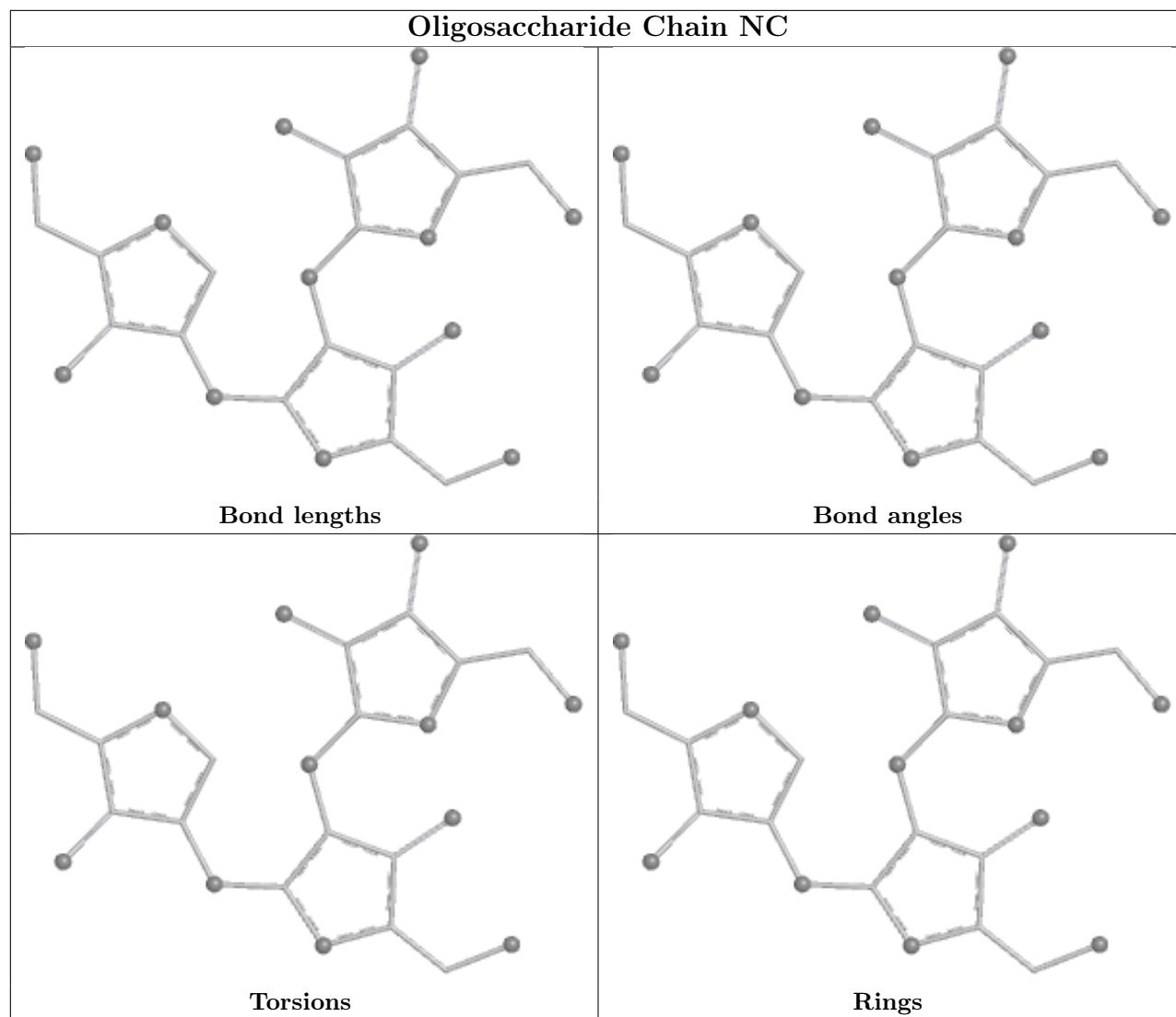
Oligosaccharide Chain GC

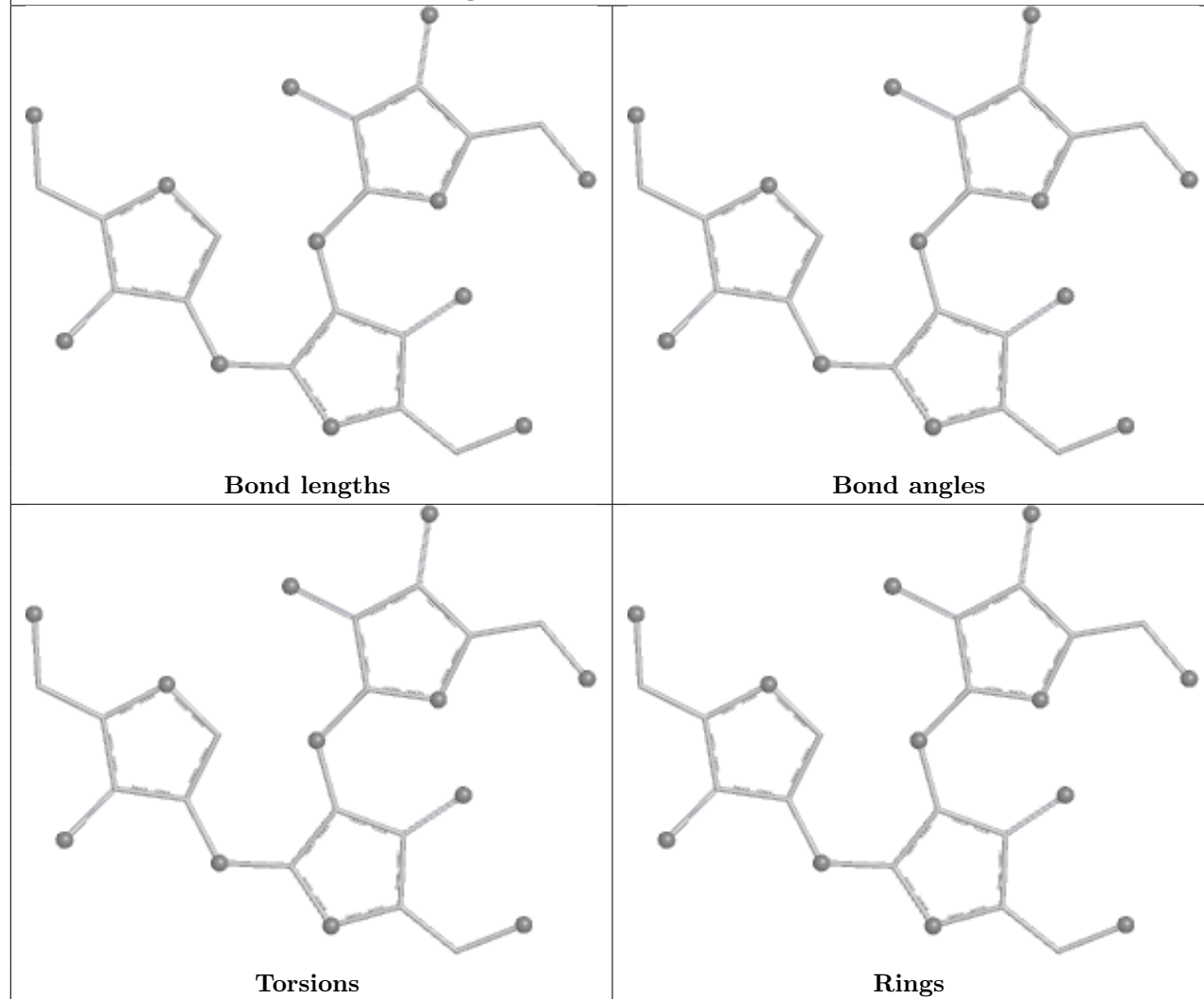
Oligosaccharide Chain HC**Bond lengths****Bond angles****Torsions****Rings**

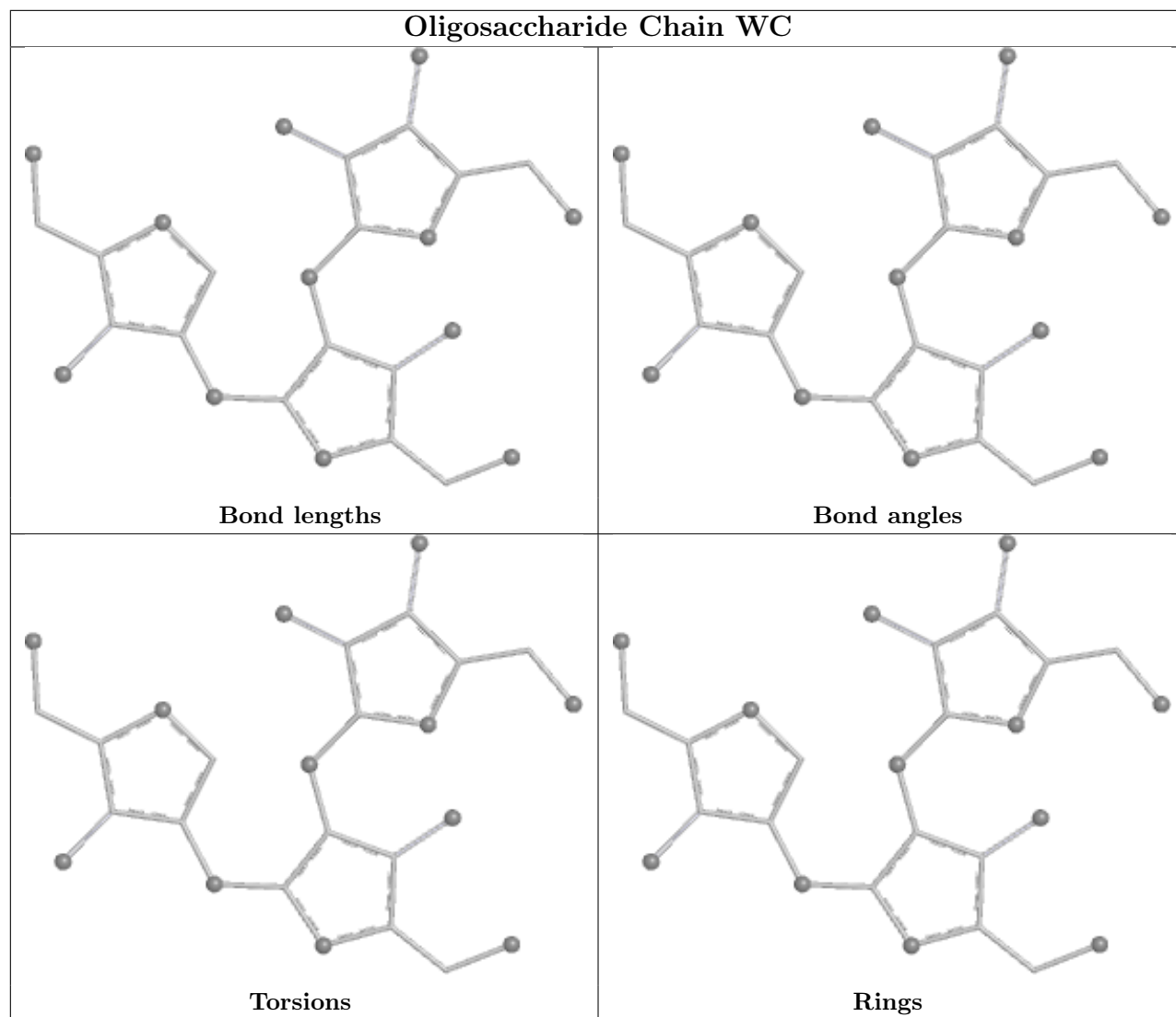


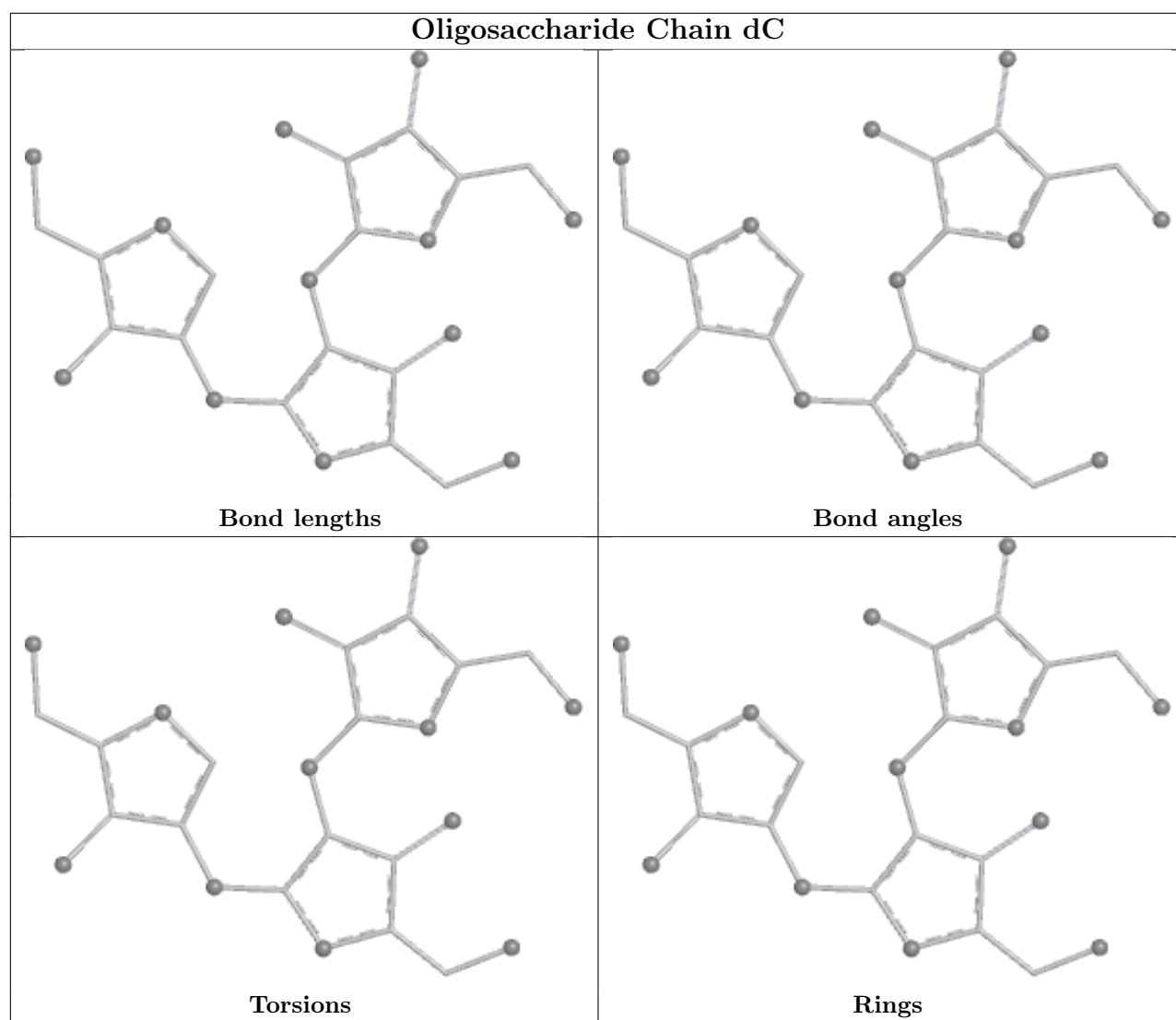


Oligosaccharide Chain NC

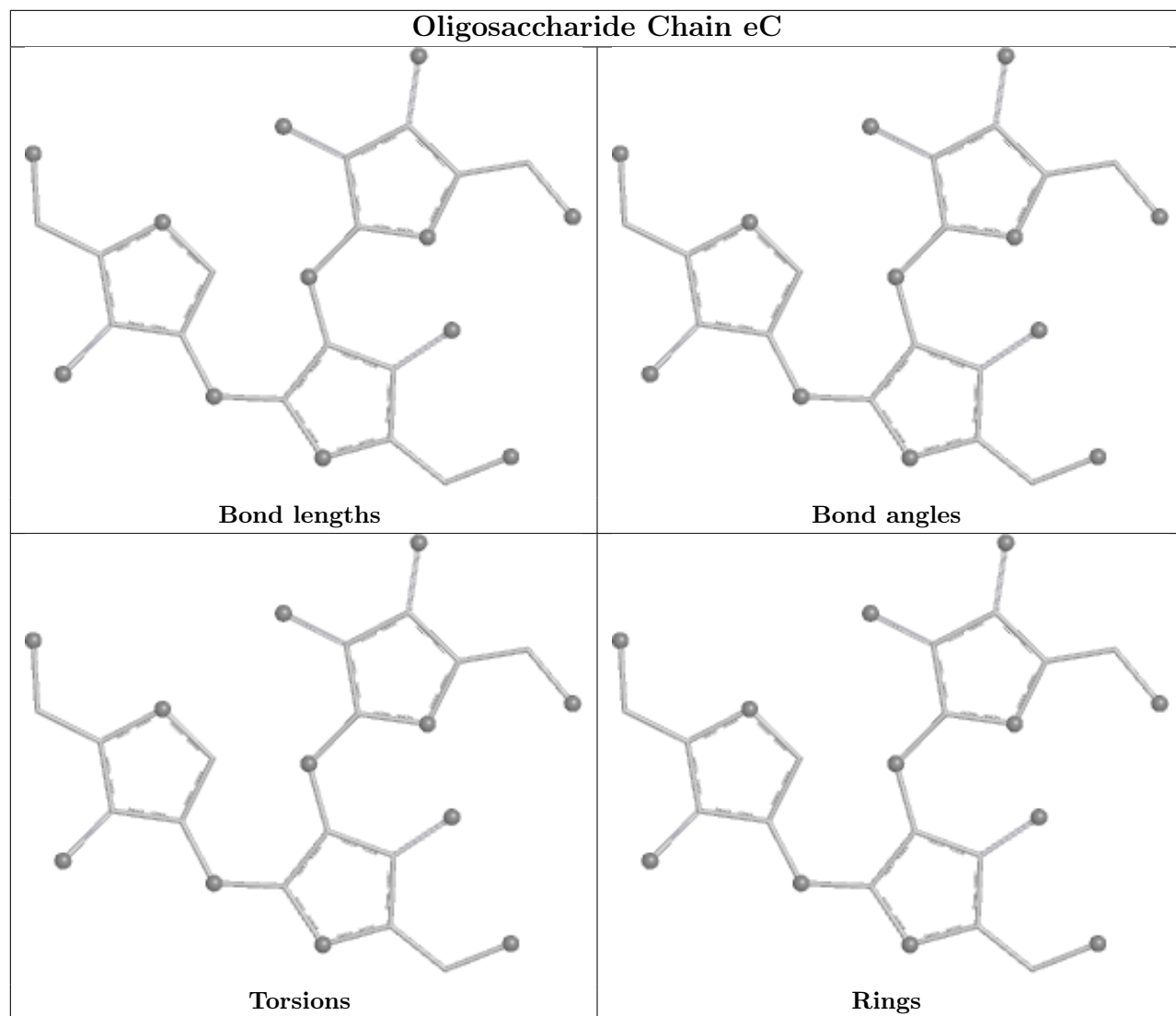


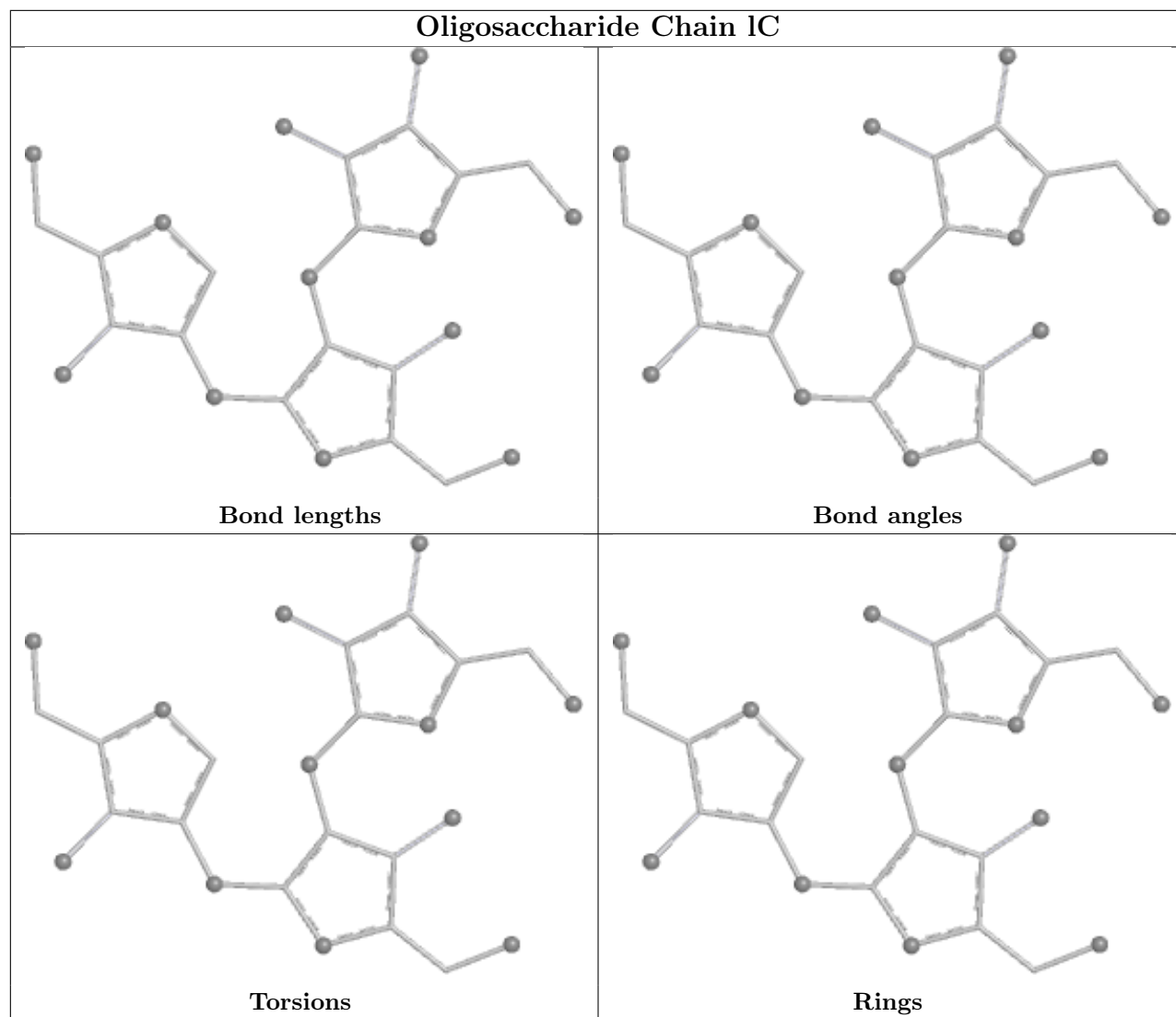
Oligosaccharide Chain TC

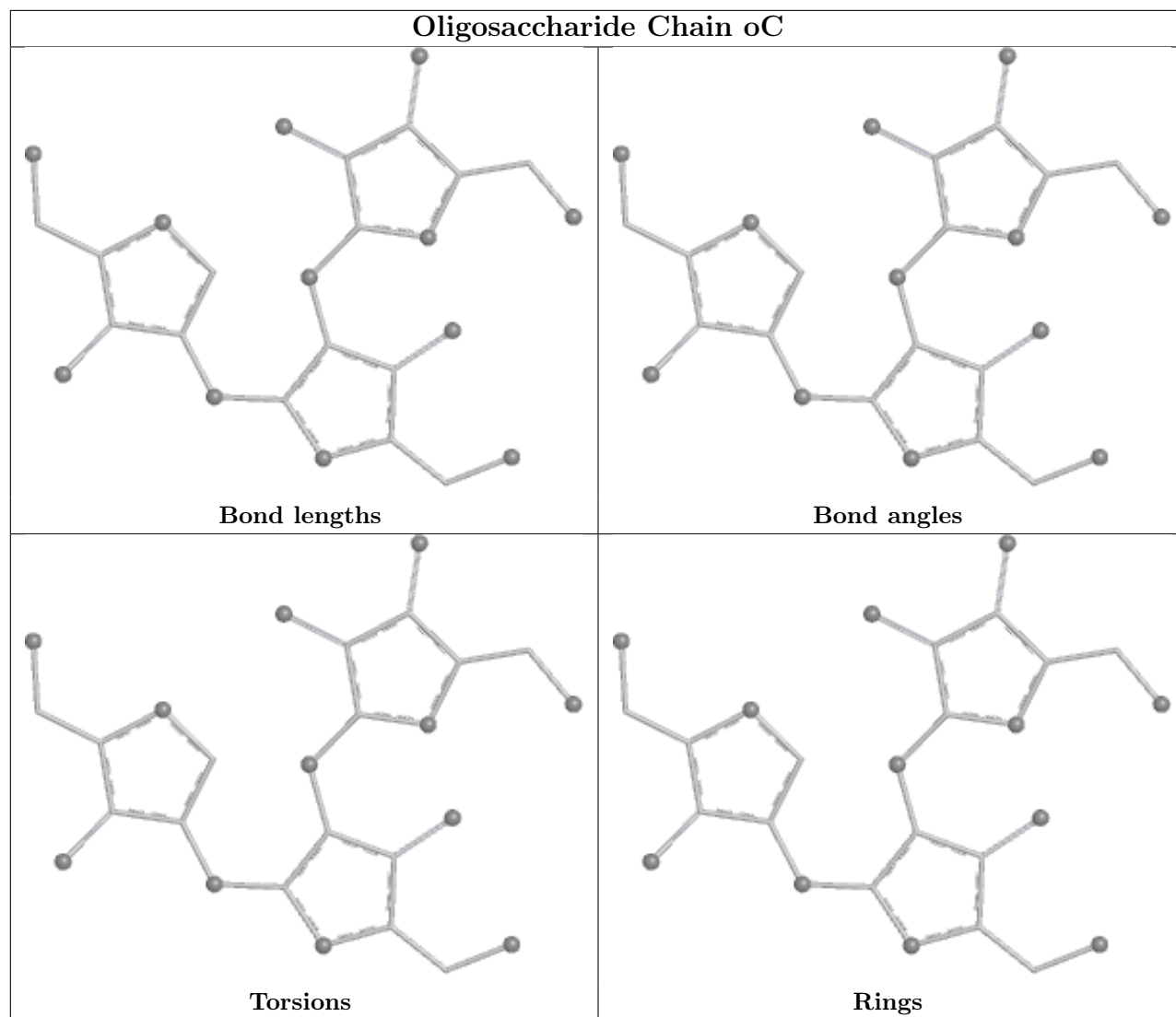


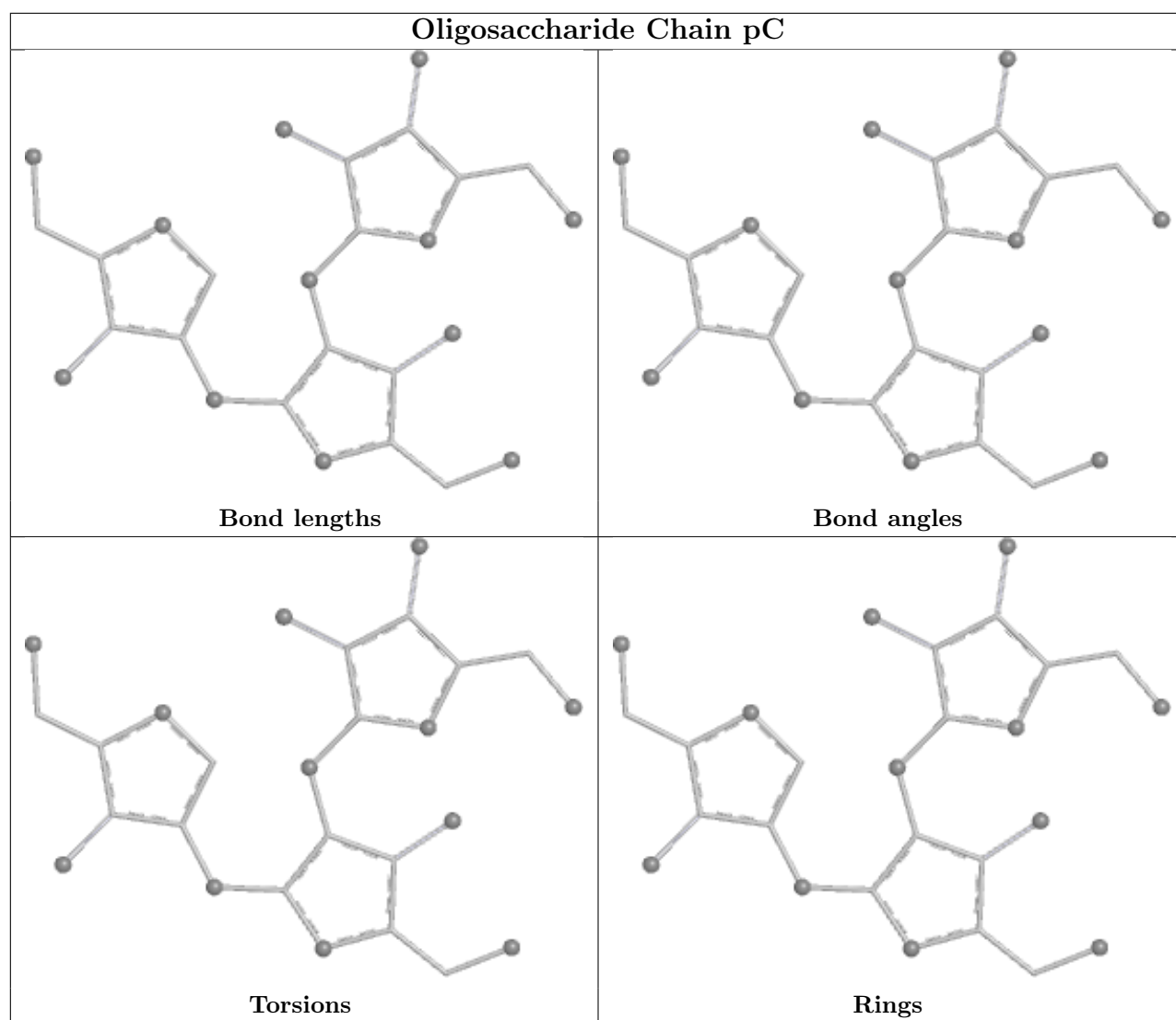


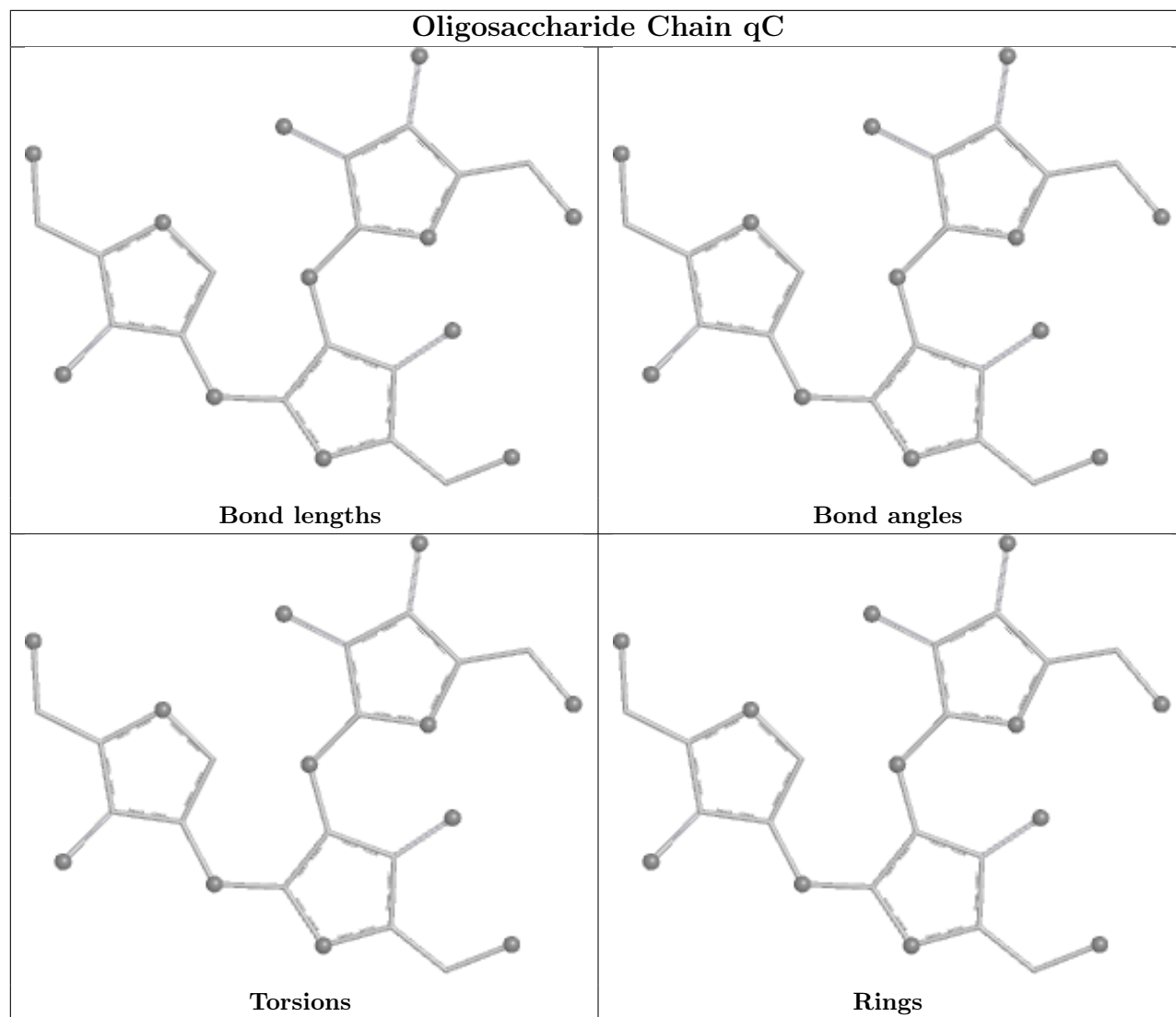
Oligosaccharide Chain eC

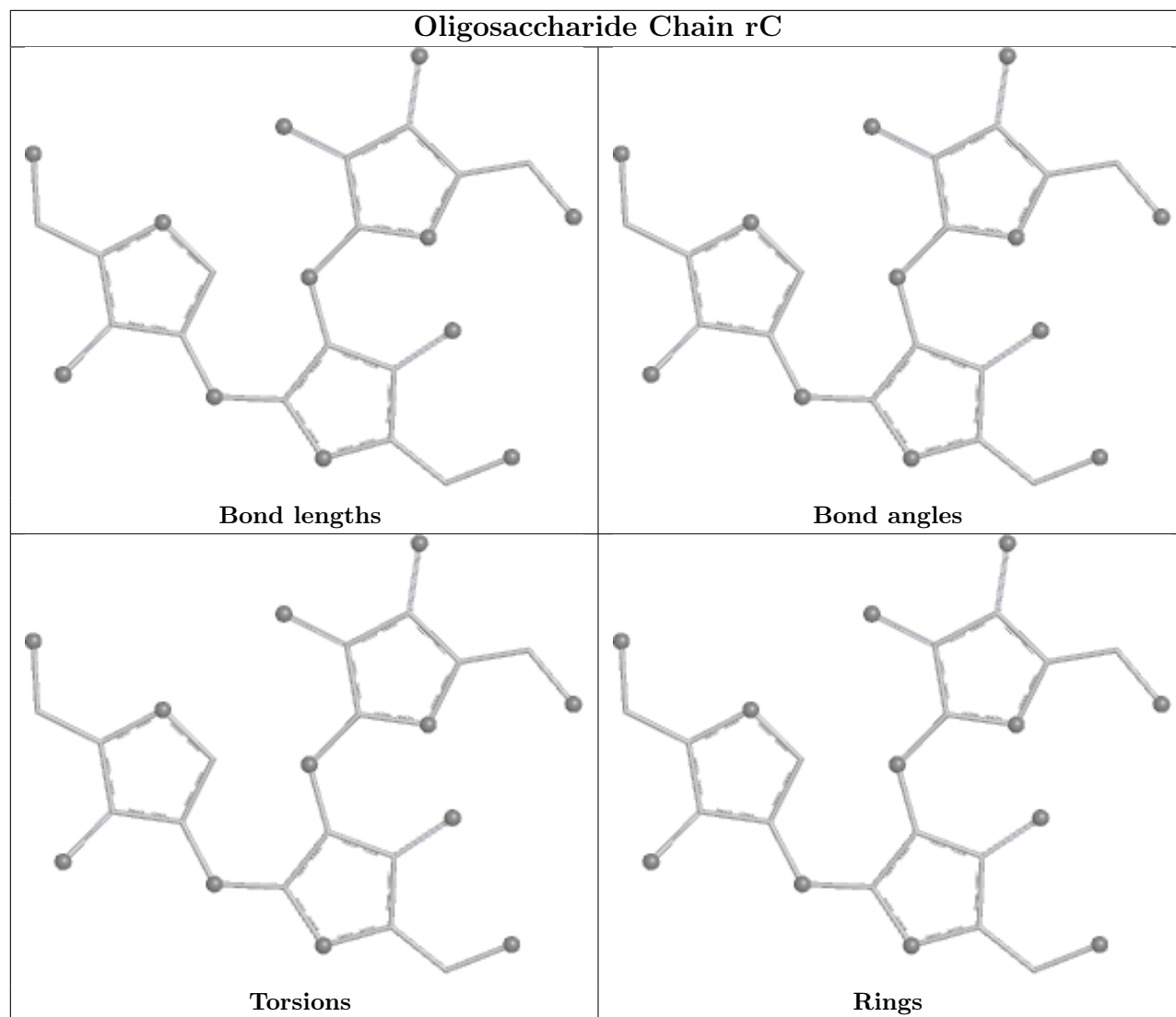


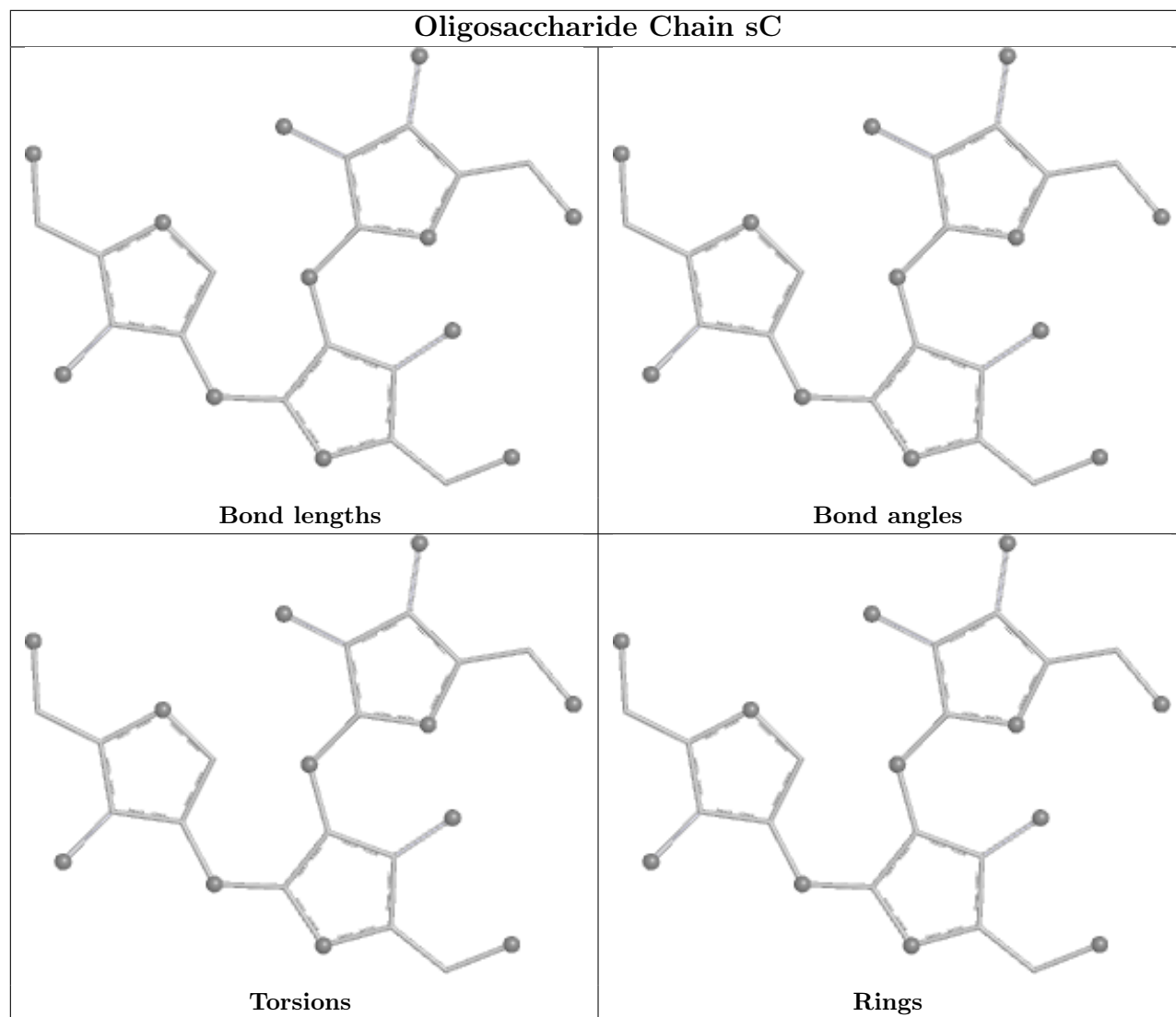


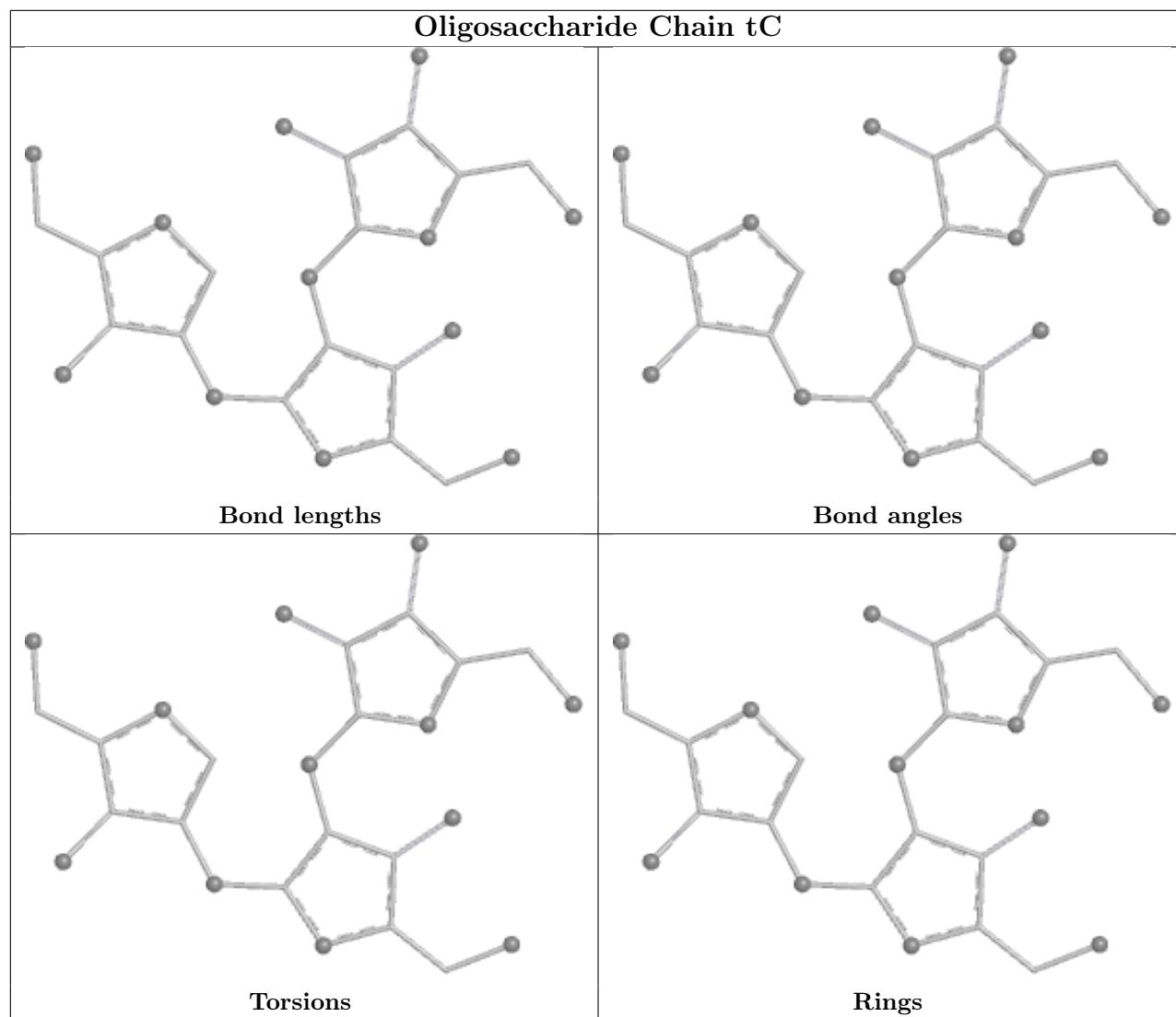


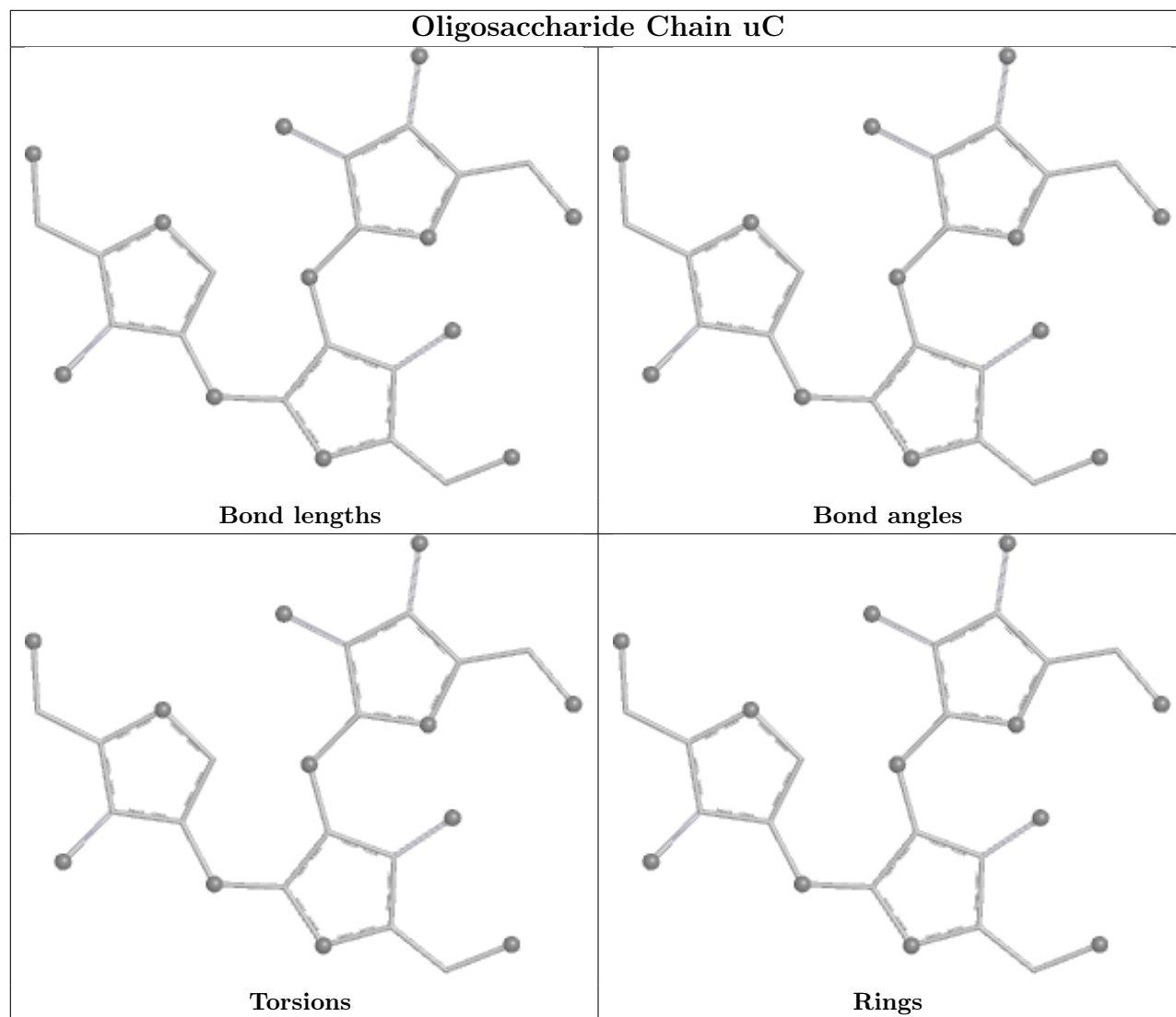




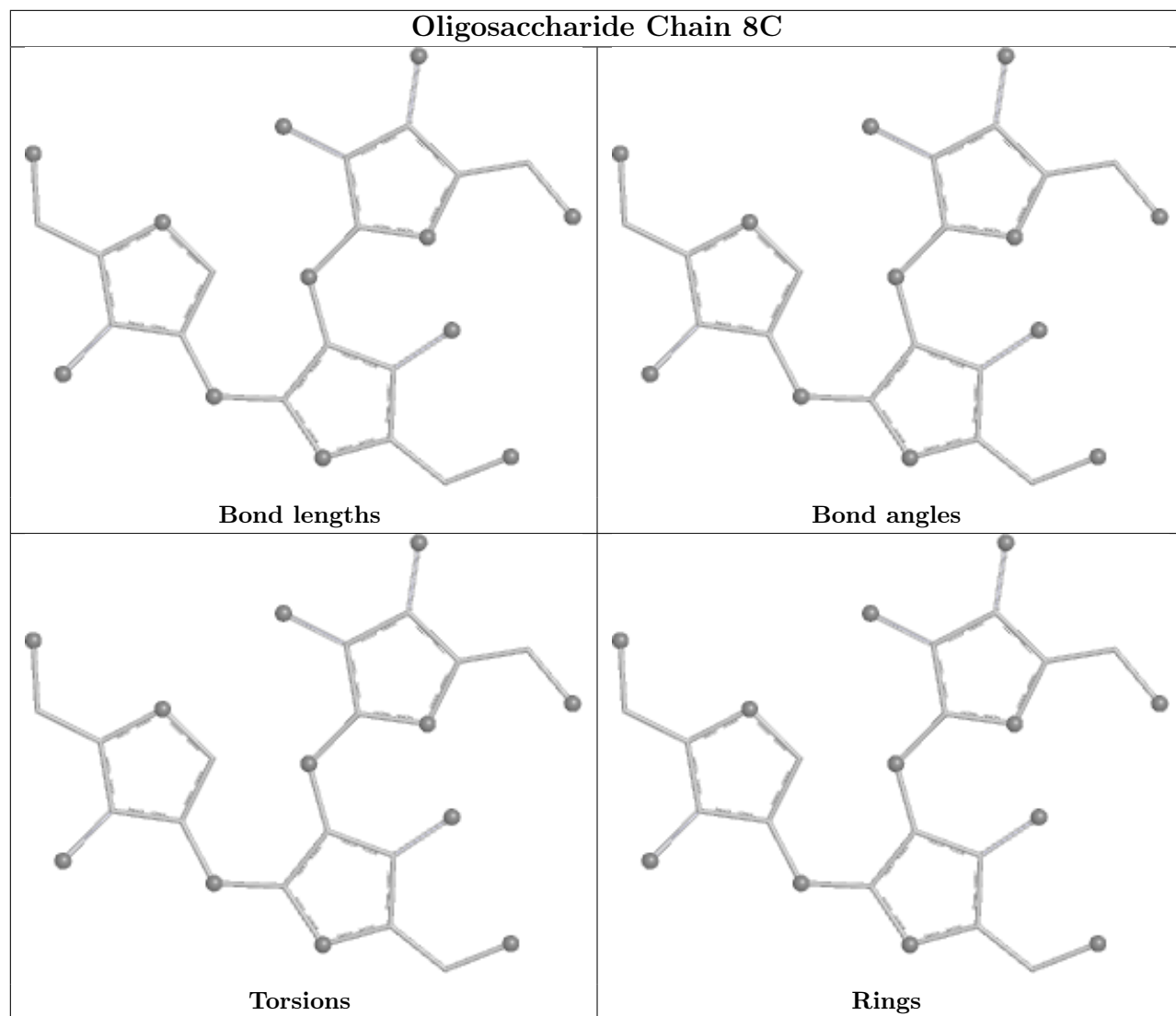




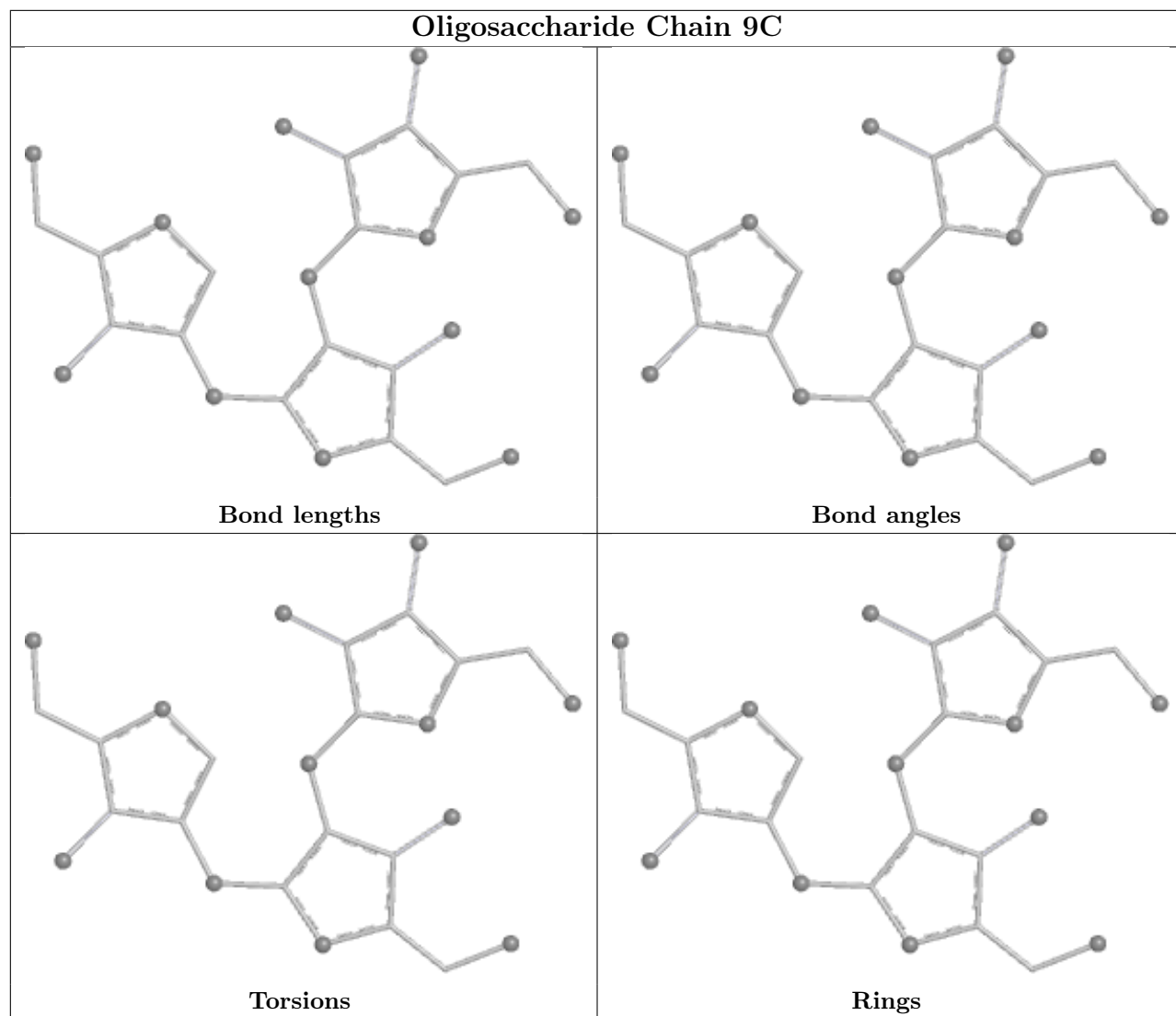


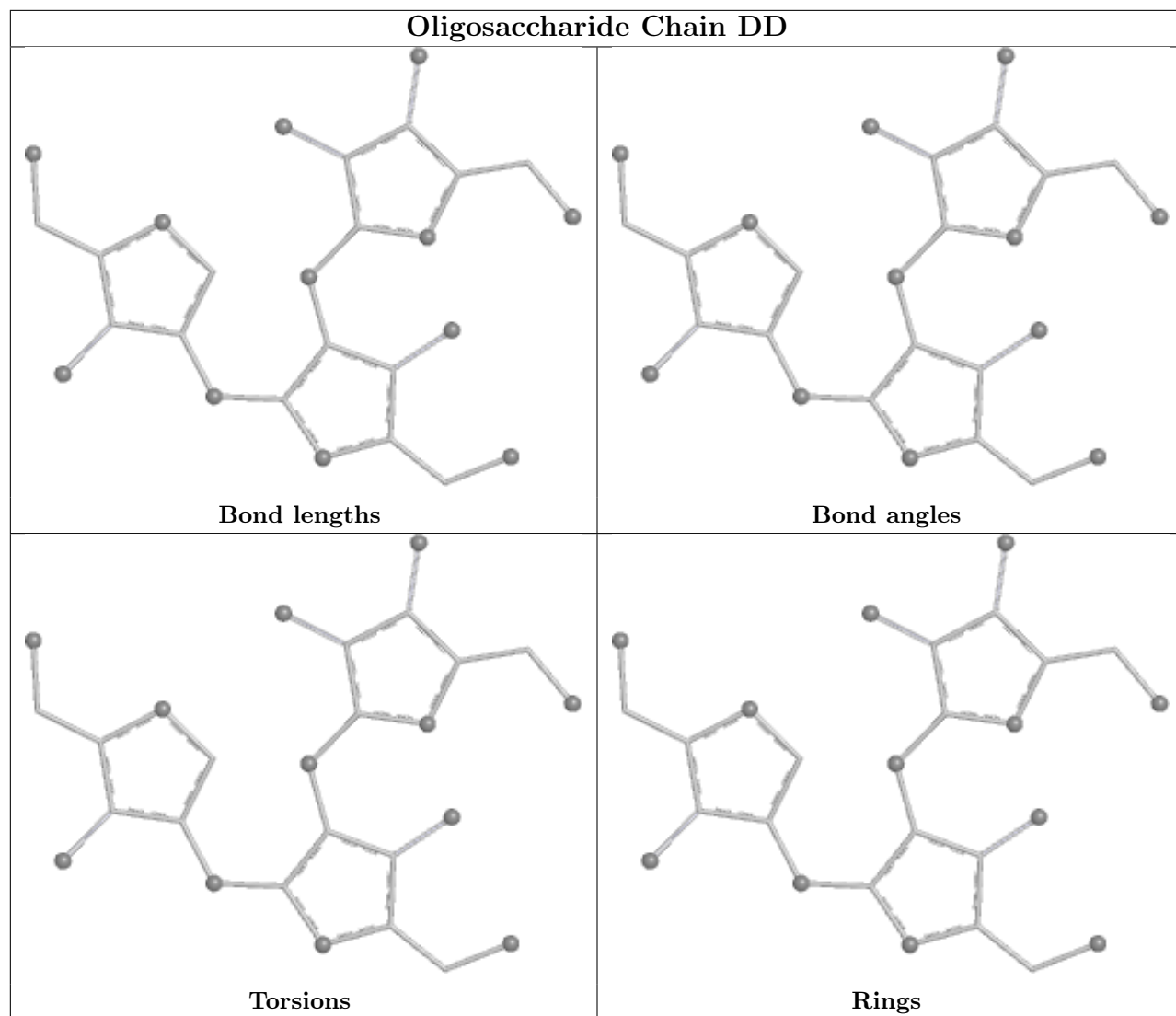


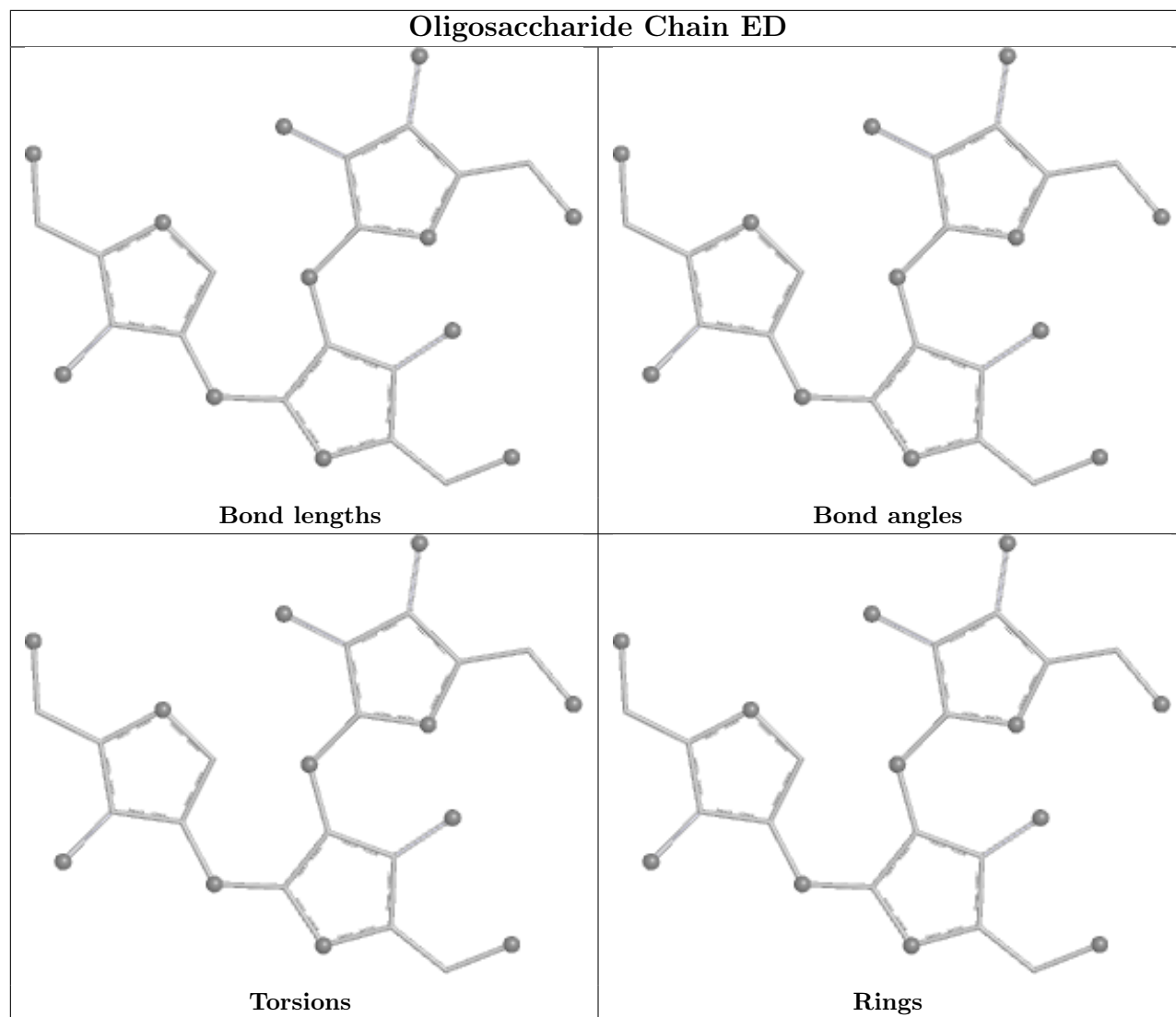
Oligosaccharide Chain 8C

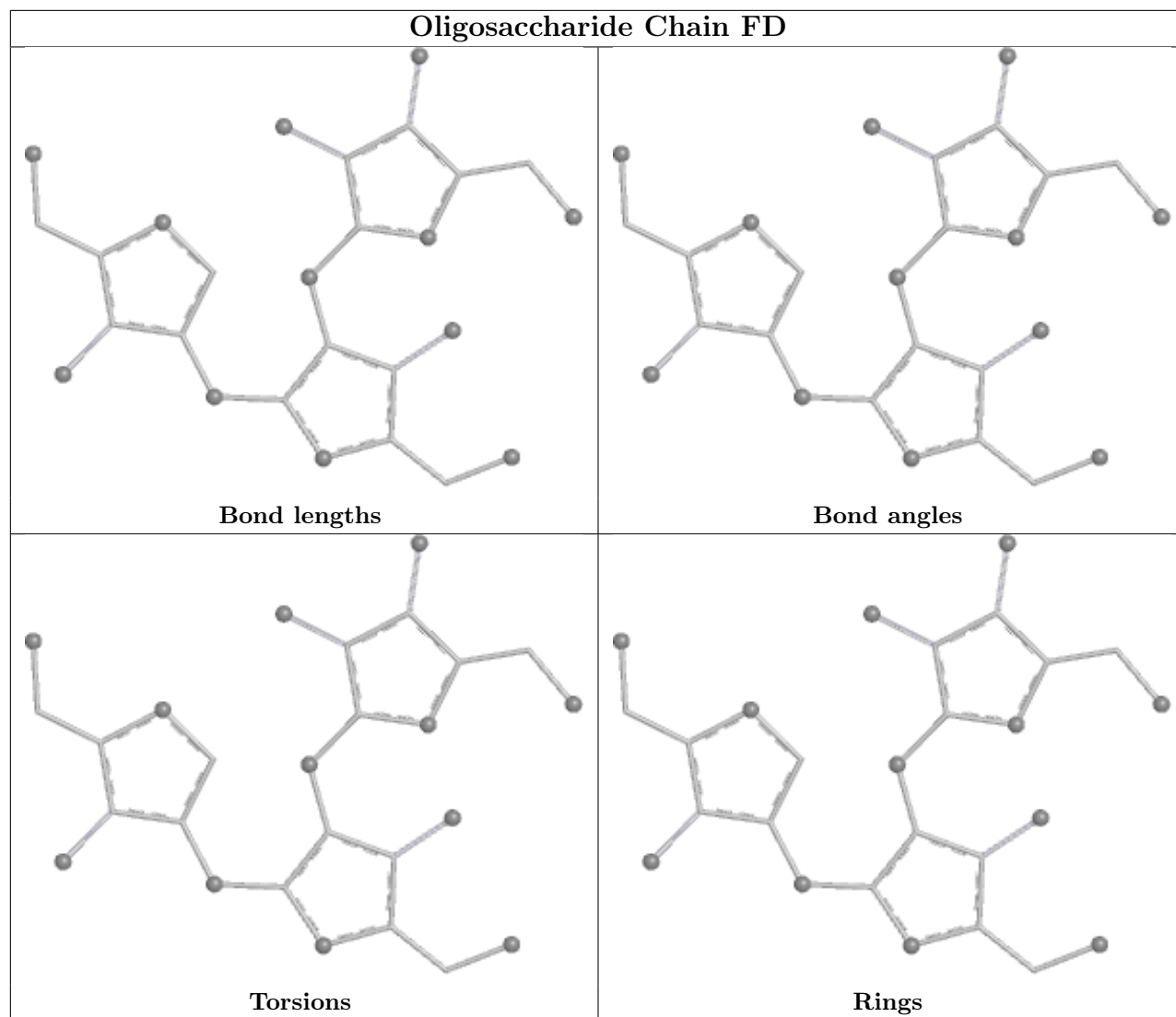


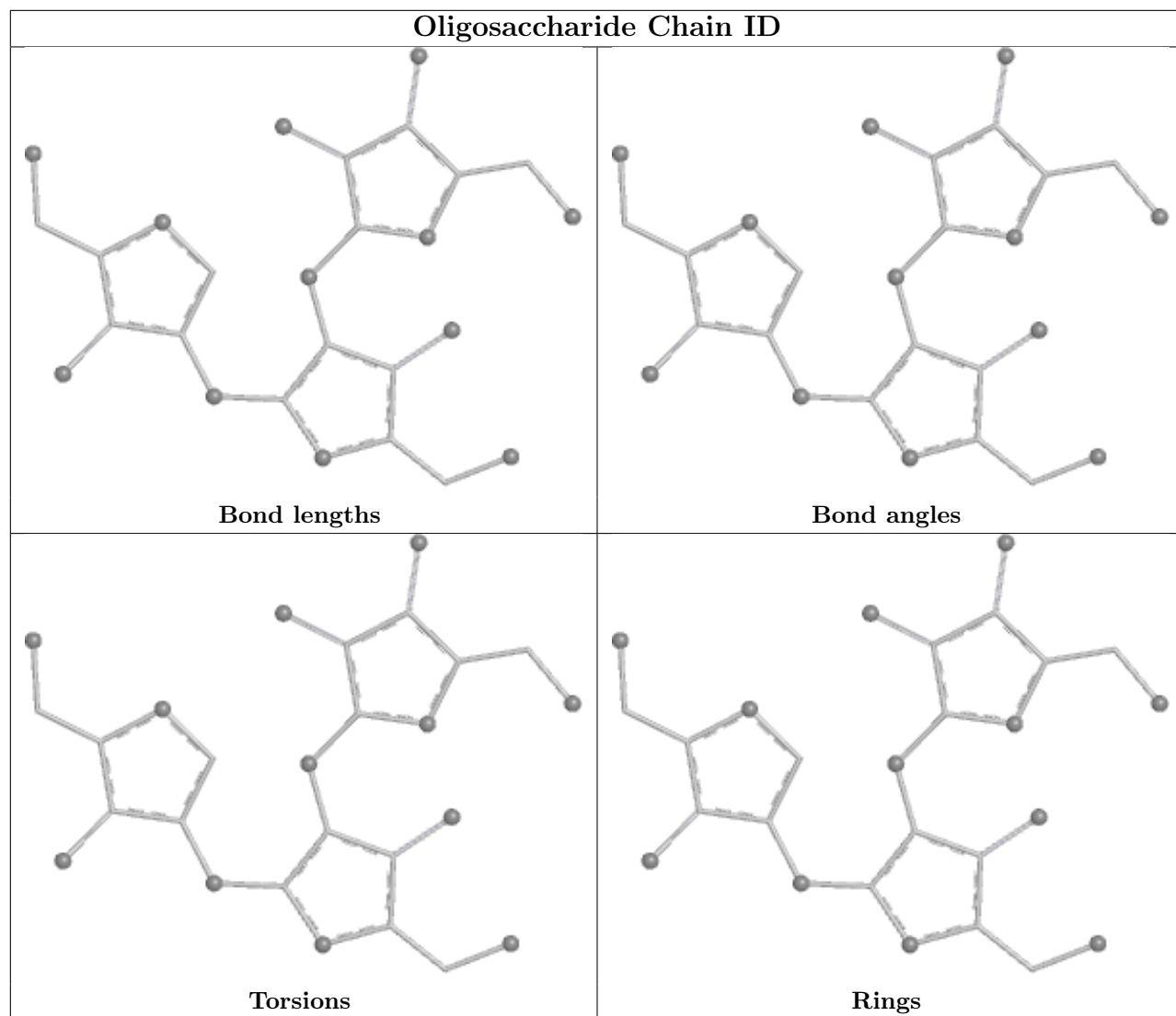
Oligosaccharide Chain 9C

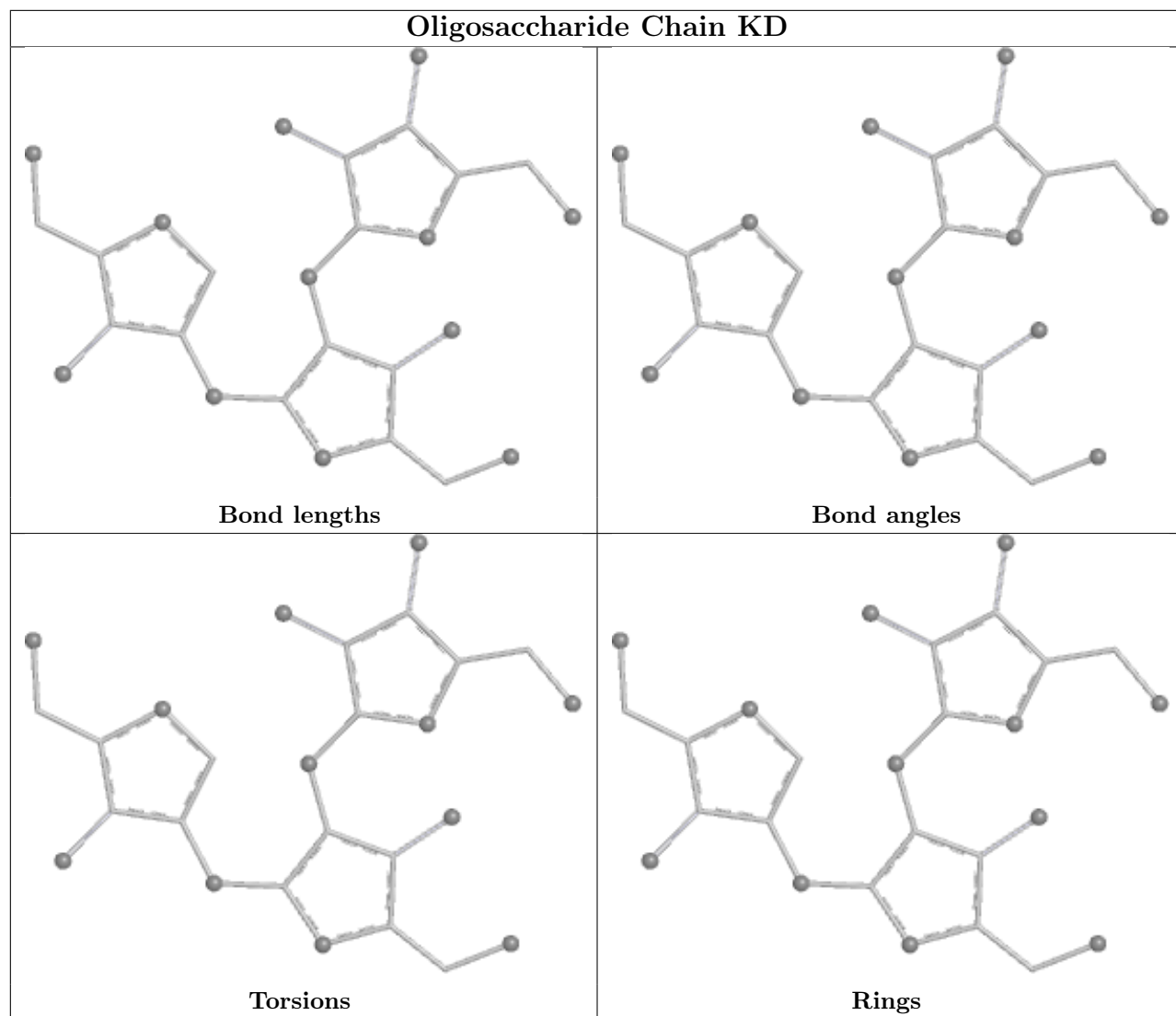


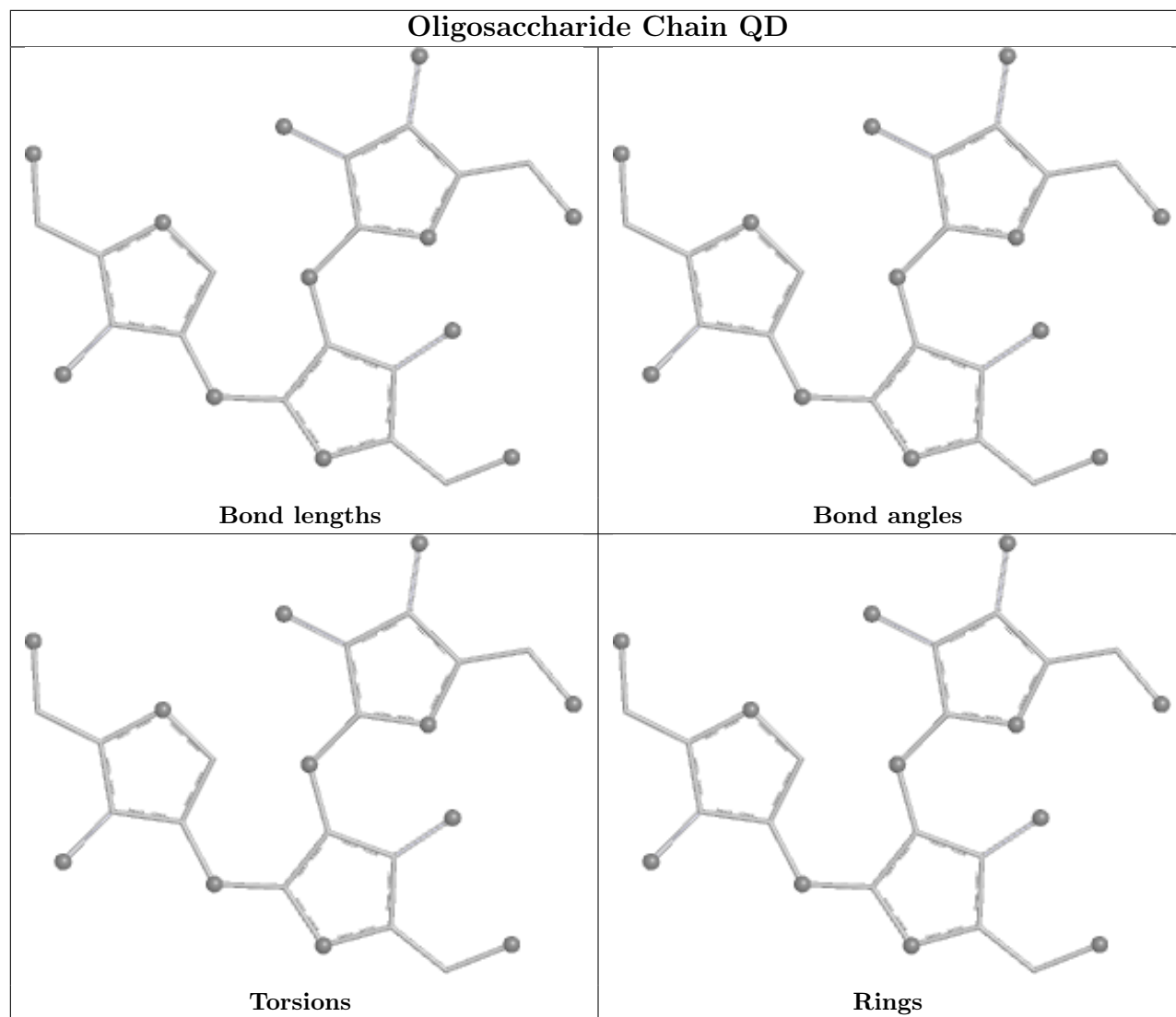


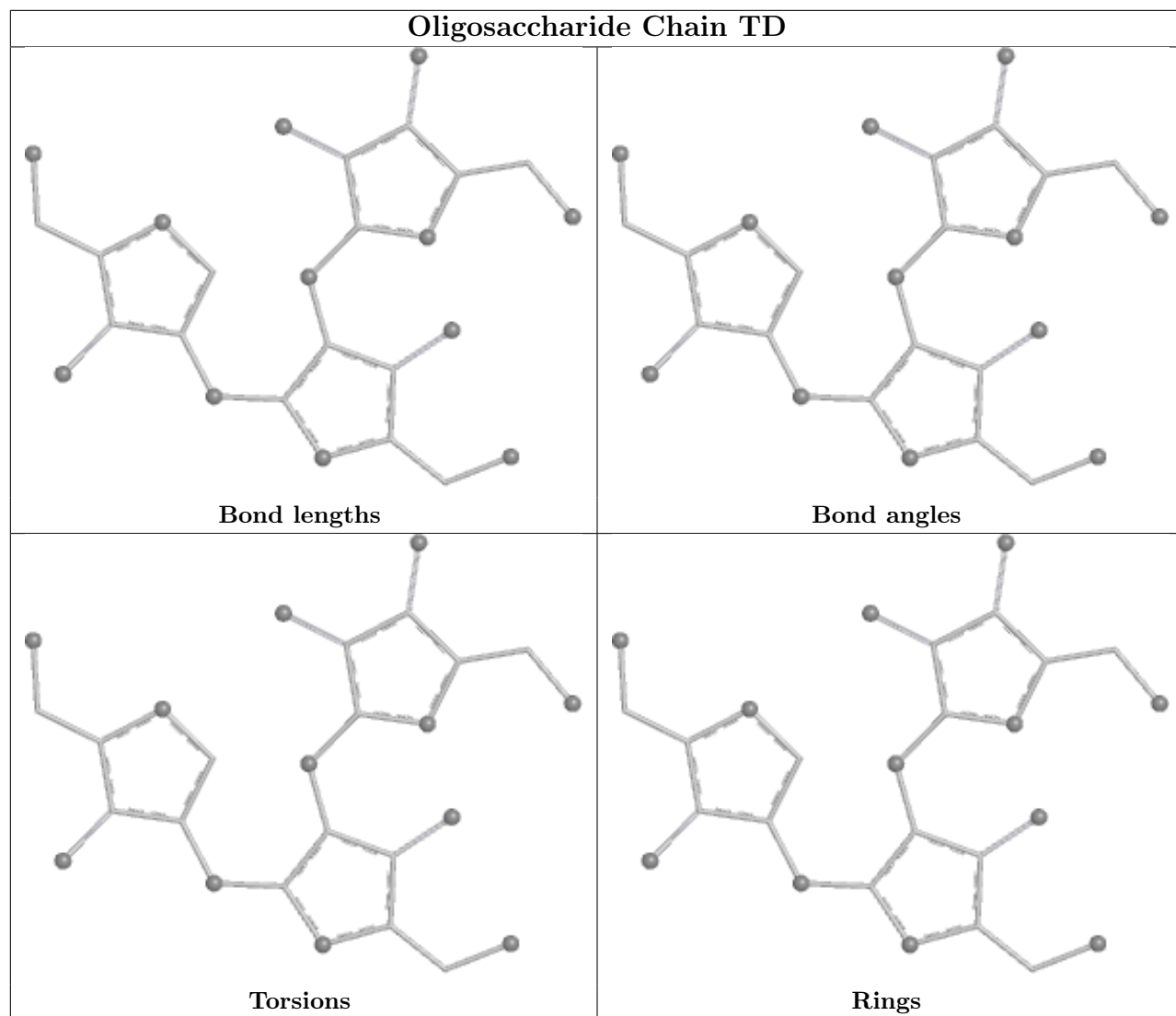


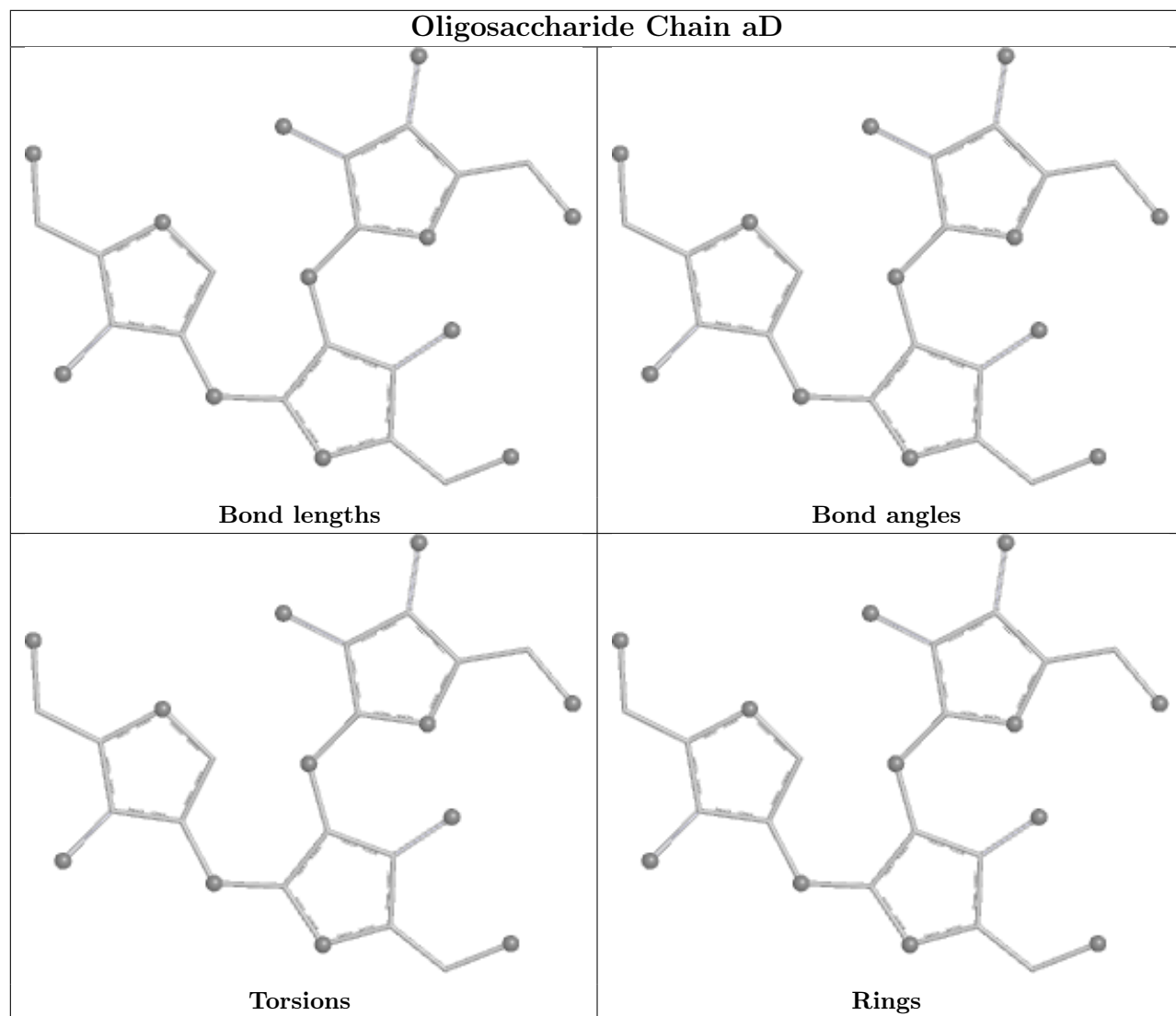


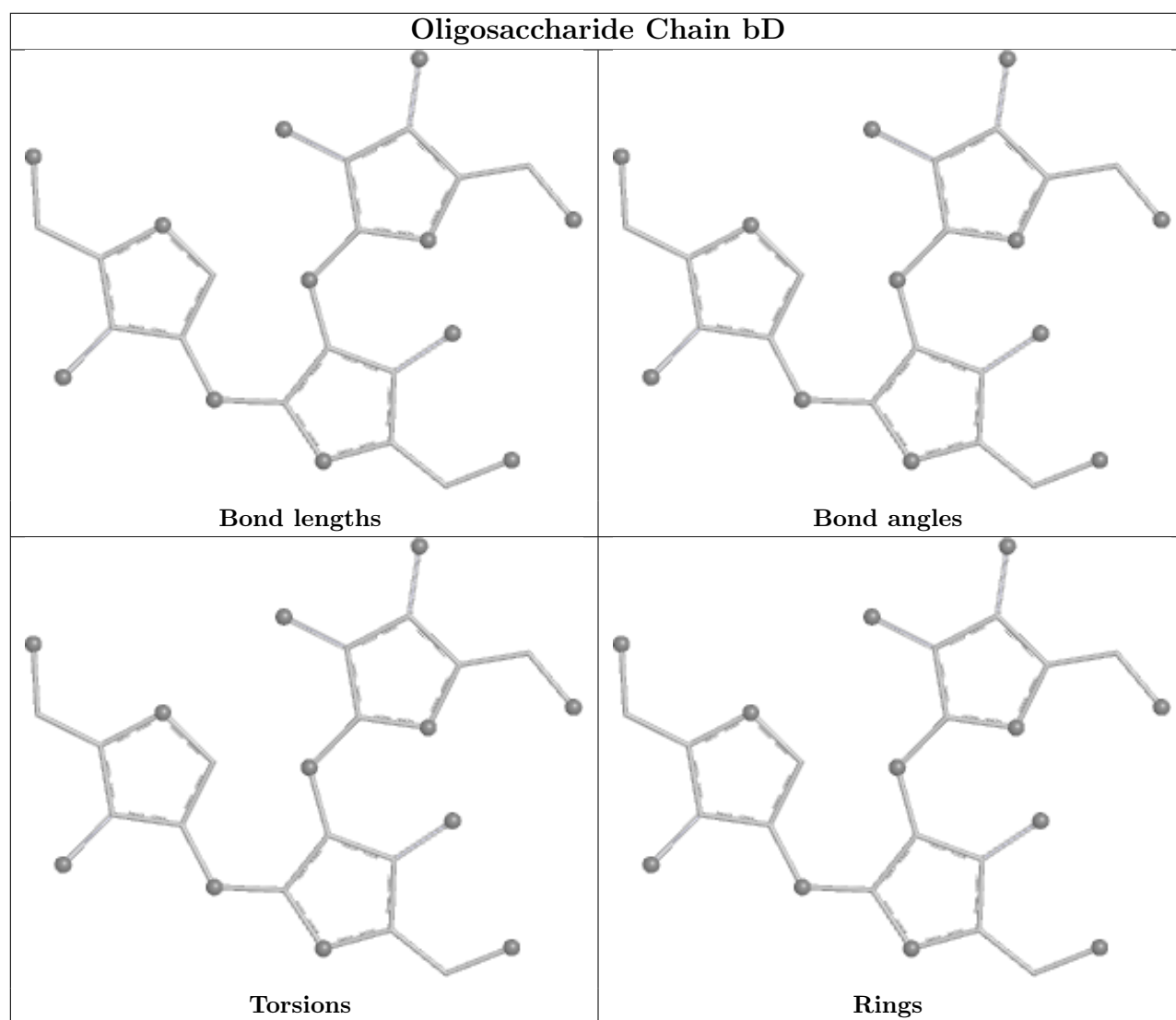


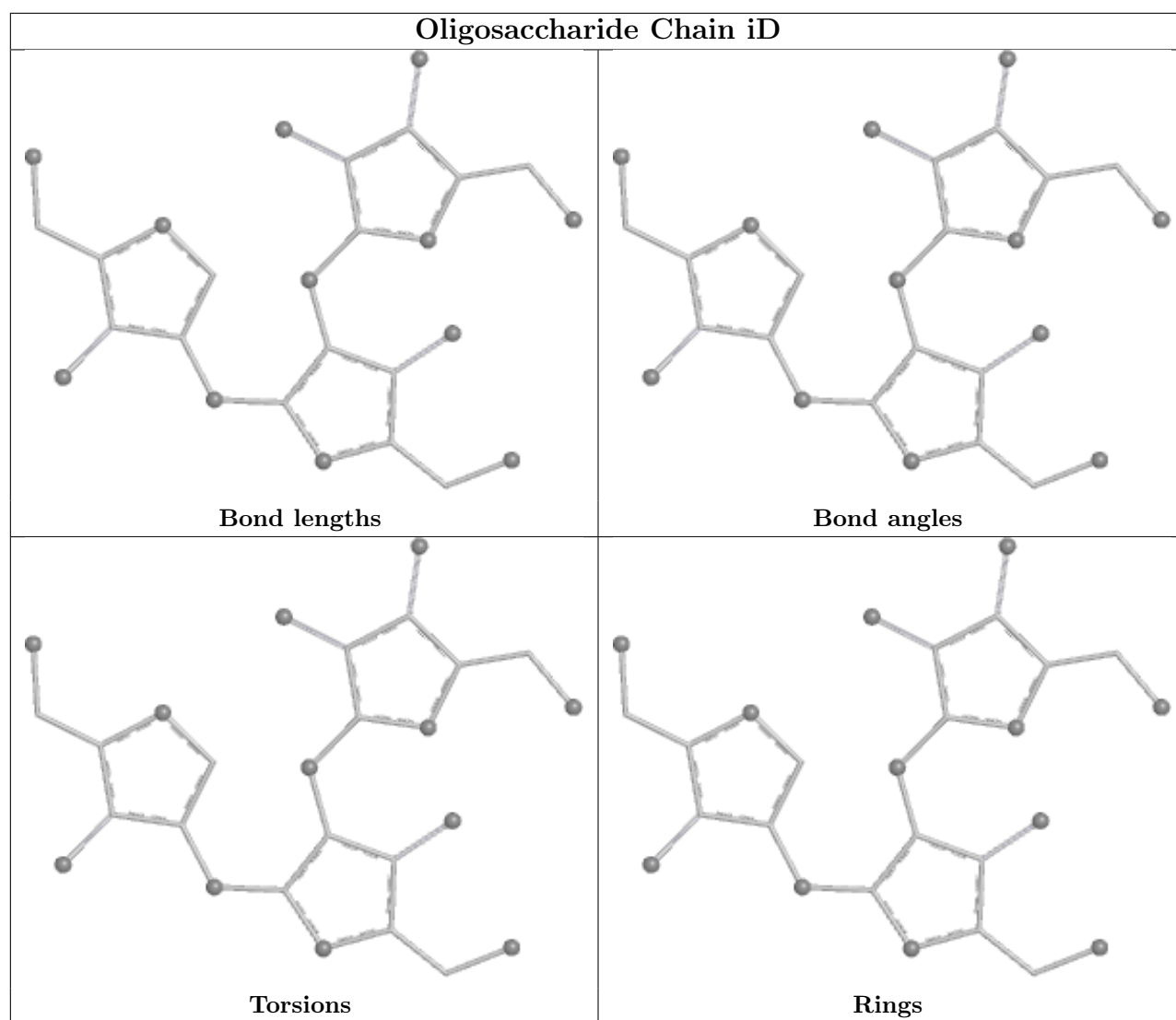


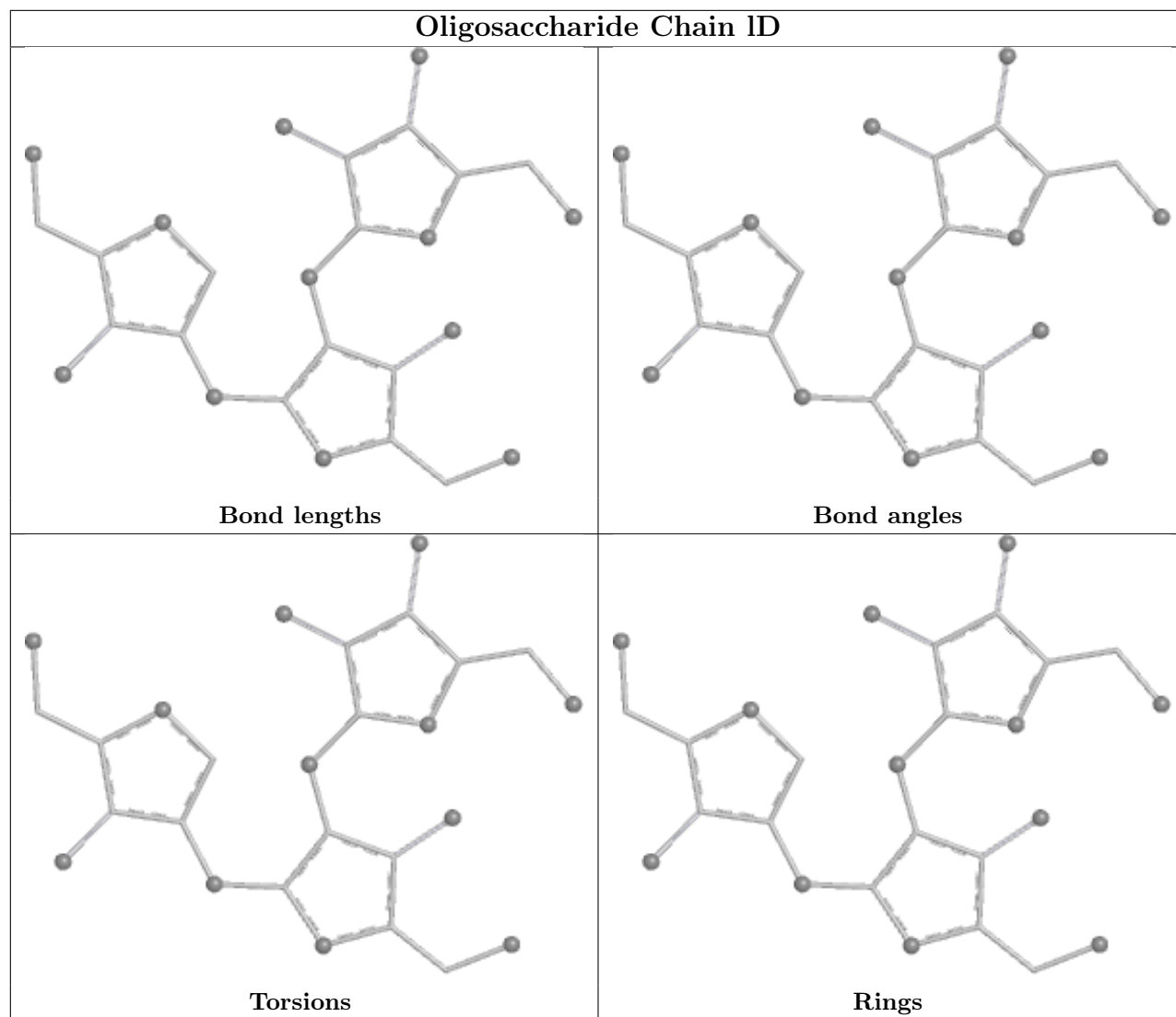


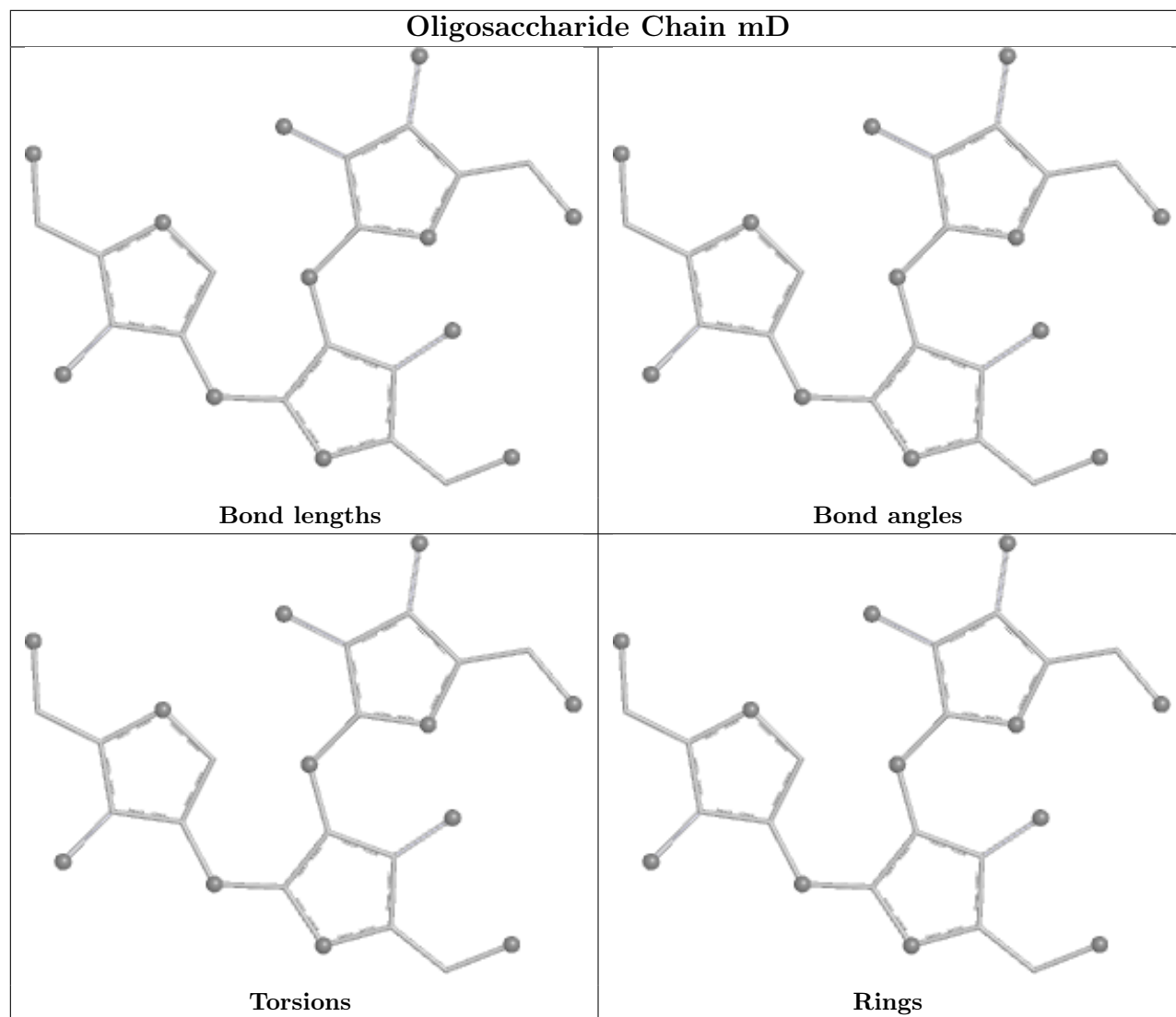
Oligosaccharide Chain TD

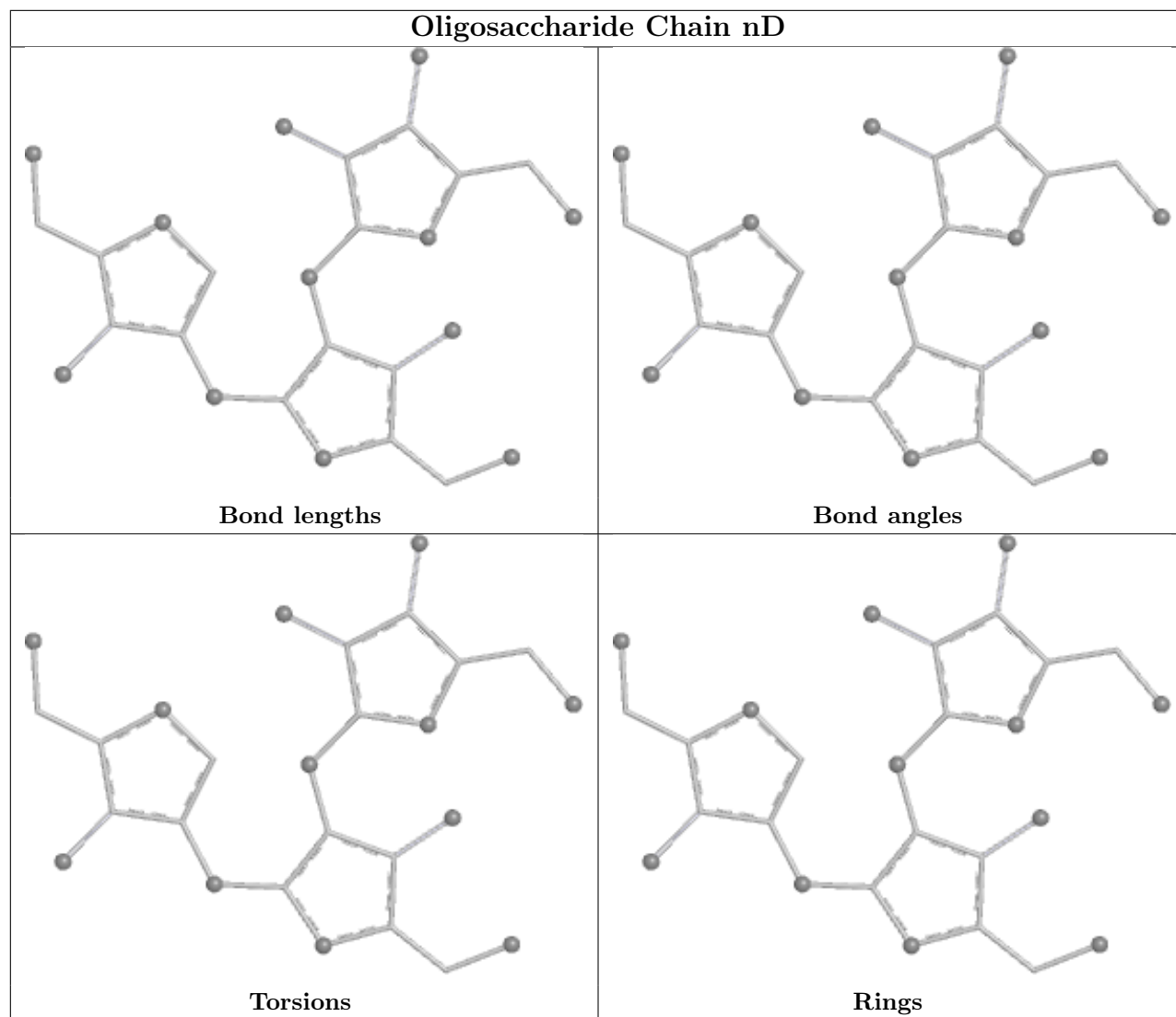


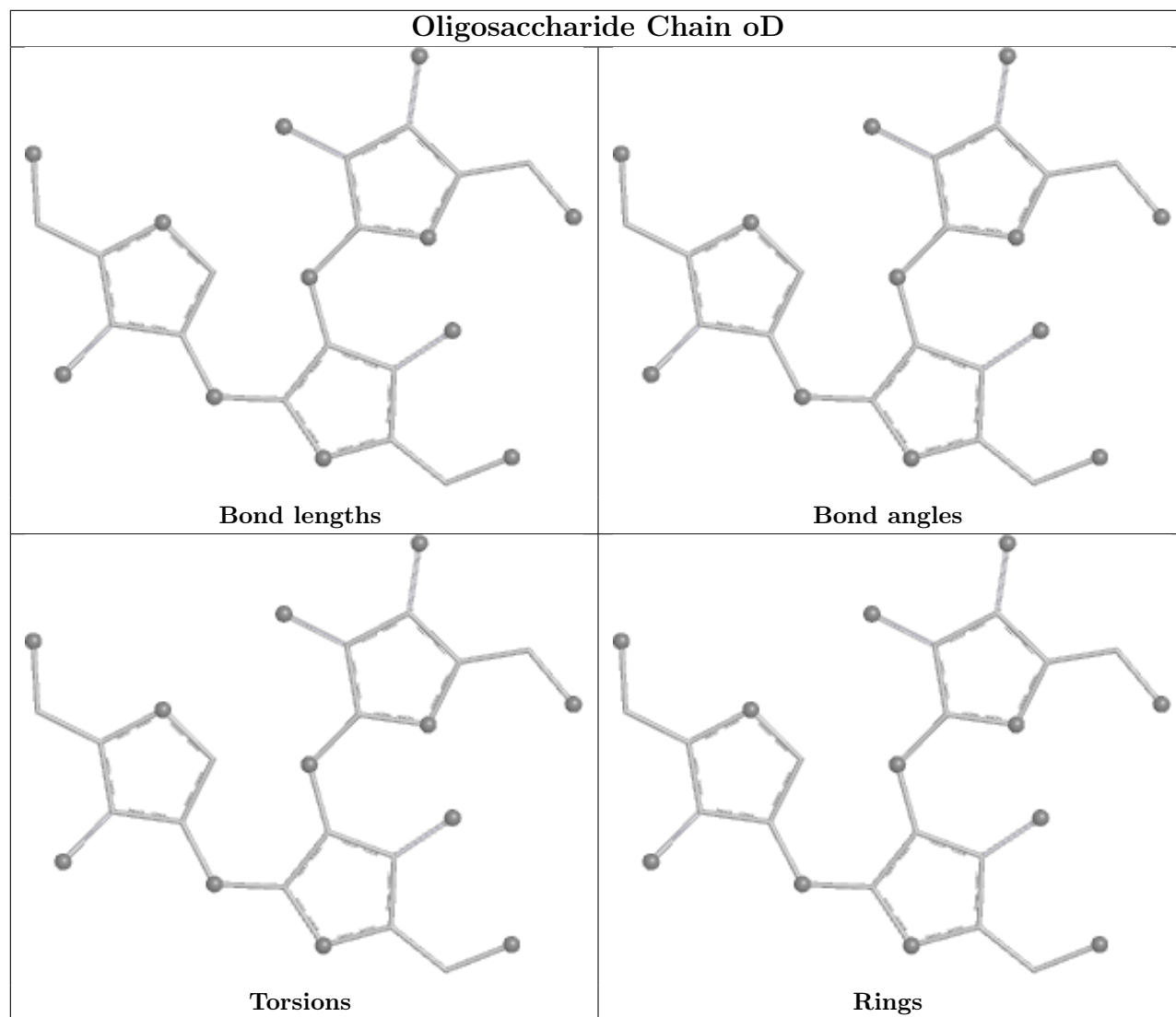


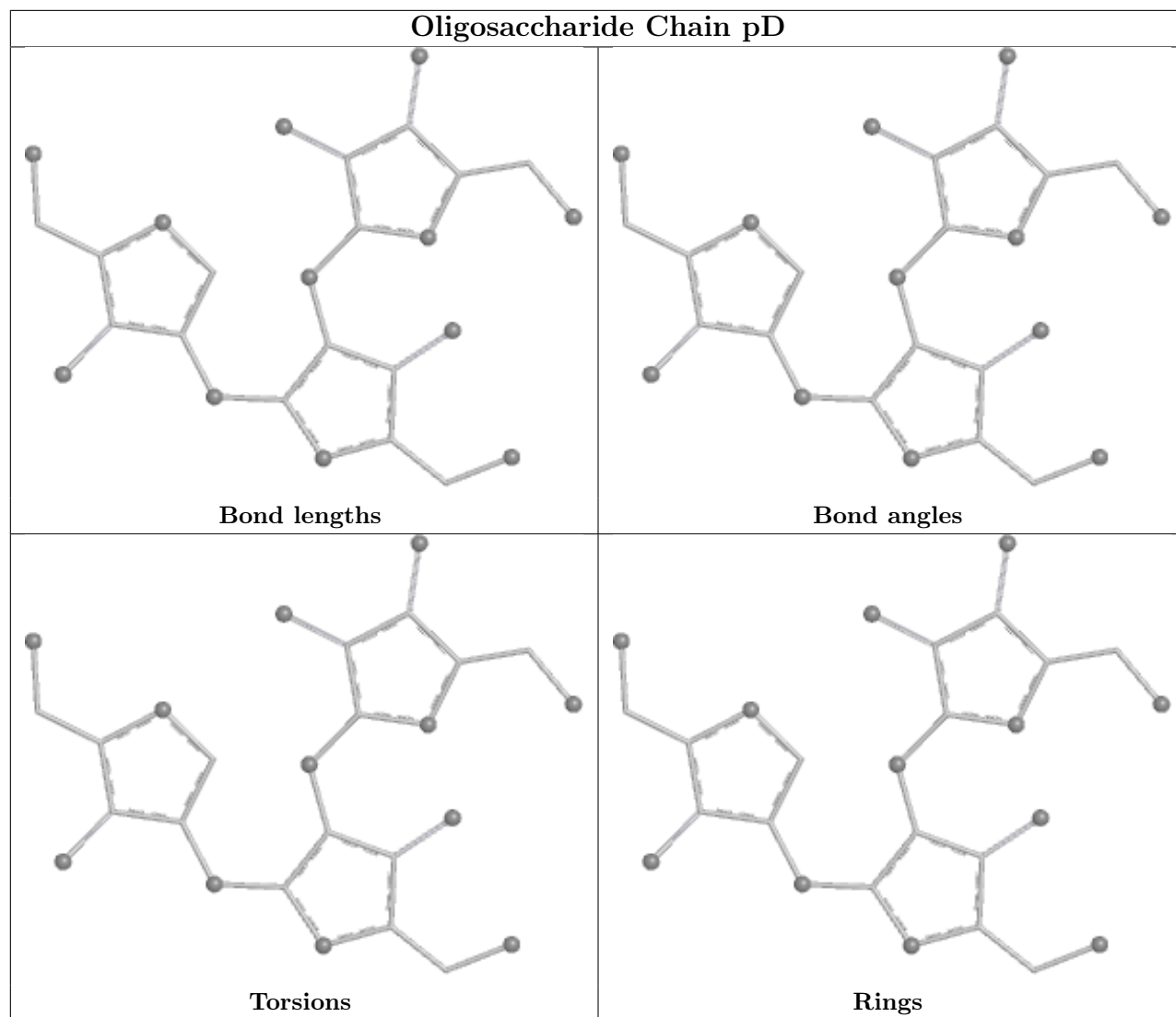


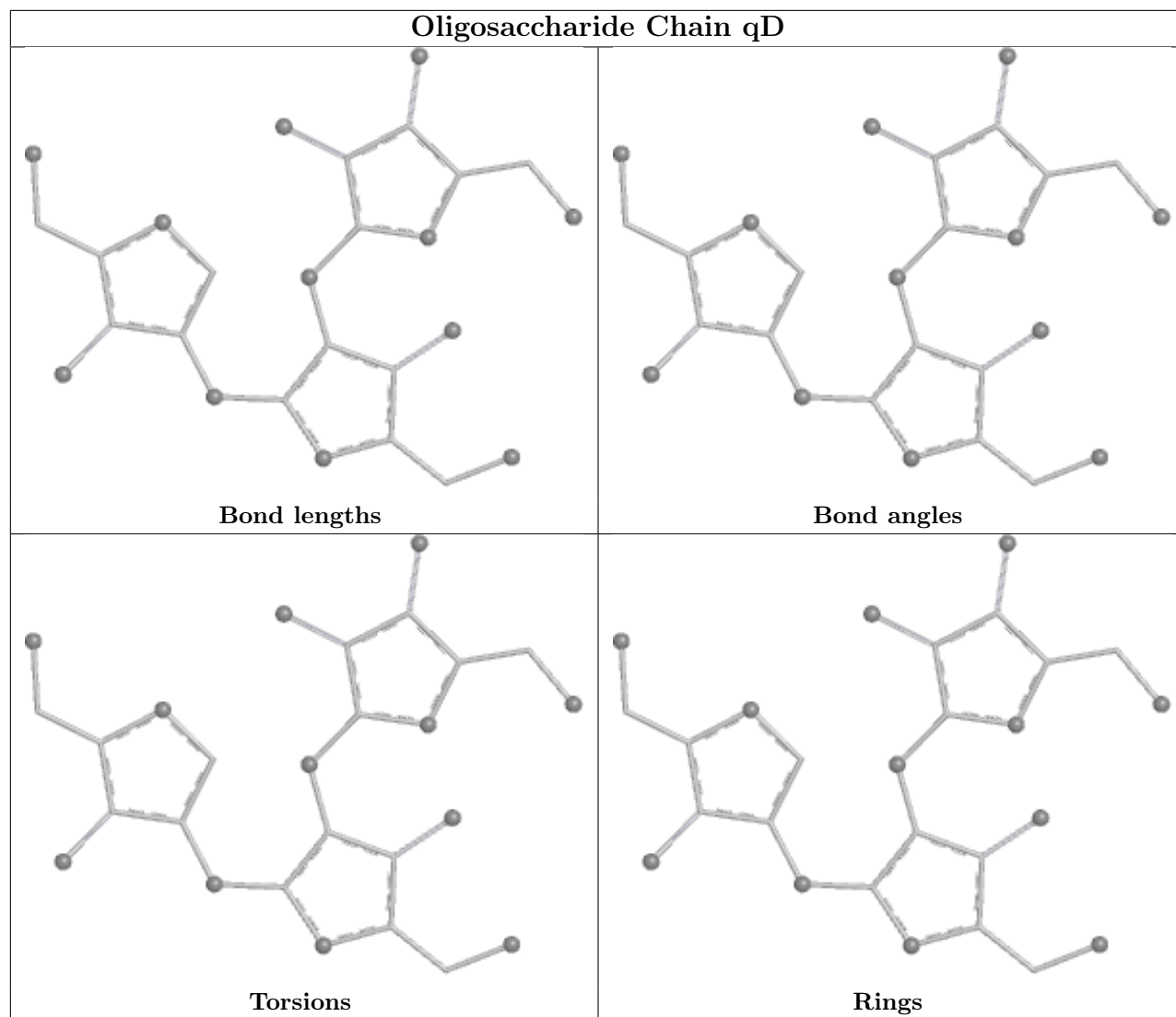


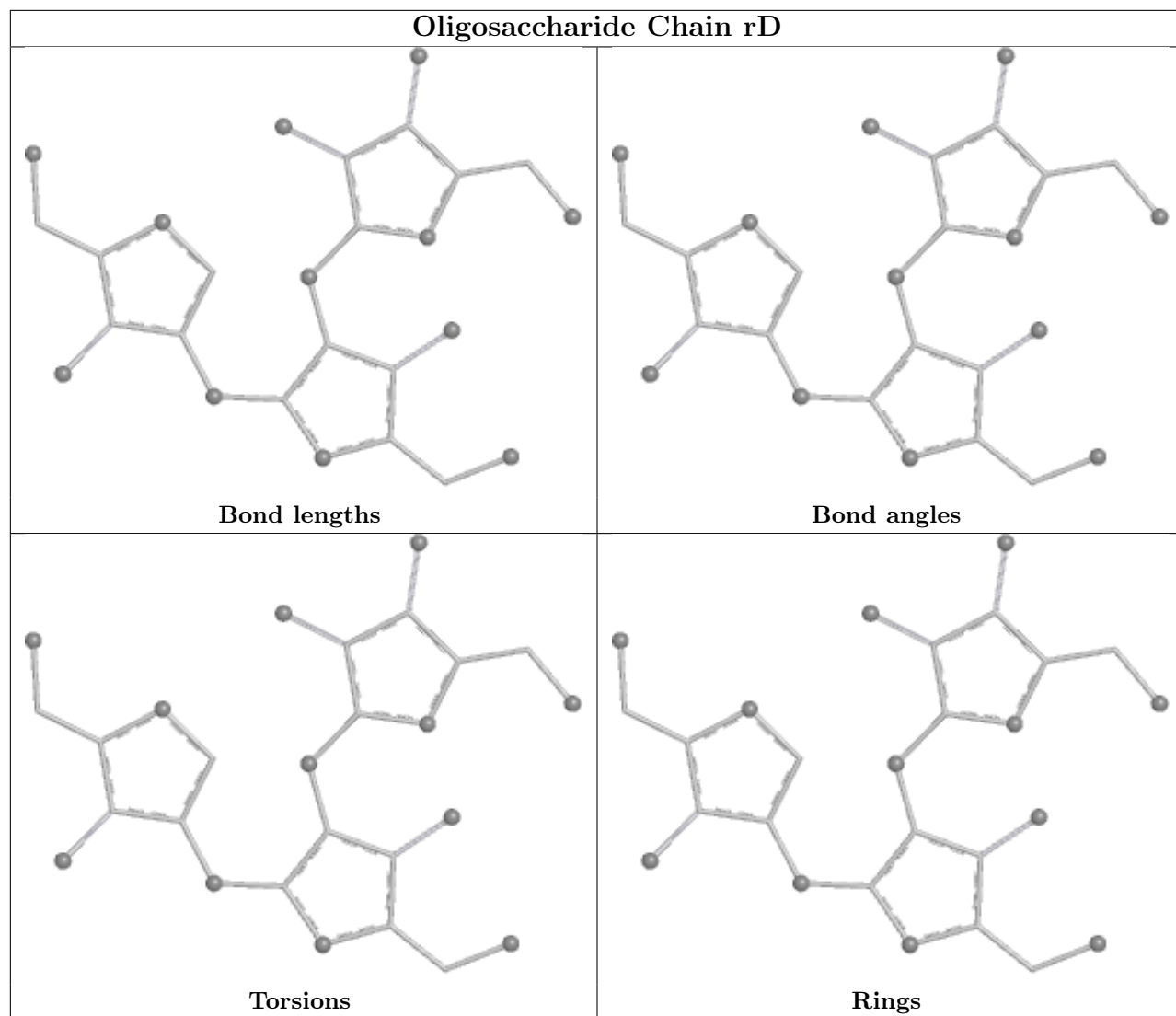


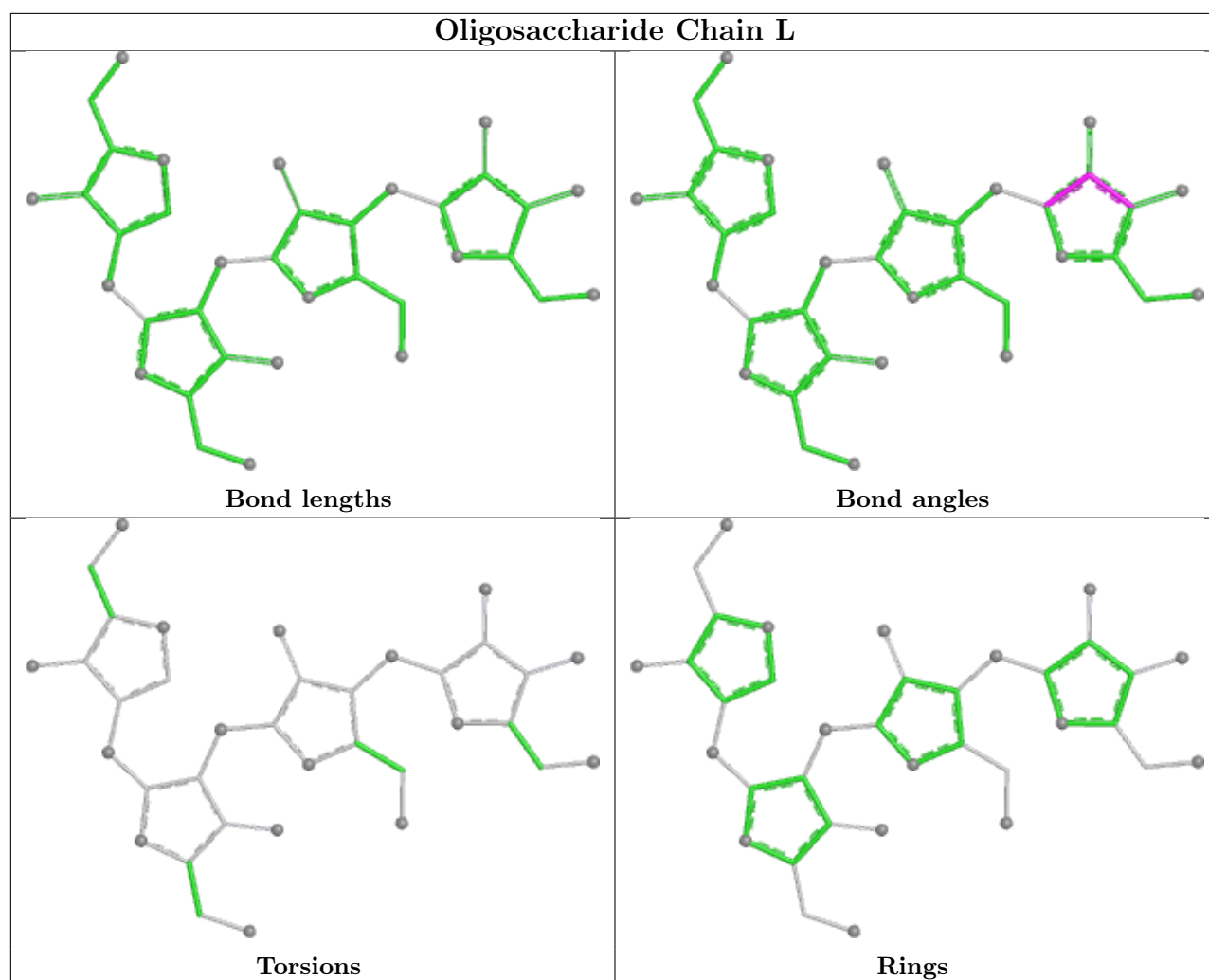


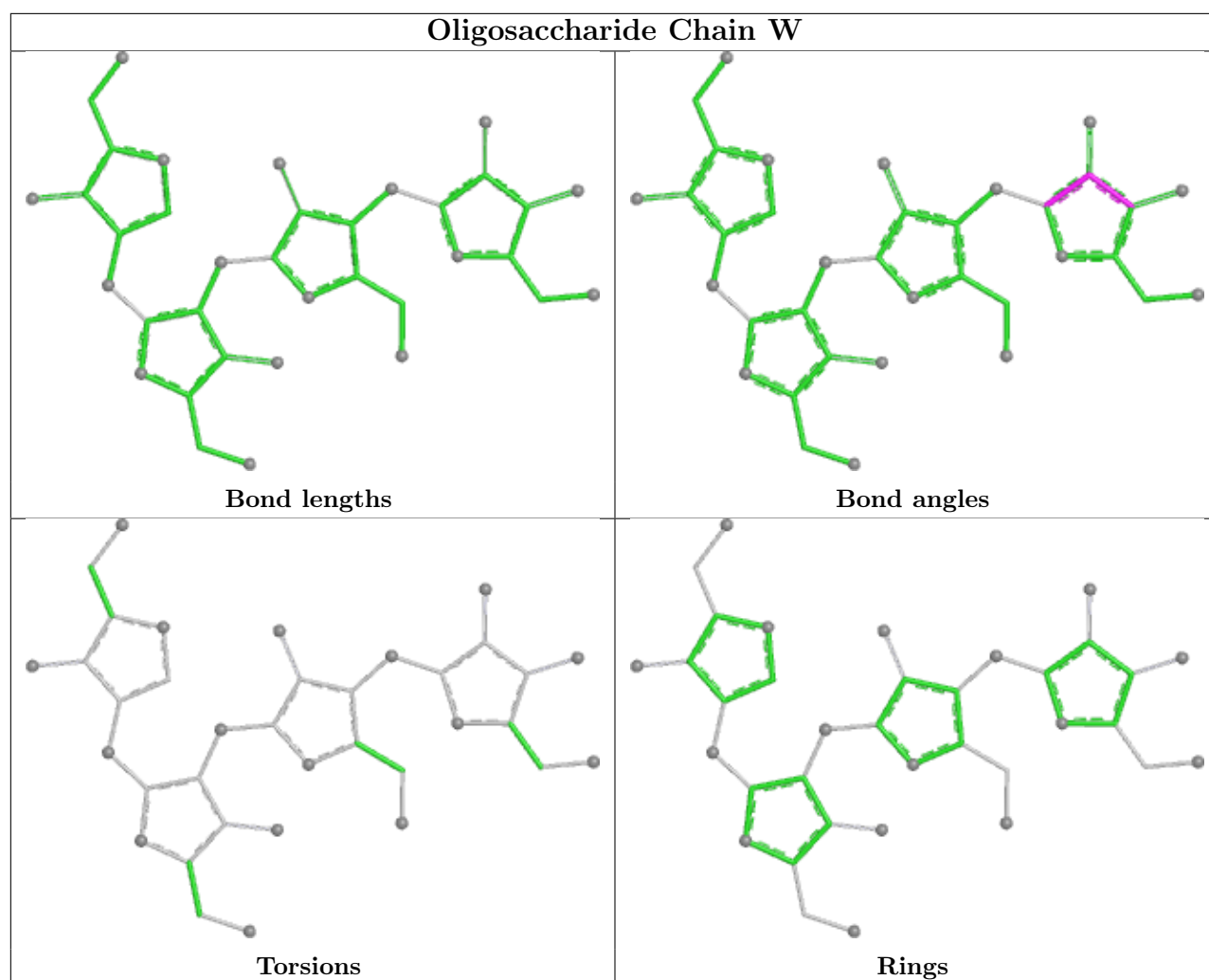


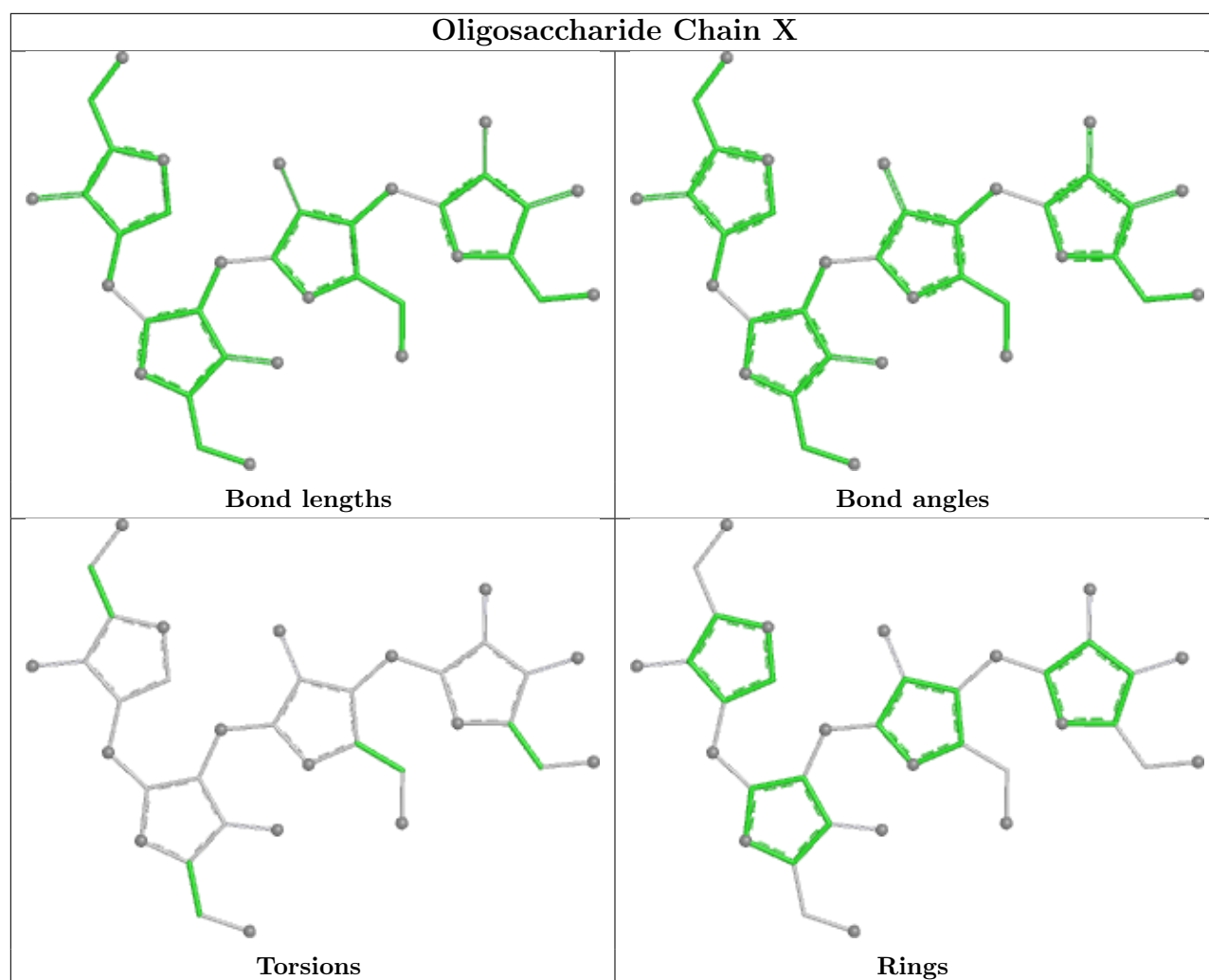


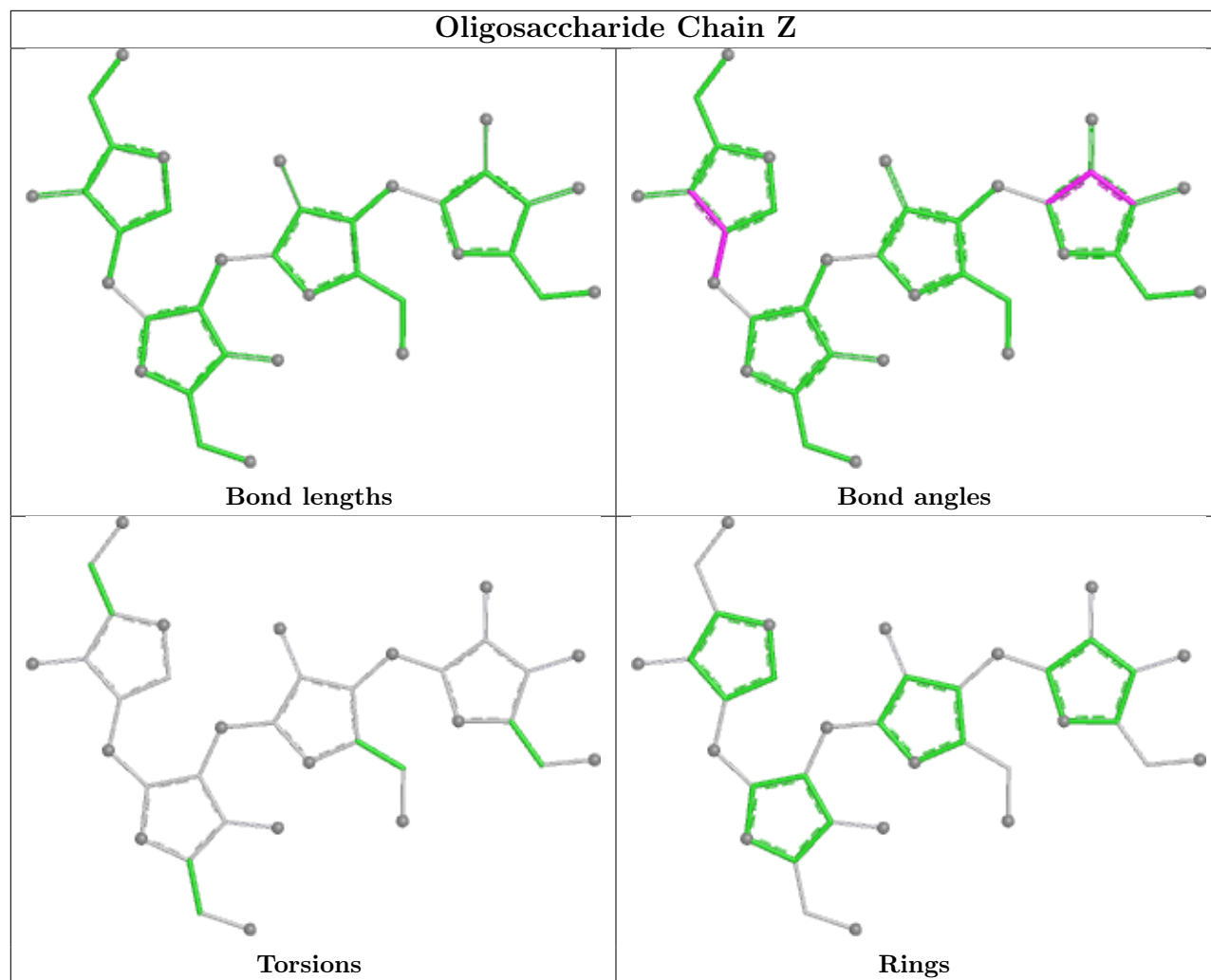


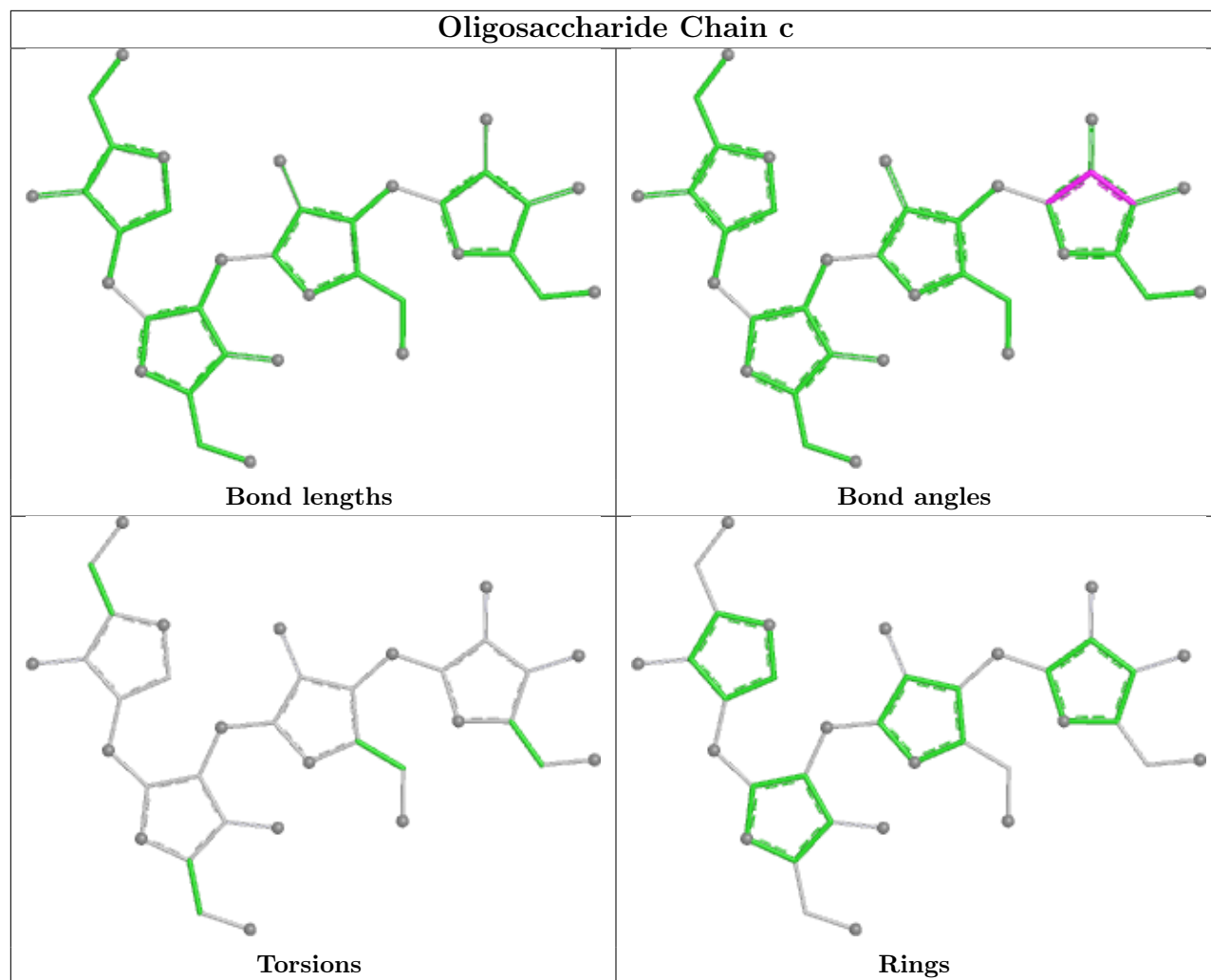


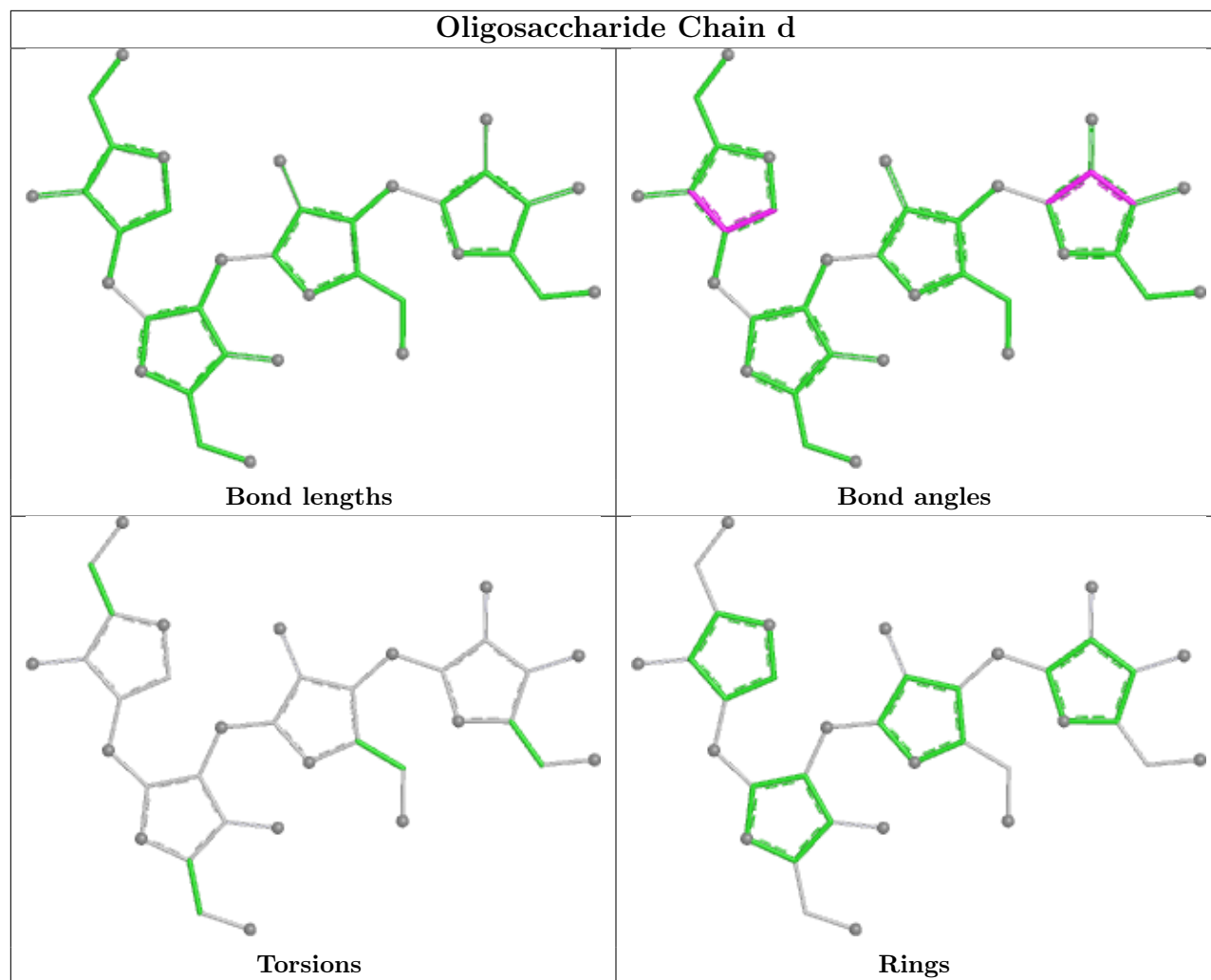


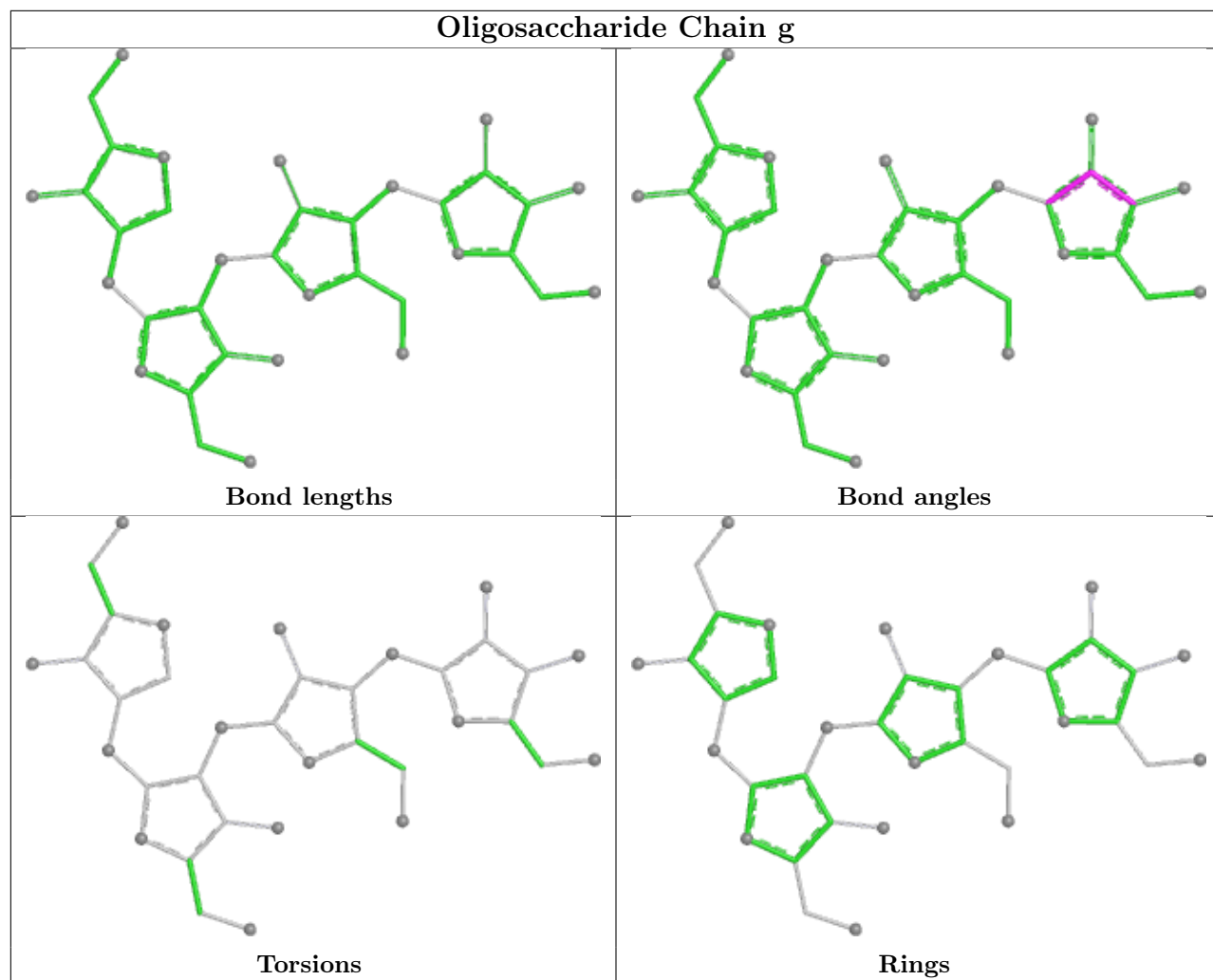


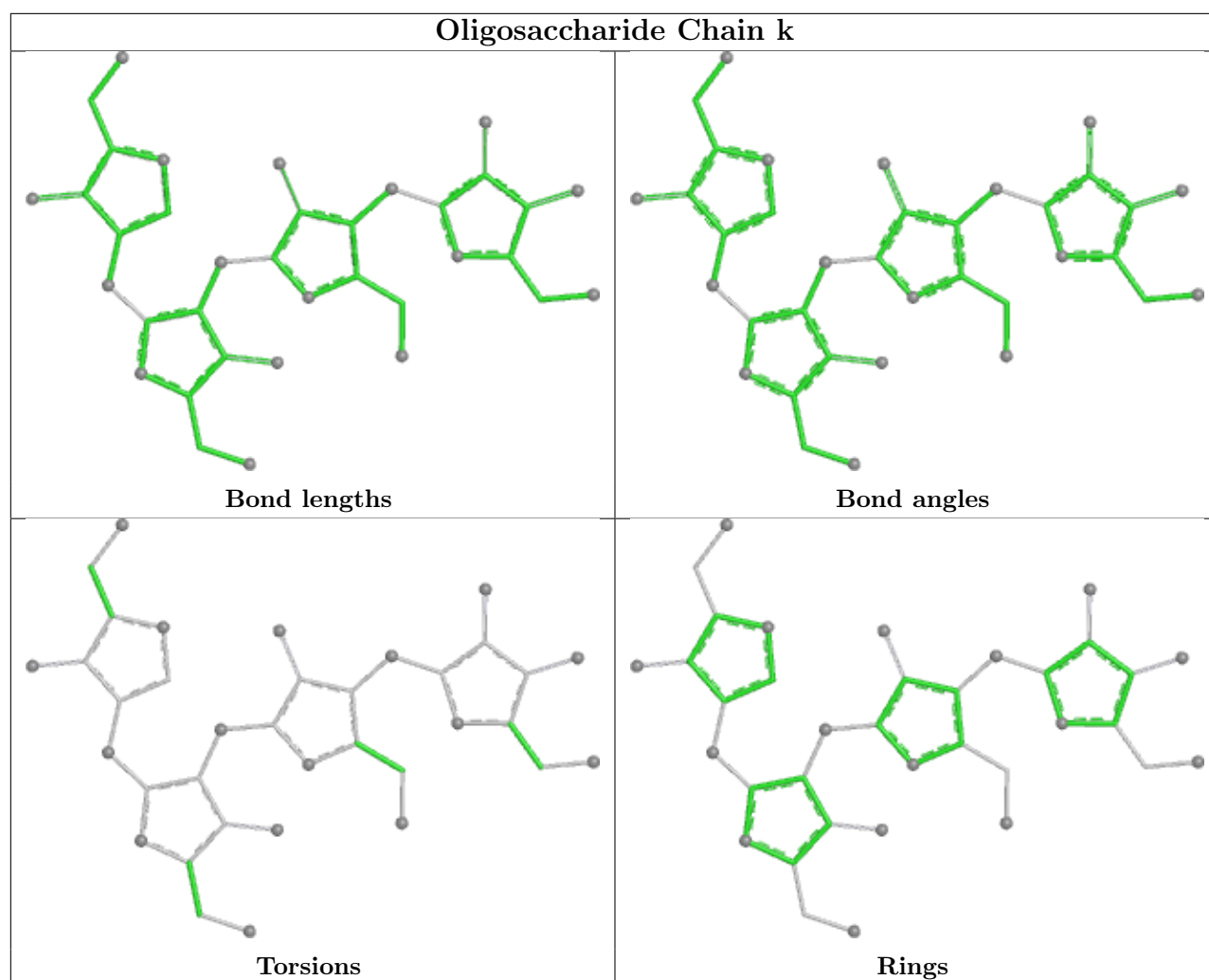


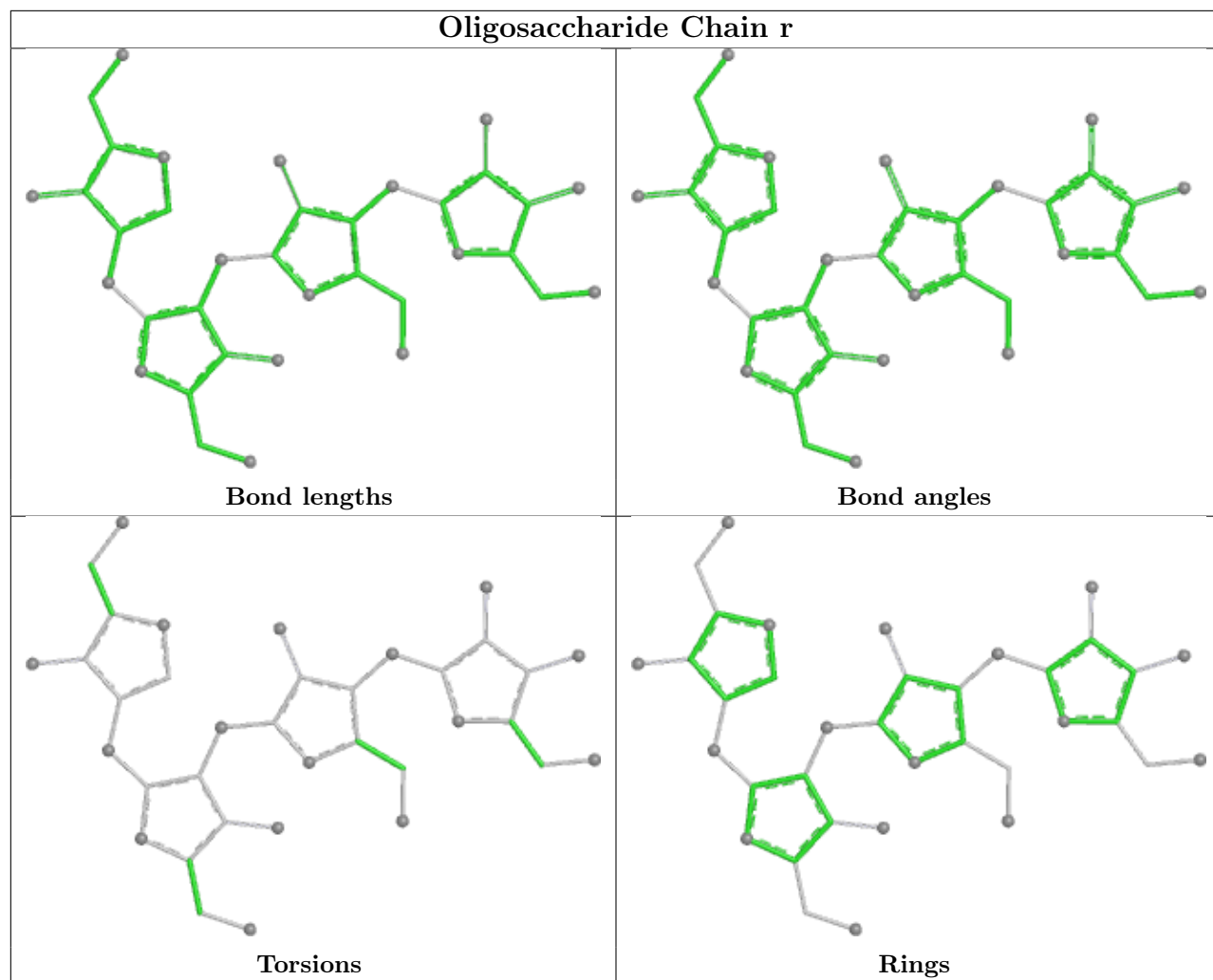


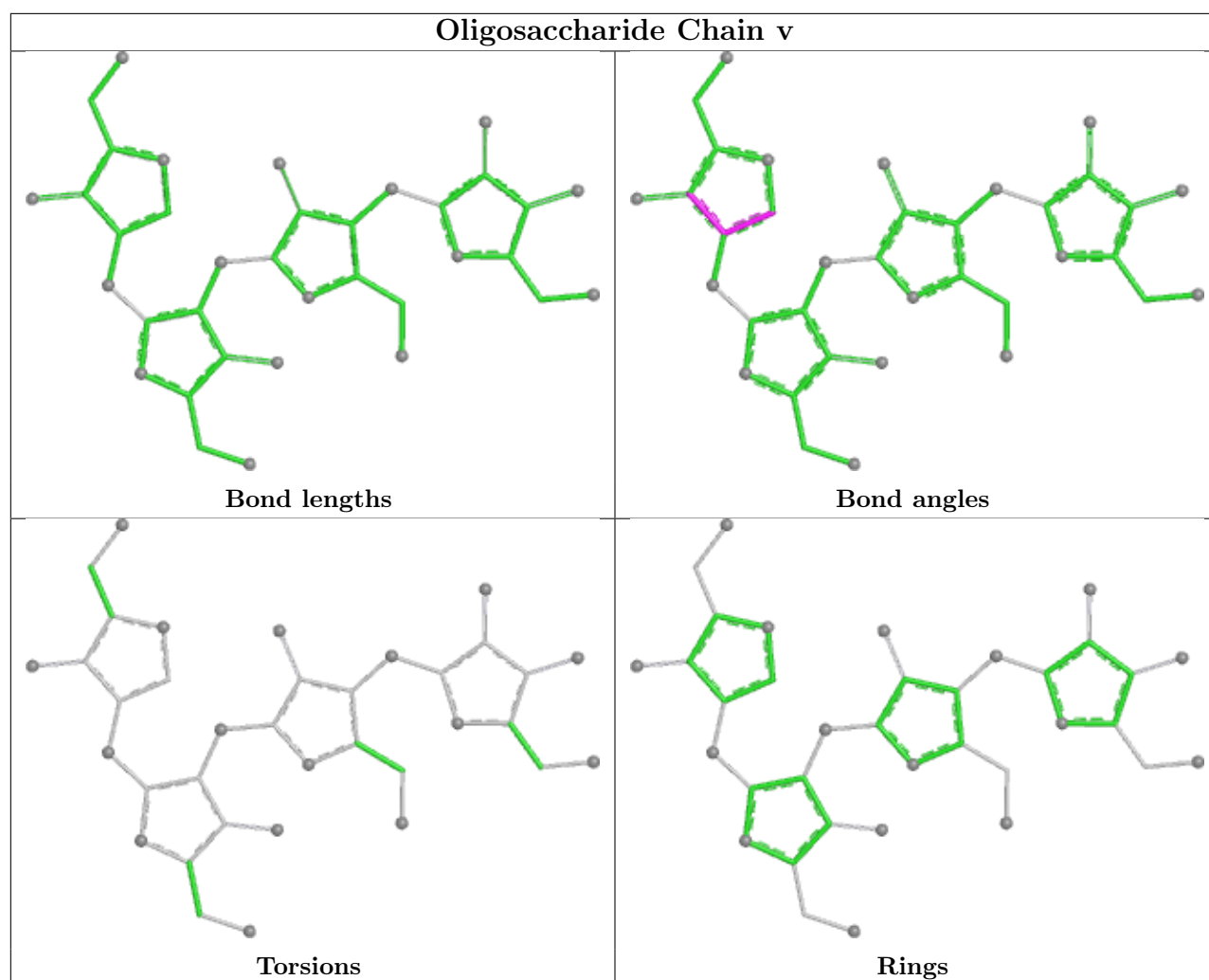


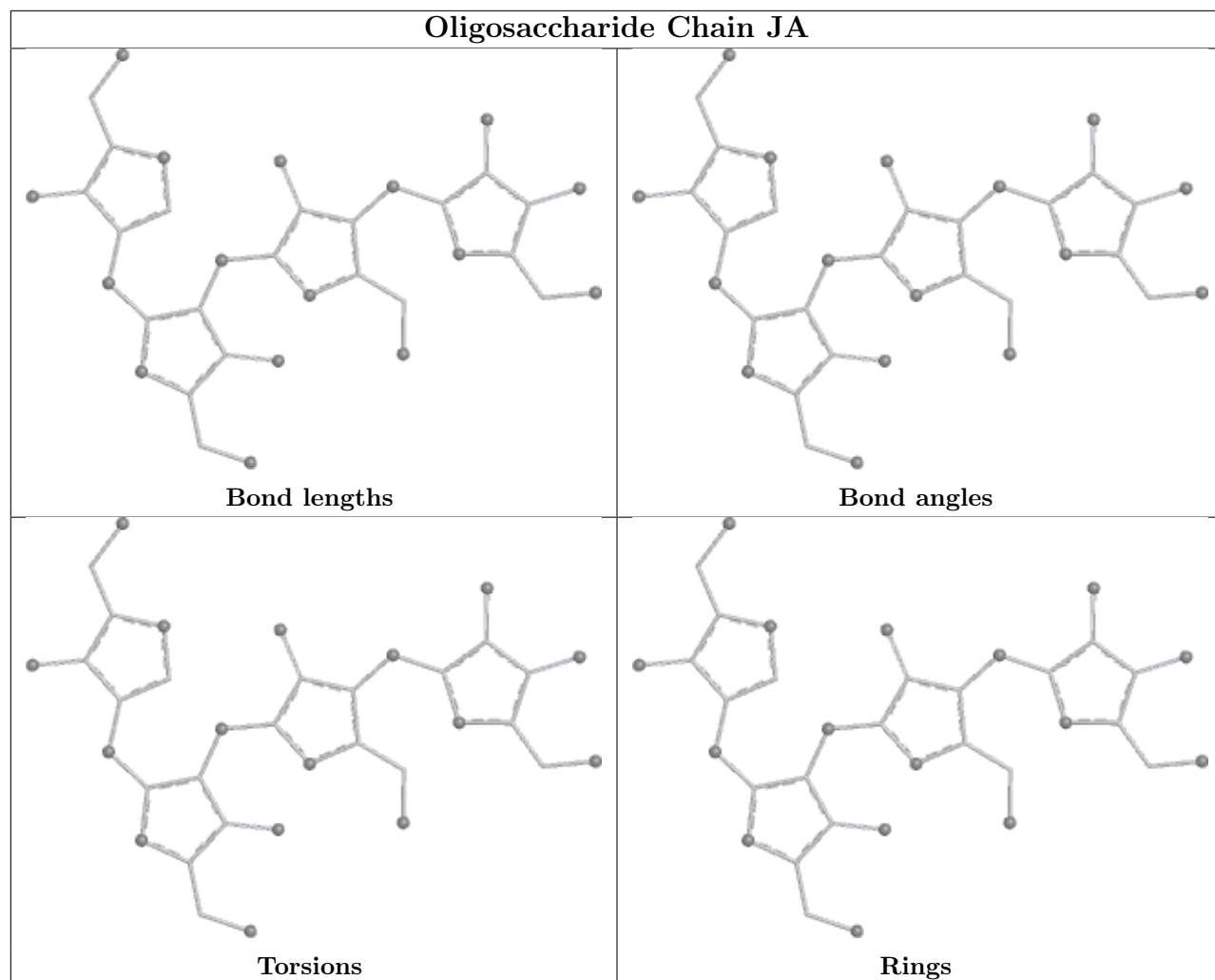


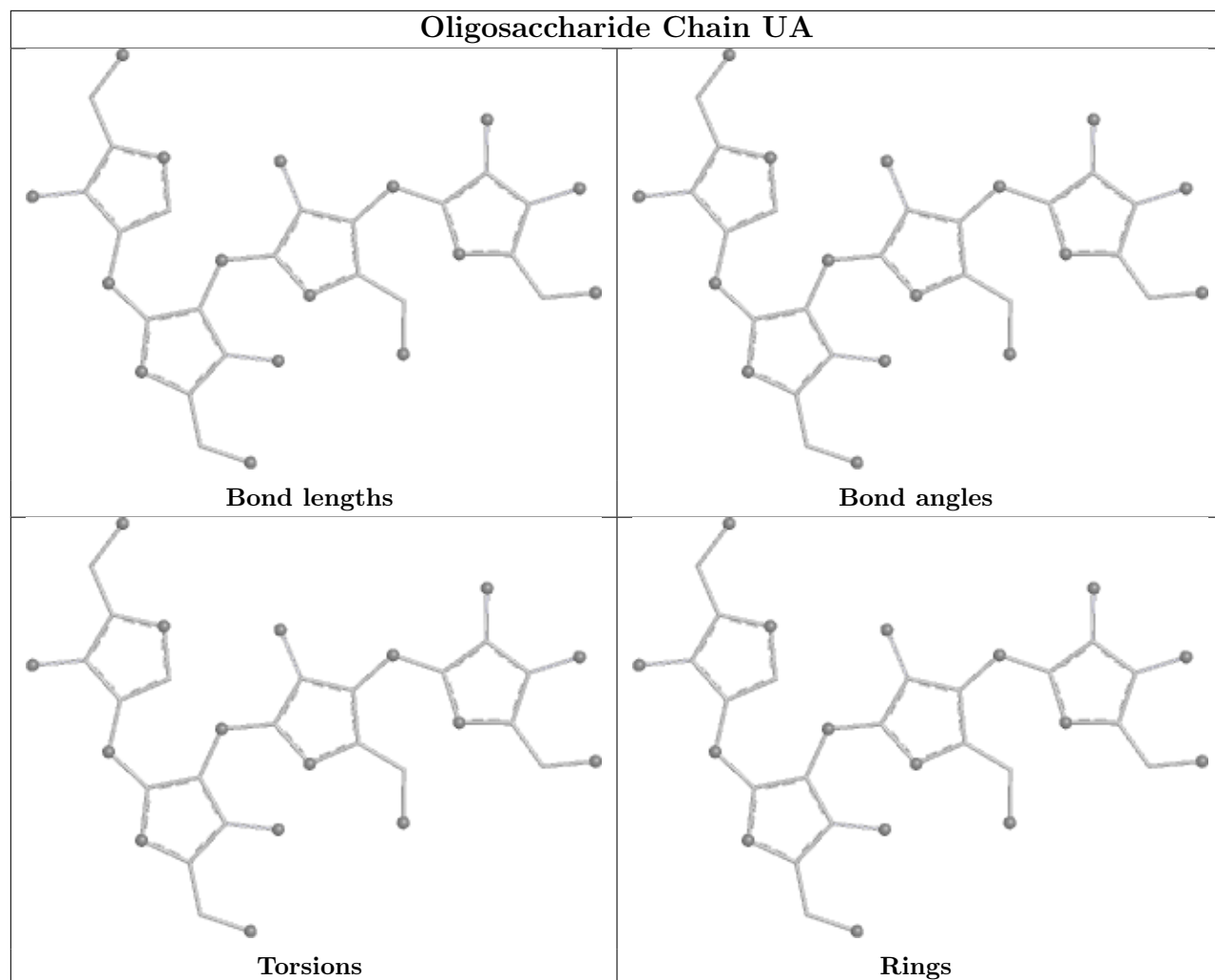


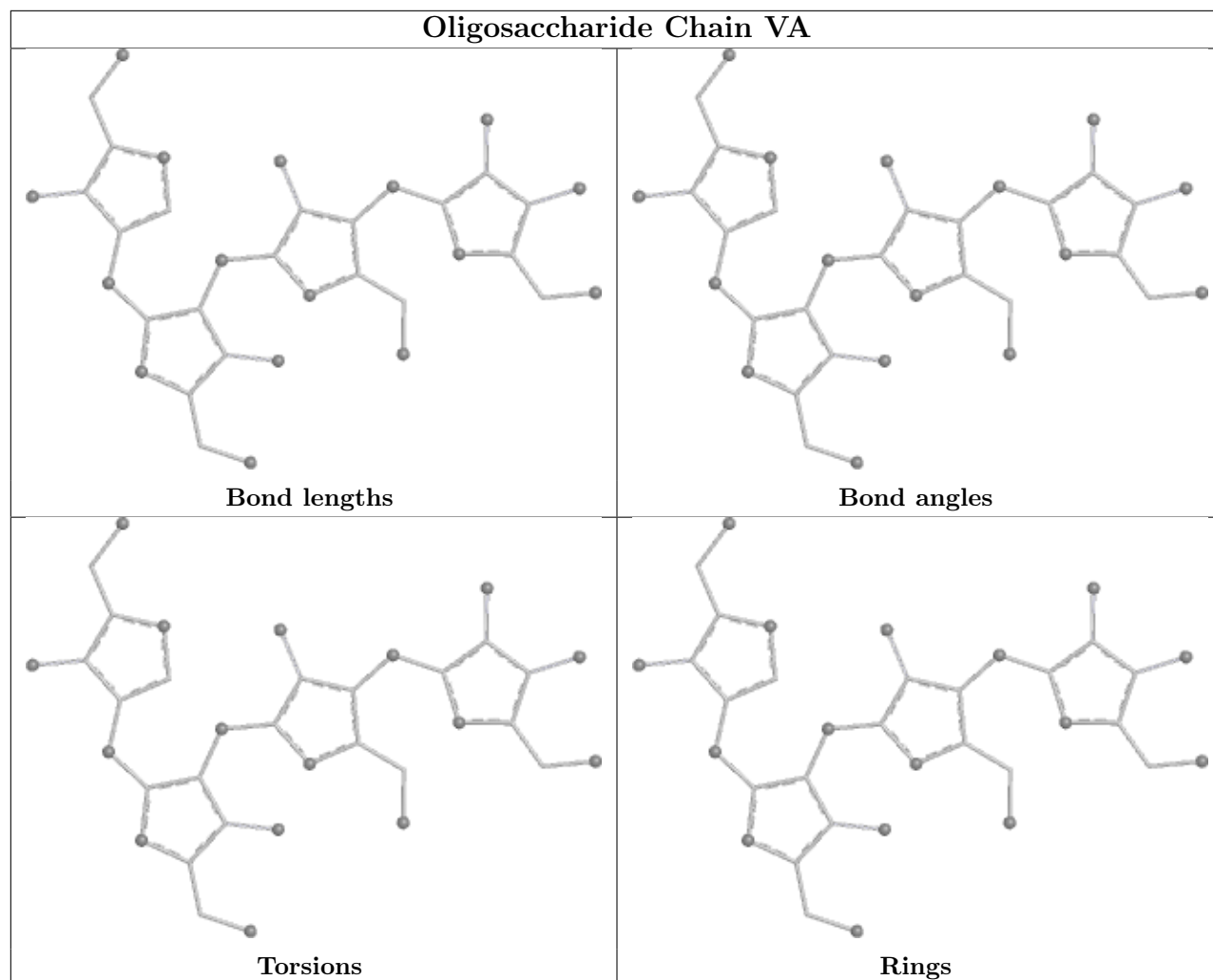


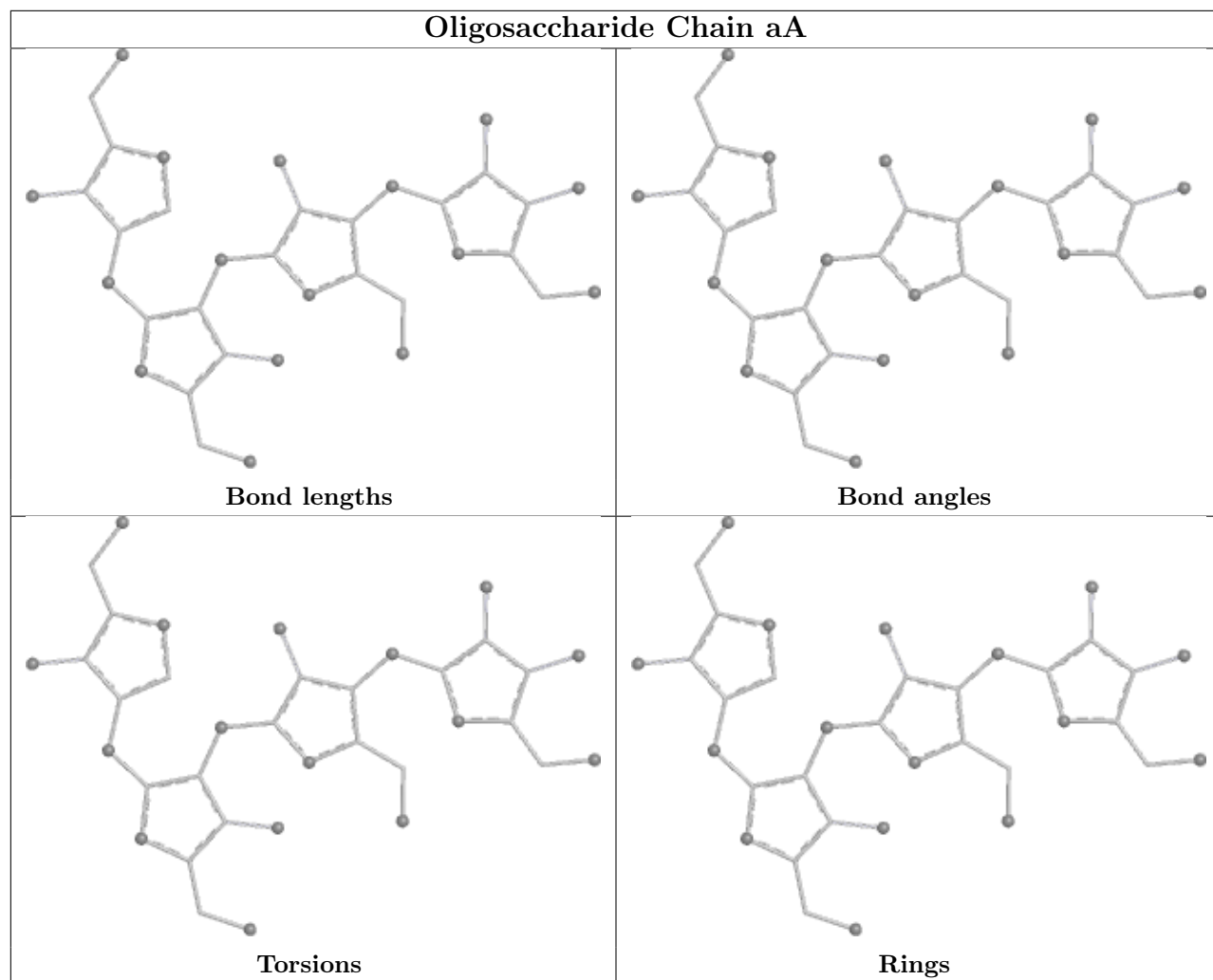


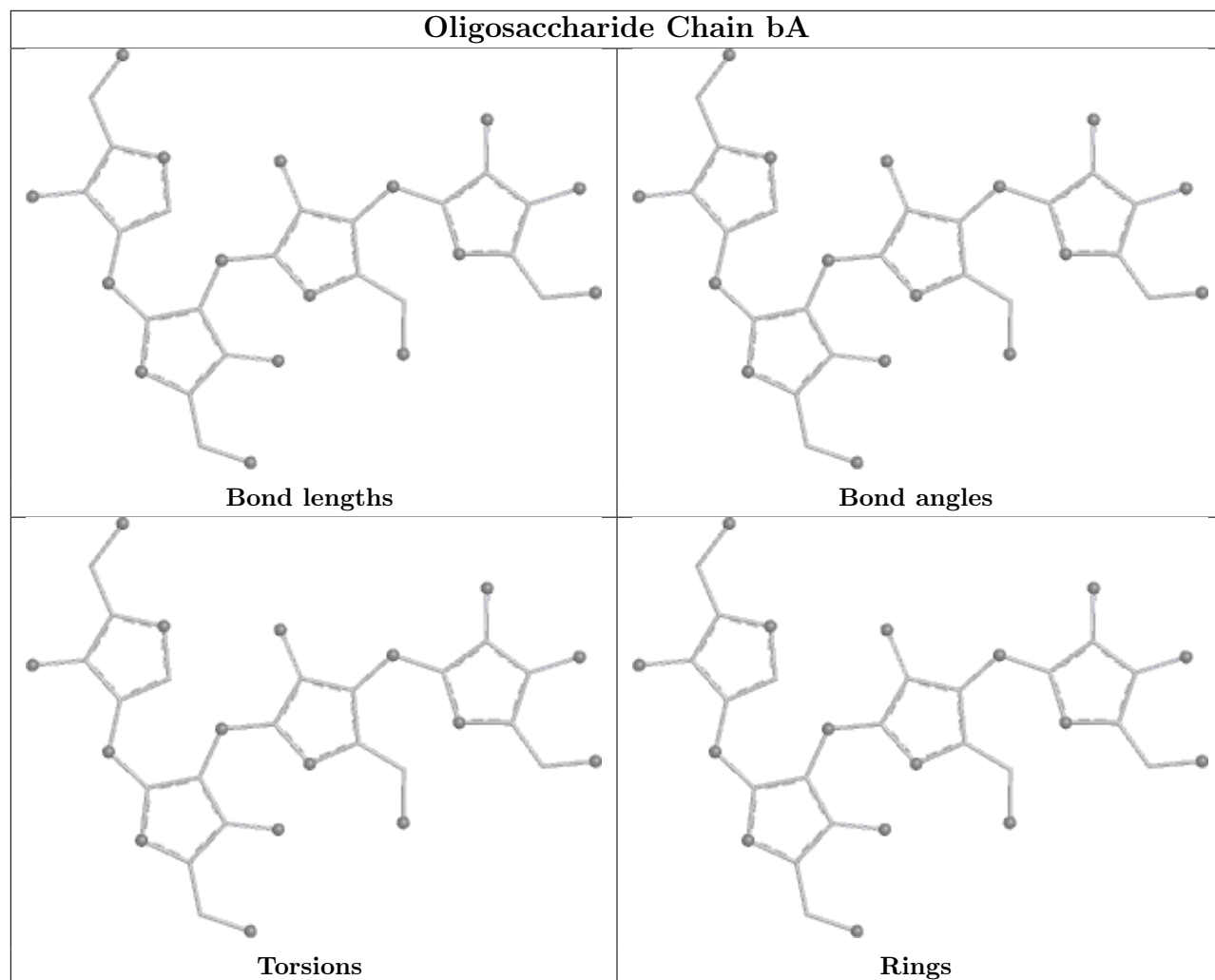


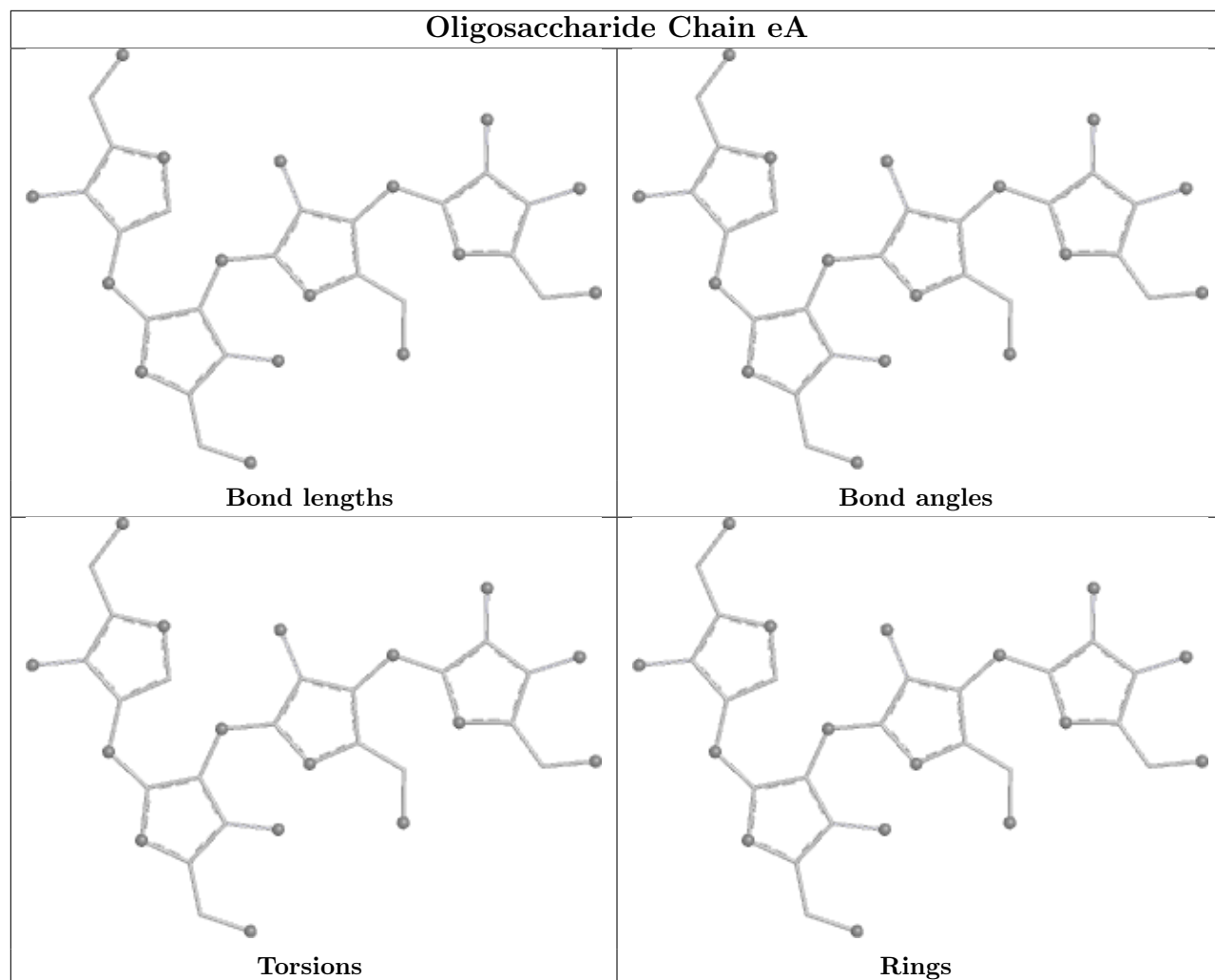
Oligosaccharide Chain JA

Oligosaccharide Chain UA

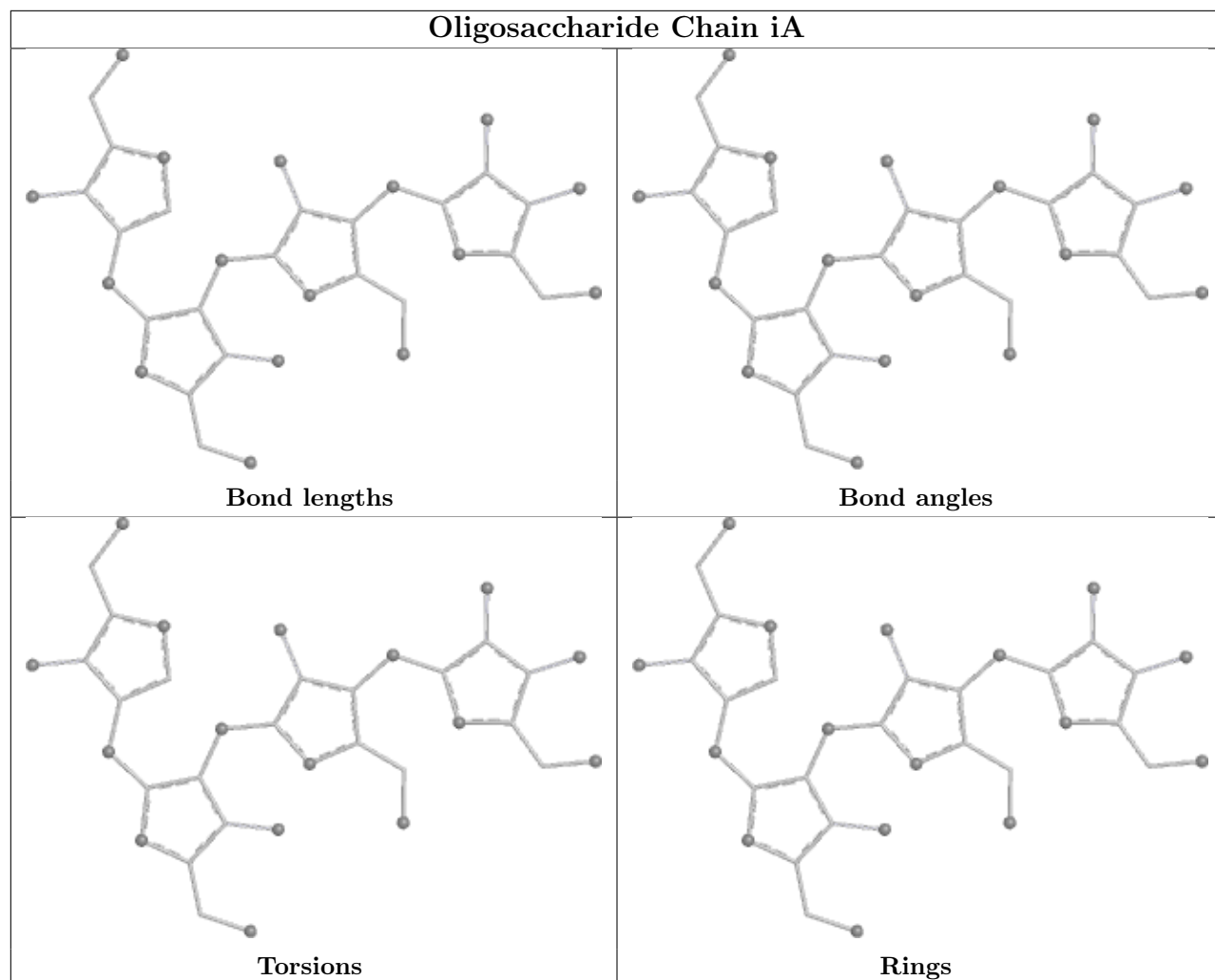
Oligosaccharide Chain VA

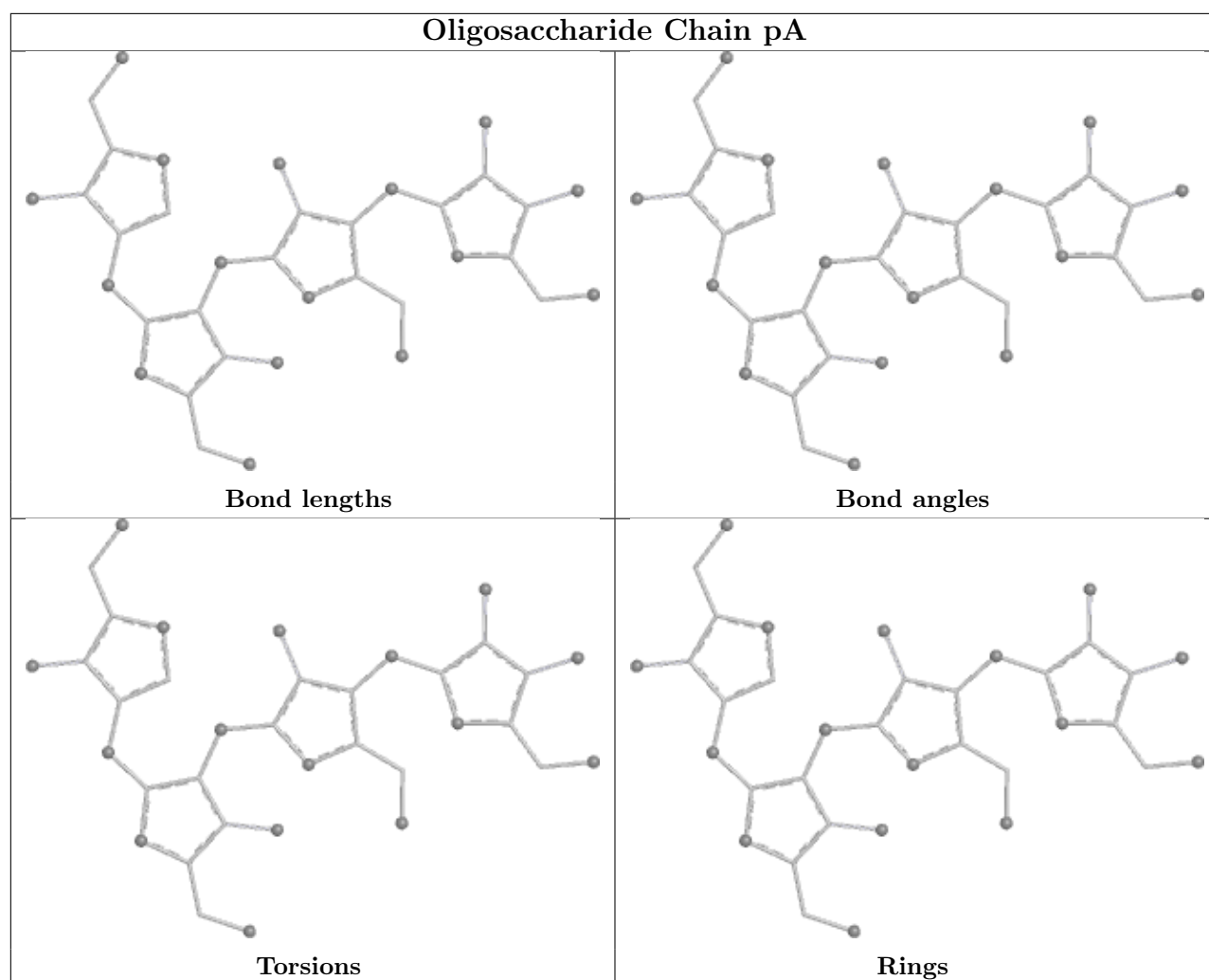


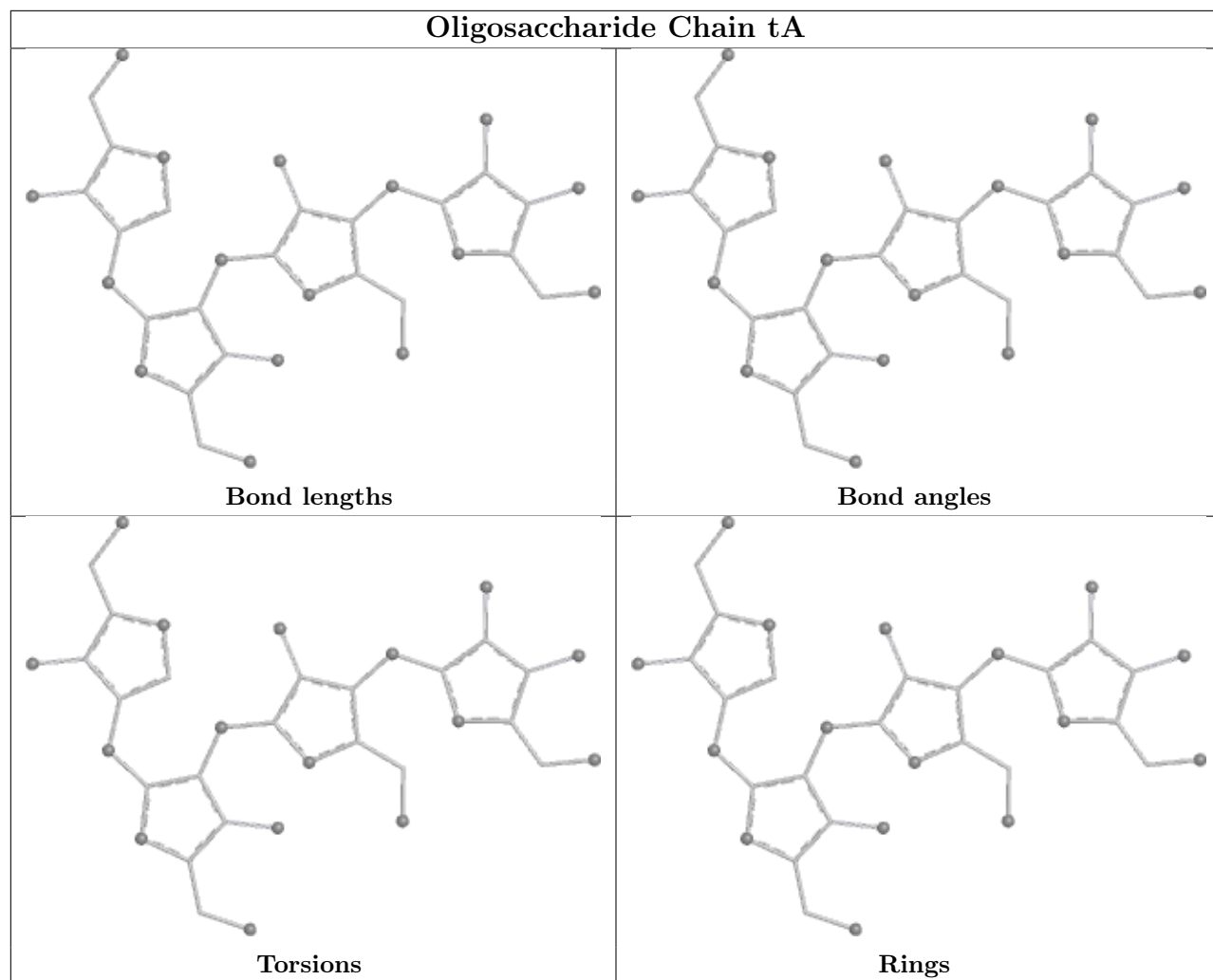
Oligosaccharide Chain bA

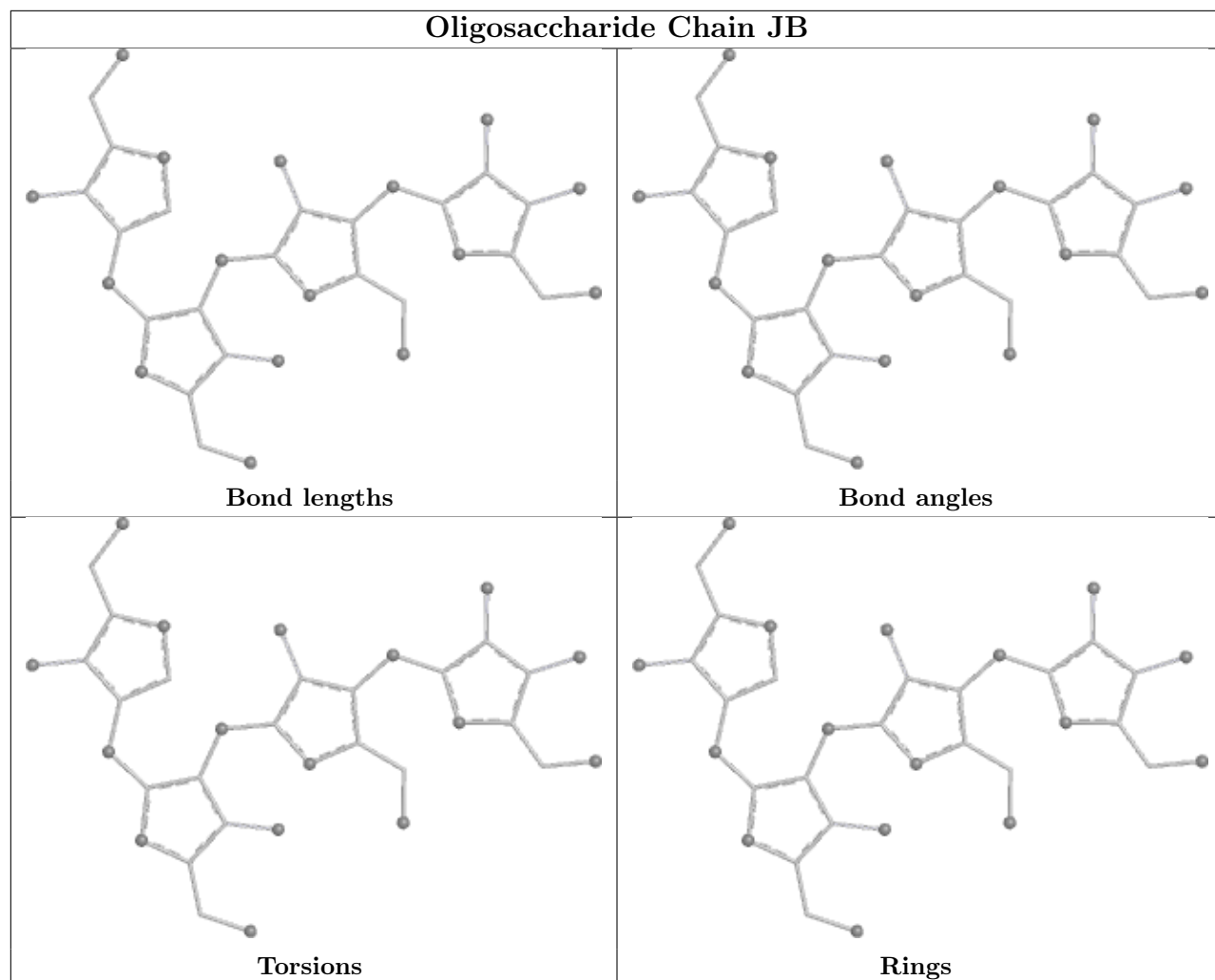
Oligosaccharide Chain eA

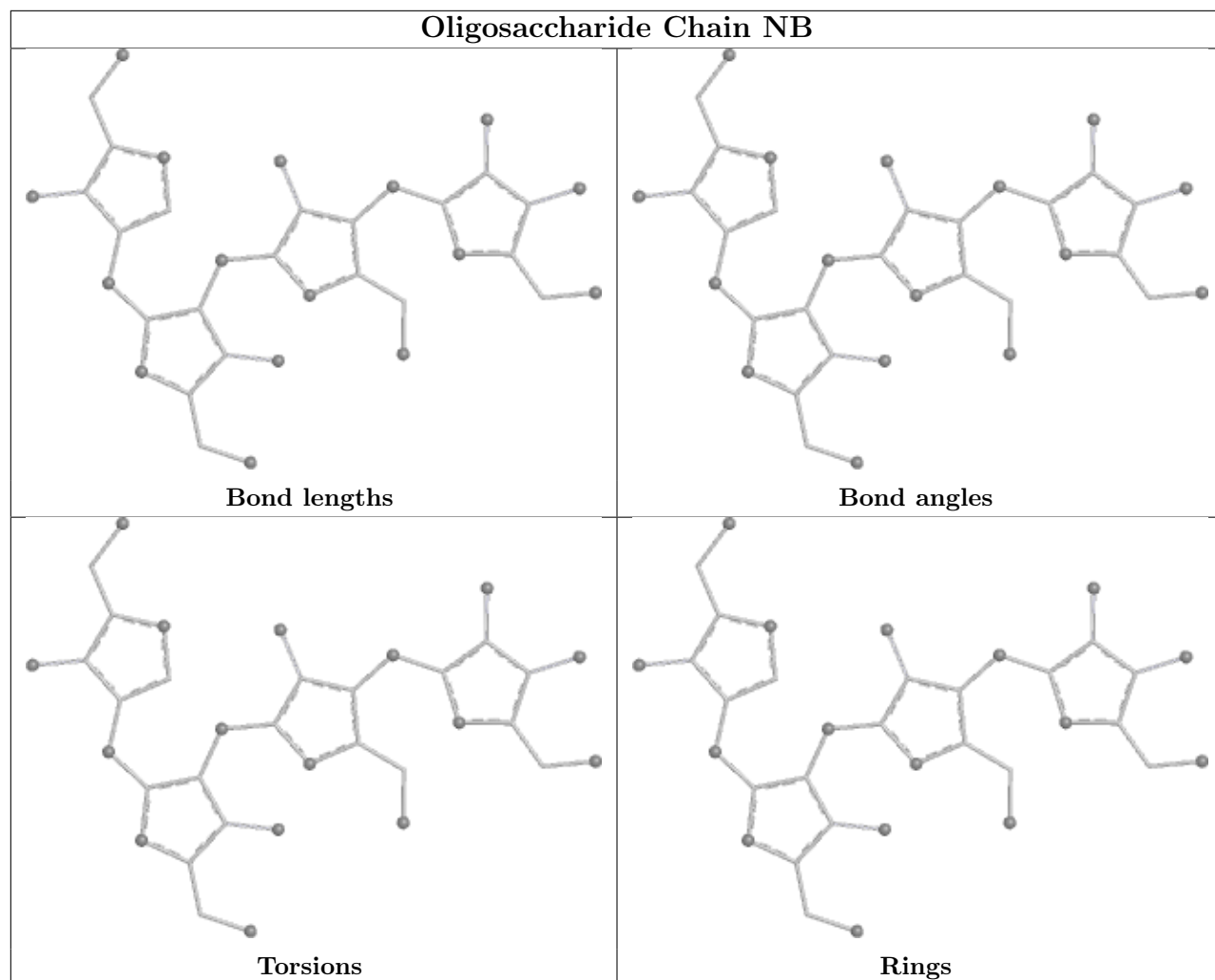
Oligosaccharide Chain iA

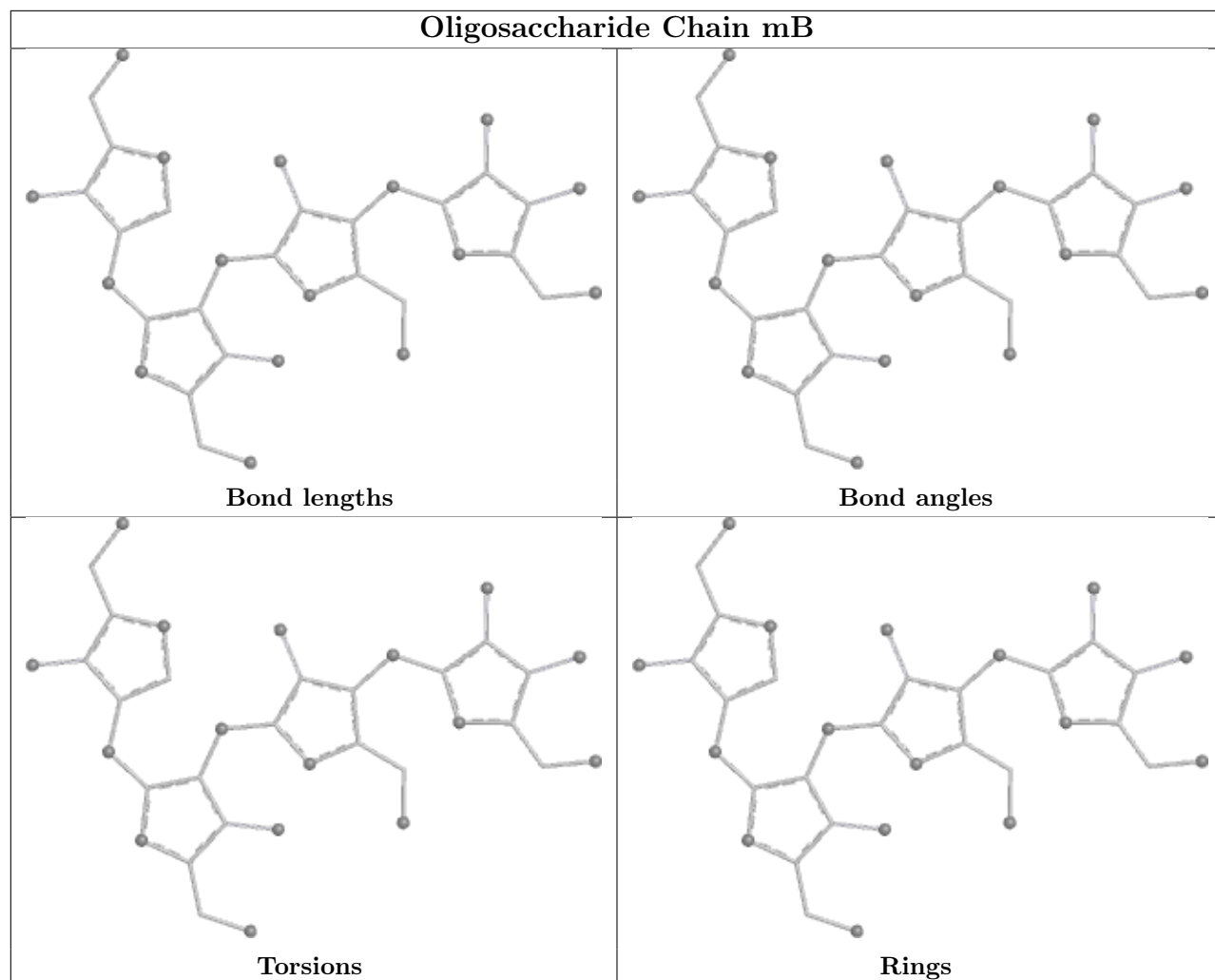


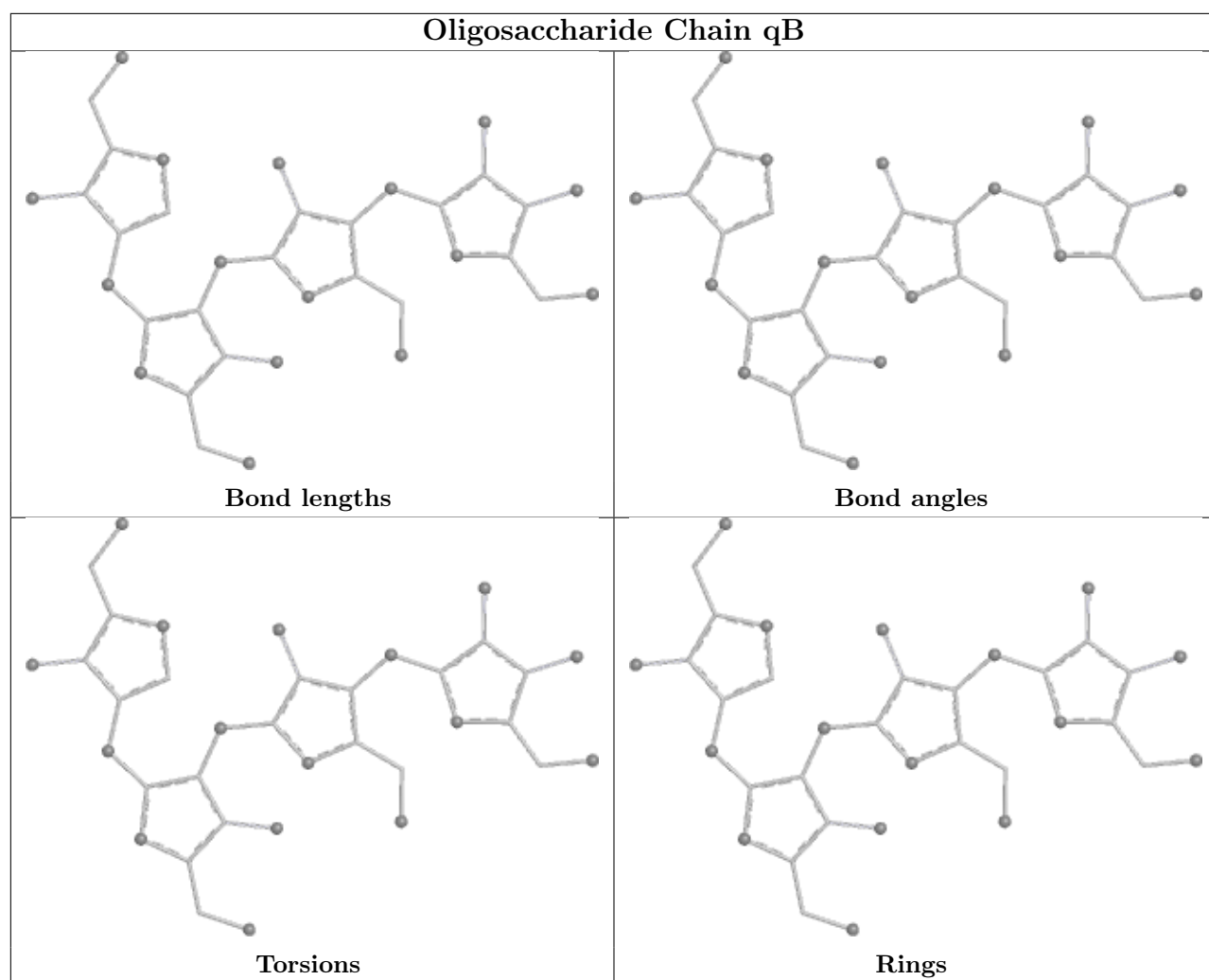


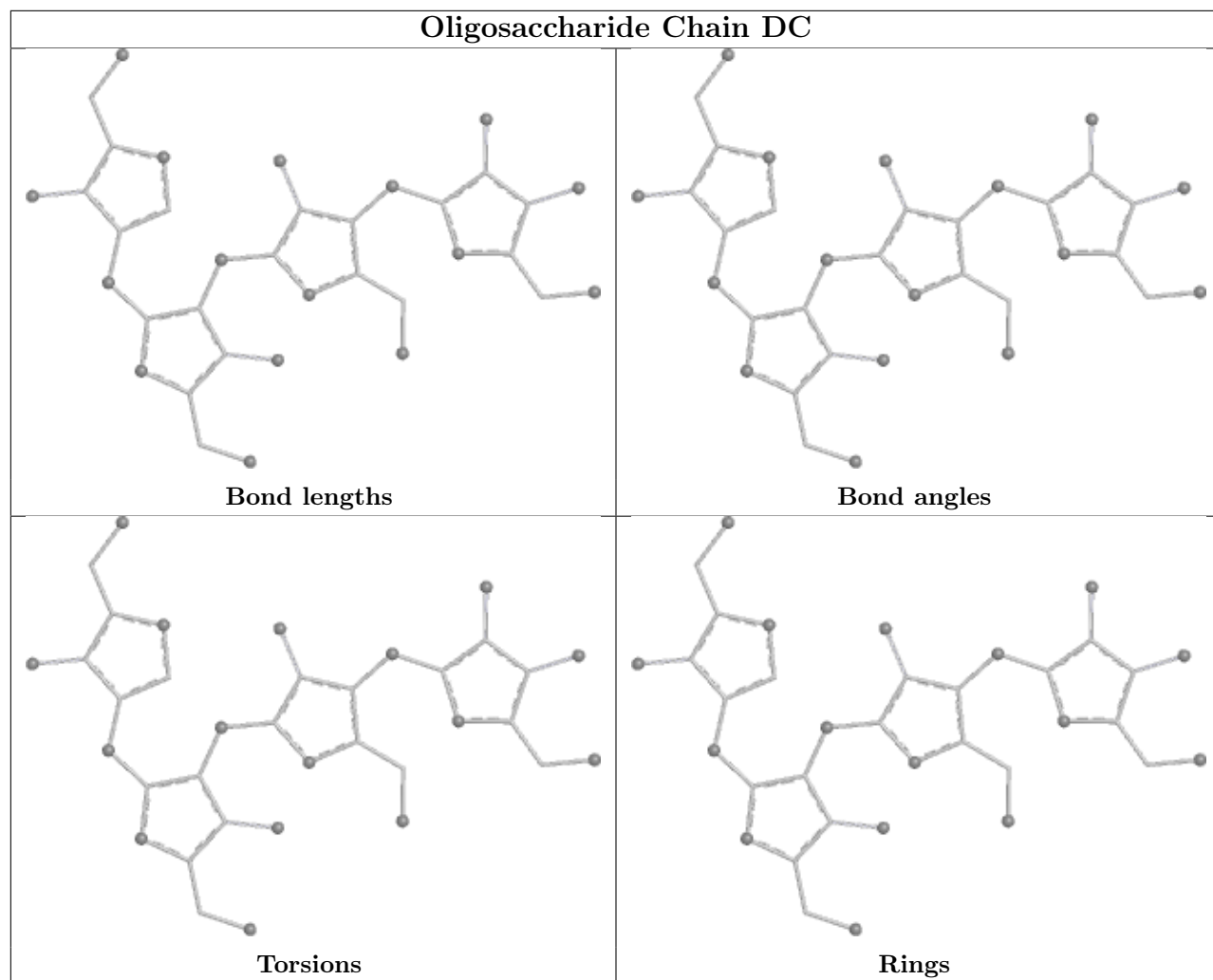


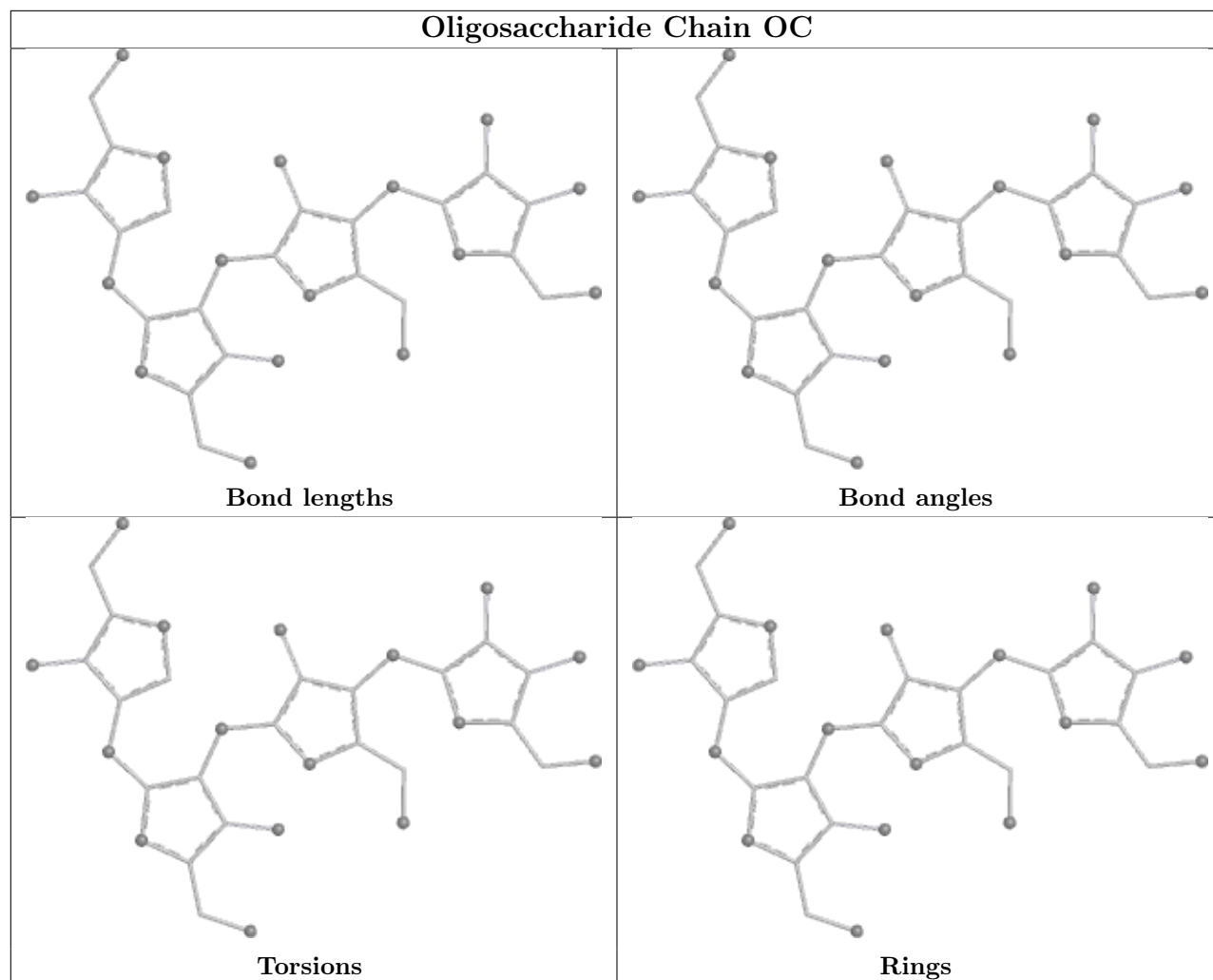
Oligosaccharide Chain JB

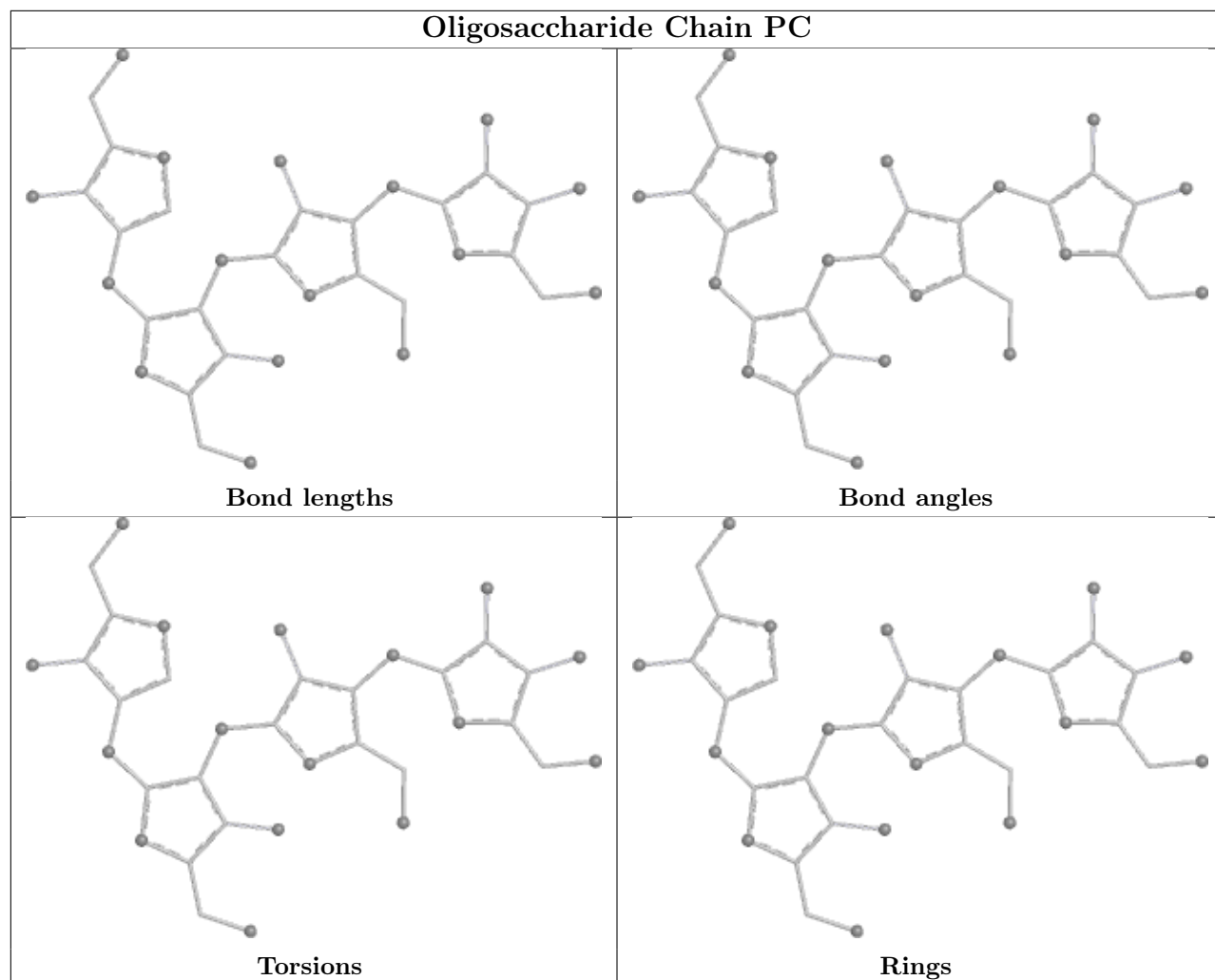
Oligosaccharide Chain NB

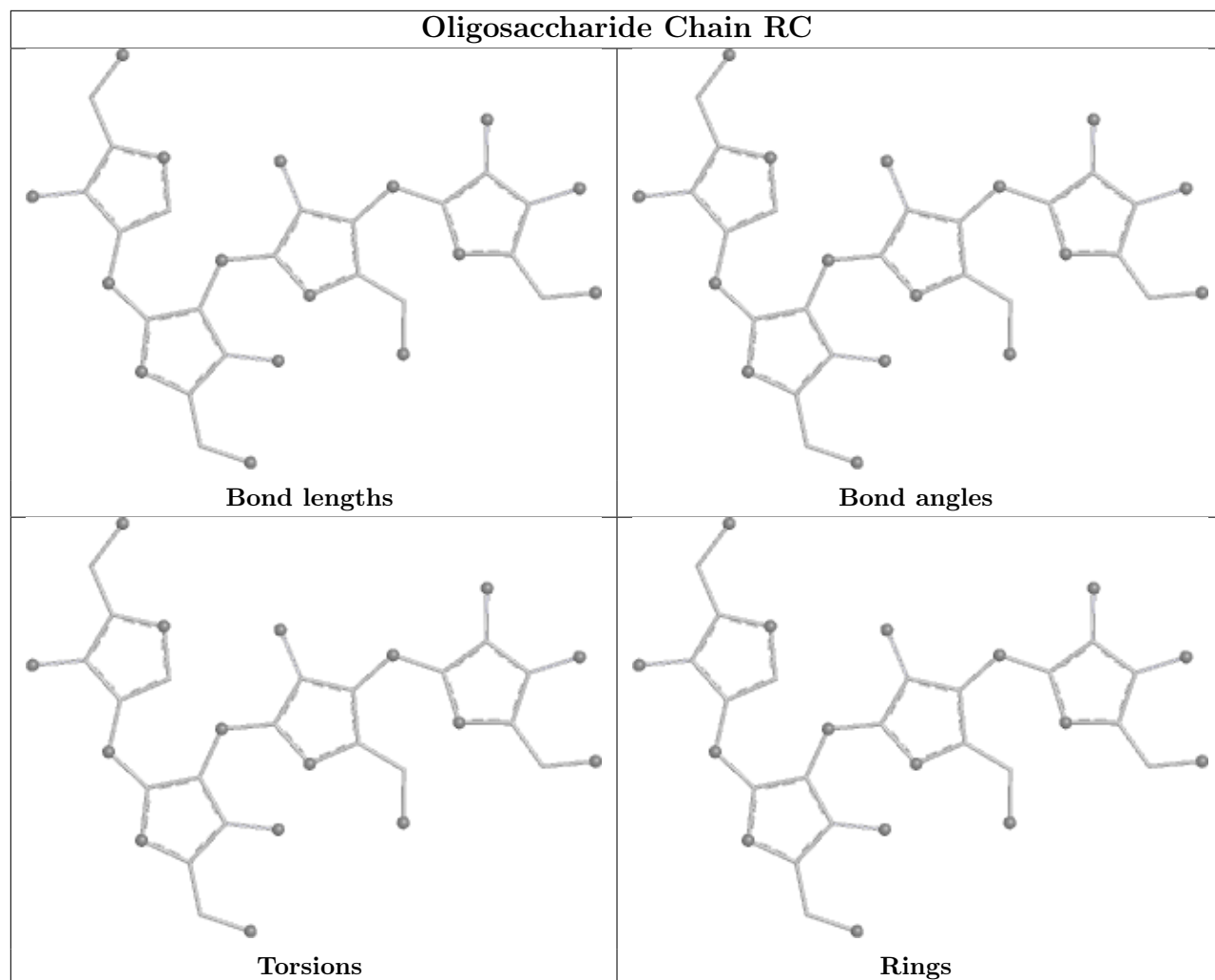
Oligosaccharide Chain mB

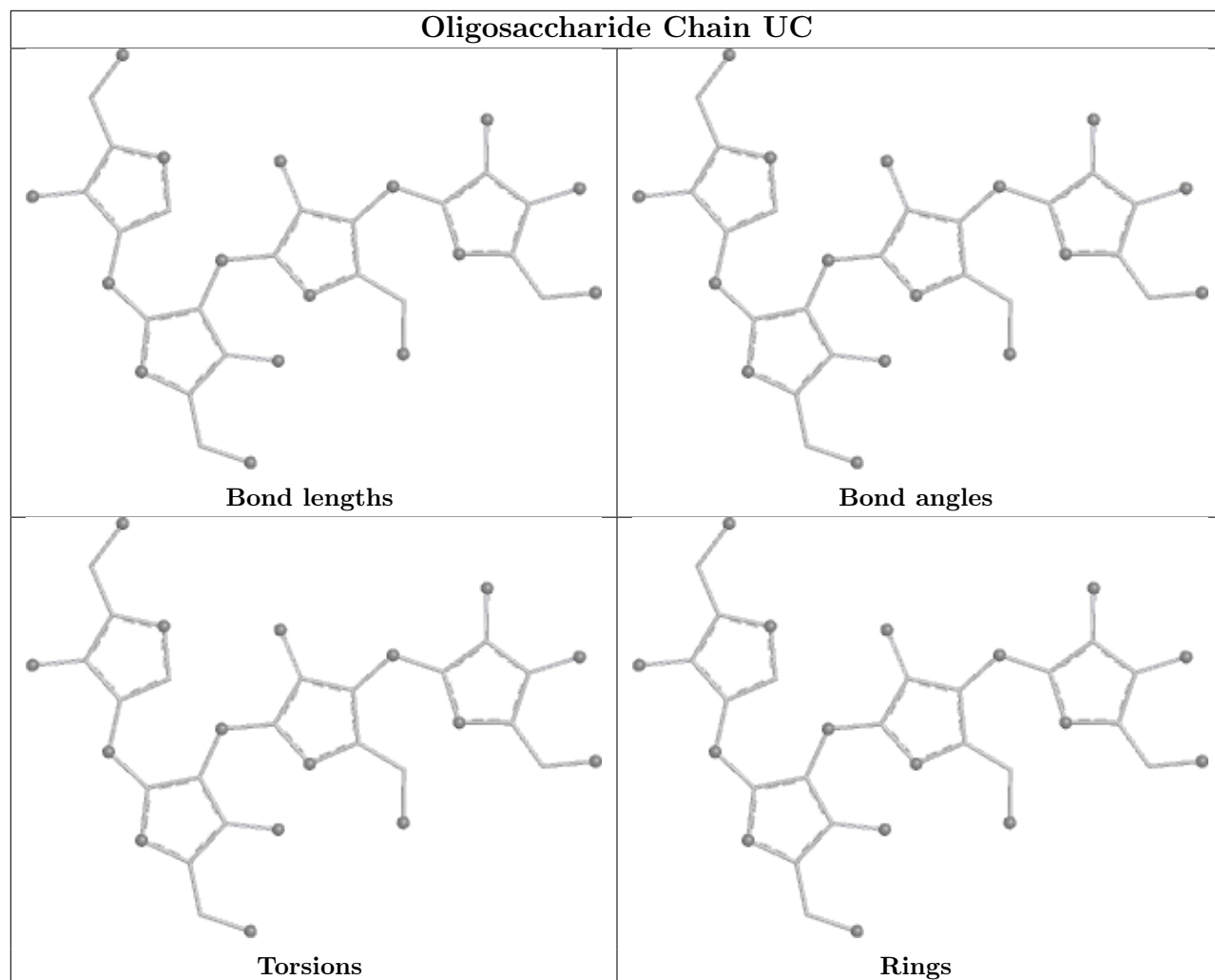


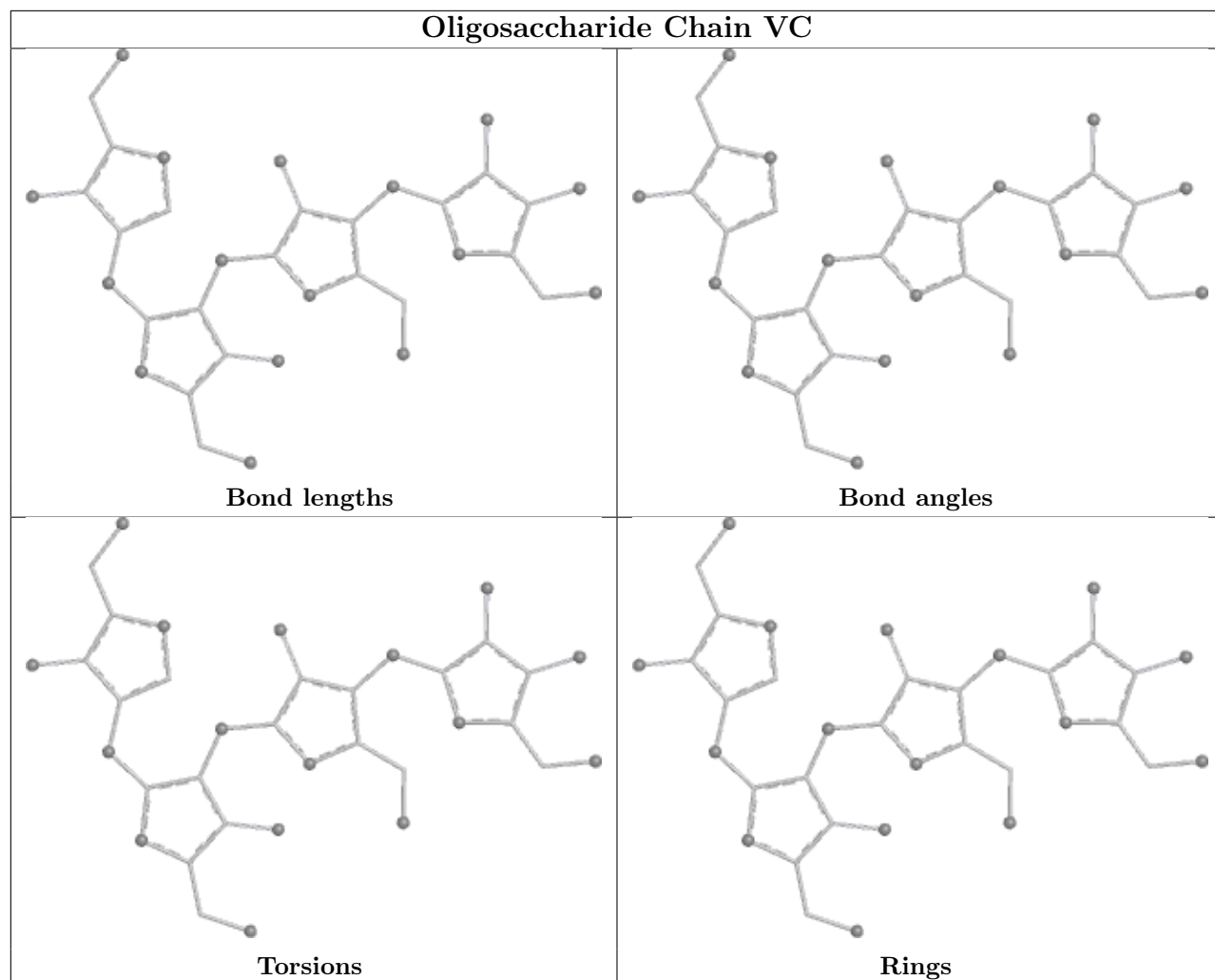
Oligosaccharide Chain DC

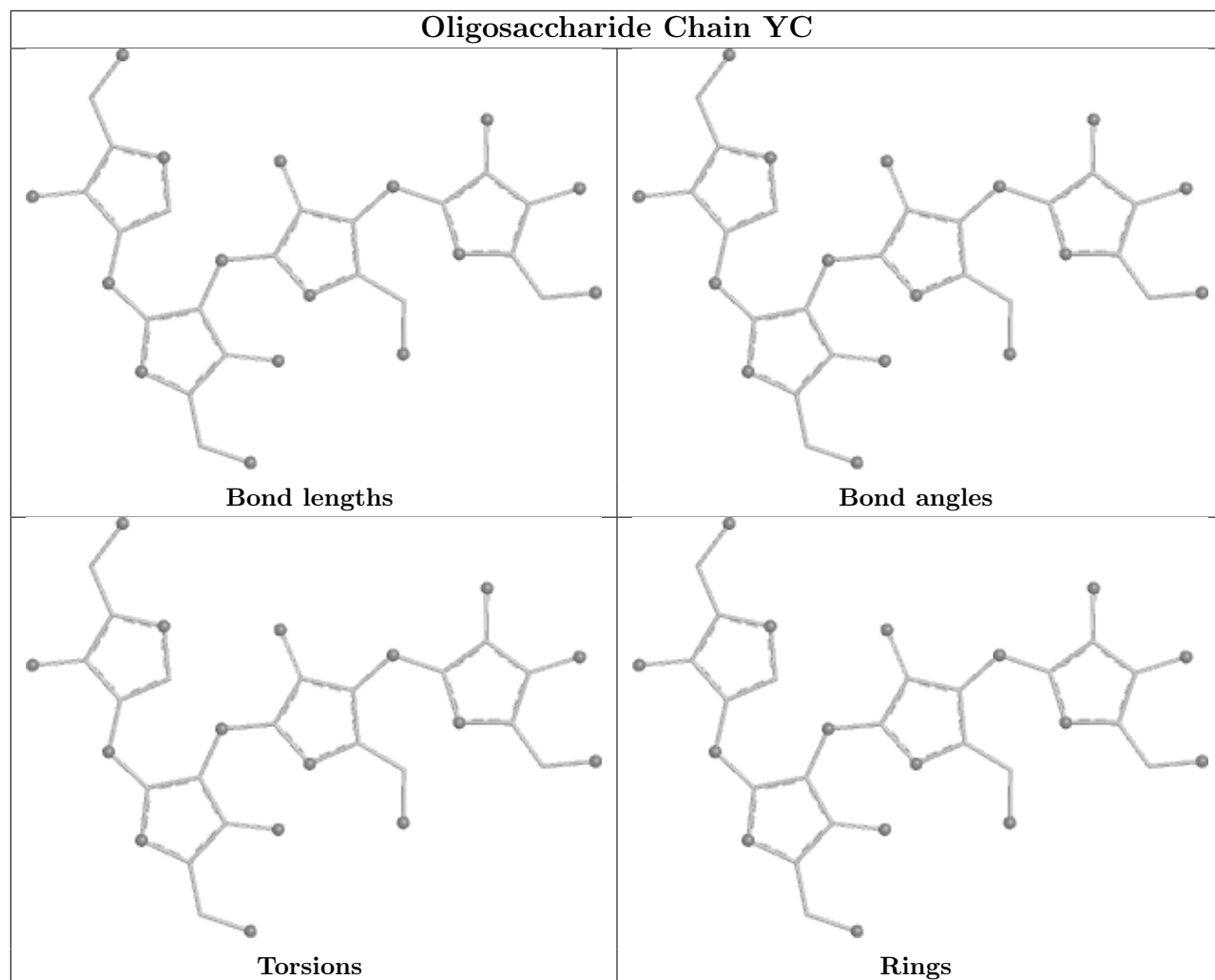
Oligosaccharide Chain OC

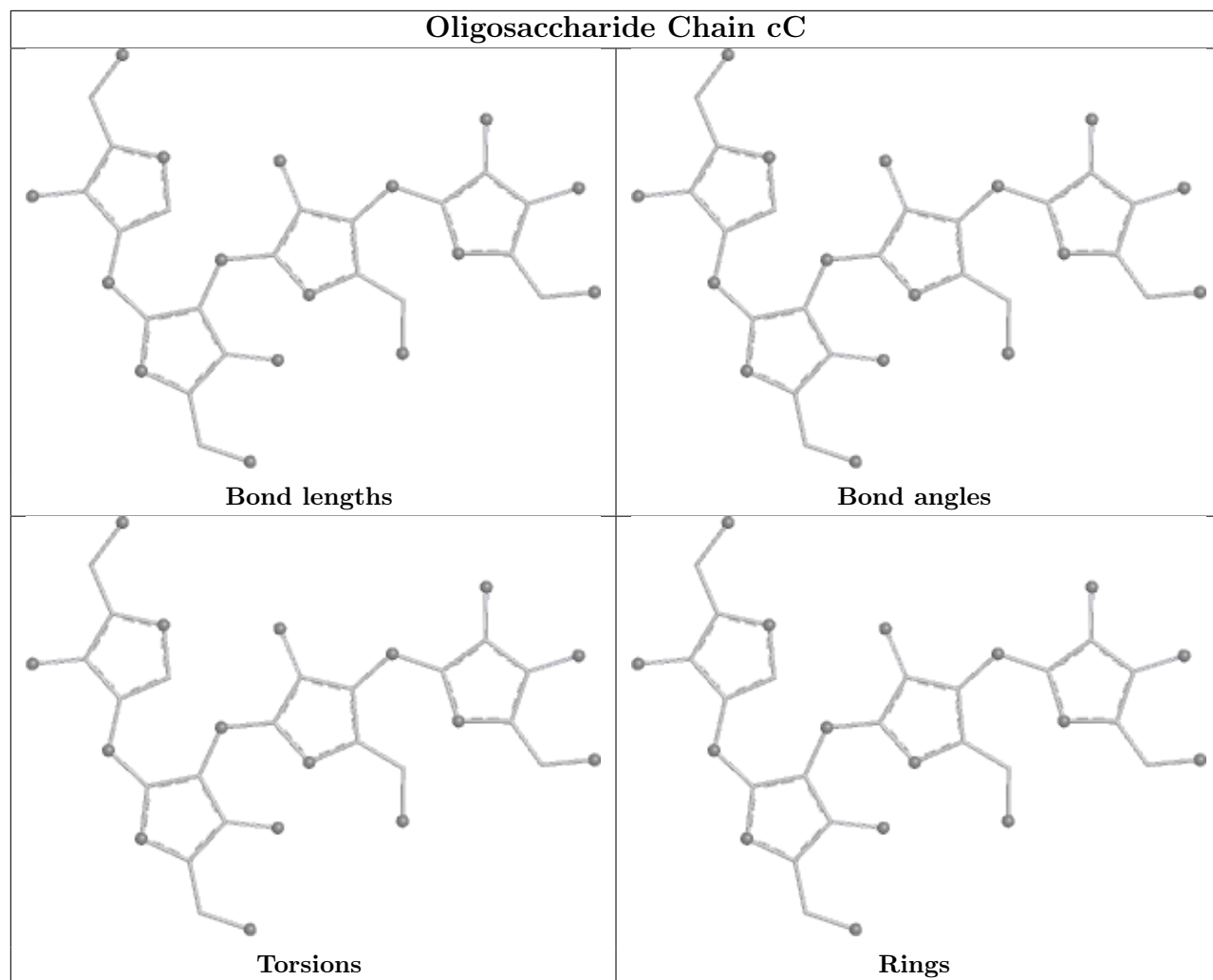
Oligosaccharide Chain PC

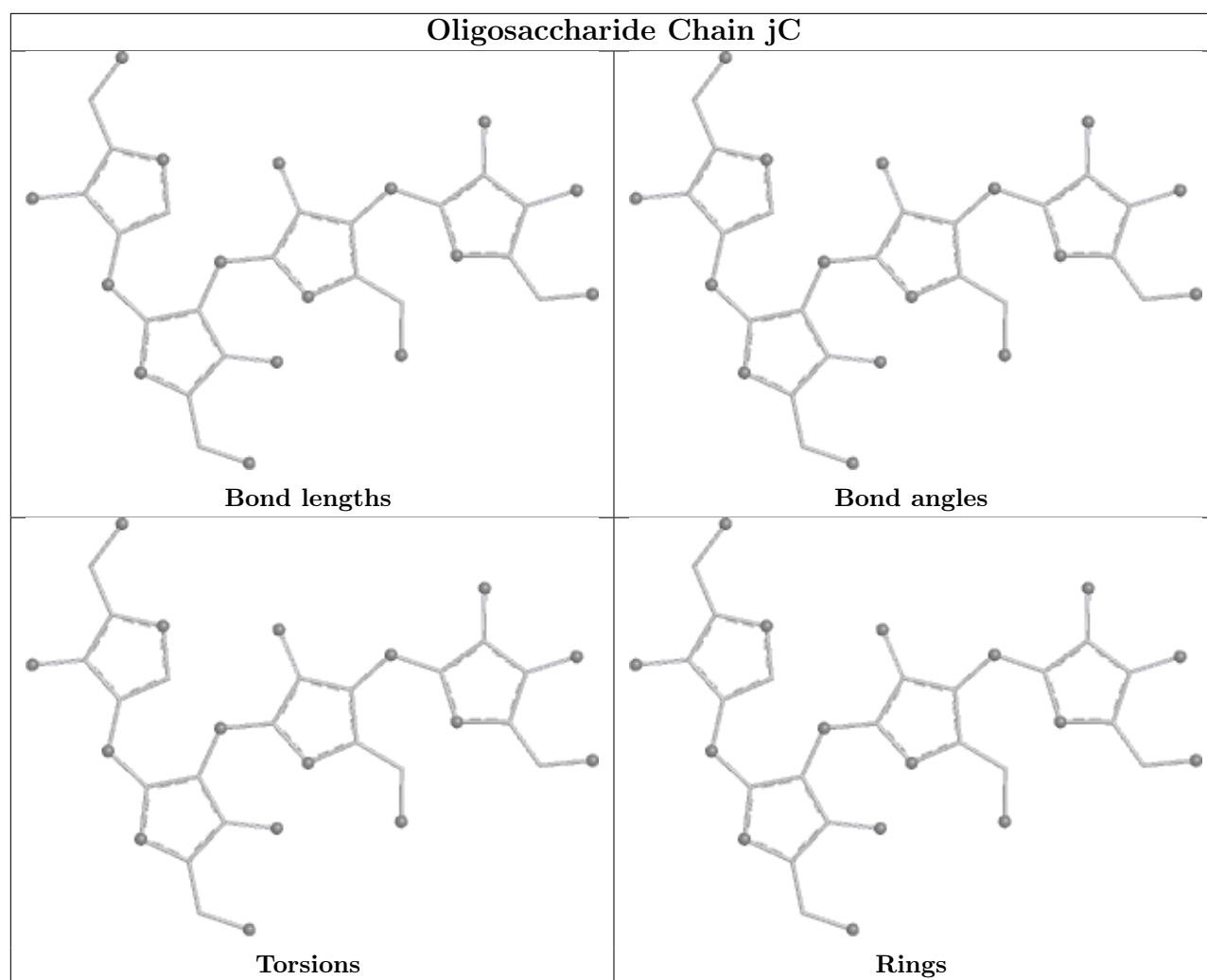
Oligosaccharide Chain RC

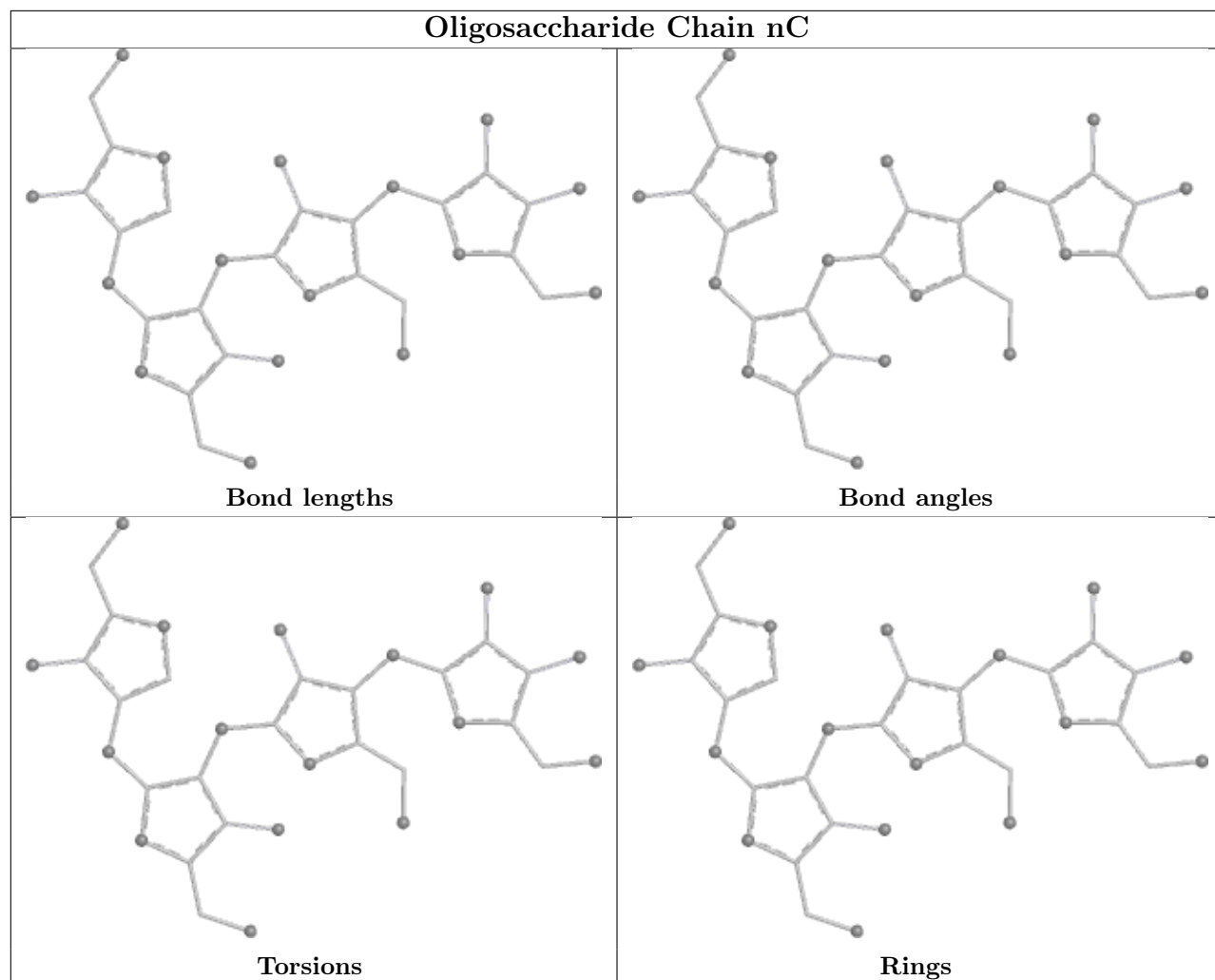
Oligosaccharide Chain UC

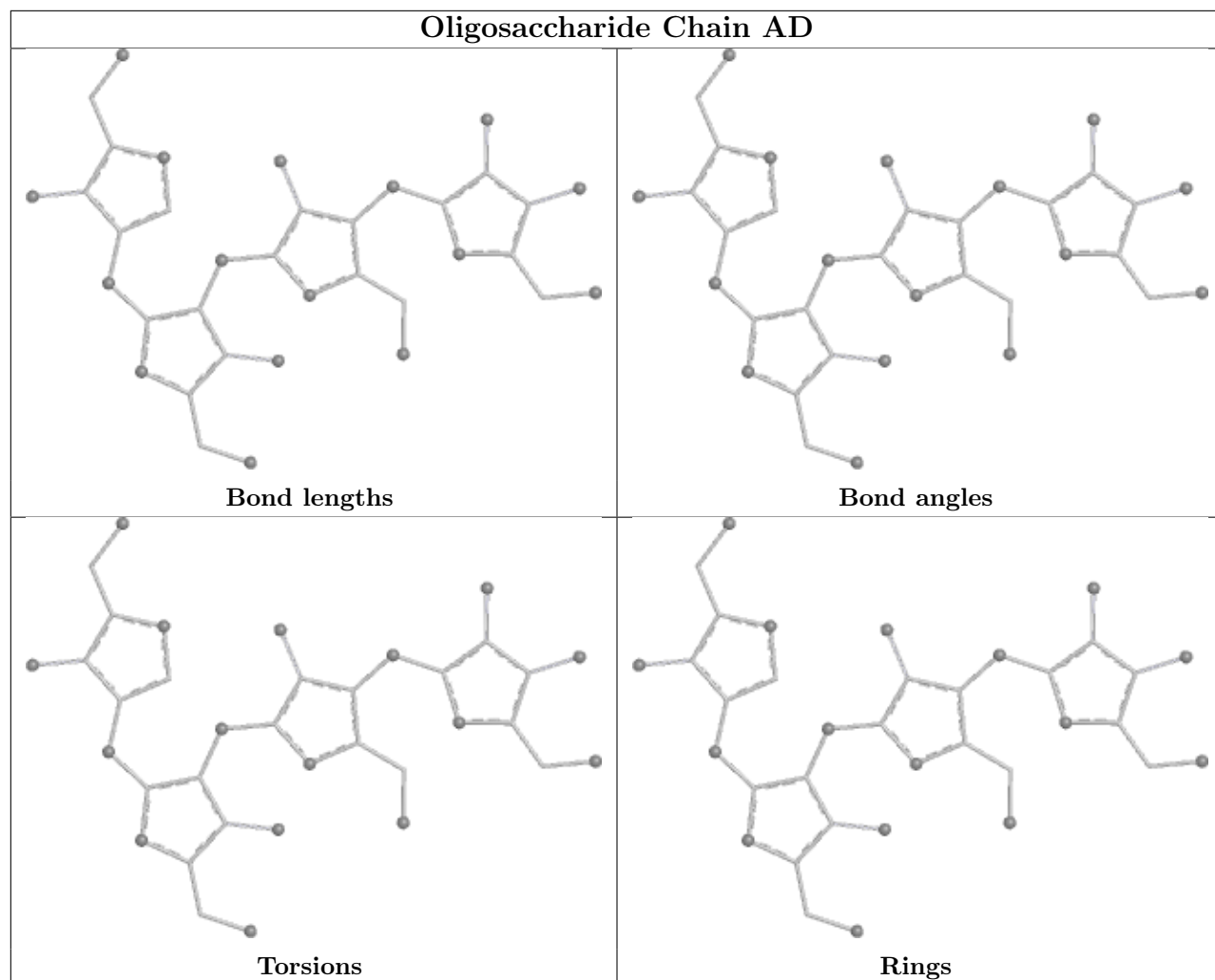
Oligosaccharide Chain VC

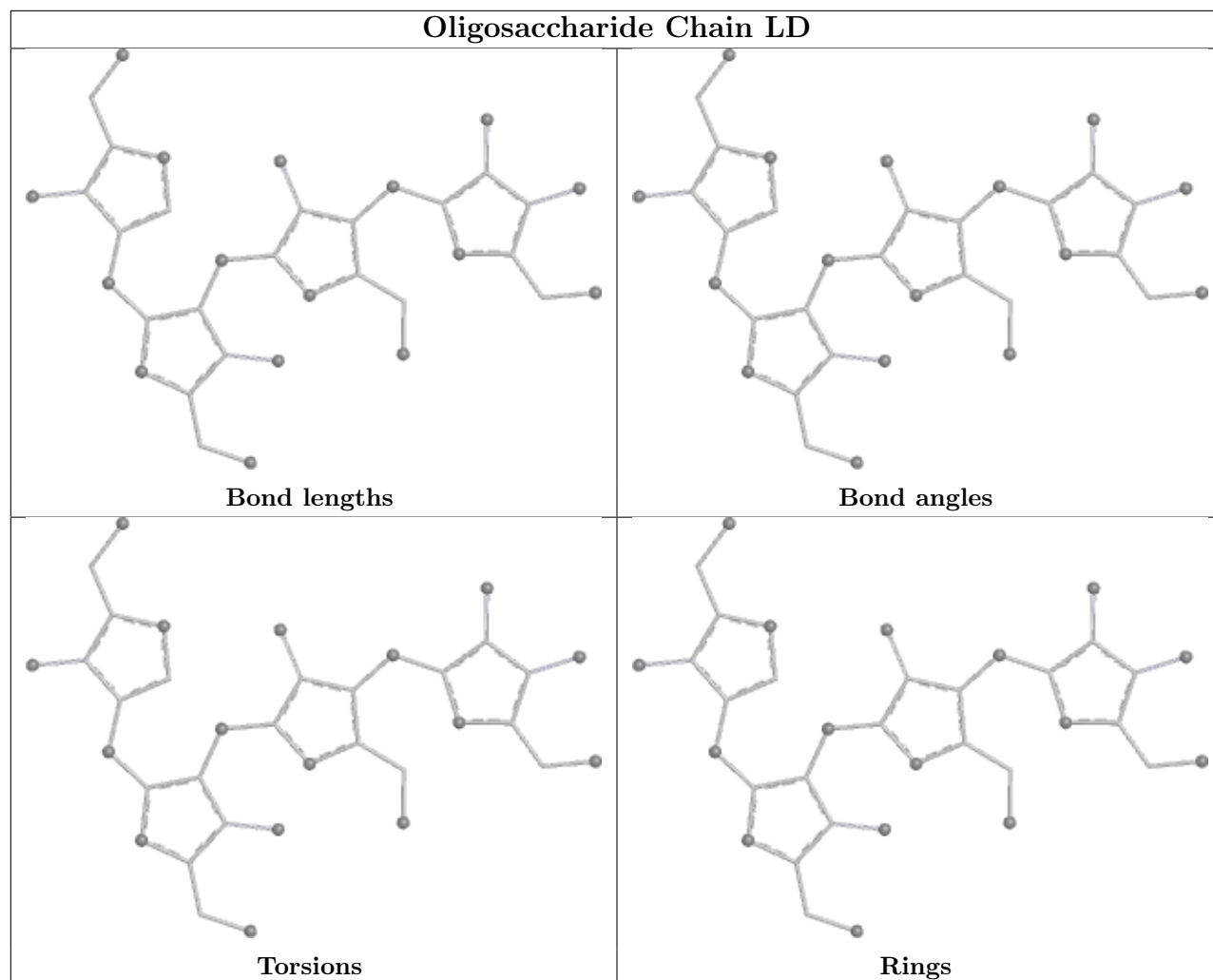
Oligosaccharide Chain YC

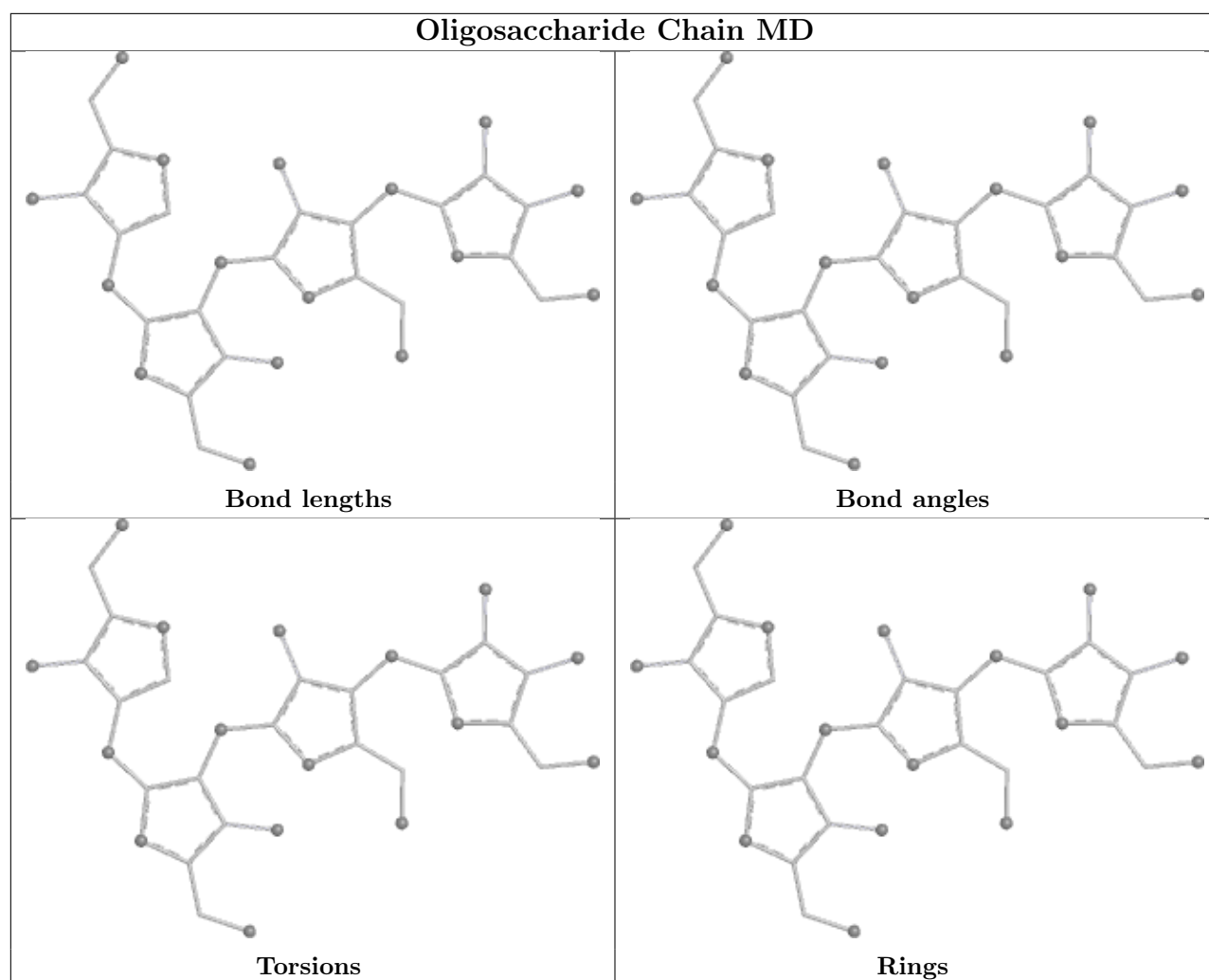
Oligosaccharide Chain cC



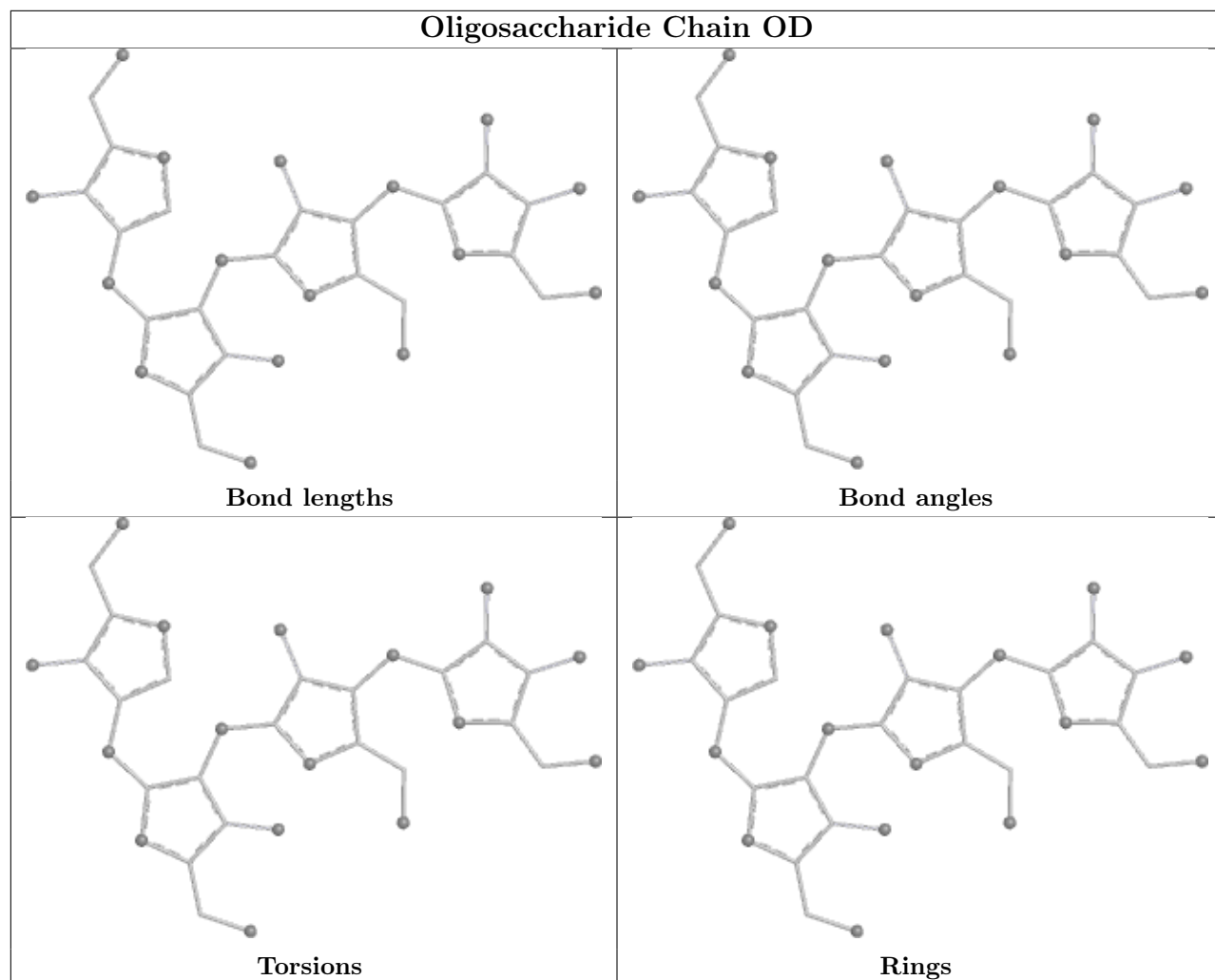
Oligosaccharide Chain nC

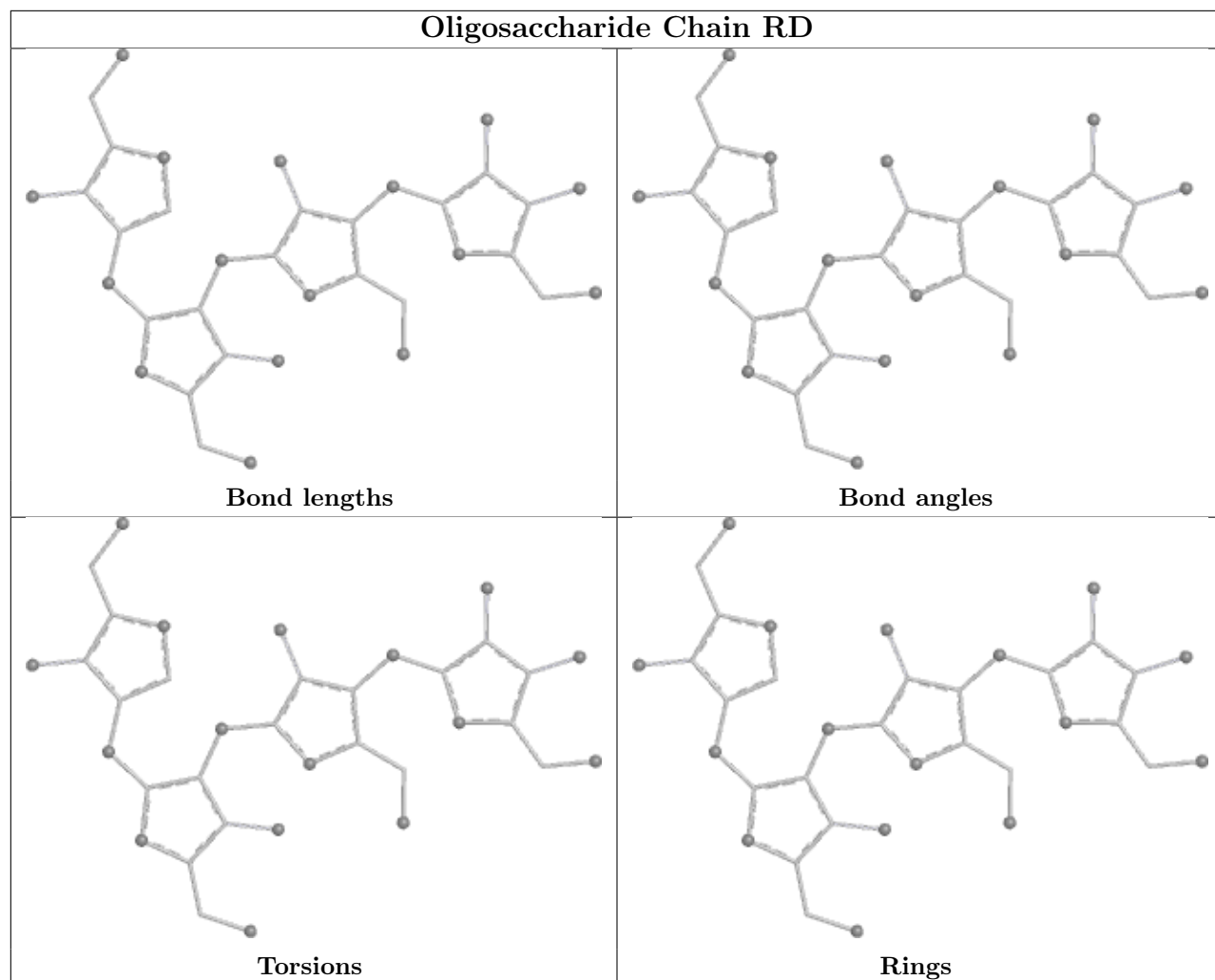
Oligosaccharide Chain AD

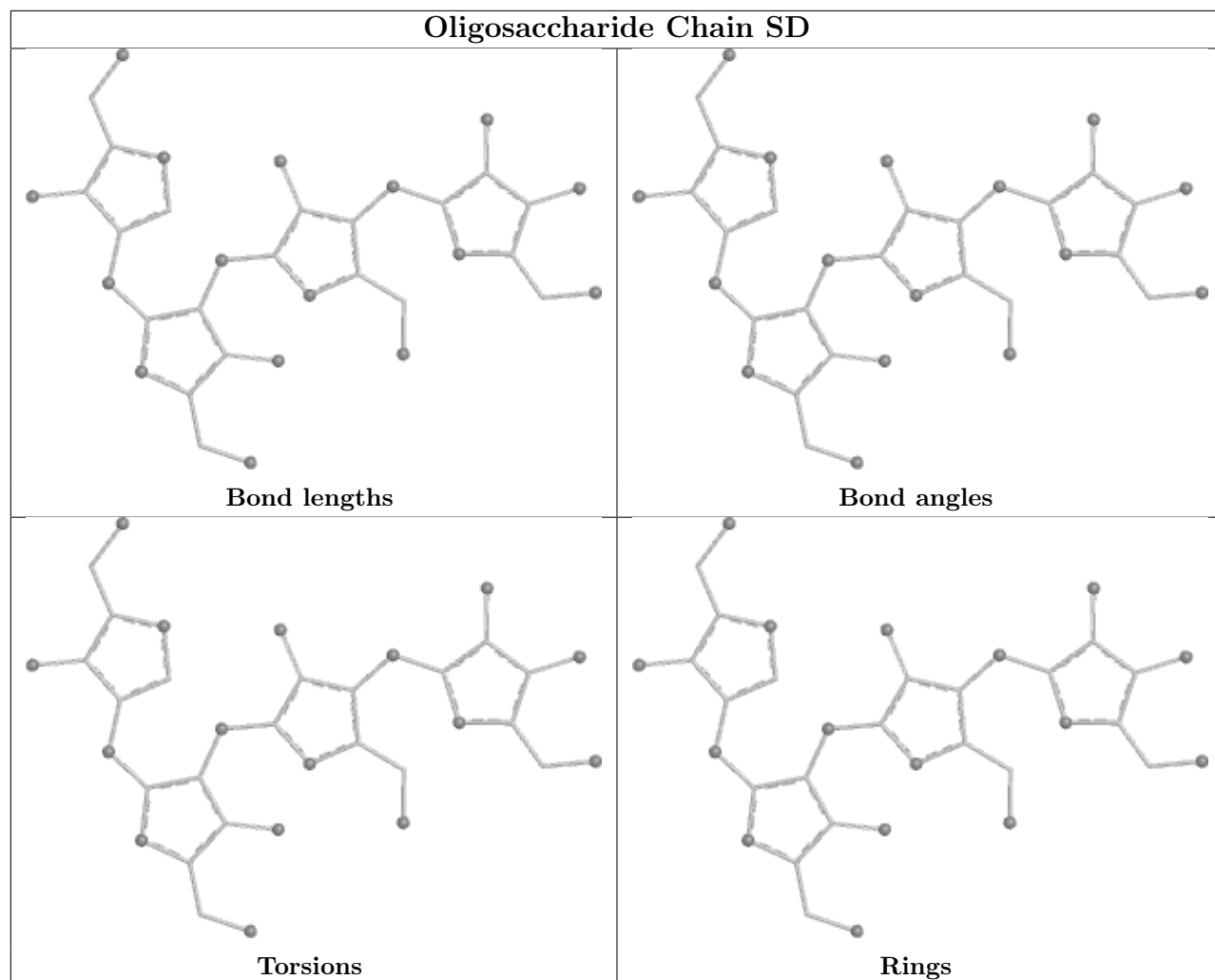
Oligosaccharide Chain LD

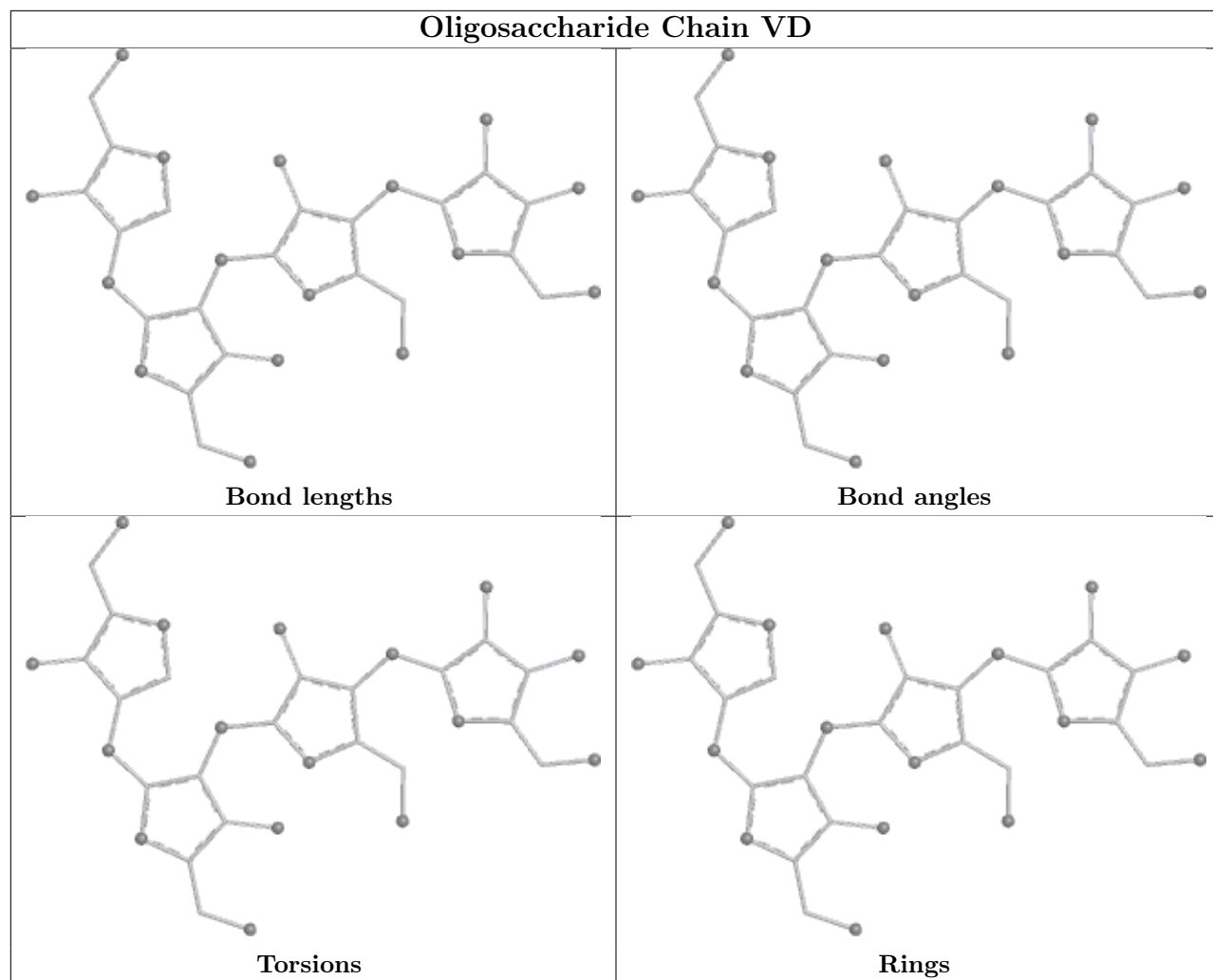


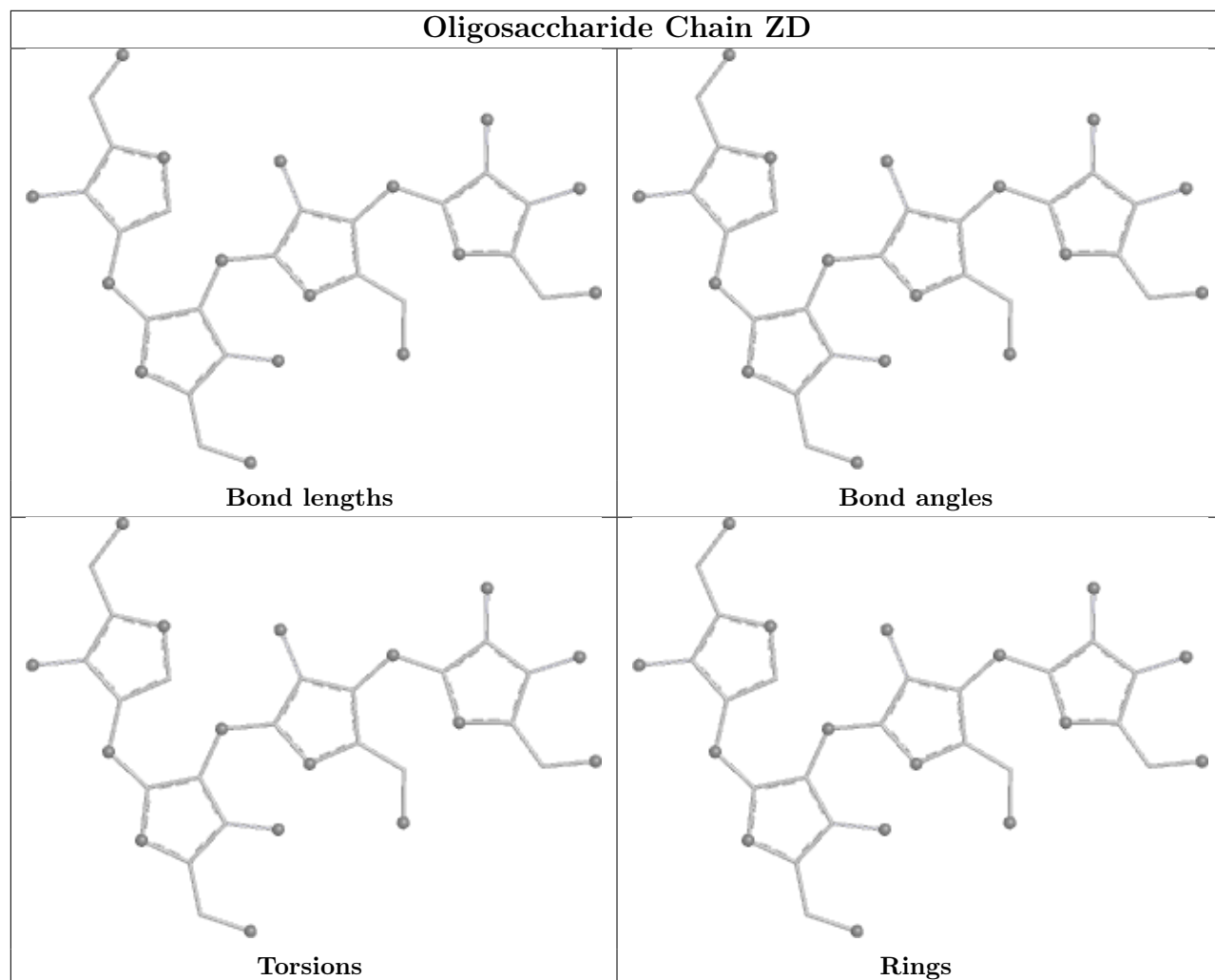
Oligosaccharide Chain OD

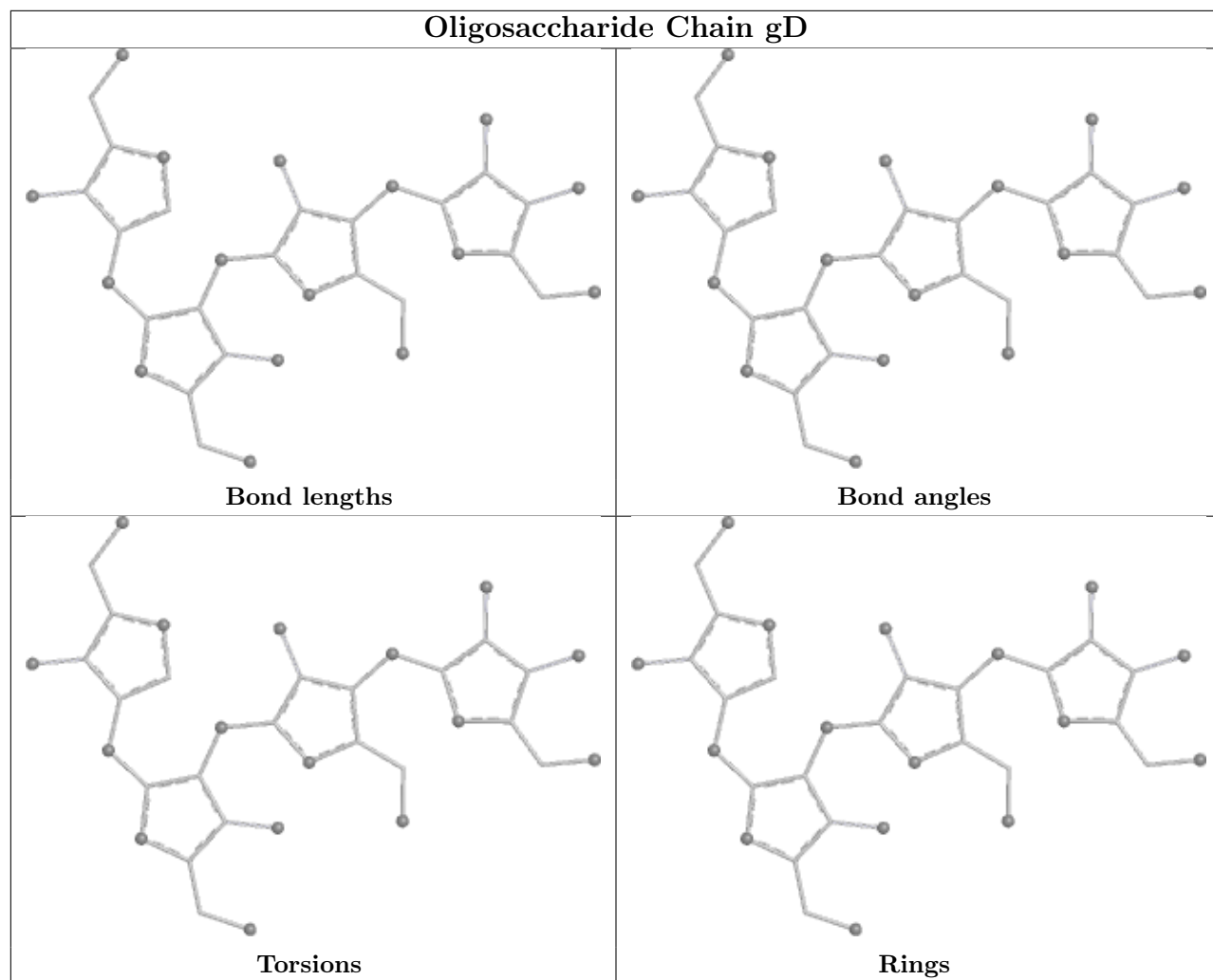


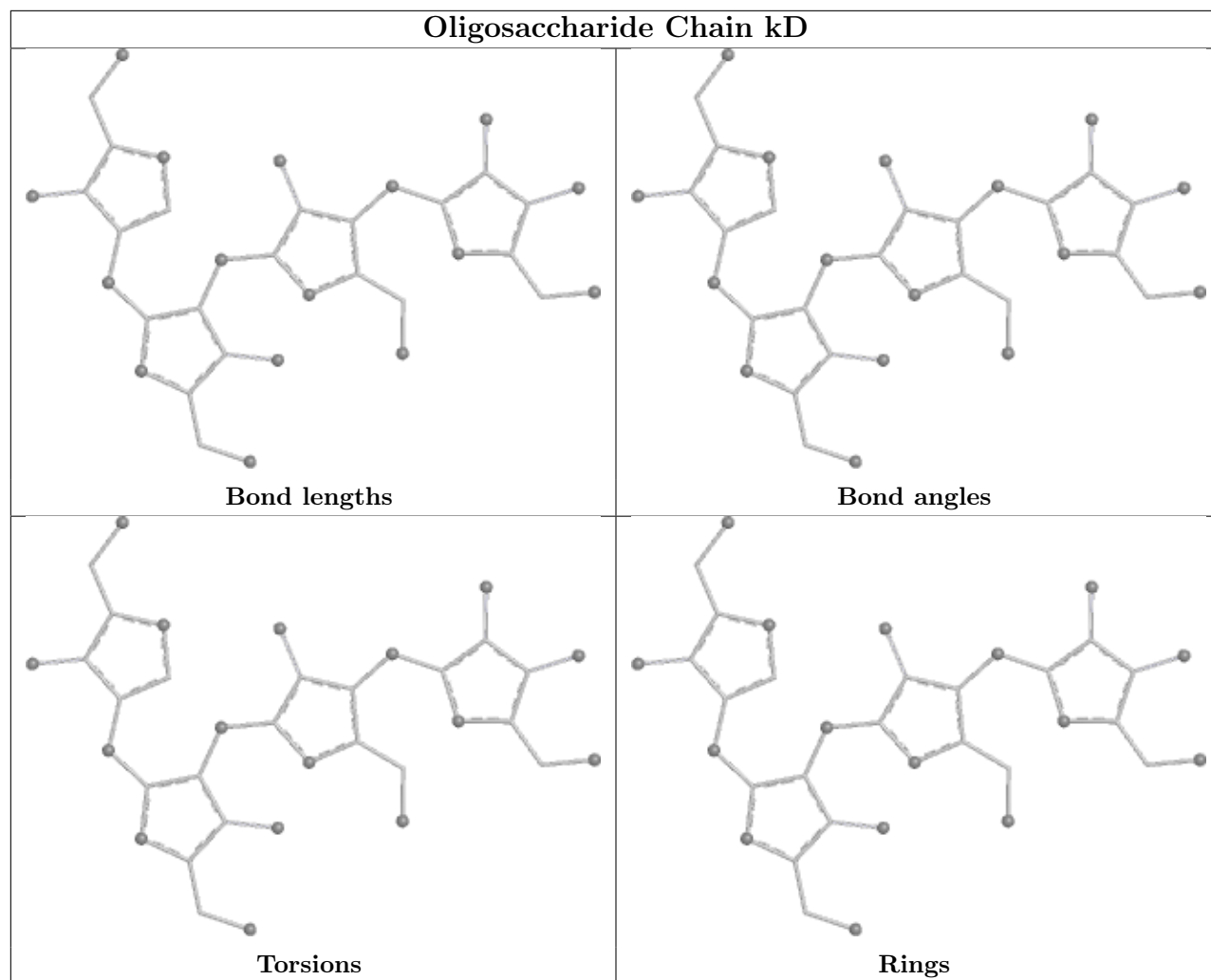
Oligosaccharide Chain RD

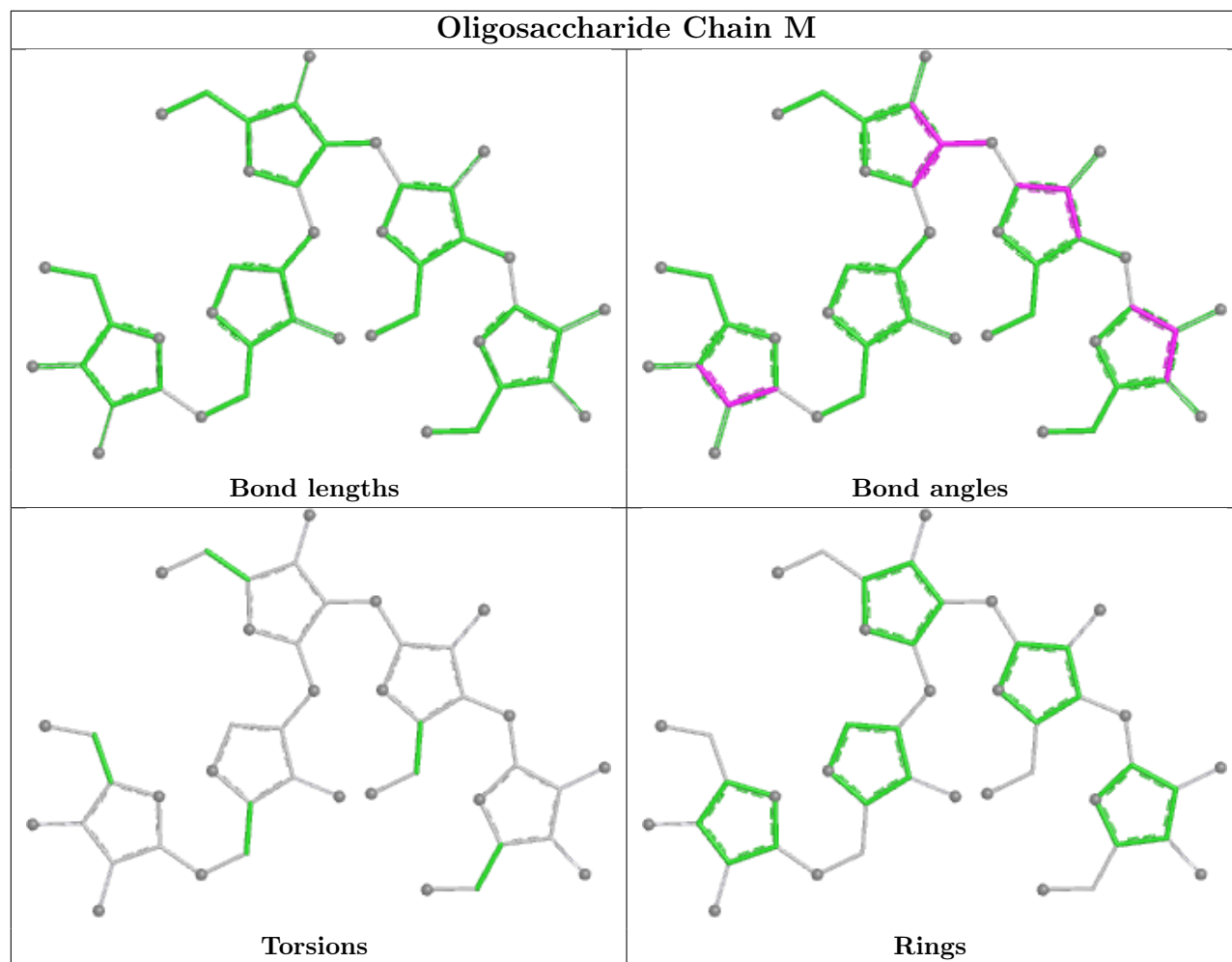
Oligosaccharide Chain SD

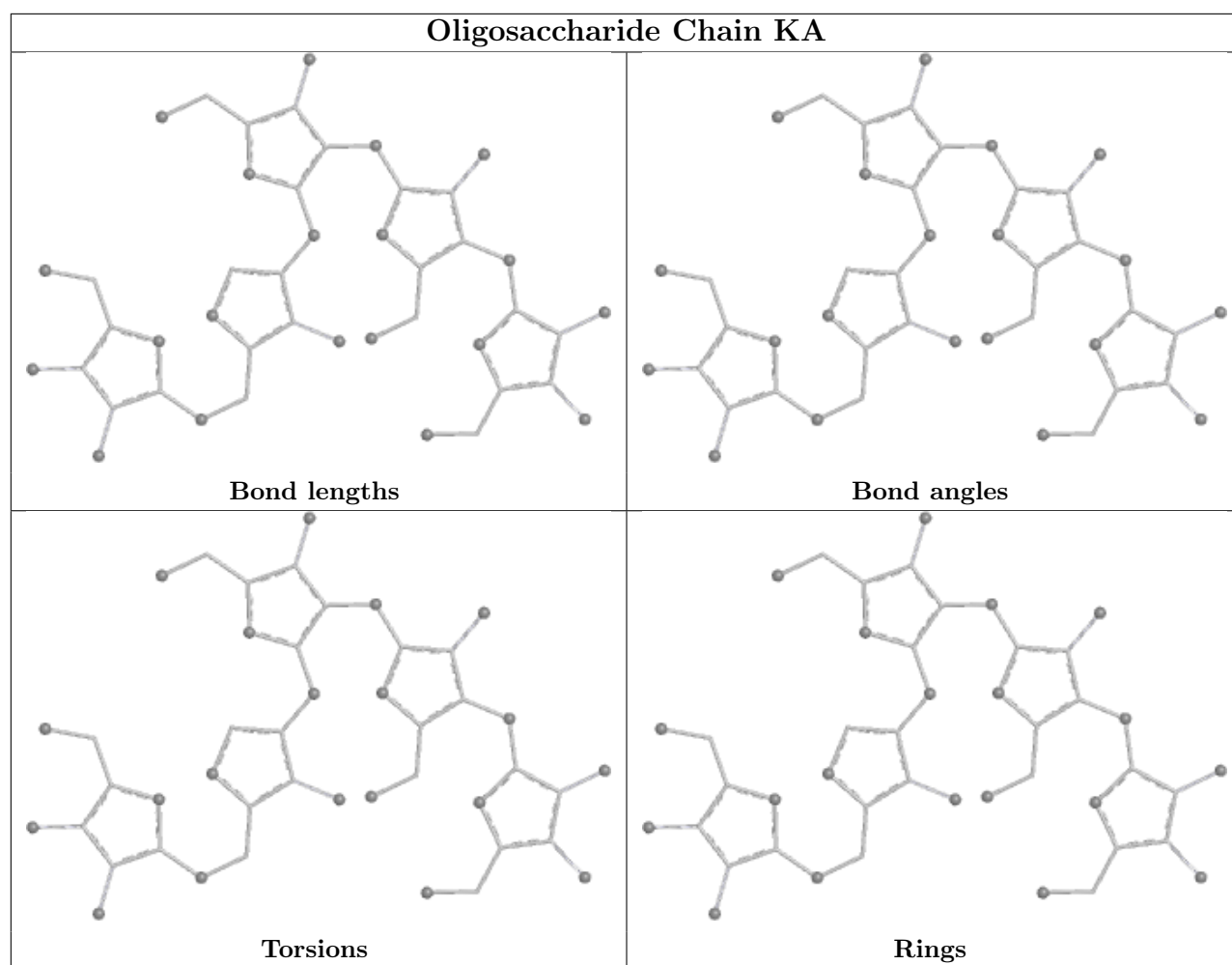
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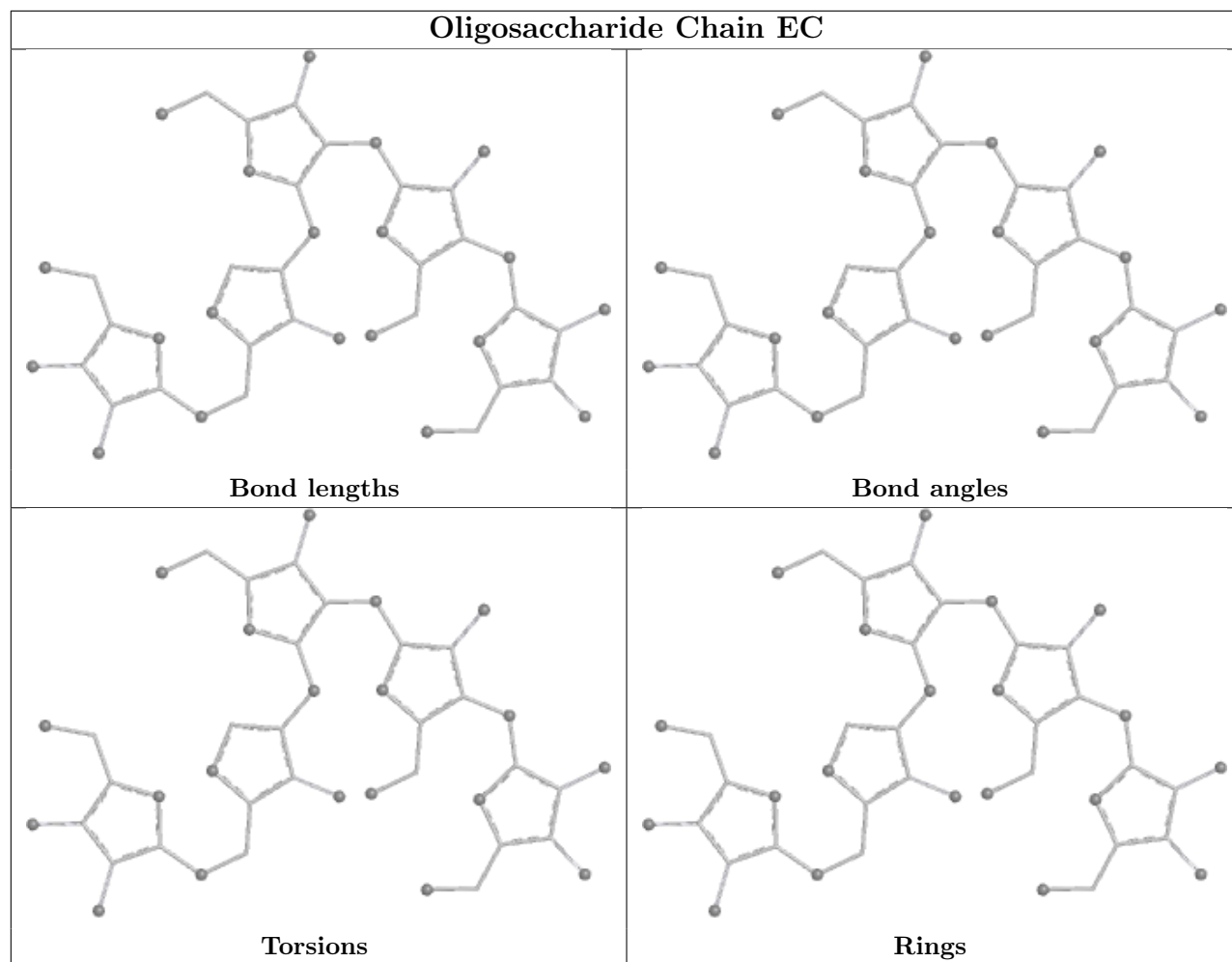
Oligosaccharide Chain ZD

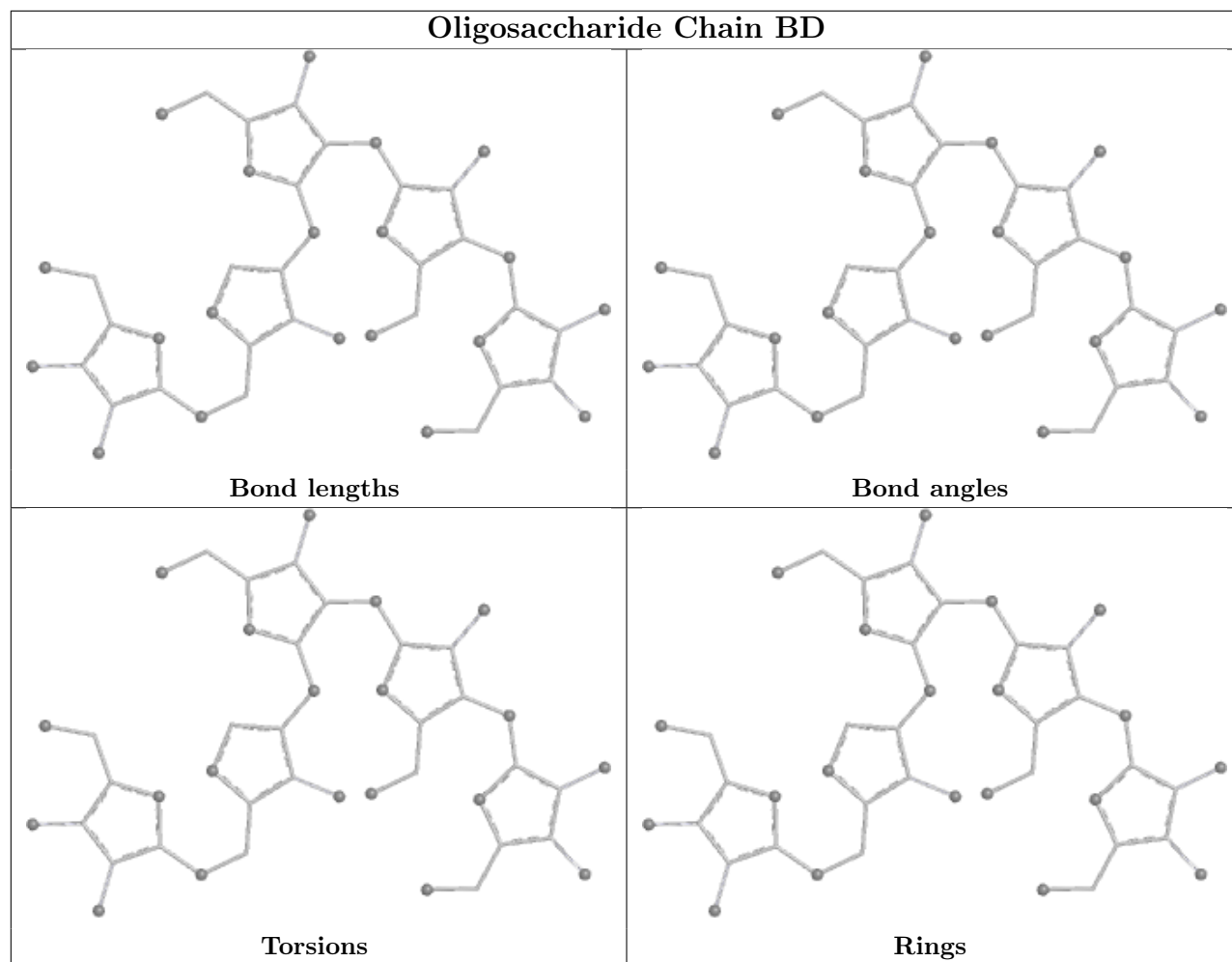


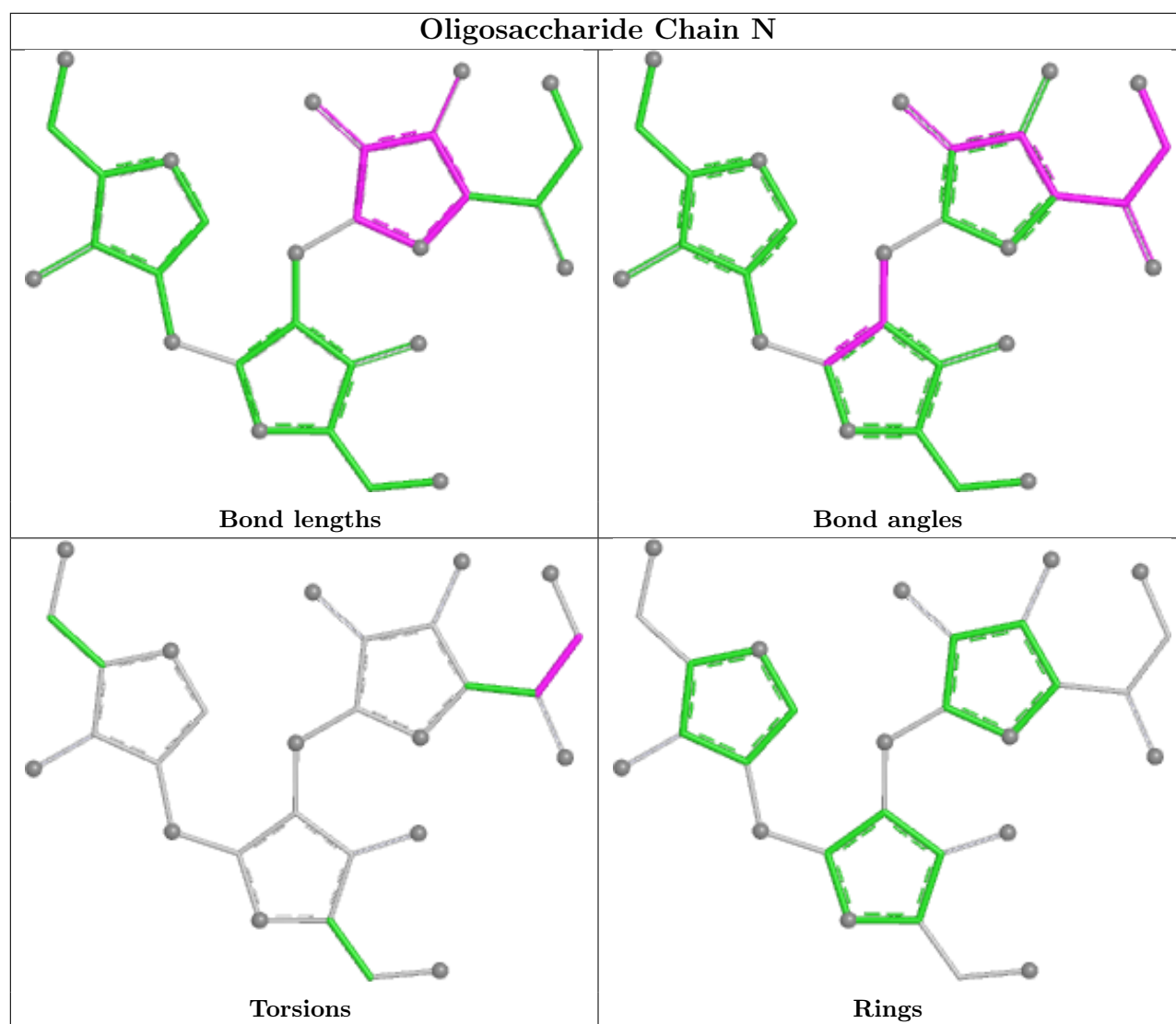


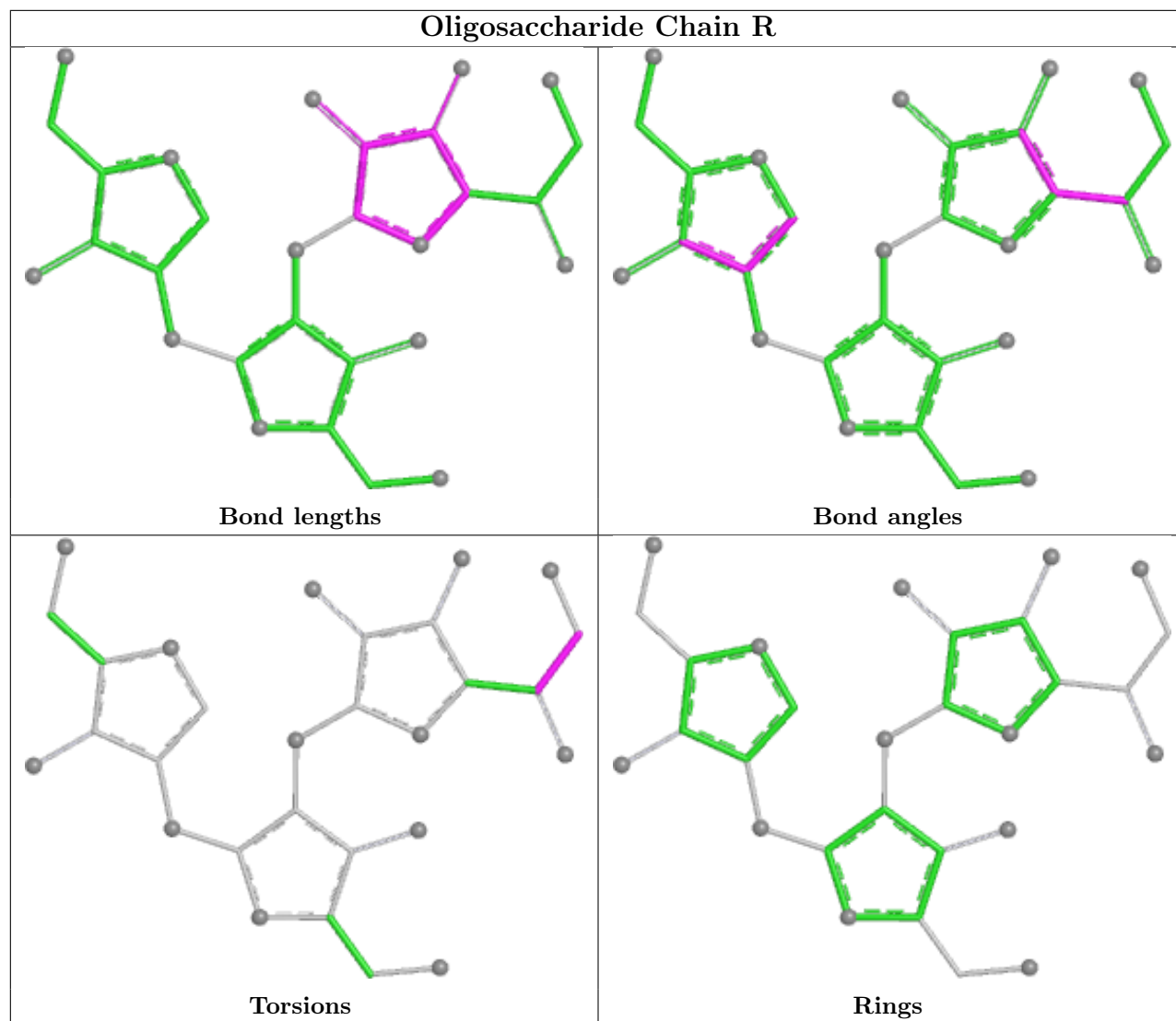


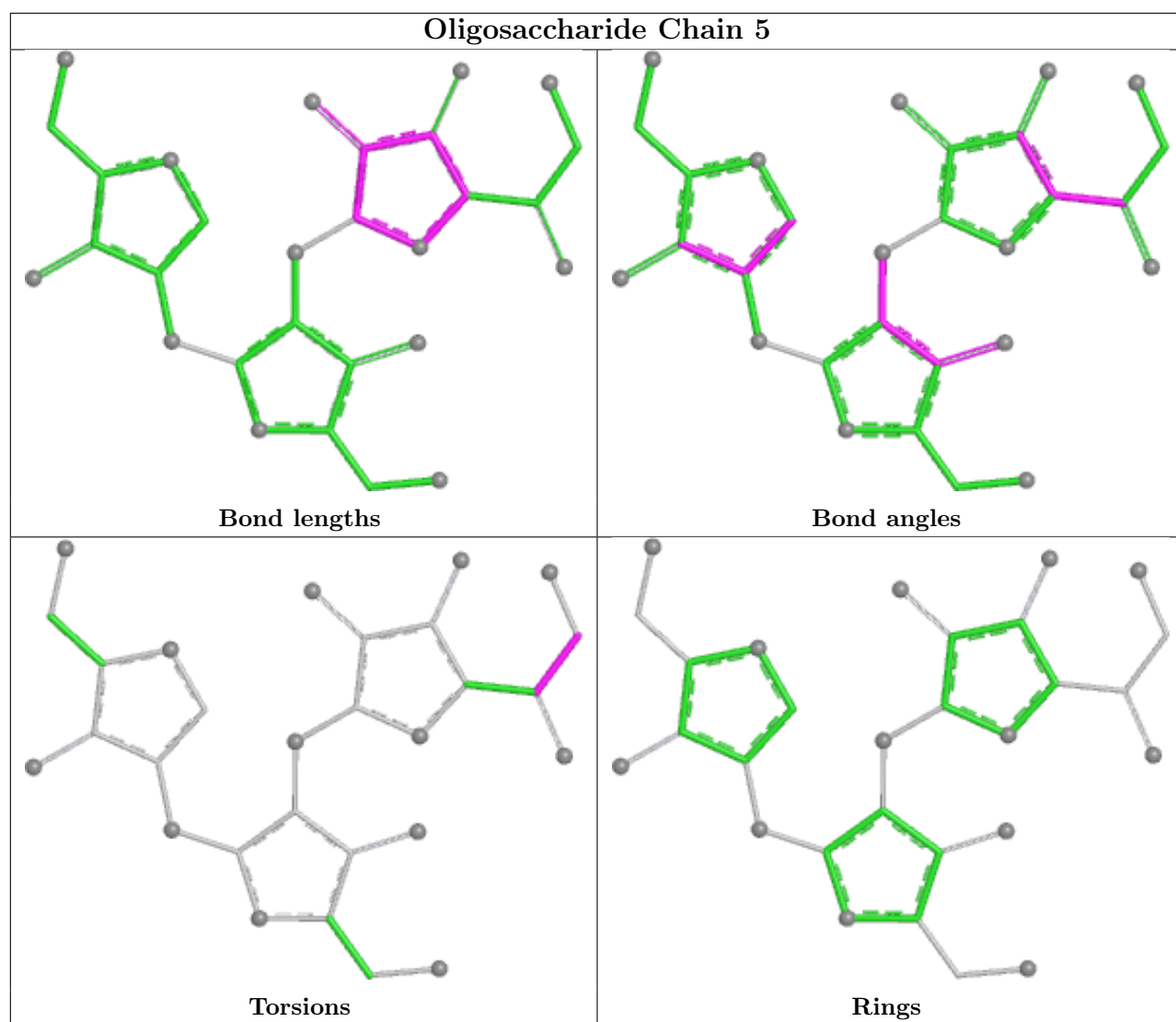




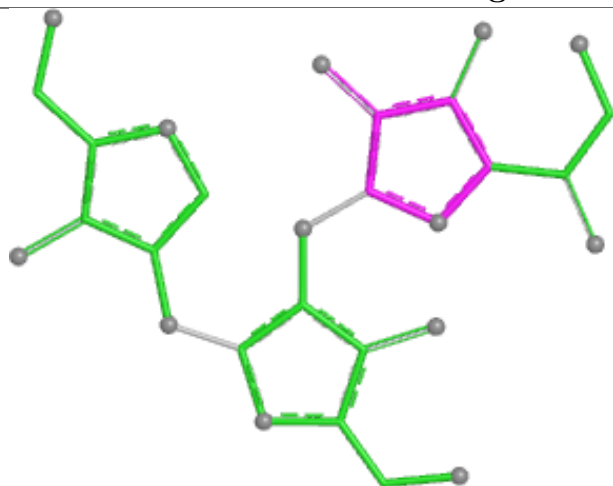




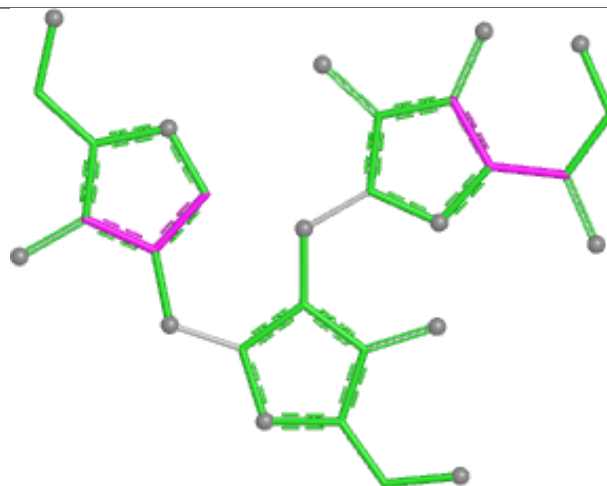




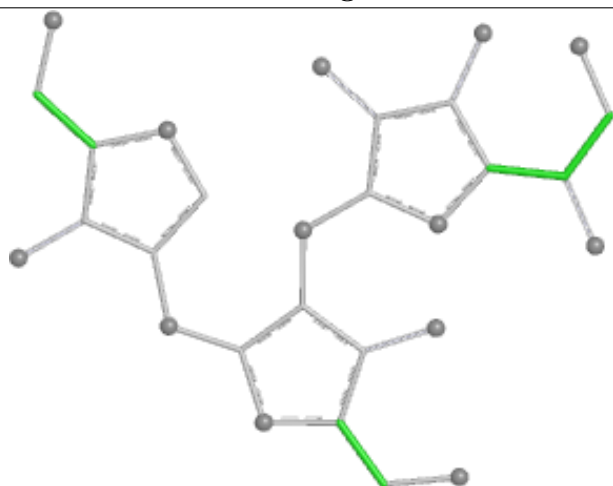
Oligosaccharide Chain 8



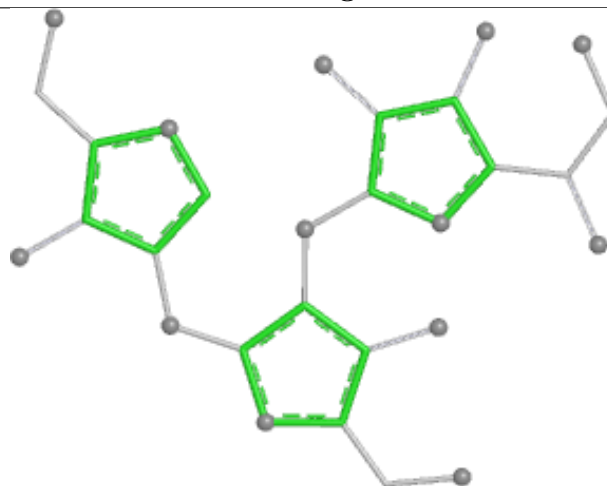
Bond lengths



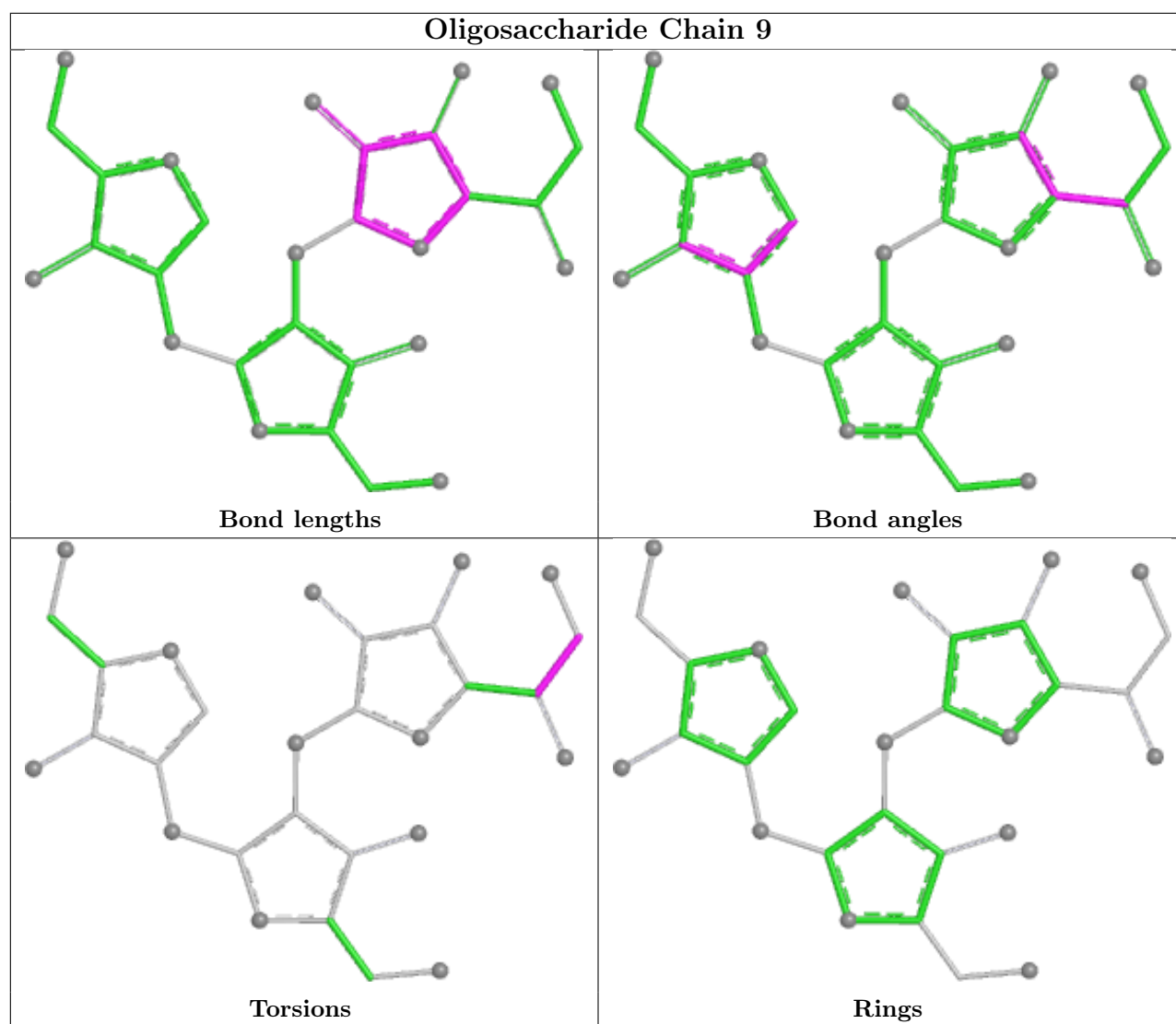
Bond angles

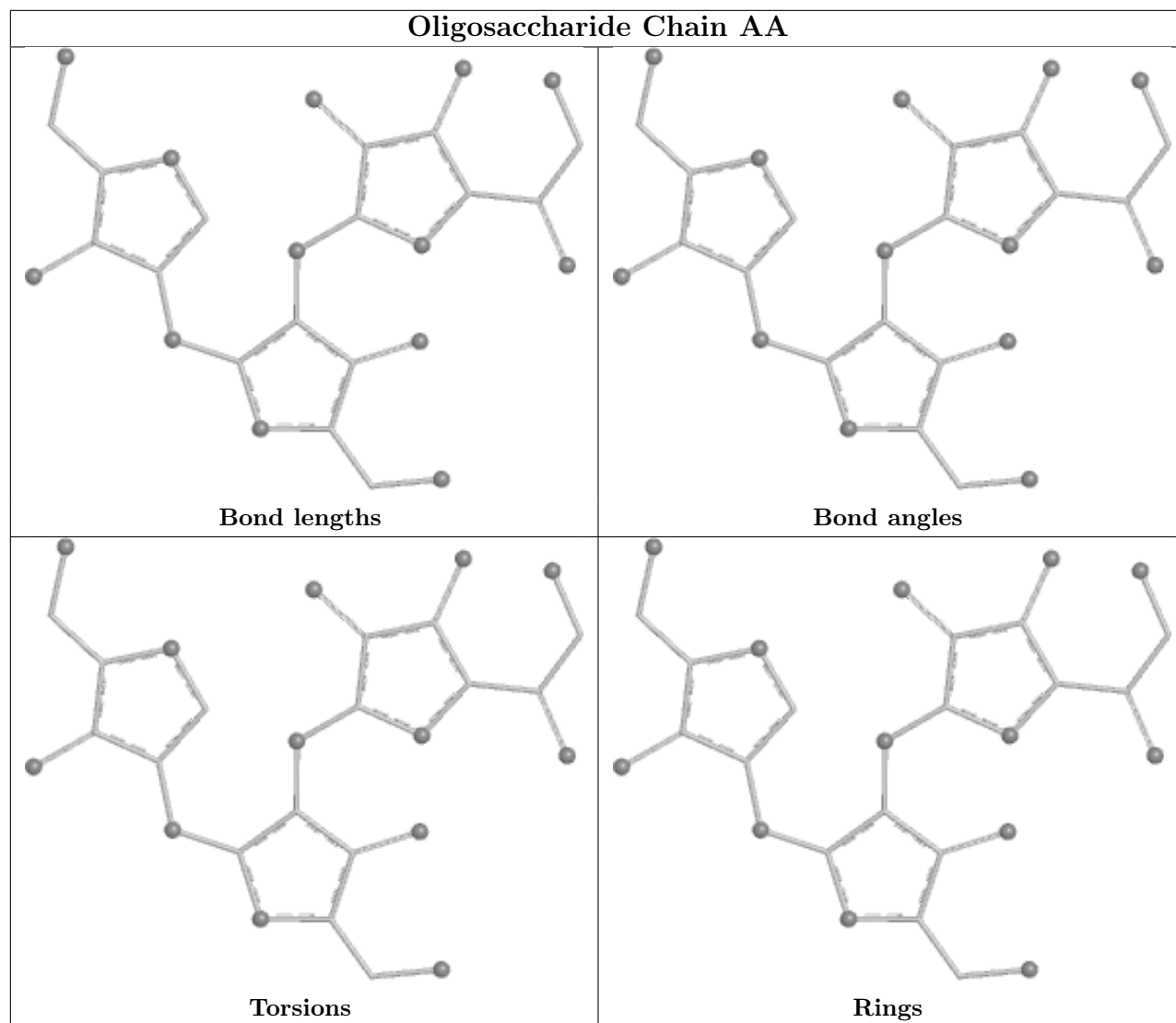


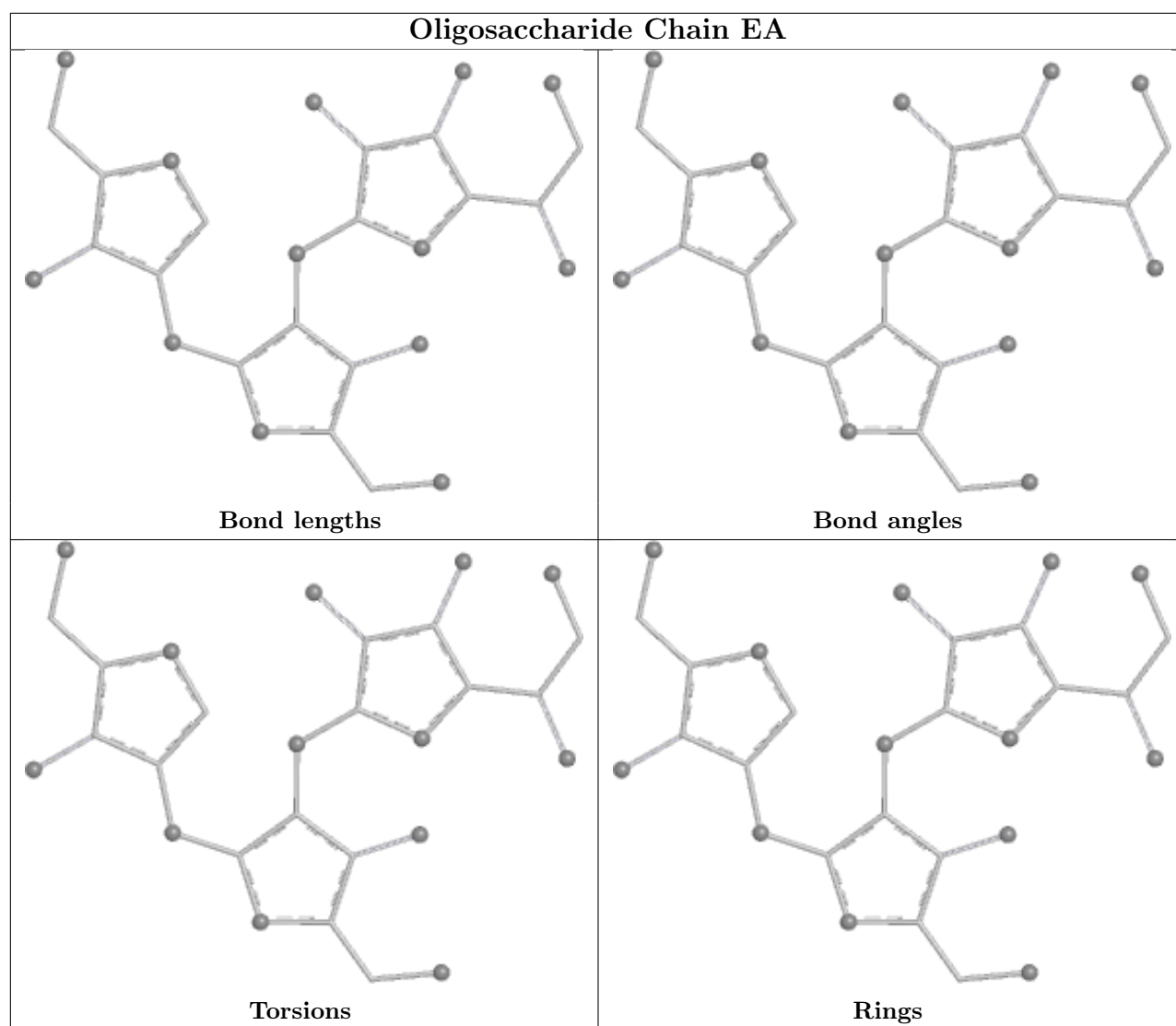
Torsions

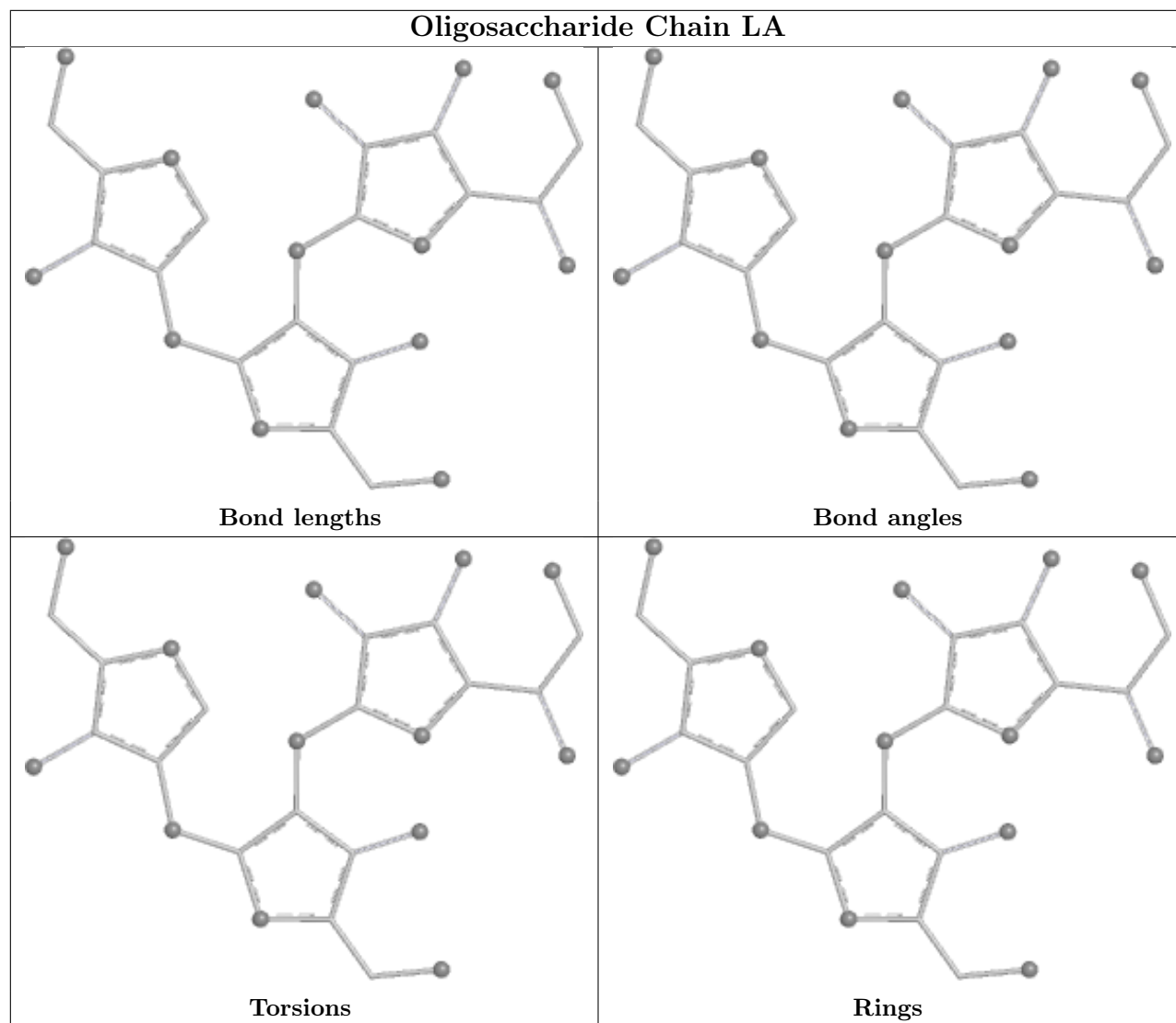


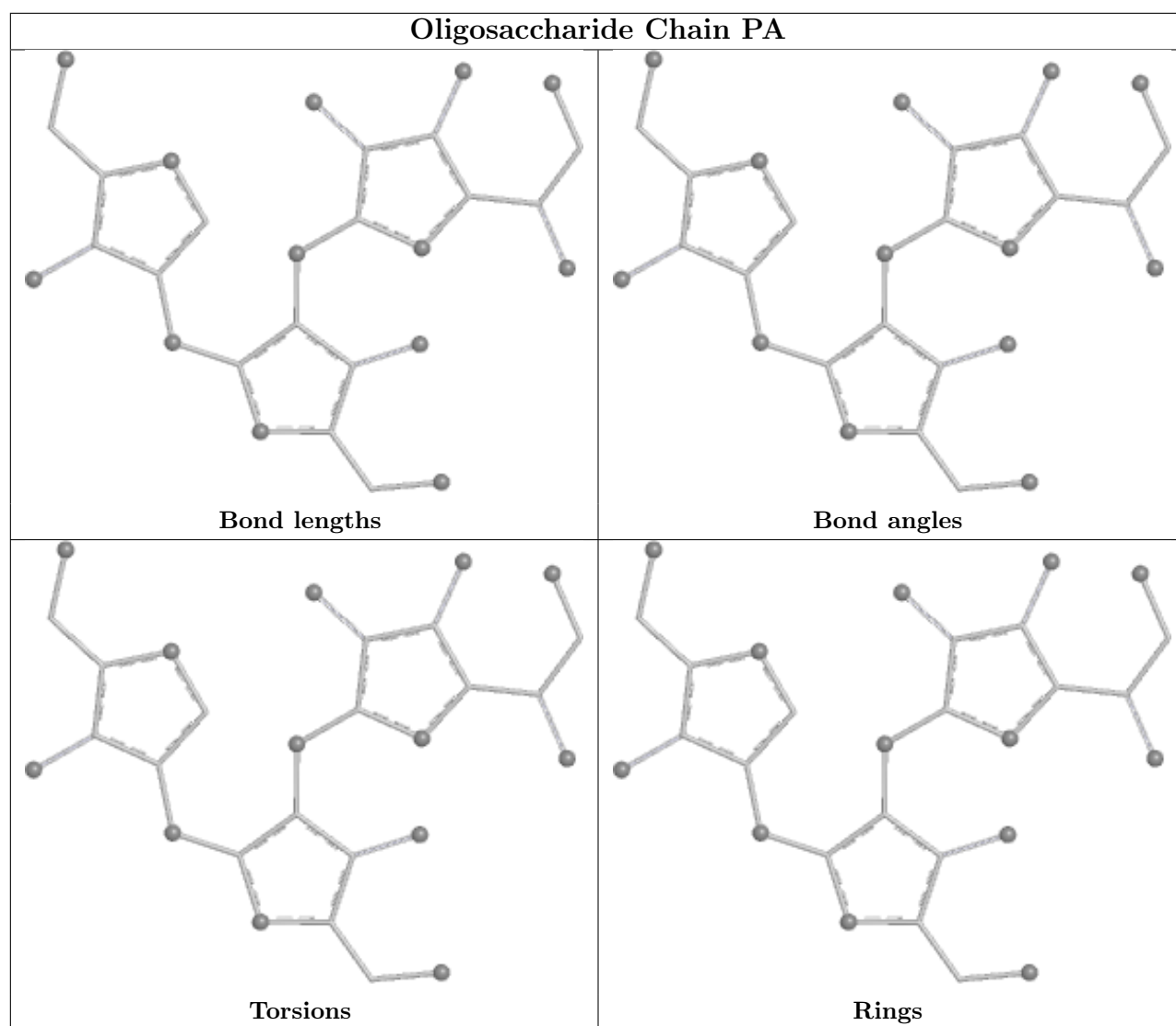
Rings

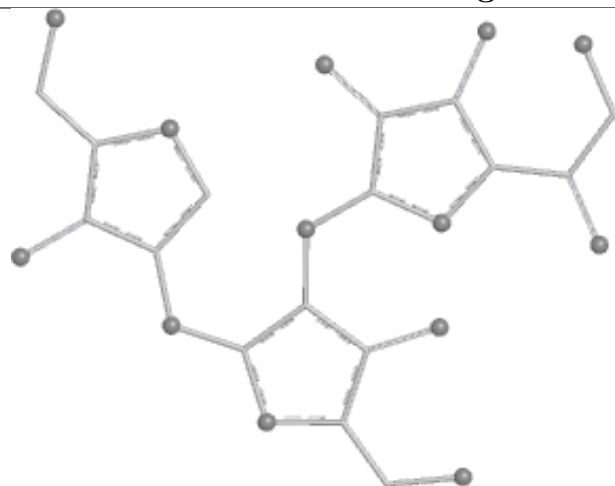
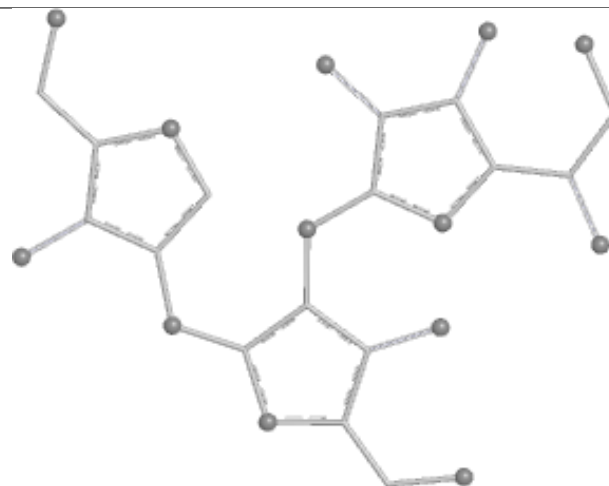
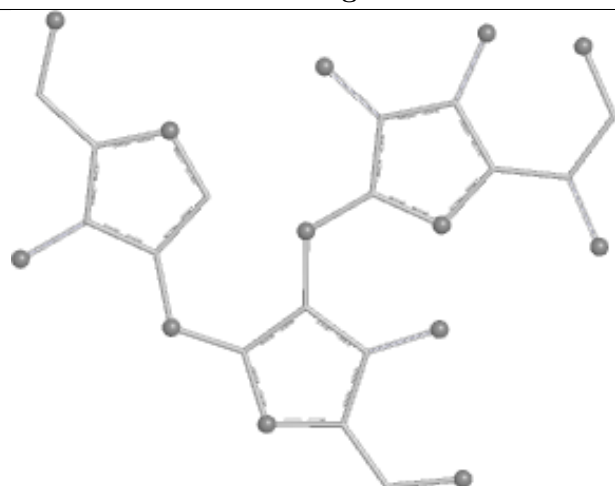
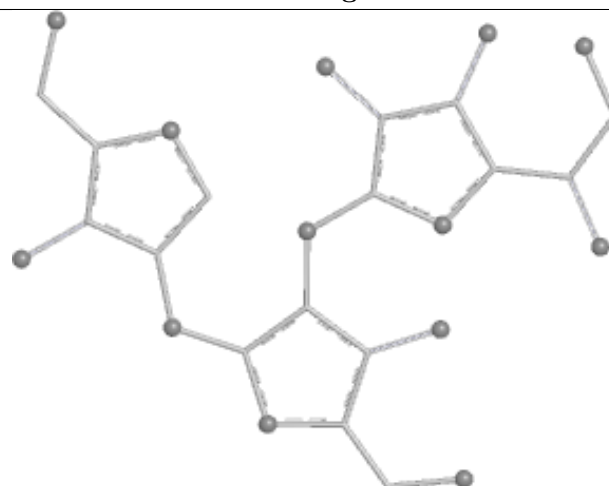




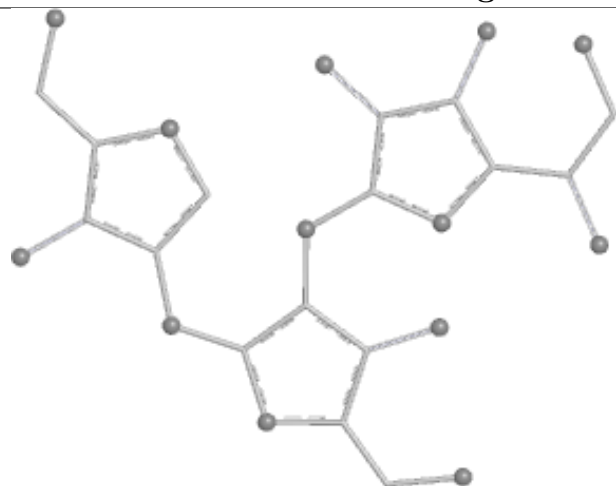




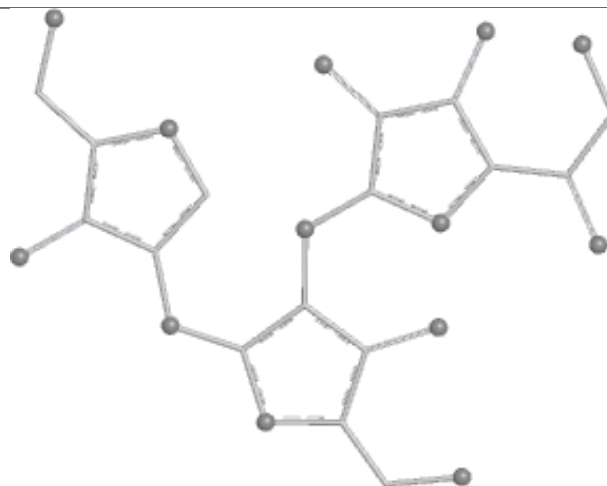


Oligosaccharide Chain 3A**Bond lengths****Bond angles****Torsions****Rings**

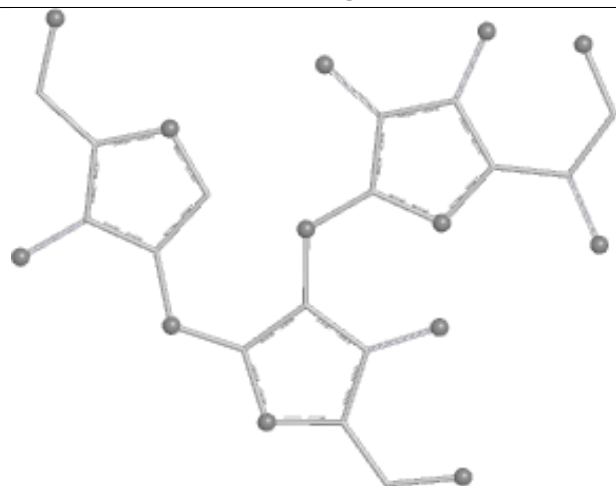
Oligosaccharide Chain 6A



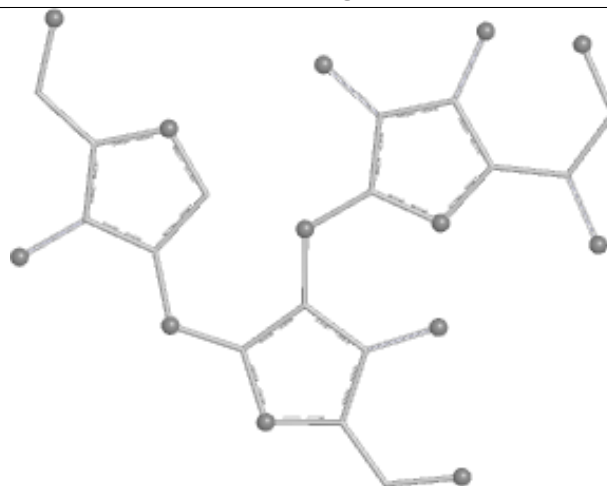
Bond lengths



Bond angles

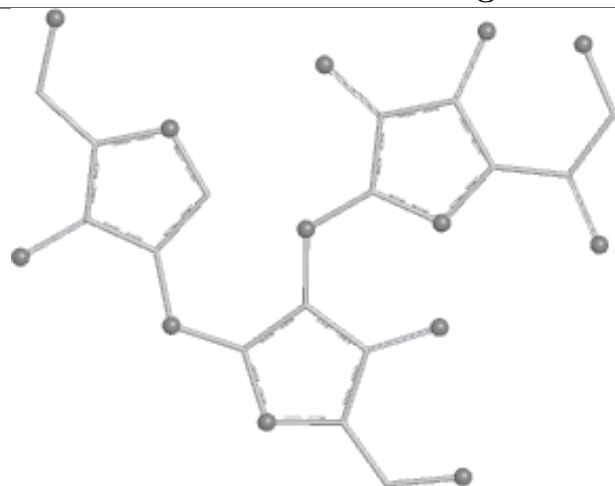


Torsions

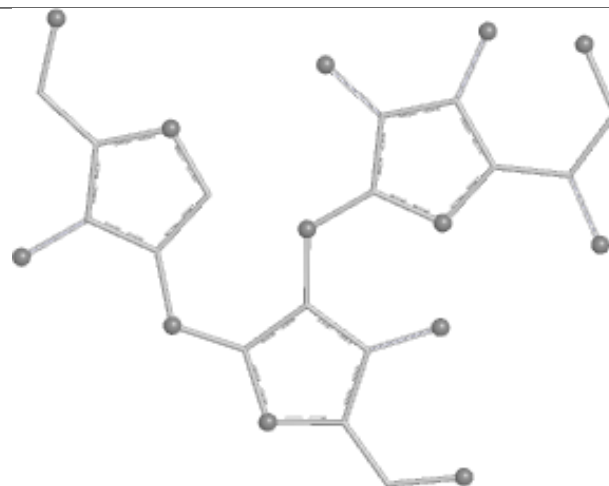


Rings

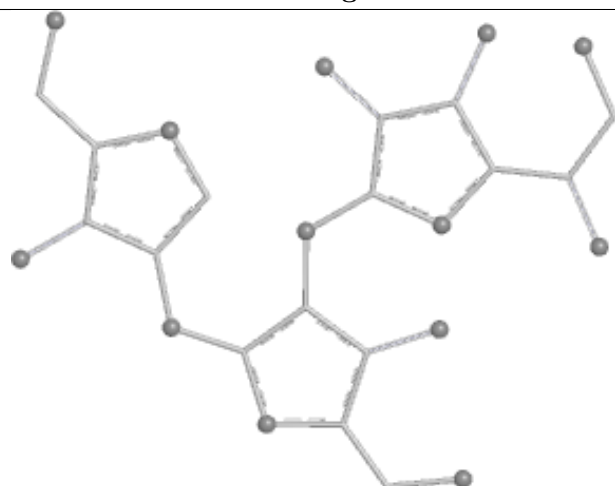
Oligosaccharide Chain 7A



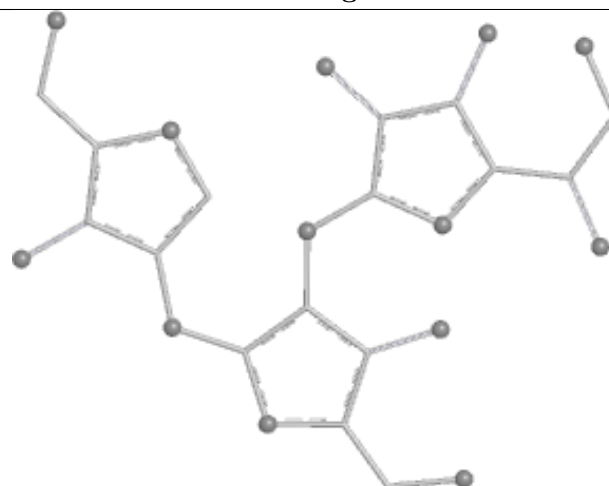
Bond lengths



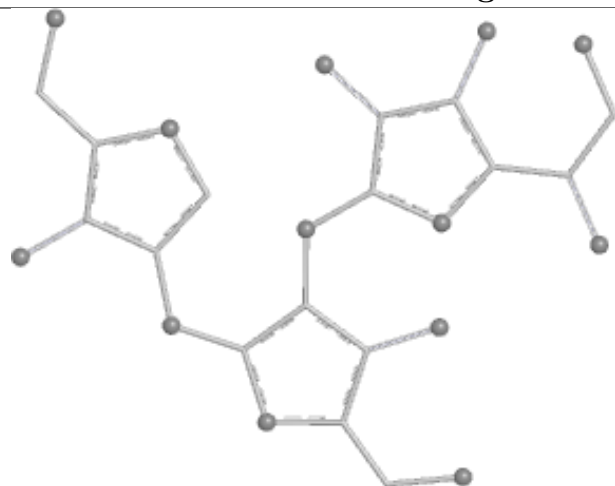
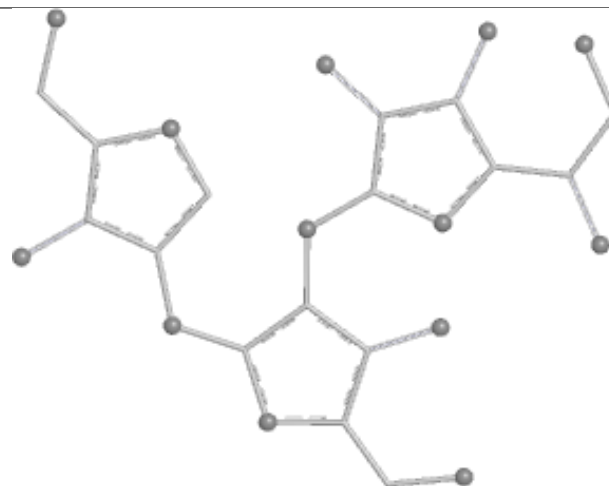
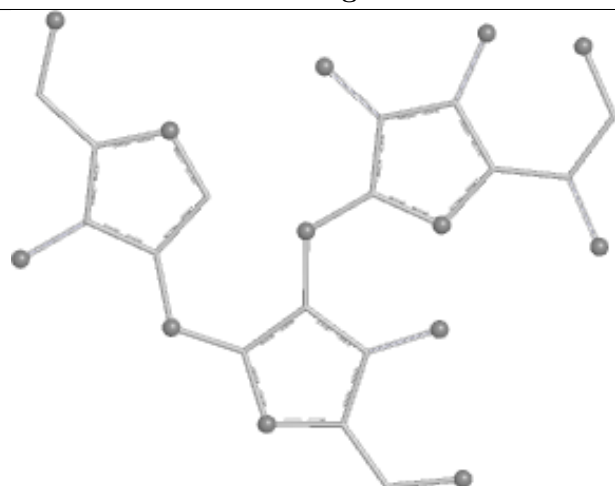
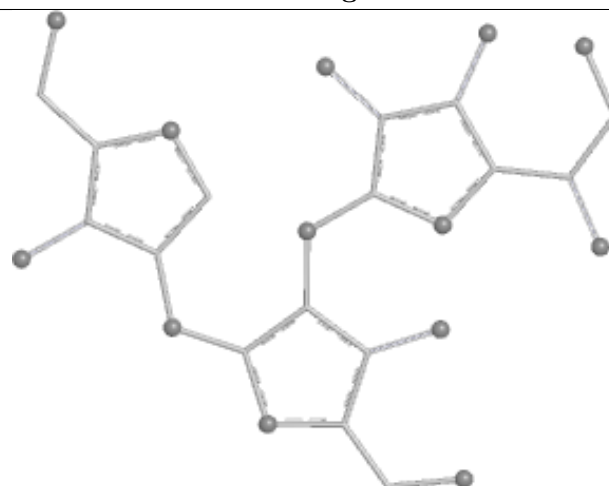
Bond angles

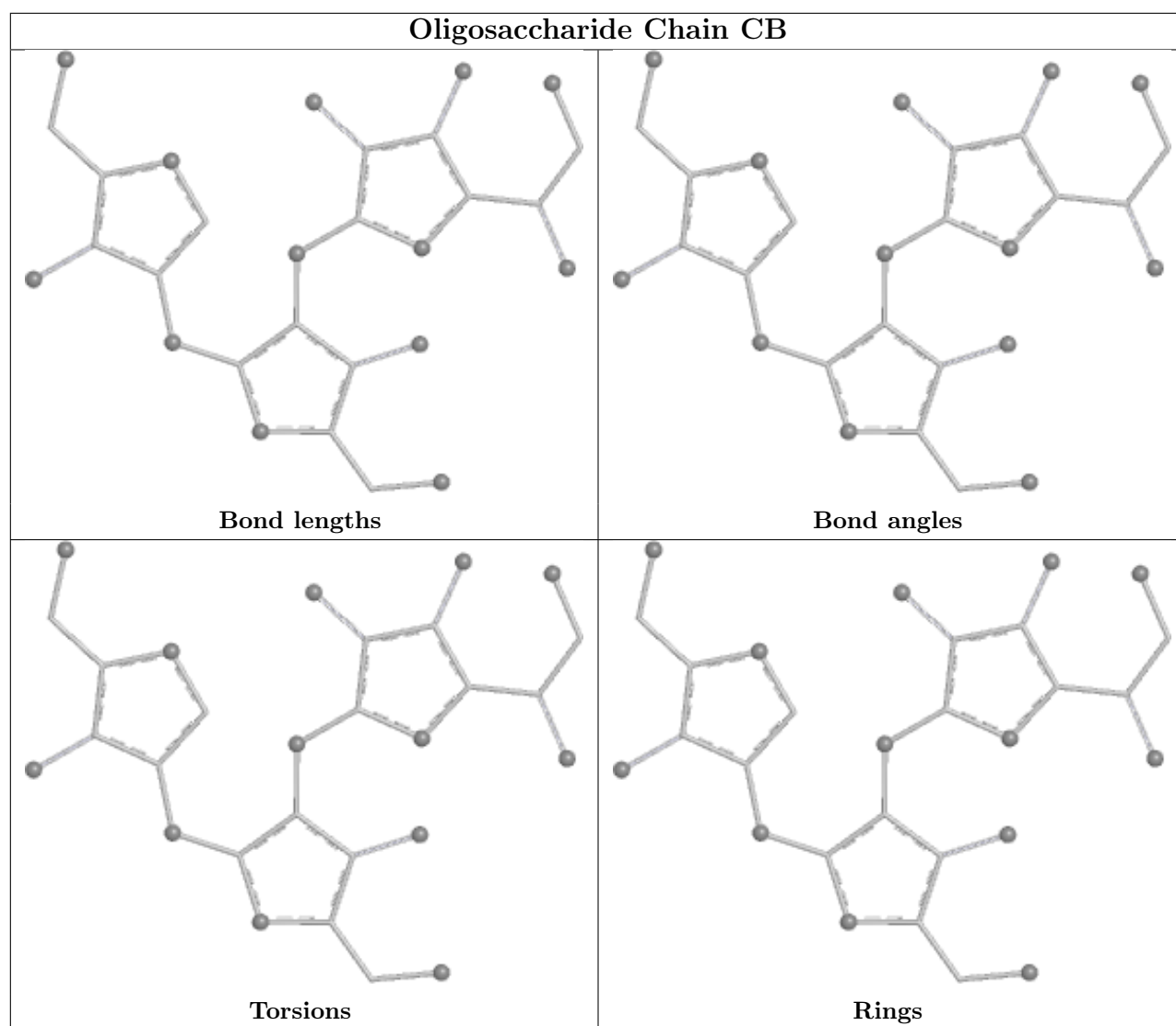


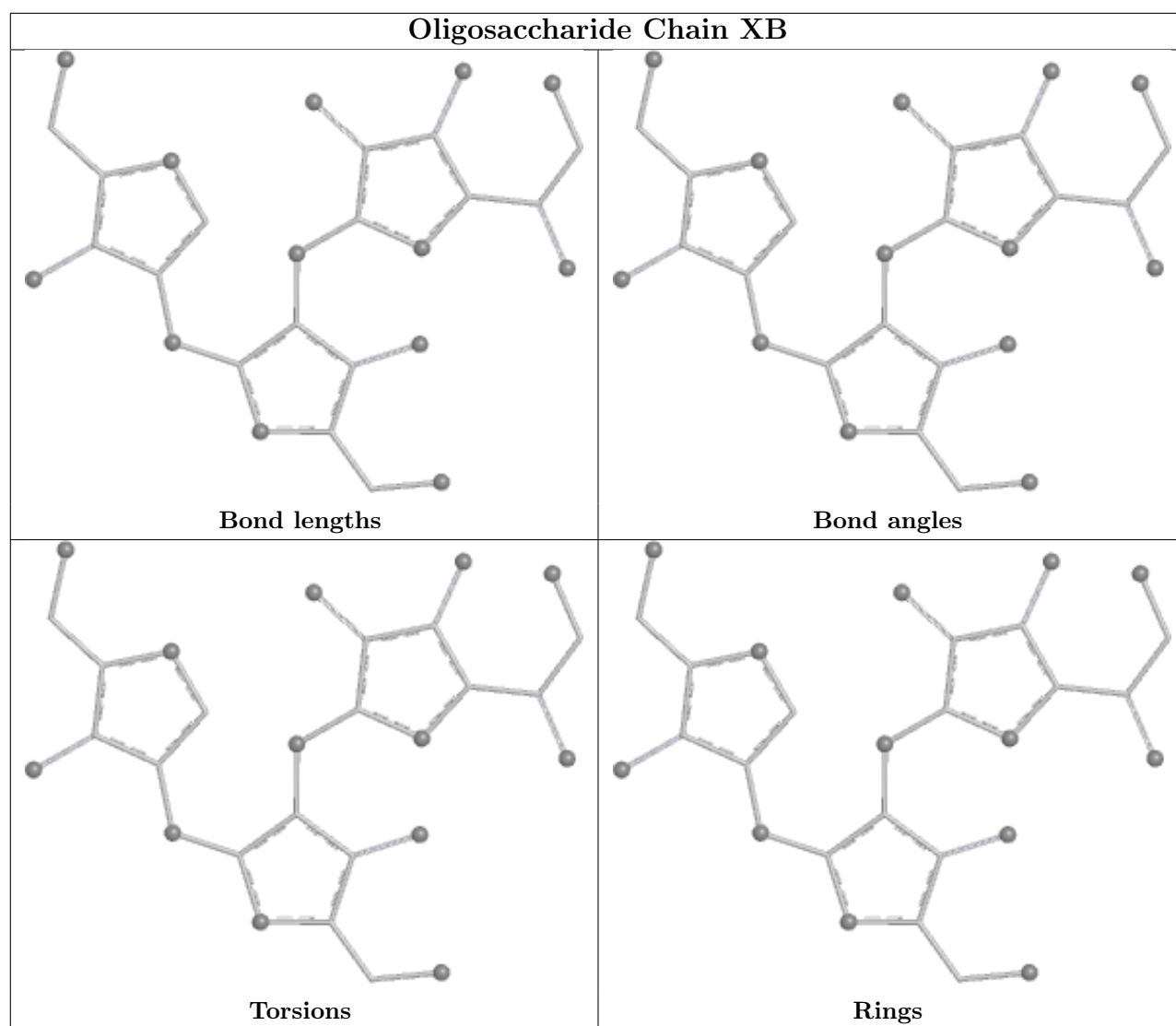
Torsions

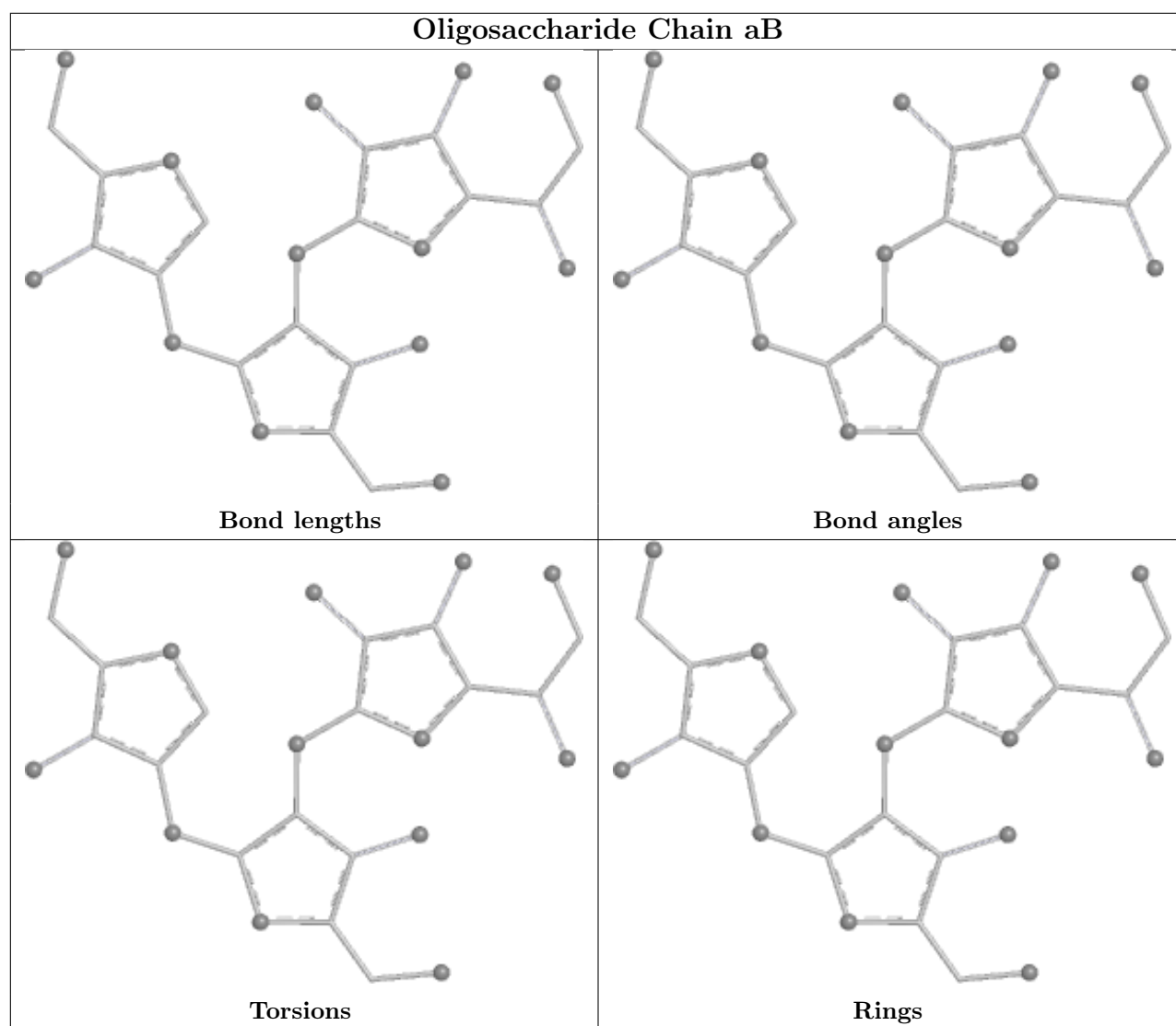


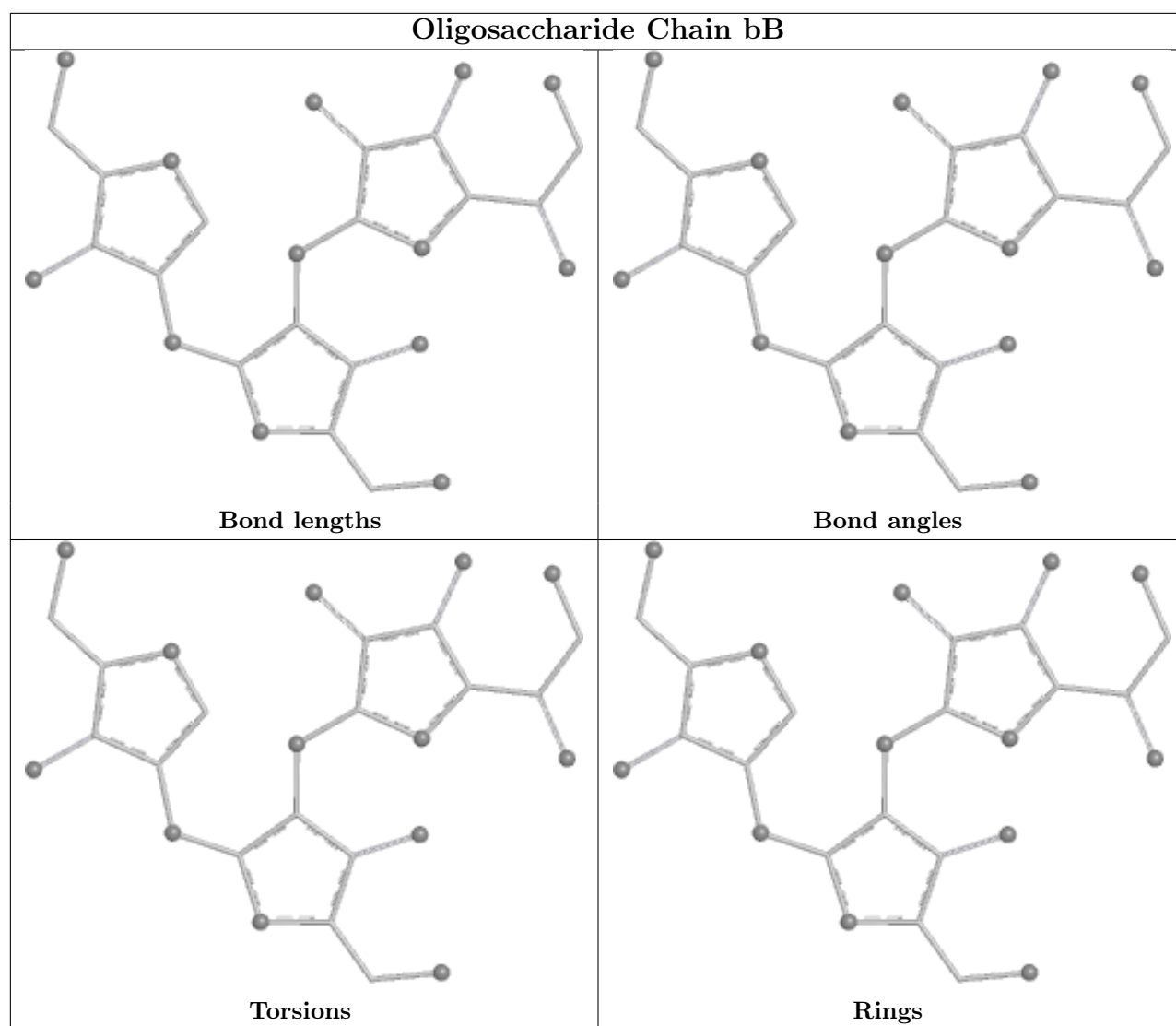
Rings

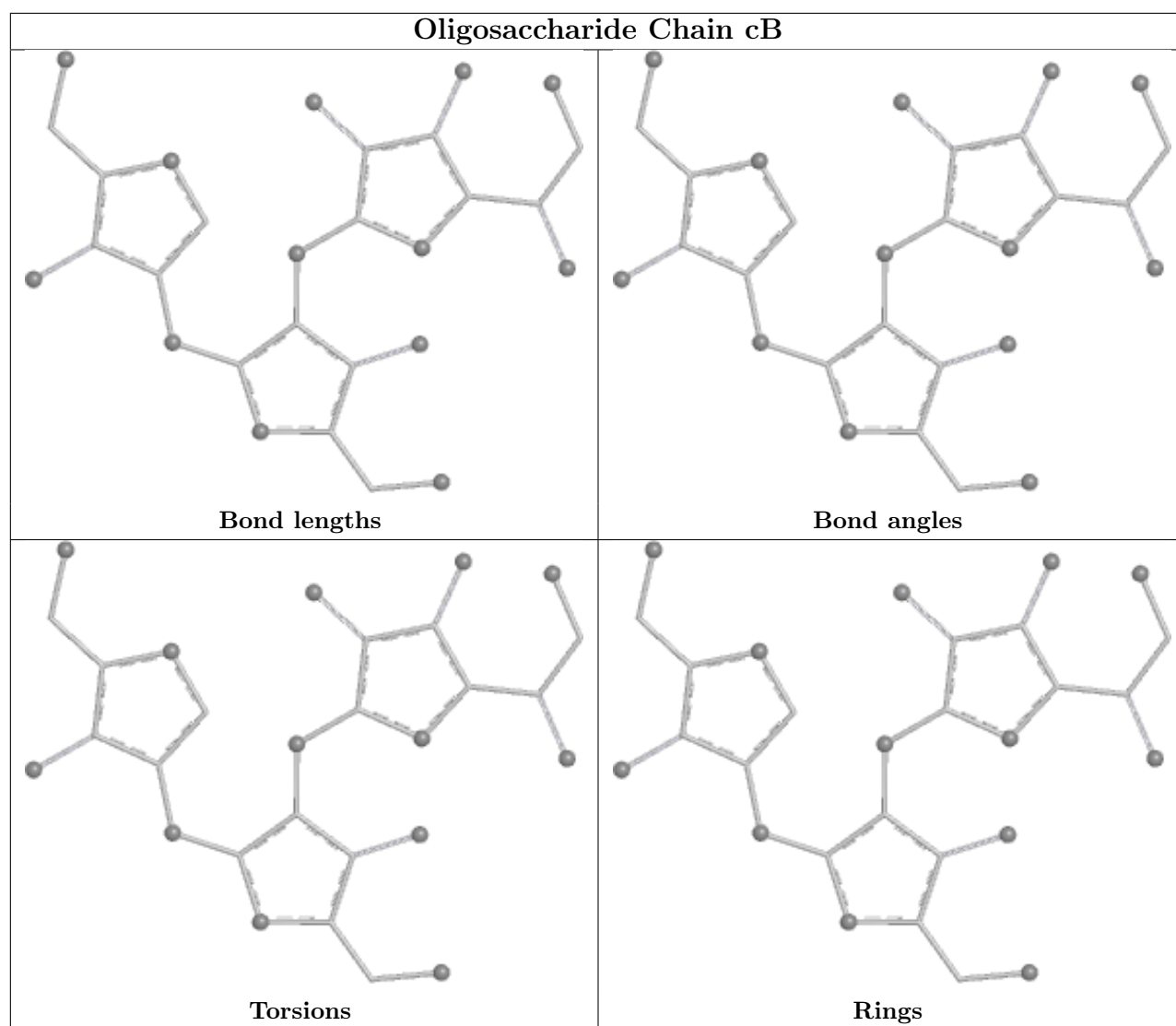
Oligosaccharide Chain 8A**Bond lengths****Bond angles****Torsions****Rings**

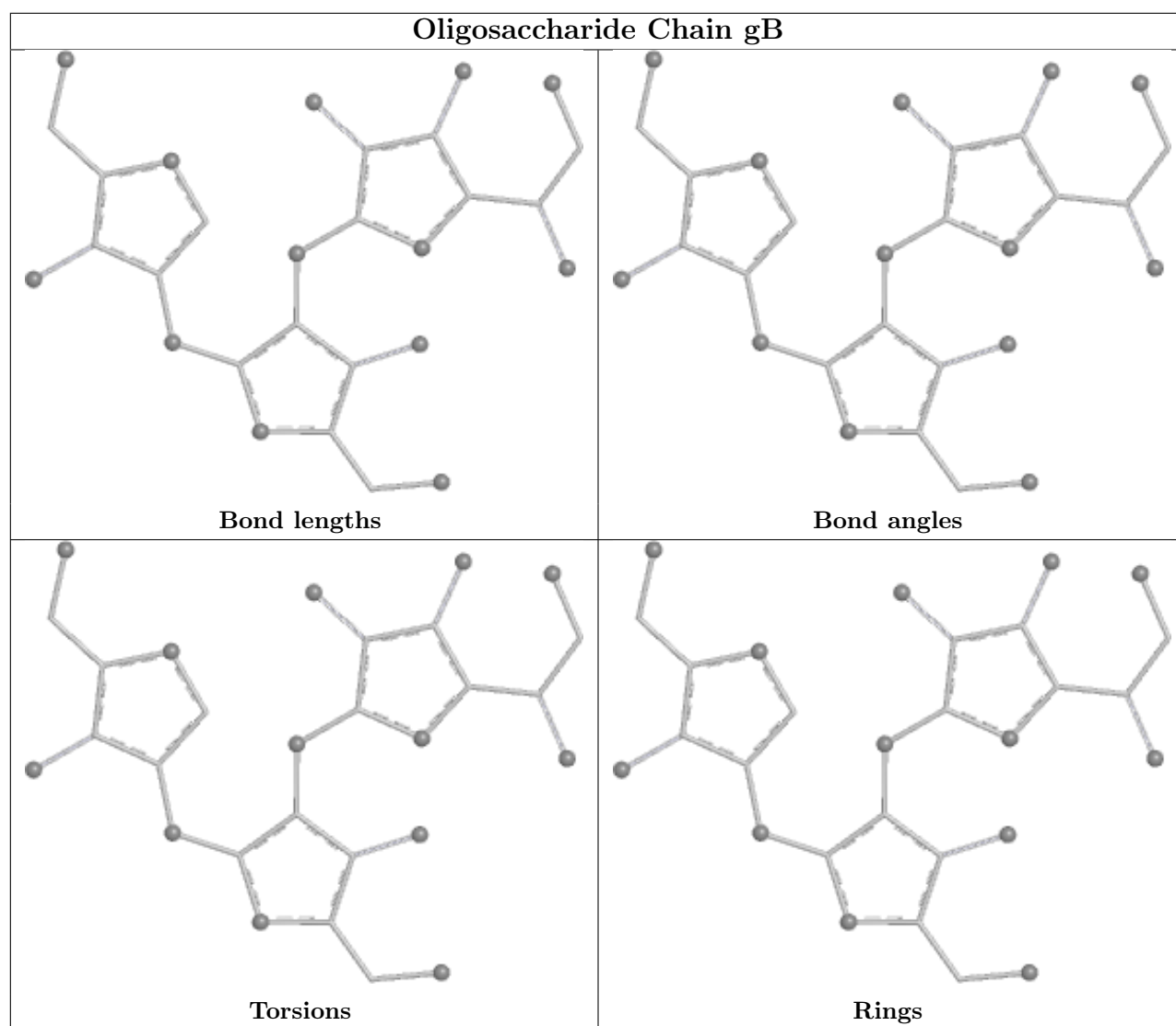


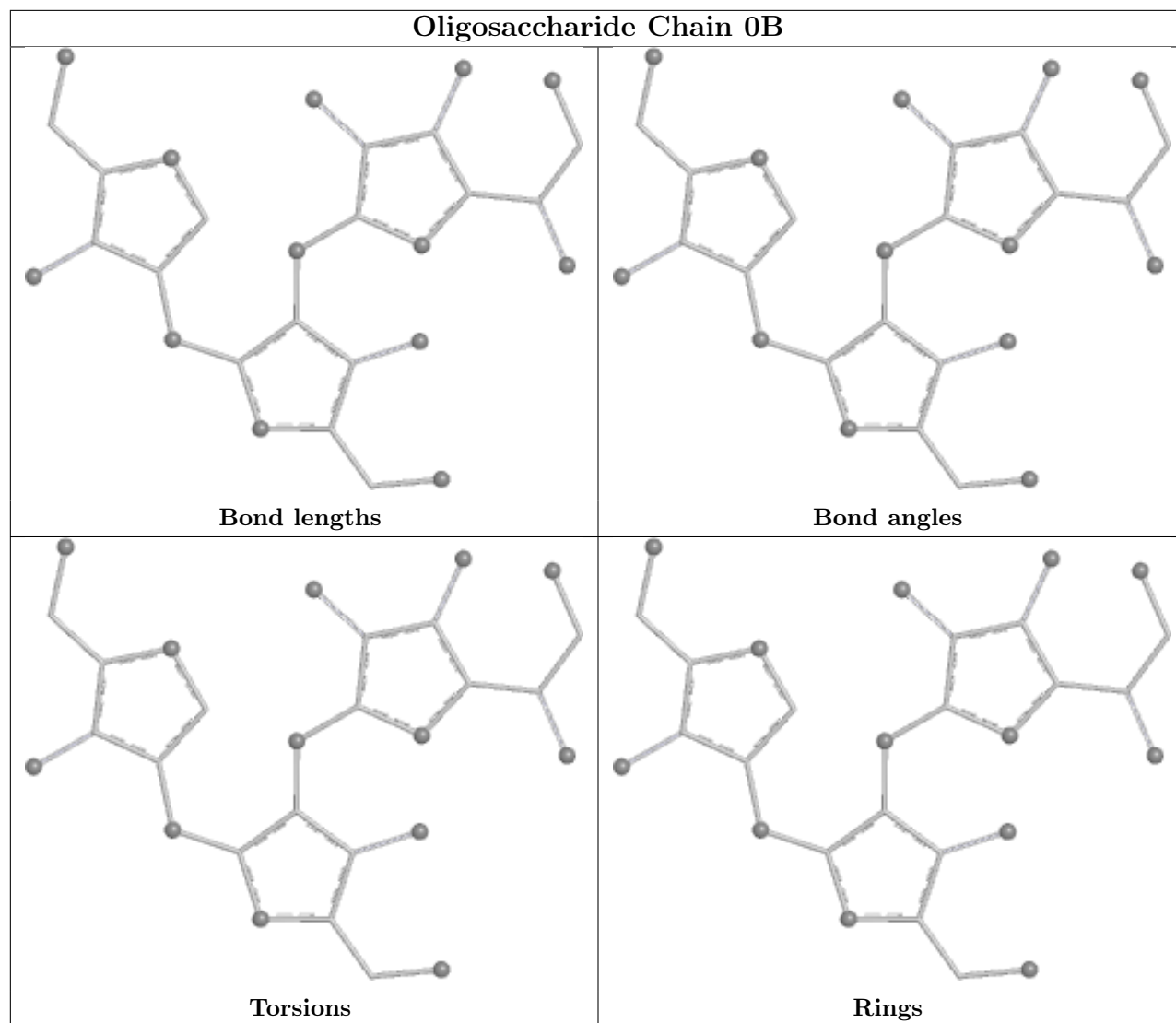


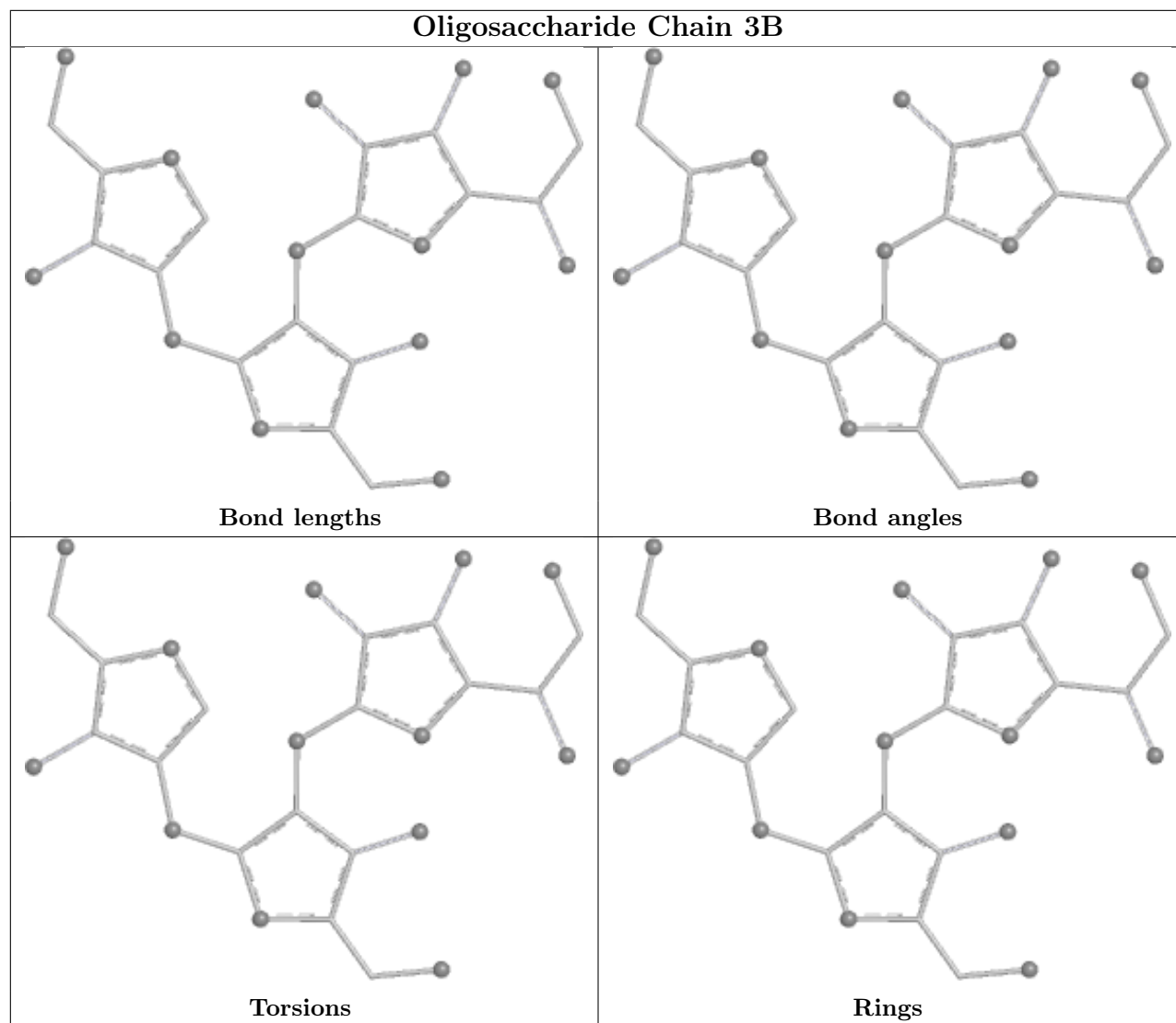




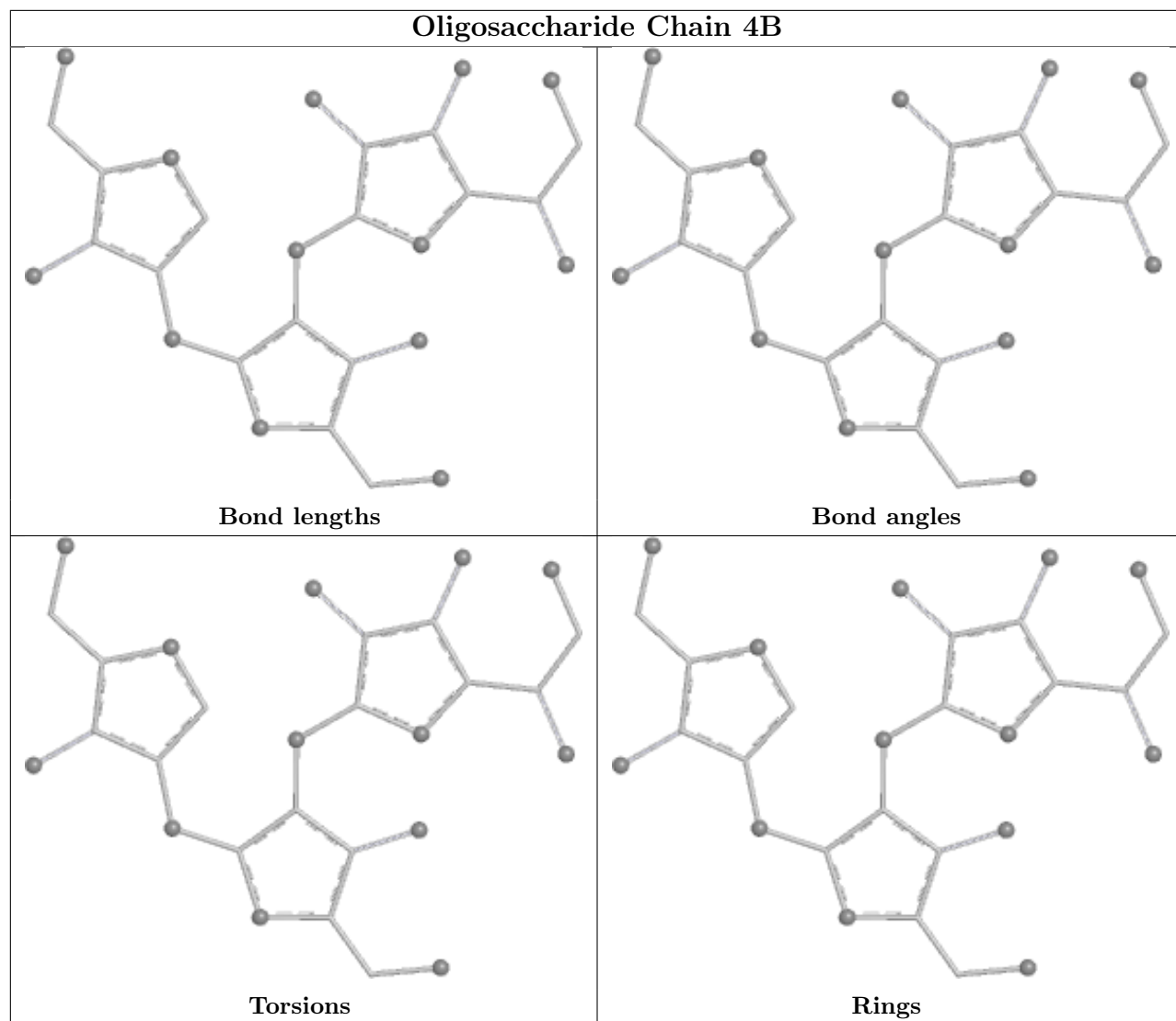


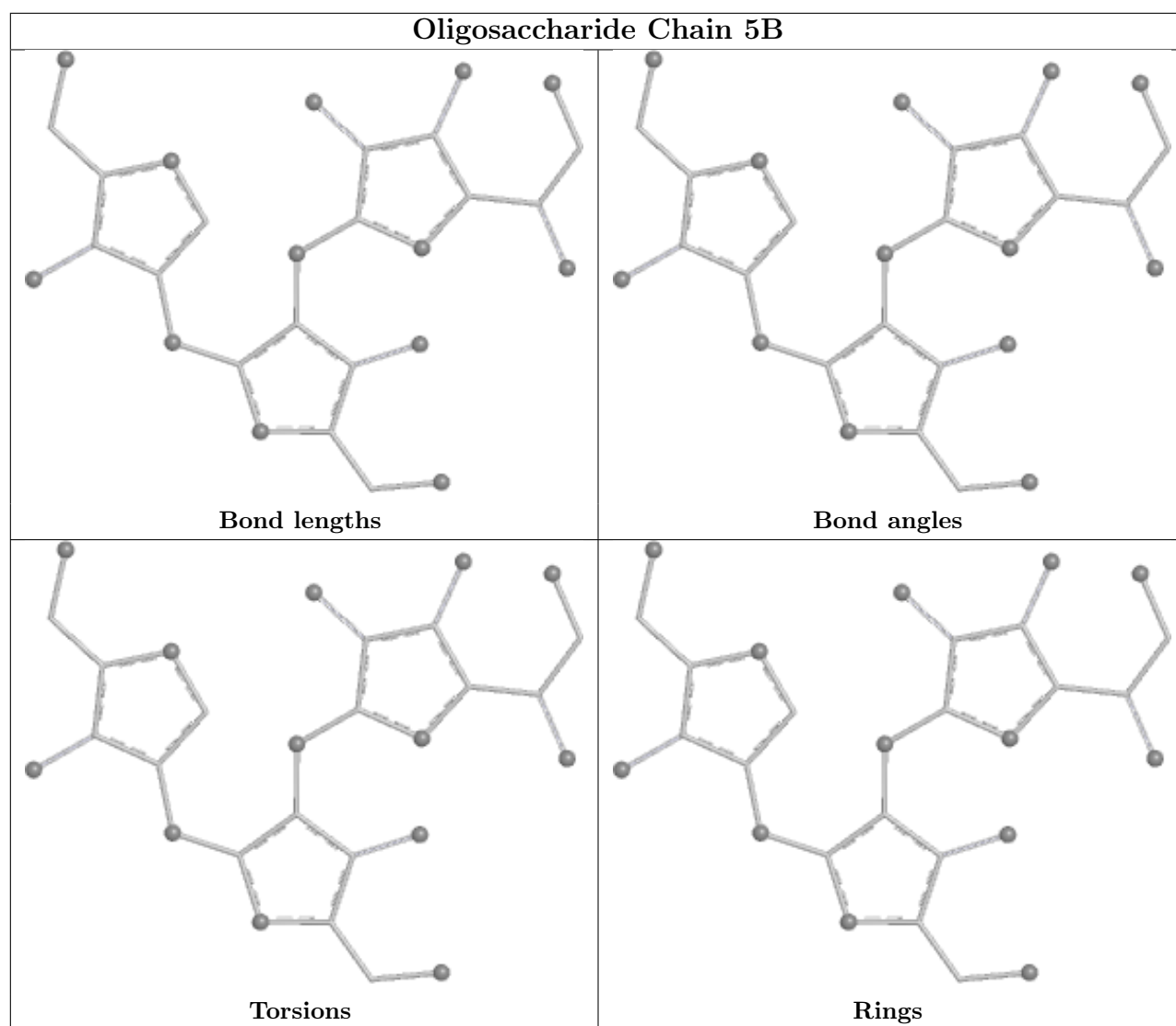




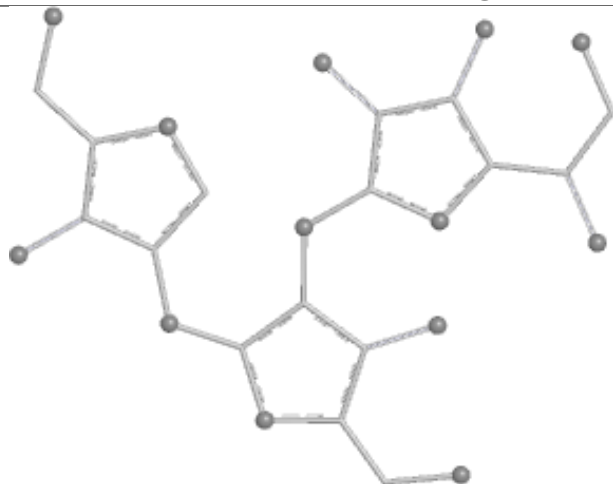


Oligosaccharide Chain 4B

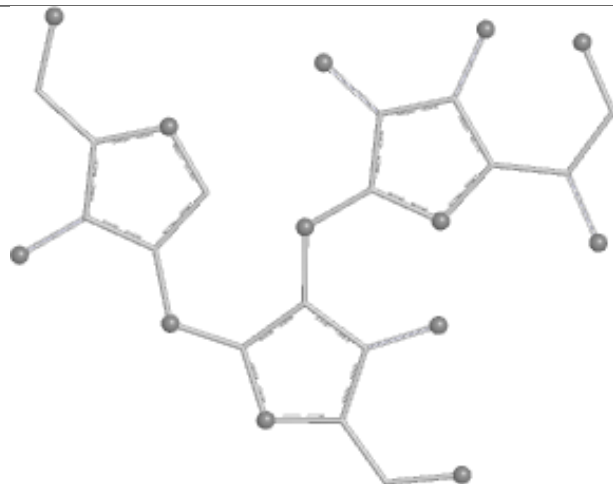




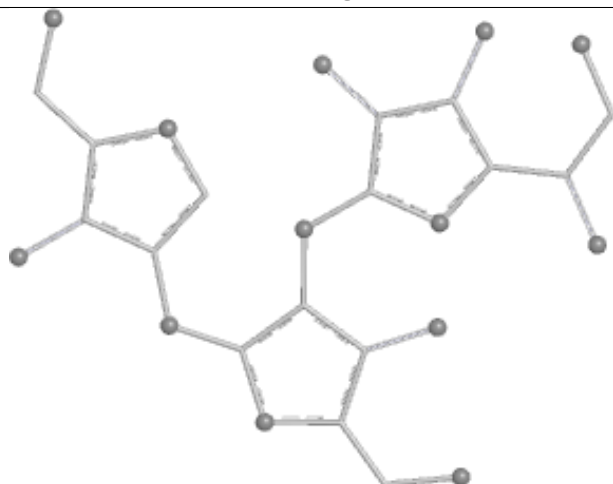
Oligosaccharide Chain 9B



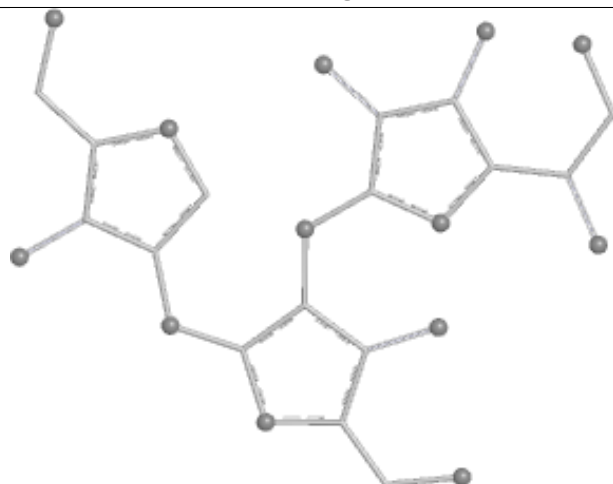
Bond lengths



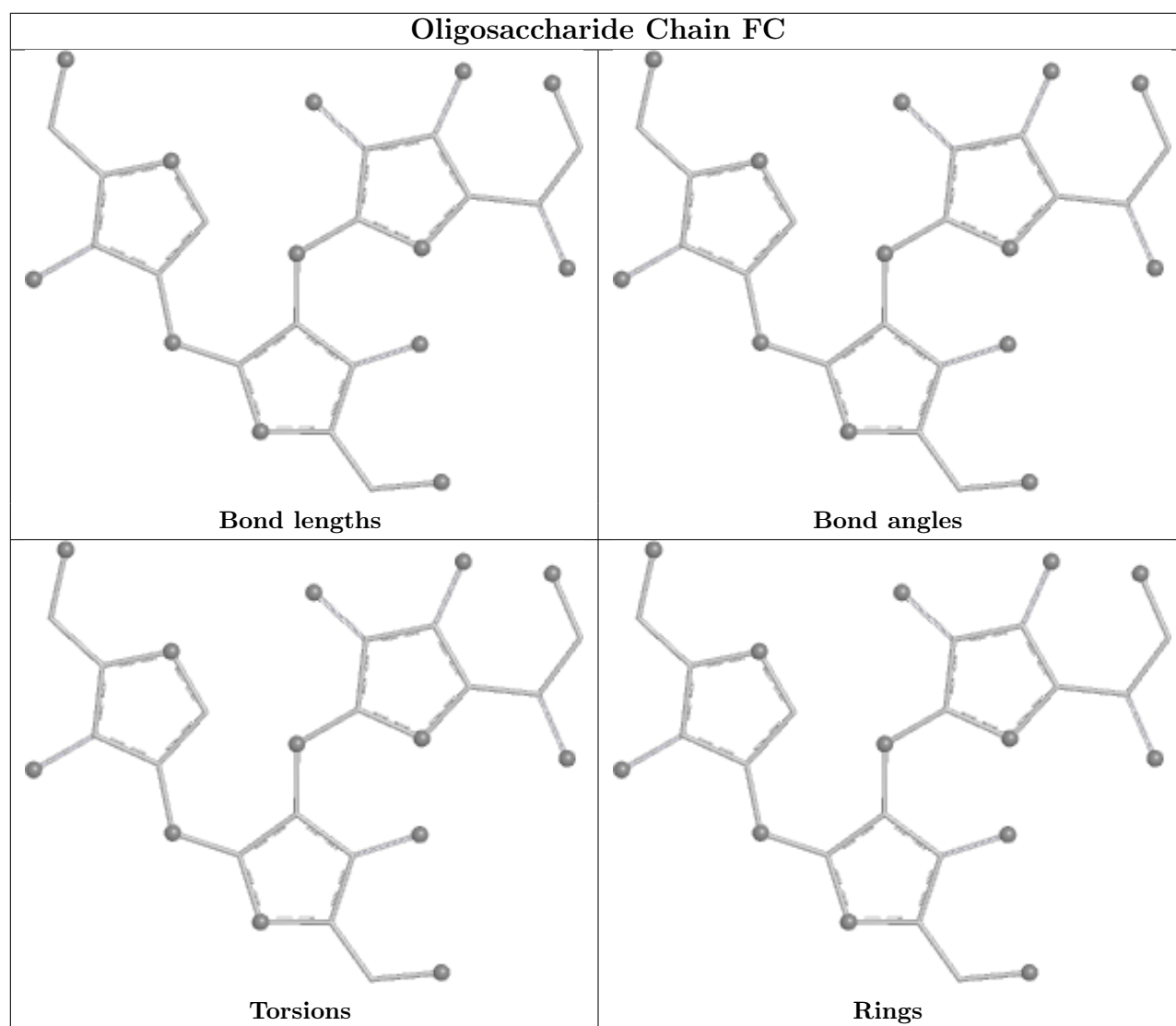
Bond angles

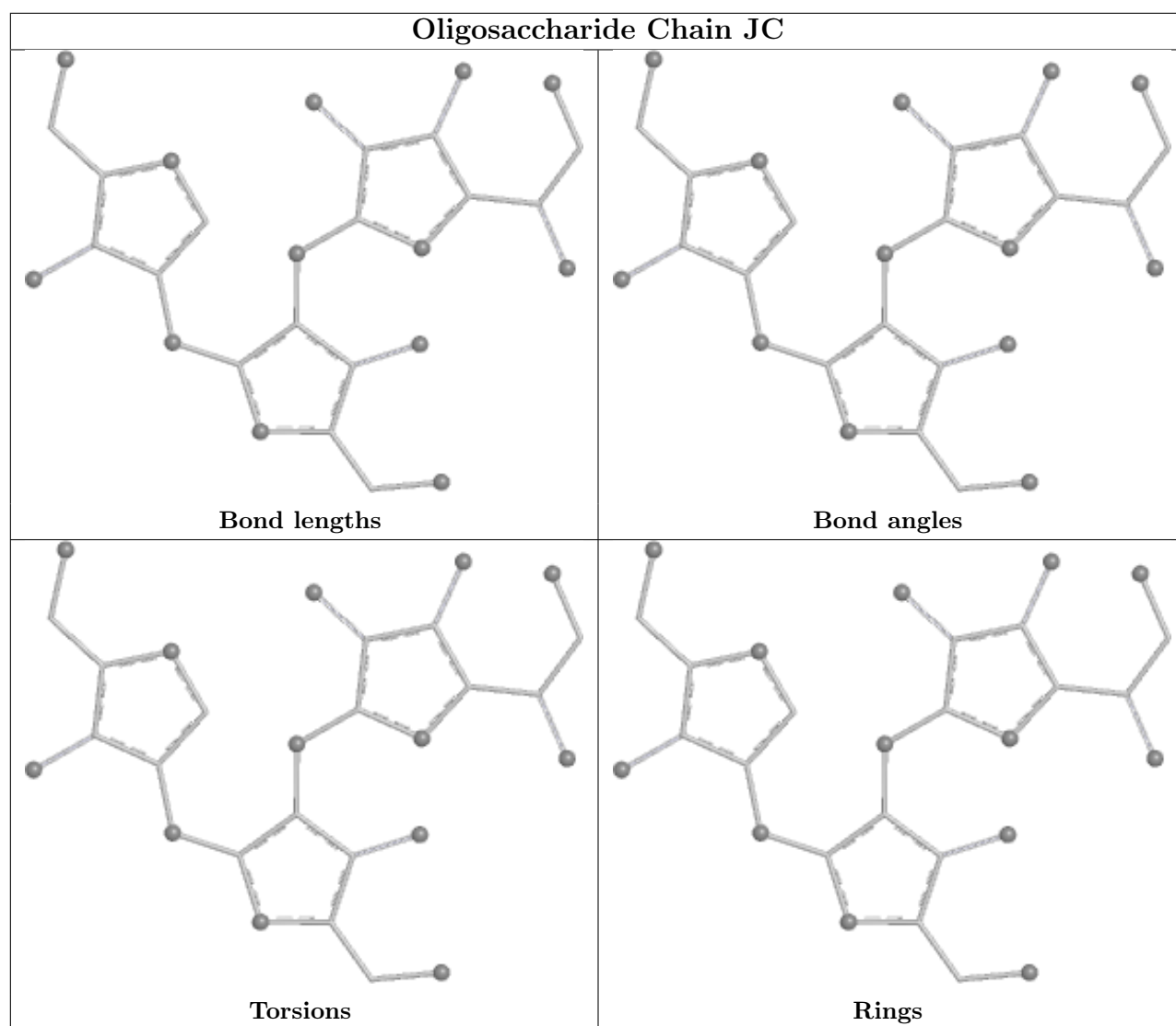


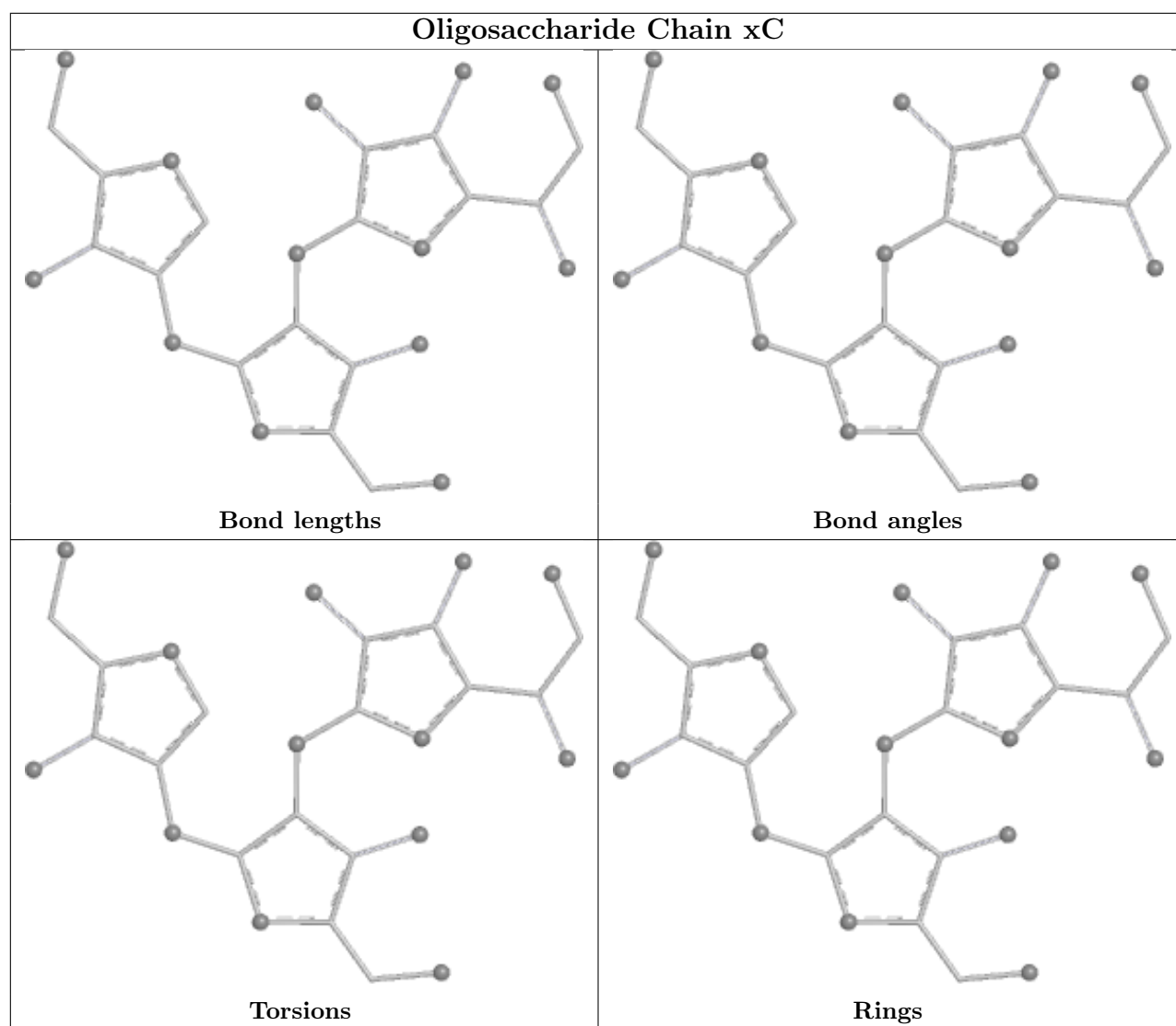
Torsions

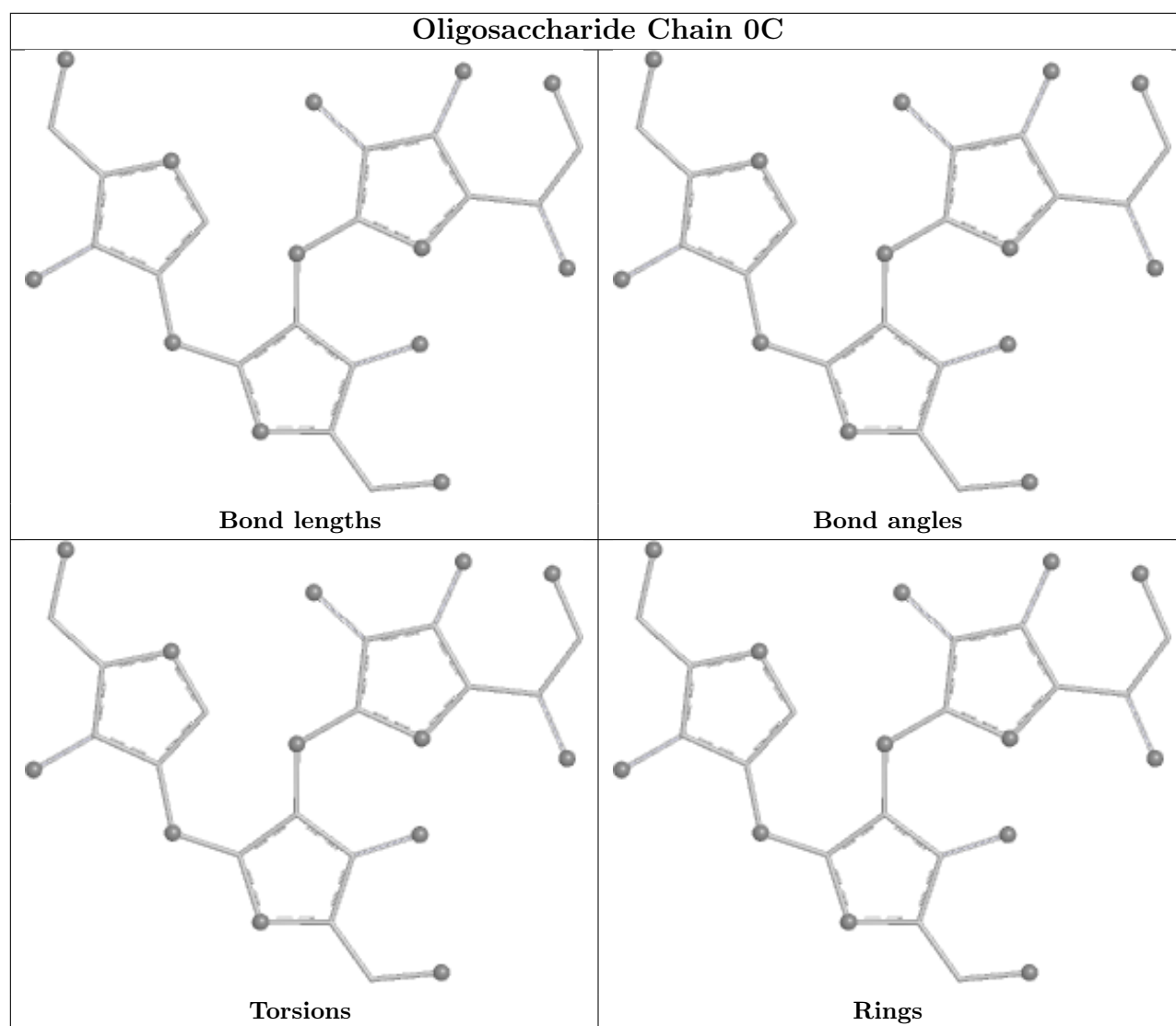


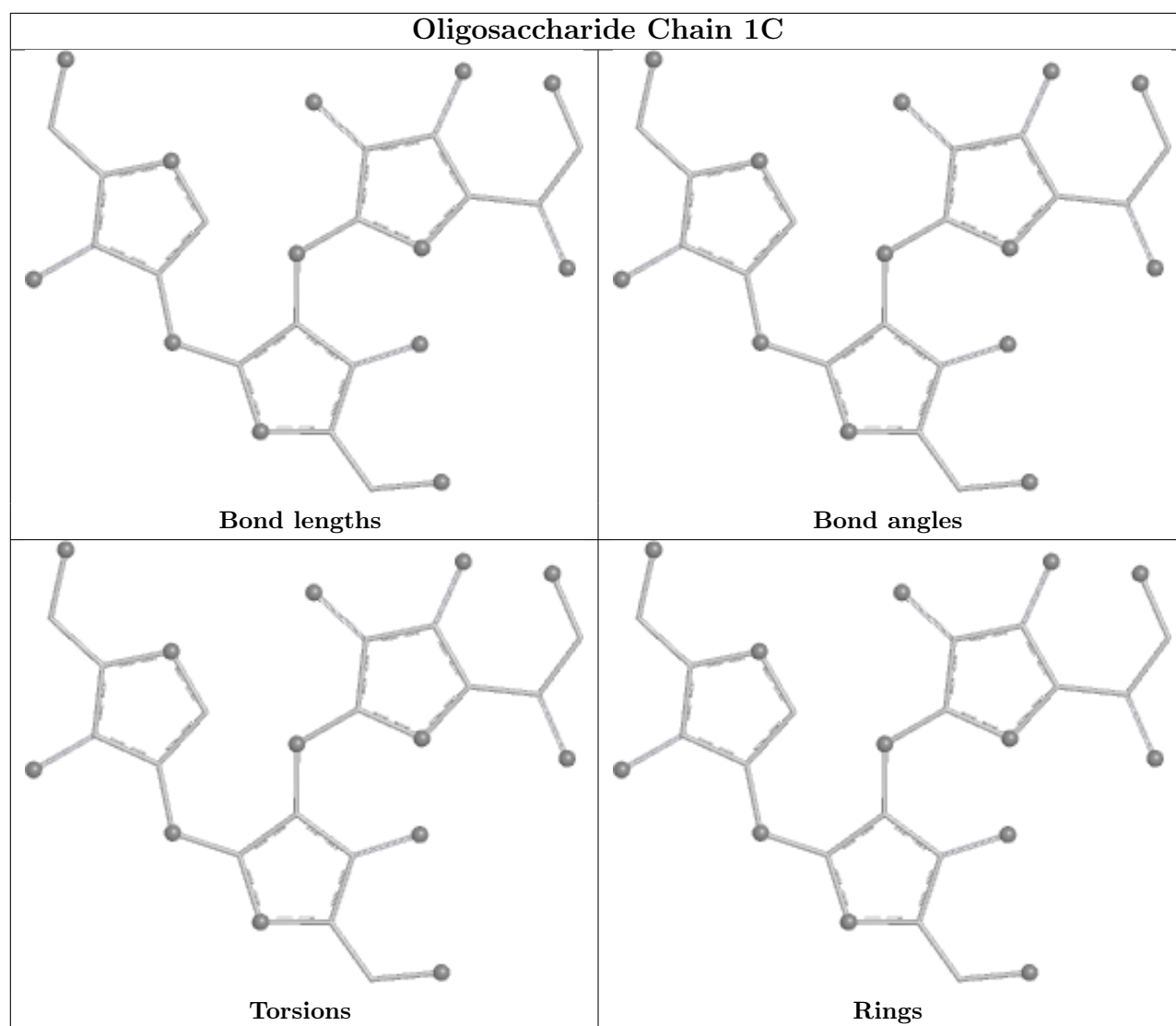
Rings



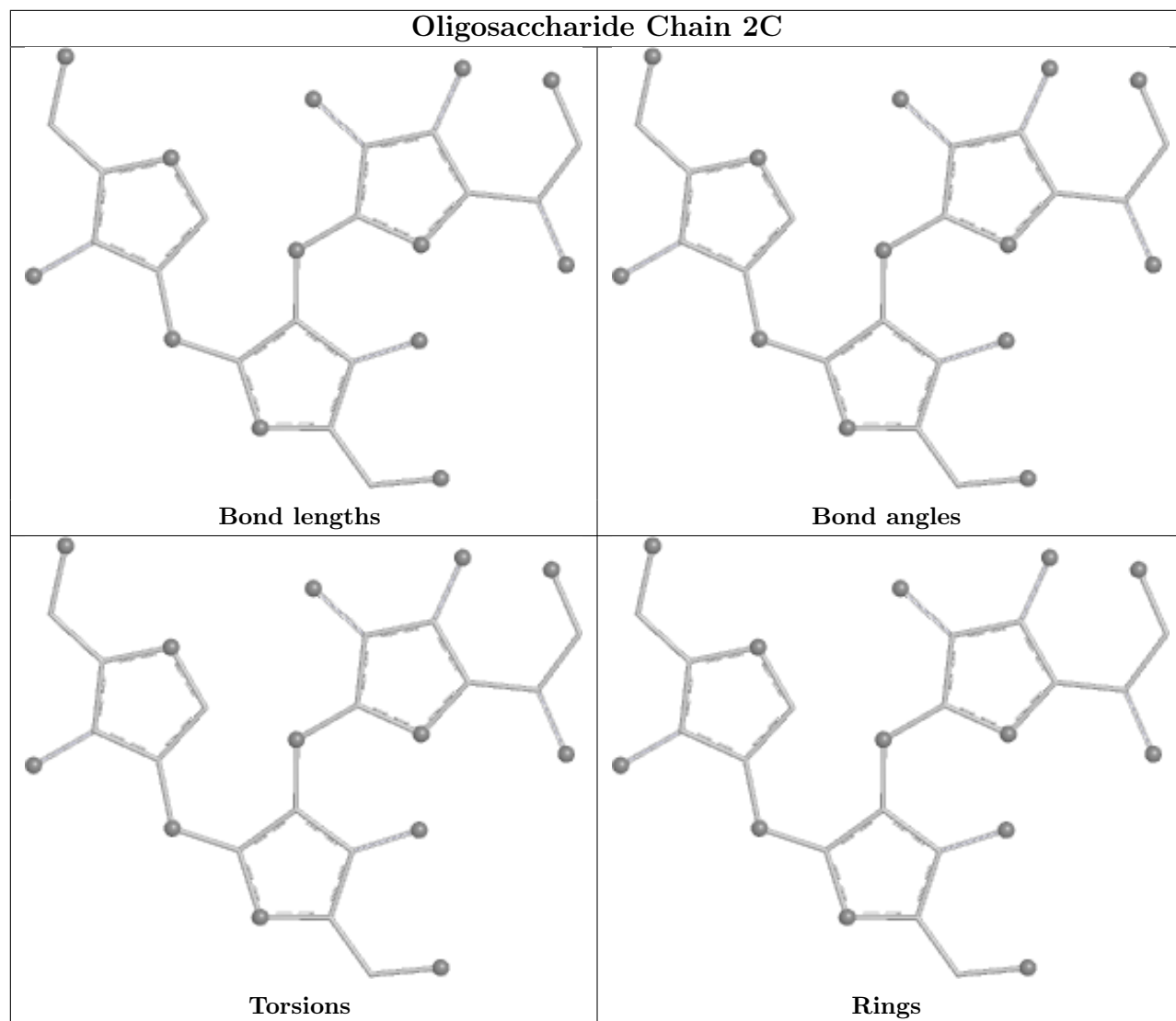




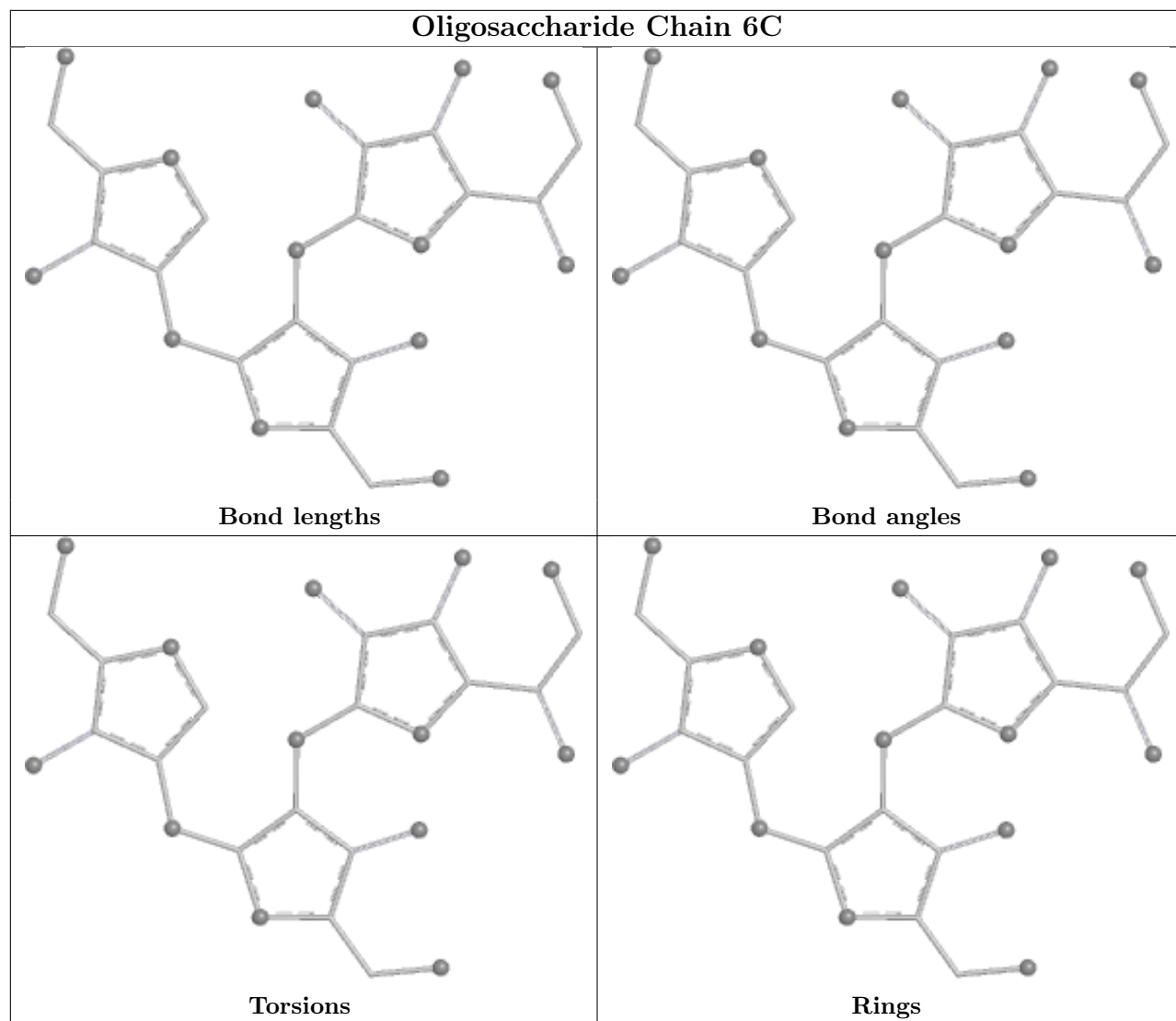


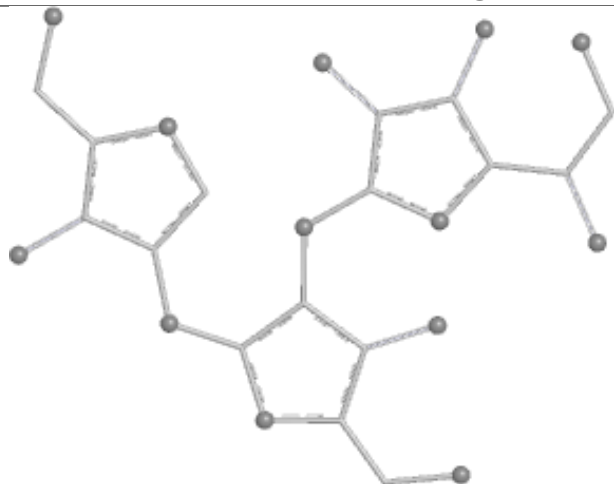
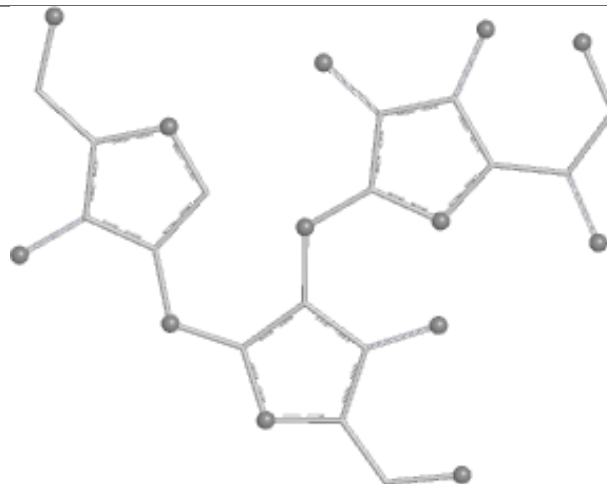
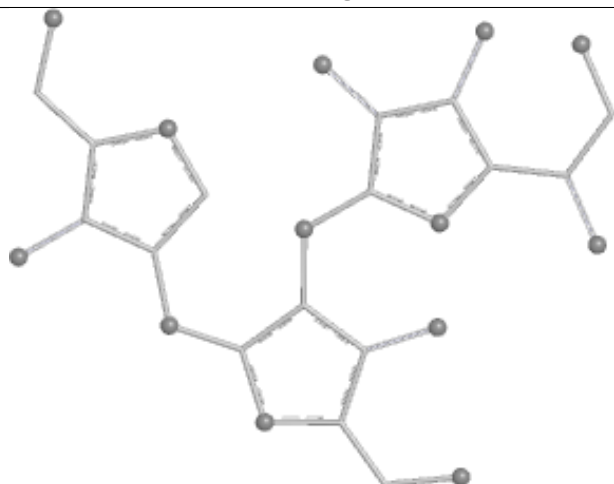
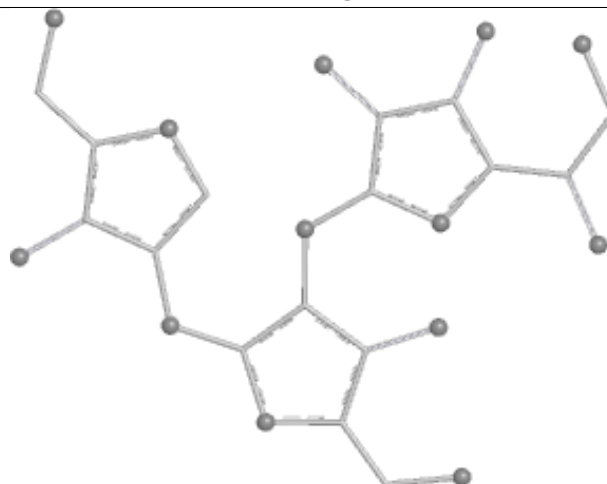


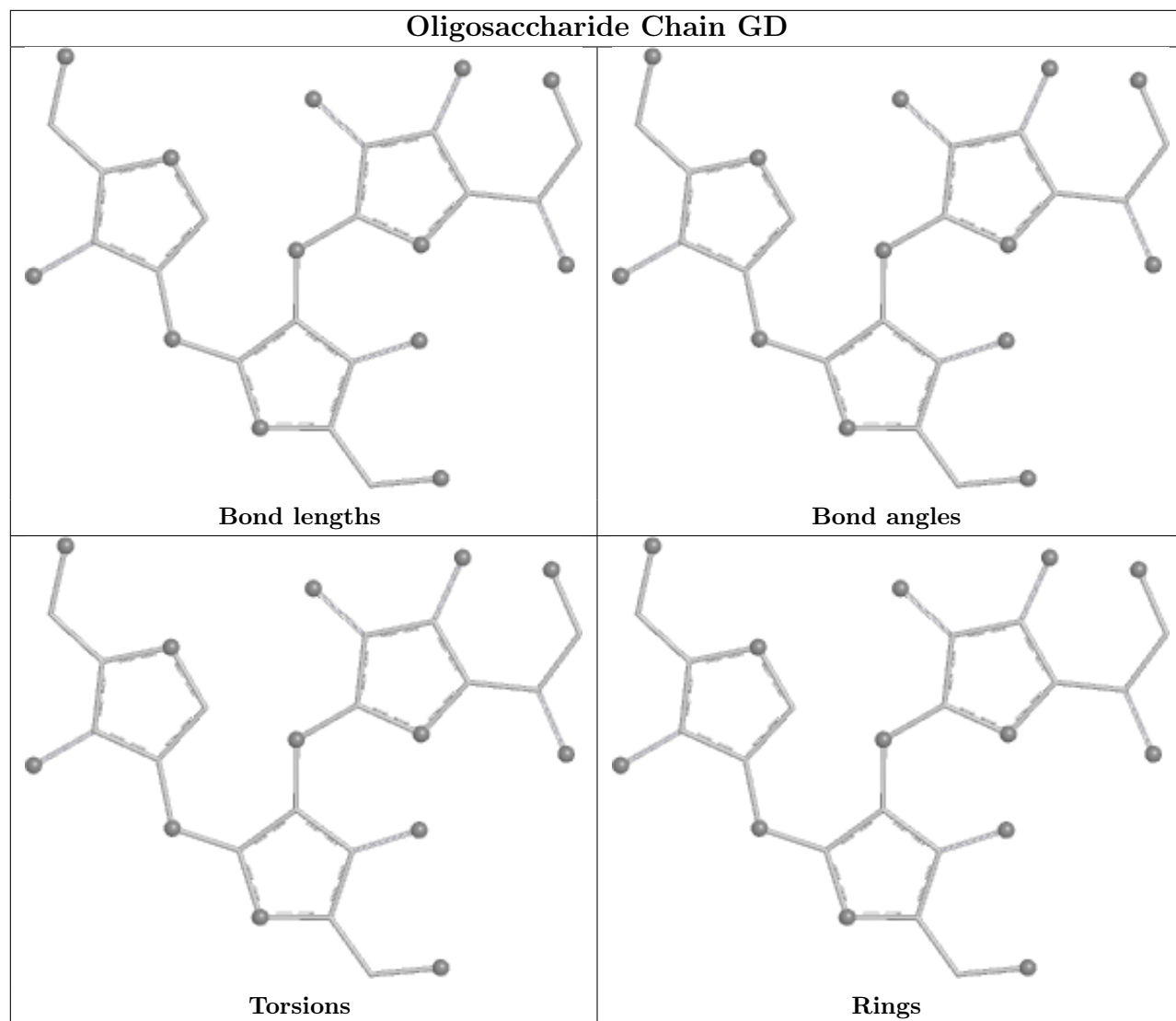
Oligosaccharide Chain 2C

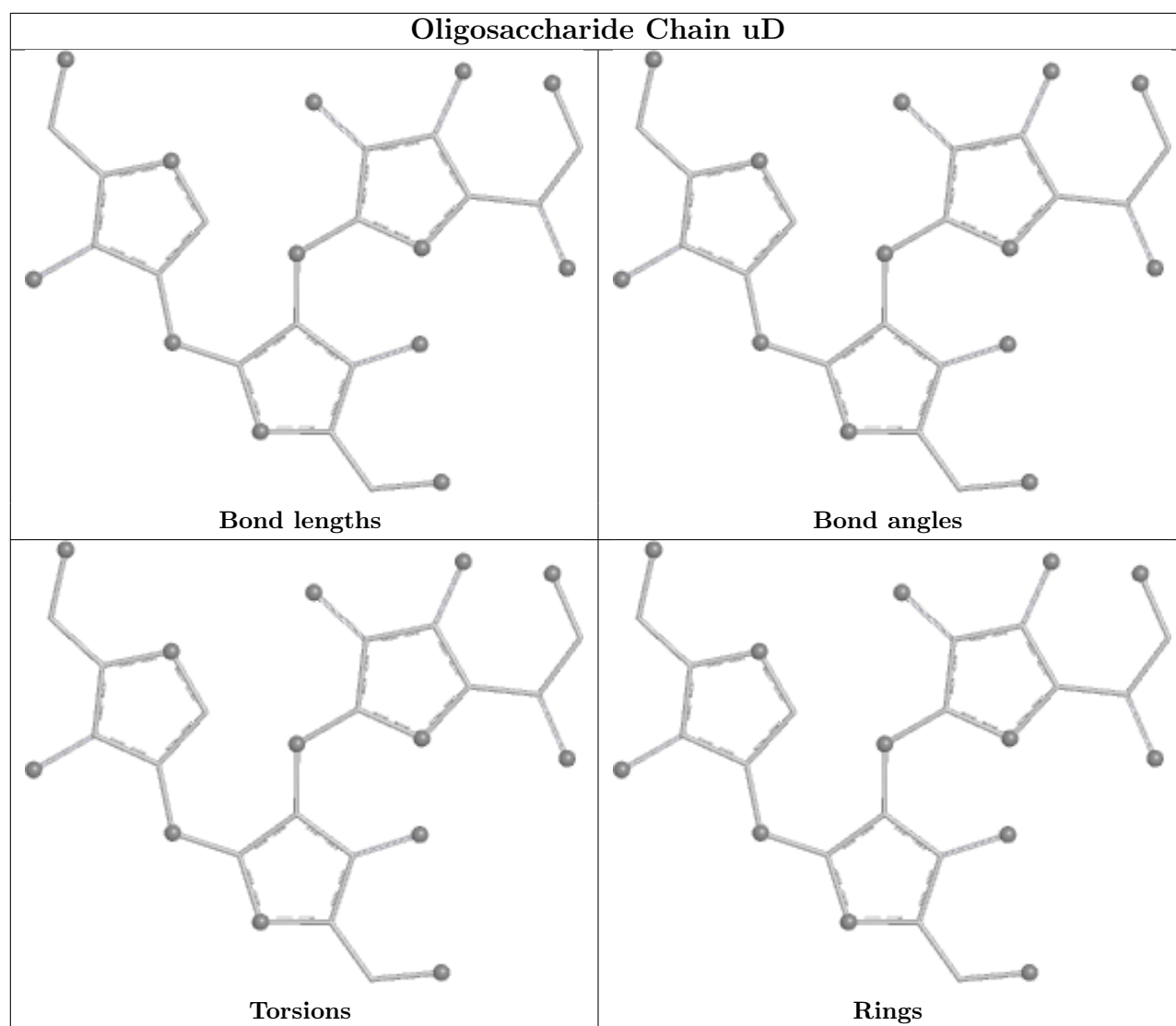


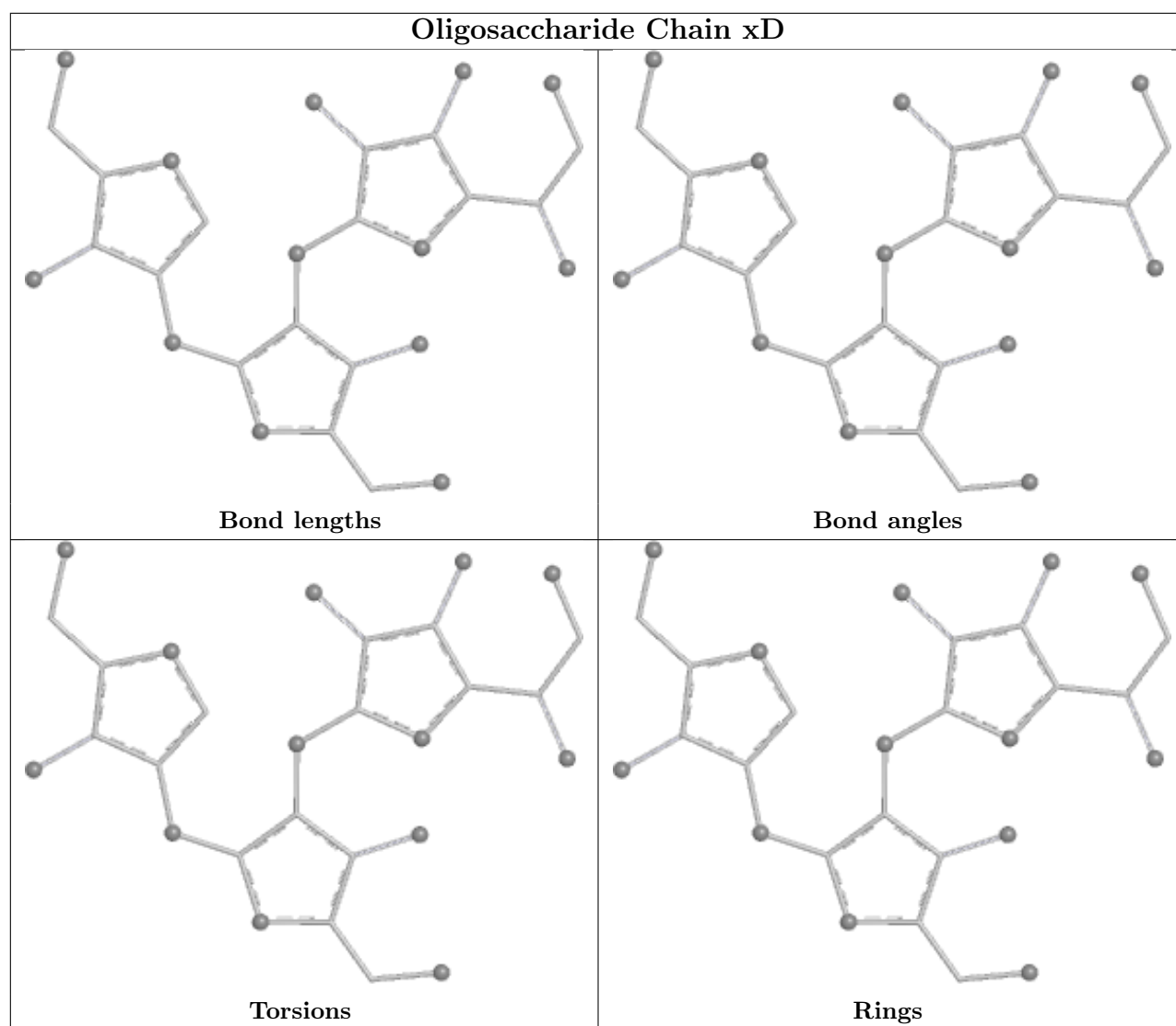
Oligosaccharide Chain 6C

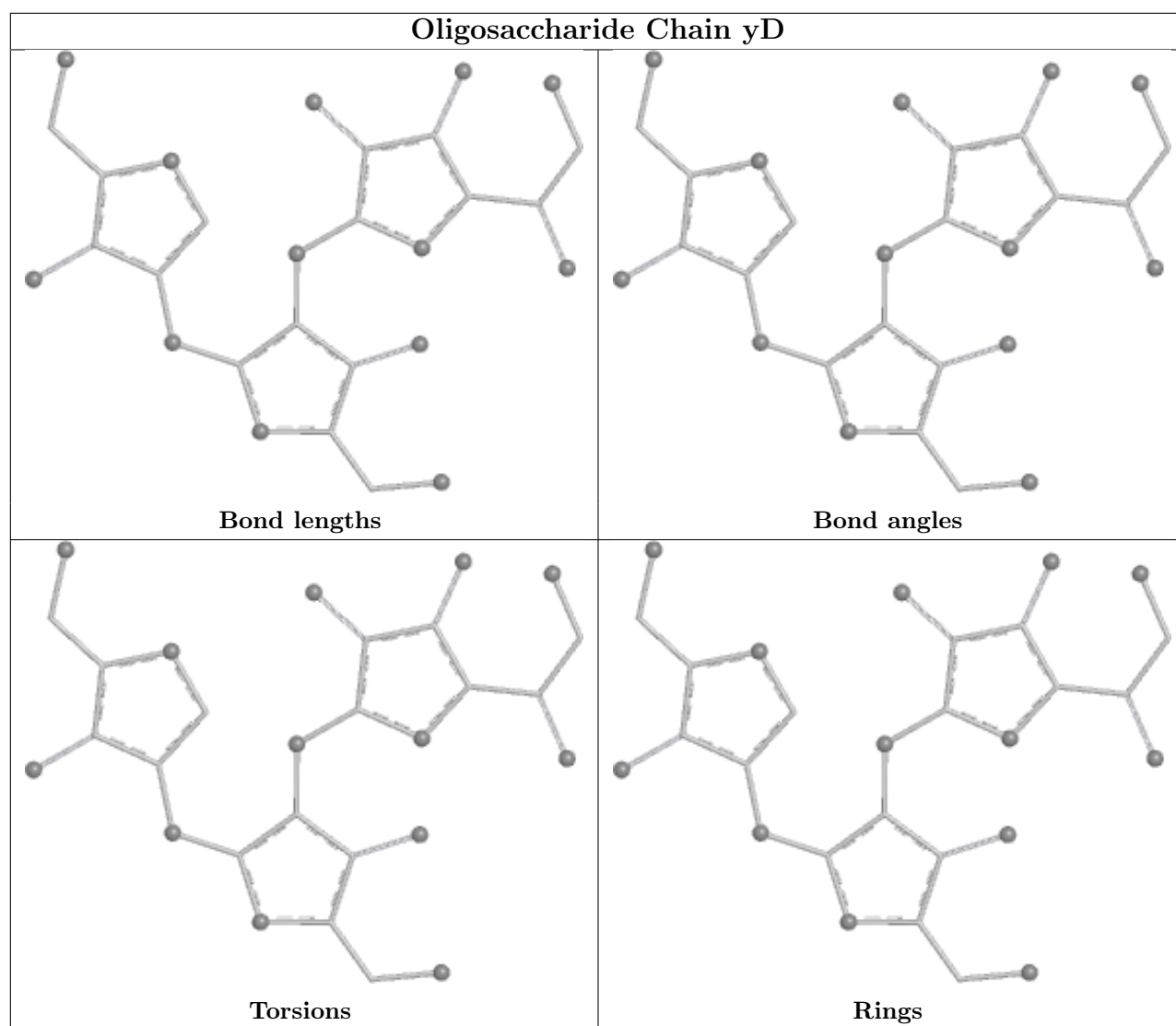


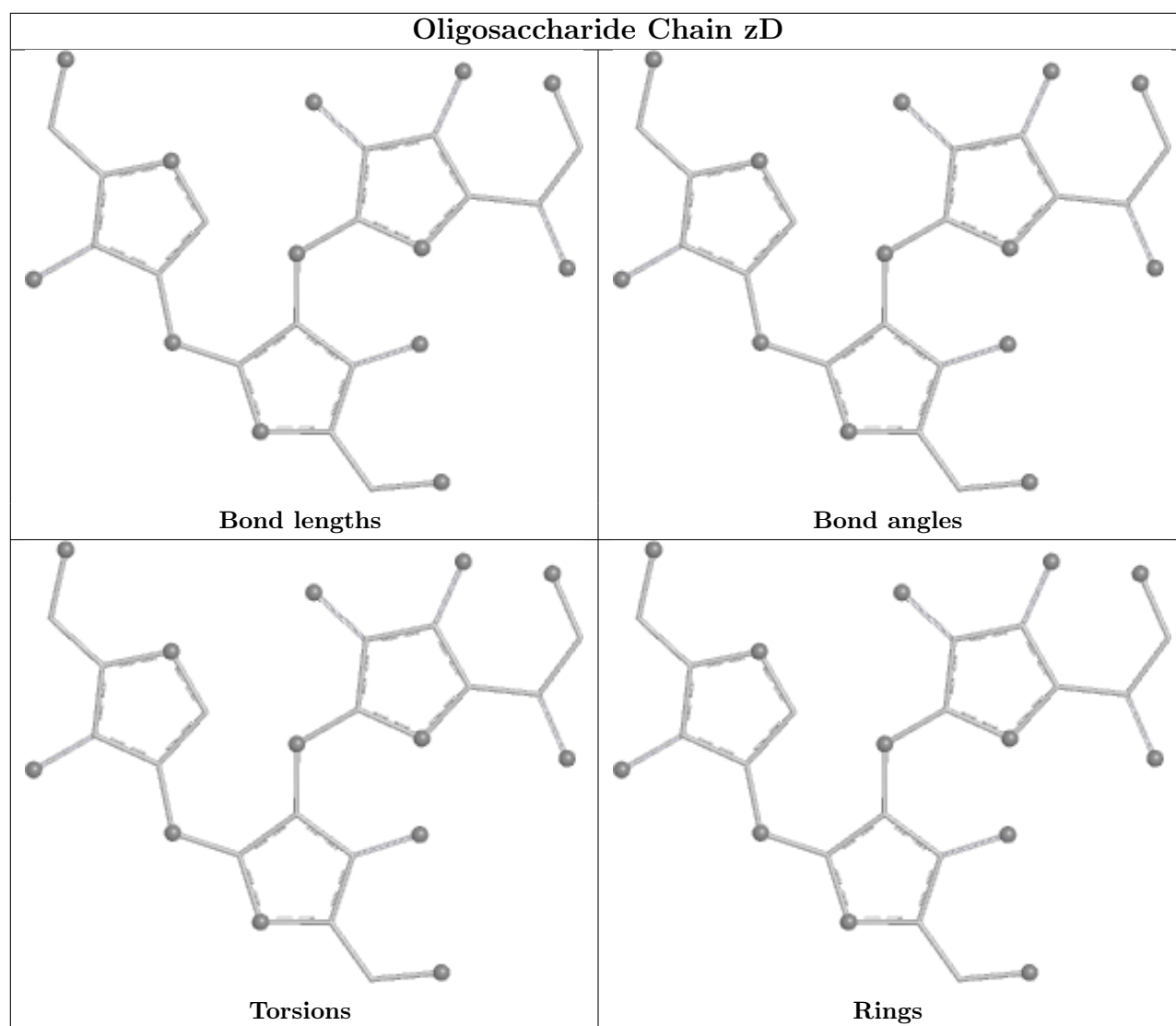
Oligosaccharide Chain CD**Bond lengths****Bond angles****Torsions****Rings**

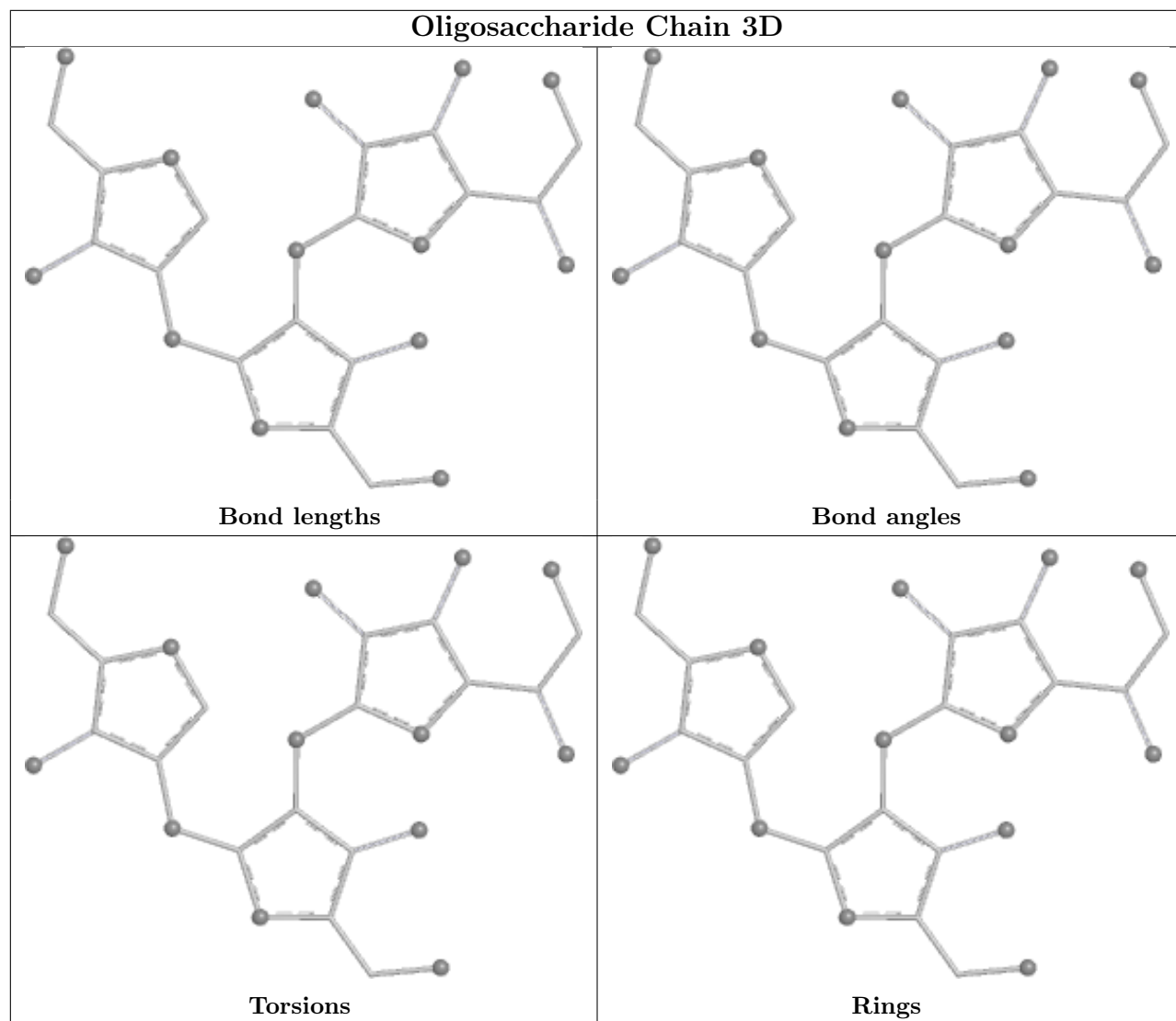




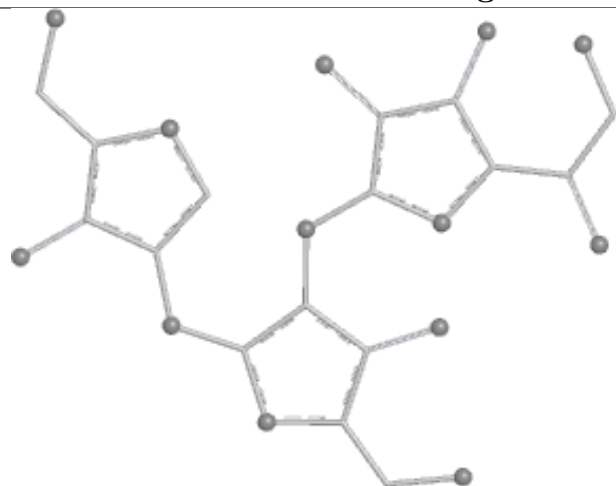




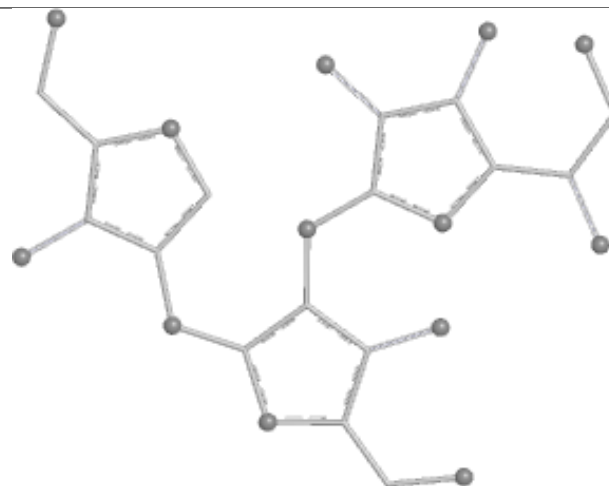




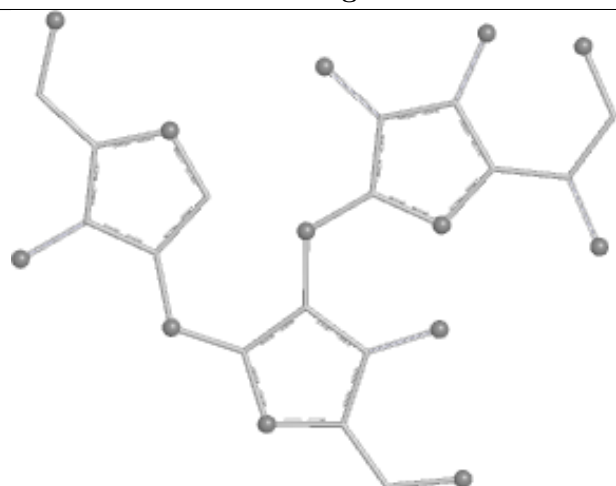
Oligosaccharide Chain 6D



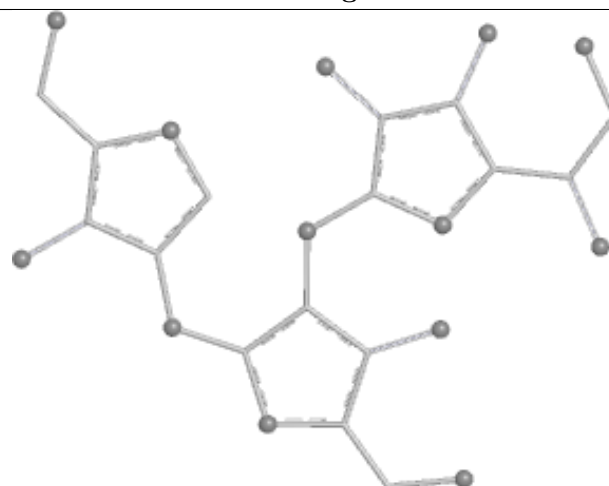
Bond lengths



Bond angles

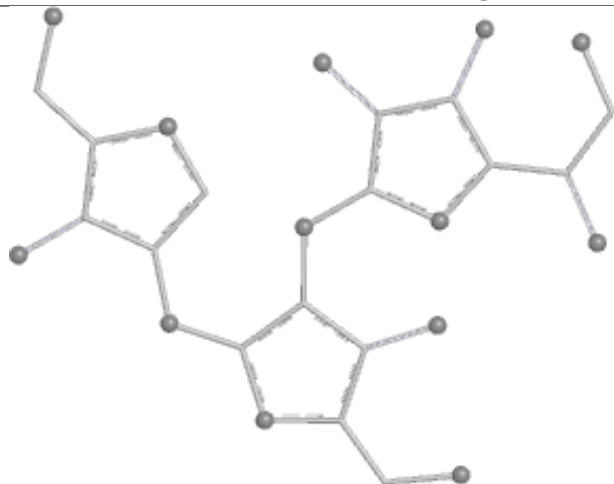


Torsions

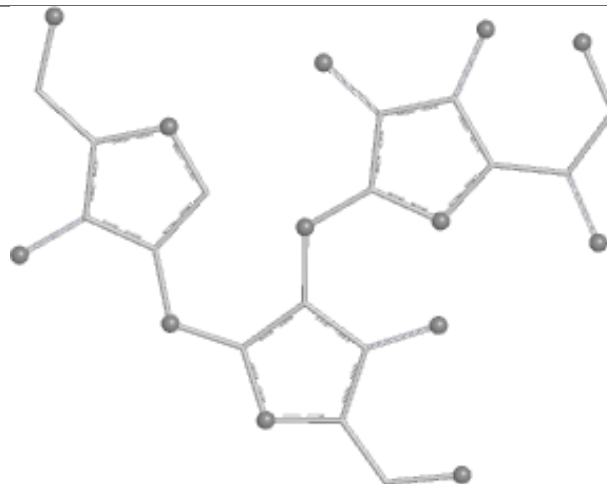


Rings

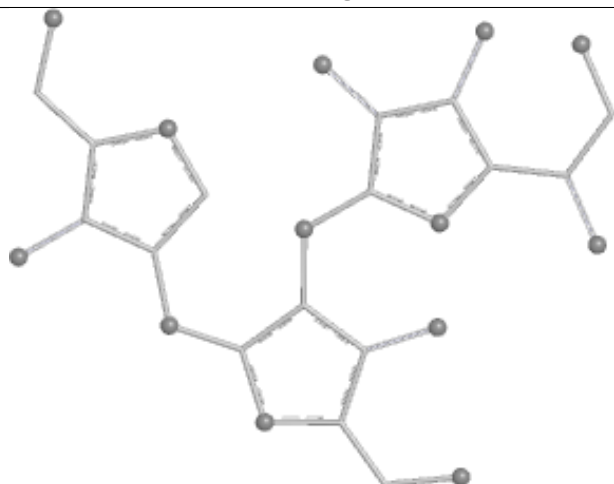
Oligosaccharide Chain 7D



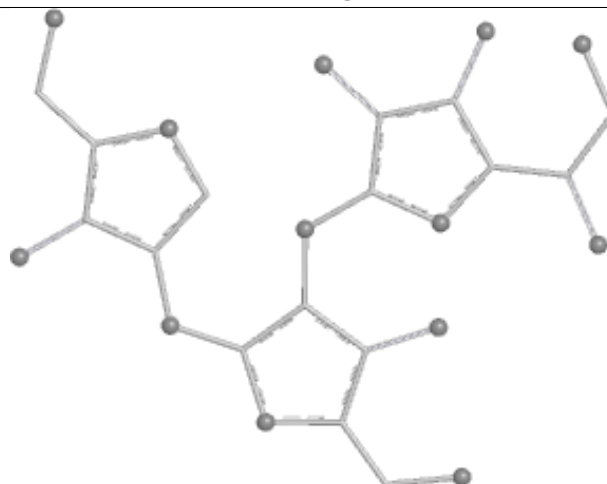
Bond lengths



Bond angles

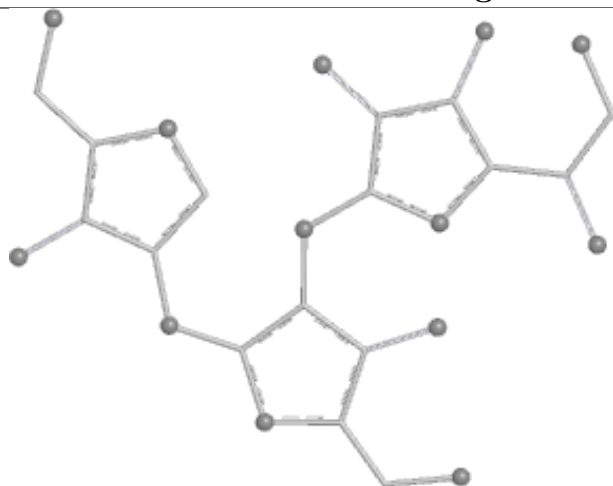


Torsions

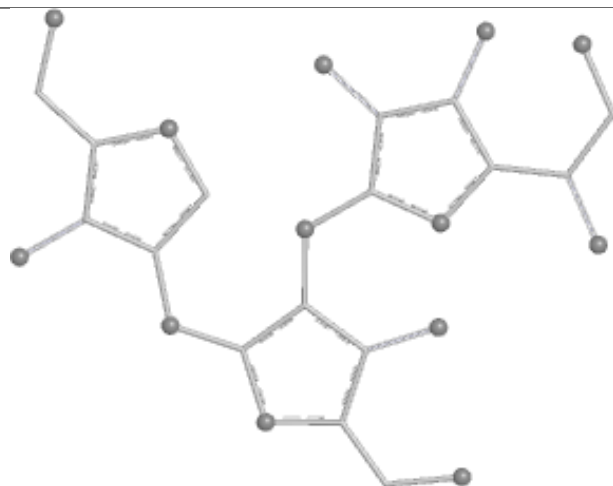


Rings

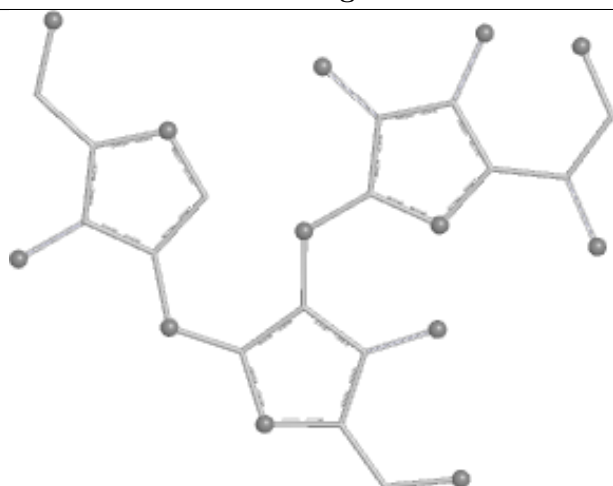
Oligosaccharide Chain 8D



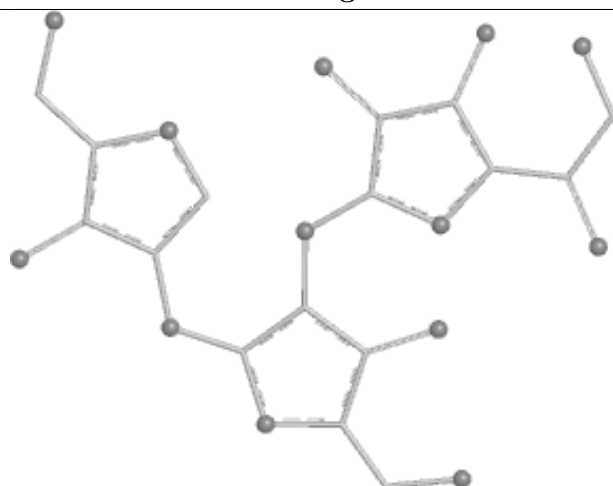
Bond lengths



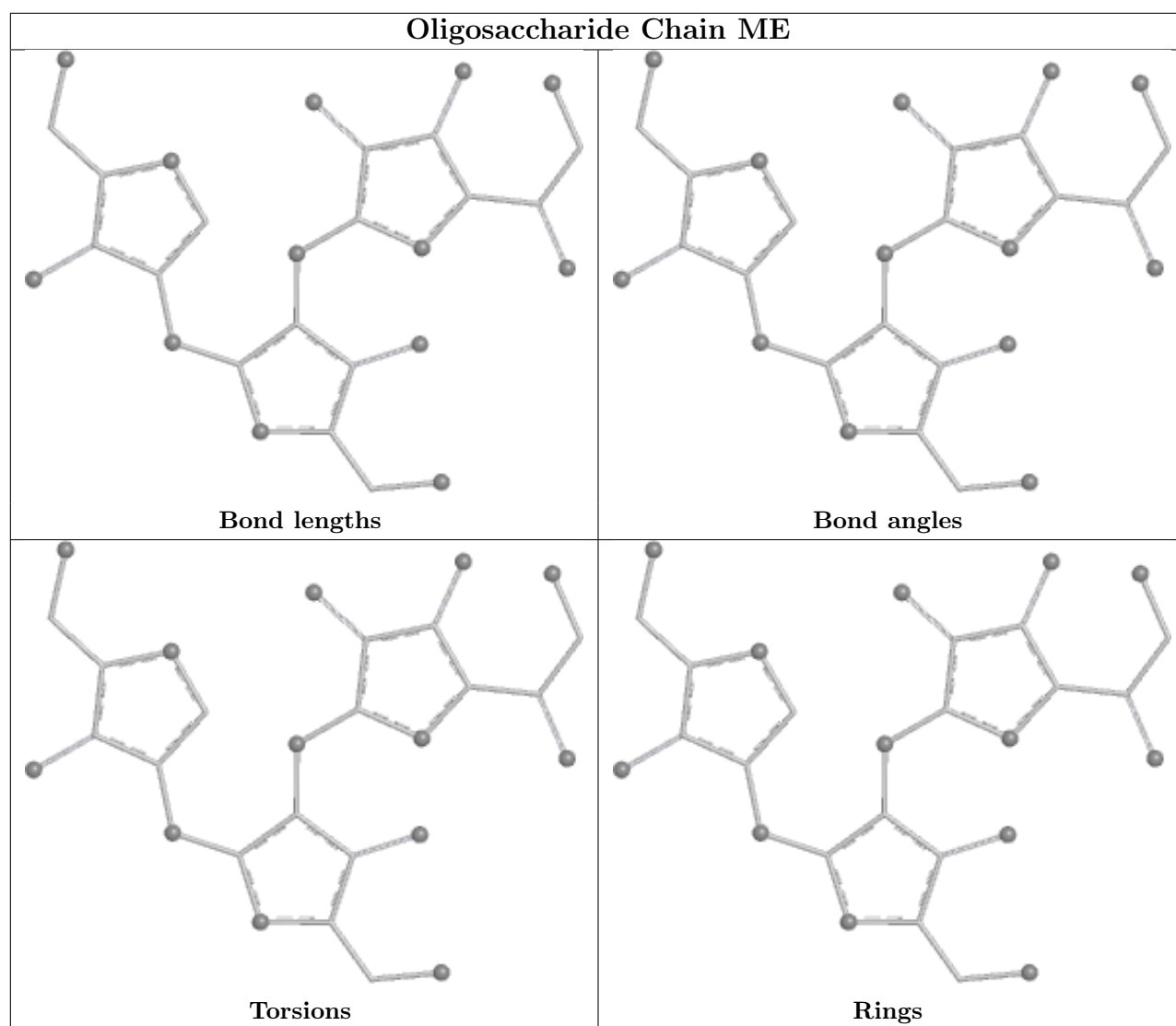
Bond angles

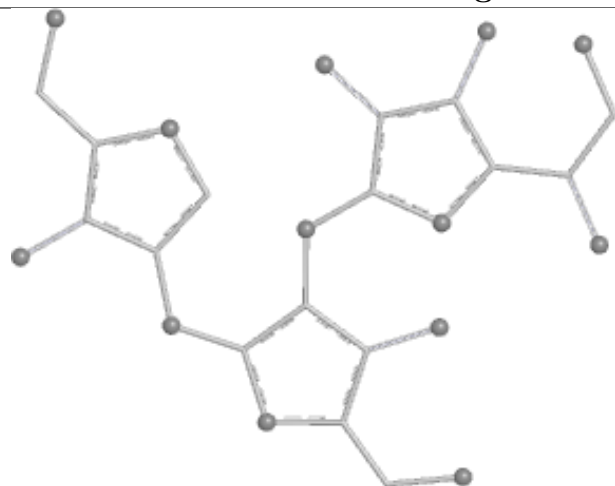
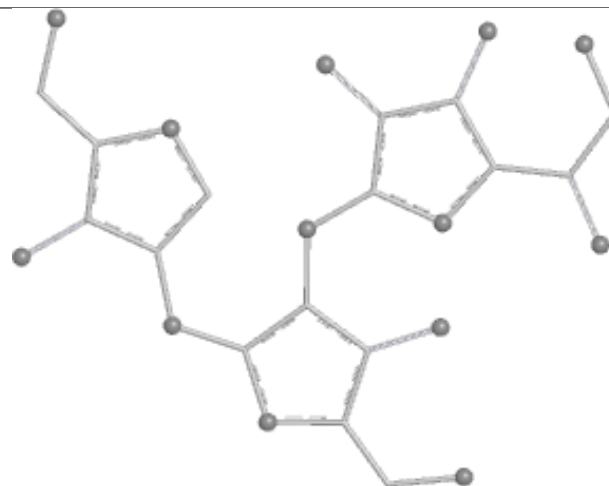
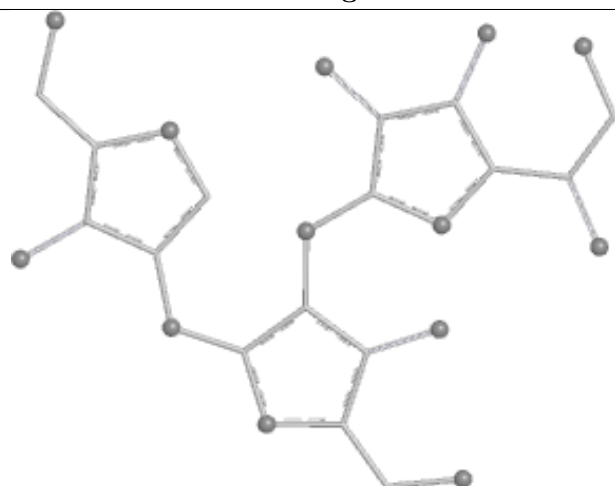
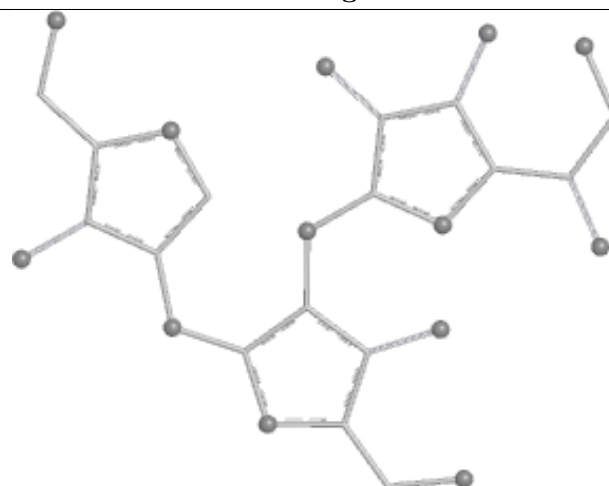


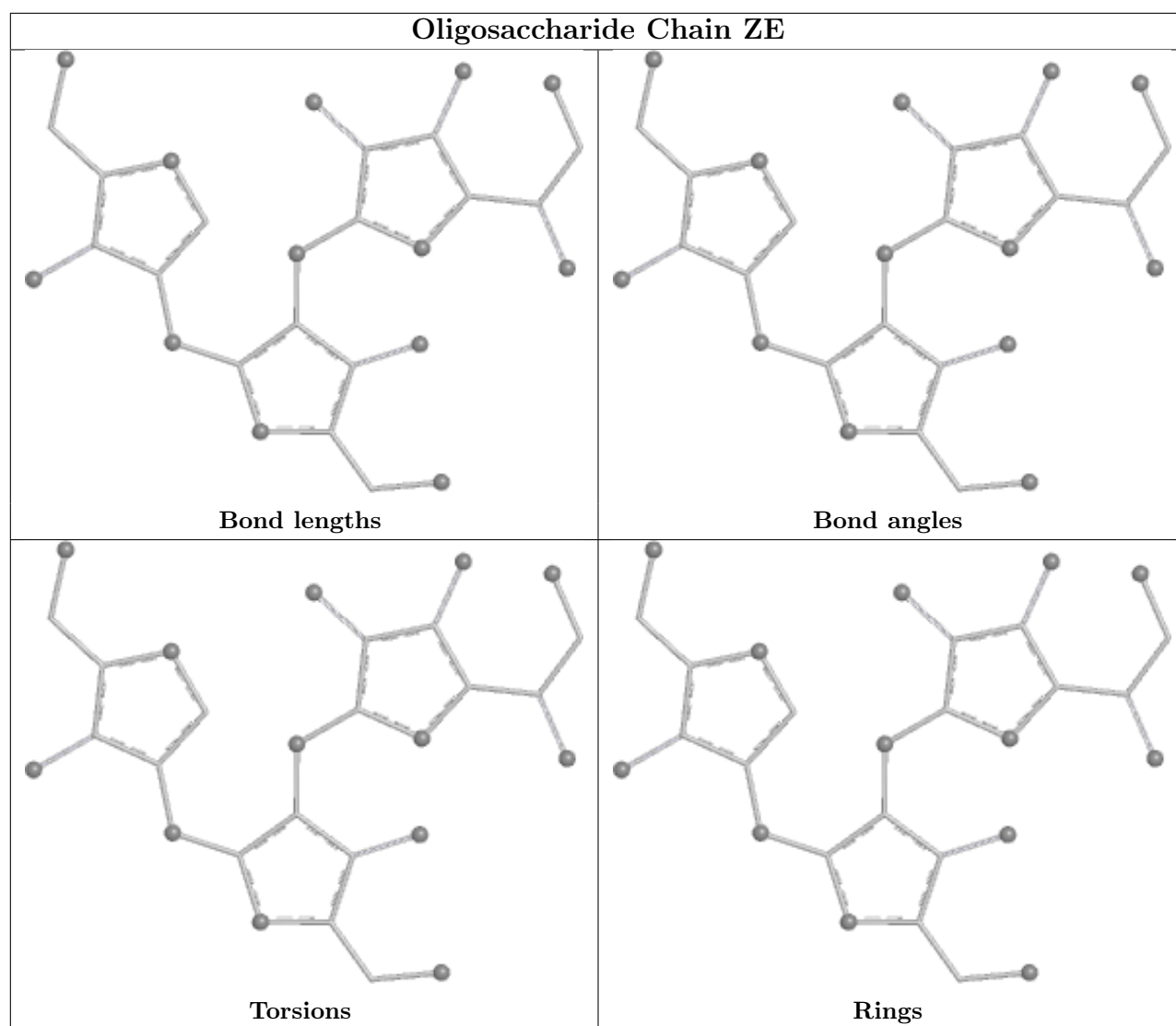
Torsions

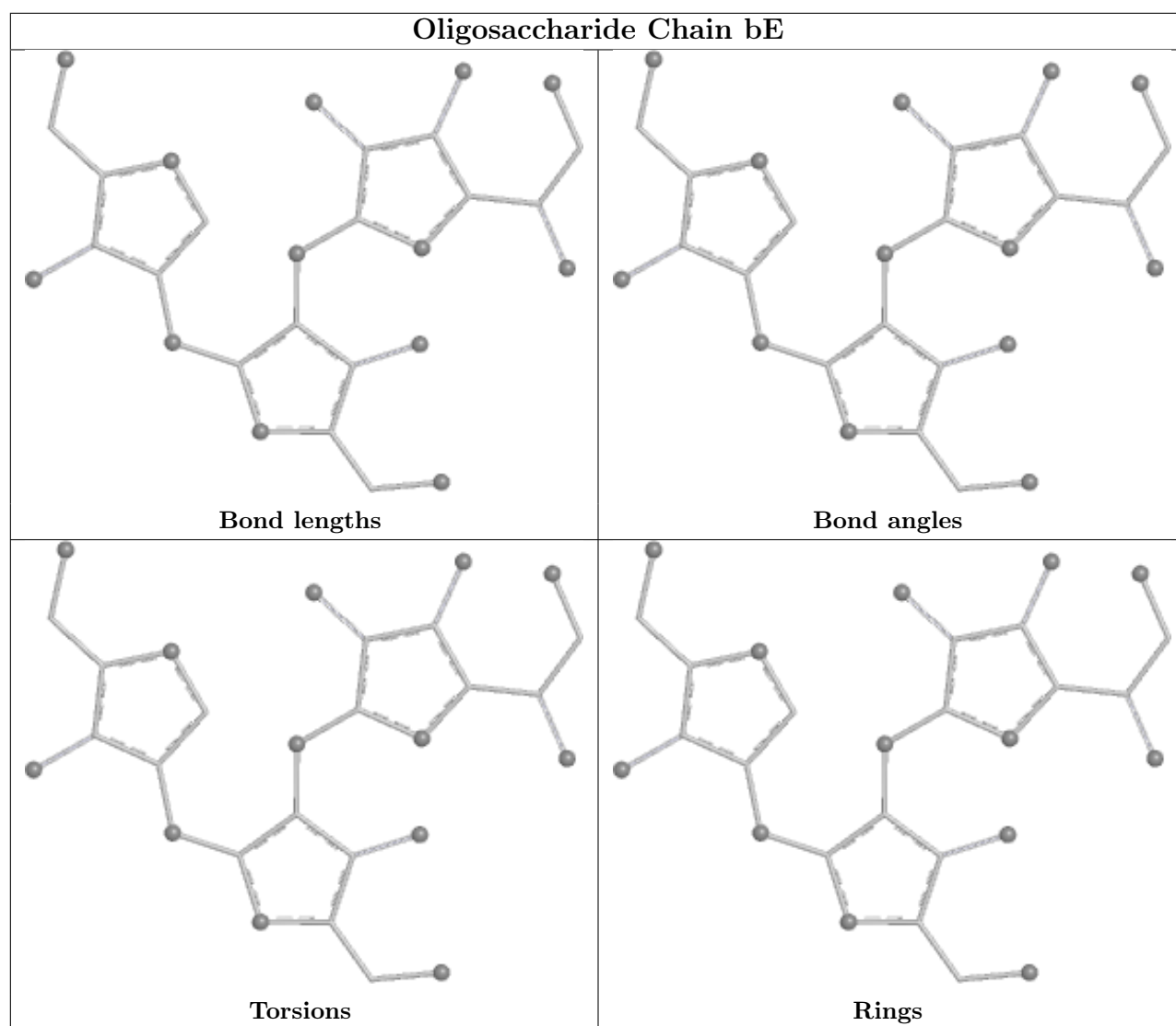


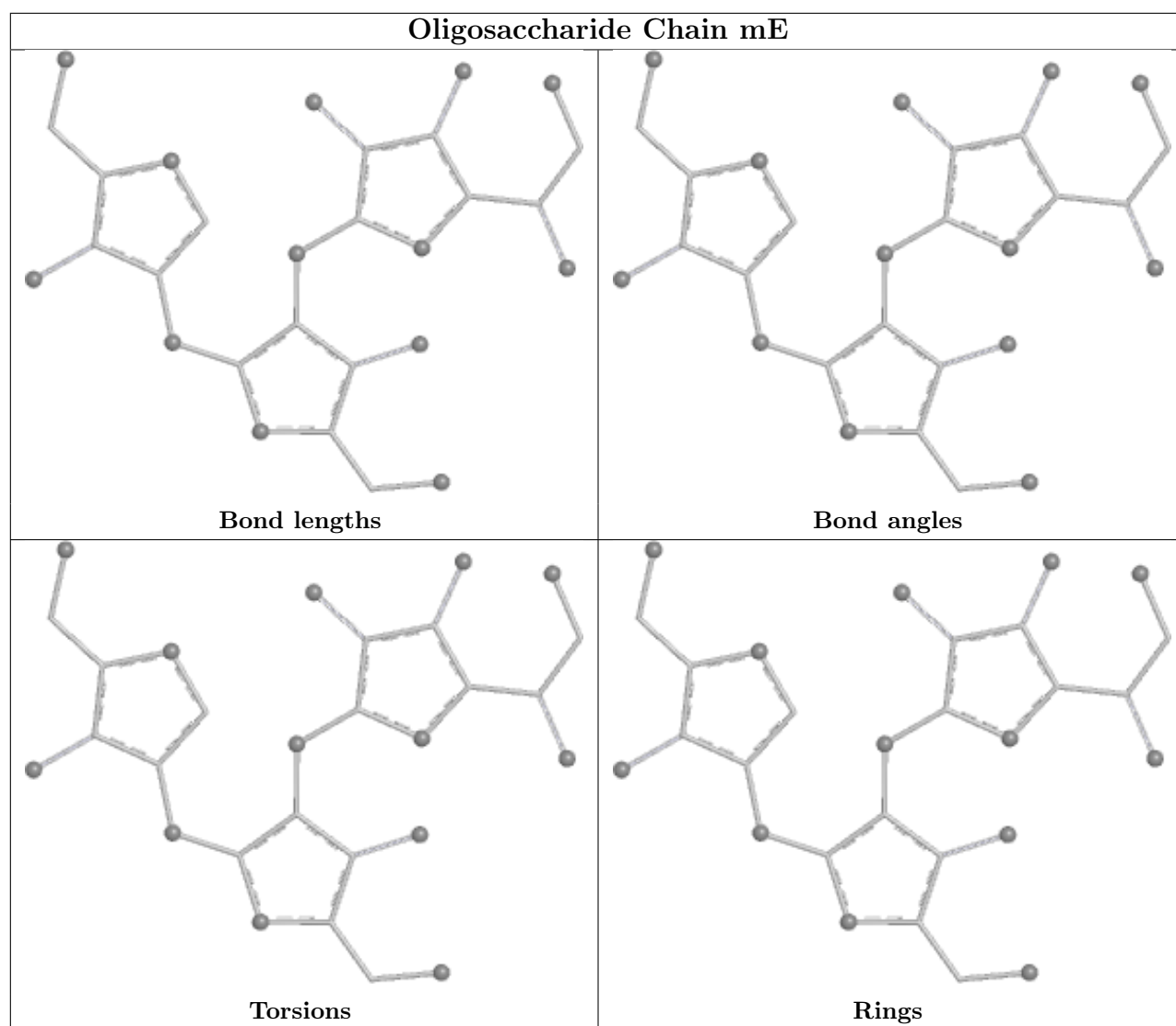
Rings

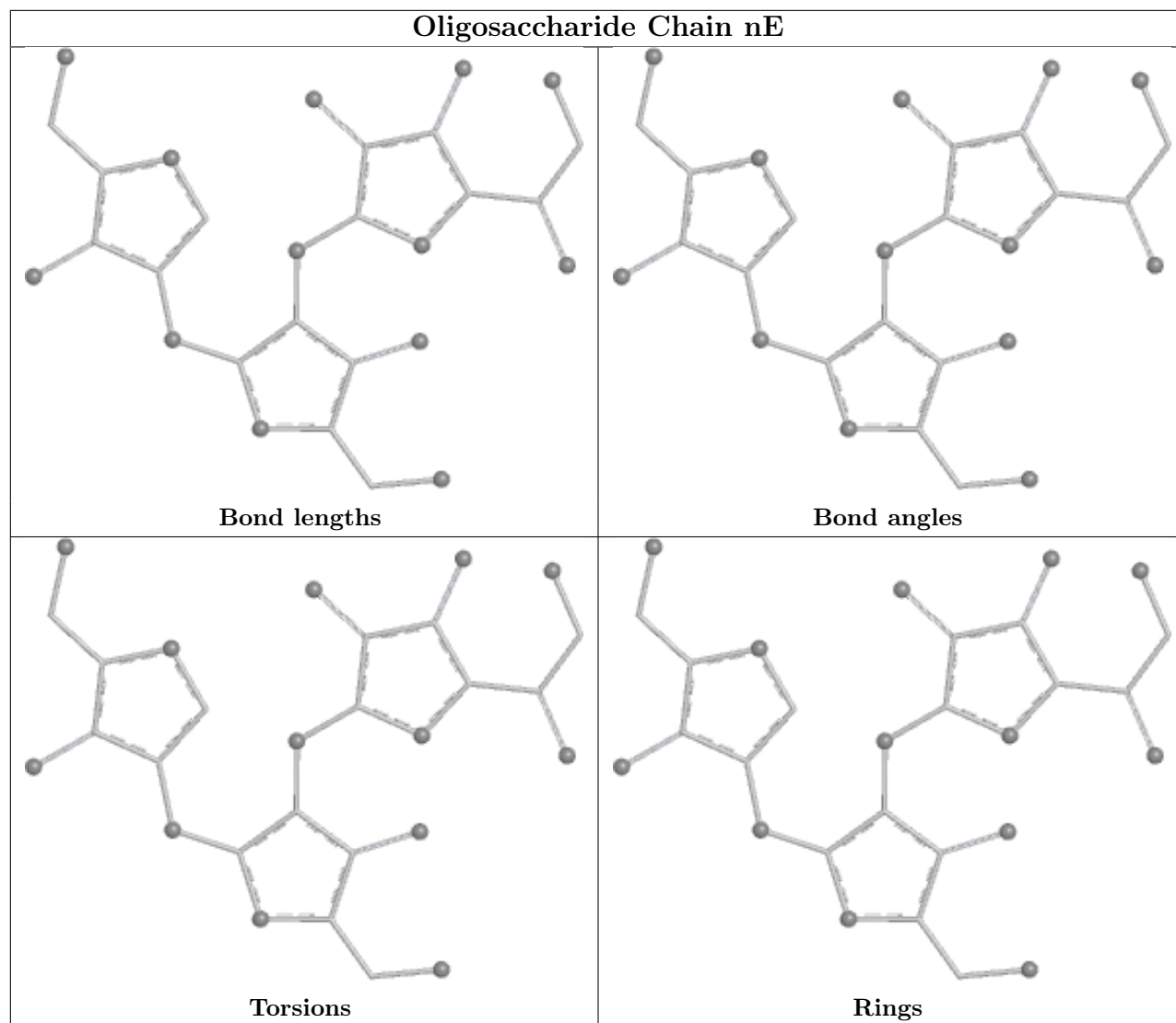


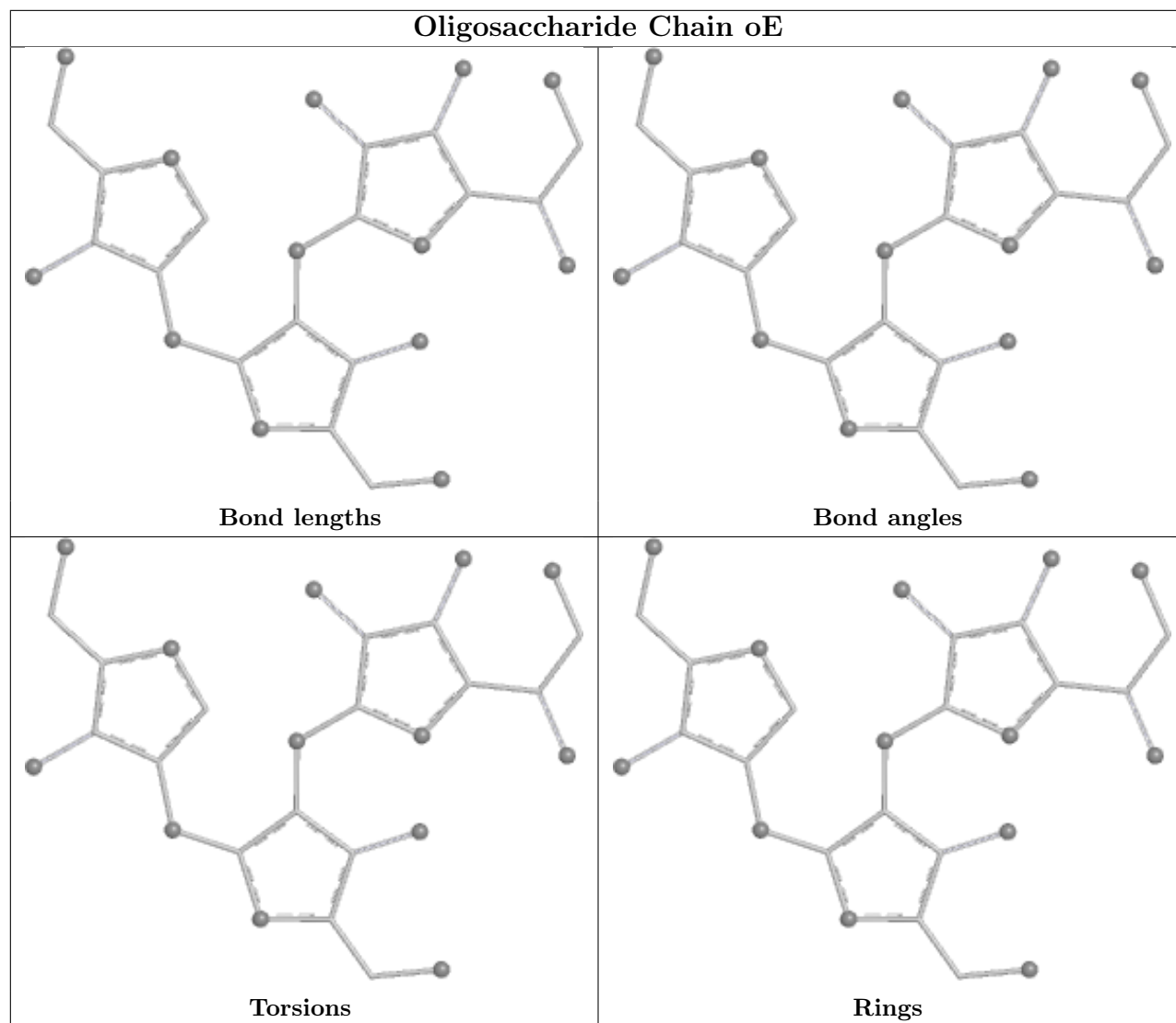
Oligosaccharide Chain OE**Bond lengths****Bond angles****Torsions****Rings**

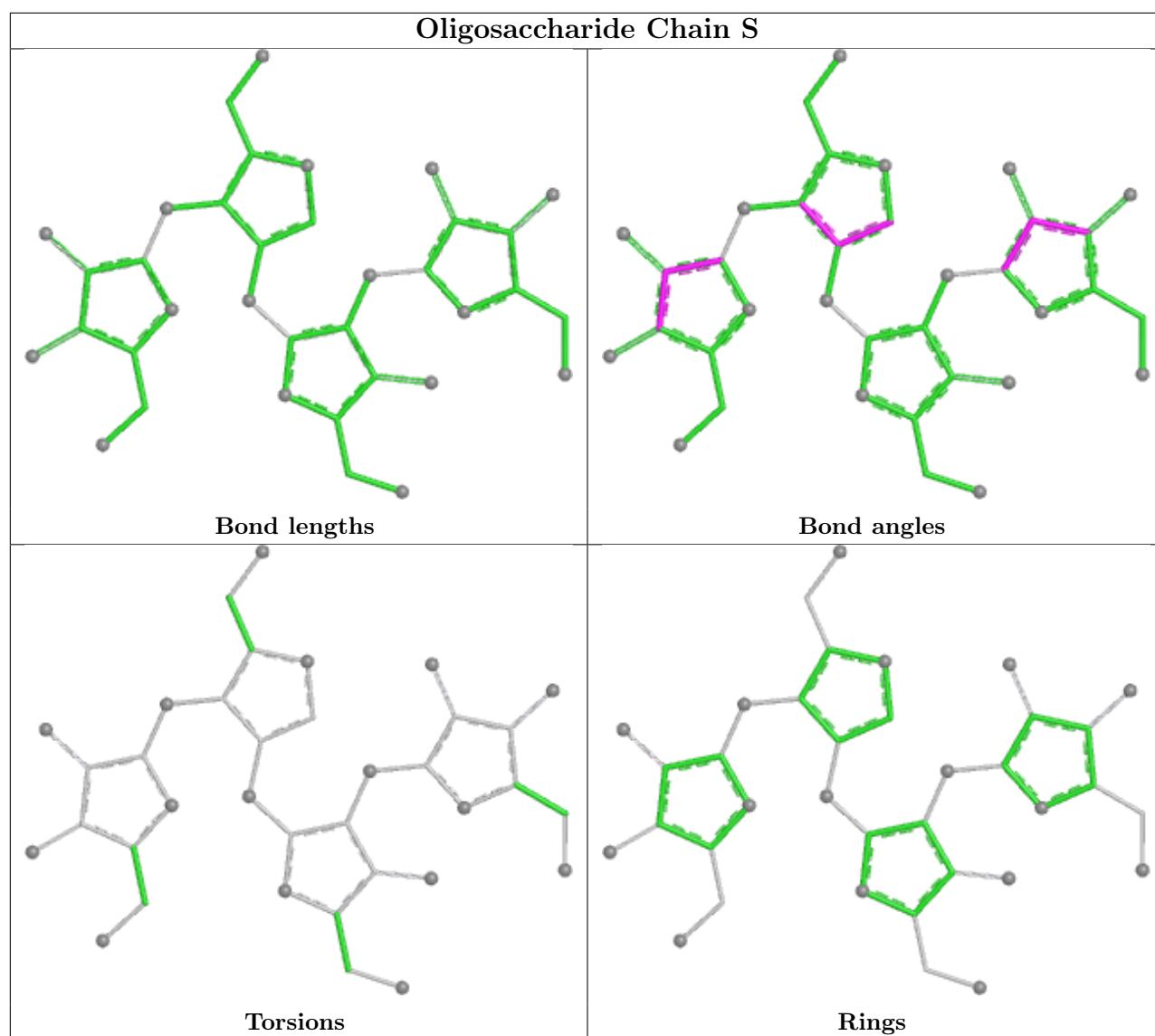


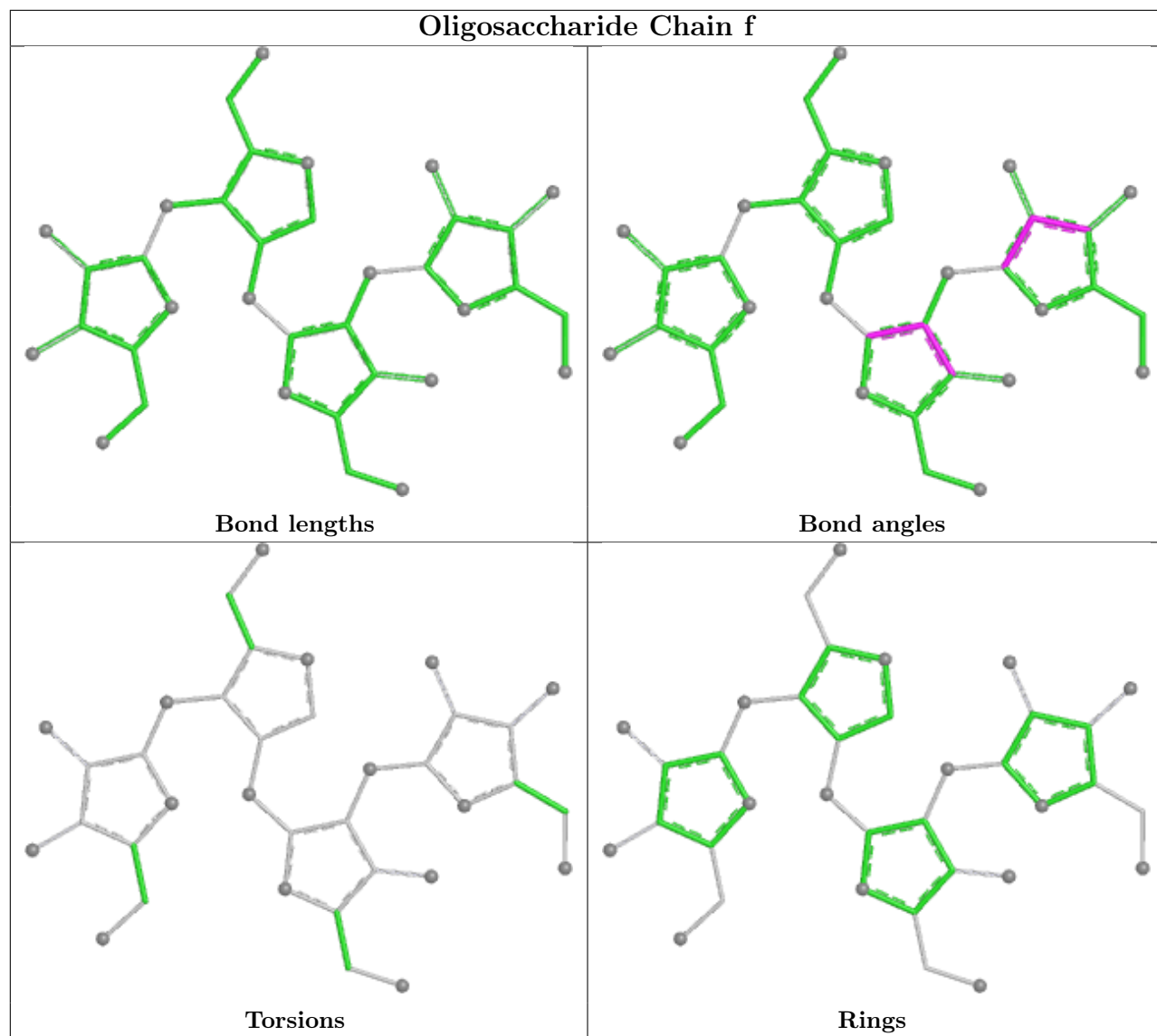


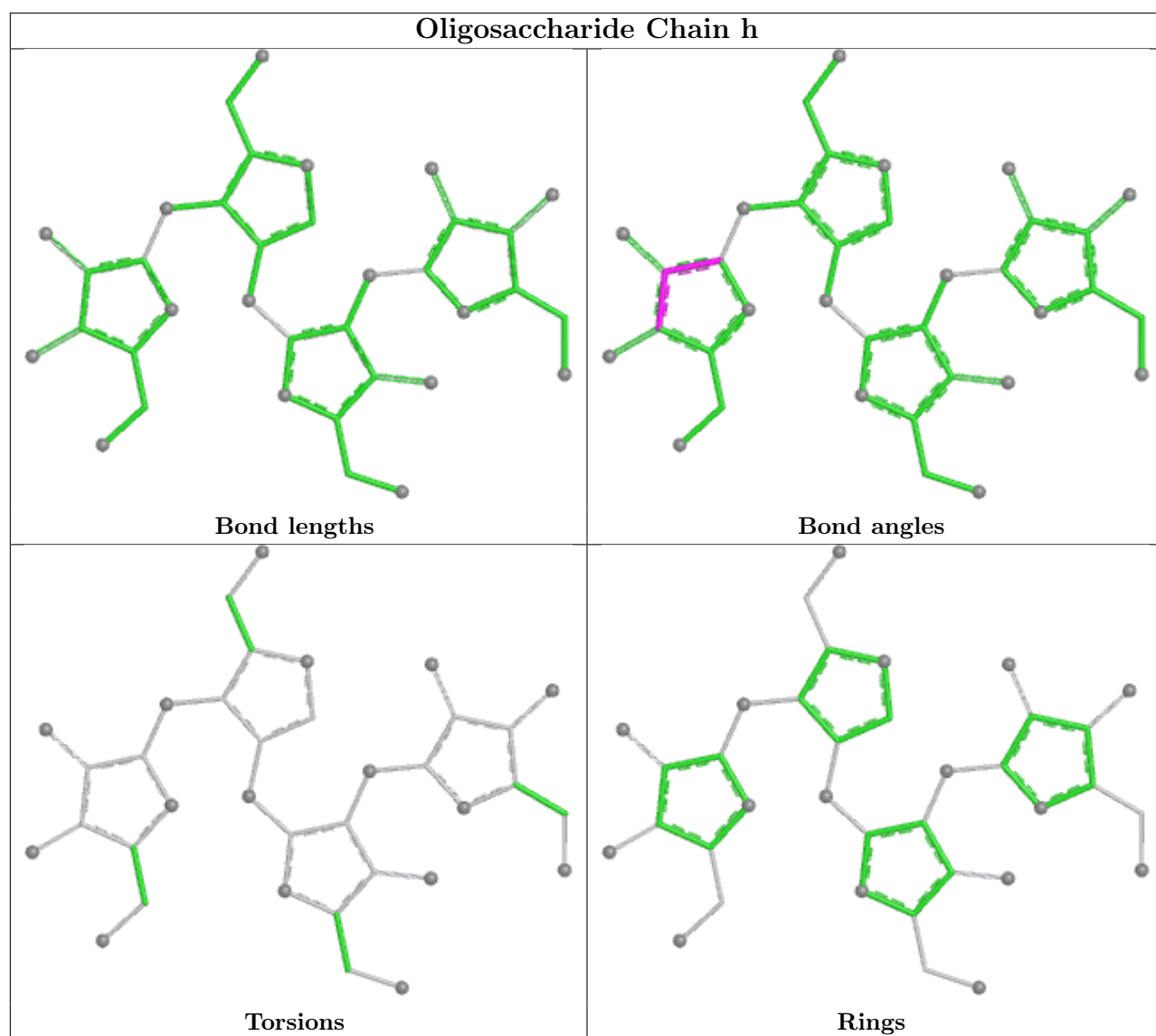


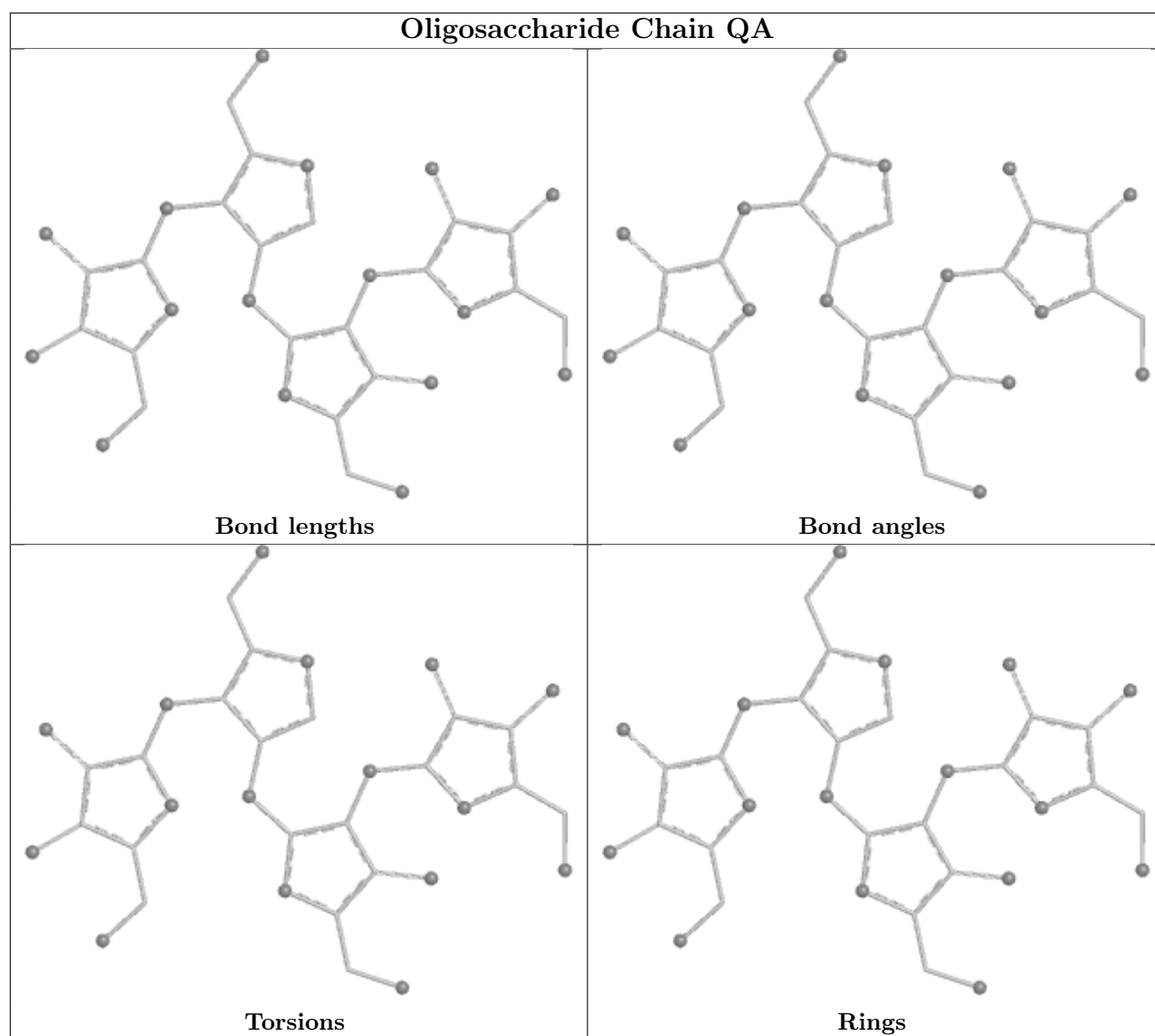


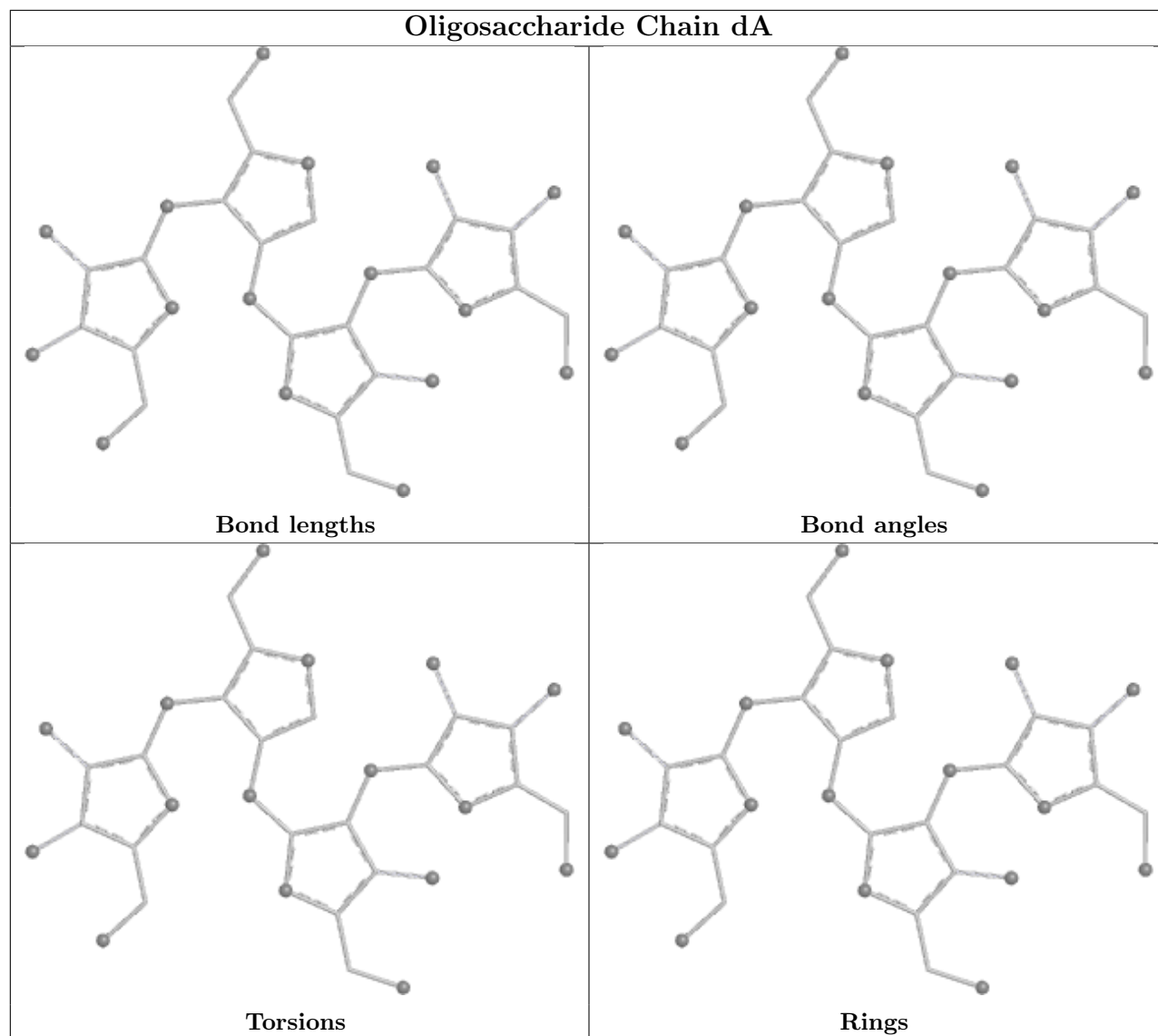


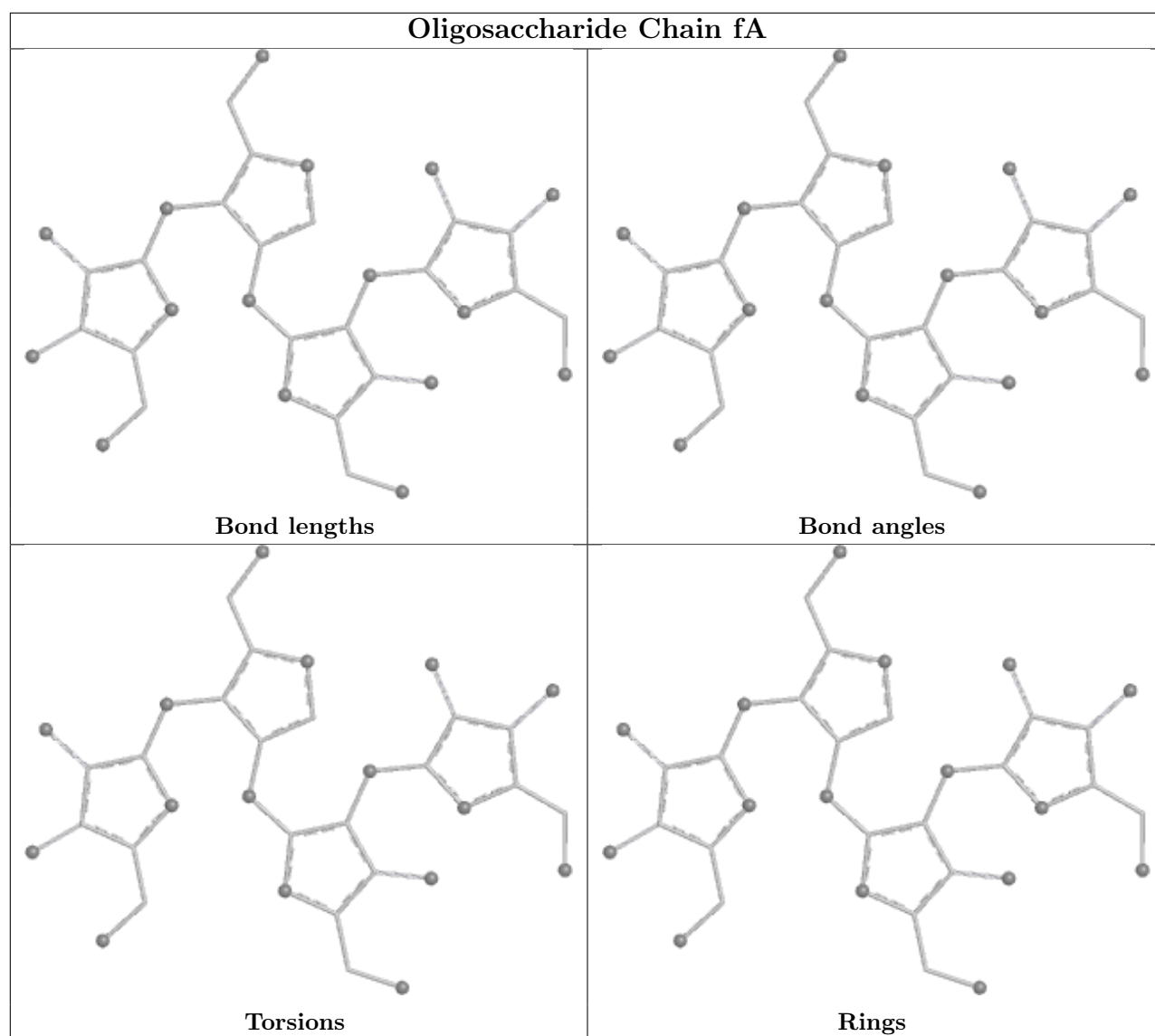


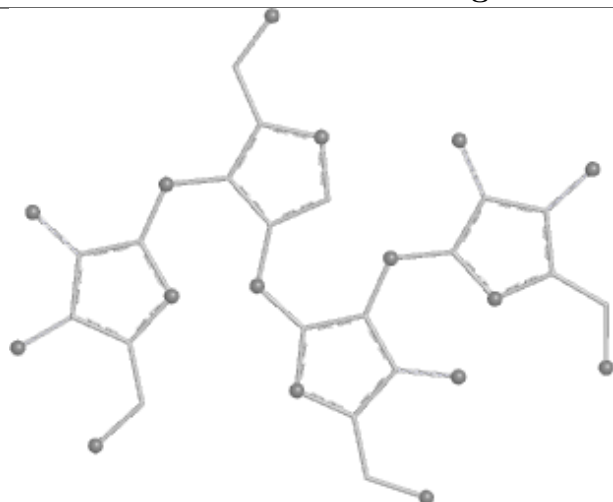
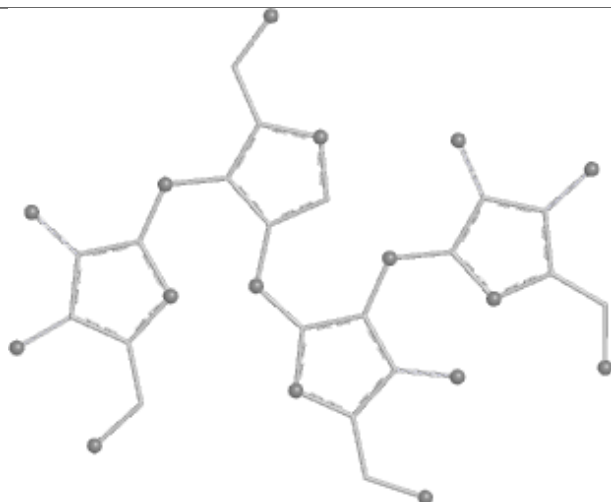
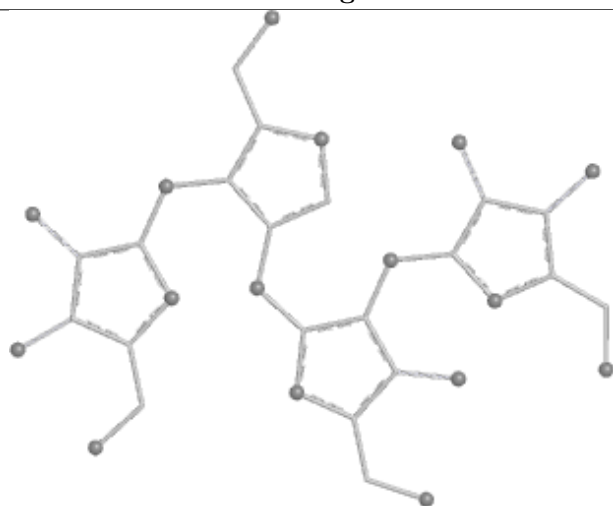
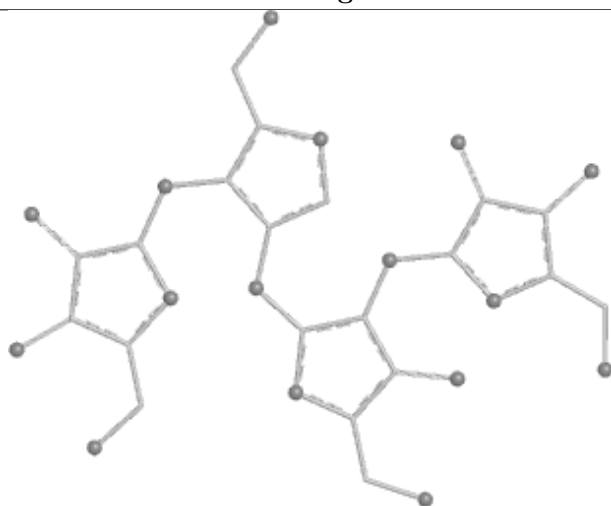


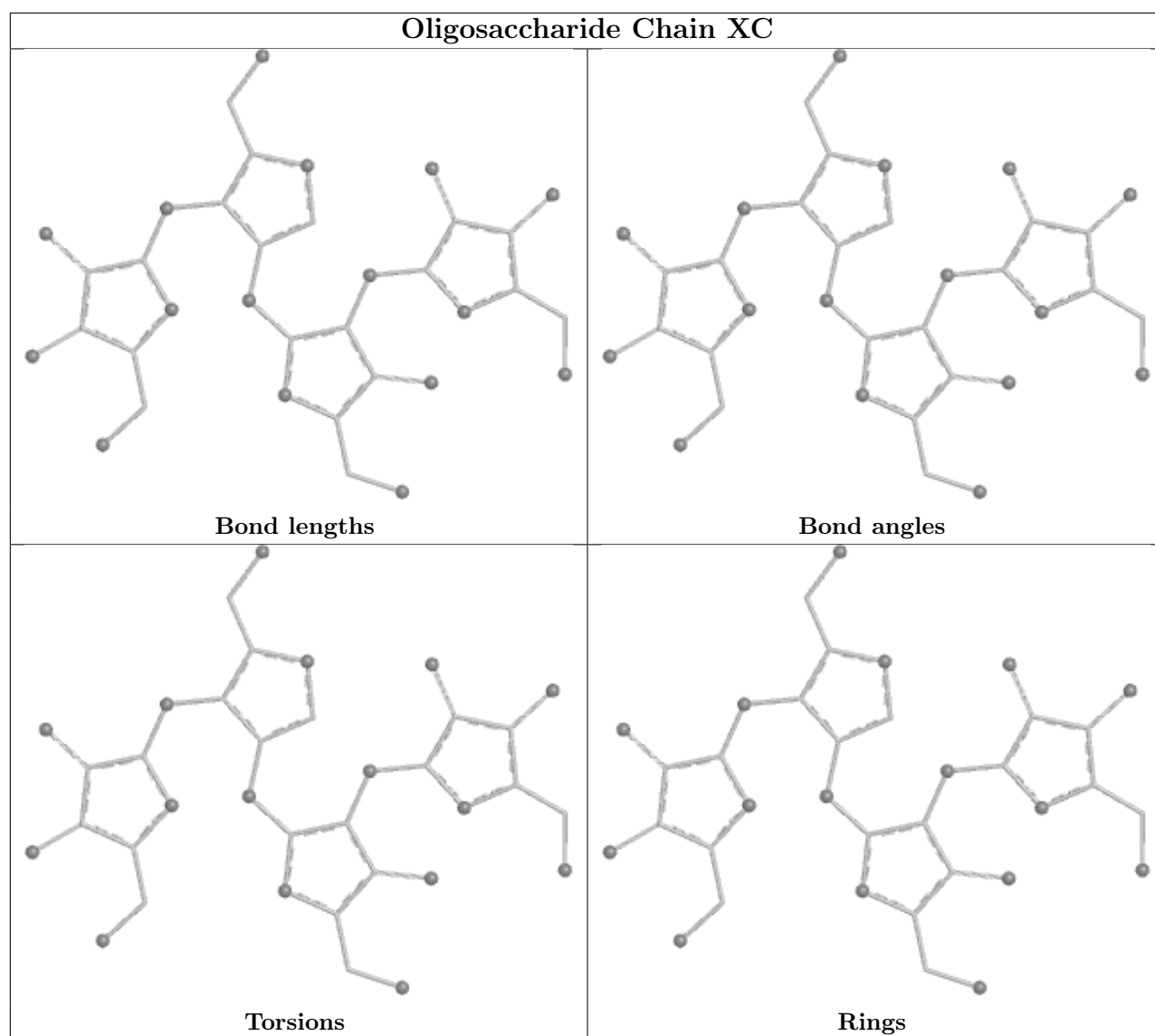


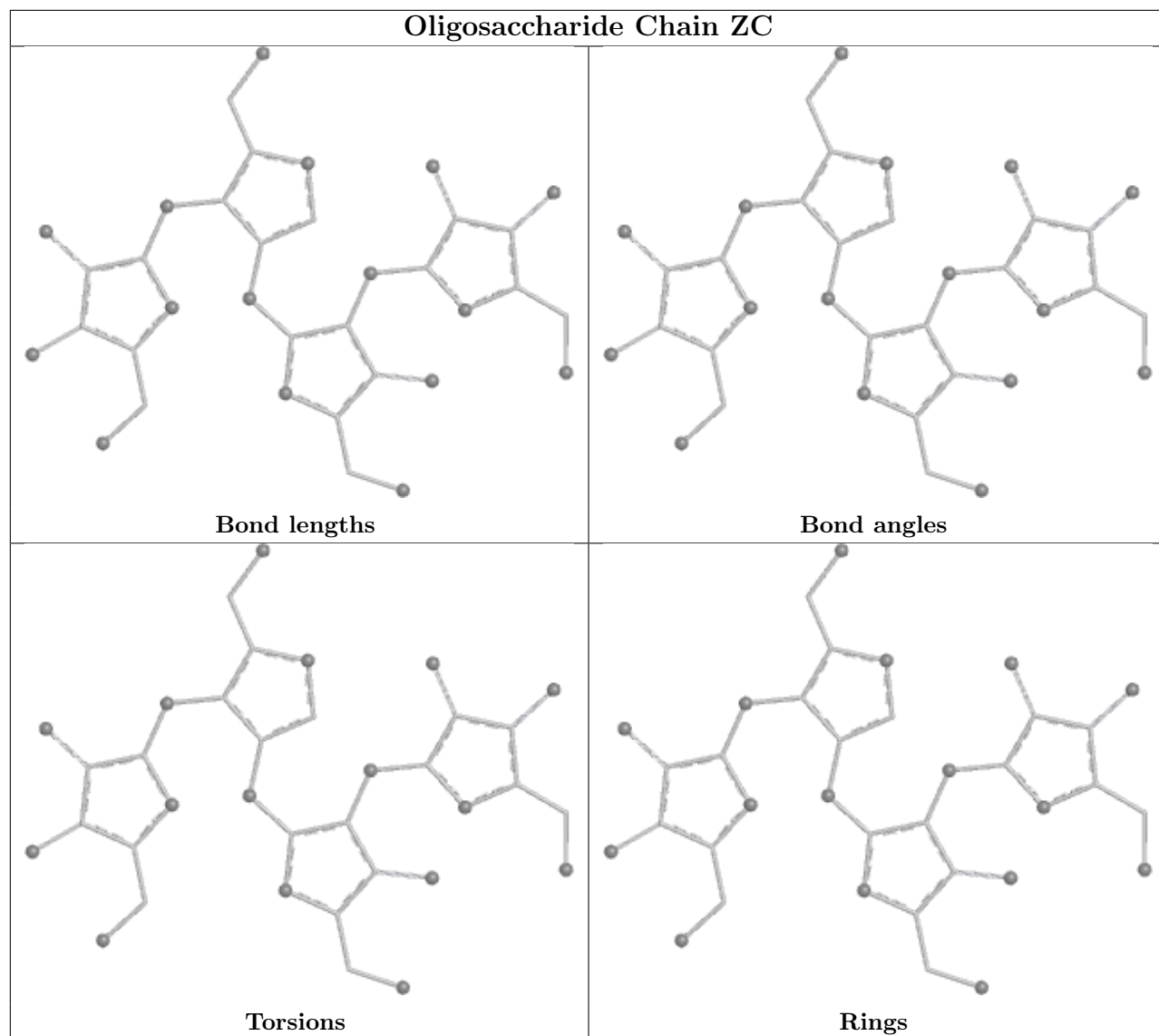


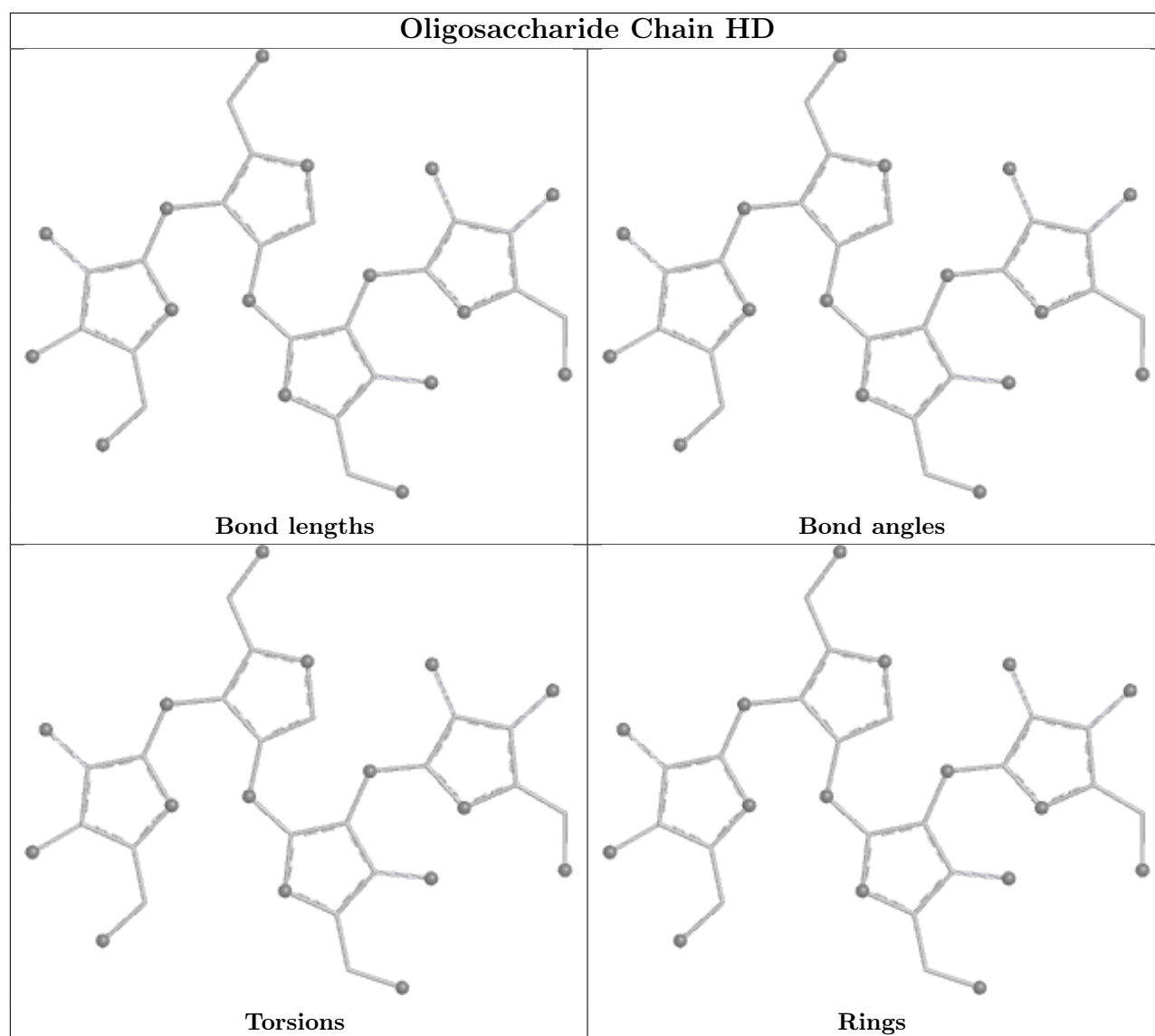


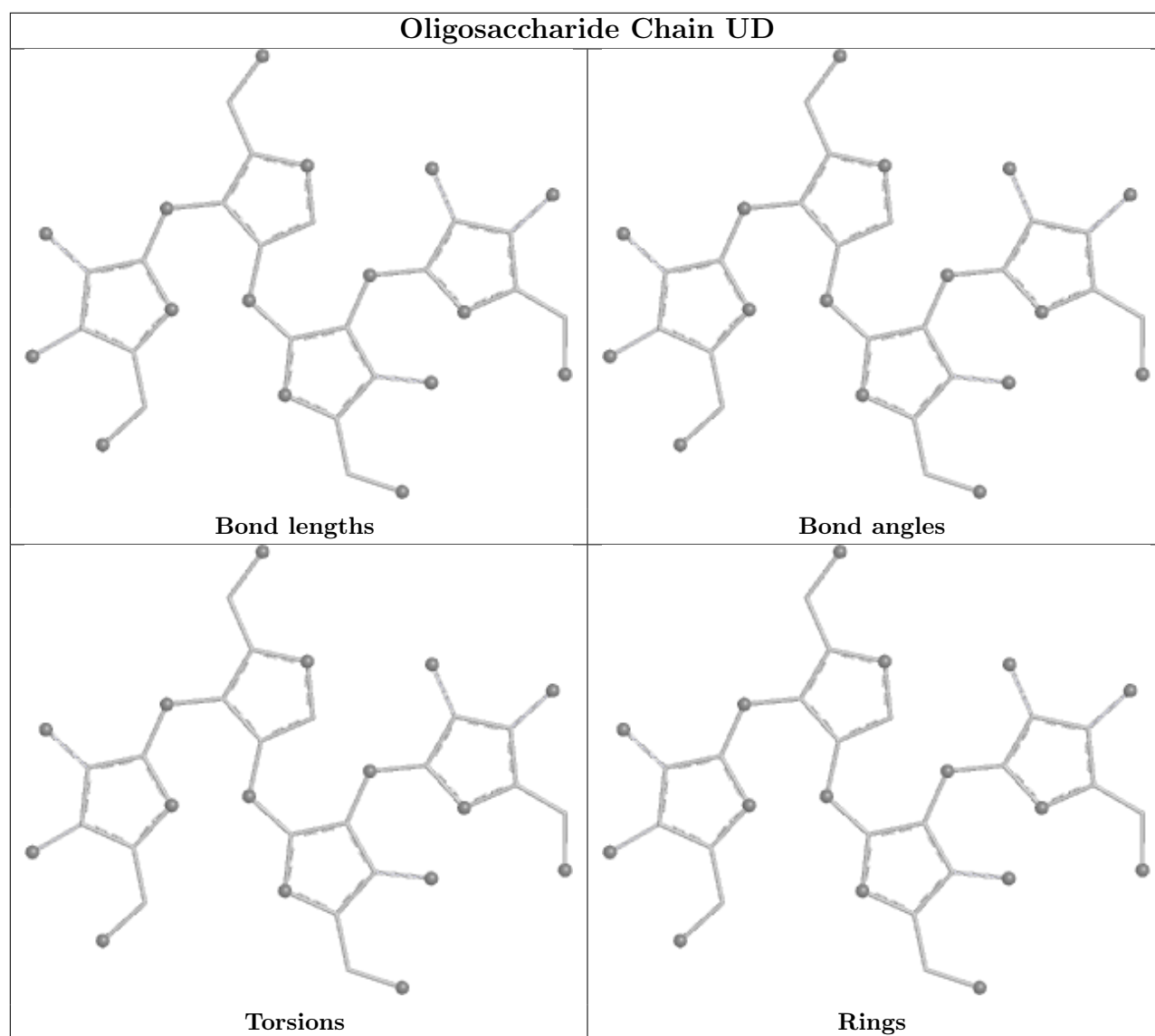


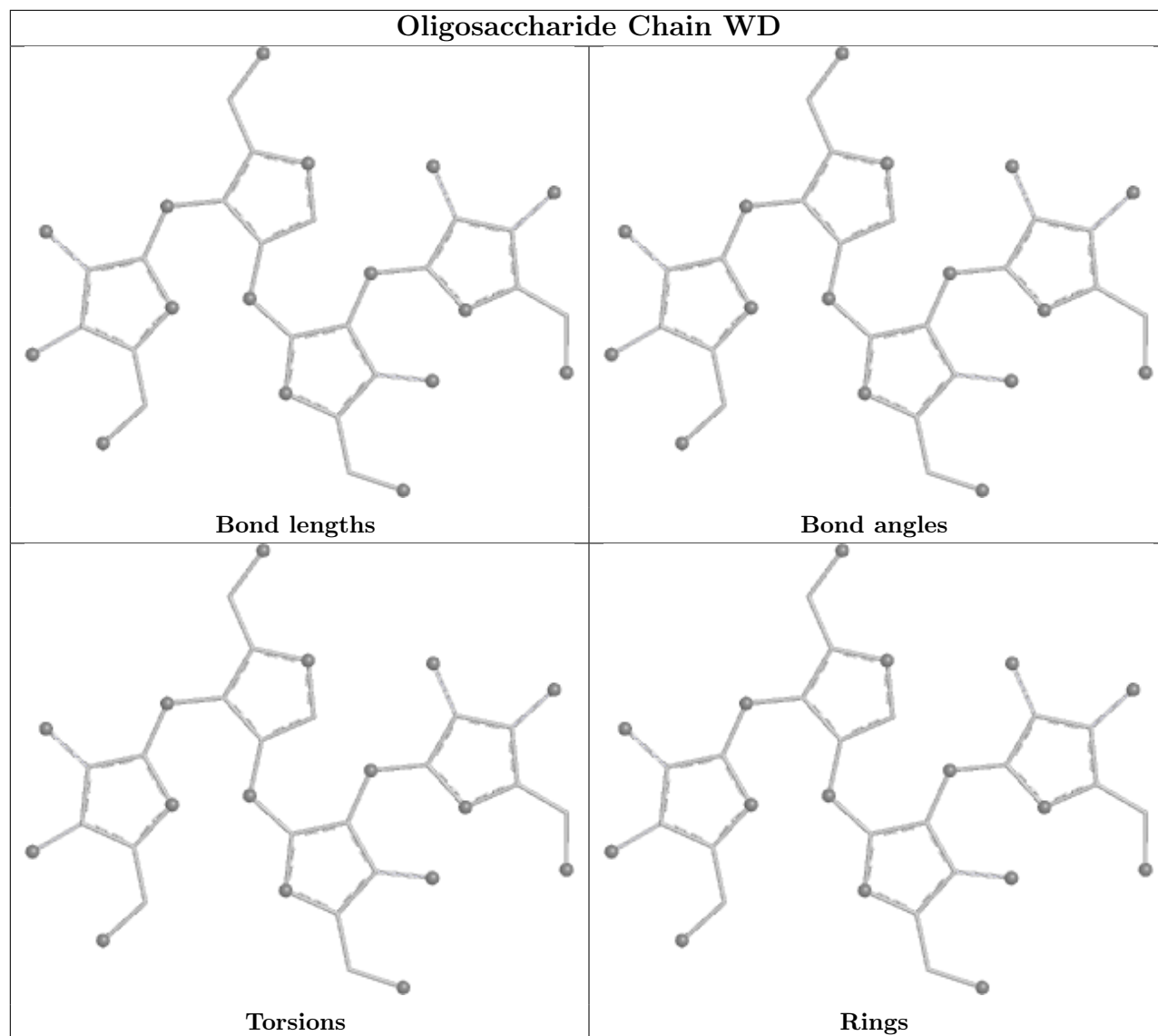
Oligosaccharide Chain KC**Bond lengths****Bond angles****Torsions****Rings**

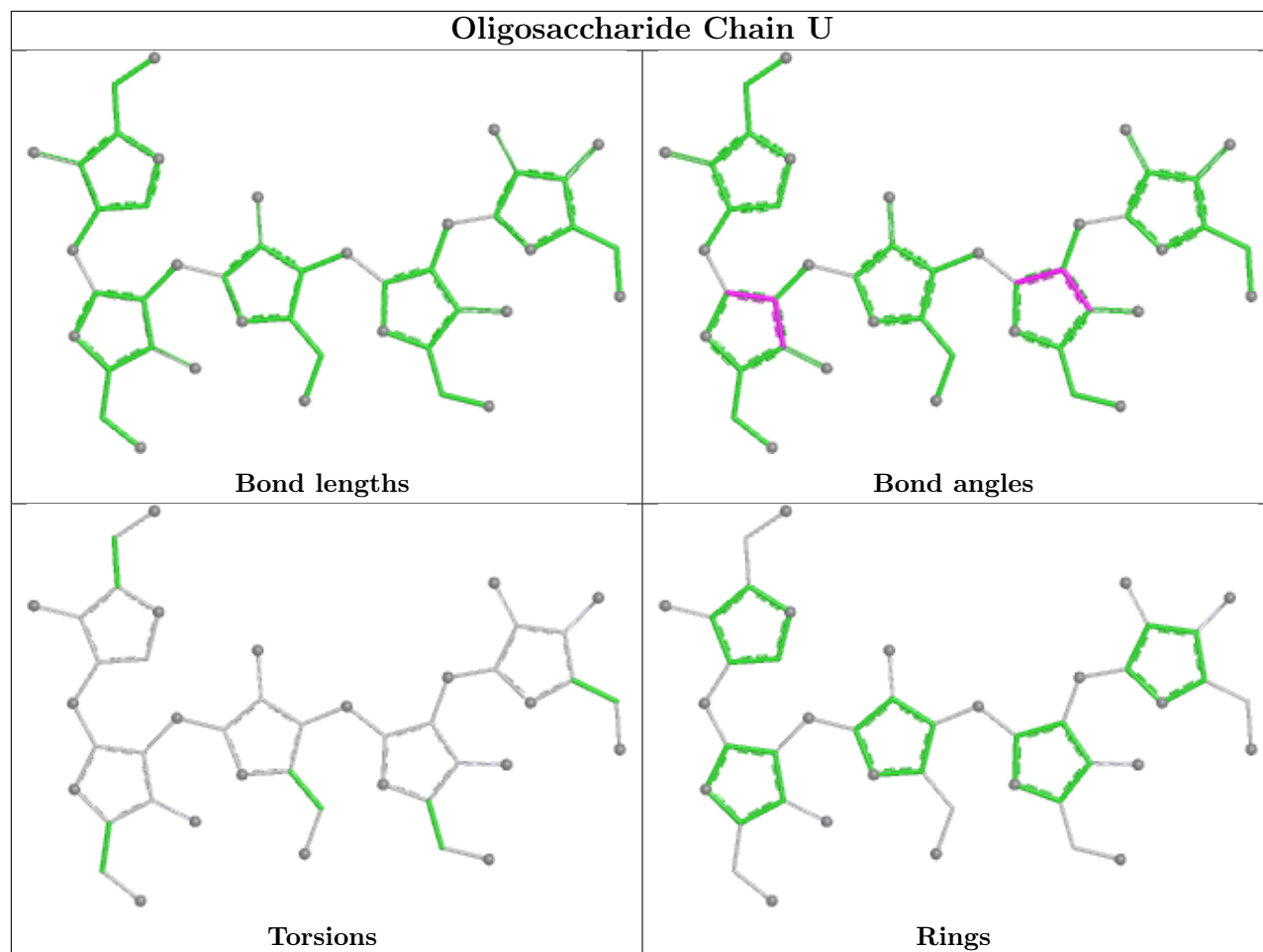


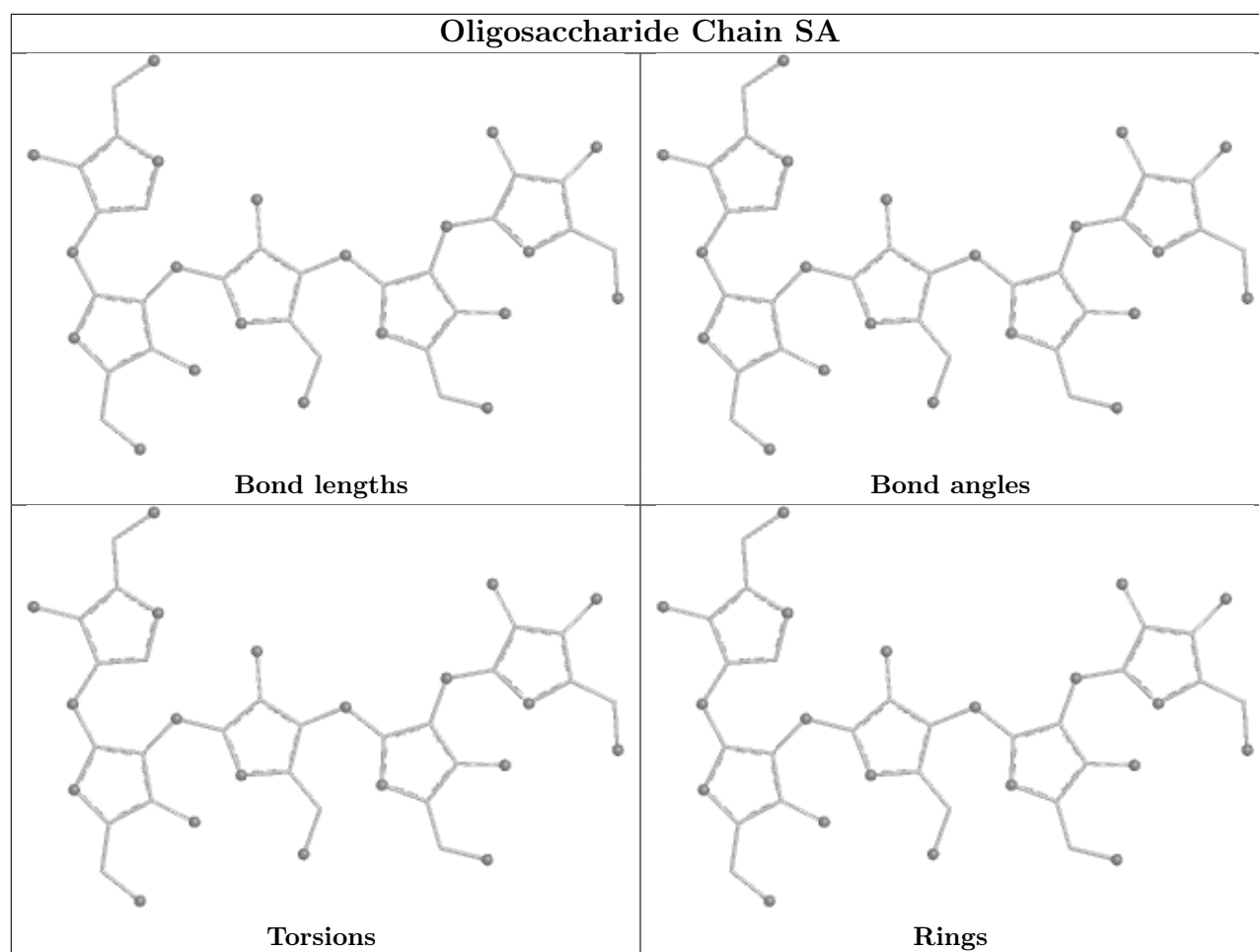


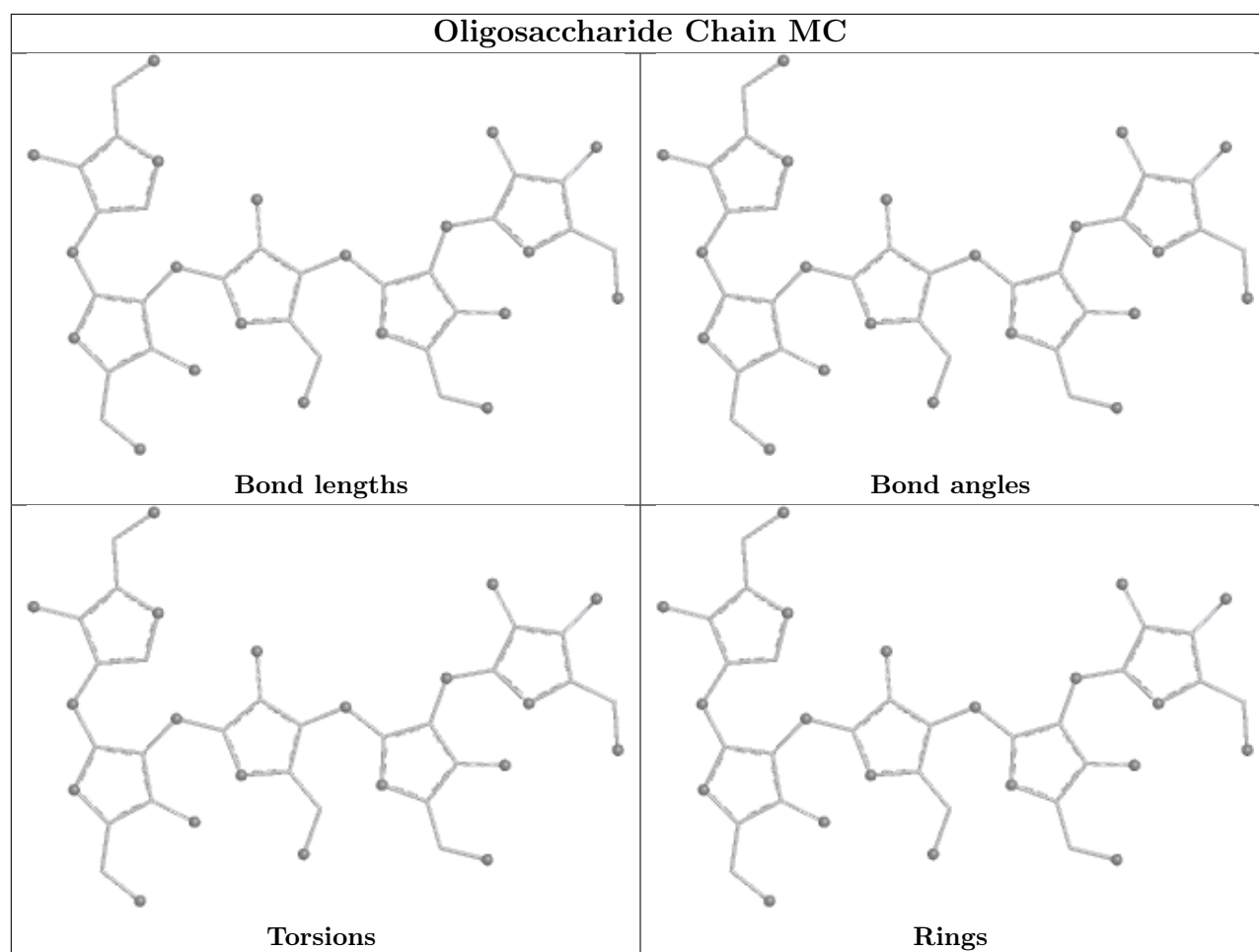


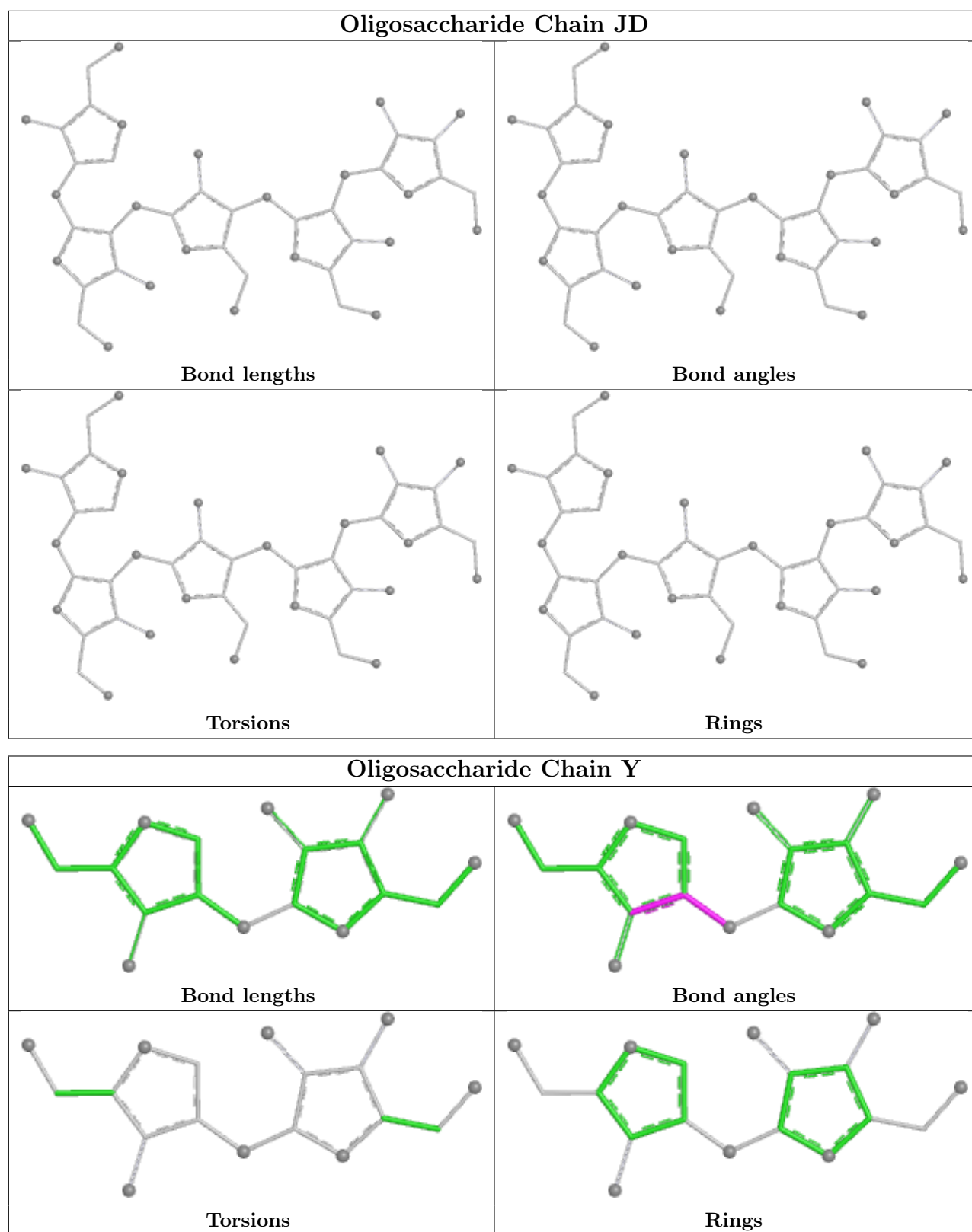


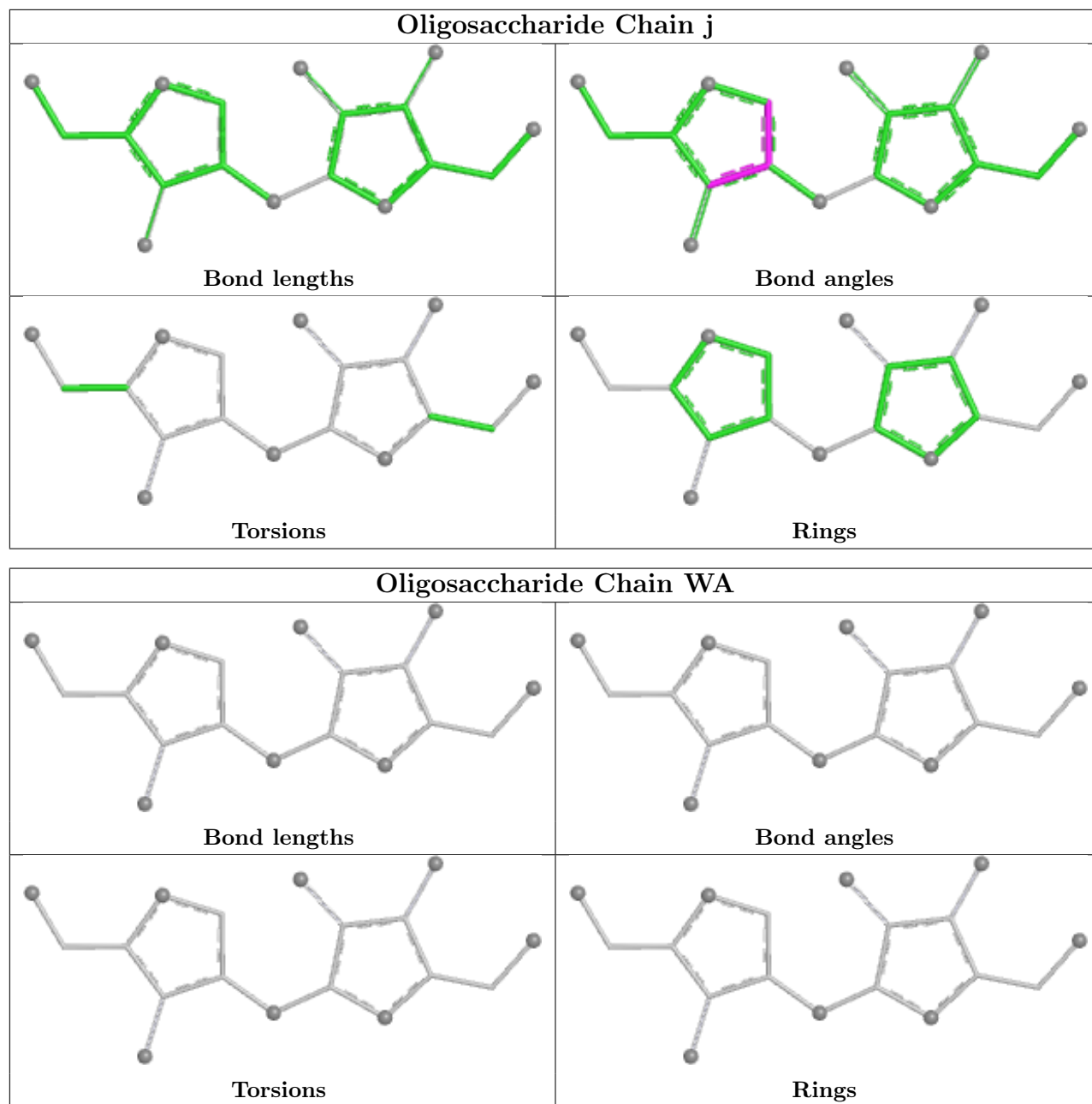


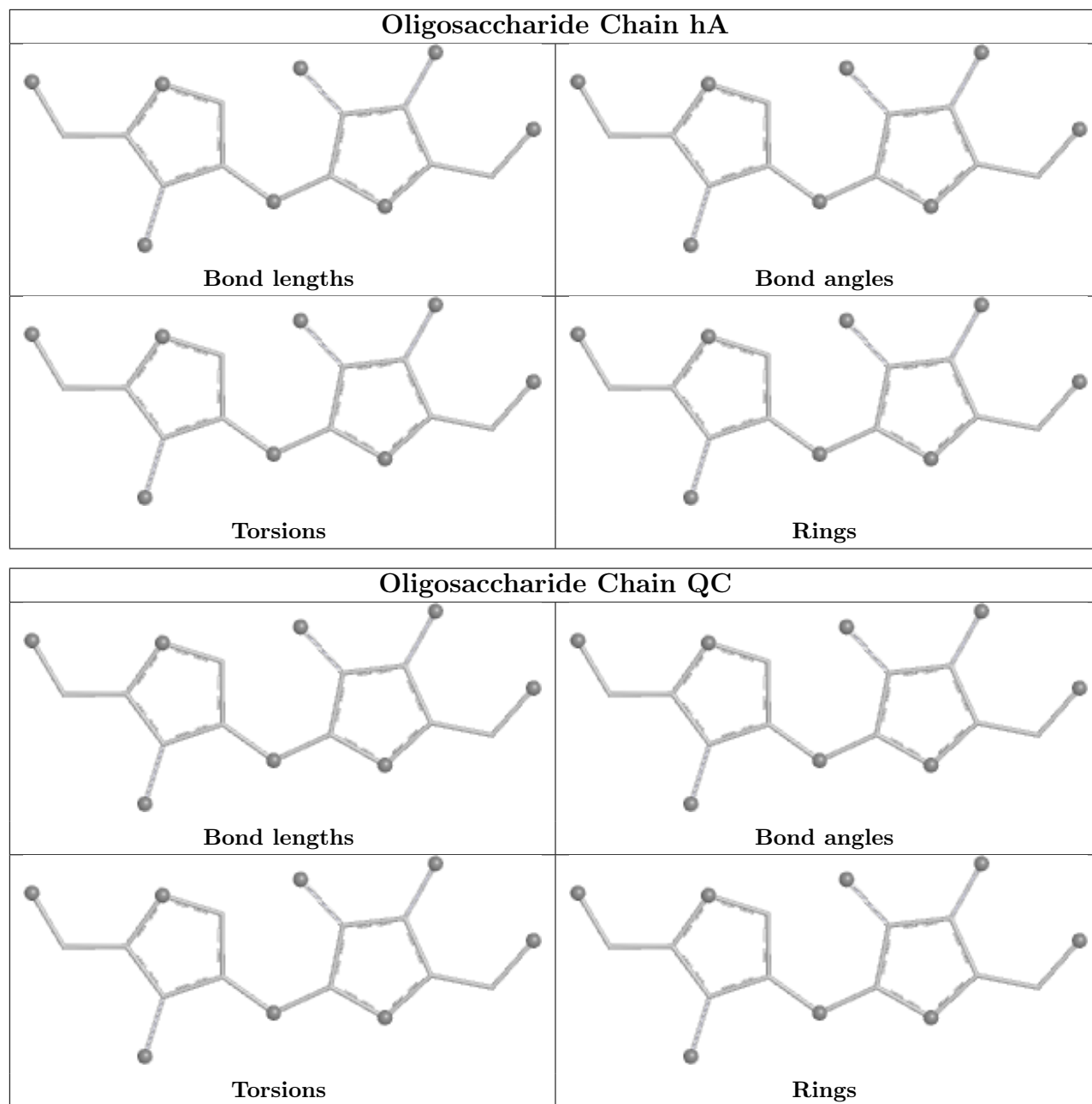


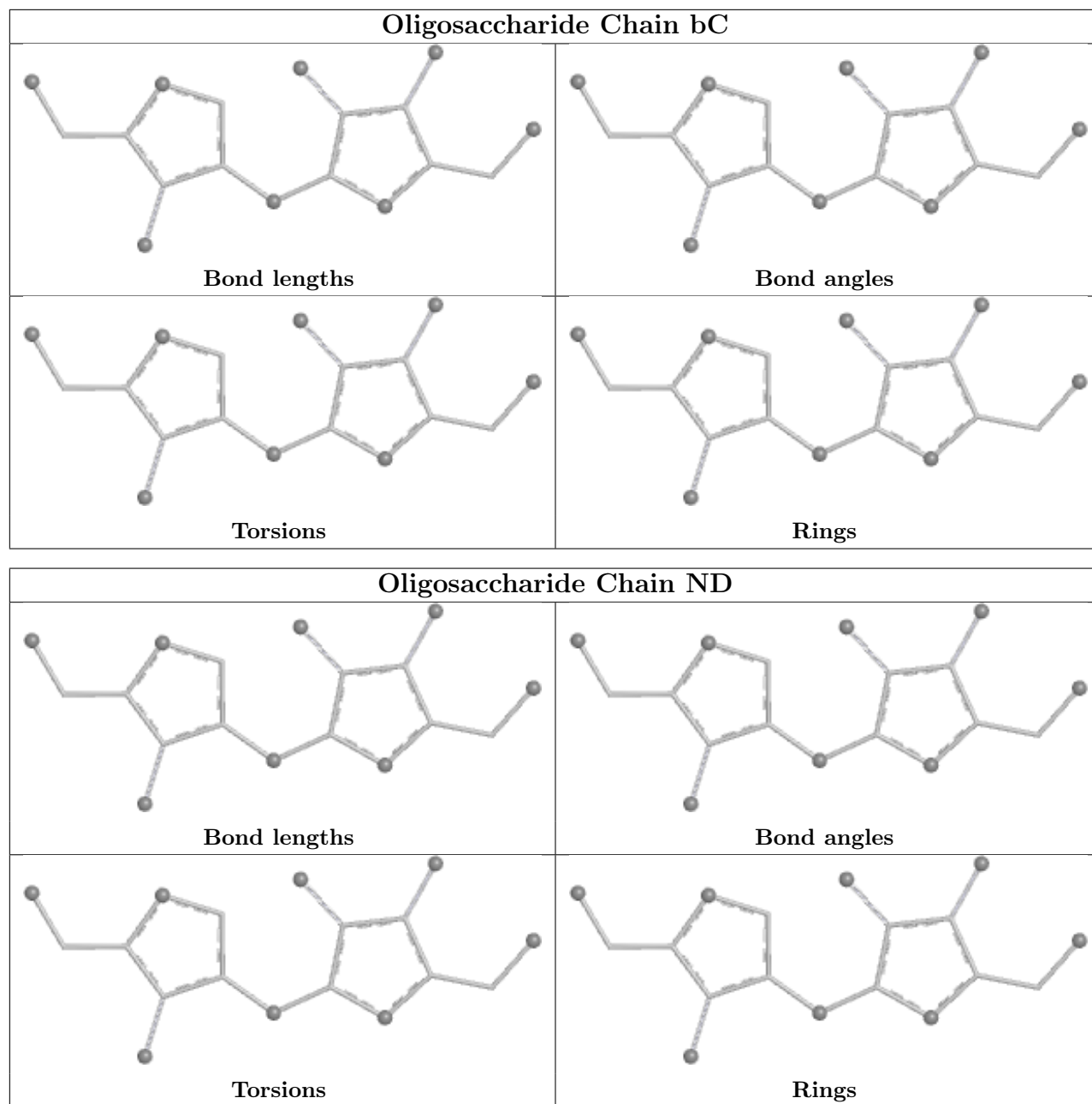


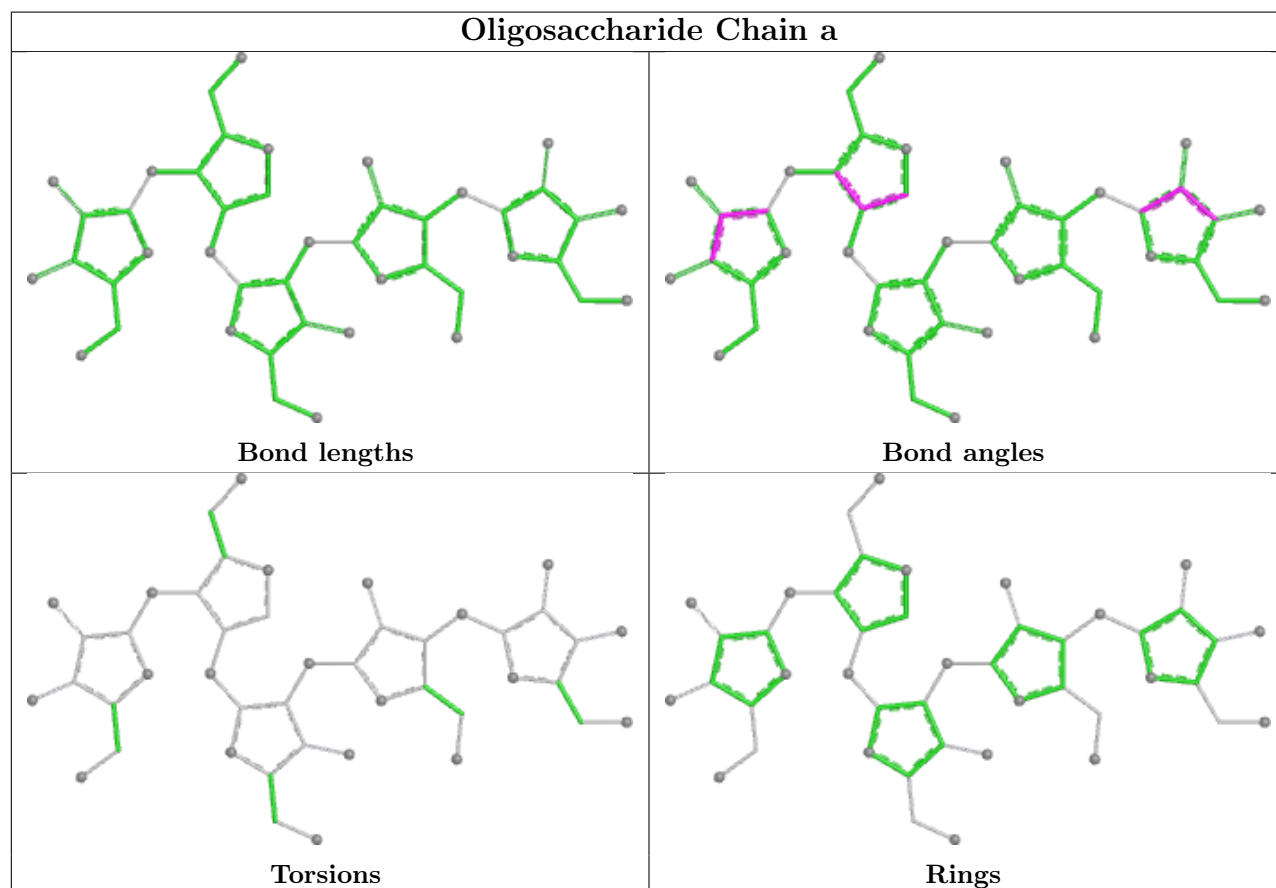
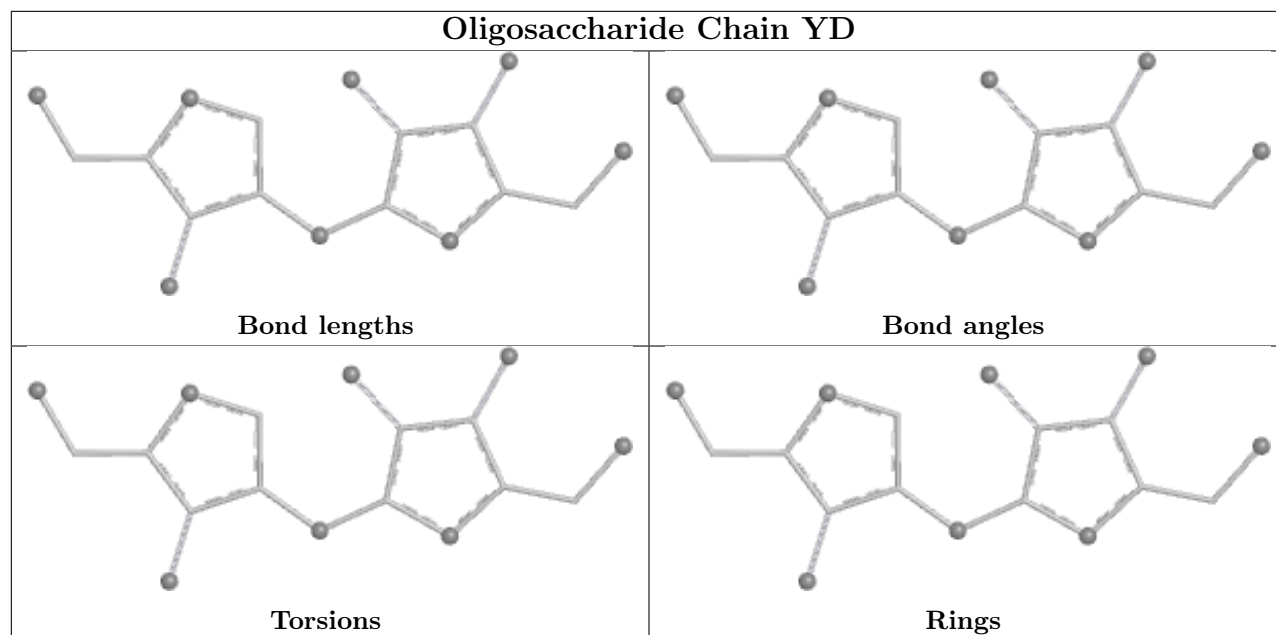


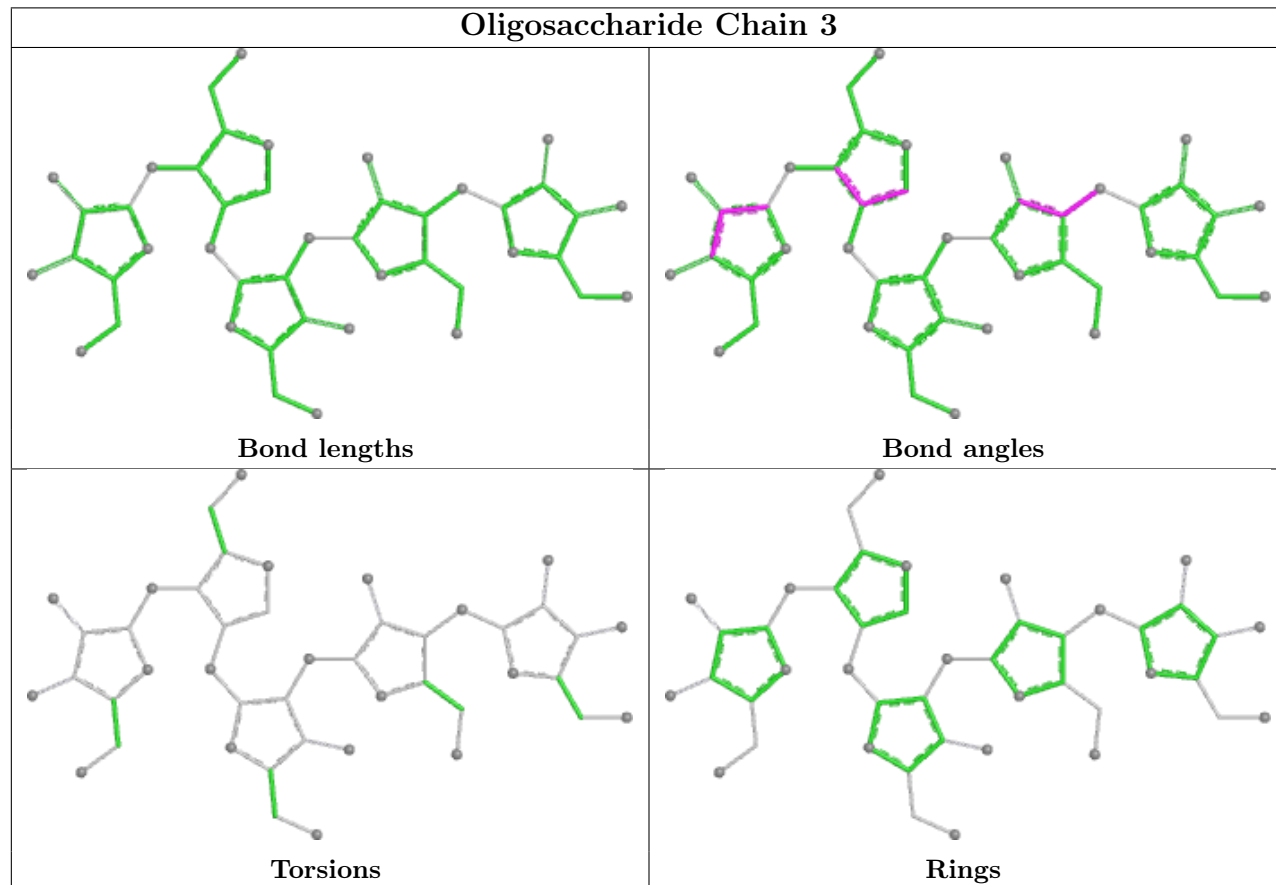
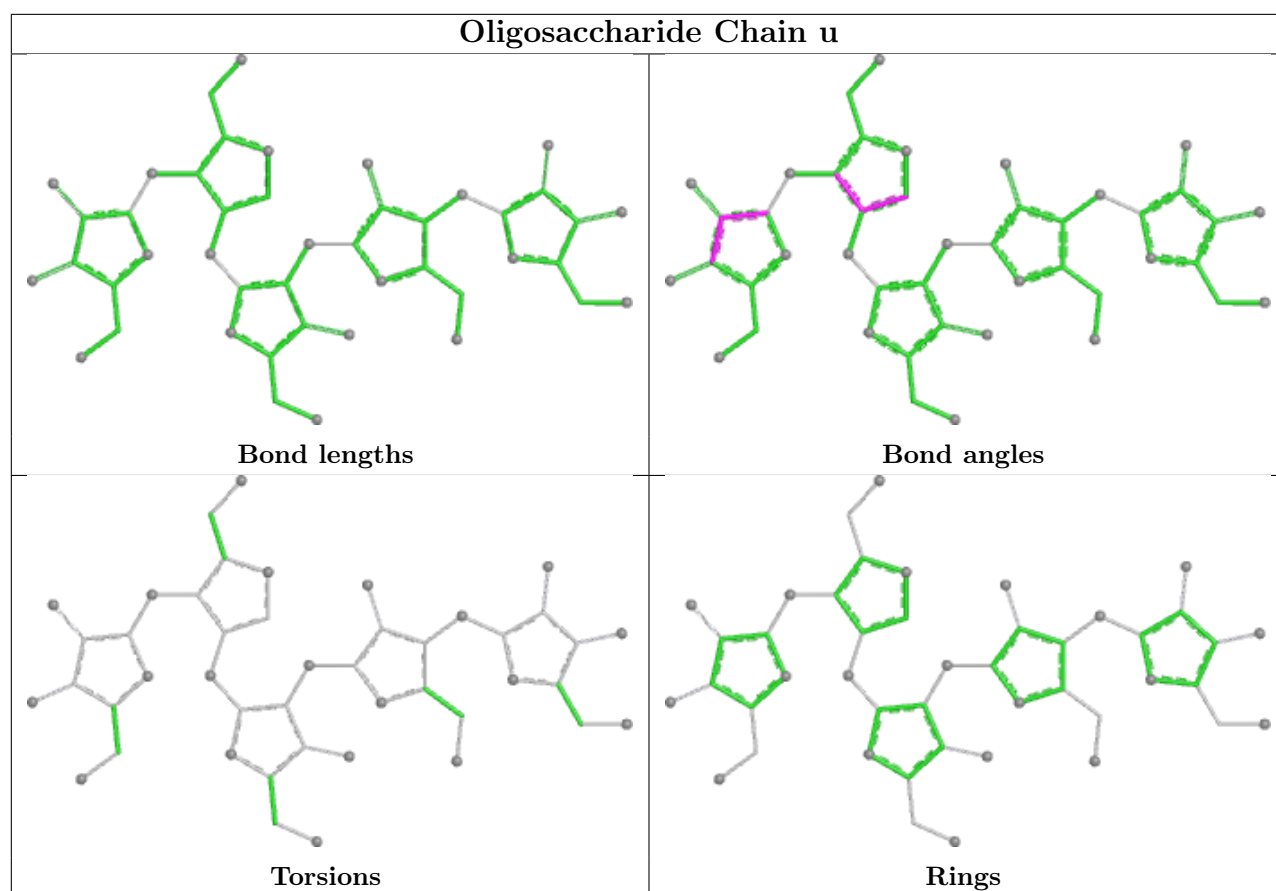


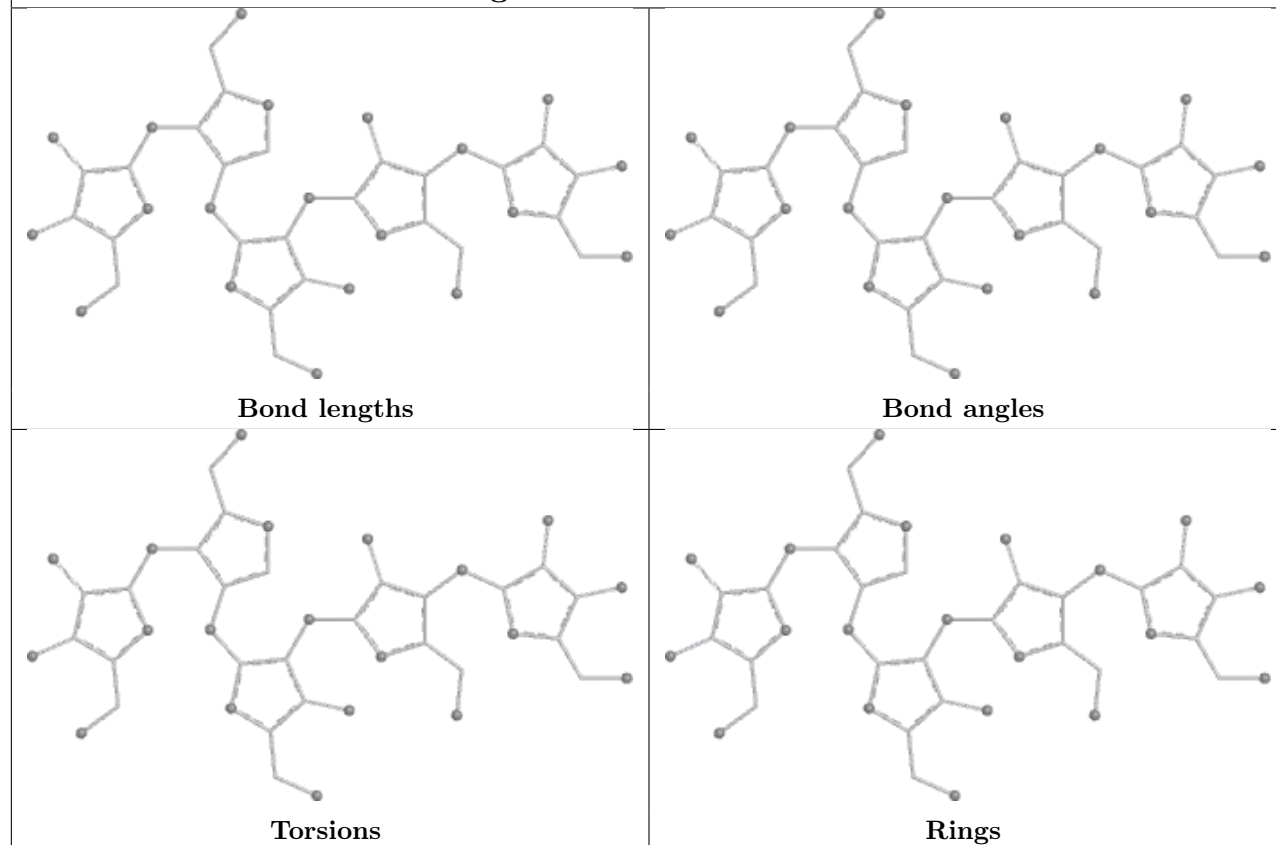
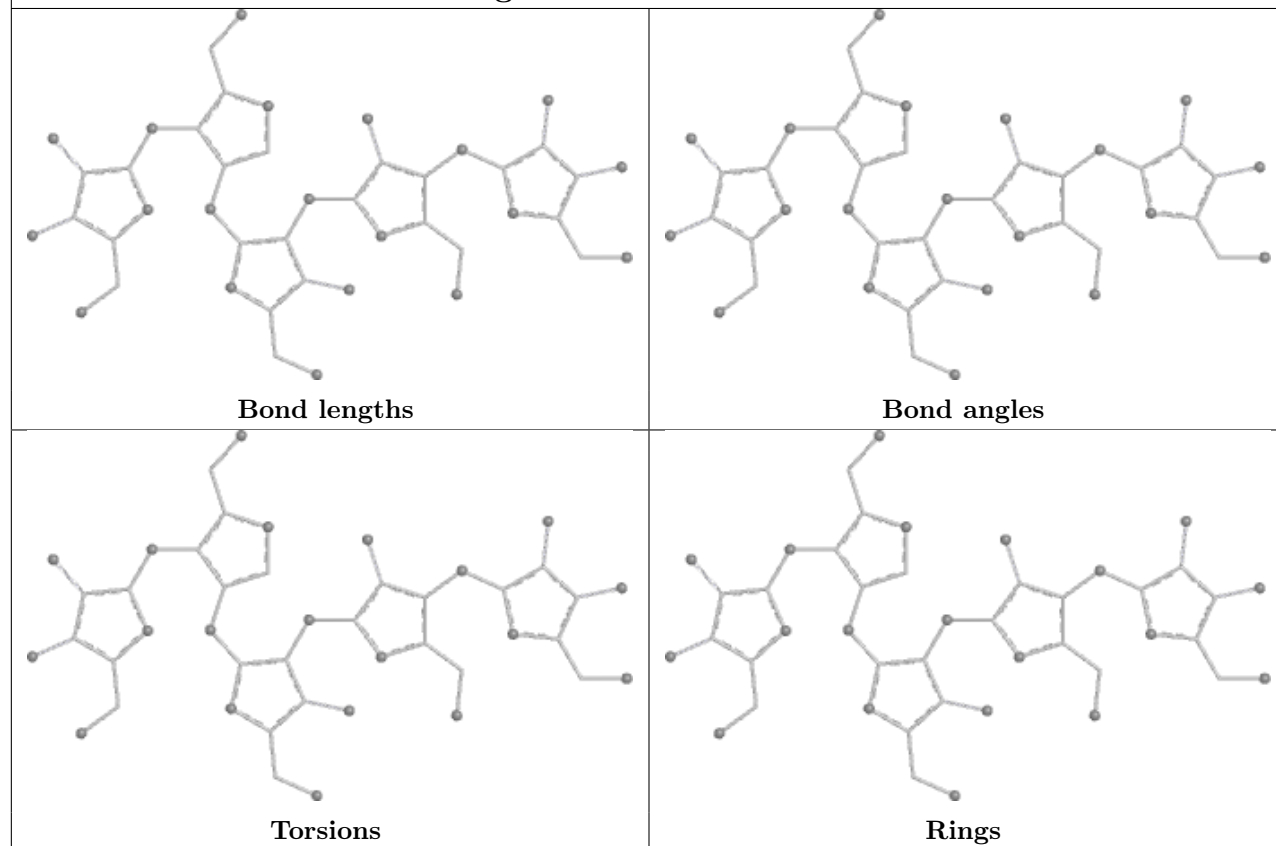


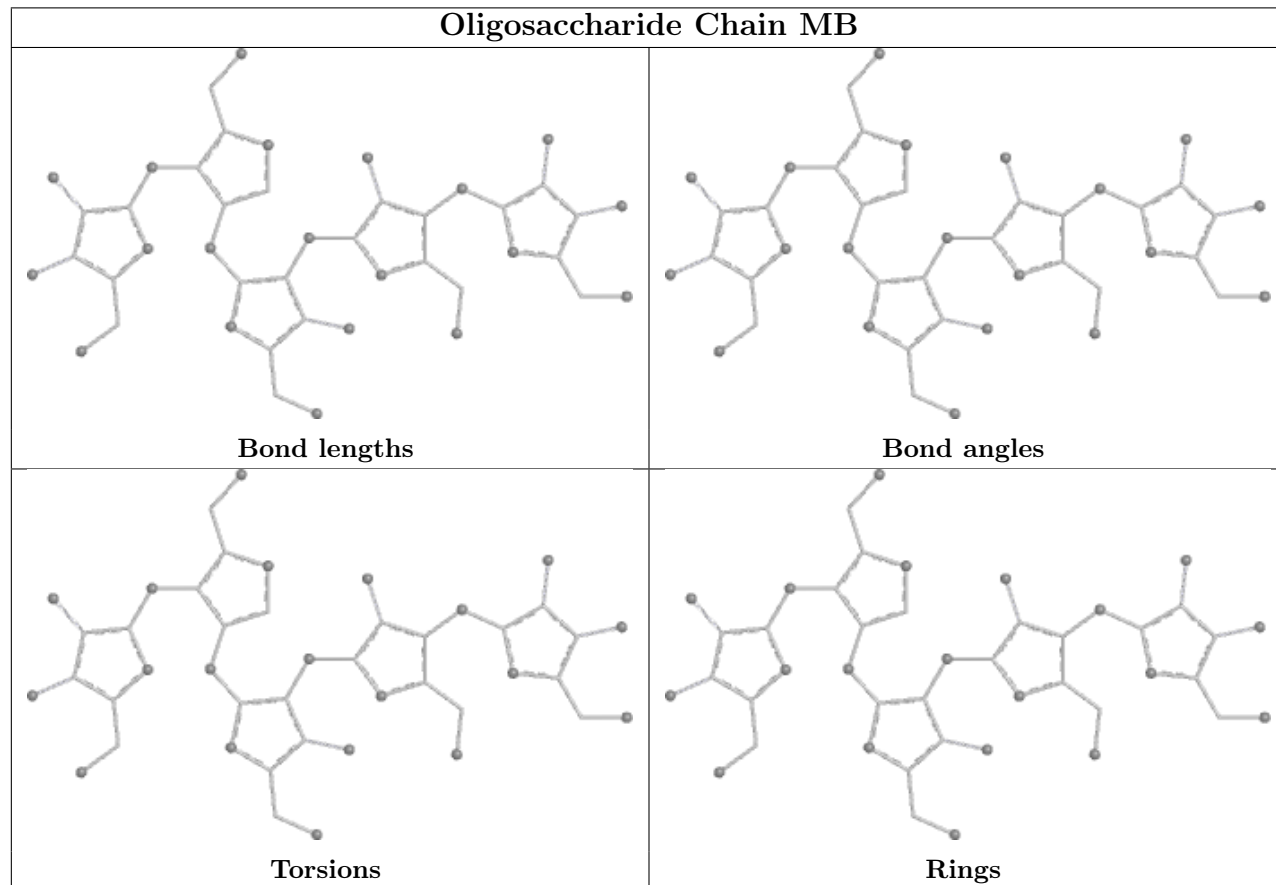
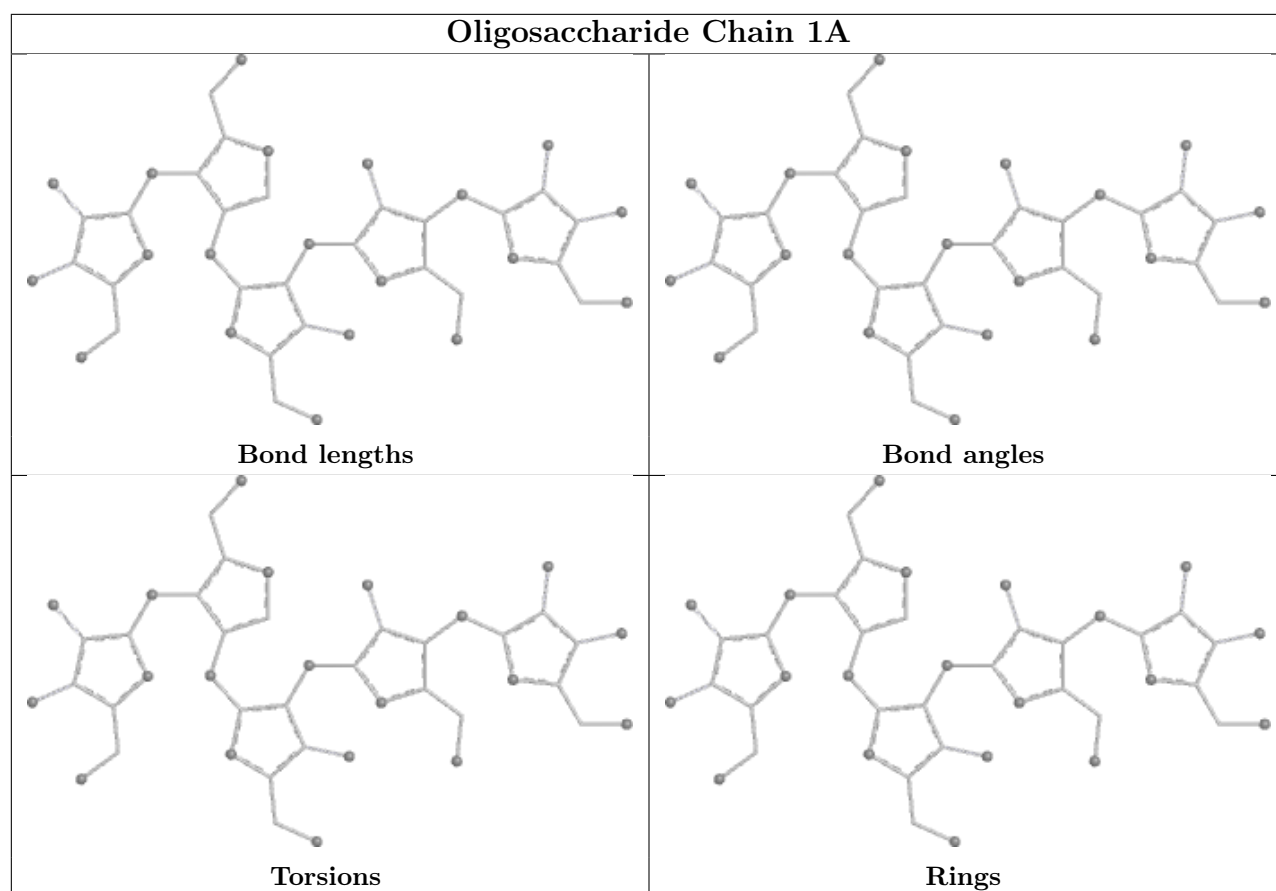


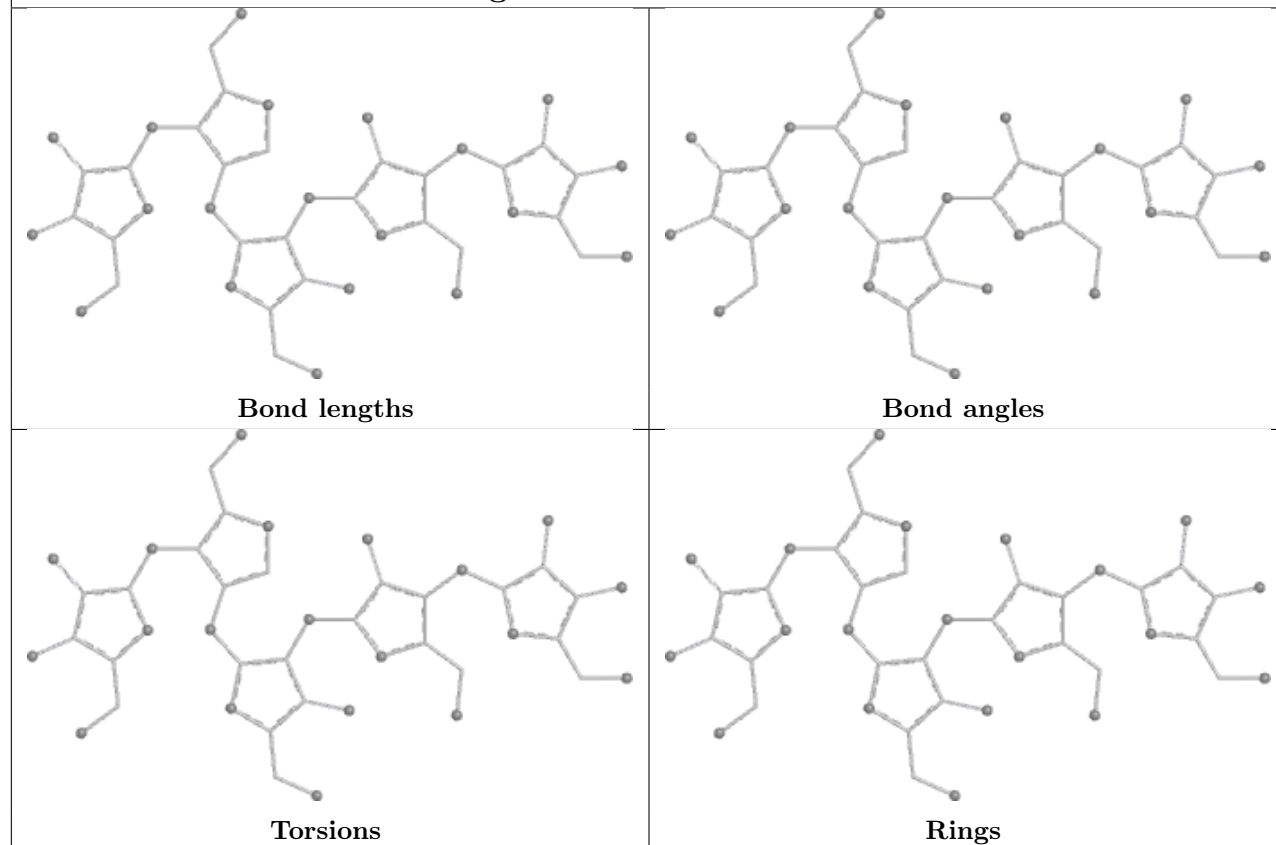
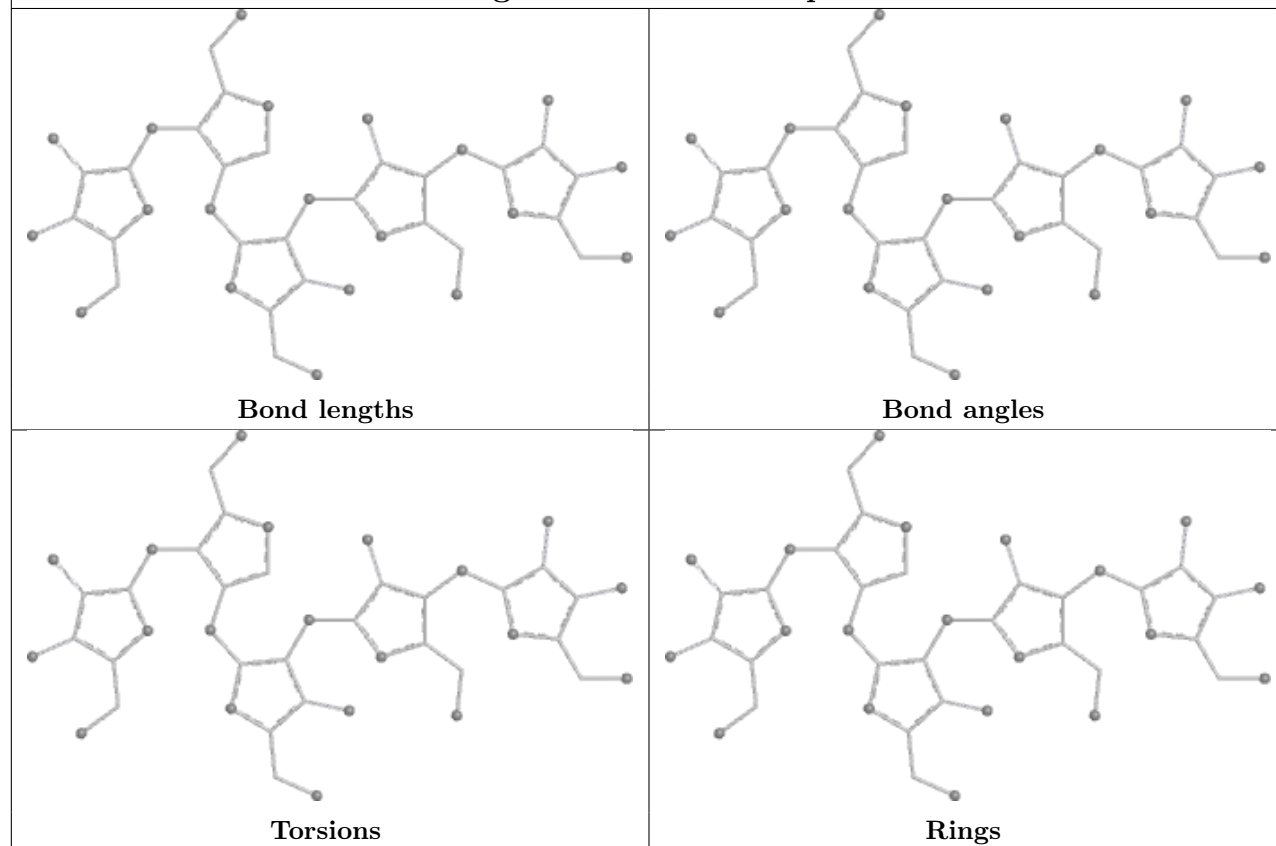


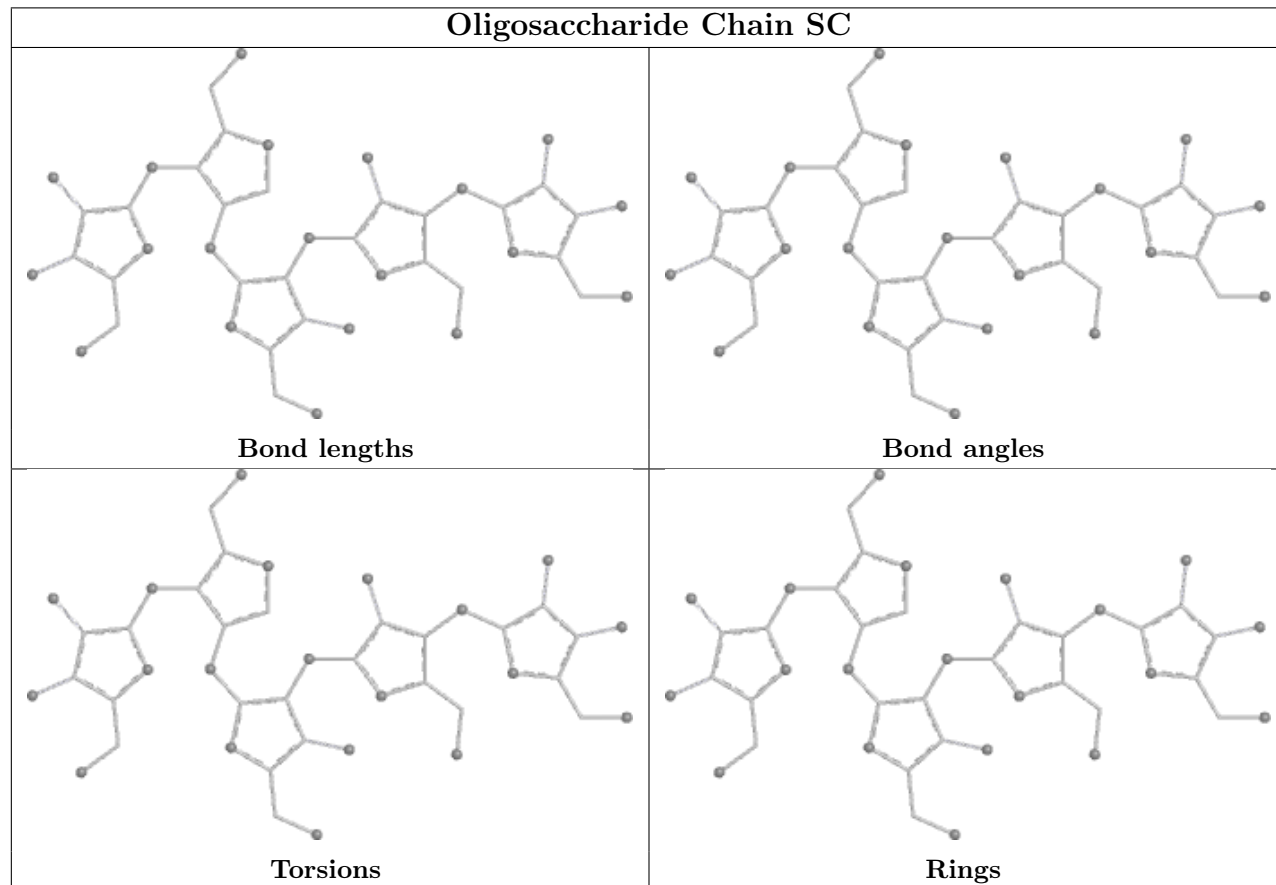
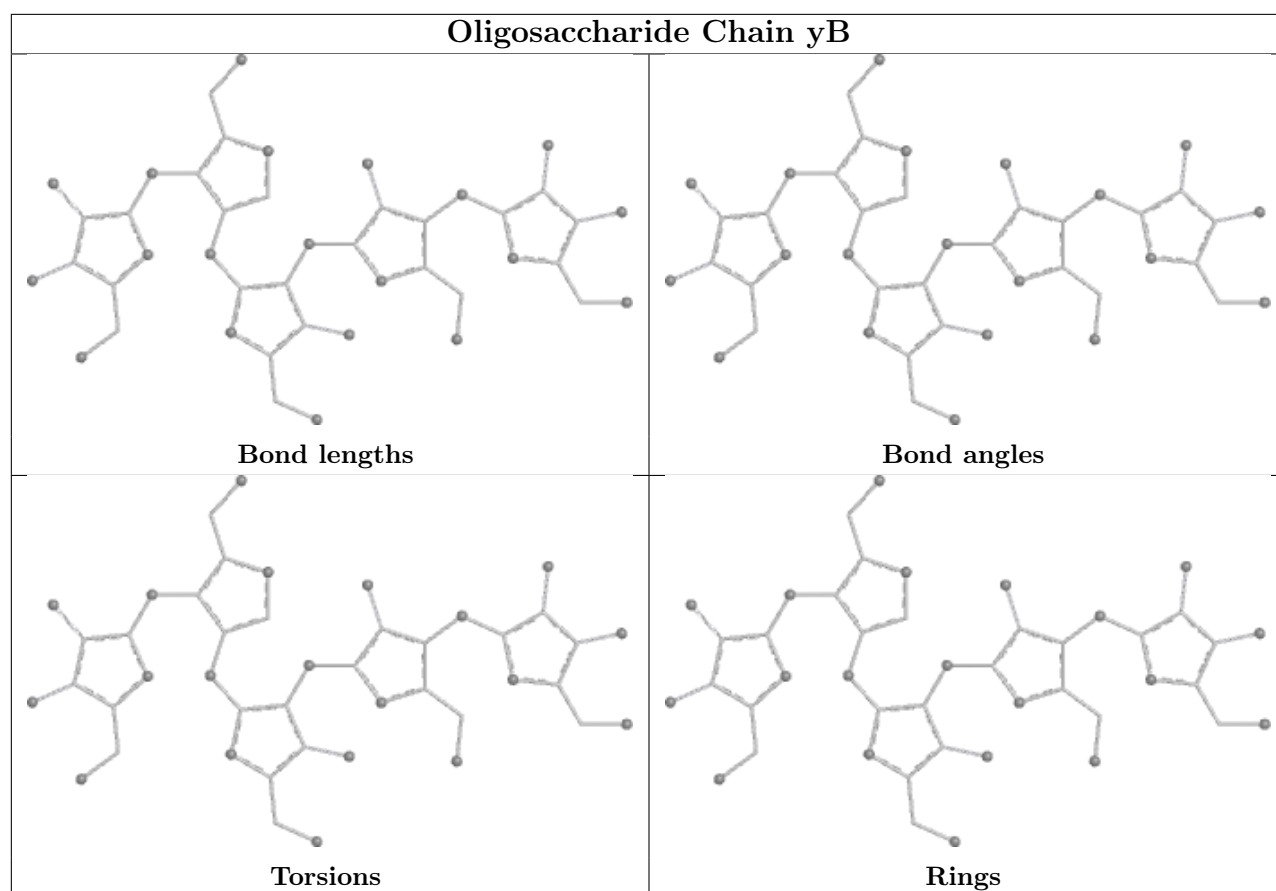


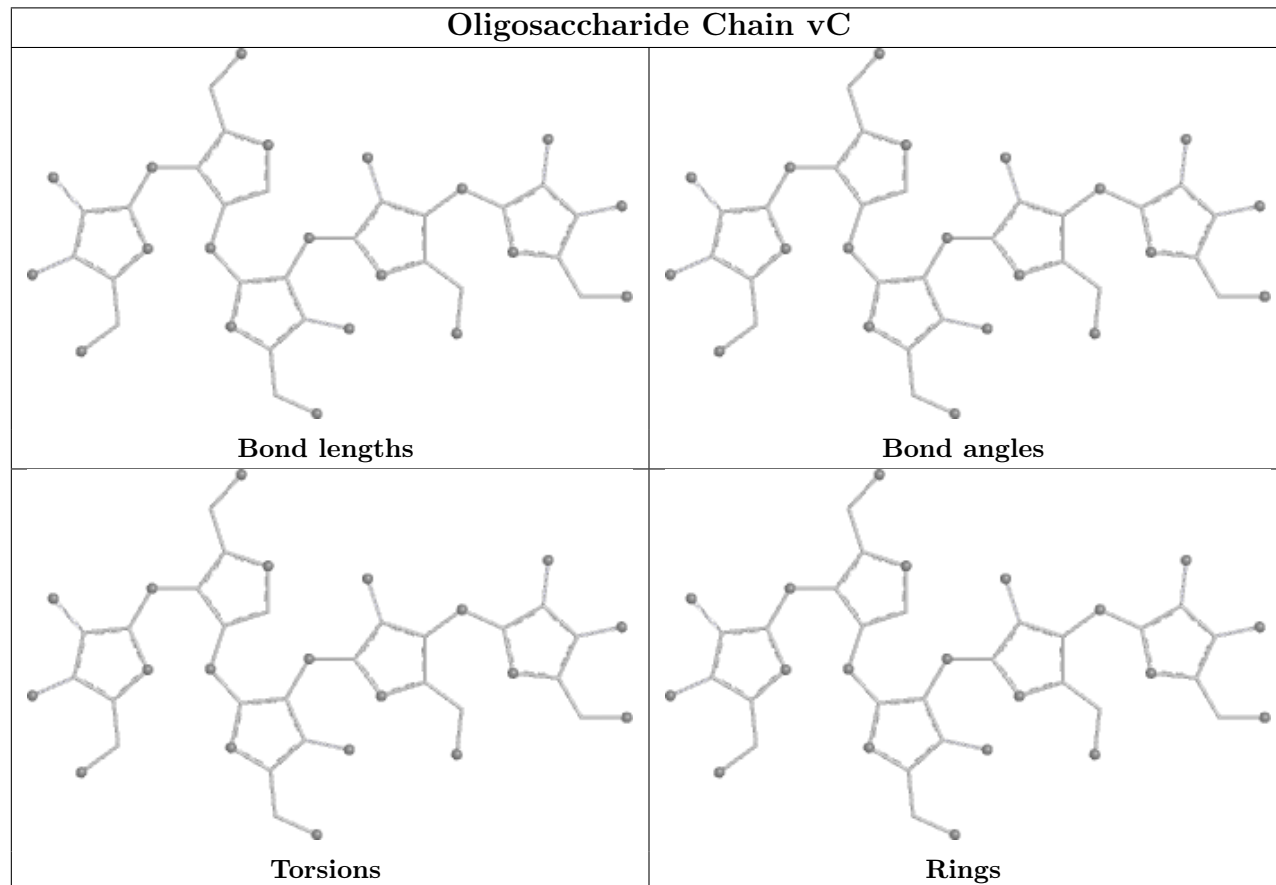
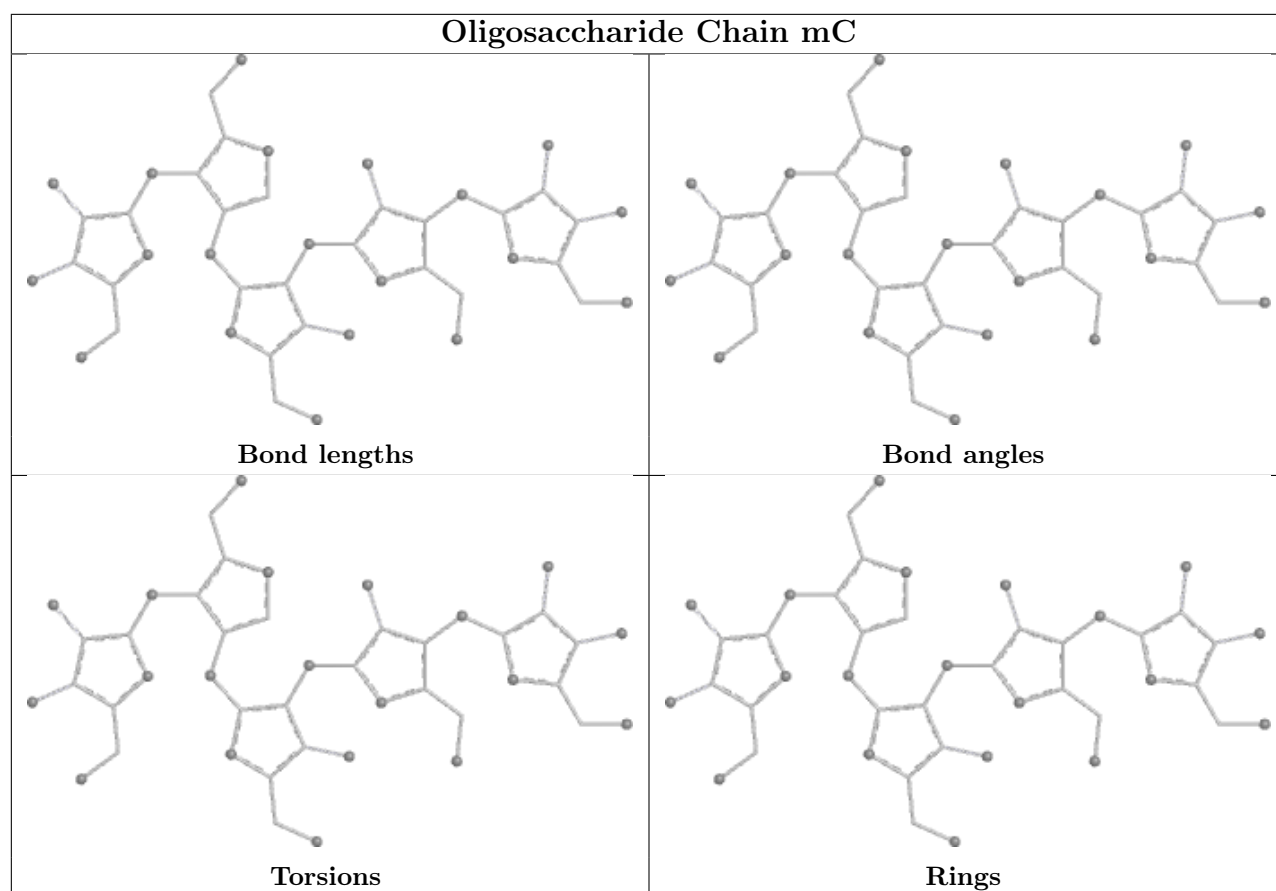


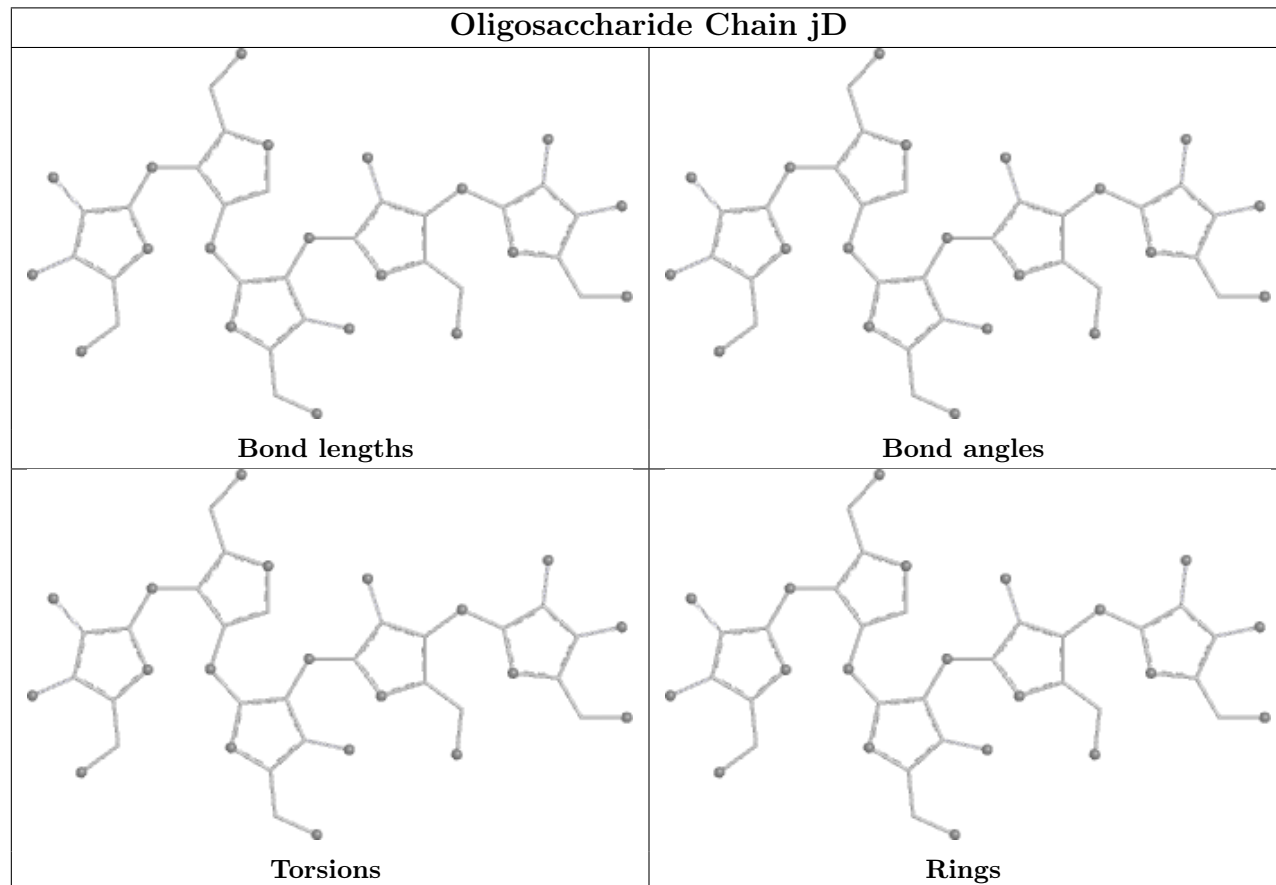
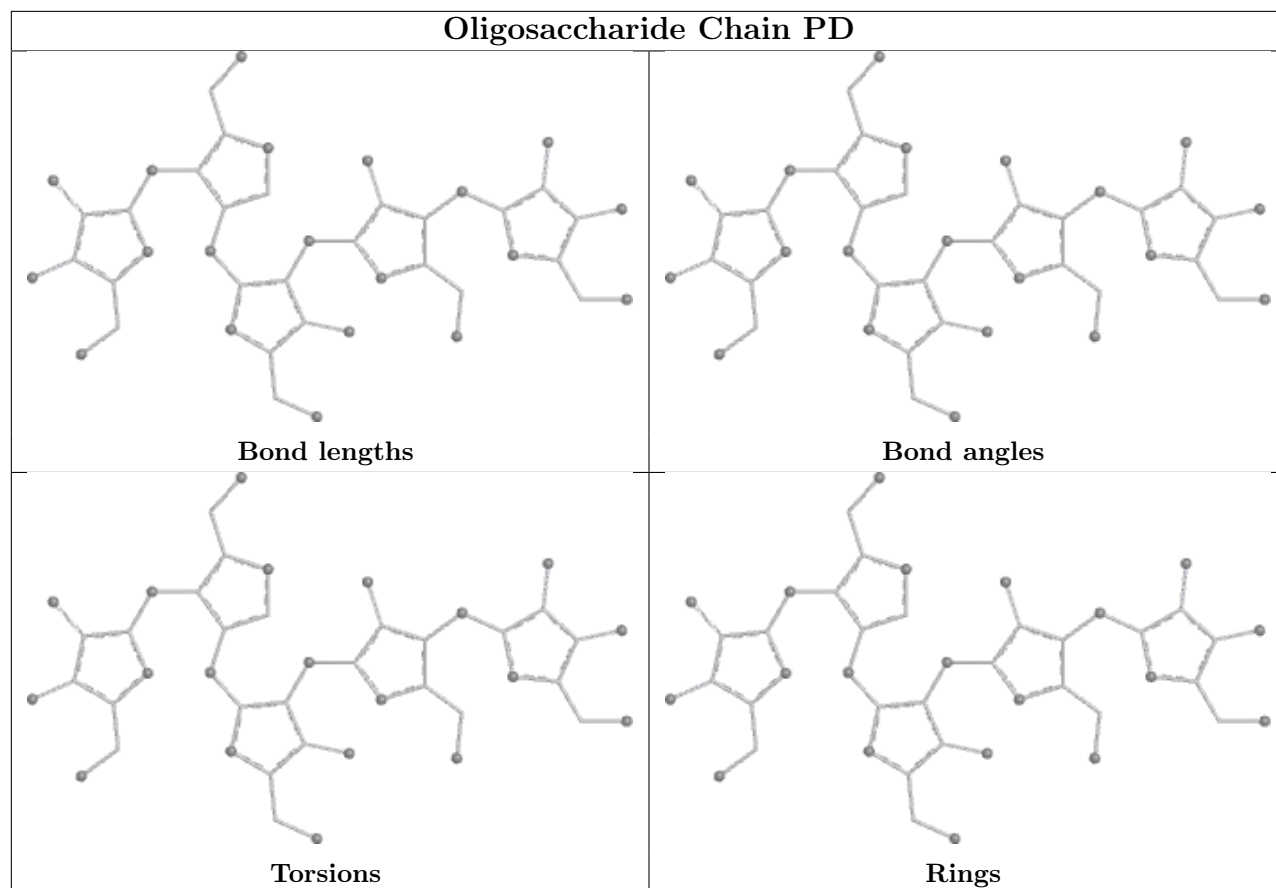
Oligosaccharide Chain YA**Oligosaccharide Chain sA**

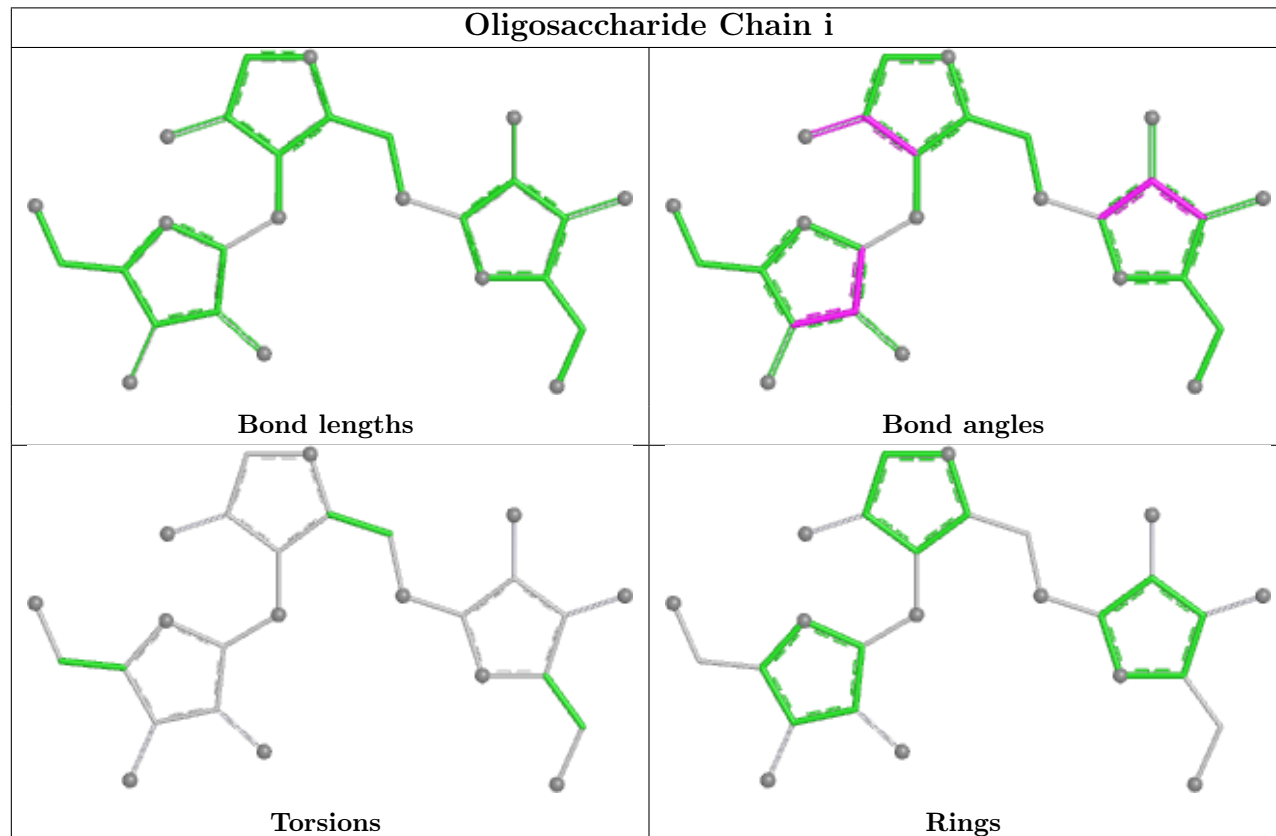
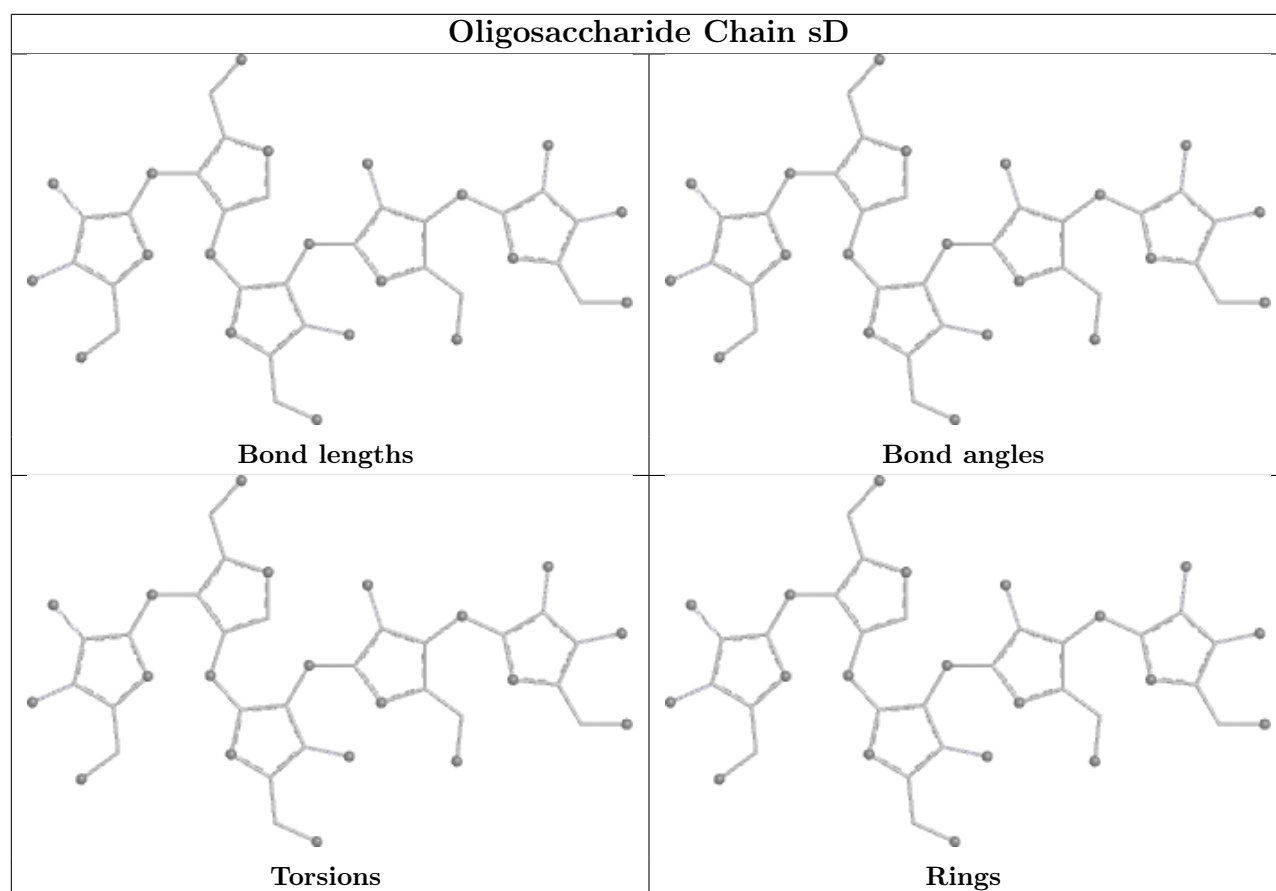


Oligosaccharide Chain VB**Oligosaccharide Chain pB**

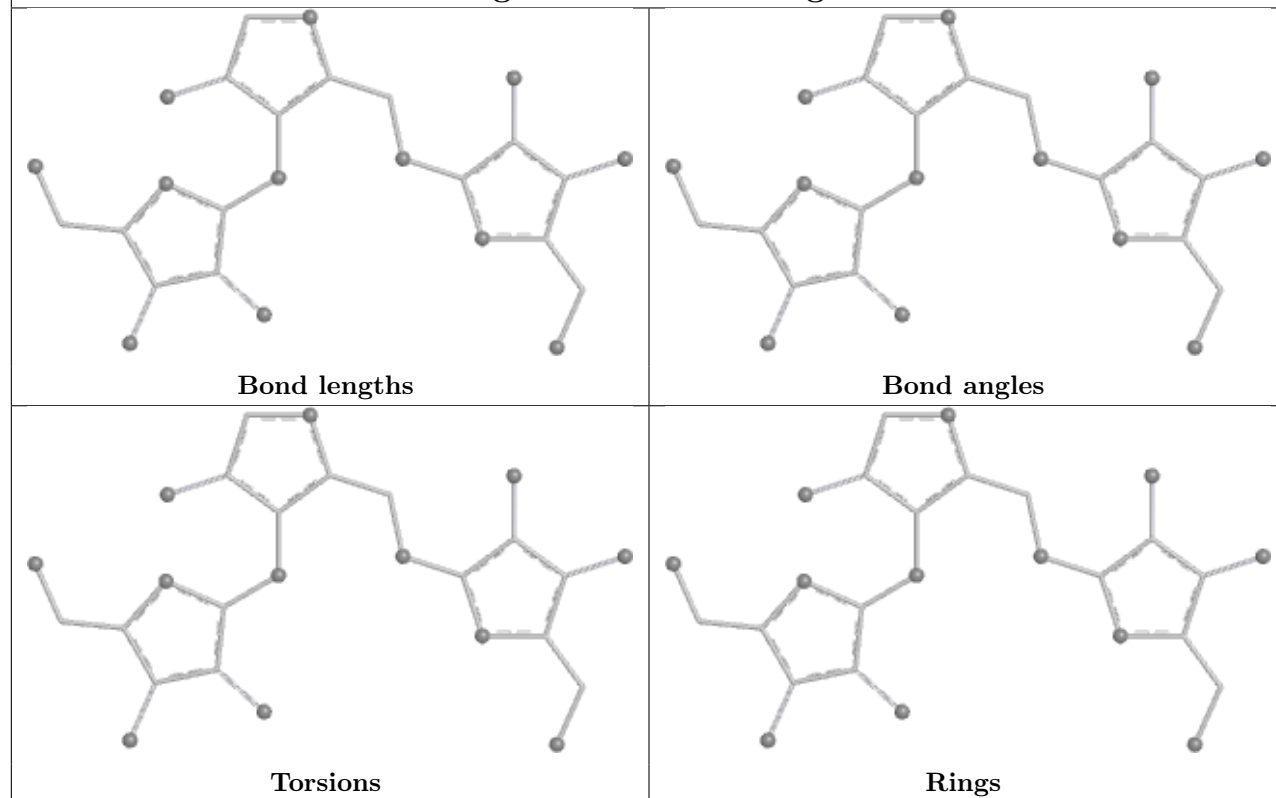




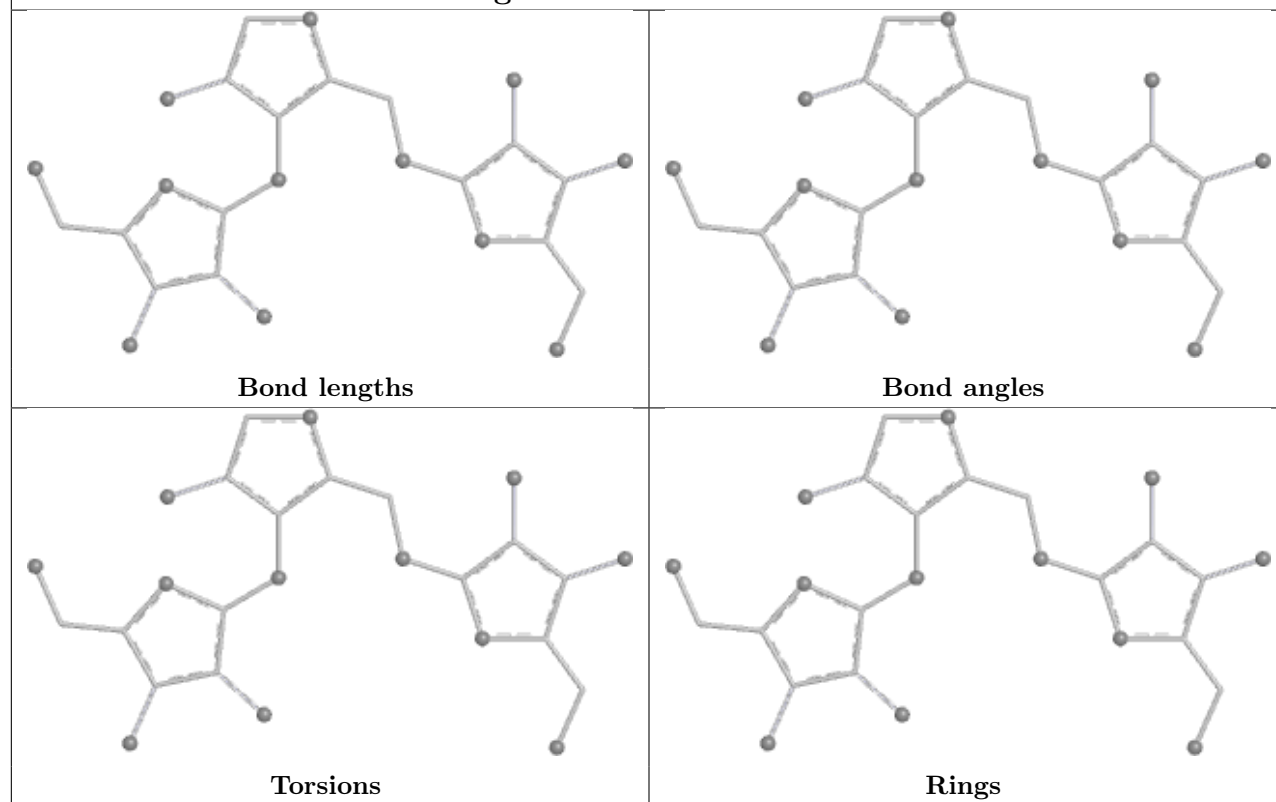


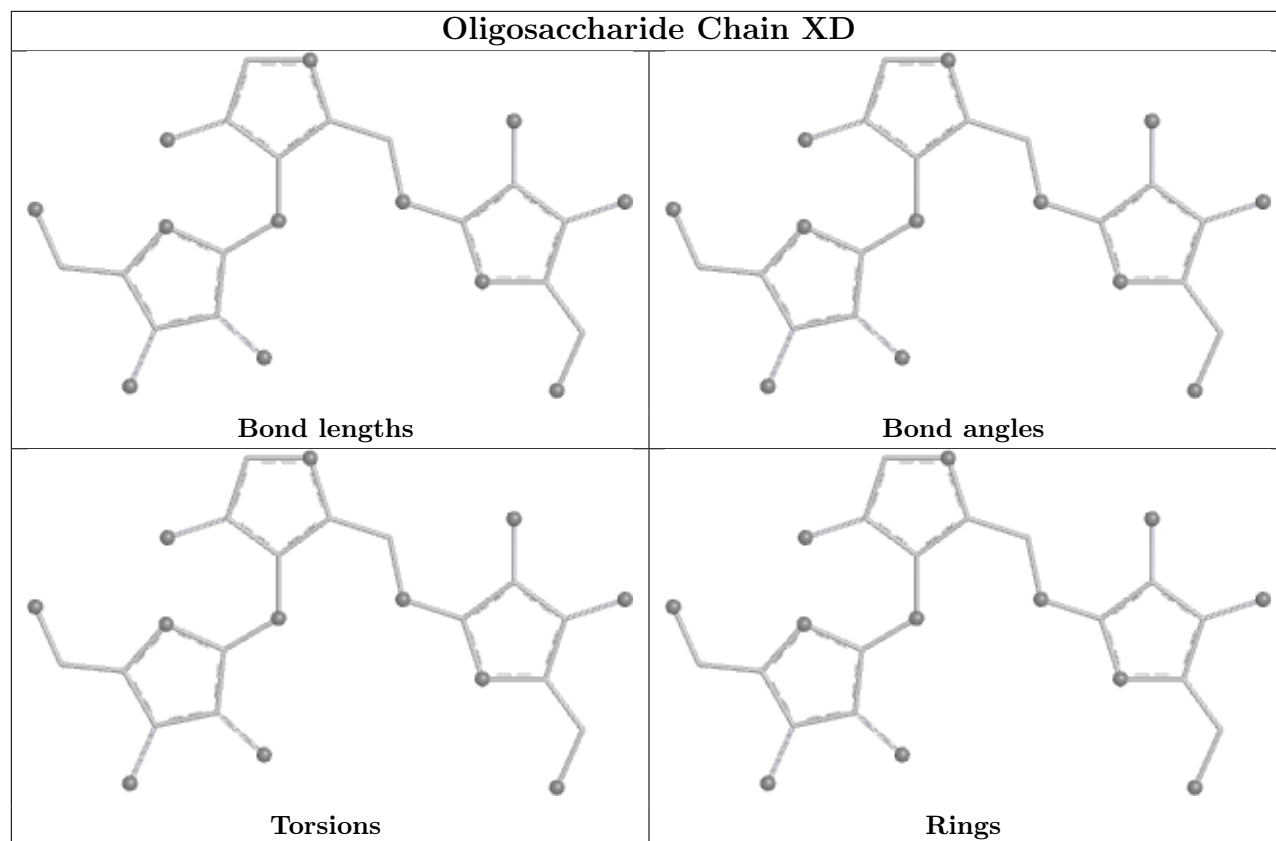


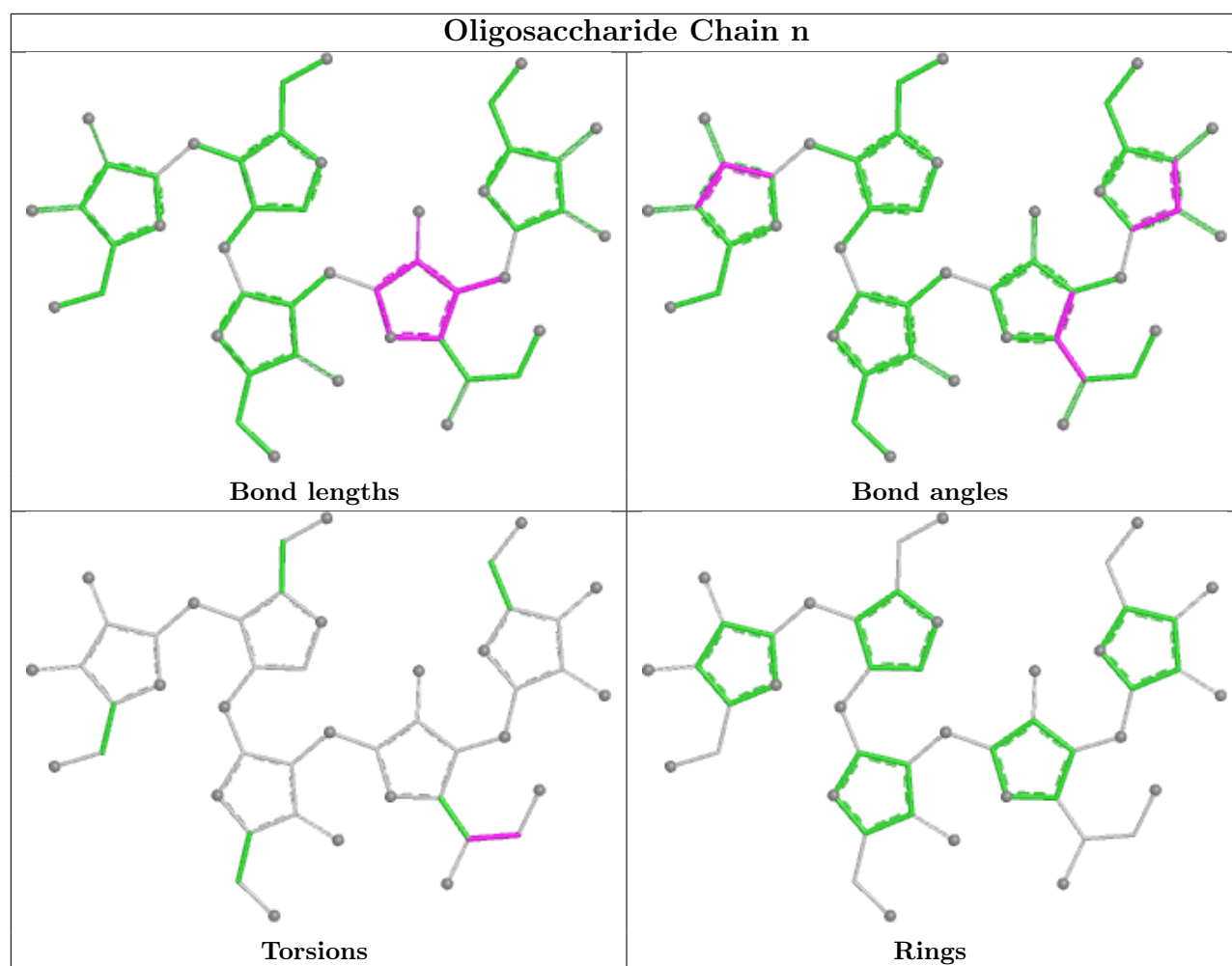
Oligosaccharide Chain gA

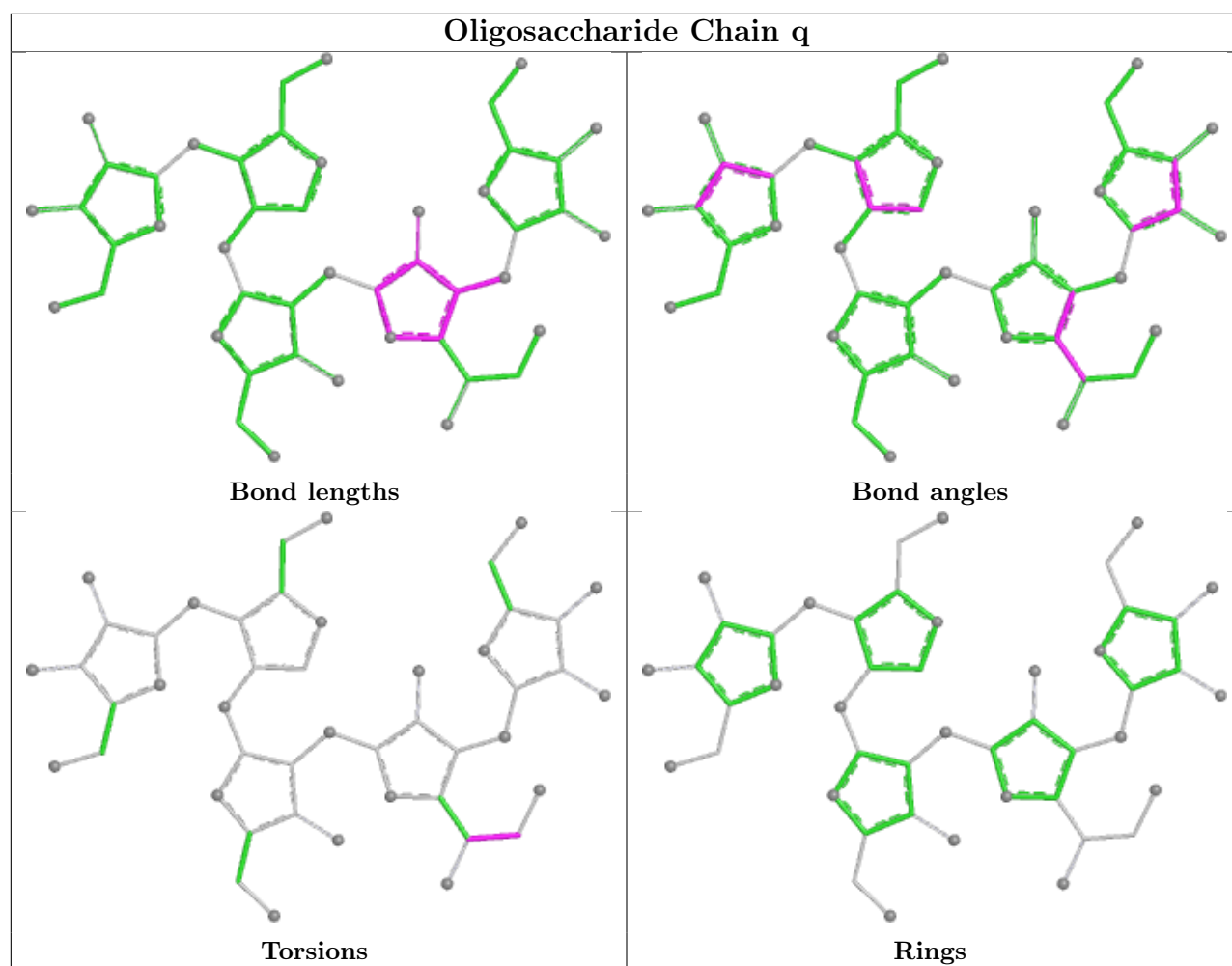


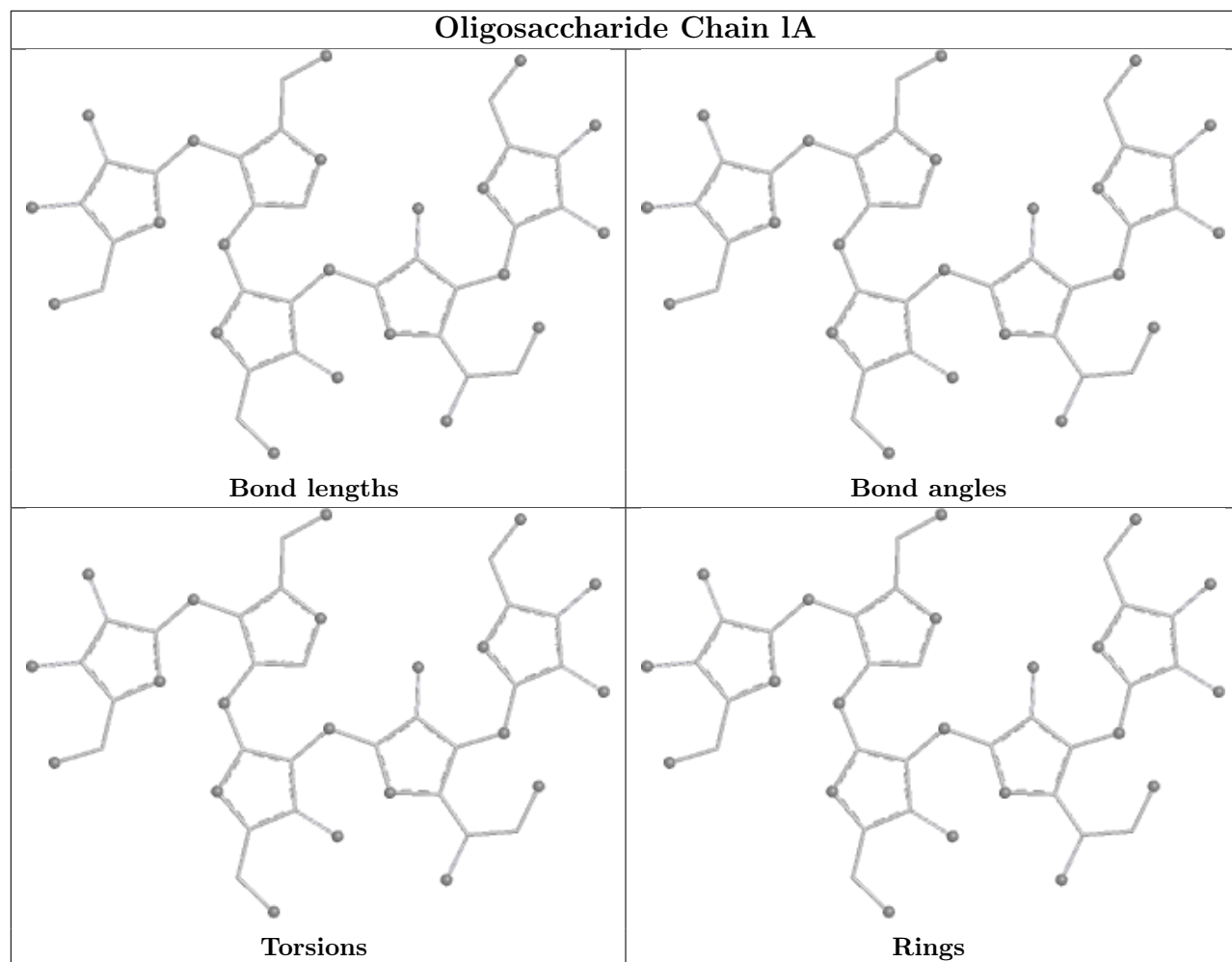
Oligosaccharide Chain aC

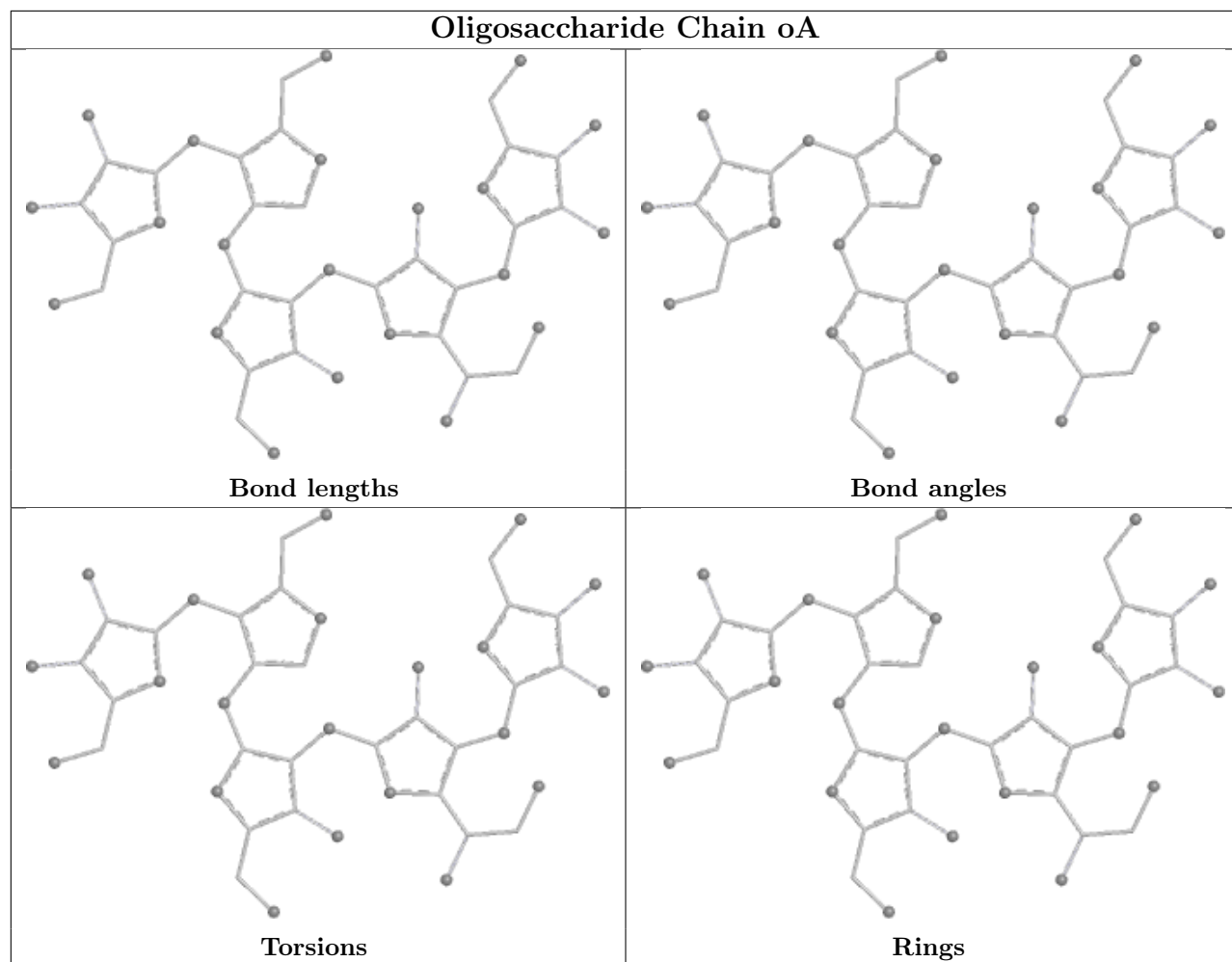


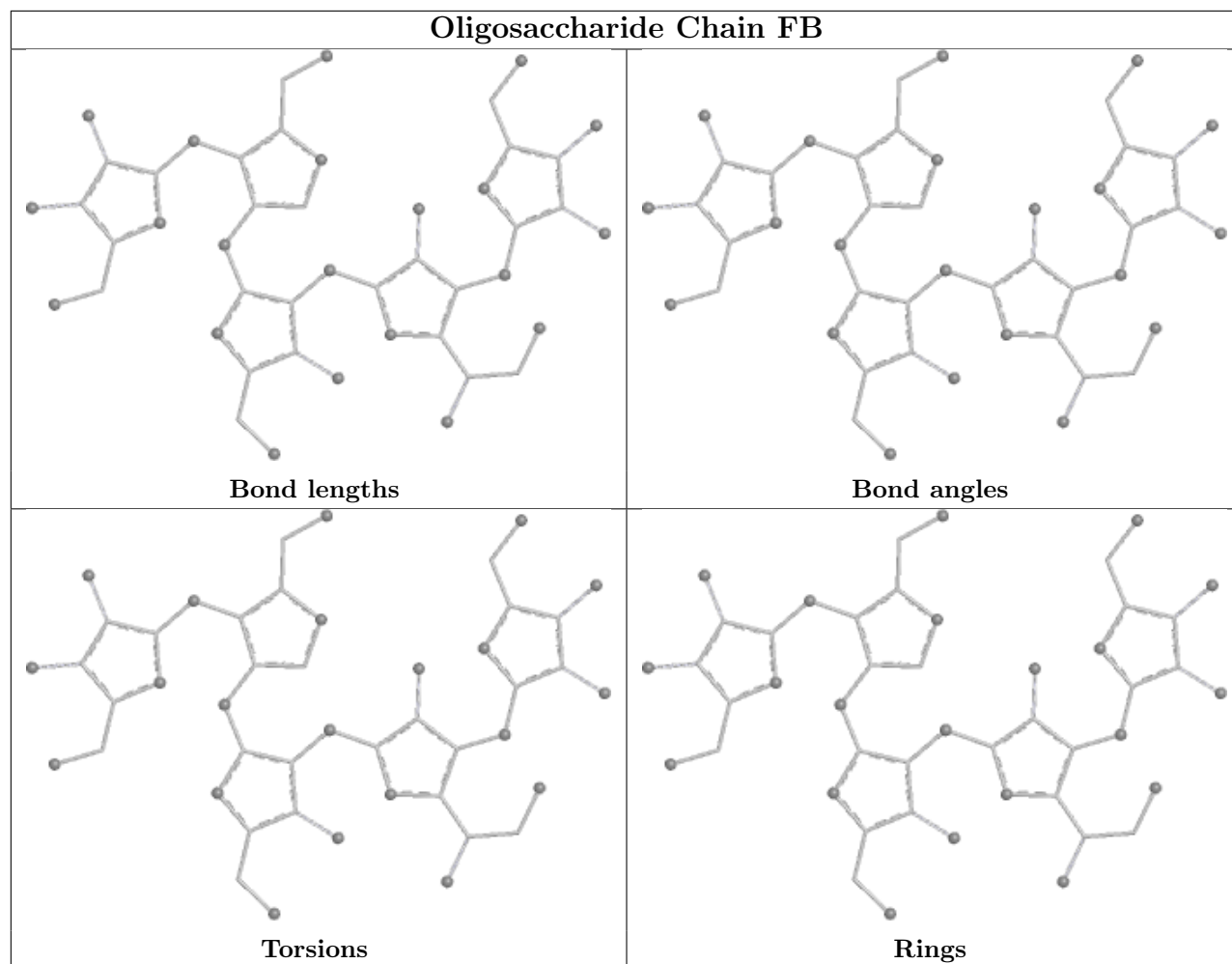


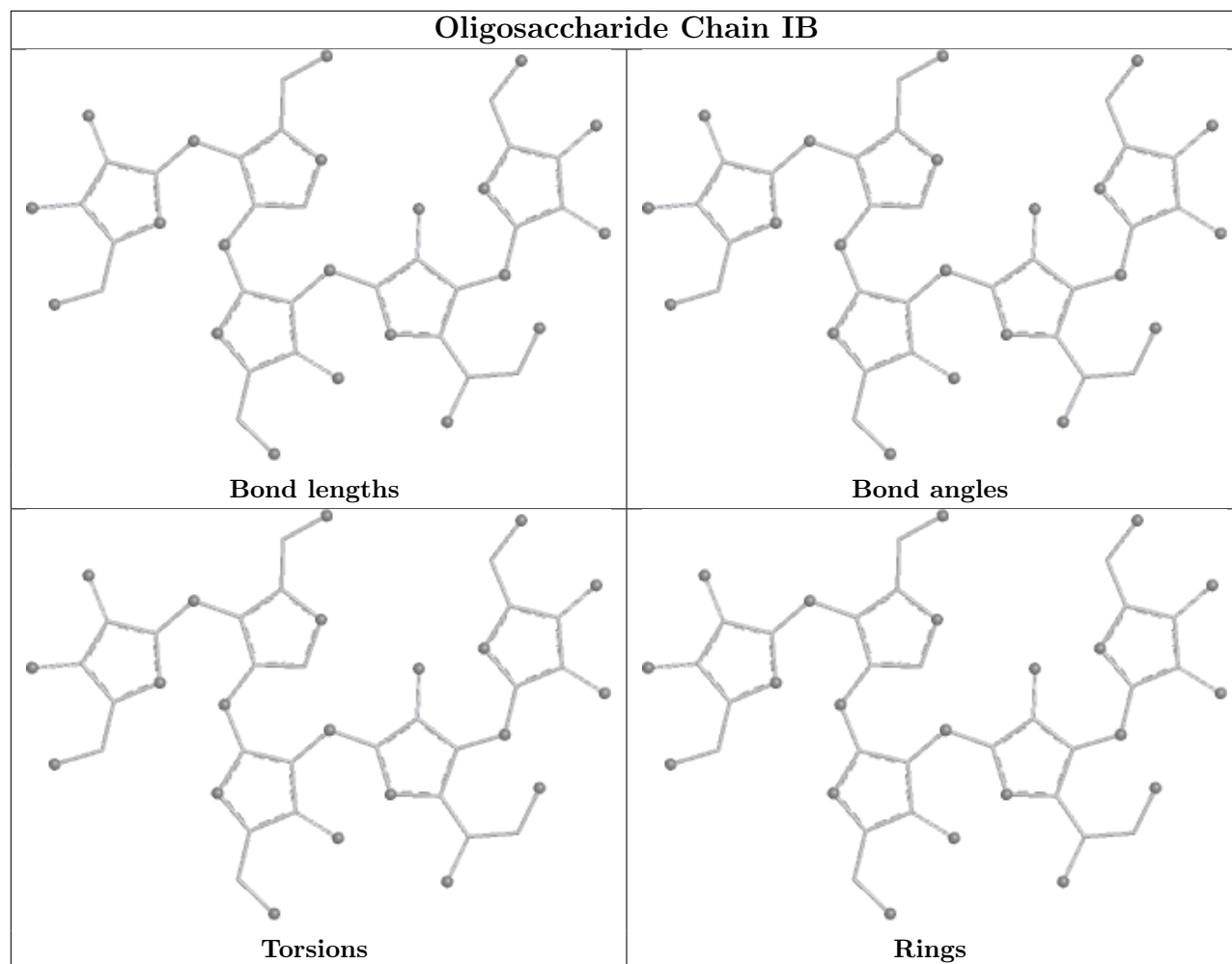


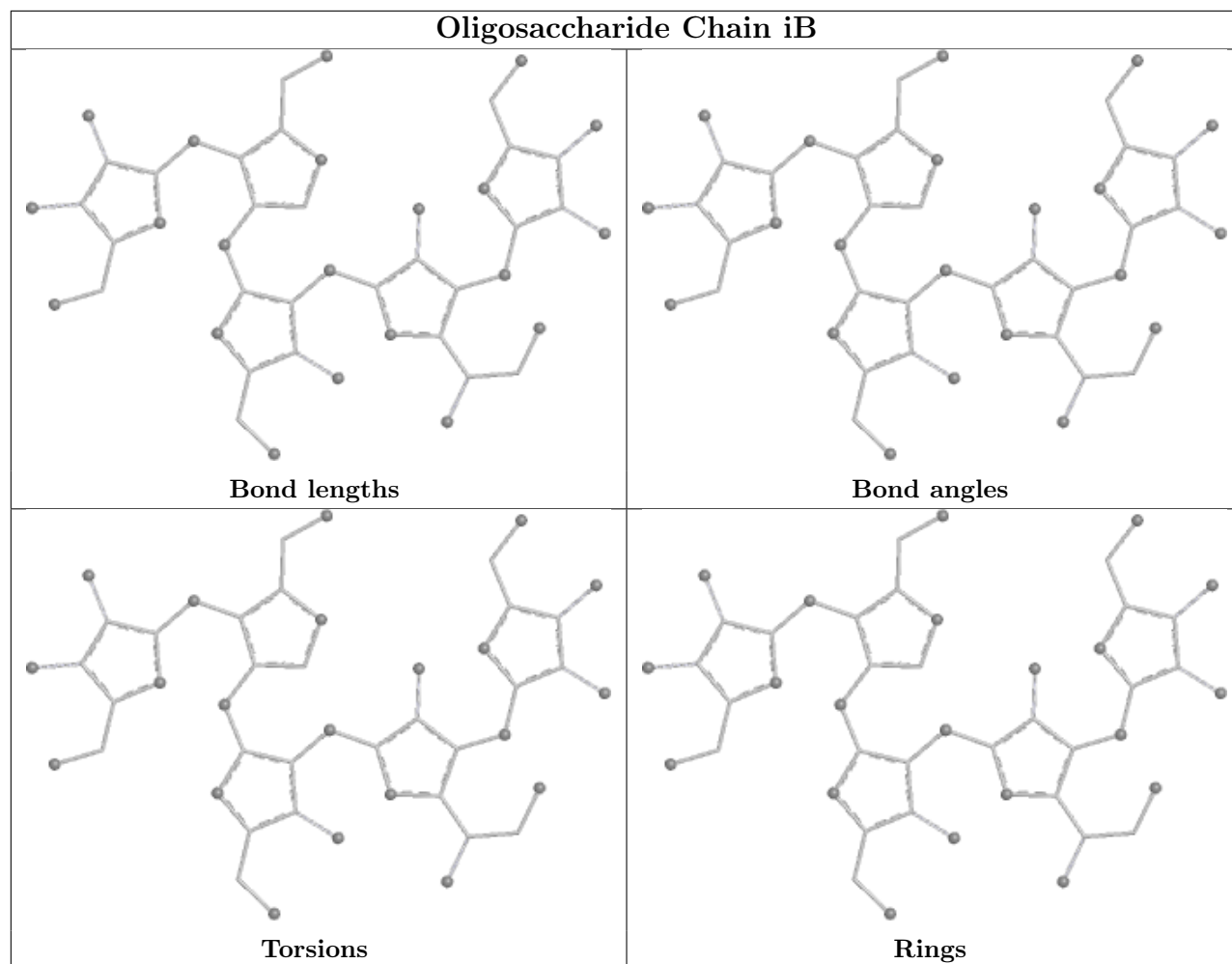


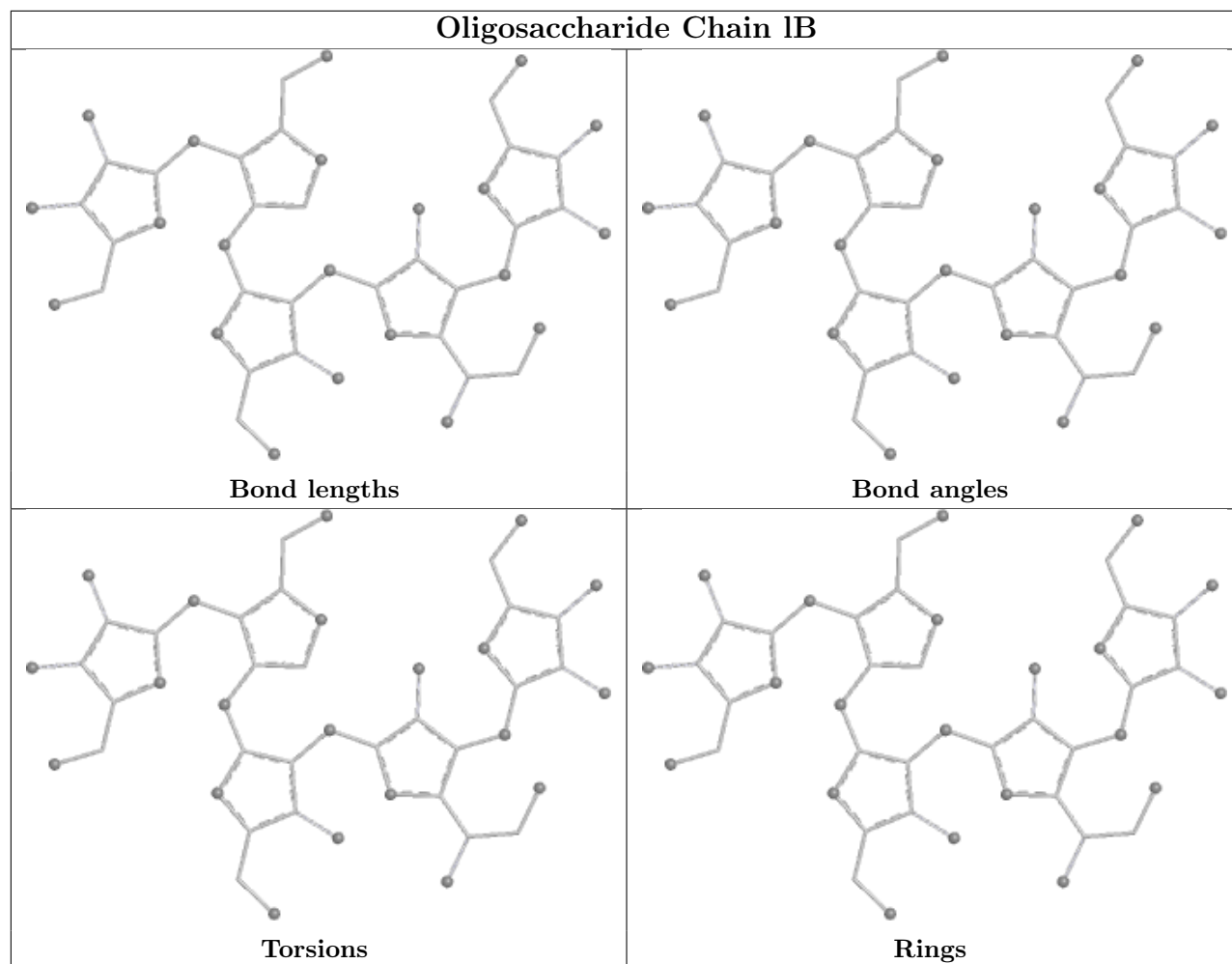


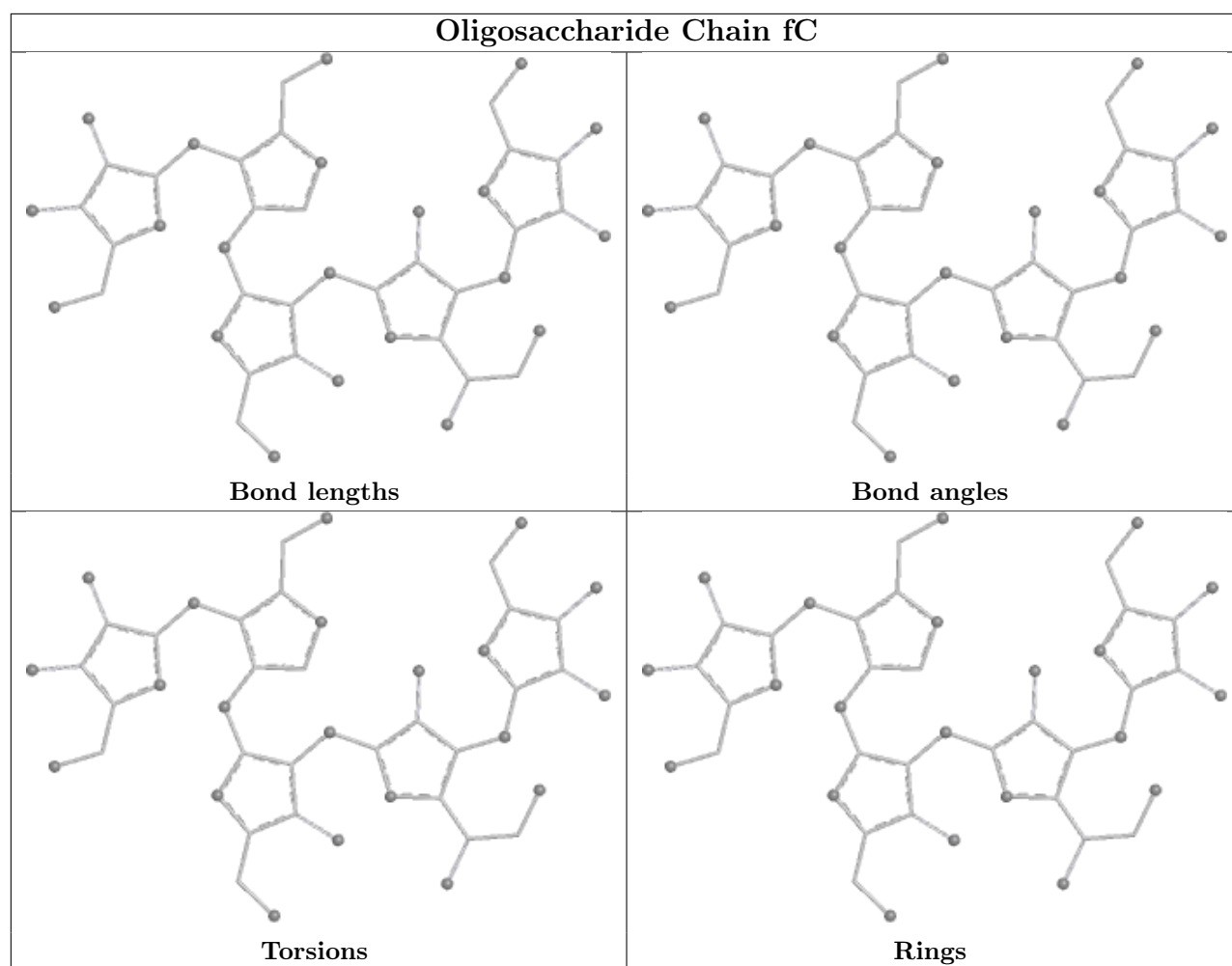


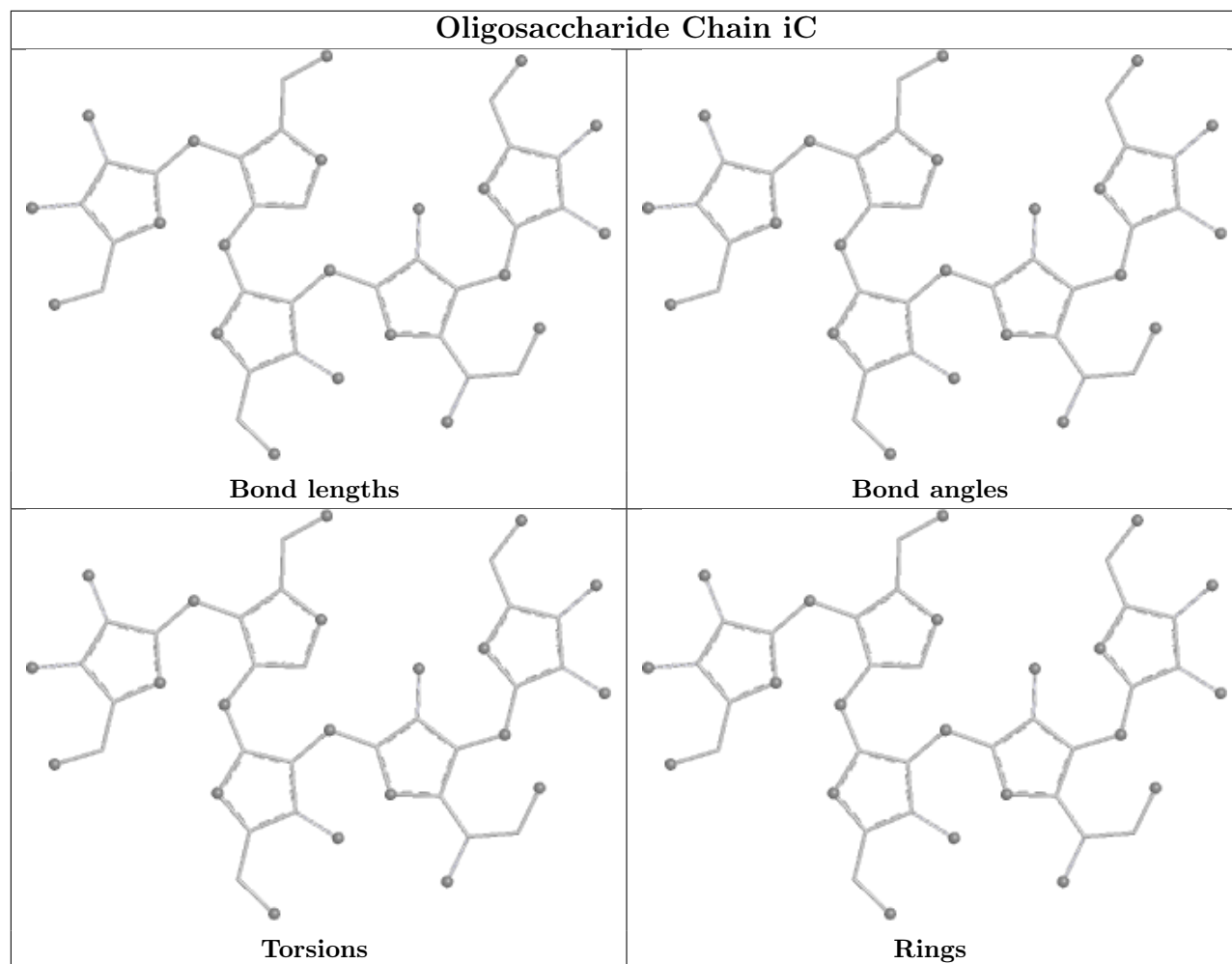


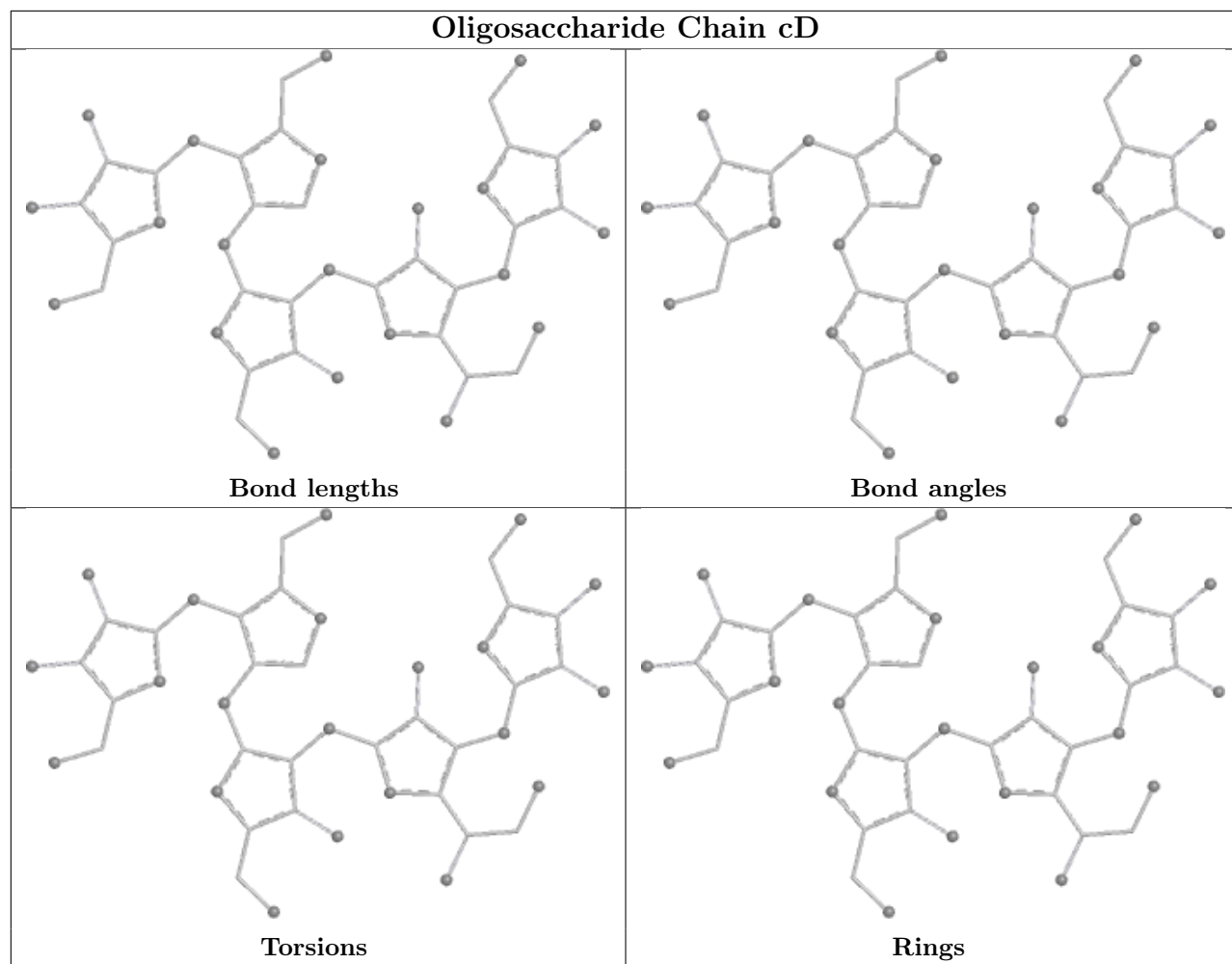


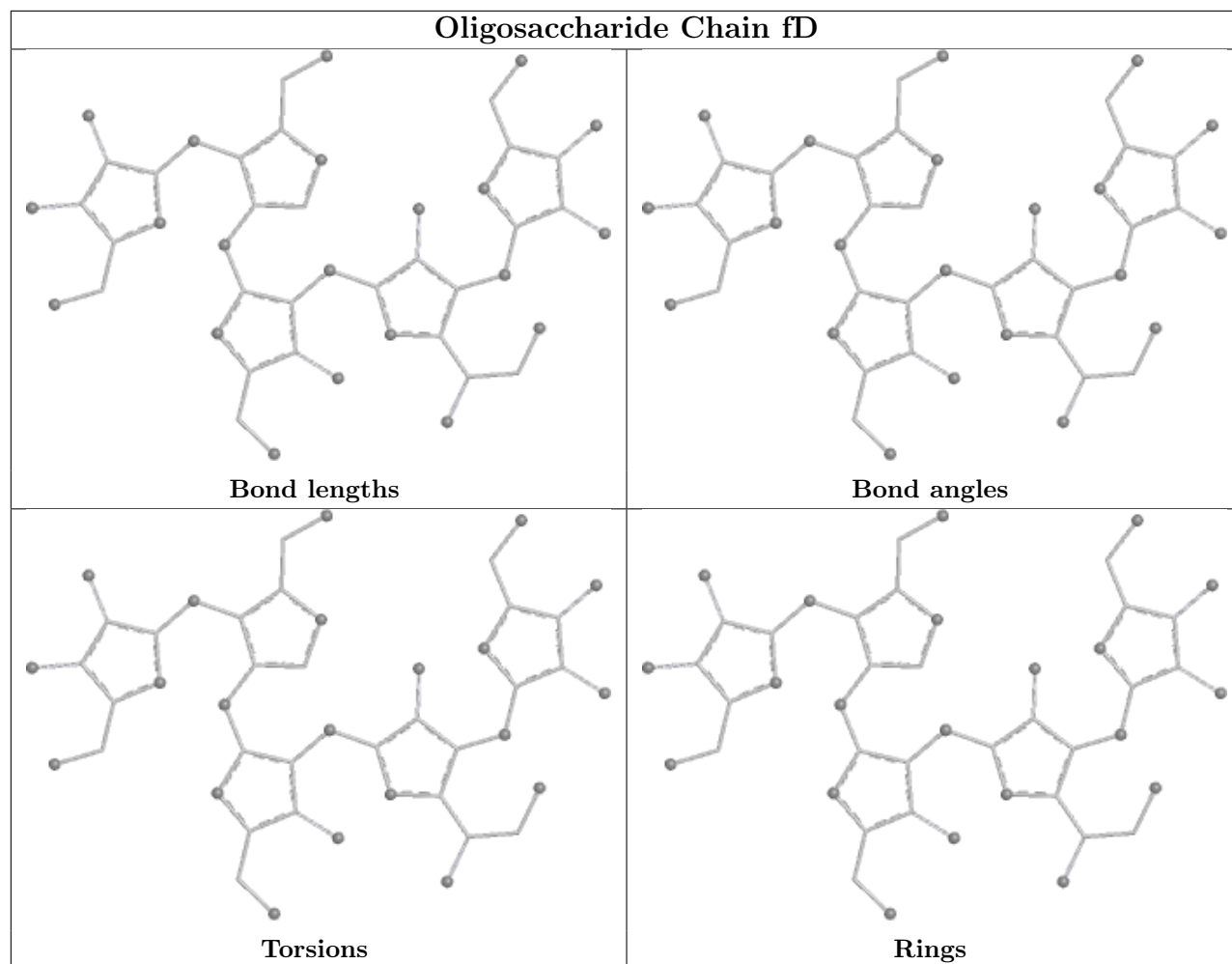


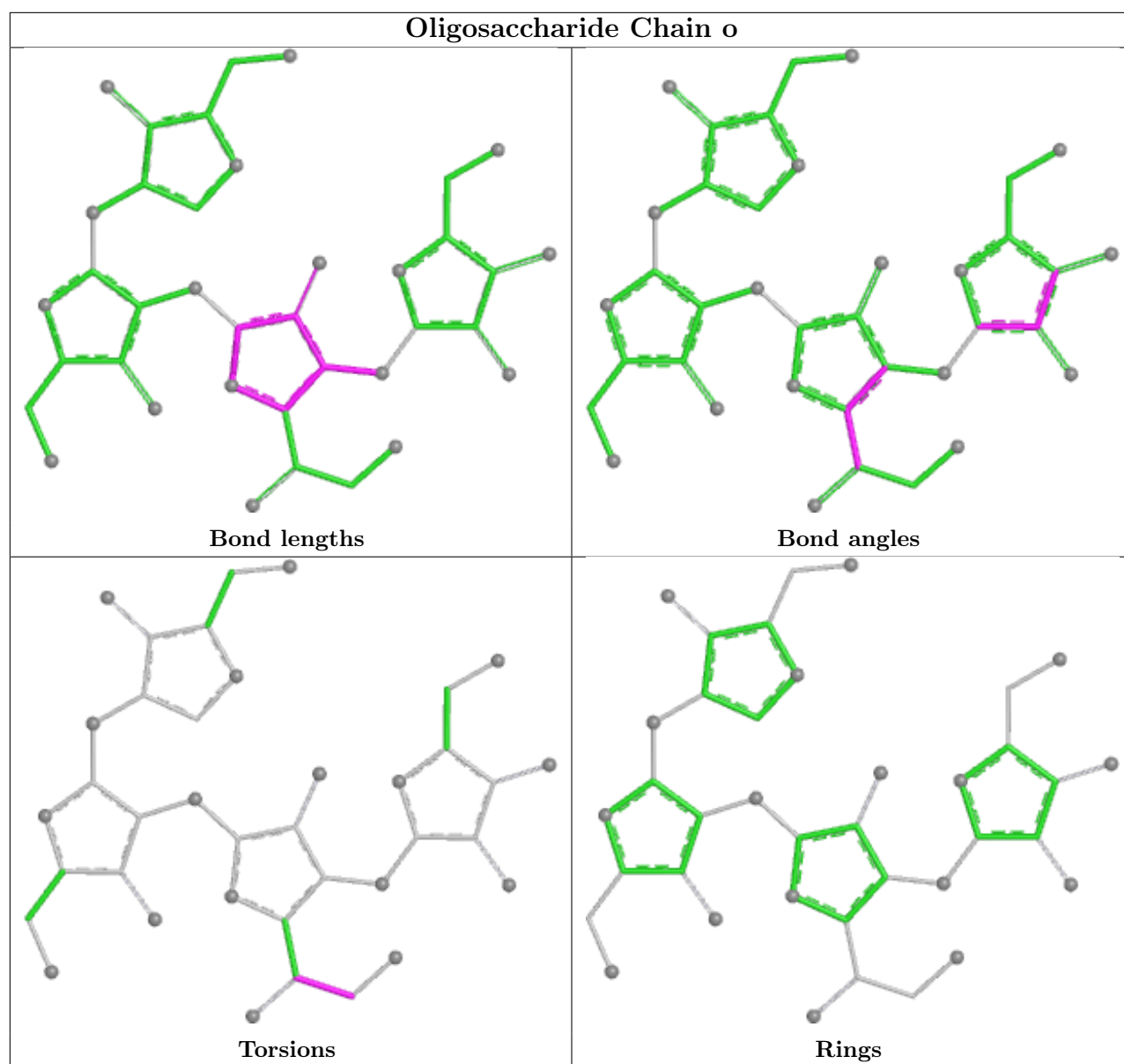


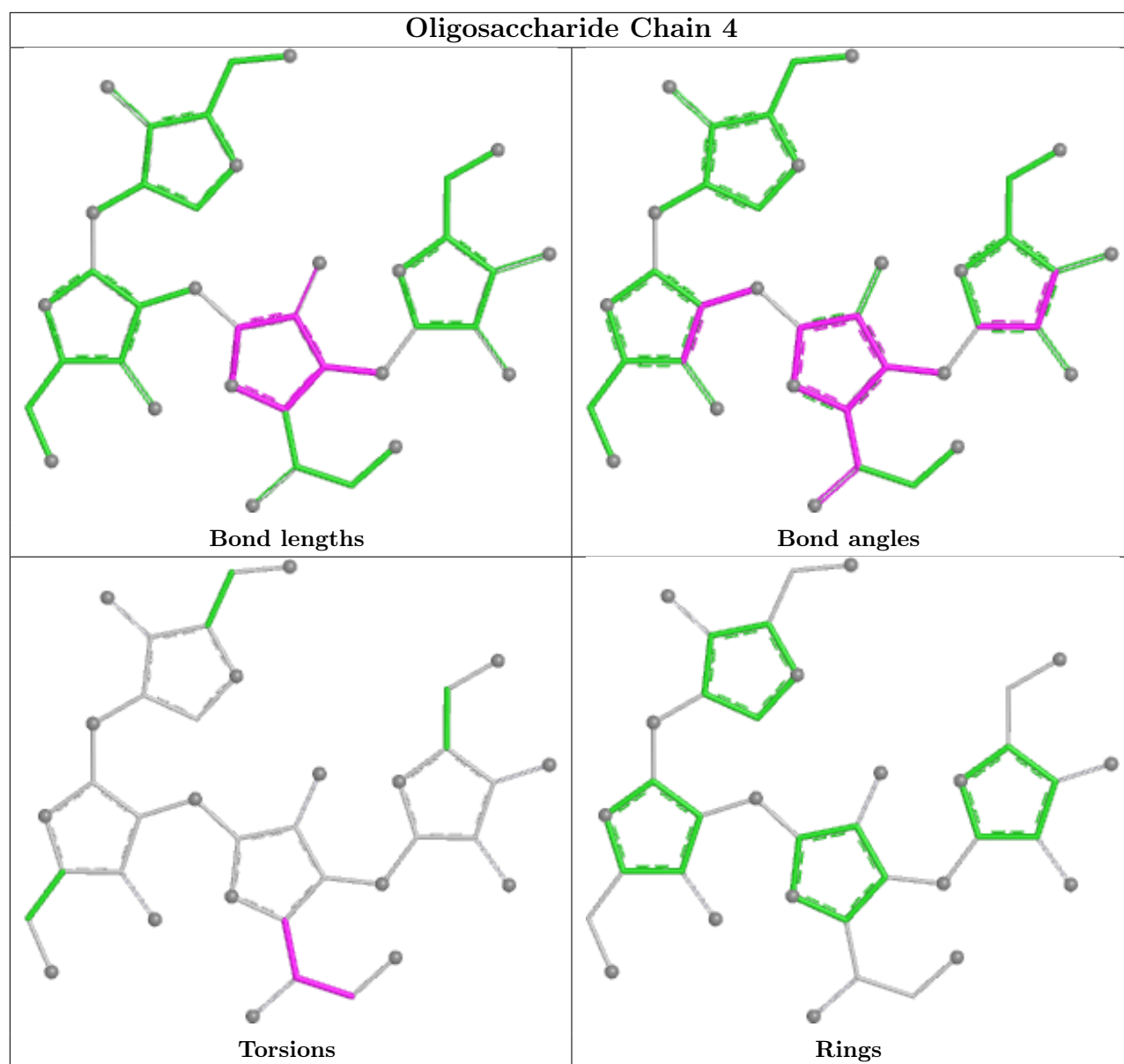


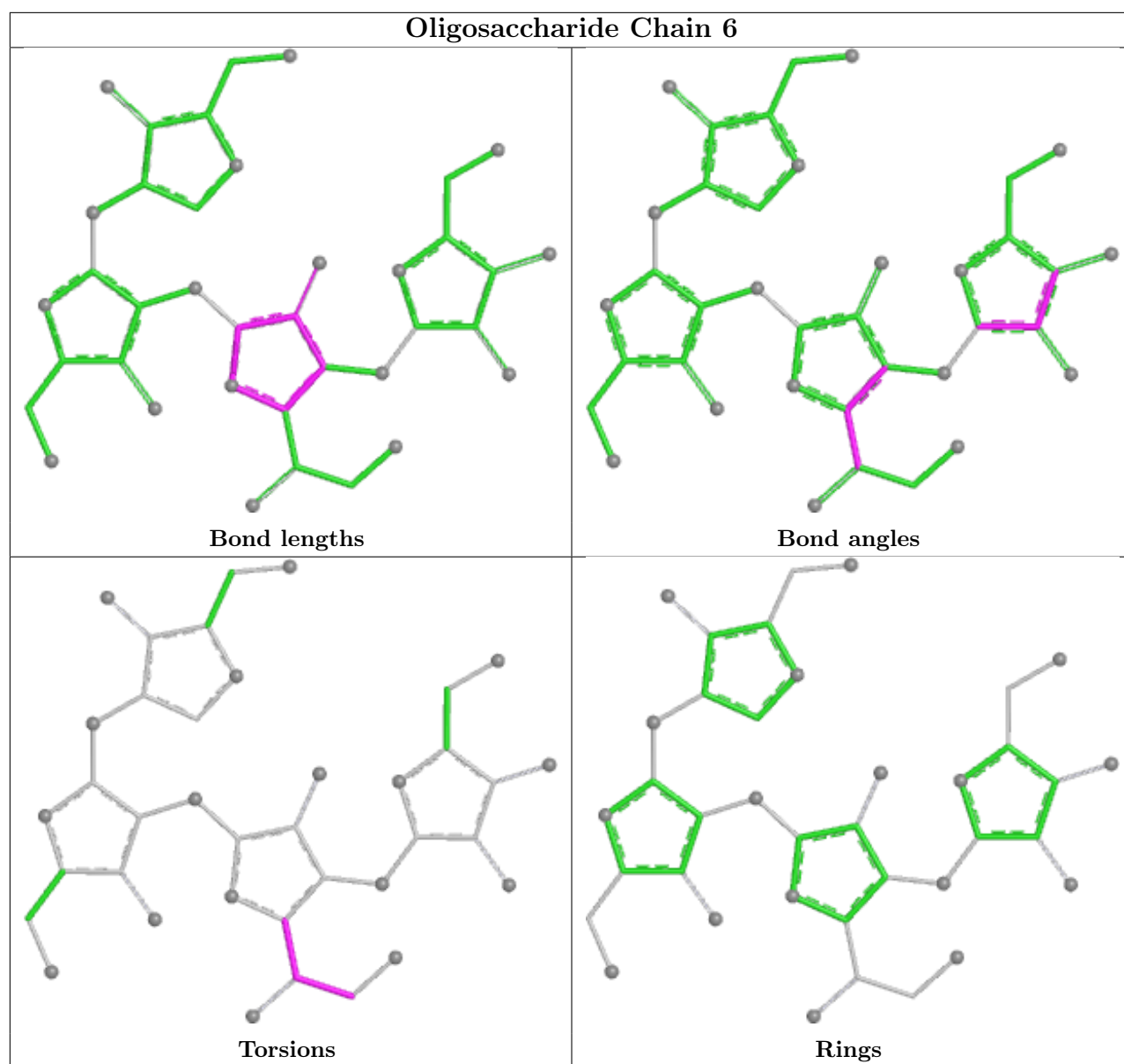


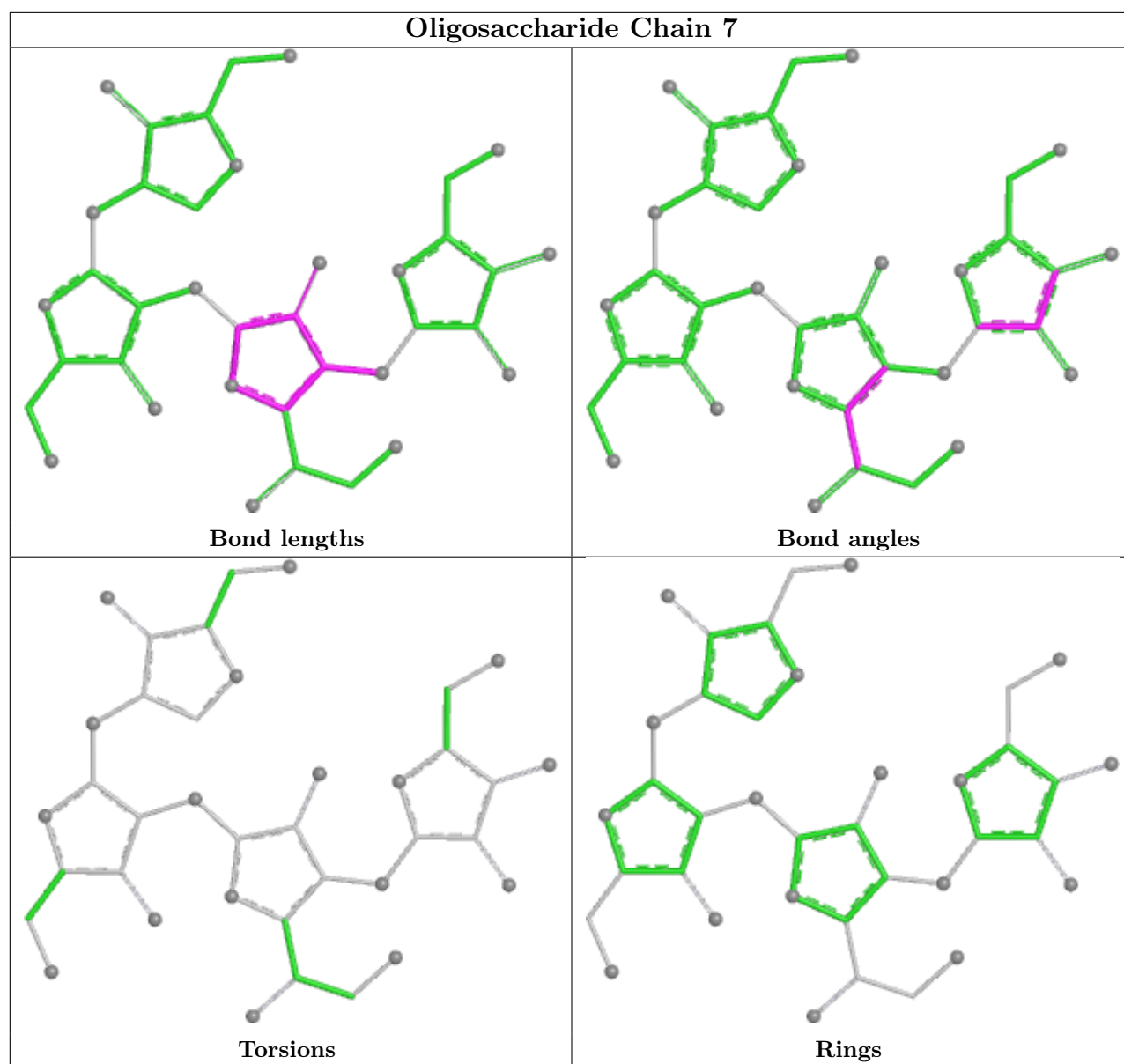


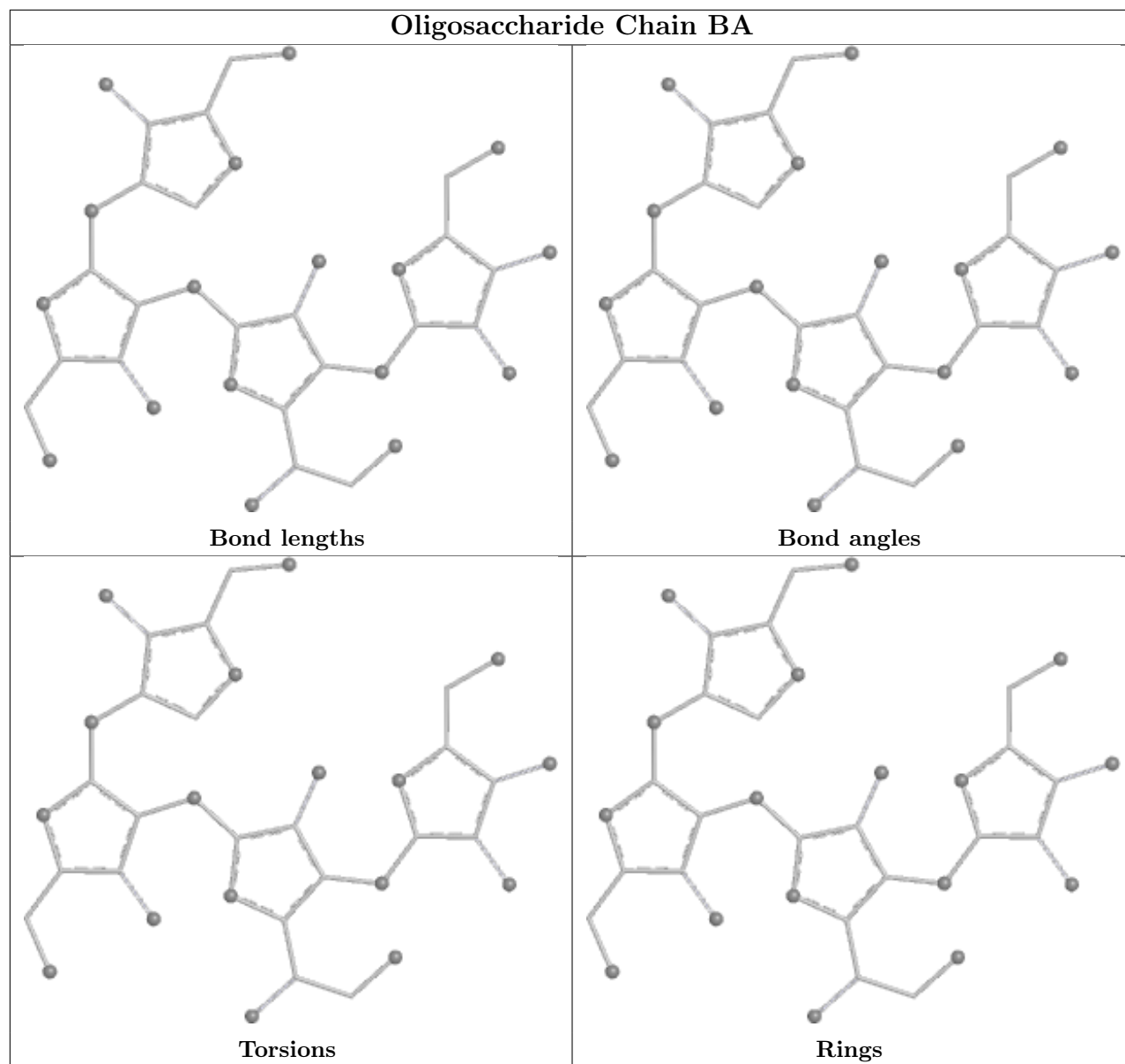


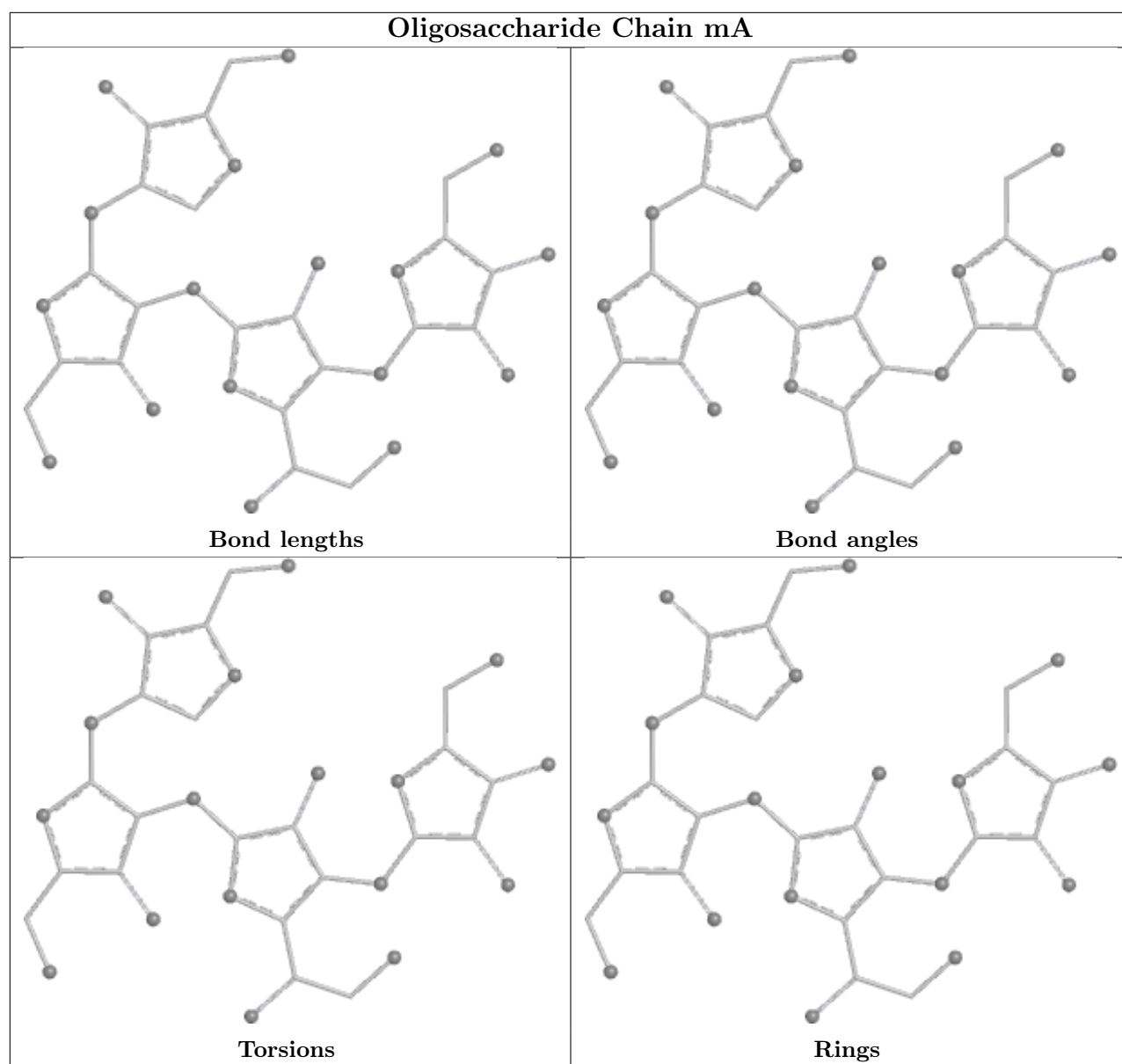


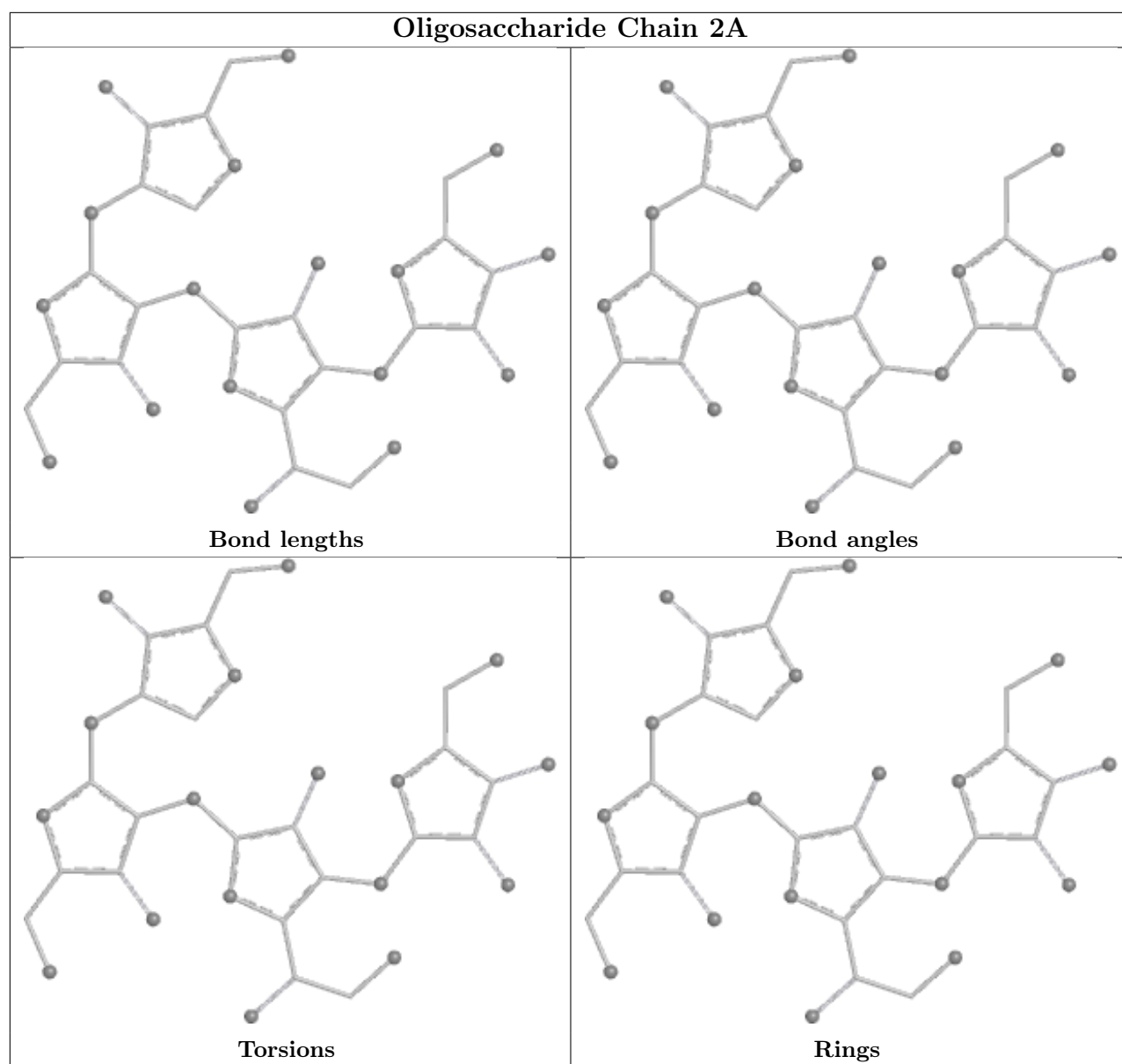


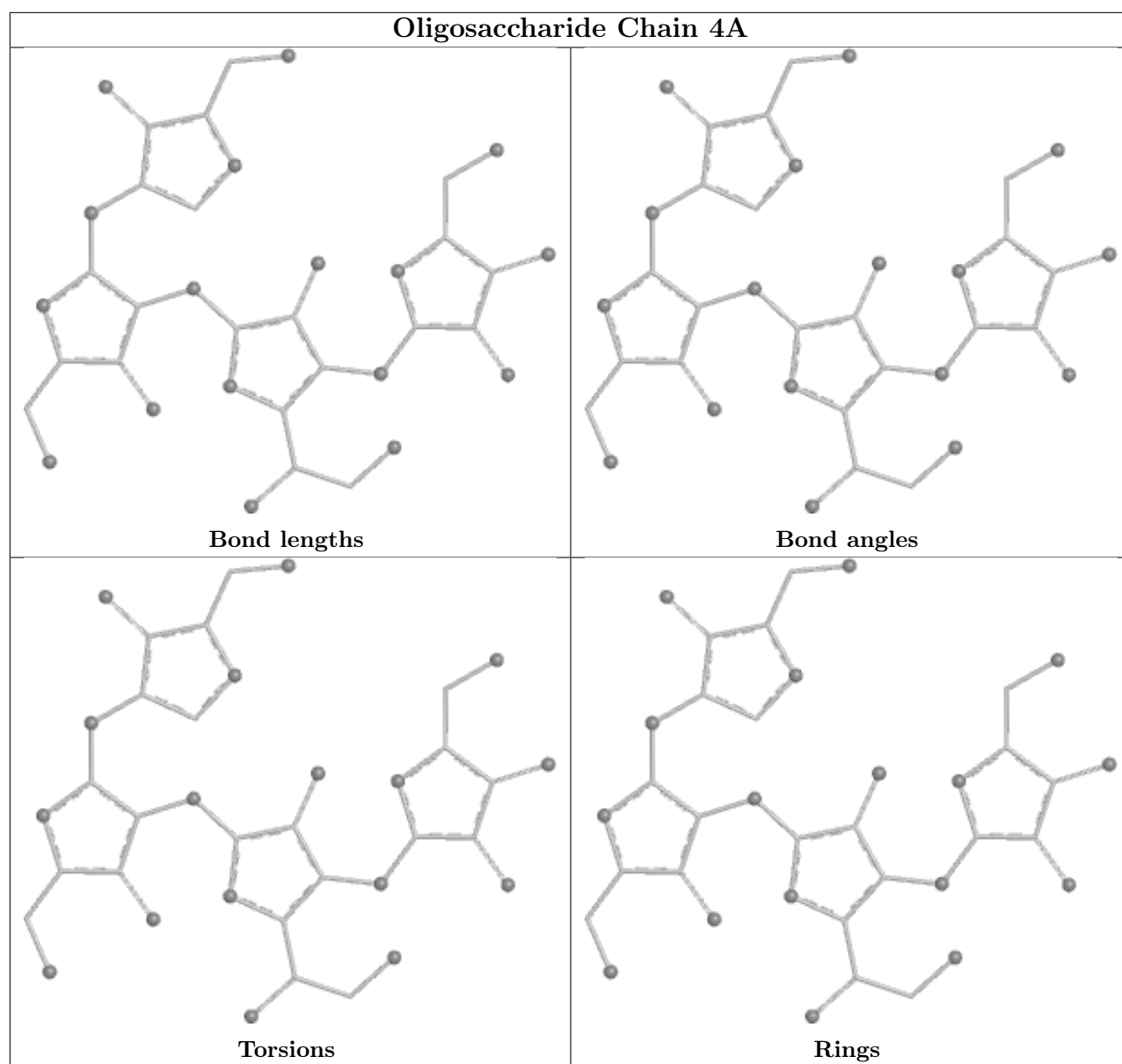




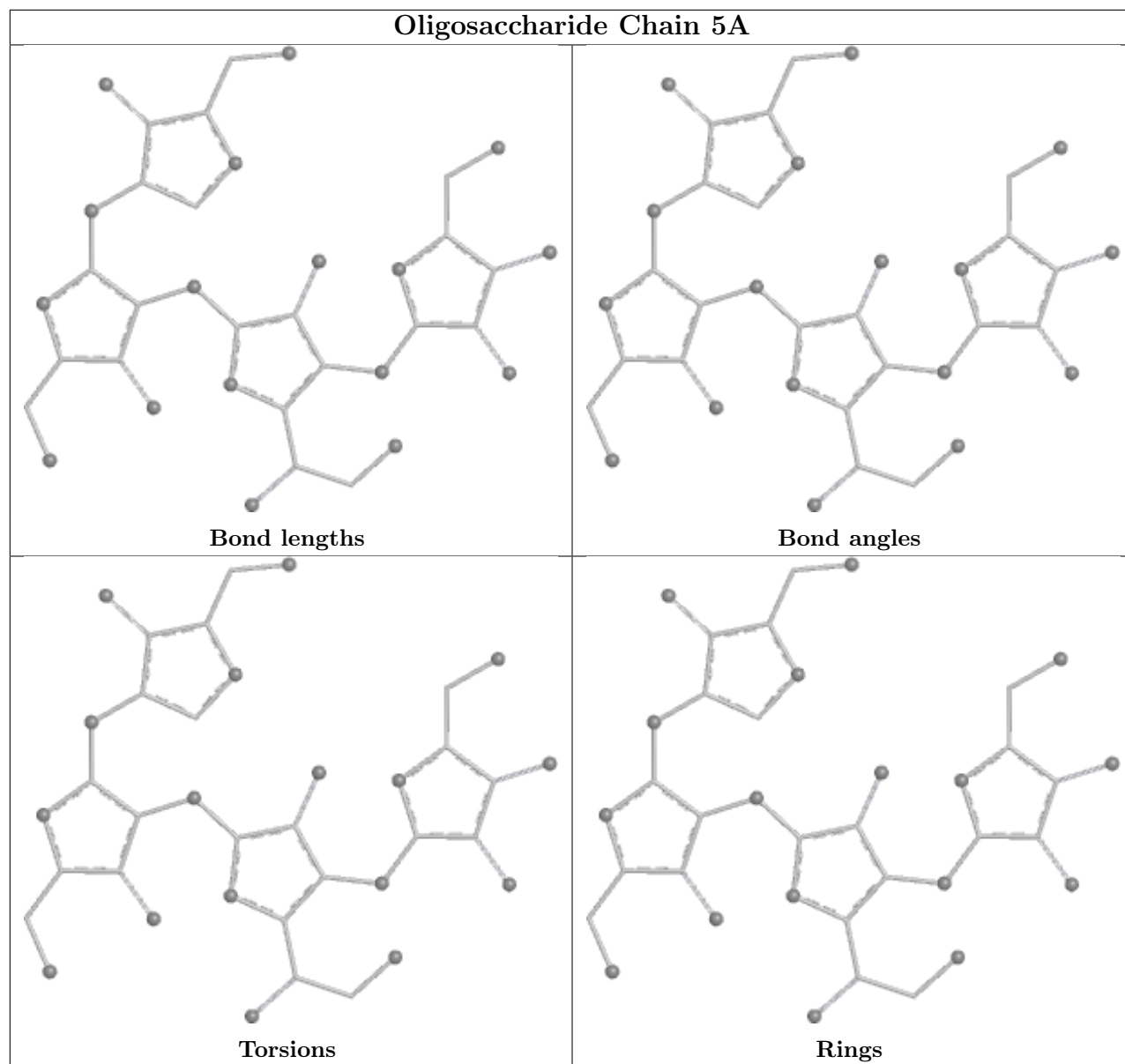


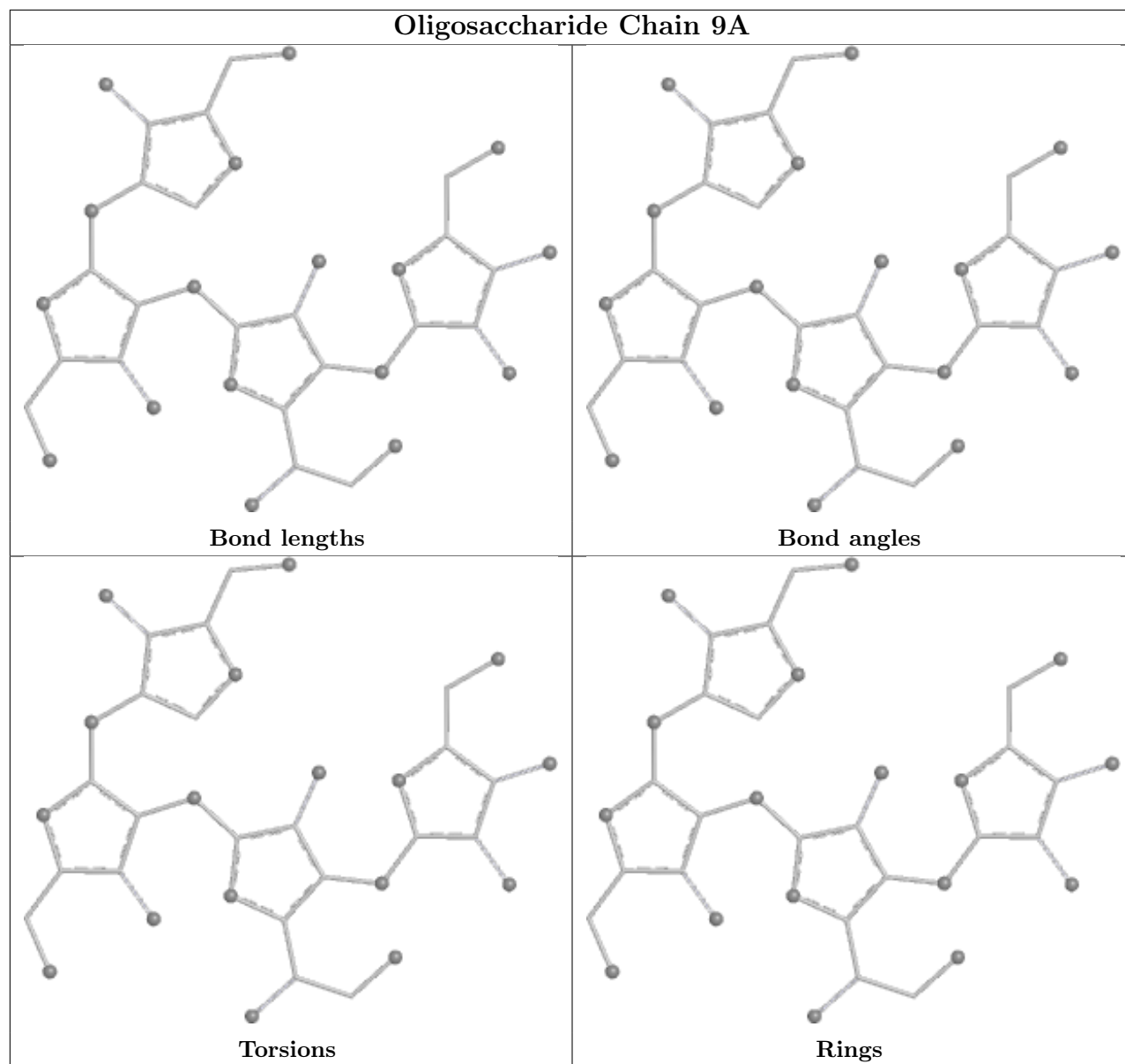


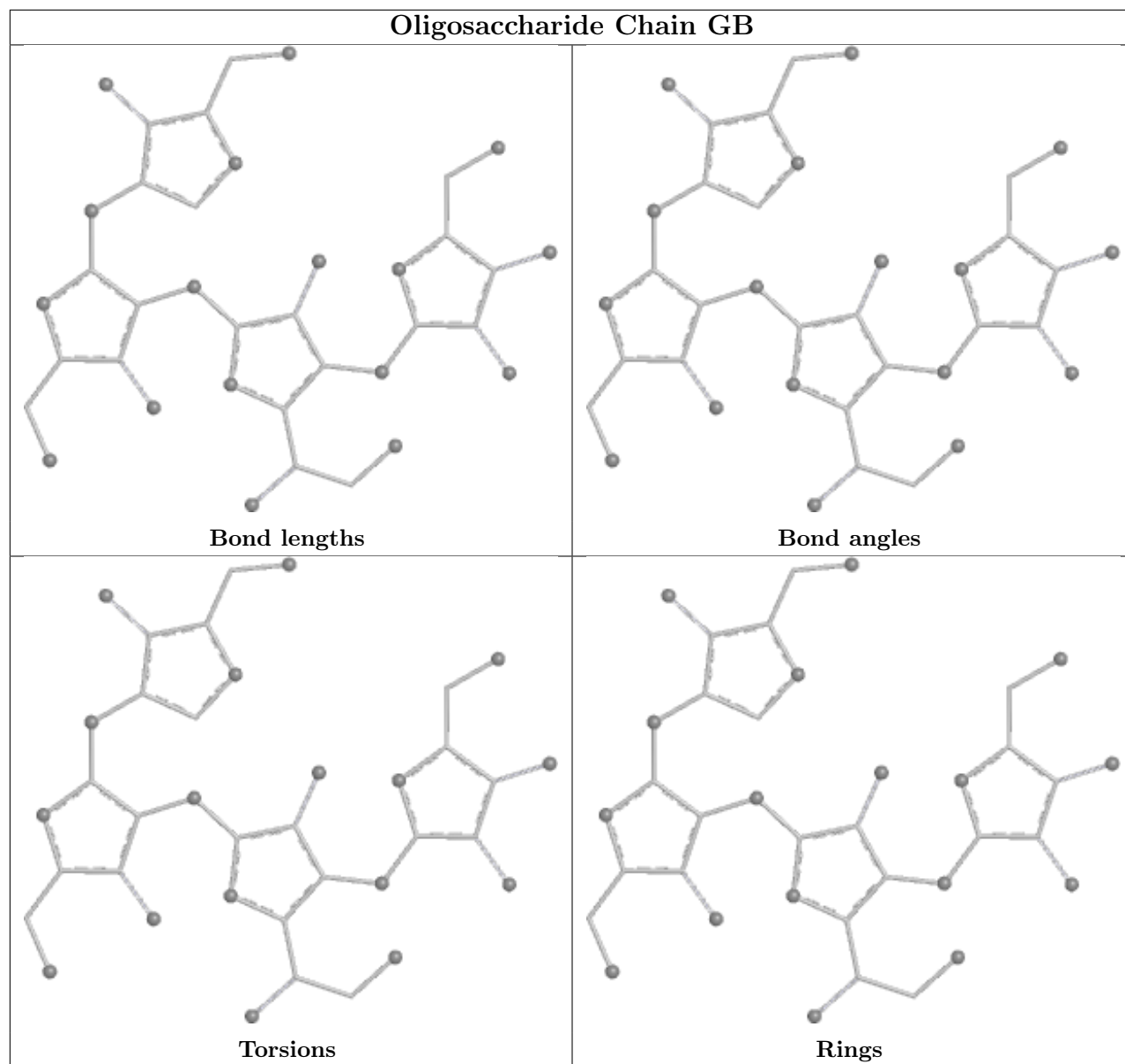


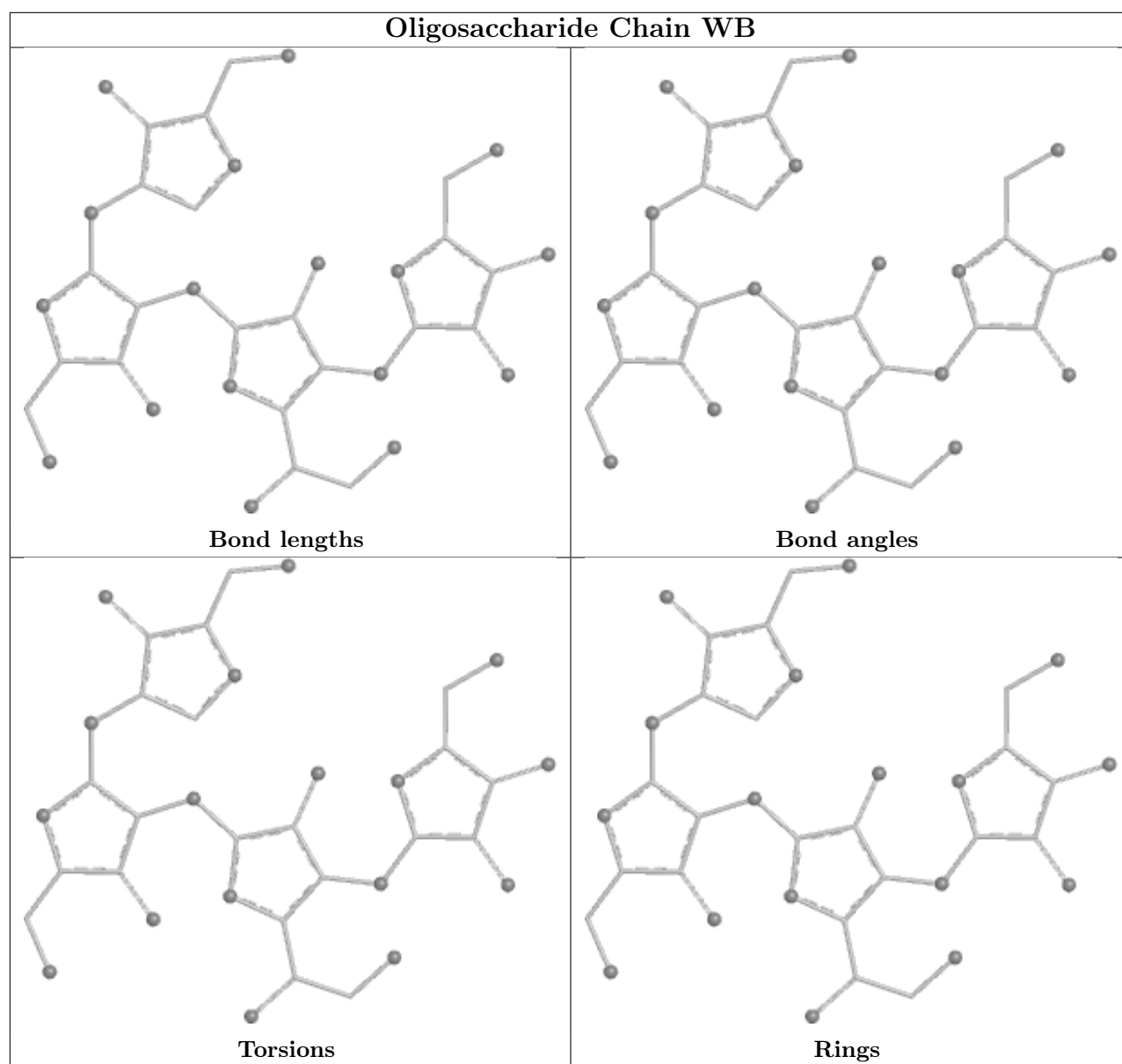


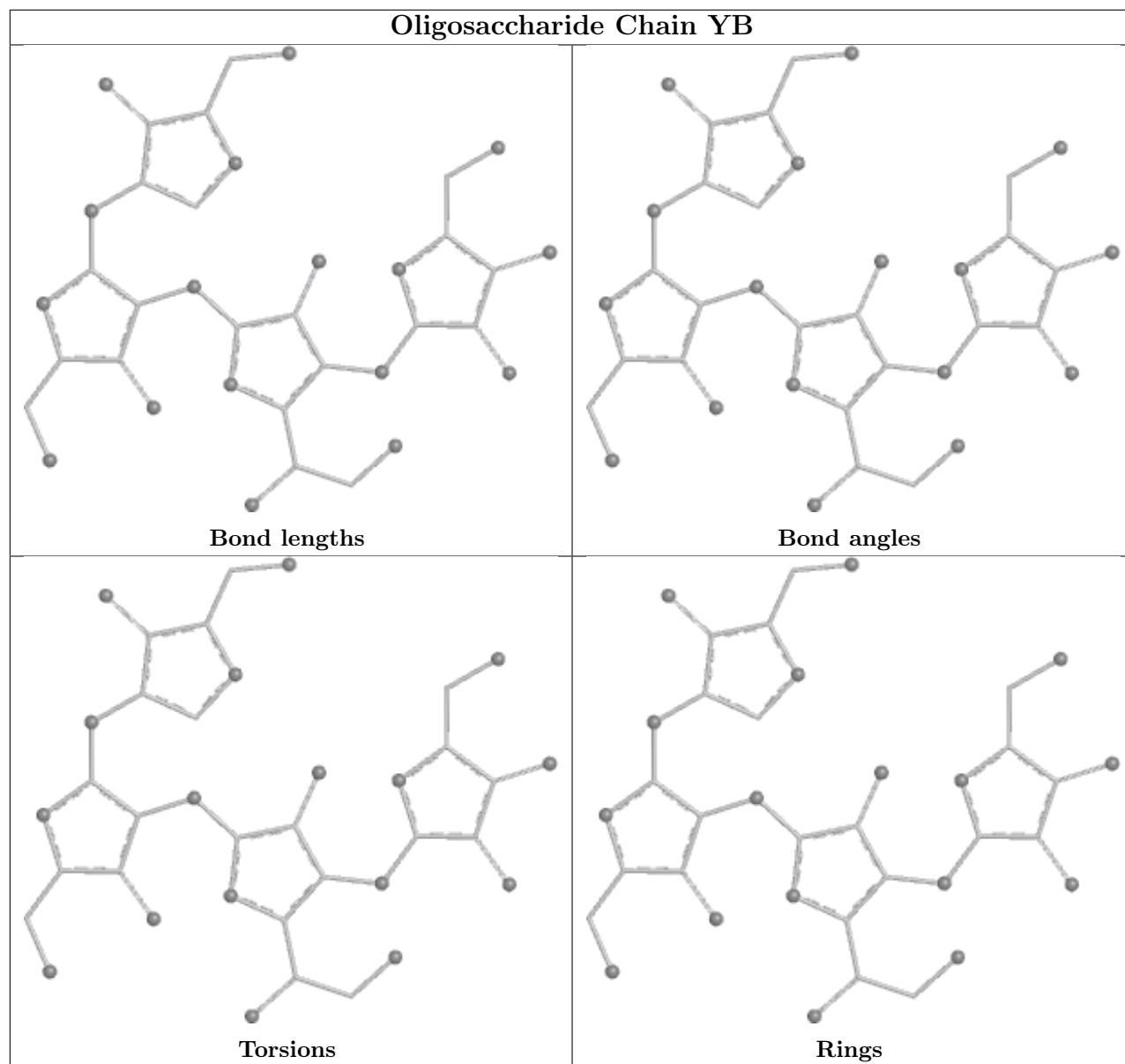
Oligosaccharide Chain 5A

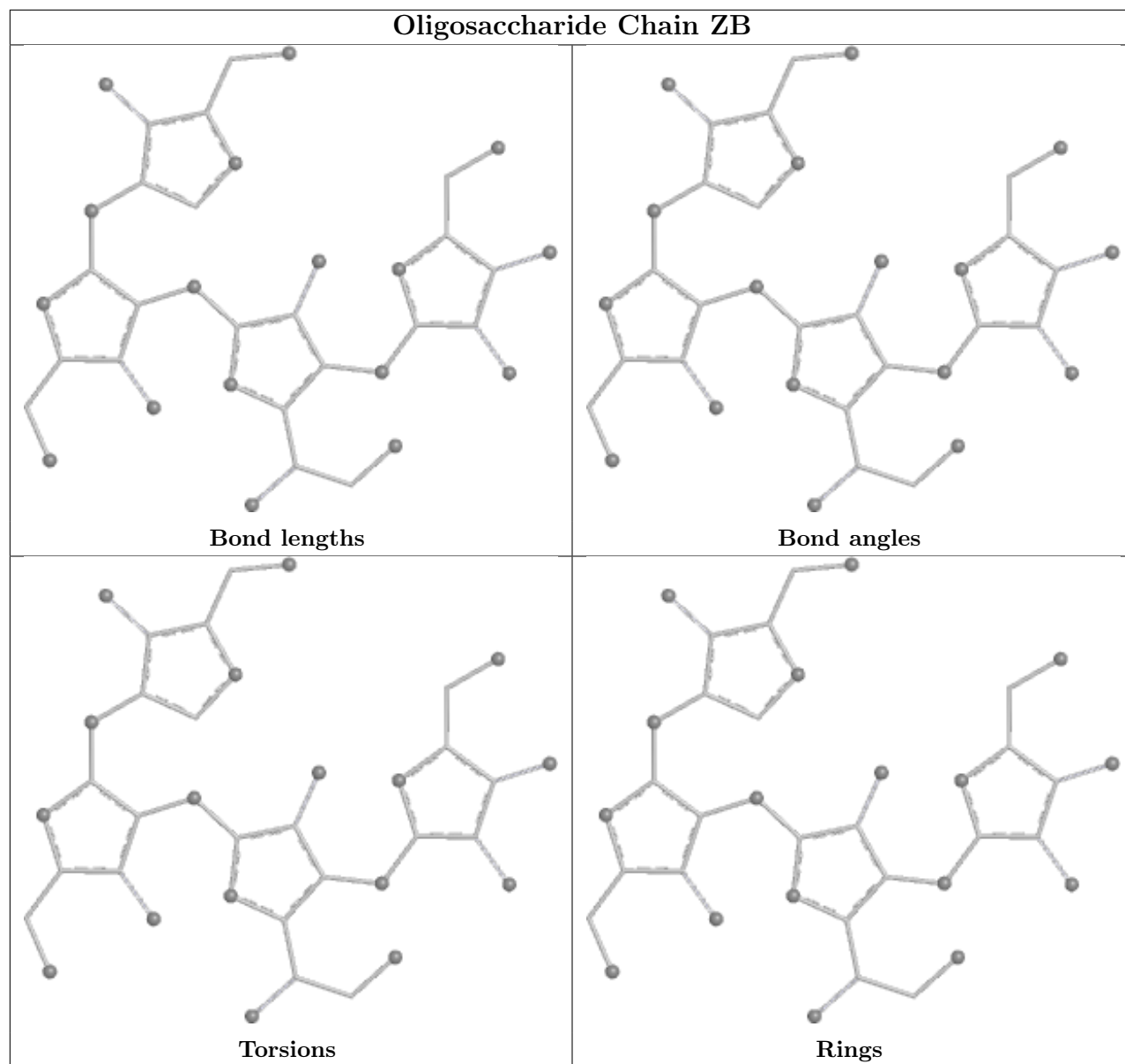


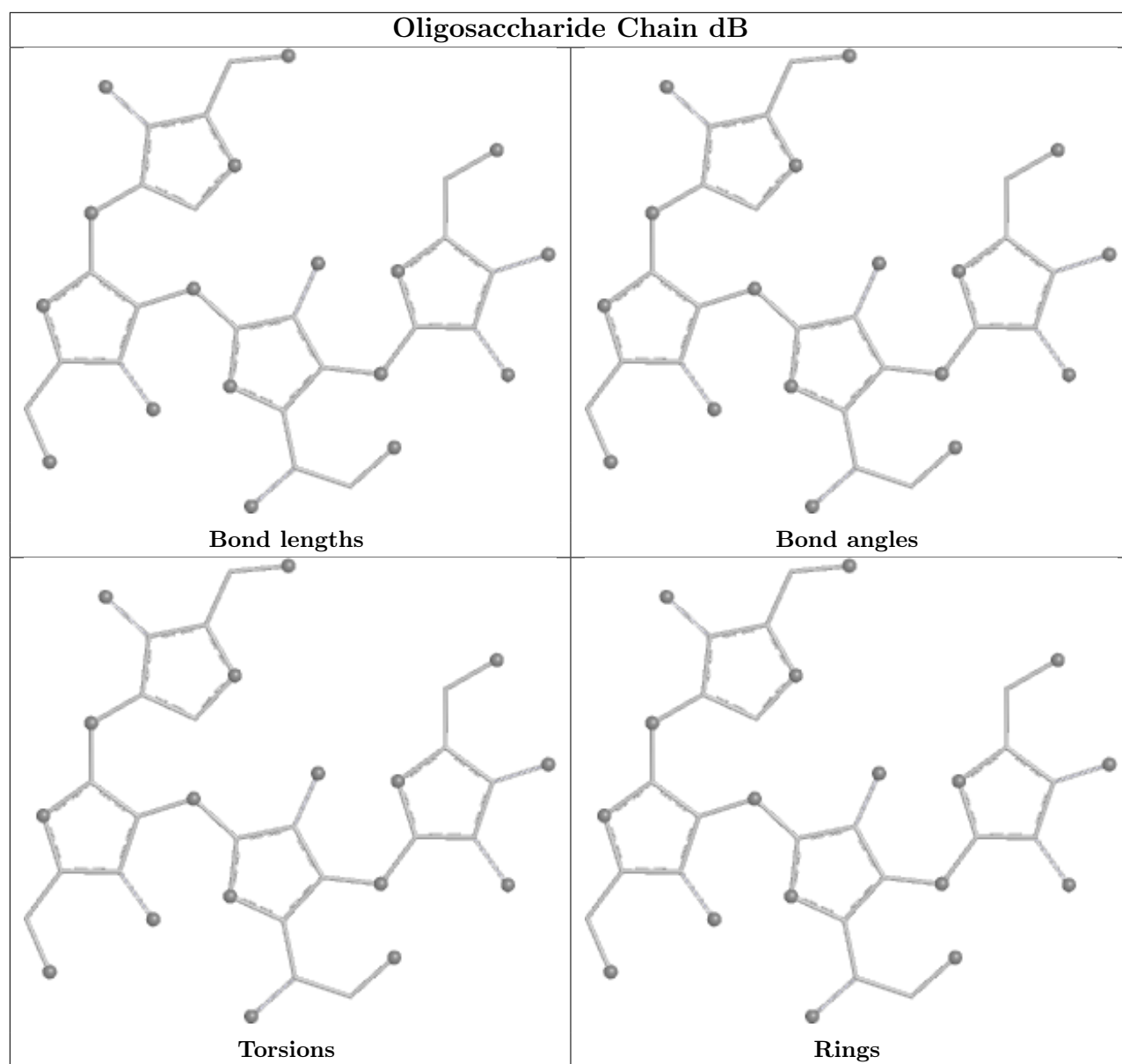


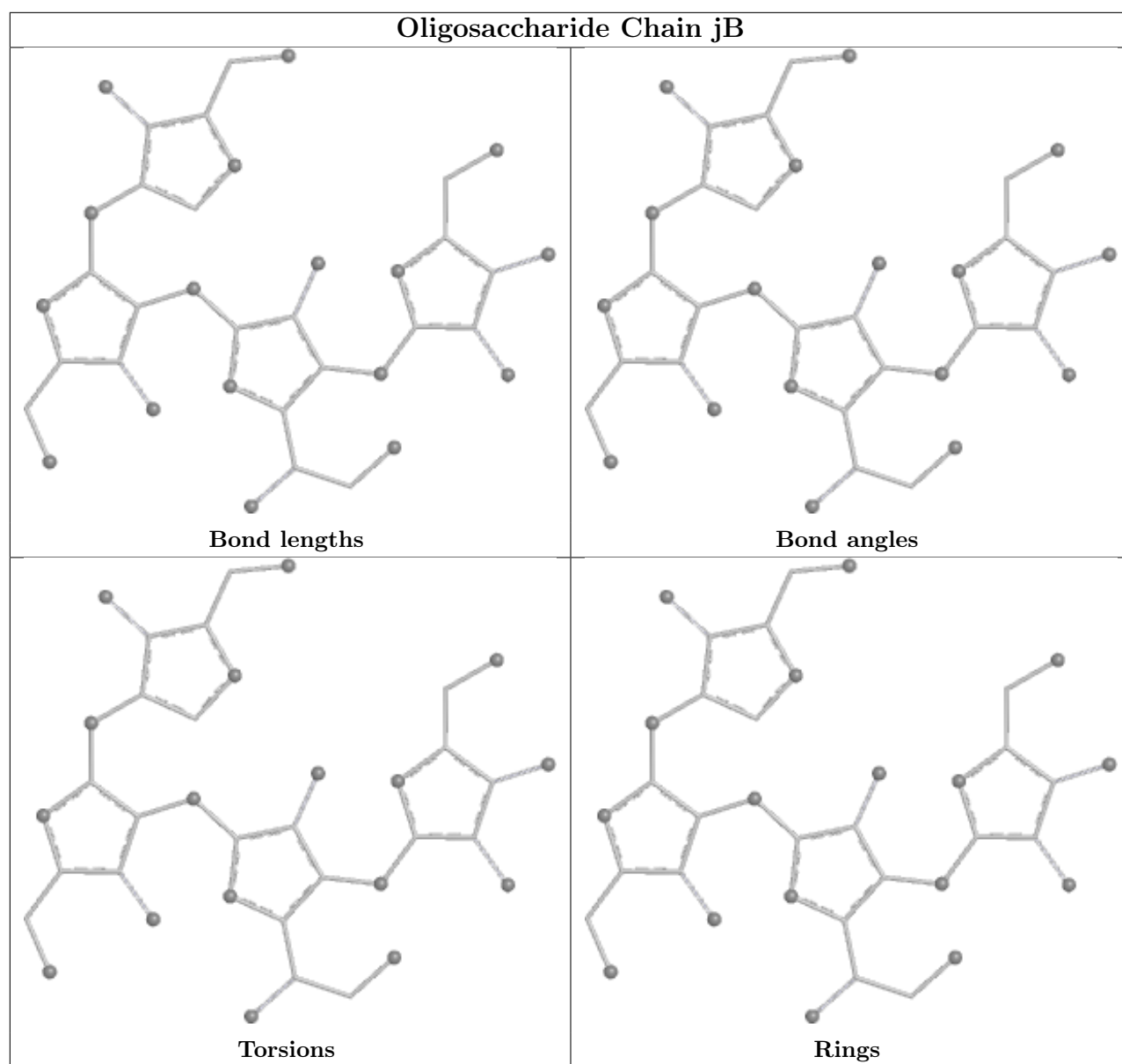


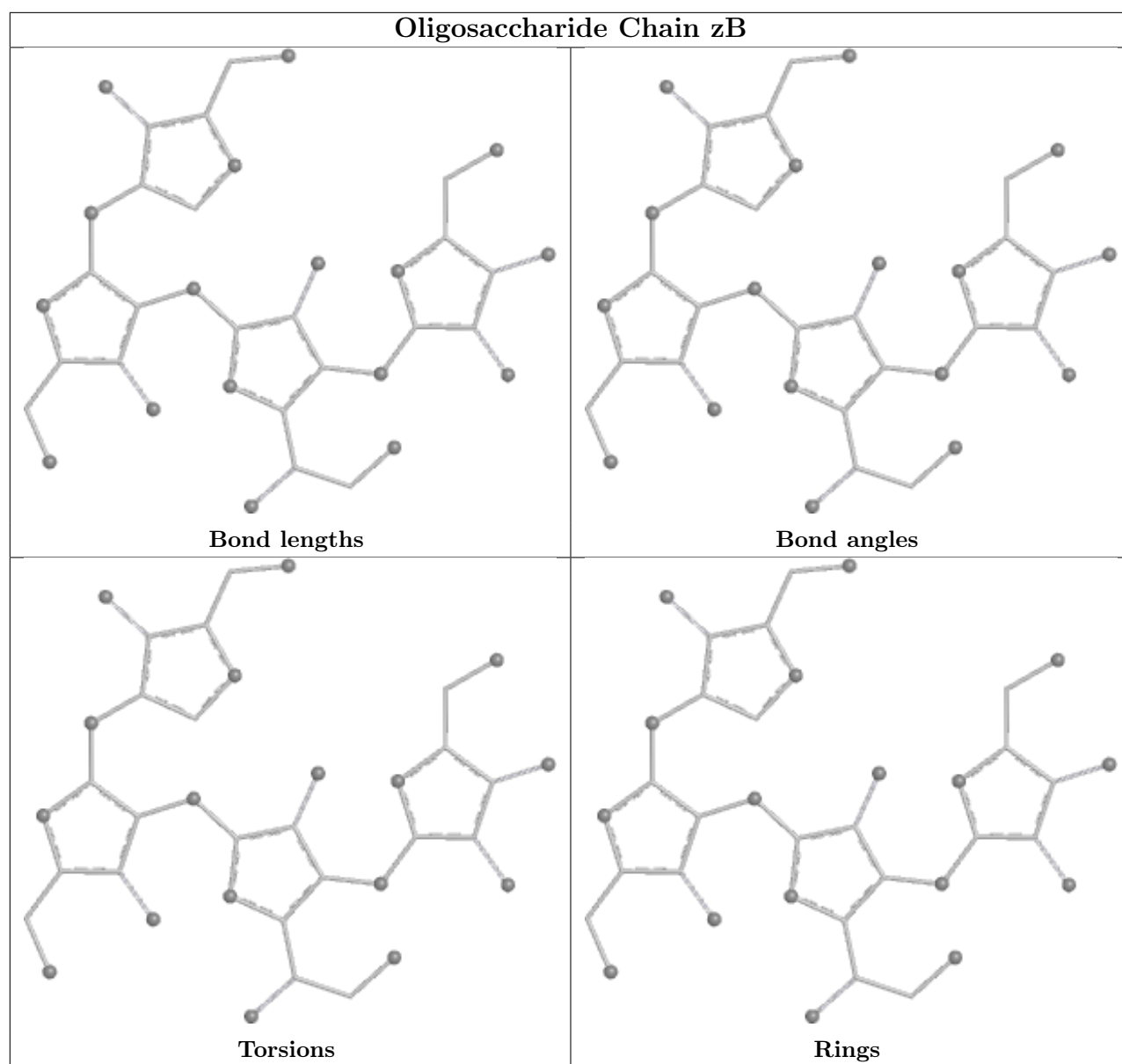


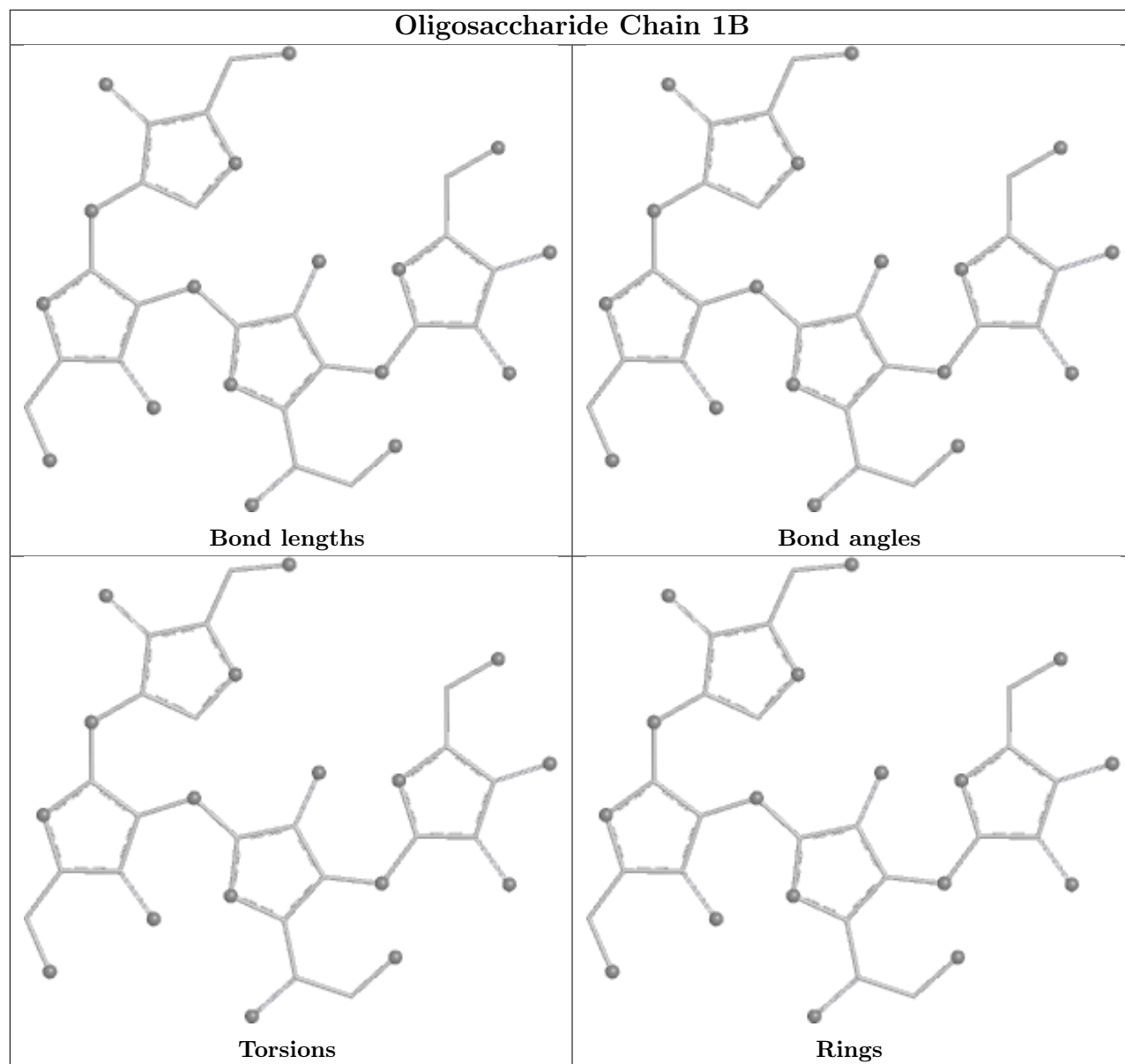
Oligosaccharide Chain YB

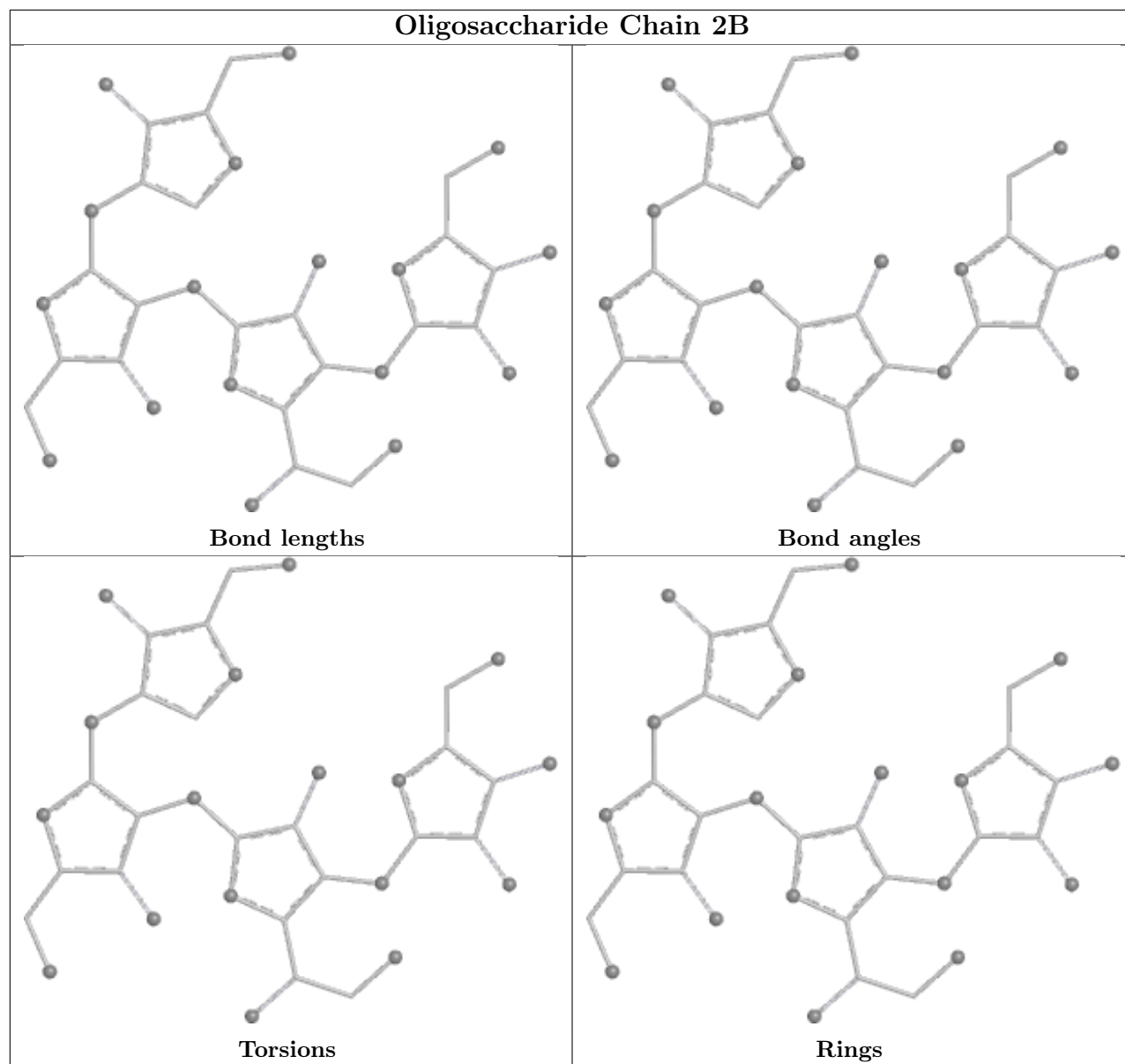


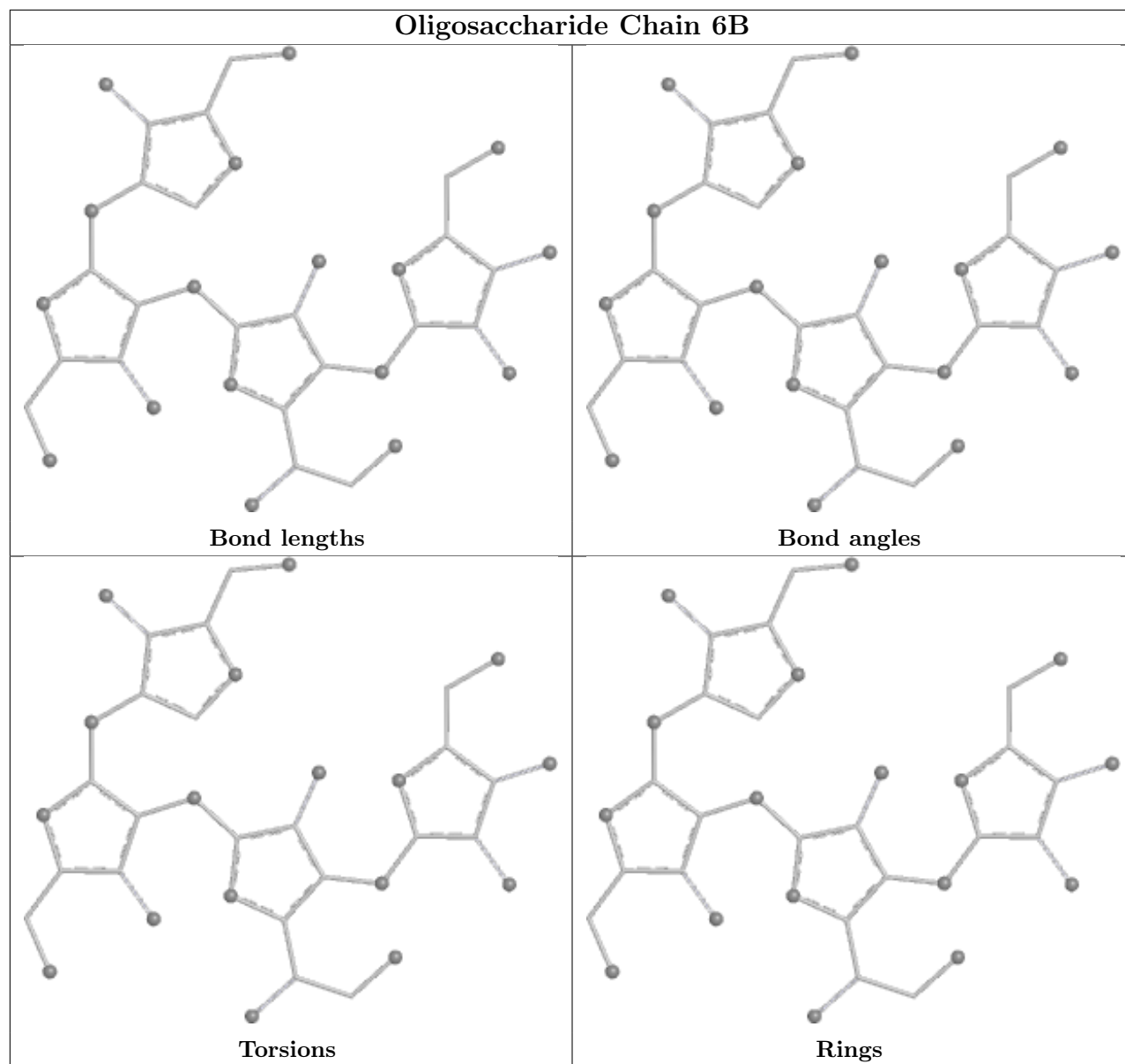


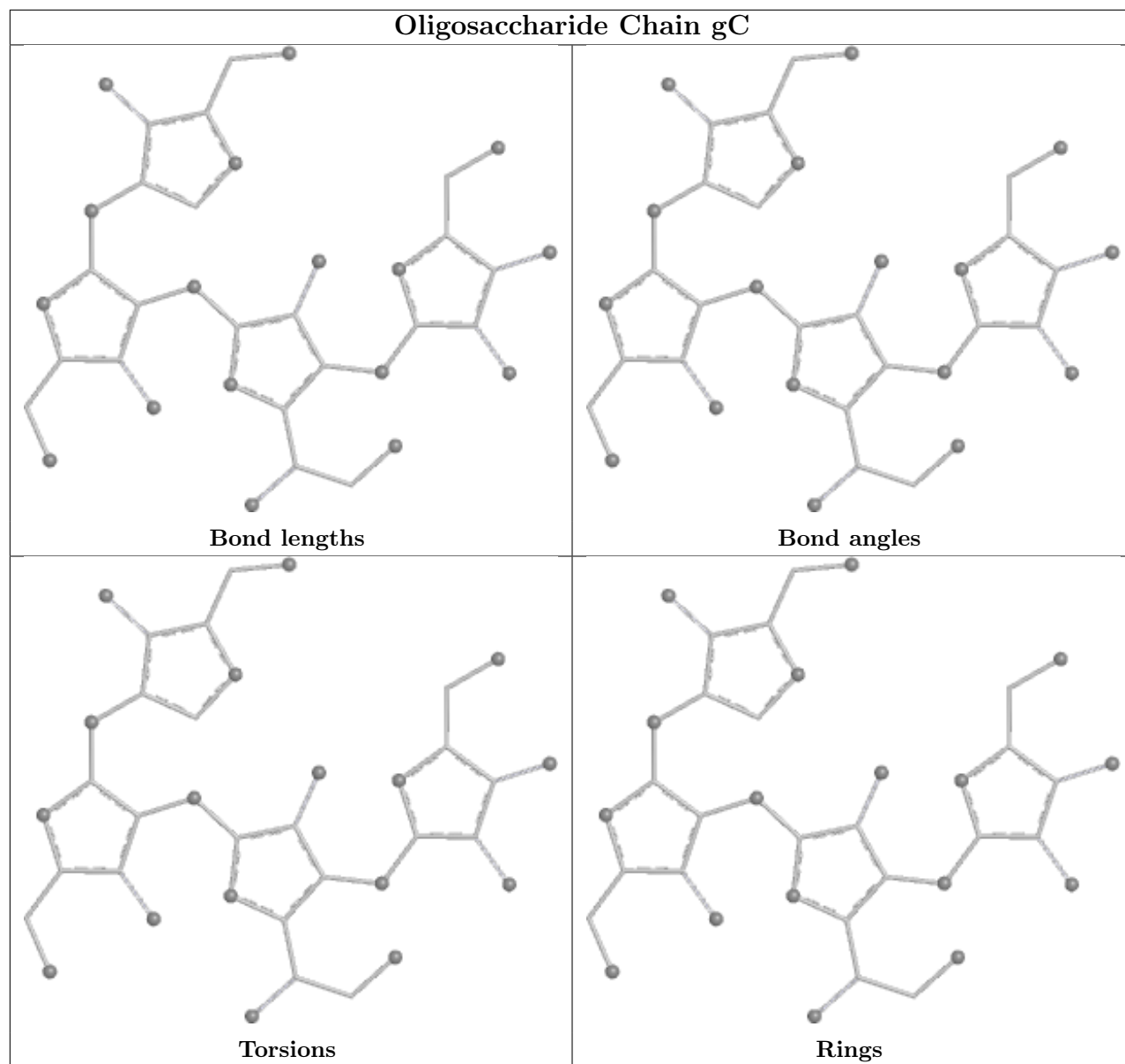


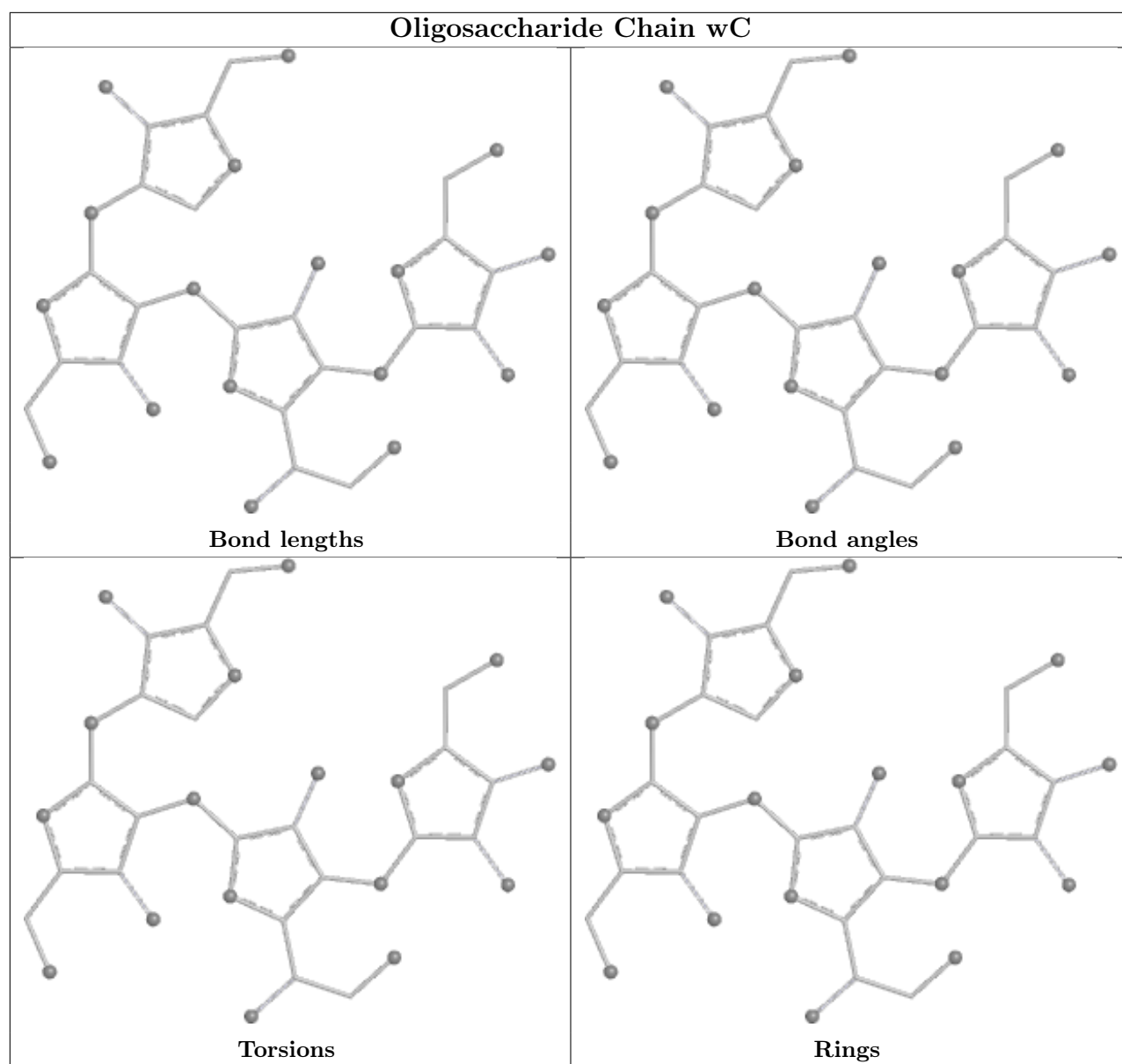


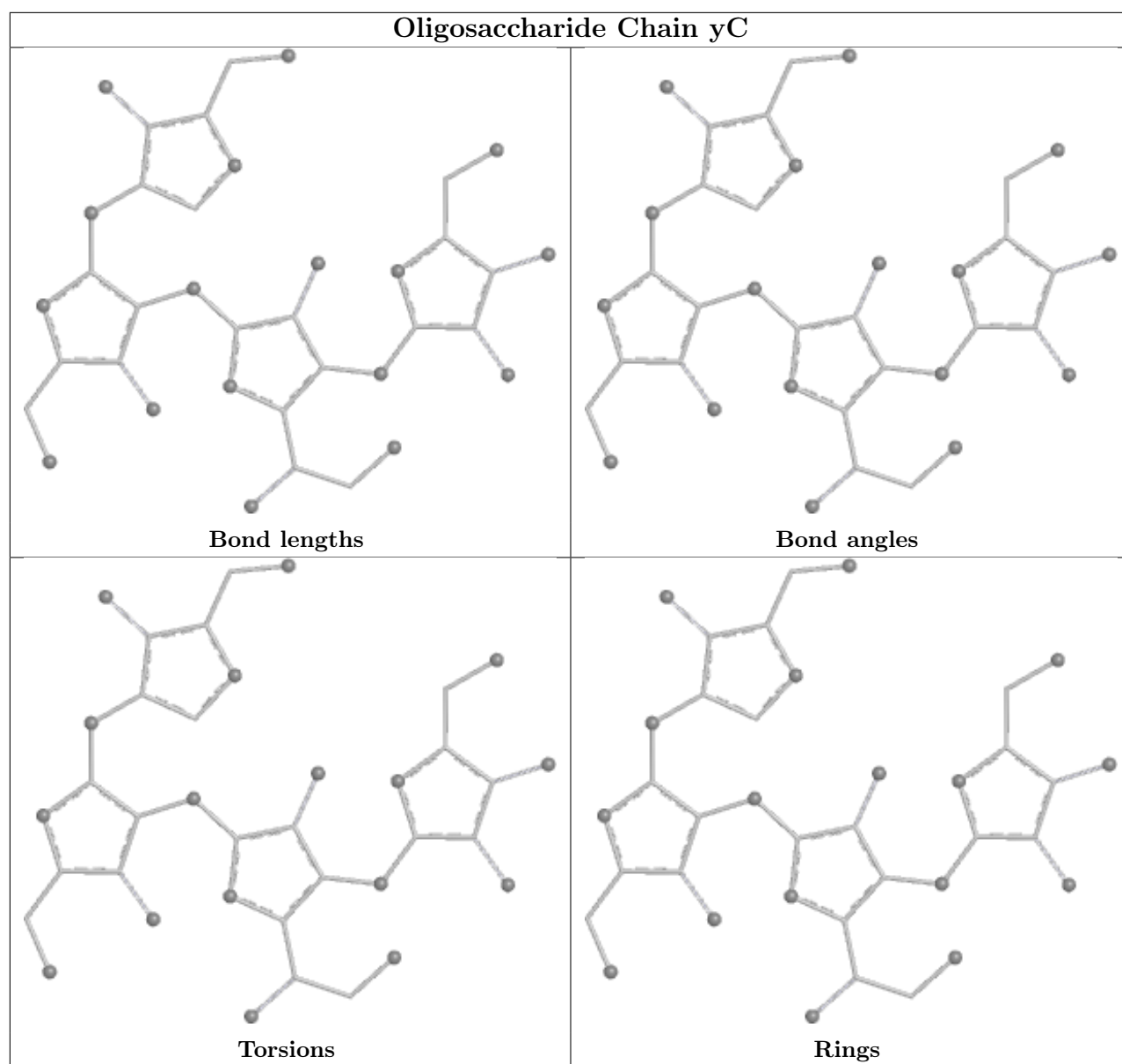


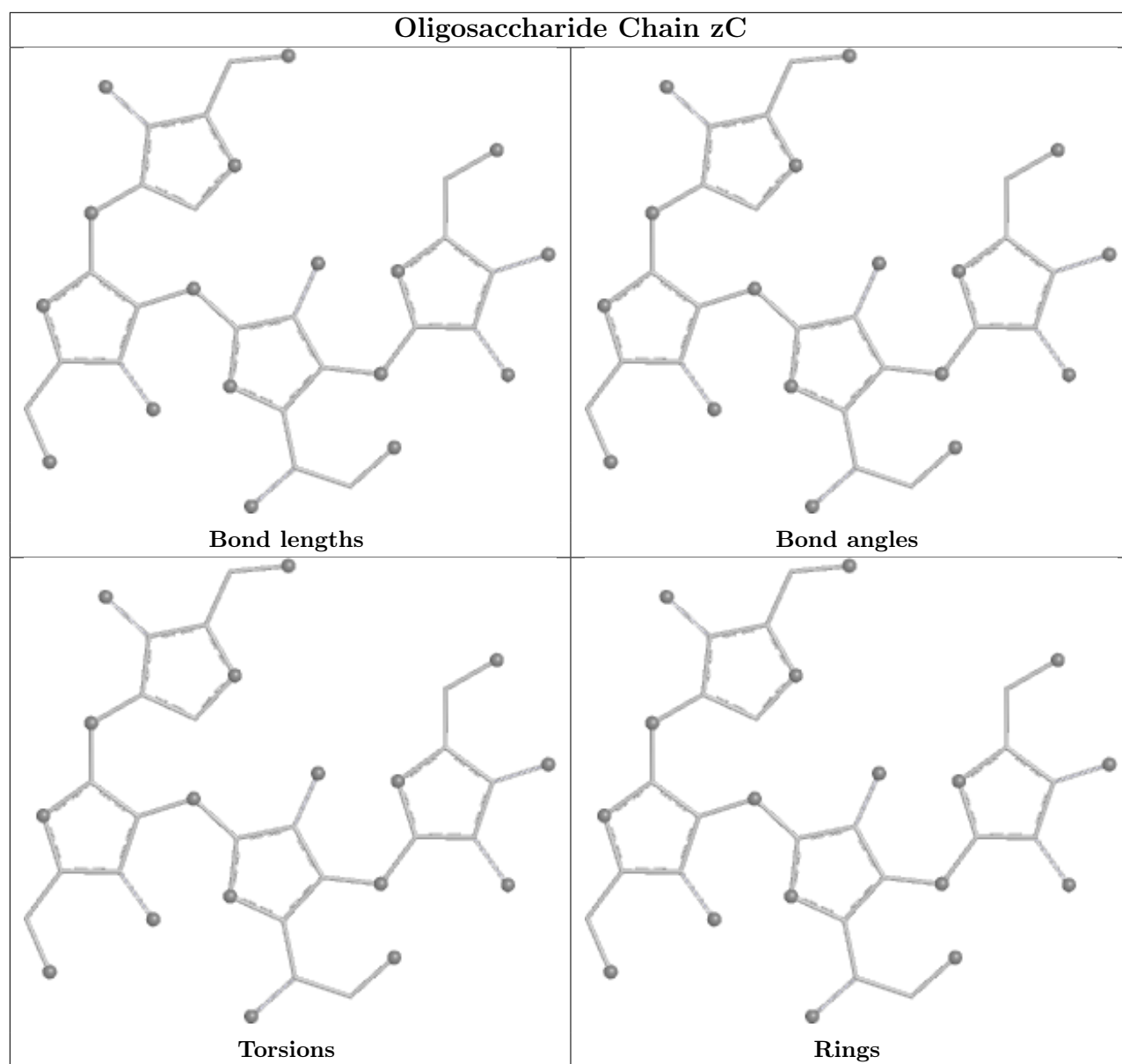


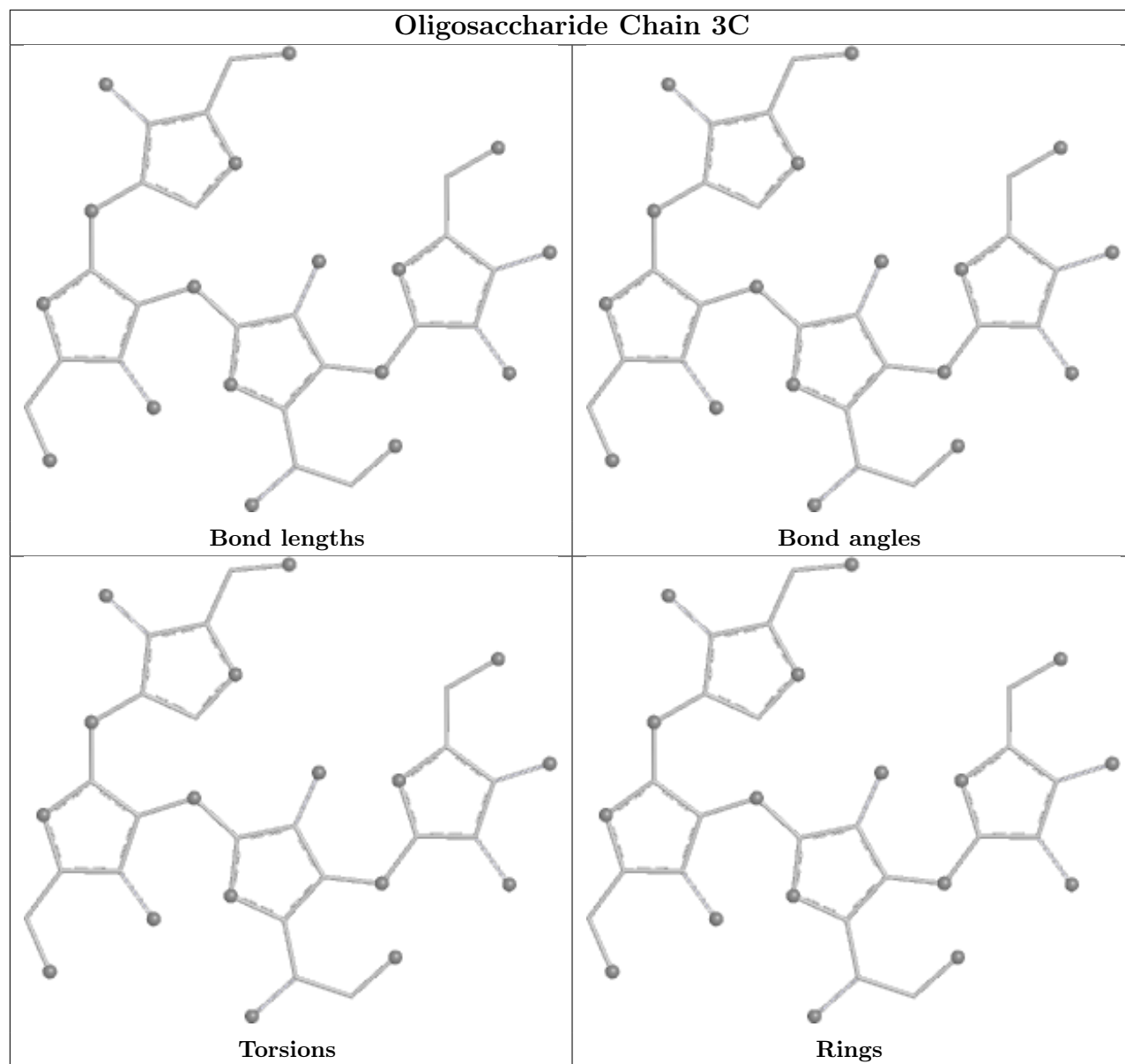


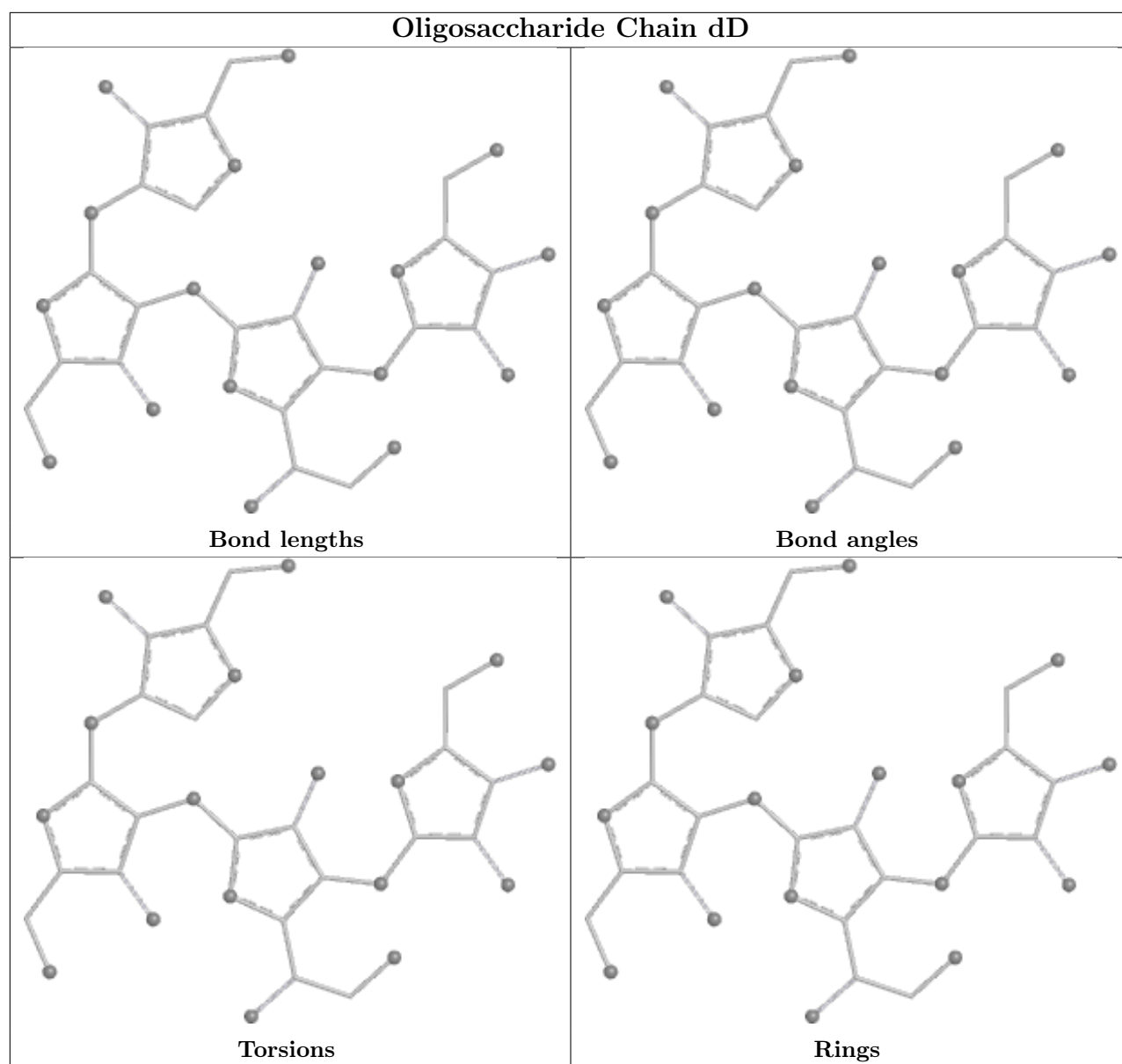


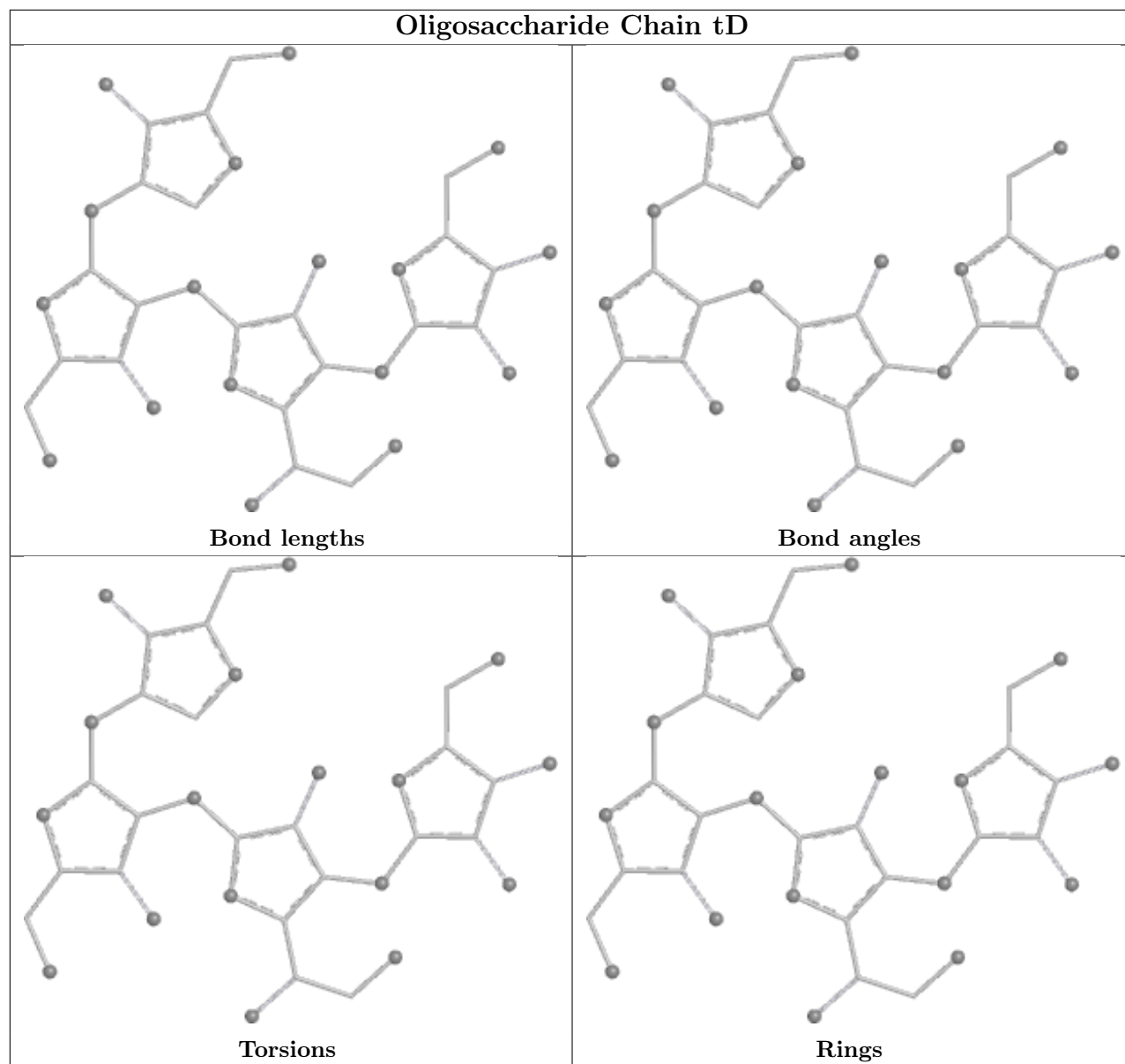


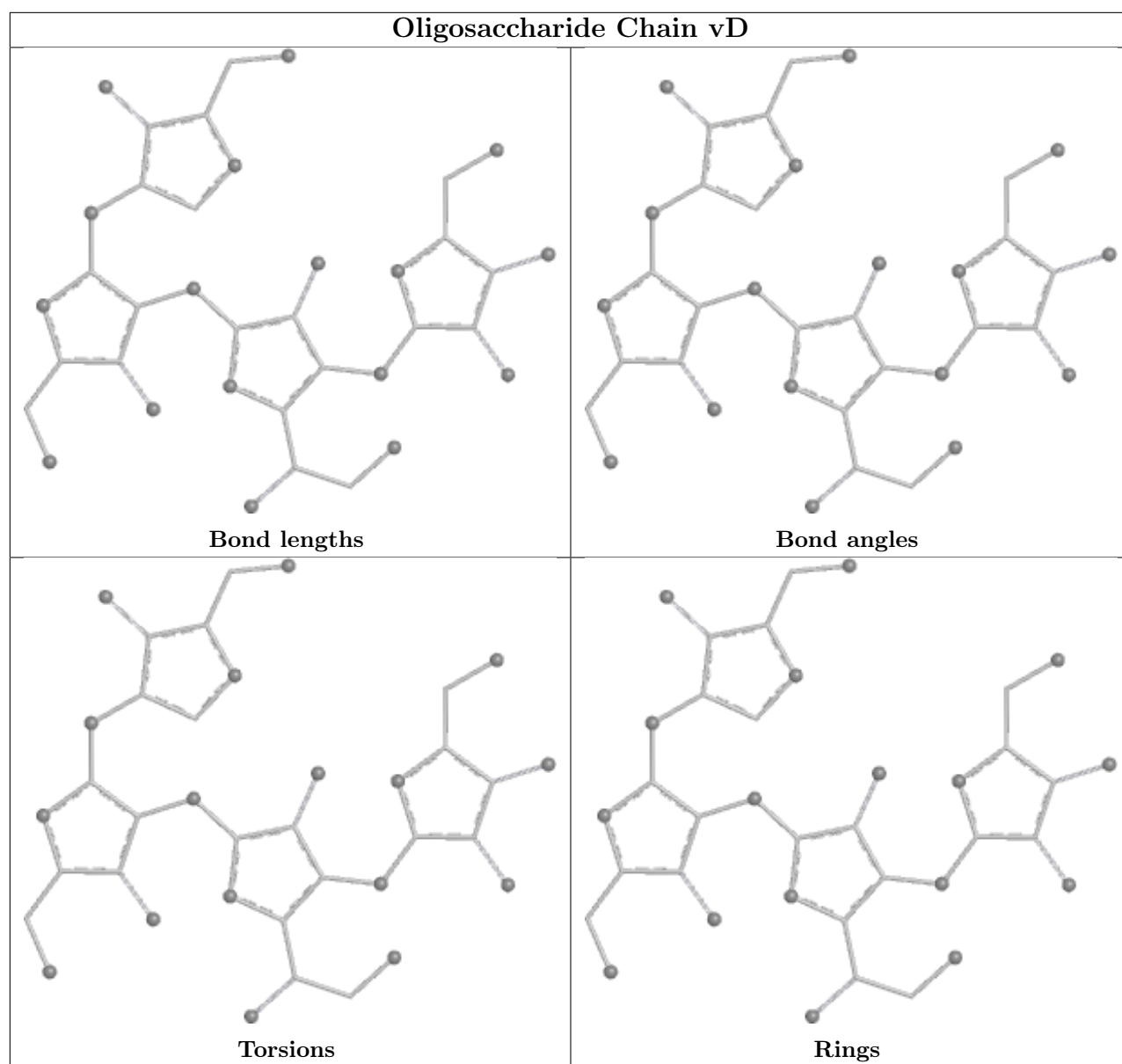


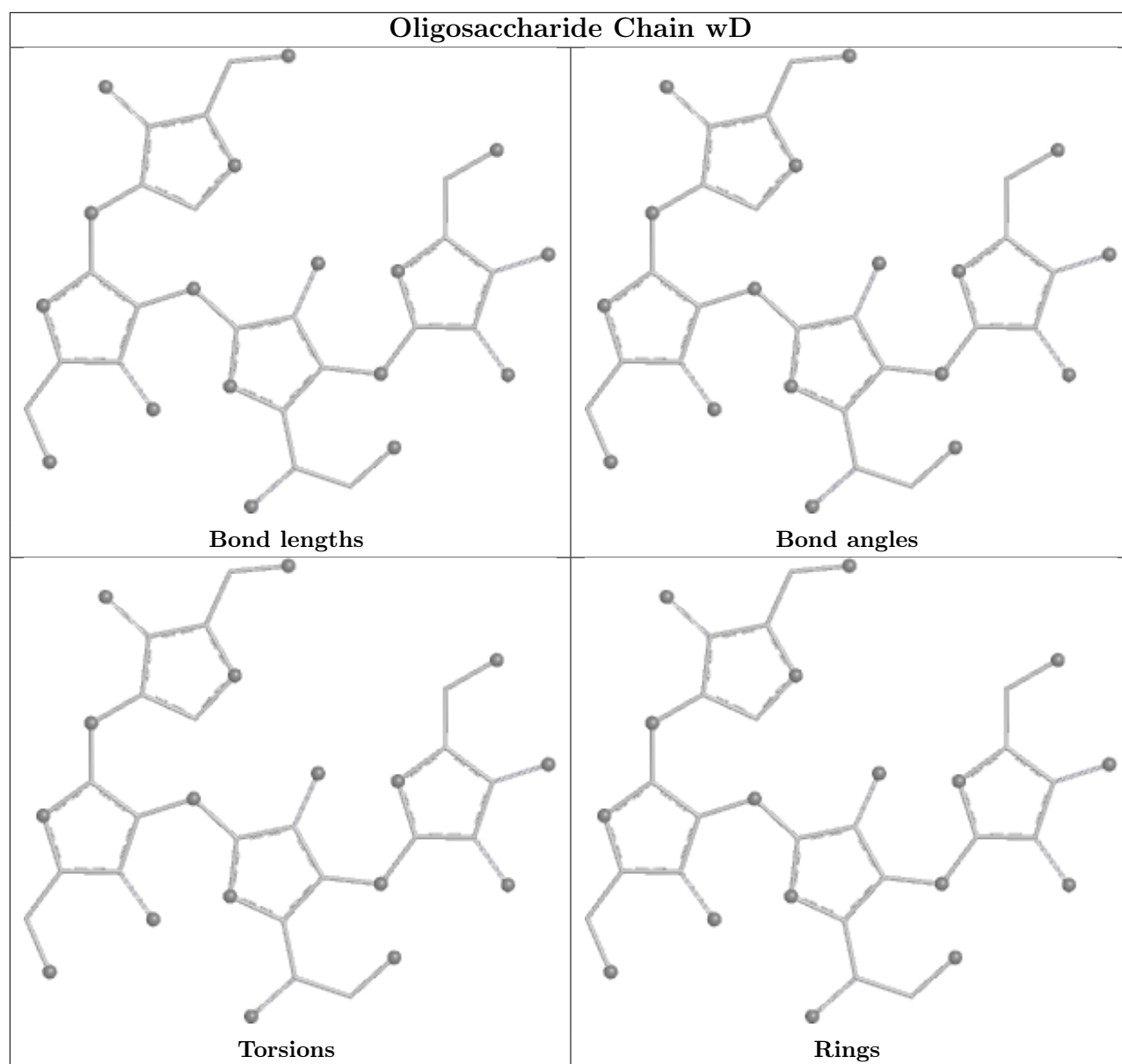


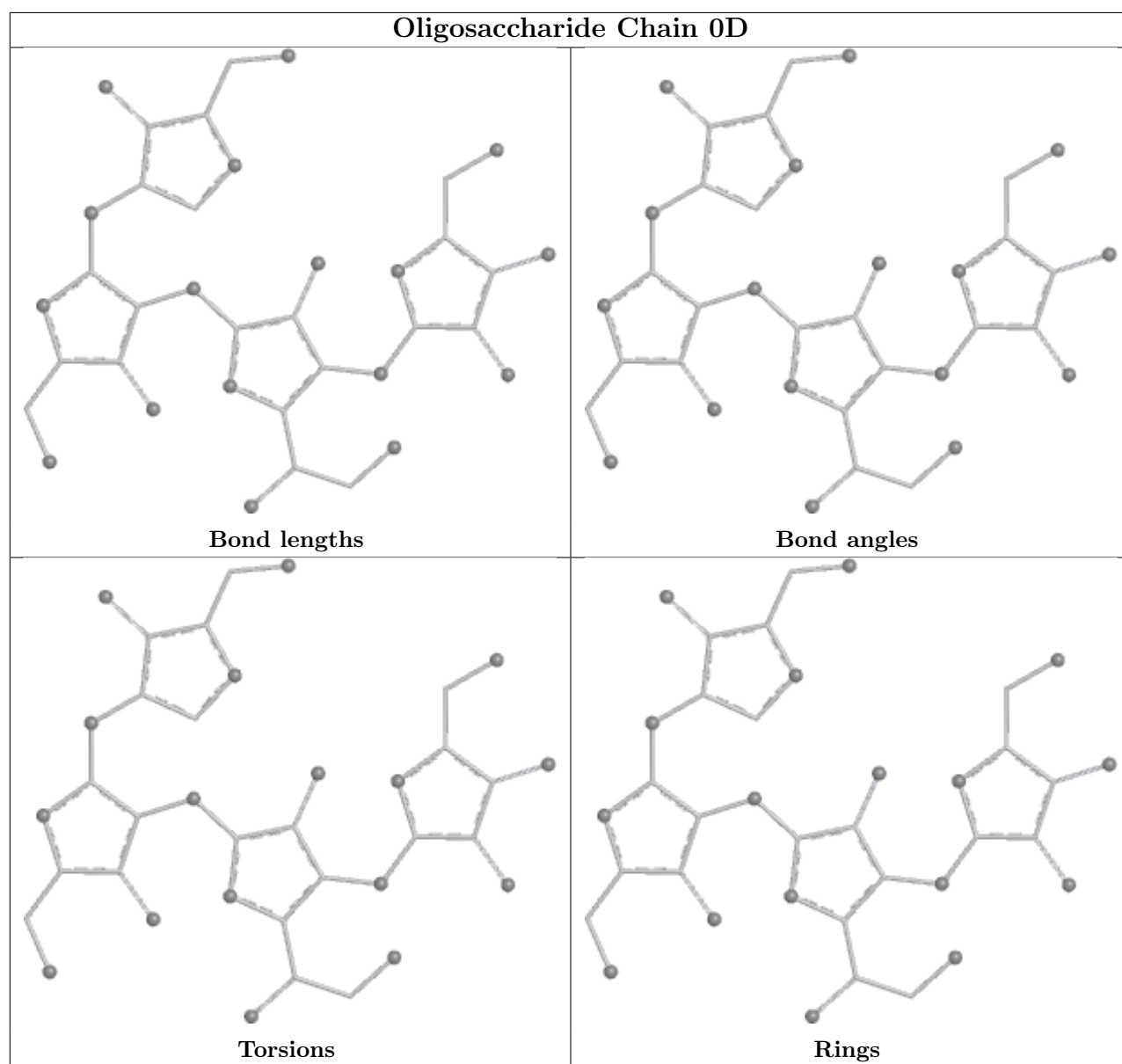


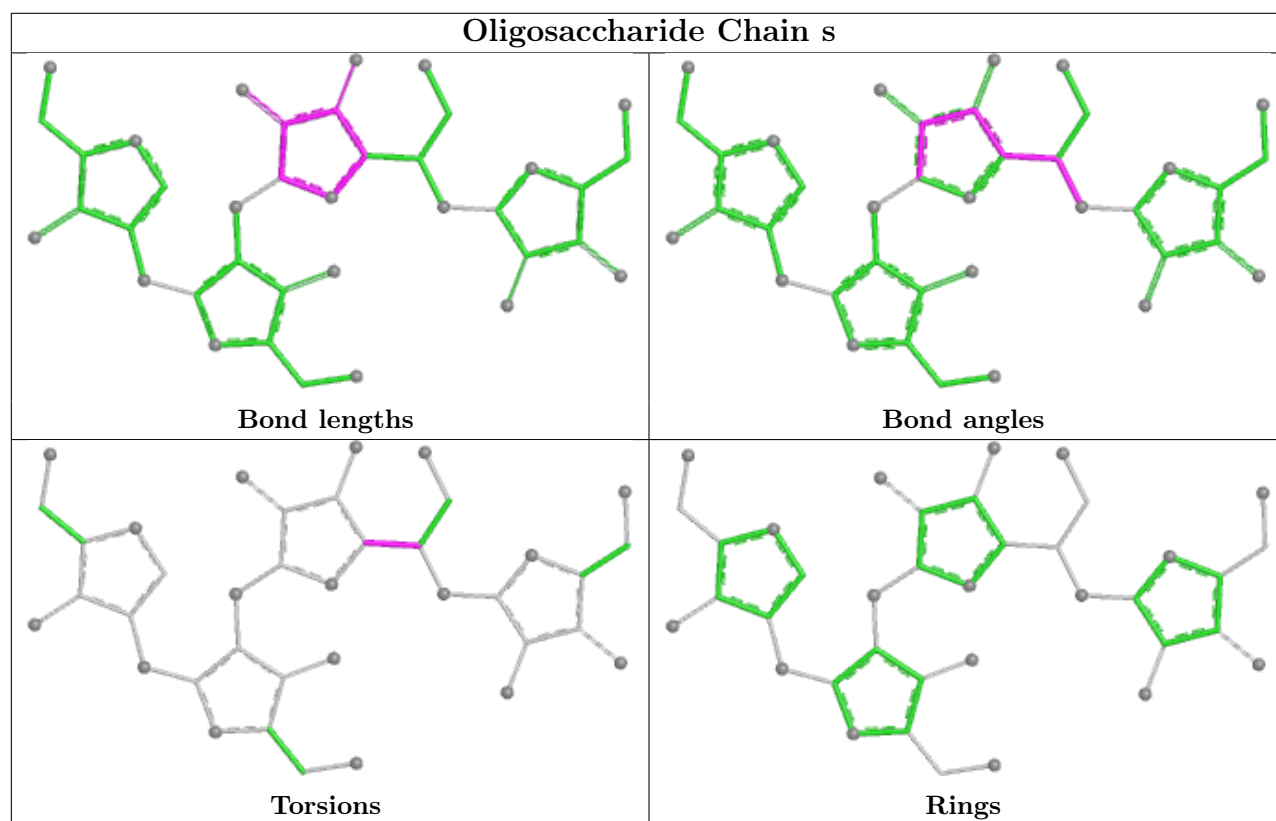
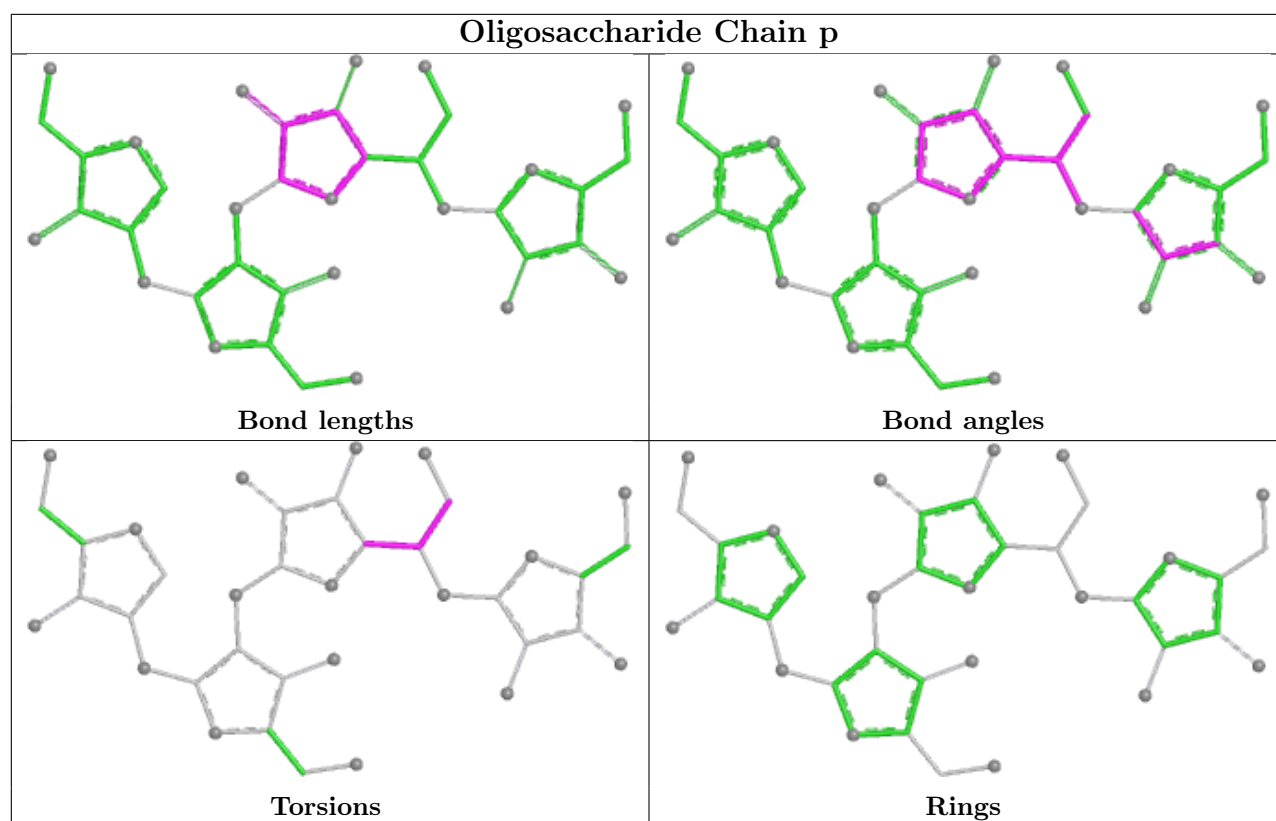


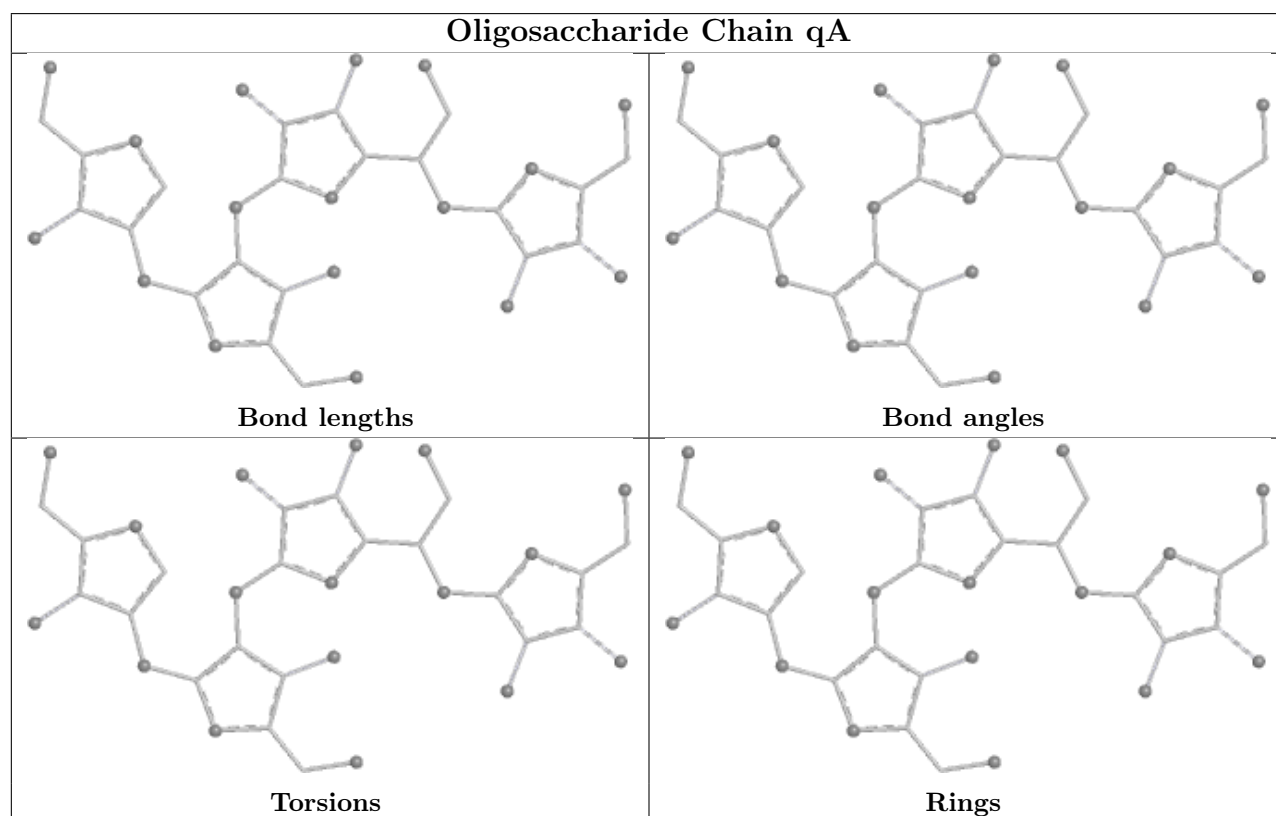
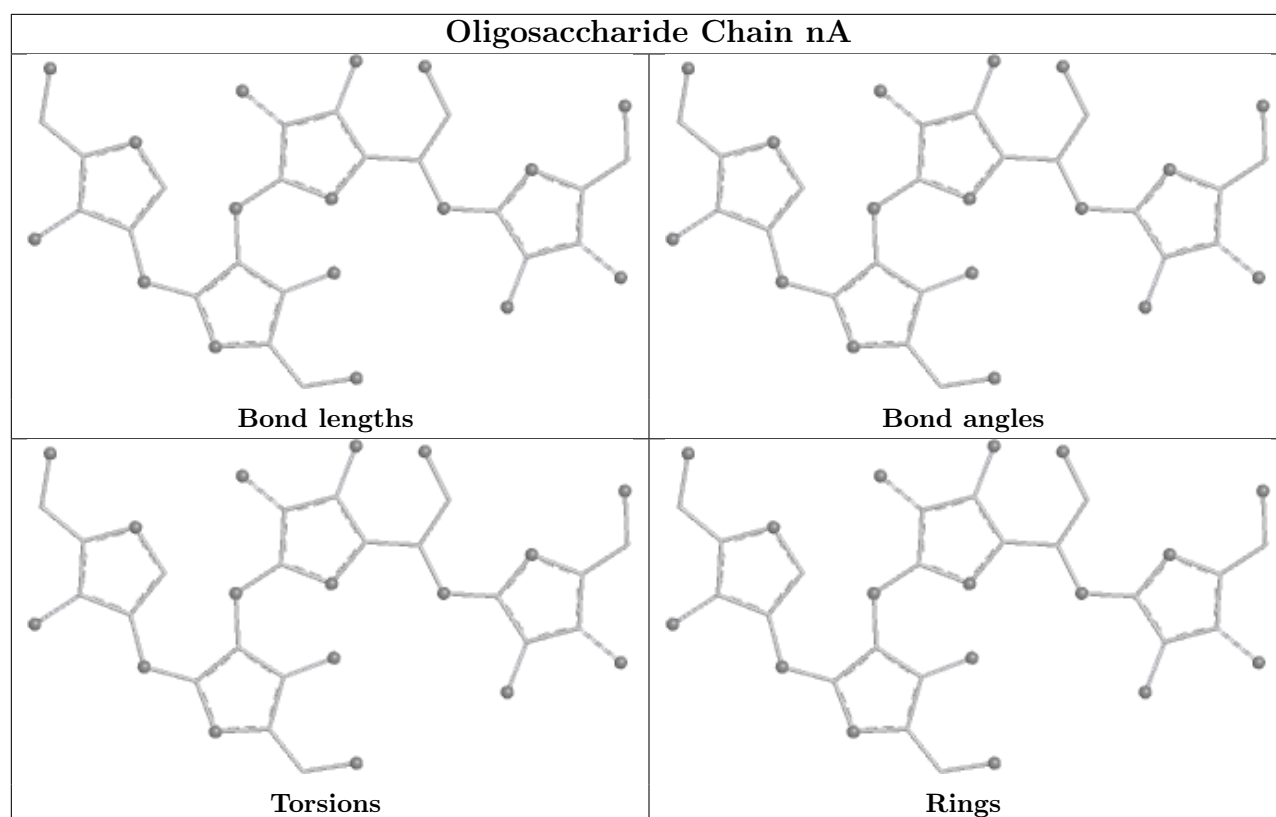


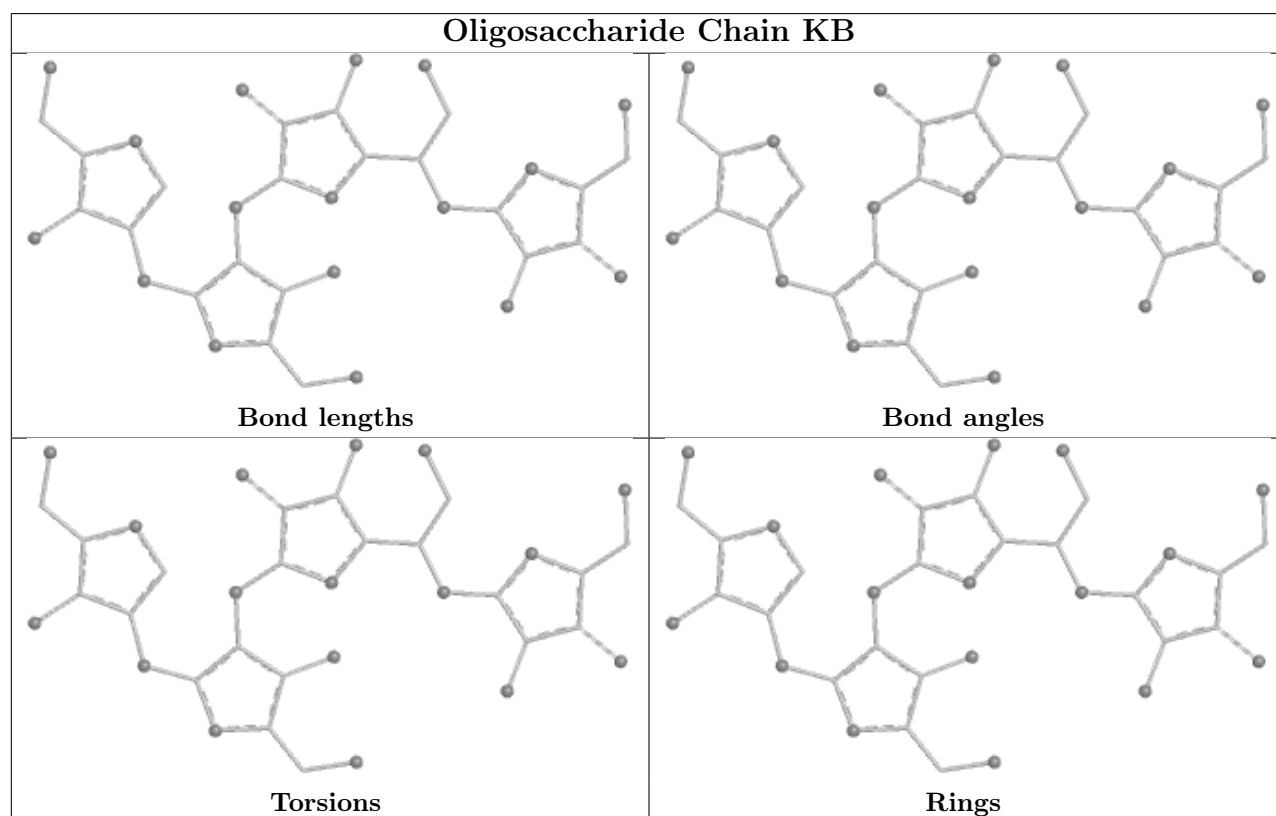
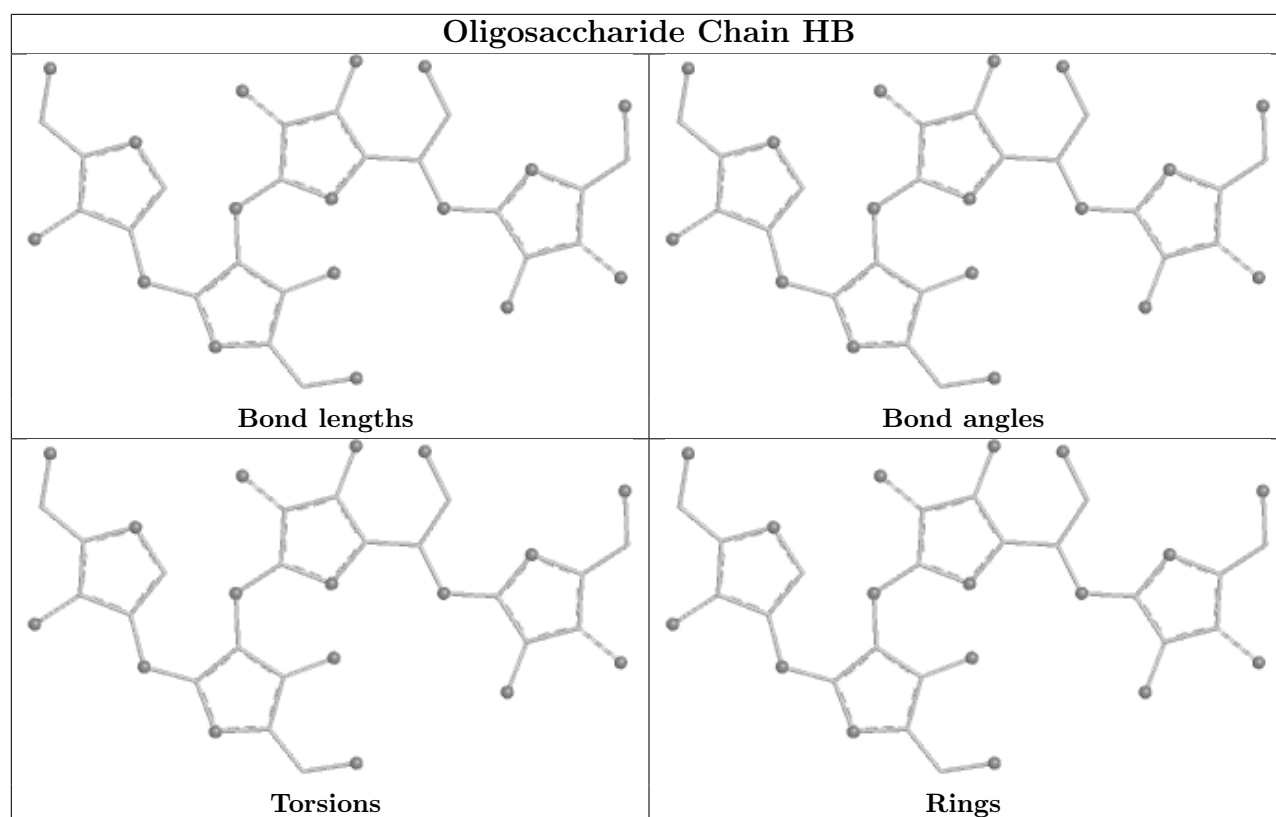


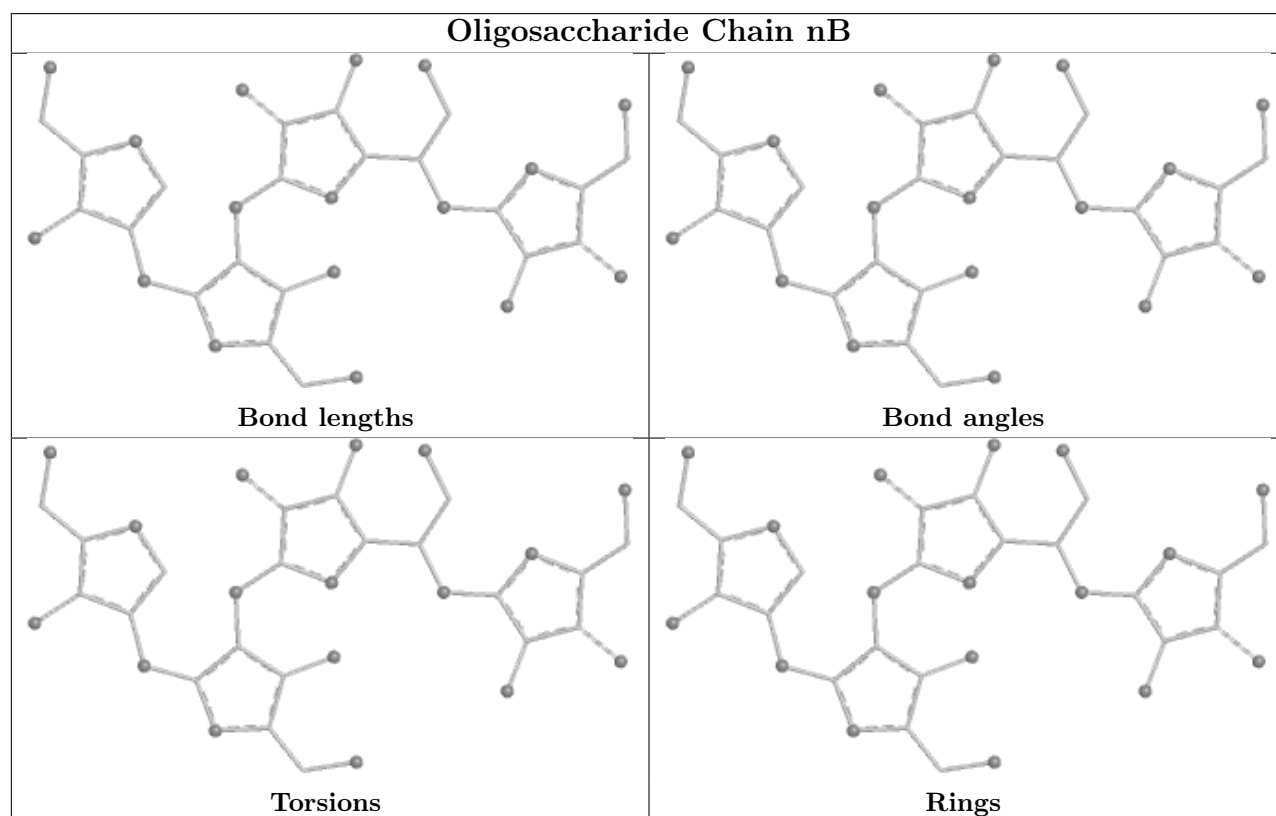
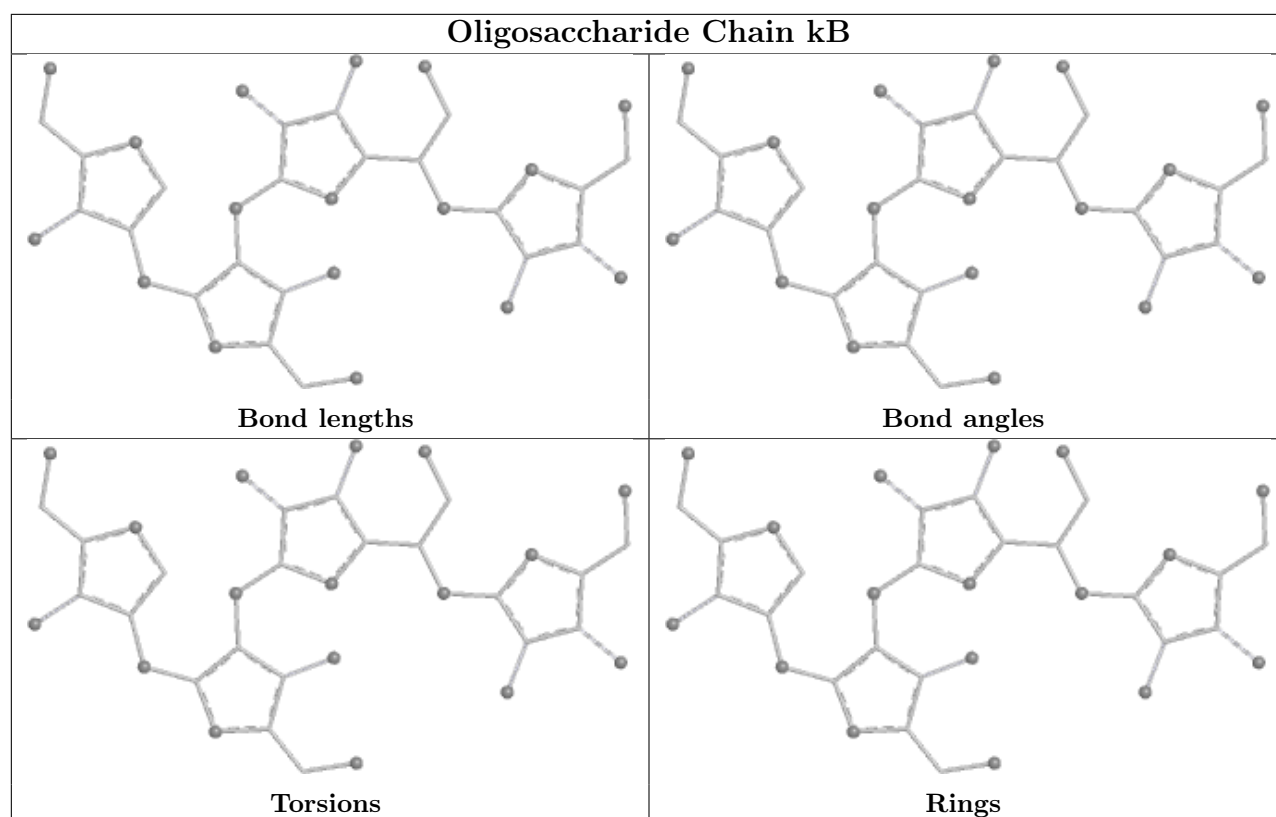


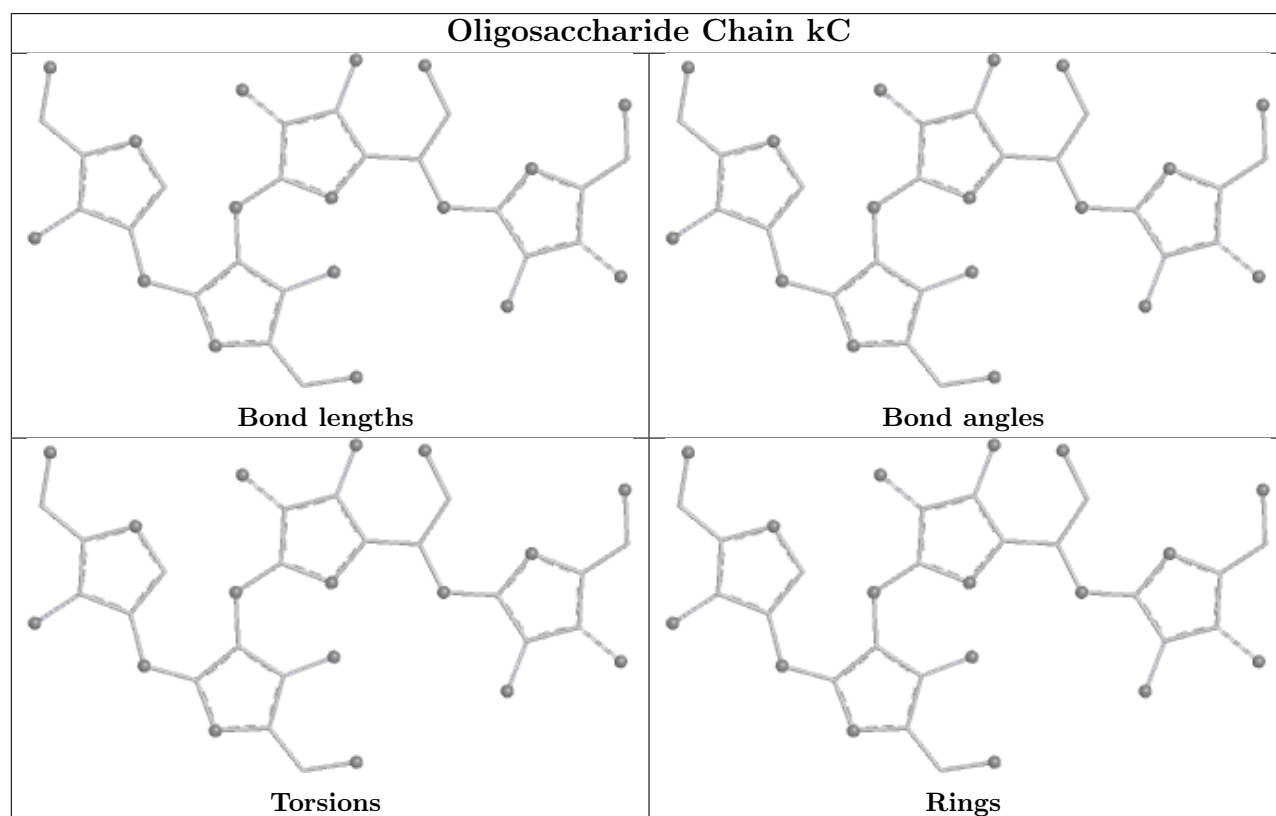
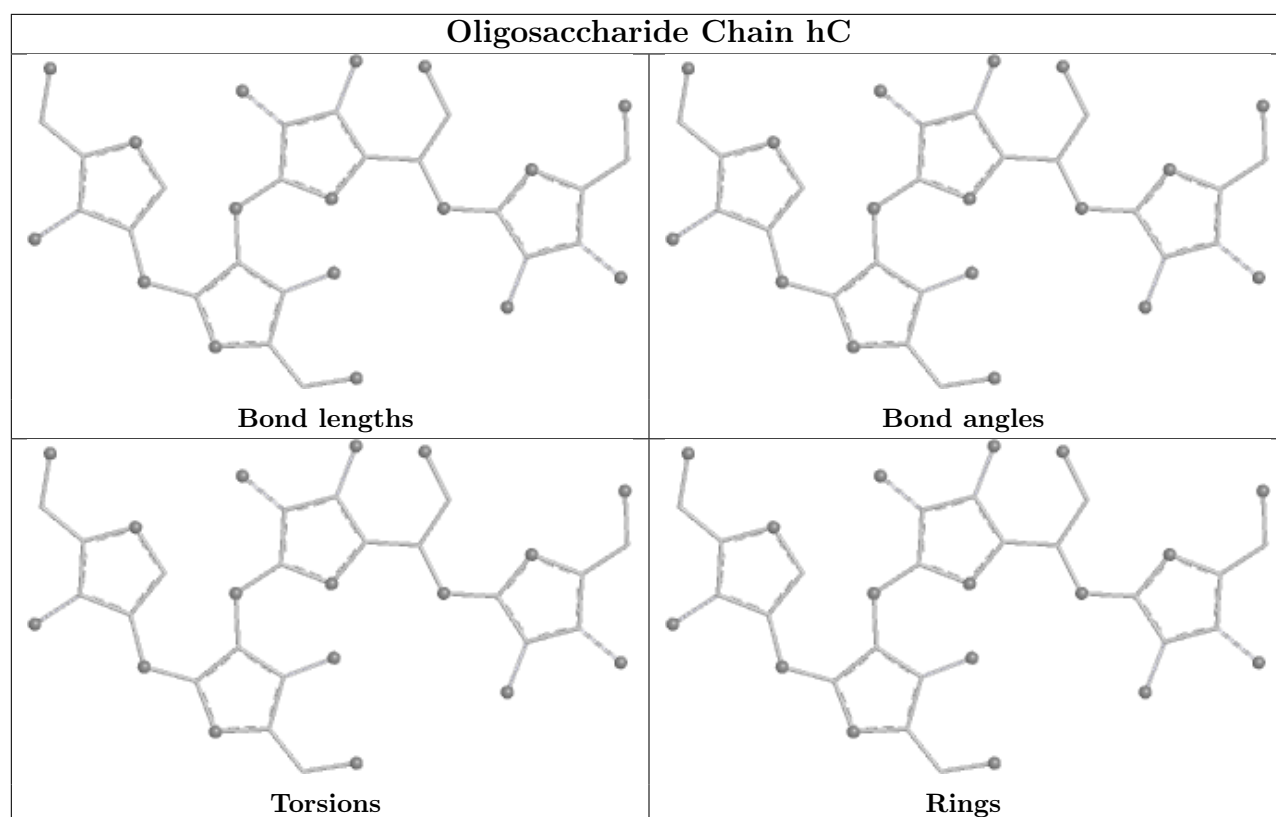


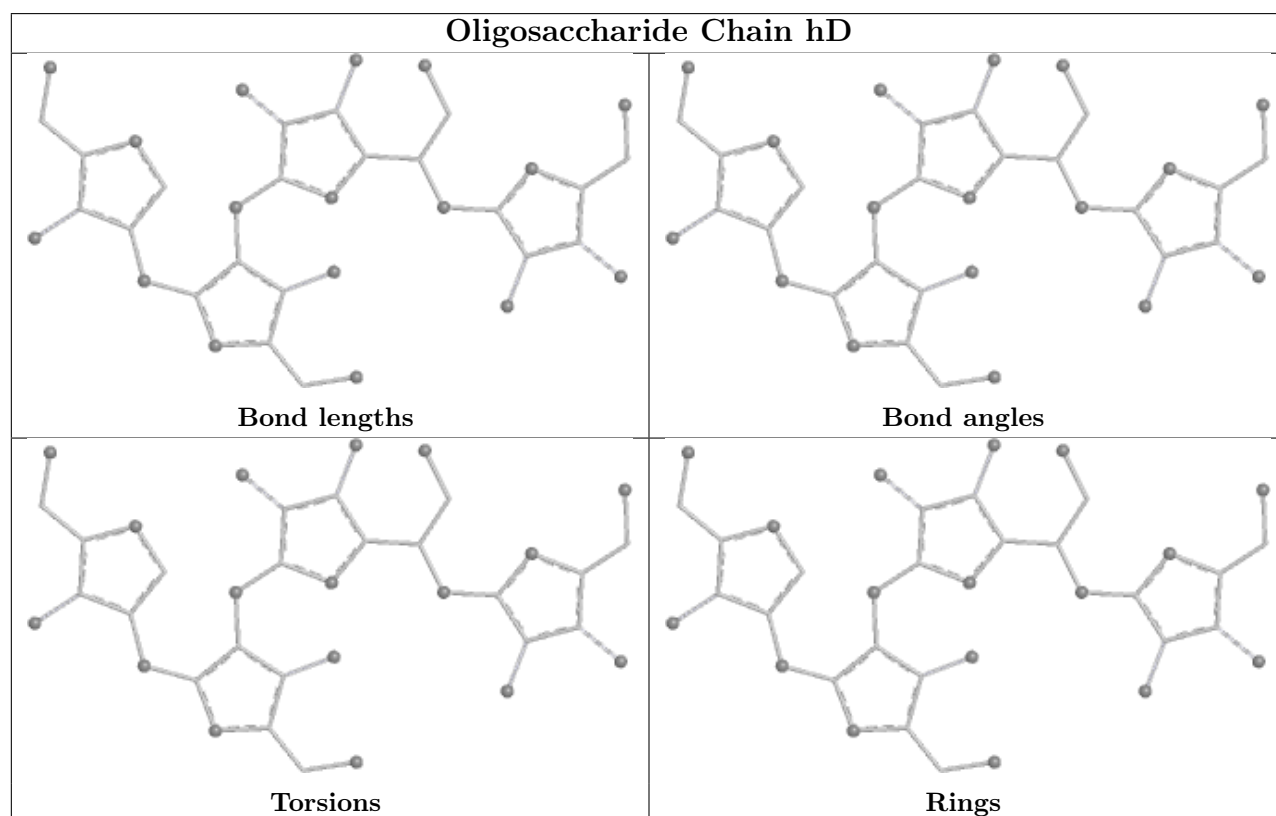
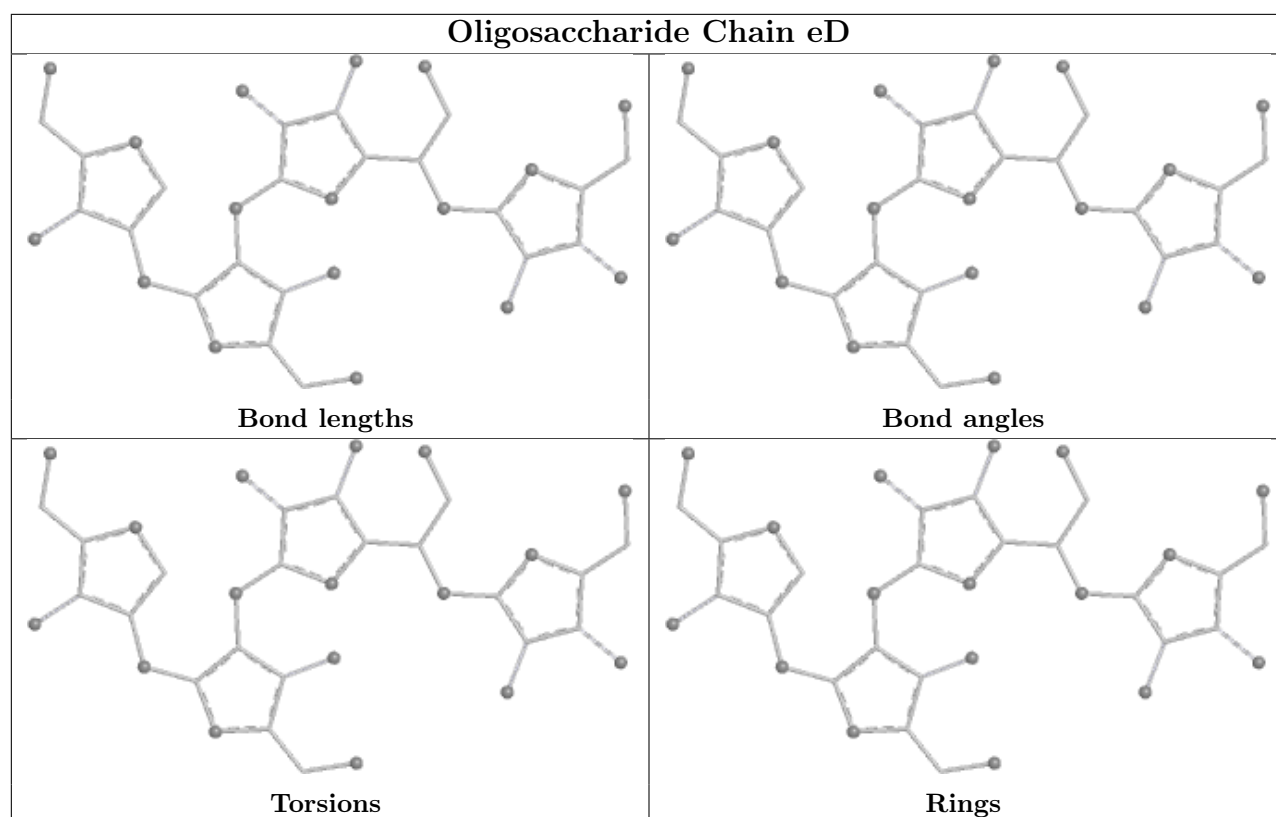


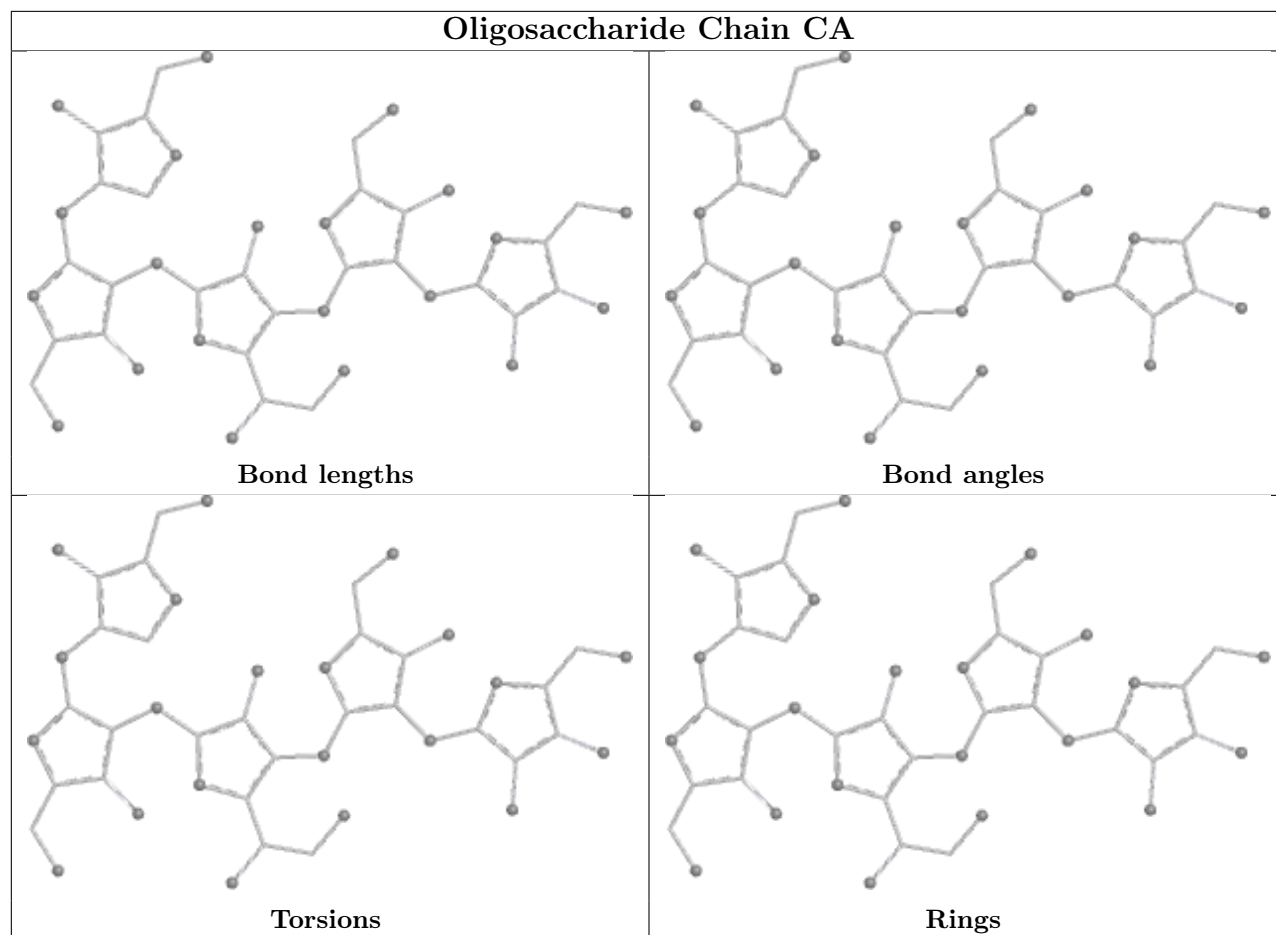


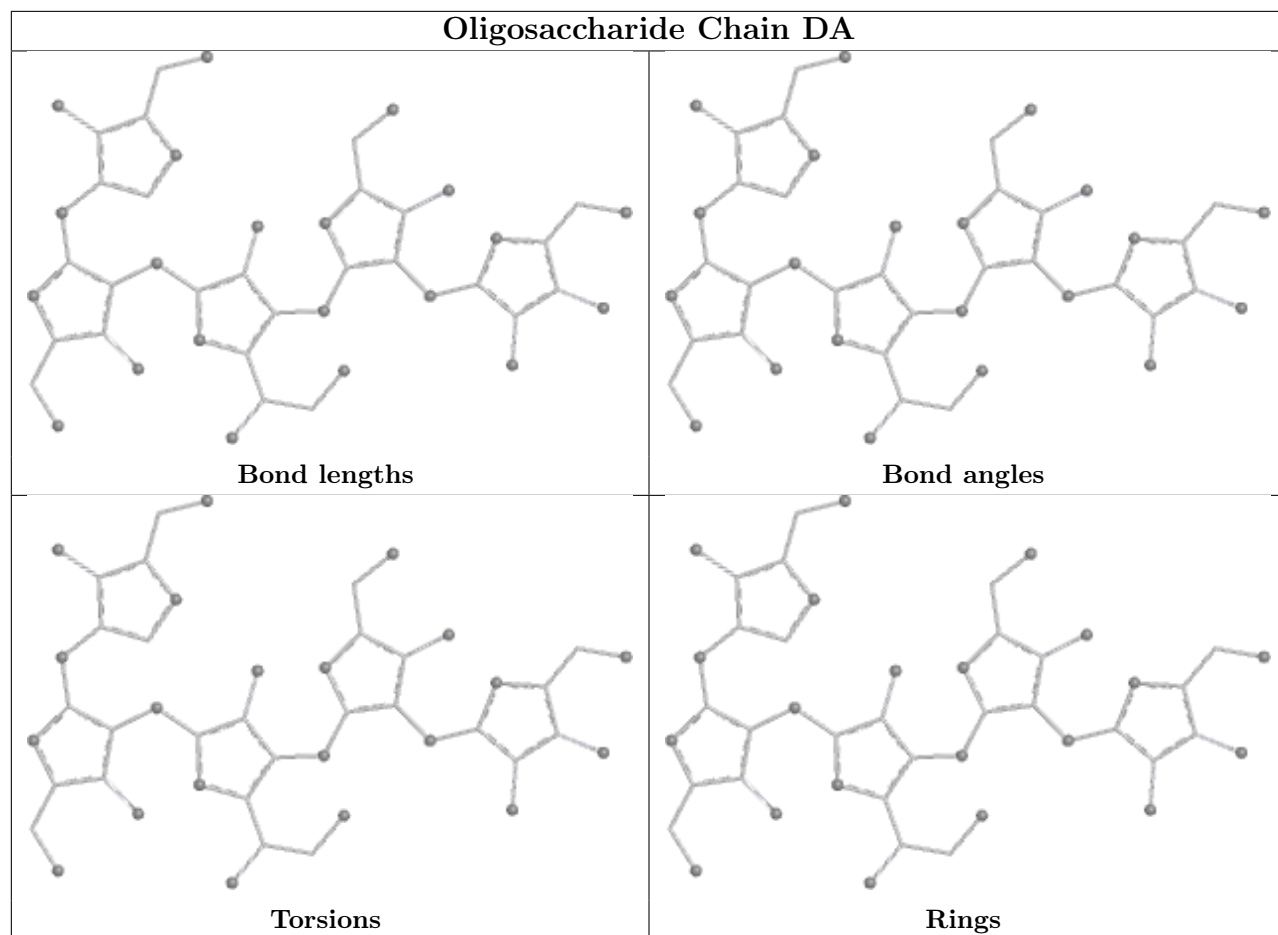


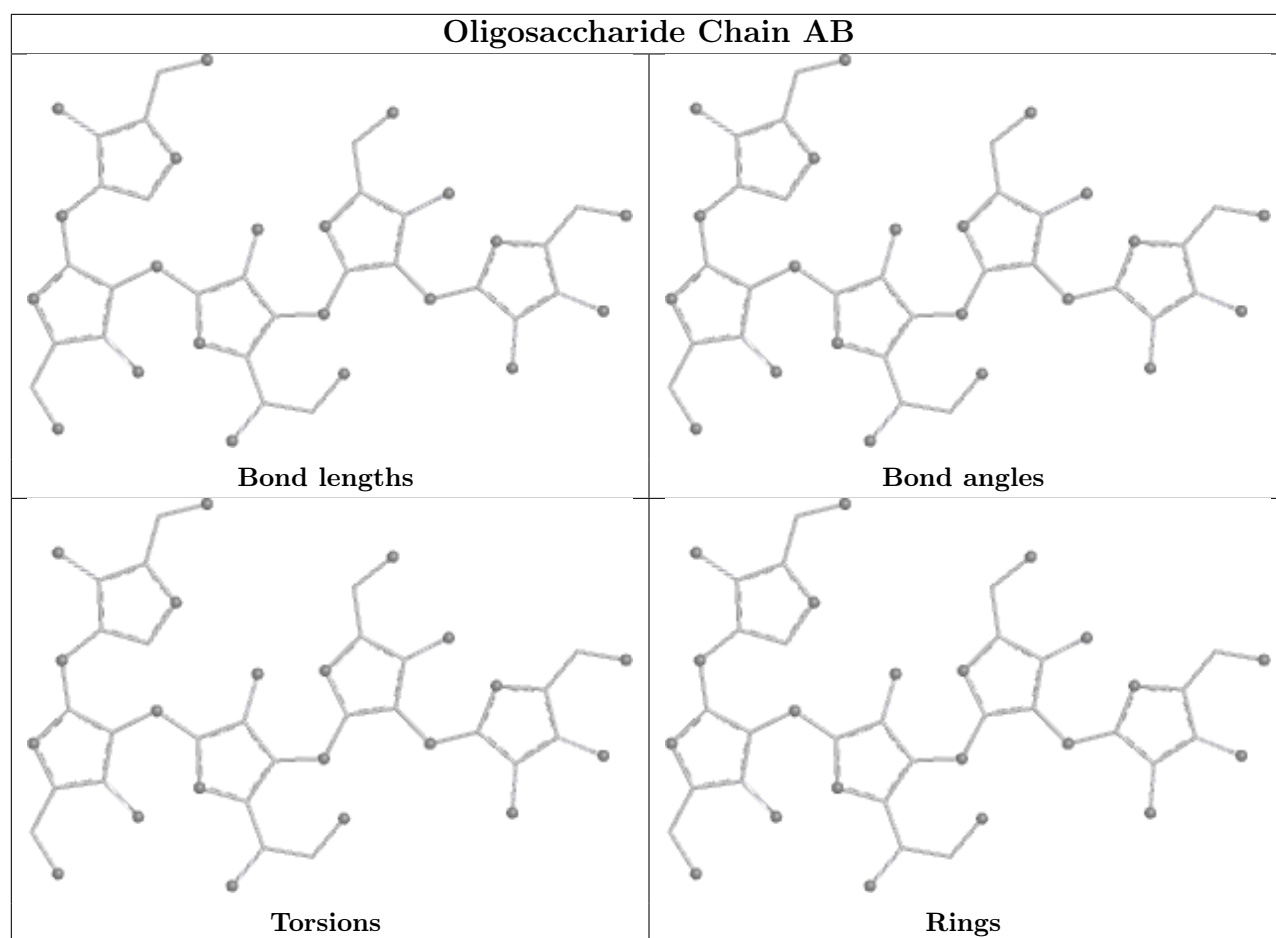


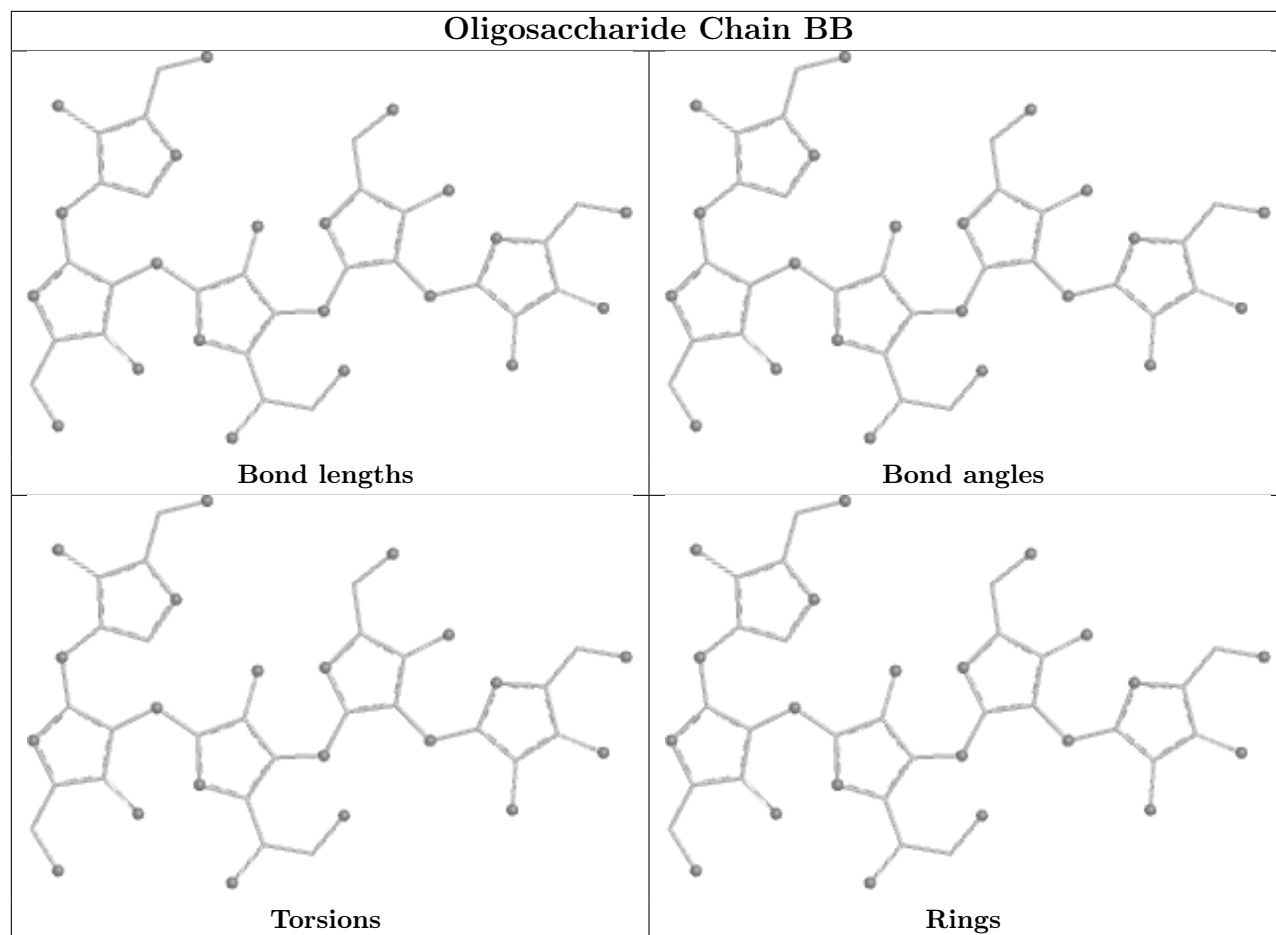


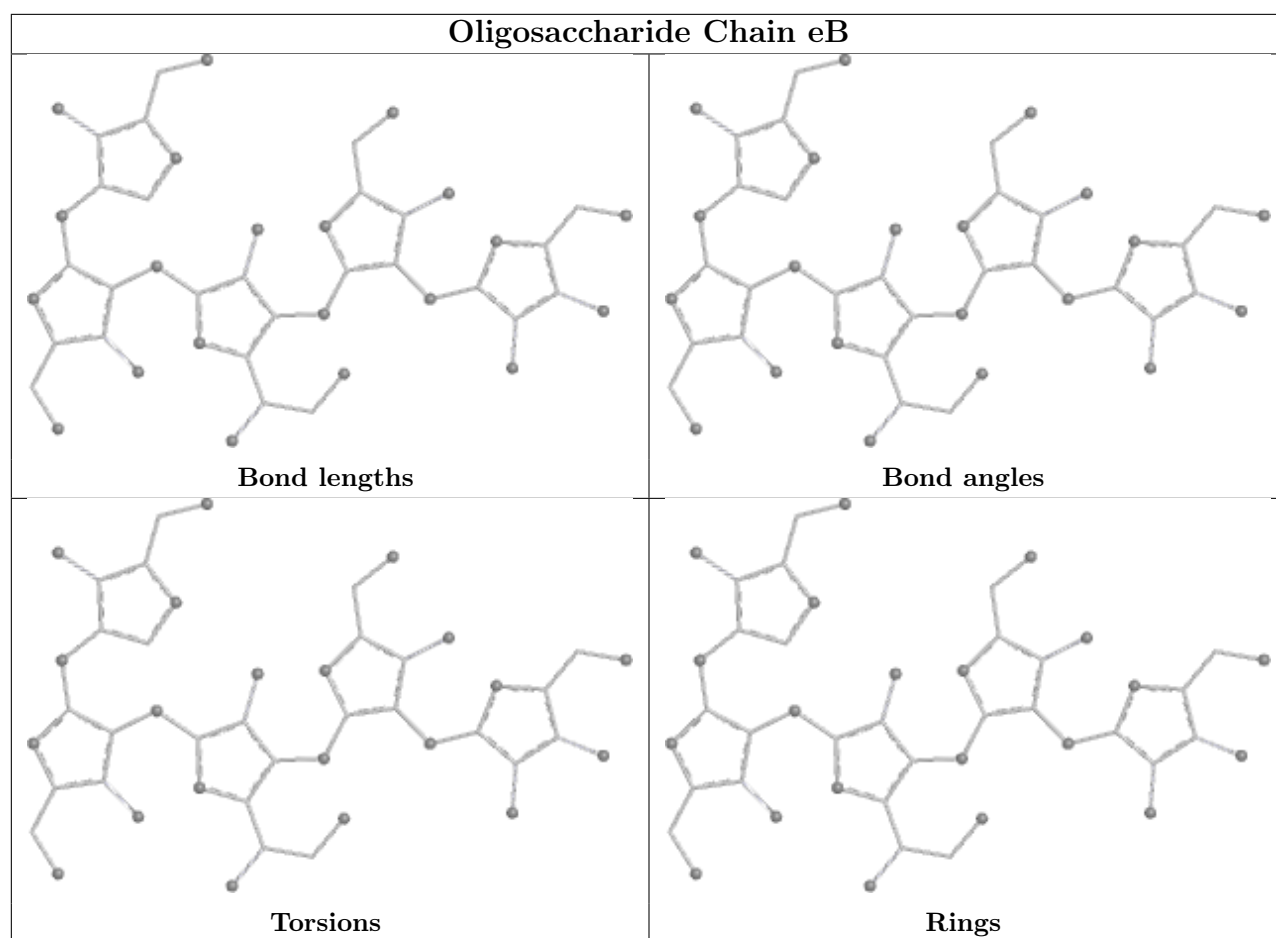


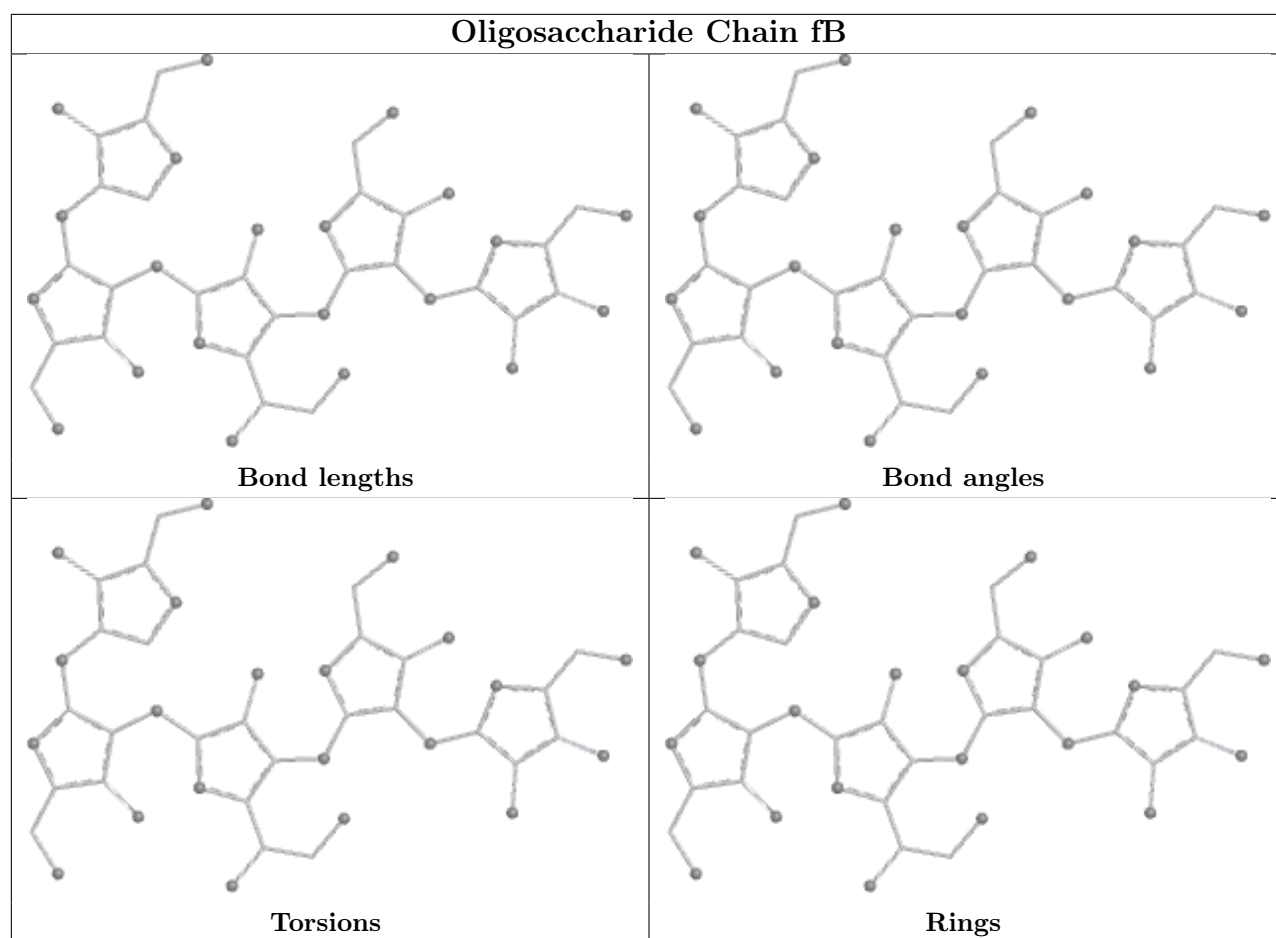


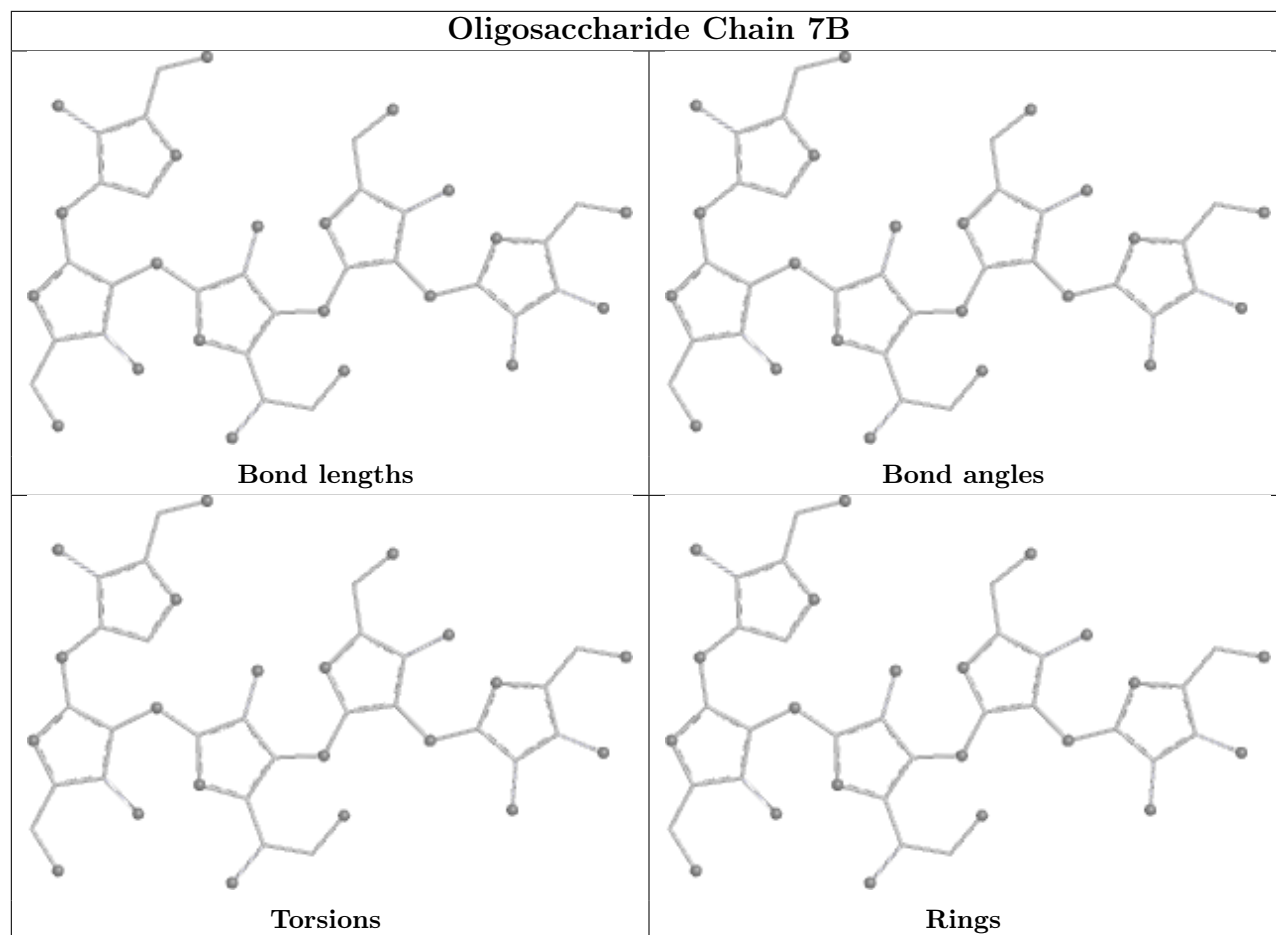


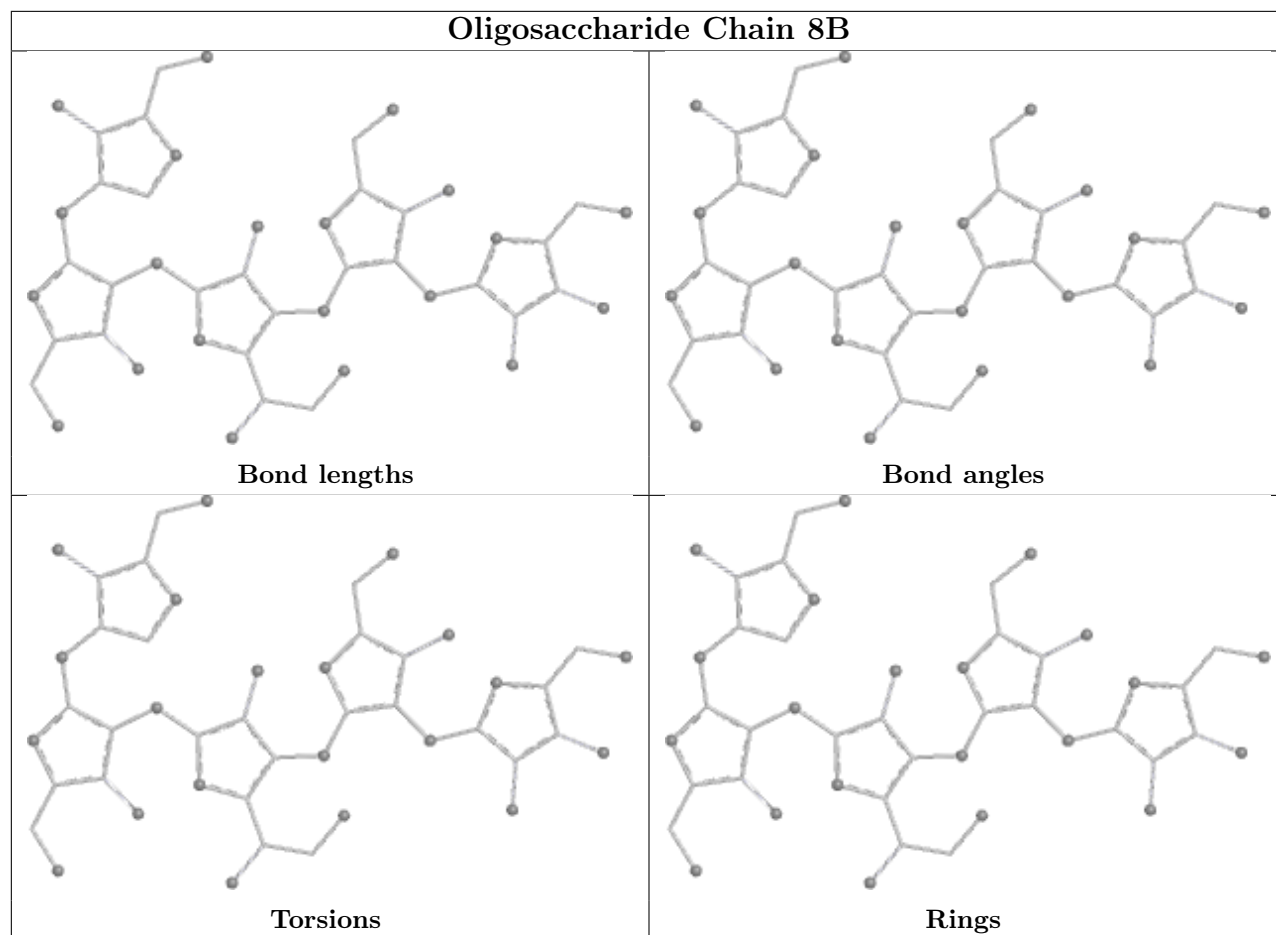


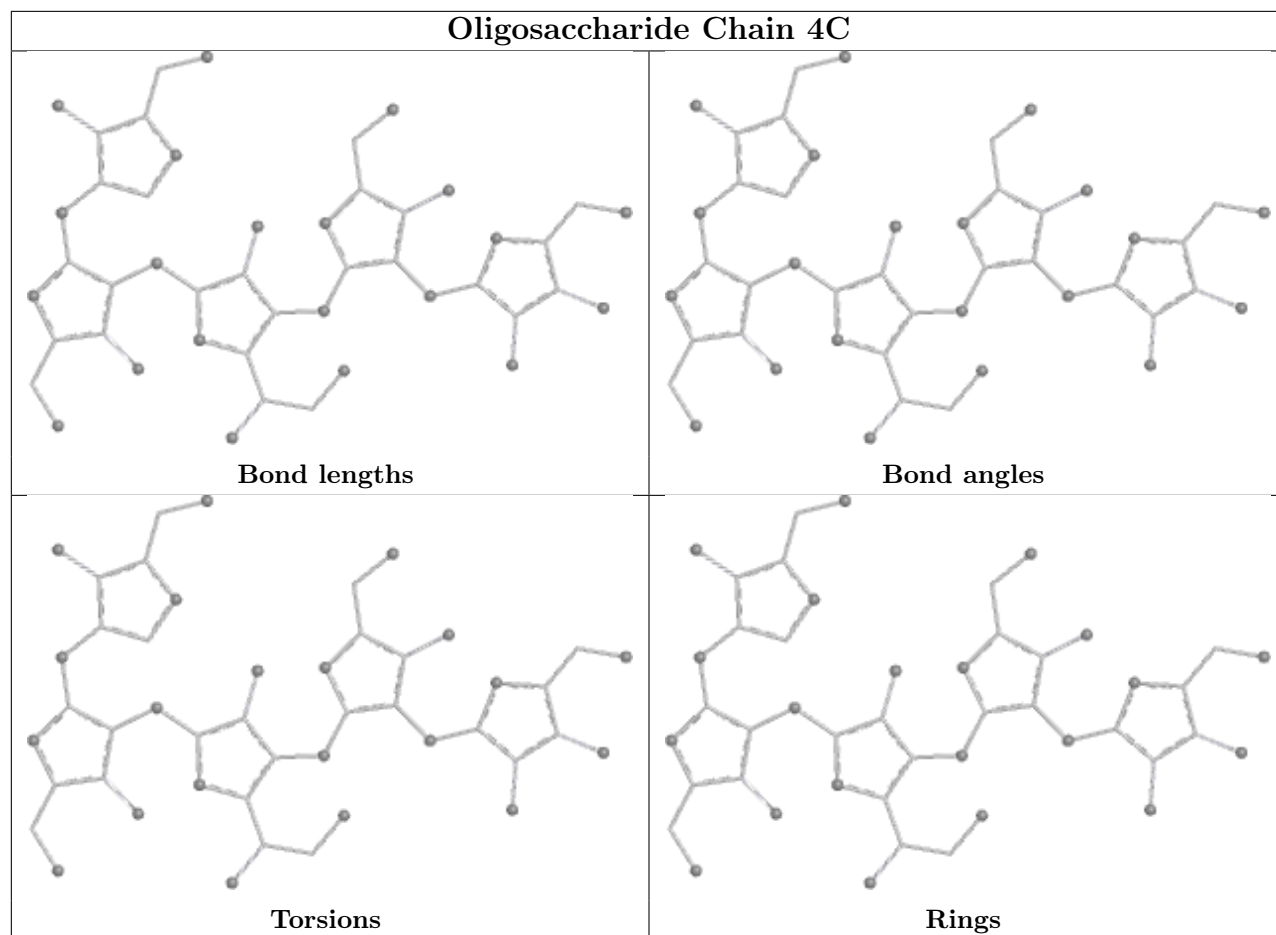


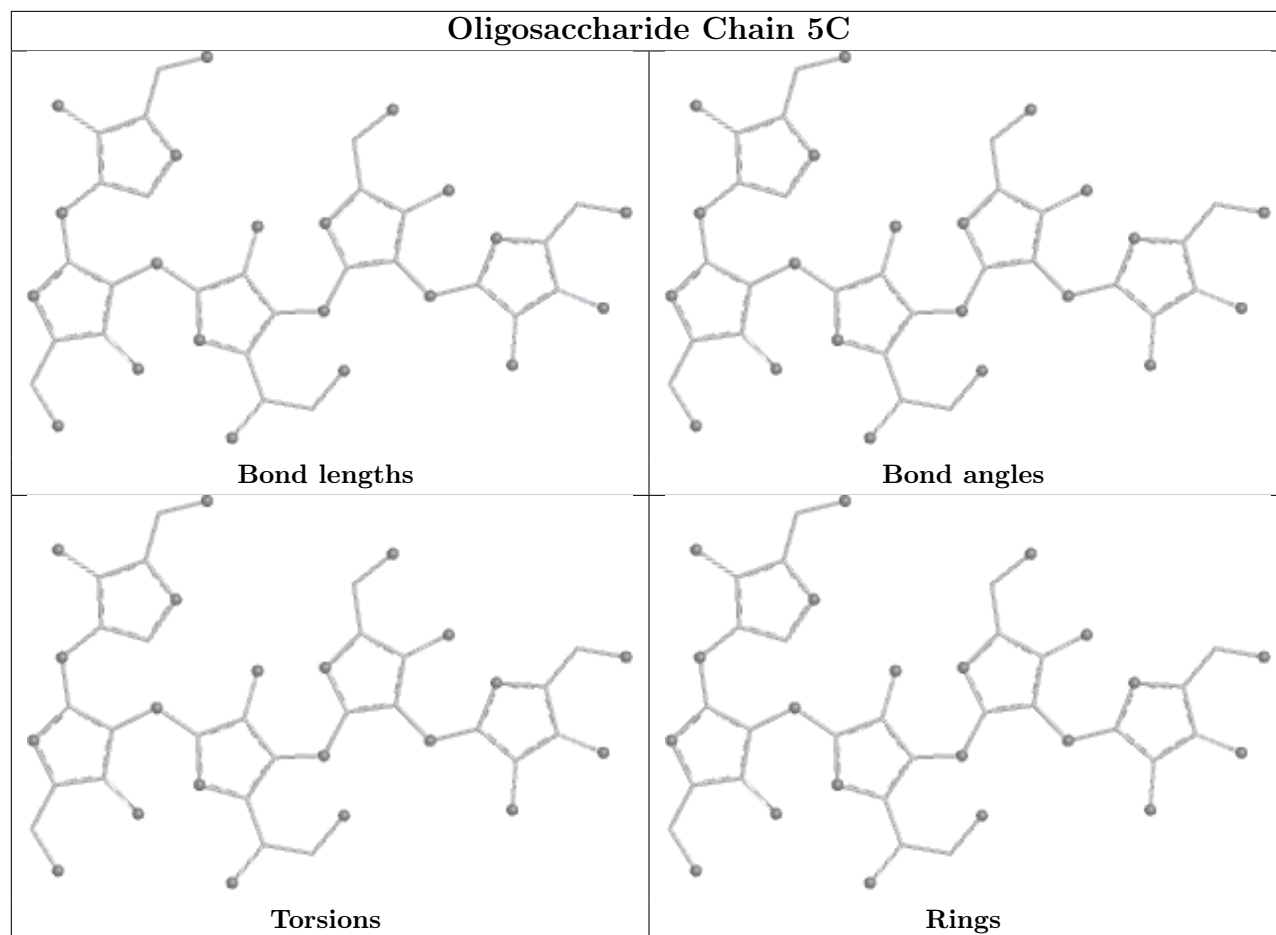


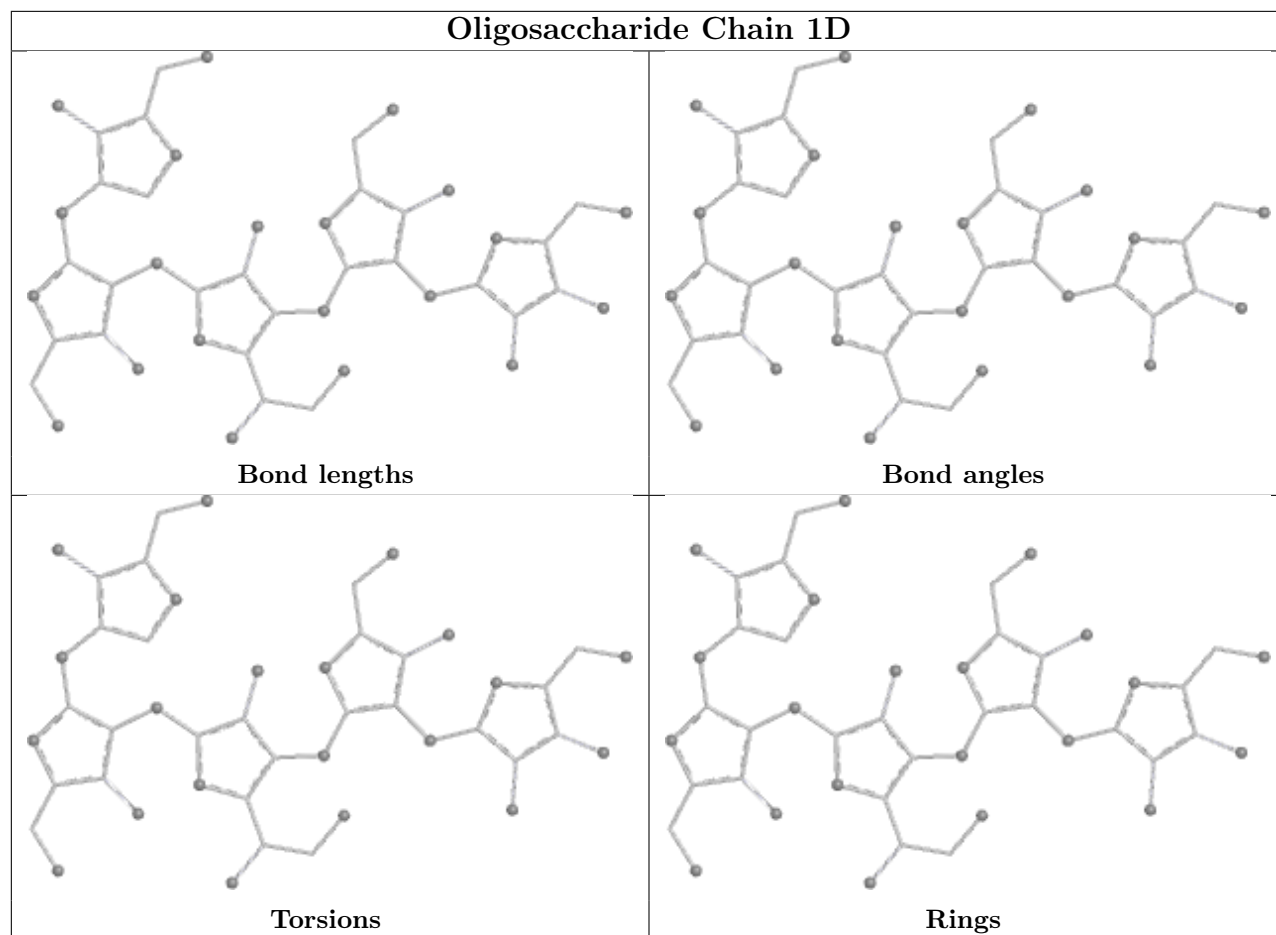


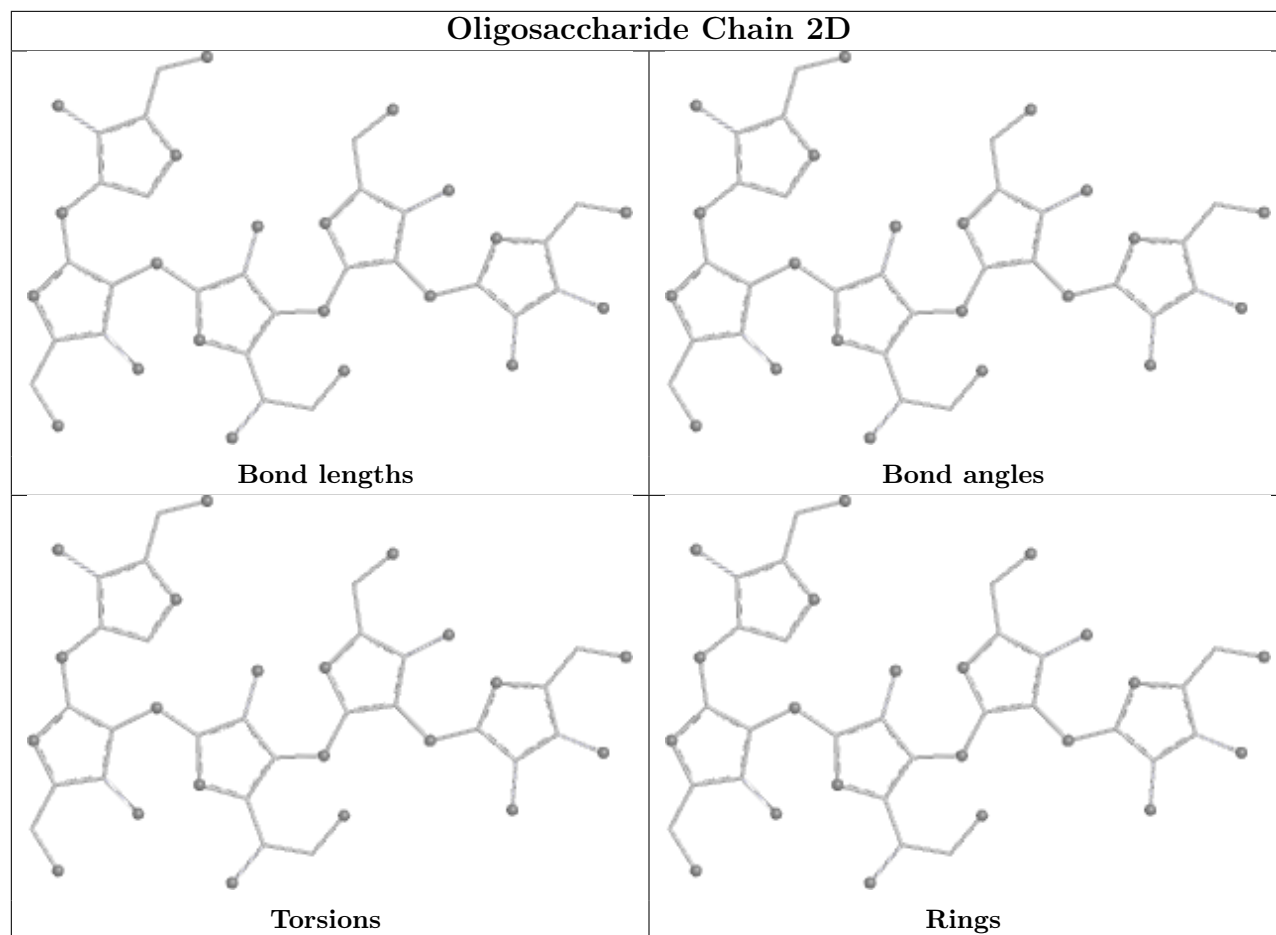


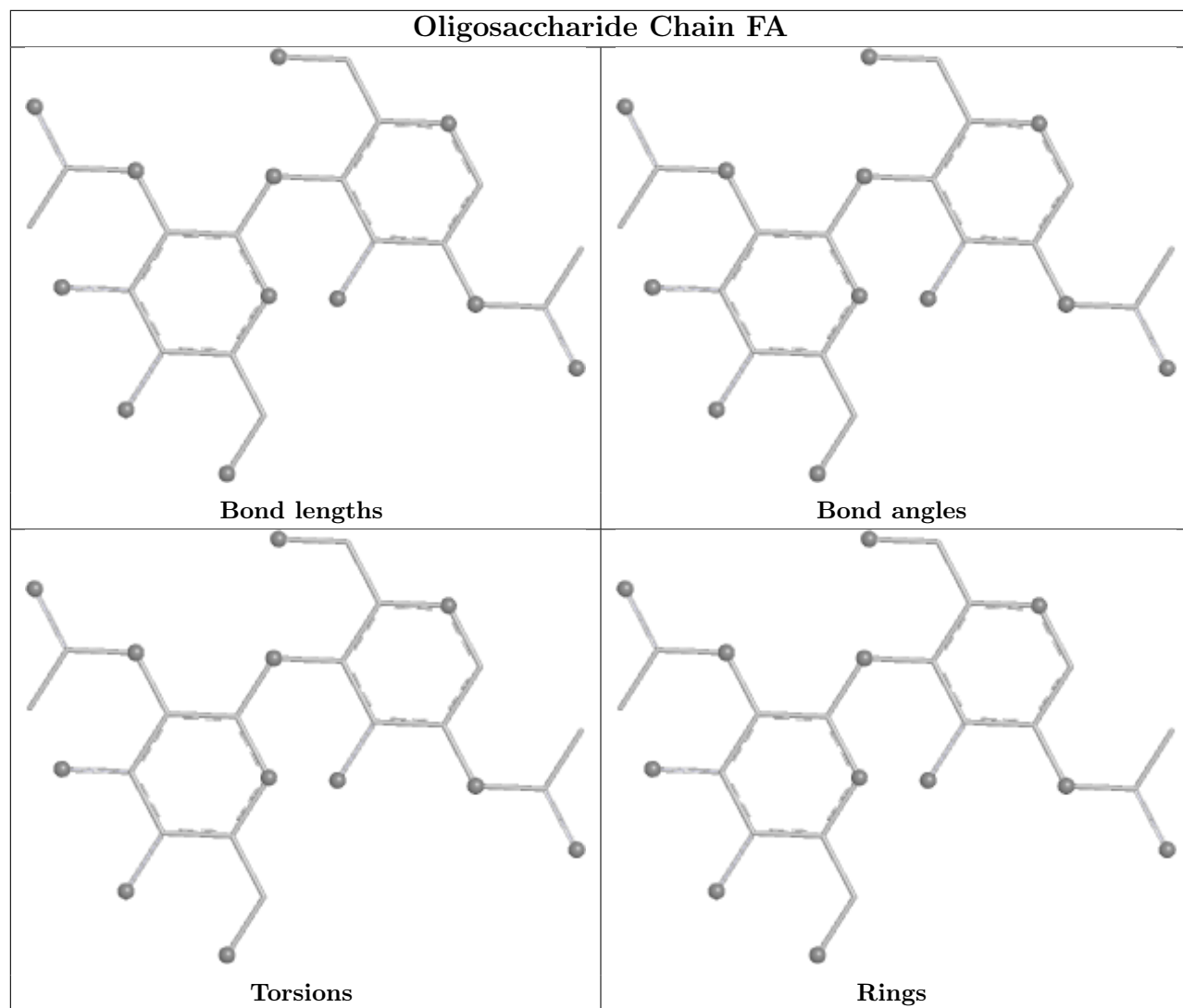


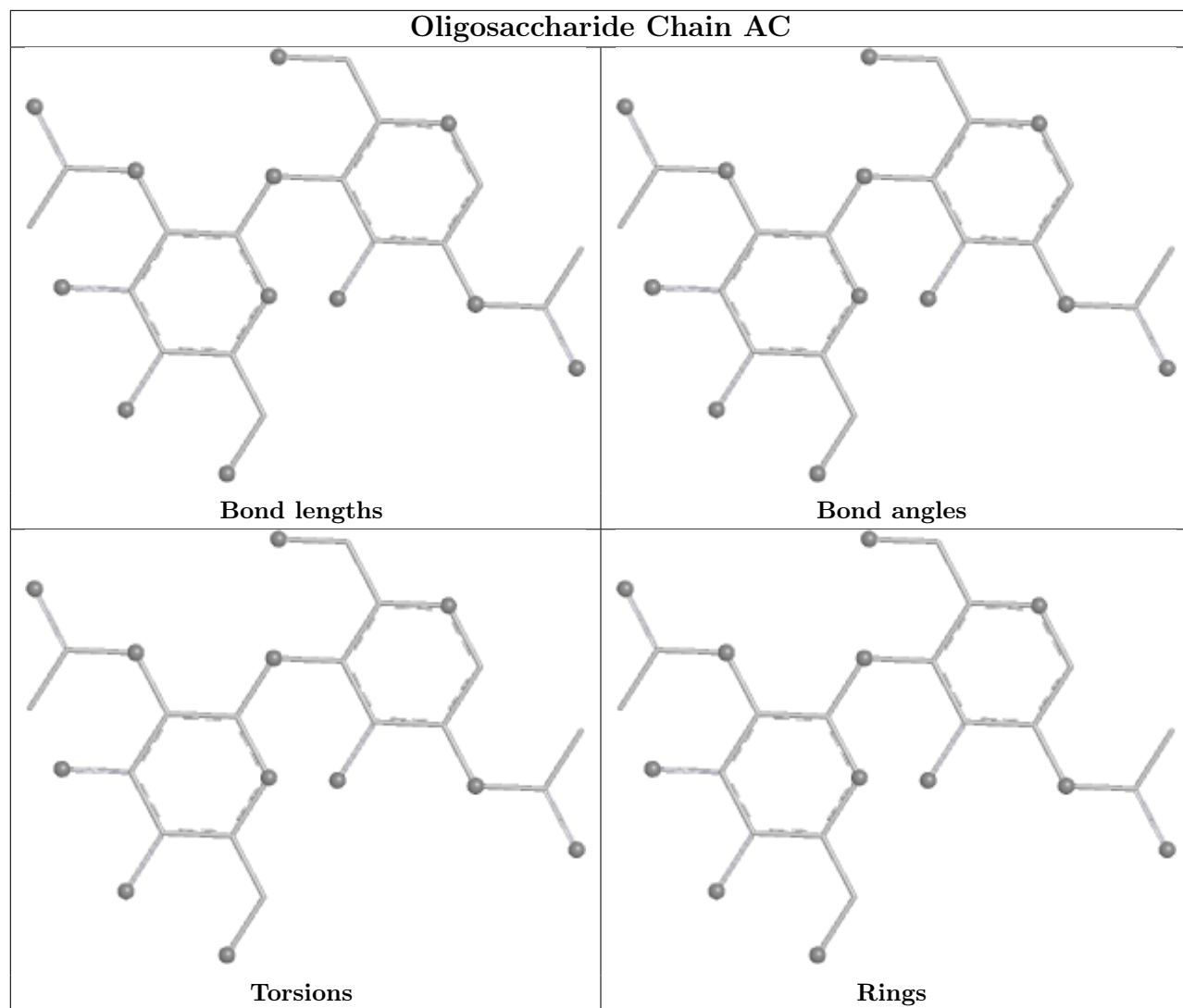


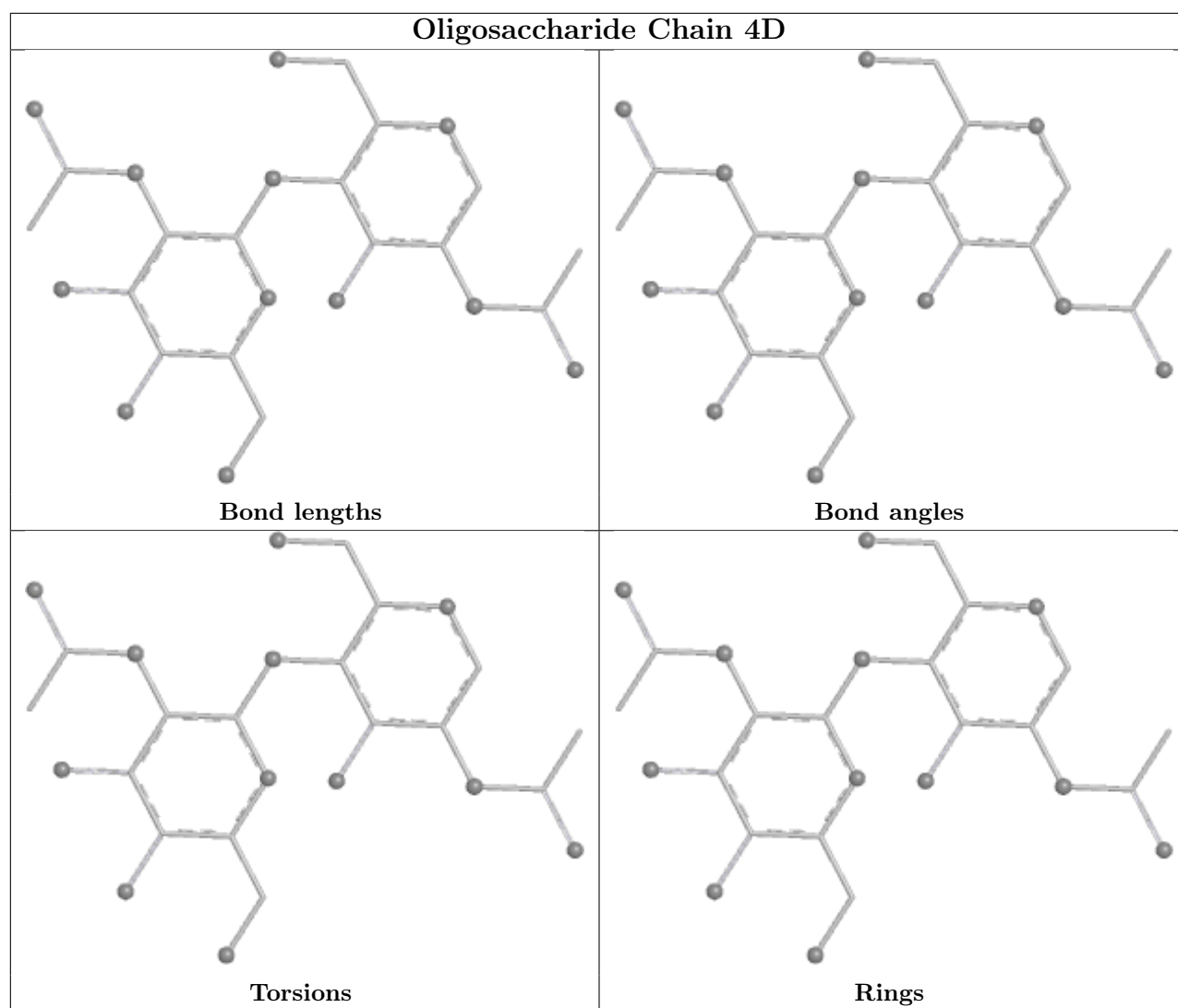


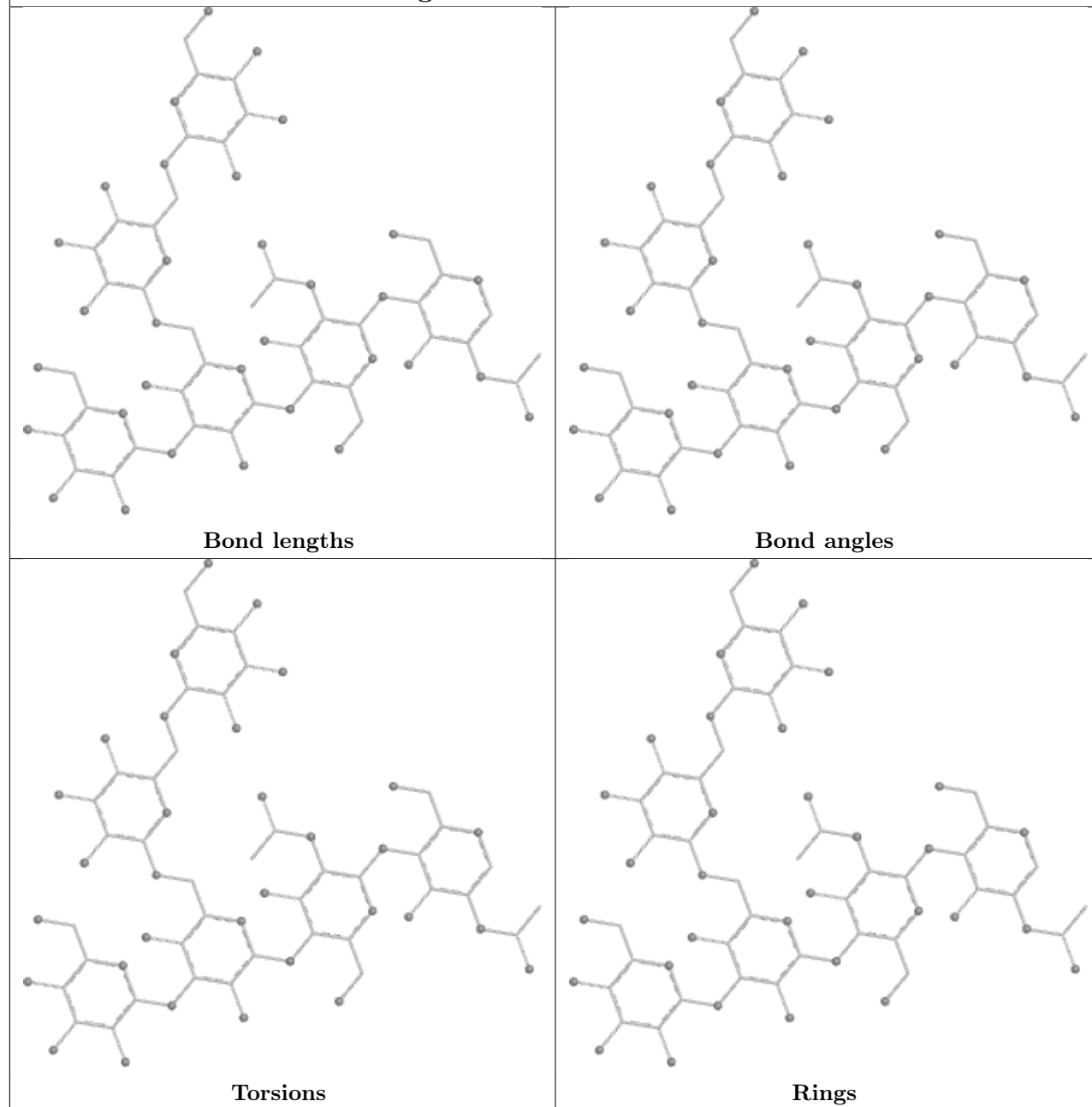


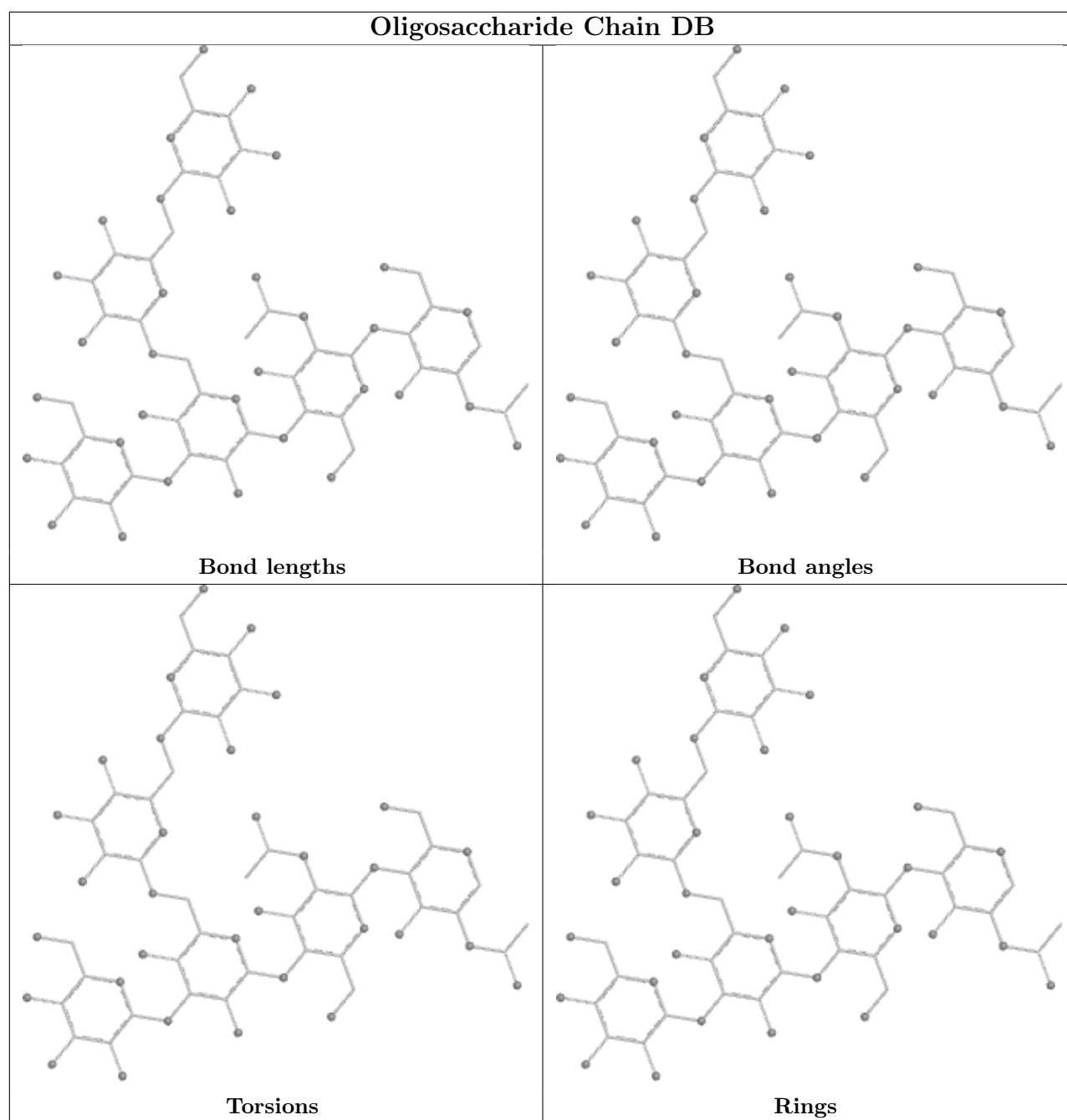


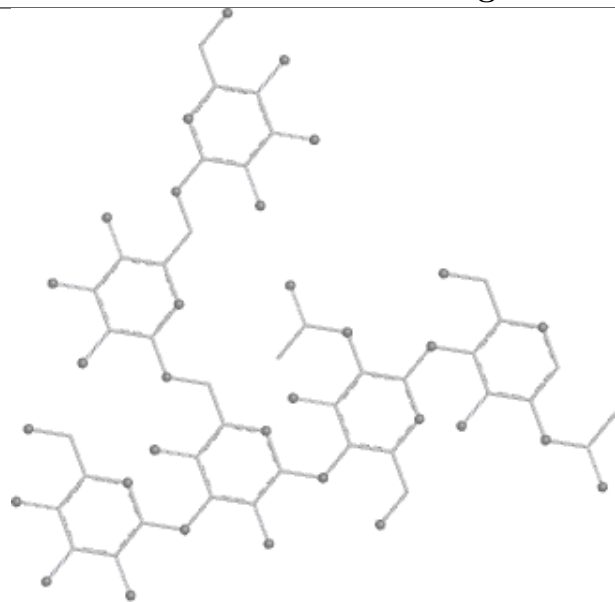
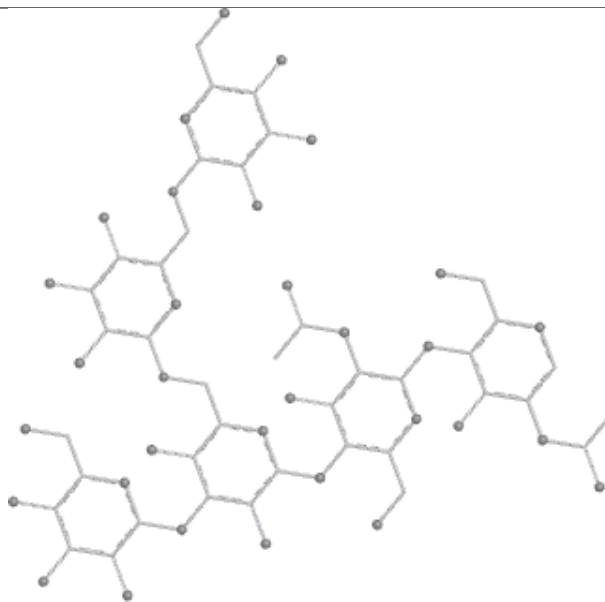
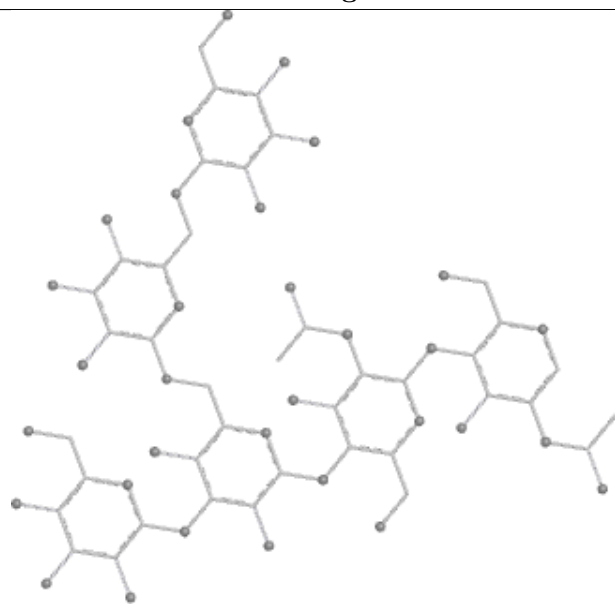
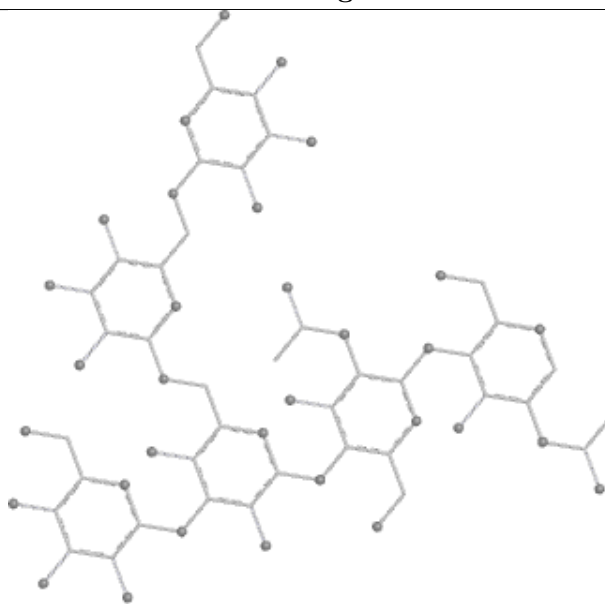


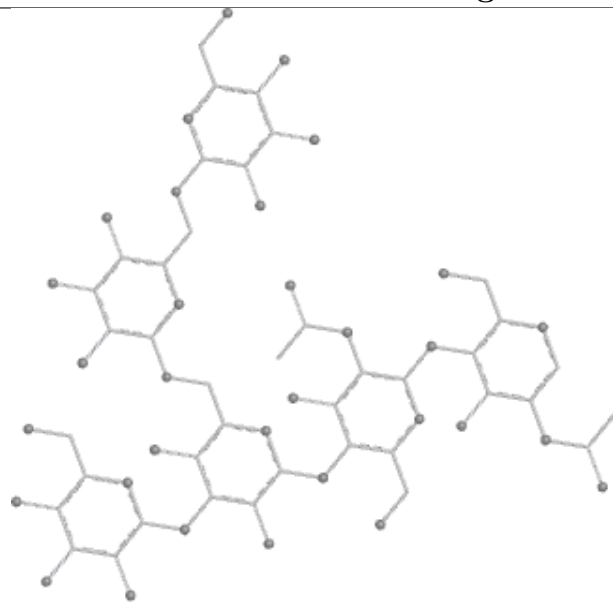
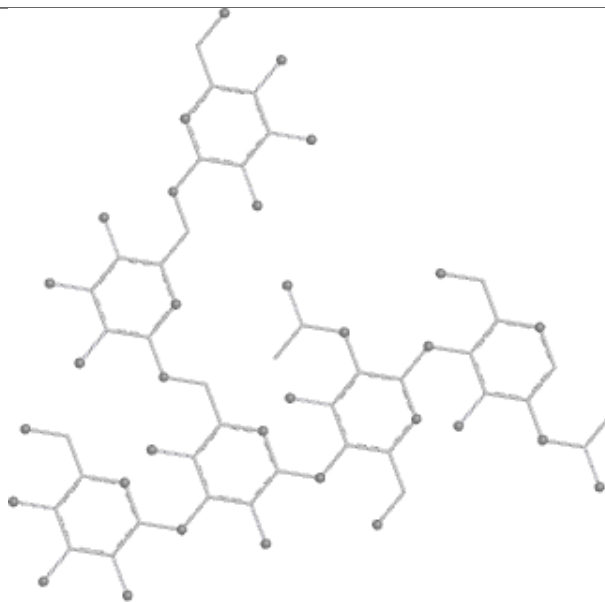
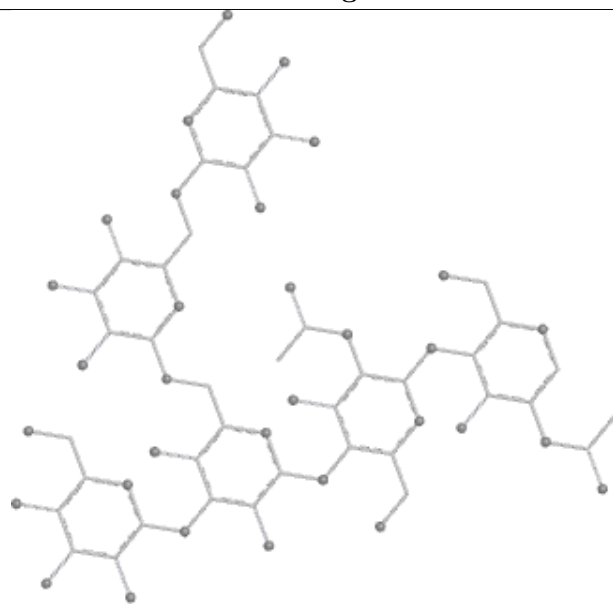
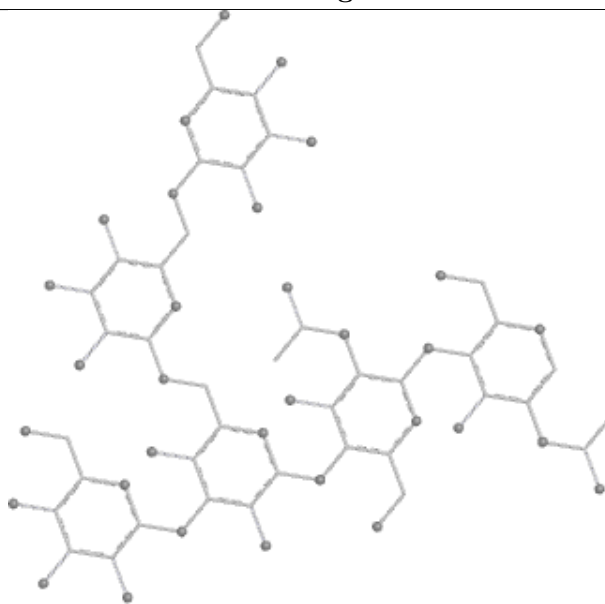


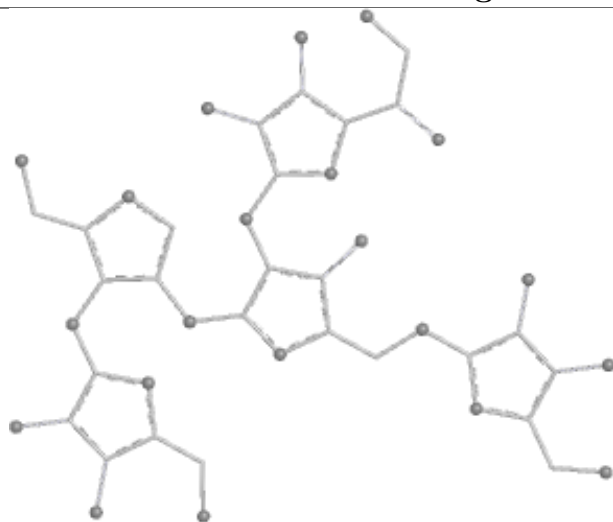
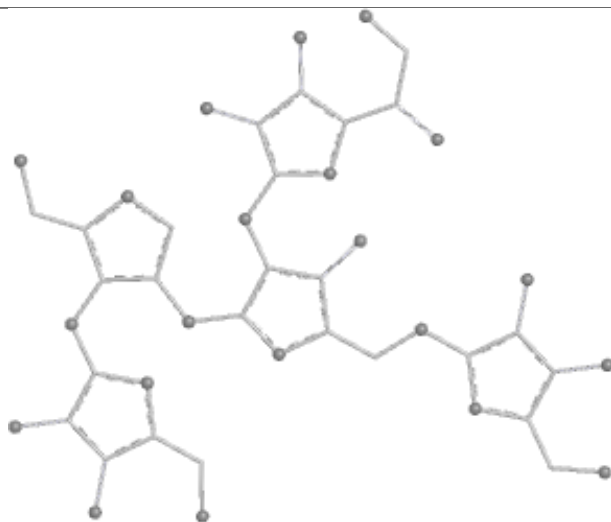
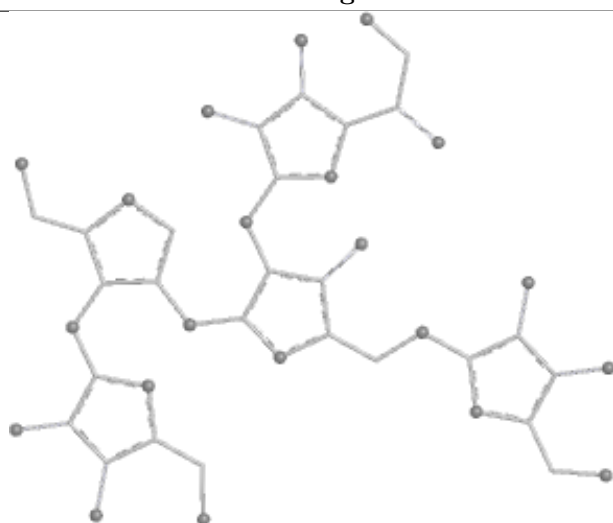
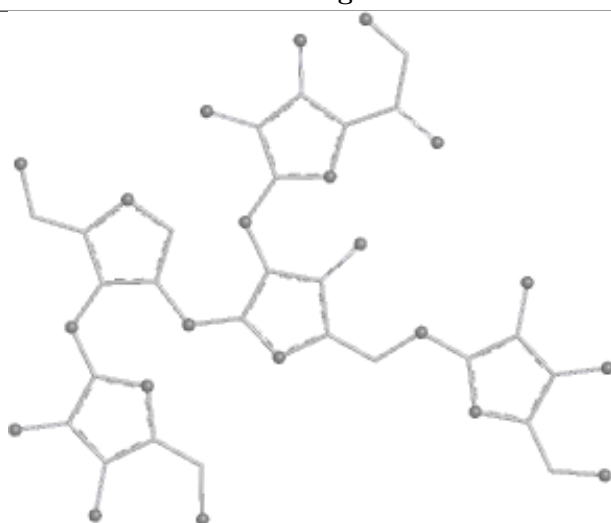


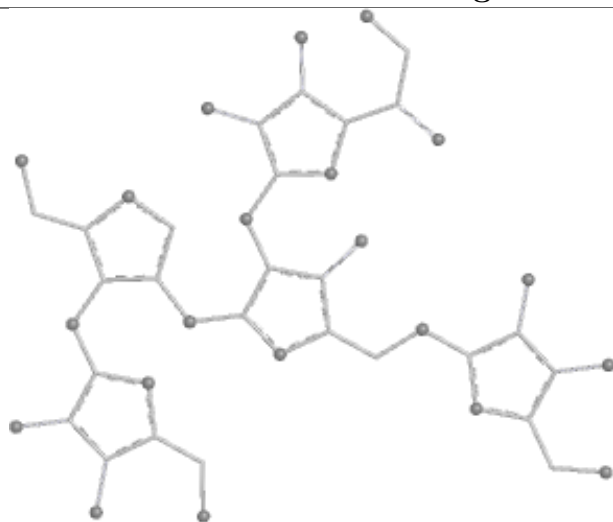
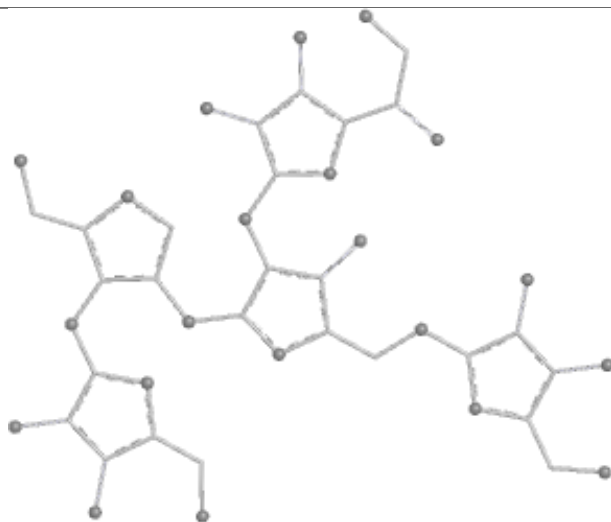
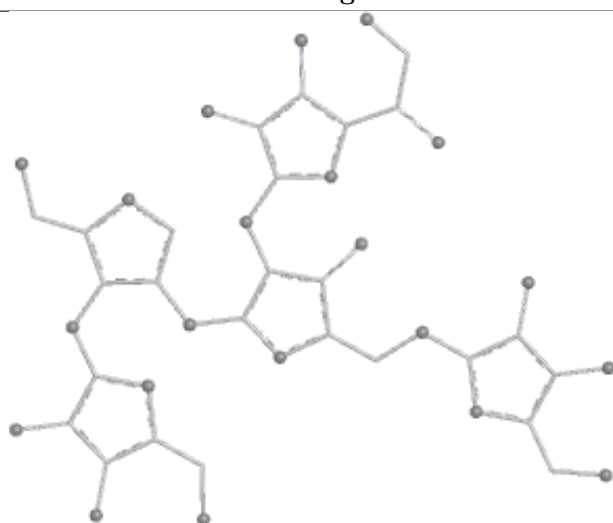
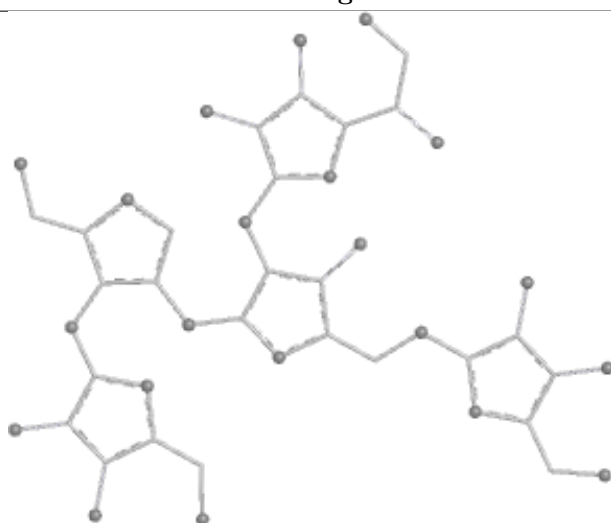
Oligosaccharide Chain GA

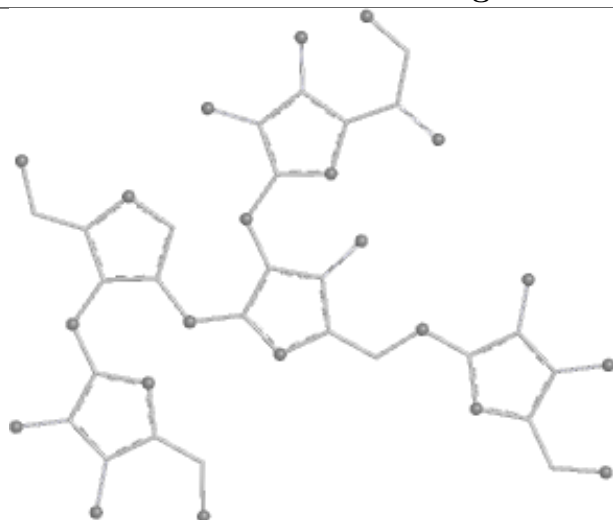
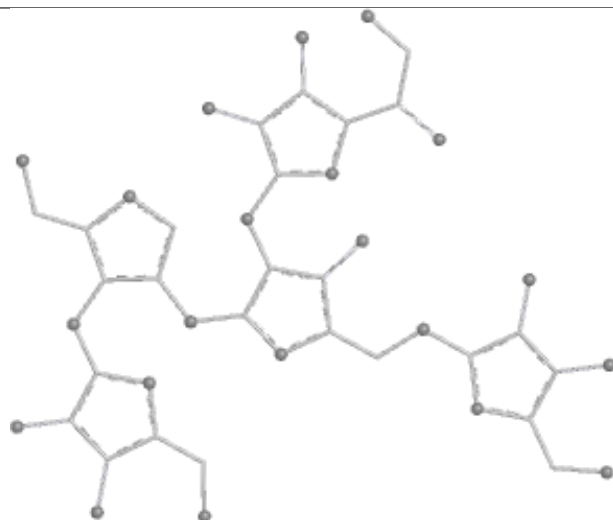
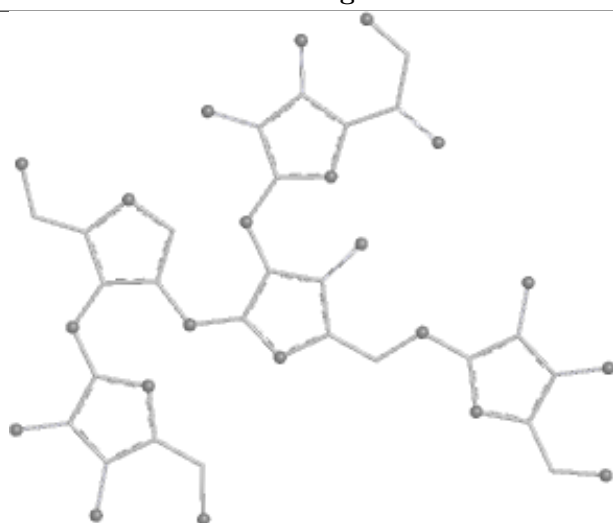
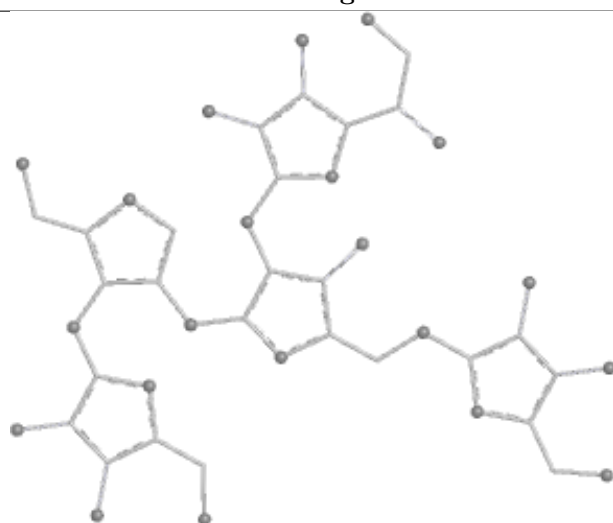


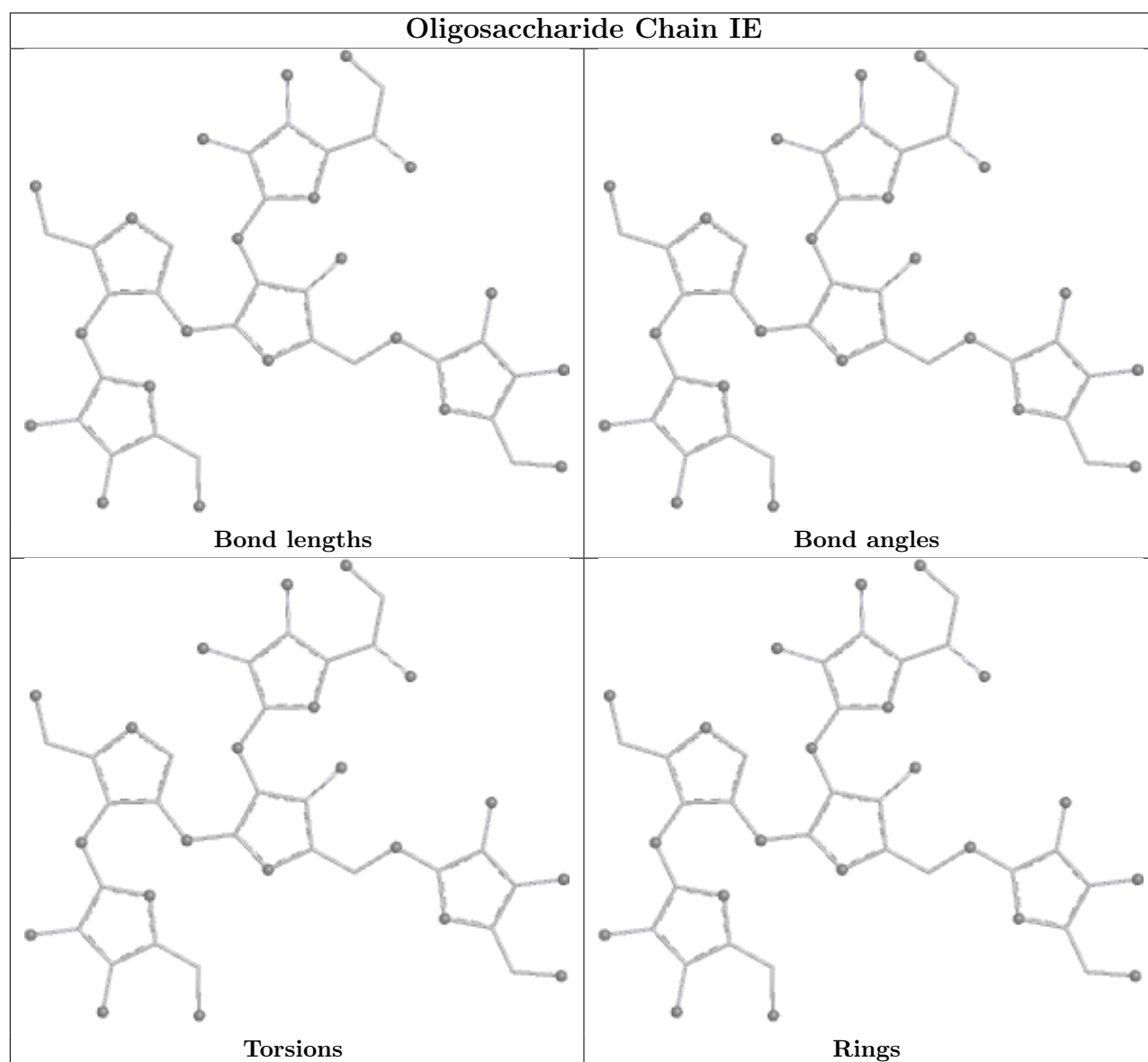
Oligosaccharide Chain 7C**Bond lengths****Bond angles****Torsions****Rings**

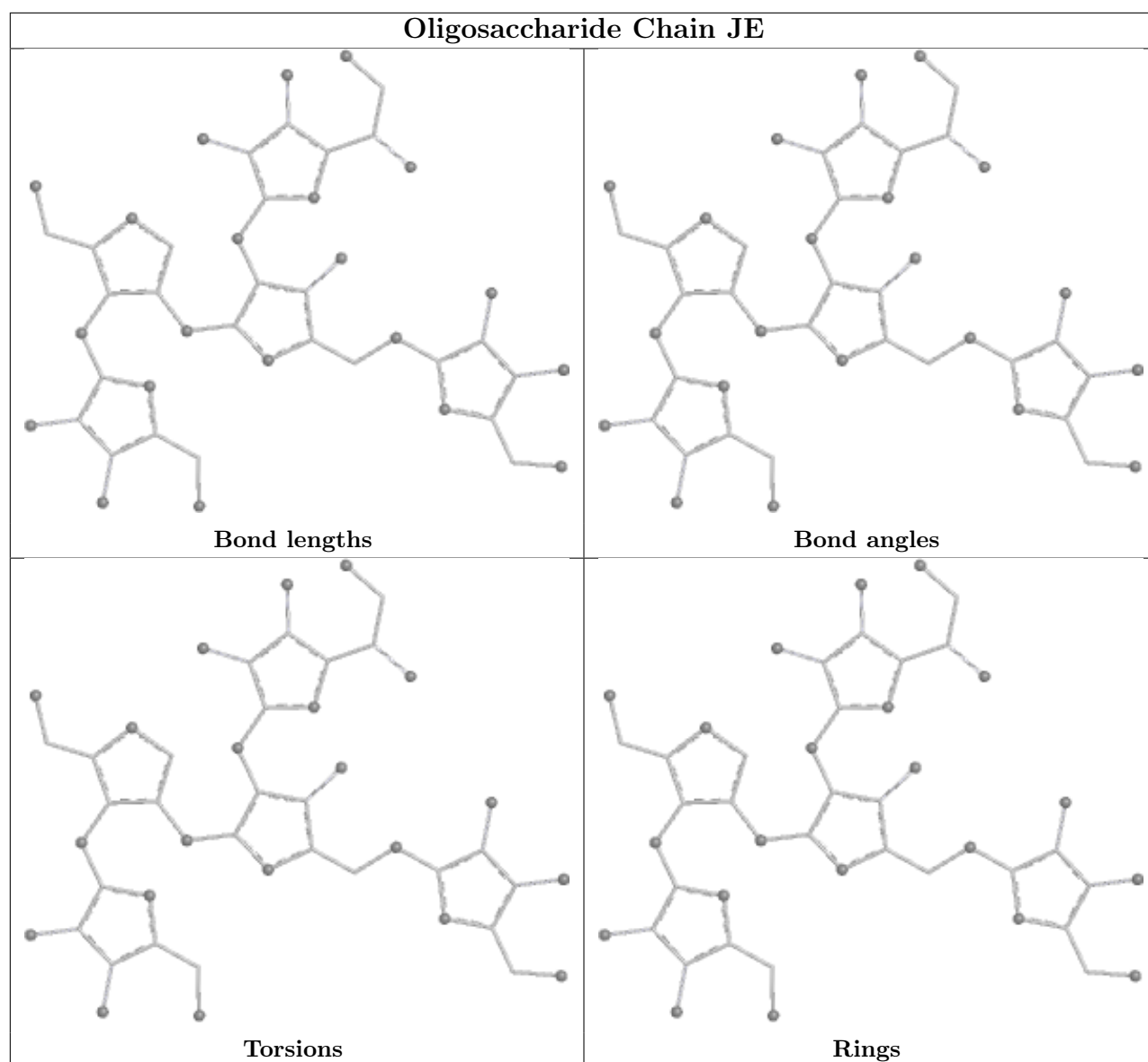
Oligosaccharide Chain 5D**Bond lengths****Bond angles****Torsions****Rings**

Oligosaccharide Chain 9D**Bond lengths****Bond angles****Torsions****Rings**

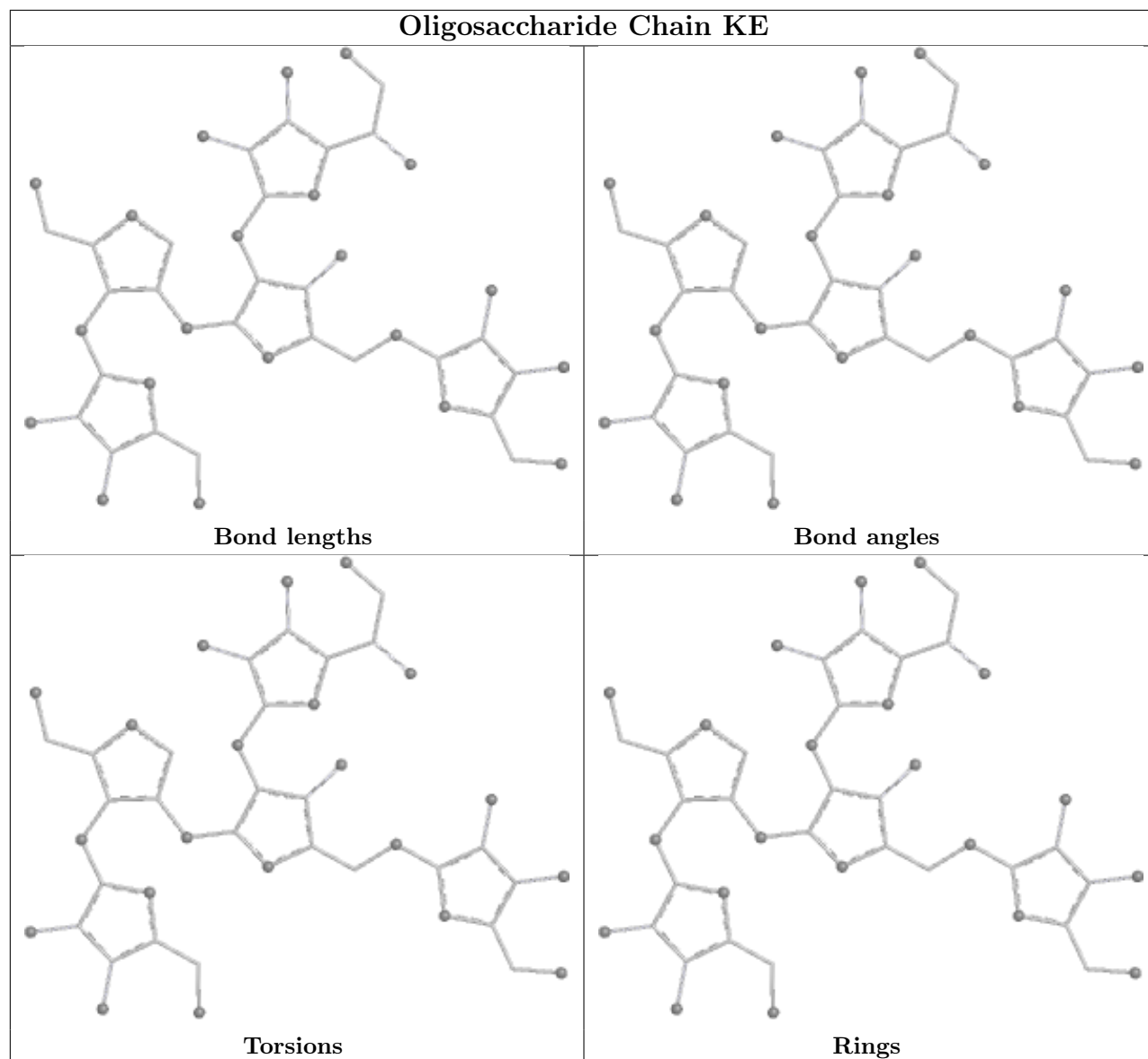
Oligosaccharide Chain BE**Bond lengths****Bond angles****Torsions****Rings**

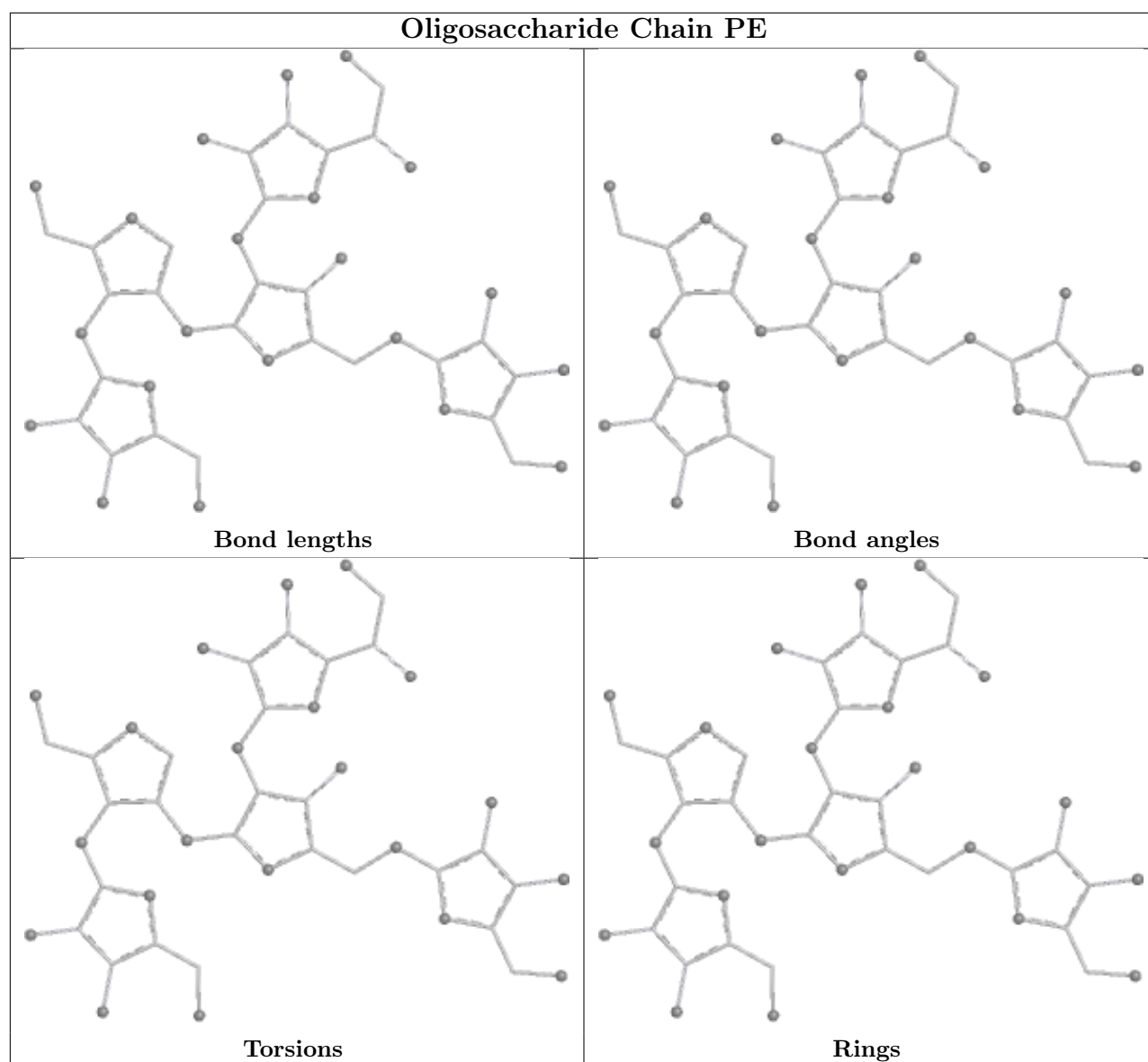
Oligosaccharide Chain DE**Bond lengths****Bond angles****Torsions****Rings**

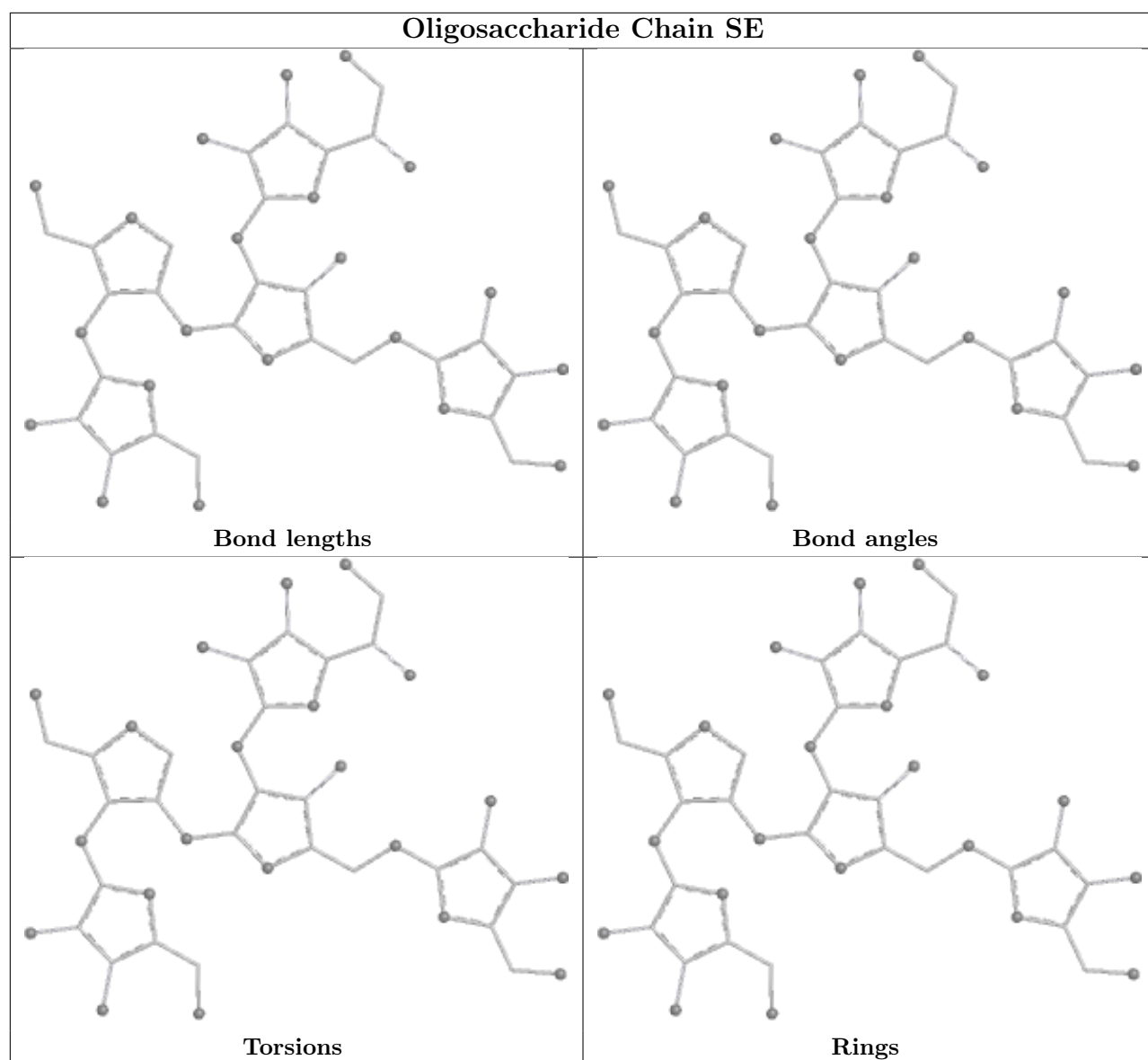


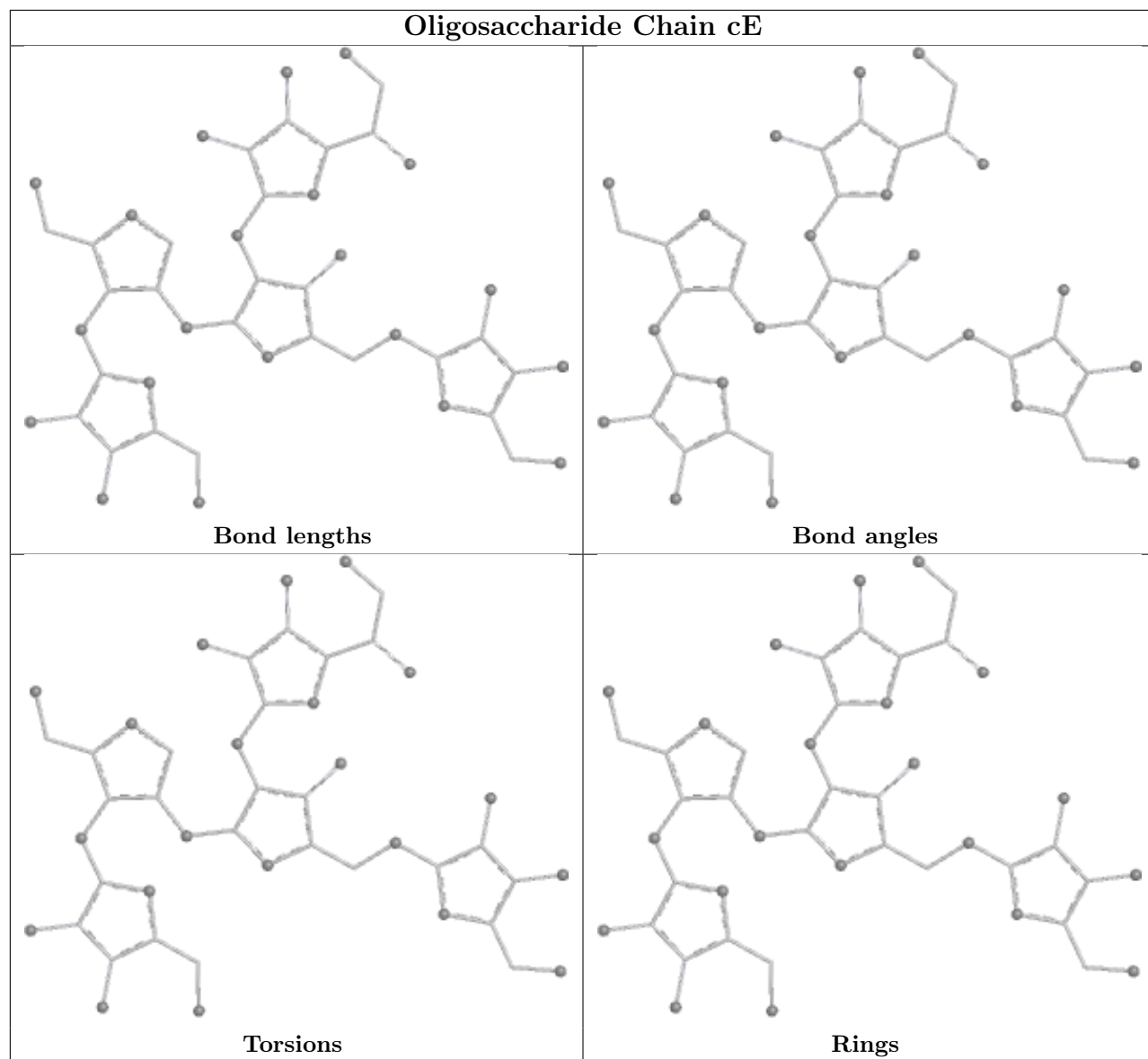


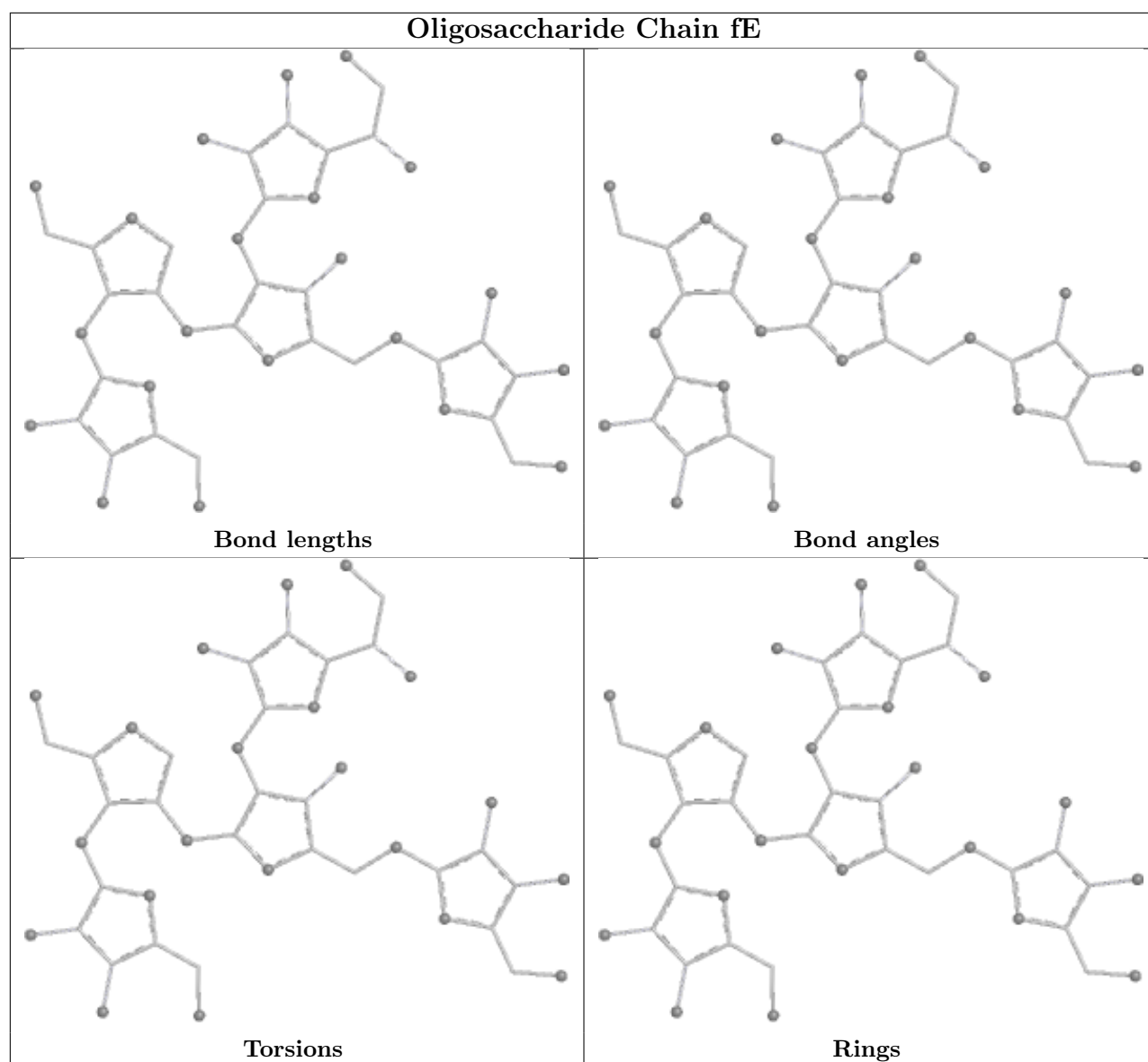
Oligosaccharide Chain KE

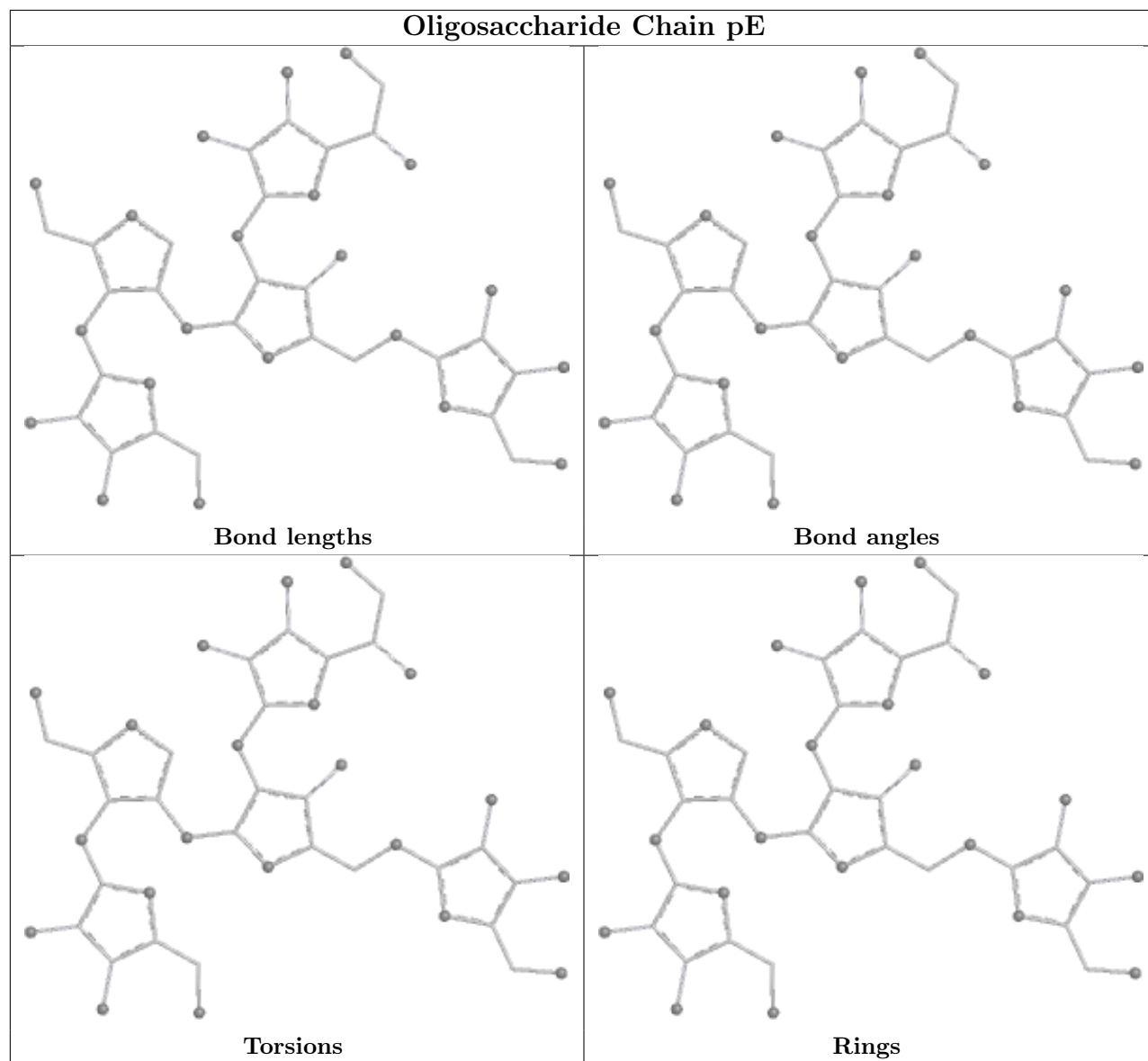


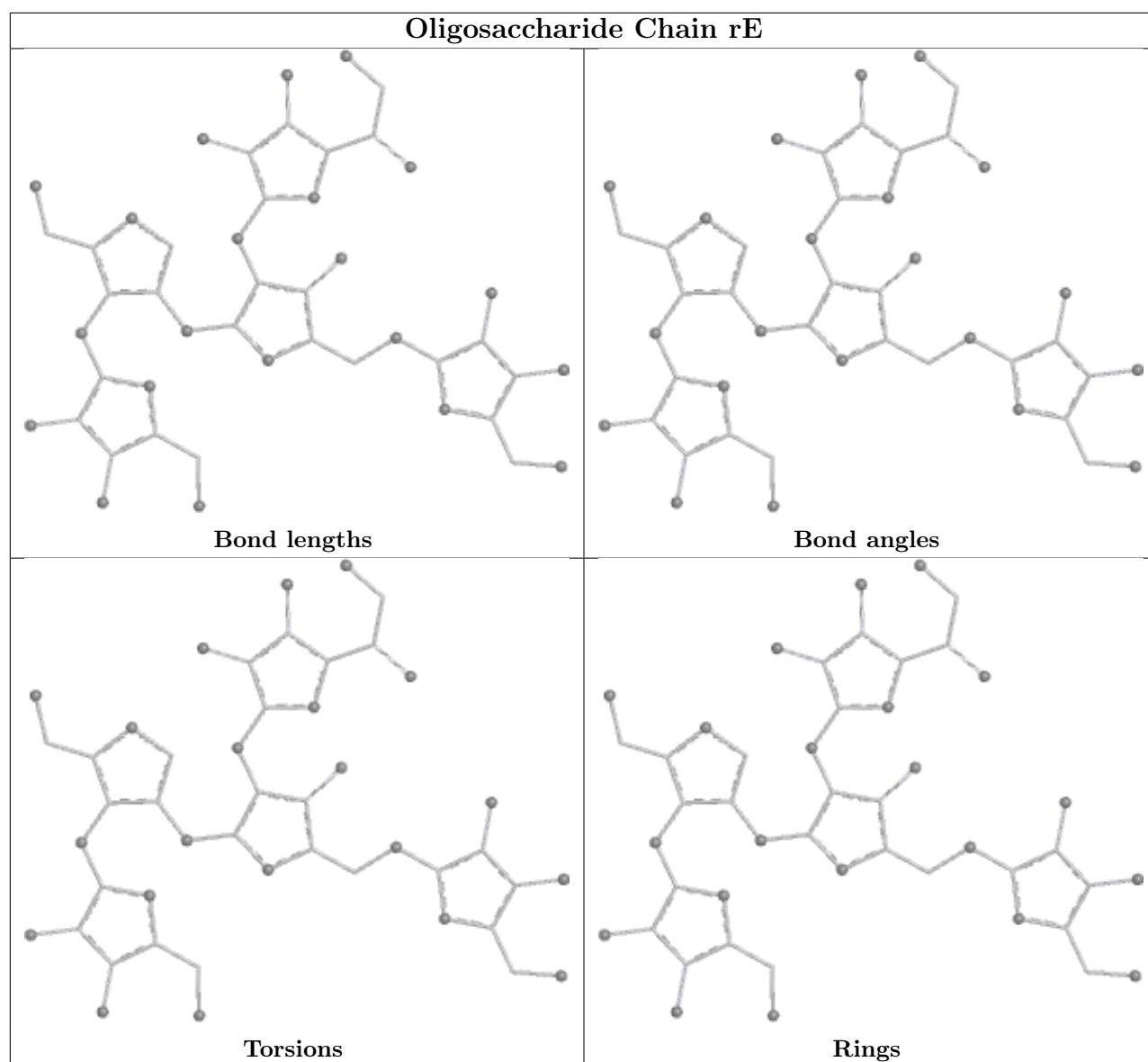


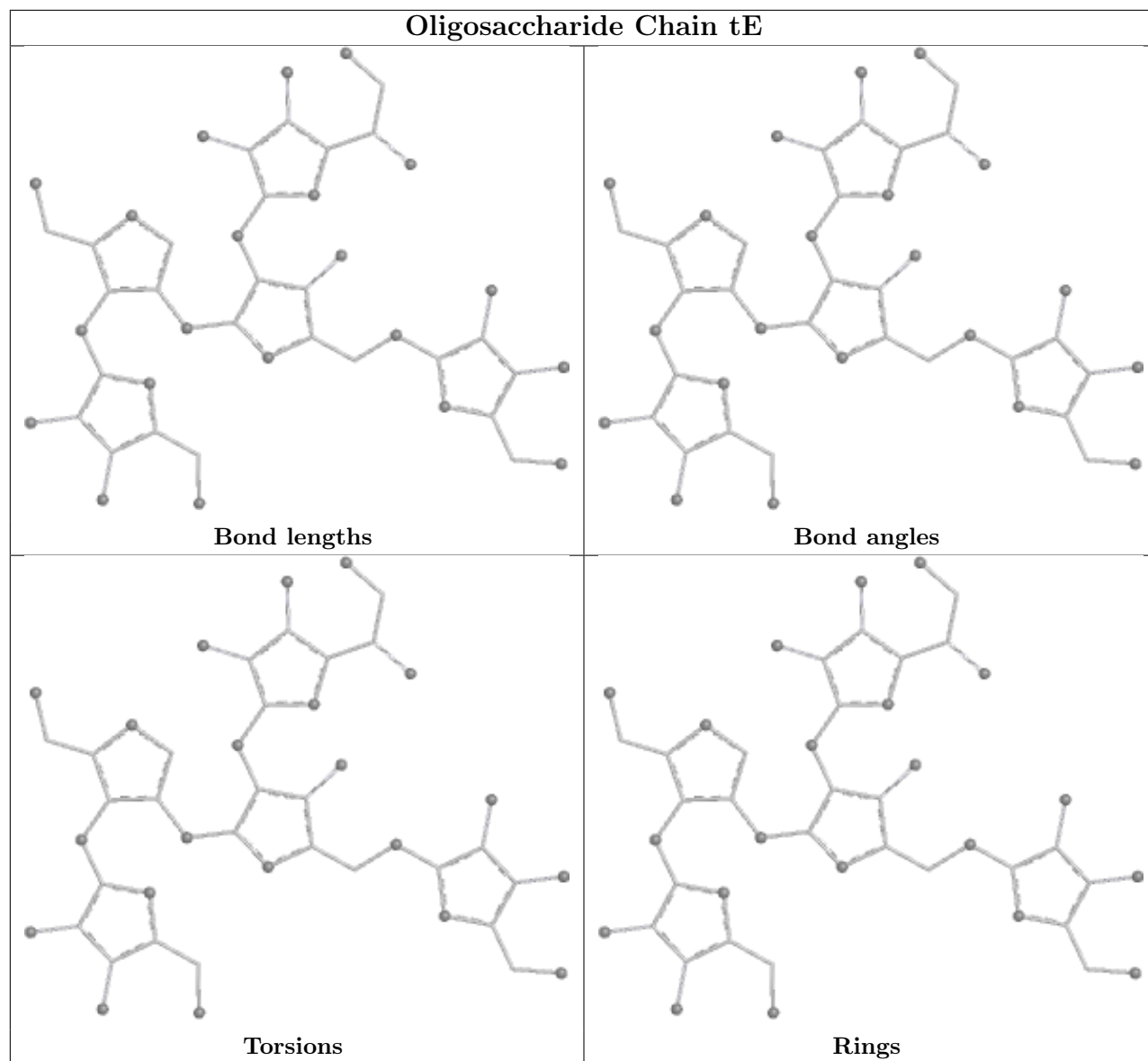


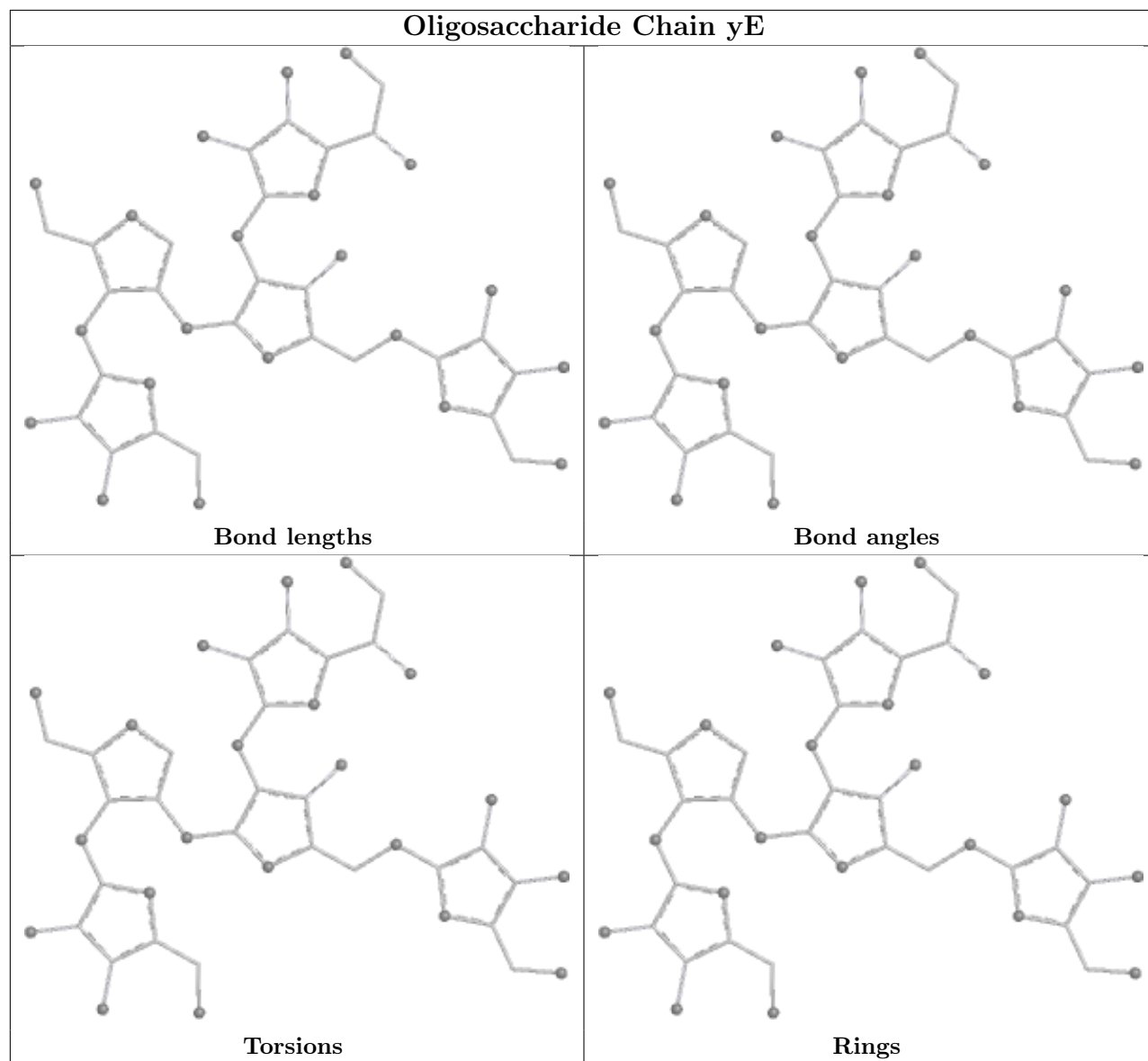


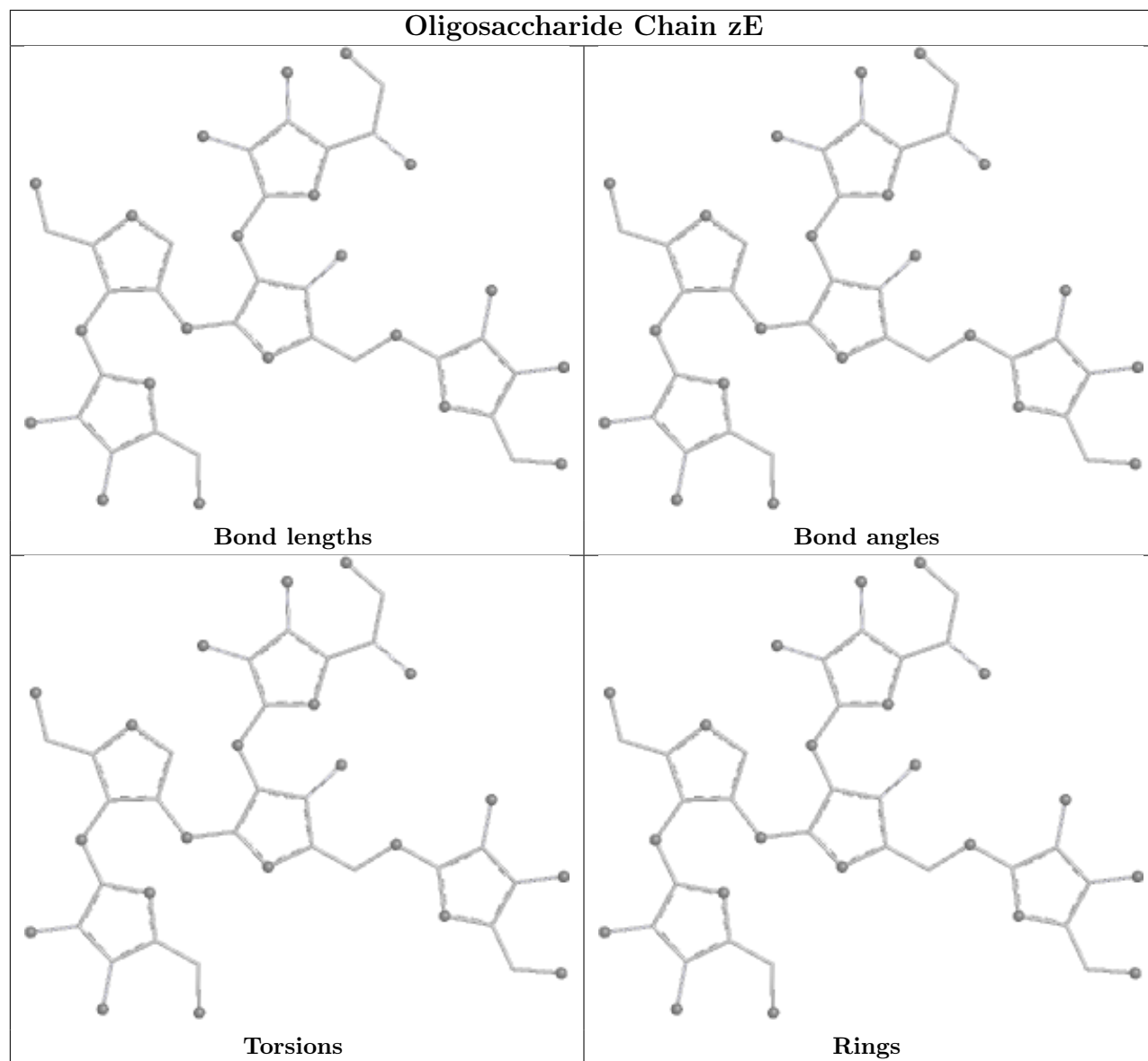


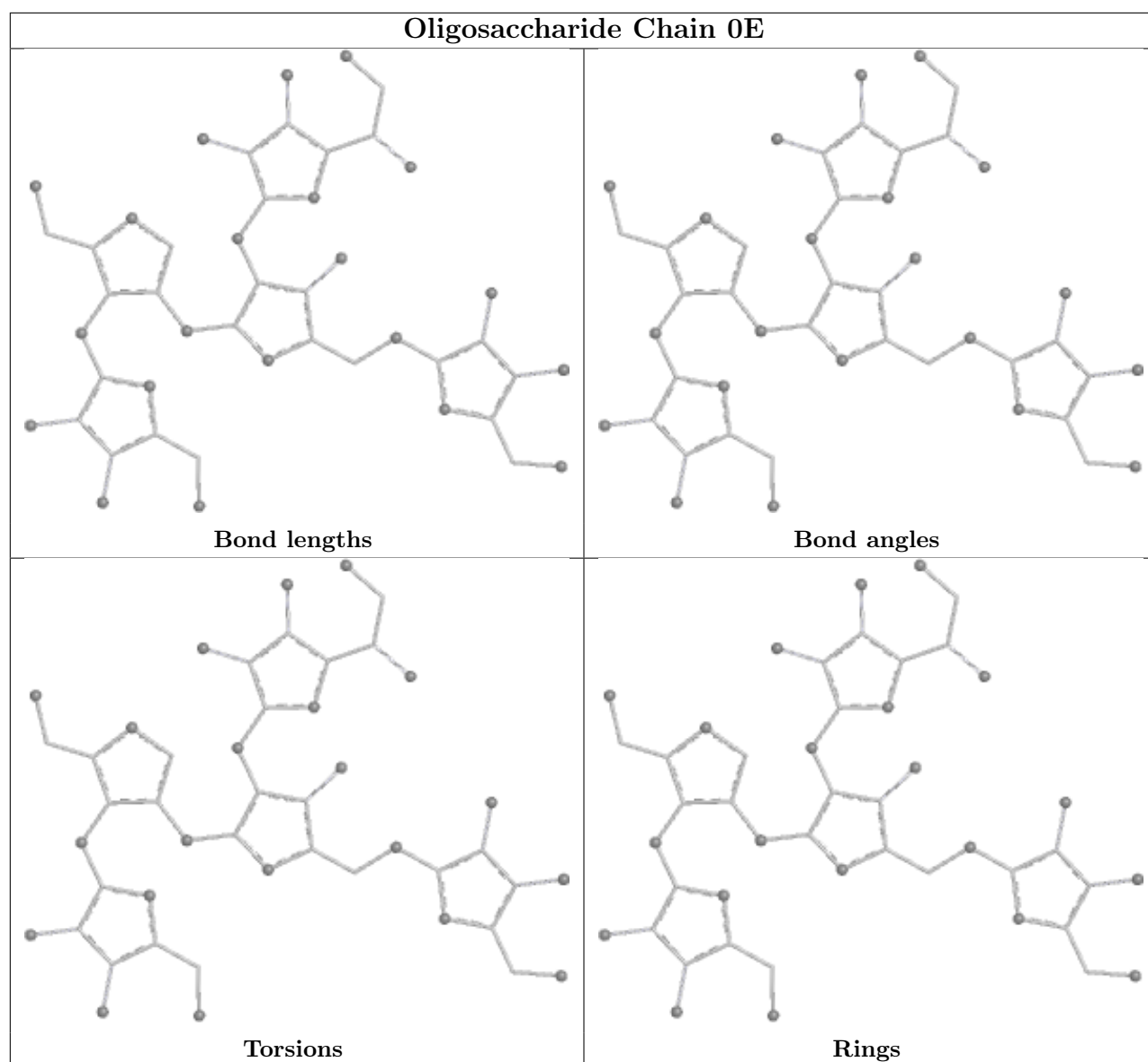


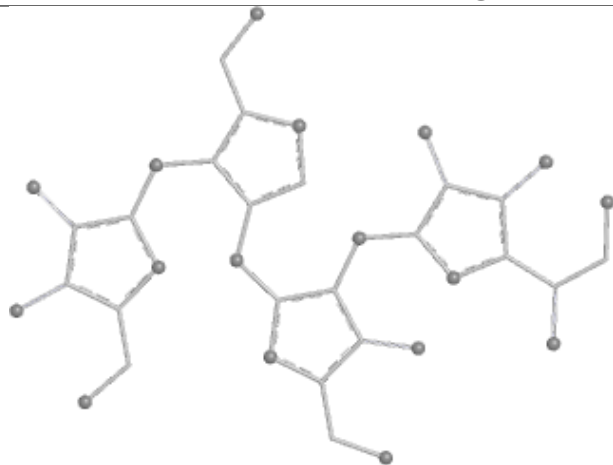
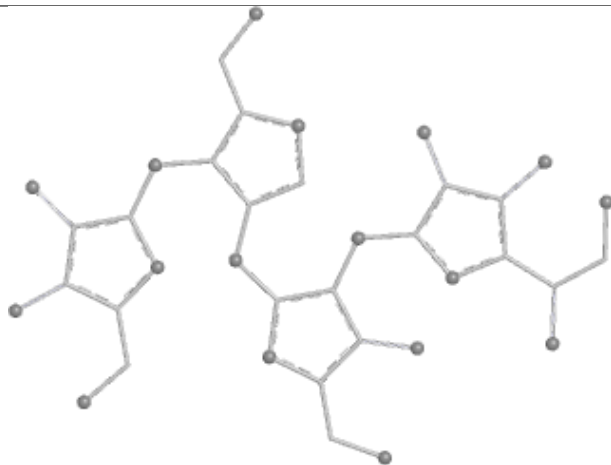
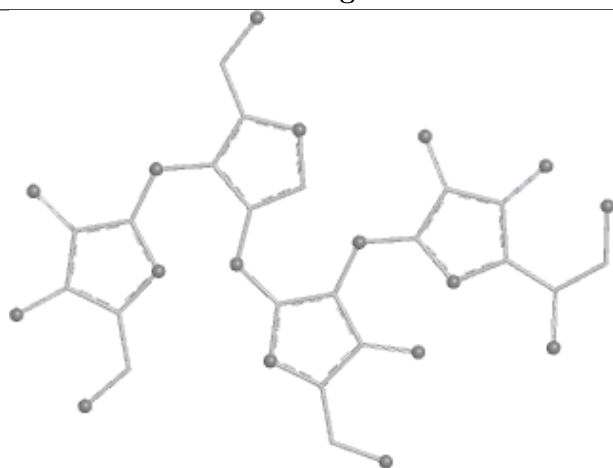
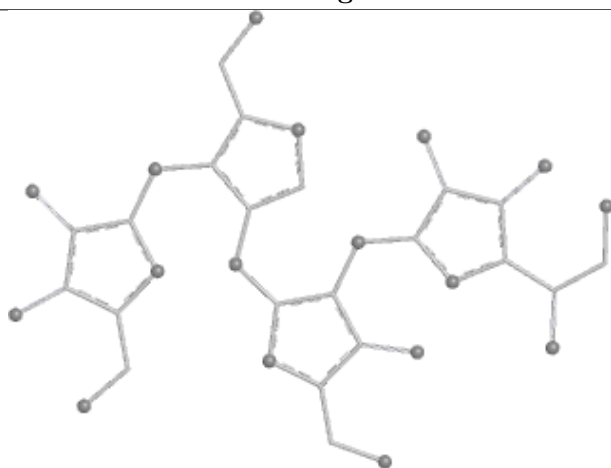


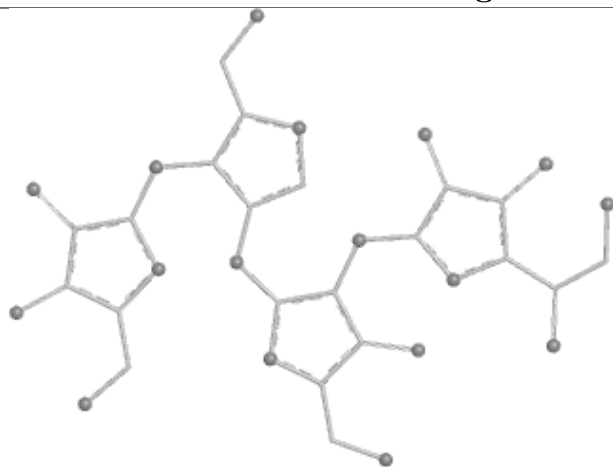
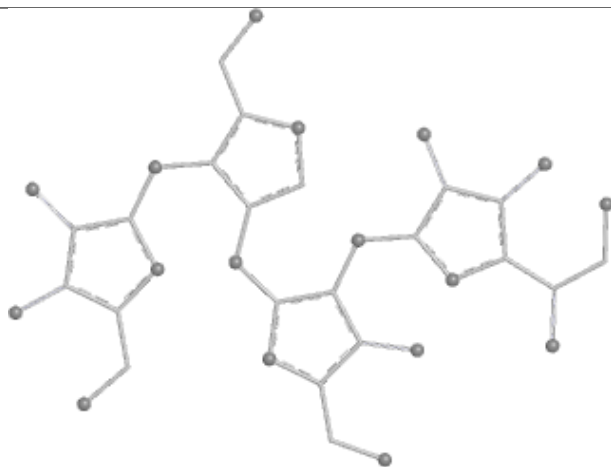
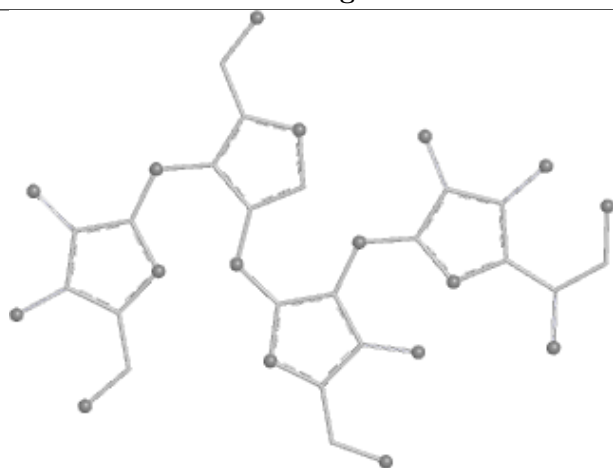
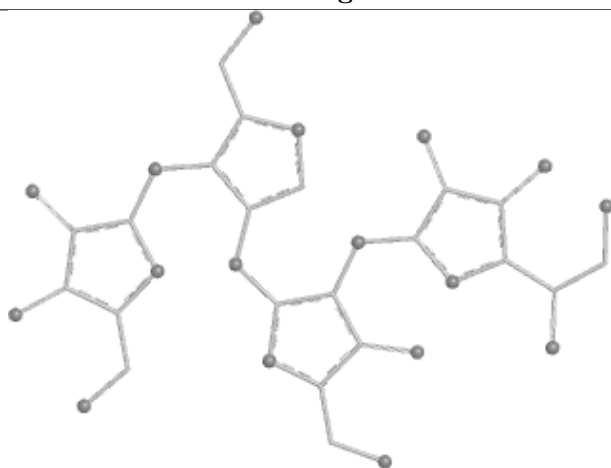




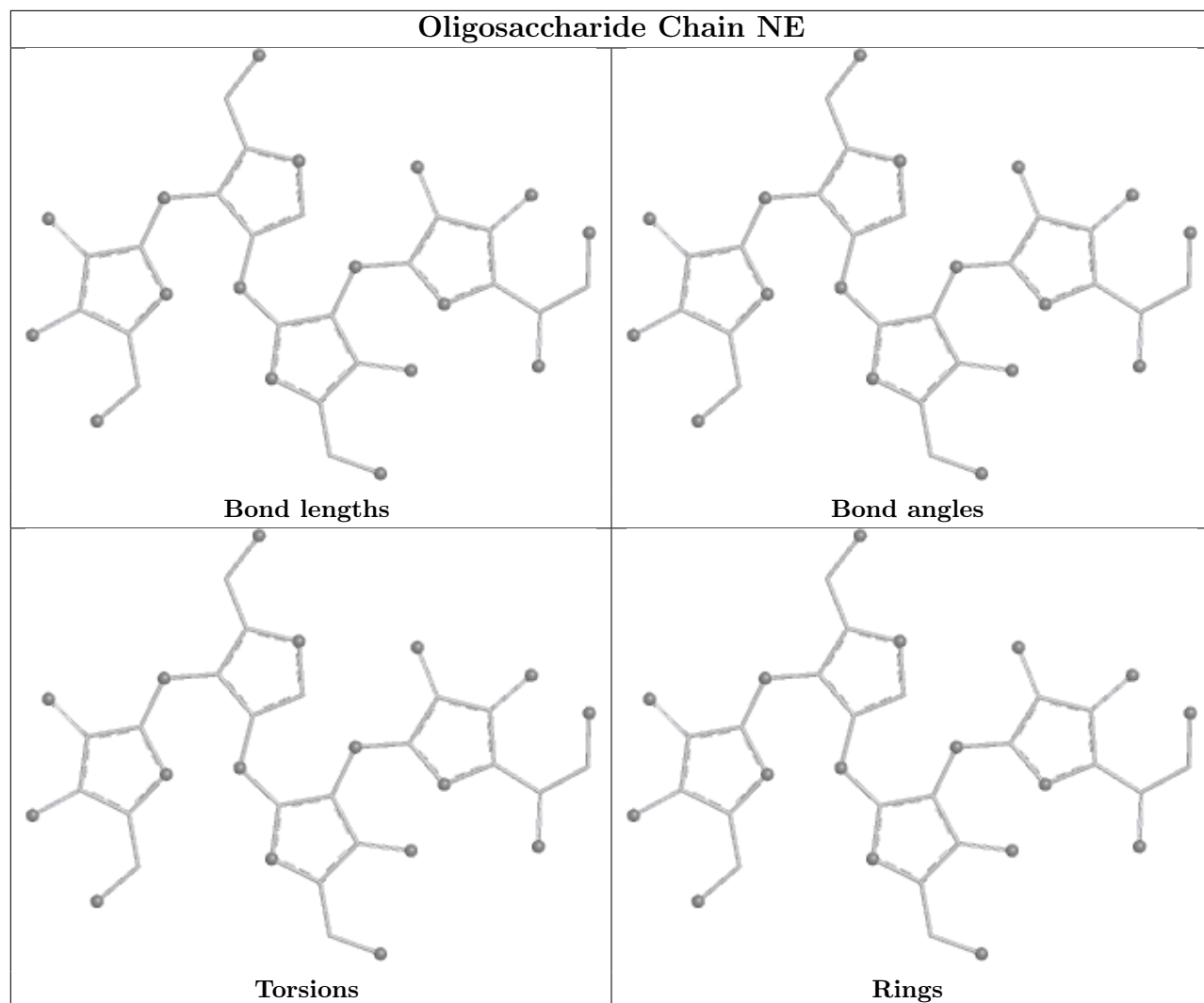


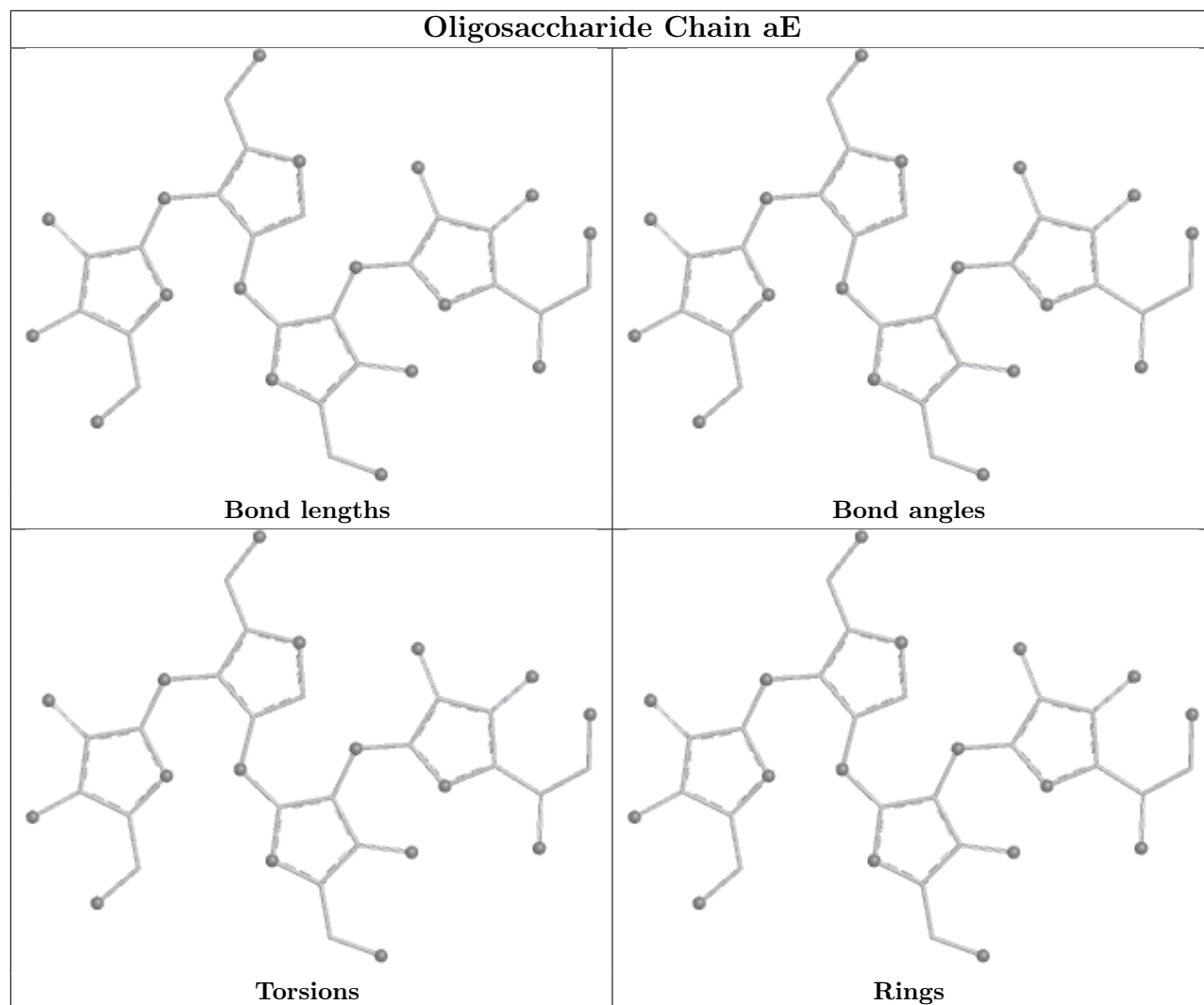


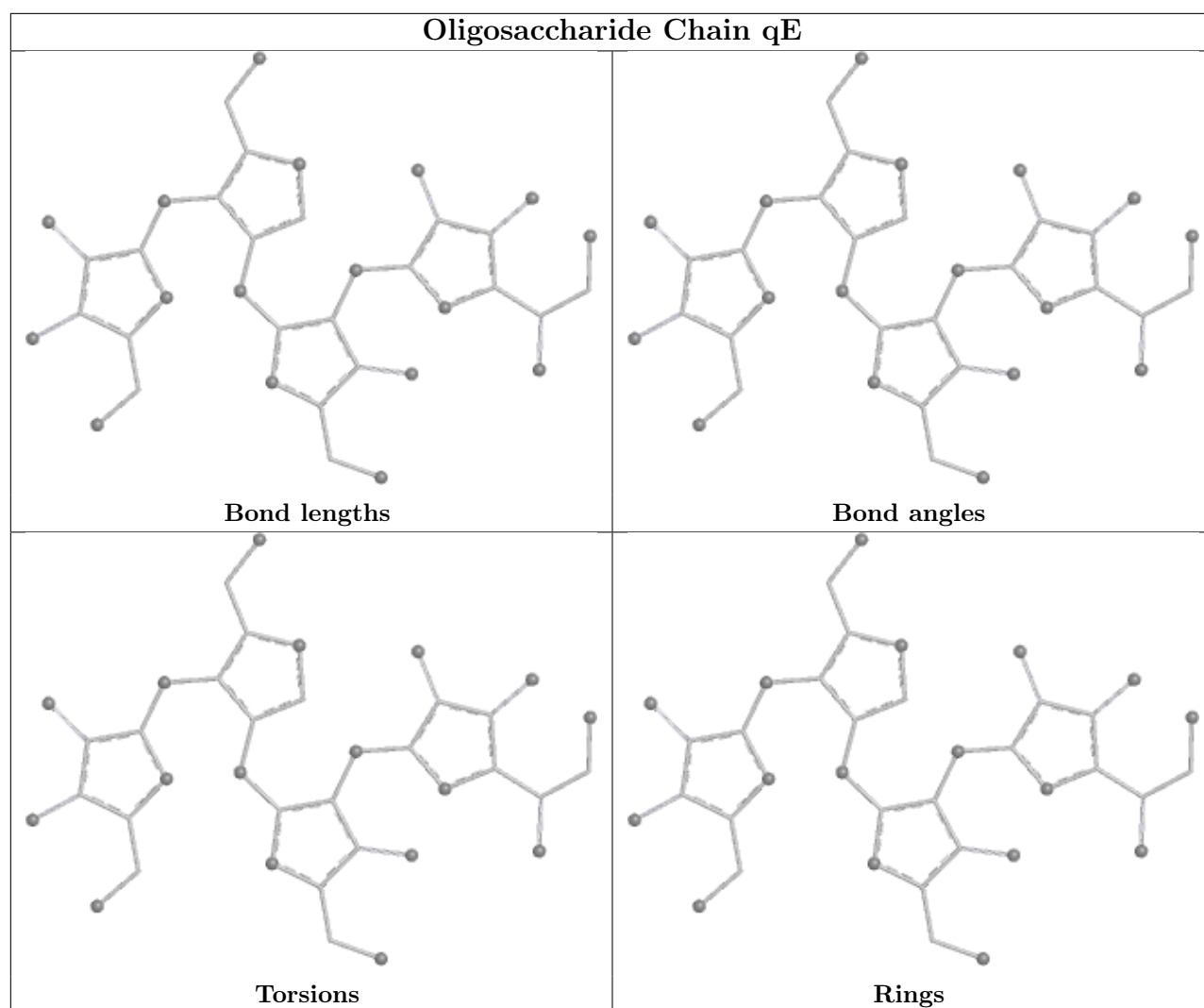
Oligosaccharide Chain AE**Bond lengths****Bond angles****Torsions****Rings**

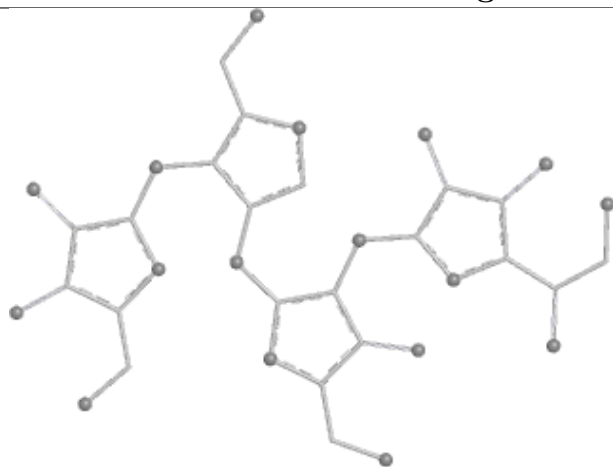
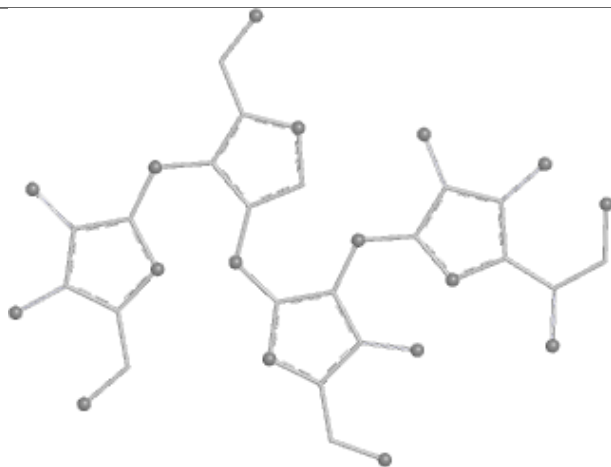
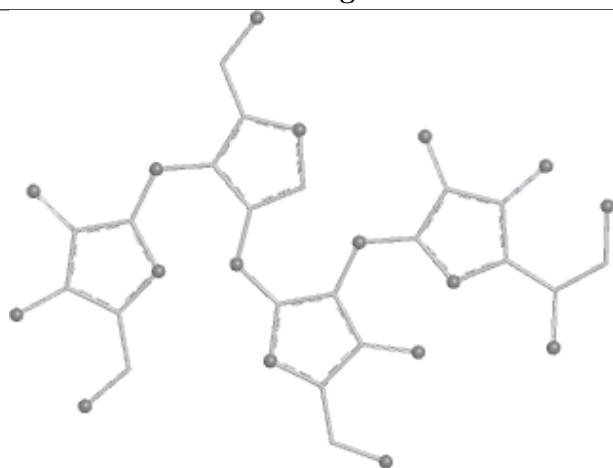
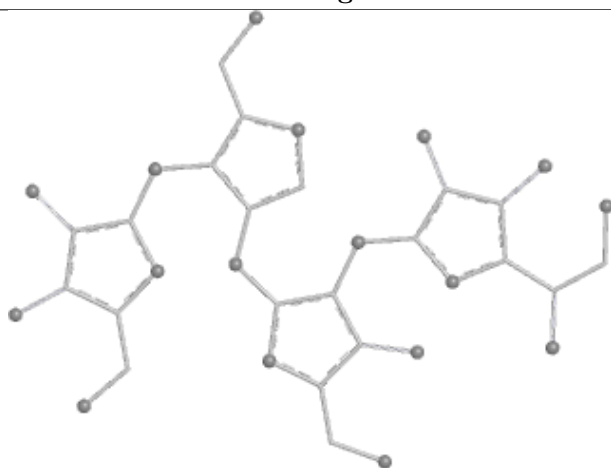
Oligosaccharide Chain LE**Bond lengths****Bond angles****Torsions****Rings**

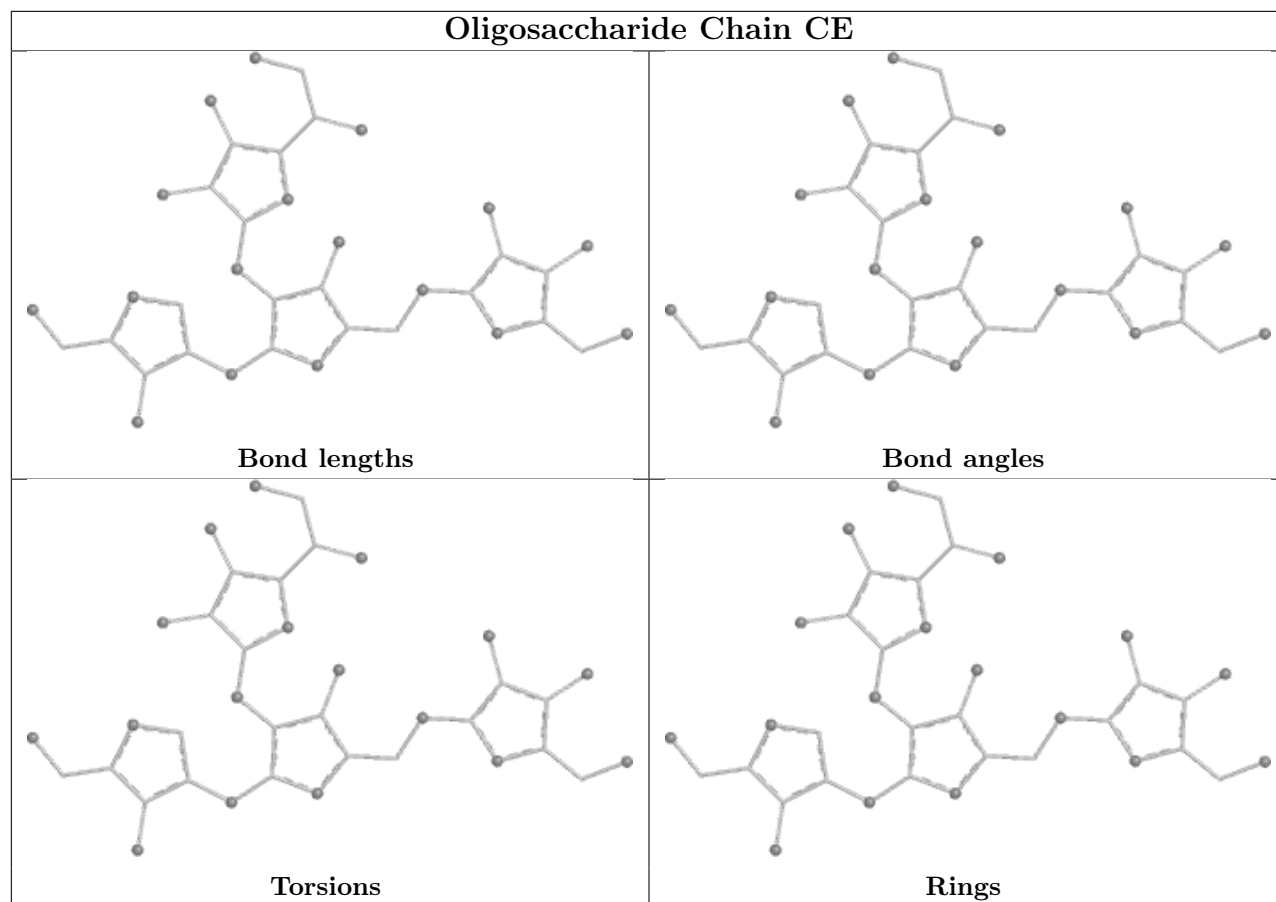
Oligosaccharide Chain NE

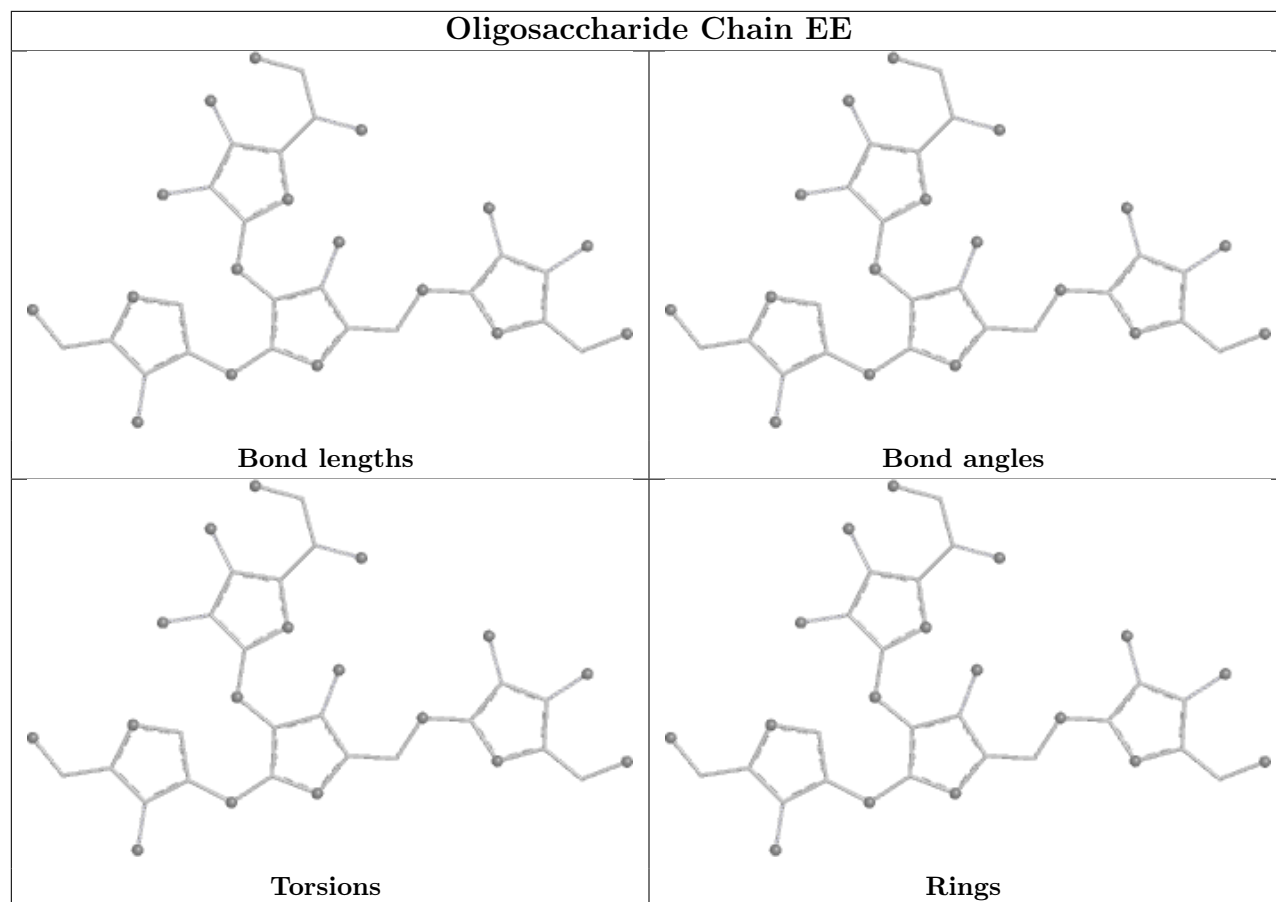


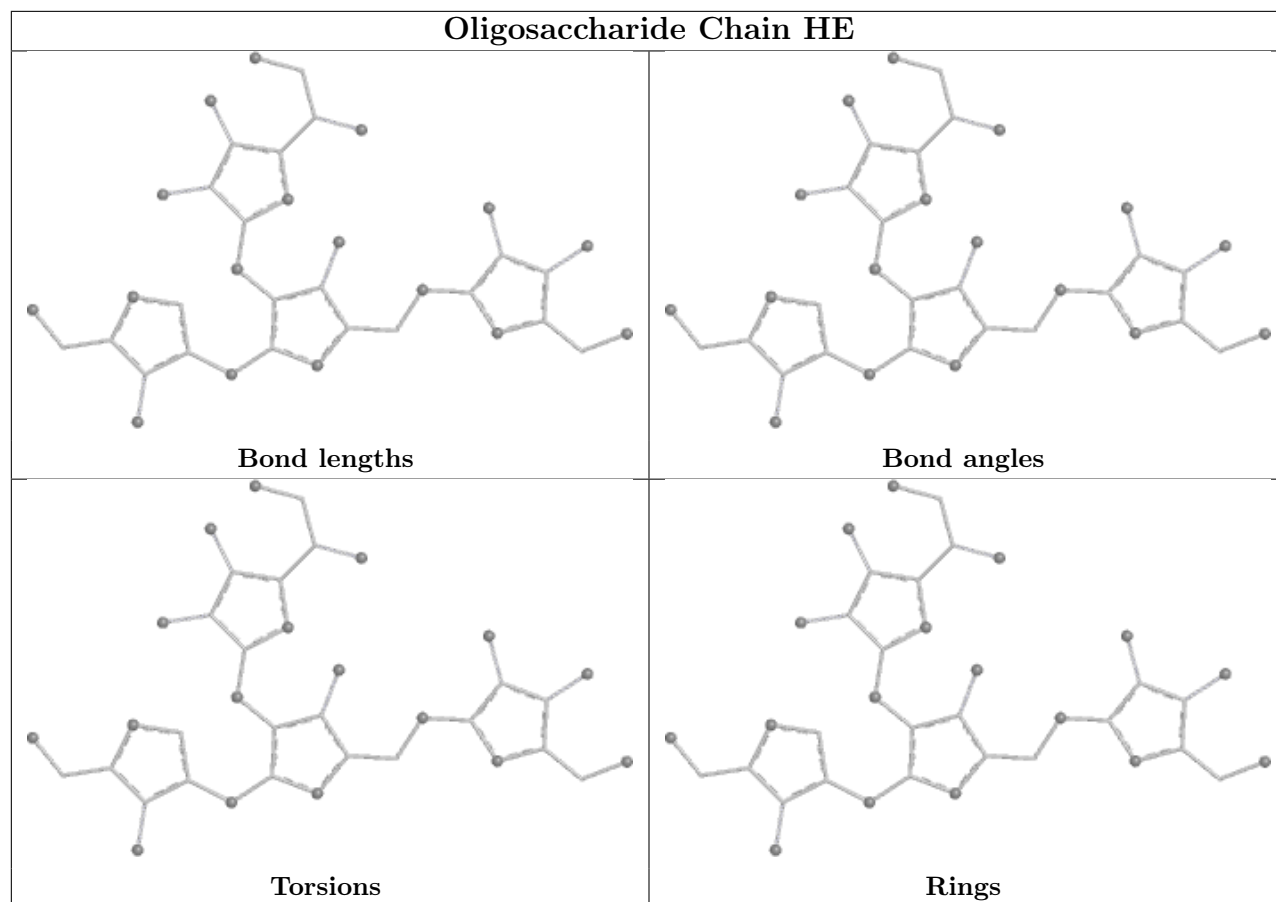


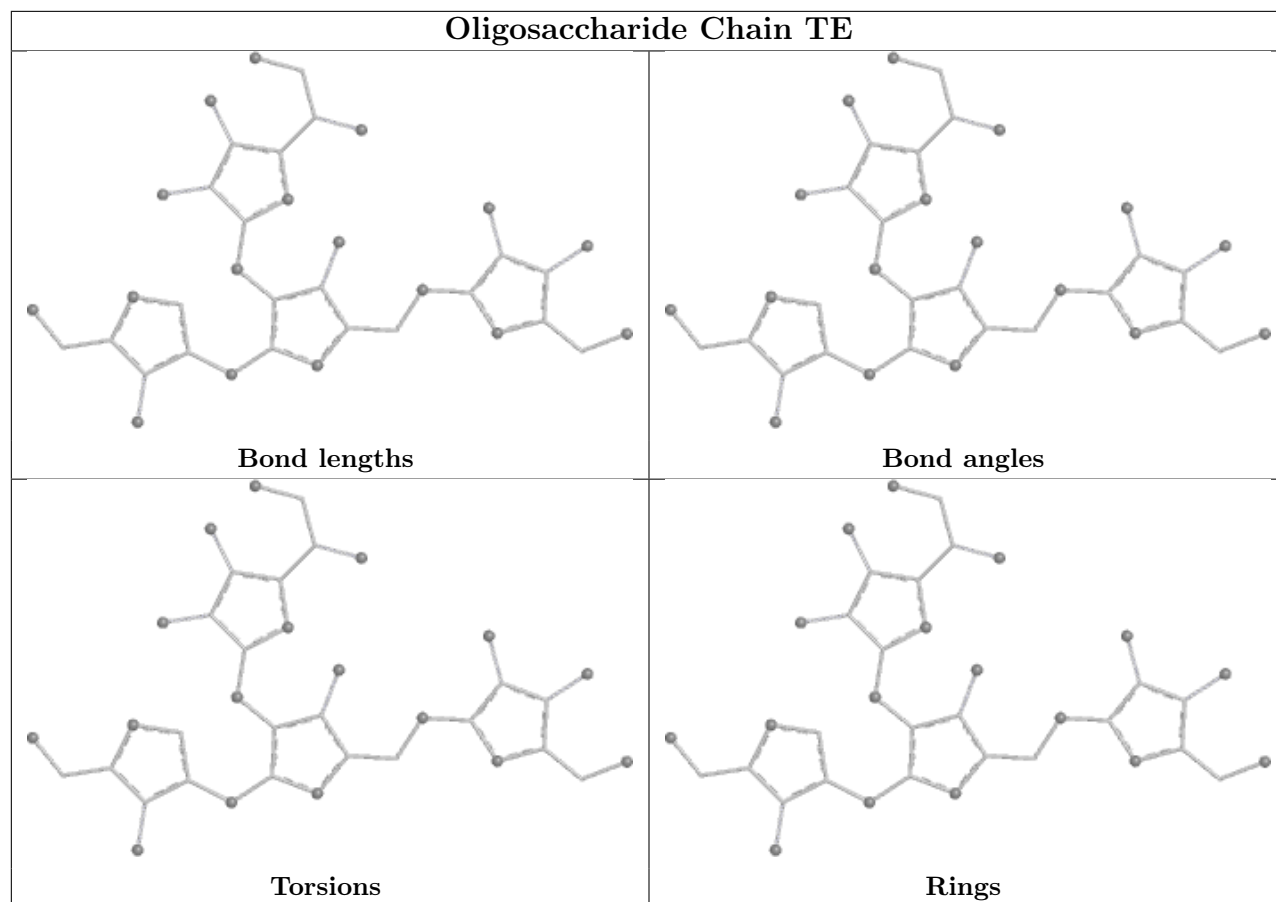


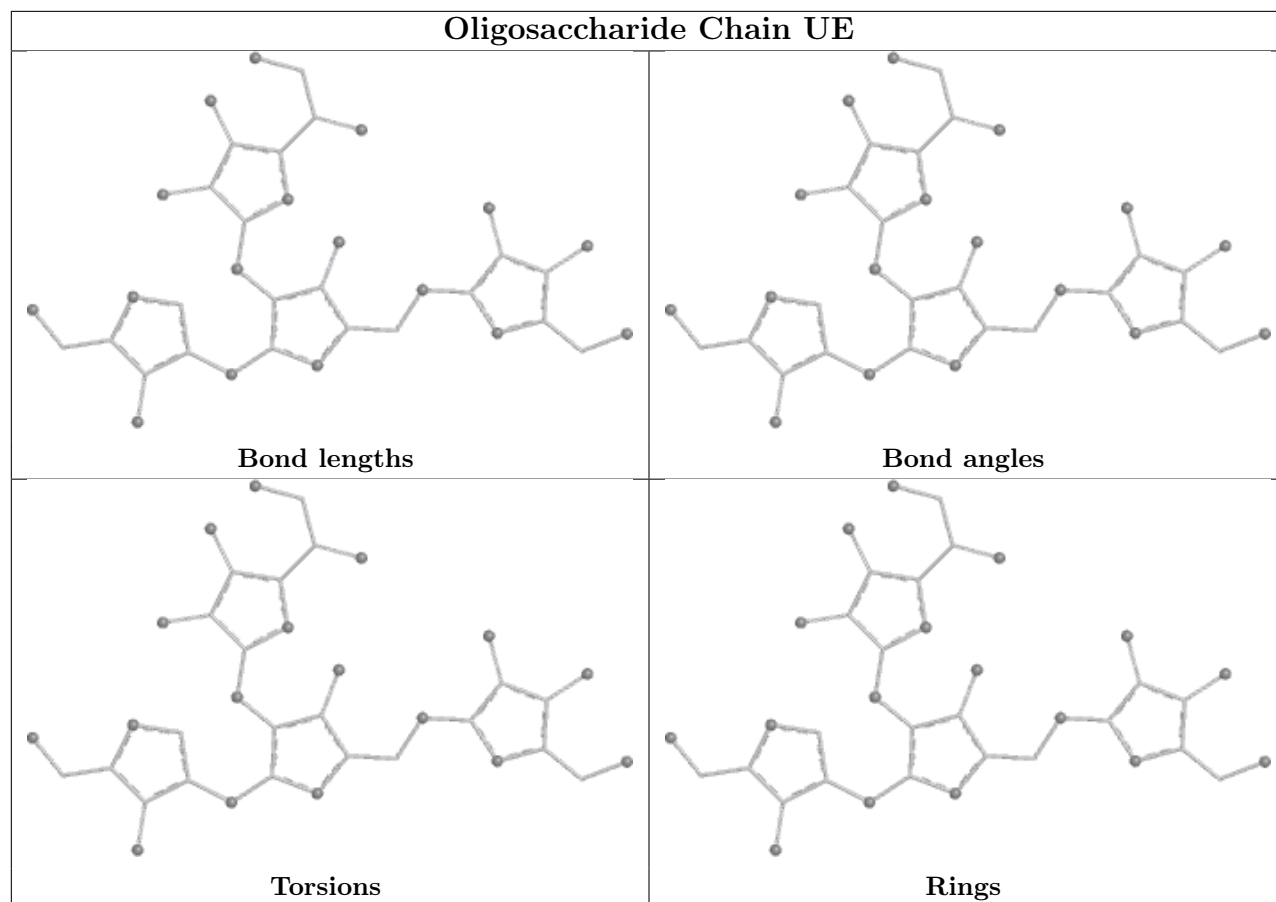
Oligosaccharide Chain 1E**Bond lengths****Bond angles****Torsions****Rings**

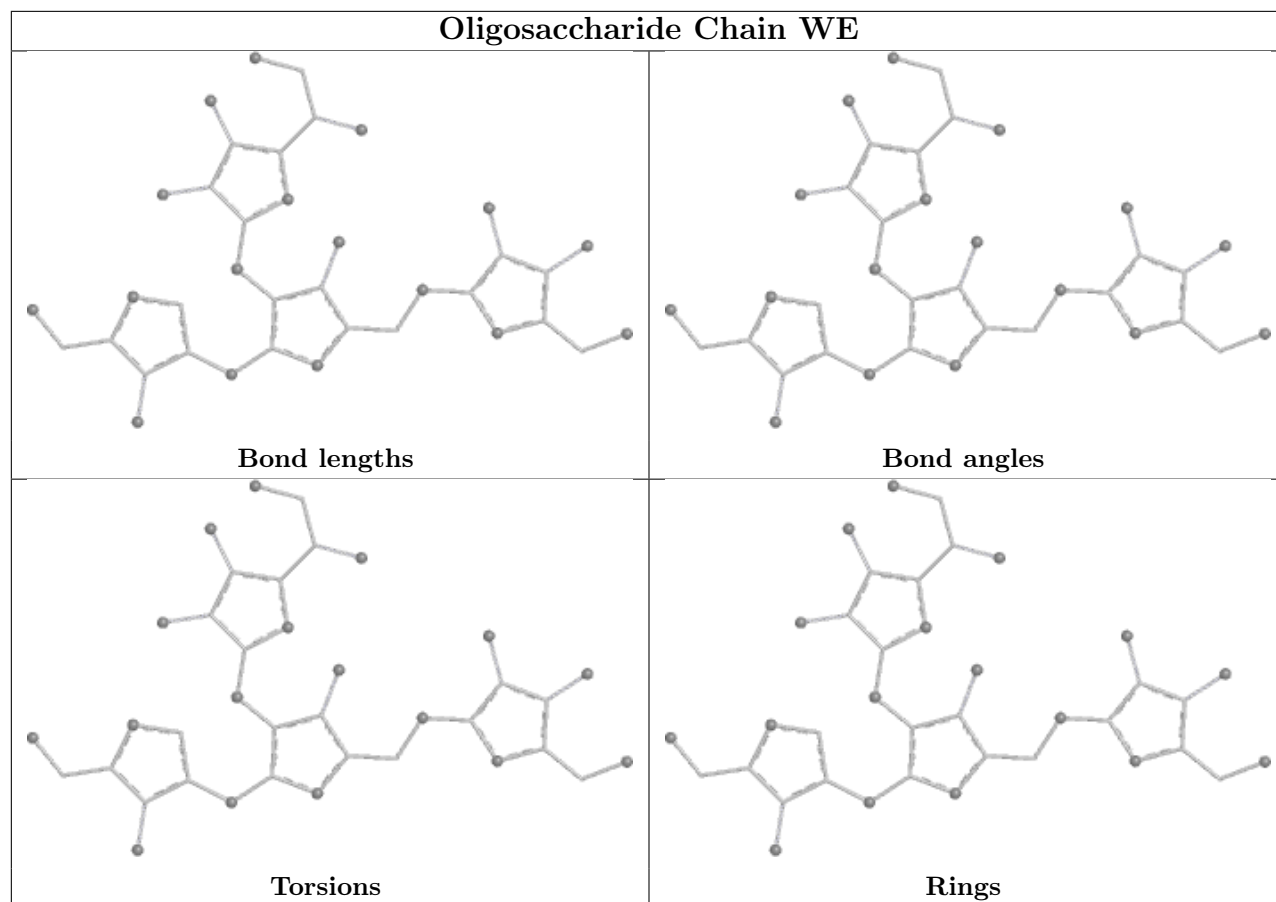


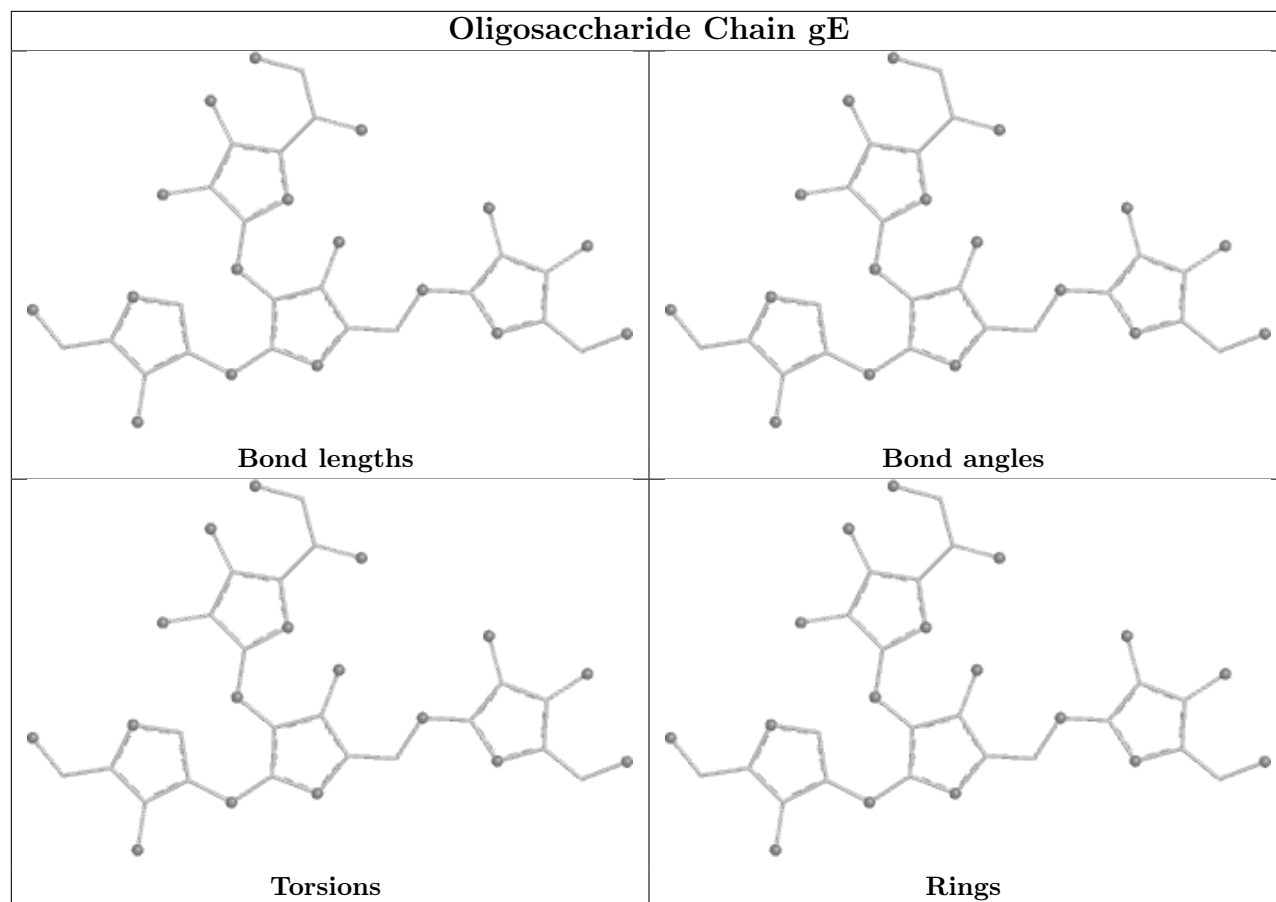


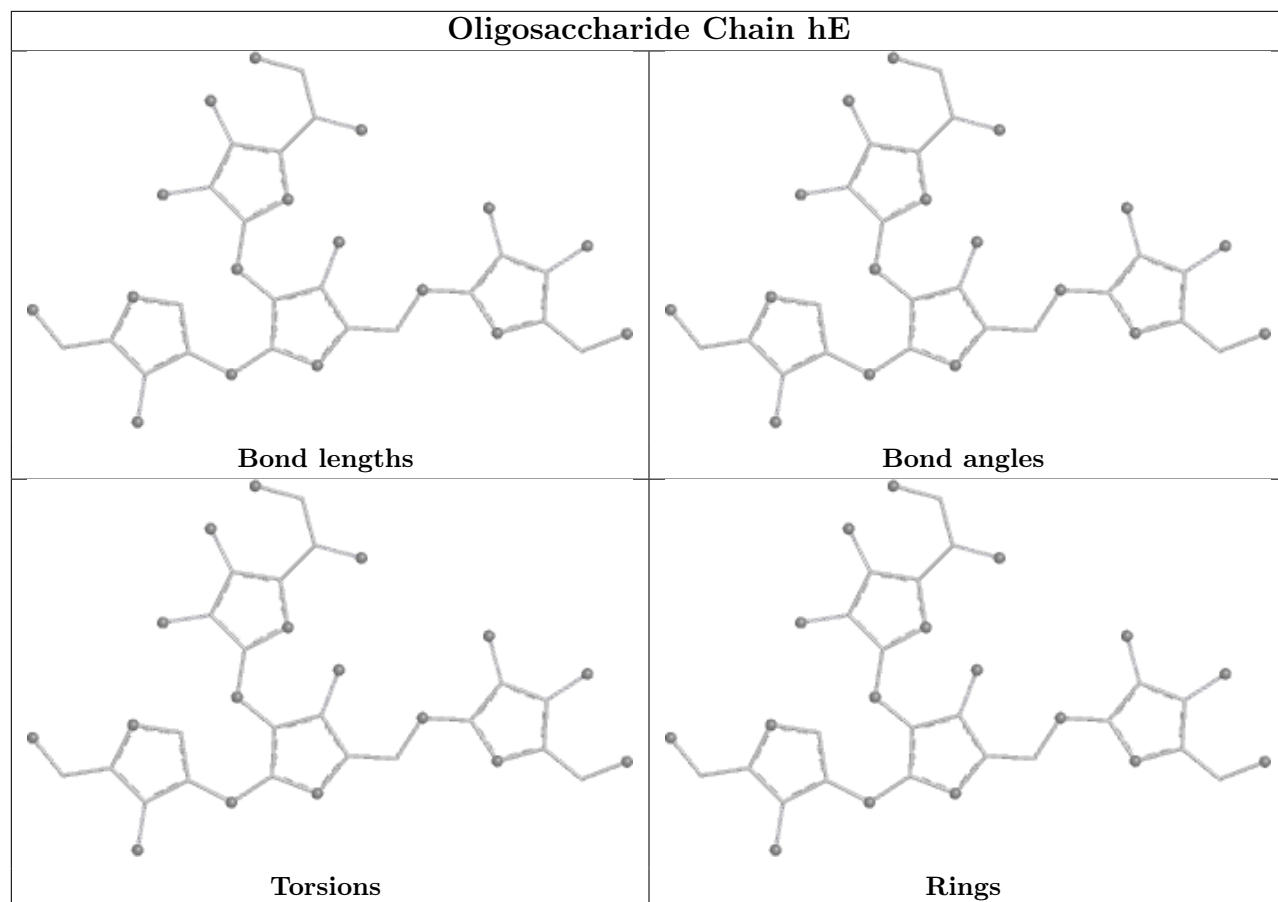


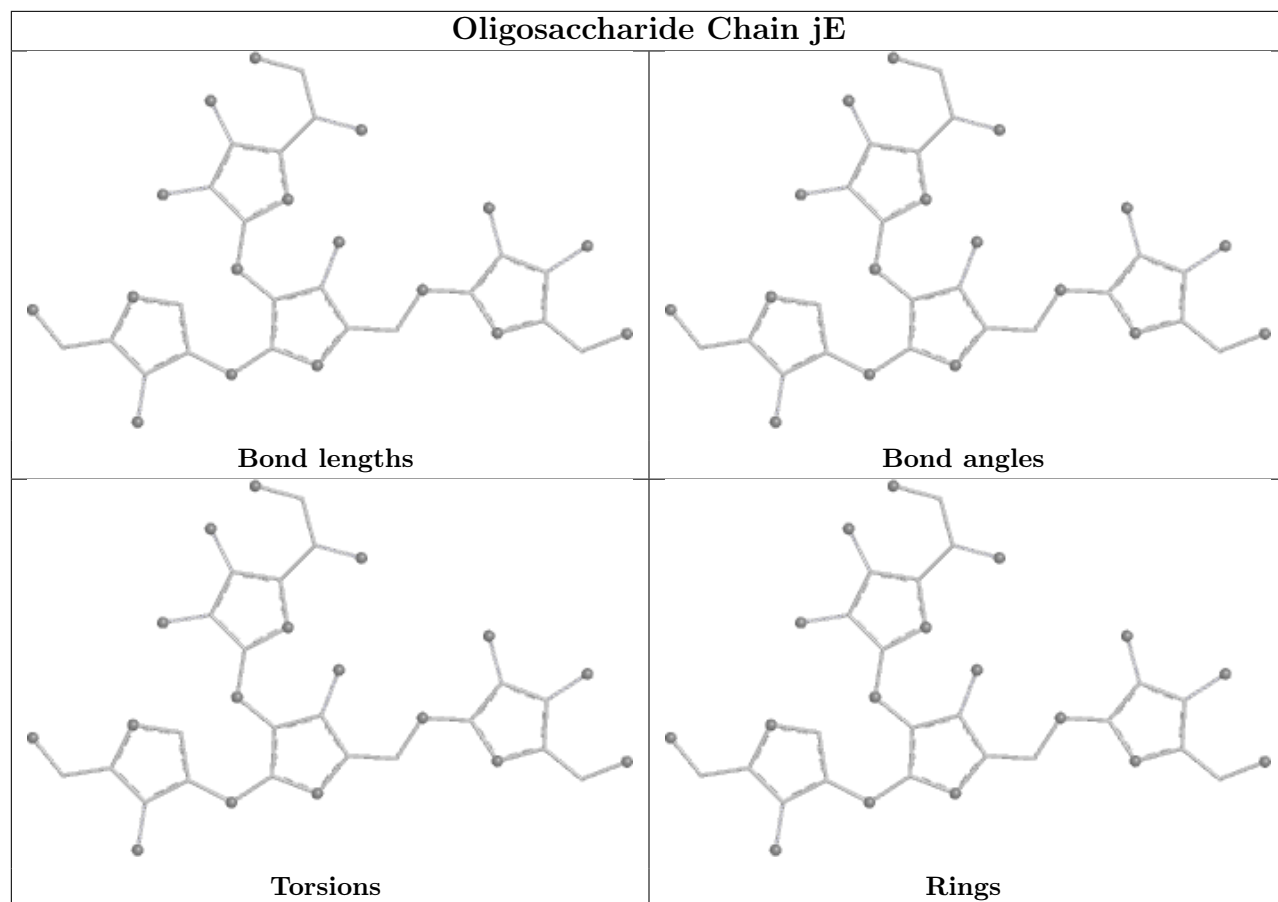


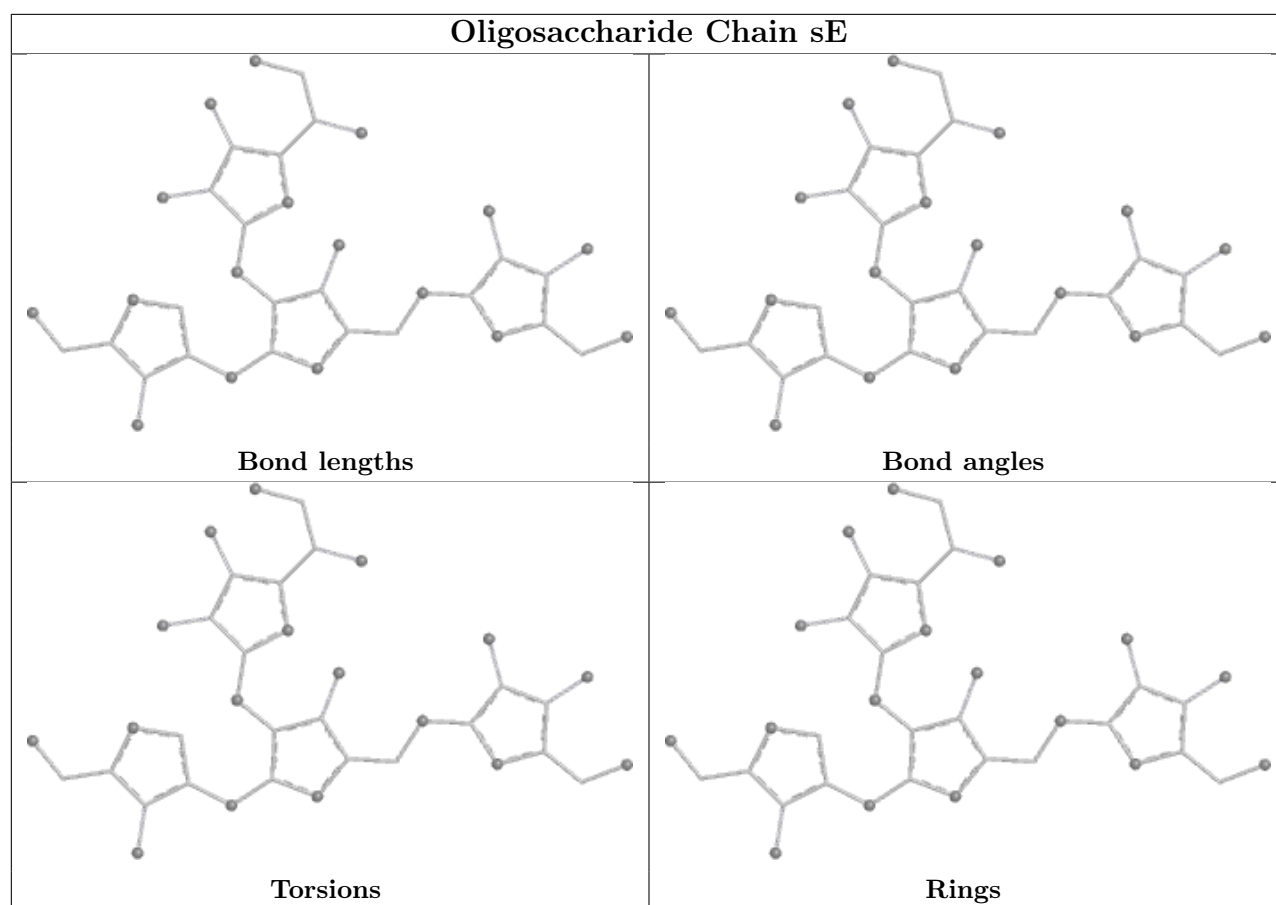


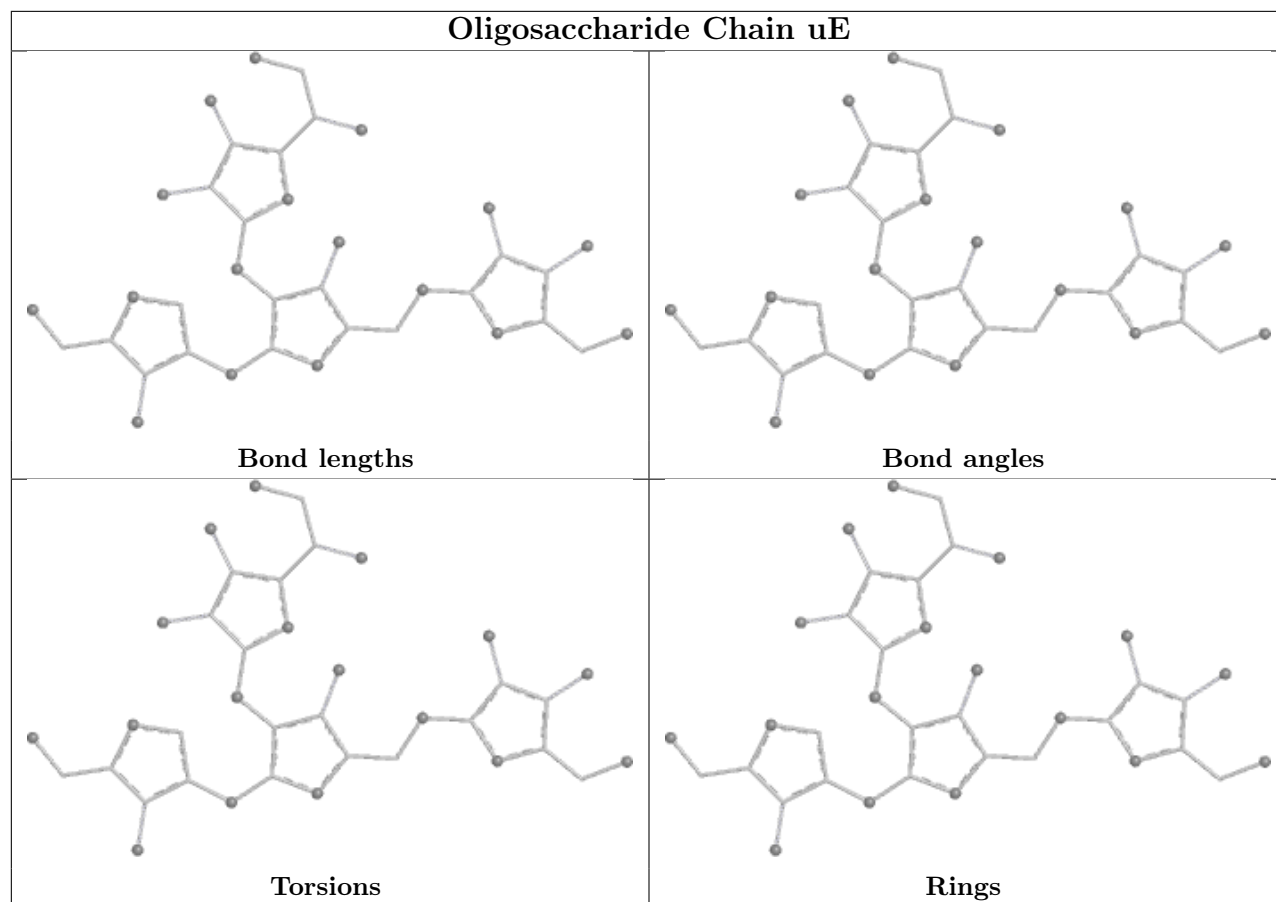


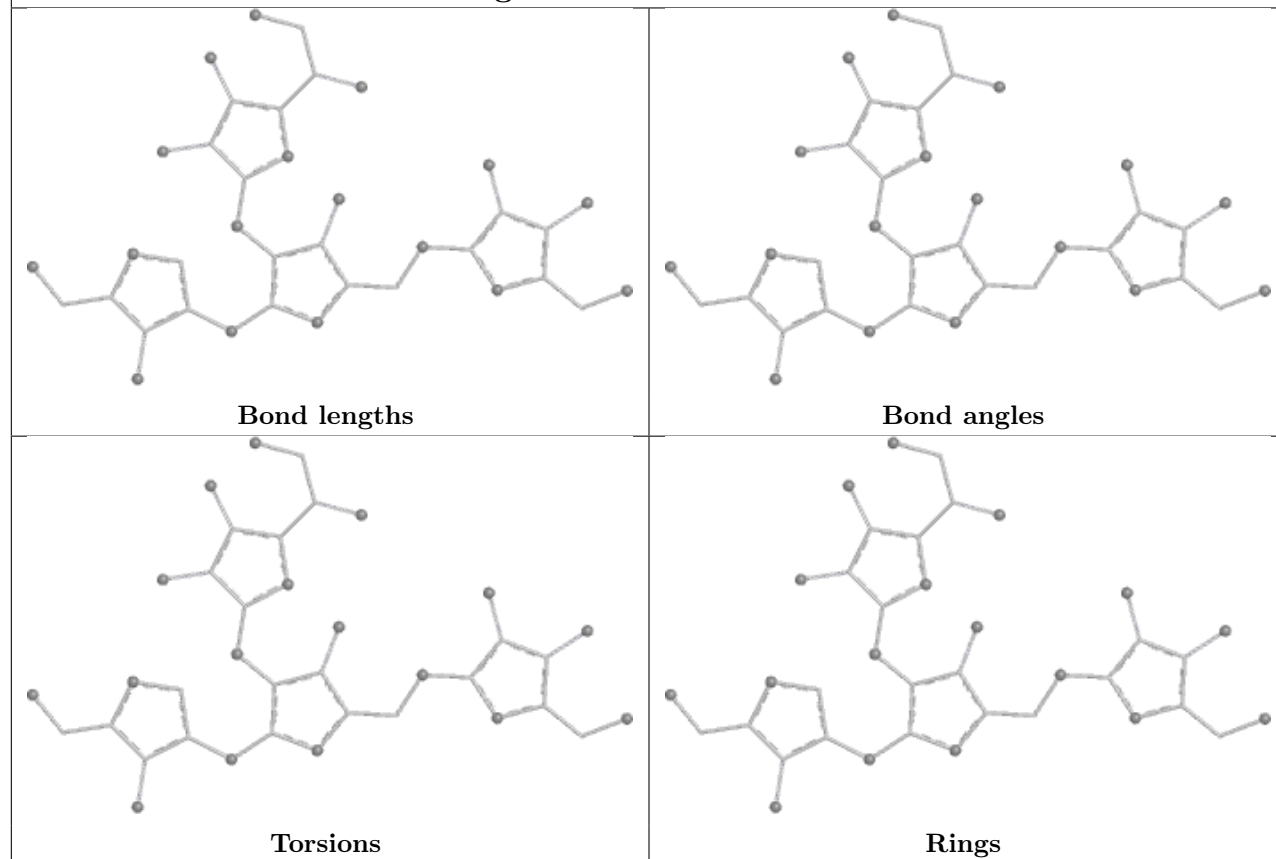
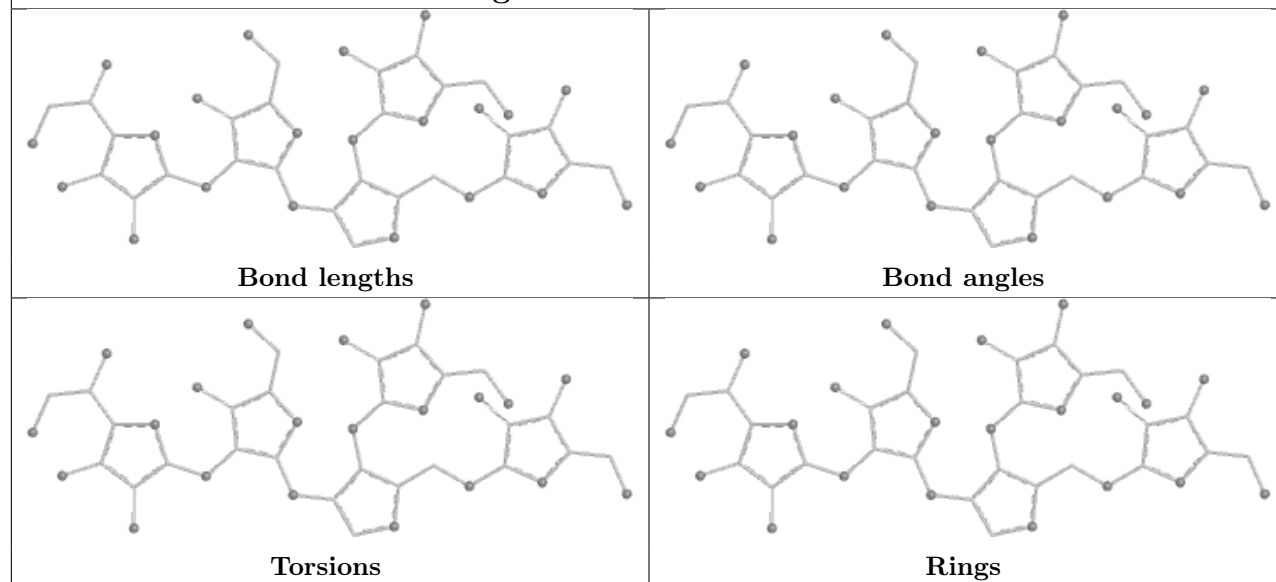


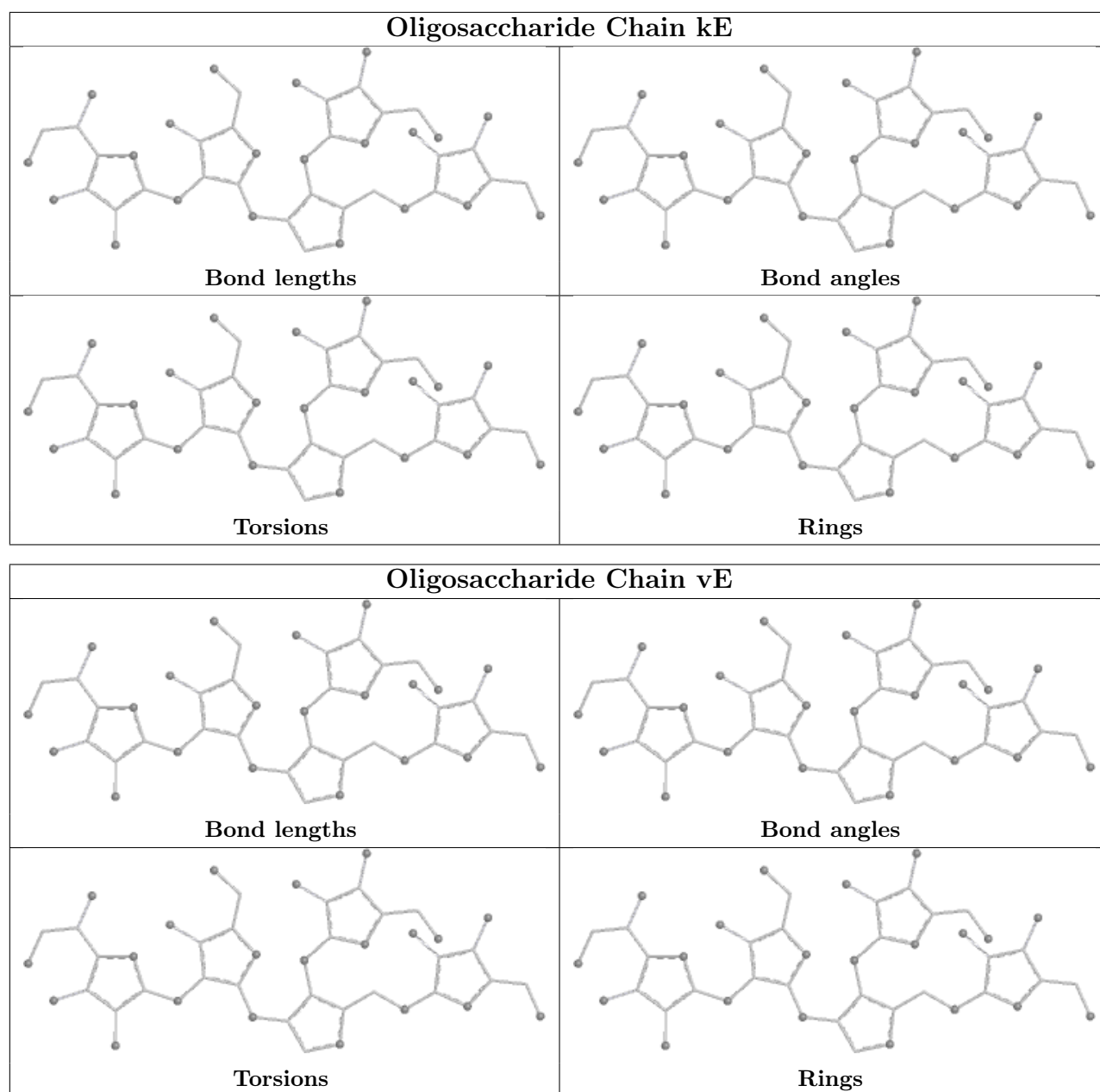


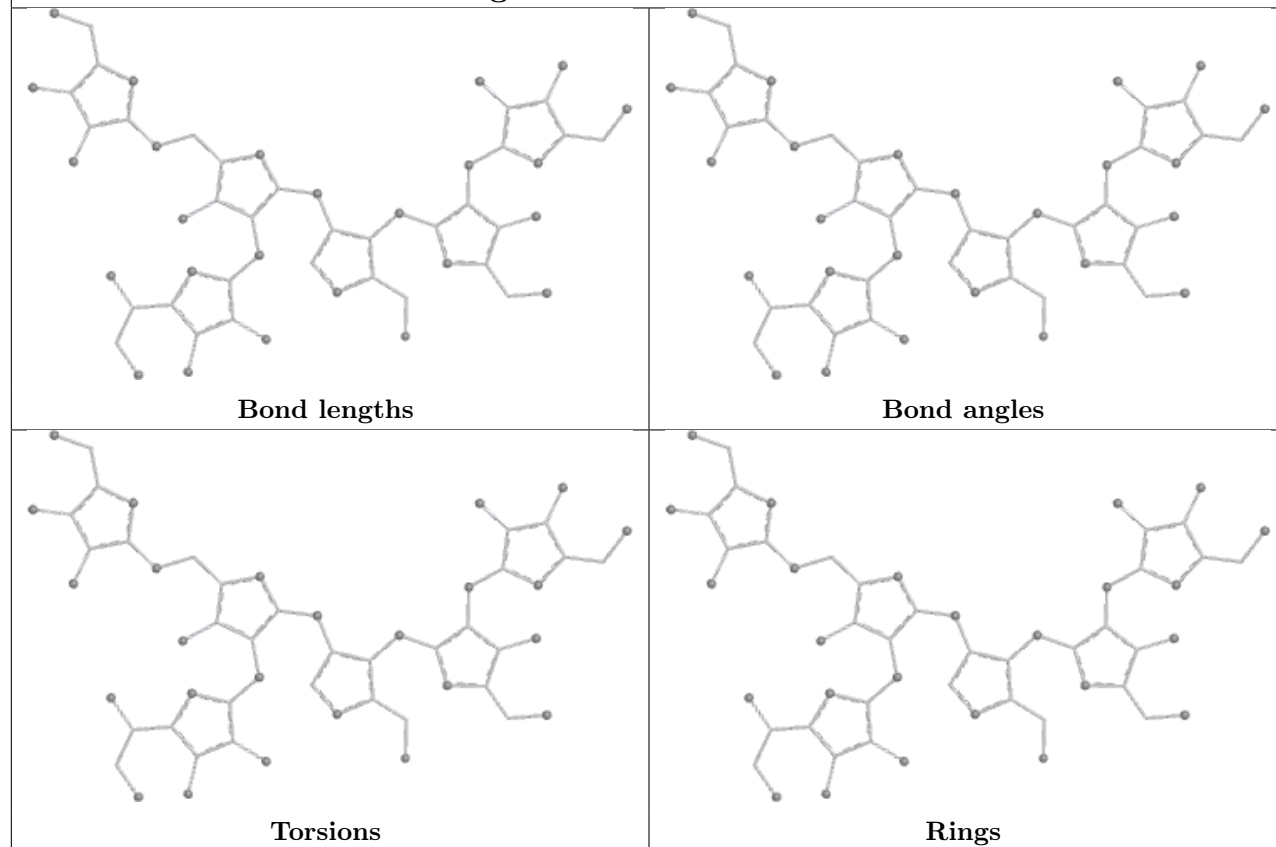
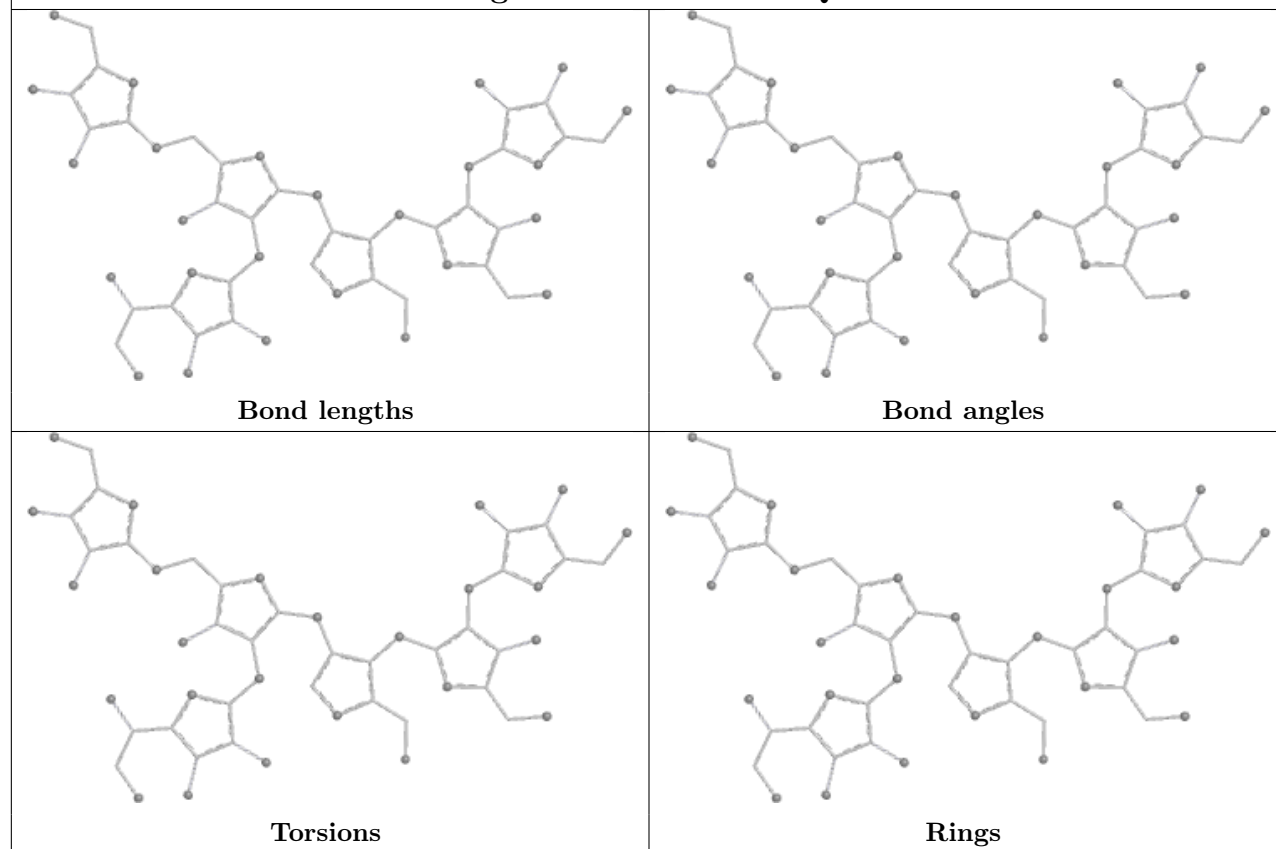


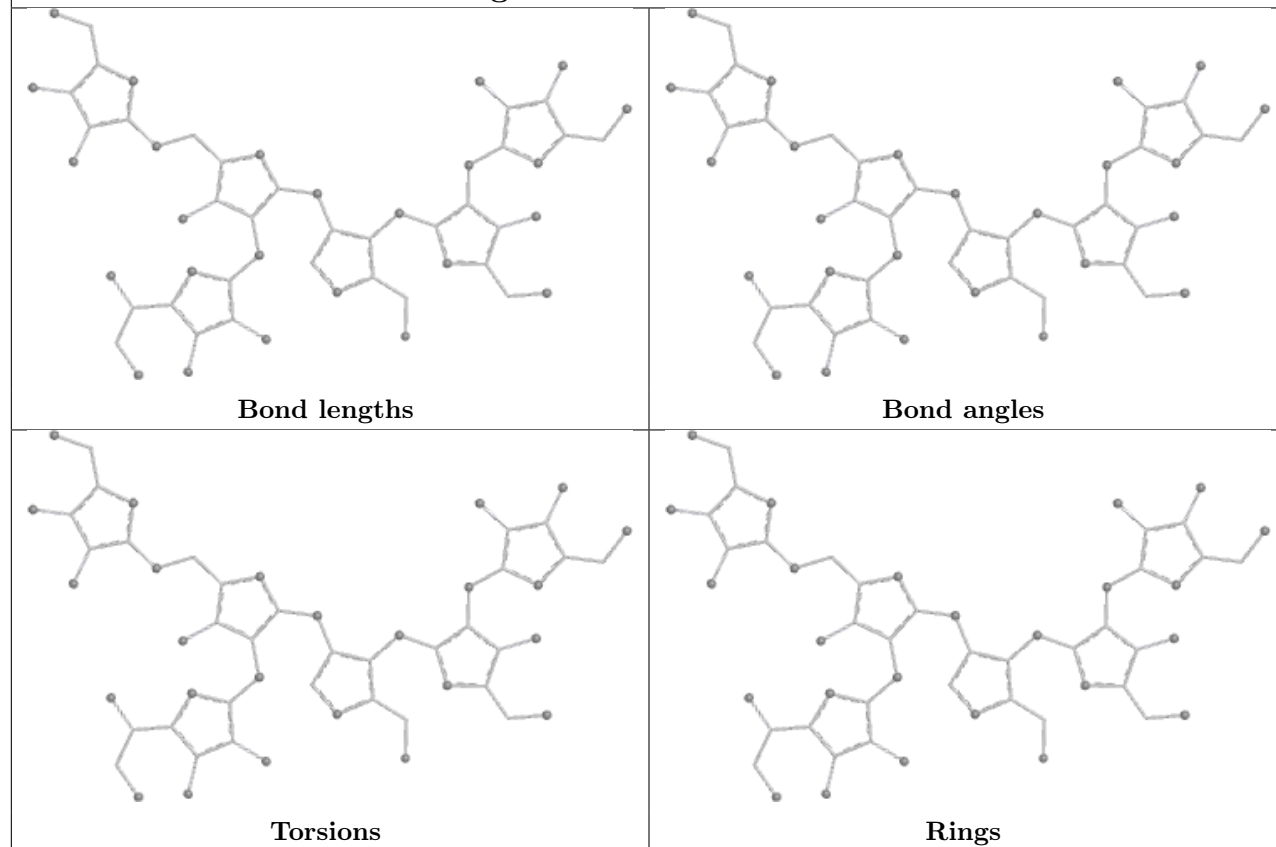
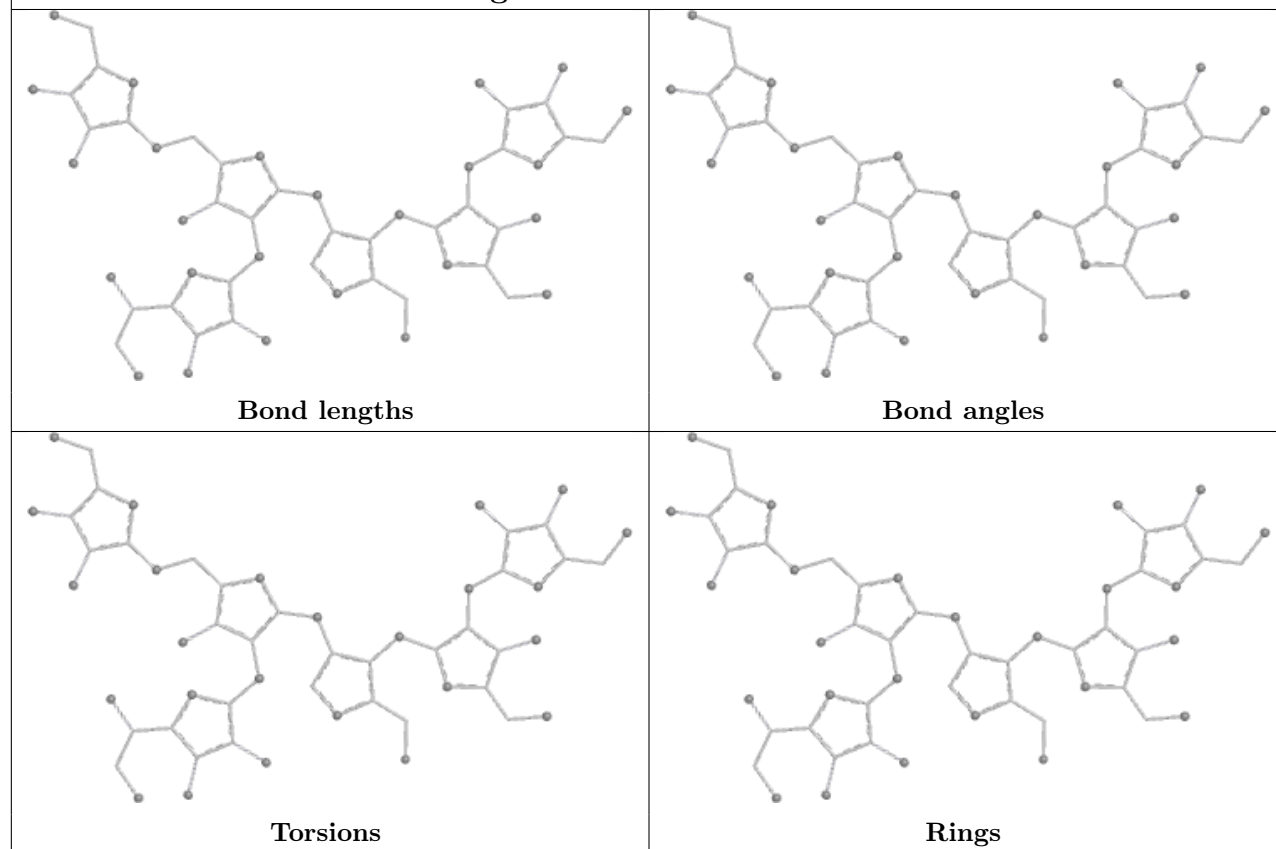


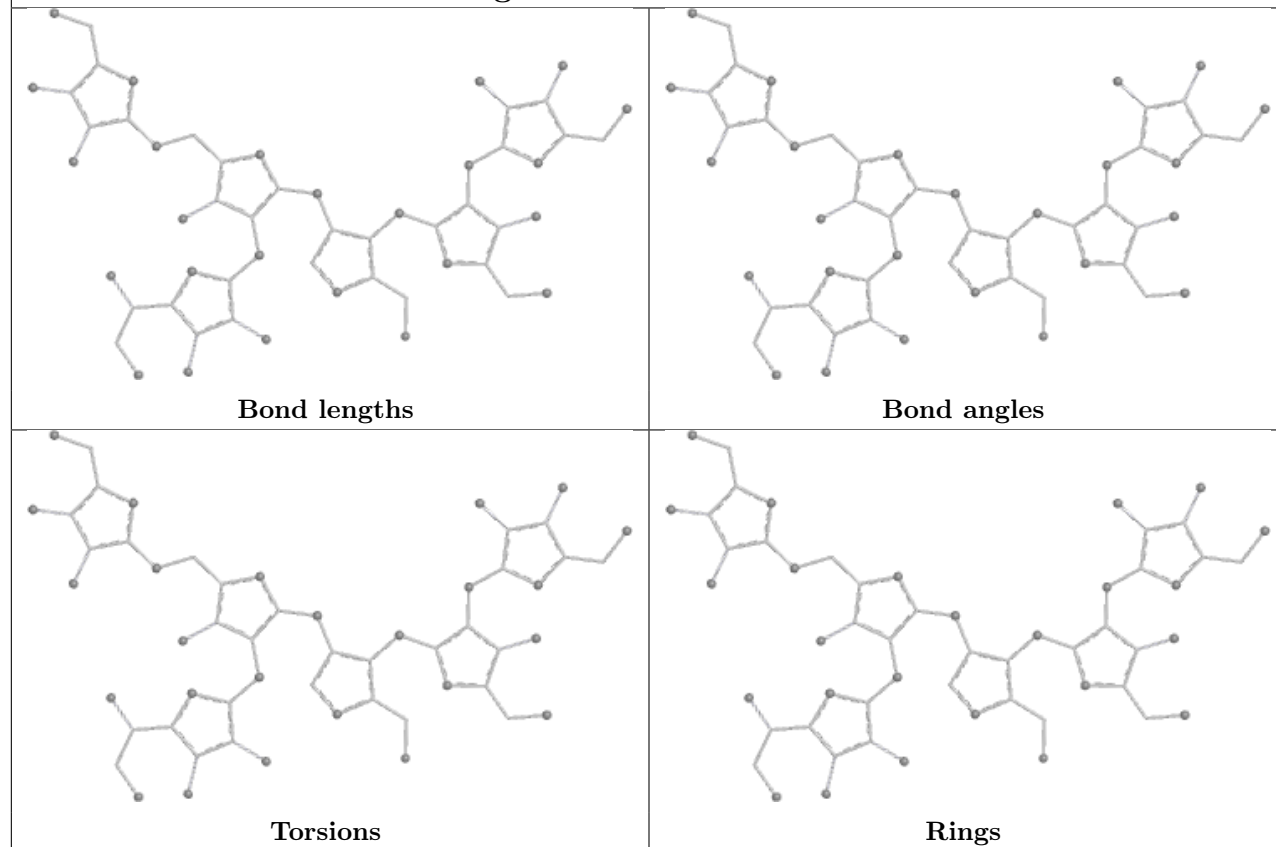
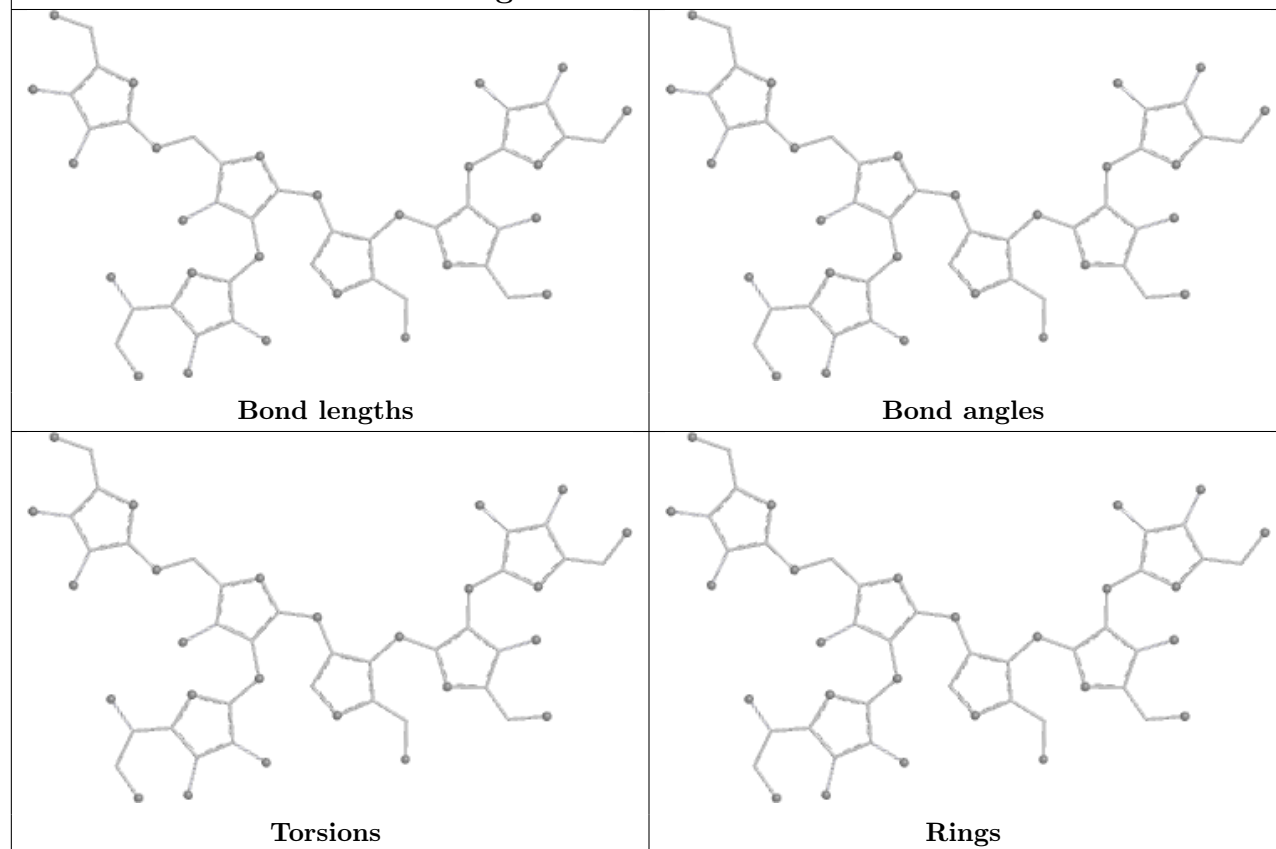


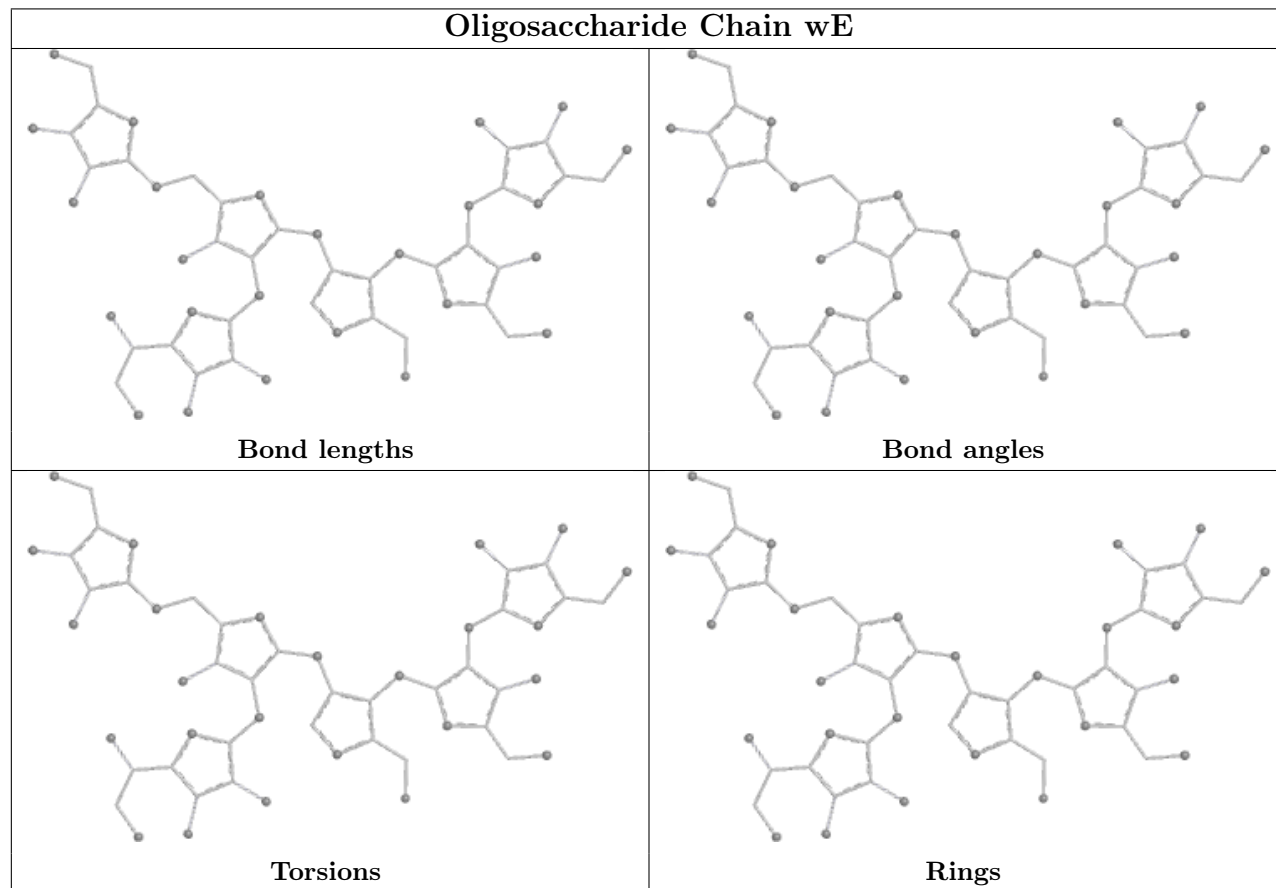
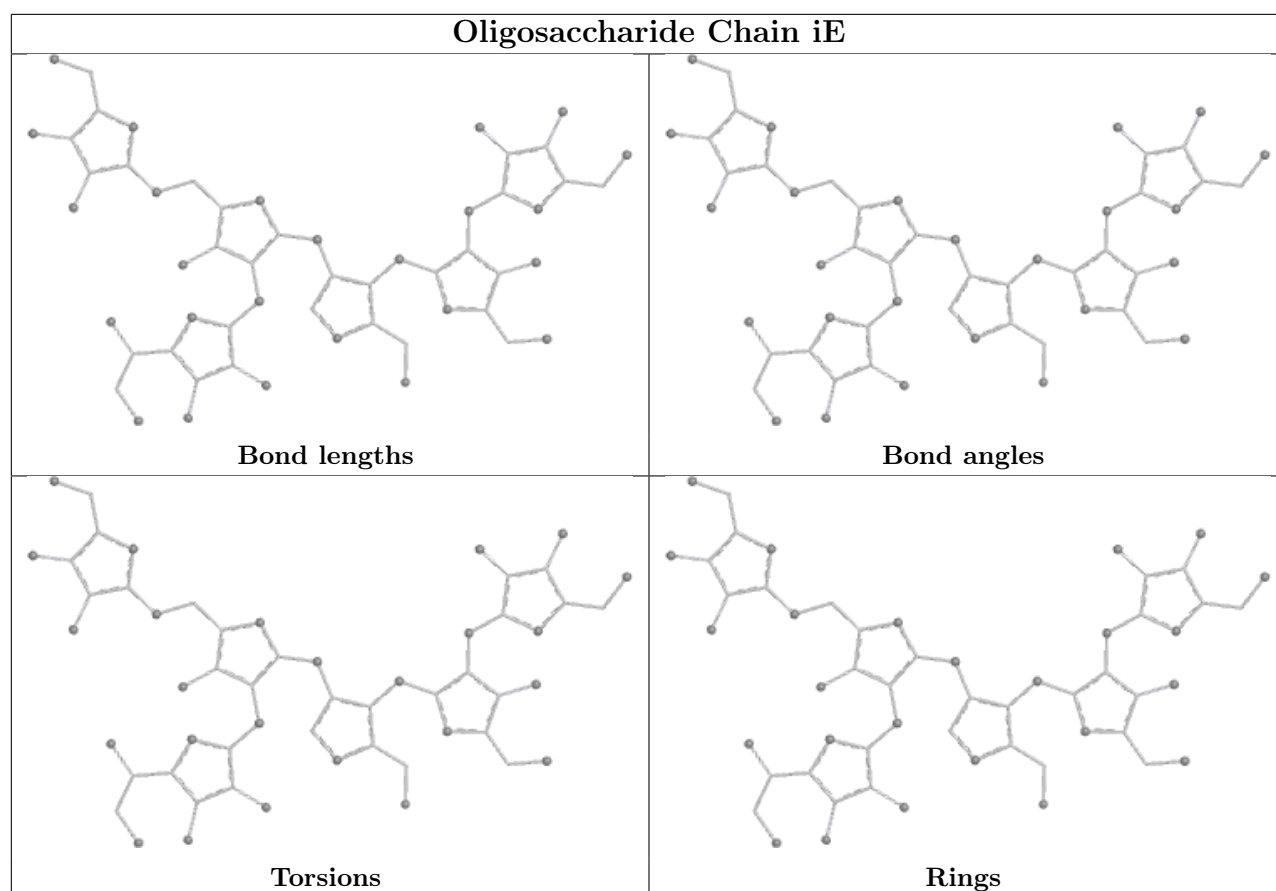
Oligosaccharide Chain xE**Oligosaccharide Chain FE**

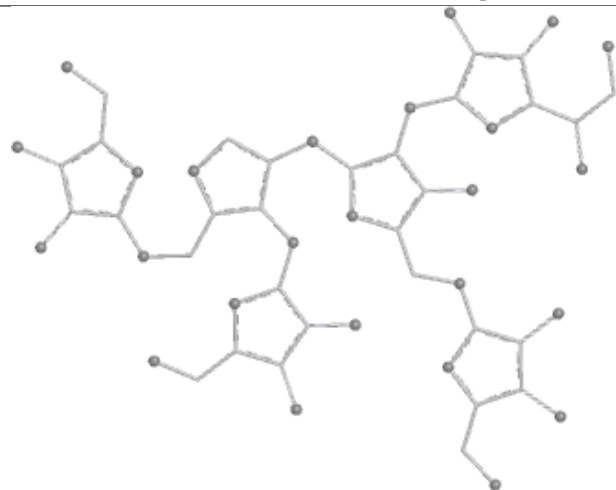
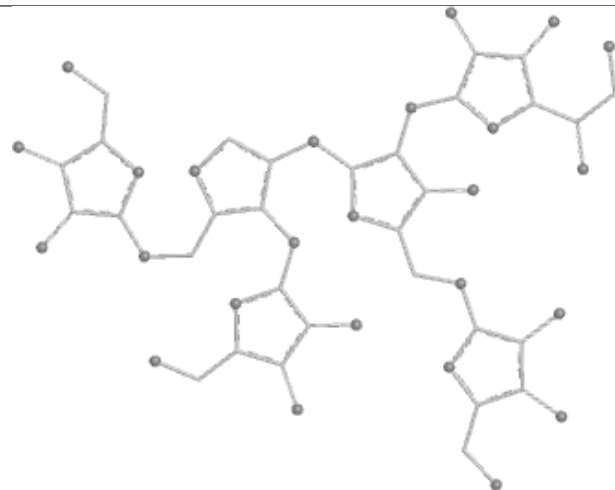
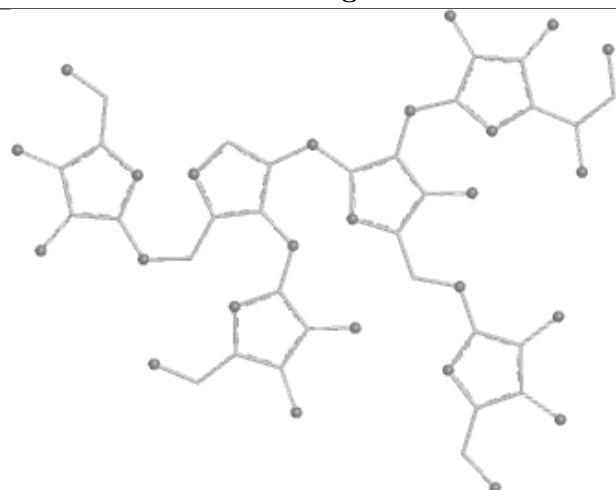
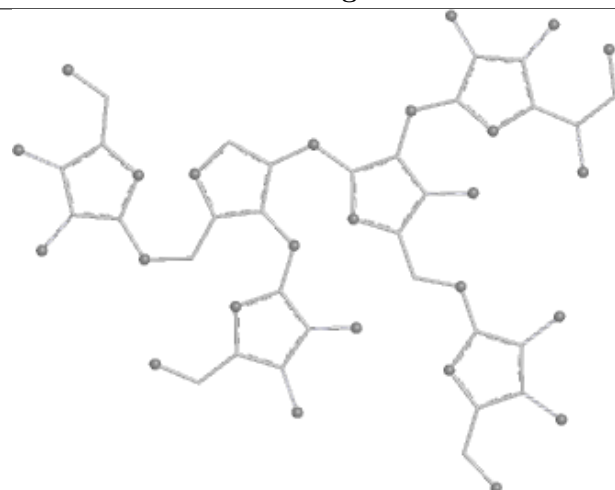


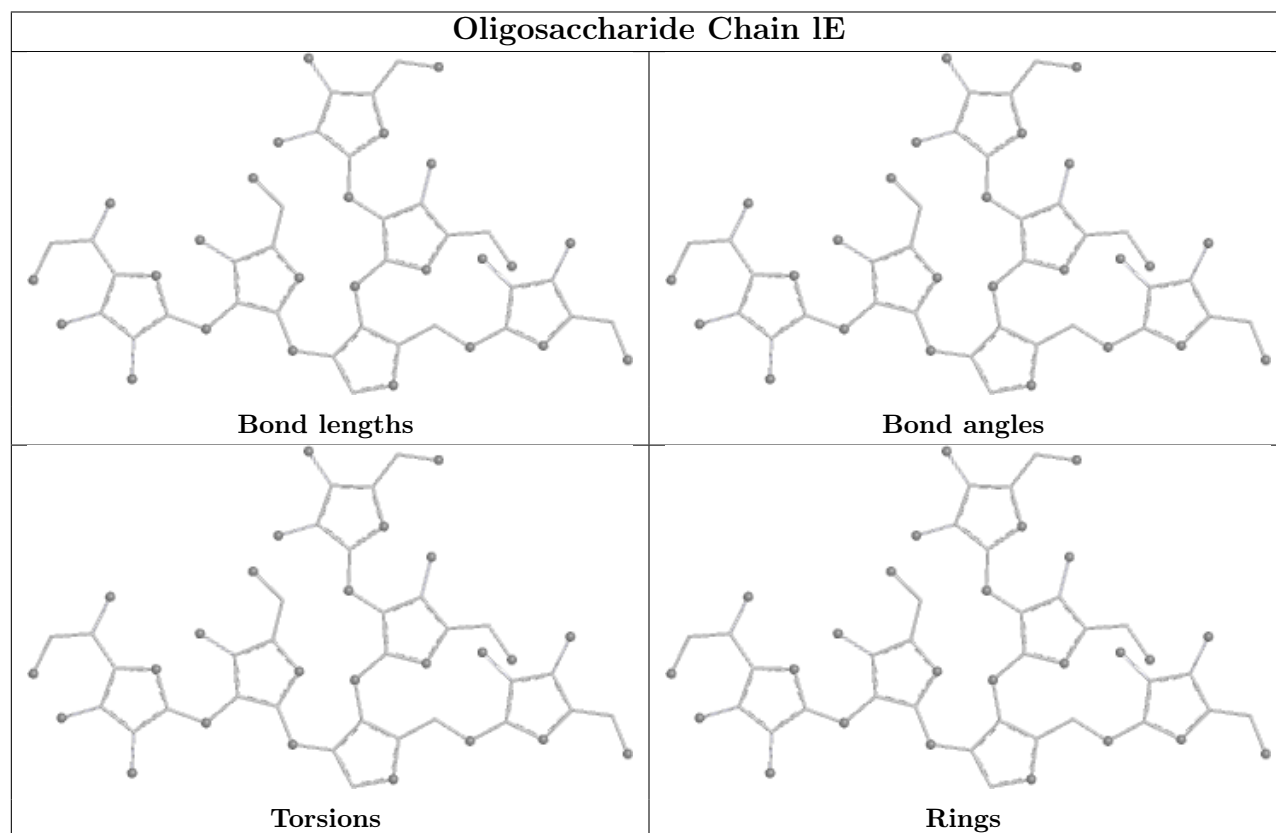
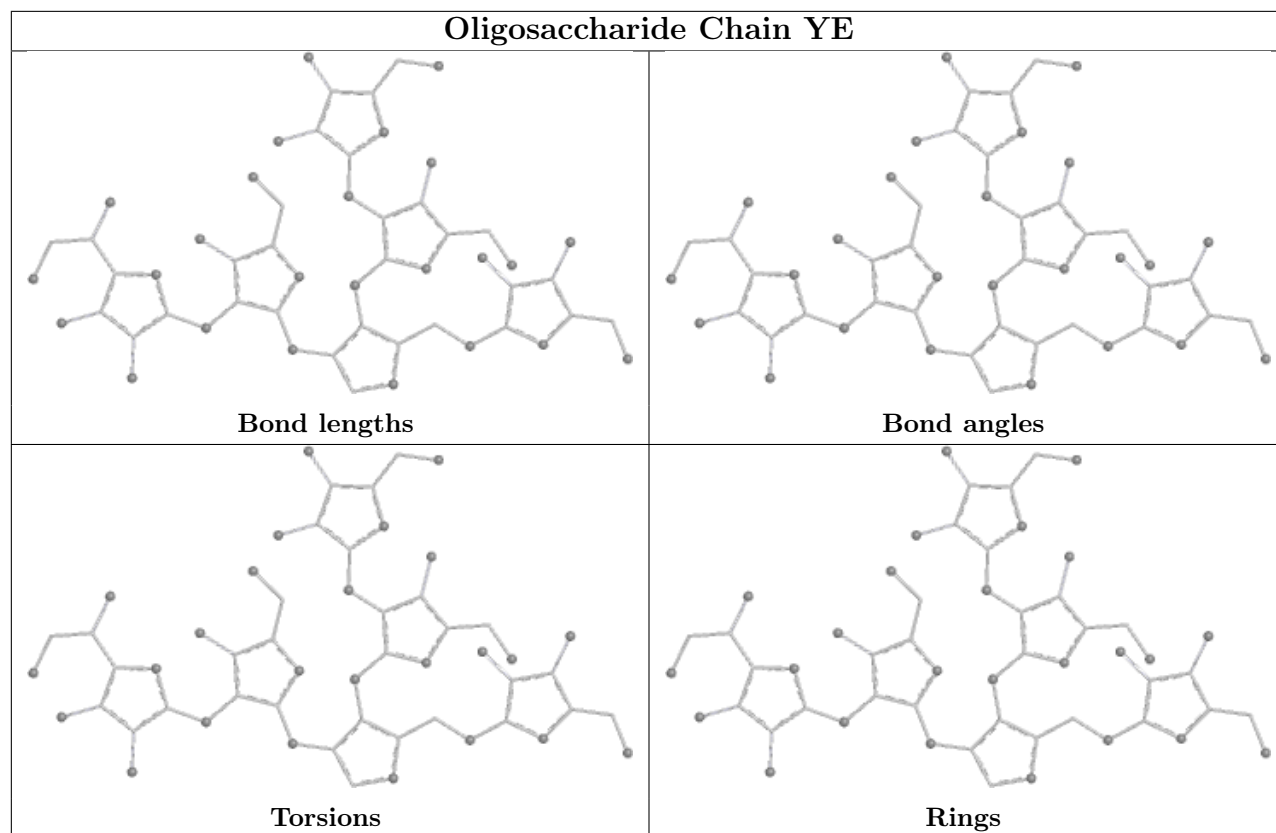
Oligosaccharide Chain GE**Oligosaccharide Chain QE**

Oligosaccharide Chain RE**Oligosaccharide Chain VE**

Oligosaccharide Chain dE**Oligosaccharide Chain eE**



Oligosaccharide Chain XE**Bond lengths****Bond angles****Torsions****Rings**



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	B	2015	1	11,11,12	1.71	3 (27%)	15,15,17	0.81	0
28	NAG	A	2017	1	14,14,15	0.32	0	17,19,21	0.64	0
26	AHR	F	2005	-	9,9,10	0.64	0	11,12,14	1.54	3 (27%)
27	GLA	C	2007	1	11,11,12	1.74	3 (27%)	15,15,17	0.82	0
26	AHR	F	2019	-	9,9,10	0.54	0	11,12,14	0.64	0
27	GLA	F	2014	1	11,11,12	1.73	3 (27%)	15,15,17	0.81	0
27	GLA	F	2017	1	11,11,12	1.69	3 (27%)	15,15,17	1.02	1 (6%)
26	AHR	A	2002	-	9,9,10	0.83	1 (11%)	11,12,14	1.36	2 (18%)
27	GLA	A	2011	1	11,11,12	1.74	3 (27%)	15,15,17	0.90	1 (6%)
27	GLA	B	2013	1	11,11,12	1.68	3 (27%)	15,15,17	0.90	0
27	GLA	A	2010	1	11,11,12	1.68	3 (27%)	15,15,17	0.87	1 (6%)
27	GLA	F	2018	1	11,11,12	1.72	3 (27%)	15,15,17	0.61	0
27	GLA	A	2007	1	11,11,12	1.71	3 (27%)	15,15,17	0.62	0
27	GLA	A	2016	1	11,11,12	1.71	3 (27%)	15,15,17	0.95	1 (6%)
27	GLA	E	2004	1	11,11,12	1.83	3 (27%)	15,15,17	1.73	4 (26%)
26	AHR	A	2019	-	9,9,10	0.54	0	11,12,14	0.81	0
27	GLA	E	2010	1	11,11,12	1.64	2 (18%)	15,15,17	1.26	1 (6%)
27	GLA	D	2006	1	11,11,12	1.65	3 (27%)	15,15,17	0.95	1 (6%)
28	NAG	C	2009	1	14,14,15	0.37	0	17,19,21	0.73	0
27	GLA	B	2010	1	11,11,12	1.72	3 (27%)	15,15,17	0.77	0
27	GLA	C	2006	1	11,11,12	1.65	3 (27%)	15,15,17	0.78	0
27	GLA	D	2005	1	11,11,12	1.73	3 (27%)	15,15,17	0.87	0
26	AHR	B	2002	-	9,9,10	0.53	0	11,12,14	1.11	1 (9%)
26	AHR	A	2018	-	9,9,10	0.54	0	11,12,14	1.04	1 (9%)
28	NAG	D	2010	1	14,14,15	0.31	0	17,19,21	0.71	0
26	AHR	F	2004	-	9,9,10	0.64	0	11,12,14	1.56	3 (27%)
27	GLA	F	2016	1	11,11,12	1.65	2 (18%)	15,15,17	0.86	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	GLA	A	2004	1	11,11,12	1.83	3 (27%)	15,15,17	1.63	4 (26%)
27	GLA	B	2012	1	11,11,12	1.75	3 (27%)	15,15,17	0.70	0
27	GLA	E	2014	1	11,11,12	1.69	3 (27%)	15,15,17	0.91	0
27	GLA	D	2008	1	11,11,12	1.72	3 (27%)	15,15,17	0.71	0
27	GLA	F	2012	1	11,11,12	1.69	3 (27%)	15,15,17	0.84	0
27	GLA	C	2008	1	11,11,12	1.74	3 (27%)	15,15,17	0.94	0
26	AHR	B	2020	-	9,9,10	0.88	0	11,12,14	0.92	1 (9%)
26	AHR	D	2003	-	9,9,10	0.82	0	11,12,14	1.70	3 (27%)
27	GLA	B	2008	1	11,11,12	1.70	3 (27%)	15,15,17	0.76	0
27	GLA	F	2013	1	11,11,12	1.71	3 (27%)	15,15,17	0.90	0
28	NAG	B	2019	1	14,14,15	0.36	0	17,19,21	0.97	1 (5%)
27	GLA	E	2009	1	11,11,12	1.68	3 (27%)	15,15,17	1.04	1 (6%)
27	GLA	D	2009	1	11,11,12	1.76	3 (27%)	15,15,17	0.78	0
27	GLA	F	2011	1	11,11,12	1.72	3 (27%)	15,15,17	0.82	0
27	GLA	F	2008	1	11,11,12	1.70	3 (27%)	15,15,17	0.96	1 (6%)
27	GLA	A	2006	1	11,11,12	1.75	3 (27%)	15,15,17	0.95	1 (6%)
27	GLA	D	2007	1	11,11,12	1.67	3 (27%)	15,15,17	0.87	0
26	AHR	D	2004	-	9,9,10	0.65	0	11,12,14	1.55	3 (27%)
27	GLA	B	2009	-	11,11,12	1.72	3 (27%)	15,15,17	1.45	1 (6%)
27	GLA	F	2009	1	11,11,12	1.63	2 (18%)	15,15,17	0.86	1 (6%)
27	GLA	C	2004	1	11,11,12	1.72	3 (27%)	15,15,17	0.74	0
28	NAG	B	2018	1	14,14,15	0.35	0	17,19,21	0.80	0
26	AHR	B	2004	-	9,9,10	0.77	0	11,12,14	1.78	4 (36%)
27	GLA	B	2006	1	11,11,12	1.72	3 (27%)	15,15,17	0.71	0
27	GLA	E	2015	1	11,11,12	1.65	2 (18%)	15,15,17	1.17	1 (6%)
27	GLA	F	2006	1	11,11,12	1.77	3 (27%)	15,15,17	1.81	4 (26%)
27	GLA	A	2012	1	11,11,12	1.70	3 (27%)	15,15,17	0.84	0
27	GLA	B	2014	1	11,11,12	1.62	2 (18%)	15,15,17	0.83	1 (6%)
27	GLA	F	2015	1	11,11,12	1.72	3 (27%)	15,15,17	0.66	0
27	GLA	B	2017	1	11,11,12	1.61	2 (18%)	15,15,17	1.33	1 (6%)
27	GLA	E	2005	1	11,11,12	1.71	3 (27%)	15,15,17	0.90	0
27	GLA	B	2016	1	11,11,12	1.79	3 (27%)	15,15,17	0.78	0
27	GLA	A	2009	1	11,11,12	1.67	3 (27%)	15,15,17	1.03	1 (6%)
27	GLA	C	2005	1	11,11,12	1.64	3 (27%)	15,15,17	0.87	1 (6%)
27	GLA	B	2007	1	11,11,12	1.75	3 (27%)	15,15,17	0.82	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	GLA	F	2010	-	11,11,12	1.74	3 (27%)	15,15,17	0.84	0
27	GLA	E	2011	1	11,11,12	1.69	3 (27%)	15,15,17	0.87	0
28	NAG	C	2010	1	14,14,15	0.32	0	17,19,21	0.91	1 (5%)
26	AHR	E	2003	-	9,9,10	0.64	0	11,12,14	1.54	3 (27%)
26	AHR	C	2001	-	9,9,10	0.53	0	11,12,14	1.61	1 (9%)
27	GLA	F	2007	1	11,11,12	1.64	3 (27%)	15,15,17	1.04	0
26	AHR	B	2003	-	9,9,10	0.90	0	11,12,14	1.88	4 (36%)
26	AHR	C	2003	-	9,9,10	0.79	0	11,12,14	1.72	4 (36%)
26	AHR	F	2003	-	9,9,10	0.55	0	11,12,14	1.59	1 (9%)
27	GLA	A	2015	1	11,11,12	1.75	3 (27%)	15,15,17	0.78	0
26	AHR	A	2003	-	9,9,10	0.75	1 (11%)	11,12,14	1.63	3 (27%)
26	AHR	D	2001	-	9,9,10	0.65	0	11,12,14	1.49	2 (18%)
27	GLA	B	2011	1	11,11,12	1.67	3 (27%)	15,15,17	0.98	1 (6%)
27	GLA	E	2006	1	11,11,12	1.73	3 (27%)	15,15,17	0.75	0
28	NAG	E	2017	1	14,14,15	0.33	0	17,19,21	0.93	1 (5%)
27	GLA	A	2005	1	11,11,12	1.66	3 (27%)	15,15,17	0.84	0
27	GLA	A	2013	1	11,11,12	1.72	3 (27%)	15,15,17	0.64	0
27	GLA	E	2016	1	11,11,12	1.79	3 (27%)	15,15,17	0.82	0
26	AHR	E	2002	-	9,9,10	0.78	1 (11%)	11,12,14	1.78	3 (27%)
27	GLA	E	2012	1	11,11,12	1.60	1 (9%)	15,15,17	1.17	1 (6%)
27	GLA	E	2013	1	11,11,12	1.76	3 (27%)	15,15,17	0.74	0
27	GLA	B	2005	1	11,11,12	1.82	3 (27%)	15,15,17	1.54	3 (20%)
27	GLA	A	2008	-	11,11,12	1.72	2 (18%)	15,15,17	1.33	1 (6%)
27	GLA	A	2014	1	11,11,12	1.73	3 (27%)	15,15,17	0.86	0
27	GLA	E	2007	1	11,11,12	1.76	3 (27%)	15,15,17	1.35	3 (20%)
26	AHR	F	2001	-	9,9,10	0.65	0	11,12,14	1.53	3 (27%)
27	GLA	E	2008	-	11,11,12	1.70	3 (27%)	15,15,17	0.99	1 (6%)

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
27	GLA	B	2015	1	-	2/2/19/22	0/1/1/1
28	NAG	A	2017	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	AHR	F	2005	-	-	2/2/15/18	0/1/1/1
27	GLA	C	2007	1	-	2/2/19/22	0/1/1/1
26	AHR	F	2019	-	-	0/2/15/18	0/1/1/1
27	GLA	F	2014	1	-	2/2/19/22	0/1/1/1
27	GLA	F	2017	1	-	2/2/19/22	0/1/1/1
26	AHR	A	2002	-	-	2/2/15/18	0/1/1/1
27	GLA	A	2011	1	-	2/2/19/22	0/1/1/1
27	GLA	B	2013	1	-	1/2/19/22	0/1/1/1
27	GLA	A	2010	1	-	2/2/19/22	0/1/1/1
27	GLA	F	2018	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	A	2016	1	-	1/2/19/22	0/1/1/1
27	GLA	E	2004	1	-	1/2/19/22	0/1/1/1
26	AHR	A	2019	-	-	0/2/15/18	0/1/1/1
27	GLA	E	2010	1	-	1/2/19/22	0/1/1/1
27	GLA	D	2006	1	-	0/2/19/22	0/1/1/1
28	NAG	C	2009	1	-	4/6/23/26	0/1/1/1
27	GLA	B	2010	1	-	2/2/19/22	0/1/1/1
27	GLA	C	2006	1	-	0/2/19/22	0/1/1/1
27	GLA	D	2005	1	-	2/2/19/22	0/1/1/1
26	AHR	A	2018	-	-	0/2/15/18	0/1/1/1
26	AHR	B	2002	-	-	0/2/15/18	0/1/1/1
28	NAG	D	2010	1	-	0/6/23/26	0/1/1/1
26	AHR	F	2004	-	-	2/2/15/18	0/1/1/1
27	GLA	F	2016	1	-	2/2/19/22	0/1/1/1
27	GLA	A	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	E	2014	1	-	2/2/19/22	0/1/1/1
27	GLA	D	2008	1	-	2/2/19/22	0/1/1/1
27	GLA	F	2012	1	-	2/2/19/22	0/1/1/1
27	GLA	C	2008	1	-	2/2/19/22	0/1/1/1
26	AHR	B	2020	-	-	1/2/15/18	0/1/1/1
26	AHR	D	2003	-	-	2/2/15/18	0/1/1/1
27	GLA	B	2008	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
28	NAG	B	2019	1	-	2/6/23/26	0/1/1/1
27	GLA	E	2009	1	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	GLA	D	2009	1	-	2/2/19/22	0/1/1/1
27	GLA	F	2011	1	-	1/2/19/22	0/1/1/1
27	GLA	F	2008	1	-	1/2/19/22	0/1/1/1
27	GLA	A	2006	1	-	1/2/19/22	0/1/1/1
27	GLA	D	2007	1	-	2/2/19/22	0/1/1/1
26	AHR	D	2004	-	-	2/2/15/18	0/1/1/1
27	GLA	B	2009	-	-	2/2/19/22	0/1/1/1
27	GLA	F	2009	1	1/1/4/5	2/2/19/22	0/1/1/1
27	GLA	C	2004	1	-	2/2/19/22	0/1/1/1
28	NAG	B	2018	1	-	4/6/23/26	0/1/1/1
26	AHR	B	2004	-	-	2/2/15/18	0/1/1/1
27	GLA	B	2006	1	-	0/2/19/22	0/1/1/1
27	GLA	E	2015	1	-	0/2/19/22	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	2014	1	1/1/4/5	0/2/19/22	0/1/1/1
27	GLA	F	2015	1	-	0/2/19/22	0/1/1/1
27	GLA	B	2017	1	-	2/2/19/22	0/1/1/1
27	GLA	E	2005	1	-	2/2/19/22	0/1/1/1
27	GLA	B	2016	1	-	2/2/19/22	0/1/1/1
27	GLA	A	2009	1	-	1/2/19/22	0/1/1/1
27	GLA	C	2005	1	-	2/2/19/22	0/1/1/1
27	GLA	B	2007	1	-	2/2/19/22	0/1/1/1
27	GLA	F	2010	-	-	2/2/19/22	0/1/1/1
27	GLA	E	2011	1	-	2/2/19/22	0/1/1/1
28	NAG	C	2010	1	-	4/6/23/26	0/1/1/1
26	AHR	E	2003	-	-	2/2/15/18	0/1/1/1
26	AHR	C	2001	-	-	2/2/15/18	0/1/1/1
27	GLA	F	2007	1	-	2/2/19/22	0/1/1/1
26	AHR	B	2003	-	-	2/2/15/18	0/1/1/1
26	AHR	C	2003	-	-	2/2/15/18	0/1/1/1
26	AHR	F	2003	-	-	1/2/15/18	0/1/1/1
27	GLA	A	2015	1	-	2/2/19/22	0/1/1/1
26	AHR	A	2003	-	-	2/2/15/18	0/1/1/1
26	AHR	D	2001	-	-	1/2/15/18	0/1/1/1
27	GLA	B	2011	1	-	1/2/19/22	0/1/1/1

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

The worst 5 of 180 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	2004	GLA	O5-C1	4.66	1.51	1.43
27	B	2005	GLA	O5-C1	4.63	1.51	1.43
27	B	2009	GLA	O5-C1	4.55	1.51	1.43
27	E	2004	GLA	O5-C1	4.51	1.51	1.43
27	A	2008	GLA	O5-C1	4.51	1.51	1.43

The worst 5 of 86 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	F	2003	AHR	O4-C1-C2	-4.29	98.37	105.76
26	C	2001	AHR	O4-C1-C2	-4.23	98.47	105.76
27	B	2009	GLA	C1-C2-C3	4.20	115.76	109.64
27	A	2008	GLA	C1-C2-C3	3.74	115.10	109.64
26	F	2004	AHR	O4-C1-C2	-3.72	99.36	105.76

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

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Mol	Chain	Res	Type	Atom
27	E	2007	GLA	C1
27	F	2009	GLA	C1

5 of 136 torsion outliers are listed below:

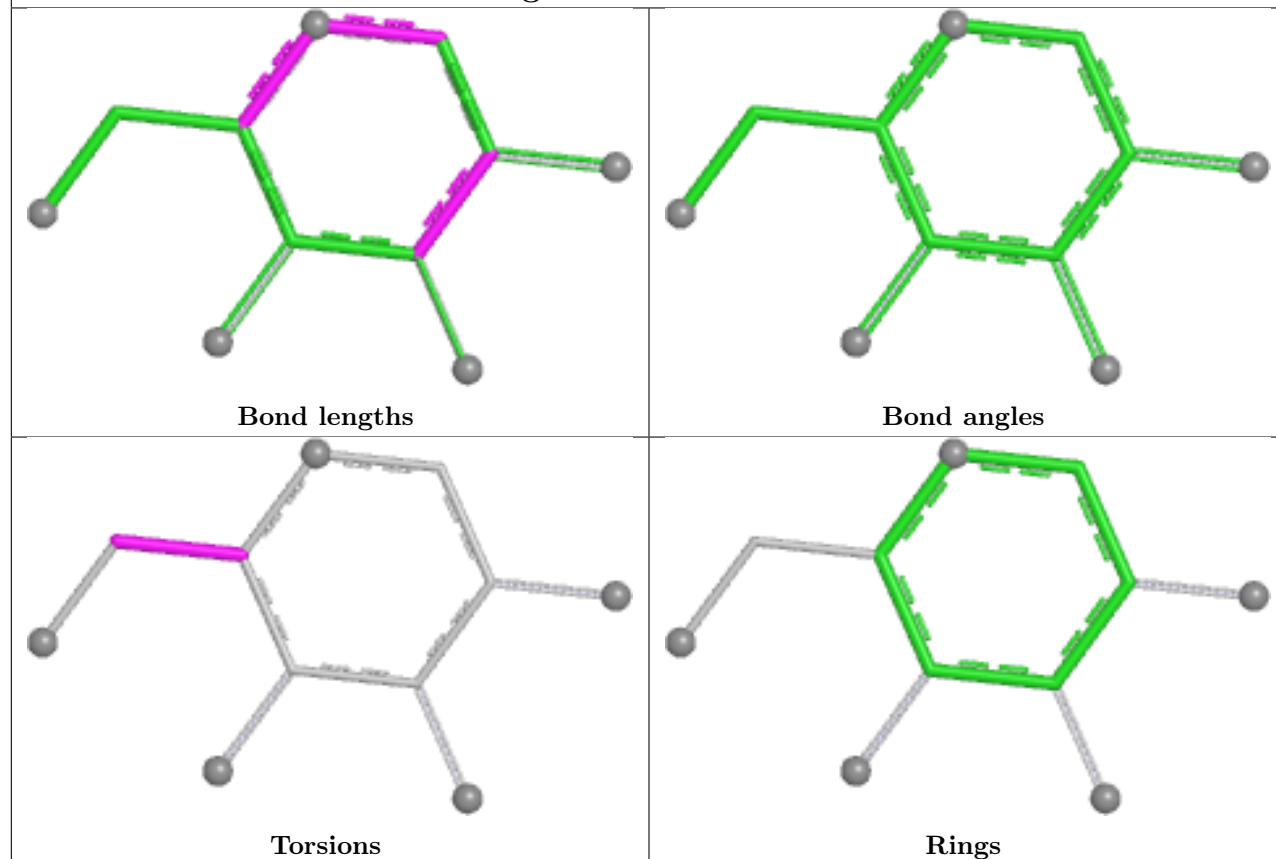
Mol	Chain	Res	Type	Atoms
28	B	2018	NAG	C3-C2-N2-C7
28	B	2018	NAG	C8-C7-N2-C2
28	B	2018	NAG	O7-C7-N2-C2
28	C	2009	NAG	C3-C2-N2-C7
28	C	2009	NAG	C8-C7-N2-C2

There are no ring outliers.

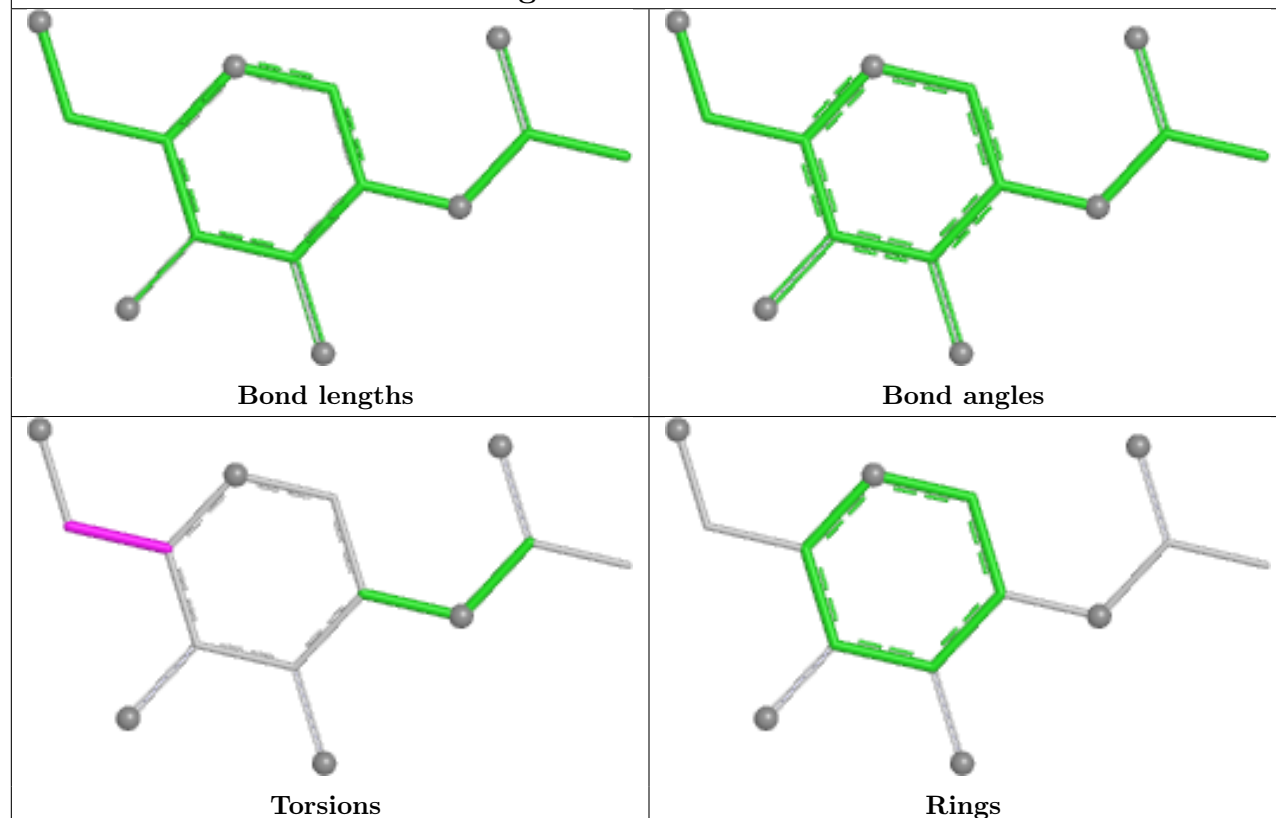
No monomer is involved in short contacts.

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.

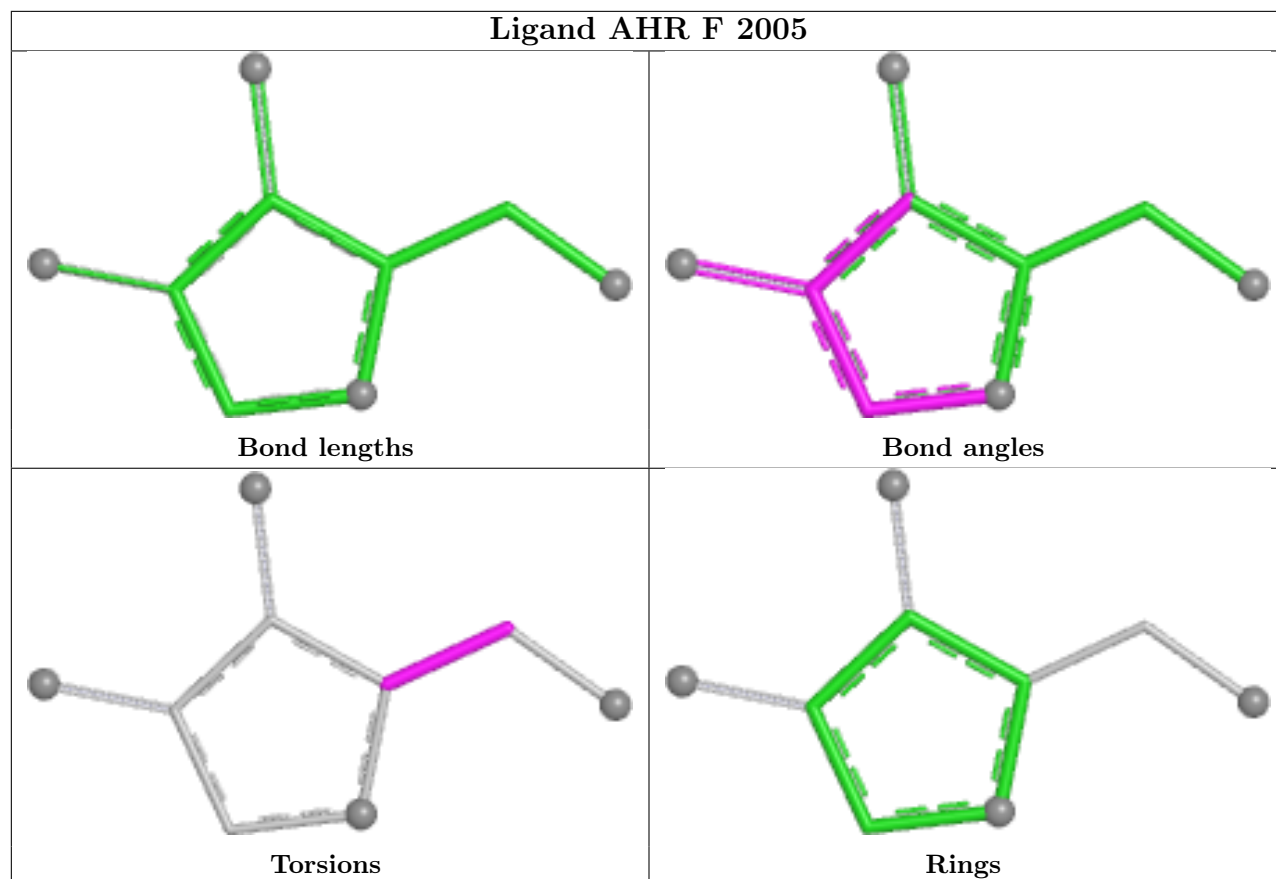
Ligand GLA B 2015



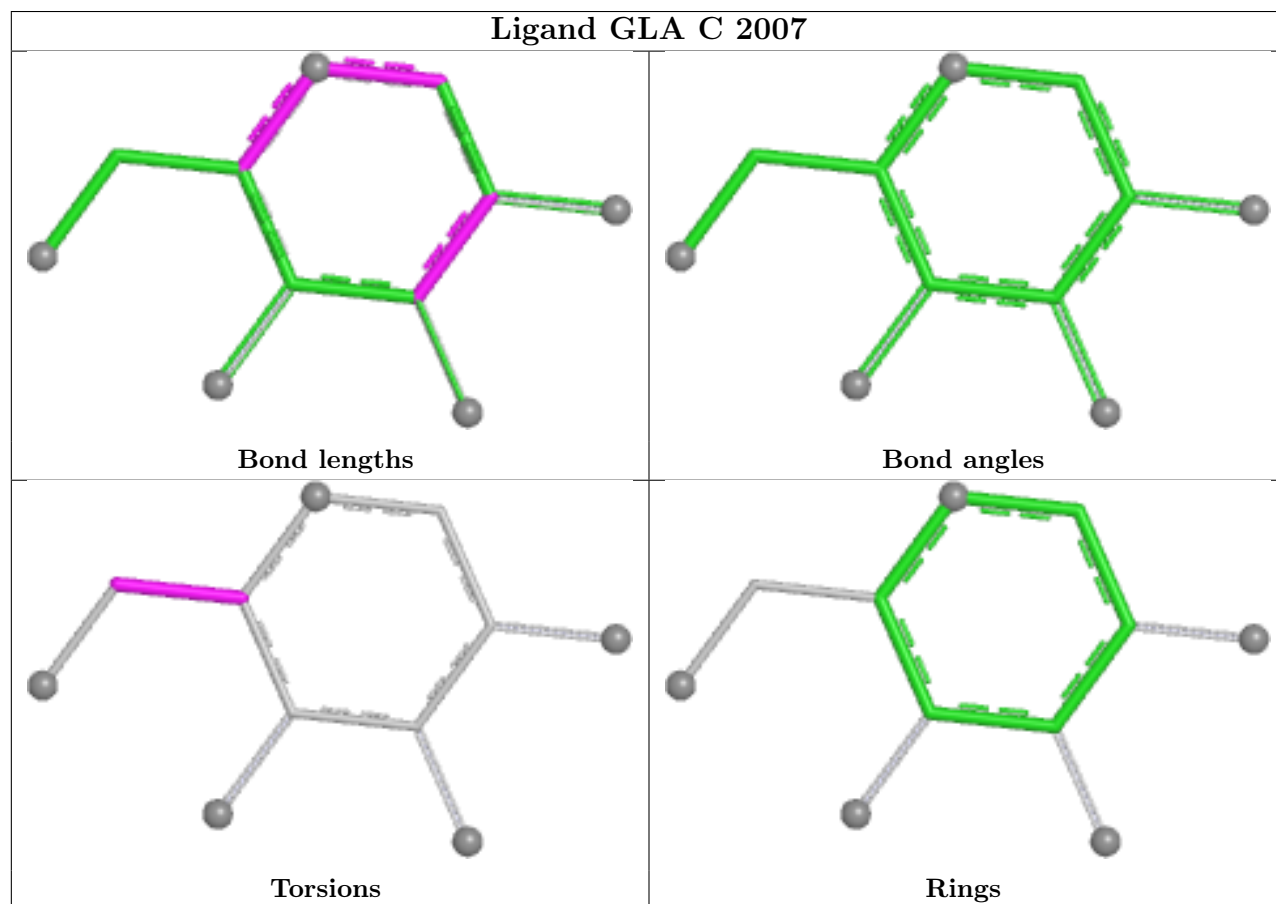
Ligand NAG A 2017



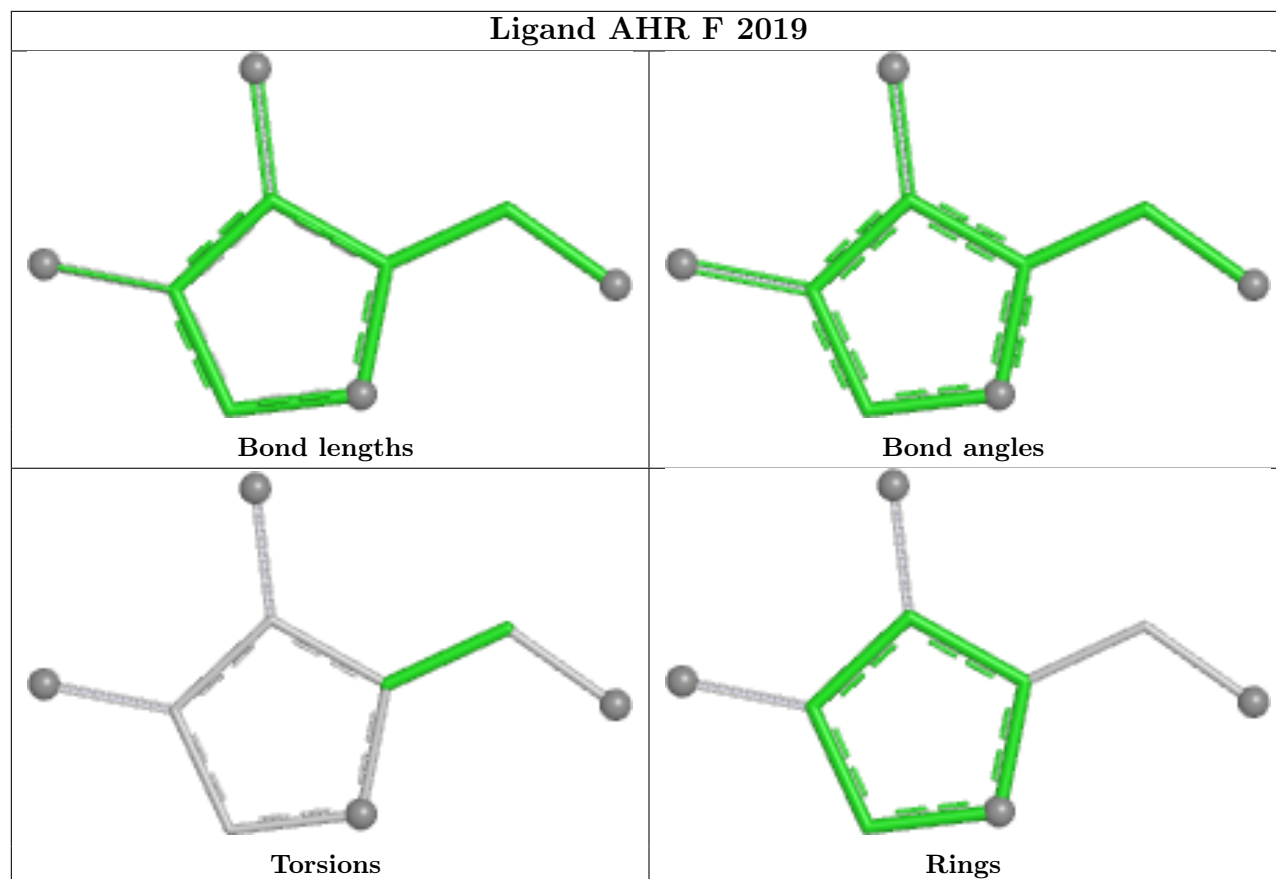
Ligand AHR F 2005



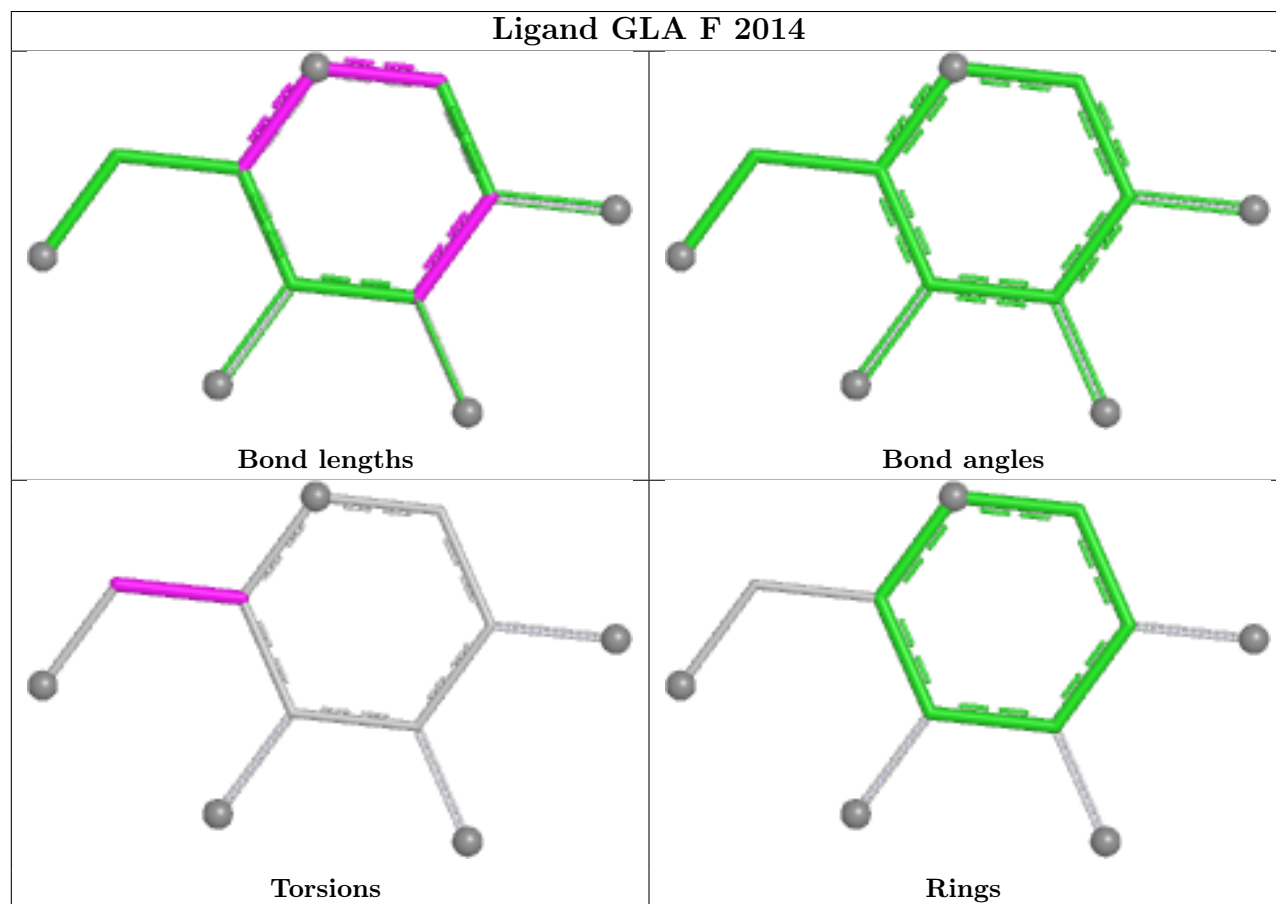
Ligand GLA C 2007



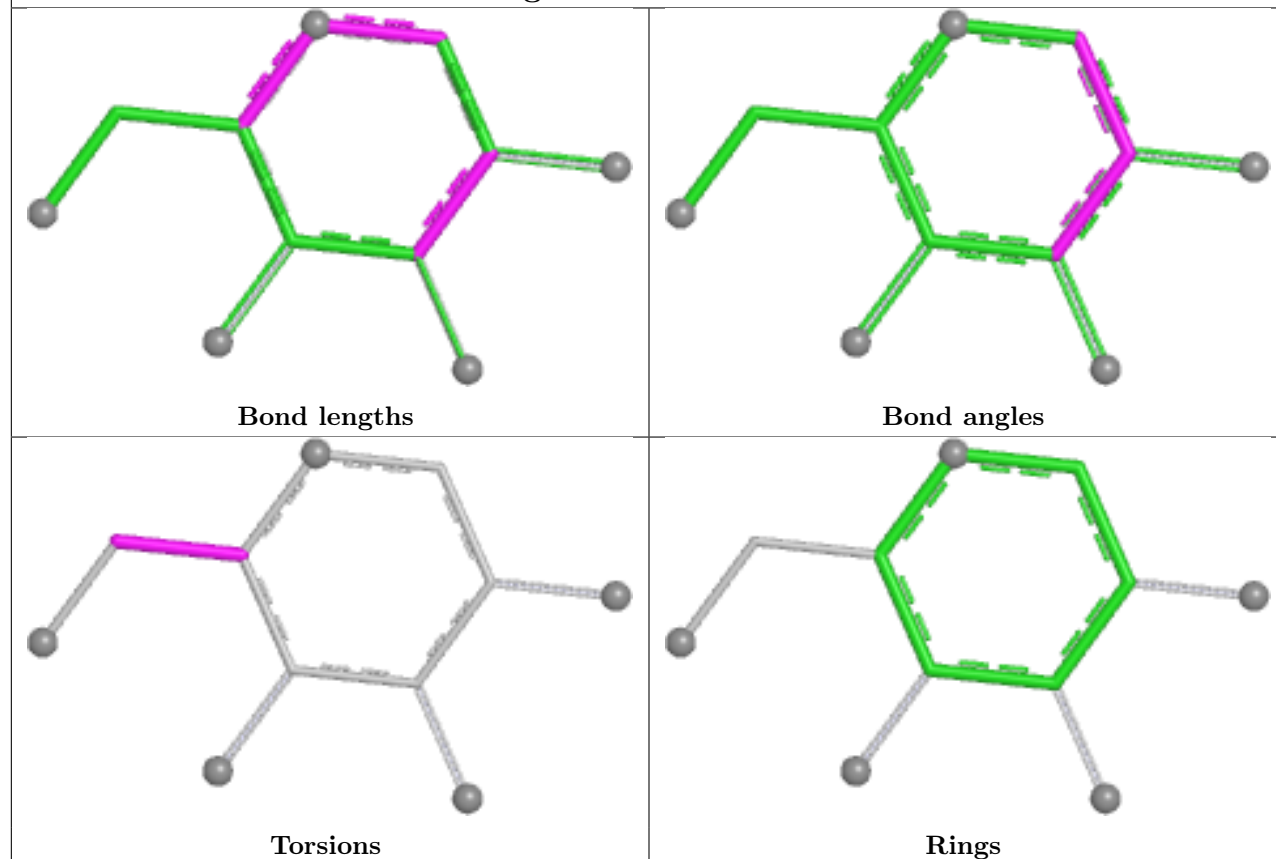
Ligand AHR F 2019



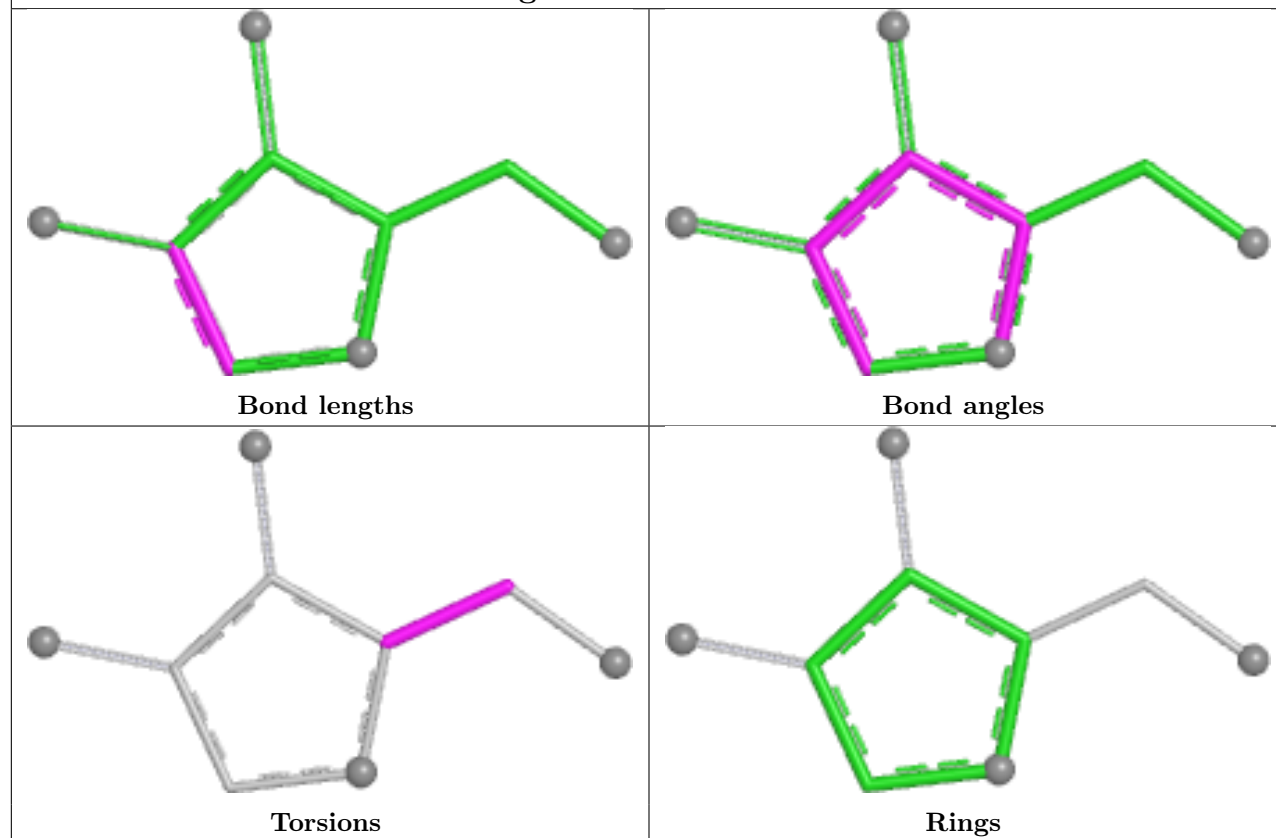
Ligand GLA F 2014

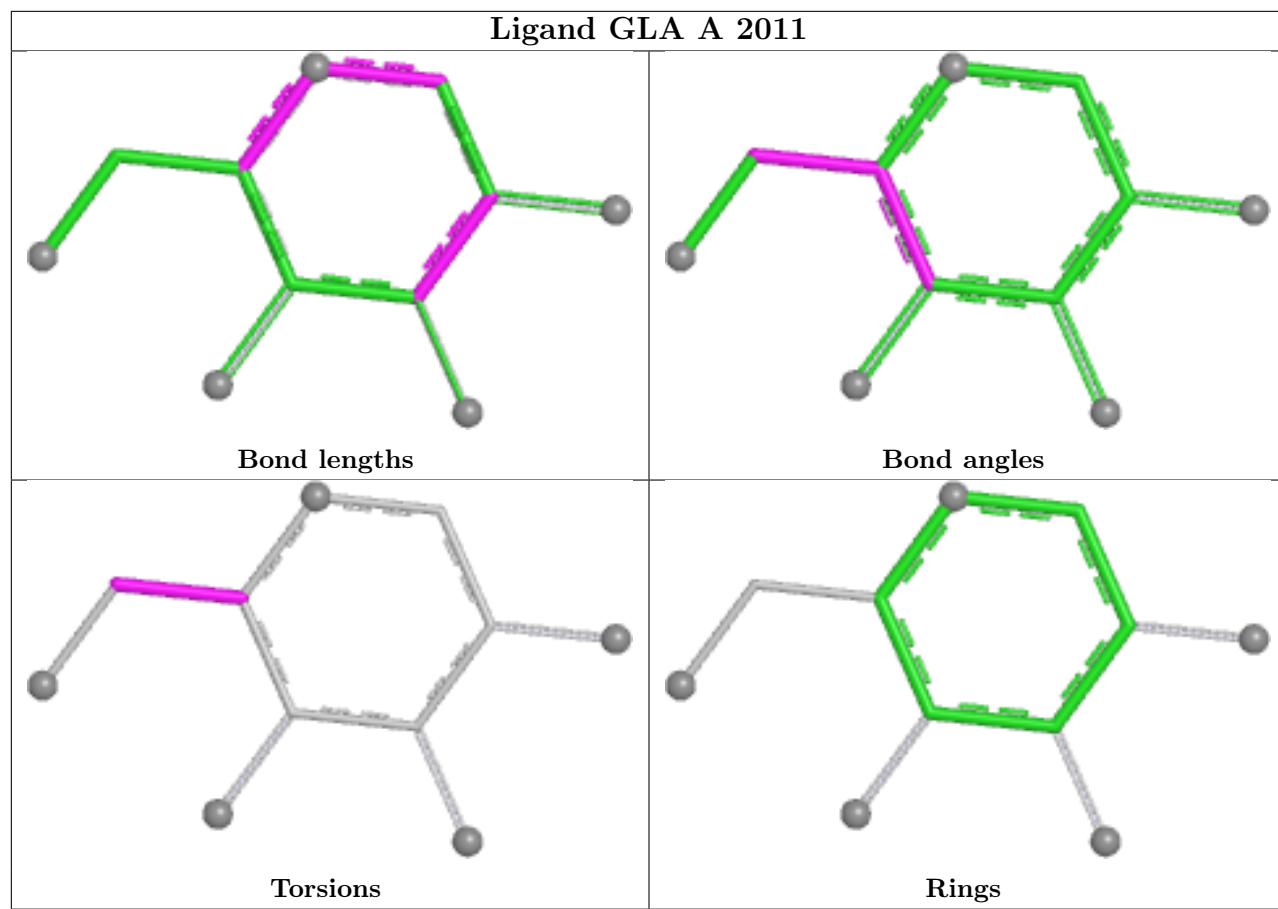


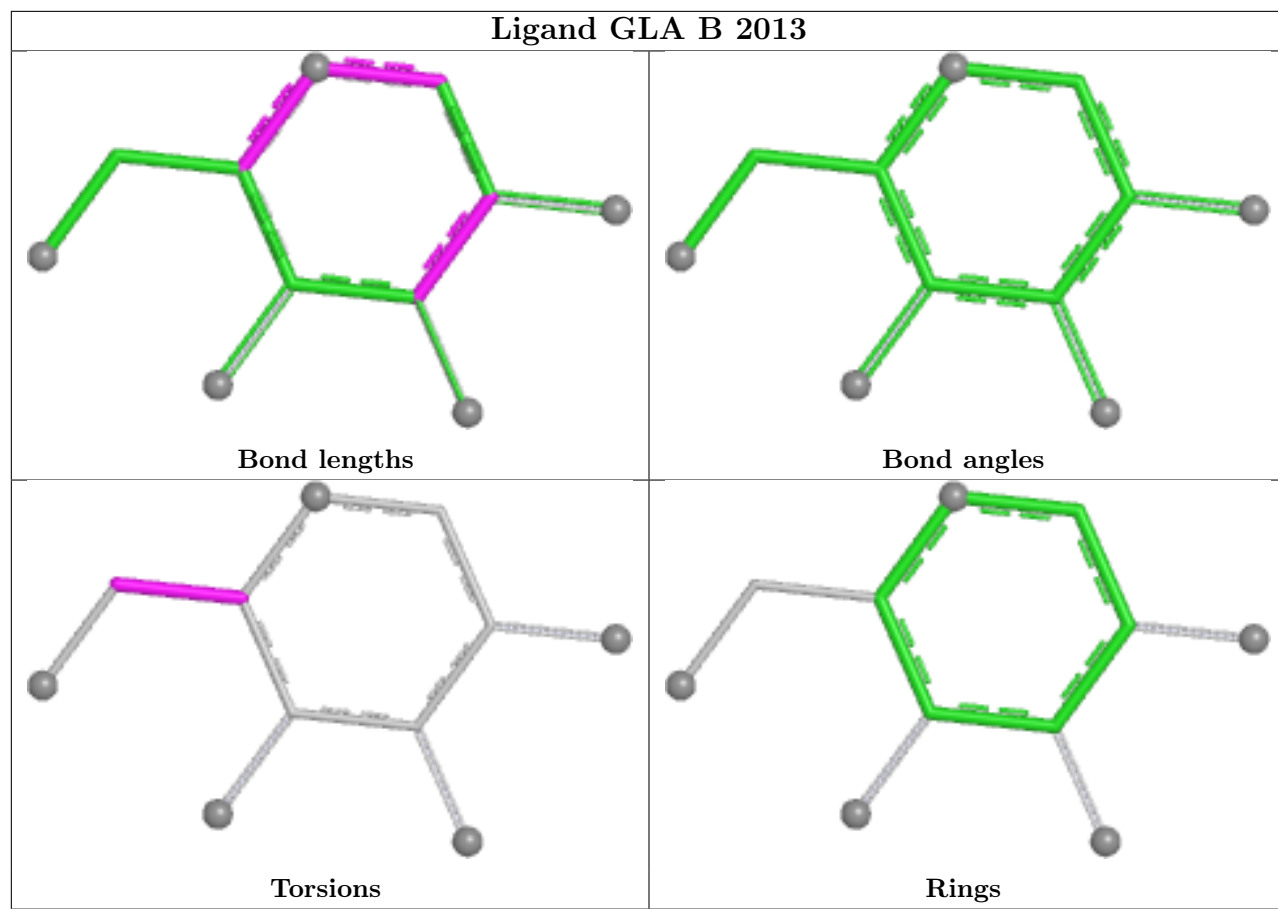
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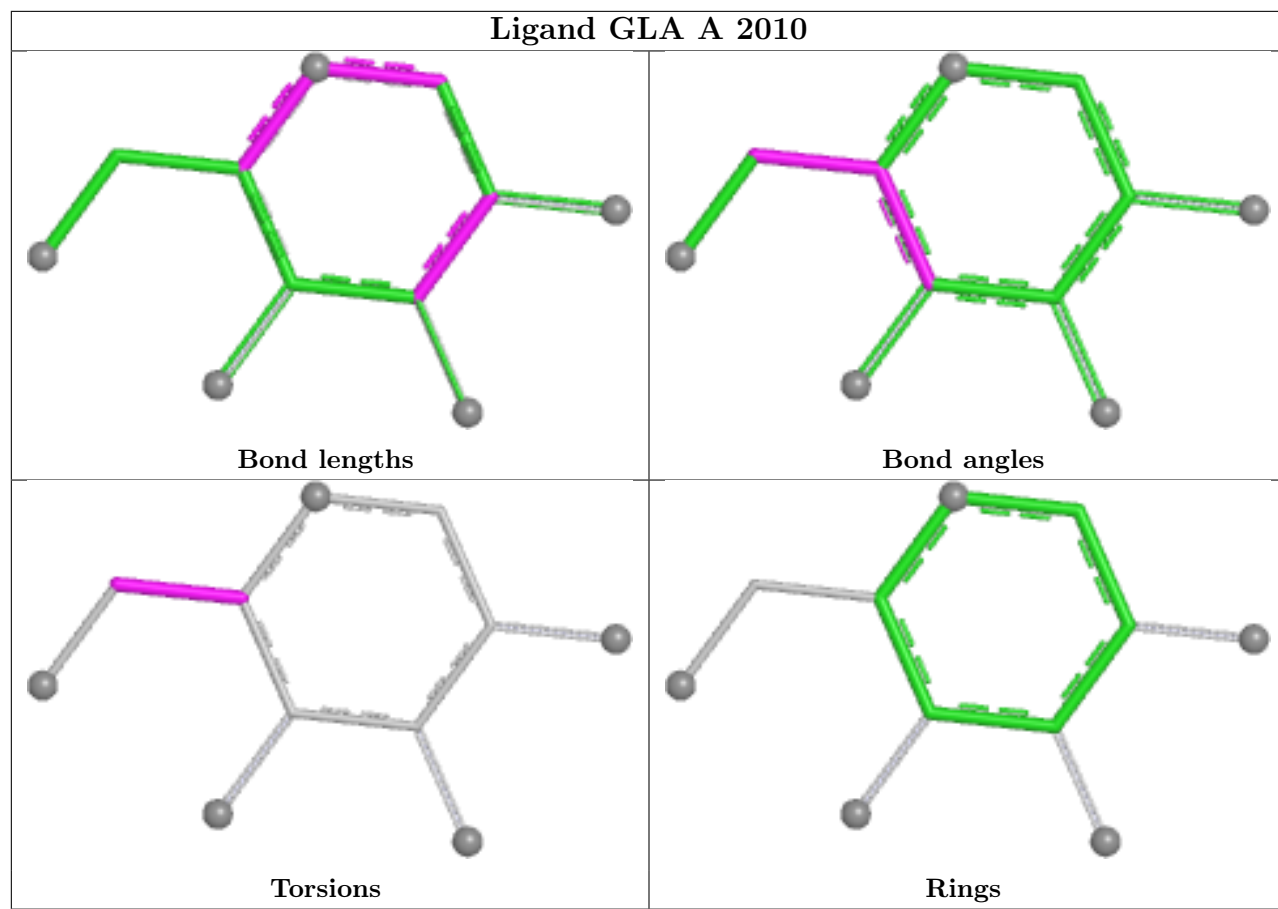


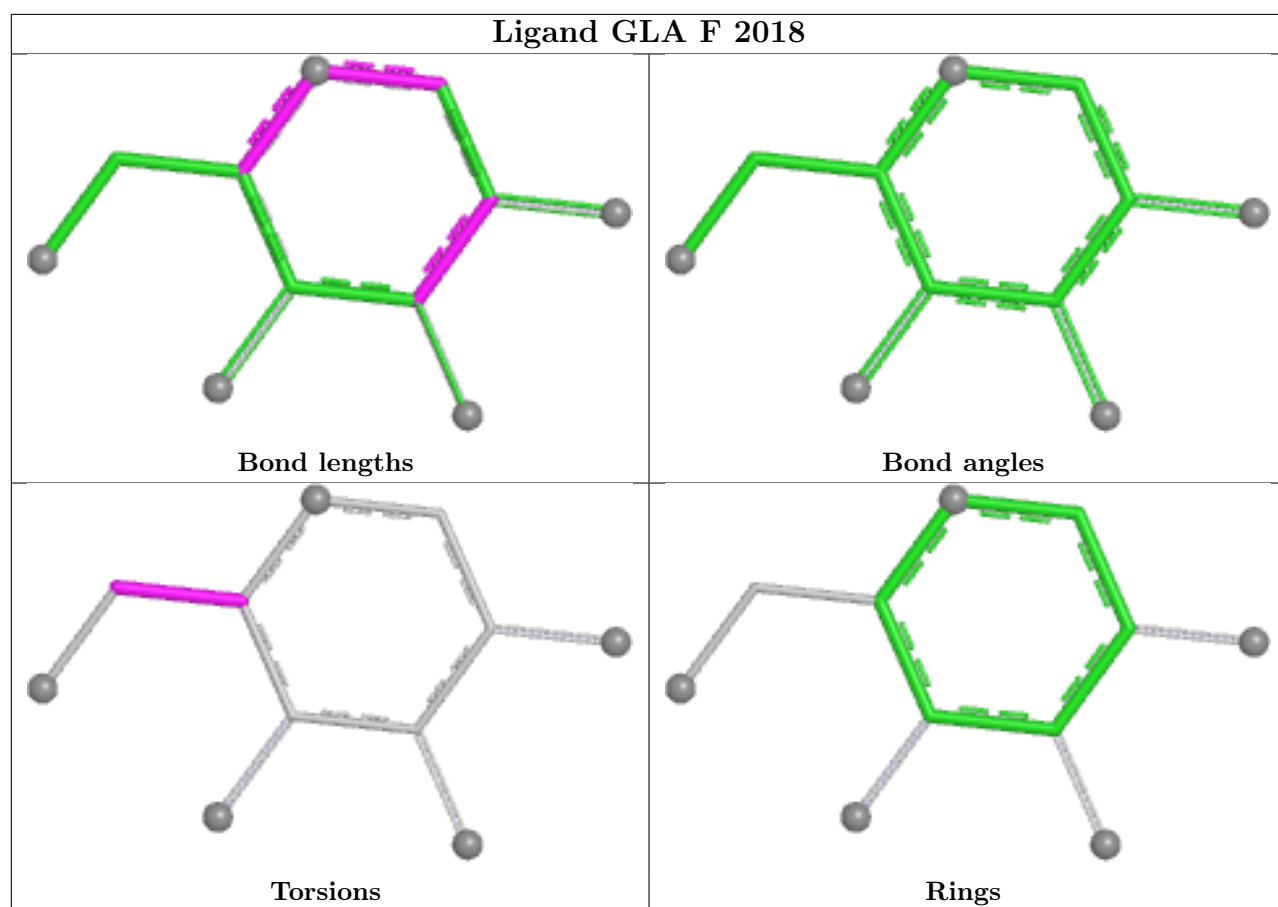
Ligand AHR A 2002

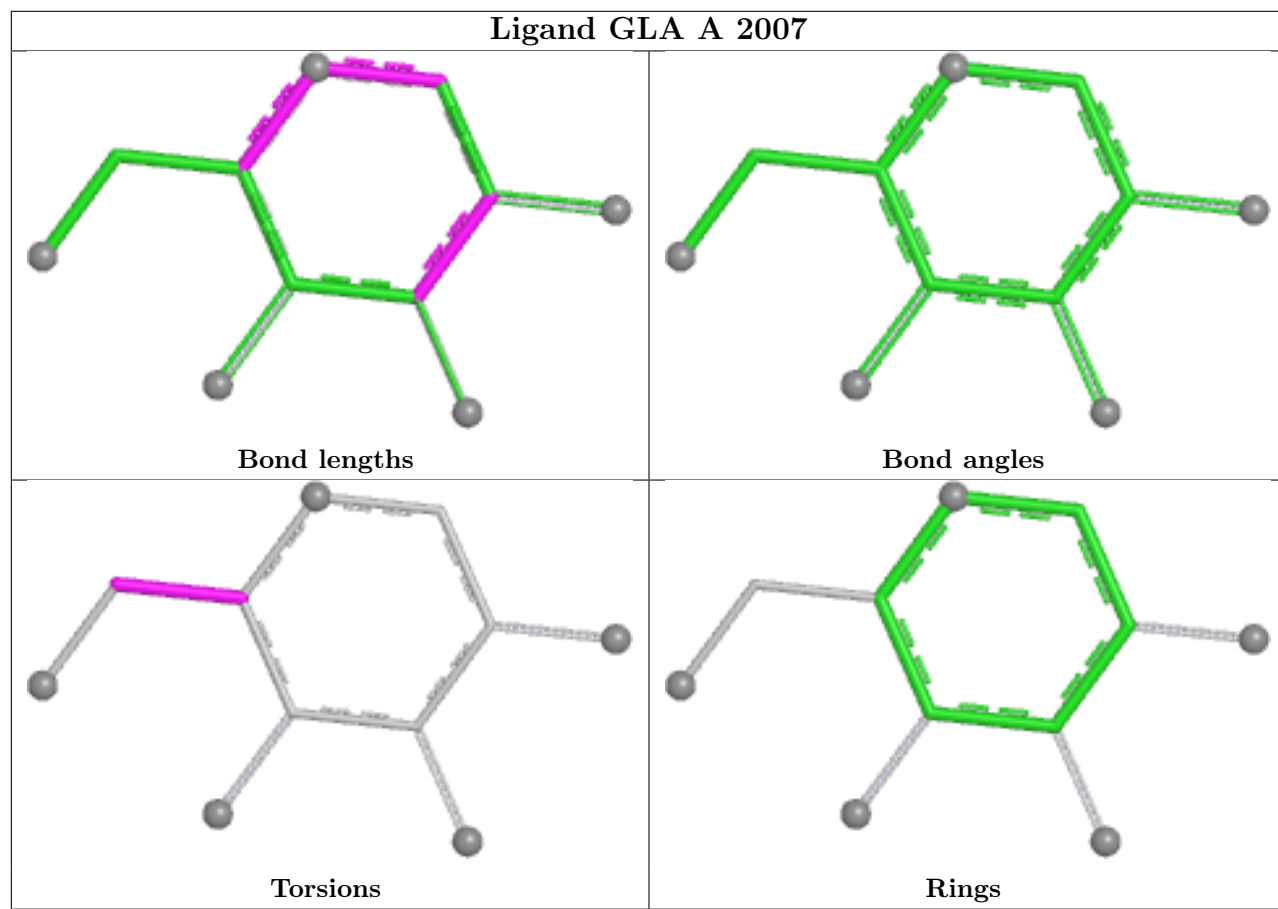


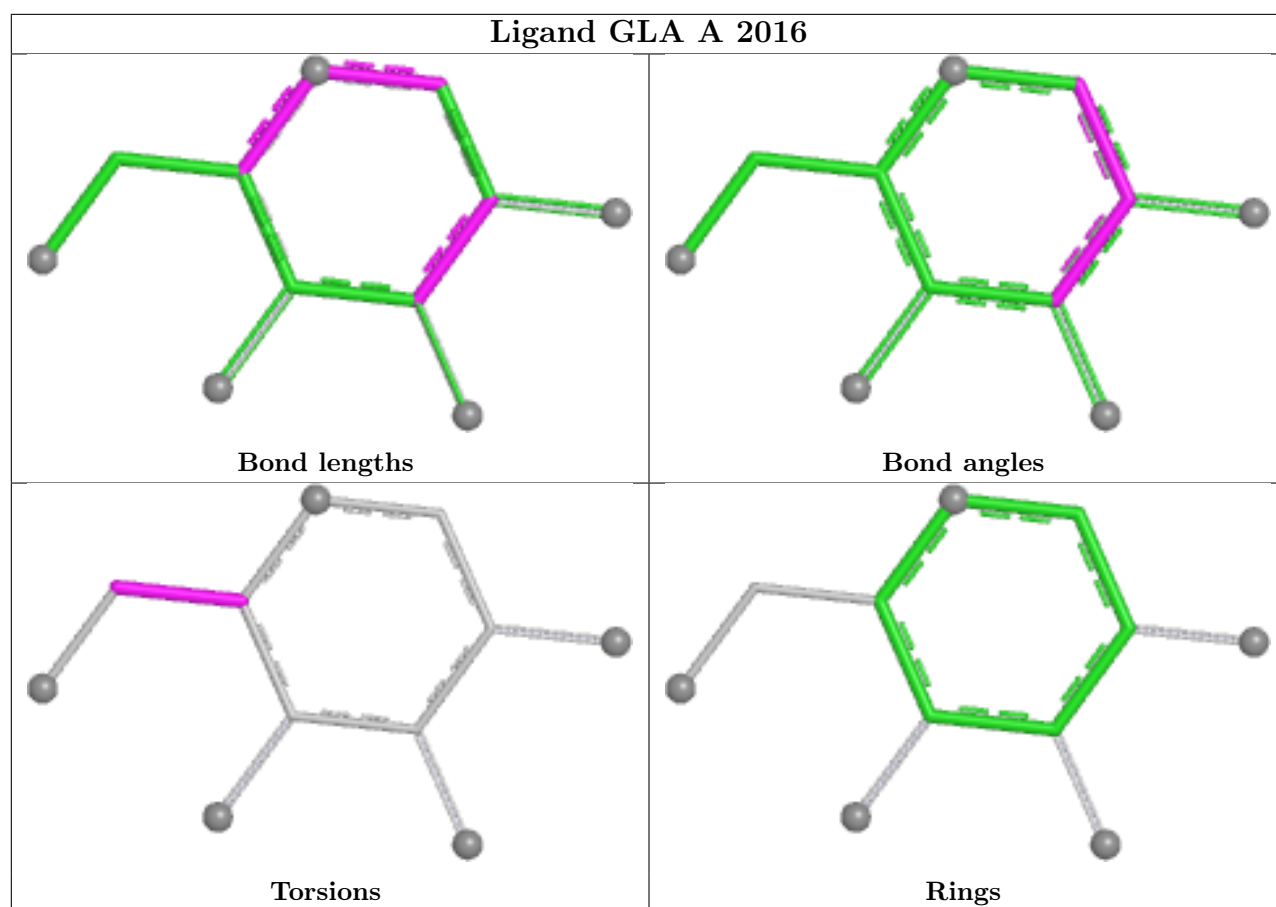




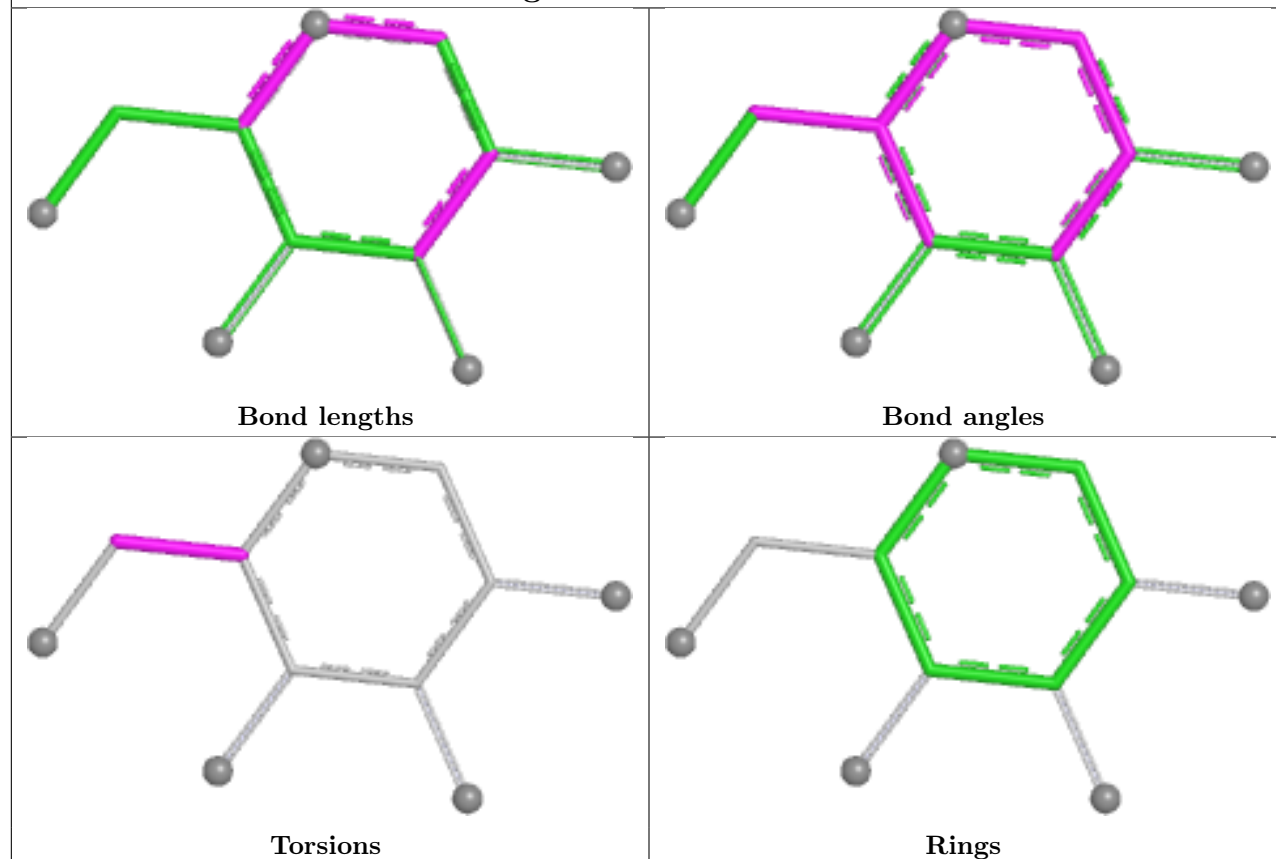




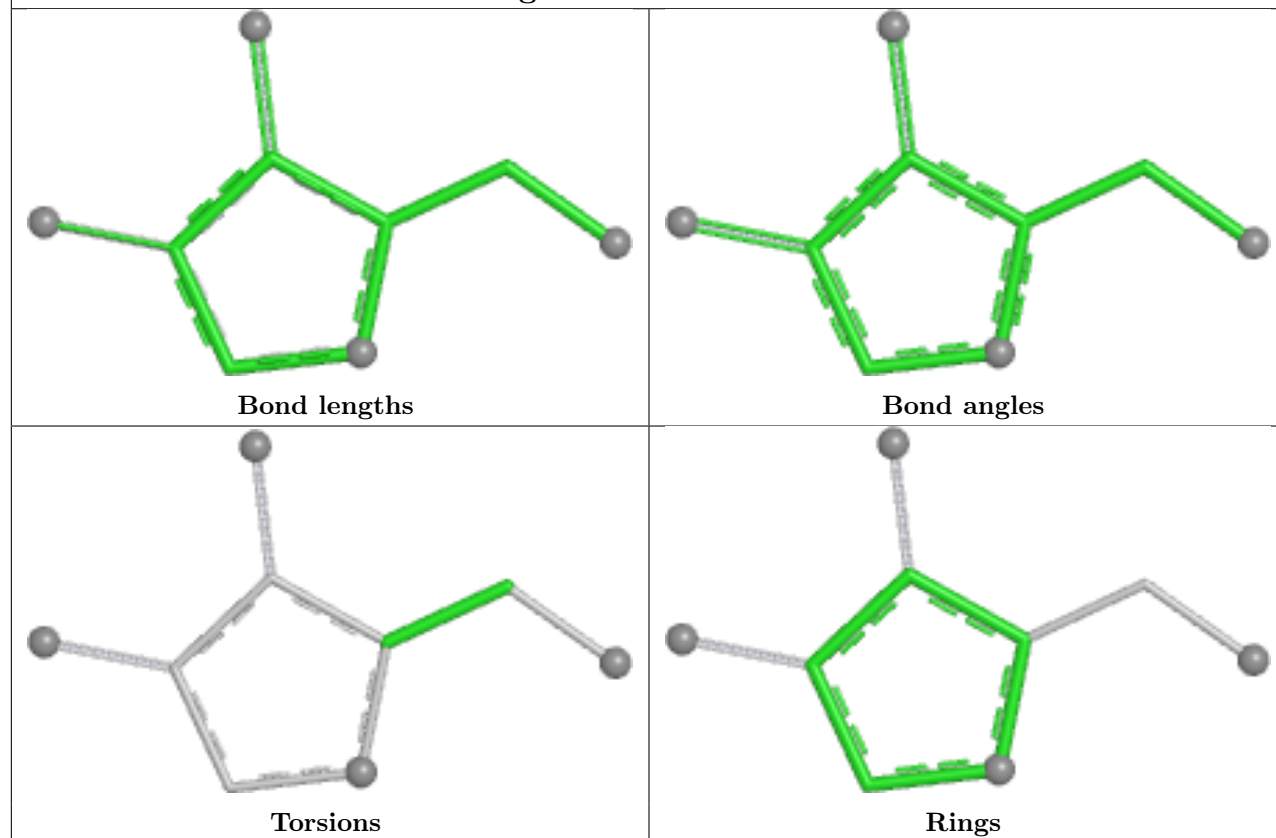


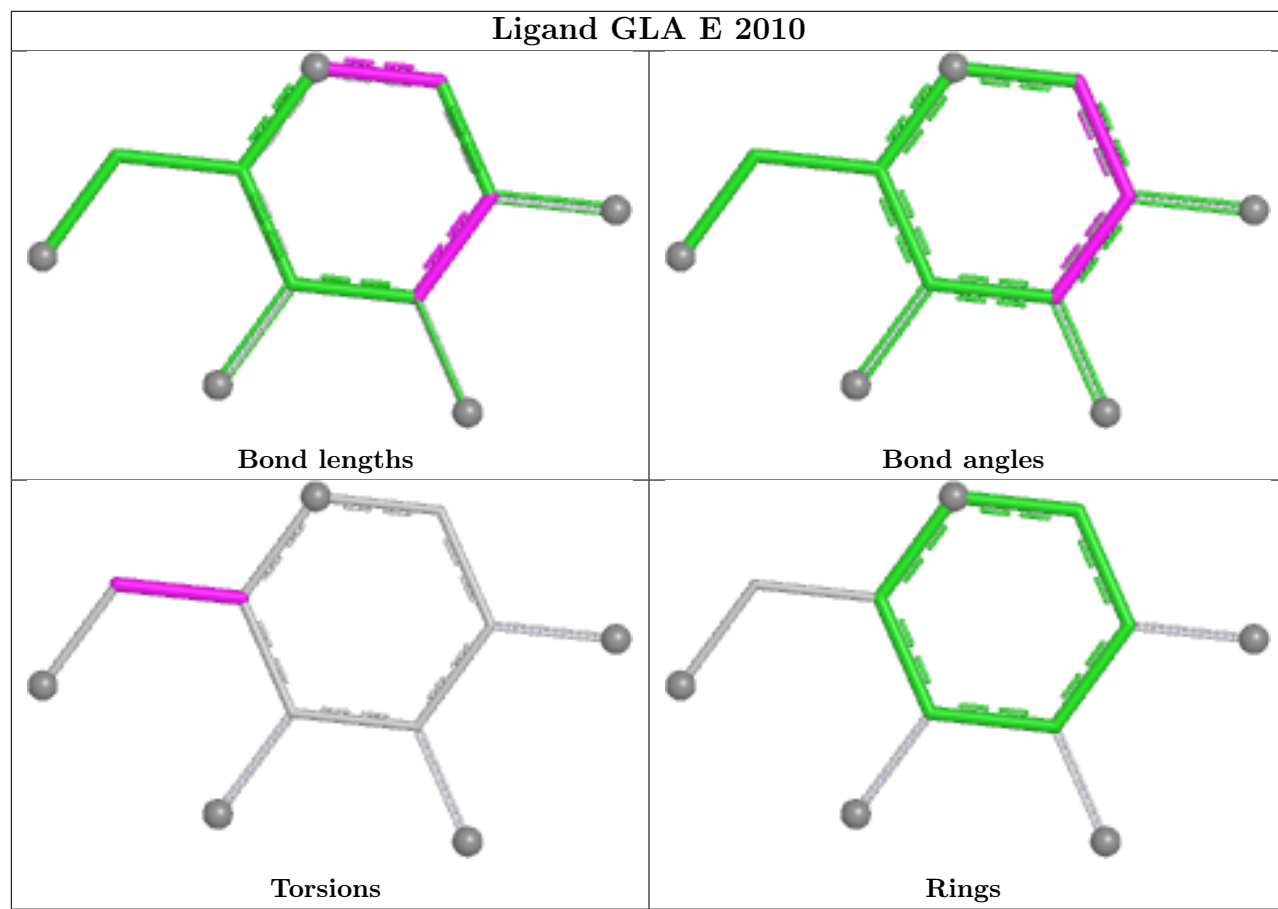


Ligand GLA E 2004

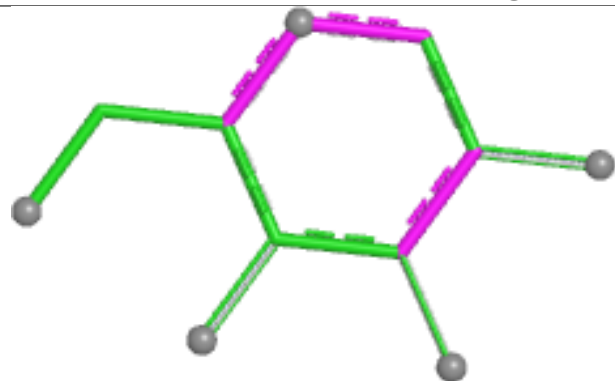


Ligand AHR A 2019

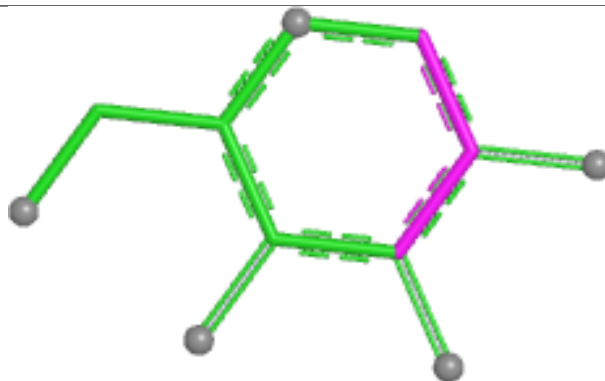




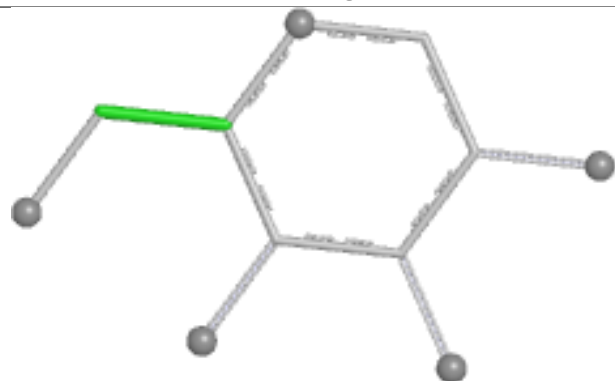
Ligand GLA D 2006



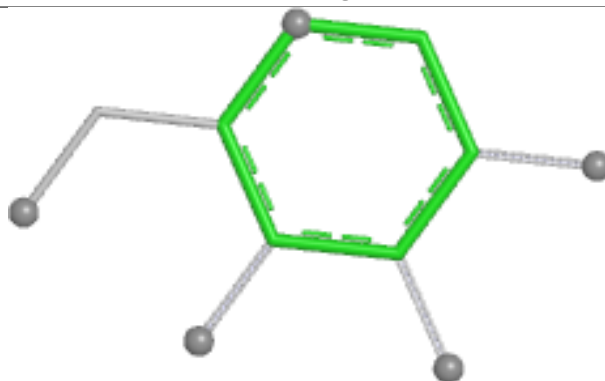
Bond lengths



Bond angles

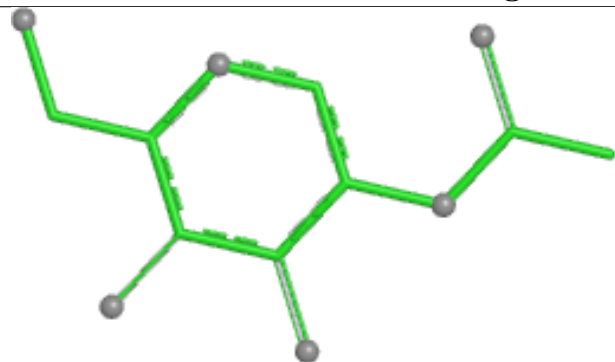


Torsions

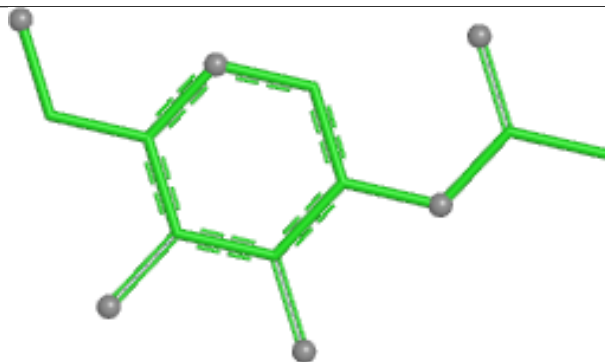


Rings

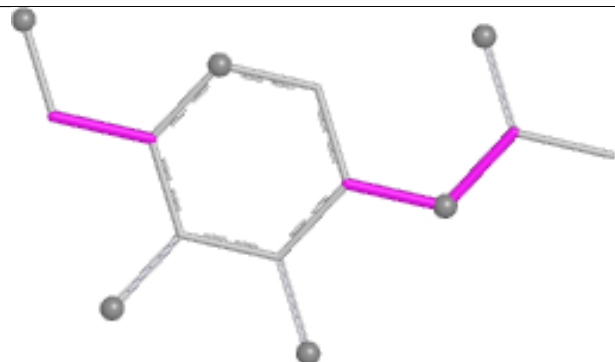
Ligand NAG C 2009



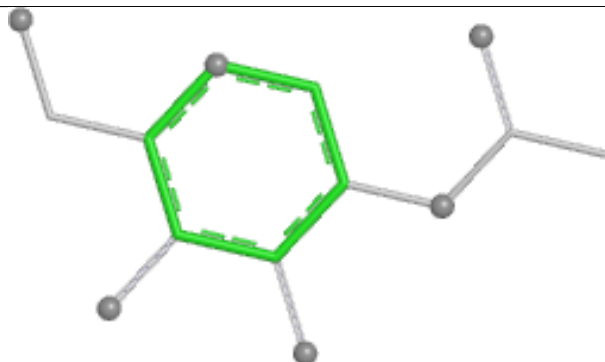
Bond lengths



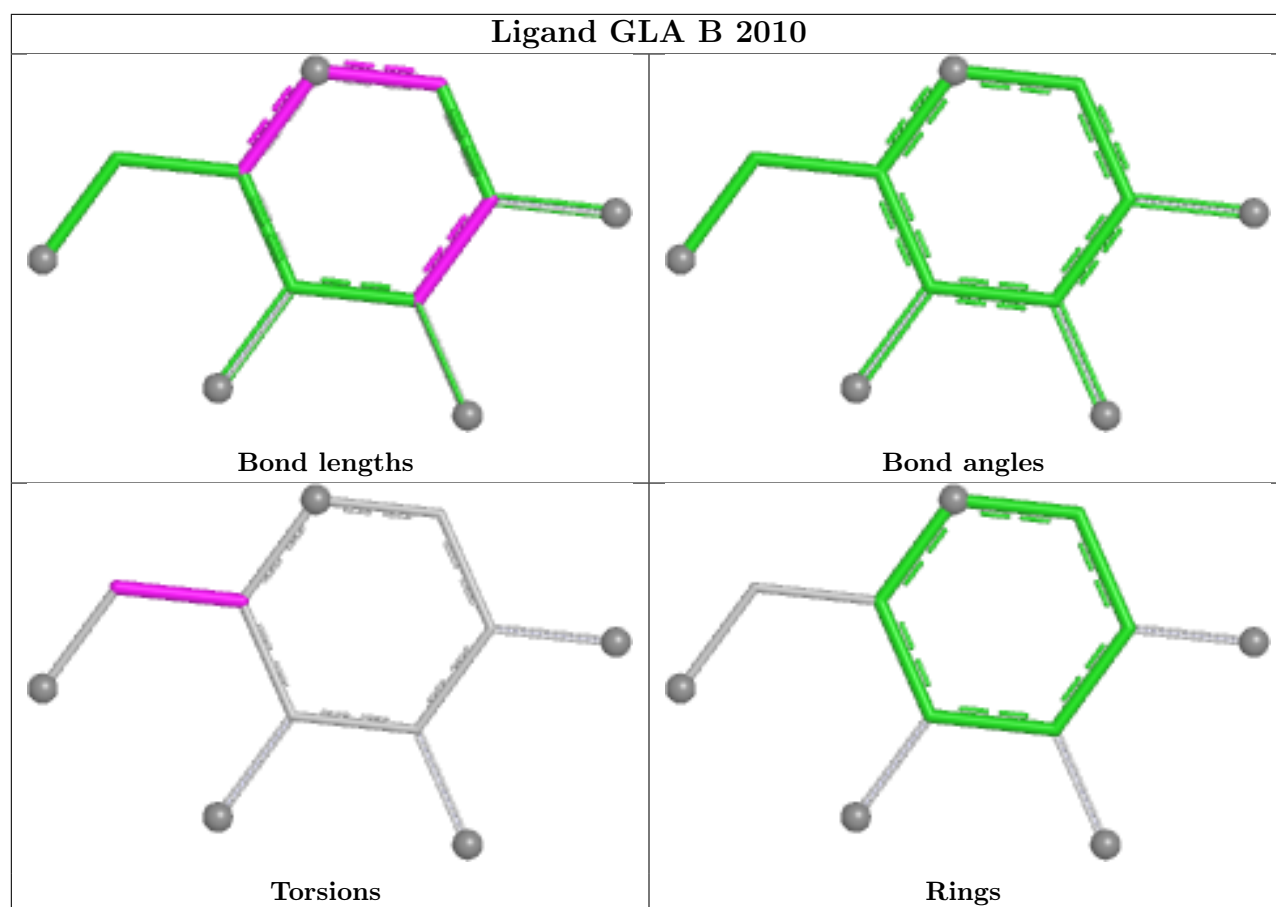
Bond angles

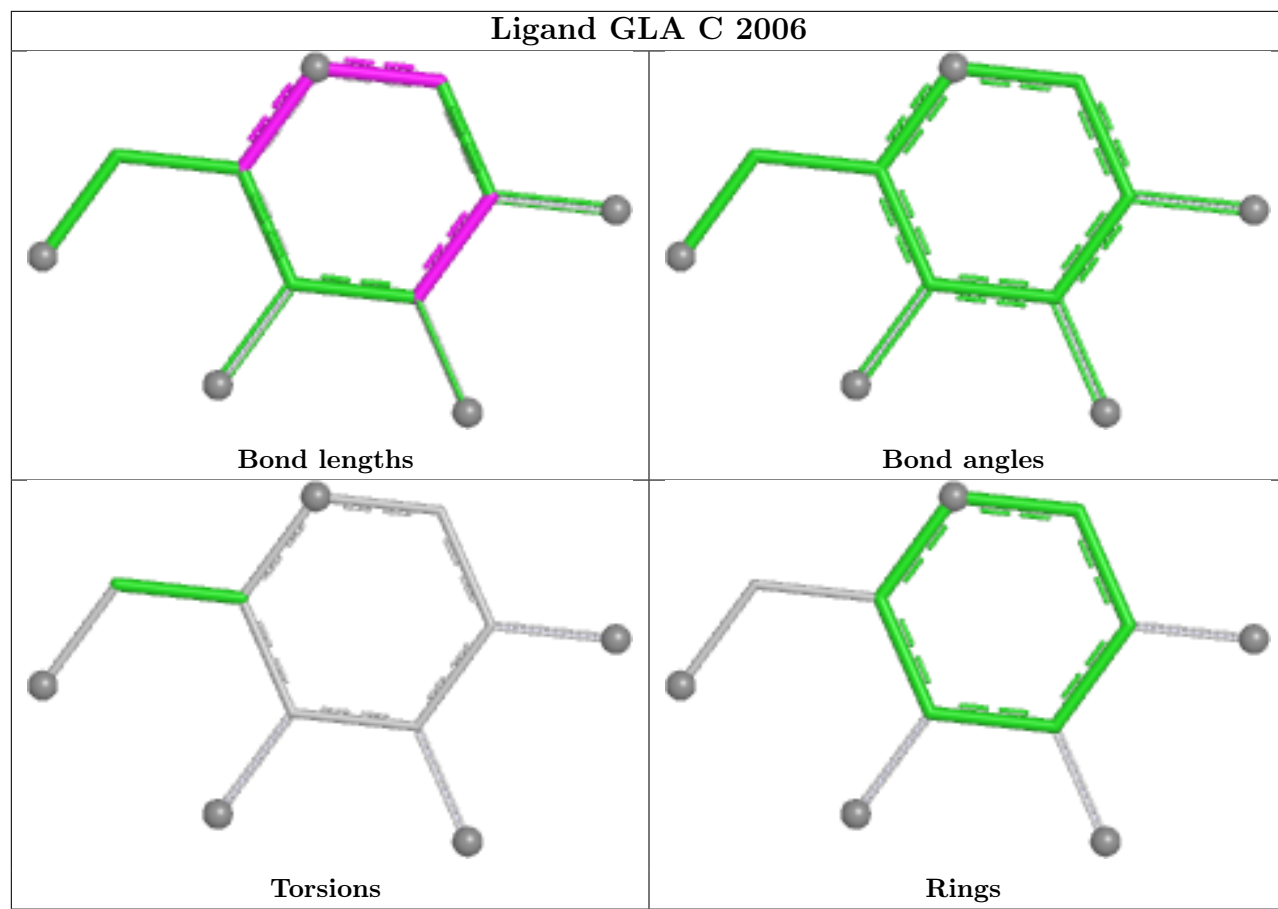


Torsions

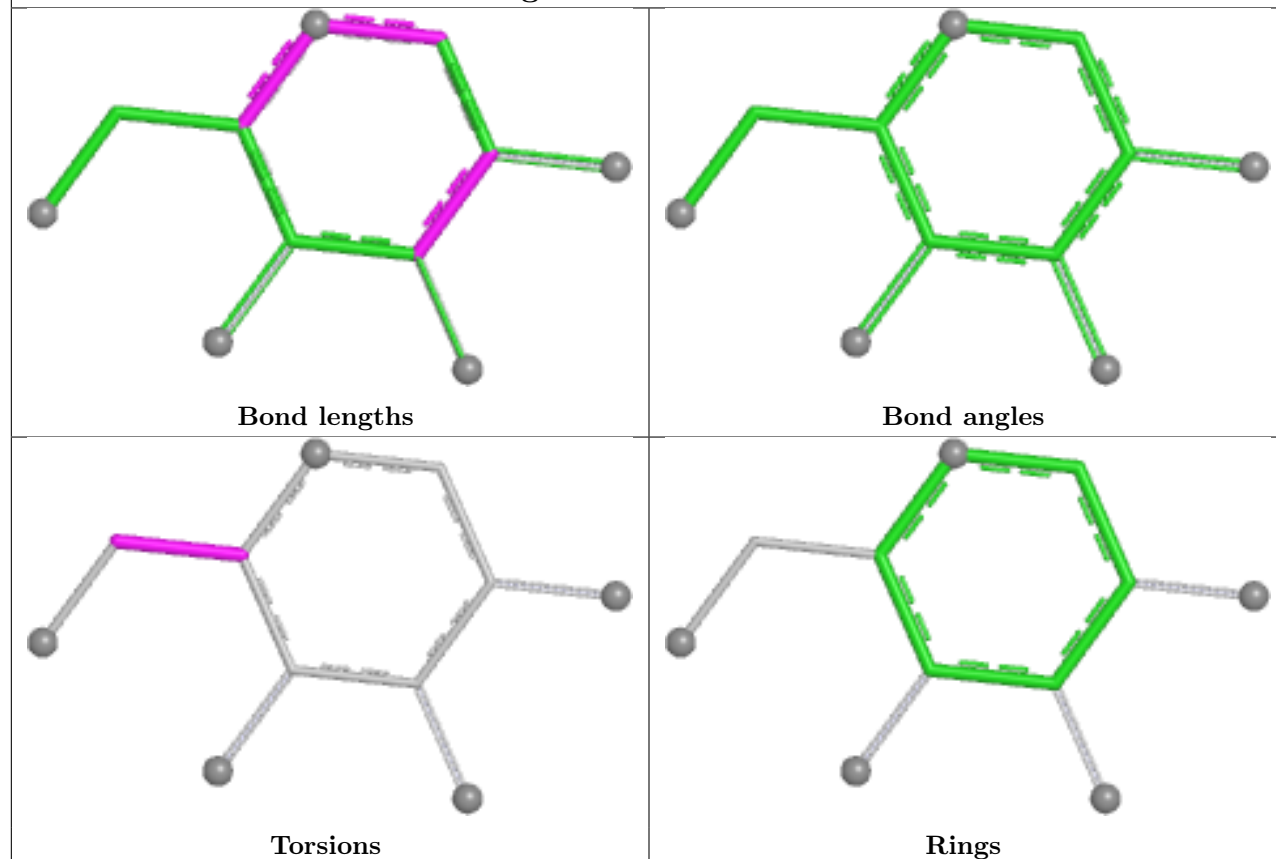


Rings

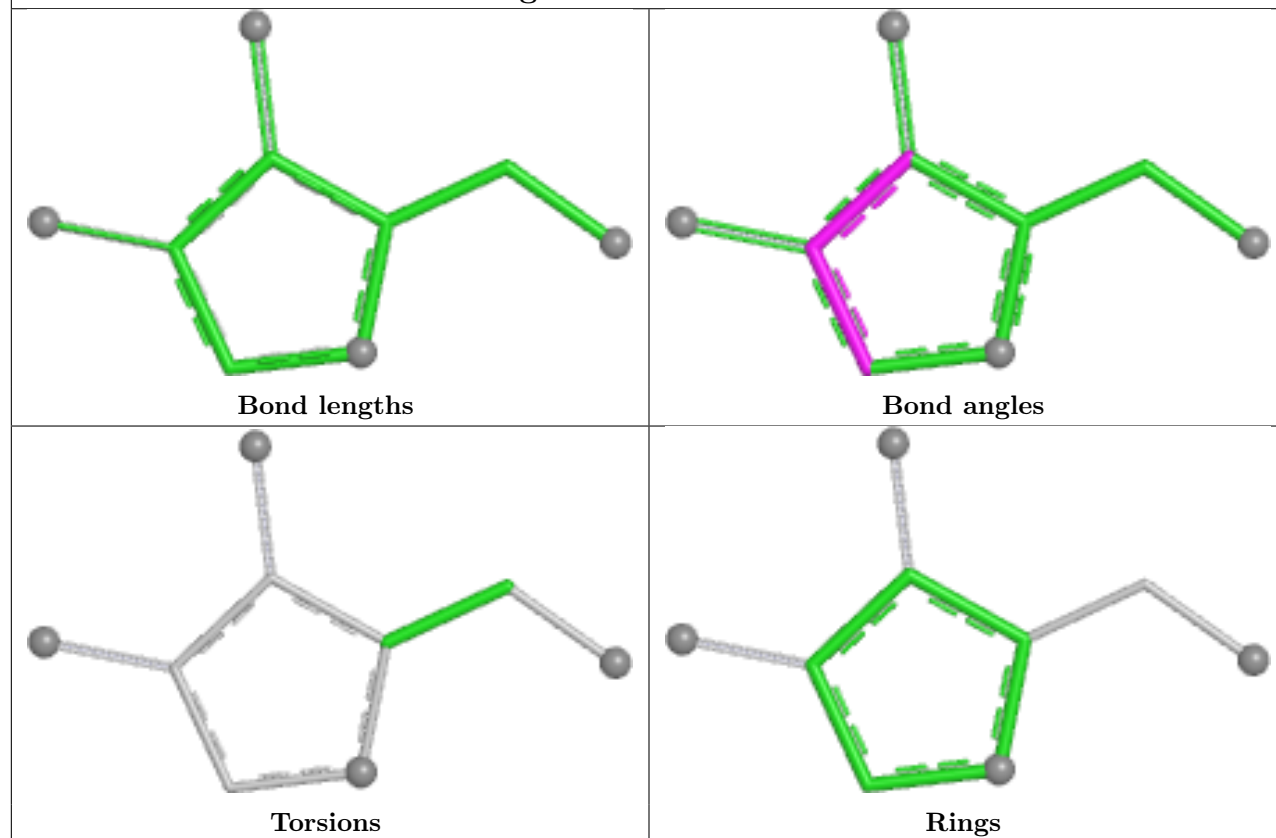




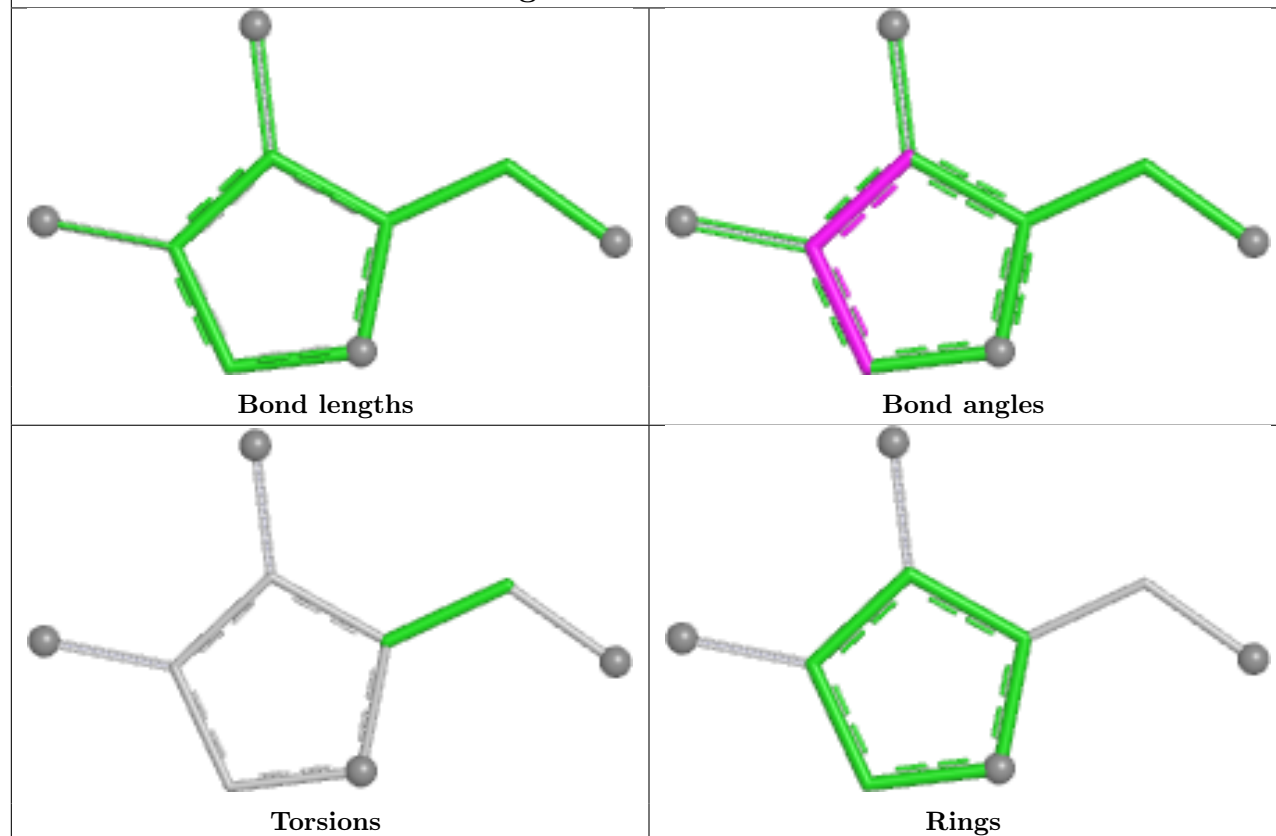
Ligand GLA D 2005



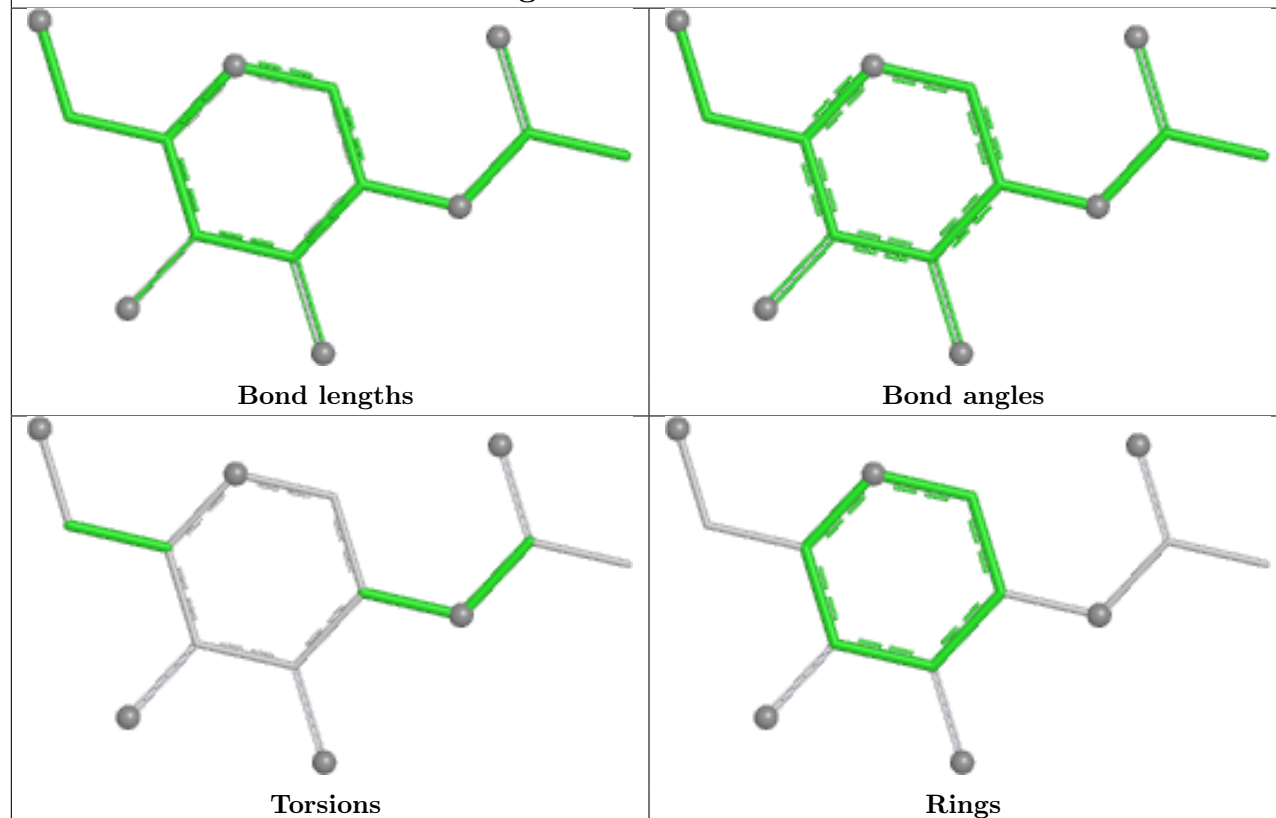
Ligand AHR B 2002



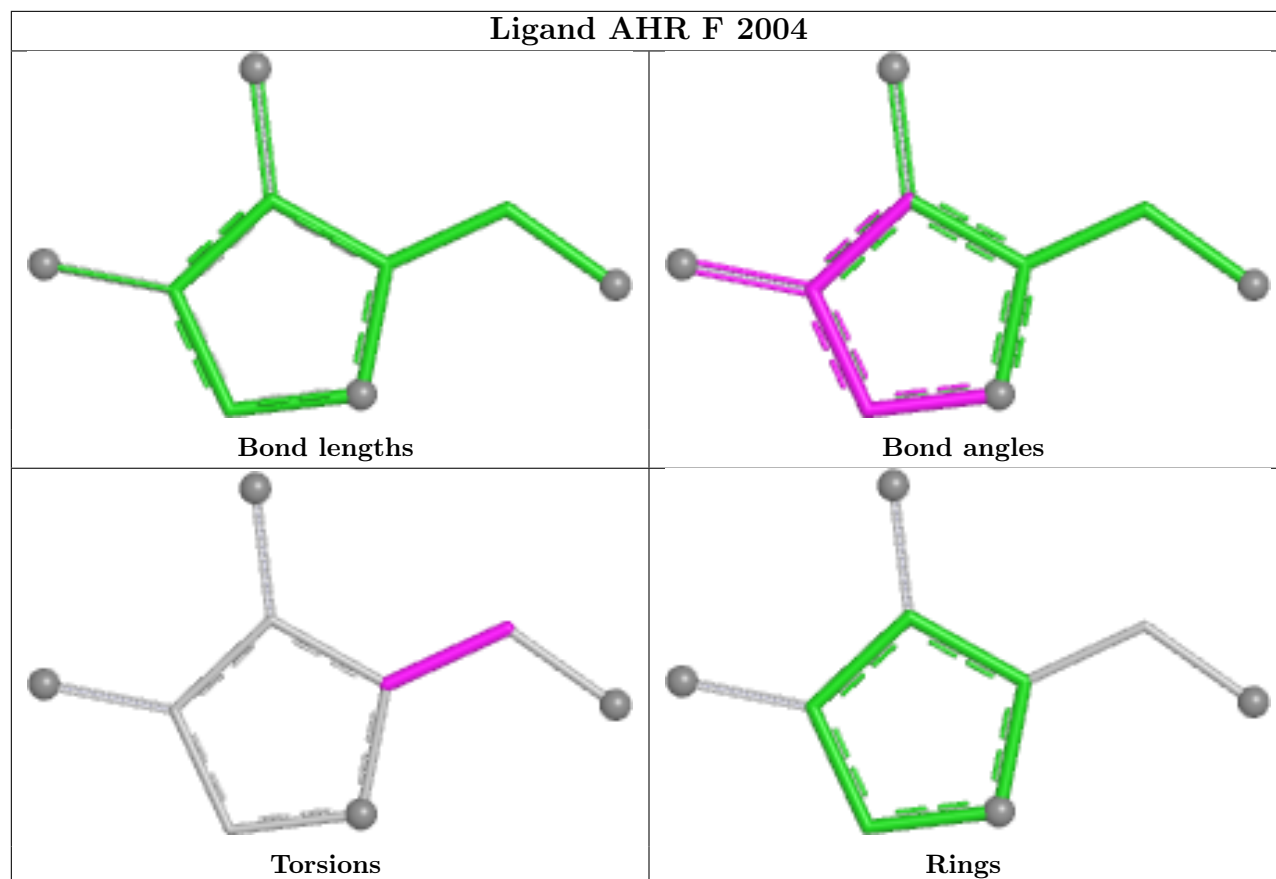
Ligand AHR A 2018



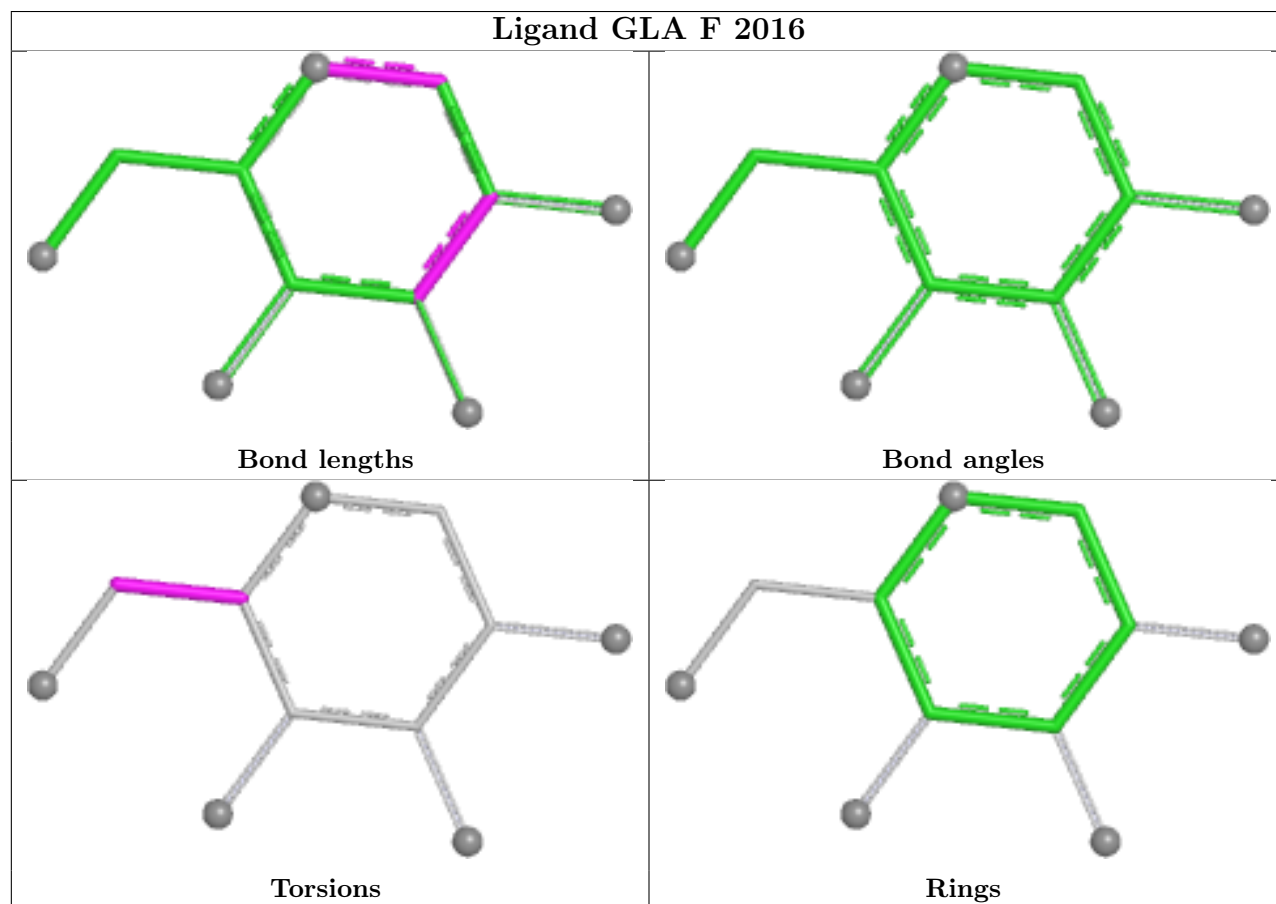
Ligand NAG D 2010

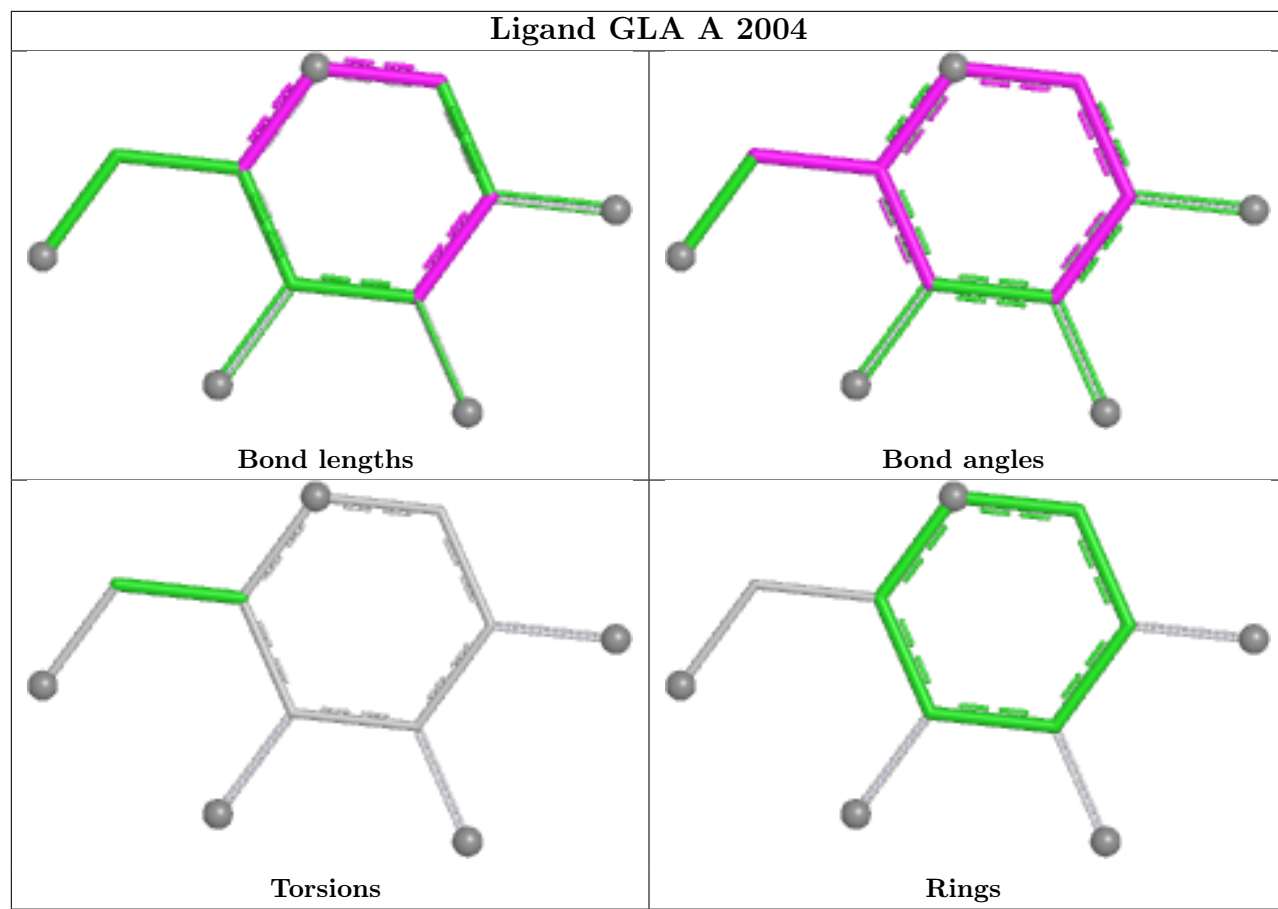


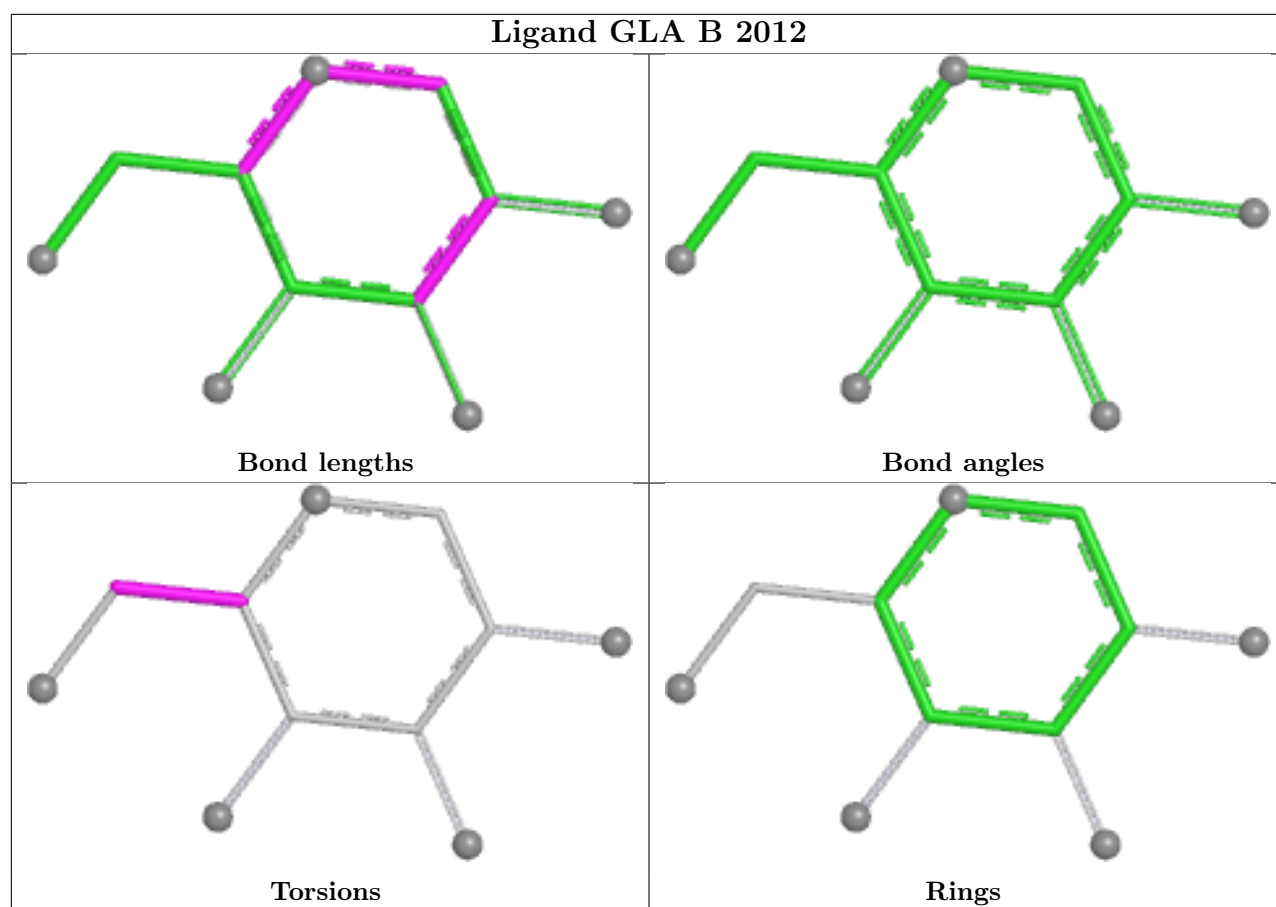
Ligand AHR F 2004

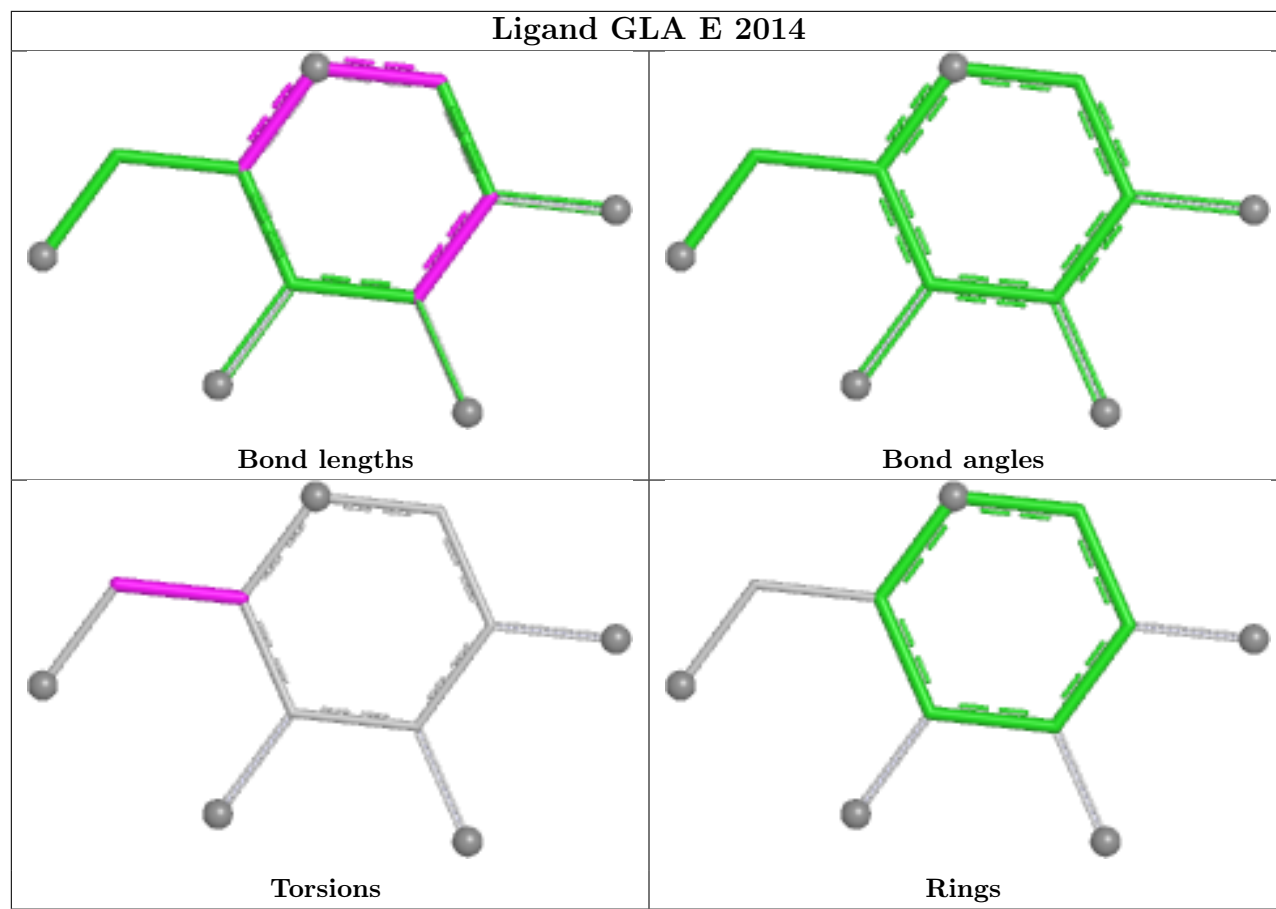


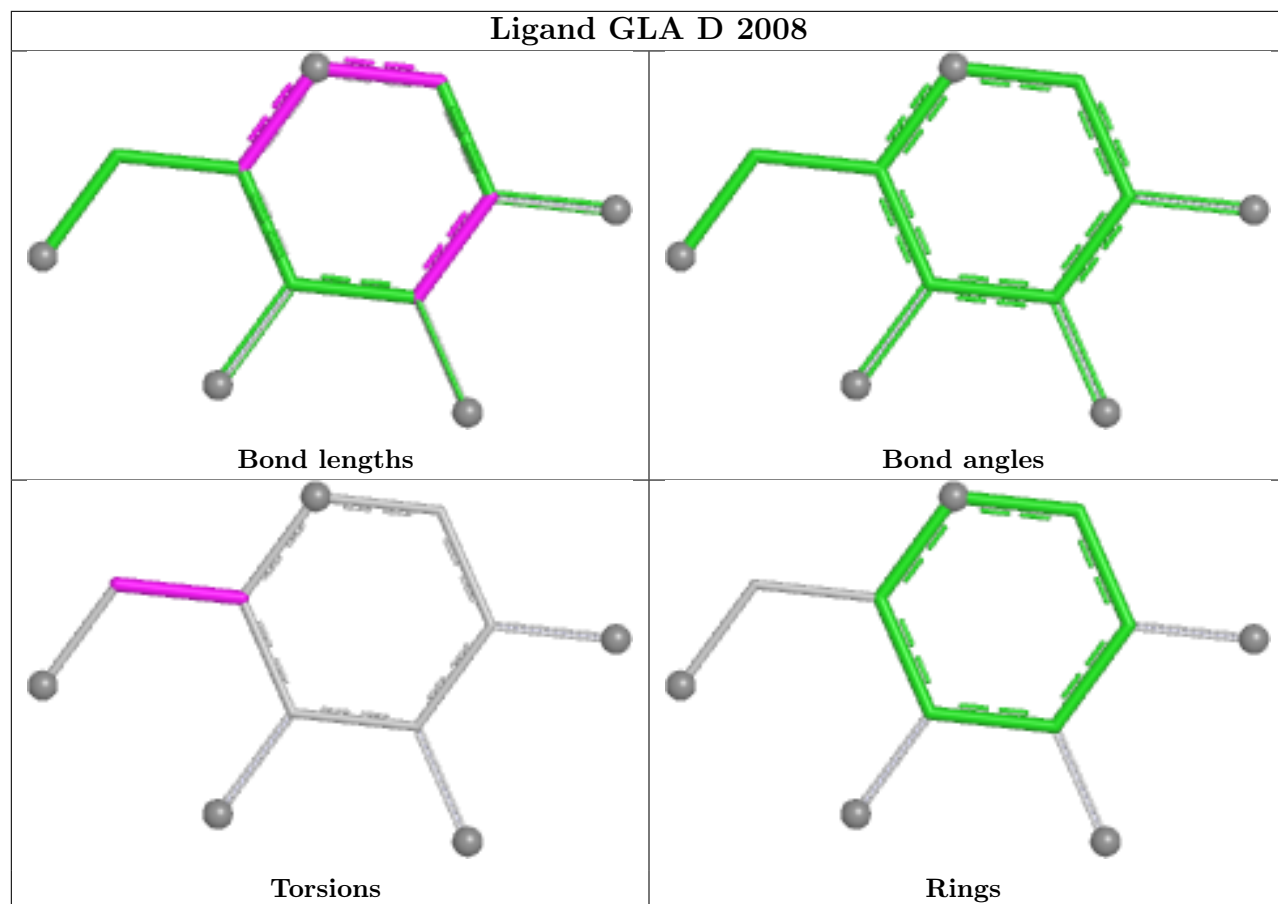
Ligand GLA F 2016

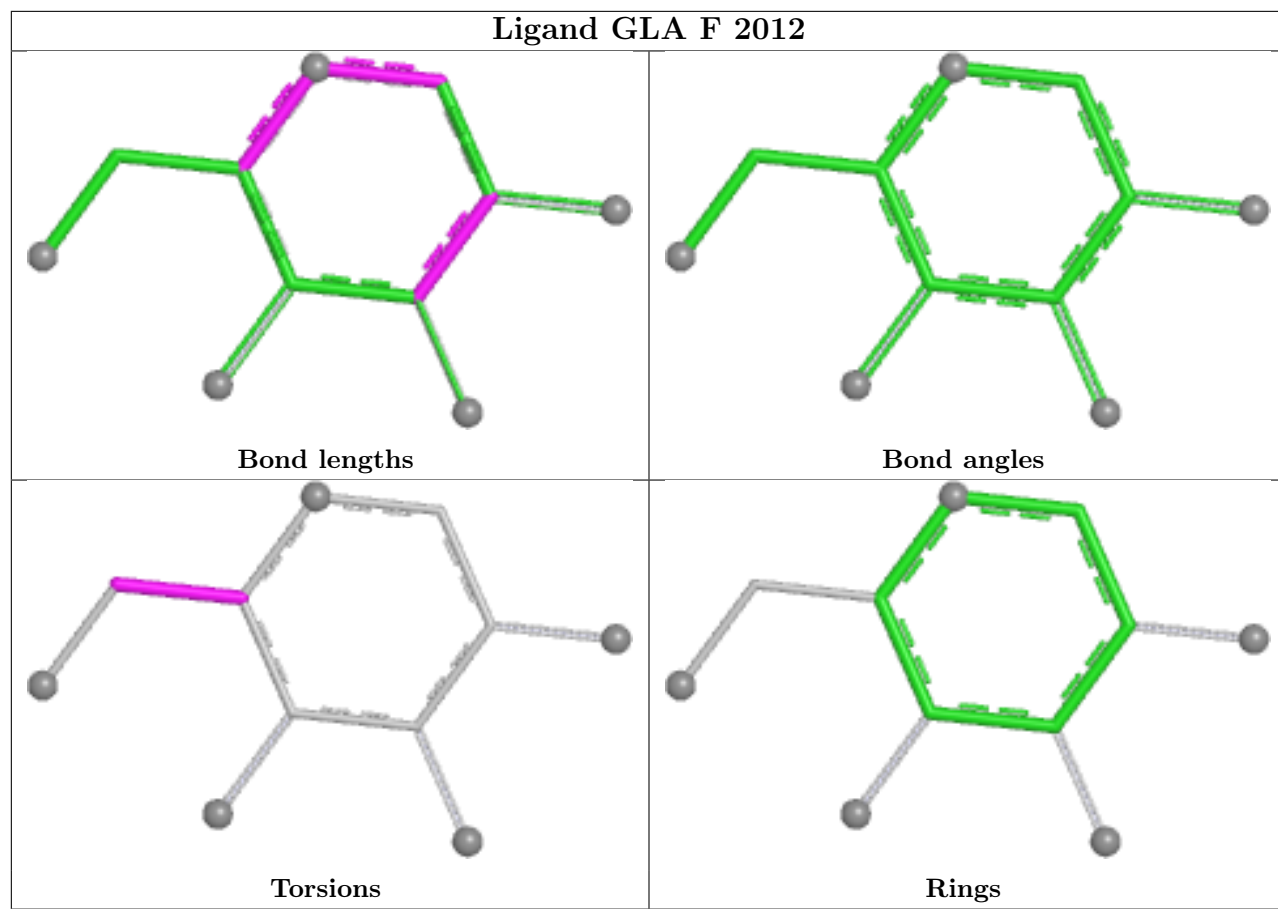




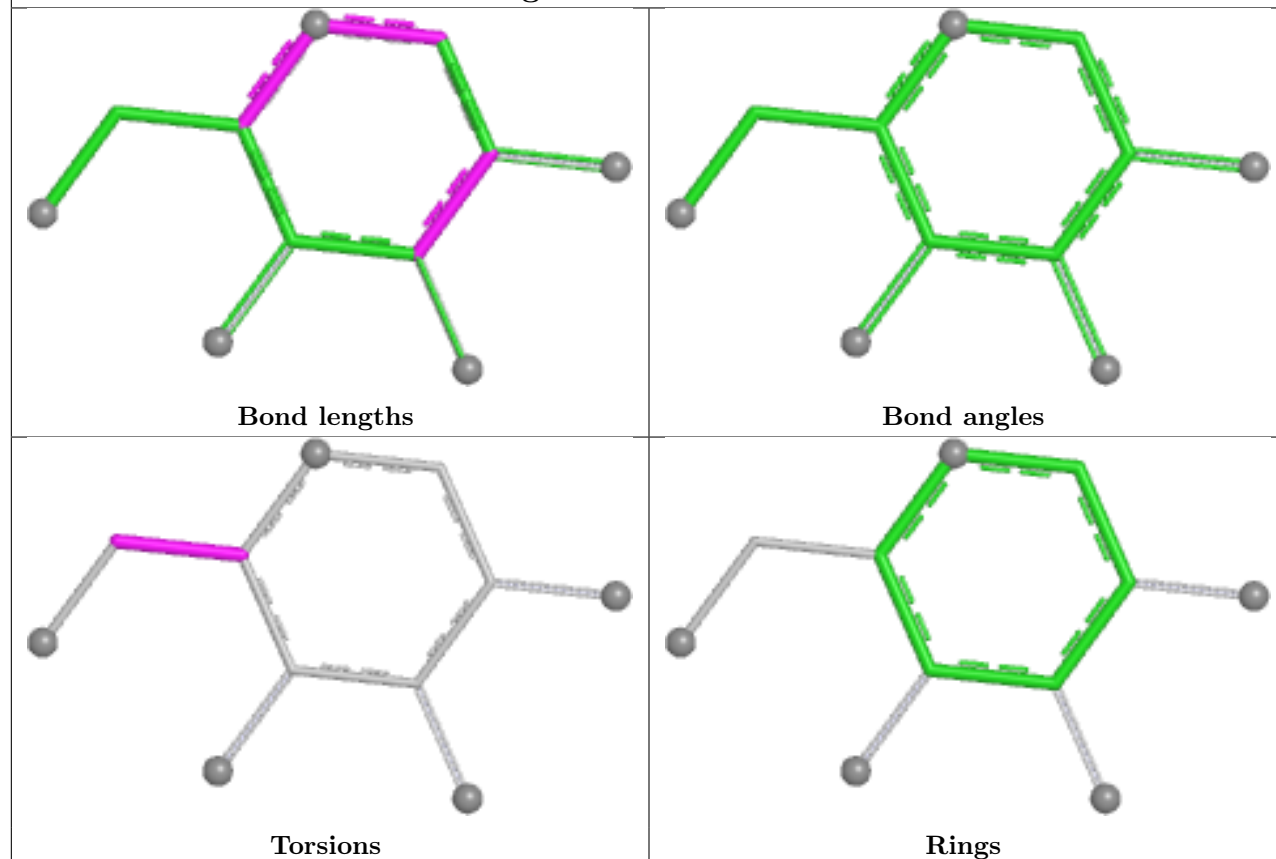




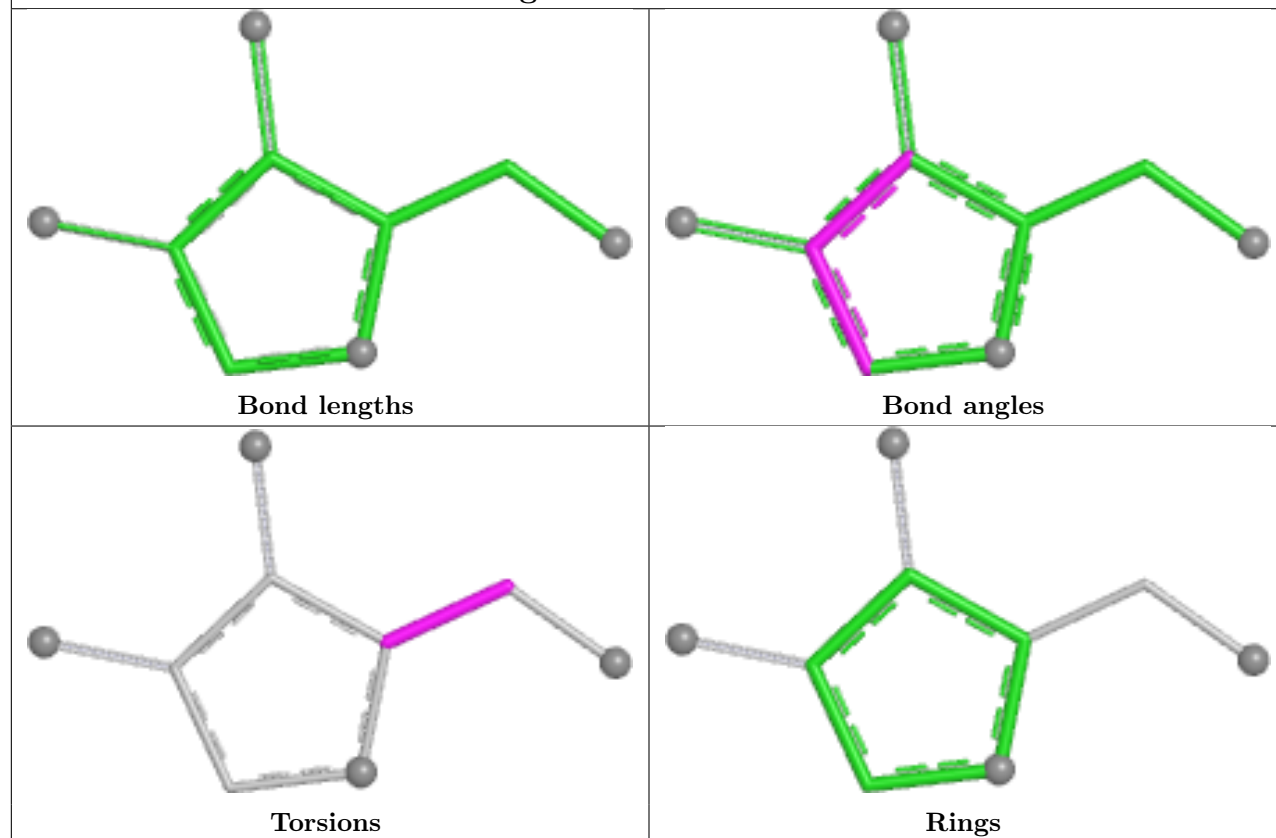




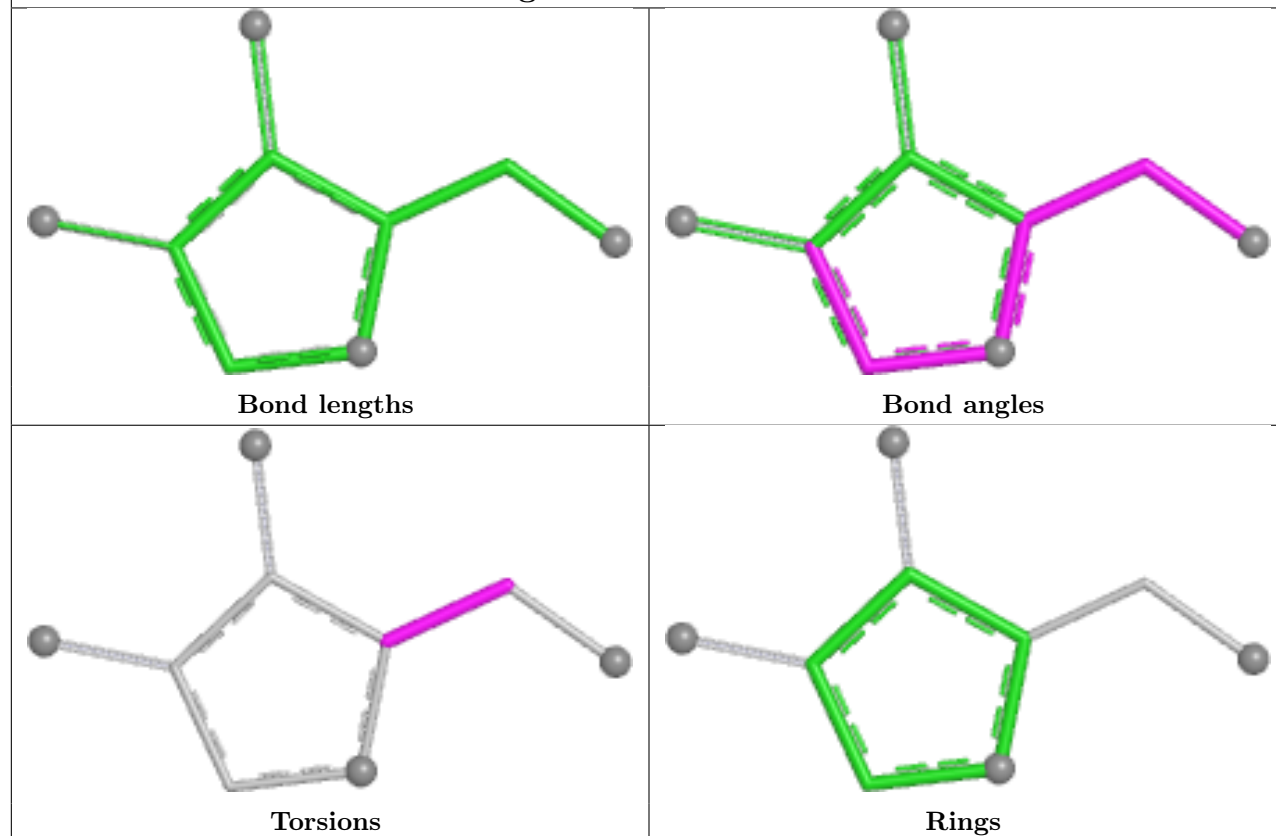
Ligand GLA C 2008



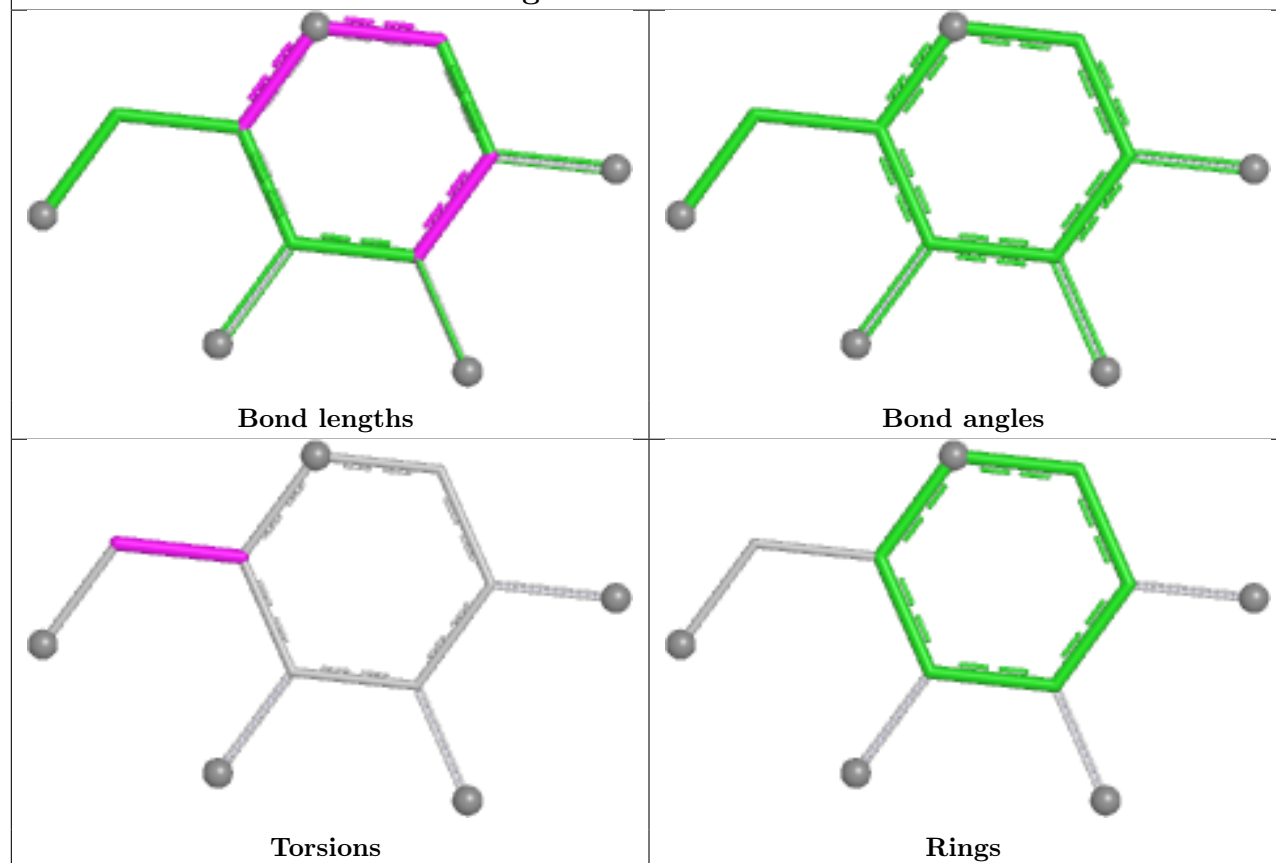
Ligand AHR B 2020

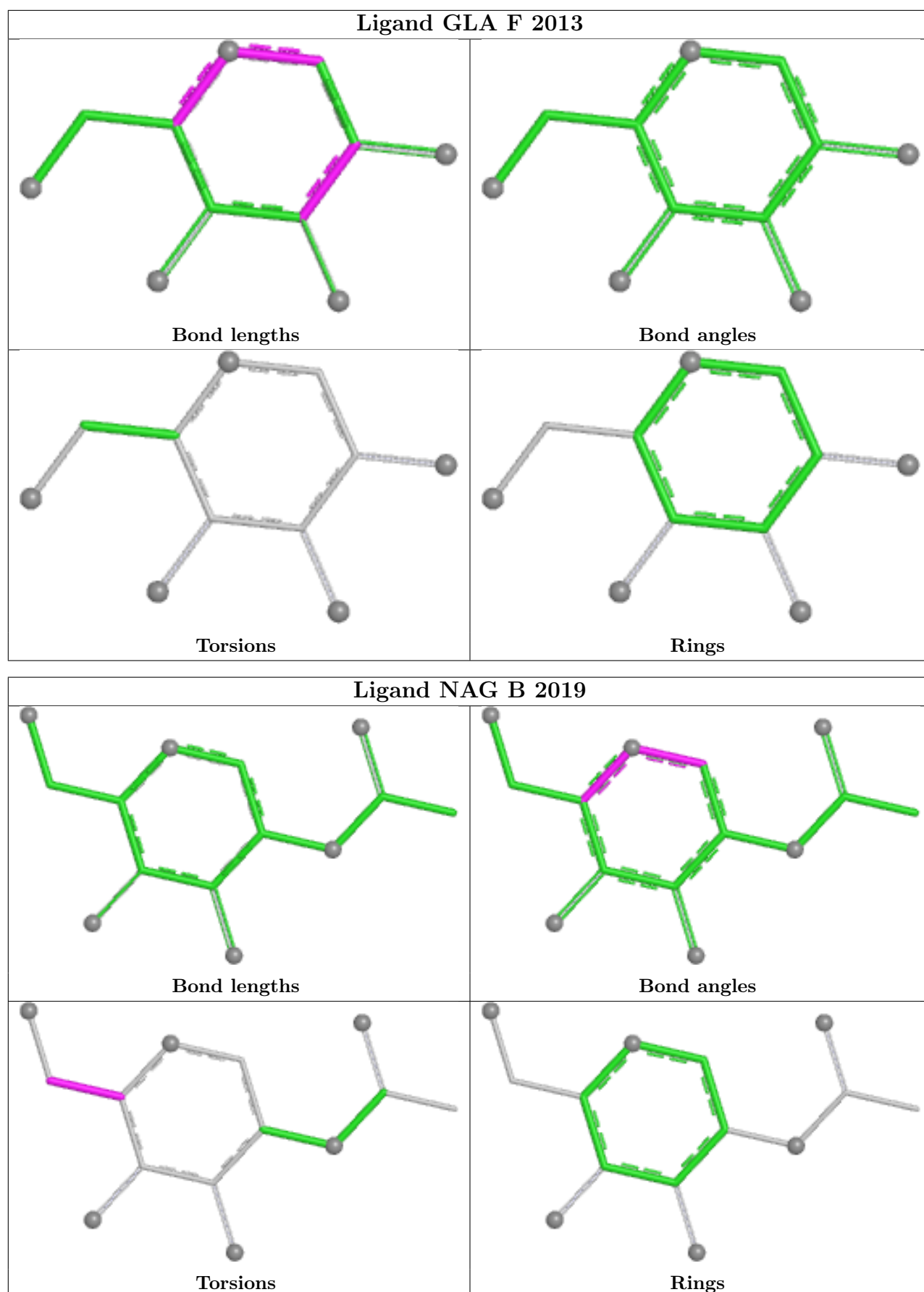


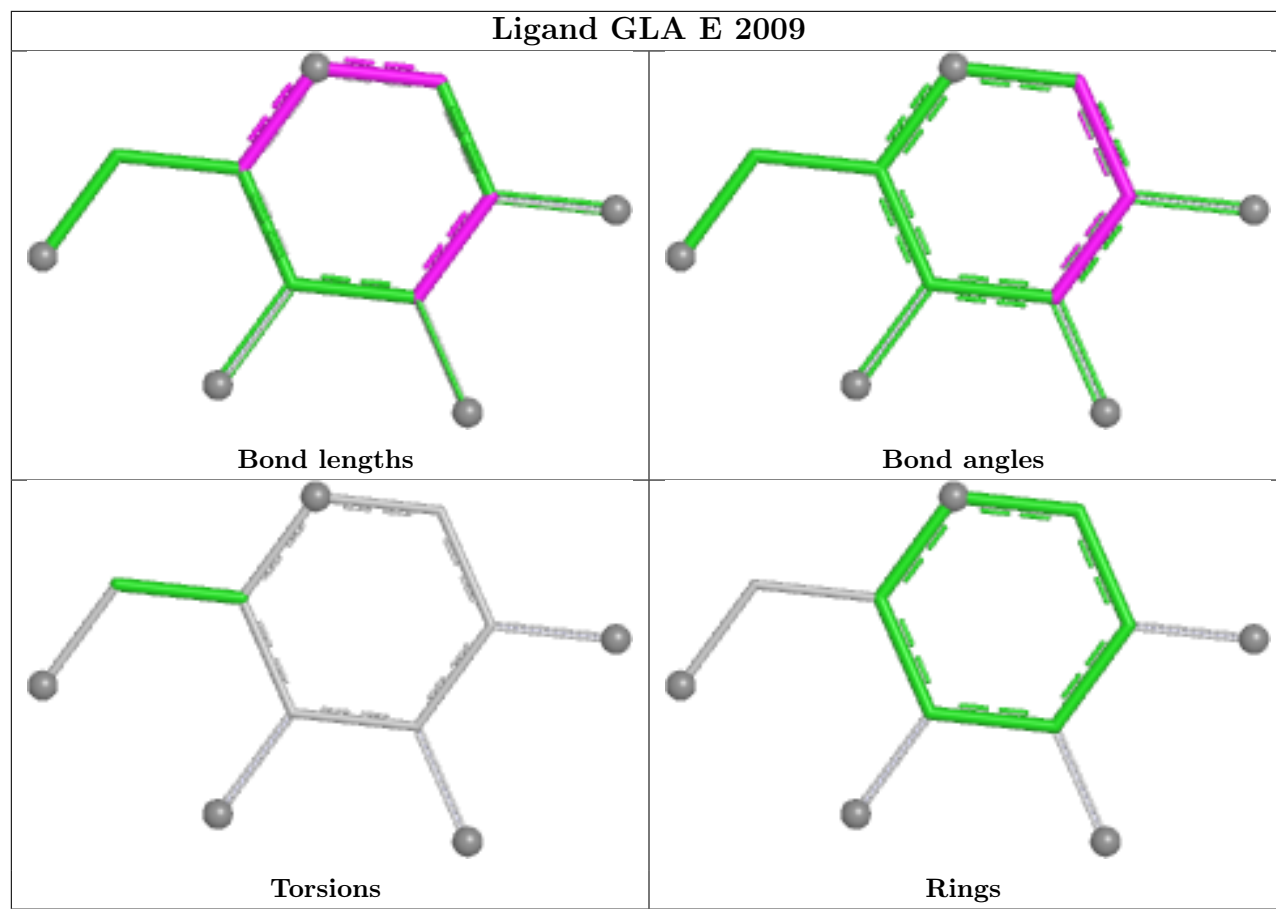
Ligand AHR D 2003

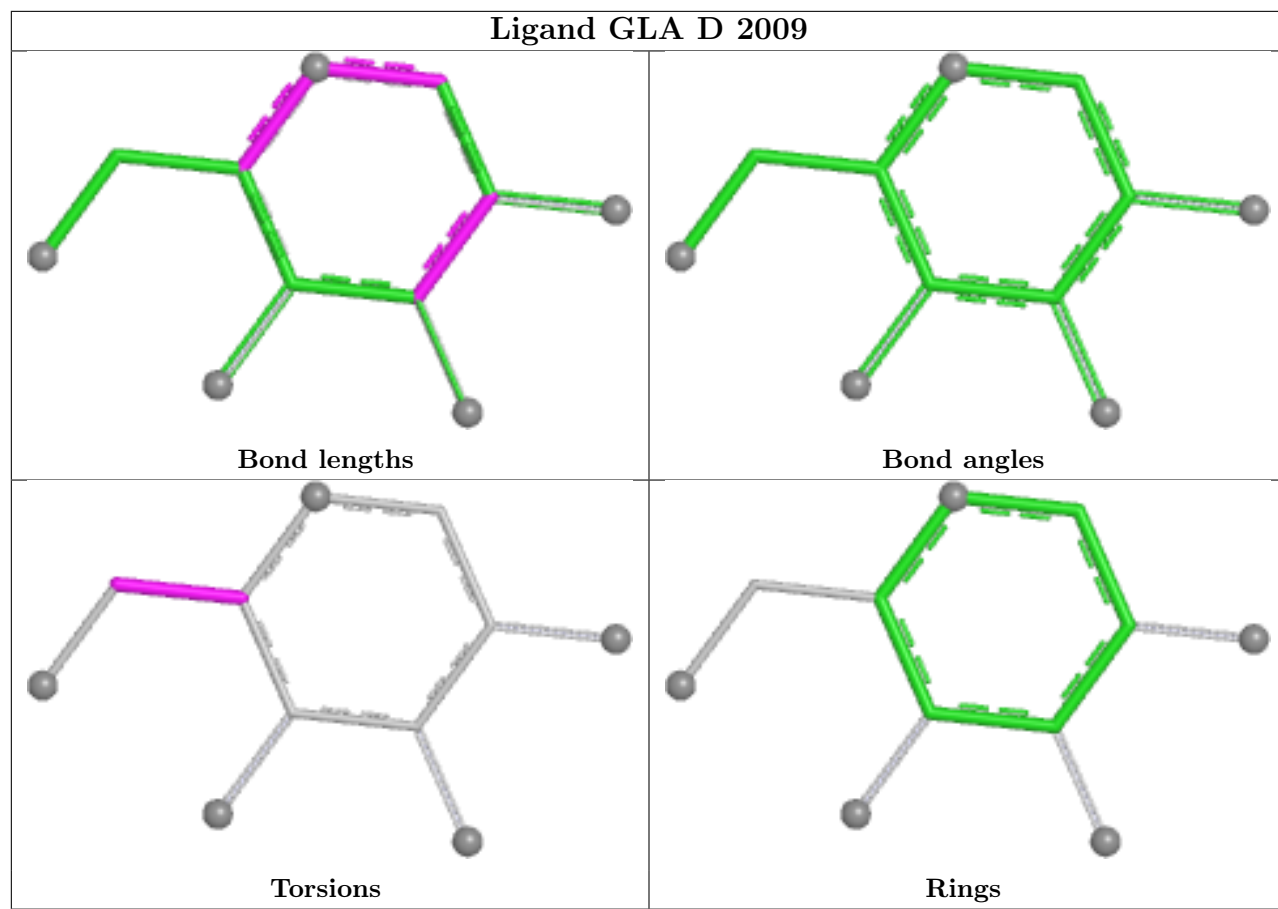


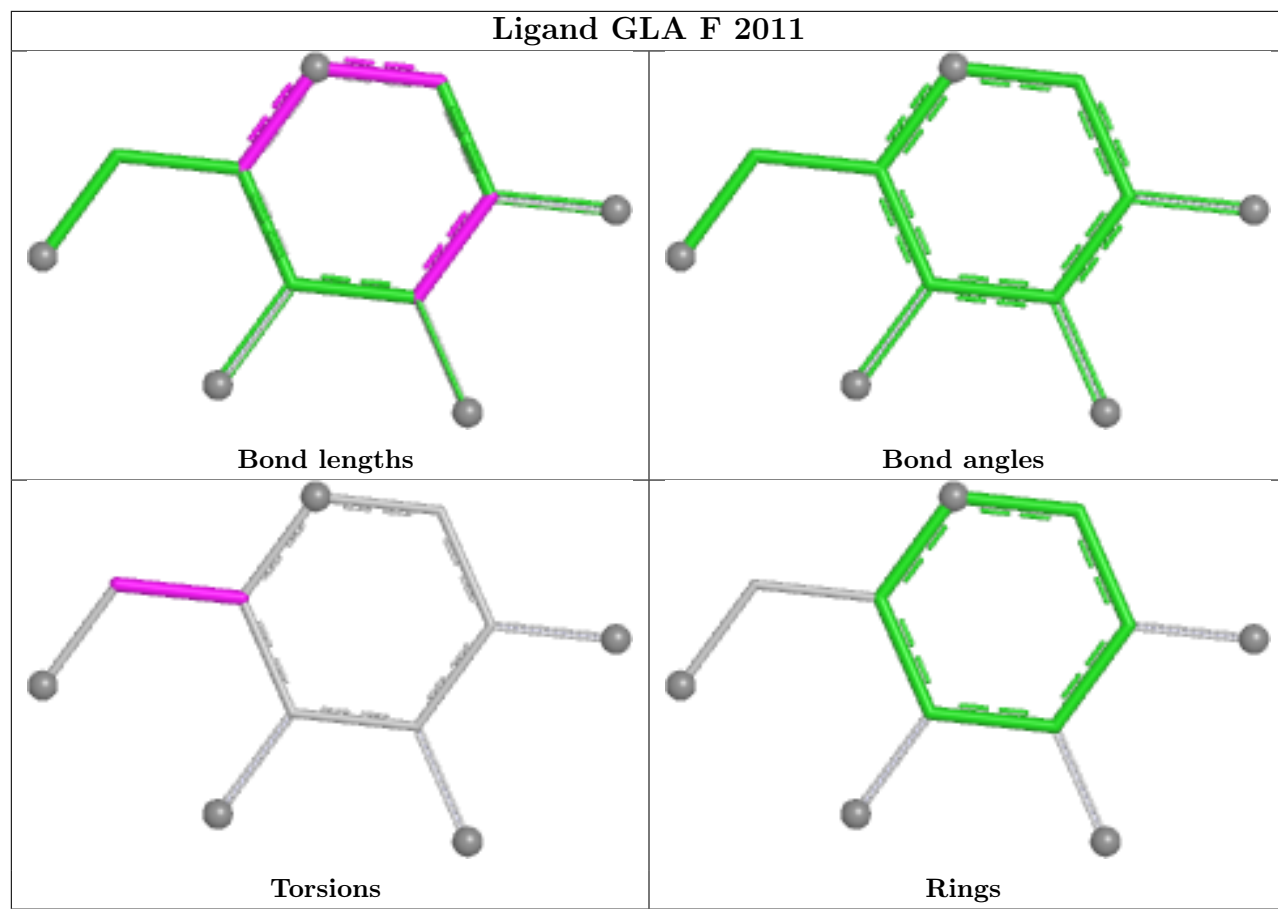
Ligand GLA B 2008

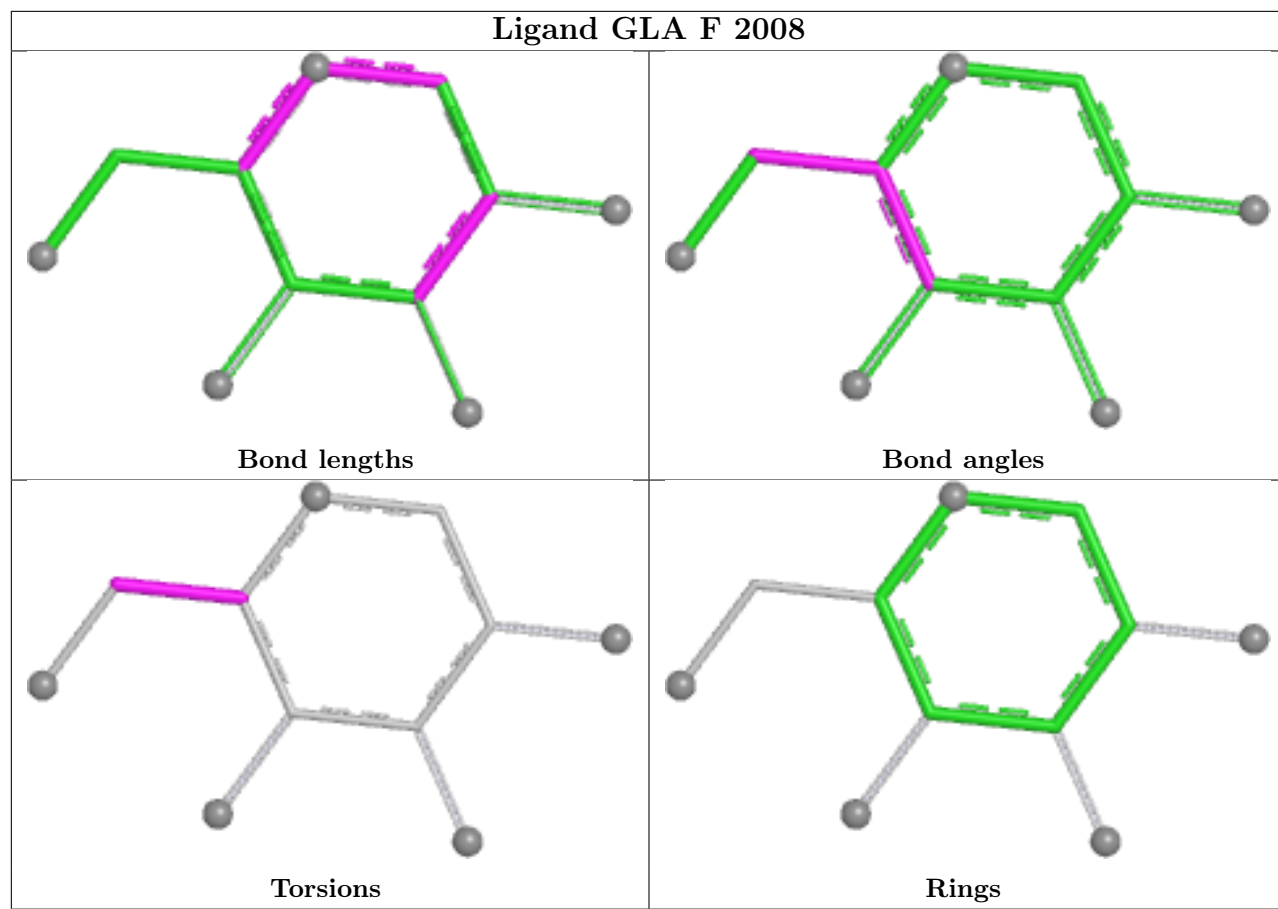


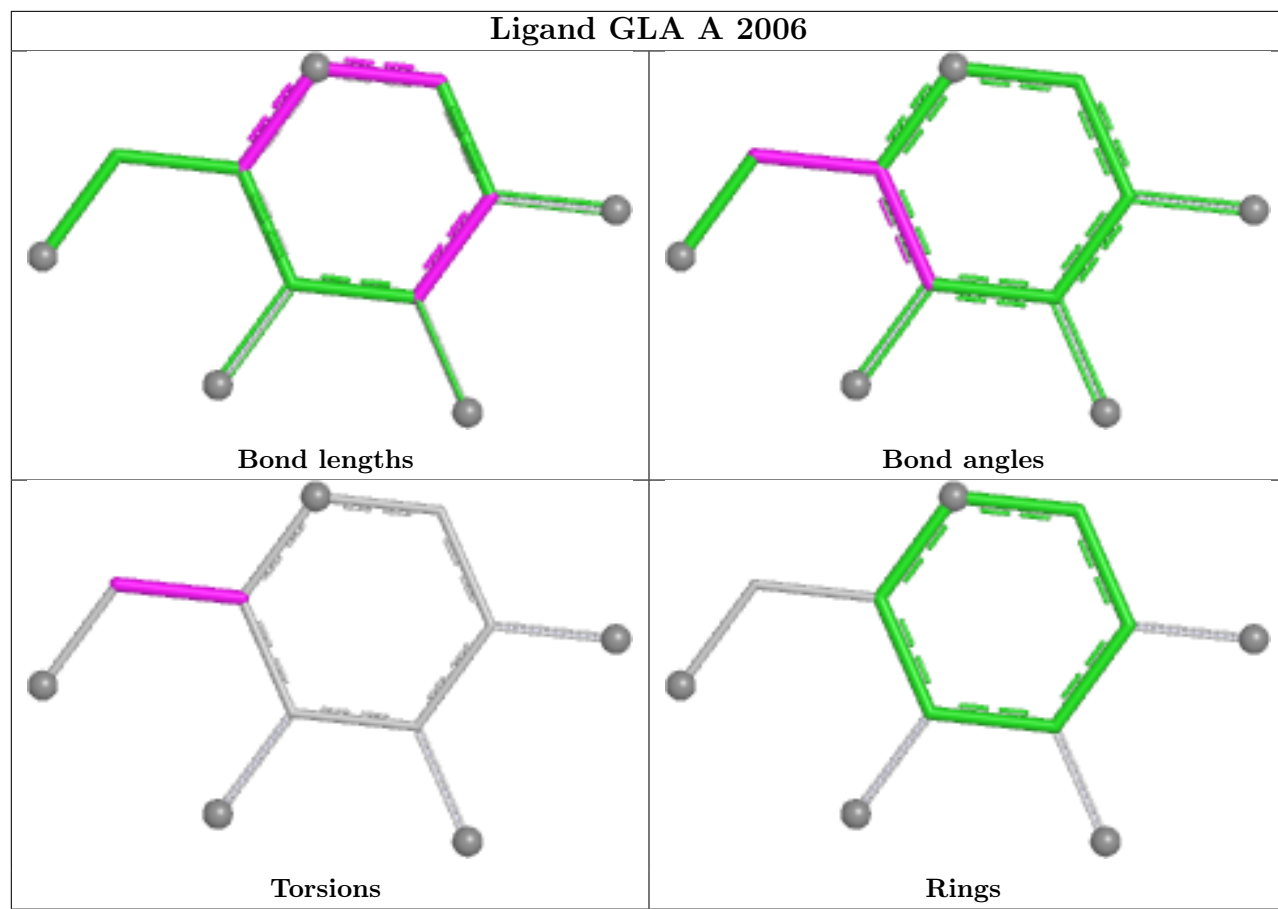




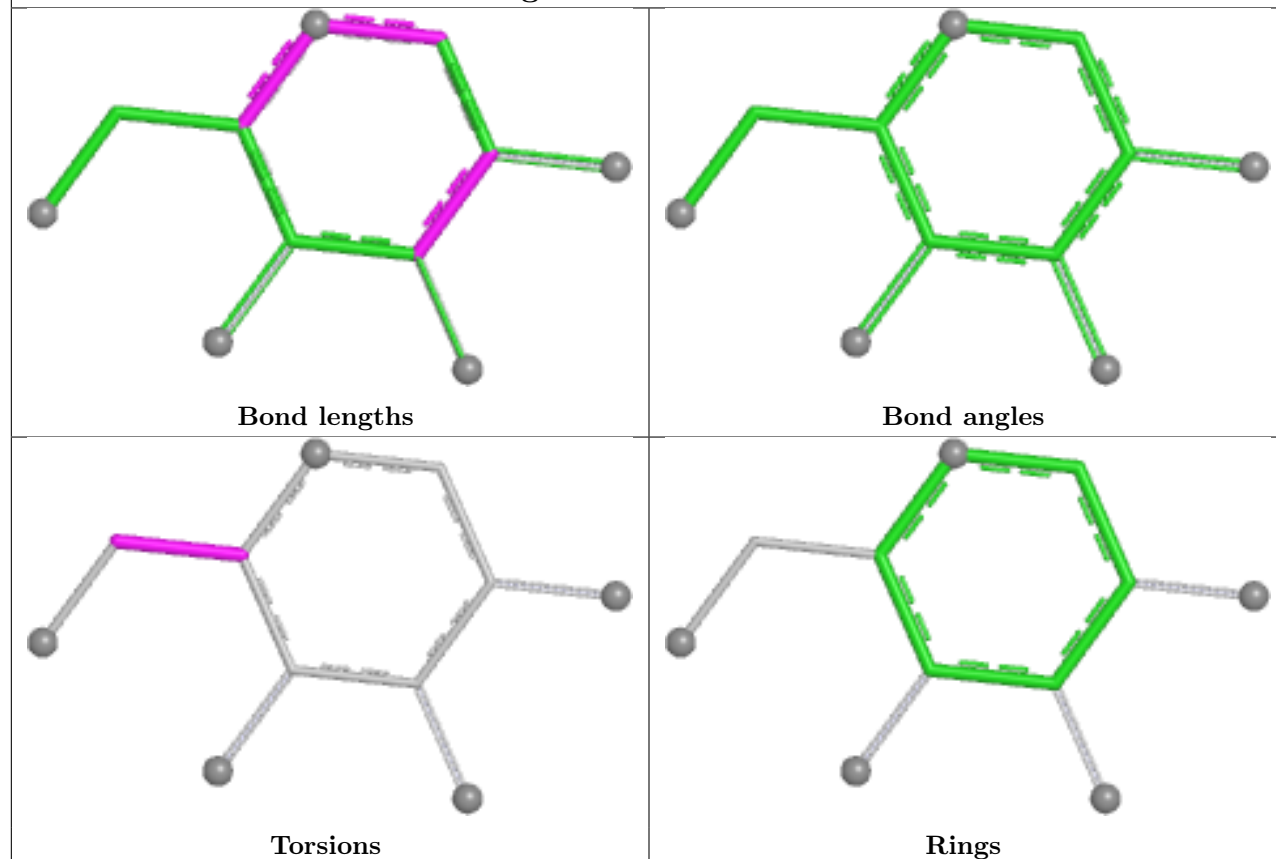




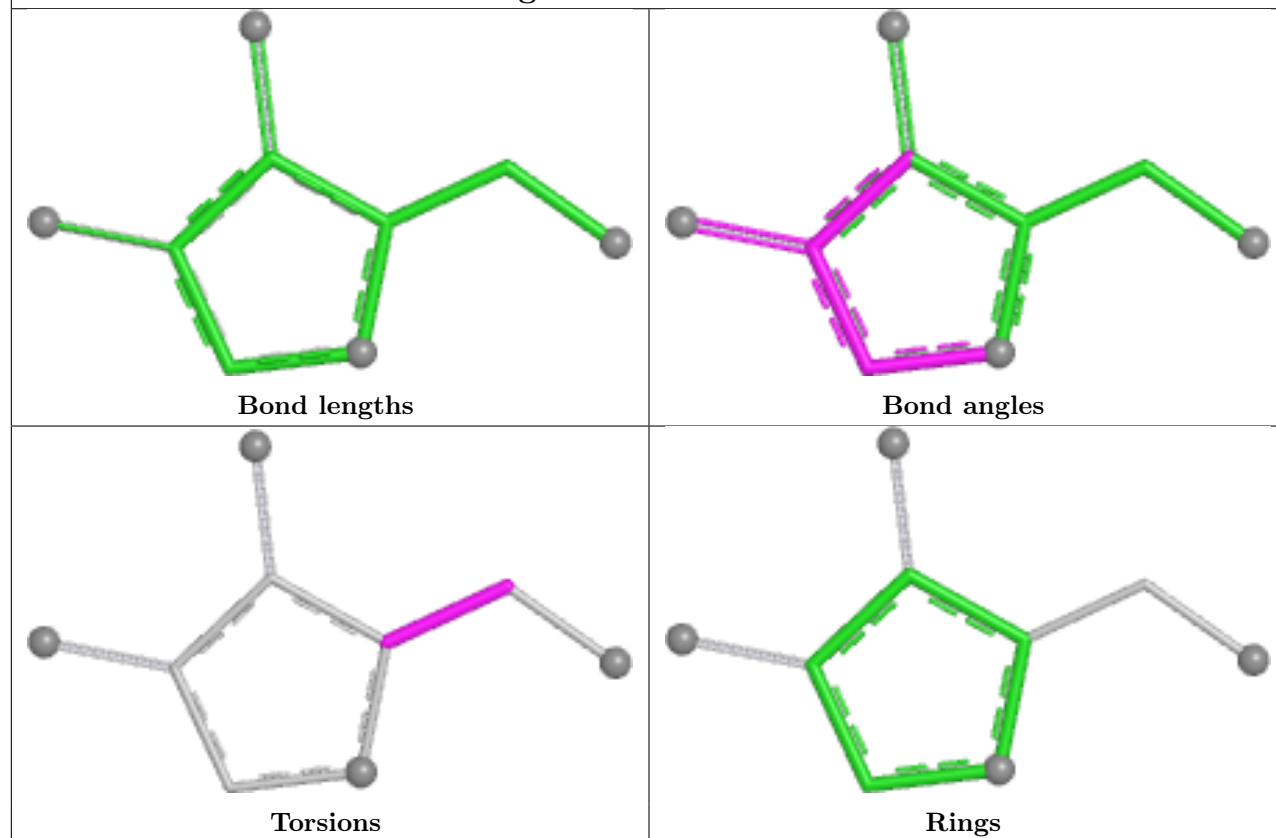


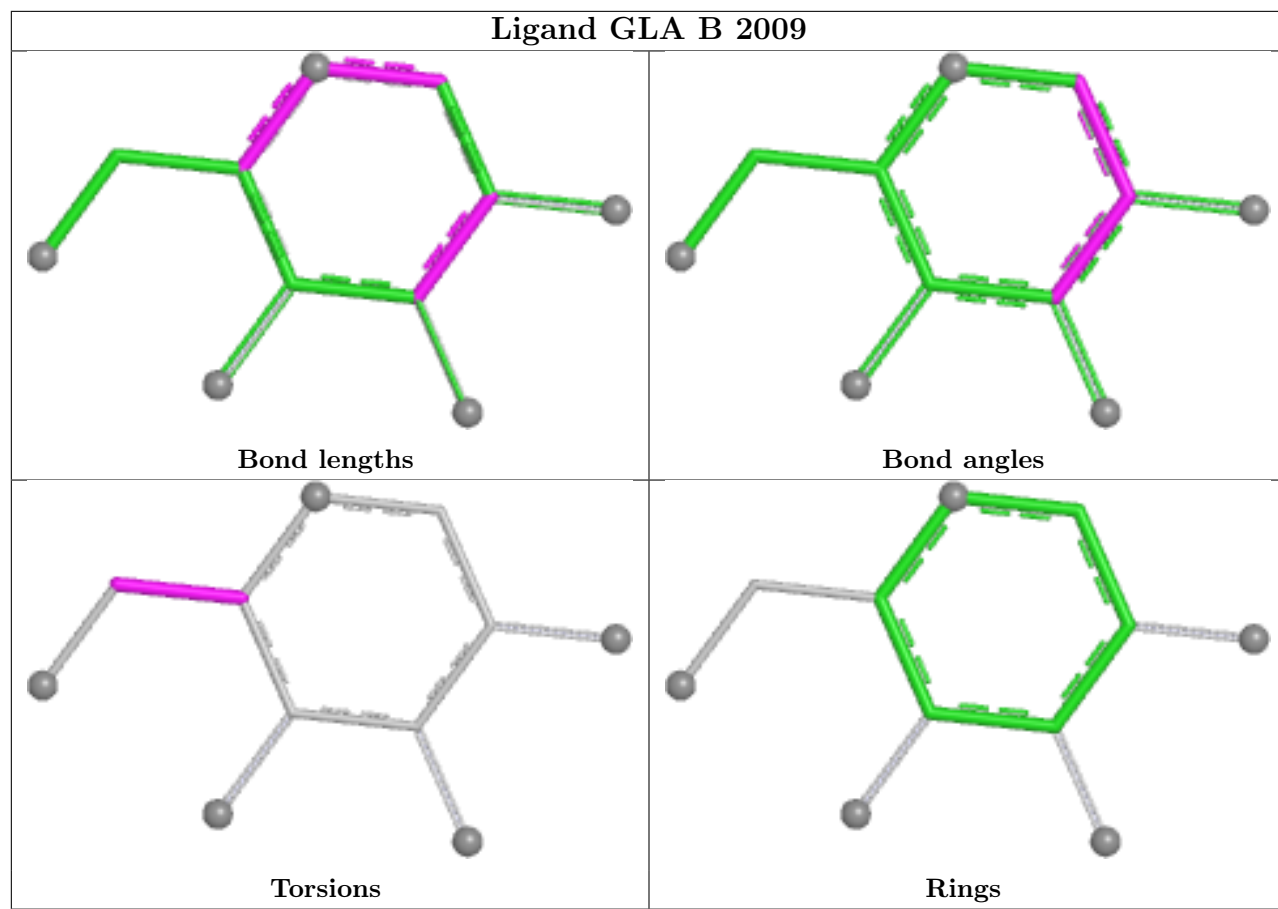


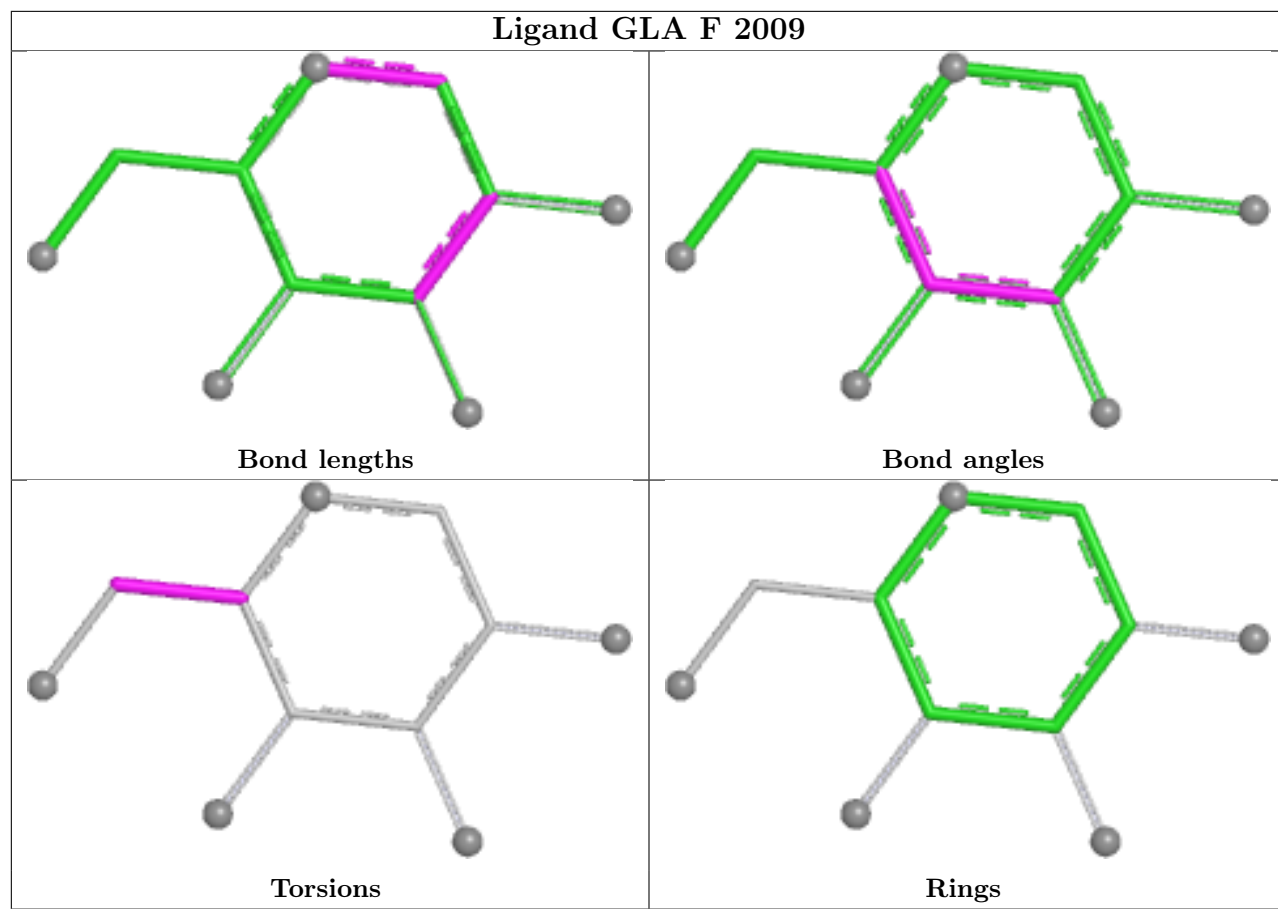
Ligand GLA D 2007



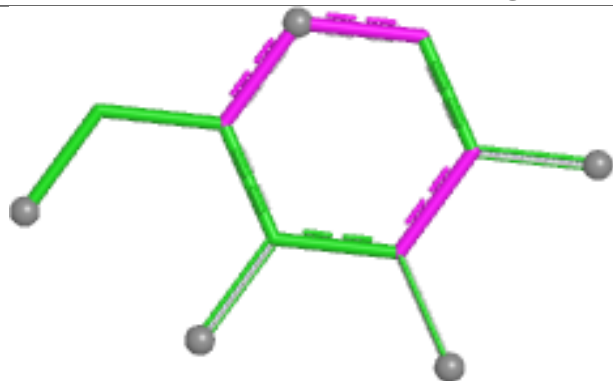
Ligand AHR D 2004



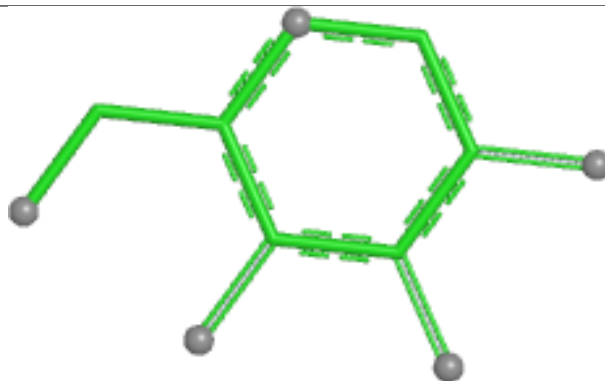




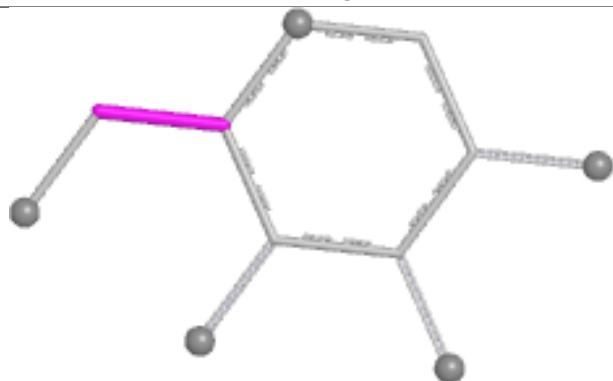
Ligand GLA C 2004



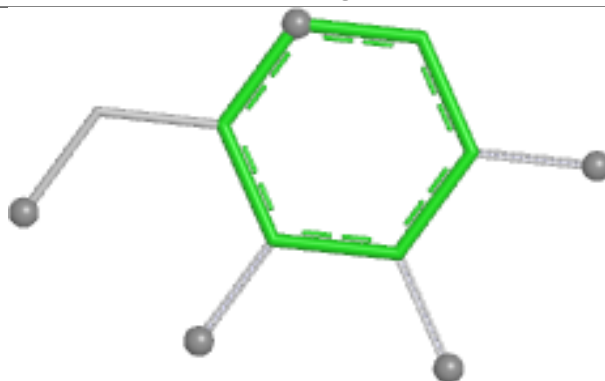
Bond lengths



Bond angles

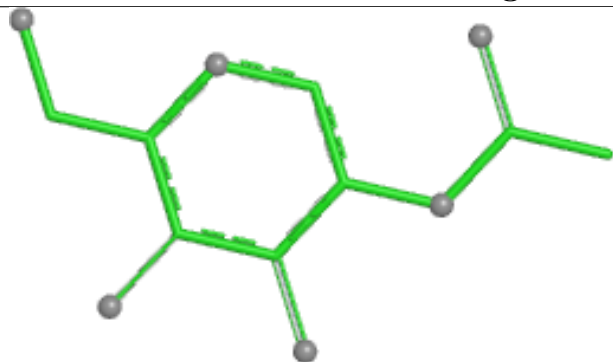


Torsions

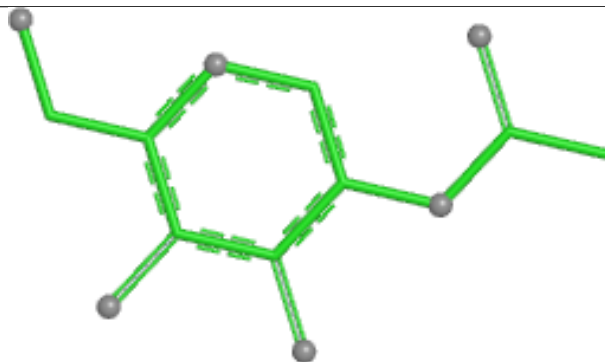


Rings

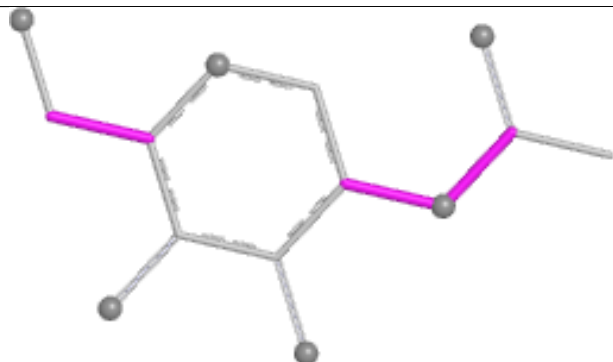
Ligand NAG B 2018



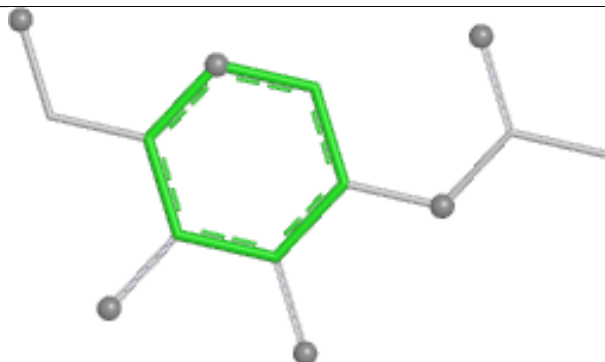
Bond lengths



Bond angles

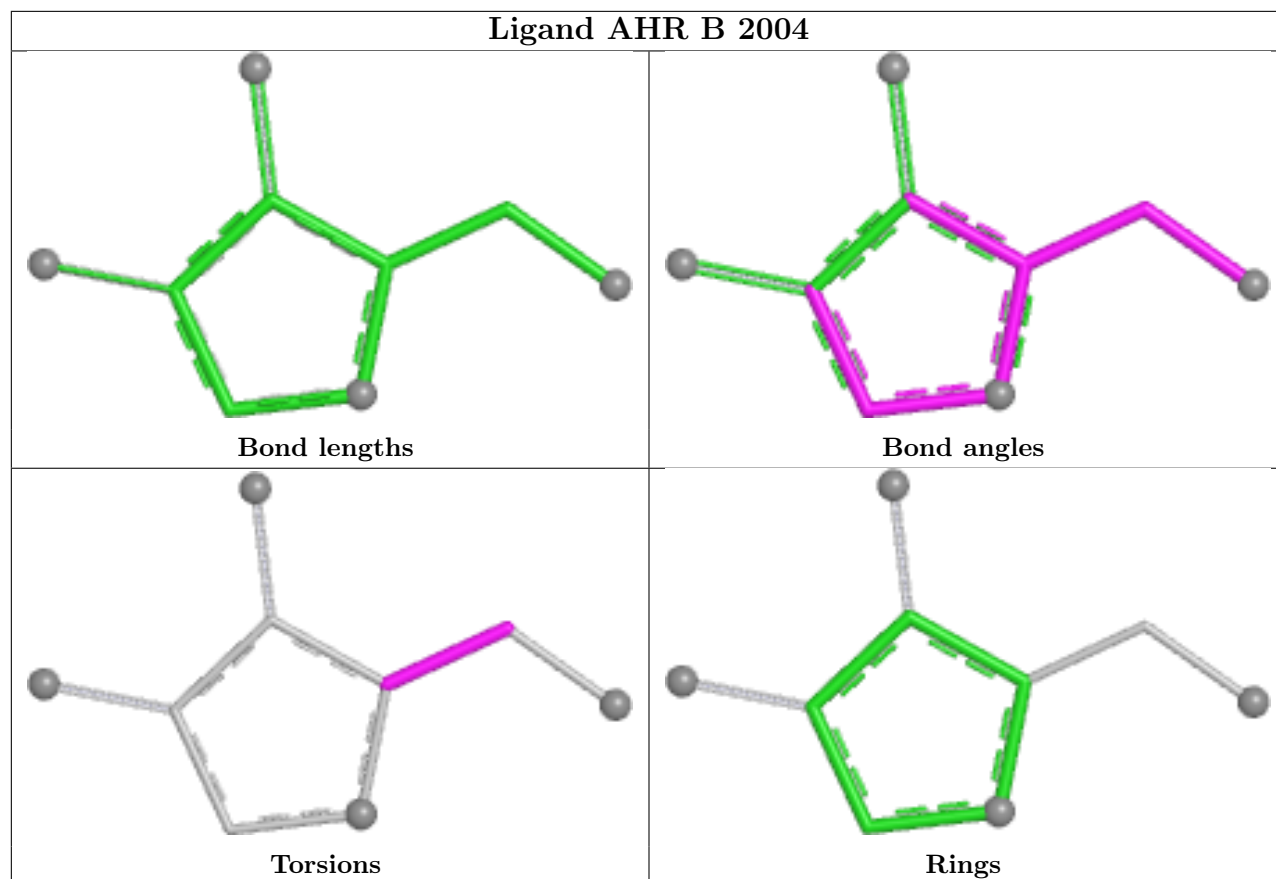


Torsions

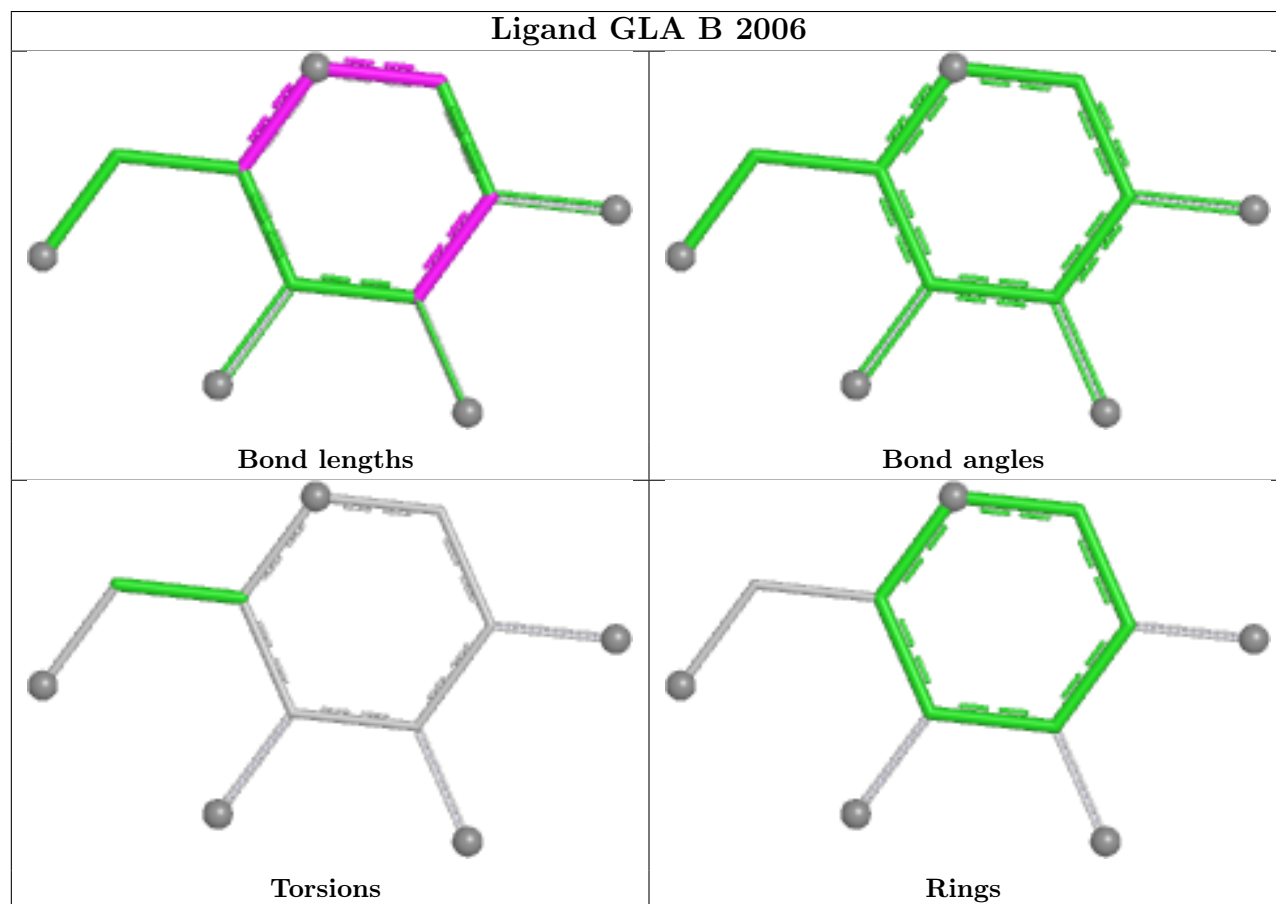


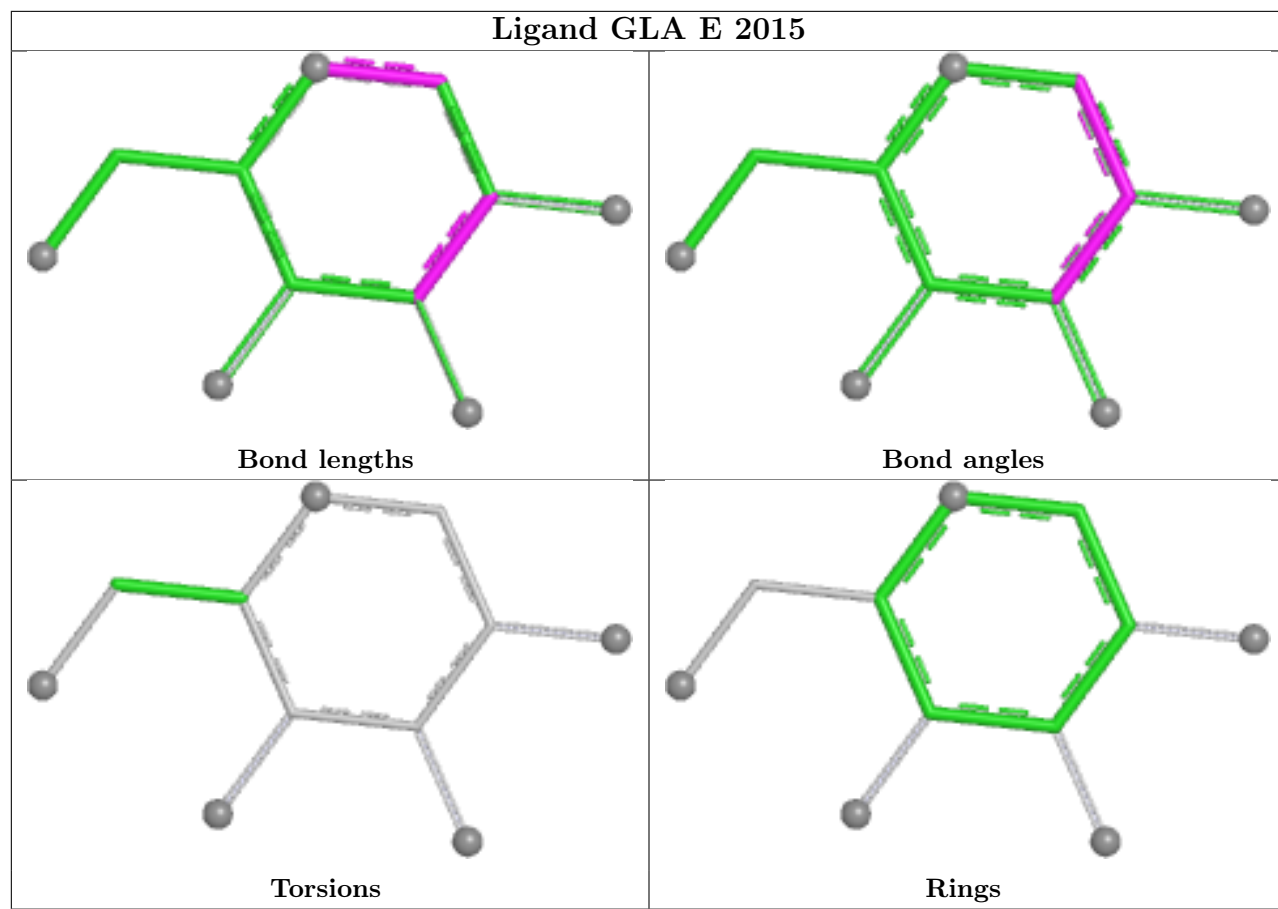
Rings

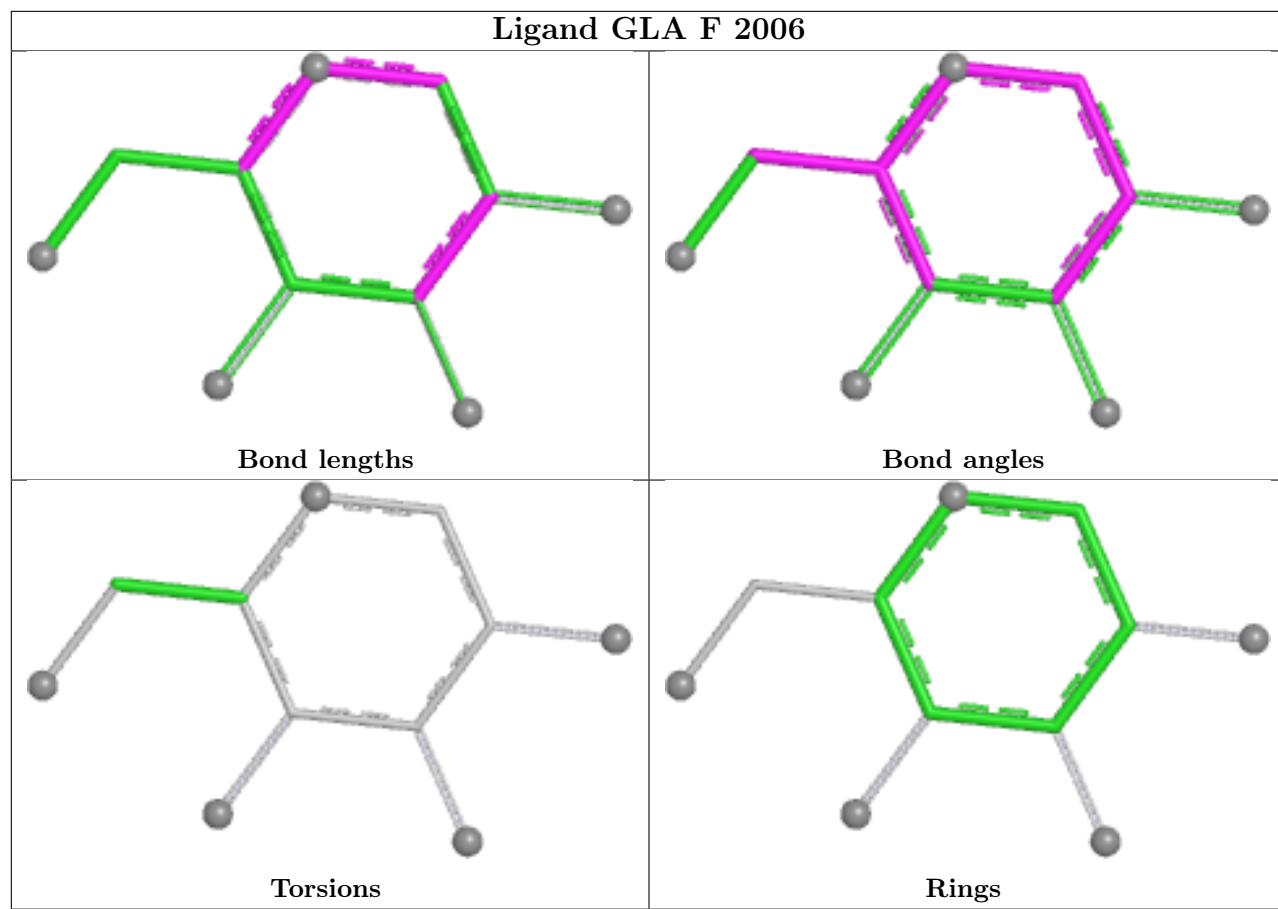
Ligand AHR B 2004

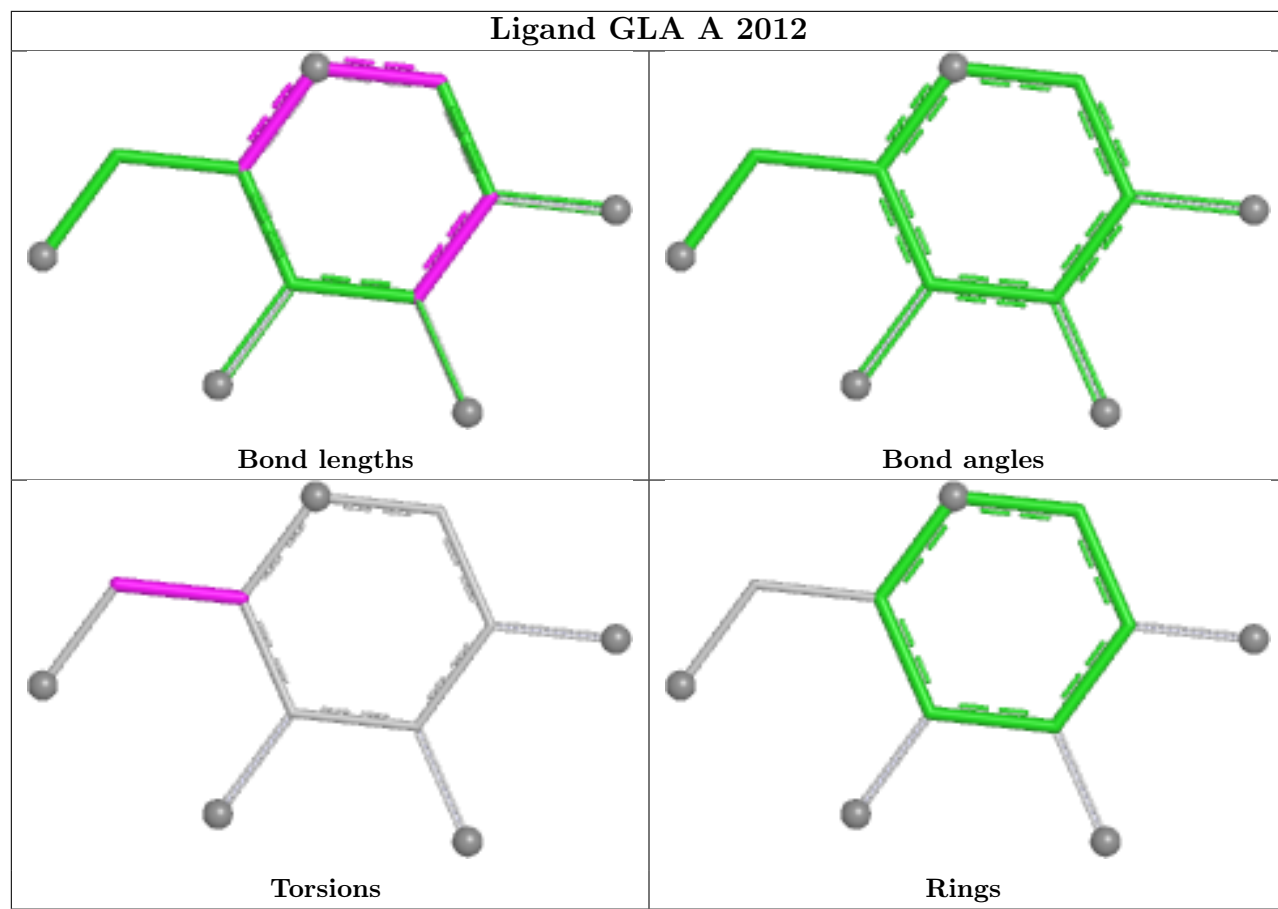


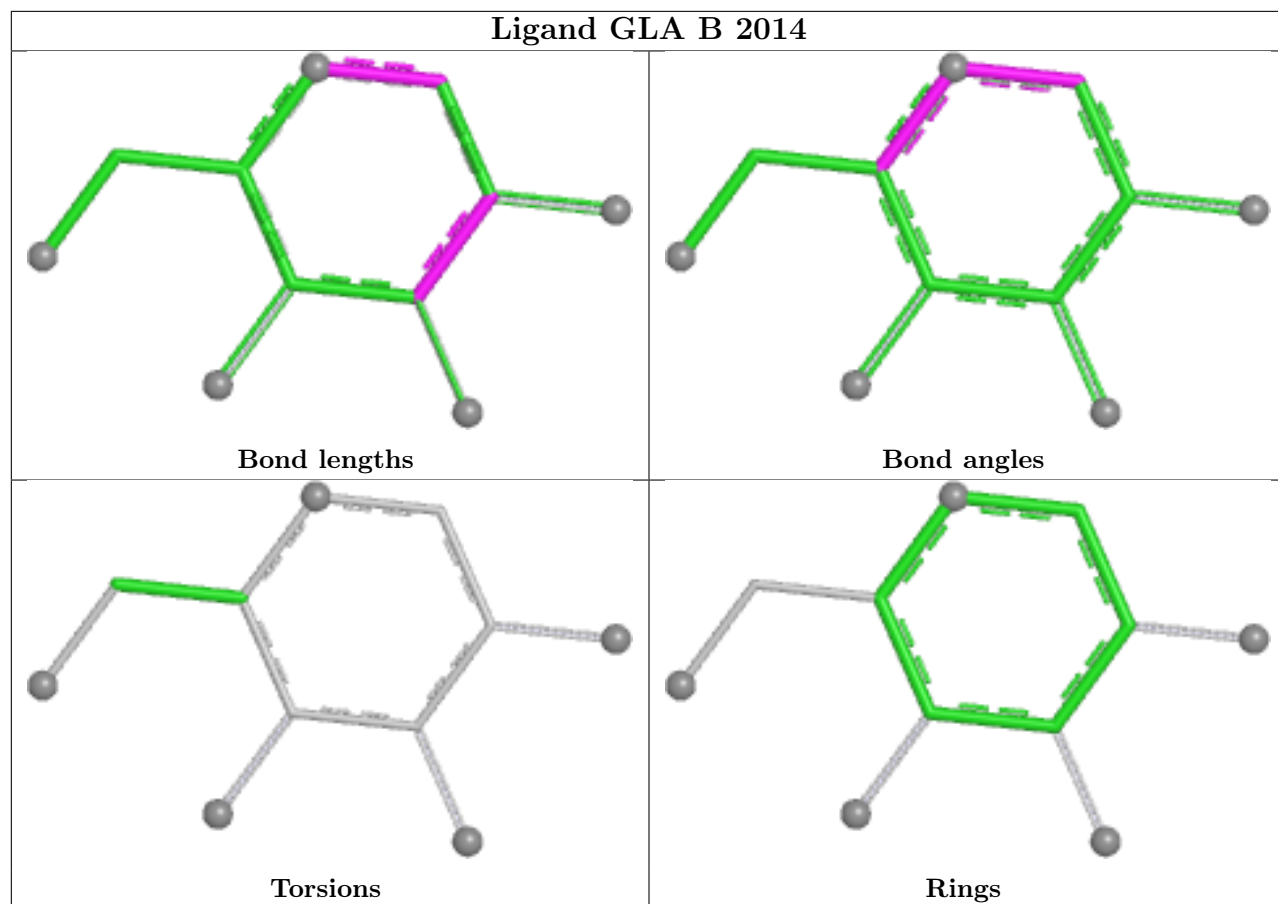
Ligand GLA B 2006

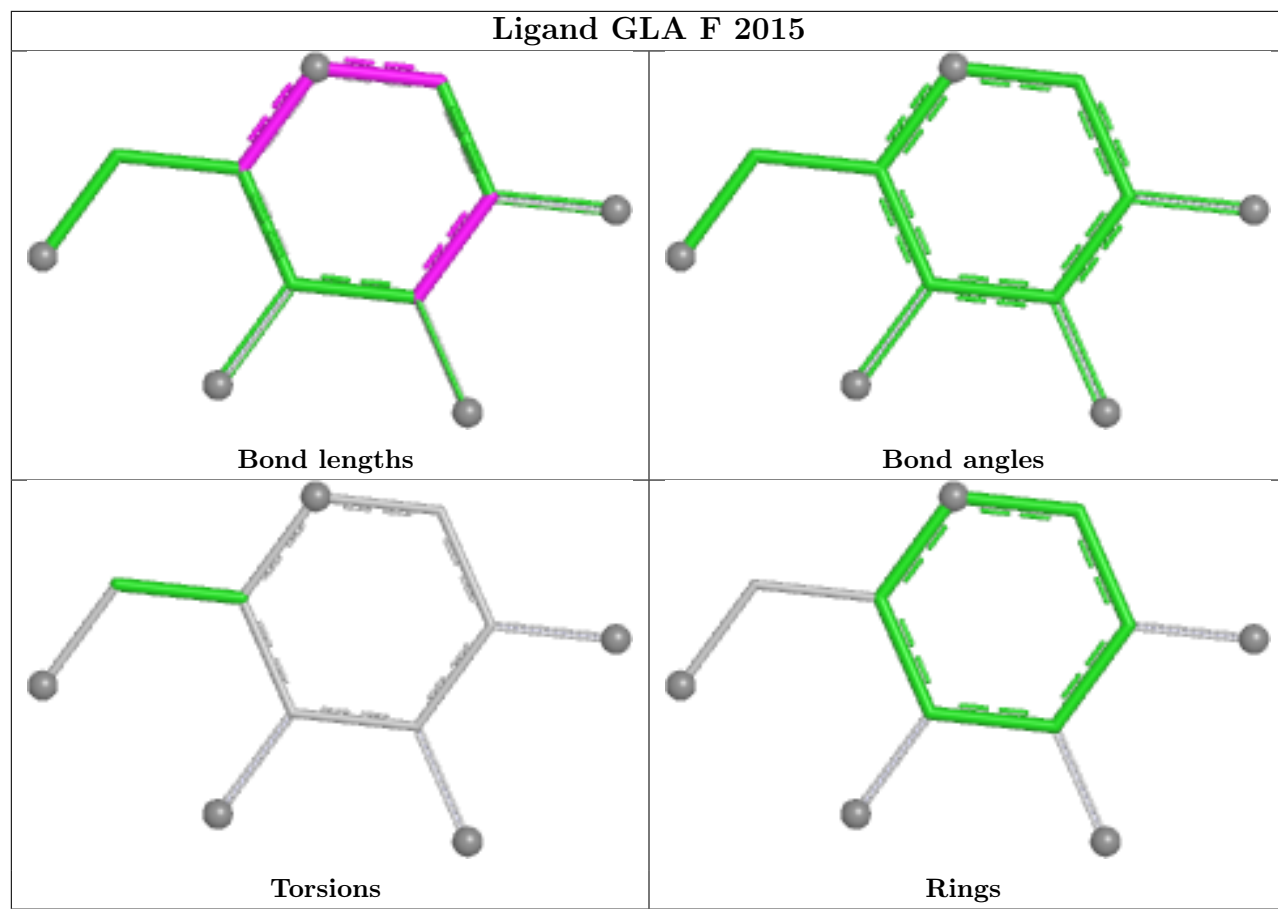


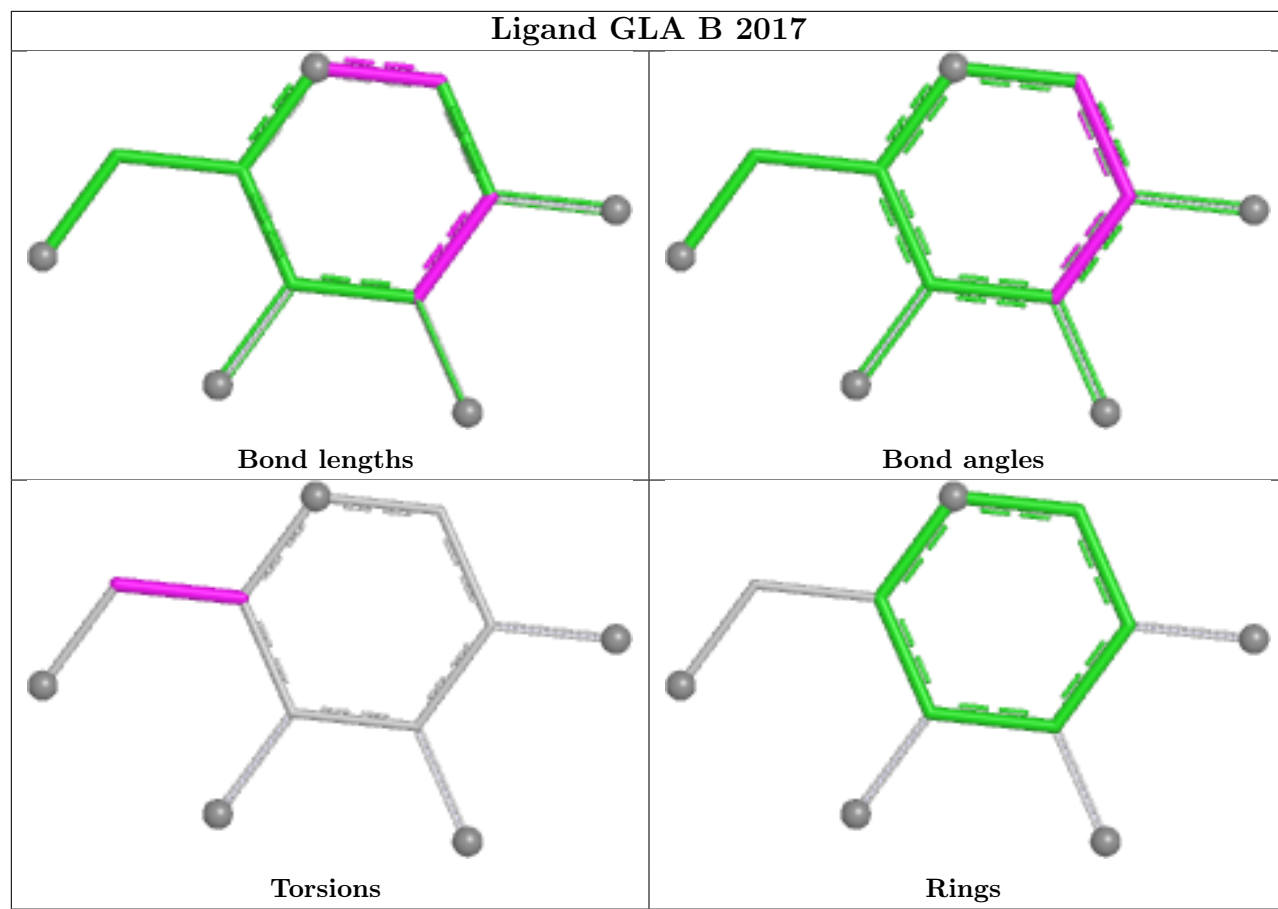


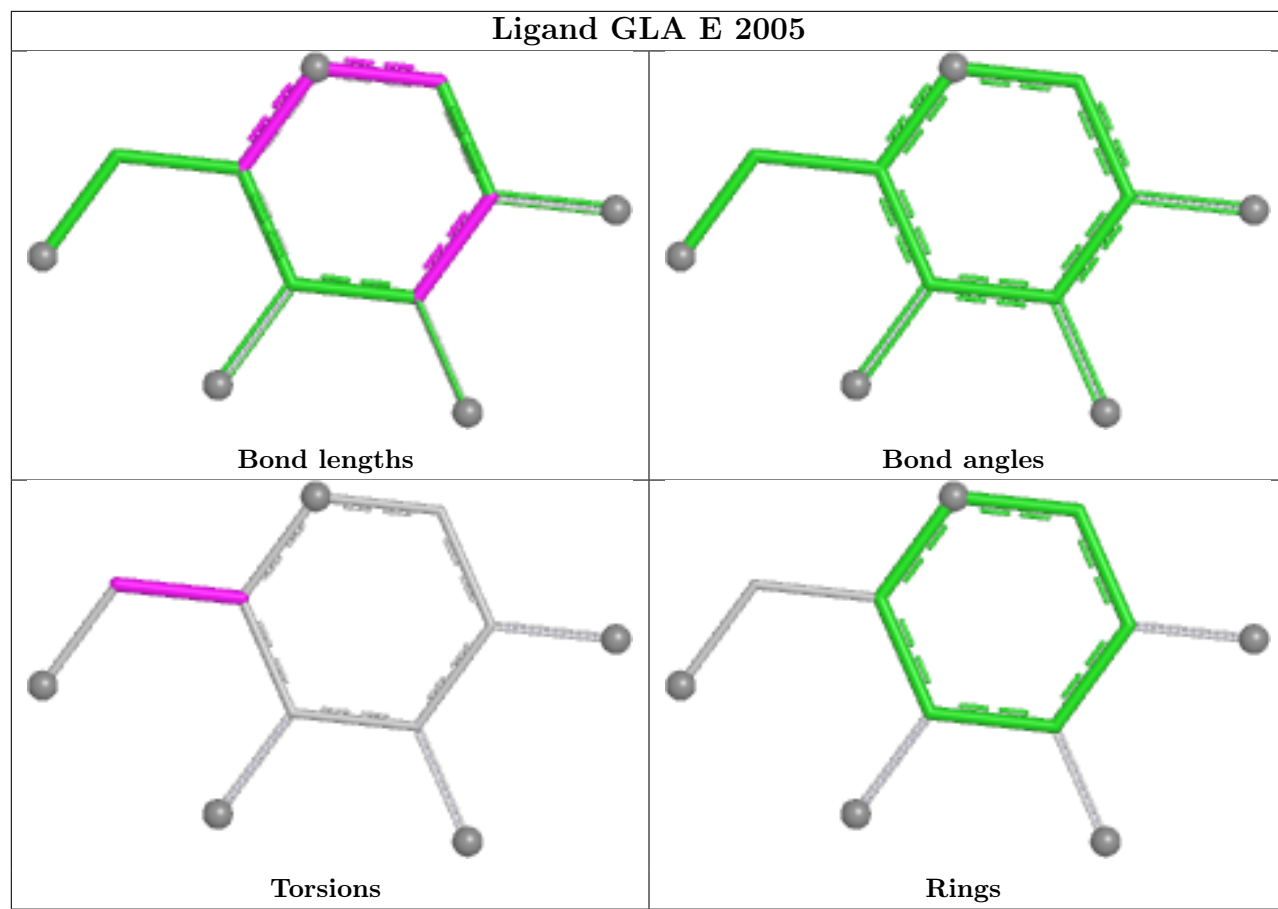


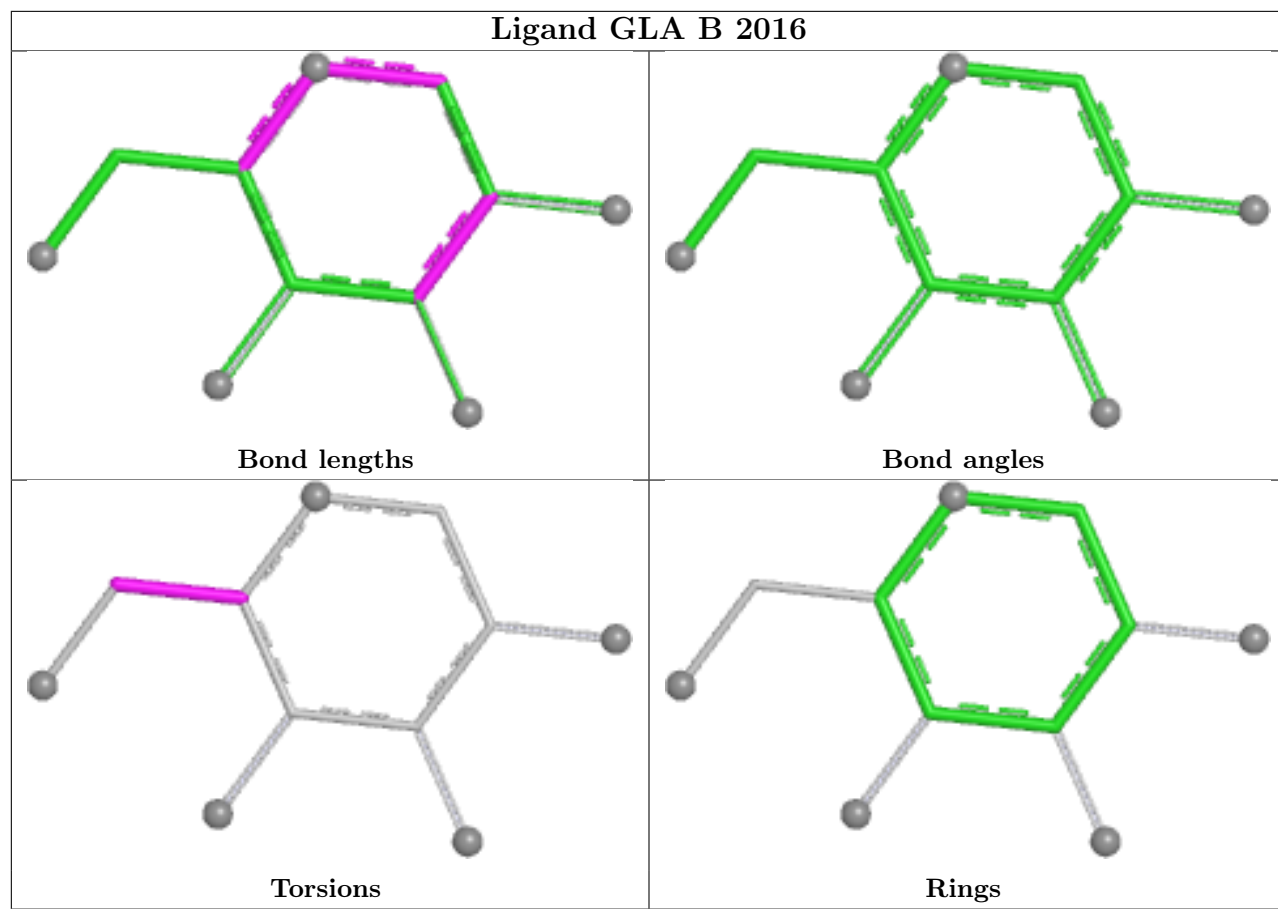


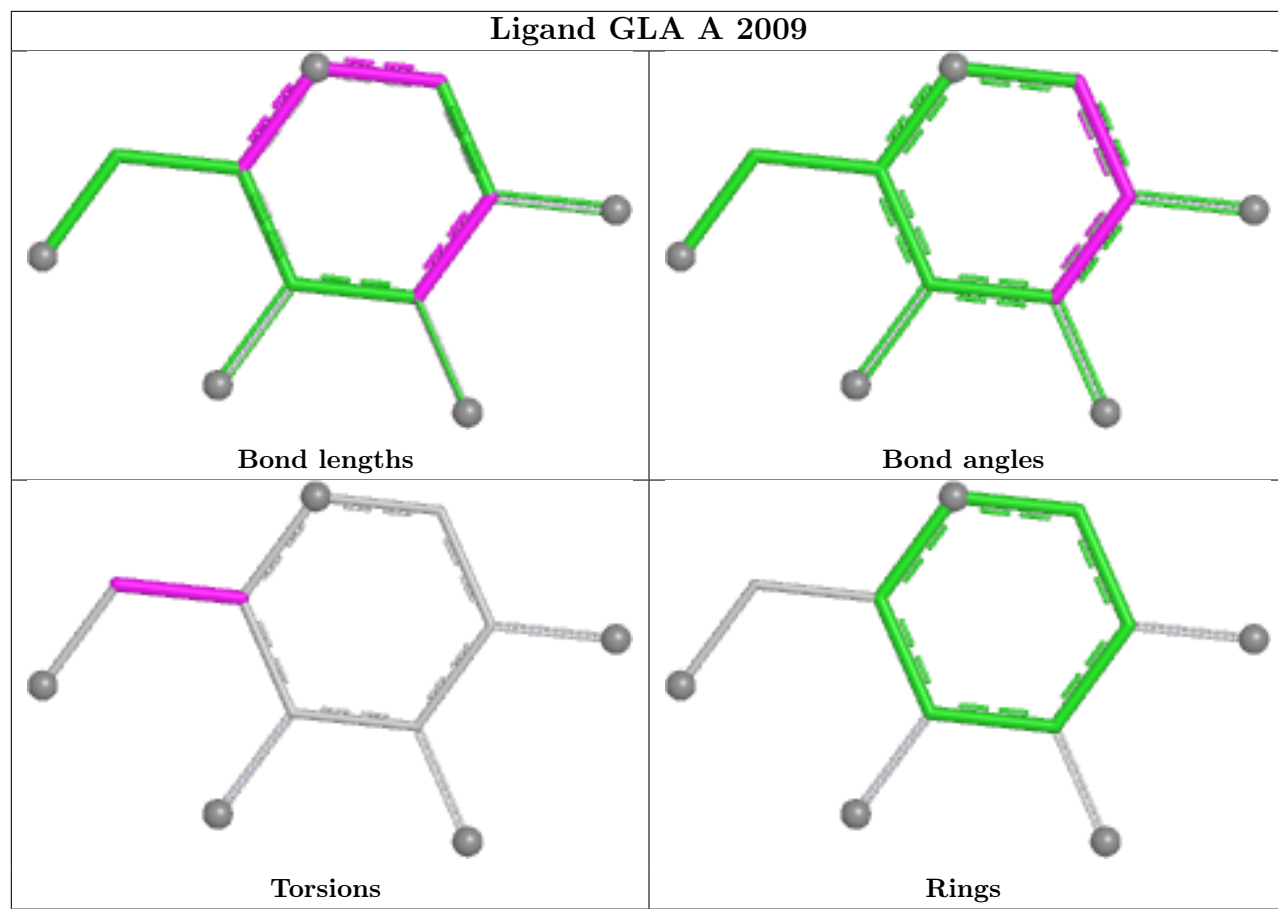


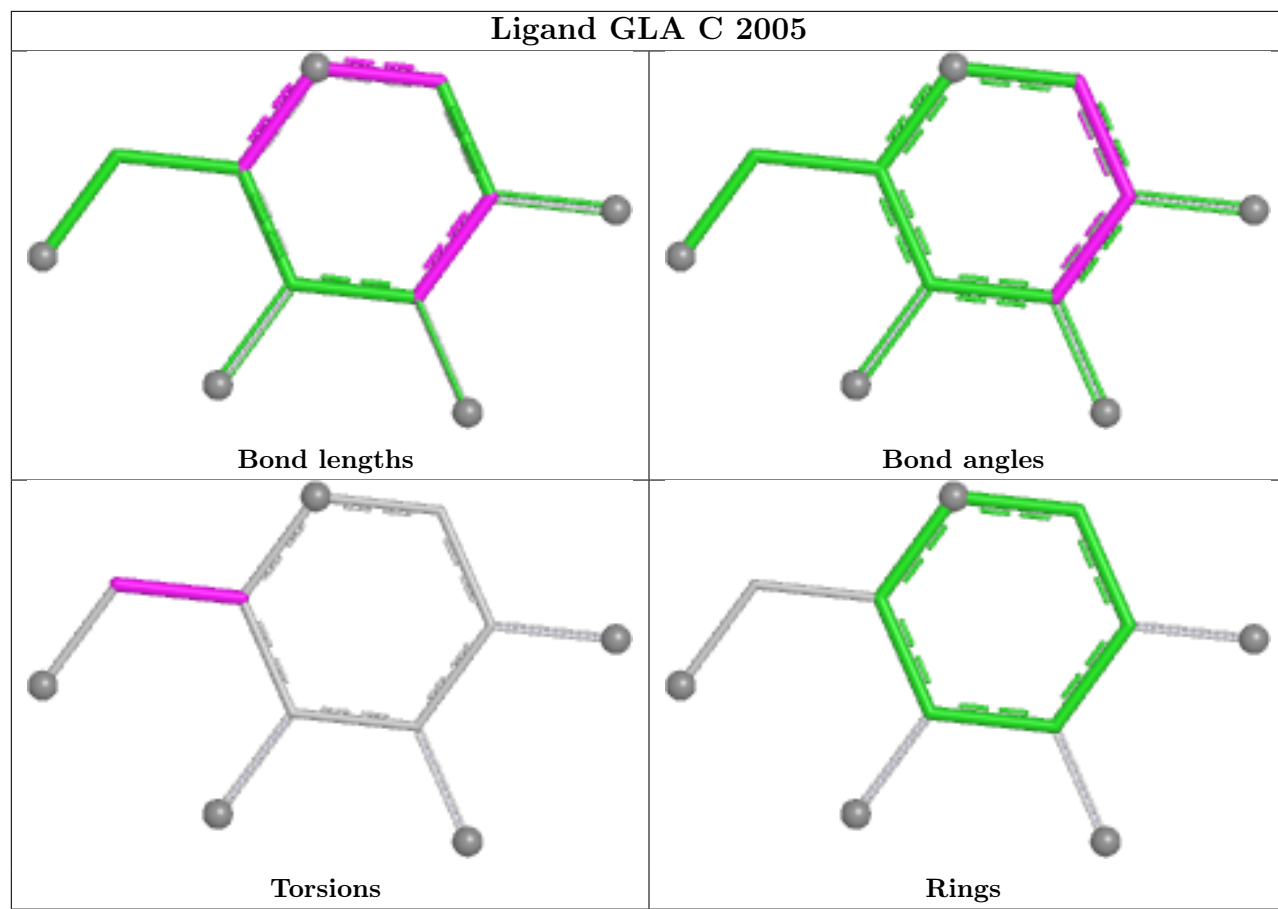


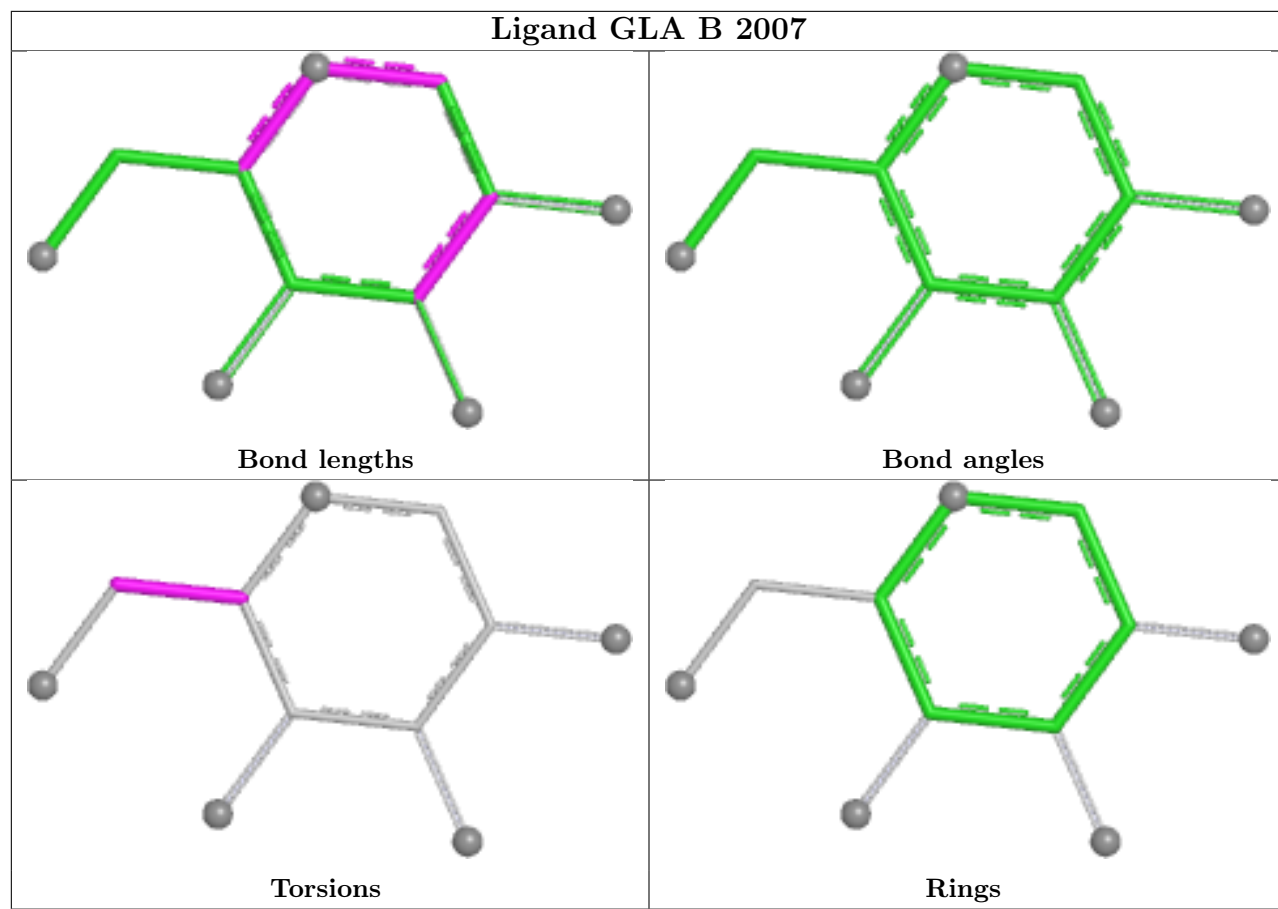


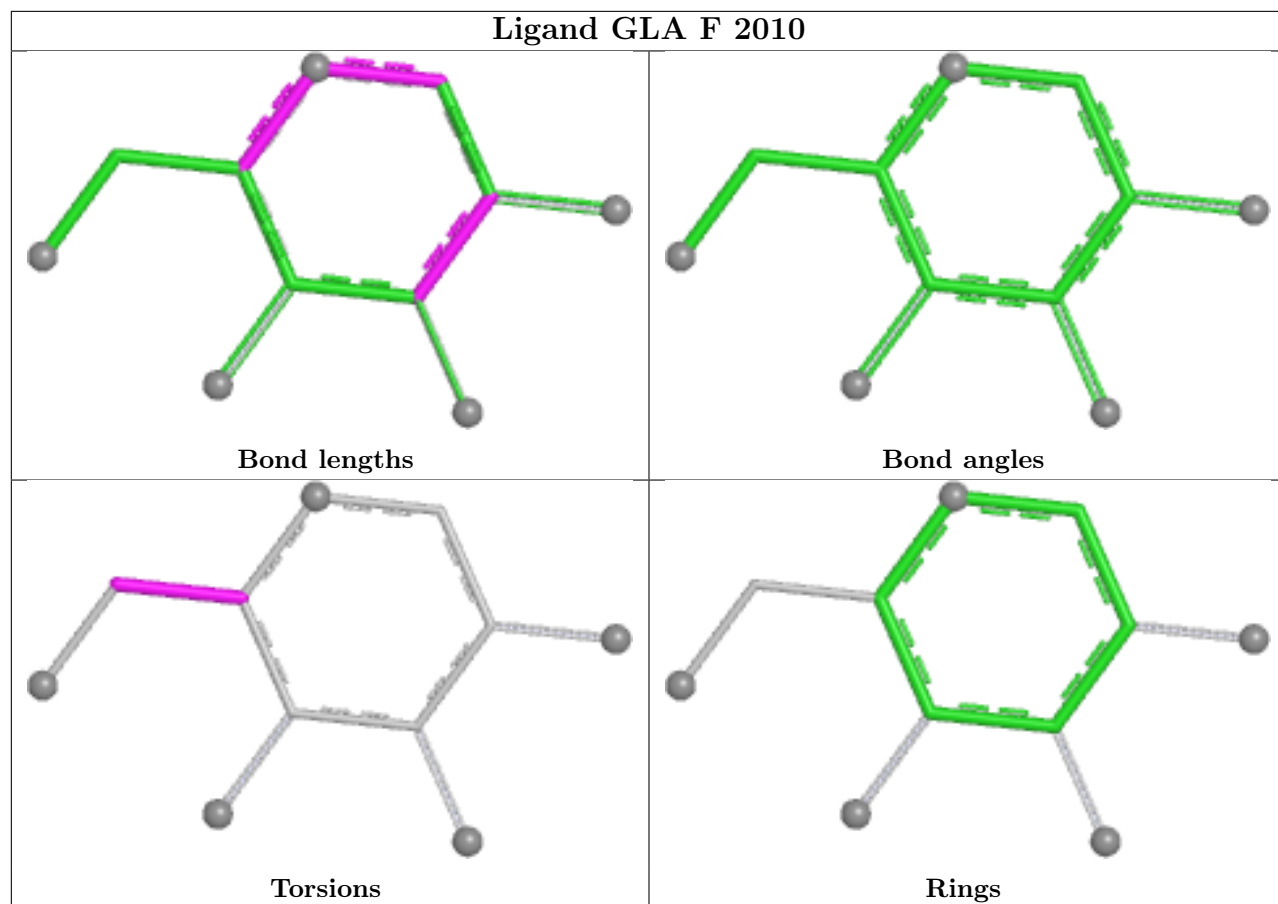




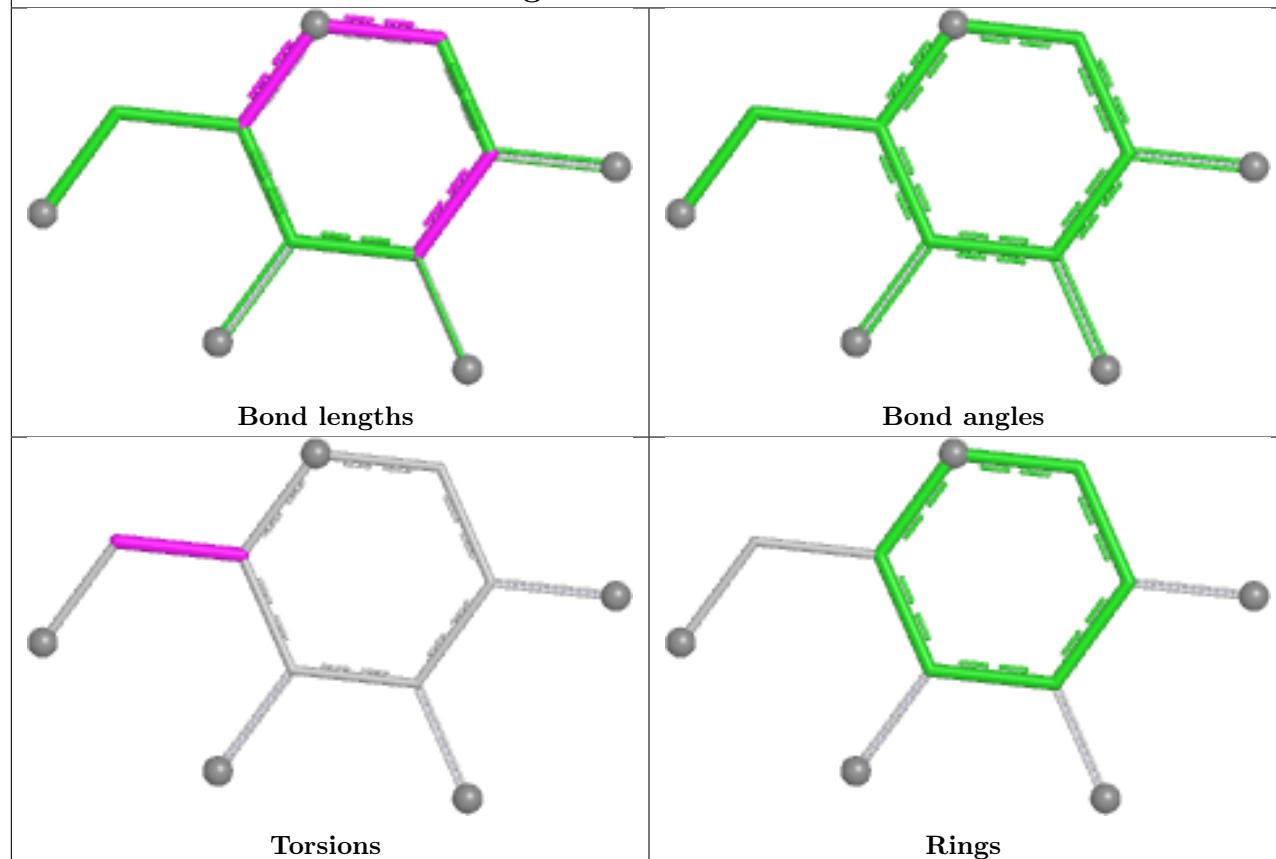




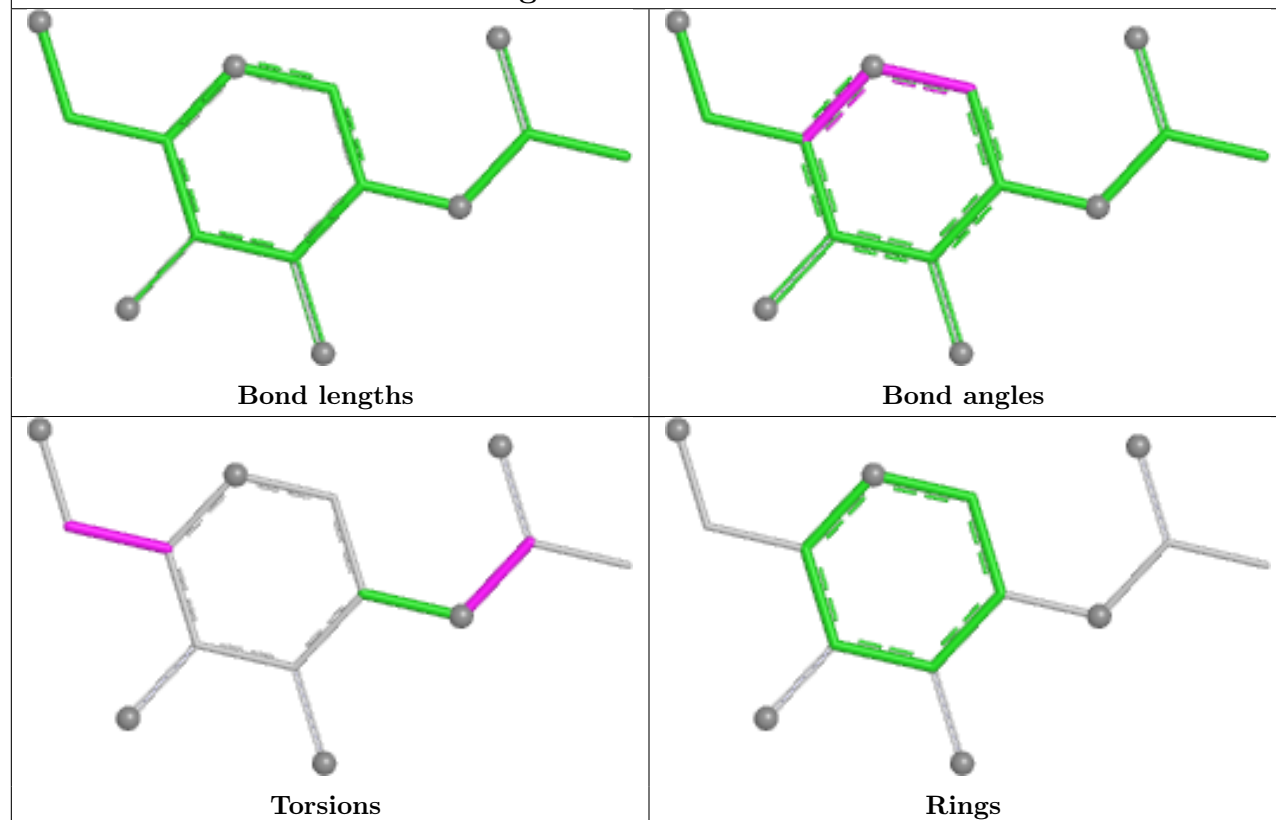




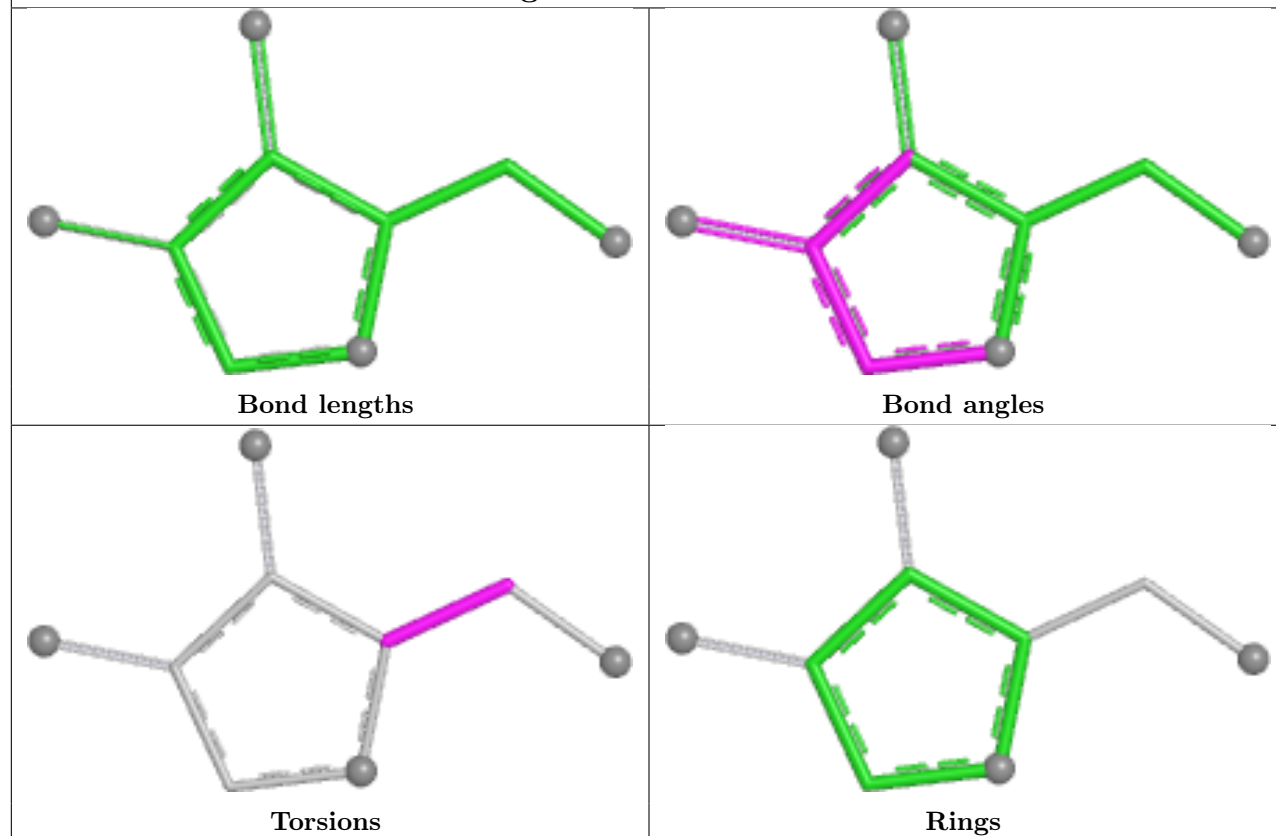
Ligand GLA E 2011



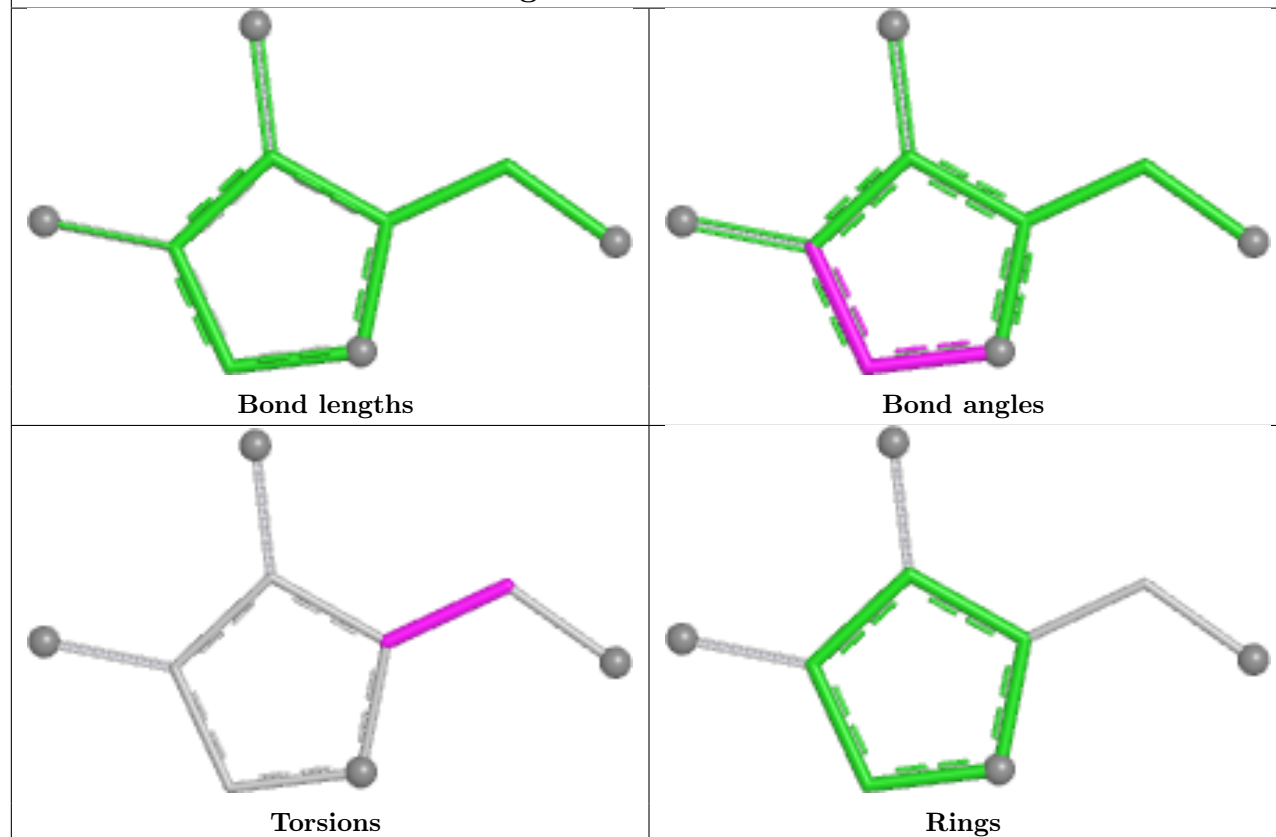
Ligand NAG C 2010



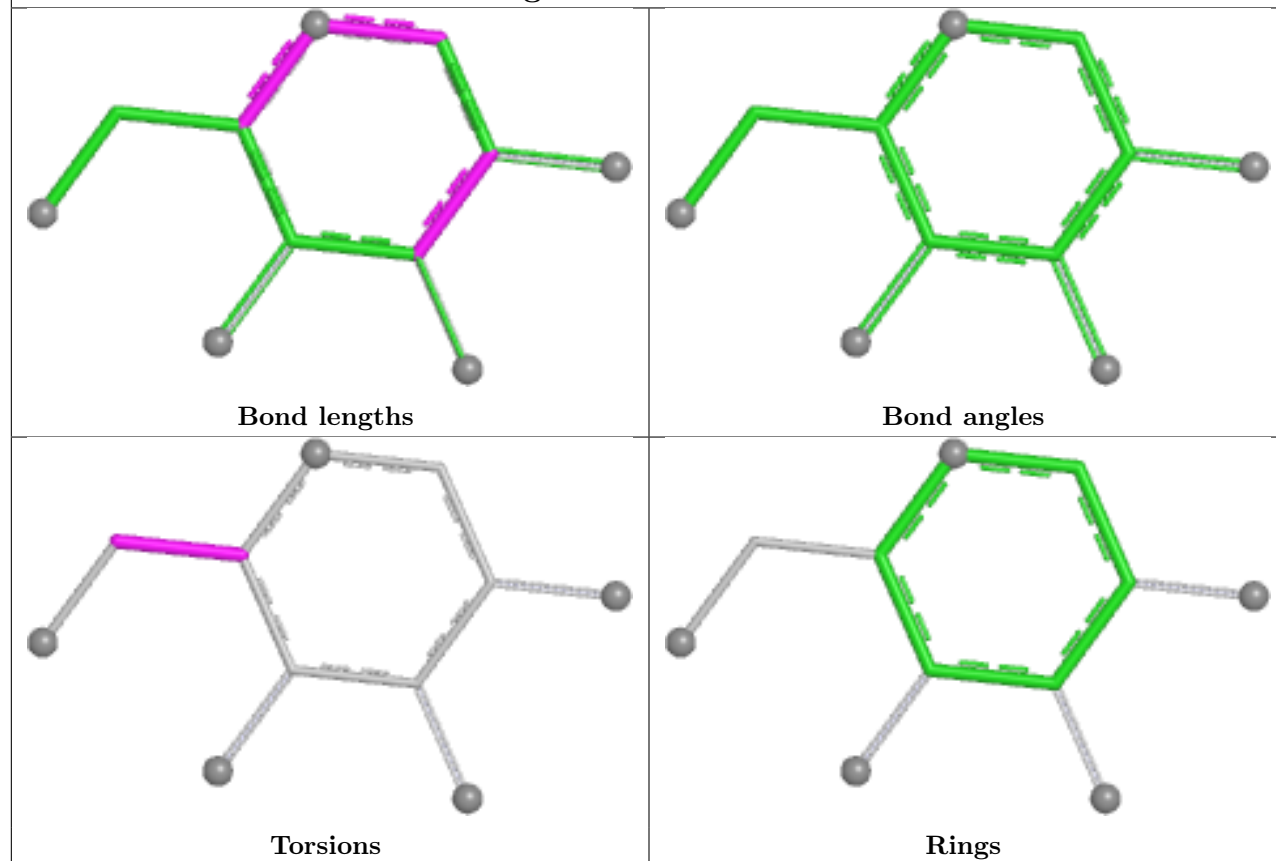
Ligand AHR E 2003



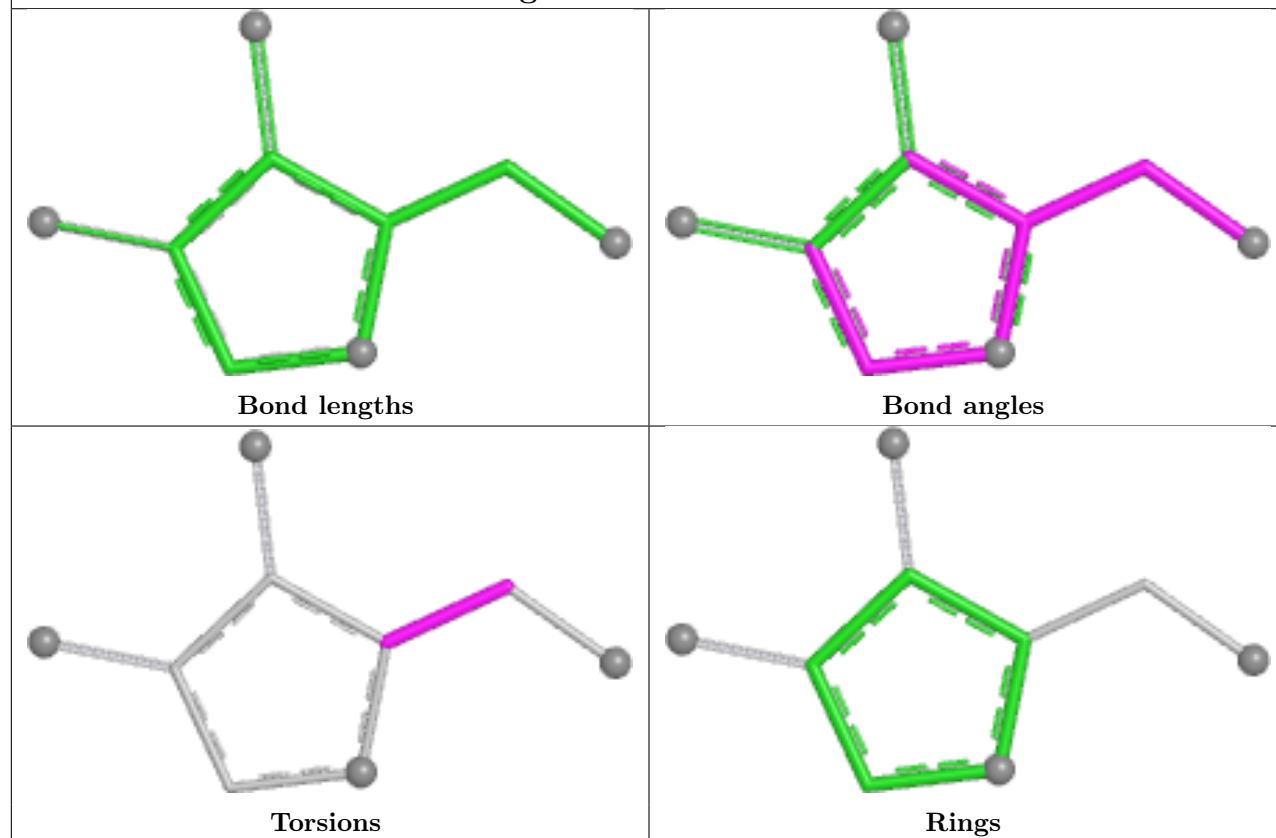
Ligand AHR C 2001



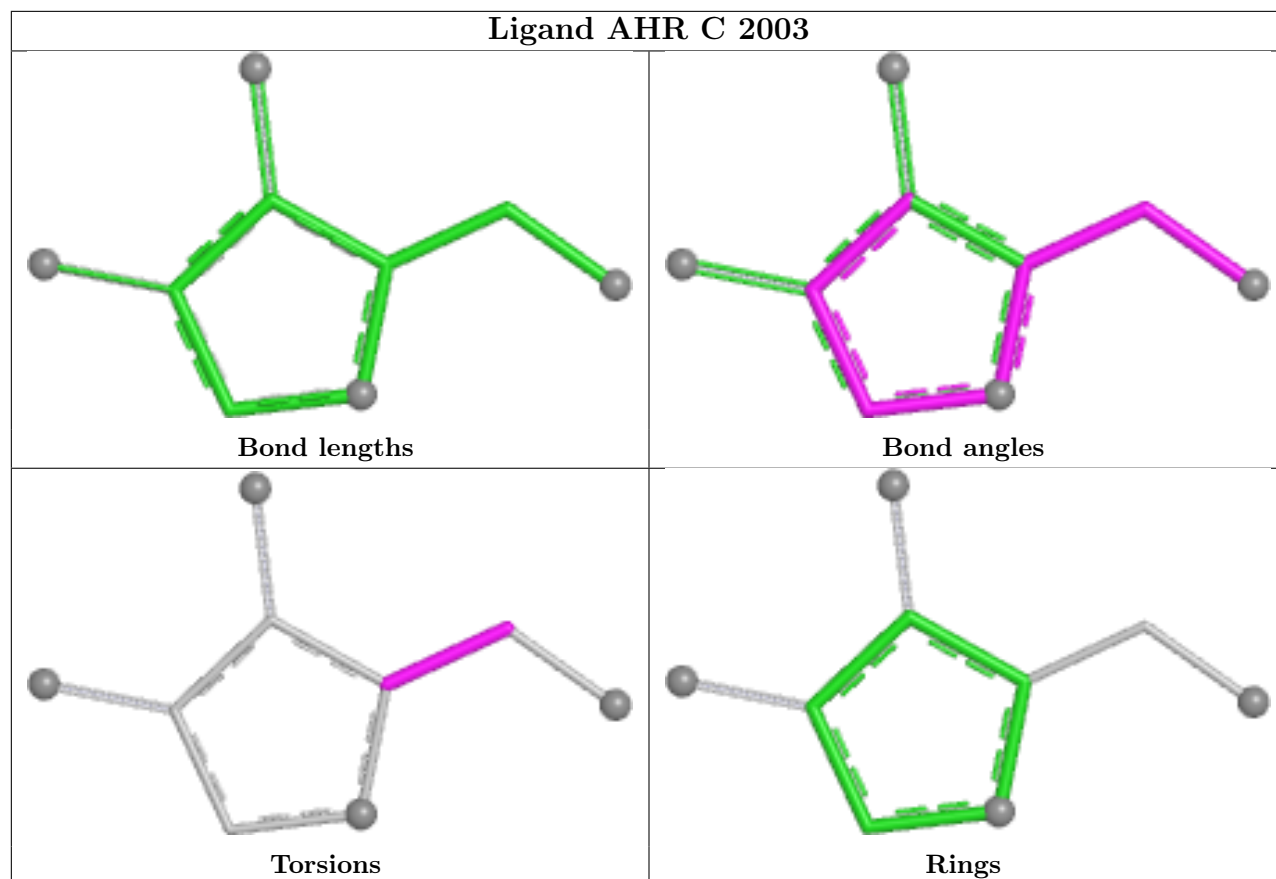
Ligand GLA F 2007



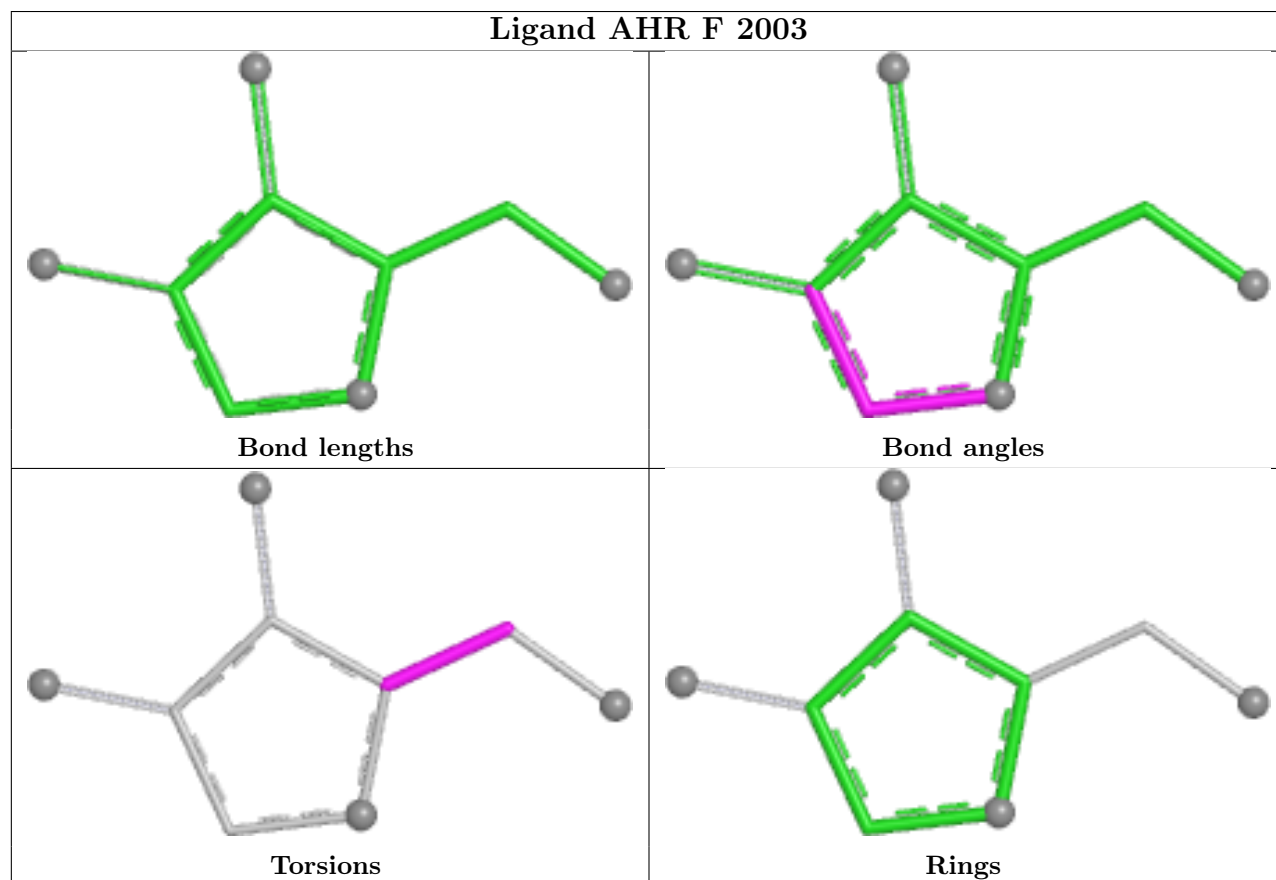
Ligand AHR B 2003



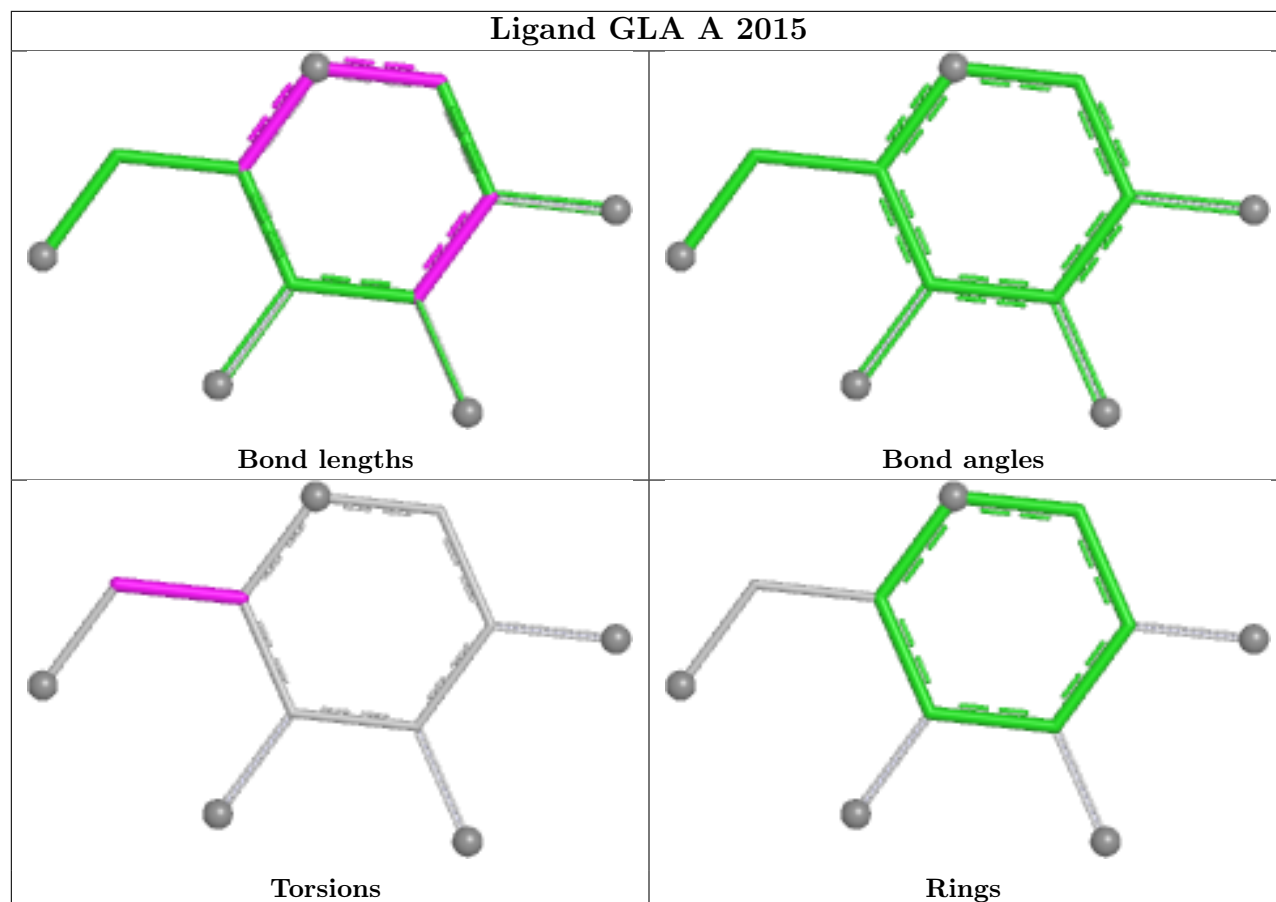
Ligand AHR C 2003



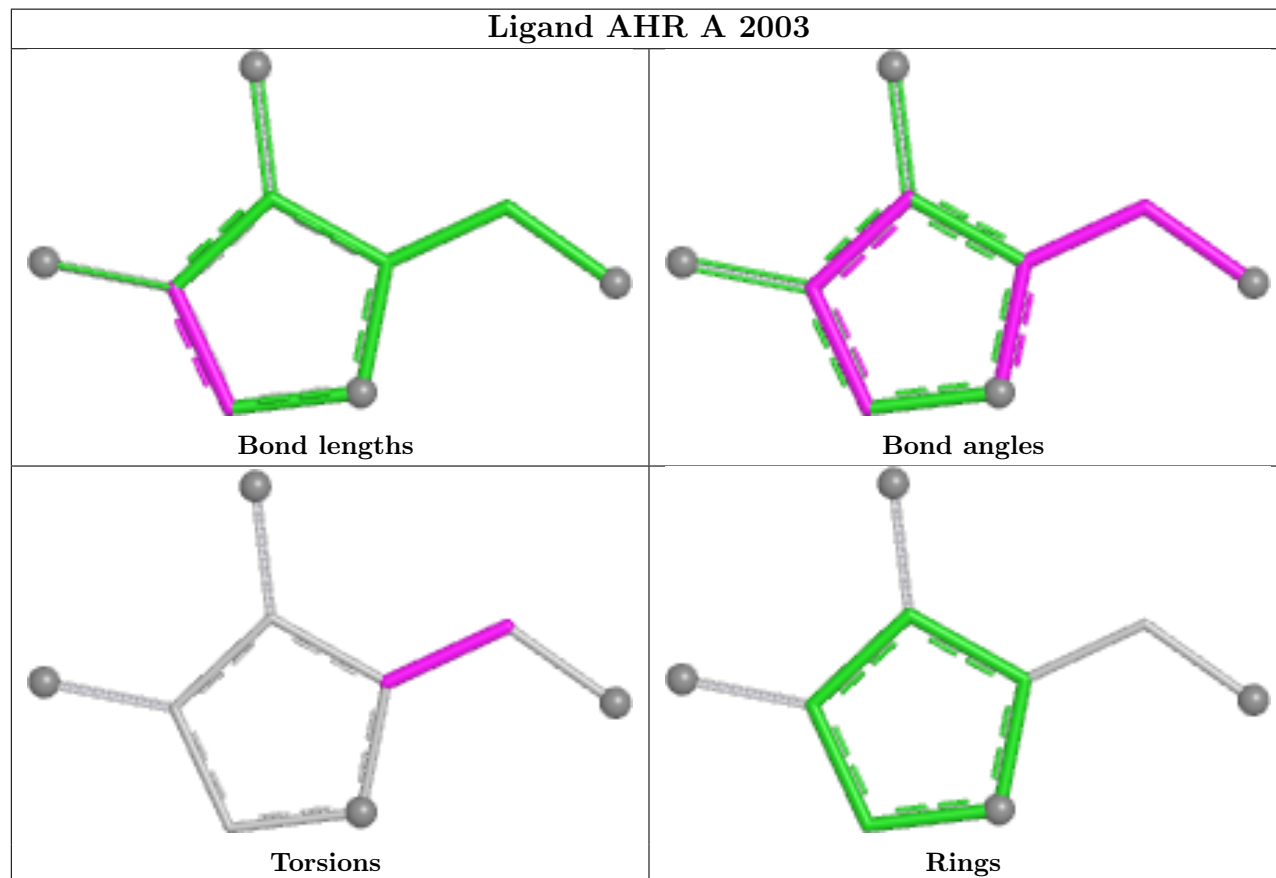
Ligand AHR F 2003



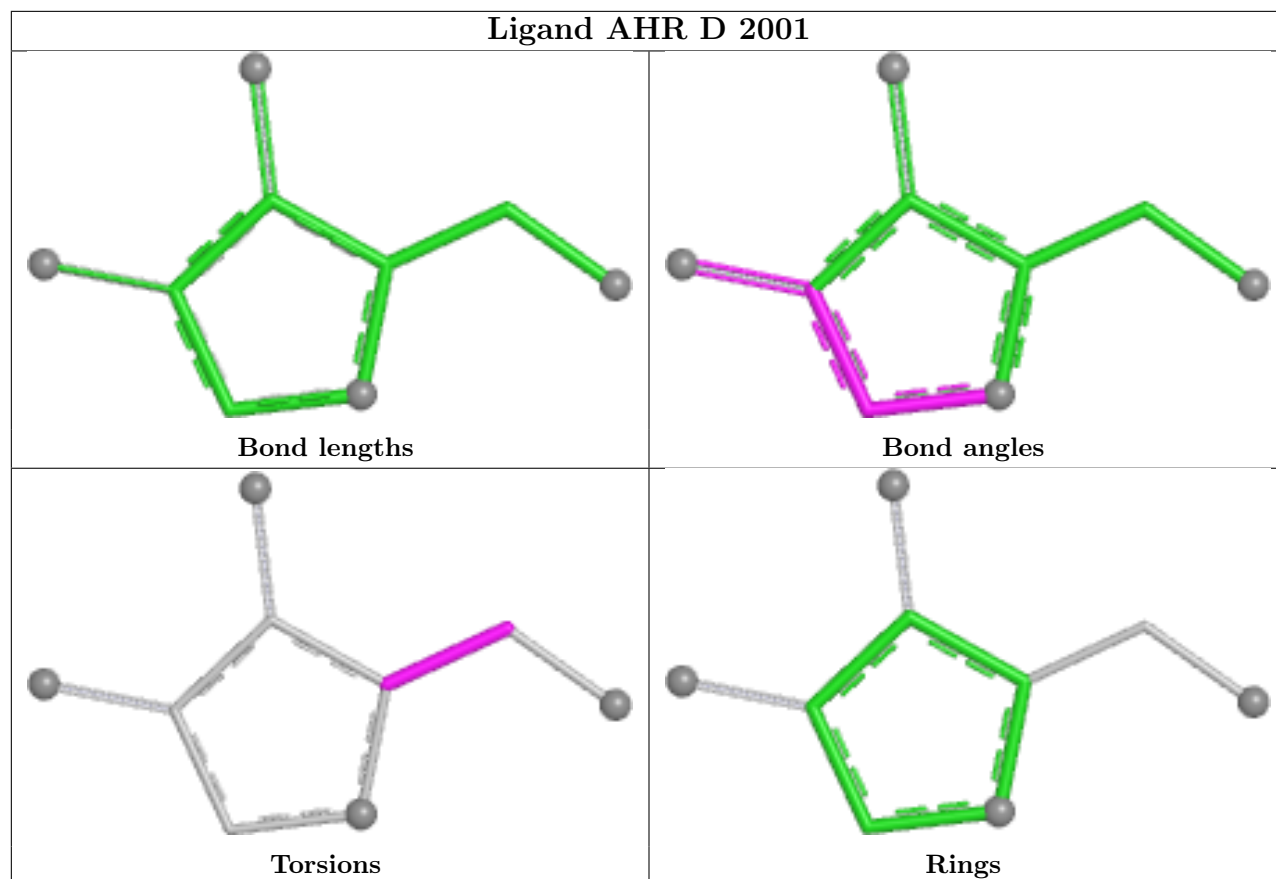
Ligand GLA A 2015



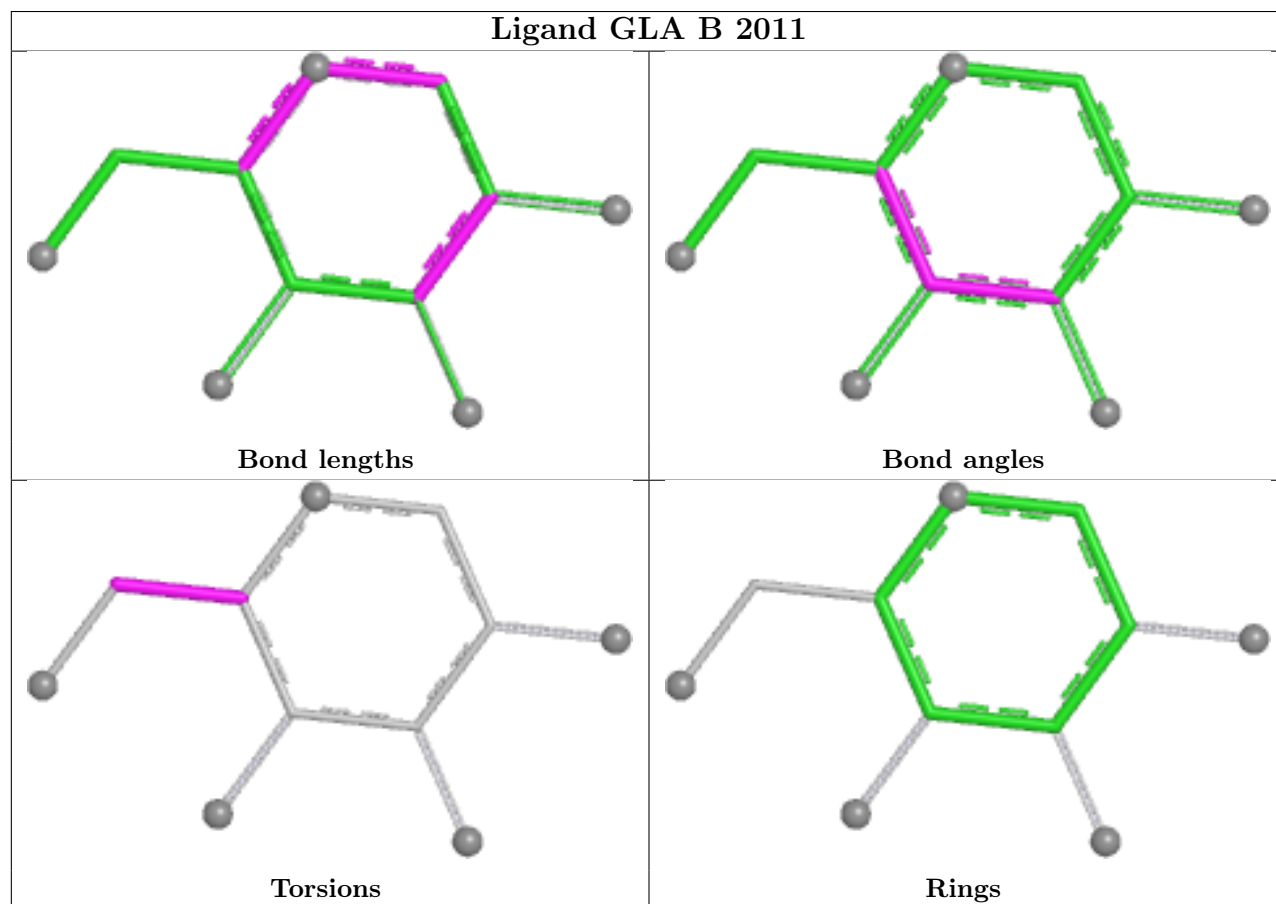
Ligand AHR A 2003



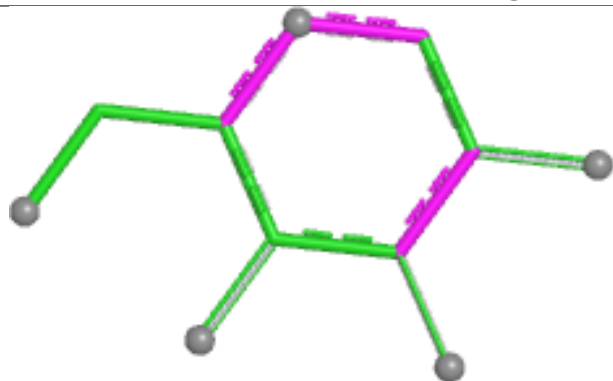
Ligand AHR D 2001



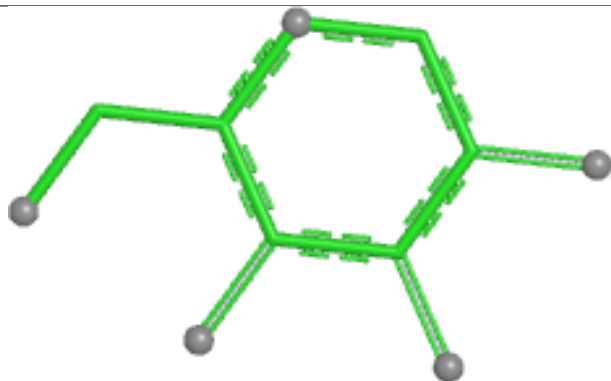
Ligand GLA B 2011



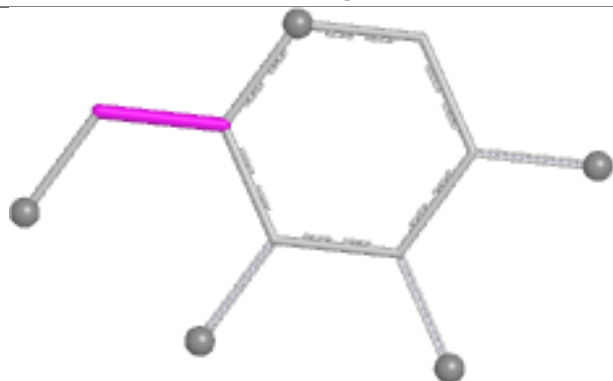
Ligand GLA E 2006



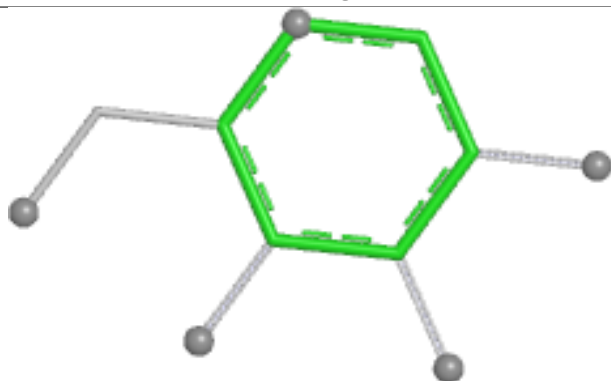
Bond lengths



Bond angles

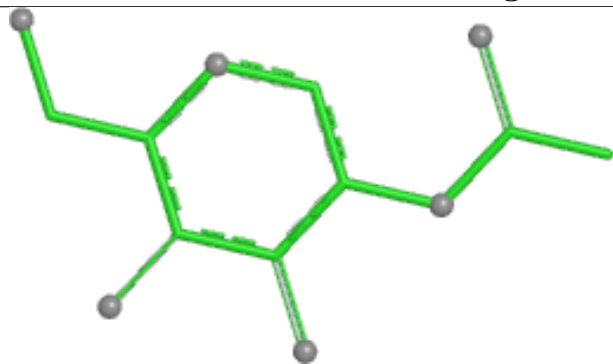


Torsions

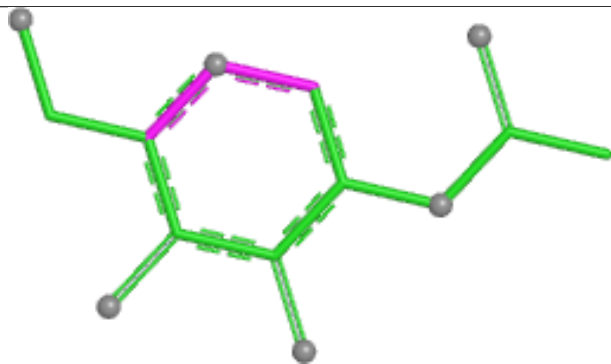


Rings

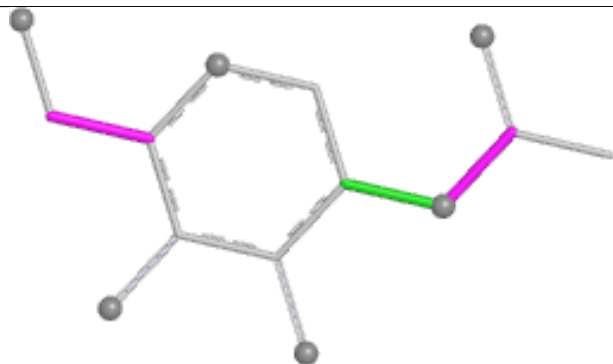
Ligand NAG E 2017



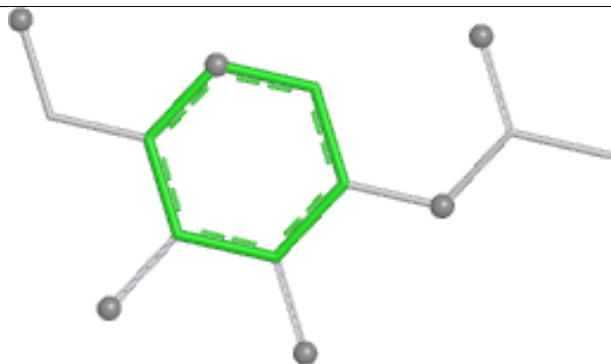
Bond lengths



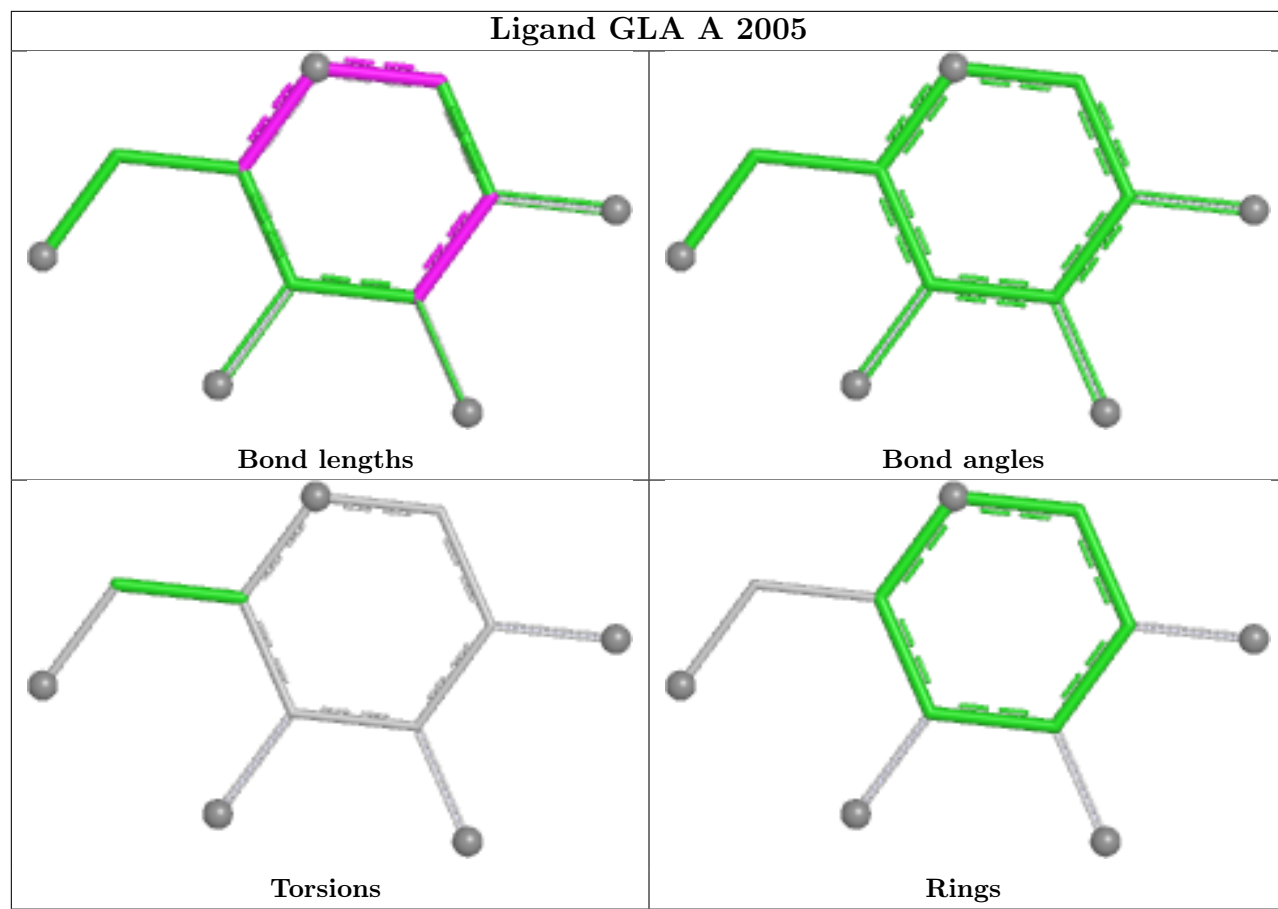
Bond angles

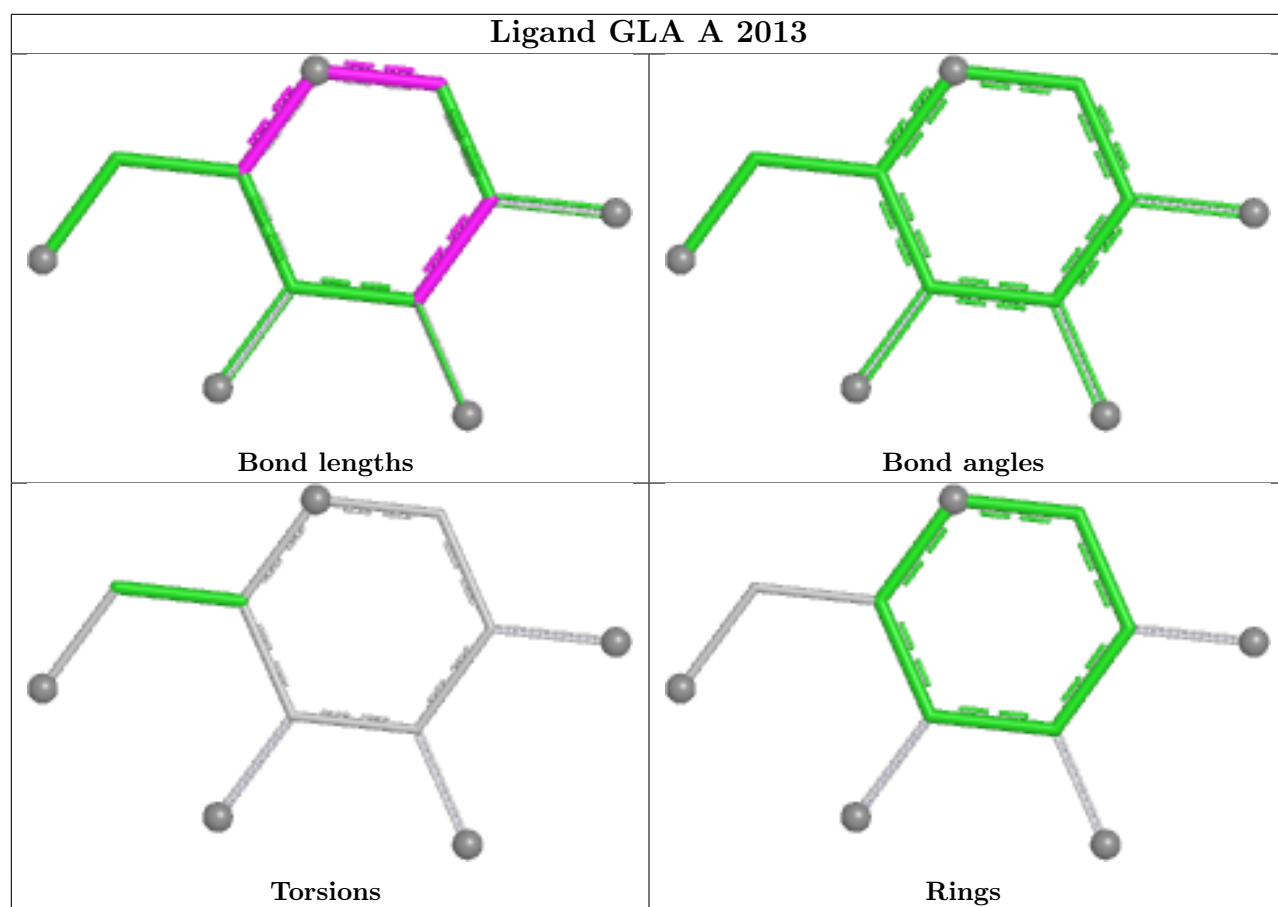


Torsions

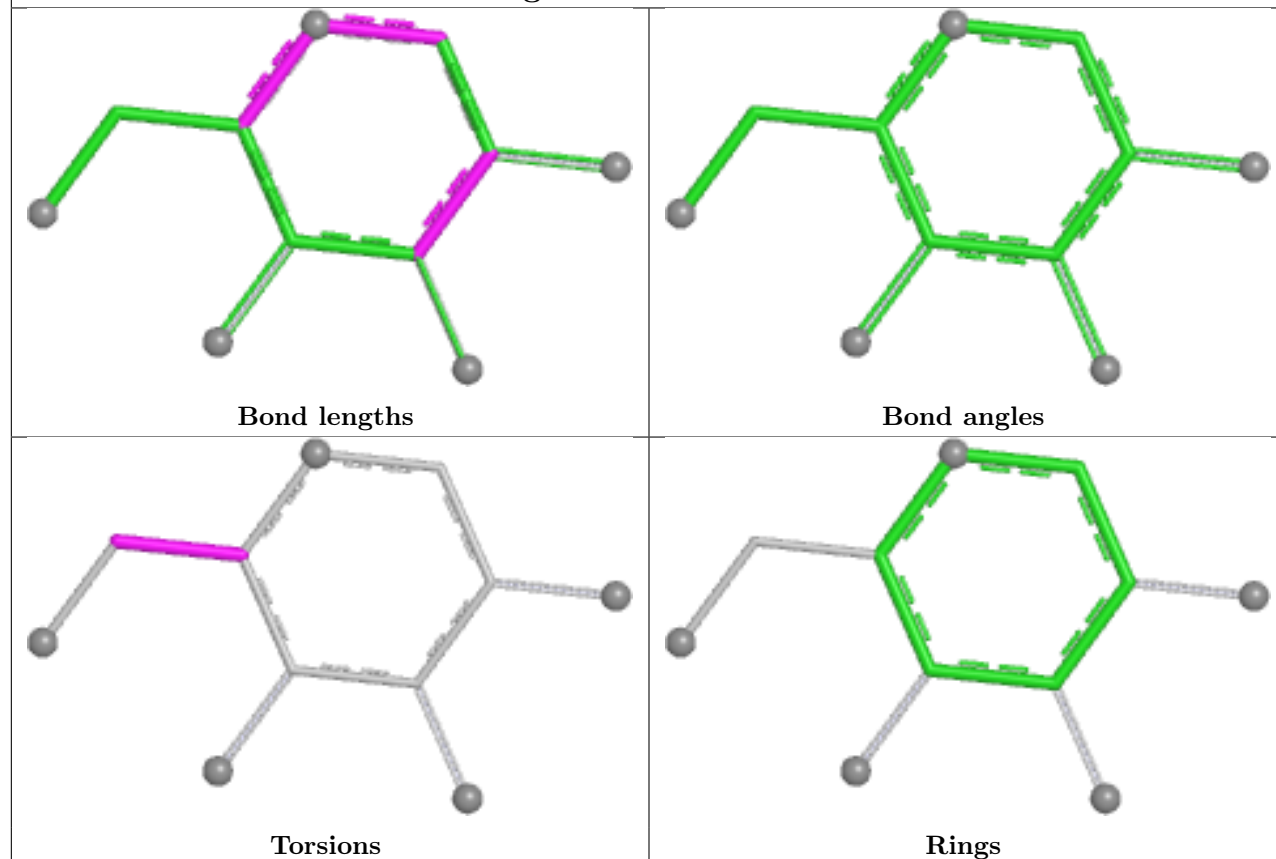


Rings

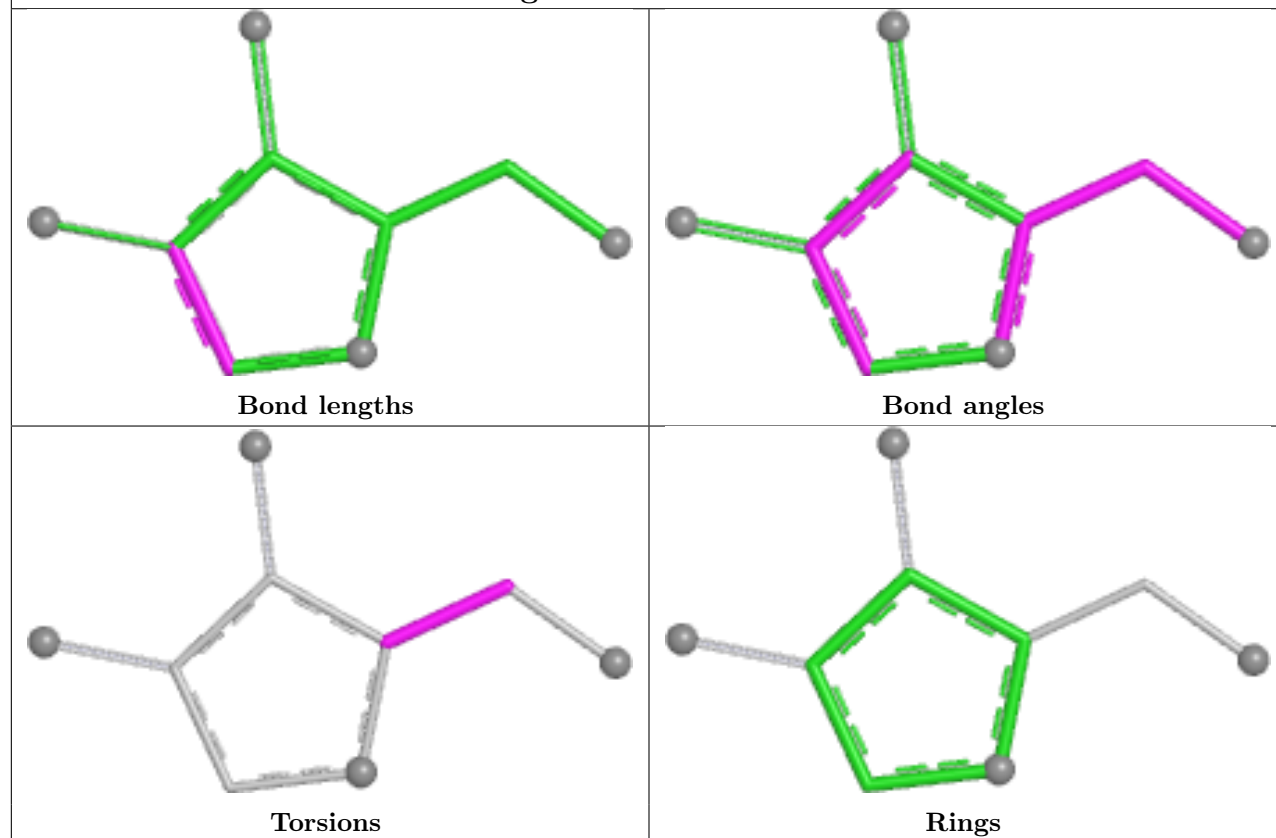


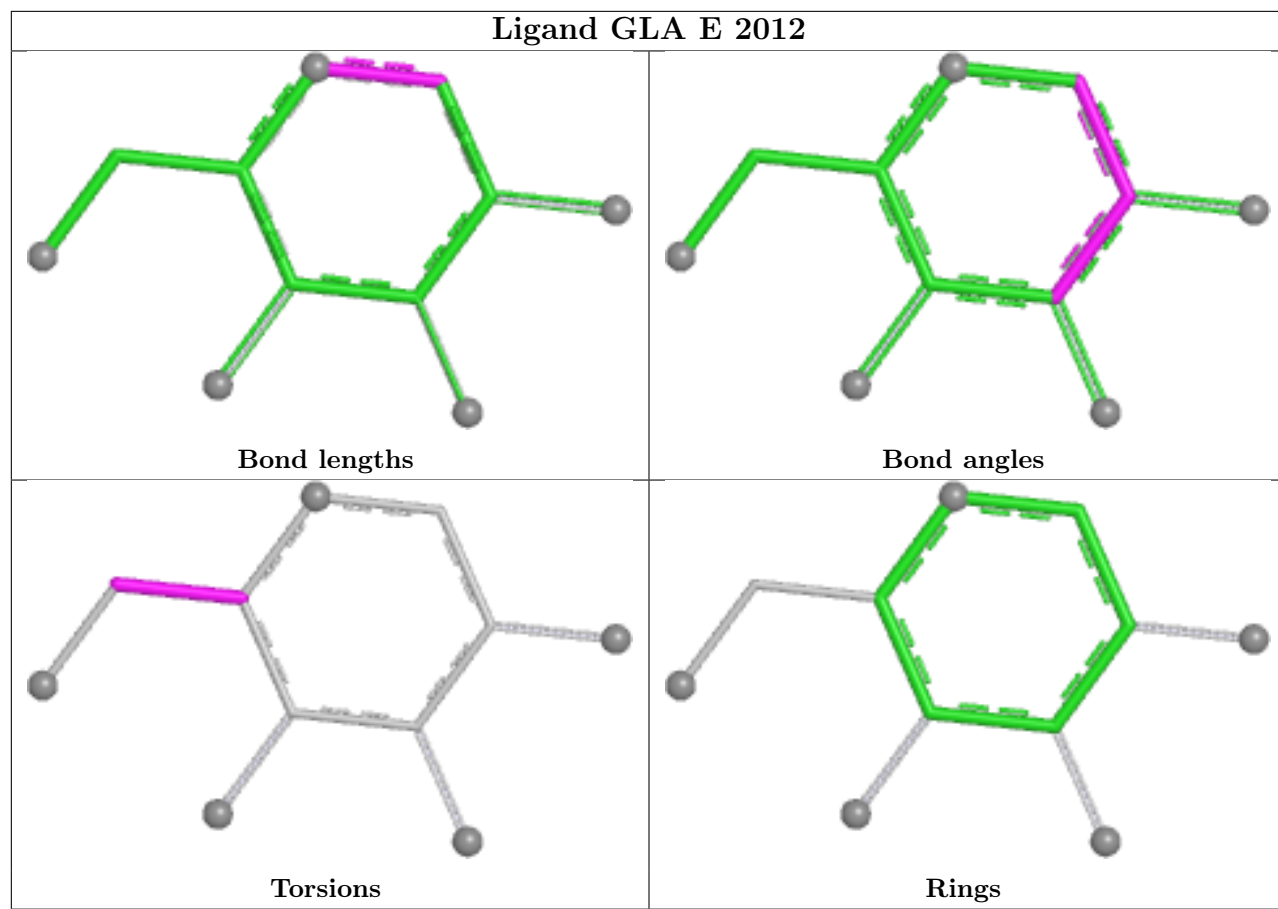


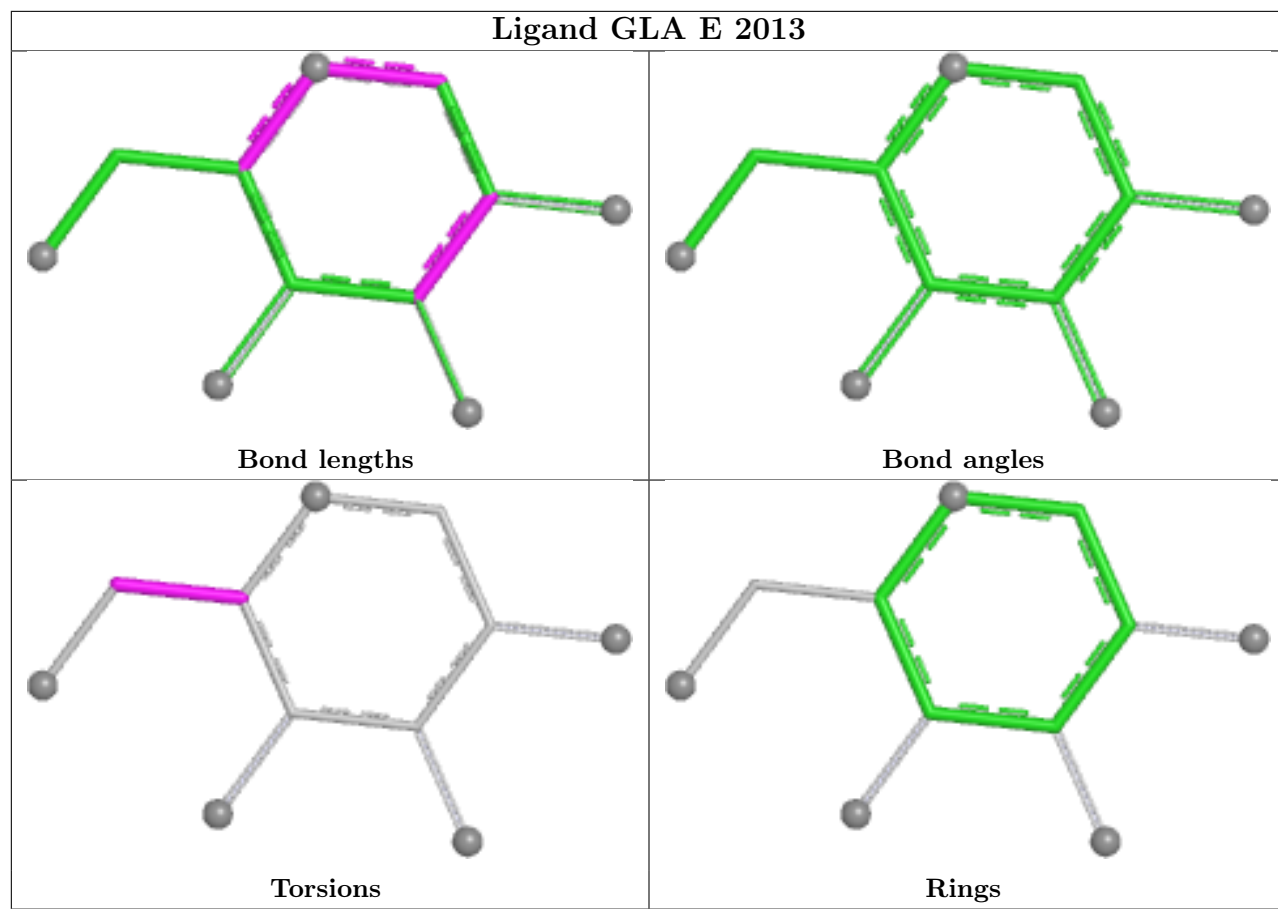
Ligand GLA E 2016

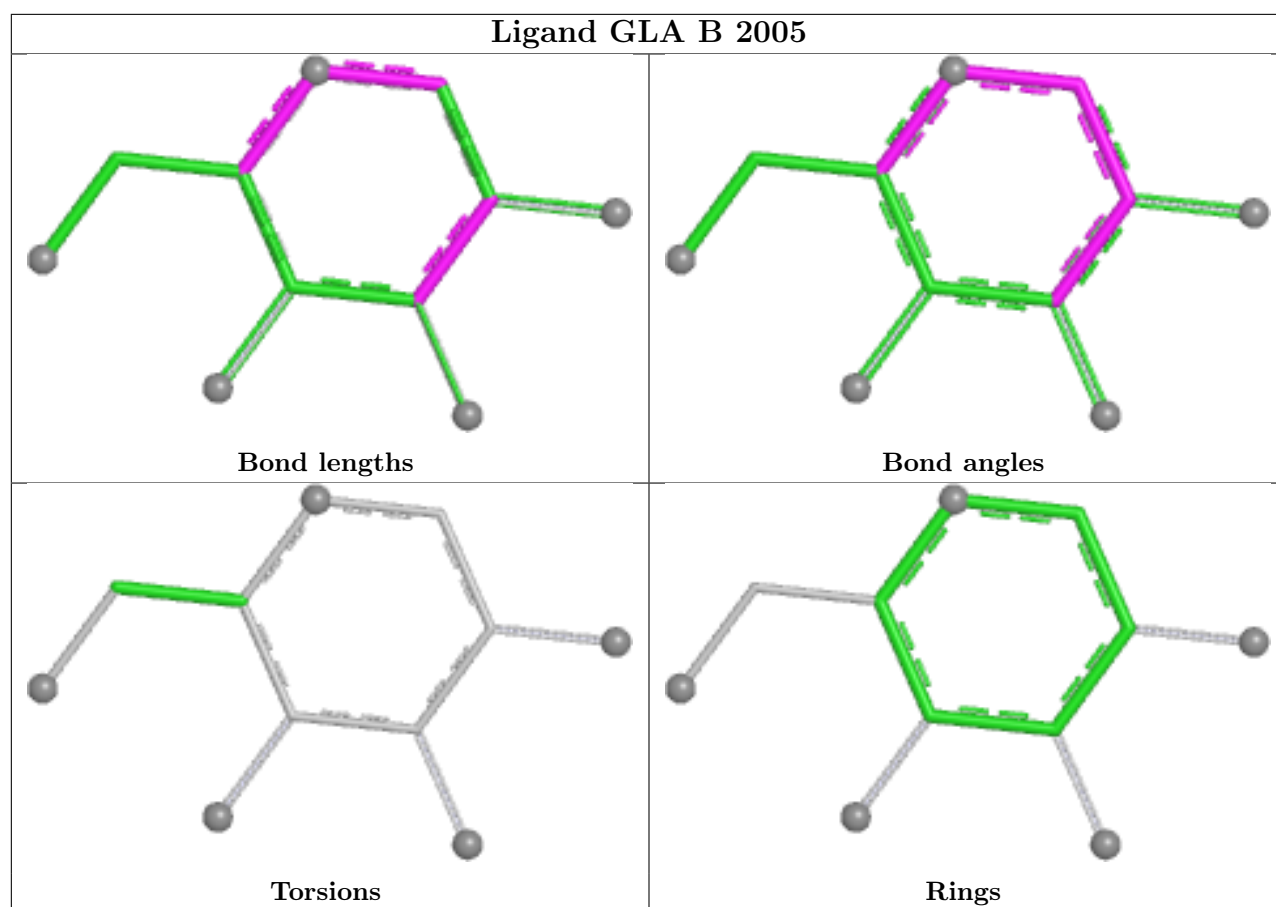


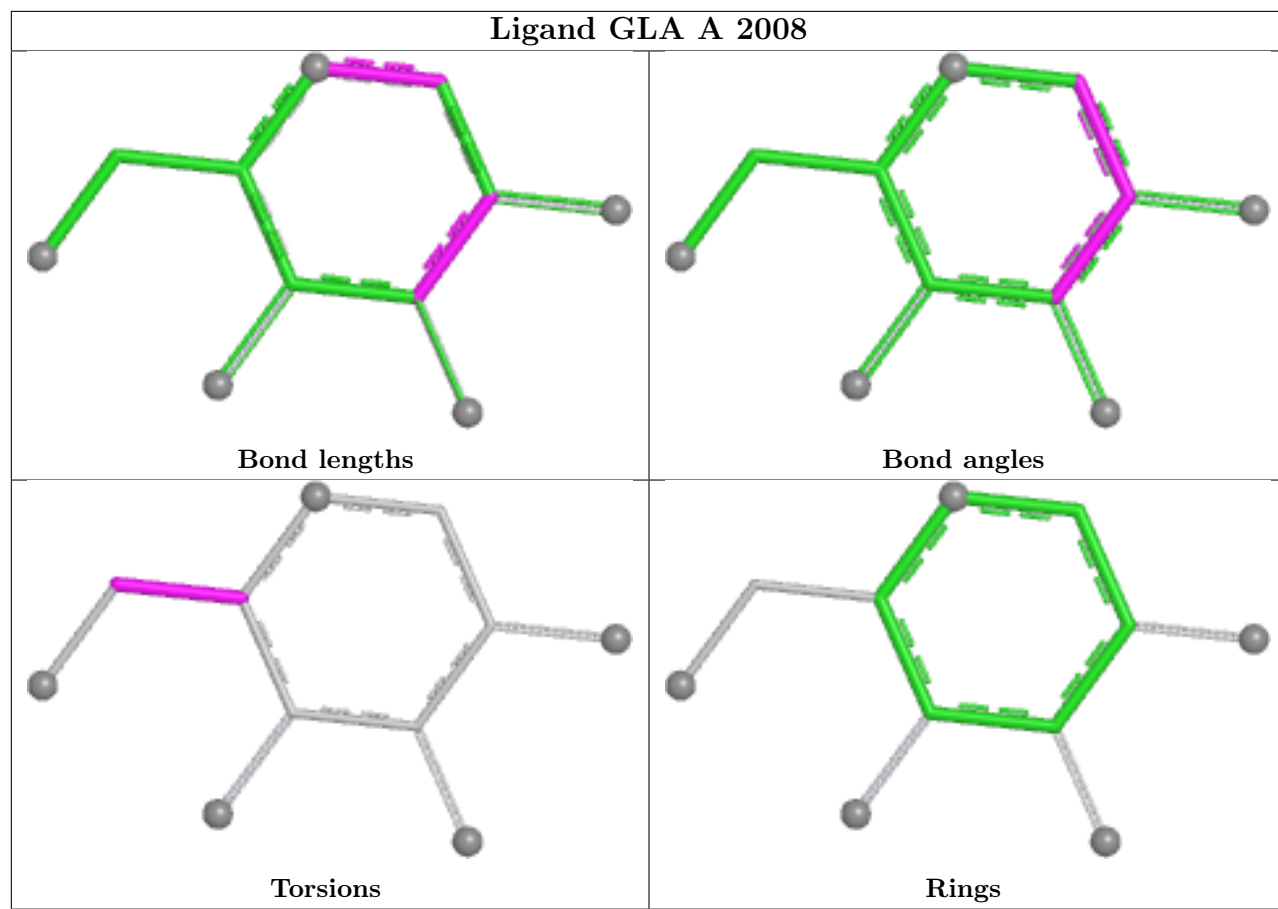
Ligand AHR E 2002

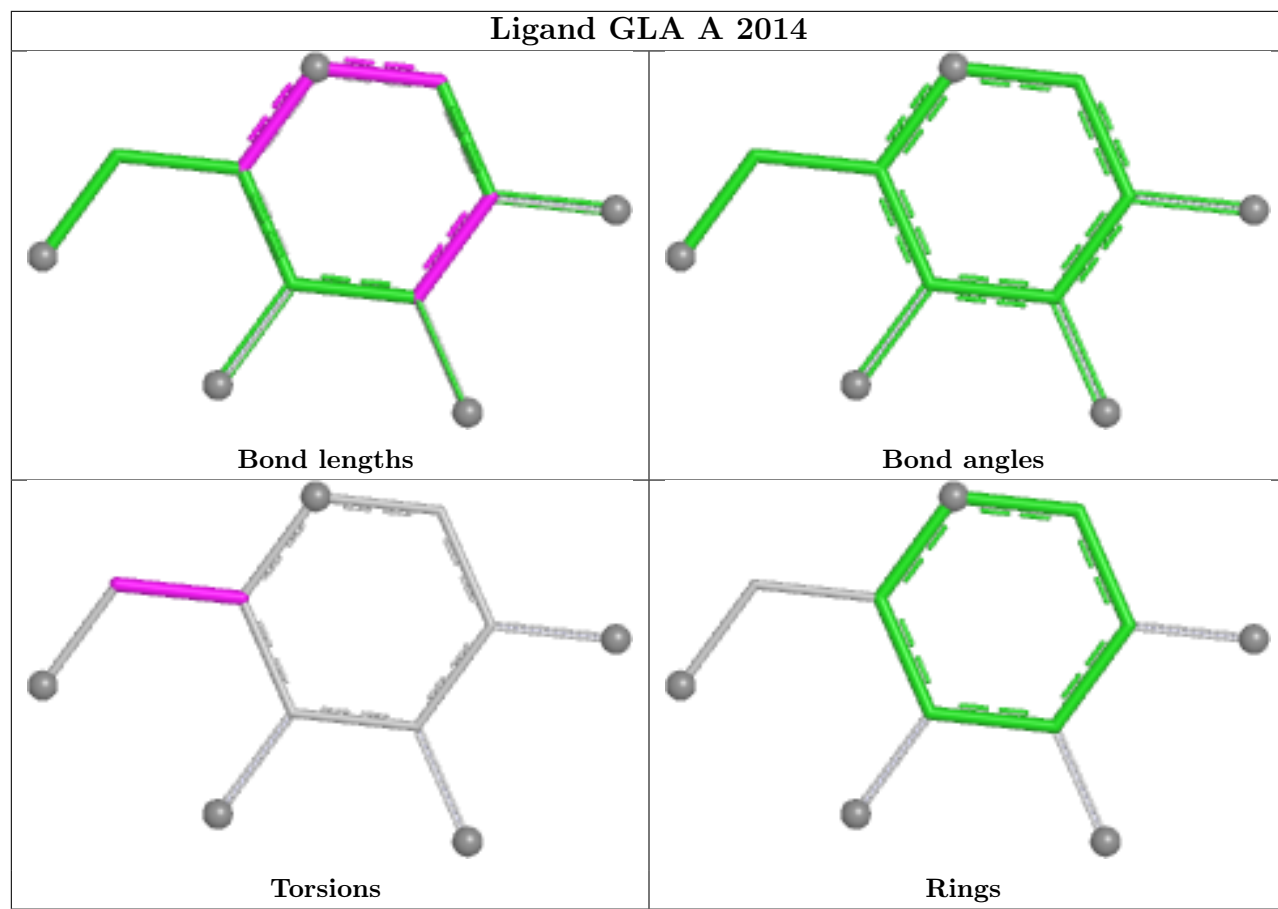




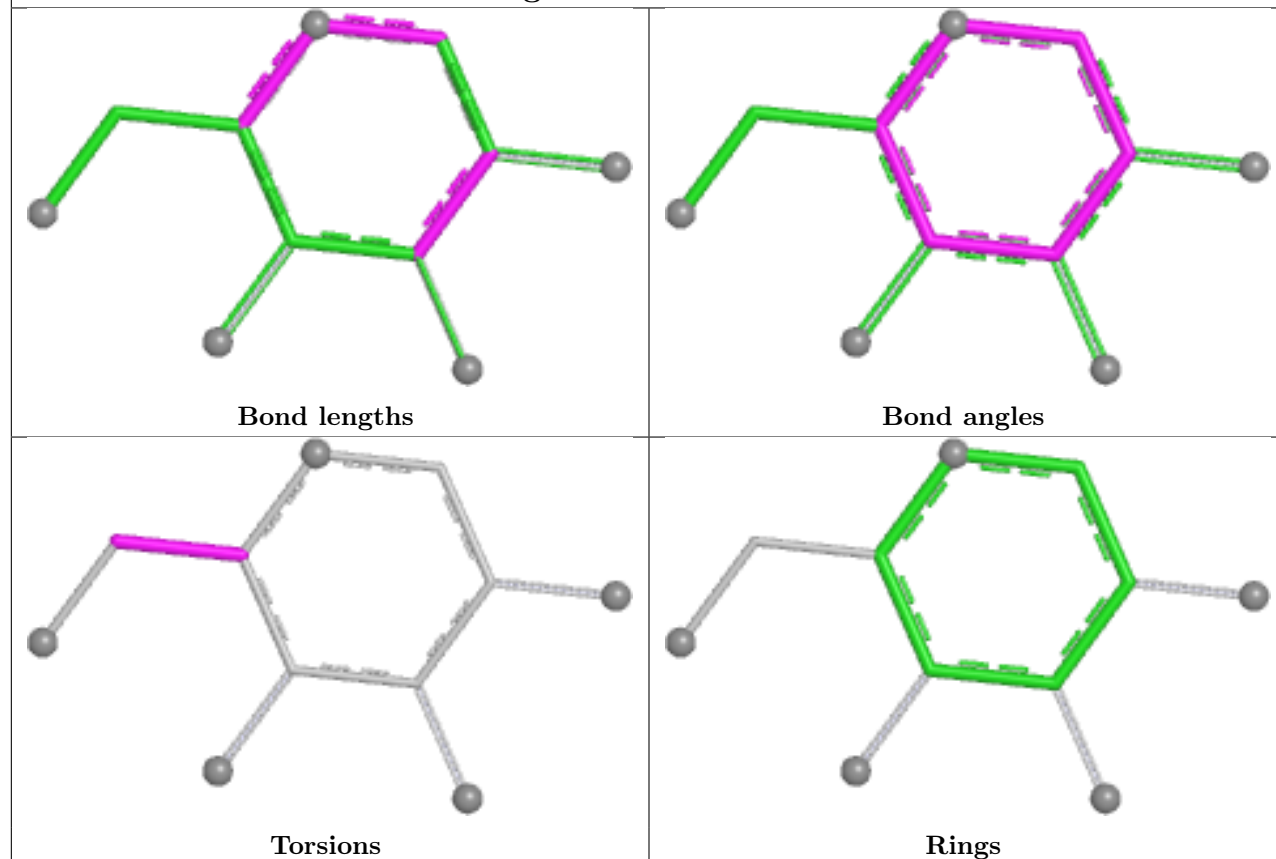




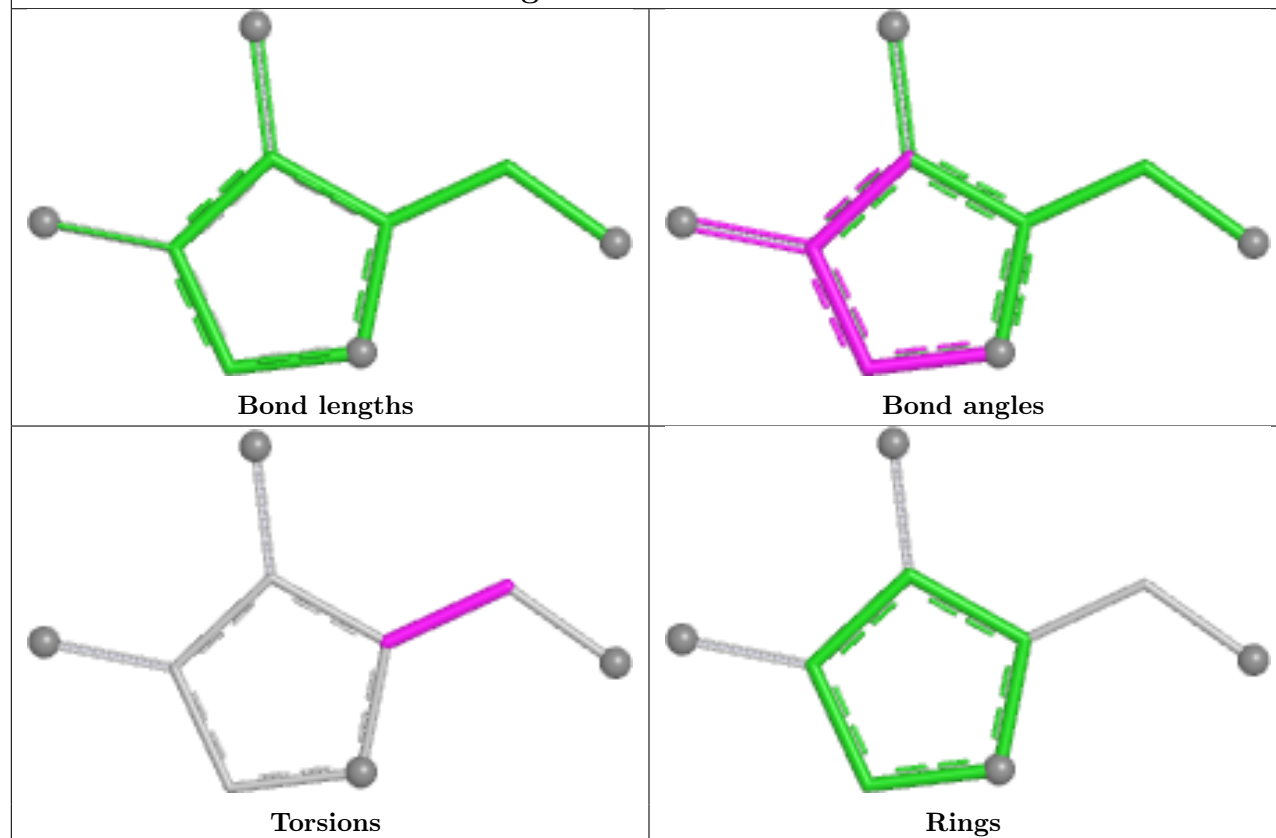


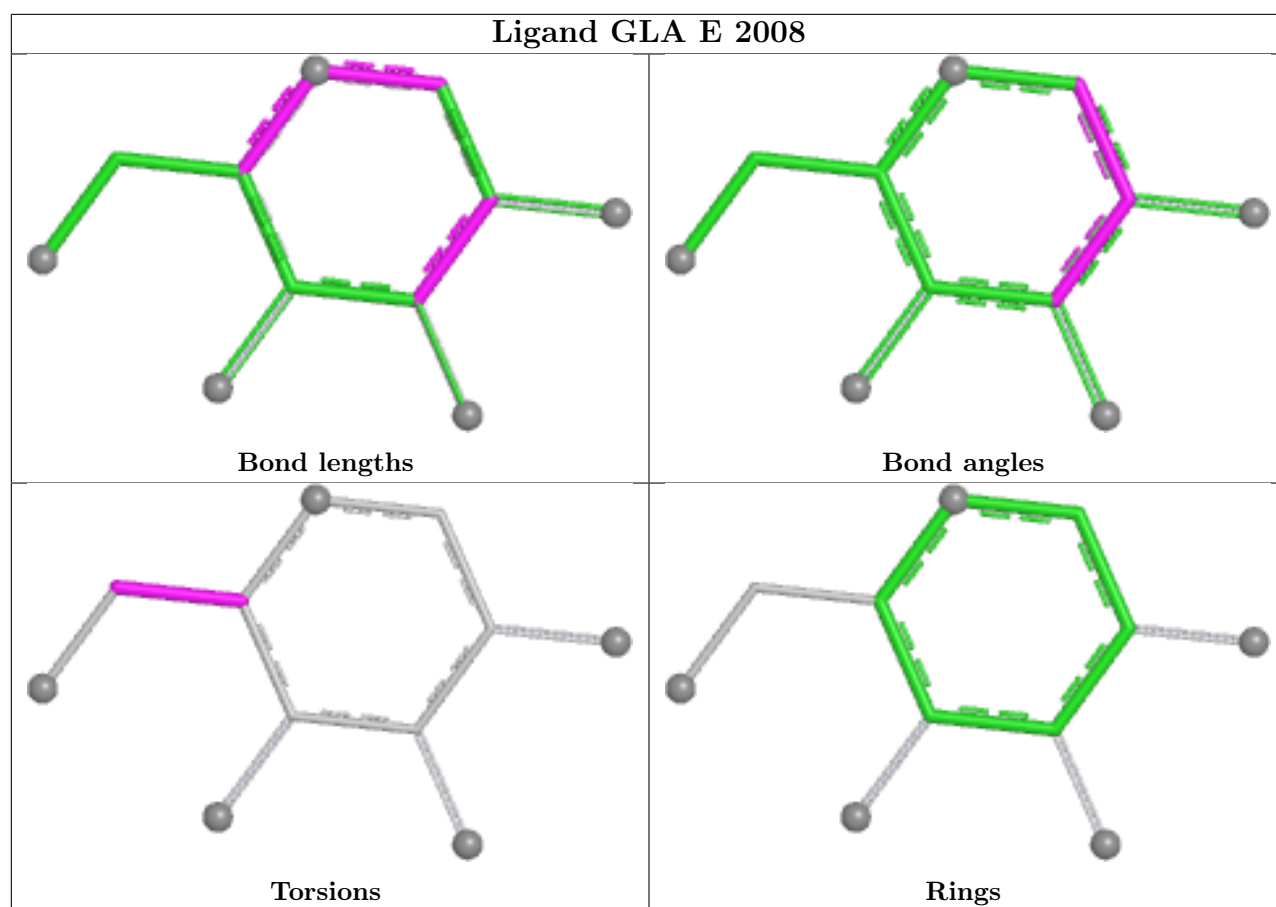


Ligand GLA E 2007



Ligand AHR F 2001





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.

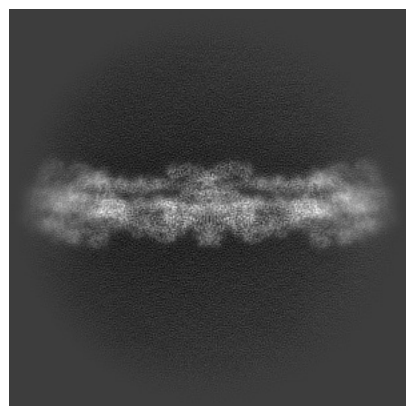
6 Map visualisation [i](#)

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.

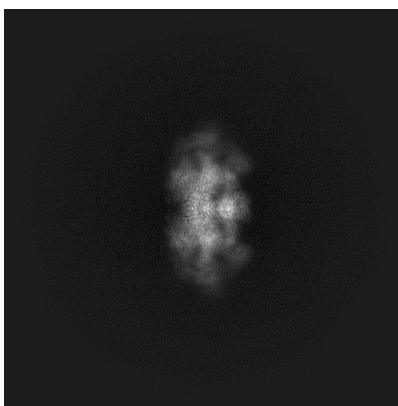
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

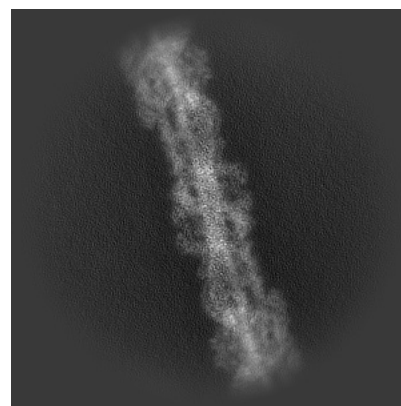
6.1.1 Primary map



X

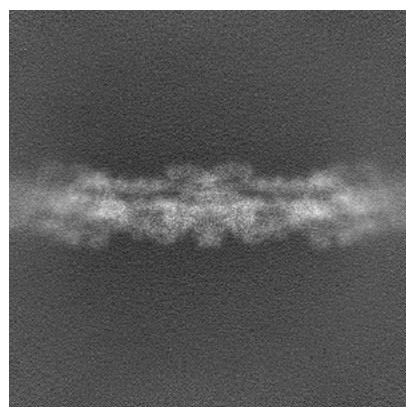


Y

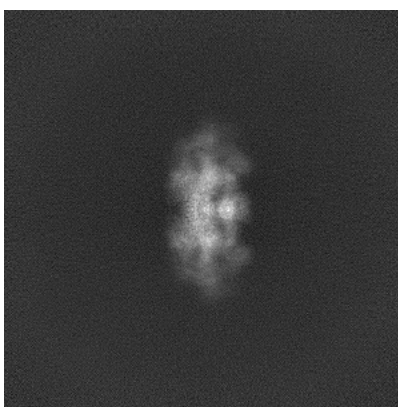


Z

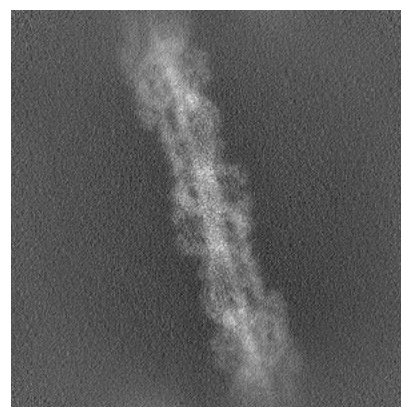
6.1.2 Raw map



X



Y

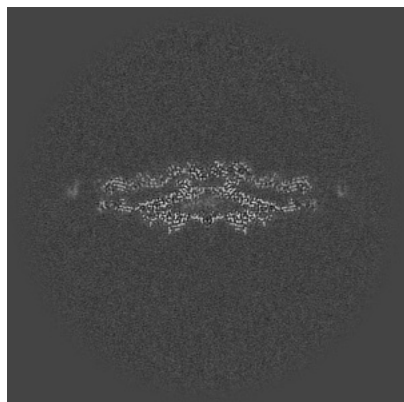


Z

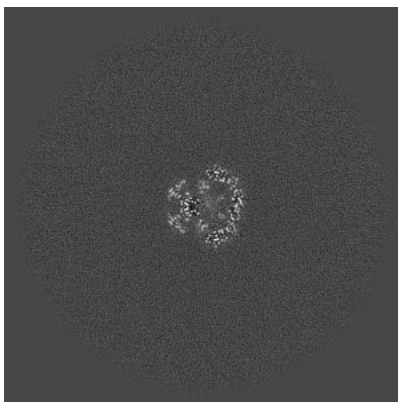
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

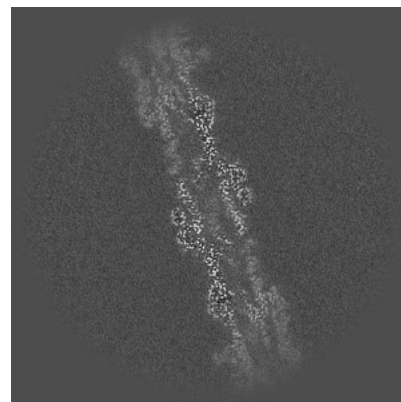
6.2.1 Primary map



X Index: 256

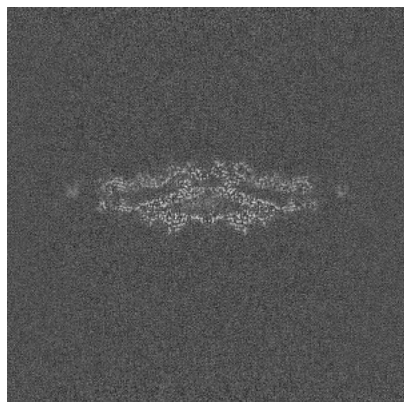


Y Index: 256

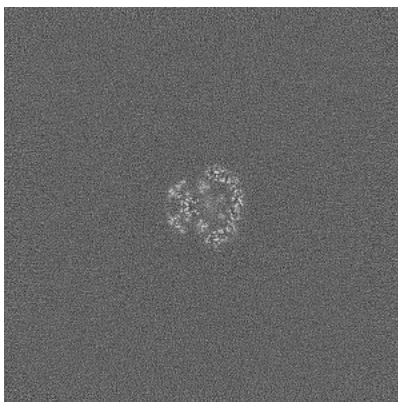


Z Index: 256

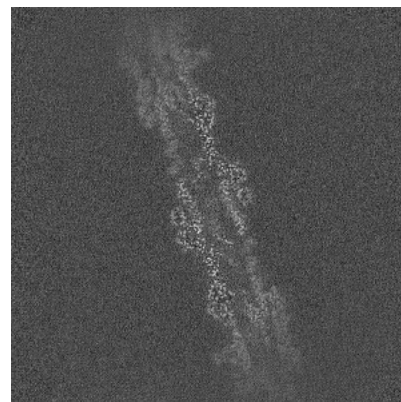
6.2.2 Raw map



X Index: 256



Y Index: 256

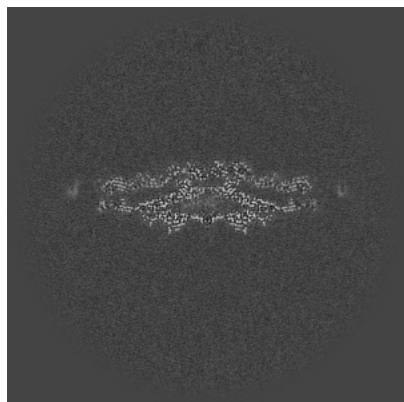


Z Index: 256

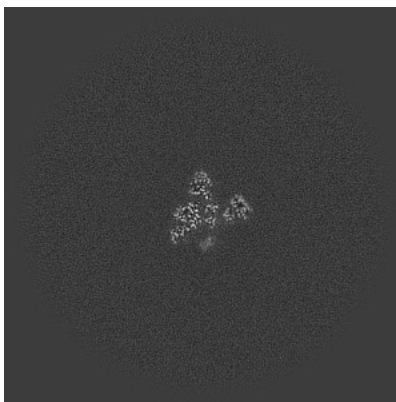
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

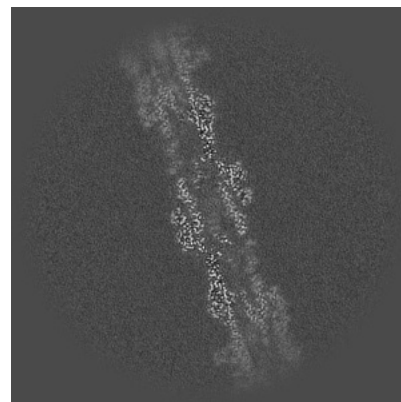
6.3.1 Primary map



X Index: 256

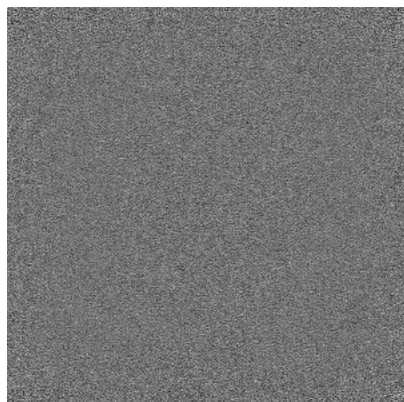


Y Index: 302

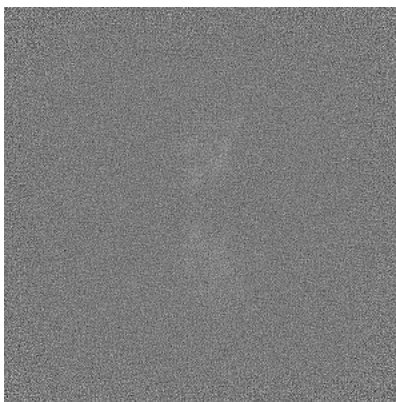


Z Index: 255

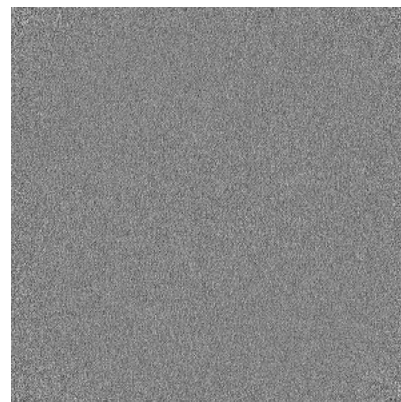
6.3.2 Raw map



X Index: 0



Y Index: 0

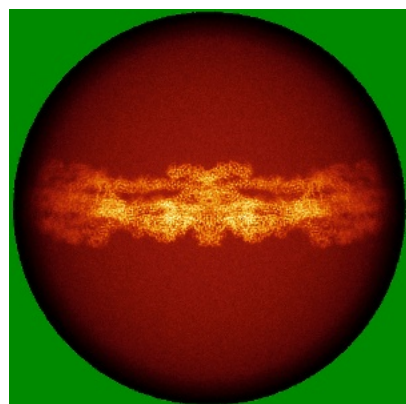


Z Index: 0

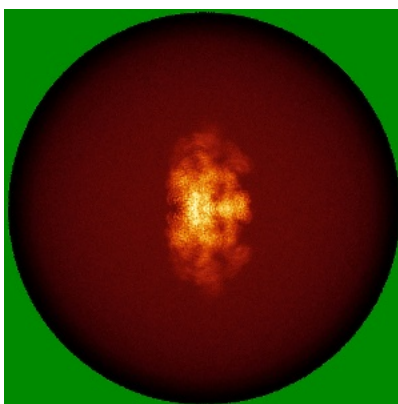
The images above show the largest variance slices of the map in three orthogonal directions.

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

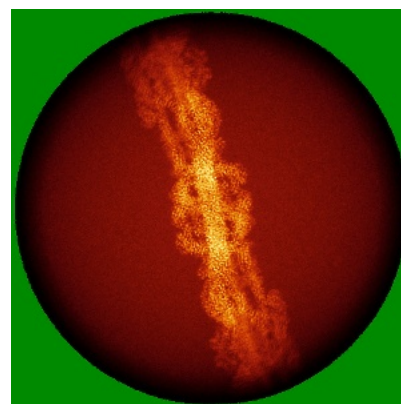
6.4.1 Primary map



X

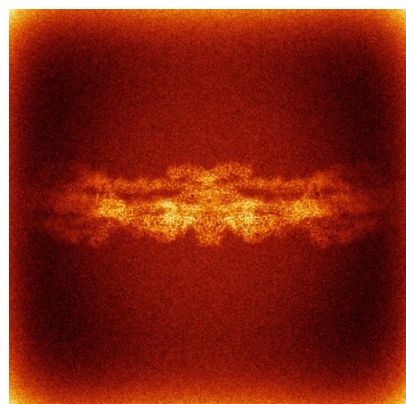


Y

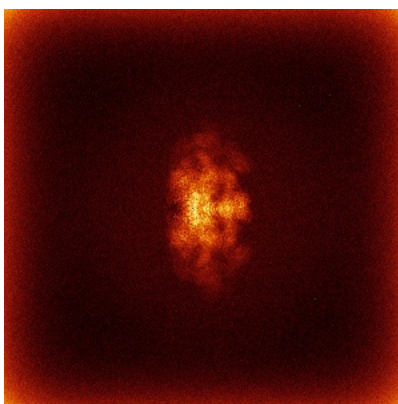


Z

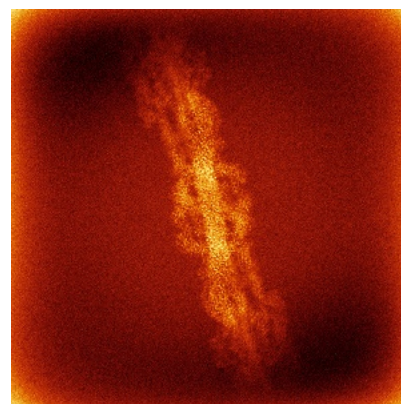
6.4.2 Raw map



X



Y

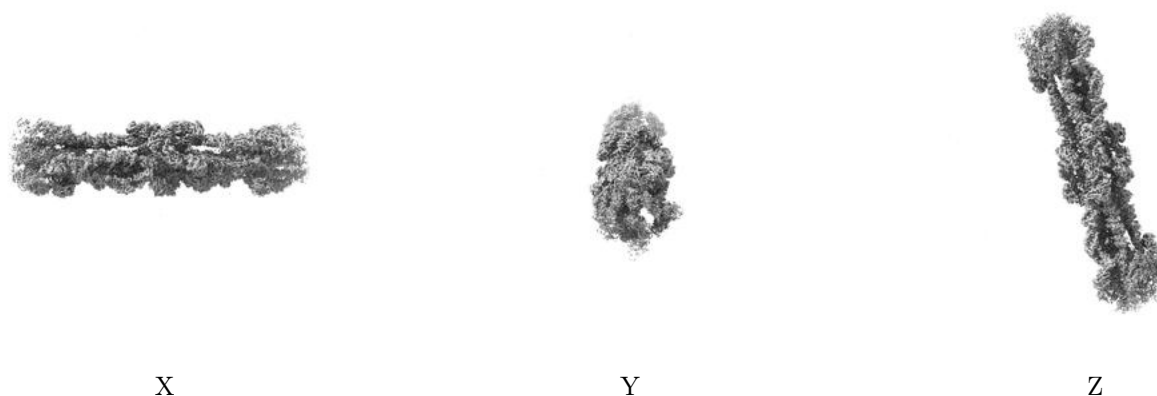


Z

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.

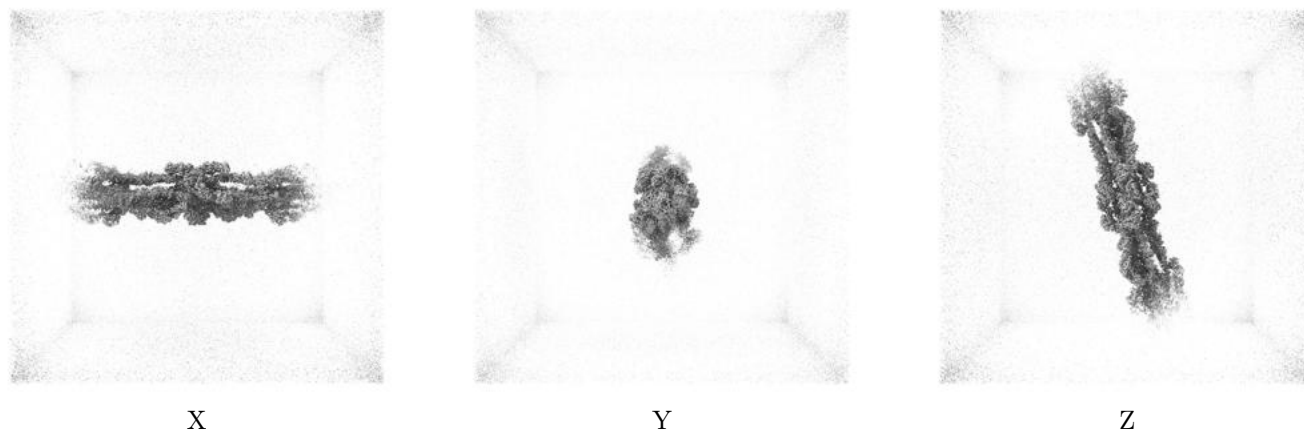
6.5 Orthogonal surface views [i](#)

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.

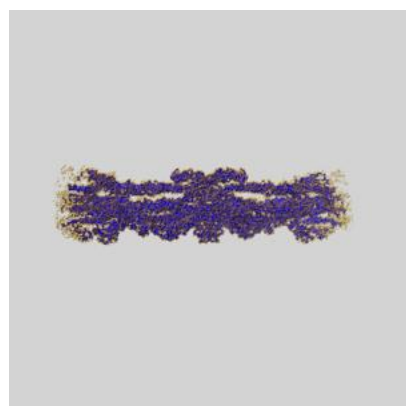
6.6 Mask visualisation [i](#)

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

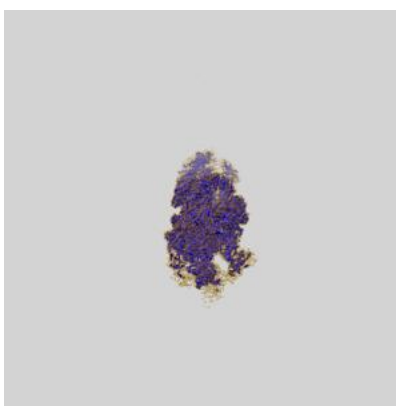
A mask typically either:

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

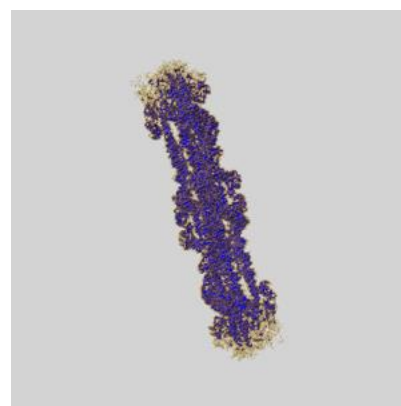
6.6.1 emd_37389_msk_1.map [i](#)



X



Y

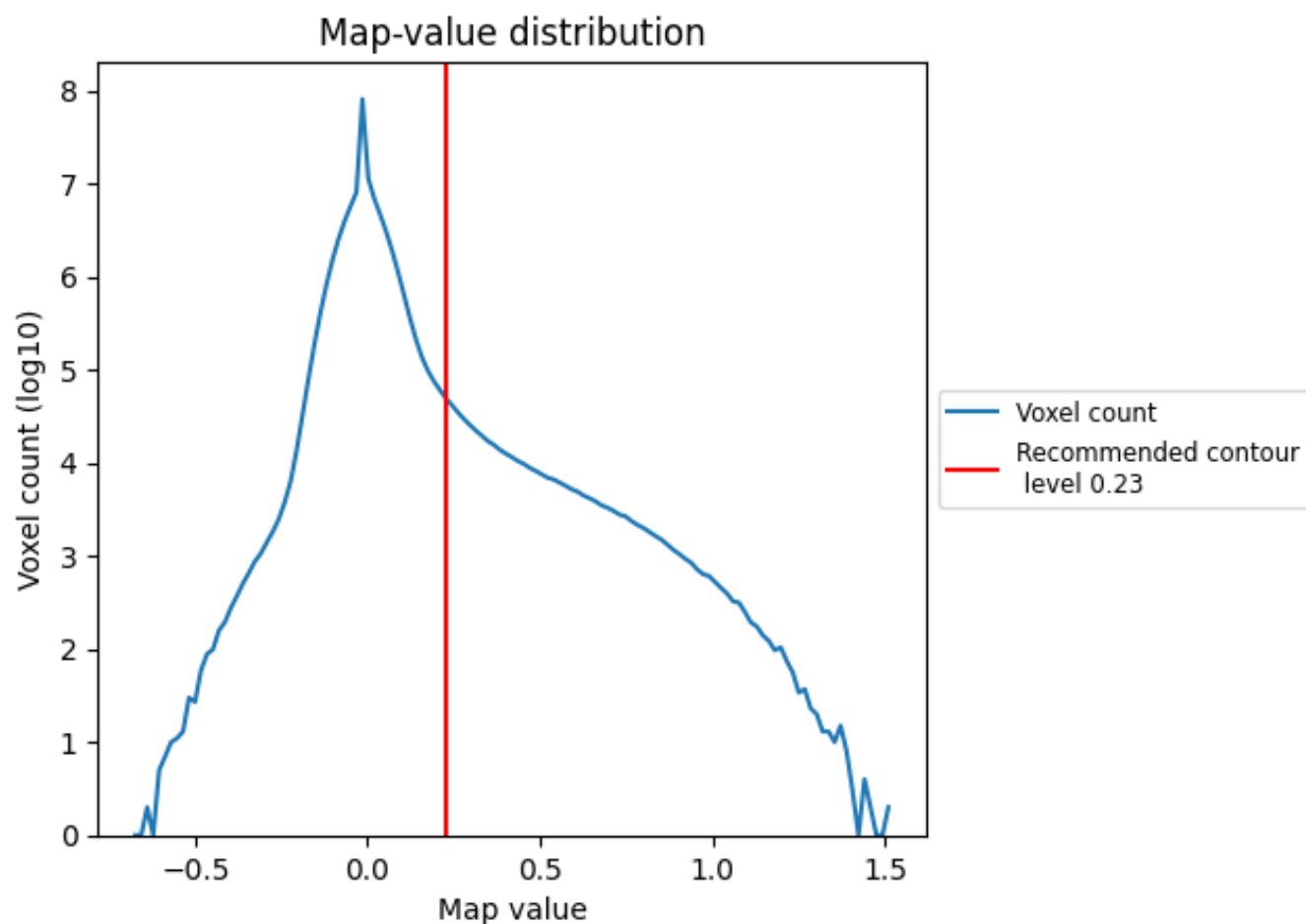


Z

7 Map analysis [i](#)

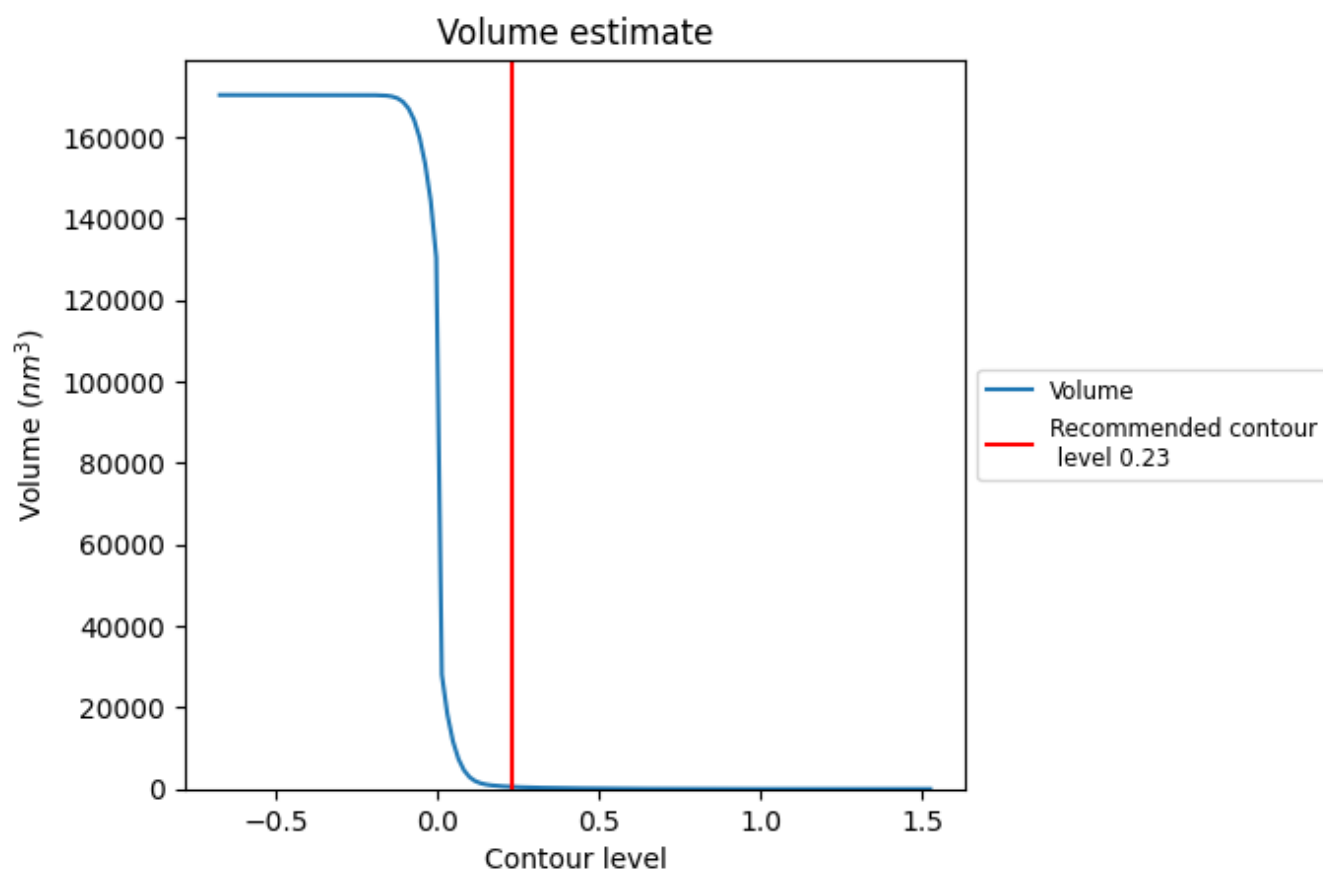
This section contains the results of statistical analysis of the map.

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.

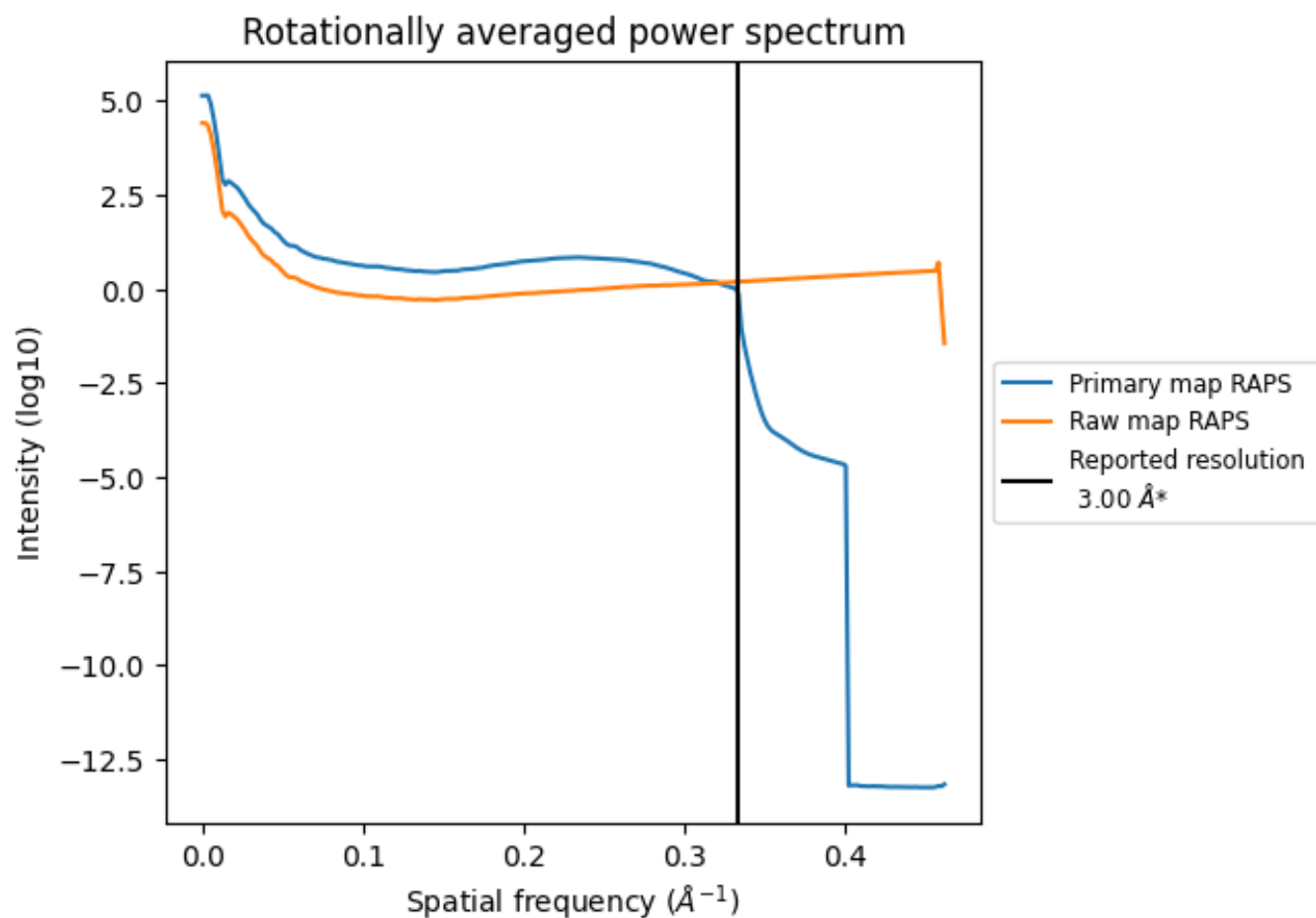
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 527 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 ⓘ

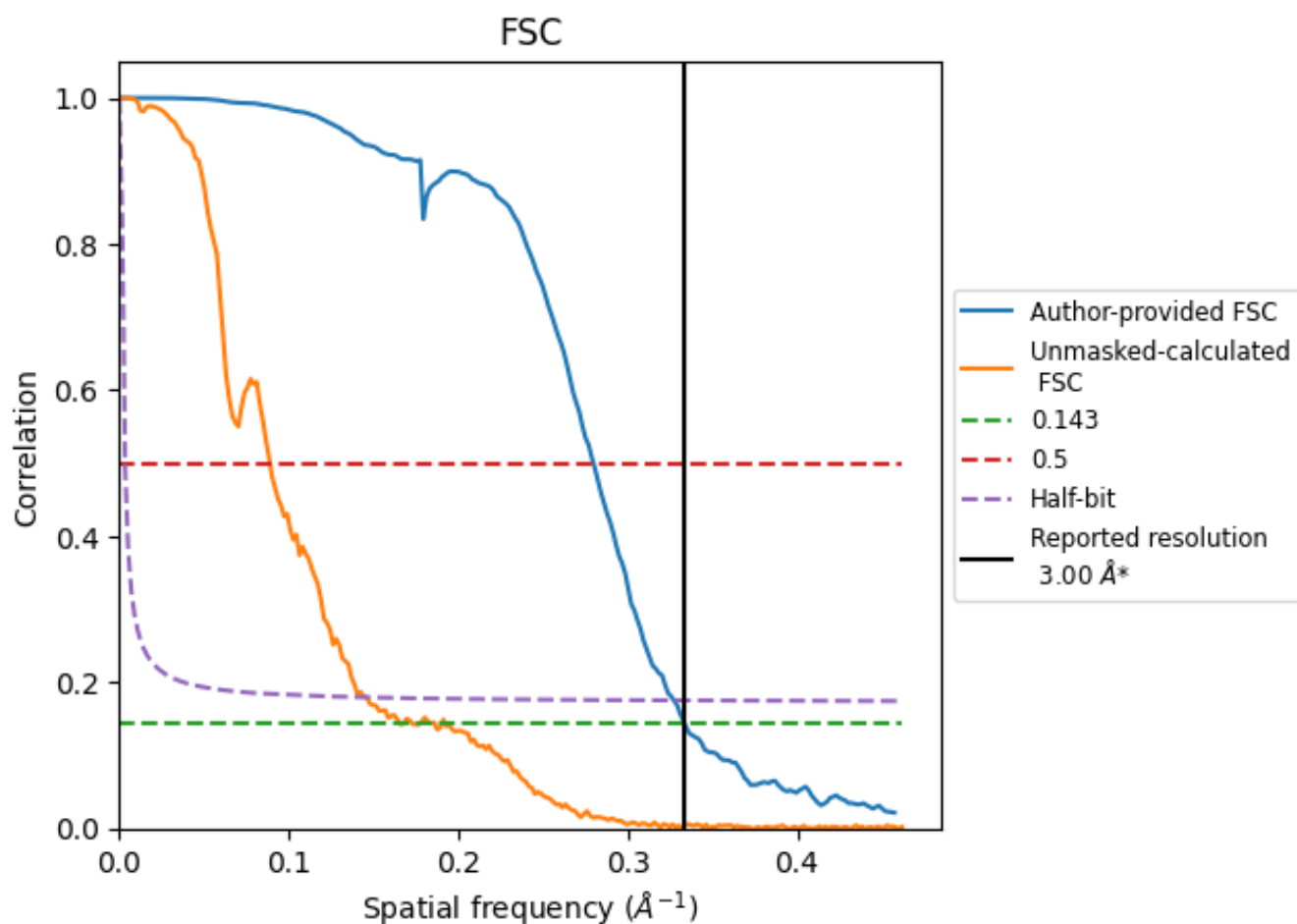


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.333 \AA^{-1}

8.2 Resolution estimates [i](#)

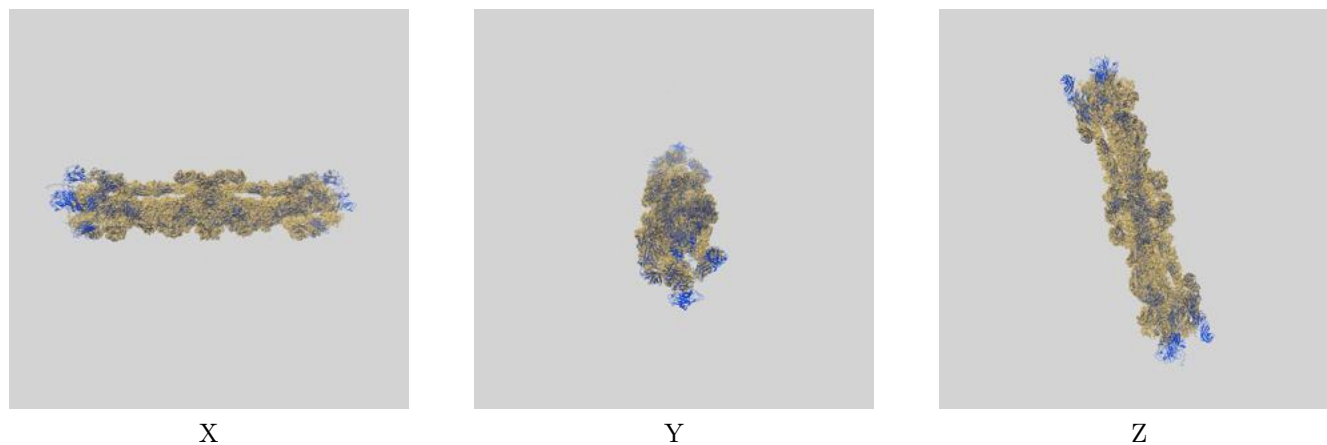
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.00	3.57	3.06
Unmasked-calculated*	6.04	11.24	6.84

*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](#)

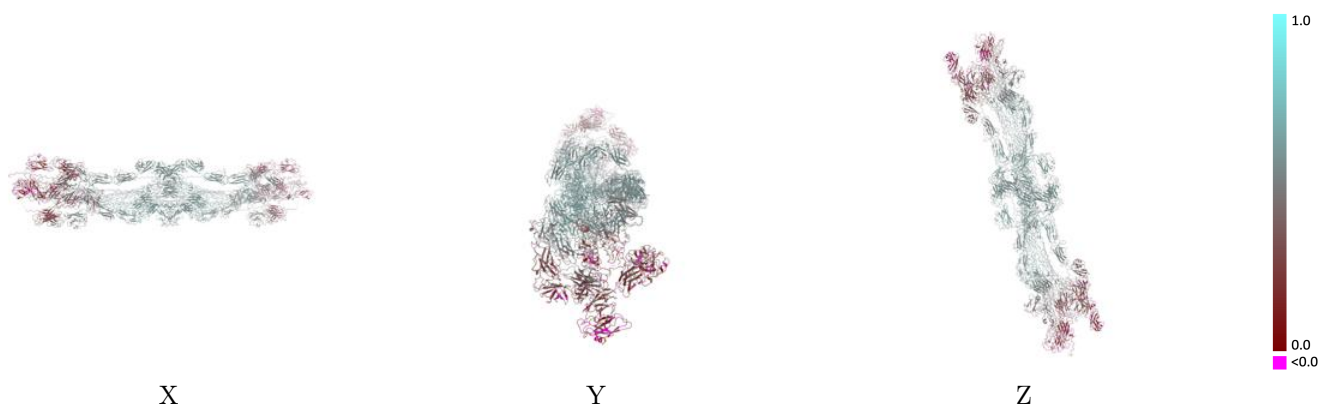
This section contains information regarding the fit between EMDB map EMD-37389 and PDB model 8WA2. Per-residue inclusion information can be found in section 3 on page 53.

9.1 Map-model overlay [i](#)



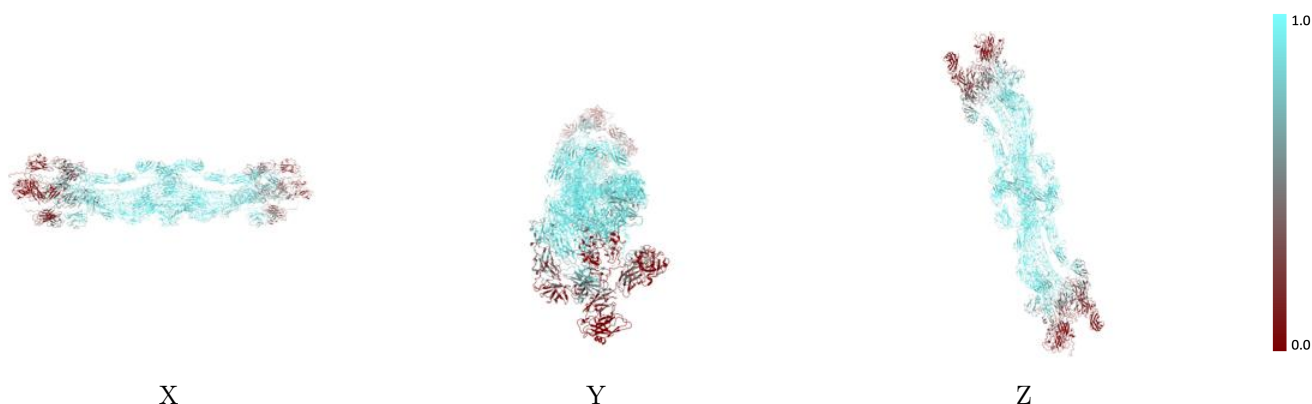
The images above show the 3D surface view of the map at the recommended contour level 0.23 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



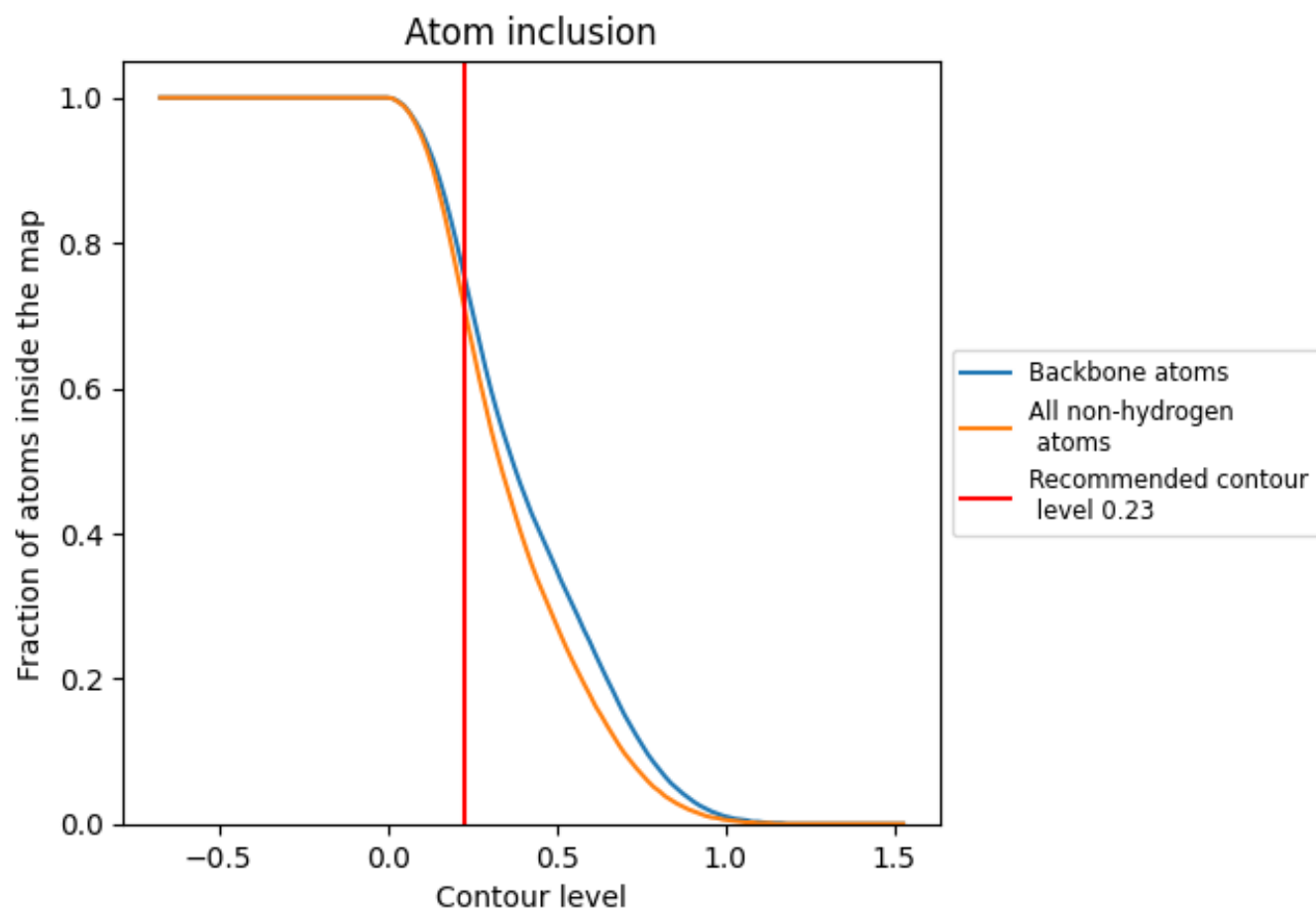
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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