



wwPDB EM Validation Summary Report ⓘ

Mar 29, 2026 – 02:44 AM UTC

PDB ID : 8WA2 / pdb_00008wa2
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:

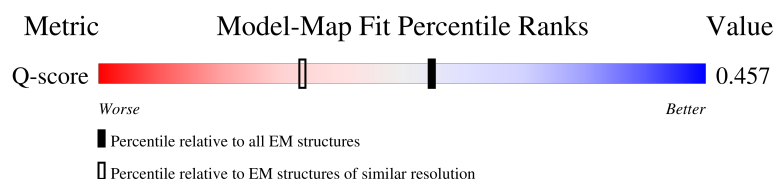
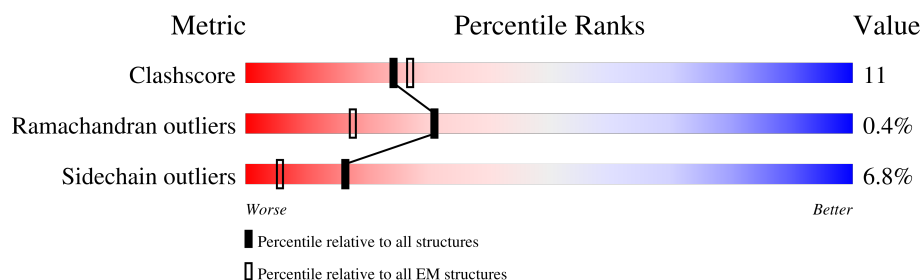
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14081 (2.50 - 3.50)

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	

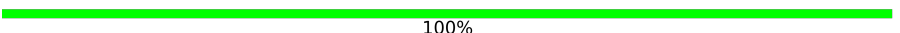
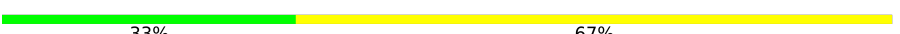
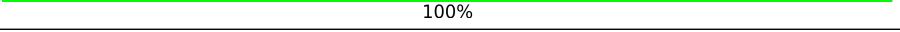
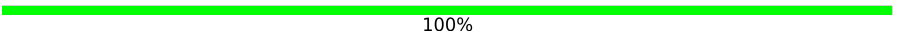
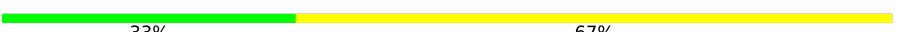
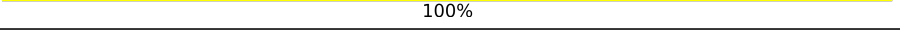
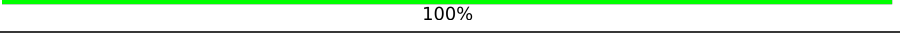
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Mol	Chain	Length	Quality of chain
1	E	1987	
1	F	1987	
2	G	64	
2	H	64	
2	I	64	
3	0	3	
3	0A	3	
3	1	3	
3	2	3	
3	8C	3	
3	9C	3	
3	BC	3	
3	CC	3	
3	DD	3	
3	EB	3	
3	ED	3	
3	FD	3	
3	GC	3	
3	HA	3	
3	HC	3	
3	IA	3	
3	IC	3	
3	ID	3	
3	J	3	
3	K	3	

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Mol	Chain	Length	Quality of chain
3	KD	3	 67%33%
3	LB	3	 67%33%
3	LC	3	 100%
3	MA	3	 33%67%
3	NA	3	 33%67%
3	NC	3	 67%33%
3	O	3	 67%33%
3	OA	3	 67%33%
3	OB	3	 100%  100%
3	P	3	 67%33%
3	PB	3	 33%67%  33%67%
3	Q	3	 67%33%
3	QB	3	 33%67%  67%33%
3	QD	3	 100%
3	RA	3	 67%33%
3	RB	3	 67%  100%
3	SB	3	 33%67%
3	T	3	 67%33%
3	TA	3	 67%33%
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%

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Mol	Chain	Length	Quality of chain
3	XA	3	
3	ZA	3	
3	aD	3	
3	b	3	
3	bD	3	
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	

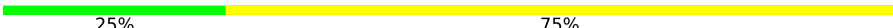
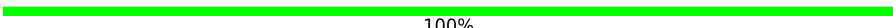
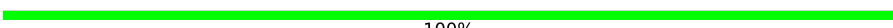
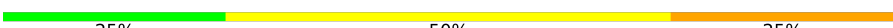
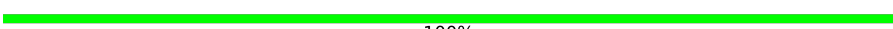
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Mol	Chain	Length	Quality of chain
3	qD	3	67% 100%
3	rA	3	67% 33%
3	rB	3	67% 33%
3	rC	3	100% 67% 33%
3	rD	3	67% 33%
3	sB	3	33% 33% 67%
3	sC	3	100% 67% 33%
3	t	3	67% 33%
3	tB	3	33% 100%
3	tC	3	33% 100%
3	uA	3	67% 33%
3	uB	3	100%
3	uC	3	67% 33%
3	vA	3	67% 33%
3	vB	3	33% 67% 33%
3	w	3	67% 33%
3	wA	3	67% 33%
3	wB	3	33% 67%
3	x	3	67% 33%
3	xA	3	33% 67%
3	xB	3	67% 33%
3	y	3	67% 33%
3	yA	3	67% 33%
3	z	3	33% 33% 33%
3	zA	3	100%

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Mol	Chain	Length	Quality of chain
4	AD	4	
4	DC	4	
4	JA	4	
4	JB	4	
4	L	4	
4	LD	4	
4	MD	4	
4	NB	4	
4	OC	4	
4	OD	4	
4	PC	4	
4	RC	4	
4	RD	4	
4	SD	4	
4	UA	4	
4	UC	4	
4	VA	4	
4	VC	4	
4	VD	4	
4	W	4	
4	X	4	
4	YC	4	
4	Z	4	
4	ZD	4	
4	aA	4	

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

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Mol	Chain	Length	Quality of chain
6	2C	3	
6	3A	3	
6	3B	3	
6	3D	3	
6	4B	3	
6	5	3	
6	5B	3	
6	6A	3	
6	6C	3	
6	6D	3	
6	7A	3	
6	7D	3	
6	8	3	
6	8A	3	
6	8D	3	
6	9	3	
6	9B	3	
6	AA	3	
6	CB	3	
6	CD	3	
6	EA	3	
6	FC	3	
6	GD	3	
6	JC	3	
6	LA	3	

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Mol	Chain	Length	Quality of chain
6	ME	3	
6	N	3	
6	OE	3	
6	PA	3	
6	R	3	
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	

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Mol	Chain	Length	Quality of chain
7	WD	4	
7	XC	4	
7	ZC	4	
7	dA	4	
7	f	4	
7	fA	4	
7	h	4	
8	JD	5	
8	MC	5	
8	SA	5	
8	U	5	
9	ND	2	
9	QC	2	
9	WA	2	
9	Y	2	
9	YD	2	
9	bC	2	
9	hA	2	
9	j	2	
10	1A	5	
10	3	5	
10	MB	5	
10	PD	5	
10	SC	5	
10	VB	5	

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Mol	Chain	Length	Quality of chain
10	YA	5	
10	a	5	
10	jD	5	
10	mC	5	
10	pB	5	
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	

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Mol	Chain	Length	Quality of chain
12	q	5	
13	0D	4	
13	1B	4	
13	2A	4	
13	2B	4	
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	

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Mol	Chain	Length	Quality of chain
13	vD	4	
13	wC	4	
13	wD	4	
13	yC	4	
13	zB	4	
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	

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Mol	Chain	Length	Quality of chain
15	BB	5	
15	CA	5	
15	DA	5	
15	eB	5	
15	fB	5	
16	4D	2	
16	AC	2	
16	FA	2	
17	5D	6	
17	7C	6	
17	DB	6	
17	GA	6	
18	0E	5	
18	9D	5	
18	BE	5	
18	DE	5	
18	IE	5	
18	JE	5	
18	KE	5	
18	PE	5	
18	SE	5	
18	cE	5	
18	fE	5	
18	pE	5	
18	rE	5	

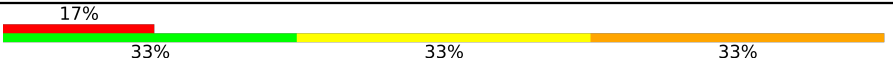
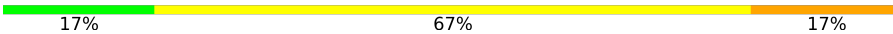
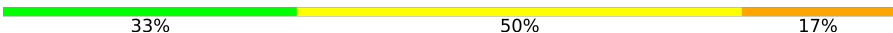
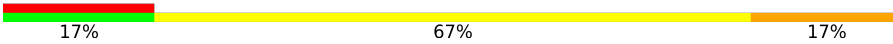
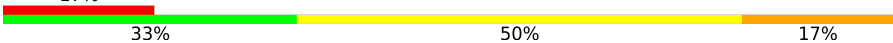
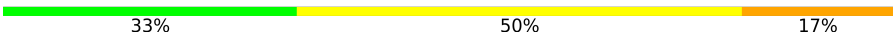
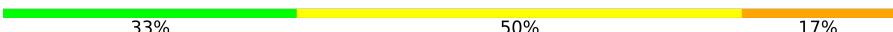
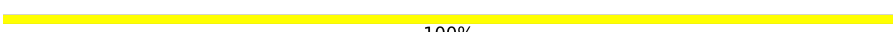
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Mol	Chain	Length	Quality of chain
18	tE	5	
18	yE	5	
18	zE	5	
19	1E	4	
19	AE	4	
19	LE	4	
19	NE	4	
19	aE	4	
19	qE	4	
20	CE	4	
20	EE	4	
20	HE	4	
20	TE	4	
20	UE	4	
20	WE	4	
20	gE	4	
20	hE	4	
20	jE	4	
20	sE	4	
20	uE	4	
20	xE	4	
21	FE	5	
21	kE	5	
21	vE	5	
22	GE	6	

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Mol	Chain	Length	Quality of chain
22	QE	6	
22	RE	6	
22	VE	6	
22	dE	6	
22	eE	6	
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
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	-	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	-	X	-
13	GZL	wD	3	X	-	-	-
13	GZL	yC	3	X	-	-	-
13	GZL	zB	3	X	-	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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	GZL	IE	3	X	-	-	-
24	AHR	IE	4	X	-	-	-
26	AHR	A	2003	-	-	X	-
26	AHR	C	2003	-	-	X	-
26	AHR	D	2003	-	-	X	-
26	AHR	E	2002	-	-	X	-
26	AHR	F	2003	-	-	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	-	-	-
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	-	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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	X	-
6	GZL	OE	3	X	-	-	-
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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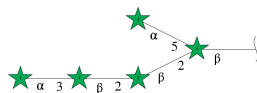
Mol	Chain	Residues	Atoms			AltConf	Trace
4	k	4	Total 36	C 20	O 16	0	0
4	r	4	Total 36	C 20	O 16	0	0
4	v	4	Total 36	C 20	O 16	0	0
4	JA	4	Total 36	C 20	O 16	0	0
4	UA	4	Total 36	C 20	O 16	0	0
4	VA	4	Total 36	C 20	O 16	0	0
4	aA	4	Total 36	C 20	O 16	0	0
4	bA	4	Total 36	C 20	O 16	0	0
4	eA	4	Total 36	C 20	O 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.



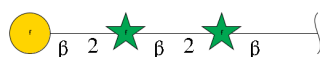
Mol	Chain	Residues	Atoms			AltConf	Trace
5	M	5	Total	C	O	0	0
			45	25	20		
5	KA	5	Total	C	O	0	0
			45	25	20		

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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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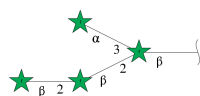
Mol	Chain	Residues	Atoms			AltConf	Trace
6	aB	3	Total	C	O	0	0
			29	16	13		
6	bB	3	Total	C	O	0	0
			29	16	13		
6	cB	3	Total	C	O	0	0
			29	16	13		
6	gB	3	Total	C	O	0	0
			29	16	13		
6	0B	3	Total	C	O	0	0
			29	16	13		
6	3B	3	Total	C	O	0	0
			29	16	13		
6	4B	3	Total	C	O	0	0
			29	16	13		
6	5B	3	Total	C	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.



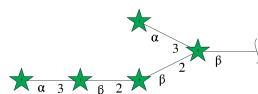
Mol	Chain	Residues	Atoms			AltConf	Trace
9	Y	2	Total	C	O	0	0
			18	10	8		

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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.



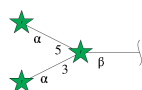
Mol	Chain	Residues	Atoms			AltConf	Trace
10	a	5	Total	C	O	0	0
			45	25	20		
10	u	5	Total	C	O	0	0
			45	25	20		
10	3	5	Total	C	O	0	0
			45	25	20		
10	YA	5	Total	C	O	0	0
			45	25	20		
10	sA	5	Total	C	O	0	0
			45	25	20		
10	1A	5	Total	C	O	0	0
			45	25	20		
10	MB	5	Total	C	O	0	0
			45	25	20		
10	VB	5	Total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

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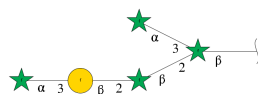
Mol	Chain	Residues	Atoms			AltConf	Trace
10	yB	5	Total	C	O	0	0
			45	25	20		
10	SC	5	Total	C	O	0	0
			45	25	20		
10	mC	5	Total	C	O	0	0
			45	25	20		
10	vC	5	Total	C	O	0	0
			45	25	20		
10	PD	5	Total	C	O	0	0
			45	25	20		
10	jD	5	Total	C	O	0	0
			45	25	20		
10	sD	5	Total	C	O	0	0
			45	25	20		

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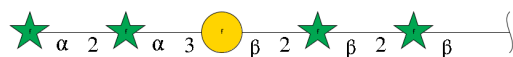
Mol	Chain	Residues	Atoms			AltConf	Trace
13	tD	4	Total	C	O	0	0
			38	21	17		
13	vD	4	Total	C	O	0	0
			38	21	17		
13	wD	4	Total	C	O	0	0
			38	21	17		
13	0D	4	Total	C	O	0	0
			38	21	17		

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



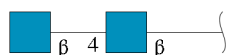
Mol	Chain	Residues	Atoms			AltConf	Trace
14	p	4	Total	C	O	0	0
			38	21	17		
14	s	4	Total	C	O	0	0
			38	21	17		
14	nA	4	Total	C	O	0	0
			38	21	17		
14	qA	4	Total	C	O	0	0
			38	21	17		
14	HB	4	Total	C	O	0	0
			38	21	17		
14	KB	4	Total	C	O	0	0
			38	21	17		
14	kB	4	Total	C	O	0	0
			38	21	17		
14	nB	4	Total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



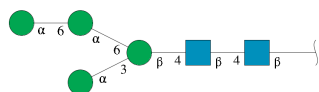
Mol	Chain	Residues	Atoms				AltConf	Trace
16	FA	2	Total	C	N	O	0	0
			28	16	2	10		

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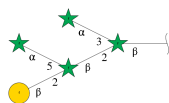
Mol	Chain	Residues	Atoms				AltConf	Trace
16	AC	2	Total	C	N	O	0	0
			28	16	2	10		
16	4D	2	Total	C	N	O	0	0
			28	16	2	10		

- 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.



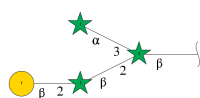
Mol	Chain	Residues	Atoms			AltConf	Trace
18	9D	5	Total	C	O	0	0
			47	26	21		
18	BE	5	Total	C	O	0	0
			47	26	21		
18	DE	5	Total	C	O	0	0
			47	26	21		
18	IE	5	Total	C	O	0	0
			47	26	21		
18	JE	5	Total	C	O	0	0
			47	26	21		

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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.



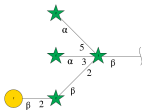
Mol	Chain	Residues	Atoms			AltConf	Trace
19	AE	4	Total	C	O	0	0
			38	21	17		
19	LE	4	Total	C	O	0	0
			38	21	17		
19	NE	4	Total	C	O	0	0
			38	21	17		
19	aE	4	Total	C	O	0	0
			38	21	17		
19	qE	4	Total	C	O	0	0
			38	21	17		
19	1E	4	Total	C	O	0	0
			38	21	17		

- 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.



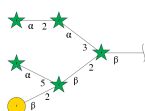
Mol	Chain	Residues	Atoms			AltConf	Trace
21	FE	5	Total	C	O	0	0
			47	26	21		

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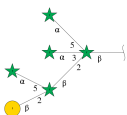
Mol	Chain	Residues	Atoms			AltConf	Trace
21	kE	5	Total	C	O	0	0
			47	26	21		
21	vE	5	Total	C	O	0	0
			47	26	21		

- 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.



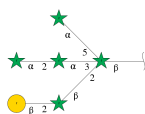
Mol	Chain	Residues	Atoms			AltConf	Trace
22	GE	6	Total	C	O	0	0
			56	31	25		
22	QE	6	Total	C	O	0	0
			56	31	25		
22	RE	6	Total	C	O	0	0
			56	31	25		
22	VE	6	Total	C	O	0	0
			56	31	25		
22	dE	6	Total	C	O	0	0
			56	31	25		
22	eE	6	Total	C	O	0	0
			56	31	25		
22	iE	6	Total	C	O	0	0
			56	31	25		
22	wE	6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

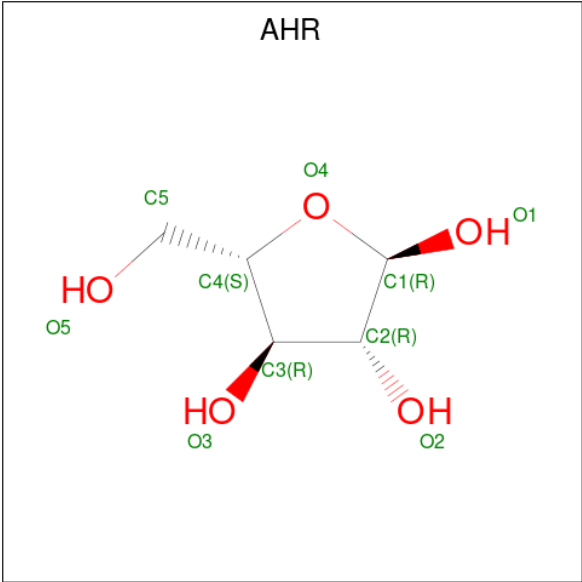


Mol	Chain	Residues	Atoms			AltConf	Trace
24	YE	6	Total	C	O	0	0
			56	31	25		
24	IE	6	Total	C	O	0	0
			56	31	25		

- Molecule 25 is CALCIUM ION (CCD ID: 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 (CCD ID: AHR) (formula: C₅H₁₀O₅) (labeled as "Ligand of Interest" by depositor).



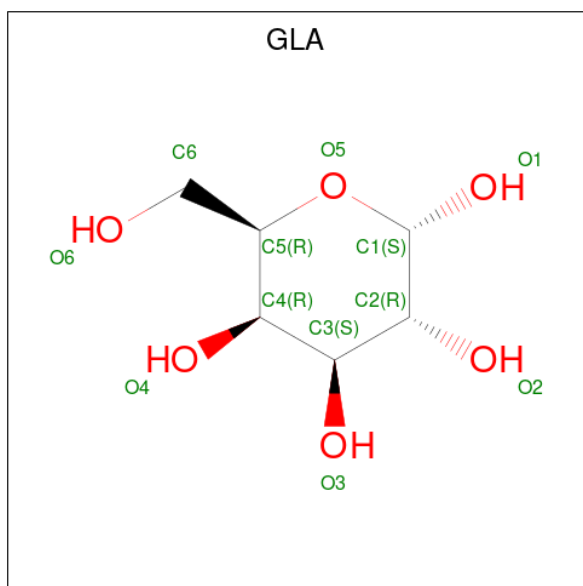
Mol	Chain	Residues	Atoms			AltConf
26	A	1	Total	C	O	0
			9	5	4	
26	A	1	Total	C	O	0
			9	5	4	
26	A	1	Total	C	O	0
			9	5	4	
26	A	1	Total	C	O	0
			9	5	4	
26	B	1	Total	C	O	0
			9	5	4	
26	B	1	Total	C	O	0
			9	5	4	
26	B	1	Total	C	O	0
			9	5	4	
26	B	1	Total	C	O	0
			9	5	4	
26	C	1	Total	C	O	0
			9	5	4	
26	C	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 (CCD ID: GLA) (formula: $C_6H_{12}O_6$) (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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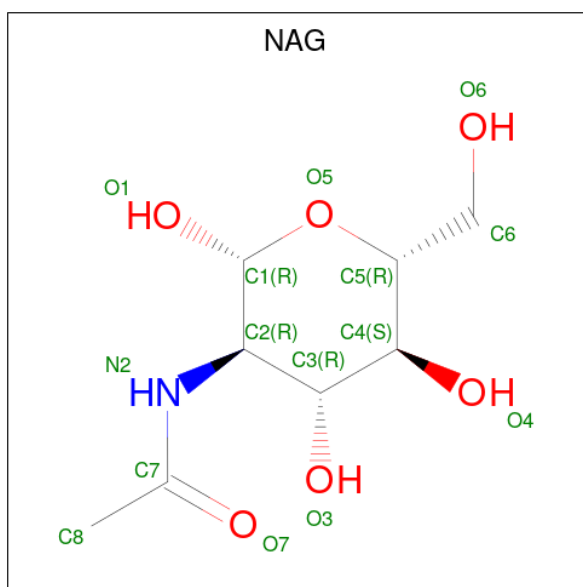
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
27	C	1	11	6	5	0
27	C	1	11	6	5	0
27	C	1	11	6	5	0
27	C	1	11	6	5	0
27	C	1	11	6	5	0
27	D	1	11	6	5	0
27	D	1	11	6	5	0
27	D	1	11	6	5	0
27	D	1	11	6	5	0
27	D	1	11	6	5	0
27	E	1	11	6	5	0
27	E	1	11	6	5	0
27	E	1	11	6	5	0
27	E	1	11	6	5	0
27	E	1	11	6	5	0
27	E	1	11	6	5	0
27	E	1	11	6	5	0
27	E	1	11	6	5	0
27	E	1	11	6	5	0
27	E	1	11	6	5	0
27	E	1	11	6	5	0
27	E	1	11	6	5	0

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Mol	Chain	Residues	Atoms			AltConf
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 (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).

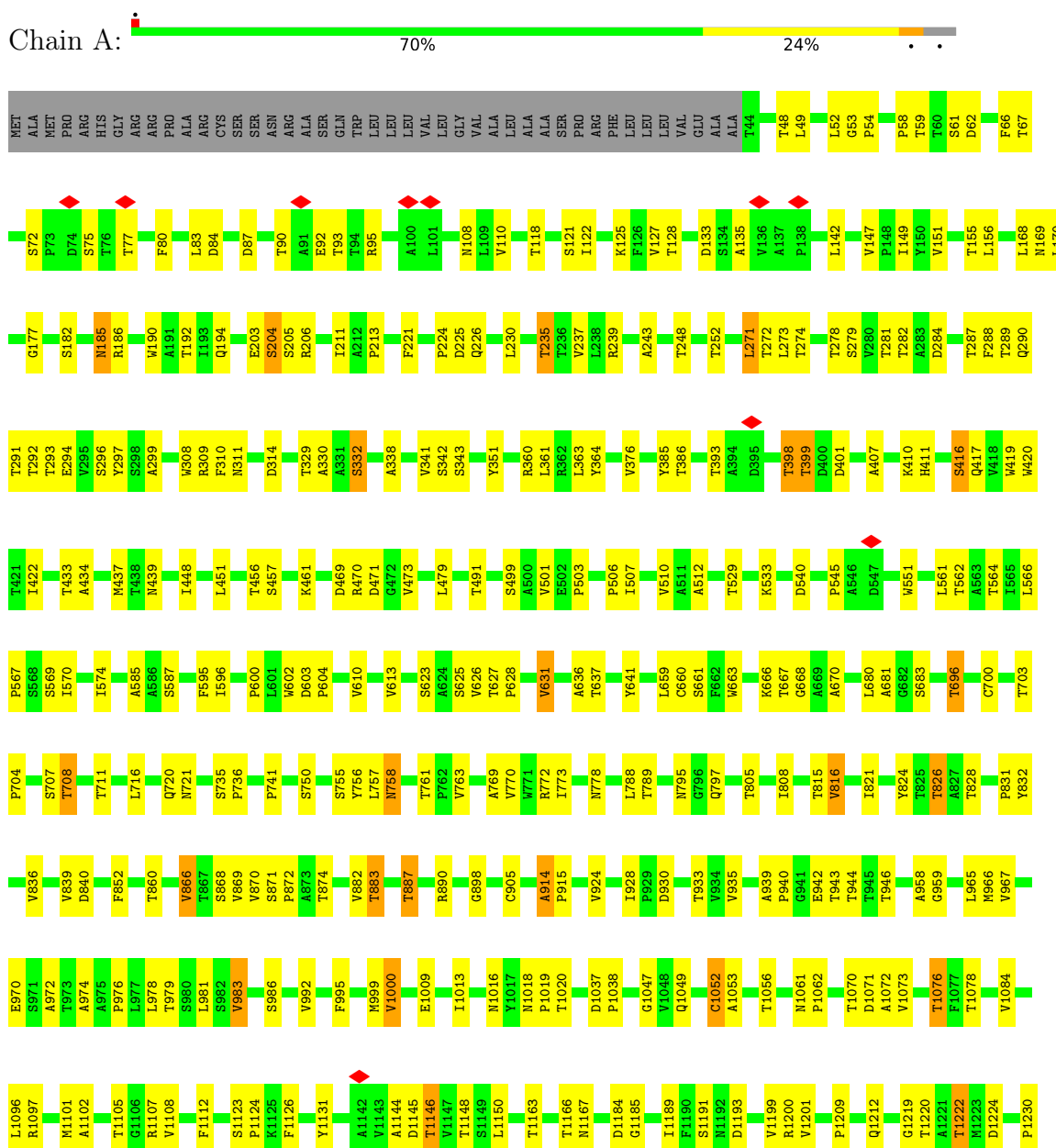


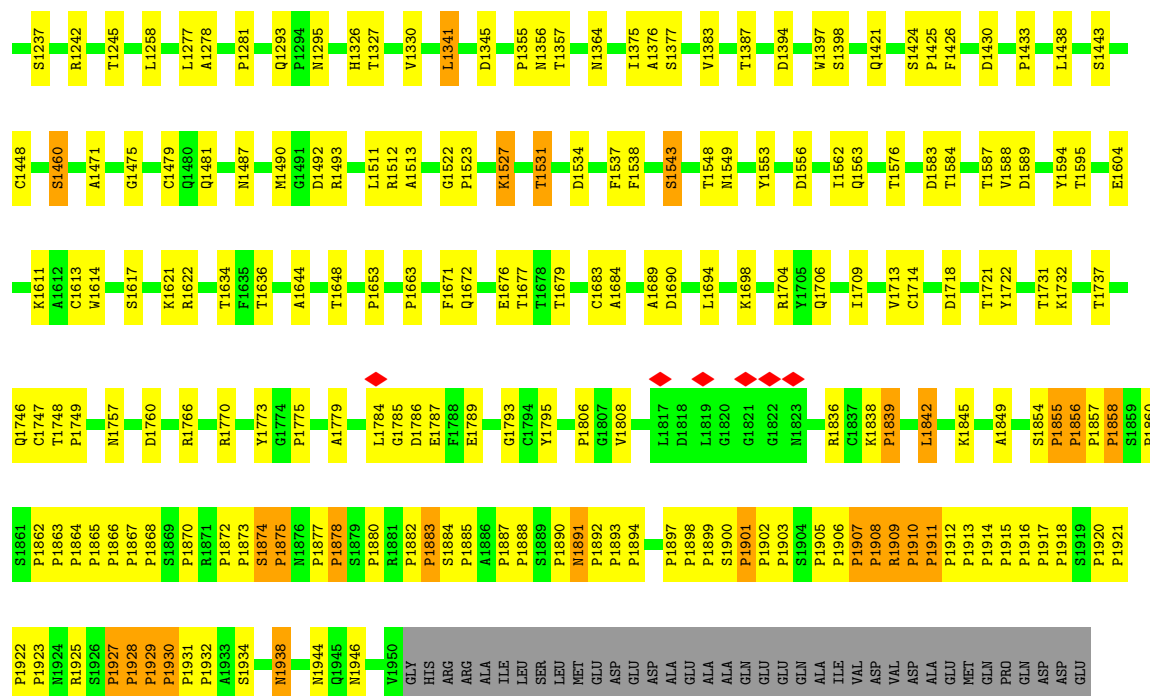
Mol	Chain	Residues	Atoms				AltConf
28	A	1	Total	C	N	O	0
			14	8	1	5	
28	B	1	Total	C	N	O	0
			14	8	1	5	
28	B	1	Total	C	N	O	0
			14	8	1	5	
28	C	1	Total	C	N	O	0
			14	8	1	5	
28	C	1	Total	C	N	O	0
			14	8	1	5	
28	D	1	Total	C	N	O	0
			14	8	1	5	
28	E	1	Total	C	N	O	0
			14	8	1	5	

3 Residue-property plots

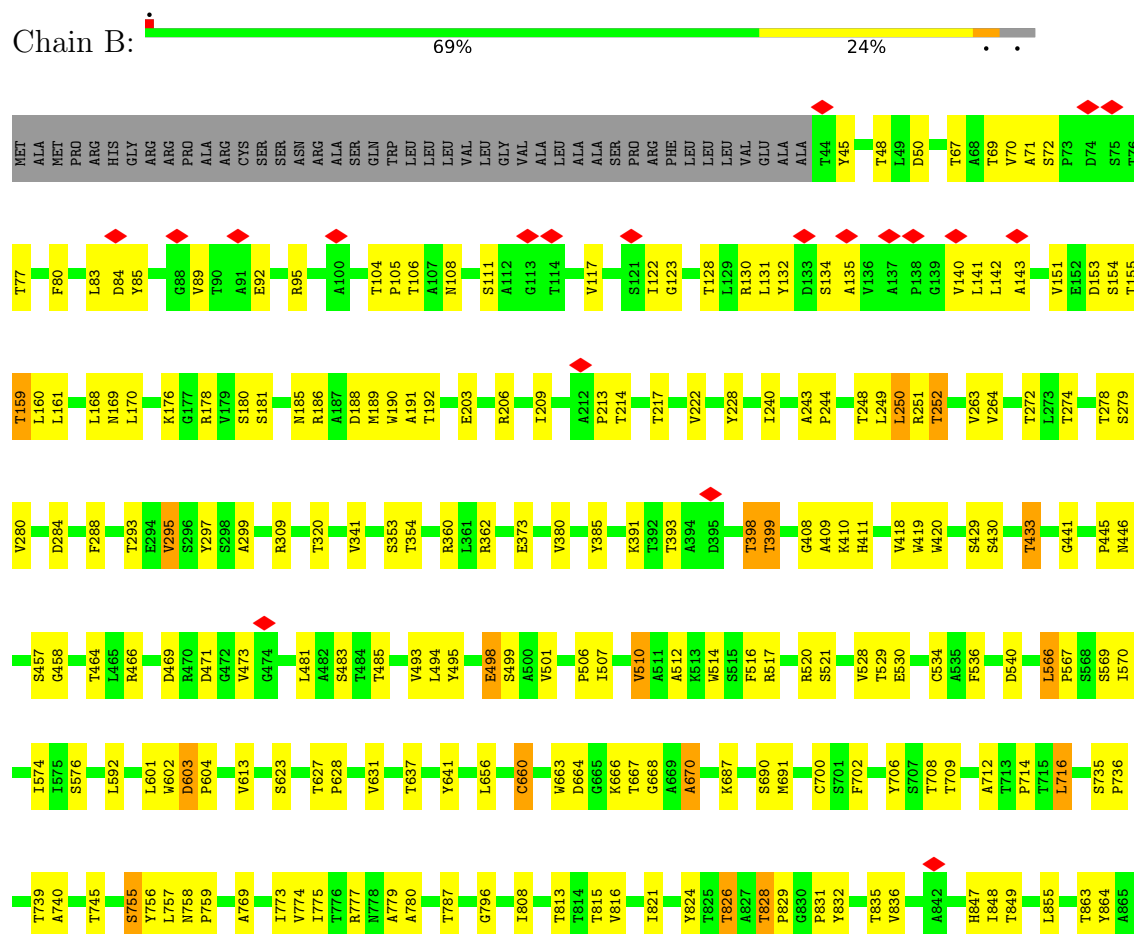
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

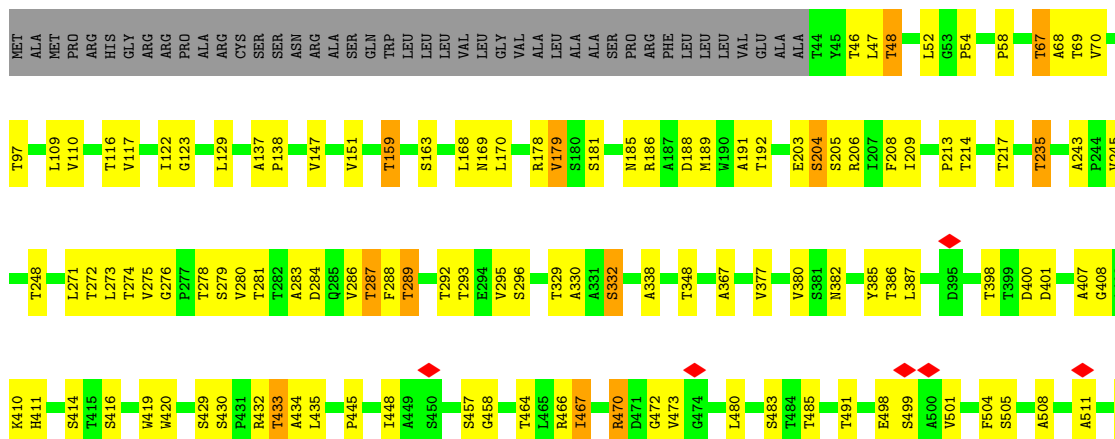
• Molecule 1: Mst1





• Molecule 1: Mst1







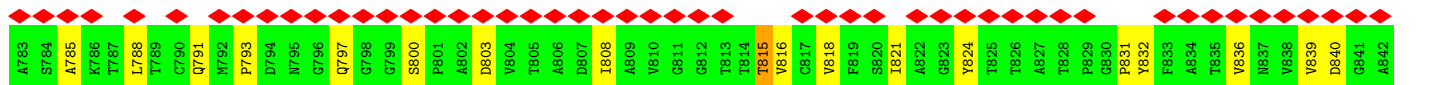
[illegible]

- Molecule 1: Mst1



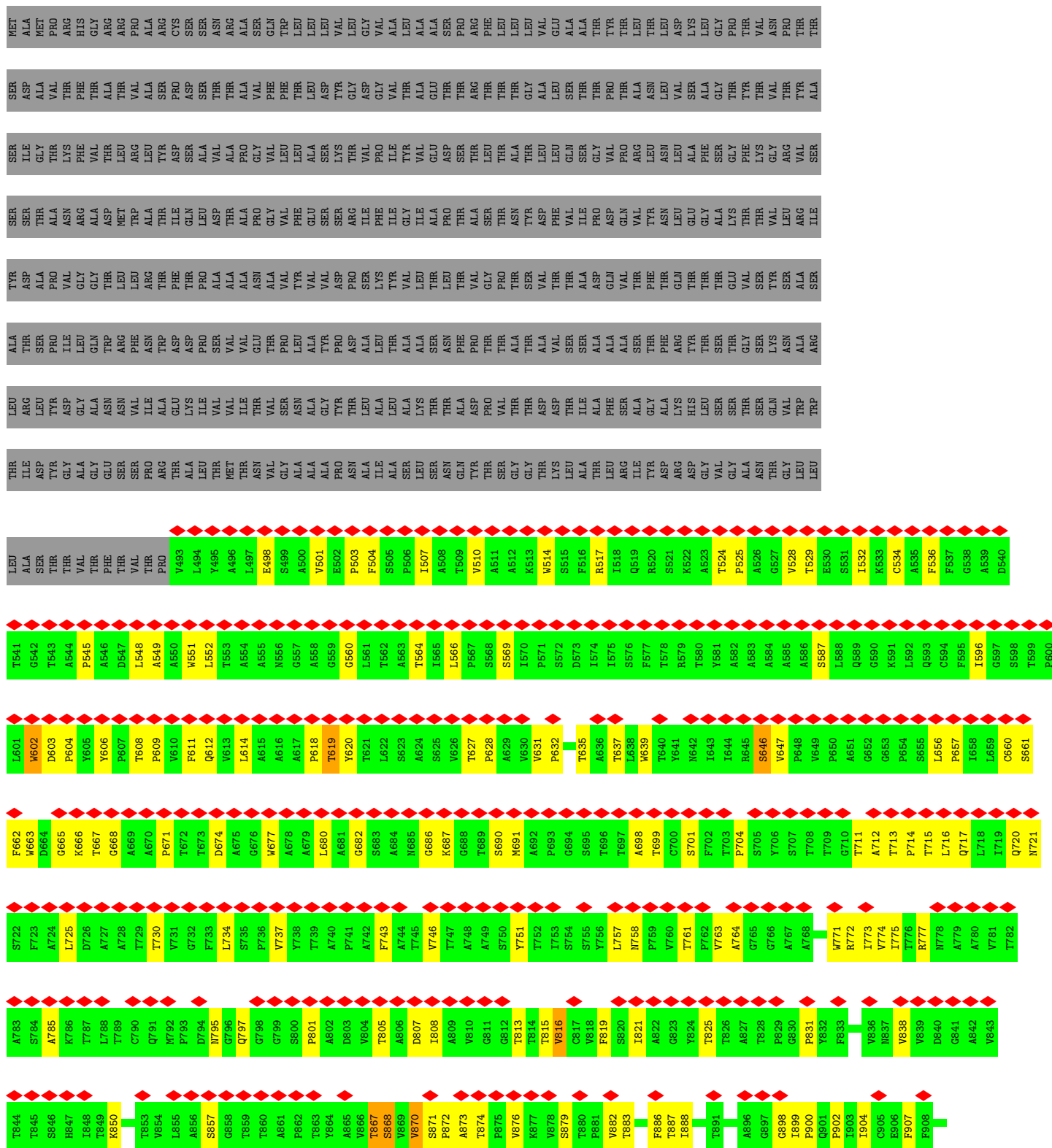
Y770	W771	R772	T773	W774	T775	T776	R777	W778	A779	W780	W781	T782	W783	W784	A785	K786	T787	L788	T789	W790	T791	W792	T793	W794	T795	W796	T797	W798	W799	S800	P801	A802	D803	W804	T805	A806	D807	I808	A809	W810	G811	G812	T813	T814	T815	W816	C817	W818	F819	S820	I821	G823	T824	T825	T826	A827	T828
Y706	S707	T708	T709	T710	T711	A712	T713	T714	T715	L716	T717	L718	T719	Q720	S721	A724	L725	D726	A727	A728	T729	F733	L734	S735	T736	T737	A740	P741	A742	T743	A744	T745	W746	T747	A748	A749	S750	T751	T752	T753	S754	T755	Y756	L757	N758	P759	W760	T761	P762	P763	A764	T765	G766	A767	A768	A769	
P632	V633	D634	T635	A636	T637	L638	P639	T640	W641	W642	I643	P648	W649	W650	A651	L656	L659	C660	S661	F662	W663	D664	G665	K666	T667	G668	A669	A670	P671	T672	A675	G676	W677	A678	A679	L680	A681	G682	S683	A684	W685	G686	K687	M691	T686	T687	A688	T689	C700	T703	S705						
A558	G559	G560	L561	T562	L566	S569	I575	S576	F577	T578	R579	T580	Y581	A582	A583	A584	A585	A586	S587	L588	Q593	C594	F595	I596	G597	S598	T599	W602	D603	Y606	P607	T608	P609	V610	L614	A615	A616	A617	P618	T619	W620	T621	L622	S623	A624	S625	V626	T627	P628	A629	V630	V631					
G474	A475	L479	L480	L481	T487	T491	L497	A500	V501	E502	P503	F504	S505	P506	I507	A508	T509	A511	A512	K513	F516	R517	I518	Q519	K522	A523	T524	P525	A526	G527	V528	S531	I532	K533	G534	A539	D540	T541	G542	T543	P545	L548	W551	M556	G557												
A338	I393	S342	R350	Y351	T352	S353	K357	T379	Y385	T386	D395	T398	T399	D400	D401	A407	K410	H411	S414	T415	S416	Q417	W418	W419	W420	T421	I422	S429	S430	T433	G441	A442	I448	Q454	L462	I467	Y468	D469	D470	A471	G472	V473															
T192	T193	Q194	E203	S204	I207	F208	I209	G210	L211	A212	P213	Y219	T223	P224	D225	Q226	E231	L238	R239	T248	T252	T272	L273	T274	V275	G276	P277	T278	S279	V280	T281	T282	A283	Q285	D284	Q286	F288	T289	Q290	T293	S296	Y297	R298	A299	T329	A330											
T67	A71	S72	S75	T76	F80	L83	R85	S102	T103	P105	V110	Y115	T116	I122	G123	R130	L131	A135	L141	L142	V151	T157	A159	T159	L161	L168	N169	L170	F175	R178	V179	S180	S181	N185	R186	A187	D188	T189	A191																		
MET	ALA	MET	PRO	ARG	HIS	GLY	ARG	ARG	PRO	ALA	ARG	CYS	ALA	SER	SER	ASN	ARG	SER	GLN	TRP	LEU	LEU	VAL	LEU	GLY	VAL	ALA	LEU	ALA	ALA	PRO	ARG	PHE	LEU	LEU	LEU	VAL	GLU	ALA	T44	Y45	T46	L47	D50	K51	L52	G53	P58	S61	V64	T65	F66					

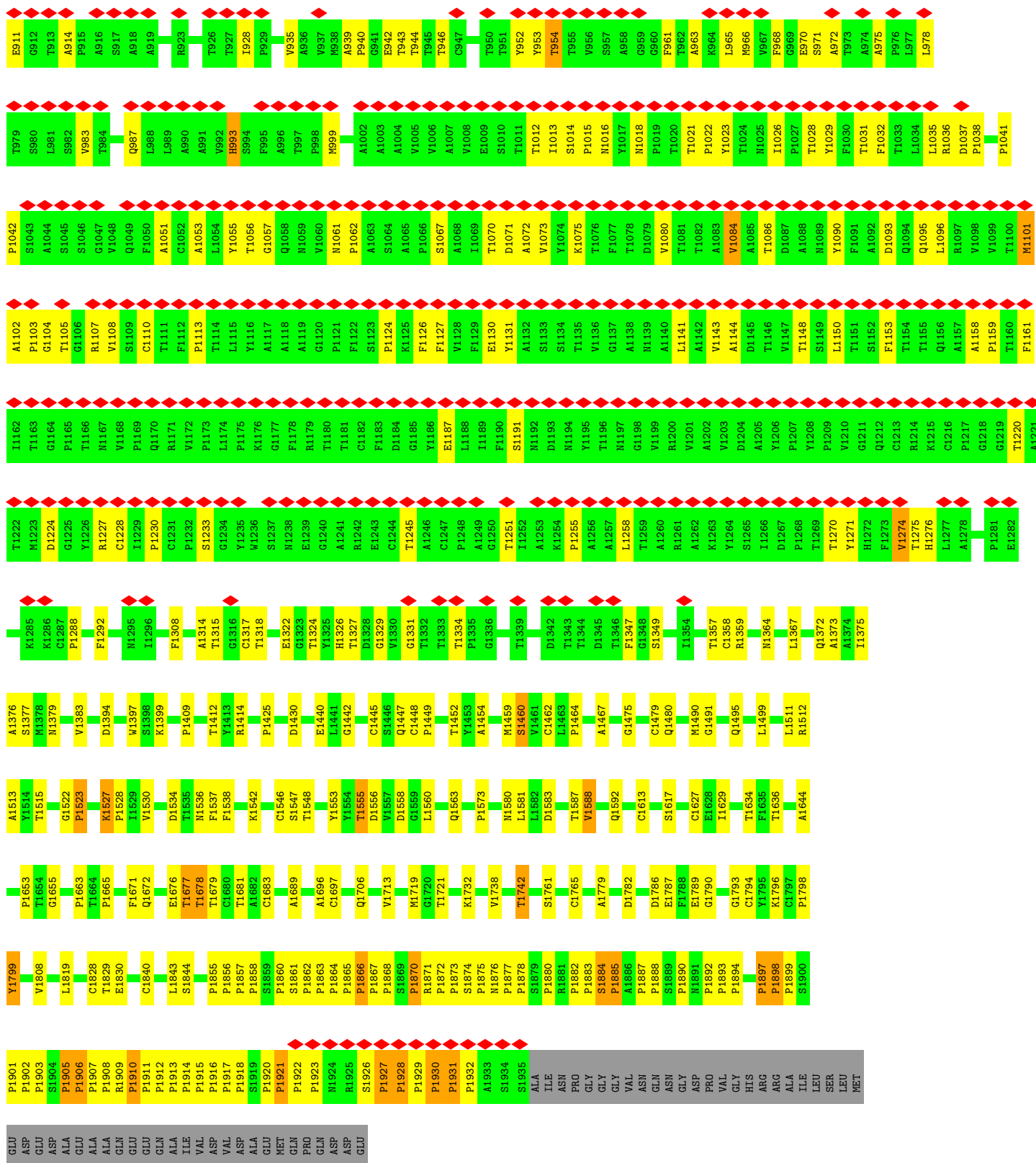
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HYP	VAL	THR	THR	CYS	LYS	PRO	D1507	Q1447	A1382	L1277	E1130	S1046	T962	A896	P831
HYP	ARG	PRO	ALA	ILE	GLY	THR	F1508	C1448		A1278	S1133	G1047	A963	G897	Y832
HYP	GLN	CYS	ASP	ALA	THR	PHE	P1509	P1449	P1388	M1279	A1138	T1056	K964	G898	F833
HYP	ALA	ALA	ALA	PRO	MET	PRO	A1510	P1450	R1390	G1280	M1139	Q1058	L965	I899	A834
HYP	ALA	GLY	ALA	GLY	ALA	PRO	L1511	P1451		P1281	M1140	G1059	L966	P900	T835
HYP	ALA	GLY	ALA	GLY	ALA	PRO	R1512	T1452	E1393	E1282	L1141	Q1058	M967	Q901	V836
HYP	ALA	GLY	ALA	GLY	ALA	PRO	A1513	Y1453	D1394	K1285	L1142	Q1059	G969	P902	N837
HYP	ALA	GLY	ALA	GLY	ALA	PRO	Y1514	P1454	G1395	K1286	A1142	V1060	E970	I903	V838
HYP	ALA	GLY	ALA	GLY	ALA	PRO	T1515	P1455	G1396	K1289	A1143	N1061	S971	I904	Y839
HYP	ALA	GLY	ALA	GLY	ALA	PRO	ILE	F1457	S1398		L1144	P1062	A972	C905	D840
HYP	ALA	GLY	ALA	GLY	ALA	PRO	SER	T1456	K1399	F1292	T1145	A1063	T973	E906	G841
HYP	ALA	GLY	ALA	GLY	ALA	PRO	GLY	F1458	K1399	Q1293	L1146	S1064	A974	F907	A842
HYP	ALA	GLY	ALA	GLY	ALA	PRO	MET	M1459	A1400	P1294	V1147			F908	V843
HYP	ALA	GLY	ALA	GLY	ALA	PRO	VAL	S1460	A1401	N1295	L1150	S1067	A975	N909	T844
HYP	ALA	GLY	ALA	GLY	ALA	PRO	ALA	V1461	A1402	T1299	T1155	A1068	P976	G910	T845
HYP	ALA	GLY	ALA	GLY	ALA	PRO	PRO	A1462	A1403			I1069	L977	E911	S846
HYP	ALA	GLY	ALA	GLY	ALA	PRO	ALA	C1463	A1404	S1306	T1160	T1070	L978	G912	
HYP	ALA	GLY	ALA	GLY	ALA	PRO	ALA	L1463	C1405	G1307	F1161	D1071	T979	T913	
HYP	ALA	GLY	ALA	GLY	ALA	PRO	ALA	P1464	Q1406	F1308		A1072	S980	H847	
HYP	ALA	GLY	ALA	GLY	ALA	PRO	ALA	C1465	K1407		P1165	T1076	L981	A914	
HYP	ALA	GLY	ALA	GLY	ALA	PRO	ALA	P1466	C1408	G1313				I849	
HYP	ALA	GLY	ALA	GLY	ALA	PRO	ALA	A1467	P1409	A1314	V1080		S982	T849	
HYP	ALA	GLY	ALA	GLY	ALA	PRO	ALA	G1468	P1410			V1084	T984	N851	
HYP	ALA	GLY	ALA	GLY	ALA	PRO	ALA	T1469	G1411	C1317		A1085	P985	F852	
HYP	ALA	GLY	ALA	GLY	ALA	PRO	ALA	F1470	T1412	T1318	D1184	T1086	S986	T853	
HYP	ALA	GLY	ALA	GLY	ALA	PRO	ALA	A1471	G1413	A1319			Q987	V854	
HYP	ALA	GLY	ALA	GLY	ALA	PRO	ALA	S1472	R1413	H1326	M1192	D1093	L855	L855	
HYP	ALA	GLY	ALA	GLY	ALA	PRO	ALA	P1473	N1414	T1327	D1193	Q1094	A856	A856	
HYP	ALA	GLY	ALA	GLY	ALA	PRO	ALA	A1474	T1416	G1329	R1200	Q1095	S857	S857	
HYP	ALA	GLY	ALA	GLY	ALA	PRO	ALA	P1475	W1417	V1330	V1201	L1096	G859	G859	
HYP	ALA	GLY	ALA	GLY	ALA	PRO	ALA	G1476	F1418	T1333	A1202	R1097	T859	T860	
HYP	ALA	GLY	ALA	GLY	ALA	PRO	ALA	A1476	S1419				A861		
HYP	ALA	GLY	ALA	GLY	ALA	PRO	ALA	T1477	G1420	A1338	V1203		P862		
HYP	ALA	GLY	ALA	GLY	ALA	PRO	ALA	A1478	Q1421	T1339	D1204		T933		
HYP	ALA	GLY	ALA	GLY	ALA	PRO	ALA	C1479	L1422		P1209	G1104	T997	V834	
HYP	ALA	GLY	ALA	GLY	ALA	PRO	ALA	Q1480	G1423	P1355		T1105	P998	V835	
HYP	ALA	GLY	ALA	GLY	ALA	PRO	ALA	Q1481	S1424	N1356	Q1212	G1106	M999	A936	
HYP	ALA	GLY	ALA	GLY	ALA	PRO	ALA	C1482	P1425	T1357	G1219	R1007	V1000	V937	
HYP	ALA	GLY	ALA	GLY	ALA	PRO	ALA	P1484	F1426	C1361	T1220	V1108	A1002	M938	
HYP	ALA	GLY	ALA	GLY	ALA	PRO	ALA	T1485	I1427	P1362	M1223	F1112	A1003	A939	
HYP	ALA	GLY	ALA	GLY	ALA	PRO	ALA	T1486	T1428	A1363	D1224	P1113	A1004	P940	
HYP	ALA	GLY	ALA	GLY	ALA	PRO	ALA	N1487	T1429	N1364		T1114	G941	G941	
HYP	ALA	GLY	ALA	GLY	ALA	PRO	ALA	S1488	D1430		I1229	L1115	E942	T943	
HYP	ALA	GLY	ALA	GLY	ALA	PRO	ALA	L1489	G1431	L1367	P1230	Y1116	T945	T945	
HYP	ALA	GLY	ALA	GLY	ALA	PRO	ALA	M1490	V1432	A1374		A1119	M1018	T946	
HYP	ALA	GLY	ALA	GLY	ALA	PRO	ALA	G1491	P1433		R1242		T1021	T946	
HYP	ALA	GLY	ALA	GLY	ALA	PRO	ALA	D1492	V1434	S1377	E1243		T1028	C947	
HYP	ALA	GLY	ALA	GLY	ALA	PRO	ALA	R1493	A1435	M1378		S1123	T951	T951	
HYP	ALA	GLY	ALA	GLY	ALA	PRO	ALA	T1494	T1436	N1379	T1251	P1124	T952	T885	
HYP	ALA	GLY	ALA	GLY	ALA	PRO	ALA	Q1495	T1437	L1350	P1256	K1125	T953	F886	
HYP	ALA	GLY	ALA	GLY	ALA	PRO	ALA	D1558	L1438					T887	
HYP	ALA	GLY	ALA	GLY	ALA	PRO	ALA	G1559	T1439					I888	
HYP	ALA	GLY	ALA	GLY	ALA	PRO	ALA	L1560	E1440					T889	
HYP	ALA	GLY	ALA	GLY	ALA	PRO	ALA	P1561	L1441					R890	
HYP	ALA	GLY	ALA	GLY	ALA	PRO	ALA	T1562	G1442					T891	
HYP	ALA	GLY	ALA	GLY	ALA	PRO	ALA	Q1563	T1444					T892	
HYP	ALA	GLY	ALA	GLY	ALA	PRO	ALA	L1564	G1445					A893	
HYP	ALA	GLY	ALA	GLY	ALA	PRO	ALA	P1565						V894	

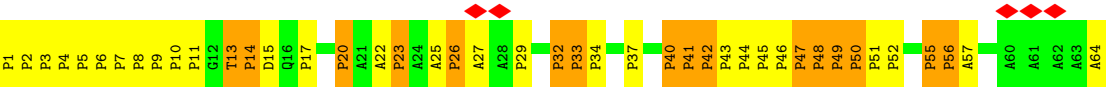


HIS	P1892	G1807	S1377	K1286	T1162	A1102	P1042	L981	G910	V843
ARG	P1893	V1808	K1376	C1287	T1163	P1103	S1043	S982	E911	T844
ARG	P1894	R1809	N1379	K1288	G1164	G1104	A1044	V933	G912	T845
ALA	P1895	T1677	T1387	P1289	P1165	T1105	S1045	T984	T913	S846
ILE	P1896	T1678	D1534	Y1291	T1166	R1107	S1046	P985	H847	H848
LEU	P1897	T1679	T1396	F1292	N1167	G1047	G1047	L988	P915	I849
SER	P1898	C1683	F1397	F1293	V1168	V1108	V1048	L989	A916	T849
LEU	P1899	C1684	S1398	N1295	P1169	S1109	Q1049	A990	S917	K850
MET	P1900	T1687	M1539	T1296	C1228	C1110	F1050	A991	A918	K851
GLU	P1901	T1688	C1405	A1297	P1230	T1111	A1051	A992	A919	F852
ASP	P1902	D1690	T1412	G1298	C1231	F1112	C1052	H993	A920	T853
GLU	P1903	D1691	L1415	C1301	P1232	P1113	A1053	S994	Y921	V854
ASP	P1904	C1697	T1416	L1302	S1233	T1114	L1054	F995	W922	L855
ALA	P1905	K1698	Q1421	F1308	G1234	L1115	Y1055	A996	V924	A856
ALA	P1906	R1704	Q1422	S1312	S1237	Y1116	T1056	T997	T927	S857
ALA	P1907	Y1705	D1430	G1313	N1238	A1117	Q1058	P998	T928	G858
GLN	P1908	Q1706	D1431	A1314	E1239	A1118	G1059	M999	I928	T859
GLU	P1909	Q1707	T1438	A1315	G1240	A1119	V1060	V1000	P929	A861
GLU	P1910	Q1708	T1439	C1317	A1241	G1120	N1061	V1001	D932	P862
GLU	P1911	Q1709	T1440	T1318	E1242	P1121	A1062	A1002	T933	T863
GLN	P1912	Q1710	T1441	A1319	E1243	F1122	P1063	A1003	V934	Y864
ALA	P1913	Q1711	T1442	T1324	C1244	S1123	A1063	A1004	A865	A866
ILE	P1914	Q1712	T1443	Y1325	T1245	P1124	S1064	V1005	V867	T867
VAL	P1915	Q1713	T1444	T1326	A1246	K1125	A1065	V1006	M938	S868
VAL	P1916	Q1714	T1445	T1327	C1247	F1126	P1066	A1007	A939	S871
ASP	P1917	Q1715	T1446	T1328	E1248	T1127	S1067	A1008	P940	P872
ASP	P1918	Q1716	T1447	Y1330	A1249	V1128	I1068	E1009	G941	A873
ASP	P1919	Q1717	T1448	T1331	K1254	F1129	I1069	S1010	E942	T874
GLU	P1920	Q1718	T1449	T1332	P1255	E1130	T1070	S1011	T943	T875
GLN	P1921	Q1719	T1450	T1333	P1256	Y1131	D1071	T1012	T945	P876
PRO	P1922	Q1720	T1451	T1334	A1257	A1132	A1072	I1013	T950	V876
GLN	P1923	Q1721	T1452	E1337	A1258	A1133	Y1073	S1014	T951	K877
ASP	P1924	Q1722	T1453	L1341	T1259	S1134	Y1074	P1015	T952	V878
ASP	P1925	Q1723	T1454	D1342	A1260	T1135	K1075	N1016	Y953	S879
ASP	P1926	Q1724	T1455	D1343	S1261	V1136	T1076	T954	T955	T880
GLU	P1927	Q1725	T1456	T1350	A1262	G1137	F1077	N1018	V956	P881
GLU	P1928	Q1726	T1457	T1351	A1263	A1138	T1078	P1019	Y884	V882
GLU	P1929	Q1727	T1458	T1352	K1263	N1139	D1079	T1020	T885	T883
GLU	P1930	Q1728	T1459	L1341	S1264	A1140	V1080	T1021	F886	T884
GLU	P1931	Q1729	T1460	D1342	S1265	L1141	T1081	P1022	G959	T885
GLU	P1932	Q1730	T1461	T1350	A1266	A1142	T1082	G960	T889	T886
GLU	P1933	Q1731	T1462	T1351	A1267	Y1143	A1083	T1023	G961	T889
GLU	P1934	Q1732	T1463	T1352	P1268	A1144	V1084	T1024	F961	T890
GLU	P1935	Q1733	T1464	T1353	T1269	D1145	A1085	N1025	T962	V882
GLU	P1936	Q1734	T1465	Q1360	A1206	T1146	T1086	I1026	A963	V883
GLU	P1937	Q1735	T1466	T1354	Y1206	T1147	D1087	P1027	K964	A896
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GLU	P1945	Q1743	T1474	T1362	R1214	T1154	Q1094	L1035	P976	F907
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GLU	P1947	Q1745	T1476	T1364	C1216	Q1156	L1096	D1037		N909
GLU	P1948	Q1746	T1477	T1365	P1217	A1157	V1098	P1038		
GLU	P1949	Q1747	T1478	T1366	G1218	A1158	V1099	V1040		
GLU	P1950	Q1748	T1479	T1367	T1220	T1160	T1100	P1041		
GLU	P1951	Q1749	T1480	T1368	A1221	F1161				
GLU	P1952	Q1750	T1481	T1369						
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GLU	P2031	Q1829	T1560	T1448						
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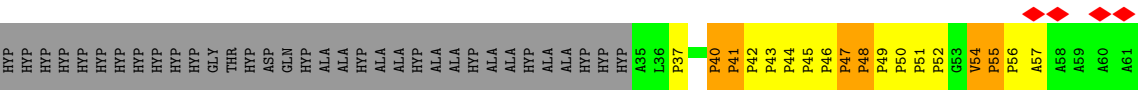
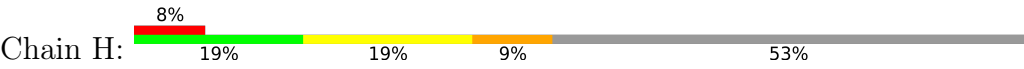
Chain F: 35% 50% 20% 27%



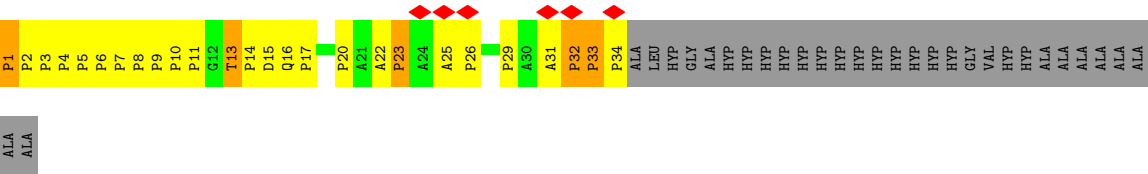




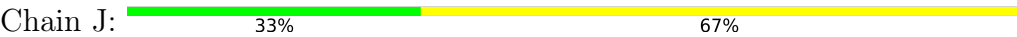
• Molecule 2: Mstax



• Molecule 2: Mstax



• 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 P:  67% 33%

FUB1
FUB2
FUB3

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

Chain Q:  67% 33%

FUB1
FUB2
FUB3

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

Chain T:  67% 33%

FUB1
FUB2
FUB3

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

Chain V:  67% 33%

FUB1
FUB2
FUB3

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

Chain b:  100%

FUB1
FUB2
FUB3

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

Chain e:  67% 33%

FUB1
FUB2
FUB3

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

Chain l:  100%

FUB1
FUB2
FUB3

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

Chain m:  33% 67%

FUB1
FUB2
FUB3

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

Chain t:  67% 33%

FUB1
FUB2
FUB3

- 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:  67% 33%

FUB1
FUB2
FUB3

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

Chain z:  33% 33% 33%

FUB1
FUB2
FUB3

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

Chain 0:  67% 33%



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

Chain 1:  67% 33%



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

Chain 2:  100%

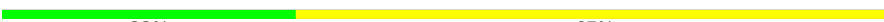


- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain HA:  67% 33%



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

Chain IA:  33% 67%



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

Chain MA:  33% 67%



- 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:  67% 33%

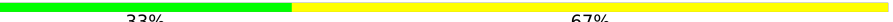


- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain XA:  33% 67% 33%

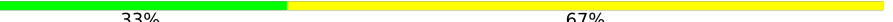


- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain ZA:  33% 67%

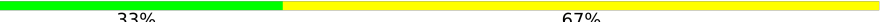


- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain cA:  33% 67%



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

Chain jA:  33% 67%



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

Chain kA:  100%

FUB1
FUB2
FUB3

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

Chain rA:  67% 33%

FUB1
FUB2
FUB3

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

Chain uA:  67% 33%

FUB1
FUB2
FUB3

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

Chain vA:  67% 33%

FUB1
FUB2
FUB3

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

Chain wA:  67% 33%

FUB1
FUB2
FUB3

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

Chain xA:  33% 67%

FUB1
FUB2
FUB3

- 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



• 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-arabinofuranos e



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



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



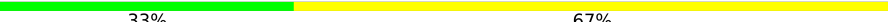
- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranos e



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



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

Chain wB:  33% 67%

FUB1
FUB2
FUB3

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

Chain xB:  67% 33%

FUB1
FUB2
FUB3

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

Chain BC:  67% 33%

FUB1
FUB2
FUB3

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

Chain CC:  33% 67%

FUB1
FUB2
FUB3

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

Chain GC:  67% 33%

FUB1
FUB2
FUB3

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

Chain HC:  67% 33%

FUB1
FUB2
FUB3

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

Chain IC:  67% 33%

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 NC:  67% 33%

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%



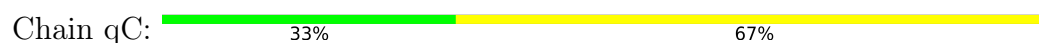
- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



- 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 ID:  67% 33%



- 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%

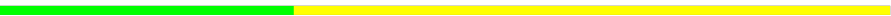


- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain bD:  100%



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

Chain iD:  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





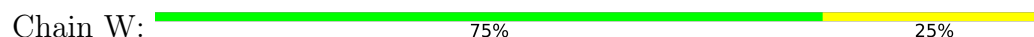
- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



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



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



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



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



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



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

Chain d:  50% 50%

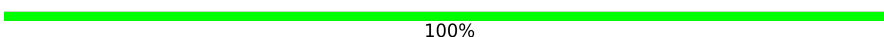


- Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

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:  75% 25%



- 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%

FUB1
FUB2
FUB3
AHR4

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

Chain VA:  75% 25%

FUB1
FUB2
FUB3
AHR4

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

Chain aA:  100%

FUB1
FUB2
FUB3
AHR4

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

Chain bA:  100%

FUB1
FUB2
FUB3
AHR4

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

Chain eA:  100%

FUB1
FUB2
FUB3
AHR4

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

Chain iA:  100%

FUB1
FUB2
FUB3
AHR4

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

Chain pA:  50% 50%



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



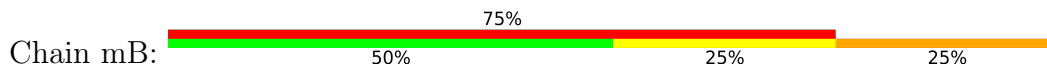
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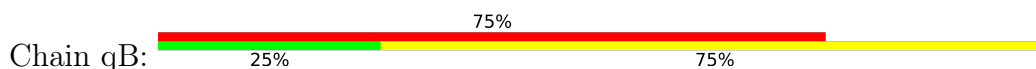
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- Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



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



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





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

Chain OC: 75% 25%



- 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



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



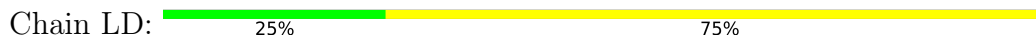
- Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



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



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



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



- Molecule 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%



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

Chain SD:  50% 50%



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

Chain VD:  25% 50% 25%



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

Chain ZD:  25% 75% 25%



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

Chain gD:  25% 50% 25% 25%



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

Chain kD:  25% 75% 25%



- 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

Chain M: 80% 20%



- 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

Chain KA: 40% 40% 20%



- 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

Chain EC: 20% 80%



- 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

Chain BD: 60% 40%



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

Chain N: 33% 33% 33%



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

Chain R: 33% 67%

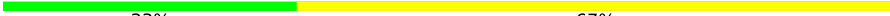


- Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 5:  33% 33% 33%



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

Chain 8:  33% 67%



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

Chain 9:  33% 33% 33%



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

Chain AA:  33% 67%



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

Chain EA:  67% 33%



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

Chain LA:  33% 33% 33%



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

Chain PA:  67% 33%



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



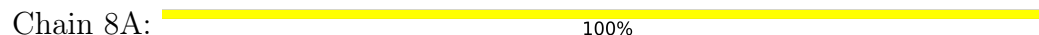
- Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



- 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

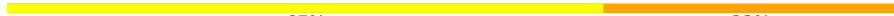


- Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain aB:  33% 67%



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

Chain bB:  67% 33%



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

Chain cB:  67% 33%



- 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%

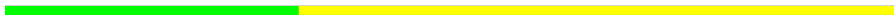


- Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

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



- 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



- 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

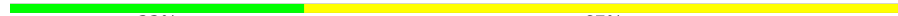


- Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 8D:  67% 33%

FUB1
FUB2
GZL3

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

Chain ME:  33% 67%

FUB1
FUB2
GZL3

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

Chain OE:  100%

FUB1
FUB2
GZL3

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

Chain ZE:  33% 67%

FUB1
FUB2
GZL3

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

Chain bE:  33% 33% 33%

FUB1
FUB2
GZL3

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

Chain mE:  67% 33%

FUB1
FUB2
GZL3

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

Chain nE:  33% 33% 33%



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



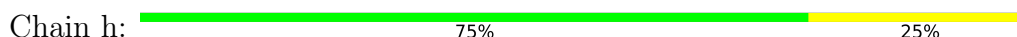
- Molecule 7: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose



- 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



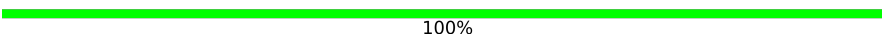
- Molecule 7: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose



- 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 fA:  100%

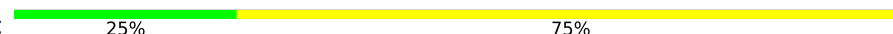


- Molecule 7: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain KC:  50% 25% 25%



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

Chain XC:  25% 75%



- 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% 25% 25%



- 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%

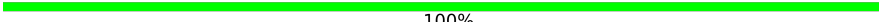


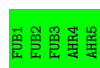
- Molecule 8: alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

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%



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

Chain MC:  40% 60%



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

Chain JD:  60% 40%



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

Chain Y:  50% 50%



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

Chain j:  50% 50%



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

Chain WA:  100%

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%

FUB1
FUB2

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

Chain bC:  100%

FUB1
FUB2

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

Chain ND:  50% 50%

FUB1
FUB2

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

Chain YD:  100%

FUB1
FUB2

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

Chain a:  40% 60%

FUB1
FUB2
FUB3
AHR4
AHR5

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

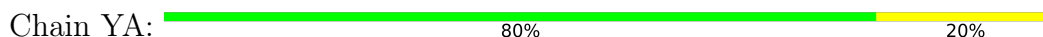
Chain u:  60% 40%



- 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



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



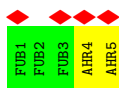
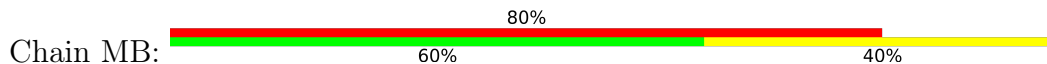
- Molecule 10: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose



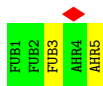
- Molecule 10: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose



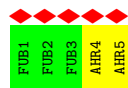
- Molecule 10: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose



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



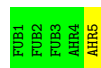
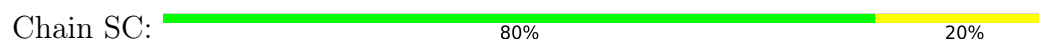
- Molecule 10: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose



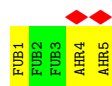
- Molecule 10: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose



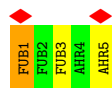
- Molecule 10: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose



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



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



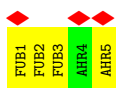
- Molecule 10: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose



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



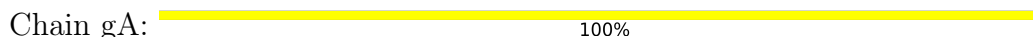
- Molecule 10: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose



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



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



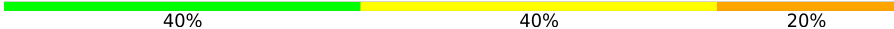
- Molecule 11: alpha-L-arabinofuranose-(1-3)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose



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

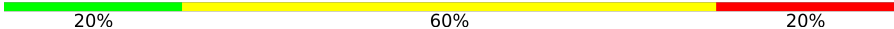


- Molecule 12: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain n: 

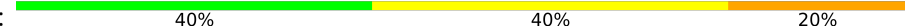


- Molecule 12: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain q: 



- 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 lA: 



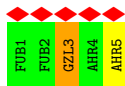
- Molecule 12: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain oA: 

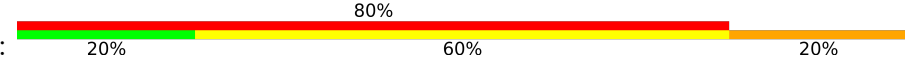


- Molecule 12: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain FB: 

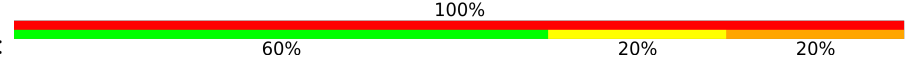


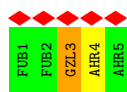
- Molecule 12: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain IB: 

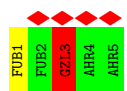
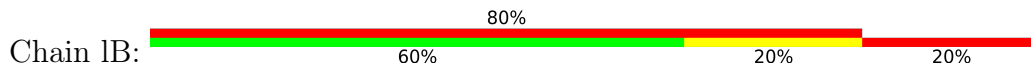


- Molecule 12: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

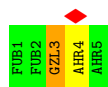
Chain iB: 



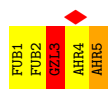
- Molecule 12: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose



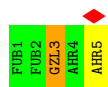
- Molecule 12: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose



- 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



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



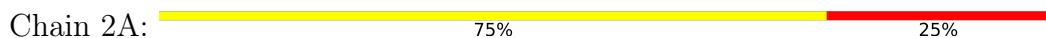
- Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



- 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

Chain 4A: 



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

Chain 5A: 



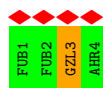
- Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 9A: 

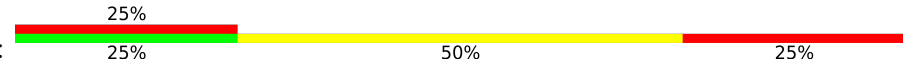


- Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain GB: 



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

Chain WB: 



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

Chain YB: 



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

Chain ZB:  75% 25%

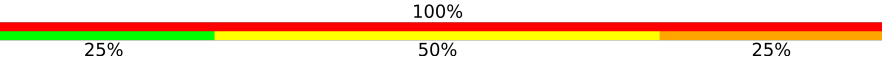


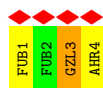
- Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain dB:  50% 50%



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

Chain jB:  25% 50% 25%



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

Chain zB:  25% 25% 25% 25%



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

Chain 1B:  75% 25%



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

Chain 2B:  50% 50%



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

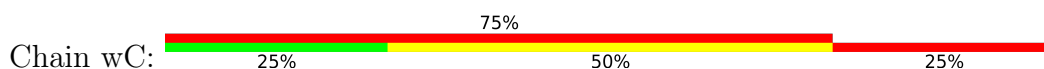
Chain 6B:  50% 50%



- 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



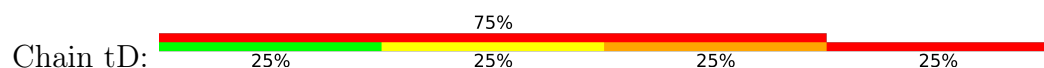
- Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



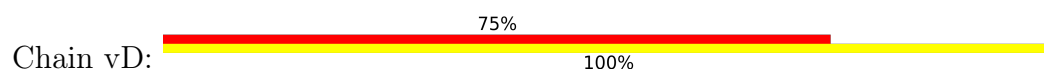
- Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



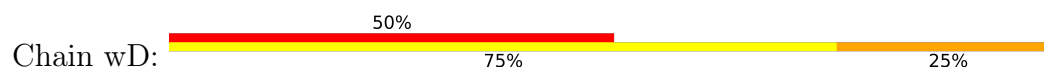
- Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



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



- 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

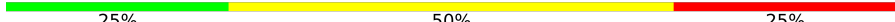


- Molecule 14: beta-L-arabinofuranose-(1-5)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain s:  75% 25%

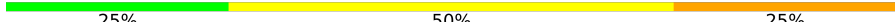


- Molecule 14: beta-L-arabinofuranose-(1-5)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain nA:  25% 50% 25%

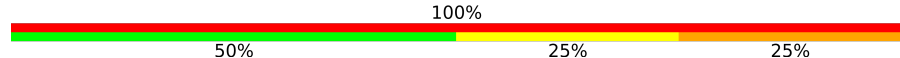


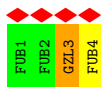
- Molecule 14: beta-L-arabinofuranose-(1-5)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain qA:  25% 50% 25%

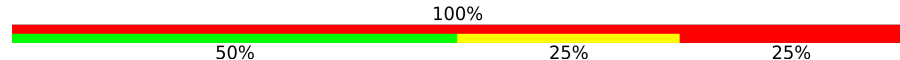


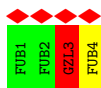
- Molecule 14: beta-L-arabinofuranose-(1-5)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain HB:  100% 50% 25% 25%

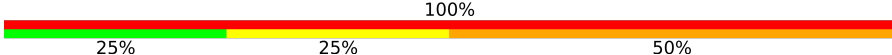


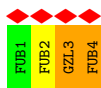
- Molecule 14: beta-L-arabinofuranose-(1-5)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain KB:  100% 50% 25% 25%

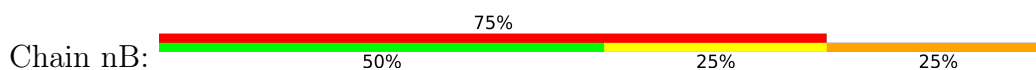


- Molecule 14: beta-L-arabinofuranose-(1-5)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain kB:  100% 25% 25% 50%



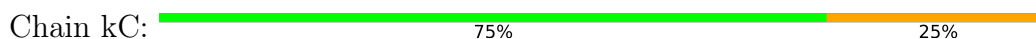
- Molecule 14: beta-L-arabinofuranose-(1-5)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



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



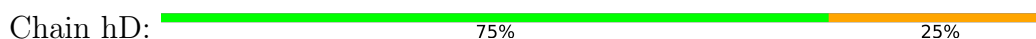
- Molecule 14: beta-L-arabinofuranose-(1-5)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



- 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 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 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



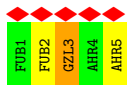
- Molecule 15: alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



- 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



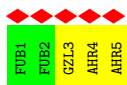
- Molecule 15: alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



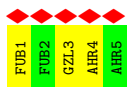
- Molecule 15: alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



- 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



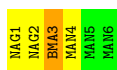
- Molecule 17: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- 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



- 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



- 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



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

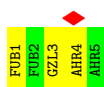
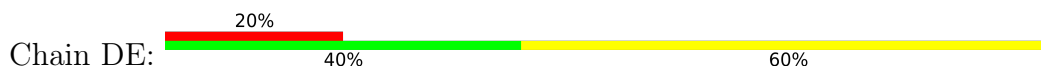




- Molecule 18: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose



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



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



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



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



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



- 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: 



- 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: 



- 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 rE: 

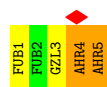
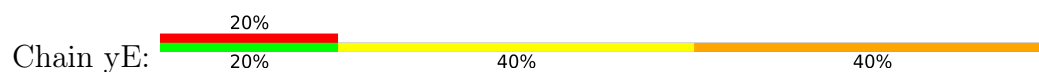


- Molecule 18: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain tE: 



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



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



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



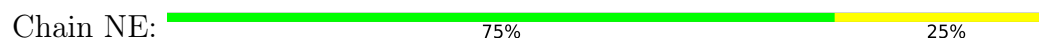
- Molecule 19: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose



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



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



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



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



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



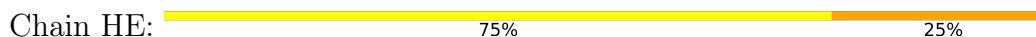
- Molecule 20: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



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



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



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





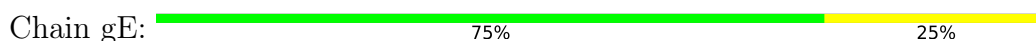
- Molecule 20: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



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



- 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 uE:  75% 25%

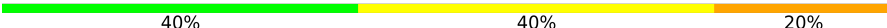


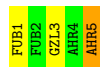
- Molecule 20: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain xE:  25% 25% 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% 40% 20%



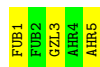
- Molecule 21: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)][alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose

Chain kE:  20% 80%

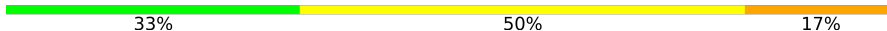


- Molecule 21: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)][alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose

Chain vE:  40% 60%

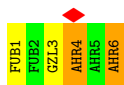


- Molecule 22: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

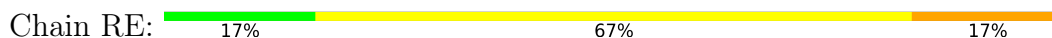
Chain GE:  33% 50% 17%



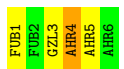
- Molecule 22: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose



- 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



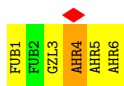
- Molecule 22: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose



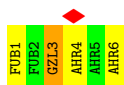
- Molecule 22: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose



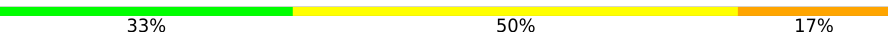
- Molecule 22: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose



- 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

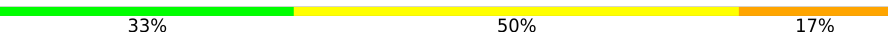


- Molecule 22: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain wE:  33% 50% 17%



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

Chain XE:  33% 50% 17%

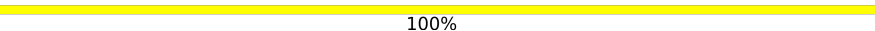


- Molecule 24: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)][alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose

Chain YE:  17% 83%



- 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 lE:  100%



4 Experimental information

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

5 Model quality

5.1 Standard geometry

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

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	0.15	0/13724	0.37	2/18848 (0.0%)
1	B	0.16	0/13724	0.37	2/18848 (0.0%)
1	C	0.13	0/10873	0.33	0/14984
1	D	0.14	0/11422	0.36	2/15734 (0.0%)
1	E	0.13	0/10283	0.33	0/14106
1	F	0.20	2/10246 (0.0%)	0.42	4/14055 (0.0%)
2	G	0.17	0/139	0.52	0/174
2	H	0.06	0/69	0.25	0/89
2	I	0.16	0/71	0.42	0/87
All	All	0.15	2/70551 (0.0%)	0.36	10/96925 (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	-10.44	0.97	1.49
1	F	632	PRO	CG-CD	-9.29	1.19	1.50

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	632	PRO	CB-CG-CD	18.16	164.20	106.10
1	F	632	PRO	N-CD-CG	-16.73	78.11	103.20
1	F	632	PRO	CA-CB-CG	-13.99	77.91	104.50
1	B	1846	PRO	CA-N-CD	-12.57	94.40	112.00
1	A	1839	PRO	CA-N-CD	-11.43	96.00	112.00

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](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	13862	0	13346	281	0
1	B	13862	0	13347	275	0
1	C	10840	0	10542	223	0
1	D	11377	0	11060	292	0
1	E	10491	0	10011	240	0
1	F	10455	0	9976	230	0
2	G	438	0	367	12	0
2	H	201	0	174	3	0
2	I	238	0	196	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	0	27	0	0	0	0
3	0A	27	0	0	0	0
3	1	27	0	0	0	0
3	2	27	0	0	0	0
3	8C	27	0	0	1	0
3	9C	27	0	0	0	0
3	BC	27	0	0	0	0
3	CC	27	0	0	0	0
3	DD	27	0	0	0	0
3	EB	27	0	0	0	0
3	ED	27	0	0	0	0
3	FD	27	0	0	0	0
3	GC	27	0	0	0	0
3	HA	27	0	0	0	0
3	HC	27	0	0	0	0
3	IA	27	0	0	1	0
3	IC	27	0	0	0	0
3	ID	27	0	0	0	0
3	J	27	0	0	1	0
3	K	27	0	0	1	0
3	KD	27	0	0	0	0
3	LB	27	0	0	2	0
3	LC	27	0	0	0	0
3	MA	27	0	0	1	0
3	NA	27	0	0	0	0
3	NC	27	0	0	1	0
3	O	27	0	0	0	0
3	OA	27	0	0	0	0
3	OB	27	0	0	0	0
3	P	27	0	0	0	0
3	PB	27	0	0	1	0
3	Q	27	0	0	0	0
3	QB	27	0	0	2	0
3	QD	27	0	0	0	0
3	RA	27	0	0	0	0
3	RB	27	0	0	2	0
3	SB	27	0	0	0	0
3	T	27	0	0	0	0
3	TA	27	0	0	1	0
3	TB	27	0	0	0	0
3	TC	27	0	0	0	0
3	TD	27	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	UB	27	0	0	0	0
3	V	27	0	0	0	0
3	WC	27	0	0	0	0
3	XA	27	0	0	0	0
3	ZA	27	0	0	1	0
3	aD	27	0	0	0	0
3	b	27	0	0	1	0
3	bD	27	0	0	0	0
3	cA	27	0	0	0	0
3	dC	27	0	0	0	0
3	e	27	0	0	0	0
3	eC	27	0	0	0	0
3	hB	27	0	0	0	0
3	iD	27	0	0	1	0
3	jA	27	0	0	0	0
3	kA	27	0	0	0	0
3	l	27	0	0	0	0
3	lC	27	0	0	0	0
3	lD	27	0	0	0	0
3	m	27	0	0	1	0
3	mD	27	0	0	1	0
3	nD	27	0	0	0	0
3	oB	27	0	0	2	0
3	oC	27	0	0	0	0
3	oD	27	0	0	1	0
3	pC	27	0	0	0	0
3	pD	27	0	0	0	0
3	qC	27	0	0	1	0
3	qD	27	0	0	0	0
3	rA	27	0	0	1	0
3	rB	27	0	0	0	0
3	rC	27	0	0	0	0
3	rD	27	0	0	0	0
3	sB	27	0	0	1	0
3	sC	27	0	0	0	0
3	t	27	0	0	1	0
3	tB	27	0	0	0	0
3	tC	27	0	0	1	0
3	uA	27	0	0	0	0
3	uB	27	0	0	0	0
3	uC	27	0	0	0	0
3	vA	27	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	vB	27	0	0	0	0
3	w	27	0	0	0	0
3	wA	27	0	0	1	0
3	wB	27	0	0	1	0
3	x	27	0	0	0	0
3	xA	27	0	0	2	0
3	xB	27	0	0	0	0
3	y	27	0	0	1	0
3	yA	27	0	0	0	0
3	z	27	0	0	2	0
3	zA	27	0	0	0	0
4	AD	36	0	0	2	0
4	DC	36	0	0	1	0
4	JA	36	0	0	1	0
4	JB	36	0	0	2	0
4	L	36	0	0	0	0
4	LD	36	0	0	1	0
4	MD	36	0	0	0	0
4	NB	36	0	0	0	0
4	OC	36	0	0	0	0
4	OD	36	0	0	0	0
4	PC	36	0	0	0	0
4	RC	36	0	0	0	0
4	RD	36	0	0	0	0
4	SD	36	0	0	0	0
4	UA	36	0	0	0	0
4	UC	36	0	0	0	0
4	VA	36	0	0	0	0
4	VC	36	0	0	0	0
4	VD	36	0	0	1	0
4	W	36	0	0	0	0
4	X	36	0	0	0	0
4	YC	36	0	0	0	0
4	Z	36	0	0	0	0
4	ZD	36	0	0	0	0
4	aA	36	0	0	0	0
4	bA	36	0	0	0	0
4	c	36	0	0	0	0
4	cC	36	0	0	0	0
4	d	36	0	0	0	0
4	eA	36	0	0	0	0
4	g	36	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	gD	36	0	0	3	0
4	iA	36	0	0	1	0
4	jC	36	0	0	2	0
4	k	36	0	0	0	0
4	kD	36	0	0	1	0
4	mB	36	0	0	1	0
4	nC	36	0	0	0	0
4	pA	36	0	0	2	0
4	qB	36	0	0	0	0
4	r	36	0	0	1	0
4	tA	36	0	0	0	0
4	v	36	0	0	0	0
5	BD	45	0	0	0	0
5	EC	45	0	0	2	0
5	KA	45	0	0	1	0
5	M	45	0	0	3	0
6	0B	29	0	7	4	0
6	0C	29	0	8	1	0
6	1C	29	0	8	1	0
6	2C	29	0	8	1	0
6	3A	29	0	7	5	0
6	3B	29	0	8	0	0
6	3D	29	0	8	0	0
6	4B	29	0	8	0	0
6	5	29	0	8	7	0
6	5B	29	0	8	0	0
6	6A	29	0	8	0	0
6	6C	29	0	8	0	0
6	6D	29	0	7	0	0
6	7A	29	0	8	0	0
6	7D	29	0	8	0	0
6	8	29	0	8	0	0
6	8A	29	0	8	0	0
6	8D	29	0	8	0	0
6	9	29	0	8	1	0
6	9B	29	0	8	0	0
6	AA	29	0	8	0	0
6	CB	29	0	8	0	0
6	CD	29	0	8	5	0
6	EA	29	0	8	0	0
6	FC	29	0	7	4	0
6	GD	29	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	JC	29	0	8	0	0
6	LA	29	0	8	4	0
6	ME	29	0	8	1	0
6	N	29	0	7	6	0
6	OE	29	0	8	1	0
6	PA	29	0	8	0	0
6	R	29	0	8	0	0
6	XB	29	0	7	4	0
6	ZE	29	0	8	0	0
6	aB	29	0	8	0	0
6	bB	29	0	8	1	0
6	bE	29	0	8	1	0
6	cB	29	0	8	1	0
6	gB	29	0	8	0	0
6	mE	29	0	8	2	0
6	nE	29	0	8	1	0
6	oE	29	0	8	0	0
6	uD	29	0	7	6	0
6	xC	29	0	7	6	0
6	xD	29	0	7	2	0
6	yD	29	0	8	0	0
6	zD	29	0	8	1	0
7	HD	36	0	0	1	0
7	KC	36	0	0	1	0
7	QA	36	0	0	0	0
7	S	36	0	0	0	0
7	UD	36	0	0	0	0
7	WD	36	0	0	0	0
7	XC	36	0	0	1	0
7	ZC	36	0	0	0	0
7	dA	36	0	0	0	0
7	f	36	0	0	2	0
7	fA	36	0	0	0	0
7	h	36	0	0	0	0
8	JD	45	0	0	1	0
8	MC	45	0	0	0	0
8	SA	45	0	0	0	0
8	U	45	0	0	0	0
9	ND	18	0	0	0	0
9	QC	18	0	0	0	0
9	WA	18	0	0	0	0
9	Y	18	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	YD	18	0	0	0	0
9	bC	18	0	0	0	0
9	hA	18	0	0	1	0
9	j	18	0	0	0	0
10	1A	45	0	0	0	0
10	3	45	0	0	1	0
10	MB	45	0	0	0	0
10	PD	45	0	0	0	0
10	SC	45	0	0	0	0
10	VB	45	0	0	0	0
10	YA	45	0	0	0	0
10	a	45	0	0	0	0
10	jD	45	0	0	0	0
10	mC	45	0	0	0	0
10	pB	45	0	0	0	0
10	sA	45	0	0	0	0
10	sD	45	0	0	2	0
10	u	45	0	0	0	0
10	vC	45	0	0	1	0
10	yB	45	0	0	1	0
11	XD	27	0	0	0	0
11	aC	27	0	0	0	0
11	gA	27	0	0	1	0
11	i	27	0	0	0	0
12	FB	47	0	7	0	0
12	IB	47	0	8	0	0
12	cD	47	0	8	0	0
12	fC	47	0	8	0	0
12	fD	47	0	8	0	0
12	iB	47	0	8	1	0
12	iC	47	0	8	2	0
12	lA	47	0	8	0	0
12	lB	47	0	8	1	0
12	n	47	0	8	0	0
12	oA	47	0	8	1	0
12	q	47	0	8	1	0
13	0D	38	0	8	2	0
13	1B	38	0	8	0	0
13	2A	38	0	8	5	0
13	2B	38	0	8	0	0
13	3C	38	0	8	0	0
13	4	38	0	7	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	4A	38	0	8	0	0
13	5A	38	0	8	0	0
13	6	38	0	8	0	0
13	6B	38	0	8	0	0
13	7	38	0	8	0	0
13	9A	38	0	8	0	0
13	BA	38	0	8	1	0
13	GB	38	0	8	0	0
13	WB	38	0	8	6	0
13	YB	38	0	8	0	0
13	ZB	38	0	8	0	0
13	dB	38	0	8	0	0
13	dD	38	0	8	1	0
13	gC	38	0	8	1	0
13	jB	38	0	8	1	0
13	mA	38	0	8	1	0
13	o	38	0	8	1	0
13	tD	38	0	8	6	0
13	vD	38	0	8	1	0
13	wC	38	0	8	6	0
13	wD	38	0	8	1	0
13	yC	38	0	8	0	0
13	zB	38	0	8	8	0
13	zC	38	0	8	2	0
14	HB	38	0	7	0	0
14	KB	38	0	6	1	0
14	eD	38	0	7	1	0
14	hC	38	0	6	0	0
14	hD	38	0	6	0	0
14	kB	38	0	7	1	0
14	kC	38	0	6	0	0
14	nA	38	0	7	3	0
14	nB	38	0	7	0	0
14	p	38	0	7	1	0
14	qA	38	0	7	1	0
14	s	38	0	7	0	0
15	1D	47	0	8	0	0
15	2D	47	0	8	0	0
15	4C	47	0	8	1	0
15	5C	47	0	8	0	0
15	7B	47	0	8	1	0
15	8B	47	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	AB	47	0	8	1	0
15	BB	47	0	8	0	0
15	CA	47	0	8	0	0
15	DA	47	0	8	0	0
15	eB	47	0	8	1	0
15	fB	47	0	8	0	0
16	4D	28	0	25	1	0
16	AC	28	0	25	2	0
16	FA	28	0	25	1	0
17	5D	72	0	61	0	0
17	7C	72	0	61	1	0
17	DB	72	0	61	0	0
17	GA	72	0	61	0	0
18	0E	47	0	8	1	0
18	9D	47	0	8	0	0
18	BE	47	0	8	2	0
18	DE	47	0	7	0	0
18	IE	47	0	7	2	0
18	JE	47	0	7	0	0
18	KE	47	0	8	0	0
18	PE	47	0	8	1	0
18	SE	47	0	8	1	0
18	cE	47	0	8	0	0
18	fE	47	0	8	1	0
18	pE	47	0	8	1	0
18	rE	47	0	8	1	0
18	tE	47	0	8	0	0
18	yE	47	0	7	2	0
18	zE	47	0	7	1	0
19	1E	38	0	7	0	0
19	AE	38	0	8	0	0
19	LE	38	0	8	1	0
19	NE	38	0	8	0	0
19	aE	38	0	7	0	0
19	qE	38	0	8	0	0
20	CE	38	0	7	1	0
20	EE	38	0	8	1	0
20	HE	38	0	7	5	0
20	TE	38	0	8	0	0
20	UE	38	0	8	1	0
20	WE	38	0	8	0	0
20	gE	38	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	hE	38	0	8	2	0
20	jE	38	0	8	0	0
20	sE	38	0	8	0	0
20	uE	38	0	8	2	0
20	xE	38	0	8	4	0
21	FE	47	0	8	1	0
21	kE	47	0	8	0	0
21	vE	47	0	8	0	0
22	GE	56	0	8	1	0
22	QE	56	0	8	1	0
22	RE	56	0	8	2	0
22	VE	56	0	8	1	0
22	dE	56	0	8	2	0
22	eE	56	0	8	0	0
22	iE	56	0	8	2	0
22	wE	56	0	8	2	0
23	XE	56	0	8	1	0
24	YE	56	0	8	0	0
24	lE	56	0	8	0	0
25	A	1	0	0	0	0
25	B	1	0	0	0	0
25	C	1	0	0	0	0
25	D	1	0	0	0	0
25	E	1	0	0	0	0
25	F	1	0	0	0	0
26	A	36	0	0	11	0
26	B	36	0	0	12	0
26	C	18	0	0	11	0
26	D	27	0	0	15	0
26	E	18	0	0	10	0
26	F	45	0	0	19	0
27	A	143	0	130	4	0
27	B	143	0	130	2	0
27	C	55	0	50	1	0
27	D	55	0	50	1	0
27	E	143	0	130	2	0
27	F	143	0	130	7	0
28	A	14	0	13	0	0
28	B	28	0	26	1	0
28	C	28	0	26	0	0
28	D	14	0	13	0	0
28	E	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	85288	0	71309	1676	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

The worst 5 of 1676 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:B:2020:AHR:C1	6:FC:3:GZL:O5	1.66	1.43
26:D:2003:AHR:C1	13:zB:3:GZL:O5	1.69	1.41
26:B:2003:AHR:C1	13:2A:3:GZL:O5	1.69	1.40
26:A:2003:AHR:C1	6:5:3:GZL:O5	1.71	1.39
26:B:2004:AHR:C1	6:3A:3:GZL:O5	1.69	1.39

There are no symmetry-related clashes.

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	65
1	B	1848/1987 (93%)	1691 (92%)	150 (8%)	7 (0%)	30	65
1	C	1461/1987 (74%)	1342 (92%)	115 (8%)	4 (0%)	36	70
1	D	1531/1987 (77%)	1411 (92%)	114 (7%)	6 (0%)	30	65
1	E	1390/1987 (70%)	1289 (93%)	97 (7%)	4 (0%)	36	70
1	F	1384/1987 (70%)	1273 (92%)	108 (8%)	3 (0%)	43	76
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	9515/12114 (78%)	8733 (92%)	743 (8%)	39 (0%)	31	65

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%)	1347 (93%)	104 (7%)	13	43
1	B	1451/1514 (96%)	1340 (92%)	111 (8%)	12	41
1	C	1149/1514 (76%)	1070 (93%)	79 (7%)	14	45
1	D	1209/1514 (80%)	1124 (93%)	85 (7%)	14	44
1	E	1081/1514 (71%)	1015 (94%)	66 (6%)	17	49
1	F	1078/1514 (71%)	1020 (95%)	58 (5%)	20	53
2	G	5/5 (100%)	5 (100%)	0	100	100
2	H	2/5 (40%)	1 (50%)	1 (50%)	0	0
2	I	3/5 (60%)	2 (67%)	1 (33%)	0	1
All	All	7429/9099 (82%)	6924 (93%)	505 (7%)	16	45

5 of 505 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	289	THR
1	E	1891	ASN
1	C	1259	THR
1	E	1832	LEU

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Mol	Chain	Res	Type
1	F	1245	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	847	HIS
1	E	1293	GLN
1	F	1835	GLN
1	B	1536	ASN
1	B	1447	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	F	1865	1	7,8,9	0.57	0	5,10,12	1.68	2 (40%)
1	HYP	B	1906	1	7,8,9	0.59	0	5,10,12	1.20	1 (20%)
1	HYP	A	1903	1	7,8,9	0.58	0	5,10,12	1.81	2 (40%)
1	HYP	E	1870	1	7,8,9	0.50	0	5,10,12	1.59	2 (40%)
1	HYP	F	1890	1	7,8,9	0.57	0	5,10,12	1.18	1 (20%)
1	HYP	E	1918	1	7,8,9	0.54	0	5,10,12	1.73	2 (40%)
1	HYP	B	1862	1	7,8,9	0.53	0	5,10,12	1.48	1 (20%)
1	HYP	B	1902	1	7,8,9	0.59	0	5,10,12	1.62	1 (20%)
1	HYP	F	1880	1	7,8,9	0.53	0	5,10,12	1.44	1 (20%)
2	HYP	H	51	2	7,8,9	0.53	0	5,10,12	1.64	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	HYP	B	1908	1	7,8,9	0.56	0	5,10,12	2.17	3 (60%)
1	HYP	B	1930	1	7,8,9	0.60	0	5,10,12	1.65	1 (20%)
1	HYP	D	1908	1	7,8,9	0.54	0	5,10,12	1.74	2 (40%)
1	HYP	F	1912	1	7,8,9	0.57	0	5,10,12	1.17	1 (20%)
2	HYP	G	51	2	7,8,9	0.57	0	5,10,12	1.62	1 (20%)
2	HYP	I	2	2	7,8,9	0.48	0	5,10,12	1.48	1 (20%)
1	HYP	E	1868	1	7,8,9	0.57	0	5,10,12	1.83	2 (40%)
1	HYP	E	1930	1	7,8,9	0.59	0	5,10,12	1.24	1 (20%)
2	HYP	H	55	2	7,8,9	0.52	0	5,10,12	1.22	1 (20%)
1	HYP	E	1893	1	7,8,9	0.58	0	5,10,12	1.26	1 (20%)
1	HYP	A	1873	1	7,8,9	0.50	0	5,10,12	1.23	1 (20%)
1	HYP	D	1922	1	7,8,9	0.56	0	5,10,12	1.42	1 (20%)
1	HYP	F	1867	1	7,8,9	0.54	0	5,10,12	1.67	1 (20%)
1	HYP	A	1932	1	7,8,9	0.54	0	5,10,12	1.82	3 (60%)
1	HYP	A	1914	1	7,8,9	0.57	0	5,10,12	1.40	1 (20%)
1	HYP	B	1901	1	7,8,9	0.57	0	5,10,12	1.20	1 (20%)
1	HYP	A	1905	1	7,8,9	0.60	0	5,10,12	1.24	1 (20%)
1	HYP	B	1880	1	7,8,9	0.54	0	5,10,12	1.38	1 (20%)
1	HYP	E	1931	1	7,8,9	0.55	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	B	1888	1	7,8,9	0.54	0	5,10,12	1.72	2 (40%)
1	HYP	D	1923	1	7,8,9	0.53	0	5,10,12	1.86	3 (60%)
2	HYP	I	17	2	7,8,9	0.56	0	5,10,12	1.24	1 (20%)
2	HYP	H	49	2	7,8,9	0.59	0	5,10,12	1.49	1 (20%)
1	HYP	E	1855	1	7,8,9	0.60	0	5,10,12	1.22	1 (20%)
1	HYP	A	1916	1	7,8,9	0.58	0	5,10,12	1.47	1 (20%)
1	HYP	E	1908	1	7,8,9	0.54	0	5,10,12	2.14	3 (60%)
1	HYP	B	1890	1	7,8,9	0.59	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	F	1929	1	7,8,9	0.57	0	5,10,12	1.22	1 (20%)
1	HYP	B	1912	1	7,8,9	0.59	0	5,10,12	1.28	1 (20%)
1	HYP	E	1920	1	7,8,9	0.56	0	5,10,12	1.47	1 (20%)
1	HYP	C	1902	1	7,8,9	0.57	0	5,10,12	1.81	2 (40%)
1	HYP	E	1911	1	7,8,9	0.56	0	5,10,12	1.25	1 (20%)
1	HYP	D	1897	1	7,8,9	0.51	0	5,10,12	1.27	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HYP	G	9	2	7,8,9	0.55	0	5,10,12	1.80	2 (40%)
2	HYP	G	50	2	7,8,9	0.58	0	5,10,12	1.21	1 (20%)
1	HYP	B	1877	1	7,8,9	0.51	0	5,10,12	1.68	1 (20%)
1	HYP	D	1898	1	7,8,9	0.56	0	5,10,12	1.26	1 (20%)
1	HYP	C	1906	1	7,8,9	0.56	0	5,10,12	1.19	1 (20%)
1	HYP	F	1882	1	7,8,9	0.53	0	5,10,12	1.20	1 (20%)
1	HYP	F	1868	1	7,8,9	0.58	0	5,10,12	2.08	3 (60%)
1	HYP	F	1897	1	7,8,9	0.55	0	5,10,12	1.30	1 (20%)
1	HYP	E	1867	1	7,8,9	0.58	0	5,10,12	1.82	2 (40%)
1	HYP	F	1877	1	7,8,9	0.54	0	5,10,12	1.58	1 (20%)
1	HYP	A	1863	1	7,8,9	0.49	0	5,10,12	1.38	1 (20%)
1	HYP	E	1865	1	7,8,9	0.55	0	5,10,12	1.66	1 (20%)
1	HYP	D	1916	1	7,8,9	0.57	0	5,10,12	1.40	1 (20%)
1	HYP	E	1878	1	7,8,9	0.51	0	5,10,12	1.96	2 (40%)
2	HYP	G	45	2	7,8,9	0.59	0	5,10,12	1.29	1 (20%)
1	HYP	F	1898	1	7,8,9	0.58	0	5,10,12	1.19	1 (20%)
1	HYP	C	1922	1	7,8,9	0.57	0	5,10,12	1.49	1 (20%)
1	HYP	F	1862	1	7,8,9	0.50	0	5,10,12	1.37	1 (20%)
1	HYP	D	1913	1	7,8,9	0.56	0	5,10,12	1.26	1 (20%)
2	HYP	H	44	2	7,8,9	0.54	0	5,10,12	1.67	1 (20%)
1	HYP	C	1901	1	7,8,9	0.56	0	5,10,12	1.20	1 (20%)
1	HYP	C	1915	1	7,8,9	0.57	0	5,10,12	1.23	1 (20%)
1	HYP	E	1862	1	7,8,9	0.54	0	5,10,12	1.49	1 (20%)
1	HYP	E	1927	1	7,8,9	0.55	0	5,10,12	1.22	1 (20%)
1	HYP	E	1902	1	7,8,9	0.52	0	5,10,12	1.70	1 (20%)
1	HYP	B	1856	1	7,8,9	0.50	0	5,10,12	1.28	1 (20%)
1	HYP	E	1857	1	7,8,9	0.54	0	5,10,12	1.59	1 (20%)
1	HYP	E	1910	1	7,8,9	0.52	0	5,10,12	1.22	1 (20%)
1	HYP	A	1862	1	7,8,9	0.54	0	5,10,12	1.45	1 (20%)
1	HYP	F	1885	1	7,8,9	0.54	0	5,10,12	1.24	1 (20%)
2	HYP	G	11	2	7,8,9	0.51	0	5,10,12	1.98	2 (40%)
1	HYP	C	1911	1	7,8,9	0.54	0	5,10,12	1.23	1 (20%)
1	HYP	C	1912	1	7,8,9	0.56	0	5,10,12	1.21	1 (20%)
1	HYP	E	1866	1	7,8,9	0.59	0	5,10,12	1.43	1 (20%)
1	HYP	F	1887	1	7,8,9	0.54	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	1888	1	7,8,9	0.54	0	5,10,12	1.55	1 (20%)
1	HYP	D	1917	1	7,8,9	0.57	0	5,10,12	1.53	1 (20%)
2	HYP	I	11	2	7,8,9	0.50	0	5,10,12	1.84	2 (40%)
2	HYP	G	26	2	7,8,9	0.55	0	5,10,12	1.19	1 (20%)
1	HYP	E	1892	1	7,8,9	0.52	0	5,10,12	1.32	1 (20%)
2	HYP	G	48	2	7,8,9	0.59	0	5,10,12	1.23	1 (20%)
1	HYP	E	1880	1	7,8,9	0.53	0	5,10,12	1.45	1 (20%)
1	HYP	F	1873	1	7,8,9	0.46	0	5,10,12	1.29	1 (20%)
1	HYP	A	1920	1	7,8,9	0.55	0	5,10,12	1.58	1 (20%)
1	HYP	A	1901	1	7,8,9	0.58	0	5,10,12	1.19	1 (20%)
1	HYP	F	1907	1	7,8,9	0.55	0	5,10,12	1.78	3 (60%)
1	HYP	C	1929	1	7,8,9	0.63	0	5,10,12	1.30	1 (20%)
1	HYP	F	1893	1	7,8,9	0.57	0	5,10,12	1.34	1 (20%)
1	HYP	F	1857	1	7,8,9	0.56	0	5,10,12	1.61	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	1875	1	7,8,9	0.55	0	5,10,12	1.20	1 (20%)
1	HYP	B	1918	1	7,8,9	0.61	0	5,10,12	1.62	1 (20%)
2	HYP	G	20	2	7,8,9	0.54	0	5,10,12	1.33	1 (20%)
1	HYP	D	1931	1	7,8,9	0.54	0	5,10,12	1.41	1 (20%)
1	HYP	D	1914	1	7,8,9	0.53	0	5,10,12	1.11	1 (20%)
1	HYP	E	1899	1	7,8,9	0.59	0	5,10,12	1.34	1 (20%)
1	HYP	A	1917	1	7,8,9	0.55	0	5,10,12	1.62	1 (20%)
1	HYP	D	1915	1	7,8,9	0.56	0	5,10,12	1.26	1 (20%)
1	HYP	F	1915	1	7,8,9	0.52	0	5,10,12	1.24	1 (20%)
2	HYP	I	20	2	7,8,9	0.55	0	5,10,12	1.28	1 (20%)
2	HYP	H	41	2	7,8,9	0.54	0	5,10,12	1.30	1 (20%)
1	HYP	F	1928	1	7,8,9	0.56	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%)
1	HYP	A	1867	1	7,8,9	0.51	0	5,10,12	1.61	1 (20%)
1	HYP	E	1913	1	7,8,9	0.56	0	5,10,12	1.22	1 (20%)
1	HYP	F	1931	1	7,8,9	0.54	0	5,10,12	1.39	1 (20%)
1	HYP	B	1855	1	7,8,9	0.54	0	5,10,12	1.20	1 (20%)
2	HYP	I	6	2	7,8,9	0.53	0	5,10,12	1.32	1 (20%)
2	HYP	G	29	2	7,8,9	0.53	0	5,10,12	1.24	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	HYP	F	1906	1	7,8,9	0.55	0	5,10,12	1.33	1 (20%)
1	HYP	A	1865	1	7,8,9	0.56	0	5,10,12	1.68	1 (20%)
1	HYP	A	1899	1	7,8,9	0.65	0	5,10,12	1.44	1 (20%)
1	HYP	E	1858	1	7,8,9	0.54	0	5,10,12	1.70	1 (20%)
1	HYP	F	1855	1	7,8,9	0.62	0	5,10,12	1.46	1 (20%)
2	HYP	G	2	2	7,8,9	0.55	0	5,10,12	1.66	2 (40%)
1	HYP	B	1866	1	7,8,9	0.51	0	5,10,12	1.32	1 (20%)
1	HYP	F	1922	1	7,8,9	0.60	0	5,10,12	1.60	1 (20%)
1	HYP	D	1921	1	7,8,9	0.59	0	5,10,12	1.25	1 (20%)
2	HYP	H	42	2	7,8,9	0.56	0	5,10,12	1.26	1 (20%)
2	HYP	H	52	2	7,8,9	0.52	0	5,10,12	1.77	2 (40%)
1	HYP	F	1903	1	7,8,9	0.57	0	5,10,12	1.74	2 (40%)
1	HYP	D	1905	1	7,8,9	0.55	0	5,10,12	1.22	1 (20%)
2	HYP	G	44	2	7,8,9	0.56	0	5,10,12	1.55	1 (20%)
1	HYP	B	1903	1	7,8,9	0.57	0	5,10,12	1.97	3 (60%)
1	HYP	B	1892	1	7,8,9	0.51	0	5,10,12	1.27	1 (20%)
2	HYP	H	50	2	7,8,9	0.57	0	5,10,12	1.23	1 (20%)
1	HYP	C	1898	1	7,8,9	0.56	0	5,10,12	1.22	1 (20%)
2	HYP	G	14	2	7,8,9	0.57	0	5,10,12	1.37	1 (20%)
1	HYP	F	1932	1	7,8,9	0.50	0	5,10,12	1.75	2 (40%)
1	HYP	F	1905	1	7,8,9	0.59	0	5,10,12	1.30	1 (20%)
2	HYP	I	8	2	7,8,9	0.55	0	5,10,12	1.52	1 (20%)
1	HYP	A	1911	1	7,8,9	0.56	0	5,10,12	1.24	1 (20%)
1	HYP	A	1902	1	7,8,9	0.61	0	5,10,12	1.63	1 (20%)
1	HYP	E	1887	1	7,8,9	0.53	0	5,10,12	1.25	1 (20%)
2	HYP	H	48	2	7,8,9	0.62	0	5,10,12	1.23	1 (20%)
1	HYP	E	1883	1	7,8,9	0.55	0	5,10,12	2.08	2 (40%)
1	HYP	F	1918	1	7,8,9	0.53	0	5,10,12	2.04	2 (40%)
1	HYP	A	1868	1	7,8,9	0.56	0	5,10,12	1.98	3 (60%)
1	HYP	E	1921	1	7,8,9	0.60	0	5,10,12	1.35	1 (20%)
1	HYP	A	1897	1	7,8,9	0.55	0	5,10,12	1.29	1 (20%)
1	HYP	F	1927	1	7,8,9	0.53	0	5,10,12	1.18	1 (20%)
1	HYP	B	1923	1	7,8,9	0.57	0	5,10,12	2.02	3 (60%)
1	HYP	F	1860	1	7,8,9	0.59	0	5,10,12	1.59	2 (40%)
2	HYP	I	3	2	7,8,9	0.54	0	5,10,12	1.66	2 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	HYP	E	1915	1	7,8,9	0.52	0	5,10,12	1.17	1 (20%)
1	HYP	E	1906	1	7,8,9	0.56	0	5,10,12	1.26	1 (20%)
1	HYP	B	1915	1	7,8,9	0.57	0	5,10,12	1.29	1 (20%)
1	HYP	A	1898	1	7,8,9	0.64	0	5,10,12	1.23	1 (20%)
1	HYP	F	1866	1	7,8,9	0.57	0	5,10,12	1.37	1 (20%)
2	HYP	G	52	2	7,8,9	0.55	0	5,10,12	1.68	2 (40%)
2	HYP	I	4	2	7,8,9	0.54	0	5,10,12	1.29	1 (20%)
1	HYP	C	1907	1	7,8,9	0.55	0	5,10,12	1.77	2 (40%)
1	HYP	F	1930	1	7,8,9	0.53	0	5,10,12	1.54	1 (20%)
1	HYP	C	1908	1	7,8,9	0.54	0	5,10,12	1.96	3 (60%)
2	HYP	G	17	2	7,8,9	0.56	0	5,10,12	1.31	1 (20%)
1	HYP	D	1929	1	7,8,9	0.59	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	A	1882	1	7,8,9	0.55	0	5,10,12	1.25	1 (20%)
1	HYP	E	1932	1	7,8,9	0.54	0	5,10,12	1.48	1 (20%)
2	HYP	H	45	2	7,8,9	0.55	0	5,10,12	1.22	1 (20%)
1	HYP	E	1894	1	7,8,9	0.59	0	5,10,12	1.29	1 (20%)
2	HYP	G	32	2	7,8,9	0.52	0	5,10,12	1.43	1 (20%)
1	HYP	B	1865	1	7,8,9	0.53	0	5,10,12	1.71	1 (20%)
1	HYP	A	1923	1	7,8,9	0.55	0	5,10,12	1.93	3 (60%)
1	HYP	B	1932	1	7,8,9	0.54	0	5,10,12	1.57	1 (20%)
1	HYP	C	1920	1	7,8,9	0.56	0	5,10,12	1.49	1 (20%)
1	HYP	B	1916	1	7,8,9	0.58	0	5,10,12	1.47	1 (20%)
1	HYP	C	1923	1	7,8,9	0.57	0	5,10,12	1.99	3 (60%)
1	HYP	E	1912	1	7,8,9	0.57	0	5,10,12	1.29	1 (20%)
2	HYP	G	37	2	7,8,9	0.55	0	5,10,12	0.98	1 (20%)
1	HYP	F	1902	1	7,8,9	0.57	0	5,10,12	1.72	2 (40%)
1	HYP	B	1931	1	7,8,9	0.56	0	5,10,12	1.43	1 (20%)
2	HYP	I	33	2	7,8,9	0.51	0	5,10,12	1.27	1 (20%)
2	HYP	G	34	2	7,8,9	0.51	0	5,10,12	1.70	2 (40%)
1	HYP	B	1910	1	7,8,9	0.54	0	5,10,12	1.18	1 (20%)
1	HYP	E	1885	1	7,8,9	0.53	0	5,10,12	1.41	1 (20%)
2	HYP	H	40	2	7,8,9	0.51	0	5,10,12	1.15	1 (20%)
1	HYP	B	1864	1	7,8,9	0.53	0	5,10,12	1.49	1 (20%)
1	HYP	A	1913	1	7,8,9	0.62	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
2	HYP	G	23	2	7,8,9	0.44	0	5,10,12	1.51	1 (20%)
1	HYP	C	1914	1	7,8,9	0.53	0	5,10,12	1.44	1 (20%)
1	HYP	B	1878	1	7,8,9	0.54	0	5,10,12	1.88	2 (40%)
1	HYP	A	1887	1	7,8,9	0.55	0	5,10,12	1.27	1 (20%)
1	HYP	F	1911	1	7,8,9	0.54	0	5,10,12	1.18	1 (20%)
1	HYP	D	1899	1	7,8,9	0.52	0	5,10,12	1.73	2 (40%)
1	HYP	C	1932	1	7,8,9	0.55	0	5,10,12	1.89	2 (40%)
2	HYP	G	47	2	7,8,9	0.61	0	5,10,12	1.31	1 (20%)
1	HYP	E	1863	1	7,8,9	0.54	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	D	1918	1	7,8,9	0.55	0	5,10,12	1.86	2 (40%)
1	HYP	A	1931	1	7,8,9	0.58	0	5,10,12	1.43	1 (20%)
1	HYP	A	1893	1	7,8,9	0.61	0	5,10,12	1.32	1 (20%)
1	HYP	F	1858	1	7,8,9	0.57	0	5,10,12	1.72	2 (40%)
1	HYP	B	1927	1	7,8,9	0.58	0	5,10,12	1.23	1 (20%)
1	HYP	E	1922	1	7,8,9	0.62	0	5,10,12	1.55	1 (20%)
1	HYP	B	1870	1	7,8,9	0.56	0	5,10,12	1.57	1 (20%)
1	HYP	C	1931	1	7,8,9	0.56	0	5,10,12	1.40	1 (20%)
1	HYP	E	1872	1	7,8,9	0.59	0	5,10,12	1.29	1 (20%)
1	HYP	B	1860	1	7,8,9	0.51	0	5,10,12	1.75	3 (60%)
2	HYP	I	34	2	7,8,9	0.52	0	5,10,12	1.63	1 (20%)
1	HYP	F	1917	1	7,8,9	0.54	0	5,10,12	1.41	1 (20%)
1	HYP	F	1892	1	7,8,9	0.57	0	5,10,12	1.28	1 (20%)
1	HYP	C	1905	1	7,8,9	0.58	0	5,10,12	1.20	1 (20%)
1	HYP	A	1866	1	7,8,9	0.56	0	5,10,12	1.48	1 (20%)
2	HYP	I	23	2	7,8,9	0.42	0	5,10,12	1.45	1 (20%)
1	HYP	B	1921	1	7,8,9	0.61	0	5,10,12	1.25	1 (20%)
1	HYP	E	1873	1	7,8,9	0.47	0	5,10,12	1.34	1 (20%)
1	HYP	B	1914	1	7,8,9	0.53	0	5,10,12	1.55	1 (20%)
1	HYP	C	1930	1	7,8,9	0.60	0	5,10,12	1.76	2 (40%)
1	HYP	E	1916	1	7,8,9	0.59	0	5,10,12	1.34	1 (20%)
2	HYP	G	4	2	7,8,9	0.59	0	5,10,12	1.40	1 (20%)
1	HYP	A	1894	1	7,8,9	0.55	0	5,10,12	1.93	2 (40%)
2	HYP	G	8	2	7,8,9	0.59	0	5,10,12	1.62	1 (20%)
2	HYP	G	10	2	7,8,9	0.62	0	5,10,12	1.67	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	HYP	F	1913	1	7,8,9	0.55	0	5,10,12	1.28	1 (20%)
1	HYP	B	1858	1	7,8,9	0.56	0	5,10,12	1.43	1 (20%)
2	HYP	H	47	2	7,8,9	0.59	0	5,10,12	1.30	1 (20%)
1	HYP	D	1928	1	7,8,9	0.57	0	5,10,12	1.16	1 (20%)
1	HYP	D	1901	1	7,8,9	0.56	0	5,10,12	1.22	1 (20%)
1	HYP	B	1875	1	7,8,9	0.56	0	5,10,12	1.20	1 (20%)
1	HYP	F	1875	1	7,8,9	0.55	0	5,10,12	1.18	1 (20%)
1	HYP	E	1864	1	7,8,9	0.58	0	5,10,12	1.58	1 (20%)
1	HYP	B	1899	1	7,8,9	0.64	0	5,10,12	1.47	1 (20%)
1	HYP	F	1870	1	7,8,9	0.52	0	5,10,12	1.60	1 (20%)
2	HYP	G	40	2	7,8,9	0.50	0	5,10,12	1.18	1 (20%)
2	HYP	I	29	2	7,8,9	0.54	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%)
1	HYP	A	1921	1	7,8,9	0.66	0	5,10,12	1.42	1 (20%)
1	HYP	B	1905	1	7,8,9	0.59	0	5,10,12	1.23	1 (20%)
1	HYP	F	1910	1	7,8,9	0.52	0	5,10,12	1.16	1 (20%)
1	HYP	A	1930	1	7,8,9	0.58	0	5,10,12	1.69	1 (20%)
1	HYP	E	1888	1	7,8,9	0.50	0	5,10,12	1.86	2 (40%)
1	HYP	E	1929	1	7,8,9	0.59	0	5,10,12	1.27	1 (20%)
1	HYP	F	1872	1	7,8,9	0.56	0	5,10,12	1.25	1 (20%)
1	HYP	D	1932	1	7,8,9	0.56	0	5,10,12	1.87	3 (60%)
1	HYP	A	1918	1	7,8,9	0.57	0	5,10,12	1.62	1 (20%)
1	HYP	B	1917	1	7,8,9	0.60	0	5,10,12	1.68	1 (20%)
1	HYP	B	1867	1	7,8,9	0.51	0	5,10,12	1.67	1 (20%)
2	HYP	G	5	2	7,8,9	0.47	0	5,10,12	1.20	1 (20%)
1	HYP	A	1906	1	7,8,9	0.59	0	5,10,12	1.39	1 (20%)
1	HYP	E	1890	1	7,8,9	0.55	0	5,10,12	1.15	1 (20%)
1	HYP	A	1860	1	7,8,9	0.53	0	5,10,12	1.82	3 (60%)
1	HYP	E	1907	1	7,8,9	0.54	0	5,10,12	1.67	2 (40%)
1	HYP	C	1910	1	7,8,9	0.55	0	5,10,12	1.20	1 (20%)
1	HYP	D	1927	1	7,8,9	0.55	0	5,10,12	1.23	1 (20%)
1	HYP	A	1883	1	7,8,9	0.55	0	5,10,12	2.22	2 (40%)
1	HYP	A	1885	1	7,8,9	0.57	0	5,10,12	1.23	1 (20%)
2	HYP	G	6	2	7,8,9	0.49	0	5,10,12	1.54	1 (20%)
1	HYP	C	1897	1	7,8,9	0.53	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	F	1920	1	7,8,9	0.56	0	5,10,12	1.58	2 (40%)
1	HYP	E	1914	1	7,8,9	0.56	0	5,10,12	1.26	1 (20%)
1	HYP	A	1855	1	7,8,9	0.61	0	5,10,12	1.20	1 (20%)
2	HYP	G	3	2	7,8,9	0.56	0	5,10,12	1.64	2 (40%)
1	HYP	A	1922	1	7,8,9	0.61	0	5,10,12	1.76	1 (20%)
2	HYP	H	43	2	7,8,9	0.55	0	5,10,12	1.50	1 (20%)
2	HYP	G	7	2	7,8,9	0.63	0	5,10,12	1.41	1 (20%)
1	HYP	E	1928	1	7,8,9	0.54	0	5,10,12	1.25	1 (20%)
1	HYP	A	1880	1	7,8,9	0.53	0	5,10,12	1.41	1 (20%)
1	HYP	D	1920	1	7,8,9	0.57	0	5,10,12	1.51	1 (20%)
1	HYP	F	1908	1	7,8,9	0.57	0	5,10,12	1.84	2 (40%)
1	HYP	B	1929	1	7,8,9	0.68	0	5,10,12	1.40	1 (20%)
1	HYP	A	1892	1	7,8,9	0.56	0	5,10,12	1.39	1 (20%)
2	HYP	H	37	2	7,8,9	0.56	0	5,10,12	1.16	1 (20%)
1	HYP	D	1906	1	7,8,9	0.54	0	5,10,12	1.37	1 (20%)
1	HYP	F	1921	1	7,8,9	0.61	0	5,10,12	1.38	1 (20%)
1	HYP	C	1917	1	7,8,9	0.57	0	5,10,12	1.48	1 (20%)
1	HYP	A	1912	1	7,8,9	0.60	0	5,10,12	1.24	1 (20%)
1	HYP	A	1908	1	7,8,9	0.52	0	5,10,12	2.25	3 (60%)
1	HYP	E	1882	1	7,8,9	0.53	0	5,10,12	1.26	1 (20%)
1	HYP	F	1894	1	7,8,9	0.51	0	5,10,12	1.98	2 (40%)
1	HYP	F	1901	1	7,8,9	0.53	0	5,10,12	1.18	1 (20%)
1	HYP	D	1907	1	7,8,9	0.50	0	5,10,12	1.61	1 (20%)
1	HYP	D	1902	1	7,8,9	0.52	0	5,10,12	1.77	2 (40%)
1	HYP	F	1914	1	7,8,9	0.54	0	5,10,12	1.48	1 (20%)
1	HYP	C	1899	1	7,8,9	0.59	0	5,10,12	1.32	1 (20%)
1	HYP	D	1910	1	7,8,9	0.50	0	5,10,12	1.17	1 (20%)
2	HYP	I	9	2	7,8,9	0.52	0	5,10,12	1.58	1 (20%)
2	HYP	G	1	2	7,8,9	0.53	0	5,10,12	1.21	1 (20%)
1	HYP	B	1883	1	7,8,9	0.54	0	5,10,12	2.07	2 (40%)
1	HYP	B	1885	1	7,8,9	0.58	0	5,10,12	1.19	1 (20%)
1	HYP	D	1930	1	7,8,9	0.63	0	5,10,12	1.30	1 (20%)
1	HYP	C	1903	1	7,8,9	0.54	0	5,10,12	1.84	3 (60%)
1	HYP	A	1858	1	7,8,9	0.56	0	5,10,12	1.26	1 (20%)
2	HYP	I	7	2	7,8,9	0.52	0	5,10,12	1.67	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	HYP	B	1887	1	7,8,9	0.58	0	5,10,12	1.30	1 (20%)
1	HYP	B	1898	1	7,8,9	0.64	0	5,10,12	1.29	1 (20%)
1	HYP	A	1857	1	7,8,9	0.57	0	5,10,12	1.34	1 (20%)
2	HYP	G	46	2	7,8,9	0.57	0	5,10,12	1.57	1 (20%)
1	HYP	B	1882	1	7,8,9	0.53	0	5,10,12	1.24	1 (20%)
1	HYP	E	1917	1	7,8,9	0.56	0	5,10,12	1.40	1 (20%)
1	HYP	C	1918	1	7,8,9	0.56	0	5,10,12	1.81	2 (40%)
1	HYP	F	1883	1	7,8,9	0.53	0	5,10,12	2.03	2 (40%)
2	HYP	G	49	2	7,8,9	0.57	0	5,10,12	1.51	1 (20%)
1	HYP	B	1911	1	7,8,9	0.57	0	5,10,12	1.21	1 (20%)
1	HYP	B	1857	1	7,8,9	0.57	0	5,10,12	1.63	2 (40%)
1	HYP	A	1927	1	7,8,9	0.55	0	5,10,12	1.43	1 (20%)
1	HYP	E	1905	1	7,8,9	0.55	0	5,10,12	1.26	1 (20%)
2	HYP	H	56	2	7,8,9	0.53	0	5,10,12	1.26	1 (20%)
2	HYP	I	5	2	7,8,9	0.55	0	5,10,12	1.47	1 (20%)
1	HYP	A	1872	1	7,8,9	0.53	0	5,10,12	1.33	1 (20%)
1	HYP	A	1907	1	7,8,9	0.53	0	5,10,12	1.91	2 (40%)
1	HYP	F	1916	1	7,8,9	0.54	0	5,10,12	1.28	1 (20%)
2	HYP	I	32	2	7,8,9	0.50	0	5,10,12	1.18	1 (20%)
2	HYP	G	42	2	7,8,9	0.61	0	5,10,12	1.29	1 (20%)
1	HYP	A	1856	1	7,8,9	0.56	0	5,10,12	1.34	1 (20%)
1	HYP	F	1899	1	7,8,9	0.61	0	5,10,12	1.33	1 (20%)
1	HYP	B	1873	1	7,8,9	0.49	0	5,10,12	1.37	1 (20%)
1	HYP	B	1893	1	7,8,9	0.56	0	5,10,12	1.26	1 (20%)
1	HYP	B	1907	1	7,8,9	0.56	0	5,10,12	1.68	1 (20%)
1	HYP	F	1878	1	7,8,9	0.57	0	5,10,12	1.57	2 (40%)
2	HYP	G	41	2	7,8,9	0.58	0	5,10,12	1.23	1 (20%)
1	HYP	F	1856	1	7,8,9	0.56	0	5,10,12	1.37	1 (20%)
2	HYP	G	33	2	7,8,9	0.51	0	5,10,12	1.65	1 (20%)
1	HYP	A	1928	1	7,8,9	0.56	0	5,10,12	1.16	1 (20%)
1	HYP	A	1875	1	7,8,9	0.58	0	5,10,12	1.21	1 (20%)
1	HYP	B	1863	1	7,8,9	0.54	0	5,10,12	1.45	1 (20%)
1	HYP	B	1868	1	7,8,9	0.52	0	5,10,12	2.03	3 (60%)
1	HYP	A	1910	1	7,8,9	0.55	0	5,10,12	1.19	1 (20%)
1	HYP	E	1897	1	7,8,9	0.52	0	5,10,12	1.22	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	HYP	B	1913	1	7,8,9	0.62	0	5,10,12	1.34	1 (20%)
1	HYP	F	1863	1	7,8,9	0.54	0	5,10,12	1.41	1 (20%)
2	HYP	G	56	2	7,8,9	0.53	0	5,10,12	1.28	1 (20%)
1	HYP	C	1921	1	7,8,9	0.57	0	5,10,12	1.23	1 (20%)
1	HYP	B	1928	1	7,8,9	0.56	0	5,10,12	1.54	1 (20%)
2	HYP	G	43	2	7,8,9	0.54	0	5,10,12	1.49	1 (20%)
2	HYP	I	26	2	7,8,9	0.54	0	5,10,12	1.51	2 (40%)
1	HYP	E	1856	1	7,8,9	0.54	0	5,10,12	1.32	1 (20%)
1	HYP	A	1878	1	7,8,9	0.52	0	5,10,12	1.75	2 (40%)
1	HYP	E	1898	1	7,8,9	0.57	0	5,10,12	1.22	1 (20%)
2	HYP	G	55	2	7,8,9	0.53	0	5,10,12	1.21	1 (20%)
1	HYP	E	1860	1	7,8,9	0.57	0	5,10,12	1.92	3 (60%)
1	HYP	A	1870	1	7,8,9	0.50	0	5,10,12	1.60	2 (40%)
2	HYP	I	14	2	7,8,9	0.57	0	5,10,12	1.31	1 (20%)
1	HYP	C	1927	1	7,8,9	0.57	0	5,10,12	1.23	1 (20%)
1	HYP	A	1929	1	7,8,9	0.62	0	5,10,12	1.27	1 (20%)
2	HYP	H	46	2	7,8,9	0.51	0	5,10,12	1.63	1 (20%)
1	HYP	F	1864	1	7,8,9	0.55	0	5,10,12	1.45	1 (20%)
1	HYP	A	1890	1	7,8,9	0.59	0	5,10,12	1.25	1 (20%)
1	HYP	D	1912	1	7,8,9	0.56	0	5,10,12	1.33	1 (20%)
2	HYP	I	10	2	7,8,9	0.57	0	5,10,12	1.73	1 (20%)
1	HYP	E	1923	1	7,8,9	0.53	0	5,10,12	2.15	2 (40%)
2	HYP	I	1	2	7,8,9	0.50	0	5,10,12	1.27	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	E	1903	1	7,8,9	0.54	0	5,10,12	1.92	3 (60%)
1	HYP	A	1864	1	7,8,9	0.54	0	5,10,12	1.50	1 (20%)
1	HYP	D	1911	1	7,8,9	0.57	0	5,10,12	1.22	1 (20%)
1	HYP	C	1913	1	7,8,9	0.57	0	5,10,12	1.27	1 (20%)
1	HYP	F	1888	1	7,8,9	0.50	0	5,10,12	1.90	2 (40%)
1	HYP	B	1894	1	7,8,9	0.55	0	5,10,12	2.01	2 (40%)
1	HYP	C	1928	1	7,8,9	0.61	0	5,10,12	1.30	1 (20%)
1	HYP	A	1915	1	7,8,9	0.57	0	5,10,12	1.27	1 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	HYP	F	1865	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1906	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1903	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1870	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1890	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1918	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1862	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1902	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1880	1	-	0/0/11/13	0/1/1/1
2	HYP	H	51	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1908	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1930	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	1912	1	-	0/0/11/13	0/1/1/1
2	HYP	G	51	2	-	0/0/11/13	0/1/1/1
2	HYP	I	2	2	-	0/0/11/13	0/1/1/1
1	HYP	E	1868	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1930	1	-	0/0/11/13	0/1/1/1
2	HYP	H	55	2	-	0/0/11/13	0/1/1/1
1	HYP	E	1893	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1873	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1922	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1867	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1932	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1914	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	1905	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1880	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1931	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1877	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1888	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1923	1	-	0/0/11/13	0/1/1/1
2	HYP	I	17	2	-	0/0/11/13	0/1/1/1
2	HYP	H	49	2	-	0/0/11/13	0/1/1/1
1	HYP	E	1855	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1916	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1908	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1890	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1922	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1929	1	-	0/0/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	HYP	B	1912	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1920	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1902	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	1897	1	-	0/0/11/13	0/1/1/1
2	HYP	G	9	2	-	0/0/11/13	0/1/1/1
2	HYP	G	50	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1877	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1898	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1906	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1882	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1868	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1897	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1867	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1877	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1863	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	1916	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1878	1	-	0/0/11/13	0/1/1/1
2	HYP	G	45	2	-	0/0/11/13	0/1/1/1
1	HYP	F	1898	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1922	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1862	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1913	1	-	0/0/11/13	0/1/1/1
2	HYP	H	44	2	-	0/0/11/13	0/1/1/1
1	HYP	C	1901	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1915	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1862	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1927	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	1856	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1857	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	1862	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	11	2	-	0/0/11/13	0/1/1/1
1	HYP	C	1911	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1912	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1866	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1887	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1888	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1917	1	-	0/0/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HYP	I	11	2	-	0/0/11/13	0/1/1/1
2	HYP	G	26	2	1/1/2/4	0/0/11/13	0/1/1/1
1	HYP	E	1892	1	-	0/0/11/13	0/1/1/1
2	HYP	G	48	2	-	0/0/11/13	0/1/1/1
1	HYP	E	1880	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1893	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1920	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	1907	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1929	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1873	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1857	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	1875	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1918	1	-	0/0/11/13	0/1/1/1
2	HYP	G	20	2	-	0/0/11/13	0/1/1/1
1	HYP	D	1931	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1914	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1899	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1917	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1915	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1915	1	-	0/0/11/13	0/1/1/1
2	HYP	I	20	2	-	0/0/11/13	0/1/1/1
2	HYP	H	41	2	-	0/0/11/13	0/1/1/1
1	HYP	F	1928	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1923	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1867	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	1931	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1855	1	-	0/0/11/13	0/1/1/1
2	HYP	I	6	2	-	0/0/11/13	0/1/1/1
2	HYP	G	29	2	-	0/0/11/13	0/1/1/1
1	HYP	F	1906	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1865	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1899	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	1855	1	-	0/0/11/13	0/1/1/1
2	HYP	G	2	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1866	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1922	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1921	1	-	0/0/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HYP	H	42	2	-	0/0/11/13	0/1/1/1
2	HYP	H	52	2	-	0/0/11/13	0/1/1/1
1	HYP	F	1903	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1905	1	-	0/0/11/13	0/1/1/1
2	HYP	G	44	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1903	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1892	1	-	0/0/11/13	0/1/1/1
2	HYP	H	50	2	-	0/0/11/13	0/1/1/1
1	HYP	C	1898	1	-	0/0/11/13	0/1/1/1
2	HYP	G	14	2	-	0/0/11/13	0/1/1/1
1	HYP	F	1932	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1905	1	-	0/0/11/13	0/1/1/1
2	HYP	I	8	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1911	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1902	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1887	1	-	0/0/11/13	0/1/1/1
2	HYP	H	48	2	-	0/0/11/13	0/1/1/1
1	HYP	E	1883	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	1868	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	1897	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1927	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1923	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1860	1	-	0/0/11/13	0/1/1/1
2	HYP	I	3	2	-	0/0/11/13	0/1/1/1
1	HYP	E	1915	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	1915	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1898	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1866	1	-	0/0/11/13	0/1/1/1
2	HYP	G	52	2	-	0/0/11/13	0/1/1/1
2	HYP	I	4	2	-	0/0/11/13	0/1/1/1
1	HYP	C	1907	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1930	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1908	1	-	0/0/11/13	0/1/1/1
2	HYP	G	17	2	-	0/0/11/13	0/1/1/1
1	HYP	D	1929	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1872	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	1932	1	-	0/0/11/13	0/1/1/1
2	HYP	H	45	2	-	0/0/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	HYP	E	1894	1	-	0/0/11/13	0/1/1/1
2	HYP	G	32	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1865	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1923	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1932	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1920	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1916	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1923	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1912	1	-	0/0/11/13	0/1/1/1
2	HYP	G	37	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	1931	1	-	0/0/11/13	0/1/1/1
2	HYP	I	33	2	-	0/0/11/13	0/1/1/1
2	HYP	G	34	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1910	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1885	1	-	0/0/11/13	0/1/1/1
2	HYP	H	40	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1864	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	23	2	1/1/2/4	0/0/11/13	0/1/1/1
1	HYP	C	1914	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1878	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1887	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1911	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1899	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1932	1	-	0/0/11/13	0/1/1/1
2	HYP	G	47	2	-	0/0/11/13	0/1/1/1
1	HYP	E	1863	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1916	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1918	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	1893	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1858	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1927	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1922	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1870	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1931	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1872	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1860	1	-	0/0/11/13	0/1/1/1
2	HYP	I	34	2	-	0/0/11/13	0/1/1/1
1	HYP	F	1917	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1892	1	-	0/0/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	HYP	C	1905	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1866	1	-	0/0/11/13	0/1/1/1
2	HYP	I	23	2	1/1/2/4	0/0/11/13	0/1/1/1
1	HYP	B	1921	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1873	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1914	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	1916	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	1894	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	10	2	-	0/0/11/13	0/1/1/1
1	HYP	F	1913	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1858	1	-	0/0/11/13	0/1/1/1
2	HYP	H	47	2	-	0/0/11/13	0/1/1/1
1	HYP	D	1928	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1901	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1875	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	1864	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1899	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1870	1	-	0/0/11/13	0/1/1/1
2	HYP	G	40	2	-	0/0/11/13	0/1/1/1
2	HYP	I	29	2	-	0/0/11/13	0/1/1/1
1	HYP	D	1903	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1921	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1905	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1910	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	1888	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1929	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	1932	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	1917	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1867	1	-	0/0/11/13	0/1/1/1
2	HYP	G	5	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1906	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	1860	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1907	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1910	1	-	0/0/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	HYP	D	1927	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1883	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1885	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	1897	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1920	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1914	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1855	1	-	0/0/11/13	0/1/1/1
2	HYP	G	3	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1922	1	-	0/0/11/13	0/1/1/1
2	HYP	H	43	2	-	0/0/11/13	0/1/1/1
2	HYP	G	7	2	-	0/0/11/13	0/1/1/1
1	HYP	E	1928	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1880	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1920	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1908	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1929	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1892	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	1906	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1921	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	1912	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1908	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1882	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1894	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1901	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	1902	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1914	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1899	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1910	1	-	0/0/11/13	0/1/1/1
2	HYP	I	9	2	-	0/0/11/13	0/1/1/1
2	HYP	G	1	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1883	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1885	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1930	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1903	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1858	1	-	0/0/11/13	0/1/1/1
2	HYP	I	7	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1887	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1898	1	-	0/0/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	HYP	A	1857	1	-	0/0/11/13	0/1/1/1
2	HYP	G	46	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1882	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1917	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1918	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1883	1	-	0/0/11/13	0/1/1/1
2	HYP	G	49	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1911	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1857	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1927	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1905	1	-	0/0/11/13	0/1/1/1
2	HYP	H	56	2	-	0/0/11/13	0/1/1/1
2	HYP	I	5	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1872	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1907	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1916	1	-	0/0/11/13	0/1/1/1
2	HYP	I	32	2	-	0/0/11/13	0/1/1/1
2	HYP	G	42	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1856	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	1873	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1893	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1907	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1878	1	-	0/0/11/13	0/1/1/1
2	HYP	G	41	2	-	0/0/11/13	0/1/1/1
1	HYP	F	1856	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	1928	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1875	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1863	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1868	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1910	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1897	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1913	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1863	1	-	0/0/11/13	0/1/1/1
2	HYP	G	56	2	-	0/0/11/13	0/1/1/1
1	HYP	C	1921	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1928	1	-	0/0/11/13	0/1/1/1
2	HYP	G	43	2	-	0/0/11/13	0/1/1/1
2	HYP	I	26	2	1/1/2/4	0/0/11/13	0/1/1/1
1	HYP	E	1856	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1878	1	-	0/0/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	HYP	E	1898	1	-	0/0/11/13	0/1/1/1
2	HYP	G	55	2	-	0/0/11/13	0/1/1/1
1	HYP	E	1860	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1870	1	-	0/0/11/13	0/1/1/1
2	HYP	I	14	2	-	0/0/11/13	0/1/1/1
1	HYP	C	1927	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1929	1	-	0/0/11/13	0/1/1/1
2	HYP	H	46	2	-	0/0/11/13	0/1/1/1
1	HYP	F	1864	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1890	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1912	1	-	0/0/11/13	0/1/1/1
2	HYP	I	10	2	-	0/0/11/13	0/1/1/1
1	HYP	E	1923	1	-	0/0/11/13	0/1/1/1
2	HYP	I	1	2	-	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	E	1903	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1864	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1911	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1913	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1888	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	1928	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1915	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.

106 monomers are involved in 80 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	1918	HYP	1	0
1	B	1930	HYP	1	0
1	E	1930	HYP	2	0
2	H	55	HYP	1	0
1	E	1931	HYP	1	0
1	E	1855	HYP	1	0
1	E	1908	HYP	1	0
1	B	1890	HYP	1	0
1	B	1912	HYP	1	0
1	C	1902	HYP	1	0
1	E	1911	HYP	2	0
1	D	1897	HYP	1	0
2	G	50	HYP	1	0
1	C	1906	HYP	1	0
1	F	1897	HYP	1	0
1	F	1898	HYP	1	0
1	C	1901	HYP	1	0
1	E	1927	HYP	1	0
1	E	1910	HYP	2	0
1	F	1885	HYP	1	0
1	C	1911	HYP	1	0
1	C	1912	HYP	1	0
2	G	26	HYP	1	0
2	G	48	HYP	1	0
1	E	1880	HYP	1	0
1	A	1901	HYP	1	0
1	B	1918	HYP	1	0
2	G	20	HYP	1	0
1	D	1931	HYP	1	0
2	H	41	HYP	1	0
1	F	1928	HYP	1	0
1	F	1931	HYP	1	0
1	F	1906	HYP	1	0
1	D	1921	HYP	1	0
1	D	1905	HYP	2	0
2	G	14	HYP	1	0
1	F	1905	HYP	1	0
1	A	1911	HYP	1	0
2	H	48	HYP	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	1883	HYP	1	0
1	F	1927	HYP	1	0
1	F	1866	HYP	1	0
1	F	1930	HYP	1	0
2	G	32	HYP	1	0
1	C	1920	HYP	1	0
1	E	1912	HYP	1	0
1	B	1931	HYP	1	0
2	I	33	HYP	1	0
1	B	1910	HYP	1	0
1	E	1885	HYP	1	0
2	H	40	HYP	1	0
2	G	23	HYP	1	0
2	G	47	HYP	1	0
1	B	1927	HYP	1	0
1	C	1931	HYP	1	0
1	E	1872	HYP	1	0
1	C	1905	HYP	1	0
2	I	23	HYP	1	0
1	B	1914	HYP	1	0
1	C	1930	HYP	1	0
2	H	47	HYP	1	0
1	D	1928	HYP	1	0
1	F	1870	HYP	1	0
2	G	40	HYP	1	0
1	B	1905	HYP	1	0
1	F	1910	HYP	1	0
1	A	1930	HYP	1	0
1	E	1929	HYP	1	0
1	E	1907	HYP	1	0
1	C	1910	HYP	2	0
1	D	1927	HYP	1	0
1	A	1883	HYP	1	0
1	C	1897	HYP	1	0
1	A	1855	HYP	1	0
1	E	1928	HYP	1	0
1	D	1920	HYP	1	0
1	D	1906	HYP	1	0
1	F	1921	HYP	1	0
1	A	1908	HYP	1	0
1	B	1883	HYP	1	0
1	D	1930	HYP	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1858	HYP	1	0
2	G	49	HYP	1	0
1	B	1911	HYP	1	0
1	A	1927	HYP	2	0
1	A	1907	HYP	1	0
2	I	32	HYP	2	0
2	G	42	HYP	1	0
1	A	1856	HYP	1	0
2	G	41	HYP	2	0
2	G	33	HYP	1	0
1	A	1928	HYP	1	0
1	A	1875	HYP	1	0
1	A	1910	HYP	2	0
1	E	1897	HYP	2	0
1	B	1913	HYP	2	0
2	G	56	HYP	1	0
1	C	1921	HYP	1	0
1	A	1878	HYP	1	0
1	E	1898	HYP	1	0
2	G	55	HYP	1	0
1	C	1927	HYP	2	0
1	A	1929	HYP	1	0
2	I	1	HYP	1	0
1	C	1913	HYP	1	0
1	C	1928	HYP	1	0

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
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	16,1	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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
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	16,1	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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
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	16,1	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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	FUB	b	2	3	9,9,10	0.54	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
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	AHR	cE	4	18	9,9,10	0.55	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%)
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	FUB	eC	1	3	9,9,10	0.53	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%)
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	GZL	fE	3	18	11,11,12	6.58	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%)
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
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

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

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

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

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	AHR	AE	4	19	-	0/2/15/18	0/1/1/1
13	FUB	BA	1	13	-	0/2/15/18	0/1/1/1
13	FUB	BA	2	13	1/1/3/4	0/2/15/18	0/1/1/1
13	GZL	BA	3	13	-	4/6/19/22	0/1/1/1
13	AHR	BA	4	13	-	0/2/15/18	0/1/1/1
15	FUB	BB	1	15	-	0/2/15/18	0/1/1/1
15	FUB	BB	2	15	-	0/2/15/18	0/1/1/1
15	GZL	BB	3	15	1/1/4/5	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	FUB	DA	1	15	-	0/2/15/18	0/1/1/1
15	FUB	DA	2	15	-	0/2/15/18	0/1/1/1
15	GZL	DA	3	15	1/1/4/5	2/6/19/22	0/1/1/1
15	AHR	DA	4	15	-	0/2/15/18	0/1/1/1
15	AHR	DA	5	15	-	0/2/15/18	0/1/1/1
17	NAG	DB	1	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	AHR	EE	4	20	-	0/2/15/18	0/1/1/1
16	NAG	FA	1	16,1	-	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
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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FUB	pD	2	3	-	0/2/15/18	0/1/1/1
3	FUB	pD	3	3	-	0/2/15/18	0/1/1/1
18	FUB	pE	1	18	-	0/2/15/18	0/1/1/1
18	FUB	pE	2	18	-	0/2/15/18	0/1/1/1
18	GZL	pE	3	18	1/1/4/5	4/6/19/22	0/1/1/1
18	AHR	pE	4	18	1/1/3/4	0/2/15/18	0/1/1/1
18	AHR	pE	5	18	-	0/2/15/18	0/1/1/1
12	FUB	q	1	12	-	0/2/15/18	0/1/1/1
12	FUB	q	2	12	-	0/2/15/18	0/1/1/1
12	GZL	q	3	12	2/2/4/5	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

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

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

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

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

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

The worst 5 of 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	C1

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.

223 monomers are involved in 222 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	wA	3	FUB	1	0
12	oA	3	GZL	1	0
14	kB	4	FUB	1	0
5	M	1	FUB	1	0
6	xD	2	FUB	1	0
20	xE	1	FUB	2	0
4	iA	2	FUB	1	0
13	zC	1	FUB	1	0
3	PB	1	FUB	1	0
12	iB	4	AHR	1	0
18	BE	3	GZL	1	0
10	3	2	FUB	1	0
4	JB	1	FUB	2	0
18	yE	5	AHR	1	0
20	hE	2	FUB	1	0
14	nA	2	FUB	2	0
18	zE	1	FUB	1	0
6	bB	2	FUB	1	0
20	HE	1	FUB	2	0
15	4C	3	GZL	1	0
15	eB	2	FUB	1	0
5	EC	5	AHR	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	8C	1	FUB	1	0
10	yB	3	FUB	1	0
4	iA	3	FUB	1	0
13	jB	4	AHR	1	0
6	1C	3	GZL	1	0
6	0C	2	FUB	1	0
14	qA	2	FUB	1	0
3	NC	3	FUB	1	0
3	b	3	FUB	1	0
4	VD	1	FUB	1	0
6	XB	2	FUB	1	0
6	zD	3	GZL	1	0
3	wB	3	FUB	1	0
13	dD	1	FUB	1	0
13	wD	3	GZL	1	0
22	dE	3	GZL	1	0
13	0D	3	GZL	1	0
4	jC	1	FUB	1	0
6	N	3	GZL	6	0
13	mA	4	AHR	1	0
3	RB	1	FUB	1	0
18	PE	4	AHR	1	0
6	0C	1	FUB	1	0
20	HE	4	AHR	1	0
3	K	2	FUB	1	0
20	uE	2	FUB	1	0
17	7C	3	BMA	1	0
13	4	4	AHR	1	0
15	AB	1	FUB	1	0
13	zB	4	AHR	1	0
4	mB	1	FUB	1	0
18	IE	4	AHR	1	0
20	uE	4	AHR	1	0
3	qC	3	FUB	1	0
3	xA	1	FUB	1	0
6	mE	1	FUB	1	0
23	XE	4	AHR	1	0
6	xD	3	GZL	1	0
3	QB	2	FUB	1	0
11	gA	2	AHR	1	0
6	bE	3	GZL	1	0
18	yE	4	AHR	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	xC	2	FUB	1	0
6	CD	3	GZL	5	0
3	z	2	FUB	2	0
6	bB	3	GZL	1	0
7	XC	3	FUB	1	0
6	0B	2	FUB	1	0
16	FA	1	NAG	1	0
3	RB	2	FUB	2	0
3	sB	3	FUB	1	0
6	nE	3	GZL	1	0
23	XE	5	AHR	1	0
3	m	3	FUB	1	0
18	pE	4	AHR	1	0
6	5	3	GZL	6	0
6	OE	1	FUB	1	0
3	QB	3	FUB	1	0
13	wC	3	GZL	6	0
4	JA	4	AHR	1	0
13	tD	3	GZL	5	0
22	QE	4	AHR	1	0
3	LB	2	FUB	2	0
18	BE	1	FUB	1	0
5	EC	2	FUB	1	0
3	TA	2	FUB	1	0
22	GE	1	FUB	1	0
14	nA	3	GZL	2	0
4	AD	4	AHR	2	0
13	gC	4	AHR	1	0
3	iD	2	FUB	1	0
7	f	4	AHR	1	0
3	ZA	3	FUB	1	0
13	2A	3	GZL	5	0
16	4D	1	NAG	1	0
22	wE	1	FUB	1	0
6	9	3	GZL	1	0
3	IA	3	FUB	1	0
20	hE	4	AHR	1	0
20	uE	3	GZL	1	0
13	dD	2	FUB	1	0
18	IE	1	FUB	1	0
22	QE	6	AHR	1	0
3	sB	2	FUB	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	fE	1	FUB	1	0
18	zE	5	AHR	1	0
8	JD	5	AHR	1	0
3	b	2	FUB	1	0
6	FC	3	GZL	4	0
22	RE	1	FUB	1	0
12	lB	3	GZL	1	0
18	yE	1	FUB	1	0
3	PB	2	FUB	1	0
13	tD	4	AHR	1	0
3	oD	1	FUB	1	0
14	qA	1	FUB	1	0
13	0D	2	FUB	1	0
14	nA	4	FUB	1	0
4	pA	1	FUB	1	0
14	KB	3	GZL	1	0
3	IA	2	FUB	1	0
14	p	3	GZL	1	0
6	0B	3	GZL	3	0
3	J	3	FUB	1	0
10	3	3	FUB	1	0
10	vC	1	FUB	1	0
13	WB	3	GZL	6	0
13	BA	3	GZL	1	0
15	7B	1	FUB	1	0
22	wE	2	FUB	1	0
20	xE	4	AHR	1	0
3	t	2	FUB	1	0
13	zB	3	GZL	7	0
12	iC	5	AHR	1	0
13	zC	2	FUB	1	0
15	4C	2	FUB	1	0
13	vD	2	FUB	1	0
6	2C	3	GZL	1	0
15	eB	3	GZL	1	0
3	TA	3	FUB	1	0
3	z	1	FUB	1	0
3	xA	2	FUB	2	0
6	XB	1	FUB	1	0
10	sD	2	FUB	2	0
3	wB	2	FUB	1	0
18	IE	5	AHR	1	0

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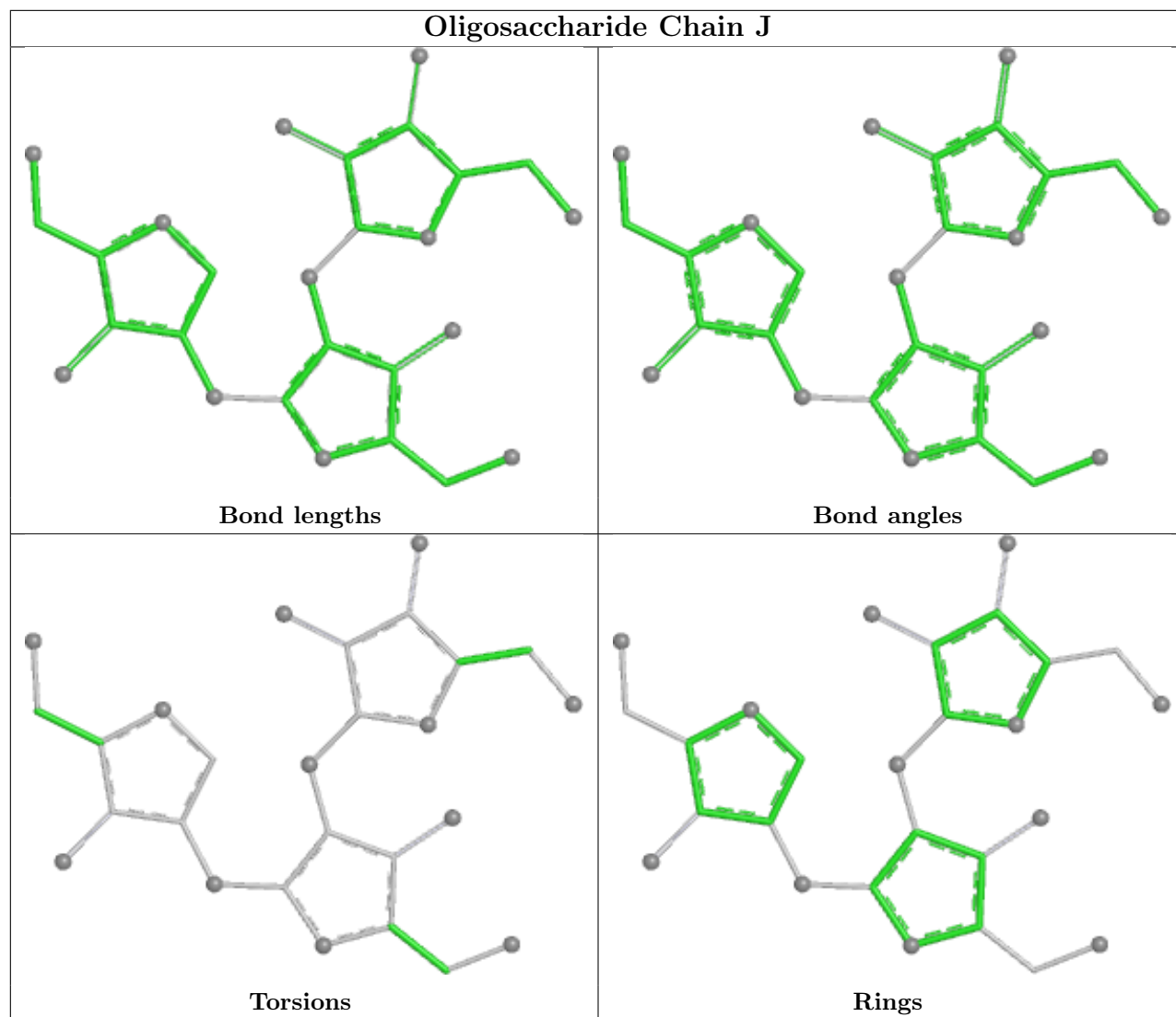
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	XB	3	GZL	3	0
21	FE	5	AHR	1	0
14	eD	3	GZL	1	0
20	CE	4	AHR	1	0
17	7C	2	NAG	1	0
22	dE	2	FUB	1	0
6	LA	3	GZL	4	0
16	AC	1	NAG	2	0
6	ME	1	FUB	1	0
3	MA	1	FUB	1	0
3	m	2	FUB	1	0
20	HE	2	FUB	1	0
22	dE	6	AHR	1	0
4	VD	2	FUB	1	0
6	xC	3	GZL	5	0
7	XC	4	AHR	1	0
3	y	3	FUB	1	0
22	iE	3	GZL	1	0
4	kD	1	FUB	1	0
18	0E	4	AHR	1	0
3	iD	3	FUB	1	0
3	tC	1	FUB	1	0
4	LD	2	FUB	1	0
3	QB	1	FUB	1	0
3	oD	2	FUB	1	0
6	OE	2	FUB	1	0
5	KA	5	AHR	1	0
12	q	3	GZL	1	0
7	HD	4	AHR	1	0
6	uD	1	FUB	1	0
6	bE	2	FUB	1	0
7	f	2	FUB	2	0
13	vD	1	FUB	1	0
6	3A	3	GZL	5	0
10	yB	2	FUB	1	0
4	gD	4	AHR	1	0
5	M	2	FUB	2	0
4	gD	1	FUB	2	0
4	r	1	FUB	1	0
20	EE	4	AHR	1	0
22	iE	4	AHR	1	0
6	mE	2	FUB	1	0

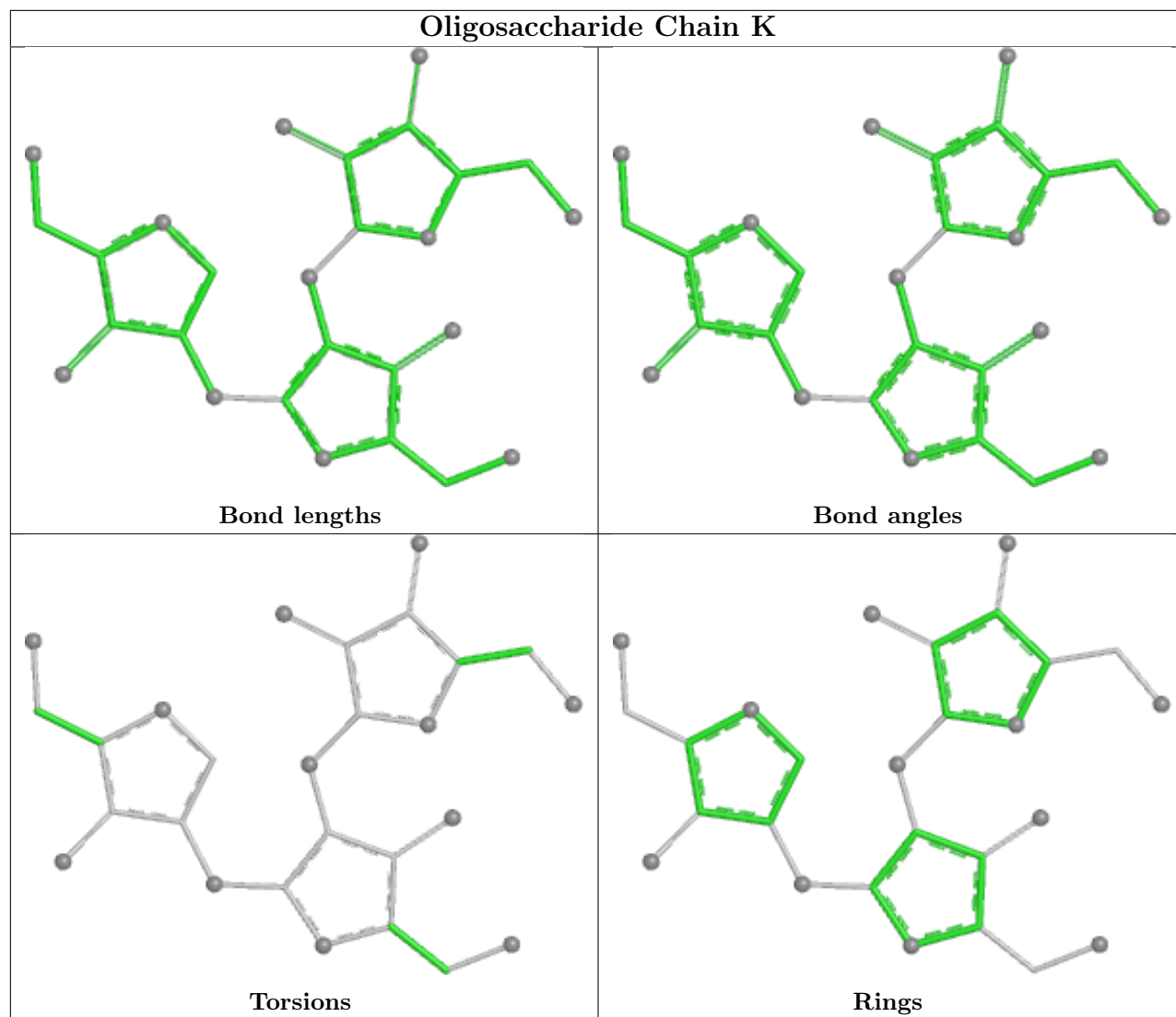
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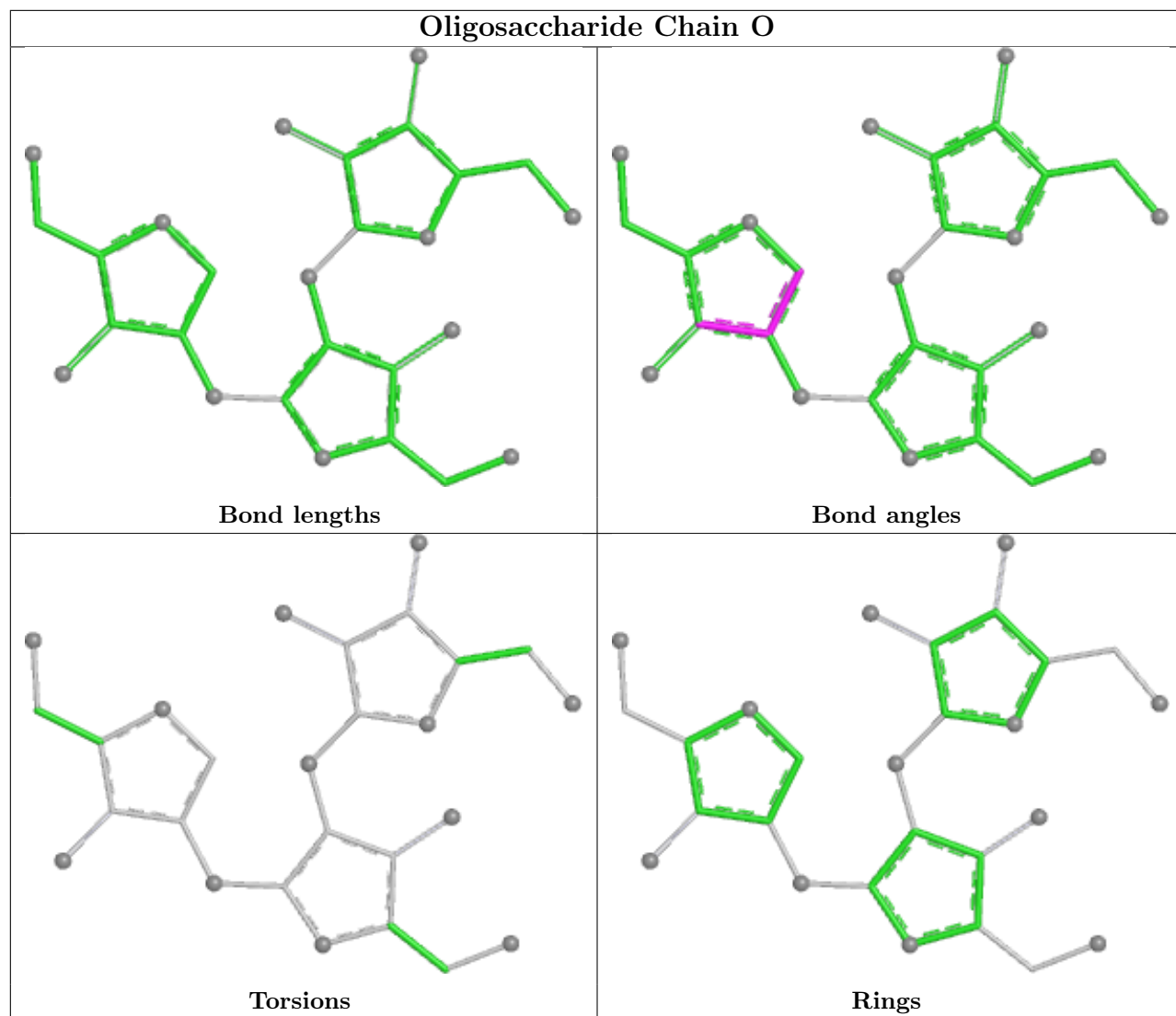
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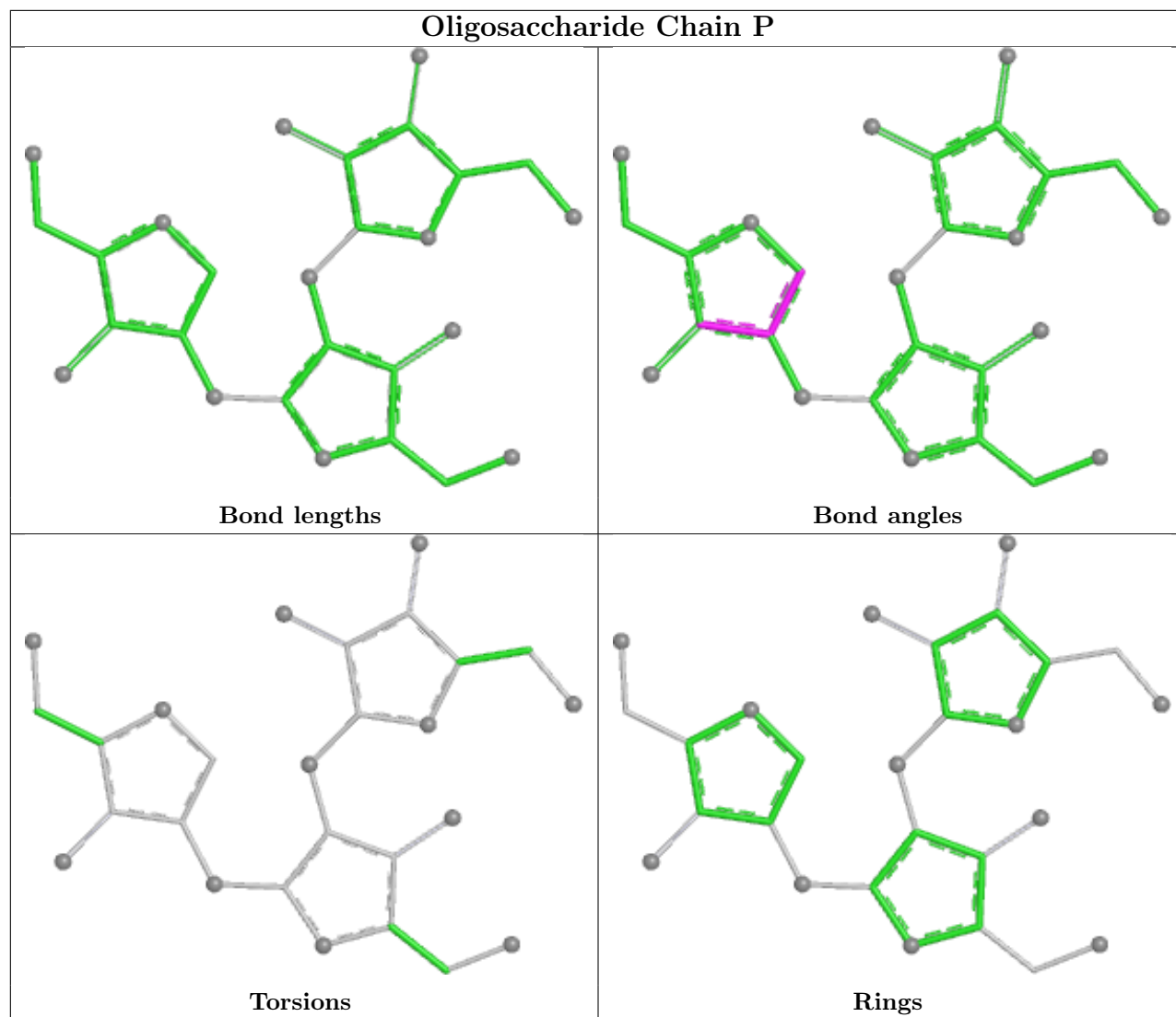
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	iC	3	GZL	1	0
9	hA	1	FUB	1	0
20	xE	3	GZL	1	0
13	wD	2	FUB	1	0
6	uD	3	GZL	5	0
3	rA	2	FUB	1	0
4	pA	4	AHR	1	0
18	SE	1	FUB	1	0
22	wE	3	GZL	1	0
6	0B	1	FUB	1	0
6	mE	3	GZL	1	0
6	5	2	FUB	1	0
3	qC	2	FUB	1	0
6	cB	3	GZL	1	0
22	RE	6	AHR	1	0
4	DC	1	FUB	1	0
3	MA	2	FUB	1	0
3	J	2	FUB	1	0
7	KC	4	AHR	1	0
13	o	4	AHR	1	0
3	tC	2	FUB	1	0
18	rE	1	FUB	1	0
3	oB	2	FUB	2	0
3	mD	2	FUB	1	0
10	sD	5	AHR	1	0
20	HE	3	GZL	2	0
4	jC	4	AHR	1	0
20	hE	3	GZL	1	0
22	VE	4	AHR	1	0
19	LE	3	GZL	1	0
13	4	3	GZL	4	0
20	UE	4	AHR	1	0
10	sD	3	FUB	1	0

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

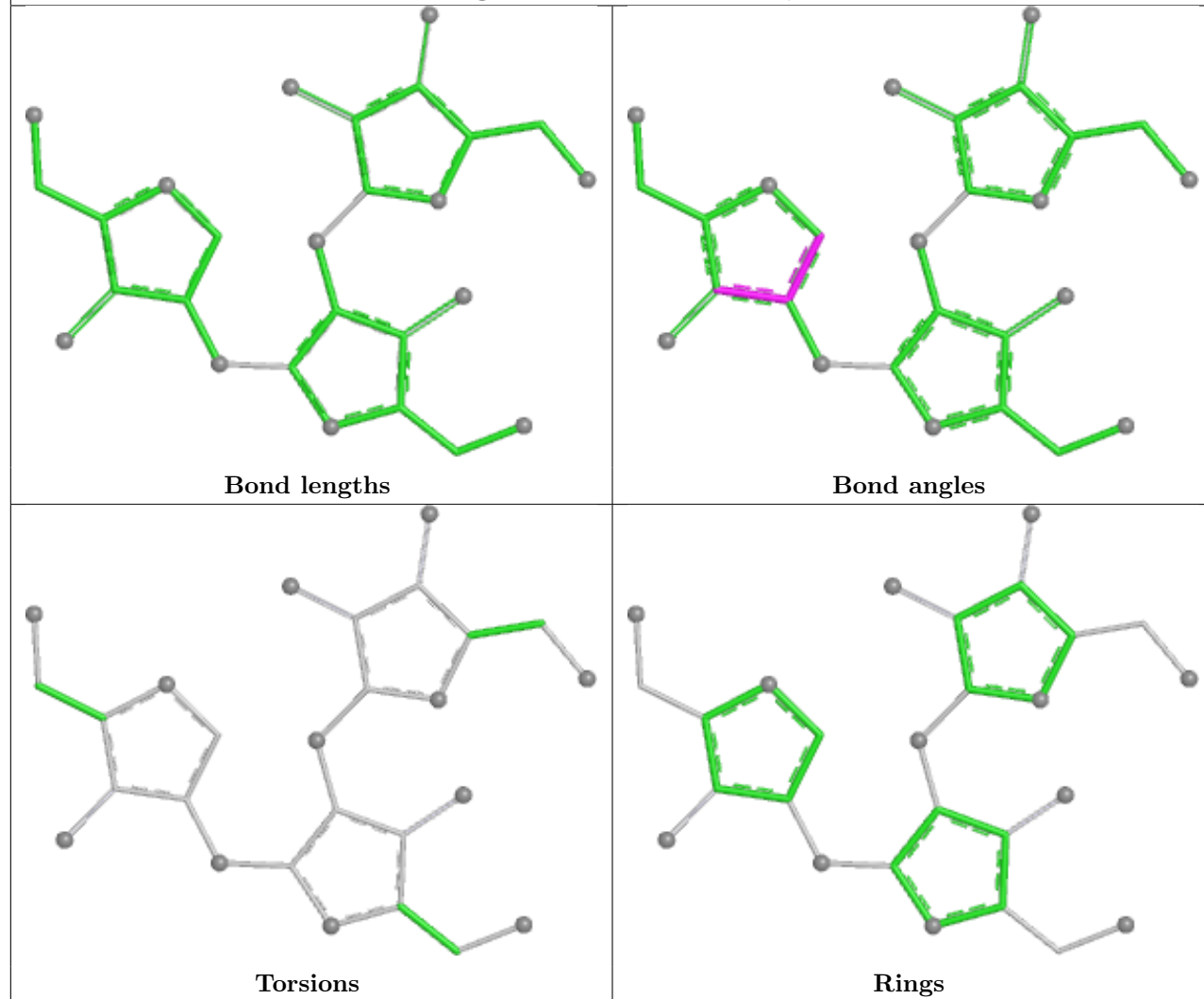


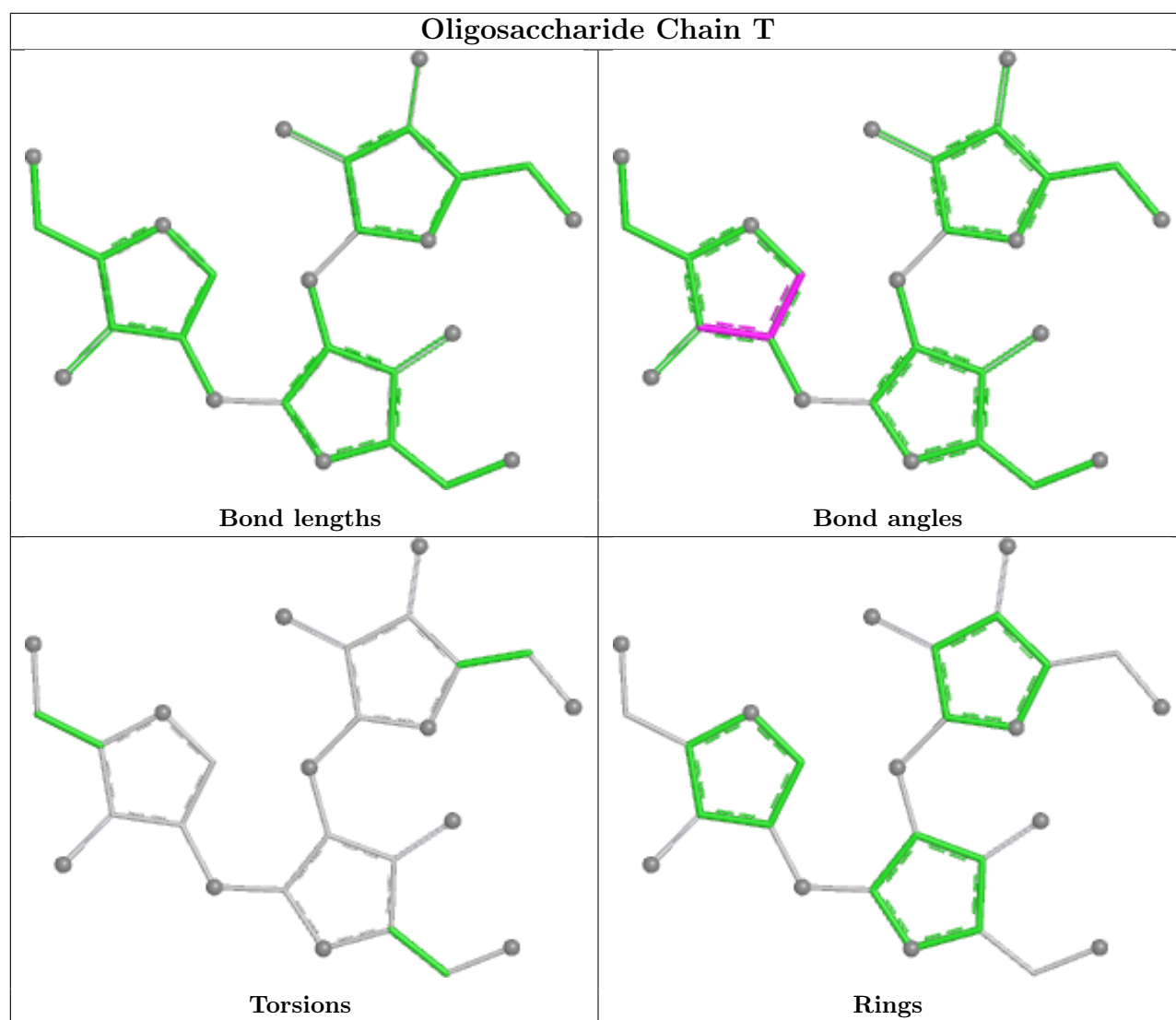


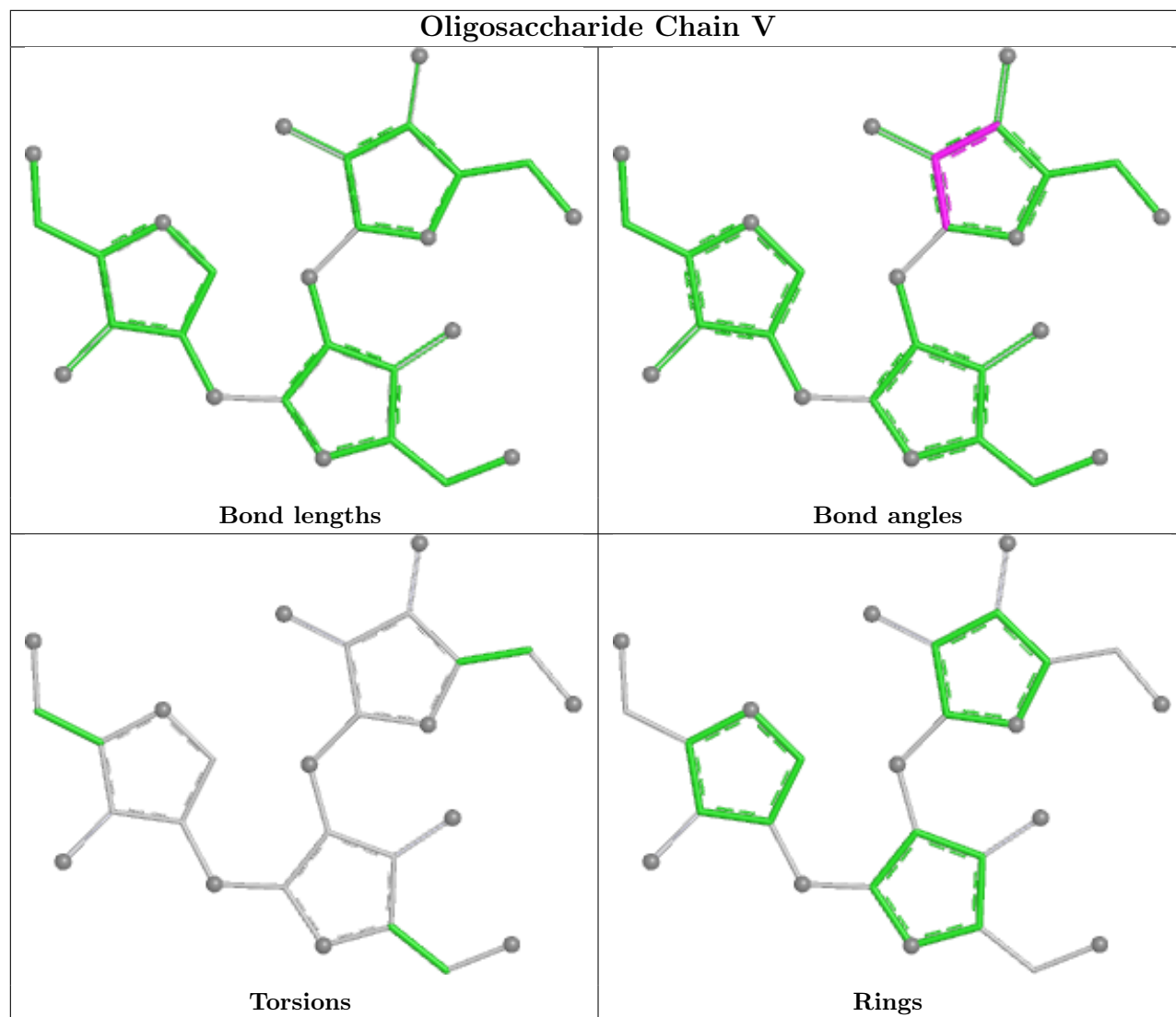


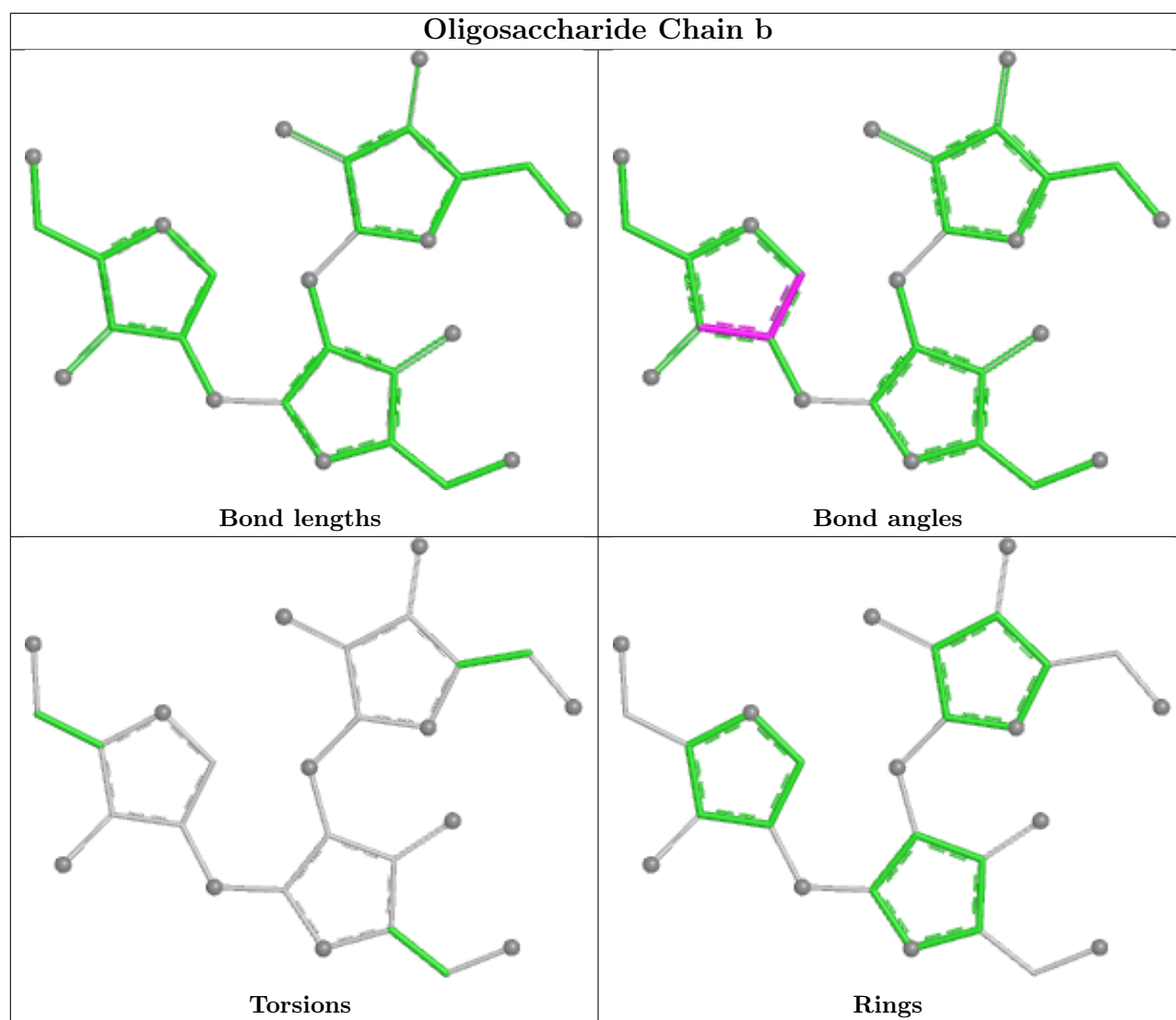


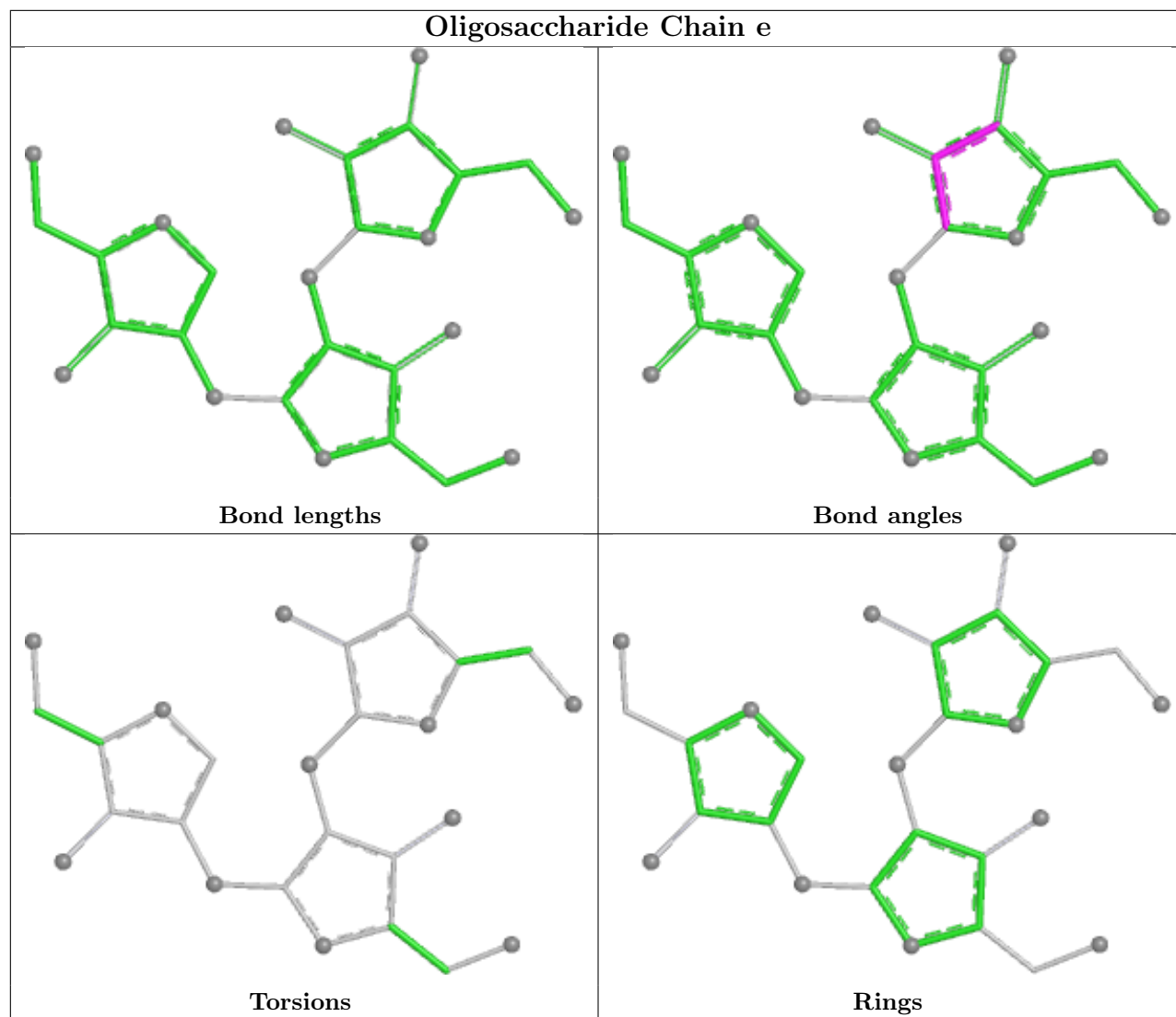
Oligosaccharide Chain Q

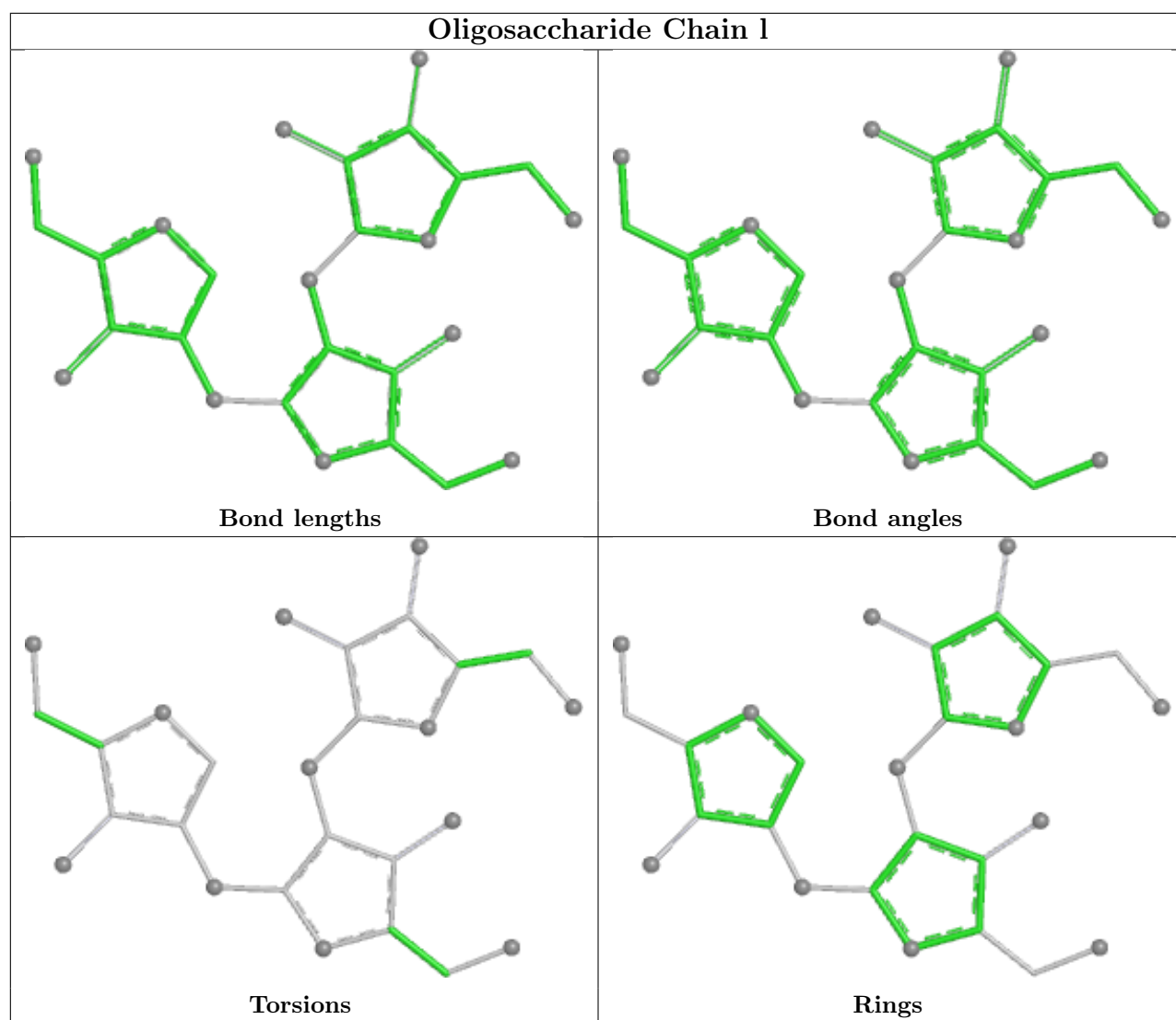


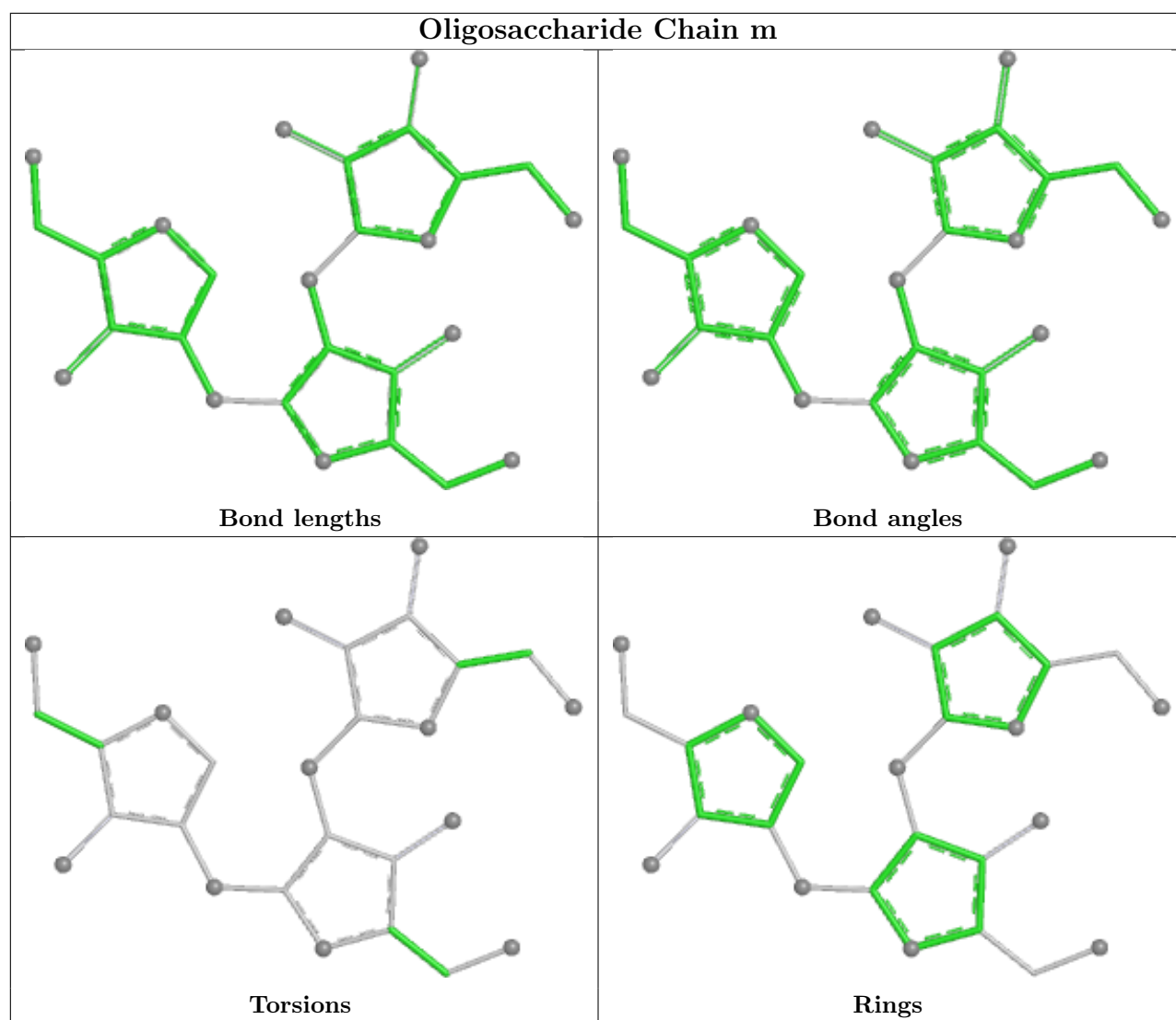


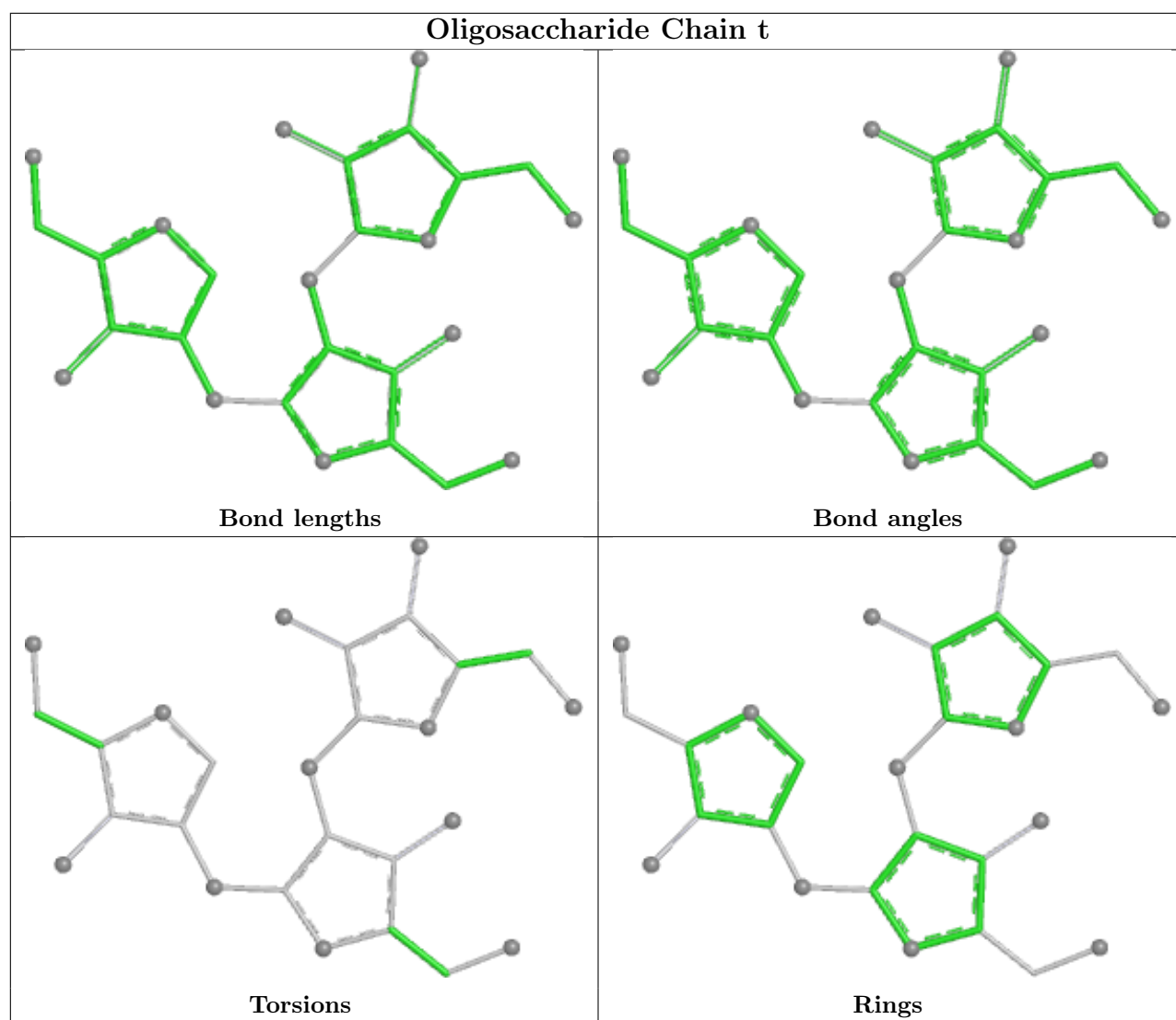


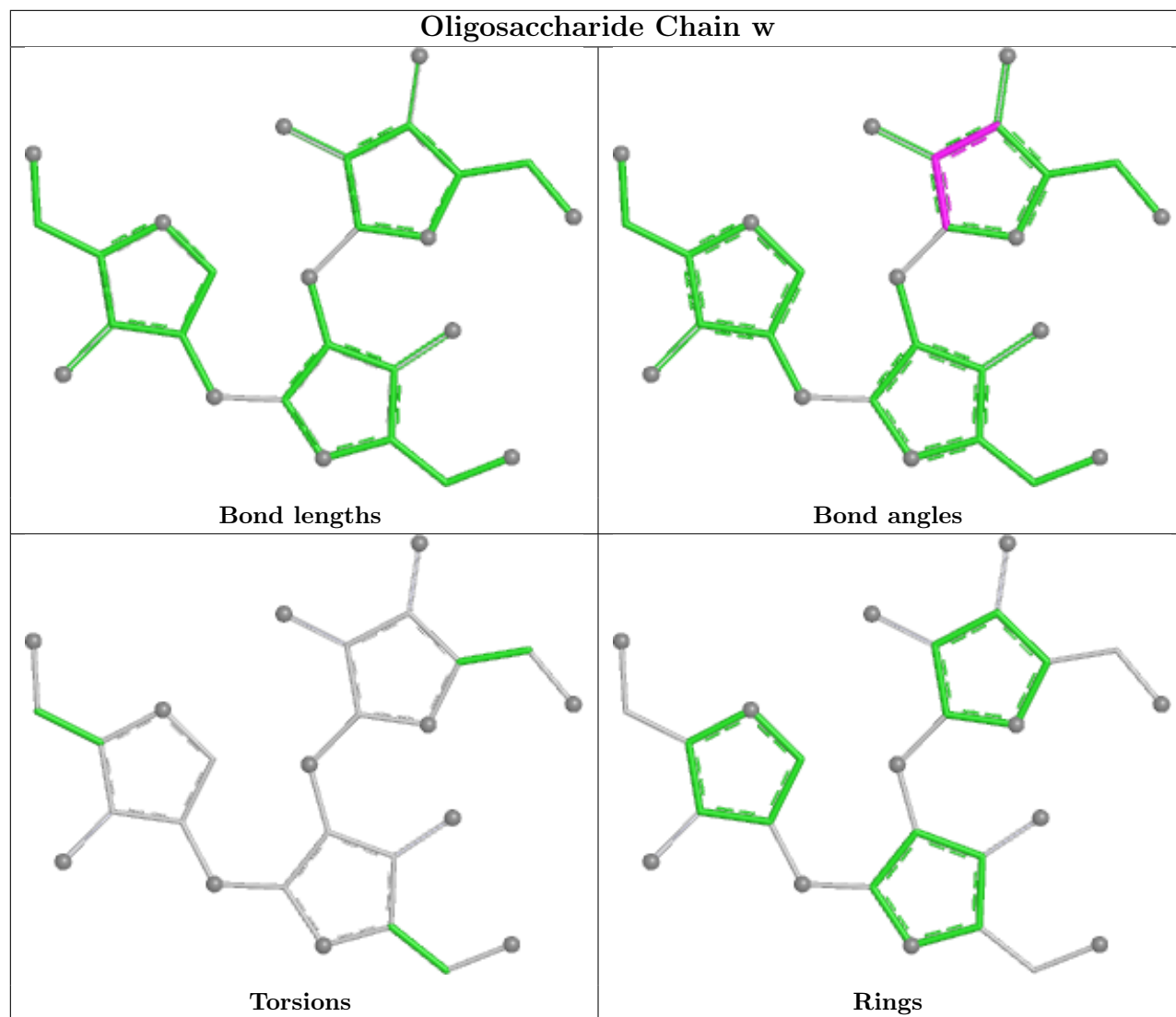


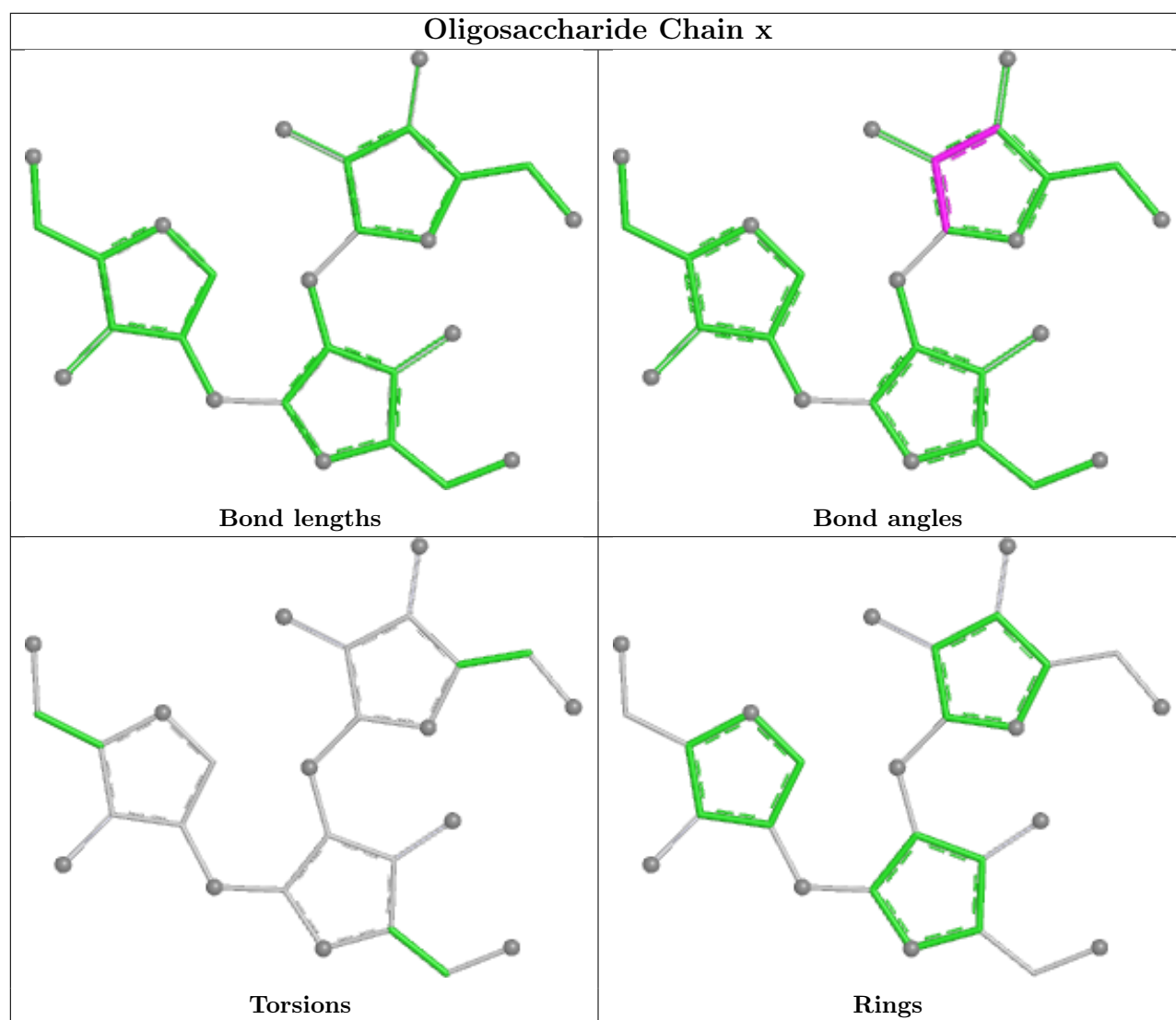


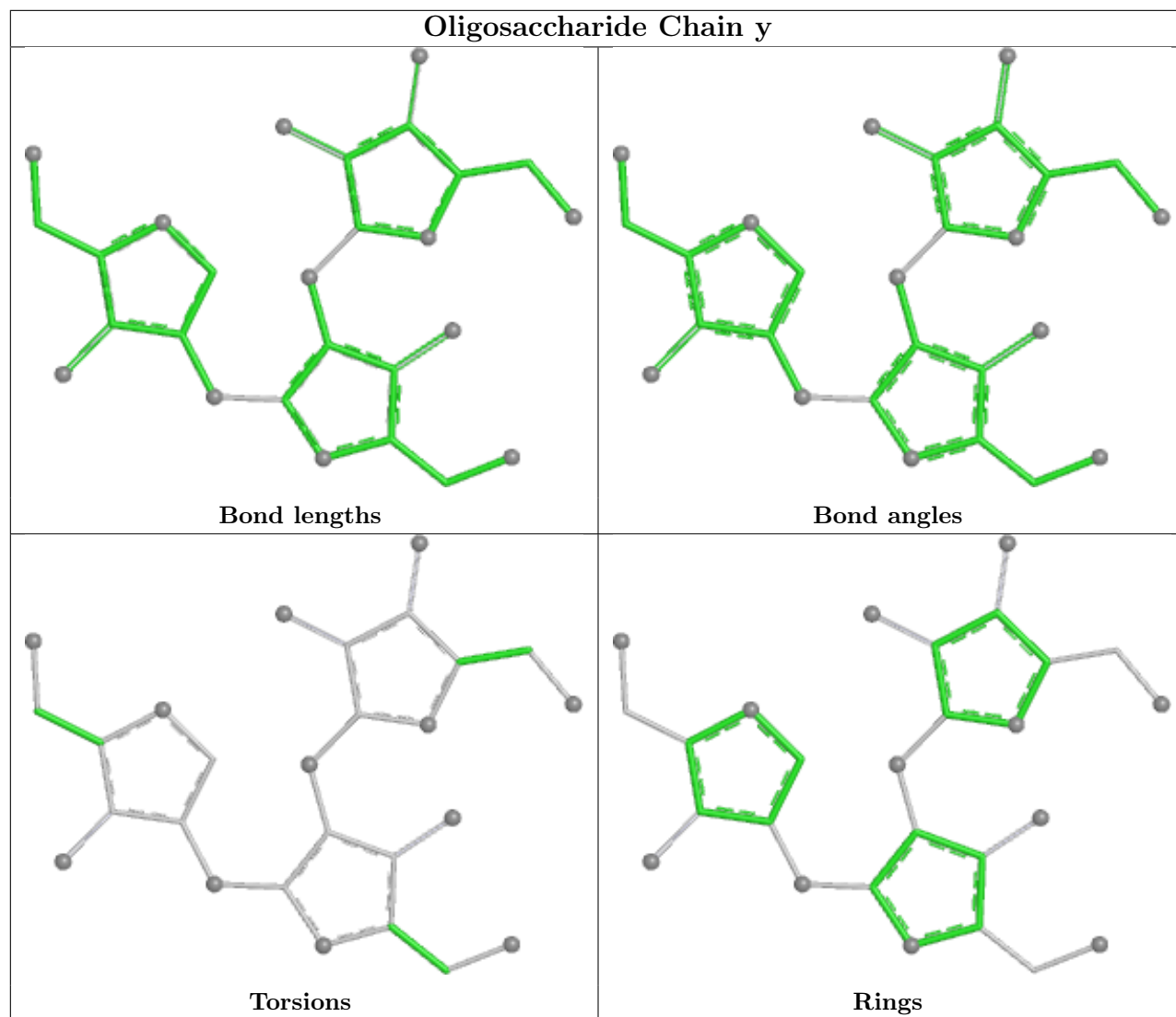


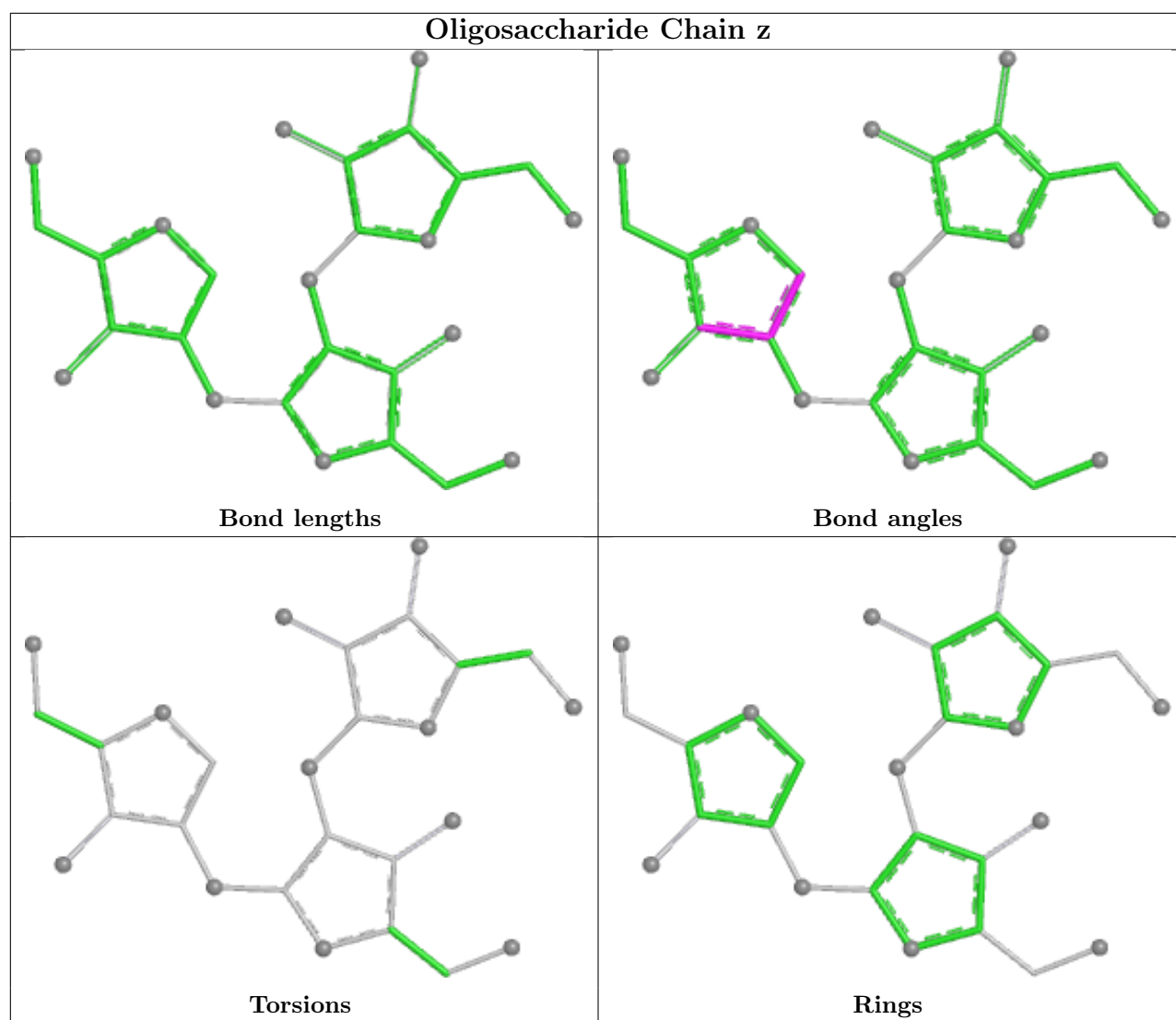


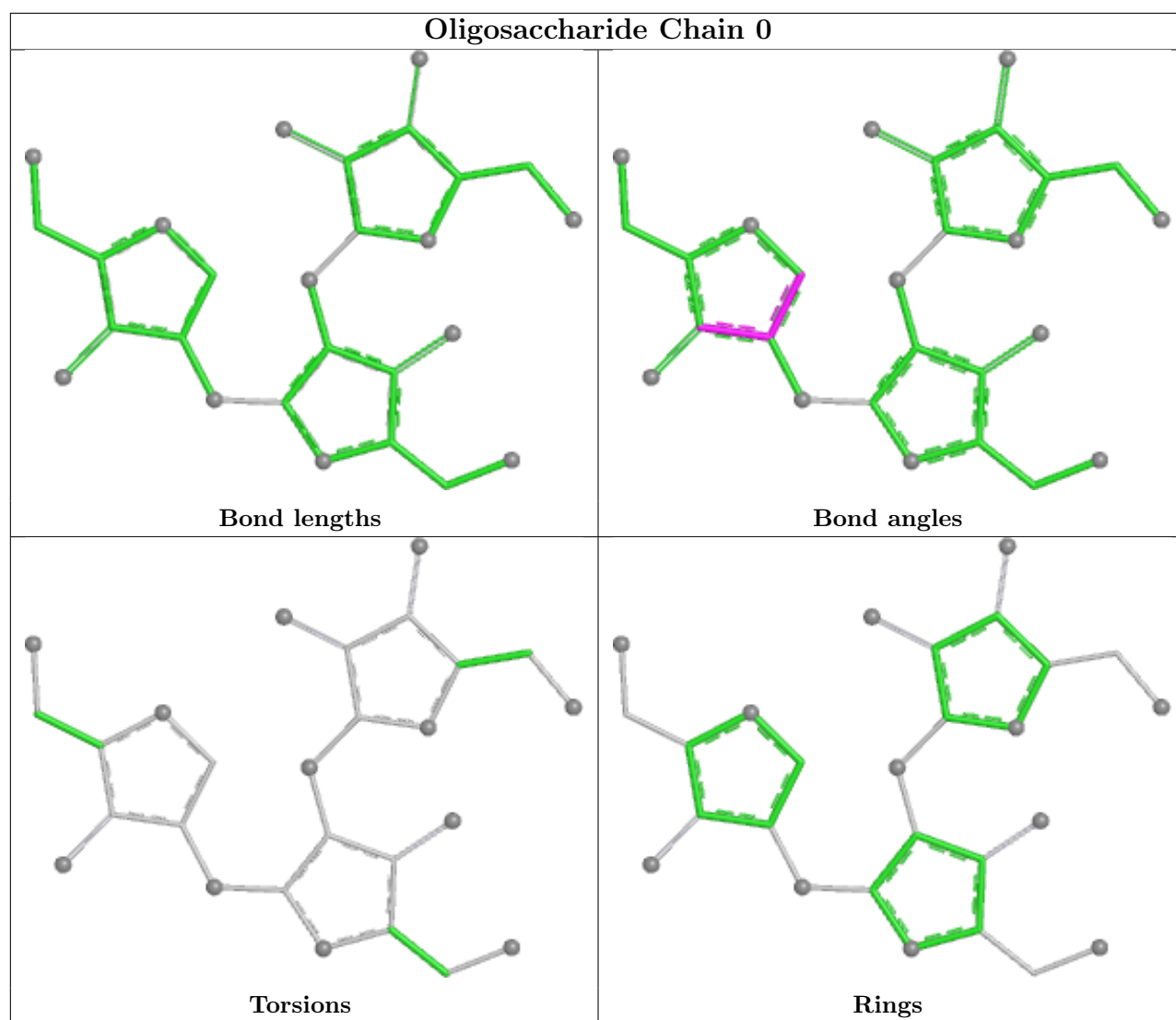


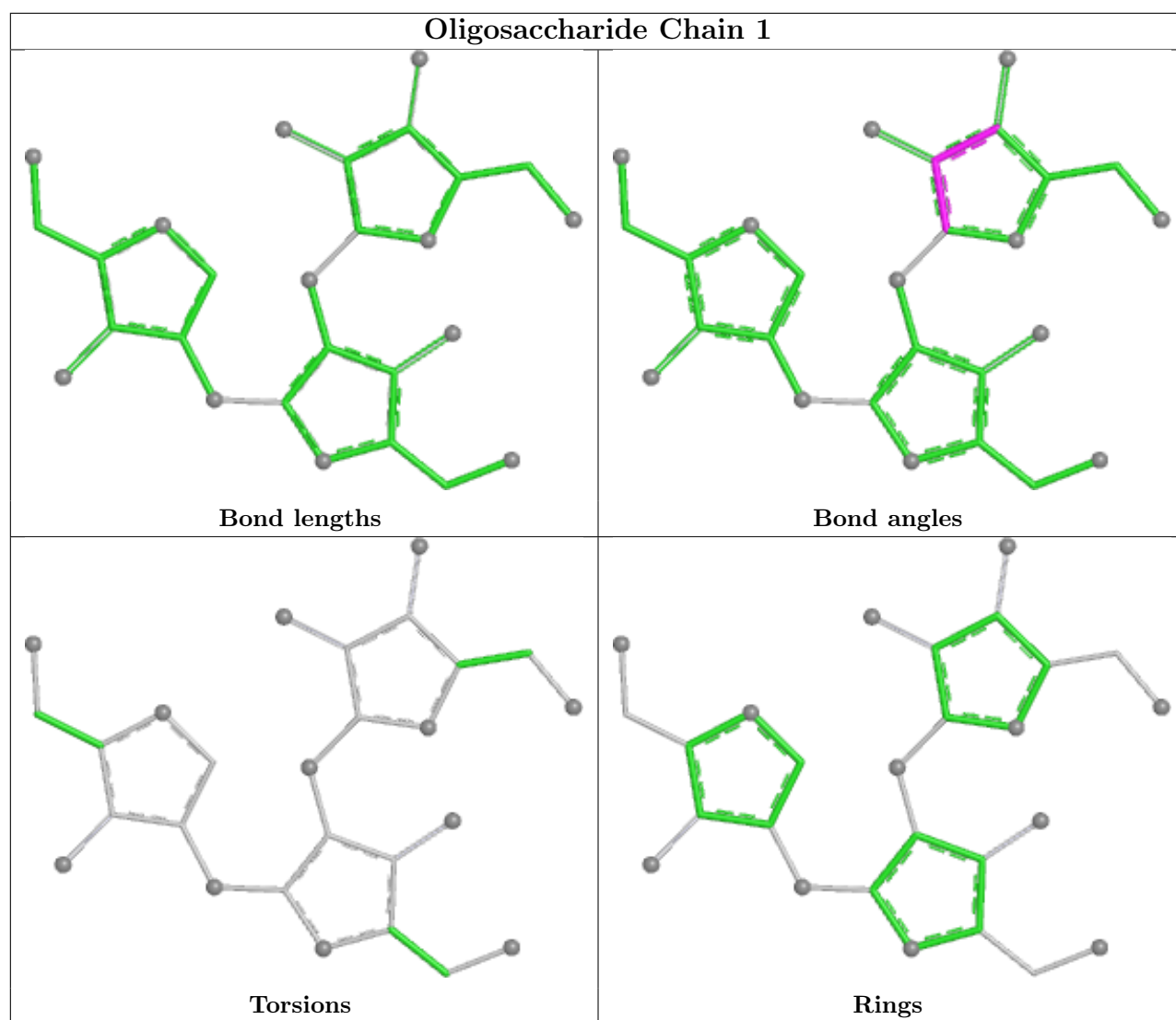


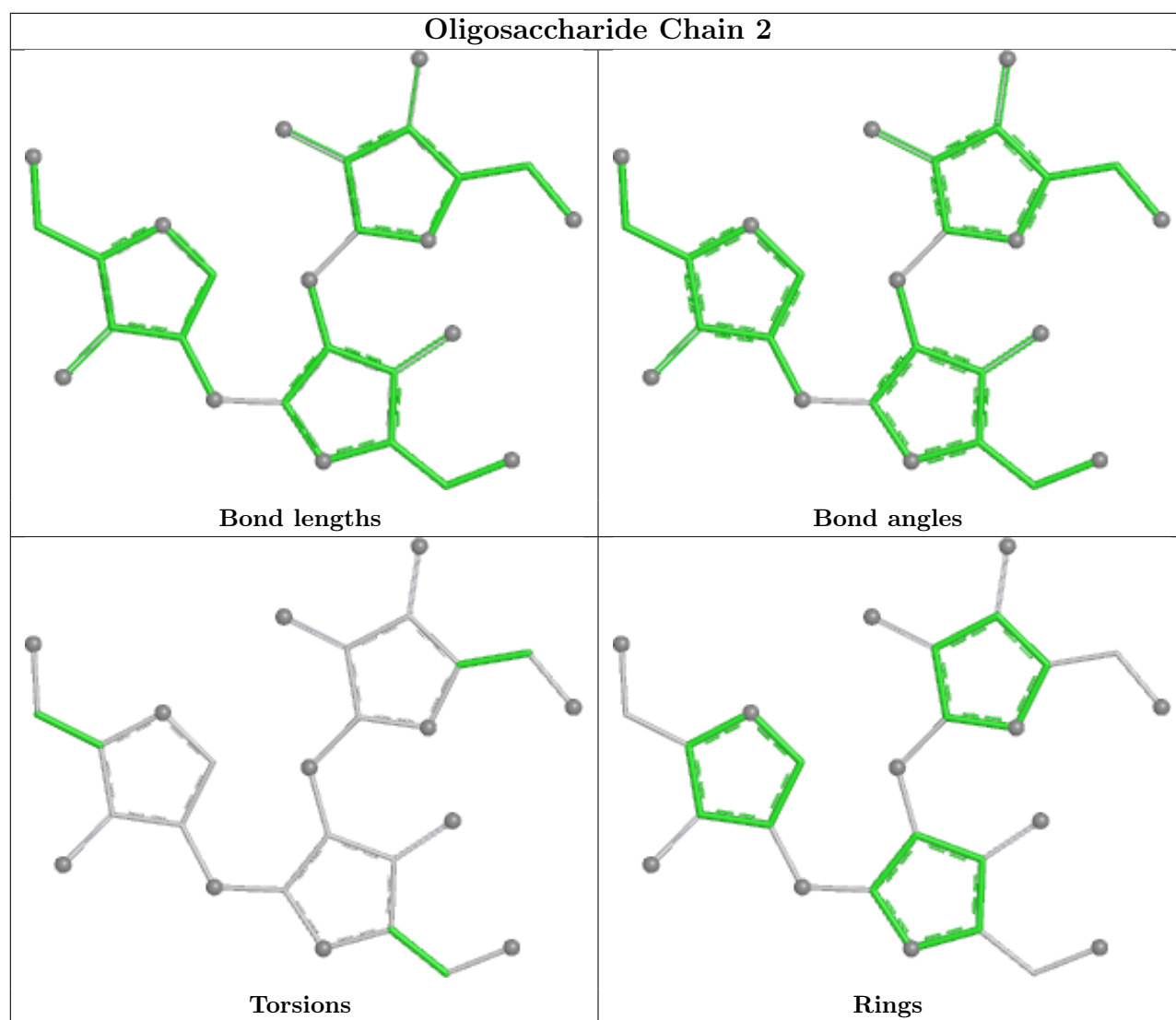


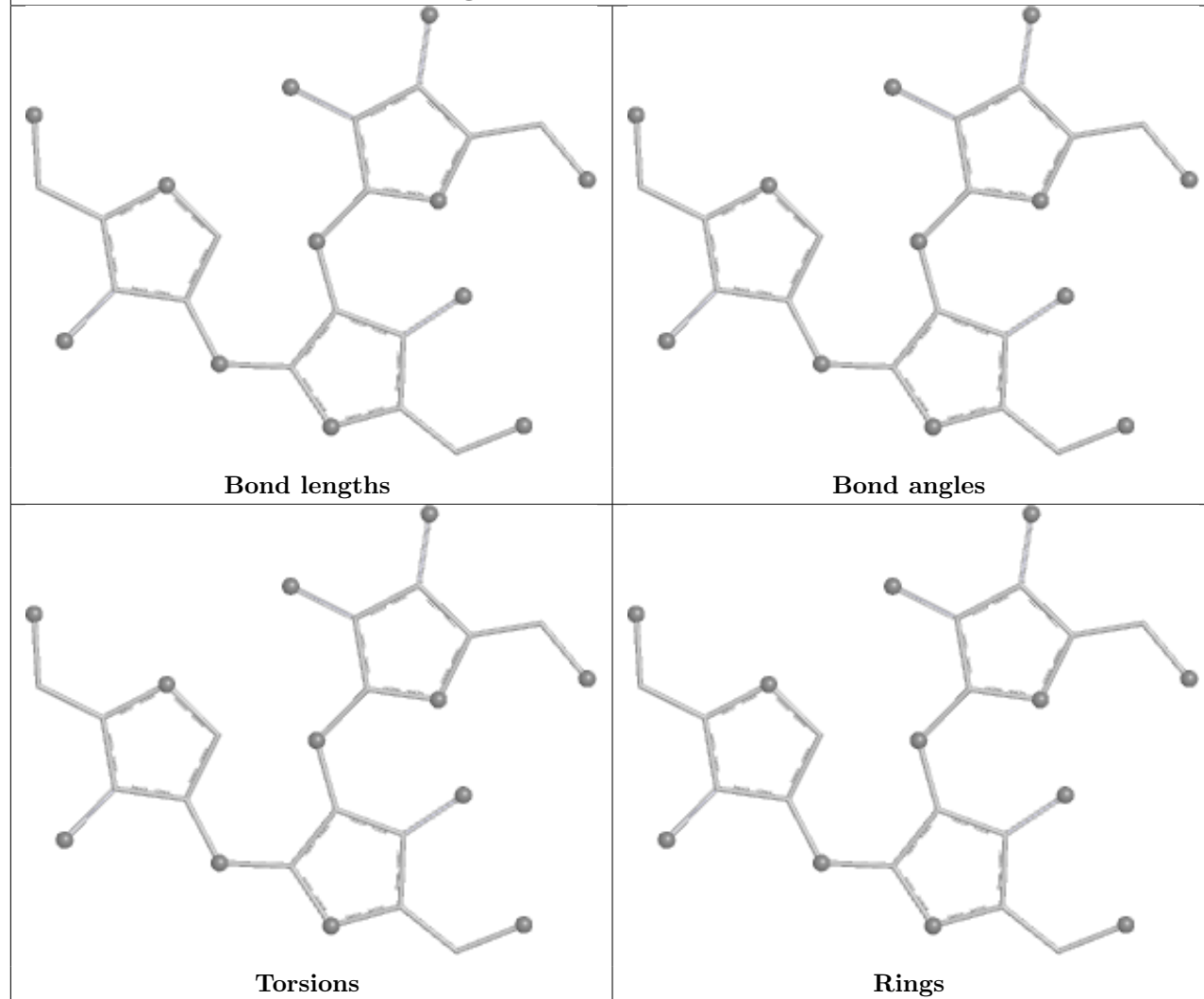


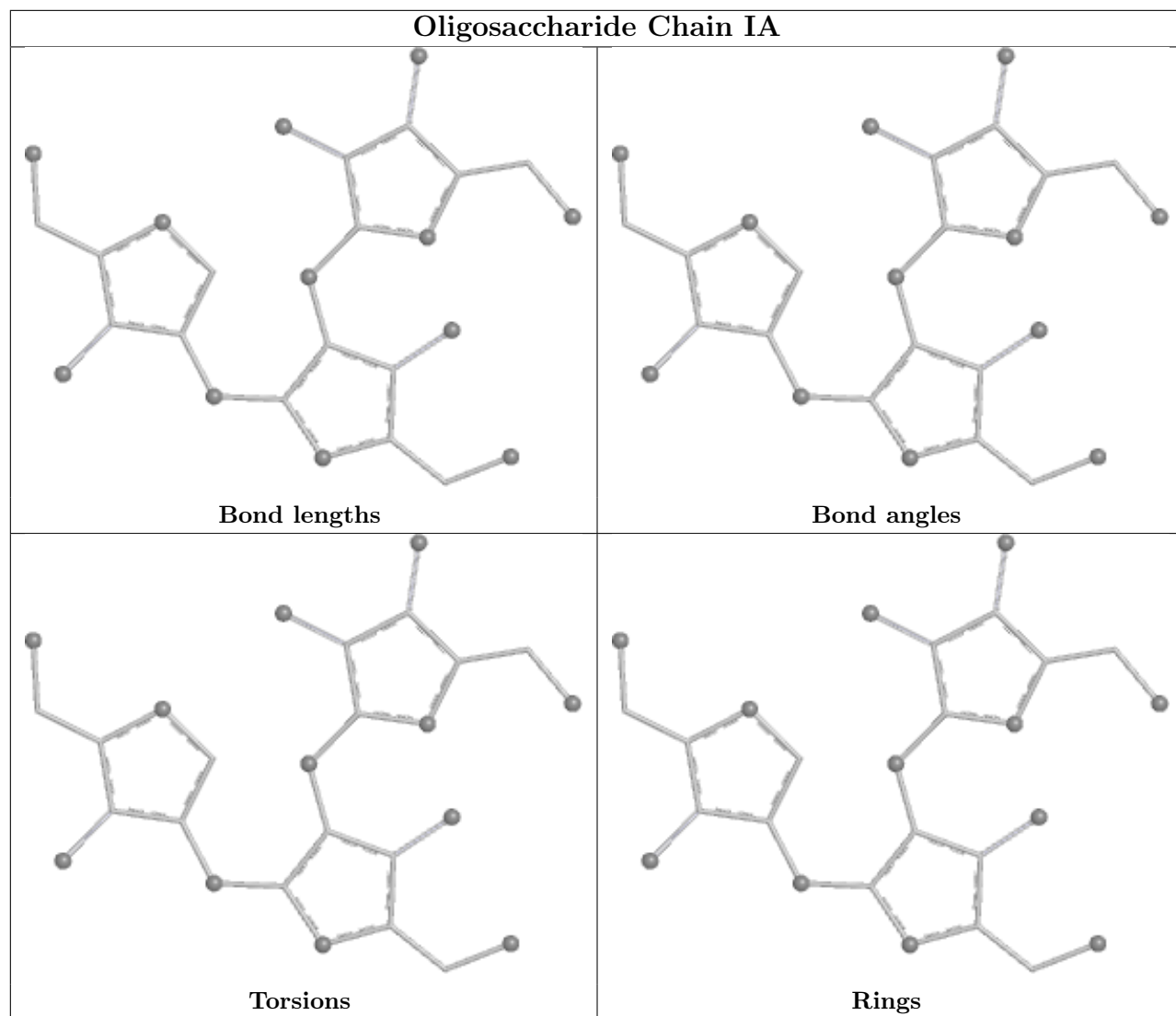


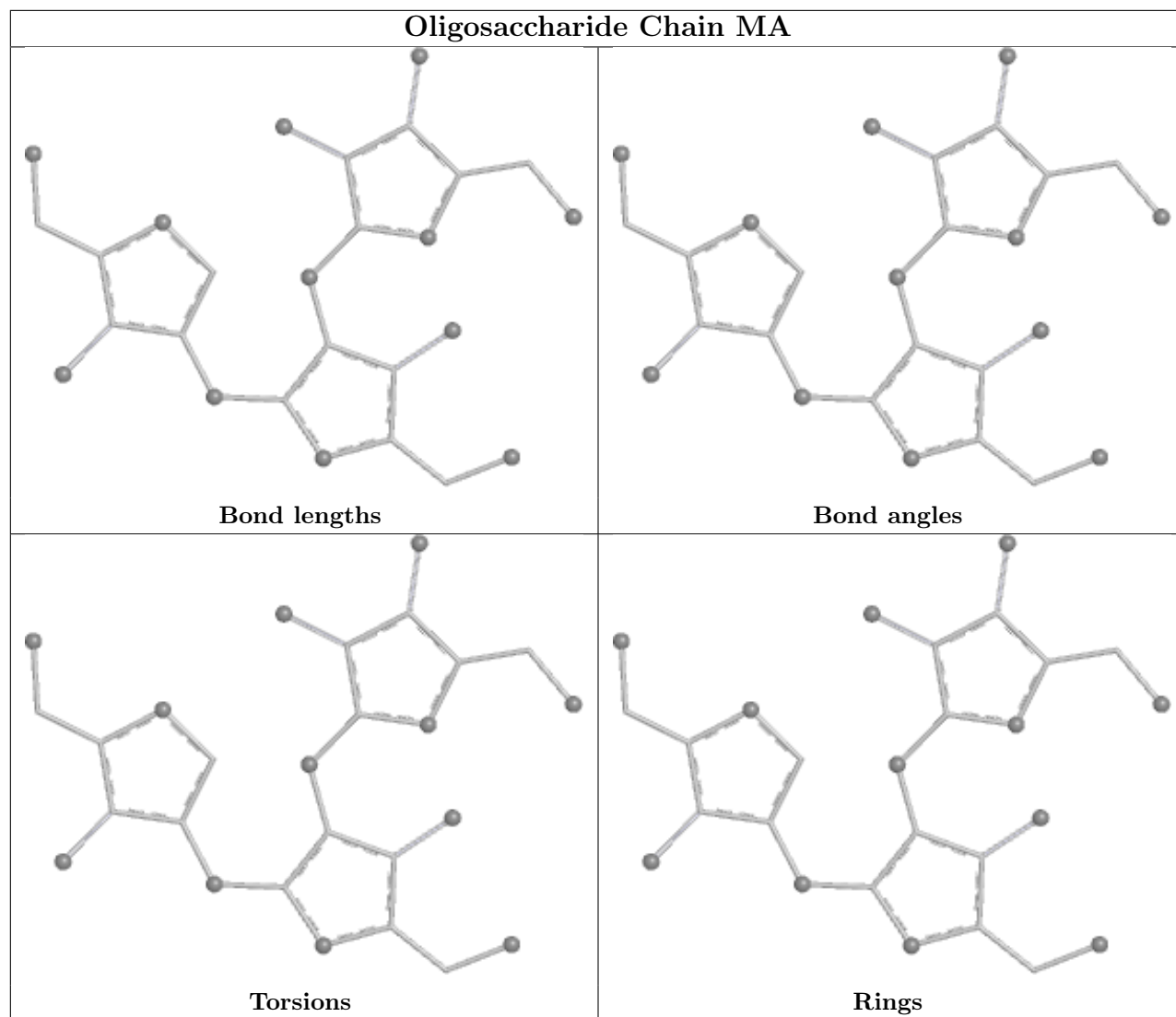


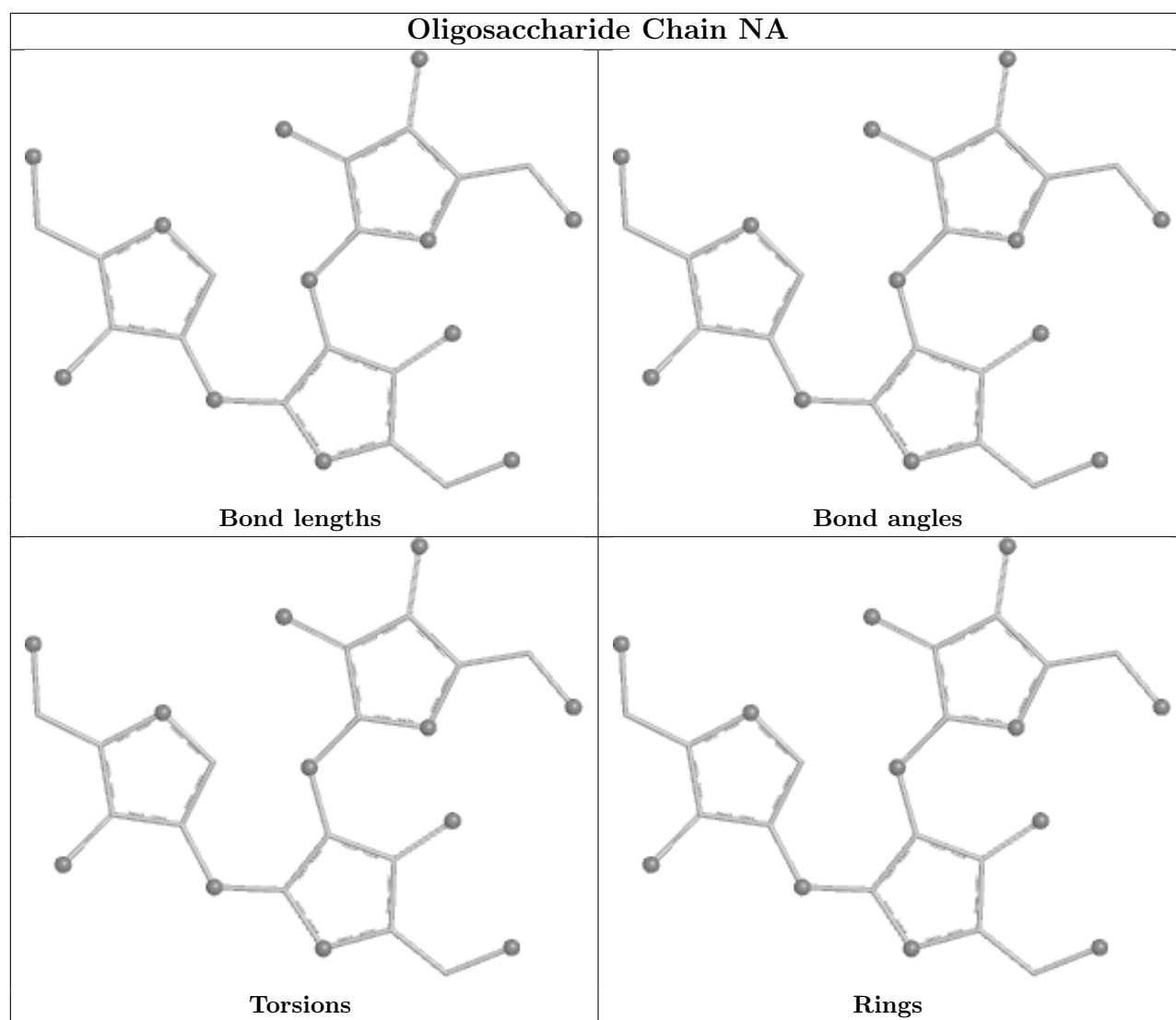


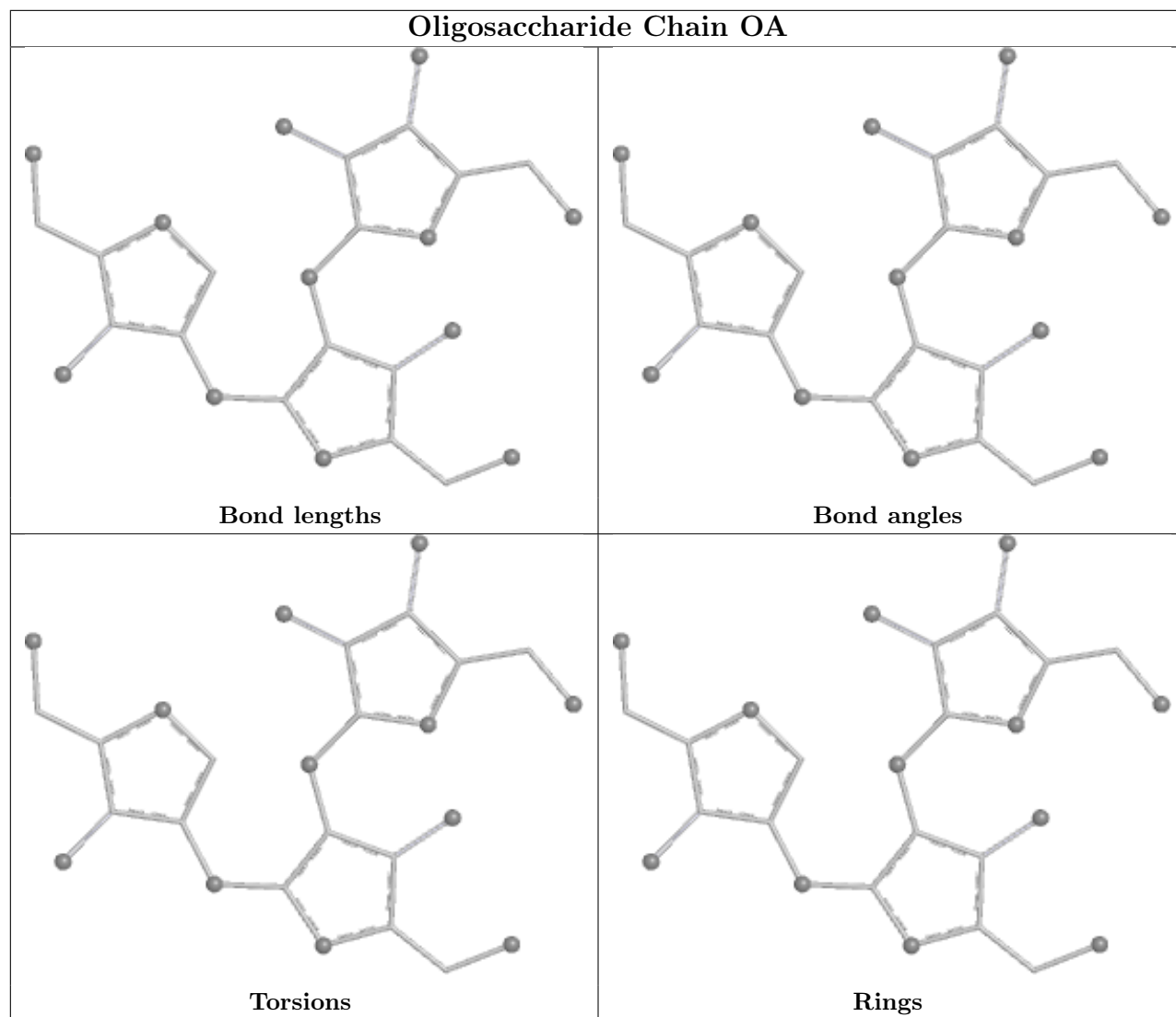


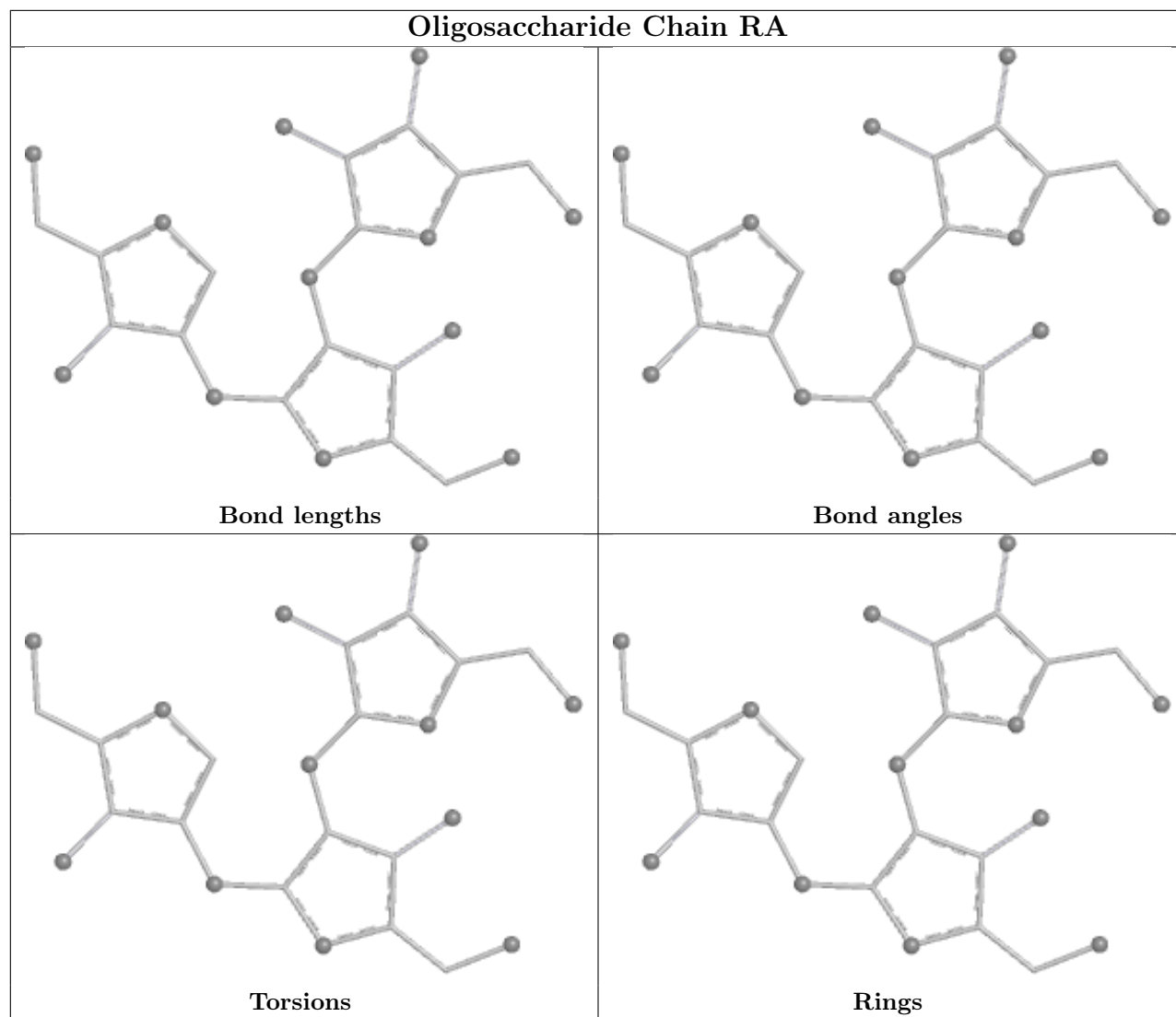
Oligosaccharide Chain HA

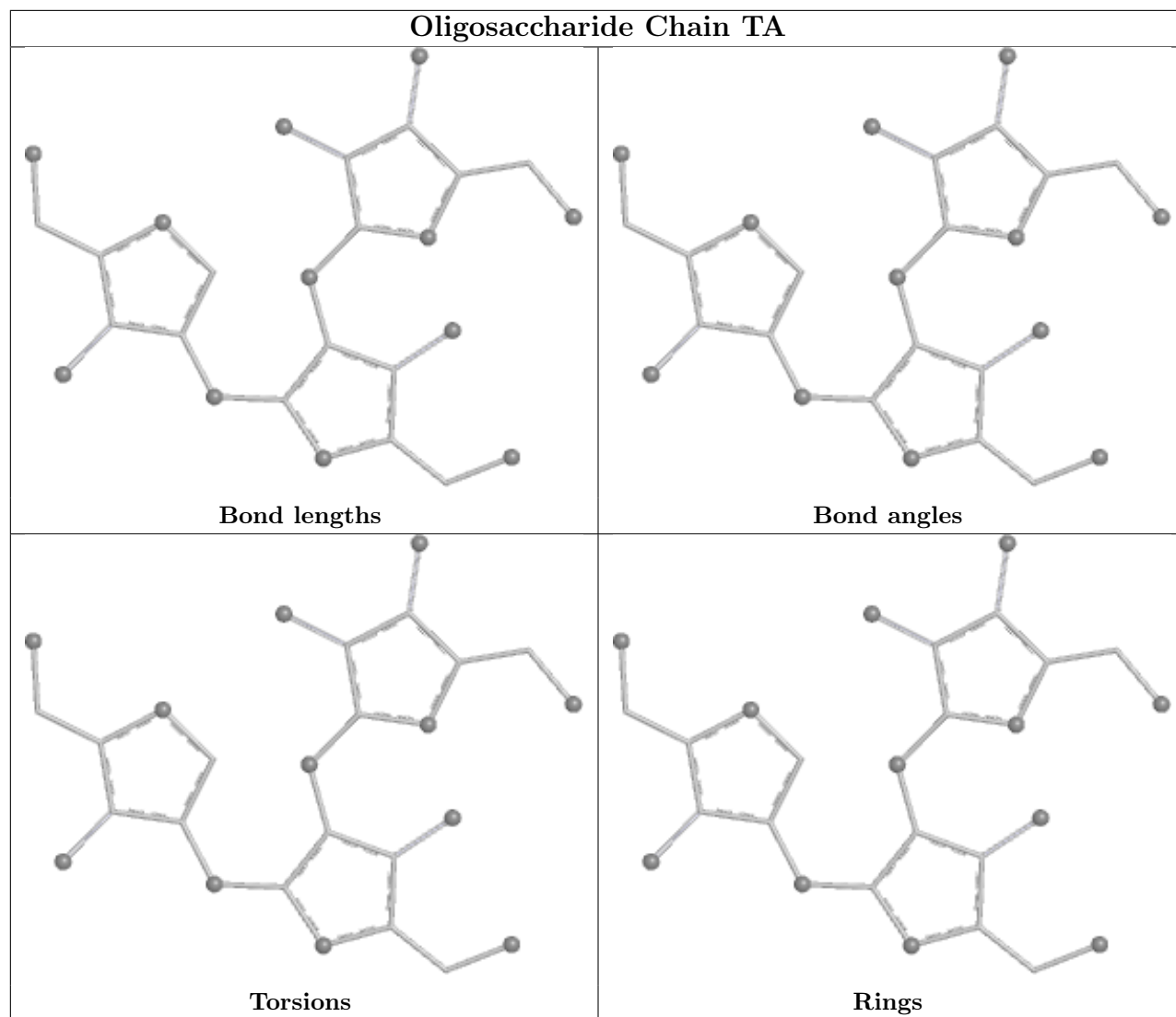


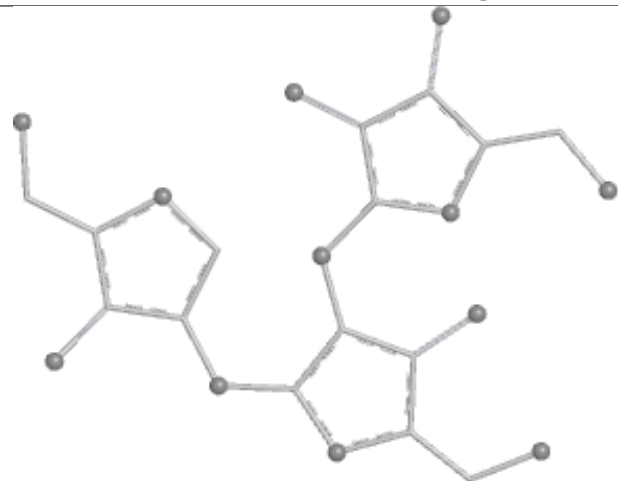
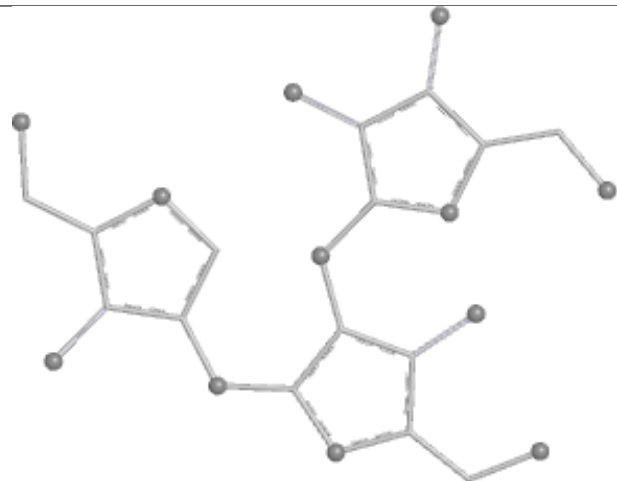
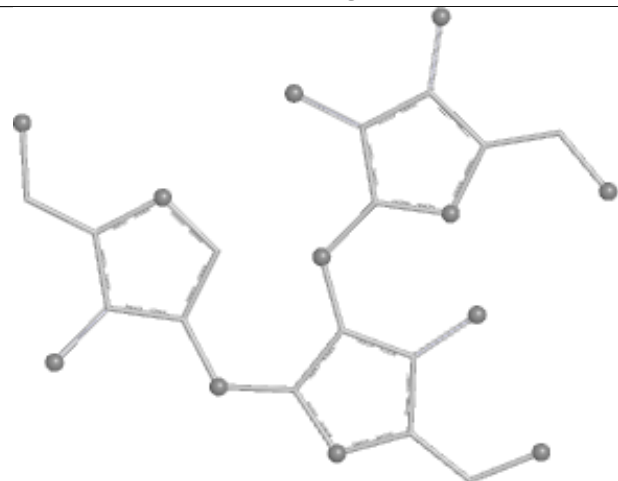
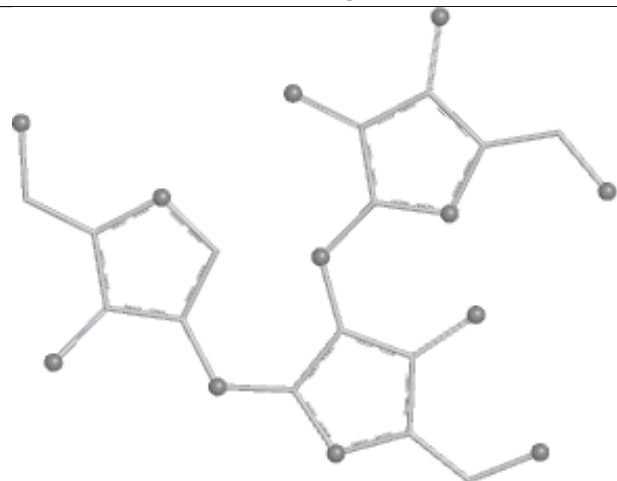


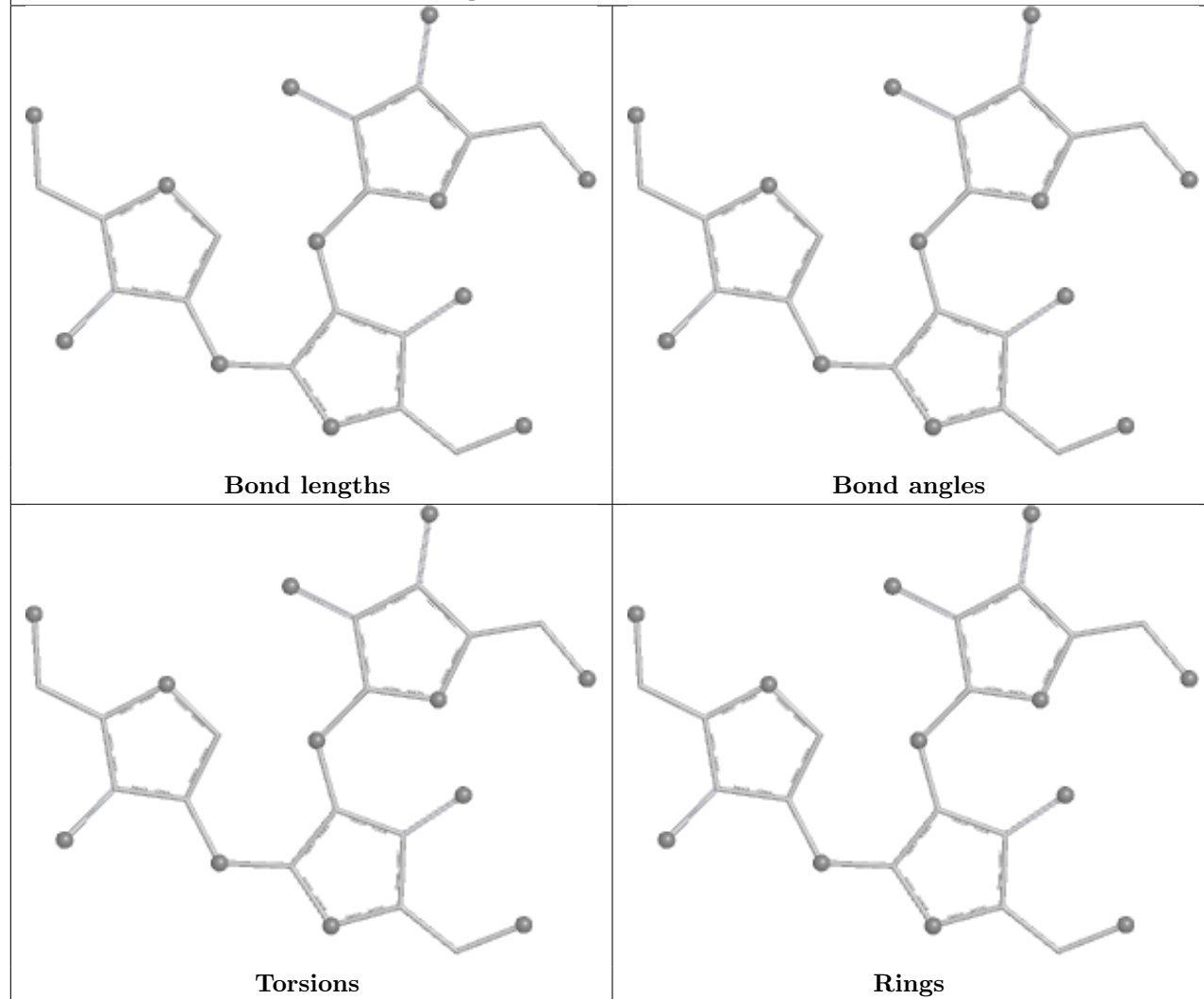


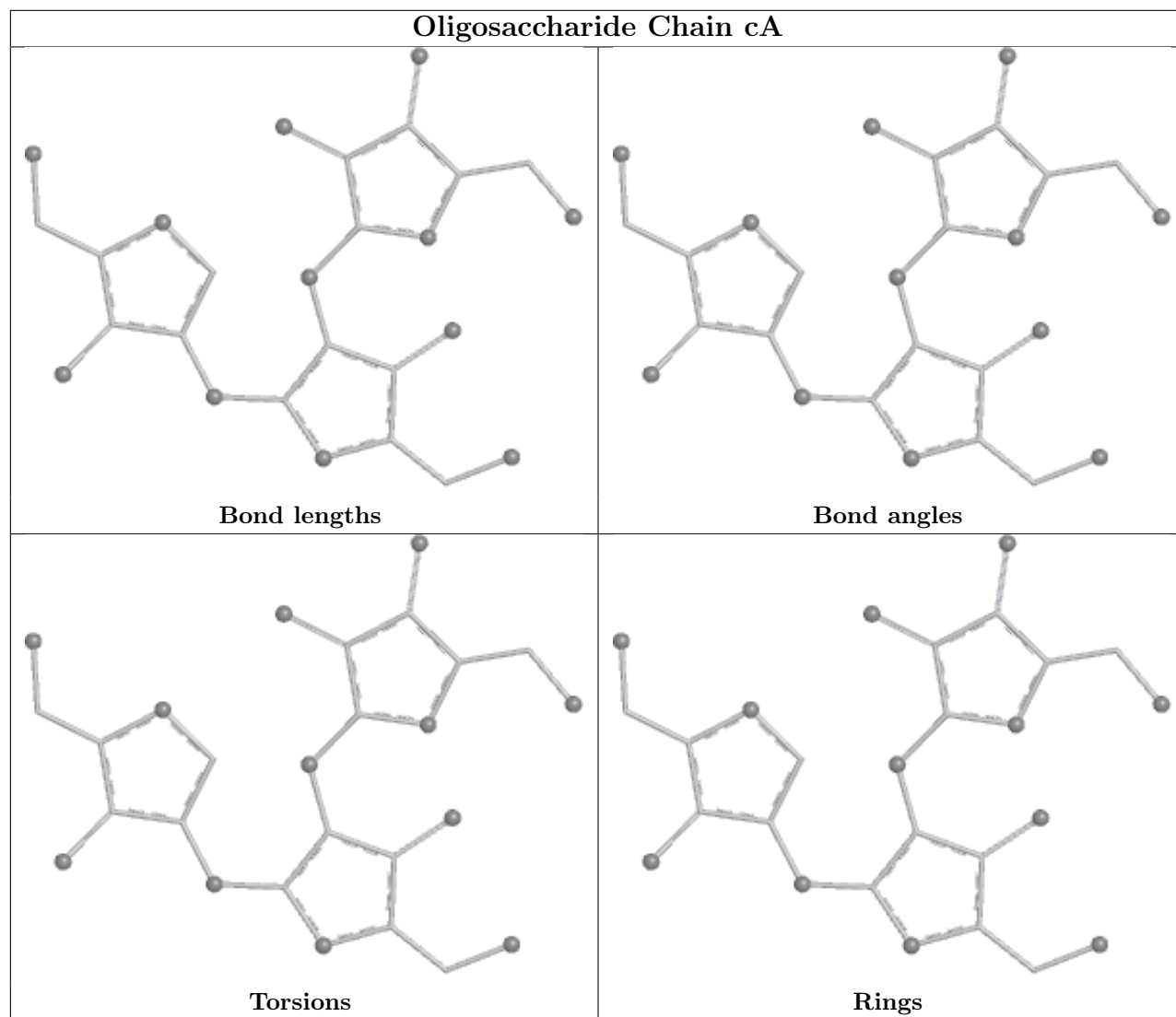


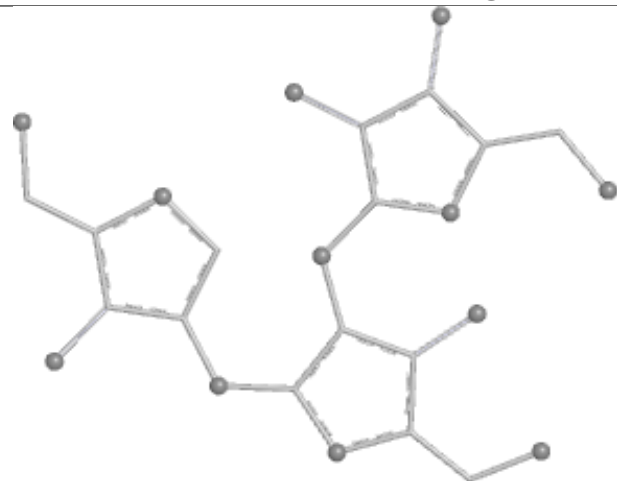
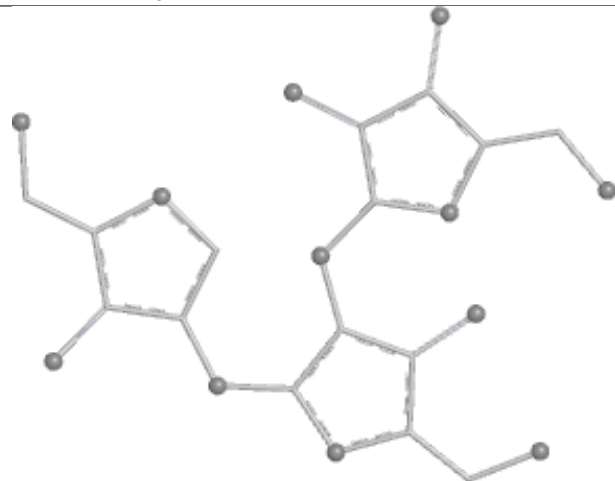
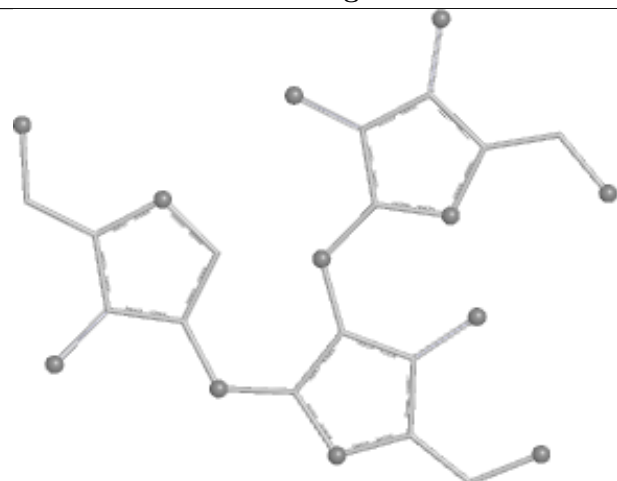
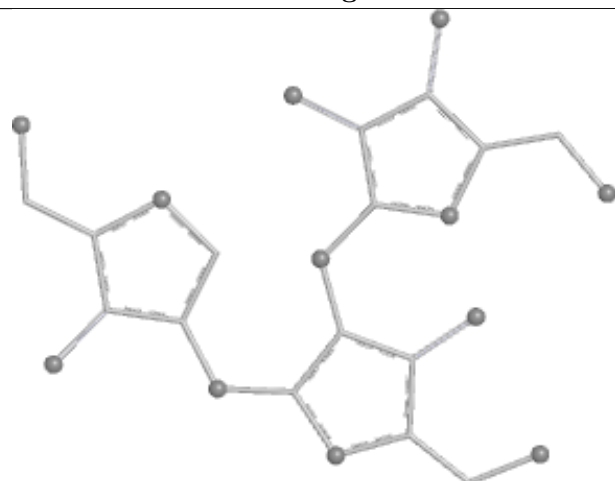


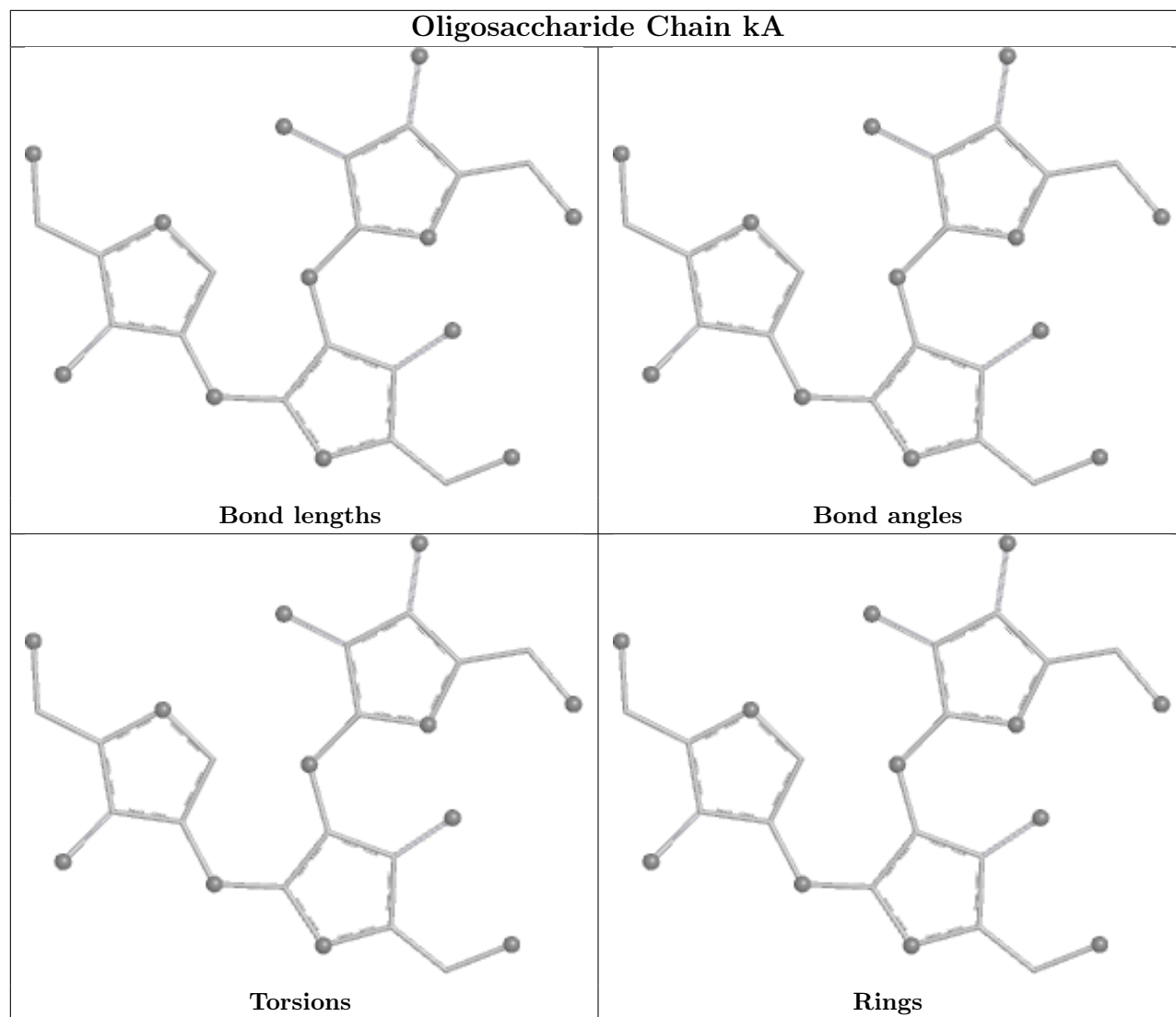


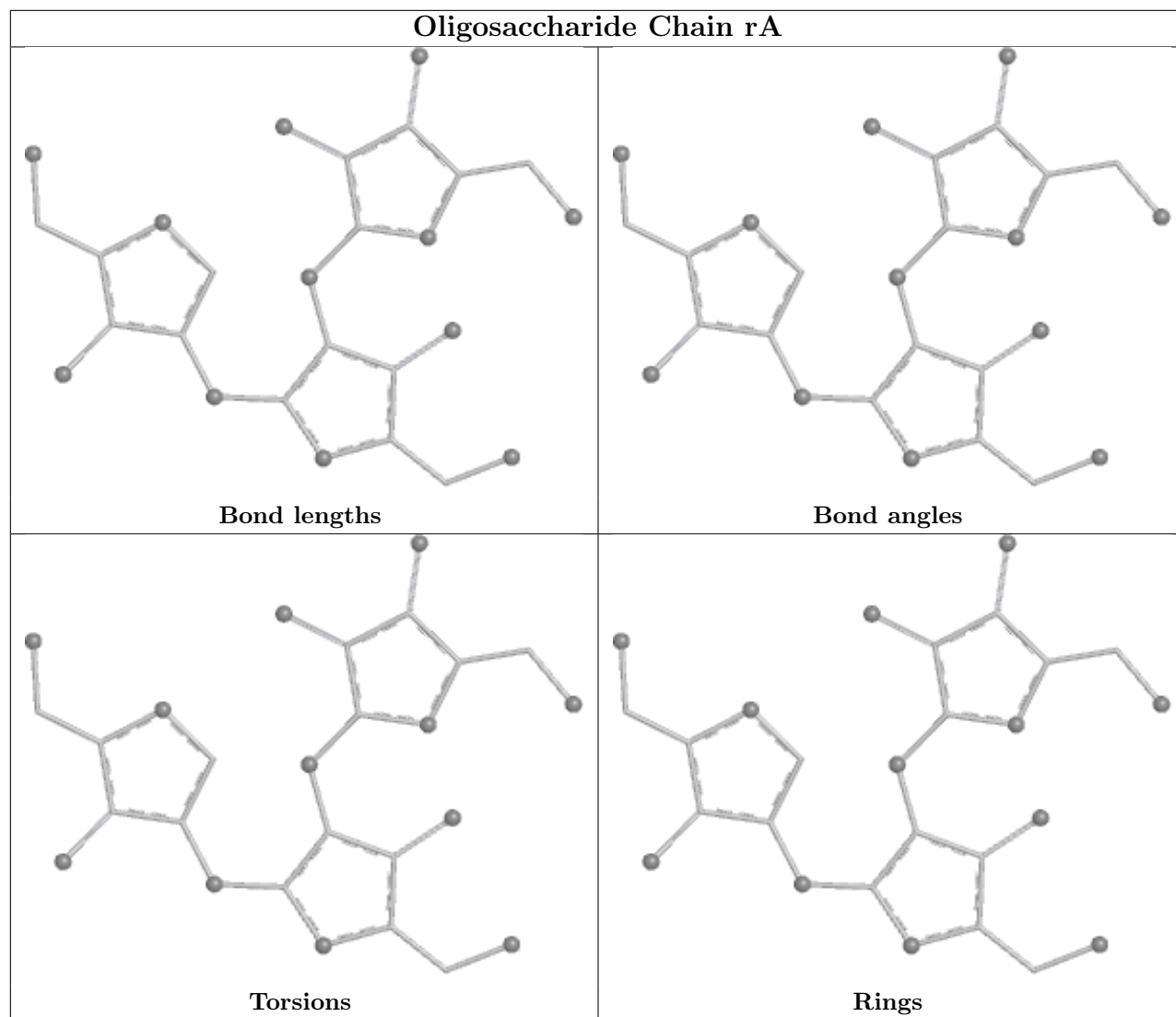
Oligosaccharide Chain XA**Bond lengths****Bond angles****Torsions****Rings**

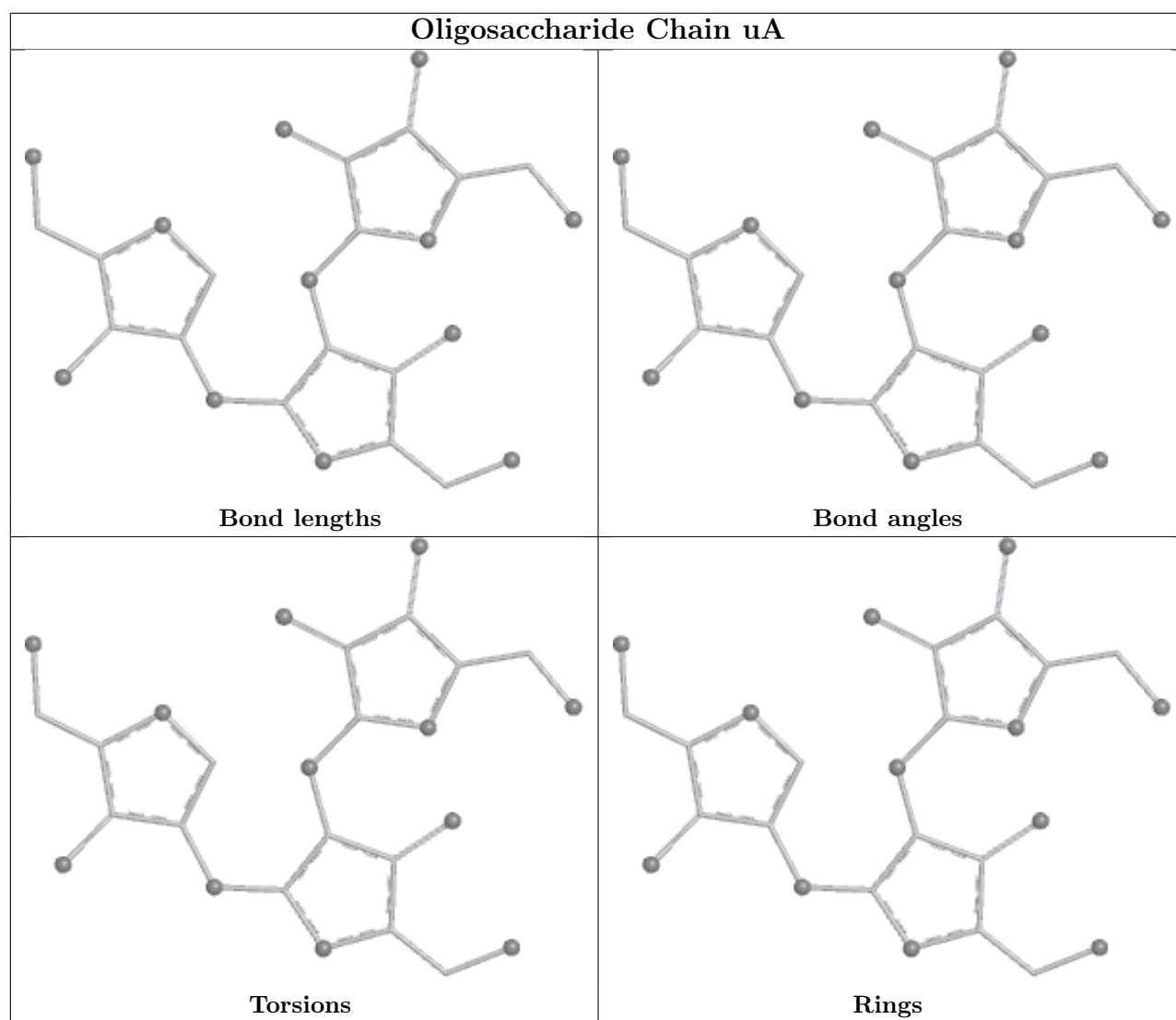
Oligosaccharide Chain ZA

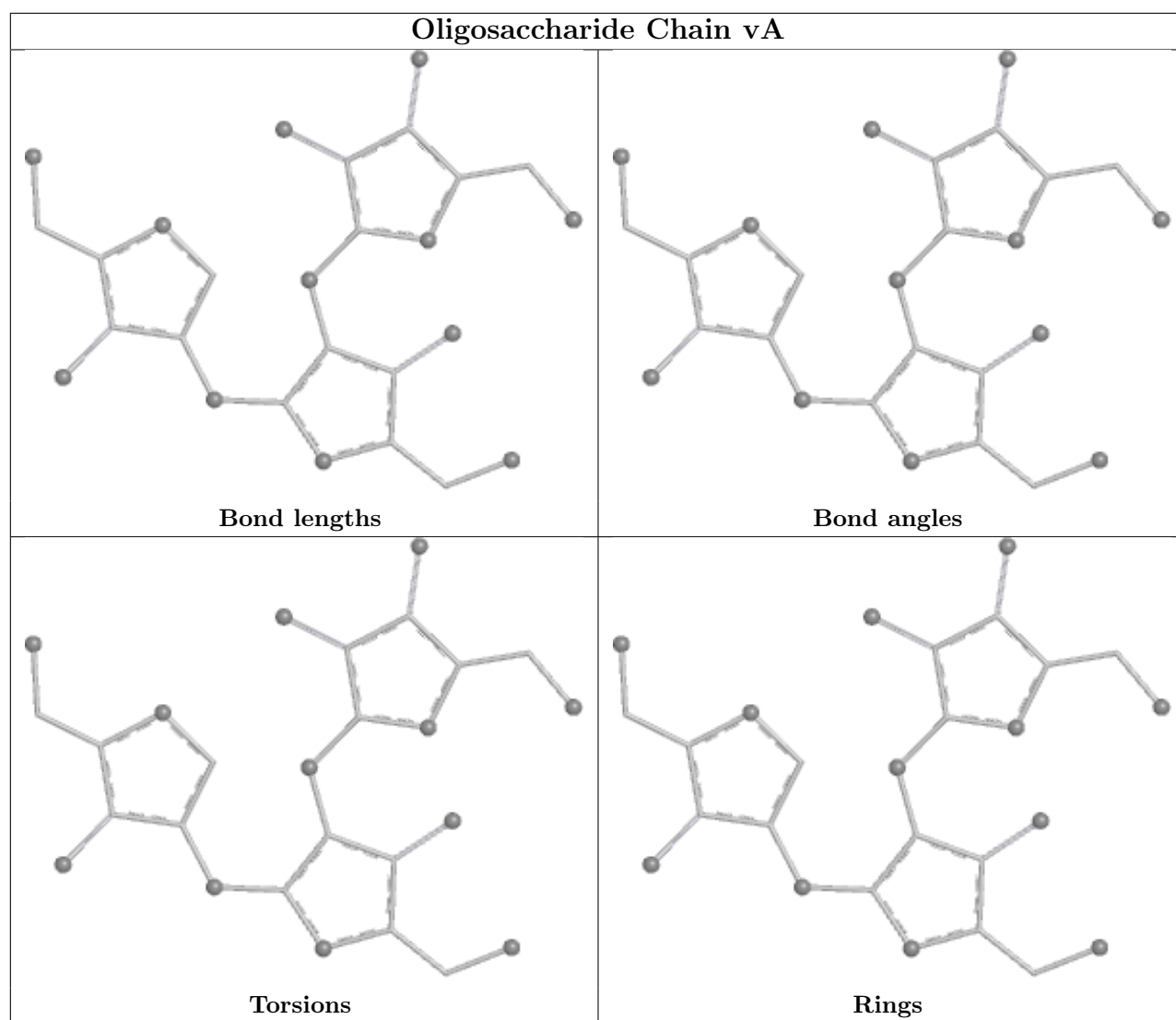


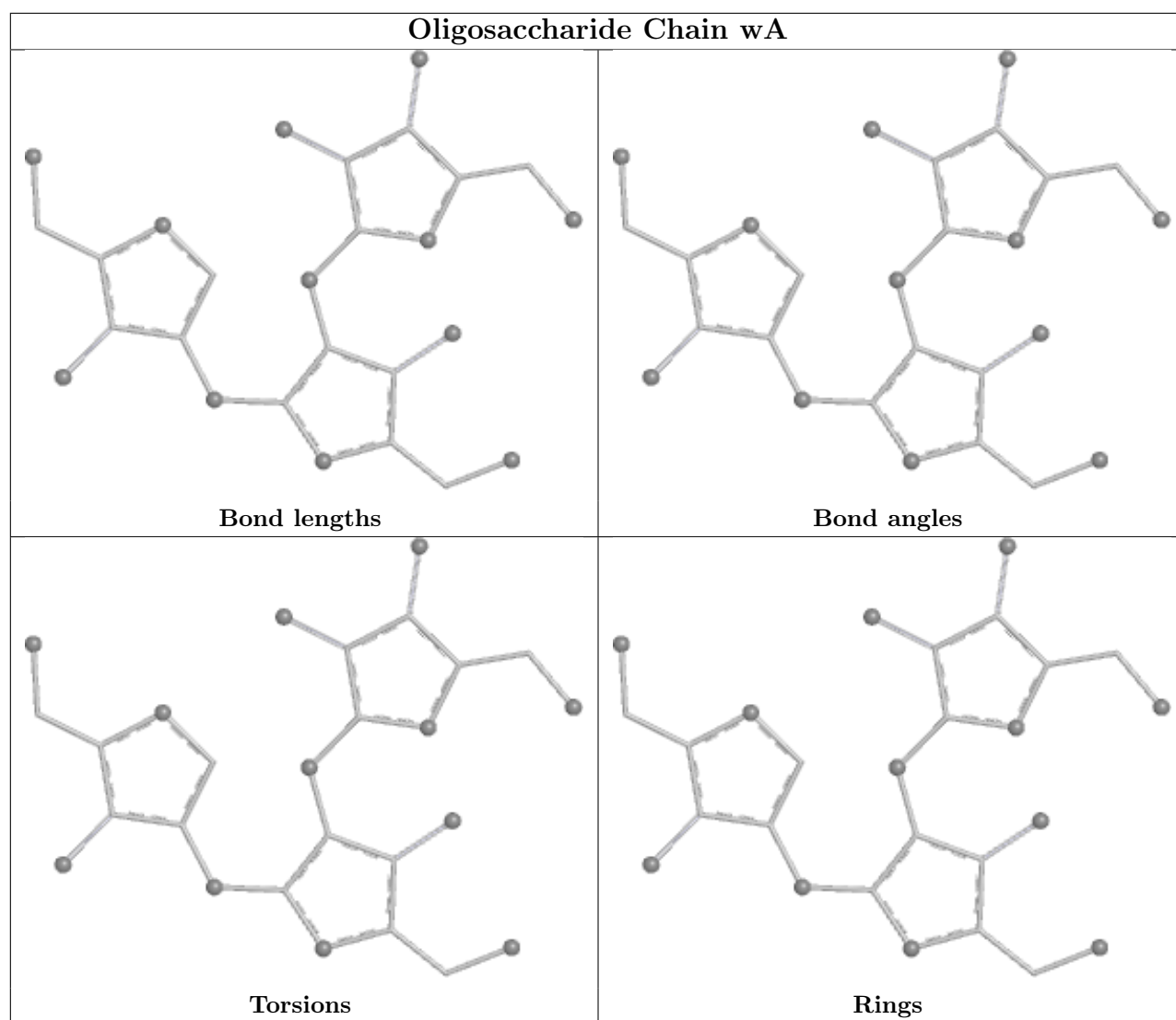
Oligosaccharide Chain jA**Bond lengths****Bond angles****Torsions****Rings**

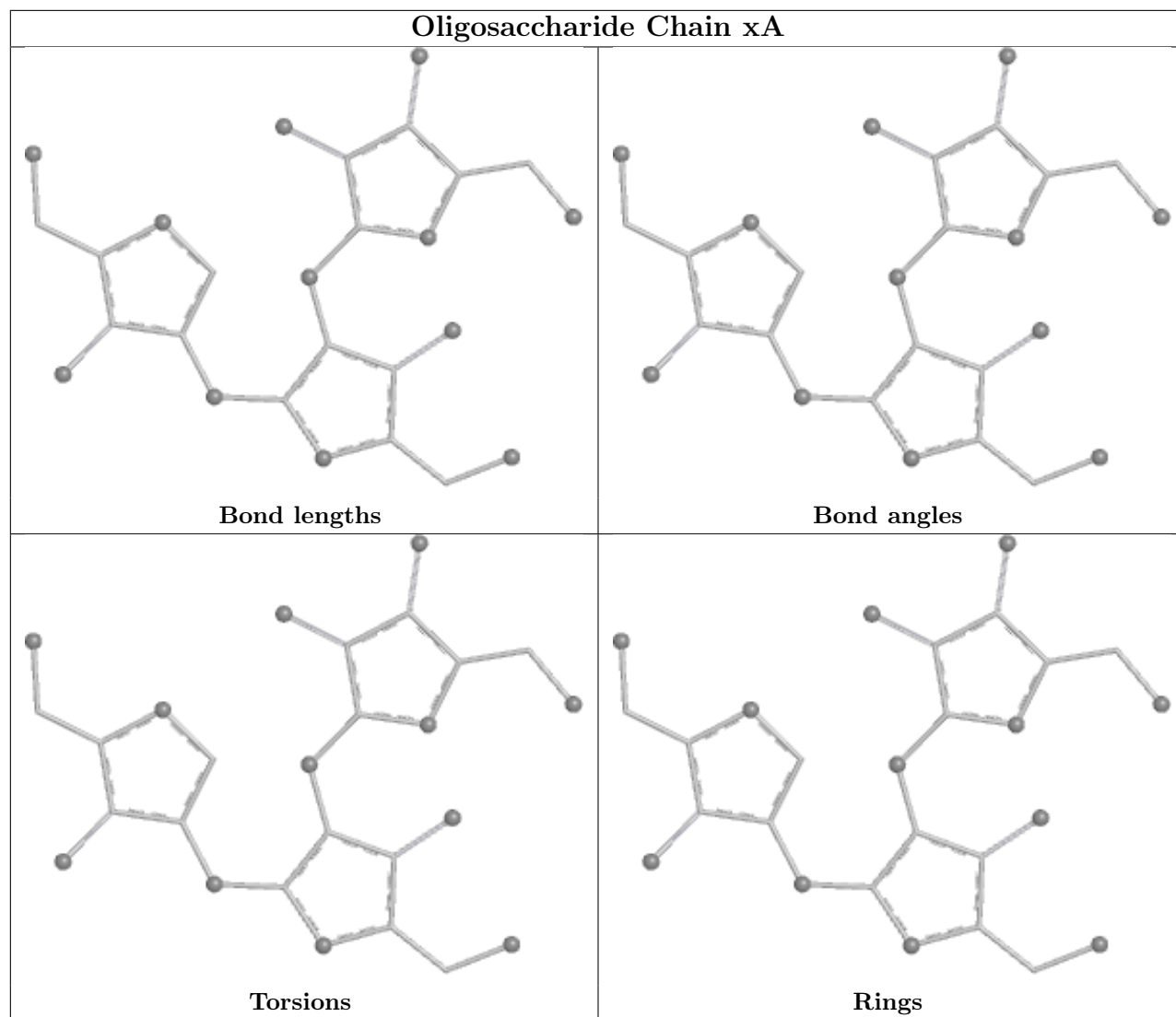


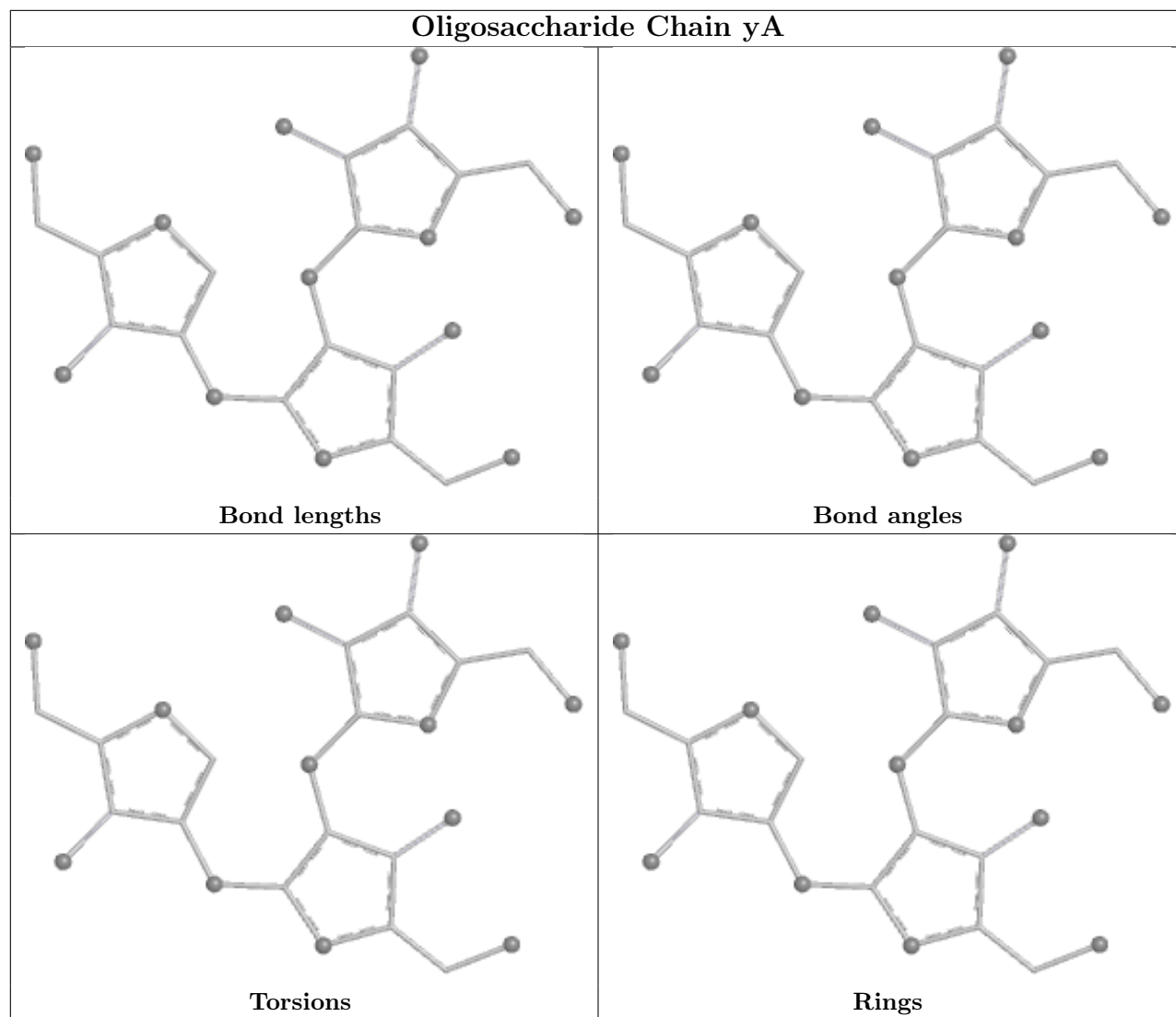


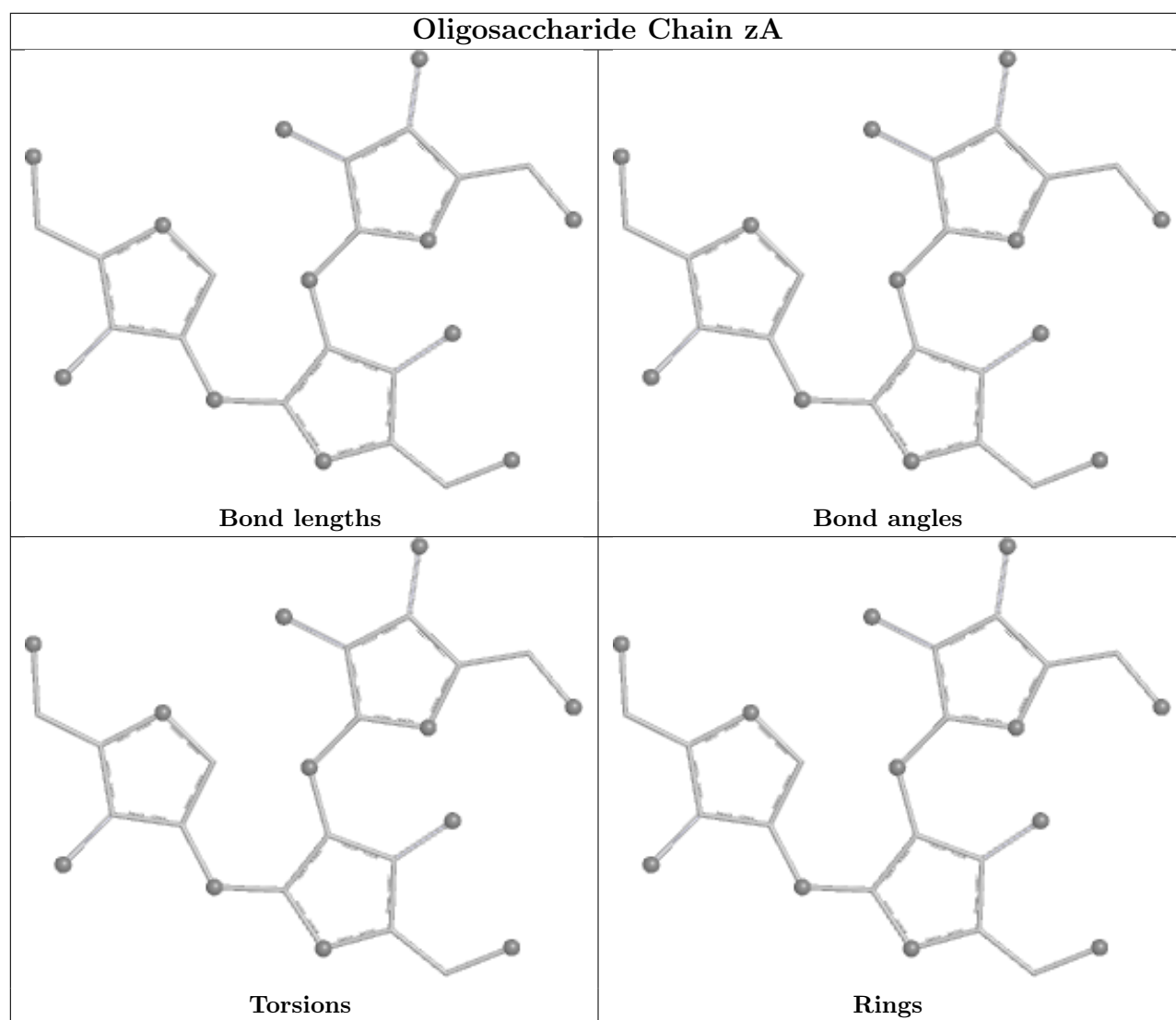




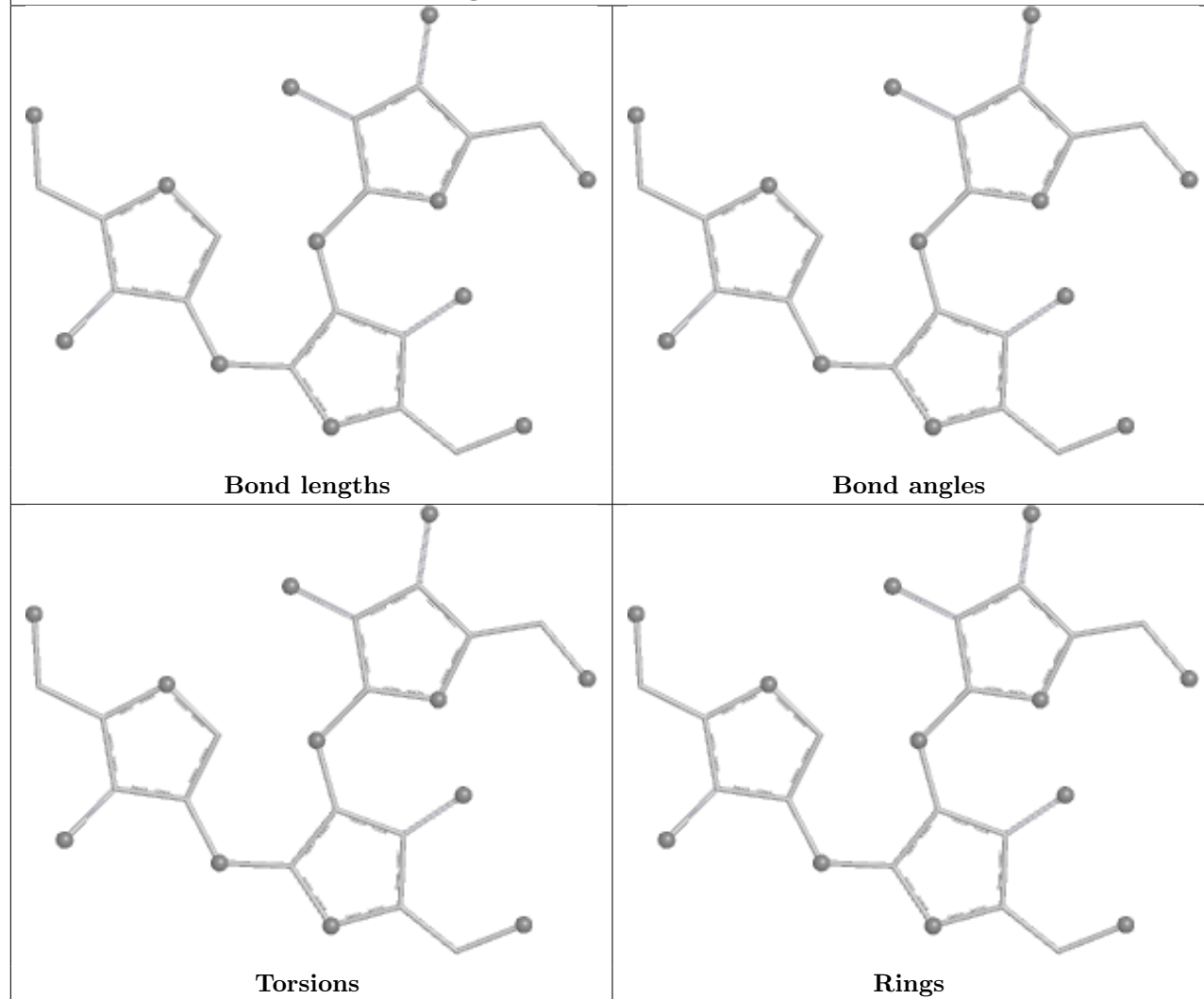


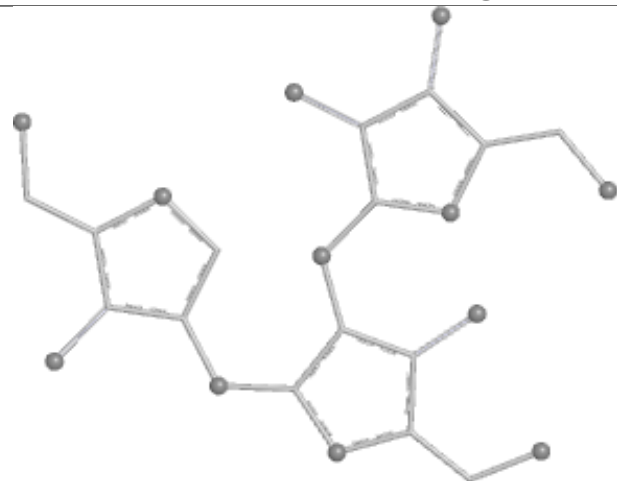
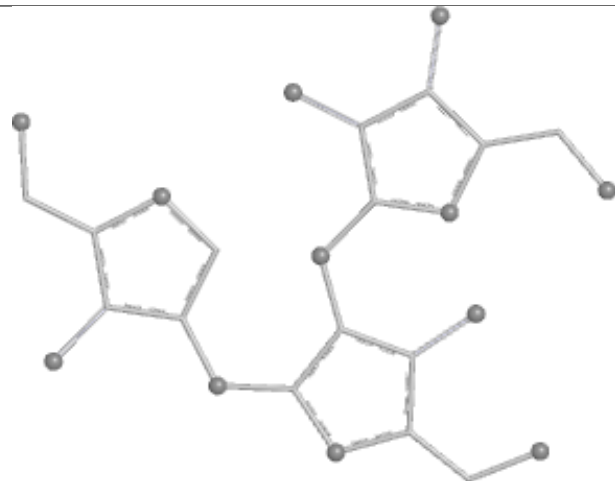
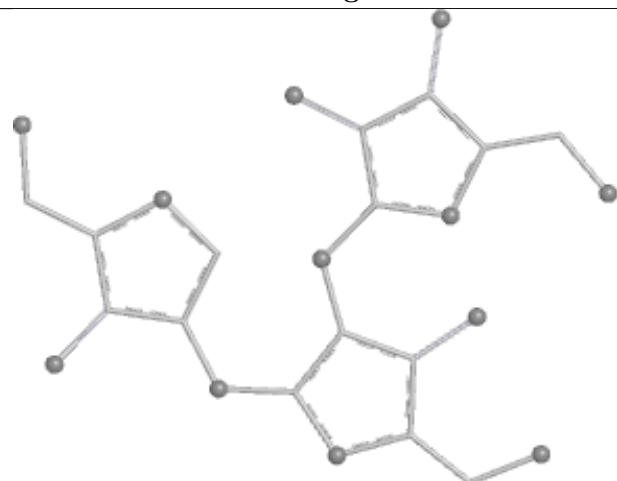
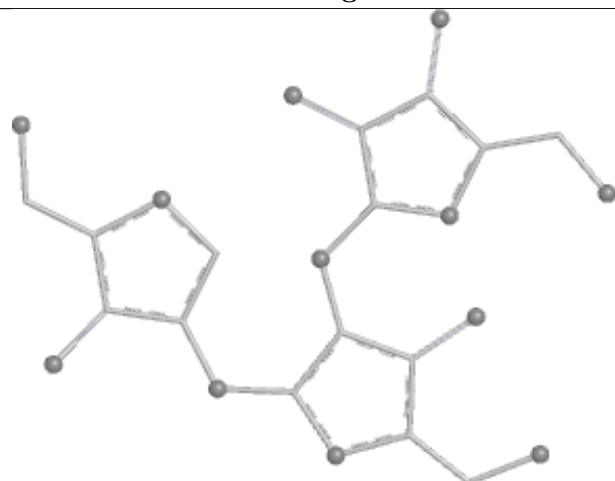


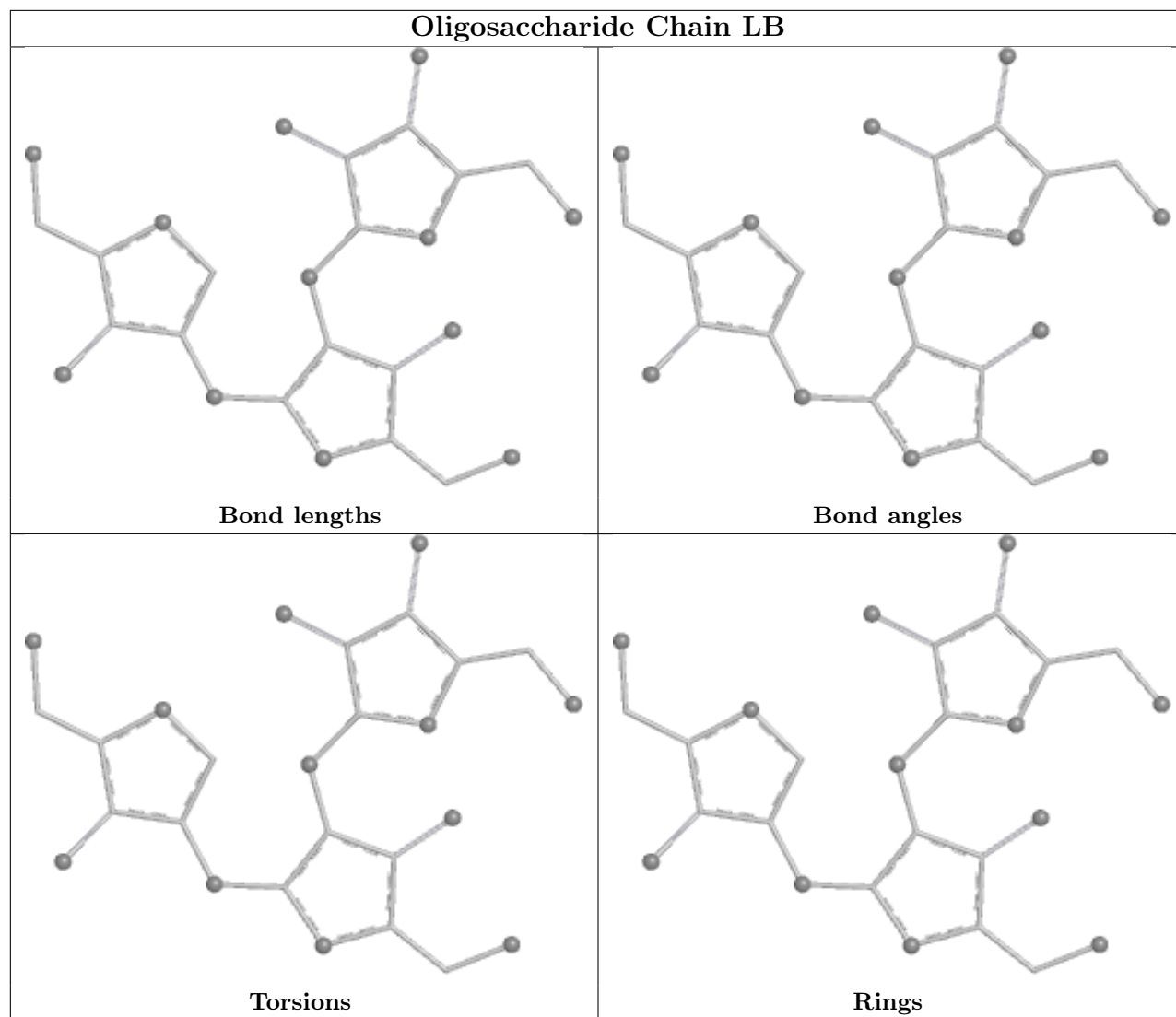


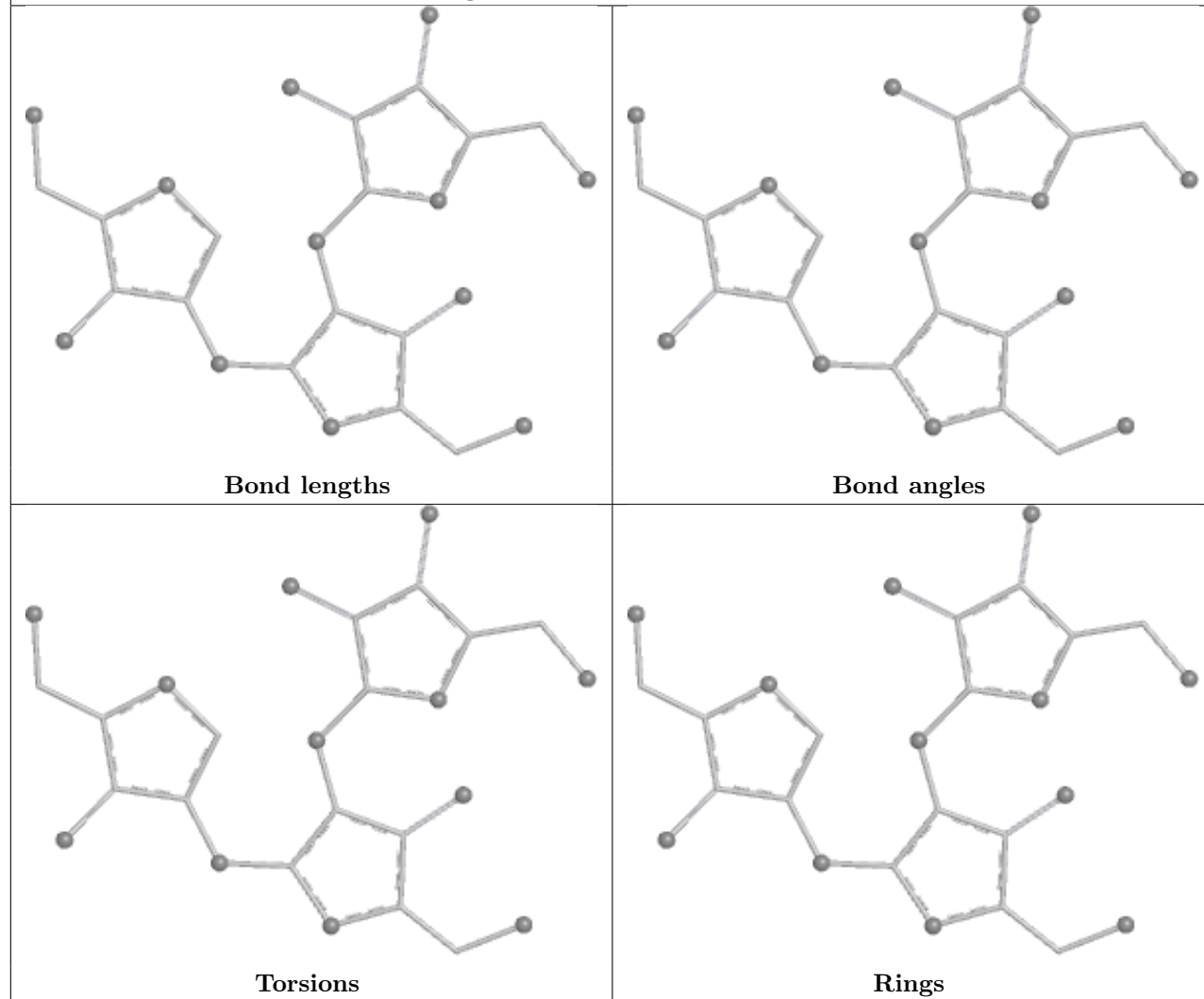


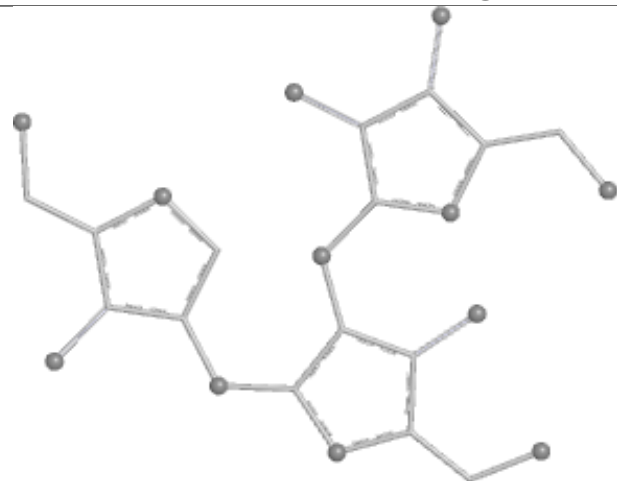
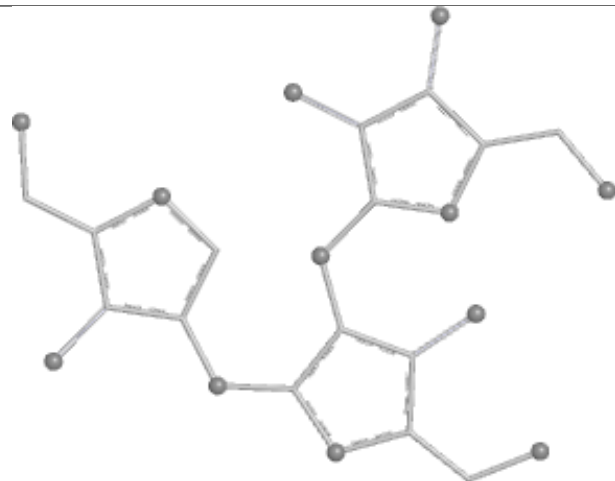
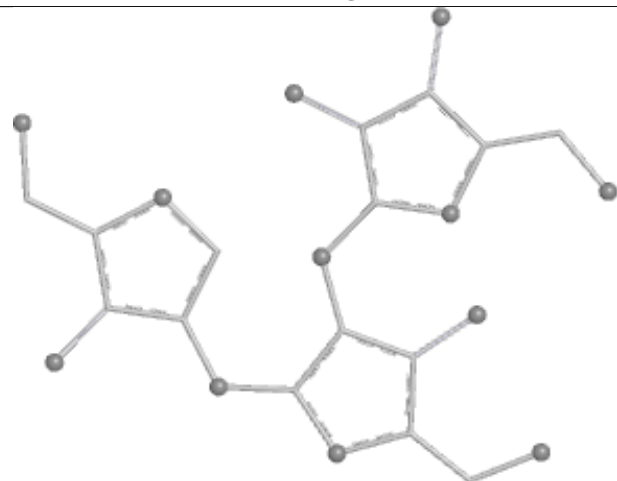
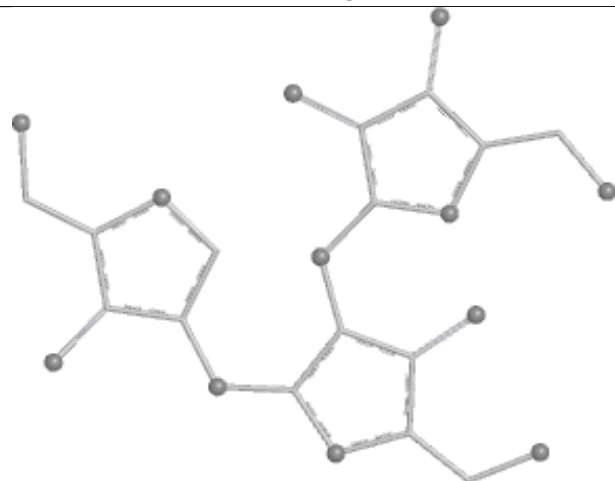
Oligosaccharide Chain 0A

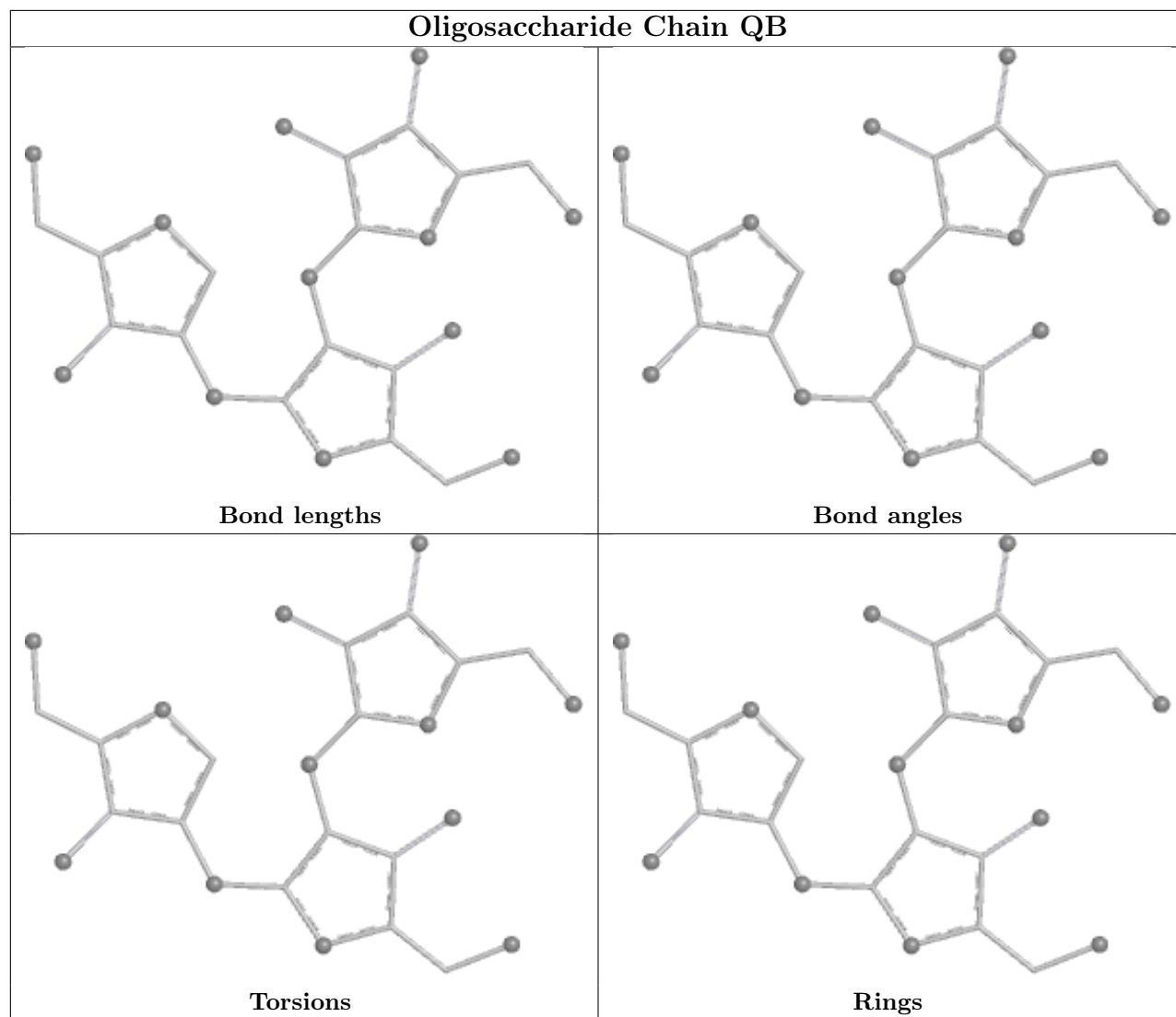


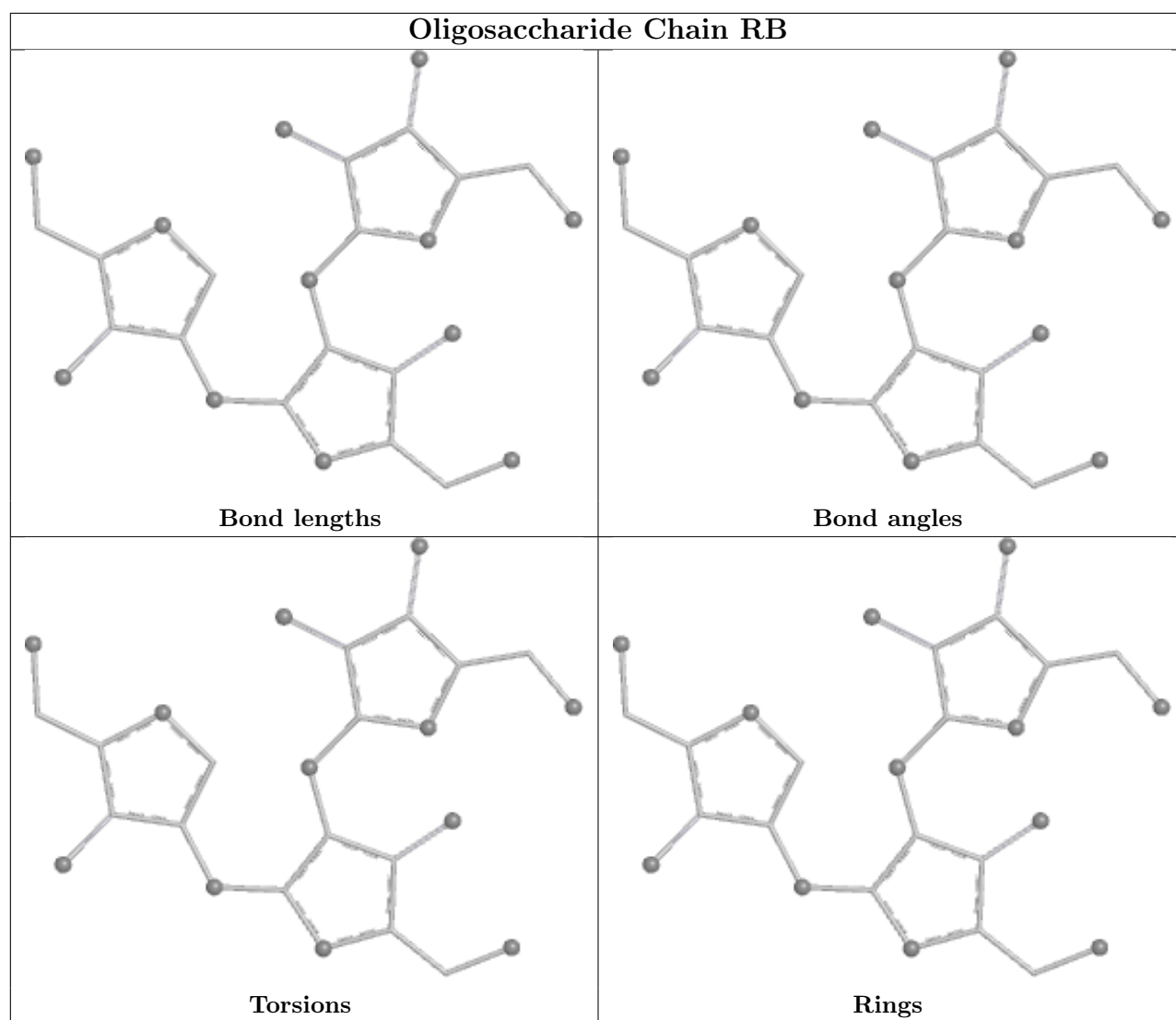
Oligosaccharide Chain EB**Bond lengths****Bond angles****Torsions****Rings**

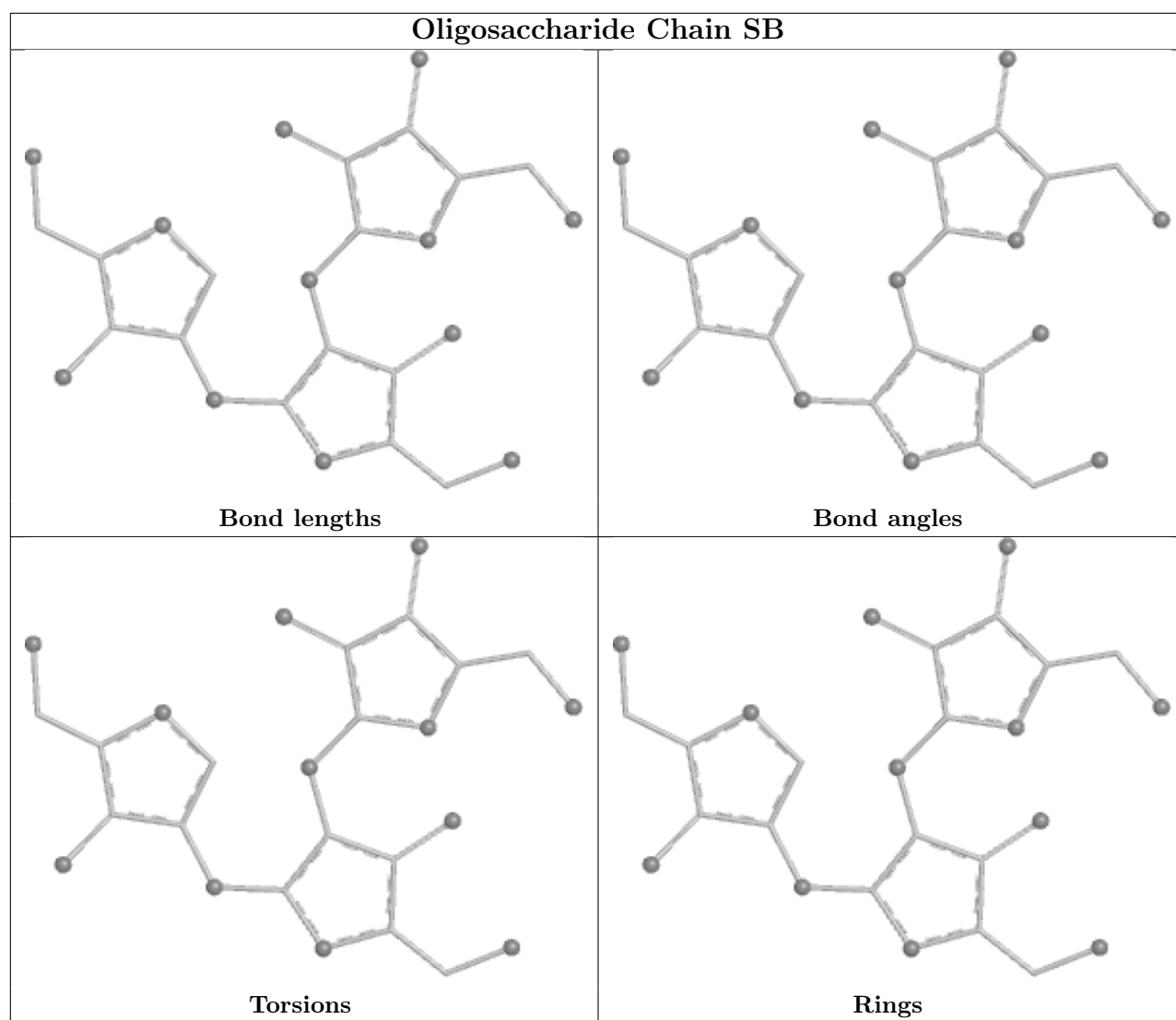


Oligosaccharide Chain OB

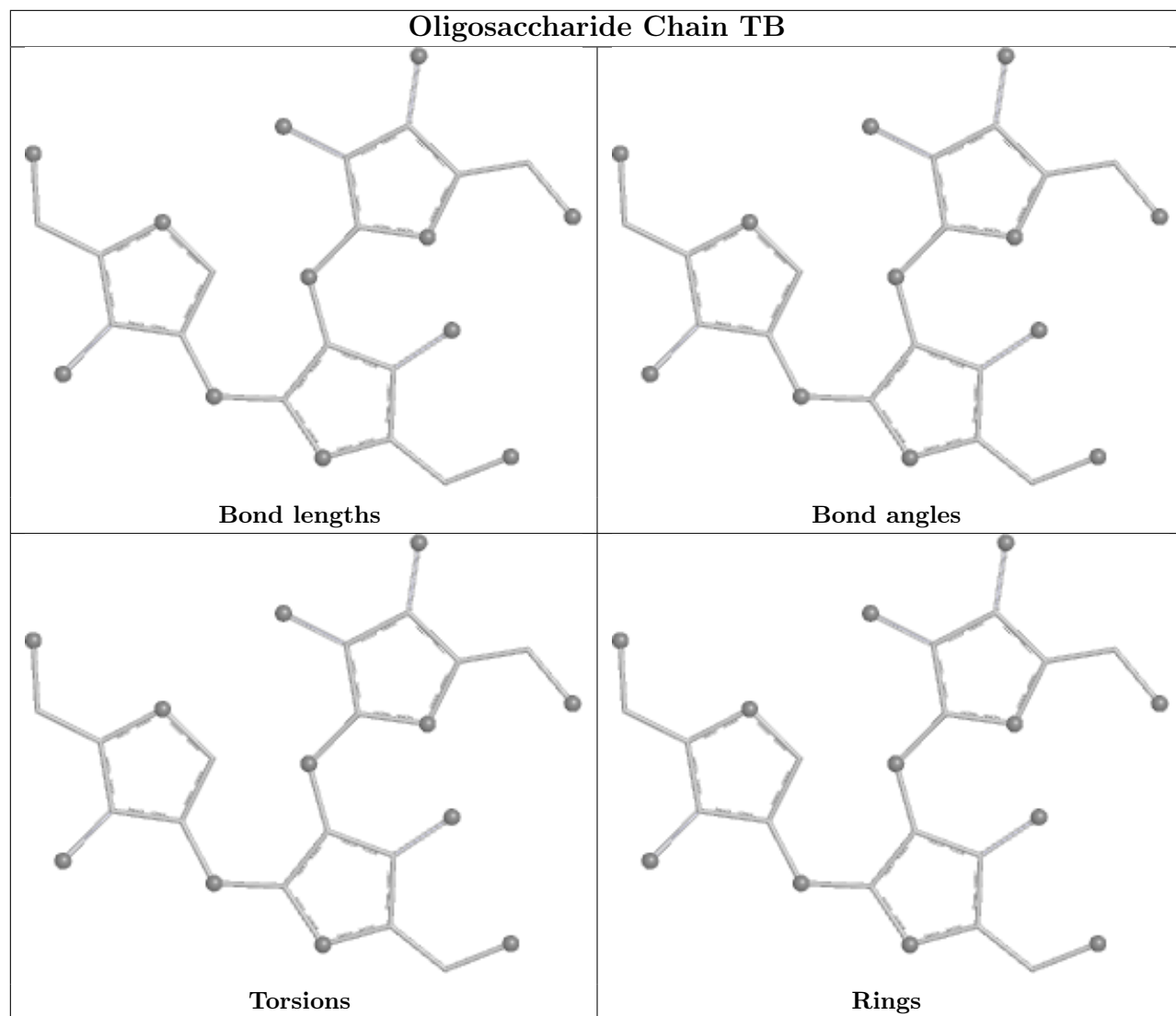
Oligosaccharide Chain PB**Bond lengths****Bond angles****Torsions****Rings**

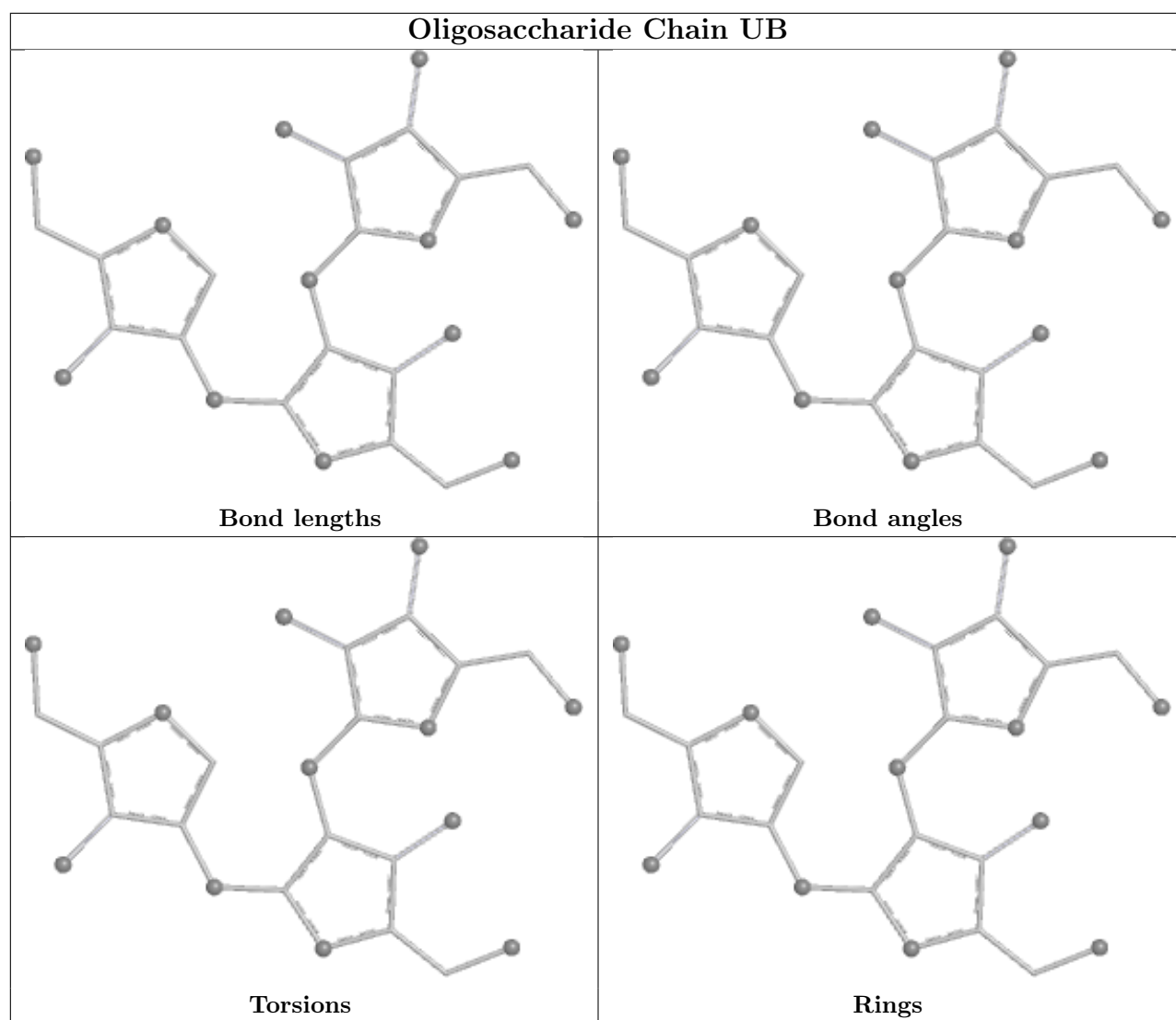


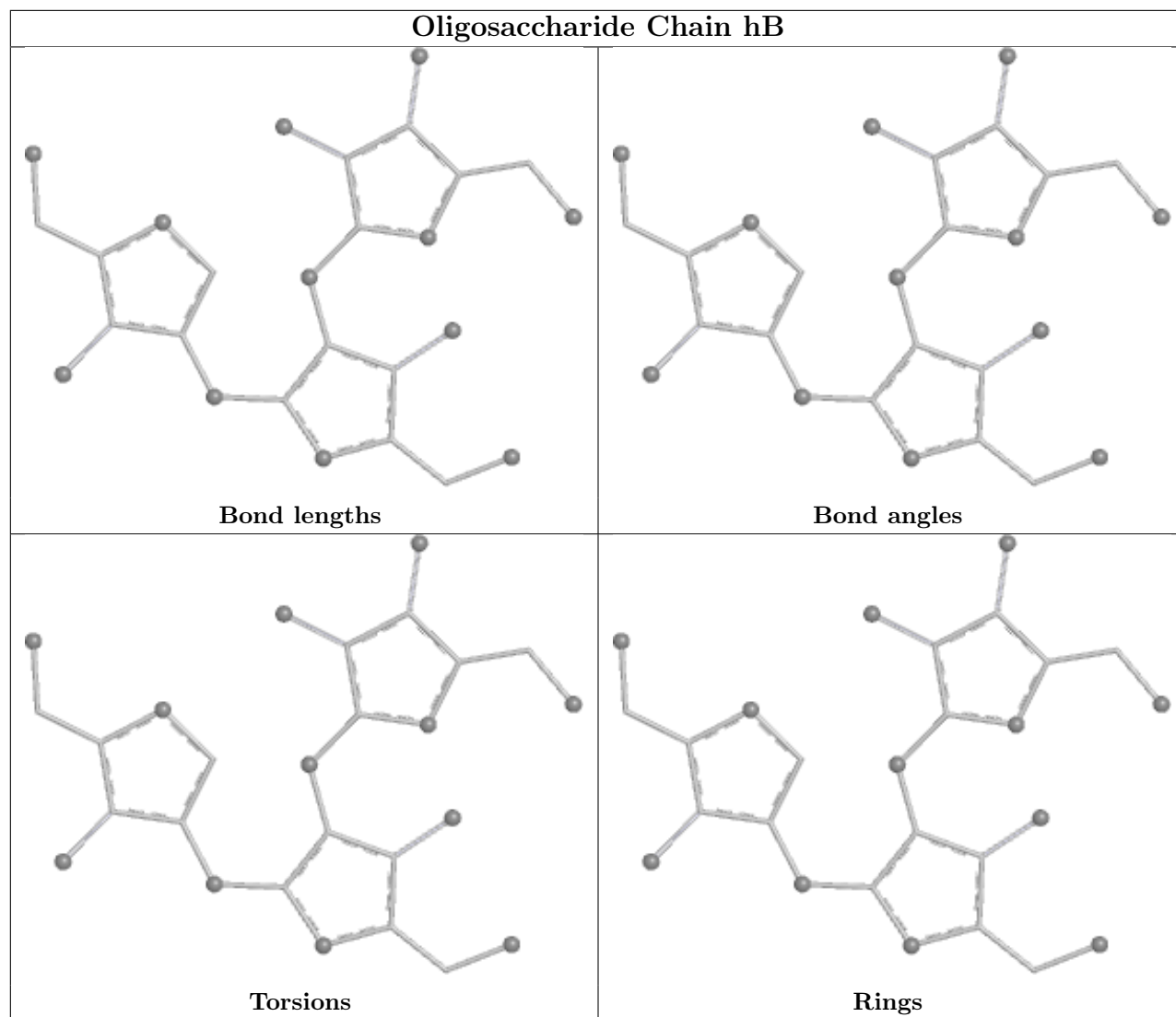


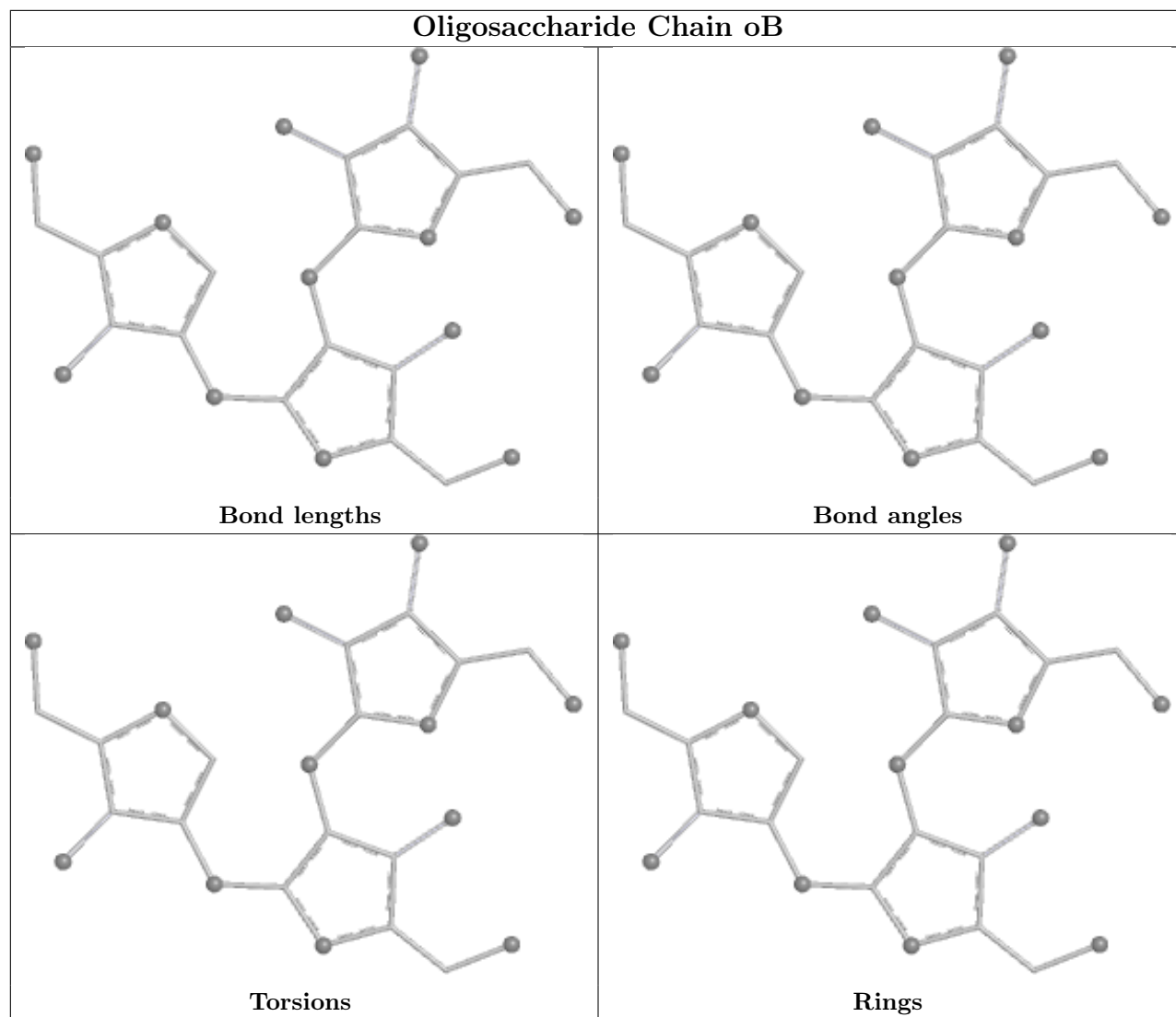


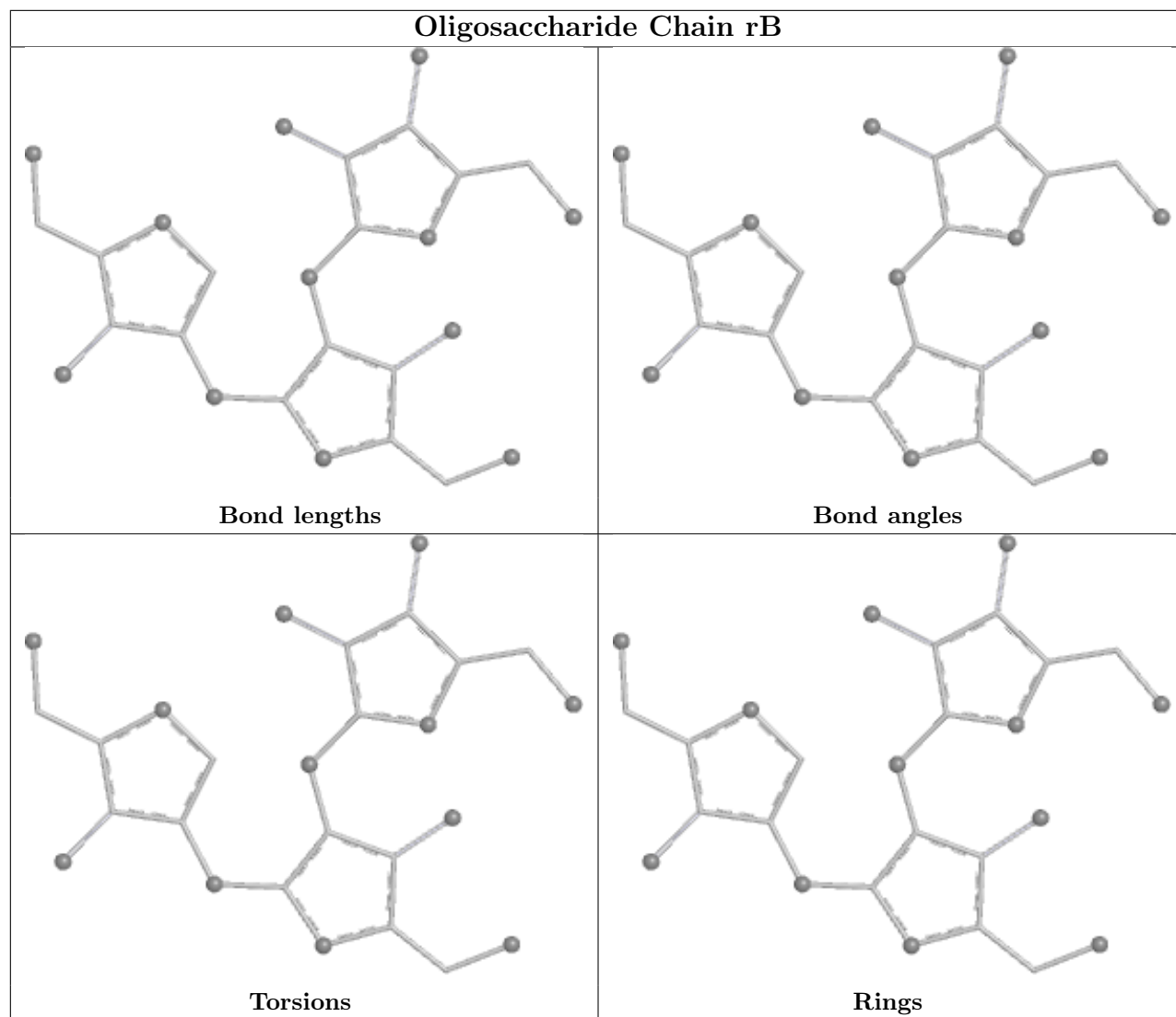
Oligosaccharide Chain TB

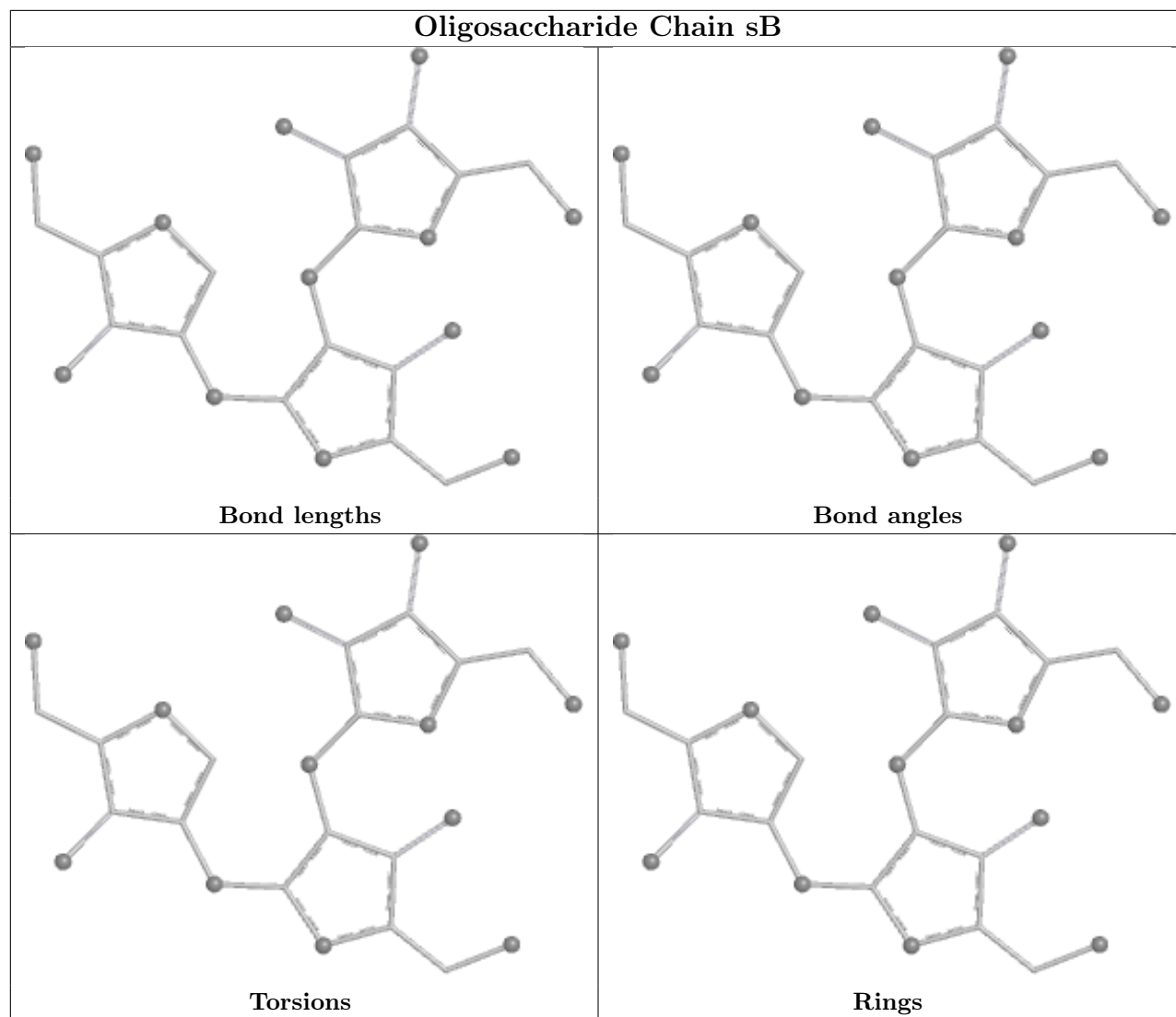


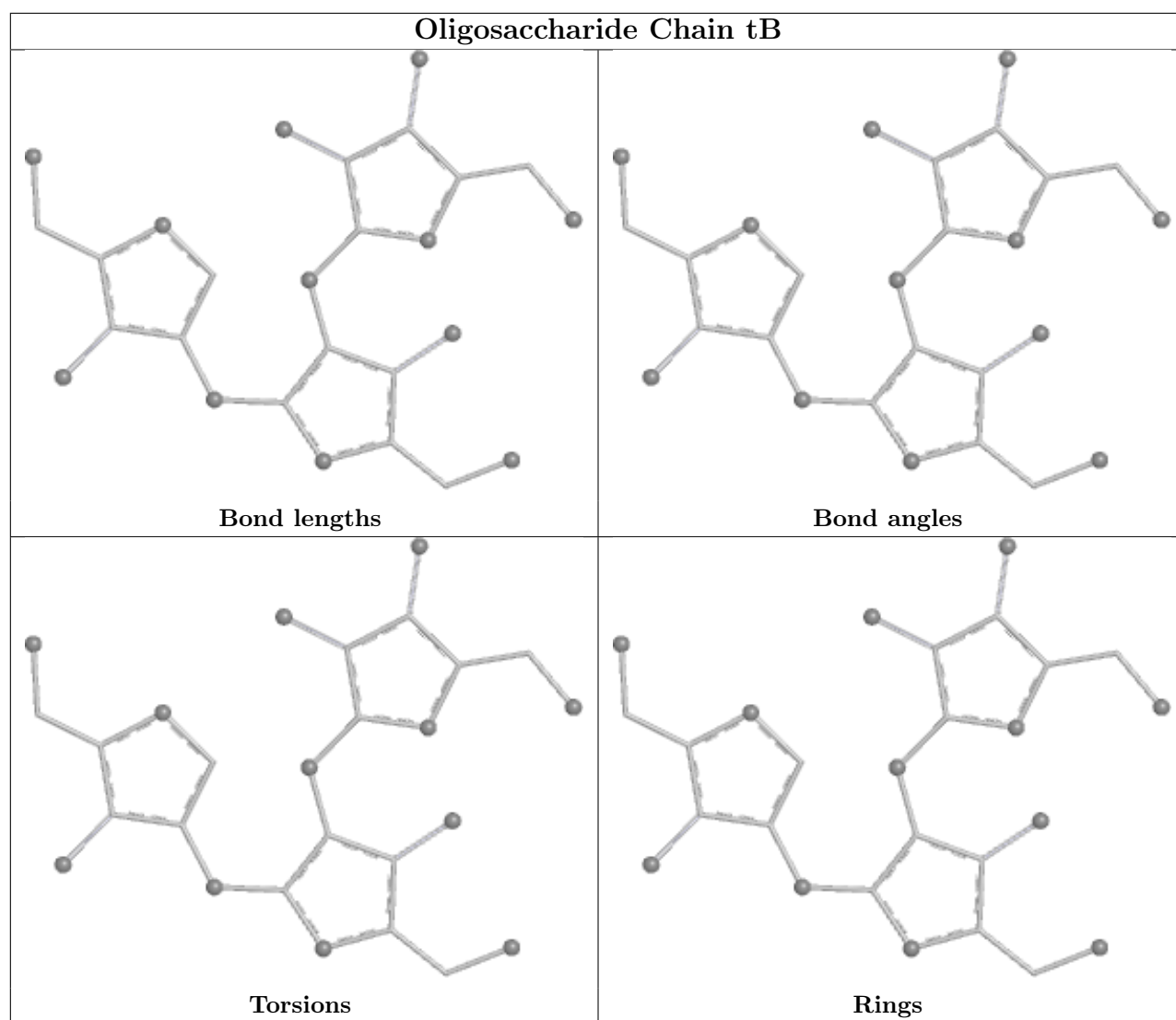


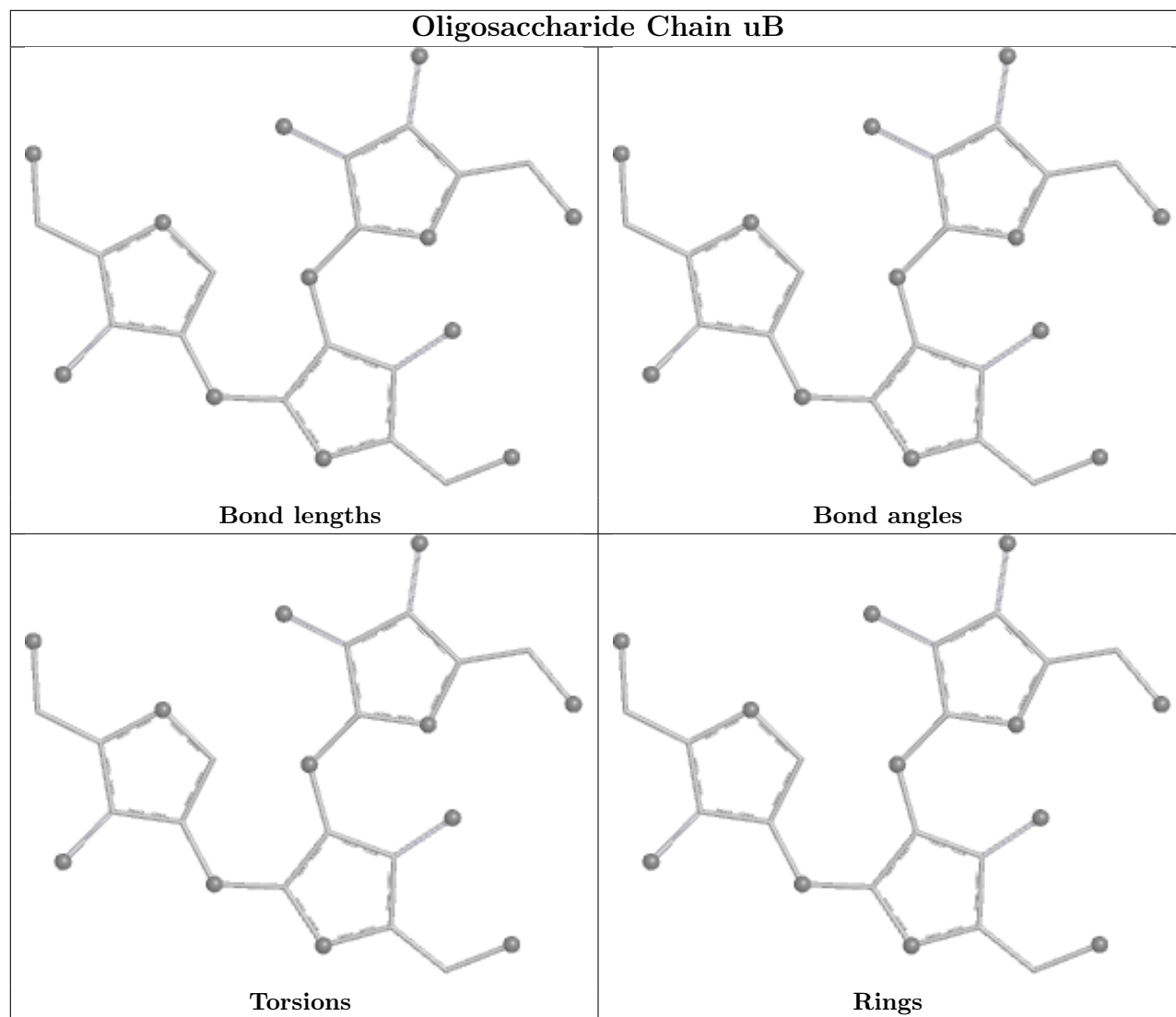


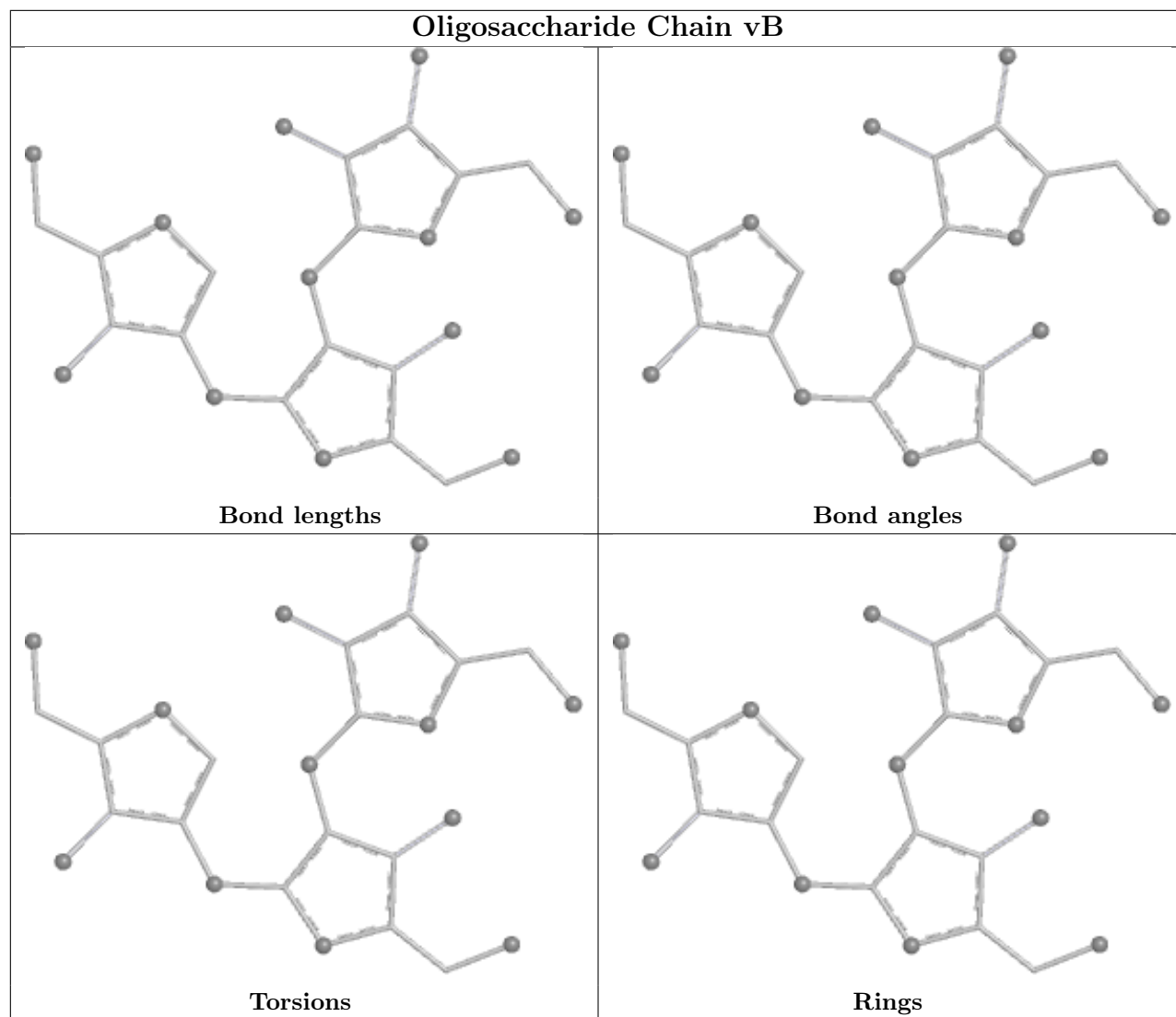


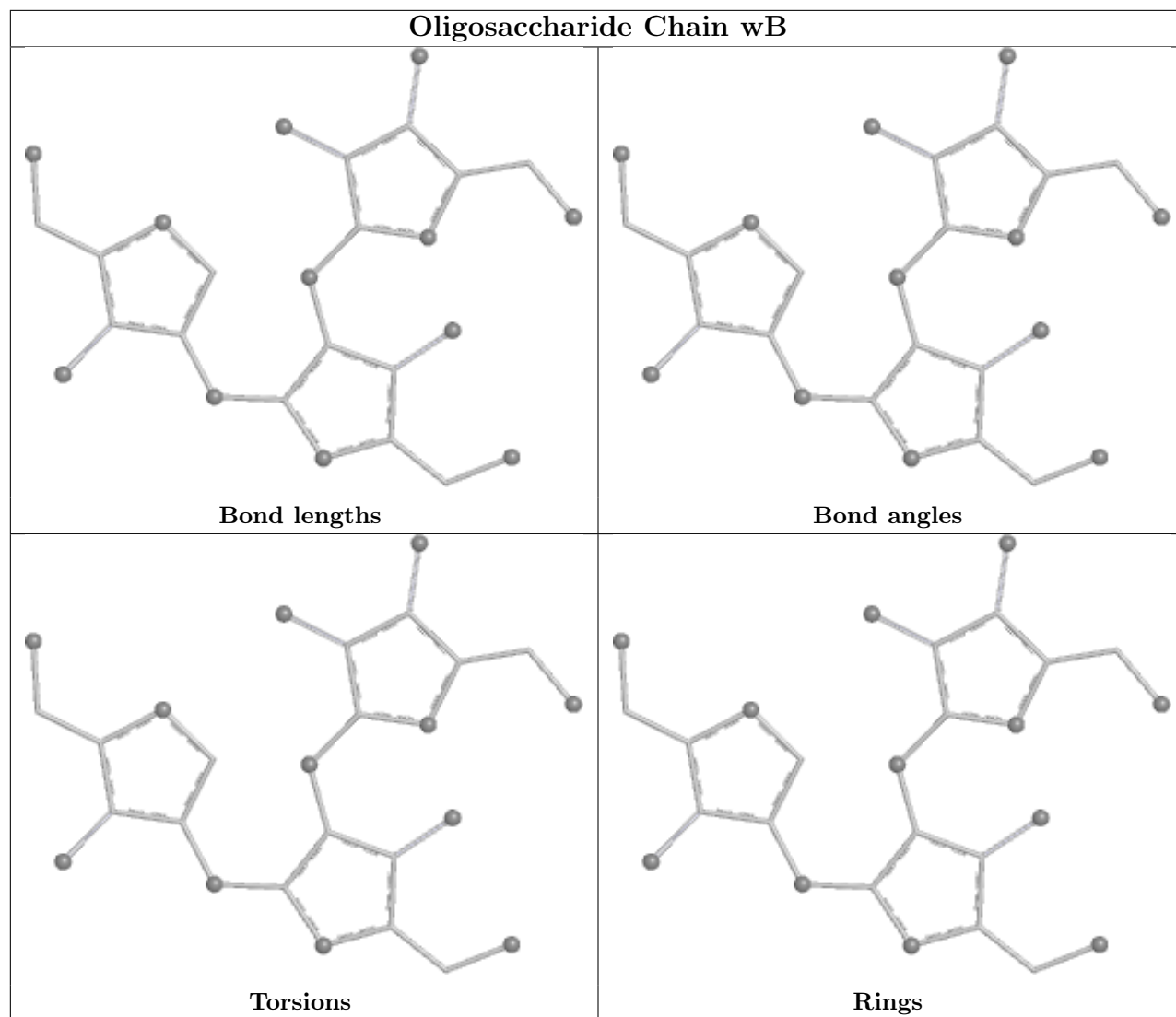


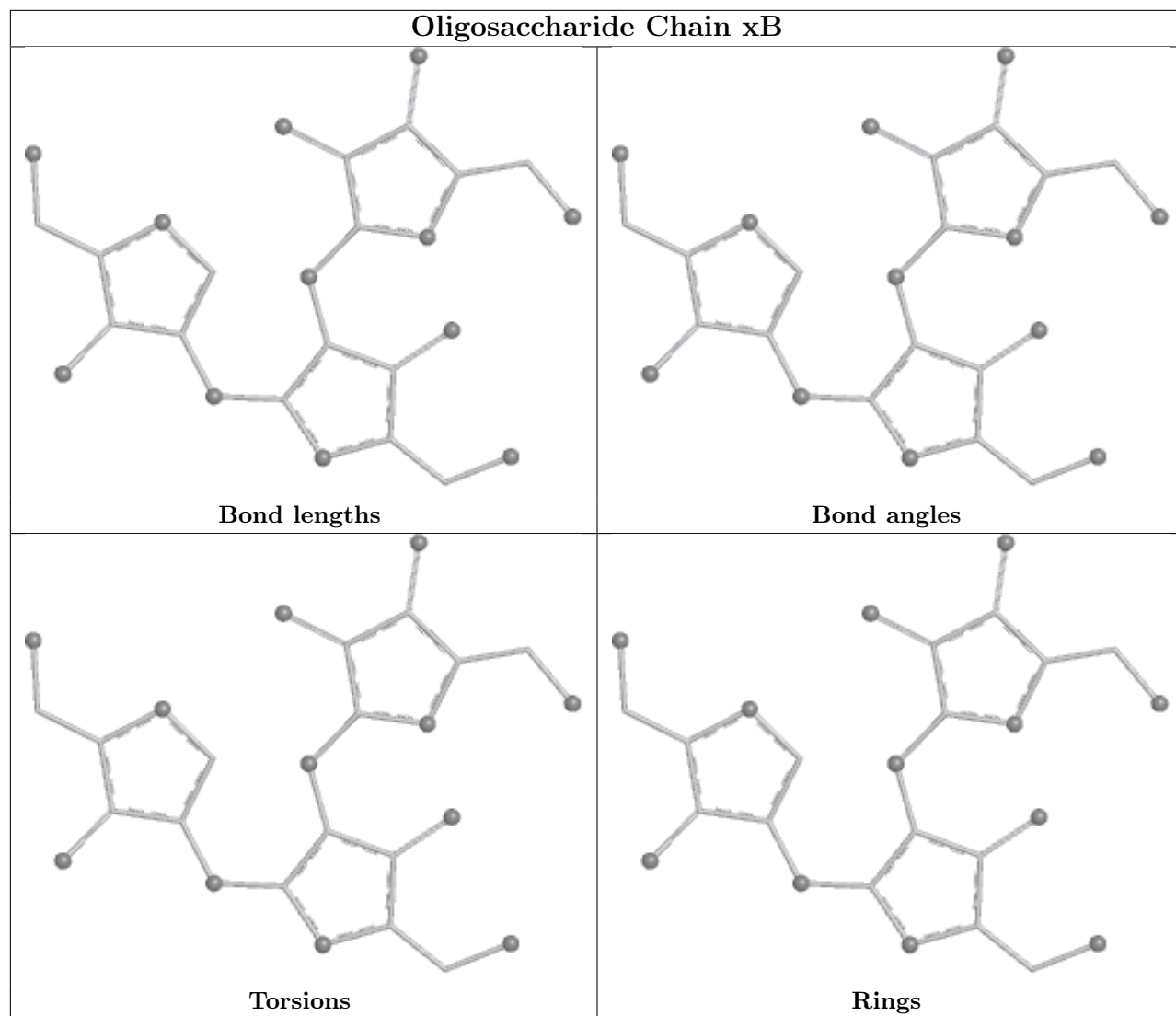


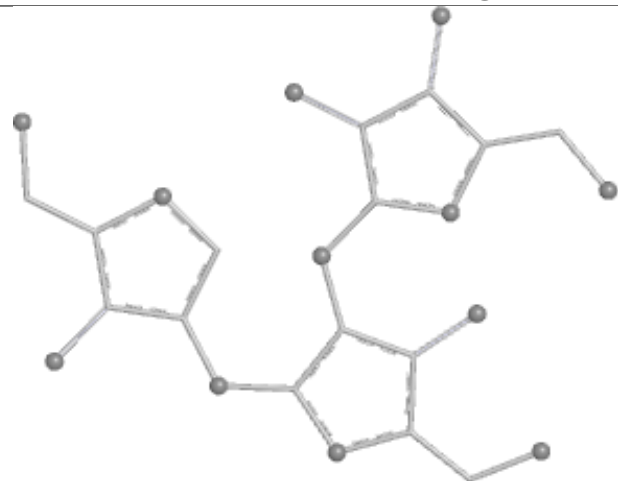
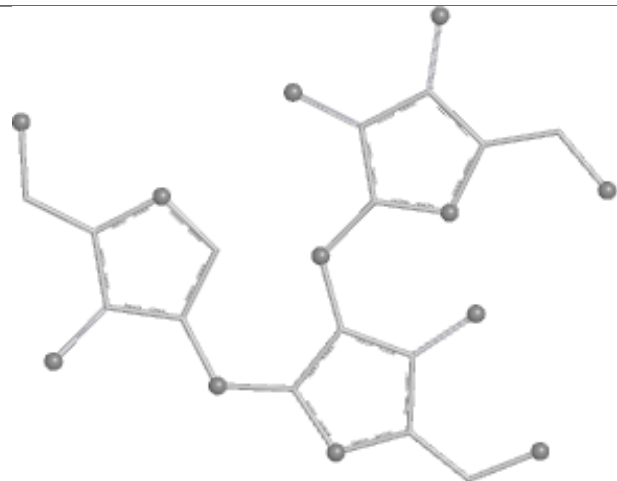
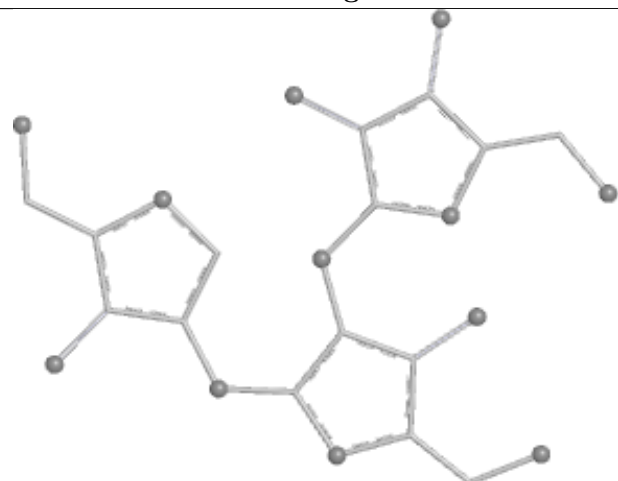
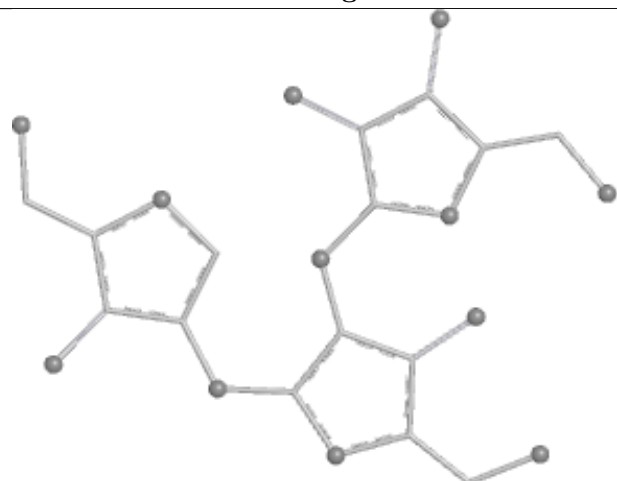


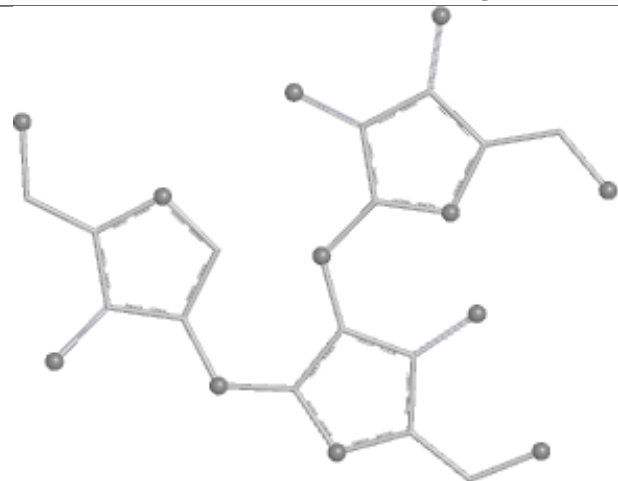
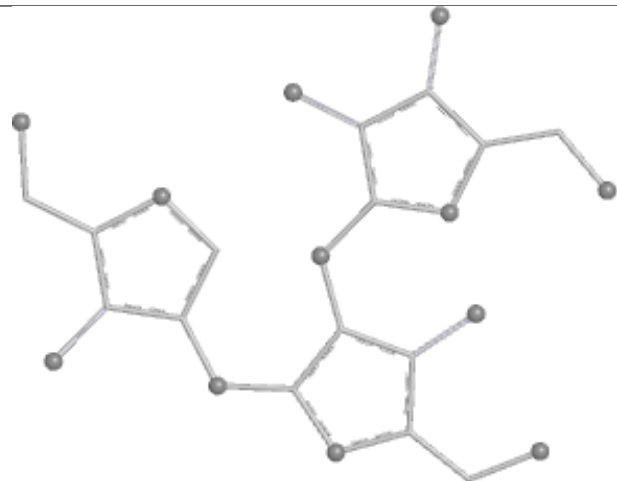
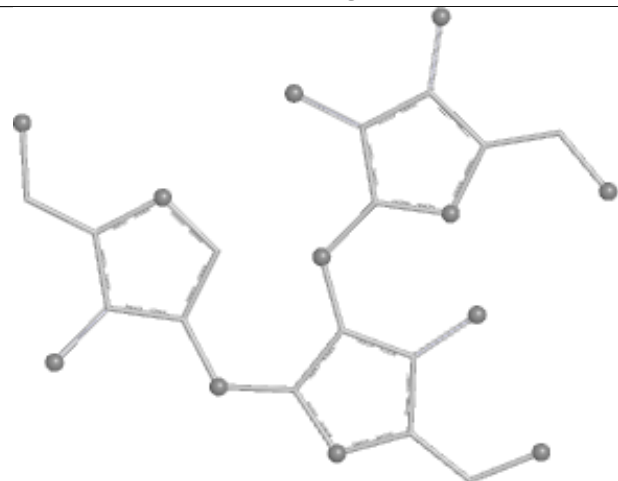
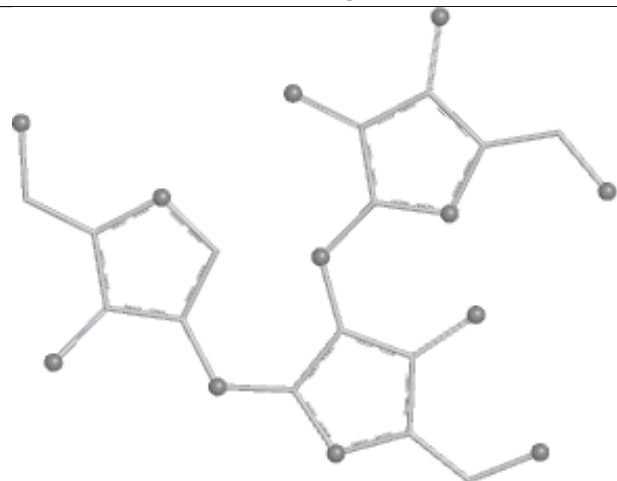


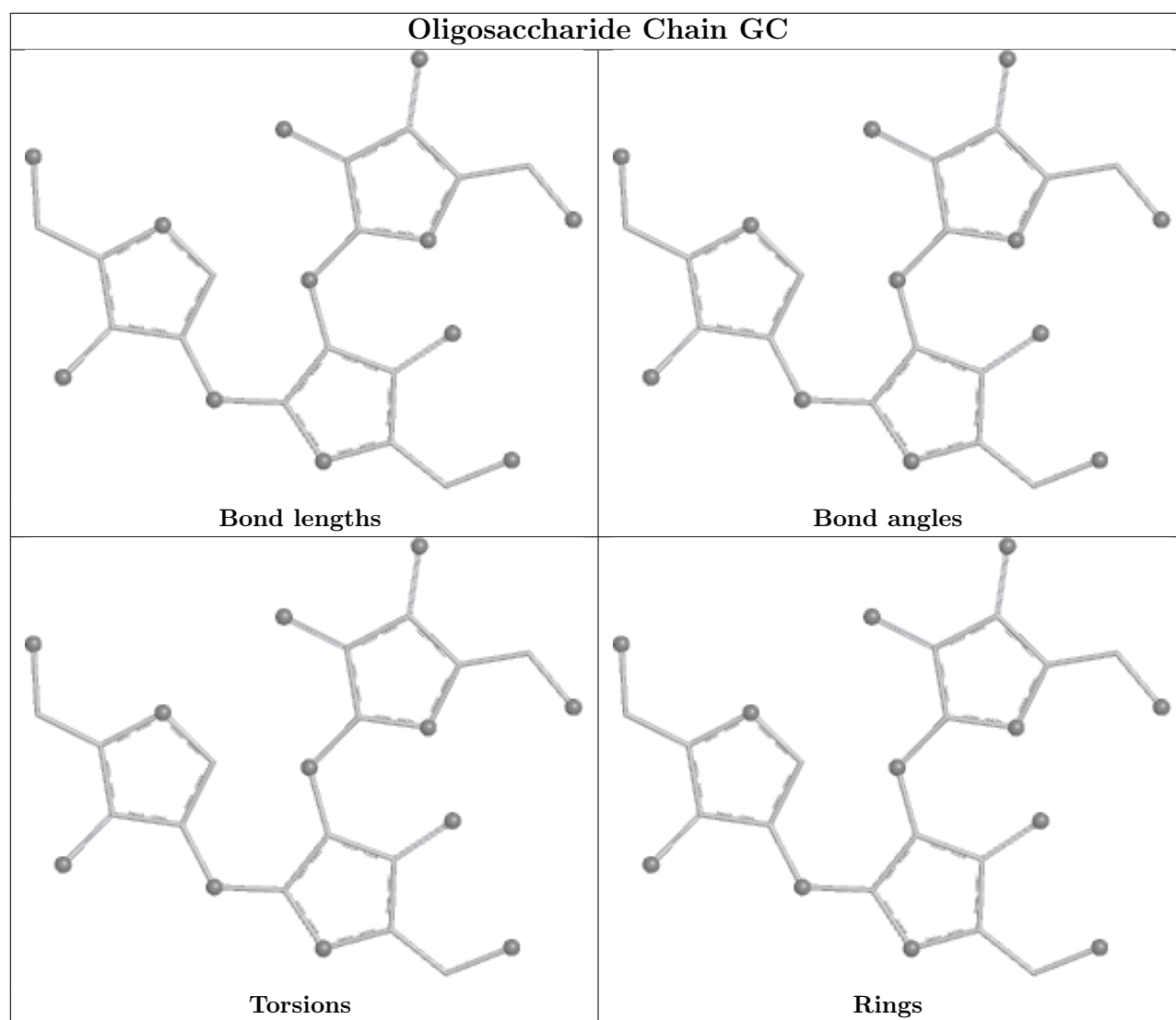


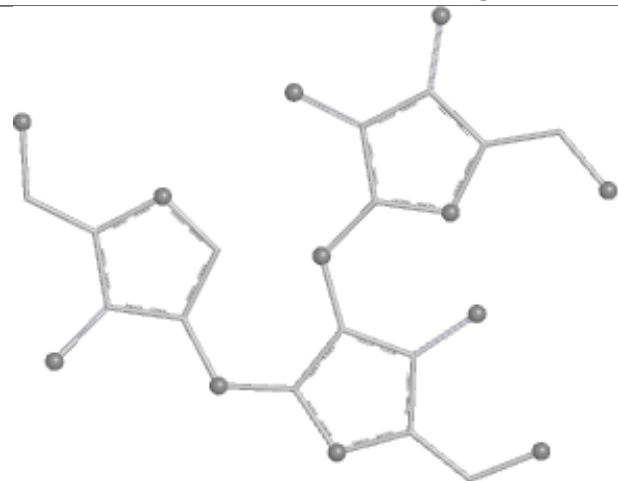
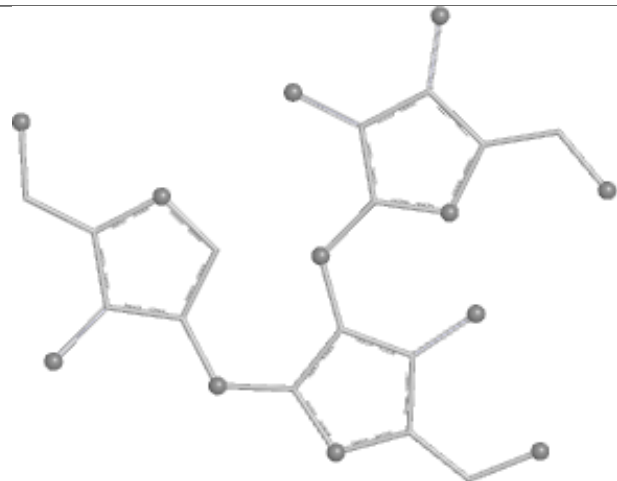
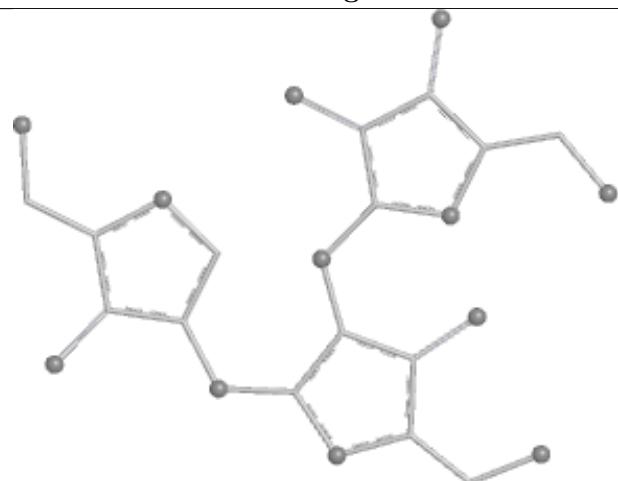
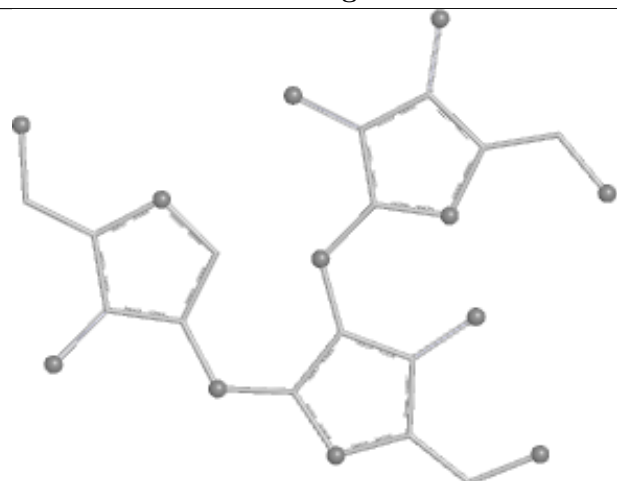


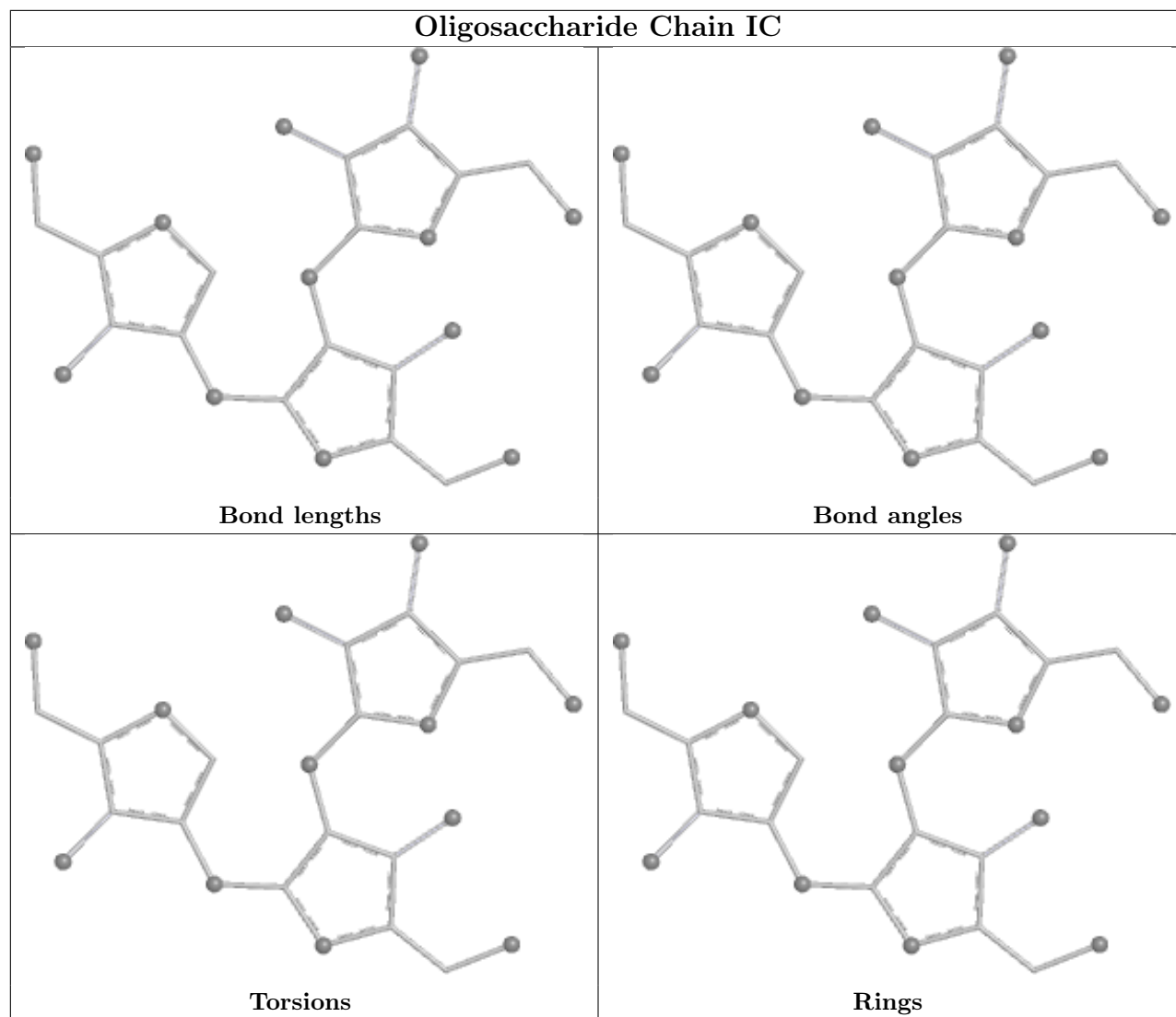


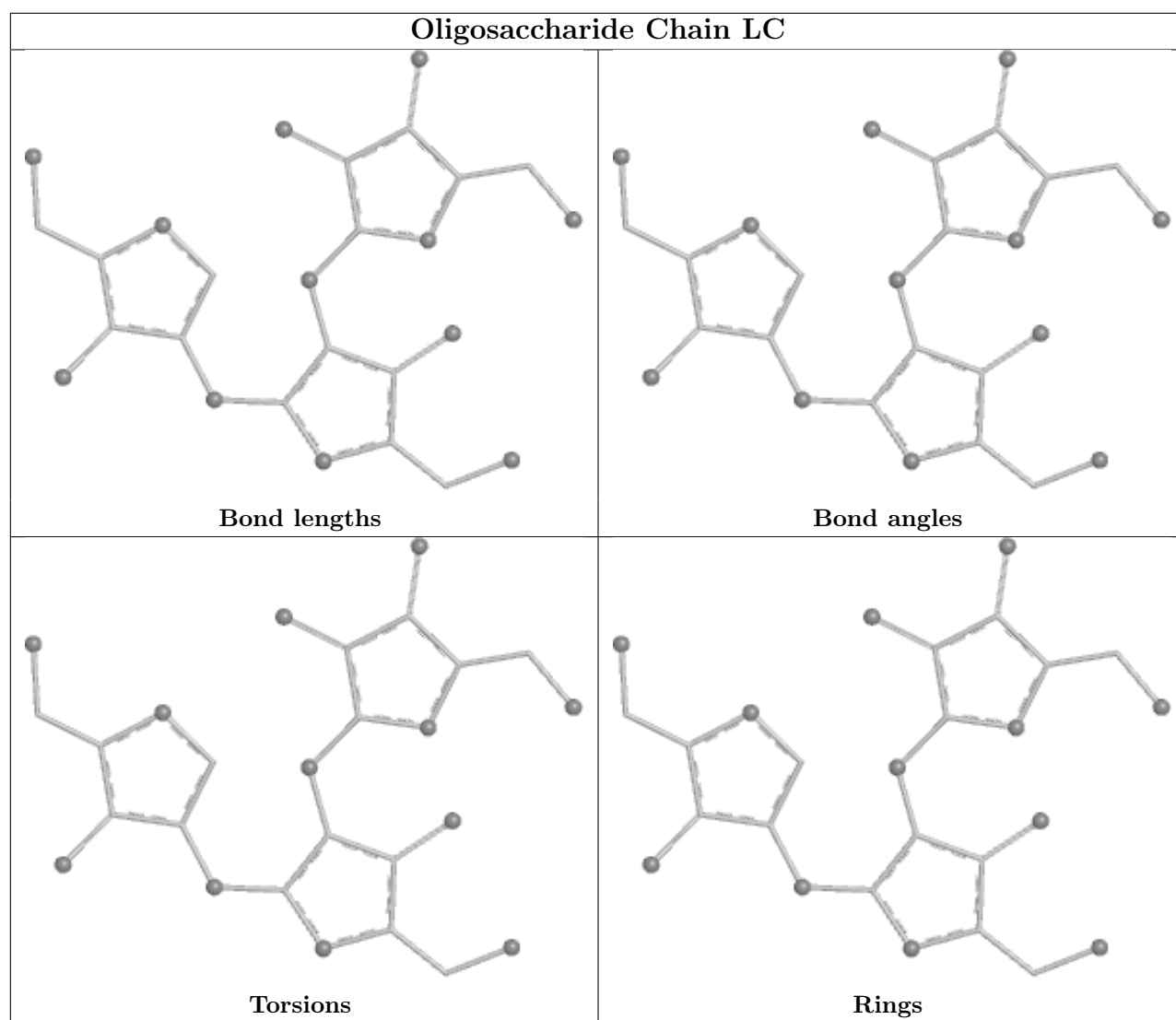
Oligosaccharide Chain BC**Bond lengths****Bond angles****Torsions****Rings**

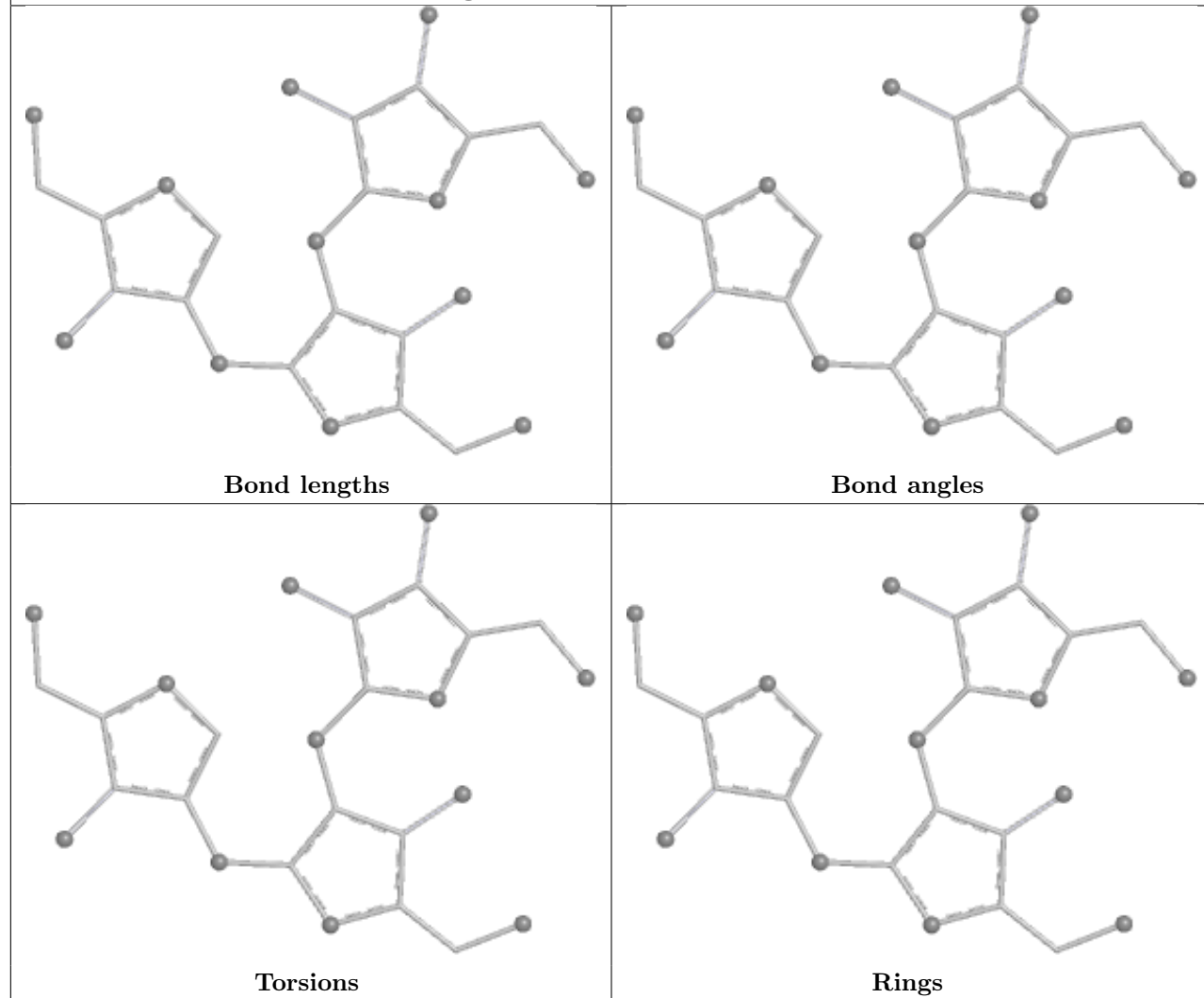
Oligosaccharide Chain CC**Bond lengths****Bond angles****Torsions****Rings**

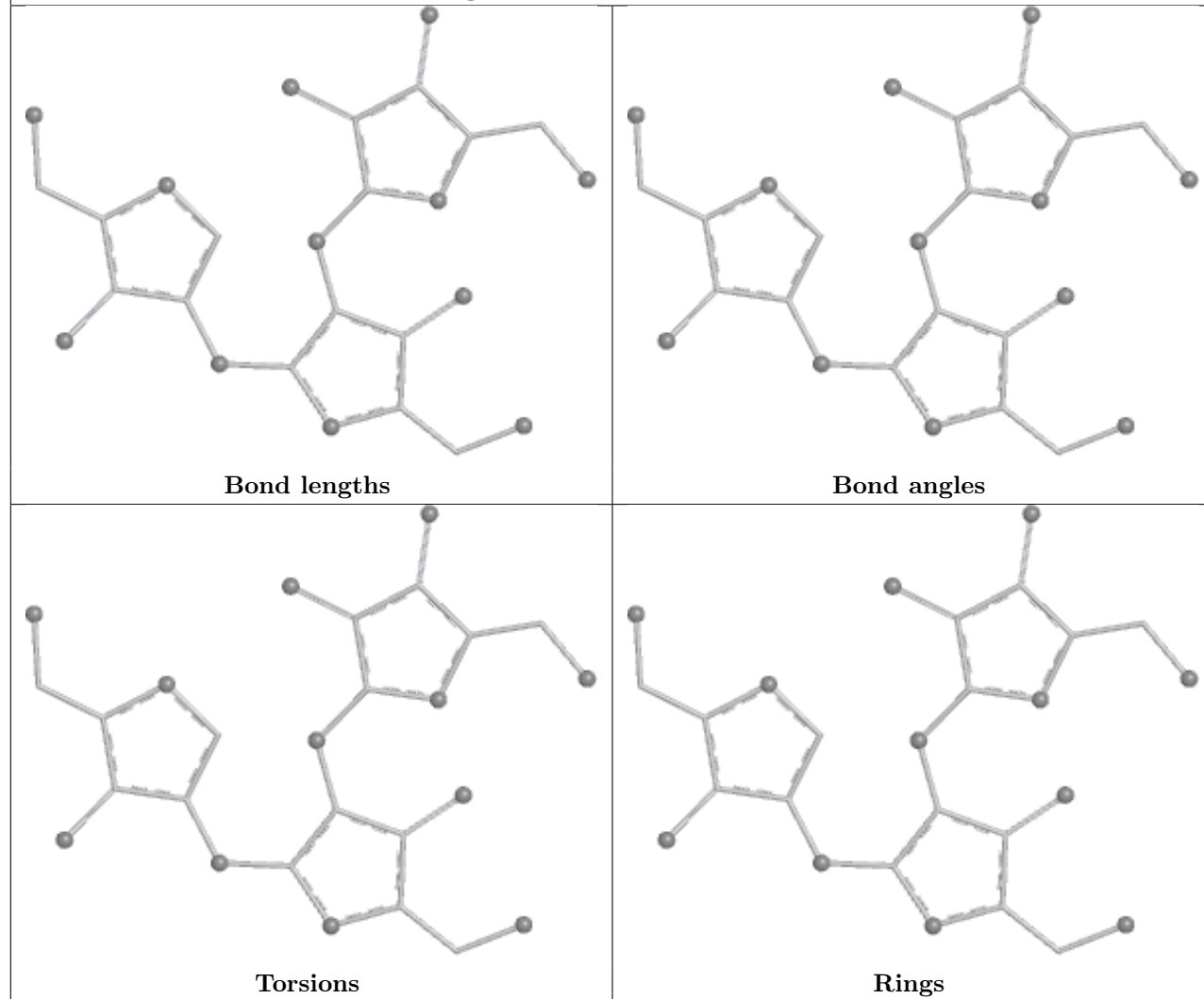


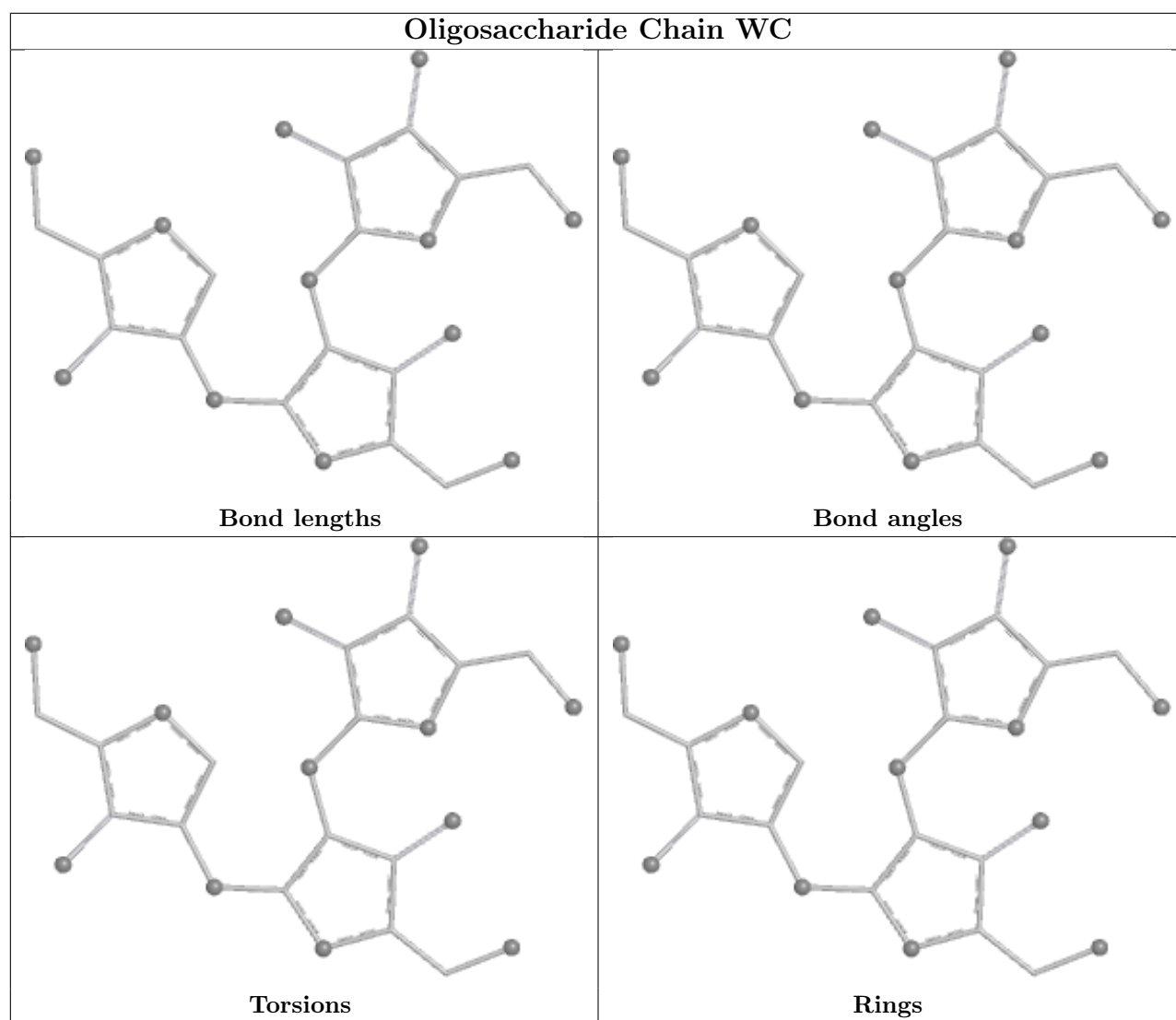
Oligosaccharide Chain HC**Bond lengths****Bond angles****Torsions****Rings**



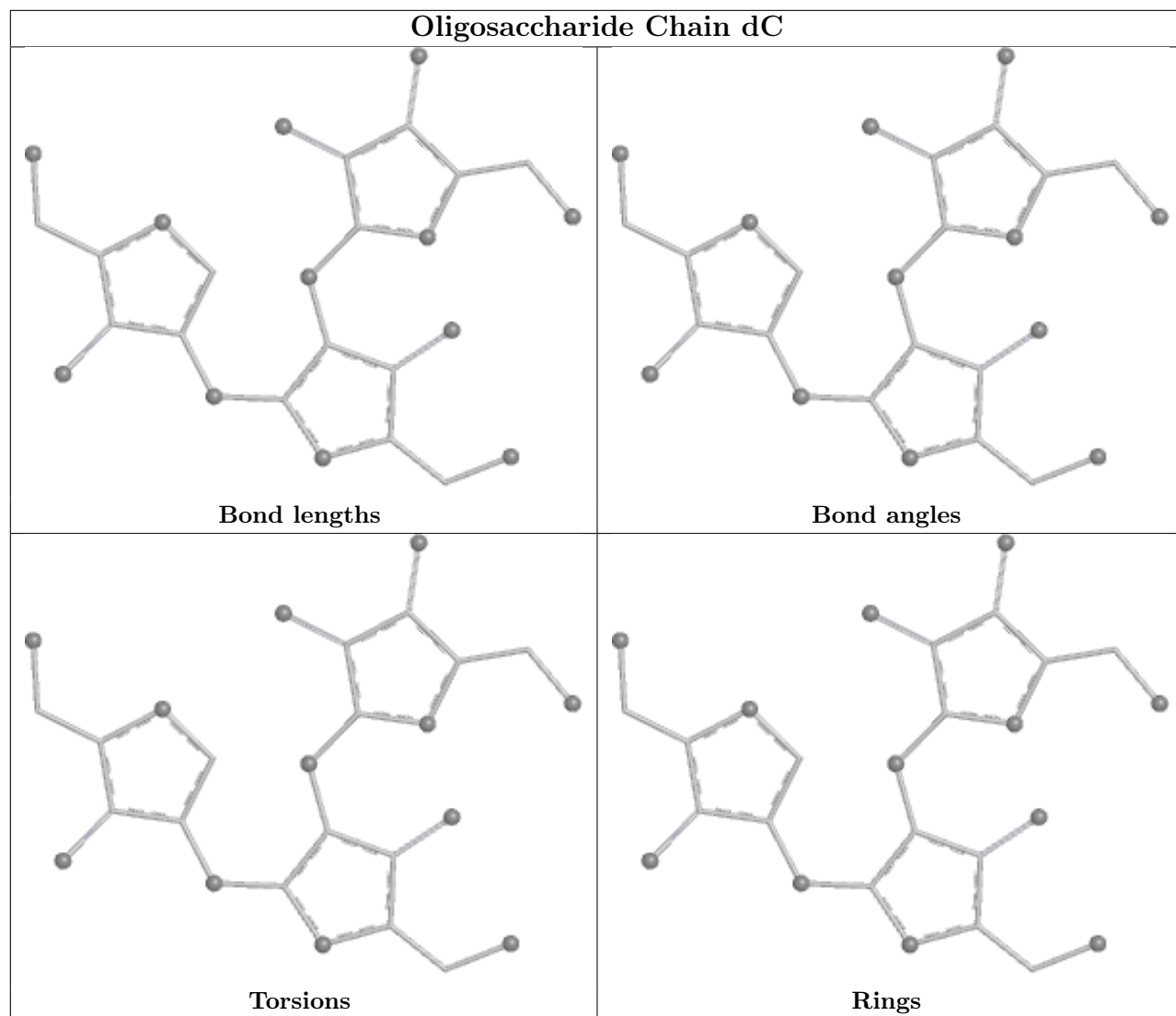


Oligosaccharide Chain NC

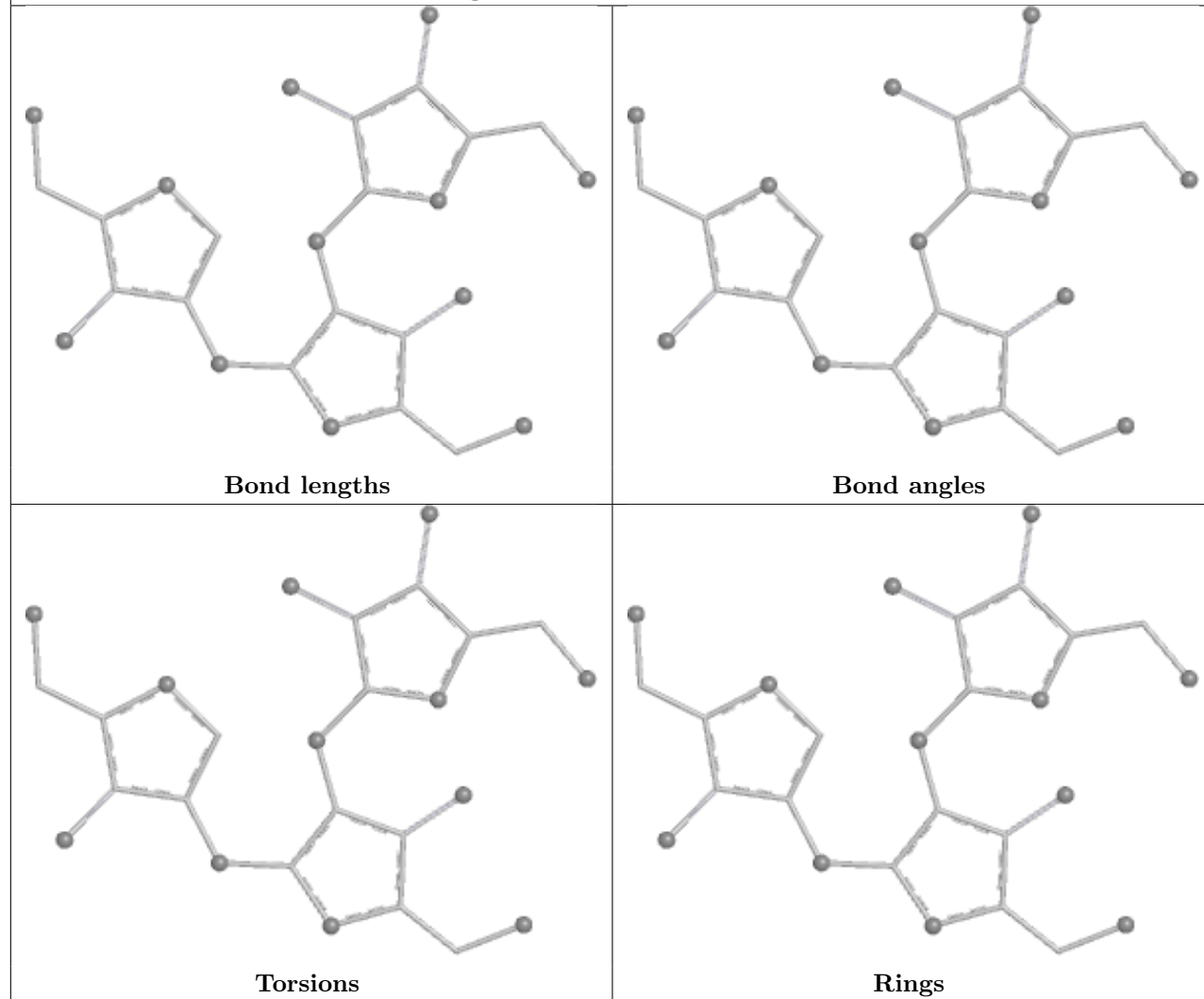
Oligosaccharide Chain TC

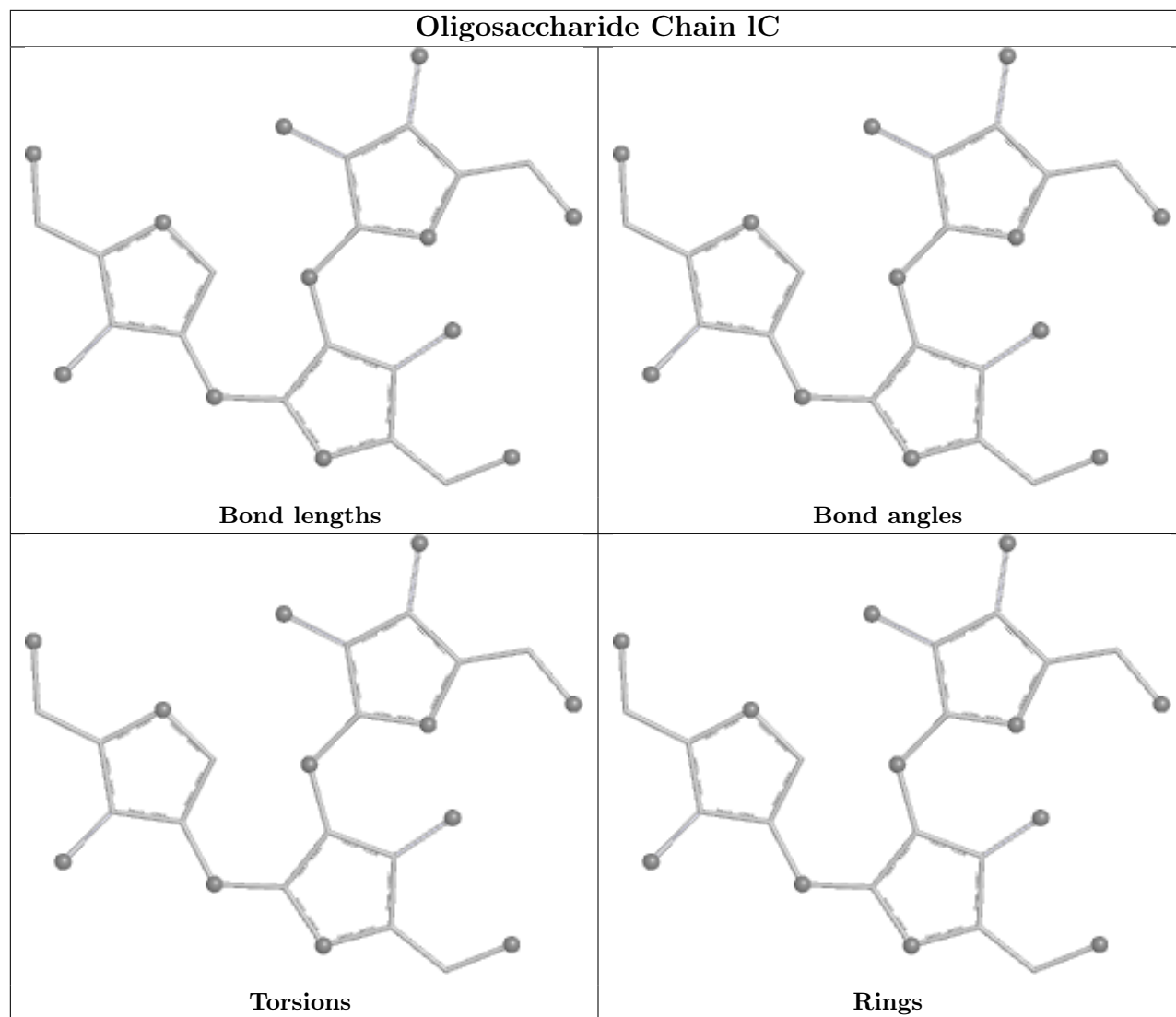


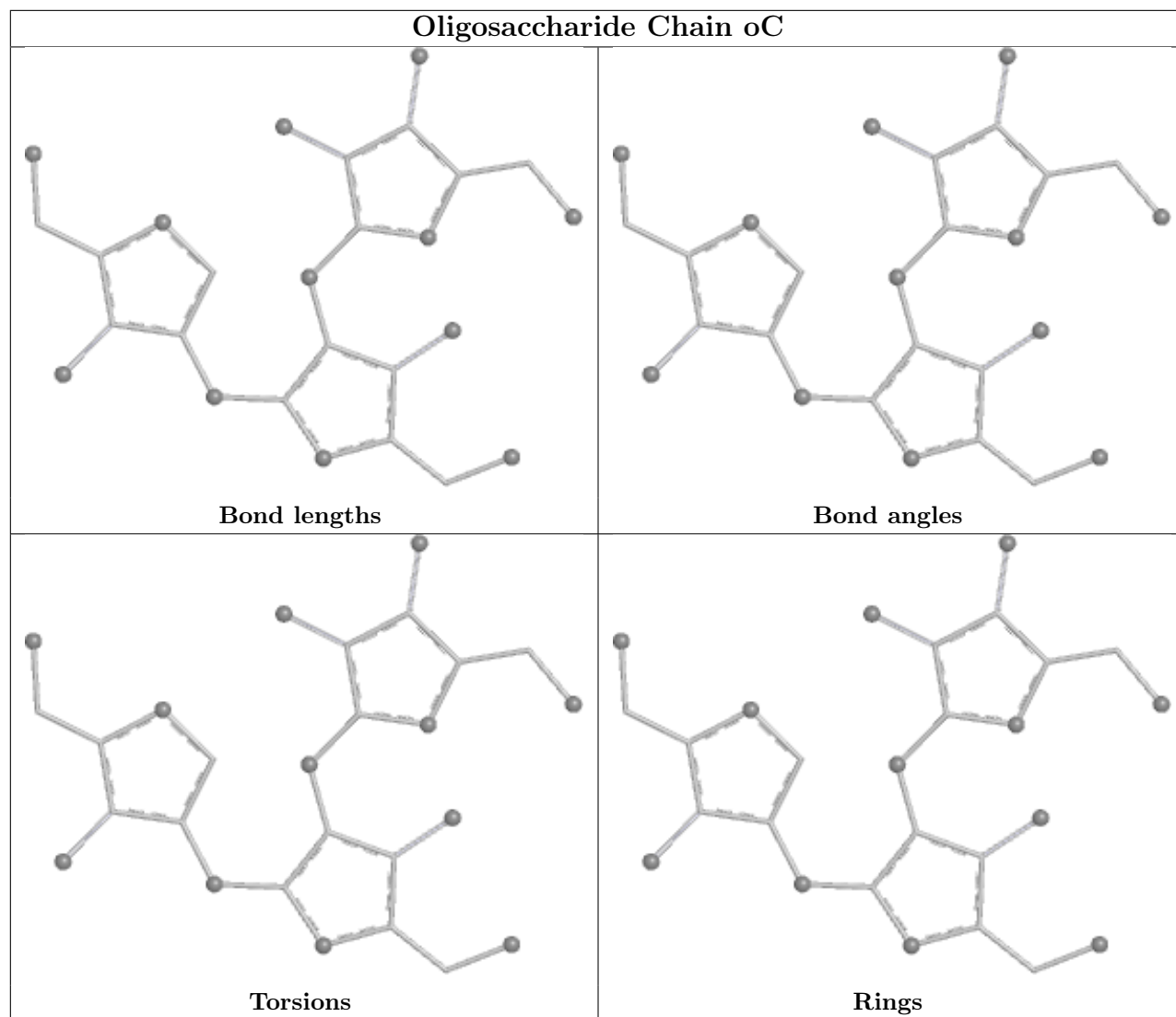
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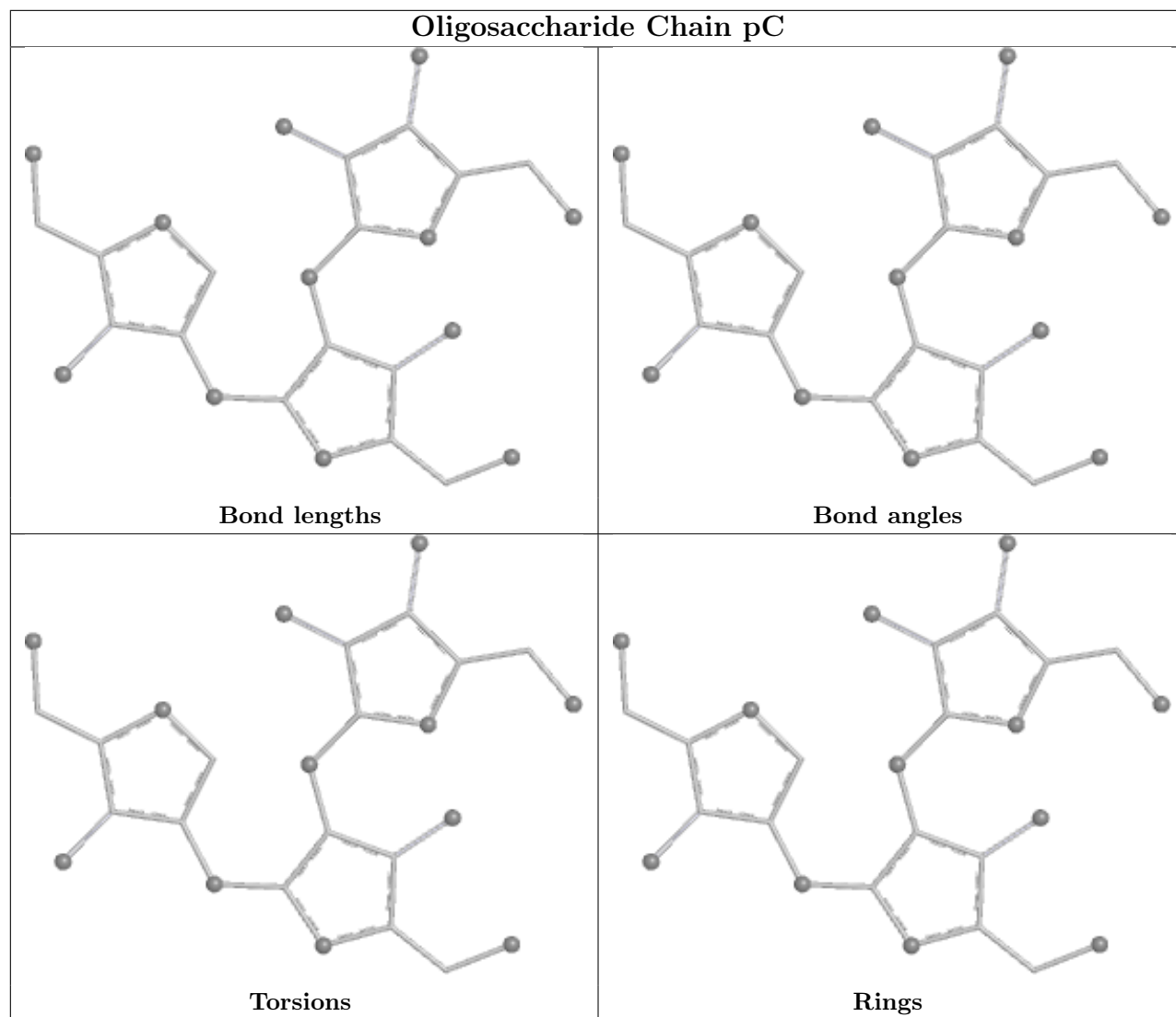


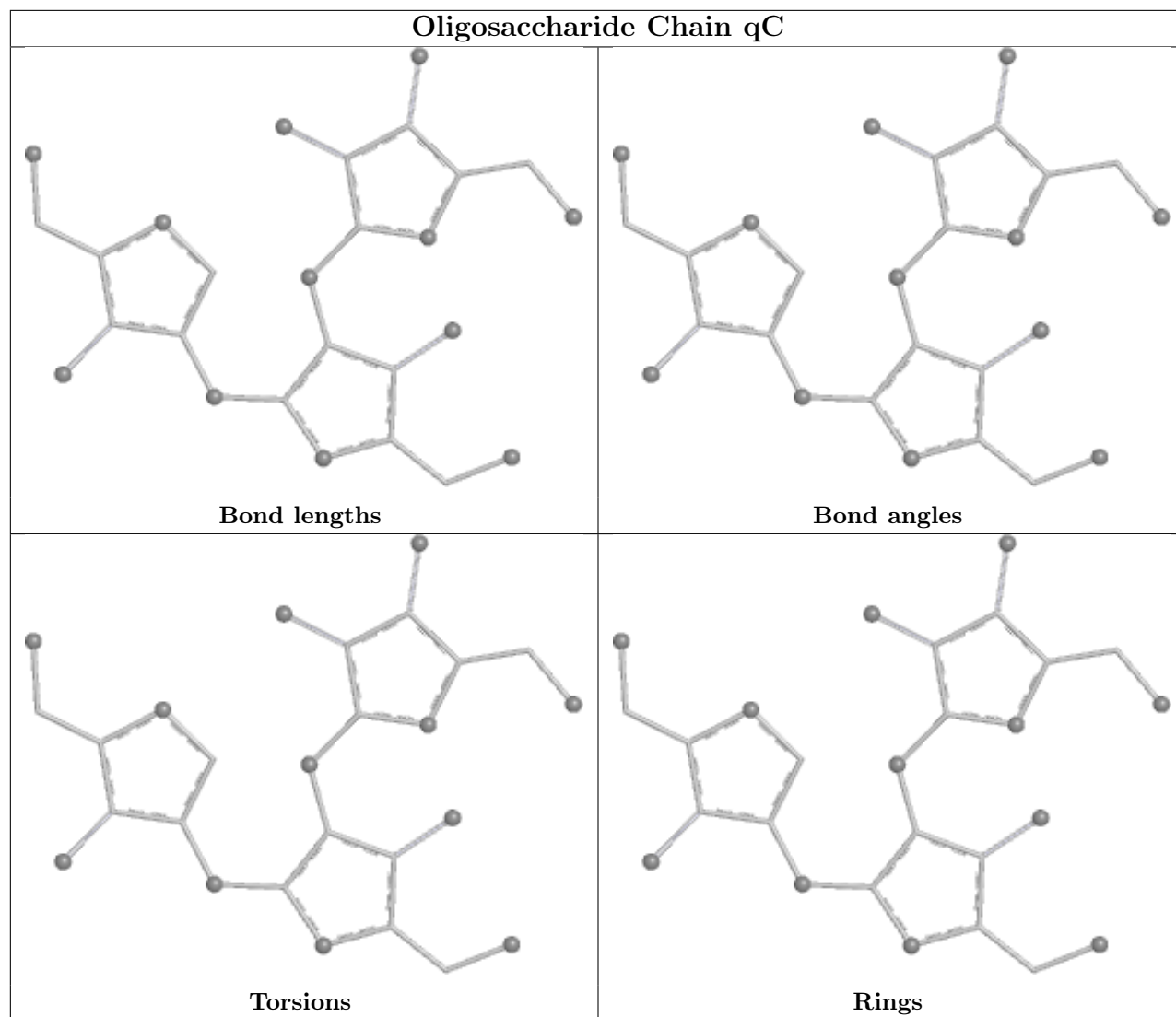
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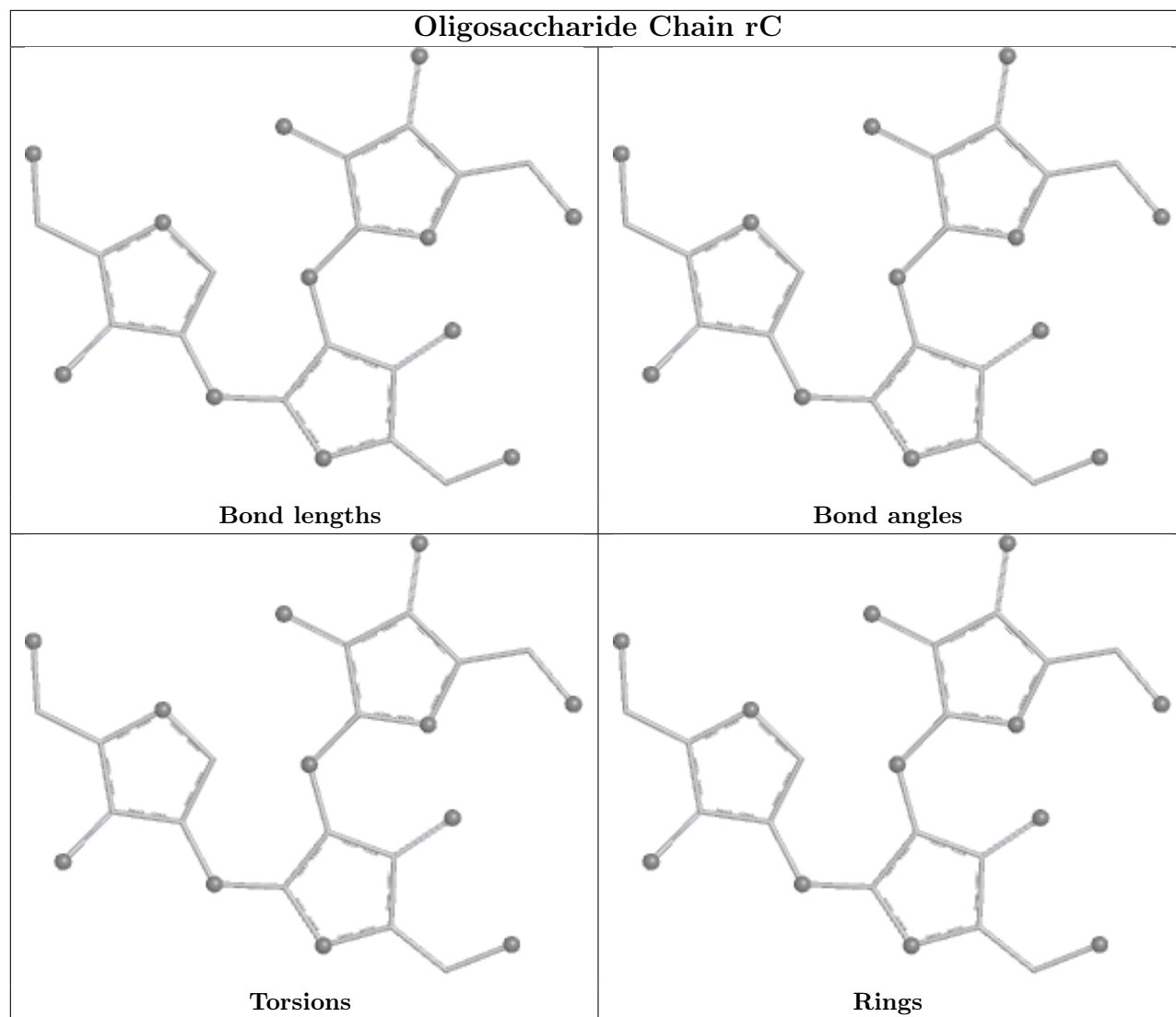


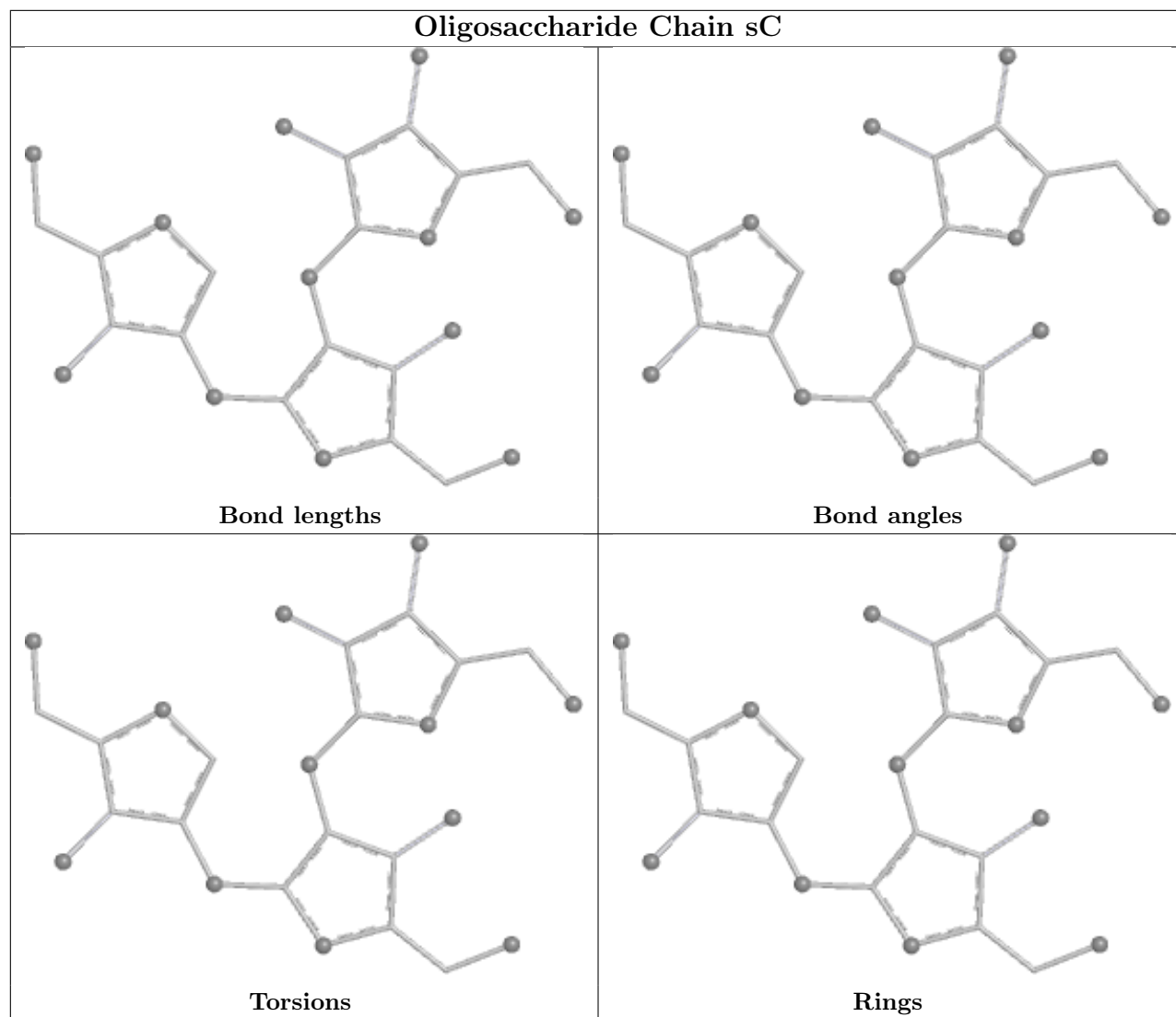


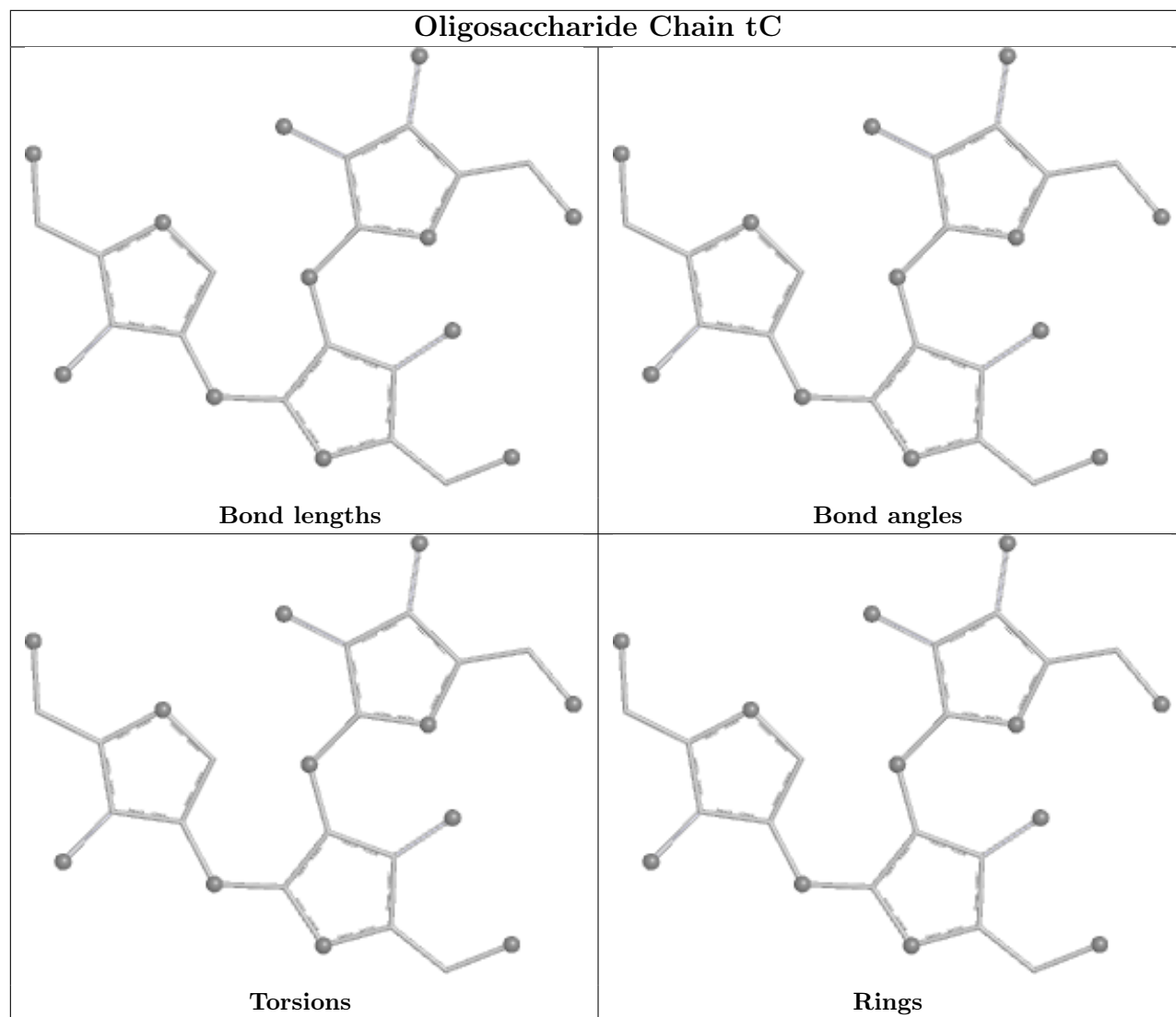


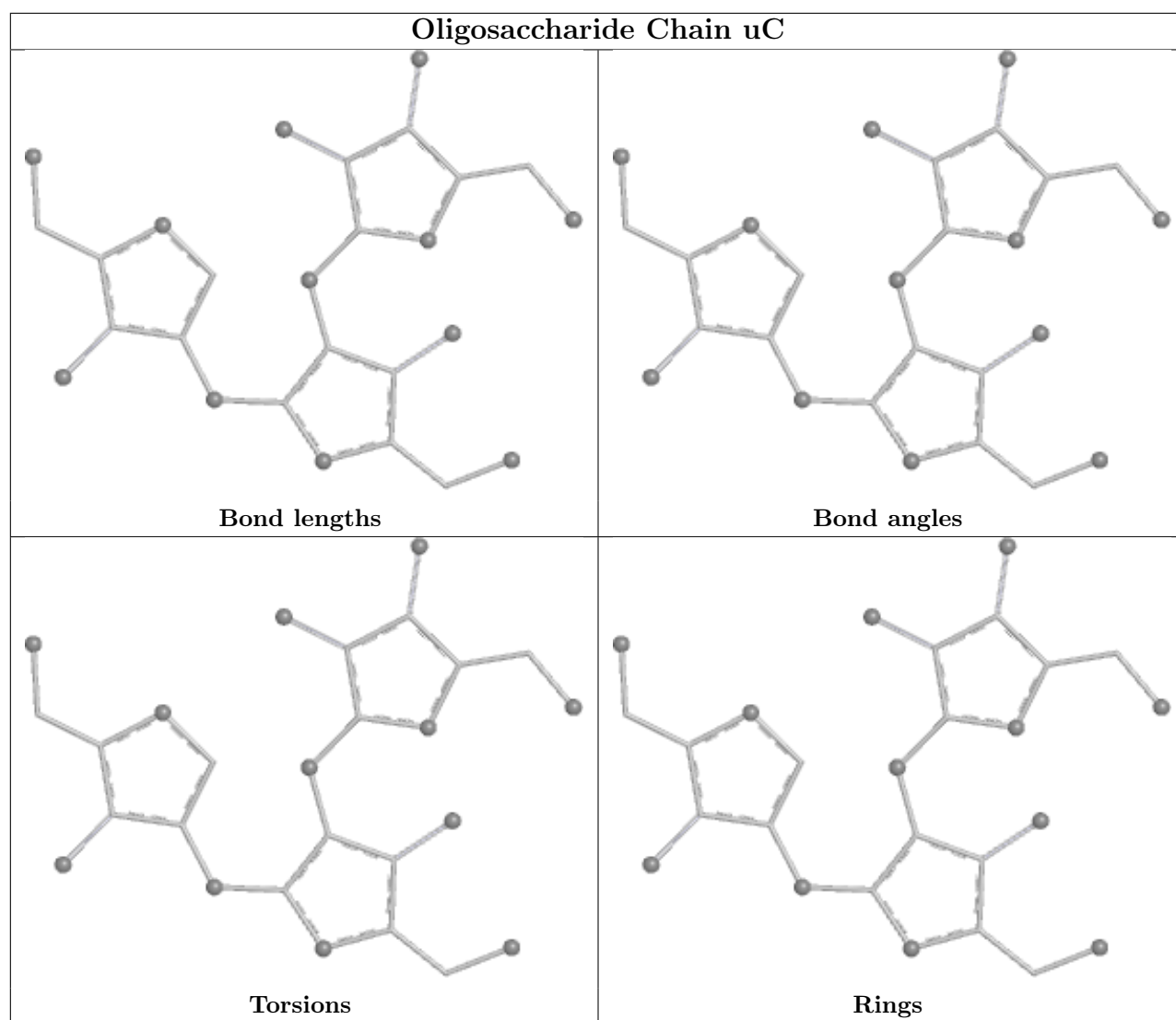


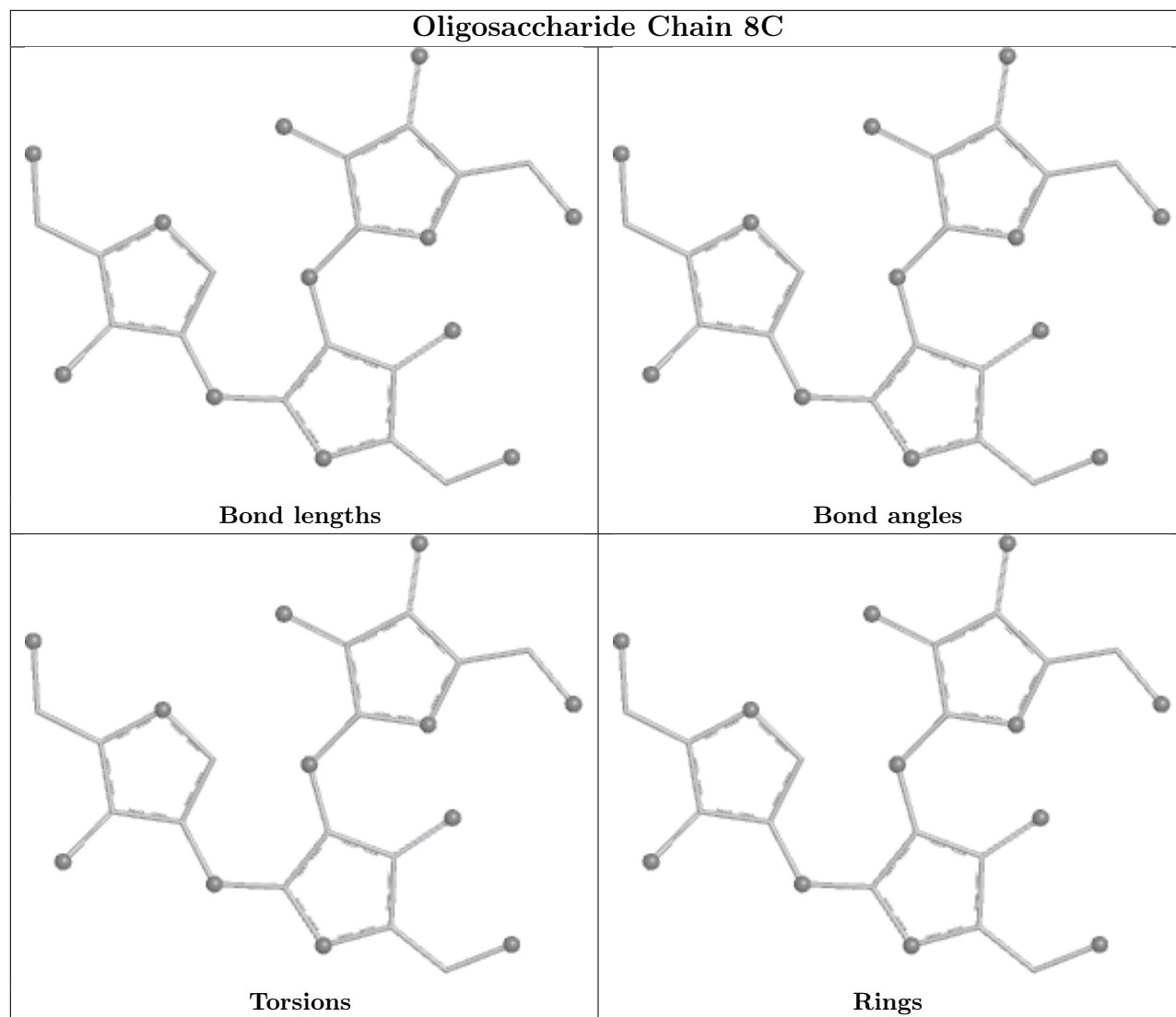




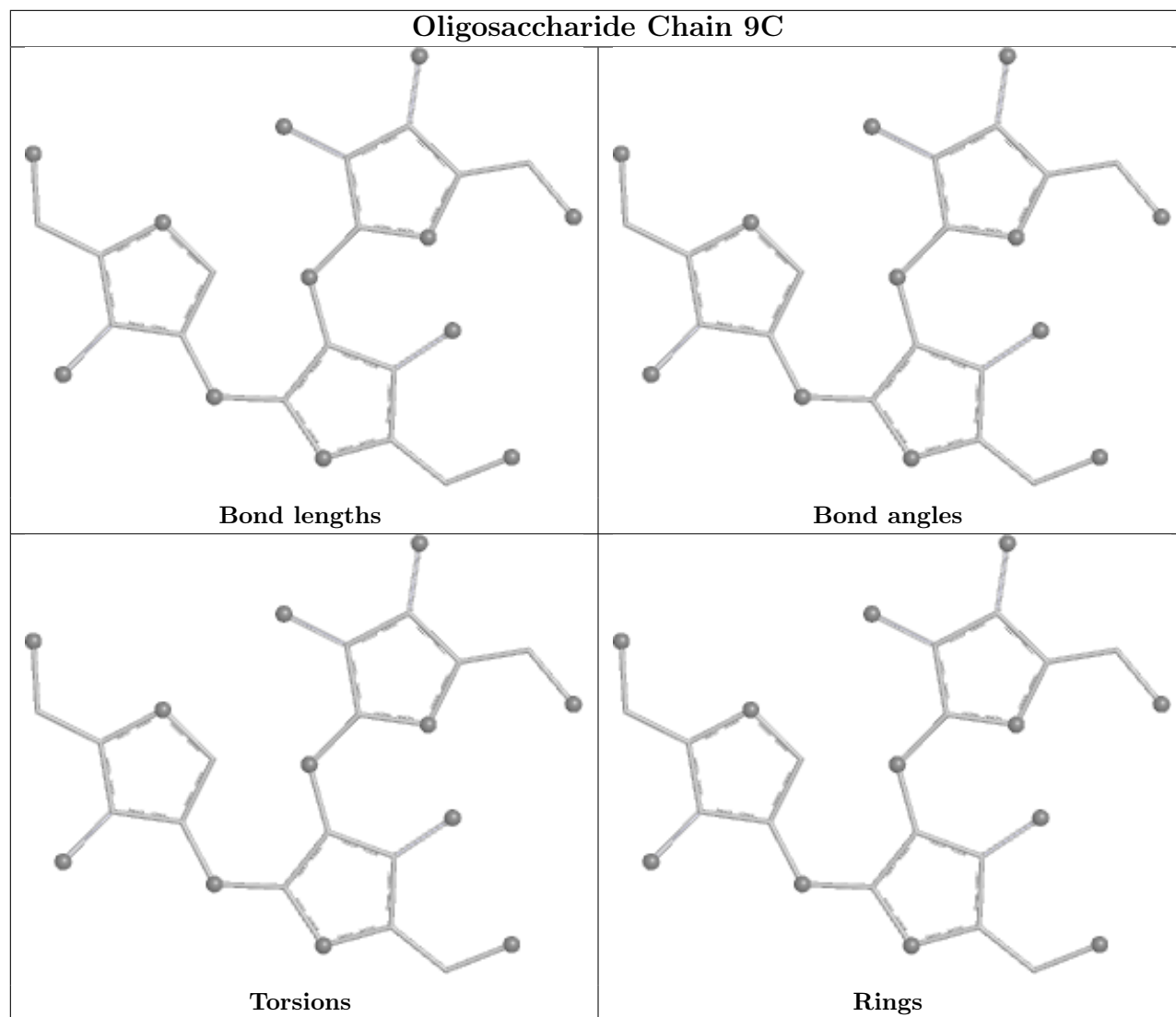


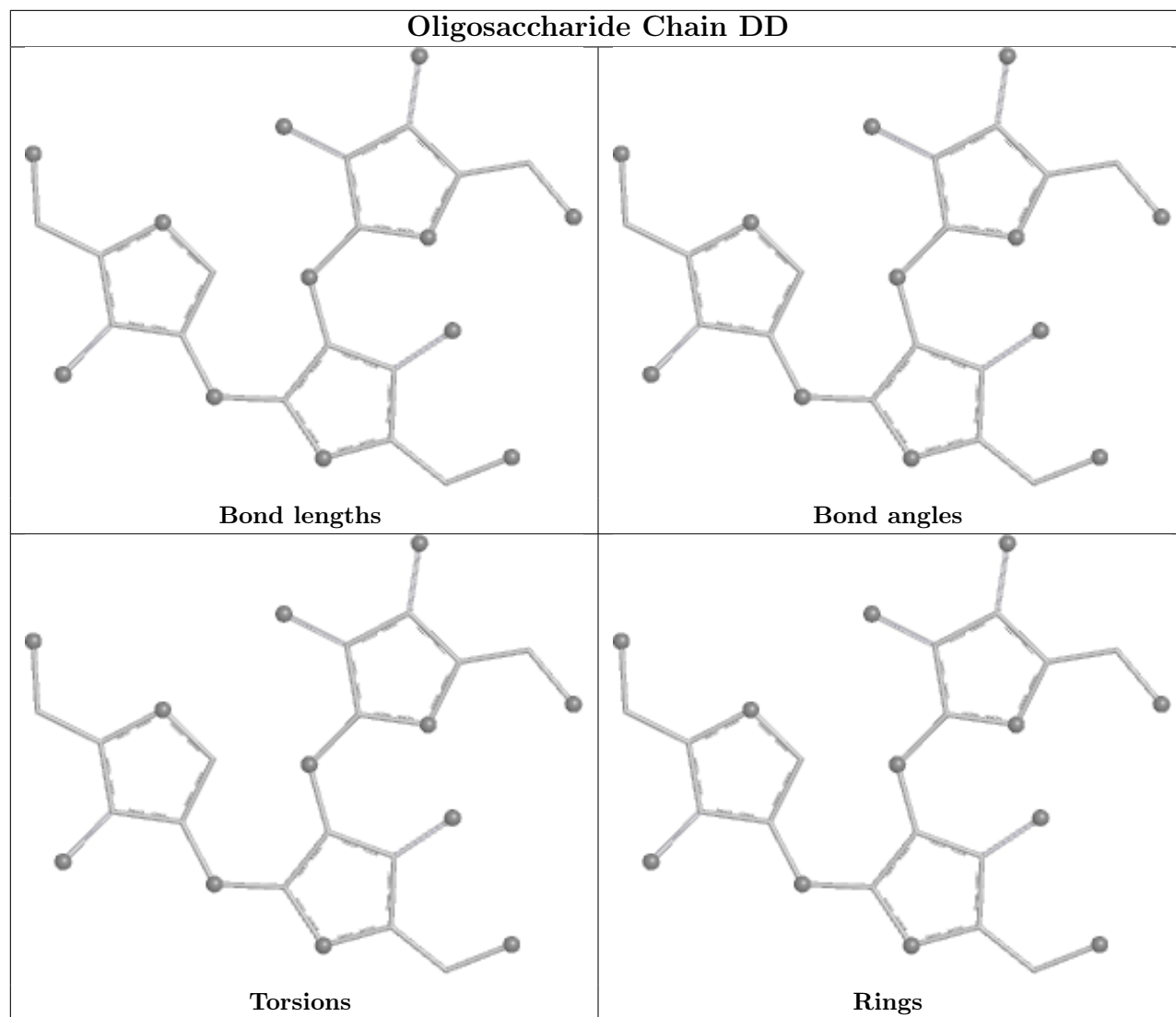


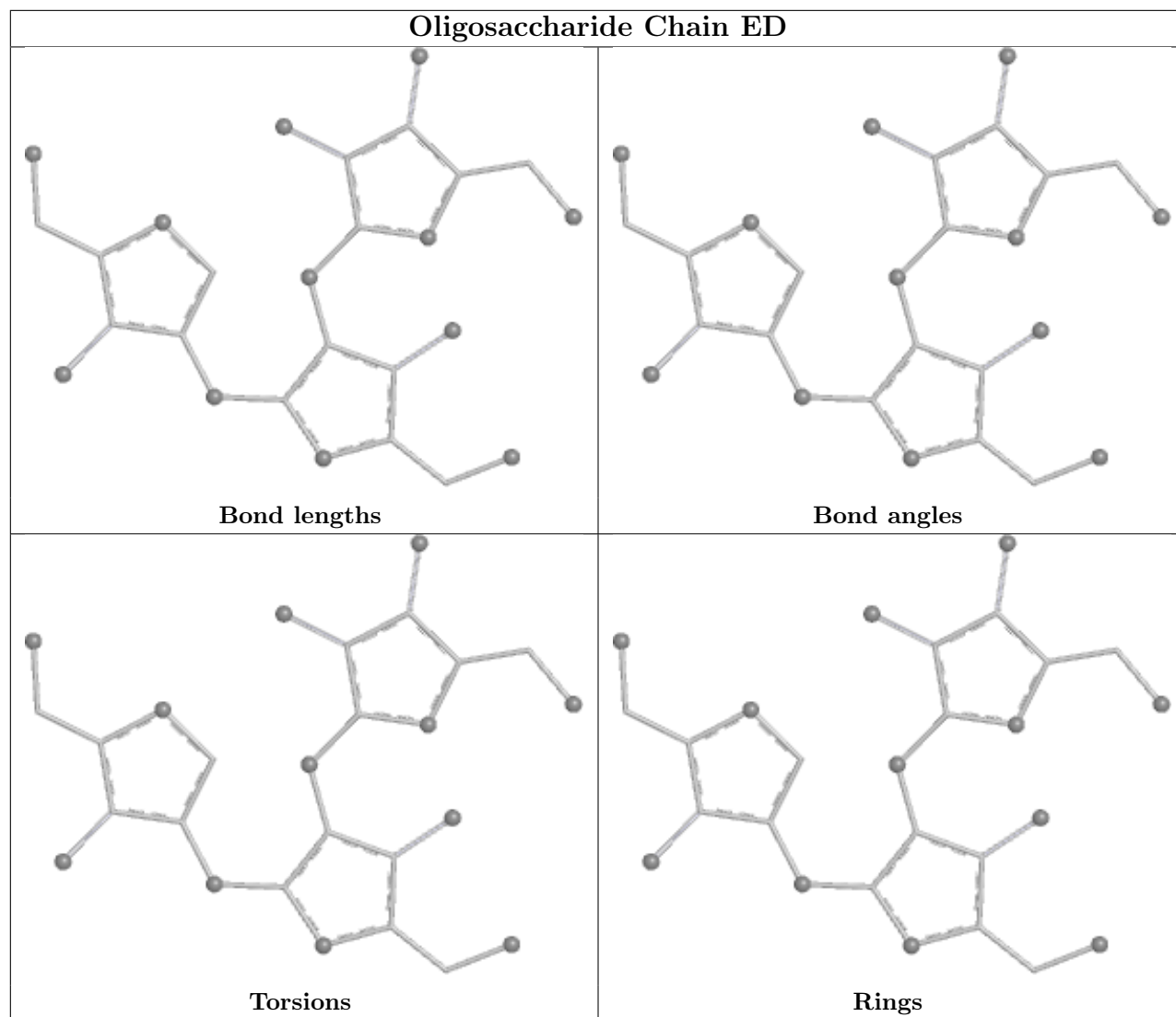


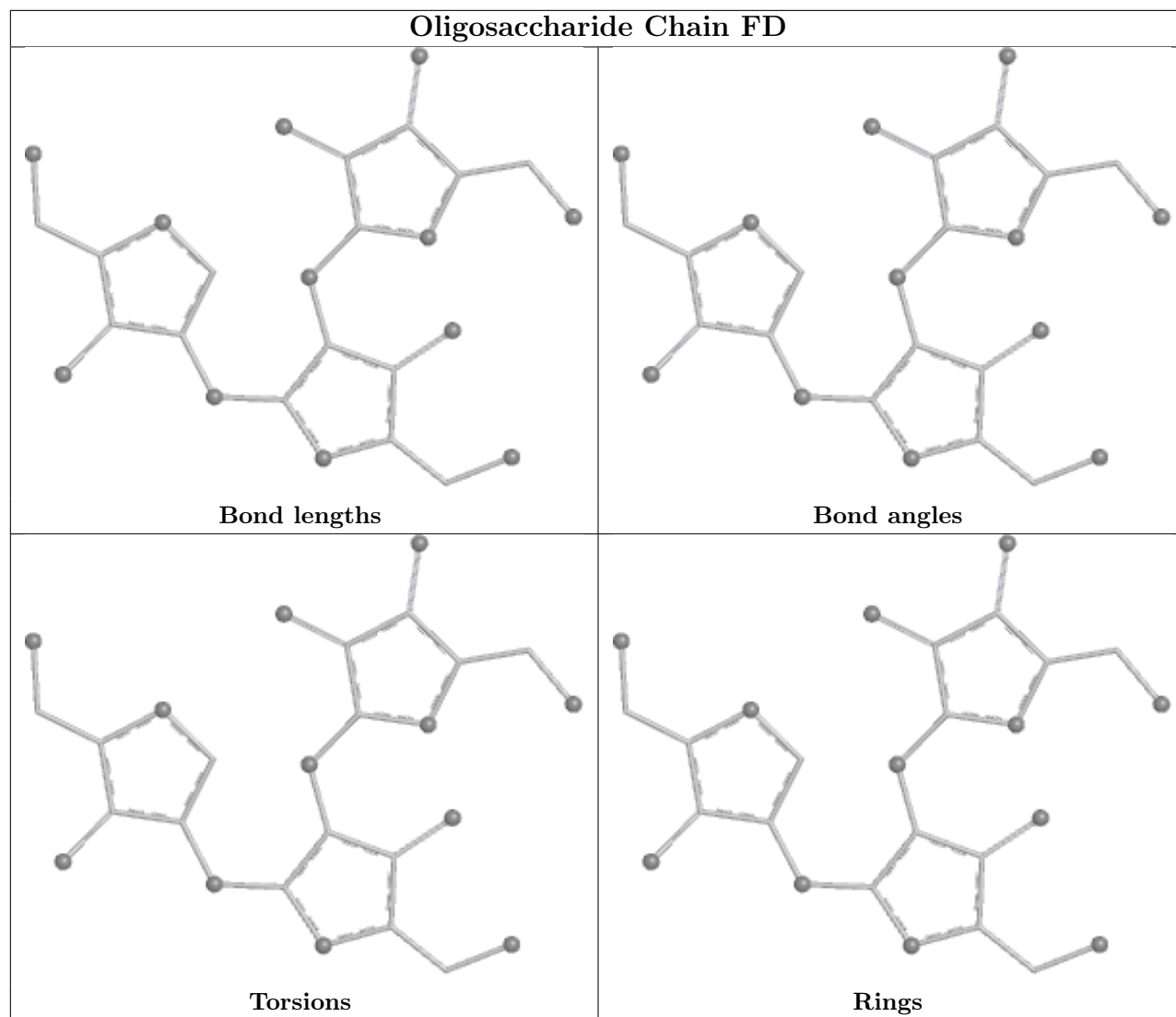


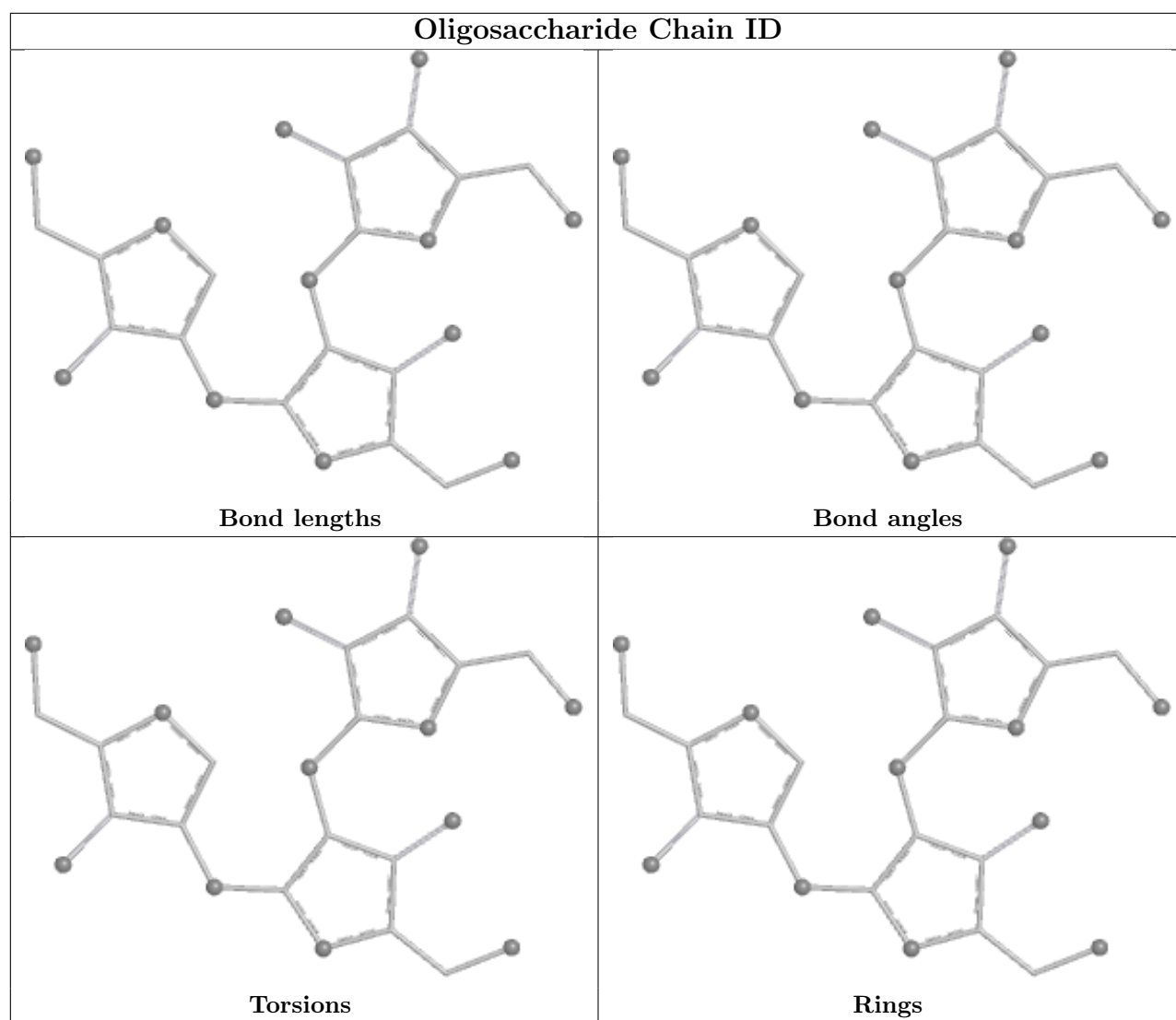
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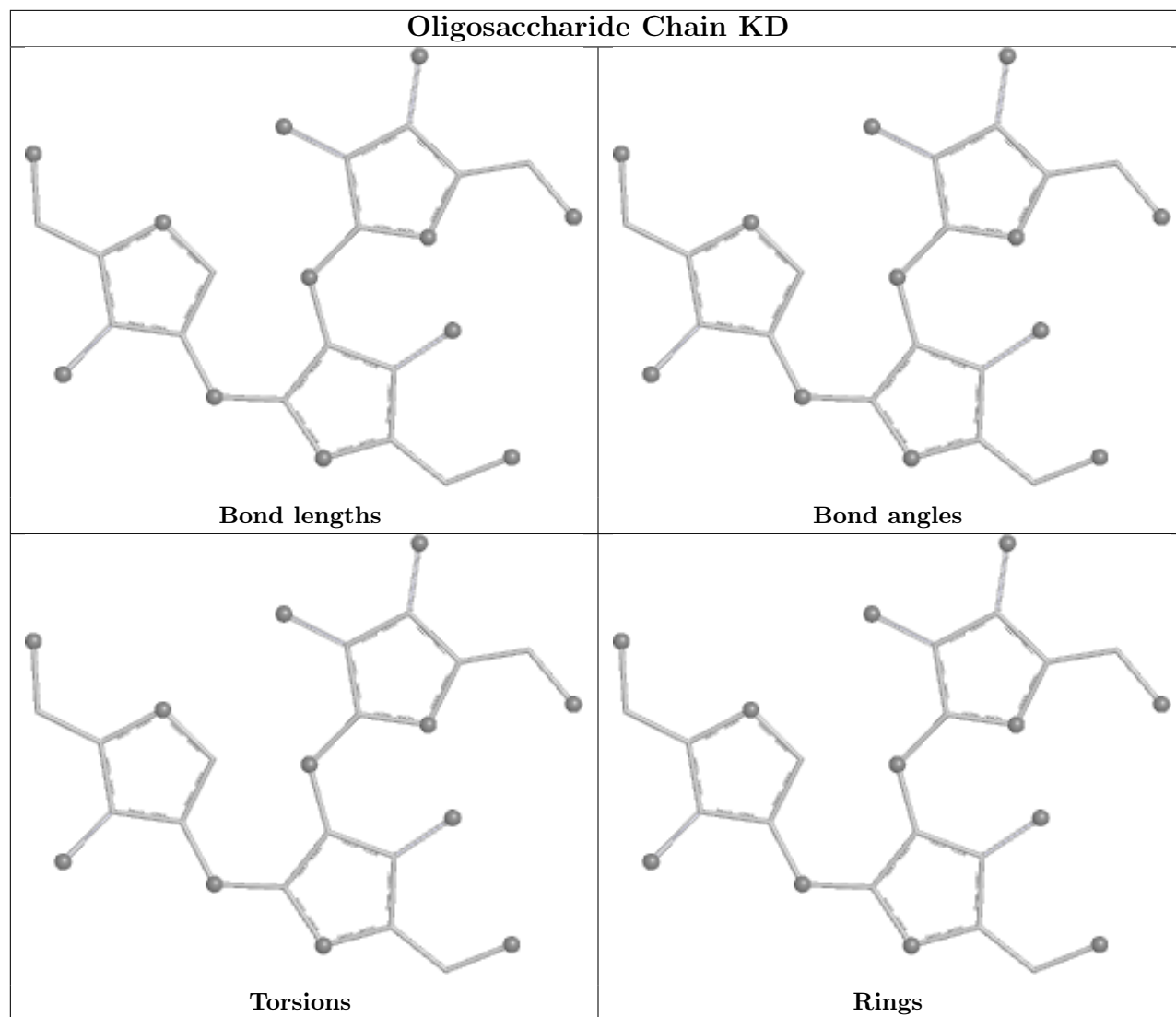


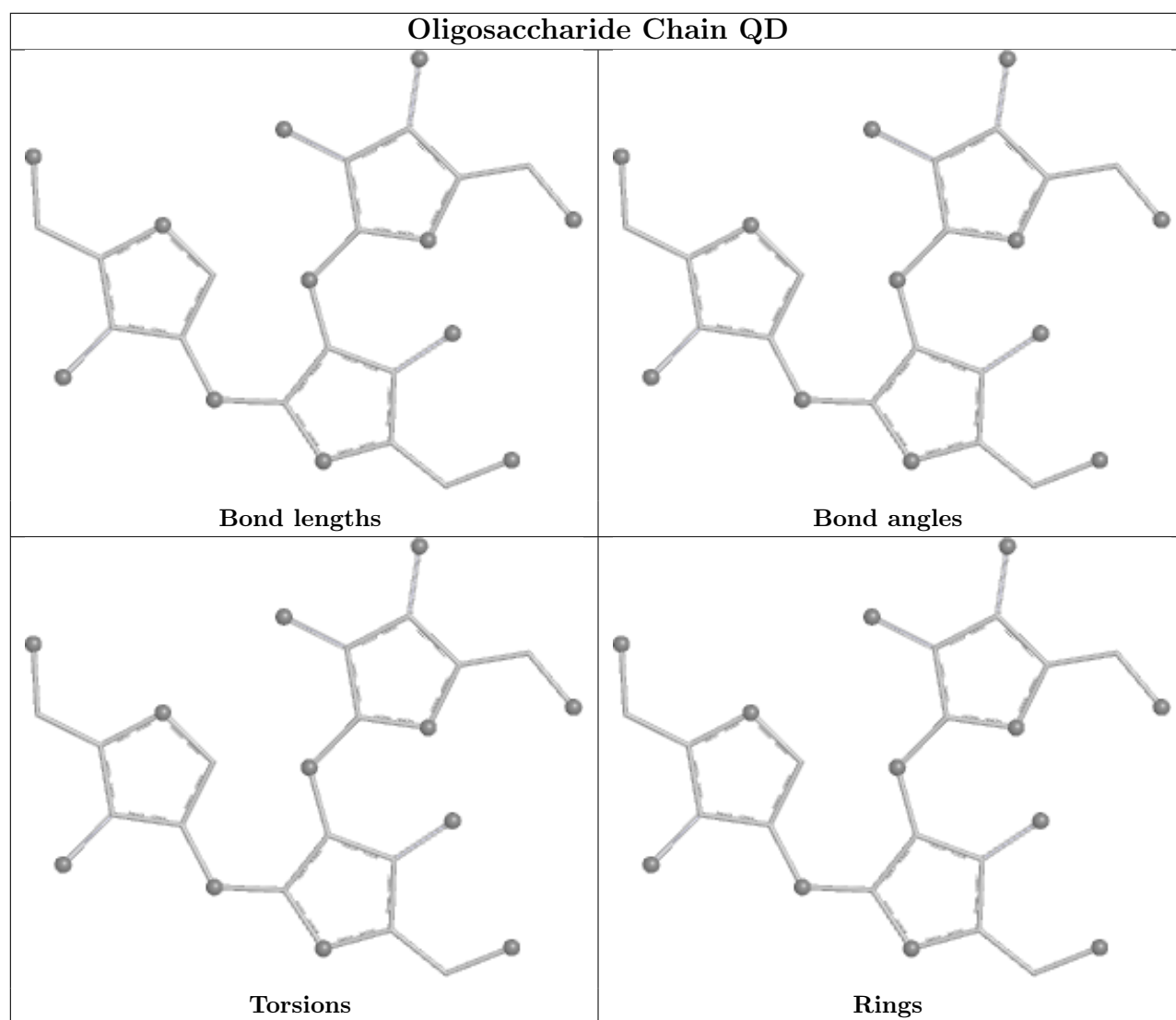


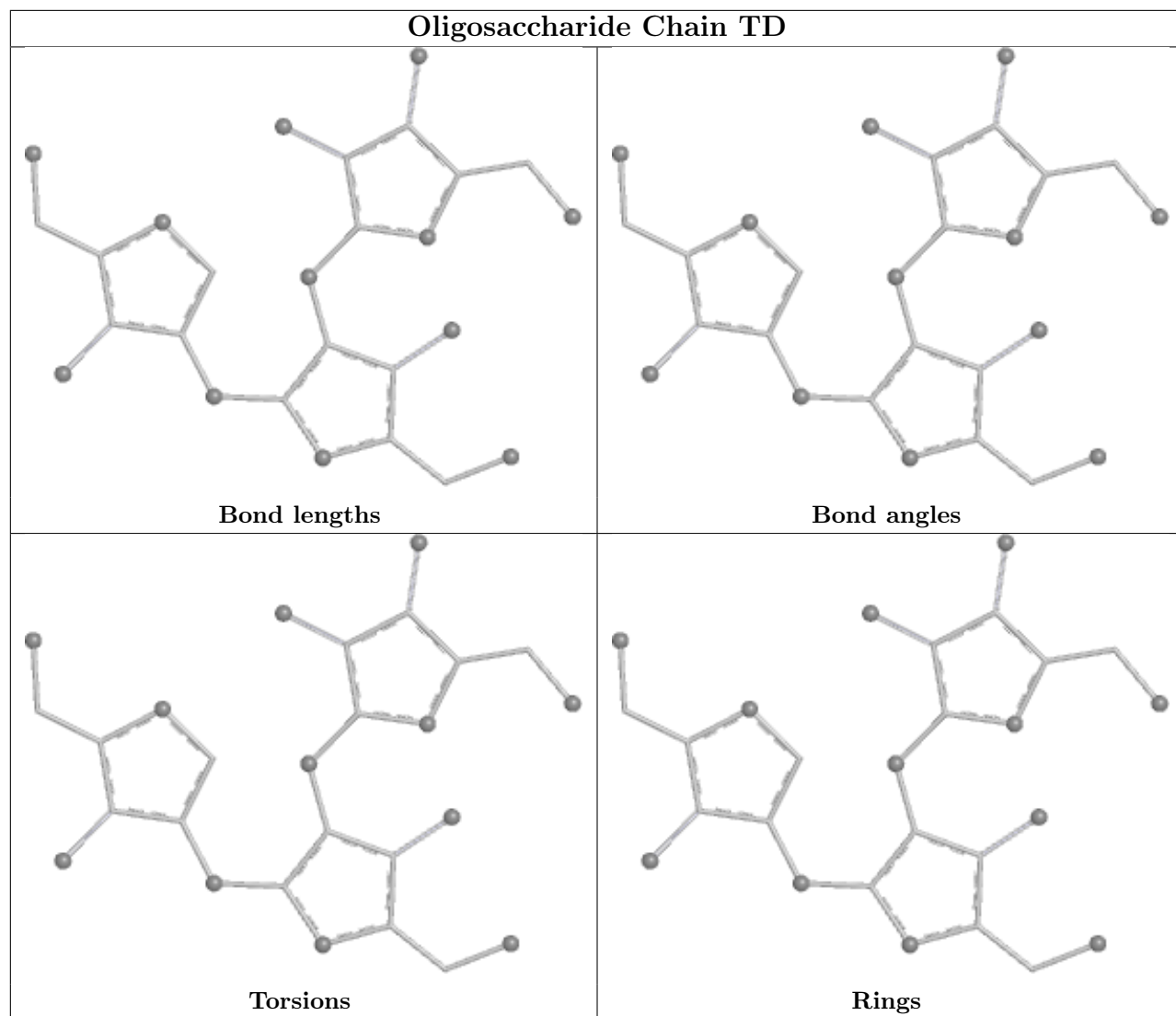


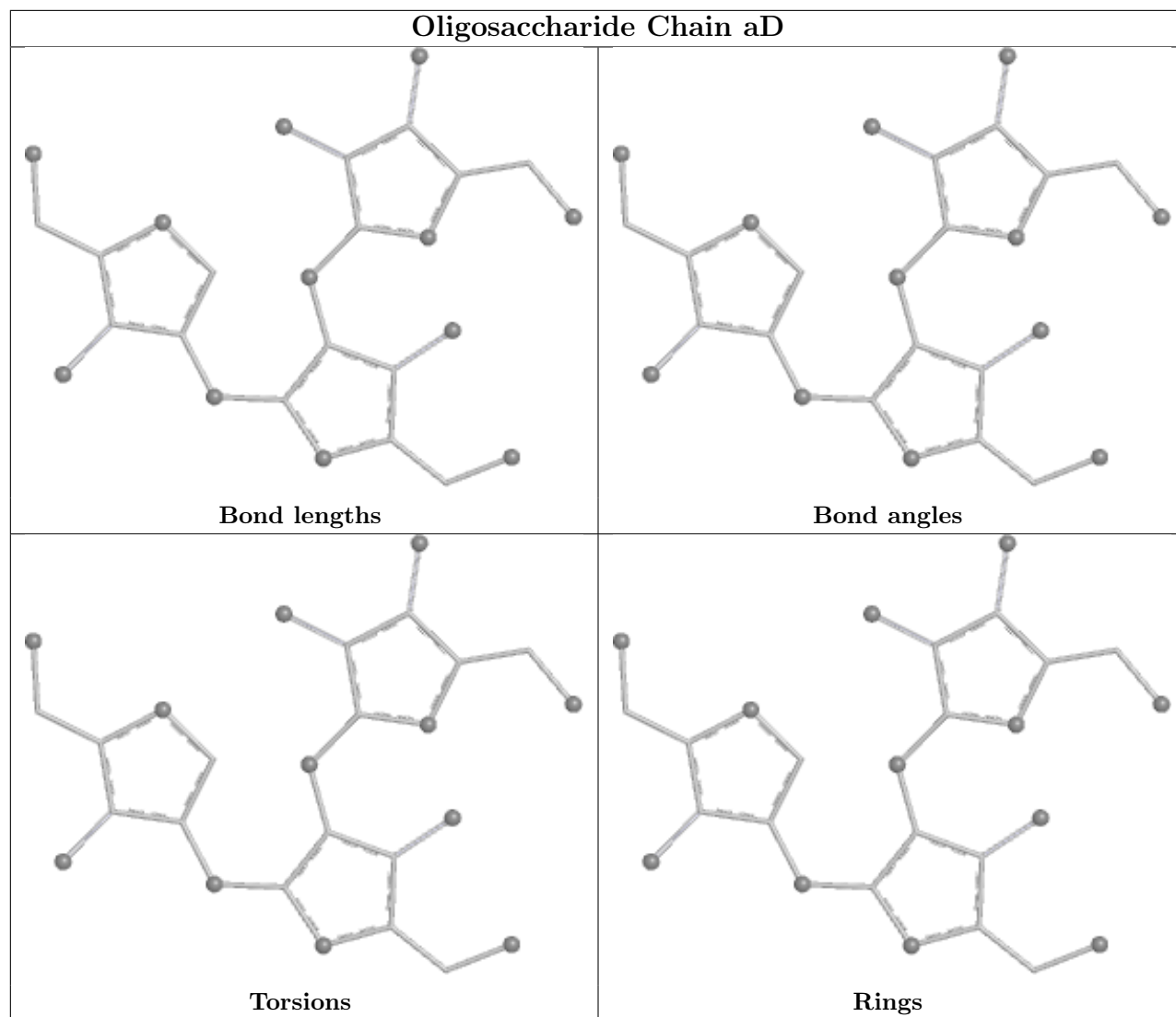


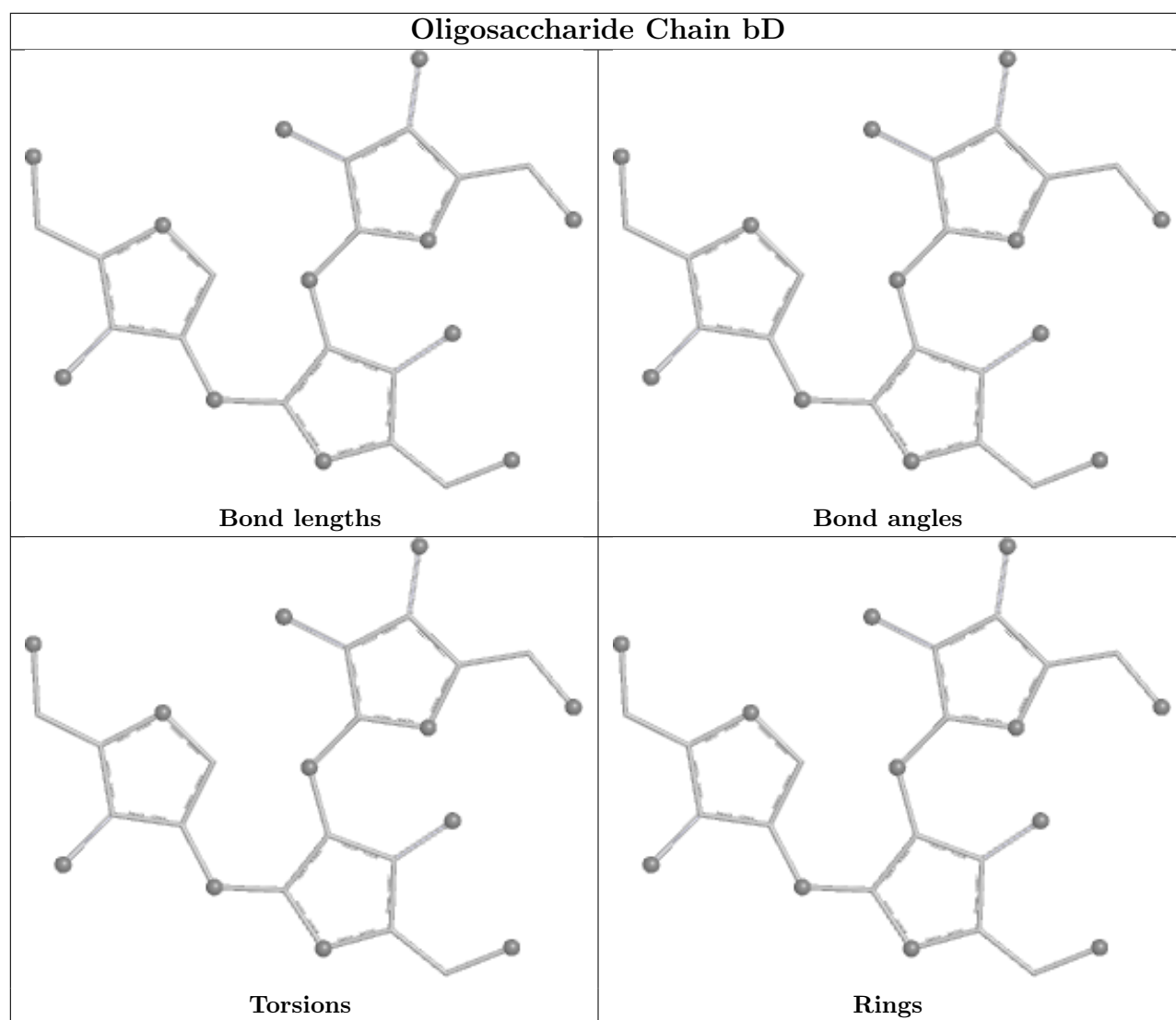


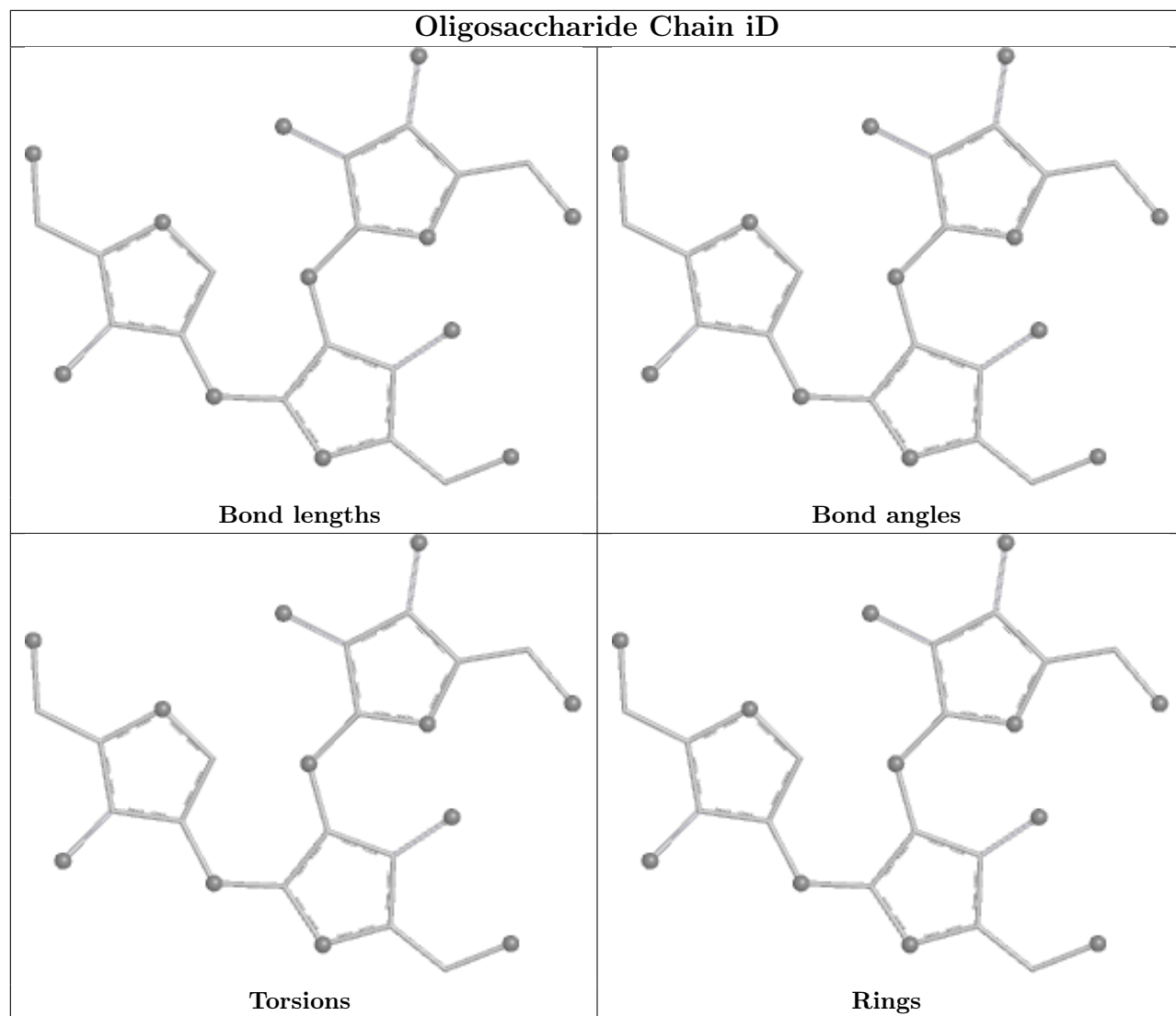


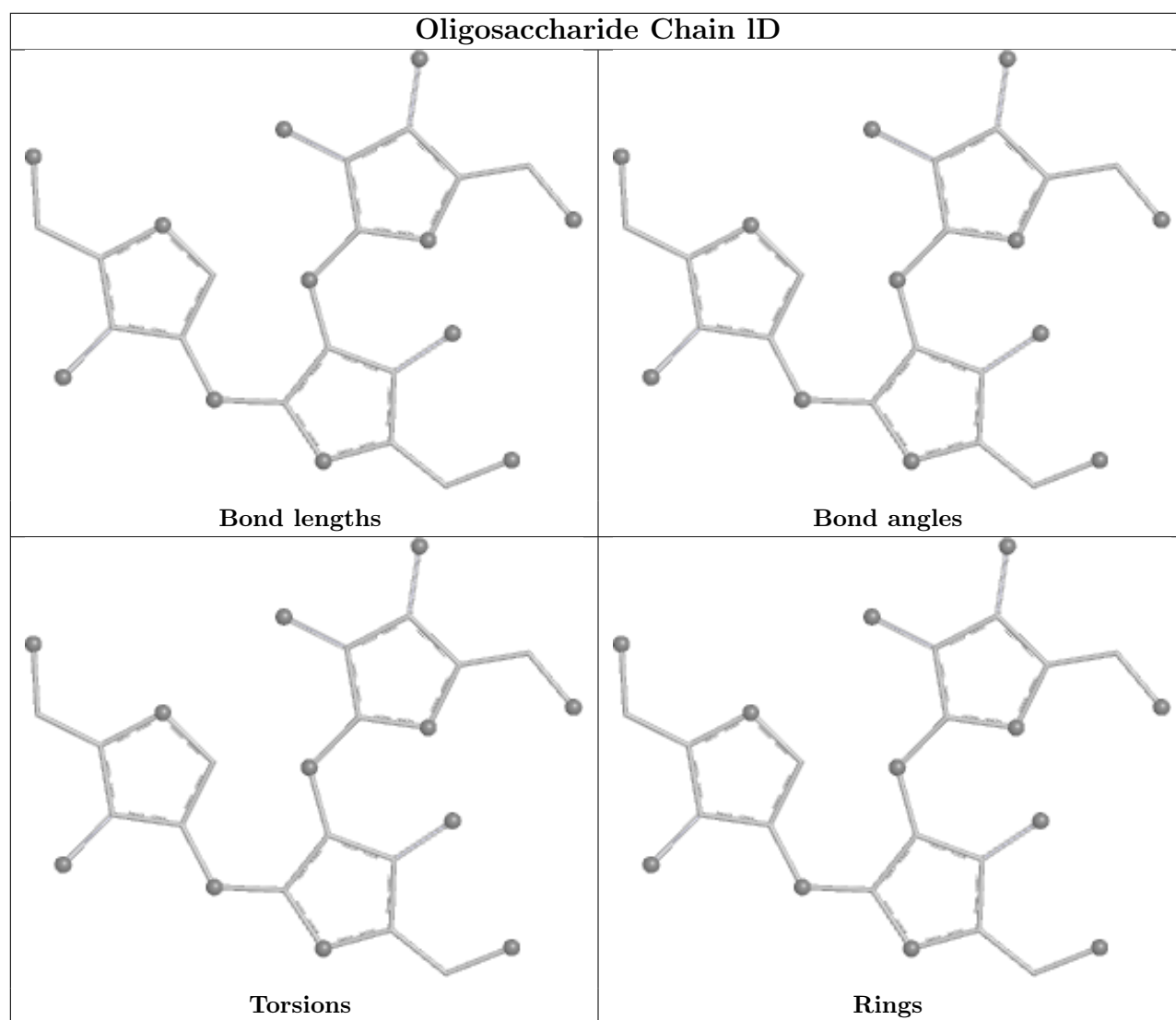


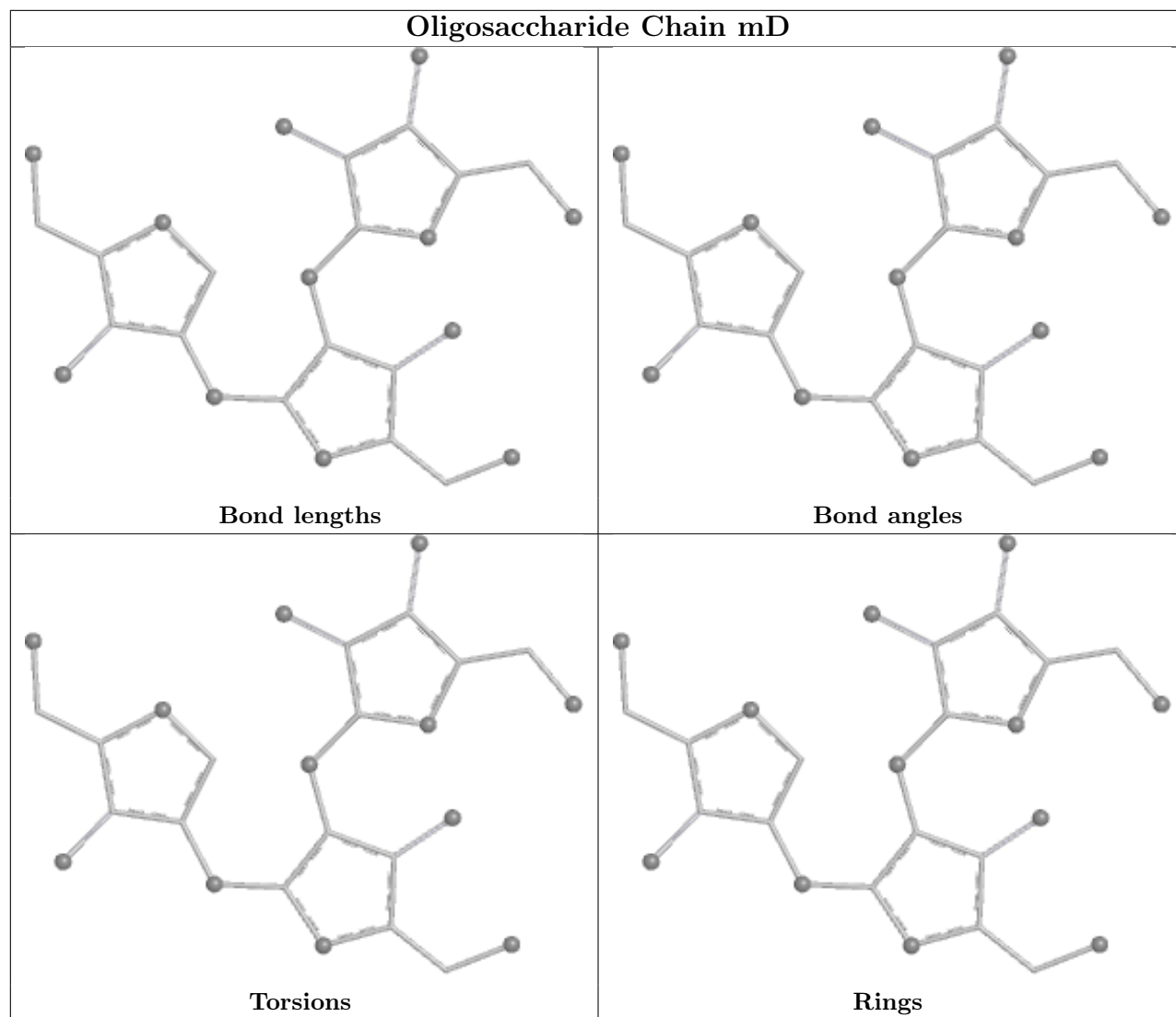


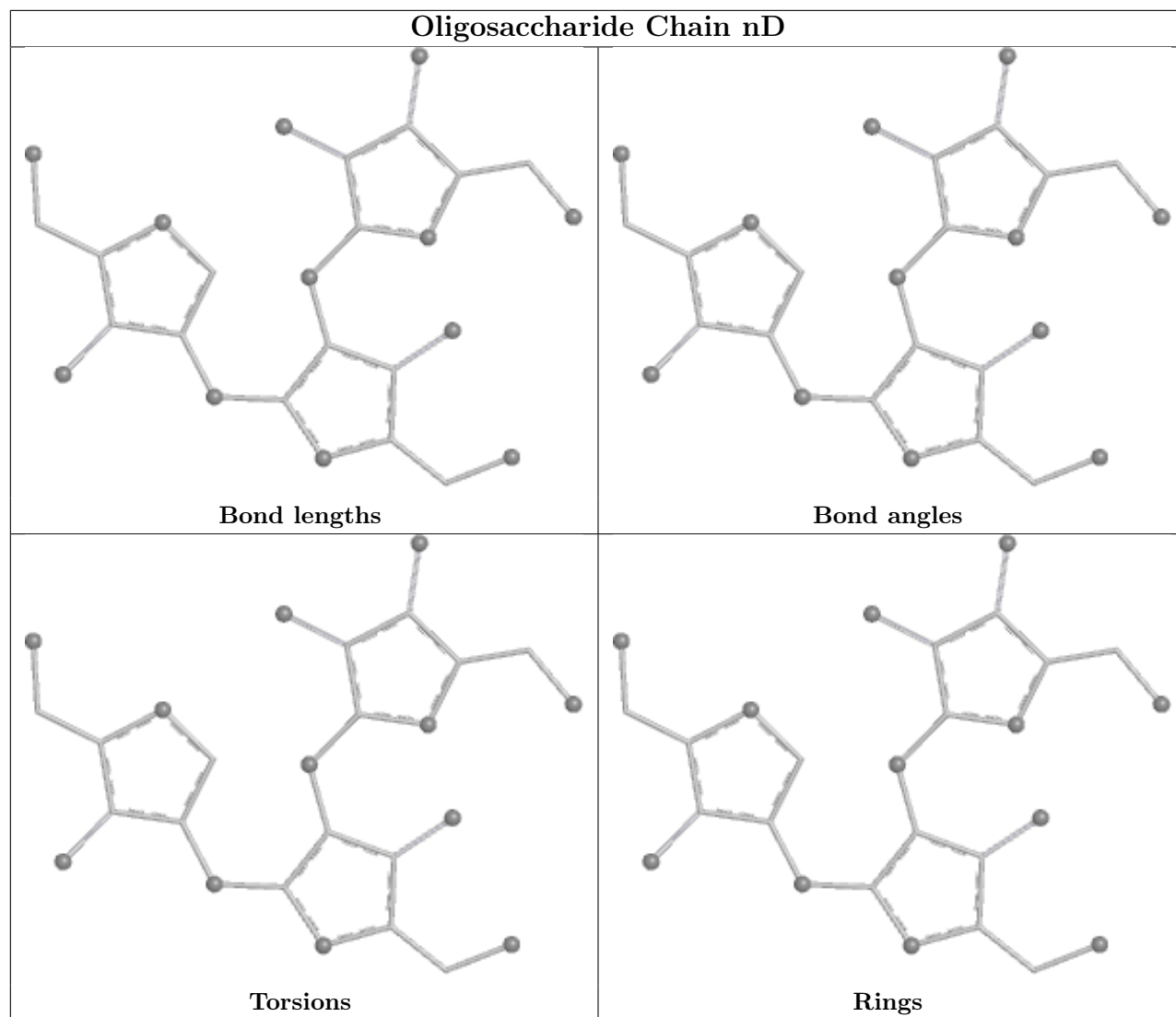


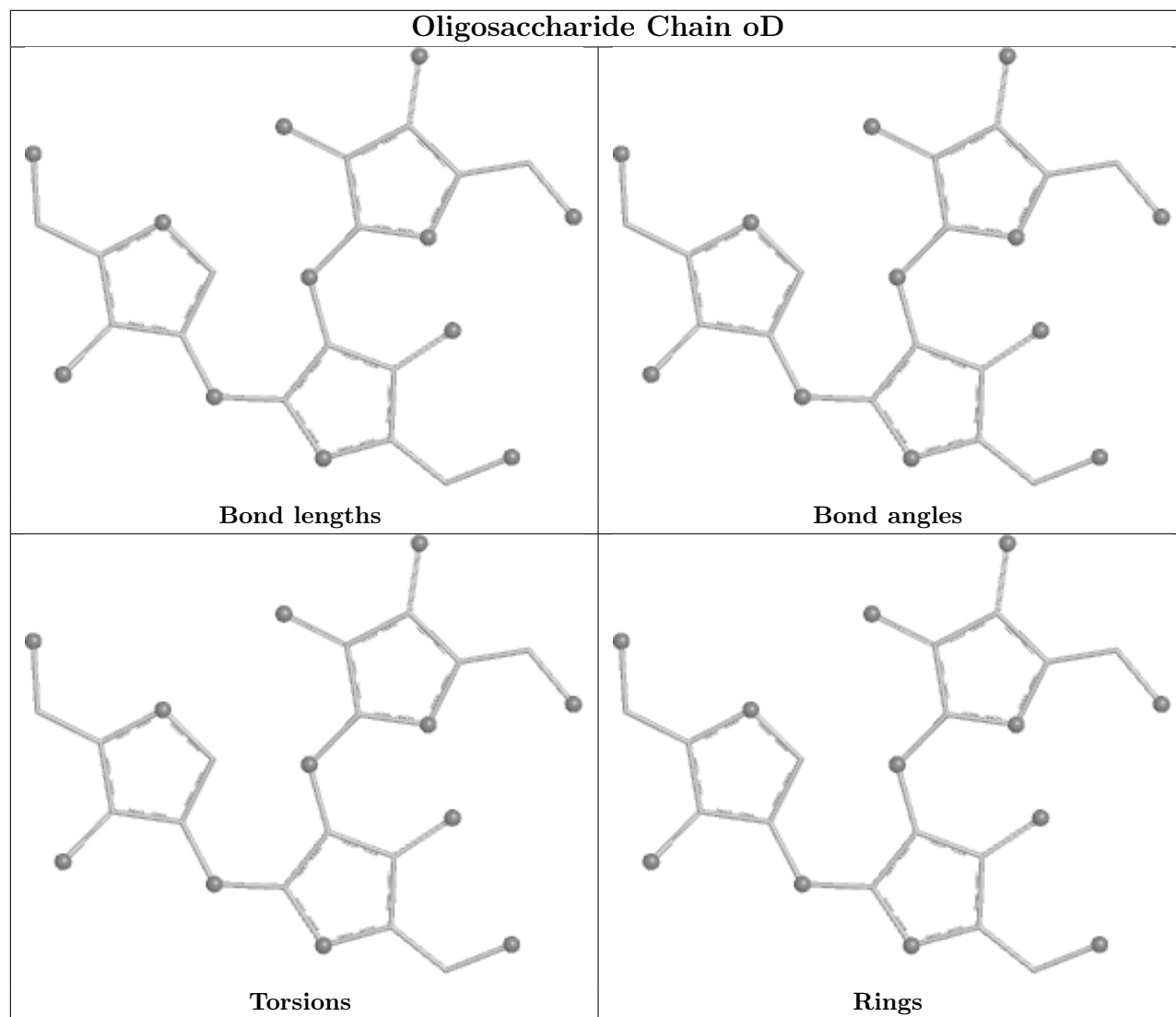


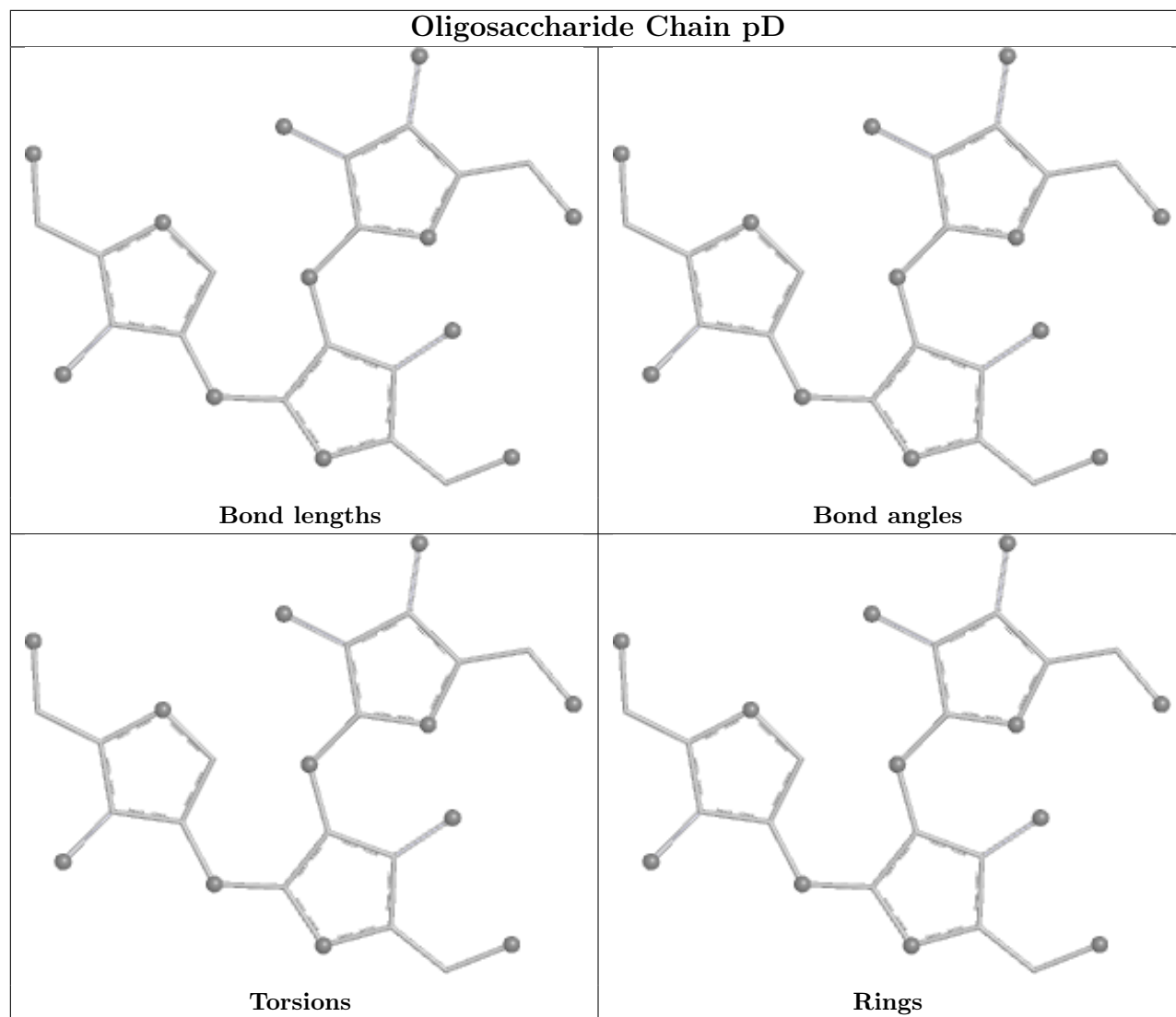


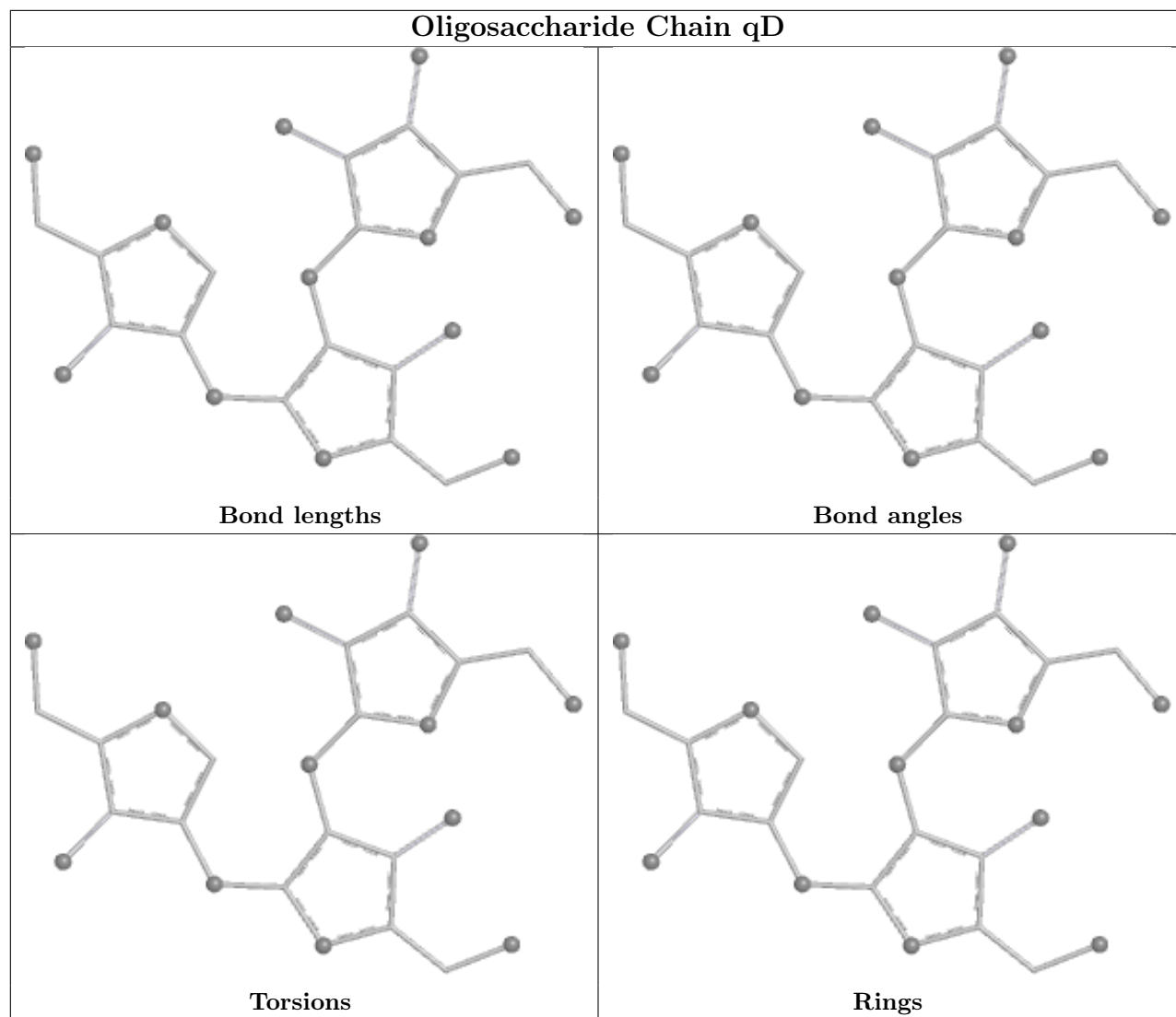


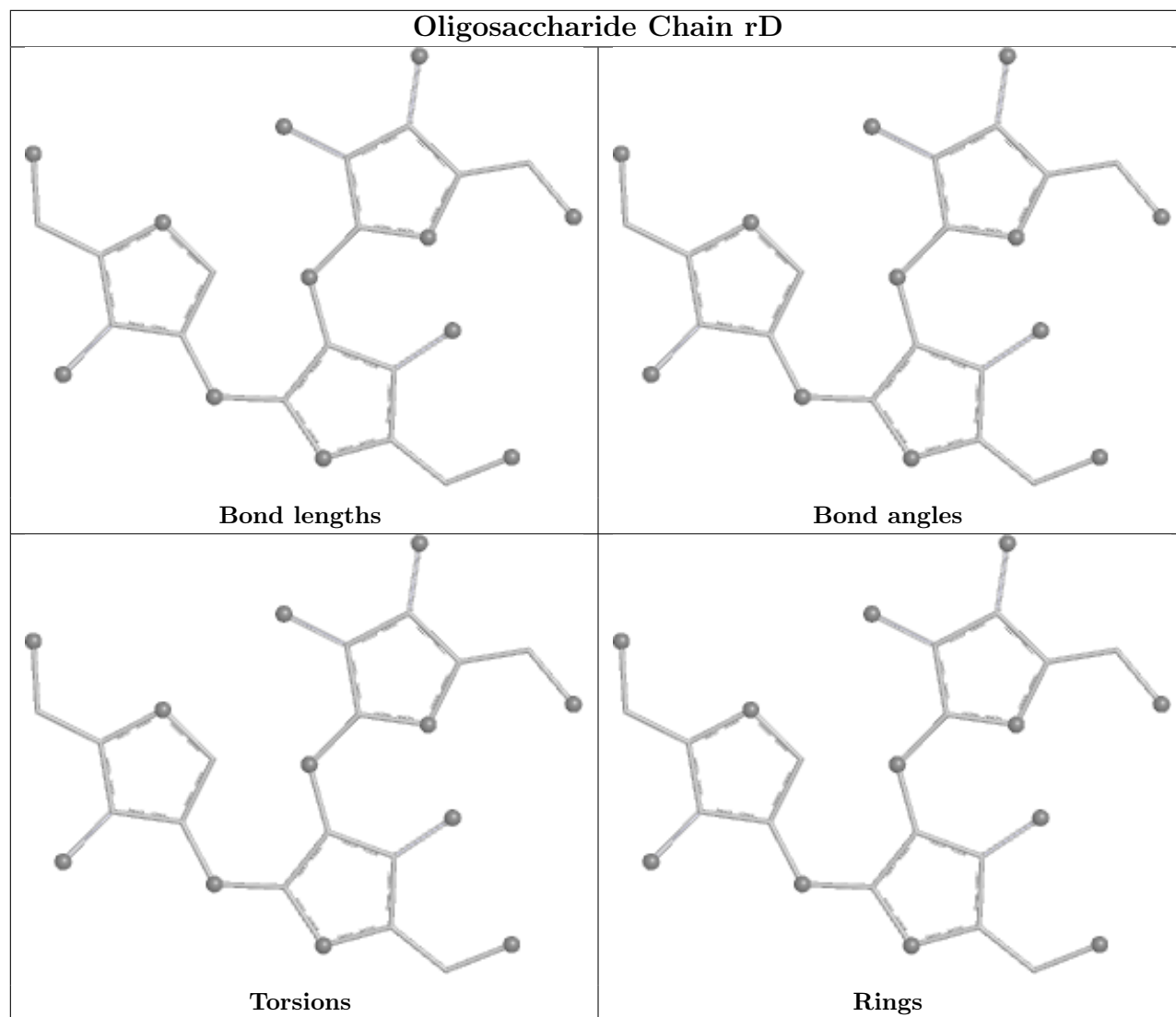


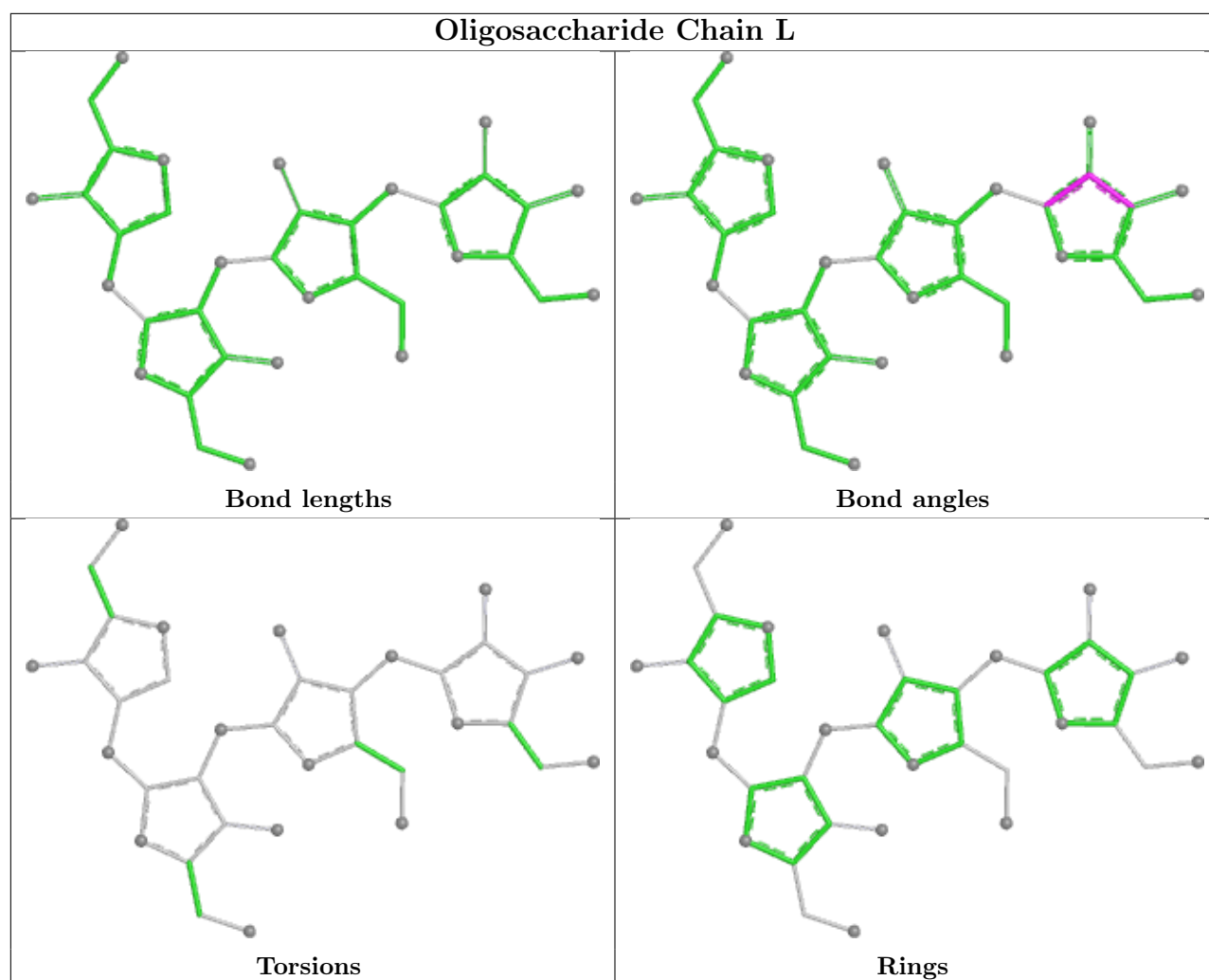


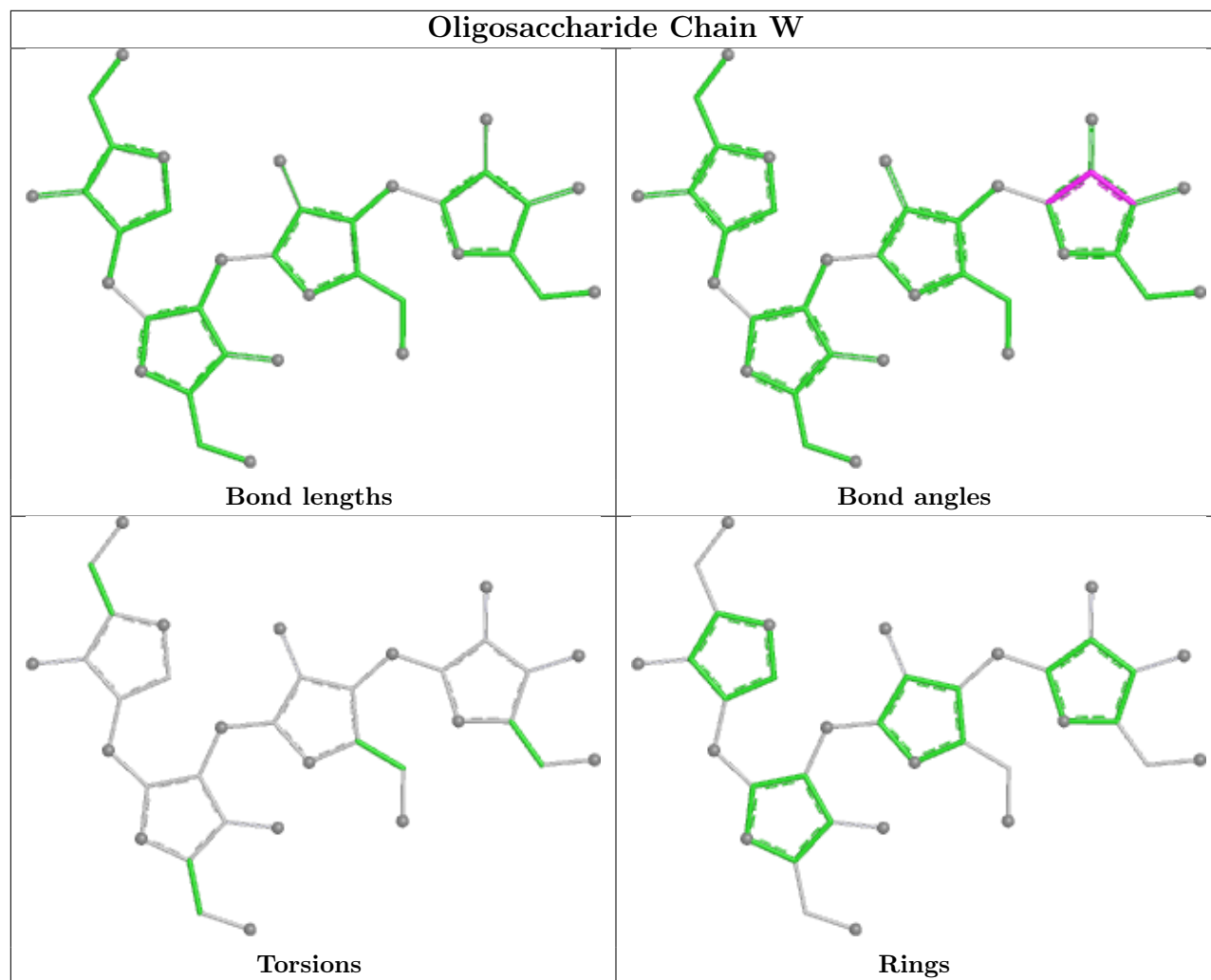


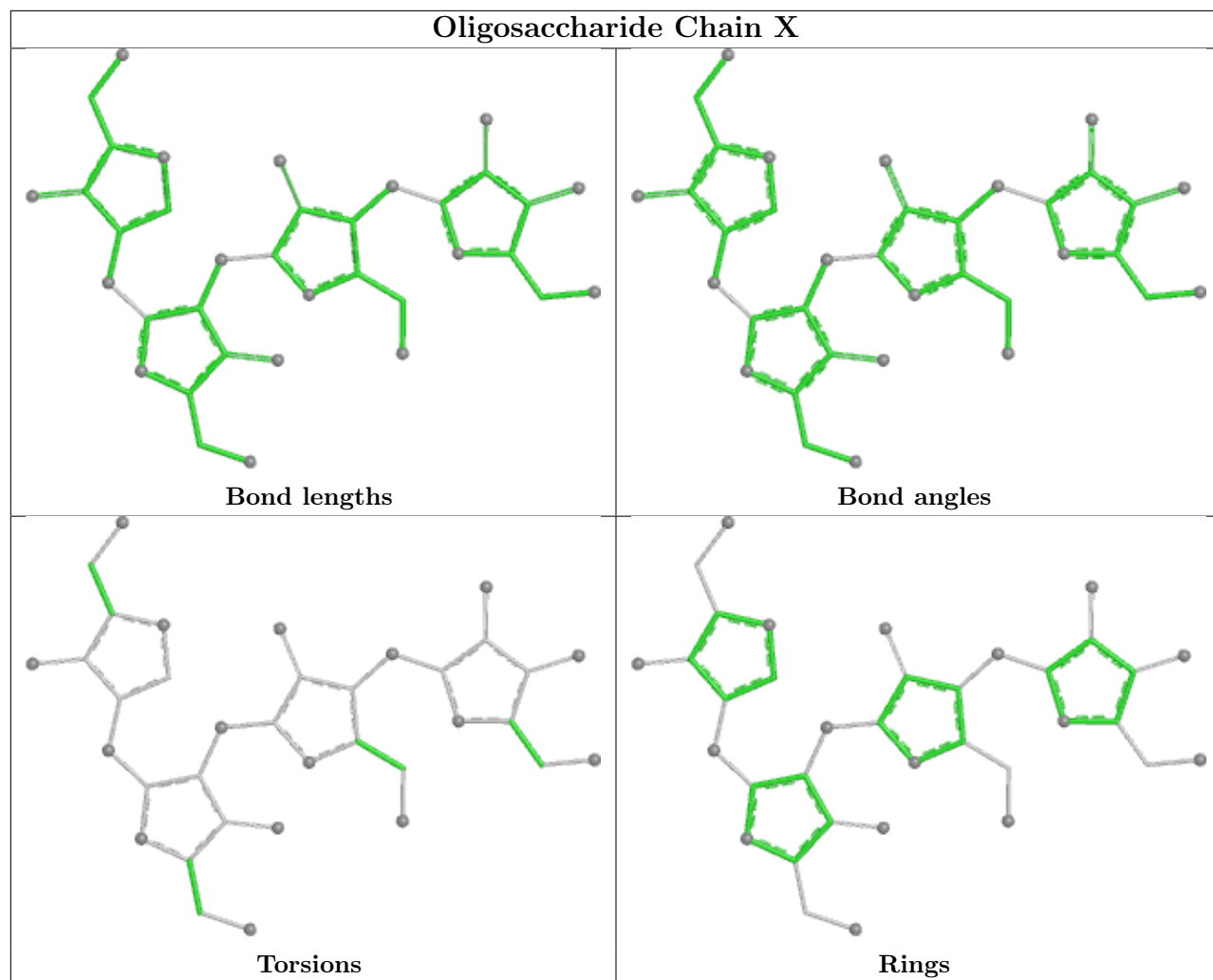


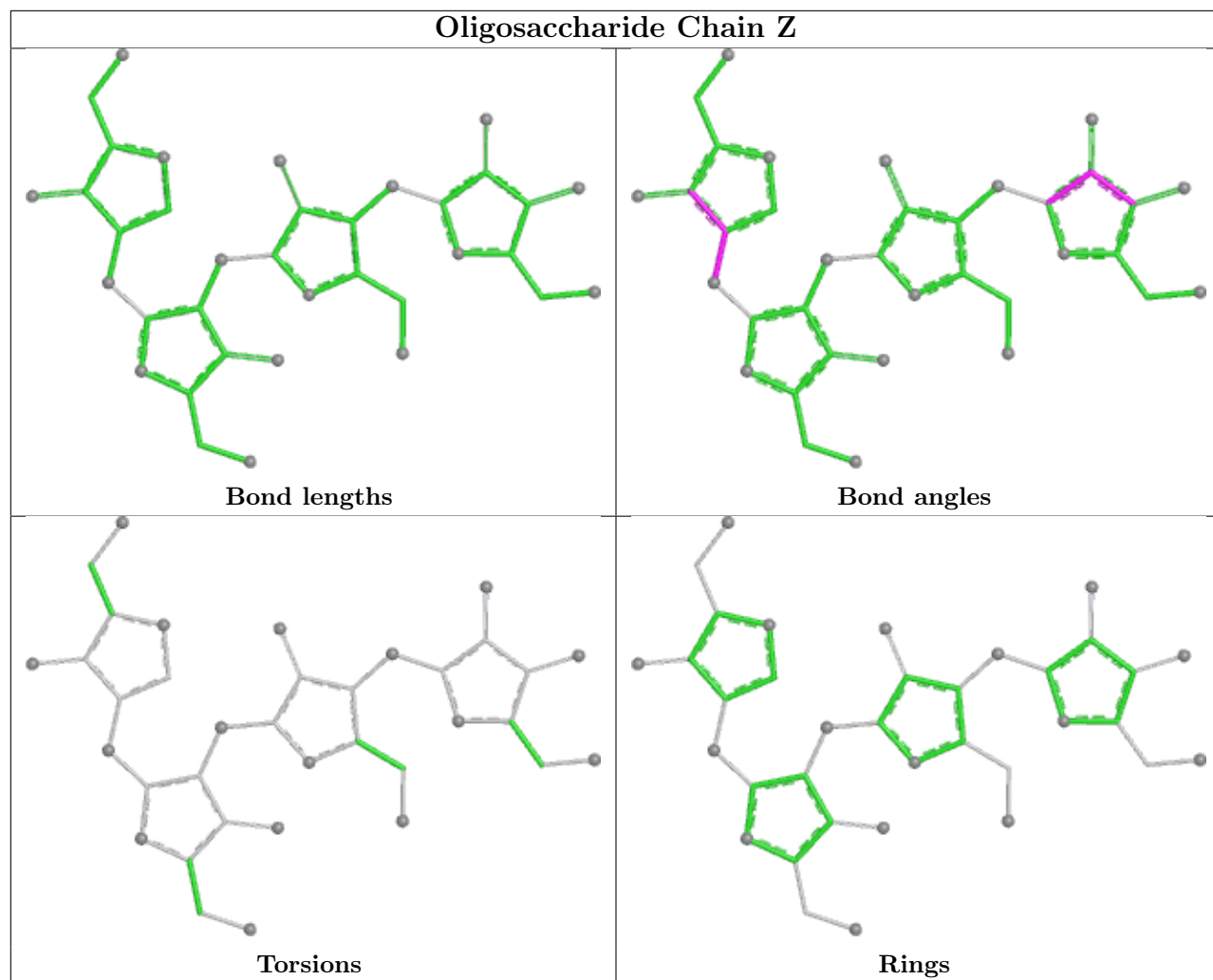


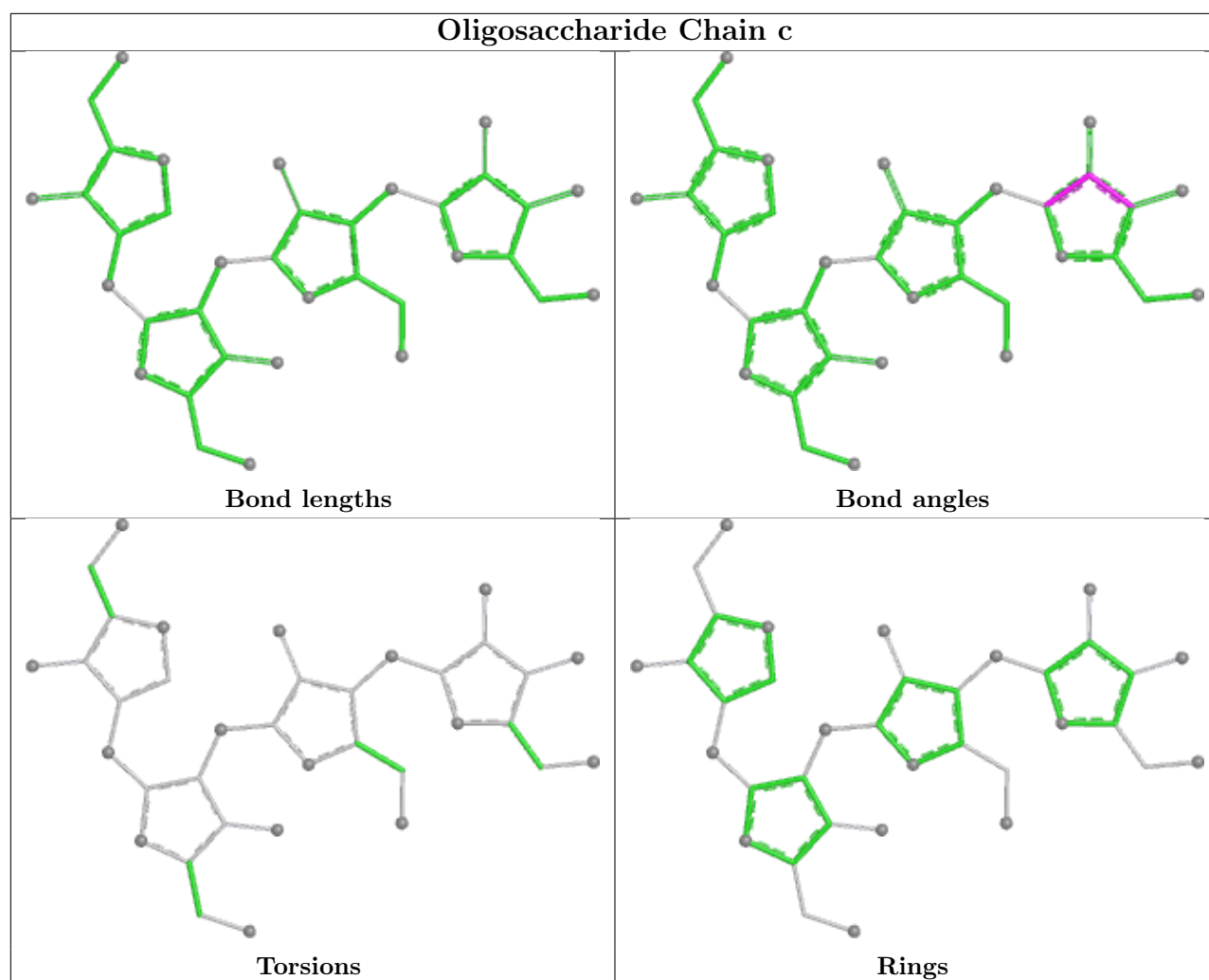


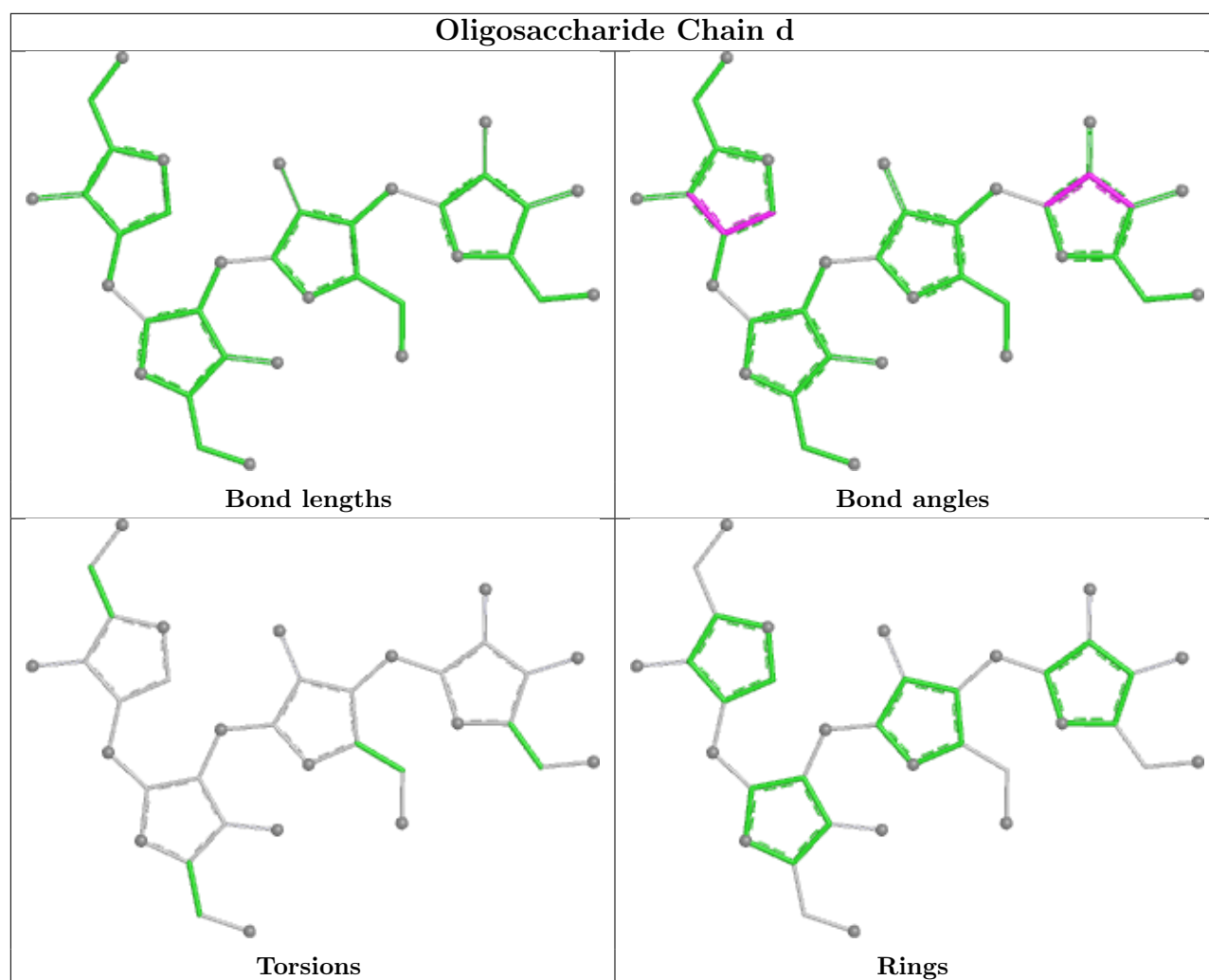


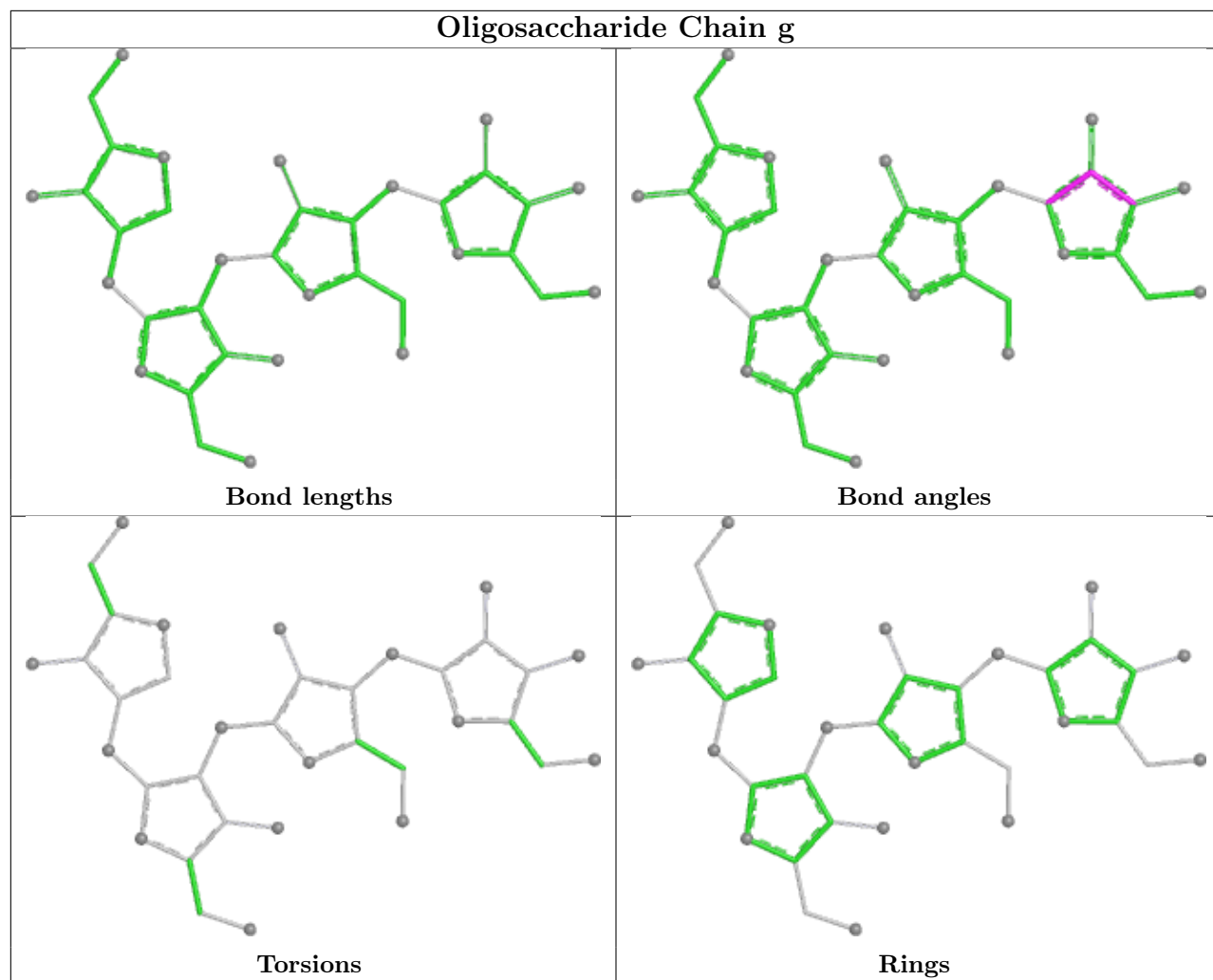


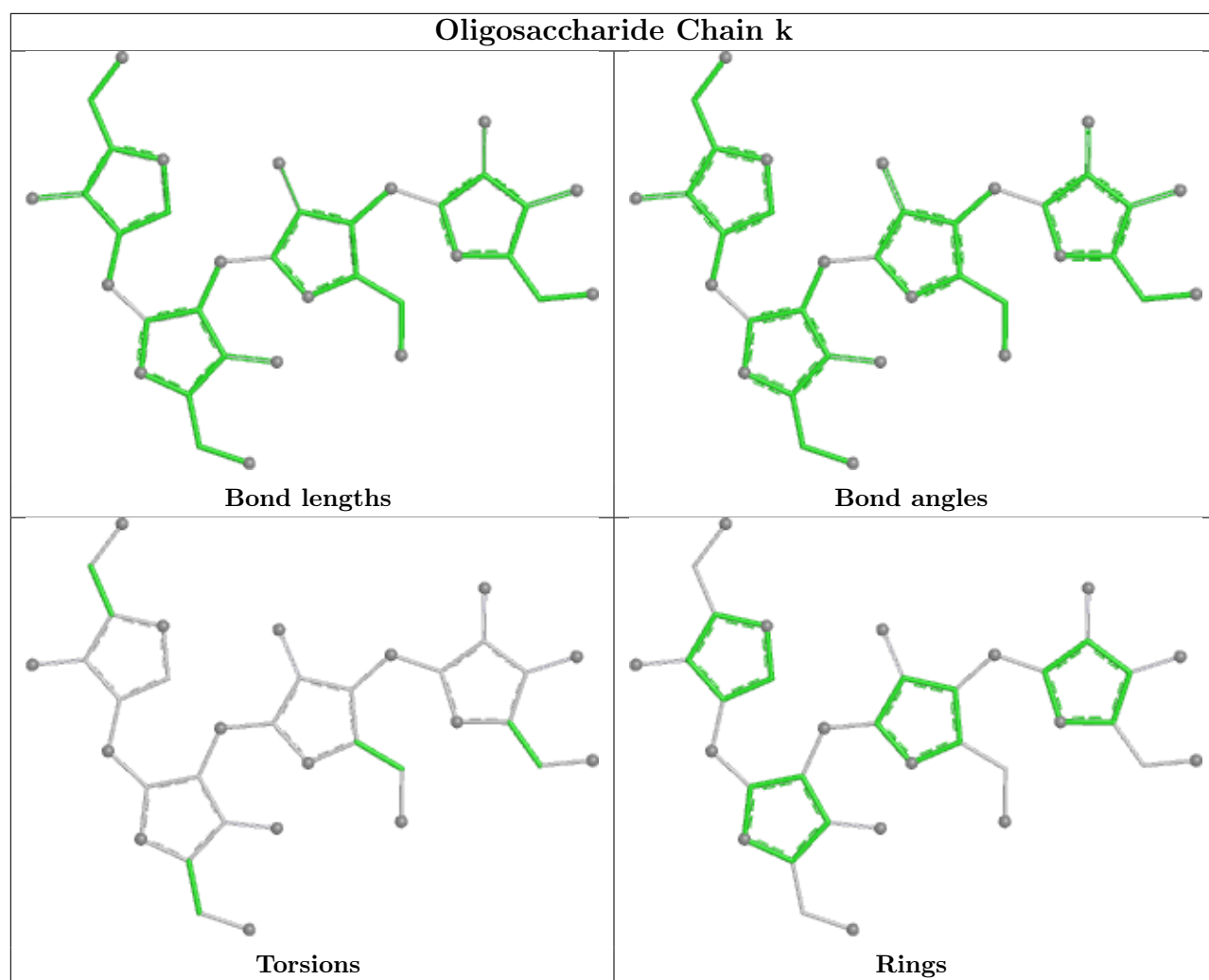


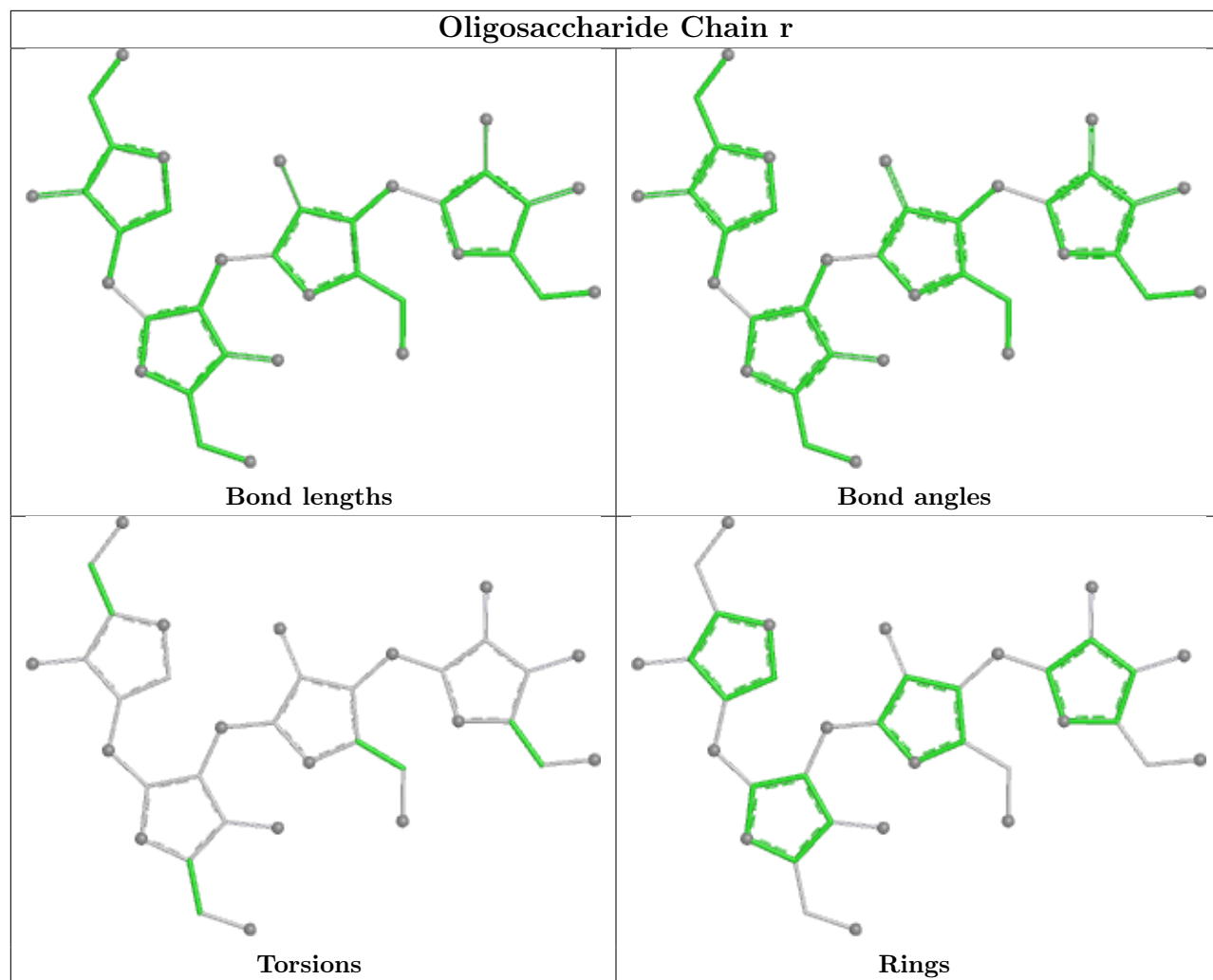


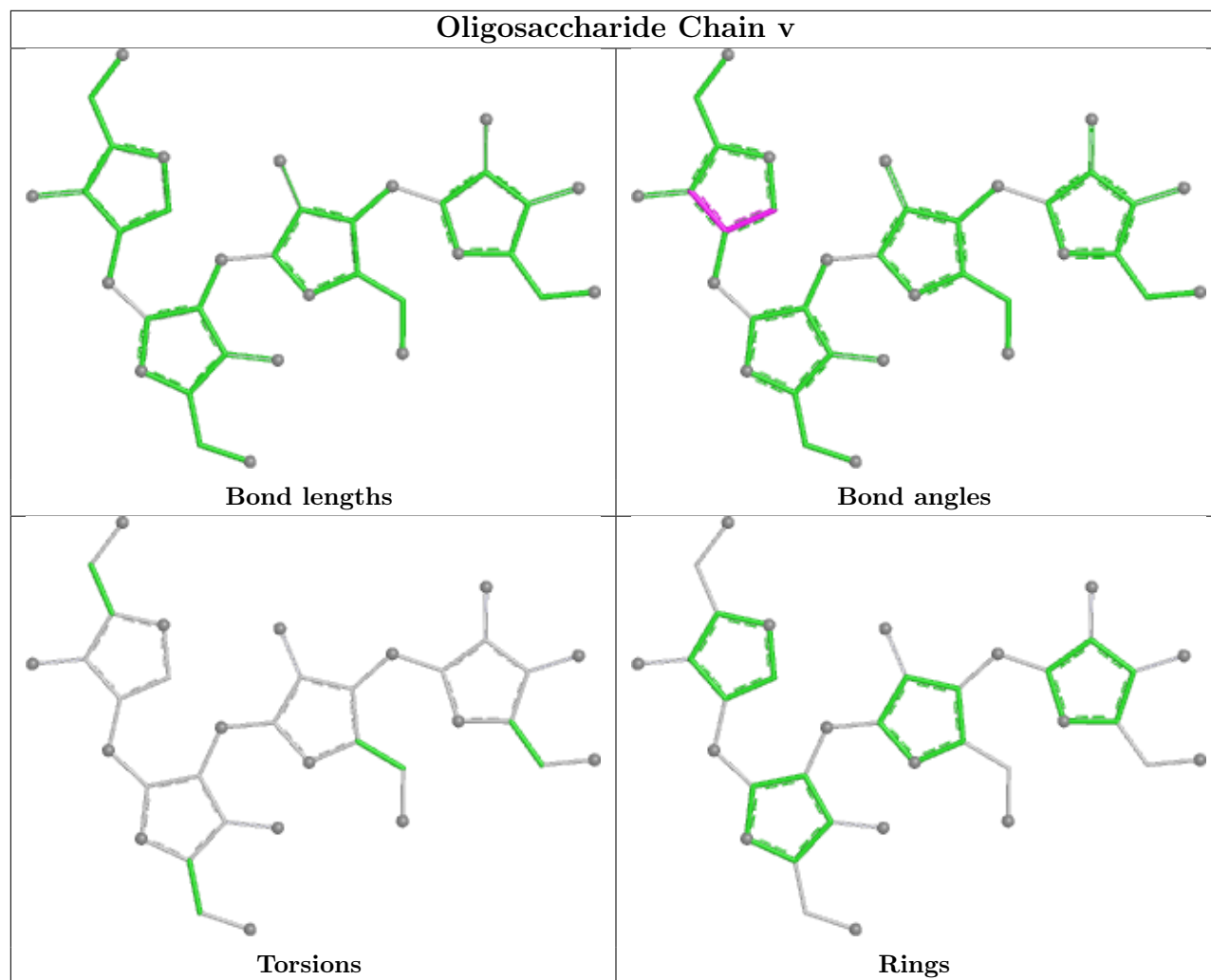


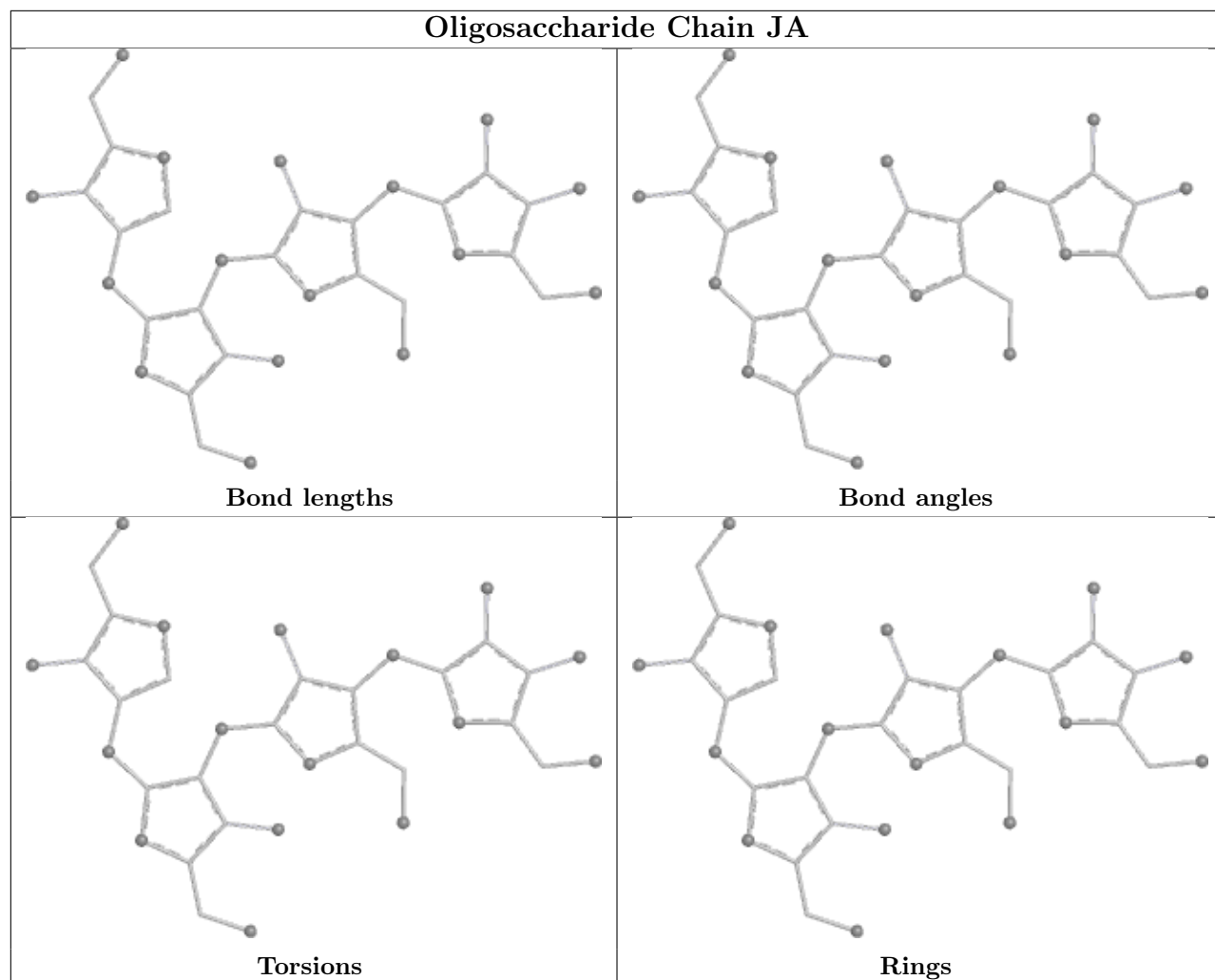


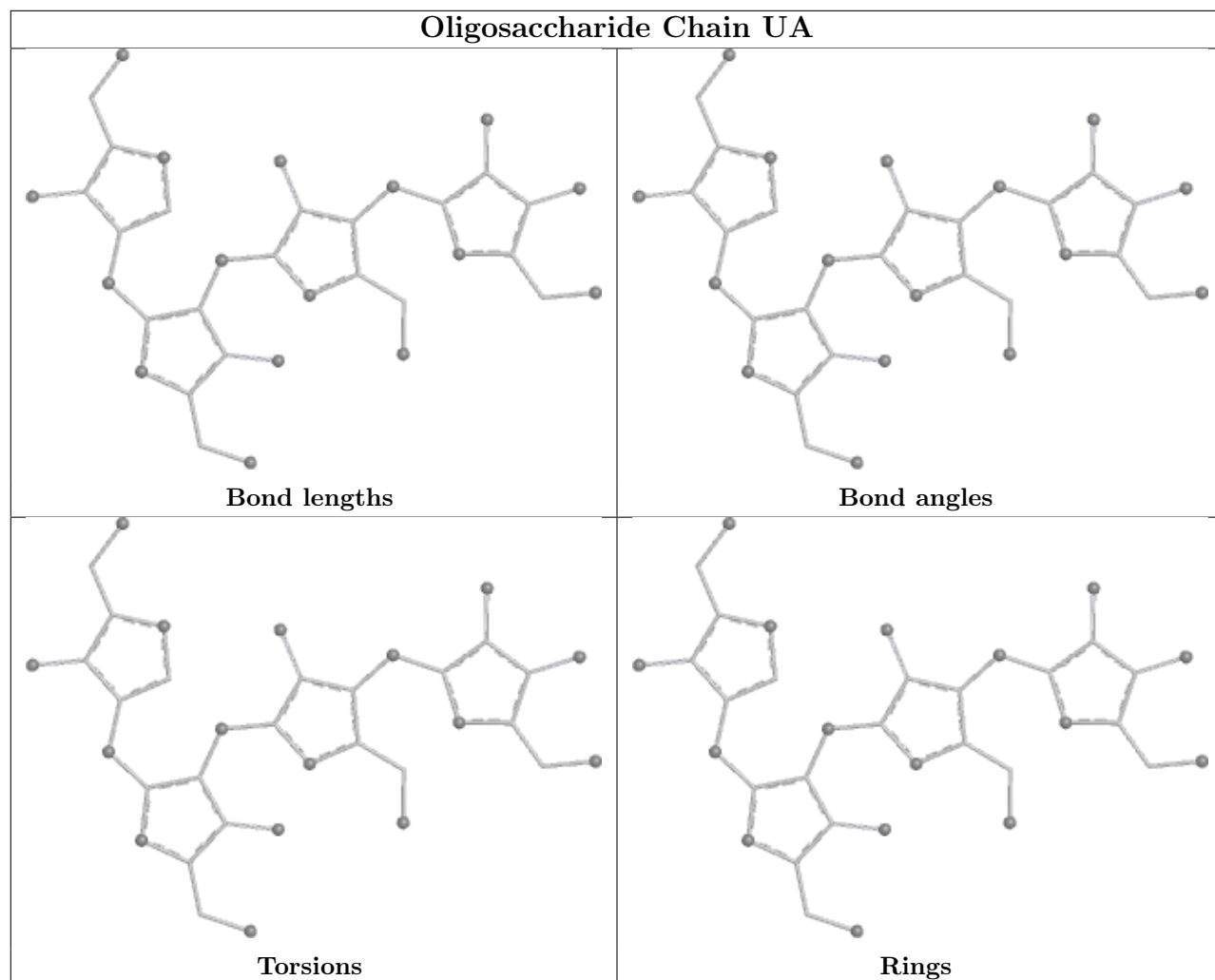


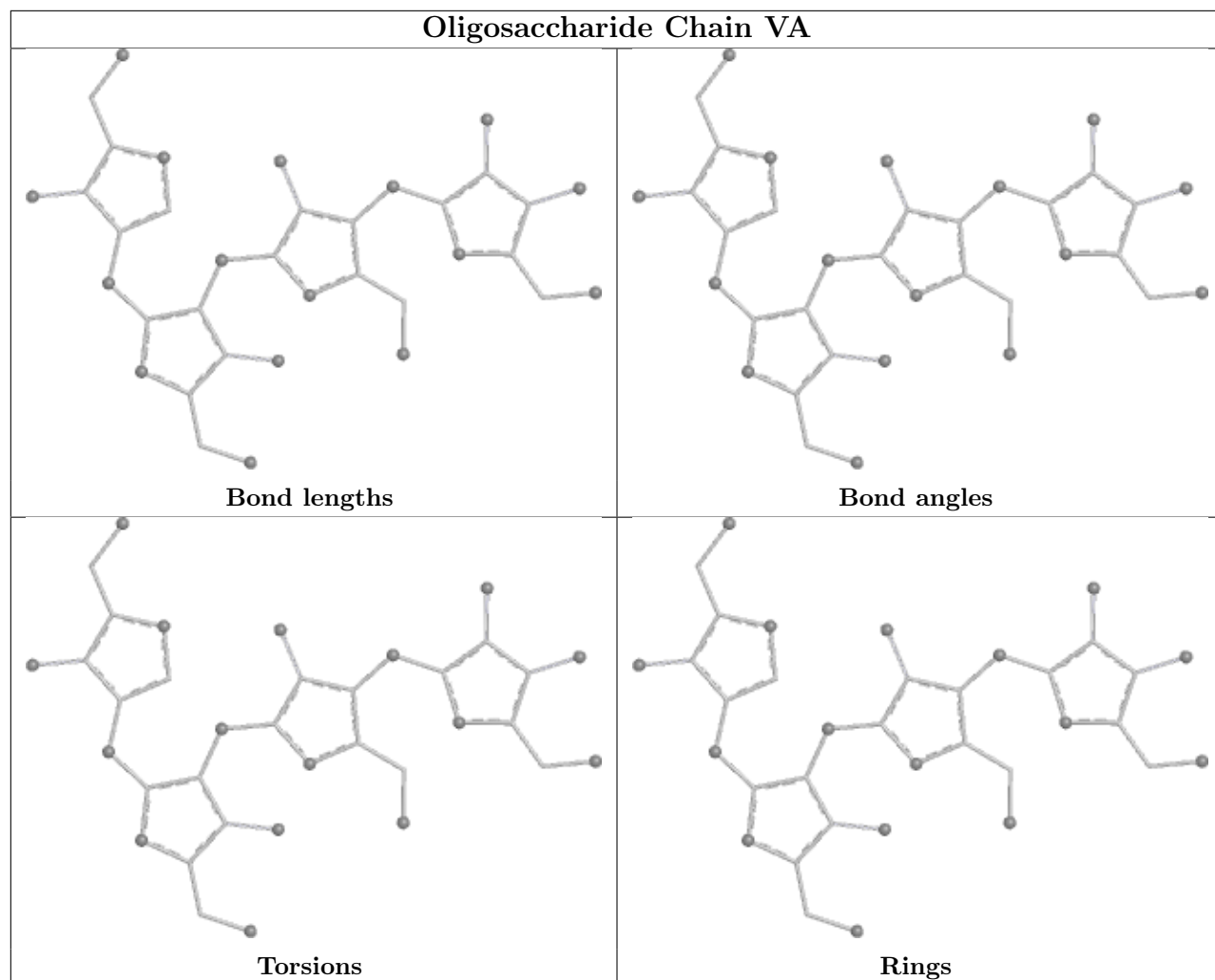




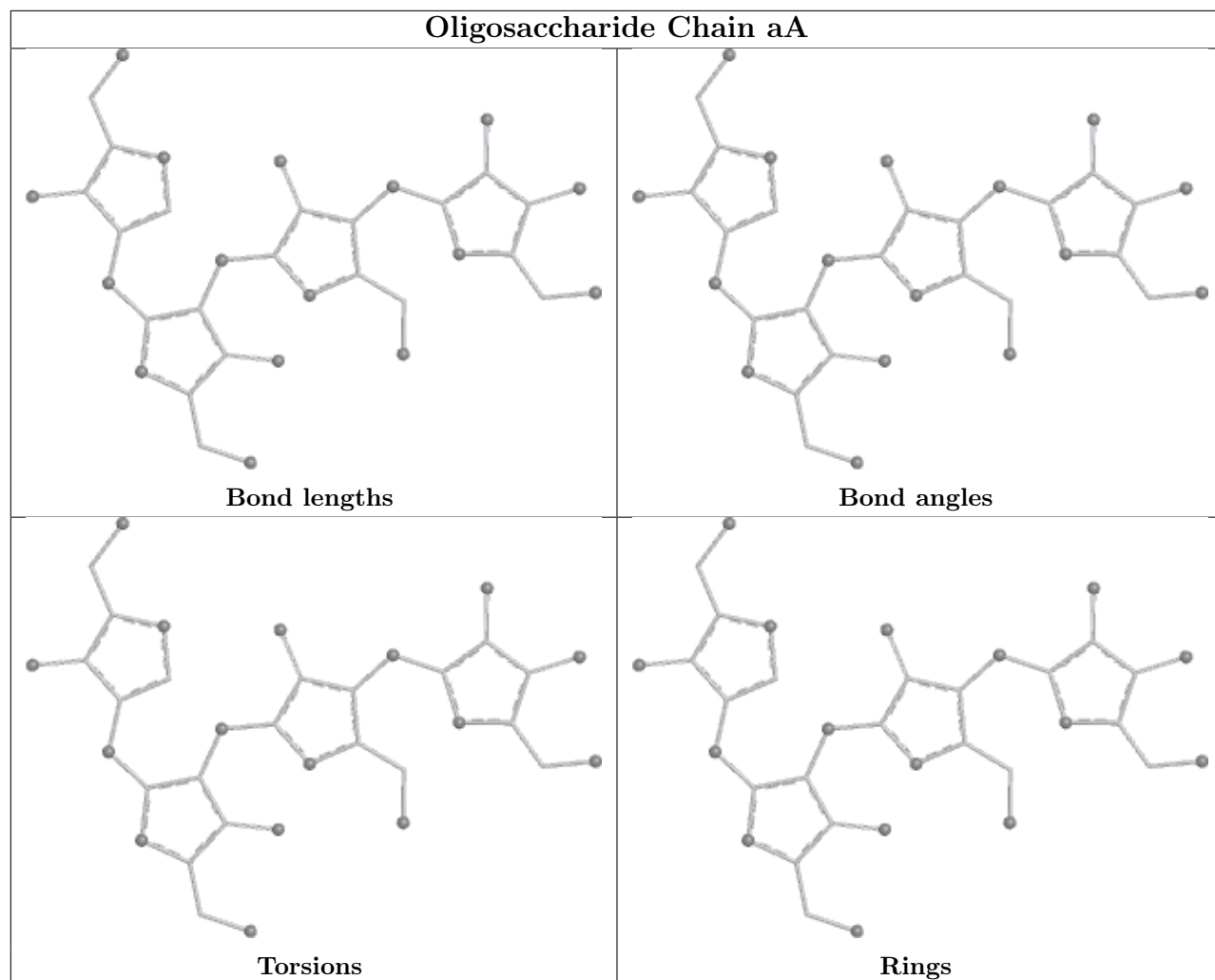


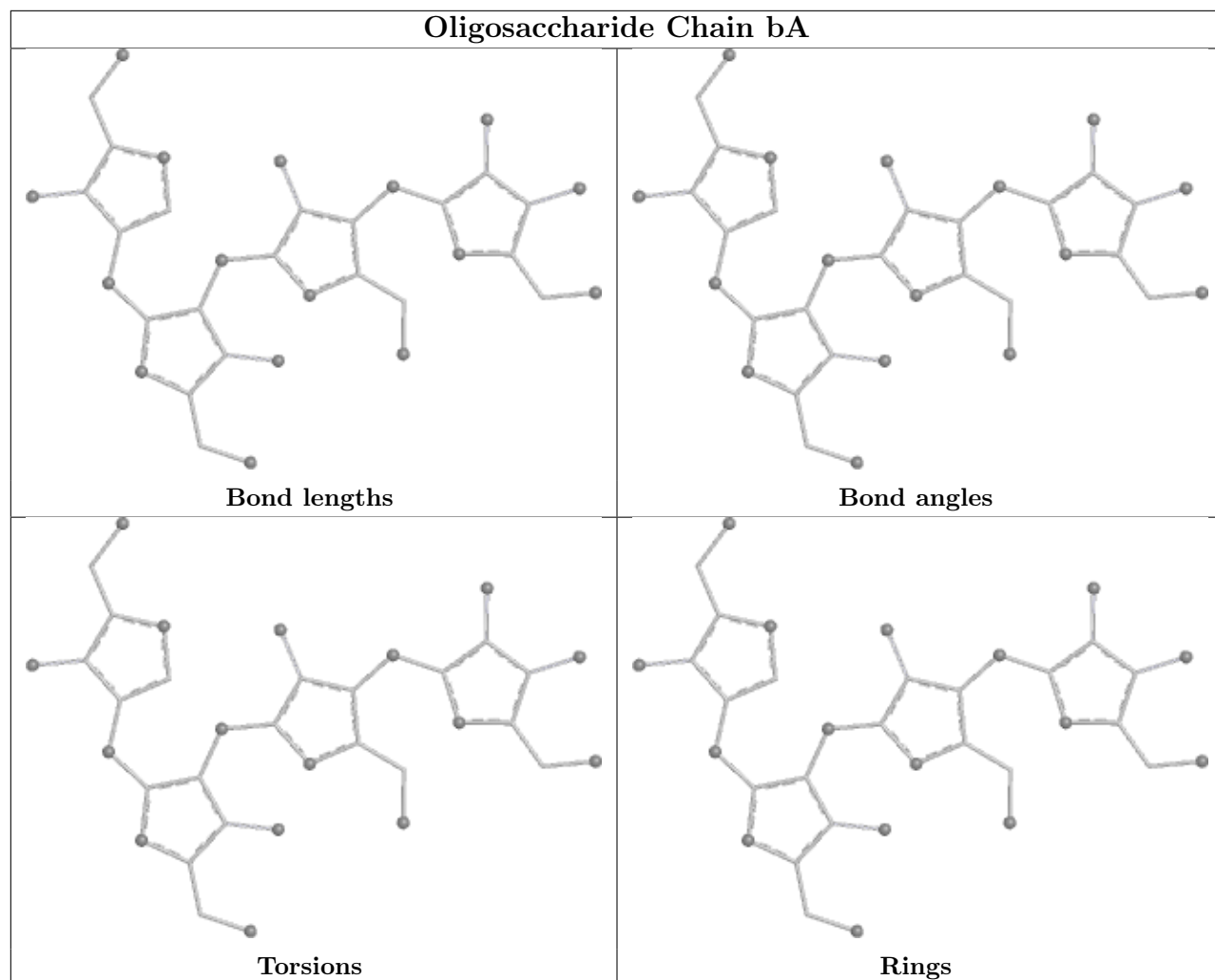
Oligosaccharide Chain JA

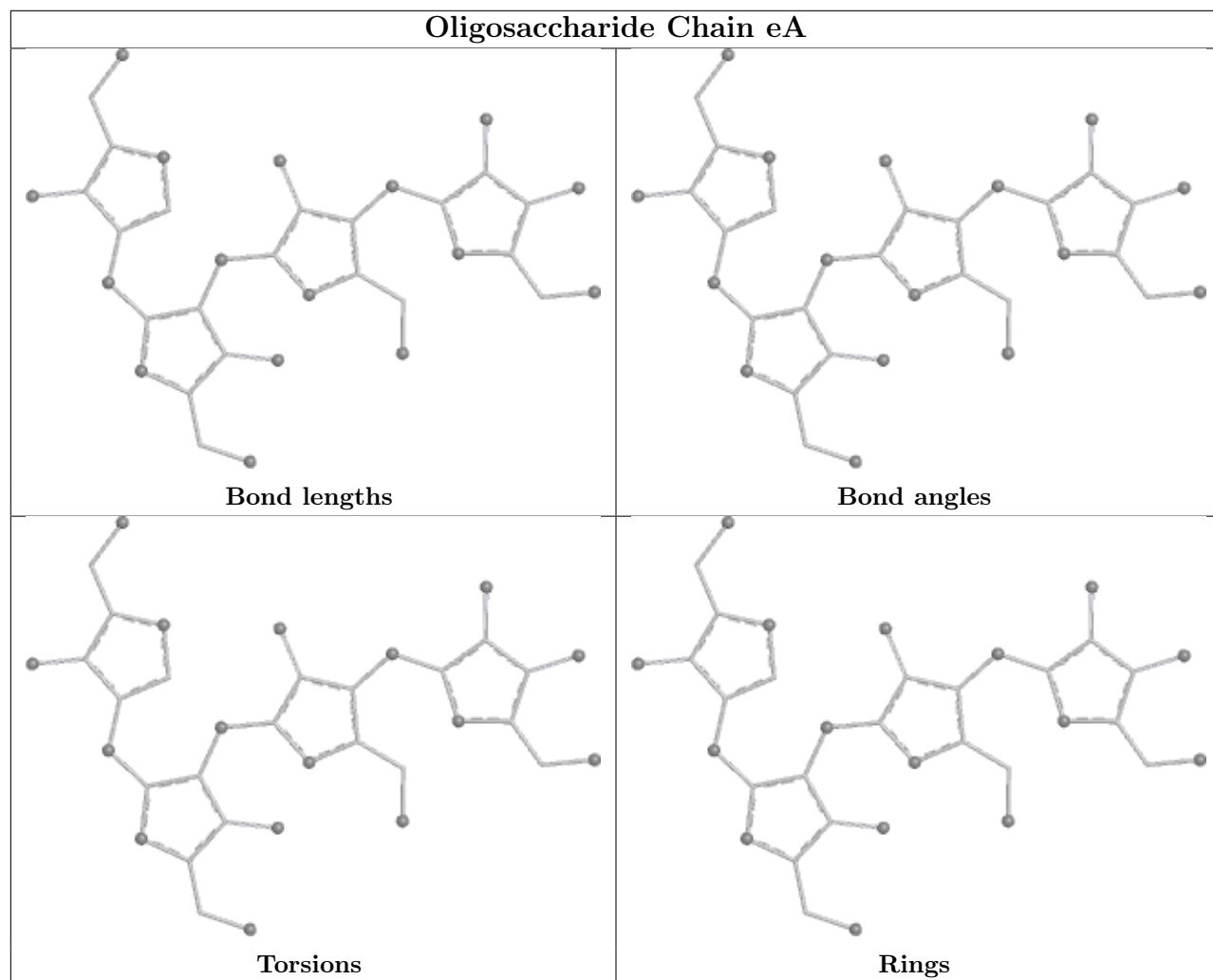
Oligosaccharide Chain UA

Oligosaccharide Chain VA

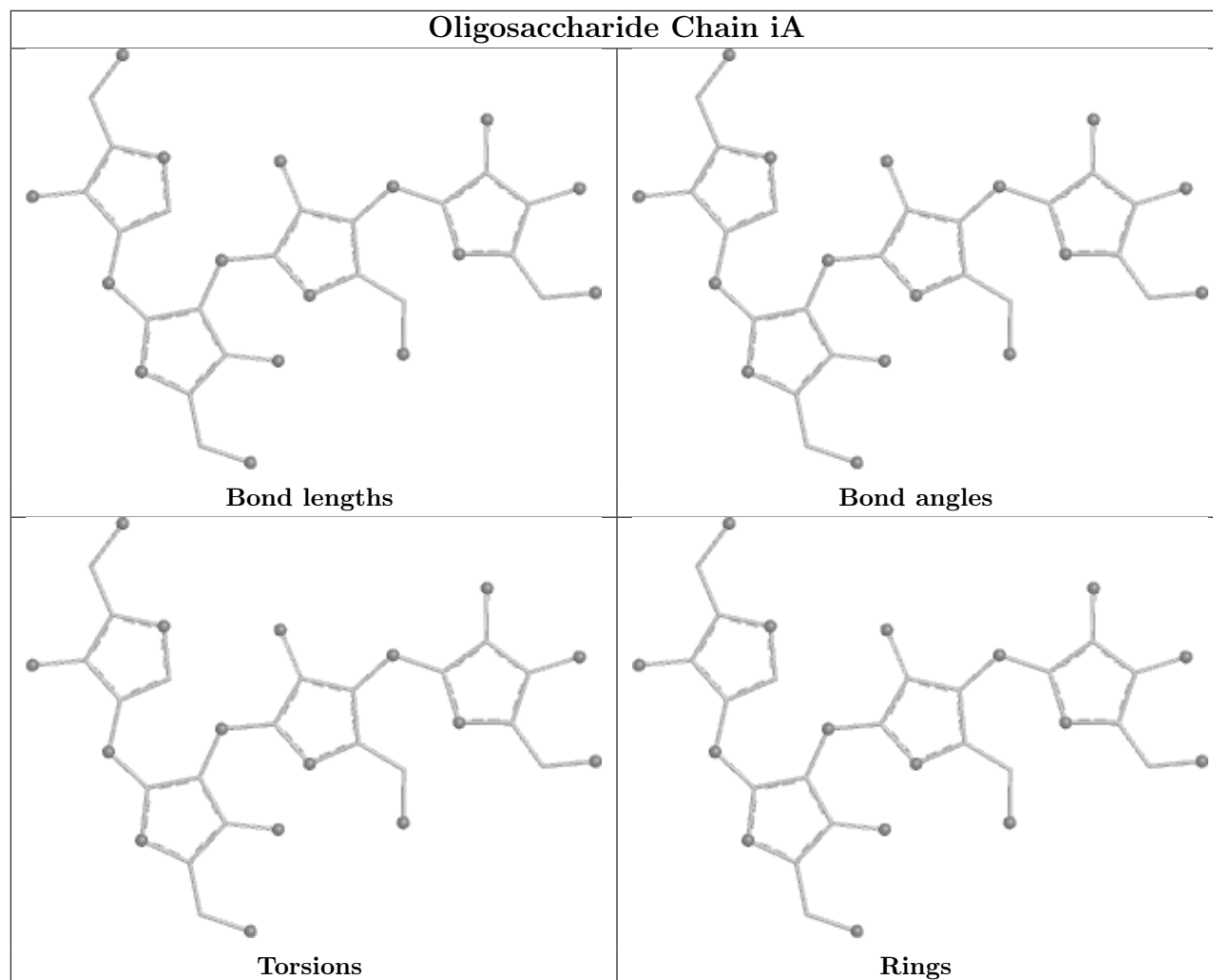
Oligosaccharide Chain aA

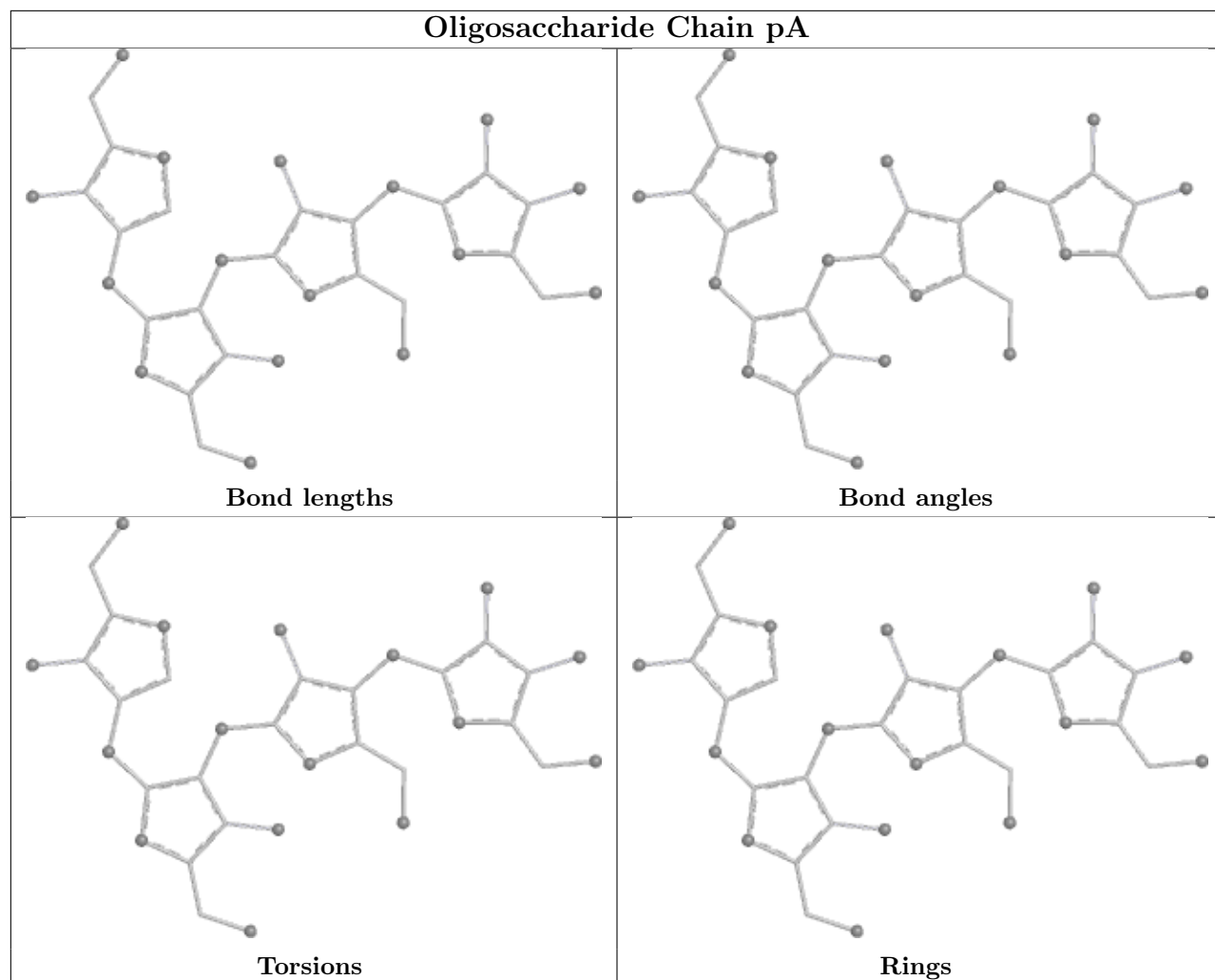


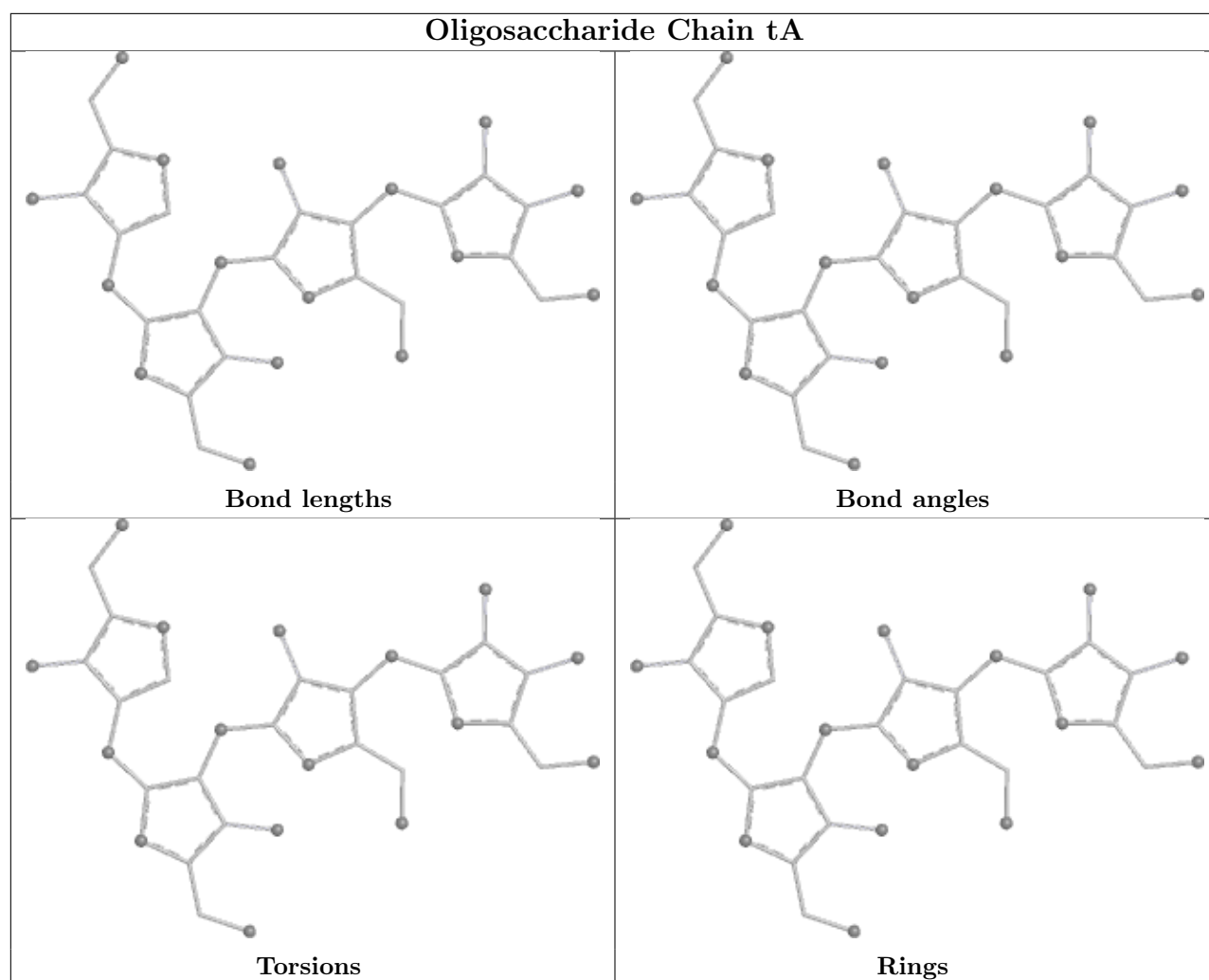
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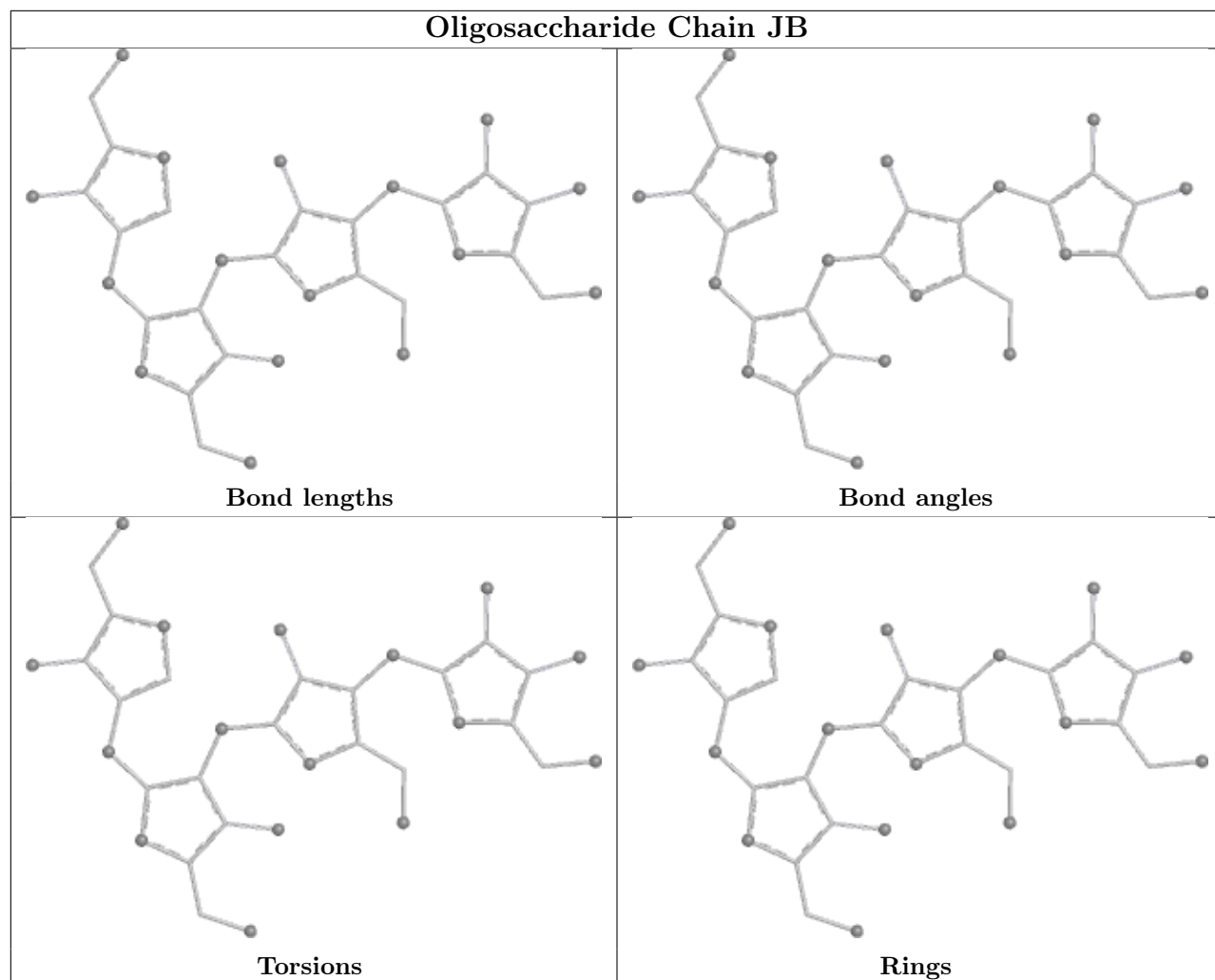


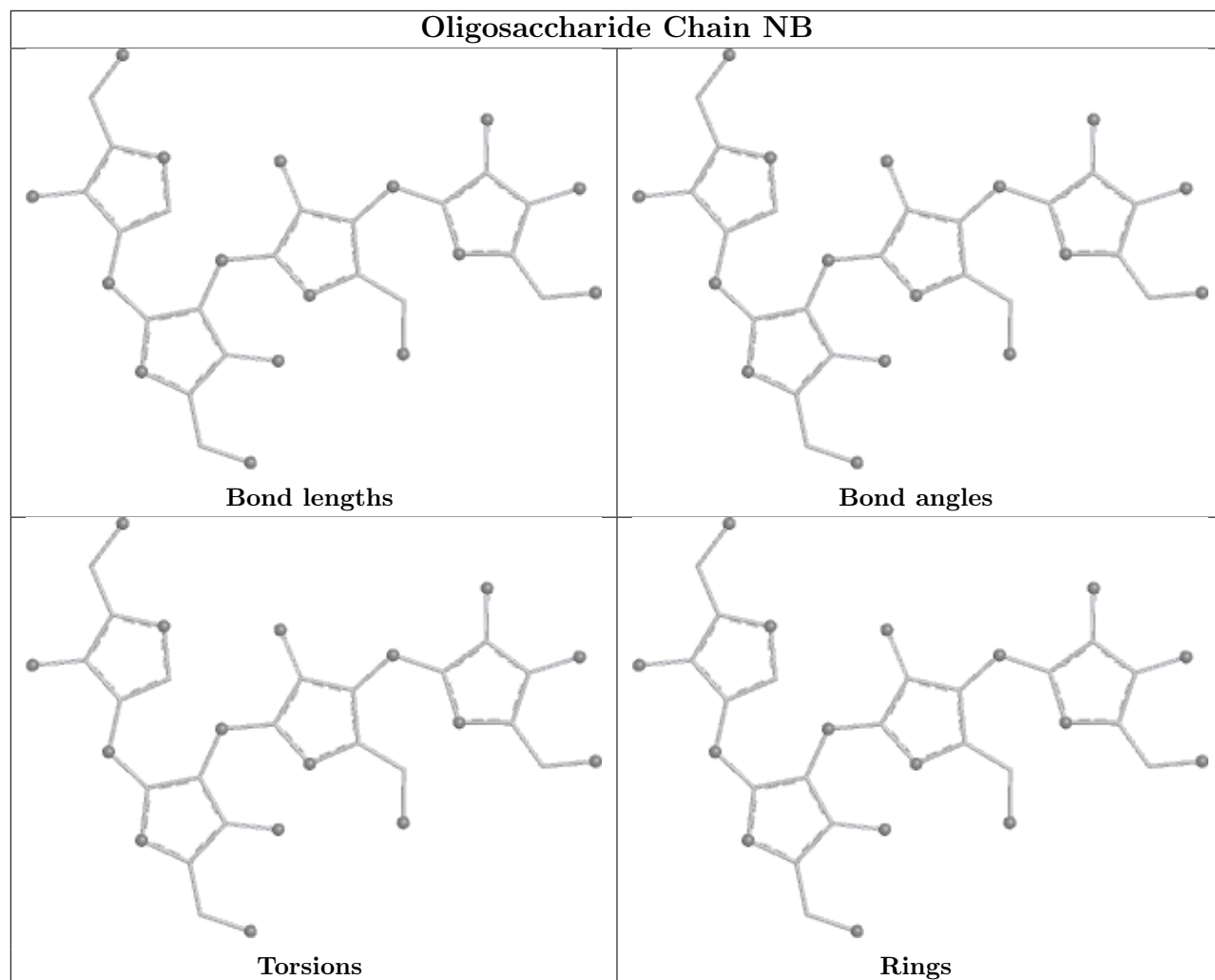
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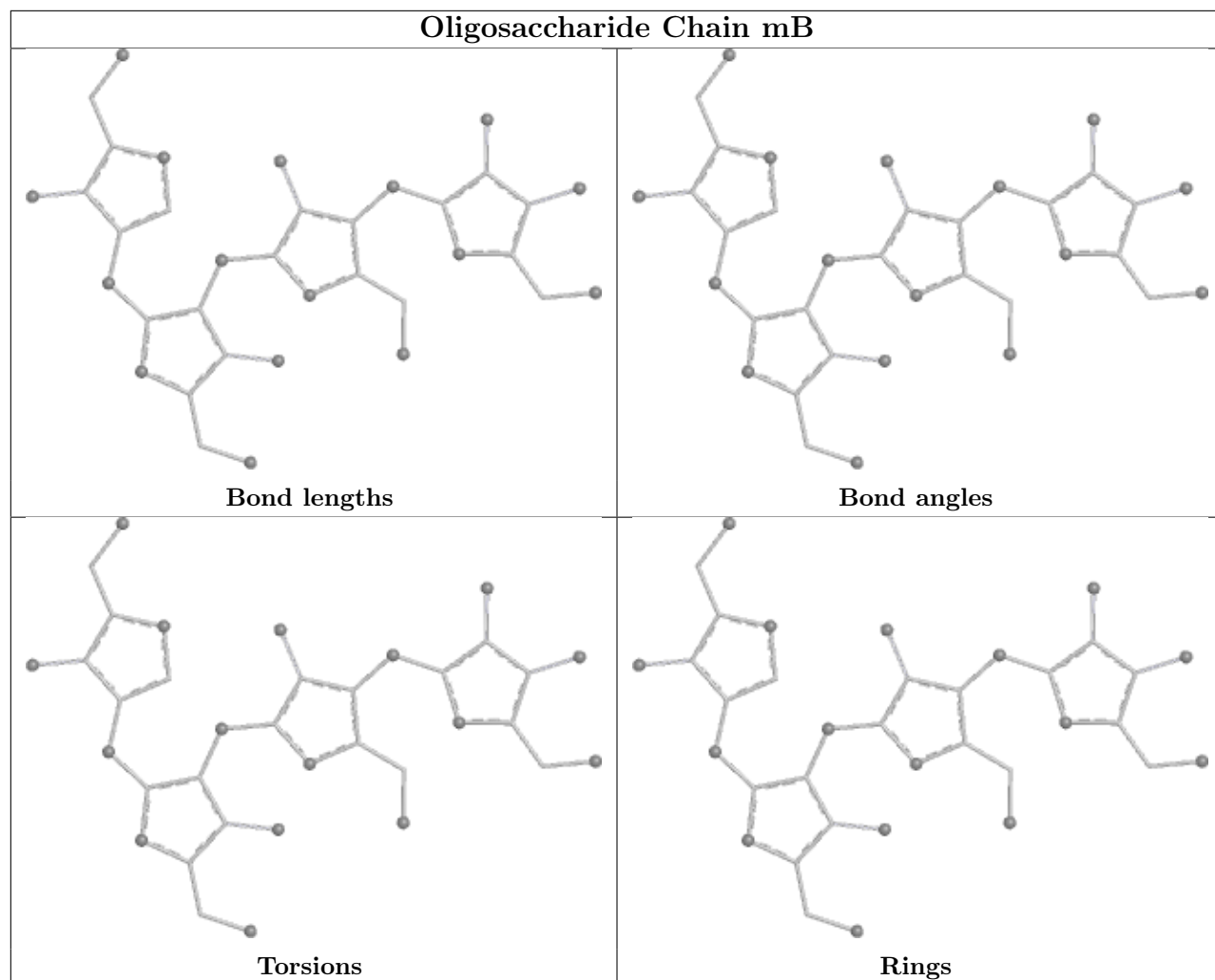


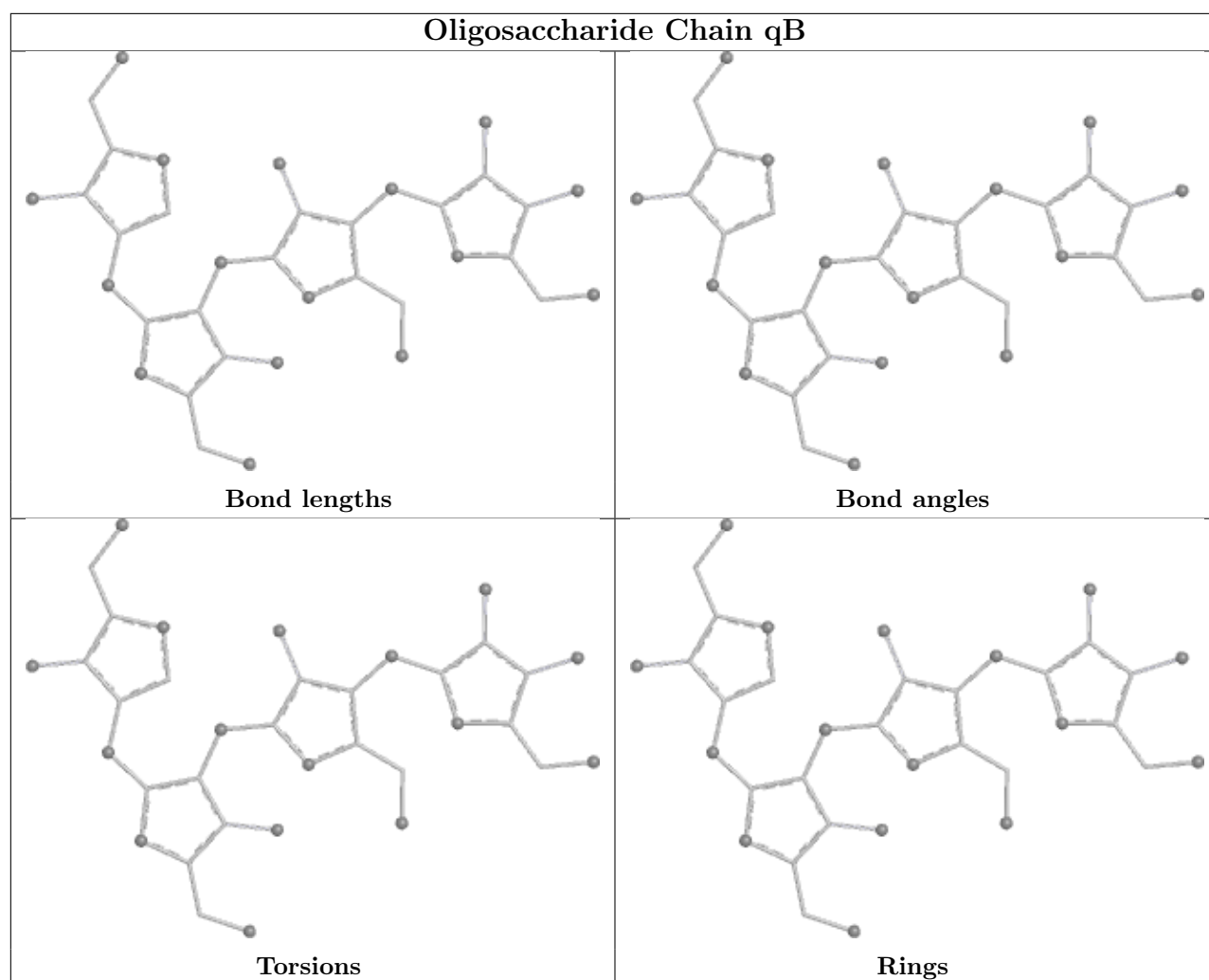
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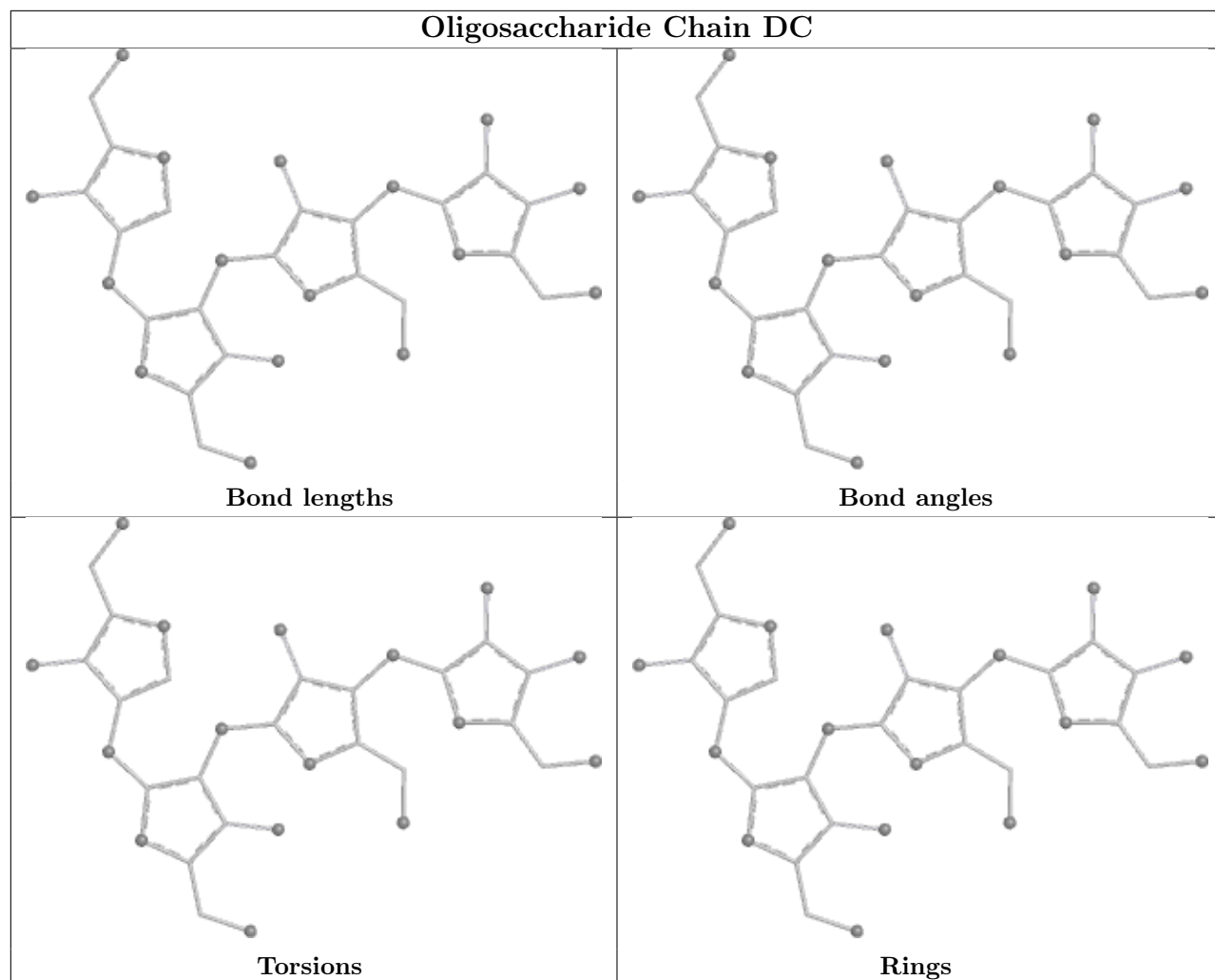


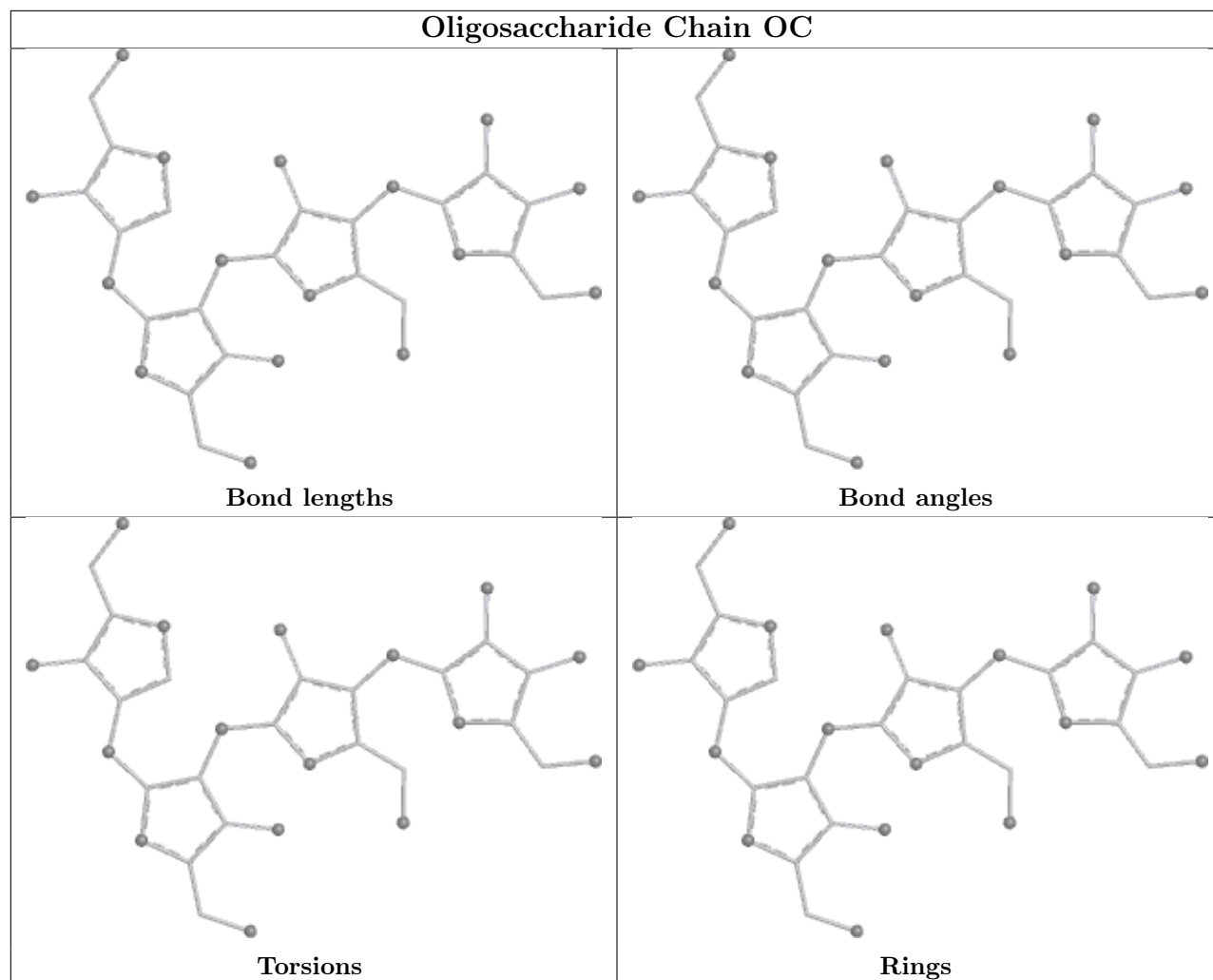
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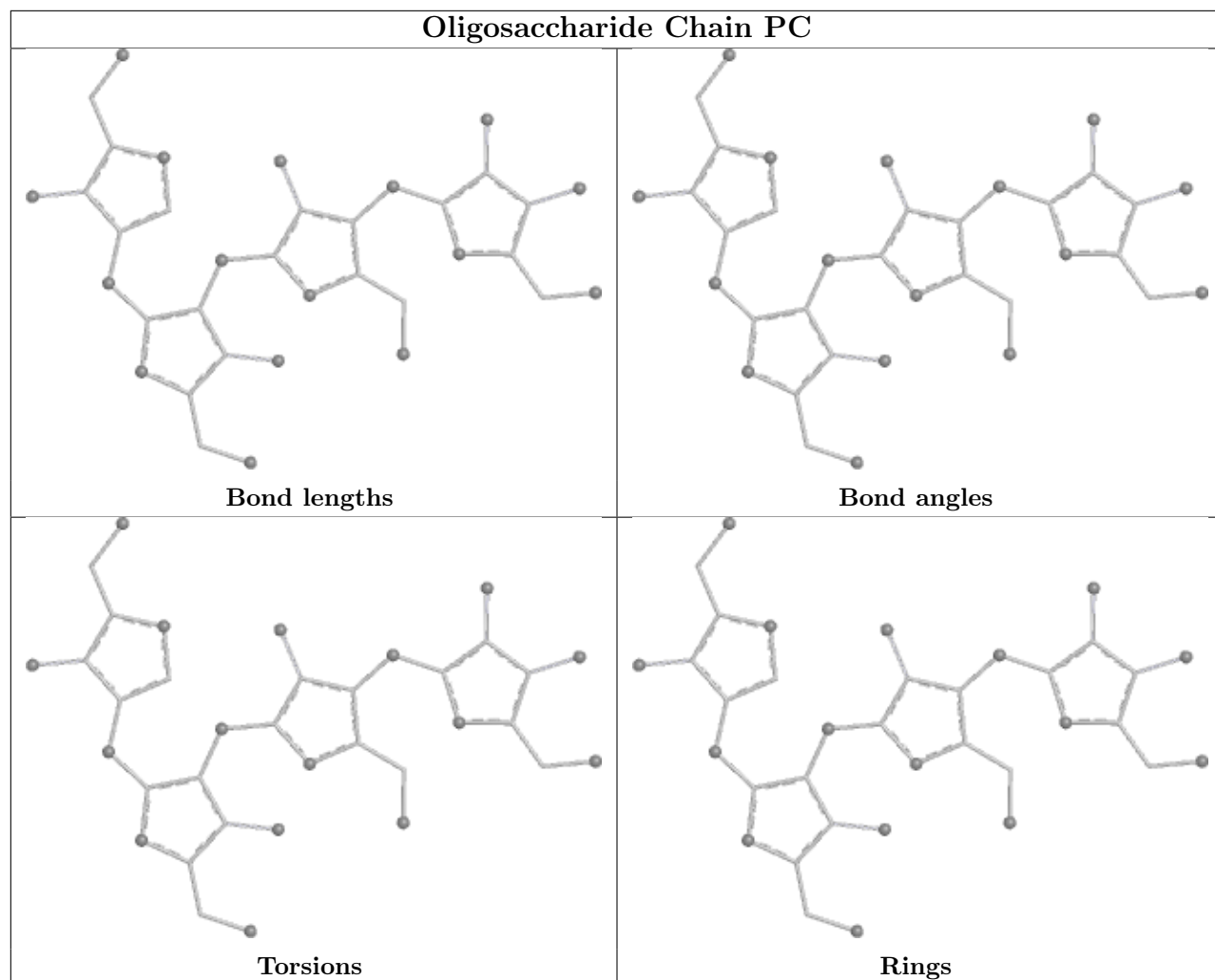
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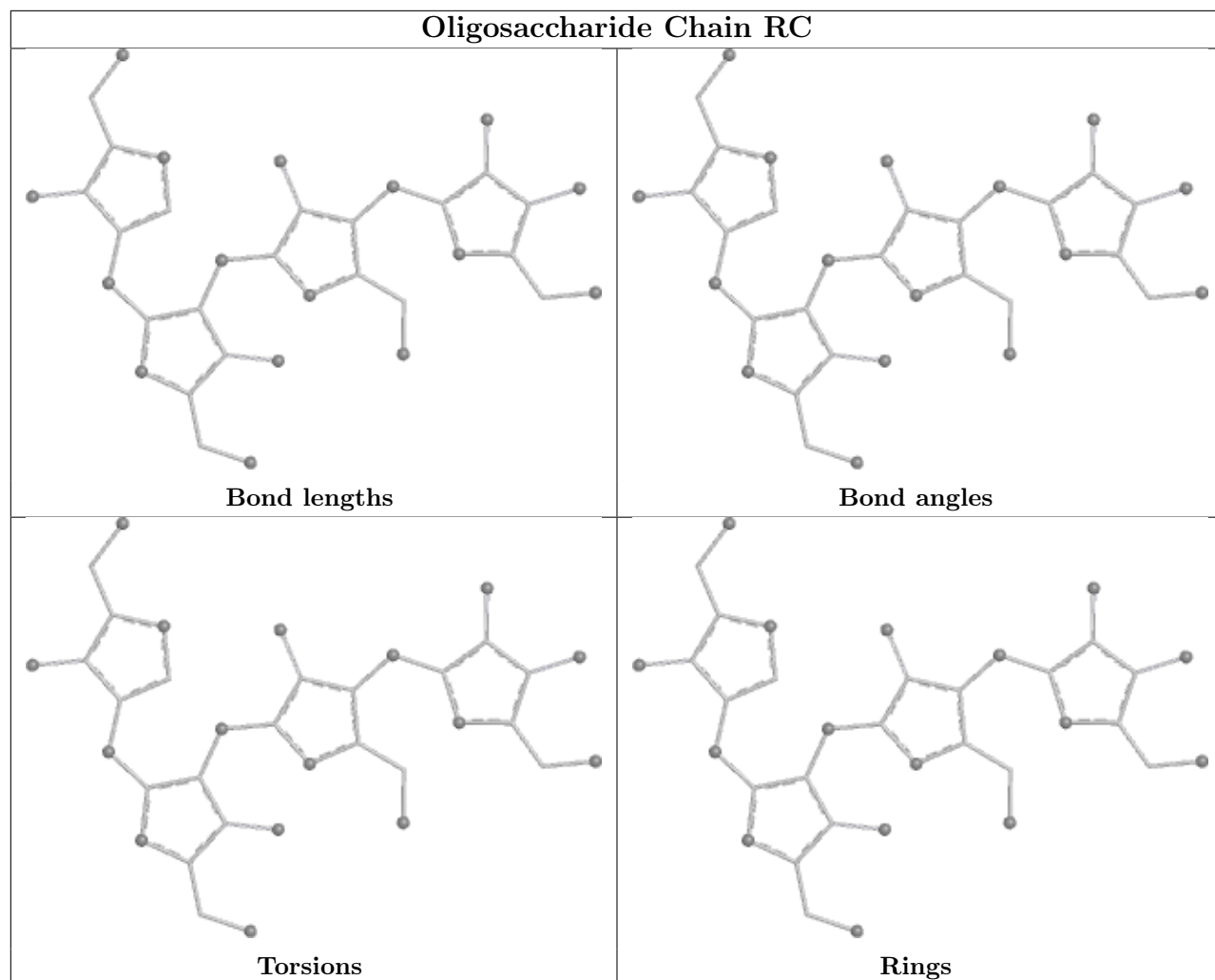
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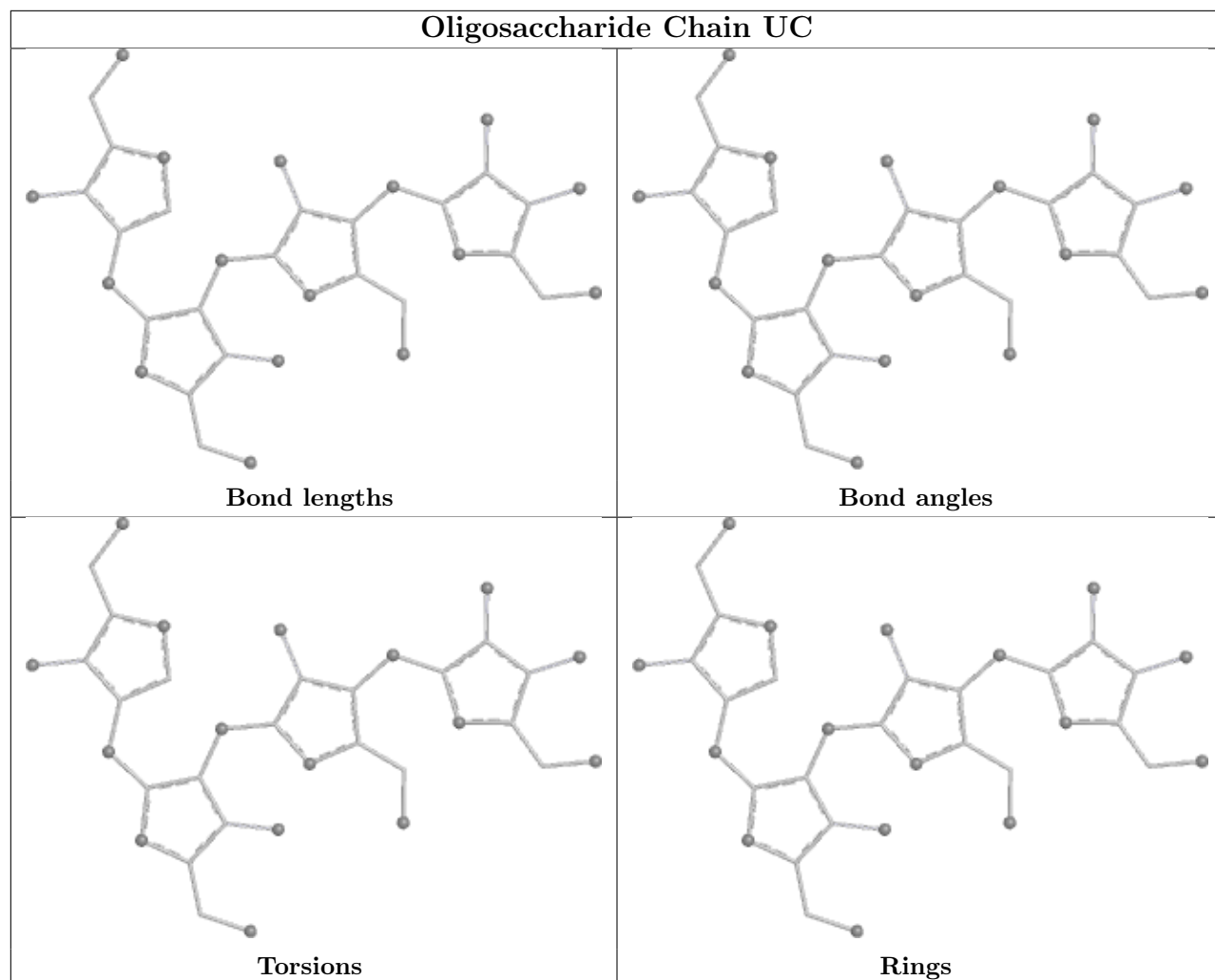


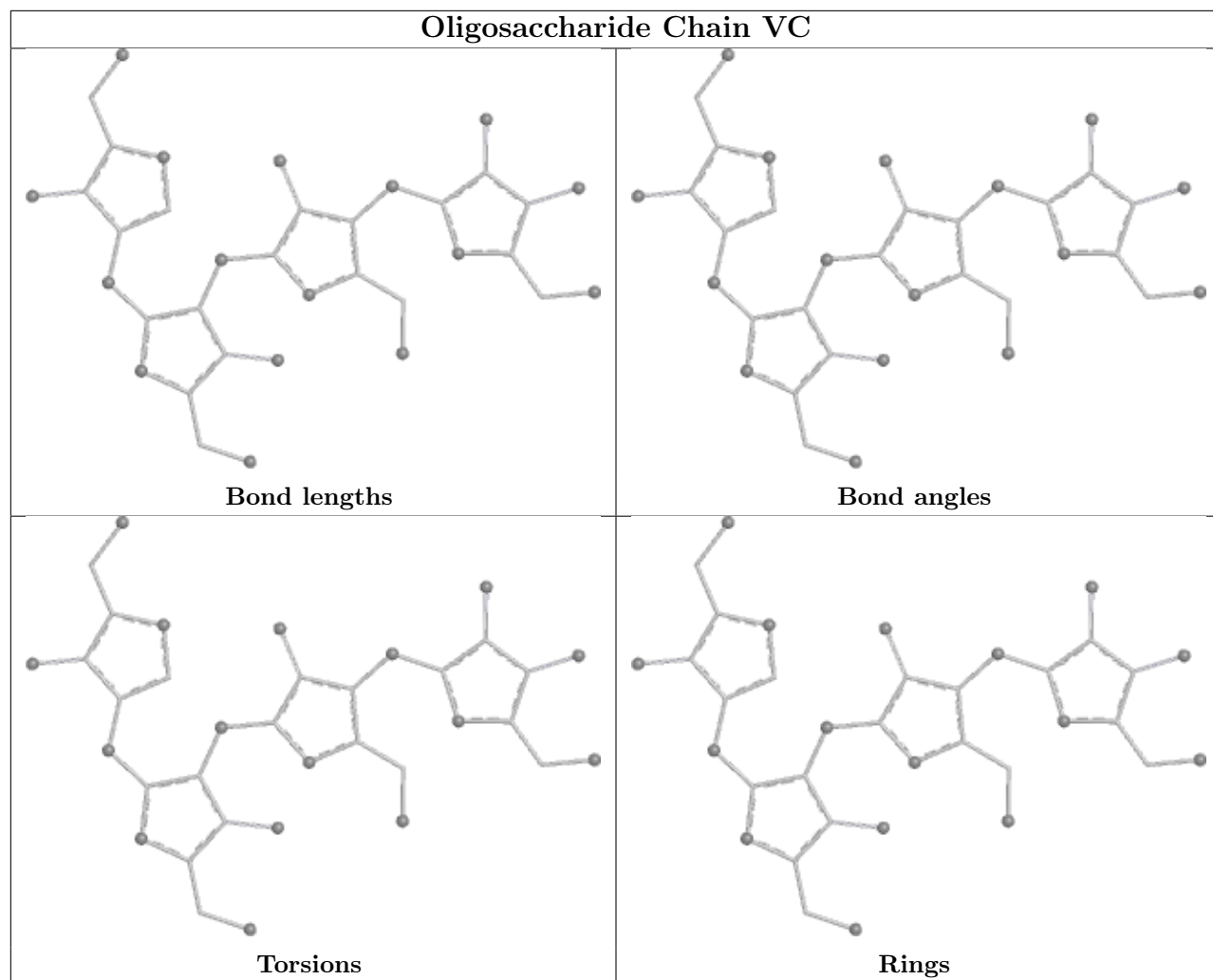
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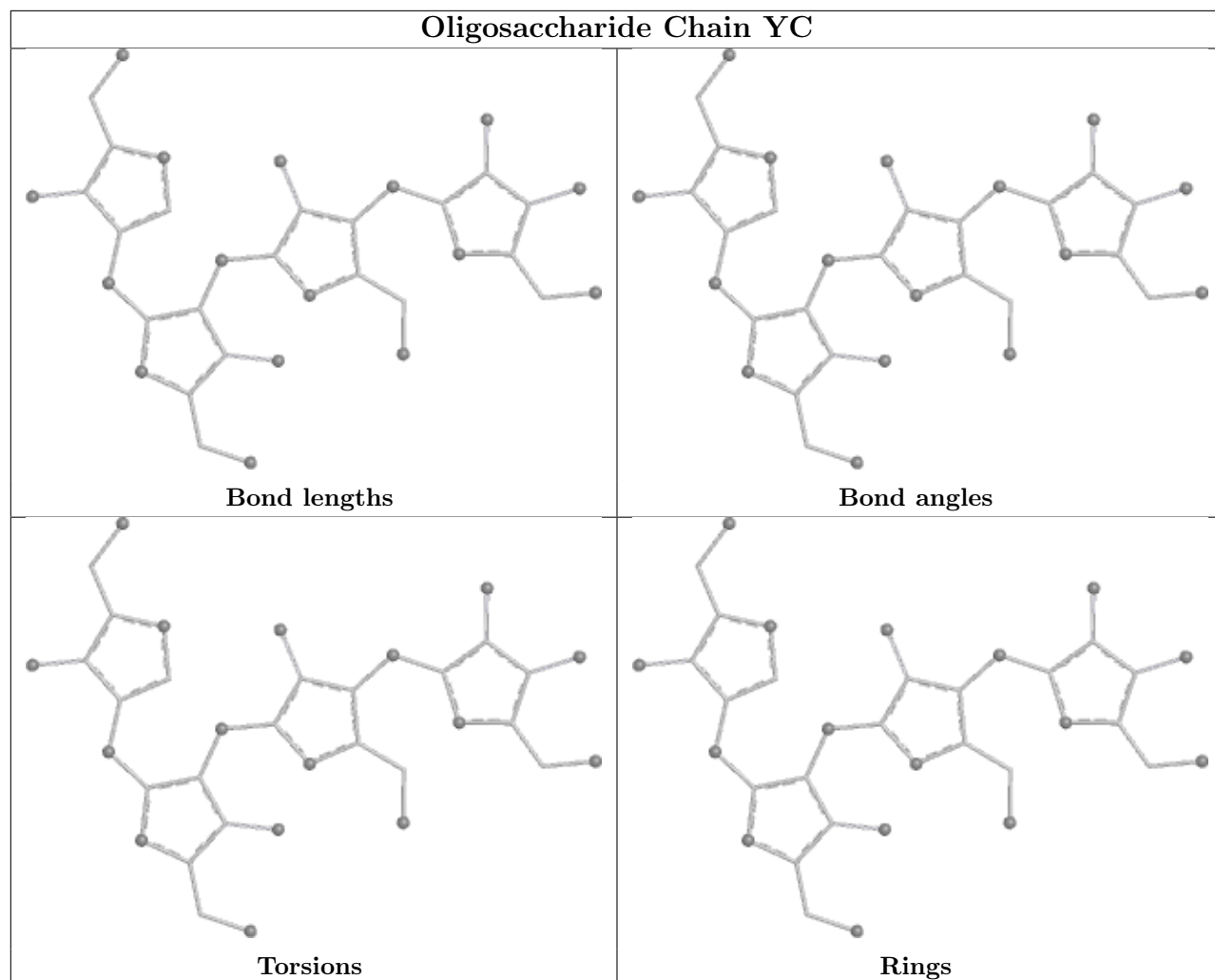
Oligosaccharide Chain OC

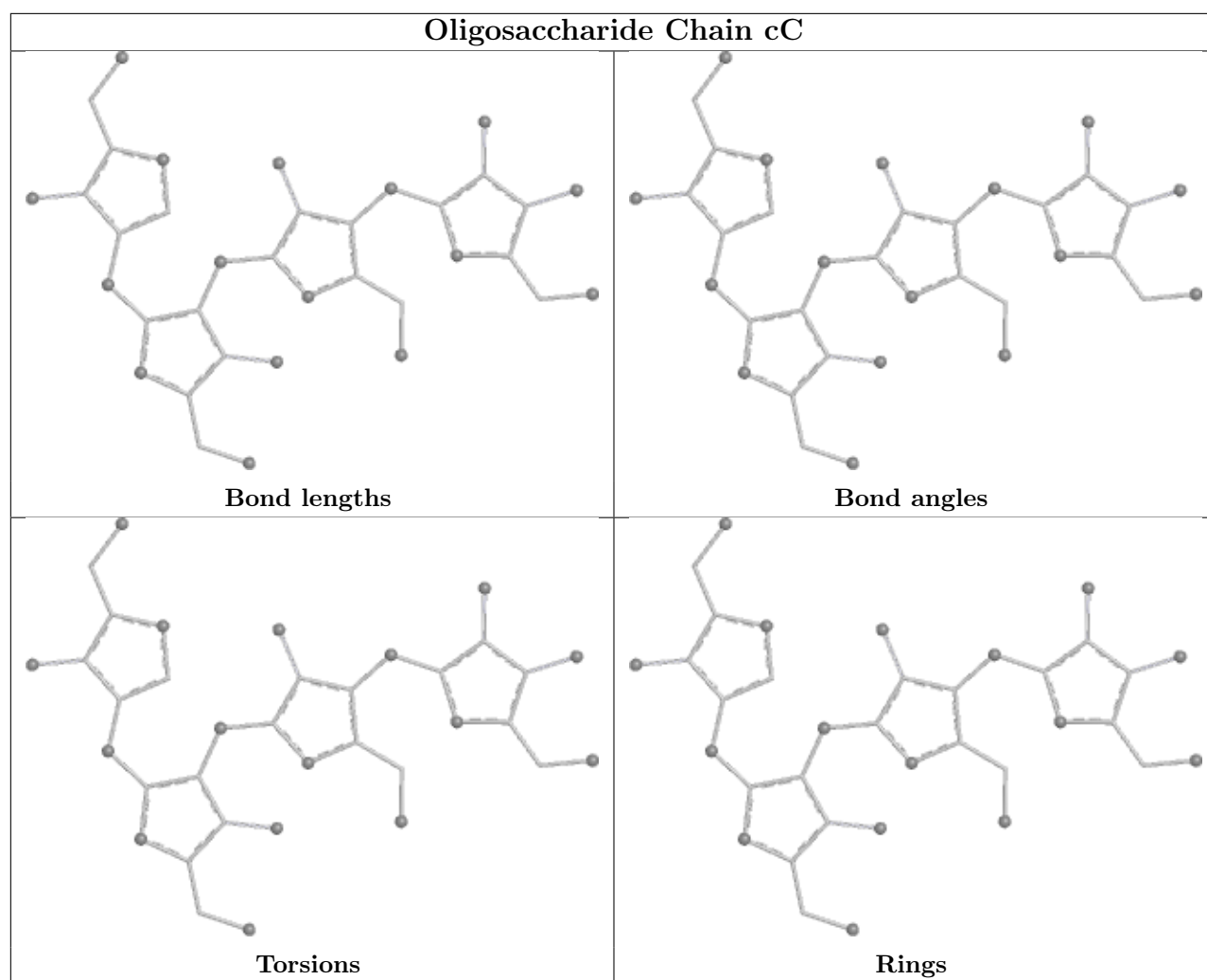
Oligosaccharide Chain PC

Oligosaccharide Chain RC

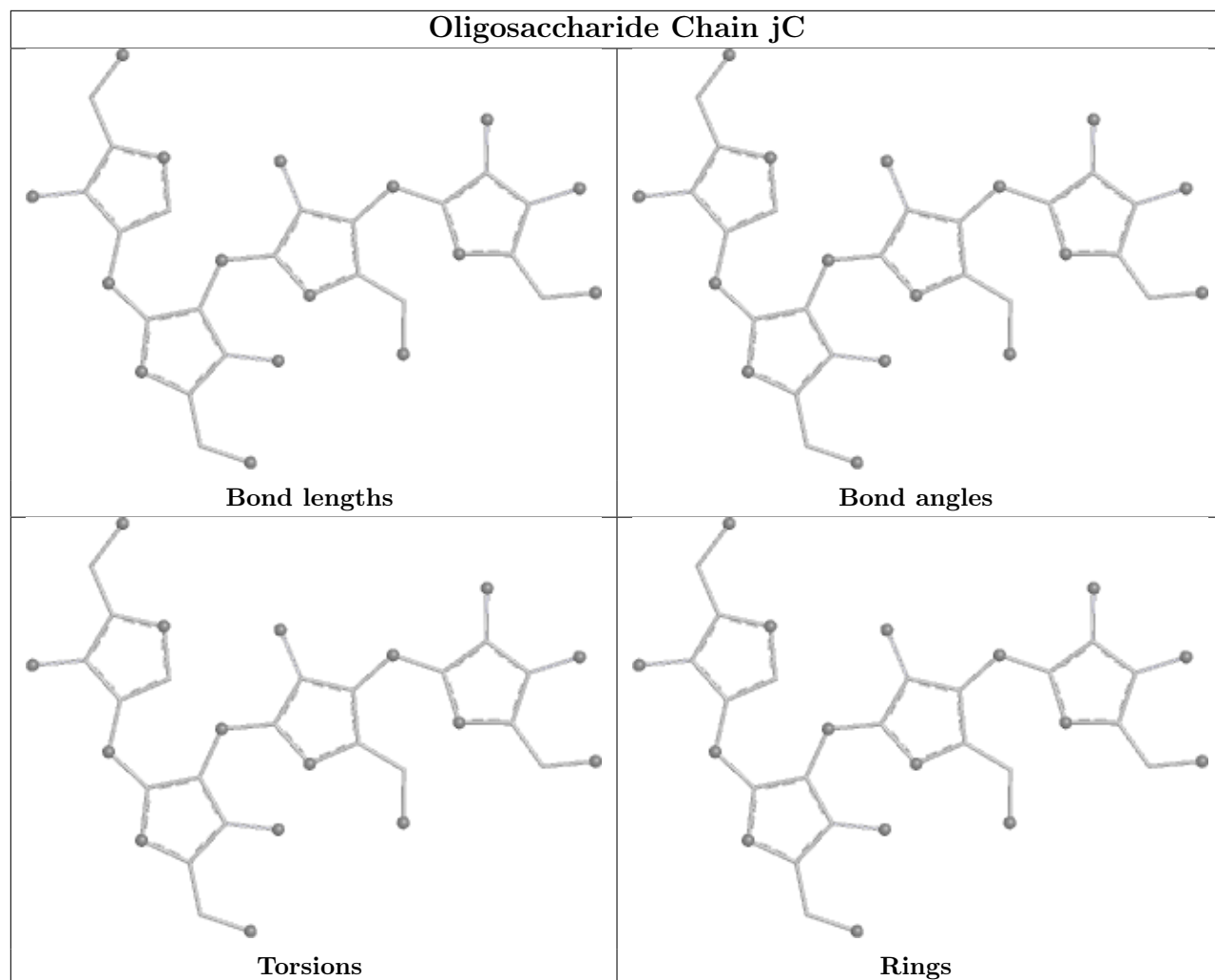
Oligosaccharide Chain UC

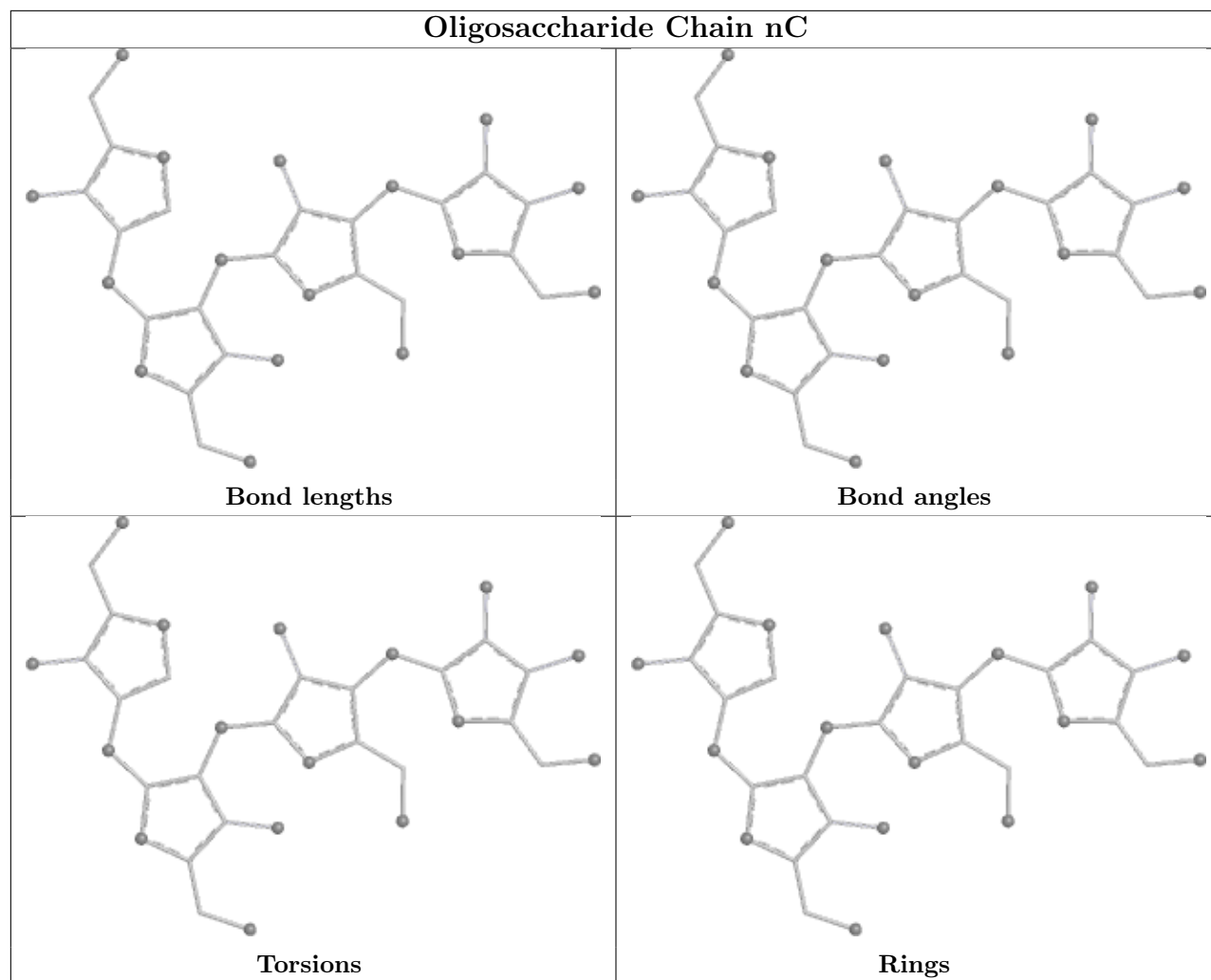
Oligosaccharide Chain VC

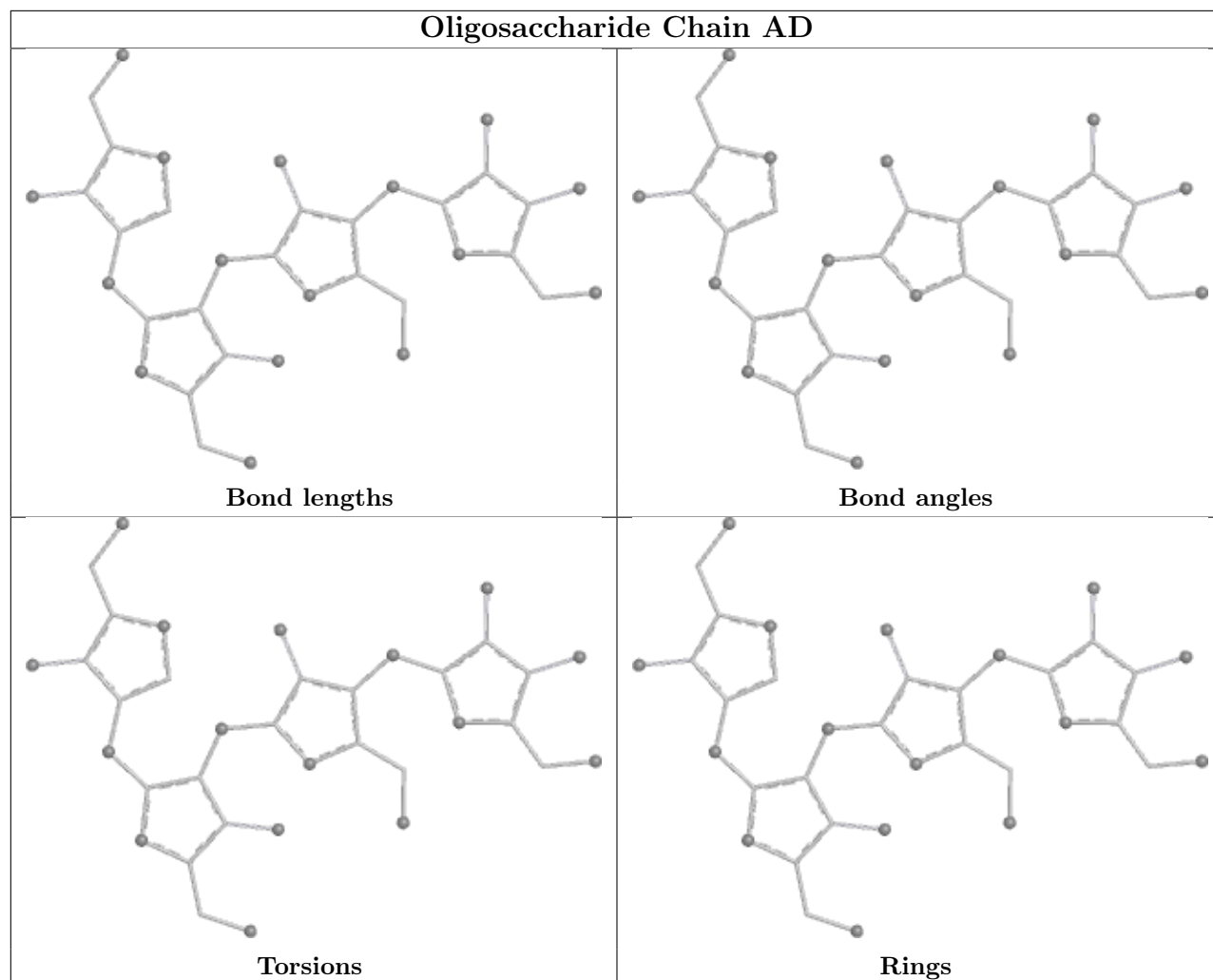
Oligosaccharide Chain YC

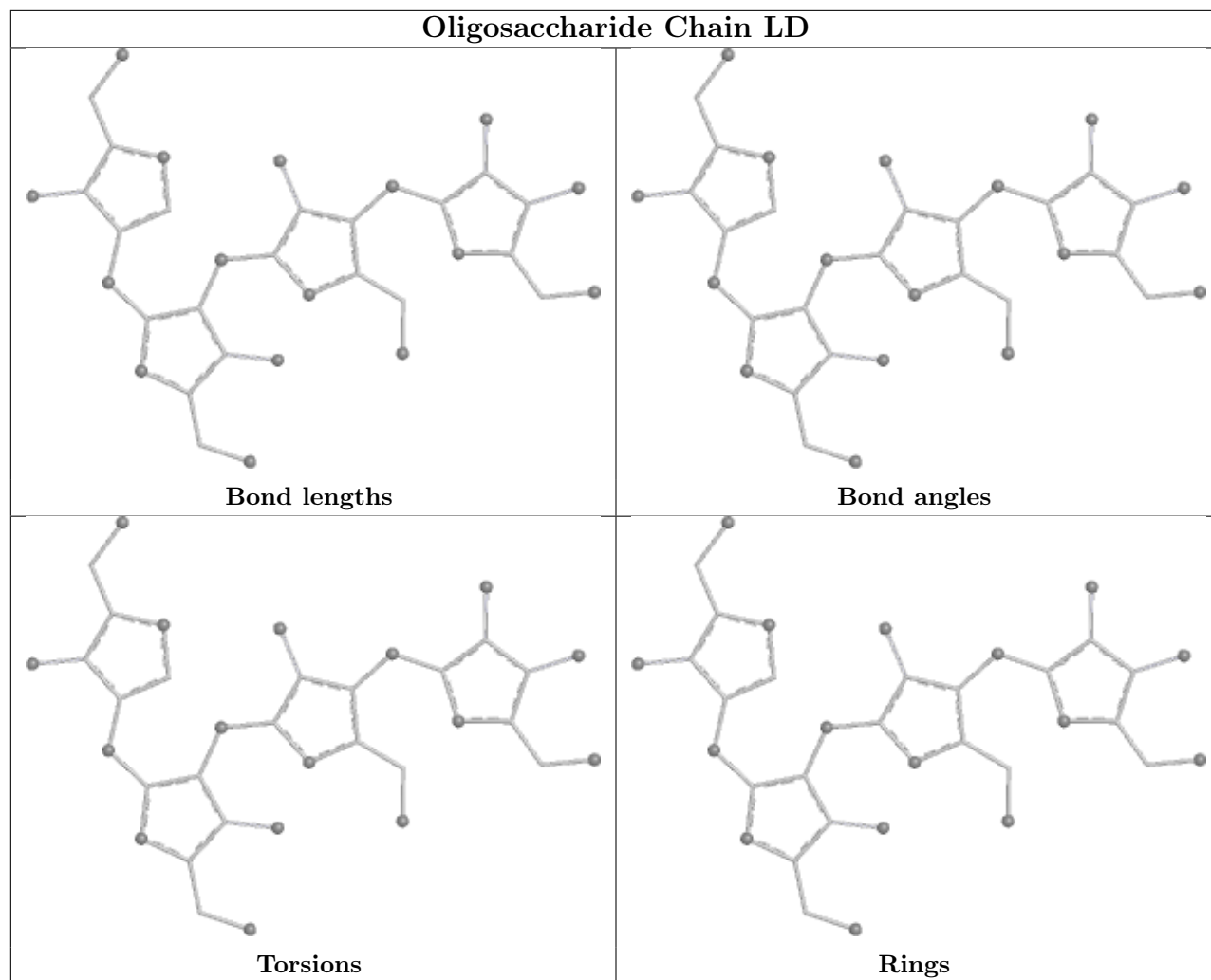


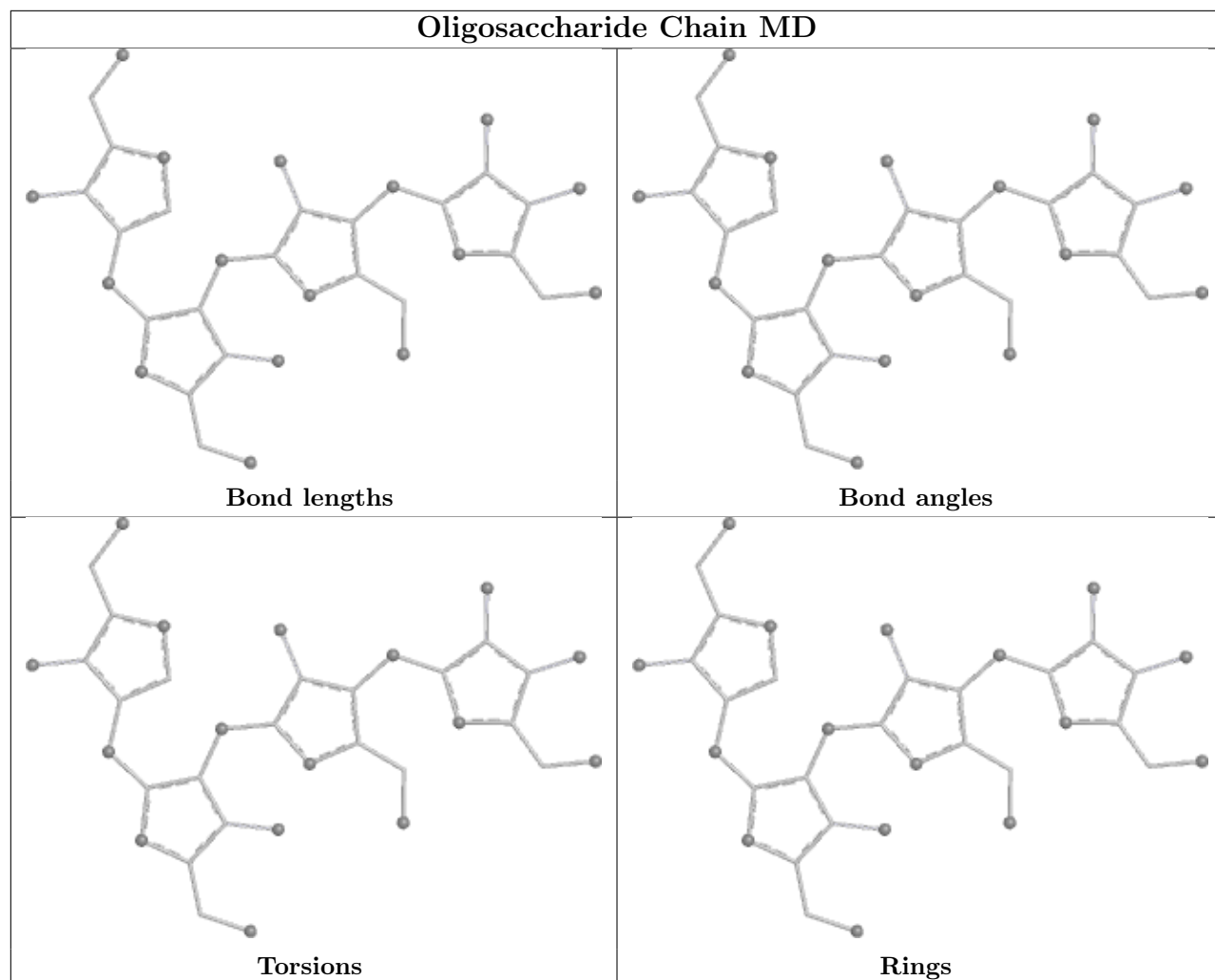
Oligosaccharide Chain jC



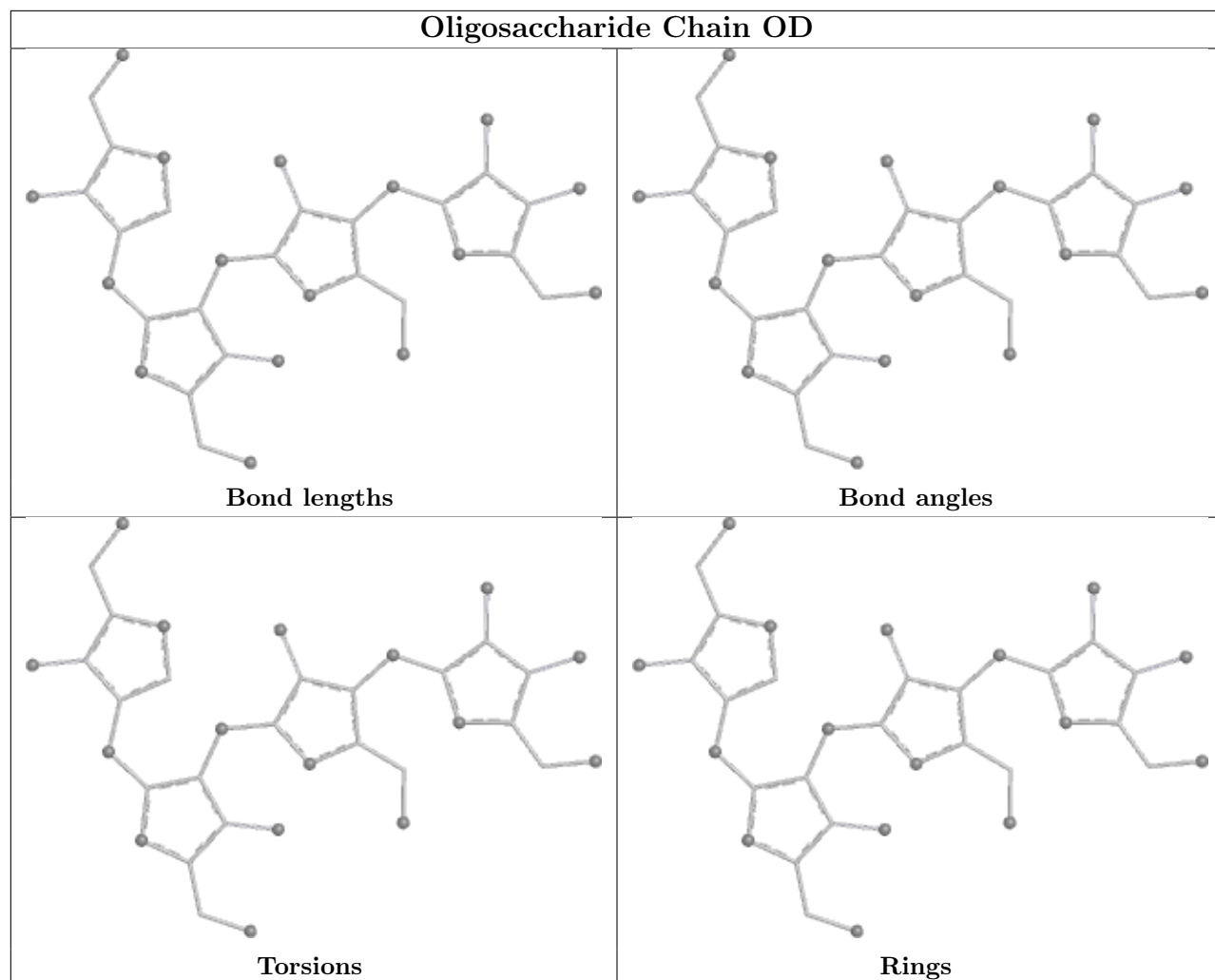


Oligosaccharide Chain AD

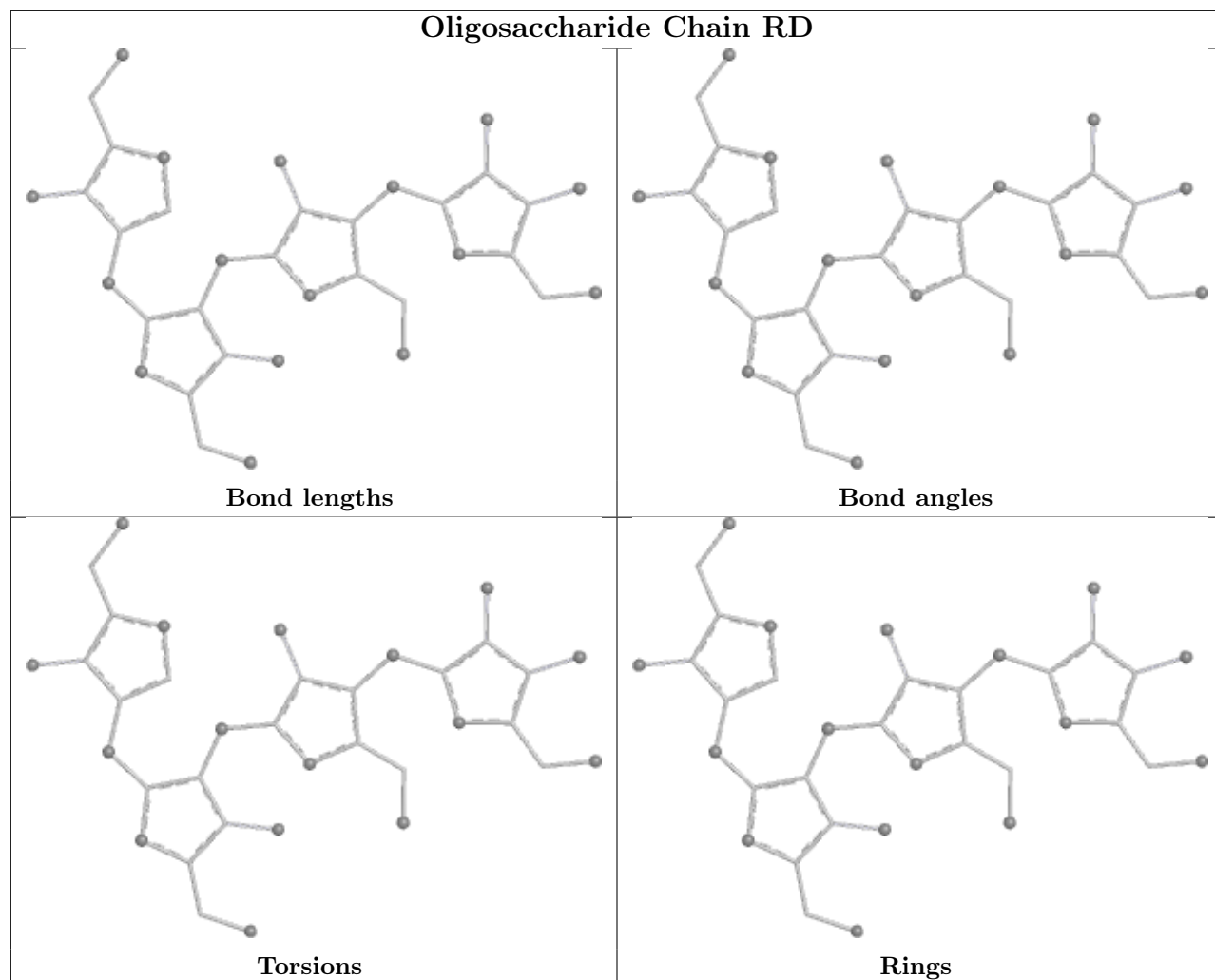


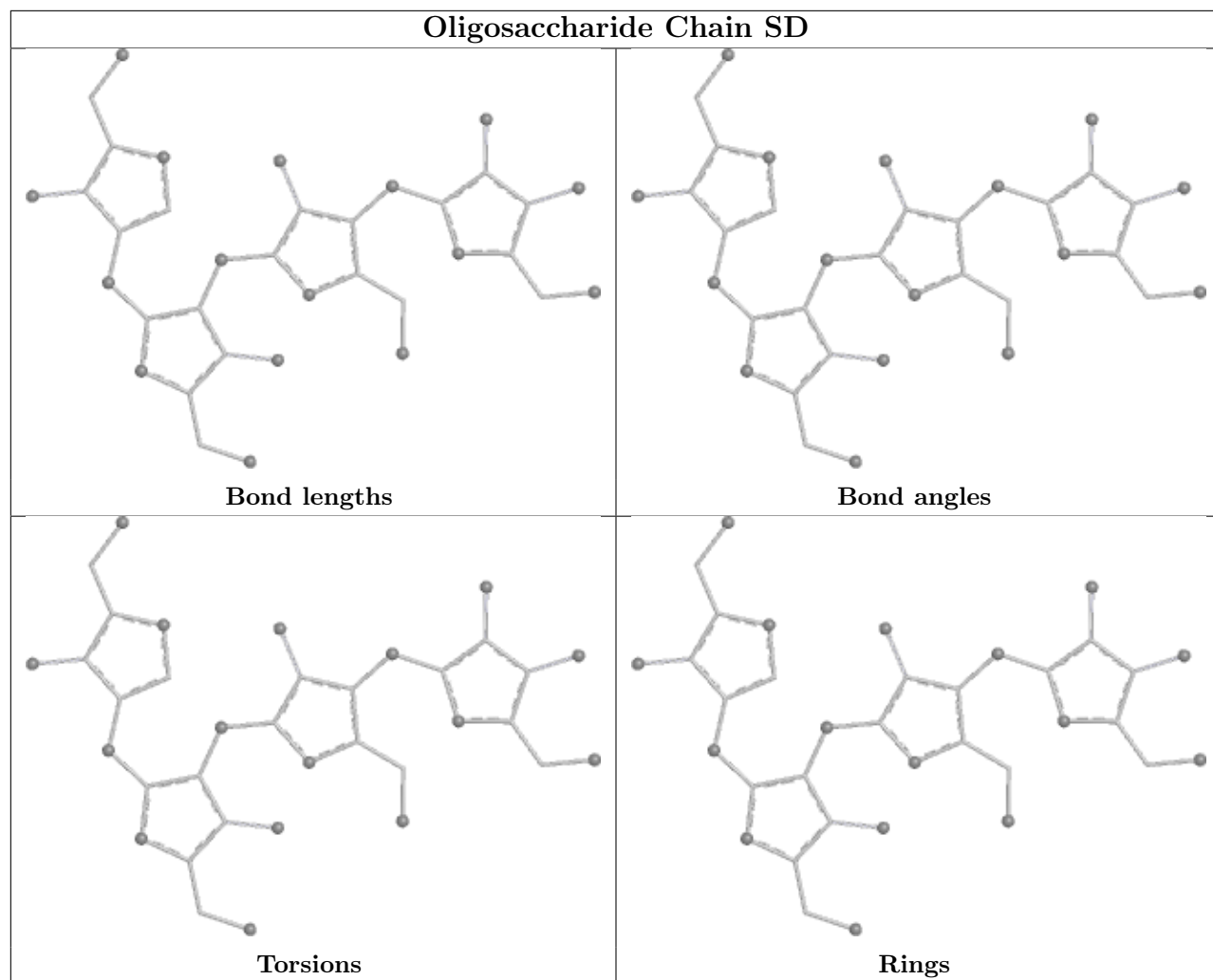
Oligosaccharide Chain MD

Oligosaccharide Chain OD

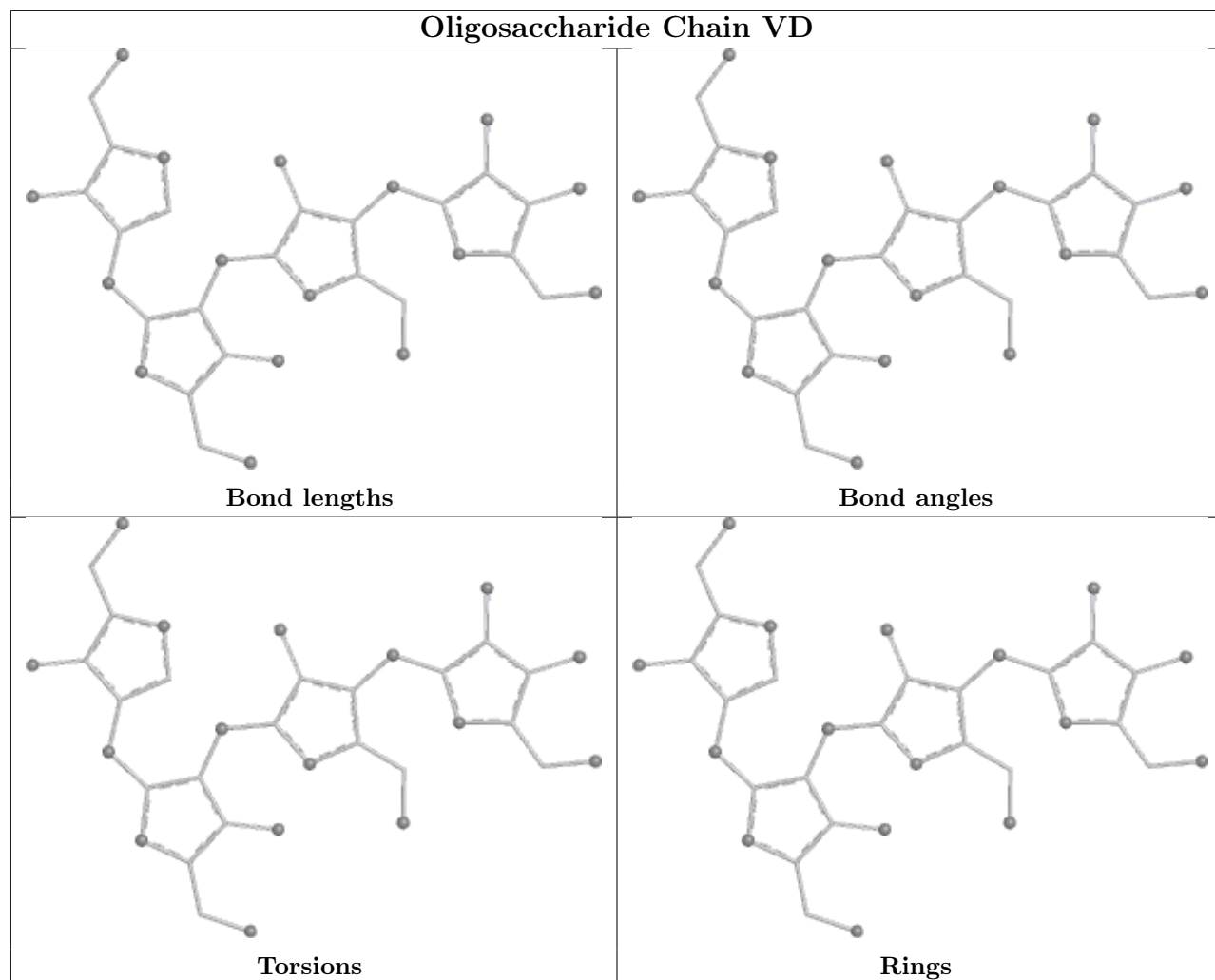


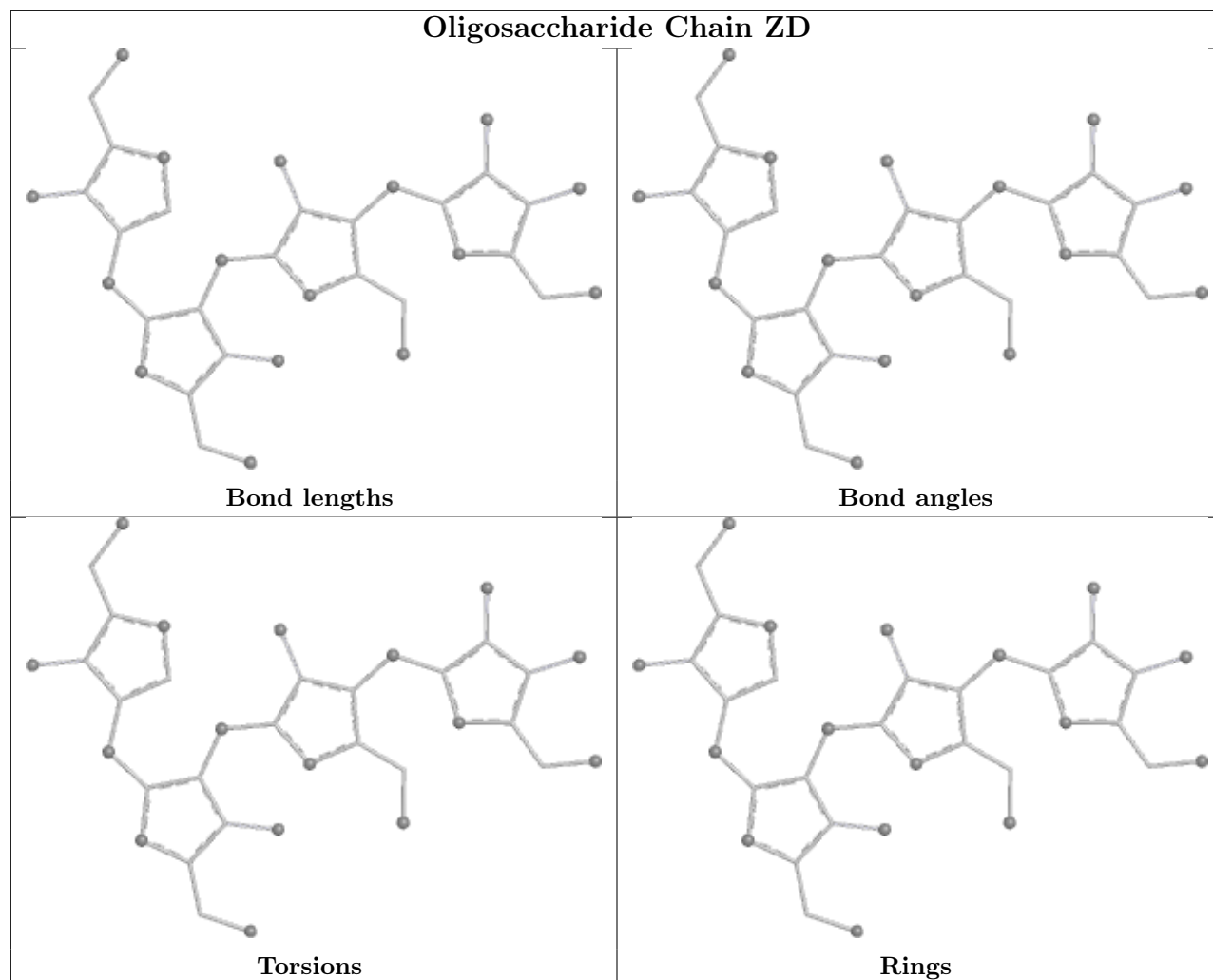
Oligosaccharide Chain RD

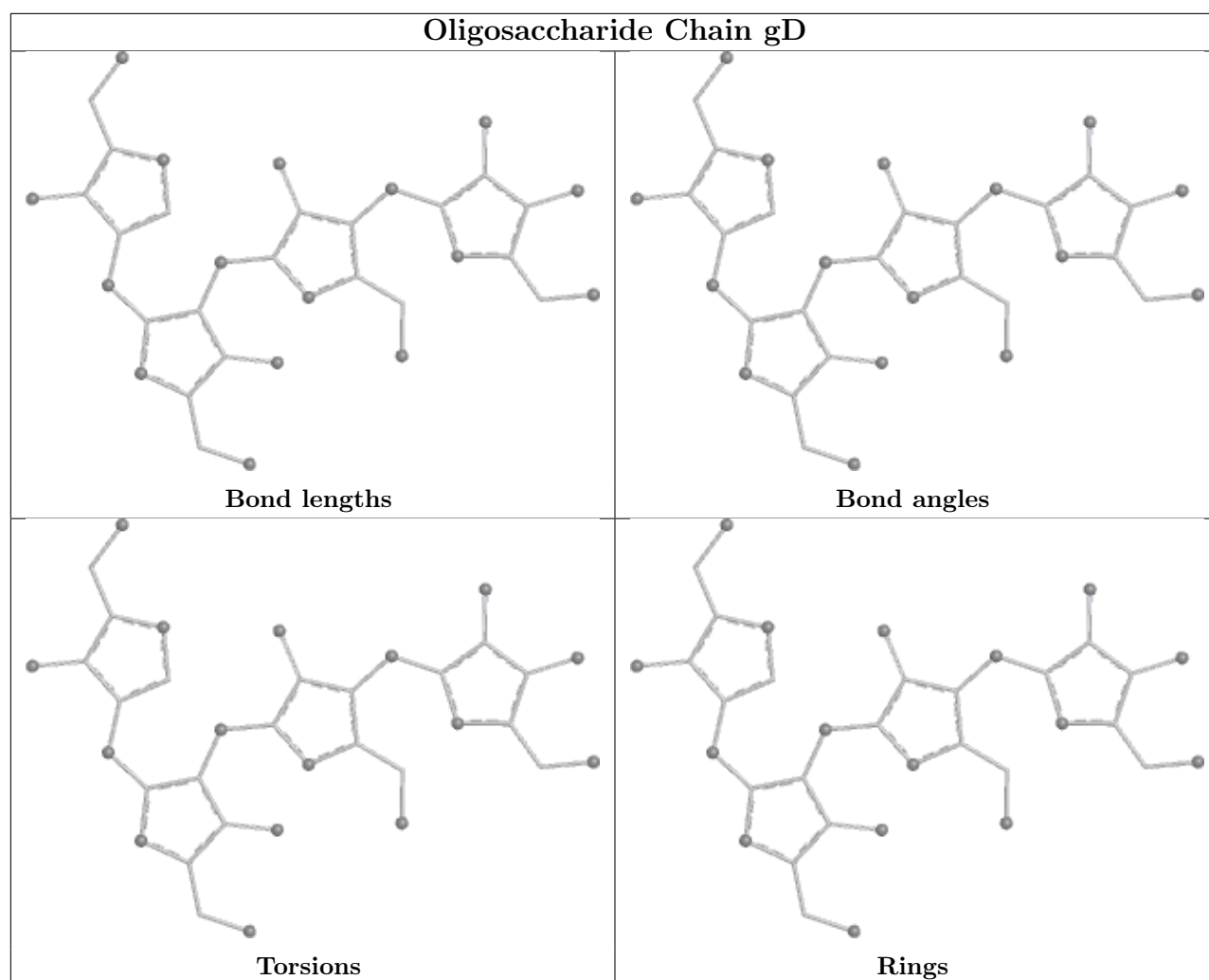


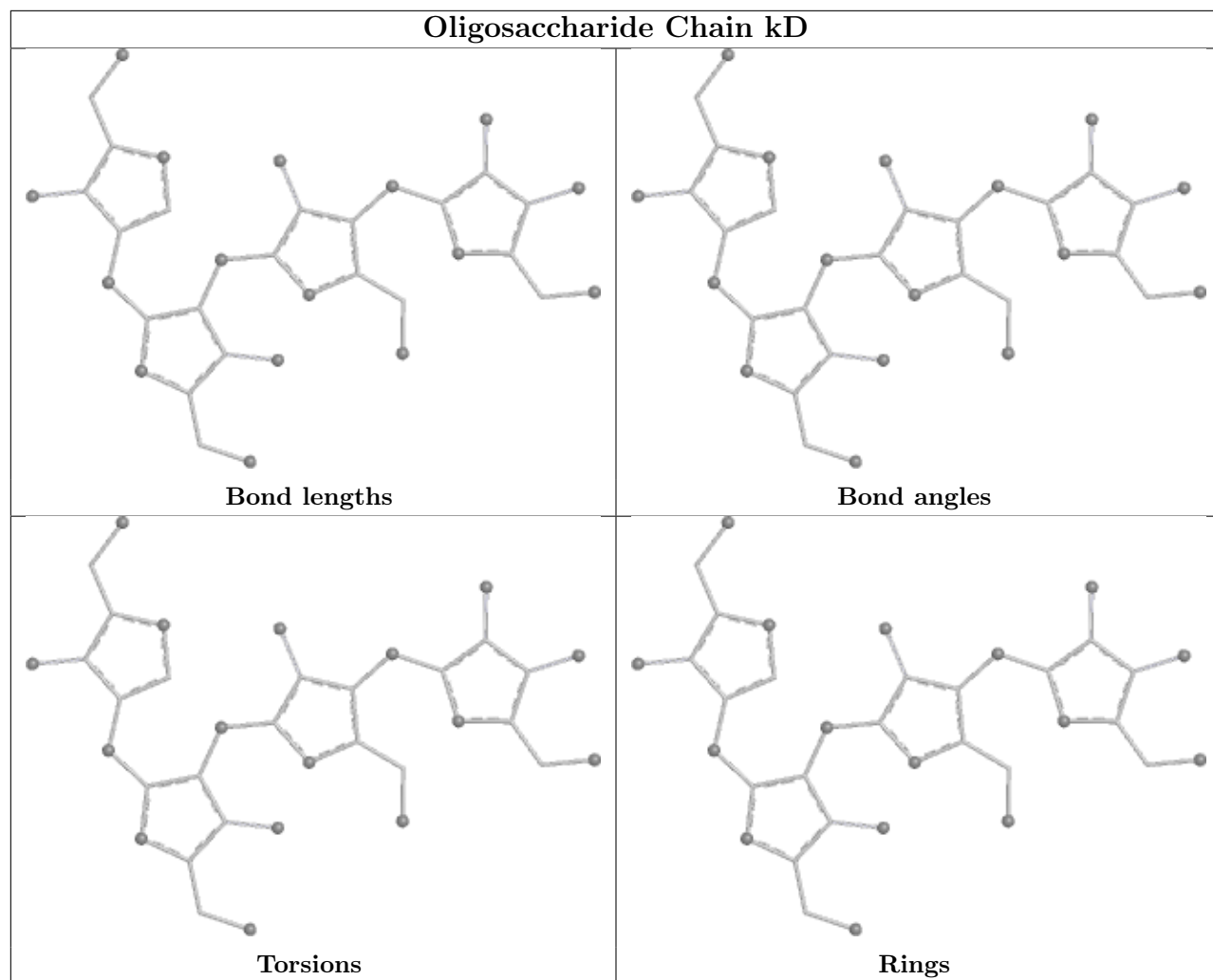
Oligosaccharide Chain SD

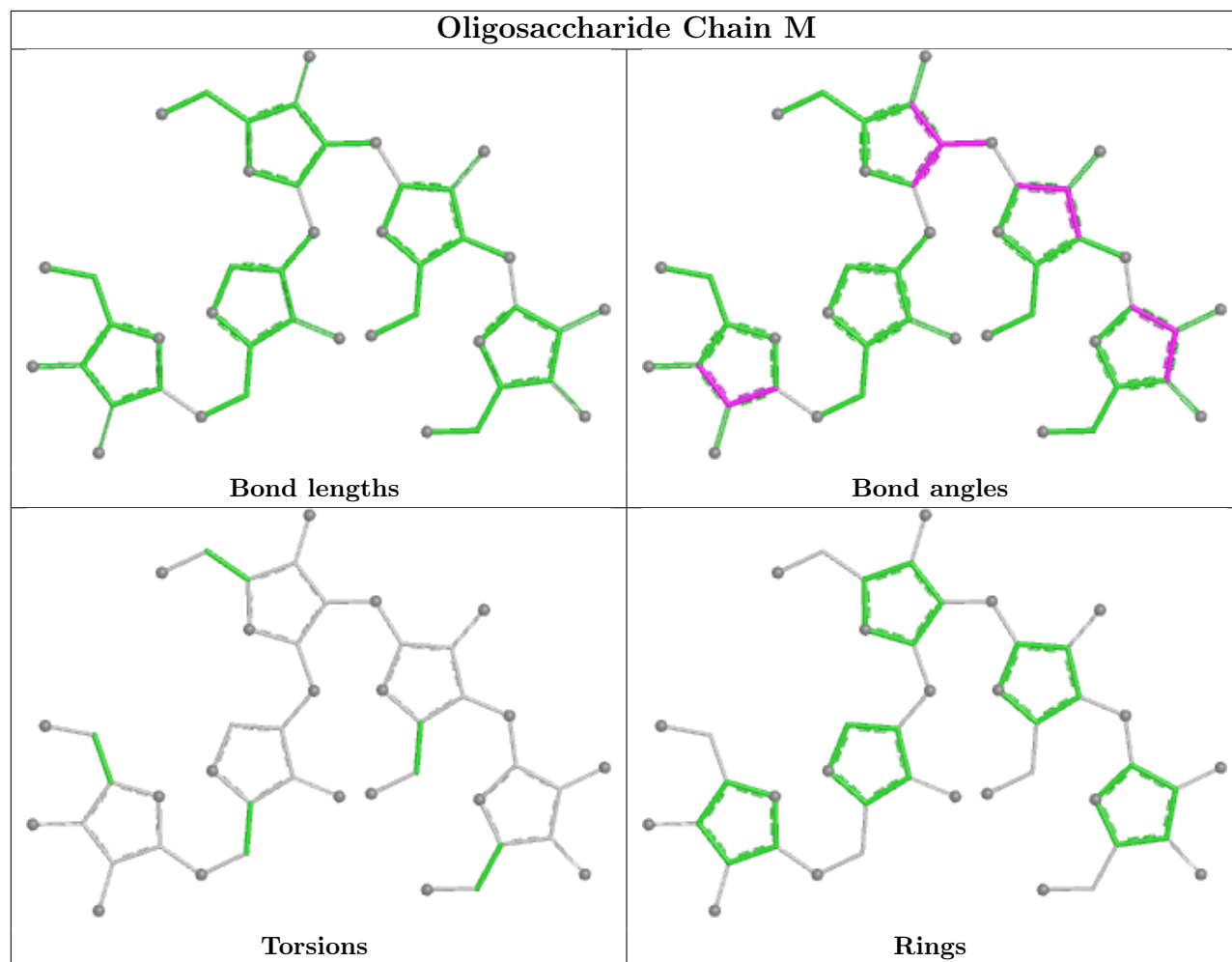
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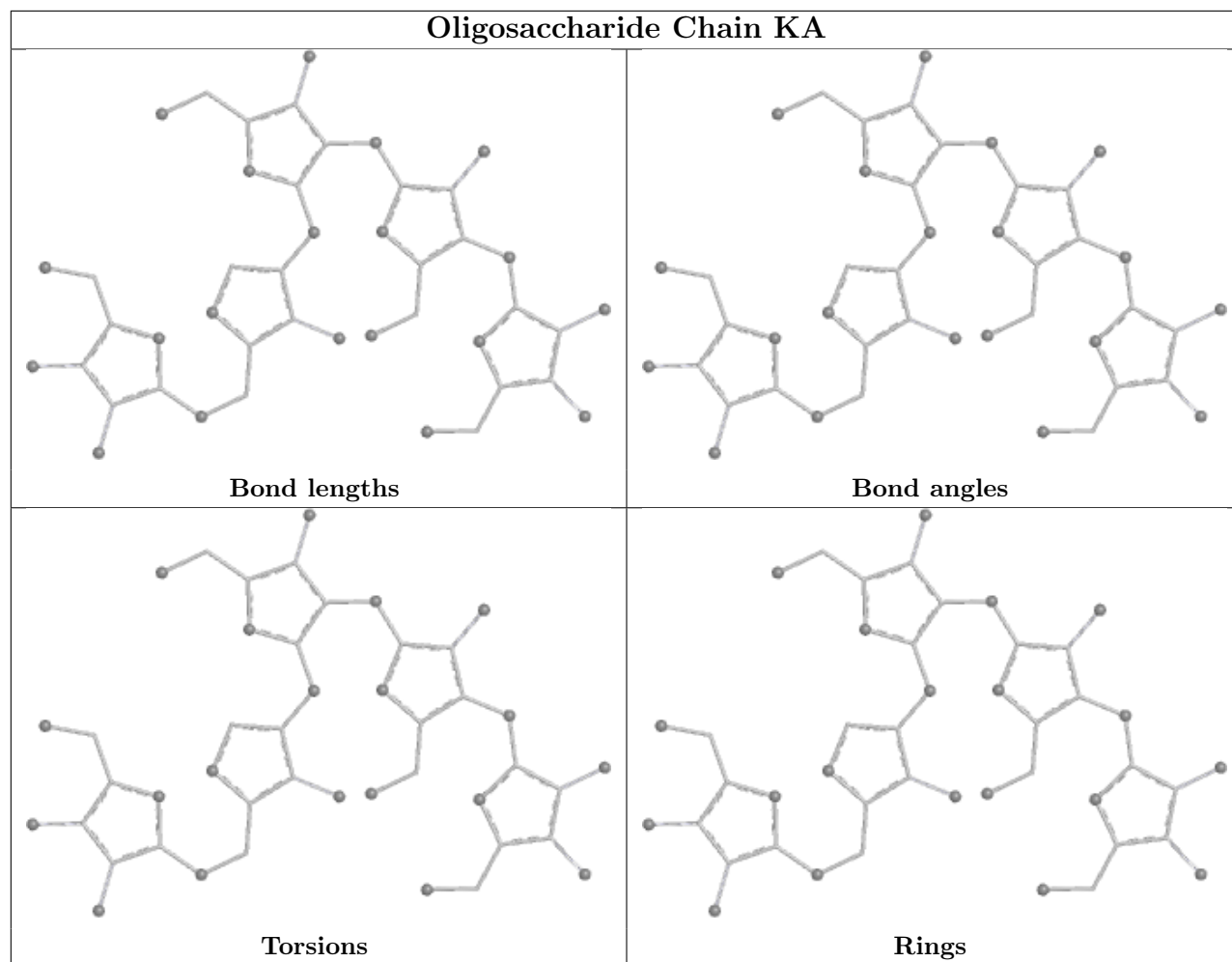


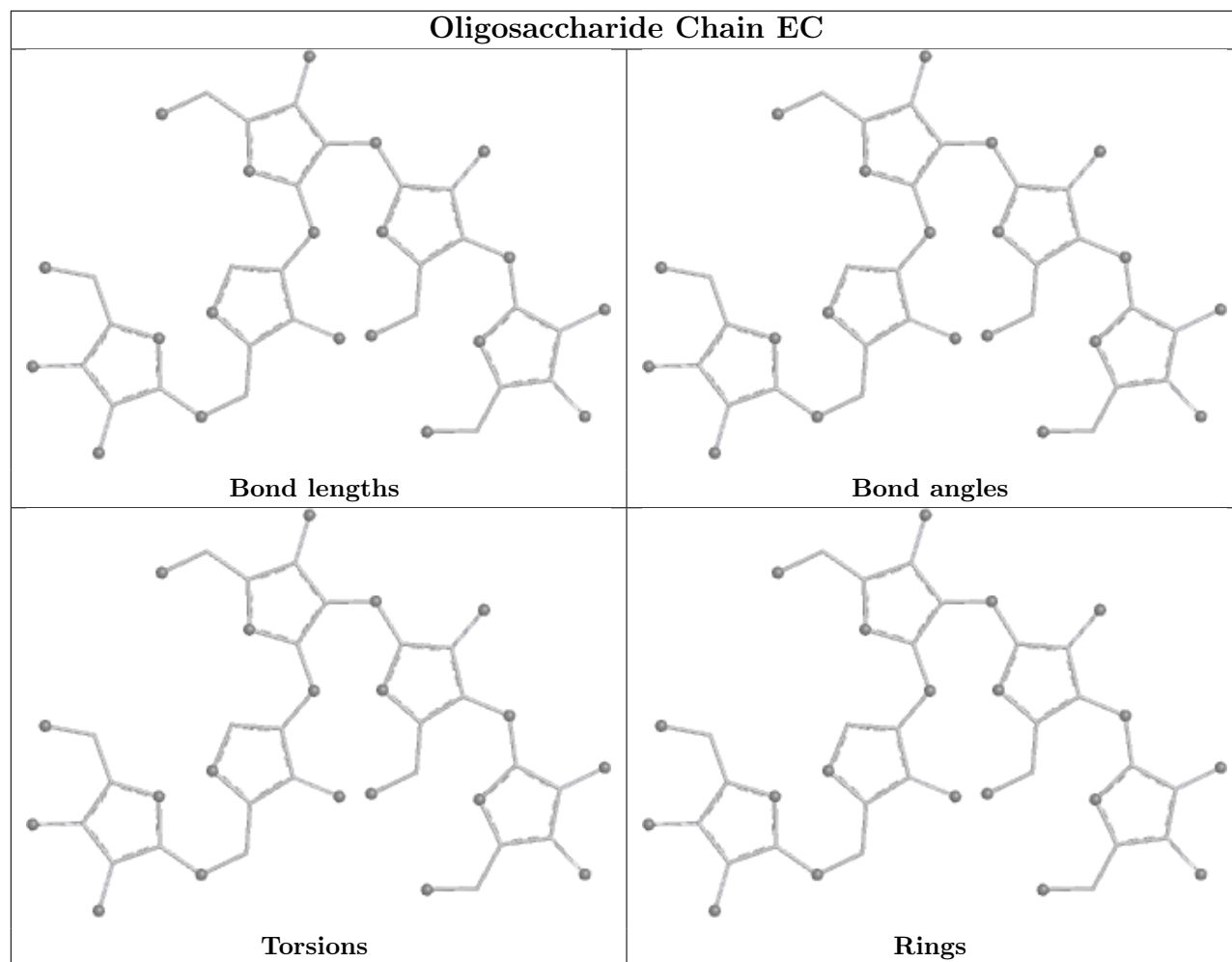
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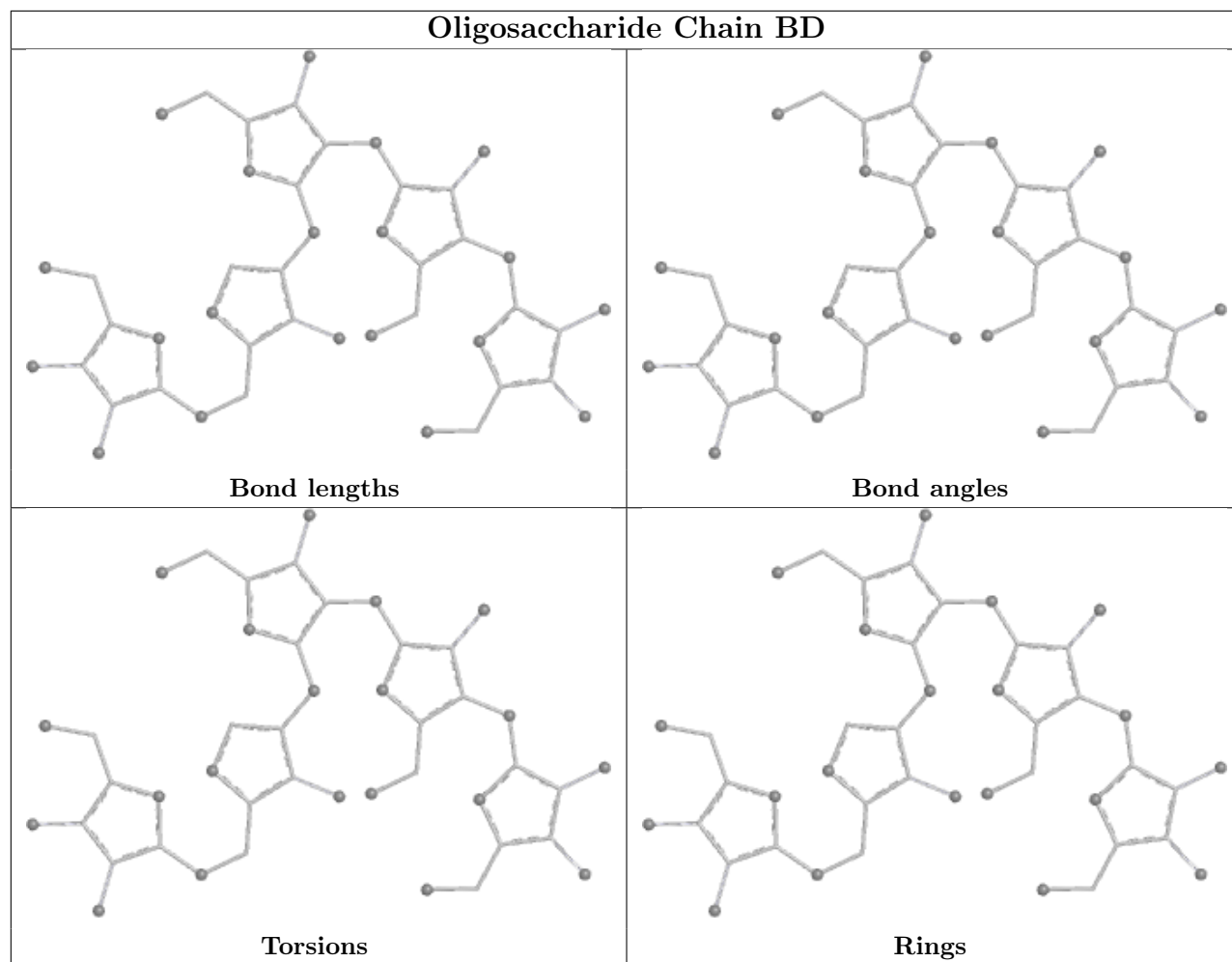


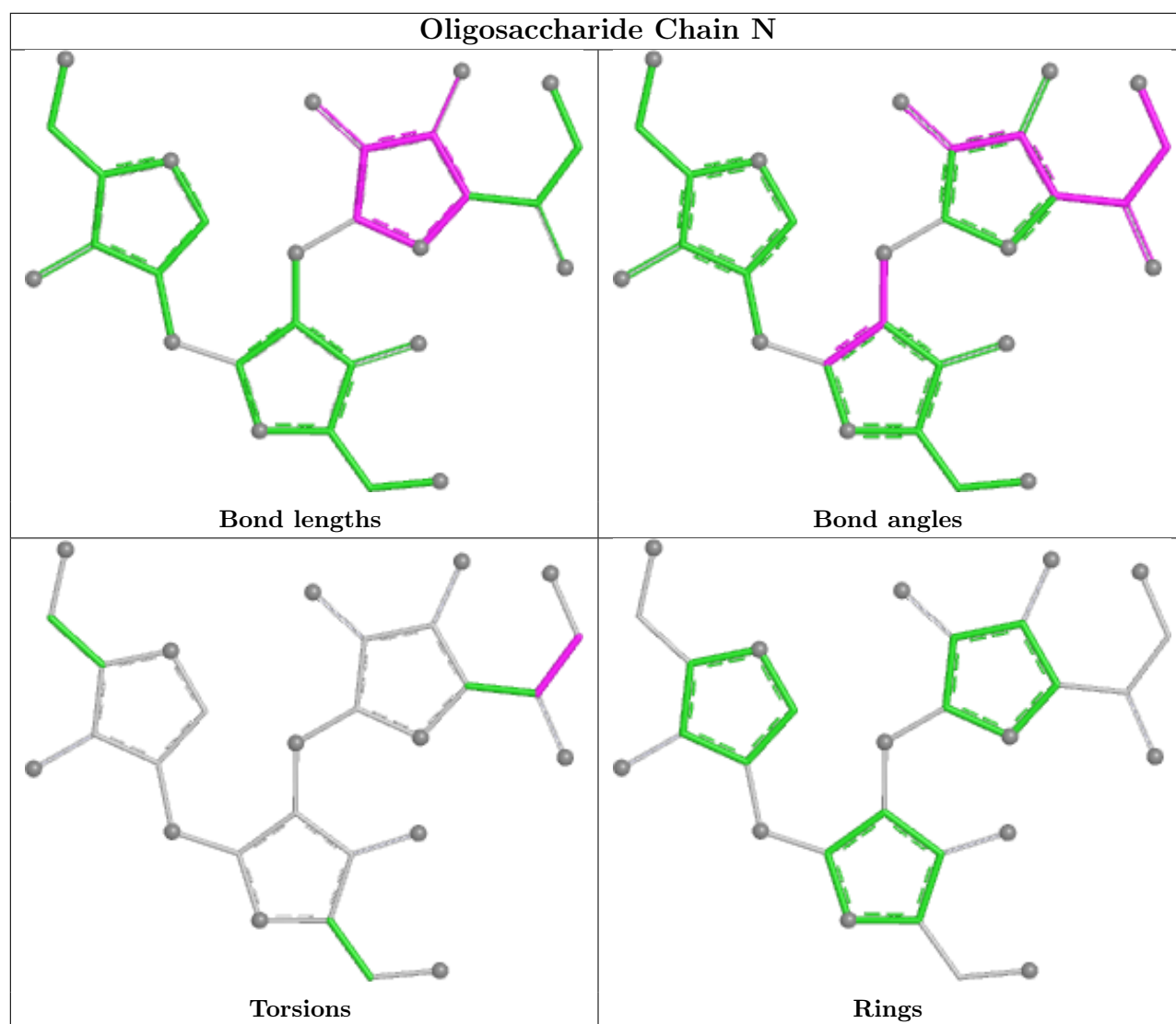


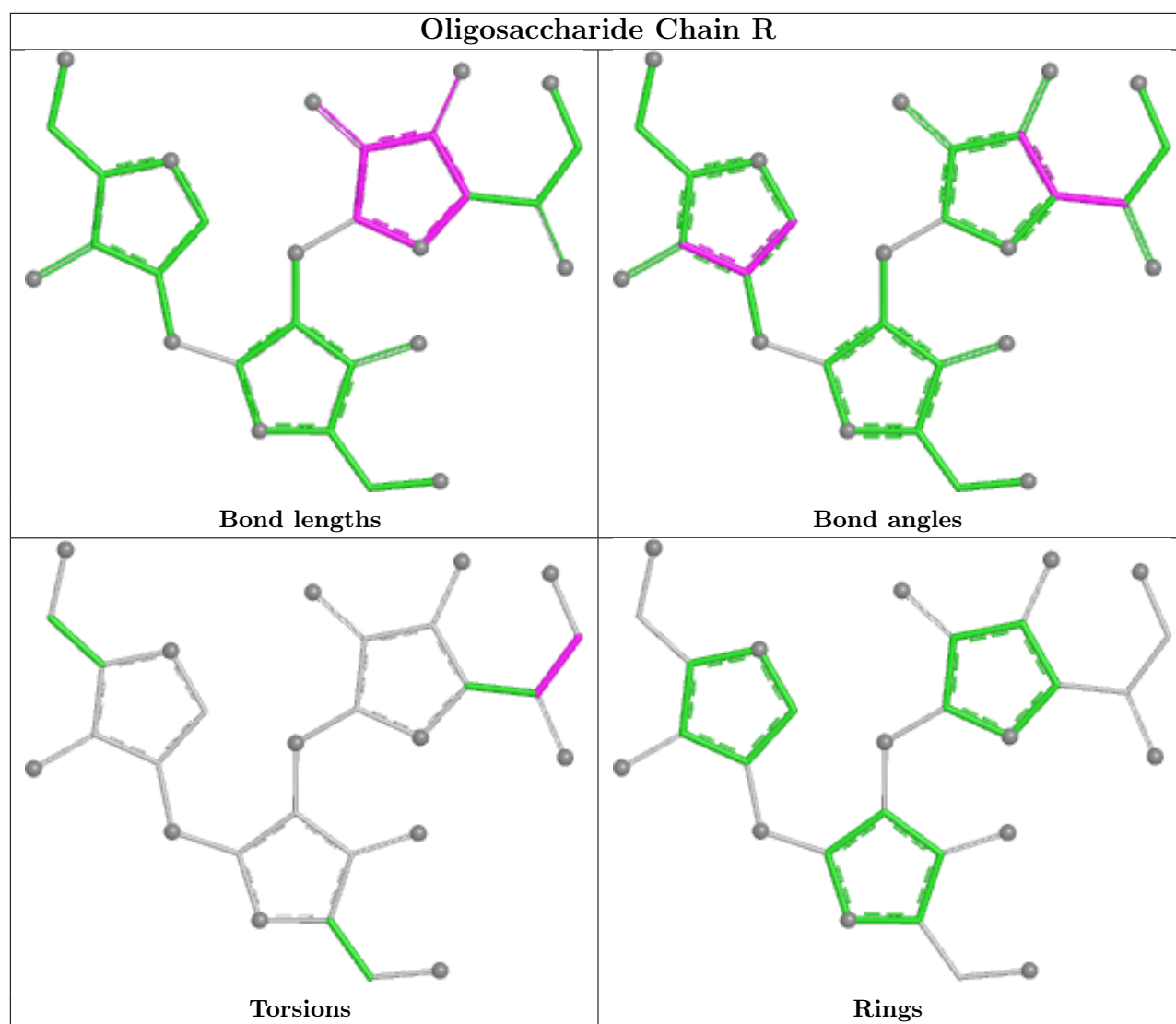




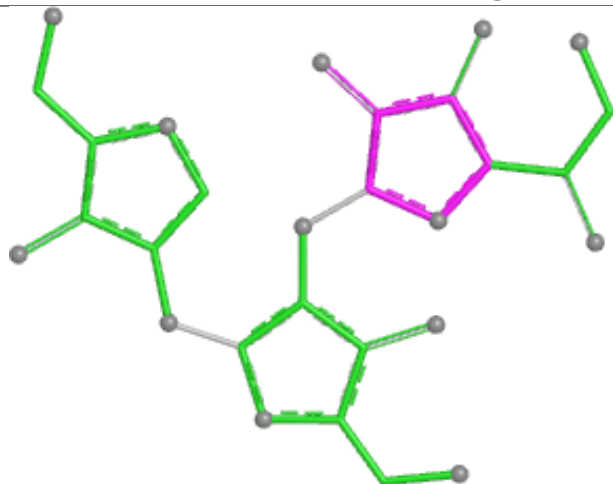




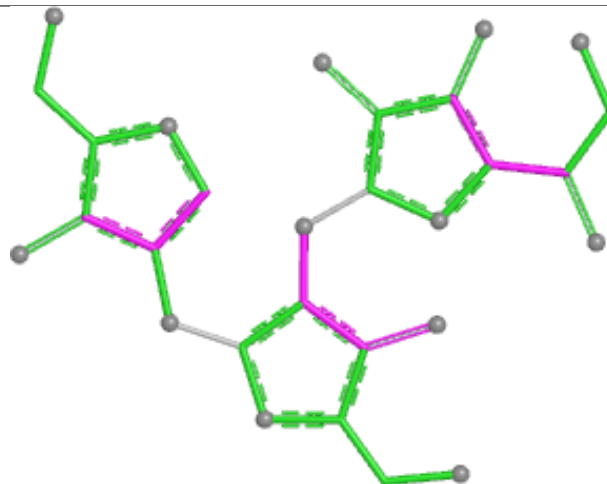




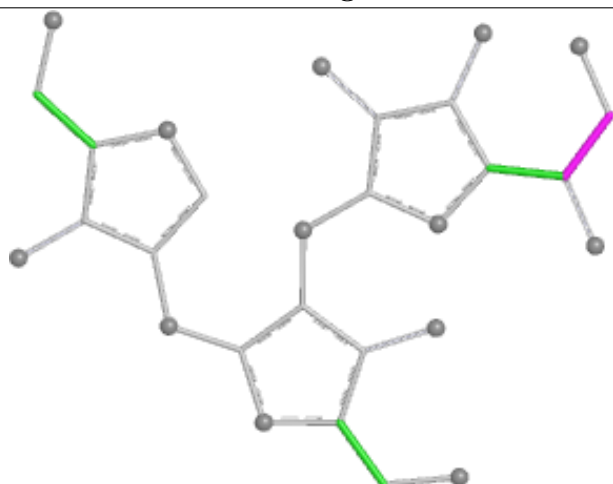
Oligosaccharide Chain 5



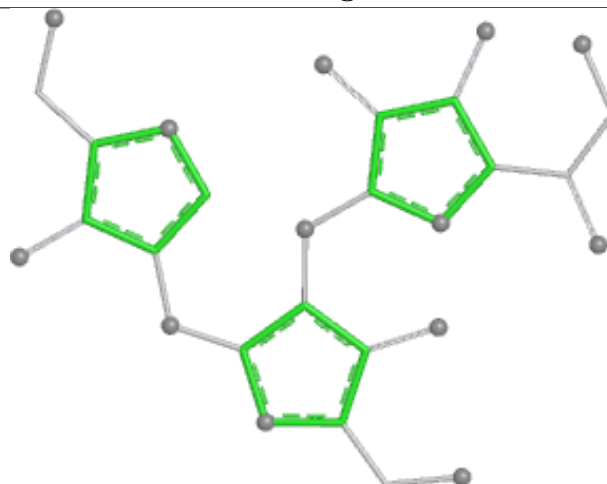
Bond lengths



Bond angles

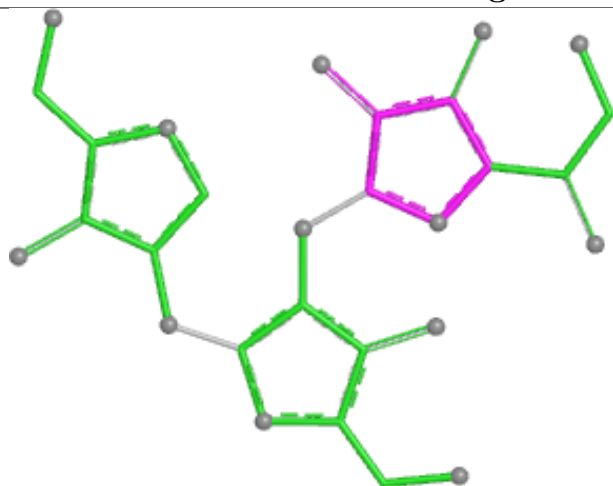


Torsions

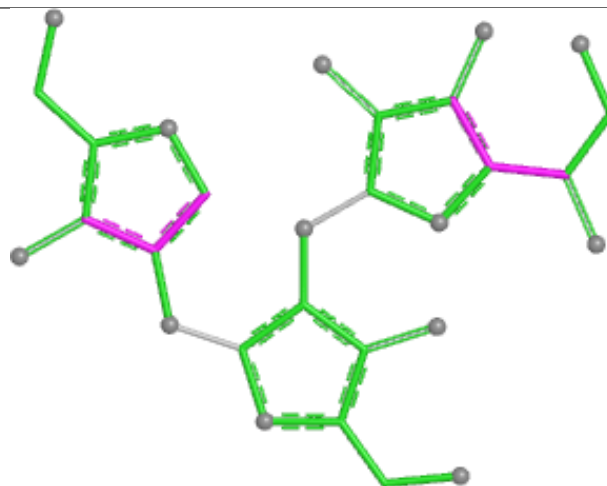


Rings

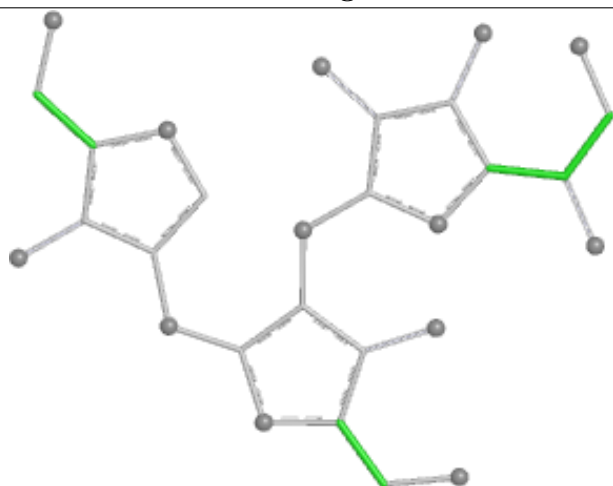
Oligosaccharide Chain 8



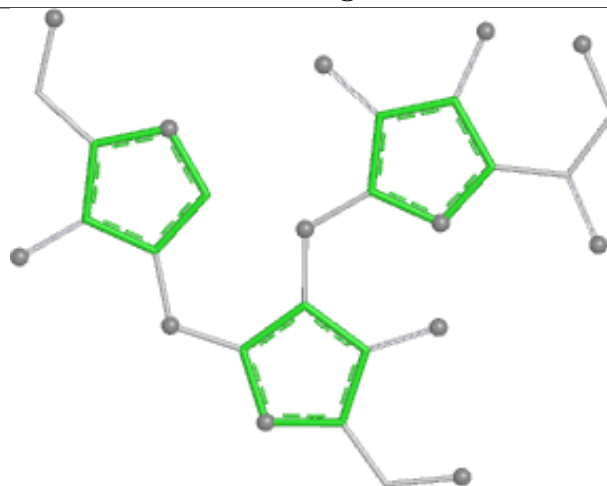
Bond lengths



Bond angles

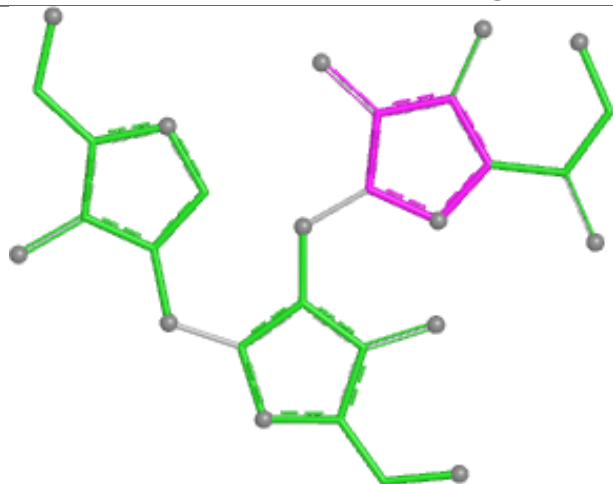


Torsions

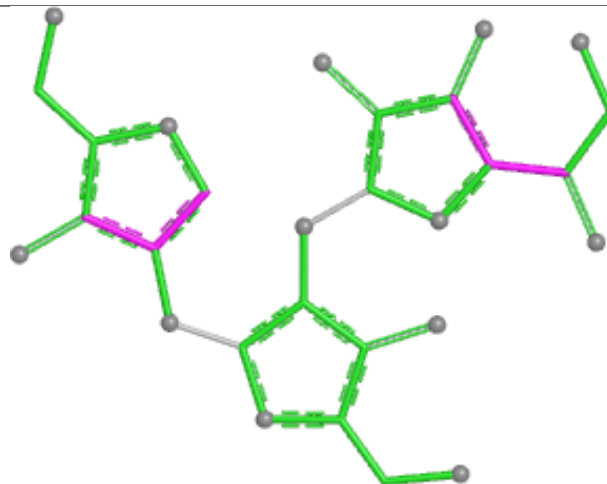


Rings

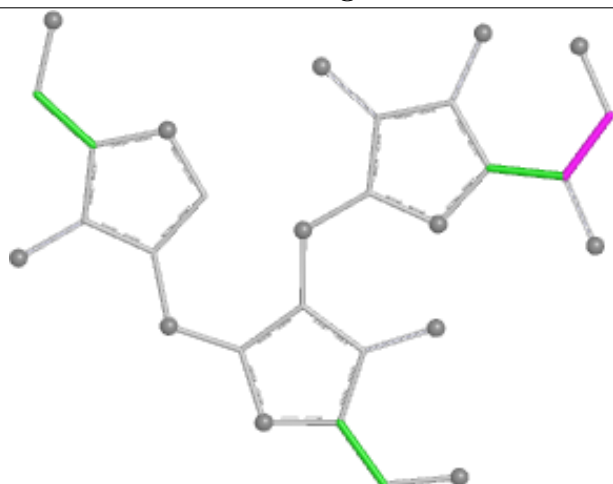
Oligosaccharide Chain 9



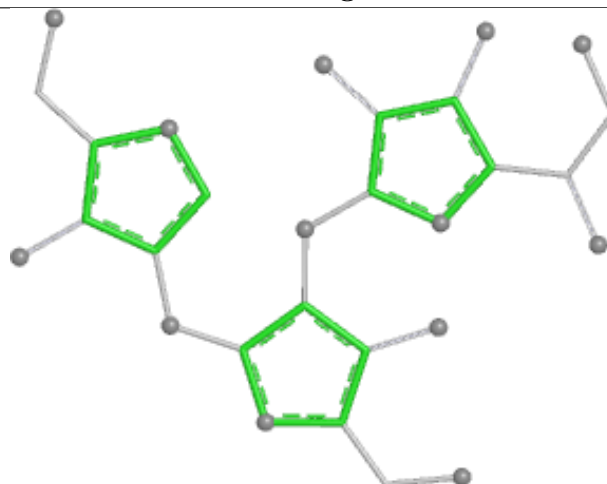
Bond lengths



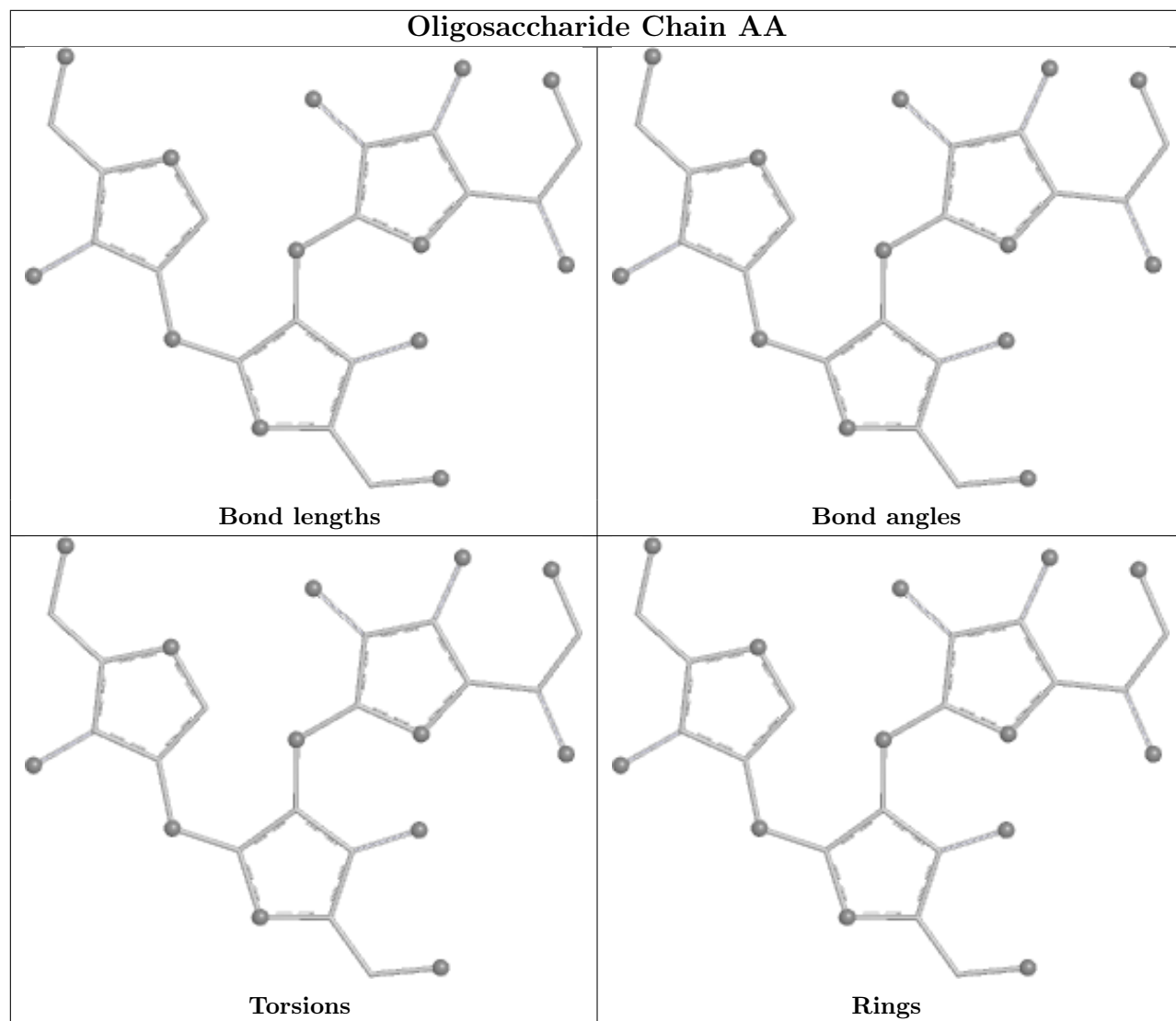
Bond angles

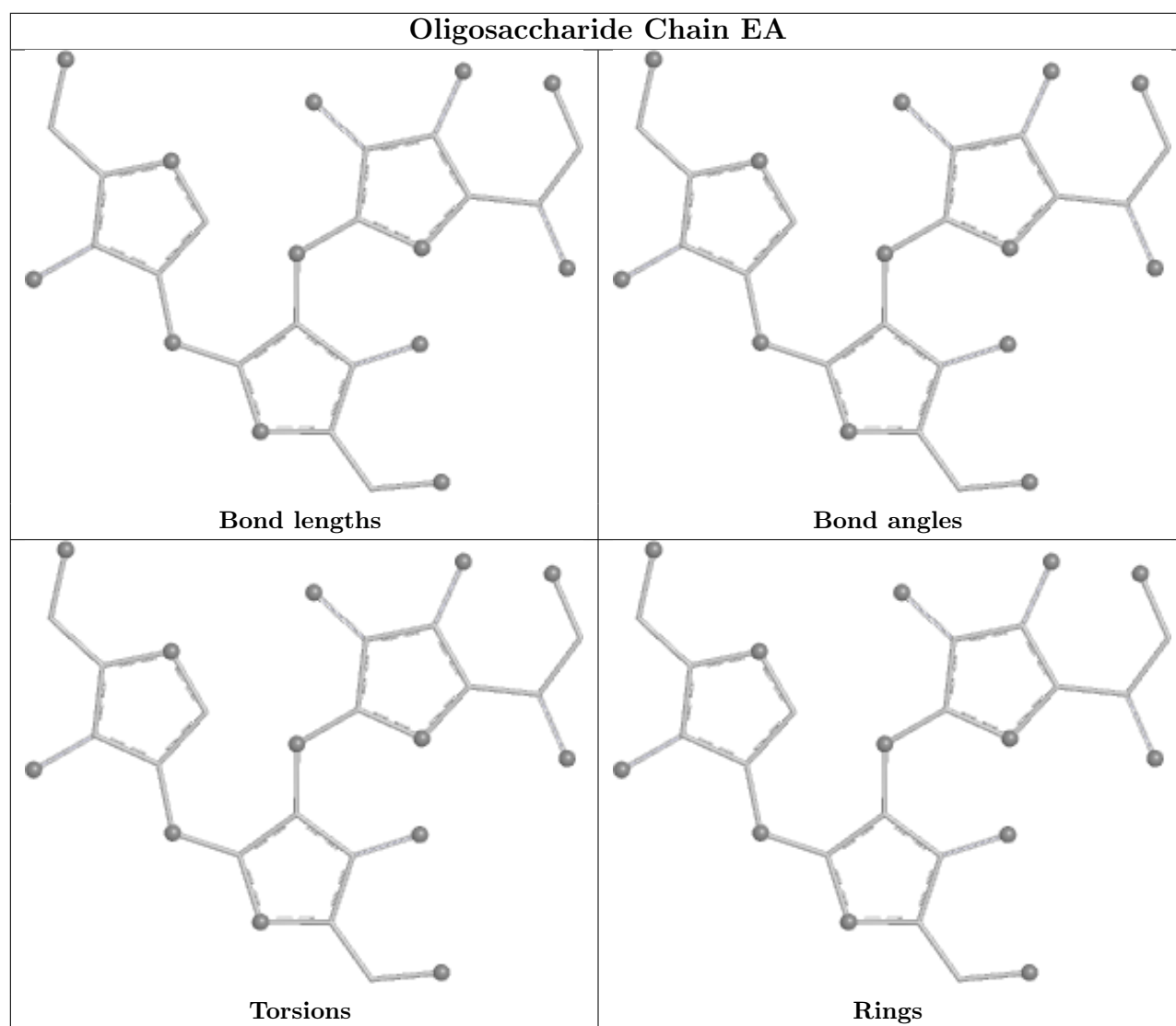


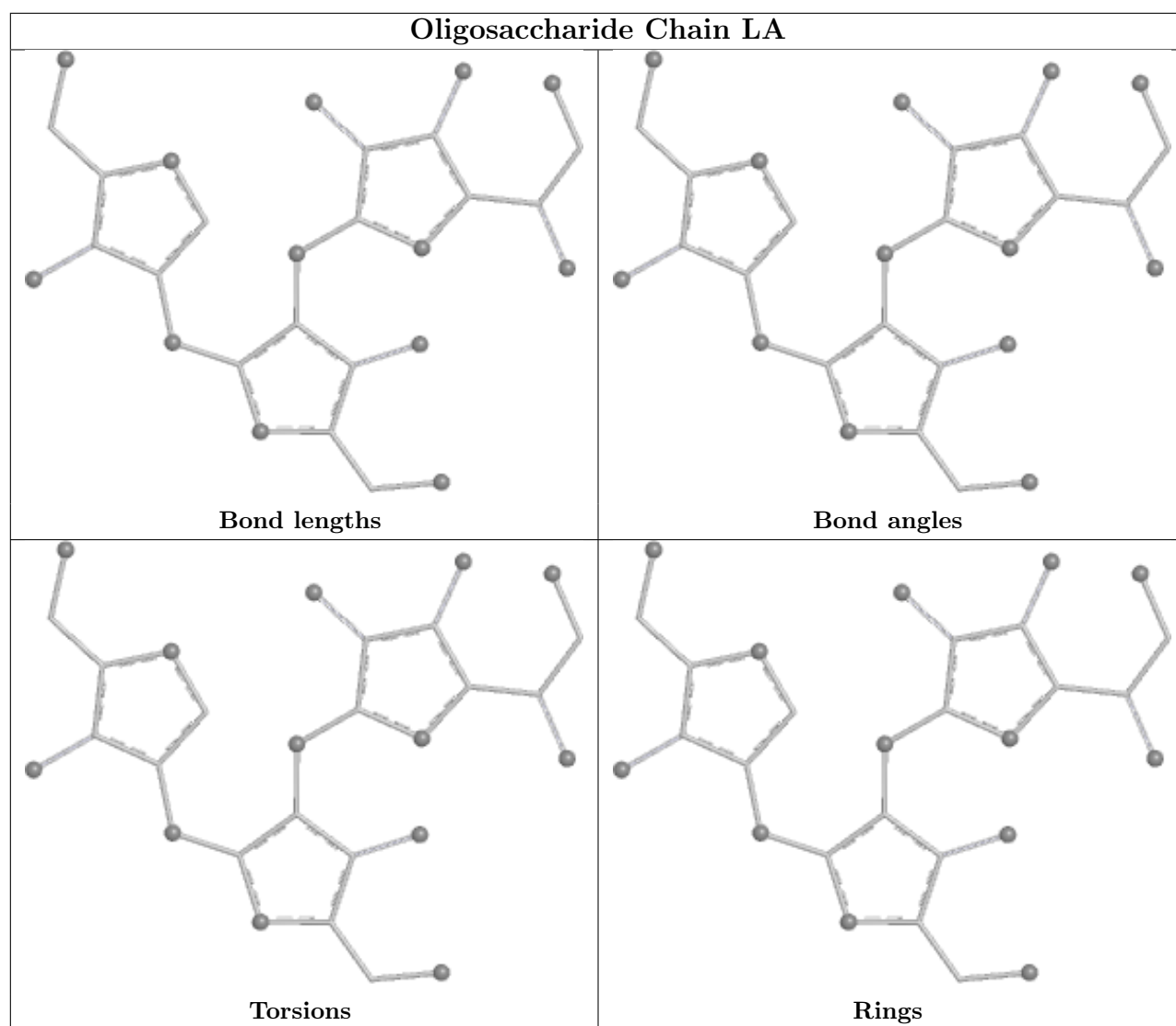
Torsions

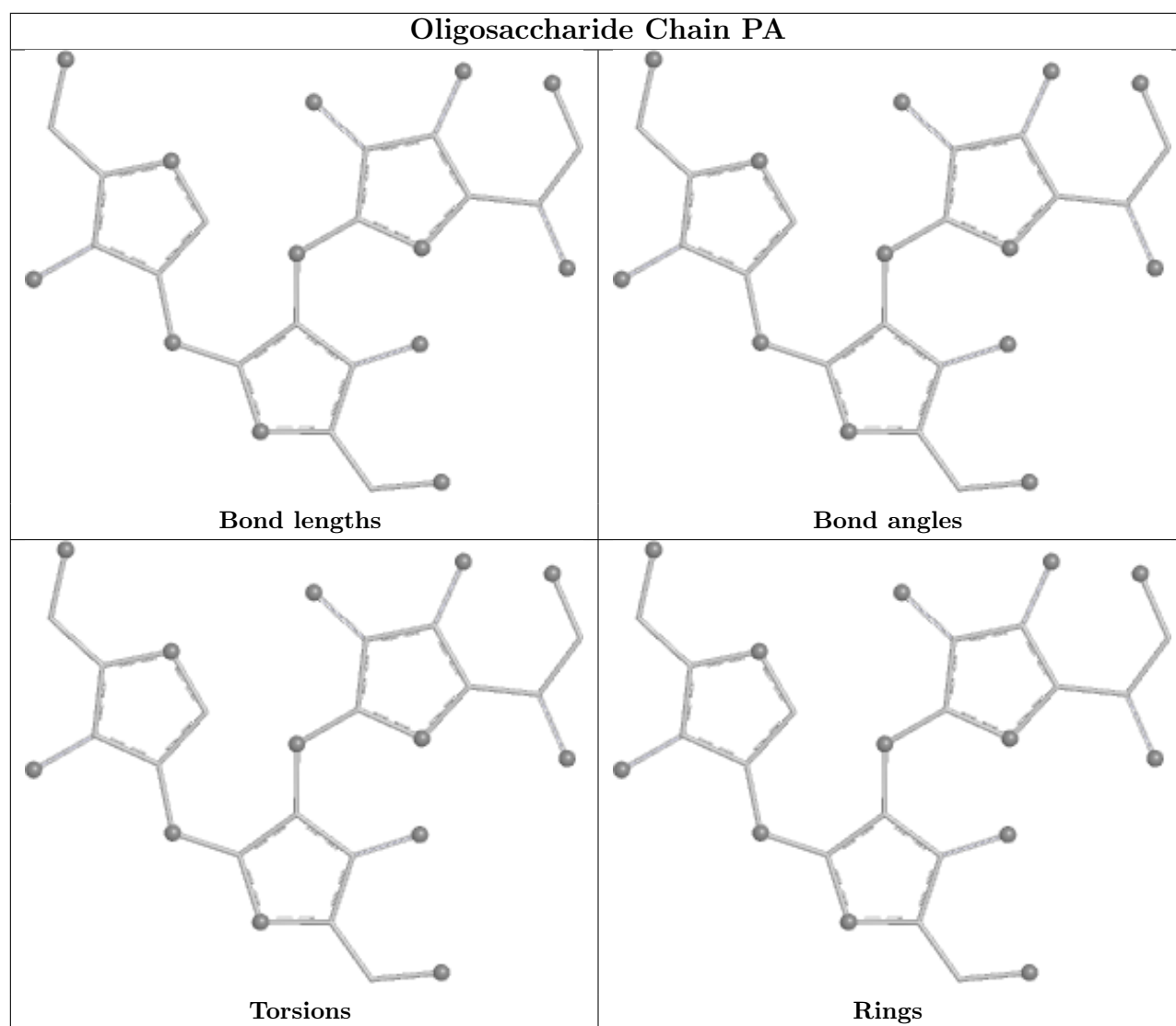


Rings

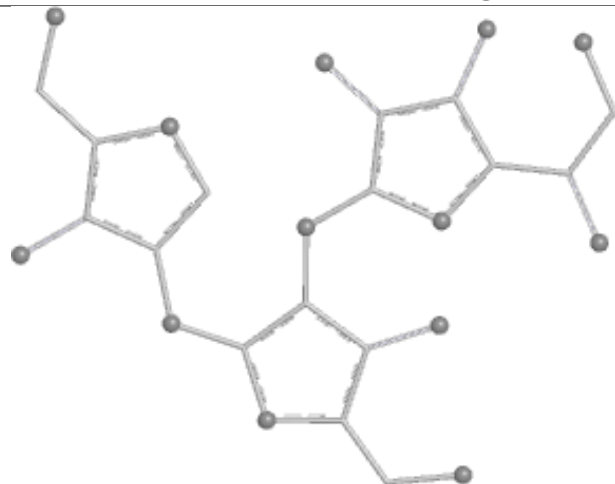




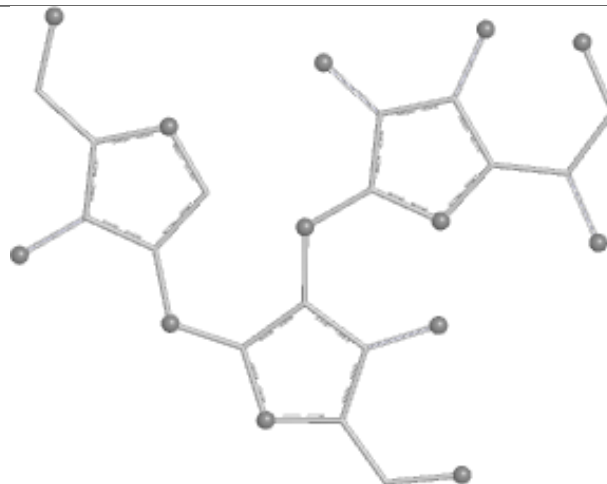




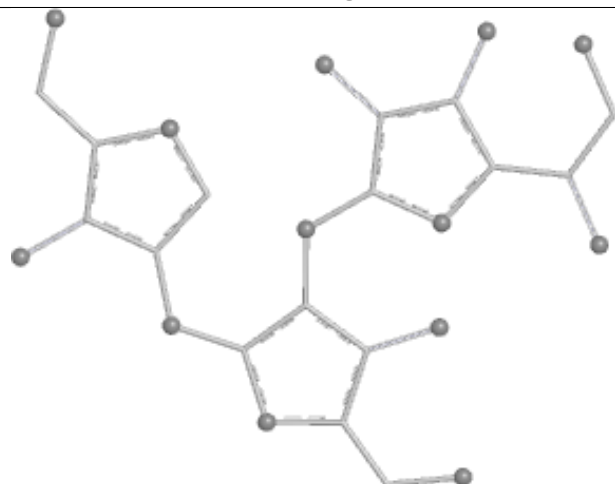
Oligosaccharide Chain 3A



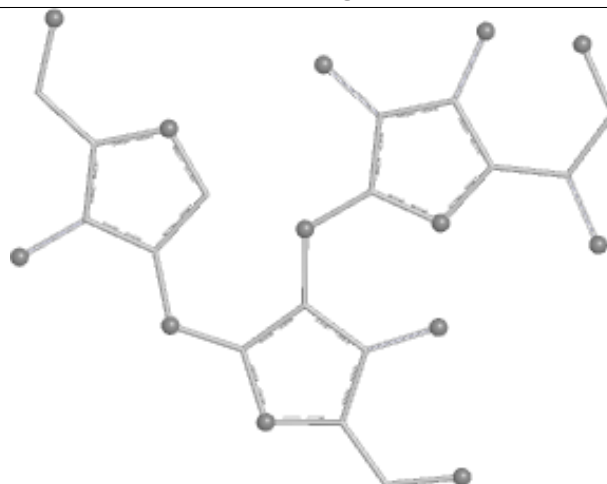
Bond lengths



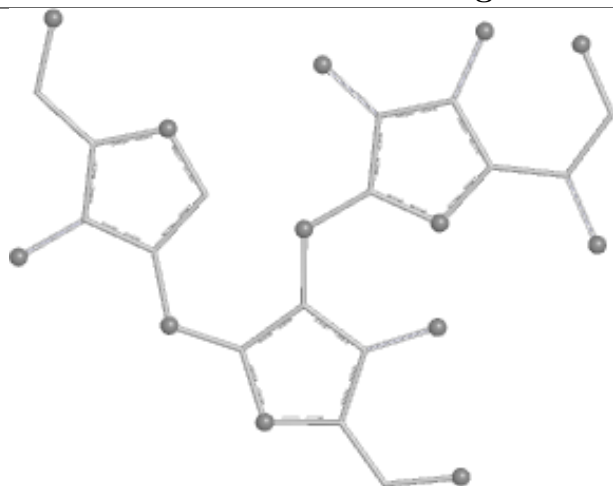
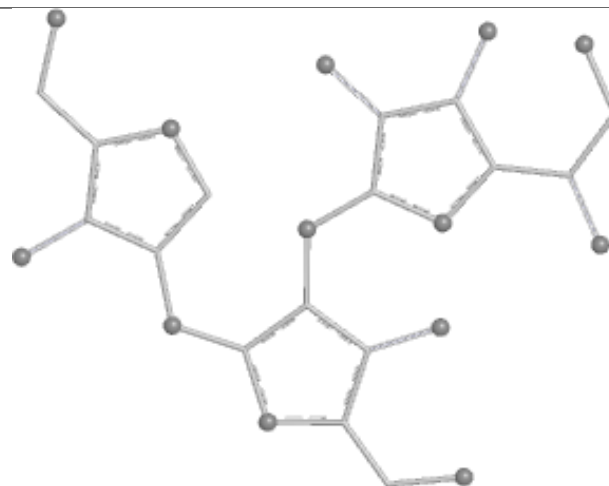
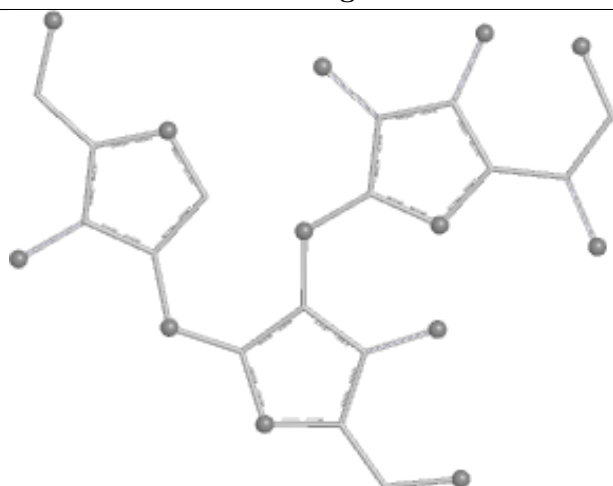
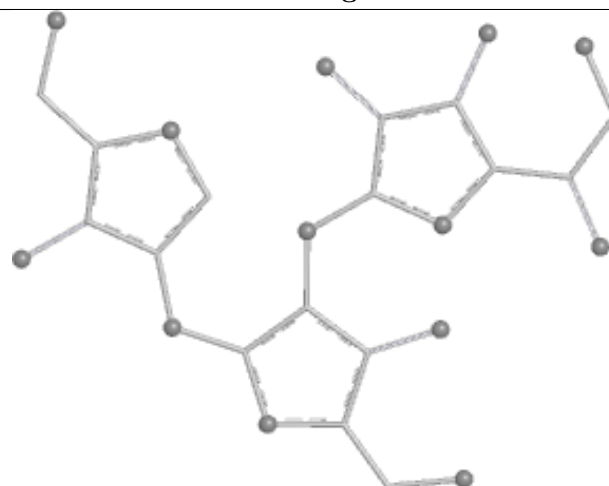
Bond angles



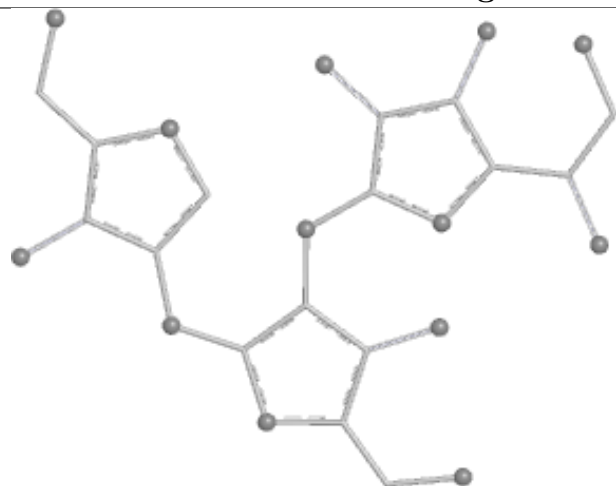
Torsions



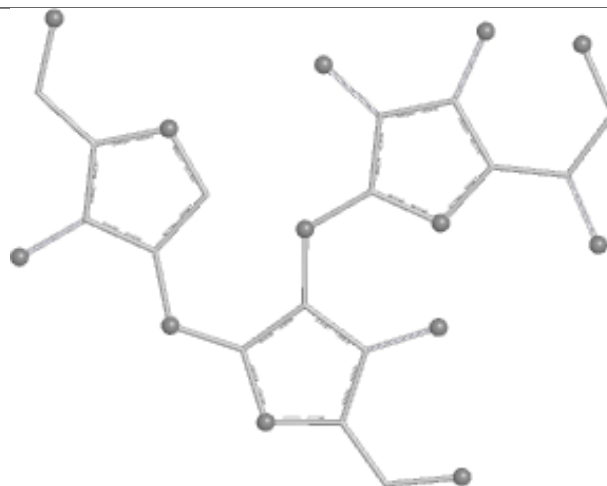
Rings

Oligosaccharide Chain 6A**Bond lengths****Bond angles****Torsions****Rings**

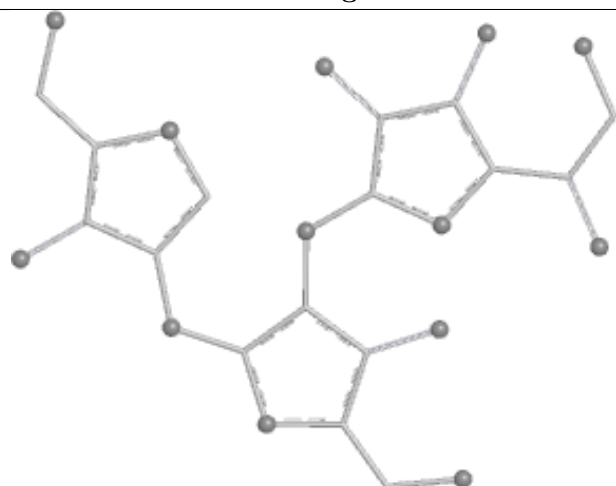
Oligosaccharide Chain 7A



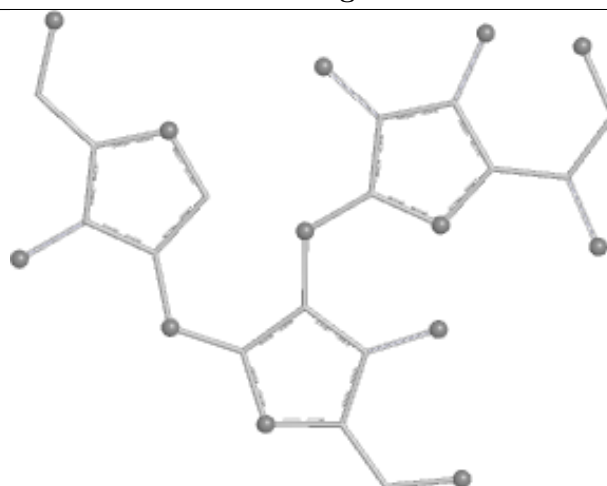
Bond lengths



Bond angles

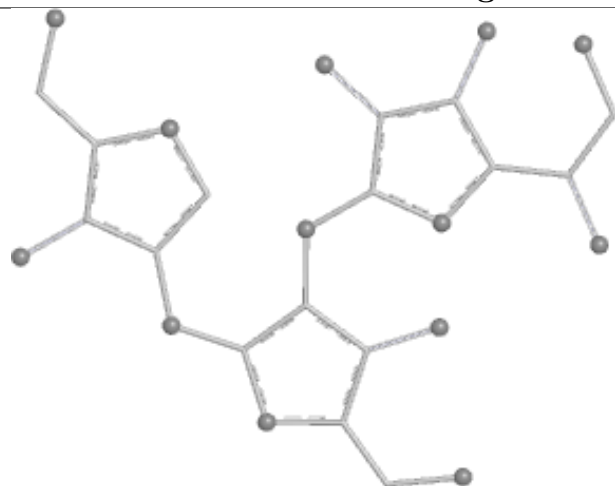


Torsions

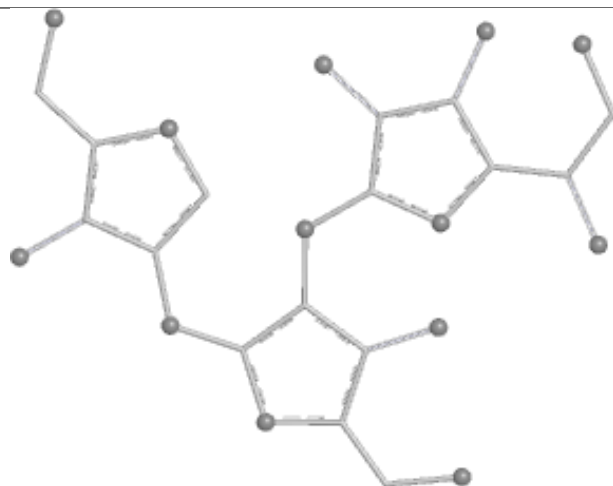


Rings

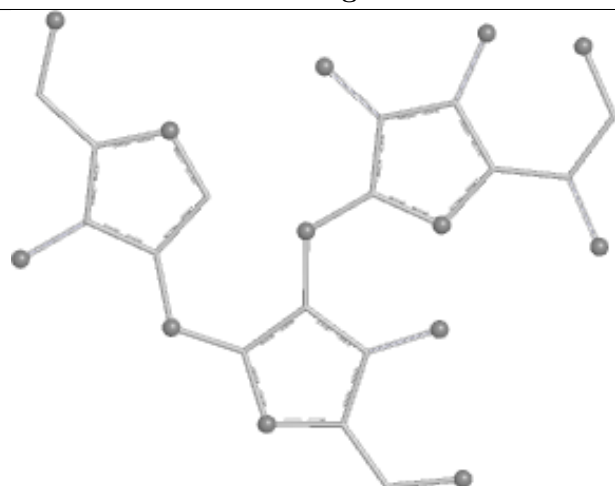
Oligosaccharide Chain 8A



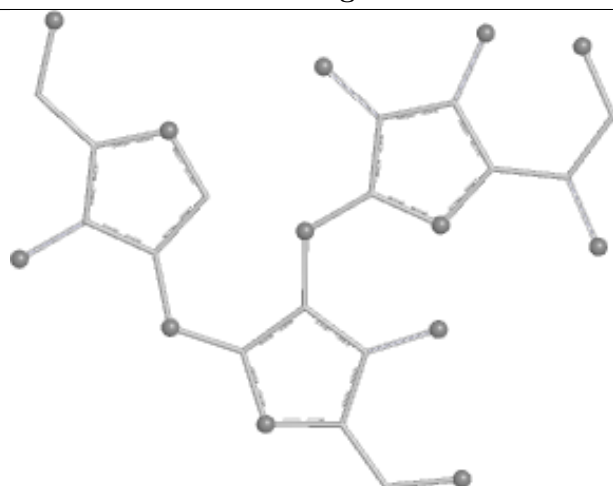
Bond lengths



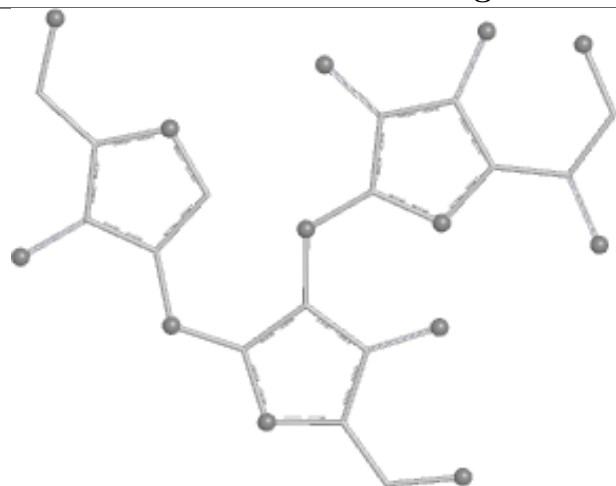
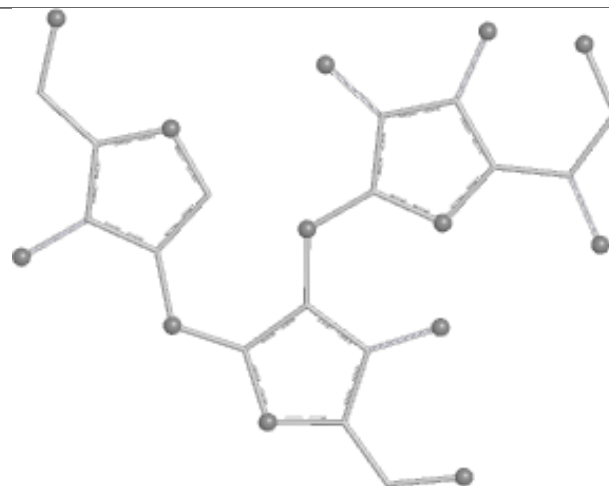
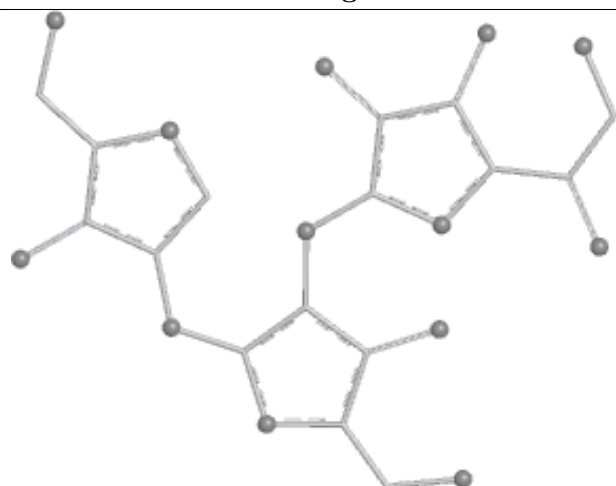
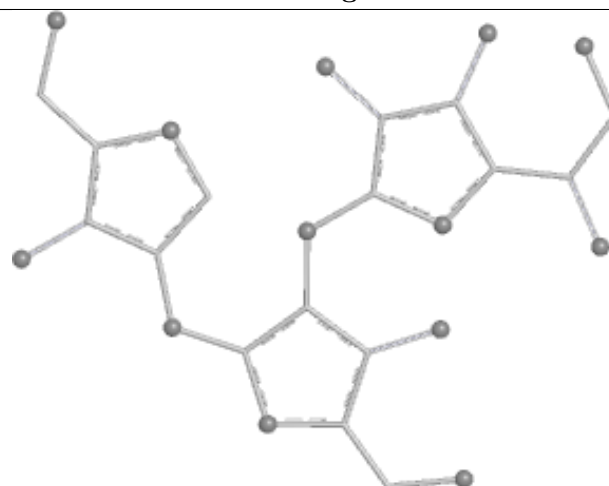
Bond angles

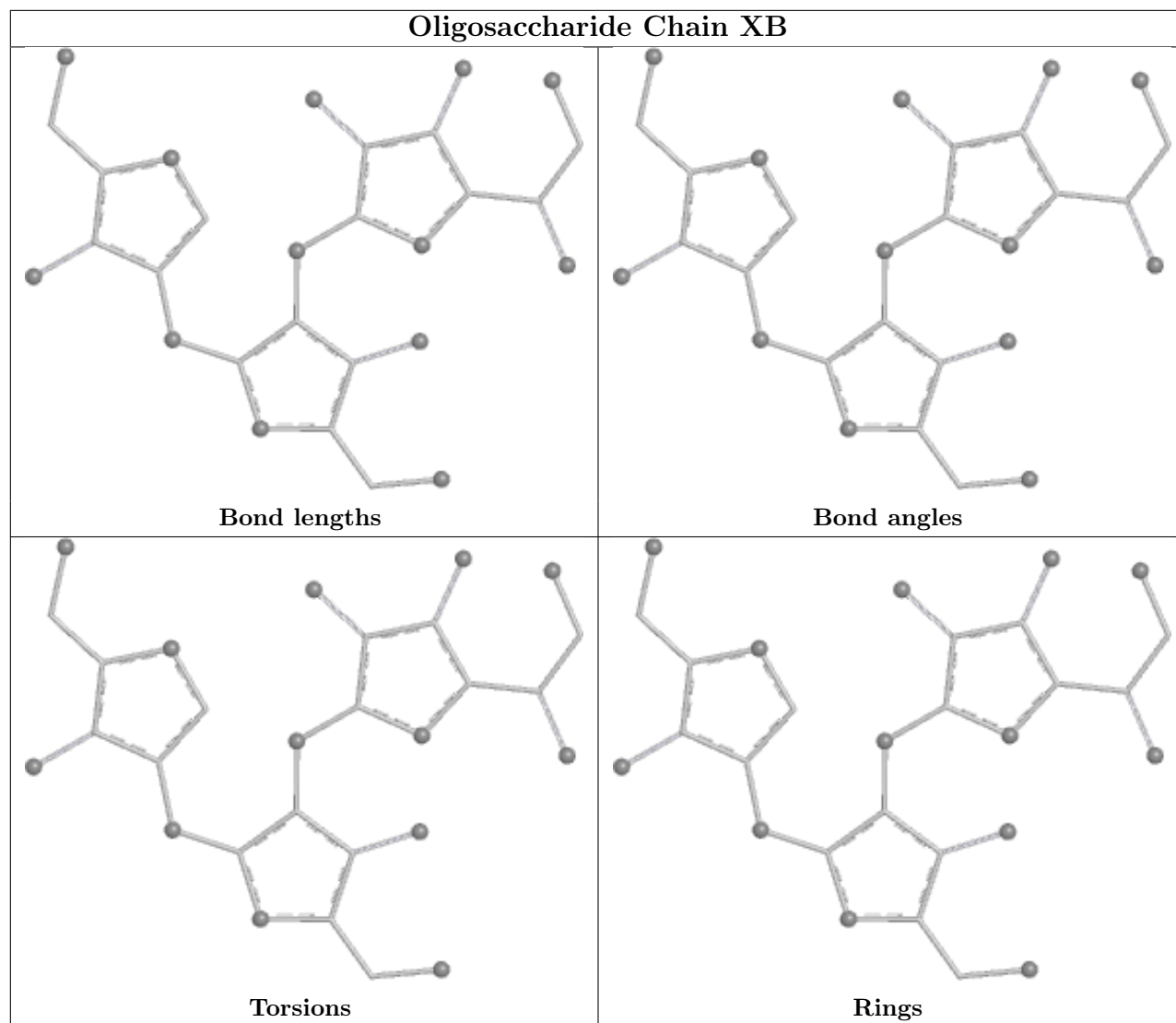


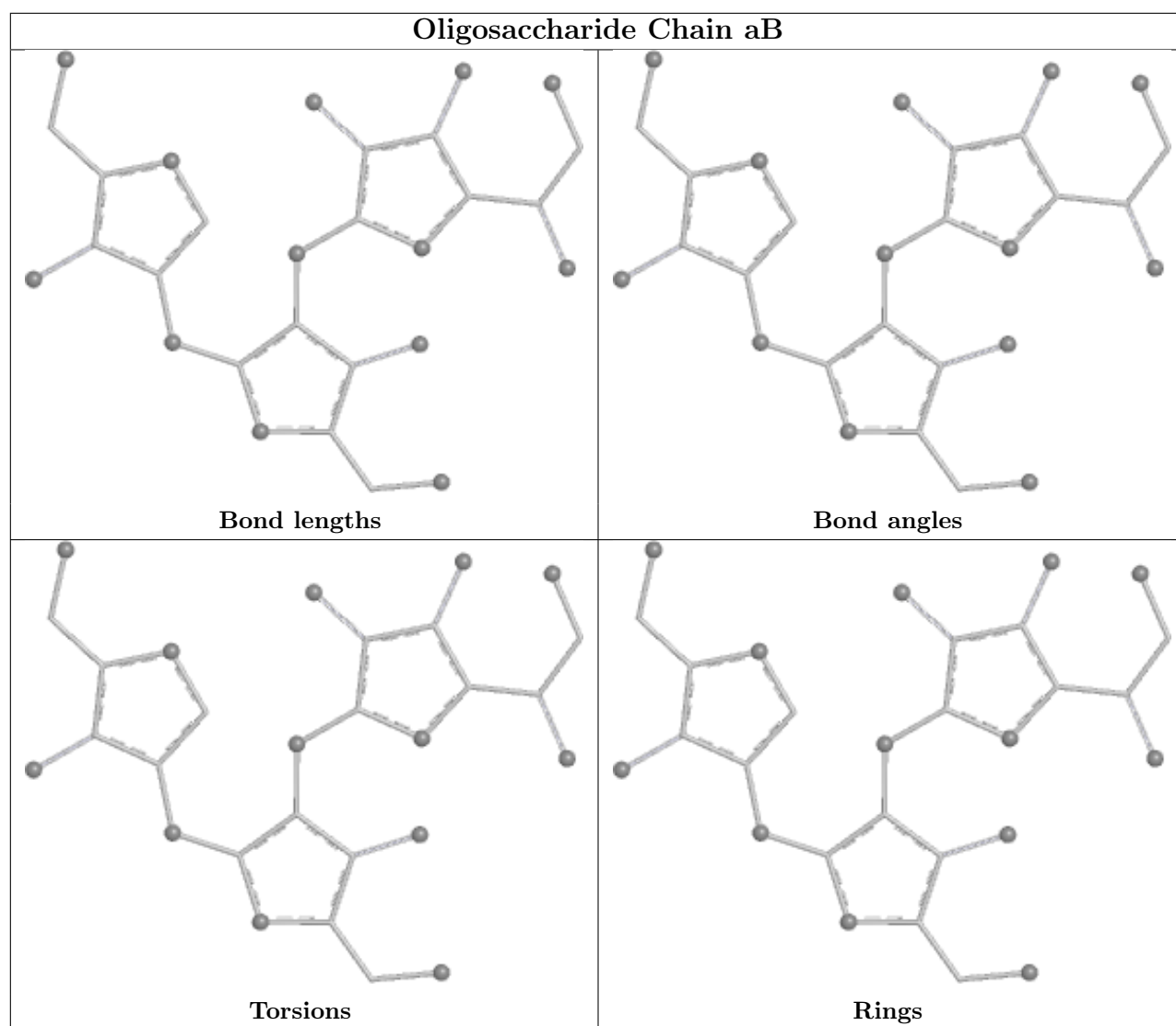
Torsions

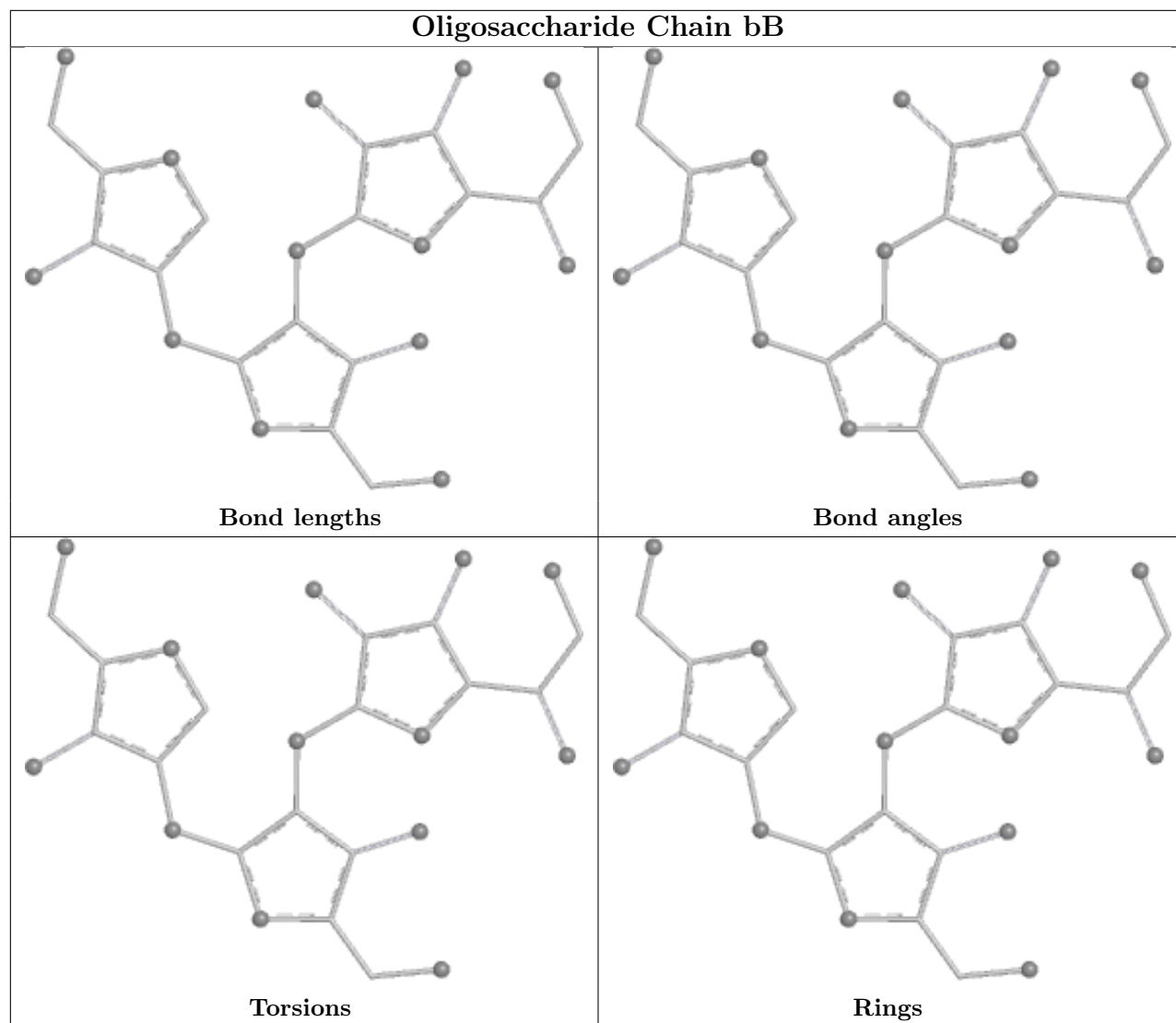


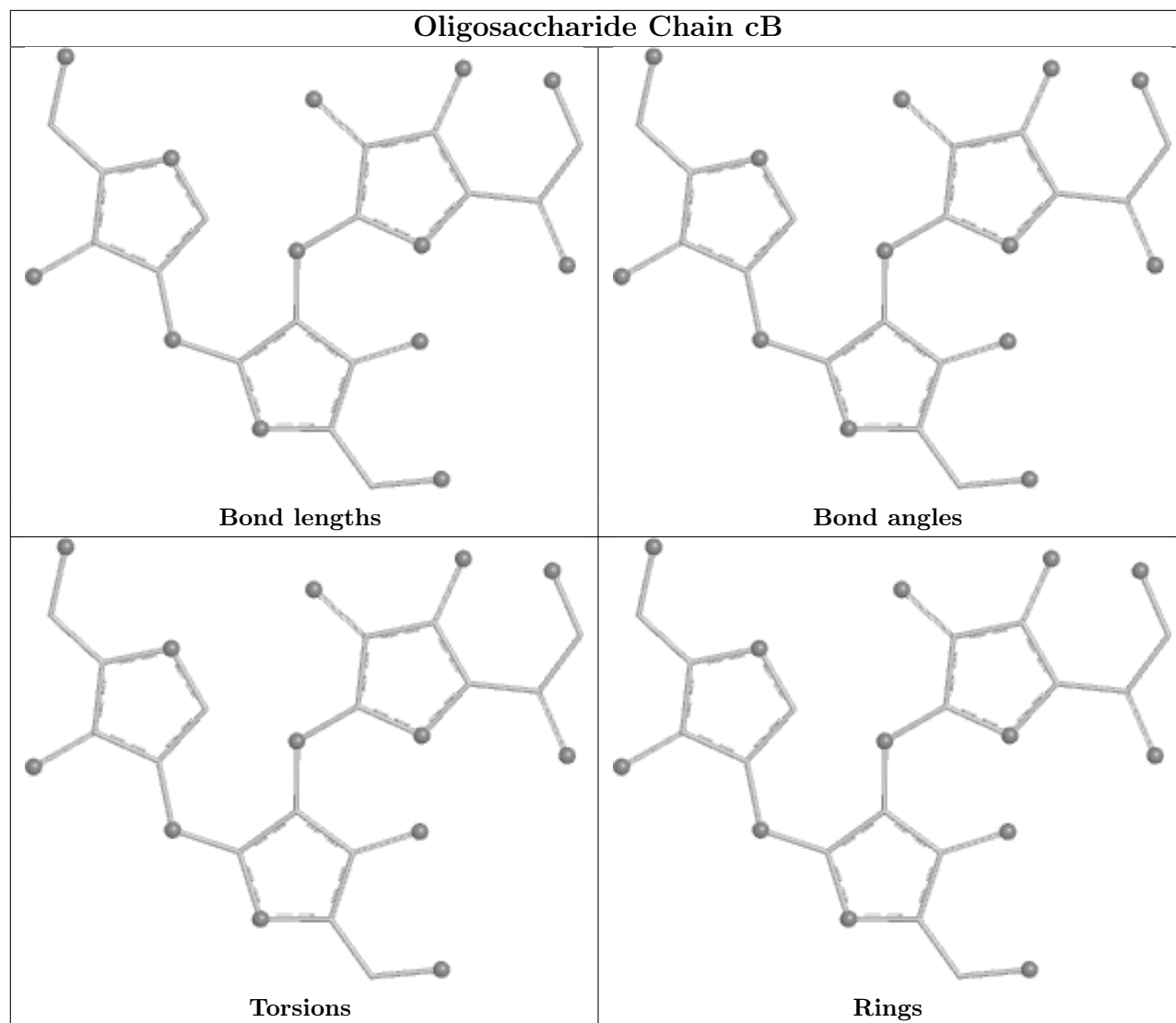
Rings

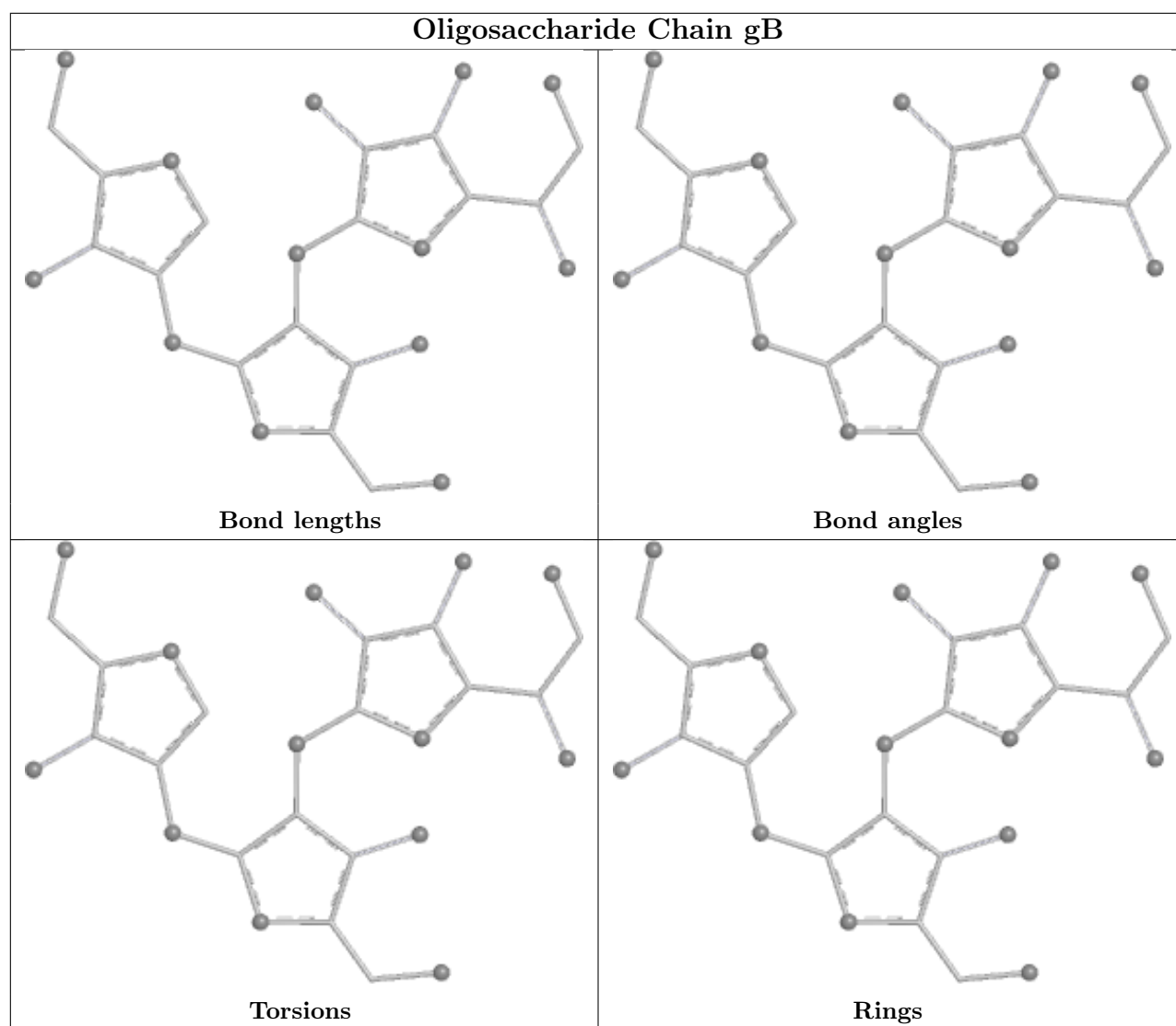
Oligosaccharide Chain CB**Bond lengths****Bond angles****Torsions****Rings**

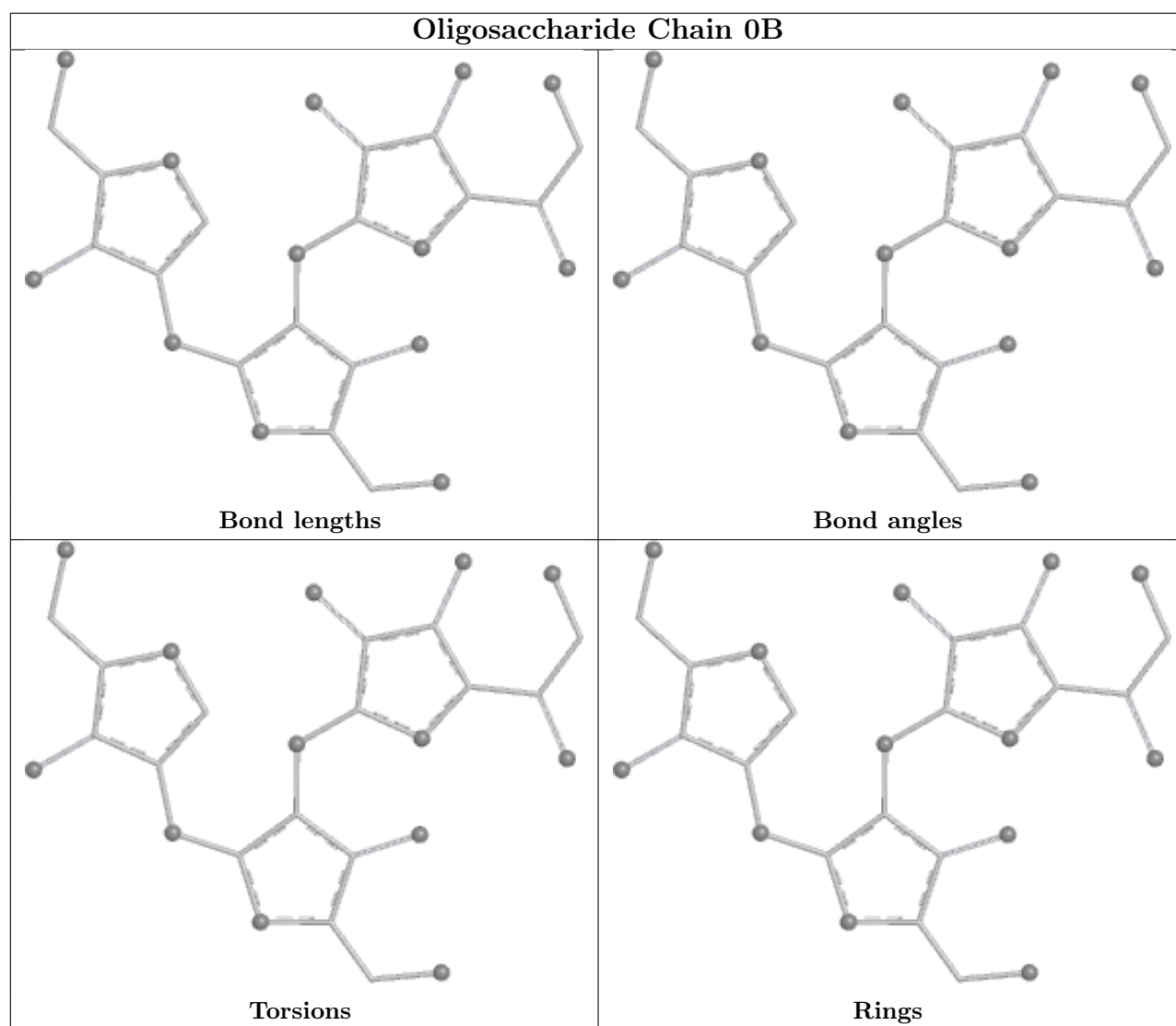


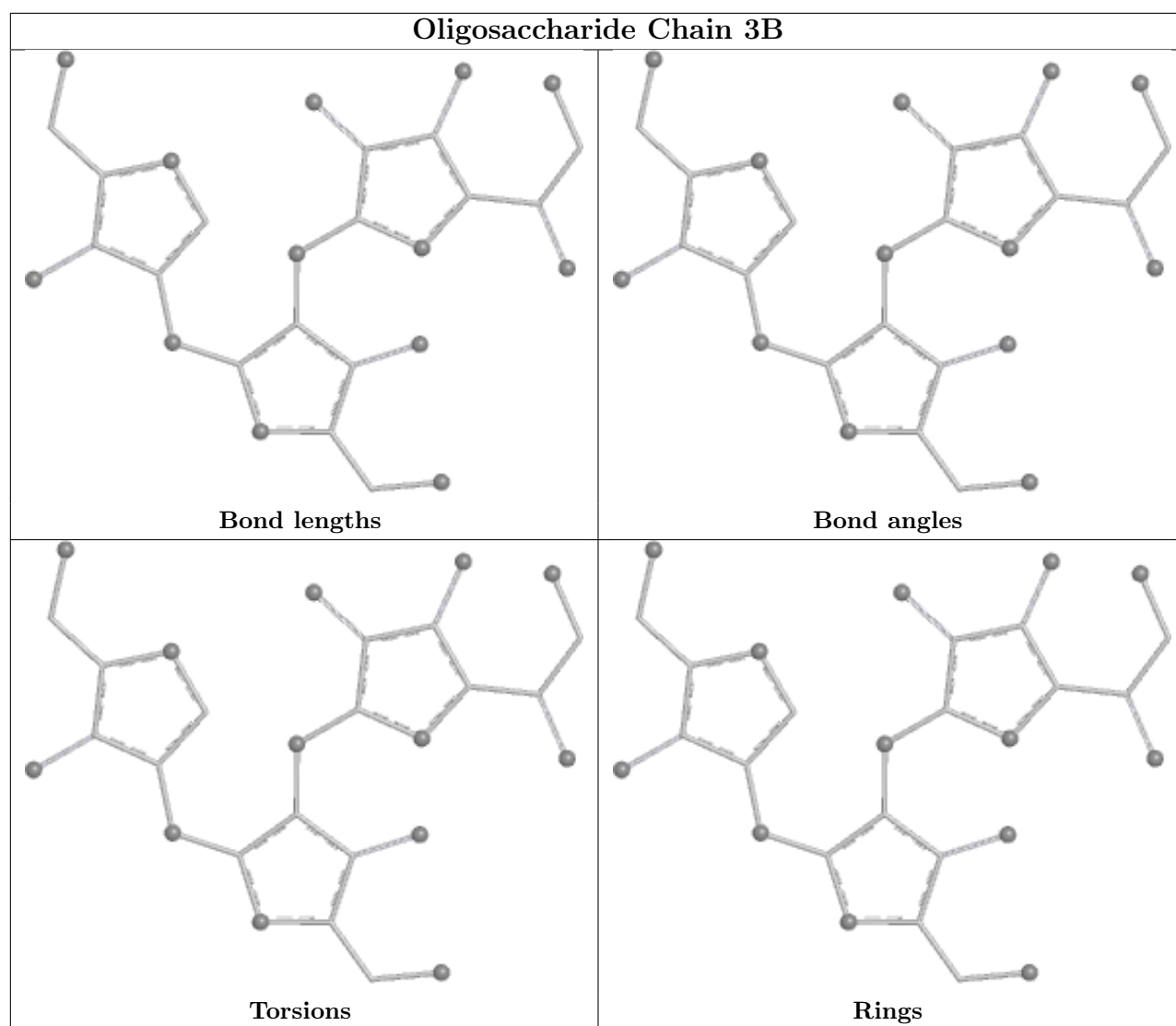


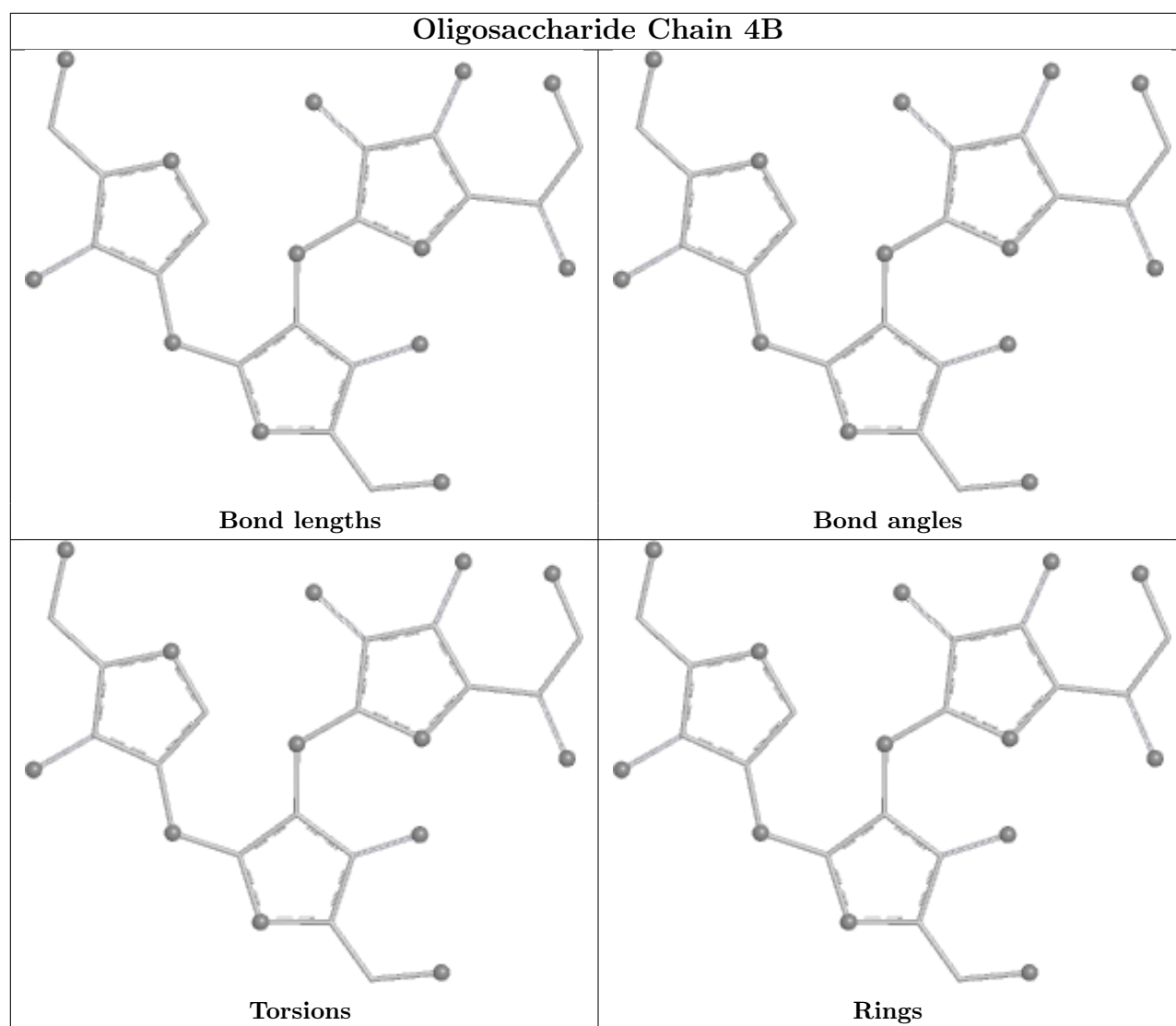


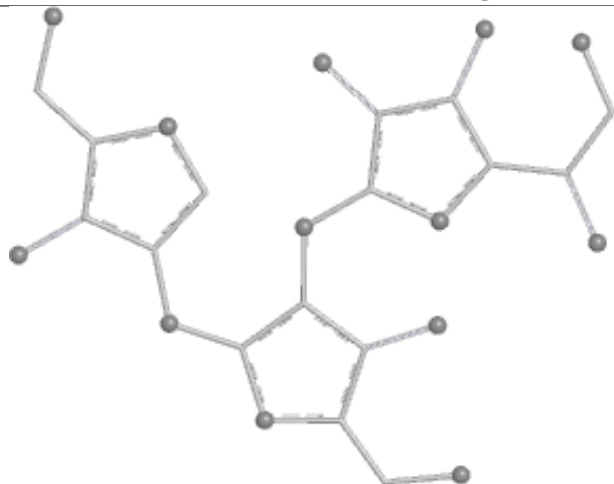
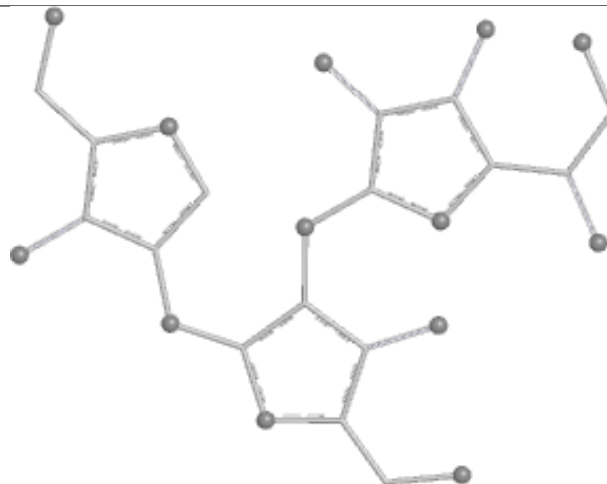
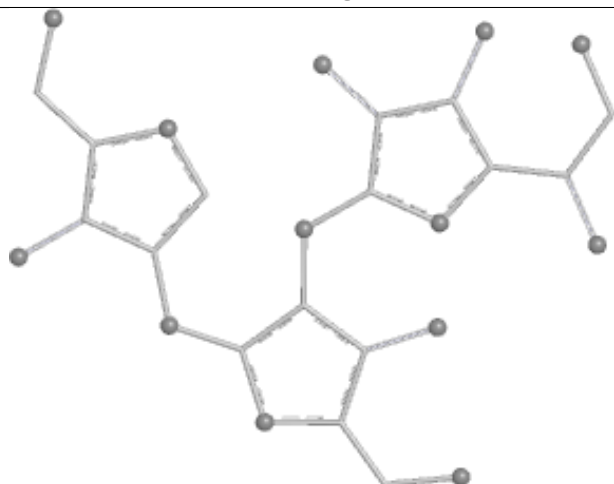
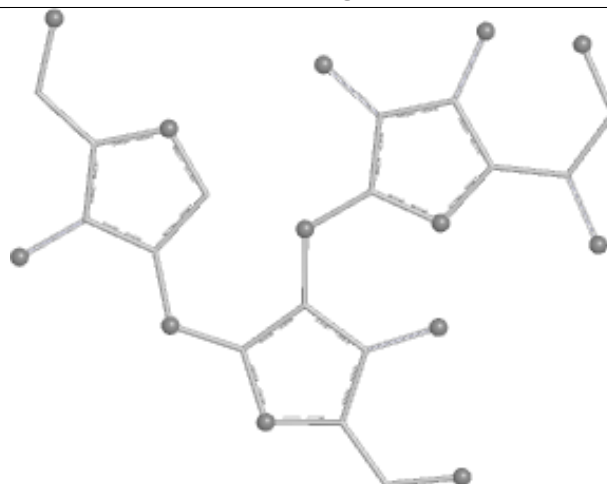


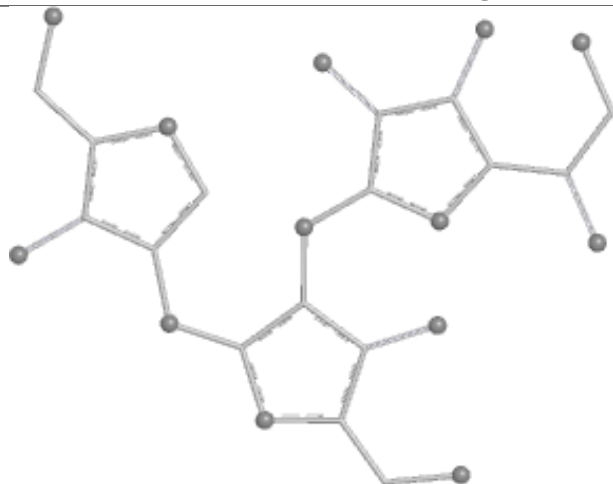
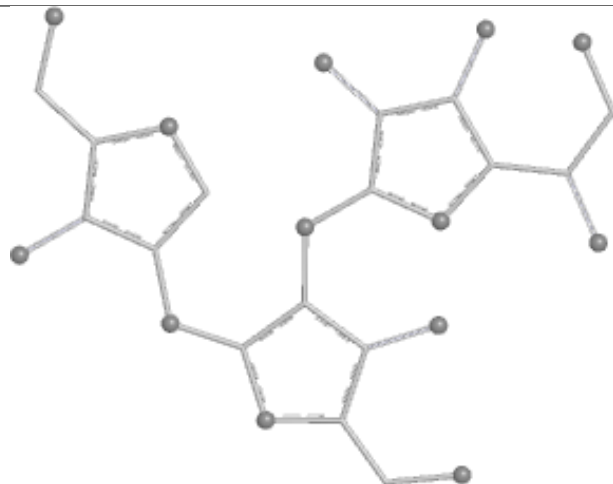
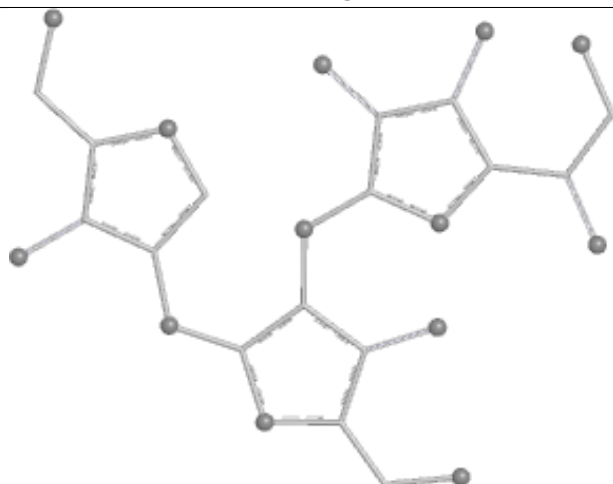
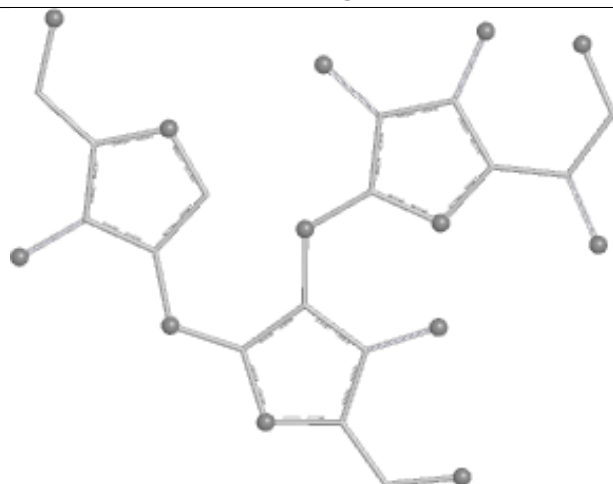


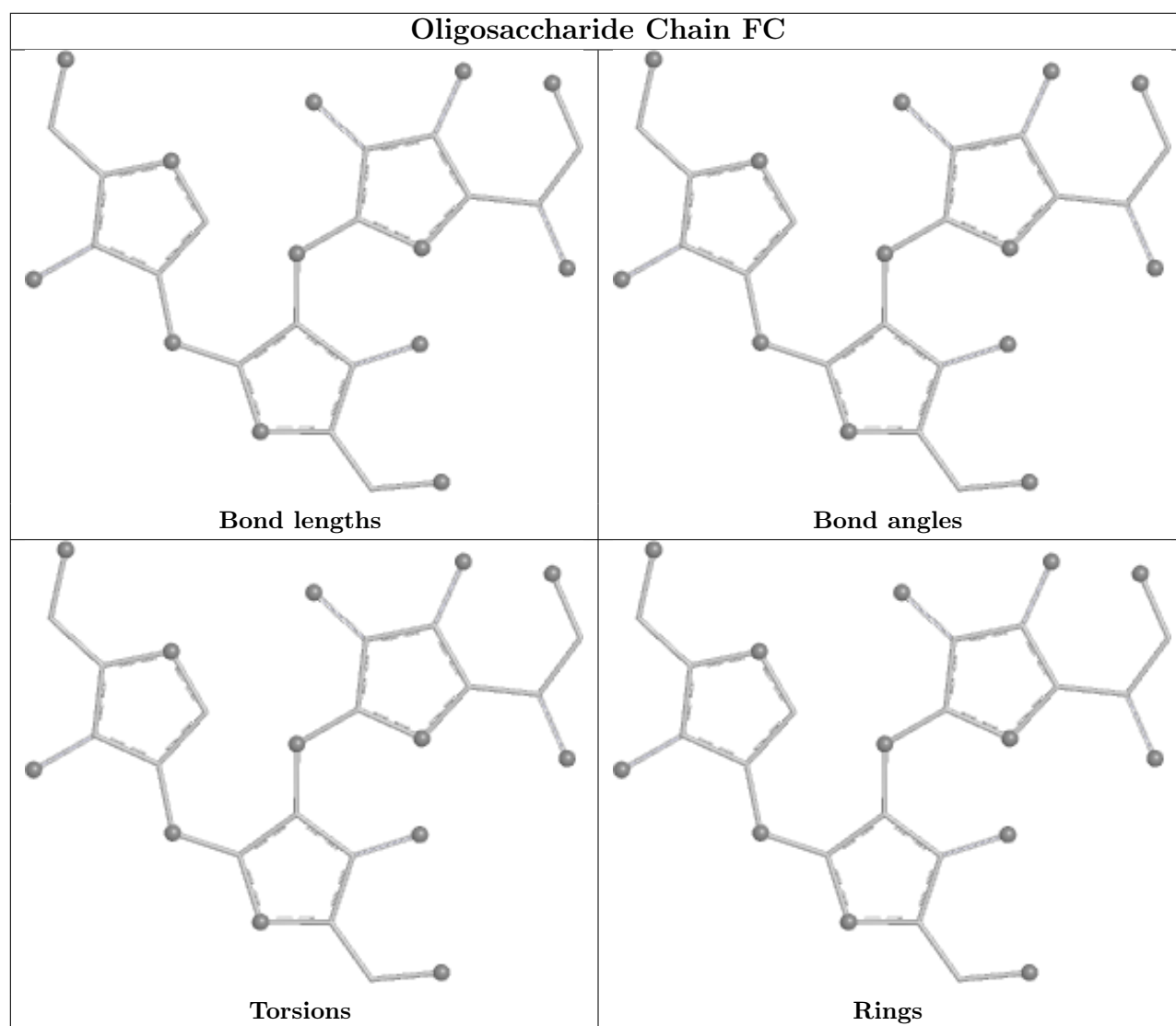




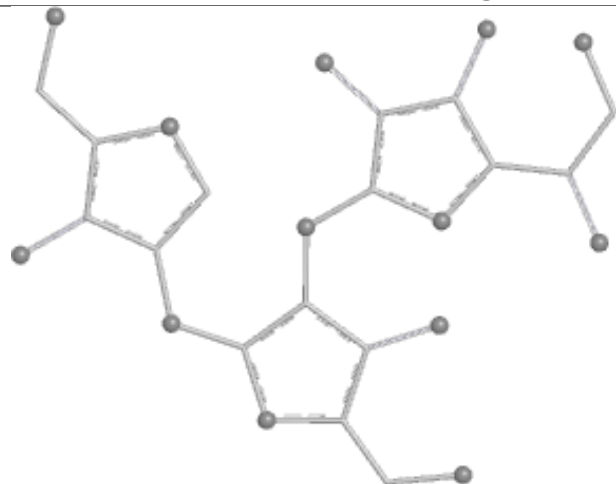


Oligosaccharide Chain 5B**Bond lengths****Bond angles****Torsions****Rings**

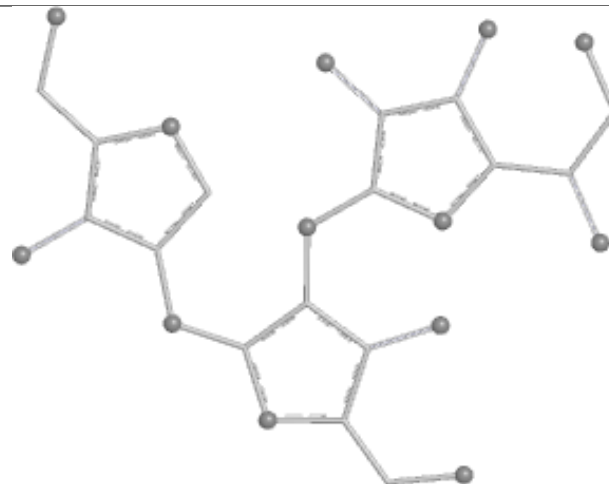
Oligosaccharide Chain 9B**Bond lengths****Bond angles****Torsions****Rings**



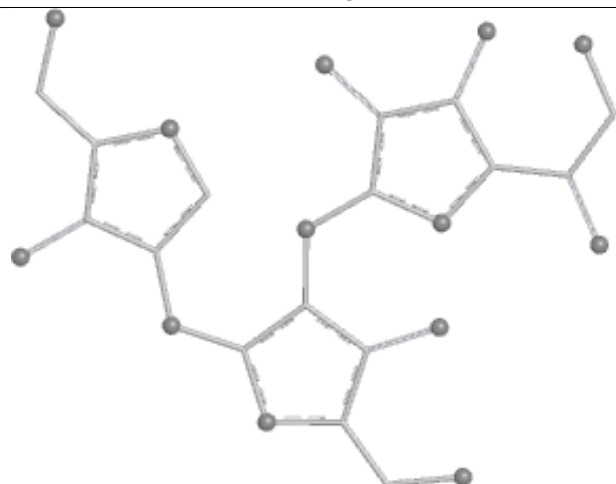
Oligosaccharide Chain JC



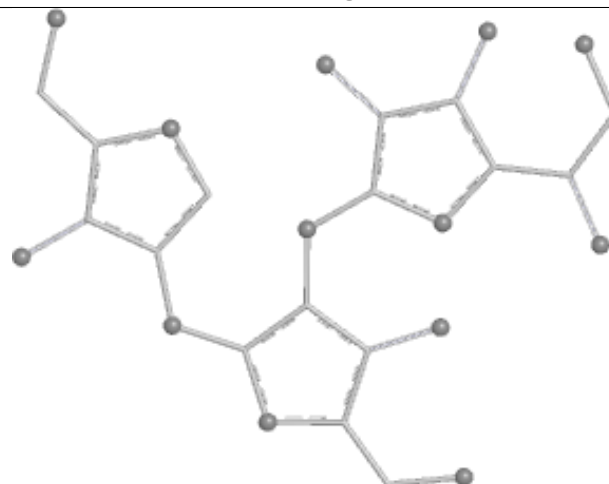
Bond lengths



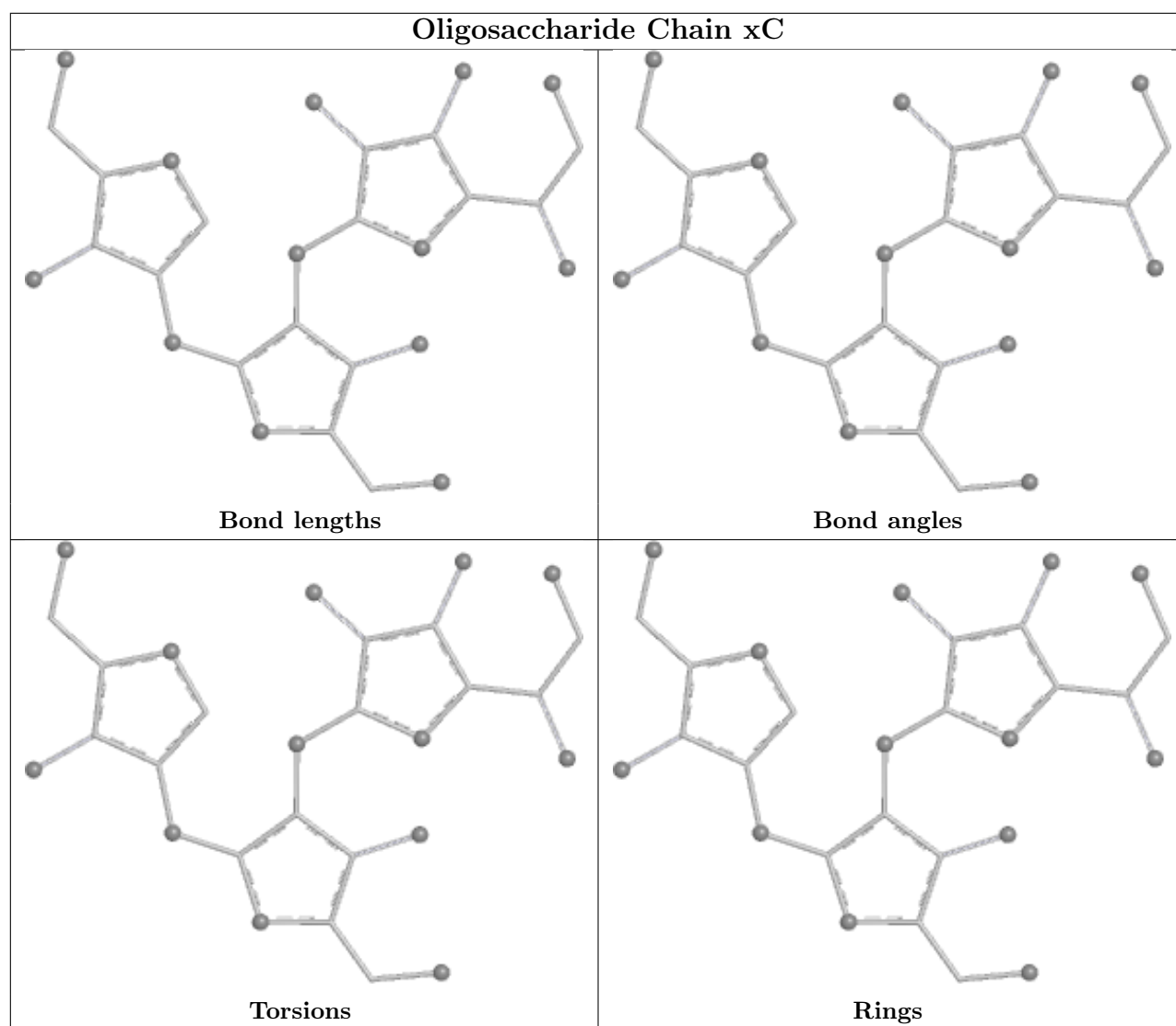
Bond angles

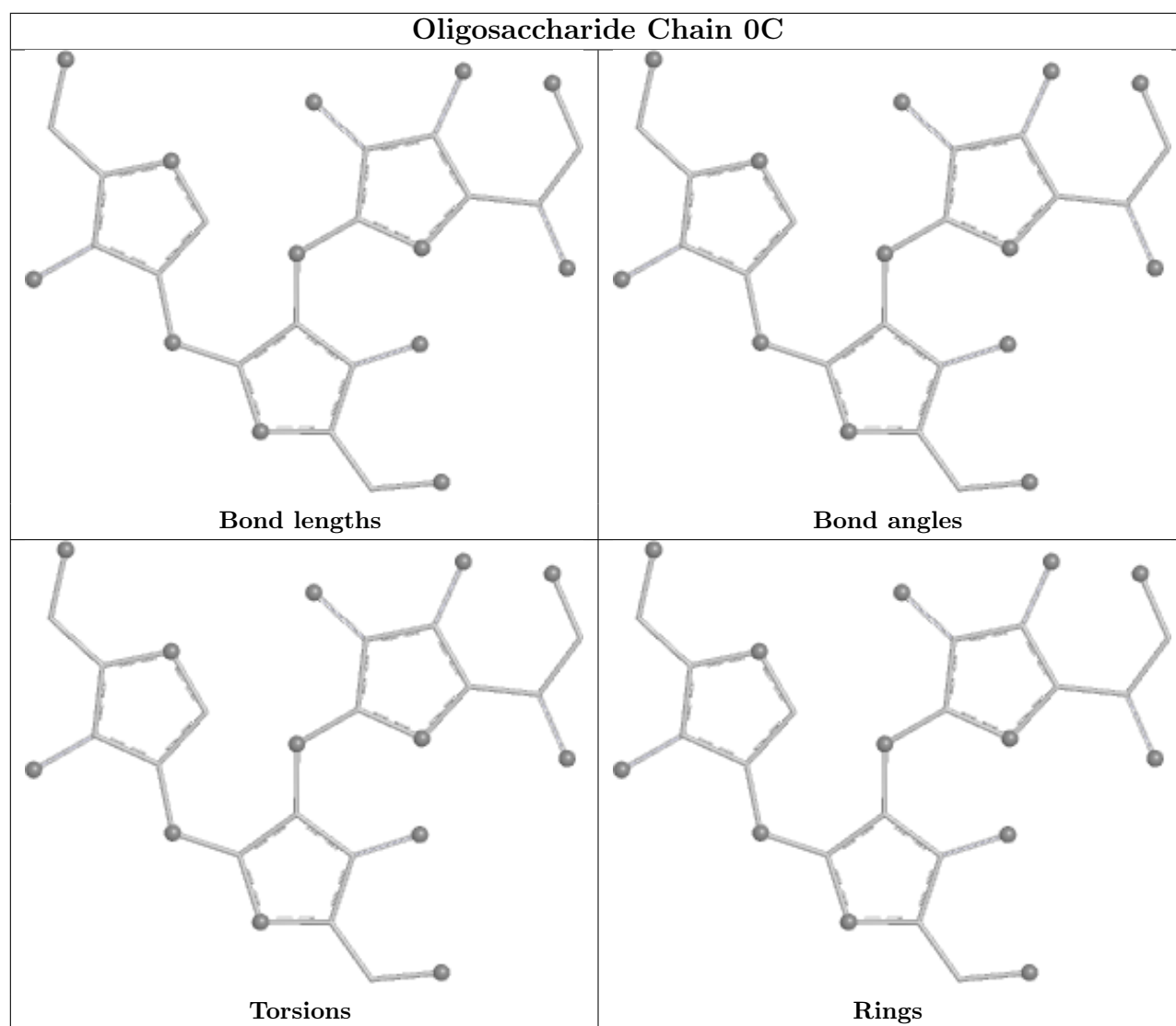


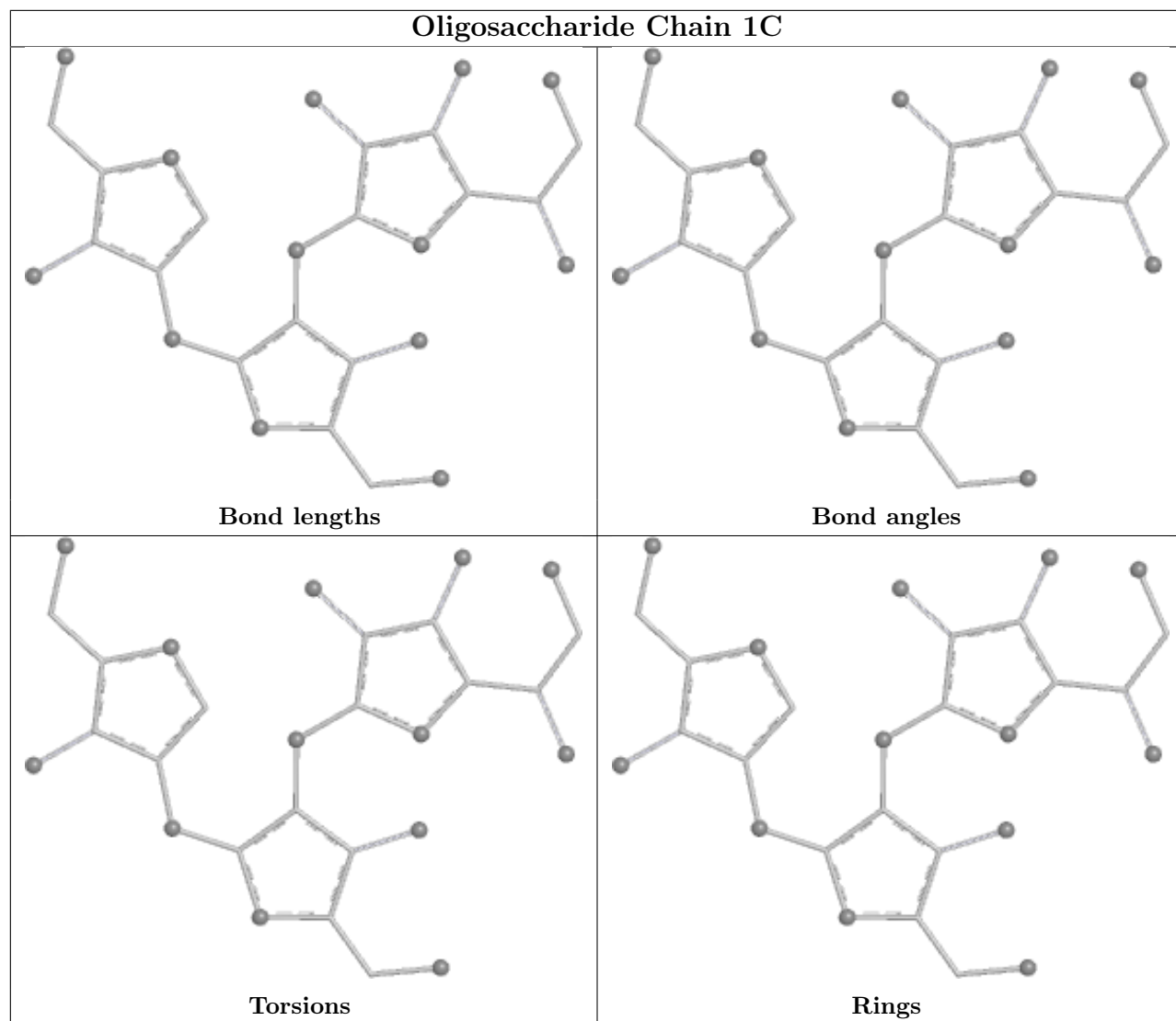
Torsions

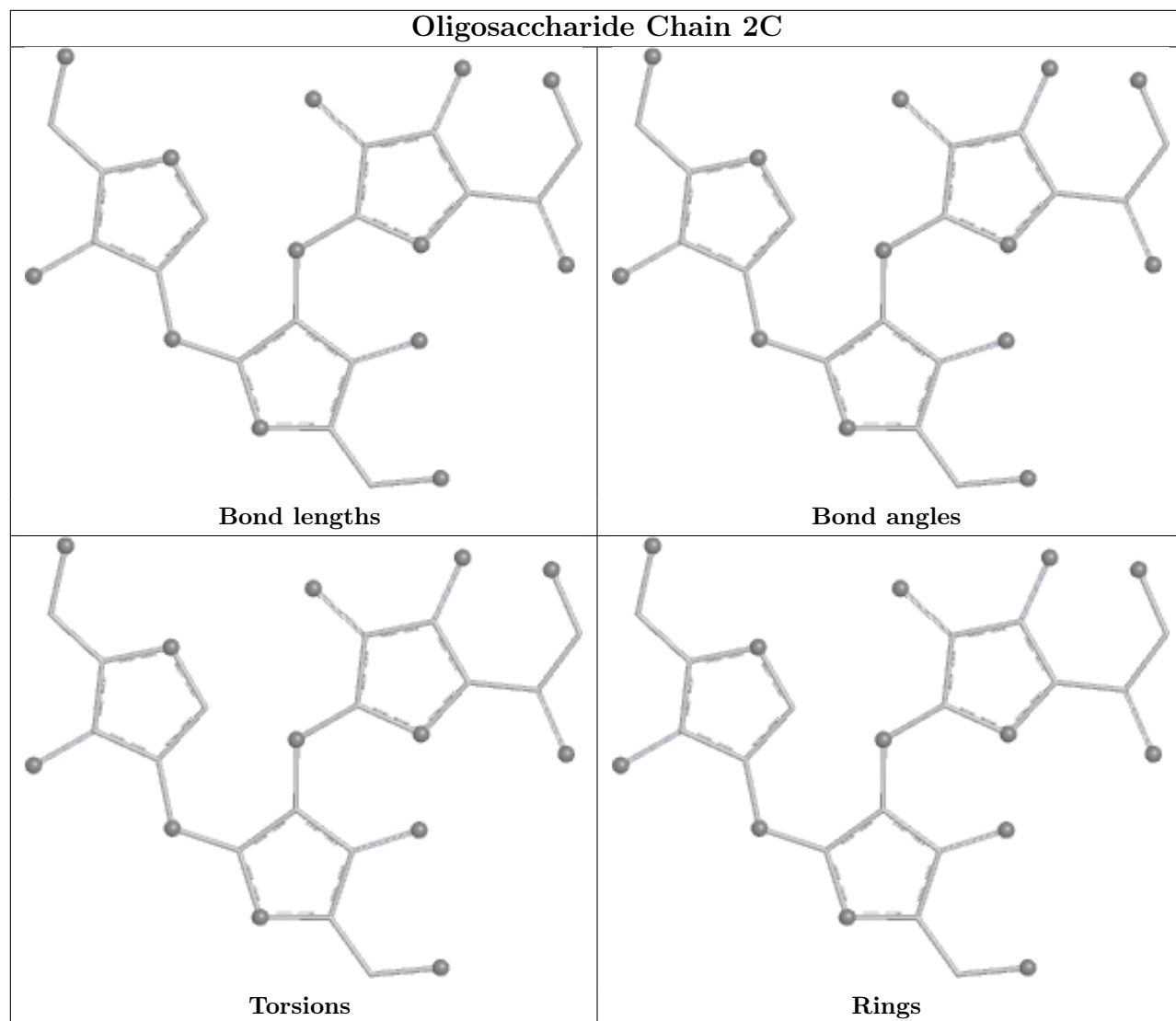


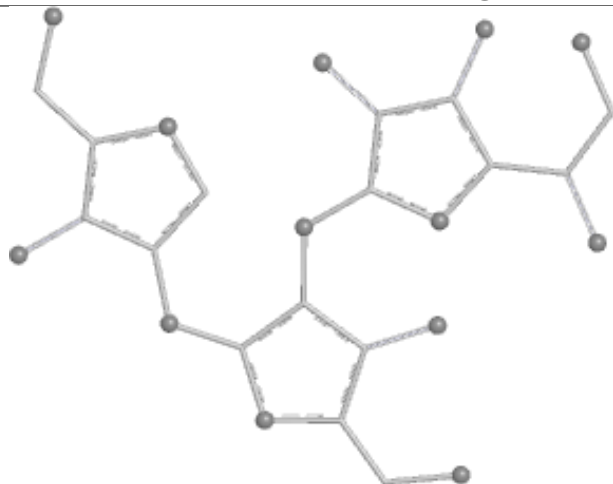
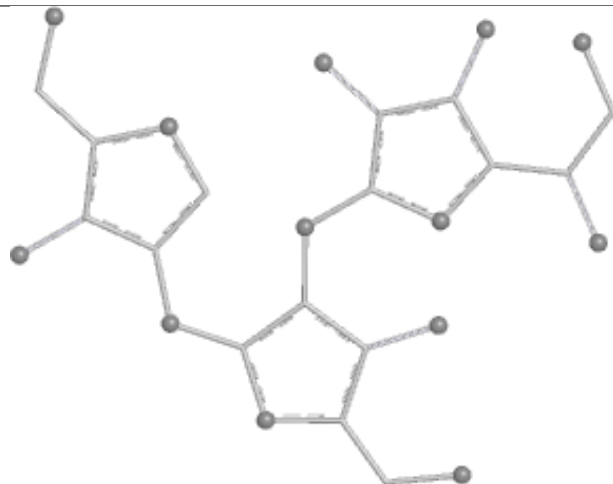
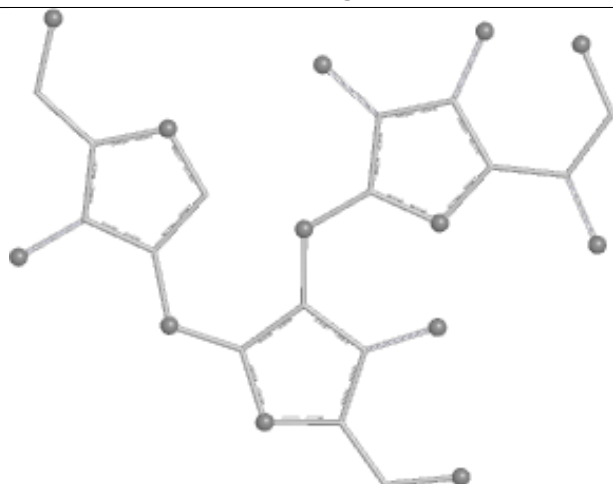
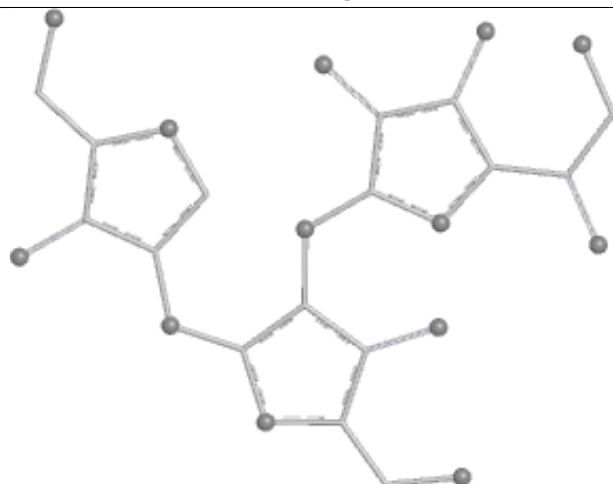
Rings

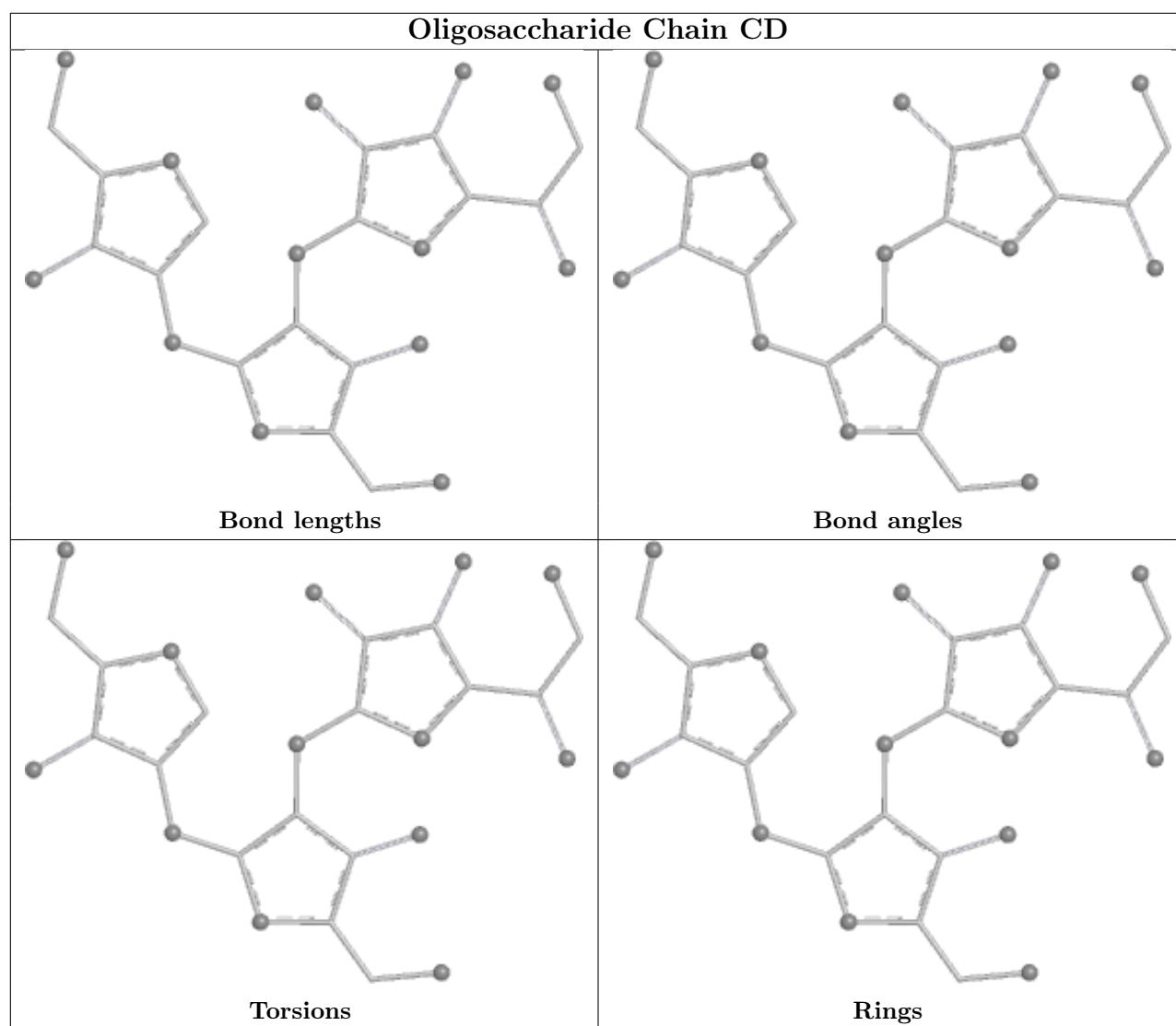


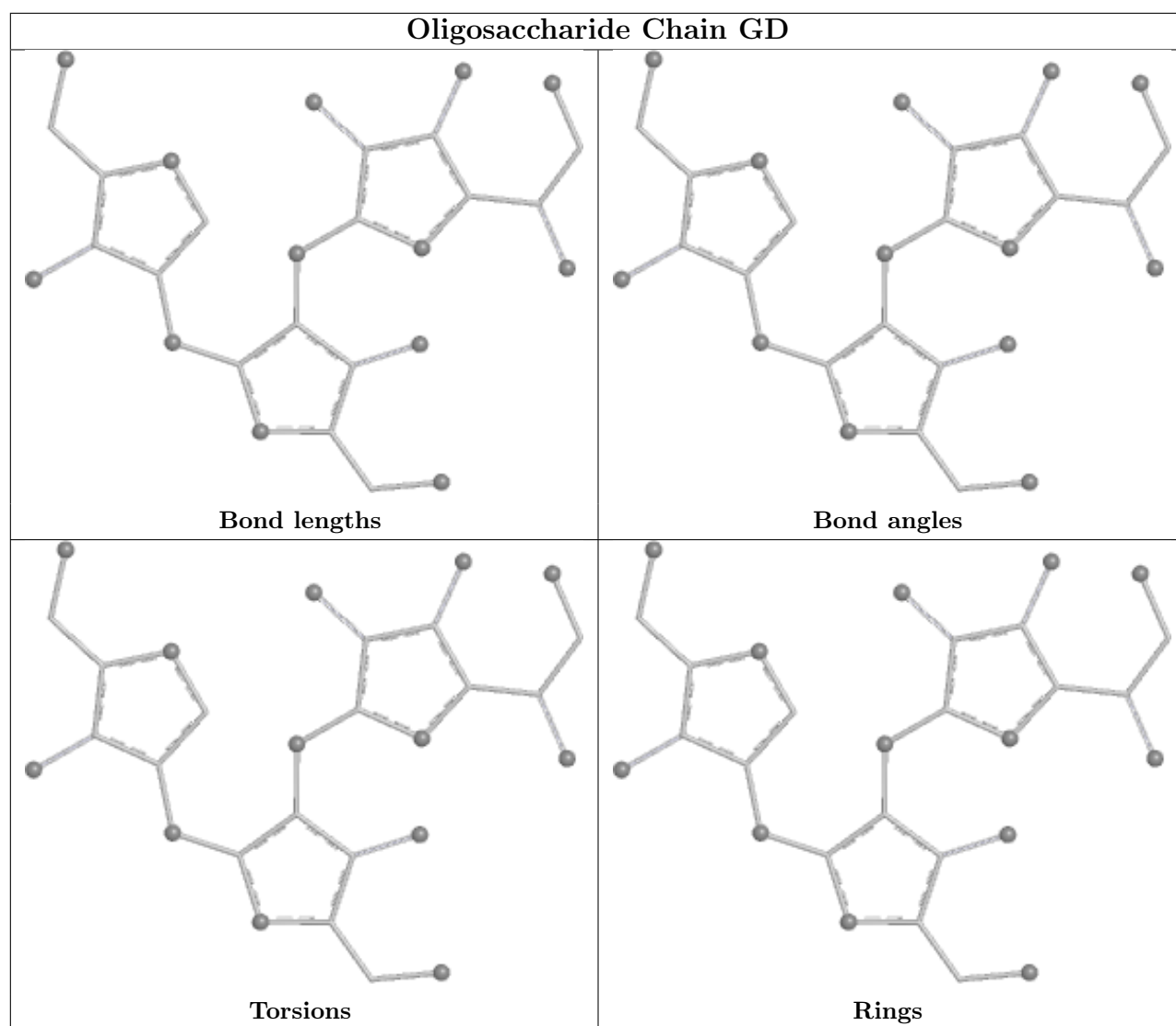


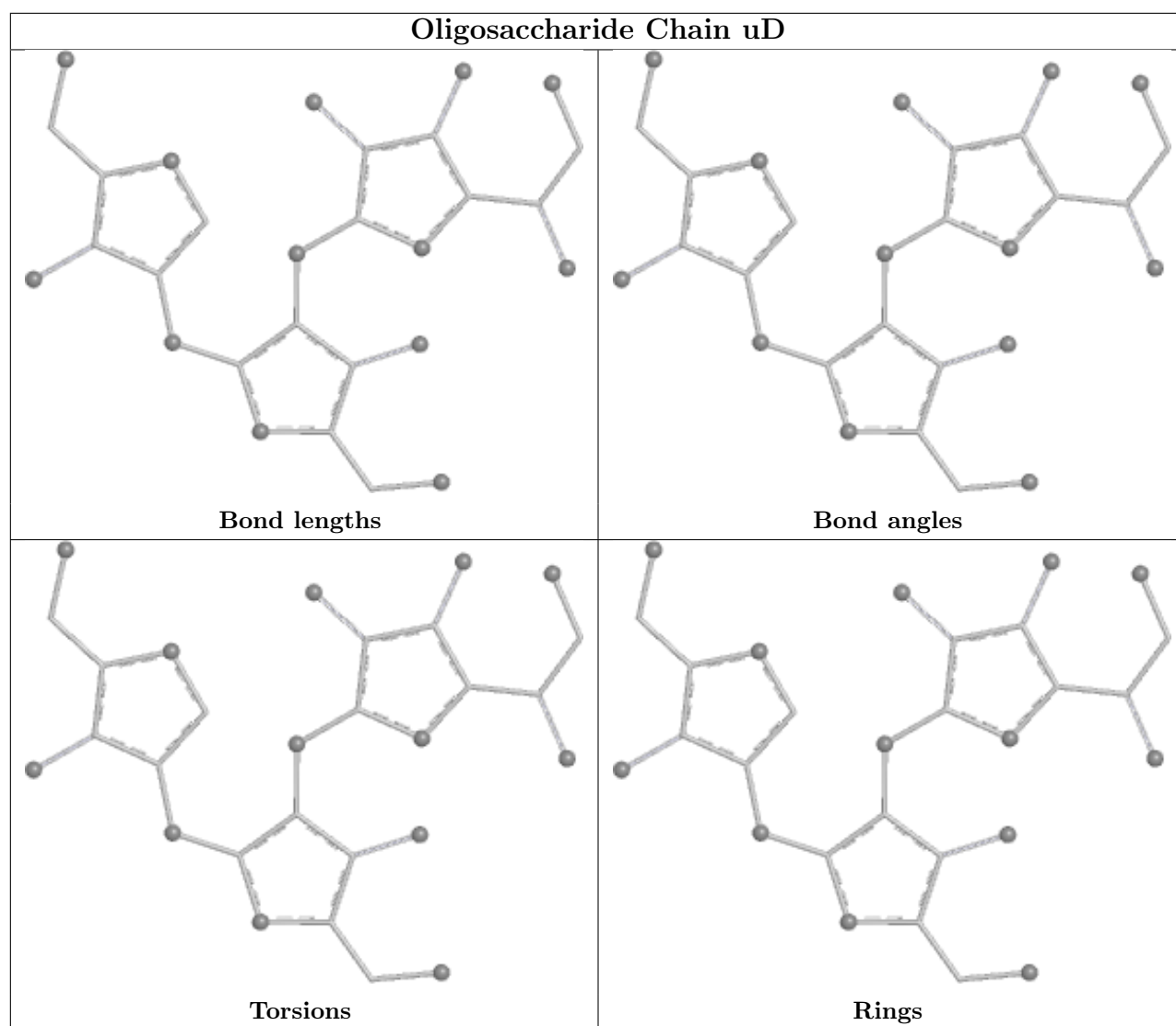


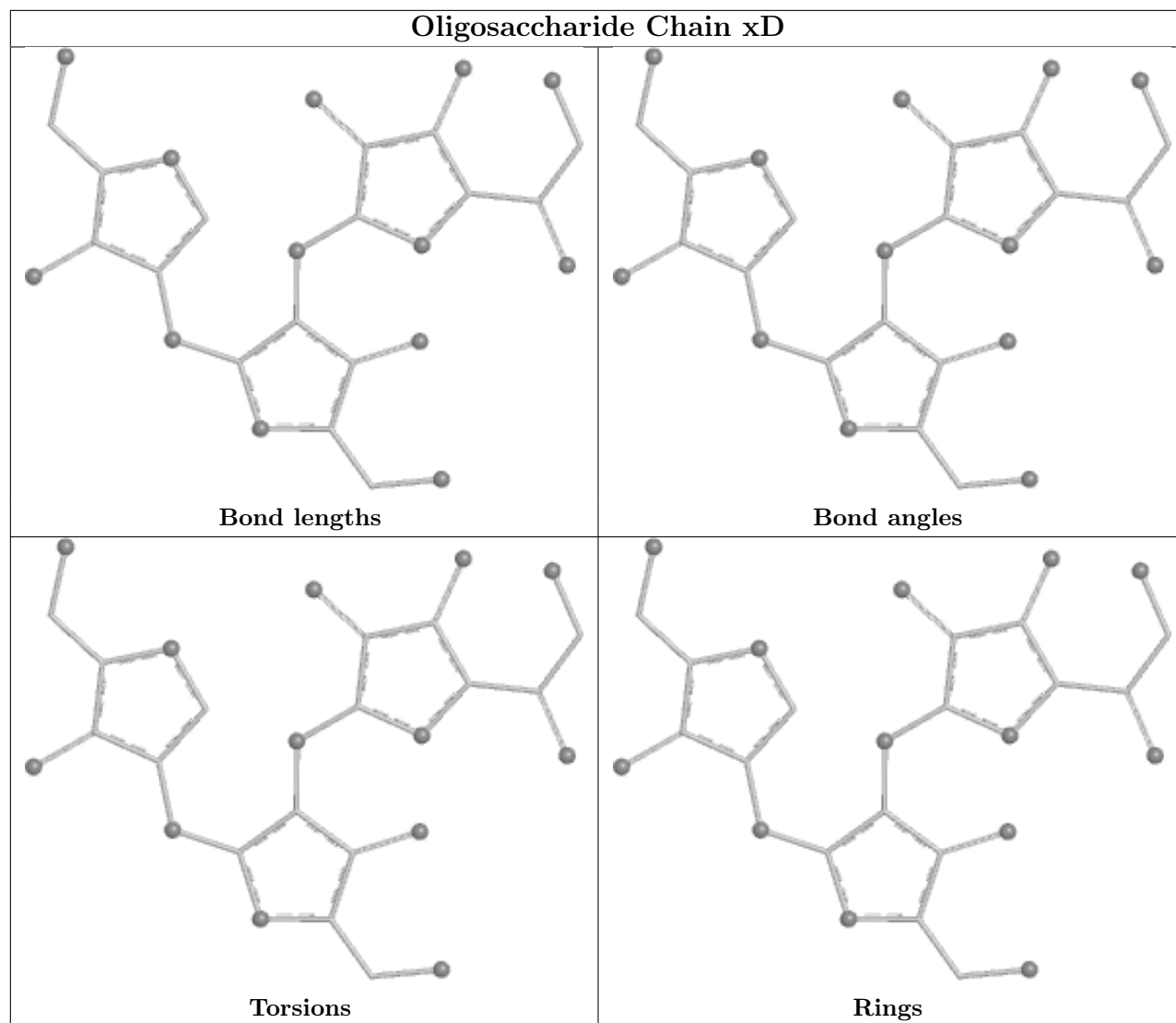


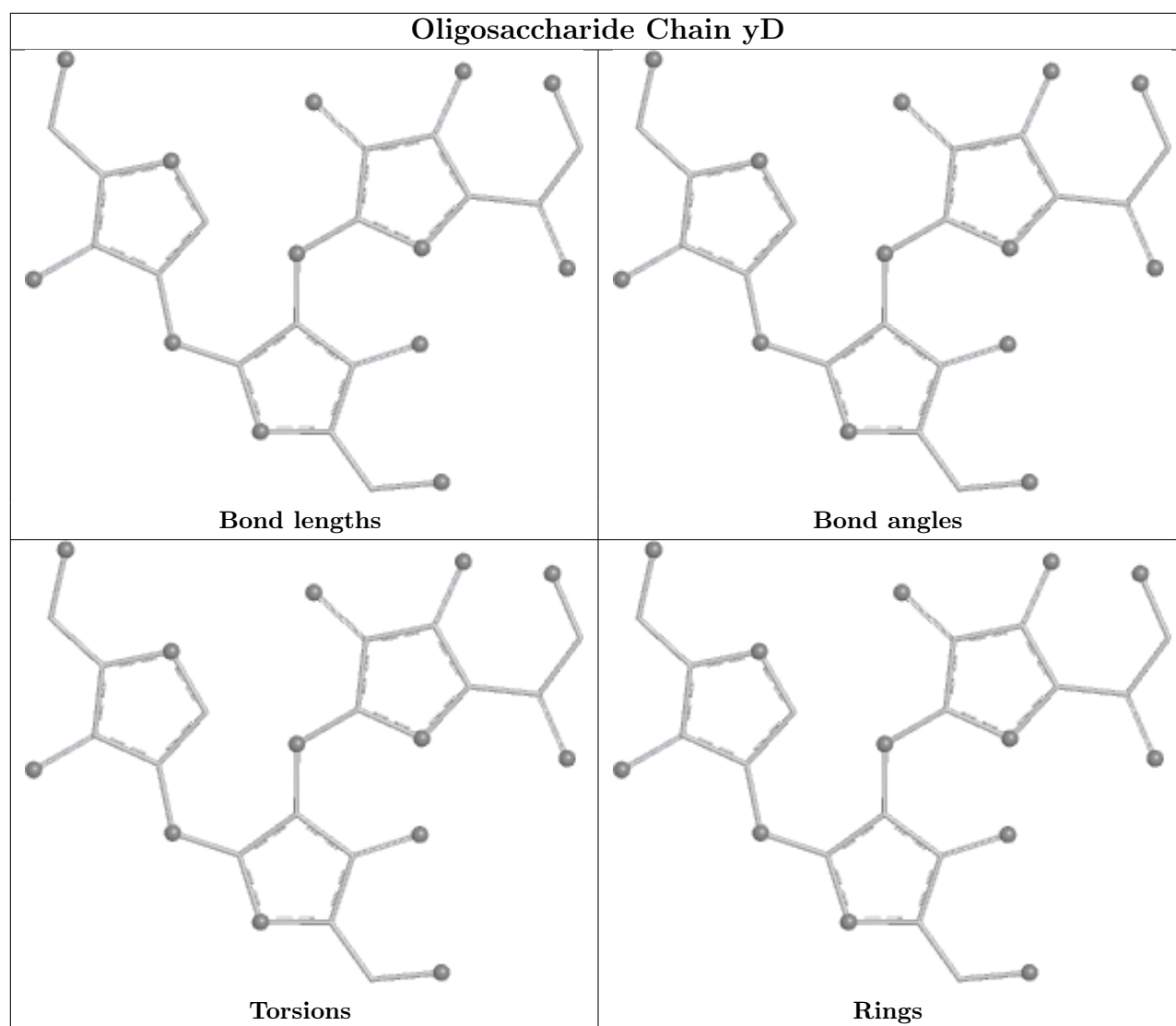
Oligosaccharide Chain 6C**Bond lengths****Bond angles****Torsions****Rings**

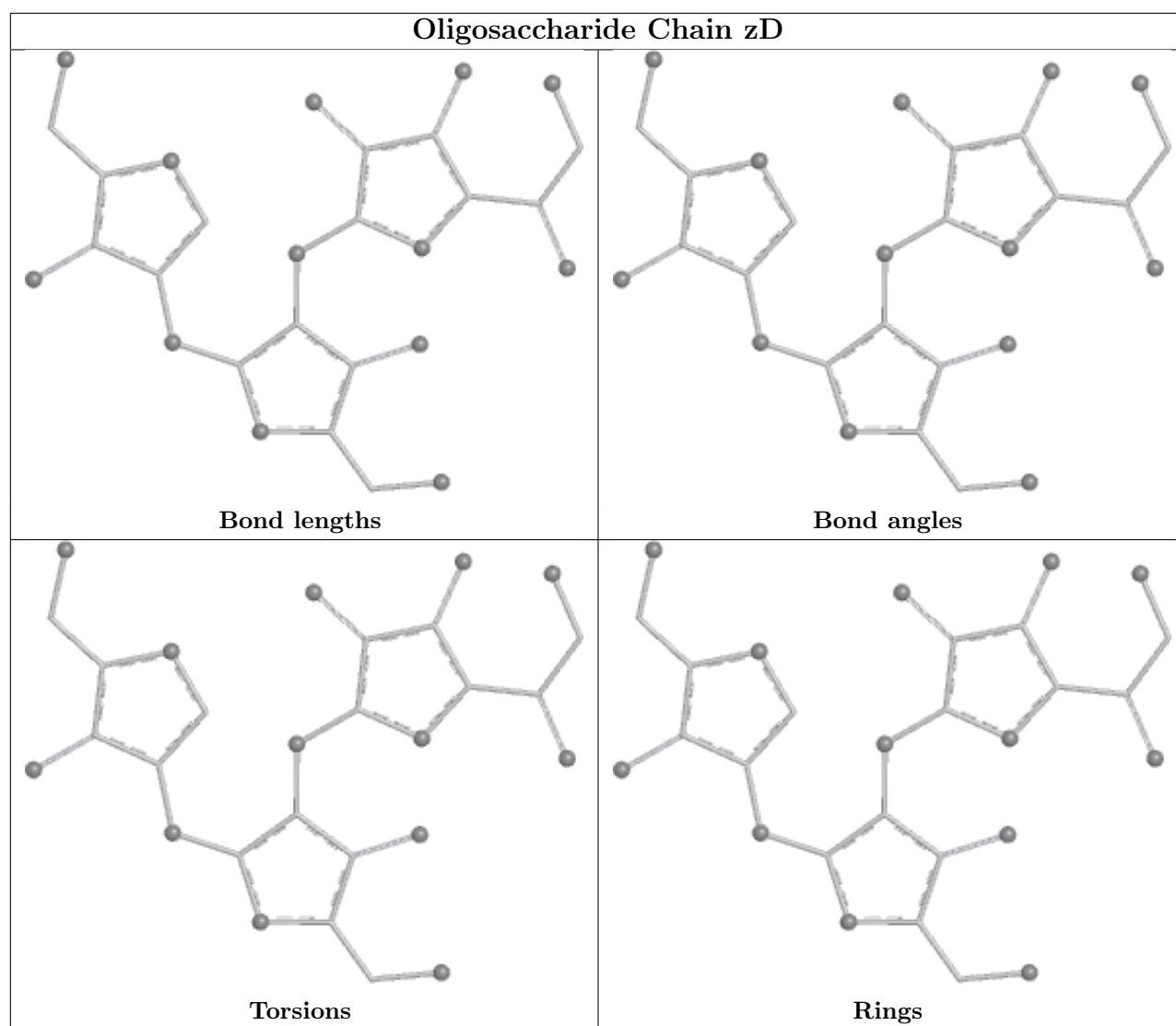


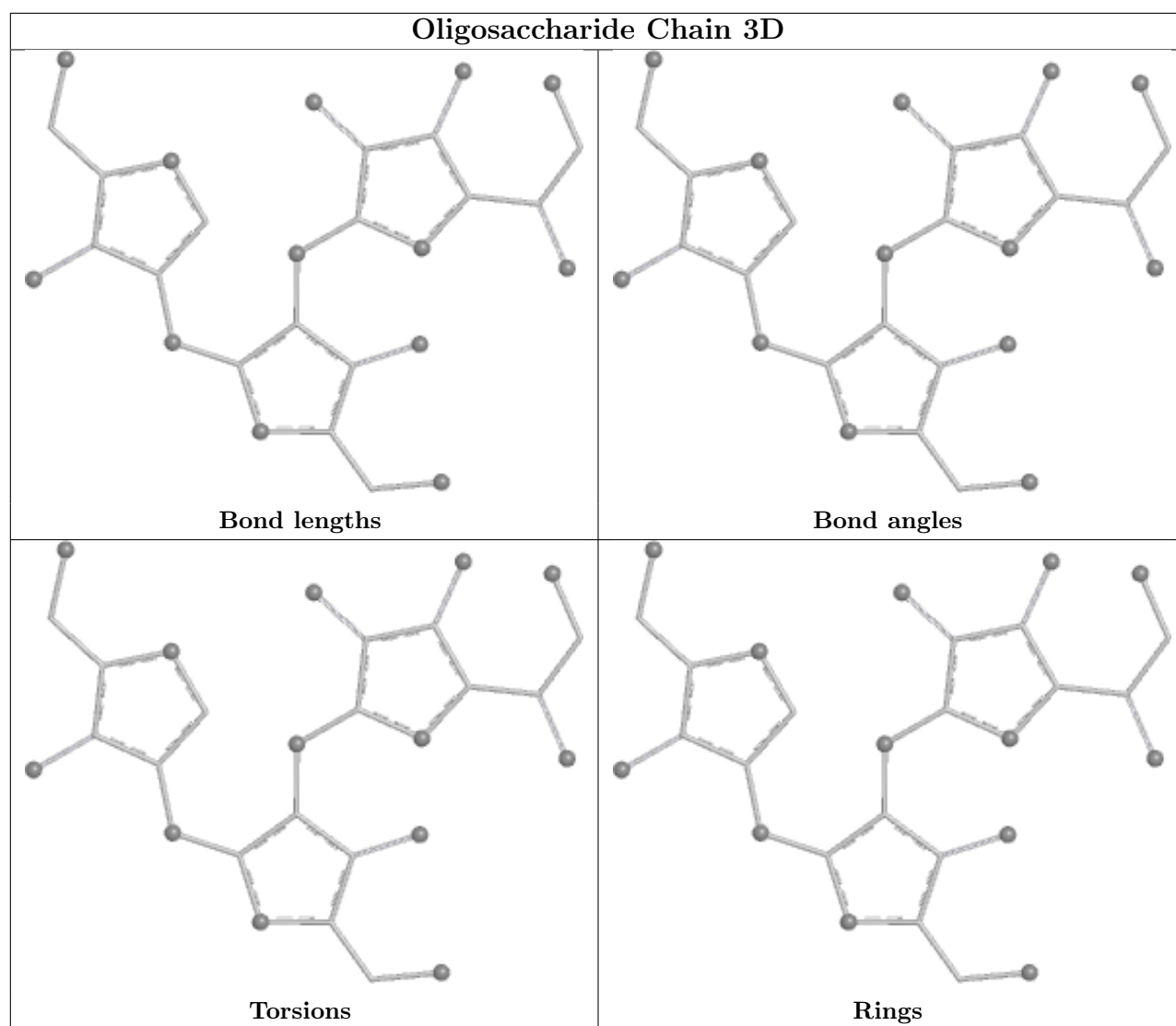


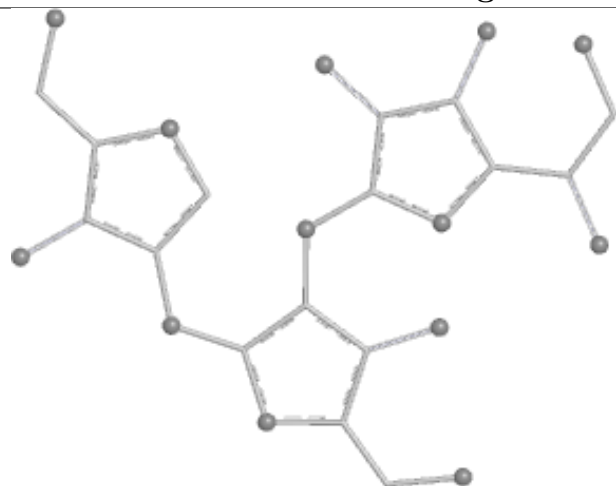
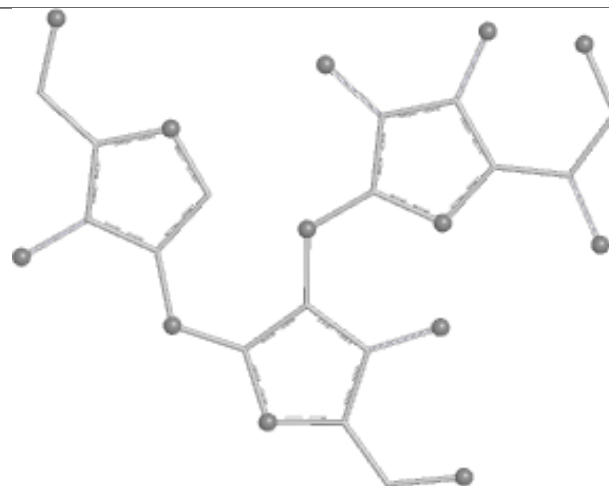
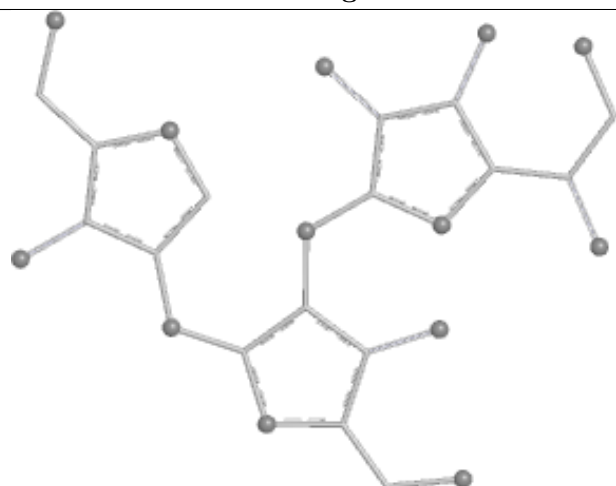
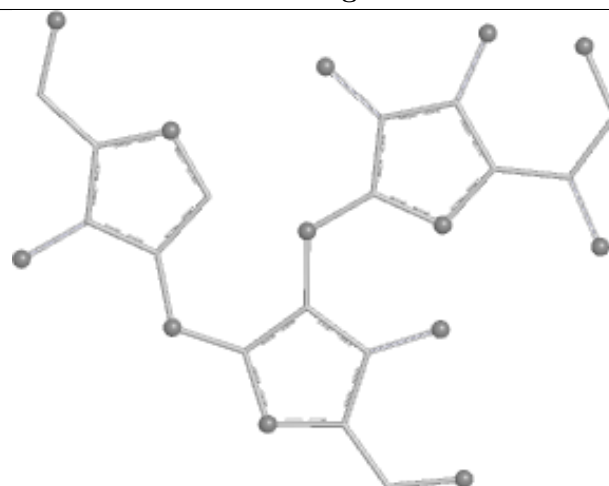




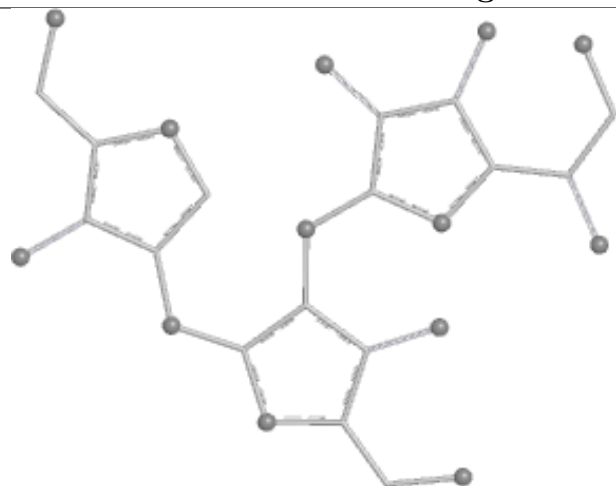




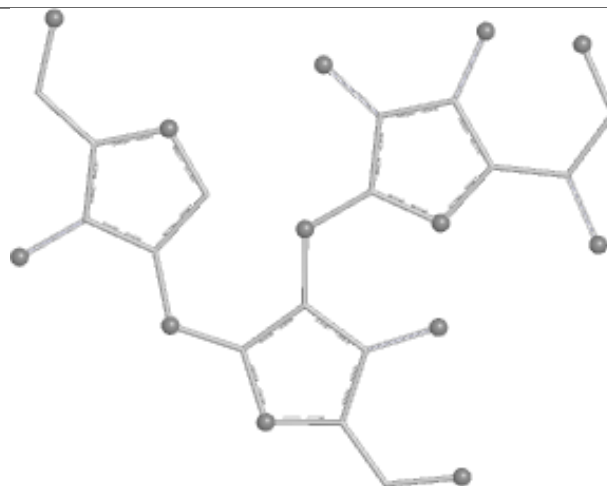


Oligosaccharide Chain 6D**Bond lengths****Bond angles****Torsions****Rings**

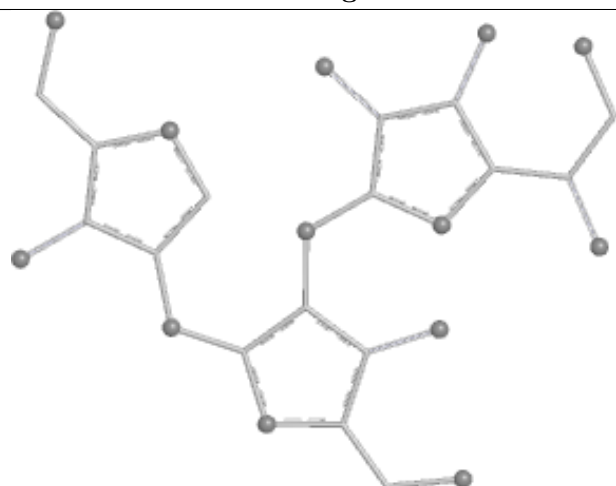
Oligosaccharide Chain 7D



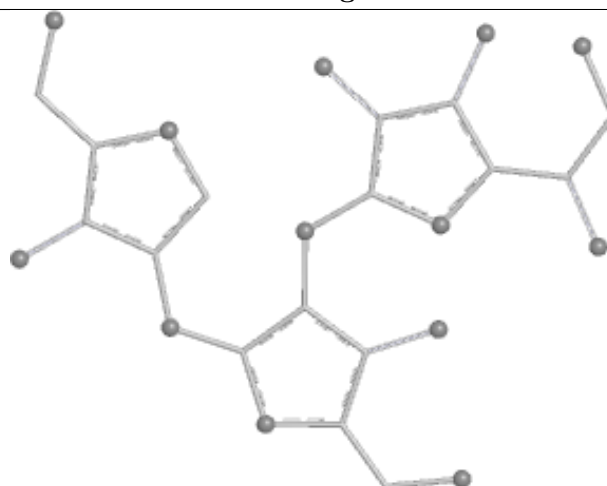
Bond lengths



Bond angles

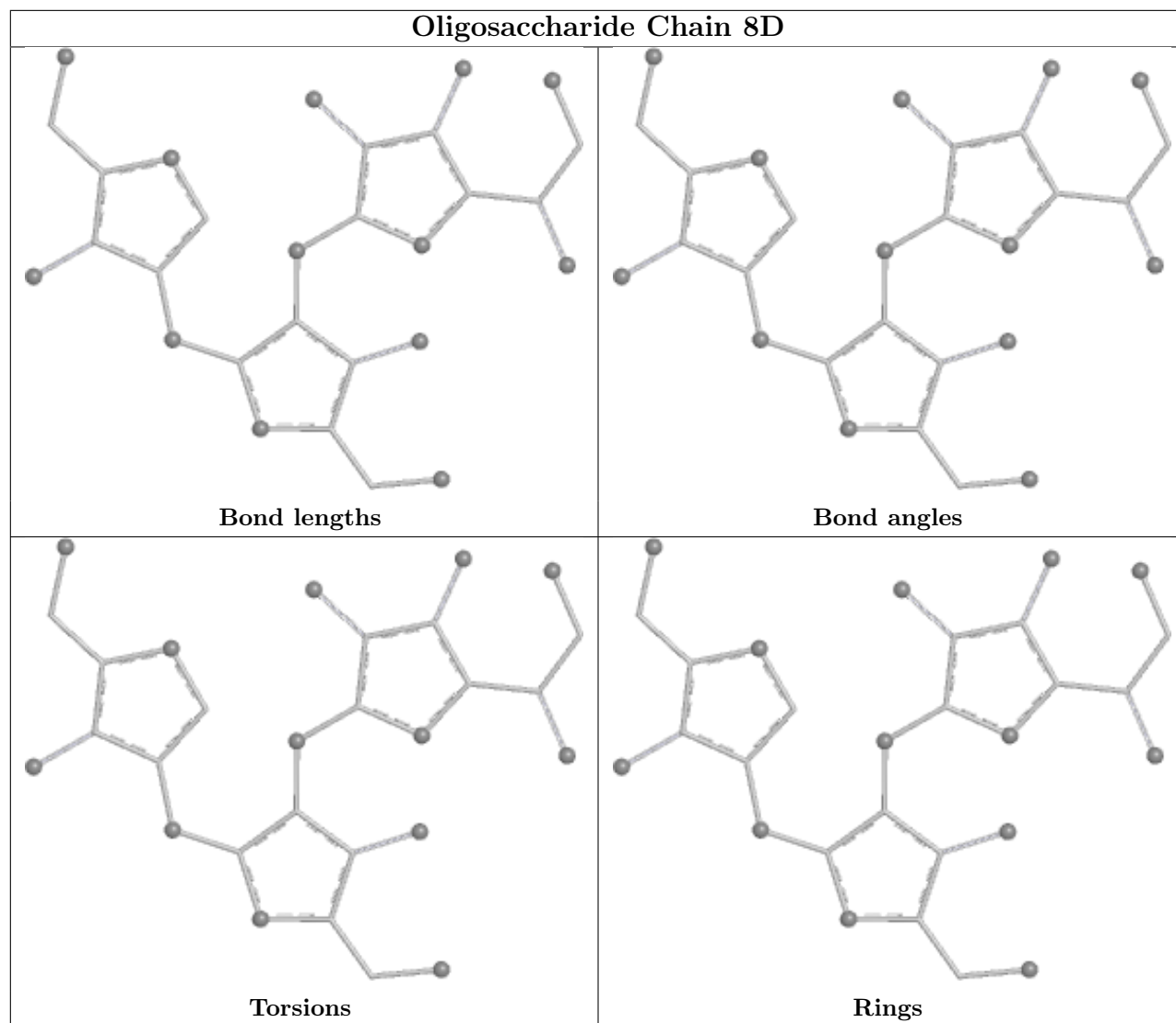


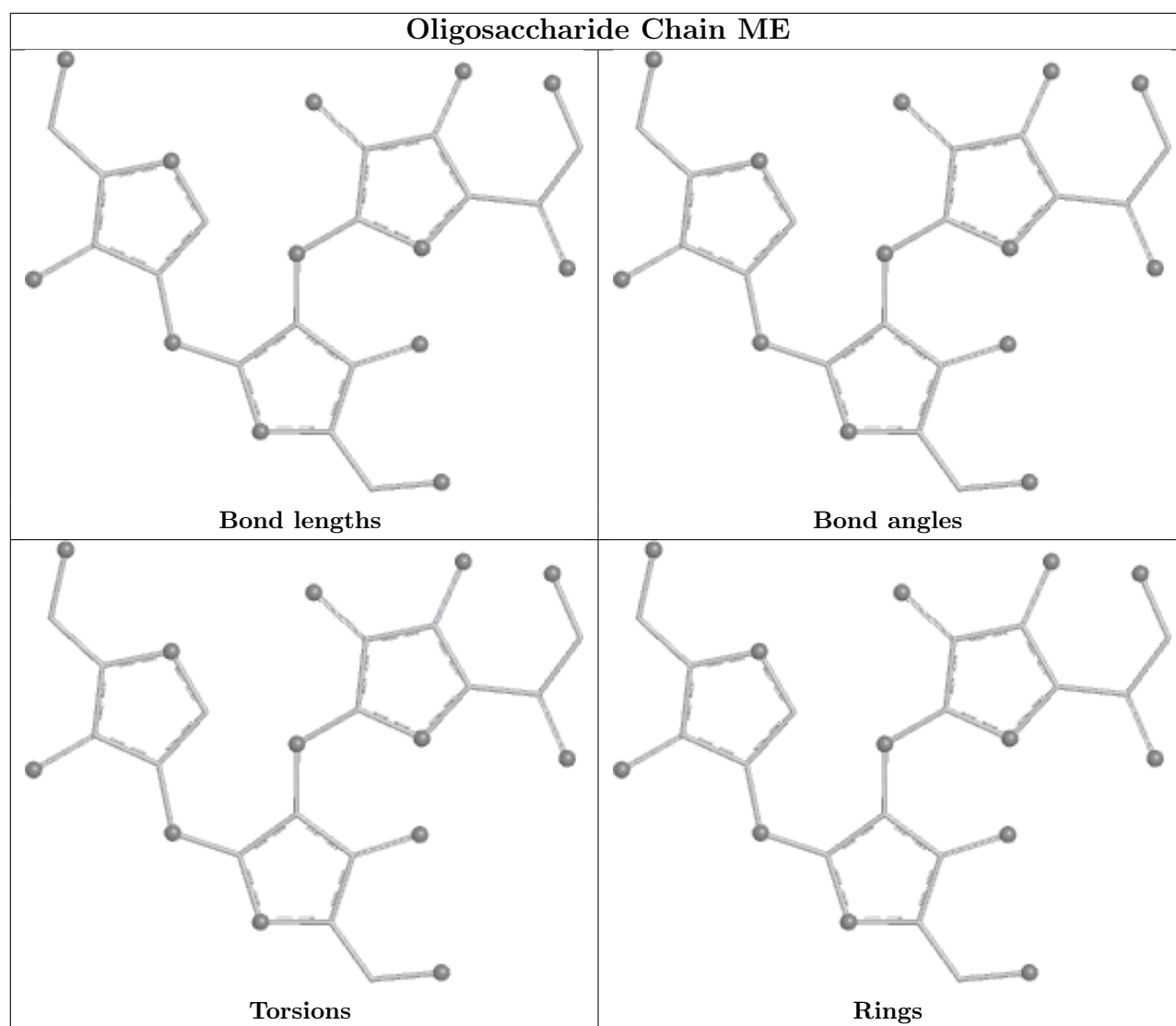
Torsions

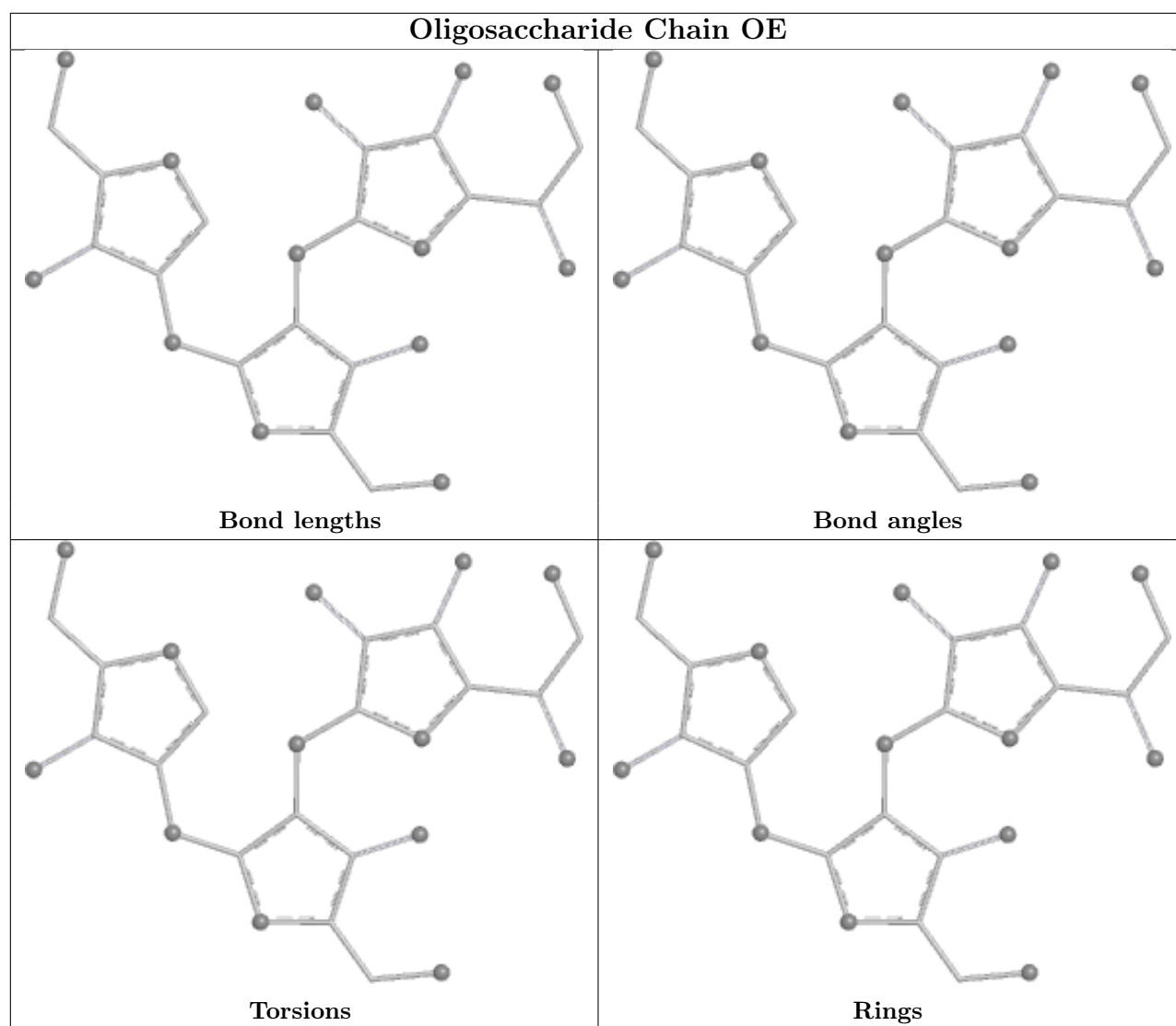


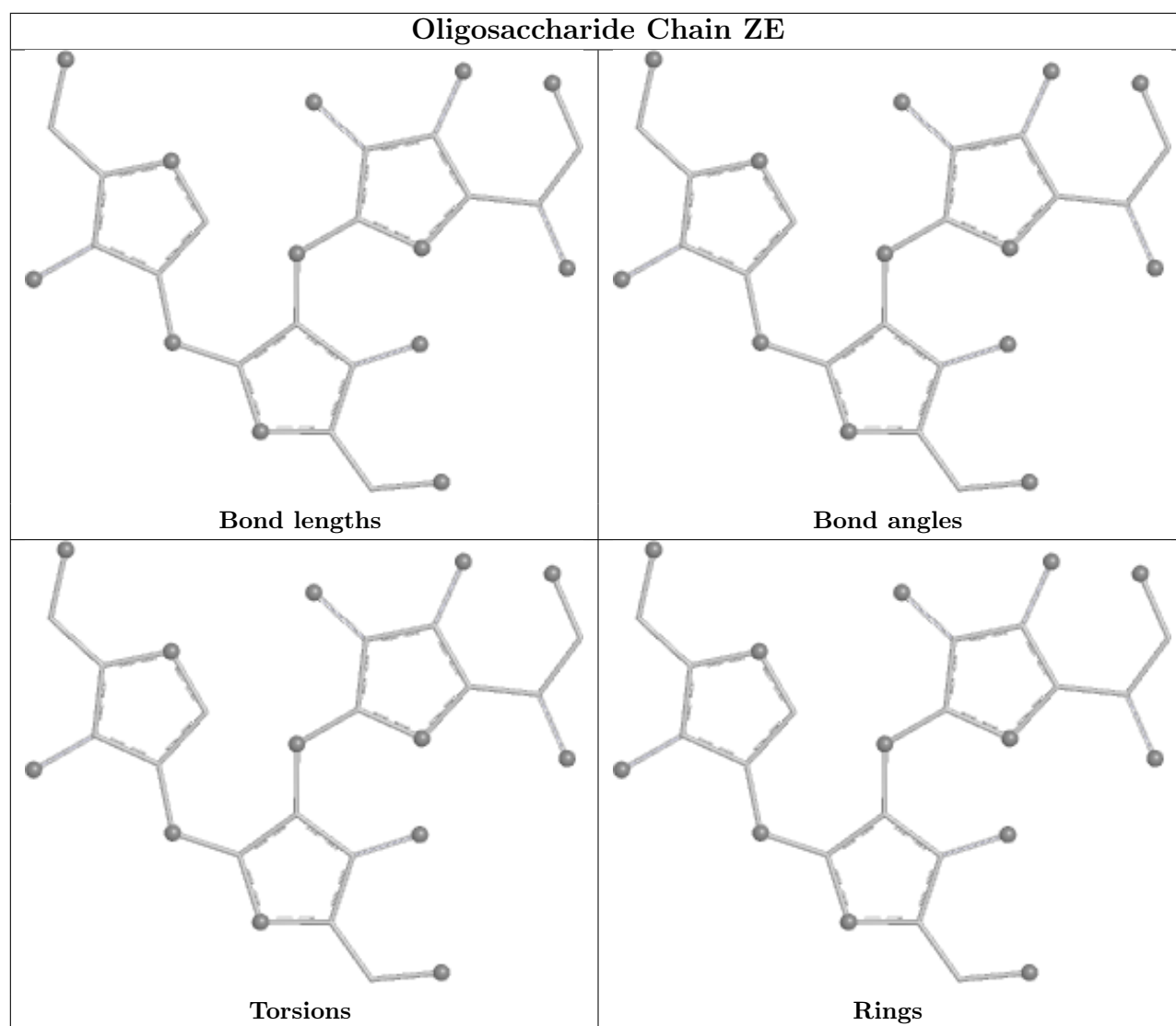
Rings

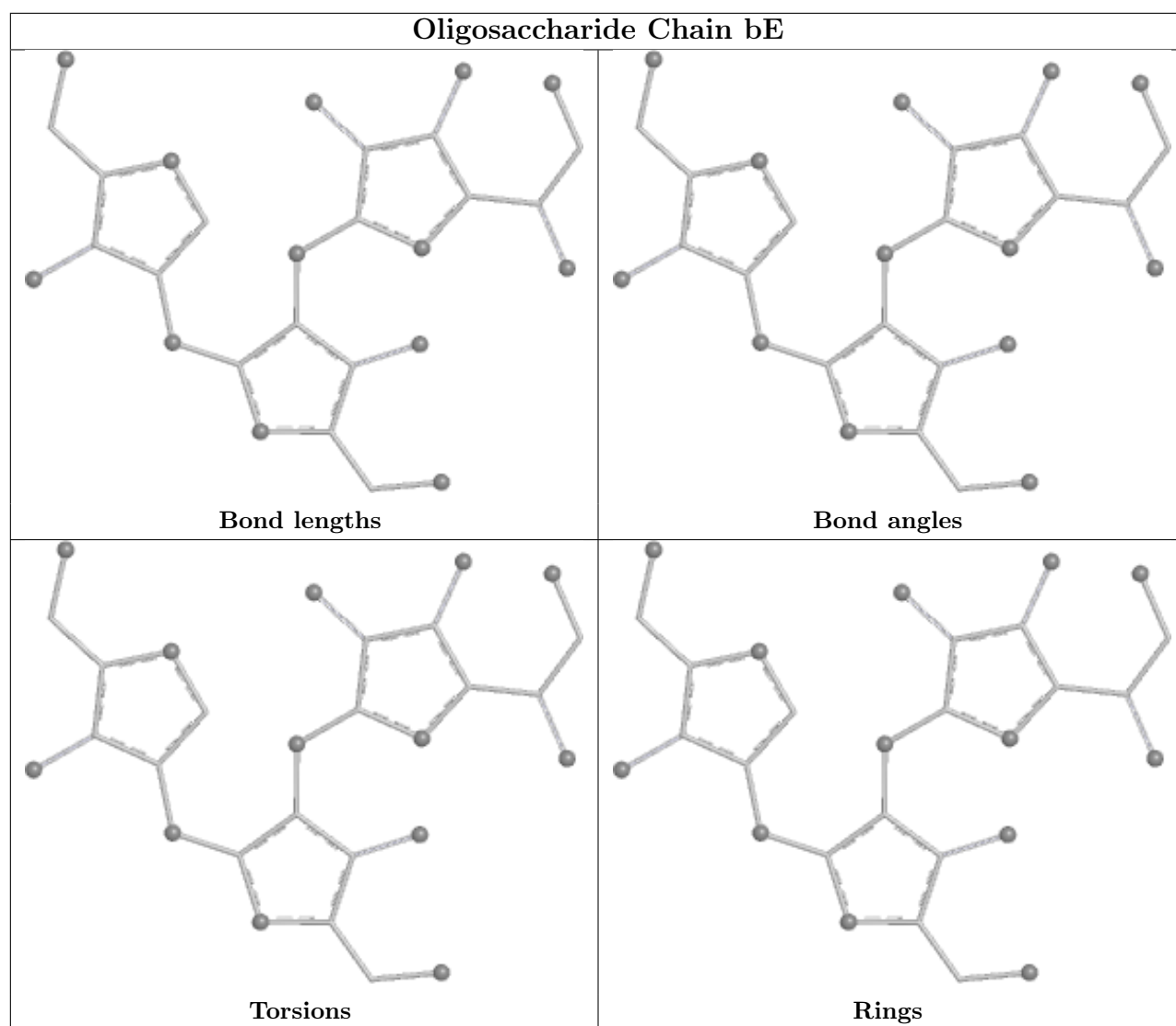
Oligosaccharide Chain 8D

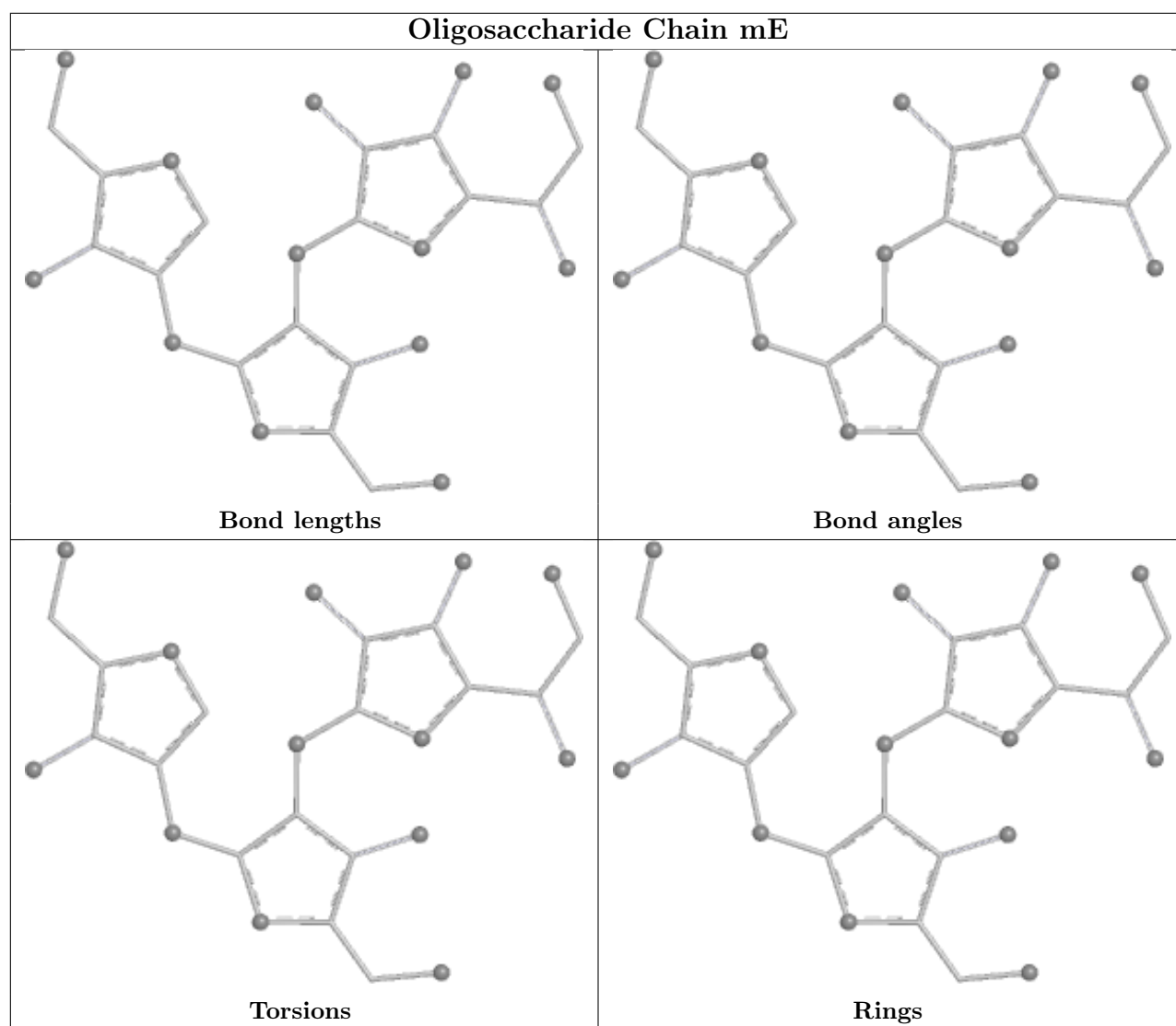


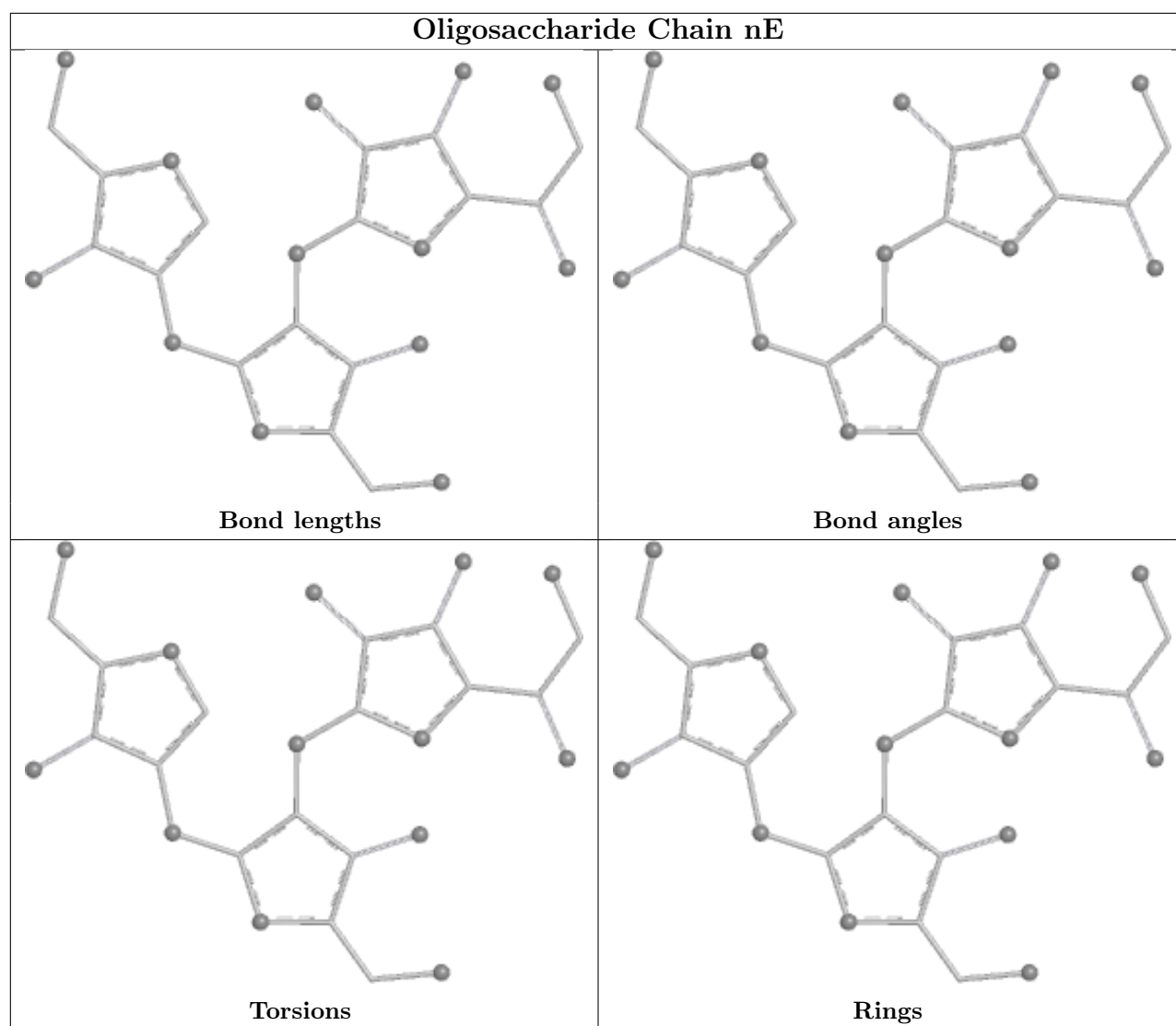


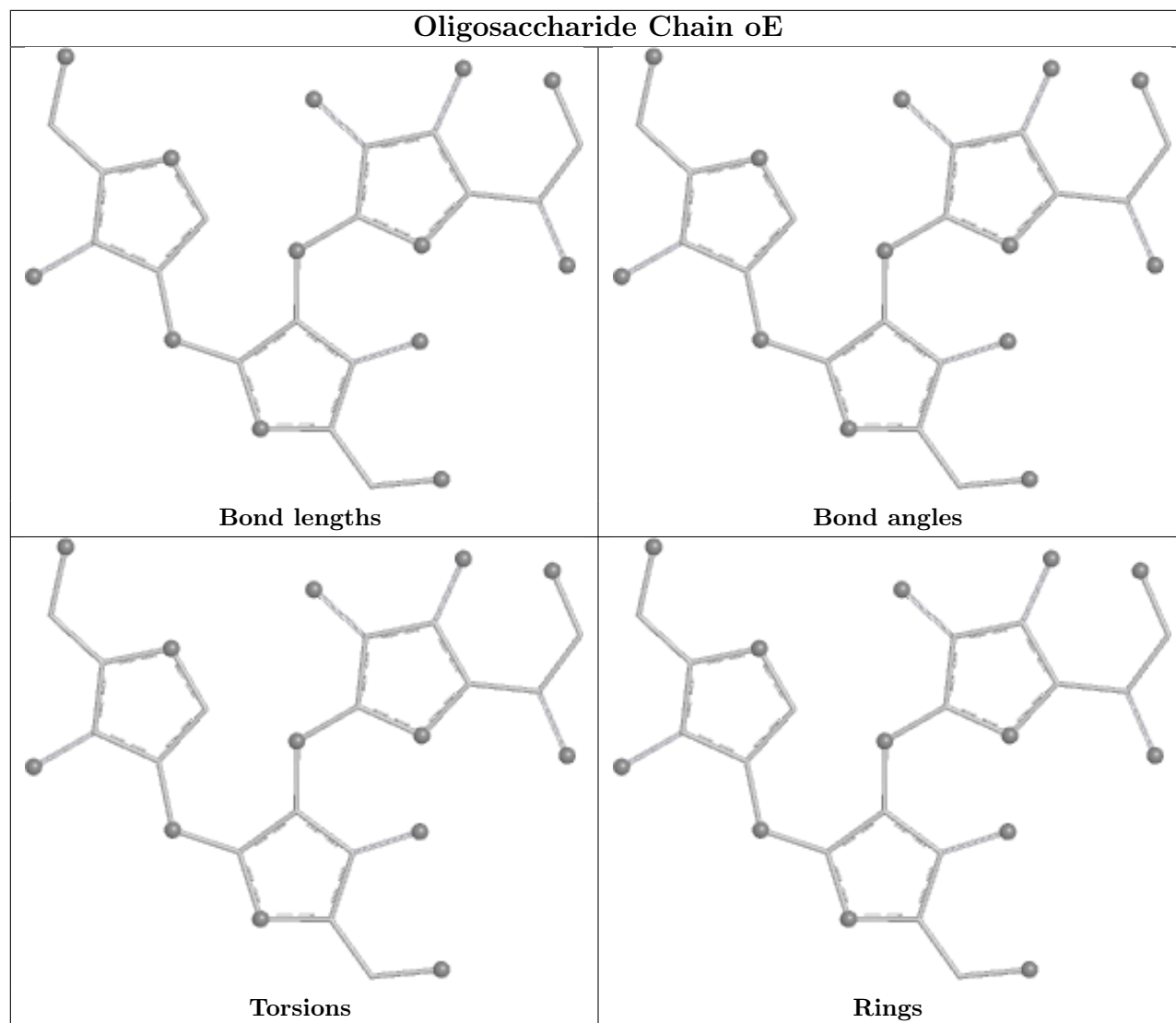


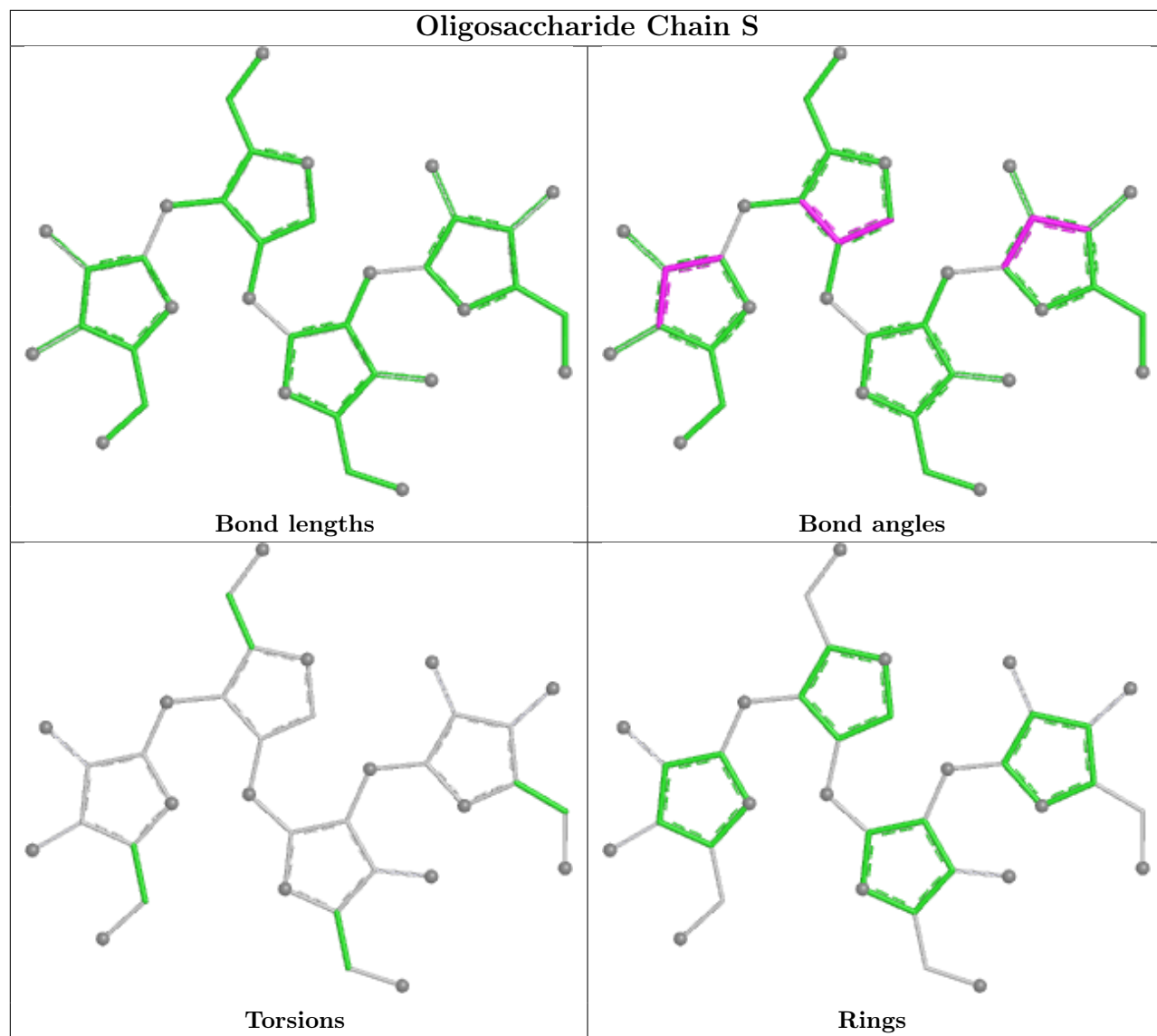


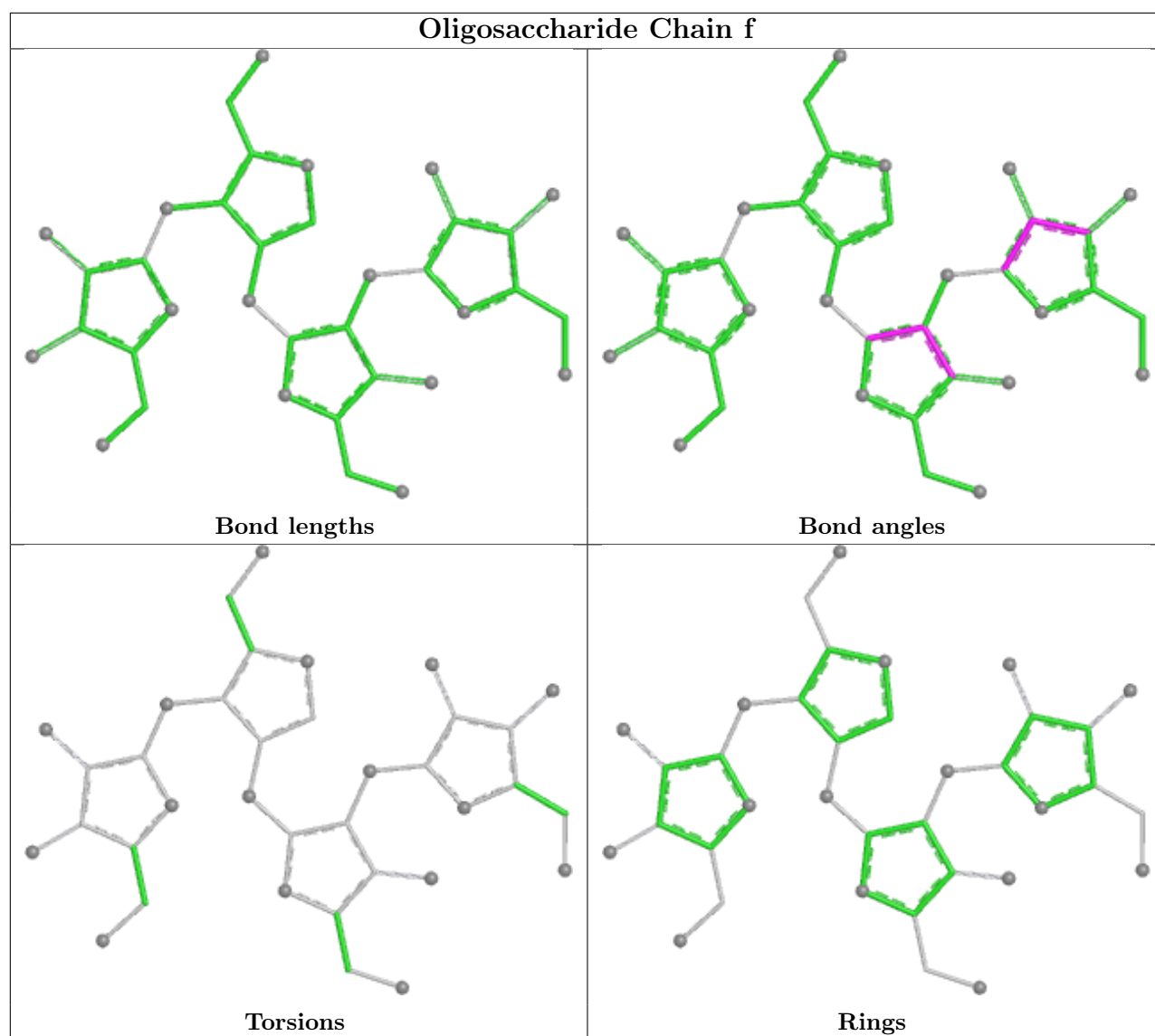


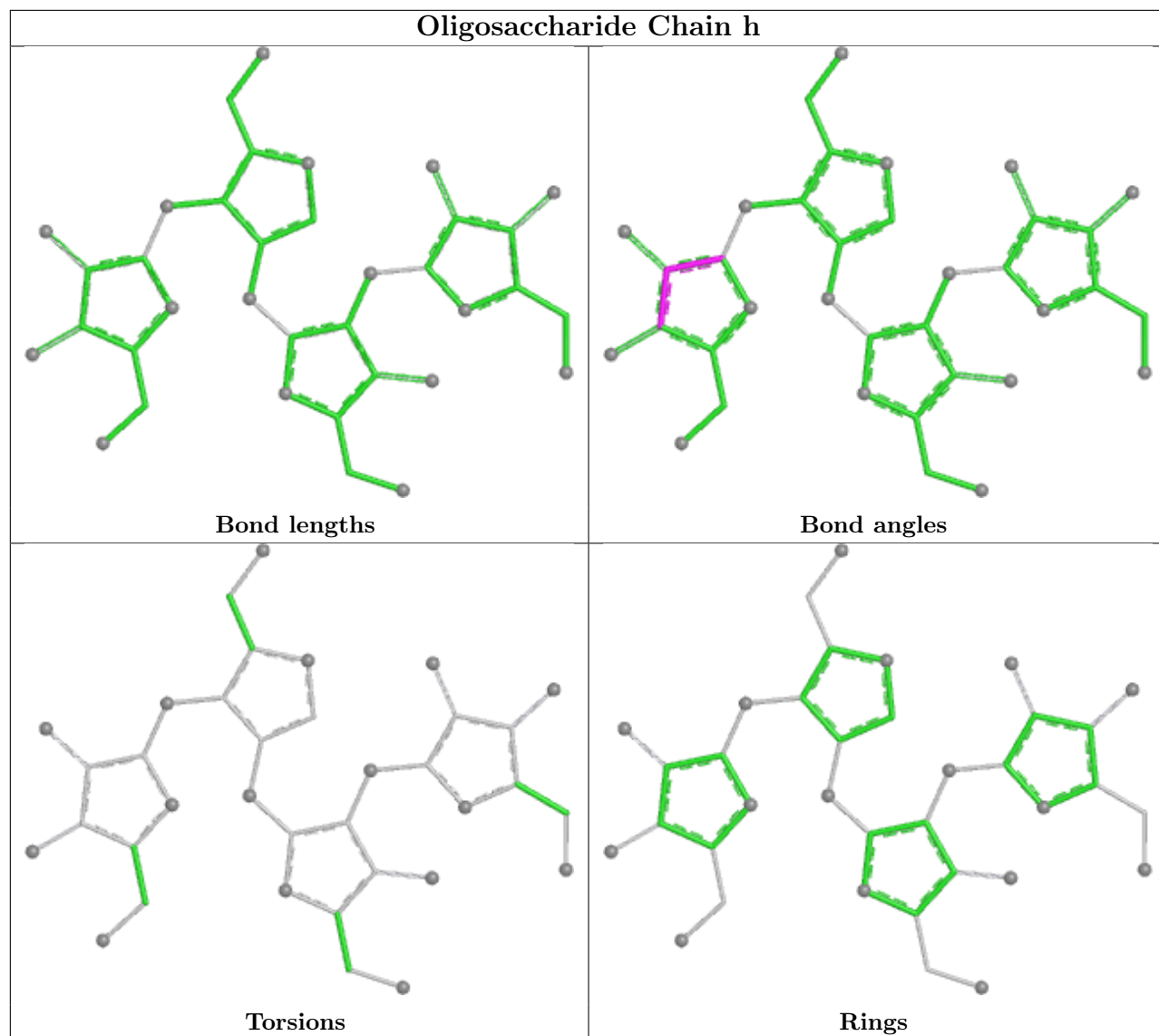


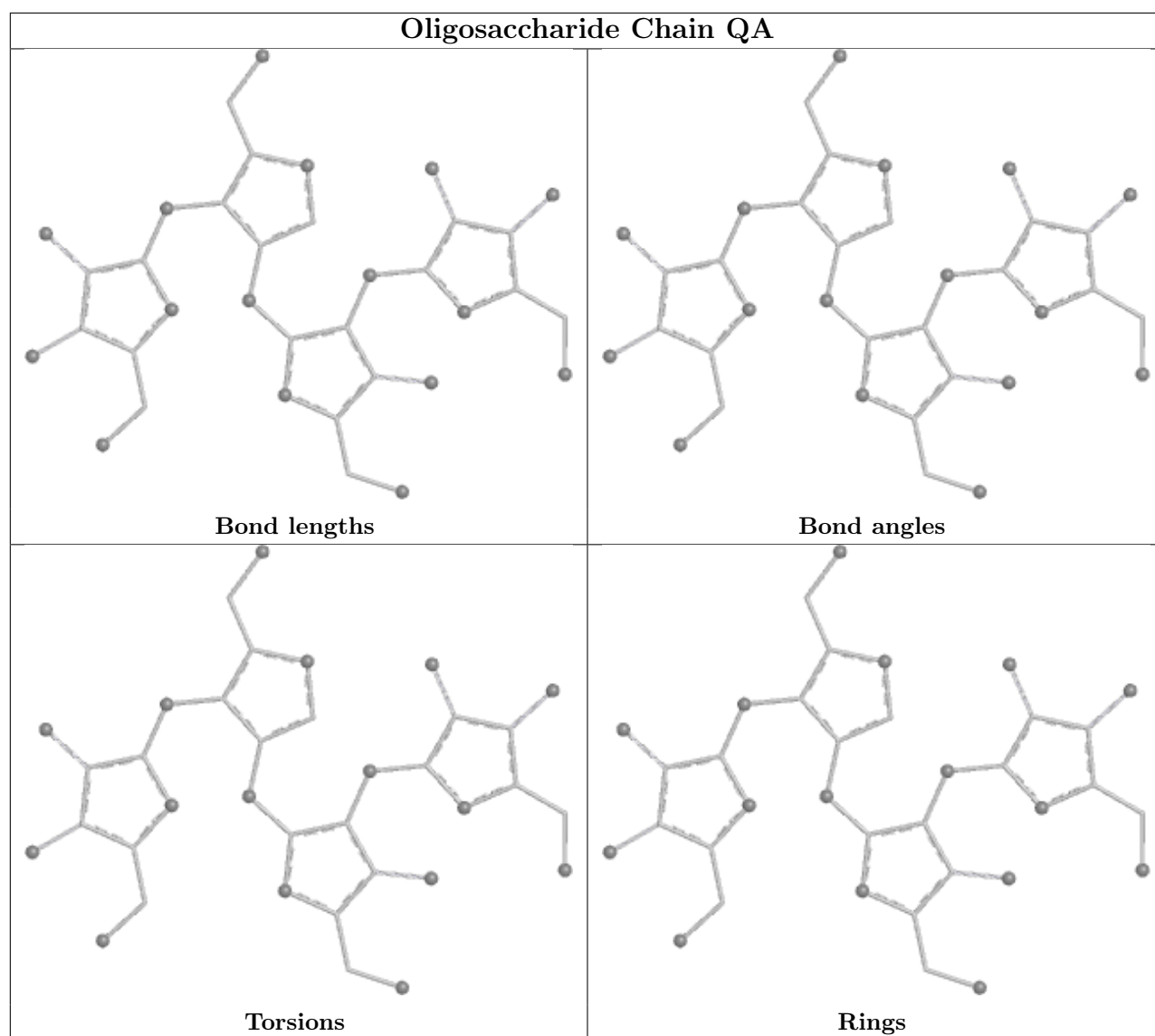


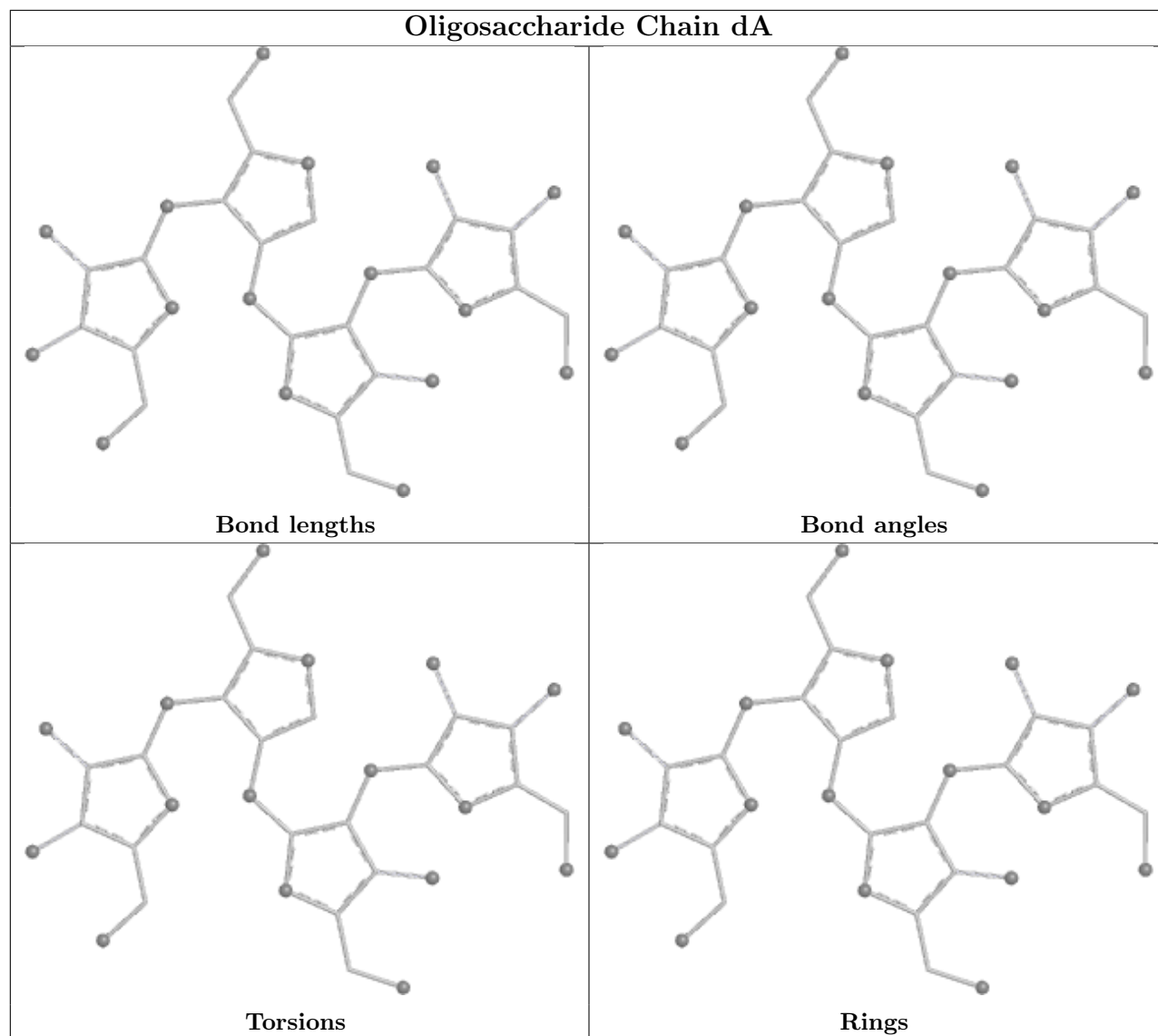


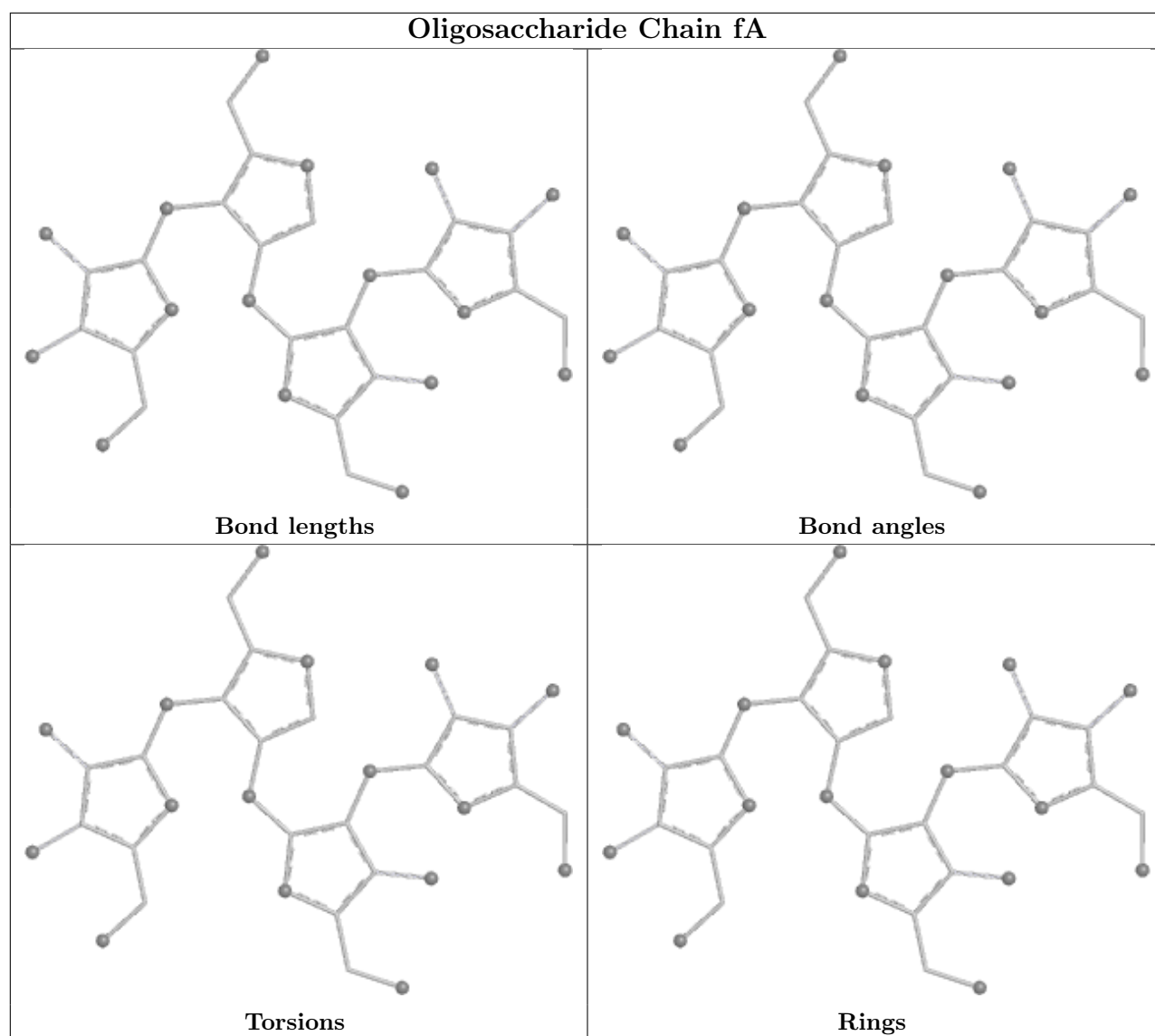


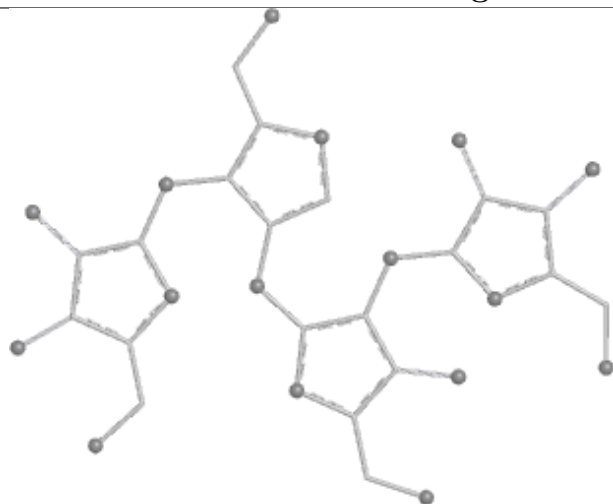
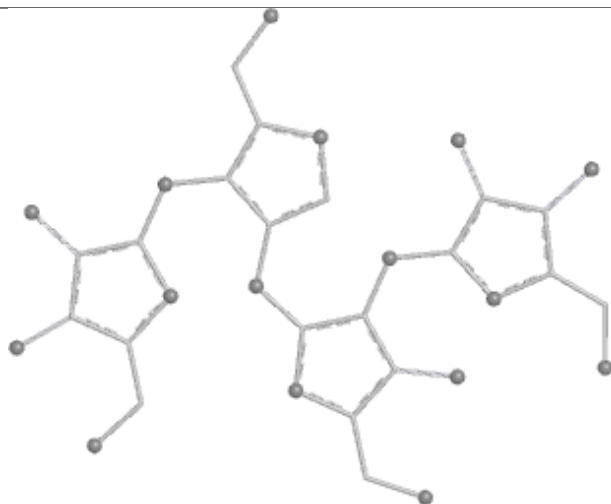
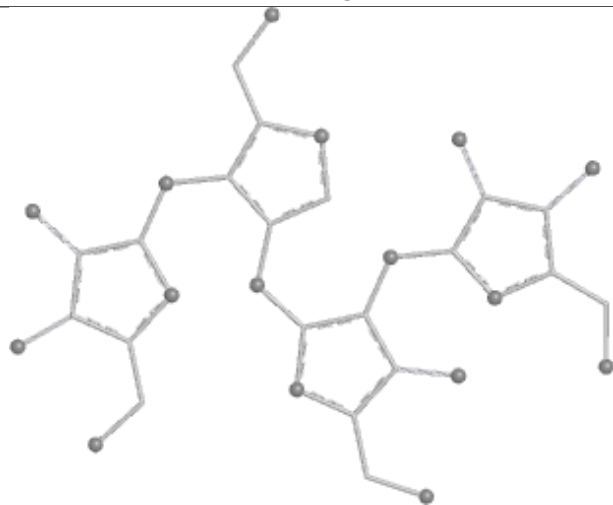
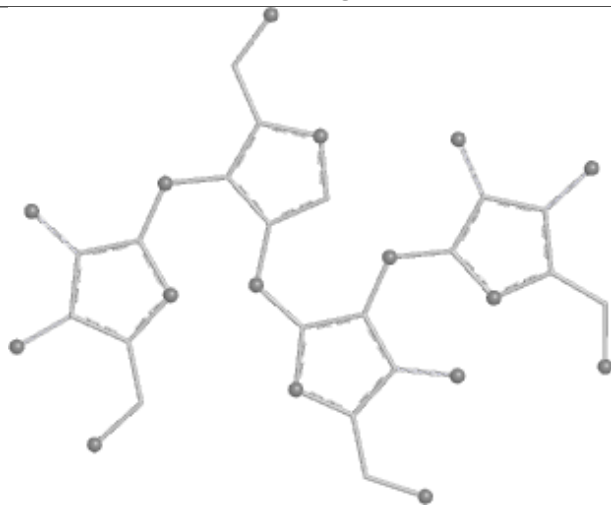


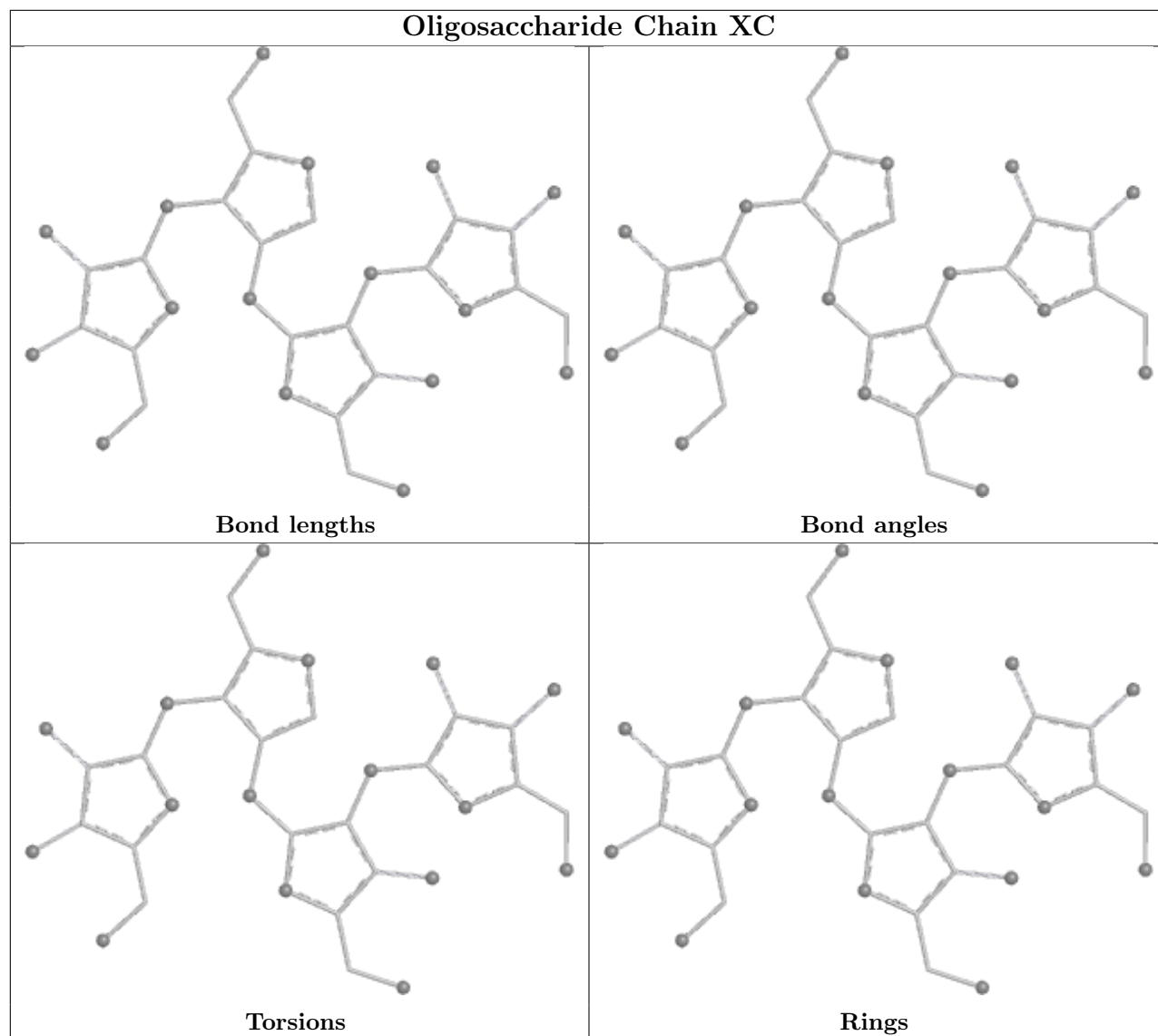


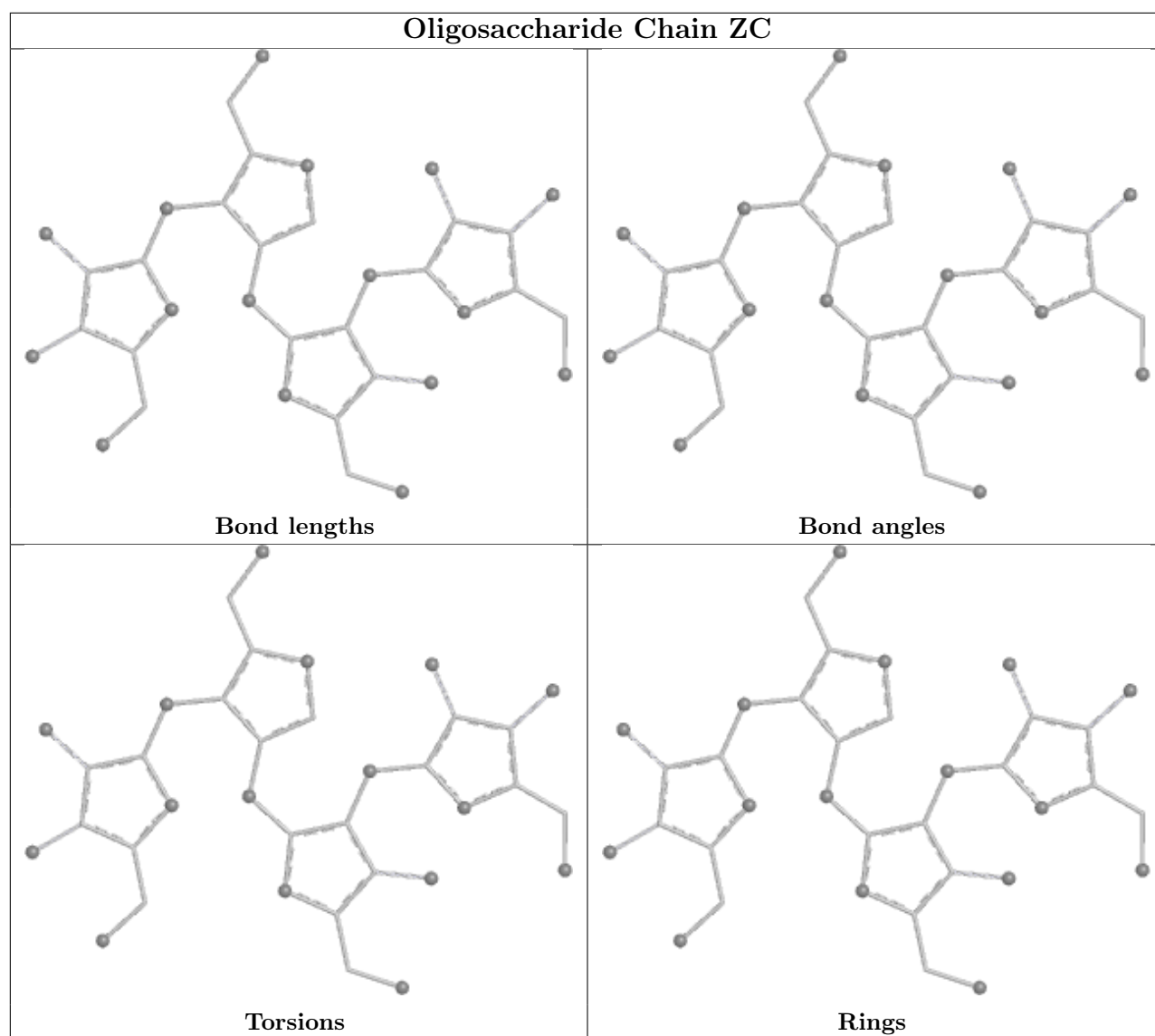


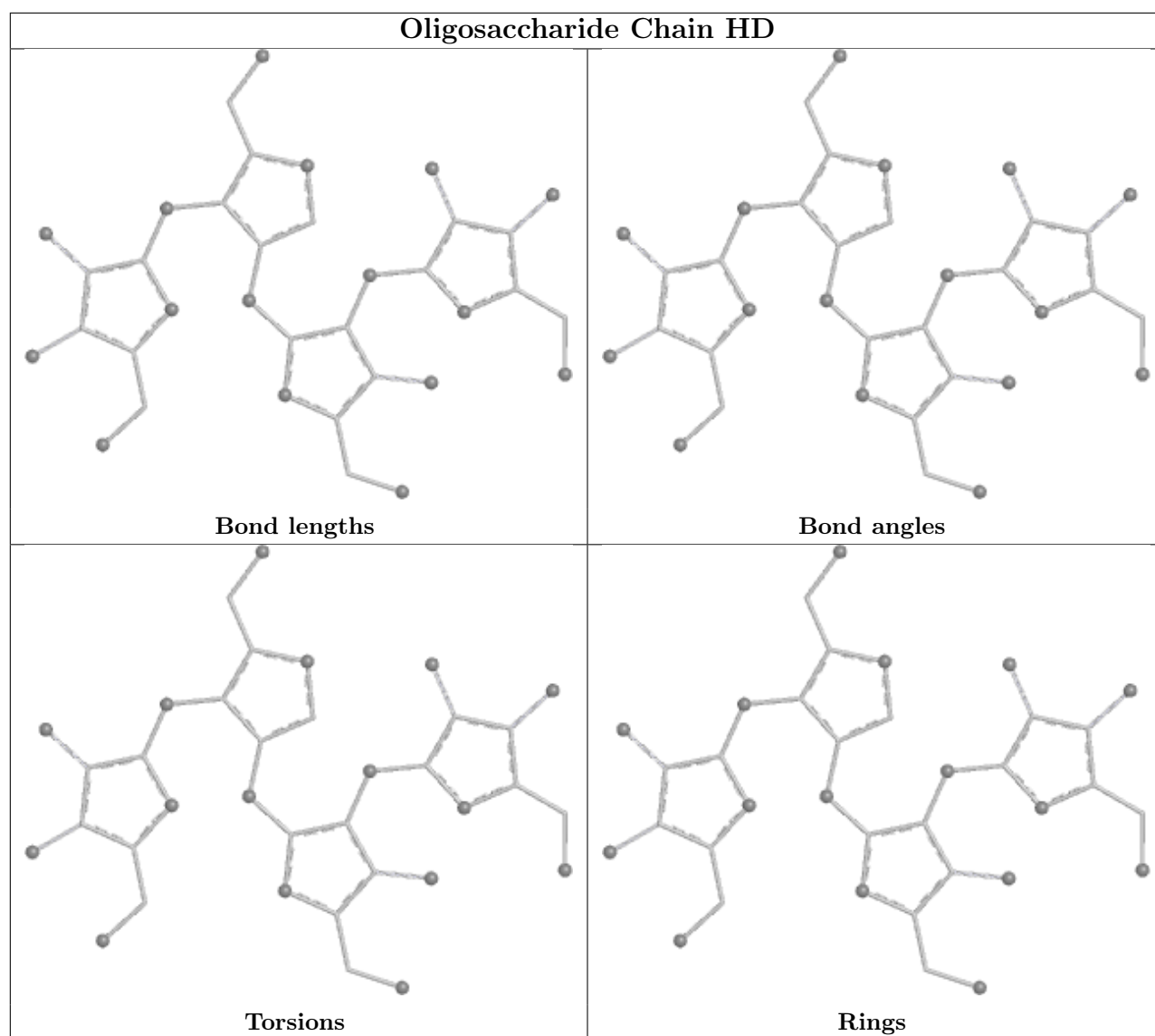


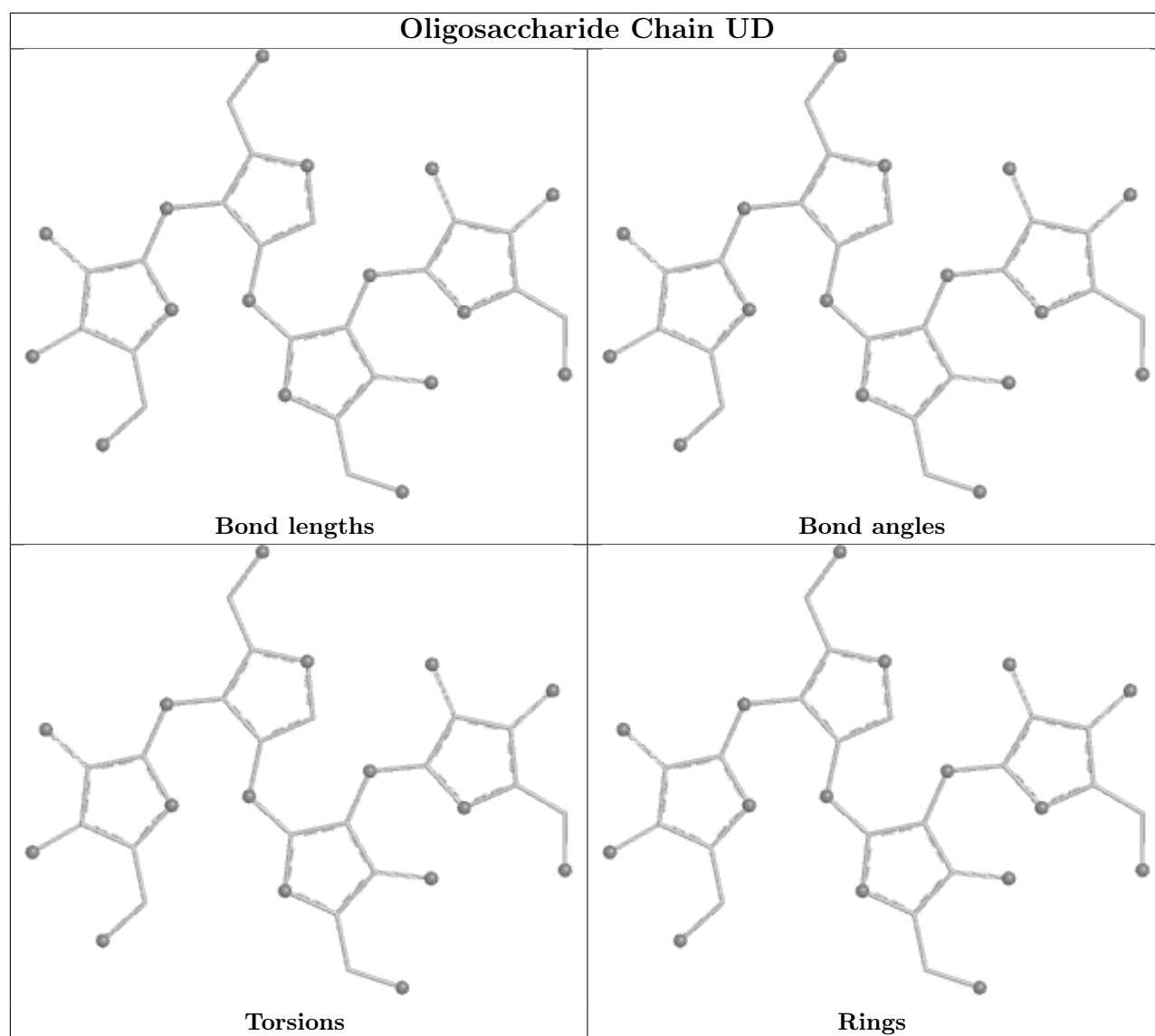


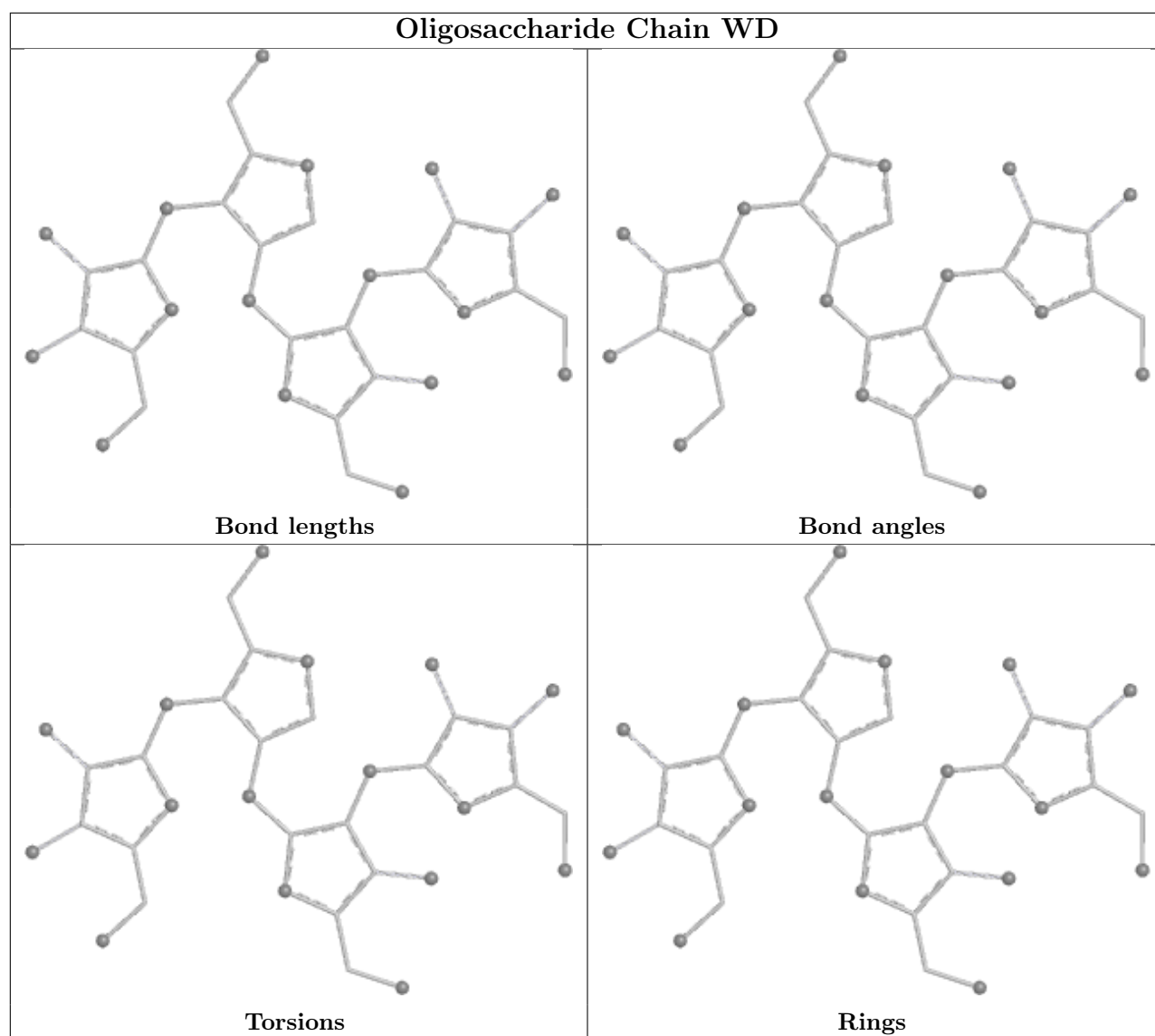
Oligosaccharide Chain KC**Bond lengths****Bond angles****Torsions****Rings**

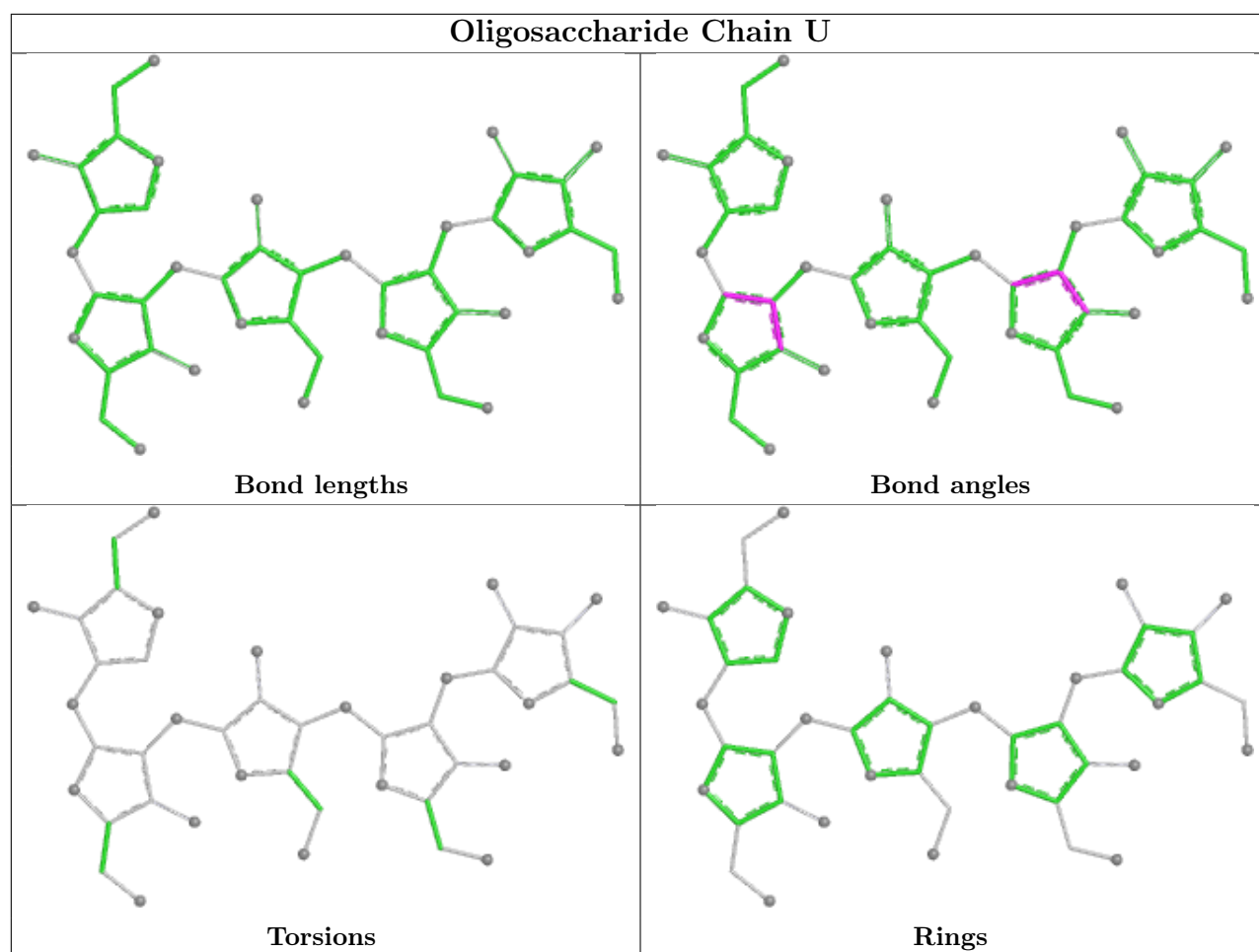


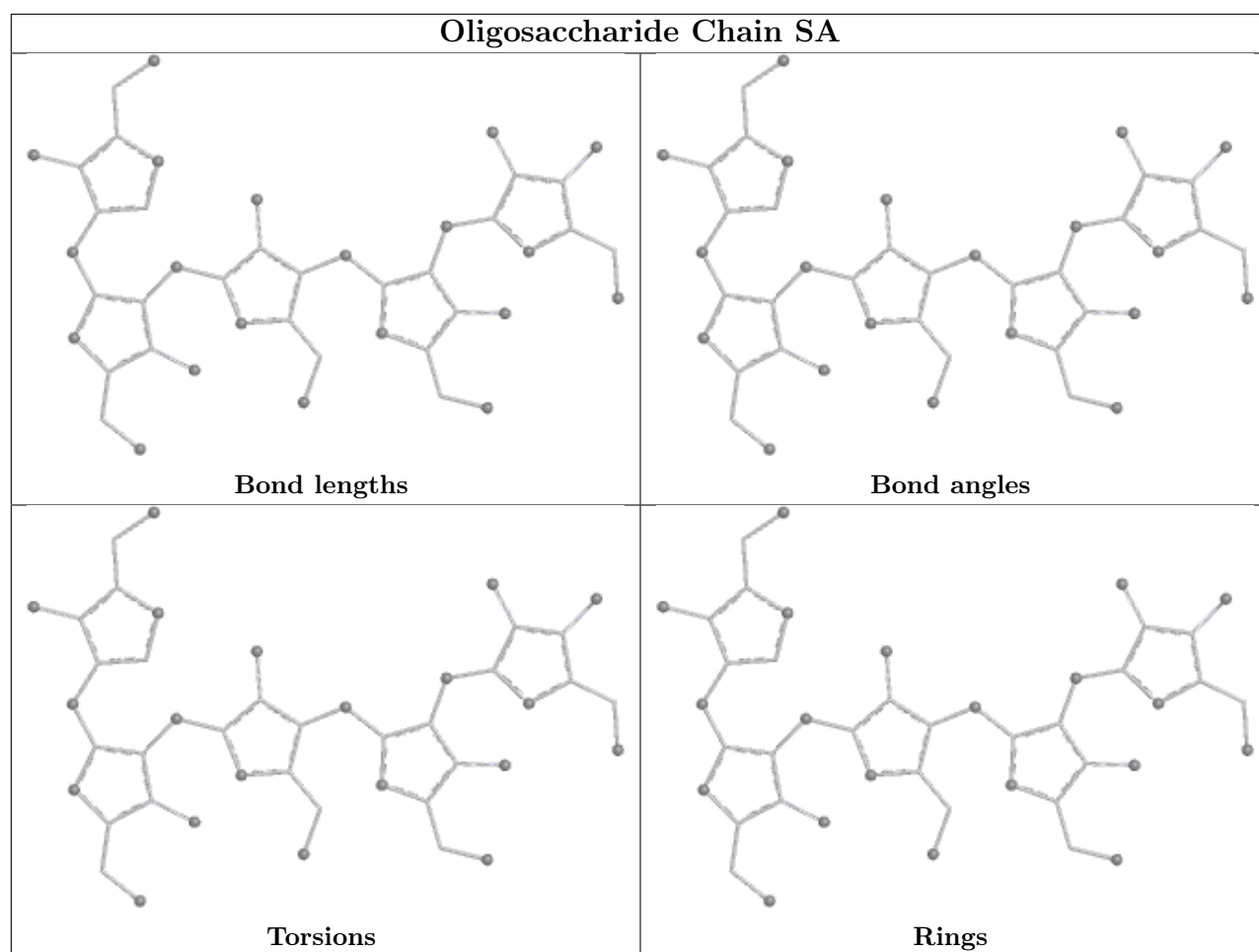


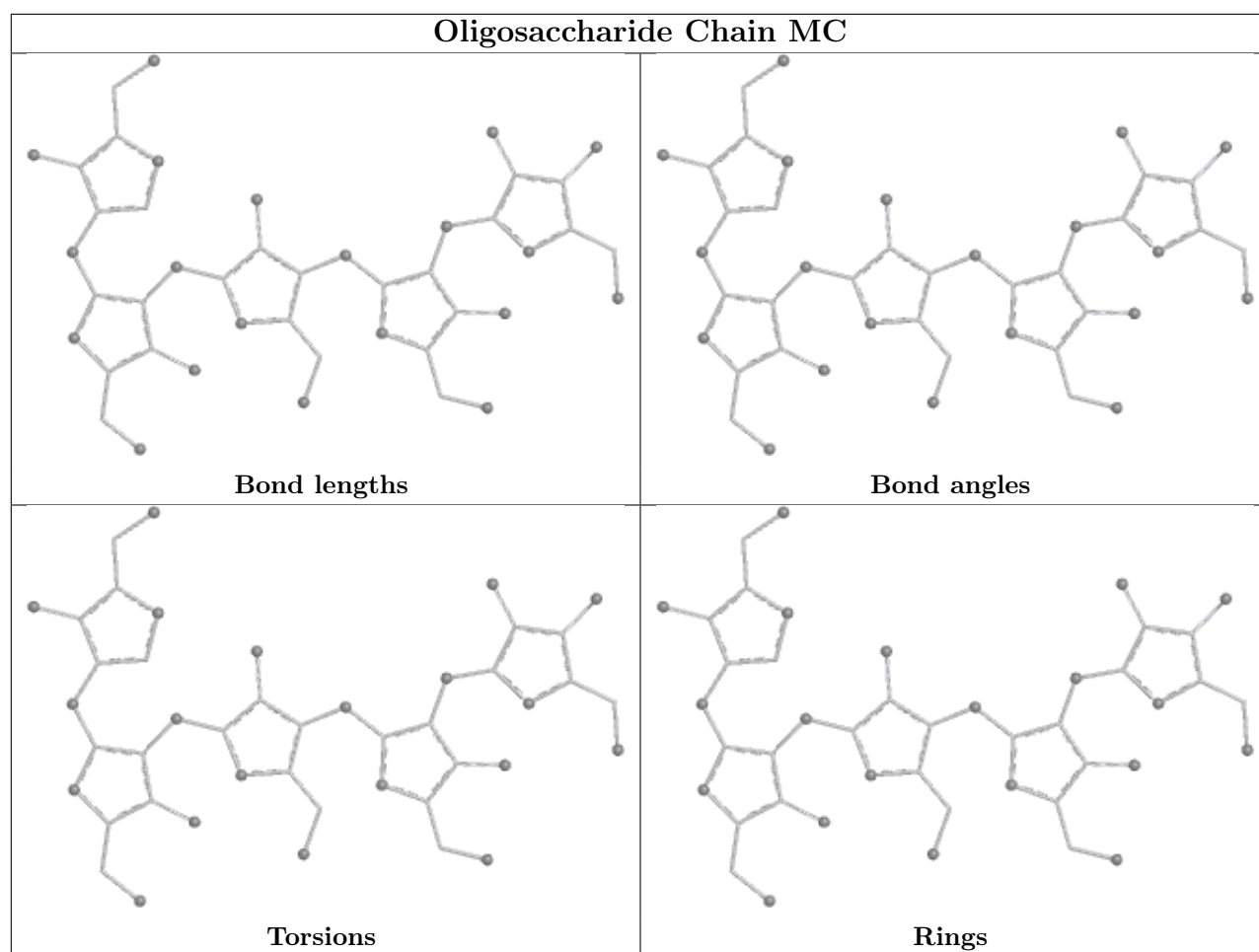


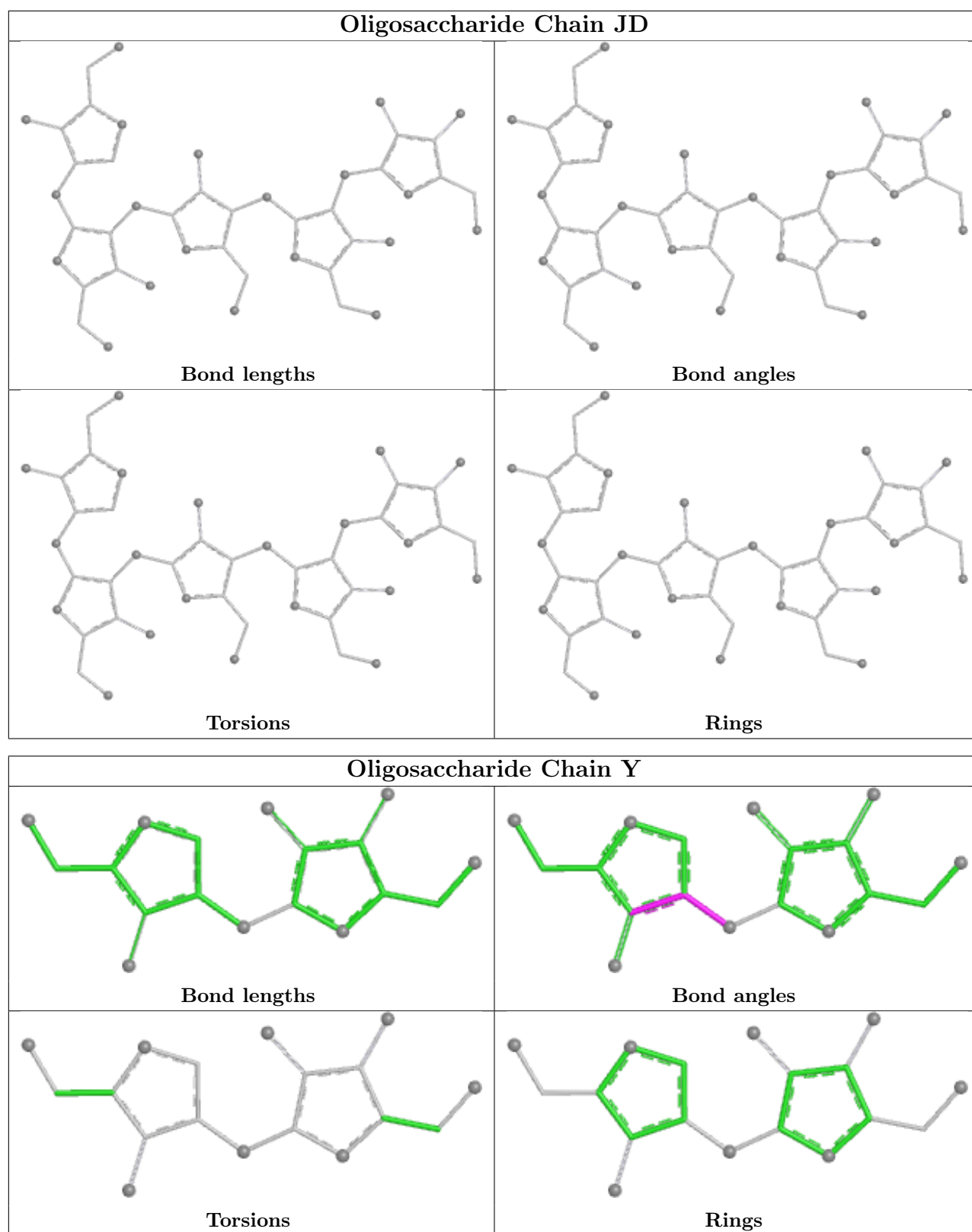


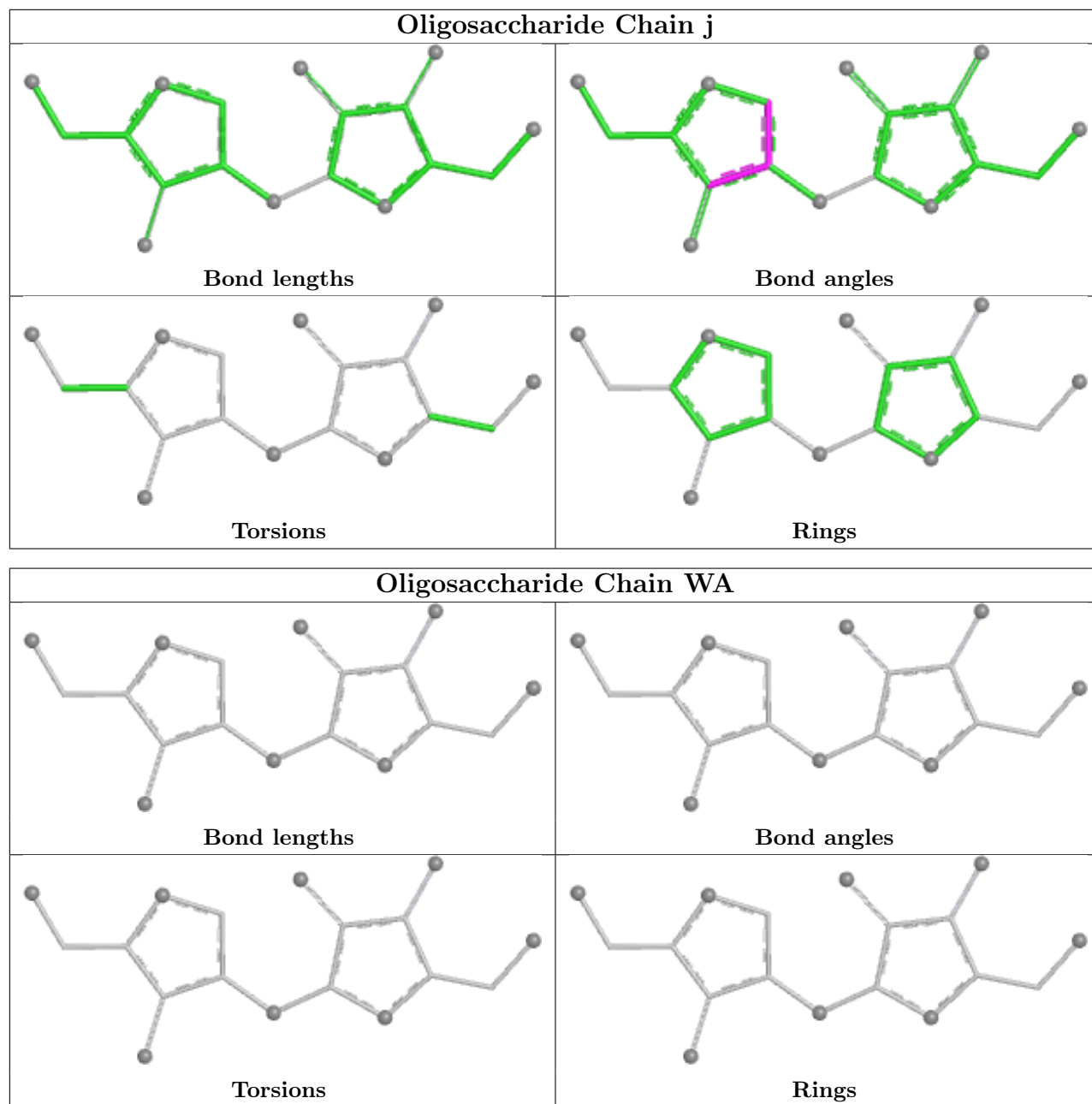


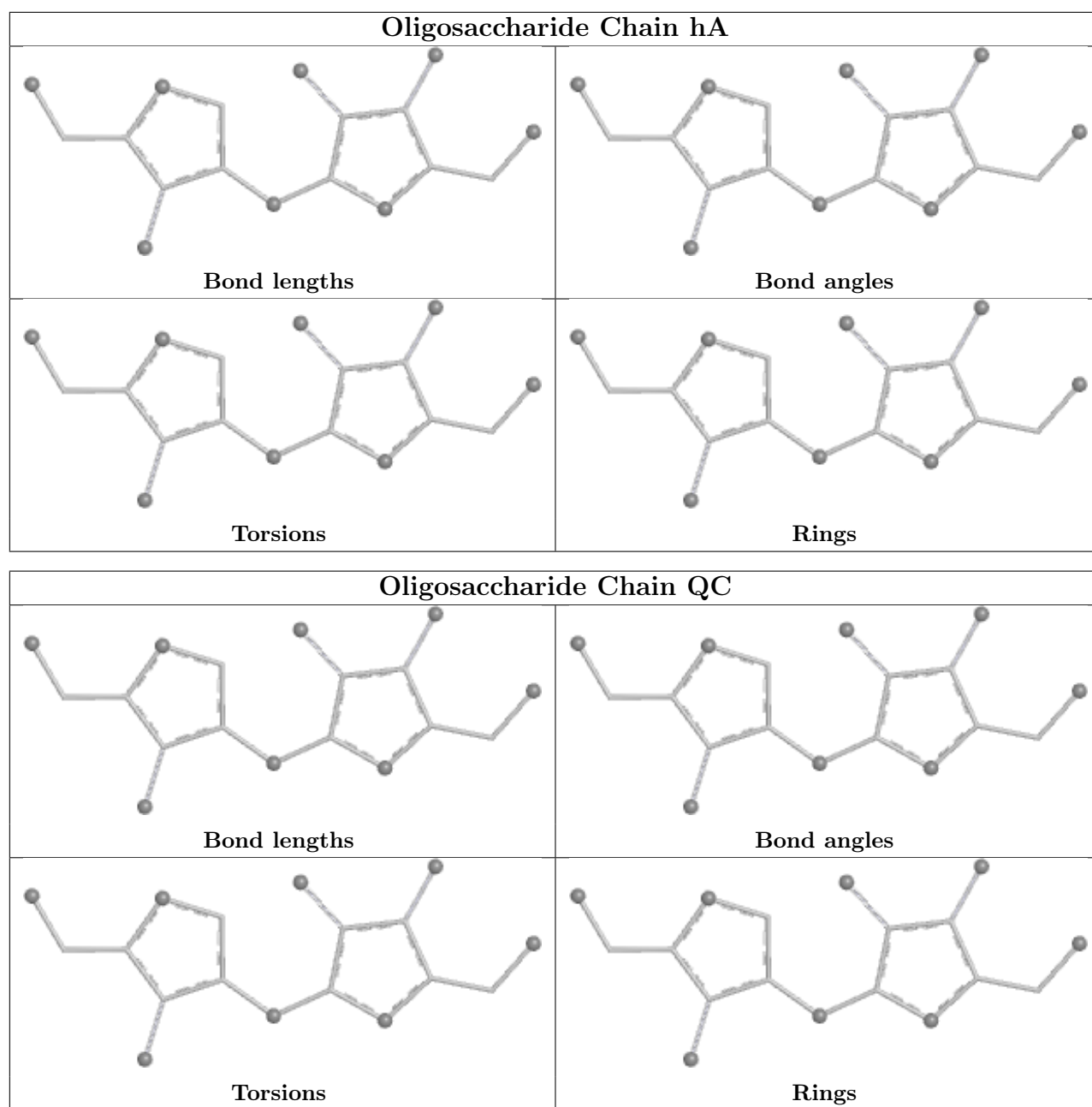


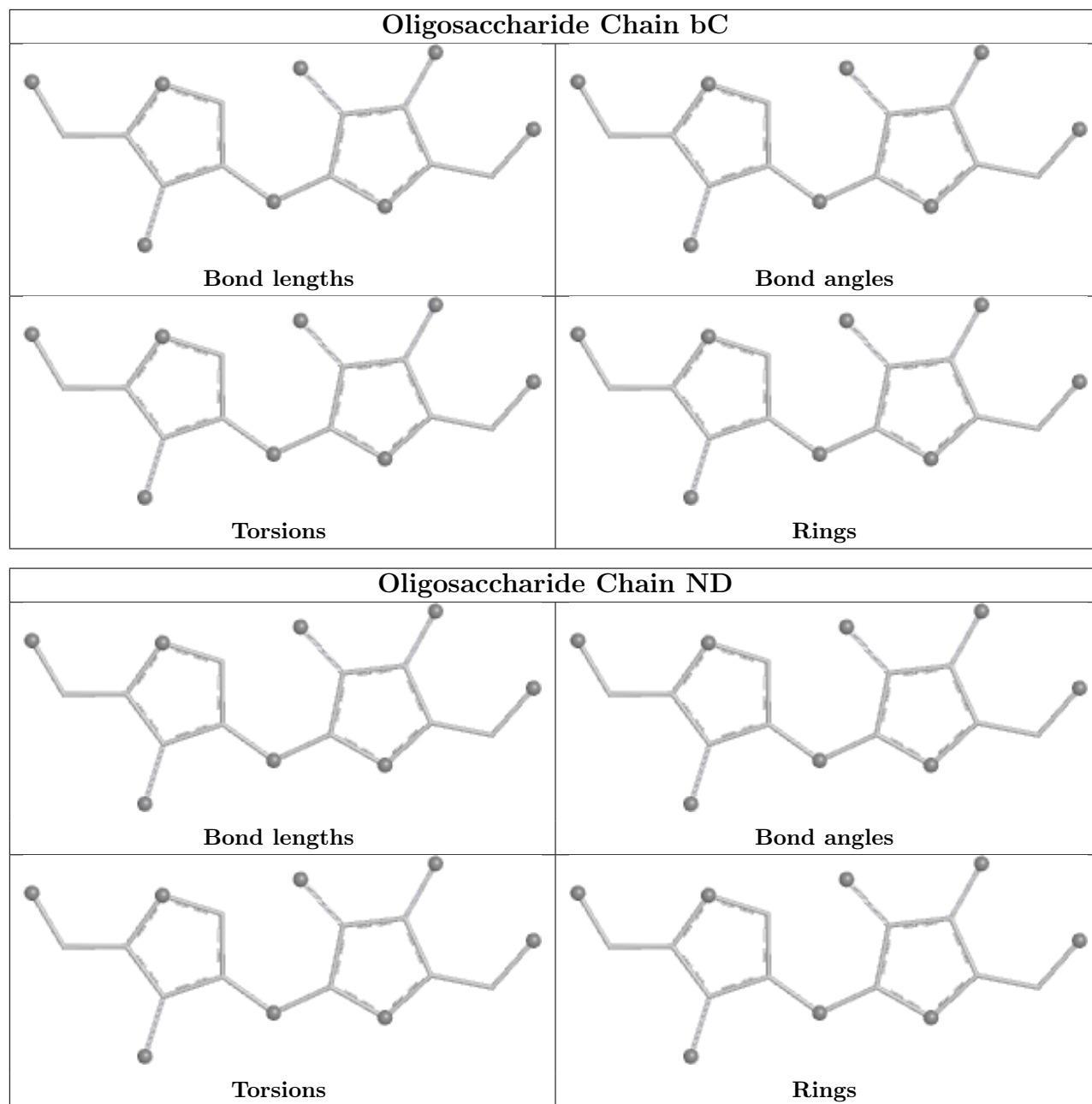


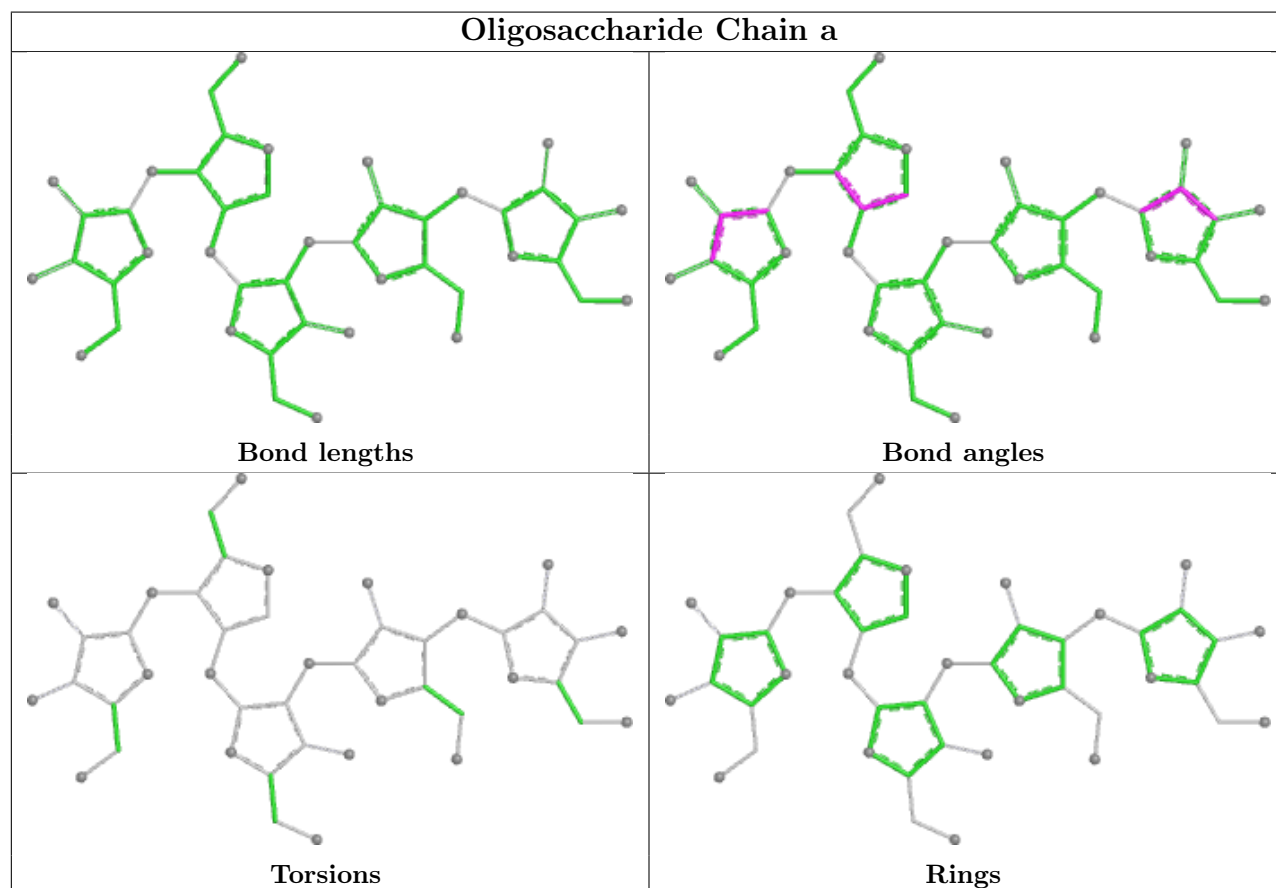
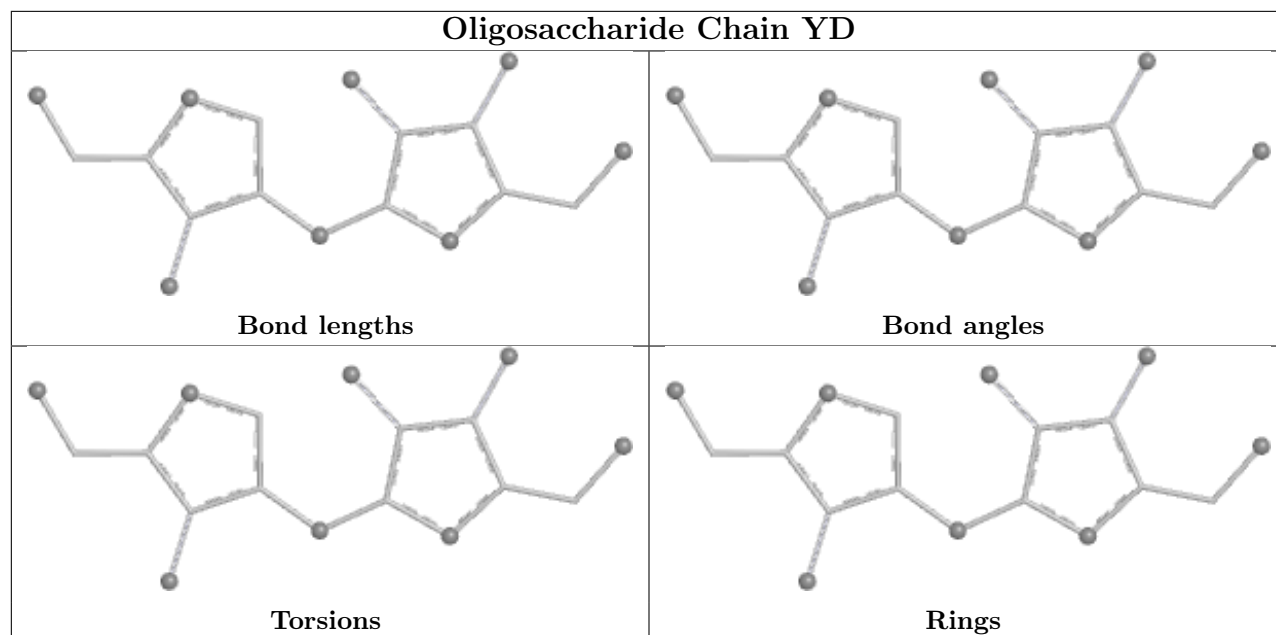


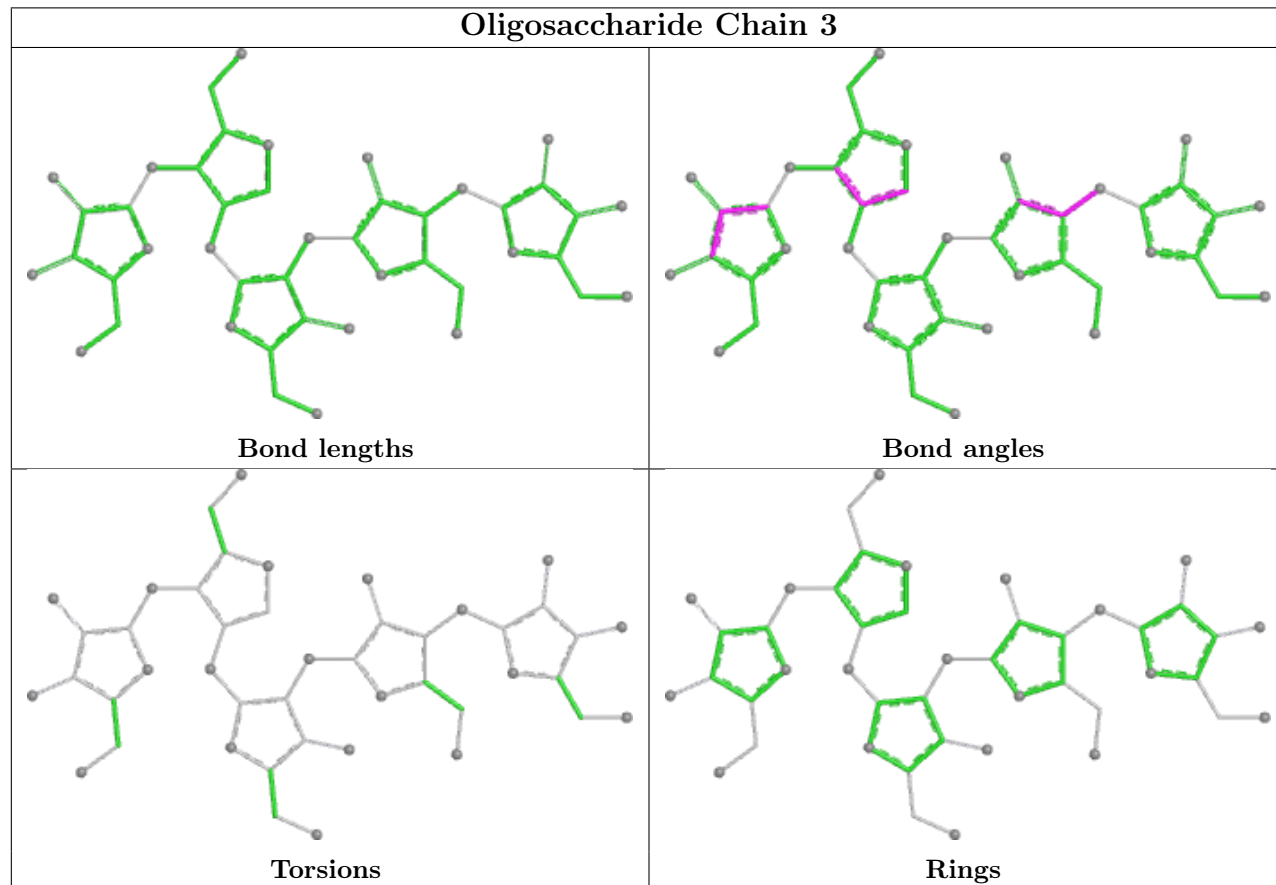
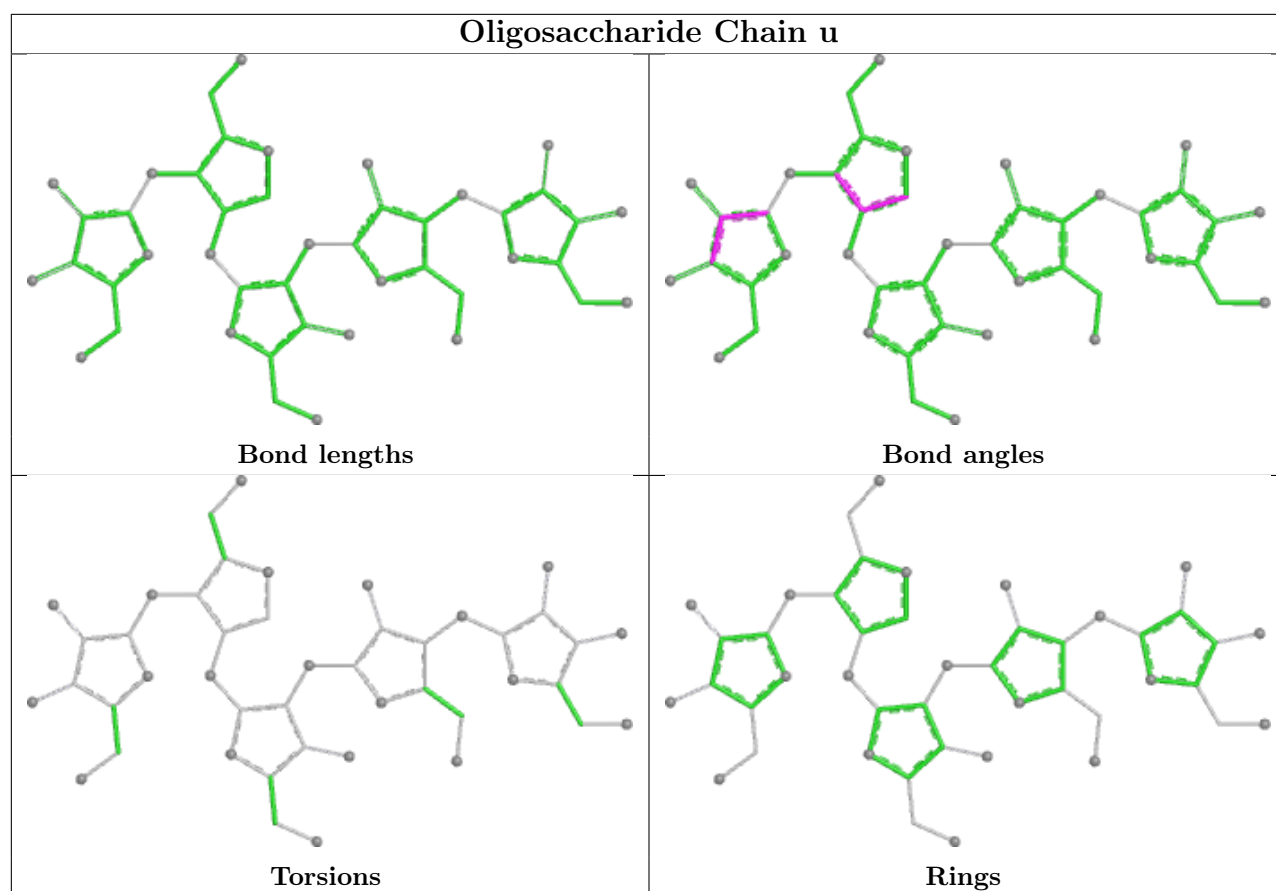


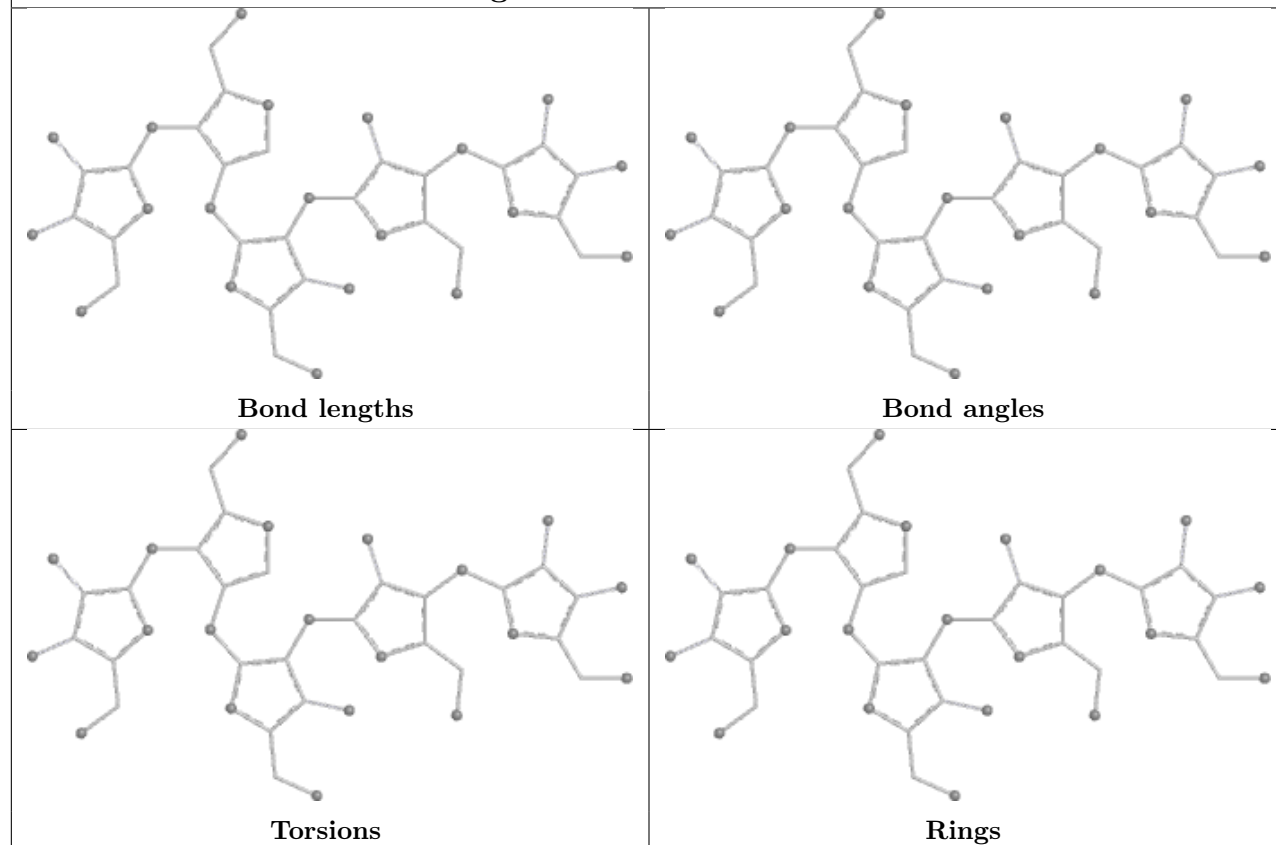
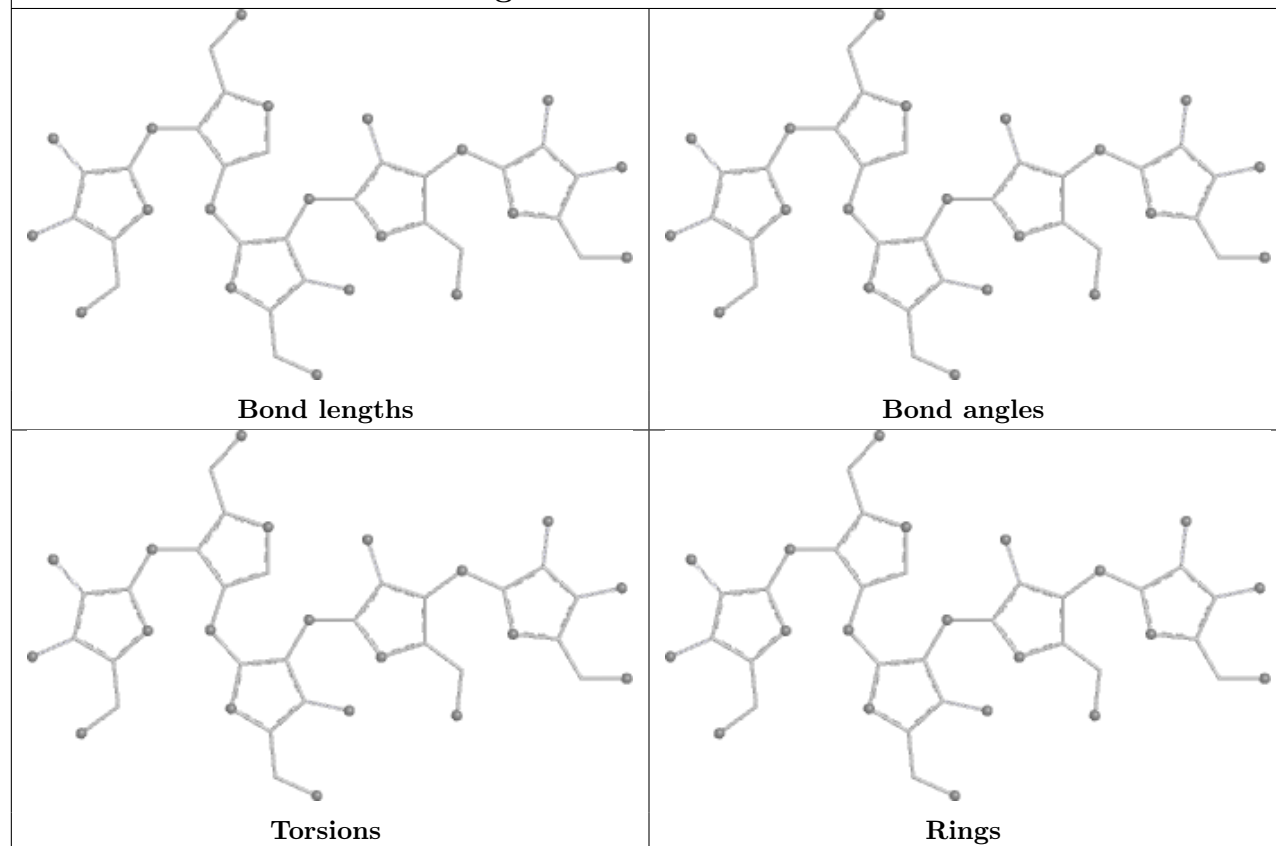


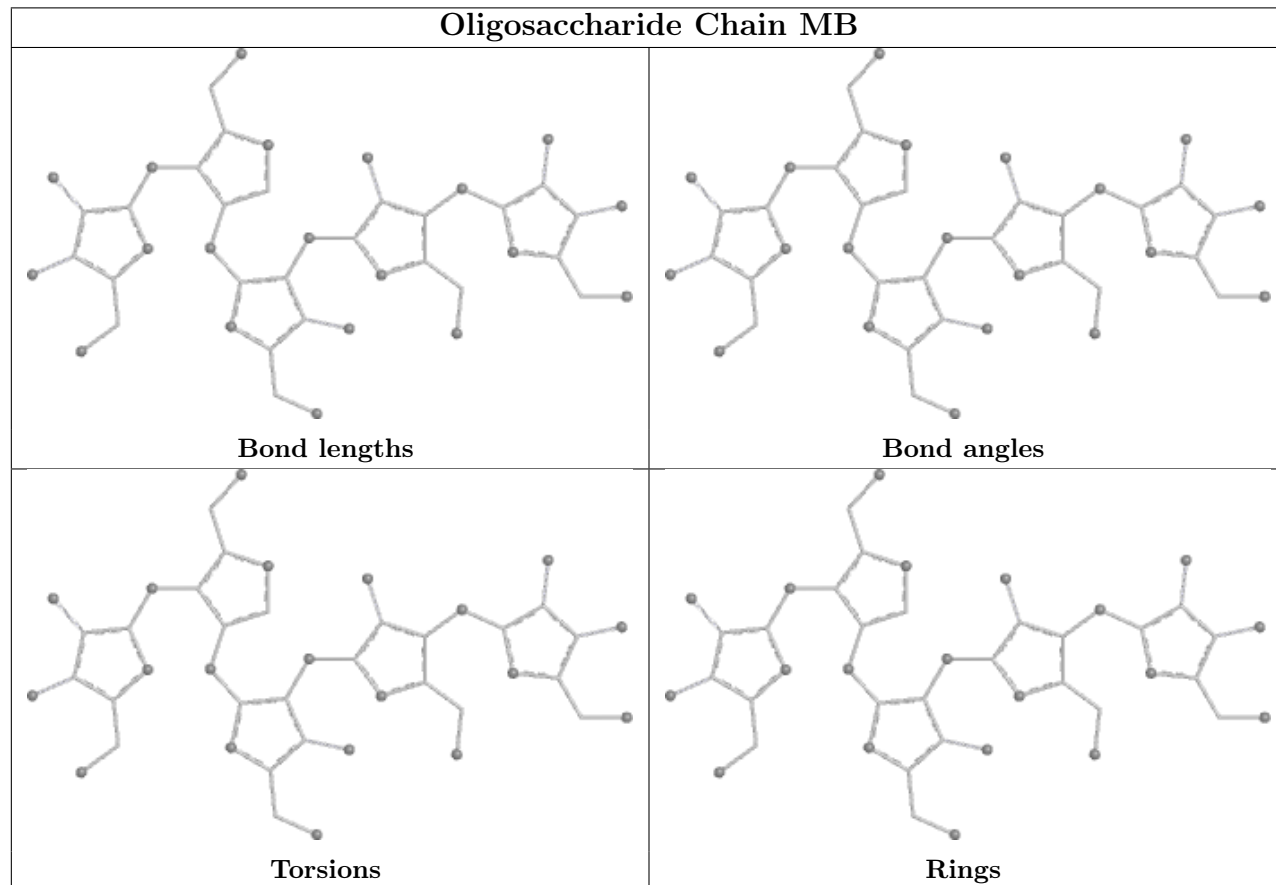
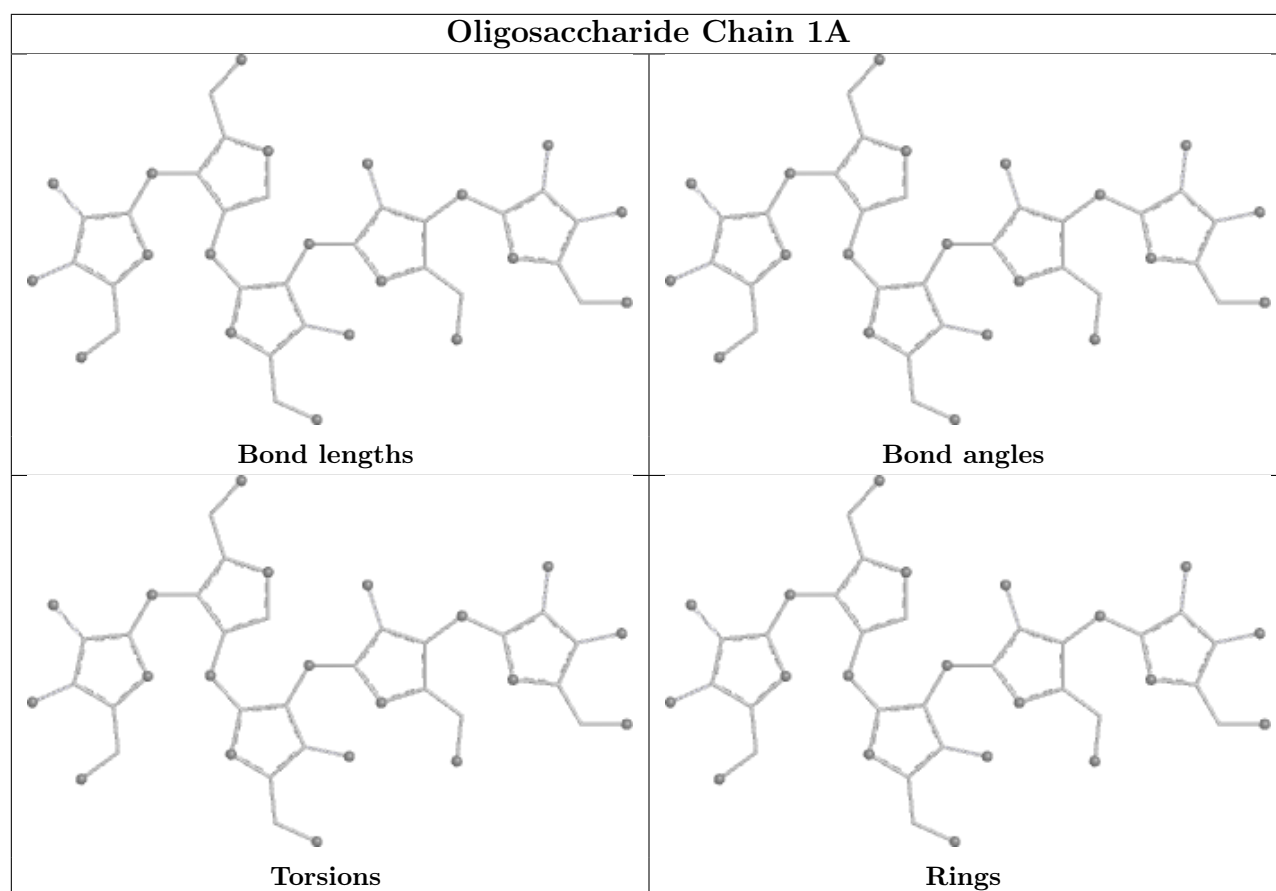


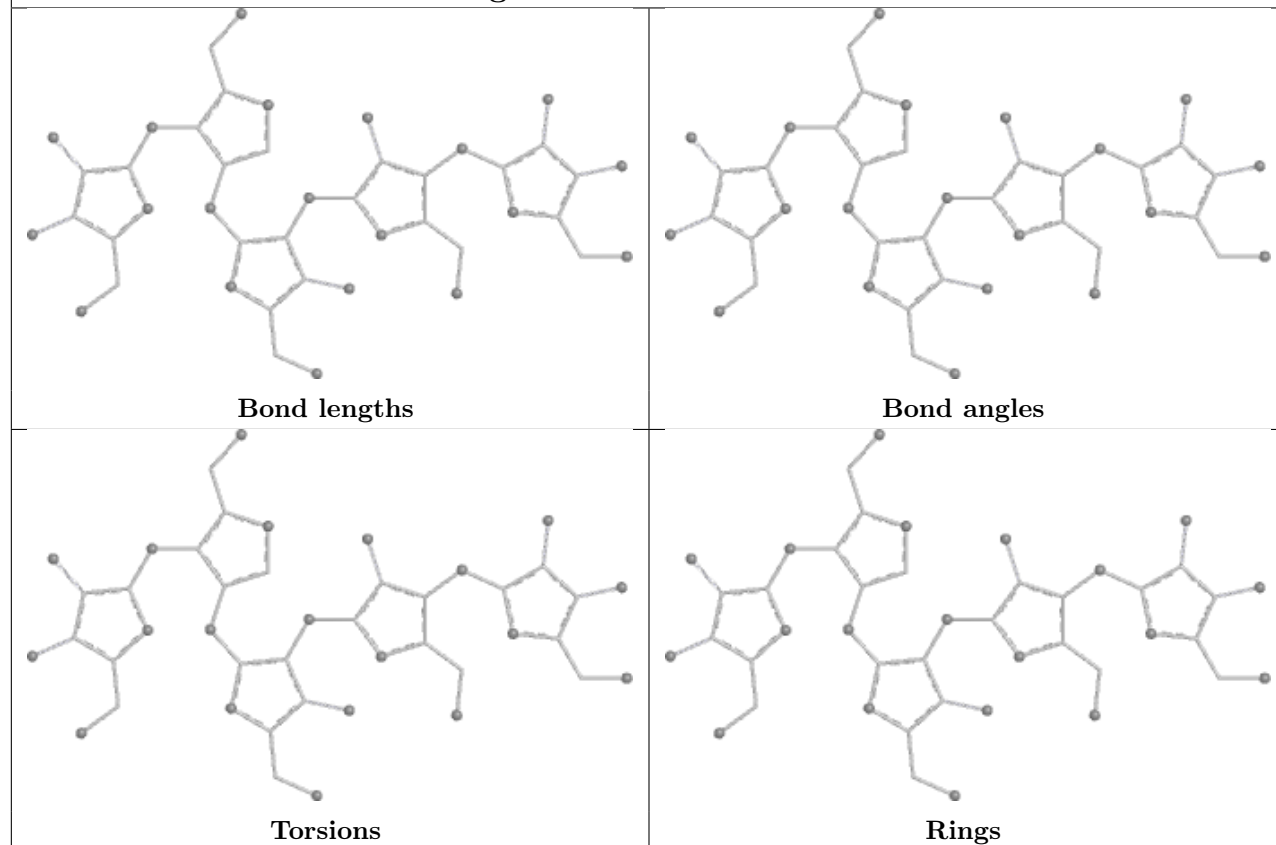
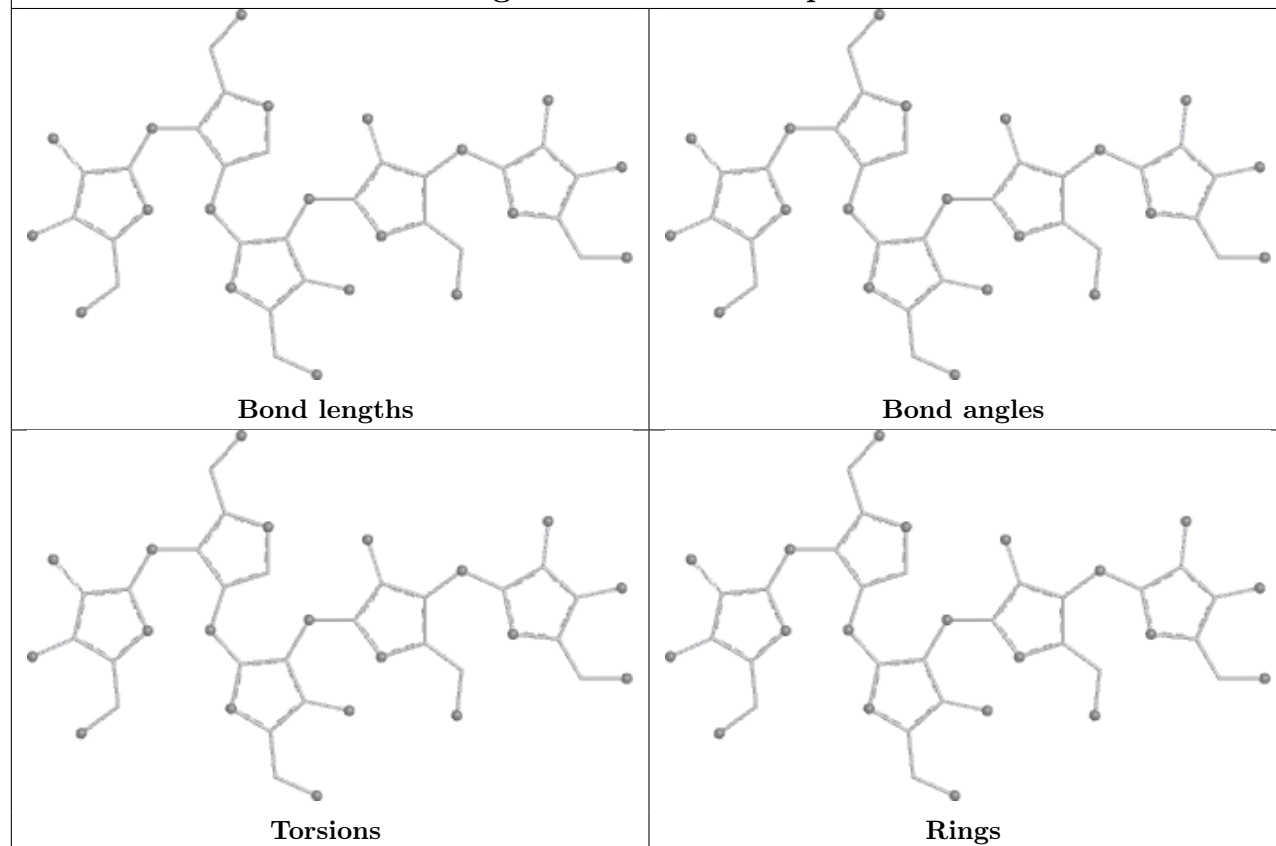


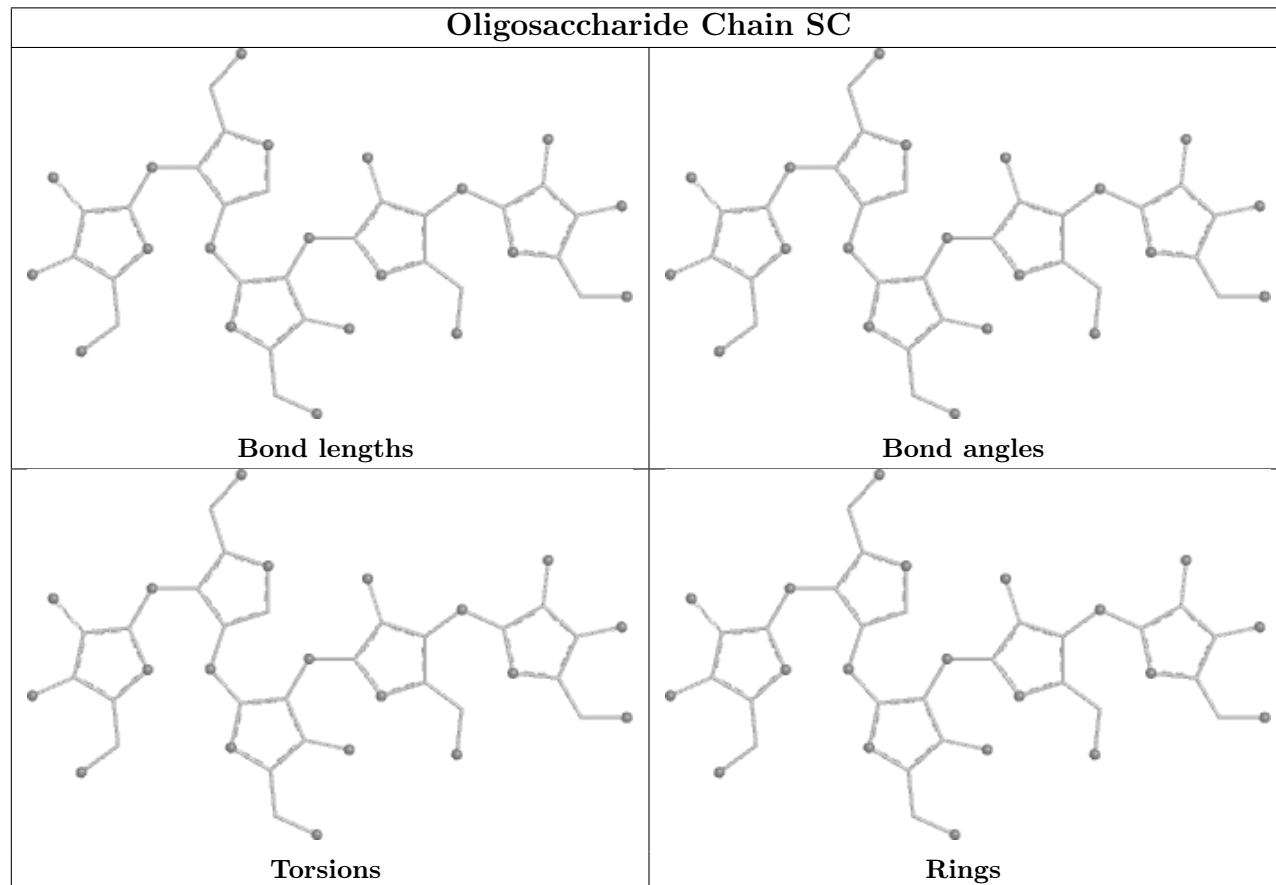
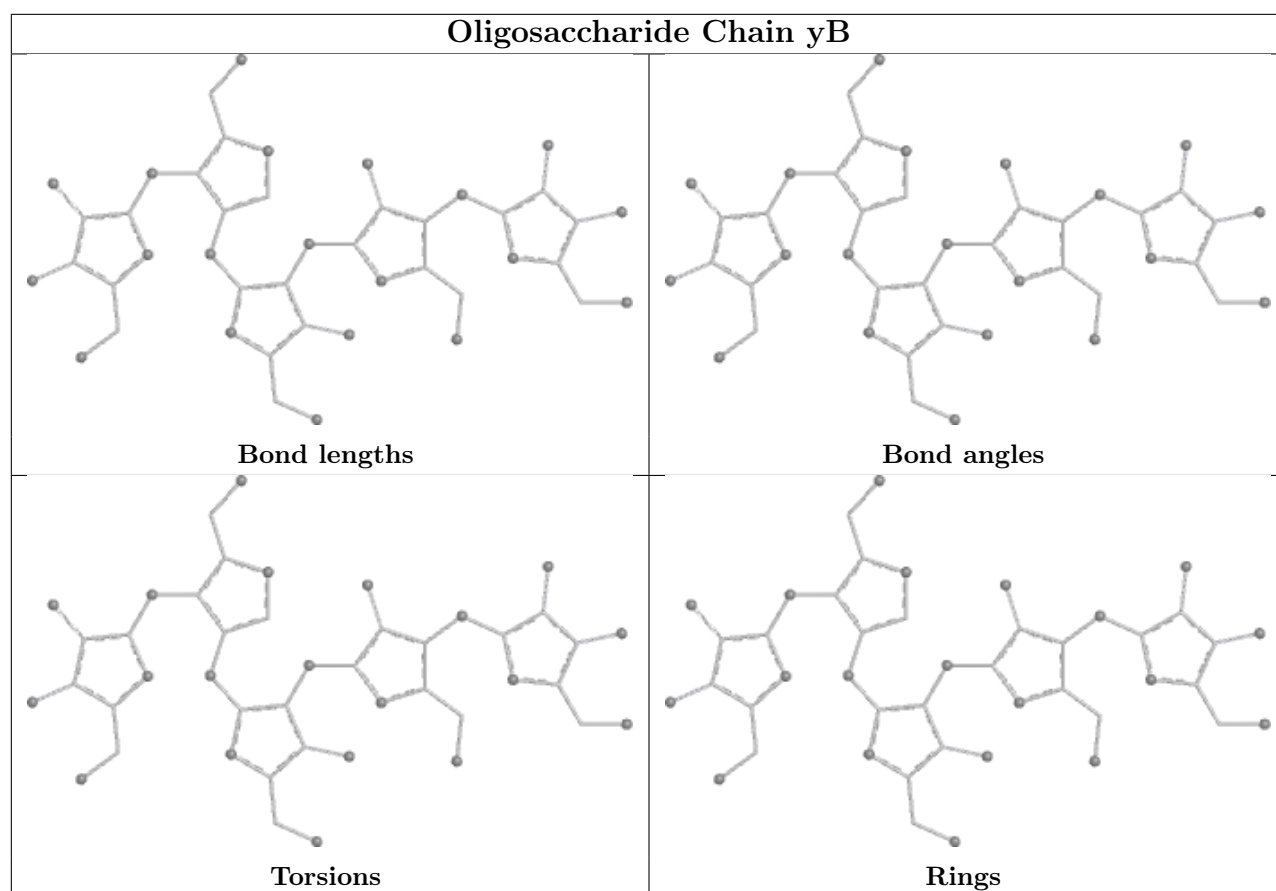


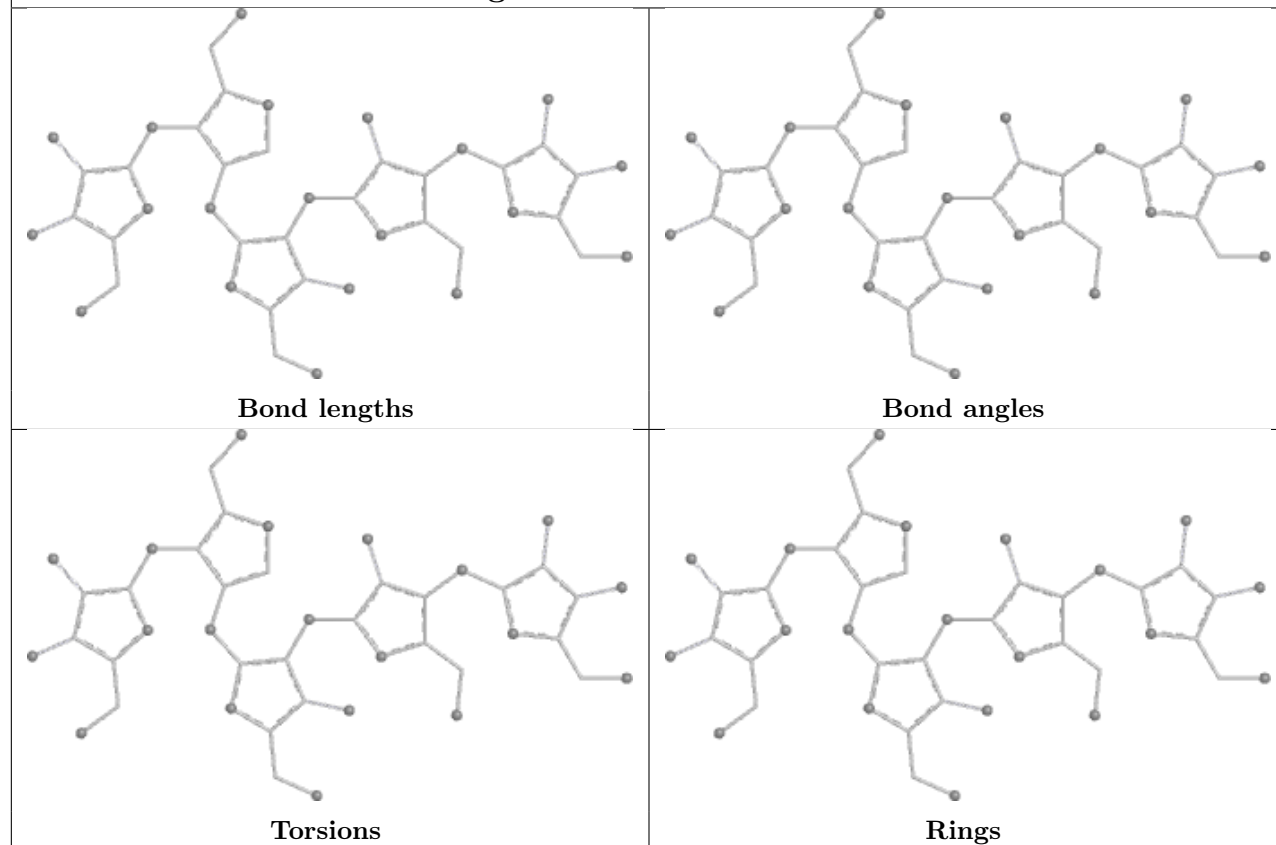
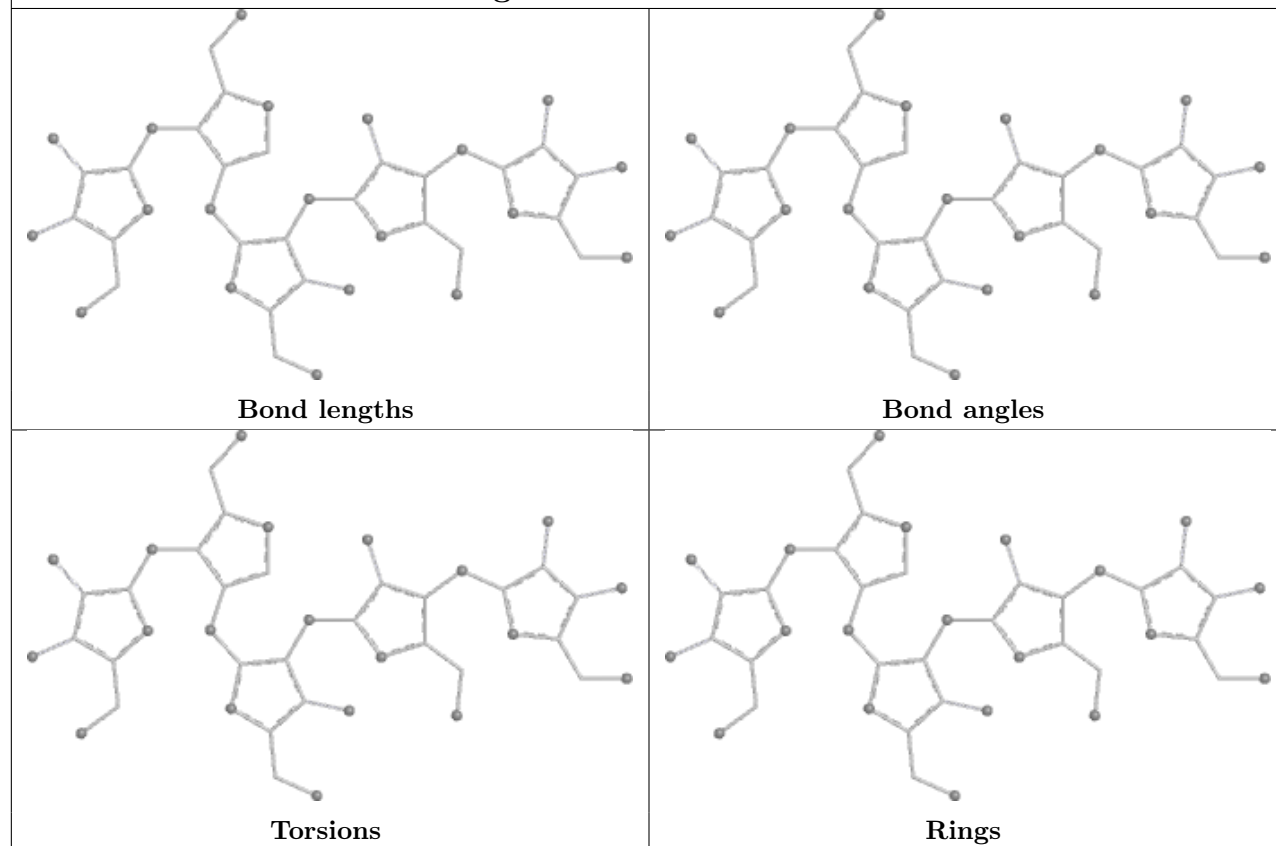


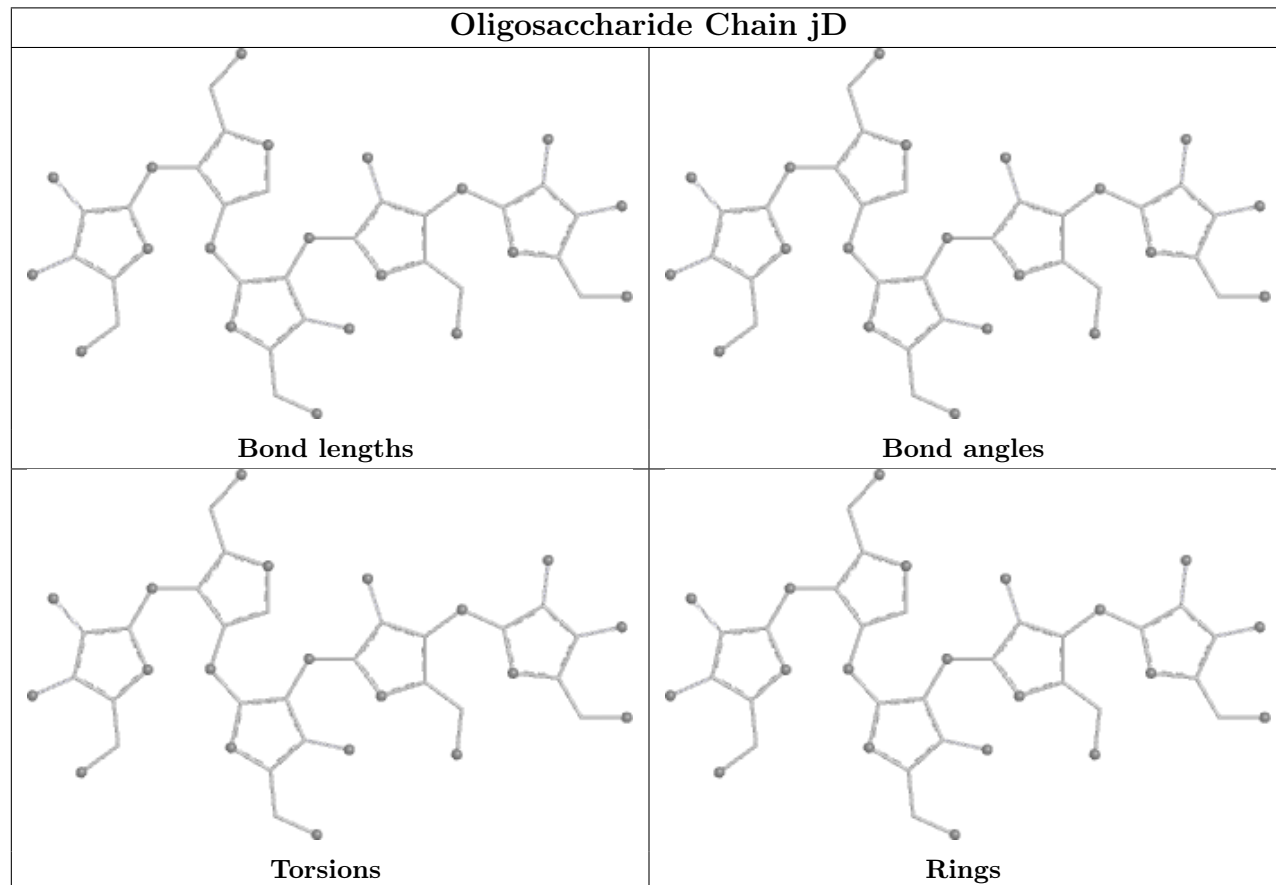
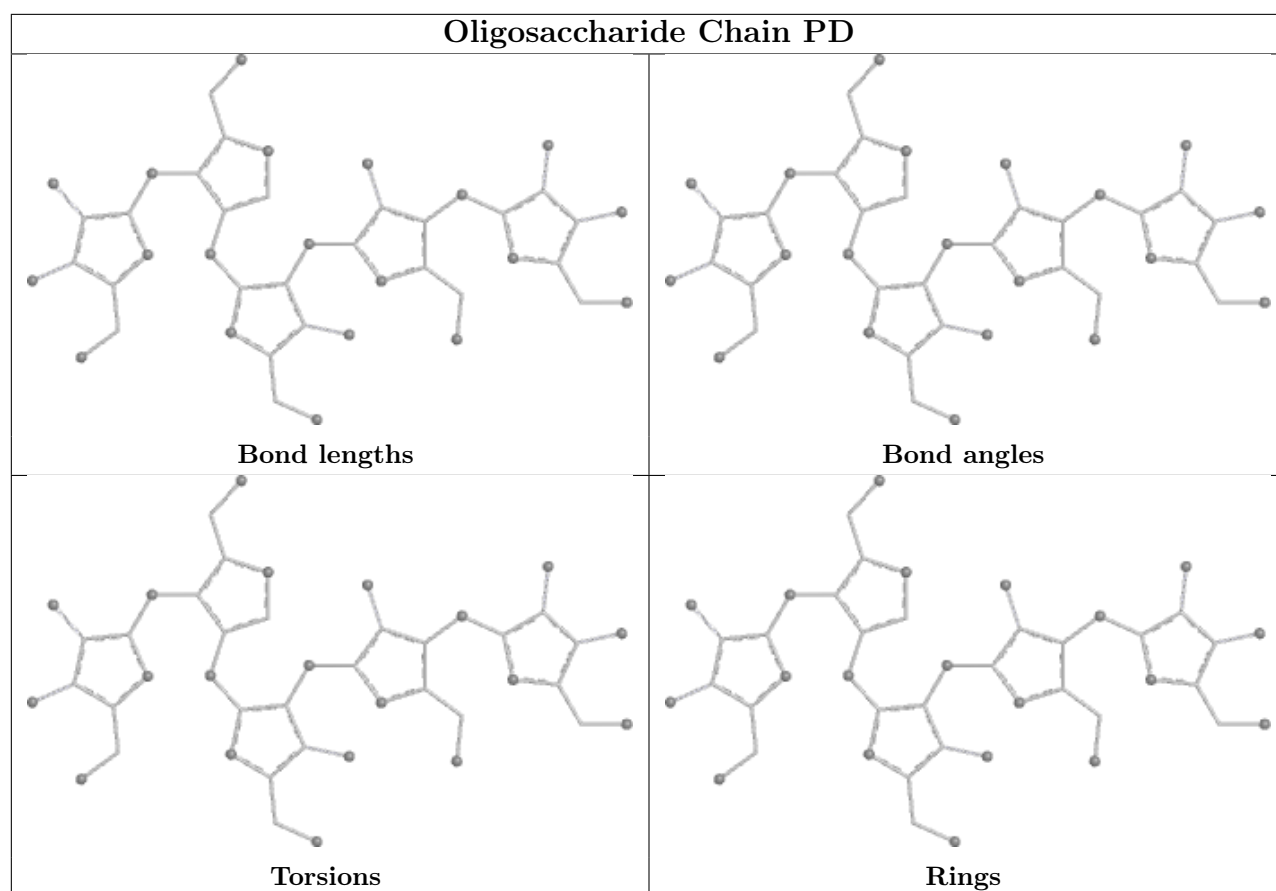
Oligosaccharide Chain YA**Oligosaccharide Chain sA**

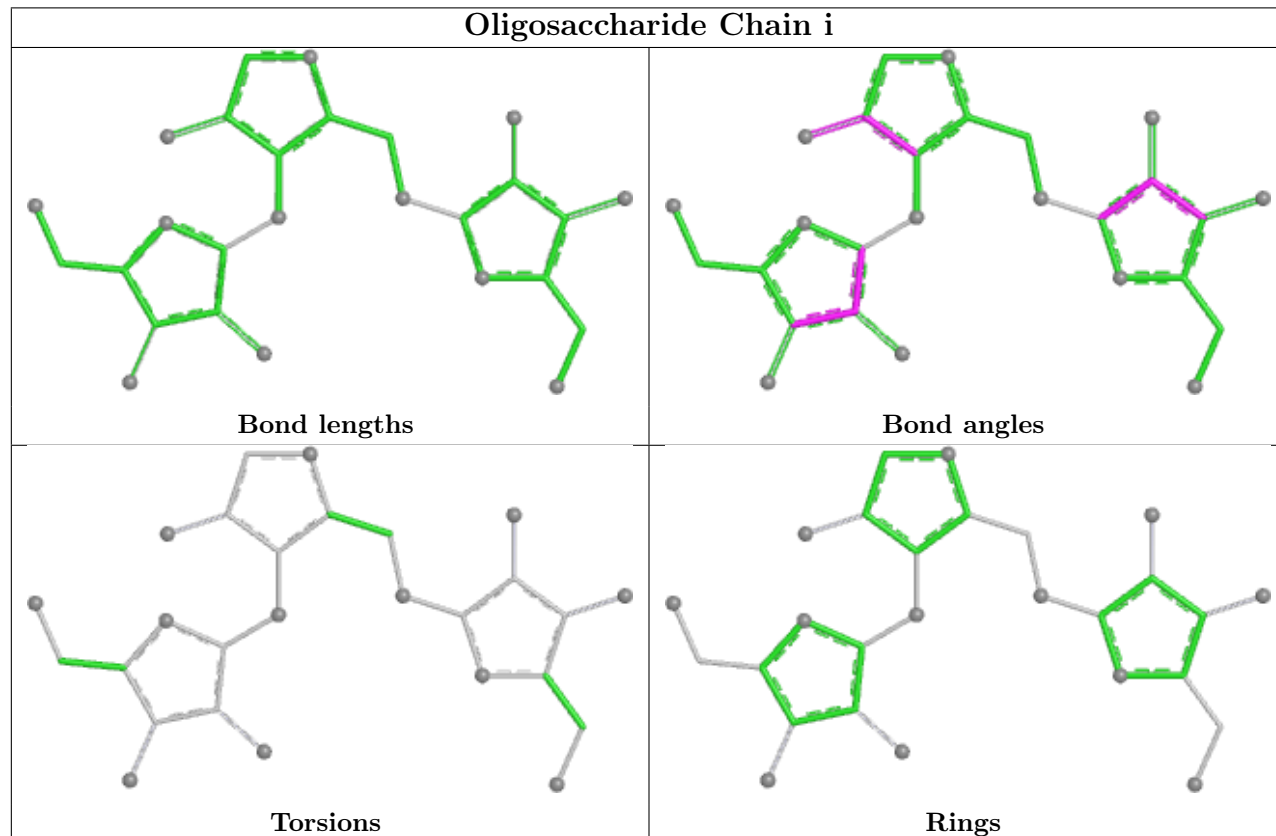
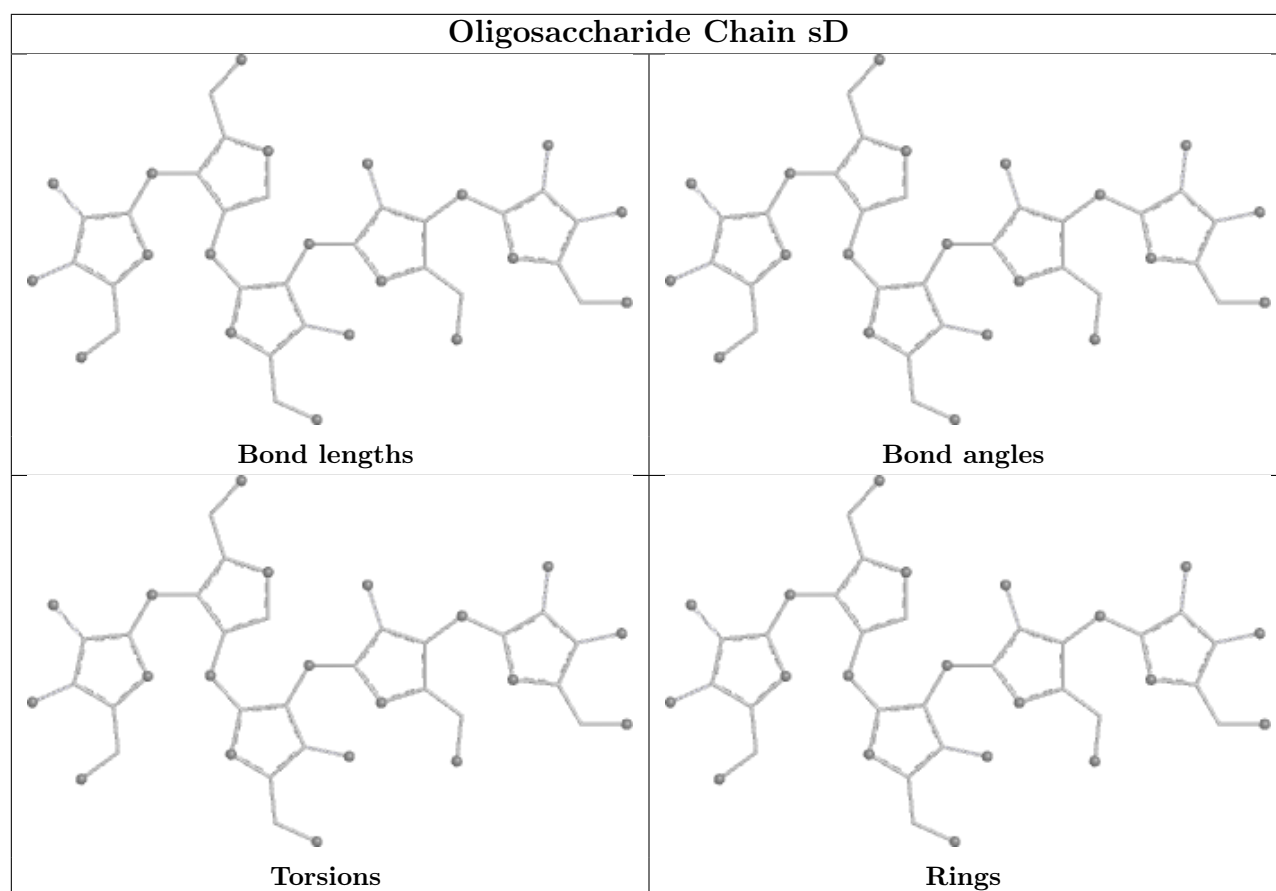


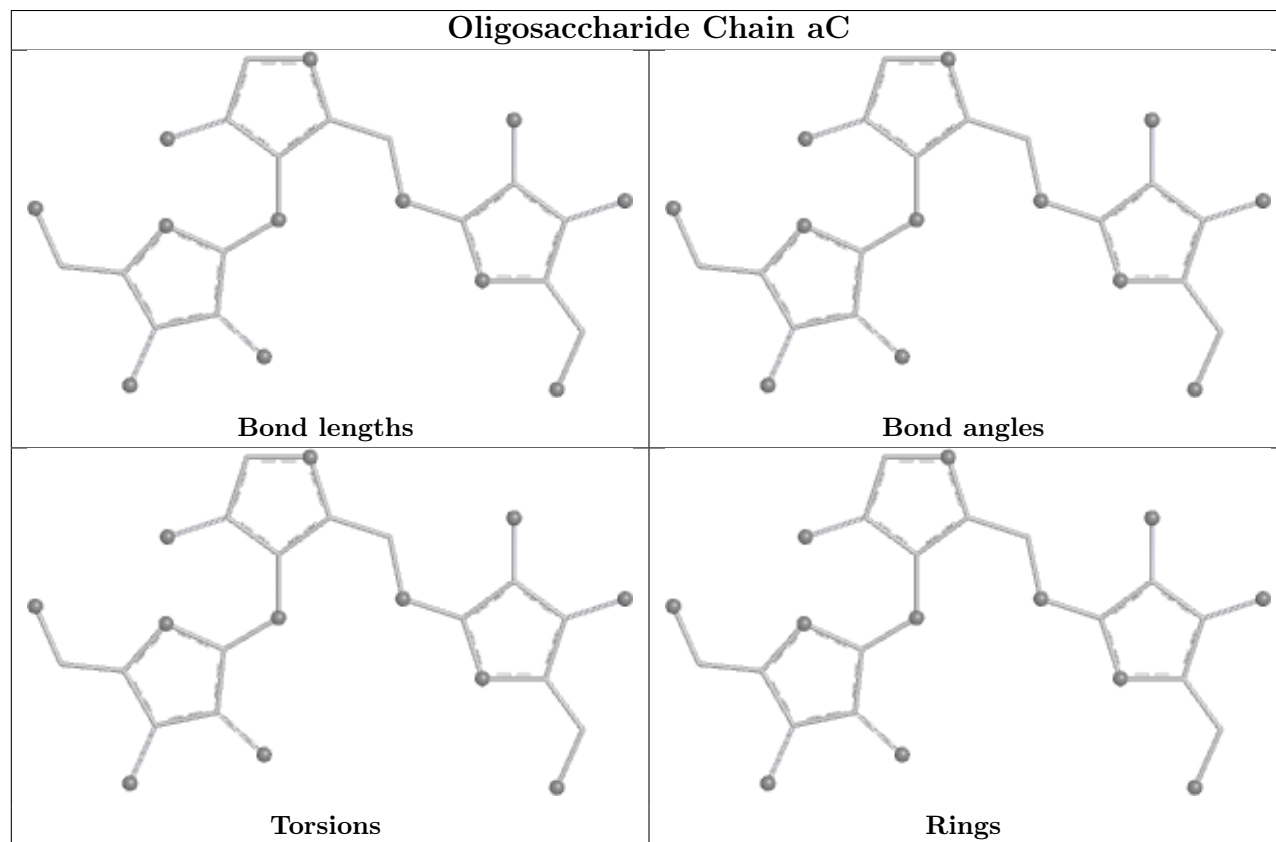
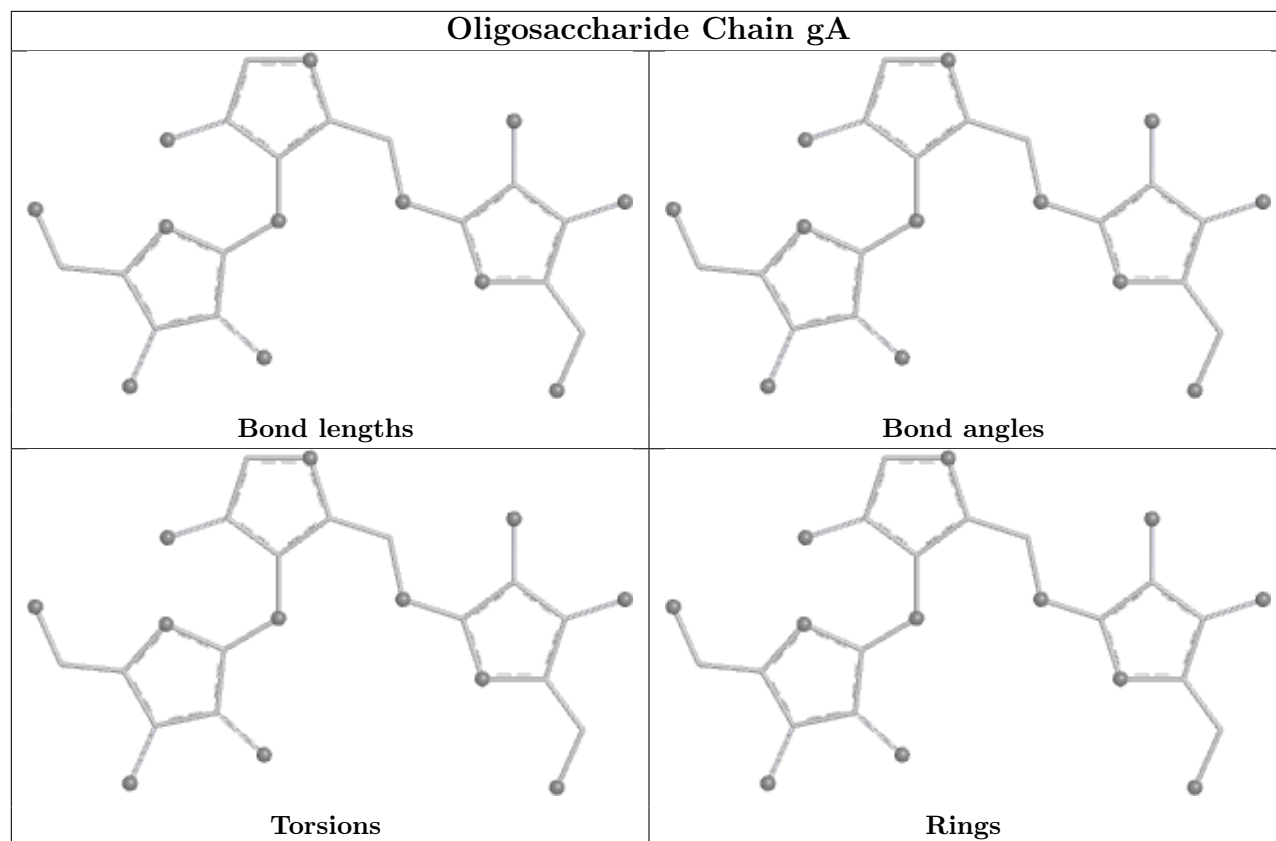
Oligosaccharide Chain VB**Oligosaccharide Chain pB**

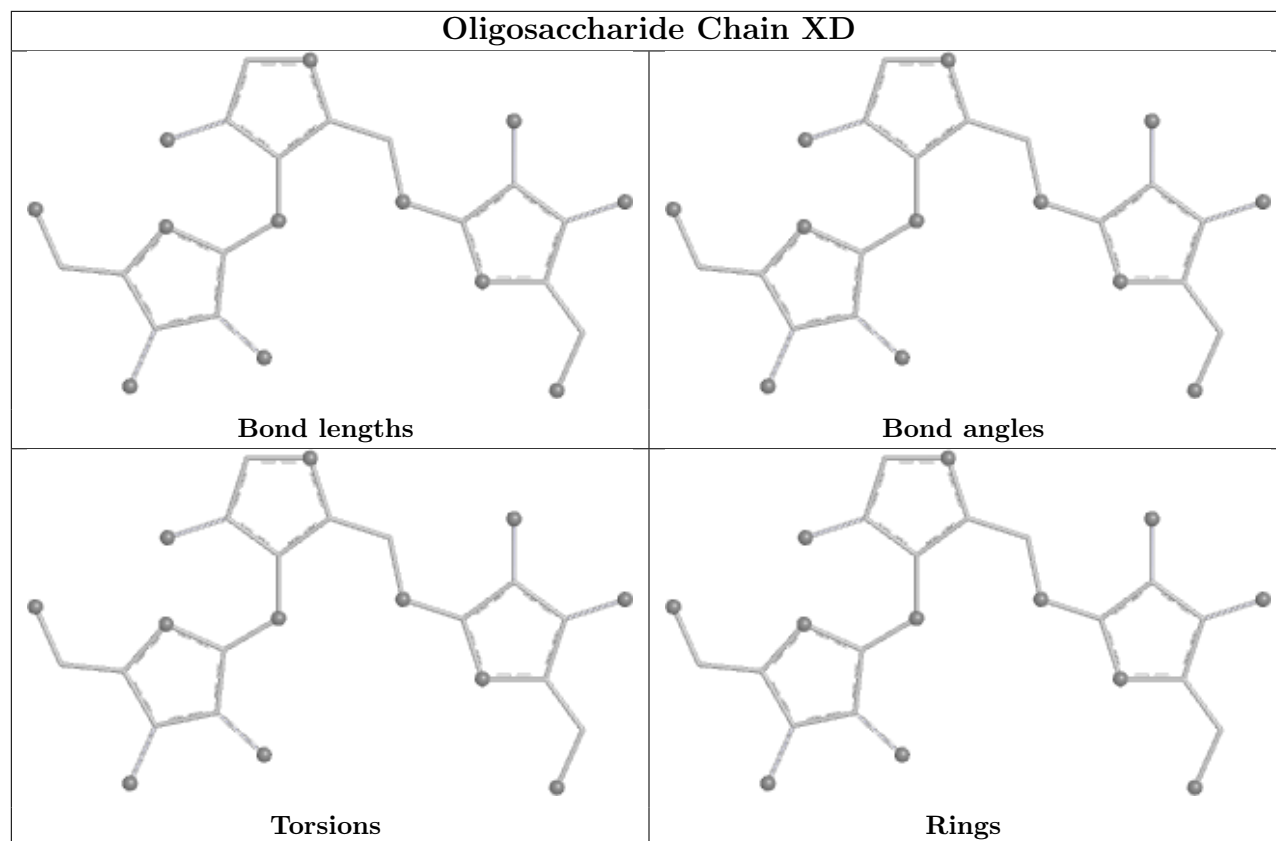


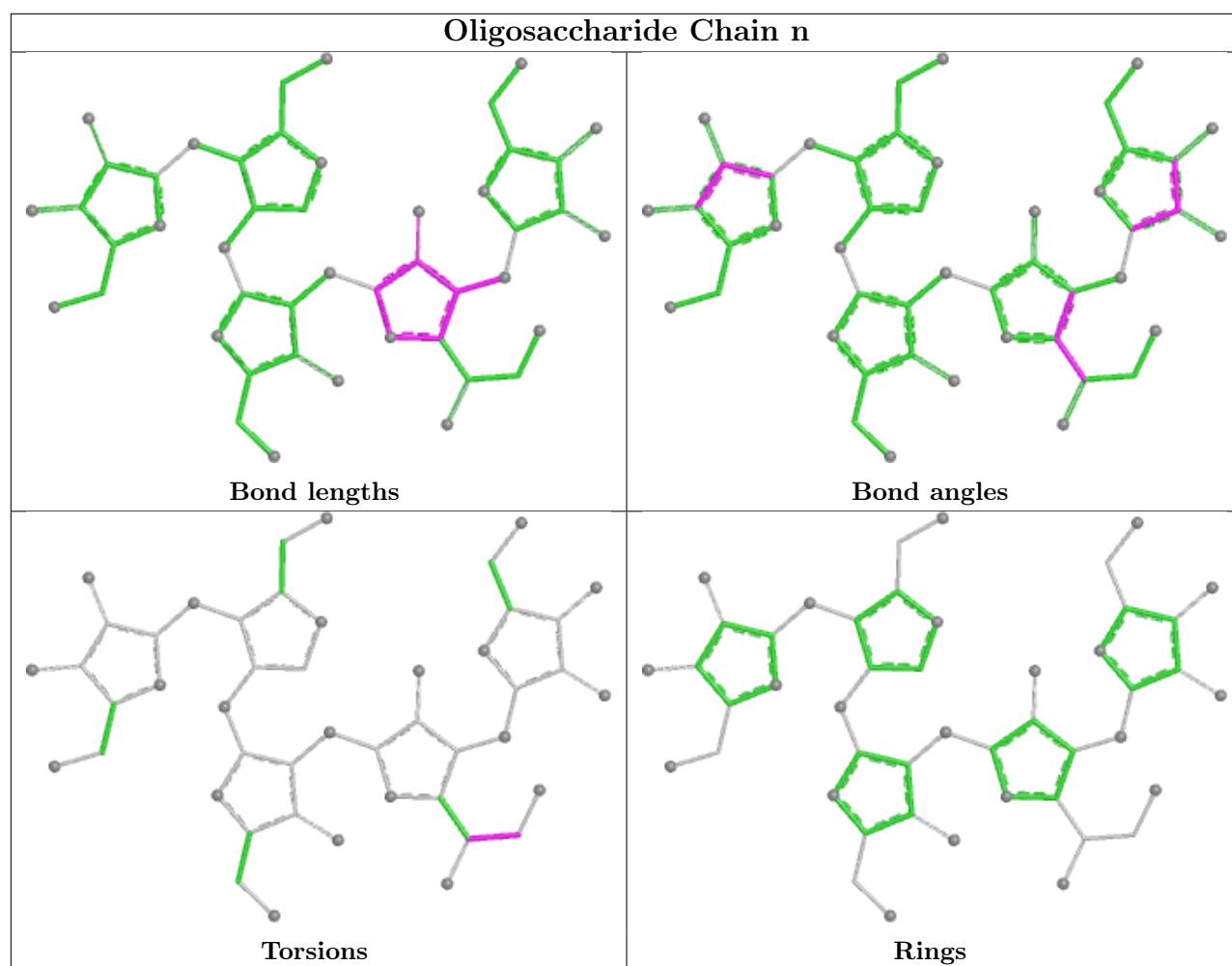
Oligosaccharide Chain mC**Oligosaccharide Chain vC**

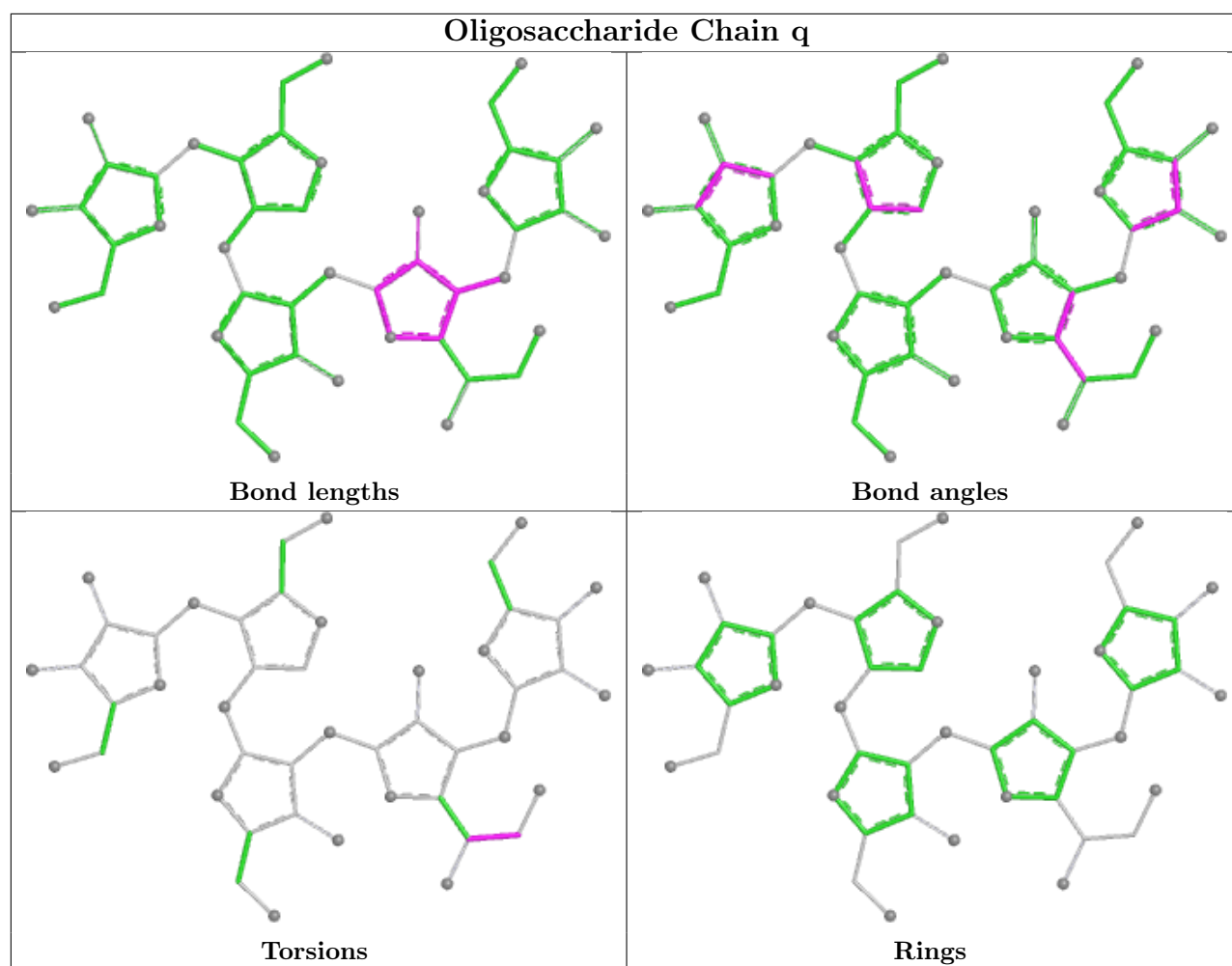


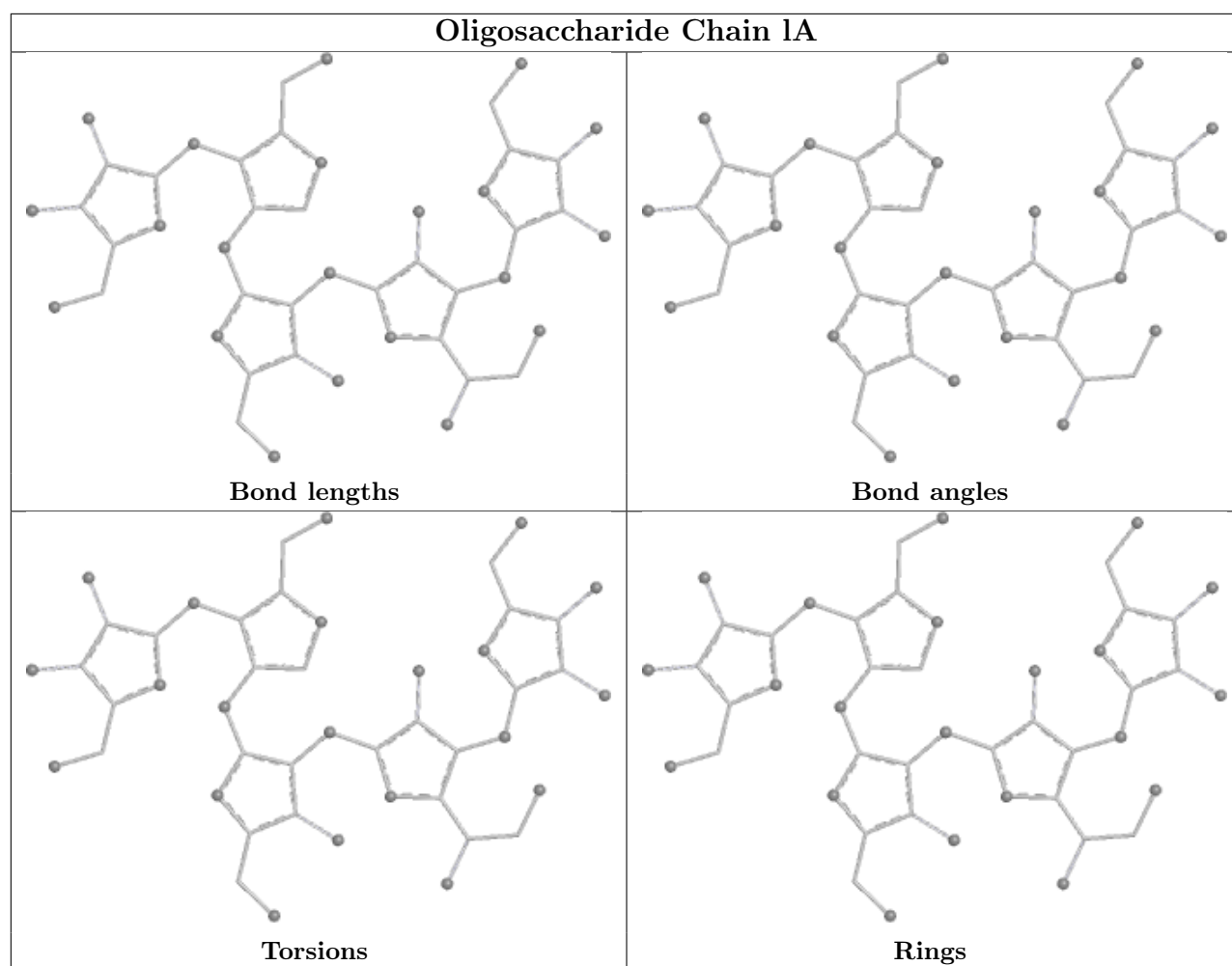


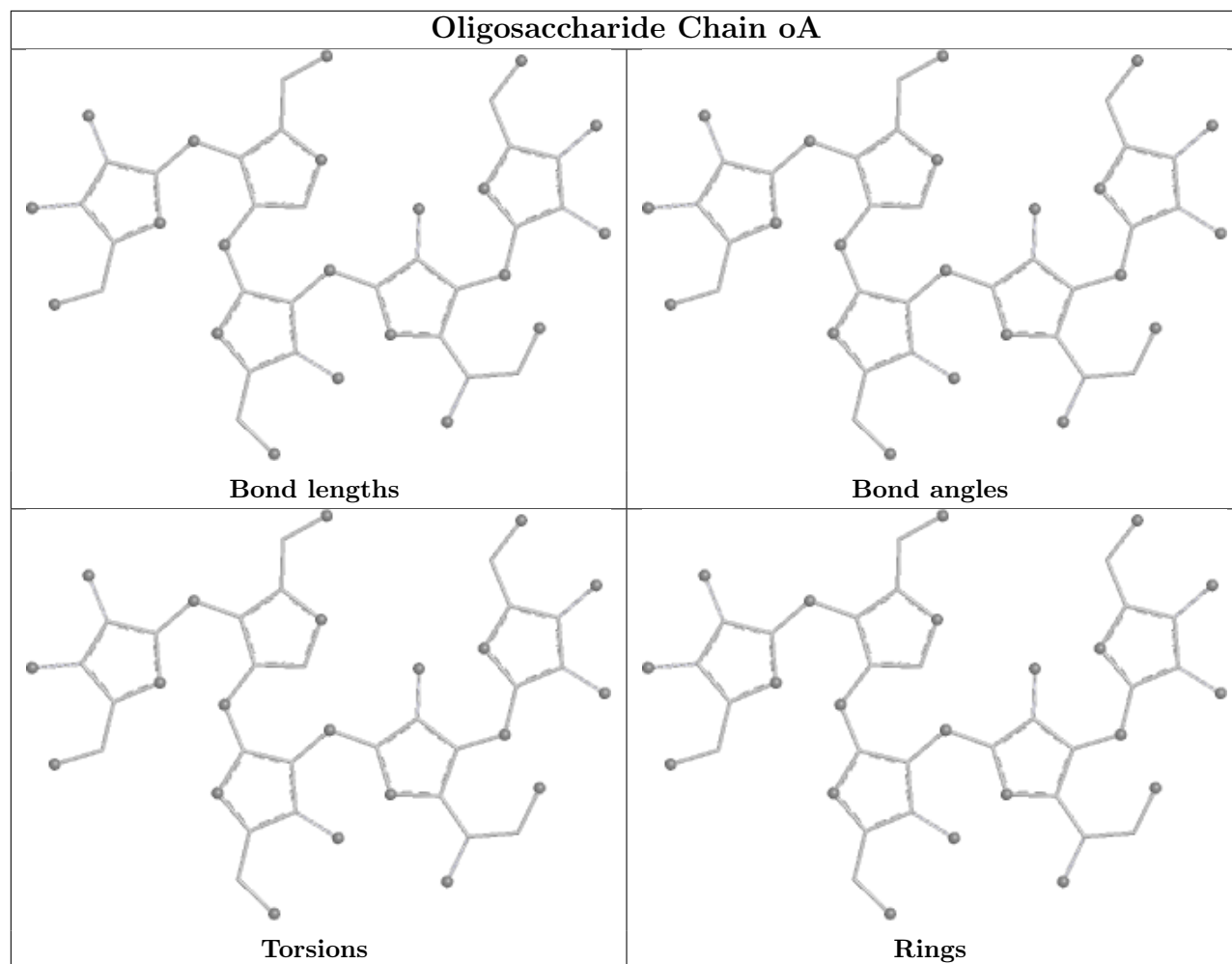


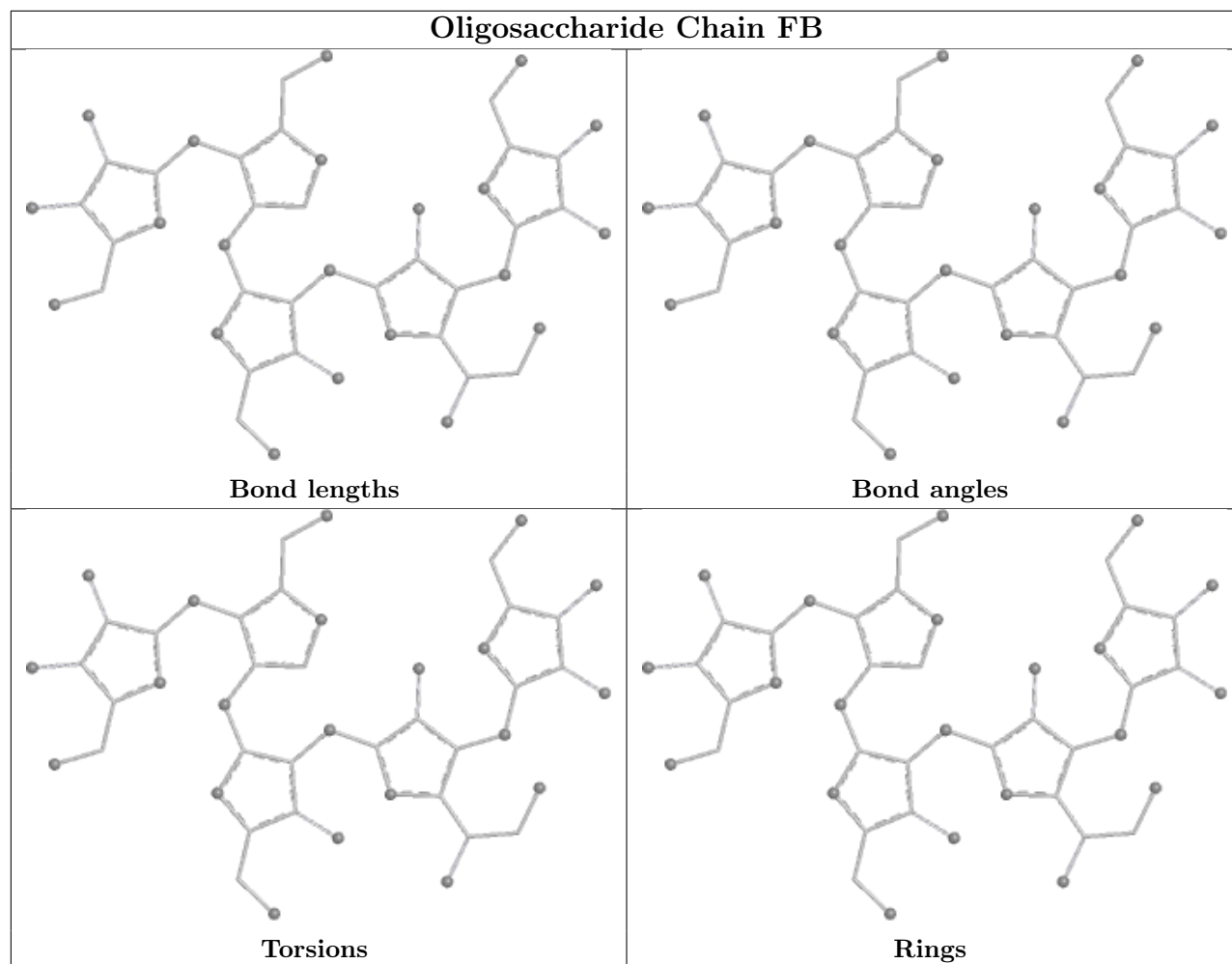


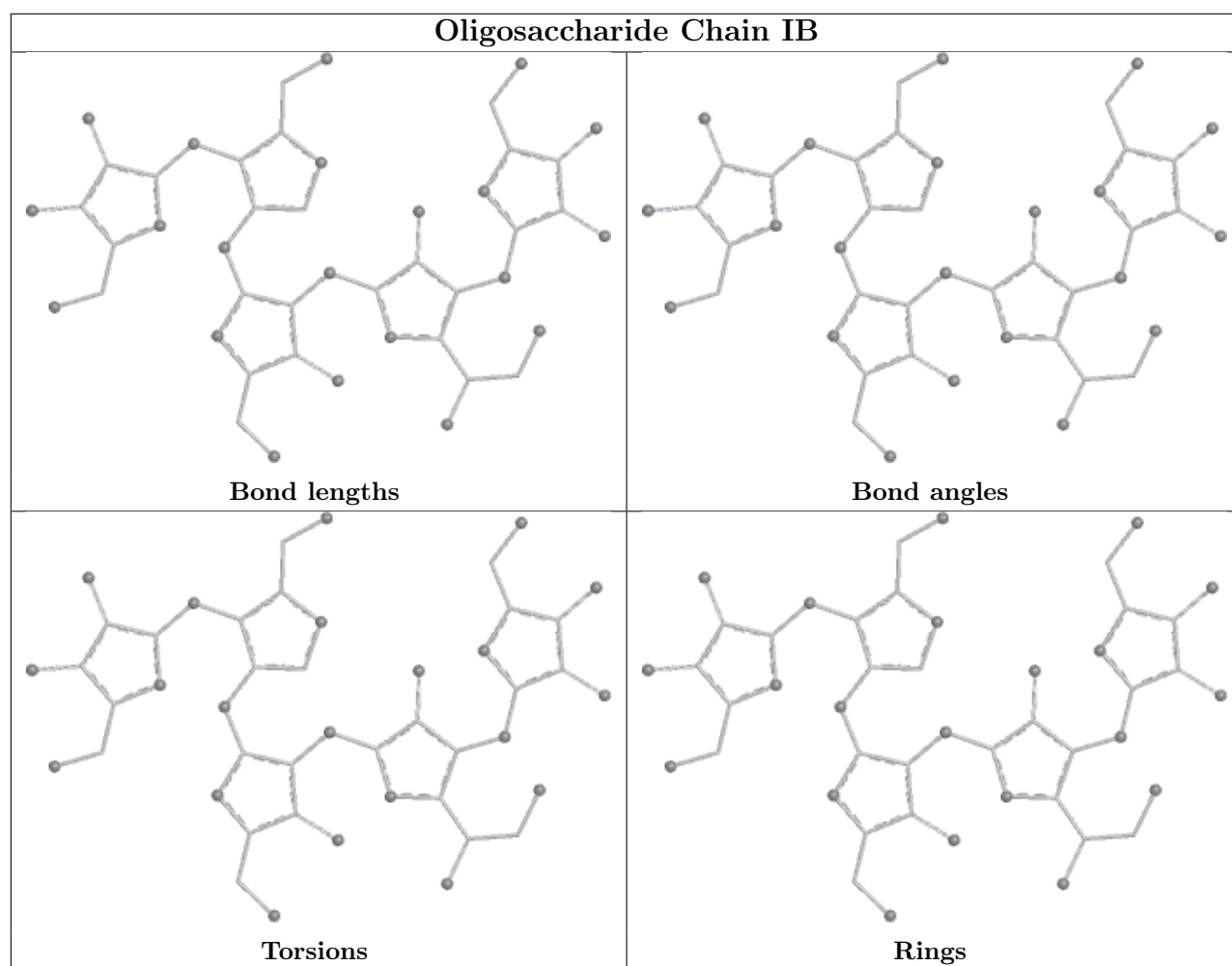


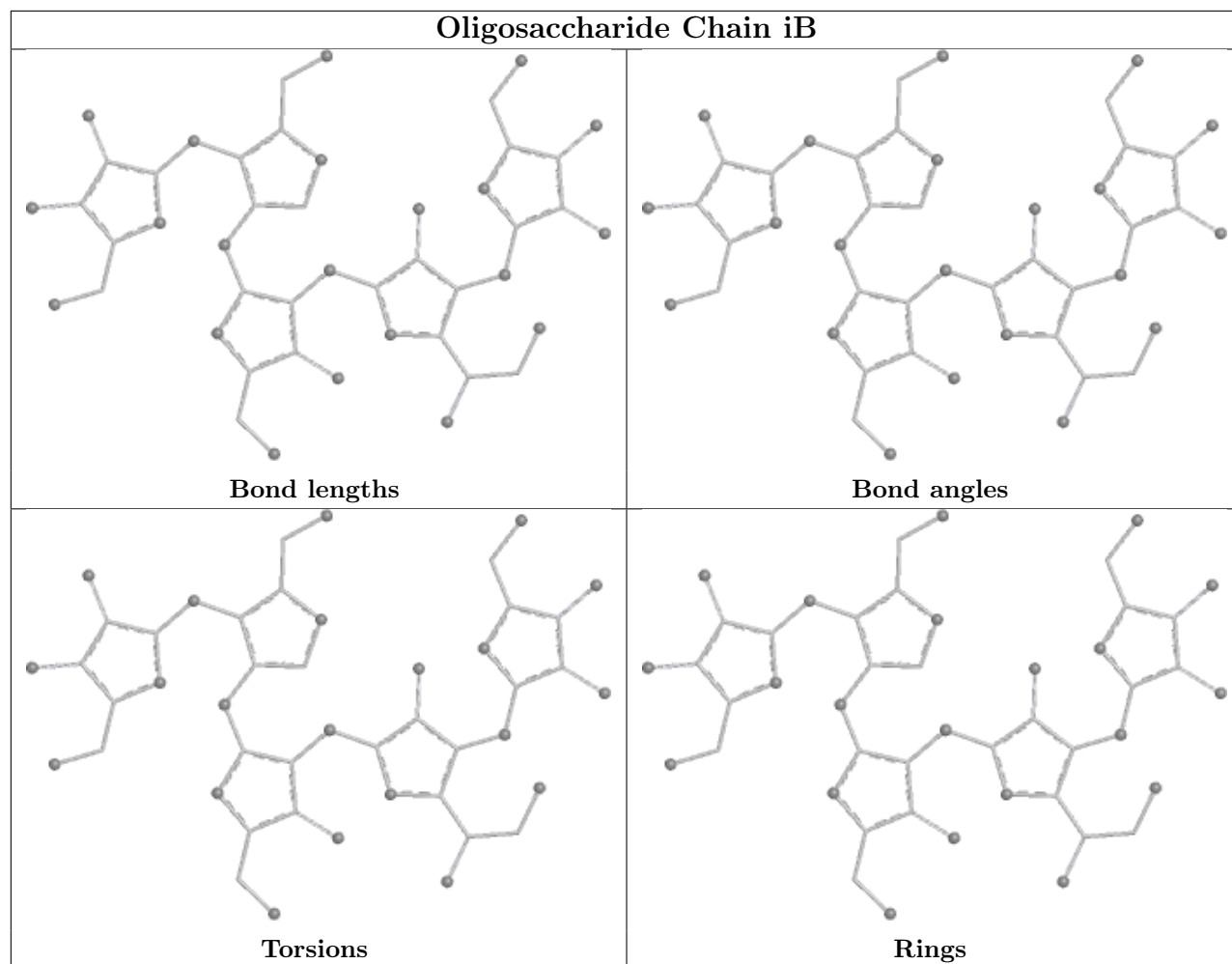


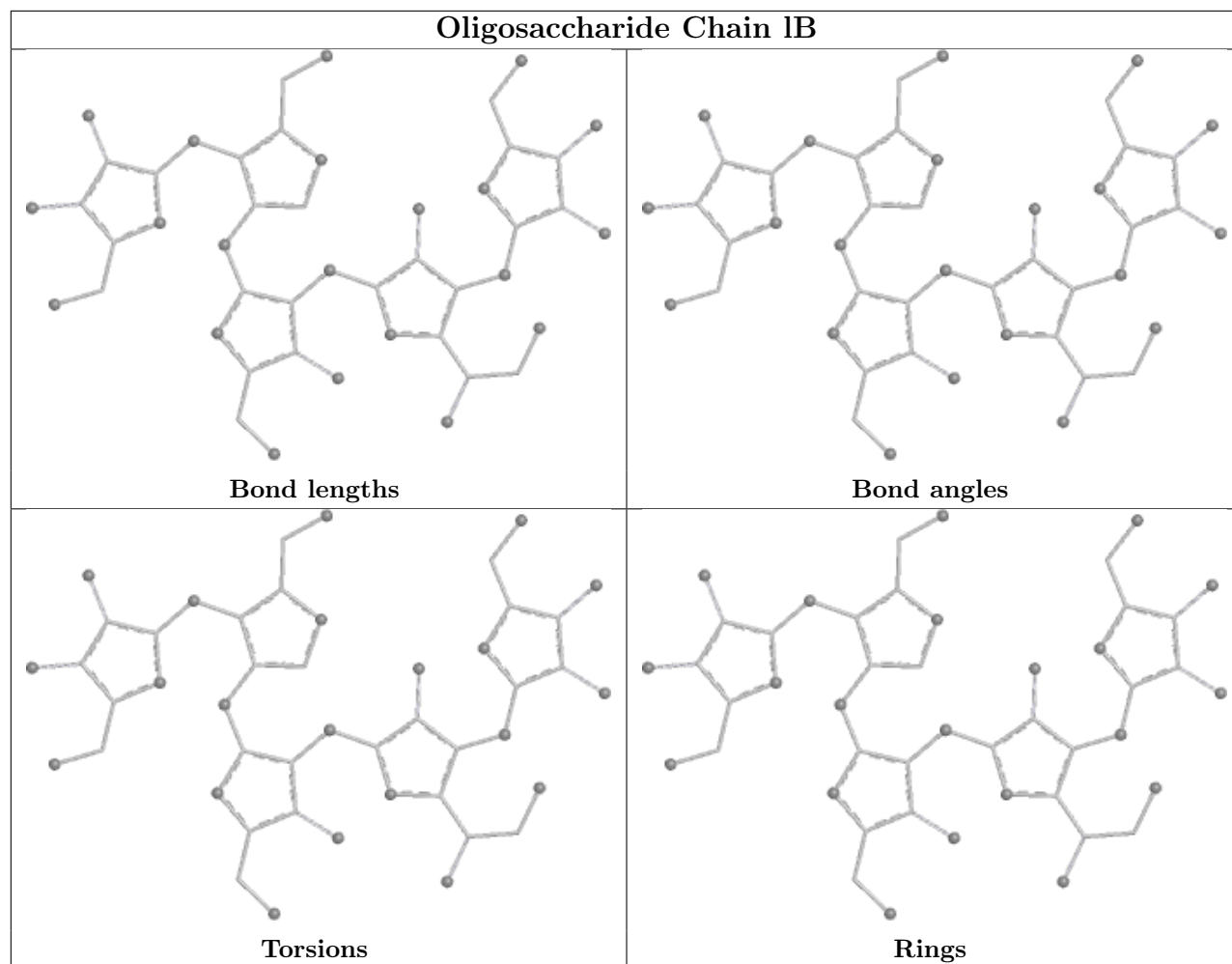


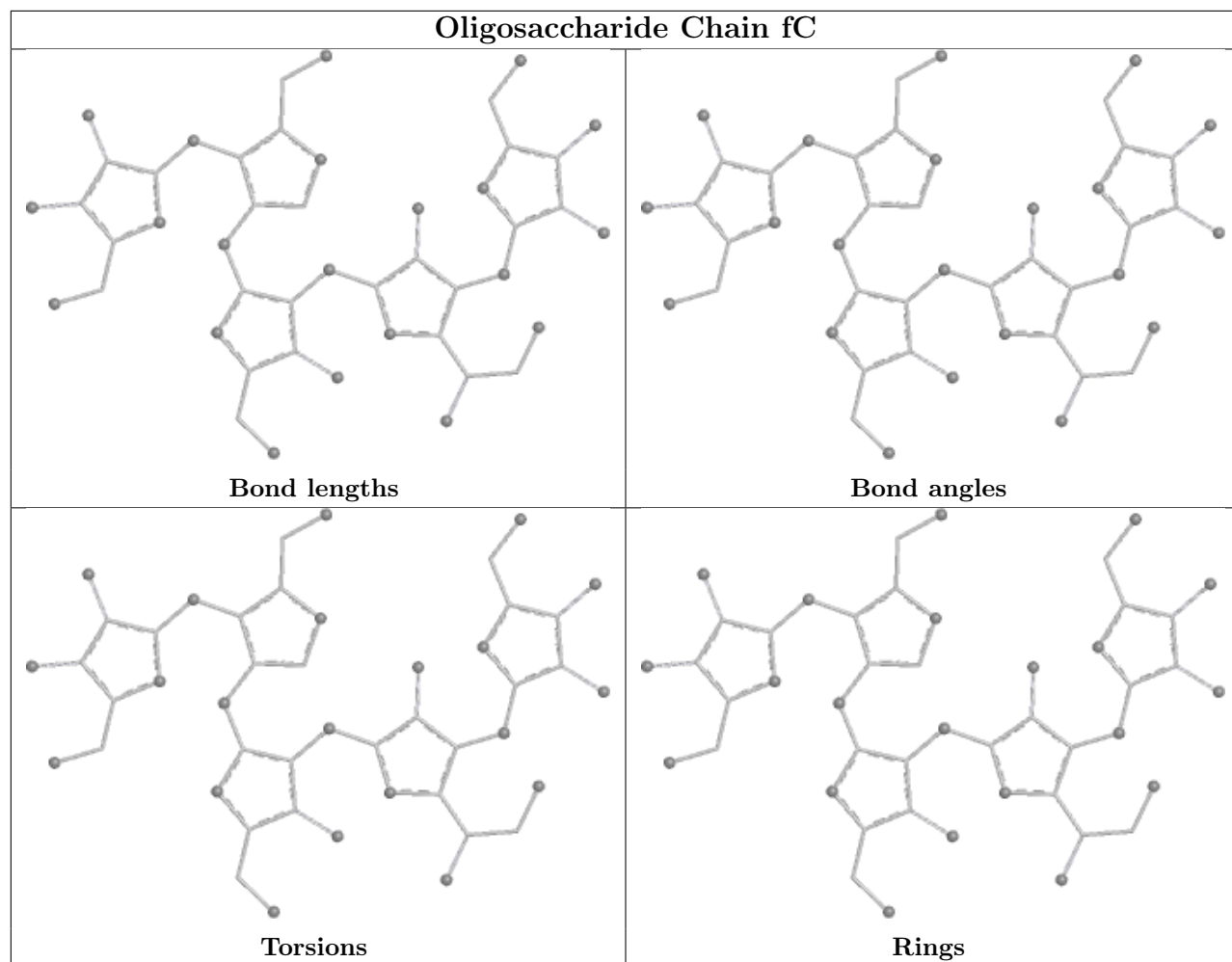


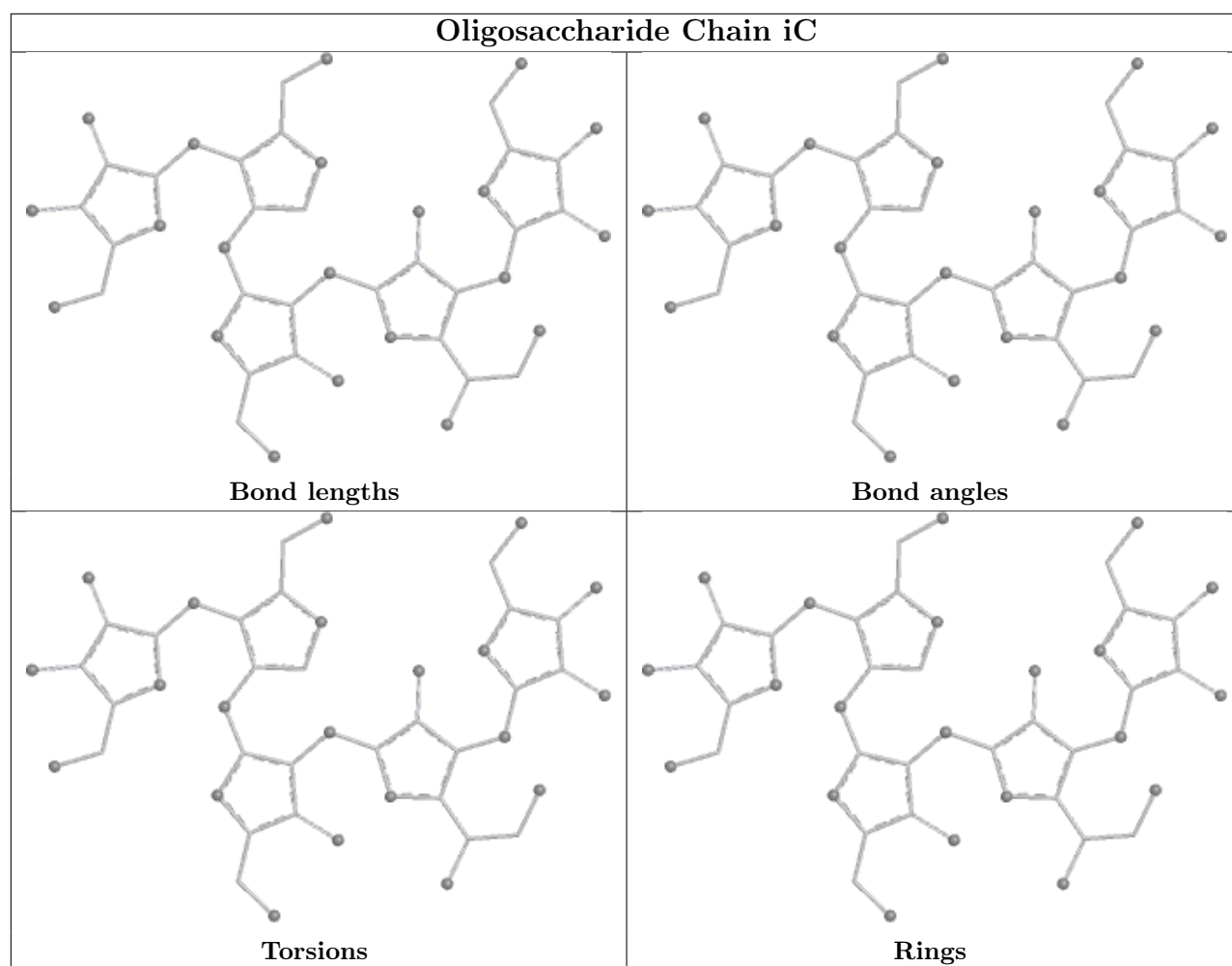


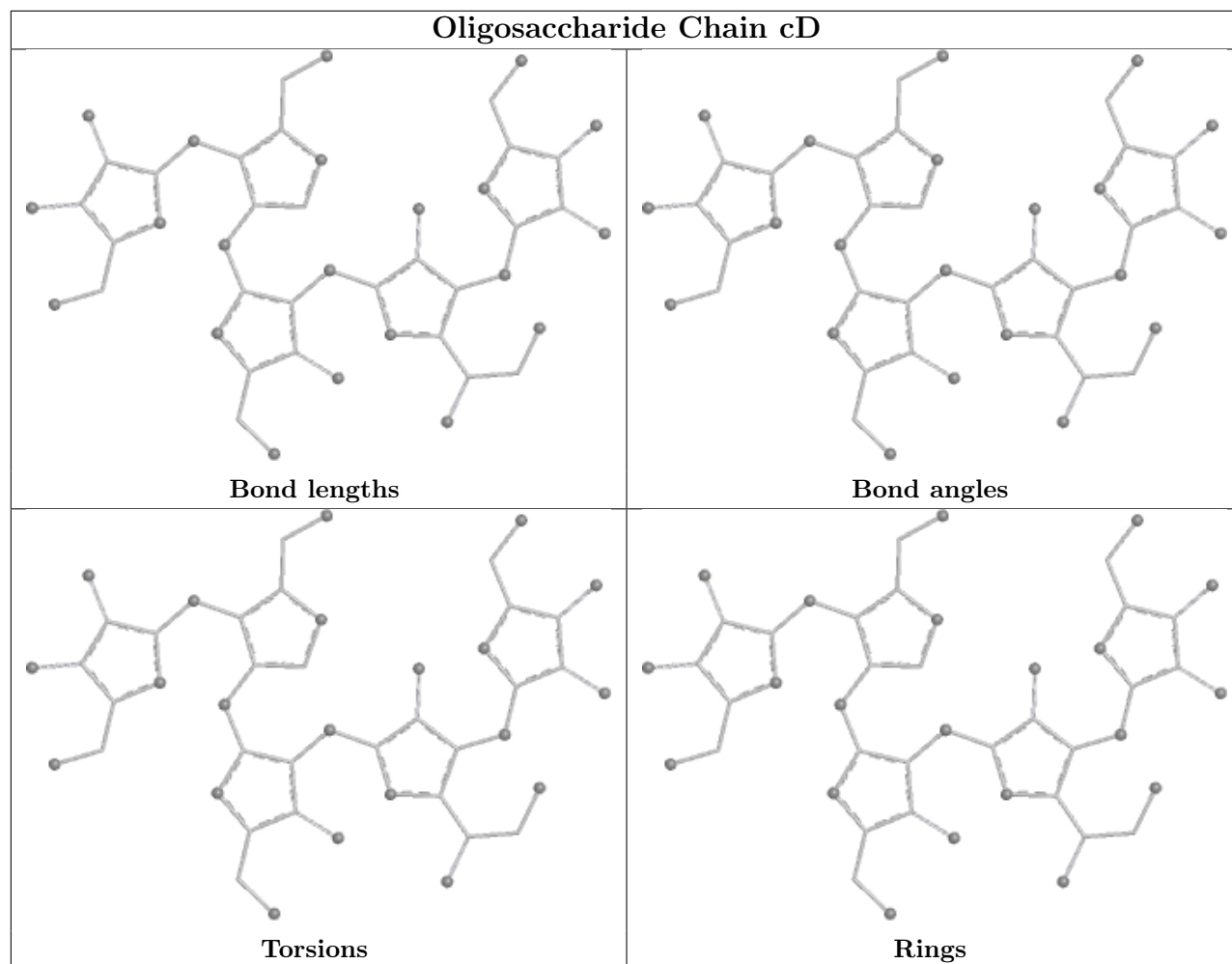


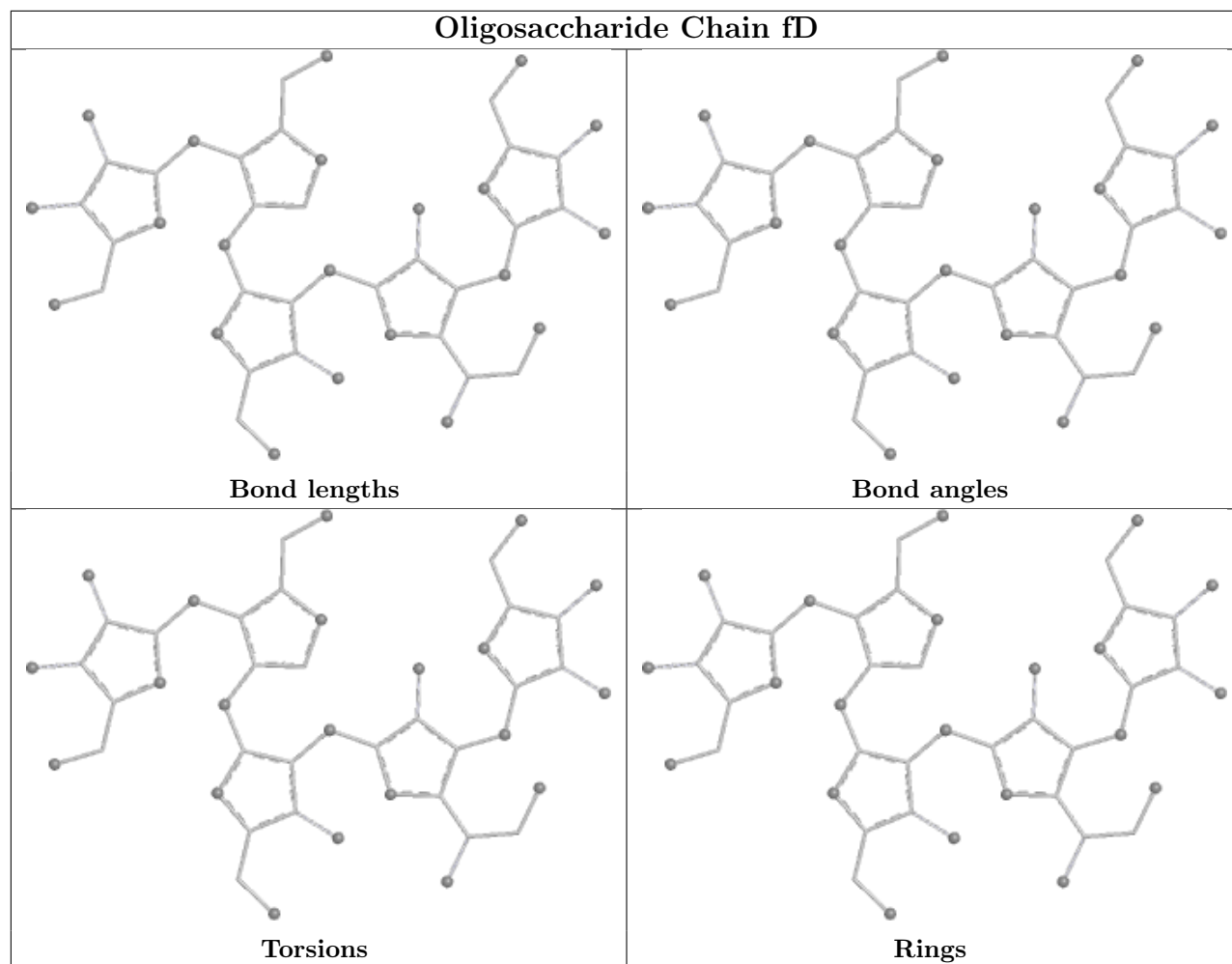


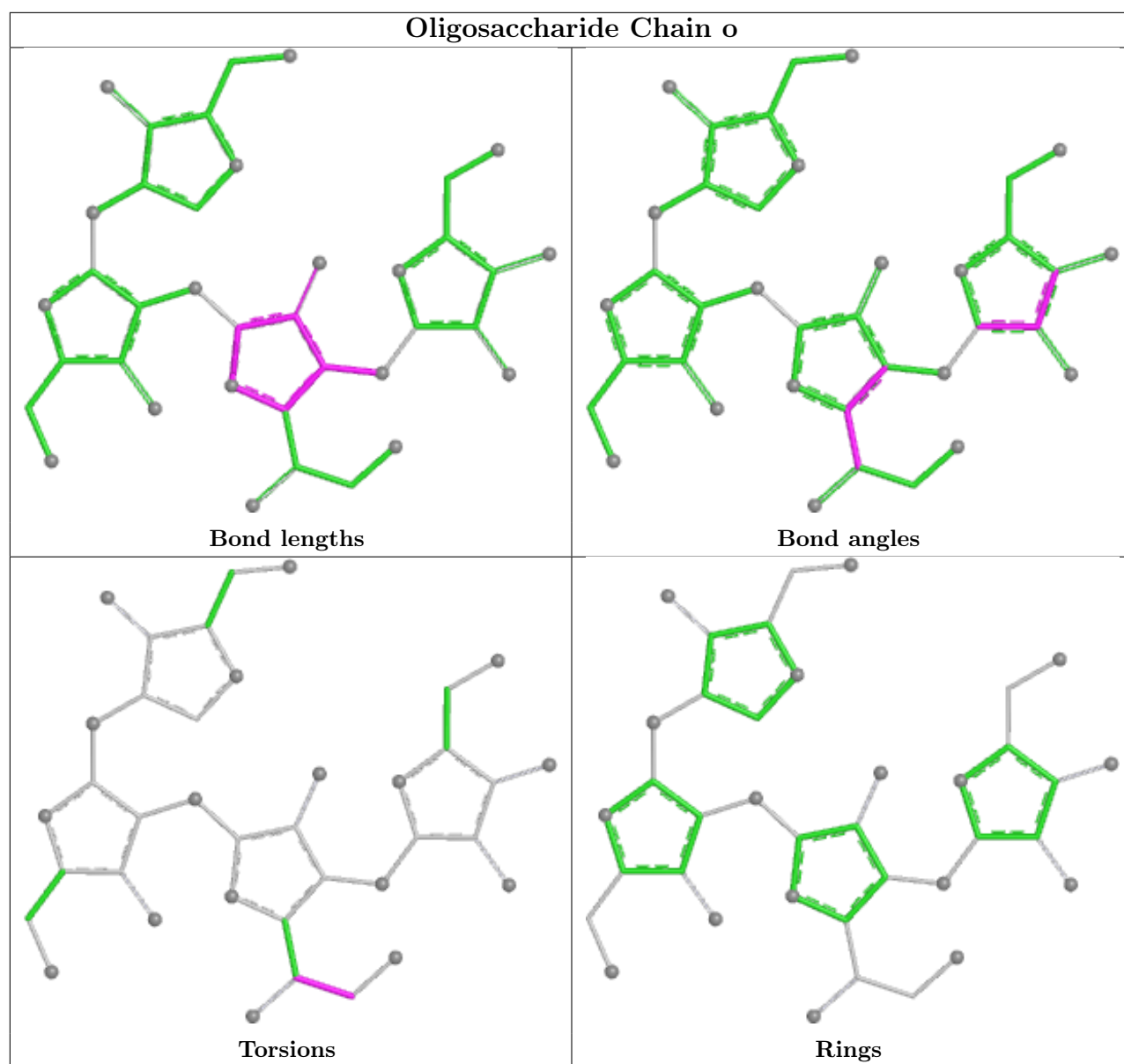


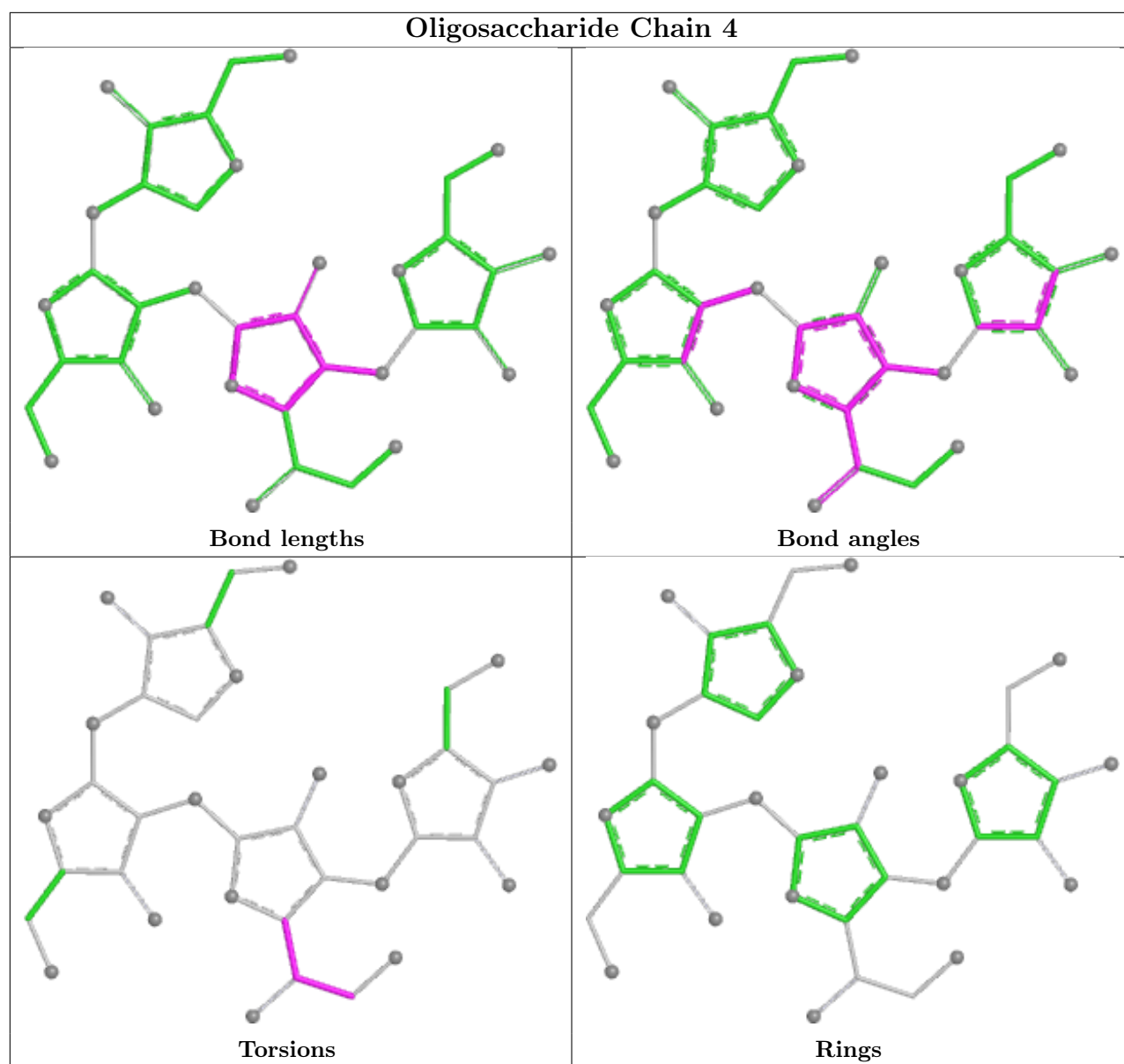


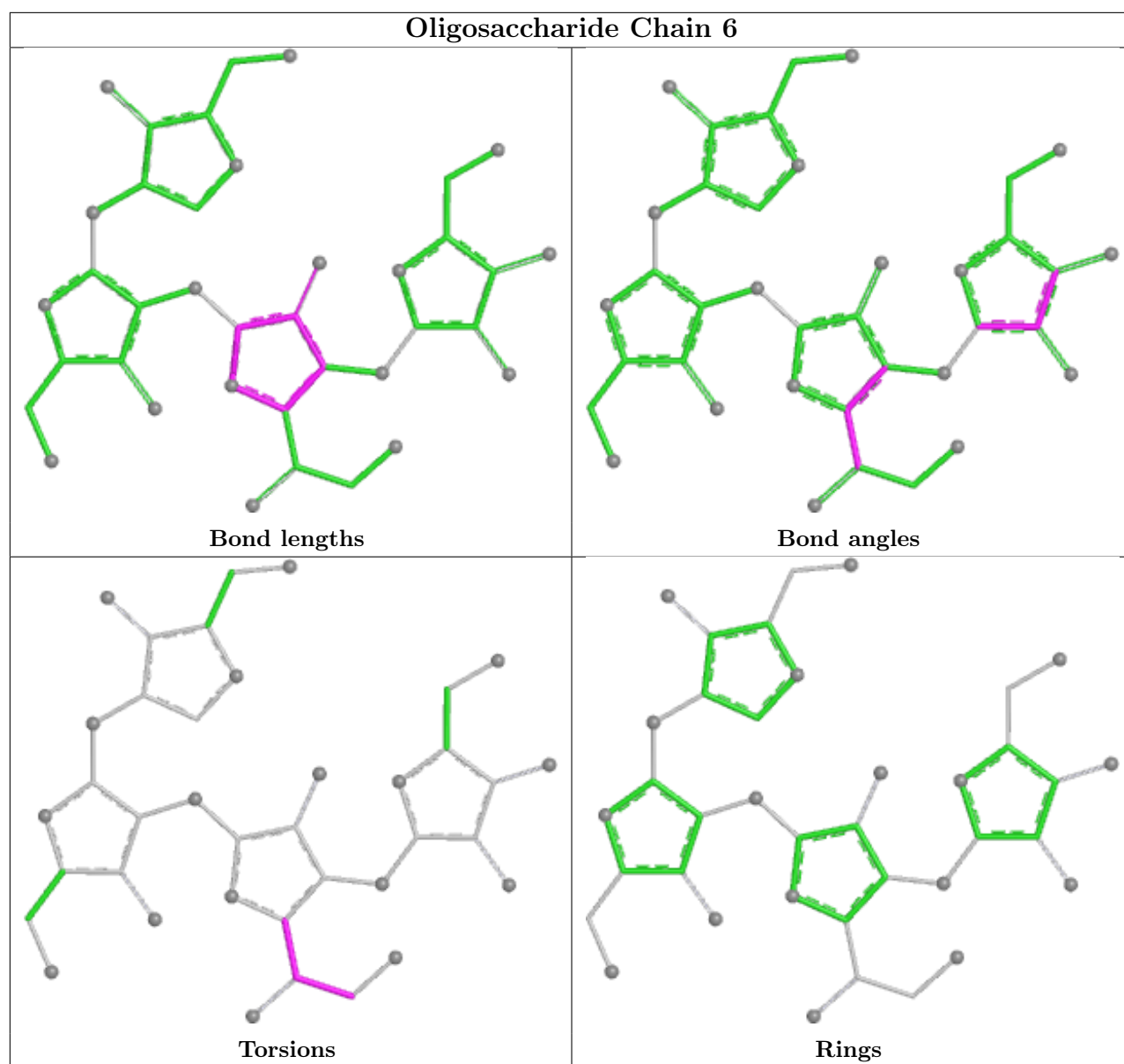


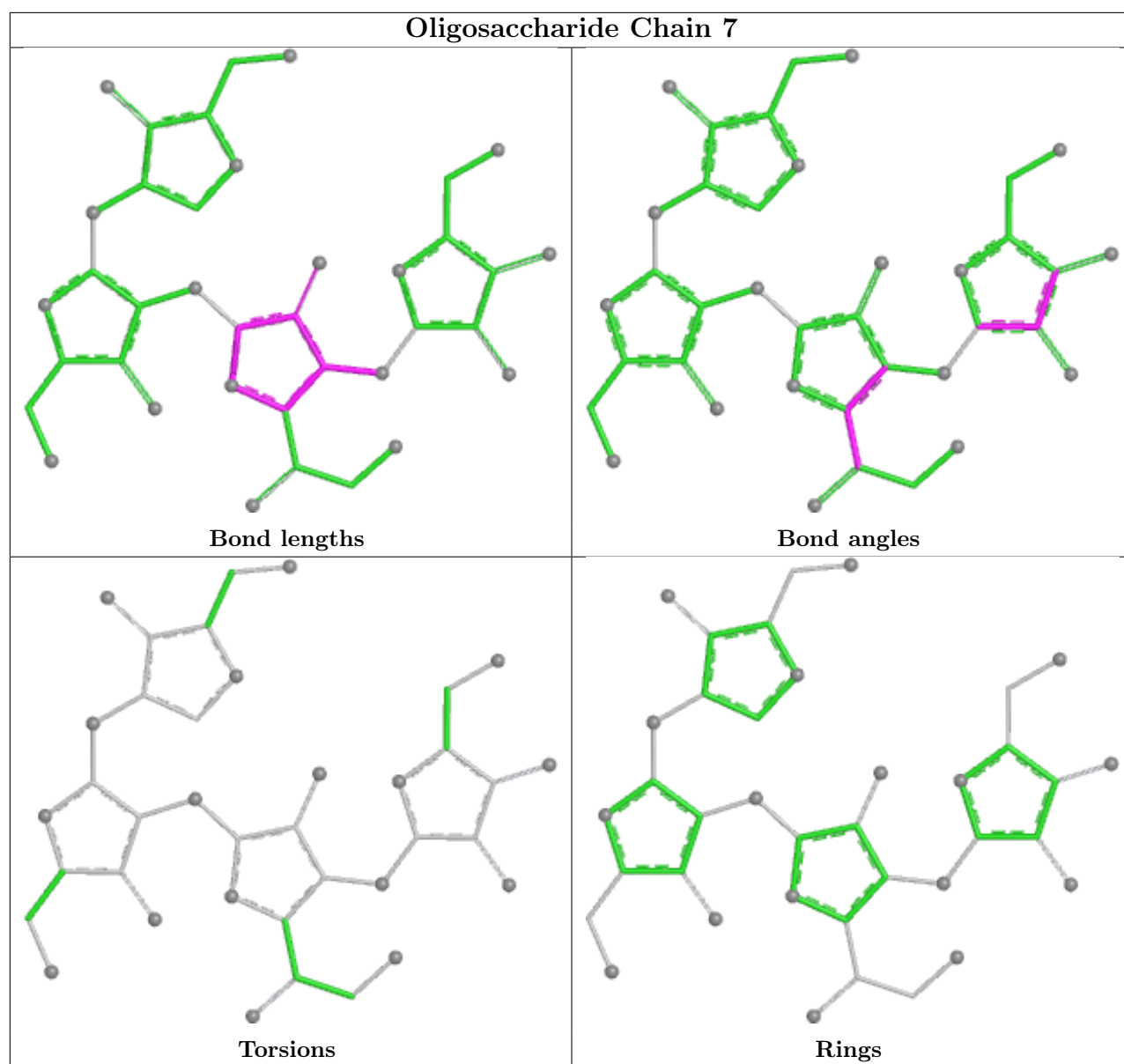


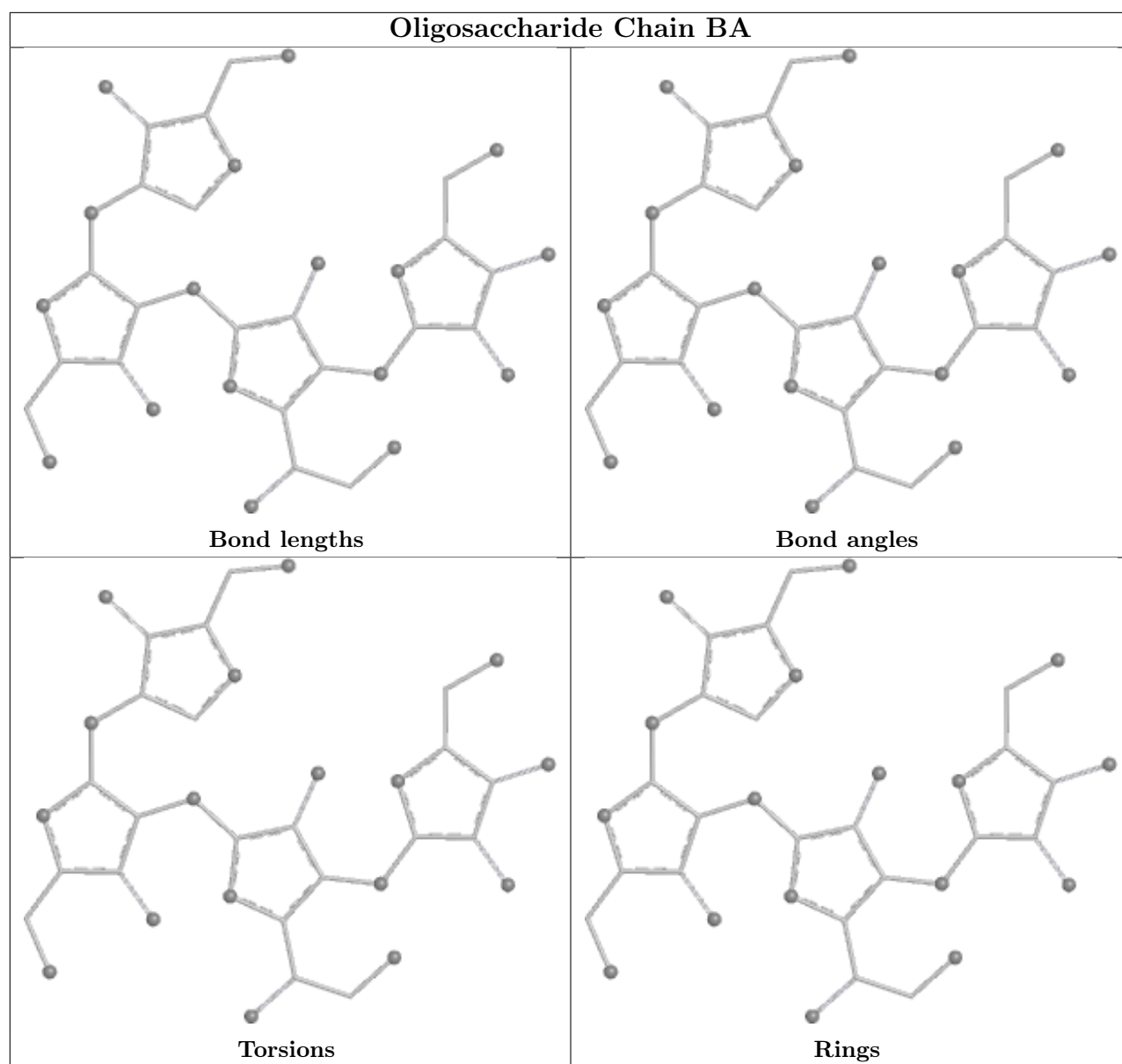


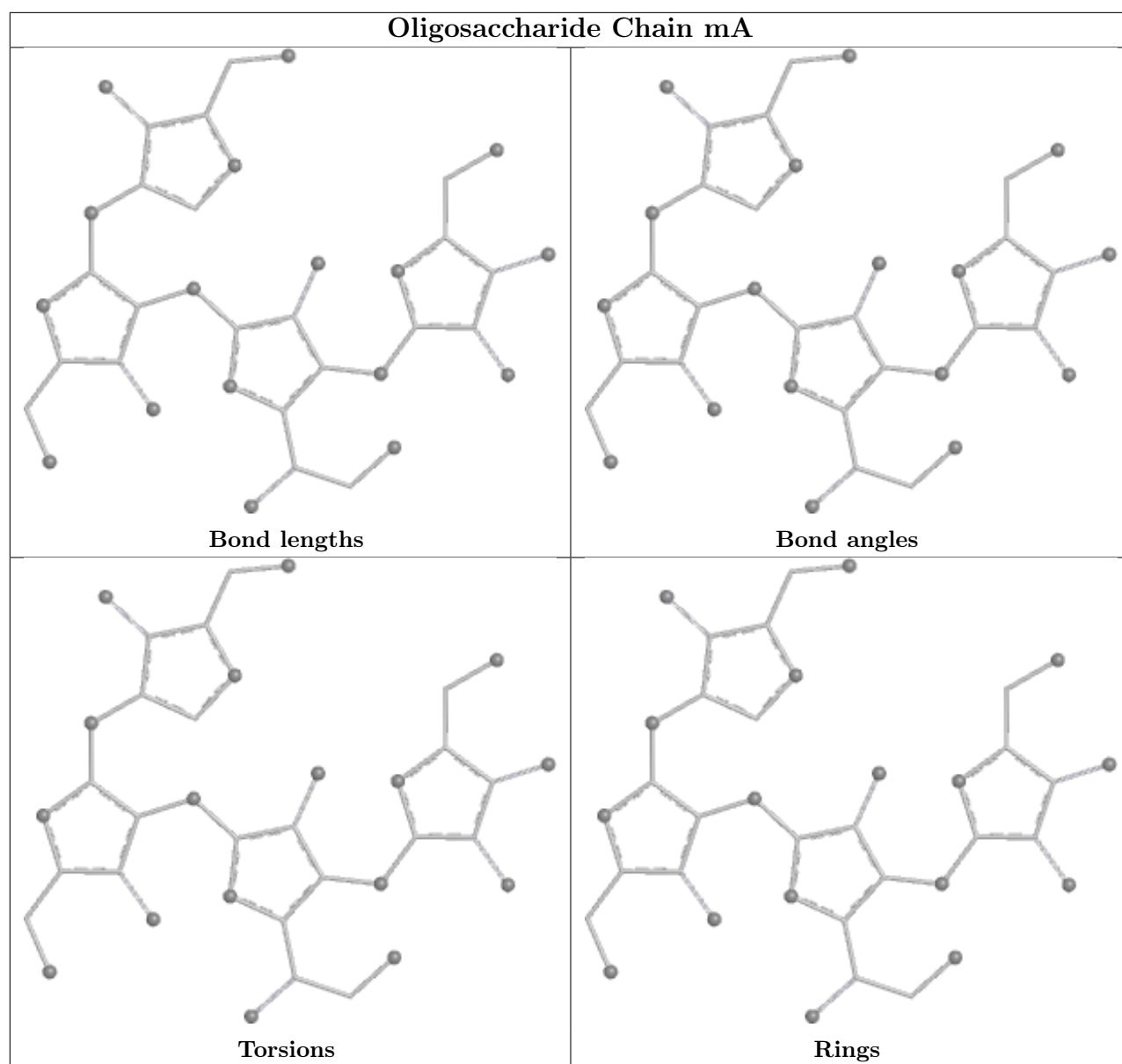


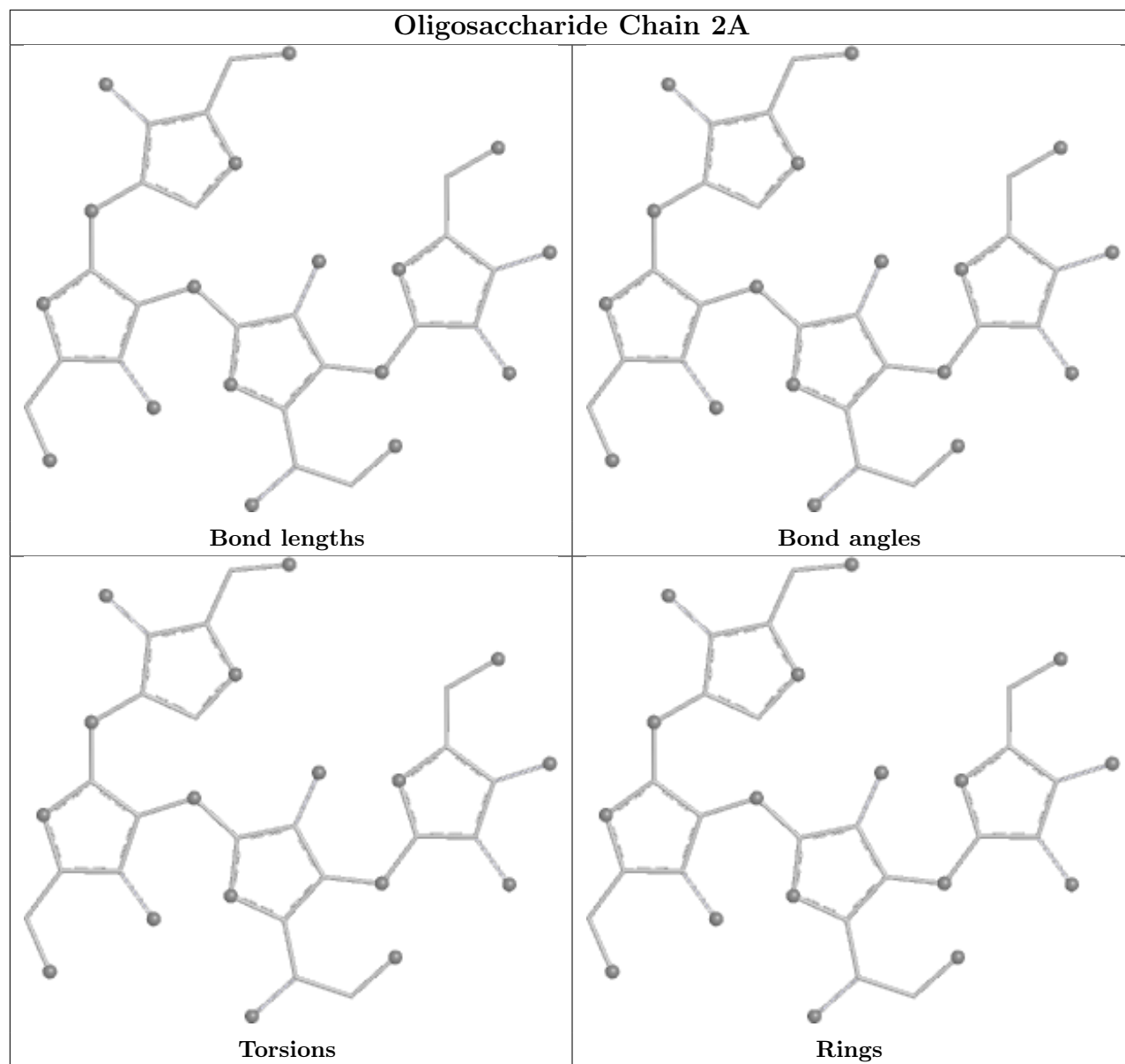


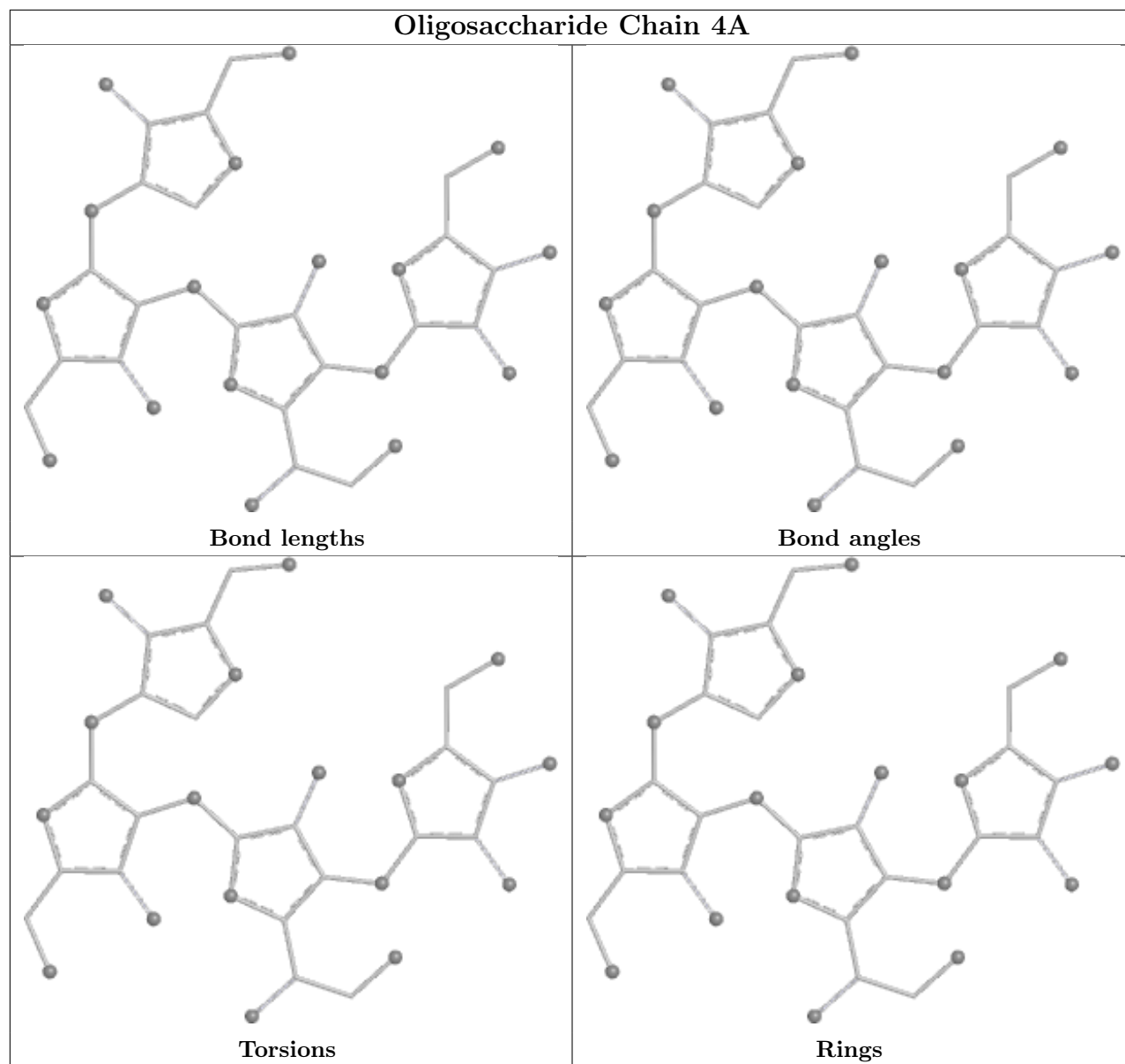


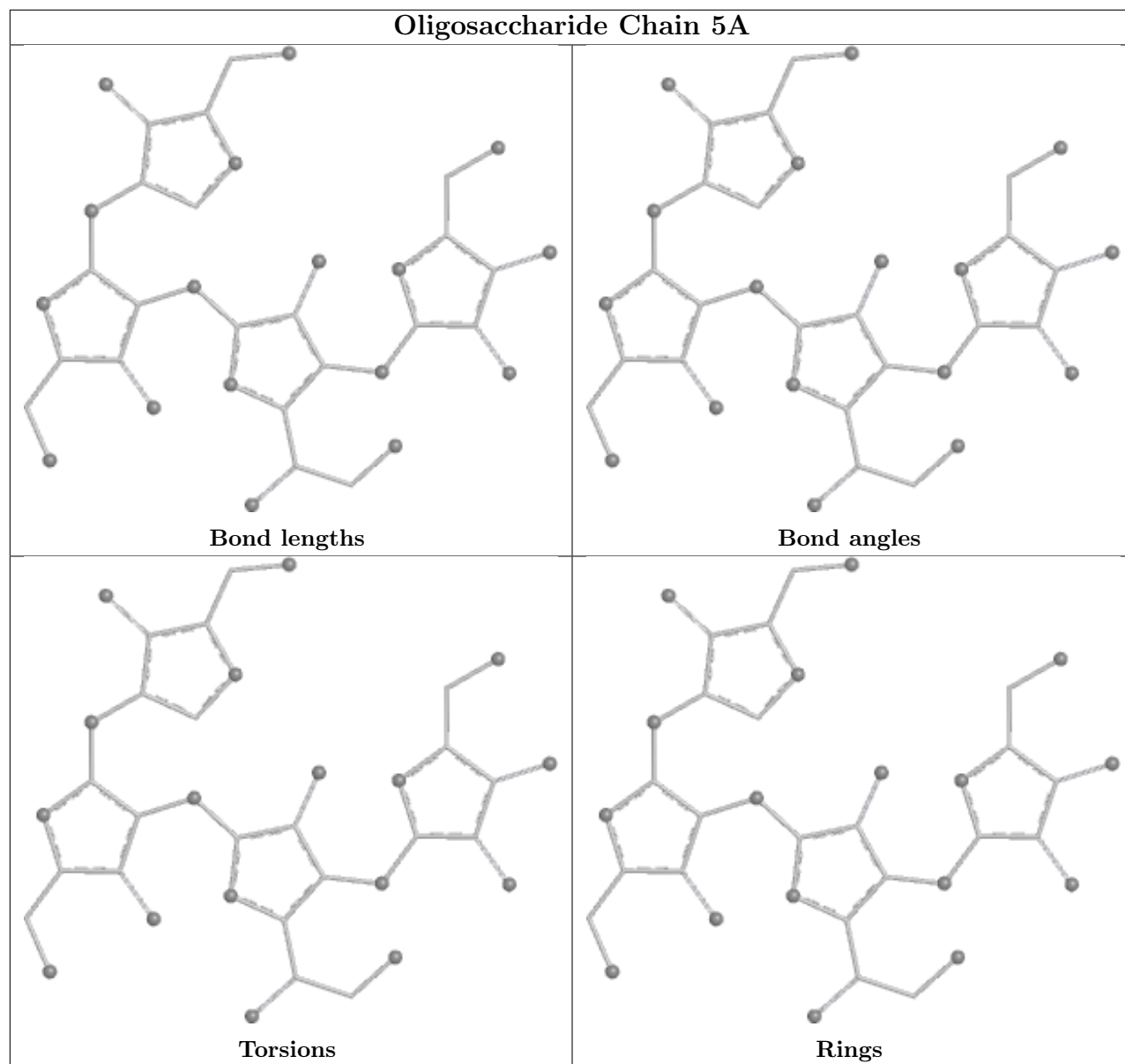


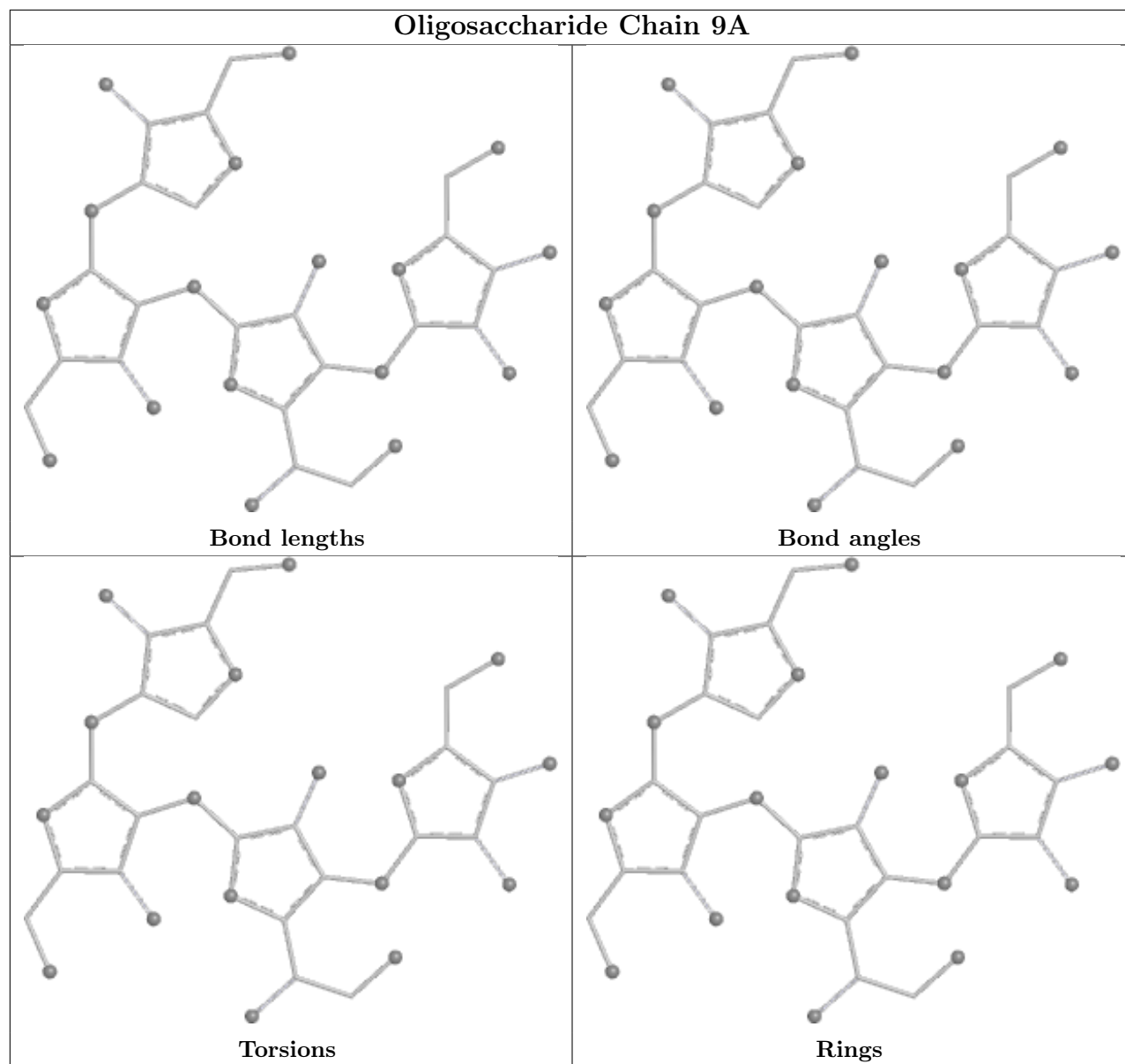


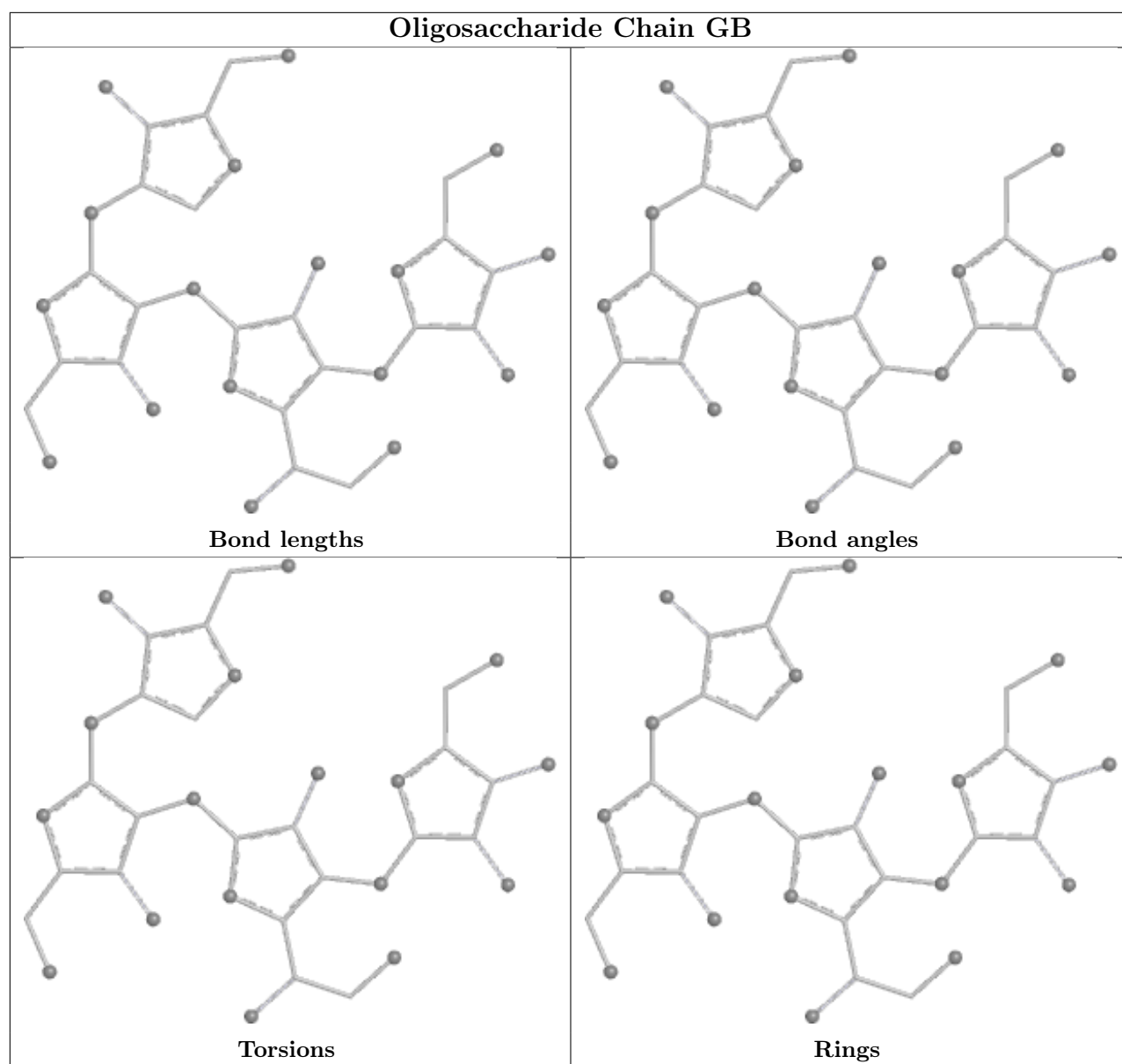


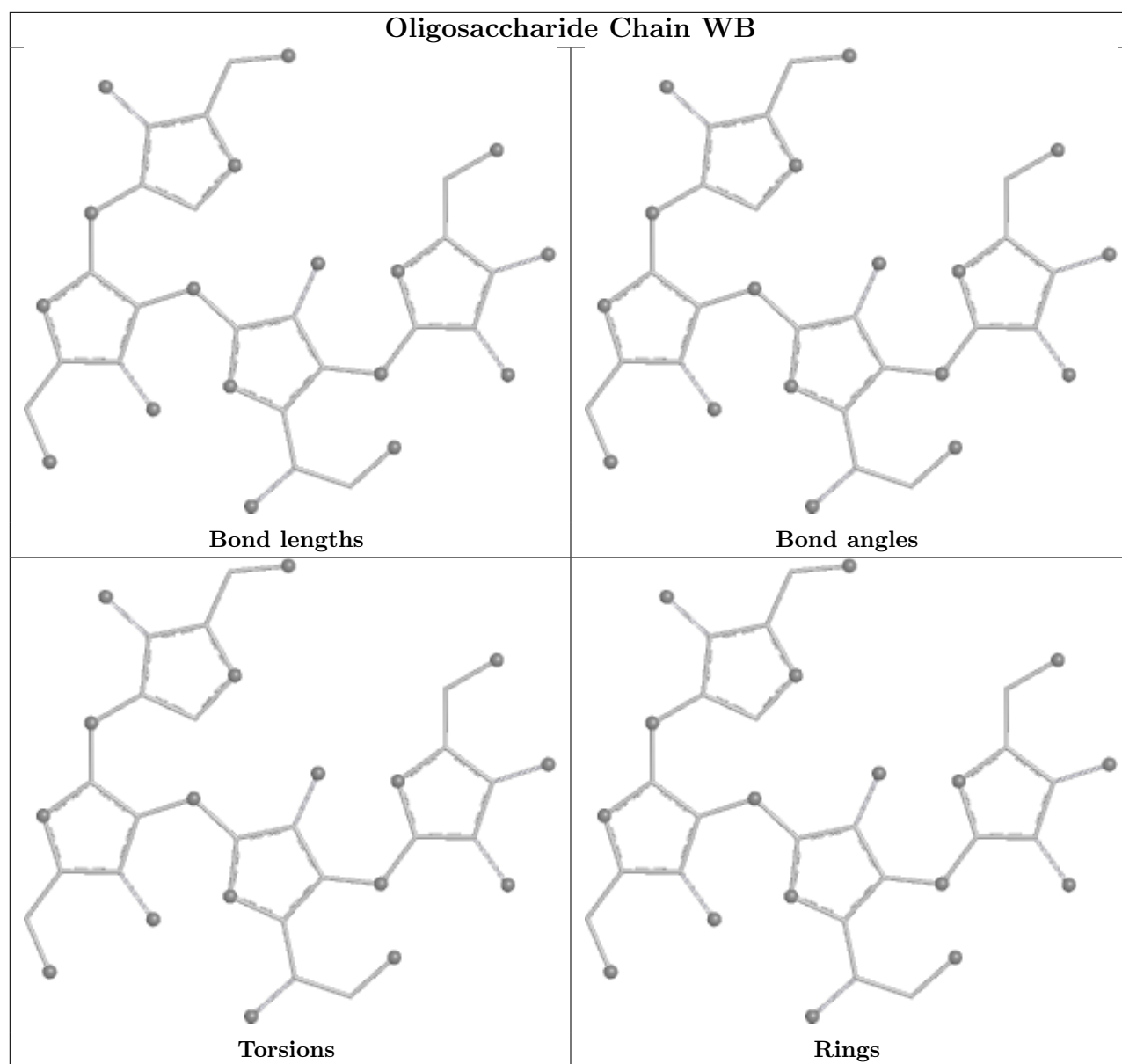


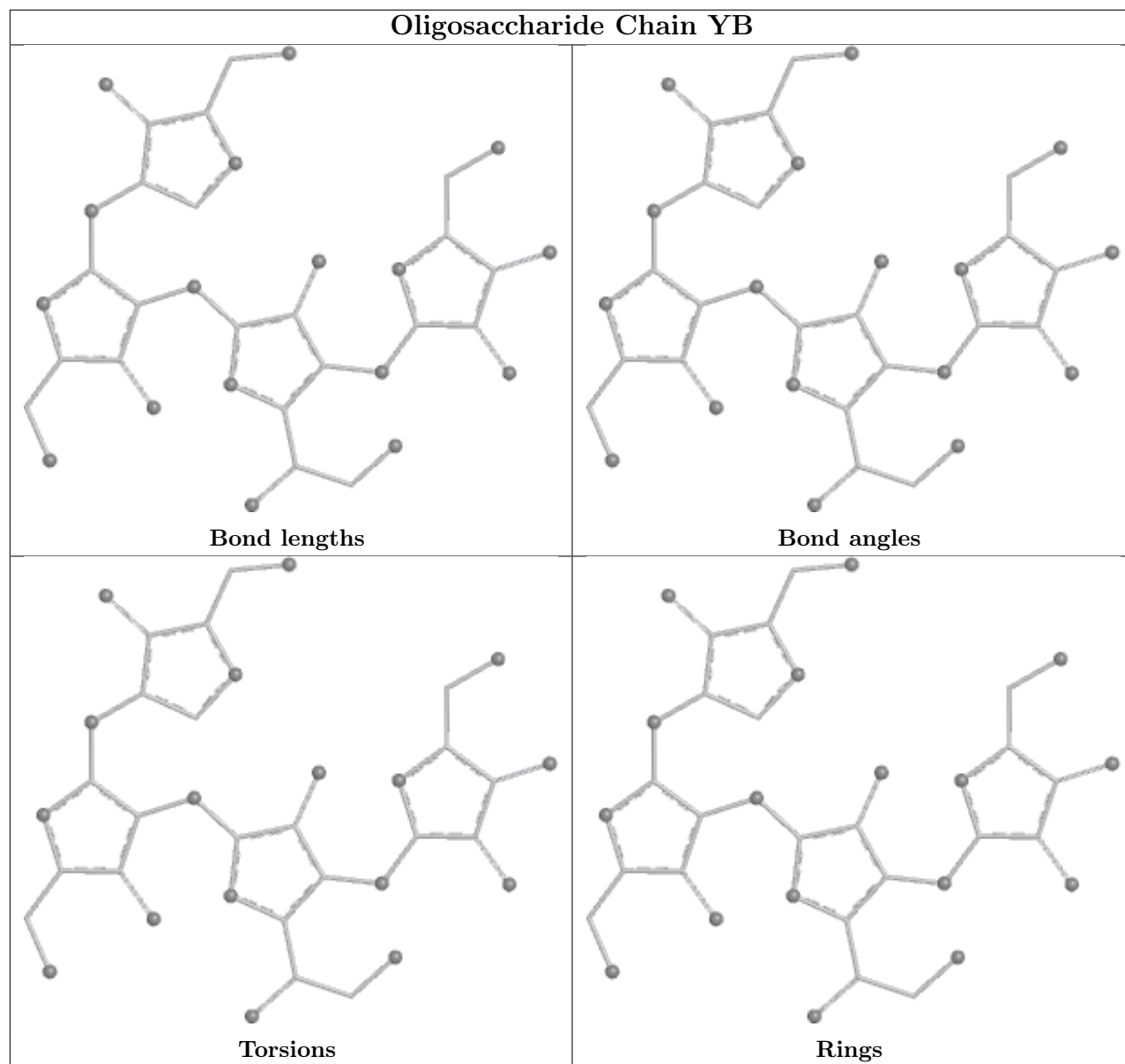


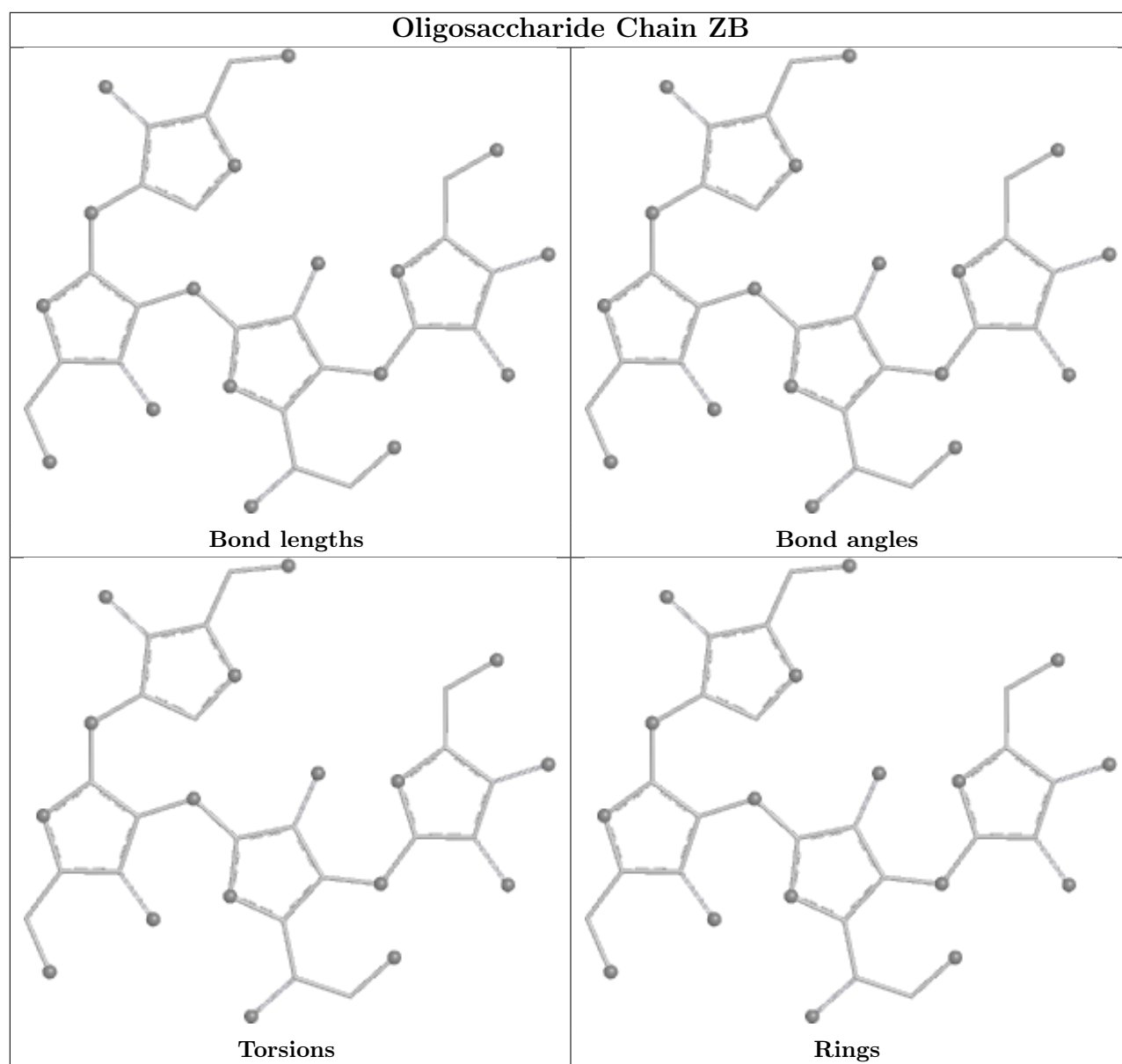


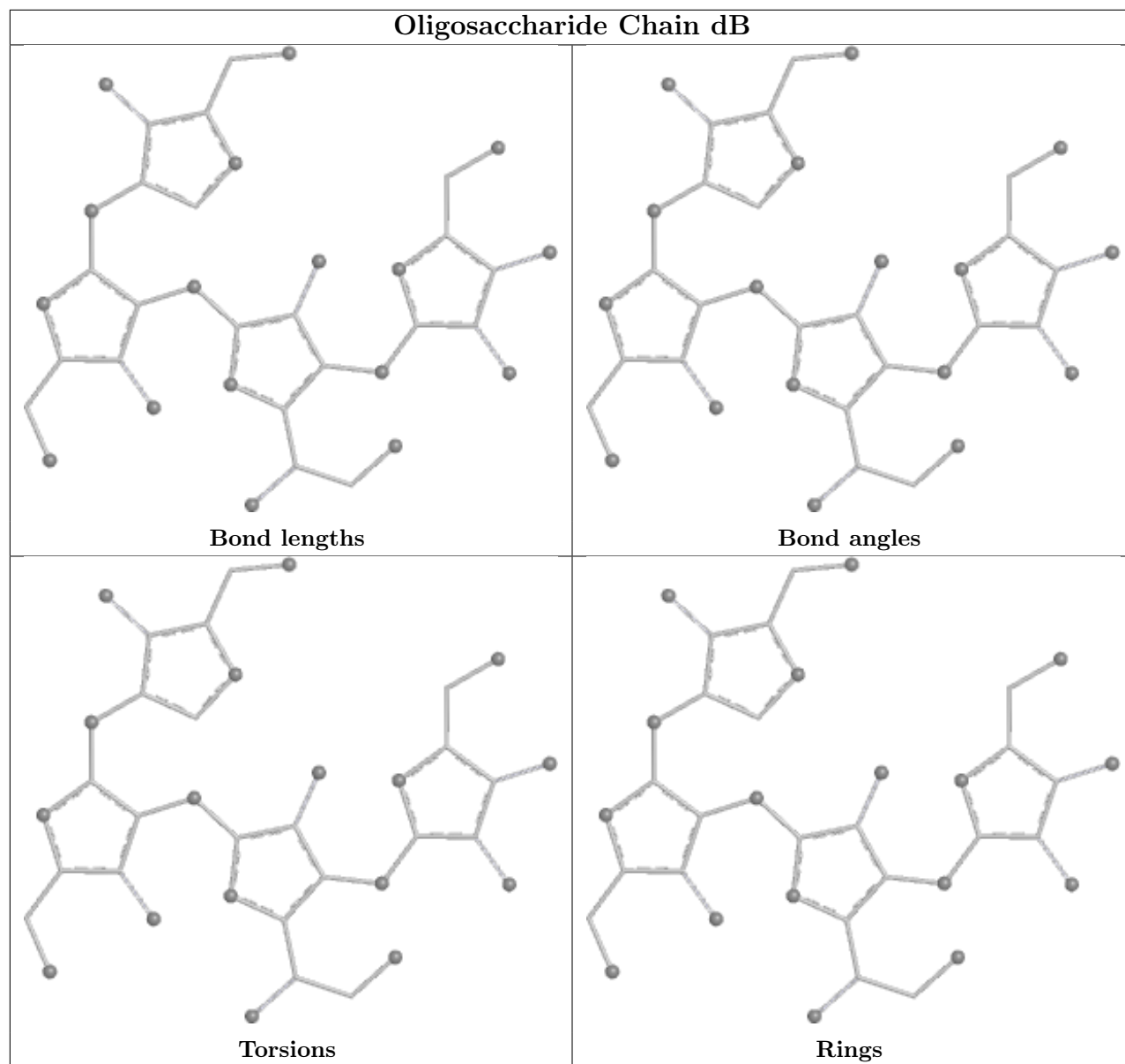


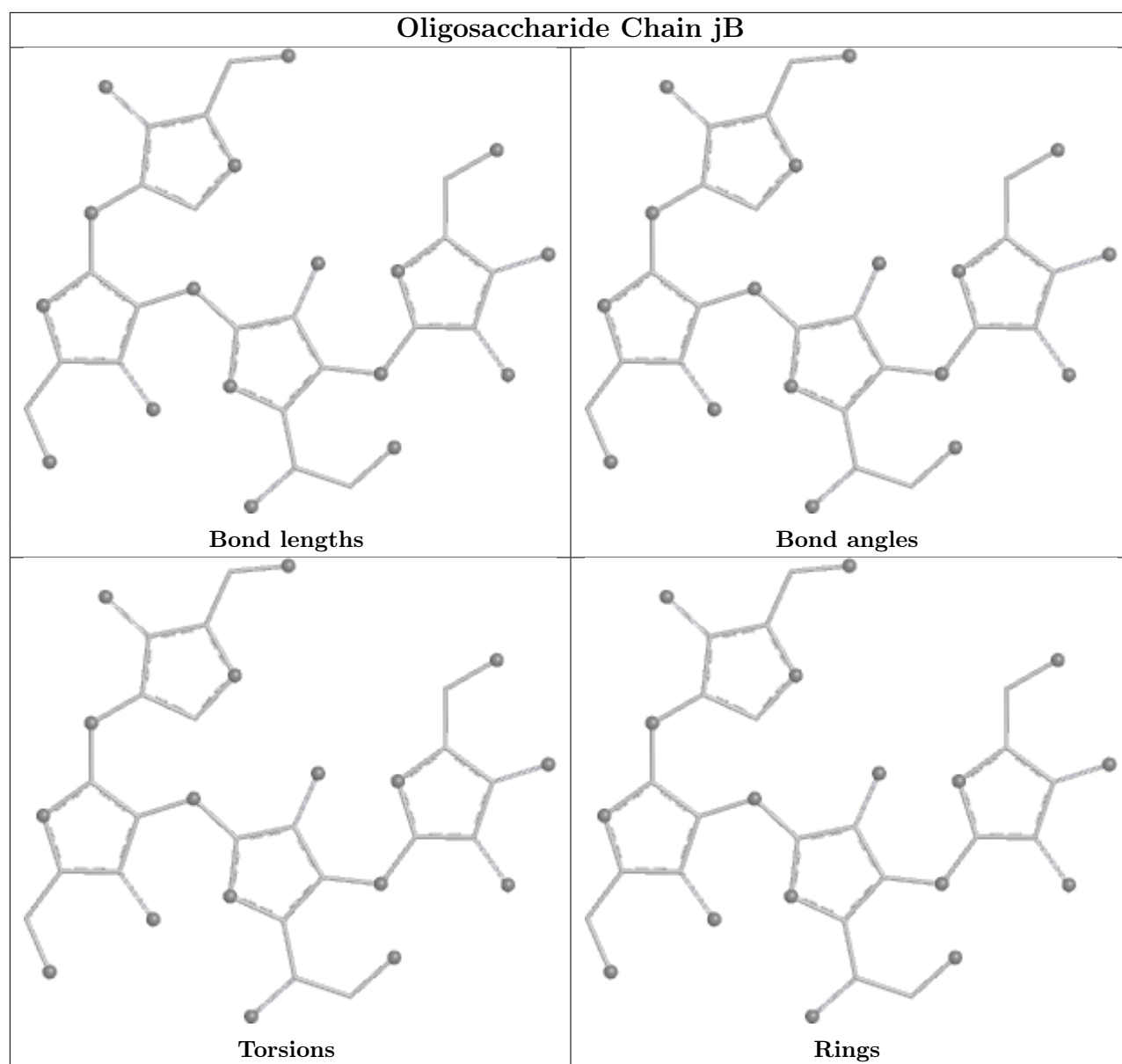


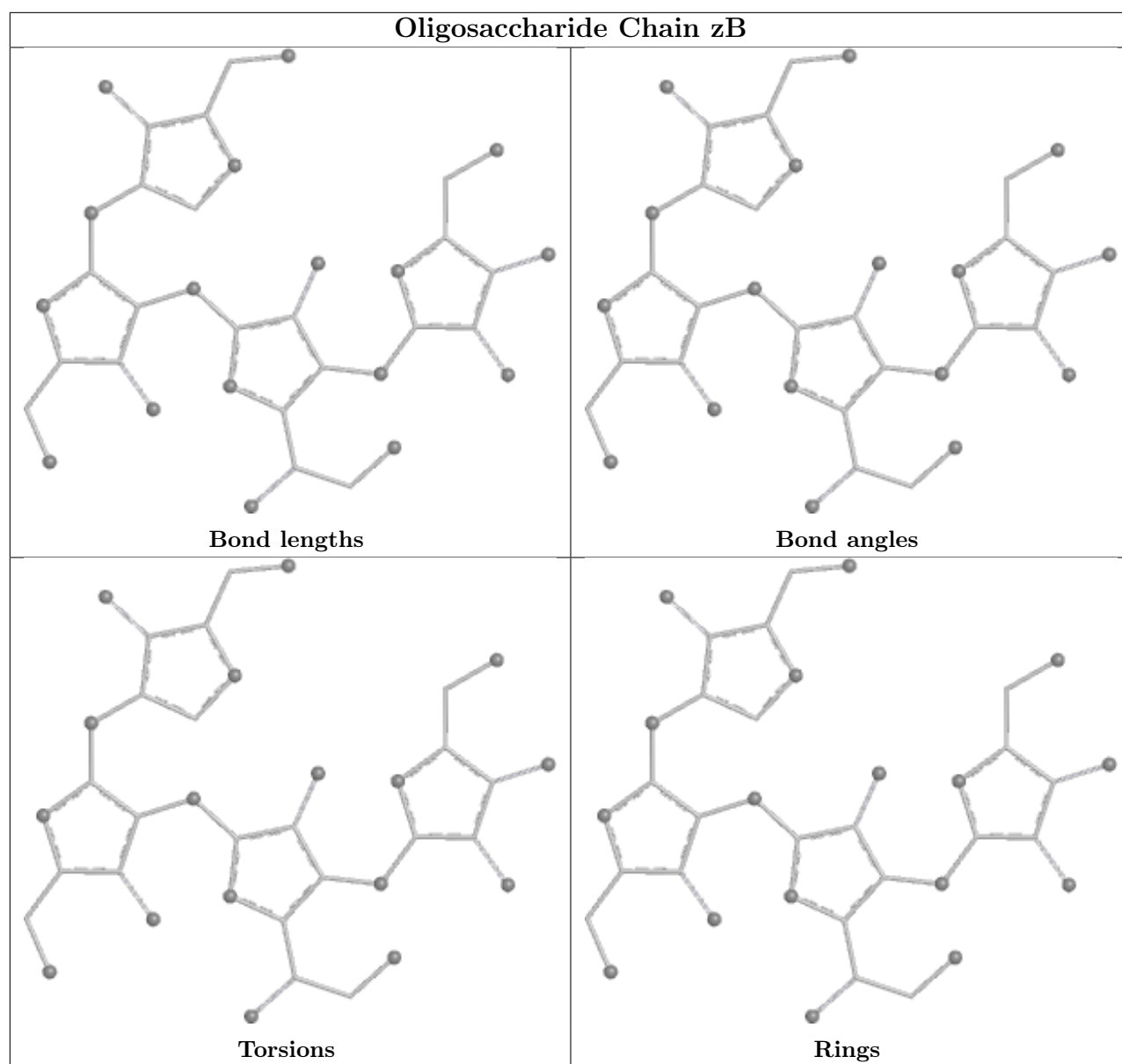


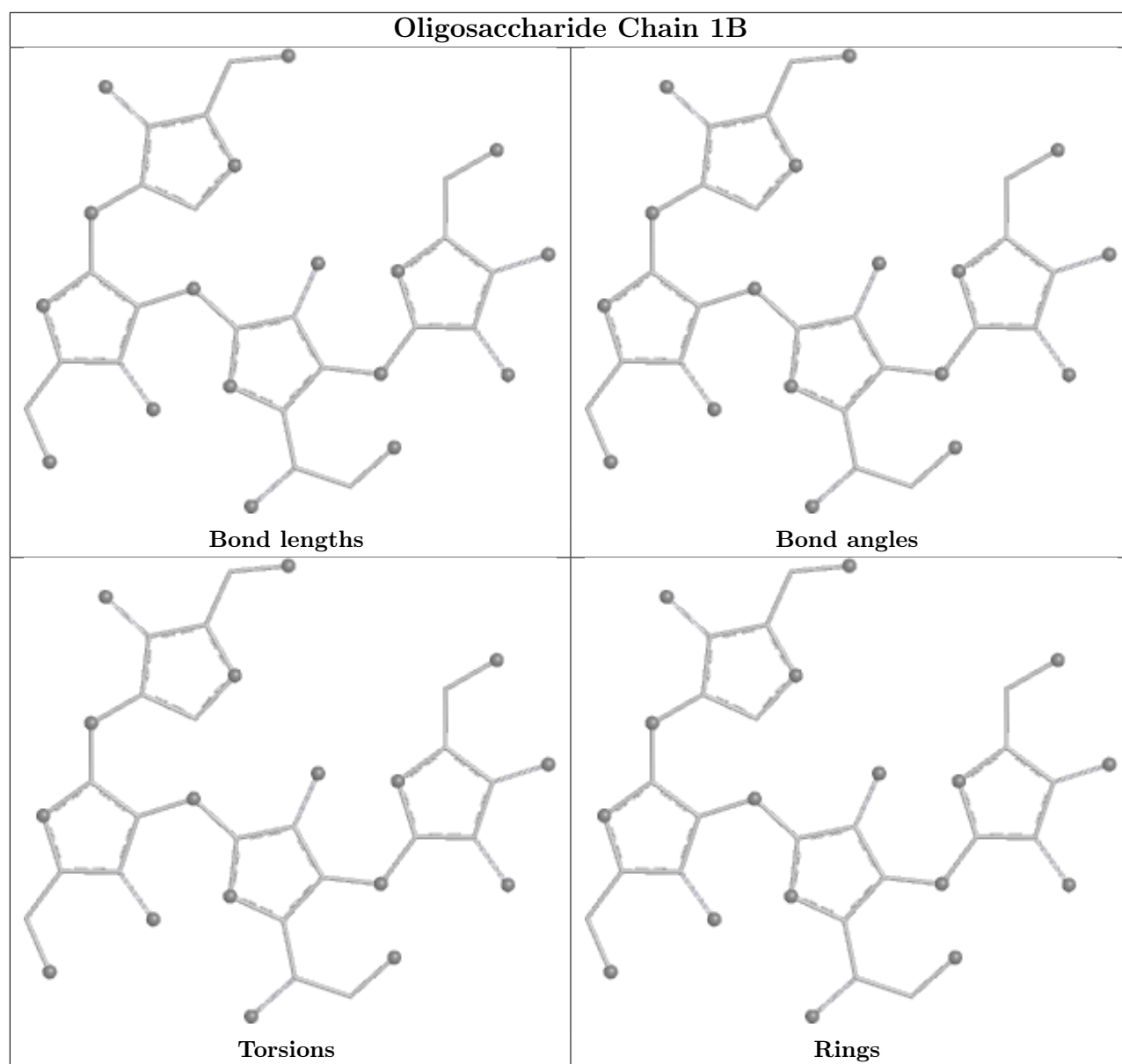
Oligosaccharide Chain YB

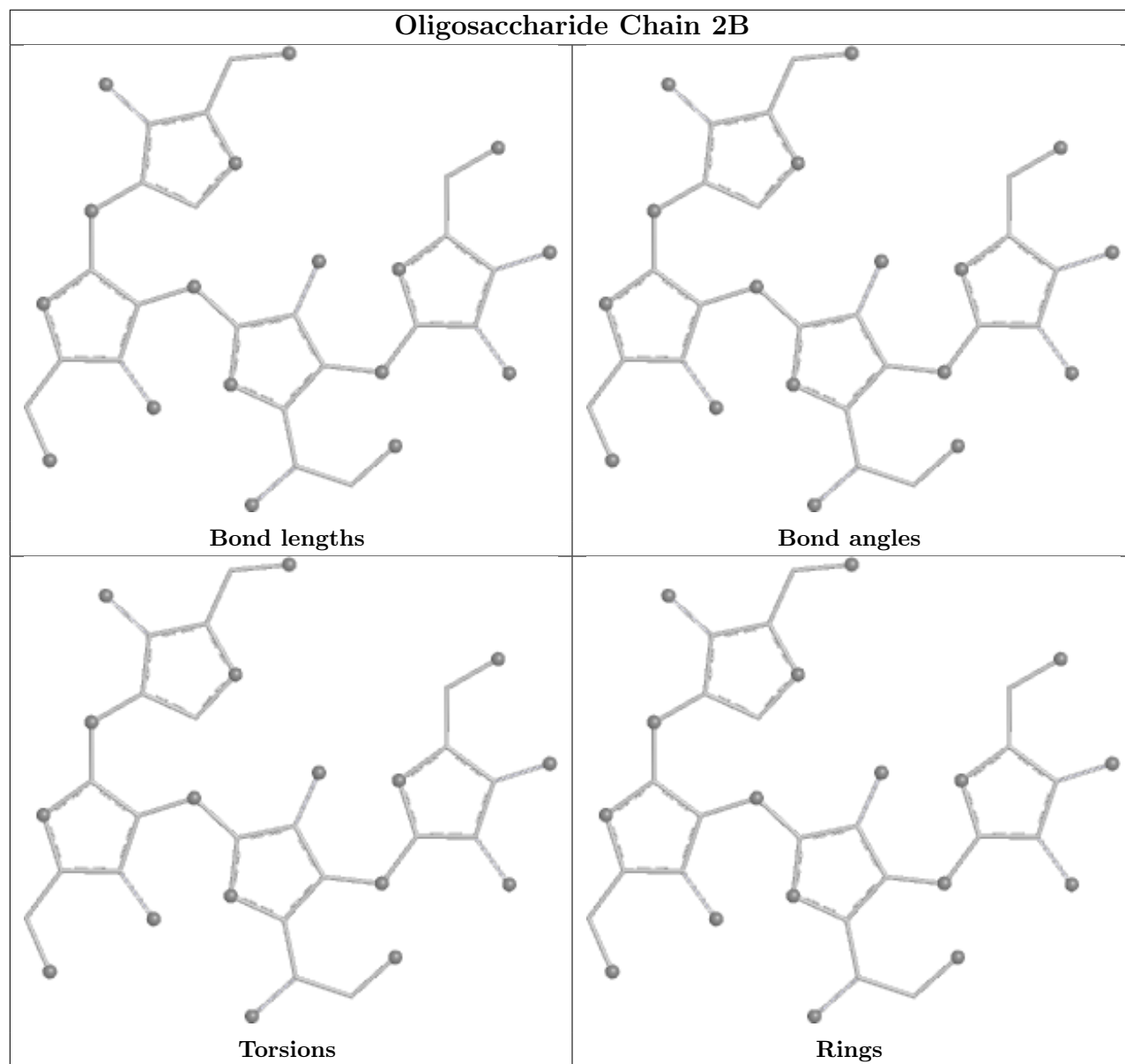


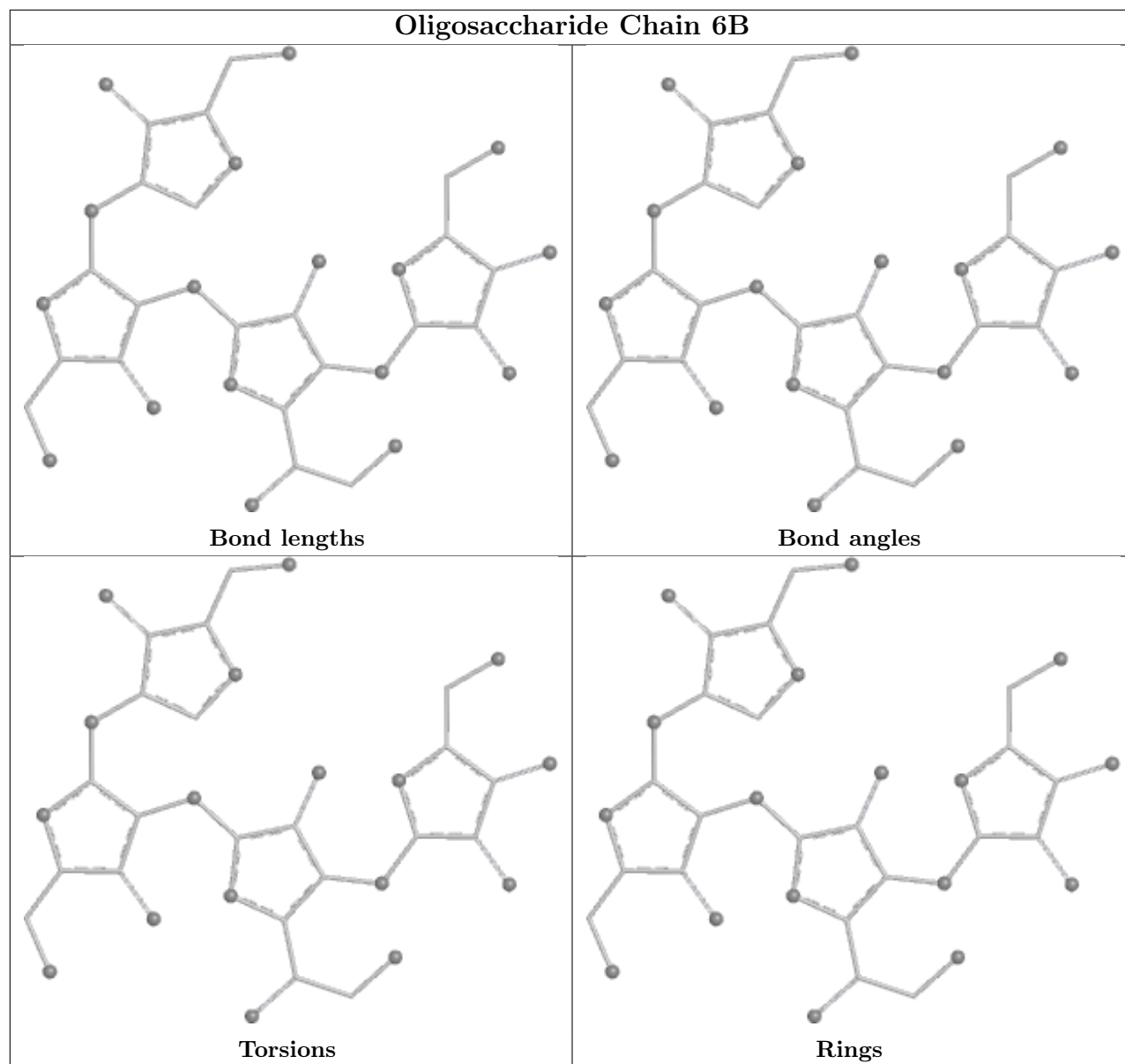


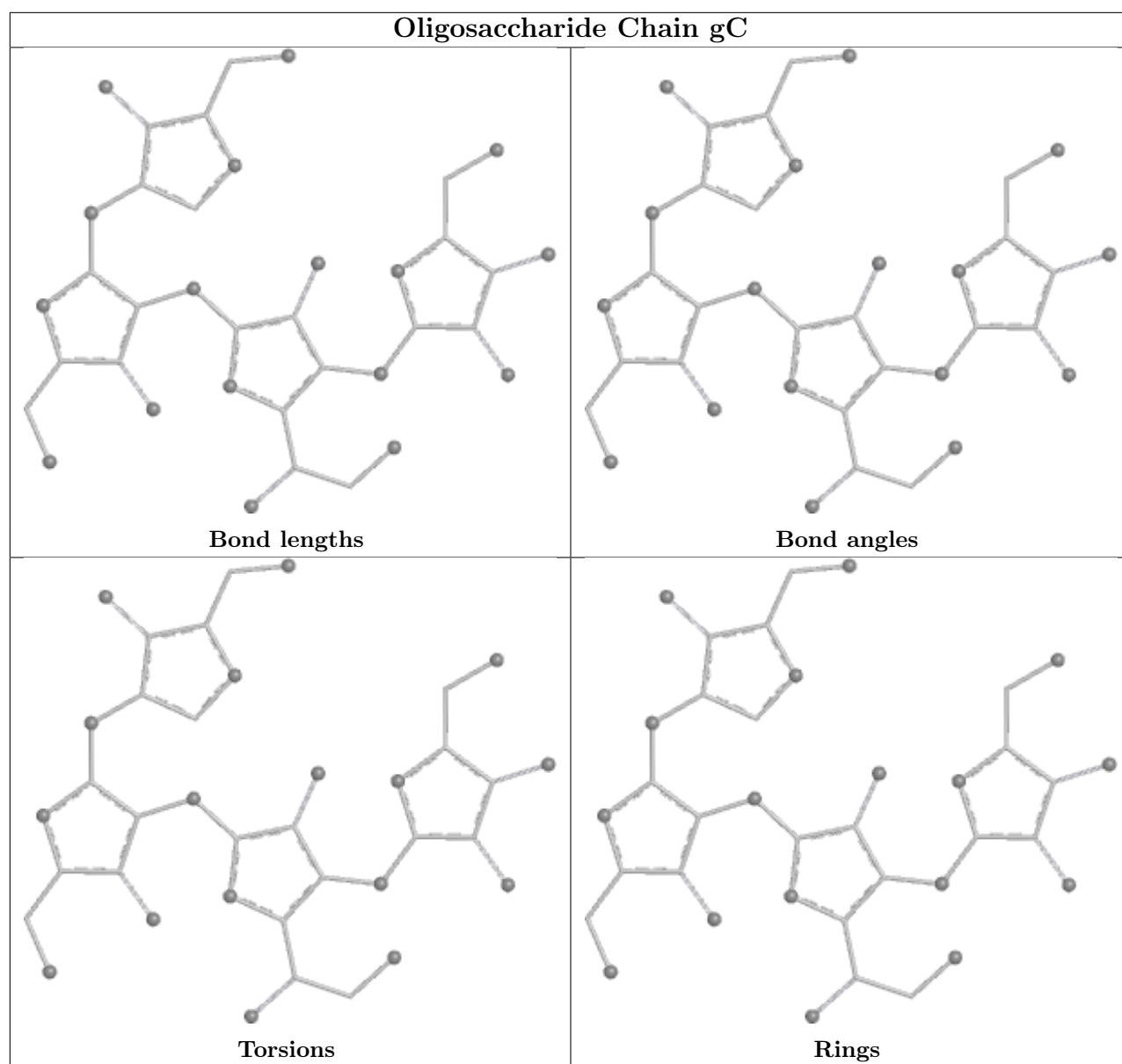


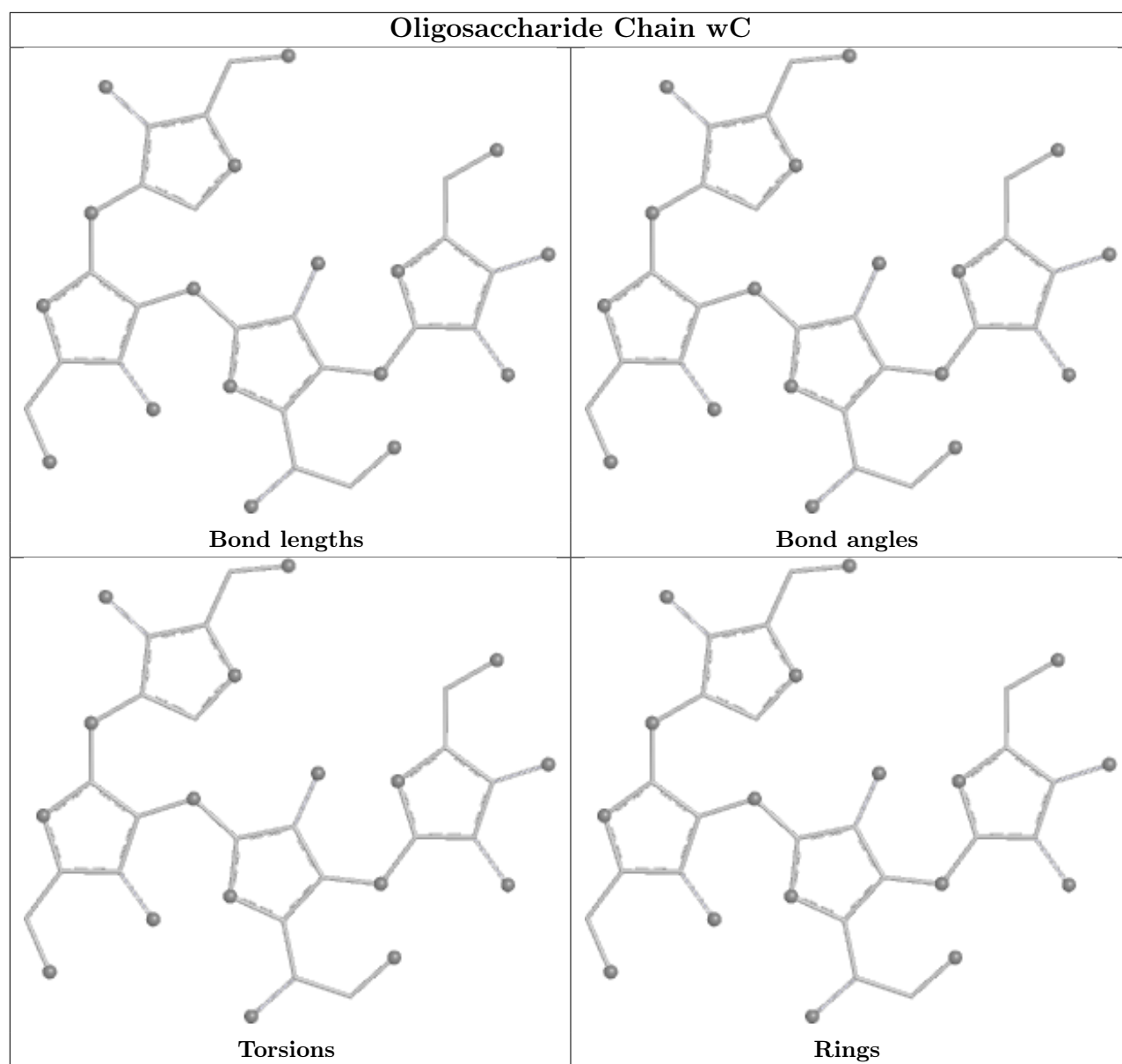


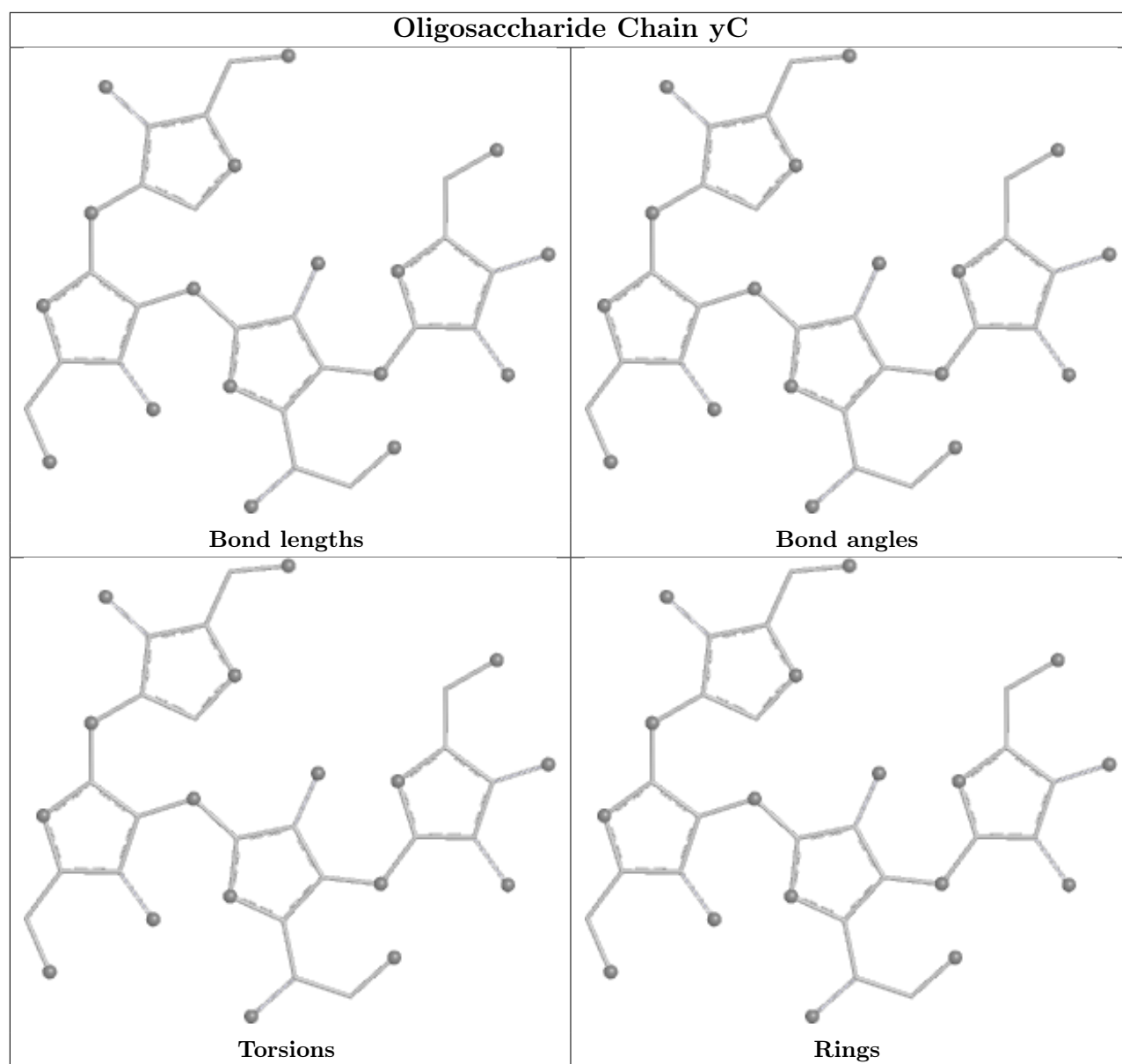


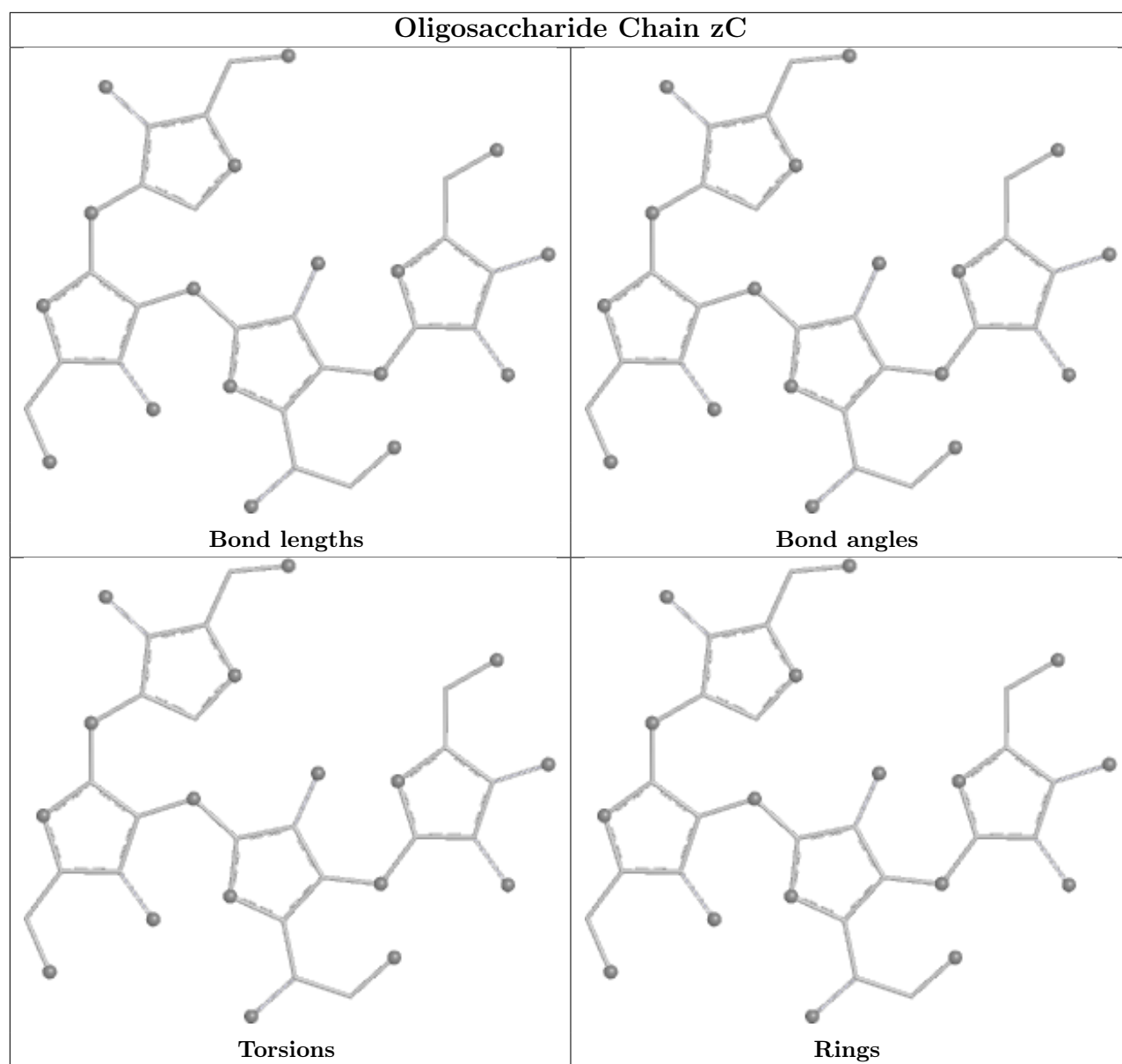


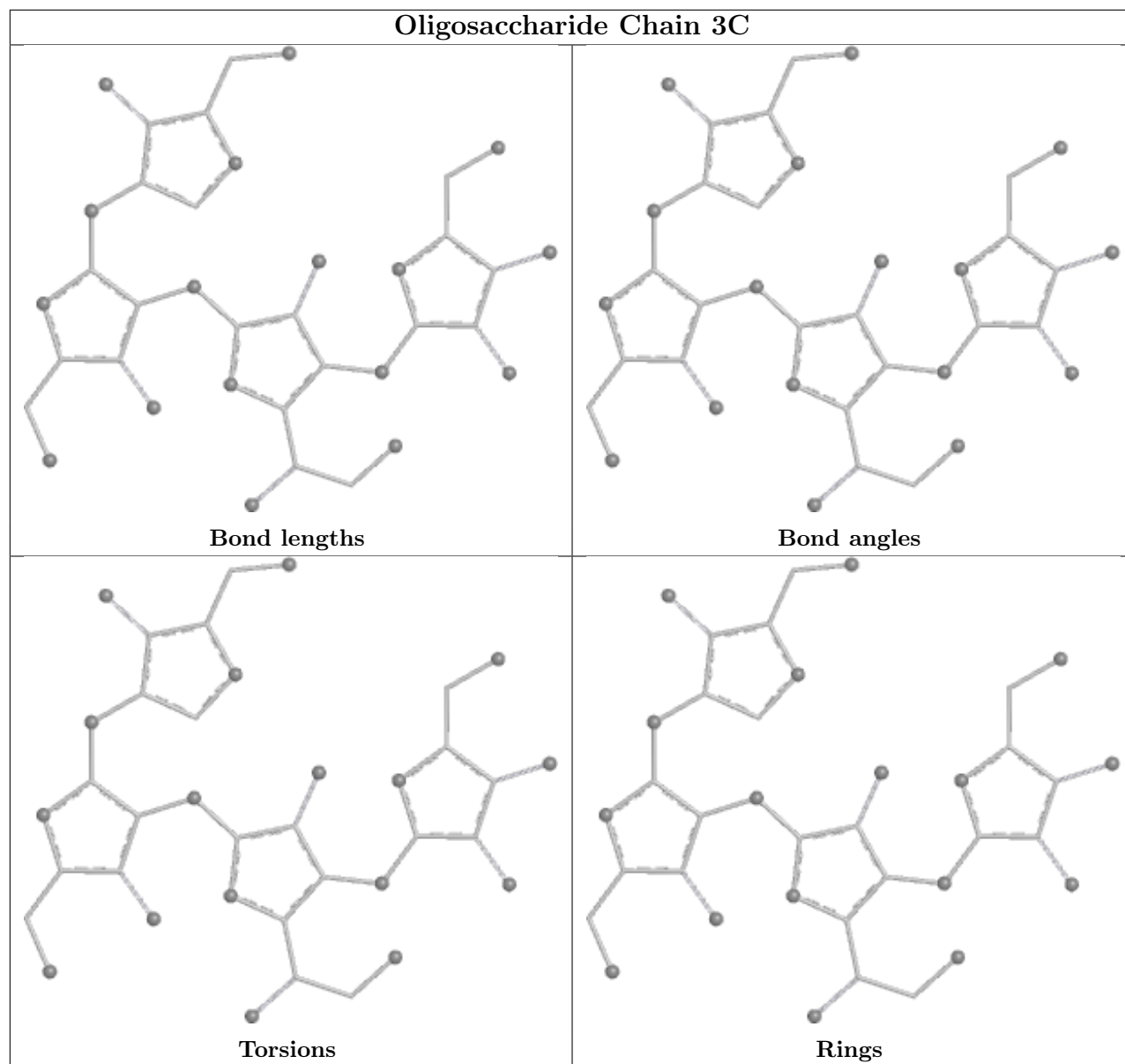


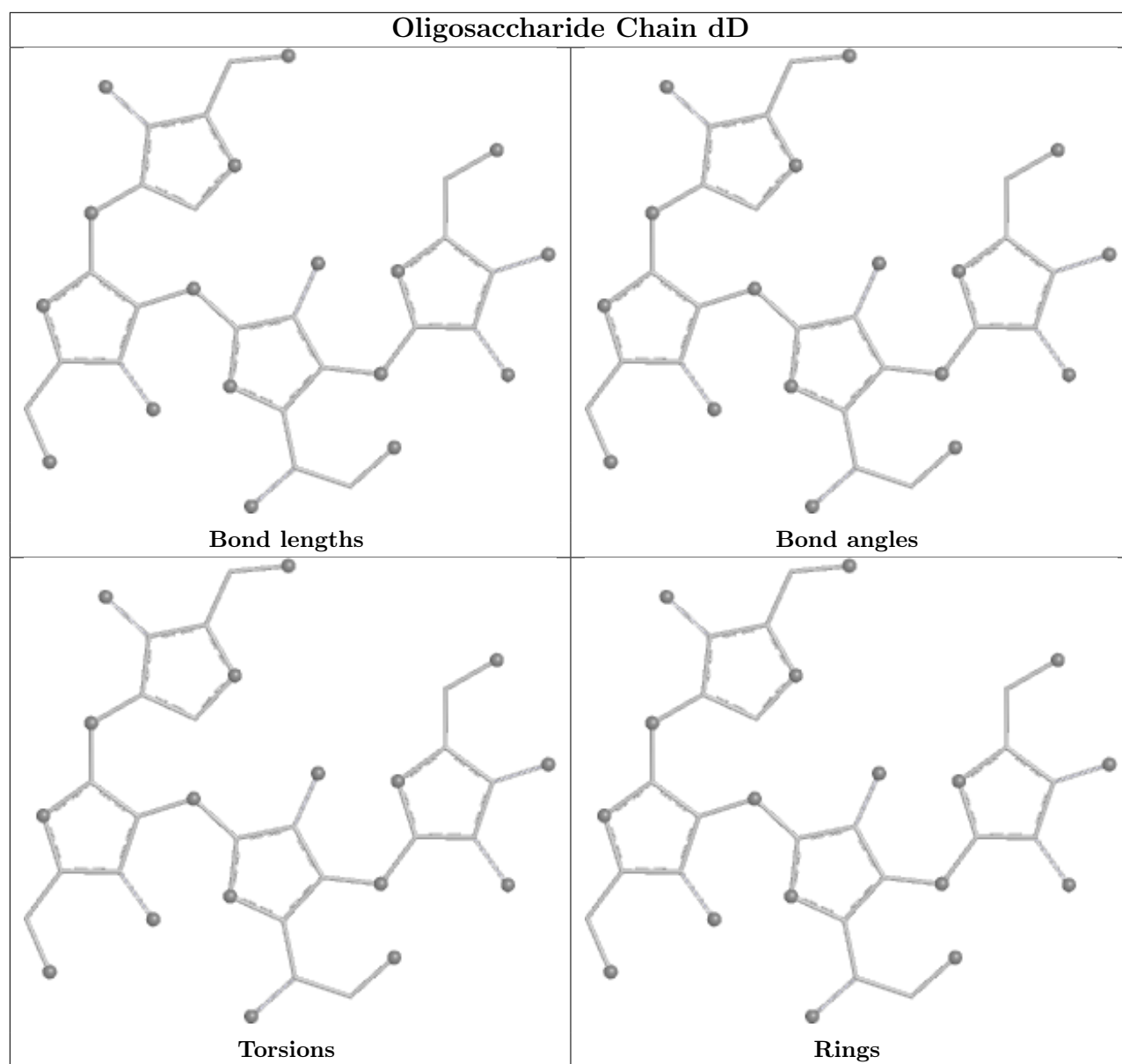


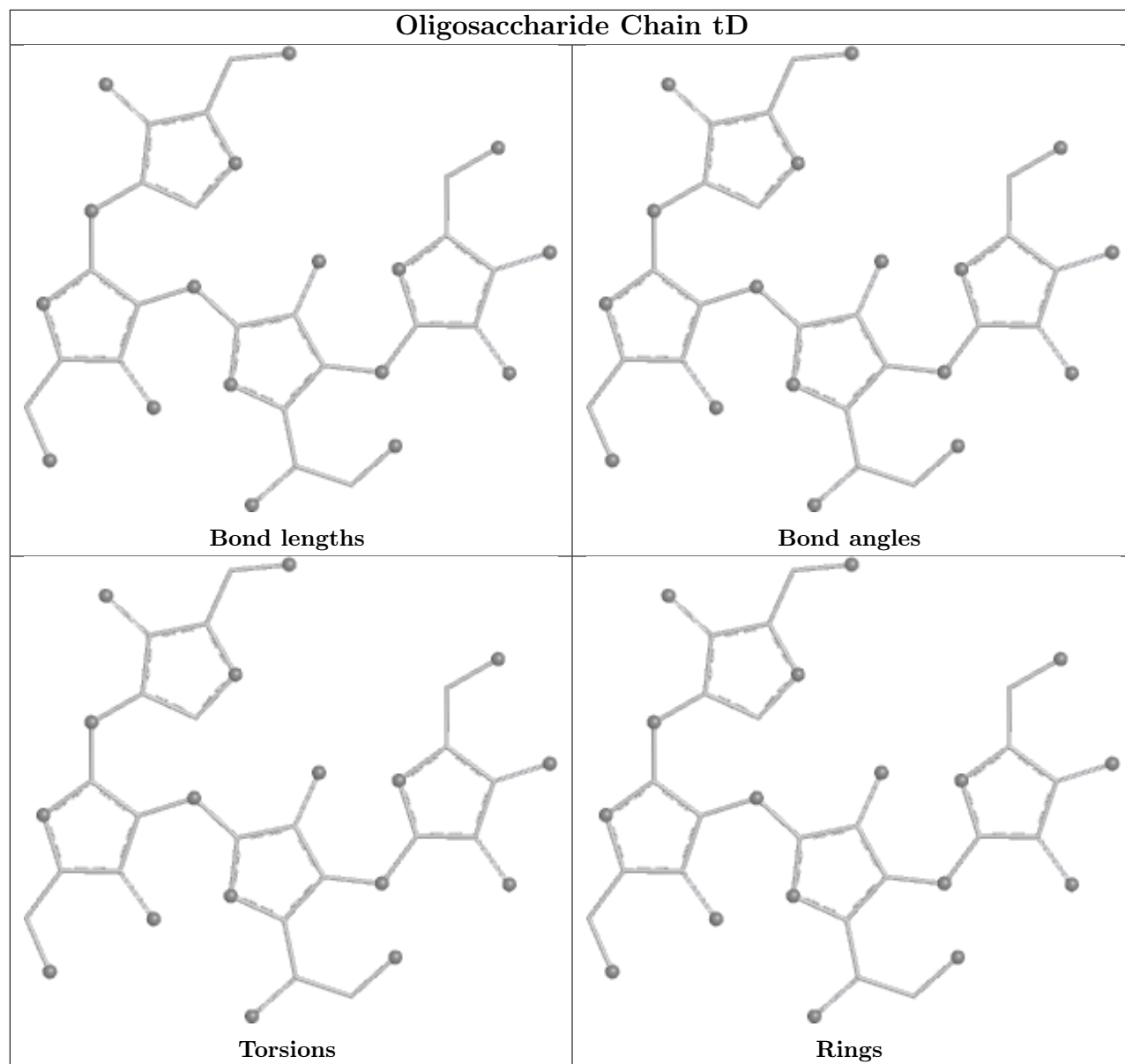


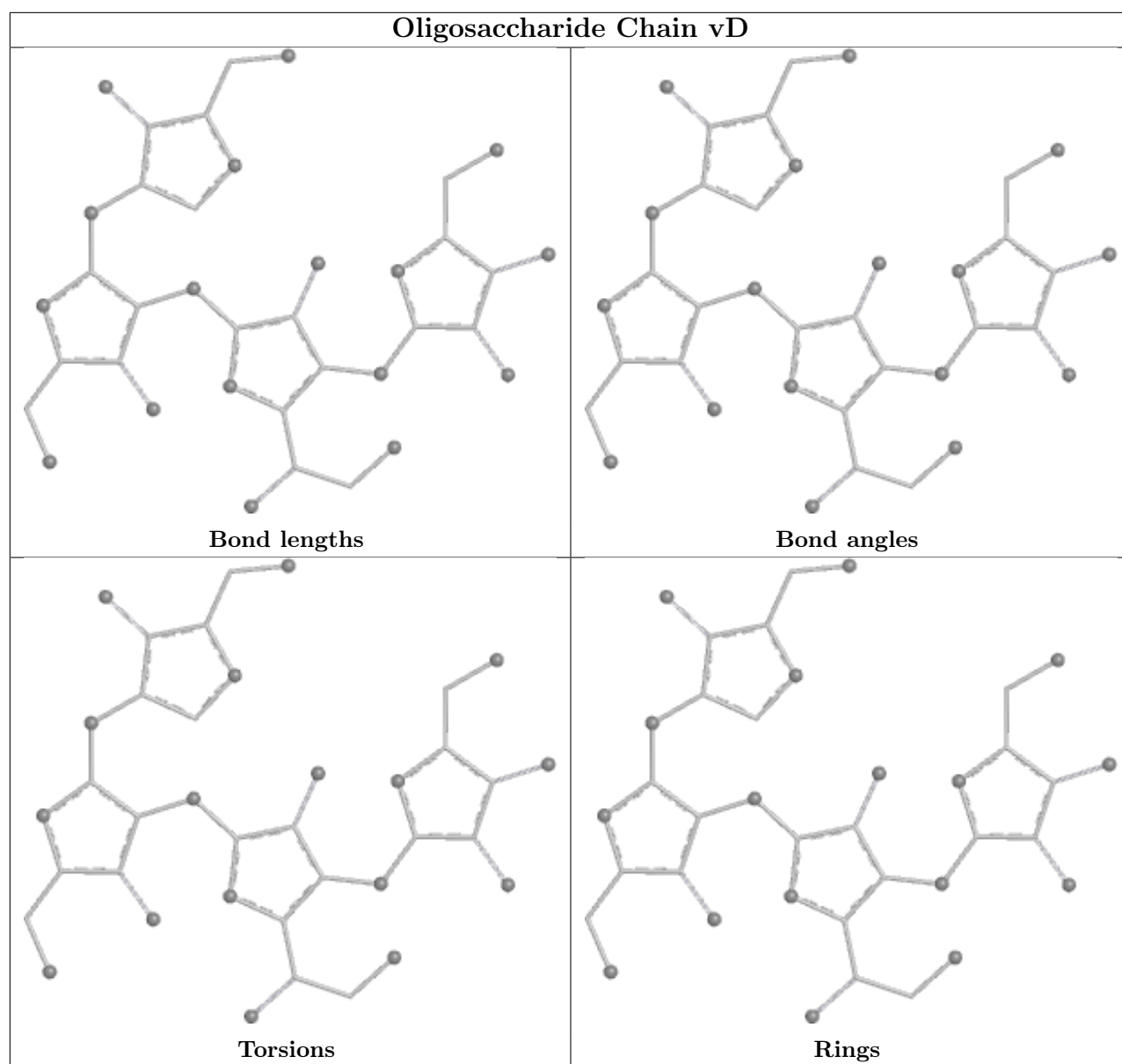


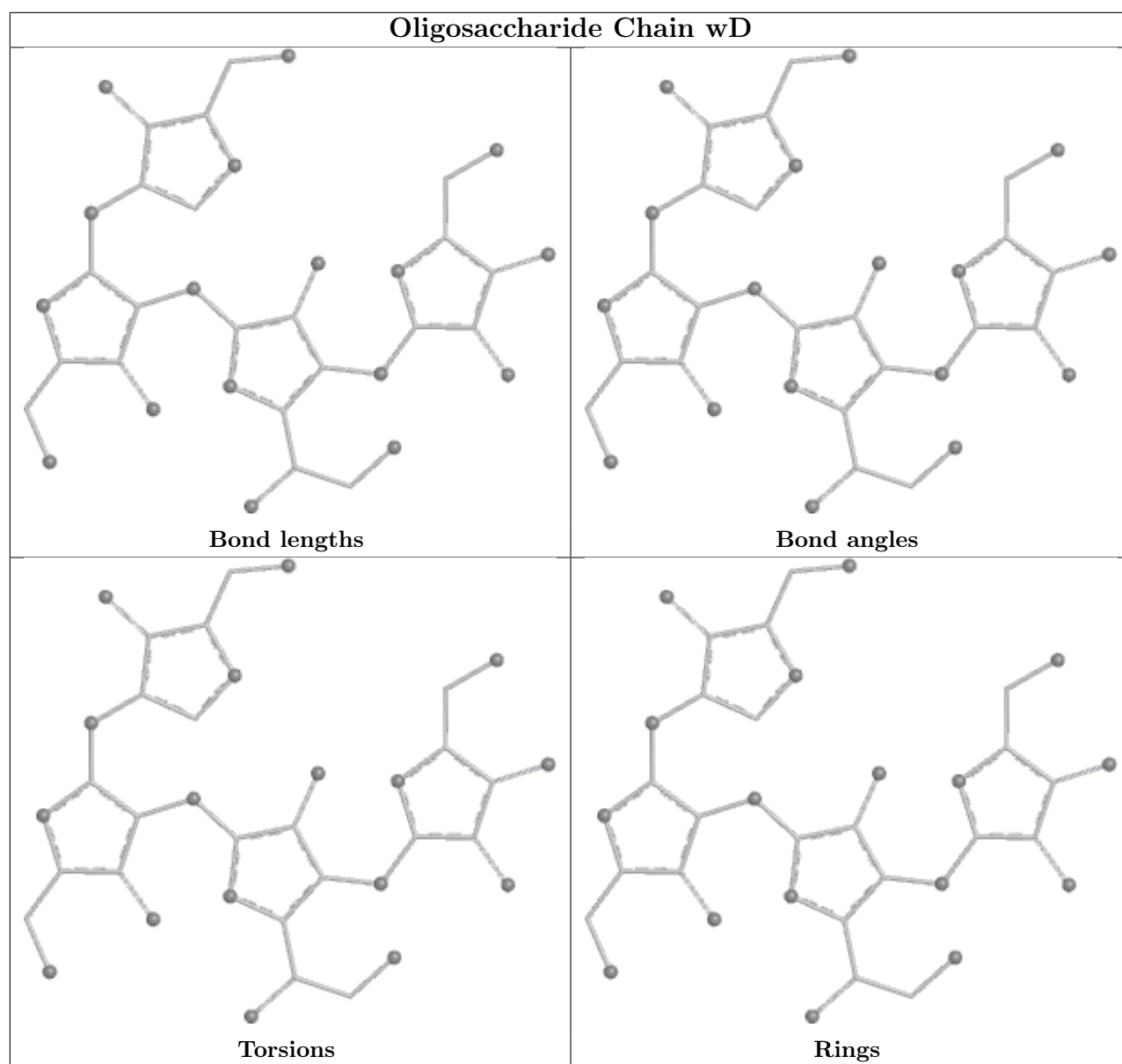


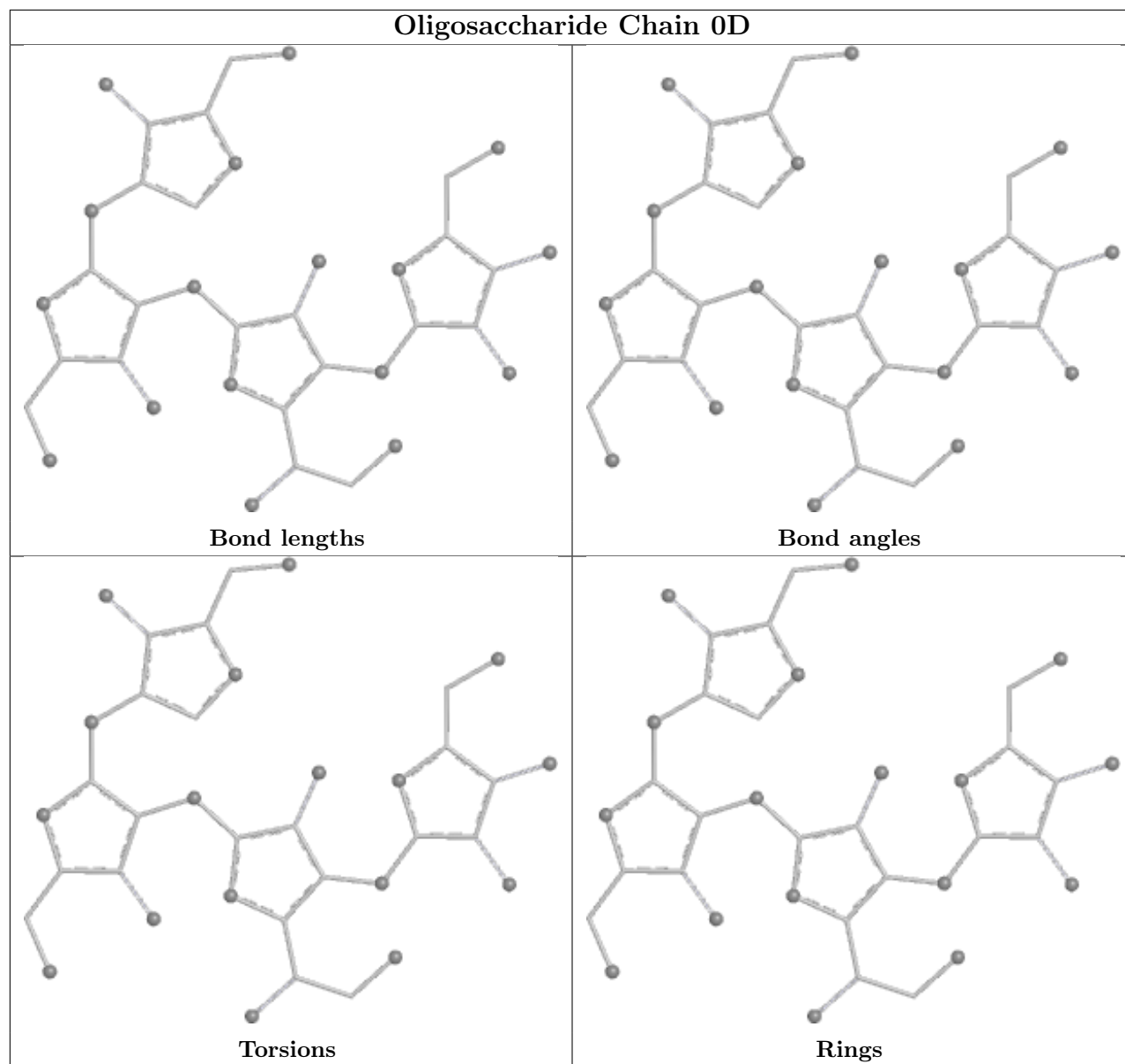


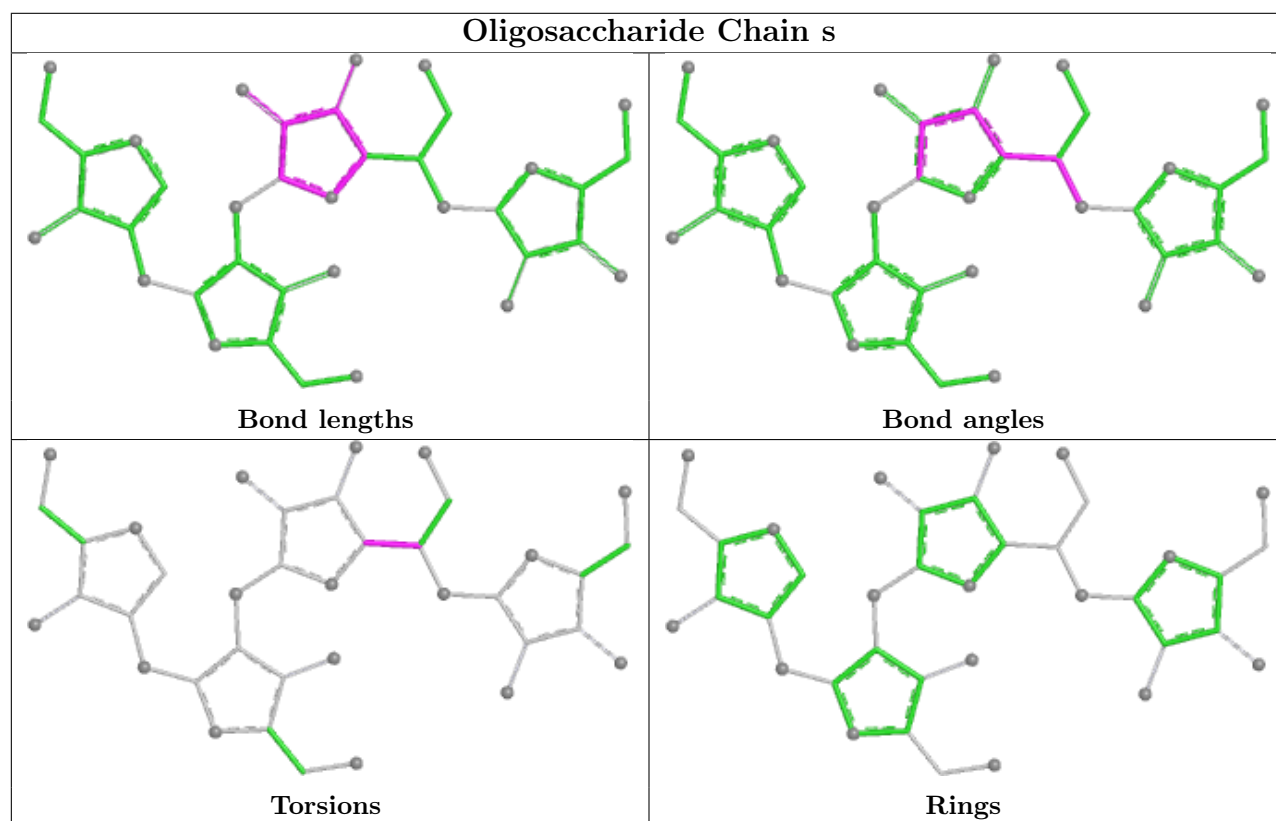
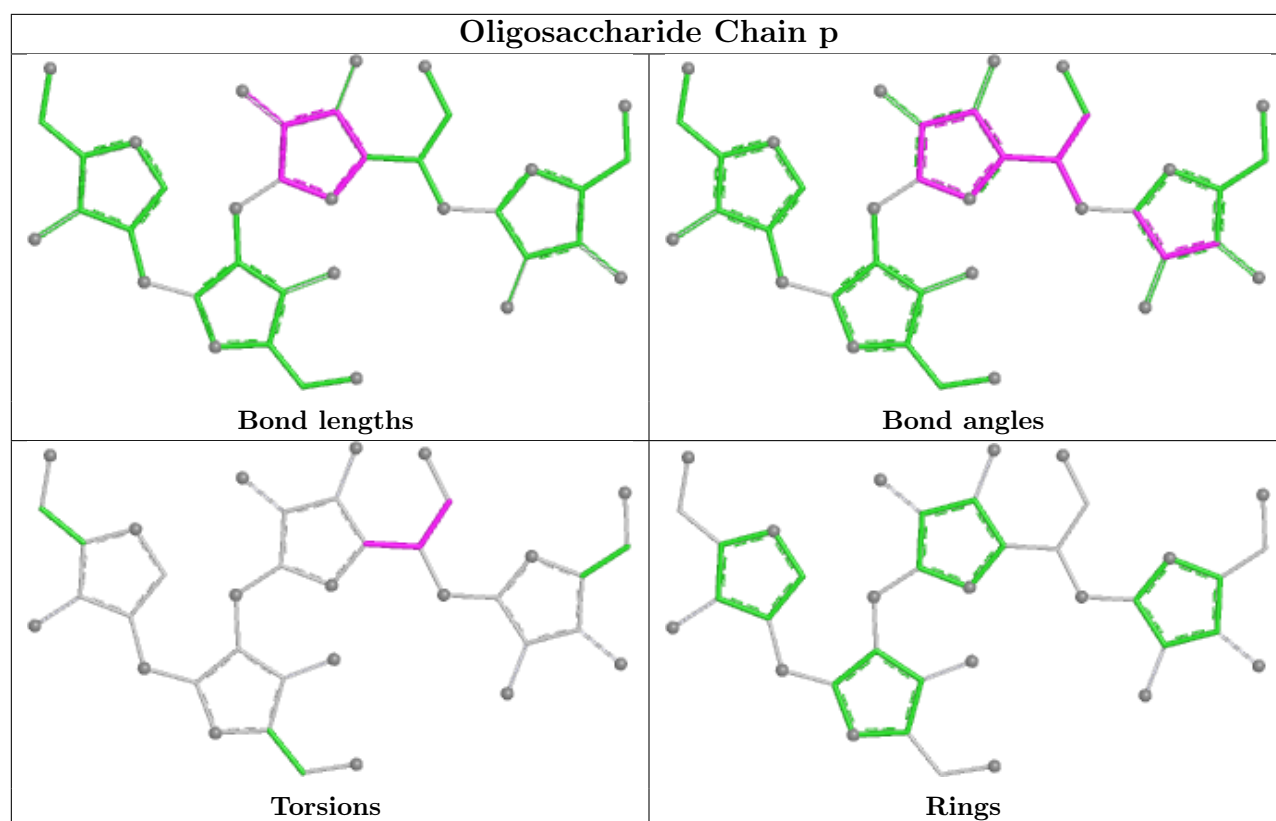


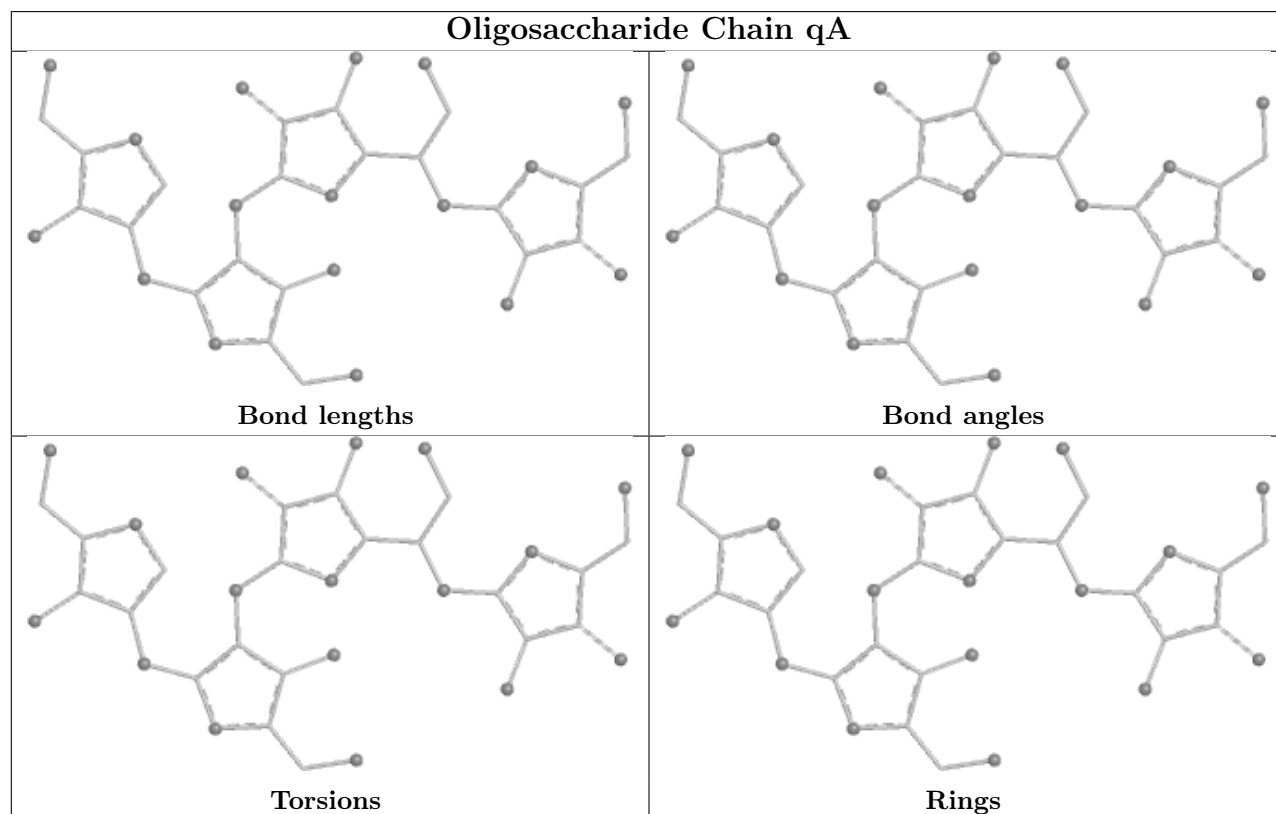
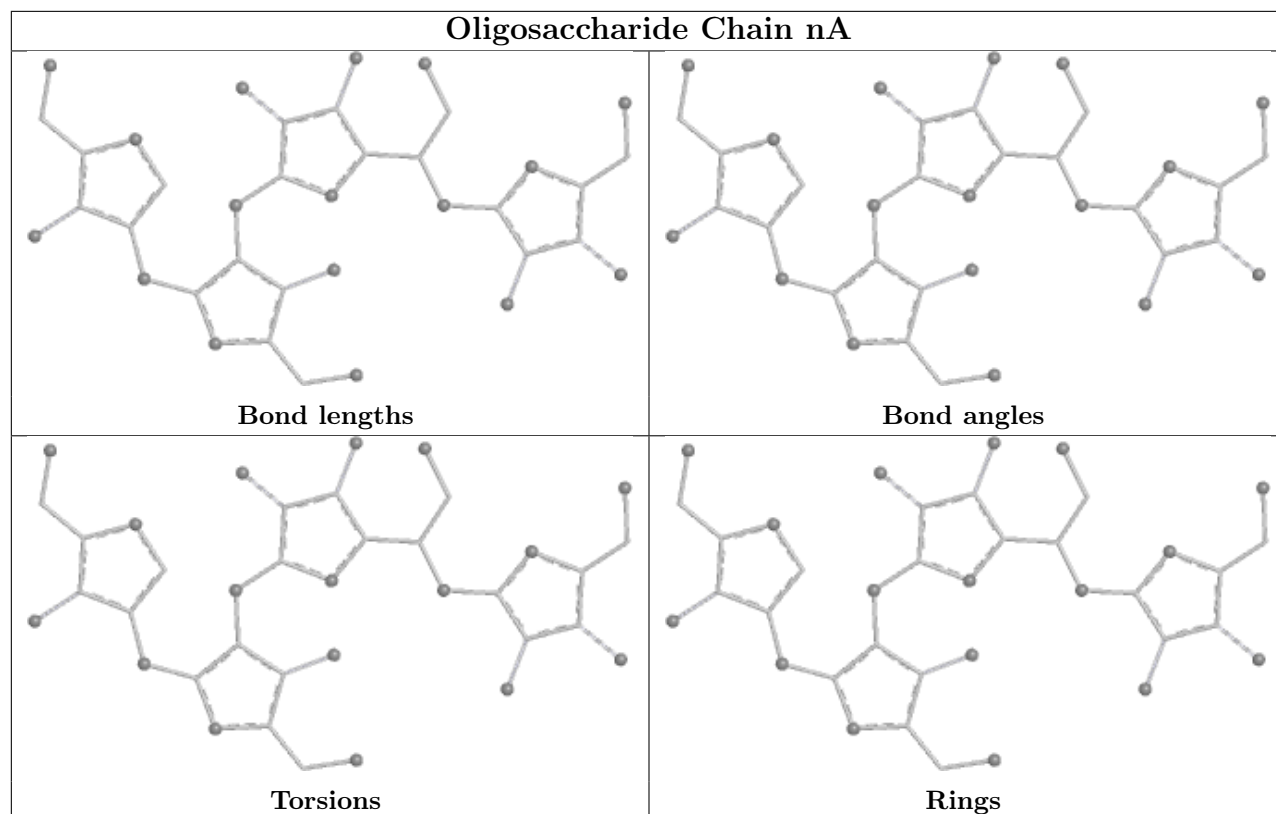


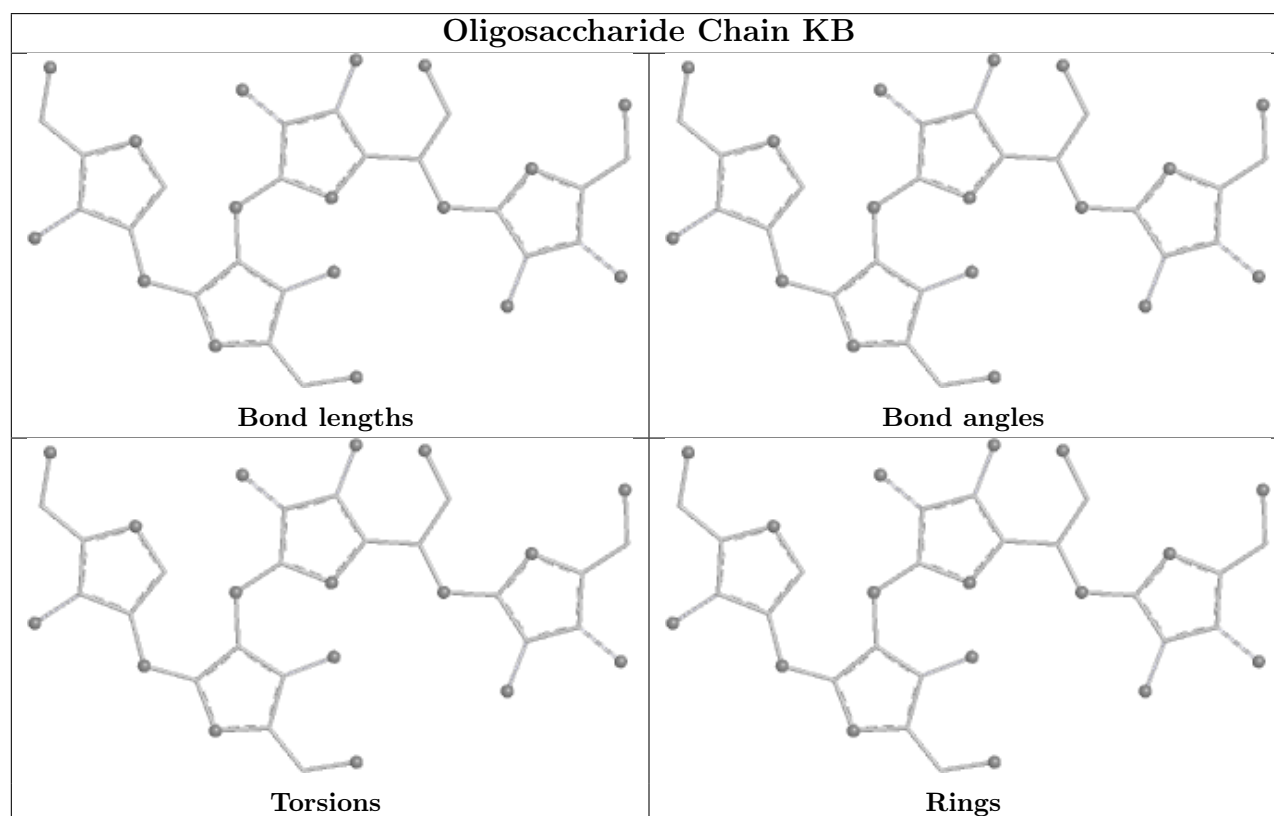
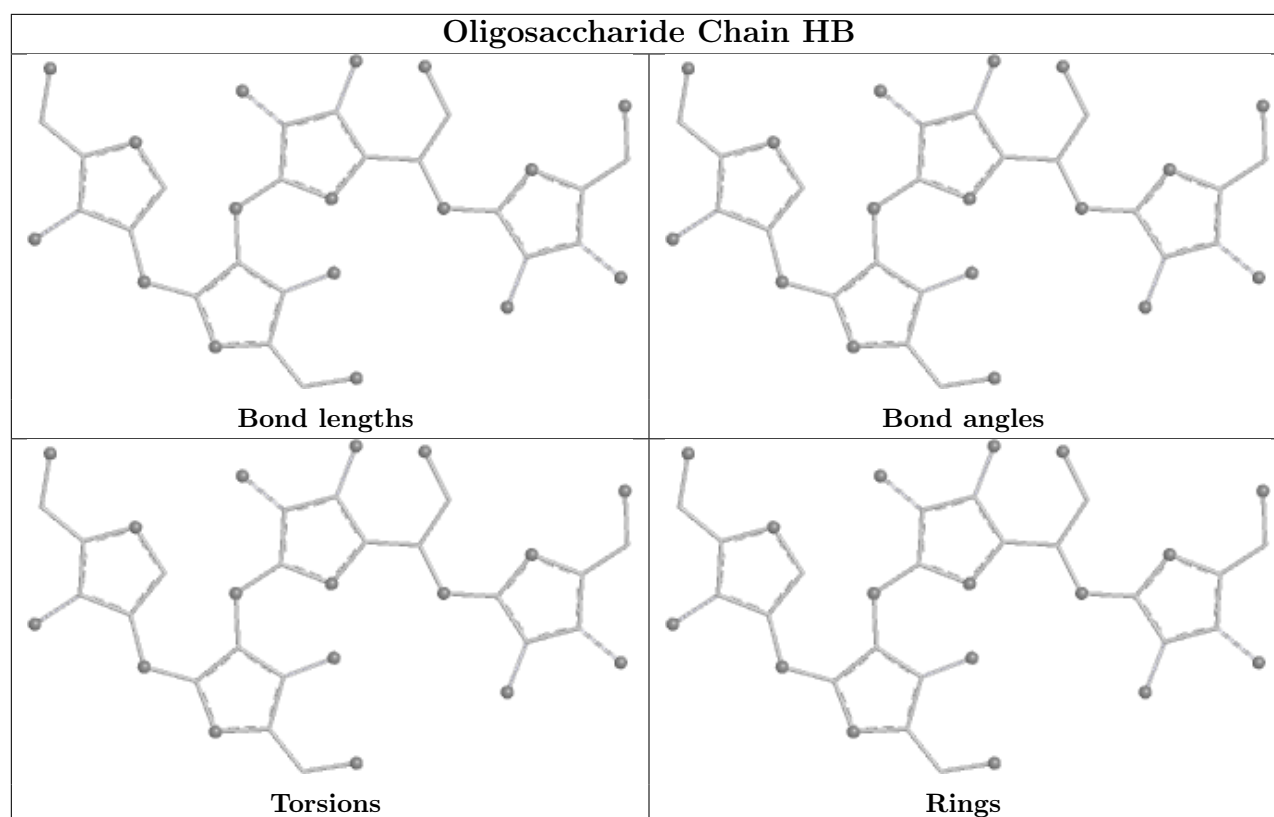


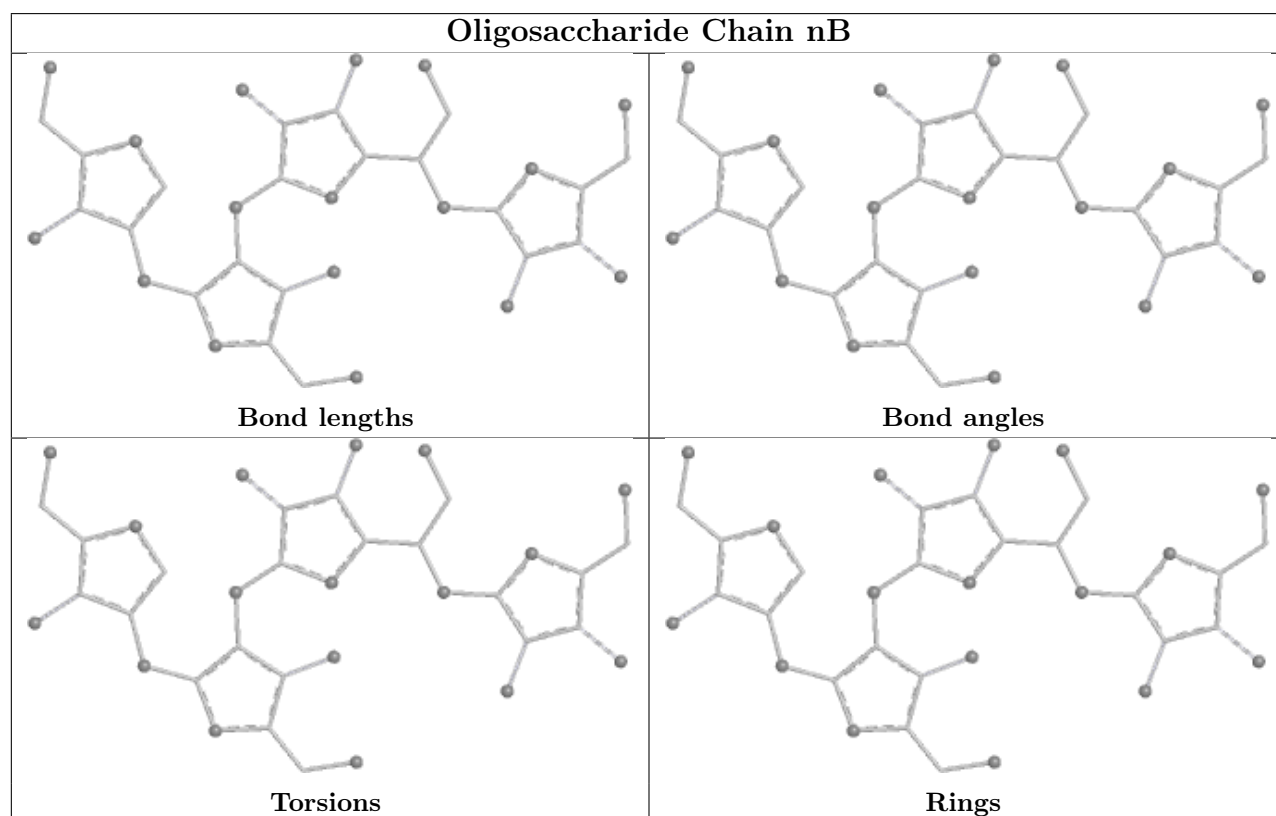
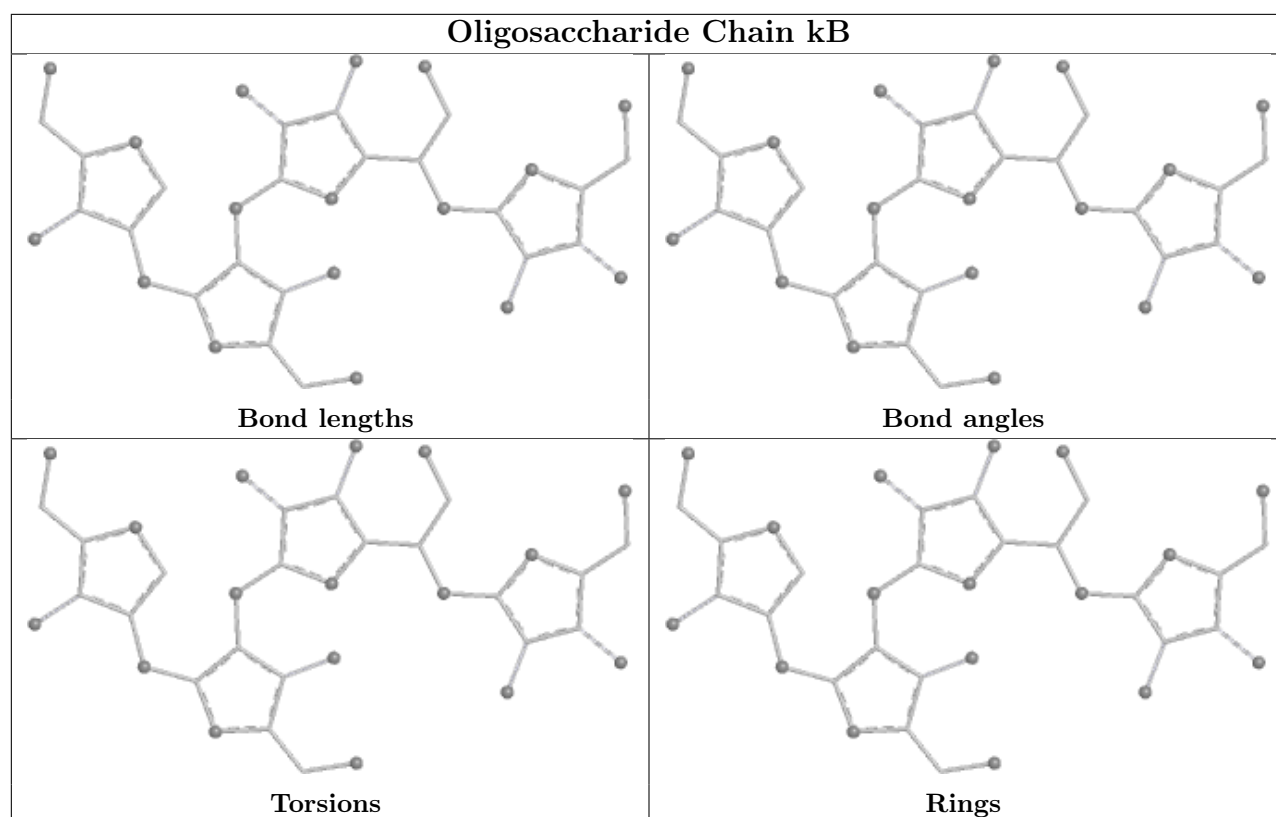


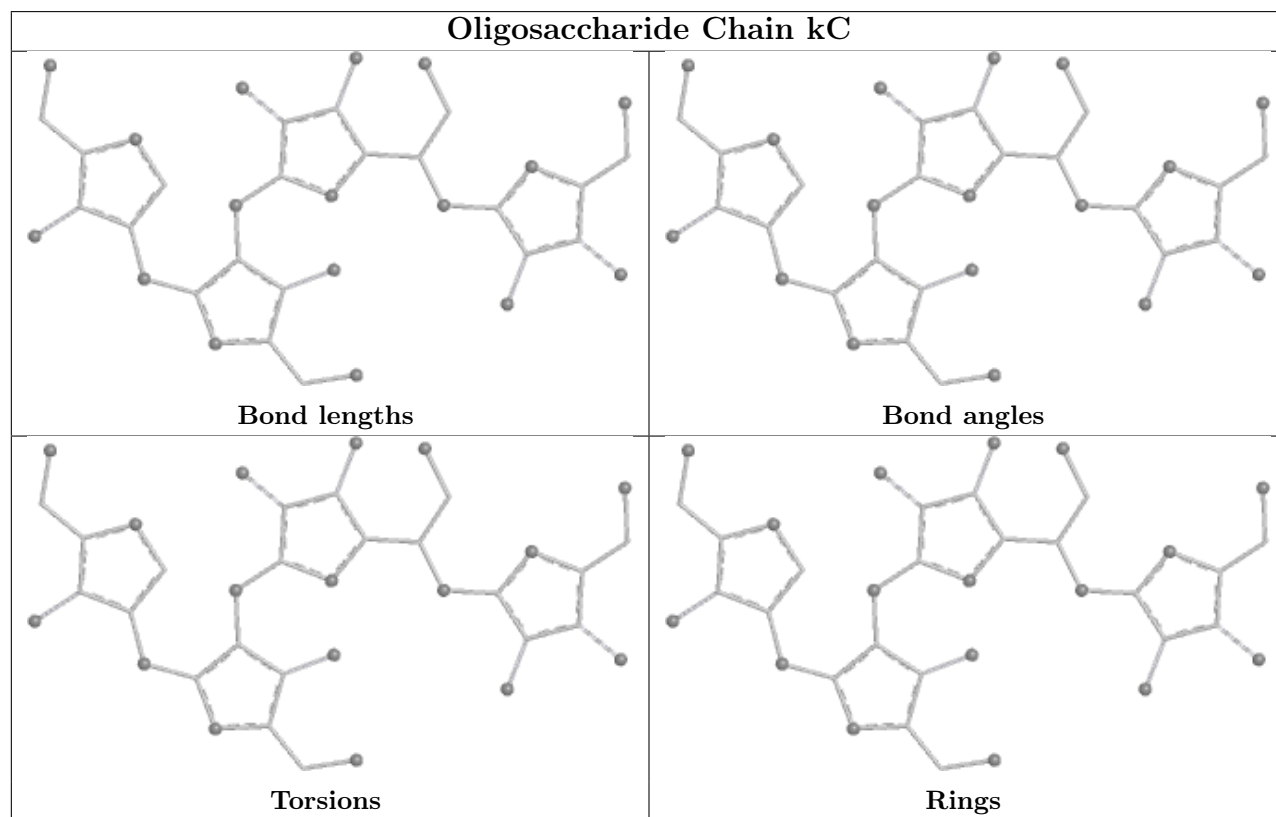
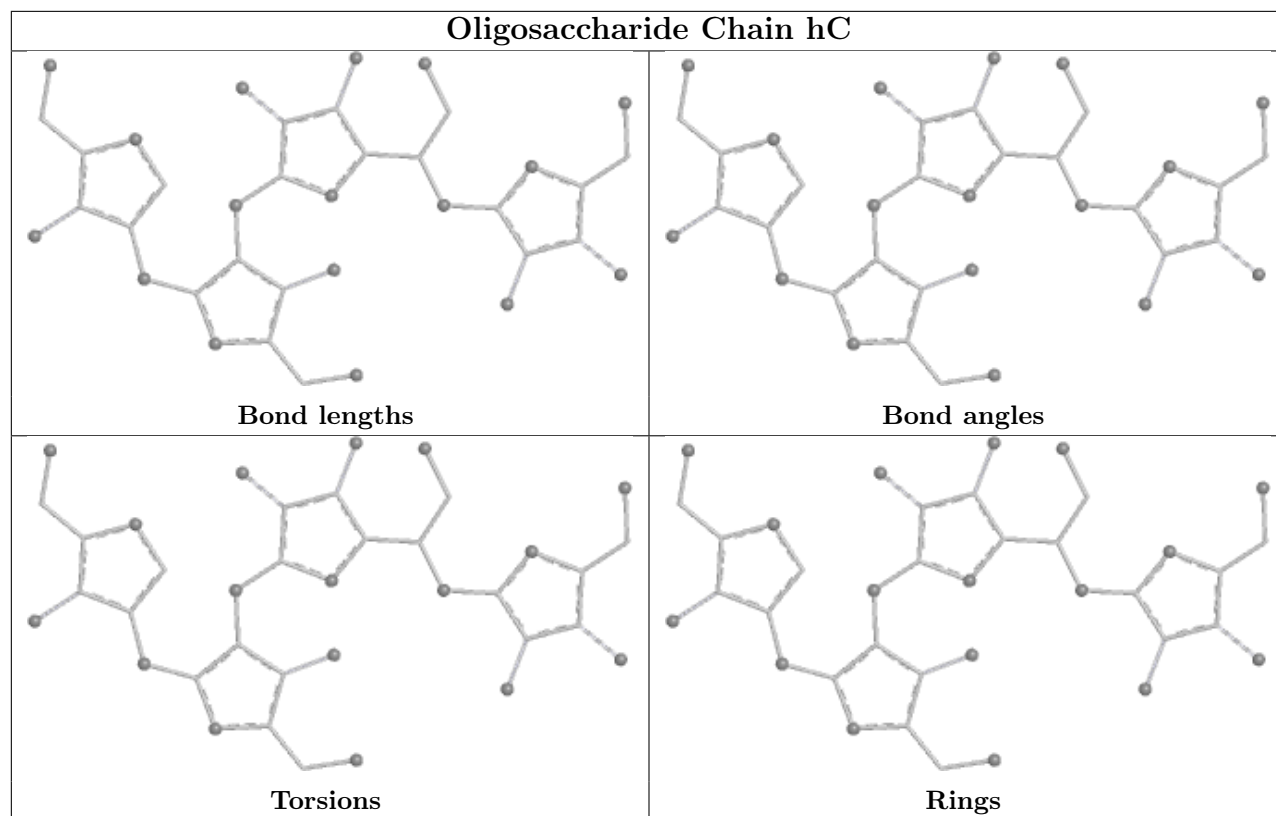


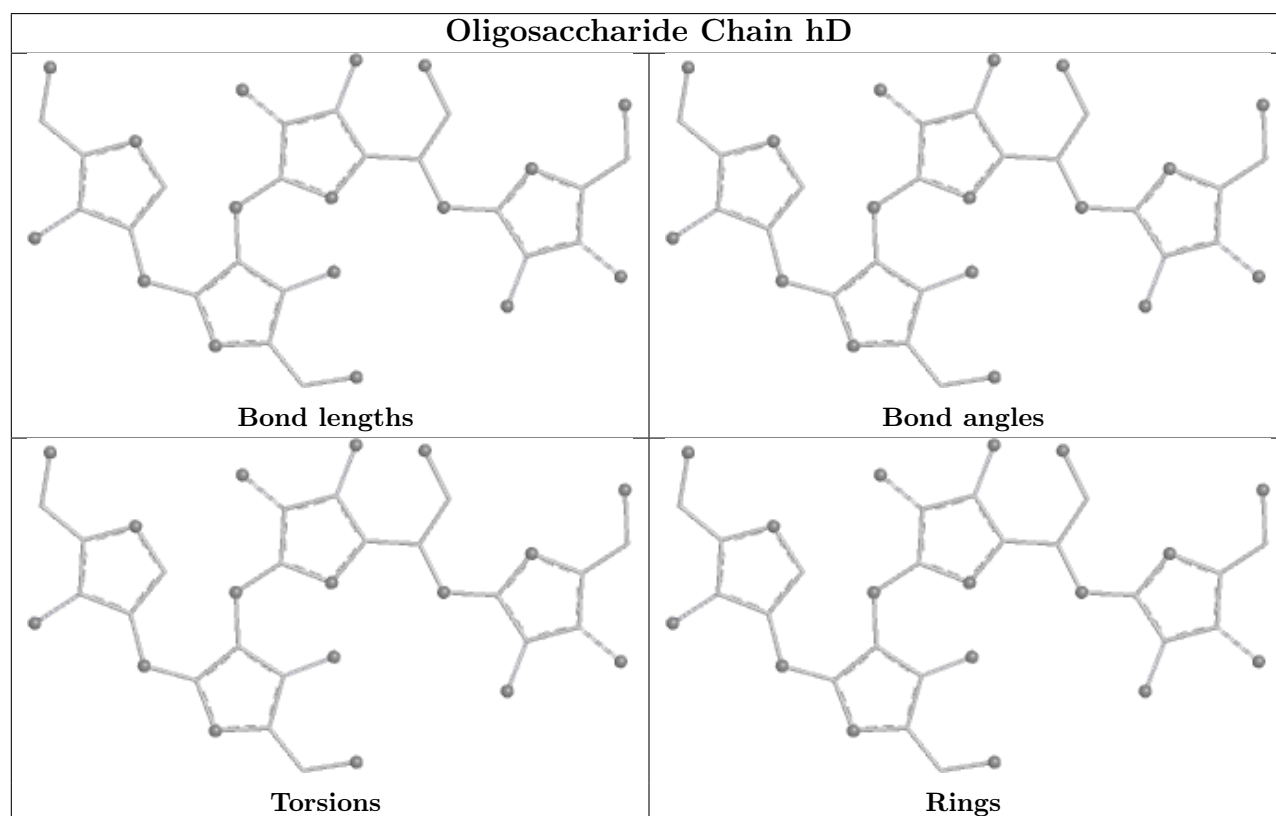
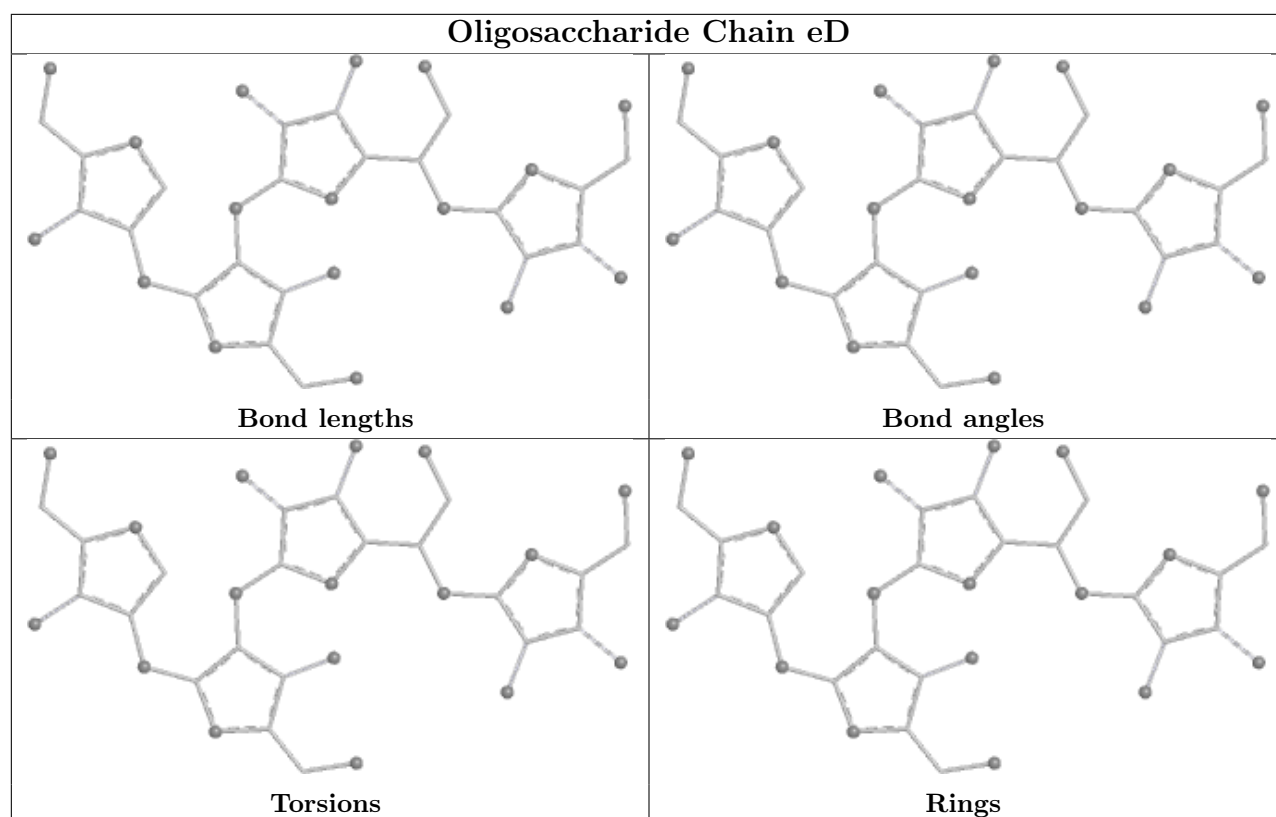


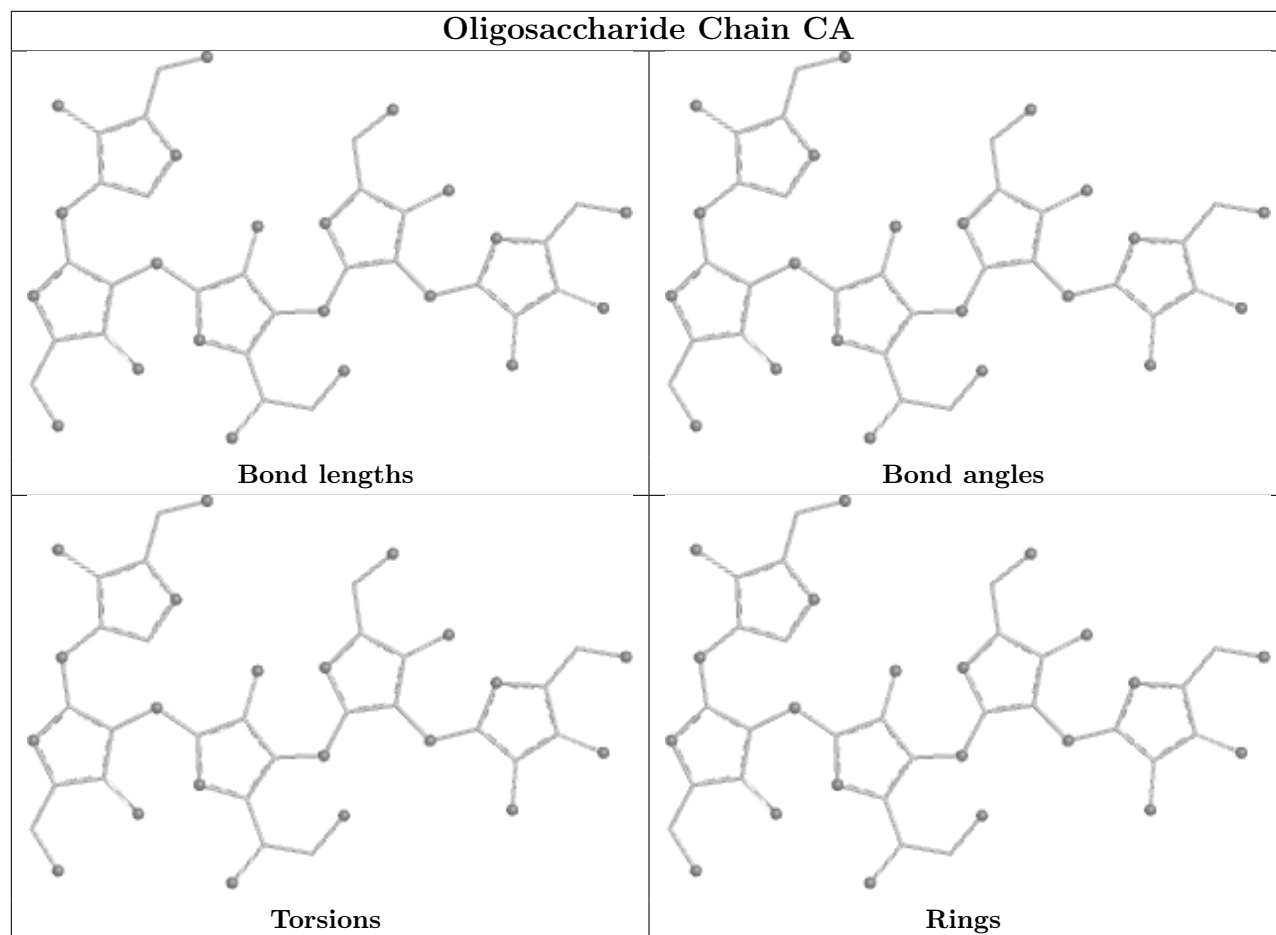


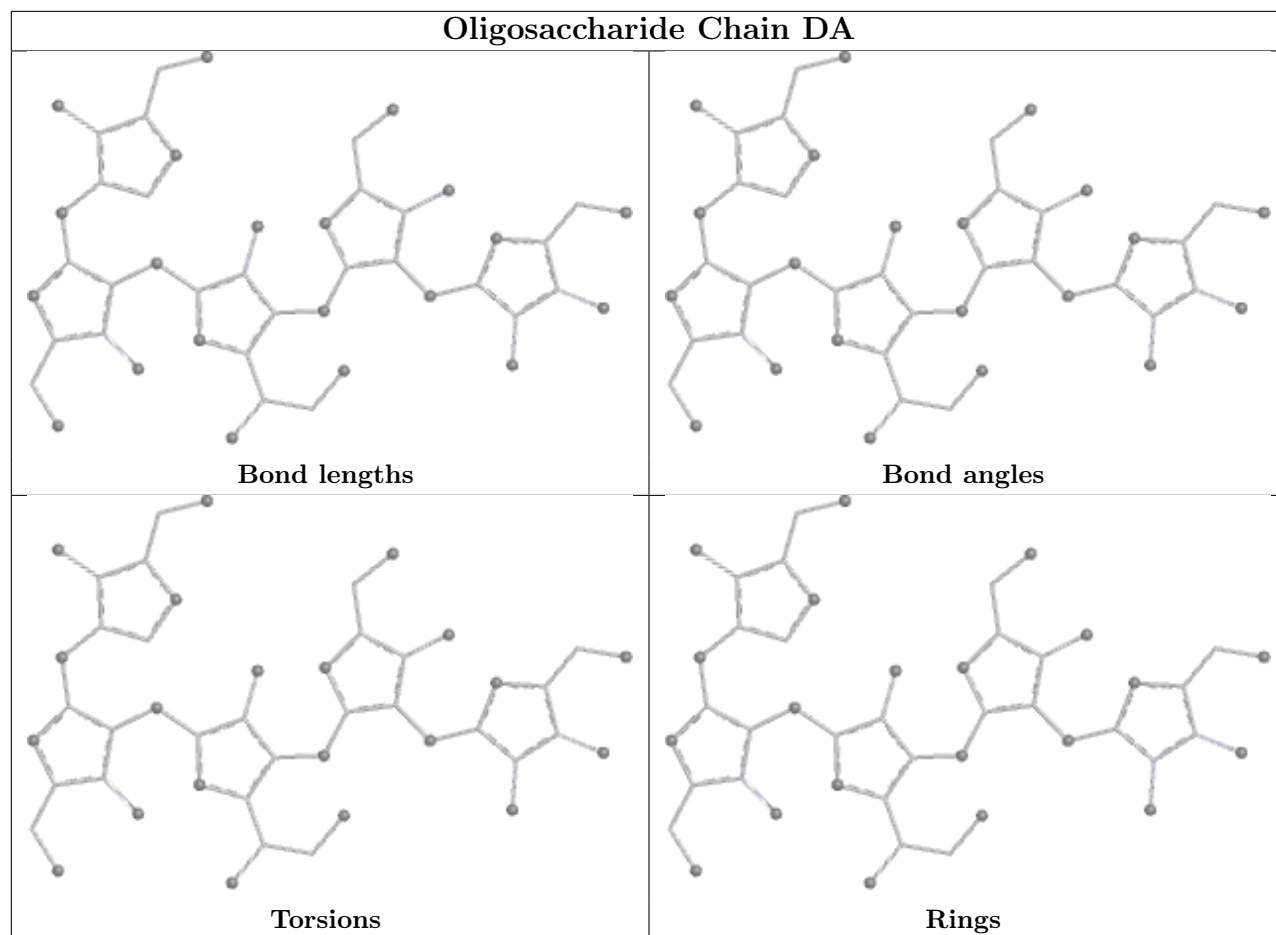


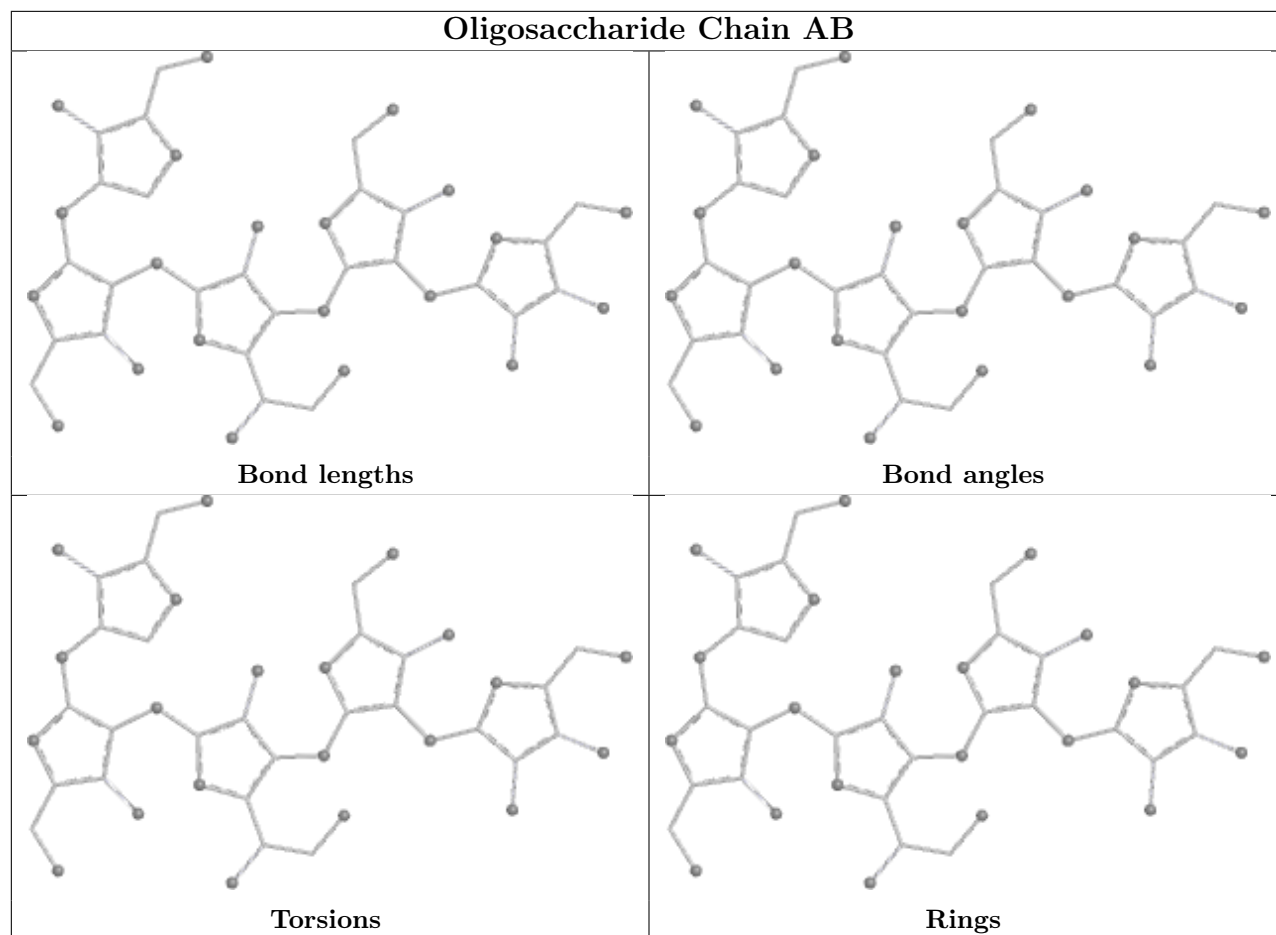


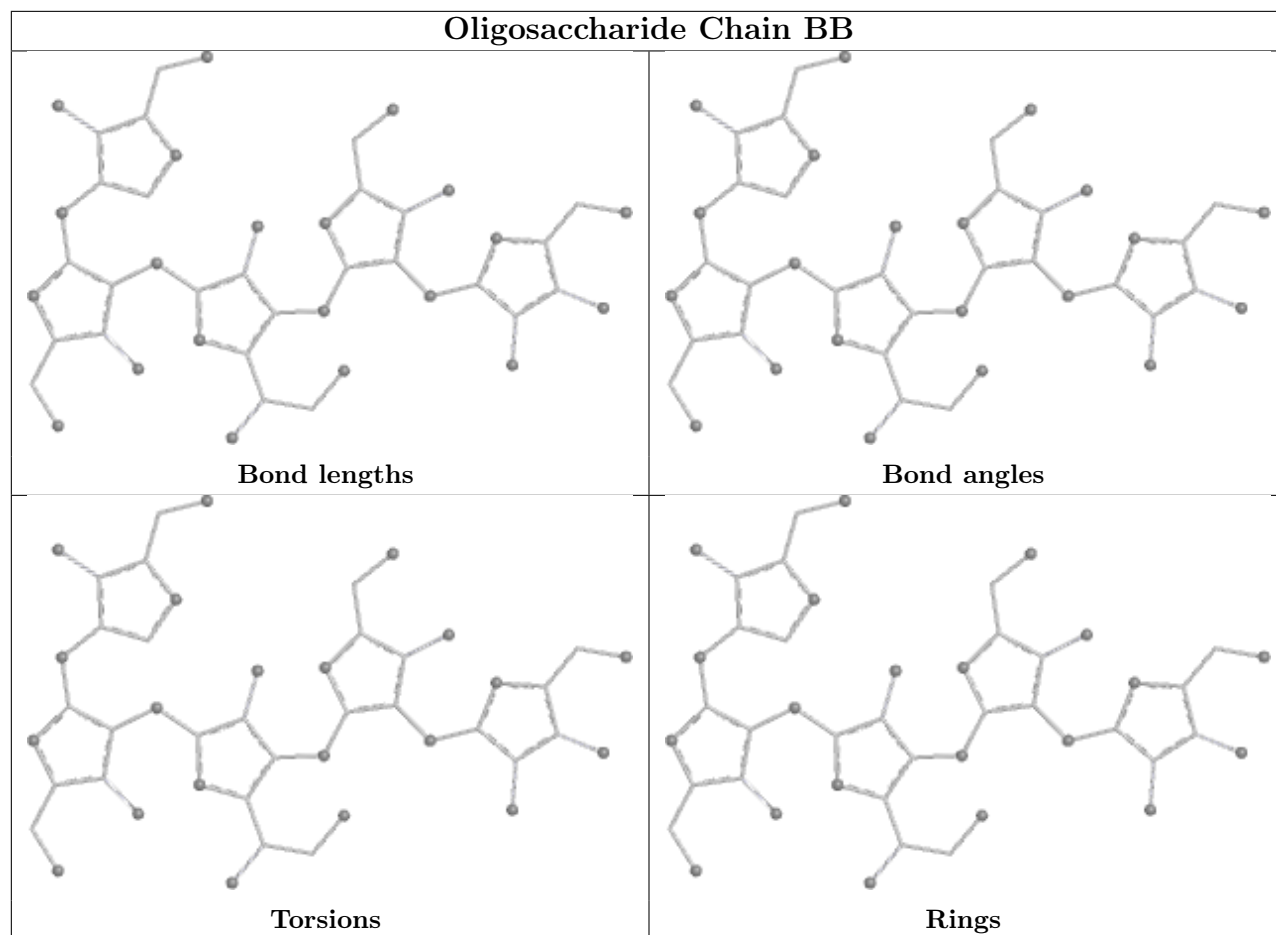


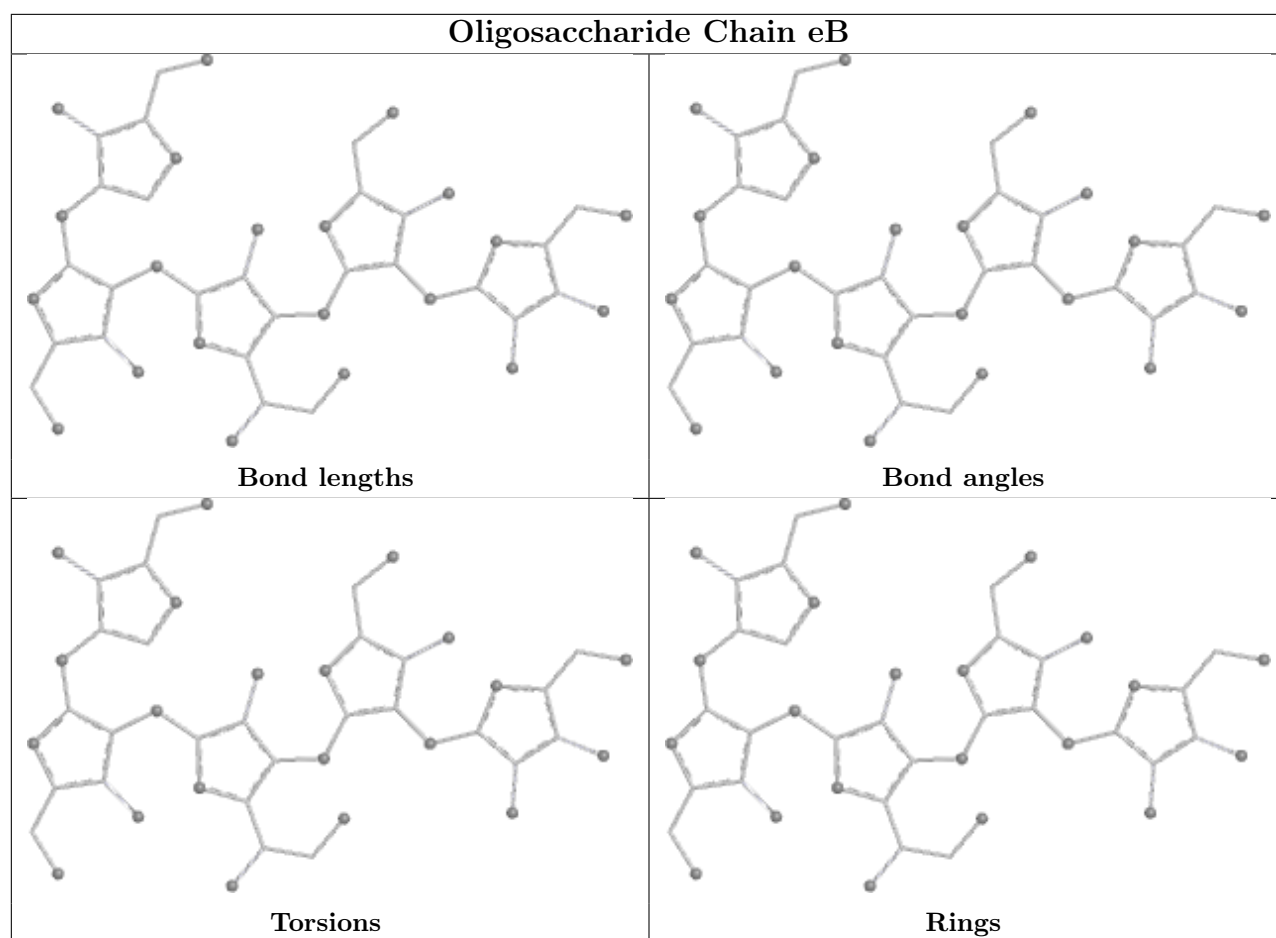


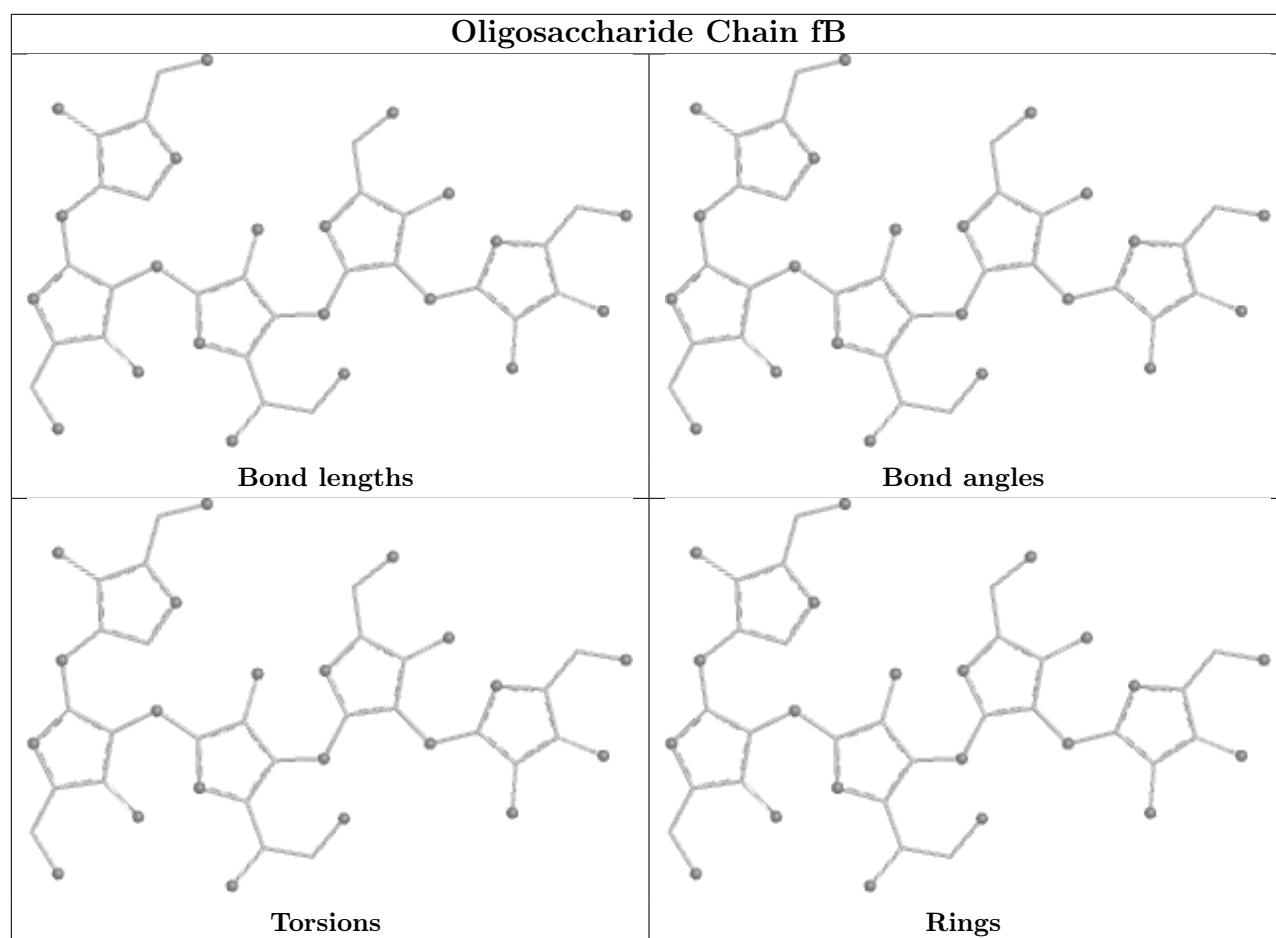


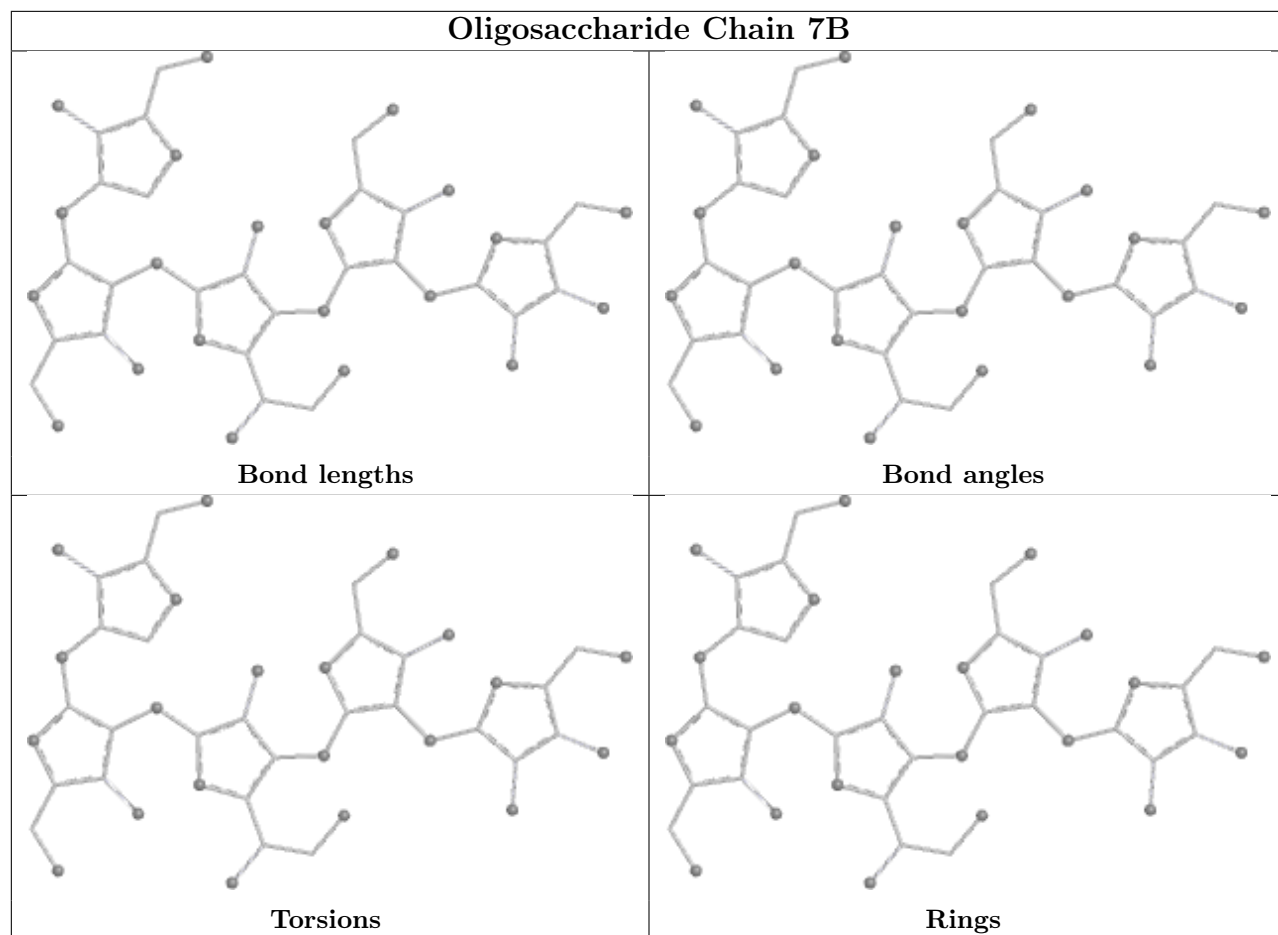


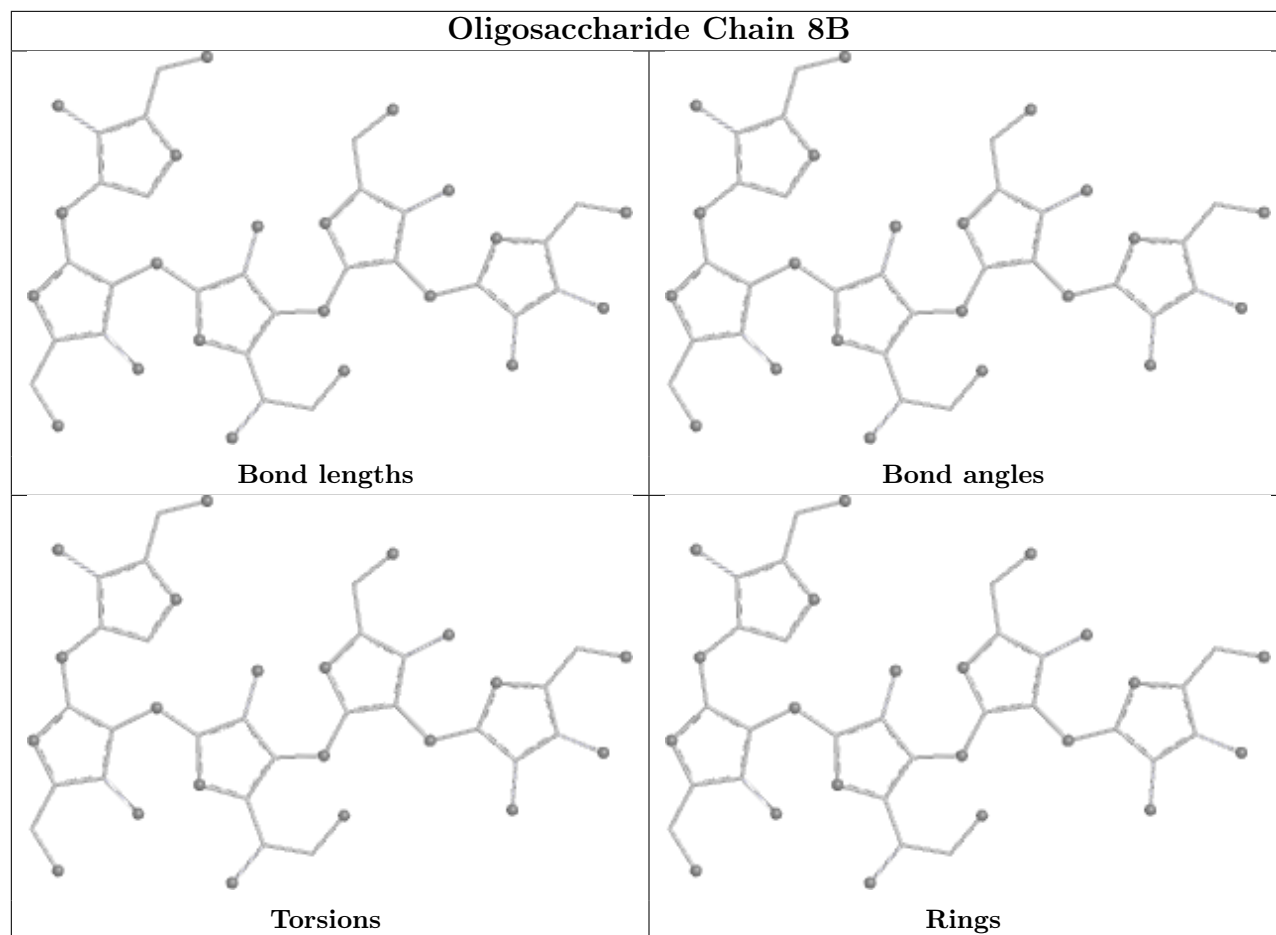


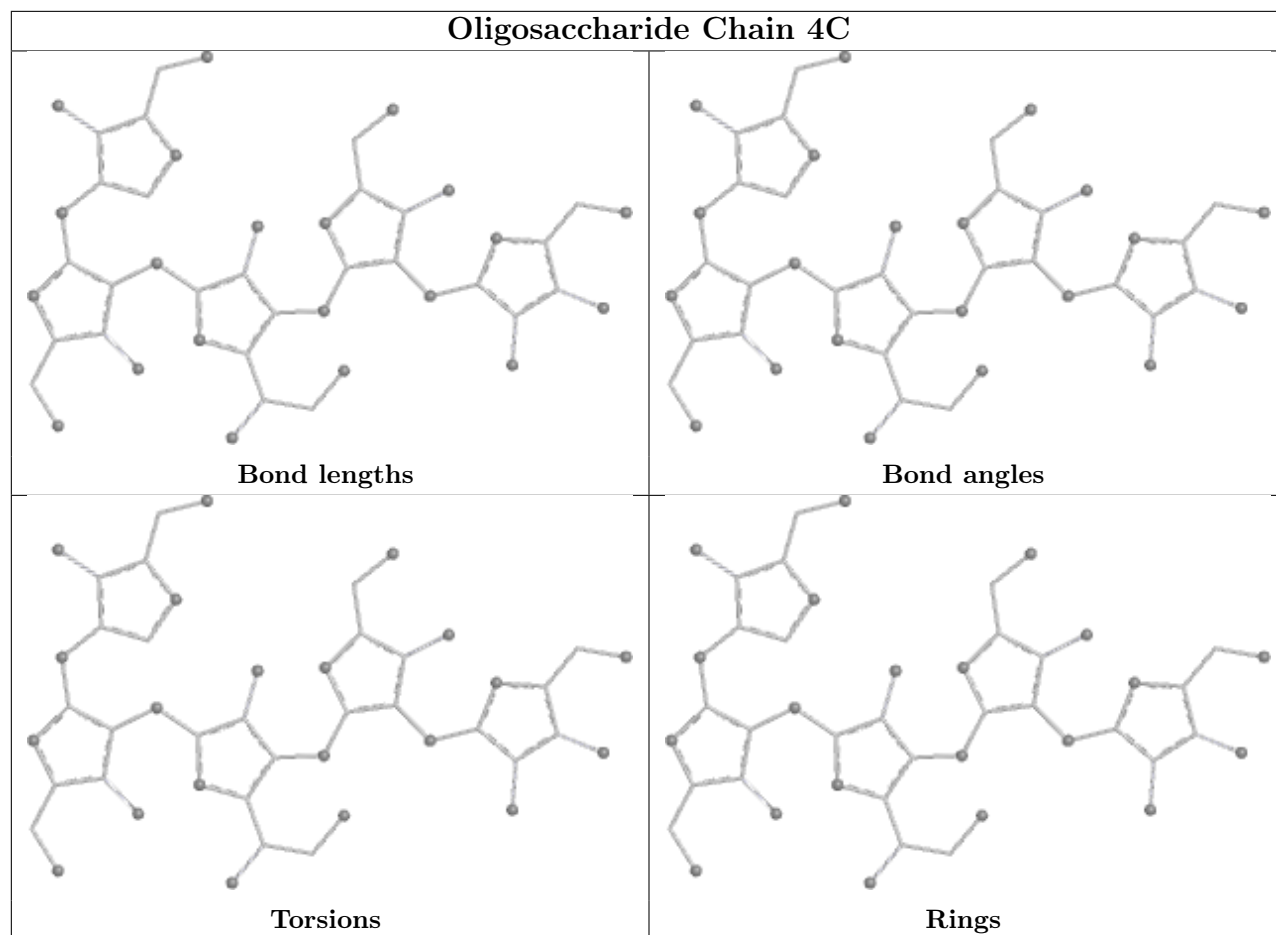


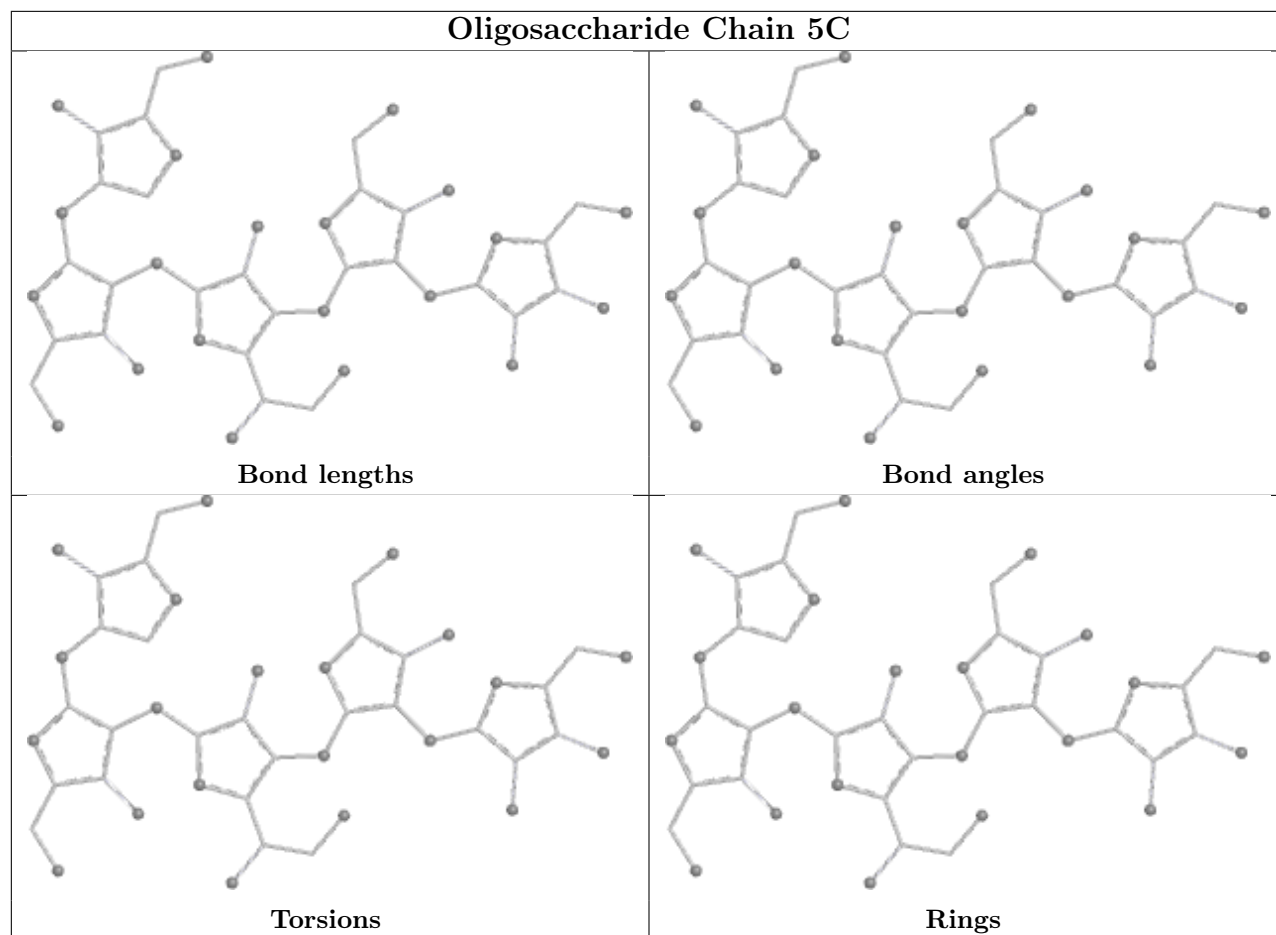


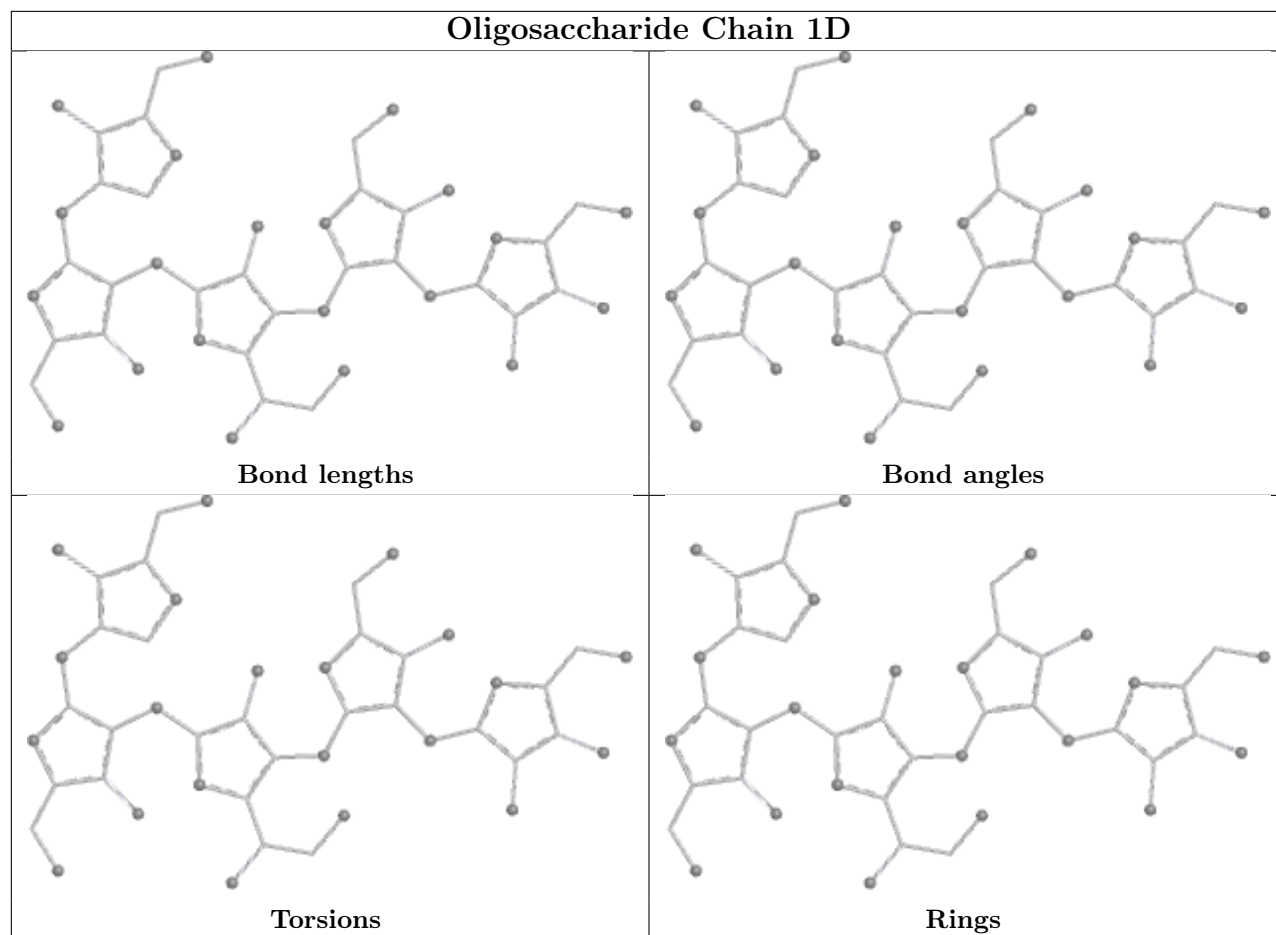


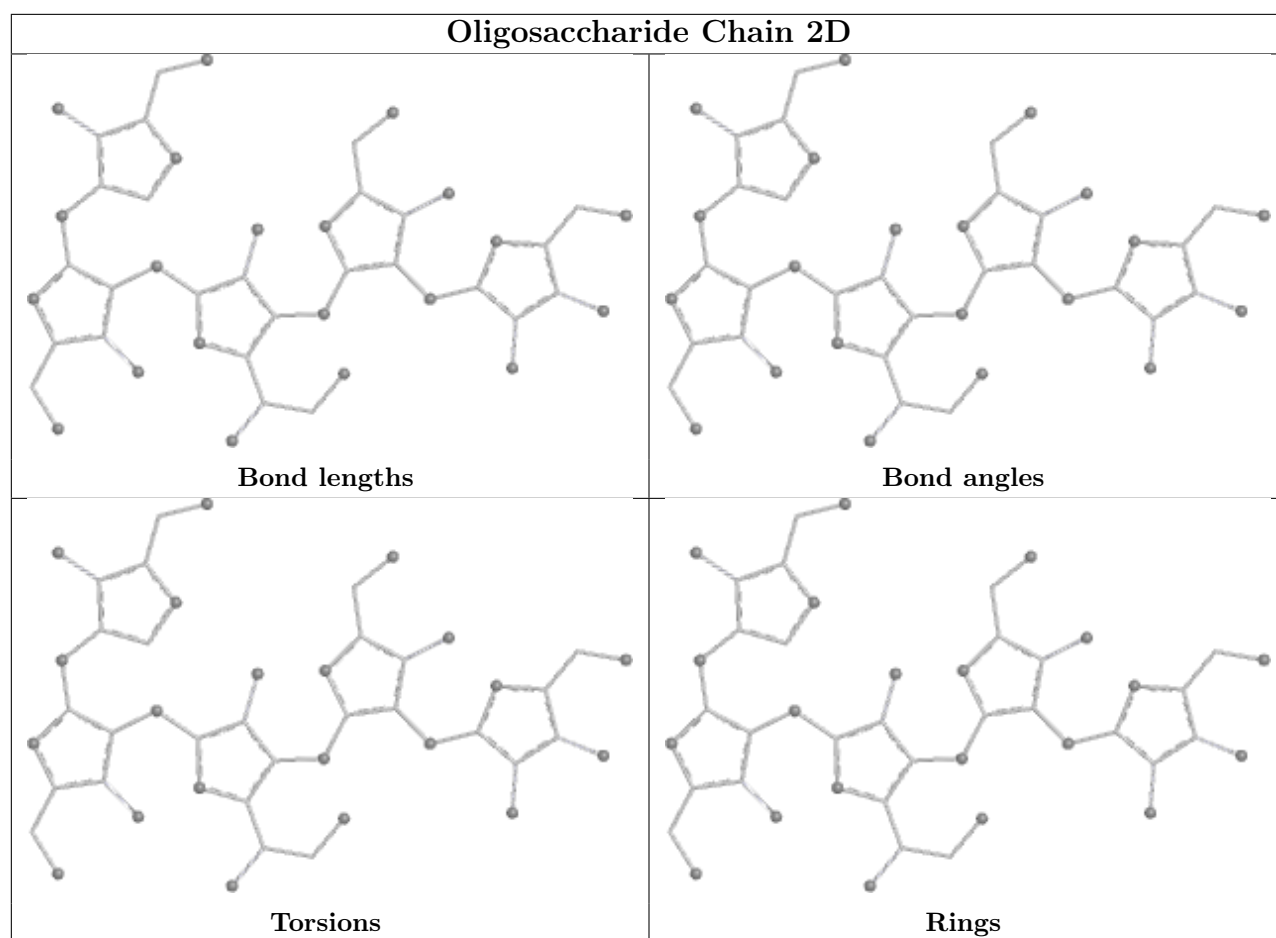
Oligosaccharide Chain 7B

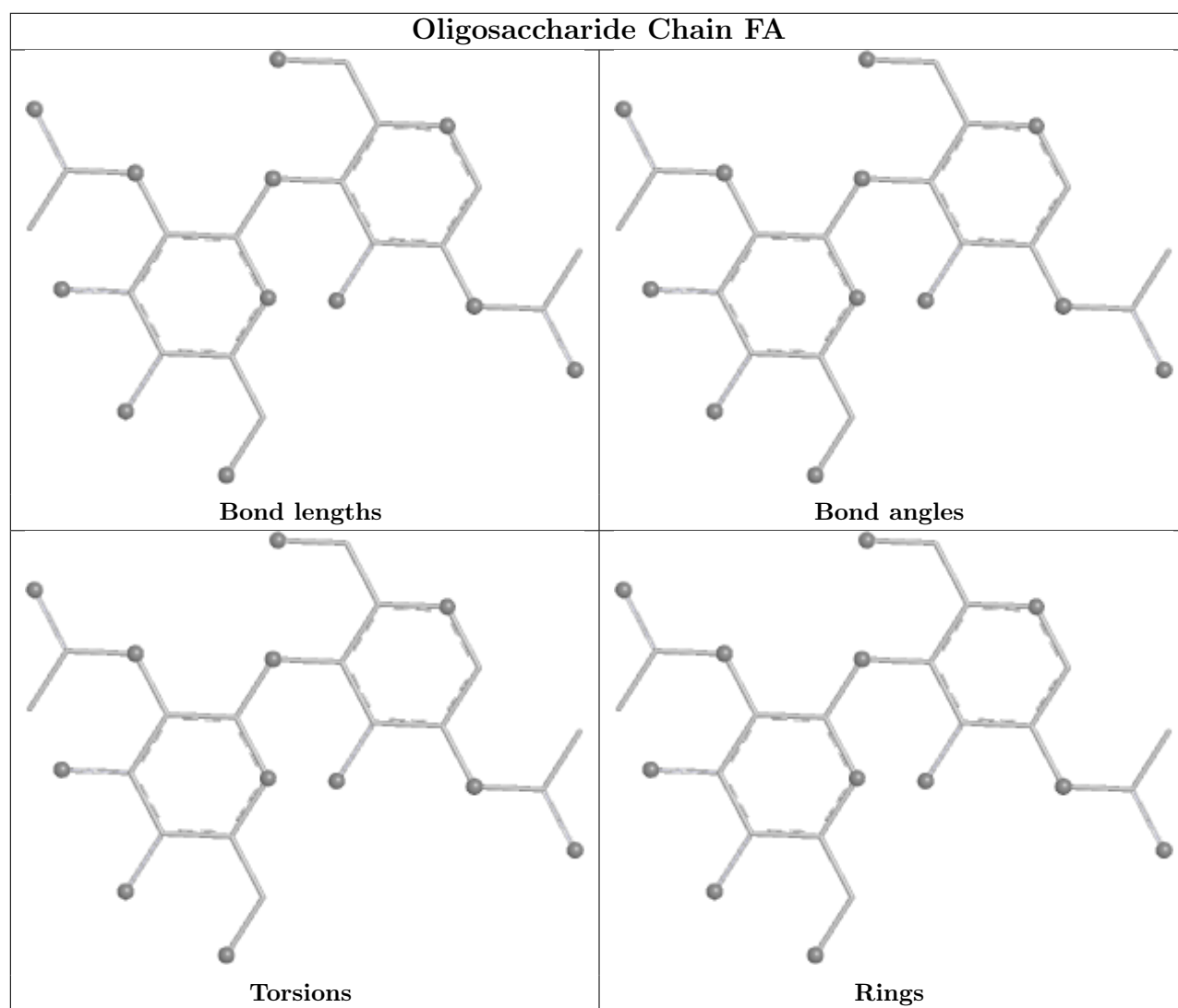


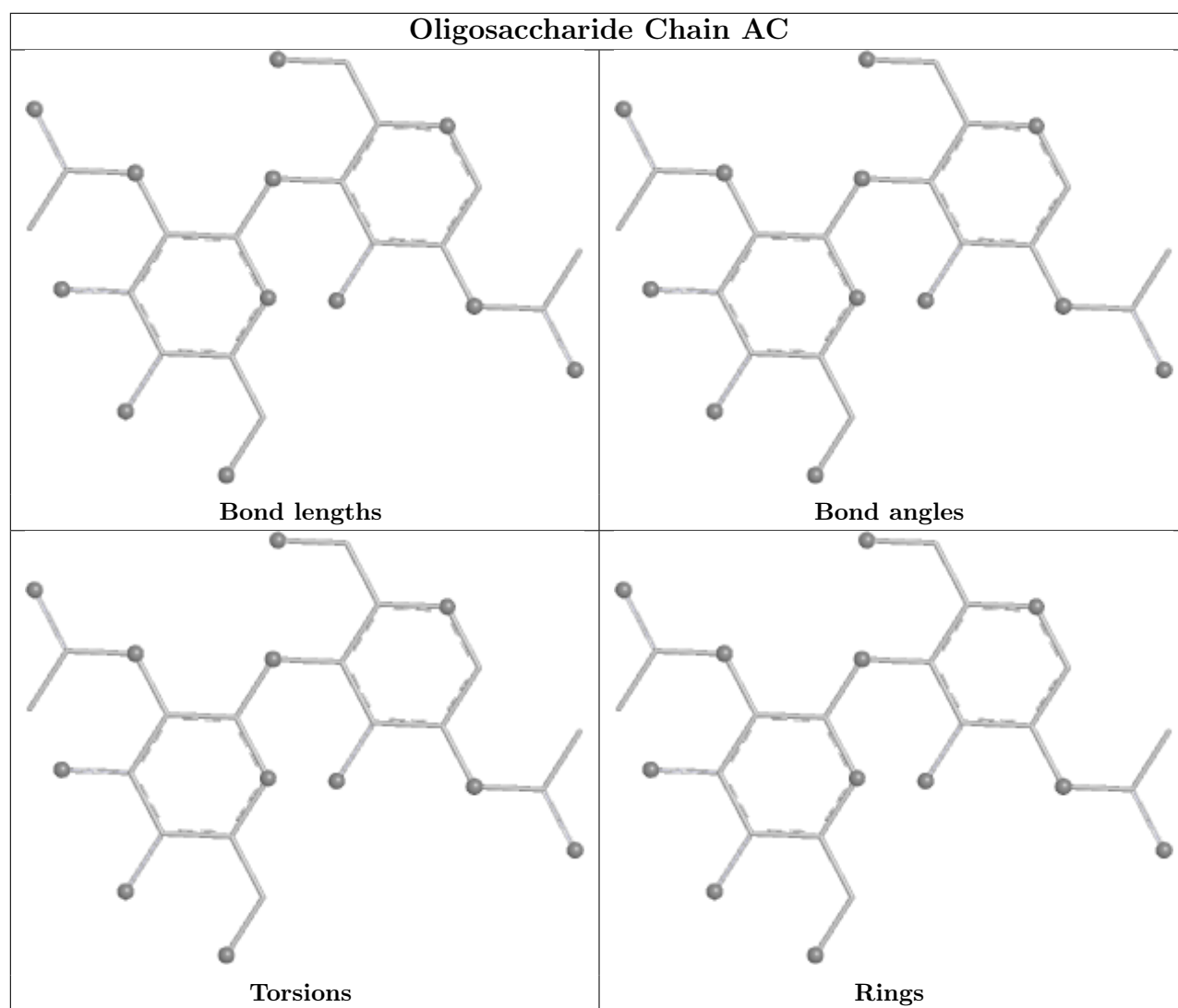


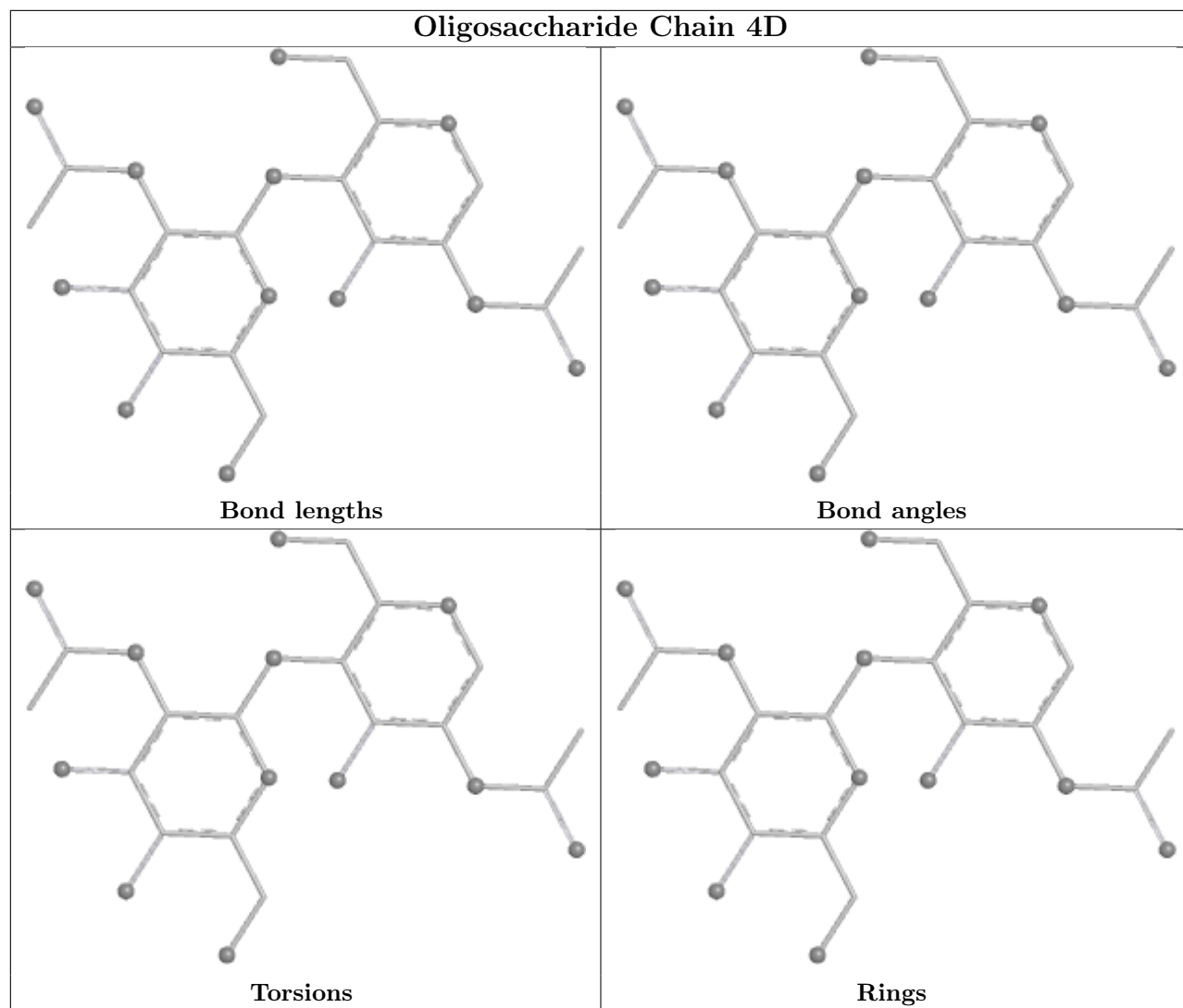


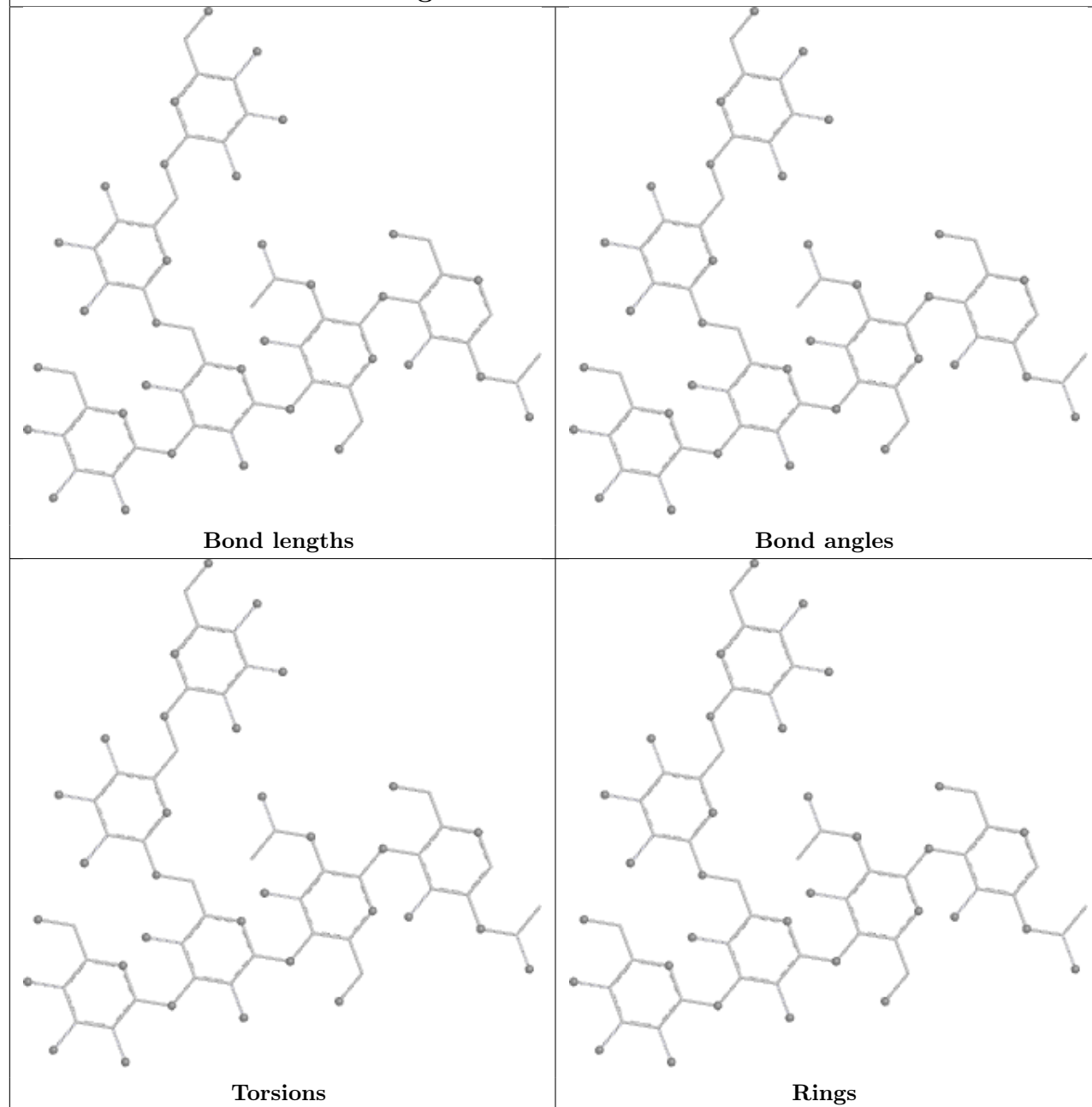


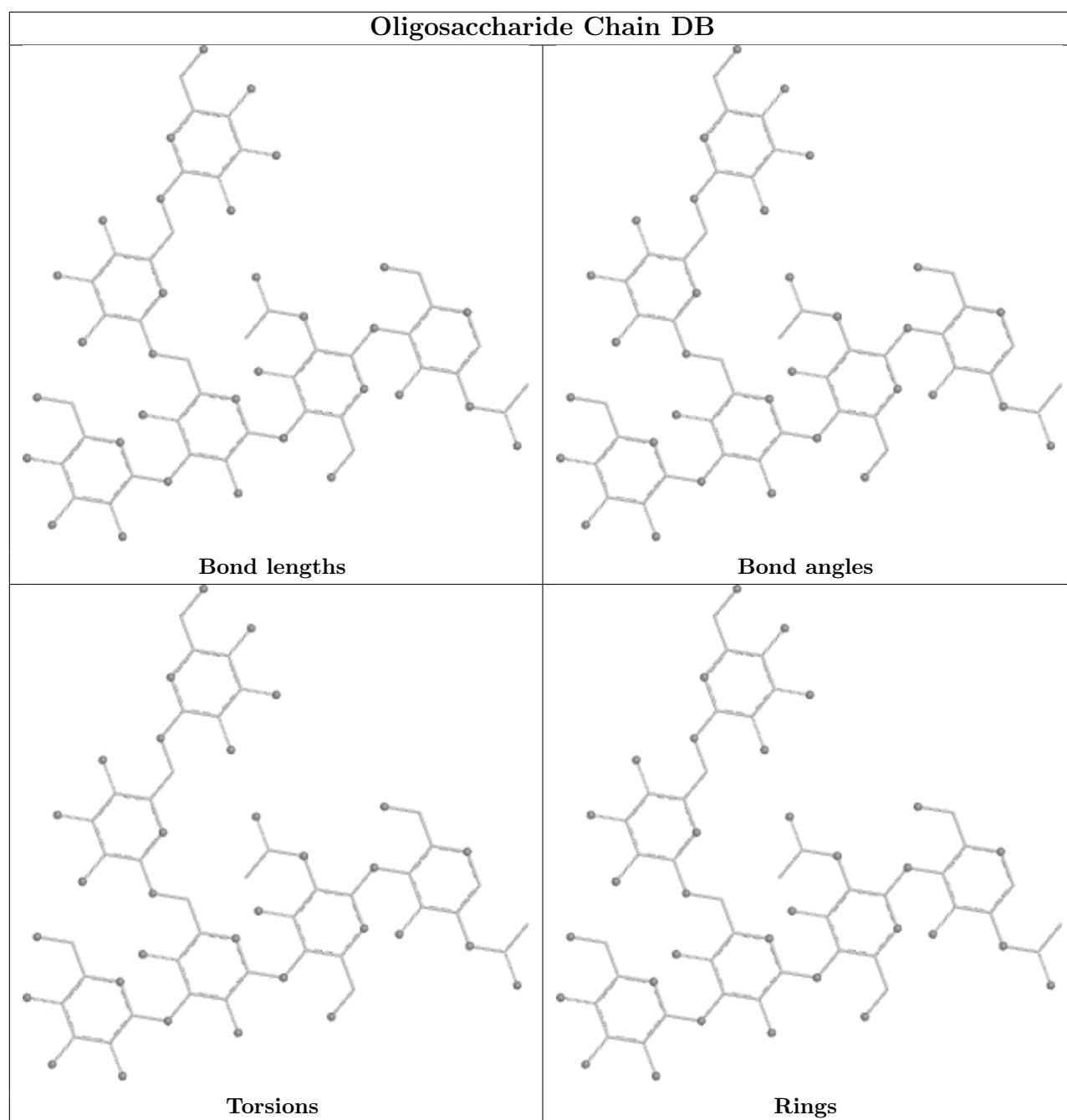


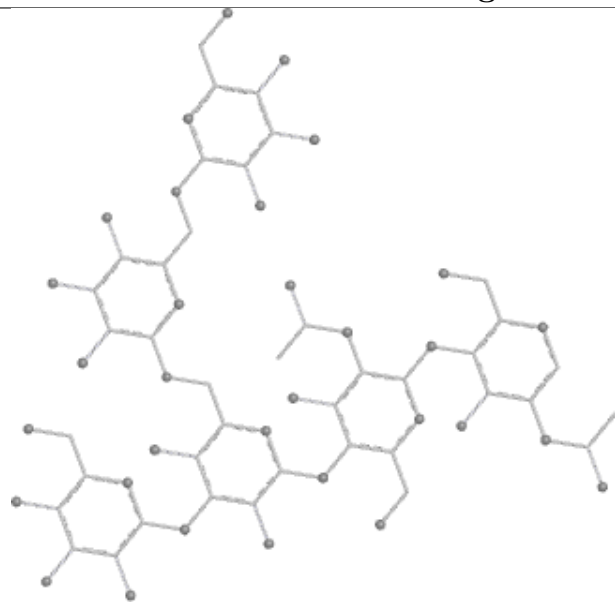
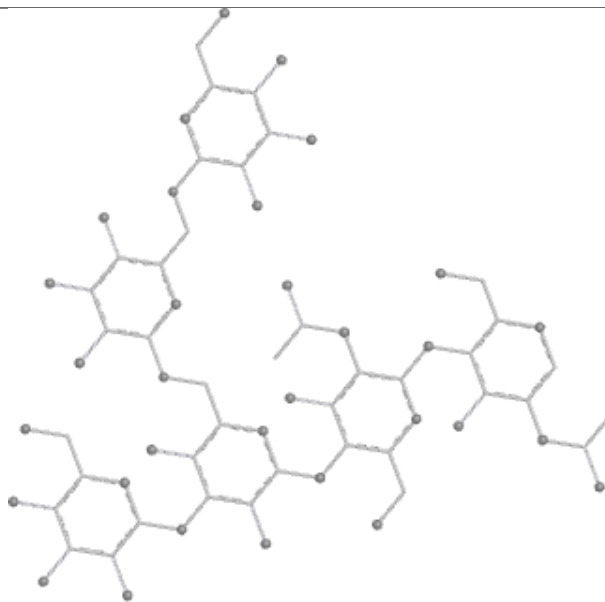
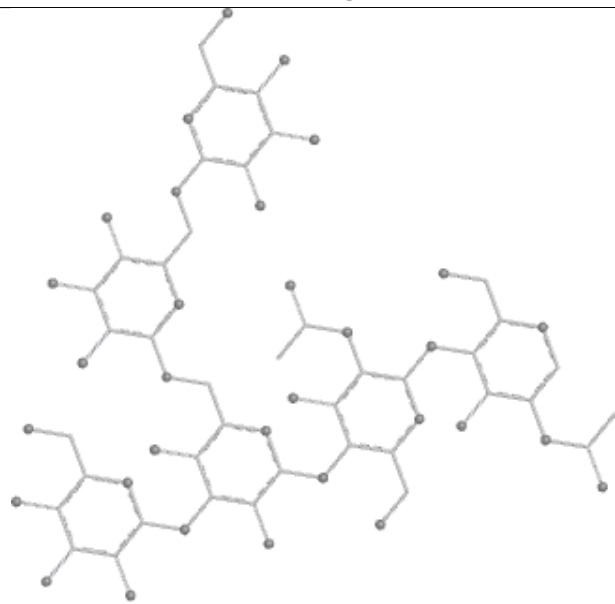
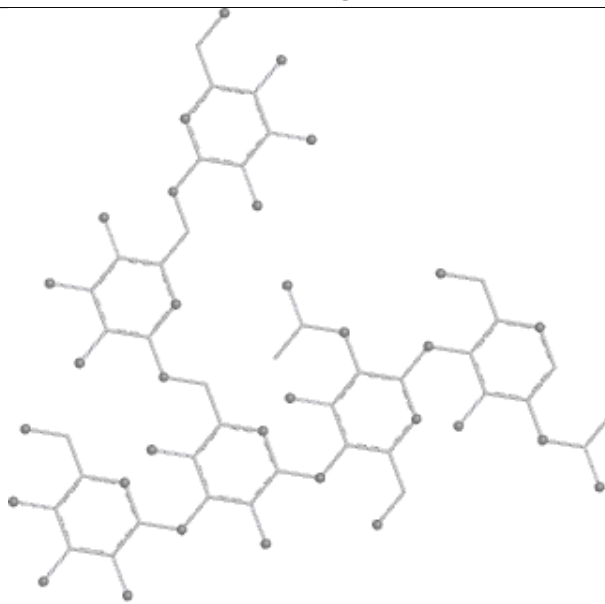


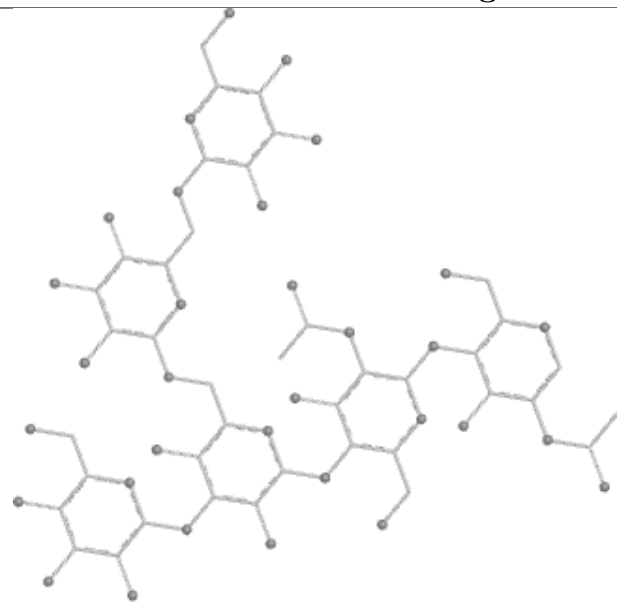
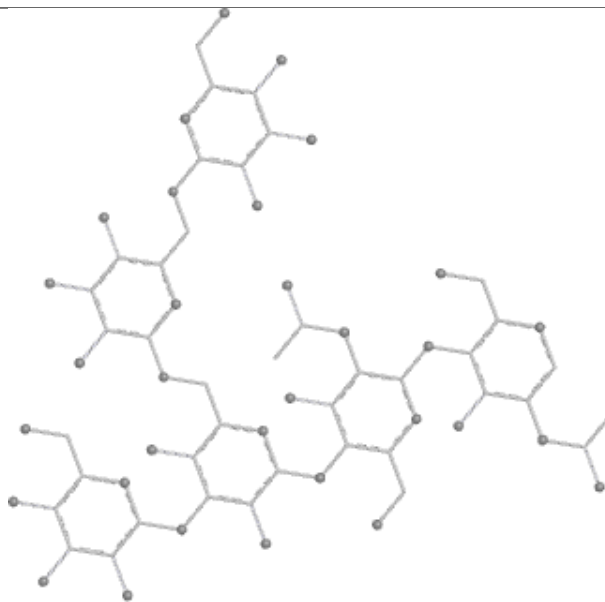
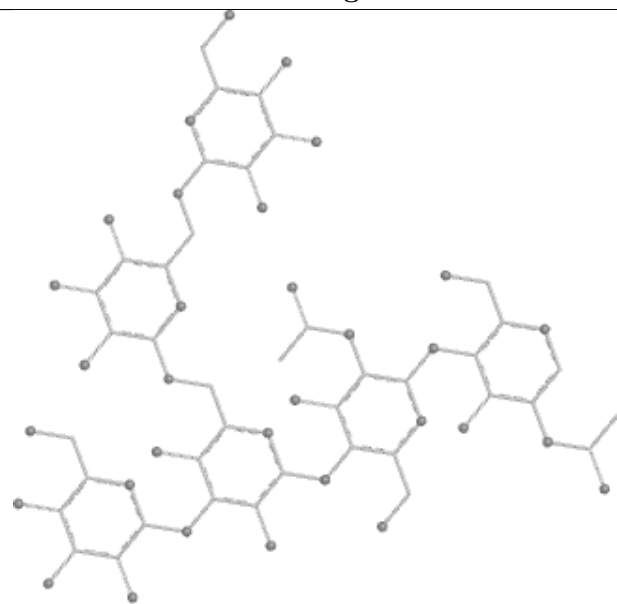
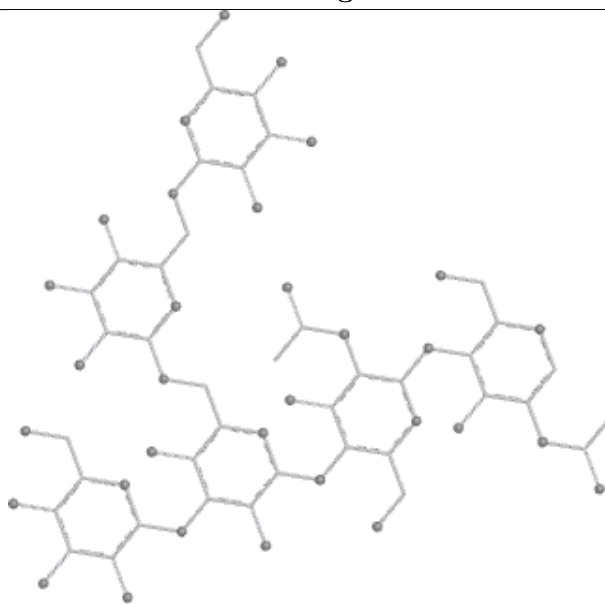




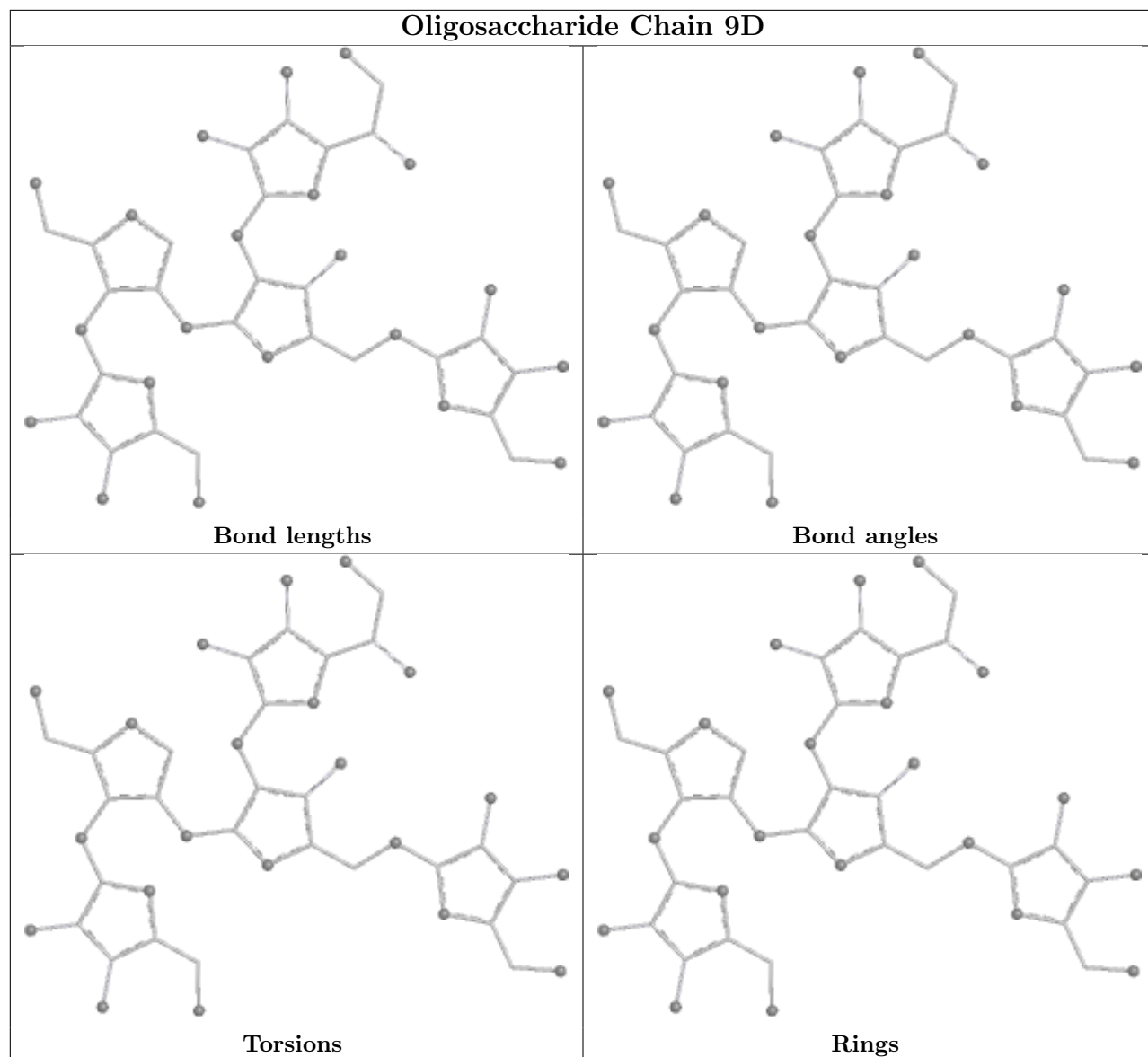
Oligosaccharide Chain GA

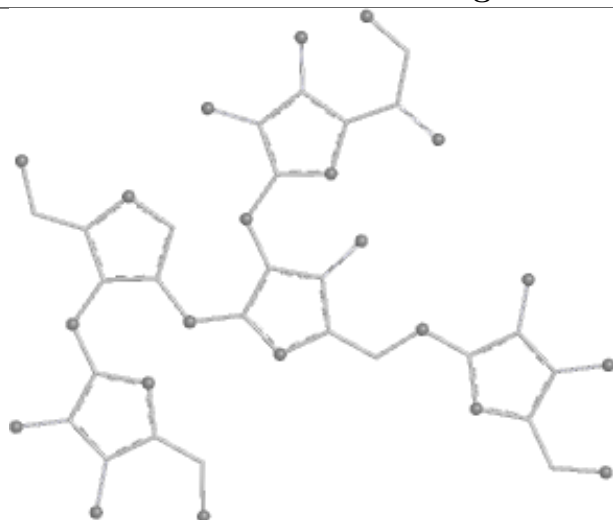
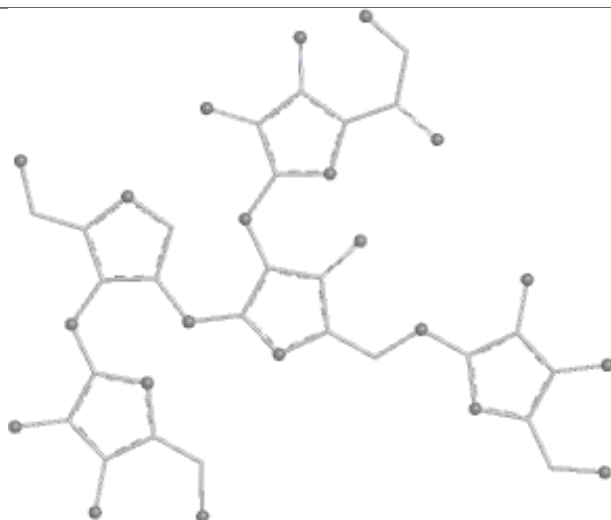
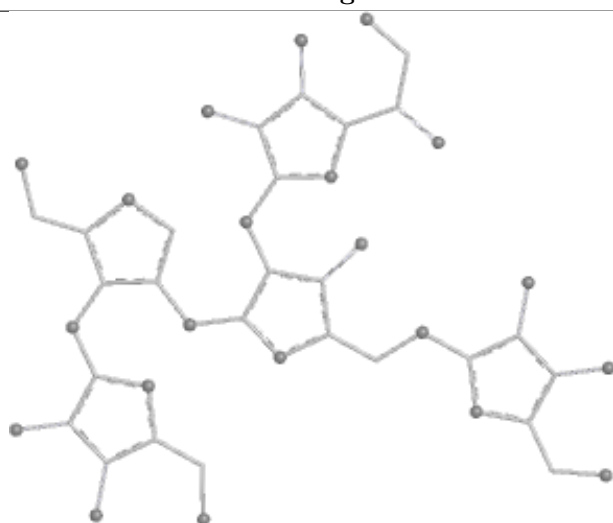
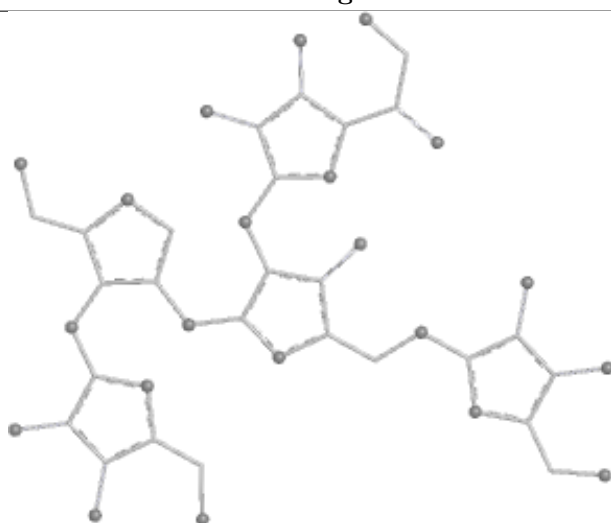


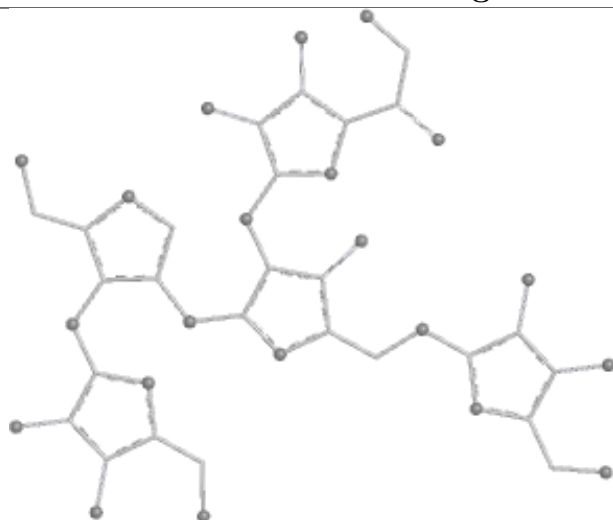
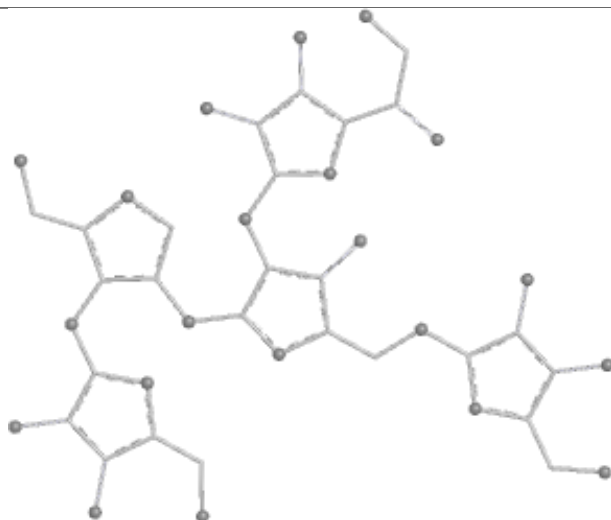
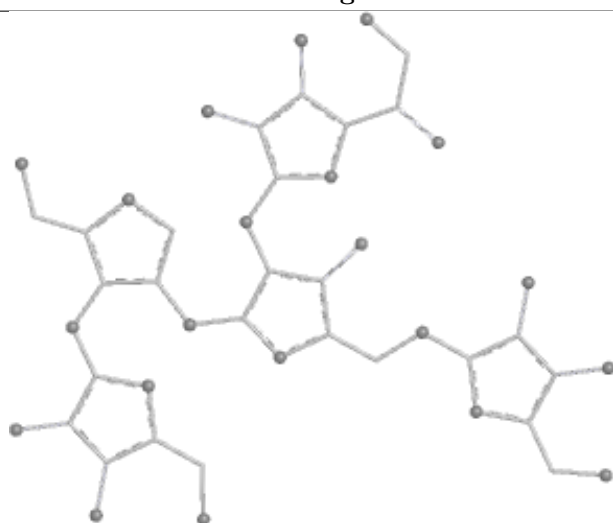
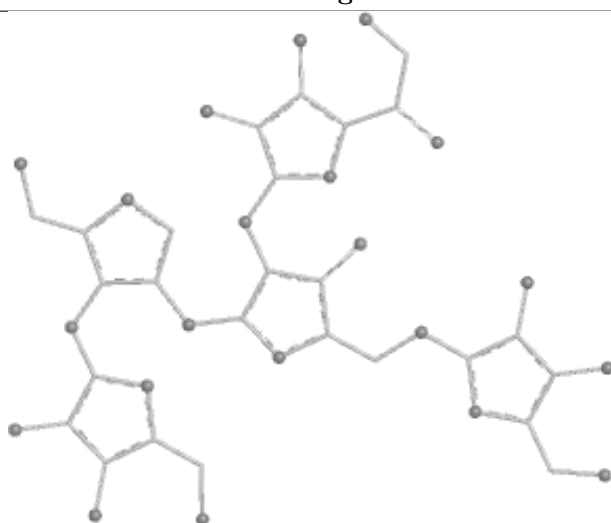
Oligosaccharide Chain 7C**Bond lengths****Bond angles****Torsions****Rings**

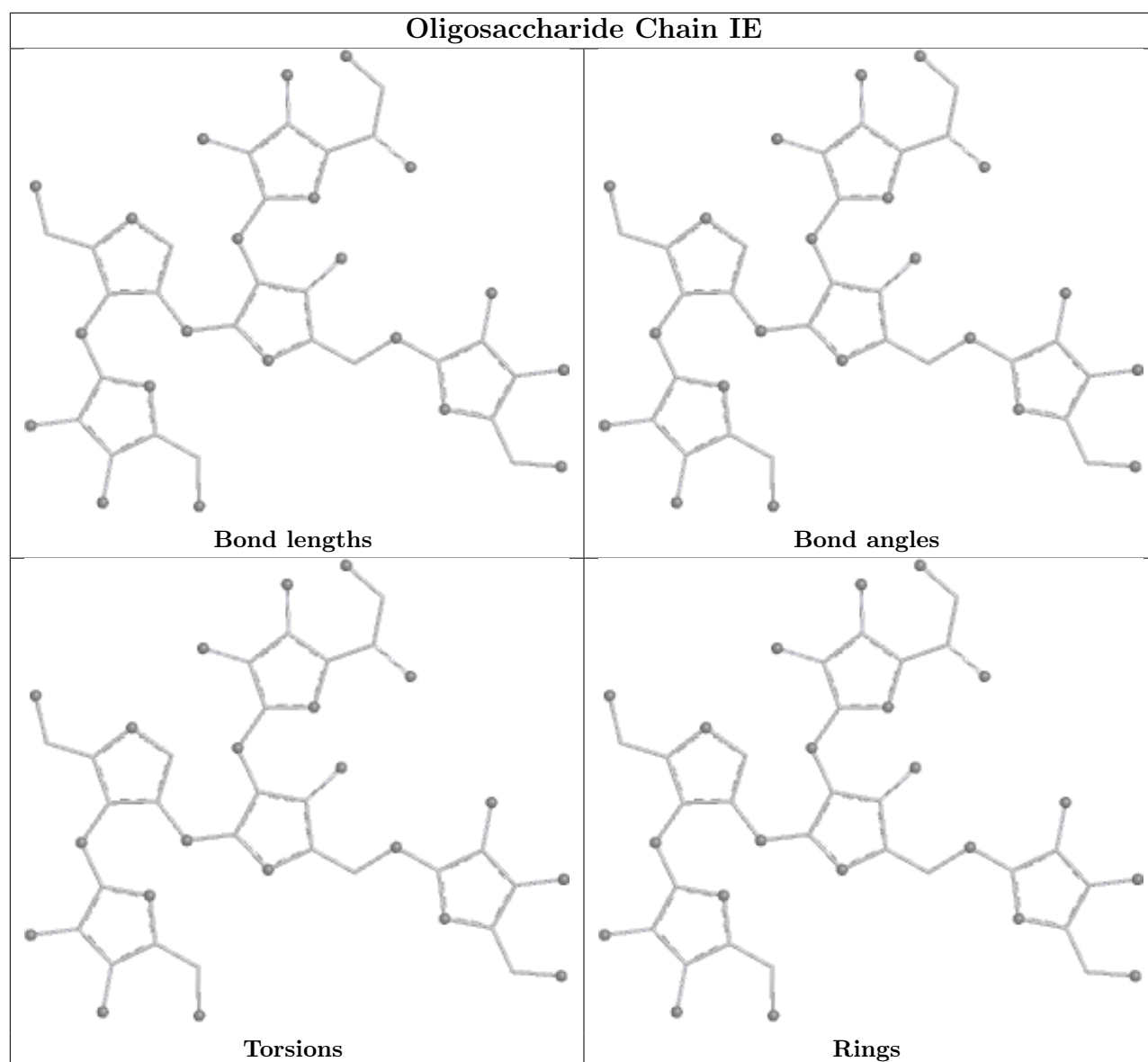
Oligosaccharide Chain 5D**Bond lengths****Bond angles****Torsions****Rings**

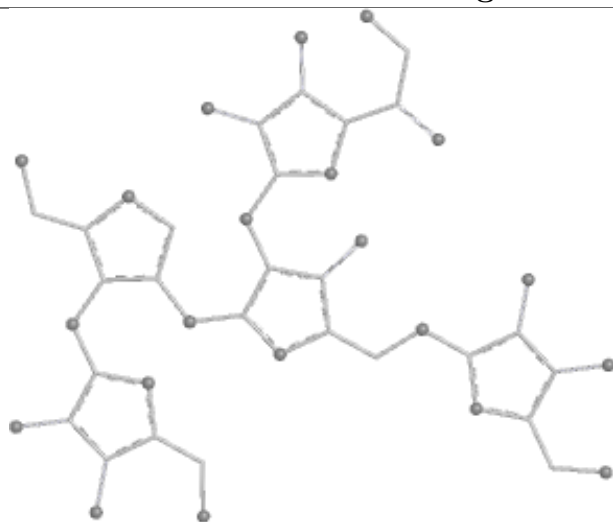
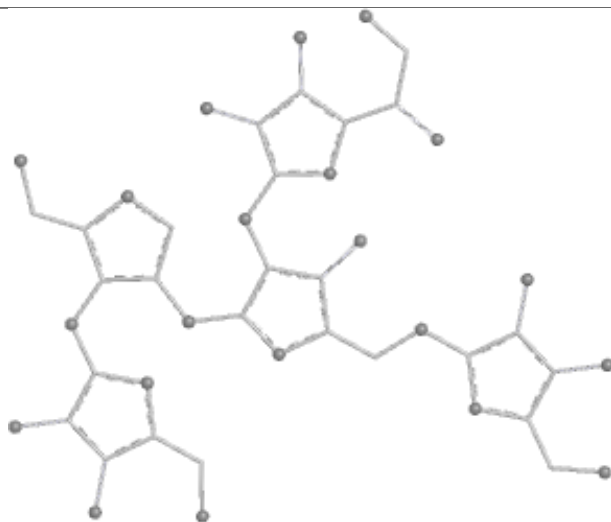
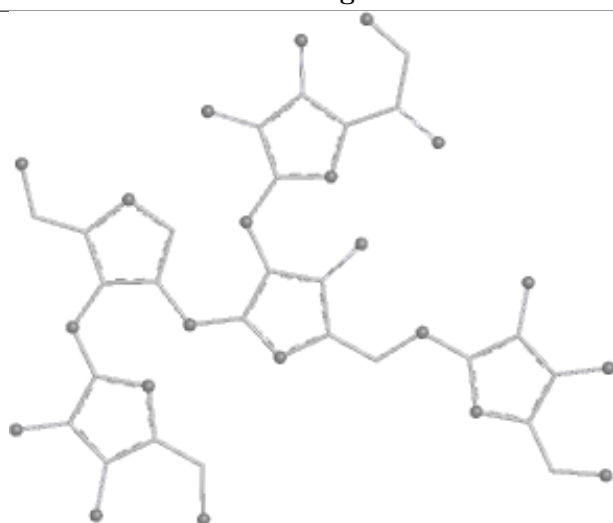
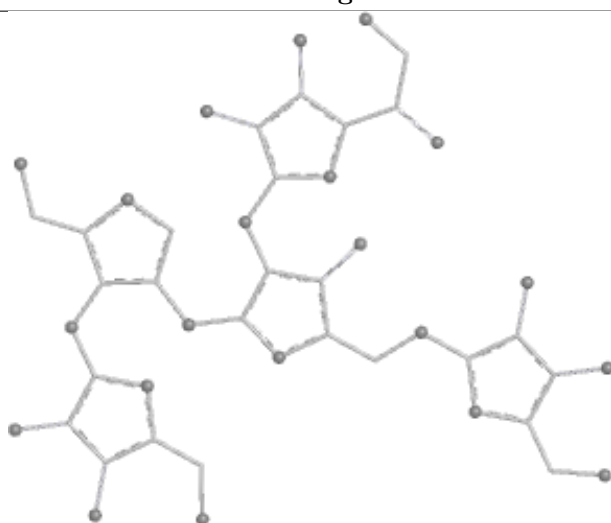
Oligosaccharide Chain 9D

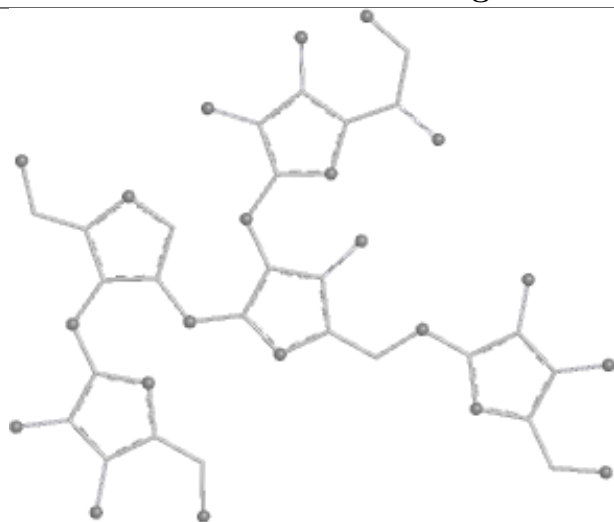
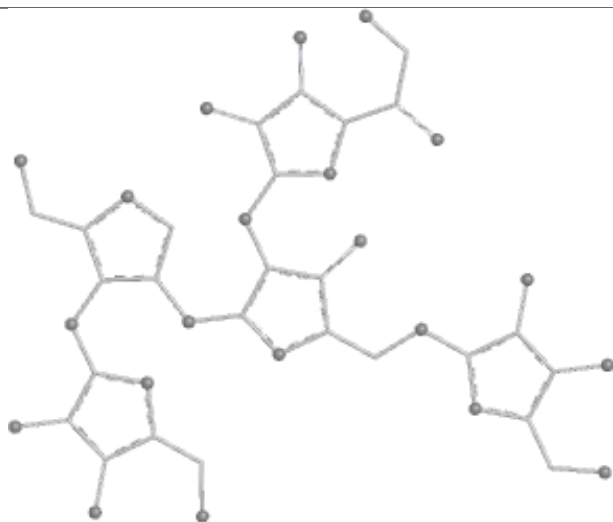
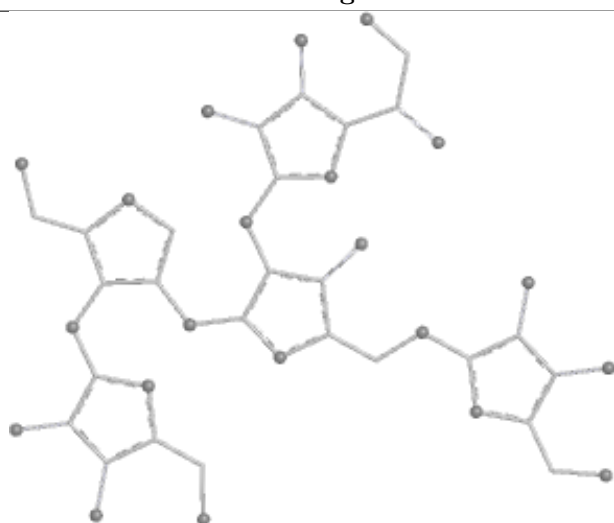
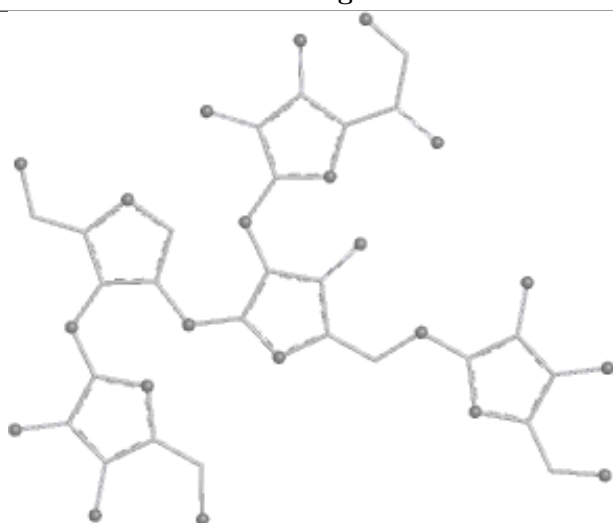


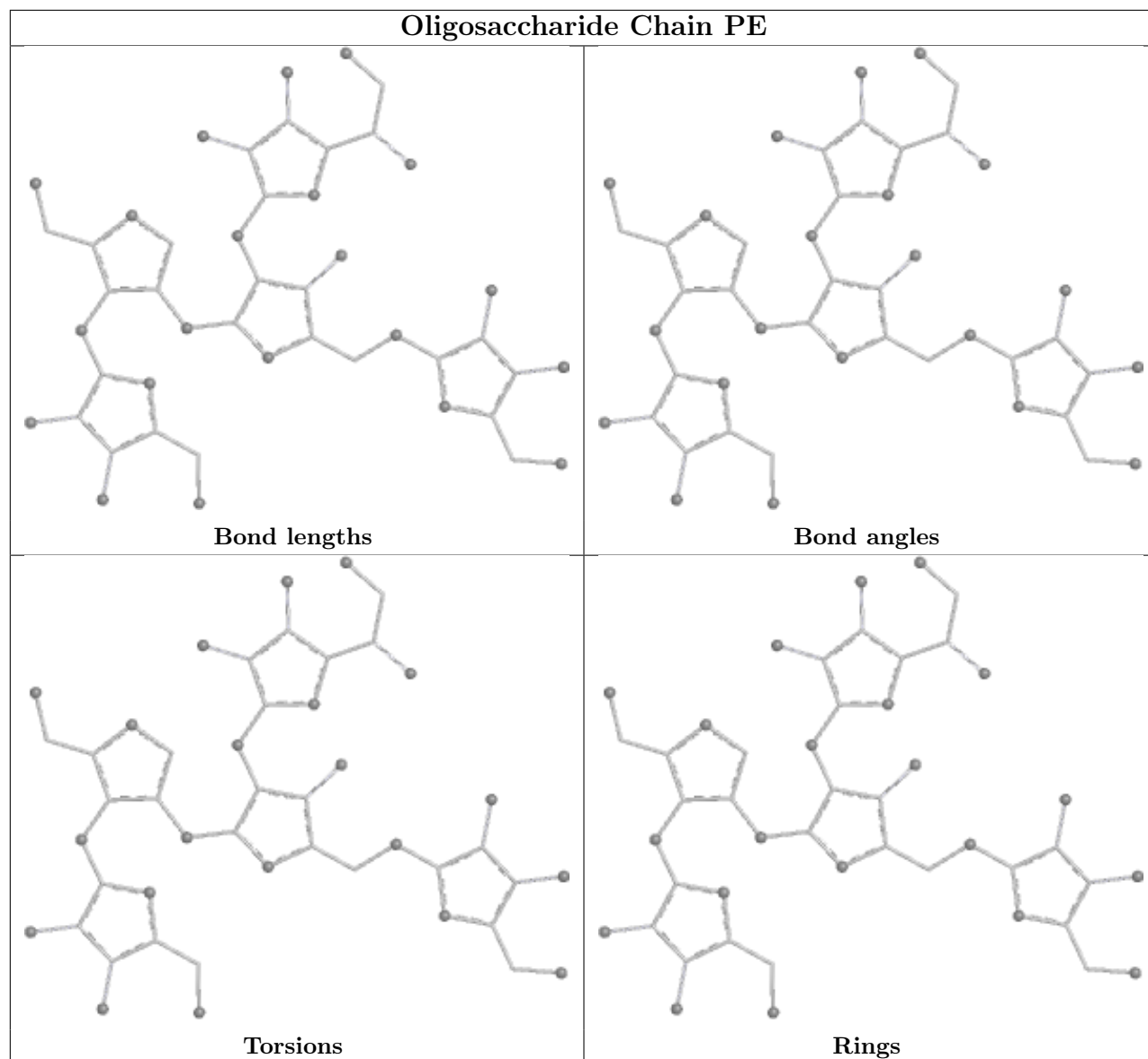
Oligosaccharide Chain BE**Bond lengths****Bond angles****Torsions****Rings**

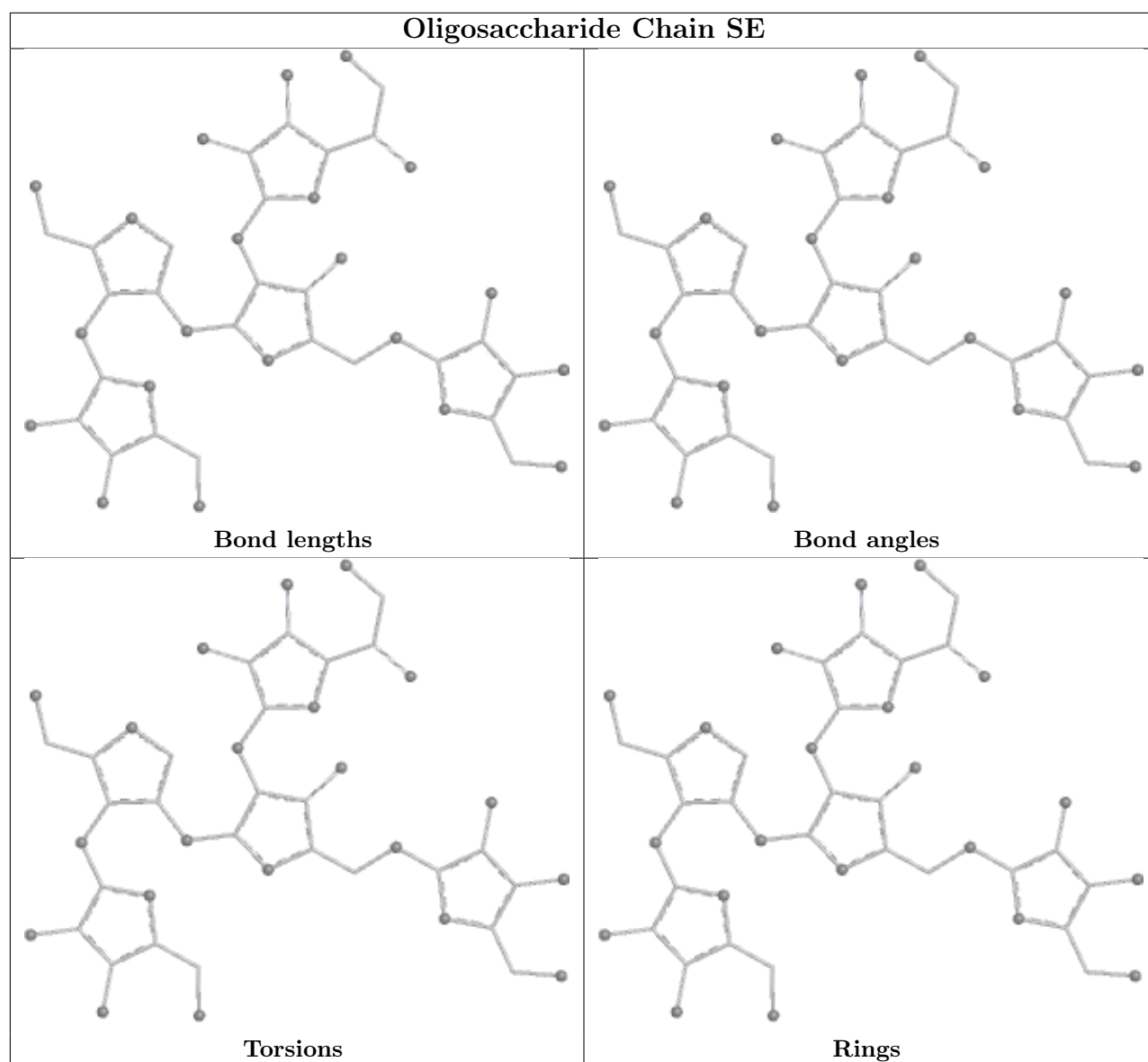
Oligosaccharide Chain DE**Bond lengths****Bond angles****Torsions****Rings**

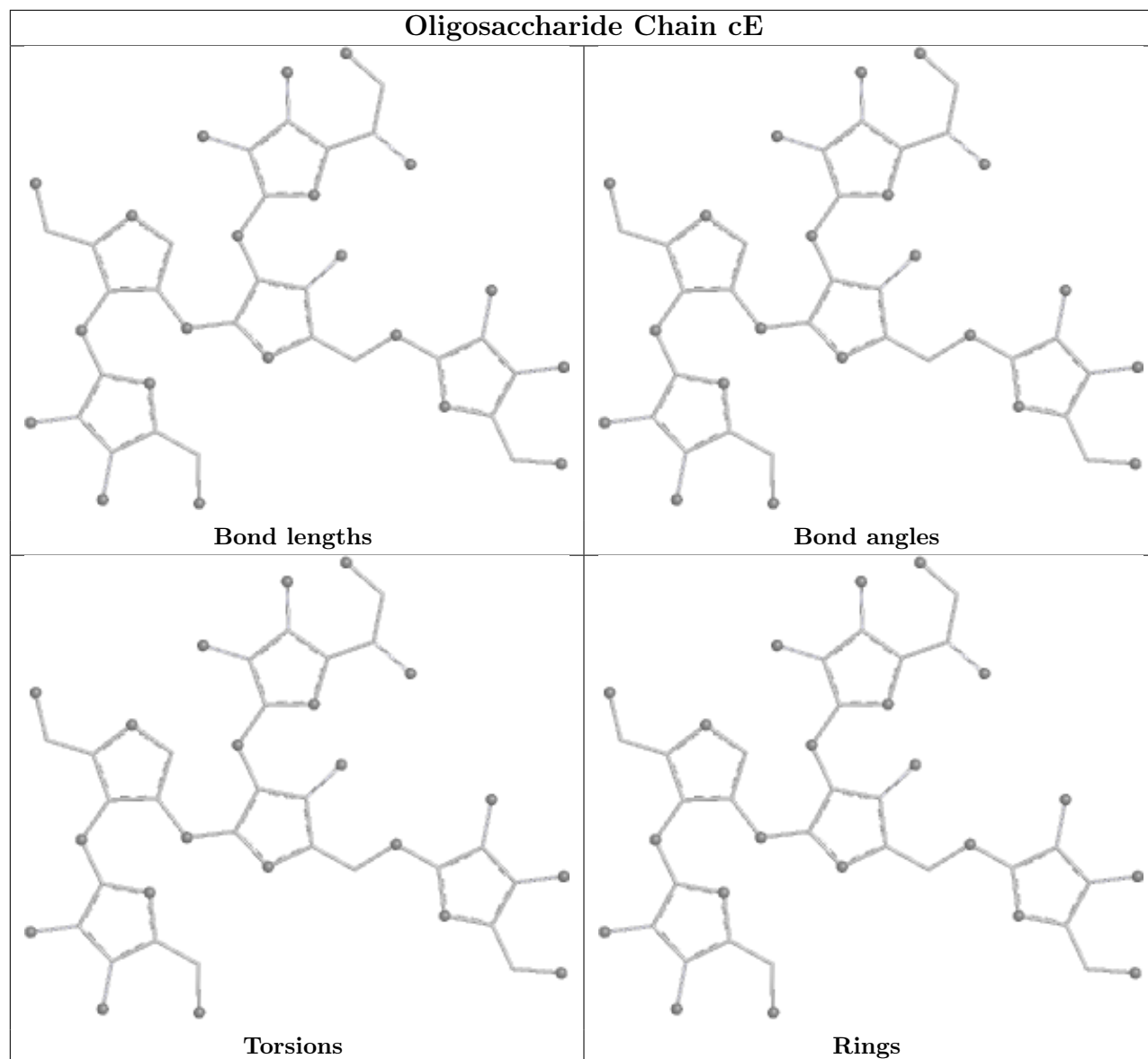


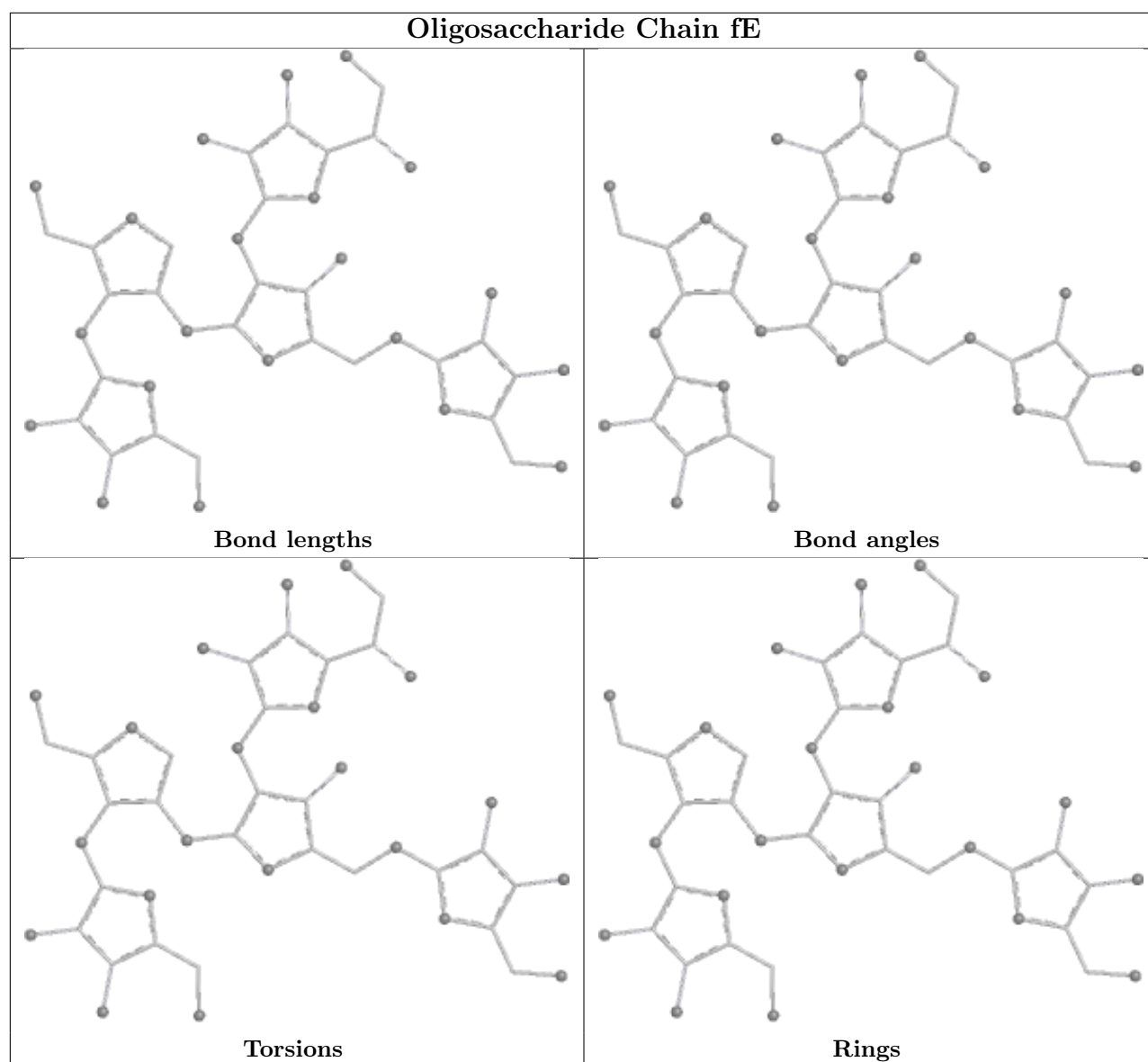
Oligosaccharide Chain JE**Bond lengths****Bond angles****Torsions****Rings**

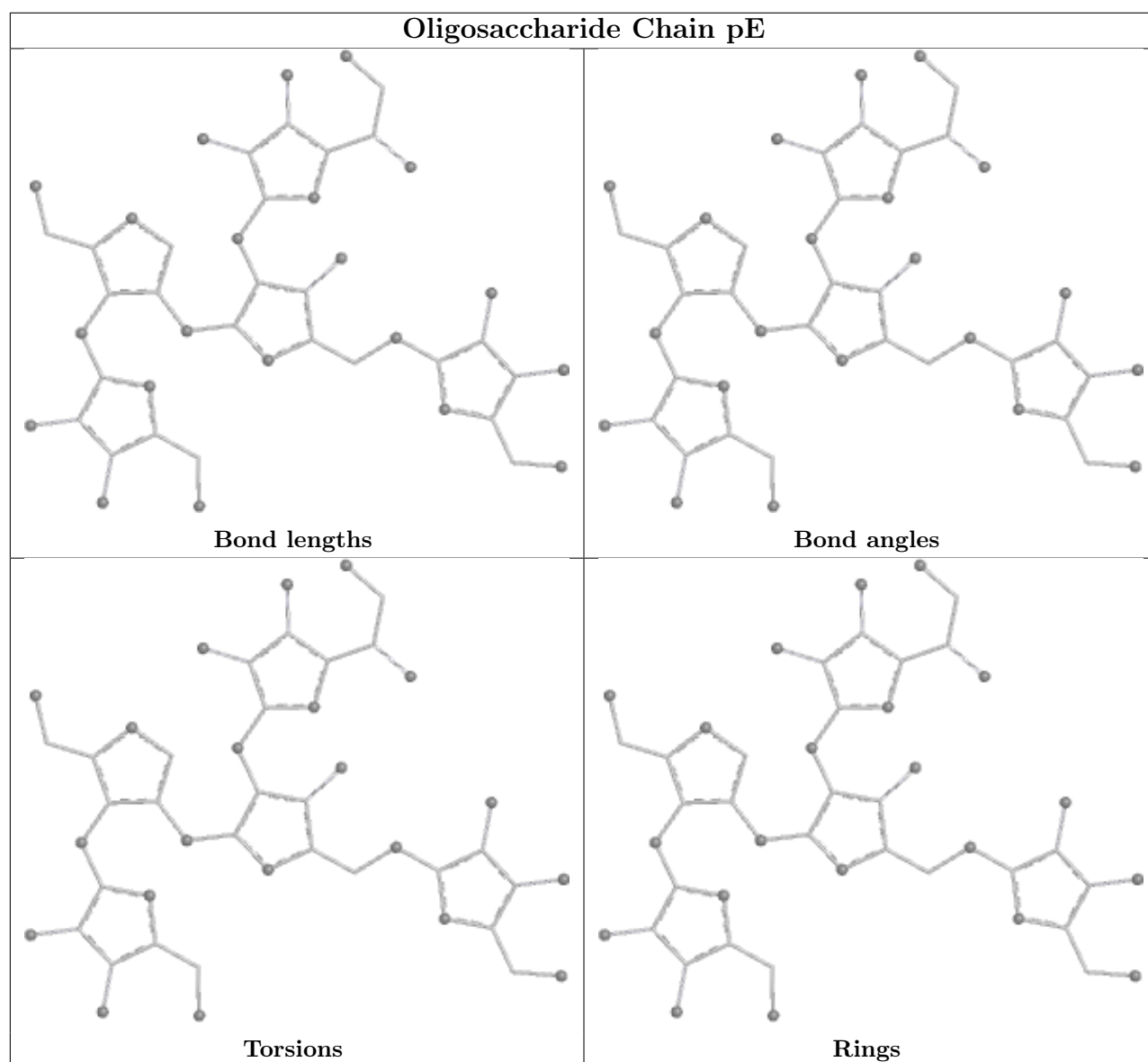
Oligosaccharide Chain KE**Bond lengths****Bond angles****Torsions****Rings**

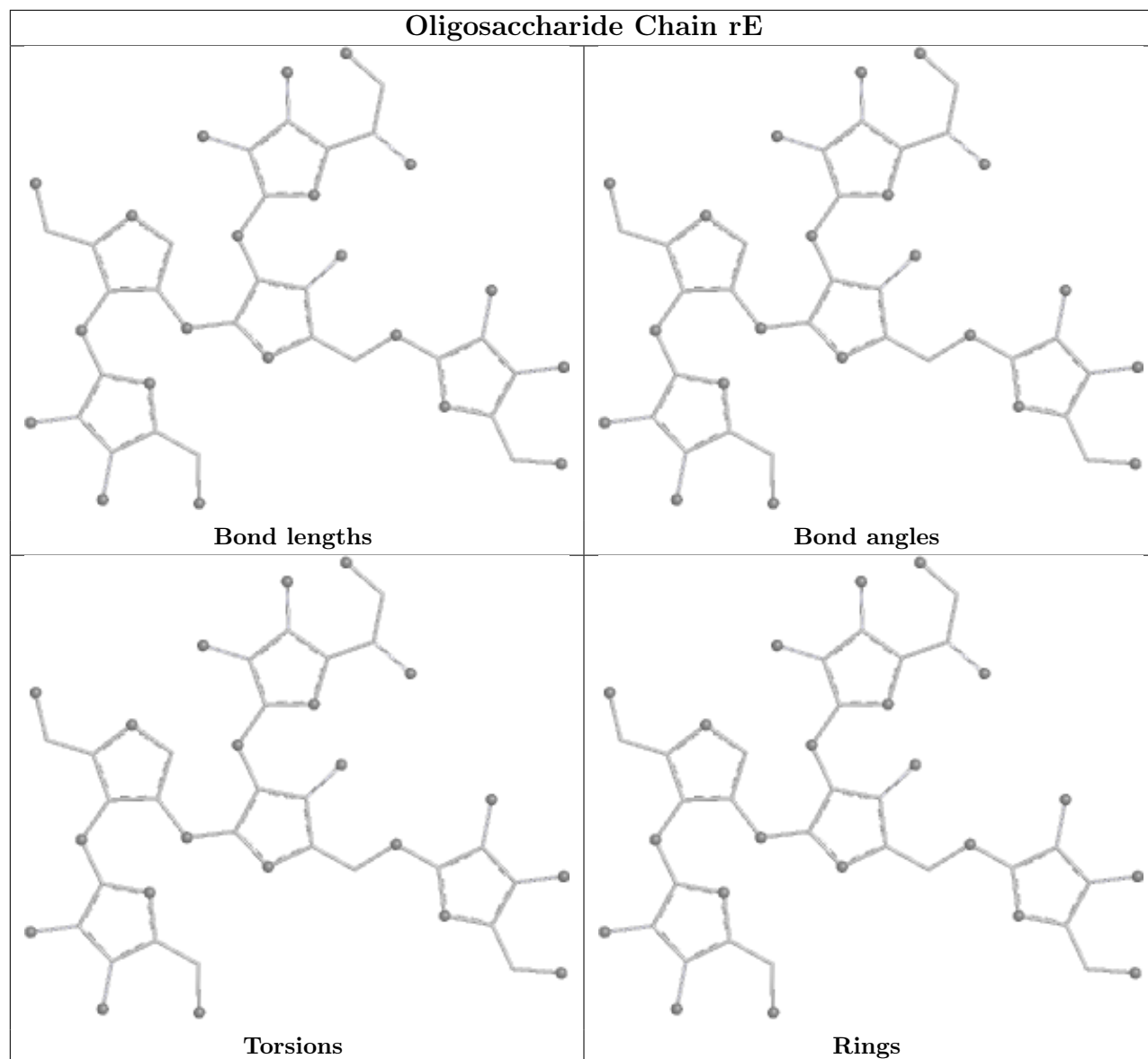


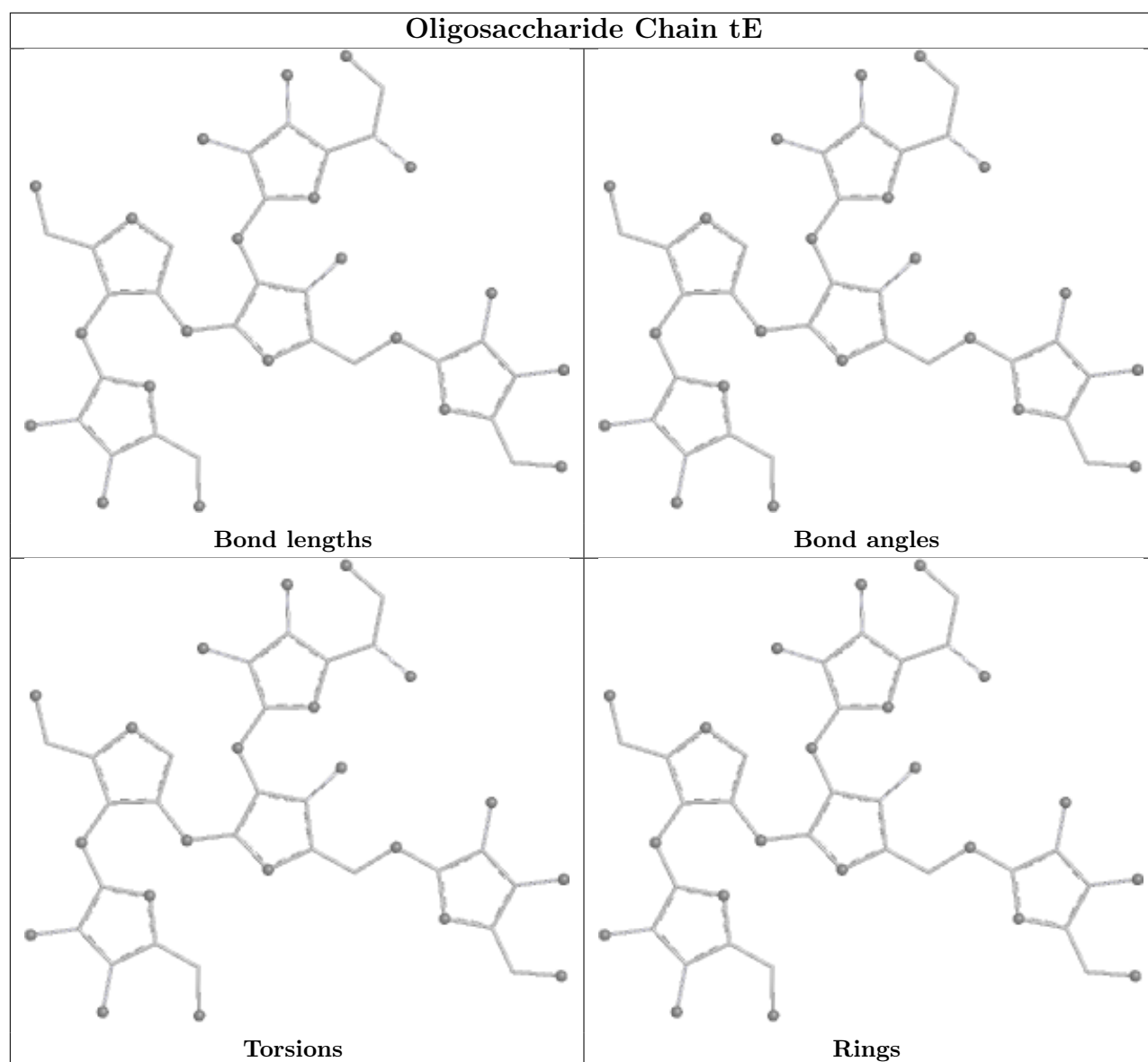


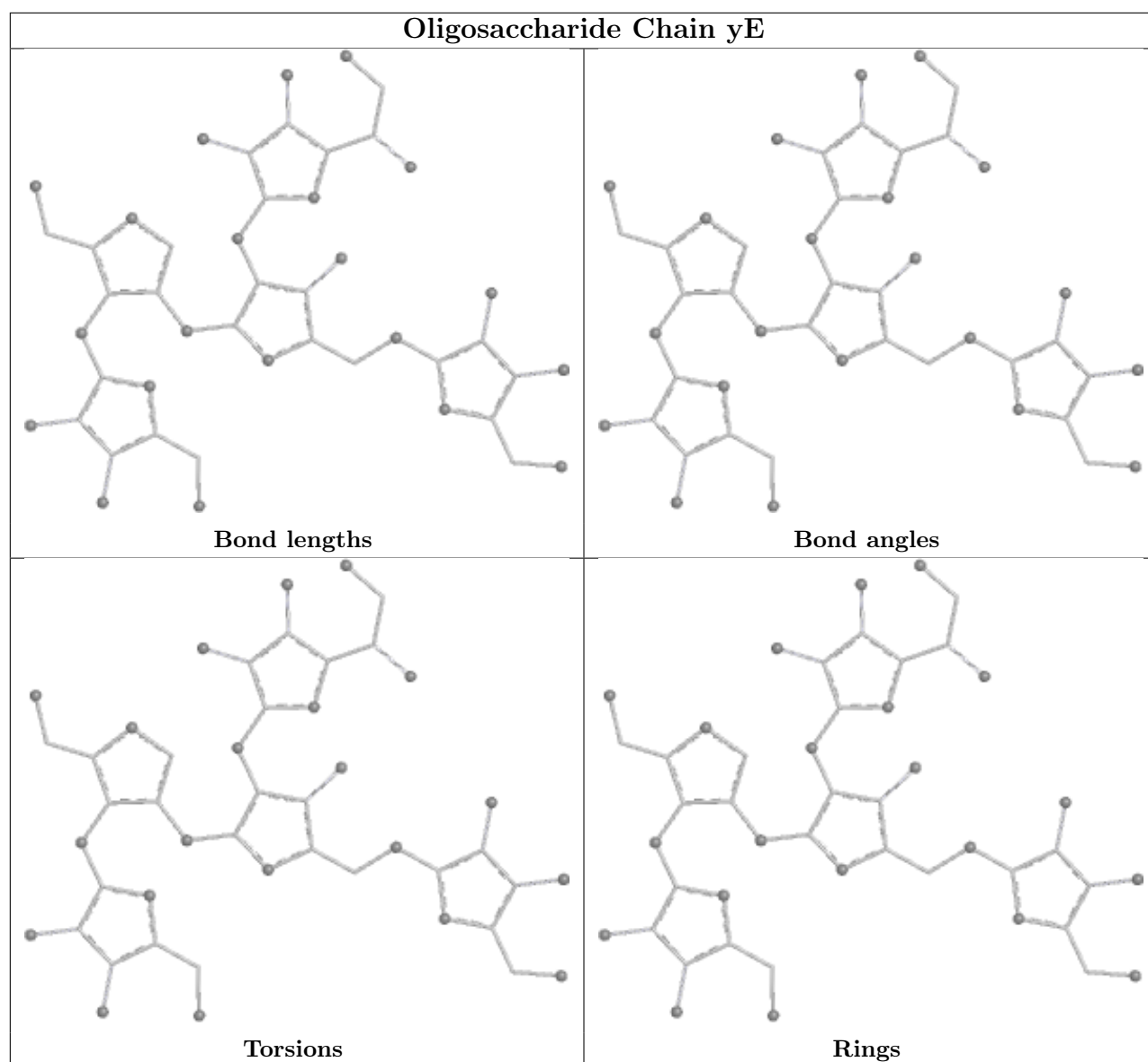


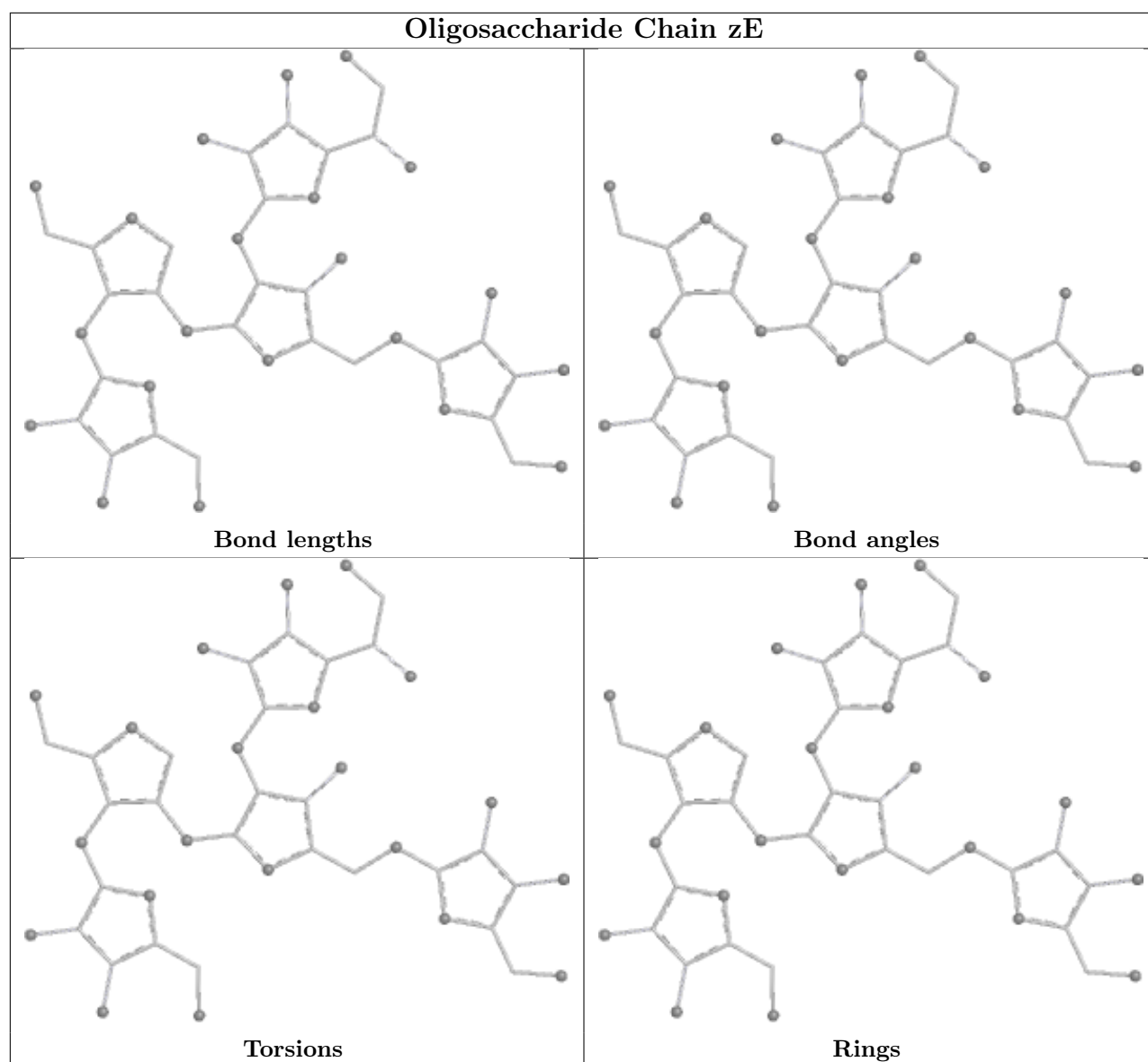


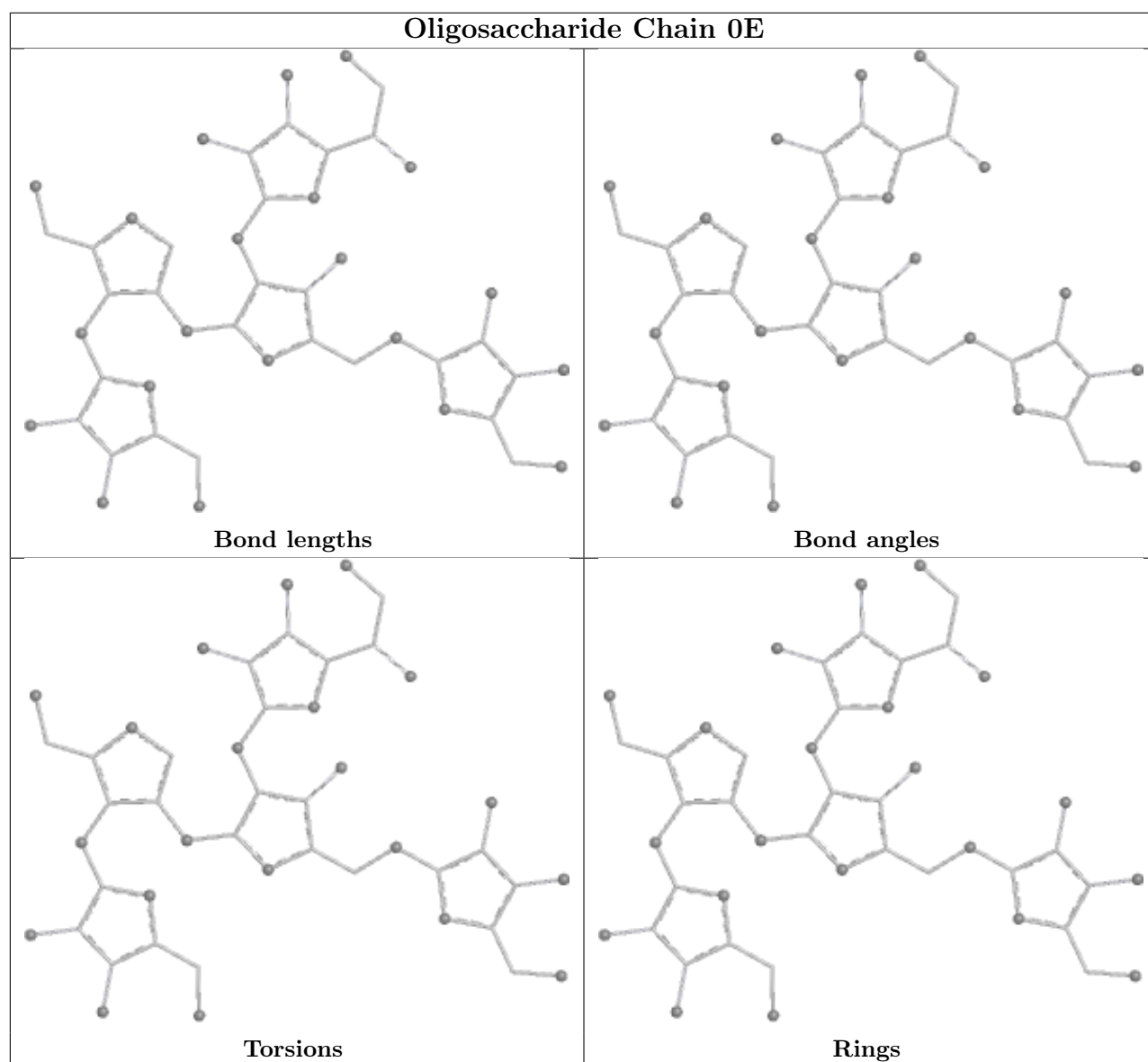


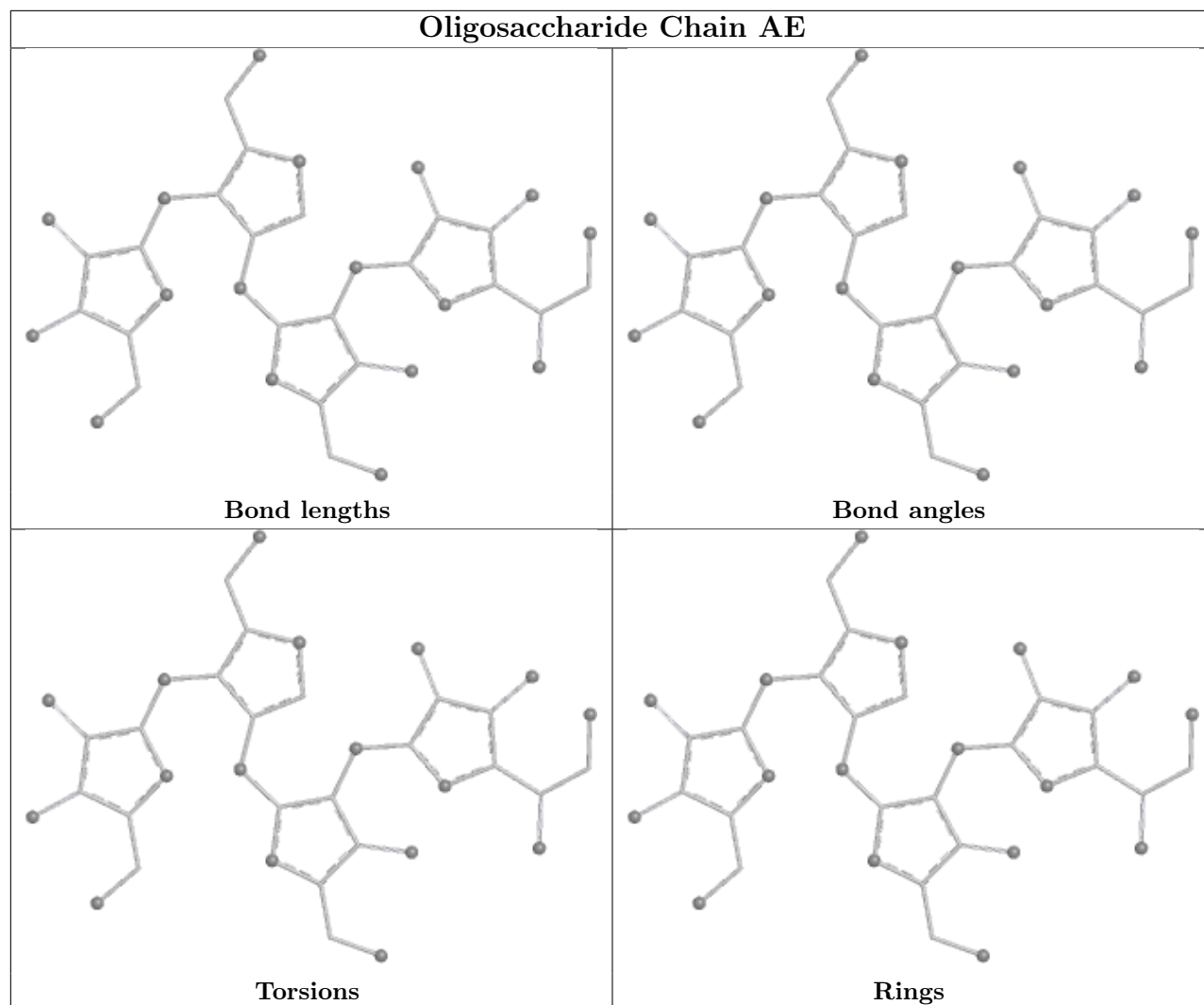


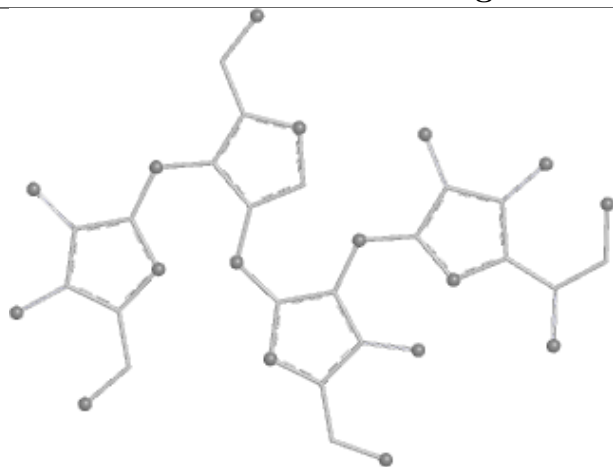
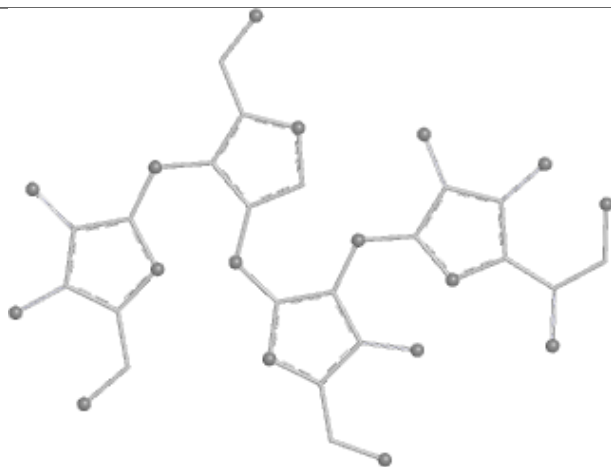
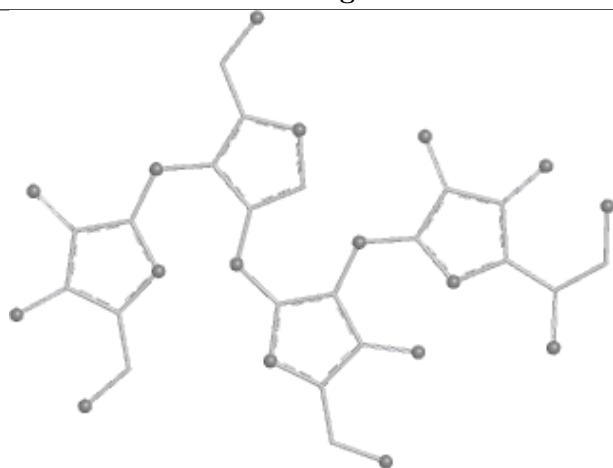
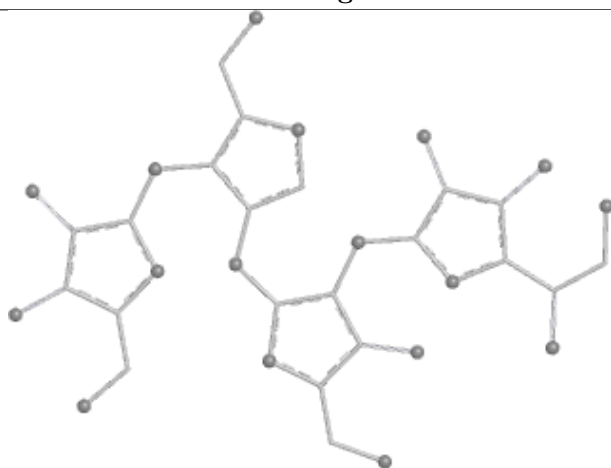




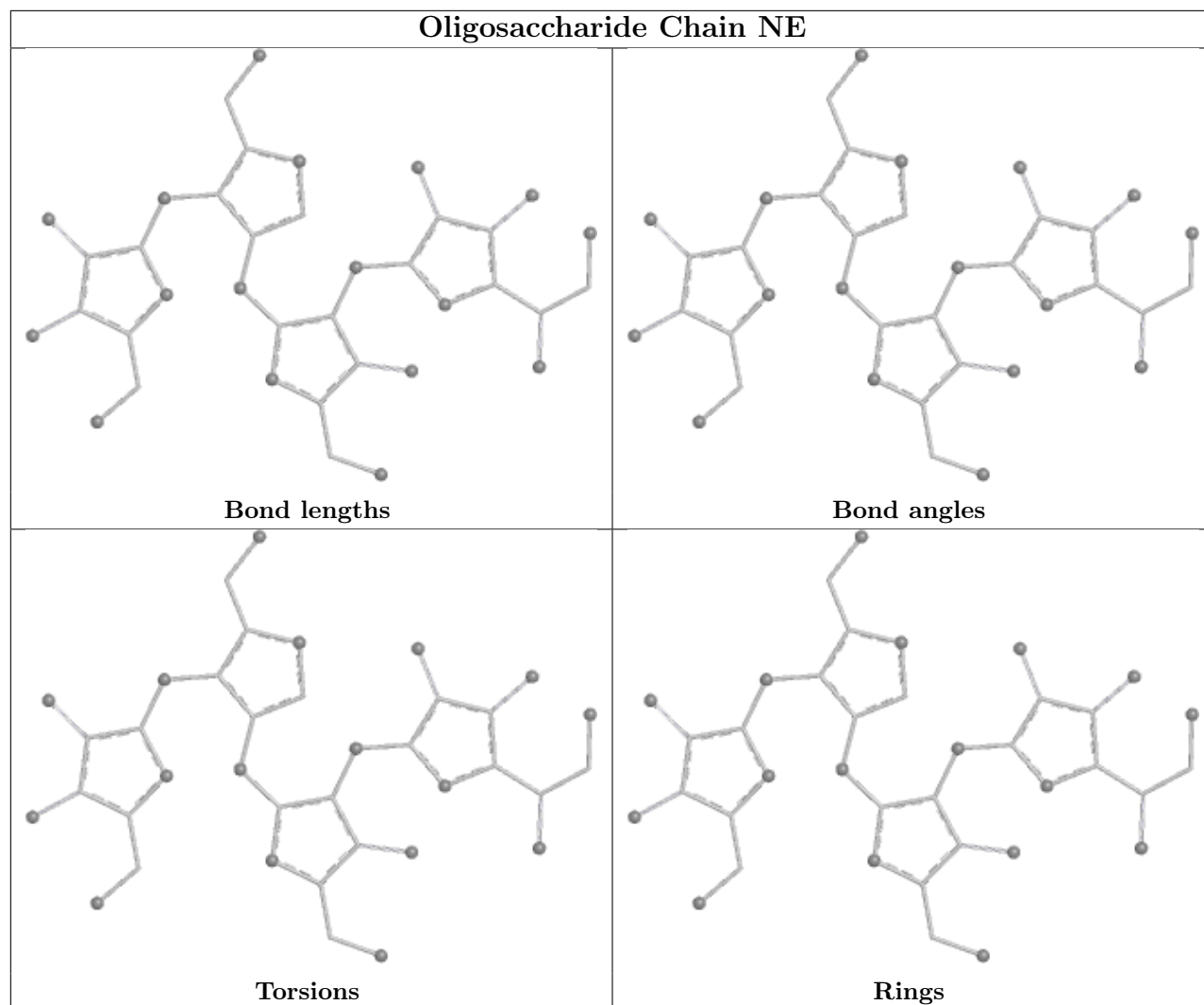


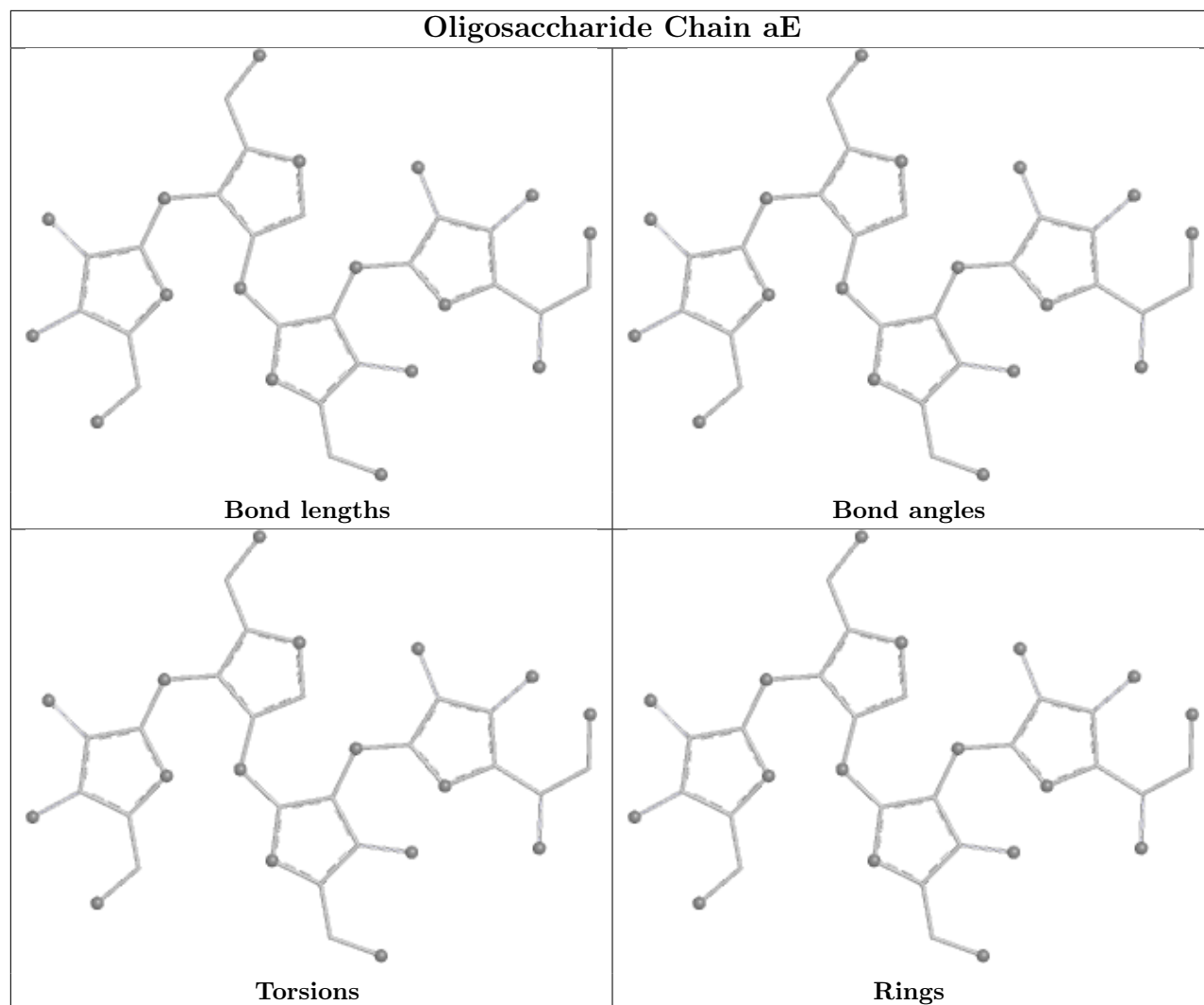


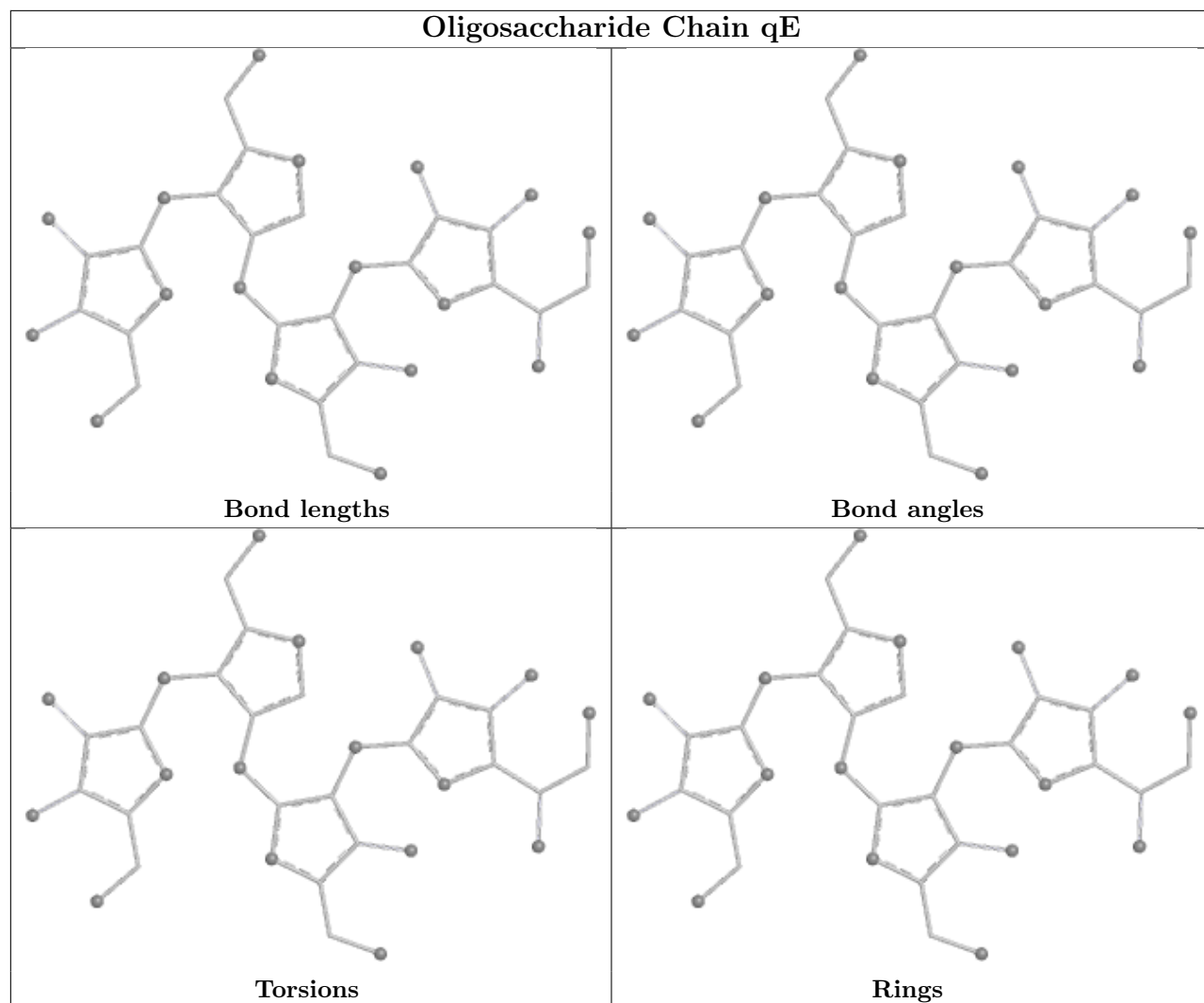


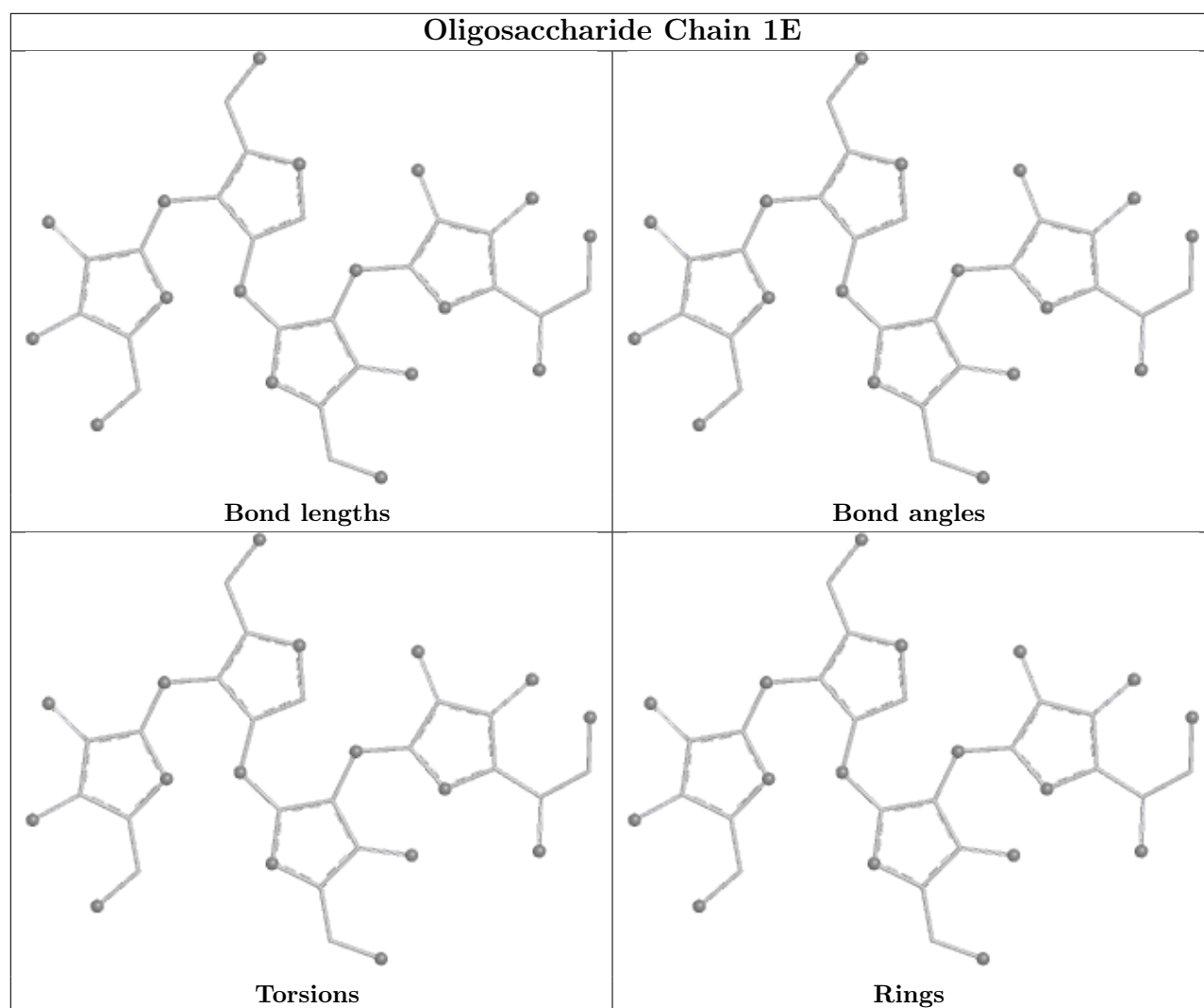
Oligosaccharide Chain LE**Bond lengths****Bond angles****Torsions****Rings**

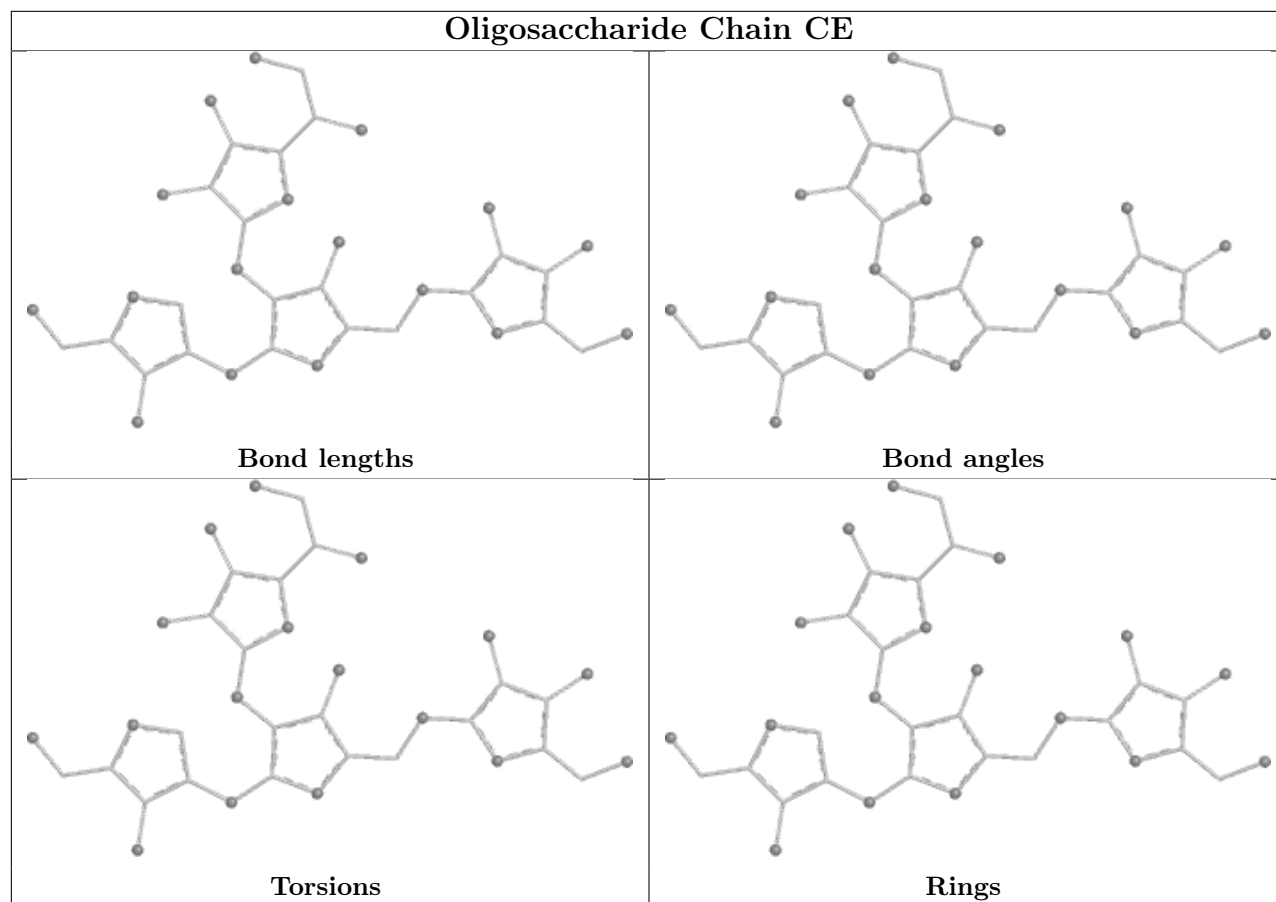
Oligosaccharide Chain NE

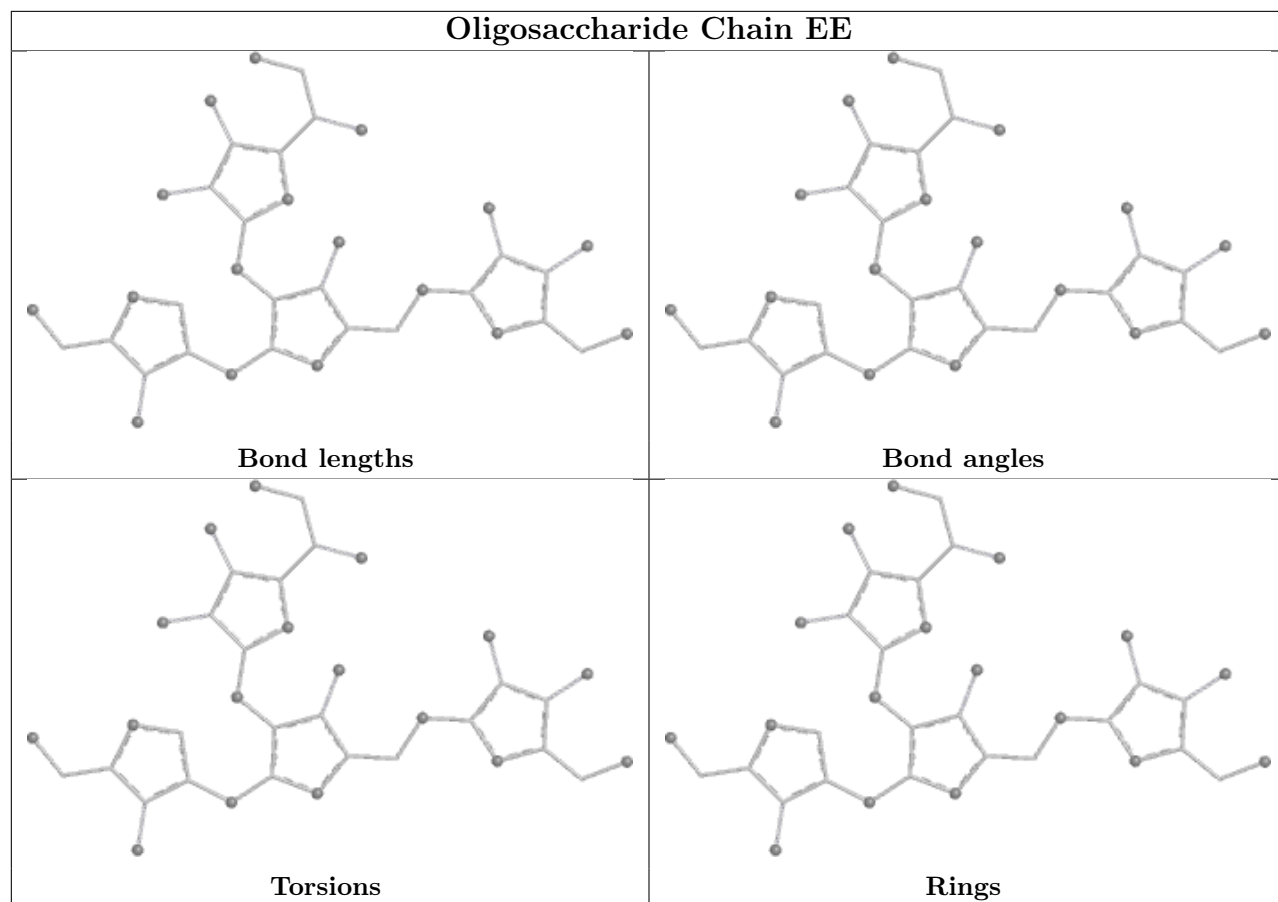


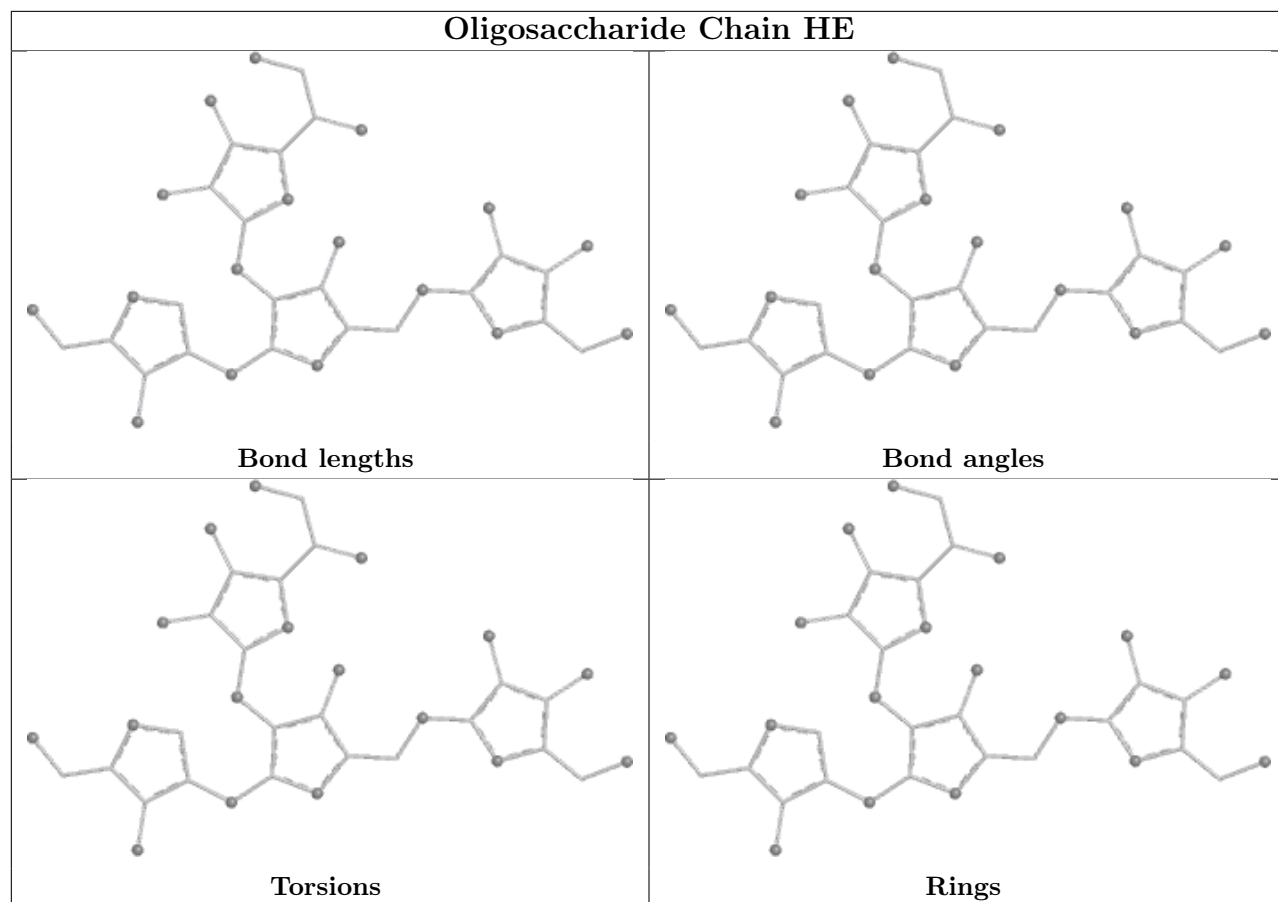


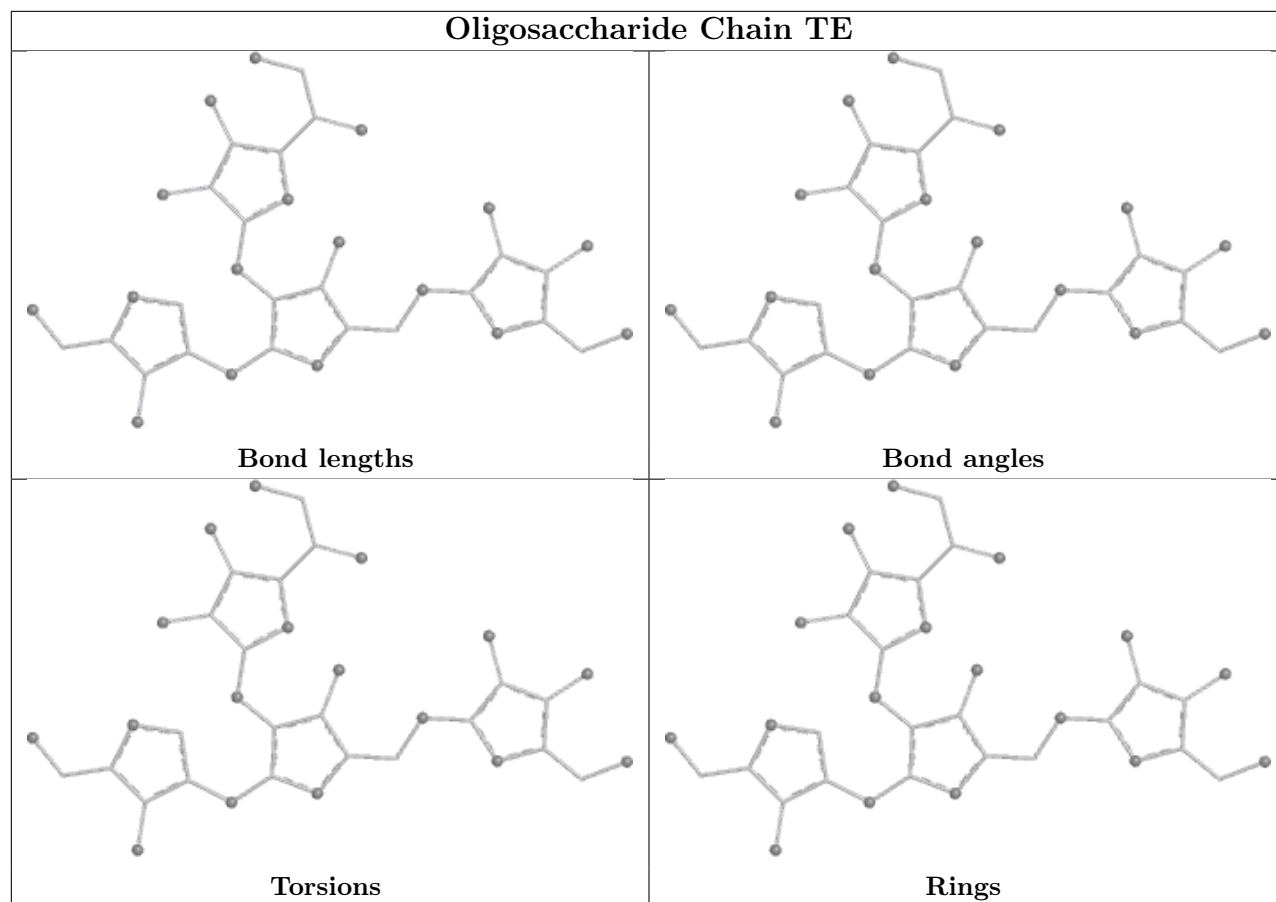


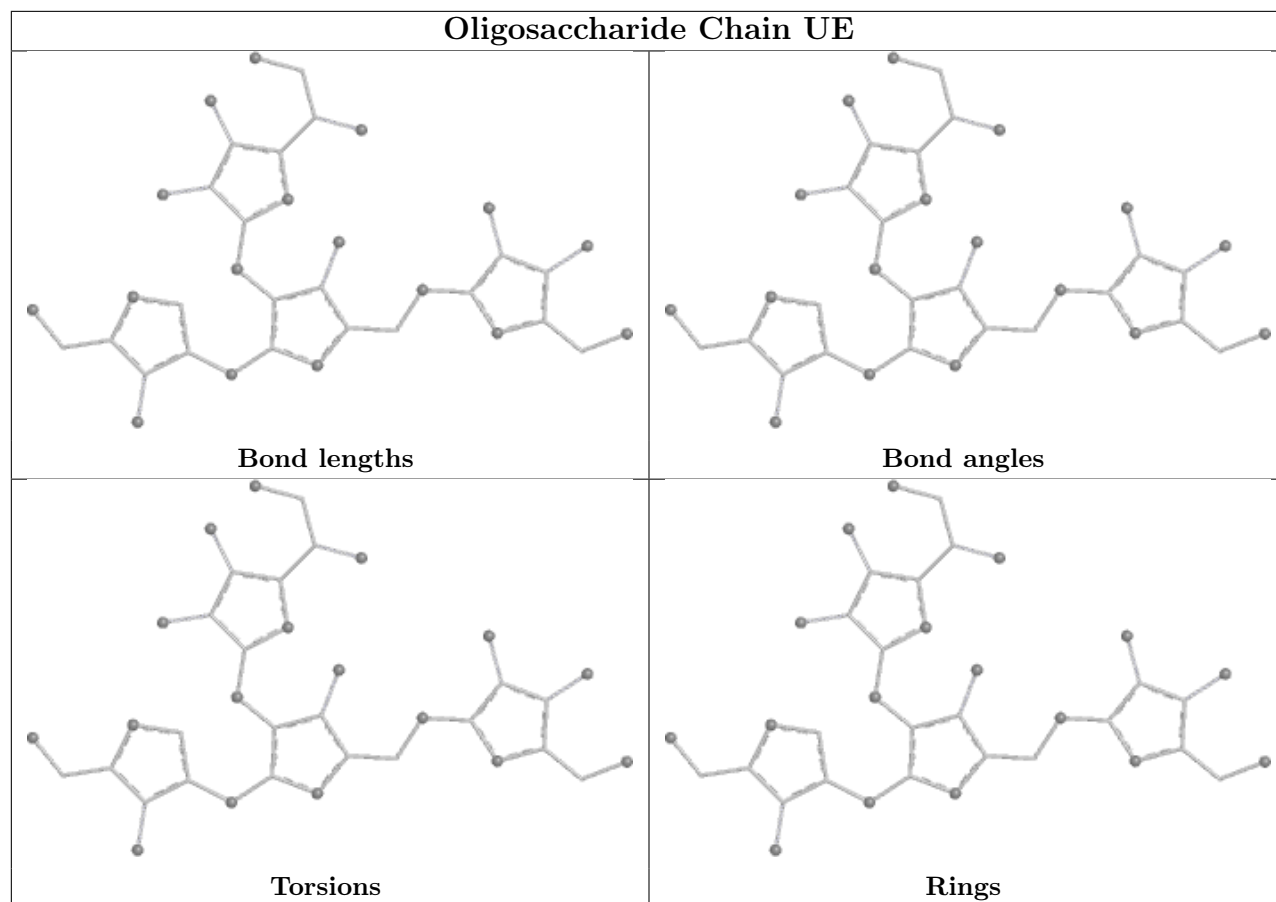


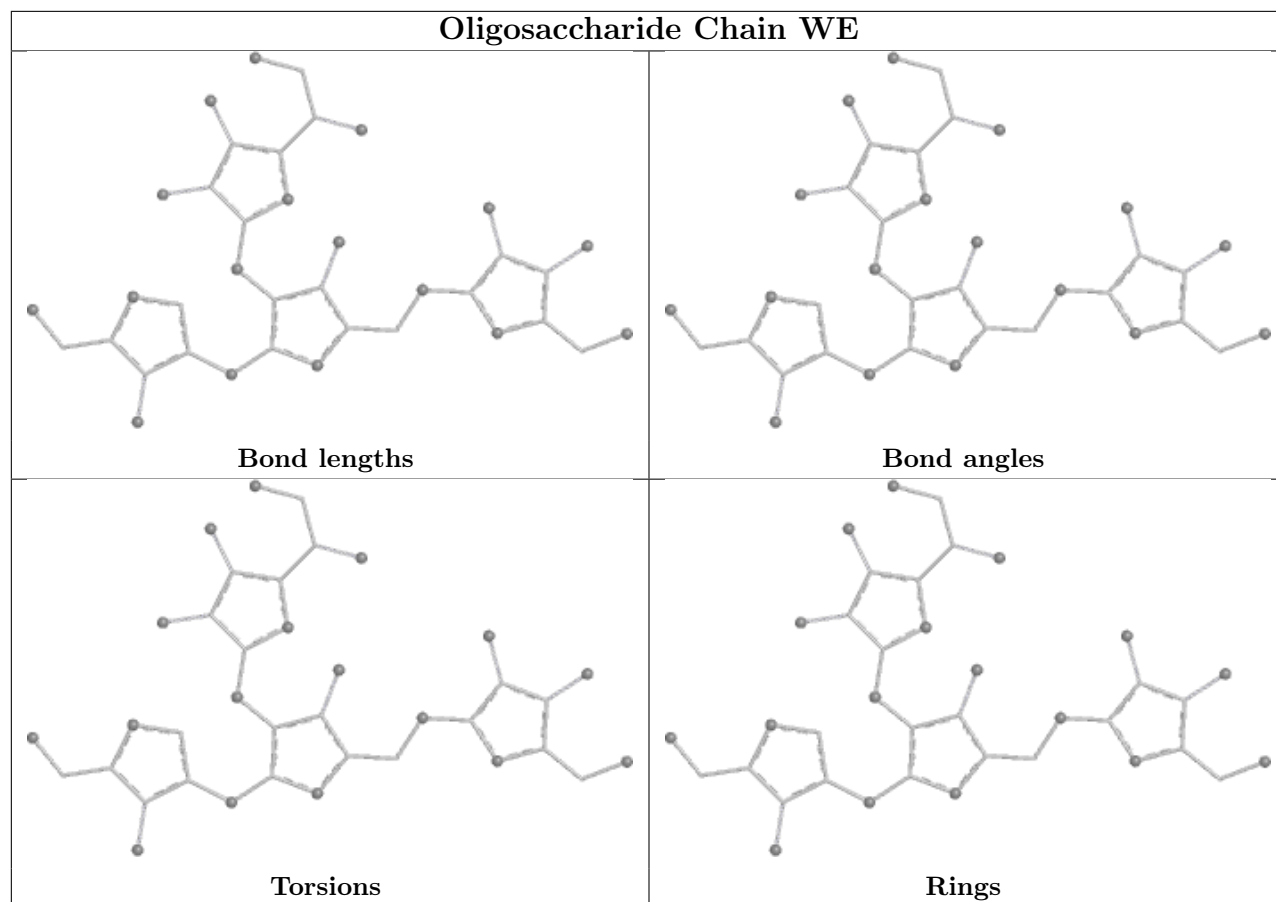


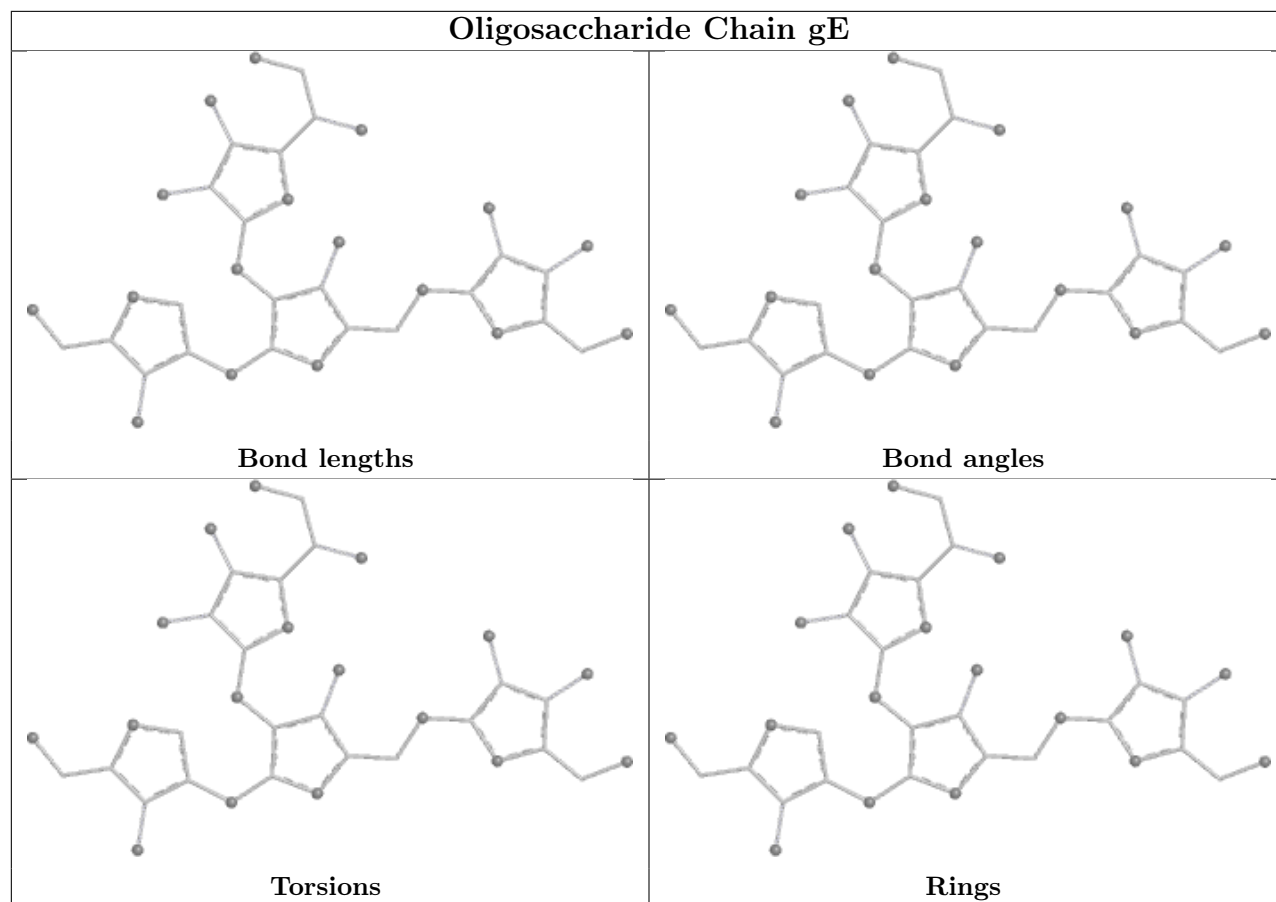


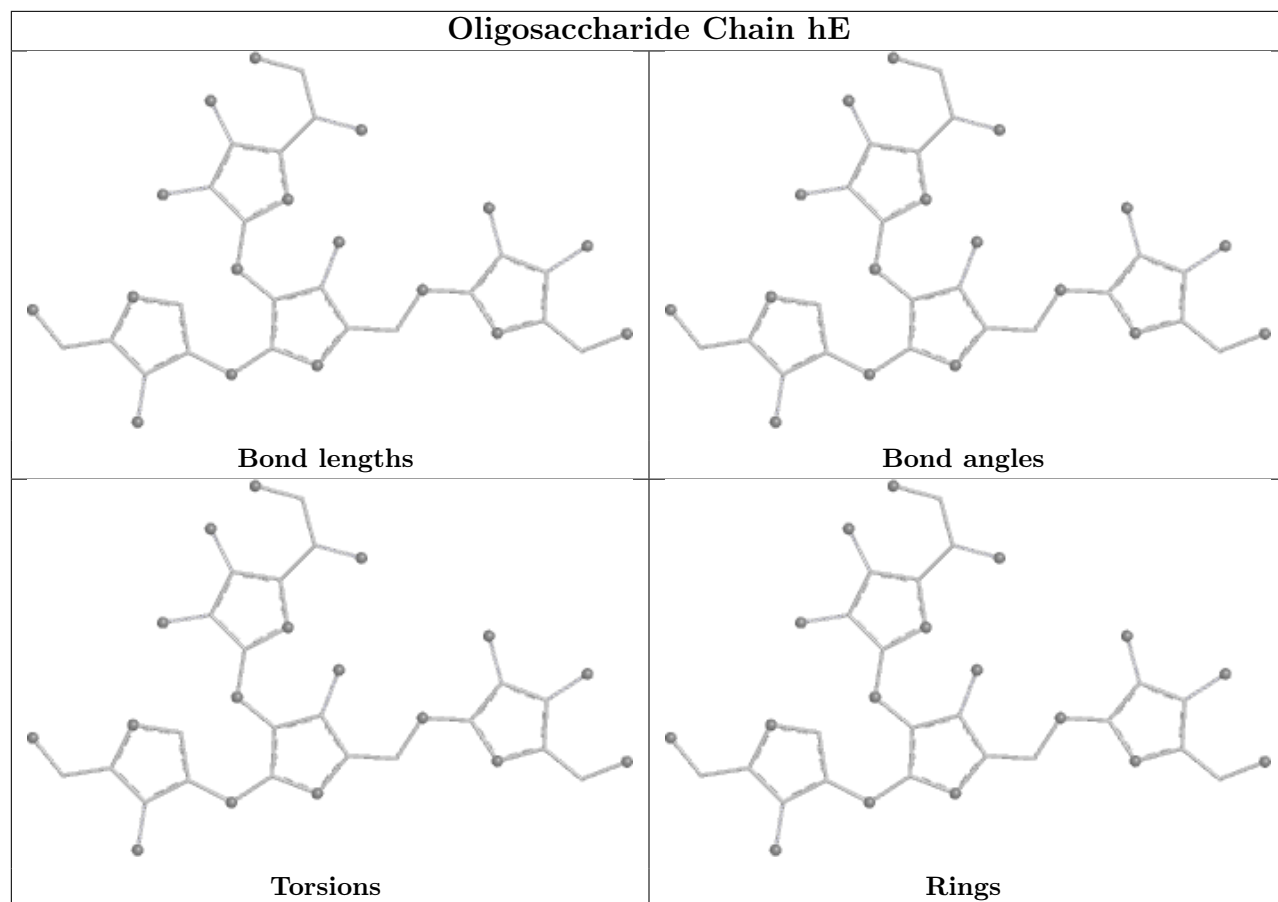
Oligosaccharide Chain HE

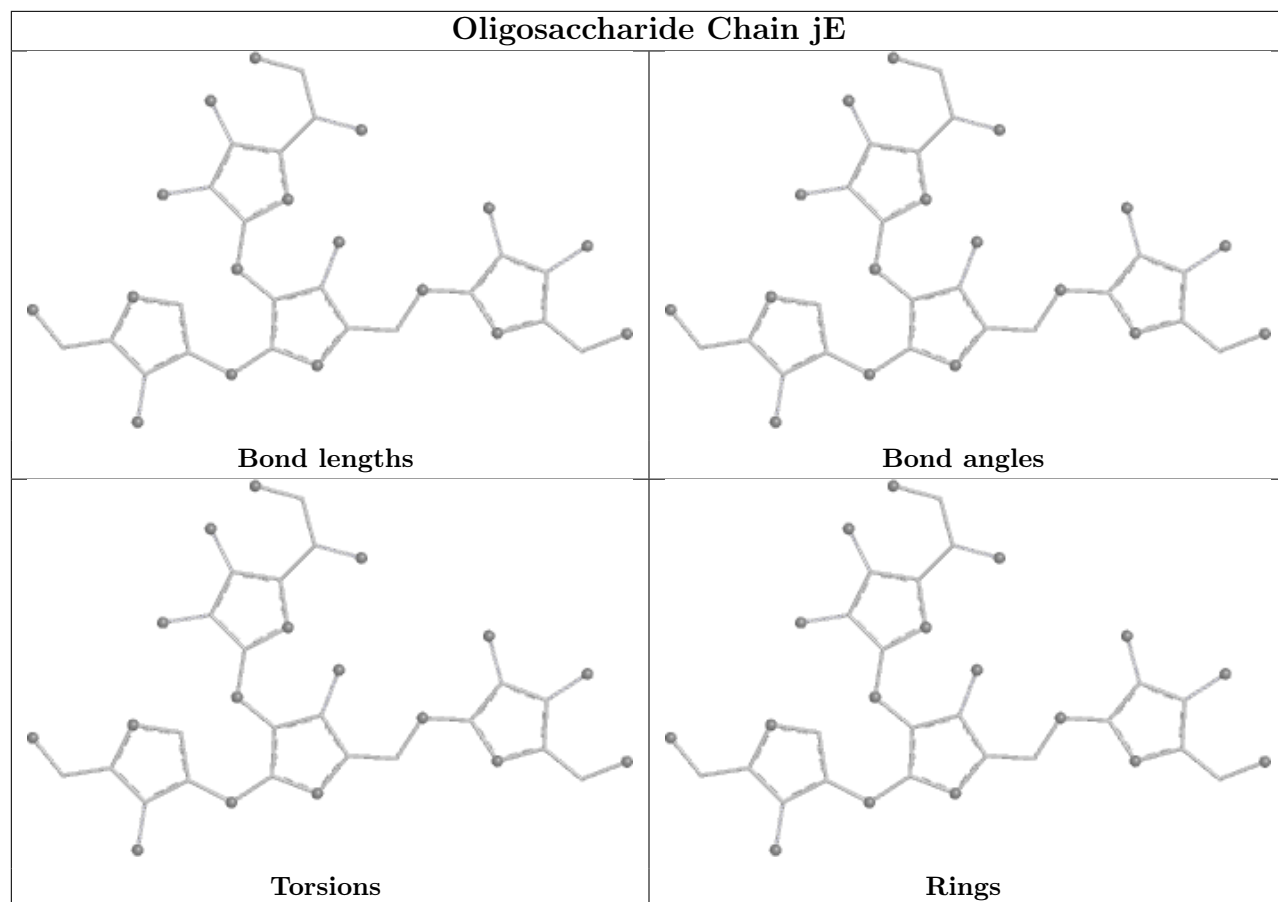


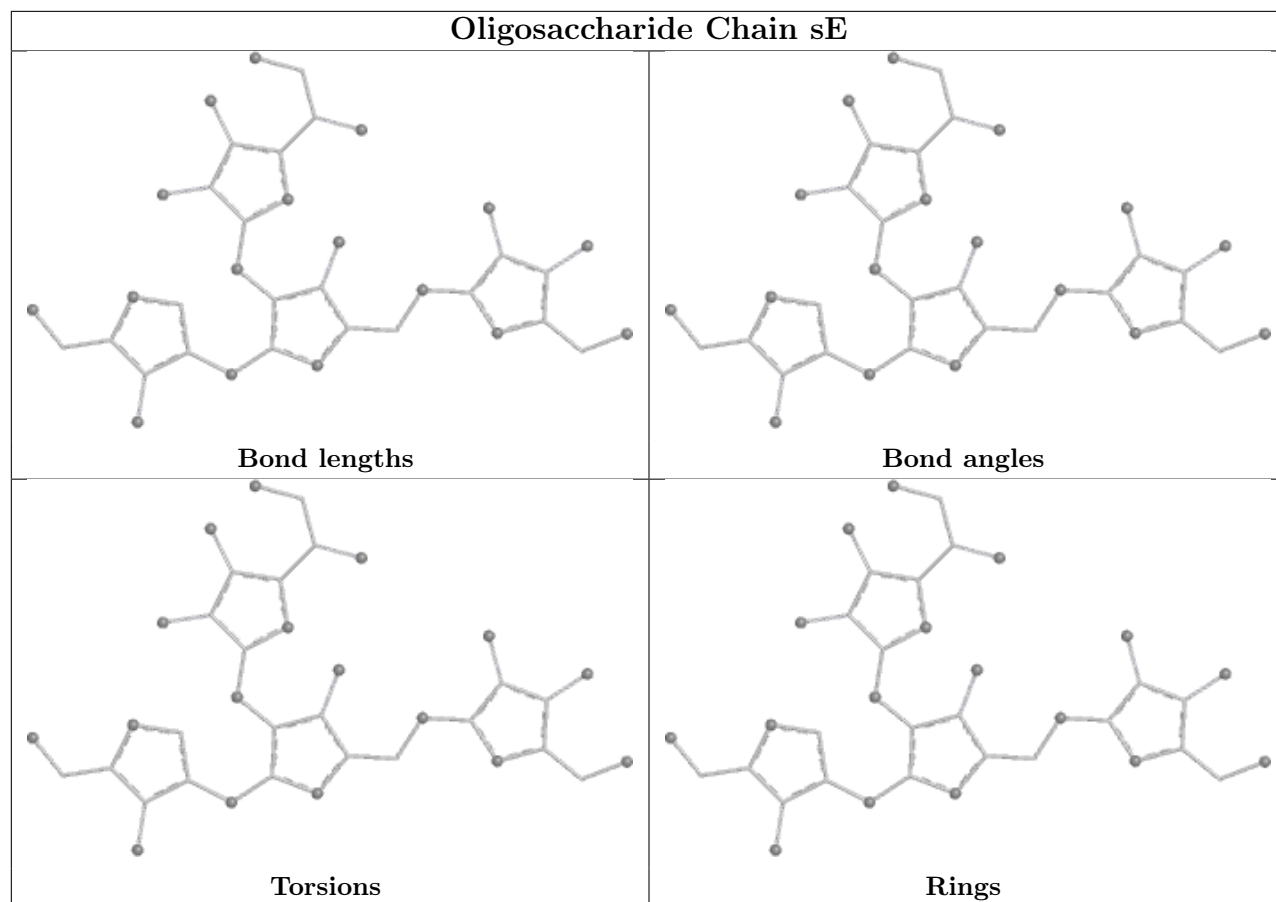


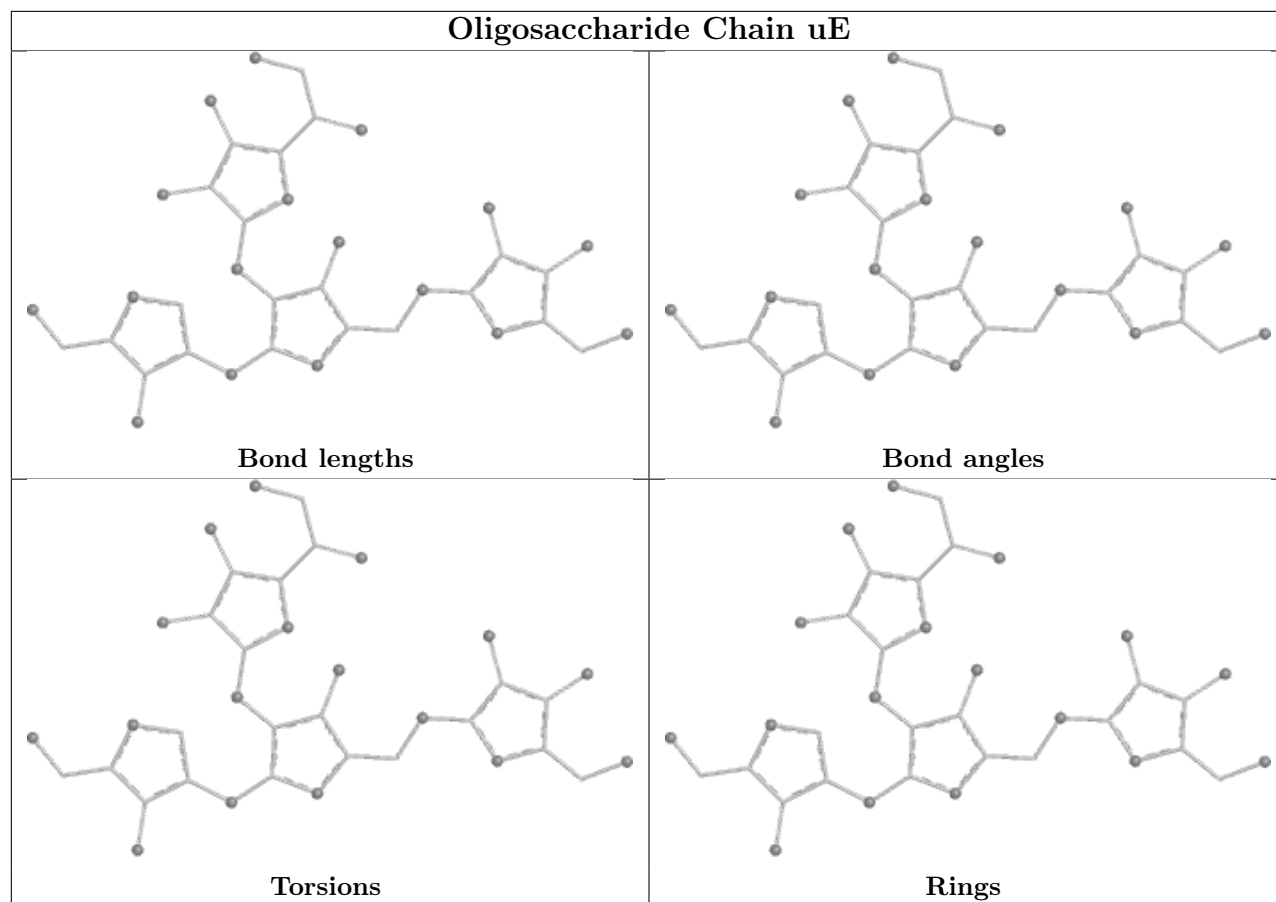


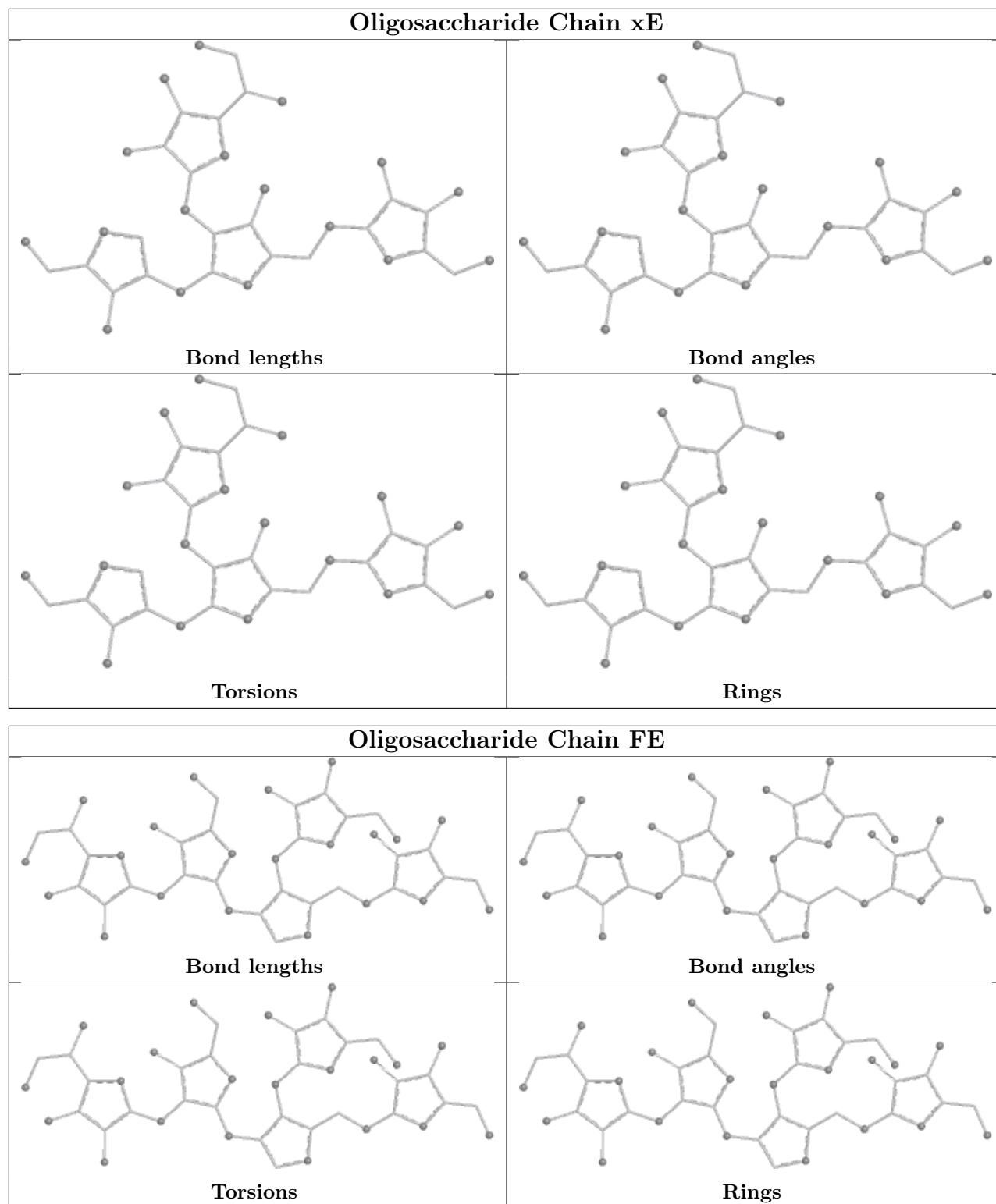


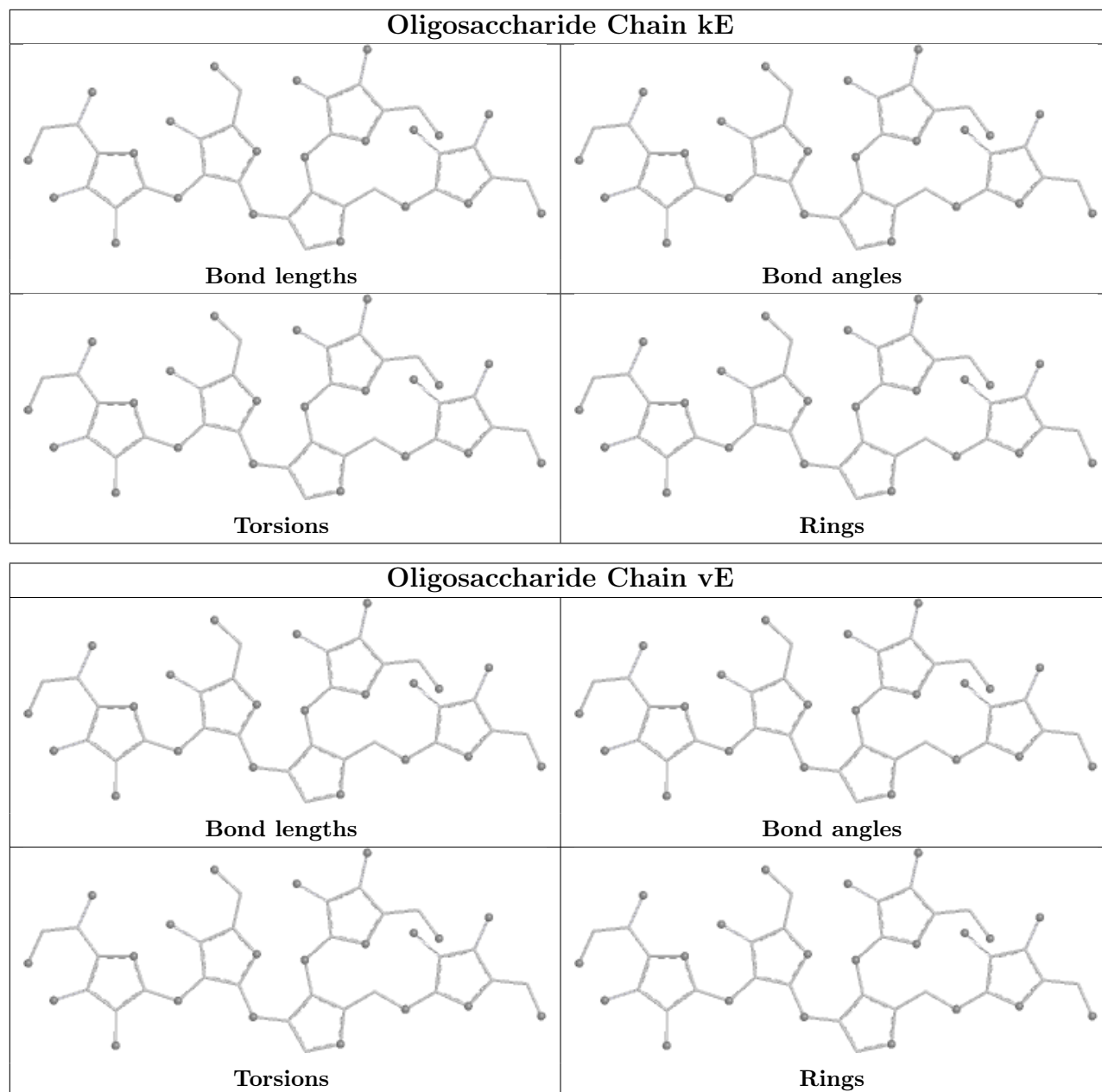


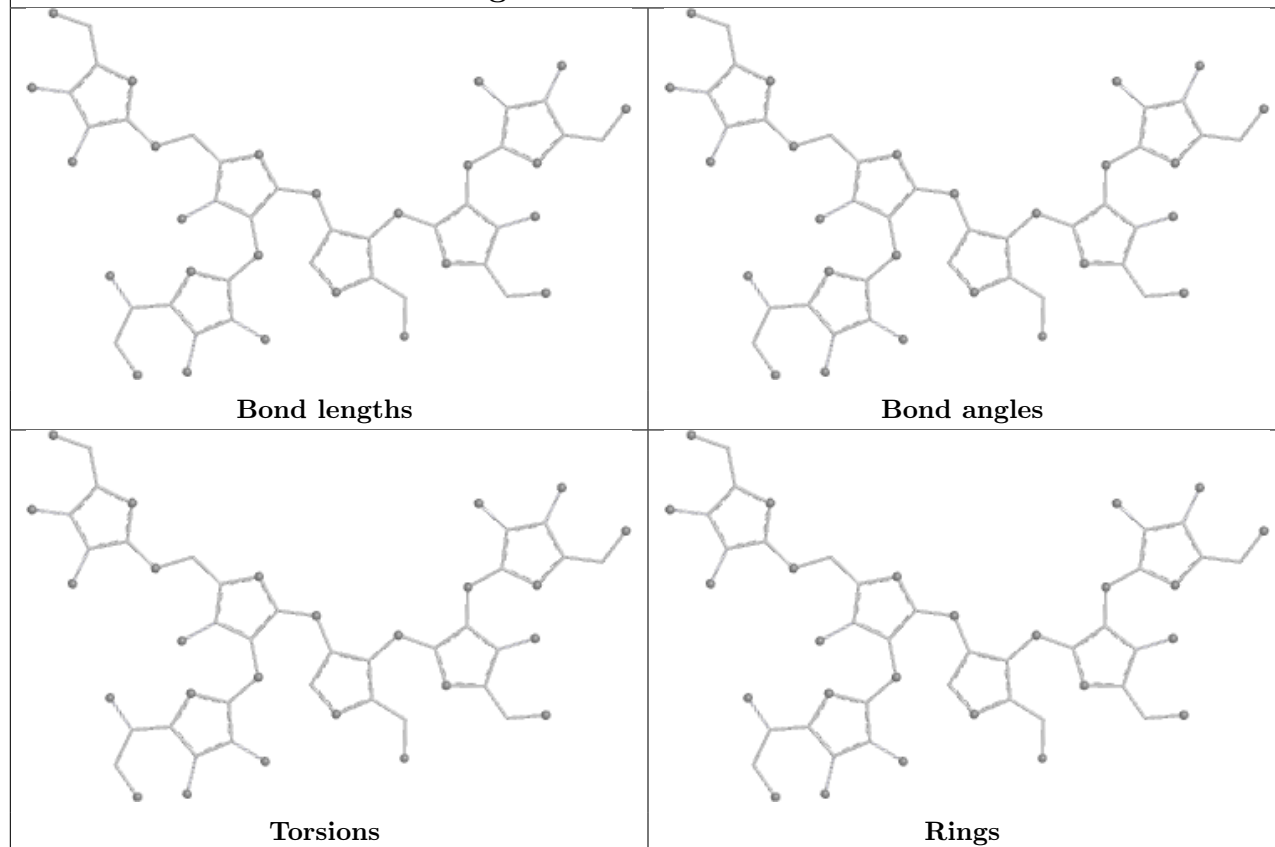
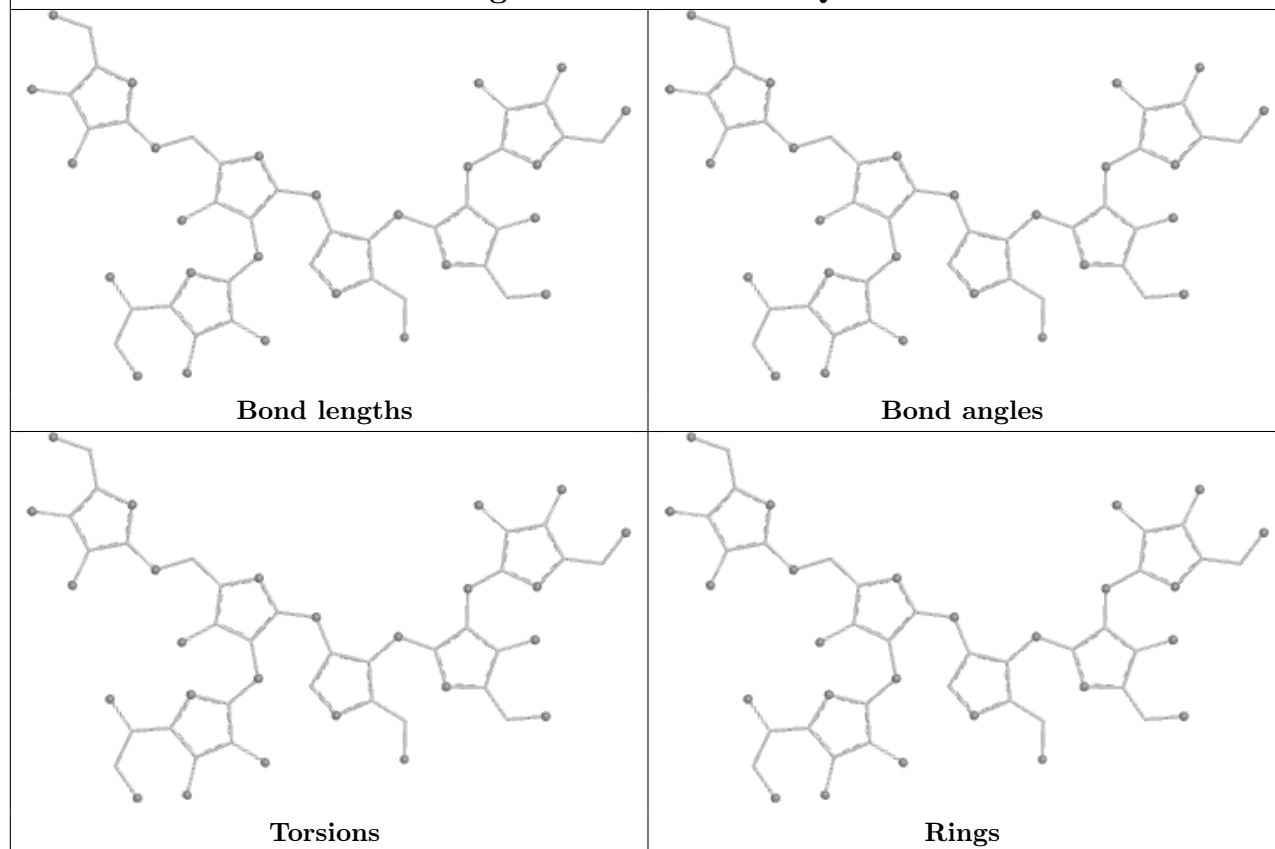


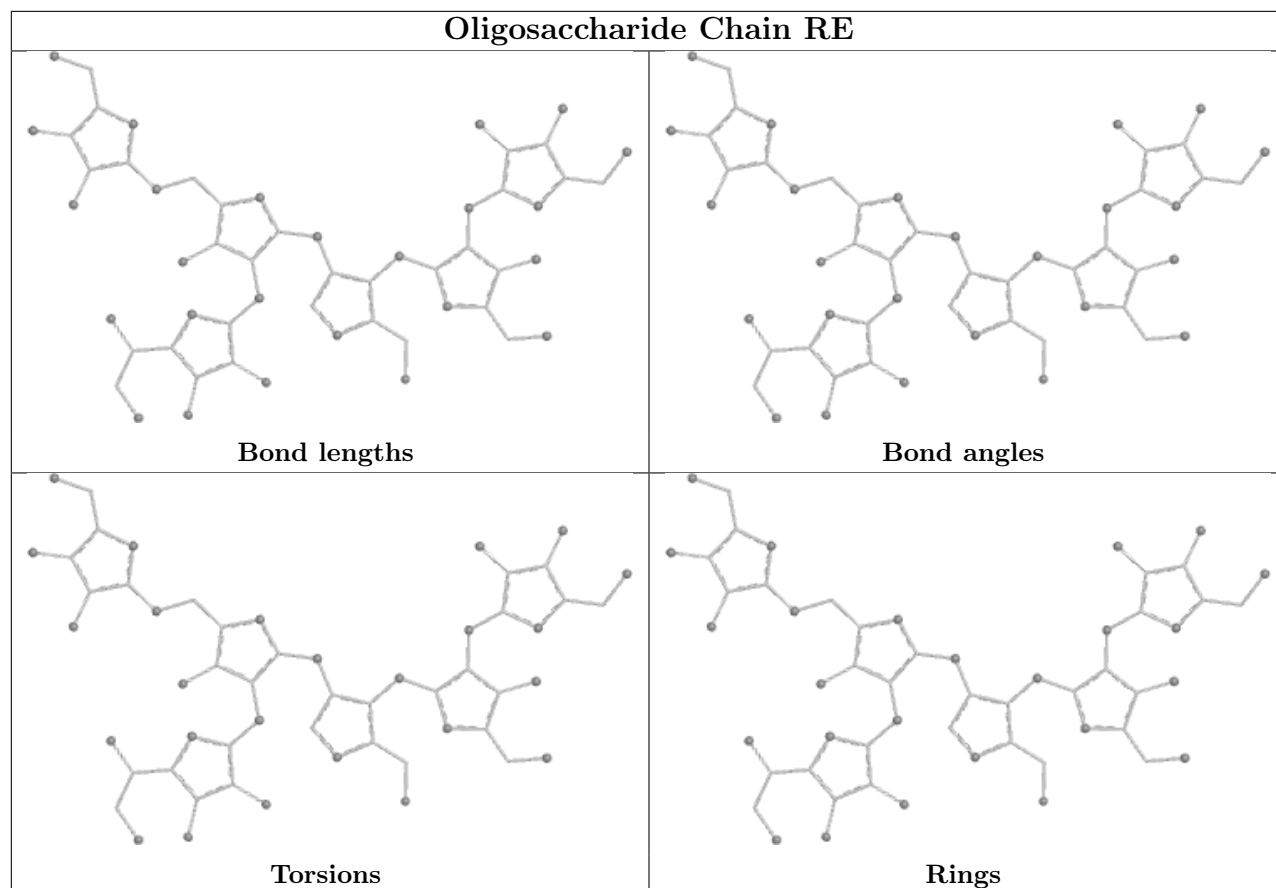
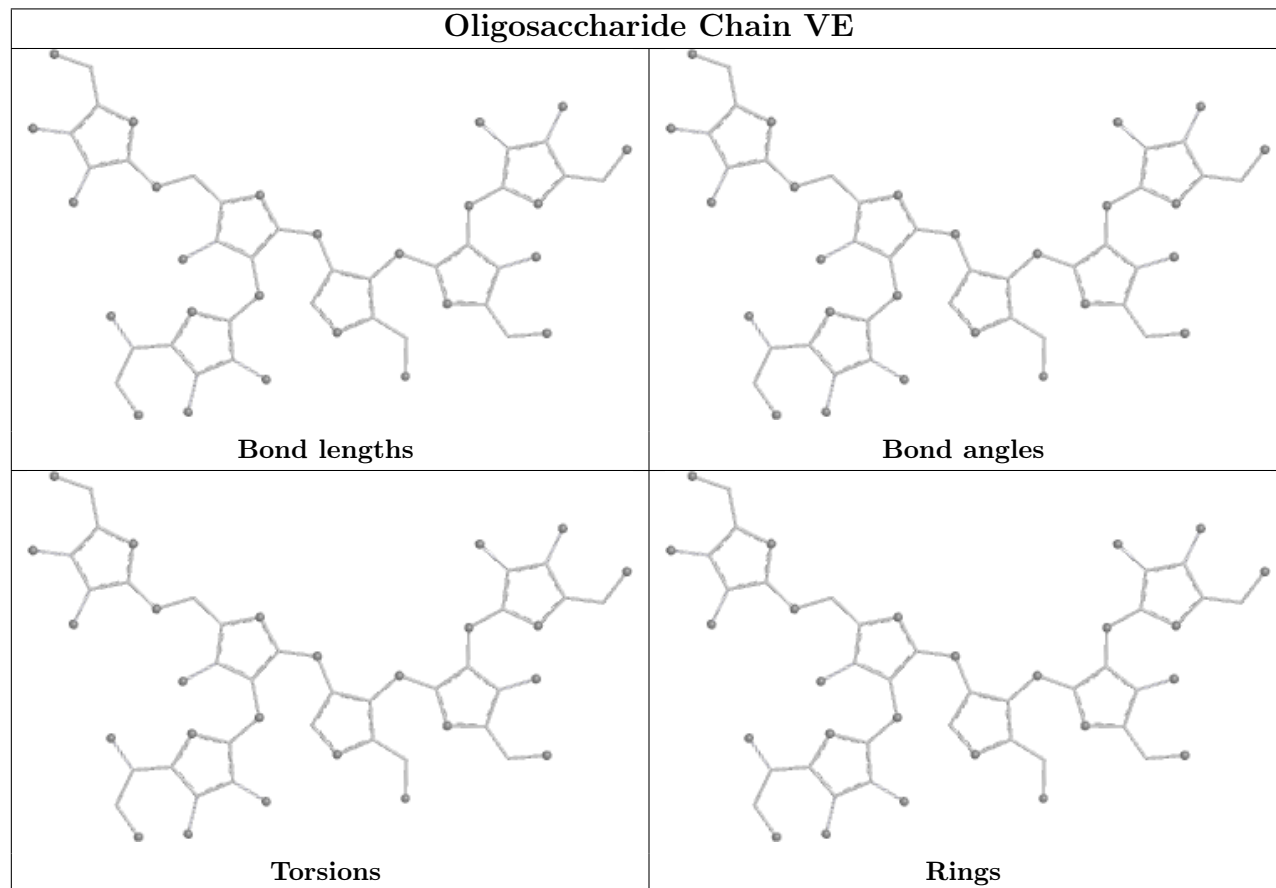


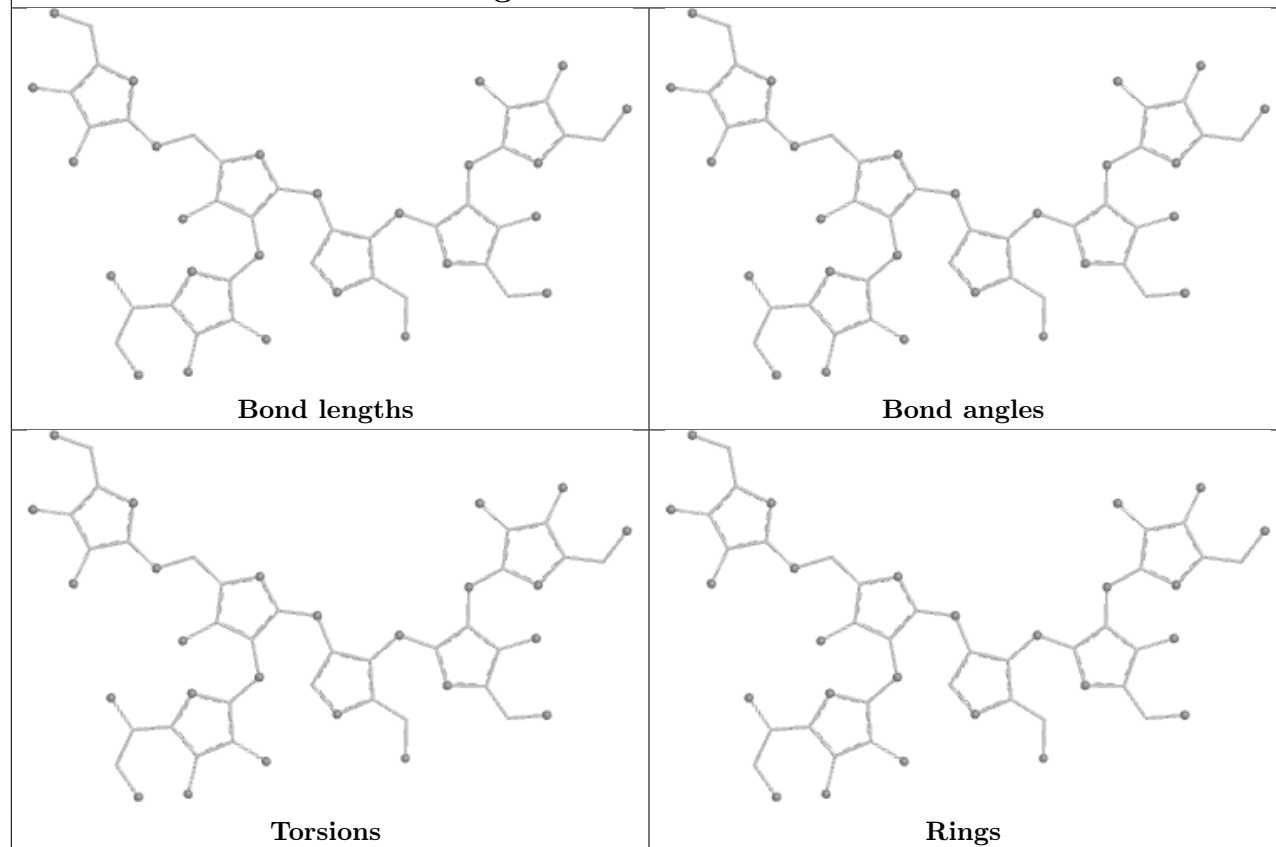
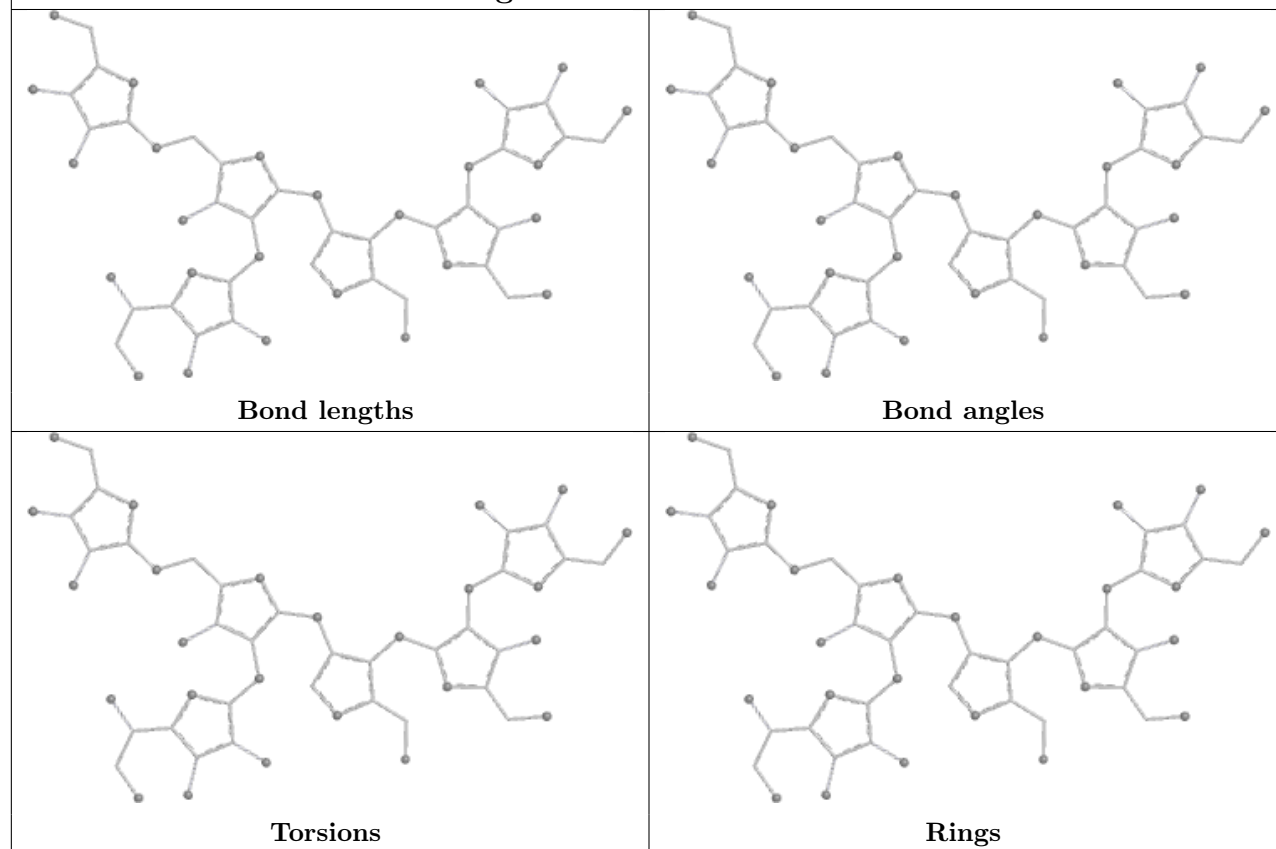




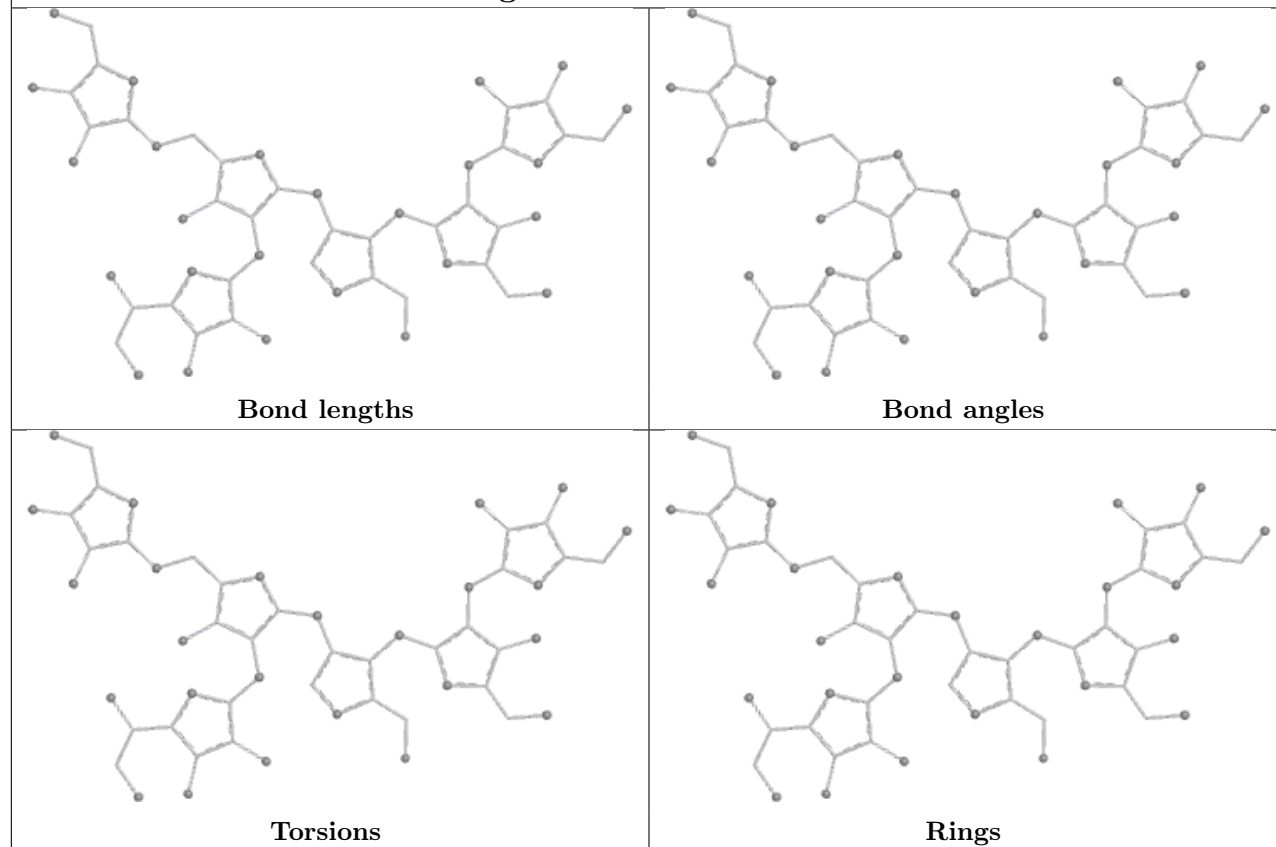


Oligosaccharide Chain GE**Oligosaccharide Chain QE**

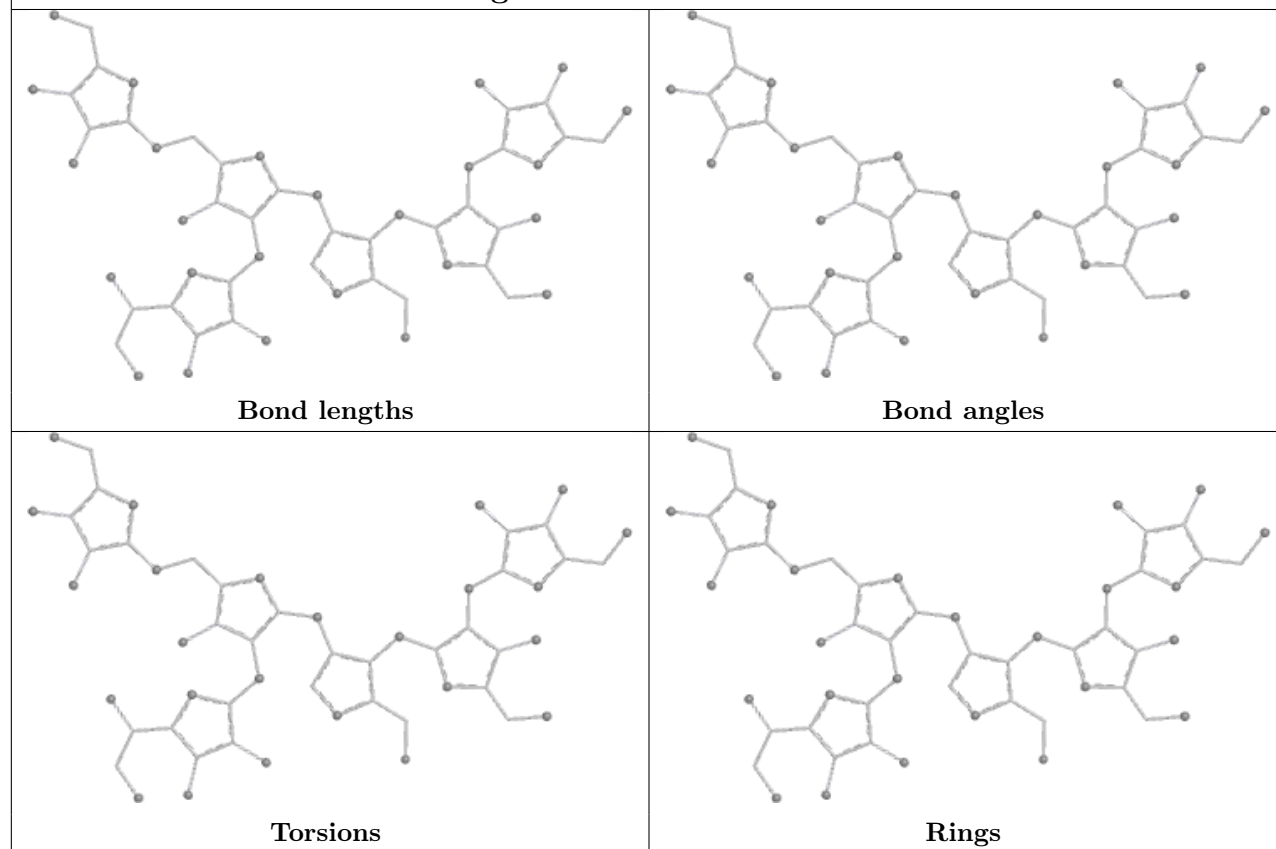
Oligosaccharide Chain RE**Oligosaccharide Chain VE**

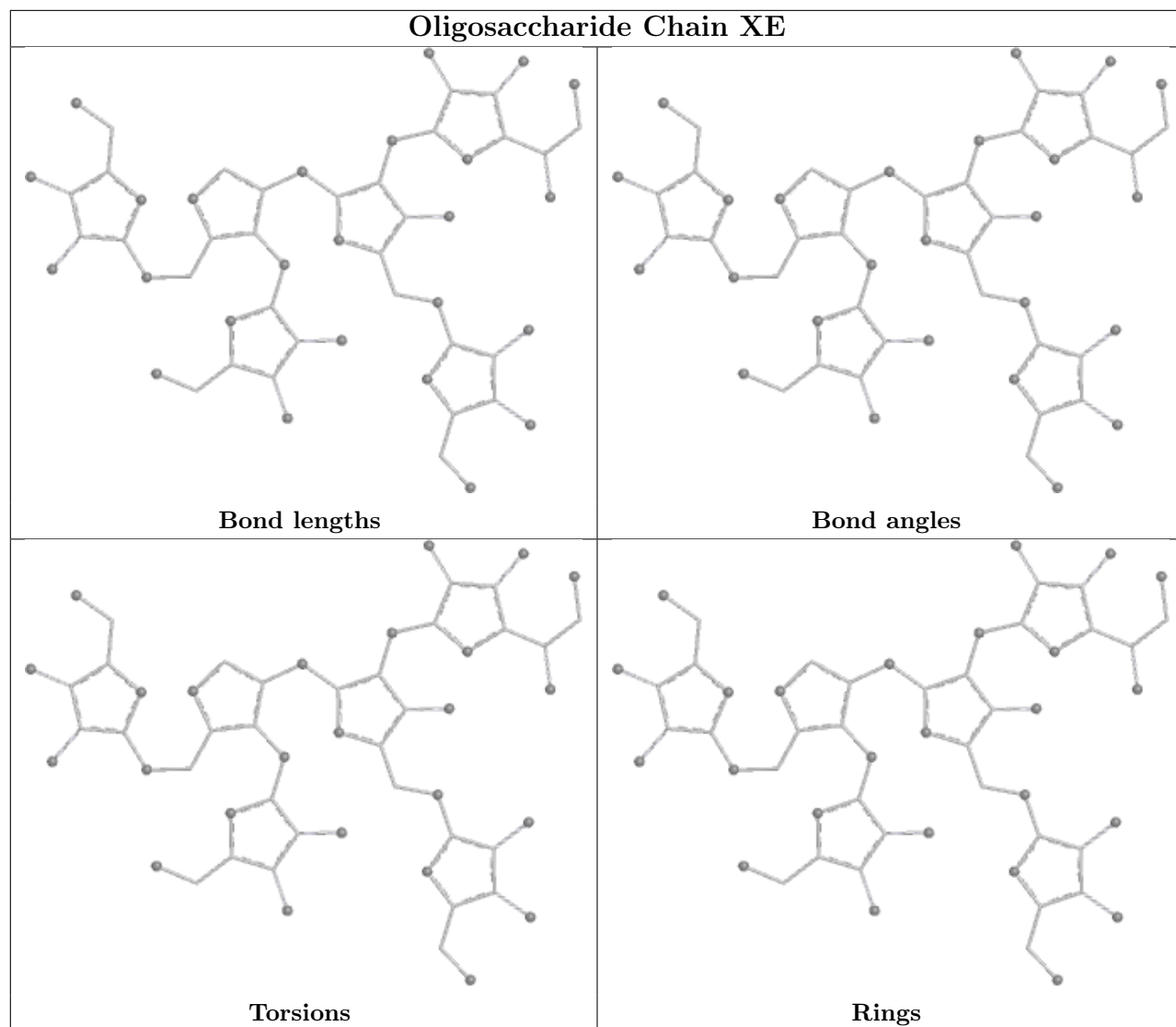
Oligosaccharide Chain dE**Oligosaccharide Chain eE**

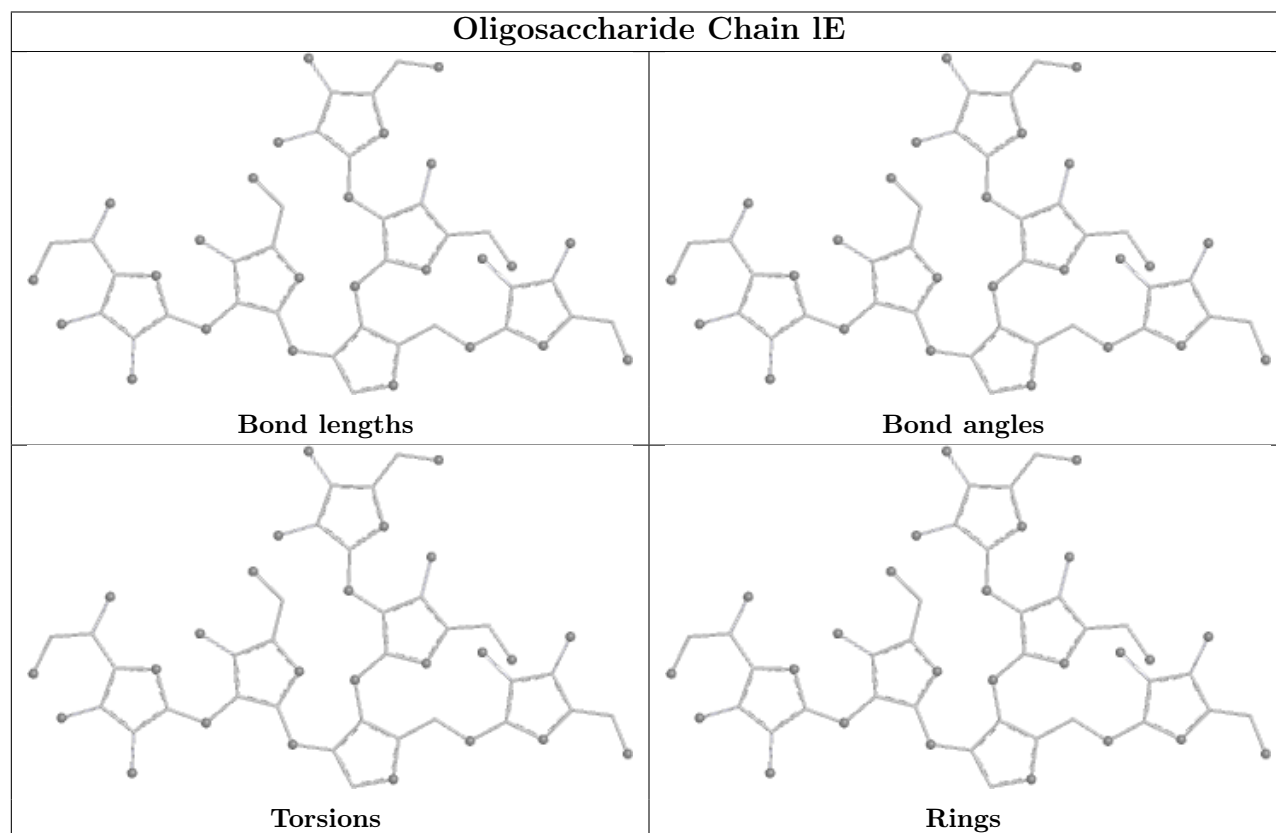
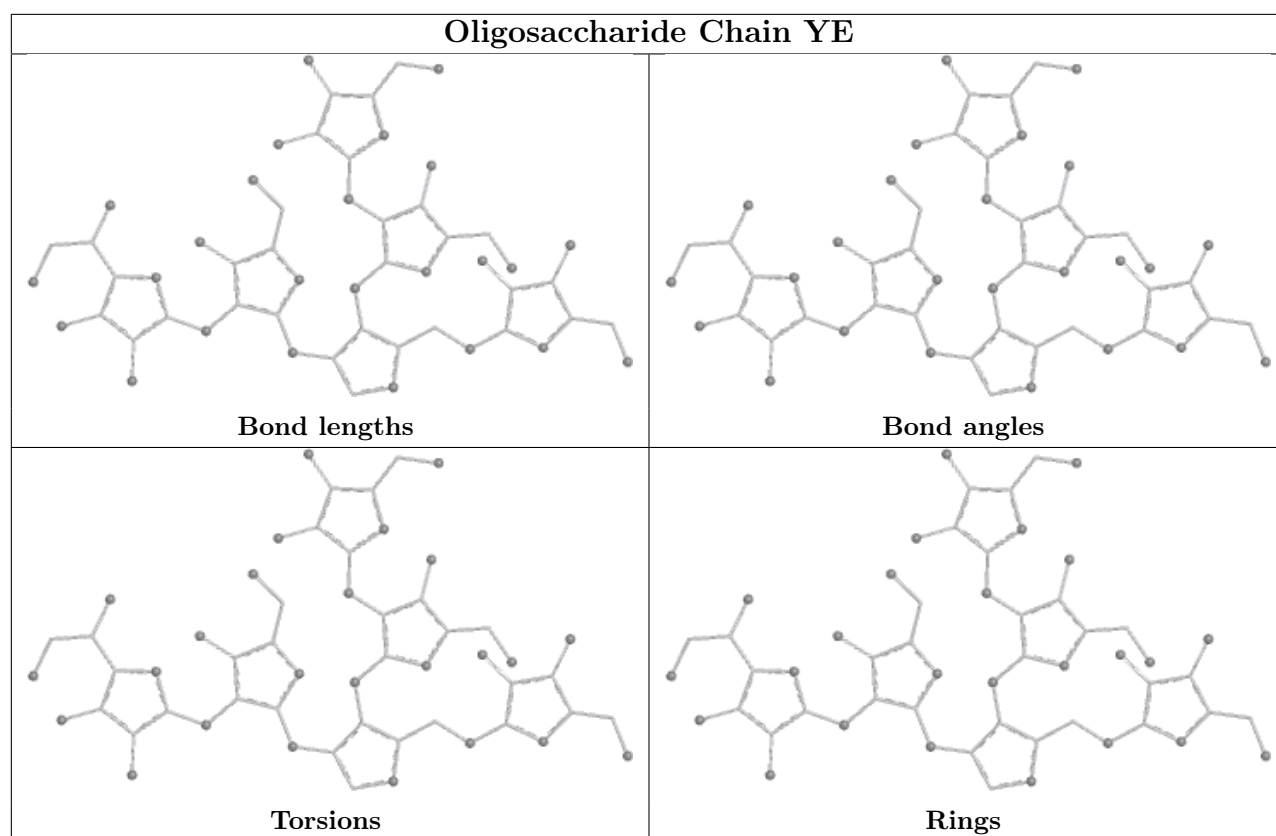
Oligosaccharide Chain iE



Oligosaccharide Chain wE







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
28	NAG	D	2010	1	14,14,15	0.31	0	17,19,21	0.71	0
26	AHR	D	2004	-	9,9,10	0.65	0	11,12,14	1.55	3 (27%)
27	GLA	F	2014	1	11,11,12	1.73	3 (27%)	15,15,17	0.81	0
27	GLA	B	2010	1	11,11,12	1.72	3 (27%)	15,15,17	0.77	0
26	AHR	B	2002	-	9,9,10	0.53	0	11,12,14	1.11	1 (9%)
27	GLA	E	2008	-	11,11,12	1.70	3 (27%)	15,15,17	0.99	1 (6%)
26	AHR	F	2005	-	9,9,10	0.64	0	11,12,14	1.54	3 (27%)
27	GLA	B	2013	1	11,11,12	1.68	3 (27%)	15,15,17	0.90	0
27	GLA	D	2008	1	11,11,12	1.72	3 (27%)	15,15,17	0.71	0
26	AHR	A	2019	-	9,9,10	0.54	0	11,12,14	0.81	0
26	AHR	F	2019	-	9,9,10	0.54	0	11,12,14	0.64	0
27	GLA	F	2017	1	11,11,12	1.69	3 (27%)	15,15,17	1.02	1 (6%)
27	GLA	A	2008	-	11,11,12	1.72	2 (18%)	15,15,17	1.33	1 (6%)
27	GLA	D	2007	1	11,11,12	1.67	3 (27%)	15,15,17	0.87	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%)
27	GLA	A	2014	1	11,11,12	1.73	3 (27%)	15,15,17	0.86	0
26	AHR	B	2004	-	9,9,10	0.77	0	11,12,14	1.78	4 (36%)
26	AHR	C	2001	-	9,9,10	0.53	0	11,12,14	1.61	1 (9%)
27	GLA	B	2012	1	11,11,12	1.75	3 (27%)	15,15,17	0.70	0
27	GLA	F	2009	1	11,11,12	1.63	2 (18%)	15,15,17	0.86	1 (6%)
26	AHR	A	2018	-	9,9,10	0.54	0	11,12,14	1.04	1 (9%)
27	GLA	C	2008	1	11,11,12	1.74	3 (27%)	15,15,17	0.94	0
26	AHR	E	2002	-	9,9,10	0.78	1 (11%)	11,12,14	1.78	3 (27%)
27	GLA	A	2013	1	11,11,12	1.72	3 (27%)	15,15,17	0.64	0
27	GLA	A	2006	1	11,11,12	1.75	3 (27%)	15,15,17	0.95	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	AHR	B	2003	-	9,9,10	0.90	0	11,12,14	1.88	4 (36%)
27	GLA	D	2005	1	11,11,12	1.73	3 (27%)	15,15,17	0.87	0
26	AHR	C	2003	-	9,9,10	0.79	0	11,12,14	1.72	4 (36%)
27	GLA	A	2015	1	11,11,12	1.75	3 (27%)	15,15,17	0.78	0
26	AHR	D	2003	-	9,9,10	0.82	0	11,12,14	1.70	3 (27%)
27	GLA	C	2006	1	11,11,12	1.65	3 (27%)	15,15,17	0.78	0
28	NAG	A	2017	1	14,14,15	0.32	0	17,19,21	0.64	0
27	GLA	B	2017	1	11,11,12	1.61	2 (18%)	15,15,17	1.33	1 (6%)
27	GLA	E	2006	1	11,11,12	1.73	3 (27%)	15,15,17	0.75	0
27	GLA	E	2016	1	11,11,12	1.79	3 (27%)	15,15,17	0.82	0
26	AHR	A	2002	-	9,9,10	0.83	1 (11%)	11,12,14	1.36	2 (18%)
27	GLA	E	2014	1	11,11,12	1.69	3 (27%)	15,15,17	0.91	0
27	GLA	A	2005	1	11,11,12	1.66	3 (27%)	15,15,17	0.84	0
27	GLA	A	2009	1	11,11,12	1.67	3 (27%)	15,15,17	1.03	1 (6%)
27	GLA	D	2006	1	11,11,12	1.65	3 (27%)	15,15,17	0.95	1 (6%)
26	AHR	A	2003	-	9,9,10	0.75	1 (11%)	11,12,14	1.63	3 (27%)
27	GLA	F	2013	1	11,11,12	1.71	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%)
26	AHR	F	2003	-	9,9,10	0.55	0	11,12,14	1.59	1 (9%)
27	GLA	F	2015	1	11,11,12	1.72	3 (27%)	15,15,17	0.66	0
26	AHR	F	2001	-	9,9,10	0.65	0	11,12,14	1.53	3 (27%)
28	NAG	B	2018	1	14,14,15	0.35	0	17,19,21	0.80	0
27	GLA	A	2011	1	11,11,12	1.74	3 (27%)	15,15,17	0.90	1 (6%)
27	GLA	A	2004	1	11,11,12	1.83	3 (27%)	15,15,17	1.63	4 (26%)
27	GLA	E	2009	1	11,11,12	1.68	3 (27%)	15,15,17	1.04	1 (6%)
26	AHR	F	2004	-	9,9,10	0.64	0	11,12,14	1.56	3 (27%)
27	GLA	B	2005	1	11,11,12	1.82	3 (27%)	15,15,17	1.54	3 (20%)
26	AHR	E	2003	-	9,9,10	0.64	0	11,12,14	1.54	3 (27%)
27	GLA	B	2016	1	11,11,12	1.79	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	A	2007	1	11,11,12	1.71	3 (27%)	15,15,17	0.62	0
27	GLA	B	2014	1	11,11,12	1.62	2 (18%)	15,15,17	0.83	1 (6%)
27	GLA	E	2012	1	11,11,12	1.60	1 (9%)	15,15,17	1.17	1 (6%)
27	GLA	E	2004	1	11,11,12	1.83	3 (27%)	15,15,17	1.73	4 (26%)
27	GLA	F	2006	1	11,11,12	1.77	3 (27%)	15,15,17	1.81	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	GLA	E	2013	1	11,11,12	1.76	3 (27%)	15,15,17	0.74	0
27	GLA	E	2010	1	11,11,12	1.64	2 (18%)	15,15,17	1.26	1 (6%)
28	NAG	B	2019	1	14,14,15	0.36	0	17,19,21	0.97	1 (5%)
27	GLA	F	2010	-	11,11,12	1.74	3 (27%)	15,15,17	0.84	0
27	GLA	B	2008	1	11,11,12	1.70	3 (27%)	15,15,17	0.76	0
27	GLA	B	2007	1	11,11,12	1.75	3 (27%)	15,15,17	0.82	0
27	GLA	F	2018	1	11,11,12	1.72	3 (27%)	15,15,17	0.61	0
27	GLA	A	2016	1	11,11,12	1.71	3 (27%)	15,15,17	0.95	1 (6%)
26	AHR	B	2020	-	9,9,10	0.88	0	11,12,14	0.92	1 (9%)
28	NAG	E	2017	1	14,14,15	0.33	0	17,19,21	0.93	1 (5%)
27	GLA	C	2007	1	11,11,12	1.74	3 (27%)	15,15,17	0.82	0
27	GLA	F	2007	1	11,11,12	1.64	3 (27%)	15,15,17	1.04	0
27	GLA	B	2011	1	11,11,12	1.67	3 (27%)	15,15,17	0.98	1 (6%)
27	GLA	F	2016	1	11,11,12	1.65	2 (18%)	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%)
27	GLA	E	2005	1	11,11,12	1.71	3 (27%)	15,15,17	0.90	0
27	GLA	D	2009	1	11,11,12	1.76	3 (27%)	15,15,17	0.78	0
27	GLA	A	2012	1	11,11,12	1.70	3 (27%)	15,15,17	0.84	0
27	GLA	E	2015	1	11,11,12	1.65	2 (18%)	15,15,17	1.17	1 (6%)
27	GLA	F	2008	1	11,11,12	1.70	3 (27%)	15,15,17	0.96	1 (6%)
27	GLA	C	2004	1	11,11,12	1.72	3 (27%)	15,15,17	0.74	0
26	AHR	D	2001	-	9,9,10	0.65	0	11,12,14	1.49	2 (18%)
27	GLA	B	2015	1	11,11,12	1.71	3 (27%)	15,15,17	0.81	0
27	GLA	C	2005	1	11,11,12	1.64	3 (27%)	15,15,17	0.87	1 (6%)
28	NAG	C	2009	1	14,14,15	0.37	0	17,19,21	0.73	0
27	GLA	B	2006	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	B	2009	-	11,11,12	1.72	3 (27%)	15,15,17	1.45	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
28	NAG	D	2010	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	AHR	D	2004	-	-	2/2/15/18	0/1/1/1
27	GLA	F	2014	1	-	2/2/19/22	0/1/1/1
27	GLA	B	2010	1	-	2/2/19/22	0/1/1/1
26	AHR	B	2002	-	-	0/2/15/18	0/1/1/1
27	GLA	E	2008	-	-	2/2/19/22	0/1/1/1
26	AHR	F	2005	-	-	2/2/15/18	0/1/1/1
27	GLA	B	2013	1	-	1/2/19/22	0/1/1/1
27	GLA	D	2008	1	-	2/2/19/22	0/1/1/1
26	AHR	A	2019	-	-	0/2/15/18	0/1/1/1
26	AHR	F	2019	-	-	0/2/15/18	0/1/1/1
27	GLA	F	2017	1	-	2/2/19/22	0/1/1/1
27	GLA	A	2008	-	-	2/2/19/22	0/1/1/1
27	GLA	D	2007	1	-	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
27	GLA	A	2014	1	-	2/2/19/22	0/1/1/1
26	AHR	B	2004	-	-	2/2/15/18	0/1/1/1
26	AHR	C	2001	-	-	2/2/15/18	0/1/1/1
27	GLA	B	2012	1	-	1/2/19/22	0/1/1/1
27	GLA	F	2009	1	1/1/4/5	2/2/19/22	0/1/1/1
26	AHR	A	2018	-	-	0/2/15/18	0/1/1/1
27	GLA	C	2008	1	-	2/2/19/22	0/1/1/1
26	AHR	E	2002	-	-	2/2/15/18	0/1/1/1
27	GLA	A	2013	1	-	0/2/19/22	0/1/1/1
27	GLA	A	2006	1	-	1/2/19/22	0/1/1/1
26	AHR	B	2003	-	-	2/2/15/18	0/1/1/1
27	GLA	D	2005	1	-	2/2/19/22	0/1/1/1
26	AHR	C	2003	-	-	2/2/15/18	0/1/1/1
27	GLA	A	2015	1	-	2/2/19/22	0/1/1/1
26	AHR	D	2003	-	-	2/2/15/18	0/1/1/1
27	GLA	C	2006	1	-	0/2/19/22	0/1/1/1
28	NAG	A	2017	1	-	2/6/23/26	0/1/1/1
27	GLA	B	2017	1	-	2/2/19/22	0/1/1/1
27	GLA	E	2006	1	-	2/2/19/22	0/1/1/1
27	GLA	E	2016	1	-	2/2/19/22	0/1/1/1
26	AHR	A	2002	-	-	2/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	GLA	E	2014	1	-	2/2/19/22	0/1/1/1
27	GLA	A	2005	1	-	0/2/19/22	0/1/1/1
27	GLA	A	2009	1	-	1/2/19/22	0/1/1/1
27	GLA	D	2006	1	-	0/2/19/22	0/1/1/1
26	AHR	A	2003	-	-	2/2/15/18	0/1/1/1
27	GLA	F	2013	1	-	0/2/19/22	0/1/1/1
27	GLA	A	2010	1	-	2/2/19/22	0/1/1/1
26	AHR	F	2003	-	-	1/2/15/18	0/1/1/1
27	GLA	F	2015	1	-	0/2/19/22	0/1/1/1
26	AHR	F	2001	-	-	2/2/15/18	0/1/1/1
28	NAG	B	2018	1	-	4/6/23/26	0/1/1/1
27	GLA	A	2011	1	-	2/2/19/22	0/1/1/1
27	GLA	A	2004	1	-	0/2/19/22	0/1/1/1
27	GLA	E	2009	1	-	0/2/19/22	0/1/1/1
26	AHR	F	2004	-	-	2/2/15/18	0/1/1/1
27	GLA	B	2005	1	-	0/2/19/22	0/1/1/1
26	AHR	E	2003	-	-	2/2/15/18	0/1/1/1
27	GLA	B	2016	1	-	2/2/19/22	0/1/1/1
27	GLA	F	2011	1	-	1/2/19/22	0/1/1/1
27	GLA	A	2007	1	1/1/4/5	2/2/19/22	0/1/1/1
27	GLA	B	2014	1	1/1/4/5	0/2/19/22	0/1/1/1
27	GLA	E	2012	1	-	1/2/19/22	0/1/1/1
27	GLA	E	2004	1	-	1/2/19/22	0/1/1/1
27	GLA	F	2006	1	-	0/2/19/22	0/1/1/1
27	GLA	E	2013	1	-	2/2/19/22	0/1/1/1
27	GLA	E	2010	1	-	1/2/19/22	0/1/1/1
28	NAG	B	2019	1	-	2/6/23/26	0/1/1/1
27	GLA	F	2010	-	-	2/2/19/22	0/1/1/1
27	GLA	B	2008	1	1/1/4/5	2/2/19/22	0/1/1/1
27	GLA	B	2007	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	2016	1	-	1/2/19/22	0/1/1/1
26	AHR	B	2020	-	-	1/2/15/18	0/1/1/1
28	NAG	E	2017	1	-	4/6/23/26	0/1/1/1
27	GLA	C	2007	1	-	2/2/19/22	0/1/1/1
27	GLA	F	2007	1	-	2/2/19/22	0/1/1/1
27	GLA	B	2011	1	-	1/2/19/22	0/1/1/1
27	GLA	F	2016	1	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	GLA	E	2007	1	1/1/4/5	2/2/19/22	0/1/1/1
27	GLA	E	2005	1	-	2/2/19/22	0/1/1/1
27	GLA	D	2009	1	-	2/2/19/22	0/1/1/1
27	GLA	A	2012	1	-	2/2/19/22	0/1/1/1
27	GLA	E	2015	1	-	0/2/19/22	0/1/1/1
27	GLA	F	2008	1	-	1/2/19/22	0/1/1/1
27	GLA	C	2004	1	-	2/2/19/22	0/1/1/1
26	AHR	D	2001	-	-	1/2/15/18	0/1/1/1
27	GLA	B	2015	1	-	2/2/19/22	0/1/1/1
27	GLA	C	2005	1	-	2/2/19/22	0/1/1/1
28	NAG	C	2009	1	-	4/6/23/26	0/1/1/1
27	GLA	B	2006	1	-	0/2/19/22	0/1/1/1
27	GLA	F	2012	1	-	2/2/19/22	0/1/1/1
27	GLA	B	2009	-	-	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.

31 monomers are involved in 96 short contacts:

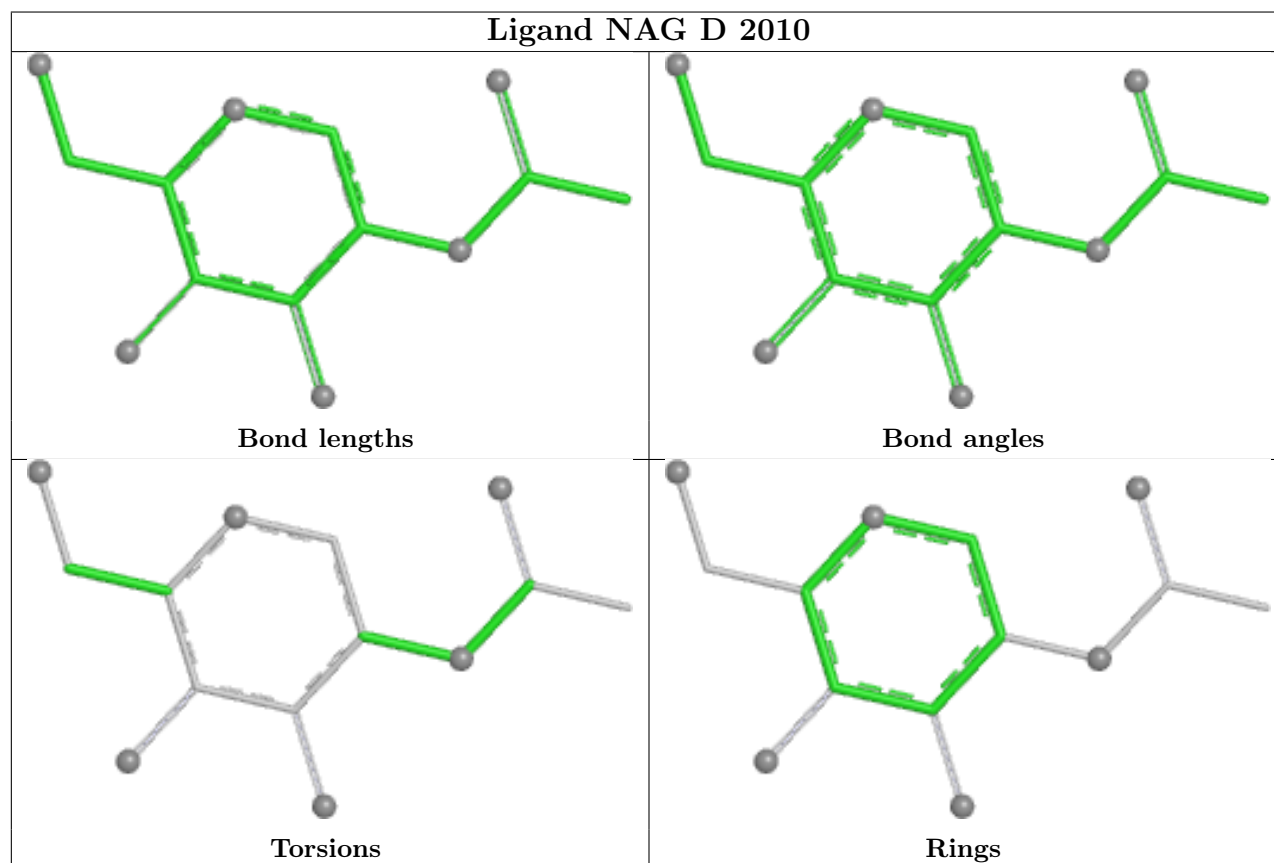
Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	D	2004	AHR	3	0
27	B	2010	GLA	1	0
26	F	2005	AHR	5	0
27	D	2008	GLA	1	0
27	A	2008	GLA	1	0
27	A	2014	GLA	1	0
26	B	2004	AHR	4	0
26	C	2001	AHR	5	0
27	F	2009	GLA	1	0
26	E	2002	AHR	6	0
27	A	2006	GLA	1	0
26	B	2003	AHR	5	0
26	C	2003	AHR	6	0
26	D	2003	AHR	7	0
27	C	2006	GLA	1	0
26	A	2002	AHR	4	0
27	A	2009	GLA	1	0
26	A	2003	AHR	7	0
26	F	2003	AHR	6	0
27	F	2015	GLA	1	0
26	F	2001	AHR	3	0
28	B	2018	NAG	1	0
27	E	2009	GLA	1	0
26	F	2004	AHR	5	0
26	E	2003	AHR	4	0
27	B	2014	GLA	1	0

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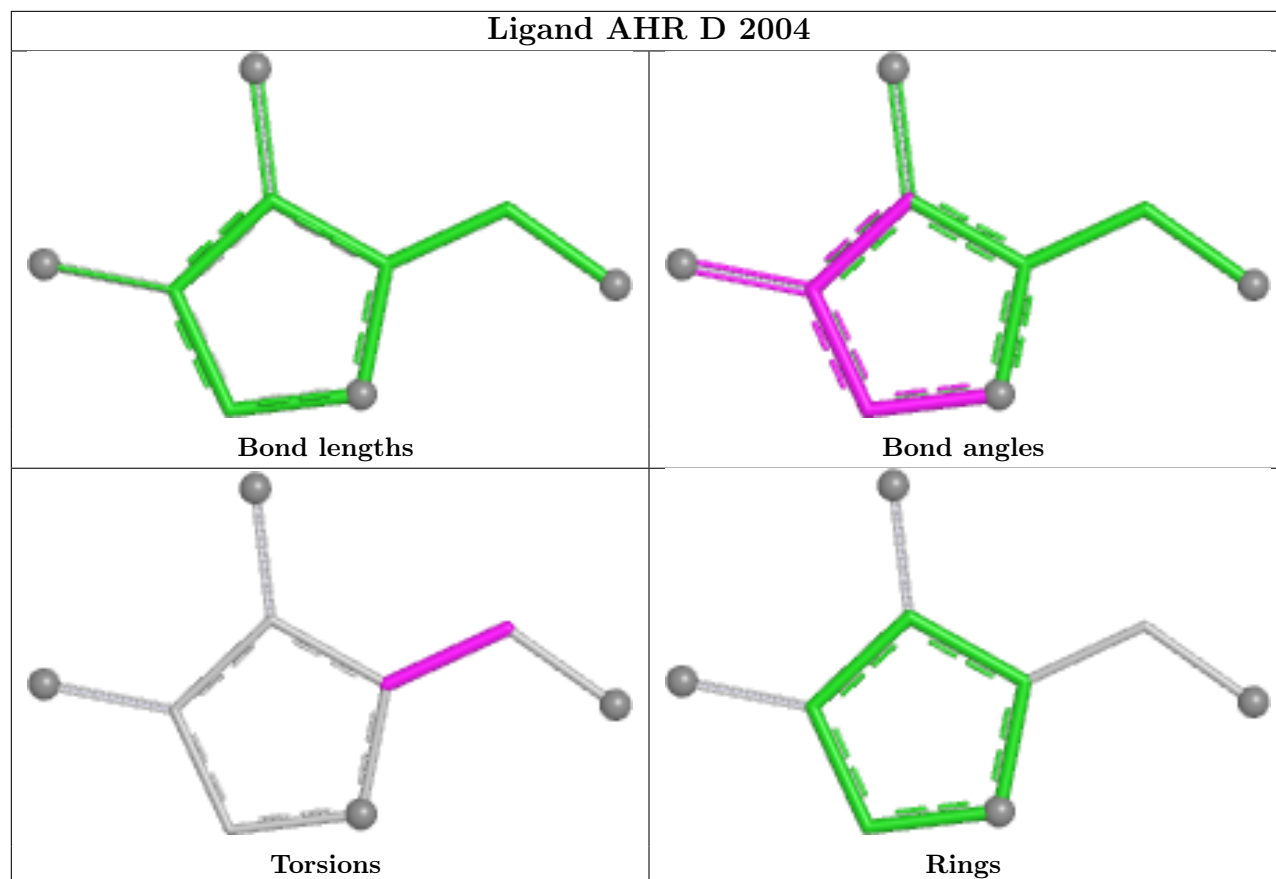
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	E	2013	GLA	1	0
26	B	2020	AHR	3	0
27	F	2016	GLA	2	0
27	F	2008	GLA	3	0
26	D	2001	AHR	5	0

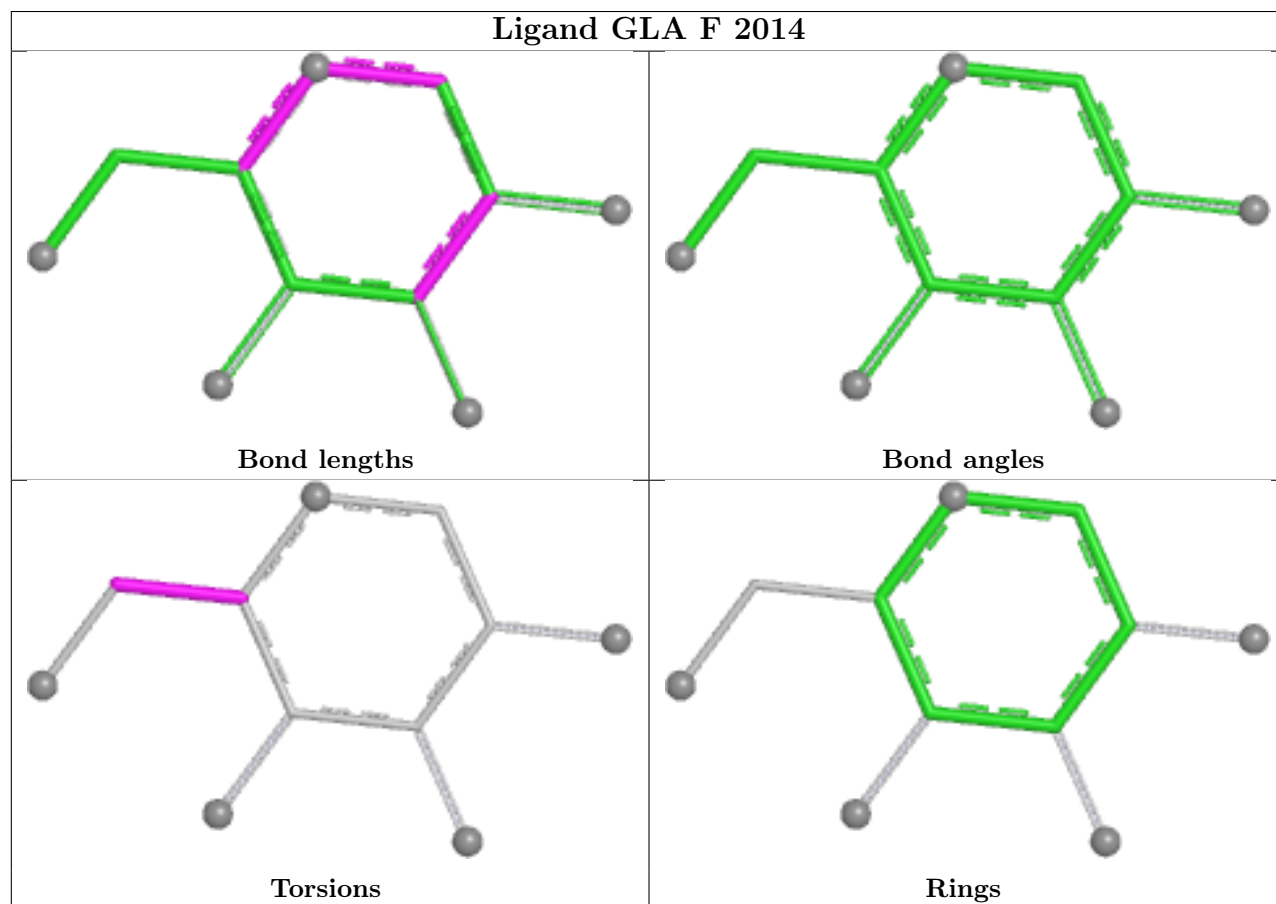
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



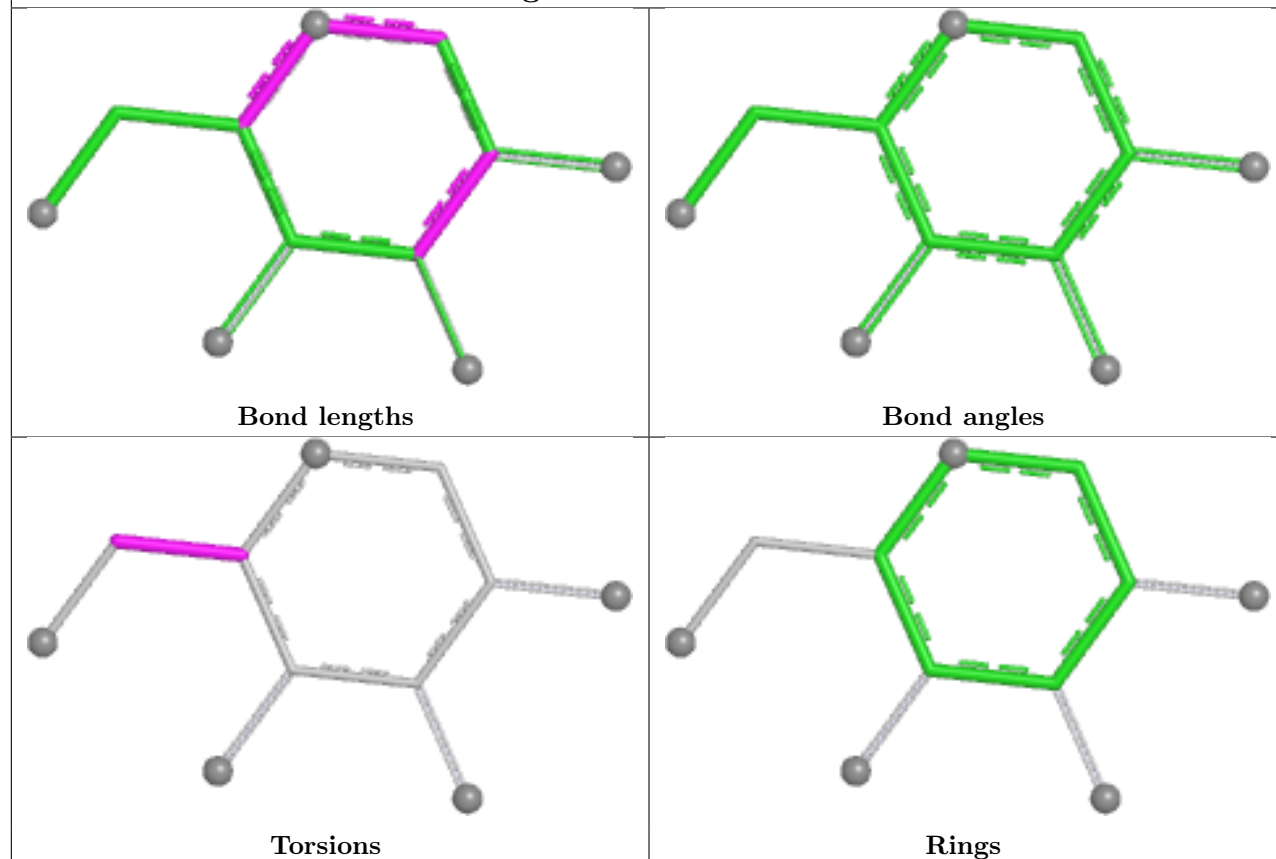
Ligand AHR D 2004



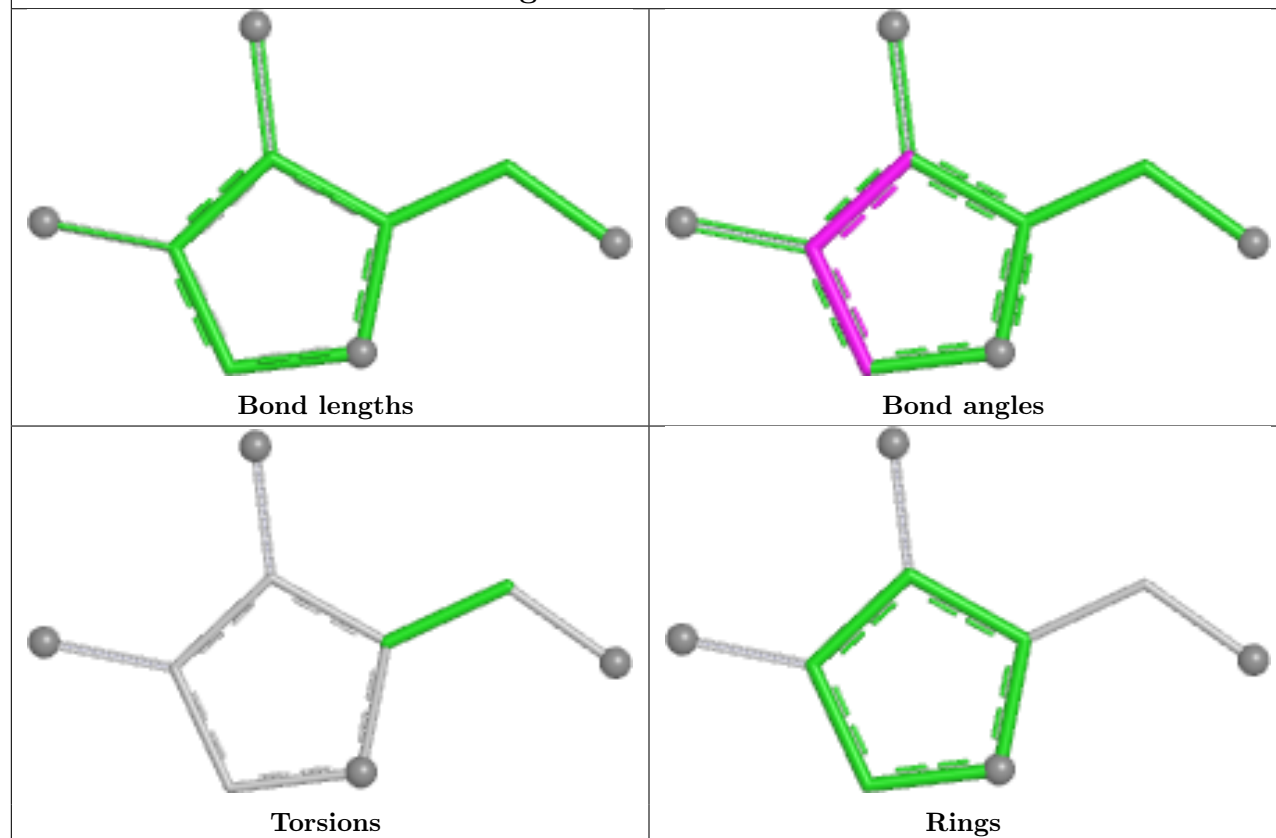
Ligand GLA F 2014



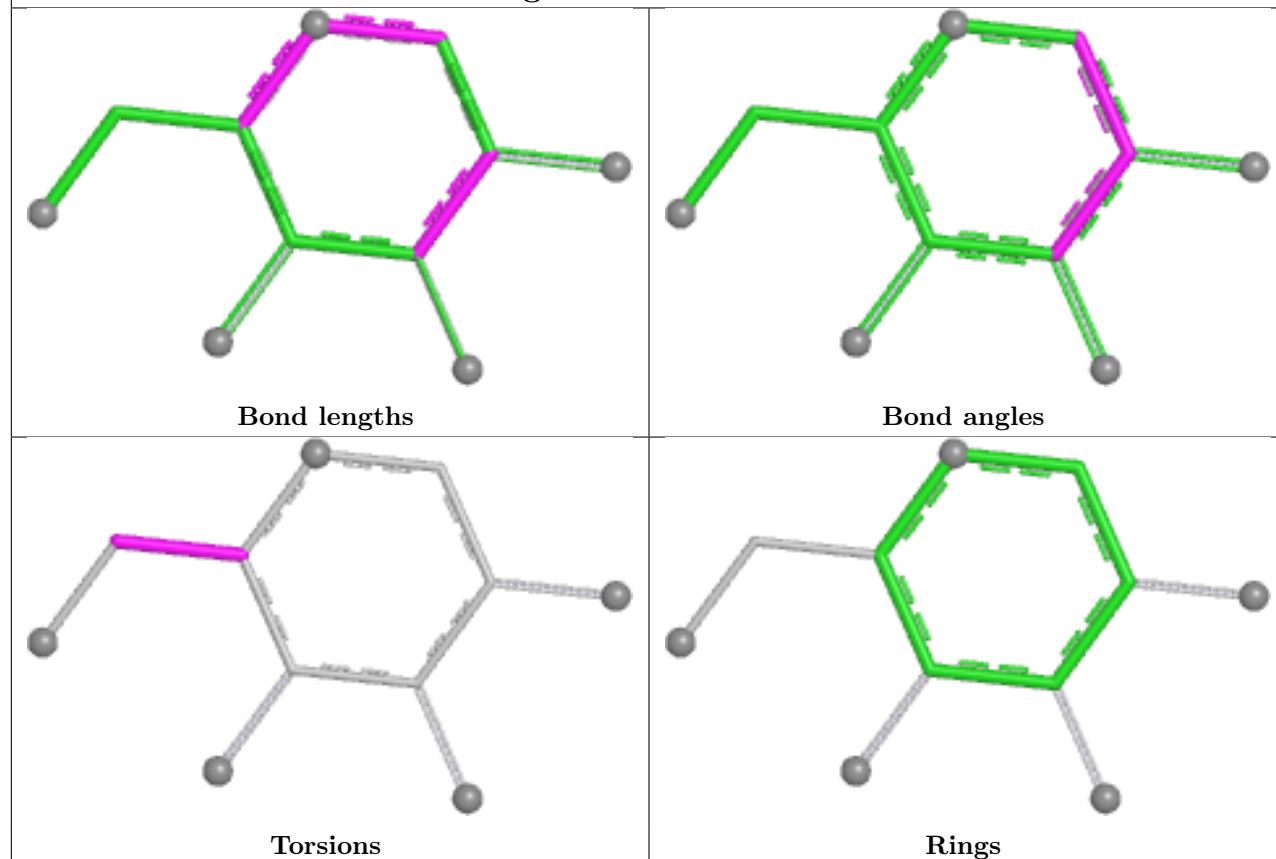
Ligand GLA B 2010



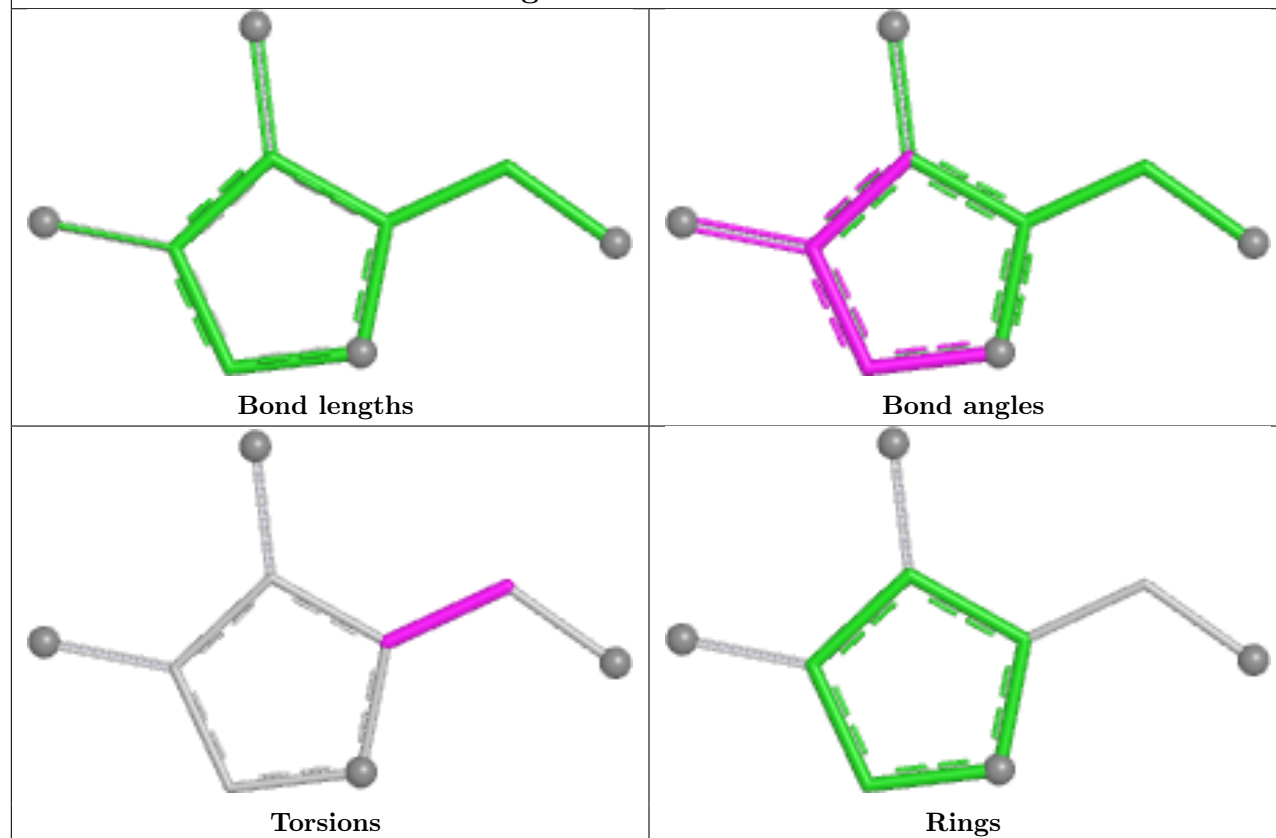
Ligand AHR B 2002

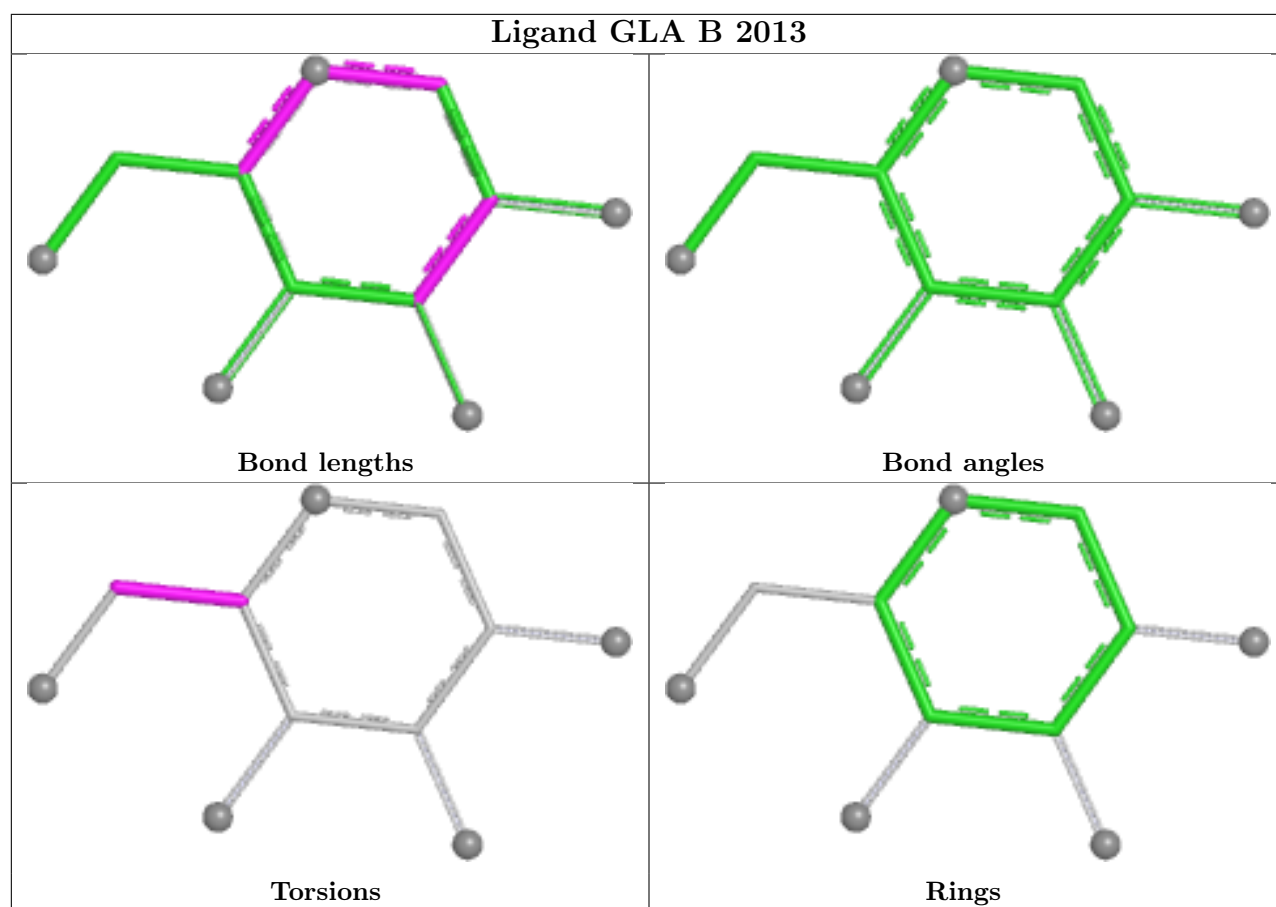


Ligand GLA E 2008

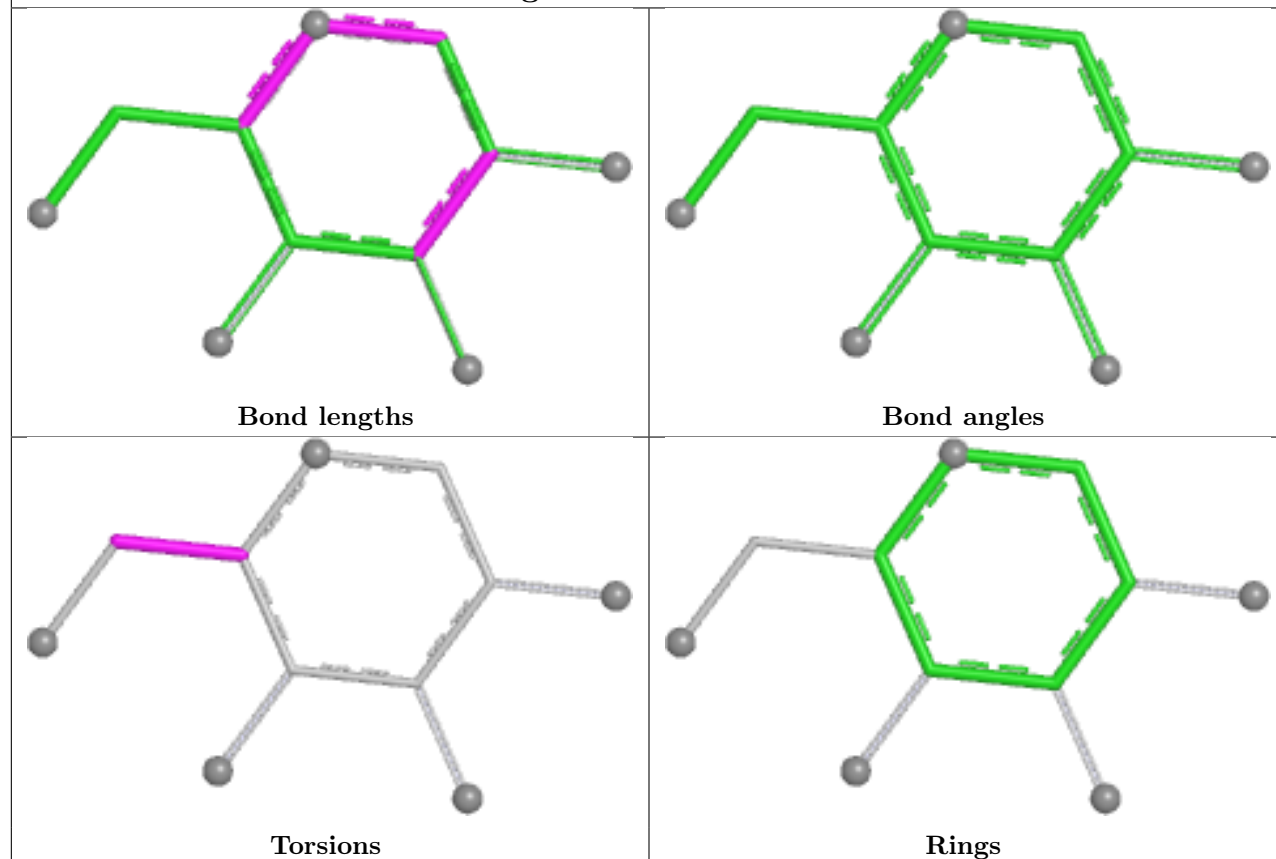


Ligand AHR F 2005

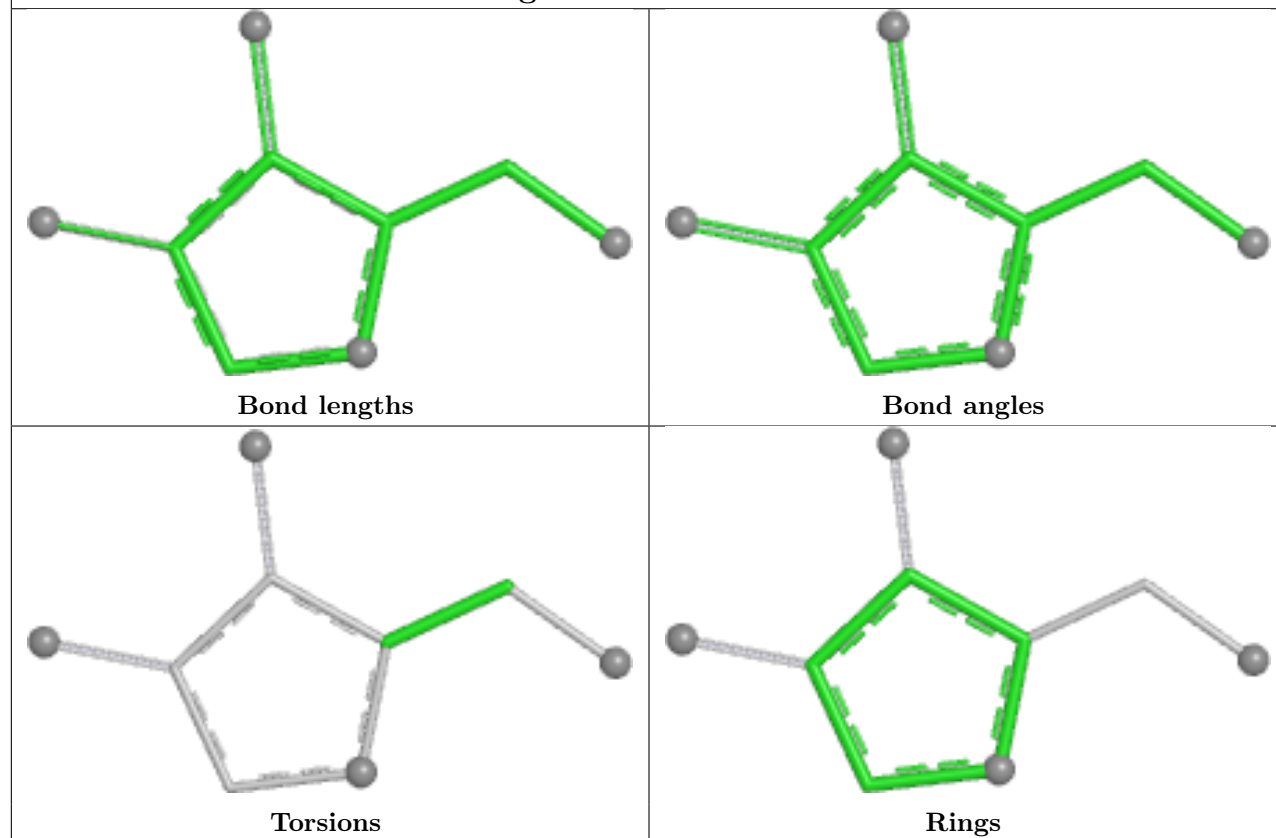




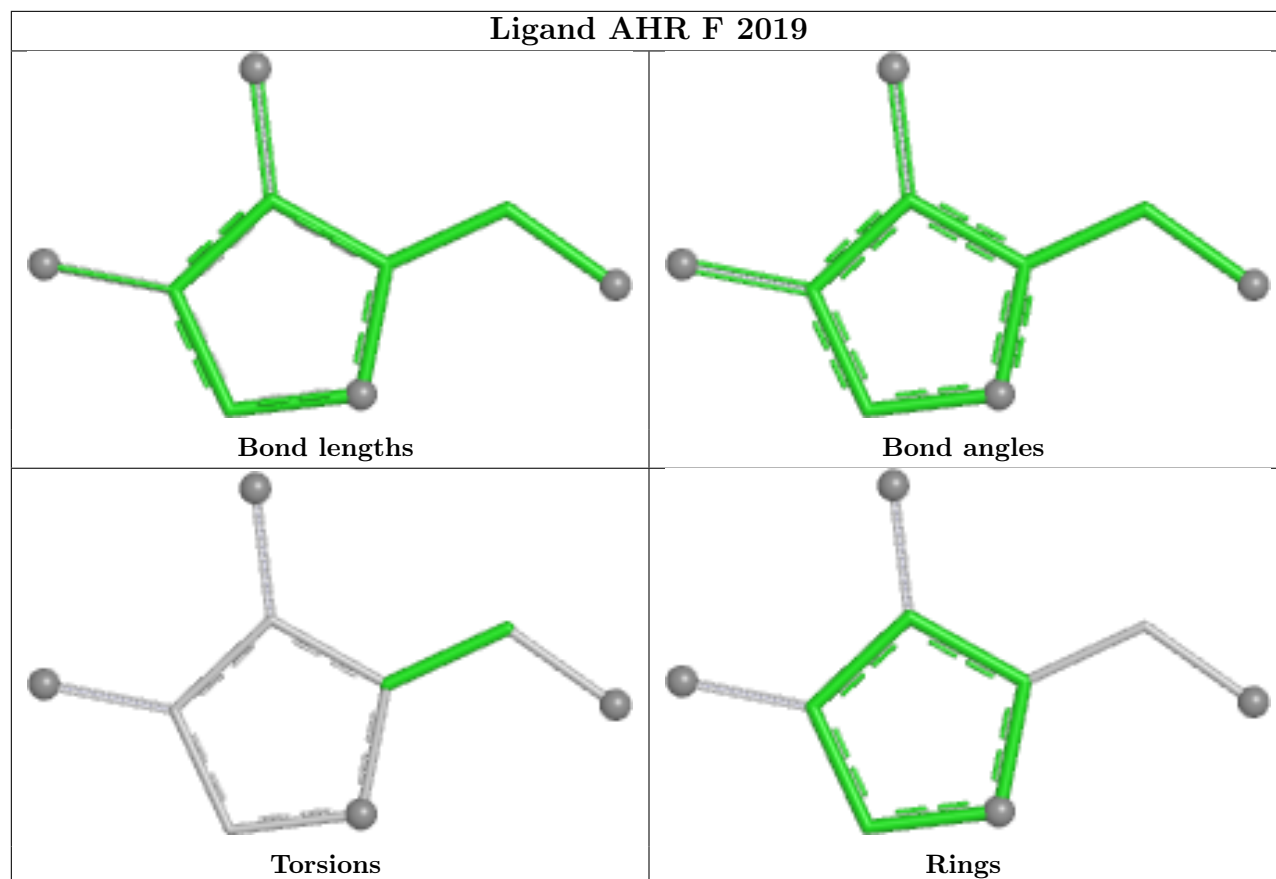
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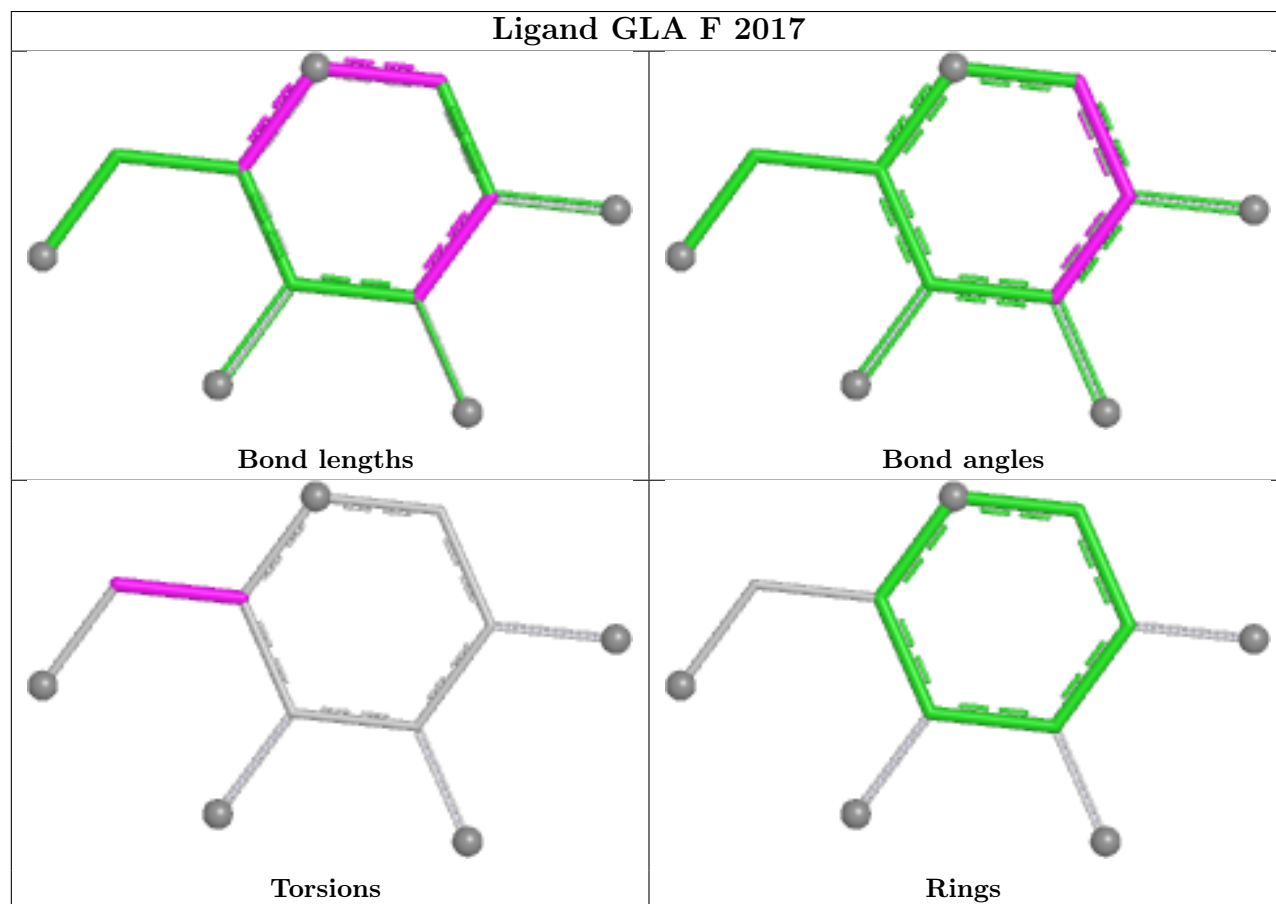
Ligand AHR A 2019

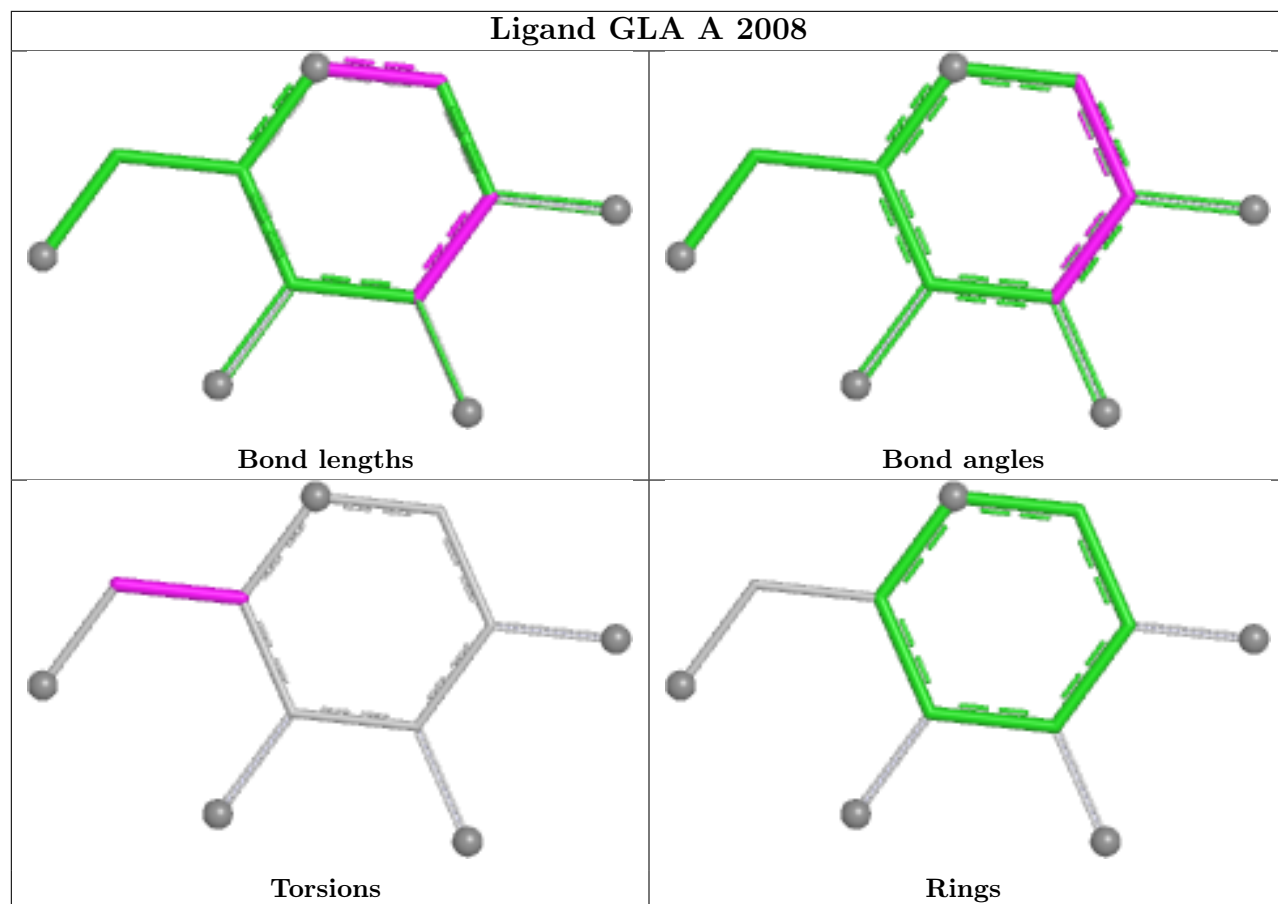


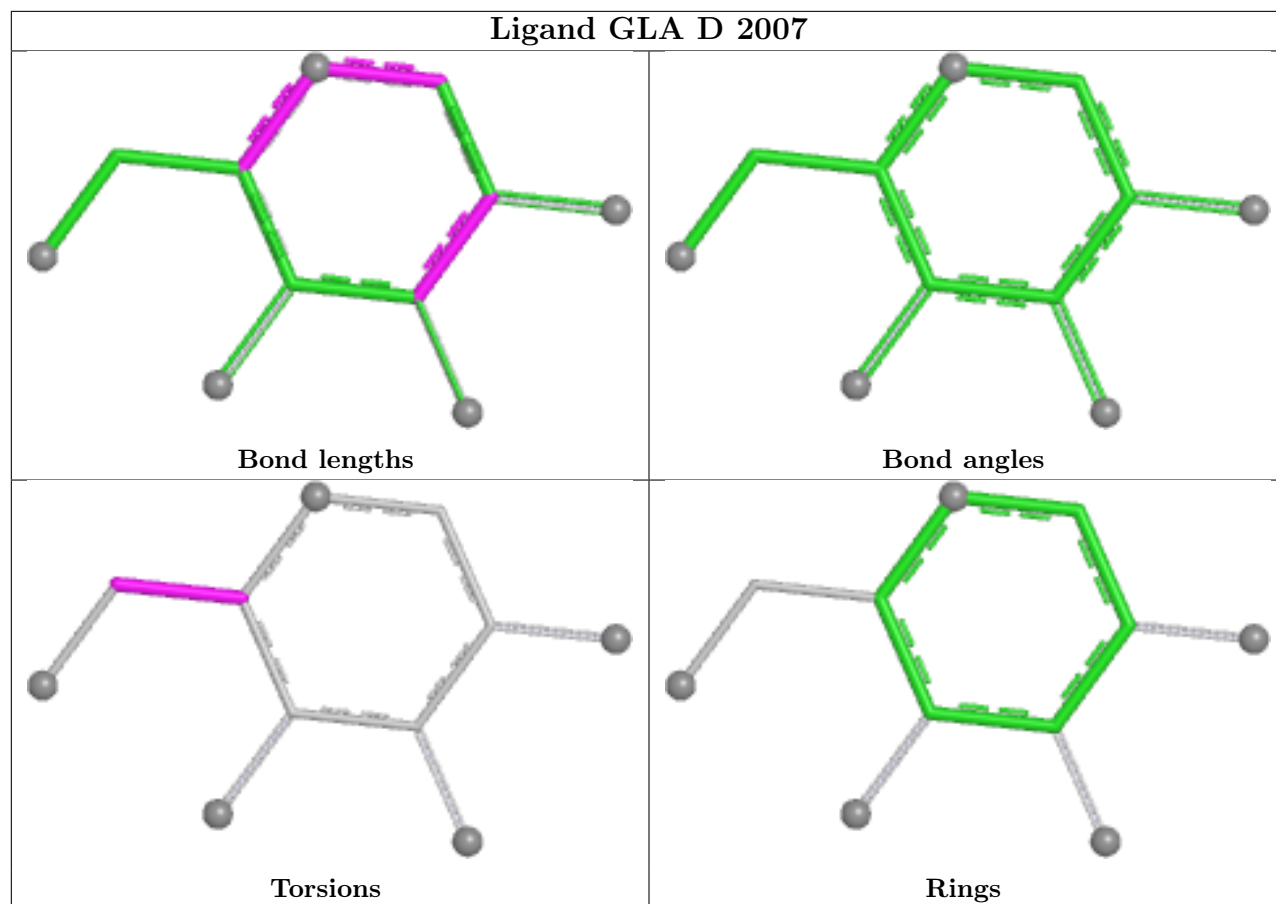
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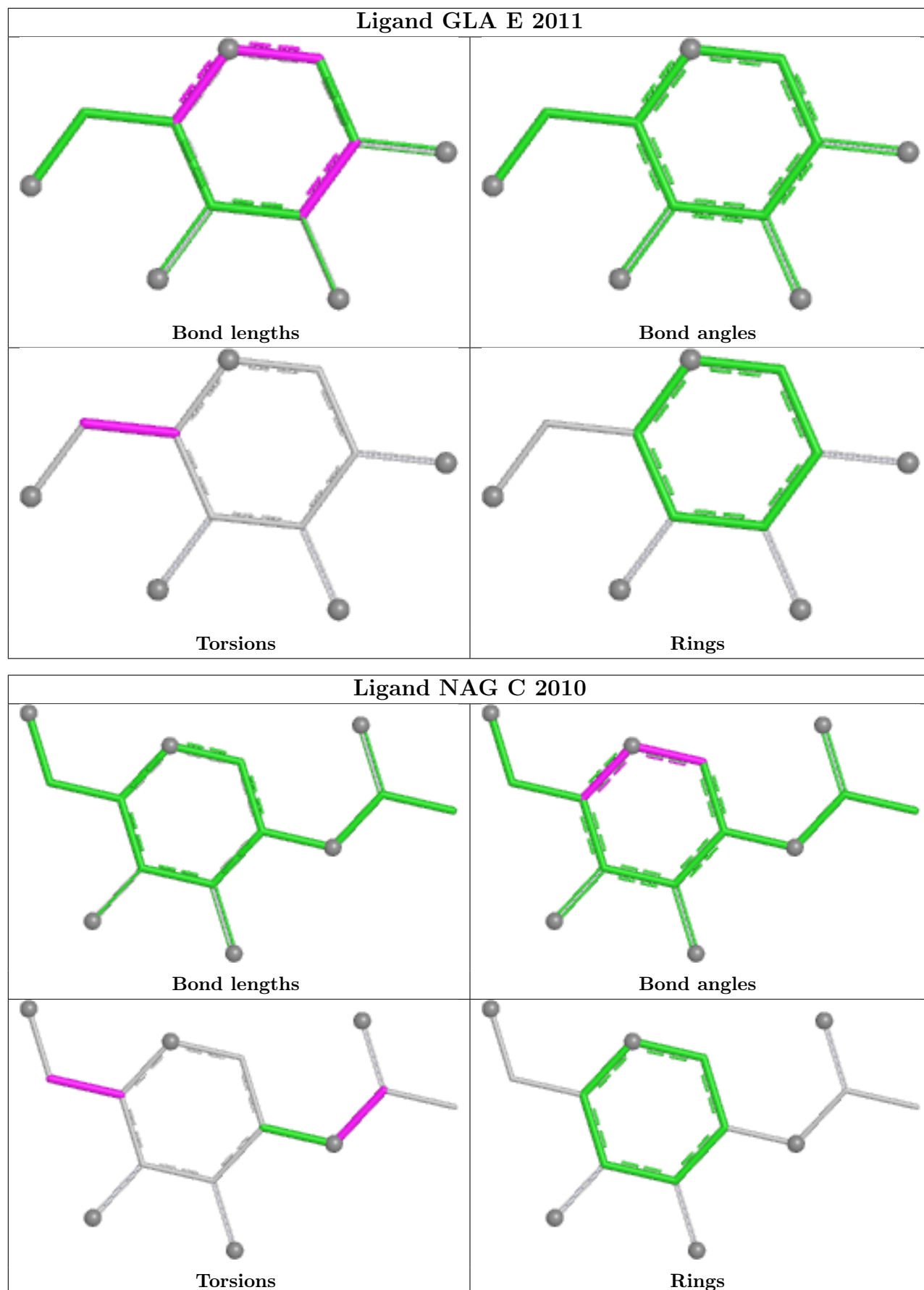


Ligand GLA F 2017

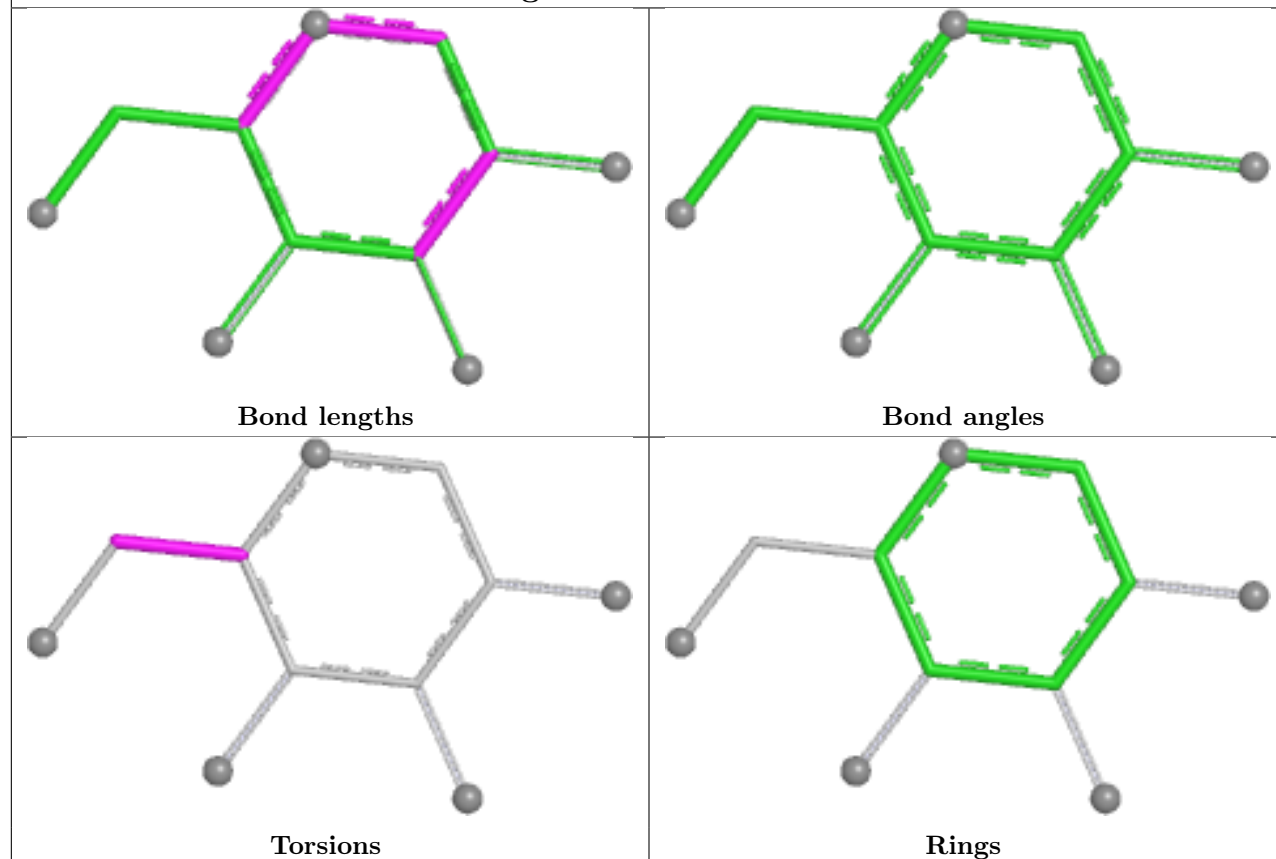




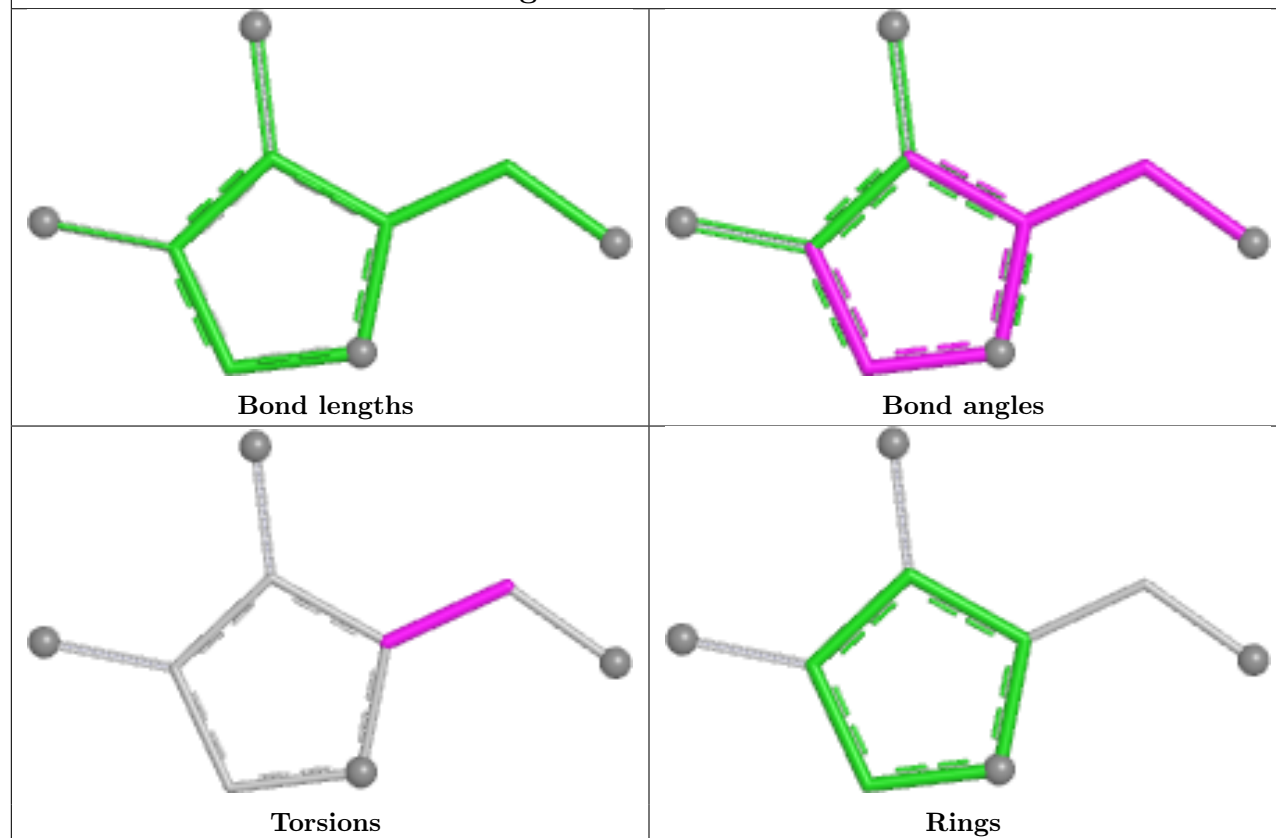




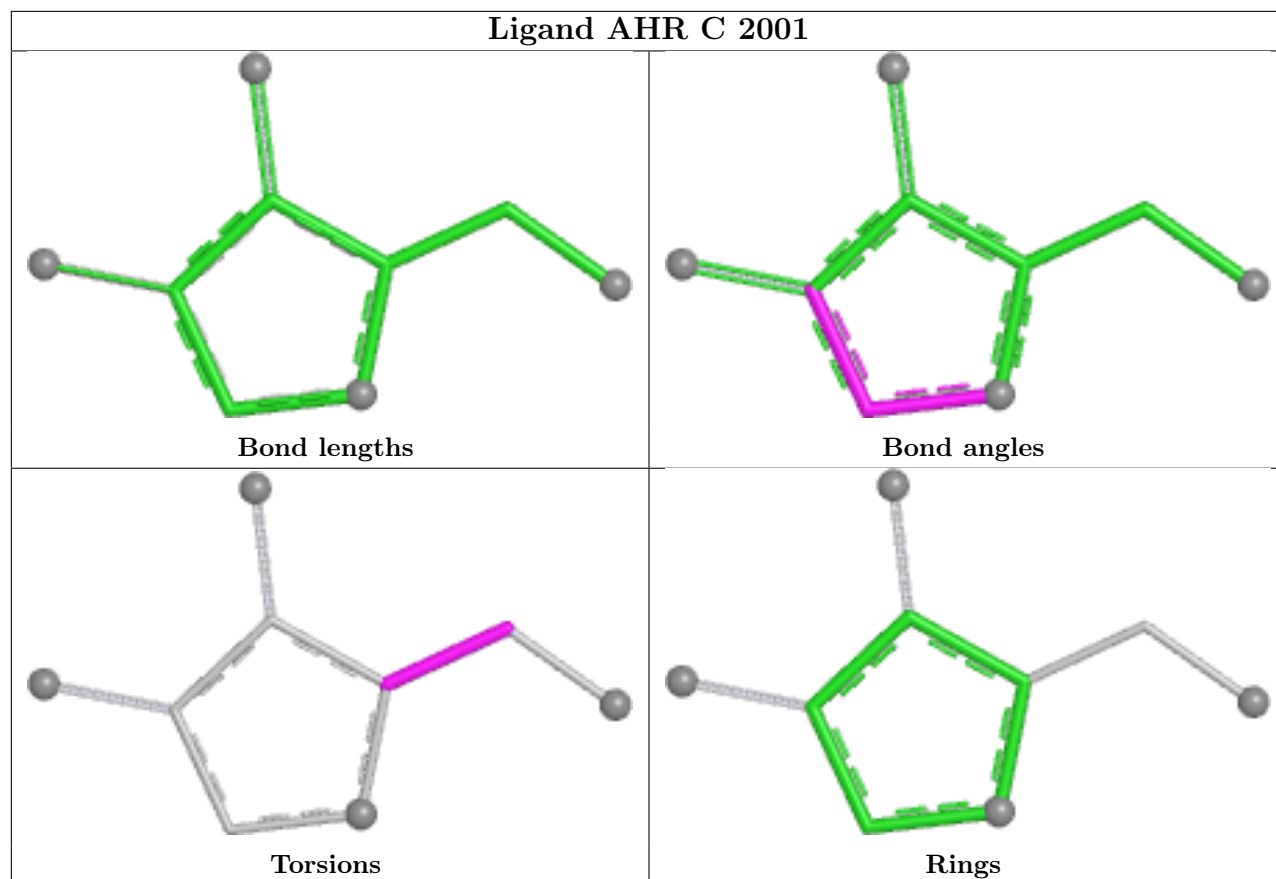
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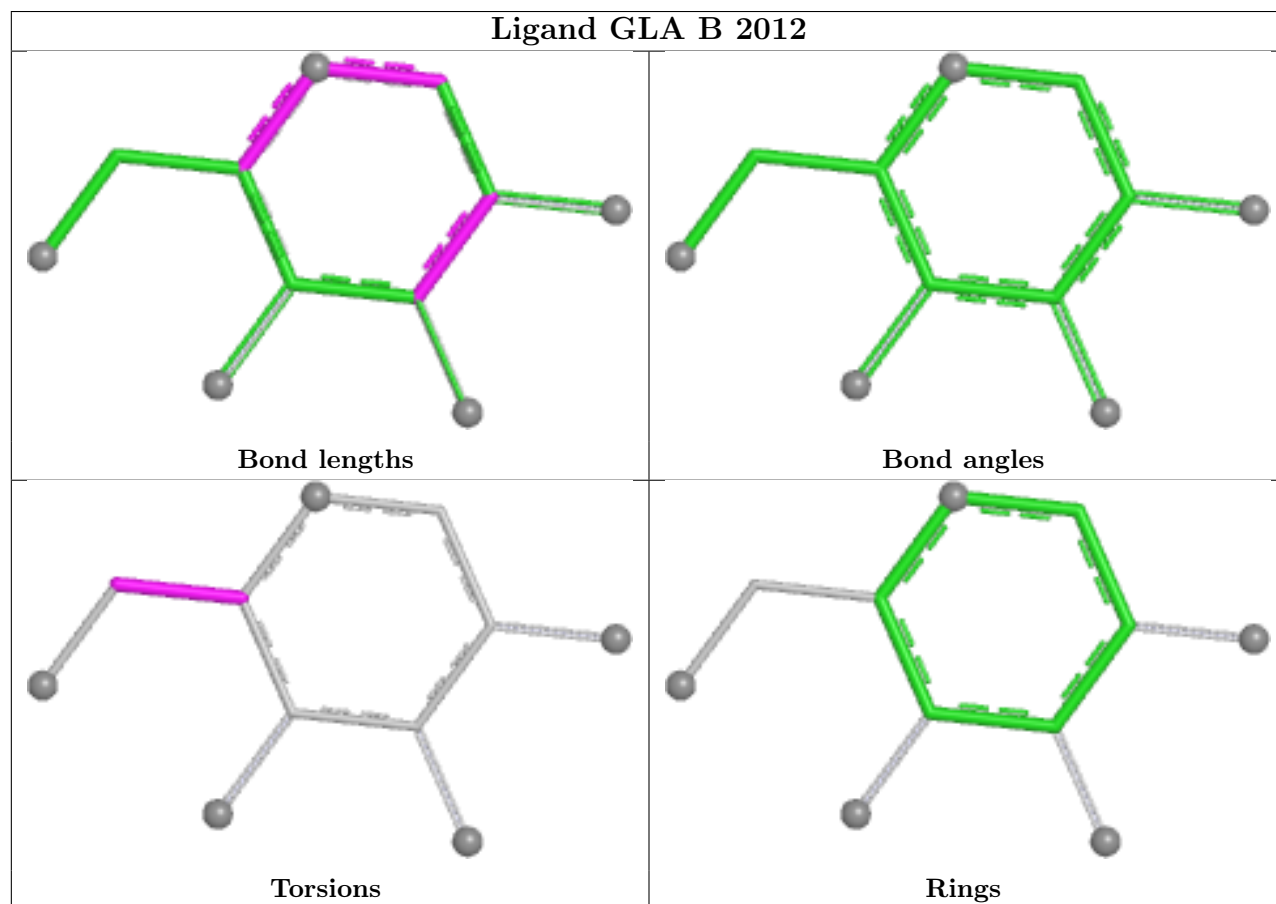
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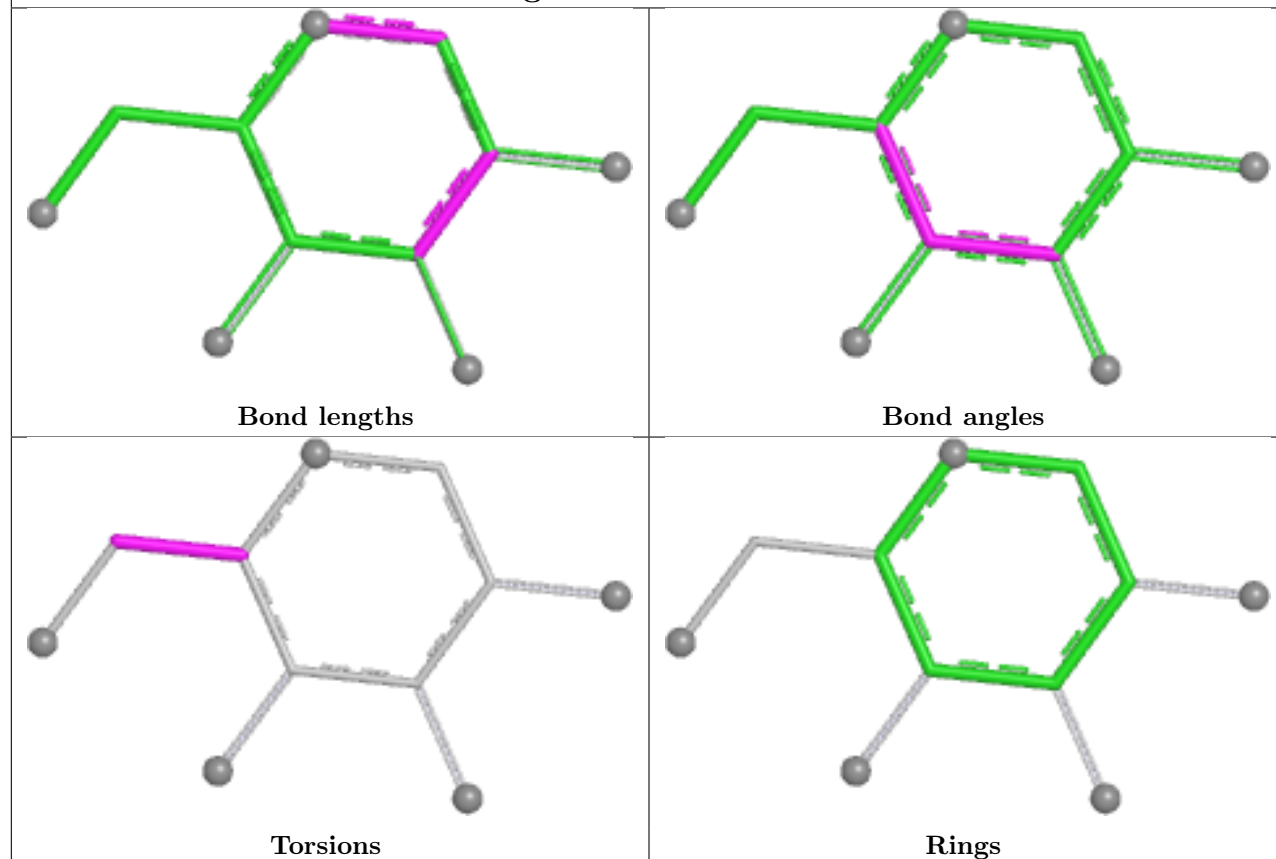
Ligand AHR C 2001



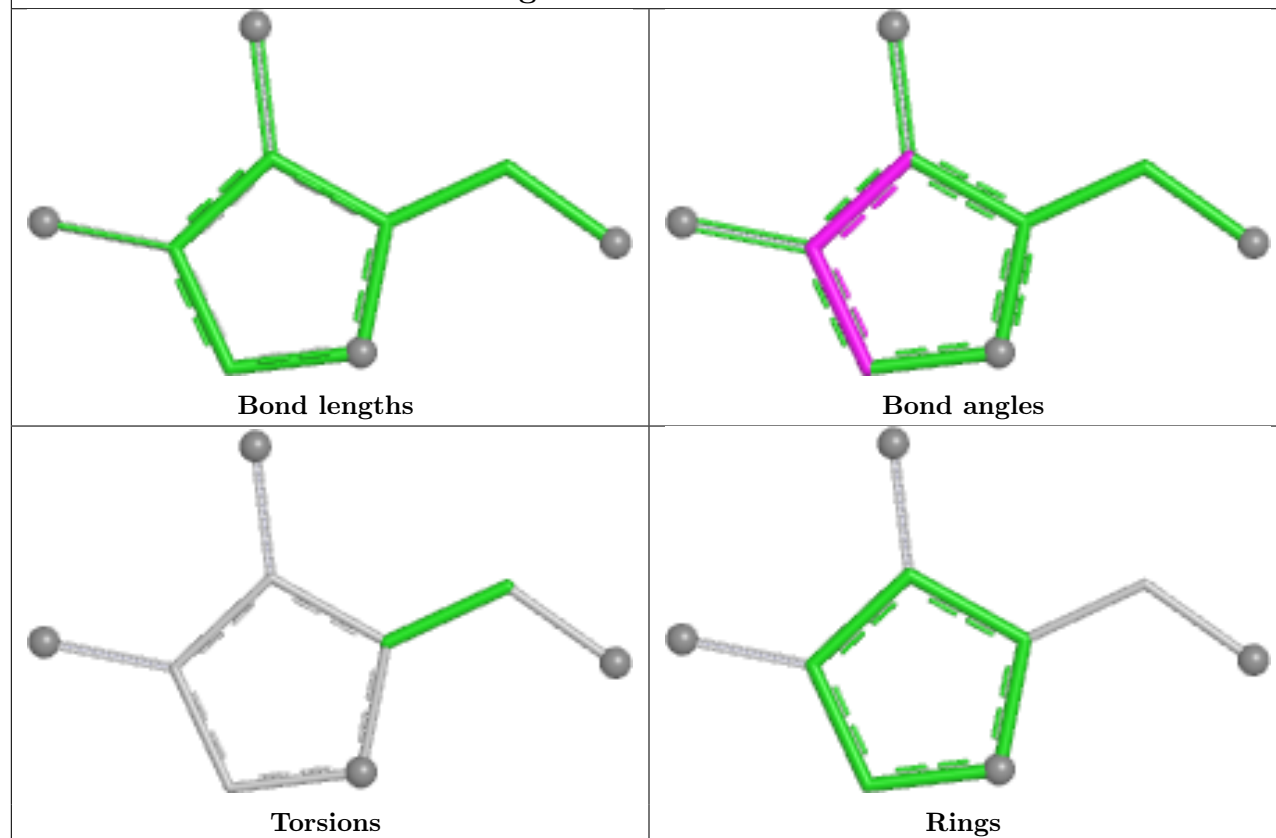
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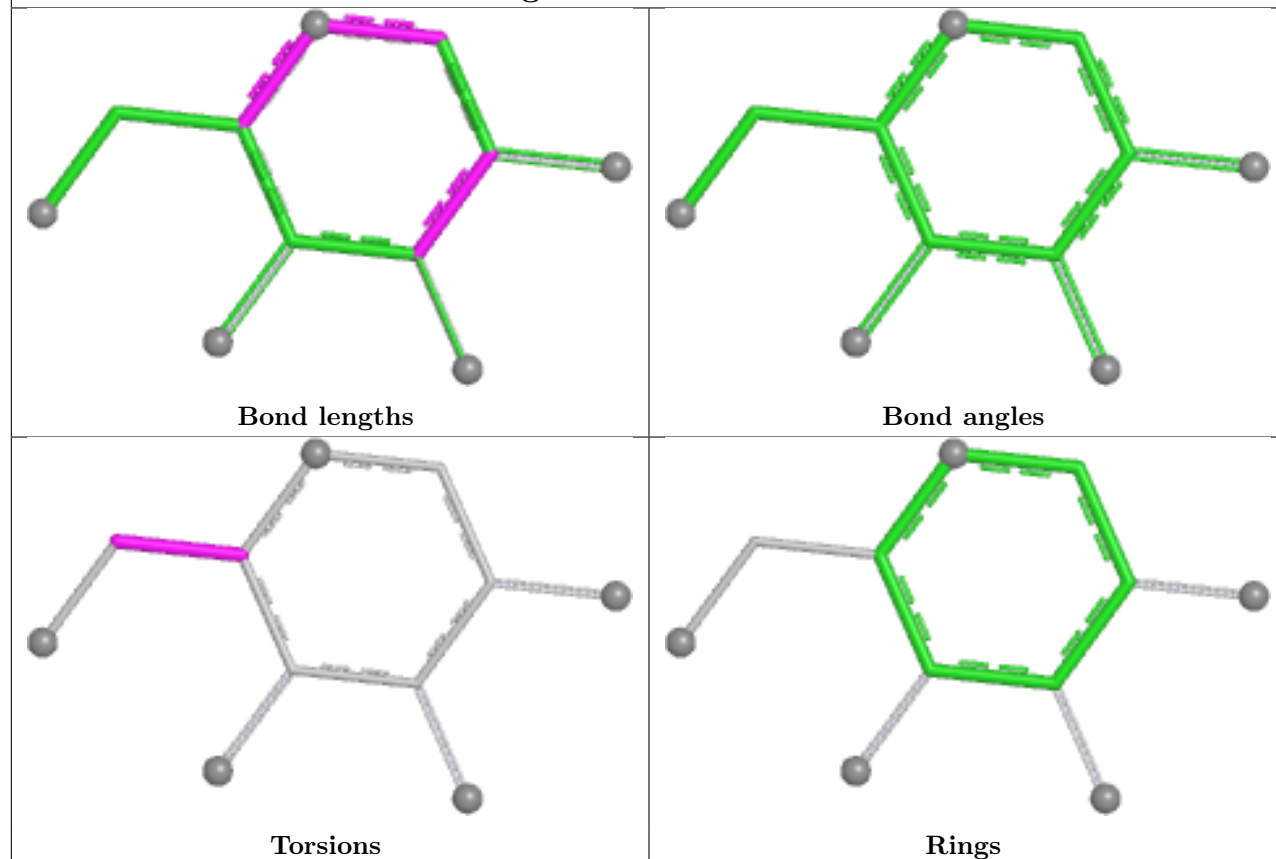
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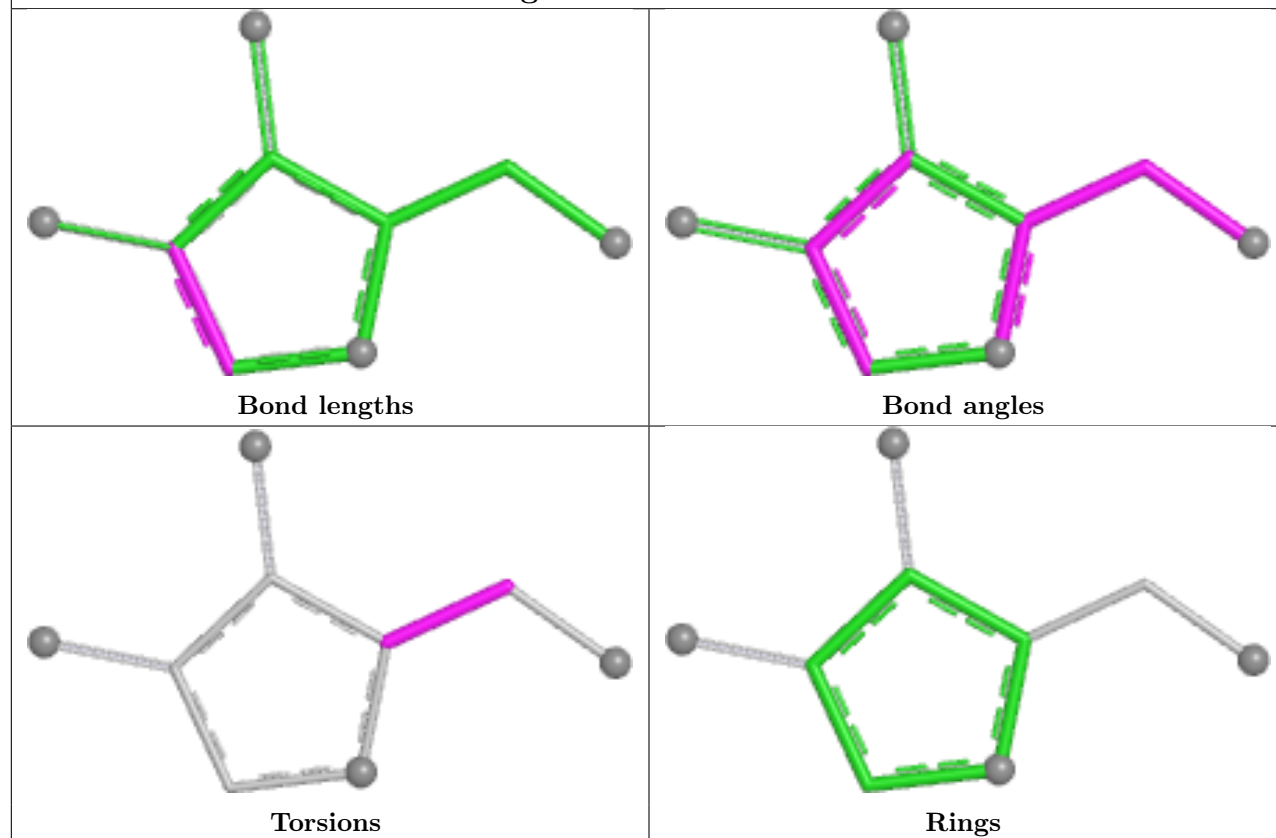
Ligand AHR A 2018

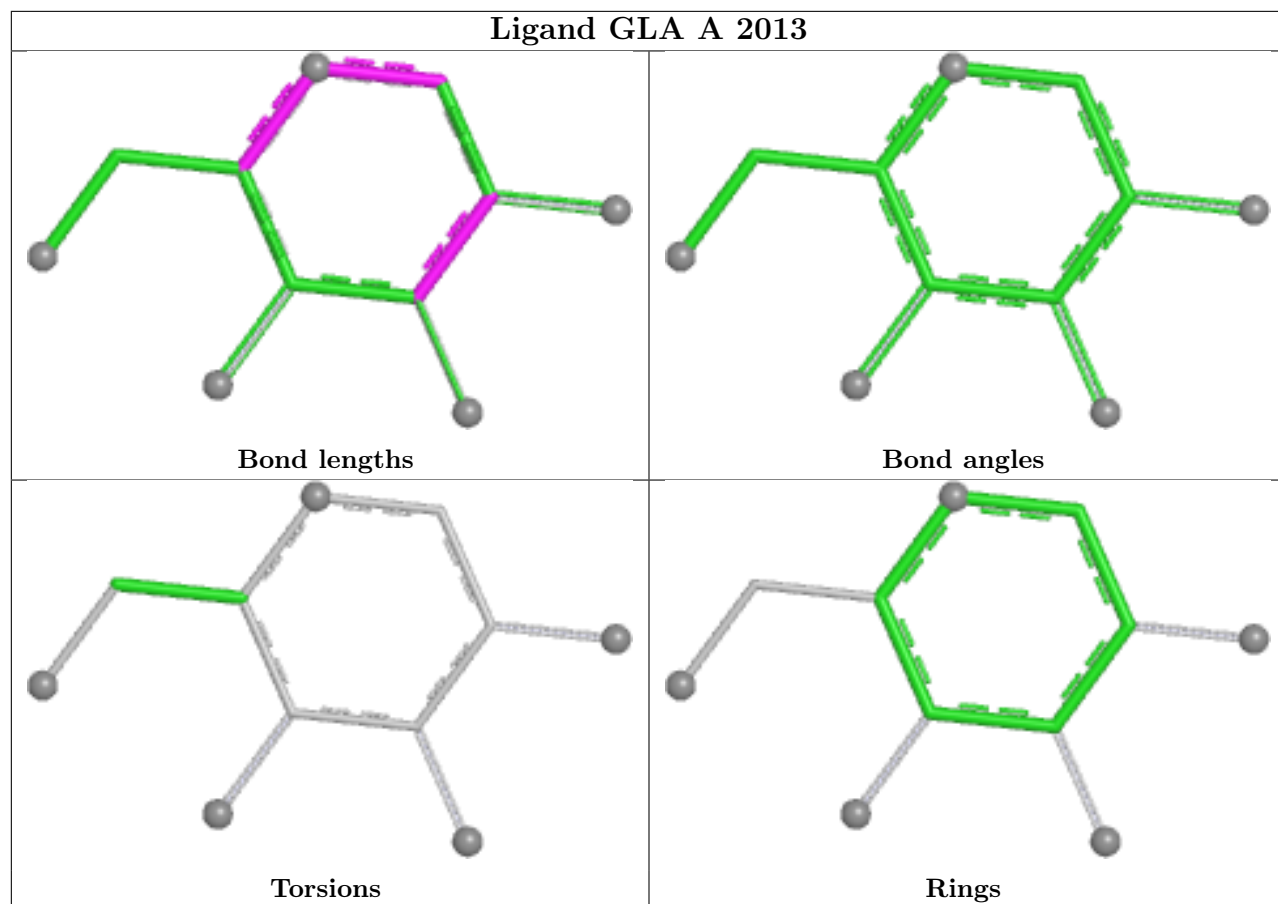


Ligand GLA C 2008

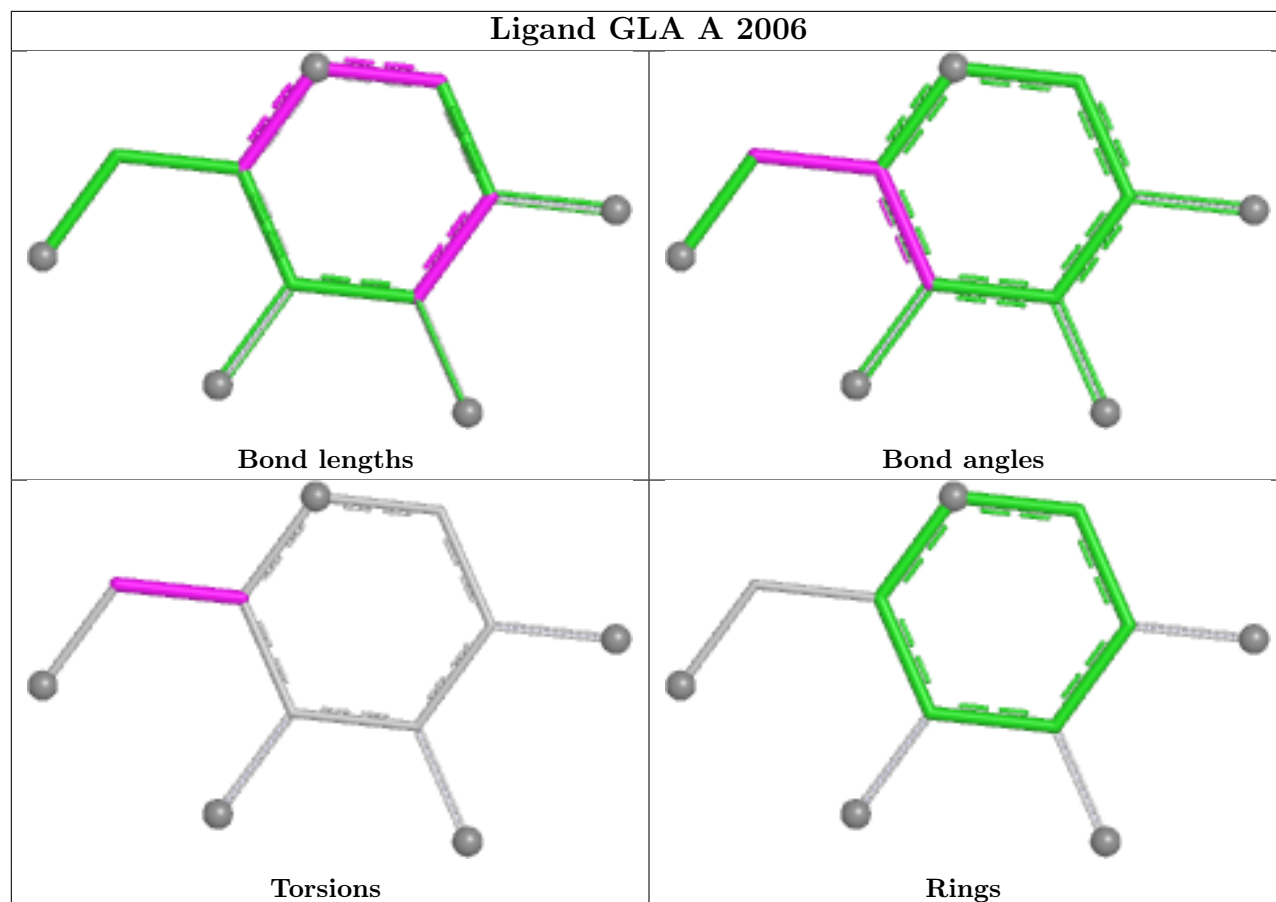


Ligand AHR E 2002

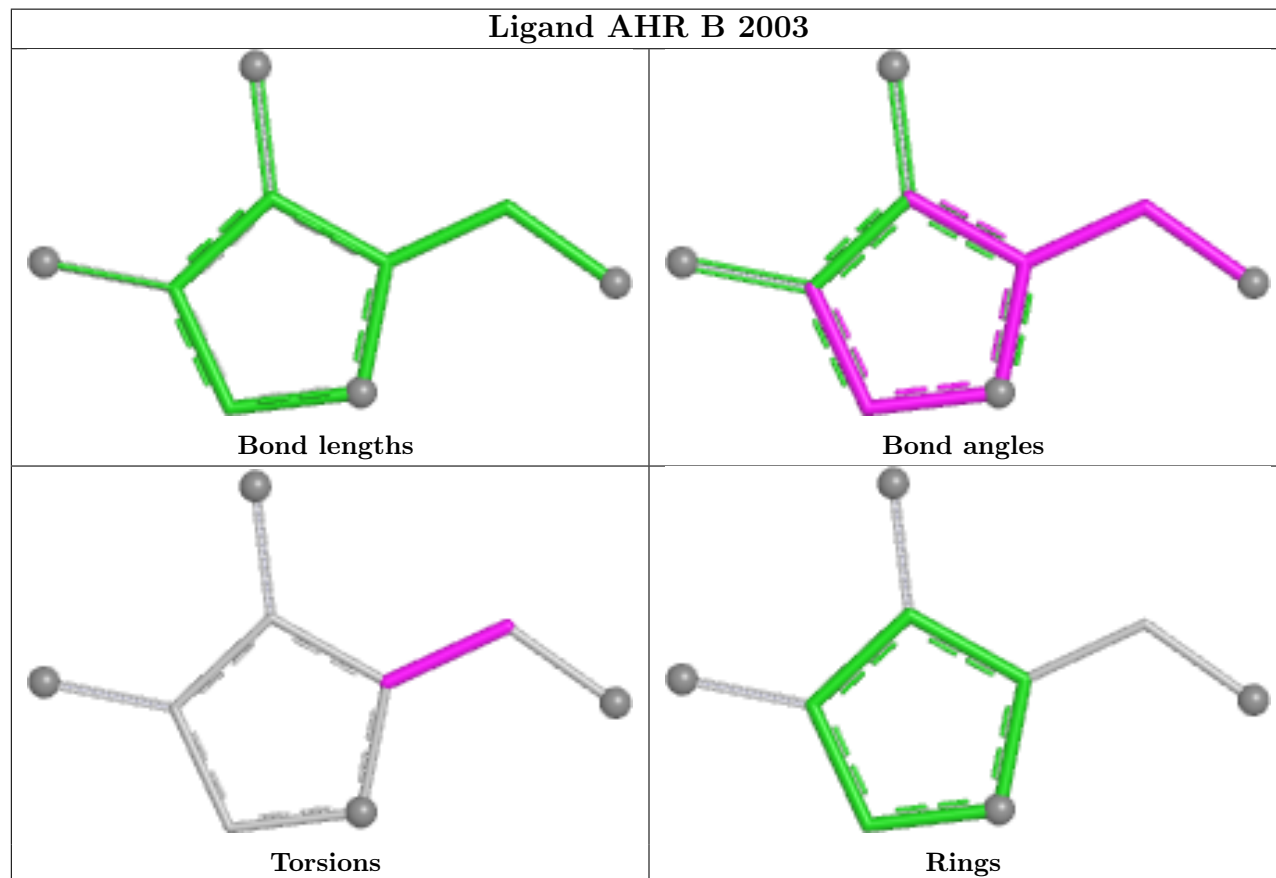




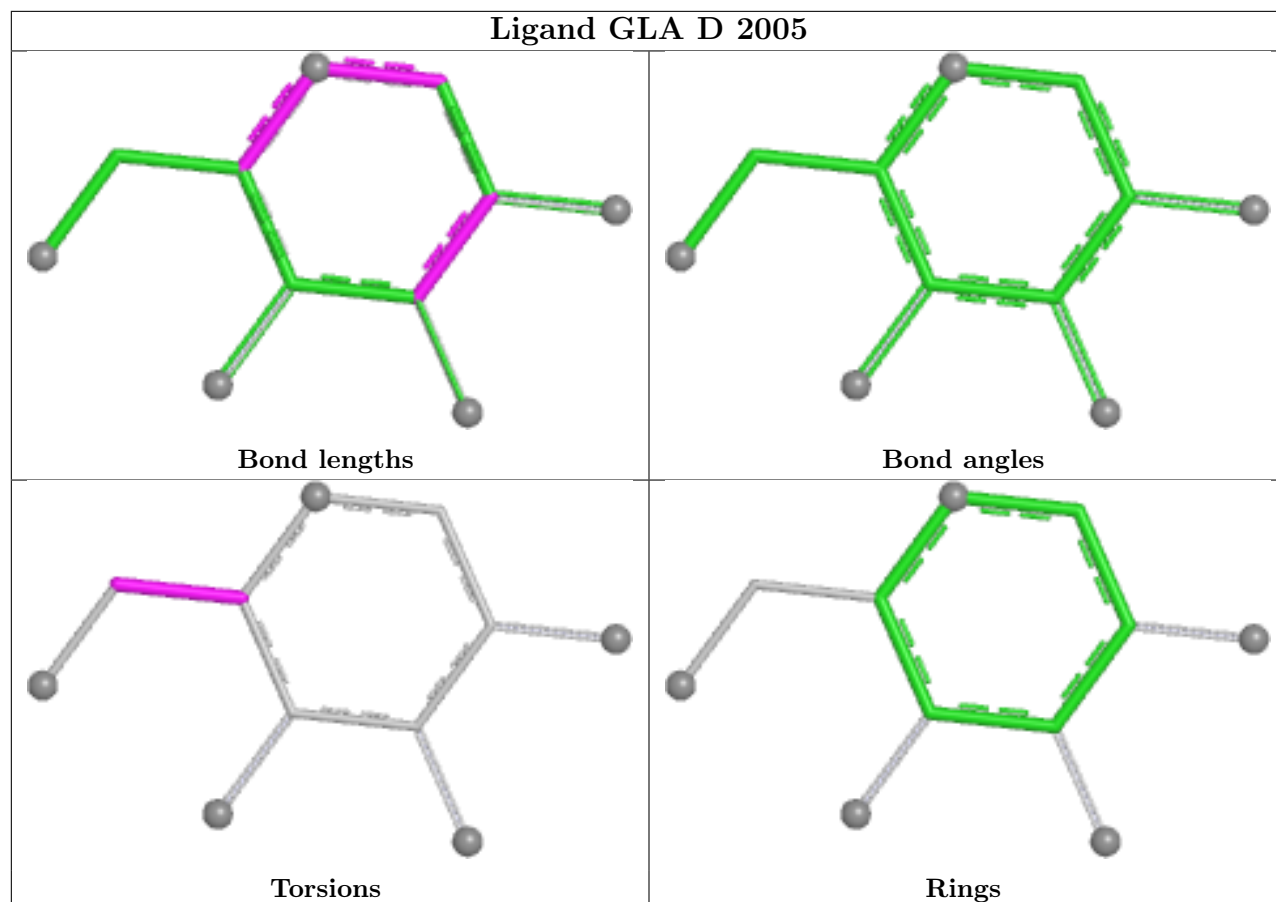
Ligand GLA A 2006



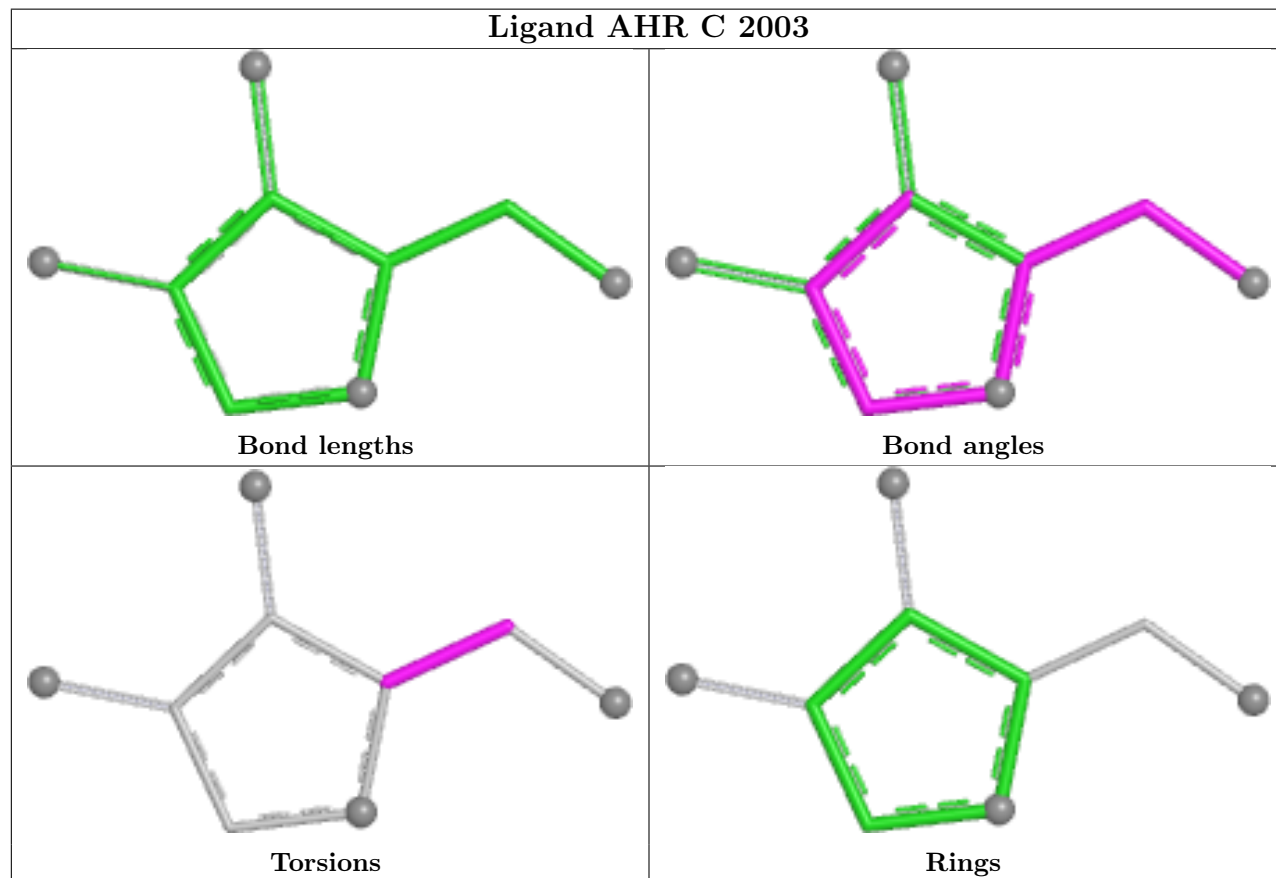
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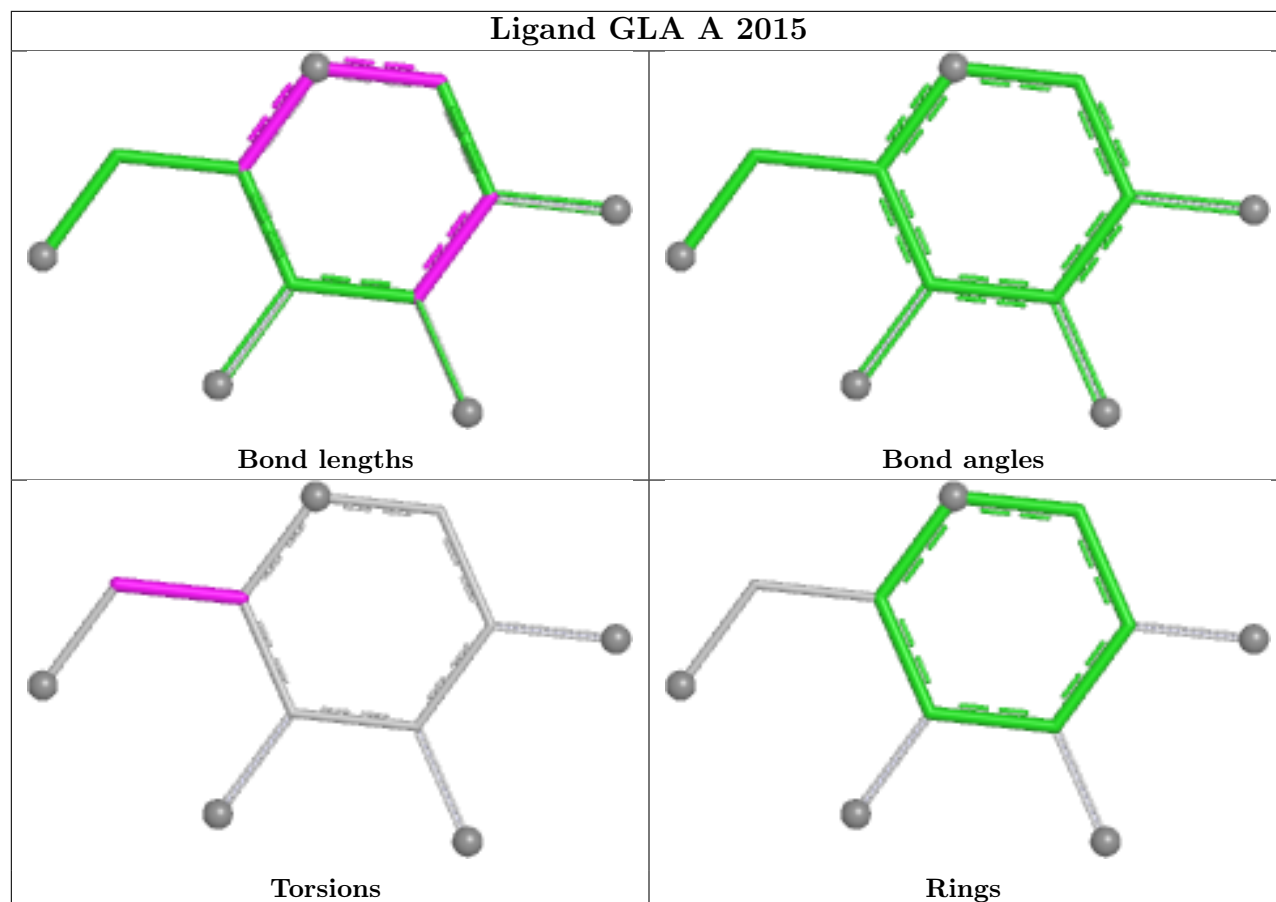
Ligand GLA D 2005



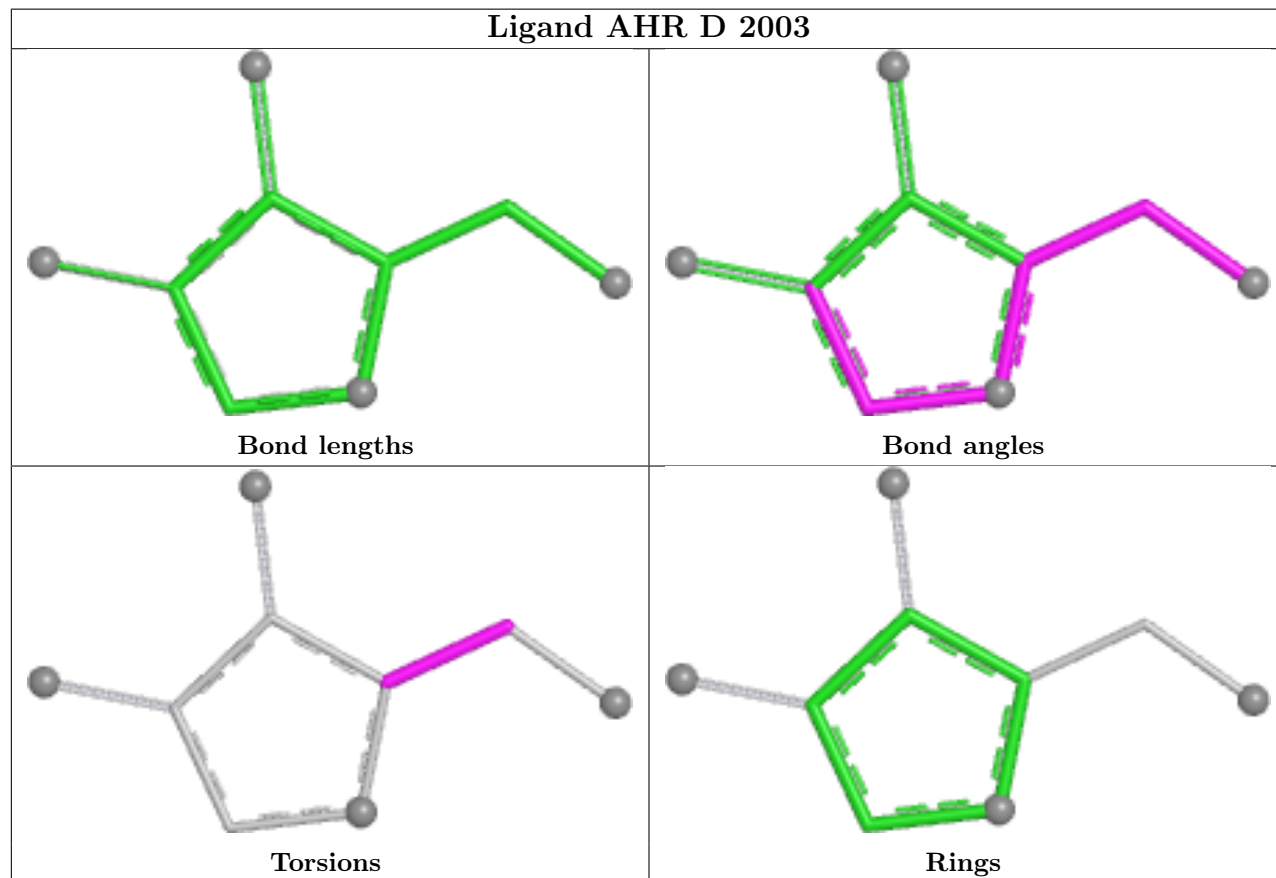
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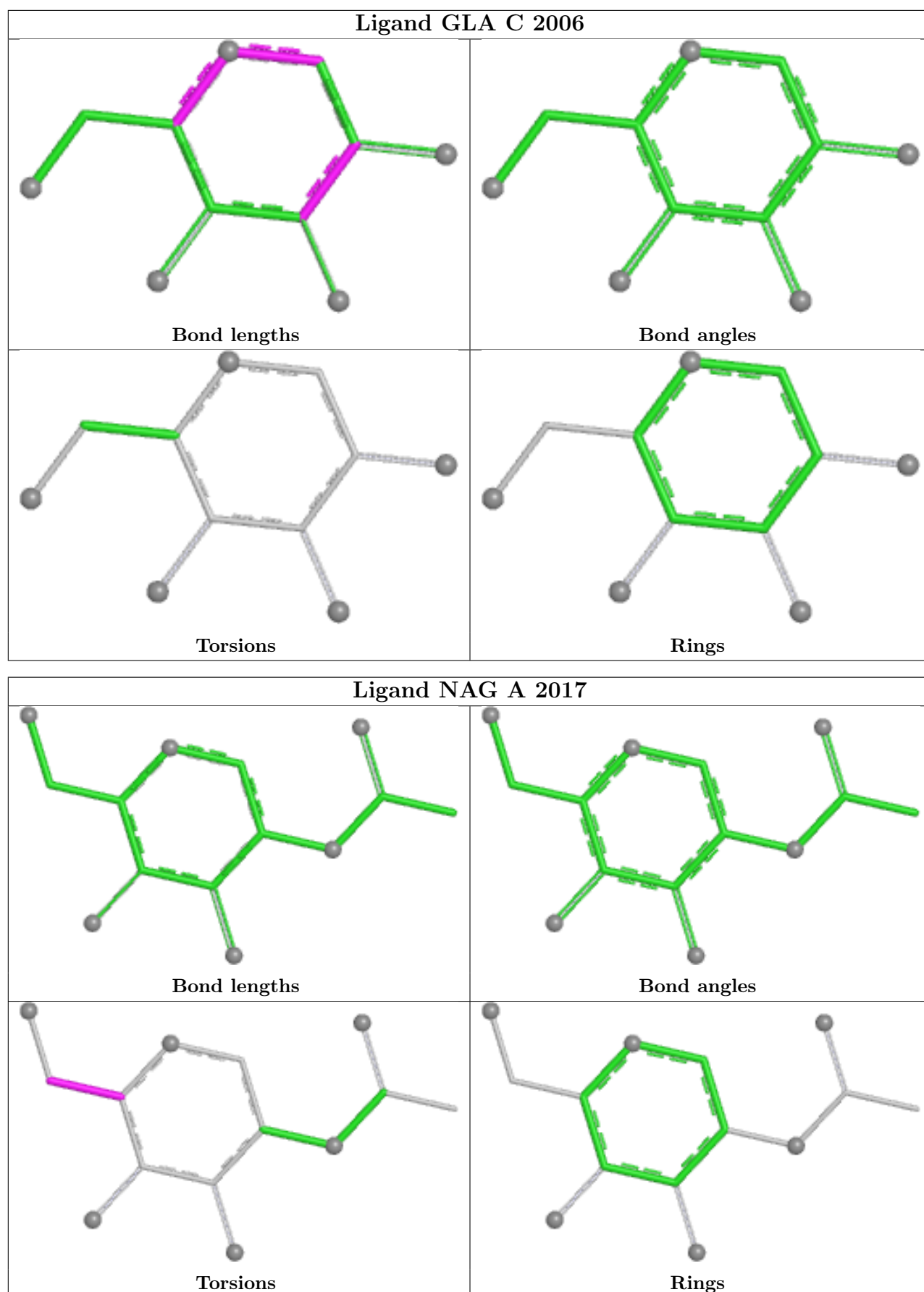


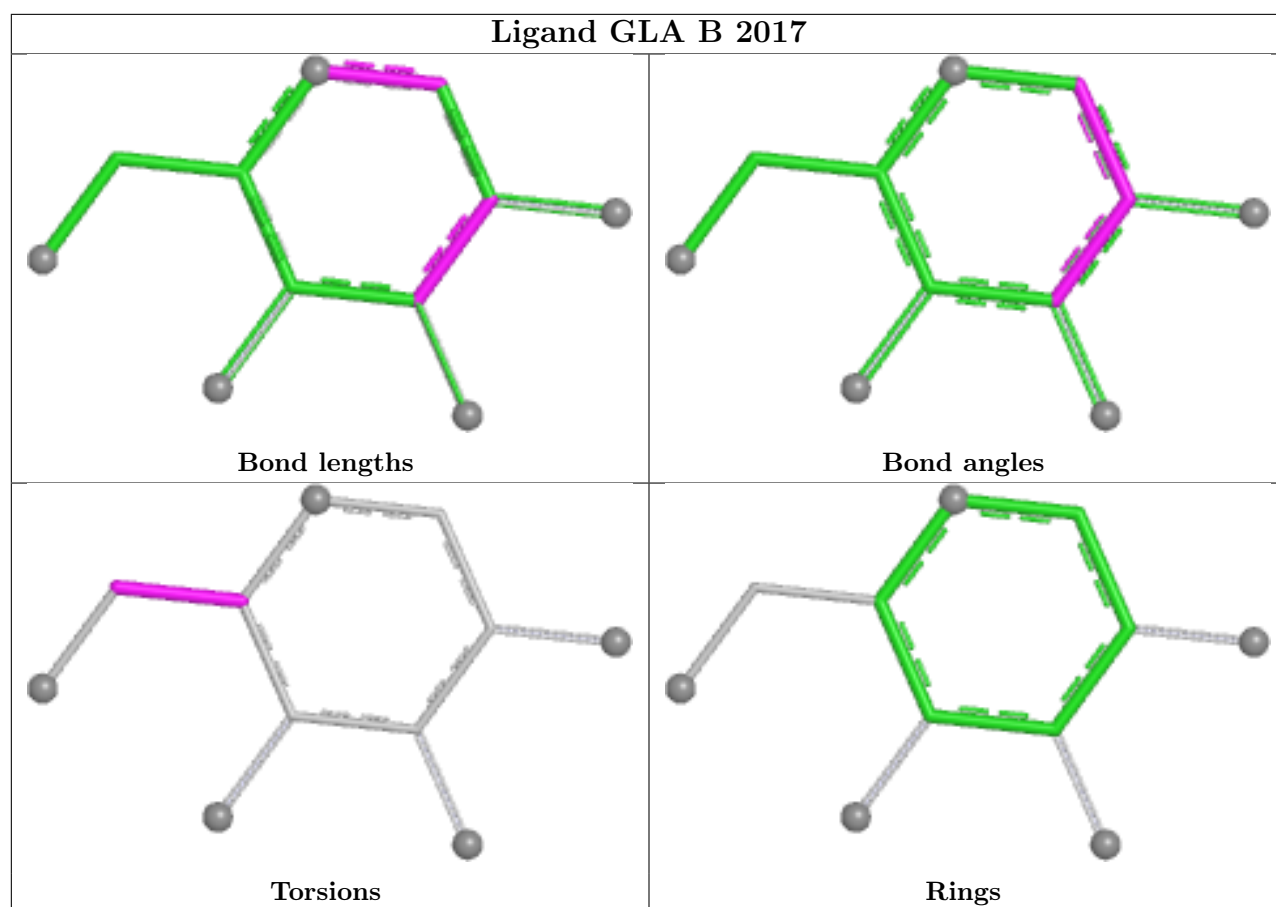
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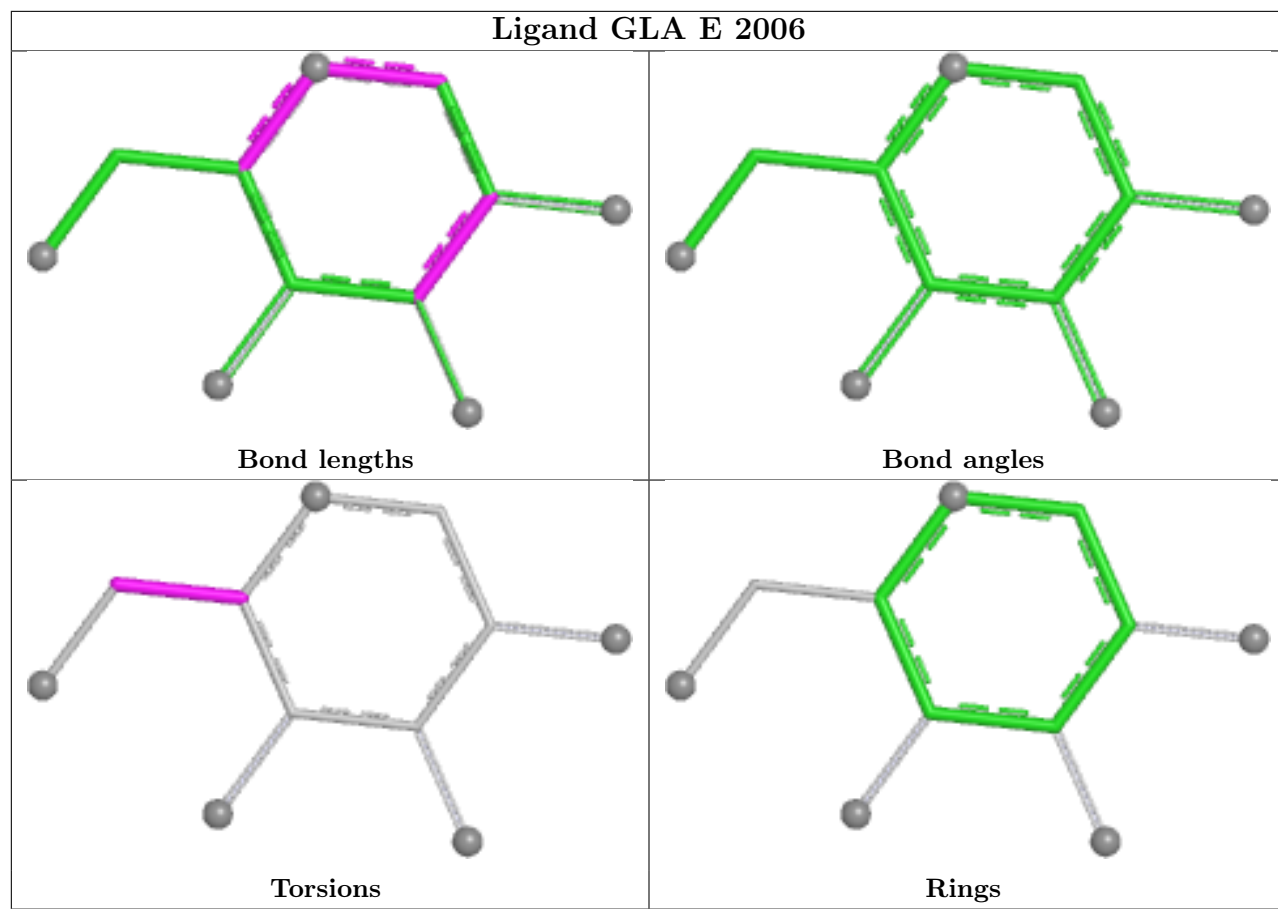


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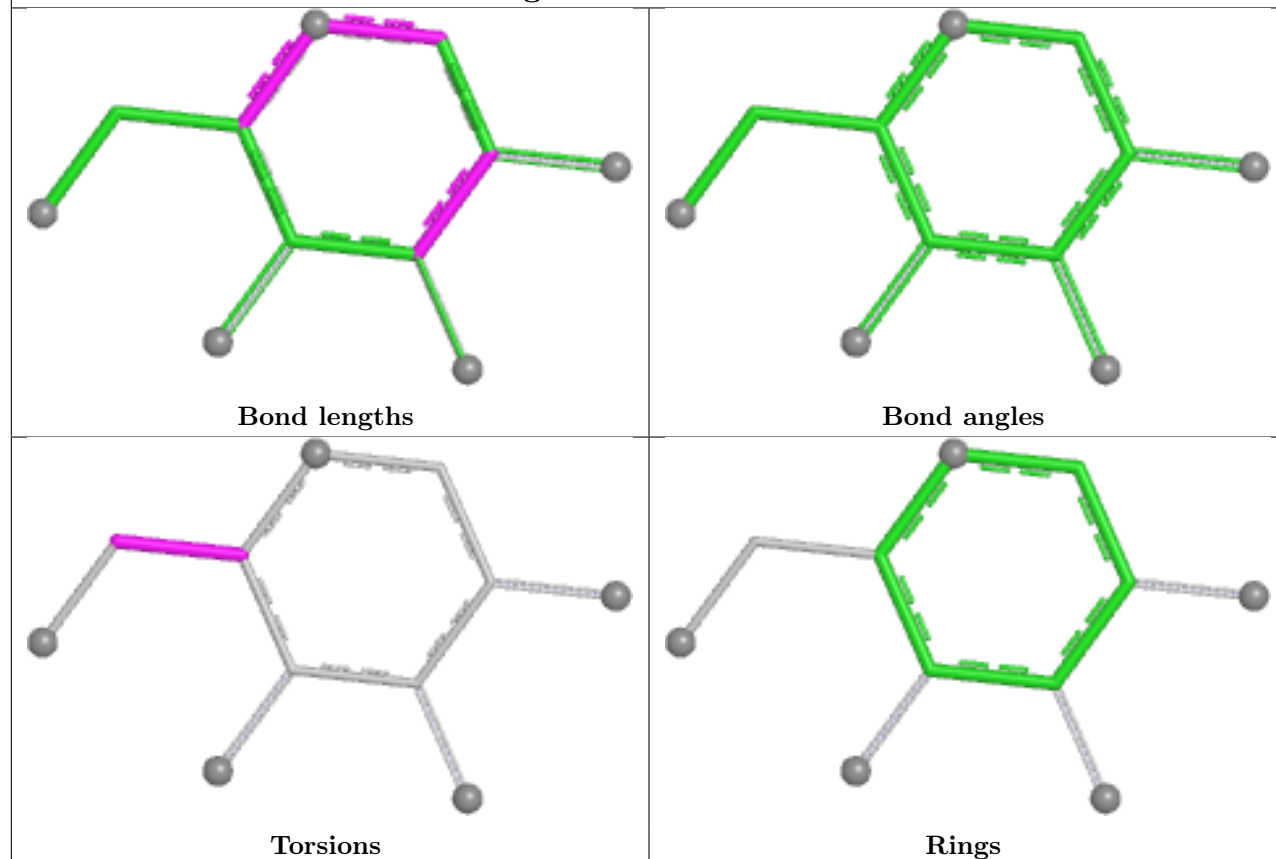




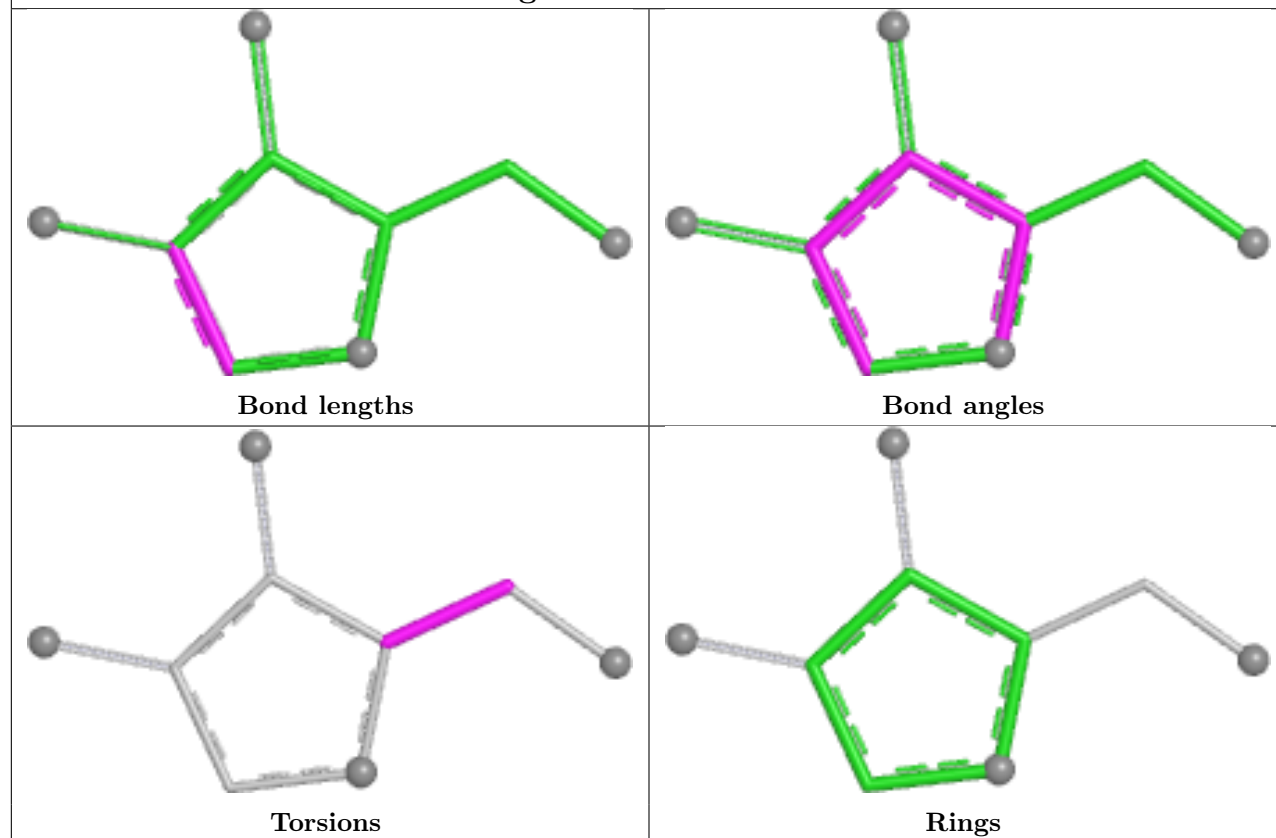


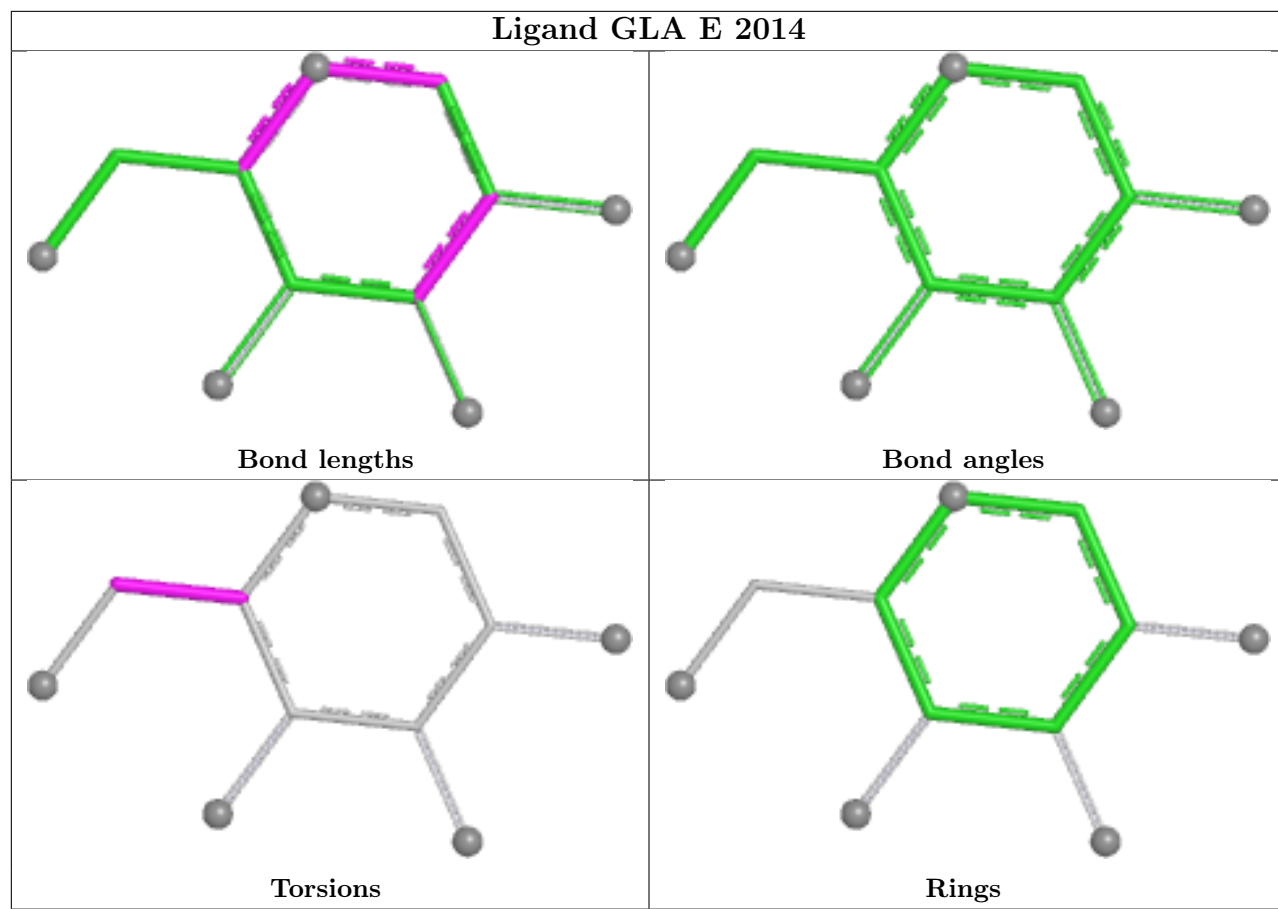


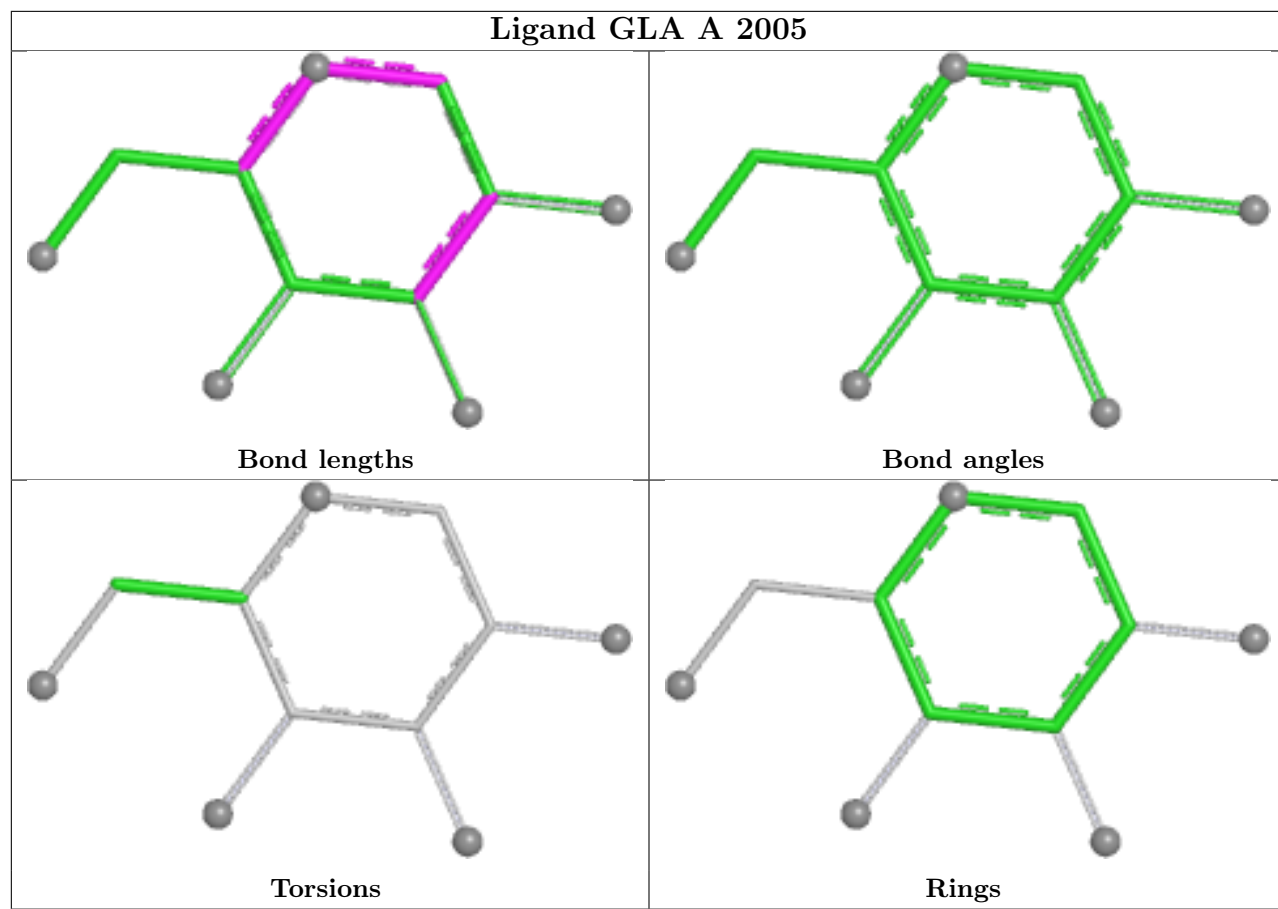
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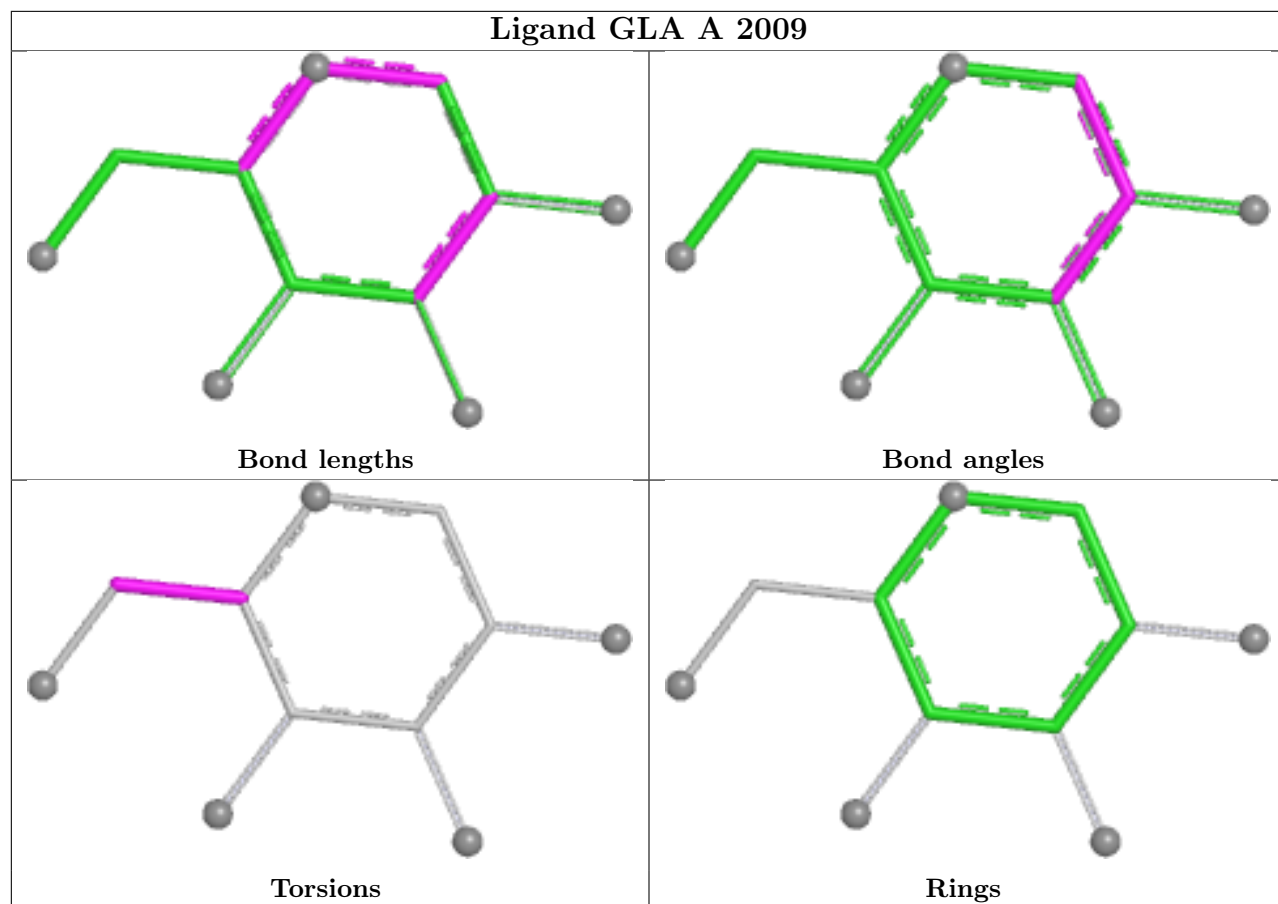


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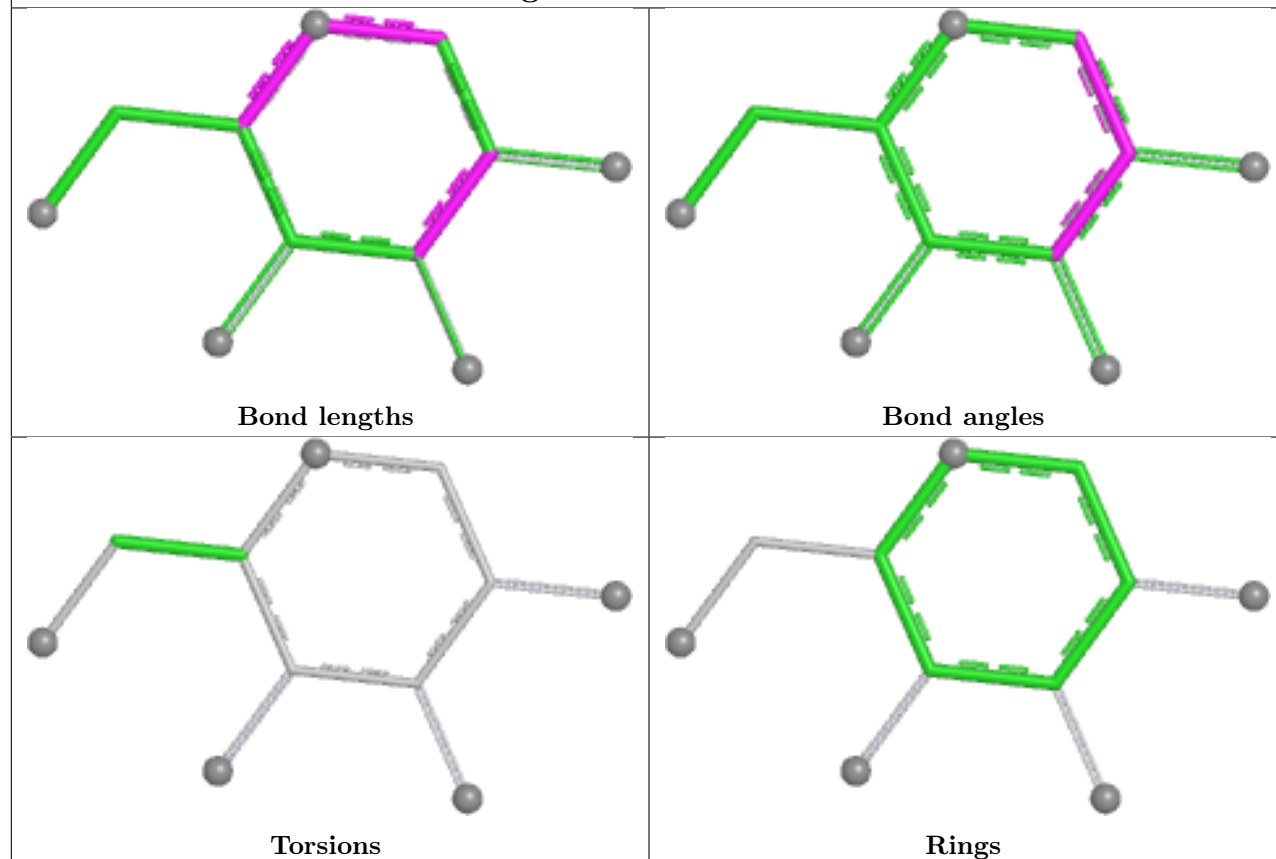




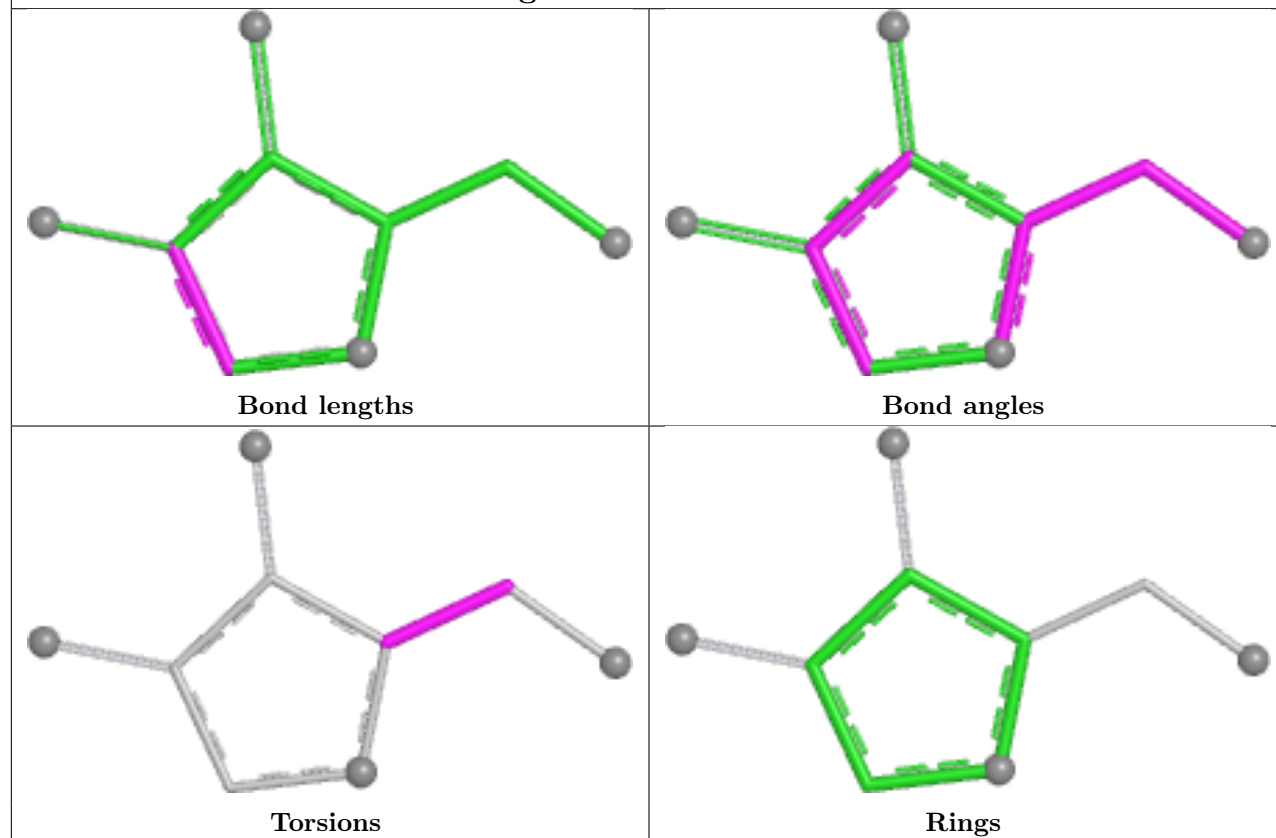


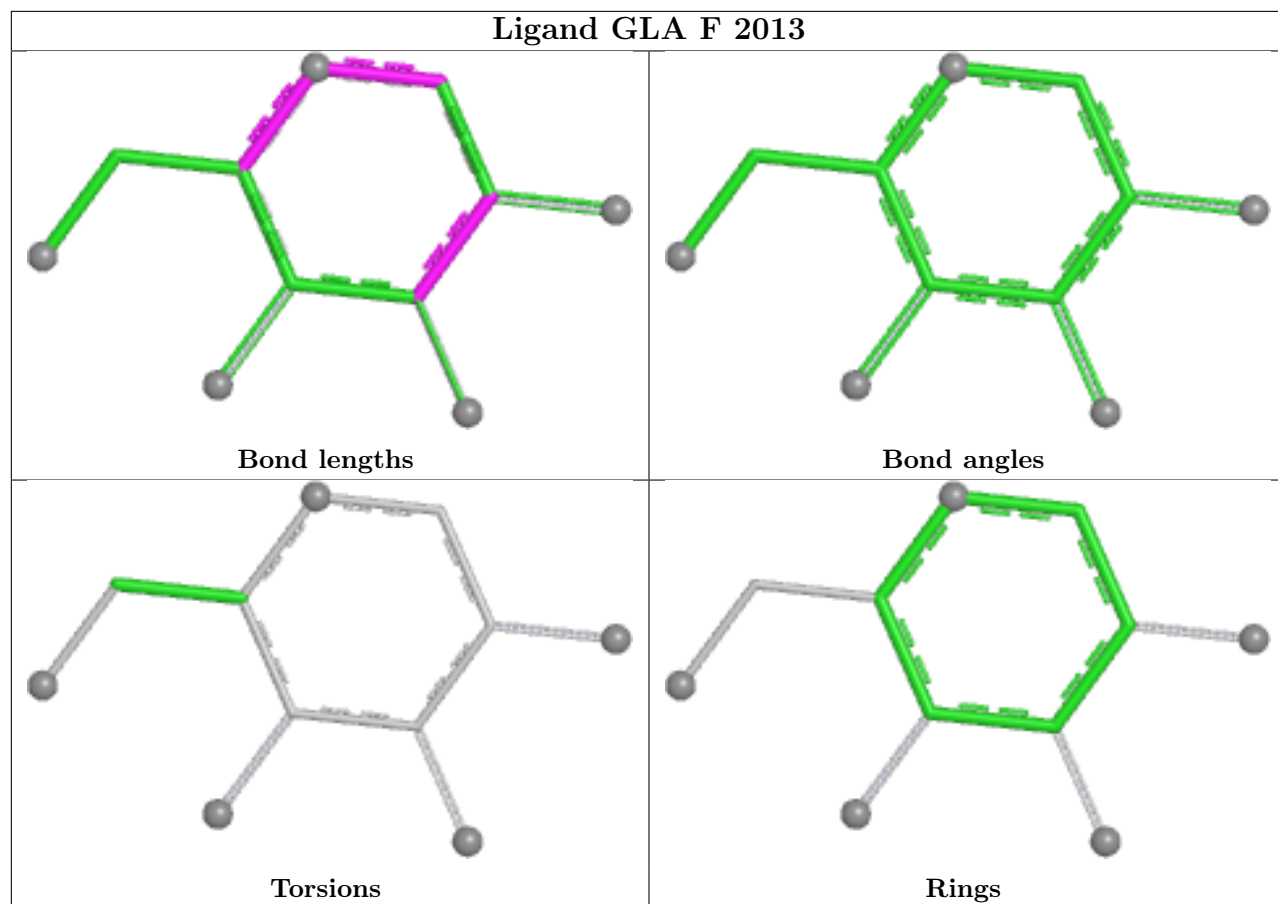


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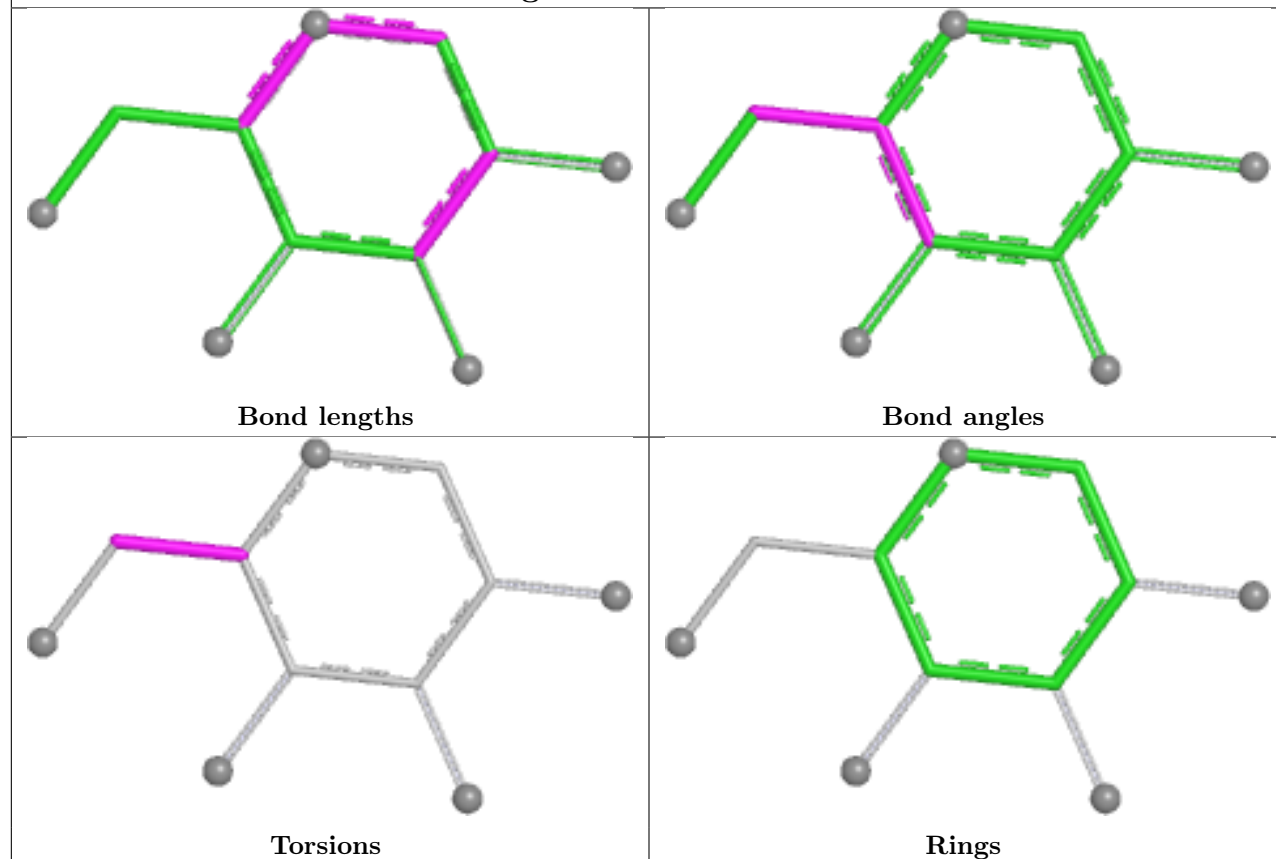


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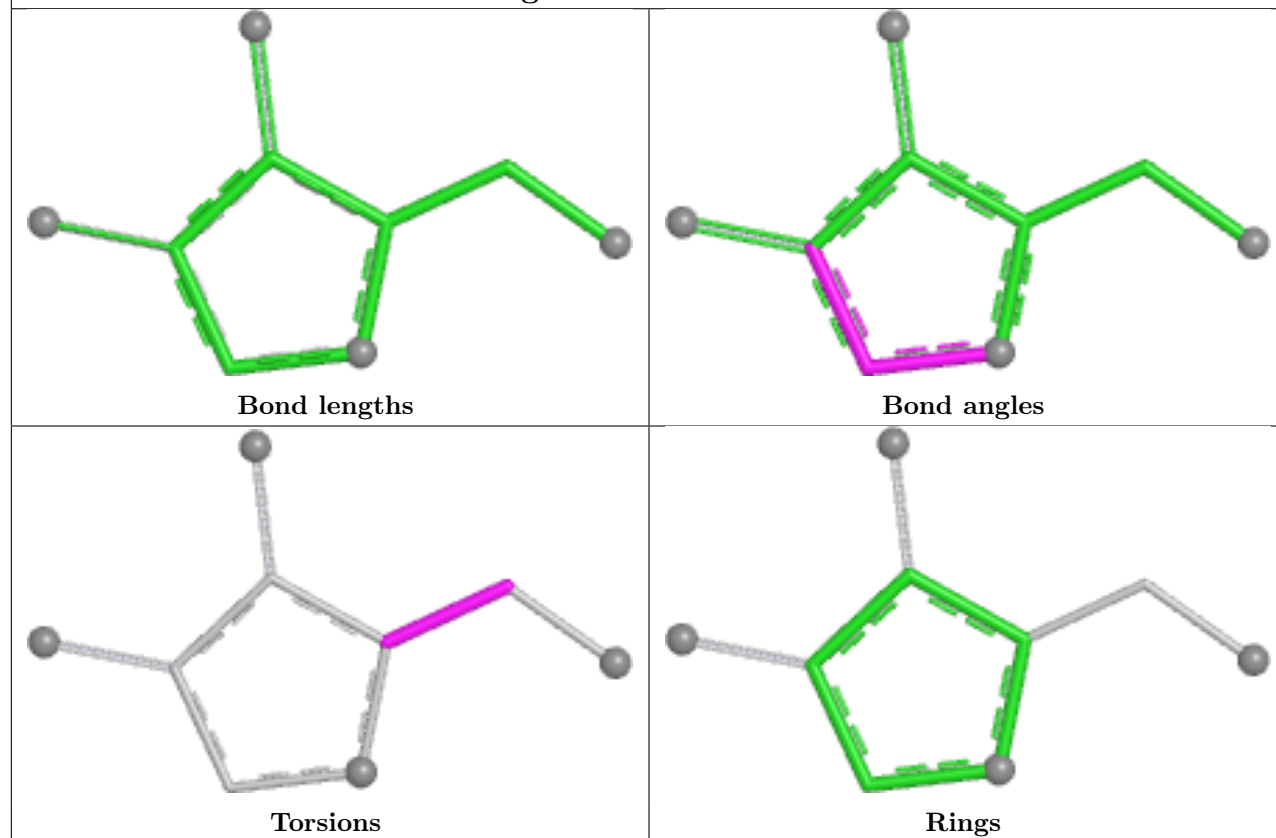




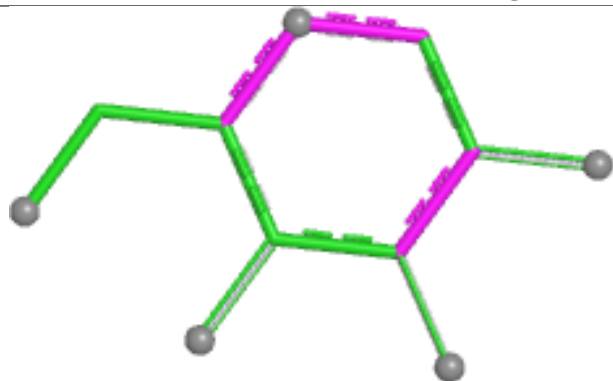
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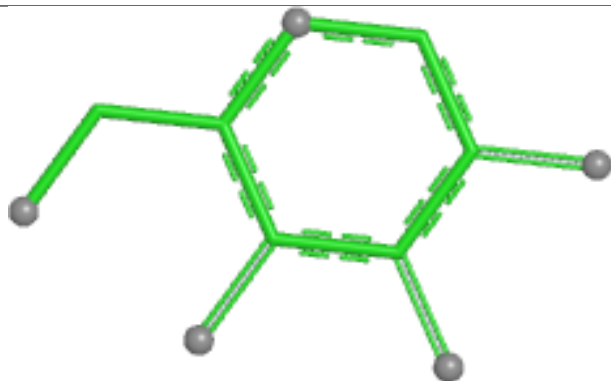
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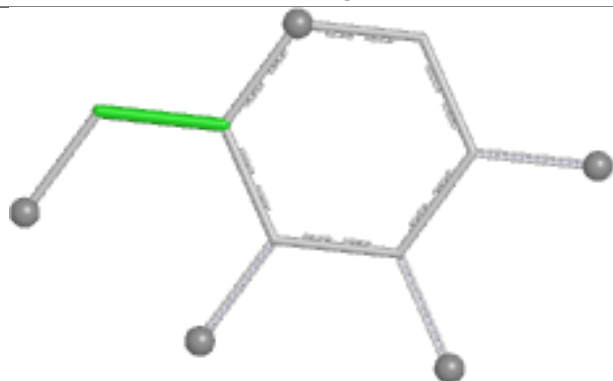
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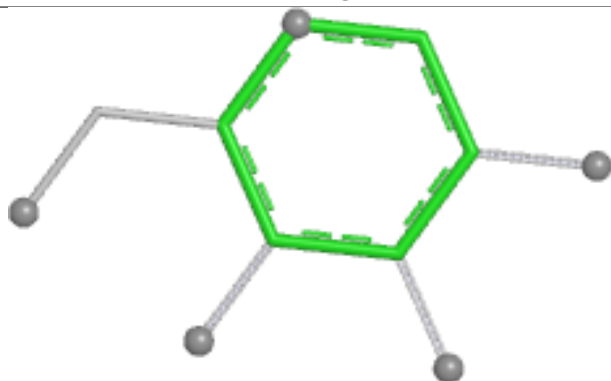
Bond lengths



Bond angles

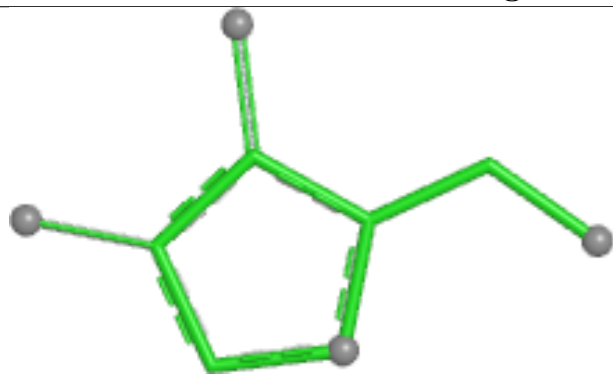


Torsions

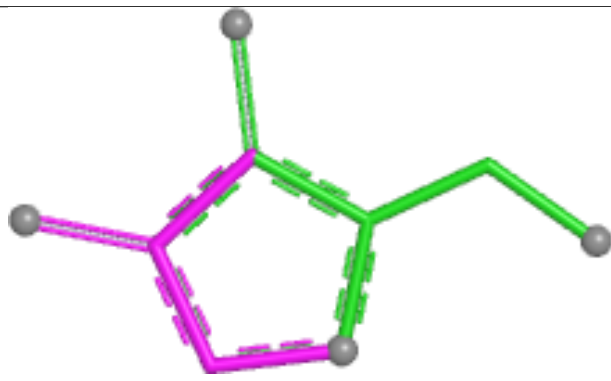


Rings

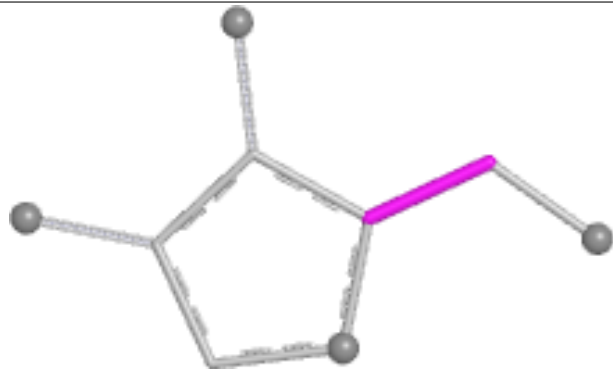
Ligand AHR F 2001



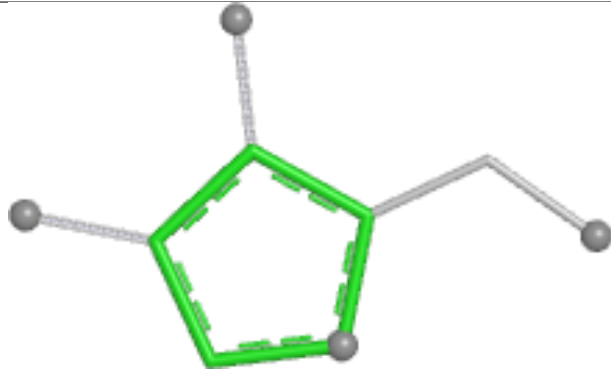
Bond lengths



Bond angles

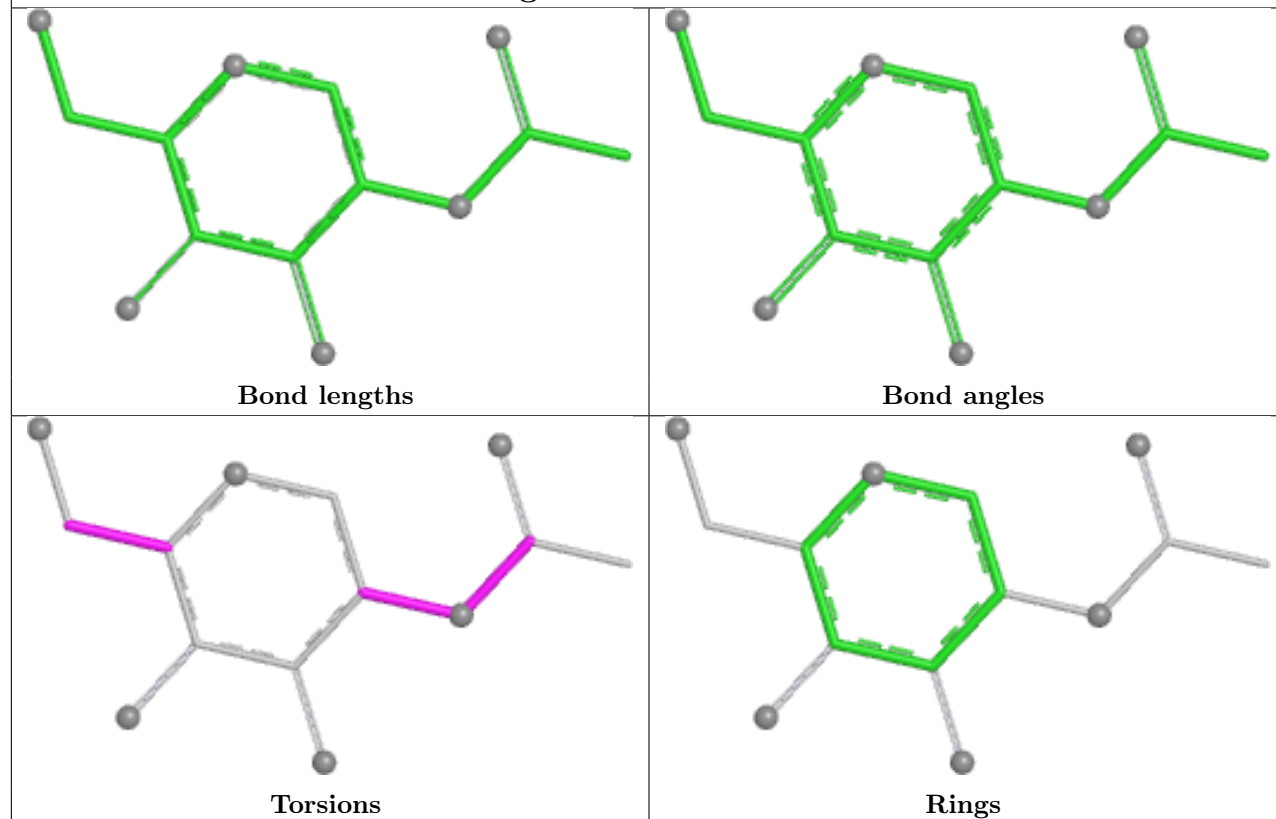


Torsions

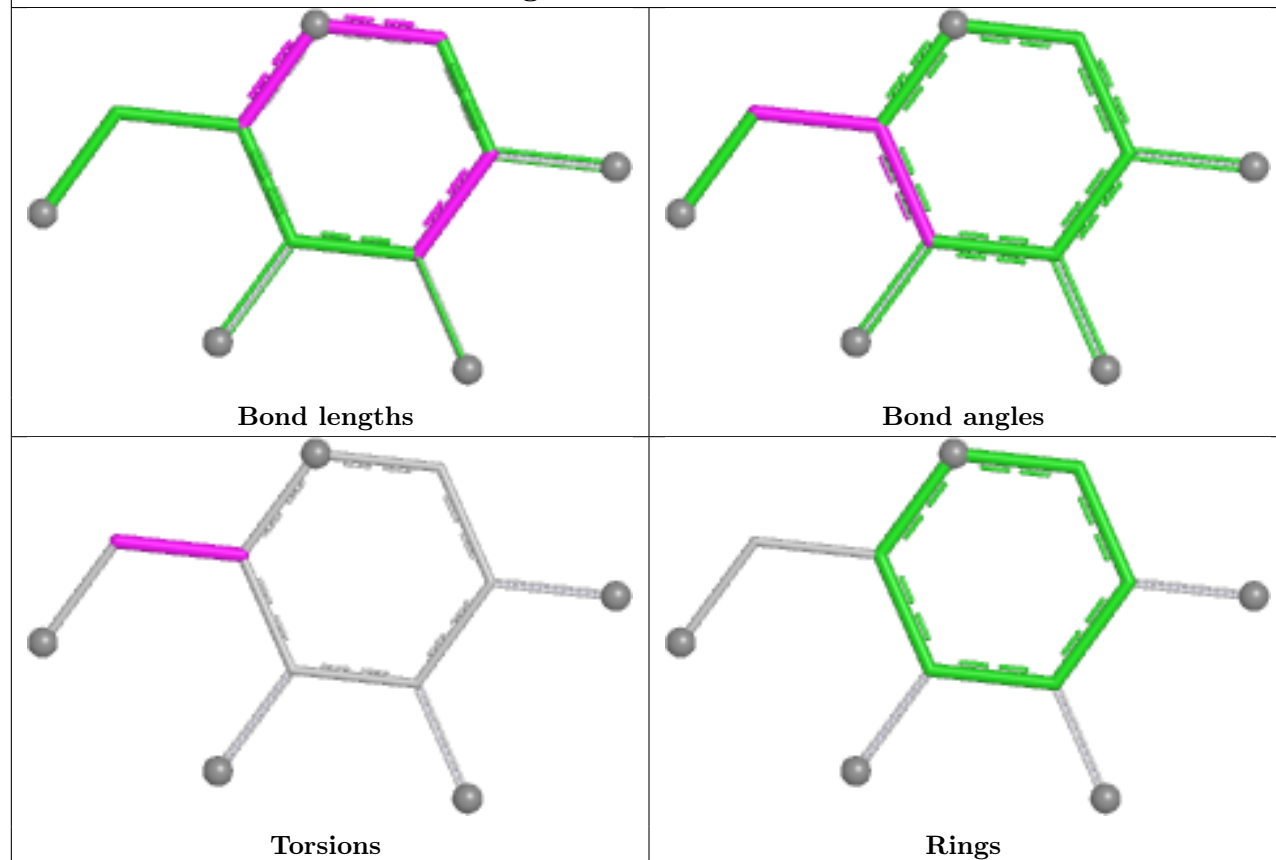


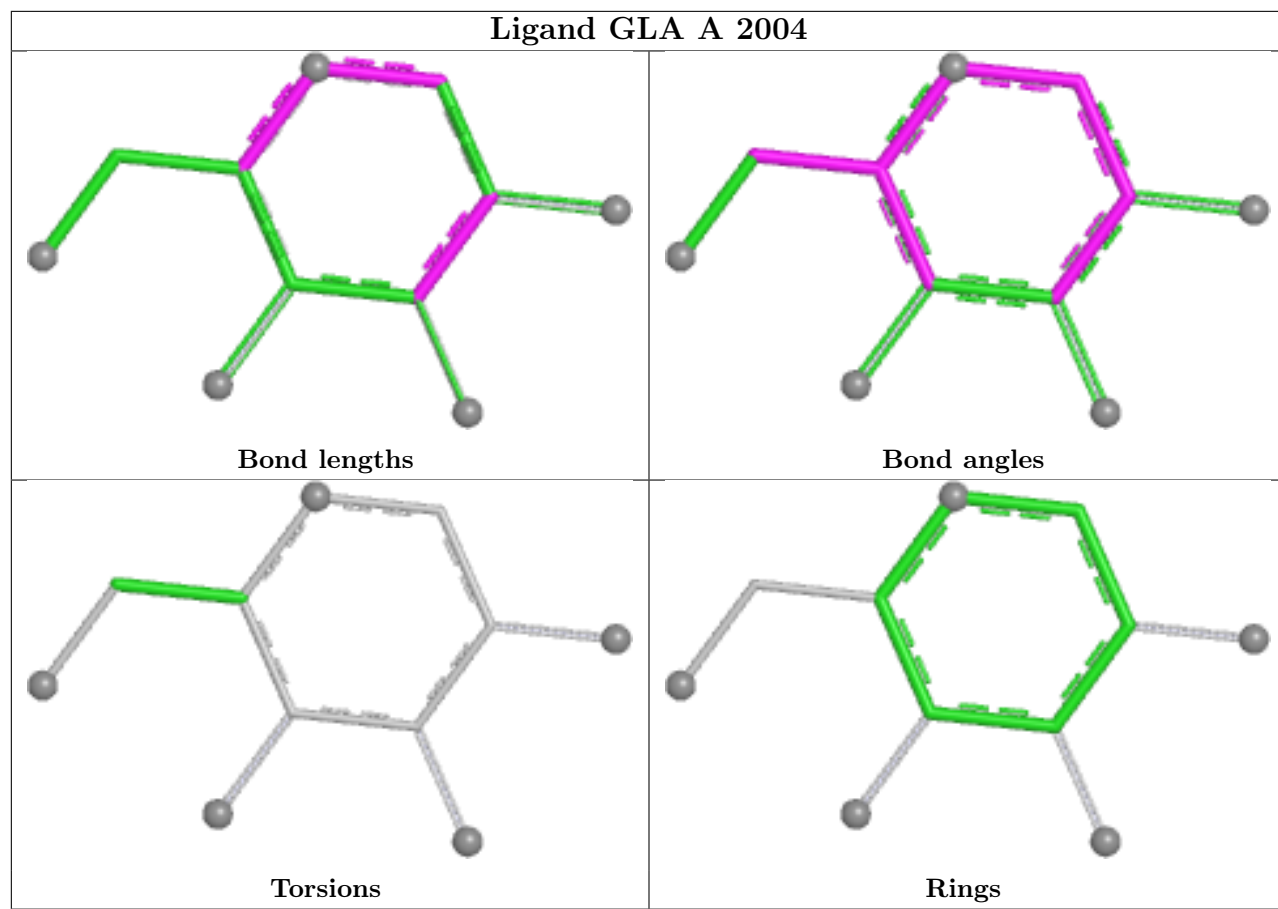
Rings

Ligand NAG B 2018

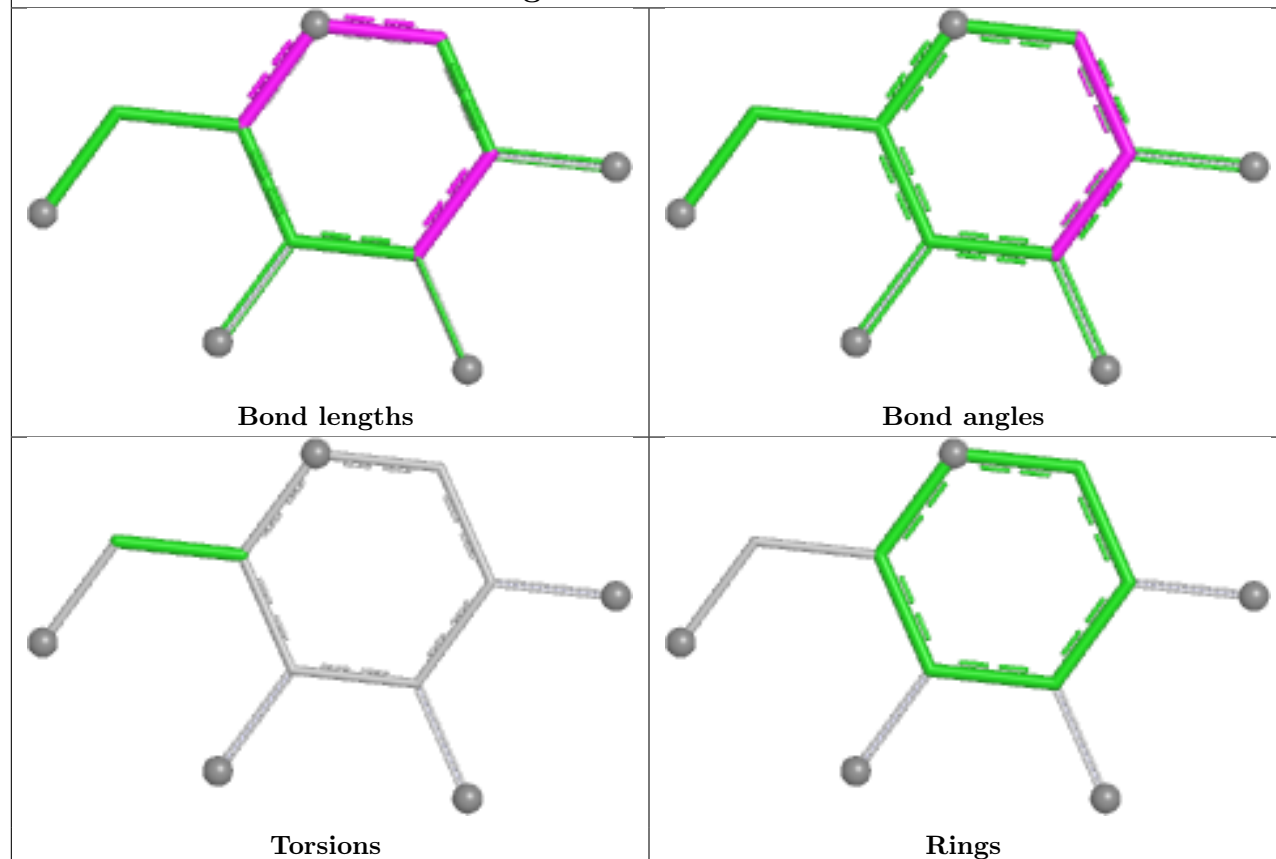


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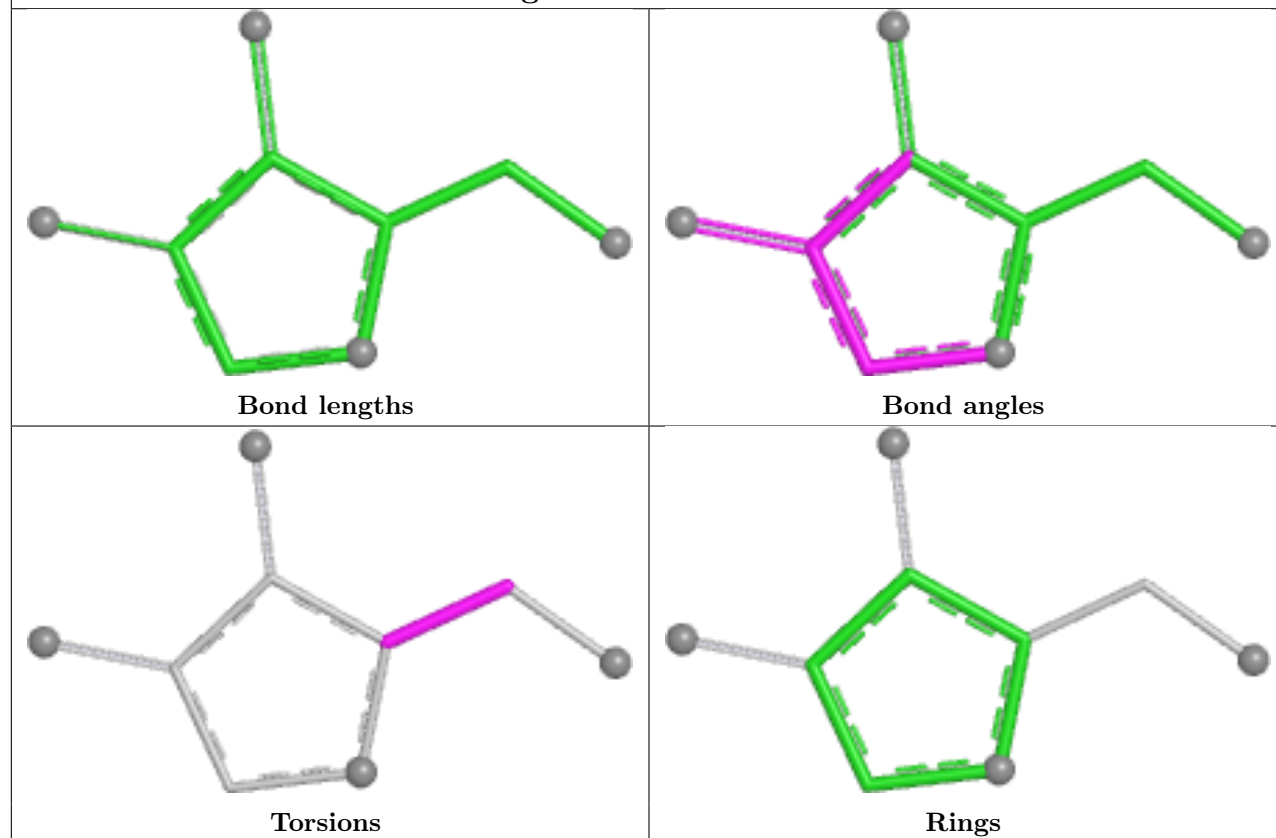




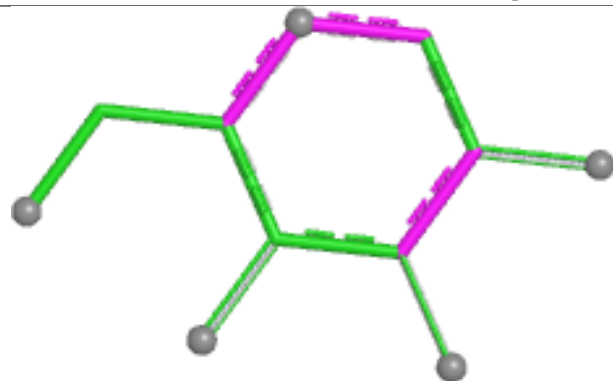
Ligand GLA E 2009



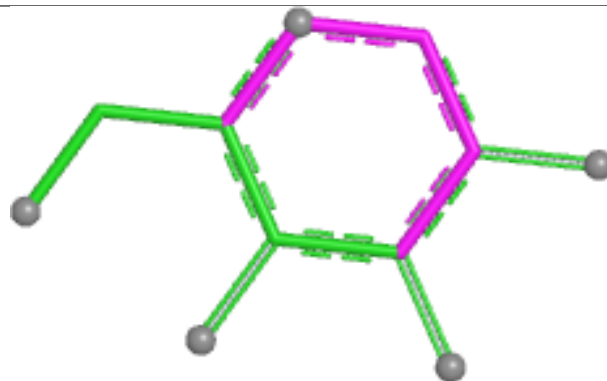
Ligand AHR F 2004



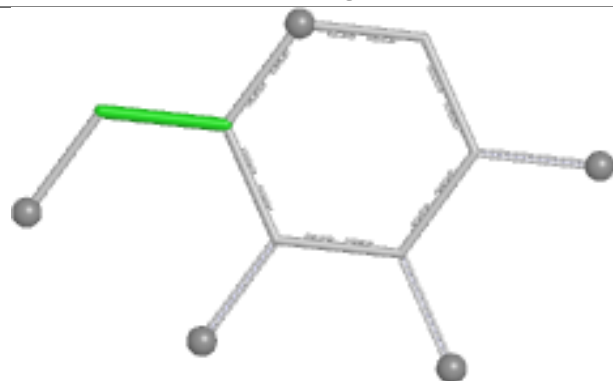
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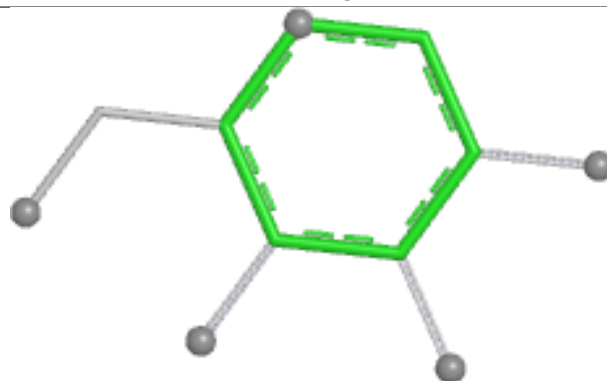
Bond lengths



Bond angles

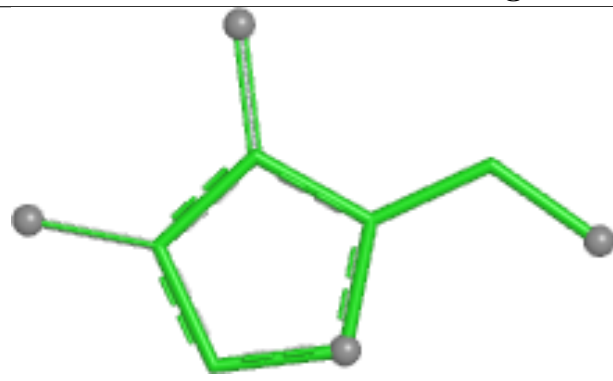


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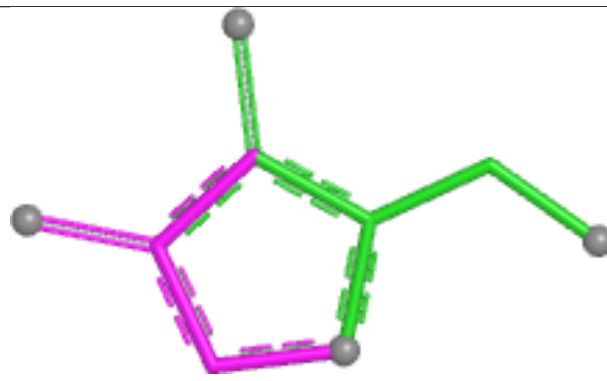


Rings

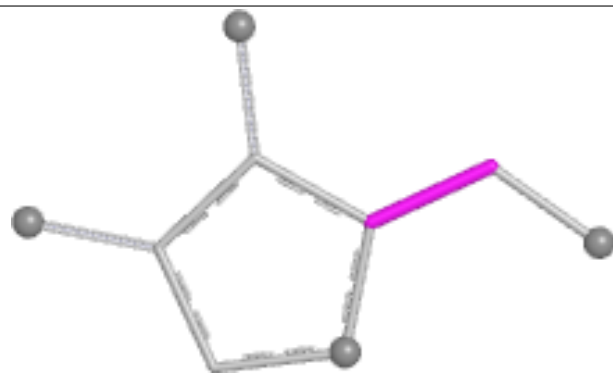
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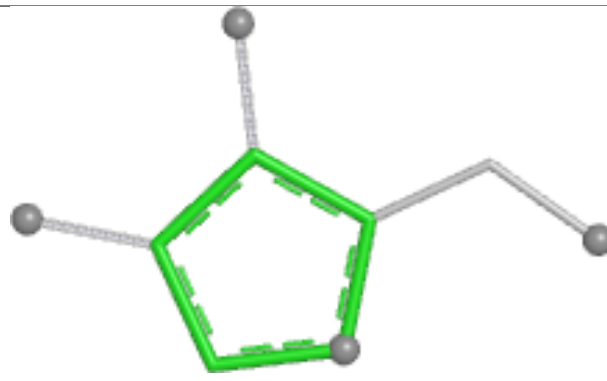
Bond lengths



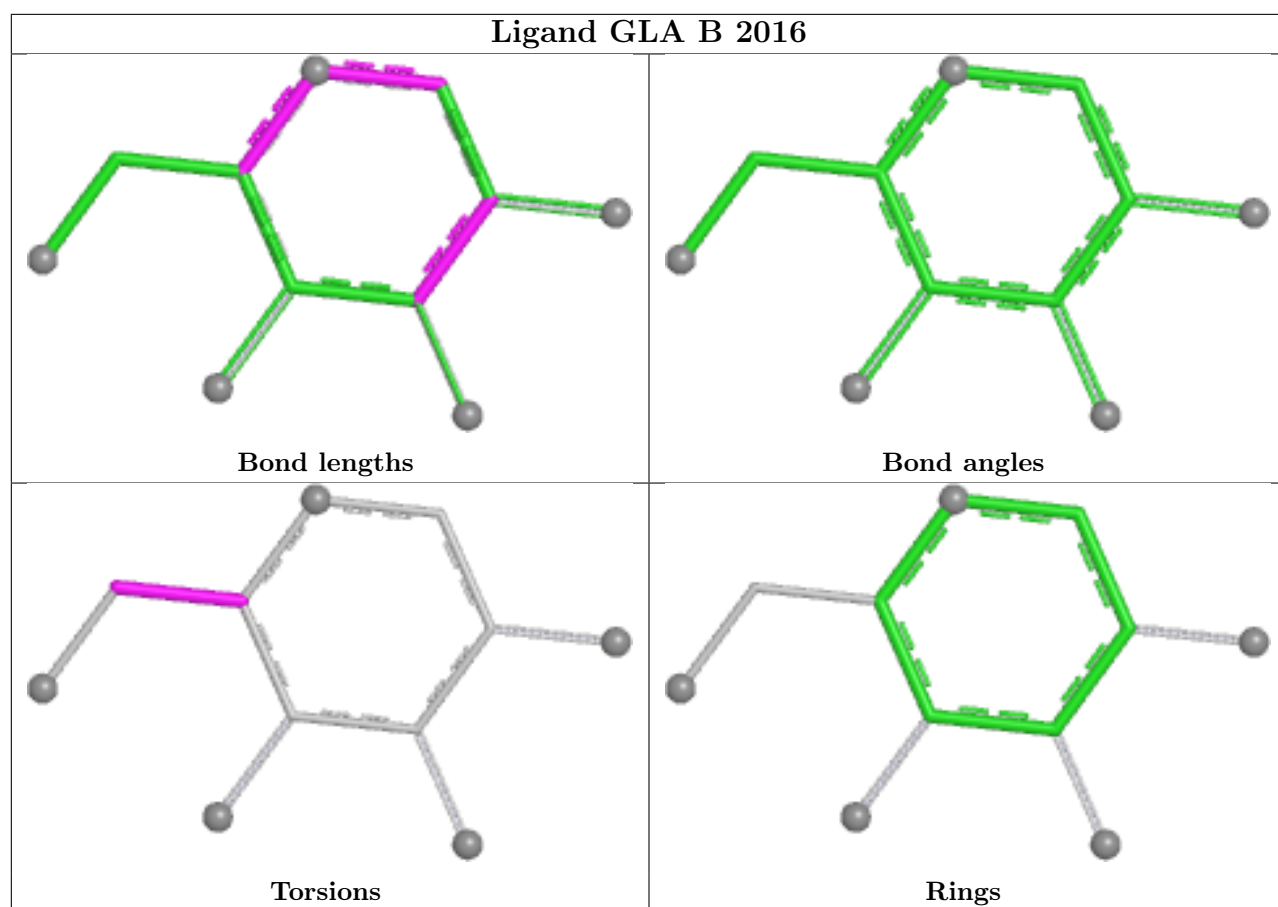
Bond angles

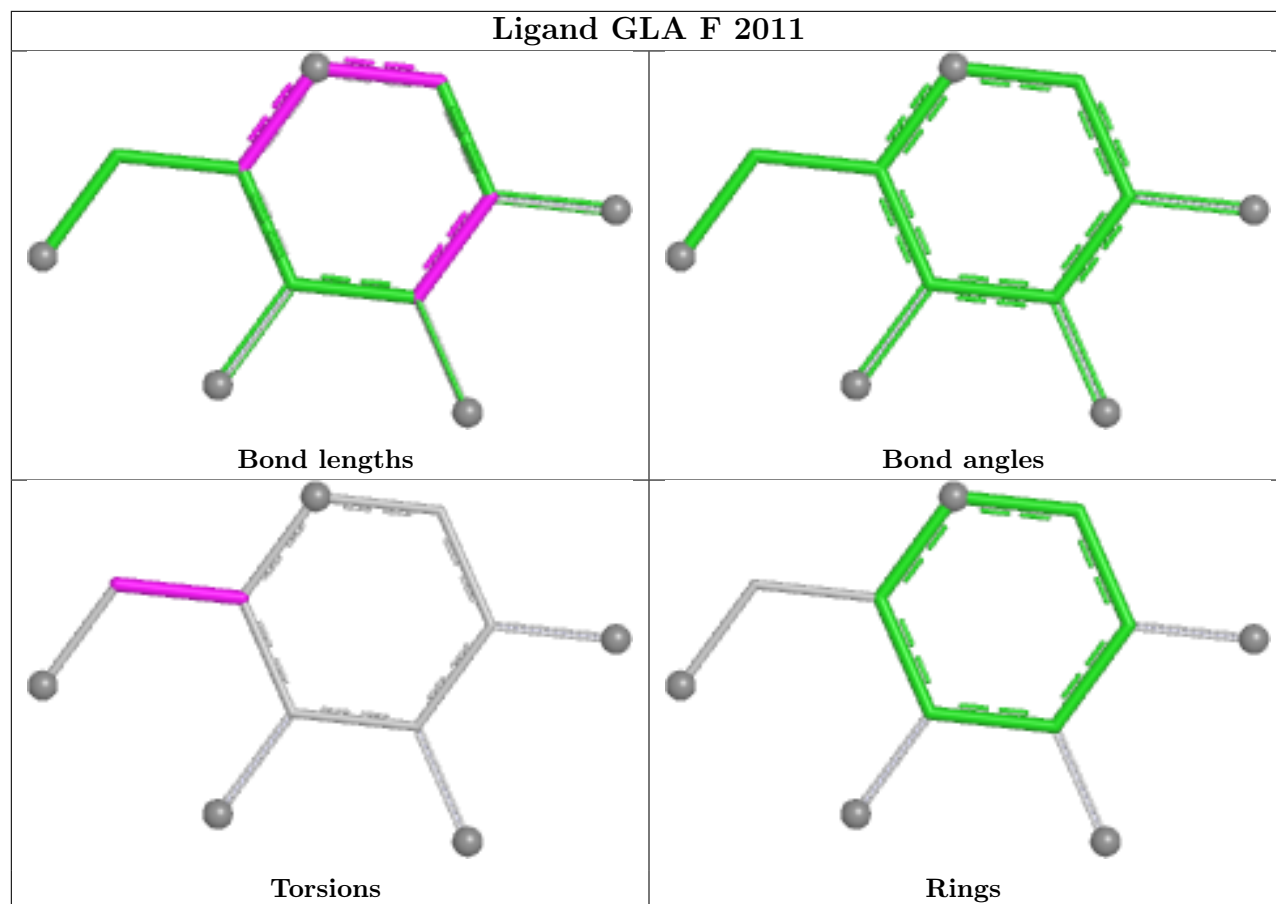


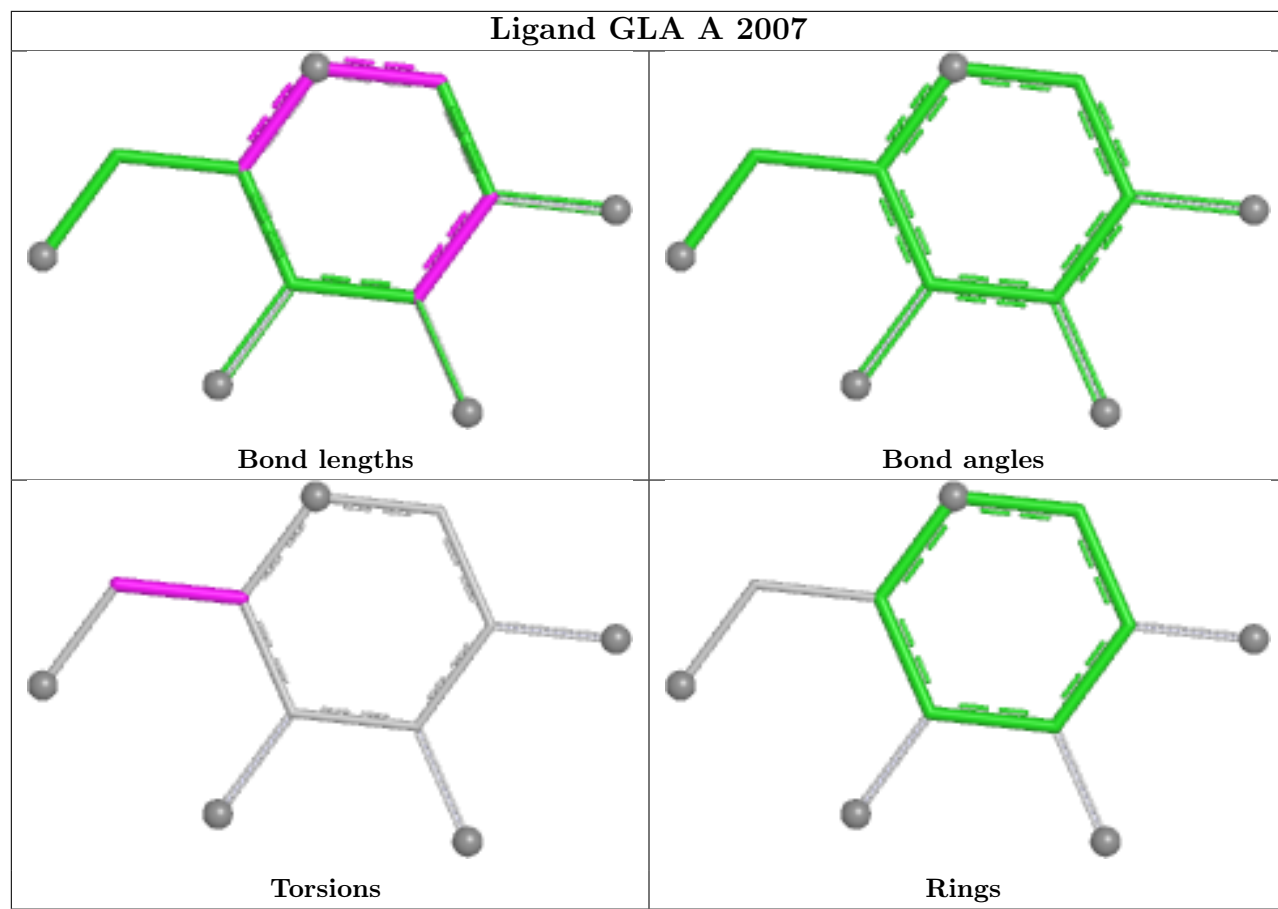
Torsions

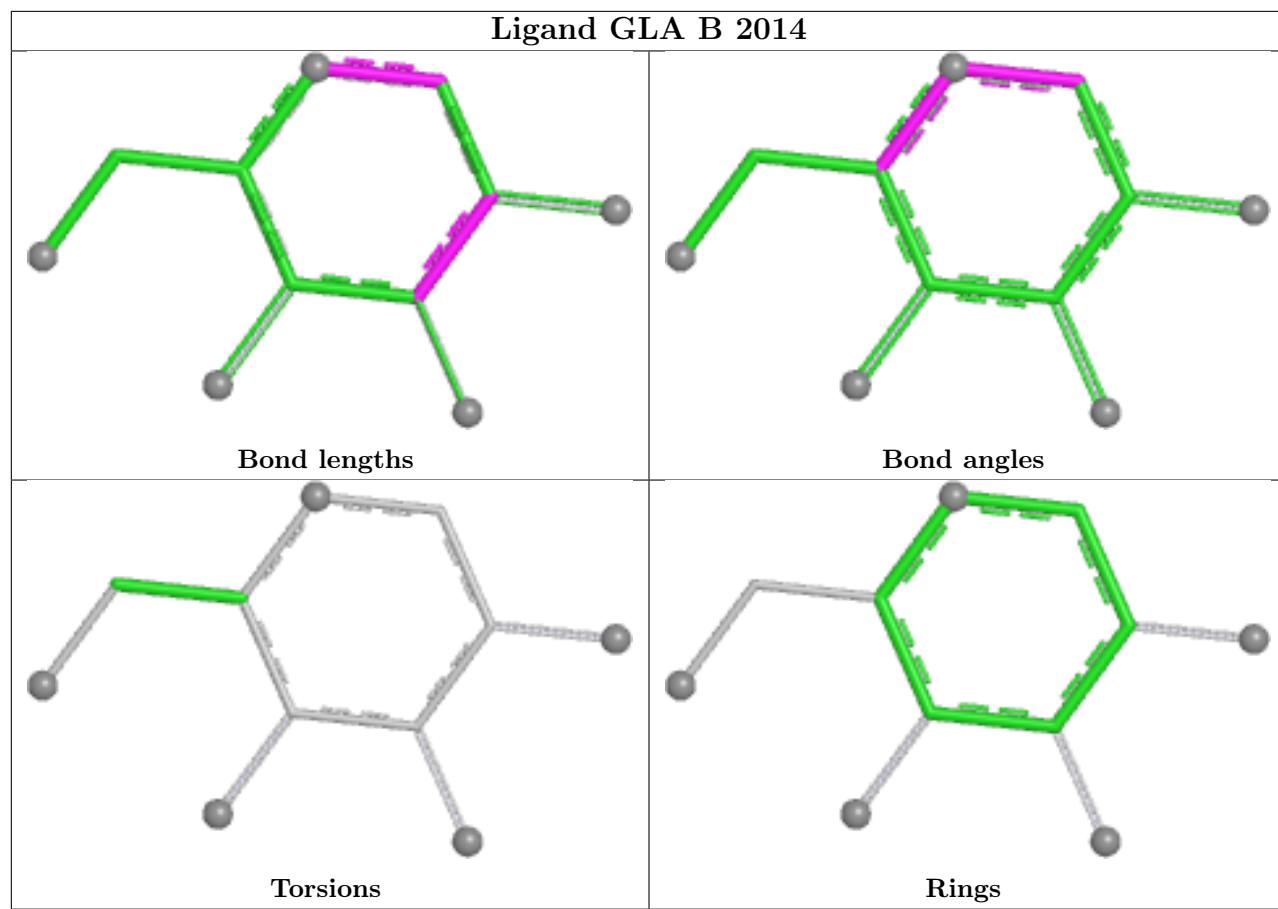


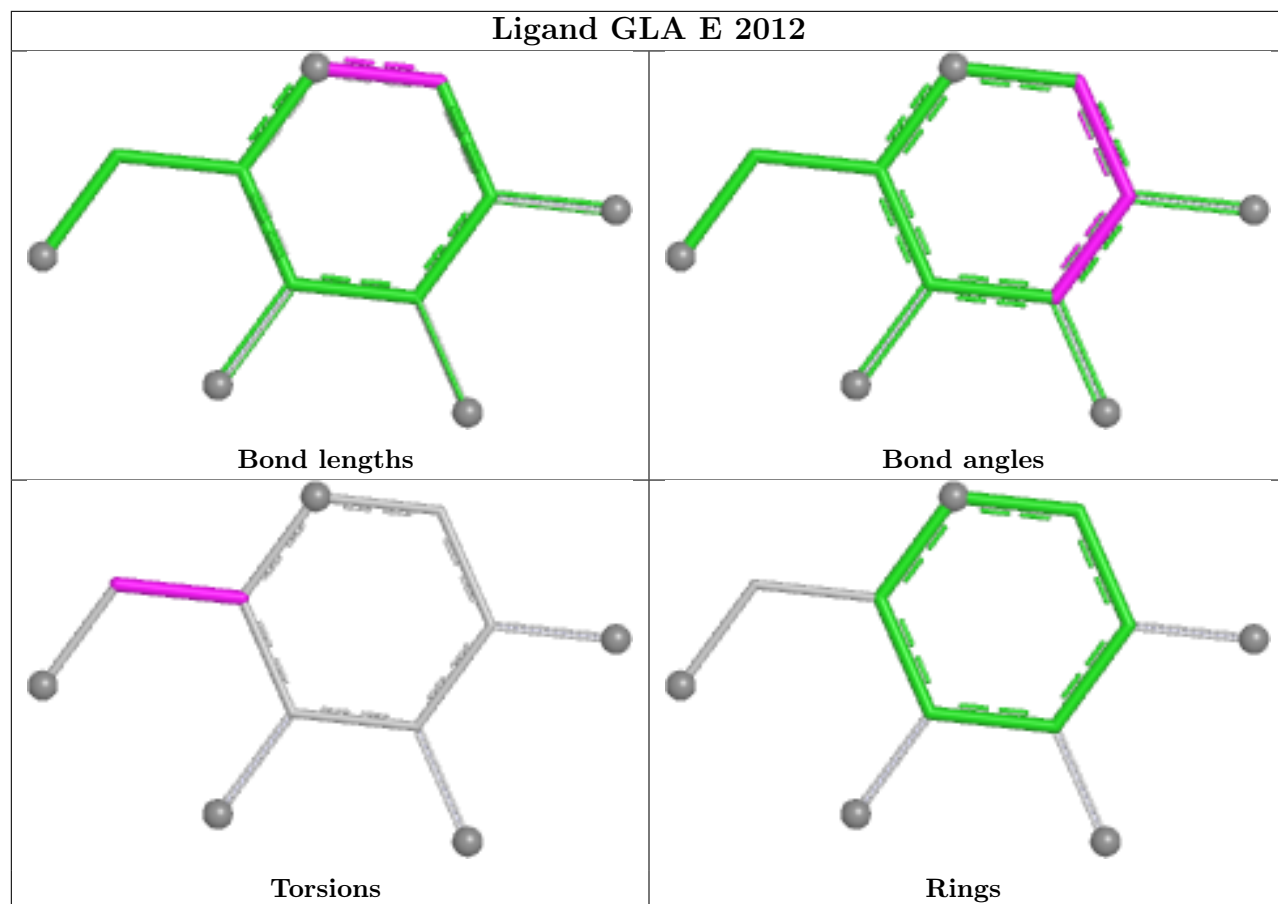
Rings

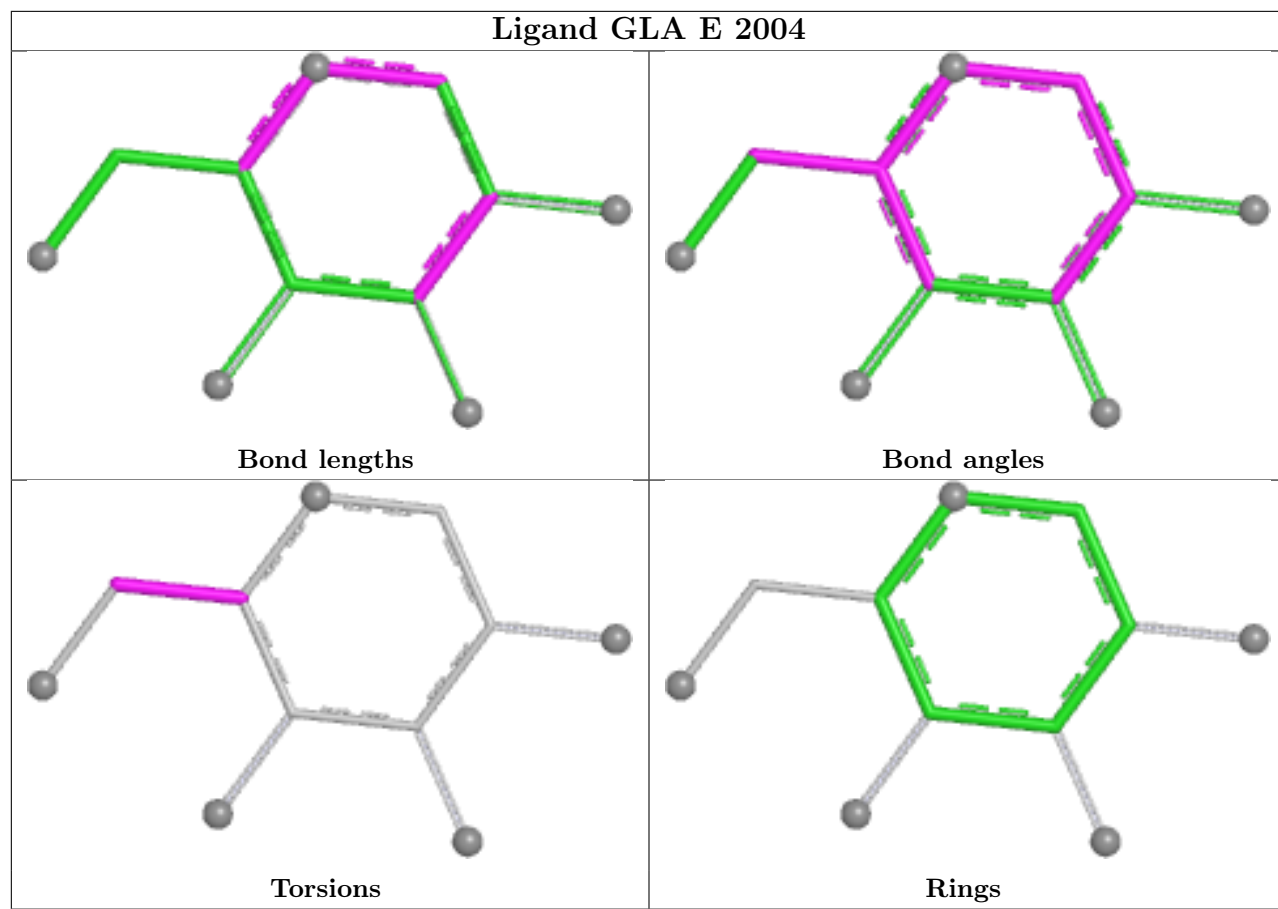


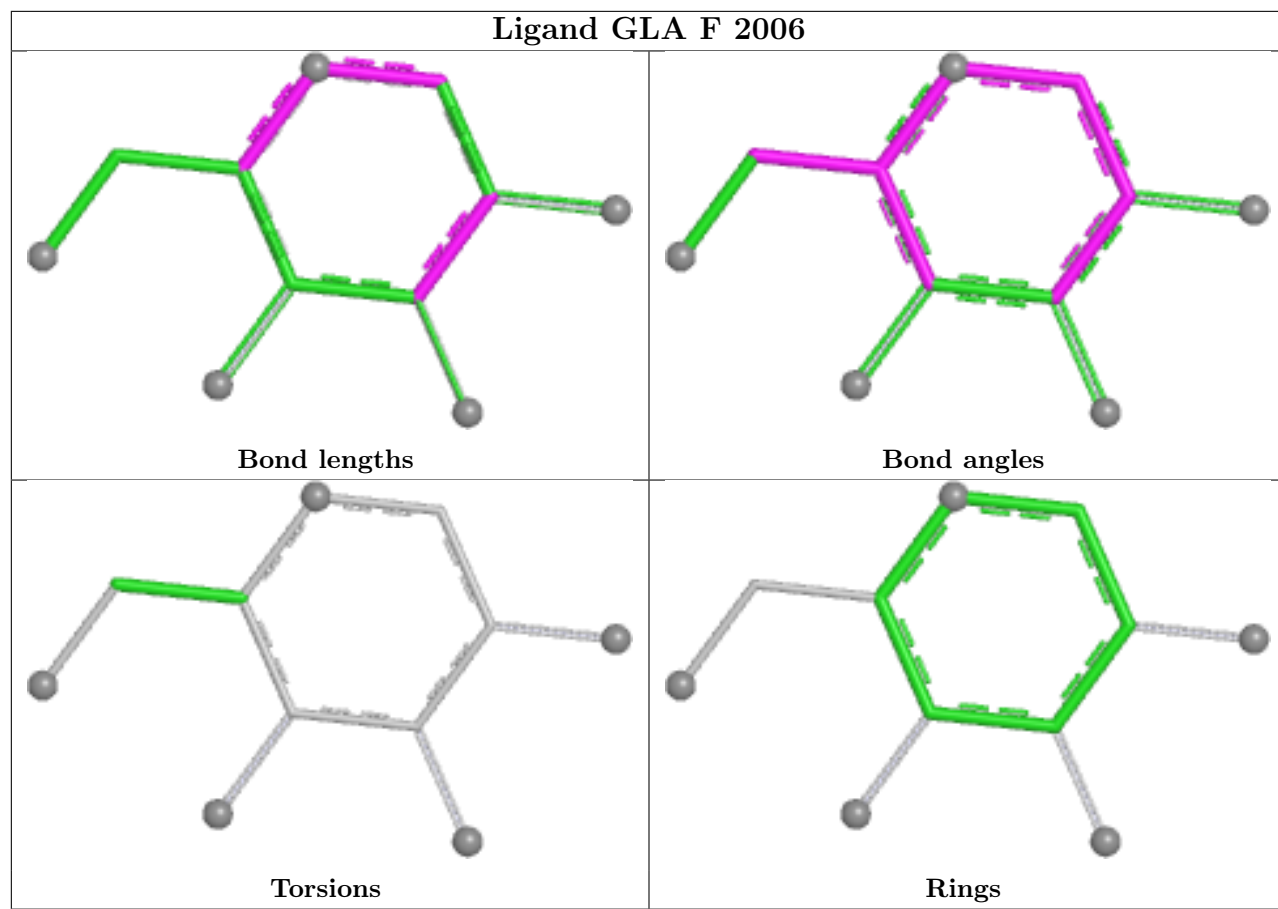


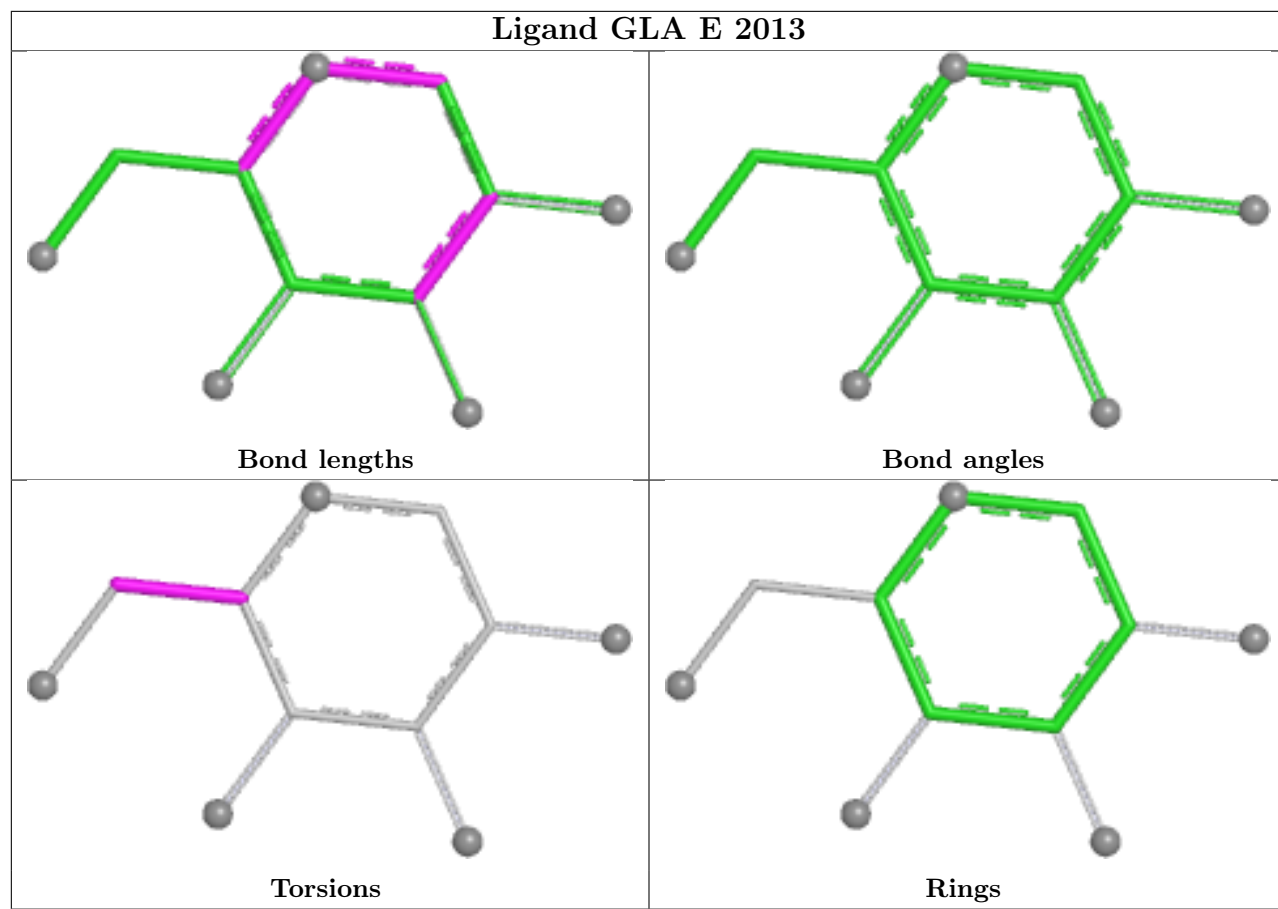


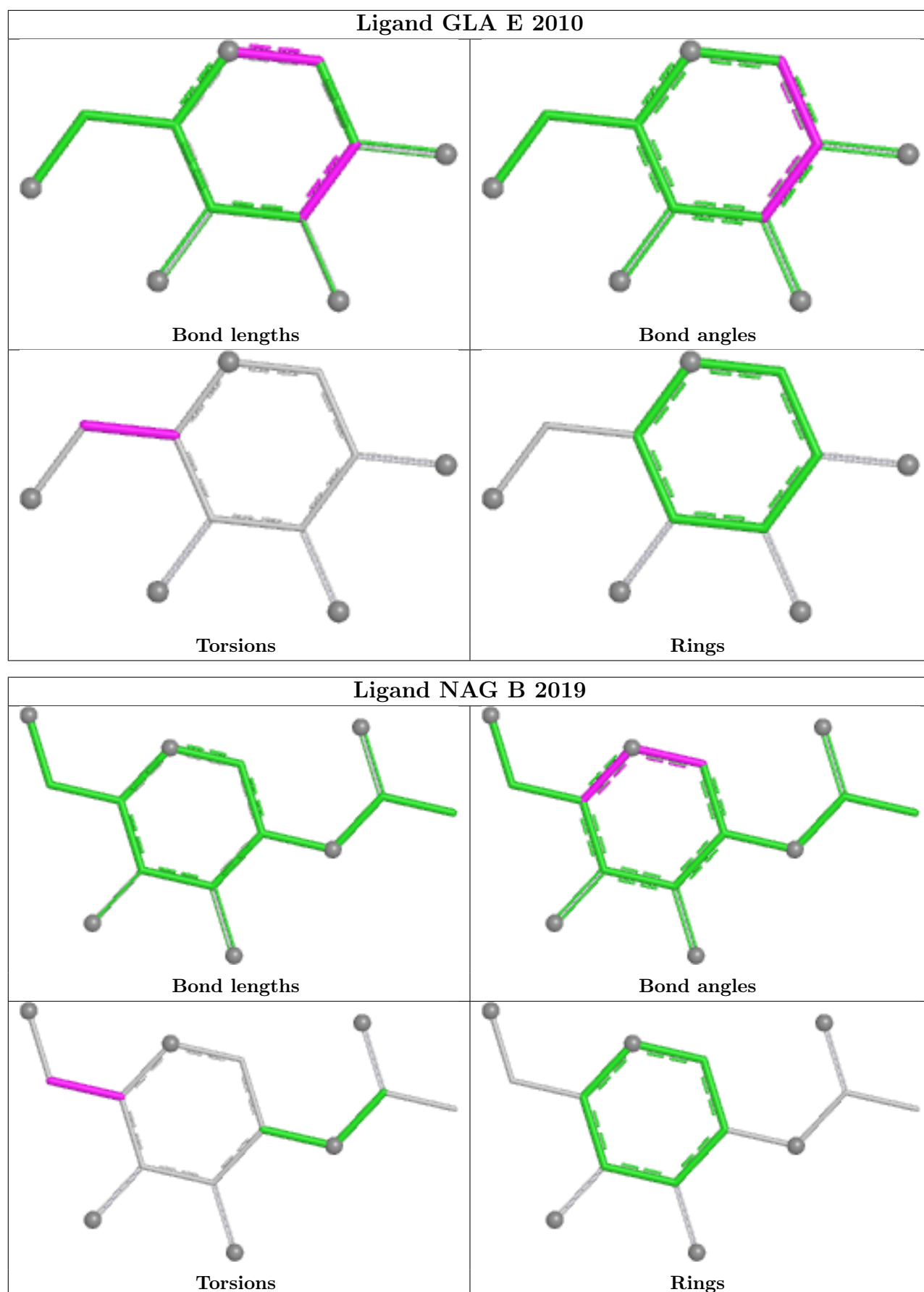


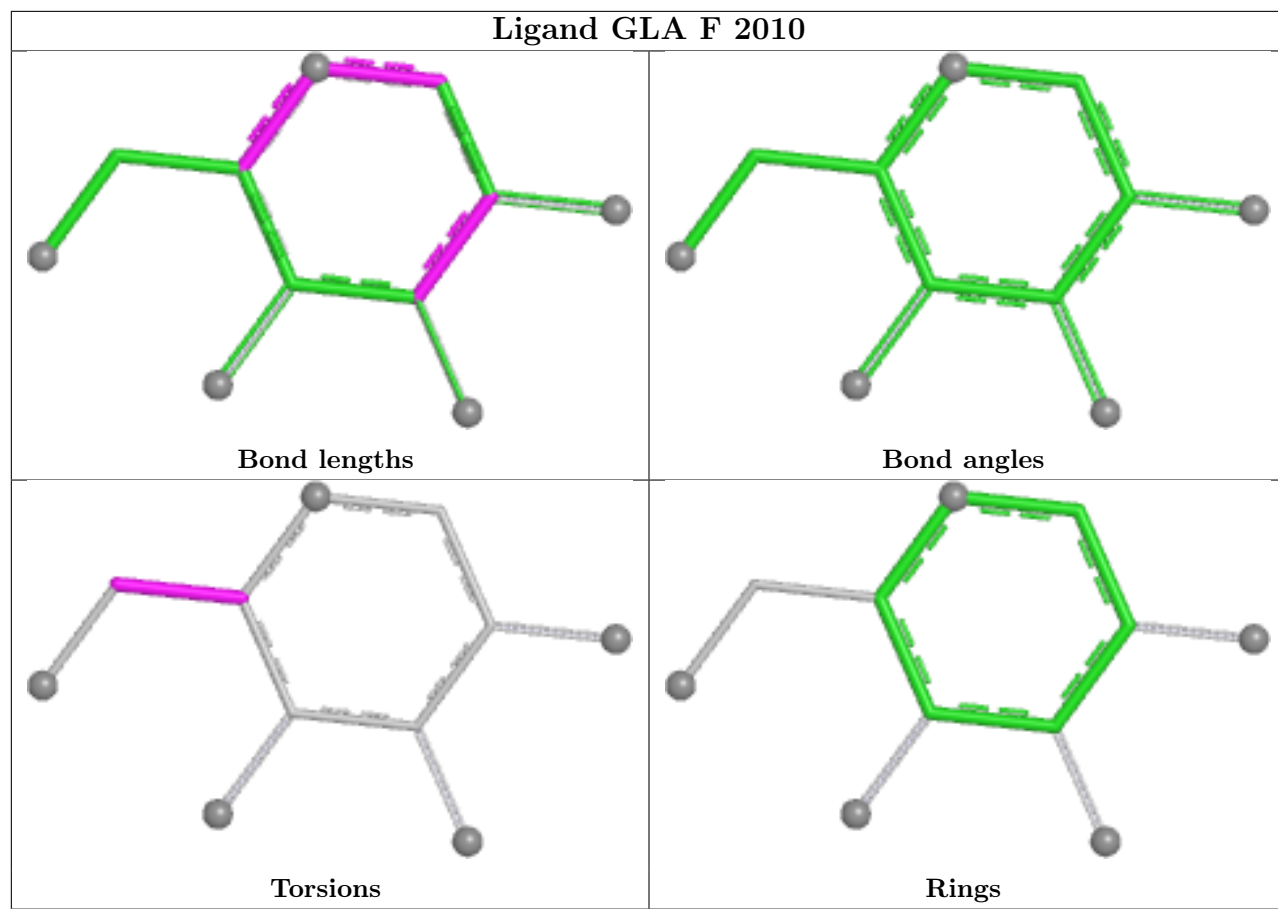


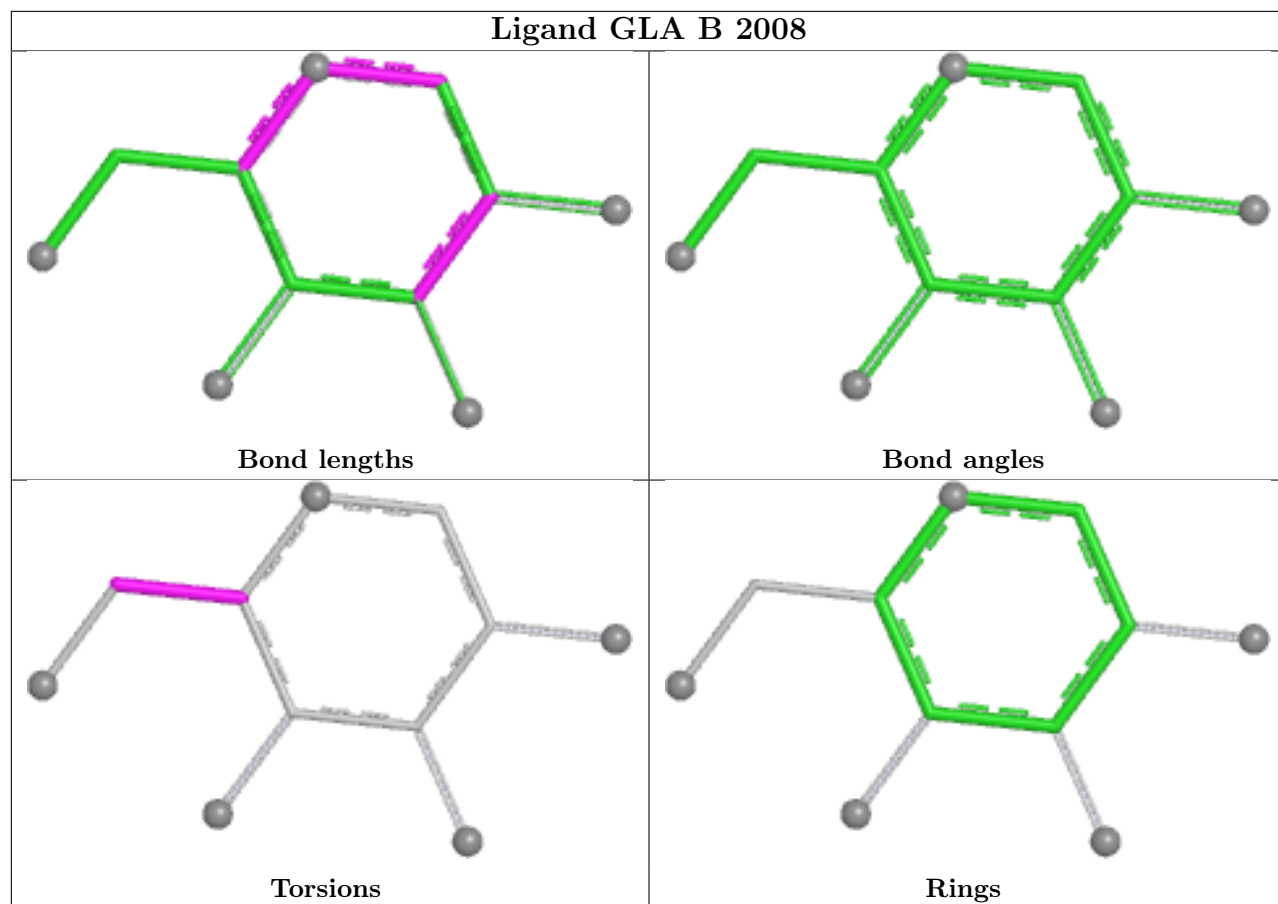


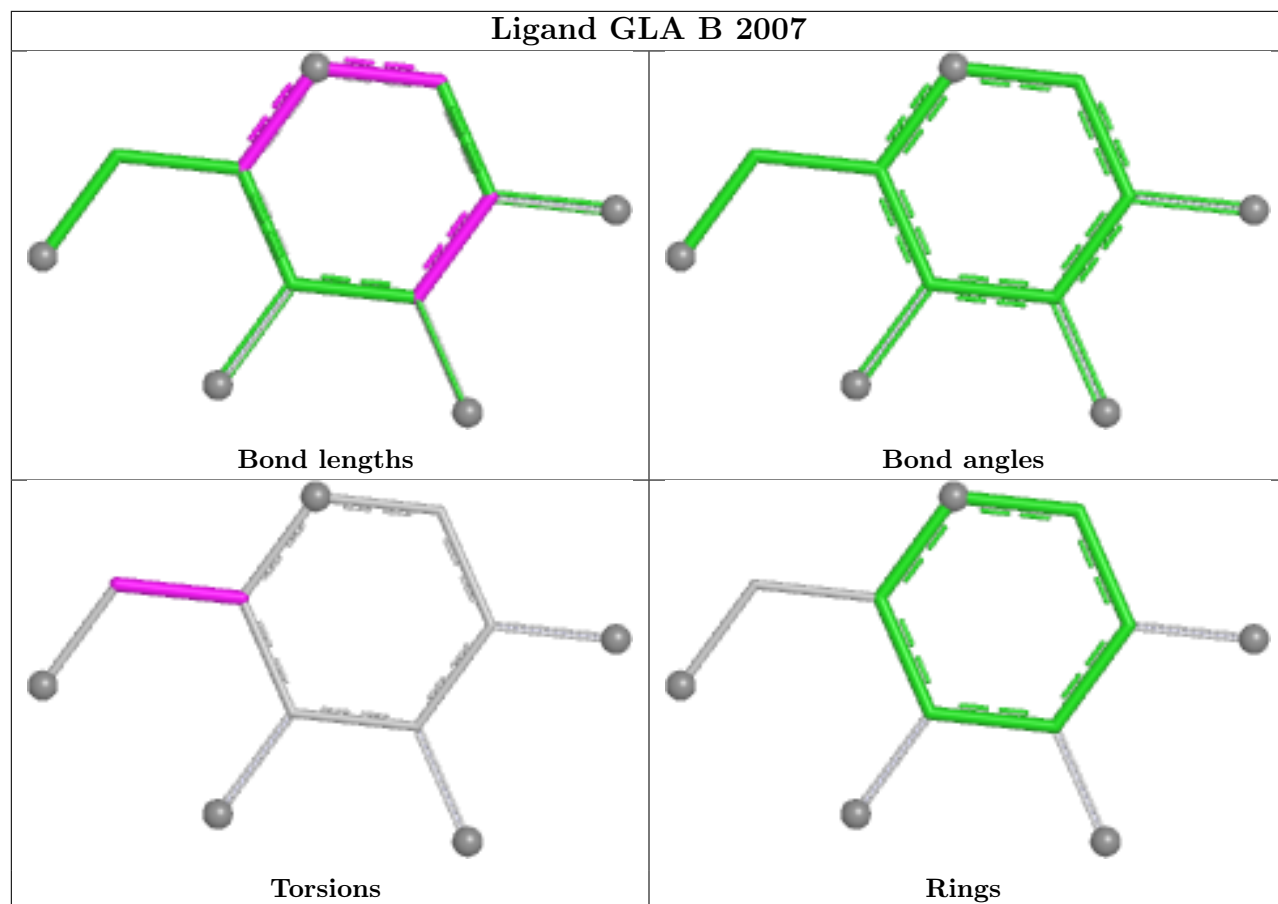


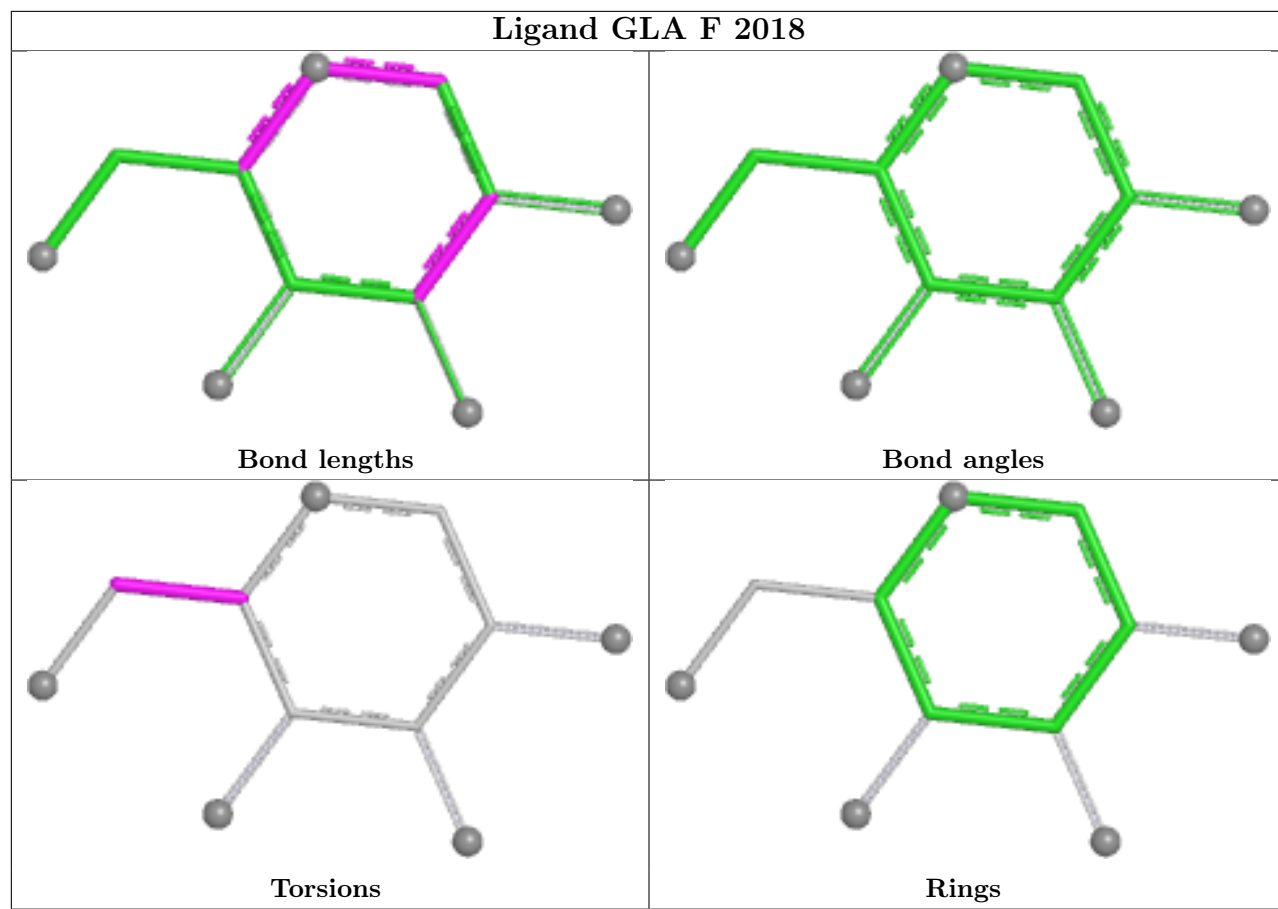




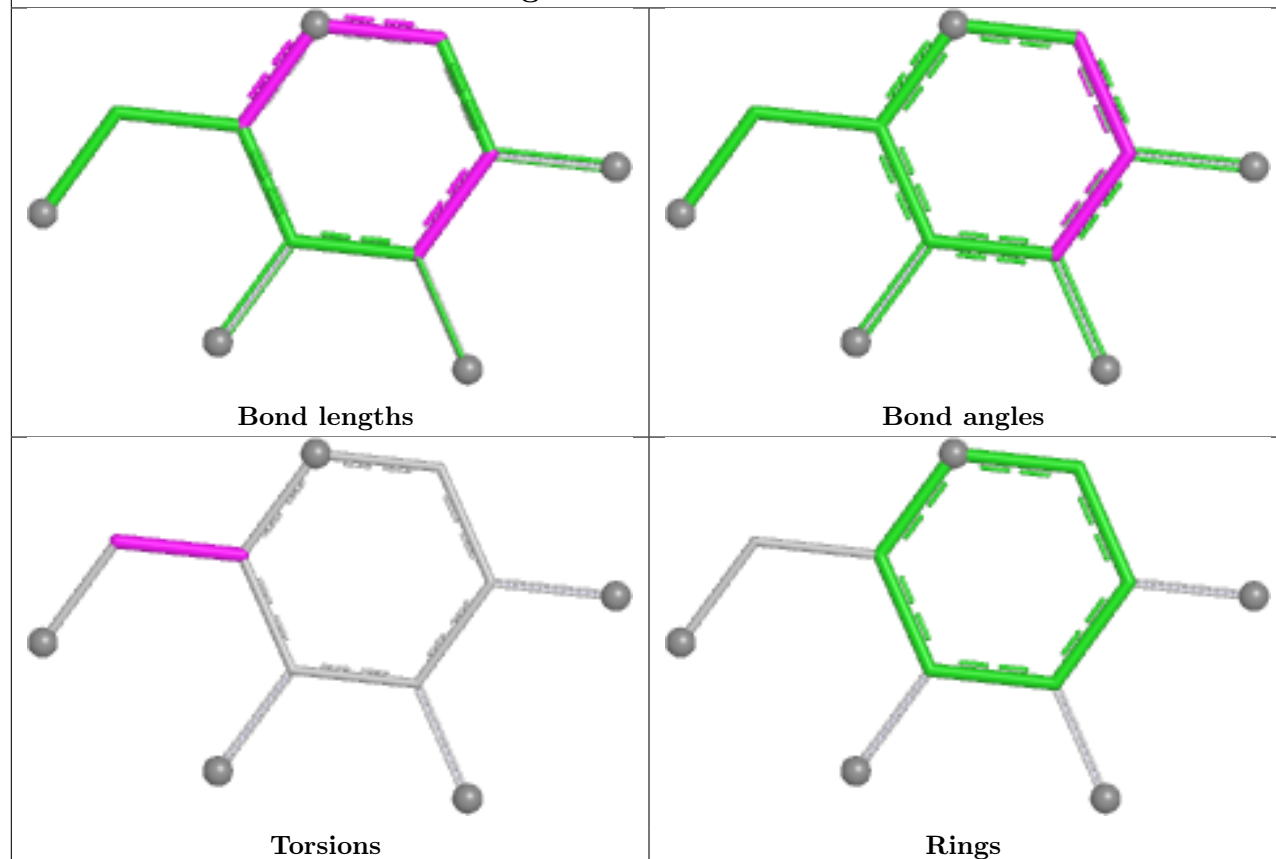




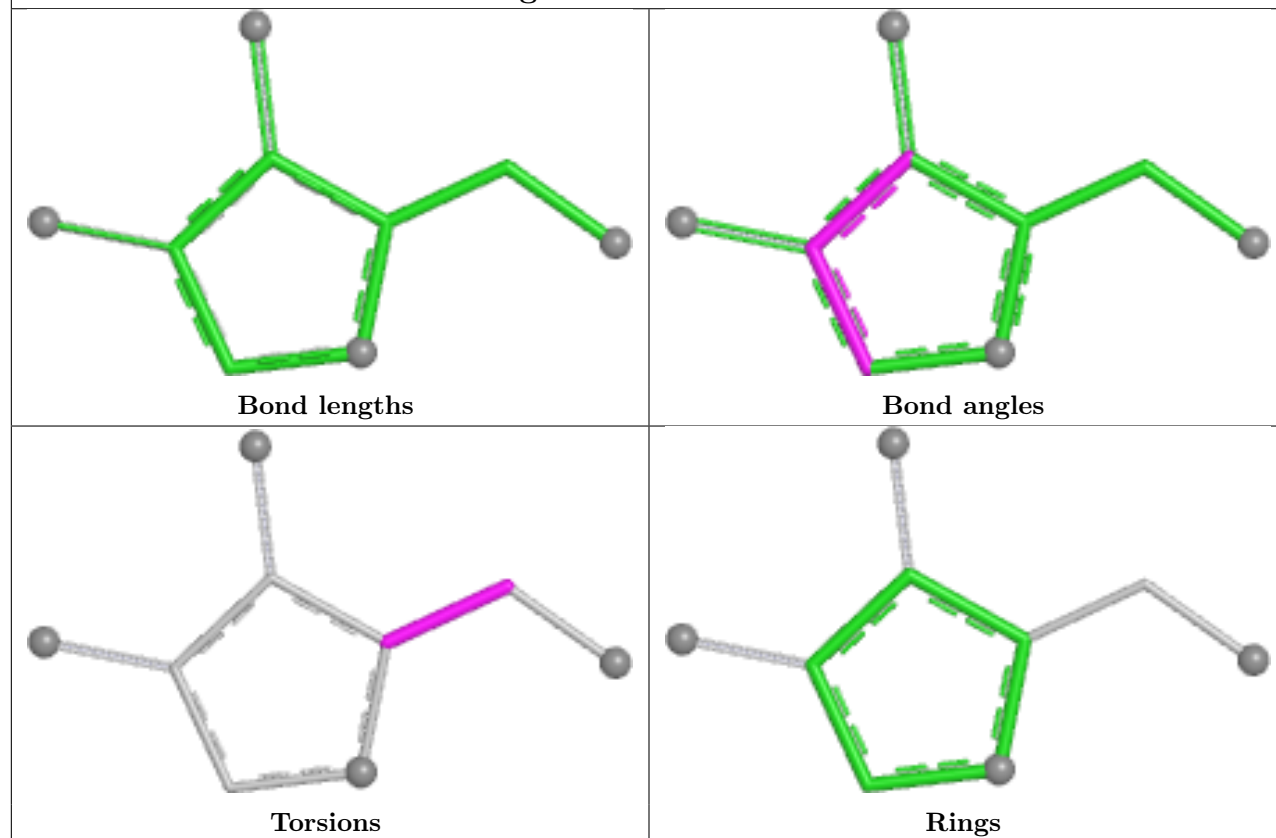


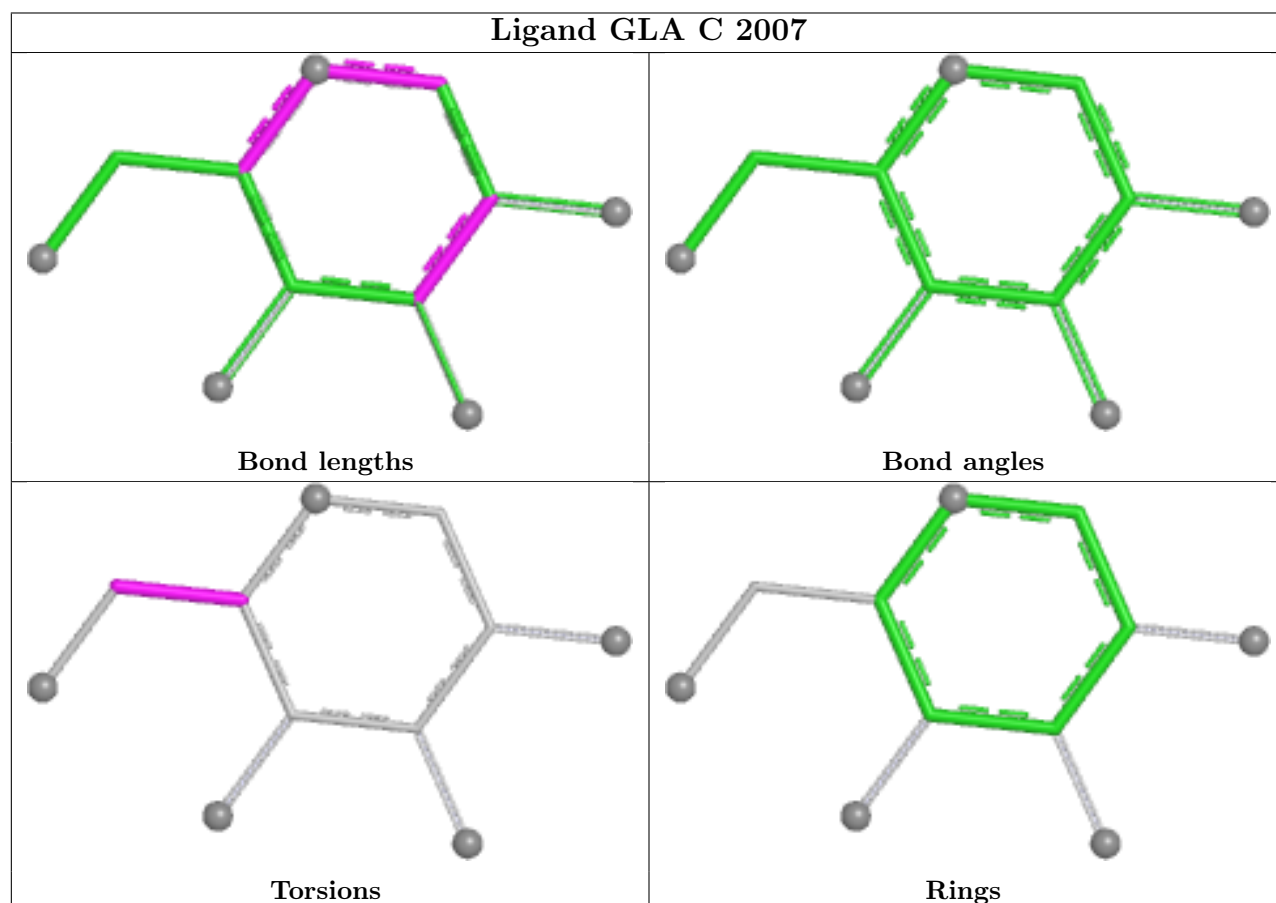
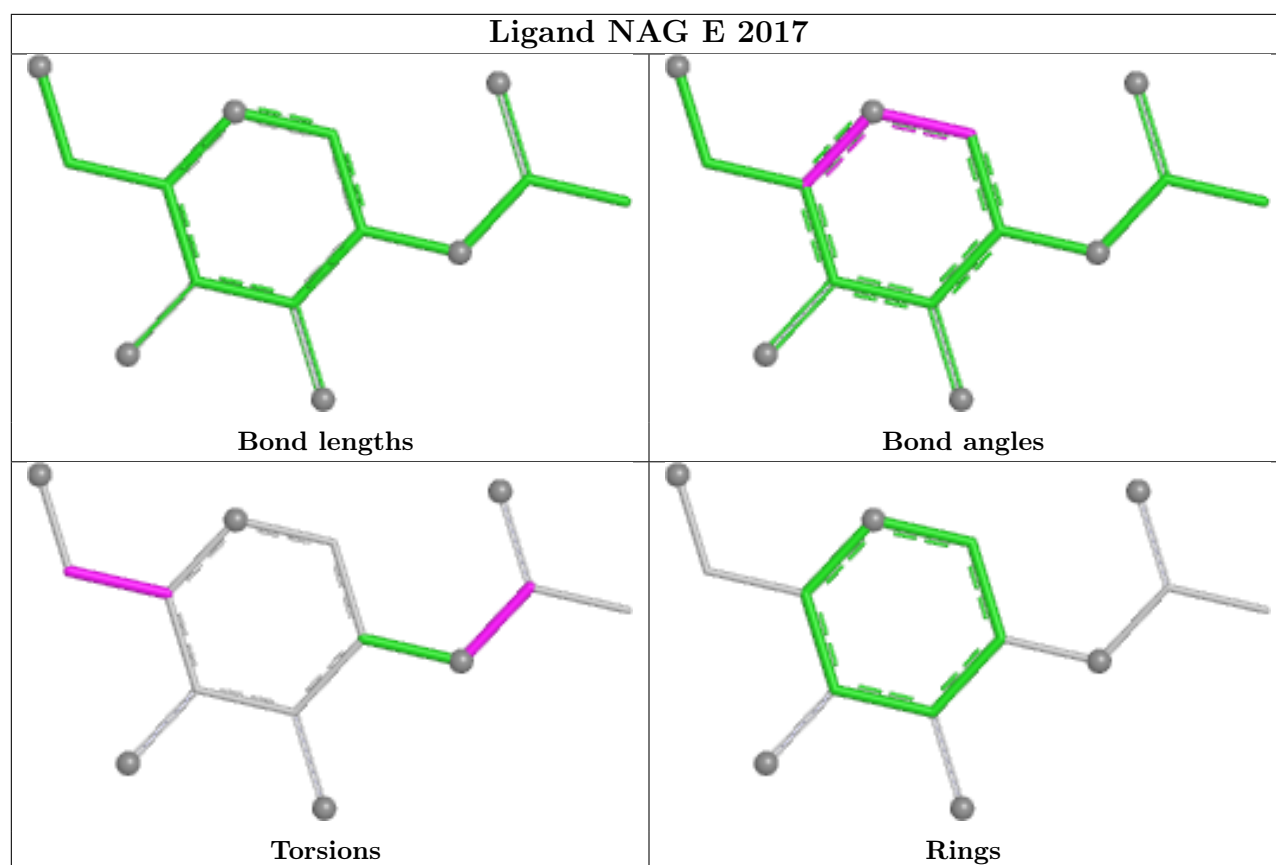


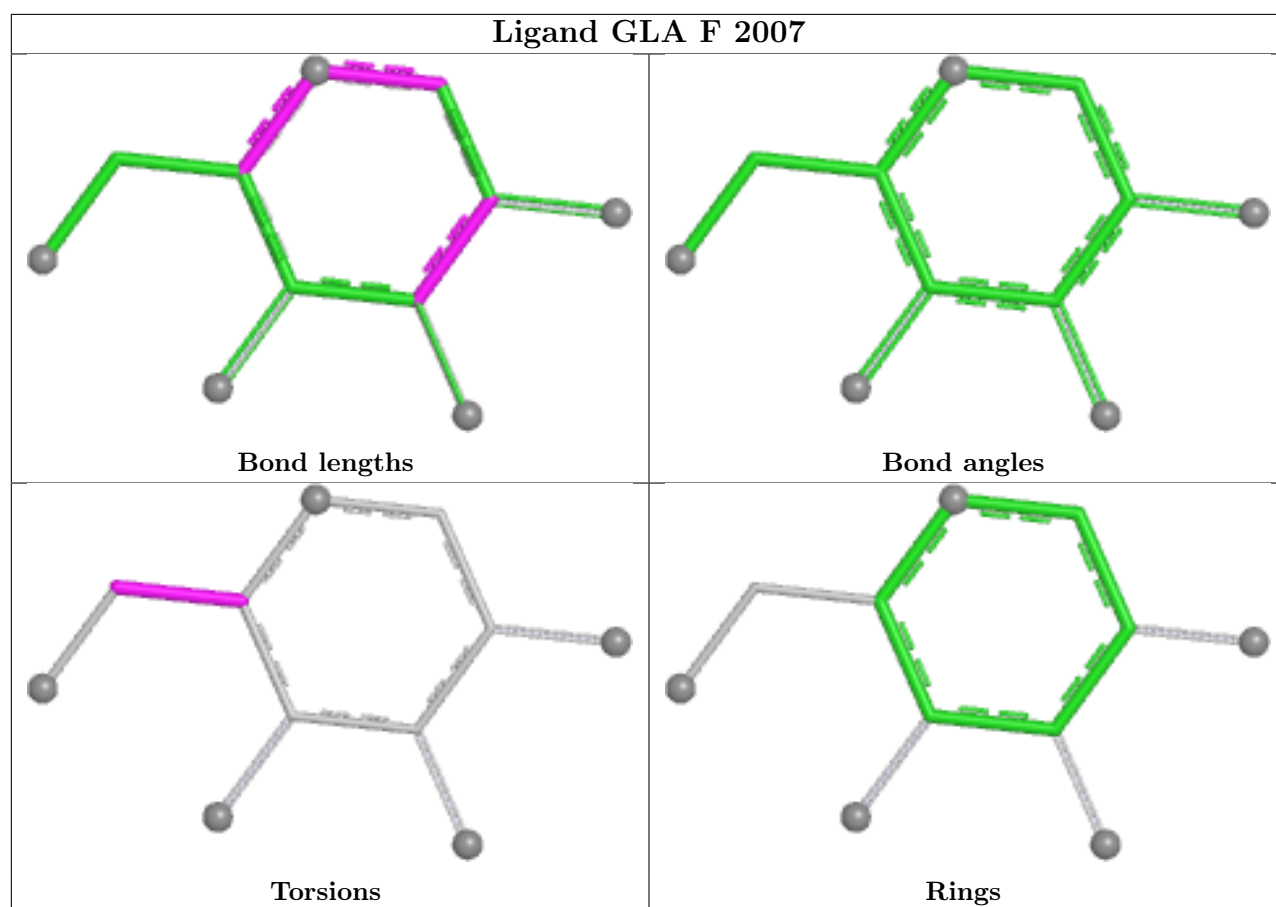
Ligand GLA A 2016

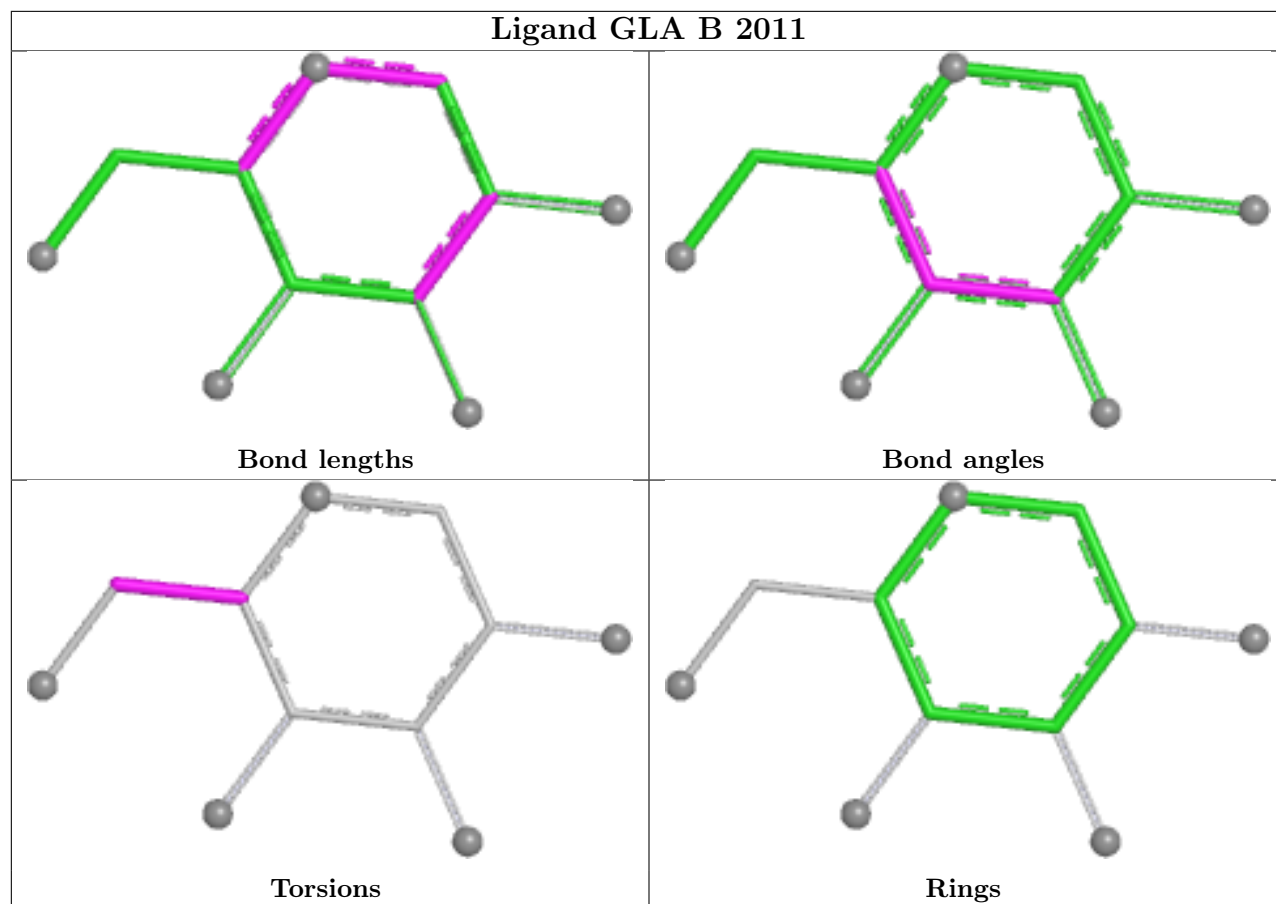


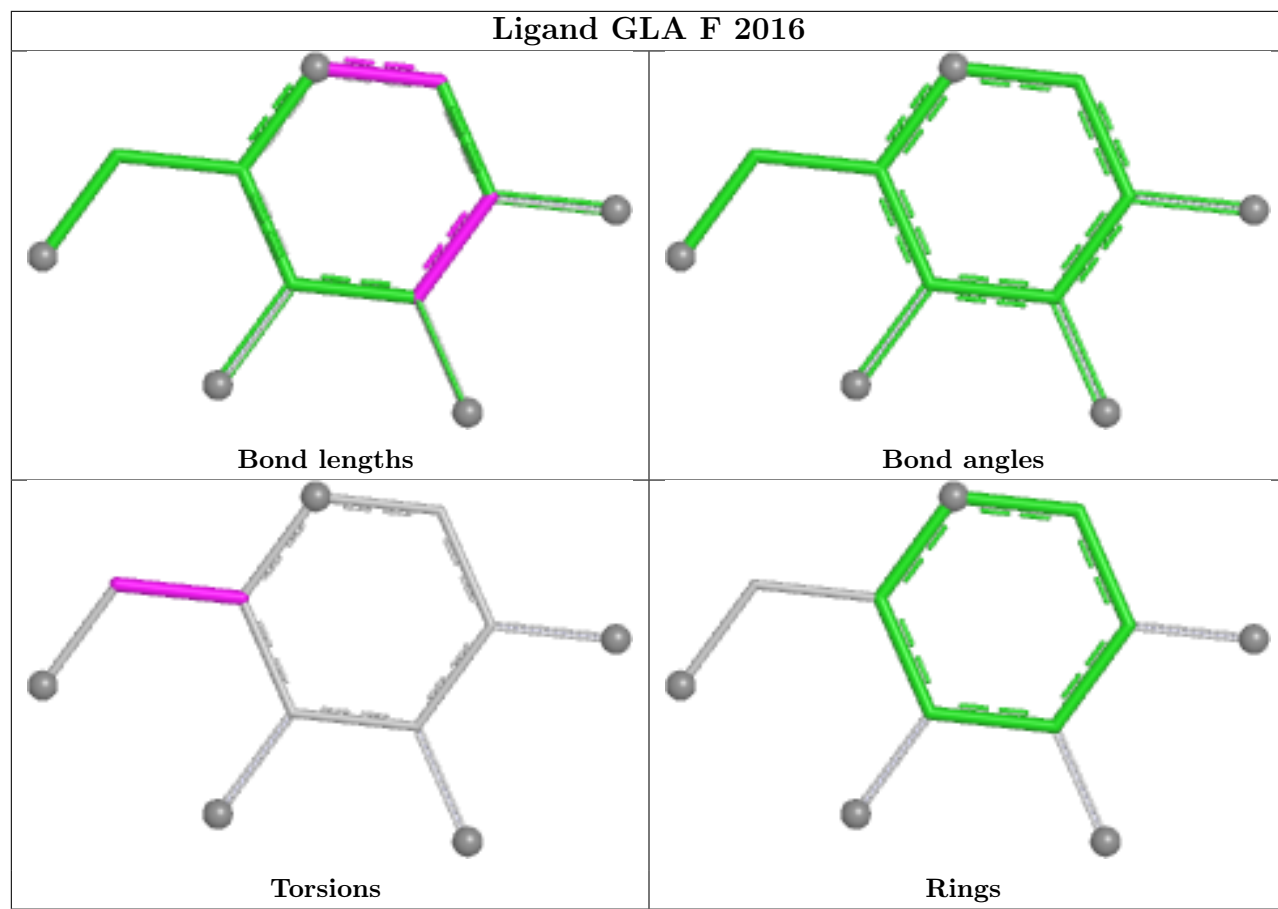
Ligand AHR B 2020

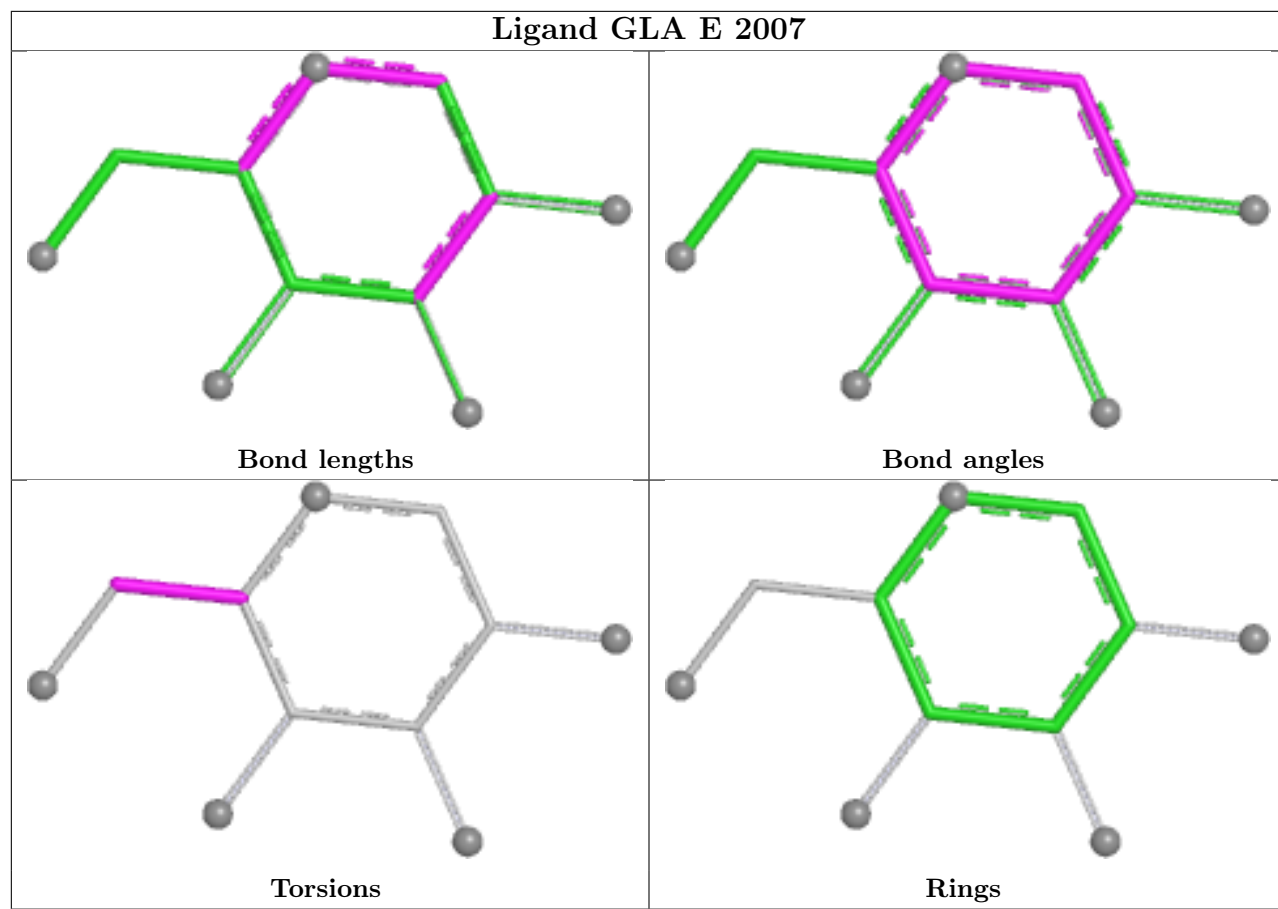


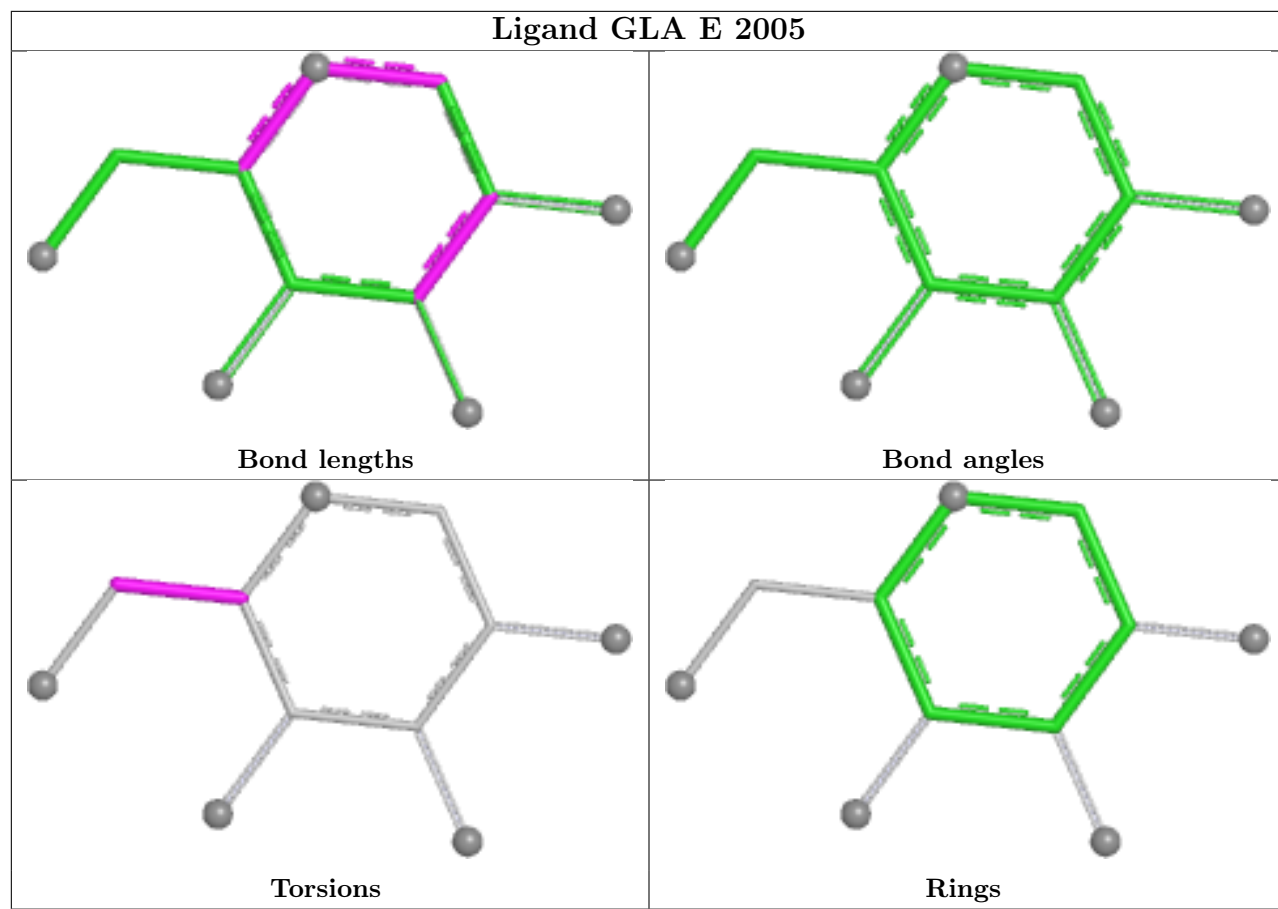


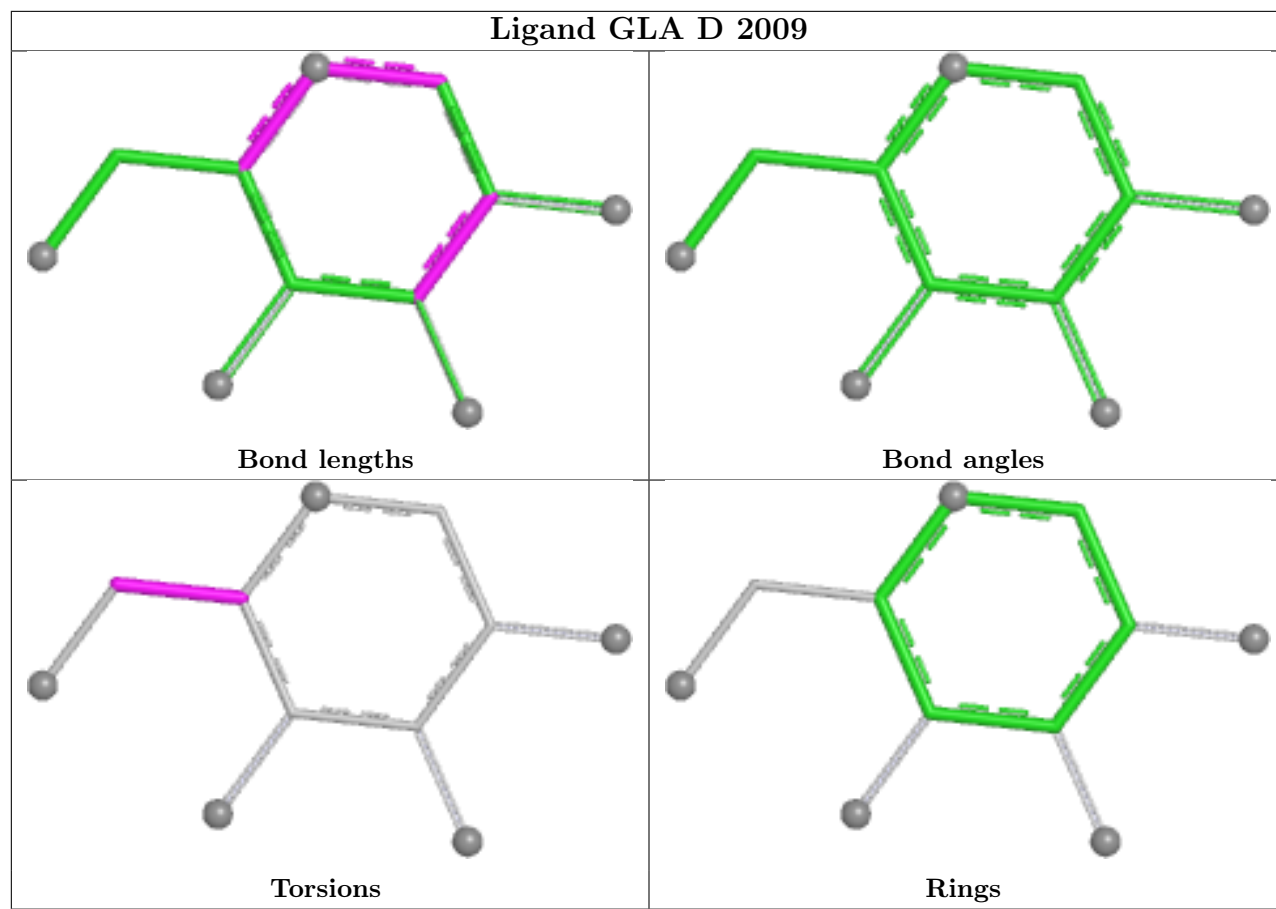


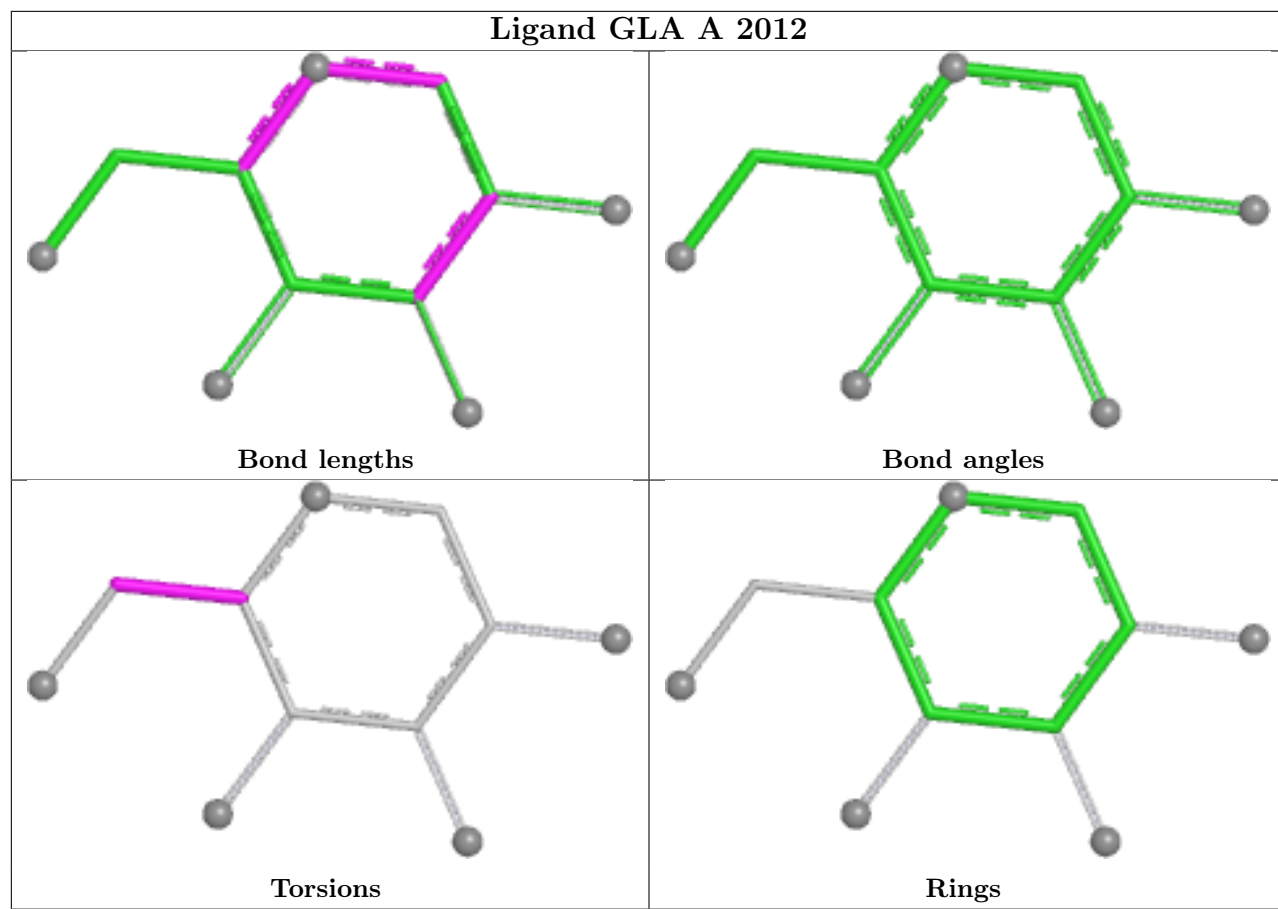


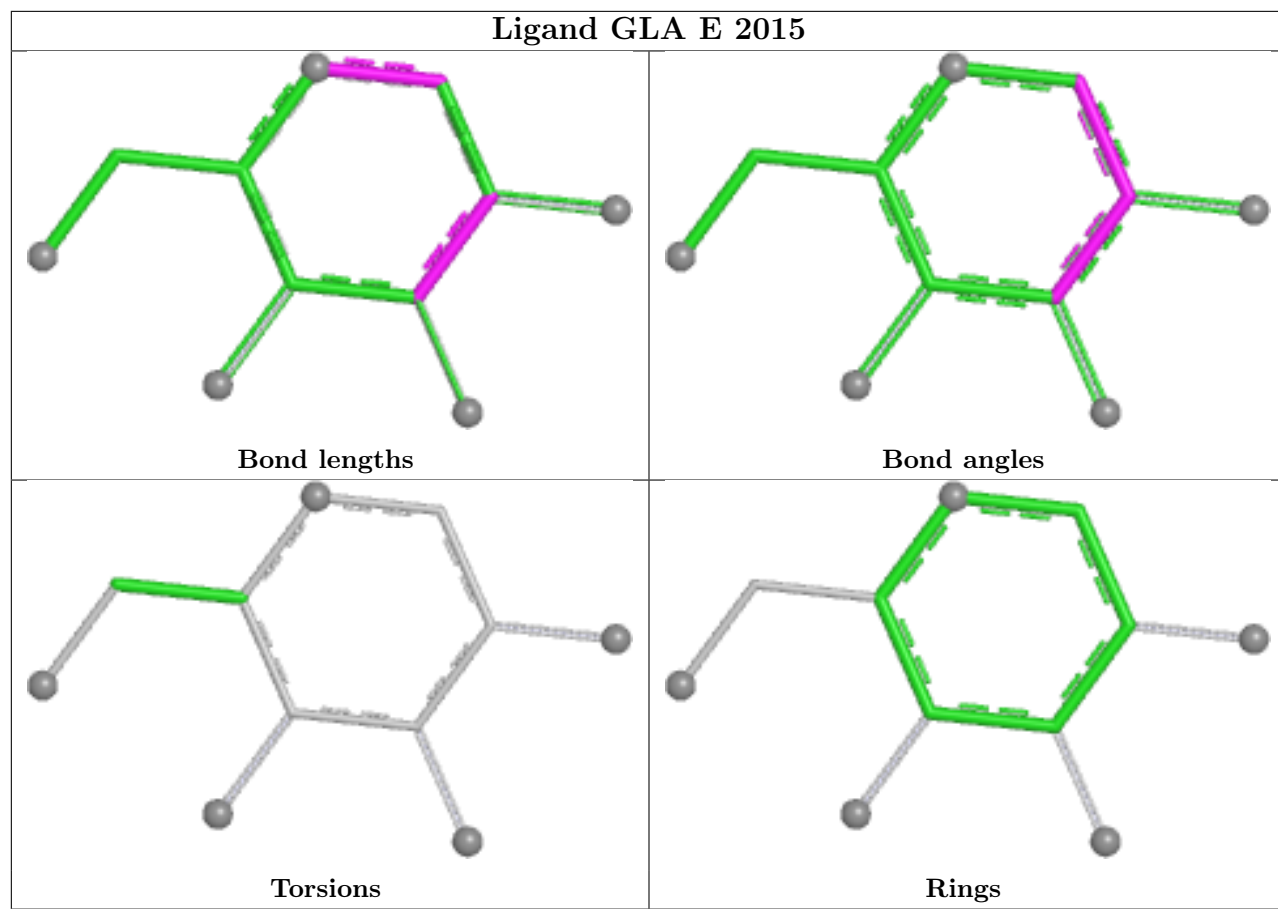


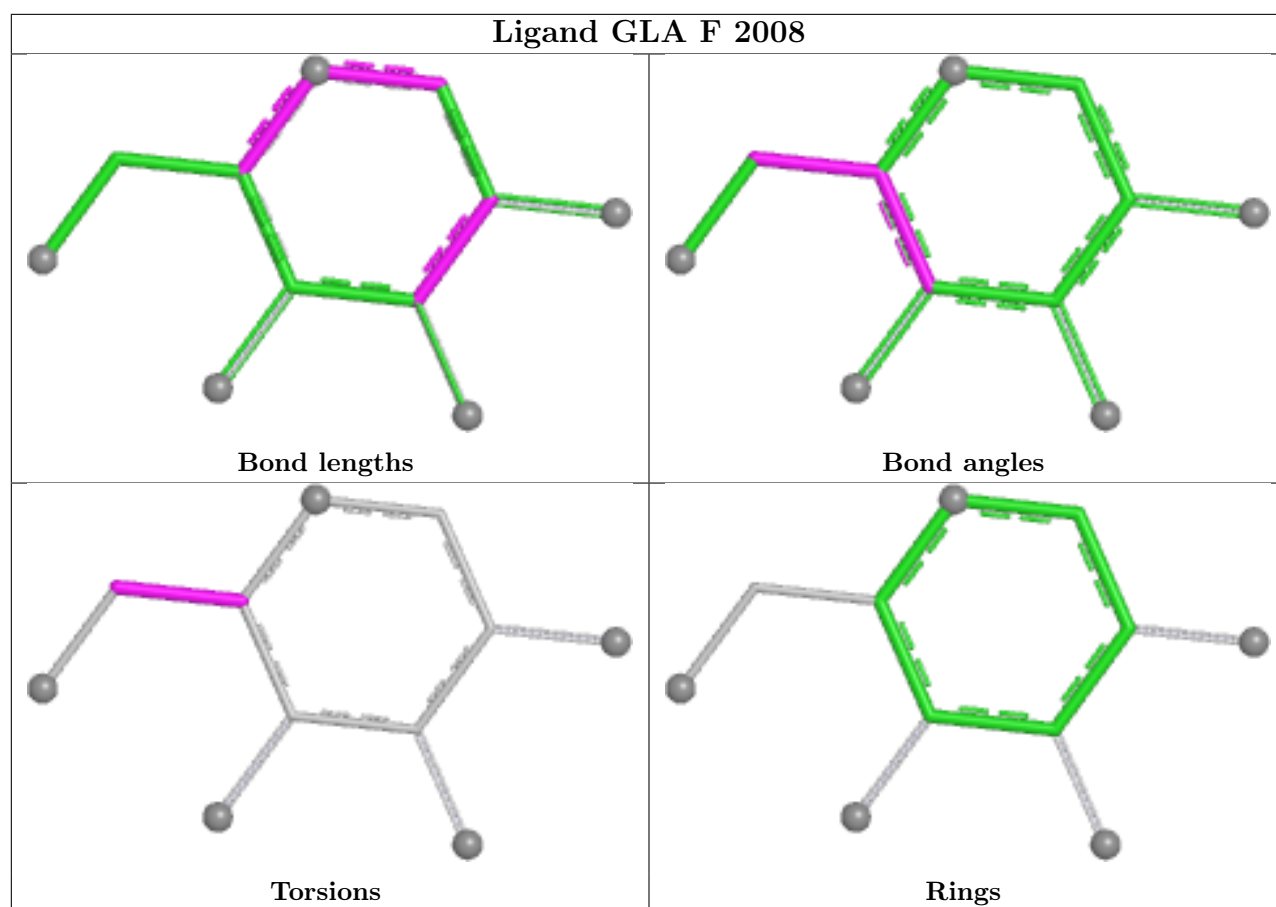




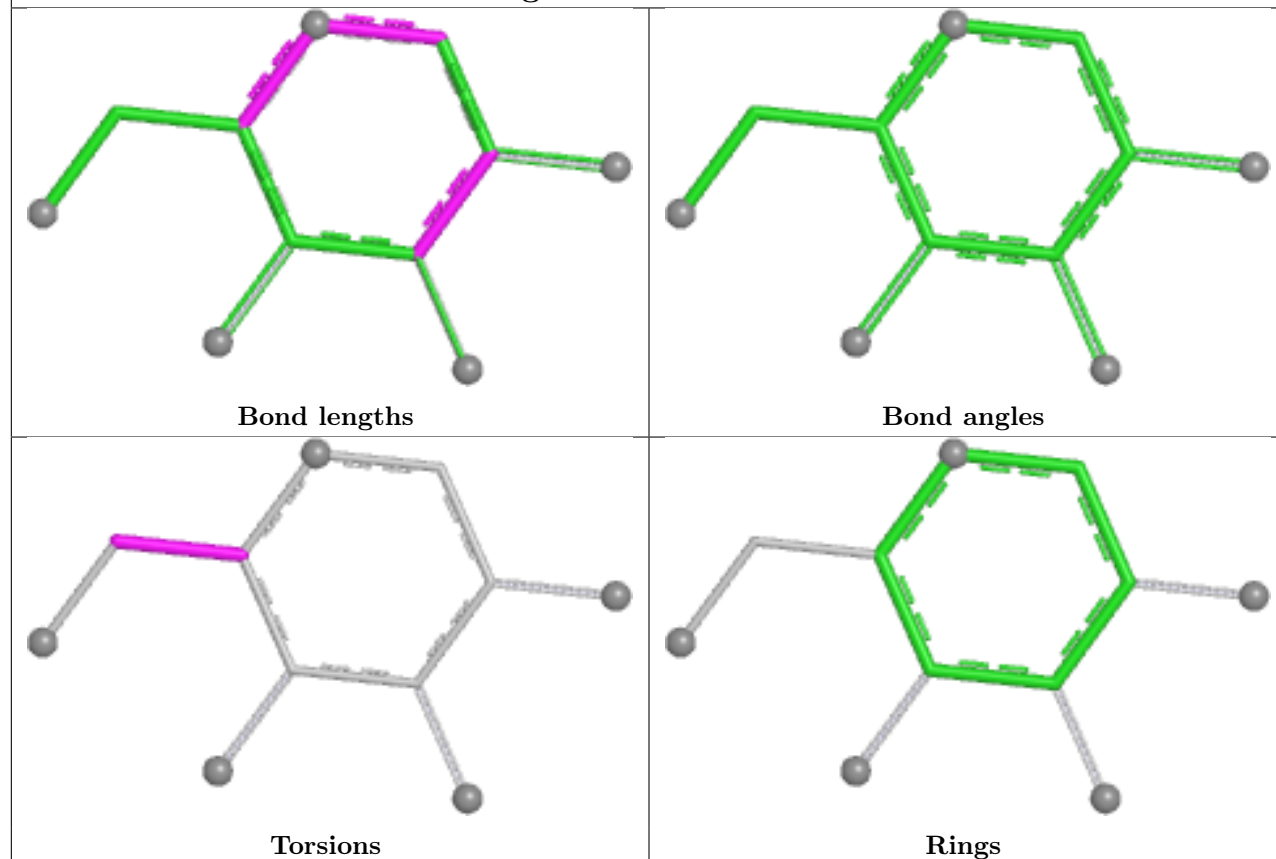




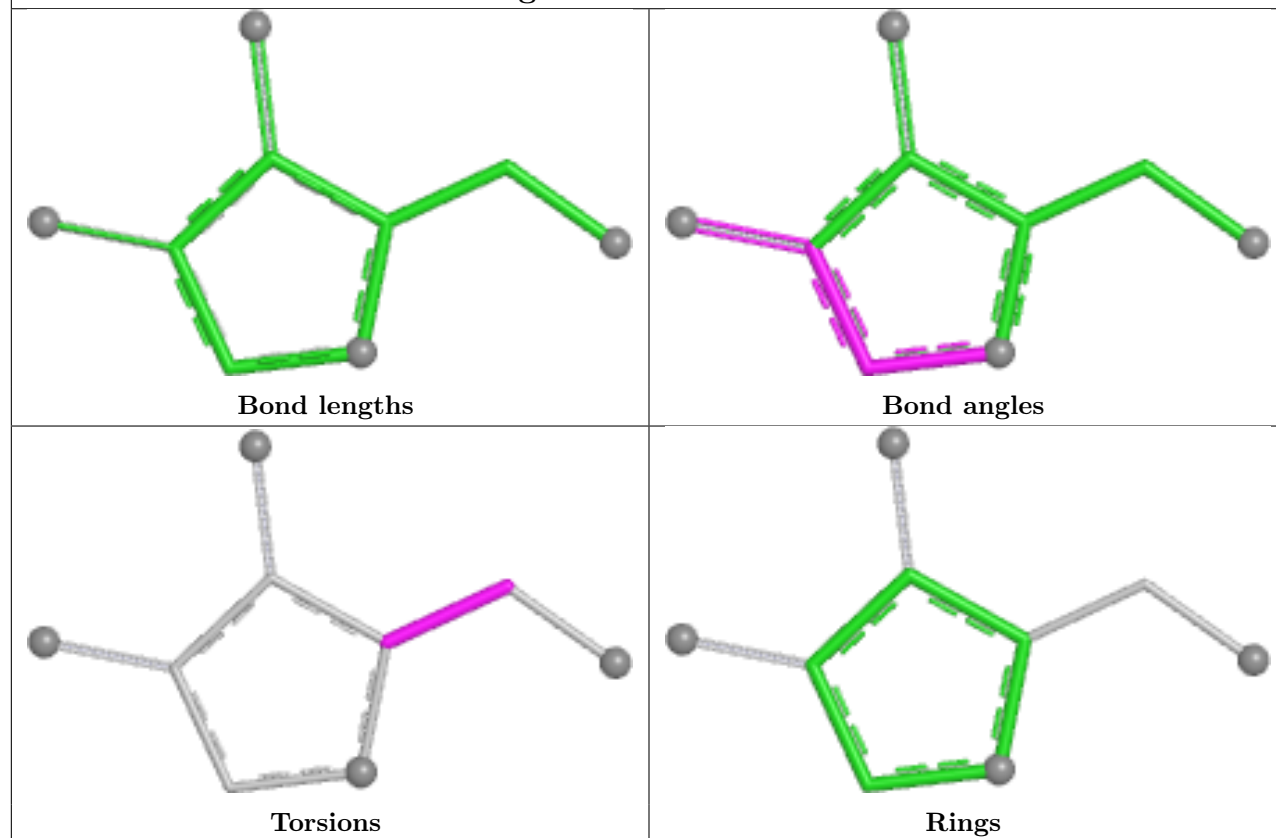


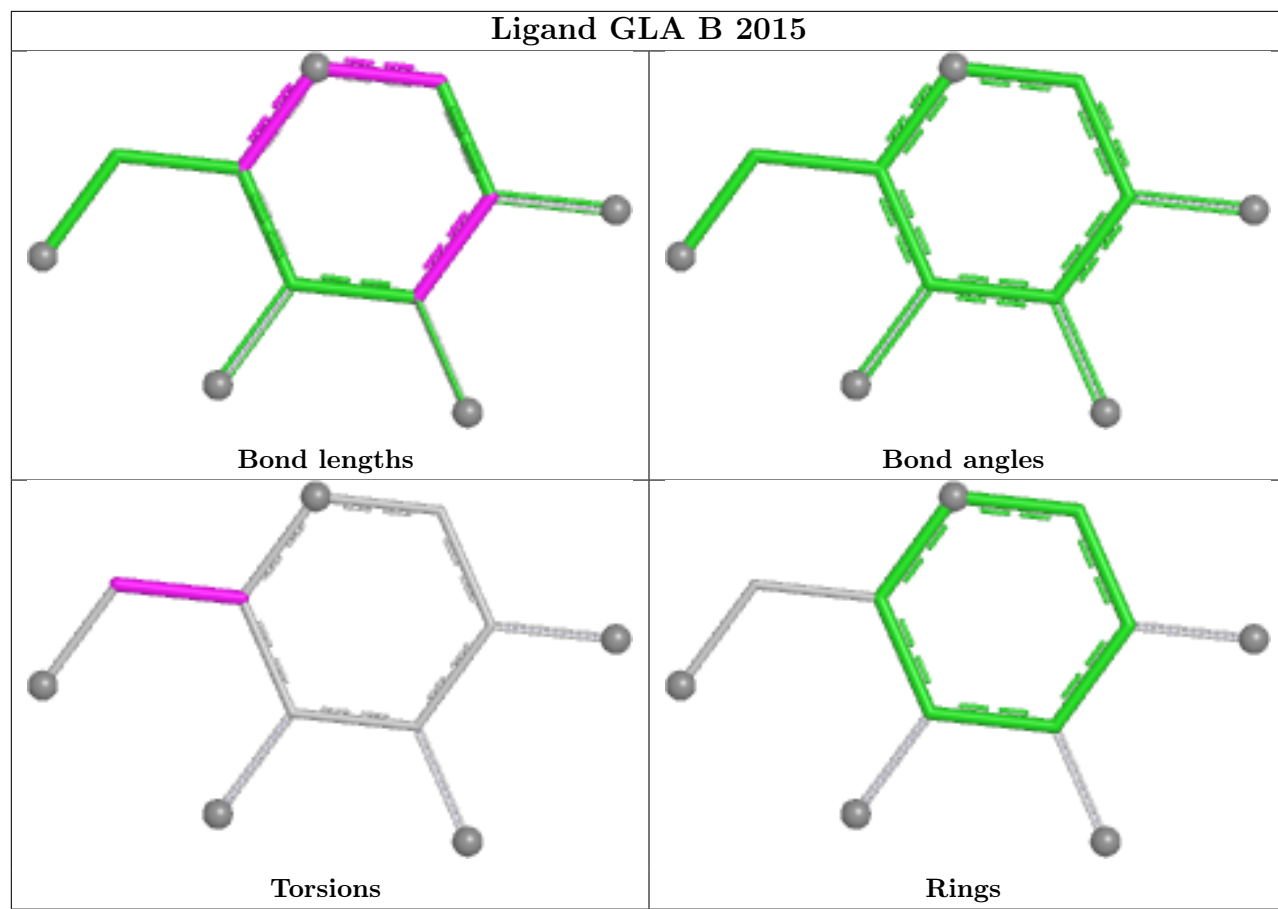


Ligand GLA C 2004

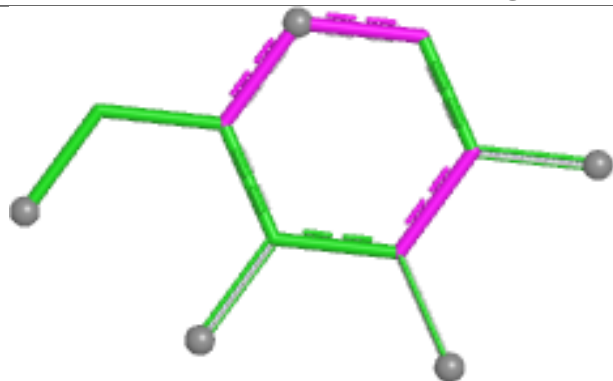


Ligand AHR D 2001

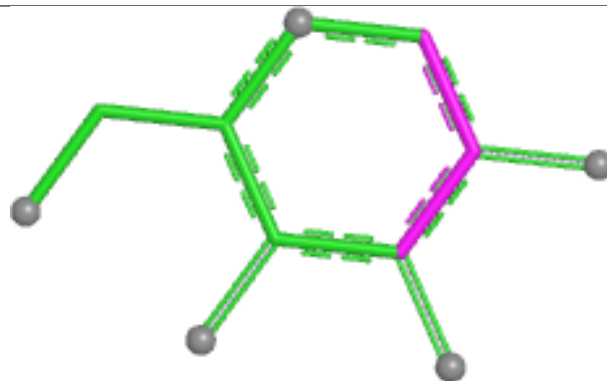




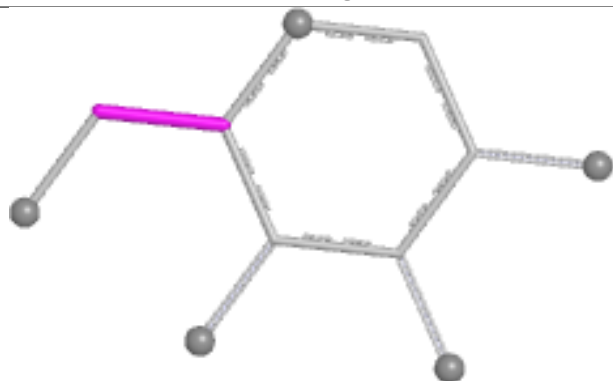
Ligand GLA C 2005



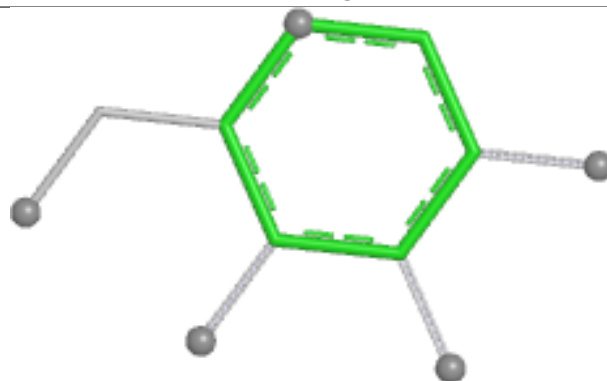
Bond lengths



Bond angles

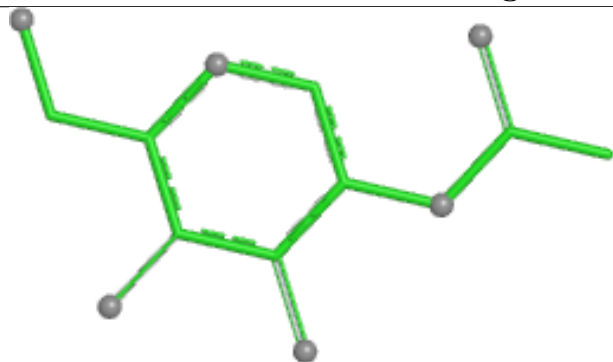


Torsions

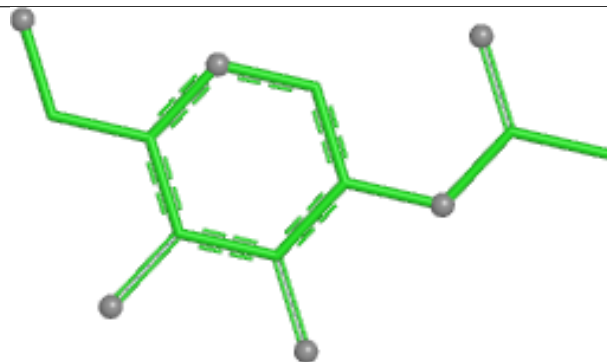


Rings

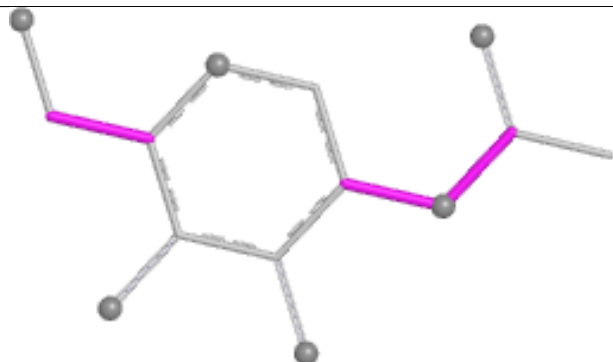
Ligand NAG C 2009



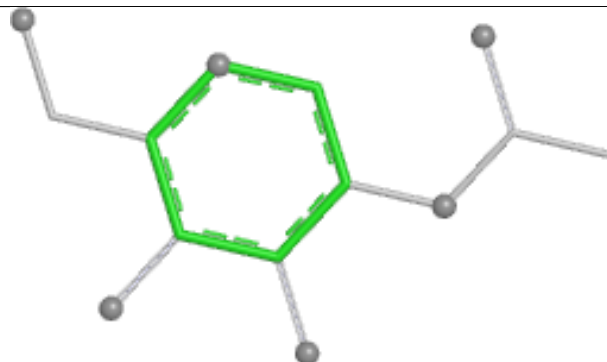
Bond lengths



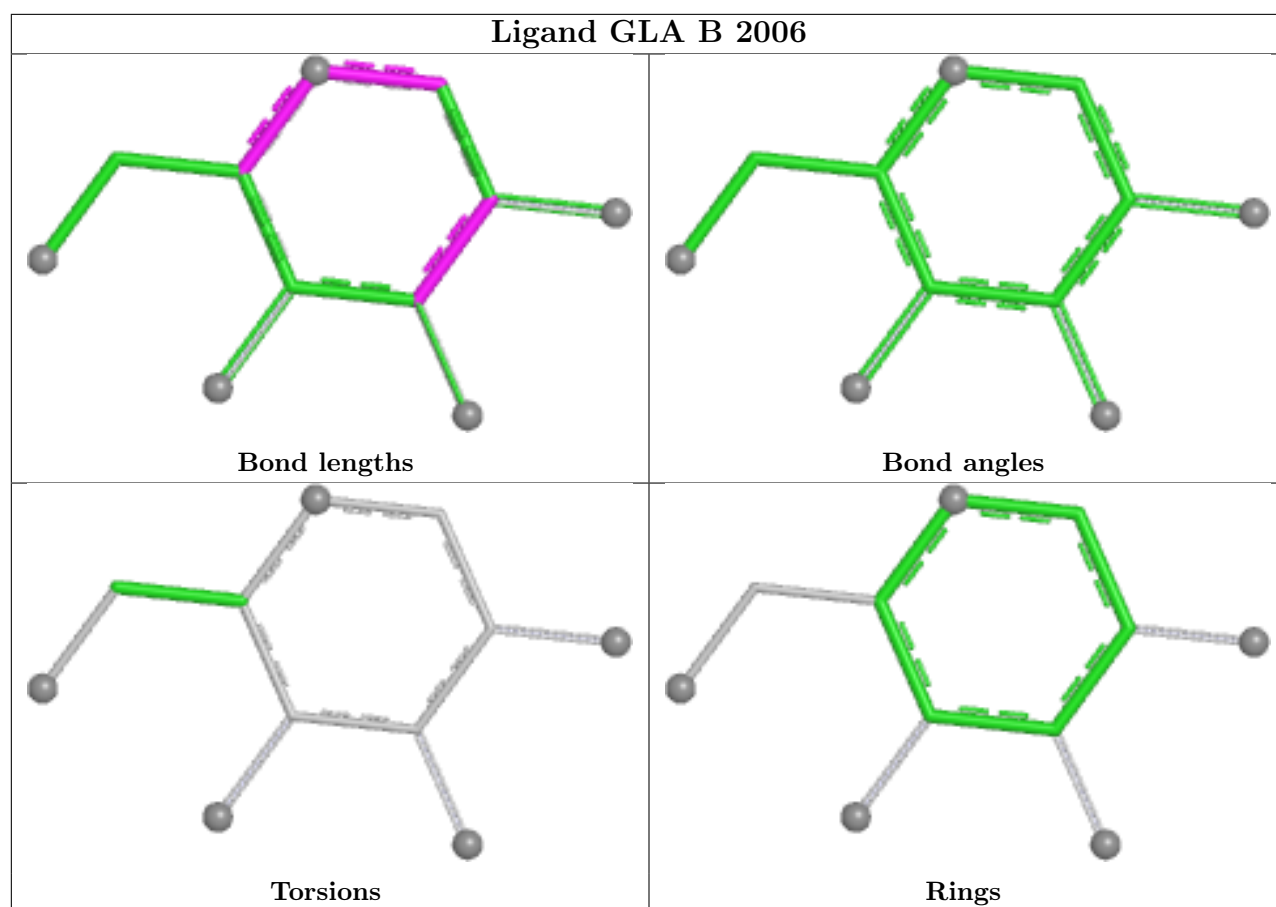
Bond angles

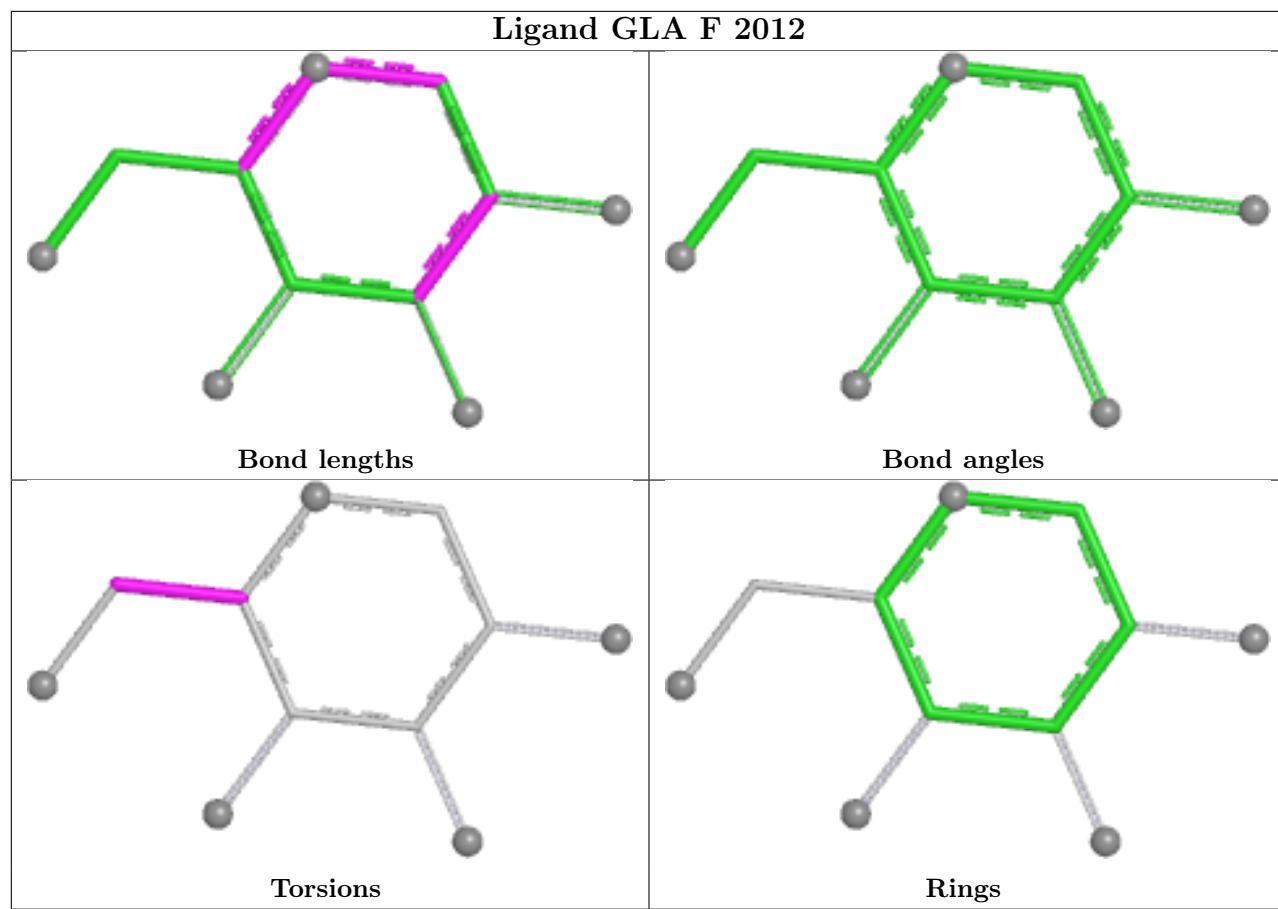


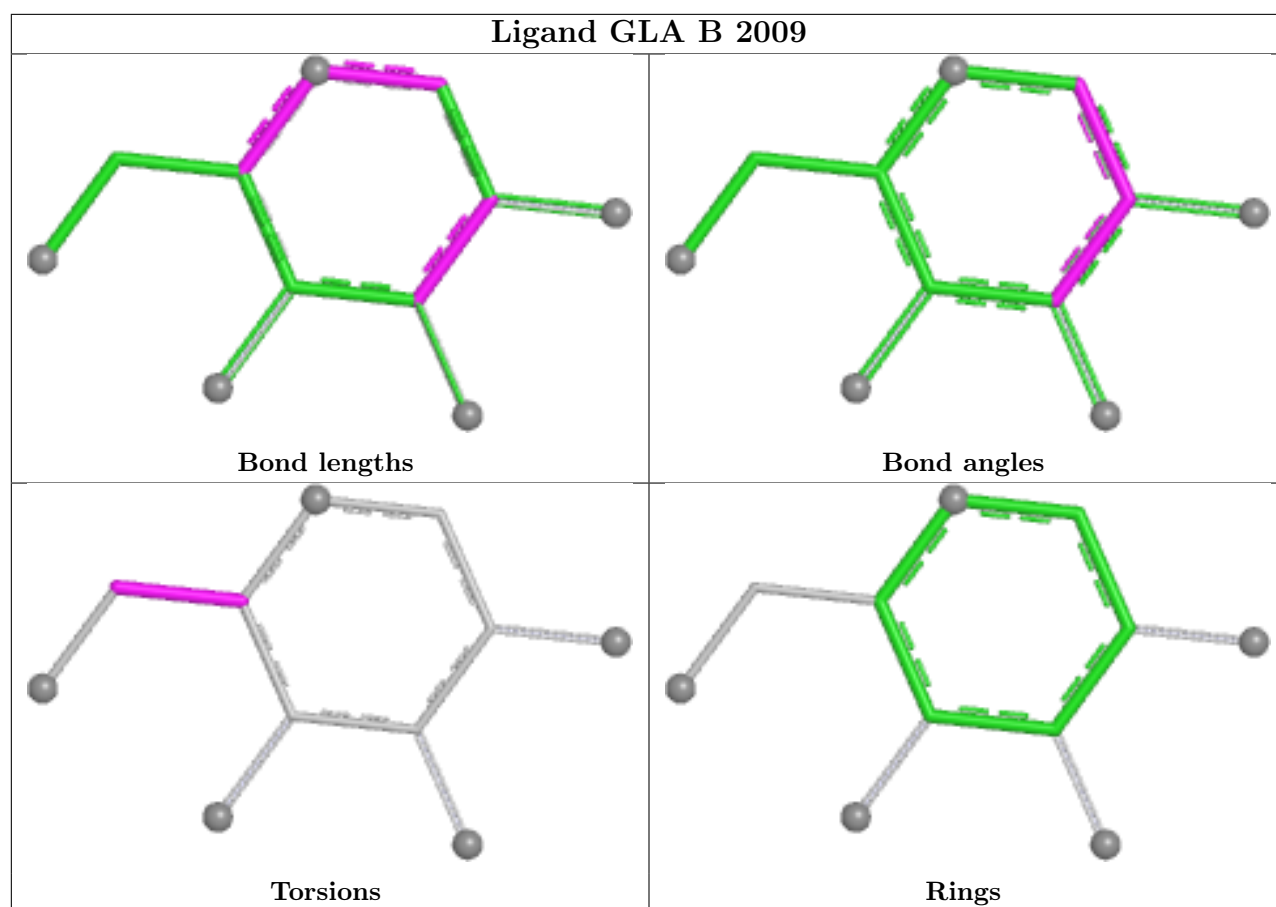
Torsions



Rings







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.

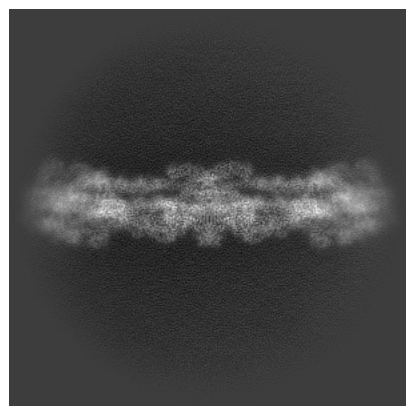
6 Map visualisation [i](#)

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.

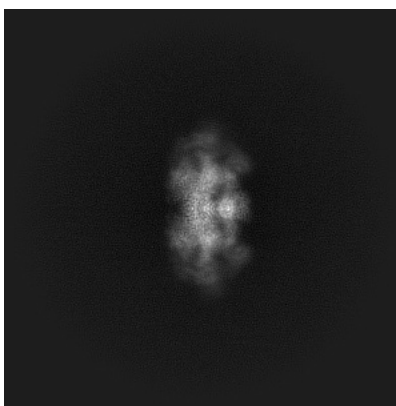
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

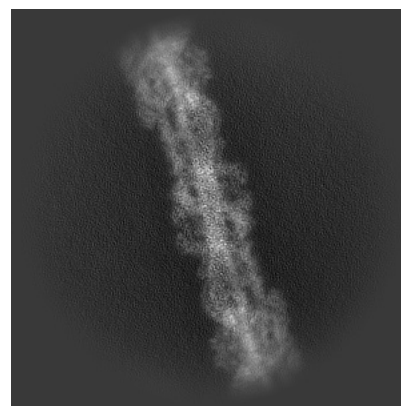
6.1.1 Primary map



X

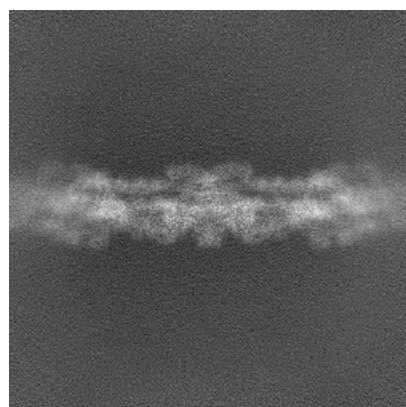


Y

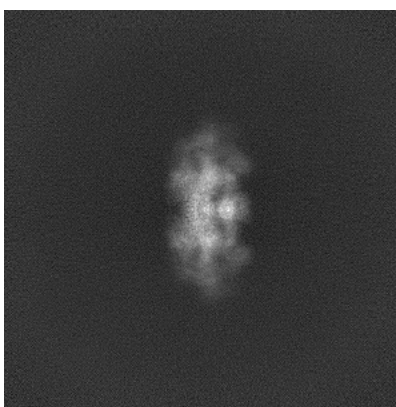


Z

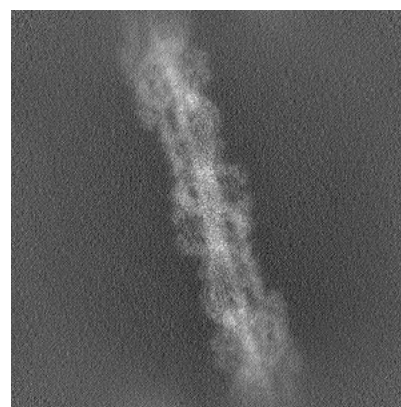
6.1.2 Raw map



X



Y

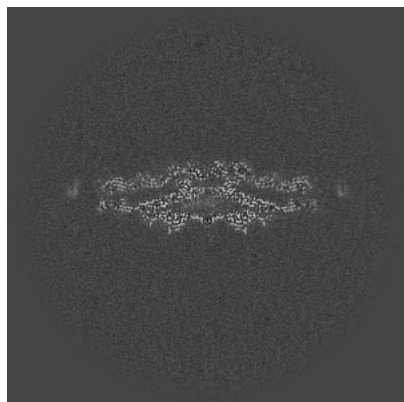


Z

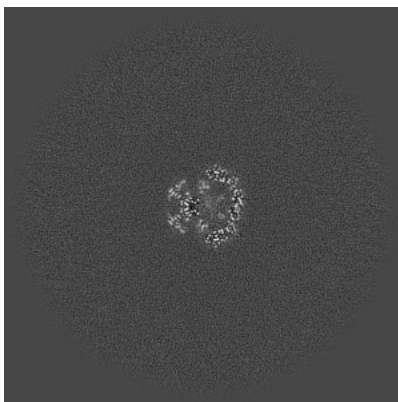
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

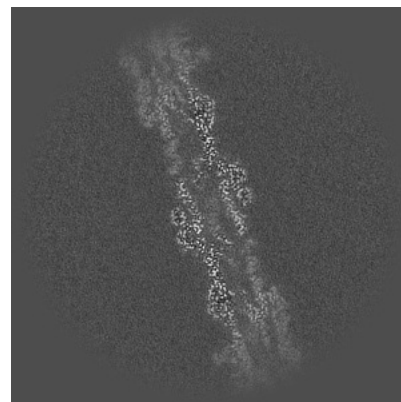
6.2.1 Primary map



X Index: 256

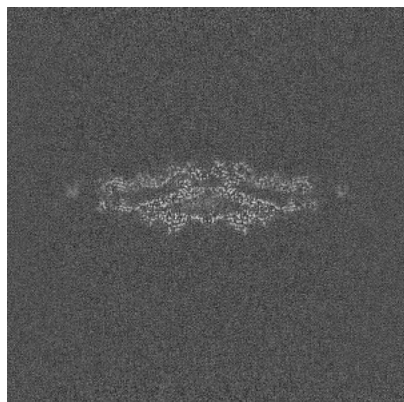


Y Index: 256

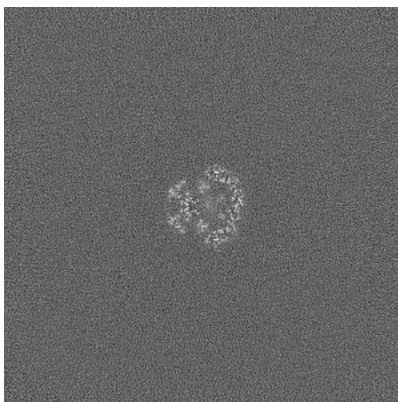


Z Index: 256

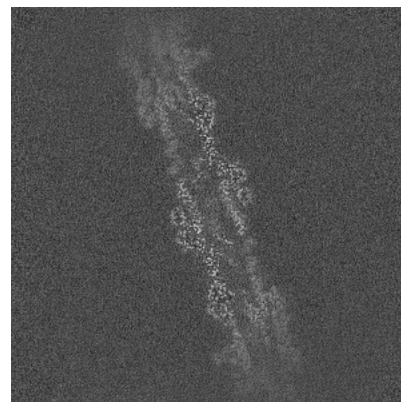
6.2.2 Raw map



X Index: 256



Y Index: 256

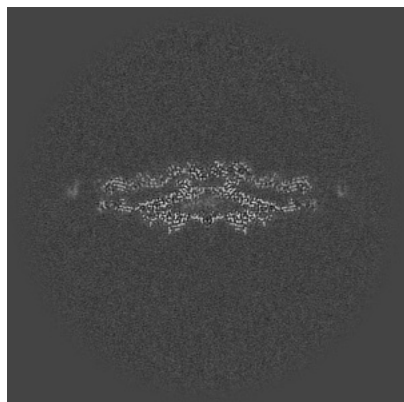


Z Index: 256

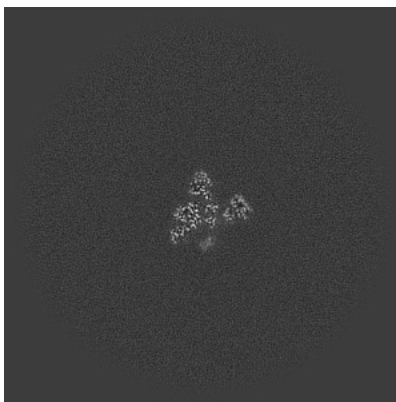
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

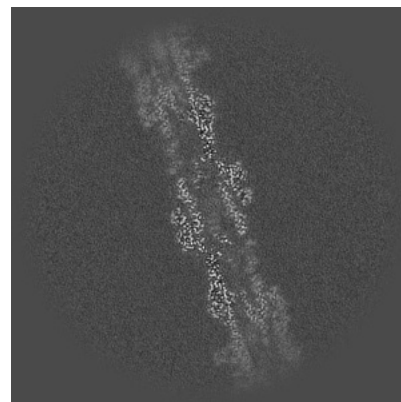
6.3.1 Primary map



X Index: 256

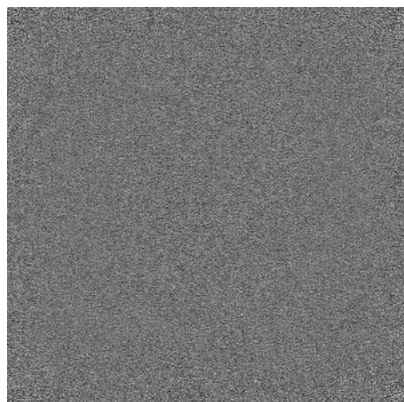


Y Index: 302

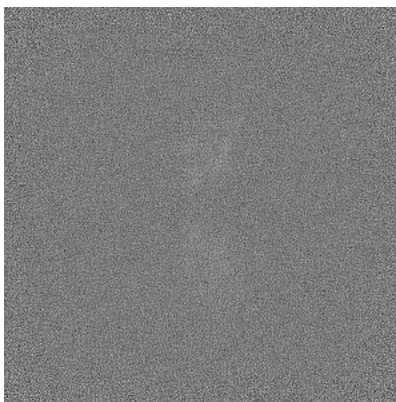


Z Index: 255

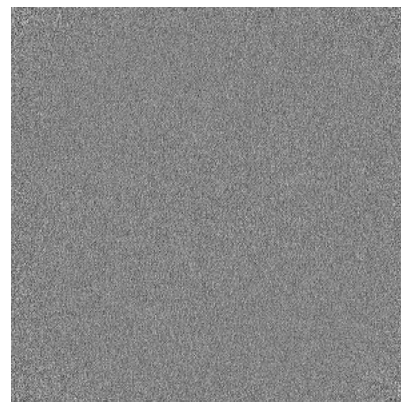
6.3.2 Raw map



X Index: 0



Y Index: 0

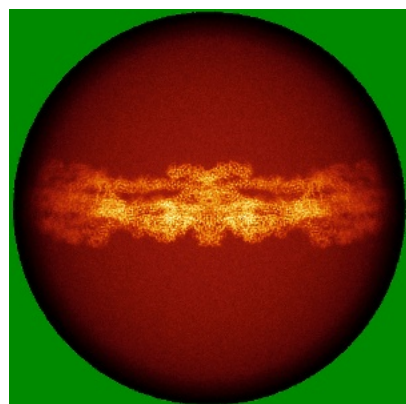


Z Index: 0

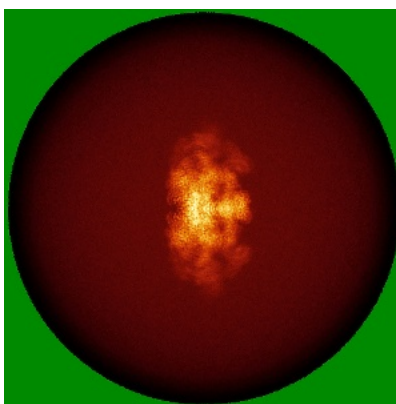
The images above show the largest variance slices of the map in three orthogonal directions.

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

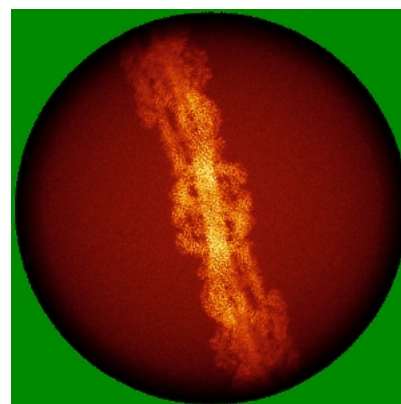
6.4.1 Primary map



X

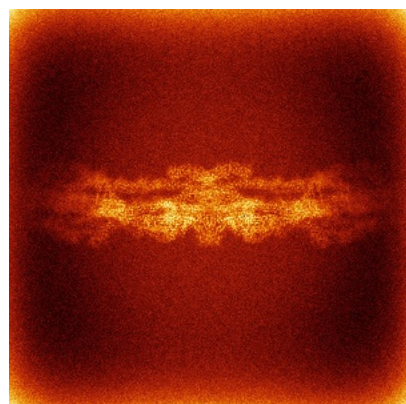


Y

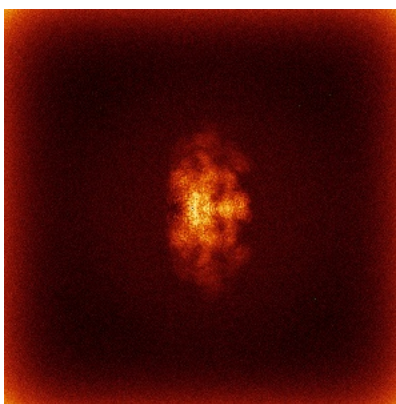


Z

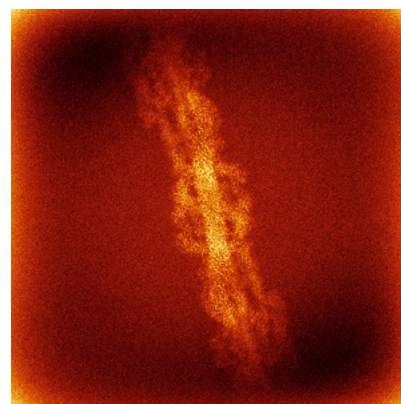
6.4.2 Raw map



X



Y

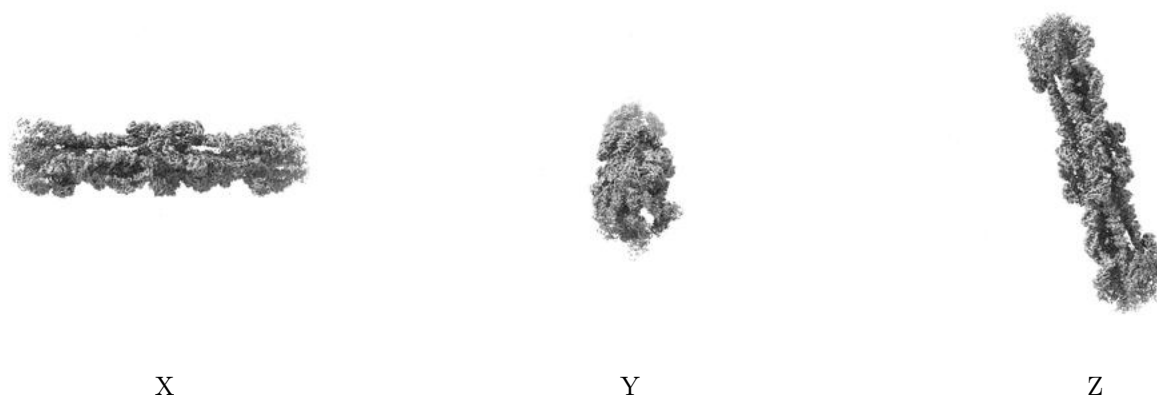


Z

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.

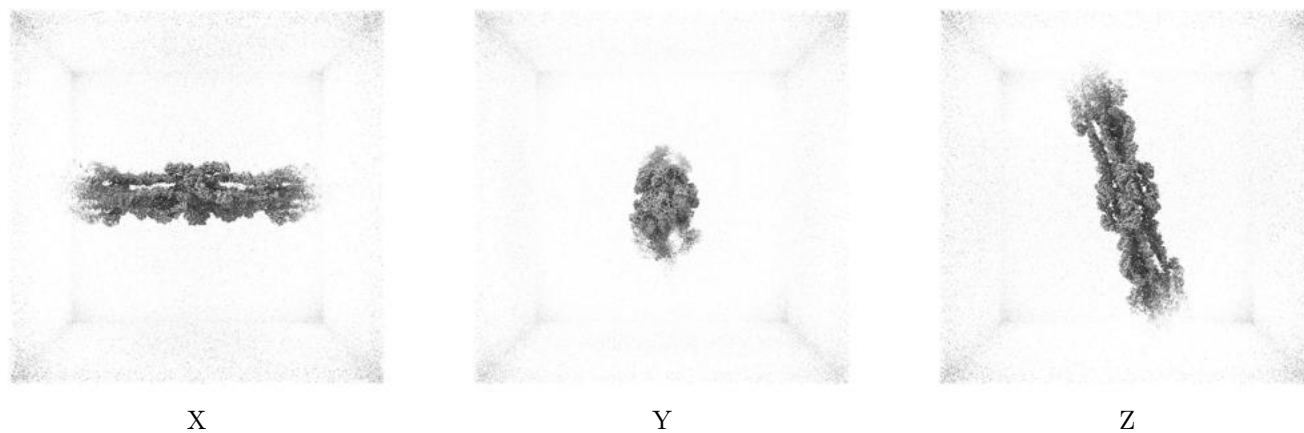
6.5 Orthogonal surface views [i](#)

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.

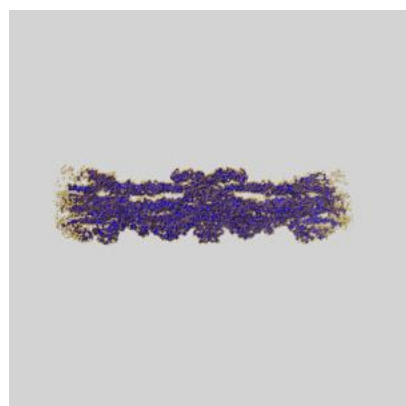
6.6 Mask visualisation [i](#)

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

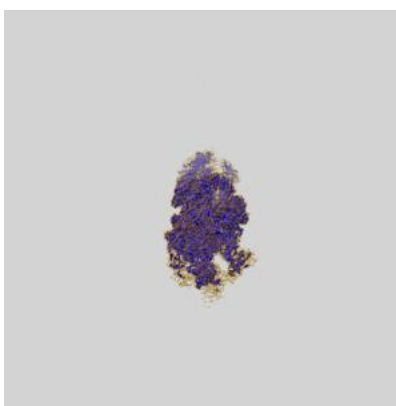
A mask typically either:

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

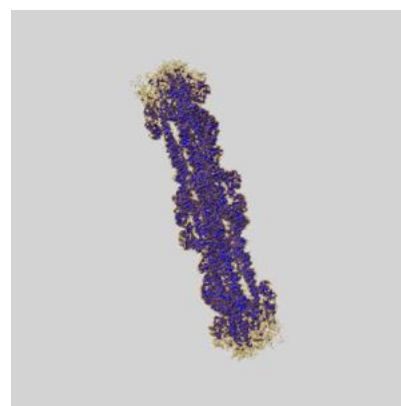
6.6.1 emd_37389_msk_1.map [i](#)



X



Y

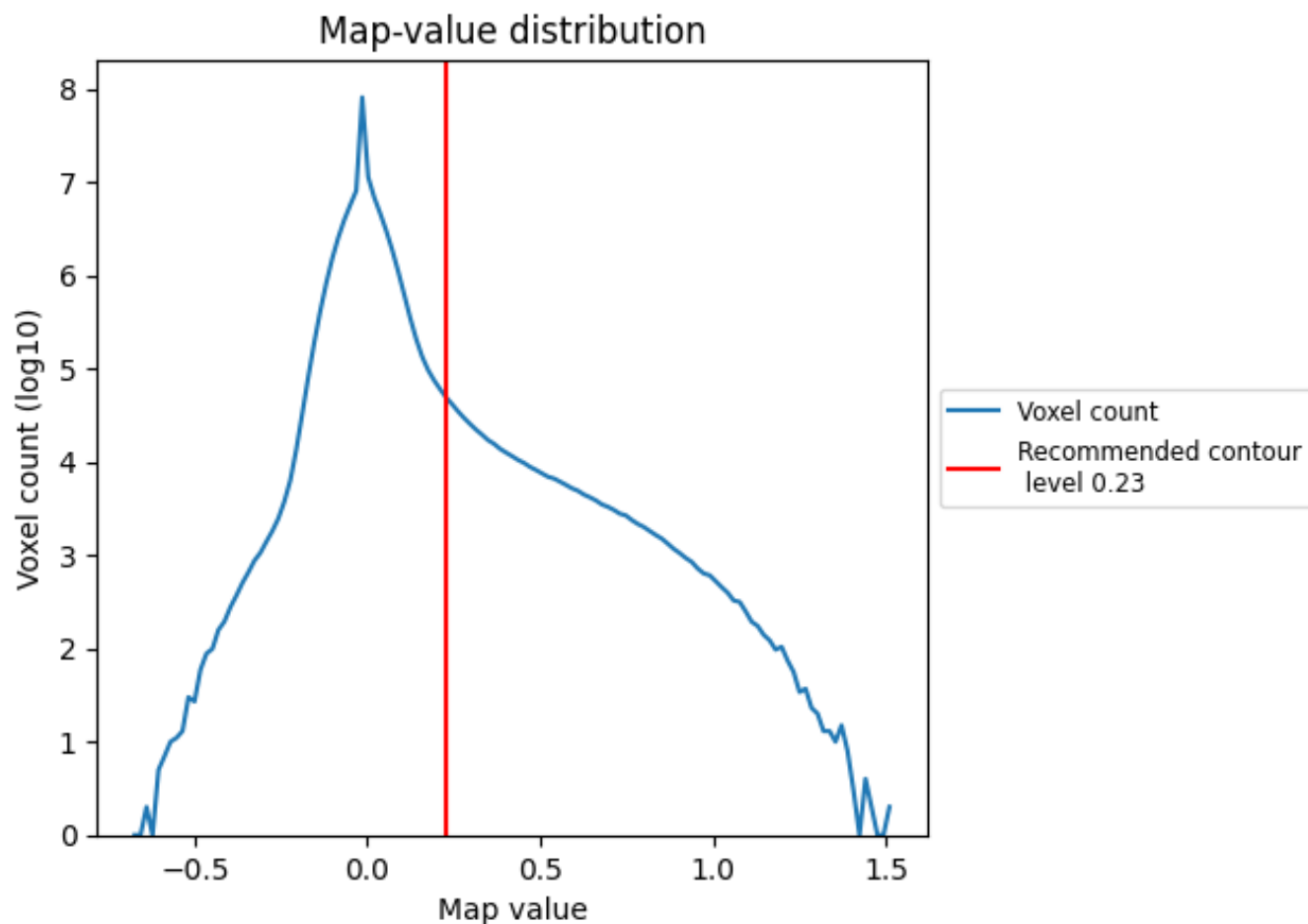


Z

7 Map analysis [i](#)

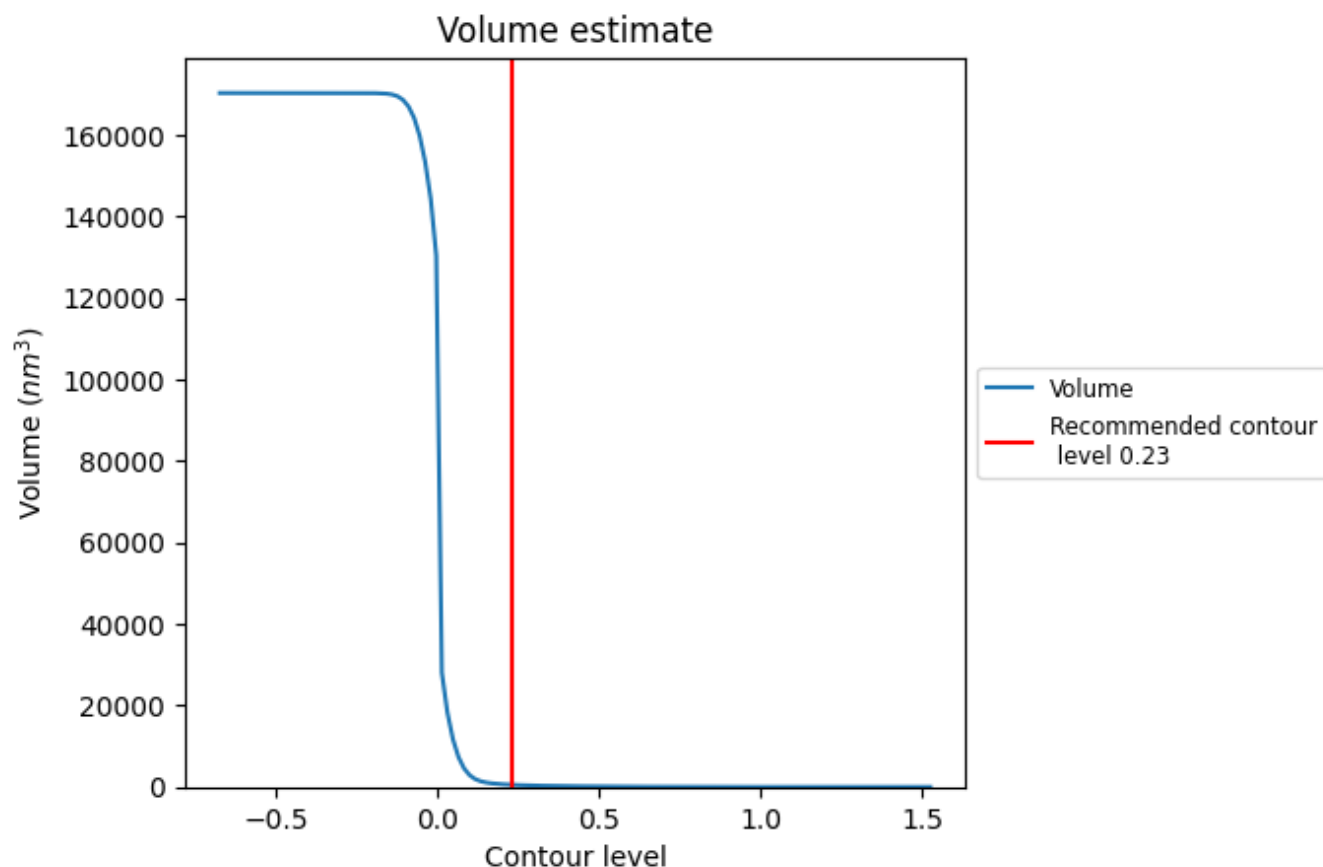
This section contains the results of statistical analysis of the map.

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.

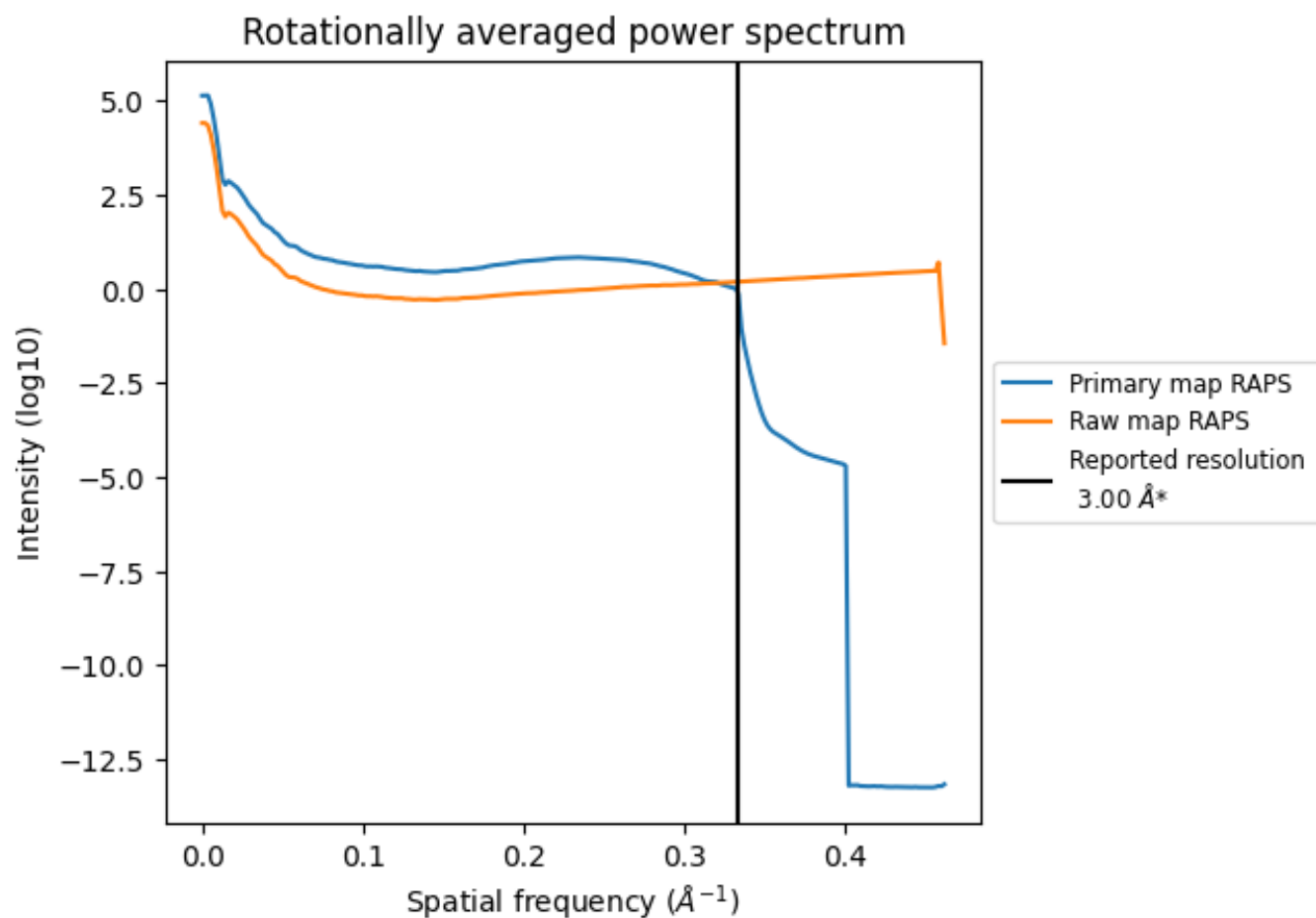
7.2 Volume estimate [i](#)



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 ⓘ

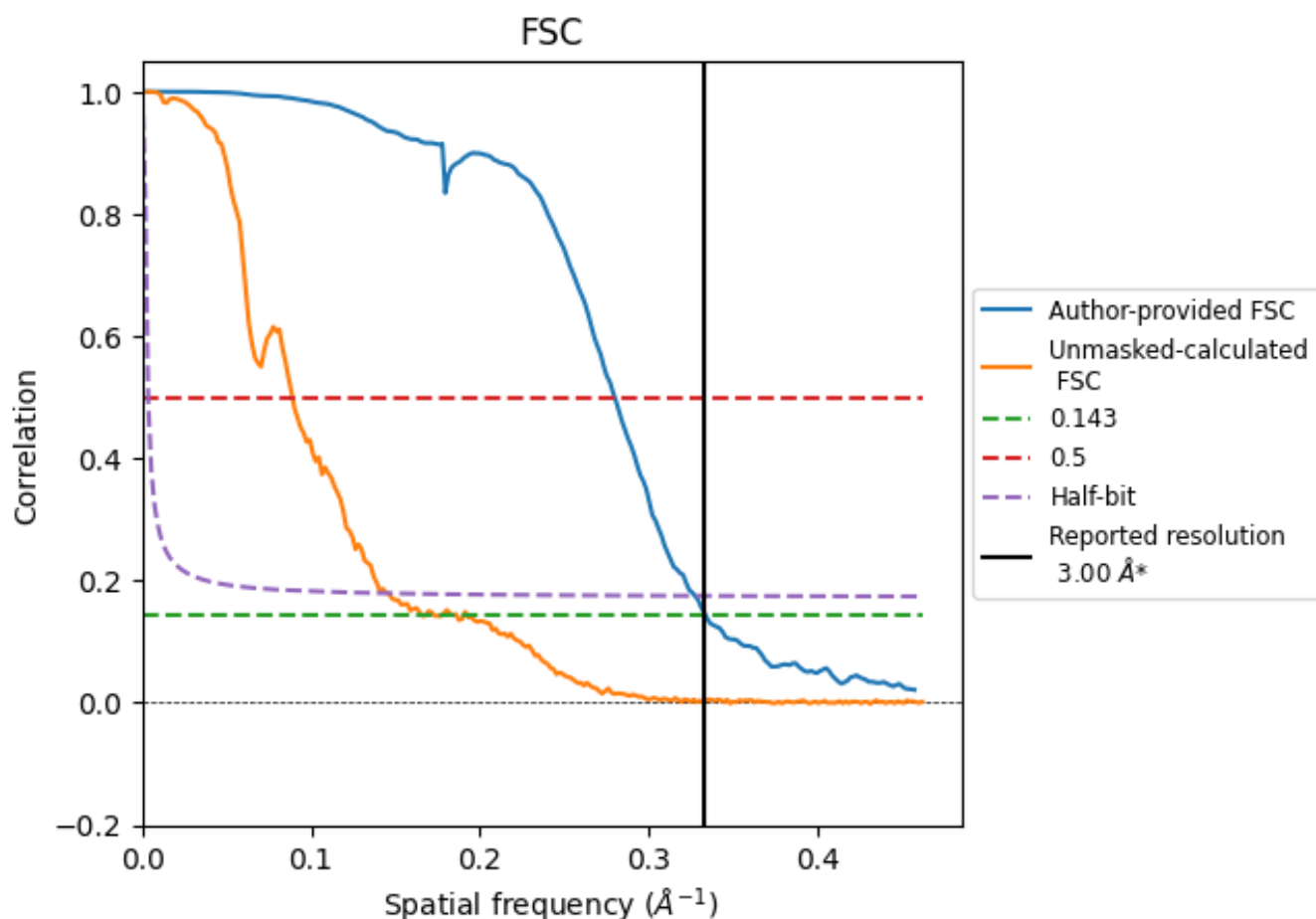


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

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 Å⁻¹

8.2 Resolution estimates [i](#)

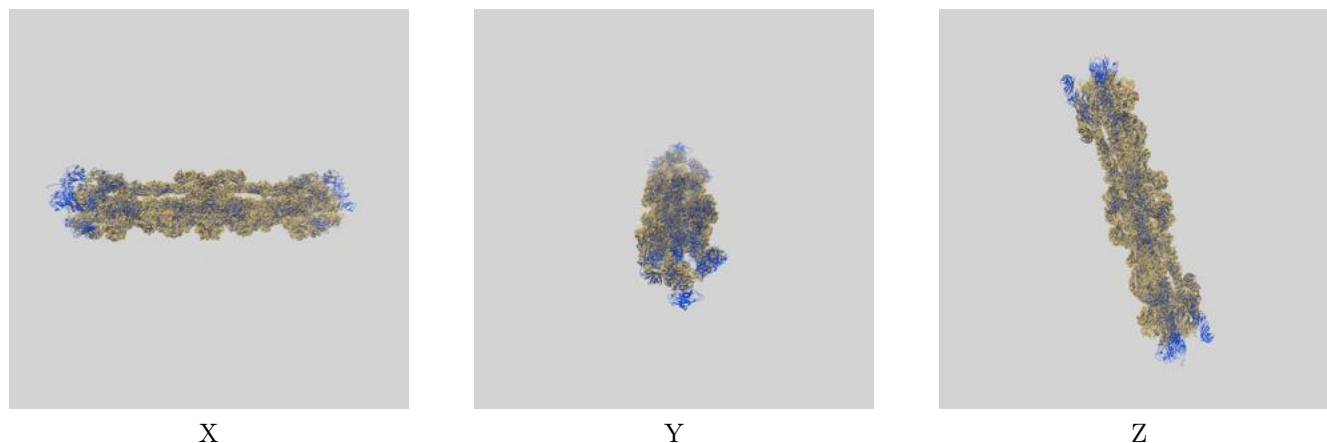
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.00	3.57	3.06
Unmasked-calculated*	6.04	11.24	6.84

*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](#)

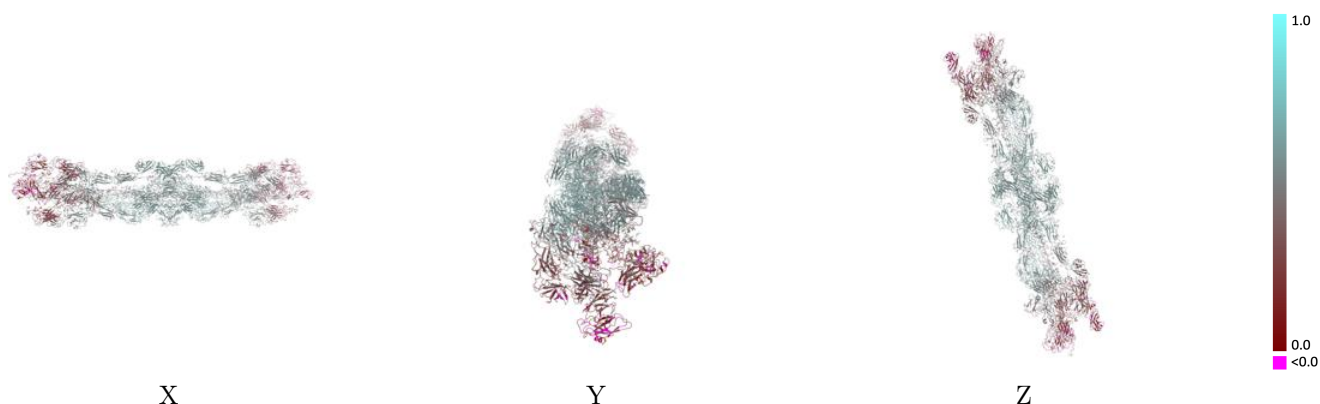
This section contains information regarding the fit between EMDB map EMD-37389 and PDB model 8WA2. Per-residue inclusion information can be found in section [3](#) on page [53](#).

9.1 Map-model overlay [i](#)



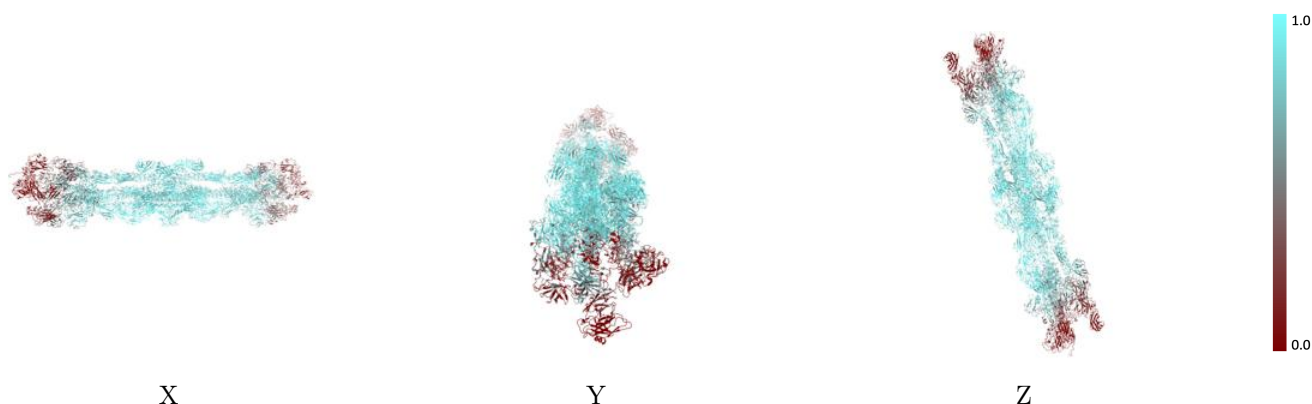
The images above show the 3D surface view of the map at the recommended contour level 0.23 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



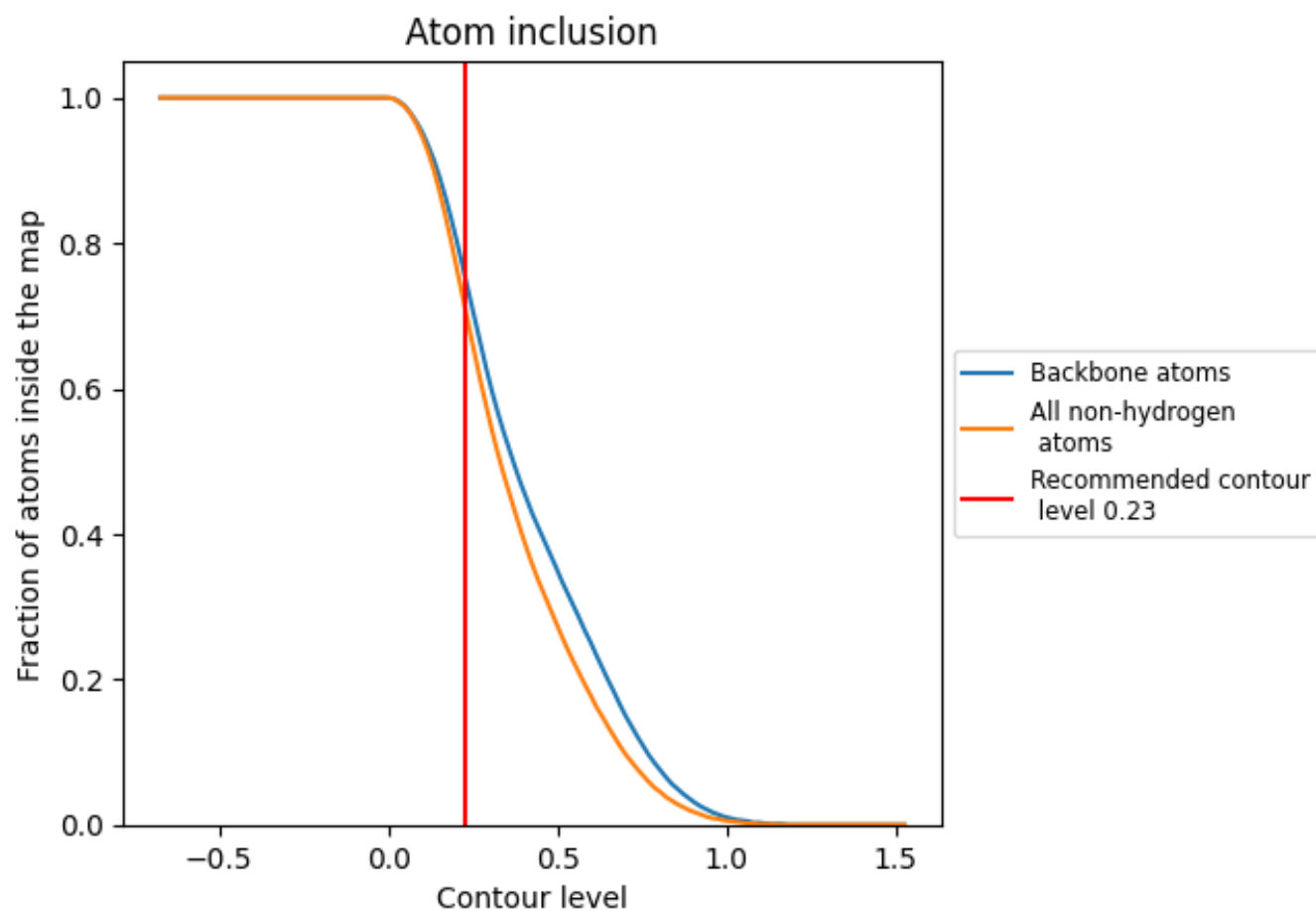
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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