



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 03:01 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 Full wwPDB EM Validation 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:

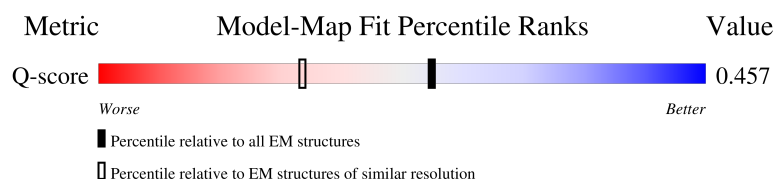
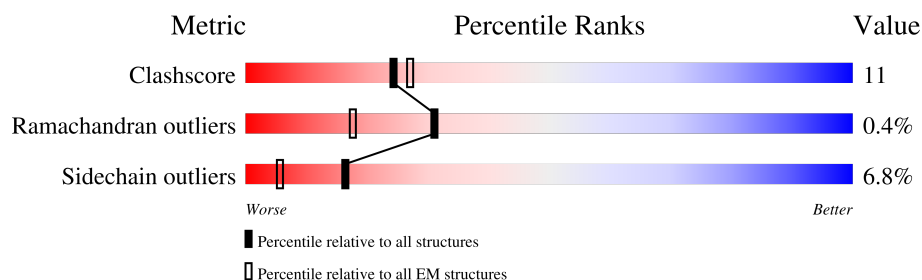
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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	

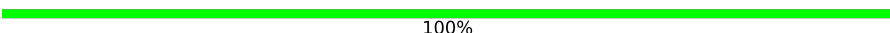
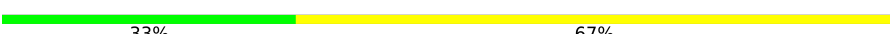
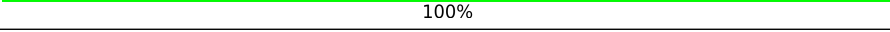
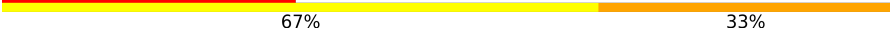
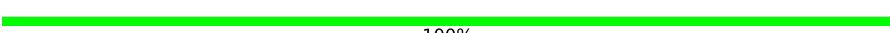
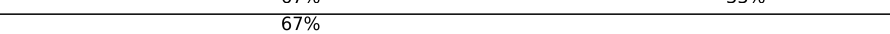
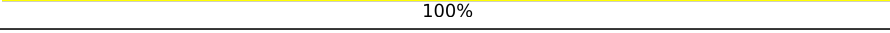
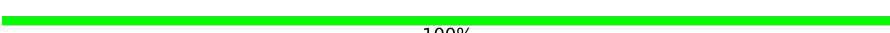
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Mol	Chain	Length	Quality of chain
1	E	1987	
1	F	1987	
2	G	64	
2	H	64	
2	I	64	
3	0	3	
3	0A	3	
3	1	3	
3	2	3	
3	8C	3	
3	9C	3	
3	BC	3	
3	CC	3	
3	DD	3	
3	EB	3	
3	ED	3	
3	FD	3	
3	GC	3	
3	HA	3	
3	HC	3	
3	IA	3	
3	IC	3	
3	ID	3	
3	J	3	
3	K	3	

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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	

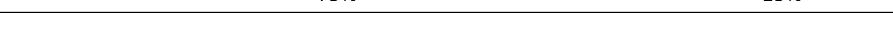
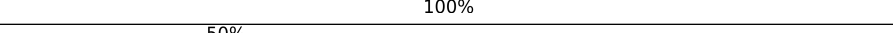
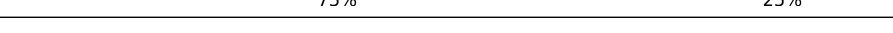
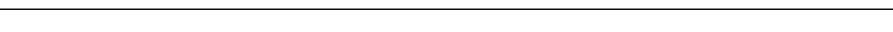
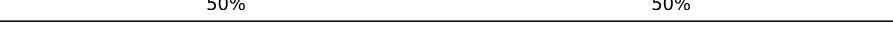
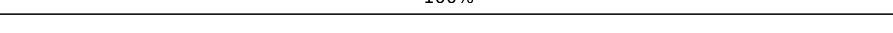
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Mol	Chain	Length	Quality of chain
3	qD	3	67% 100%
3	rA	3	67% 33%
3	rB	3	67% 33%
3	rC	3	100% 67% 33%
3	rD	3	67% 33%
3	sB	3	33% 33% 67%
3	sC	3	100% 67% 33%
3	t	3	67% 33%
3	tB	3	33% 100%
3	tC	3	33% 100%
3	uA	3	67% 33%
3	uB	3	100%
3	uC	3	67% 33%
3	vA	3	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%
4	cC	4	50%
4	d	4	50%
4	eA	4	100%
4	g	4	75%
4	gD	4	25%
4	iA	4	100%
4	jC	4	50%
4	k	4	100%
4	kD	4	25%
4	mB	4	75%
4	nC	4	25%
4	pA	4	50%
4	qB	4	75%
4	r	4	75%
4	tA	4	50%
4	v	4	75%
5	BD	5	60%
5	EC	5	20%
5	KA	5	40%
5	M	5	80%
6	0B	3	33%
6	0C	3	100%
6	1C	3	67%

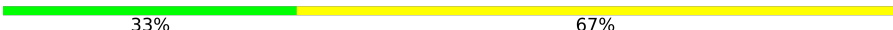
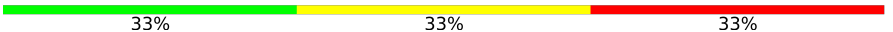
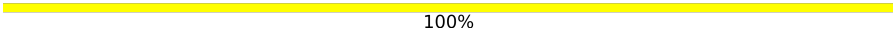
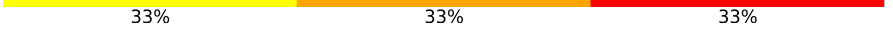
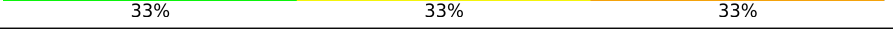
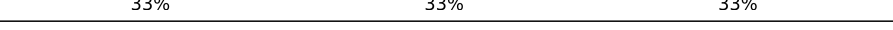
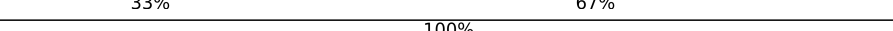
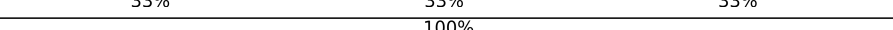
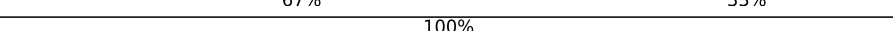
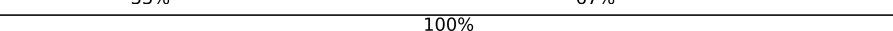
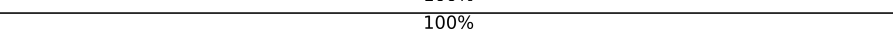
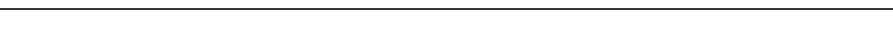
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Mol	Chain	Length	Quality of chain
6	2C	3	
6	3A	3	
6	3B	3	
6	3D	3	
6	4B	3	
6	5	3	
6	5B	3	
6	6A	3	
6	6C	3	
6	6D	3	
6	7A	3	
6	7D	3	
6	8	3	
6	8A	3	
6	8D	3	
6	9	3	
6	9B	3	
6	AA	3	
6	CB	3	
6	CD	3	
6	EA	3	
6	FC	3	
6	GD	3	
6	JC	3	
6	LA	3	

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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	

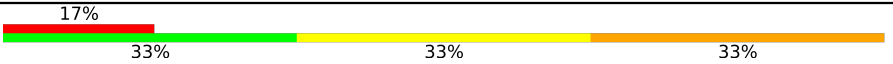
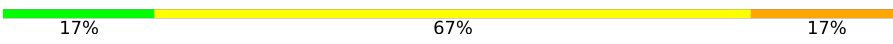
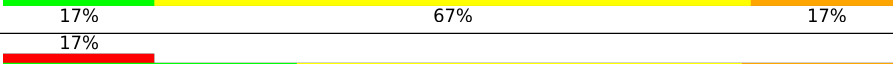
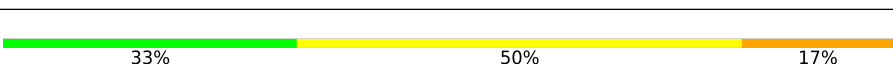
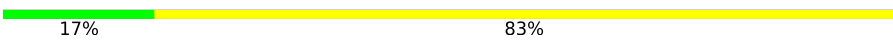
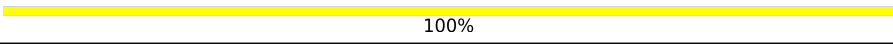
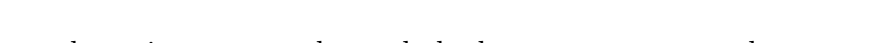
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Mol	Chain	Length	Quality of chain
18	tE	5	
18	yE	5	
18	zE	5	
19	1E	4	
19	AE	4	
19	LE	4	
19	NE	4	
19	aE	4	
19	qE	4	
20	CE	4	
20	EE	4	
20	HE	4	
20	TE	4	
20	UE	4	
20	WE	4	
20	gE	4	
20	hE	4	
20	jE	4	
20	sE	4	
20	uE	4	
20	xE	4	
21	FE	5	
21	kE	5	
21	vE	5	
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 27	C 15	O 12	0	0
3	O	3	Total 27	C 15	O 12	0	0
3	P	3	Total 27	C 15	O 12	0	0
3	Q	3	Total 27	C 15	O 12	0	0
3	T	3	Total 27	C 15	O 12	0	0
3	V	3	Total 27	C 15	O 12	0	0
3	b	3	Total 27	C 15	O 12	0	0
3	e	3	Total 27	C 15	O 12	0	0
3	l	3	Total 27	C 15	O 12	0	0
3	m	3	Total 27	C 15	O 12	0	0
3	t	3	Total 27	C 15	O 12	0	0
3	w	3	Total 27	C 15	O 12	0	0
3	x	3	Total 27	C 15	O 12	0	0
3	y	3	Total 27	C 15	O 12	0	0
3	z	3	Total 27	C 15	O 12	0	0
3	0	3	Total 27	C 15	O 12	0	0
3	1	3	Total 27	C 15	O 12	0	0
3	2	3	Total 27	C 15	O 12	0	0
3	HA	3	Total 27	C 15	O 12	0	0
3	IA	3	Total 27	C 15	O 12	0	0
3	MA	3	Total 27	C 15	O 12	0	0

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

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

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

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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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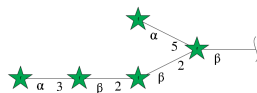
Mol	Chain	Residues	Atoms			AltConf	Trace
4	k	4	Total 36	C 20	O 16	0	0
4	r	4	Total 36	C 20	O 16	0	0
4	v	4	Total 36	C 20	O 16	0	0
4	JA	4	Total 36	C 20	O 16	0	0
4	UA	4	Total 36	C 20	O 16	0	0
4	VA	4	Total 36	C 20	O 16	0	0
4	aA	4	Total 36	C 20	O 16	0	0
4	bA	4	Total 36	C 20	O 16	0	0
4	eA	4	Total 36	C 20	O 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.



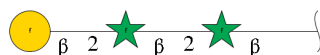
Mol	Chain	Residues	Atoms			AltConf	Trace
5	M	5	Total	C	O	0	0
			45	25	20		
5	KA	5	Total	C	O	0	0
			45	25	20		

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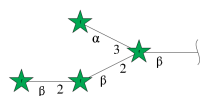
Mol	Chain	Residues	Atoms			AltConf	Trace
6	aB	3	Total	C	O	0	0
			29	16	13		
6	bB	3	Total	C	O	0	0
			29	16	13		
6	cB	3	Total	C	O	0	0
			29	16	13		
6	gB	3	Total	C	O	0	0
			29	16	13		
6	0B	3	Total	C	O	0	0
			29	16	13		
6	3B	3	Total	C	O	0	0
			29	16	13		
6	4B	3	Total	C	O	0	0
			29	16	13		
6	5B	3	Total	C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



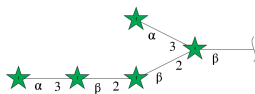
Mol	Chain	Residues	Atoms			AltConf	Trace
9	Y	2	Total	C	O	0	0
			18	10	8		

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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.



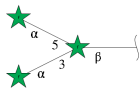
Mol	Chain	Residues	Atoms			AltConf	Trace
10	a	5	Total	C	O	0	0
			45	25	20		
10	u	5	Total	C	O	0	0
			45	25	20		
10	3	5	Total	C	O	0	0
			45	25	20		
10	YA	5	Total	C	O	0	0
			45	25	20		
10	sA	5	Total	C	O	0	0
			45	25	20		
10	1A	5	Total	C	O	0	0
			45	25	20		
10	MB	5	Total	C	O	0	0
			45	25	20		
10	VB	5	Total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

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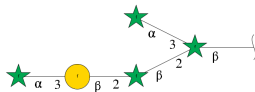
Mol	Chain	Residues	Atoms			AltConf	Trace
10	yB	5	Total	C	O	0	0
			45	25	20		
10	SC	5	Total	C	O	0	0
			45	25	20		
10	mC	5	Total	C	O	0	0
			45	25	20		
10	vC	5	Total	C	O	0	0
			45	25	20		
10	PD	5	Total	C	O	0	0
			45	25	20		
10	jD	5	Total	C	O	0	0
			45	25	20		
10	sD	5	Total	C	O	0	0
			45	25	20		

- 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	C	O	0	0
			38	21	17		
13	2A	4	Total	C	O	0	0
			38	21	17		
13	4A	4	Total	C	O	0	0
			38	21	17		
13	5A	4	Total	C	O	0	0
			38	21	17		
13	9A	4	Total	C	O	0	0
			38	21	17		
13	GB	4	Total	C	O	0	0
			38	21	17		
13	WB	4	Total	C	O	0	0
			38	21	17		
13	YB	4	Total	C	O	0	0
			38	21	17		
13	ZB	4	Total	C	O	0	0
			38	21	17		
13	dB	4	Total	C	O	0	0
			38	21	17		
13	jB	4	Total	C	O	0	0
			38	21	17		
13	zB	4	Total	C	O	0	0
			38	21	17		
13	1B	4	Total	C	O	0	0
			38	21	17		
13	2B	4	Total	C	O	0	0
			38	21	17		
13	6B	4	Total	C	O	0	0
			38	21	17		
13	gC	4	Total	C	O	0	0
			38	21	17		
13	wC	4	Total	C	O	0	0
			38	21	17		
13	yC	4	Total	C	O	0	0
			38	21	17		
13	zC	4	Total	C	O	0	0
			38	21	17		
13	3C	4	Total	C	O	0	0
			38	21	17		
13	dD	4	Total	C	O	0	0
			38	21	17		

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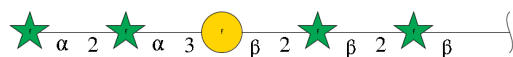
Mol	Chain	Residues	Atoms			AltConf	Trace
13	tD	4	Total	C	O	0	0
			38	21	17		
13	vD	4	Total	C	O	0	0
			38	21	17		
13	wD	4	Total	C	O	0	0
			38	21	17		
13	0D	4	Total	C	O	0	0
			38	21	17		

- 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.



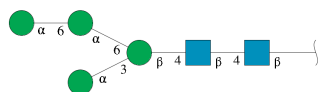
Mol	Chain	Residues	Atoms				AltConf	Trace
16	FA	2	Total	C	N	O	0	0
			28	16	2	10		

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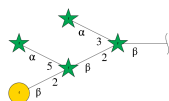
Mol	Chain	Residues	Atoms				AltConf	Trace
16	AC	2	Total	C	N	O	0	0
			28	16	2	10		
16	4D	2	Total	C	N	O	0	0
			28	16	2	10		

- 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.



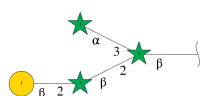
Mol	Chain	Residues	Atoms			AltConf	Trace
18	9D	5	Total	C	O	0	0
			47	26	21		
18	BE	5	Total	C	O	0	0
			47	26	21		
18	DE	5	Total	C	O	0	0
			47	26	21		
18	IE	5	Total	C	O	0	0
			47	26	21		
18	JE	5	Total	C	O	0	0
			47	26	21		

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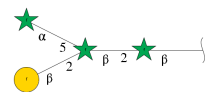
Mol	Chain	Residues	Atoms			AltConf	Trace
18	KE	5	Total	C	O	0	0
			47	26	21		
18	PE	5	Total	C	O	0	0
			47	26	21		
18	SE	5	Total	C	O	0	0
			47	26	21		
18	cE	5	Total	C	O	0	0
			47	26	21		
18	fE	5	Total	C	O	0	0
			47	26	21		
18	pE	5	Total	C	O	0	0
			47	26	21		
18	rE	5	Total	C	O	0	0
			47	26	21		
18	tE	5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



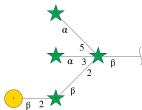
Mol	Chain	Residues	Atoms			AltConf	Trace
19	AE	4	Total	C	O	0	0
			38	21	17		
19	LE	4	Total	C	O	0	0
			38	21	17		
19	NE	4	Total	C	O	0	0
			38	21	17		
19	aE	4	Total	C	O	0	0
			38	21	17		
19	qE	4	Total	C	O	0	0
			38	21	17		
19	1E	4	Total	C	O	0	0
			38	21	17		

- 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.



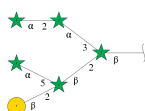
Mol	Chain	Residues	Atoms			AltConf	Trace
21	FE	5	Total	C	O	0	0
			47	26	21		

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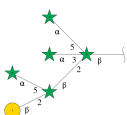
Mol	Chain	Residues	Atoms			AltConf	Trace
21	kE	5	Total	C	O	0	0
			47	26	21		
21	vE	5	Total	C	O	0	0
			47	26	21		

- 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.



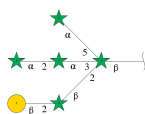
Mol	Chain	Residues	Atoms			AltConf	Trace
22	GE	6	Total	C	O	0	0
			56	31	25		
22	QE	6	Total	C	O	0	0
			56	31	25		
22	RE	6	Total	C	O	0	0
			56	31	25		
22	VE	6	Total	C	O	0	0
			56	31	25		
22	dE	6	Total	C	O	0	0
			56	31	25		
22	eE	6	Total	C	O	0	0
			56	31	25		
22	iE	6	Total	C	O	0	0
			56	31	25		
22	wE	6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

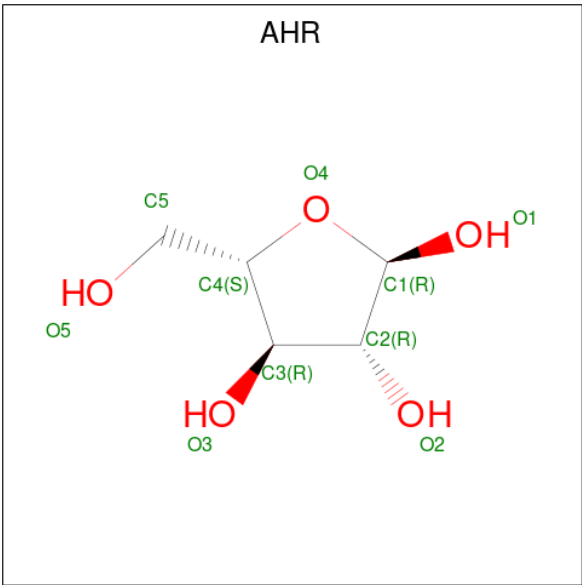


Mol	Chain	Residues	Atoms			AltConf	Trace
24	YE	6	Total	C	O	0	0
			56	31	25		
24	IE	6	Total	C	O	0	0
			56	31	25		

- 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).



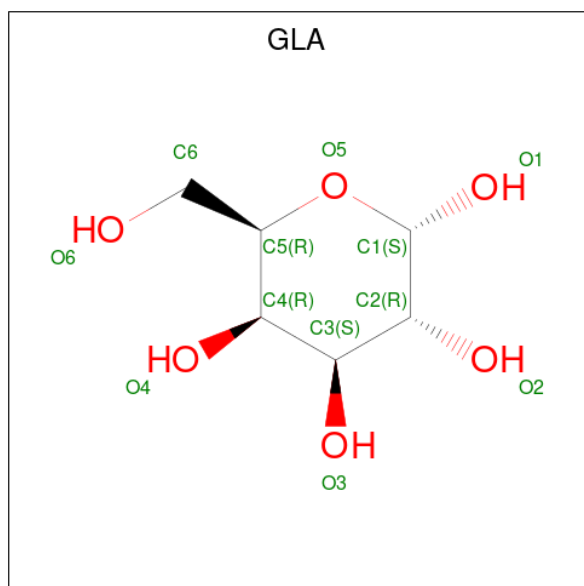
Mol	Chain	Residues	Atoms			AltConf
26	A	1	Total	C	O	0
			9	5	4	
26	A	1	Total	C	O	0
			9	5	4	
26	A	1	Total	C	O	0
			9	5	4	
26	A	1	Total	C	O	0
			9	5	4	
26	B	1	Total	C	O	0
			9	5	4	
26	B	1	Total	C	O	0
			9	5	4	
26	B	1	Total	C	O	0
			9	5	4	
26	B	1	Total	C	O	0
			9	5	4	
26	C	1	Total	C	O	0
			9	5	4	
26	C	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
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	
27	A	1	Total	C	O	0
			11	6	5	
27	B	1	Total	C	O	0
			11	6	5	
27	B	1	Total	C	O	0
			11	6	5	
27	B	1	Total	C	O	0
			11	6	5	
27	B	1	Total	C	O	0
			11	6	5	
27	B	1	Total	C	O	0
			11	6	5	
27	B	1	Total	C	O	0
			11	6	5	
27	B	1	Total	C	O	0
			11	6	5	
27	B	1	Total	C	O	0
			11	6	5	
27	B	1	Total	C	O	0
			11	6	5	
27	B	1	Total	C	O	0
			11	6	5	
27	B	1	Total	C	O	0
			11	6	5	

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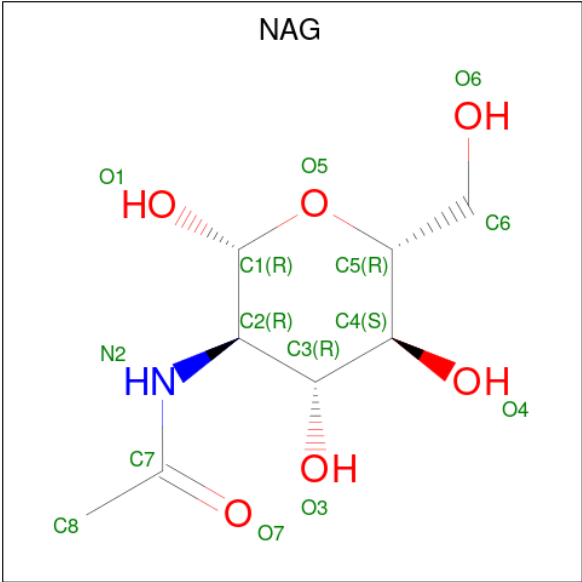
Mol	Chain	Residues	Atoms			AltConf
27	C	1	Total	C	O	0
			11	6	5	
27	C	1	Total	C	O	0
			11	6	5	
27	C	1	Total	C	O	0
			11	6	5	
27	C	1	Total	C	O	0
			11	6	5	
27	C	1	Total	C	O	0
			11	6	5	
27	D	1	Total	C	O	0
			11	6	5	
27	D	1	Total	C	O	0
			11	6	5	
27	D	1	Total	C	O	0
			11	6	5	
27	D	1	Total	C	O	0
			11	6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

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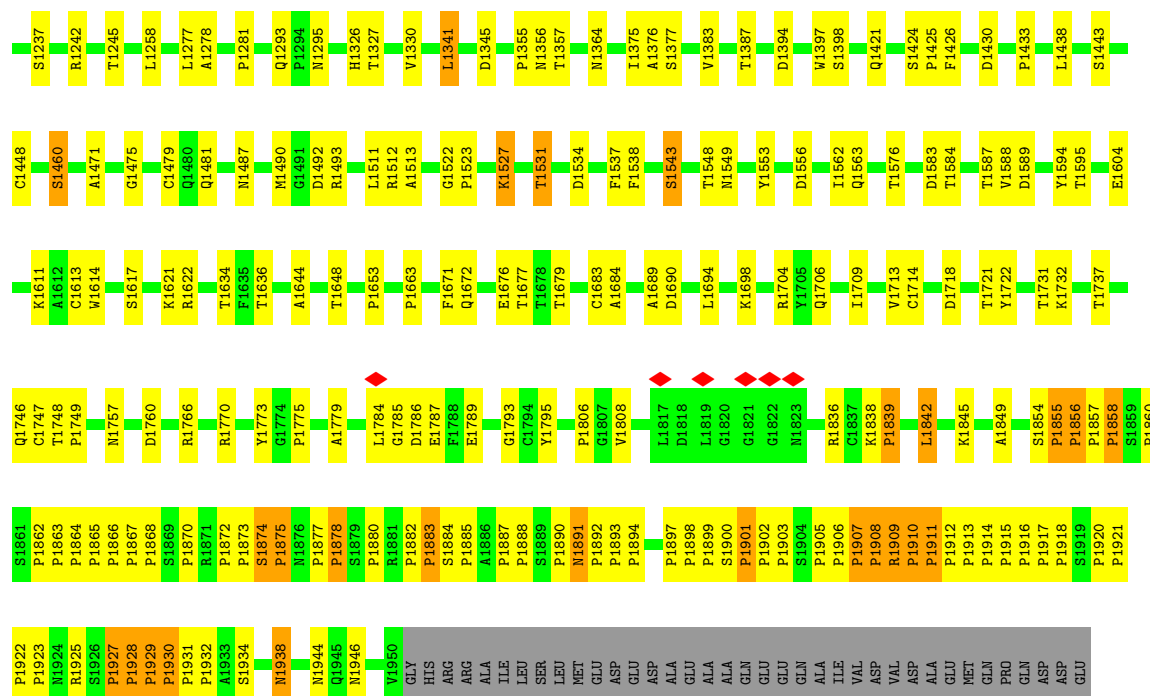
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Mol	Chain	Residues	Atoms			AltConf
27	E	1	Total	C	O	0
			11	6	5	
27	E	1	Total	C	O	0
			11	6	5	
27	F	1	Total	C	O	0
			11	6	5	
27	F	1	Total	C	O	0
			11	6	5	
27	F	1	Total	C	O	0
			11	6	5	
27	F	1	Total	C	O	0
			11	6	5	
27	F	1	Total	C	O	0
			11	6	5	
27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

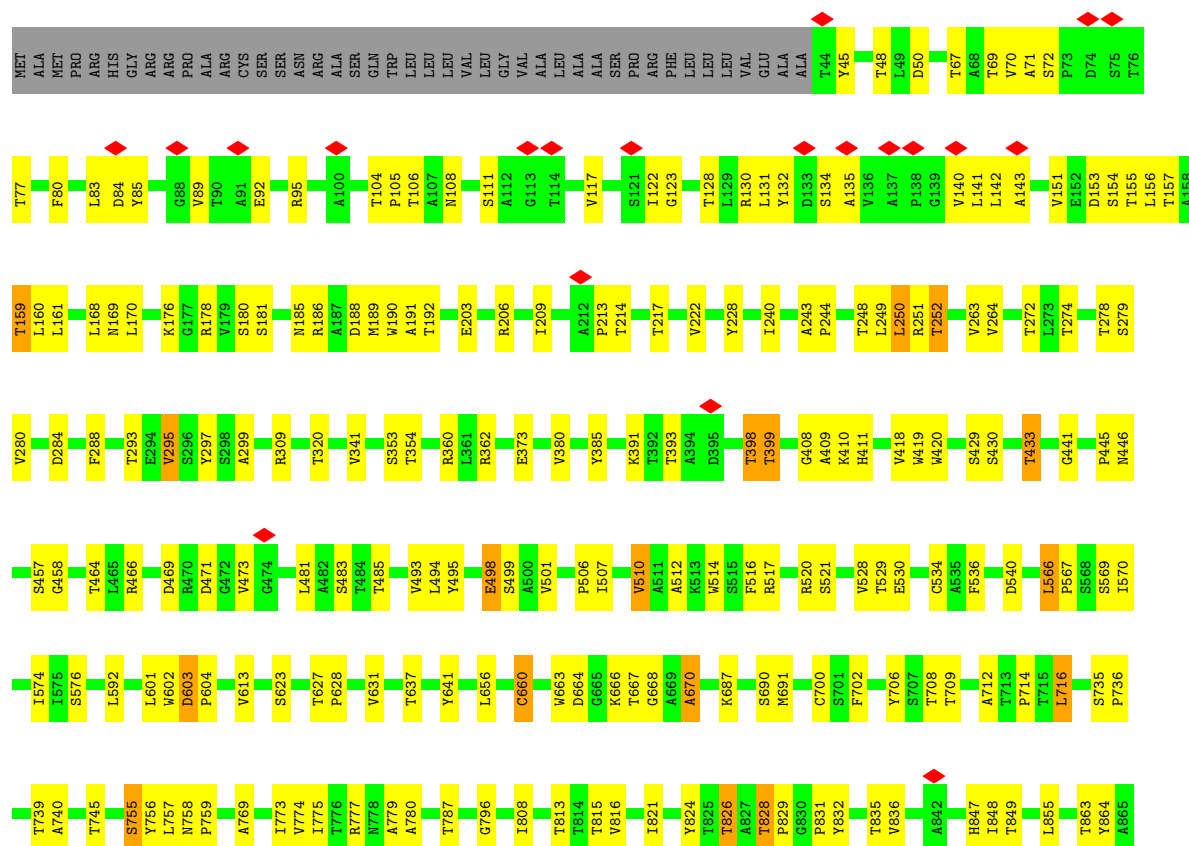


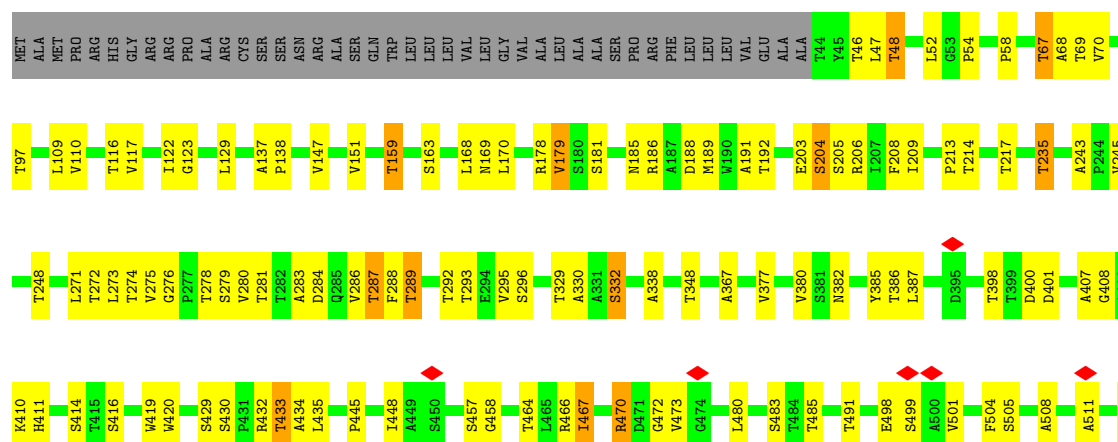
Mol	Chain	Residues	Atoms				AltConf
28	A	1	Total	C	N	O	0
			14	8	1	5	
28	B	1	Total	C	N	O	0
			14	8	1	5	
28	B	1	Total	C	N	O	0
			14	8	1	5	
28	C	1	Total	C	N	O	0
			14	8	1	5	
28	C	1	Total	C	N	O	0
			14	8	1	5	
28	D	1	Total	C	N	O	0
			14	8	1	5	
28	E	1	Total	C	N	O	0
			14	8	1	5	



• Molecule 1: Mst1

Chain B: 69% 24%









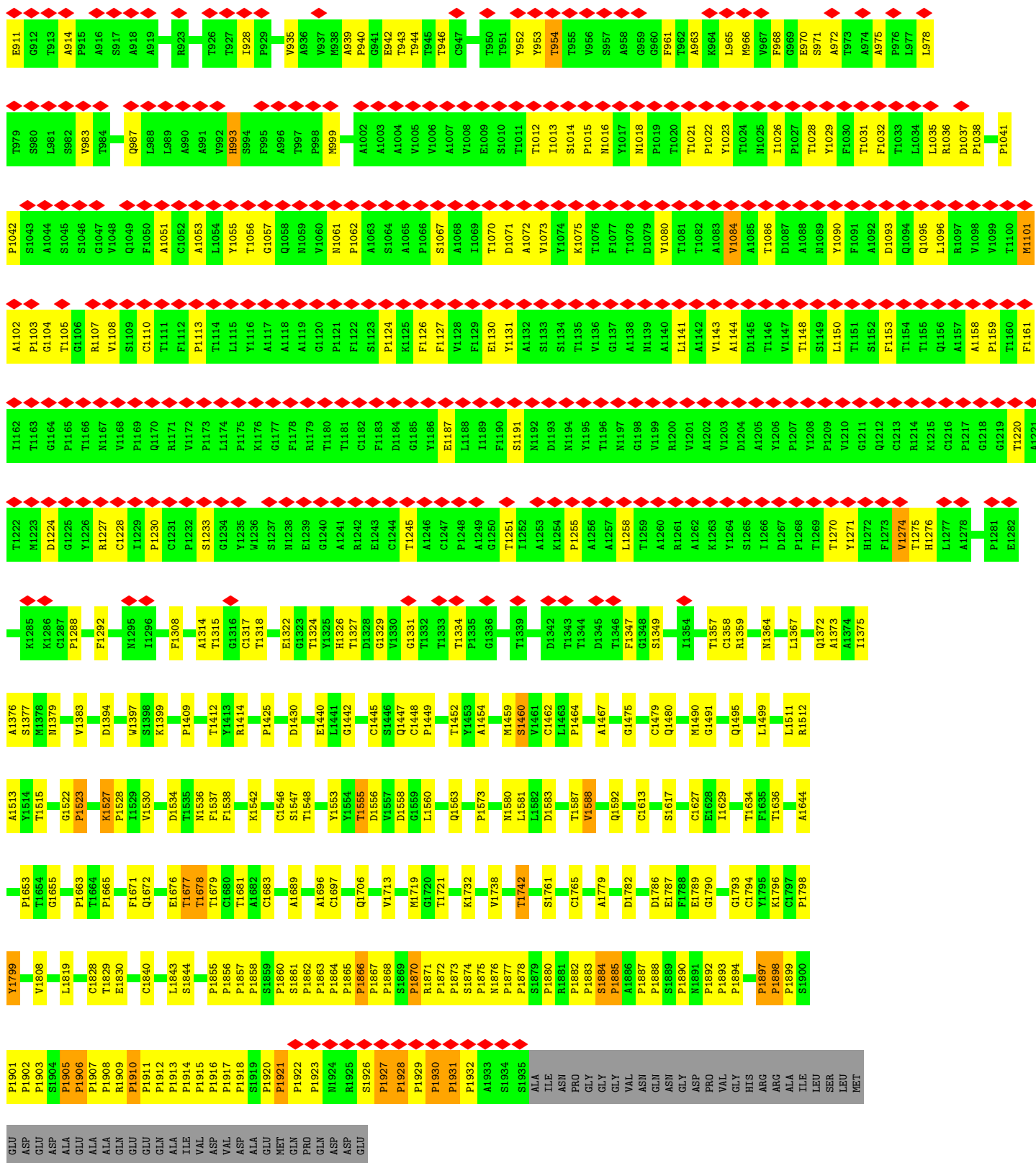






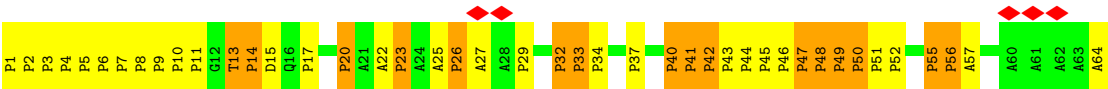
Chain F:



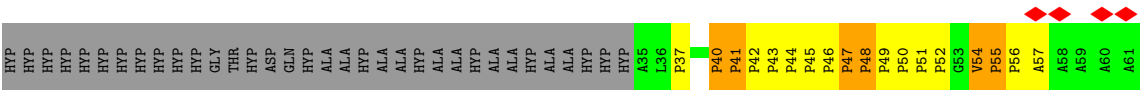
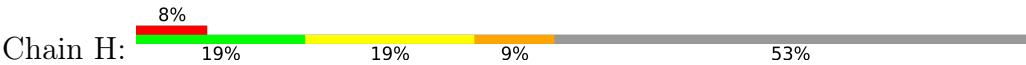


● Molecule 2: Mstax

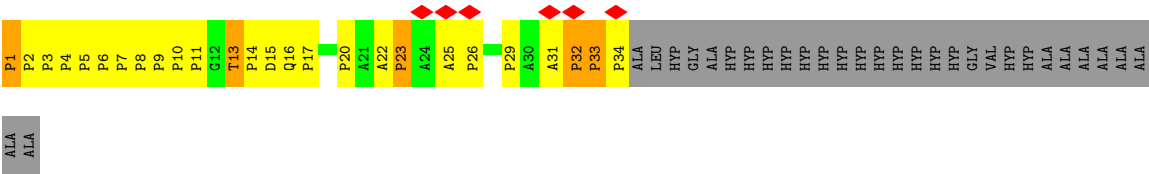




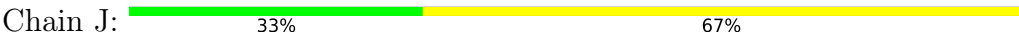
• Molecule 2: Mstax



• 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%



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

Chain t:  67% 33%



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

Chain w:  67% 33%



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

Chain x:  67% 33%



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

Chain y:  67% 33%



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

Chain z:  33% 33% 33%



- 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%

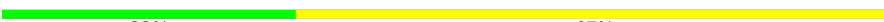


- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

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%



- 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 uA:  67%  33%



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

Chain vA:  67%  33%



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

Chain wA:  67%  33%



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

Chain xA:  33%  67%



- 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



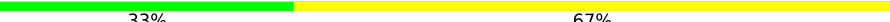
- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranos e



- 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-arabinofuranos e

Chain xB:  67% 33%

FUB1
FUB2
FUB3

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

Chain BC:  67% 33%

FUB1
FUB2
FUB3

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

Chain CC:  33% 67%

FUB1
FUB2
FUB3

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

Chain GC:  67% 33%

FUB1
FUB2
FUB3

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

Chain HC:  67% 33%

FUB1
FUB2
FUB3

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

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%



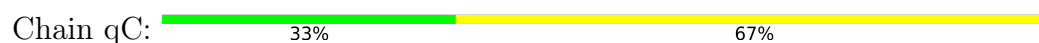
- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



- 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%

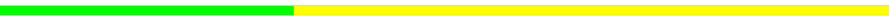


- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

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

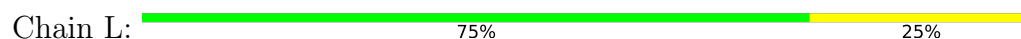




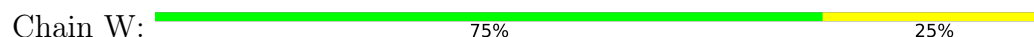
- Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



- 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



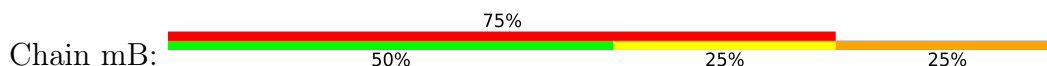
- Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



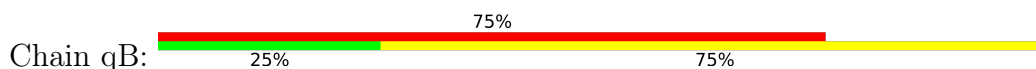
- Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



- 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 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%

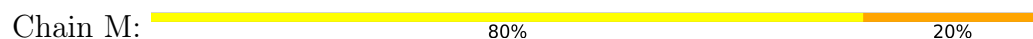


- Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

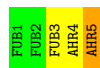
Chain kD:  25% 75% 25%



- 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



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



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



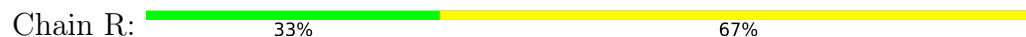
- Molecule 5: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose



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



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

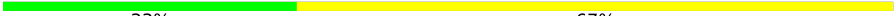


- Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

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%

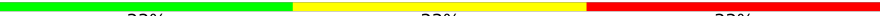


- Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

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



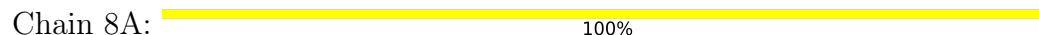
- Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



- 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

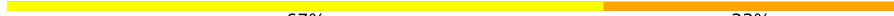


- Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

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%

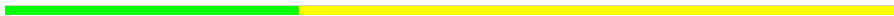


- Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

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

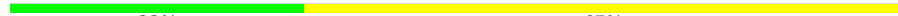


- Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 8D:  67% 33%



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

Chain ME:  33% 67%



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

Chain OE:  100%



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

Chain ZE:  33% 67%



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

Chain bE:  33% 33% 33%



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

Chain mE:  67% 33%



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

Chain nE:  33% 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



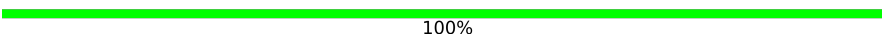
- Molecule 7: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose



- 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%

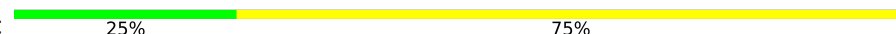


- Molecule 7: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

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%

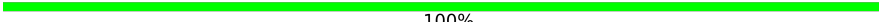


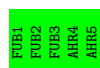
- Molecule 8: alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

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

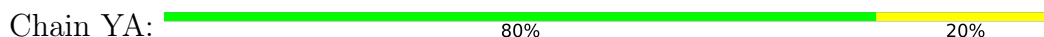
Chain u:  60% 40%



- 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



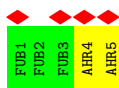
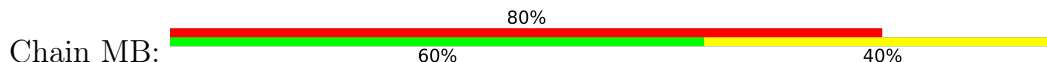
- Molecule 10: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose



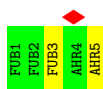
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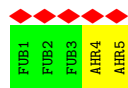
- Molecule 10: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose



- 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



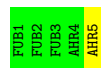
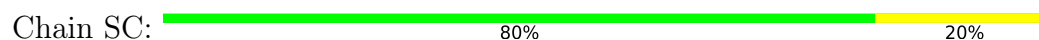
- Molecule 10: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose



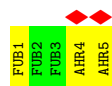
- Molecule 10: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose



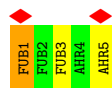
- Molecule 10: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose



- 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



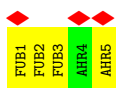
- Molecule 10: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose



- 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



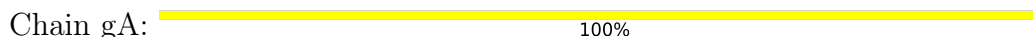
- Molecule 10: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose



- 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



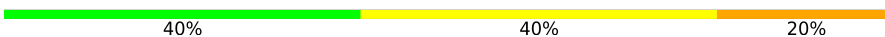
- Molecule 11: alpha-L-arabinofuranose-(1-3)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose



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

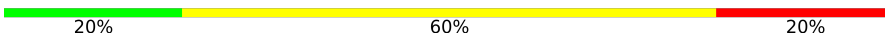


- Molecule 12: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

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: 



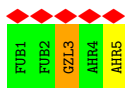
- Molecule 12: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain oA: 

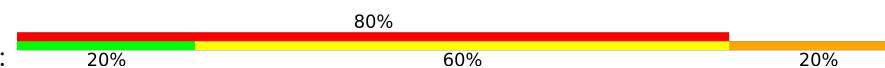


- Molecule 12: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain FB: 



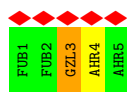
- Molecule 12: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain IB: 

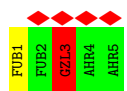
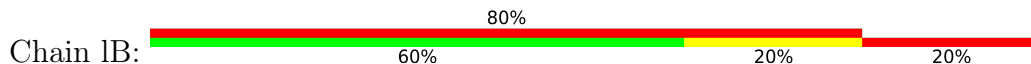


- Molecule 12: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

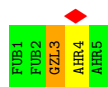
Chain iB: 



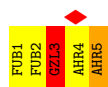
- Molecule 12: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose



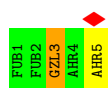
- Molecule 12: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose



- 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



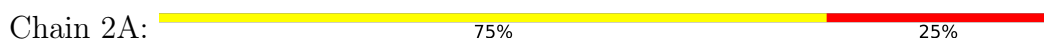
- Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



- 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: 



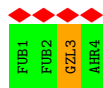
- Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 9A: 

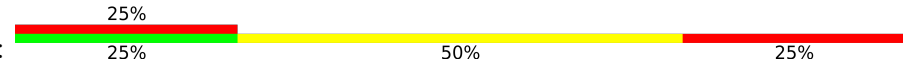


- Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

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%

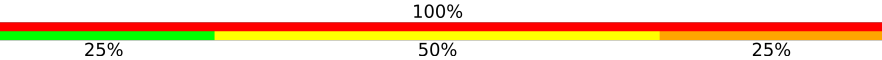


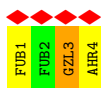
- Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

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:  100% 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

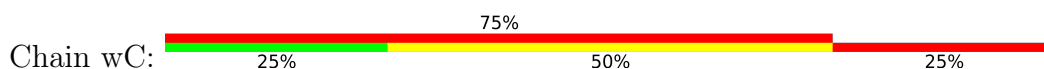
Chain 6B:  50% 50%



- 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



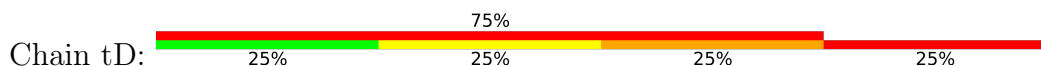
- Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



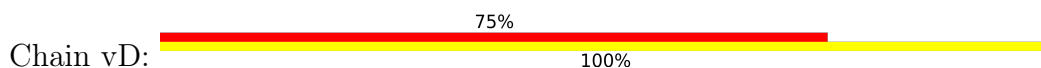
- Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



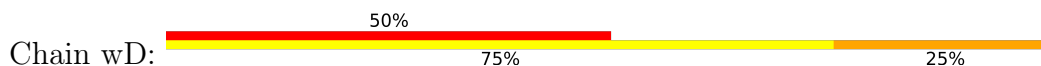
- Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



- 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

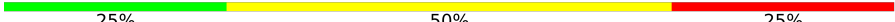


- Molecule 14: beta-L-arabinofuranose-(1-5)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain s:  75% 25%

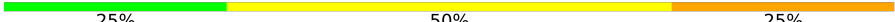


- Molecule 14: beta-L-arabinofuranose-(1-5)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain nA:  25% 50% 25%

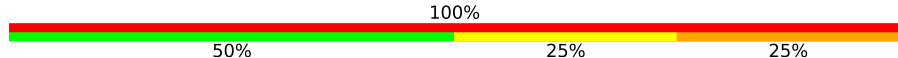


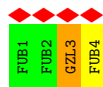
- Molecule 14: beta-L-arabinofuranose-(1-5)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain qA:  25% 50% 25%

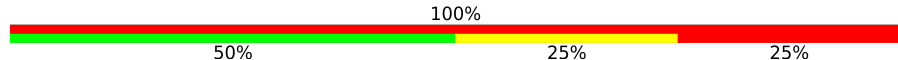


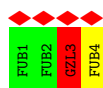
- Molecule 14: beta-L-arabinofuranose-(1-5)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain HB:  100% 50% 25% 25%

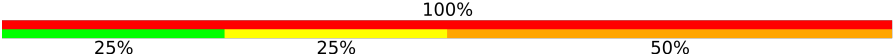


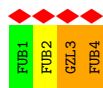
- Molecule 14: beta-L-arabinofuranose-(1-5)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain KB:  100% 50% 25% 25%

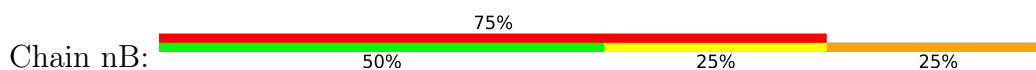


- Molecule 14: beta-L-arabinofuranose-(1-5)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain kB:  100% 25% 25% 50%



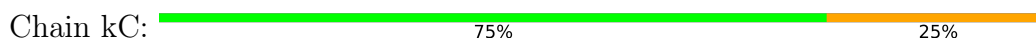
- Molecule 14: beta-L-arabinofuranose-(1-5)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



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



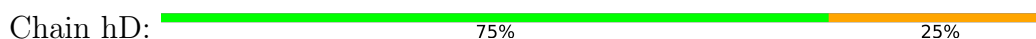
- Molecule 14: beta-L-arabinofuranose-(1-5)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



- 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



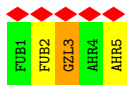
- Molecule 15: alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



- 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



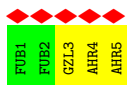
- Molecule 15: alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



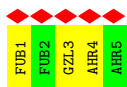
- Molecule 15: alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



- 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



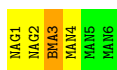
- Molecule 17: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- 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

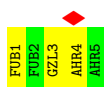
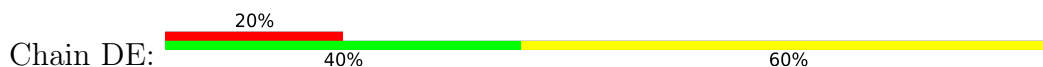




- Molecule 18: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose



- 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: 

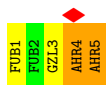
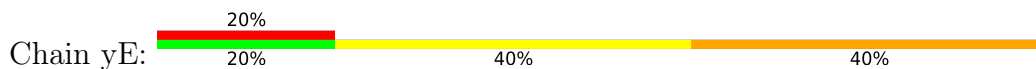


- Molecule 18: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

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



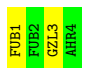
- Molecule 18: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose



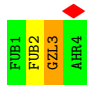
- Molecule 18: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose



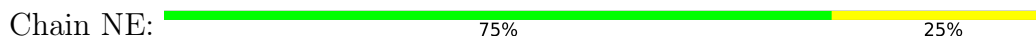
- Molecule 19: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose



- 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



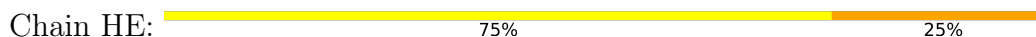
- Molecule 20: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



- 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





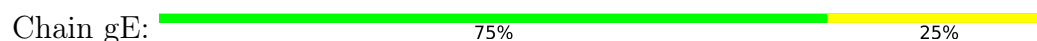
- Molecule 20: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



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



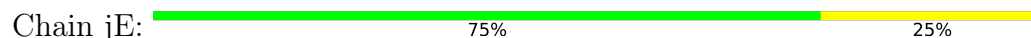
- Molecule 20: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose



- 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%

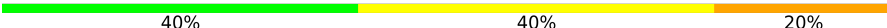


- Molecule 20: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

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%

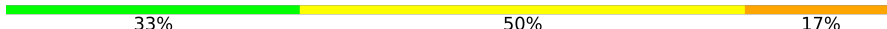


- Molecule 21: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)][alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose

Chain vE:  40% 60%

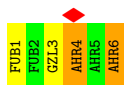


- Molecule 22: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

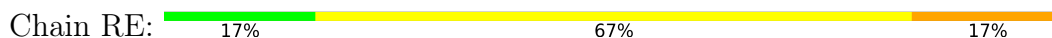
Chain GE:  33% 50% 17%



- 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



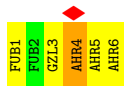
- Molecule 22: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose



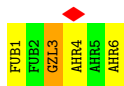
- Molecule 22: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose



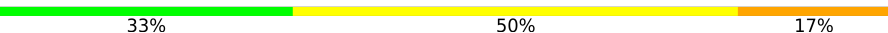
- Molecule 22: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose



- 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

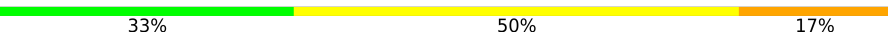


- Molecule 22: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

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%

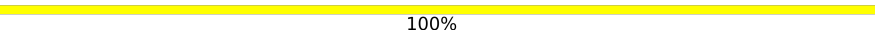


- Molecule 24: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)][alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose

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

All (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
1	B	1846	PRO	N-CD-CG	-6.07	94.10	103.20
1	D	534	CYS	CA-CB-SG	6.00	128.20	114.40
1	D	915	PRO	CA-N-CD	-5.98	103.63	112.00
1	F	632	PRO	CA-N-CD	-5.94	103.69	112.00
1	A	1842	LEU	CA-CB-CG	5.62	135.98	116.30

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

All (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
1	F	1527	LYS	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	13862	0	13346	281	0
1	B	13862	0	13347	275	0
1	C	10840	0	10542	223	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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.

All (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
26:C:2003:AHR:C1	13:WB:3:GZL:O5	1.69	1.38
26:E:2002:AHR:C1	13:wC:3:GZL:O5	1.70	1.38
26:F:2001:AHR:C1	6:XB:3:GZL:O5	1.72	1.38
26:E:2003:AHR:C1	6:xC:3:GZL:O5	1.72	1.38
26:D:2001:AHR:C1	6:N:3:GZL:O5	1.72	1.36
26:D:2004:AHR:C1	6:0B:3:GZL:O5	1.72	1.36
26:F:2005:AHR:C1	6:uD:3:GZL:O5	1.72	1.36
26:F:2003:AHR:C1	6:CD:3:GZL:O5	1.74	1.36
26:A:2002:AHR:C1	13:4:3:GZL:O5	1.72	1.35
26:C:2001:AHR:C1	6:LA:3:GZL:O5	1.74	1.35
26:F:2004:AHR:C1	13:tD:3:GZL:O5	1.73	1.34
26:F:2001:AHR:C1	6:XB:3:GZL:H5	1.60	1.08
1:D:534:CYS:HB2	1:D:594:CYS:HA	1.36	1.06
26:D:2004:AHR:C1	6:0B:3:GZL:H5	1.59	1.02
26:E:2003:AHR:C1	6:xC:3:GZL:H5	1.60	1.00
26:C:2001:AHR:C1	6:LA:3:GZL:H5	1.75	0.99
26:A:2002:AHR:C1	13:4:3:GZL:H5	1.64	0.98
26:A:2002:AHR:C1	13:4:3:GZL:H41	2.03	0.89
1:D:1047:GLY:HA3	1:D:1101:MET:O	1.71	0.89
1:A:419:TRP:CZ3	1:A:471:ASP:HA	2.09	0.87
26:A:2003:AHR:C1	6:5:3:GZL:H5	1.86	0.86
1:D:808:ILE:HG13	1:D:815:THR:HB	1.58	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:667:THR:HG22	1:A:668:GLY:H	1.43	0.83
1:B:189:MET:HB3	1:B:240:ILE:HD11	1.59	0.83
1:B:45:TYR:HE2	1:B:142:LEU:HB2	1.45	0.82
26:F:2003:THR:HG22	6:CD:3:GZL:H5	1.92	0.81
1:B:278:THR:HG22	1:B:279:SER:H	1.44	0.81
26:F:2005:THR:HG22	6:uD:3:GZL:H5	1.95	0.80
1:D:534:CYS:CB	1:D:594:CYS:HA	2.10	0.80
1:F:501:VAL:HG12	1:F:503:PRO:HD2	1.64	0.79
26:C:2003:THR:HG22	13:WB:3:GZL:H5	1.93	0.79
1:A:872:PRO:HG2	1:A:882:VAL:HA	1.64	0.78
1:C:52:LEU:HD23	1:C:67:THR:HG22	1.66	0.78
26:E:2002:THR:HG22	13:wC:3:GZL:H5	1.95	0.77
26:B:2020:THR:HG22	6:FC:3:GZL:O2	2.01	0.77
1:D:497:LEU:HD21	1:D:516:PHE:HB3	1.65	0.77
1:C:1292:PHE:HA	1:C:1314:ALA:HB1	1.66	0.77
26:B:2004:THR:HG22	6:3A:3:GZL:H5	1.96	0.76
1:B:1047:GLY:HA3	1:B:1101:MET:O	1.84	0.76
1:D:661:SER:HB3	1:D:680:LEU:HD12	1.66	0.76
26:F:2004:THR:HG22	13:tD:3:GZL:H5	1.97	0.76
1:A:84:ASP:HB2	1:A:92:GLU:HG2	1.68	0.76
1:A:898:GLY:HA2	1:A:940:PRO:HB3	1.67	0.75
1:F:939:ALA:HB3	1:F:942:GLU:HG2	1.69	0.75
1:B:898:GLY:HA2	1:B:940:PRO:HB3	1.66	0.75
1:F:850:LYS:HD2	1:F:899:ILE:HA	1.68	0.74
1:C:612:GLN:HB3	1:C:650:PRO:HG3	1.68	0.74
26:A:2003:THR:HG22	6:5:3:GZL:H21	2.17	0.74
1:F:1490:MET:HE3	1:F:1538:PHE:HB2	1.67	0.74
1:D:191:ALA:HB2	1:D:209:ILE:HD11	1.70	0.74
1:F:1779:ALA:HB1	1:F:1793:GLY:HA2	1.67	0.73
1:A:1779:ALA:HB1	1:A:1793:GLY:HA2	1.71	0.73
26:A:2003:THR:HG22	6:5:3:GZL:O3	2.05	0.73
1:E:1255:PRO:HB2	1:E:1276:HIS:HB3	1.68	0.73
1:F:667:THR:HG22	1:F:668:GLY:H	1.54	0.73
1:A:1672:GLN:NE2	1:A:1679:THR:O	2.22	0.73
1:E:872:PRO:HG2	1:E:882:VAL:HA	1.70	0.73
1:E:1779:ALA:HB1	1:E:1793:GLY:HA2	1.71	0.73
1:A:294:GLU:HB3	1:A:338:ALA:HB1	1.70	0.72
1:D:662:PHE:O	1:D:685:ASN:ND2	2.23	0.72
1:C:1200:ARG:NH2	1:F:1534:ASP:O	2.21	0.72
1:A:501:VAL:HG12	1:A:503:PRO:HD2	1.71	0.72
1:C:872:PRO:HG2	1:C:882:VAL:HA	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1946:ASN:O	1:E:1622:ARG:NH1	2.21	0.72
1:D:561:LEU:HD13	1:D:575:ILE:HG23	1.72	0.72
26:D:2003:AHR:C1	13:zB:3:GZL:H21	2.20	0.72
1:E:1706:GLN:NE2	1:E:1713:VAL:O	2.22	0.72
1:E:928:ILE:HG13	1:E:929:PRO:HD3	1.72	0.71
1:B:1471:ALA:HB2	1:B:1479:CYS:HB3	1.72	0.71
1:B:1779:ALA:HB1	1:B:1793:GLY:HA2	1.72	0.71
1:B:1672:GLN:NE2	1:B:1679:THR:O	2.23	0.71
14:nA:3:GZL:O6	14:nA:3:GZL:O4	2.05	0.71
1:F:525:PRO:HG2	1:F:528:VAL:HB	1.72	0.71
1:F:872:PRO:HG2	1:F:882:VAL:HA	1.73	0.71
1:C:501:VAL:HG23	1:C:504:PHE:HA	1.73	0.71
1:D:525:PRO:HG2	1:D:528:VAL:HB	1.71	0.71
1:E:1124:PRO:HG2	1:E:1150:LEU:HB2	1.71	0.71
1:D:185:ASN:HA	1:D:213:PRO:HA	1.73	0.71
1:A:471:ASP:OD1	1:A:471:ASP:N	2.22	0.71
26:E:2002:AHR:C1	13:wC:3:GZL:H21	2.20	0.71
1:A:1471:ALA:HB2	1:A:1479:CYS:HB3	1.71	0.71
26:C:2003:AHR:C1	13:WB:3:GZL:H21	2.21	0.71
1:F:715:THR:HG22	1:F:737:VAL:HG12	1.72	0.70
1:E:1672:GLN:NE2	1:E:1679:THR:O	2.23	0.70
1:F:1270:THR:HG22	1:F:1271:TYR:H	1.56	0.70
1:E:1326:HIS:HE2	1:E:1356:ASN:HA	1.55	0.70
1:B:872:PRO:HG2	1:B:882:VAL:HA	1.72	0.70
1:A:757:LEU:HD11	1:A:769:ALA:HB1	1.74	0.70
1:A:1622:ARG:NH1	1:B:1946:ASN:O	2.24	0.70
1:E:501:VAL:HG12	1:E:503:PRO:HD2	1.74	0.70
26:B:2003:AHR:C1	13:2A:3:GZL:H21	2.21	0.70
1:C:1047:GLY:HA3	1:C:1101:MET:O	1.92	0.70
1:D:1293:GLN:NE2	1:D:1295:ASN:O	2.25	0.70
1:A:663:TRP:NE1	1:A:668:GLY:O	2.24	0.70
1:D:1292:PHE:HA	1:D:1314:ALA:HB1	1.72	0.70
1:B:667:THR:HG22	1:B:668:GLY:H	1.56	0.69
1:E:622:LEU:HD11	1:E:641:TYR:HB3	1.73	0.69
1:A:808:ILE:HG12	1:A:815:THR:HB	1.75	0.69
26:B:2003:AHR:O4	13:2A:3:GZL:O5	2.08	0.69
1:A:1839:PRO:HD2	1:A:1839:PRO:O	1.92	0.69
26:A:2003:AHR:O2	6:5:2:FUB:O3	2.10	0.69
1:E:1126:PHE:HB3	1:E:1148:THR:HB	1.75	0.68
1:F:942:GLU:OE1	4:gD:1:FUB:O5	2.11	0.68
1:C:159:THR:HG23	1:C:178:ARG:HB3	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1327:THR:HG22	1:D:1328:ASP:H	1.58	0.68
1:A:1786:ASP:HB3	1:A:1789:GLU:HB2	1.76	0.68
26:F:2005:AHR:O5	6:uD:3:GZL:O3	2.12	0.68
1:C:1361:CYS:HB2	1:C:1401:GLY:HA2	1.75	0.68
1:A:1326:HIS:HE2	1:A:1356:ASN:HA	1.59	0.68
1:B:663:TRP:NE1	1:B:668:GLY:O	2.26	0.68
1:C:792:MET:HE1	1:C:836:VAL:HG13	1.75	0.68
26:F:2001:AHR:O5	6:XB:3:GZL:O3	2.12	0.68
1:C:1102:ALA:O	1:C:1105:THR:OG1	2.10	0.68
1:D:989:LEU:HD22	1:D:990:ALA:H	1.57	0.68
1:E:751:TYR:HB3	1:E:775:ILE:HD11	1.75	0.68
1:E:904:ILE:HG12	1:E:935:VAL:HG22	1.76	0.68
1:E:997:THR:HG23	1:E:999:MET:HE1	1.75	0.68
26:E:2003:AHR:O5	6:xC:3:GZL:O3	2.12	0.68
1:C:530:GLU:HB2	1:C:565:ILE:HB	1.77	0.67
1:D:1193:ASP:O	1:D:1212:GLN:NE2	2.28	0.67
1:E:757:LEU:HD11	1:E:769:ALA:HB1	1.76	0.67
1:D:656:LEU:HB3	1:D:691:MET:HB2	1.76	0.67
1:D:1421:GLN:HE22	1:D:1438:LEU:H	1.40	0.67
1:C:808:ILE:HG12	1:C:815:THR:HB	1.75	0.67
1:D:1481:GLN:NE2	1:E:1165:PRO:O	2.27	0.67
1:A:1424:SER:HB3	1:A:1543:SER:HB2	1.74	0.67
1:D:872:PRO:HG2	1:D:882:VAL:HA	1.77	0.67
1:A:1193:ASP:O	1:A:1212:GLN:NE2	2.28	0.67
1:C:905:CYS:HB3	1:C:965:LEU:HD11	1.76	0.67
1:D:159:THR:HG23	1:D:178:ARG:HB3	1.76	0.67
1:F:1255:PRO:HB2	1:F:1276:HIS:HB3	1.76	0.67
1:D:507:ILE:HD12	1:D:507:ILE:H	1.60	0.67
26:D:2004:AHR:O5	6:OB:3:GZL:O3	2.13	0.67
1:A:410:LYS:HA	1:A:437:MET:HE1	1.76	0.66
1:B:130:ARG:HG2	1:B:141:LEU:HD21	1.75	0.66
1:F:876:VAL:HG22	1:F:999:MET:HE2	1.77	0.66
1:B:1193:ASP:O	1:B:1212:GLN:NE2	2.28	0.66
1:B:1689:ALA:HB2	1:B:1697:CYS:HB3	1.76	0.66
1:C:1902:HYP:HD22	27:C:2006:GLA:H62	1.77	0.66
1:D:1367:LEU:HD21	1:D:1389:CYS:HA	1.77	0.66
1:E:901:GLN:HB3	1:E:938:MET:HB2	1.77	0.66
1:A:1946:ASN:O	1:B:1622:ARG:NH1	2.29	0.66
1:C:593:GLN:NE2	1:C:602:TRP:O	2.28	0.66
1:D:1124:PRO:HG2	1:D:1150:LEU:HB2	1.77	0.66
1:D:1200:ARG:NH2	1:E:1534:ASP:O	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1672:GLN:NE2	1:F:1679:THR:O	2.27	0.66
1:B:274:THR:H	1:B:293:THR:HG22	1.60	0.66
1:B:757:LEU:HD11	1:B:769:ALA:HB1	1.76	0.66
1:D:691:MET:SD	1:D:698:ALA:HB2	2.36	0.66
26:D:2001:AHR:O5	6:N:3:GZL:O2	2.14	0.66
26:F:2003:AHR:O4	6:CD:3:GZL:H21	1.96	0.66
1:D:1467:ALA:HA	1:D:1539:MET:HE1	1.76	0.65
26:D:2003:AHR:O4	13:zB:3:GZL:O5	2.14	0.65
1:E:1613:CYS:SG	1:E:1617:SER:OG	2.54	0.65
1:D:192:THR:OG1	1:D:203:GLU:OE2	2.15	0.65
1:F:764:ALA:HB3	1:F:857:SER:HB2	1.79	0.65
1:A:419:TRP:HZ3	1:A:471:ASP:HA	1.61	0.65
1:C:281:THR:HG23	1:C:283:ALA:H	1.61	0.65
26:C:2003:AHR:O4	13:WB:3:GZL:O5	2.13	0.65
1:C:271:LEU:HD23	1:C:295:VAL:HG12	1.79	0.65
1:C:935:VAL:HG11	1:C:972:ALA:HB2	1.79	0.65
26:F:2004:AHR:O5	13:tD:3:GZL:O3	2.15	0.65
1:A:1047:GLY:HA3	1:A:1101:MET:O	1.96	0.64
1:B:903:ILE:HD11	1:B:945:THR:HG21	1.78	0.64
1:A:1613:CYS:SG	1:A:1617:SER:OG	2.55	0.64
1:C:191:ALA:HB2	1:C:209:ILE:HD11	1.77	0.64
26:A:2002:AHR:C1	13:4:3:GZL:C4	2.74	0.64
1:B:185:ASN:HA	1:B:213:PRO:HA	1.79	0.64
1:B:909:ASN:ND2	1:B:951:THR:OG1	2.31	0.64
1:F:1706:GLN:NE2	1:F:1713:VAL:O	2.28	0.64
1:B:206:ARG:NH1	1:B:243:ALA:O	2.31	0.64
1:C:505:SER:OG	1:C:612:GLN:NE2	2.30	0.64
1:C:1465:CYS:SG	1:C:1469:THR:OG1	2.54	0.64
1:F:501:VAL:HB	1:F:504:PHE:HA	1.79	0.64
1:C:420:TRP:NE1	1:C:433:THR:HG1	1.94	0.64
1:F:1013:ILE:HG21	1:F:1022:PRO:HB3	1.80	0.64
1:F:1124:PRO:HB2	1:F:1150:LEU:HD23	1.78	0.64
1:A:756:TYR:OH	1:A:970:GLU:OE1	2.16	0.63
1:B:1223:MET:O	20:HE:1:FUB:O5	2.16	0.63
1:A:185:ASN:HA	1:A:213:PRO:HA	1.80	0.63
1:A:206:ARG:NH1	1:A:243:ALA:O	2.30	0.63
1:A:1534:ASP:O	1:B:1200:ARG:NH2	2.32	0.63
1:C:192:THR:OG1	1:C:203:GLU:OE2	2.15	0.63
1:C:1374:ALA:HA	1:C:1388:PRO:HD3	1.80	0.63
1:D:420:TRP:NE1	1:D:433:THR:HG1	1.96	0.63
1:E:536:PHE:HB2	1:E:592:LEU:HD23	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:E:2002:HR:O4	13:wC:3:GZL:O5	2.16	0.63
1:F:1613:CYS:SG	1:F:1617:SER:OG	2.56	0.63
1:B:918:ALA:HB1	1:B:966:MET:HE3	1.80	0.63
1:B:1706:GLN:NE2	1:B:1713:VAL:O	2.31	0.63
1:C:276:GLY:N	1:C:287:THR:O	2.31	0.63
1:C:1293:GLN:NE2	1:C:1295:ASN:O	2.32	0.63
1:D:774:VAL:HG11	1:D:974:ALA:HB2	1.80	0.63
1:F:898:GLY:HA2	1:F:940:PRO:HB3	1.81	0.63
1:D:1071:ASP:N	1:D:1145:ASP:OD2	2.31	0.63
1:A:1858:HYP:N	6:N:3:GZL:H61	2.14	0.63
1:A:1891:ASN:N	1:A:1891:ASN:OD1	2.32	0.63
1:B:506:PRO:HG2	1:B:613:VAL:HG22	1.80	0.63
1:C:1412:THR:HG22	1:C:1447:GLN:HA	1.81	0.63
3:xA:1:FUB:O3	3:xA:2:FUB:O5	2.16	0.63
1:A:311:ASN:HB3	1:A:360:ARG:HG2	1.80	0.62
1:E:1718:ASP:OD2	15:AB:1:FUB:O3	2.17	0.62
1:E:959:GLY:H	1:E:1000:VAL:HG13	1.64	0.62
1:E:1871:ARG:NH2	3:NC:3:FUB:O3	2.32	0.62
1:B:889:THR:HG22	1:B:944:THR:HG23	1.81	0.62
1:B:1293:GLN:NE2	1:B:1295:ASN:O	2.32	0.62
1:C:1329:GLY:N	1:C:1357:THR:OG1	2.32	0.62
1:E:507:ILE:HG23	1:E:509:THR:H	1.65	0.62
1:F:656:LEU:HB3	1:F:691:MET:HB2	1.82	0.62
1:A:121:SER:OG	1:A:125:LYS:NZ	2.32	0.62
1:B:354:THR:HA	1:B:380:VAL:HG23	1.81	0.62
1:B:666:LYS:HD3	1:B:712:ALA:HB2	1.82	0.62
1:D:1047:GLY:CA	1:D:1101:MET:O	2.46	0.62
1:C:624:ALA:HB3	1:C:741:PRO:HD2	1.81	0.62
1:E:808:ILE:HG12	1:E:815:THR:HB	1.80	0.62
1:F:870:VAL:HG22	1:F:873:ALA:H	1.63	0.62
26:C:2001:HR:O4	6:LA:3:GZL:H21	1.99	0.62
1:A:1200:ARG:NH2	1:B:1534:ASP:O	2.33	0.62
1:C:797:GLN:NE2	1:C:825:THR:O	2.29	0.62
1:E:1289:LYS:HE2	1:E:1312:SER:HB2	1.81	0.62
1:D:288:PHE:HE1	1:D:293:THR:HG21	1.65	0.62
1:E:1804:ASP:OD1	1:E:1804:ASP:N	2.33	0.62
1:F:661:SER:HB3	1:F:680:LEU:HD12	1.82	0.62
1:F:1454:ALA:HA	1:F:1459:MET:HE1	1.80	0.61
1:A:417:GLN:HG2	1:A:419:TRP:HE1	1.65	0.61
1:D:471:ASP:OD1	1:D:472:GLY:N	2.33	0.61
1:A:696:THR:O	1:A:696:THR:OG1	2.19	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:ASN:OD1	1:B:111:SER:N	2.33	0.61
1:B:191:ALA:HB2	1:B:209:ILE:HD11	1.81	0.61
1:B:1328:ASP:O	1:B:1359:ARG:NH1	2.34	0.61
1:C:663:TRP:NE1	1:C:668:GLY:O	2.33	0.61
1:D:83:LEU:HD13	1:D:110:VAL:HG11	1.81	0.61
1:D:1209:PRO:HD3	1:E:1515:THR:HG22	1.80	0.61
6:0B:1:FUB:O3	6:0B:2:FUB:O5	2.19	0.61
1:C:1480:GLN:HB3	1:F:1161:PHE:HB3	1.82	0.61
1:F:887:THR:HG22	1:F:946:THR:HG22	1.83	0.61
1:C:1017:TYR:HD2	1:C:1156:GLN:HG3	1.65	0.61
1:C:1328:ASP:O	1:C:1359:ARG:NH1	2.34	0.61
1:F:871:SER:HB3	1:F:883:THR:HB	1.82	0.61
1:F:1071:ASP:HB3	1:F:1075:LYS:HE3	1.81	0.61
1:C:1449:PRO:O	1:C:1452:THR:OG1	2.17	0.61
1:E:507:ILE:HG22	1:E:510:VAL:HG12	1.82	0.61
1:E:532:ILE:HG22	1:E:563:ALA:HB3	1.83	0.61
1:B:1396:THR:HB	1:B:1405:CYS:HB3	1.83	0.61
1:C:1328:ASP:OD2	1:F:1379:ASN:ND2	2.33	0.61
1:F:666:LYS:HG2	1:F:712:ALA:HB2	1.83	0.61
1:A:1102:ALA:O	1:A:1105:THR:OG1	2.17	0.60
1:B:391:LYS:NZ	1:B:393:THR:O	2.33	0.60
1:B:398:THR:OG1	1:B:399:THR:N	2.32	0.60
1:B:603:ASP:OD2	7:KC:4:AHR:O2	2.18	0.60
1:B:756:TYR:OH	1:B:970:GLU:OE1	2.19	0.60
1:D:831:PRO:HD2	16:AC:1:NAG:H82	1.83	0.60
1:F:1292:PHE:HA	1:F:1314:ALA:HB1	1.83	0.60
1:A:1426:PHE:HZ	1:A:1490:MET:HE2	1.66	0.60
1:E:1292:PHE:HA	1:E:1314:ALA:HB1	1.82	0.60
1:A:660:CYS:HB3	1:A:716:LEU:HD11	1.83	0.60
1:A:1706:GLN:NE2	1:A:1713:VAL:O	2.34	0.60
1:D:906:GLU:HG2	1:D:933:THR:HG23	1.82	0.60
1:F:1448:CYS:HB2	1:F:1475:GLY:HA2	1.83	0.60
1:B:1047:GLY:CA	1:B:1101:MET:O	2.49	0.60
1:D:524:THR:HG22	1:D:525:PRO:HD2	1.83	0.60
1:E:791:GLN:OE1	1:E:791:GLN:N	2.34	0.60
1:F:660:CYS:HB3	1:F:716:LEU:HD11	1.83	0.60
1:F:1014:SER:OG	1:F:1015:PRO:HD3	2.01	0.60
1:A:870:VAL:HG21	1:A:999:MET:HE1	1.82	0.60
1:C:498:GLU:OE1	1:C:517:ARG:NH1	2.34	0.60
1:D:540:ASP:OD1	1:D:540:ASP:N	2.32	0.60
1:D:1058:GLN:NE2	1:D:1115:LEU:O	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1102:ALA:O	1:E:1105:THR:OG1	2.14	0.60
14:p:3:GZL:O4	14:p:3:GZL:O6	2.16	0.60
1:A:398:THR:OG1	1:A:399:THR:N	2.34	0.60
1:C:122:ILE:HD12	1:C:248:THR:HG21	1.83	0.60
1:E:762:PRO:HG2	1:E:854:VAL:HG22	1.82	0.60
1:F:1799:TYR:O	1:F:1829:THR:OG1	2.16	0.60
1:B:1881:ARG:NH2	3:ZA:3:FUB:O3	2.35	0.60
4:JB:1:FUB:O5	3:LB:2:FUB:O5	2.19	0.60
1:C:288:PHE:HE1	1:C:293:THR:HG21	1.66	0.60
1:F:911:GLU:OE2	1:F:954:THR:OG1	2.20	0.60
1:F:1053:ALA:HB3	1:F:1127:PHE:HB2	1.84	0.60
1:F:1786:ASP:OD1	1:F:1787:GLU:N	2.35	0.60
1:C:966:MET:HB2	1:C:992:VAL:HG12	1.83	0.59
26:C:2001:AHR:O3	4:JA:4:AHR:O2	2.20	0.59
1:D:664:ASP:HB2	1:D:706:TYR:HE1	1.66	0.59
1:A:795:ASN:O	1:A:824:TYR:OH	2.20	0.59
1:F:1644:ALA:HB1	1:F:1653:PRO:HB2	1.84	0.59
1:D:467:ILE:HG23	1:D:481:LEU:HB2	1.82	0.59
1:E:770:VAL:HG12	1:E:818:VAL:HG22	1.84	0.59
1:F:1270:THR:HB	1:F:1274:VAL:HG11	1.85	0.59
1:B:758:ASN:HB3	1:B:759:PRO:HD3	1.83	0.59
1:E:1058:GLN:HG2	1:E:1060:VAL:HG23	1.83	0.59
1:A:211:ILE:HD12	1:A:213:PRO:HD3	1.84	0.59
1:A:540:ASP:OD1	1:A:540:ASP:N	2.35	0.59
1:A:1070:THR:HG22	1:A:1072:ALA:H	1.68	0.59
1:B:1124:PRO:HG2	1:B:1150:LEU:HB2	1.83	0.59
1:C:278:THR:HG22	1:C:279:SER:H	1.68	0.59
1:C:664:ASP:N	1:C:664:ASP:OD1	2.36	0.59
1:D:1328:ASP:HB3	1:D:1355:PRO:HB3	1.84	0.59
1:F:874:THR:HA	1:F:999:MET:HE1	1.85	0.59
1:A:1242:ARG:NH2	22:RE:1:FUB:O4	2.32	0.59
1:D:649:VAL:HG21	1:D:691:MET:HB3	1.85	0.59
1:A:1644:ALA:HB1	1:A:1653:PRO:HB2	1.83	0.59
1:B:420:TRP:NE1	1:B:433:THR:OG1	2.36	0.59
1:A:1061:ASN:HB3	1:A:1062:PRO:HD3	1.84	0.59
1:B:893:ALA:HA	1:B:943:THR:HB	1.84	0.59
1:E:831:PRO:HB2	1:E:851:ASN:HD22	1.67	0.59
1:F:671:PRO:O	1:F:677:TRP:NE1	2.36	0.59
1:F:1101:MET:HE1	1:F:1108:VAL:HB	1.84	0.59
10:3:2:FUB:O3	10:3:3:FUB:O5	2.21	0.59
4:kD:1:FUB:O5	3:mD:2:FUB:O3	2.21	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:THR:O	1:A:235:THR:OG1	2.18	0.58
1:A:1053:ALA:HB2	1:A:1096:LEU:HD12	1.84	0.58
1:C:884:TYR:OH	1:C:953:TYR:OH	2.21	0.58
1:C:1166:THR:HG22	1:F:1467:ALA:O	2.03	0.58
1:D:418:VAL:HG21	1:D:467:ILE:HD11	1.84	0.58
1:D:1167:ASN:ND2	1:E:1558:ASP:O	2.36	0.58
10:sD:2:FUB:O5	10:sD:5:AHR:O3	2.21	0.58
1:C:432:ARG:NH1	1:C:470:ARG:O	2.36	0.58
1:E:1489:LEU:HD13	1:E:1539:MET:HE3	1.85	0.58
1:A:192:THR:OG1	1:A:203:GLU:OE2	2.21	0.58
1:A:507:ILE:HB	1:A:510:VAL:HG12	1.84	0.58
1:B:660:CYS:HB3	1:B:716:LEU:HD11	1.85	0.58
1:C:168:LEU:O	1:C:170:LEU:N	2.36	0.58
1:C:655:SER:HA	1:C:693:PRO:HD3	1.84	0.58
1:C:1261:ARG:HD3	1:C:1268:PRO:HB3	1.84	0.58
1:D:1308:PHE:O	1:D:1326:HIS:NE2	2.36	0.58
1:D:1361:CYS:HB2	1:D:1401:GLY:HA2	1.85	0.58
1:E:1556:ASP:OD1	1:E:1556:ASP:N	2.33	0.58
23:XE:4:AHR:O3	23:XE:5:AHR:O2	2.21	0.58
1:A:566:LEU:O	1:A:569:SER:OG	2.19	0.58
1:E:566:LEU:O	1:E:569:SER:OG	2.22	0.58
1:E:596:ILE:HG13	1:E:599:THR:HB	1.84	0.58
1:F:1671:PHE:HD2	1:F:1696:ALA:HA	1.67	0.58
26:F:2004:AHR:C1	13:tD:3:GZL:H21	2.33	0.58
1:B:1037:ASP:HB3	1:B:1038:PRO:HD3	1.84	0.58
1:C:1223:MET:O	20:xE:1:FUB:O5	2.21	0.58
1:D:181:SER:HB2	1:D:186:ARG:HD2	1.85	0.58
1:F:1495:GLN:HB3	1:F:1511:LEU:HD12	1.83	0.58
1:A:758:ASN:OD1	1:A:772:ARG:NH2	2.29	0.58
1:D:1130:GLU:OE2	1:D:1138:ALA:N	2.37	0.58
1:B:506:PRO:HB3	1:B:512:ALA:HB2	1.84	0.58
1:E:1396:THR:HB	1:E:1405:CYS:HB3	1.85	0.58
1:E:1891:ASN:OD1	1:E:1891:ASN:N	2.33	0.58
1:F:721:ASN:HA	1:F:725:LEU:HD22	1.86	0.58
1:F:1224:ASP:OD1	1:F:1224:ASP:N	2.36	0.58
1:B:1058:GLN:HB3	1:B:1093:ASP:OD2	2.04	0.58
1:D:1255:PRO:HB2	1:D:1276:HIS:HB3	1.85	0.58
1:E:913:THR:O	1:E:913:THR:OG1	2.21	0.58
1:F:797:GLN:NE2	1:F:825:THR:O	2.37	0.58
1:F:978:LEU:HD22	1:F:983:VAL:HG13	1.86	0.58
27:F:2008:GLA:O2	4:LD:2:FUB:O3	2.22	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1787:GLU:OE1	1:A:1787:GLU:N	2.35	0.57
1:C:901:GLN:HB3	1:C:938:MET:HB3	1.86	0.57
1:E:942:GLU:OE1	4:jC:1:FUB:O5	2.21	0.57
1:E:955:THR:HG23	1:E:961:PHE:HZ	1.69	0.57
1:A:735:SER:OG	1:A:736:PRO:HD3	2.03	0.57
1:D:532:ILE:HG22	1:D:596:ILE:HB	1.86	0.57
1:A:890:ARG:O	1:A:943:THR:OG1	2.21	0.57
1:A:905:CYS:HB3	1:A:965:LEU:HD11	1.86	0.57
1:C:534:CYS:O	1:C:560:GLY:HA3	2.04	0.57
1:E:793:PRO:O	1:E:800:SER:OG	2.22	0.57
1:B:71:ALA:HB2	1:B:105:PRO:HA	1.85	0.57
1:C:627:THR:HG22	1:C:628:PRO:HD3	1.85	0.57
1:C:1193:ASP:O	1:C:1212:GLN:NE2	2.38	0.57
1:C:235:THR:O	1:C:235:THR:OG1	2.22	0.57
1:C:273:LEU:HA	1:C:293:THR:HG22	1.86	0.57
1:C:274:THR:H	1:C:293:THR:HG22	1.69	0.57
1:D:168:LEU:O	1:D:170:LEU:N	2.38	0.57
1:A:928:ILE:HD11	1:A:976:PRO:HG3	1.87	0.57
1:C:886:PHE:CG	1:C:965:LEU:HD23	2.39	0.57
1:C:906:GLU:OE1	1:C:933:THR:OG1	2.21	0.57
1:C:1464:PRO:O	1:F:1227:ARG:NH1	2.37	0.57
1:D:1102:ALA:O	1:D:1105:THR:OG1	2.15	0.57
3:PB:1:FUB:O3	3:PB:2:FUB:O5	2.22	0.57
6:XB:1:FUB:O3	6:XB:2:FUB:O5	2.21	0.57
1:C:188:ASP:HB3	1:C:208:PHE:HE1	1.70	0.57
1:C:663:TRP:CG	1:C:670:ALA:HB2	2.39	0.57
1:C:1327:THR:O	1:C:1357:THR:OG1	2.21	0.57
1:B:1701:GLN:HG3	1:C:1170:GLN:HG2	1.87	0.57
6:bB:2:FUB:O3	6:bB:3:GZL:O5	2.21	0.57
1:A:1481:GLN:NE2	1:B:1165:PRO:O	2.38	0.57
1:B:1613:CYS:SG	1:B:1617:SER:OG	2.60	0.57
1:D:353:SER:OG	1:D:357:LYS:NZ	2.31	0.57
1:E:532:ILE:HG13	1:E:596:ILE:HG23	1.87	0.57
1:E:757:LEU:HG	1:E:759:PRO:HD2	1.87	0.57
1:A:133:ASP:HB3	1:A:142:LEU:HD11	1.87	0.56
1:E:939:ALA:HB3	1:E:942:GLU:HG2	1.87	0.56
1:A:1421:GLN:HE22	1:A:1438:LEU:HB2	1.69	0.56
1:A:1718:ASP:OD2	15:7B:1:FUB:O3	2.23	0.56
1:D:1448:CYS:O	1:D:1475:GLY:N	2.38	0.56
1:F:566:LEU:O	1:F:569:SER:OG	2.21	0.56
1:A:274:THR:H	1:A:293:THR:HG22	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1883:HYP:O	27:B:2010:GLA:O6	2.24	0.56
1:C:1070:THR:HG22	1:C:1072:ALA:H	1.69	0.56
1:D:1422:LEU:HG	1:D:1433:PRO:HB2	1.87	0.56
1:D:1558:ASP:O	1:E:1167:ASN:ND2	2.38	0.56
1:E:761:THR:OG1	1:E:890:ARG:NH2	2.38	0.56
1:E:1198:GLY:HA3	1:E:1215:LYS:HG3	1.87	0.56
1:F:886:PHE:CG	1:F:965:LEU:HD22	2.40	0.56
10:sD:2:FUB:O3	10:sD:3:FUB:O5	2.23	0.56
1:B:663:TRP:CD2	1:B:670:ALA:HB2	2.39	0.56
1:C:501:VAL:O	1:C:720:GLN:NE2	2.36	0.56
1:E:1553:TYR:HB3	1:E:1563:GLN:HB3	1.87	0.56
18:rE:1:FUB:O4	20:uE:4:AHR:O2	2.24	0.56
1:A:1836:ARG:HH12	1:A:1838:LYS:HG3	1.70	0.56
1:D:641:TYR:HB2	1:D:700:CYS:SG	2.46	0.56
1:A:1383:VAL:HG21	1:B:1337:GLU:HG2	1.86	0.56
1:B:288:PHE:HE1	1:B:293:THR:HG21	1.71	0.56
1:C:281:THR:OG1	1:C:382:ASN:OD1	2.22	0.56
1:D:274:THR:H	1:D:293:THR:HG22	1.70	0.56
1:A:1842:LEU:HD13	1:A:1842:LEU:O	2.06	0.56
1:B:85:TYR:CD2	1:B:117:VAL:HG21	2.41	0.56
1:B:278:THR:CG2	1:B:279:SER:H	2.16	0.56
1:C:47:LEU:HD23	1:C:129:LEU:HD23	1.86	0.56
1:E:963:ALA:O	1:E:995:PHE:N	2.38	0.56
26:E:2002:AHR:O5	13:wC:3:GZL:O3	2.23	0.56
1:F:758:ASN:OD1	1:F:772:ARG:NH2	2.37	0.56
1:F:1449:PRO:O	1:F:1452:THR:OG1	2.23	0.56
6:OE:1:FUB:O3	6:OE:2:FUB:O5	2.23	0.56
1:A:1047:GLY:CA	1:A:1101:MET:O	2.54	0.56
1:B:1364:ASN:HA	1:B:1397:TRP:O	2.05	0.56
1:B:1757:ASN:HB3	1:B:1766:ARG:HD3	1.88	0.56
1:C:1047:GLY:CA	1:C:1101:MET:O	2.54	0.56
1:D:666:LYS:NZ	1:D:708:THR:OG1	2.27	0.56
1:D:1165:PRO:O	1:E:1481:GLN:NE2	2.39	0.56
1:E:1027:PRO:HB3	1:E:1091:PHE:HZ	1.69	0.56
4:pA:1:FUB:O5	3:rA:2:FUB:O5	2.23	0.56
1:A:603:ASP:OD1	7:HD:4:AHR:O2	2.23	0.56
1:D:45:TYR:HE2	1:D:142:LEU:HD22	1.70	0.56
1:D:506:PRO:HB3	1:D:512:ALA:HB2	1.87	0.56
1:D:643:ILE:HB	1:D:698:ALA:HB3	1.86	0.56
1:B:1337:GLU:N	1:B:1337:GLU:OE1	2.37	0.56
1:C:1132:ALA:HB3	1:C:1135:THR:HG23	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:26:HYP:O	19:LE:3:GZL:O2	2.24	0.56
1:A:1281:PRO:HB2	1:C:245:VAL:HG23	1.88	0.55
1:B:1830:GLU:HG3	1:B:1838:LYS:HE3	1.88	0.55
1:D:942:GLU:OE1	3:O:B:2:FUB:O3	2.24	0.55
1:D:1018:ASN:OD1	1:D:1021:THR:N	2.39	0.55
1:D:1189:ILE:HB	1:E:1537:PHE:HB2	1.88	0.55
1:E:1055:TYR:O	1:E:1124:PRO:HA	2.05	0.55
1:A:272:THR:O	1:A:293:THR:HA	2.06	0.55
1:A:1364:ASN:HA	1:A:1397:TRP:O	2.07	0.55
27:A:2014:GLA:O2	13:4:4:AHR:O3	2.23	0.55
1:B:1553:TYR:HB3	1:B:1563:GLN:HB3	1.88	0.55
1:B:1701:GLN:HE22	1:C:1171:ARG:HG2	1.71	0.55
1:D:276:GLY:N	1:D:287:THR:O	2.39	0.55
1:D:888:ILE:HD11	1:D:967:VAL:HG11	1.88	0.55
1:D:1374:ALA:HA	1:D:1388:PRO:HD3	1.88	0.55
1:A:155:THR:O	1:A:182:SER:N	2.39	0.55
1:D:1390:ARG:HD3	1:E:1302:LEU:HD13	1.88	0.55
1:E:909:ASN:O	1:E:953:TYR:OH	2.24	0.55
18:BE:1:FUB:O4	20:EE:4:AHR:O2	2.24	0.55
1:C:272:THR:O	1:C:293:THR:HA	2.07	0.55
1:C:649:VAL:HG23	1:C:691:MET:HE2	1.89	0.55
26:D:2001:AHR:C1	6:N:3:GZL:H5	2.09	0.55
1:A:156:LEU:HD23	1:A:186:ARG:HH12	1.72	0.55
1:E:788:LEU:HD22	1:E:840:ASP:HB2	1.88	0.55
1:D:918:ALA:HA	1:D:921:TYR:HD2	1.72	0.55
2:G:15:ASP:OD2	20:HE:3:GZL:O3	2.25	0.55
1:B:828:THR:HG22	1:B:829:PRO:HD2	1.89	0.55
1:B:943:THR:O	1:B:943:THR:OG1	2.23	0.55
1:B:1412:THR:HG22	1:B:1447:GLN:HA	1.89	0.55
1:C:1306:SER:HA	1:F:1375:ILE:HD11	1.88	0.55
1:A:420:TRP:NE1	1:A:433:THR:OG1	2.40	0.55
1:B:1326:HIS:HE2	1:B:1356:ASN:HA	1.72	0.55
1:D:519:GLN:HA	1:D:519:GLN:OE1	2.07	0.55
1:D:566:LEU:O	1:D:569:SER:OG	2.21	0.55
1:E:889:THR:HG22	1:E:944:THR:HG23	1.89	0.55
1:F:532:ILE:HG23	1:F:596:ILE:HG13	1.88	0.55
1:F:1678:THR:O	1:F:1678:THR:OG1	2.21	0.55
1:A:420:TRP:NE1	1:A:433:THR:HG1	2.04	0.55
1:B:188:ASP:OD1	1:B:190:TRP:NE1	2.40	0.55
26:B:2004:AHR:O4	6:3A:3:GZL:O3	2.24	0.55
1:D:420:TRP:NE1	1:D:433:THR:OG1	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:LEU:O	1:A:170:LEU:N	2.40	0.54
1:C:866:VAL:HG13	1:C:993:HIS:ND1	2.23	0.54
1:F:968:PHE:HE1	1:F:987:GLN:HG3	1.72	0.54
1:B:603:ASP:OD1	1:B:603:ASP:N	2.31	0.54
1:D:157:THR:OG1	1:D:180:SER:OG	2.25	0.54
1:D:273:LEU:HA	1:D:293:THR:HG22	1.89	0.54
1:F:831:PRO:HD2	16:4D:1:NAG:H82	1.89	0.54
1:A:121:SER:O	1:A:125:LYS:NZ	2.36	0.54
1:A:401:ASP:OD1	1:A:401:ASP:N	2.40	0.54
1:C:907:PHE:HE1	1:C:963:ALA:HB1	1.72	0.54
1:E:641:TYR:HB2	1:E:700:CYS:SG	2.48	0.54
6:0C:1:FUB:O3	6:0C:2:FUB:O5	2.26	0.54
4:VD:1:FUB:O3	4:VD:2:FUB:O5	2.25	0.54
1:A:663:TRP:CD2	1:A:670:ALA:HB2	2.42	0.54
1:A:1589:ASP:OD1	1:A:1589:ASP:N	2.40	0.54
1:B:249:LEU:HD11	1:B:252:THR:HG22	1.89	0.54
1:B:457:SER:OG	1:B:458:GLY:N	2.41	0.54
1:C:420:TRP:NE1	1:C:433:THR:OG1	2.39	0.54
1:D:123:GLY:HA2	1:D:248:THR:HG23	1.88	0.54
1:D:696:THR:O	1:D:696:THR:OG1	2.26	0.54
1:E:1843:LEU:HD21	1:E:1846:PRO:HA	1.90	0.54
1:F:507:ILE:HD11	1:F:510:VAL:HG12	1.88	0.54
1:F:1394:ASP:HB3	1:F:1460:SER:HB3	1.89	0.54
3:RB:1:FUB:O3	3:RB:2:FUB:O5	2.26	0.54
1:D:1307:GLY:HA2	1:D:1326:HIS:HB2	1.90	0.54
1:F:691:MET:SD	1:F:698:ALA:HB2	2.47	0.54
22:QE:4:ADR:O5	22:QE:6:ADR:O5	2.26	0.54
1:B:1421:GLN:HE22	1:B:1438:LEU:HB2	1.73	0.54
1:C:899:ILE:H	1:C:940:PRO:HB3	1.71	0.54
26:D:2003:ADR:C1	13:zB:3:GZL:H5	2.11	0.54
1:F:966:MET:HE3	1:F:966:MET:C	2.33	0.54
1:F:1036:ARG:HG2	1:F:1038:PRO:HD2	1.90	0.54
20:hE:2:FUB:O3	20:hE:3:GZL:O5	2.23	0.54
1:A:419:TRP:CZ3	1:A:471:ASP:CA	2.88	0.54
1:A:666:LYS:HZ3	1:A:708:THR:HG23	1.72	0.54
1:A:1448:CYS:HB2	1:A:1475:GLY:HA2	1.89	0.54
26:B:2003:ADR:O4	13:2A:3:GZL:C5	2.56	0.54
1:D:80:PHE:HB3	1:D:95:ARG:HG2	1.89	0.54
1:F:1840:CYS:HA	1:F:1843:LEU:HD23	1.89	0.54
1:D:386:THR:OG1	1:D:410:LYS:HG2	2.08	0.54
1:D:624:ALA:HB1	1:D:639:TRP:HZ3	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1412:THR:HB	1:D:1445:CYS:HB3	1.90	0.54
1:B:864:TYR:OH	1:B:901:GLN:OE1	2.13	0.54
1:F:663:TRP:O	1:F:714:PRO:HA	2.07	0.54
20:HE:2:FUB:O3	20:HE:3:GZL:O5	2.25	0.54
1:D:385:TYR:CE2	1:D:411:HIS:HD2	2.25	0.53
1:B:835:THR:HG22	1:B:848:ILE:HG12	1.90	0.53
1:B:978:LEU:HD13	1:B:983:VAL:HG13	1.90	0.53
1:D:671:PRO:HG3	1:D:680:LEU:HD11	1.91	0.53
1:E:561:LEU:HD23	1:E:575:ILE:HG23	1.90	0.53
1:E:906:GLU:OE2	1:E:933:THR:OG1	2.26	0.53
4:r:1:FUB:O5	3:t:2:FUB:O5	2.25	0.53
1:A:628:PRO:HB2	1:A:631:VAL:HG13	1.89	0.53
1:F:663:TRP:CZ2	1:F:665:GLY:HA2	2.44	0.53
1:F:1329:GLY:N	1:F:1357:THR:OG1	2.42	0.53
20:uE:2:FUB:O3	20:uE:3:GZL:O5	2.26	0.53
1:A:978:LEU:HD13	1:A:983:VAL:HG13	1.90	0.53
1:B:494:LEU:HD12	1:B:521:SER:HB2	1.90	0.53
1:B:1770:ARG:NH2	18:0E:4:AHR:O3	2.41	0.53
1:C:464:THR:HG22	1:C:485:THR:HG23	1.91	0.53
13:o:4:AHR:O2	12:q:3:GZL:O5	2.25	0.53
1:C:1184:ASP:HB3	1:C:1242:ARG:HB3	1.89	0.53
1:D:709:THR:HA	1:D:746:VAL:HB	1.90	0.53
1:F:1556:ASP:OD1	1:F:1556:ASP:N	2.36	0.53
6:uD:1:FUB:O5	6:xD:2:FUB:O3	2.26	0.53
1:B:826:THR:O	1:B:826:THR:OG1	2.27	0.53
1:A:773:ILE:HD13	1:A:836:VAL:HG11	1.89	0.53
1:A:1537:PHE:HB2	1:B:1189:ILE:HB	1.90	0.53
1:B:905:CYS:HB3	1:B:965:LEU:HD11	1.91	0.53
1:C:386:THR:OG1	1:C:410:LYS:HG2	2.08	0.53
1:D:71:ALA:HB2	1:D:105:PRO:HA	1.90	0.53
1:D:664:ASP:OD1	1:D:664:ASP:N	2.37	0.53
1:E:497:LEU:HD11	1:E:516:PHE:HB3	1.89	0.53
1:E:1364:ASN:HA	1:E:1397:TRP:O	2.09	0.53
1:E:1589:ASP:N	1:E:1589:ASP:OD1	2.41	0.53
1:F:587:SER:HA	1:F:612:GLN:HA	1.89	0.53
13:vD:1:FUB:O3	13:vD:2:FUB:O5	2.25	0.53
1:D:1282:GLU:OE2	1:D:1285:LYS:NZ	2.42	0.53
1:E:898:GLY:HA2	1:E:940:PRO:HB3	1.91	0.53
1:E:964:LYS:HA	1:E:994:SER:HA	1.91	0.53
1:F:1555:THR:HG22	1:F:1560:LEU:HD12	1.89	0.53
3:MA:1:FUB:O3	3:MA:2:FUB:O5	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:757:LEU:HD12	1:A:758:ASN:H	1.74	0.53
1:B:45:TYR:CE2	1:B:142:LEU:HB2	2.34	0.53
1:E:1109:SER:OG	13:zC:1:FUB:O3	2.23	0.53
1:F:1412:THR:HG22	1:F:1447:GLN:HA	1.90	0.53
1:F:1440:GLU:OE1	1:F:1442:GLY:N	2.42	0.53
1:D:1123:SER:O	1:D:1123:SER:OG	2.27	0.53
1:D:1443:SER:OG	1:D:1444:GLY:N	2.42	0.53
1:E:1721:THR:HB	1:E:1730:CYS:HB2	1.91	0.53
14:qA:1:FUB:O3	14:qA:2:FUB:O5	2.26	0.53
1:A:666:LYS:NZ	1:A:708:THR:O	2.42	0.52
1:D:959:GLY:H	1:D:1000:VAL:HG12	1.74	0.52
1:A:641:TYR:HB2	1:A:700:CYS:SG	2.49	0.52
27:B:2014:GLA:O2	4:pA:4:AHR:O3	2.27	0.52
1:D:764:ALA:HB3	1:D:857:SER:HB2	1.90	0.52
1:D:1426:PHE:CD1	1:D:1490:MET:HE1	2.45	0.52
1:F:1364:ASN:HA	1:F:1397:TRP:O	2.09	0.52
1:A:1397:TRP:CG	1:A:1443:SER:HG	2.26	0.52
1:B:536:PHE:HD1	1:B:592:LEU:HB2	1.74	0.52
1:C:419:TRP:CD1	1:C:434:ALA:HA	2.45	0.52
1:C:534:CYS:O	1:C:560:GLY:CA	2.57	0.52
1:A:939:ALA:HB3	1:A:942:GLU:HG2	1.92	0.52
1:A:1855:HYP:HB3	5:M:2:FUB:O3	2.09	0.52
1:A:1878:HYP:O	27:A:2008:GLA:O6	2.26	0.52
1:C:457:SER:OG	1:C:458:GLY:N	2.42	0.52
1:D:224:PRO:O	1:D:226:GLN:NE2	2.33	0.52
1:F:627:THR:OG1	1:F:628:PRO:HD3	2.09	0.52
2:I:15:ASP:OD2	20:xE:3:GZL:O3	2.26	0.52
1:A:824:TYR:HE2	1:A:852:PHE:HE2	1.57	0.52
1:B:157:THR:OG1	1:B:180:SER:OG	2.28	0.52
1:C:179:VAL:HG11	1:C:189:MET:HE1	1.92	0.52
1:C:626:VAL:HG12	1:C:628:PRO:HD2	1.92	0.52
1:D:1220:THR:HG22	1:D:1230:PRO:HA	1.91	0.52
1:E:911:GLU:OE2	1:E:954:THR:OG1	2.22	0.52
14:nA:2:FUB:O3	14:nA:4:FUB:O5	2.28	0.52
1:A:1326:HIS:NE2	1:A:1356:ASN:HA	2.25	0.52
1:B:1787:GLU:OE1	1:B:1787:GLU:N	2.37	0.52
1:C:886:PHE:CD2	1:C:965:LEU:HD23	2.44	0.52
1:D:756:TYR:OH	1:D:970:GLU:OE1	2.27	0.52
1:E:773:ILE:HD13	1:E:836:VAL:HG11	1.92	0.52
1:F:1021:THR:HG22	1:F:1153:PHE:HB2	1.91	0.52
1:A:1224:ASP:OD1	1:A:1224:ASP:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:68:ALA:HB1	1:C:129:LEU:HD22	1.92	0.52
1:D:821:ILE:HG22	1:D:823:GLY:H	1.74	0.52
1:E:511:ALA:HA	1:E:580:THR:HA	1.92	0.52
1:E:1671:PHE:CD1	1:E:1683:CYS:HB3	2.43	0.52
1:E:1773:TYR:HD2	1:E:1810:GLN:HA	1.74	0.52
26:F:2003:AHR:O3	4:AD:4:AHR:O2	2.28	0.52
14:nA:2:FUB:O3	14:nA:3:GZL:O6	2.27	0.52
1:A:278:THR:HG22	1:A:279:SER:H	1.74	0.52
1:A:1614:TRP:NE1	1:A:1676:GLU:OE2	2.33	0.52
1:B:84:ASP:HB2	1:B:92:GLU:CD	2.35	0.52
1:B:1448:CYS:HB2	1:B:1475:GLY:HA2	1.91	0.52
1:C:841:GLY:H	1:C:843:VAL:HG22	1.75	0.52
1:F:529:THR:HG23	1:F:566:LEU:HA	1.92	0.52
27:F:2015:GLA:O2	4:gD:4:AHR:O3	2.26	0.52
1:A:1293:GLN:NE2	1:A:1295:ASN:O	2.41	0.52
1:B:866:VAL:HG12	1:B:888:ILE:HG23	1.92	0.52
1:B:1755:TYR:CZ	1:B:1766:ARG:HG3	2.45	0.52
1:F:797:GLN:HE22	1:F:825:THR:H	1.58	0.52
14:KB:3:GZL:O3	3:LB:2:FUB:O4	2.28	0.52
1:A:399:THR:O	1:A:399:THR:OG1	2.29	0.51
1:B:168:LEU:O	1:B:170:LEU:N	2.43	0.51
1:B:410:LYS:NZ	1:B:441:GLY:O	2.42	0.51
1:C:185:ASN:OD1	1:C:185:ASN:N	2.43	0.51
1:C:466:ARG:HG2	1:C:483:SER:HB3	1.91	0.51
1:D:211:ILE:HG13	1:D:213:PRO:HD3	1.91	0.51
1:E:1069:ILE:HA	1:E:1074:TYR:HE2	1.75	0.51
1:E:1883:HYP:O	27:E:2009:GLA:O6	2.28	0.51
6:mE:2:FUB:O3	6:mE:3:GZL:O5	2.23	0.51
27:A:2006:GLA:O6	27:A:2006:GLA:O4	2.28	0.51
1:B:469:ASP:HB3	1:B:481:LEU:HD13	1.92	0.51
1:B:1804:ASP:HB3	1:B:1835:GLN:HB2	1.93	0.51
1:F:501:VAL:O	1:F:720:GLN:NE2	2.44	0.51
1:F:772:ARG:NH2	1:F:970:GLU:OE2	2.42	0.51
4:mB:1:FUB:O5	3:oB:2:FUB:O5	2.28	0.51
1:A:1770:ARG:NH1	1:A:1806:PRO:HG3	2.26	0.51
1:C:965:LEU:HD12	1:C:966:MET:N	2.26	0.51
1:D:624:ALA:HB1	1:D:639:TRP:CZ3	2.46	0.51
1:D:687:LYS:NZ	1:D:700:CYS:HB2	2.26	0.51
1:E:666:LYS:HB2	1:E:706:TYR:HD1	1.75	0.51
1:E:1080:VAL:O	1:E:1097:ARG:NH1	2.43	0.51
1:F:662:PHE:HE1	1:F:714:PRO:HB3	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:nE:3:GZL:O4	6:nE:3:GZL:O6	2.19	0.51
1:B:131:LEU:HB2	1:B:143:ALA:HB3	1.92	0.51
1:C:593:GLN:HG2	1:C:605:TYR:HA	1.91	0.51
1:D:875:PRO:HB3	1:D:1000:VAL:HG23	1.93	0.51
1:D:1161:PHE:HB3	1:E:1480:GLN:HB3	1.92	0.51
1:F:868:SER:HB3	1:F:886:PHE:CD2	2.46	0.51
1:A:470:ARG:HG3	1:A:471:ASP:OD1	2.10	0.51
1:A:501:VAL:O	1:A:720:GLN:NE2	2.44	0.51
1:A:1376:ALA:HB2	1:B:1376:ALA:HA	1.92	0.51
1:D:282:THR:OG1	1:D:469:ASP:OD2	2.27	0.51
1:D:551:TRP:CE3	1:D:593:GLN:HB2	2.46	0.51
1:D:1327:THR:O	1:D:1357:THR:OG1	2.25	0.51
1:E:1490:MET:SD	1:E:1538:PHE:HB2	2.51	0.51
1:F:1689:ALA:HB2	1:F:1697:CYS:HB2	1.92	0.51
1:B:155:THR:OG1	1:B:186:ARG:NH2	2.43	0.51
1:C:185:ASN:HA	1:C:213:PRO:HA	1.93	0.51
1:D:1224:ASP:OD1	1:D:1224:ASP:N	2.44	0.51
1:D:1397:TRP:CG	1:D:1443:SER:HG	2.29	0.51
1:D:1490:MET:O	1:D:1496:GLN:NE2	2.35	0.51
1:F:1870:HYP:O	8:JD:5:AHR:O5	2.28	0.51
1:A:1052:CYS:HB2	1:A:1112:PHE:HZ	1.76	0.51
1:B:45:TYR:HD2	1:B:143:ALA:HB2	1.76	0.51
1:C:123:GLY:HA2	1:C:248:THR:HG23	1.93	0.51
1:D:1286:LYS:HE3	1:D:1313:GLY:HA2	1.91	0.51
1:E:1448:CYS:HB2	1:E:1475:GLY:HA2	1.93	0.51
1:F:850:LYS:HE3	1:F:900:PRO:HD2	1.91	0.51
1:F:1542:LYS:HE2	1:F:1546:CYS:HA	1.92	0.51
1:F:1921:HYP:HB3	6:xD:3:GZL:H41	1.93	0.51
1:A:469:ASP:OD1	1:A:479:LEU:N	2.38	0.51
1:B:1492:ASP:OD1	1:B:1493:ARG:N	2.43	0.51
1:C:504:PHE:CE2	1:C:656:LEU:HB2	2.46	0.51
1:D:110:VAL:HG12	1:D:115:TYR:CG	2.46	0.51
1:D:231:GLU:OE1	1:D:297:TYR:OH	2.29	0.51
1:A:1037:ASP:HB3	1:A:1038:PRO:HD3	1.92	0.51
1:A:1925:ARG:NH2	6:9:3:GZL:O6	2.44	0.51
1:D:625:SER:HA	1:E:742:ALA:HA	1.91	0.51
1:D:775:ILE:HG12	1:D:838:VAL:HG21	1.93	0.51
1:D:1251:THR:HG22	1:D:1286:LYS:HA	1.91	0.51
1:A:386:THR:OG1	1:A:410:LYS:HG2	2.10	0.51
1:B:190:TRP:CZ2	1:B:244:PRO:HG3	2.44	0.51
1:C:1130:GLU:O	1:C:1137:GLY:N	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:58:PRO:HG2	1:D:151:VAL:HG12	1.93	0.51
1:D:239:ARG:HG2	1:D:252:THR:HG22	1.93	0.51
1:D:663:TRP:O	1:D:714:PRO:HA	2.10	0.51
1:D:1426:PHE:CE1	1:D:1490:MET:HE1	2.46	0.51
7:XC:3:FUB:O2	7:XC:4:AHR:O5	2.28	0.51
3:iD:2:FUB:O3	3:iD:3:FUB:O5	2.29	0.51
3:oD:1:FUB:O3	3:oD:2:FUB:O5	2.29	0.51
1:A:329:THR:OG1	1:A:330:ALA:N	2.43	0.50
1:B:495:TYR:OH	1:B:530:GLU:OE1	2.26	0.50
1:C:1125:LYS:HB3	1:C:1147:VAL:HG21	1.93	0.50
1:E:797:GLN:HE22	1:E:824:TYR:HA	1.76	0.50
3:m:2:FUB:O3	3:m:3:FUB:O5	2.29	0.50
1:B:153:ASP:OD2	1:B:186:ARG:NH2	2.43	0.50
1:D:869:VAL:HG12	1:D:885:THR:HB	1.93	0.50
1:A:329:THR:O	1:A:332:SER:OG	2.29	0.50
1:A:1737:THR:OG1	1:A:1747:CYS:HB3	2.11	0.50
1:B:666:LYS:NZ	1:B:709:THR:O	2.35	0.50
1:D:407:ALA:HB3	1:D:448:ILE:HB	1.91	0.50
1:D:633:VAL:HG21	1:D:777:ARG:HH22	1.77	0.50
1:A:239:ARG:HG2	1:A:252:THR:HG22	1.93	0.50
1:A:959:GLY:H	1:A:1000:VAL:HG13	1.76	0.50
1:A:1185:GLY:H	1:A:1222:THR:HG22	1.75	0.50
1:C:890:ARG:NE	1:C:892:THR:O	2.44	0.50
1:E:1189:ILE:HD13	1:E:1214:ARG:HB2	1.94	0.50
1:E:1327:THR:O	1:E:1357:THR:OG1	2.28	0.50
1:F:775:ILE:HG12	1:F:838:VAL:HG21	1.93	0.50
1:A:758:ASN:ND2	1:A:986:SER:OG	2.44	0.50
1:B:228:TYR:CG	1:B:263:VAL:HG21	2.47	0.50
1:B:1770:ARG:HH11	1:B:1770:ARG:HB2	1.76	0.50
1:C:874:THR:HG23	1:C:1000:VAL:HG12	1.94	0.50
1:D:385:TYR:CE2	1:D:481:LEU:HD23	2.47	0.50
1:E:680:LEU:HD13	1:E:685:ASN:HB3	1.92	0.50
1:E:791:GLN:HG3	1:E:803:ASP:OD2	2.11	0.50
13:gC:4:AHR:O2	12:iC:3:GZL:O5	2.29	0.50
3:qC:2:FUB:O3	3:qC:3:FUB:O5	2.29	0.50
1:A:190:TRP:HB3	1:A:206:ARG:HB3	1.93	0.50
1:B:360:ARG:HH11	1:B:362:ARG:HD2	1.77	0.50
1:B:1784:LEU:HD23	1:B:1785:GLY:H	1.77	0.50
1:C:329:THR:OG1	1:C:330:ALA:N	2.44	0.50
1:C:1034:LEU:HB2	1:C:1108:VAL:HG12	1.94	0.50
1:D:398:THR:OG1	1:D:399:THR:N	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:501:VAL:HB	1:E:504:PHE:HA	1.92	0.50
1:E:1193:ASP:O	1:E:1212:GLN:NE2	2.45	0.50
1:A:824:TYR:CE2	1:A:852:PHE:HE2	2.30	0.50
1:B:627:THR:OG1	1:B:628:PRO:HD3	2.12	0.50
1:B:808:ILE:HG12	1:B:815:THR:HB	1.92	0.50
1:B:1549:ASN:HD22	1:B:1563:GLN:HG2	1.75	0.50
1:D:283:ALA:O	1:D:416:SER:OG	2.23	0.50
1:D:890:ARG:NE	1:D:892:THR:O	2.45	0.50
1:D:898:GLY:HA2	1:D:940:PRO:HG2	1.94	0.50
1:E:874:THR:OG1	1:E:1000:VAL:HG23	2.12	0.50
13:wD:2:FUB:O3	13:wD:3:GZL:O5	2.27	0.50
1:B:161:LEU:HG	1:B:176:LYS:HG2	1.93	0.50
1:B:420:TRP:NE1	1:B:433:THR:HG1	2.10	0.50
1:B:1430:ASP:OD1	1:B:1430:ASP:N	2.45	0.50
1:C:602:TRP:CE3	1:C:606:TYR:HB2	2.46	0.50
1:D:1013:ILE:HG23	1:D:1028:THR:HG23	1.94	0.50
1:E:662:PHE:HE2	1:E:704:PRO:HG3	1.75	0.50
1:E:785:ALA:HA	1:E:808:ILE:O	2.11	0.50
1:A:95:ARG:HD2	1:A:135:ALA:HA	1.94	0.50
1:A:1721:THR:HG22	1:A:1732:LYS:HA	1.92	0.50
1:D:639:TRP:CE2	1:D:714:PRO:HG3	2.46	0.50
1:E:1308:PHE:HA	1:E:1319:ALA:HA	1.94	0.50
3:TA:2:FUB:O3	3:TA:3:FUB:O5	2.29	0.50
1:A:587:SER:HB2	1:A:610:VAL:CG2	2.42	0.49
1:A:966:MET:HB2	1:A:992:VAL:HG12	1.94	0.49
1:A:1220:THR:HG22	1:A:1230:PRO:HA	1.94	0.49
1:B:466:ARG:HG2	1:B:483:SER:HB3	1.94	0.49
26:B:2020:AHR:C1	6:FC:3:GZL:C5	2.83	0.49
1:C:1029:TYR:HH	1:C:1090:TYR:HH	1.53	0.49
3:y:3:FUB:O3	3:z:2:FUB:O4	2.30	0.49
1:A:84:ASP:HB3	1:A:128:THR:HG22	1.94	0.49
1:B:1328:ASP:HB3	1:B:1355:PRO:HB3	1.94	0.49
1:B:1527:LYS:HB3	1:B:1528:PRO:HD3	1.94	0.49
1:D:626:VAL:HG12	1:D:628:PRO:HD2	1.93	0.49
1:D:664:ASP:OD2	1:D:667:THR:OG1	2.30	0.49
1:E:1018:ASN:OD1	1:E:1021:THR:N	2.45	0.49
1:F:993:HIS:ND1	1:F:993:HIS:C	2.69	0.49
13:dD:1:FUB:O3	13:dD:2:FUB:O5	2.29	0.49
1:A:204:SER:OG	1:A:205:SER:N	2.45	0.49
1:A:1671:PHE:CE1	1:A:1683:CYS:HB3	2.47	0.49
1:C:385:TYR:CZ	1:C:411:HIS:HD2	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:663:TRP:CZ2	1:C:665:GLY:HA2	2.46	0.49
1:D:596:ILE:O	1:D:599:THR:HB	2.12	0.49
1:E:643:ILE:HB	1:E:698:ALA:HB3	1.94	0.49
1:E:662:PHE:CE2	1:E:704:PRO:HG3	2.47	0.49
1:F:1080:VAL:HG11	1:F:1095:GLN:HB3	1.93	0.49
1:A:821:ILE:HD13	1:A:824:TYR:CE1	2.47	0.49
1:A:1184:ASP:OD1	20:UE:4:AHR:O2	2.30	0.49
26:D:2001:AHR:O5	6:N:3:GZL:H51	2.12	0.49
1:F:1671:PHE:CD1	1:F:1683:CYS:HB3	2.47	0.49
3:wA:3:FUB:O3	3:xA:2:FUB:O4	2.29	0.49
1:A:194:GLN:HB3	1:A:237:VAL:HG23	1.94	0.49
1:A:506:PRO:HB3	1:A:512:ALA:HB2	1.94	0.49
1:B:498:GLU:OE2	1:B:517:ARG:NE	2.33	0.49
1:B:1436:THR:OG1	1:B:1437:THR:N	2.44	0.49
1:B:1551:PRO:HG3	1:B:1574:PHE:HD1	1.78	0.49
1:B:1846:PRO:O	1:B:1846:PRO:HD2	2.12	0.49
1:E:965:LEU:HD22	1:E:966:MET:H	1.77	0.49
3:QB:3:FUB:O3	3:RB:2:FUB:O4	2.31	0.49
1:A:1690:ASP:OD1	1:A:1698:LYS:NZ	2.30	0.49
1:B:84:ASP:HB3	1:B:128:THR:HG22	1.95	0.49
1:C:504:PHE:CG	1:C:656:LEU:HD13	2.47	0.49
1:E:527:GLY:H	1:E:567:PRO:HB3	1.76	0.49
1:E:753:ILE:HG13	1:E:775:ILE:HD13	1.93	0.49
1:E:1058:GLN:NE2	1:E:1116:TYR:HD1	2.10	0.49
1:E:1224:ASP:OD1	1:E:1224:ASP:N	2.40	0.49
1:F:1677:THR:OG1	1:F:1678:THR:N	2.45	0.49
1:B:123:GLY:HA2	1:B:248:THR:HG23	1.95	0.49
1:C:1272:HIS:CD2	1:F:1425:PRO:HD3	2.47	0.49
1:D:1421:GLN:HA	1:D:1449:PRO:HG3	1.94	0.49
1:E:1855:HYP:HB3	5:EC:2:FUB:O3	2.12	0.49
1:F:1367:LEU:HD21	1:F:1372:GLN:HG3	1.94	0.49
18:zE:1:FUB:O5	18:zE:5:AHR:O2	2.30	0.49
1:B:297:TYR:CZ	1:B:299:ALA:HB3	2.48	0.49
1:B:714:PRO:HD2	1:B:740:ALA:HB3	1.94	0.49
1:F:902:PRO:HB2	1:F:971:SER:HA	1.95	0.49
1:B:280:VAL:HB	1:B:284:ASP:HB2	1.94	0.49
1:C:1029:TYR:OH	1:C:1090:TYR:OH	2.20	0.49
1:E:1097:ARG:HG3	1:E:1112:PHE:CE1	2.48	0.49
6:mE:1:FUB:O5	18:pE:4:AHR:O2	2.30	0.49
1:A:67:THR:OG1	1:A:108:ASN:ND2	2.46	0.49
1:A:789:THR:HB	1:A:839:VAL:HG23	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1022:PRO:HG2	1:C:1155:THR:HG22	1.95	0.49
1:E:497:LEU:HD22	1:E:592:LEU:HD12	1.95	0.49
1:A:1845:LYS:HB2	1:A:1849:ALA:HB3	1.94	0.48
1:B:67:THR:HA	1:B:108:ASN:HD21	1.79	0.48
1:B:131:LEU:HD12	1:B:143:ALA:HB3	1.94	0.48
1:D:758:ASN:HB3	1:D:759:PRO:HD3	1.95	0.48
1:A:273:LEU:HD23	1:A:376:VAL:HG23	1.94	0.48
1:B:566:LEU:O	1:B:569:SER:OG	2.28	0.48
1:D:1084:VAL:HG13	1:D:1086:THR:H	1.78	0.48
1:D:1306:SER:OG	1:E:1373:ALA:O	2.30	0.48
1:E:712:ALA:HB3	1:E:744:ALA:HB3	1.95	0.48
1:D:72:SER:OG	1:D:75:SER:O	2.31	0.48
1:D:1412:THR:HA	1:D:1447:GLN:HA	1.96	0.48
1:E:627:THR:OG1	1:E:628:PRO:HD3	2.13	0.48
1:E:1421:GLN:NE2	1:E:1438:LEU:H	2.11	0.48
1:A:59:THR:OG1	1:A:62:ASP:OD1	2.31	0.48
1:A:290:GLN:OE1	1:A:342:SER:OG	2.23	0.48
1:B:469:ASP:HB3	1:B:481:LEU:CD1	2.44	0.48
1:C:632:PRO:HD2	1:C:635:THR:HG21	1.96	0.48
26:C:2001:AHR:C1	6:LA:3:GZL:H21	2.43	0.48
1:D:51:LYS:HE2	1:D:58:PRO:HD3	1.94	0.48
1:D:1229:ILE:HG23	1:E:1464:PRO:HD2	1.95	0.48
1:A:741:PRO:HB2	1:B:739:THR:HG21	1.94	0.48
1:B:1786:ASP:HB3	1:B:1789:GLU:HB2	1.95	0.48
1:D:939:ALA:HB3	1:D:942:GLU:HG2	1.95	0.48
1:F:757:LEU:HD13	1:F:771:TRP:CD1	2.49	0.48
3:b:2:FUB:O3	3:b:3:FUB:O5	2.31	0.48
1:A:627:THR:OG1	1:A:628:PRO:HD3	2.13	0.48
1:B:278:THR:HG22	1:B:279:SER:N	2.20	0.48
1:B:1798:PRO:HD2	1:B:1801:PHE:HB2	1.96	0.48
1:D:497:LEU:HB3	1:D:606:TYR:CZ	2.48	0.48
1:E:588:LEU:HB2	1:E:611:PHE:CZ	2.49	0.48
1:B:264:VAL:HG23	1:B:297:TYR:CZ	2.49	0.48
1:B:1672:GLN:CD	1:B:1677:THR:HG21	2.39	0.48
1:D:1243:GLU:OE2	22:dE:6:AHR:O3	2.31	0.48
1:E:757:LEU:HD13	1:E:771:TRP:CD1	2.49	0.48
1:E:864:TYR:OH	1:E:901:GLN:OE1	2.32	0.48
1:E:1069:ILE:HD12	1:E:1069:ILE:O	2.14	0.48
1:F:711:THR:HG23	1:F:743:PHE:CD2	2.49	0.48
1:F:1015:PRO:HB2	1:F:1023:TYR:HD2	1.78	0.48
1:A:225:ASP:OD1	1:A:225:ASP:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1884:SER:OG	7:f:2:FUB:O3	2.32	0.48
1:C:163:SER:O	1:C:367:ALA:HB2	2.13	0.48
1:C:1397:TRP:CD1	1:C:1397:TRP:H	2.31	0.48
1:D:102:SER:OG	1:D:104:THR:OG1	2.28	0.48
1:D:793:PRO:O	1:D:800:SER:OG	2.31	0.48
1:F:1499:LEU:HD23	1:F:1512:ARG:HG2	1.96	0.48
6:bE:2:FUB:O3	6:bE:3:GZL:O5	2.26	0.48
1:A:192:THR:HG22	1:A:206:ARG:HA	1.95	0.48
1:A:965:LEU:HG	1:A:966:MET:N	2.28	0.48
1:B:1537:PHE:HD1	1:B:1537:PHE:O	1.96	0.48
1:F:1016:ASN:ND2	1:F:1018:ASN:O	2.47	0.48
1:C:1171:ARG:HD2	1:C:1171:ARG:HA	1.59	0.48
1:E:1016:ASN:OD1	1:E:1016:ASN:N	2.46	0.48
1:E:1644:ALA:HB1	1:E:1653:PRO:HB2	1.96	0.48
1:F:602:TRP:CE3	1:F:606:TYR:HB2	2.48	0.48
27:F:2016:GLA:O2	13:tD:4:AHR:O3	2.31	0.48
1:A:1326:HIS:NE2	1:A:1355:PRO:O	2.47	0.47
1:B:664:ASP:HB2	1:B:706:TYR:HE1	1.77	0.47
1:B:1049:GLN:HB3	1:B:1131:TYR:HB3	1.96	0.47
14:eD:3:GZL:O4	14:eD:3:GZL:O6	2.21	0.47
1:A:1636:THR:HG22	1:A:1663:PRO:HA	1.96	0.47
26:A:2003:AHR:O4	6:5:3:GZL:O5	2.28	0.47
26:D:2003:AHR:O4	13:zB:3:GZL:C5	2.61	0.47
1:E:1128:VAL:HB	1:E:1140:ALA:HB3	1.96	0.47
1:A:1124:PRO:HG2	1:A:1150:LEU:HD13	1.96	0.47
1:A:1757:ASN:HD22	1:A:1766:ARG:NH2	2.13	0.47
1:B:1684:ALA:HA	1:B:1709:ILE:HG22	1.95	0.47
1:C:532:ILE:HG13	1:C:596:ILE:HB	1.95	0.47
1:C:797:GLN:OE1	1:C:825:THR:N	2.36	0.47
1:C:1090:TYR:OH	6:cB:3:GZL:O5	2.30	0.47
1:E:504:PHE:HB2	1:E:720:GLN:HE22	1.78	0.47
1:E:524:THR:OG1	1:E:568:SER:N	2.47	0.47
1:E:1107:ARG:O	13:zC:2:FUB:O5	2.31	0.47
1:F:1721:THR:HG22	1:F:1732:LYS:HA	1.96	0.47
1:A:958:ALA:HA	1:A:1000:VAL:HG12	1.96	0.47
1:B:601:LEU:H	1:B:601:LEU:HD12	1.78	0.47
1:C:1453:TYR:CD2	1:C:1455:PRO:HD3	2.49	0.47
1:D:47:LEU:HD21	1:D:131:LEU:HG	1.95	0.47
1:F:1126:PHE:HB3	1:F:1148:THR:OG1	2.14	0.47
1:F:1159:PRO:HB2	1:F:1161:PHE:HD2	1.78	0.47
3:IA:2:FUB:O5	3:IA:3:FUB:O5	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1018:ASN:O	1:A:1020:THR:N	2.47	0.47
1:A:1394:ASP:HB2	1:B:1299:THR:HG21	1.97	0.47
1:D:982:SER:O	1:D:982:SER:OG	2.27	0.47
1:D:1125:LYS:HB3	1:D:1147:VAL:HG21	1.94	0.47
1:F:1553:TYR:HB3	1:F:1563:GLN:HB3	1.96	0.47
1:F:1819:LEU:HD23	1:F:1819:LEU:H	1.78	0.47
1:B:419:TRP:CH2	1:B:471:ASP:HB3	2.49	0.47
1:C:47:LEU:HG	1:C:70:VAL:HG12	1.96	0.47
1:C:511:ALA:HA	1:C:580:THR:HA	1.95	0.47
1:E:1925:ARG:NH2	6:1C:3:GZL:O6	2.46	0.47
1:F:953:TYR:CZ	1:F:961:PHE:CE1	3.02	0.47
1:F:1636:THR:HG22	1:F:1663:PRO:HA	1.97	0.47
1:A:87:ASP:HB2	1:A:90:THR:HG22	1.97	0.47
1:A:308:TRP:HZ3	1:A:310:PHE:HB2	1.79	0.47
1:A:1049:GLN:HB3	1:A:1131:TYR:HB3	1.95	0.47
1:A:1511:LEU:O	1:A:1513:ALA:N	2.47	0.47
1:A:1622:ARG:HD3	1:B:1944:ASN:O	2.15	0.47
1:B:1097:ARG:HG3	1:B:1112:PHE:CE2	2.50	0.47
1:B:1773:TYR:CD2	1:B:1810:GLN:HA	2.49	0.47
1:C:70:VAL:HG22	1:C:109:LEU:HD11	1.97	0.47
1:D:185:ASN:OD1	1:D:185:ASN:N	2.48	0.47
1:D:415:THR:HG22	1:D:415:THR:O	2.15	0.47
1:D:1459:MET:HE1	1:D:1462:CYS:HA	1.97	0.47
1:E:758:ASN:HB3	1:E:759:PRO:HD3	1.97	0.47
1:E:871:SER:HB3	1:E:883:THR:HB	1.96	0.47
1:E:1127:PHE:CZ	1:E:1147:VAL:HG22	2.50	0.47
26:E:2002:AHR:O4	13:wC:3:GZL:C5	2.63	0.47
1:F:773:ILE:O	1:F:816:VAL:HA	2.15	0.47
1:F:1035:LEU:HD12	1:F:1107:ARG:HG3	1.95	0.47
13:jB:4:AHR:O2	12:lB:3:GZL:O5	2.27	0.47
20:HE:1:FUB:O4	18:IE:4:AHR:O2	2.32	0.47
1:C:1307:GLY:HA2	1:C:1326:HIS:HB3	1.96	0.47
1:D:545:PRO:HG2	1:D:551:TRP:CD2	2.50	0.47
1:D:1097:ARG:HG3	1:D:1112:PHE:CE1	2.50	0.47
1:F:639:TRP:CH2	1:F:714:PRO:HG3	2.50	0.47
3:tC:1:FUB:O3	3:tC:2:FUB:O5	2.33	0.47
1:A:66:PHE:CE2	1:A:127:VAL:HG21	2.50	0.47
1:A:826:THR:O	1:A:826:THR:OG1	2.28	0.47
1:C:588:LEU:HB2	1:C:611:PHE:CE1	2.50	0.47
1:F:501:VAL:HG22	1:F:514:TRP:CZ3	2.50	0.47
1:A:296:SER:HB3	1:A:338:ALA:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:636:ALA:HB1	1:A:703:THR:HG22	1.95	0.47
1:B:1511:LEU:O	1:B:1513:ALA:N	2.48	0.47
1:B:1555:THR:HG22	1:B:1560:LEU:HD12	1.97	0.47
1:D:1061:ASN:HB3	1:D:1062:PRO:HD3	1.96	0.47
1:F:674:ASP:OD2	1:F:730:THR:HG23	2.14	0.47
1:F:751:TYR:CE1	1:F:777:ARG:HG3	2.49	0.47
1:F:1828:CYS:HB2	1:F:1840:CYS:HB3	1.56	0.47
1:F:1876:ASN:OD1	1:F:1876:ASN:N	2.46	0.47
1:A:419:TRP:CD1	1:A:434:ALA:HA	2.50	0.46
1:B:1844:SER:OG	1:B:1845:LYS:N	2.48	0.46
1:C:280:VAL:HB	1:C:284:ASP:HB2	1.96	0.46
1:C:432:ARG:HD2	1:C:472:GLY:N	2.30	0.46
26:C:2003:AHR:O4	13:WB:3:GZL:C5	2.63	0.46
1:D:851:ASN:HB3	16:AC:1:NAG:H2	1.96	0.46
1:D:1396:THR:HB	1:D:1405:CYS:HB3	1.96	0.46
1:E:1070:THR:HG22	1:E:1072:ALA:H	1.80	0.46
1:F:656:LEU:HD12	1:F:657:PRO:HD2	1.97	0.46
1:A:637:THR:O	1:A:703:THR:HA	2.15	0.46
1:A:1016:ASN:HD22	1:A:1019:PRO:HA	1.80	0.46
1:B:159:THR:HG22	1:B:178:ARG:HB3	1.97	0.46
1:B:664:ASP:HB2	1:B:706:TYR:CE1	2.49	0.46
1:B:836:VAL:HG23	1:B:847:HIS:HB3	1.97	0.46
1:B:1644:ALA:HB1	1:B:1653:PRO:HB2	1.97	0.46
1:B:1770:ARG:HG2	1:B:1804:ASP:O	2.15	0.46
1:B:1804:ASP:HB2	1:B:1805:ARG:NH2	2.30	0.46
2:G:22:ALA:HA	2:G:23:HYP:HD23	1.75	0.46
22:GE:1:FUB:O5	20:HE:4:AHR:O2	2.33	0.46
1:A:52:LEU:HG	1:A:53:GLY:H	1.79	0.46
1:B:156:LEU:HD13	1:B:181:SER:HB2	1.97	0.46
1:B:409:ALA:O	1:B:446:ASN:ND2	2.48	0.46
1:B:493:VAL:HG11	1:B:520:ARG:CZ	2.46	0.46
1:B:660:CYS:HB2	1:B:702:PHE:HZ	1.79	0.46
1:B:831:PRO:HD2	28:B:2018:NAG:H82	1.97	0.46
1:B:1549:ASN:ND2	1:B:1563:GLN:HG2	2.30	0.46
1:D:894:VAL:HB	1:D:940:PRO:HA	1.97	0.46
1:E:1687:THR:HB	1:E:1697:CYS:SG	2.54	0.46
10:~C:1:FUB:O5	6:~C:2:FUB:O3	2.32	0.46
1:A:288:PHE:HE1	1:A:293:THR:HG21	1.79	0.46
1:A:667:THR:HG22	1:A:668:GLY:N	2.20	0.46
1:B:48:THR:OG1	1:B:69:THR:OG1	2.27	0.46
1:B:1280:GLY:O	1:B:1282:GLU:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:188:ASP:HB3	1:D:208:PHE:HE1	1.80	0.46
1:D:773:ILE:CG2	1:D:817:CYS:HB2	2.45	0.46
1:D:966:MET:HE1	1:D:968:PHE:CG	2.51	0.46
1:D:1328:ASP:OD2	1:E:1377:SER:HA	2.16	0.46
1:E:1329:GLY:N	1:E:1357:THR:OG1	2.48	0.46
1:E:1879:SER:HA	1:E:1880:HYP:HD22	1.79	0.46
1:F:1104:GLY:O	27:F:2016:GLA:O3	2.30	0.46
1:B:1698:LYS:H	1:B:1698:LYS:HG2	1.39	0.46
1:D:533:LYS:O	1:D:534:CYS:HB3	2.15	0.46
1:F:1327:THR:O	1:F:1357:THR:OG1	2.28	0.46
1:F:1399:LYS:HB2	1:F:1399:LYS:HE2	1.68	0.46
26:F:2003:AHR:O5	6:CD:3:GZL:H41	2.14	0.46
1:A:54:PRO:HG2	1:A:58:PRO:HB3	1.97	0.46
1:A:297:TYR:CE2	1:A:299:ALA:HB3	2.50	0.46
1:A:1219:GLY:HA2	1:A:1278:ALA:O	2.15	0.46
1:B:534:CYS:HB3	1:B:592:LEU:HD11	1.98	0.46
1:C:414:SER:HG	1:C:416:SER:HG	1.64	0.46
1:C:1251:THR:HG22	1:C:1286:LYS:HG3	1.97	0.46
1:C:1364:ASN:HA	1:C:1397:TRP:O	2.15	0.46
27:D:2008:GLA:O2	13:zB:4:AHR:O3	2.29	0.46
15:4C:2:FUB:O3	15:4C:3:GZL:O5	2.33	0.46
1:B:902:PRO:HB2	1:B:971:SER:HA	1.97	0.46
1:C:1324:THR:HG22	1:C:1360:GLN:HA	1.98	0.46
1:C:1337:GLU:OE1	1:C:1355:PRO:HA	2.16	0.46
1:D:886:PHE:CE2	1:D:965:LEU:HB2	2.51	0.46
1:B:192:THR:OG1	1:B:203:GLU:OE2	2.32	0.46
1:B:1668:MET:HE3	1:F:1592:GLN:HG2	1.97	0.46
1:C:48:THR:O	1:C:68:ALA:HA	2.16	0.46
1:C:1438:LEU:HG	1:C:1447:GLN:HG3	1.97	0.46
1:F:1671:PHE:CD2	1:F:1696:ALA:HA	2.49	0.46
1:A:122:ILE:HA	1:A:151:VAL:HG23	1.98	0.46
1:A:417:GLN:CG	1:A:419:TRP:HE1	2.28	0.46
1:A:1487:ASN:CG	1:A:1563:GLN:HE21	2.24	0.46
1:B:1062:PRO:HD3	1:B:1093:ASP:HB2	1.97	0.46
1:C:1189:ILE:HB	1:F:1537:PHE:HB2	1.97	0.46
1:D:272:THR:O	1:D:293:THR:HA	2.16	0.46
1:D:561:LEU:HD23	1:D:562:THR:H	1.81	0.46
1:D:878:VAL:N	1:D:1002:ALA:O	2.49	0.46
1:D:904:ILE:HG12	1:D:935:VAL:HG22	1.98	0.46
1:D:1223:MET:O	20:hE:4:AHR:O3	2.34	0.46
1:E:1037:ASP:HB3	1:E:1038:PRO:HD3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1534:ASP:N	1:E:1534:ASP:OD1	2.49	0.46
27:F:2009:GLA:O6	27:F:2009:GLA:O4	2.24	0.46
1:A:533:LYS:HD2	1:A:533:LYS:HA	1.69	0.46
1:A:1123:SER:O	1:A:1123:SER:OG	2.26	0.46
1:C:540:ASP:OD1	1:C:540:ASP:N	2.39	0.46
1:C:902:PRO:HB2	1:C:971:SER:HA	1.98	0.46
1:D:411:HIS:CG	1:D:414:SER:HB3	2.50	0.46
1:D:637:THR:O	1:D:703:THR:HA	2.17	0.46
1:F:935:VAL:HG11	1:F:972:ALA:HB2	1.97	0.46
12:iB:4:THR:O2	14:kB:4:FUB:O3	2.34	0.46
1:A:80:PHE:CD1	1:A:80:PHE:N	2.84	0.45
1:A:868:SER:HB2	1:A:995:PHE:CE1	2.51	0.45
1:A:1909:ARG:HA	1:A:1910:HYP:HD22	1.77	0.45
1:B:185:ASN:ND2	12:iC:5:THR:O5	2.41	0.45
1:B:603:ASP:HB2	1:B:604:PRO:HD3	1.97	0.45
1:B:1393:GLU:H	1:B:1393:GLU:HG3	1.39	0.45
1:C:181:SER:HB2	1:C:186:ARG:HD2	1.96	0.45
1:D:410:LYS:HD2	1:D:441:GLY:O	2.16	0.45
1:D:540:ASP:OD2	1:D:579:ARG:NE	2.42	0.45
1:F:785:ALA:HA	1:F:808:ILE:O	2.17	0.45
1:F:911:GLU:HB2	1:F:961:PHE:CE2	2.51	0.45
1:F:928:ILE:HD12	1:F:975:ALA:HB3	1.97	0.45
1:F:952:TYR:CD2	1:F:1041:PRO:HG3	2.51	0.45
2:G:64:ALA:HA	2:I:1:HYP:HD23	1.82	0.45
3:z:1:FUB:O3	3:z:2:FUB:O5	2.33	0.45
6:zD:3:GZL:O6	13:0D:2:FUB:O5	2.29	0.45
1:A:177:GLY:HA3	1:A:221:PHE:CZ	2.50	0.45
1:B:128:THR:HG21	1:B:130:ARG:NH2	2.31	0.45
1:B:1935:SER:O	1:E:1711:GLN:NE2	2.48	0.45
1:C:407:ALA:HB3	1:C:448:ILE:HB	1.97	0.45
1:D:1048:VAL:O	1:D:1101:MET:HB2	2.16	0.45
1:E:1219:GLY:HA3	1:E:1277:LEU:HG	1.97	0.45
10:yB:2:FUB:O3	10:yB:3:FUB:O5	2.35	0.45
1:A:758:ASN:HB2	1:A:770:VAL:HG23	1.99	0.45
1:A:1537:PHE:HD1	1:A:1537:PHE:O	2.00	0.45
1:B:1948:ASP:HB3	1:E:1637:ASN:O	2.16	0.45
1:D:511:ALA:HA	1:D:580:THR:HA	1.99	0.45
1:D:1034:LEU:O	1:D:1107:ARG:HA	2.16	0.45
1:E:1636:THR:HG22	1:E:1663:PRO:HA	1.99	0.45
1:E:1690:ASP:OD1	1:E:1698:LYS:NZ	2.37	0.45
1:F:1515:THR:HB	1:F:1530:VAL:HB	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:BE:3:GZL:O6	20:CE:4:AHR:O2	2.25	0.45
1:A:1070:THR:HA	1:A:1145:ASP:OD2	2.16	0.45
1:A:1425:PRO:HB3	1:A:1433:PRO:HD3	1.98	0.45
1:C:756:TYR:OH	1:C:901:GLN:HA	2.16	0.45
1:C:1909:ARG:HA	1:C:1910:HYP:HD22	1.61	0.45
1:D:789:THR:HB	1:D:839:VAL:HG23	1.98	0.45
1:D:1005:VAL:HG13	1:D:1037:ASP:HB2	1.98	0.45
1:F:619:THR:N	1:F:646:SER:OG	2.48	0.45
18:fE:1:FUB:O5	22:iE:4:AHR:O2	2.33	0.45
1:A:282:THR:HG23	1:A:351:TYR:O	2.17	0.45
1:C:1017:TYR:CD2	1:C:1156:GLN:HG3	2.50	0.45
1:D:168:LEU:HD12	1:D:168:LEU:HA	1.81	0.45
1:E:1573:PRO:HG2	1:E:1588:VAL:HG11	1.98	0.45
1:E:1871:ARG:HG2	1:E:1872:HYP:HD23	1.99	0.45
1:F:1324:THR:HB	1:F:1358:CYS:HB3	1.98	0.45
27:F:2008:GLA:O6	27:F:2008:GLA:O4	2.31	0.45
1:A:469:ASP:OD1	1:A:469:ASP:N	2.50	0.45
1:A:1209:PRO:HD3	1:B:1515:THR:HG22	1.99	0.45
1:A:1562:ILE:HD11	1:B:1190:PHE:HD1	1.81	0.45
1:A:1587:THR:O	1:A:1594:TYR:OH	2.23	0.45
1:D:1467:ALA:HB2	1:E:1226:TYR:HB3	1.99	0.45
1:F:1905:HYP:HA	1:F:1906:HYP:HD22	1.72	0.45
1:A:407:ALA:HB3	1:A:448:ILE:HB	1.98	0.45
1:B:1013:ILE:HB	1:B:1016:ASN:HB3	1.99	0.45
1:B:1326:HIS:NE2	1:B:1356:ASN:HA	2.32	0.45
1:C:671:PRO:HG2	1:C:677:TRP:CD2	2.52	0.45
1:C:1052:CYS:HB3	1:C:1126:PHE:HE1	1.82	0.45
1:E:507:ILE:HD11	1:E:616:ALA:C	2.41	0.45
1:E:850:LYS:NZ	1:E:900:PRO:HD3	2.32	0.45
1:E:907:PHE:HE1	1:E:963:ALA:HB1	1.81	0.45
1:F:751:TYR:HE1	1:F:777:ARG:HG3	1.80	0.45
1:F:907:PHE:CE1	1:F:963:ALA:HB1	2.51	0.45
1:F:1377:SER:OG	1:F:1383:VAL:O	2.24	0.45
2:G:13:THR:HA	2:G:14:HYP:HD22	1.76	0.45
1:A:1070:THR:HG22	1:A:1072:ALA:N	2.31	0.45
1:A:1490:MET:SD	1:A:1538:PHE:HB2	2.57	0.45
1:B:1061:ASN:HB3	1:B:1062:PRO:HD3	1.98	0.45
1:B:1490:MET:SD	1:B:1538:PHE:HB2	2.57	0.45
1:D:122:ILE:HA	1:D:151:VAL:HG23	1.98	0.45
1:D:1058:GLN:HE22	1:D:1116:TYR:HA	1.81	0.45
1:F:1288:PRO:HD3	1:F:1347:PHE:HE2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:dE:2:FUB:O3	22:dE:3:GZL:O5	2.29	0.45
1:A:1883:HYP:O	27:A:2009:GLA:O6	2.35	0.45
1:B:540:ASP:OD1	1:B:540:ASP:N	2.45	0.45
1:B:687:LYS:HG3	1:B:702:PHE:CE2	2.51	0.45
1:B:1126:PHE:HB3	1:B:1148:THR:HB	1.99	0.45
1:C:420:TRP:HD1	1:C:435:LEU:HG	1.82	0.45
1:D:868:SER:HB2	1:D:995:PHE:CE2	2.51	0.45
1:D:1439:THR:HG22	1:D:1446:SER:HA	1.98	0.45
1:F:867:THR:HG22	1:F:887:THR:OG1	2.16	0.45
1:B:419:TRP:N	1:B:419:TRP:CD1	2.84	0.45
1:B:999:MET:HE2	1:B:999:MET:HB2	1.83	0.45
26:B:2004:AHR:O4	6:3A:3:GZL:O5	2.26	0.45
1:D:398:THR:HG21	1:D:522:LYS:HE3	1.99	0.45
1:F:631:VAL:HB	1:F:635:THR:OG1	2.16	0.45
1:F:1909:ARG:HA	1:F:1910:HYP:HD22	1.74	0.45
1:A:595:PHE:CE1	1:A:600:PRO:HB3	2.52	0.44
1:A:1097:ARG:HG3	1:A:1112:PHE:CE2	2.51	0.44
1:B:1425:PRO:HB3	1:B:1433:PRO:HD3	1.99	0.44
1:C:137:ALA:HB3	1:C:138:PRO:HD3	1.99	0.44
1:C:387:LEU:HD22	1:C:467:ILE:HG22	2.00	0.44
1:D:596:ILE:HG23	1:D:599:THR:HB	1.99	0.44
1:D:663:TRP:HE3	1:D:715:THR:HG22	1.82	0.44
1:E:963:ALA:HB3	1:E:995:PHE:HD2	1.81	0.44
1:F:1029:TYR:CE2	1:F:1113:PRO:HB3	2.52	0.44
1:F:1927:HYP:HA	1:F:1928:HYP:HD22	1.81	0.44
18:IE:1:FUB:O5	18:IE:5:AHR:O4	2.35	0.44
1:A:1704:ARG:HB3	1:A:1714:CYS:HB3	1.99	0.44
1:B:796:GLY:O	1:B:832:TYR:HB3	2.18	0.44
1:C:296:SER:HB3	1:C:338:ALA:HA	2.00	0.44
1:C:1289:LYS:HB2	1:C:1338:ALA:HB2	1.98	0.44
1:D:95:ARG:HD2	1:D:135:ALA:HA	1.99	0.44
1:D:285:GLN:HG3	1:D:350:ARG:HG3	1.99	0.44
1:D:907:PHE:HE1	1:D:963:ALA:HB1	1.82	0.44
1:D:966:MET:HE3	1:D:966:MET:C	2.43	0.44
1:D:1289:LYS:HB2	1:D:1338:ALA:HB2	1.99	0.44
1:E:664:ASP:OD1	1:E:664:ASP:N	2.48	0.44
1:E:1029:TYR:OH	6:2C:3:GZL:O5	2.28	0.44
1:F:1187:GLU:HB3	1:F:1228:CYS:SG	2.57	0.44
1:A:797:GLN:HB3	1:A:832:TYR:CD2	2.52	0.44
1:A:1938:ASN:OD1	1:A:1938:ASN:N	2.43	0.44
1:D:179:VAL:HG23	1:D:219:TYR:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:754:SER:O	1:D:773:ILE:HD12	2.17	0.44
1:D:1308:PHE:HB3	1:D:1317:CYS:HB3	1.99	0.44
1:E:905:CYS:HB2	1:E:934:VAL:CG1	2.47	0.44
1:E:1516:ILE:HG23	1:E:1529:ILE:HD12	1.97	0.44
1:A:329:THR:N	1:A:332:SER:OG	2.46	0.44
1:A:1856:HYP:O	5:M:2:FUB:O3	2.36	0.44
1:B:1219:GLY:HA2	1:B:1278:ALA:O	2.18	0.44
1:B:1721:THR:HG22	1:B:1730:CYS:HB2	1.99	0.44
1:B:1809:ARG:NH2	5:KA:5:AHR:O3	2.50	0.44
26:C:2003:AHR:O4	13:WB:3:GZL:H21	2.18	0.44
1:D:677:TRP:CZ2	1:D:737:VAL:HG11	2.52	0.44
1:D:1129:PHE:HD1	1:D:1139:ASN:HA	1.82	0.44
1:E:528:VAL:HG12	1:E:530:GLU:OE1	2.17	0.44
1:E:1014:SER:OG	1:E:1015:PRO:HD3	2.17	0.44
1:E:1786:ASP:OD1	1:E:1786:ASP:N	2.51	0.44
1:F:1084:VAL:HG13	1:F:1086:THR:H	1.82	0.44
3:sB:2:FUB:O3	3:sB:3:FUB:O5	2.36	0.44
1:A:1189:ILE:HB	1:B:1537:PHE:HB2	2.00	0.44
1:B:385:TYR:CZ	1:B:411:HIS:HD2	2.34	0.44
1:B:1022:PRO:HB3	1:B:1028:THR:HG21	1.99	0.44
1:C:54:PRO:HG2	1:C:58:PRO:HB3	1.98	0.44
1:C:904:ILE:HG23	1:C:933:THR:HG23	1.99	0.44
1:E:1141:LEU:HB3	1:E:1143:VAL:HG22	1.97	0.44
1:F:1055:TYR:CZ	1:F:1057:GLY:HA2	2.53	0.44
1:F:1275:THR:O	1:F:1276:HIS:ND1	2.50	0.44
1:A:1126:PHE:HB3	1:A:1148:THR:HB	2.00	0.44
1:A:1326:HIS:CE1	1:B:1375:ILE:HG12	2.52	0.44
1:A:1784:LEU:HD12	1:A:1785:GLY:N	2.33	0.44
1:B:80:PHE:HE2	1:B:135:ALA:HB2	1.83	0.44
1:B:1424:SER:HB3	1:B:1543:SER:HB2	2.00	0.44
1:C:1306:SER:OG	1:F:1373:ALA:O	2.35	0.44
1:C:1927:HYP:HA	1:C:1928:HYP:HD22	1.86	0.44
1:D:753:ILE:HG23	1:D:847:HIS:HB2	2.00	0.44
1:D:1280:GLY:O	1:D:1282:GLU:N	2.51	0.44
1:E:1124:PRO:HB2	1:E:1150:LEU:HD23	1.99	0.44
1:E:1412:THR:HG22	1:E:1447:GLN:HA	2.00	0.44
1:F:797:GLN:NE2	1:F:825:THR:H	2.15	0.44
1:A:663:TRP:CG	1:A:670:ALA:HB2	2.52	0.44
1:A:681:ALA:C	1:A:683:SER:H	2.26	0.44
1:A:1394:ASP:HB3	1:A:1460:SER:HB3	2.00	0.44
1:B:1032:PHE:O	1:B:1109:SER:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1930:HYP:HA	1:B:1931:HYP:HD22	1.73	0.44
1:D:1393:GLU:H	1:D:1393:GLU:CD	2.25	0.44
1:E:1511:LEU:O	1:E:1513:ALA:N	2.49	0.44
1:F:548:LEU:HD13	1:F:552:LEU:HD23	1.98	0.44
1:F:1061:ASN:HB3	1:F:1062:PRO:HD3	2.00	0.44
1:B:1087:ASP:OD1	1:B:1087:ASP:N	2.51	0.44
1:C:1067:SER:HB2	1:C:1073:VAL:HG21	2.00	0.44
1:C:1167:ASN:ND2	1:F:1558:ASP:O	2.51	0.44
1:D:1184:ASP:HB3	1:D:1242:ARG:HB2	2.00	0.44
1:D:1364:ASN:HA	1:D:1397:TRP:O	2.18	0.44
1:F:1067:SER:HB2	1:F:1073:VAL:HG21	2.00	0.44
2:G:40:HYP:HA	2:G:41:HYP:HD22	1.77	0.44
1:A:122:ILE:HD12	1:A:248:THR:HG21	1.99	0.44
1:A:170:LEU:HD12	1:A:170:LEU:H	1.83	0.44
1:B:250:LEU:HD12	1:B:250:LEU:HA	1.77	0.44
1:B:514:TRP:O	1:B:576:SER:HA	2.17	0.44
1:B:690:SER:OG	4:DC:1:FUB:O5	2.31	0.44
1:C:566:LEU:O	1:C:569:SER:OG	2.27	0.44
1:C:1061:ASN:HB3	1:C:1062:PRO:HD3	1.99	0.44
1:E:1085:ALA:HA	1:E:1090:TYR:CG	2.53	0.44
1:E:1451:GLY:N	1:E:1471:ALA:O	2.46	0.44
27:E:2013:GLA:O2	4:jC:4:AHR:O3	2.30	0.44
1:F:1866:HYP:HB3	27:F:2008:GLA:H61	2.00	0.44
3:QB:1:FUB:O3	3:QB:2:FUB:O5	2.36	0.44
22:wE:1:FUB:O5	20:xE:4:AHR:O2	2.36	0.44
18:yE:1:FUB:O5	18:yE:5:AHR:O4	2.35	0.44
1:A:1144:ALA:O	1:A:1146:THR:HG22	2.18	0.43
1:A:1492:ASP:OD1	1:A:1493:ARG:N	2.50	0.43
1:B:84:ASP:HB3	1:B:128:THR:CG2	2.48	0.43
1:C:188:ASP:OD1	1:C:188:ASP:N	2.50	0.43
1:C:918:ALA:O	1:C:921:TYR:HB2	2.18	0.43
1:D:497:LEU:HD23	1:D:518:ILE:HD13	2.00	0.43
1:D:1927:HYP:HA	1:D:1928:HYP:HD22	1.70	0.43
1:E:622:LEU:CD1	1:E:643:ILE:HG12	2.48	0.43
1:E:1909:ARG:HA	1:E:1910:HYP:HD22	1.82	0.43
1:F:609:PRO:HG2	1:F:611:PHE:CE2	2.53	0.43
17:7C:2:NAG:H4	17:7C:3:BMA:H2	1.82	0.43
1:A:273:LEU:HA	1:A:293:THR:HG22	2.00	0.43
1:A:545:PRO:HG2	1:A:551:TRP:CE2	2.54	0.43
1:A:831:PRO:HD2	16:FA:1:NAG:H82	1.99	0.43
1:A:1426:PHE:CZ	1:A:1490:MET:HE2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1927:HYP:HD22	13:BA:3:GZL:O4	2.18	0.43
26:A:2003:HR:O4	6:5:3:GZL:H21	2.17	0.43
1:B:1671:PHE:CE1	1:B:1683:CYS:HB3	2.53	0.43
1:B:1773:TYR:HD2	1:B:1810:GLN:HA	1.83	0.43
1:C:470:ARG:HD3	1:C:470:ARG:HA	1.75	0.43
1:C:1415:ASN:ND2	1:C:1460:SER:O	2.51	0.43
1:C:1905:HYP:HA	1:C:1906:HYP:HD22	1.73	0.43
1:D:400:ASP:OD2	1:D:525:PRO:HD3	2.18	0.43
1:D:513:LYS:HE2	1:D:513:LYS:HB3	1.81	0.43
1:E:1059:ASN:HD21	1:E:1065:ALA:HB2	1.82	0.43
1:F:1629:ILE:HG23	1:F:1676:GLU:HB2	1.99	0.43
1:F:1884:SER:HA	1:F:1885:HYP:HD22	1.82	0.43
18:SE:1:FUB:O5	22:VE:4:HR:O2	2.36	0.43
1:C:1395:GLY:H	1:C:1414:ARG:HB3	1.83	0.43
1:D:660:CYS:HB3	1:D:716:LEU:HD11	2.00	0.43
1:E:1013:ILE:HG23	1:E:1028:THR:HG23	2.00	0.43
3:K:2:FUB:O2	3:K:2:FUB:O5	2.36	0.43
1:A:930:ASP:OD1	1:A:933:THR:N	2.51	0.43
1:B:251:ARG:HD2	1:B:251:ARG:HA	1.84	0.43
1:C:596:ILE:O	1:C:599:THR:HB	2.18	0.43
1:D:627:THR:OG1	1:D:628:PRO:HD3	2.17	0.43
1:E:1217:PRO:O	1:E:1220:THR:OG1	2.36	0.43
1:E:1717:CYS:SG	1:E:1730:CYS:HB3	2.57	0.43
1:E:1907:HYP:HA	1:E:1908:HYP:HD23	1.86	0.43
1:E:1911:HYP:HA	1:E:1912:HYP:HD22	1.77	0.43
1:A:185:ASN:OD1	1:A:185:ASN:N	2.51	0.43
1:A:1634:THR:HB	1:A:1663:PRO:HB2	2.01	0.43
1:A:1704:ARG:NH2	1:D:1168:VAL:O	2.47	0.43
1:B:153:ASP:OD1	1:B:154:SER:N	2.51	0.43
1:B:974:ALA:O	1:B:978:LEU:HD23	2.19	0.43
1:C:499:SER:HA	1:C:515:SER:O	2.18	0.43
1:C:1132:ALA:N	1:C:1135:THR:O	2.51	0.43
1:C:1224:ASP:N	1:C:1224:ASP:OD1	2.42	0.43
1:D:497:LEU:HB3	1:D:606:TYR:CE1	2.54	0.43
1:D:666:LYS:HD3	1:D:712:ALA:HB2	1.99	0.43
1:D:965:LEU:HG	1:D:966:MET:N	2.33	0.43
1:D:1465:CYS:HB3	1:D:1469:THR:OG1	2.18	0.43
1:E:602:TRP:CD2	1:E:606:TYR:HB2	2.53	0.43
1:E:1036:ARG:HG2	1:E:1038:PRO:HD2	2.00	0.43
1:B:191:ALA:CB	1:B:209:ILE:HD11	2.48	0.43
1:B:1052:CYS:HB3	1:B:1126:PHE:CE1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1421:GLN:HG2	1:B:1436:THR:HG23	2.01	0.43
1:B:1876:ASN:OD1	1:B:1876:ASN:N	2.51	0.43
1:D:503:PRO:C	1:D:505:SER:H	2.25	0.43
1:D:1425:PRO:HB3	1:D:1433:PRO:N	2.33	0.43
1:E:540:ASP:OD1	1:E:541:THR:N	2.47	0.43
1:E:561:LEU:HD12	1:E:561:LEU:HA	1.88	0.43
1:E:743:PHE:HE2	1:E:745:THR:HG22	1.84	0.43
1:E:1061:ASN:HB3	1:E:1062:PRO:HD3	2.00	0.43
1:E:1074:TYR:HA	1:E:1077:PHE:CE1	2.53	0.43
1:F:1634:THR:HG22	1:F:1665:PRO:HA	2.00	0.43
1:F:1765:CYS:H	22:RE:6:AHR:C5	2.31	0.43
1:A:628:PRO:HG2	1:A:637:THR:HG23	2.00	0.43
1:B:863:THR:O	1:B:891:THR:HG23	2.19	0.43
1:C:411:HIS:CG	1:C:414:SER:HB3	2.54	0.43
1:C:1052:CYS:HB3	1:C:1126:PHE:CE1	2.54	0.43
1:D:130:ARG:HB3	1:D:141:LEU:HD11	2.01	0.43
1:D:603:ASP:OD1	1:D:603:ASP:C	2.61	0.43
1:D:663:TRP:CG	1:D:670:ALA:HB2	2.53	0.43
1:E:570:ILE:HB	1:E:571:PRO:HD3	2.01	0.43
1:F:637:THR:O	1:F:704:PRO:HD2	2.19	0.43
1:F:886:PHE:CD2	1:F:965:LEU:HD22	2.54	0.43
1:F:1897:HYP:HA	1:F:1898:HYP:HD22	1.82	0.43
1:A:1341:LEU:HA	1:A:1345:ASP:HB2	2.01	0.43
1:B:1394:ASP:OD1	1:B:1416:THR:OG1	2.37	0.43
1:C:943:THR:H	4:JB:1:FUB:C5	2.32	0.43
1:C:1326:HIS:NE2	1:C:1356:ASN:HA	2.34	0.43
1:D:194:GLN:OE1	1:D:239:ARG:NH1	2.45	0.43
1:D:290:GLN:OE1	1:D:342:SER:OG	2.32	0.43
1:D:632:PRO:O	1:D:635:THR:OG1	2.29	0.43
1:D:995:PHE:HD1	1:D:997:THR:H	1.67	0.43
1:D:1080:VAL:HG21	1:D:1095:GLN:HB3	2.01	0.43
1:D:1139:ASN:OD1	1:D:1140:ALA:N	2.51	0.43
26:D:2001:AHR:O2	6:N:3:GZL:H31	2.17	0.43
1:F:666:LYS:HD2	1:F:666:LYS:HA	1.72	0.43
1:F:1143:VAL:HG22	1:F:1144:ALA:H	1.84	0.43
1:F:1326:HIS:HB3	1:F:1373:ALA:HB2	2.00	0.43
11:gA:2:AHR:O2	9:hA:1:FUB:O5	2.37	0.43
1:A:1684:ALA:HA	1:A:1709:ILE:HG22	2.00	0.43
1:A:1907:HYP:HA	1:A:1908:HYP:HD23	1.79	0.43
1:B:641:TYR:HB2	1:B:700:CYS:SG	2.59	0.43
1:C:398:THR:HG22	1:C:491:THR:HB	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:914:ALA:HA	1:C:915:PRO:HD3	1.88	0.43
1:E:1280:GLY:O	1:E:1283:SER:OG	2.30	0.43
1:E:1324:THR:HG22	1:E:1360:GLN:HA	2.00	0.43
1:E:1415:ASN:OD1	1:E:1416:THR:N	2.52	0.43
1:F:1022:PRO:HD2	1:F:1153:PHE:CD2	2.53	0.43
2:G:32:HYP:HA	2:G:33:HYP:HD22	1.94	0.43
13:0D:3:GZL:O4	13:0D:3:GZL:O6	2.34	0.43
1:A:828:THR:HB	1:A:832:TYR:HE2	1.83	0.43
1:B:295:VAL:HG13	1:B:341:VAL:HG22	2.01	0.43
1:D:400:ASP:O	1:D:454:GLN:NE2	2.50	0.43
1:D:622:LEU:HD21	1:D:718:LEU:HD11	2.01	0.43
1:D:886:PHE:CD2	1:D:965:LEU:HD22	2.54	0.43
1:E:1583:ASP:OD1	1:E:1597:GLN:NE2	2.52	0.43
1:F:1331:GLY:H	1:F:1359:ARG:NH2	2.17	0.43
2:I:22:ALA:HA	2:I:23:HYP:HD23	1.80	0.43
1:A:788:LEU:HD22	1:A:840:ASP:HB2	2.01	0.42
1:D:868:SER:HB3	1:D:886:PHE:HE1	1.83	0.42
1:D:1219:GLY:HA2	1:D:1278:ALA:O	2.19	0.42
1:D:1920:HYP:HA	1:D:1921:HYP:HD22	1.78	0.42
1:E:577:PHE:HB3	1:E:579:ARG:NH1	2.33	0.42
1:E:761:THR:HG22	1:E:855:LEU:HG	2.00	0.42
1:E:1439:THR:HG22	1:E:1446:SER:HA	2.01	0.42
1:E:1884:SER:HA	1:E:1885:HYP:HD22	1.84	0.42
1:F:888:ILE:O	1:F:944:THR:HA	2.19	0.42
1:F:1258:LEU:HD21	1:F:1274:VAL:HG13	1.99	0.42
1:F:1452:THR:HB	1:F:1462:CYS:HB3	2.00	0.42
1:F:1511:LEU:O	1:F:1513:ALA:N	2.52	0.42
26:F:2004:HR:A2	13:tD:3:GZL:H21	2.49	0.42
26:F:2005:HR:A3	6:uD:3:GZL:H21	2.49	0.42
2:G:41:HYP:HA	2:G:42:HYP:HD22	1.74	0.42
7:f:2:FUB:O5	7:f:4:HR:O5	2.37	0.42
6:ME:1:FUB:O4	18:PE:4:HR:O2	2.37	0.42
22:wE:2:FUB:O3	22:wE:3:GZL:O6	2.35	0.42
1:A:1512:ARG:NH1	1:A:1531:THR:O	2.50	0.42
1:C:278:THR:O	1:C:280:VAL:HG13	2.18	0.42
1:C:1261:ARG:HH22	1:F:1536:ASN:ND2	2.17	0.42
1:C:1920:HYP:HA	1:C:1921:HYP:HD22	1.81	0.42
1:D:1418:PHE:HZ	1:D:1461:VAL:HG12	1.84	0.42
1:F:687:LYS:HD2	1:F:701:SER:O	2.18	0.42
1:F:801:PRO:HG3	1:F:821:ILE:HG21	2.00	0.42
1:F:879:SER:HB2	1:F:1036:ARG:NH2	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:54:VAL:HA	2:H:55:HYP:HD22	1.83	0.42
1:C:866:VAL:HA	1:C:887:THR:O	2.19	0.42
1:C:1397:TRP:H	1:C:1397:TRP:HD1	1.66	0.42
1:D:666:LYS:HZ2	1:D:708:THR:HG1	1.59	0.42
1:D:1056:THR:OG1	1:D:1093:ASP:OD1	2.29	0.42
1:D:1425:PRO:O	1:D:1431:GLY:HA2	2.19	0.42
1:D:1930:HYP:HA	1:D:1931:HYP:HD22	1.96	0.42
1:F:534:CYS:O	1:F:560:GLY:HA2	2.18	0.42
1:F:1782:ASP:OD1	1:F:1790:GLY:HA2	2.19	0.42
1:A:293:THR:O	1:A:341:VAL:HG23	2.19	0.42
1:A:309:ARG:HB2	1:A:364:TYR:HE1	1.85	0.42
1:A:637:THR:O	1:A:704:PRO:HD2	2.20	0.42
1:A:1375:ILE:HD11	1:B:1306:SER:HA	2.00	0.42
1:B:309:ARG:HG2	1:B:320:THR:O	2.19	0.42
1:B:1327:THR:O	1:B:1357:THR:OG1	2.32	0.42
1:D:1904:SER:HA	1:D:1905:HYP:HD22	1.85	0.42
1:E:663:TRP:NE1	1:E:667:THR:OG1	2.52	0.42
1:E:1341:LEU:O	1:E:1345:ASP:HB3	2.18	0.42
1:E:1549:ASN:HD22	1:E:1563:GLN:HG2	1.84	0.42
1:E:1634:THR:HB	1:E:1663:PRO:HB2	2.00	0.42
1:F:777:ARG:HB3	1:F:813:THR:HG23	2.01	0.42
1:F:1930:HYP:HA	1:F:1931:HYP:HD22	1.82	0.42
4:iA:2:FUB:O3	4:iA:3:FUB:O5	2.37	0.42
1:A:271:LEU:HD11	1:A:363:LEU:HD11	2.01	0.42
1:A:439:ASN:OD1	1:A:439:ASN:N	2.51	0.42
1:A:561:LEU:HD23	1:A:561:LEU:HA	1.89	0.42
1:A:974:ALA:O	1:A:978:LEU:HD23	2.20	0.42
1:C:168:LEU:HD12	1:C:168:LEU:HA	1.81	0.42
1:C:633:VAL:HG12	1:C:746:VAL:HG12	2.02	0.42
1:C:663:TRP:CH2	1:C:665:GLY:HA2	2.54	0.42
1:D:682:GLY:HA2	1:D:686:GLY:O	2.20	0.42
1:D:780:ALA:HA	1:D:813:THR:HG22	2.01	0.42
1:E:506:PRO:HB3	1:E:512:ALA:HB2	2.01	0.42
1:E:532:ILE:HD11	1:E:601:LEU:HD12	2.01	0.42
1:E:1287:CYS:HA	1:E:1347:PHE:HE2	1.84	0.42
1:E:1430:ASP:O	1:E:1503:ASN:ND2	2.43	0.42
1:E:1741:LYS:HE2	21:FE:5:AHR:O3	2.19	0.42
1:F:1220:THR:HG22	1:F:1230:PRO:HA	2.02	0.42
1:A:871:SER:HB3	1:A:883:THR:HG22	2.01	0.42
1:A:1277:LEU:HD23	1:A:1277:LEU:HA	1.89	0.42
1:A:1553:TYR:HB3	1:A:1563:GLN:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1900:SER:HA	1:A:1901:HYP:HD22	1.87	0.42
1:B:777:ARG:NH1	1:B:779:ALA:O	2.40	0.42
1:C:1900:SER:HA	1:C:1901:HYP:HD22	1.88	0.42
1:D:329:THR:OG1	1:D:330:ALA:N	2.52	0.42
1:D:1119:ALA:HA	1:D:1155:THR:OG1	2.19	0.42
1:D:1896:SER:HA	1:D:1897:HYP:HD22	1.90	0.42
1:E:967:VAL:HG23	1:E:988:LEU:HB2	2.02	0.42
1:E:1614:TRP:NE1	1:E:1676:GLU:OE2	2.38	0.42
1:F:904:ILE:HG12	1:F:935:VAL:HG22	2.01	0.42
2:G:55:HYP:HA	2:G:56:HYP:HD22	1.76	0.42
20:xE:1:FUB:O4	18:yE:4:AHR:O2	2.38	0.42
1:A:48:THR:O	1:A:48:THR:OG1	2.34	0.42
1:A:1071:ASP:OD1	1:A:1071:ASP:N	2.52	0.42
1:A:1326:HIS:ND1	1:B:1375:ILE:HG12	2.34	0.42
1:B:780:ALA:HA	1:B:813:THR:HG22	2.02	0.42
1:B:1634:THR:HB	1:B:1663:PRO:HB2	2.01	0.42
1:B:1889:SER:HA	1:B:1890:HYP:HD22	1.86	0.42
1:D:53:GLY:N	1:D:65:THR:O	2.52	0.42
1:D:587:SER:OG	1:D:610:VAL:HG13	2.19	0.42
1:D:788:LEU:HD22	1:D:840:ASP:HB2	2.02	0.42
1:E:839:VAL:HG12	1:E:844:THR:HA	2.00	0.42
1:E:935:VAL:HG11	1:E:972:ALA:HB2	2.02	0.42
1:E:1602:ASN:O	1:E:1625:PRO:HA	2.20	0.42
1:F:628:PRO:HG2	1:F:637:THR:HA	2.02	0.42
1:F:1042:PRO:HA	1:F:1103:PRO:HB3	2.02	0.42
1:F:1452:THR:HG22	1:F:1464:PRO:HA	2.01	0.42
1:A:385:TYR:CZ	1:A:411:HIS:HD2	2.37	0.42
1:A:1773:TYR:CE1	1:A:1795:TYR:HB2	2.55	0.42
1:B:132:TYR:CE2	1:B:141:LEU:HD23	2.55	0.42
1:B:821:ILE:HD11	1:B:824:TYR:CE2	2.54	0.42
1:C:214:THR:O	1:C:217:THR:HG22	2.19	0.42
1:C:408:GLY:HA3	1:C:445:PRO:HB2	2.02	0.42
1:C:1910:HYP:HA	1:C:1911:HYP:HD22	1.77	0.42
1:C:1912:HYP:HA	1:C:1913:HYP:HD22	1.74	0.42
1:D:976:PRO:O	1:D:980:SER:OG	2.28	0.42
1:D:1560:LEU:HD23	1:D:1560:LEU:HA	1.84	0.42
1:F:1055:TYR:HA	1:F:1093:ASP:O	2.19	0.42
1:F:1102:ALA:O	1:F:1105:THR:OG1	2.30	0.42
1:F:1270:THR:HG22	1:F:1271:TYR:N	2.30	0.42
13:mA:4:AHR:O2	12:oA:3:GZL:O5	2.35	0.42
1:A:750:SER:H	1:A:778:ASN:HB2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1119:ALA:O	1:B:1154:THR:HG23	2.19	0.42
1:B:1186:TYR:O	1:B:1225:GLY:HA2	2.20	0.42
1:C:1443:SER:OG	1:C:1444:GLY:N	2.52	0.42
1:D:882:VAL:HB	1:D:951:THR:O	2.19	0.42
1:D:1062:PRO:CD	1:D:1093:ASP:HB2	2.50	0.42
1:D:1415:ASN:OD1	1:D:1416:THR:N	2.53	0.42
1:E:663:TRP:CD2	1:E:670:ALA:HB2	2.55	0.42
1:E:922:TRP:HA	1:E:922:TRP:CE3	2.55	0.42
1:E:966:MET:HG3	1:E:967:VAL:N	2.35	0.42
1:F:545:PRO:HG2	1:F:551:TRP:CE2	2.55	0.42
1:F:1409:PRO:HG2	1:F:1440:GLU:HG3	2.02	0.42
22:iE:3:GZL:O4	22:iE:3:GZL:O6	2.32	0.42
1:A:1073:VAL:O	1:A:1076:THR:OG1	2.37	0.42
1:B:886:PHE:CD2	1:B:965:LEU:HD13	2.55	0.42
1:B:1918:HYP:O	6:3A:3:GZL:O2	2.35	0.42
1:C:1452:THR:HG22	1:C:1464:PRO:HA	2.02	0.42
1:C:1926:SER:HA	1:C:1927:HYP:HD22	1.85	0.42
1:D:175:PHE:HB3	1:D:223:ILE:HD12	2.01	0.42
1:D:297:TYR:CZ	1:D:299:ALA:HB3	2.55	0.42
1:D:1308:PHE:HA	1:D:1319:ALA:HA	2.02	0.42
1:D:1450:PRO:HB2	1:D:1543:SER:HB2	2.02	0.42
1:E:1101:MET:HE3	1:E:1106:GLY:N	2.34	0.42
1:F:1023:TYR:HB3	1:F:1158:ALA:HB2	2.01	0.42
1:F:1522:GLY:O	1:F:1523:PRO:C	2.62	0.42
2:G:49:HYP:HA	2:G:50:HYP:HD22	1.84	0.42
1:A:773:ILE:O	1:A:816:VAL:HA	2.19	0.41
1:A:1874:SER:HA	1:A:1875:HYP:HD22	1.77	0.41
1:A:1929:HYP:HA	1:A:1930:HYP:HD23	1.97	0.41
1:A:1944:ASN:O	1:B:1622:ARG:HD3	2.20	0.41
1:B:83:LEU:HD22	1:B:85:TYR:CE1	2.55	0.41
1:B:1803:ALA:HB2	1:B:1811:CYS:HA	2.02	0.41
1:C:400:ASP:OD2	1:C:522:LYS:NZ	2.49	0.41
1:C:1021:THR:HG22	1:C:1153:PHE:HB2	2.02	0.41
1:C:1326:HIS:HA	1:C:1357:THR:O	2.19	0.41
1:D:52:LEU:HD23	1:D:67:THR:HB	2.02	0.41
1:D:663:TRP:NE1	1:D:668:GLY:O	2.54	0.41
1:D:762:PRO:HG2	1:D:854:VAL:HG22	2.02	0.41
1:D:938:MET:HE2	1:D:945:THR:HB	2.02	0.41
1:D:1080:VAL:HG23	1:D:1097:ARG:HG2	2.00	0.41
1:D:1421:GLN:NE2	1:D:1438:LEU:H	2.13	0.41
1:E:757:LEU:HD22	1:E:771:TRP:NE1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1927:HYP:HA	1:E:1928:HYP:HD22	1.81	0.41
26:F:2005:HR:A2	6:uD:3:GZL:H21	2.50	0.41
2:H:40:HYP:HA	2:H:41:HYP:HD22	1.80	0.41
5:EC:5:HR:O2	6:FC:3:GZL:H61	2.20	0.41
1:A:1737:THR:HA	1:A:1749:PRO:HA	2.03	0.41
1:B:84:ASP:OD1	1:B:85:TYR:N	2.53	0.41
1:C:329:THR:O	1:C:332:SER:OG	2.36	0.41
1:C:793:PRO:HG2	1:C:835:THR:OG1	2.20	0.41
1:C:1376:ALA:HB2	1:F:1376:ALA:HA	2.02	0.41
1:D:659:LEU:N	1:D:721:ASN:HB2	2.36	0.41
1:D:1192:ASN:OD1	1:D:1204:ASP:HA	2.20	0.41
1:E:1291:TYR:HB3	1:E:1301:CYS:HB3	2.01	0.41
1:E:1514:TYR:HB2	1:E:1550:LEU:HD22	2.02	0.41
1:F:1037:ASP:HB3	1:F:1038:PRO:HD3	2.02	0.41
1:F:1573:PRO:HG2	1:F:1588:VAL:HG11	2.03	0.41
1:F:1719:MET:HG2	1:F:1742:THR:HG22	2.01	0.41
1:A:49:LEU:O	1:A:147:VAL:HG21	2.19	0.41
1:C:735:SER:OG	1:C:736:PRO:HD3	2.19	0.41
1:D:909:ASN:OD1	1:D:951:THR:OG1	2.20	0.41
1:D:1330:VAL:HG21	1:E:1379:ASN:HB2	2.02	0.41
1:E:1918:HYP:HD22	6:xC:3:GZL:O2	2.20	0.41
1:F:677:TRP:CE3	1:F:717:GLN:HB3	2.56	0.41
1:F:682:GLY:HA2	1:F:686:GLY:O	2.21	0.41
26:F:2003:HR:C1	6:CD:3:GZL:H41	2.51	0.41
2:G:47:HYP:HA	2:G:48:HYP:HD22	1.83	0.41
1:A:83:LEU:O	1:A:93:THR:OG1	2.30	0.41
1:B:464:THR:HG22	1:B:485:THR:HG23	2.01	0.41
1:B:1034:LEU:HB2	1:B:1108:VAL:HG12	2.03	0.41
1:C:289:THR:O	1:C:289:THR:OG1	2.37	0.41
1:C:908:PHE:CE2	1:C:914:ALA:HA	2.56	0.41
1:C:1451:GLY:HA2	1:C:1471:ALA:HB3	2.01	0.41
1:D:663:TRP:CD2	1:D:670:ALA:HB2	2.54	0.41
1:E:1736:GLY:HA2	1:E:1780:TYR:HB3	2.02	0.41
1:E:1930:HYP:HA	1:E:1931:HYP:HD22	1.76	0.41
1:F:1430:ASP:OD1	1:F:1430:ASP:N	2.52	0.41
1:A:1327:THR:O	1:A:1357:THR:OG1	2.36	0.41
1:A:1910:HYP:HA	1:A:1911:HYP:HD22	1.82	0.41
1:B:1293:GLN:NE2	1:B:1298:GLY:HA3	2.35	0.41
1:E:1823:ASN:ND2	1:F:1844:SER:O	2.54	0.41
1:E:1896:SER:HA	1:E:1897:HYP:HD22	1.91	0.41
1:E:1897:HYP:HA	1:E:1898:HYP:HD22	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:801:PRO:HG2	1:F:819:PHE:CE1	2.56	0.41
1:F:850:LYS:H	1:F:850:LYS:HG2	1.58	0.41
1:F:1026:ILE:HD13	1:F:1026:ILE:HA	1.91	0.41
2:I:16:GLN:OE1	2:I:16:GLN:N	2.34	0.41
2:I:32:HYP:HA	2:I:33:HYP:HD22	1.89	0.41
1:B:1799:TYR:CZ	1:B:1850:ARG:HD2	2.56	0.41
1:C:58:PRO:O	1:C:151:VAL:HA	2.21	0.41
1:C:551:TRP:CE3	1:C:593:GLN:HB2	2.56	0.41
1:C:993:HIS:CD2	1:C:993:HIS:C	2.99	0.41
1:C:1071:ASP:OD1	1:C:1071:ASP:N	2.52	0.41
1:D:662:PHE:HZ	1:D:704:PRO:HG3	1.84	0.41
1:D:1036:ARG:HG2	1:D:1038:PRO:HD2	2.02	0.41
1:D:1515:THR:HG22	1:E:1209:PRO:HD3	2.02	0.41
1:D:1905:HYP:HA	1:D:1906:HYP:HD22	1.75	0.41
26:D:2003:HR:A1	13:zB:3:GZL:C5	2.87	0.41
1:E:720:GLN:HB2	1:E:733:PHE:CE1	2.56	0.41
1:E:1798:PRO:HB2	1:E:1801:PHE:CD1	2.56	0.41
1:E:1929:HYP:HA	1:E:1930:HYP:HD22	1.80	0.41
1:F:498:GLU:OE1	1:F:517:ARG:HD2	2.20	0.41
1:A:1527:LYS:HD2	1:A:1527:LYS:HA	1.77	0.41
1:A:1760:ASP:OD1	1:A:1760:ASP:N	2.53	0.41
1:B:1566:CYS:SG	1:B:1572:MET:HB2	2.61	0.41
1:B:1760:ASP:OD1	1:B:1761:SER:N	2.51	0.41
1:C:1061:ASN:HD22	1:C:1092:ALA:HA	1.86	0.41
1:C:1930:HYP:HA	1:C:1931:HYP:HD22	1.85	0.41
1:F:943:THR:H	4:gD:1:FUB:C5	2.33	0.41
1:F:1308:PHE:HB3	1:F:1317:CYS:HB3	2.03	0.41
1:F:1491:GLY:O	1:F:1547:SER:HB3	2.20	0.41
1:A:659:LEU:HB2	1:A:721:ASN:HB2	2.02	0.41
1:A:935:VAL:HG11	1:A:972:ALA:HB2	2.02	0.41
1:A:1927:HYP:HA	1:A:1928:HYP:HD22	1.76	0.41
1:B:362:ARG:NE	1:B:373:GLU:OE1	2.49	0.41
1:B:529:THR:OG1	1:B:567:PRO:HD3	2.21	0.41
1:B:1168:VAL:O	1:E:1704:ARG:NH2	2.48	0.41
1:B:1511:LEU:HB3	1:B:1536:ASN:ND2	2.36	0.41
1:B:1637:ASN:O	1:C:1948:ASP:HB3	2.21	0.41
1:B:1904:SER:HA	1:B:1905:HYP:HD22	1.84	0.41
1:C:401:ASP:OD1	1:C:401:ASP:N	2.49	0.41
1:C:545:PRO:HG2	1:C:551:TRP:CD2	2.56	0.41
1:C:868:SER:HB3	1:C:886:PHE:CE2	2.56	0.41
1:C:976:PRO:HG2	1:C:977:LEU:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:535:ALA:HB2	1:E:555:ALA:HA	2.02	0.41
1:E:602:TRP:CE3	1:E:606:TYR:HB2	2.56	0.41
1:E:1805:ARG:H	1:E:1805:ARG:HG2	1.60	0.41
1:F:620:TYR:HB2	1:F:734:LEU:HD21	2.03	0.41
1:F:1141:LEU:C	1:F:1143:VAL:H	2.28	0.41
15:eB:2:FUB:O3	15:eB:3:GZL:O5	2.39	0.41
1:A:1167:ASN:ND2	1:B:1558:ASP:O	2.54	0.41
1:A:1689:ALA:HB1	1:A:1694:LEU:HD12	2.03	0.41
1:B:80:PHE:HB3	1:B:95:ARG:HG2	2.01	0.41
1:B:385:TYR:CE2	1:B:411:HIS:HD2	2.39	0.41
1:B:869:VAL:HG13	1:B:885:THR:HB	2.03	0.41
1:C:922:TRP:HZ2	1:C:975:ALA:HA	1.86	0.41
1:C:1018:ASN:OD1	1:C:1021:THR:N	2.46	0.41
1:C:1161:PHE:HB3	1:F:1480:GLN:HB3	2.02	0.41
1:D:462:LEU:HB3	1:D:487:THR:HG22	2.02	0.41
26:D:2003:HR:O4	13:zB:3:GZL:H21	2.20	0.41
1:E:518:ILE:HA	1:E:518:ILE:HD13	1.81	0.41
1:E:622:LEU:HD23	1:E:738:TYR:CG	2.56	0.41
1:E:1519:MET:HE3	1:E:1519:MET:HB2	1.89	0.41
1:E:1806:PRO:HD2	2:G:20:HYP:HD22	2.01	0.41
1:E:1876:ASN:OD1	1:E:1876:ASN:N	2.54	0.41
1:F:609:PRO:HG2	1:F:611:PHE:HE2	1.86	0.41
1:F:1032:PHE:HB2	1:F:1110:CYS:SG	2.61	0.41
2:H:47:HYP:HA	2:H:48:HYP:HD22	1.82	0.41
3:J:2:FUB:O3	3:J:3:FUB:O5	2.39	0.41
1:A:72:SER:OG	1:A:75:SER:O	2.20	0.41
1:A:284:ASP:HA	1:A:416:SER:OG	2.21	0.41
1:A:457:SER:O	1:A:461:LYS:HE2	2.21	0.41
1:A:1722:TYR:CD2	1:A:1746:GLN:HA	2.55	0.41
1:B:278:THR:CG2	1:B:279:SER:N	2.81	0.41
1:B:1926:SER:HA	1:B:1927:HYP:HD22	1.77	0.41
1:C:508:ALA:N	1:C:614:LEU:O	2.53	0.41
1:C:1896:SER:HA	1:C:1897:HYP:HD22	1.82	0.41
1:D:720:GLN:O	1:D:725:LEU:HD13	2.21	0.41
1:E:1077:PHE:N	1:E:1077:PHE:CD1	2.89	0.41
1:F:603:ASP:HB2	1:F:604:PRO:HD3	2.03	0.41
1:F:1070:THR:HG22	1:F:1072:ALA:H	1.86	0.41
1:F:1580:ASN:O	1:F:1581:LEU:C	2.64	0.41
1:A:224:PRO:O	1:A:226:GLN:NE2	2.38	0.40
1:A:666:LYS:NZ	1:A:708:THR:HG23	2.37	0.40
1:A:866:VAL:HA	1:A:887:THR:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:914:ALA:HA	1:A:915:PRO:HD3	1.92	0.40
1:A:1009:GLU:OE2	1:A:1107:ARG:HD3	2.22	0.40
1:A:1493:ARG:NH1	1:A:1549:ASN:O	2.52	0.40
1:B:214:THR:O	1:B:217:THR:HG22	2.21	0.40
1:B:408:GLY:HA3	1:B:445:PRO:HB2	2.03	0.40
1:B:1847:LYS:CE	1:B:1847:LYS:H	2.34	0.40
1:B:1910:HYP:HA	1:B:1911:HYP:HD22	1.87	0.40
1:B:1912:HYP:HA	1:B:1913:HYP:HD22	1.82	0.40
1:C:280:VAL:O	1:C:380:VAL:HA	2.22	0.40
1:C:1029:TYR:CZ	1:C:1113:PRO:HB3	2.57	0.40
1:D:296:SER:HB3	1:D:338:ALA:HA	2.03	0.40
1:D:595:PHE:HA	1:D:599:THR:O	2.21	0.40
1:D:753:ILE:CG1	1:D:773:ILE:HD11	2.51	0.40
1:E:504:PHE:CE2	1:E:656:LEU:HB2	2.56	0.40
1:E:1030:PHE:HB3	1:E:1032:PHE:CE2	2.56	0.40
1:F:1051:ALA:HB2	1:F:1131:TYR:HD1	1.85	0.40
1:F:1796:LYS:O	3:8C:1:FUB:O5	2.39	0.40
1:A:999:MET:HB2	1:A:999:MET:HE2	1.75	0.40
1:A:1166:THR:HG21	1:B:1561:PRO:HB3	2.02	0.40
1:A:1430:ASP:OD1	1:A:1430:ASP:N	2.48	0.40
1:A:1604:GLU:OE1	1:A:1611:LYS:NZ	2.36	0.40
1:A:1775:PRO:HG3	5:M:1:FUB:O3	2.21	0.40
1:B:70:VAL:O	1:B:106:THR:HG23	2.22	0.40
1:B:122:ILE:H	1:B:122:ILE:HG13	1.77	0.40
1:B:507:ILE:HB	1:B:510:VAL:HG22	2.03	0.40
1:B:656:LEU:HD23	1:B:691:MET:HE3	2.03	0.40
1:B:755:SER:HB2	1:B:773:ILE:HD12	2.03	0.40
1:B:1018:ASN:OD1	1:B:1021:THR:HG23	2.21	0.40
1:B:1184:ASP:HB3	1:B:1242:ARG:HB3	2.02	0.40
1:B:1522:GLY:O	1:B:1523:PRO:C	2.64	0.40
1:C:206:ARG:NH1	1:C:243:ALA:O	2.50	0.40
1:C:1326:HIS:NE2	1:C:1355:PRO:O	2.36	0.40
1:D:419:TRP:CD1	1:D:419:TRP:N	2.89	0.40
1:D:664:ASP:CG	1:D:667:THR:HG1	2.29	0.40
1:D:1414:ARG:HB2	1:D:1445:CYS:SG	2.61	0.40
1:E:932:ASP:OD1	1:E:932:ASP:N	2.52	0.40
1:E:952:TYR:HD2	1:E:1041:PRO:HB3	1.85	0.40
1:E:1326:HIS:NE2	1:E:1356:ASN:HA	2.31	0.40
1:E:1910:HYP:HA	1:E:1911:HYP:HD22	1.89	0.40
1:F:536:PHE:HE1	1:F:608:THR:HG21	1.86	0.40
1:F:808:ILE:HG12	1:F:815:THR:HB	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:566:LEU:HB2	1:A:567:PRO:HD2	2.02	0.40
1:B:206:ARG:HD2	1:B:244:PRO:O	2.21	0.40
1:B:272:THR:O	1:B:293:THR:HA	2.22	0.40
1:B:574:ILE:HD12	1:B:574:ILE:O	2.21	0.40
1:B:855:LEU:HD23	1:B:855:LEU:HA	1.93	0.40
26:B:2003:HR:O4	13:2A:3:GZL:H51	2.19	0.40
1:C:1006:VAL:HG21	1:C:1050:PHE:CZ	2.56	0.40
1:D:278:THR:O	1:D:279:SER:C	2.64	0.40
1:D:399:THR:O	1:D:399:THR:OG1	2.34	0.40
1:D:540:ASP:HA	1:D:581:TYR:HE1	1.87	0.40
1:D:771:TRP:HB2	1:D:819:PHE:HB2	2.03	0.40
1:E:904:ILE:O	1:E:967:VAL:HA	2.21	0.40
1:E:908:PHE:HD2	1:E:964:LYS:HB2	1.87	0.40
1:F:618:PRO:HB3	1:F:647:VAL:HG22	2.03	0.40
1:F:1130:GLU:H	1:F:1130:GLU:HG3	1.78	0.40
1:F:1644:ALA:HA	1:F:1655:GLY:O	2.21	0.40
1:F:1789:GLU:HG2	1:F:1794:CYS:O	2.21	0.40
1:F:1798:PRO:HG2	4:AD:4:HR:O5	2.22	0.40
2:I:31:ALA:HA	2:I:32:HYP:HD22	1.87	0.40
1:A:52:LEU:HG	1:A:53:GLY:N	2.35	0.40
1:A:661:SER:HB3	1:A:680:LEU:HD12	2.03	0.40
1:B:1913:HYP:HA	1:B:1914:HYP:HD23	1.97	0.40
1:C:1925:ARG:HB2	1:C:1925:ARG:HH11	1.86	0.40
1:D:1034:LEU:HB2	1:D:1108:VAL:HG12	2.02	0.40
1:D:1040:VAL:HG12	1:D:1103:PRO:HA	2.03	0.40
1:D:1101:MET:HE2	1:D:1106:GLY:HA2	2.04	0.40
1:D:1422:LEU:HD12	1:D:1422:LEU:HA	1.87	0.40
1:E:775:ILE:HG23	1:E:815:THR:HG22	2.02	0.40
1:E:832:TYR:O	1:E:851:ASN:HA	2.22	0.40
26:E:2003:HR:C2	6:xC:3:GZL:H21	2.51	0.40
1:F:549:ALA:O	1:F:552:LEU:HG	2.22	0.40
1:A:422:ILE:HD13	1:A:451:LEU:HD13	2.03	0.40
1:B:499:SER:HB3	1:B:516:PHE:CD1	2.57	0.40
1:B:735:SER:OG	1:B:736:PRO:HD3	2.21	0.40
1:B:1010:SER:HB3	1:B:1033:THR:HB	2.03	0.40
1:C:204:SER:OG	1:C:205:SER:N	2.54	0.40
1:C:1097:ARG:HG3	1:C:1112:PHE:CZ	2.57	0.40
1:C:1110:CYS:HB3	1:C:1112:PHE:HE1	1.86	0.40
1:D:401:ASP:OD1	1:D:401:ASP:N	2.38	0.40
1:D:545:PRO:HG2	1:D:551:TRP:CE2	2.56	0.40
1:D:633:VAL:HG12	1:D:746:VAL:HG12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:781:VAL:HG21	1:D:808:ILE:HG22	2.03	0.40
1:D:1361:CYS:SG	1:D:1367:LEU:HD23	2.62	0.40
1:E:1522:GLY:O	1:E:1523:PRO:C	2.63	0.40
1:F:1012:THR:OG1	1:F:1031:THR:HB	2.22	0.40
1:F:1090:TYR:CZ	1:F:1113:PRO:HG3	2.56	0.40
1:F:1414:ARG:HG3	1:F:1445:CYS:HA	2.04	0.40
1:F:1459:MET:HE2	1:F:1459:MET:HB2	1.87	0.40
1:F:1527:LYS:O	1:F:1528:PRO:C	2.65	0.40
3:wB:2:FUB:O3	3:wB:3:FUB:O5	2.39	0.40

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
All	All	9515/12114 (78%)	8733 (92%)	743 (8%)	39 (0%)	31	65

All (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
1	A	473	VAL
1	B	473	VAL
1	C	169	ASN
1	C	473	VAL
1	D	169	ASN
1	D	473	VAL
1	D	585	ALA
2	G	27	ALA
1	A	1909	ARG
1	B	602	TRP
1	C	602	TRP
1	D	1909	ARG
1	E	1909	ARG
1	F	602	TRP
1	A	169	ASN
1	A	602	TRP
1	A	914	ALA
1	D	602	TRP
1	E	602	TRP
2	G	25	ALA
2	G	57	ALA
2	H	57	ALA
2	I	13	THR
2	I	25	ALA
1	B	914	ALA
1	C	914	ALA
1	D	914	ALA
2	G	13	THR
1	B	169	ASN
1	B	1398	SER
1	E	1398	SER
1	F	914	ALA
1	A	604	PRO
1	B	670	ALA

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

All (505) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	SER
1	A	77	THR
1	A	110	VAL
1	A	118	THR
1	A	149	ILE
1	A	185	ASN
1	A	204	SER
1	A	230	LEU
1	A	235	THR
1	A	271	LEU
1	A	281	THR
1	A	287	THR
1	A	289	THR
1	A	291	THR
1	A	292	THR
1	A	314	ASP
1	A	332	SER
1	A	343	SER

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Mol	Chain	Res	Type
1	A	361	LEU
1	A	393	THR
1	A	398	THR
1	A	399	THR
1	A	416	SER
1	A	456	THR
1	A	491	THR
1	A	499	SER
1	A	529	THR
1	A	562	THR
1	A	564	THR
1	A	570	ILE
1	A	574	ILE
1	A	596	ILE
1	A	613	VAL
1	A	623	SER
1	A	625	SER
1	A	626	VAL
1	A	631	VAL
1	A	696	THR
1	A	707	SER
1	A	708	THR
1	A	711	THR
1	A	755	SER
1	A	758	ASN
1	A	761	THR
1	A	763	VAL
1	A	805	THR
1	A	816	VAL
1	A	826	THR
1	A	860	THR
1	A	866	VAL
1	A	869	VAL
1	A	874	THR
1	A	883	THR
1	A	887	THR
1	A	924	VAL
1	A	944	THR
1	A	946	THR
1	A	967	VAL
1	A	979	THR
1	A	981	LEU

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Mol	Chain	Res	Type
1	A	983	VAL
1	A	1000	VAL
1	A	1013	ILE
1	A	1052	CYS
1	A	1056	THR
1	A	1076	THR
1	A	1078	THR
1	A	1084	VAL
1	A	1108	VAL
1	A	1146	THR
1	A	1163	THR
1	A	1191	SER
1	A	1199	VAL
1	A	1201	VAL
1	A	1222	THR
1	A	1237	SER
1	A	1245	THR
1	A	1258	LEU
1	A	1330	VAL
1	A	1341	LEU
1	A	1377	SER
1	A	1387	THR
1	A	1398	SER
1	A	1460	SER
1	A	1531	THR
1	A	1543	SER
1	A	1548	THR
1	A	1556	ASP
1	A	1576	THR
1	A	1583	ASP
1	A	1584	THR
1	A	1588	VAL
1	A	1595	THR
1	A	1621	LYS
1	A	1648	THR
1	A	1677	THR
1	A	1731	THR
1	A	1748	THR
1	A	1808	VAL
1	A	1854	SER
1	A	1874	SER
1	A	1891	ASN

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Mol	Chain	Res	Type
1	A	1934	SER
1	A	1938	ASN
1	B	50	ASP
1	B	72	SER
1	B	77	THR
1	B	89	VAL
1	B	104	THR
1	B	134	SER
1	B	140	VAL
1	B	151	VAL
1	B	159	THR
1	B	160	LEU
1	B	222	VAL
1	B	250	LEU
1	B	252	THR
1	B	295	VAL
1	B	353	SER
1	B	398	THR
1	B	399	THR
1	B	418	VAL
1	B	429	SER
1	B	430	SER
1	B	433	THR
1	B	498	GLU
1	B	501	VAL
1	B	510	VAL
1	B	528	VAL
1	B	566	LEU
1	B	570	ILE
1	B	603	ASP
1	B	623	SER
1	B	631	VAL
1	B	637	THR
1	B	660	CYS
1	B	708	THR
1	B	716	LEU
1	B	745	THR
1	B	755	SER
1	B	774	VAL
1	B	775	ILE
1	B	787	THR
1	B	816	VAL

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Mol	Chain	Res	Type
1	B	826	THR
1	B	828	THR
1	B	849	THR
1	B	867	THR
1	B	869	VAL
1	B	871	SER
1	B	924	VAL
1	B	927	THR
1	B	943	THR
1	B	944	THR
1	B	955	THR
1	B	956	VAL
1	B	962	THR
1	B	965	LEU
1	B	967	VAL
1	B	977	LEU
1	B	983	VAL
1	B	997	THR
1	B	1000	VAL
1	B	1012	THR
1	B	1035	LEU
1	B	1052	CYS
1	B	1076	THR
1	B	1084	VAL
1	B	1087	ASP
1	B	1100	THR
1	B	1108	VAL
1	B	1110	CYS
1	B	1145	ASP
1	B	1146	THR
1	B	1147	VAL
1	B	1166	THR
1	B	1237	SER
1	B	1245	THR
1	B	1259	THR
1	B	1263	LYS
1	B	1270	THR
1	B	1302	LEU
1	B	1318	THR
1	B	1330	VAL
1	B	1367	LEU
1	B	1377	SER

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Mol	Chain	Res	Type
1	B	1380	LEU
1	B	1387	THR
1	B	1393	GLU
1	B	1436	THR
1	B	1437	THR
1	B	1460	SER
1	B	1486	THR
1	B	1501	VAL
1	B	1538	PHE
1	B	1543	SER
1	B	1545	THR
1	B	1548	THR
1	B	1555	THR
1	B	1576	THR
1	B	1588	VAL
1	B	1622	ARG
1	B	1627	CYS
1	B	1638	VAL
1	B	1648	THR
1	B	1654	THR
1	B	1683	CYS
1	B	1687	THR
1	B	1742	THR
1	B	1764	SER
1	B	1799	TYR
1	B	1874	SER
1	B	1884	SER
1	B	1904	SER
1	B	1934	SER
1	C	46	THR
1	C	48	THR
1	C	67	THR
1	C	69	THR
1	C	97	THR
1	C	110	VAL
1	C	116	THR
1	C	117	VAL
1	C	147	VAL
1	C	159	THR
1	C	179	VAL
1	C	204	SER
1	C	235	THR

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Mol	Chain	Res	Type
1	C	275	VAL
1	C	286	VAL
1	C	287	THR
1	C	289	THR
1	C	292	THR
1	C	332	SER
1	C	348	THR
1	C	377	VAL
1	C	429	SER
1	C	430	SER
1	C	433	THR
1	C	467	ILE
1	C	470	ARG
1	C	480	LEU
1	C	529	THR
1	C	552	LEU
1	C	619	THR
1	C	622	LEU
1	C	627	THR
1	C	631	VAL
1	C	642	ASN
1	C	667	THR
1	C	689	THR
1	C	699	THR
1	C	700	CYS
1	C	726	ASP
1	C	737	VAL
1	C	745	THR
1	C	760	VAL
1	C	761	THR
1	C	781	VAL
1	C	821	ILE
1	C	825	THR
1	C	843	VAL
1	C	869	VAL
1	C	921	TYR
1	C	924	VAL
1	C	943	THR
1	C	944	THR
1	C	950	THR
1	C	962	THR
1	C	967	VAL

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Mol	Chain	Res	Type
1	C	973	THR
1	C	978	LEU
1	C	979	THR
1	C	1011	THR
1	C	1033	THR
1	C	1071	ASP
1	C	1076	THR
1	C	1078	THR
1	C	1128	VAL
1	C	1135	THR
1	C	1172	VAL
1	C	1199	VAL
1	C	1201	VAL
1	C	1239	GLU
1	C	1245	THR
1	C	1258	LEU
1	C	1259	THR
1	C	1269	THR
1	C	1295	ASN
1	C	1365	THR
1	C	1379	ASN
1	C	1384	SER
1	C	1438	LEU
1	C	1925	ARG
1	D	46	THR
1	D	50	ASP
1	D	61	SER
1	D	64	VAL
1	D	76	THR
1	D	110	VAL
1	D	116	THR
1	D	159	THR
1	D	160	LEU
1	D	161	LEU
1	D	179	VAL
1	D	181	SER
1	D	185	ASN
1	D	204	SER
1	D	207	ILE
1	D	231	GLU
1	D	238	LEU
1	D	278	THR

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Mol	Chain	Res	Type
1	D	280	VAL
1	D	281	THR
1	D	287	THR
1	D	289	THR
1	D	352	THR
1	D	379	THR
1	D	398	THR
1	D	399	THR
1	D	416	SER
1	D	422	ILE
1	D	429	SER
1	D	433	THR
1	D	479	LEU
1	D	487	THR
1	D	491	THR
1	D	501	VAL
1	D	509	THR
1	D	524	THR
1	D	531	SER
1	D	540	ASP
1	D	561	LEU
1	D	587	SER
1	D	596	ILE
1	D	608	THR
1	D	619	THR
1	D	623	SER
1	D	664	ASP
1	D	667	THR
1	D	696	THR
1	D	697	THR
1	D	729	THR
1	D	735	SER
1	D	745	THR
1	D	747	THR
1	D	750	SER
1	D	810	VAL
1	D	832	TYR
1	D	869	VAL
1	D	888	ILE
1	D	909	ASN
1	D	934	VAL
1	D	943	THR

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Mol	Chain	Res	Type
1	D	962	THR
1	D	983	VAL
1	D	1000	VAL
1	D	1005	VAL
1	D	1028	THR
1	D	1046	SER
1	D	1059	ASN
1	D	1096	LEU
1	D	1100	THR
1	D	1114	THR
1	D	1128	VAL
1	D	1133	SER
1	D	1160	THR
1	D	1192	ASN
1	D	1201	VAL
1	D	1203	VAL
1	D	1223	MET
1	D	1229	ILE
1	D	1242	ARG
1	D	1299	THR
1	D	1339	THR
1	D	1377	SER
1	D	1398	SER
1	D	1479	CYS
1	D	1490	MET
1	E	507	ILE
1	E	518	ILE
1	E	529	THR
1	E	532	ILE
1	E	562	THR
1	E	568	SER
1	E	610	VAL
1	E	623	SER
1	E	635	THR
1	E	640	THR
1	E	701	SER
1	E	745	THR
1	E	761	THR
1	E	770	VAL
1	E	774	VAL
1	E	815	THR
1	E	816	VAL

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Mol	Chain	Res	Type
1	E	821	ILE
1	E	846	SER
1	E	848	ILE
1	E	913	THR
1	E	924	VAL
1	E	962	THR
1	E	983	VAL
1	E	1000	VAL
1	E	1008	VAL
1	E	1012	THR
1	E	1058	GLN
1	E	1078	THR
1	E	1128	VAL
1	E	1146	THR
1	E	1259	THR
1	E	1318	THR
1	E	1334	THR
1	E	1369	LEU
1	E	1387	THR
1	E	1416	THR
1	E	1460	SER
1	E	1479	CYS
1	E	1501	VAL
1	E	1515	THR
1	E	1548	THR
1	E	1555	THR
1	E	1578	THR
1	E	1588	VAL
1	E	1648	THR
1	E	1677	THR
1	E	1678	THR
1	E	1721	THR
1	E	1730	CYS
1	E	1737	THR
1	E	1738	VAL
1	E	1744	SER
1	E	1786	ASP
1	E	1788	PHE
1	E	1799	TYR
1	E	1808	VAL
1	E	1819	LEU
1	E	1829	THR

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Mol	Chain	Res	Type
1	E	1832	LEU
1	E	1841	SER
1	E	1844	SER
1	E	1861	SER
1	E	1884	SER
1	E	1891	ASN
1	E	1895	THR
1	F	524	THR
1	F	564	THR
1	F	614	LEU
1	F	619	THR
1	F	646	SER
1	F	690	SER
1	F	699	THR
1	F	713	THR
1	F	746	VAL
1	F	761	THR
1	F	763	VAL
1	F	774	VAL
1	F	795	ASN
1	F	805	THR
1	F	807	ASP
1	F	816	VAL
1	F	867	THR
1	F	868	SER
1	F	870	VAL
1	F	954	THR
1	F	993	HIS
1	F	1028	THR
1	F	1056	THR
1	F	1084	VAL
1	F	1096	LEU
1	F	1101	MET
1	F	1191	SER
1	F	1233	SER
1	F	1245	THR
1	F	1251	THR
1	F	1274	VAL
1	F	1315	THR
1	F	1318	THR
1	F	1322	GLU
1	F	1334	THR

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Mol	Chain	Res	Type
1	F	1349	SER
1	F	1460	SER
1	F	1479	CYS
1	F	1548	THR
1	F	1555	THR
1	F	1583	ASP
1	F	1587	THR
1	F	1588	VAL
1	F	1627	CYS
1	F	1677	THR
1	F	1678	THR
1	F	1681	THR
1	F	1738	VAL
1	F	1742	THR
1	F	1761	SER
1	F	1799	TYR
1	F	1808	VAL
1	F	1830	GLU
1	F	1861	SER
1	F	1871	ARG
1	F	1874	SER
1	F	1884	SER
1	F	1926	SER
2	H	54	VAL
2	I	13	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1167	ASN
1	A	1192	ASN
1	A	1272	HIS
1	A	1421	GLN
1	A	1487	ASN
1	A	1536	ASN
1	A	1563	GLN
1	B	909	ASN
1	B	1192	ASN
1	B	1293	GLN
1	B	1406	GLN
1	B	1447	GLN
1	B	1536	ASN

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Mol	Chain	Res	Type
1	B	1549	ASN
1	B	1563	GLN
1	B	1631	GLN
1	B	1672	GLN
1	B	1701	GLN
1	B	1891	ASN
1	C	358	ASN
1	C	612	GLN
1	C	717	GLN
1	C	1295	ASN
1	D	358	ASN
1	D	1212	GLN
1	D	1480	GLN
1	E	717	GLN
1	E	720	GLN
1	E	847	HIS
1	E	1293	GLN
1	E	1597	GLN
1	E	1672	GLN
1	F	1835	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%)

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

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

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

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

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

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

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

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

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

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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.

All (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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
1	F	1883	HYP	CG-CB-CA	-3.29	99.95	103.75
1	A	1908	HYP	CG-CB-CA	-3.24	100.00	103.75
2	G	11	HYP	CG-CB-CA	-3.17	100.09	103.75
1	F	1894	HYP	CG-CB-CA	-3.12	100.14	103.75
1	B	1894	HYP	CG-CB-CA	-3.08	100.19	103.75
1	F	1923	HYP	CG-CB-CA	-3.06	100.22	103.75
1	F	1888	HYP	CG-CB-CA	-3.05	100.22	103.75
1	B	1868	HYP	CG-CB-CA	-3.01	100.27	103.75
1	A	1907	HYP	CG-CB-CA	-3.01	100.27	103.75
1	E	1888	HYP	CG-CB-CA	-3.00	100.28	103.75
2	I	10	HYP	O-C-CA	-2.98	117.10	124.77
2	I	34	HYP	O-C-CA	-2.98	117.11	124.77
2	G	10	HYP	O-C-CA	-2.97	117.12	124.77
1	A	1908	HYP	O-C-CA	-2.92	117.25	124.77
2	I	11	HYP	CG-CB-CA	-2.92	100.37	103.75
1	B	1908	HYP	O-C-CA	-2.91	117.29	124.77
1	F	1868	HYP	CG-CB-CA	-2.88	100.42	103.75
1	B	1907	HYP	O-C-CA	-2.88	117.37	124.77
1	E	1867	HYP	O-C-CA	-2.86	117.42	124.77
1	E	1878	HYP	CG-CB-CA	-2.86	100.45	103.75
1	E	1908	HYP	CG-CB-CA	-2.83	100.48	103.75
1	F	1857	HYP	O-C-CA	-2.83	117.49	124.77
1	A	1922	HYP	O-C-CA	-2.83	117.50	124.77
2	G	4	HYP	O-C-CA	-2.82	117.52	124.77
1	E	1860	HYP	CG-CB-CA	-2.81	100.50	103.75
1	D	1906	HYP	O-C-CA	-2.81	117.55	124.77
1	A	1907	HYP	O-C-CA	-2.81	117.55	124.77
1	B	1931	HYP	O-C-CA	-2.80	117.57	124.77
1	E	1868	HYP	O-C-CA	-2.79	117.60	124.77
1	B	1917	HYP	O-C-CA	-2.79	117.60	124.77
1	F	1865	HYP	O-C-CA	-2.78	117.62	124.77
1	B	1872	HYP	O-C-CA	-2.77	117.63	124.77
1	A	1865	HYP	O-C-CA	-2.77	117.64	124.77
1	B	1858	HYP	O-C-CA	-2.77	117.64	124.77
1	D	1918	HYP	O-C-CA	-2.77	117.64	124.77
1	A	1917	HYP	O-C-CA	-2.76	117.67	124.77
1	F	1893	HYP	O-C-CA	-2.75	117.69	124.77
1	B	1914	HYP	O-C-CA	-2.75	117.70	124.77
1	E	1858	HYP	O-C-CA	-2.75	117.70	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	1868	HYP	O-C-CA	-2.75	117.70	124.77
1	F	1880	HYP	O-C-CA	-2.75	117.70	124.77
1	B	1902	HYP	O-C-CA	-2.74	117.72	124.77
1	A	1902	HYP	O-C-CA	-2.74	117.73	124.77
1	B	1923	HYP	O-C-CA	-2.74	117.73	124.77
1	A	1931	HYP	O-C-CA	-2.73	117.74	124.77
2	I	5	HYP	O-C-CA	-2.73	117.74	124.77
1	E	1865	HYP	O-C-CA	-2.73	117.74	124.77
1	F	1864	HYP	O-C-CA	-2.73	117.75	124.77
1	B	1932	HYP	O-C-CA	-2.73	117.75	124.77
1	A	1868	HYP	O-C-CA	-2.73	117.75	124.77
2	H	44	HYP	O-C-CA	-2.73	117.76	124.77
1	E	1857	HYP	O-C-CA	-2.73	117.76	124.77
1	C	1932	HYP	O-C-CA	-2.72	117.77	124.77
1	C	1930	HYP	O-C-CA	-2.72	117.77	124.77
1	A	1923	HYP	O-C-CA	-2.72	117.77	124.77
1	E	1916	HYP	O-C-CA	-2.72	117.78	124.77
1	E	1908	HYP	O-C-CA	-2.72	117.78	124.77
1	F	1863	HYP	O-C-CA	-2.72	117.78	124.77
1	E	1864	HYP	O-C-CA	-2.72	117.78	124.77
2	G	3	HYP	O-C-CA	-2.71	117.80	124.77
1	F	1877	HYP	O-C-CA	-2.71	117.80	124.77
1	A	1916	HYP	O-C-CA	-2.71	117.81	124.77
1	C	1923	HYP	CG-CB-CA	-2.70	100.63	103.75
1	E	1903	HYP	CG-CB-CA	-2.70	100.63	103.75
2	G	11	HYP	O-C-CA	-2.70	117.83	124.77
2	G	42	HYP	O-C-CA	-2.70	117.83	124.77
1	A	1880	HYP	O-C-CA	-2.70	117.84	124.77
1	D	1908	HYP	O-C-CA	-2.70	117.84	124.77
1	A	1894	HYP	O-C-CA	-2.69	117.84	124.77
1	A	1893	HYP	O-C-CA	-2.69	117.84	124.77
1	B	1908	HYP	CG-CB-CA	-2.69	100.64	103.75
1	F	1931	HYP	O-C-CA	-2.69	117.86	124.77
1	D	1902	HYP	O-C-CA	-2.69	117.86	124.77
1	B	1865	HYP	O-C-CA	-2.69	117.86	124.77
1	D	1931	HYP	O-C-CA	-2.68	117.87	124.77
1	C	1923	HYP	O-C-CA	-2.68	117.89	124.77
1	B	1922	HYP	O-C-CA	-2.68	117.89	124.77
2	G	43	HYP	O-C-CA	-2.67	117.89	124.77
2	H	43	HYP	O-C-CA	-2.67	117.90	124.77
1	D	1921	HYP	O-C-CA	-2.67	117.90	124.77
2	G	8	HYP	O-C-CA	-2.67	117.90	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1878	HYP	O-C-CA	-2.67	117.91	124.77
1	E	1922	HYP	O-C-CA	-2.67	117.91	124.77
1	F	1858	HYP	O-C-CA	-2.67	117.91	124.77
1	B	1915	HYP	O-C-CA	-2.67	117.91	124.77
1	B	1887	HYP	O-C-CA	-2.67	117.91	124.77
1	A	1857	HYP	O-C-CA	-2.67	117.92	124.77
2	G	45	HYP	O-C-CA	-2.66	117.92	124.77
2	H	51	HYP	O-C-CA	-2.66	117.92	124.77
1	A	1894	HYP	CG-CB-CA	-2.66	100.68	103.75
1	C	1907	HYP	O-C-CA	-2.66	117.93	124.77
1	A	1918	HYP	O-C-CA	-2.66	117.94	124.77
2	I	3	HYP	O-C-CA	-2.66	117.94	124.77
2	I	8	HYP	O-C-CA	-2.66	117.94	124.77
1	B	1913	HYP	O-C-CA	-2.66	117.94	124.77
2	H	49	HYP	O-C-CA	-2.65	117.94	124.77
1	A	1899	HYP	O-C-CA	-2.65	117.95	124.77
1	A	1914	HYP	O-C-CA	-2.65	117.95	124.77
1	B	1863	HYP	O-C-CA	-2.65	117.95	124.77
1	E	1907	HYP	O-C-CA	-2.65	117.95	124.77
1	F	1902	HYP	O-C-CA	-2.65	117.95	124.77
1	B	1899	HYP	O-C-CA	-2.65	117.96	124.77
1	F	1855	HYP	O-C-CA	-2.65	117.96	124.77
2	I	4	HYP	O-C-CA	-2.65	117.96	124.77
2	G	51	HYP	O-C-CA	-2.65	117.96	124.77
1	A	1866	HYP	O-C-CA	-2.65	117.96	124.77
1	E	1918	HYP	O-C-CA	-2.65	117.96	124.77
1	E	1877	HYP	O-C-CA	-2.65	117.96	124.77
1	A	1927	HYP	O-C-CA	-2.65	117.97	124.77
1	C	1931	HYP	O-C-CA	-2.65	117.97	124.77
1	F	1906	HYP	O-C-CA	-2.64	117.97	124.77
1	B	1903	HYP	O-C-CA	-2.64	117.97	124.77
1	E	1863	HYP	O-C-CA	-2.64	117.97	124.77
1	F	1922	HYP	O-C-CA	-2.64	117.97	124.77
1	D	1918	HYP	CG-CB-CA	-2.64	100.70	103.75
1	F	1914	HYP	O-C-CA	-2.64	117.97	124.77
1	F	1866	HYP	O-C-CA	-2.64	117.97	124.77
1	A	1903	HYP	O-C-CA	-2.64	117.98	124.77
1	A	1862	HYP	O-C-CA	-2.64	117.99	124.77
1	A	1864	HYP	O-C-CA	-2.64	117.99	124.77
1	C	1908	HYP	O-C-CA	-2.63	118.00	124.77
1	F	1873	HYP	O-C-CA	-2.63	118.00	124.77
1	D	1915	HYP	O-C-CA	-2.63	118.00	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	1899	HYP	O-C-CA	-2.63	118.00	124.77
1	D	1923	HYP	O-C-CA	-2.63	118.00	124.77
1	F	1862	HYP	O-C-CA	-2.63	118.00	124.77
1	B	1916	HYP	O-C-CA	-2.63	118.01	124.77
1	B	1921	HYP	O-C-CA	-2.63	118.02	124.77
1	D	1922	HYP	O-C-CA	-2.63	118.02	124.77
2	G	49	HYP	O-C-CA	-2.63	118.02	124.77
1	A	1930	HYP	O-C-CA	-2.62	118.02	124.77
1	E	1902	HYP	O-C-CA	-2.62	118.02	124.77
1	C	1899	HYP	O-C-CA	-2.62	118.02	124.77
1	A	1888	HYP	O-C-CA	-2.62	118.03	124.77
1	A	1872	HYP	O-C-CA	-2.62	118.03	124.77
1	E	1862	HYP	O-C-CA	-2.62	118.03	124.77
2	G	9	HYP	CG-CB-CA	-2.62	100.72	103.75
1	B	1930	HYP	O-C-CA	-2.62	118.04	124.77
1	F	1856	HYP	O-C-CA	-2.62	118.04	124.77
1	F	1872	HYP	O-C-CA	-2.62	118.04	124.77
1	F	1907	HYP	O-C-CA	-2.62	118.04	124.77
1	A	1921	HYP	O-C-CA	-2.62	118.04	124.77
1	F	1867	HYP	O-C-CA	-2.62	118.04	124.77
1	E	1880	HYP	O-C-CA	-2.61	118.05	124.77
2	G	46	HYP	O-C-CA	-2.61	118.05	124.77
2	H	46	HYP	O-C-CA	-2.61	118.05	124.77
2	H	41	HYP	O-C-CA	-2.61	118.06	124.77
1	B	1918	HYP	O-C-CA	-2.61	118.06	124.77
1	D	1898	HYP	O-C-CA	-2.61	118.07	124.77
2	H	42	HYP	O-C-CA	-2.60	118.07	124.77
1	A	1890	HYP	O-C-CA	-2.60	118.08	124.77
1	B	1857	HYP	O-C-CA	-2.60	118.08	124.77
2	G	2	HYP	O-C-CA	-2.60	118.08	124.77
1	B	1856	HYP	O-C-CA	-2.60	118.08	124.77
2	G	47	HYP	O-C-CA	-2.60	118.09	124.77
1	D	1907	HYP	O-C-CA	-2.60	118.09	124.77
1	D	1930	HYP	O-C-CA	-2.60	118.09	124.77
1	E	1872	HYP	O-C-CA	-2.60	118.09	124.77
1	F	1915	HYP	O-C-CA	-2.60	118.09	124.77
1	E	1912	HYP	O-C-CA	-2.60	118.09	124.77
1	D	1913	HYP	O-C-CA	-2.59	118.10	124.77
1	C	1917	HYP	O-C-CA	-2.59	118.10	124.77
1	B	1928	HYP	O-C-CA	-2.59	118.10	124.77
1	C	1918	HYP	O-C-CA	-2.59	118.11	124.77
1	A	1887	HYP	O-C-CA	-2.59	118.11	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1902	HYP	O-C-CA	-2.59	118.11	124.77
1	E	1914	HYP	O-C-CA	-2.59	118.11	124.77
1	D	1916	HYP	O-C-CA	-2.59	118.11	124.77
1	C	1914	HYP	O-C-CA	-2.59	118.11	124.77
1	E	1866	HYP	O-C-CA	-2.59	118.11	124.77
1	A	1877	HYP	O-C-CA	-2.59	118.11	124.77
1	B	1880	HYP	O-C-CA	-2.59	118.11	124.77
1	E	1918	HYP	CG-CB-CA	-2.59	100.76	103.75
1	B	1893	HYP	O-C-CA	-2.59	118.11	124.77
1	D	1899	HYP	O-C-CA	-2.59	118.11	124.77
2	I	20	HYP	O-C-CA	-2.59	118.12	124.77
1	E	1887	HYP	O-C-CA	-2.58	118.12	124.77
2	I	6	HYP	O-C-CA	-2.58	118.12	124.77
2	G	52	HYP	O-C-CA	-2.58	118.12	124.77
1	F	1913	HYP	O-C-CA	-2.58	118.13	124.77
1	F	1908	HYP	O-C-CA	-2.58	118.13	124.77
1	A	1915	HYP	O-C-CA	-2.58	118.13	124.77
1	B	1877	HYP	O-C-CA	-2.58	118.13	124.77
1	E	1885	HYP	O-C-CA	-2.58	118.14	124.77
1	F	1897	HYP	O-C-CA	-2.58	118.14	124.77
2	G	14	HYP	O-C-CA	-2.58	118.14	124.77
1	A	1868	HYP	CG-CB-CA	-2.58	100.77	103.75
2	G	7	HYP	O-C-CA	-2.58	118.14	124.77
1	E	1888	HYP	O-C-CA	-2.58	118.14	124.77
1	F	1928	HYP	O-C-CA	-2.58	118.15	124.77
1	A	1883	HYP	O-C-CA	-2.57	118.15	124.77
1	C	1921	HYP	O-C-CA	-2.57	118.15	124.77
1	F	1885	HYP	O-C-CA	-2.57	118.15	124.77
1	A	1898	HYP	O-C-CA	-2.57	118.15	124.77
1	D	1927	HYP	O-C-CA	-2.57	118.16	124.77
1	E	1856	HYP	O-C-CA	-2.57	118.16	124.77
1	D	1903	HYP	O-C-CA	-2.57	118.16	124.77
1	C	1915	HYP	O-C-CA	-2.57	118.16	124.77
2	G	56	HYP	O-C-CA	-2.57	118.17	124.77
1	A	1875	HYP	O-C-CA	-2.57	118.17	124.77
1	B	1927	HYP	O-C-CA	-2.57	118.17	124.77
1	B	1888	HYP	O-C-CA	-2.56	118.18	124.77
1	C	1929	HYP	O-C-CA	-2.56	118.18	124.77
1	F	1923	HYP	O-C-CA	-2.56	118.18	124.77
2	H	56	HYP	O-C-CA	-2.56	118.18	124.77
1	C	1903	HYP	O-C-CA	-2.56	118.19	124.77
1	E	1923	HYP	O-C-CA	-2.56	118.19	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1878	HYP	CG-CB-CA	-2.56	100.79	103.75
1	E	1921	HYP	O-C-CA	-2.56	118.19	124.77
1	A	1855	HYP	O-C-CA	-2.56	118.19	124.77
1	B	1898	HYP	O-C-CA	-2.56	118.19	124.77
1	E	1882	HYP	O-C-CA	-2.56	118.19	124.77
1	C	1908	HYP	CG-CB-CA	-2.56	100.80	103.75
1	E	1928	HYP	O-C-CA	-2.55	118.20	124.77
1	F	1894	HYP	O-C-CA	-2.55	118.20	124.77
1	B	1882	HYP	O-C-CA	-2.55	118.20	124.77
2	G	33	HYP	O-C-CA	-2.55	118.20	124.77
2	G	44	HYP	O-C-CA	-2.55	118.20	124.77
1	C	1927	HYP	O-C-CA	-2.55	118.20	124.77
1	C	1897	HYP	O-C-CA	-2.55	118.20	124.77
1	E	1893	HYP	O-C-CA	-2.55	118.21	124.77
1	B	1867	HYP	O-C-CA	-2.55	118.21	124.77
1	C	1922	HYP	O-C-CA	-2.55	118.21	124.77
1	E	1873	HYP	O-C-CA	-2.55	118.21	124.77
1	E	1905	HYP	O-C-CA	-2.55	118.22	124.77
1	A	1892	HYP	O-C-CA	-2.55	118.22	124.77
1	C	1913	HYP	O-C-CA	-2.55	118.22	124.77
1	A	1885	HYP	O-C-CA	-2.55	118.22	124.77
1	B	1894	HYP	O-C-CA	-2.55	118.22	124.77
2	G	6	HYP	O-C-CA	-2.55	118.22	124.77
2	I	14	HYP	O-C-CA	-2.55	118.22	124.77
1	A	1929	HYP	O-C-CA	-2.55	118.22	124.77
1	A	1911	HYP	O-C-CA	-2.54	118.22	124.77
1	E	1911	HYP	O-C-CA	-2.54	118.23	124.77
1	A	1897	HYP	O-C-CA	-2.54	118.23	124.77
2	G	20	HYP	O-C-CA	-2.54	118.23	124.77
1	A	1863	HYP	O-C-CA	-2.54	118.23	124.77
1	E	1929	HYP	O-C-CA	-2.54	118.23	124.77
1	F	1888	HYP	O-C-CA	-2.54	118.23	124.77
1	F	1892	HYP	O-C-CA	-2.54	118.24	124.77
1	B	1929	HYP	O-C-CA	-2.54	118.24	124.77
1	E	1931	HYP	O-C-CA	-2.54	118.24	124.77
1	F	1929	HYP	O-C-CA	-2.54	118.24	124.77
1	A	1906	HYP	O-C-CA	-2.54	118.24	124.77
2	I	17	HYP	O-C-CA	-2.54	118.25	124.77
1	F	1921	HYP	O-C-CA	-2.53	118.25	124.77
1	B	1862	HYP	O-C-CA	-2.53	118.26	124.77
1	F	1917	HYP	O-C-CA	-2.53	118.26	124.77
1	B	1923	HYP	CG-CB-CA	-2.53	100.83	103.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	48	HYP	O-C-CA	-2.53	118.26	124.77
1	D	1905	HYP	O-C-CA	-2.53	118.26	124.77
2	H	48	HYP	O-C-CA	-2.53	118.26	124.77
1	A	1882	HYP	O-C-CA	-2.53	118.27	124.77
1	B	1908	HYP	CB-CG-CD	-2.53	100.34	103.16
1	A	1913	HYP	O-C-CA	-2.53	118.27	124.77
2	I	1	HYP	O-C-CA	-2.53	118.27	124.77
1	B	1855	HYP	O-C-CA	-2.53	118.27	124.77
1	B	1883	HYP	O-C-CA	-2.53	118.28	124.77
1	E	1855	HYP	O-C-CA	-2.53	118.28	124.77
1	F	1930	HYP	O-C-CA	-2.52	118.28	124.77
1	E	1927	HYP	O-C-CA	-2.52	118.28	124.77
1	A	1912	HYP	O-C-CA	-2.52	118.29	124.77
1	C	1928	HYP	O-C-CA	-2.52	118.29	124.77
2	H	52	HYP	O-C-CA	-2.52	118.29	124.77
1	A	1856	HYP	O-C-CA	-2.52	118.30	124.77
1	E	1894	HYP	O-C-CA	-2.52	118.30	124.77
2	G	32	HYP	O-C-CA	-2.51	118.30	124.77
1	B	1903	HYP	CG-CB-CA	-2.51	100.85	103.75
1	B	1868	HYP	O-C-CA	-2.51	118.31	124.77
1	F	1916	HYP	O-C-CA	-2.51	118.31	124.77
2	I	11	HYP	O-C-CA	-2.51	118.31	124.77
1	C	1912	HYP	O-C-CA	-2.51	118.32	124.77
2	G	29	HYP	O-C-CA	-2.51	118.32	124.77
1	B	1905	HYP	O-C-CA	-2.51	118.32	124.77
1	B	1912	HYP	O-C-CA	-2.51	118.32	124.77
1	F	1918	HYP	O-C-CA	-2.51	118.32	124.77
2	G	41	HYP	O-C-CA	-2.51	118.32	124.77
1	B	1870	HYP	O-C-CA	-2.51	118.32	124.77
2	I	33	HYP	O-C-CA	-2.50	118.33	124.77
1	F	1903	HYP	O-C-CA	-2.50	118.33	124.77
1	E	1899	HYP	O-C-CA	-2.50	118.33	124.77
1	D	1911	HYP	O-C-CA	-2.50	118.34	124.77
1	D	1932	HYP	O-C-CA	-2.50	118.34	124.77
1	E	1875	HYP	O-C-CA	-2.50	118.34	124.77
1	E	1908	HYP	CB-CG-CD	-2.50	100.37	103.16
1	B	1866	HYP	O-C-CA	-2.50	118.34	124.77
1	C	1932	HYP	CG-CB-CA	-2.50	100.86	103.75
2	G	26	HYP	O-C-CA	-2.50	118.35	124.77
1	E	1903	HYP	O-C-CA	-2.50	118.35	124.77
1	B	1890	HYP	O-C-CA	-2.49	118.36	124.77
2	H	50	HYP	O-C-CA	-2.49	118.36	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1860	HYP	CG-CB-CA	-2.49	100.87	103.75
1	E	1898	HYP	O-C-CA	-2.49	118.37	124.77
1	E	1878	HYP	O-C-CA	-2.49	118.37	124.77
1	D	1912	HYP	O-C-CA	-2.49	118.37	124.77
1	F	1898	HYP	O-C-CA	-2.49	118.37	124.77
2	I	7	HYP	O-C-CA	-2.49	118.37	124.77
1	C	1906	HYP	O-C-CA	-2.49	118.38	124.77
2	G	17	HYP	O-C-CA	-2.49	118.38	124.77
2	I	29	HYP	O-C-CA	-2.48	118.38	124.77
1	B	1911	HYP	O-C-CA	-2.48	118.38	124.77
1	A	1905	HYP	O-C-CA	-2.48	118.39	124.77
1	A	1932	HYP	O-C-CA	-2.48	118.39	124.77
2	G	9	HYP	O-C-CA	-2.48	118.39	124.77
1	A	1867	HYP	O-C-CA	-2.48	118.39	124.77
1	C	1910	HYP	O-C-CA	-2.48	118.39	124.77
1	C	1905	HYP	O-C-CA	-2.48	118.39	124.77
2	H	47	HYP	O-C-CA	-2.48	118.39	124.77
1	B	1885	HYP	O-C-CA	-2.48	118.40	124.77
1	C	1911	HYP	O-C-CA	-2.48	118.40	124.77
1	A	1873	HYP	O-C-CA	-2.48	118.40	124.77
2	I	2	HYP	O-C-CA	-2.48	118.40	124.77
2	G	5	HYP	O-C-CA	-2.47	118.41	124.77
1	A	1858	HYP	O-C-CA	-2.47	118.42	124.77
1	B	1910	HYP	O-C-CA	-2.47	118.42	124.77
1	F	1932	HYP	O-C-CA	-2.47	118.42	124.77
1	F	1882	HYP	O-C-CA	-2.47	118.42	124.77
1	D	1917	HYP	O-C-CA	-2.47	118.42	124.77
2	G	50	HYP	O-C-CA	-2.46	118.43	124.77
1	D	1899	HYP	CG-CB-CA	-2.46	100.91	103.75
1	B	1901	HYP	O-C-CA	-2.46	118.44	124.77
1	B	1920	HYP	O-C-CA	-2.46	118.44	124.77
2	I	9	HYP	O-C-CA	-2.46	118.45	124.77
1	C	1898	HYP	O-C-CA	-2.46	118.45	124.77
1	F	1883	HYP	O-C-CA	-2.46	118.45	124.77
1	D	1929	HYP	O-C-CA	-2.46	118.45	124.77
1	F	1905	HYP	O-C-CA	-2.45	118.46	124.77
1	E	1892	HYP	O-C-CA	-2.45	118.46	124.77
1	F	1911	HYP	O-C-CA	-2.45	118.46	124.77
1	A	1910	HYP	O-C-CA	-2.45	118.46	124.77
1	F	1875	HYP	O-C-CA	-2.45	118.47	124.77
1	F	1912	HYP	O-C-CA	-2.45	118.47	124.77
1	C	1920	HYP	O-C-CA	-2.45	118.48	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	55	HYP	O-C-CA	-2.44	118.48	124.77
1	E	1910	HYP	O-C-CA	-2.44	118.49	124.77
2	G	55	HYP	O-C-CA	-2.44	118.49	124.77
1	C	1916	HYP	O-C-CA	-2.44	118.49	124.77
1	E	1901	HYP	O-C-CA	-2.44	118.50	124.77
2	G	34	HYP	O-C-CA	-2.44	118.50	124.77
1	B	1875	HYP	O-C-CA	-2.44	118.50	124.77
2	G	40	HYP	O-C-CA	-2.44	118.50	124.77
1	D	1897	HYP	O-C-CA	-2.43	118.51	124.77
1	E	1917	HYP	O-C-CA	-2.43	118.51	124.77
2	I	32	HYP	O-C-CA	-2.43	118.52	124.77
1	B	1892	HYP	O-C-CA	-2.43	118.52	124.77
1	F	1878	HYP	O-C-CA	-2.43	118.52	124.77
1	A	1878	HYP	CG-CB-CA	-2.43	100.95	103.75
2	H	45	HYP	O-C-CA	-2.42	118.54	124.77
1	E	1907	HYP	CG-CB-CA	-2.42	100.96	103.75
1	B	1906	HYP	O-C-CA	-2.42	118.55	124.77
1	A	1901	HYP	O-C-CA	-2.41	118.56	124.77
1	F	1887	HYP	O-C-CA	-2.41	118.57	124.77
1	F	1890	HYP	O-C-CA	-2.41	118.57	124.77
1	E	1913	HYP	O-C-CA	-2.41	118.57	124.77
1	A	1928	HYP	O-C-CA	-2.41	118.57	124.77
1	D	1928	HYP	O-C-CA	-2.41	118.58	124.77
2	H	40	HYP	O-C-CA	-2.41	118.58	124.77
1	B	1864	HYP	O-C-CA	-2.41	118.58	124.77
1	B	1897	HYP	O-C-CA	-2.40	118.59	124.77
1	C	1903	HYP	CG-CB-CA	-2.40	100.98	103.75
1	E	1920	HYP	O-C-CA	-2.40	118.60	124.77
1	A	1920	HYP	O-C-CA	-2.40	118.61	124.77
1	F	1910	HYP	O-C-CA	-2.40	118.61	124.77
1	F	1927	HYP	O-C-CA	-2.39	118.61	124.77
1	F	1923	HYP	CB-CG-CD	-2.39	100.50	103.16
2	G	1	HYP	O-C-CA	-2.39	118.64	124.77
1	F	1870	HYP	O-C-CA	-2.38	118.64	124.77
1	E	1932	HYP	O-C-CA	-2.38	118.64	124.77
1	A	1923	HYP	CG-CB-CA	-2.38	101.00	103.75
1	B	1873	HYP	O-C-CA	-2.37	118.66	124.77
1	E	1890	HYP	O-C-CA	-2.37	118.67	124.77
1	D	1920	HYP	O-C-CA	-2.37	118.68	124.77
1	B	1860	HYP	CG-CB-CA	-2.37	101.02	103.75
1	E	1915	HYP	O-C-CA	-2.36	118.69	124.77
2	I	26	HYP	O-C-CA	-2.36	118.70	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	37	HYP	O-C-CA	-2.36	118.70	124.77
1	E	1930	HYP	O-C-CA	-2.36	118.71	124.77
1	E	1897	HYP	O-C-CA	-2.36	118.71	124.77
1	E	1906	HYP	O-C-CA	-2.36	118.71	124.77
2	H	52	HYP	CG-CB-CA	-2.35	101.03	103.75
1	F	1908	HYP	CB-CG-CD	-2.35	100.54	103.16
2	G	34	HYP	CG-CB-CA	-2.35	101.03	103.75
1	D	1914	HYP	O-C-CA	-2.35	118.73	124.77
1	C	1901	HYP	O-C-CA	-2.35	118.74	124.77
1	E	1883	HYP	O-C-CA	-2.34	118.75	124.77
1	F	1860	HYP	O-C-CA	-2.33	118.77	124.77
1	D	1910	HYP	O-C-CA	-2.32	118.80	124.77
1	A	1860	HYP	O-C-CA	-2.32	118.81	124.77
1	D	1923	HYP	CG-CB-CA	-2.31	101.08	103.75
1	F	1920	HYP	O-C-CA	-2.31	118.82	124.77
1	B	1923	HYP	CB-CG-CD	-2.31	100.58	103.16
1	D	1932	HYP	CB-CG-CD	-2.30	100.59	103.16
1	A	1870	HYP	O-C-CA	-2.30	118.85	124.77
1	F	1901	HYP	O-C-CA	-2.30	118.86	124.77
1	E	1860	HYP	O-C-CA	-2.29	118.89	124.77
1	C	1918	HYP	CG-CB-CA	-2.28	101.11	103.75
2	G	23	HYP	O-C-CA	-2.28	118.90	124.77
1	C	1908	HYP	CB-CG-CD	-2.28	100.61	103.16
1	B	1903	HYP	CB-CG-CD	-2.28	100.62	103.16
1	A	1878	HYP	O-C-CA	-2.28	118.91	124.77
2	I	23	HYP	O-C-CA	-2.28	118.91	124.77
1	E	1870	HYP	O-C-CA	-2.28	118.91	124.77
1	B	1860	HYP	O-C-CA	-2.27	118.93	124.77
1	D	1901	HYP	O-C-CA	-2.25	118.97	124.77
1	E	1877	HYP	CG-CB-CA	-2.25	101.15	103.75
1	A	1932	HYP	CG-CB-CA	-2.25	101.15	103.75
1	D	1903	HYP	CB-CG-CD	-2.24	100.66	103.16
1	F	1932	HYP	CG-CB-CA	-2.24	101.16	103.75
1	D	1902	HYP	CG-CB-CA	-2.22	101.19	103.75
1	F	1903	HYP	CB-CG-CD	-2.22	100.69	103.16
1	A	1903	HYP	CB-CG-CD	-2.21	100.70	103.16
1	D	1932	HYP	CG-CB-CA	-2.20	101.21	103.75
1	A	1908	HYP	CB-CG-CD	-2.19	100.72	103.16
1	A	1923	HYP	CB-CG-CD	-2.18	100.72	103.16
1	D	1908	HYP	CB-CG-CD	-2.18	100.72	103.16
1	C	1907	HYP	CG-CB-CA	-2.17	101.24	103.75
1	E	1870	HYP	CG-CB-CA	-2.17	101.24	103.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	26	HYP	CB-CG-CD	-2.16	100.75	103.16
1	A	1868	HYP	CB-CG-CD	-2.15	100.76	103.16
1	F	1907	HYP	CG-CB-CA	-2.14	101.27	103.75
1	E	1860	HYP	CB-CG-CD	-2.14	100.77	103.16
1	B	1888	HYP	CB-CG-CD	-2.14	100.78	103.16
1	C	1902	HYP	CB-CG-CD	-2.13	100.78	103.16
1	D	1923	HYP	CB-CG-CD	-2.12	100.79	103.16
1	F	1868	HYP	CB-CG-CD	-2.12	100.80	103.16
1	E	1868	HYP	CB-CG-CD	-2.12	100.80	103.16
2	G	37	HYP	O-C-CA	-2.12	119.33	124.77
1	A	1932	HYP	CB-CG-CD	-2.11	100.80	103.16
2	I	3	HYP	CB-CG-CD	-2.10	100.82	103.16
1	C	1923	HYP	CB-CG-CD	-2.10	100.82	103.16
1	A	1860	HYP	CB-CG-CD	-2.09	100.83	103.16
1	A	1870	HYP	CG-CB-CA	-2.09	101.34	103.75
1	F	1860	HYP	CB-CG-CD	-2.09	100.83	103.16
1	E	1903	HYP	CB-CG-CD	-2.08	100.84	103.16
1	B	1868	HYP	CB-CG-CD	-2.07	100.85	103.16
1	C	1903	HYP	CB-CG-CD	-2.06	100.86	103.16
1	F	1878	HYP	CB-CG-CD	-2.06	100.86	103.16
1	F	1920	HYP	CB-CG-CD	-2.04	100.88	103.16
1	E	1867	HYP	CB-CG-CD	-2.04	100.89	103.16
2	G	3	HYP	CB-CG-CD	-2.03	100.89	103.16
1	F	1907	HYP	CB-CG-CD	-2.03	100.89	103.16
1	B	1857	HYP	CB-CG-CD	-2.03	100.89	103.16
1	F	1858	HYP	CB-CG-CD	-2.03	100.90	103.16
2	G	2	HYP	CB-CG-CD	-2.02	100.90	103.16
1	B	1860	HYP	CB-CG-CD	-2.02	100.90	103.16
2	G	52	HYP	CB-CG-CD	-2.01	100.92	103.16
1	F	1902	HYP	CB-CG-CD	-2.01	100.92	103.16
1	F	1865	HYP	CB-CG-CD	-2.00	100.93	103.16
1	C	1930	HYP	CB-CG-CD	-2.00	100.93	103.16

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
1	E	1883	HYP	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
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
1	A	1858	HYP	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
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
3	FUB	0A	1	3	9,9,10	0.54	0	11,12,14	0.95	1 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
19	FUB	1E	1	19	9,9,10	0.53	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
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%)
13	AHR	3C	4	13	9,9,10	0.56	0	11,12,14	0.86	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
17	NAG	5D	1	1,17	14,14,15	0.32	0	17,19,21	0.99	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
17	MAN	7C	4	17	11,11,12	0.31	0	15,15,17	1.08	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
18	GZL	9D	3	18	11,11,12	6.60	7 (63%)	13,15,17	1.29	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
18	FUB	BE	1	18	9,9,10	0.58	0	11,12,14	0.92	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
3	FUB	DD	1	3	9,9,10	0.54	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	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
21	FUB	FE	1	21	9,9,10	0.53	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
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
7	FUB	HD	3	7	9,9,10	0.54	0	11,12,14	0.96	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
8	FUB	JD	1	8	9,9,10	0.53	0	11,12,14	0.81	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
6	FUB	LA	2	6	9,9,10	0.54	0	11,12,14	1.15	1 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
6	FUB	ME	2	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	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
6	GZL	OE	3	6	11,11,12	6.59	6 (54%)	13,15,17	1.46	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
22	FUB	QE	2	22	9,9,10	0.54	0	11,12,14	0.93	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
3	FUB	SB	3	3	9,9,10	0.55	0	11,12,14	0.99	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	FUB	SC	1	10	9,9,10	0.54	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
4	FUB	UA	1	4	9,9,10	0.55	0	11,12,14	1.02	1 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	FUB	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%)
22	FUB	VE	2	22	9,9,10	0.52	0	11,12,14	0.92	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	GZL	VE	3	22	11,11,12	6.59	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
7	AHR	XC	4	7	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
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%)
3	FUB	ZA	2	3	9,9,10	0.54	0	11,12,14	0.88	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	FUB	ZA	3	3	9,9,10	0.54	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%)
3	FUB	b	2	3	9,9,10	0.54	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	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%)
18	AHR	cE	4	18	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
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
3	FUB	eC	1	3	9,9,10	0.53	0	11,12,14	0.72	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
18	GZL	fE	3	18	11,11,12	6.58	6 (54%)	13,15,17	1.28	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
14	GZL	hD	3	14	11,11,12	6.48	7 (63%)	13,15,17	1.57	2 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
13	FUB	jB	2	13	9,9,10	0.54	0	11,12,14	0.88	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
3	FUB	l	1	3	9,9,10	0.55	0	11,12,14	0.90	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
10	AHR	mC	4	10	9,9,10	0.54	0	11,12,14	0.99	1 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
12	AHR	oA	5	12	9,9,10	0.57	0	11,12,14	1.02	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
12	GZL	q	3	12	11,11,12	6.58	7 (63%)	13,15,17	1.30	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
18	AHR	rE	4	18	9,9,10	0.53	0	11,12,14	0.78	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
13	FUB	tD	2	13	9,9,10	0.53	0	11,12,14	1.11	1 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
10	FUB	vC	1	10	9,9,10	0.53	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
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
3	FUB	x	3	3	9,9,10	0.54	0	11,12,14	0.99	1 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
18	AHR	yE	5	18	9,9,10	0.53	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	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
6	FUB	0C	2	6	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
13	AHR	2A	4	13	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
6	GZL	4B	3	6	1/1/4/5	4/6/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
13	AHR	6B	4	13	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
3	FUB	8C	2	3	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
19	AHR	AE	4	19	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
15	FUB	DA	1	15	-	0/2/15/18	0/1/1/1

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
22	AHR	GE	6	22	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
4	FUB	JA	1	4	1/1/3/4	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
18	GZL	KE	3	18	1/1/4/5	4/6/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
4	FUB	MD	1	4	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
4	AHR	OD	4	4	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
22	FUB	QE	1	22	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
10	FUB	SC	1	10	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
3	FUB	UB	1	3	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
4	FUB	W	2	4	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
23	AHR	XE	5	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	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
4	FUB	ZD	3	4	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
3	FUB	bD	3	3	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
3	FUB	dC	2	3	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
7	FUB	fA	1	7	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
4	AHR	gD	4	4	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
12	AHR	iC	4	12	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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

All (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
13	4	3	GZL	C2-C3	-18.56	1.22	1.53
6	0B	3	GZL	C2-C3	-18.56	1.22	1.53
6	3A	3	GZL	C2-C3	-18.44	1.22	1.53
13	6	3	GZL	C2-C3	-18.27	1.23	1.53
13	wC	3	GZL	C2-C3	-18.22	1.23	1.53
13	YB	3	GZL	C2-C3	-18.20	1.23	1.53
13	4A	3	GZL	C2-C3	-18.20	1.23	1.53
6	5	3	GZL	C2-C3	-18.18	1.23	1.53
13	WB	3	GZL	C2-C3	-18.18	1.23	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	rE	3	GZL	C2-C3	-18.13	1.23	1.53
21	FE	3	GZL	C2-C3	-18.13	1.23	1.53
13	mA	3	GZL	C2-C3	-18.12	1.23	1.53
6	bE	3	GZL	C2-C3	-18.12	1.23	1.53
13	dB	3	GZL	C2-C3	-18.12	1.23	1.53
13	1B	3	GZL	C2-C3	-18.11	1.23	1.53
12	oA	3	GZL	C2-C3	-18.10	1.23	1.53
15	BB	3	GZL	C2-C3	-18.10	1.23	1.53
18	9D	3	GZL	C2-C3	-18.10	1.23	1.53
15	DA	3	GZL	C2-C3	-18.10	1.23	1.53
22	wE	3	GZL	C2-C3	-18.09	1.23	1.53
15	eB	3	GZL	C2-C3	-18.09	1.23	1.53
18	SE	3	GZL	C2-C3	-18.08	1.23	1.53
20	UE	3	GZL	C2-C3	-18.08	1.23	1.53
22	iE	3	GZL	C2-C3	-18.08	1.23	1.53
13	o	3	GZL	C2-C3	-18.08	1.23	1.53
18	PE	3	GZL	C2-C3	-18.08	1.23	1.53
6	OE	3	GZL	C2-C3	-18.07	1.23	1.53
15	fB	3	GZL	C2-C3	-18.07	1.23	1.53
6	9	3	GZL	C2-C3	-18.07	1.23	1.53
6	5B	3	GZL	C2-C3	-18.06	1.23	1.53
15	CA	3	GZL	C2-C3	-18.06	1.23	1.53
6	yD	3	GZL	C2-C3	-18.05	1.23	1.53
13	gC	3	GZL	C2-C3	-18.05	1.23	1.53
22	RE	3	GZL	C2-C3	-18.04	1.23	1.53
6	FC	3	GZL	C2-C3	-18.04	1.23	1.53
13	zB	3	GZL	C2-C3	-18.04	1.23	1.53
22	QE	3	GZL	C2-C3	-18.04	1.23	1.53
6	7D	3	GZL	C2-C3	-18.04	1.23	1.53
20	HE	3	GZL	C2-C3	-18.03	1.23	1.53
12	fC	3	GZL	C2-C3	-18.03	1.23	1.53
13	tD	3	GZL	C2-C3	-18.03	1.23	1.53
6	ME	3	GZL	C2-C3	-18.03	1.23	1.53
22	eE	3	GZL	C2-C3	-18.03	1.23	1.53
6	cB	3	GZL	C2-C3	-18.03	1.23	1.53
6	AA	3	GZL	C2-C3	-18.03	1.23	1.53
15	8B	3	GZL	C2-C3	-18.03	1.23	1.53
18	fE	3	GZL	C2-C3	-18.02	1.23	1.53
15	7B	3	GZL	C2-C3	-18.02	1.23	1.53
15	2D	3	GZL	C2-C3	-18.02	1.23	1.53
20	sE	3	GZL	C2-C3	-18.02	1.23	1.53
21	kE	3	GZL	C2-C3	-18.01	1.23	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	1D	3	GZL	C2-C3	-18.01	1.23	1.53
22	VE	3	GZL	C2-C3	-18.01	1.23	1.53
6	6A	3	GZL	C2-C3	-18.00	1.23	1.53
6	8A	3	GZL	C2-C3	-18.00	1.23	1.53
15	4C	3	GZL	C2-C3	-18.00	1.23	1.53
18	cE	3	GZL	C2-C3	-17.99	1.23	1.53
13	9A	3	GZL	C2-C3	-17.99	1.23	1.53
13	7	3	GZL	C2-C3	-17.99	1.23	1.53
12	q	3	GZL	C2-C3	-17.98	1.23	1.53
15	AB	3	GZL	C2-C3	-17.98	1.23	1.53
18	0E	3	GZL	C2-C3	-17.98	1.23	1.53
23	XE	3	GZL	C2-C3	-17.98	1.23	1.53
24	YE	3	GZL	C2-C3	-17.98	1.23	1.53
20	WE	3	GZL	C2-C3	-17.98	1.23	1.53
19	AE	3	GZL	C2-C3	-17.98	1.23	1.53
6	JC	3	GZL	C2-C3	-17.98	1.23	1.53
13	GB	3	GZL	C2-C3	-17.98	1.23	1.53
19	LE	3	GZL	C2-C3	-17.98	1.23	1.53
20	TE	3	GZL	C2-C3	-17.97	1.23	1.53
6	R	3	GZL	C2-C3	-17.97	1.23	1.53
20	EE	3	GZL	C2-C3	-17.97	1.23	1.53
22	GE	3	GZL	C2-C3	-17.97	1.23	1.53
20	gE	3	GZL	C2-C3	-17.97	1.23	1.53
14	qA	3	GZL	C2-C3	-17.97	1.23	1.53
6	8D	3	GZL	C2-C3	-17.96	1.23	1.53
12	lA	3	GZL	C2-C3	-17.96	1.23	1.53
21	vE	3	GZL	C2-C3	-17.96	1.23	1.53
19	NE	3	GZL	C2-C3	-17.96	1.23	1.53
13	2A	3	GZL	C2-C3	-17.95	1.23	1.53
22	dE	3	GZL	C2-C3	-17.95	1.23	1.53
6	8	3	GZL	C2-C3	-17.95	1.23	1.53
6	1C	3	GZL	C2-C3	-17.95	1.23	1.53
6	EA	3	GZL	C2-C3	-17.95	1.23	1.53
19	1E	3	GZL	C2-C3	-17.94	1.23	1.53
13	ZB	3	GZL	C2-C3	-17.94	1.23	1.53
6	zD	3	GZL	C2-C3	-17.94	1.23	1.53
20	uE	3	GZL	C2-C3	-17.94	1.23	1.53
13	jB	3	GZL	C2-C3	-17.94	1.23	1.53
6	bB	3	GZL	C2-C3	-17.94	1.23	1.53
6	mE	3	GZL	C2-C3	-17.94	1.23	1.53
12	cD	3	GZL	C2-C3	-17.94	1.23	1.53
18	tE	3	GZL	C2-C3	-17.94	1.23	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	DE	3	GZL	C2-C3	-17.93	1.23	1.53
20	CE	3	GZL	C2-C3	-17.93	1.23	1.53
6	aB	3	GZL	C2-C3	-17.93	1.23	1.53
6	7A	3	GZL	C2-C3	-17.92	1.23	1.53
12	n	3	GZL	C2-C3	-17.91	1.23	1.53
13	6B	3	GZL	C2-C3	-17.91	1.23	1.53
6	PA	3	GZL	C2-C3	-17.91	1.23	1.53
13	dD	3	GZL	C2-C3	-17.91	1.23	1.53
19	qE	3	GZL	C2-C3	-17.90	1.23	1.53
20	xE	3	GZL	C2-C3	-17.90	1.23	1.53
6	GD	3	GZL	C2-C3	-17.90	1.23	1.53
18	pE	3	GZL	C2-C3	-17.90	1.23	1.53
12	lB	3	GZL	C2-C3	-17.90	1.23	1.53
6	6C	3	GZL	C2-C3	-17.90	1.23	1.53
6	CB	3	GZL	C2-C3	-17.89	1.23	1.53
13	5A	3	GZL	C2-C3	-17.89	1.23	1.53
20	hE	3	GZL	C2-C3	-17.89	1.23	1.53
20	jE	3	GZL	C2-C3	-17.89	1.23	1.53
14	nA	3	GZL	C2-C3	-17.89	1.23	1.53
12	lB	3	GZL	C2-C3	-17.88	1.23	1.53
13	vD	3	GZL	C2-C3	-17.88	1.23	1.53
15	5C	3	GZL	C2-C3	-17.87	1.23	1.53
13	wD	3	GZL	C2-C3	-17.87	1.23	1.53
6	3D	3	GZL	C2-C3	-17.86	1.23	1.53
6	4B	3	GZL	C2-C3	-17.86	1.23	1.53
12	fD	3	GZL	C2-C3	-17.85	1.23	1.53
13	2B	3	GZL	C2-C3	-17.85	1.23	1.53
24	lE	3	GZL	C2-C3	-17.85	1.23	1.53
18	JE	3	GZL	C2-C3	-17.85	1.23	1.53
18	BE	3	GZL	C2-C3	-17.84	1.23	1.53
13	0D	3	GZL	C2-C3	-17.83	1.23	1.53
6	2C	3	GZL	C2-C3	-17.83	1.23	1.53
18	lE	3	GZL	C2-C3	-17.83	1.23	1.53
6	gB	3	GZL	C2-C3	-17.82	1.23	1.53
13	BA	3	GZL	C2-C3	-17.82	1.23	1.53
13	zC	3	GZL	C2-C3	-17.81	1.23	1.53
14	s	3	GZL	C2-C3	-17.81	1.23	1.53
6	nE	3	GZL	C2-C3	-17.79	1.23	1.53
18	KE	3	GZL	C2-C3	-17.78	1.23	1.53
14	p	3	GZL	C2-C3	-17.78	1.23	1.53
19	aE	3	GZL	C2-C3	-17.77	1.24	1.53
13	3C	3	GZL	C2-C3	-17.77	1.24	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	yC	3	GZL	C2-C3	-17.77	1.24	1.53
12	iB	3	GZL	C2-C3	-17.76	1.24	1.53
6	ZE	3	GZL	C2-C3	-17.76	1.24	1.53
14	hC	3	GZL	C2-C3	-17.76	1.24	1.53
6	6D	3	GZL	C2-C3	-17.76	1.24	1.53
12	iC	3	GZL	C2-C3	-17.76	1.24	1.53
6	oE	3	GZL	C2-C3	-17.75	1.24	1.53
14	eD	3	GZL	C2-C3	-17.75	1.24	1.53
6	9B	3	GZL	C2-C3	-17.73	1.24	1.53
6	0C	3	GZL	C2-C3	-17.72	1.24	1.53
6	3B	3	GZL	C2-C3	-17.69	1.24	1.53
14	nB	3	GZL	C2-C3	-17.67	1.24	1.53
14	kC	3	GZL	C2-C3	-17.66	1.24	1.53
18	zE	3	GZL	C2-C3	-17.64	1.24	1.53
14	HB	3	GZL	C2-C3	-17.61	1.24	1.53
18	yE	3	GZL	C2-C3	-17.61	1.24	1.53
12	FB	3	GZL	C2-C3	-17.57	1.24	1.53
14	kB	3	GZL	C2-C3	-17.56	1.24	1.53
14	KB	3	GZL	C2-C3	-17.54	1.24	1.53
6	xD	3	GZL	C2-C3	-17.51	1.24	1.53
14	hD	3	GZL	C2-C3	-17.49	1.24	1.53
6	N	3	GZL	C2-C3	-17.25	1.24	1.53
6	CD	3	GZL	O4-C4	-8.15	1.26	1.43
6	LA	3	GZL	O4-C4	-8.02	1.26	1.43
6	3A	3	GZL	O4-C4	-7.99	1.26	1.43
6	0B	3	GZL	O4-C4	-7.94	1.26	1.43
6	XB	3	GZL	O4-C4	-7.91	1.26	1.43
6	uD	3	GZL	O4-C4	-7.89	1.26	1.43
6	xC	3	GZL	O4-C4	-7.84	1.26	1.43
6	N	3	GZL	O4-C4	-7.57	1.27	1.43
13	2A	3	GZL	O4-C4	-7.57	1.27	1.43
14	hC	3	GZL	O4-C4	-7.49	1.27	1.43
18	BE	3	GZL	O4-C4	-7.48	1.27	1.43
6	3B	3	GZL	O4-C4	-7.47	1.27	1.43
14	nA	3	GZL	O4-C4	-7.47	1.27	1.43
14	p	3	GZL	O4-C4	-7.46	1.27	1.43
6	oE	3	GZL	O4-C4	-7.45	1.27	1.43
6	8D	3	GZL	O4-C4	-7.45	1.27	1.43
22	QE	3	GZL	O4-C4	-7.44	1.27	1.43
14	eD	3	GZL	O4-C4	-7.44	1.27	1.43
6	EA	3	GZL	O4-C4	-7.43	1.27	1.43
14	s	3	GZL	O4-C4	-7.42	1.27	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	8A	3	GZL	O4-C4	-7.42	1.27	1.43
6	9B	3	GZL	O4-C4	-7.42	1.27	1.43
13	tD	3	GZL	O4-C4	-7.42	1.27	1.43
15	7B	3	GZL	O4-C4	-7.41	1.27	1.43
6	CB	3	GZL	O4-C4	-7.41	1.27	1.43
14	qA	3	GZL	O4-C4	-7.41	1.27	1.43
6	PA	3	GZL	O4-C4	-7.40	1.27	1.43
6	xD	3	GZL	O4-C4	-7.40	1.27	1.43
22	RE	3	GZL	O4-C4	-7.40	1.27	1.43
14	kB	3	GZL	O4-C4	-7.39	1.27	1.43
6	4B	3	GZL	O4-C4	-7.39	1.27	1.43
20	TE	3	GZL	O4-C4	-7.39	1.27	1.43
24	lE	3	GZL	O4-C4	-7.39	1.27	1.43
6	gB	3	GZL	O4-C4	-7.39	1.27	1.43
14	KB	3	GZL	O4-C4	-7.39	1.27	1.43
21	vE	3	GZL	O4-C4	-7.39	1.27	1.43
12	FB	3	GZL	O4-C4	-7.38	1.27	1.43
14	HB	3	GZL	O4-C4	-7.37	1.27	1.43
6	GD	3	GZL	O4-C4	-7.37	1.27	1.43
13	4	3	GZL	O4-C4	-7.37	1.27	1.43
22	eE	3	GZL	O4-C4	-7.37	1.27	1.43
15	AB	3	GZL	O4-C4	-7.37	1.27	1.43
14	hD	3	GZL	O4-C4	-7.37	1.27	1.43
20	UE	3	GZL	O4-C4	-7.37	1.27	1.43
14	nB	3	GZL	O4-C4	-7.37	1.27	1.43
22	dE	3	GZL	O4-C4	-7.36	1.27	1.43
14	kC	3	GZL	O4-C4	-7.36	1.27	1.43
18	SE	3	GZL	O4-C4	-7.36	1.27	1.43
6	ZE	3	GZL	O4-C4	-7.36	1.27	1.43
12	iB	3	GZL	O4-C4	-7.35	1.27	1.43
13	2B	3	GZL	O4-C4	-7.35	1.27	1.43
6	mE	3	GZL	O4-C4	-7.35	1.27	1.43
19	qE	3	GZL	O4-C4	-7.35	1.27	1.43
6	cB	3	GZL	O4-C4	-7.35	1.27	1.43
20	gE	3	GZL	O4-C4	-7.35	1.27	1.43
23	XE	3	GZL	O4-C4	-7.35	1.27	1.43
15	CA	3	GZL	O4-C4	-7.34	1.27	1.43
21	kE	3	GZL	O4-C4	-7.34	1.27	1.43
19	AE	3	GZL	O4-C4	-7.34	1.27	1.43
6	0C	3	GZL	O4-C4	-7.34	1.27	1.43
20	WE	3	GZL	O4-C4	-7.33	1.27	1.43
6	9	3	GZL	O4-C4	-7.33	1.27	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	hE	3	GZL	O4-C4	-7.33	1.27	1.43
13	BA	3	GZL	O4-C4	-7.32	1.27	1.43
15	eB	3	GZL	O4-C4	-7.32	1.27	1.43
20	jE	3	GZL	O4-C4	-7.32	1.27	1.43
6	JC	3	GZL	O4-C4	-7.32	1.27	1.43
12	n	3	GZL	O4-C4	-7.32	1.27	1.43
13	o	3	GZL	O4-C4	-7.32	1.27	1.43
13	6	3	GZL	O4-C4	-7.32	1.27	1.43
6	3D	3	GZL	O4-C4	-7.32	1.27	1.43
20	EE	3	GZL	O4-C4	-7.32	1.27	1.43
6	7A	3	GZL	O4-C4	-7.31	1.27	1.43
18	PE	3	GZL	O4-C4	-7.31	1.27	1.43
21	FE	3	GZL	O4-C4	-7.31	1.27	1.43
6	8	3	GZL	O4-C4	-7.31	1.27	1.43
6	R	3	GZL	O4-C4	-7.31	1.27	1.43
18	IE	3	GZL	O4-C4	-7.30	1.27	1.43
6	bE	3	GZL	O4-C4	-7.30	1.27	1.43
18	yE	3	GZL	O4-C4	-7.30	1.27	1.43
6	AA	3	GZL	O4-C4	-7.30	1.27	1.43
12	iC	3	GZL	O4-C4	-7.30	1.27	1.43
13	4A	3	GZL	O4-C4	-7.29	1.27	1.43
6	6D	3	GZL	O4-C4	-7.29	1.27	1.43
13	wD	3	GZL	O4-C4	-7.29	1.27	1.43
18	zE	3	GZL	O4-C4	-7.29	1.27	1.43
13	jB	3	GZL	O4-C4	-7.29	1.28	1.43
15	DA	3	GZL	O4-C4	-7.29	1.28	1.43
13	mA	3	GZL	O4-C4	-7.28	1.28	1.43
13	5A	3	GZL	O4-C4	-7.28	1.28	1.43
24	YE	3	GZL	O4-C4	-7.28	1.28	1.43
6	ME	3	GZL	O4-C4	-7.28	1.28	1.43
15	BB	3	GZL	O4-C4	-7.27	1.28	1.43
22	VE	3	GZL	O4-C4	-7.27	1.28	1.43
13	wC	3	GZL	O4-C4	-7.27	1.28	1.43
13	yC	3	GZL	O4-C4	-7.27	1.28	1.43
20	CE	3	GZL	O4-C4	-7.26	1.28	1.43
6	bB	3	GZL	O4-C4	-7.26	1.28	1.43
15	8B	3	GZL	O4-C4	-7.26	1.28	1.43
12	oA	3	GZL	O4-C4	-7.26	1.28	1.43
13	ZB	3	GZL	O4-C4	-7.26	1.28	1.43
20	uE	3	GZL	O4-C4	-7.26	1.28	1.43
19	LE	3	GZL	O4-C4	-7.25	1.28	1.43
12	fC	3	GZL	O4-C4	-7.25	1.28	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	pE	3	GZL	O4-C4	-7.24	1.28	1.43
13	zC	3	GZL	O4-C4	-7.24	1.28	1.43
6	2C	3	GZL	O4-C4	-7.24	1.28	1.43
6	5B	3	GZL	O4-C4	-7.24	1.28	1.43
6	OE	3	GZL	O4-C4	-7.24	1.28	1.43
20	sE	3	GZL	O4-C4	-7.23	1.28	1.43
22	wE	3	GZL	O4-C4	-7.23	1.28	1.43
19	NE	3	GZL	O4-C4	-7.23	1.28	1.43
13	dD	3	GZL	O4-C4	-7.23	1.28	1.43
12	q	3	GZL	O4-C4	-7.23	1.28	1.43
12	lA	3	GZL	O4-C4	-7.23	1.28	1.43
18	rE	3	GZL	O4-C4	-7.22	1.28	1.43
20	HE	3	GZL	O4-C4	-7.22	1.28	1.43
15	fB	3	GZL	O4-C4	-7.22	1.28	1.43
13	1B	3	GZL	O4-C4	-7.22	1.28	1.43
6	6C	3	GZL	O4-C4	-7.22	1.28	1.43
18	JE	3	GZL	O4-C4	-7.21	1.28	1.43
15	5C	3	GZL	O4-C4	-7.21	1.28	1.43
13	zB	3	GZL	O4-C4	-7.21	1.28	1.43
19	1E	3	GZL	O4-C4	-7.20	1.28	1.43
13	7	3	GZL	O4-C4	-7.20	1.28	1.43
13	gC	3	GZL	O4-C4	-7.20	1.28	1.43
20	xE	3	GZL	O4-C4	-7.20	1.28	1.43
6	nE	3	GZL	O4-C4	-7.19	1.28	1.43
18	DE	3	GZL	O4-C4	-7.19	1.28	1.43
22	GE	3	GZL	O4-C4	-7.19	1.28	1.43
22	iE	3	GZL	O4-C4	-7.19	1.28	1.43
6	zD	3	GZL	O4-C4	-7.19	1.28	1.43
12	IB	3	GZL	O4-C4	-7.19	1.28	1.43
18	KE	3	GZL	O4-C4	-7.19	1.28	1.43
19	aE	3	GZL	O4-C4	-7.19	1.28	1.43
18	cE	3	GZL	O4-C4	-7.19	1.28	1.43
18	tE	3	GZL	O4-C4	-7.18	1.28	1.43
18	0E	3	GZL	O4-C4	-7.18	1.28	1.43
18	9D	3	GZL	O4-C4	-7.17	1.28	1.43
6	1C	3	GZL	O4-C4	-7.17	1.28	1.43
12	fD	3	GZL	O4-C4	-7.16	1.28	1.43
15	4C	3	GZL	O4-C4	-7.16	1.28	1.43
12	cD	3	GZL	O4-C4	-7.16	1.28	1.43
13	YB	3	GZL	O4-C4	-7.16	1.28	1.43
6	aB	3	GZL	O4-C4	-7.16	1.28	1.43
13	WB	3	GZL	O4-C4	-7.16	1.28	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	1D	3	GZL	O4-C4	-7.15	1.28	1.43
6	6A	3	GZL	O4-C4	-7.15	1.28	1.43
18	fE	3	GZL	O4-C4	-7.15	1.28	1.43
13	9A	3	GZL	C3-C4	7.15	1.68	1.53
13	GB	3	GZL	O4-C4	-7.14	1.28	1.43
15	2D	3	GZL	O4-C4	-7.12	1.28	1.43
6	yD	3	GZL	O4-C4	-7.12	1.28	1.43
13	6B	3	GZL	O4-C4	-7.12	1.28	1.43
13	9A	3	GZL	O4-C4	-7.12	1.28	1.43
13	0D	3	GZL	O4-C4	-7.12	1.28	1.43
6	5	3	GZL	O4-C4	-7.11	1.28	1.43
13	3C	3	GZL	O4-C4	-7.11	1.28	1.43
13	dB	3	GZL	O4-C4	-7.10	1.28	1.43
6	7D	3	GZL	O4-C4	-7.10	1.28	1.43
13	vD	3	GZL	O4-C4	-7.09	1.28	1.43
12	lB	3	GZL	O4-C4	-7.09	1.28	1.43
13	dB	3	GZL	C3-C4	7.08	1.68	1.53
13	BA	3	GZL	C3-C4	7.08	1.68	1.53
13	6B	3	GZL	C3-C4	7.04	1.68	1.53
13	2A	3	GZL	C3-C4	6.92	1.68	1.53
13	3C	3	GZL	C3-C4	6.89	1.68	1.53
13	0D	3	GZL	C3-C4	6.86	1.68	1.53
6	nE	3	GZL	C3-C4	6.82	1.67	1.53
18	0E	3	GZL	C3-C4	6.79	1.67	1.53
13	wC	3	GZL	C3-C4	6.78	1.67	1.53
18	zE	3	GZL	C3-C4	6.78	1.67	1.53
14	hD	3	GZL	C3-C4	6.77	1.67	1.53
18	KE	3	GZL	C3-C4	6.74	1.67	1.53
15	2D	3	GZL	C3-C4	6.74	1.67	1.53
18	JE	3	GZL	C3-C4	6.73	1.67	1.53
6	FC	3	GZL	O4-C4	-6.72	1.29	1.43
13	vD	3	GZL	C3-C4	6.71	1.67	1.53
12	cD	3	GZL	C3-C4	6.70	1.67	1.53
6	1C	3	GZL	C3-C4	6.69	1.67	1.53
6	7D	3	GZL	C3-C4	6.69	1.67	1.53
13	7	3	GZL	C3-C4	6.68	1.67	1.53
18	9D	3	GZL	C3-C4	6.68	1.67	1.53
19	1E	3	GZL	C3-C4	6.68	1.67	1.53
13	ZB	3	GZL	C3-C4	6.68	1.67	1.53
13	5A	3	GZL	C3-C4	6.67	1.67	1.53
19	aE	3	GZL	C3-C4	6.67	1.67	1.53
18	yE	3	GZL	C3-C4	6.67	1.67	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	sE	3	GZL	C3-C4	6.67	1.67	1.53
18	tE	3	GZL	C3-C4	6.67	1.67	1.53
13	zB	3	GZL	C3-C4	6.65	1.67	1.53
14	kB	3	GZL	C3-C4	6.65	1.67	1.53
20	xE	3	GZL	C3-C4	6.65	1.67	1.53
13	WB	3	GZL	C3-C4	6.64	1.67	1.53
12	FB	3	GZL	C3-C4	6.64	1.67	1.53
6	aB	3	GZL	C3-C4	6.64	1.67	1.53
18	rE	3	GZL	C3-C4	6.63	1.67	1.53
18	IE	3	GZL	C3-C4	6.62	1.67	1.53
13	tD	3	GZL	C3-C4	6.62	1.67	1.53
13	zC	3	GZL	C3-C4	6.62	1.67	1.53
12	lB	3	GZL	C3-C4	6.61	1.67	1.53
13	yC	3	GZL	C3-C4	6.61	1.67	1.53
15	8B	3	GZL	C3-C4	6.61	1.67	1.53
6	2C	3	GZL	C3-C4	6.61	1.67	1.53
15	5C	3	GZL	C3-C4	6.60	1.67	1.53
19	NE	3	GZL	C3-C4	6.60	1.67	1.53
6	xD	3	GZL	C3-C4	6.60	1.67	1.53
12	fD	3	GZL	C3-C4	6.59	1.67	1.53
13	wD	3	GZL	C3-C4	6.59	1.67	1.53
14	HB	3	GZL	C3-C4	6.59	1.67	1.53
6	zD	3	GZL	C3-C4	6.58	1.67	1.53
6	yD	3	GZL	C3-C4	6.58	1.67	1.53
14	hC	3	GZL	C3-C4	6.57	1.67	1.53
20	HE	3	GZL	C3-C4	6.57	1.67	1.53
18	eE	3	GZL	C3-C4	6.57	1.67	1.53
13	GB	3	GZL	C3-C4	6.56	1.67	1.53
12	IB	3	GZL	C3-C4	6.56	1.67	1.53
15	4C	3	GZL	C3-C4	6.56	1.67	1.53
14	KB	3	GZL	C3-C4	6.55	1.67	1.53
14	eD	3	GZL	C3-C4	6.55	1.67	1.53
22	GE	3	GZL	C3-C4	6.55	1.67	1.53
20	CE	3	GZL	C3-C4	6.55	1.67	1.53
12	lA	3	GZL	C3-C4	6.54	1.67	1.53
18	pE	3	GZL	C3-C4	6.54	1.67	1.53
15	eB	3	GZL	C3-C4	6.54	1.67	1.53
6	OE	3	GZL	C3-C4	6.53	1.67	1.53
6	9B	3	GZL	C3-C4	6.52	1.67	1.53
13	dD	3	GZL	C3-C4	6.52	1.67	1.53
6	6D	3	GZL	C3-C4	6.52	1.67	1.53
18	DE	3	GZL	C3-C4	6.51	1.67	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	6C	3	GZL	C3-C4	6.51	1.67	1.53
6	3D	3	GZL	C3-C4	6.51	1.67	1.53
14	kC	3	GZL	C3-C4	6.51	1.67	1.53
6	R	3	GZL	C3-C4	6.51	1.67	1.53
6	6A	3	GZL	C3-C4	6.51	1.67	1.53
12	iB	3	GZL	C3-C4	6.51	1.67	1.53
6	5B	3	GZL	C3-C4	6.50	1.67	1.53
15	CA	3	GZL	C3-C4	6.50	1.67	1.53
12	iC	3	GZL	C3-C4	6.50	1.67	1.53
14	s	3	GZL	C3-C4	6.49	1.67	1.53
19	qE	3	GZL	C3-C4	6.49	1.67	1.53
20	uE	3	GZL	C3-C4	6.49	1.67	1.53
14	p	3	GZL	C3-C4	6.49	1.67	1.53
15	BB	3	GZL	C3-C4	6.48	1.67	1.53
14	nB	3	GZL	C3-C4	6.48	1.67	1.53
22	wE	3	GZL	C3-C4	6.48	1.67	1.53
6	bB	3	GZL	C3-C4	6.48	1.67	1.53
6	GD	3	GZL	C3-C4	6.48	1.67	1.53
6	0C	3	GZL	C3-C4	6.48	1.67	1.53
15	fB	3	GZL	C3-C4	6.48	1.67	1.53
18	fE	3	GZL	C3-C4	6.48	1.67	1.53
22	eE	3	GZL	C3-C4	6.48	1.67	1.53
14	nA	3	GZL	C3-C4	6.48	1.67	1.53
12	fC	3	GZL	C3-C4	6.48	1.67	1.53
22	iE	3	GZL	C3-C4	6.47	1.67	1.53
6	4B	3	GZL	C3-C4	6.47	1.67	1.53
13	jB	3	GZL	C3-C4	6.47	1.67	1.53
6	JC	3	GZL	C3-C4	6.46	1.67	1.53
20	jE	3	GZL	C3-C4	6.46	1.67	1.53
6	ZE	3	GZL	C3-C4	6.46	1.67	1.53
6	3B	3	GZL	C3-C4	6.45	1.67	1.53
13	gC	3	GZL	C3-C4	6.45	1.67	1.53
6	bE	3	GZL	C3-C4	6.45	1.67	1.53
20	hE	3	GZL	C3-C4	6.45	1.67	1.53
20	EE	3	GZL	C3-C4	6.45	1.67	1.53
19	LE	3	GZL	C3-C4	6.44	1.67	1.53
19	AE	3	GZL	C3-C4	6.44	1.67	1.53
6	ME	3	GZL	C3-C4	6.44	1.67	1.53
6	gB	3	GZL	C3-C4	6.44	1.67	1.53
12	n	3	GZL	C3-C4	6.44	1.67	1.53
6	AA	3	GZL	C3-C4	6.44	1.67	1.53
13	o	3	GZL	C3-C4	6.43	1.67	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	1D	3	GZL	C3-C4	6.43	1.67	1.53
24	1E	3	GZL	C3-C4	6.43	1.67	1.53
13	2B	3	GZL	C3-C4	6.42	1.67	1.53
12	q	3	GZL	C3-C4	6.42	1.67	1.53
13	YB	3	GZL	C3-C4	6.42	1.67	1.53
22	dE	3	GZL	C3-C4	6.42	1.67	1.53
24	YE	3	GZL	C3-C4	6.41	1.67	1.53
6	8	3	GZL	C3-C4	6.41	1.67	1.53
6	cB	3	GZL	C3-C4	6.40	1.67	1.53
20	WE	3	GZL	C3-C4	6.40	1.67	1.53
13	4A	3	GZL	C3-C4	6.39	1.67	1.53
21	FE	3	GZL	C3-C4	6.39	1.67	1.53
6	8D	3	GZL	C3-C4	6.39	1.67	1.53
22	QE	3	GZL	C3-C4	6.39	1.67	1.53
21	kE	3	GZL	C3-C4	6.39	1.67	1.53
6	oE	3	GZL	C3-C4	6.38	1.66	1.53
12	oA	3	GZL	C3-C4	6.38	1.66	1.53
15	AB	3	GZL	C3-C4	6.38	1.66	1.53
15	DA	3	GZL	C3-C4	6.38	1.66	1.53
20	gE	3	GZL	C3-C4	6.37	1.66	1.53
18	PE	3	GZL	C3-C4	6.37	1.66	1.53
6	mE	3	GZL	C3-C4	6.36	1.66	1.53
6	PA	3	GZL	C3-C4	6.36	1.66	1.53
22	RE	3	GZL	C3-C4	6.36	1.66	1.53
6	8A	3	GZL	C3-C4	6.36	1.66	1.53
22	VE	3	GZL	C3-C4	6.36	1.66	1.53
21	vE	3	GZL	C3-C4	6.36	1.66	1.53
6	9	3	GZL	C3-C4	6.36	1.66	1.53
6	EA	3	GZL	C3-C4	6.36	1.66	1.53
18	BE	3	GZL	C3-C4	6.35	1.66	1.53
13	mA	3	GZL	C3-C4	6.35	1.66	1.53
15	7B	3	GZL	C3-C4	6.35	1.66	1.53
6	CB	3	GZL	C3-C4	6.35	1.66	1.53
13	1B	3	GZL	C3-C4	6.35	1.66	1.53
14	qA	3	GZL	C3-C4	6.34	1.66	1.53
18	SE	3	GZL	C3-C4	6.34	1.66	1.53
20	TE	3	GZL	C3-C4	6.31	1.66	1.53
23	XE	3	GZL	C3-C4	6.31	1.66	1.53
13	6	3	GZL	C3-C4	6.31	1.66	1.53
20	UE	3	GZL	C3-C4	6.28	1.66	1.53
6	7A	3	GZL	C3-C4	6.28	1.66	1.53
6	N	3	GZL	C3-C4	6.23	1.66	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	0B	3	GZL	C1-C2	6.21	1.62	1.51
6	5	3	GZL	C3-C4	6.18	1.66	1.53
6	LA	3	GZL	C1-C2	6.16	1.62	1.51
6	XB	3	GZL	C1-C2	6.16	1.62	1.51
6	xC	3	GZL	C1-C2	6.13	1.62	1.51
6	uD	3	GZL	C1-C2	6.08	1.62	1.51
13	4	3	GZL	C3-C4	5.99	1.66	1.53
6	CD	3	GZL	C1-C2	5.98	1.62	1.51
6	FC	3	GZL	C3-C4	5.95	1.66	1.53
6	N	3	GZL	C1-C2	5.92	1.62	1.51
6	LA	3	GZL	C3-C4	5.89	1.65	1.53
6	CD	3	GZL	C3-C4	5.74	1.65	1.53
6	3A	3	GZL	C1-C2	5.50	1.61	1.51
13	2A	3	GZL	C1-C2	5.47	1.61	1.51
6	uD	3	GZL	C3-C4	5.40	1.64	1.53
6	XB	3	GZL	C3-C4	5.37	1.64	1.53
6	0B	3	GZL	C3-C4	5.36	1.64	1.53
6	xC	3	GZL	C3-C4	5.31	1.64	1.53
6	3A	3	GZL	C3-C4	5.30	1.64	1.53
13	tD	3	GZL	C1-C2	4.97	1.60	1.51
6	5	3	GZL	C1-C2	4.93	1.60	1.51
6	3B	3	GZL	C1-C2	4.91	1.60	1.51
13	WB	3	GZL	C1-C2	4.89	1.60	1.51
6	0C	3	GZL	C1-C2	4.88	1.60	1.51
13	wC	3	GZL	C1-C2	4.87	1.60	1.51
6	CB	3	GZL	C1-C2	4.84	1.60	1.51
14	kB	3	GZL	C1-C2	4.84	1.60	1.51
14	nB	3	GZL	C1-C2	4.83	1.60	1.51
12	iB	3	GZL	C1-C2	4.83	1.60	1.51
13	jB	3	GZL	C1-C2	4.80	1.60	1.51
6	ZE	3	GZL	C1-C2	4.80	1.60	1.51
14	p	3	GZL	C1-C2	4.80	1.60	1.51
14	hC	3	GZL	C1-C2	4.79	1.60	1.51
13	zB	3	GZL	C1-C2	4.79	1.60	1.51
6	xD	3	GZL	C1-C2	4.78	1.60	1.51
6	9B	3	GZL	C1-C2	4.77	1.60	1.51
12	FB	3	GZL	C1-C2	4.76	1.60	1.51
6	gB	3	GZL	C1-C2	4.76	1.60	1.51
14	HB	3	GZL	C1-C2	4.76	1.60	1.51
14	kC	3	GZL	C1-C2	4.76	1.60	1.51
14	eD	3	GZL	C1-C2	4.75	1.60	1.51
14	KB	3	GZL	C1-C2	4.74	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	EA	3	GZL	C1-C2	4.74	1.60	1.51
19	qE	3	GZL	C1-C2	4.74	1.60	1.51
6	3D	3	GZL	C1-C2	4.74	1.60	1.51
12	n	3	GZL	C1-C2	4.73	1.60	1.51
13	4	3	GZL	C1-C2	4.73	1.60	1.51
6	PA	3	GZL	C1-C2	4.73	1.60	1.51
19	LE	3	GZL	C1-C2	4.72	1.60	1.51
13	2B	3	GZL	C1-C2	4.72	1.60	1.51
14	nA	3	GZL	C1-C2	4.72	1.60	1.51
21	vE	3	GZL	C1-C2	4.72	1.60	1.51
6	7A	3	GZL	C1-C2	4.71	1.60	1.51
19	AE	3	GZL	C1-C2	4.71	1.60	1.51
6	4B	3	GZL	C1-C2	4.71	1.60	1.51
6	6C	3	GZL	C1-C2	4.70	1.59	1.51
20	gE	3	GZL	C1-C2	4.70	1.59	1.51
14	qA	3	GZL	C1-C2	4.69	1.59	1.51
20	TE	3	GZL	C1-C2	4.68	1.59	1.51
13	1B	3	GZL	C1-C2	4.67	1.59	1.51
6	oE	3	GZL	C1-C2	4.67	1.59	1.51
6	bB	3	GZL	C1-C2	4.65	1.59	1.51
20	jE	3	GZL	C1-C2	4.65	1.59	1.51
12	IB	3	GZL	C1-C2	4.65	1.59	1.51
13	yC	3	GZL	C1-C2	4.65	1.59	1.51
13	wD	3	GZL	C1-C2	4.65	1.59	1.51
6	2C	3	GZL	C1-C2	4.64	1.59	1.51
13	GB	3	GZL	C1-C2	4.64	1.59	1.51
14	s	3	GZL	C1-C2	4.63	1.59	1.51
12	fC	3	GZL	C1-C2	4.63	1.59	1.51
13	zC	3	GZL	C1-C2	4.63	1.59	1.51
21	kE	3	GZL	C1-C2	4.63	1.59	1.51
15	1D	3	GZL	C1-C2	4.62	1.59	1.51
18	BE	3	GZL	C1-C2	4.62	1.59	1.51
20	hE	3	GZL	C1-C2	4.62	1.59	1.51
24	lE	3	GZL	C1-C2	4.61	1.59	1.51
6	6D	3	GZL	C1-C2	4.61	1.59	1.51
6	bE	3	GZL	C1-C2	4.61	1.59	1.51
6	8D	3	GZL	C1-C2	4.60	1.59	1.51
18	cE	3	GZL	C1-C2	4.60	1.59	1.51
13	dD	3	GZL	C1-C2	4.59	1.59	1.51
19	aE	3	GZL	C1-C2	4.59	1.59	1.51
13	o	3	GZL	C1-C2	4.59	1.59	1.51
6	cB	3	GZL	C1-C2	4.59	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	8	3	GZL	C1-C2	4.59	1.59	1.51
12	lA	3	GZL	C1-C2	4.58	1.59	1.51
24	YE	3	GZL	C1-C2	4.58	1.59	1.51
15	7B	3	GZL	C1-C2	4.58	1.59	1.51
6	uD	3	GZL	O4-C1	4.58	1.53	1.43
6	mE	3	GZL	C1-C2	4.57	1.59	1.51
15	AB	3	GZL	C1-C2	4.57	1.59	1.51
13	gC	3	GZL	C1-C2	4.57	1.59	1.51
6	R	3	GZL	C1-C2	4.56	1.59	1.51
13	4A	3	GZL	C1-C2	4.56	1.59	1.51
6	xC	3	GZL	O4-C1	4.55	1.53	1.43
20	UE	3	GZL	C1-C2	4.55	1.59	1.51
22	VE	3	GZL	C1-C2	4.55	1.59	1.51
12	iC	3	GZL	C1-C2	4.54	1.59	1.51
20	WE	3	GZL	C1-C2	4.54	1.59	1.51
15	5C	3	GZL	C1-C2	4.54	1.59	1.51
20	EE	3	GZL	C1-C2	4.54	1.59	1.51
15	CA	3	GZL	C1-C2	4.54	1.59	1.51
22	dE	3	GZL	C1-C2	4.53	1.59	1.51
6	zD	3	GZL	C1-C2	4.53	1.59	1.51
18	SE	3	GZL	C1-C2	4.53	1.59	1.51
6	8A	3	GZL	C1-C2	4.52	1.59	1.51
13	ZB	3	GZL	C1-C2	4.52	1.59	1.51
12	cD	3	GZL	C1-C2	4.52	1.59	1.51
23	XE	3	GZL	C1-C2	4.52	1.59	1.51
18	zE	3	GZL	C1-C2	4.51	1.59	1.51
6	XB	3	GZL	O4-C1	4.51	1.53	1.43
18	PE	3	GZL	C1-C2	4.51	1.59	1.51
6	GD	3	GZL	C1-C2	4.51	1.59	1.51
22	iE	3	GZL	C1-C2	4.51	1.59	1.51
12	lB	3	GZL	C1-C2	4.50	1.59	1.51
22	RE	3	GZL	C1-C2	4.50	1.59	1.51
6	ME	3	GZL	C1-C2	4.49	1.59	1.51
6	9	3	GZL	C1-C2	4.49	1.59	1.51
18	yE	3	GZL	C1-C2	4.49	1.59	1.51
14	hD	3	GZL	C1-C2	4.49	1.59	1.51
6	aB	3	GZL	C1-C2	4.49	1.59	1.51
6	yD	3	GZL	C1-C2	4.48	1.59	1.51
18	fE	3	GZL	C1-C2	4.48	1.59	1.51
19	lE	3	GZL	C1-C2	4.48	1.59	1.51
21	FE	3	GZL	C1-C2	4.48	1.59	1.51
13	mA	3	GZL	C1-C2	4.48	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	AA	3	GZL	C1-C2	4.48	1.59	1.51
22	eE	3	GZL	C1-C2	4.48	1.59	1.51
6	LA	3	GZL	O4-C1	4.48	1.53	1.43
18	pE	3	GZL	C1-C2	4.47	1.59	1.51
12	q	3	GZL	C1-C2	4.47	1.59	1.51
12	oA	3	GZL	C1-C2	4.47	1.59	1.51
13	YB	3	GZL	C1-C2	4.46	1.59	1.51
6	JC	3	GZL	C1-C2	4.46	1.59	1.51
6	0B	3	GZL	O4-C1	4.46	1.53	1.43
13	vD	3	GZL	C1-C2	4.46	1.59	1.51
18	DE	3	GZL	C1-C2	4.45	1.59	1.51
15	DA	3	GZL	C1-C2	4.44	1.59	1.51
20	uE	3	GZL	C1-C2	4.44	1.59	1.51
15	4C	3	GZL	C1-C2	4.44	1.59	1.51
15	eB	3	GZL	C1-C2	4.43	1.59	1.51
12	fD	3	GZL	C1-C2	4.43	1.59	1.51
6	6A	3	GZL	C1-C2	4.43	1.59	1.51
22	QE	3	GZL	C1-C2	4.43	1.59	1.51
15	BB	3	GZL	C1-C2	4.42	1.59	1.51
15	fB	3	GZL	C1-C2	4.42	1.59	1.51
15	2D	3	GZL	C1-C2	4.42	1.59	1.51
18	JE	3	GZL	C1-C2	4.41	1.59	1.51
18	tE	3	GZL	C1-C2	4.41	1.59	1.51
22	wE	3	GZL	C1-C2	4.41	1.59	1.51
20	sE	3	GZL	C1-C2	4.40	1.59	1.51
6	5B	3	GZL	C1-C2	4.40	1.59	1.51
6	OE	3	GZL	C1-C2	4.40	1.59	1.51
6	1C	3	GZL	C1-C2	4.39	1.59	1.51
13	0D	3	GZL	C1-C2	4.39	1.59	1.51
18	KE	3	GZL	C1-C2	4.38	1.59	1.51
6	nE	3	GZL	C1-C2	4.38	1.59	1.51
13	7	3	GZL	C1-C2	4.38	1.59	1.51
13	5A	3	GZL	C1-C2	4.36	1.59	1.51
13	6	3	GZL	C1-C2	4.35	1.59	1.51
13	3C	3	GZL	C1-C2	4.35	1.59	1.51
19	NE	3	GZL	C1-C2	4.35	1.59	1.51
15	8B	3	GZL	C1-C2	4.34	1.59	1.51
18	IE	3	GZL	C1-C2	4.32	1.59	1.51
6	CD	3	GZL	O4-C1	4.32	1.53	1.43
13	YB	3	GZL	O4-C1	4.30	1.53	1.43
15	1D	3	GZL	O4-C1	4.30	1.53	1.43
13	1B	3	GZL	O4-C1	4.29	1.53	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	GE	3	GZL	C1-C2	4.28	1.59	1.51
18	0E	3	GZL	C1-C2	4.27	1.59	1.51
20	HE	3	GZL	C1-C2	4.27	1.59	1.51
20	CE	3	GZL	C1-C2	4.27	1.59	1.51
18	rE	3	GZL	C1-C2	4.27	1.59	1.51
13	wC	3	GZL	O4-C1	4.26	1.53	1.43
20	xE	3	GZL	C1-C2	4.25	1.59	1.51
13	WB	3	GZL	O4-C1	4.25	1.53	1.43
19	LE	3	GZL	O4-C1	4.23	1.53	1.43
13	jB	3	GZL	O4-C1	4.23	1.53	1.43
13	zB	3	GZL	O4-C1	4.23	1.52	1.43
6	7D	3	GZL	C1-C2	4.22	1.59	1.51
13	tD	3	GZL	O4-C1	4.21	1.52	1.43
13	o	3	GZL	O4-C1	4.21	1.52	1.43
13	2A	3	GZL	O4-C1	4.21	1.52	1.43
15	4C	3	GZL	O4-C1	4.20	1.52	1.43
13	gC	3	GZL	O4-C1	4.20	1.52	1.43
20	gE	3	GZL	O4-C1	4.19	1.52	1.43
18	9D	3	GZL	C1-C2	4.19	1.59	1.51
6	N	3	GZL	O4-C1	4.19	1.52	1.43
6	5	3	GZL	O4-C1	4.19	1.52	1.43
22	VE	3	GZL	O4-C1	4.19	1.52	1.43
12	IB	3	GZL	O4-C1	4.18	1.52	1.43
13	GB	3	GZL	O4-C1	4.18	1.52	1.43
15	fB	3	GZL	O4-C1	4.18	1.52	1.43
22	iE	3	GZL	O4-C1	4.18	1.52	1.43
6	6A	3	GZL	O4-C1	4.18	1.52	1.43
13	mA	3	GZL	O4-C1	4.18	1.52	1.43
23	XE	3	GZL	O4-C1	4.17	1.52	1.43
12	q	3	GZL	O4-C1	4.17	1.52	1.43
13	6B	3	GZL	C1-C2	4.17	1.59	1.51
12	lB	3	GZL	O4-C1	4.16	1.52	1.43
13	dD	3	GZL	O4-C1	4.16	1.52	1.43
21	kE	3	GZL	O4-C1	4.16	1.52	1.43
12	fC	3	GZL	O4-C1	4.15	1.52	1.43
6	3B	3	GZL	O4-C1	4.15	1.52	1.43
14	qA	3	GZL	O4-C1	4.15	1.52	1.43
20	TE	3	GZL	O4-C1	4.15	1.52	1.43
6	zD	3	GZL	O4-C1	4.15	1.52	1.43
24	YE	3	GZL	O4-C1	4.15	1.52	1.43
12	oA	3	GZL	O4-C1	4.15	1.52	1.43
6	ZE	3	GZL	O4-C1	4.15	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	fE	3	GZL	O4-C1	4.14	1.52	1.43
6	7A	3	GZL	O4-C1	4.14	1.52	1.43
6	oE	3	GZL	O4-C1	4.14	1.52	1.43
13	6	3	GZL	O4-C1	4.14	1.52	1.43
22	wE	3	GZL	O4-C1	4.14	1.52	1.43
21	vE	3	GZL	O4-C1	4.14	1.52	1.43
13	yC	3	GZL	O4-C1	4.13	1.52	1.43
15	7B	3	GZL	O4-C1	4.13	1.52	1.43
18	pE	3	GZL	O4-C1	4.13	1.52	1.43
6	ME	3	GZL	O4-C1	4.12	1.52	1.43
6	mE	3	GZL	O4-C1	4.12	1.52	1.43
6	FC	3	GZL	O4-C1	4.12	1.52	1.43
19	AE	3	GZL	O4-C1	4.12	1.52	1.43
15	DA	3	GZL	O4-C1	4.11	1.52	1.43
15	AB	3	GZL	O4-C1	4.11	1.52	1.43
24	lE	3	GZL	O4-C1	4.11	1.52	1.43
12	lA	3	GZL	O4-C1	4.11	1.52	1.43
6	0C	3	GZL	O4-C1	4.11	1.52	1.43
12	fD	3	GZL	O4-C1	4.11	1.52	1.43
18	SE	3	GZL	O4-C1	4.10	1.52	1.43
6	bB	3	GZL	O4-C1	4.10	1.52	1.43
6	3D	3	GZL	O4-C1	4.10	1.52	1.43
12	iB	3	GZL	O4-C1	4.10	1.52	1.43
20	UE	3	GZL	O4-C1	4.10	1.52	1.43
6	AA	3	GZL	O4-C1	4.10	1.52	1.43
6	PA	3	GZL	O4-C1	4.10	1.52	1.43
6	6C	3	GZL	O4-C1	4.09	1.52	1.43
6	yD	3	GZL	O4-C1	4.09	1.52	1.43
13	2B	3	GZL	O4-C1	4.09	1.52	1.43
14	nA	3	GZL	O4-C1	4.09	1.52	1.43
14	s	3	GZL	O4-C1	4.09	1.52	1.43
20	WE	3	GZL	O4-C1	4.09	1.52	1.43
6	CB	3	GZL	O4-C1	4.09	1.52	1.43
18	PE	3	GZL	O4-C1	4.09	1.52	1.43
12	iC	3	GZL	O4-C1	4.09	1.52	1.43
20	jE	3	GZL	O4-C1	4.09	1.52	1.43
18	cE	3	GZL	O4-C1	4.09	1.52	1.43
6	FC	3	GZL	C1-C2	4.09	1.58	1.51
15	2D	3	GZL	O4-C1	4.09	1.52	1.43
13	4A	3	GZL	O4-C1	4.08	1.52	1.43
15	BB	3	GZL	O4-C1	4.08	1.52	1.43
12	n	3	GZL	O4-C1	4.08	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	8	3	GZL	O4-C1	4.08	1.52	1.43
6	xD	3	GZL	O4-C1	4.08	1.52	1.43
14	p	3	GZL	O4-C1	4.08	1.52	1.43
6	3A	3	GZL	O4-C1	4.07	1.52	1.43
6	EA	3	GZL	O4-C1	4.07	1.52	1.43
6	9	3	GZL	O4-C1	4.07	1.52	1.43
6	6D	3	GZL	O4-C1	4.07	1.52	1.43
22	RE	3	GZL	O4-C1	4.07	1.52	1.43
15	8B	3	GZL	O4-C1	4.07	1.52	1.43
6	aB	3	GZL	O4-C1	4.07	1.52	1.43
14	eD	3	GZL	O4-C1	4.06	1.52	1.43
6	5B	3	GZL	O4-C1	4.06	1.52	1.43
6	bE	3	GZL	O4-C1	4.06	1.52	1.43
19	qE	3	GZL	O4-C1	4.06	1.52	1.43
22	GE	3	GZL	O4-C1	4.06	1.52	1.43
6	8D	3	GZL	O4-C1	4.05	1.52	1.43
20	hE	3	GZL	O4-C1	4.05	1.52	1.43
6	2C	3	GZL	O4-C1	4.05	1.52	1.43
22	dE	3	GZL	O4-C1	4.05	1.52	1.43
15	CA	3	GZL	O4-C1	4.05	1.52	1.43
13	wD	3	GZL	O4-C1	4.05	1.52	1.43
20	EE	3	GZL	O4-C1	4.05	1.52	1.43
6	cB	3	GZL	O4-C1	4.05	1.52	1.43
12	cD	3	GZL	O4-C1	4.04	1.52	1.43
13	zC	3	GZL	O4-C1	4.04	1.52	1.43
15	5C	3	GZL	O4-C1	4.04	1.52	1.43
13	vD	3	GZL	O4-C1	4.04	1.52	1.43
6	8A	3	GZL	O4-C1	4.04	1.52	1.43
22	eE	3	GZL	O4-C1	4.03	1.52	1.43
19	1E	3	GZL	O4-C1	4.03	1.52	1.43
6	gB	3	GZL	O4-C1	4.03	1.52	1.43
21	FE	3	GZL	O4-C1	4.03	1.52	1.43
18	9D	3	GZL	O4-C1	4.02	1.52	1.43
22	QE	3	GZL	O4-C1	4.02	1.52	1.43
13	7	3	GZL	O4-C1	4.02	1.52	1.43
20	uE	3	GZL	O4-C1	4.02	1.52	1.43
14	nB	3	GZL	O4-C1	4.02	1.52	1.43
13	dB	3	GZL	C1-C2	4.02	1.58	1.51
14	kC	3	GZL	O4-C1	4.01	1.52	1.43
6	1C	3	GZL	O4-C1	4.01	1.52	1.43
6	JC	3	GZL	O4-C1	4.01	1.52	1.43
6	R	3	GZL	O4-C1	4.01	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	KB	3	GZL	O4-C1	4.00	1.52	1.43
18	0E	3	GZL	O4-C1	4.00	1.52	1.43
13	ZB	3	GZL	O4-C1	4.00	1.52	1.43
20	xE	3	GZL	O4-C1	3.99	1.52	1.43
19	NE	3	GZL	O4-C1	3.99	1.52	1.43
12	FB	3	GZL	O4-C1	3.99	1.52	1.43
6	4B	3	GZL	O4-C1	3.99	1.52	1.43
6	7D	3	GZL	O4-C1	3.98	1.52	1.43
18	DE	3	GZL	O4-C1	3.98	1.52	1.43
15	eB	3	GZL	O4-C1	3.98	1.52	1.43
18	rE	3	GZL	O4-C1	3.98	1.52	1.43
13	0D	3	GZL	O4-C1	3.96	1.52	1.43
14	hC	3	GZL	O4-C1	3.96	1.52	1.43
19	aE	3	GZL	O4-C1	3.95	1.52	1.43
18	JE	3	GZL	O4-C1	3.94	1.52	1.43
6	GD	3	GZL	O4-C1	3.94	1.52	1.43
14	HB	3	GZL	O4-C1	3.94	1.52	1.43
20	HE	3	GZL	O4-C1	3.93	1.52	1.43
18	tE	3	GZL	O4-C1	3.93	1.52	1.43
6	9B	3	GZL	O4-C1	3.93	1.52	1.43
18	KE	3	GZL	O4-C1	3.92	1.52	1.43
13	5A	3	GZL	O4-C1	3.92	1.52	1.43
6	nE	3	GZL	O4-C1	3.91	1.52	1.43
13	3C	3	GZL	O4-C1	3.91	1.52	1.43
14	hC	3	GZL	O2-C2	3.91	1.51	1.43
19	aE	3	GZL	O2-C2	3.91	1.51	1.43
12	FB	3	GZL	O2-C2	3.91	1.51	1.43
20	sE	3	GZL	O4-C1	3.90	1.52	1.43
18	BE	3	GZL	O4-C1	3.90	1.52	1.43
6	OE	3	GZL	O4-C1	3.90	1.52	1.43
6	0C	3	GZL	O2-C2	3.90	1.51	1.43
18	yE	3	GZL	O4-C1	3.90	1.52	1.43
13	4	3	GZL	O2-C2	3.90	1.51	1.43
14	nB	3	GZL	O2-C2	3.90	1.51	1.43
14	kB	3	GZL	O4-C1	3.89	1.52	1.43
12	iB	3	GZL	O2-C2	3.89	1.51	1.43
13	yC	3	GZL	O2-C2	3.89	1.51	1.43
18	zE	3	GZL	O2-C2	3.89	1.51	1.43
13	9A	3	GZL	C1-C2	3.89	1.58	1.51
18	zE	3	GZL	O4-C1	3.89	1.52	1.43
13	zC	3	GZL	O2-C2	3.88	1.51	1.43
6	zD	3	GZL	O2-C2	3.88	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	5C	3	GZL	O2-C2	3.88	1.51	1.43
12	IB	3	GZL	O2-C2	3.88	1.51	1.43
12	lB	3	GZL	O2-C2	3.88	1.51	1.43
13	zB	3	GZL	O2-C2	3.87	1.51	1.43
19	qE	3	GZL	O2-C2	3.87	1.51	1.43
15	4C	3	GZL	O2-C2	3.87	1.51	1.43
6	xD	3	GZL	O2-C2	3.86	1.51	1.43
13	dD	3	GZL	O2-C2	3.86	1.51	1.43
20	jE	3	GZL	O2-C2	3.86	1.51	1.43
6	nE	3	GZL	O2-C2	3.86	1.51	1.43
6	8D	3	GZL	O2-C2	3.86	1.51	1.43
18	0E	3	GZL	O2-C2	3.86	1.51	1.43
13	vD	3	GZL	O2-C2	3.86	1.51	1.43
15	2D	3	GZL	O2-C2	3.86	1.51	1.43
6	2C	3	GZL	O2-C2	3.86	1.51	1.43
14	HB	3	GZL	O2-C2	3.86	1.51	1.43
14	kB	3	GZL	O2-C2	3.86	1.51	1.43
6	ZE	3	GZL	O2-C2	3.86	1.51	1.43
6	9B	3	GZL	O2-C2	3.86	1.51	1.43
6	6C	3	GZL	O2-C2	3.86	1.51	1.43
6	3D	3	GZL	O2-C2	3.86	1.51	1.43
18	JE	3	GZL	O2-C2	3.86	1.51	1.43
18	cE	3	GZL	O2-C2	3.86	1.51	1.43
14	KB	3	GZL	O2-C2	3.85	1.51	1.43
13	lB	3	GZL	O2-C2	3.85	1.51	1.43
13	wD	3	GZL	O2-C2	3.85	1.51	1.43
13	6B	3	GZL	O4-C1	3.85	1.52	1.43
15	1D	3	GZL	O2-C2	3.85	1.51	1.43
20	CE	3	GZL	O4-C1	3.85	1.52	1.43
6	1C	3	GZL	O2-C2	3.85	1.51	1.43
13	gC	3	GZL	O2-C2	3.85	1.51	1.43
19	AE	3	GZL	O2-C2	3.85	1.51	1.43
20	hE	3	GZL	O2-C2	3.85	1.51	1.43
6	oE	3	GZL	O2-C2	3.84	1.51	1.43
14	hD	3	GZL	O2-C2	3.84	1.51	1.43
13	jB	3	GZL	O2-C2	3.84	1.51	1.43
6	3B	3	GZL	O2-C2	3.84	1.51	1.43
14	eD	3	GZL	O2-C2	3.84	1.51	1.43
12	fD	3	GZL	O2-C2	3.84	1.51	1.43
24	lE	3	GZL	O2-C2	3.84	1.51	1.43
13	WB	3	GZL	O2-C2	3.84	1.51	1.43
13	dB	3	GZL	O4-C1	3.84	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	s	3	GZL	O2-C2	3.84	1.51	1.43
13	YB	3	GZL	O2-C2	3.84	1.51	1.43
18	pE	3	GZL	O2-C2	3.84	1.51	1.43
12	iC	3	GZL	O2-C2	3.83	1.51	1.43
6	6D	3	GZL	O2-C2	3.83	1.51	1.43
13	GB	3	GZL	O2-C2	3.83	1.51	1.43
22	iE	3	GZL	O2-C2	3.83	1.51	1.43
20	HE	3	GZL	O2-C2	3.83	1.51	1.43
6	bB	3	GZL	O2-C2	3.83	1.51	1.43
20	TE	3	GZL	O2-C2	3.83	1.51	1.43
22	QE	3	GZL	O2-C2	3.83	1.51	1.43
6	4B	3	GZL	O2-C2	3.82	1.51	1.43
20	gE	3	GZL	O2-C2	3.82	1.51	1.43
20	uE	3	GZL	O2-C2	3.82	1.51	1.43
6	R	3	GZL	O2-C2	3.82	1.51	1.43
14	kC	3	GZL	O2-C2	3.82	1.51	1.43
13	3C	3	GZL	O2-C2	3.82	1.51	1.43
18	yE	3	GZL	O2-C2	3.82	1.51	1.43
6	7D	3	GZL	O2-C2	3.82	1.51	1.43
6	gB	3	GZL	O2-C2	3.82	1.51	1.43
19	NE	3	GZL	O2-C2	3.82	1.51	1.43
13	tD	3	GZL	O2-C2	3.82	1.51	1.43
13	wC	3	GZL	O2-C2	3.81	1.51	1.43
18	tE	3	GZL	O2-C2	3.81	1.51	1.43
6	ME	3	GZL	O2-C2	3.81	1.51	1.43
22	VE	3	GZL	O2-C2	3.81	1.51	1.43
22	eE	3	GZL	O2-C2	3.81	1.51	1.43
6	PA	3	GZL	O2-C2	3.81	1.51	1.43
15	7B	3	GZL	O2-C2	3.81	1.51	1.43
18	PE	3	GZL	O2-C2	3.81	1.51	1.43
18	KE	3	GZL	O2-C2	3.81	1.51	1.43
13	0D	3	GZL	O2-C2	3.81	1.51	1.43
18	BE	3	GZL	O2-C2	3.81	1.51	1.43
6	8	3	GZL	O2-C2	3.81	1.51	1.43
13	2A	3	GZL	O2-C2	3.81	1.51	1.43
6	yD	3	GZL	O2-C2	3.81	1.51	1.43
13	o	3	GZL	O2-C2	3.80	1.51	1.43
13	ZB	3	GZL	O2-C2	3.80	1.51	1.43
6	cB	3	GZL	O2-C2	3.80	1.51	1.43
6	GD	3	GZL	O2-C2	3.80	1.51	1.43
6	mE	3	GZL	O2-C2	3.80	1.51	1.43
14	qA	3	GZL	O2-C2	3.80	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	rE	3	GZL	O2-C2	3.80	1.51	1.43
15	fB	3	GZL	O2-C2	3.80	1.51	1.43
23	XE	3	GZL	O2-C2	3.80	1.51	1.43
22	GE	3	GZL	O2-C2	3.80	1.51	1.43
6	aB	3	GZL	O2-C2	3.80	1.51	1.43
12	lA	3	GZL	O2-C2	3.80	1.51	1.43
6	JC	3	GZL	O2-C2	3.80	1.51	1.43
20	xE	3	GZL	O2-C2	3.80	1.51	1.43
22	wE	3	GZL	O2-C2	3.80	1.51	1.43
18	9D	3	GZL	O2-C2	3.80	1.51	1.43
14	p	3	GZL	O2-C2	3.79	1.51	1.43
13	BA	3	GZL	C1-C2	3.79	1.58	1.51
18	IE	3	GZL	O4-C1	3.79	1.52	1.43
6	EA	3	GZL	O2-C2	3.79	1.51	1.43
13	5A	3	GZL	O2-C2	3.79	1.51	1.43
6	7A	3	GZL	O2-C2	3.79	1.51	1.43
13	7	3	GZL	O2-C2	3.79	1.51	1.43
13	2B	3	GZL	O2-C2	3.79	1.51	1.43
21	kE	3	GZL	O2-C2	3.79	1.51	1.43
18	IE	3	GZL	O2-C2	3.79	1.51	1.43
13	mA	3	GZL	O2-C2	3.79	1.51	1.43
19	1E	3	GZL	O2-C2	3.79	1.51	1.43
12	fC	3	GZL	O2-C2	3.79	1.51	1.43
12	cD	3	GZL	O2-C2	3.79	1.51	1.43
22	RE	3	GZL	O2-C2	3.79	1.51	1.43
6	LA	3	GZL	O2-C2	3.78	1.51	1.43
6	OE	3	GZL	O2-C2	3.78	1.51	1.43
18	DE	3	GZL	O2-C2	3.78	1.51	1.43
18	fE	3	GZL	O2-C2	3.78	1.51	1.43
20	sE	3	GZL	O2-C2	3.78	1.51	1.43
6	6A	3	GZL	O2-C2	3.78	1.51	1.43
20	EE	3	GZL	O2-C2	3.78	1.51	1.43
24	YE	3	GZL	O2-C2	3.77	1.51	1.43
20	CE	3	GZL	O2-C2	3.77	1.51	1.43
6	bE	3	GZL	O2-C2	3.77	1.51	1.43
13	6	3	GZL	O2-C2	3.77	1.51	1.43
20	WE	3	GZL	O2-C2	3.77	1.51	1.43
12	q	3	GZL	O2-C2	3.77	1.51	1.43
18	SE	3	GZL	O2-C2	3.77	1.51	1.43
22	dE	3	GZL	O2-C2	3.77	1.51	1.43
6	8A	3	GZL	O2-C2	3.77	1.51	1.43
6	CB	3	GZL	O2-C2	3.76	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	UE	3	GZL	O2-C2	3.76	1.51	1.43
15	8B	3	GZL	O2-C2	3.76	1.51	1.43
14	hD	3	GZL	O4-C1	3.76	1.51	1.43
15	BB	3	GZL	O2-C2	3.76	1.51	1.43
21	vE	3	GZL	O2-C2	3.75	1.51	1.43
15	eB	3	GZL	O2-C2	3.75	1.51	1.43
12	n	3	GZL	O2-C2	3.74	1.51	1.43
13	9A	3	GZL	O4-C1	3.74	1.51	1.43
6	CD	3	GZL	O2-C2	3.74	1.51	1.43
13	4A	3	GZL	O2-C2	3.74	1.51	1.43
6	5B	3	GZL	O2-C2	3.74	1.51	1.43
13	6B	3	GZL	O2-C2	3.74	1.51	1.43
15	AB	3	GZL	O2-C2	3.74	1.51	1.43
21	FE	3	GZL	O2-C2	3.73	1.51	1.43
6	uD	3	GZL	O2-C2	3.73	1.51	1.43
15	DA	3	GZL	O2-C2	3.73	1.51	1.43
6	AA	3	GZL	O2-C2	3.73	1.51	1.43
6	9	3	GZL	O2-C2	3.72	1.51	1.43
12	oA	3	GZL	O2-C2	3.72	1.51	1.43
14	nA	3	GZL	O2-C2	3.72	1.51	1.43
13	dB	3	GZL	O2-C2	3.72	1.51	1.43
15	CA	3	GZL	O2-C2	3.70	1.51	1.43
6	XB	3	GZL	O2-C2	3.69	1.51	1.43
13	9A	3	GZL	O2-C2	3.69	1.51	1.43
19	LE	3	GZL	O2-C2	3.69	1.51	1.43
13	BA	3	GZL	O2-C2	3.67	1.51	1.43
6	N	3	GZL	O2-C2	3.67	1.51	1.43
6	FC	3	GZL	O2-C2	3.65	1.51	1.43
6	xC	3	GZL	O2-C2	3.64	1.51	1.43
6	0B	3	GZL	O2-C2	3.60	1.50	1.43
13	BA	3	GZL	O4-C1	3.57	1.51	1.43
6	3A	3	GZL	O2-C2	3.46	1.50	1.43
13	4	3	GZL	O4-C1	3.28	1.50	1.43
6	5	3	GZL	O2-C2	3.26	1.50	1.43
12	fD	3	GZL	O3-C3	2.20	1.48	1.43
13	6B	3	GZL	O3-C3	2.15	1.48	1.43
12	FB	3	GZL	O3-C3	2.15	1.48	1.43
13	3C	3	GZL	O3-C3	2.14	1.48	1.43
13	0D	3	GZL	O3-C3	2.13	1.48	1.43
13	4	3	GZL	O3-C3	2.13	1.48	1.43
13	zC	3	GZL	O3-C3	2.13	1.48	1.43
13	5A	3	GZL	O3-C3	2.12	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	yC	3	GZL	O3-C3	2.11	1.48	1.43
12	lB	3	GZL	O3-C3	2.11	1.48	1.43
12	iC	3	GZL	O3-C3	2.11	1.48	1.43
13	ZB	3	GZL	O3-C3	2.09	1.48	1.43
13	dD	3	GZL	O3-C3	2.09	1.48	1.43
6	xD	3	GZL	O3-C3	2.09	1.48	1.43
20	EE	3	GZL	O3-C3	2.09	1.48	1.43
14	eD	3	GZL	O3-C3	2.09	1.48	1.43
13	9A	3	GZL	O3-C3	2.09	1.48	1.43
12	n	3	GZL	O3-C3	2.08	1.48	1.43
13	GB	3	GZL	O3-C3	2.08	1.48	1.43
13	BA	3	GZL	O3-C3	2.08	1.48	1.43
18	KE	3	GZL	O3-C3	2.07	1.48	1.43
13	o	3	GZL	O3-C3	2.07	1.48	1.43
13	jB	3	GZL	O3-C3	2.07	1.48	1.43
13	wD	3	GZL	O3-C3	2.07	1.48	1.43
14	kB	3	GZL	O3-C3	2.07	1.48	1.43
18	zE	3	GZL	O3-C3	2.07	1.48	1.43
6	GD	3	GZL	O3-C3	2.07	1.48	1.43
6	6C	3	GZL	O3-C3	2.07	1.48	1.43
6	2C	3	GZL	O3-C3	2.06	1.48	1.43
15	5C	3	GZL	O3-C3	2.06	1.48	1.43
14	KB	3	GZL	O3-C3	2.06	1.48	1.43
13	2B	3	GZL	O3-C3	2.06	1.48	1.43
15	1D	3	GZL	O3-C3	2.06	1.48	1.43
6	zD	3	GZL	O3-C3	2.06	1.48	1.43
12	lA	3	GZL	O3-C3	2.06	1.48	1.43
12	IB	3	GZL	O3-C3	2.06	1.48	1.43
6	nE	3	GZL	O3-C3	2.06	1.48	1.43
6	N	3	GZL	O3-C3	2.06	1.48	1.43
6	0C	3	GZL	O3-C3	2.06	1.48	1.43
13	1B	3	GZL	O3-C3	2.05	1.48	1.43
12	q	3	GZL	O3-C3	2.05	1.48	1.43
14	HB	3	GZL	O3-C3	2.05	1.48	1.43
6	ZE	3	GZL	O3-C3	2.05	1.48	1.43
19	aE	3	GZL	O3-C3	2.05	1.48	1.43
6	3B	3	GZL	O3-C3	2.05	1.48	1.43
19	NE	3	GZL	O3-C3	2.05	1.48	1.43
6	3D	3	GZL	O3-C3	2.04	1.48	1.43
12	cD	3	GZL	O3-C3	2.04	1.48	1.43
6	bB	3	GZL	O3-C3	2.04	1.48	1.43
12	iB	3	GZL	O3-C3	2.04	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	zB	3	GZL	O3-C3	2.04	1.48	1.43
6	4B	3	GZL	O3-C3	2.04	1.48	1.43
14	hD	3	GZL	O3-C3	2.04	1.48	1.43
15	8B	3	GZL	O3-C3	2.04	1.48	1.43
22	dE	3	GZL	O3-C3	2.04	1.48	1.43
13	7	3	GZL	O3-C3	2.04	1.48	1.43
18	0E	3	GZL	O3-C3	2.04	1.48	1.43
6	gB	3	GZL	O3-C3	2.03	1.48	1.43
15	4C	3	GZL	O3-C3	2.03	1.48	1.43
22	GE	3	GZL	O3-C3	2.03	1.48	1.43
18	pE	3	GZL	O3-C3	2.03	1.48	1.43
20	gE	3	GZL	O3-C3	2.03	1.48	1.43
20	xE	3	GZL	O3-C3	2.03	1.48	1.43
20	WE	3	GZL	O3-C3	2.03	1.48	1.43
14	s	3	GZL	O3-C3	2.03	1.48	1.43
18	BE	3	GZL	O3-C3	2.03	1.48	1.43
20	HE	3	GZL	O3-C3	2.02	1.48	1.43
20	TE	3	GZL	O3-C3	2.02	1.48	1.43
19	1E	3	GZL	O3-C3	2.02	1.48	1.43
6	yD	3	GZL	O3-C3	2.02	1.48	1.43
13	dB	3	GZL	O3-C3	2.02	1.48	1.43
15	CA	3	GZL	O3-C3	2.02	1.48	1.43
18	DE	3	GZL	O3-C3	2.02	1.48	1.43
20	uE	3	GZL	O3-C3	2.02	1.48	1.43
6	1C	3	GZL	O3-C3	2.02	1.48	1.43
18	9D	3	GZL	O3-C3	2.02	1.48	1.43
18	rE	3	GZL	O3-C3	2.02	1.48	1.43
18	yE	3	GZL	O3-C3	2.02	1.48	1.43
6	9B	3	GZL	O3-C3	2.02	1.48	1.43
13	vD	3	GZL	O3-C3	2.02	1.48	1.43
19	LE	3	GZL	O3-C3	2.02	1.48	1.43
18	JE	3	GZL	O3-C3	2.02	1.47	1.43
13	wC	3	GZL	O3-C3	2.02	1.47	1.43
14	nB	3	GZL	O3-C3	2.01	1.47	1.43
18	IE	3	GZL	O3-C3	2.01	1.47	1.43
20	hE	3	GZL	O3-C3	2.01	1.47	1.43
6	oE	3	GZL	O3-C3	2.01	1.47	1.43
13	gC	3	GZL	O3-C3	2.01	1.47	1.43
6	5B	3	GZL	O3-C3	2.01	1.47	1.43
13	WB	3	GZL	O3-C3	2.01	1.47	1.43
18	tE	3	GZL	O3-C3	2.01	1.47	1.43
6	R	3	GZL	O3-C3	2.01	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	hC	3	GZL	O3-C3	2.01	1.47	1.43
18	cE	3	GZL	O3-C3	2.01	1.47	1.43
24	YE	3	GZL	O3-C3	2.01	1.47	1.43
15	2D	3	GZL	O3-C3	2.01	1.47	1.43
24	lE	3	GZL	O3-C3	2.01	1.47	1.43
6	CB	3	GZL	O3-C3	2.00	1.47	1.43
6	AA	3	GZL	O3-C3	2.00	1.47	1.43
6	8A	3	GZL	O3-C3	2.00	1.47	1.43
6	aB	3	GZL	O3-C3	2.00	1.47	1.43
22	wE	3	GZL	O3-C3	2.00	1.47	1.43
6	bE	3	GZL	O3-C3	2.00	1.47	1.43
14	kC	3	GZL	O3-C3	2.00	1.47	1.43

All (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
6	N	3	GZL	C5-C4-C3	-9.30	102.60	115.95
13	4	3	GZL	O5-C5-C4	-9.28	87.02	109.18
6	XB	3	GZL	C1-O4-C4	-9.17	89.53	107.84
6	xC	3	GZL	C1-O4-C4	-9.11	89.65	107.84
6	3A	3	GZL	O5-C5-C4	-9.09	87.47	109.18
6	0B	3	GZL	O5-C5-C4	-8.12	89.78	109.18
6	uD	3	GZL	O5-C5-C4	-8.06	89.92	109.18
6	xC	3	GZL	O5-C5-C4	-7.99	90.10	109.18
6	XB	3	GZL	O5-C5-C4	-7.95	90.19	109.18
6	CD	3	GZL	O5-C5-C4	-7.80	90.56	109.18
6	LA	3	GZL	O4-C4-C5	7.68	125.67	109.08
6	3A	3	GZL	O4-C4-C5	7.59	125.49	109.08
6	CD	3	GZL	O4-C4-C5	7.56	125.43	109.08
6	LA	3	GZL	O5-C5-C4	-7.47	91.35	109.18
6	uD	3	GZL	O4-C4-C5	7.30	124.86	109.08
6	xC	3	GZL	O4-C4-C5	7.24	124.73	109.08
6	0B	3	GZL	O4-C4-C5	7.20	124.64	109.08
6	XB	3	GZL	O4-C4-C5	7.13	124.49	109.08
6	FC	3	GZL	C5-C4-C3	-6.95	105.97	115.95
6	N	3	GZL	O2-C2-C3	5.64	122.53	111.43
14	s	3	GZL	C5-C4-C3	-5.63	107.86	115.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	9D	1	FUB	O2-C2-C3	5.49	122.23	111.43
14	kC	3	GZL	C5-C4-C3	-5.38	108.23	115.95
17	5D	4	MAN	C1-C2-C3	4.95	116.85	109.64
14	nA	3	GZL	C5-C4-C3	-4.91	108.90	115.95
6	6D	3	GZL	C5-C4-C3	-4.90	108.91	115.95
14	qA	3	GZL	C5-C4-C3	-4.85	108.98	115.95
17	5D	4	MAN	C1-O5-C5	4.81	118.63	112.19
18	pE	1	FUB	O2-C2-C3	4.76	120.80	111.43
14	eD	3	GZL	C5-C4-C3	-4.73	109.16	115.95
6	4B	3	GZL	C5-C4-C3	-4.62	109.31	115.95
14	KB	3	GZL	C5-C4-C3	-4.61	109.33	115.95
6	mE	3	GZL	C5-C4-C3	-4.59	109.36	115.95
18	DE	3	GZL	C5-C4-C3	-4.58	109.37	115.95
22	eE	3	GZL	C5-C4-C3	-4.54	109.43	115.95
6	OE	3	GZL	C5-C4-C3	-4.48	109.51	115.95
18	cE	3	GZL	C5-C4-C3	-4.46	109.55	115.95
15	5C	3	GZL	C5-C4-C3	-4.45	109.55	115.95
20	CE	3	GZL	C5-C4-C3	-4.45	109.57	115.95
18	yE	3	GZL	C5-C4-C3	-4.44	109.57	115.95
14	hC	3	GZL	C5-C4-C3	-4.43	109.59	115.95
6	cB	3	GZL	C5-C4-C3	-4.43	109.59	115.95
6	nE	3	GZL	C5-C4-C3	-4.42	109.60	115.95
20	jE	3	GZL	C5-C4-C3	-4.42	109.61	115.95
19	aE	3	GZL	C5-C4-C3	-4.41	109.62	115.95
18	IE	3	GZL	C5-C4-C3	-4.41	109.62	115.95
20	HE	3	GZL	C5-C4-C3	-4.40	109.63	115.95
19	1E	3	GZL	C5-C4-C3	-4.39	109.64	115.95
6	oE	3	GZL	C5-C4-C3	-4.39	109.65	115.95
22	dE	3	GZL	C5-C4-C3	-4.37	109.67	115.95
20	TE	3	GZL	C5-C4-C3	-4.36	109.68	115.95
6	8A	3	GZL	C5-C4-C3	-4.35	109.70	115.95
6	bE	3	GZL	C5-C4-C3	-4.35	109.71	115.95
18	pE	3	GZL	C5-C4-C3	-4.34	109.72	115.95
18	zE	3	GZL	C5-C4-C3	-4.33	109.73	115.95
20	uE	3	GZL	C5-C4-C3	-4.29	109.78	115.95
20	xE	3	GZL	C5-C4-C3	-4.29	109.79	115.95
6	R	3	GZL	C5-C4-C3	-4.29	109.80	115.95
13	9A	3	GZL	C1-C2-C3	-4.28	94.78	101.63
6	8D	3	GZL	C5-C4-C3	-4.27	109.81	115.95
13	4A	3	GZL	C5-C4-C3	-4.27	109.81	115.95
6	ME	3	GZL	C5-C4-C3	-4.27	109.81	115.95
20	sE	3	GZL	C5-C4-C3	-4.26	109.83	115.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	1C	3	GZL	C5-C4-C3	-4.26	109.83	115.95
13	yC	3	GZL	C5-C4-C3	-4.26	109.84	115.95
20	EE	3	GZL	C5-C4-C3	-4.25	109.84	115.95
22	VE	3	GZL	C5-C4-C3	-4.25	109.85	115.95
6	yD	3	GZL	C5-C4-C3	-4.23	109.88	115.95
15	4C	3	GZL	C5-C4-C3	-4.20	109.92	115.95
13	vD	3	GZL	C5-C4-C3	-4.19	109.93	115.95
19	NE	3	GZL	C5-C4-C3	-4.18	109.95	115.95
14	HB	3	GZL	C5-C4-C3	-4.17	109.96	115.95
6	2C	3	GZL	C5-C4-C3	-4.17	109.97	115.95
13	wD	3	GZL	C5-C4-C3	-4.16	109.98	115.95
12	FB	3	GZL	C5-C4-C3	-4.15	109.99	115.95
6	zD	3	GZL	C5-C4-C3	-4.14	110.00	115.95
18	tE	3	GZL	C5-C4-C3	-4.12	110.04	115.95
18	9D	1	FUB	C1-C2-C3	-4.11	95.05	101.63
6	6C	3	GZL	C5-C4-C3	-4.10	110.06	115.95
6	bB	3	GZL	C5-C4-C3	-4.09	110.07	115.95
19	qE	3	GZL	C5-C4-C3	-4.09	110.08	115.95
18	JE	3	GZL	C5-C4-C3	-4.09	110.08	115.95
24	lE	3	GZL	C5-C4-C3	-4.09	110.08	115.95
18	SE	3	GZL	C5-C4-C3	-4.08	110.09	115.95
22	QE	3	GZL	C5-C4-C3	-4.07	110.10	115.95
15	eB	3	GZL	C5-C4-C3	-4.07	110.10	115.95
13	1B	3	GZL	C5-C4-C3	-4.07	110.11	115.95
13	2B	3	GZL	C5-C4-C3	-4.06	110.11	115.95
15	2D	3	GZL	C5-C4-C3	-4.06	110.11	115.95
6	6A	3	GZL	C5-C4-C3	-4.06	110.12	115.95
12	iB	3	GZL	C5-C4-C3	-4.06	110.12	115.95
6	JC	3	GZL	C5-C4-C3	-4.06	110.13	115.95
20	hE	3	GZL	C5-C4-C3	-4.05	110.14	115.95
6	7D	3	GZL	C5-C4-C3	-4.04	110.14	115.95
22	iE	3	GZL	C5-C4-C3	-4.04	110.15	115.95
18	rE	3	GZL	C5-C4-C3	-4.03	110.16	115.95
13	6	3	GZL	C5-C4-C3	-4.02	110.18	115.95
18	PE	3	GZL	C5-C4-C3	-4.02	110.18	115.95
22	GE	3	GZL	C5-C4-C3	-4.01	110.19	115.95
12	IB	3	GZL	C5-C4-C3	-4.01	110.19	115.95
18	BE	3	GZL	C5-C4-C3	-4.01	110.19	115.95
6	9B	3	GZL	C5-C4-C3	-4.00	110.20	115.95
6	xD	3	GZL	C5-C4-C3	-4.00	110.20	115.95
23	XE	3	GZL	C5-C4-C3	-4.00	110.20	115.95
6	PA	3	GZL	C5-C4-C3	-4.00	110.21	115.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	YE	3	GZL	C5-C4-C3	-4.00	110.21	115.95
6	8	3	GZL	C5-C4-C3	-3.99	110.22	115.95
19	AE	3	GZL	C5-C4-C3	-3.99	110.22	115.95
6	7A	3	GZL	C5-C4-C3	-3.98	110.23	115.95
6	GD	3	GZL	C5-C4-C3	-3.97	110.25	115.95
13	4	3	GZL	C5-C4-C3	3.97	121.66	115.95
6	aB	3	GZL	C5-C4-C3	-3.97	110.25	115.95
15	DA	3	GZL	C5-C4-C3	-3.97	110.25	115.95
22	wE	3	GZL	C5-C4-C3	-3.97	110.26	115.95
14	kB	3	GZL	C5-C4-C3	-3.96	110.26	115.95
12	iC	3	GZL	C5-C4-C3	-3.95	110.28	115.95
6	5	3	GZL	C5-C4-C3	-3.94	110.29	115.95
15	7B	3	GZL	C5-C4-C3	-3.94	110.29	115.95
20	WE	3	GZL	C5-C4-C3	-3.93	110.30	115.95
6	3B	3	GZL	C5-C4-C3	-3.92	110.33	115.95
18	KE	3	GZL	C5-C4-C3	-3.91	110.33	115.95
13	zC	3	GZL	C5-C4-C3	-3.90	110.35	115.95
14	p	3	GZL	C5-C4-C3	-3.90	110.35	115.95
6	5B	3	GZL	C5-C4-C3	-3.90	110.36	115.95
6	0C	3	GZL	C5-C4-C3	-3.89	110.37	115.95
6	9	3	GZL	C5-C4-C3	-3.87	110.39	115.95
13	ZB	3	GZL	C5-C4-C3	-3.87	110.39	115.95
18	fE	3	GZL	C5-C4-C3	-3.87	110.39	115.95
6	gB	3	GZL	C5-C4-C3	-3.87	110.40	115.95
13	BA	3	GZL	C1-C2-C3	-3.86	95.45	101.63
12	lB	3	GZL	C5-C4-C3	-3.85	110.42	115.95
21	FE	3	GZL	C5-C4-C3	-3.85	110.42	115.95
13	3C	3	GZL	C5-C4-C3	-3.85	110.43	115.95
19	LE	3	GZL	C5-C4-C3	-3.84	110.43	115.95
6	6A	2	FUB	O2-C2-C3	3.84	118.98	111.43
12	q	3	GZL	C5-C4-C3	-3.83	110.44	115.95
18	0E	3	GZL	C5-C4-C3	-3.83	110.45	115.95
15	1D	3	GZL	C5-C4-C3	-3.83	110.45	115.95
15	fB	3	GZL	C5-C4-C3	-3.83	110.45	115.95
16	FA	2	NAG	O5-C1-C2	3.82	117.20	111.29
12	cD	3	GZL	C5-C4-C3	-3.81	110.48	115.95
13	mA	3	GZL	C5-C4-C3	-3.80	110.49	115.95
14	nB	3	GZL	C5-C4-C3	-3.80	110.49	115.95
22	RE	3	GZL	C5-C4-C3	-3.80	110.49	115.95
6	ZE	3	GZL	C5-C4-C3	-3.79	110.51	115.95
13	GB	3	GZL	C5-C4-C3	-3.79	110.51	115.95
6	3D	3	GZL	C5-C4-C3	-3.76	110.55	115.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	vE	3	GZL	C5-C4-C3	-3.76	110.55	115.95
13	dB	3	GZL	C1-C2-C3	-3.74	95.64	101.63
13	0D	3	GZL	C5-C4-C3	-3.74	110.58	115.95
14	hD	3	GZL	C5-C4-C3	-3.73	110.59	115.95
13	gC	3	GZL	C5-C4-C3	-3.73	110.60	115.95
18	9D	3	GZL	C5-C4-C3	-3.72	110.60	115.95
18	pE	1	FUB	C1-C2-C3	-3.70	95.70	101.63
20	UE	3	GZL	C5-C4-C3	-3.70	110.64	115.95
12	fC	3	GZL	C5-C4-C3	-3.69	110.66	115.95
6	AA	3	GZL	C5-C4-C3	-3.68	110.66	115.95
12	oA	3	GZL	C5-C4-C3	-3.68	110.66	115.95
6	EA	3	GZL	C5-C4-C3	-3.68	110.67	115.95
6	CB	3	GZL	C5-C4-C3	-3.64	110.72	115.95
13	dD	3	GZL	C5-C4-C3	-3.64	110.73	115.95
16	4D	2	NAG	C1-O5-C5	3.64	117.06	112.19
16	AC	2	NAG	O5-C1-C2	3.63	116.90	111.29
6	XB	3	GZL	C1-C2-C3	-3.62	95.84	101.63
6	CD	3	GZL	C5-C4-C3	-3.61	110.77	115.95
13	6B	3	GZL	C5-C4-C3	-3.61	110.77	115.95
20	gE	3	GZL	C5-C4-C3	-3.59	110.80	115.95
6	LA	3	GZL	C5-C4-C3	-3.59	110.80	115.95
13	4	3	GZL	O3-C3-C2	-3.59	103.47	111.97
13	o	3	GZL	C5-C4-C3	-3.57	110.83	115.95
6	xC	3	GZL	C1-C2-C3	-3.56	95.93	101.63
13	WB	3	GZL	C5-C4-C3	-3.56	110.84	115.95
13	jB	3	GZL	C5-C4-C3	-3.55	110.85	115.95
13	7	3	GZL	C5-C4-C3	-3.55	110.85	115.95
17	GA	3	BMA	C1-O5-C5	3.49	116.87	112.19
21	kE	3	GZL	C5-C4-C3	-3.46	110.99	115.95
13	zB	3	GZL	C5-C4-C3	-3.45	110.99	115.95
12	fD	3	GZL	C5-C4-C3	-3.44	111.02	115.95
16	FA	2	NAG	C1-O5-C5	3.42	116.77	112.19
6	uD	3	GZL	C1-C2-C3	-3.40	96.19	101.63
13	6B	3	GZL	C1-C2-C3	-3.39	96.21	101.63
6	xD	3	GZL	C1-C2-C3	3.38	107.04	101.63
13	dB	3	GZL	C5-C4-C3	-3.36	111.12	115.95
17	5D	1	NAG	C1-O5-C5	3.35	116.68	112.19
6	LA	3	GZL	O5-C5-C6	3.30	116.53	109.03
15	8B	3	GZL	C5-C4-C3	-3.28	111.23	115.95
13	BA	3	GZL	C1-O4-C4	-3.23	101.39	107.84
6	FC	3	GZL	O4-C1-C2	-3.21	100.23	105.76
12	FB	3	GZL	C1-C2-C3	3.21	106.75	101.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	6D	3	GZL	C1-C2-C3	3.20	106.75	101.63
12	n	3	GZL	C5-C4-C3	-3.20	111.36	115.95
13	9A	3	GZL	C1-O4-C4	-3.19	101.47	107.84
6	0B	3	GZL	C1-C2-C3	-3.19	96.53	101.63
14	KB	3	GZL	C1-C2-C3	3.15	106.67	101.63
13	2A	2	FUB	O2-C2-C3	3.15	117.62	111.43
6	FC	2	FUB	O2-C2-C1	3.15	120.68	110.89
17	DB	6	MAN	C3-C4-C5	3.14	115.92	110.23
14	HB	3	GZL	C1-C2-C3	3.13	106.63	101.63
17	7C	1	NAG	C1-O5-C5	3.10	116.34	112.19
17	7C	4	MAN	C1-O5-C5	3.09	116.32	112.19
16	4D	2	NAG	O5-C1-C2	3.08	116.05	111.29
13	BA	3	GZL	C5-C4-C3	-3.08	111.53	115.95
19	qE	1	FUB	C1-C2-C3	3.07	106.53	101.63
17	5D	4	MAN	O5-C1-C2	3.07	118.10	110.79
14	p	3	GZL	O5-C5-C6	3.06	115.99	109.03
15	AB	3	GZL	C5-C4-C3	-3.06	111.56	115.95
24	lE	1	FUB	C1-C2-C3	3.01	106.45	101.63
15	BB	3	GZL	C5-C4-C3	-3.01	111.62	115.95
24	YE	1	FUB	C1-C2-C3	3.01	106.44	101.63
13	YB	3	GZL	C5-C4-C3	-2.98	111.67	115.95
6	3B	3	GZL	C1-C2-C3	2.98	106.39	101.63
6	3B	2	FUB	O2-C2-C3	2.94	117.22	111.43
15	CA	3	GZL	C5-C4-C3	-2.93	111.75	115.95
13	dB	3	GZL	O4-C1-C2	-2.92	100.72	105.76
6	LA	2	FUB	C1-C2-C3	2.91	106.28	101.63
13	BA	3	GZL	O4-C1-C2	-2.91	100.75	105.76
12	lA	3	GZL	C5-C4-C3	-2.91	111.77	115.95
6	N	3	GZL	O5-C5-C6	2.91	115.64	109.03
6	CD	3	GZL	O5-C5-C6	2.90	115.61	109.03
13	4	3	GZL	O4-C1-C2	-2.89	100.78	105.76
21	FE	1	FUB	C1-C2-C3	2.88	106.24	101.63
6	cB	2	FUB	C1-C2-C3	2.87	106.22	101.63
13	6B	3	GZL	O4-C1-C2	-2.86	100.83	105.76
6	5B	2	FUB	C1-C2-C3	2.86	106.19	101.63
4	DC	1	FUB	C1-C2-C3	2.85	106.19	101.63
20	TE	1	FUB	C1-C2-C3	2.85	106.18	101.63
18	cE	1	FUB	C1-C2-C3	2.84	106.16	101.63
13	5A	3	GZL	C5-C4-C3	-2.83	111.89	115.95
7	KC	1	FUB	C1-C2-C3	2.82	106.13	101.63
13	9A	3	GZL	O4-C1-C2	-2.82	100.91	105.76
3	NA	1	FUB	C1-C2-C3	2.82	106.13	101.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	2C	2	FUB	C1-C2-C3	2.82	106.13	101.63
4	d	4	AHR	C1-C2-C3	2.81	106.12	101.63
7	QA	1	FUB	C1-C2-C3	2.80	106.10	101.63
13	9A	3	GZL	C5-C4-C3	-2.80	111.93	115.95
18	yE	3	GZL	C1-C2-C3	2.80	106.10	101.63
6	FC	1	FUB	O2-C2-C3	2.79	116.93	111.43
18	9D	5	AHR	C1-C2-C3	2.79	106.09	101.63
12	oA	1	FUB	C1-C2-C3	2.79	106.09	101.63
7	S	1	FUB	C1-C2-C3	2.78	106.08	101.63
13	4	2	FUB	O2-C2-C3	2.78	116.90	111.43
18	DE	1	FUB	C1-C2-C3	2.78	106.07	101.63
6	5	2	FUB	O2-C2-C3	2.77	116.89	111.43
16	AC	1	NAG	C4-C3-C2	2.77	115.08	111.02
19	AE	1	FUB	C1-C2-C3	2.77	106.05	101.63
14	kB	3	GZL	C1-C2-C3	2.77	106.05	101.63
7	HD	1	FUB	C1-C2-C3	2.76	106.05	101.63
13	dB	3	GZL	C1-O4-C4	-2.76	102.33	107.84
10	mC	5	AHR	C1-C2-C3	2.76	106.03	101.63
12	lB	1	FUB	C1-C2-C3	2.75	106.03	101.63
6	9B	3	GZL	C1-C2-C3	2.75	106.03	101.63
10	3	1	FUB	C1-C2-C3	2.75	106.02	101.63
15	DA	4	AHR	C1-C2-C3	2.73	105.99	101.63
14	nA	3	GZL	O5-C5-C6	2.72	115.20	109.03
11	i	1	FUB	O2-C2-C3	2.72	116.77	111.43
4	PC	4	AHR	O2-C2-C1	2.71	119.34	110.89
12	n	4	AHR	C1-C2-C3	2.71	105.97	101.63
10	MB	5	AHR	C1-C2-C3	2.71	105.97	101.63
4	OC	4	AHR	C1-C2-C3	2.71	105.97	101.63
17	GA	3	BMA	C2-C3-C4	-2.71	106.09	110.86
6	AA	2	FUB	C1-C2-C3	2.70	105.95	101.63
13	4	3	GZL	C1-C2-C3	2.70	105.94	101.63
7	UD	1	FUB	C1-C2-C3	2.68	105.91	101.63
4	RD	4	AHR	C1-C2-C3	2.68	105.91	101.63
3	vB	1	FUB	C1-C2-C3	2.67	105.90	101.63
6	4B	3	GZL	C1-C2-C3	2.67	105.90	101.63
10	VB	3	FUB	O3-C3-C2	2.67	118.29	111.97
22	VE	1	FUB	O2-C2-C3	2.67	116.68	111.43
13	6B	3	GZL	C1-O4-C4	-2.66	102.52	107.84
10	1A	1	FUB	C1-C2-C3	2.66	105.88	101.63
6	zD	2	FUB	C1-C2-C3	2.65	105.87	101.63
10	a	4	AHR	C1-C2-C3	2.65	105.87	101.63
22	dE	4	AHR	C1-C2-C3	2.65	105.87	101.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	8A	2	FUB	C1-C2-C3	2.65	105.86	101.63
6	7D	3	GZL	O4-C1-C2	-2.64	101.20	105.76
3	rD	1	FUB	C1-C2-C3	2.64	105.85	101.63
8	MC	4	AHR	C1-C2-C3	2.63	105.84	101.63
6	oE	3	GZL	C1-C2-C3	2.63	105.84	101.63
6	bB	1	FUB	C1-C2-C3	2.62	105.83	101.63
18	pE	5	AHR	C1-C2-C3	2.62	105.83	101.63
14	eD	3	GZL	C1-C2-C3	2.62	105.82	101.63
12	lA	4	AHR	C1-C2-C3	2.62	105.82	101.63
16	AC	2	NAG	C1-O5-C5	2.62	115.70	112.19
4	tA	4	AHR	C1-C2-C3	2.62	105.82	101.63
6	nE	1	FUB	C1-C2-C3	2.62	105.82	101.63
22	GE	5	AHR	O2-C2-C1	2.62	119.04	110.89
18	PE	1	FUB	C1-C2-C3	2.62	105.81	101.63
5	M	5	AHR	C1-C2-C3	2.62	105.81	101.63
13	wC	3	GZL	C5-C4-C3	-2.61	112.20	115.95
4	Z	4	AHR	C1-C2-C3	2.61	105.80	101.63
4	iA	4	AHR	C1-C2-C3	2.61	105.80	101.63
6	0C	2	FUB	O2-C2-C3	2.61	116.56	111.43
7	dA	2	FUB	C1-C2-C3	2.61	105.80	101.63
3	ZA	1	FUB	C1-C2-C3	2.61	105.80	101.63
18	rE	2	FUB	C1-C2-C3	2.60	105.79	101.63
11	gA	1	FUB	O2-C2-C3	2.60	116.55	111.43
6	0B	2	FUB	O2-C2-C3	2.60	116.55	111.43
9	j	1	FUB	C1-C2-C3	2.60	105.79	101.63
13	BA	2	FUB	C1-C2-C3	2.60	105.78	101.63
14	hC	3	GZL	C1-C2-C3	2.60	105.78	101.63
18	IE	5	AHR	C1-C2-C3	2.58	105.76	101.63
17	GA	1	NAG	C1-O5-C5	2.58	115.64	112.19
13	4A	4	AHR	C1-C2-C3	2.58	105.75	101.63
6	GD	1	FUB	C1-C2-C3	2.57	105.74	101.63
10	pB	5	AHR	C1-C2-C3	2.57	105.74	101.63
10	u	5	AHR	C1-C2-C3	2.57	105.73	101.63
22	wE	5	AHR	O2-C2-C3	2.57	116.48	111.43
3	sC	1	FUB	C1-C2-C3	2.56	105.73	101.63
13	vD	4	AHR	C1-C2-C3	2.56	105.73	101.63
22	wE	5	AHR	O2-C2-C1	2.56	118.86	110.89
10	PD	1	FUB	C1-C2-C3	2.55	105.71	101.63
10	sA	5	AHR	C1-C2-C3	2.55	105.71	101.63
19	lE	1	FUB	C1-C2-C3	2.55	105.70	101.63
3	b	1	FUB	C1-C2-C3	2.55	105.70	101.63
18	rE	5	AHR	C1-C2-C3	2.55	105.70	101.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	6D	2	FUB	C1-C2-C3	2.54	105.69	101.63
18	9D	1	FUB	O3-C3-C4	2.54	118.38	111.08
13	7	4	AHR	C1-C2-C3	2.54	105.69	101.63
22	VE	4	AHR	C1-C2-C3	2.54	105.69	101.63
17	7C	3	BMA	C2-C3-C4	-2.54	106.40	110.86
18	yE	5	AHR	C1-C2-C3	2.54	105.68	101.63
17	GA	3	BMA	C3-C4-C5	-2.53	105.64	110.23
6	gB	3	GZL	C1-C2-C3	2.53	105.67	101.63
4	gD	1	FUB	C1-C2-C3	2.53	105.67	101.63
4	iA	1	FUB	C1-C2-C3	2.53	105.67	101.63
5	BD	4	AHR	C1-C2-C3	2.52	105.66	101.63
24	lE	2	FUB	C1-C2-C3	2.52	105.66	101.63
18	BE	5	AHR	C1-C2-C3	2.52	105.65	101.63
10	sD	1	FUB	C1-C2-C3	2.51	105.65	101.63
12	lA	5	AHR	C1-C2-C3	2.51	105.65	101.63
18	zE	3	GZL	C1-C2-C3	2.51	105.65	101.63
15	AB	5	AHR	C1-C2-C3	2.51	105.64	101.63
4	Z	1	FUB	O2-C2-C3	2.51	116.37	111.43
22	iE	6	AHR	C1-C2-C3	2.51	105.64	101.63
17	DB	3	BMA	C2-C3-C4	-2.51	106.45	110.86
4	AD	1	FUB	C1-C2-C3	2.51	105.64	101.63
20	WE	4	AHR	C1-C2-C3	2.51	105.64	101.63
22	dE	1	FUB	C1-C2-C3	2.51	105.64	101.63
12	iC	1	FUB	C1-C2-C3	2.51	105.63	101.63
7	f	2	FUB	C1-C2-C3	2.50	105.63	101.63
6	N	2	FUB	O2-C2-C1	2.50	118.67	110.89
18	lE	4	AHR	C1-C2-C3	2.50	105.63	101.63
10	PD	4	AHR	C1-C2-C3	2.49	105.61	101.63
18	BE	2	FUB	C1-C2-C3	2.49	105.61	101.63
13	4	3	GZL	C1-O4-C4	-2.49	102.87	107.84
17	5D	3	BMA	C2-C3-C4	-2.49	106.49	110.86
6	yD	2	FUB	C1-C2-C3	2.48	105.59	101.63
18	yE	4	AHR	C1-C2-C3	2.47	105.58	101.63
13	YB	4	AHR	C1-C2-C3	2.47	105.58	101.63
4	AD	4	AHR	C1-C2-C3	2.47	105.58	101.63
4	tA	1	FUB	C1-C2-C3	2.47	105.57	101.63
18	9D	1	FUB	O3-C3-C2	2.46	117.81	111.97
22	eE	1	FUB	O2-C2-C3	2.46	116.27	111.43
12	fC	4	AHR	C1-C2-C3	2.46	105.56	101.63
11	XD	3	AHR	C1-C2-C3	2.46	105.56	101.63
22	iE	1	FUB	O2-C2-C3	2.46	116.26	111.43
3	e	3	FUB	C1-C2-C3	2.45	105.55	101.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	a	1	FUB	C1-C2-C3	2.45	105.55	101.63
24	lE	6	AHR	C1-C2-C3	2.45	105.55	101.63
10	sA	4	AHR	C1-C2-C3	2.45	105.54	101.63
3	SB	2	FUB	C1-C2-C3	2.45	105.54	101.63
22	QE	4	AHR	C1-C2-C3	2.44	105.54	101.63
3	T	1	FUB	C1-C2-C3	2.44	105.53	101.63
19	LE	2	FUB	C1-C2-C3	2.44	105.53	101.63
6	FC	3	GZL	O2-C2-C1	2.44	118.49	110.89
7	ZC	3	FUB	C1-C2-C3	2.44	105.53	101.63
6	N	3	GZL	O6-C6-C5	-2.44	106.03	111.16
10	VB	5	AHR	C1-C2-C3	2.44	105.53	101.63
20	sE	1	FUB	C1-C2-C3	2.43	105.52	101.63
3	uA	3	FUB	C1-C2-C3	2.43	105.52	101.63
3	vA	3	FUB	C1-C2-C3	2.43	105.52	101.63
13	3C	2	FUB	C1-C2-C3	2.43	105.52	101.63
15	CA	4	AHR	O2-C2-C1	2.42	118.42	110.89
13	gC	4	AHR	C1-C2-C3	2.42	105.49	101.63
13	wC	4	AHR	C1-C2-C3	2.42	105.49	101.63
18	pE	1	FUB	O3-C3-C2	2.42	117.69	111.97
6	mE	3	GZL	C1-C2-C3	2.42	105.49	101.63
3	SB	1	FUB	C1-C2-C3	2.41	105.49	101.63
17	DB	6	MAN	O5-C1-C2	-2.41	105.03	110.79
3	TC	3	FUB	C1-C2-C3	2.41	105.48	101.63
17	DB	4	MAN	C1-C2-C3	2.41	113.15	109.64
3	dC	3	FUB	C1-C2-C3	2.41	105.48	101.63
22	GE	5	AHR	O2-C2-C3	2.41	116.17	111.43
15	5C	1	FUB	C1-C2-C3	2.40	105.47	101.63
3	TA	2	FUB	C1-C2-C3	2.40	105.47	101.63
6	aB	2	FUB	O2-C2-C3	2.40	116.16	111.43
6	0C	3	GZL	C1-C2-C3	2.40	105.47	101.63
21	kE	5	AHR	C1-C2-C3	2.39	105.46	101.63
6	9B	2	FUB	C1-C2-C3	2.38	105.44	101.63
3	xB	1	FUB	C1-C2-C3	2.38	105.44	101.63
12	IB	5	AHR	C1-C2-C3	2.38	105.44	101.63
10	mC	1	FUB	C1-C2-C3	2.38	105.44	101.63
24	YE	5	AHR	C1-C2-C3	2.38	105.43	101.63
10	1A	3	FUB	O3-C3-C2	2.38	117.60	111.97
10	vC	1	FUB	C1-C2-C3	2.38	105.43	101.63
22	QE	6	AHR	C1-C2-C3	2.38	105.43	101.63
4	YC	4	AHR	C1-C2-C3	2.37	105.42	101.63
4	OD	4	AHR	C1-C2-C3	2.37	105.42	101.63
14	s	3	GZL	C1-C2-C3	2.37	105.42	101.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	dE	6	AHR	C1-C2-C3	2.37	105.42	101.63
22	RE	5	AHR	C1-C2-C3	2.37	105.42	101.63
22	wE	5	AHR	C1-C2-C3	2.37	105.41	101.63
14	nA	3	GZL	C1-O4-C4	-2.37	103.11	107.84
13	6B	2	FUB	O3-C3-C2	2.36	117.57	111.97
6	3D	2	FUB	C1-C2-C3	2.36	105.41	101.63
15	AB	4	AHR	O2-C2-C1	2.36	118.24	110.89
3	WC	1	FUB	O2-C2-C3	2.36	116.07	111.43
14	kC	3	GZL	C1-C2-C3	2.36	105.40	101.63
4	jC	1	FUB	C1-C2-C3	2.36	105.40	101.63
19	1E	4	AHR	C1-C2-C3	2.35	105.39	101.63
3	RA	1	FUB	C1-C2-C3	2.35	105.38	101.63
12	iB	3	GZL	C1-C2-C3	2.35	105.38	101.63
13	zC	3	GZL	C1-C2-C3	2.35	105.38	101.63
10	yB	1	FUB	C1-C2-C3	2.35	105.38	101.63
13	tD	4	AHR	C1-C2-C3	2.35	105.38	101.63
13	4	4	AHR	C1-C2-C3	2.34	105.37	101.63
13	6	4	AHR	C1-C2-C3	2.34	105.37	101.63
4	g	4	AHR	C1-C2-C3	2.34	105.37	101.63
3	HC	1	FUB	C1-C2-C3	2.34	105.37	101.63
12	fD	1	FUB	C1-C2-C3	2.34	105.37	101.63
13	zB	4	AHR	C1-C2-C3	2.34	105.36	101.63
6	CD	2	FUB	O2-C2-C3	2.33	116.02	111.43
10	YA	5	AHR	C1-C2-C3	2.33	105.36	101.63
24	lE	5	AHR	C1-C2-C3	2.33	105.36	101.63
20	xE	1	FUB	C1-C2-C3	2.33	105.36	101.63
15	1D	5	AHR	C1-C2-C3	2.33	105.35	101.63
13	WB	4	AHR	C1-C2-C3	2.32	105.34	101.63
11	i	3	AHR	C1-C2-C3	2.32	105.34	101.63
22	GE	1	FUB	O2-C2-C3	2.32	116.00	111.43
6	8A	1	FUB	C1-C2-C3	2.32	105.34	101.63
3	TC	1	FUB	C1-C2-C3	2.32	105.34	101.63
18	9D	4	AHR	C1-C2-C3	2.32	105.34	101.63
22	RE	6	AHR	C1-C2-C3	2.32	105.34	101.63
22	GE	2	FUB	O2-C2-C3	2.32	115.99	111.43
15	5C	5	AHR	C1-C2-C3	2.32	105.34	101.63
22	eE	6	AHR	C1-C2-C3	2.32	105.33	101.63
23	XE	1	FUB	C1-C2-C3	2.31	105.33	101.63
3	V	3	FUB	C1-C2-C3	2.31	105.32	101.63
5	KA	3	FUB	C1-C2-C3	2.31	105.32	101.63
6	7A	1	FUB	C1-C2-C3	2.31	105.32	101.63
13	2A	1	FUB	C1-C2-C3	2.31	105.32	101.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	4	AHR	C1-C2-C3	2.31	105.32	101.63
3	9C	2	FUB	C1-C2-C3	2.31	105.32	101.63
10	1A	5	AHR	C1-C2-C3	2.31	105.31	101.63
13	BA	2	FUB	O3-C3-C2	2.30	117.43	111.97
8	JD	4	AHR	C1-C2-C3	2.30	105.31	101.63
15	8B	5	AHR	C1-C2-C3	2.30	105.31	101.63
4	VD	4	AHR	C1-C2-C3	2.30	105.31	101.63
4	v	1	FUB	C1-C2-C3	2.30	105.31	101.63
13	ZB	3	GZL	C1-C2-C3	2.30	105.31	101.63
14	hD	3	GZL	O4-C1-C2	-2.30	101.80	105.76
3	O	1	FUB	C1-C2-C3	2.30	105.31	101.63
6	xC	1	FUB	C1-C2-C3	2.30	105.30	101.63
14	nB	3	GZL	C1-C2-C3	2.30	105.30	101.63
3	tC	3	FUB	C1-C2-C3	2.30	105.30	101.63
3	oB	1	FUB	C1-C2-C3	2.29	105.30	101.63
18	BE	3	GZL	C1-C2-C3	2.29	105.29	101.63
5	M	2	FUB	C1-C2-C3	2.29	105.29	101.63
11	i	2	AHR	C1-C2-C3	2.29	105.29	101.63
3	DD	1	FUB	C1-C2-C3	2.29	105.29	101.63
3	P	1	FUB	C1-C2-C3	2.29	105.28	101.63
6	3A	2	FUB	O2-C2-C3	2.28	115.92	111.43
3	XA	3	FUB	C1-C2-C3	2.28	105.28	101.63
3	OA	1	FUB	C1-C2-C3	2.28	105.27	101.63
4	SD	4	AHR	C1-C2-C3	2.28	105.27	101.63
4	JA	4	AHR	C1-C2-C3	2.28	105.27	101.63
3	jA	3	FUB	C1-C2-C3	2.28	105.27	101.63
6	N	3	GZL	C6-C5-C4	2.28	116.58	112.05
12	iC	4	AHR	C1-C2-C3	2.27	105.26	101.63
17	DB	1	NAG	C1-O5-C5	2.27	115.23	112.19
22	GE	5	AHR	C1-C2-C3	2.27	105.25	101.63
10	3	3	FUB	O3-C3-C2	2.27	117.34	111.97
24	lE	4	AHR	C1-C2-C3	2.27	105.25	101.63
3	TB	2	FUB	C1-C2-C3	2.26	105.25	101.63
13	o	4	AHR	C1-C2-C3	2.26	105.24	101.63
13	jB	1	FUB	C1-C2-C3	2.26	105.24	101.63
3	0	1	FUB	C1-C2-C3	2.26	105.24	101.63
8	U	4	AHR	C1-C2-C3	2.26	105.24	101.63
12	fD	2	FUB	C1-C2-C3	2.26	105.24	101.63
4	qB	4	AHR	C1-C2-C3	2.26	105.24	101.63
5	KA	4	AHR	C1-C2-C3	2.26	105.23	101.63
12	IB	4	AHR	C1-C2-C3	2.26	105.23	101.63
8	MC	5	AHR	C1-C2-C3	2.25	105.23	101.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	nB	4	FUB	C1-C2-C3	2.25	105.23	101.63
18	KE	4	AHR	C1-C2-C3	2.25	105.22	101.63
4	mB	1	FUB	C1-C2-C3	2.25	105.22	101.63
18	tE	1	FUB	C1-C2-C3	2.25	105.22	101.63
13	2A	2	FUB	O3-C3-C2	2.25	117.30	111.97
3	cA	3	FUB	C1-C2-C3	2.25	105.22	101.63
4	W	4	AHR	C1-C2-C3	2.25	105.22	101.63
6	3A	3	GZL	O2-C2-C3	-2.25	107.00	111.43
13	mA	4	AHR	C1-C2-C3	2.24	105.22	101.63
12	iC	5	AHR	C1-C2-C3	2.24	105.22	101.63
15	fB	5	AHR	C1-C2-C3	2.24	105.22	101.63
6	FC	1	FUB	O2-C2-C1	2.24	117.87	110.89
13	2A	4	AHR	C1-C2-C3	2.24	105.21	101.63
3	z	1	FUB	C1-C2-C3	2.24	105.21	101.63
4	LD	1	FUB	O2-C2-C3	2.23	115.83	111.43
13	WB	2	FUB	O2-C2-C3	2.23	115.83	111.43
6	8D	3	GZL	C1-C2-C3	2.23	105.20	101.63
17	DB	4	MAN	C1-O5-C5	2.23	115.18	112.19
6	R	1	FUB	C1-C2-C3	2.23	105.20	101.63
14	qA	3	GZL	O5-C5-C4	2.23	114.51	109.18
6	7D	2	FUB	C1-C2-C3	2.23	105.20	101.63
6	oE	2	FUB	C1-C2-C3	2.23	105.20	101.63
6	3D	1	FUB	C1-C2-C3	2.23	105.20	101.63
14	kB	3	GZL	O5-C5-C4	2.23	114.50	109.18
3	UB	1	FUB	C1-C2-C3	2.23	105.19	101.63
12	n	5	AHR	C1-C2-C3	2.23	105.19	101.63
22	VE	5	AHR	C1-C2-C3	2.22	105.18	101.63
7	WD	4	AHR	C1-C2-C3	2.22	105.18	101.63
14	p	3	GZL	C1-O4-C4	-2.22	103.40	107.84
13	zB	2	FUB	O2-C2-C3	2.22	115.80	111.43
19	qE	3	GZL	C1-C2-C3	2.22	105.18	101.63
14	p	3	GZL	C1-C2-C3	2.22	105.18	101.63
4	LD	4	AHR	C1-C2-C3	2.22	105.17	101.63
13	0D	3	GZL	O4-C1-C2	-2.22	101.94	105.76
21	kE	2	FUB	C1-C2-C3	2.22	105.17	101.63
4	qB	1	FUB	C1-C2-C3	2.21	105.17	101.63
17	5D	3	BMA	C1-O5-C5	2.21	115.15	112.19
4	cC	4	AHR	C1-C2-C3	2.21	105.17	101.63
3	IC	1	FUB	C1-C2-C3	2.21	105.16	101.63
14	nA	3	GZL	C1-C2-C3	2.21	105.16	101.63
18	SE	1	FUB	C1-C2-C3	2.21	105.16	101.63
24	YE	4	AHR	C1-C2-C3	2.21	105.16	101.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	ND	2	FUB	C1-C2-C3	2.21	105.16	101.63
14	nB	3	GZL	C1-O4-C4	-2.21	103.44	107.84
3	FD	1	FUB	C1-C2-C3	2.20	105.15	101.63
10	jD	1	FUB	C1-C2-C3	2.20	105.15	101.63
13	wD	4	AHR	C1-C2-C3	2.20	105.15	101.63
13	9A	2	FUB	O3-C3-C2	2.20	117.19	111.97
5	M	3	FUB	C1-C2-C3	2.20	105.15	101.63
10	a	5	AHR	C1-C2-C3	2.20	105.15	101.63
20	sE	4	AHR	C1-C2-C3	2.20	105.15	101.63
14	kB	2	FUB	C1-C2-C3	2.20	105.14	101.63
4	cC	1	FUB	C1-C2-C3	2.20	105.14	101.63
6	6C	2	FUB	C1-C2-C3	2.20	105.14	101.63
13	wC	2	FUB	O2-C2-C3	2.20	115.75	111.43
6	yD	1	FUB	C1-C2-C3	2.19	105.14	101.63
5	EC	4	AHR	C1-C2-C3	2.19	105.13	101.63
4	SD	2	FUB	C1-C2-C3	2.19	105.13	101.63
15	BB	4	AHR	C1-C2-C3	2.19	105.13	101.63
13	BA	2	FUB	O2-C2-C3	2.19	115.74	111.43
12	fD	5	AHR	C1-C2-C3	2.19	105.13	101.63
6	cB	1	FUB	C1-C2-C3	2.19	105.13	101.63
14	hC	1	FUB	C1-C2-C3	2.19	105.13	101.63
14	HB	4	FUB	C1-C2-C3	2.19	105.13	101.63
19	aE	3	GZL	C1-C2-C3	2.19	105.13	101.63
15	fB	4	AHR	C1-C2-C3	2.19	105.12	101.63
4	YC	2	FUB	C1-C2-C3	2.19	105.12	101.63
13	tD	3	GZL	C5-C4-C3	-2.18	112.81	115.95
15	2D	4	AHR	C1-C2-C3	2.18	105.12	101.63
17	DB	2	NAG	C4-C3-C2	-2.18	107.82	111.02
4	NB	1	FUB	C1-C2-C3	2.18	105.11	101.63
22	eE	5	AHR	C1-C2-C3	2.18	105.11	101.63
13	2B	3	GZL	C1-C2-C3	2.18	105.11	101.63
10	pB	4	AHR	C1-C2-C3	2.18	105.11	101.63
18	0E	5	AHR	C1-C2-C3	2.18	105.11	101.63
15	AB	1	FUB	C1-C2-C3	2.18	105.11	101.63
13	5A	4	AHR	C1-C2-C3	2.17	105.11	101.63
3	RB	3	FUB	C1-C2-C3	2.17	105.10	101.63
6	9	1	FUB	C1-C2-C3	2.17	105.10	101.63
9	hA	1	FUB	C1-C2-C3	2.17	105.10	101.63
18	JE	1	FUB	C1-C2-C3	2.17	105.10	101.63
21	vE	1	FUB	C1-C2-C3	2.17	105.10	101.63
4	qB	2	FUB	C1-C2-C3	2.17	105.09	101.63
4	nC	1	FUB	C1-C2-C3	2.16	105.08	101.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	4	AHR	C1-C2-C3	2.16	105.08	101.63
13	6B	2	FUB	O2-C2-C3	2.16	115.68	111.43
13	wD	3	GZL	C1-C2-C3	2.16	105.08	101.63
4	UA	1	FUB	O2-C2-C3	2.16	115.67	111.43
19	aE	4	AHR	C1-C2-C3	2.16	105.08	101.63
8	MC	1	FUB	C1-C2-C3	2.15	105.07	101.63
18	9D	1	FUB	O2-C2-C1	2.15	117.59	110.89
10	vC	3	FUB	O3-C3-C2	2.15	117.07	111.97
15	8B	4	AHR	C1-C2-C3	2.15	105.07	101.63
10	MB	4	AHR	C1-C2-C3	2.15	105.07	101.63
12	FB	5	AHR	C1-C2-C3	2.15	105.06	101.63
3	ED	1	FUB	C1-C2-C3	2.15	105.06	101.63
15	eB	4	AHR	O2-C2-C1	2.15	117.56	110.89
7	S	3	FUB	C1-C2-C3	2.14	105.06	101.63
5	BD	1	FUB	C1-C2-C3	2.14	105.05	101.63
3	rC	1	FUB	C1-C2-C3	2.14	105.05	101.63
7	QA	3	FUB	C1-C2-C3	2.14	105.05	101.63
6	CB	3	GZL	C1-O4-C4	-2.14	103.57	107.84
6	3A	1	FUB	C1-C2-C3	2.14	105.05	101.63
15	4C	5	AHR	C1-C2-C3	2.14	105.05	101.63
3	wA	3	FUB	O4-C4-C3	2.14	106.61	104.63
3	BC	1	FUB	C1-C2-C3	2.14	105.04	101.63
3	oD	3	FUB	C1-C2-C3	2.14	105.04	101.63
13	tD	2	FUB	O2-C2-C3	2.13	115.63	111.43
7	dA	1	FUB	C1-C2-C3	2.13	105.03	101.63
20	jE	3	GZL	C1-C2-C3	2.13	105.03	101.63
3	mD	3	FUB	C1-C2-C3	2.13	105.03	101.63
18	DE	4	AHR	C1-C2-C3	2.12	105.02	101.63
6	CB	1	FUB	C1-C2-C3	2.12	105.02	101.63
3	TC	2	FUB	C1-C2-C3	2.12	105.02	101.63
4	VD	2	FUB	C1-C2-C3	2.12	105.02	101.63
12	q	1	FUB	C1-C2-C3	2.12	105.02	101.63
6	4B	1	FUB	C1-C2-C3	2.12	105.02	101.63
15	2D	1	FUB	C1-C2-C3	2.12	105.01	101.63
3	pD	3	FUB	C1-C2-C3	2.12	105.01	101.63
14	kB	4	FUB	C1-C2-C3	2.11	105.01	101.63
7	KC	4	AHR	C1-C2-C3	2.11	105.01	101.63
3	QB	1	FUB	C1-C2-C3	2.11	105.00	101.63
6	aB	2	FUB	C1-C2-C3	2.11	105.00	101.63
15	DA	5	AHR	C1-C2-C3	2.11	105.00	101.63
20	uE	1	FUB	C1-C2-C3	2.11	105.00	101.63
4	VC	4	AHR	C1-C2-C3	2.11	105.00	101.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	0A	1	FUB	C1-C2-C3	2.11	105.00	101.63
3	pC	1	FUB	C1-C2-C3	2.10	104.99	101.63
14	s	3	GZL	O5-C5-C4	2.10	114.20	109.18
11	gA	3	AHR	C1-C2-C3	2.10	104.99	101.63
10	vC	5	AHR	C1-C2-C3	2.10	104.98	101.63
3	yA	1	FUB	C1-C2-C3	2.09	104.97	101.63
15	7B	4	AHR	O2-C2-C1	2.09	117.40	110.89
3	KD	1	FUB	C1-C2-C3	2.09	104.97	101.63
6	XB	2	FUB	O2-C2-C3	2.09	115.54	111.43
15	CA	4	AHR	C1-C2-C3	2.09	104.97	101.63
15	1D	4	AHR	C1-C2-C3	2.09	104.97	101.63
5	KA	5	AHR	C1-C2-C3	2.09	104.96	101.63
9	Y	1	FUB	O2-C2-C3	2.09	115.53	111.43
3	oB	3	FUB	C1-C2-C3	2.08	104.96	101.63
18	IE	1	FUB	O2-C2-C3	2.08	115.53	111.43
6	xD	2	FUB	O2-C2-C3	2.08	115.53	111.43
11	aC	2	AHR	C1-C2-C3	2.08	104.95	101.63
3	TA	1	FUB	C1-C2-C3	2.07	104.94	101.63
14	HB	3	GZL	O5-C5-C4	2.07	114.13	109.18
18	pE	1	FUB	O3-C3-C4	2.07	117.03	111.08
23	XE	4	AHR	O4-C4-C3	2.07	106.55	104.63
15	eB	1	FUB	C1-C2-C3	2.07	104.94	101.63
22	QE	1	FUB	C1-C2-C3	2.07	104.94	101.63
13	3C	3	GZL	O4-C1-C2	-2.07	102.19	105.76
3	w	3	FUB	C1-C2-C3	2.07	104.93	101.63
4	mB	4	AHR	C1-C2-C3	2.07	104.93	101.63
3	Q	1	FUB	C1-C2-C3	2.06	104.93	101.63
3	NA	3	FUB	C1-C2-C3	2.06	104.93	101.63
3	ID	1	FUB	C1-C2-C3	2.06	104.93	101.63
3	rB	1	FUB	C1-C2-C3	2.06	104.92	101.63
4	RC	4	AHR	C1-C2-C3	2.06	104.92	101.63
10	SC	5	AHR	C1-C2-C3	2.06	104.92	101.63
14	KB	4	FUB	C1-C2-C3	2.06	104.92	101.63
10	mC	4	AHR	C1-C2-C3	2.06	104.92	101.63
3	EB	1	FUB	C1-C2-C3	2.06	104.92	101.63
3	uC	3	FUB	C1-C2-C3	2.06	104.92	101.63
5	EC	3	FUB	C1-C2-C3	2.06	104.92	101.63
13	zC	2	FUB	C1-C2-C3	2.05	104.91	101.63
22	eE	4	AHR	C1-C2-C3	2.05	104.91	101.63
14	p	4	FUB	C1-C2-C3	2.05	104.91	101.63
10	jD	5	AHR	C1-C2-C3	2.05	104.91	101.63
7	XC	2	FUB	C1-C2-C3	-2.05	98.35	101.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	dB	2	FUB	O3-C3-C2	2.05	116.83	111.97
12	q	4	AHR	C1-C2-C3	2.05	104.90	101.63
6	uD	1	FUB	C1-C2-C3	2.05	104.90	101.63
22	dE	2	FUB	C1-C2-C3	2.05	104.90	101.63
18	fE	1	FUB	C1-C2-C3	2.05	104.90	101.63
6	CB	3	GZL	C1-C2-C3	2.05	104.90	101.63
13	9A	2	FUB	O2-C2-C3	2.04	115.45	111.43
6	5	1	FUB	C1-C2-C3	2.04	104.89	101.63
20	EE	2	FUB	O4-C4-C3	2.04	106.52	104.63
21	kE	1	FUB	O4-C4-C3	2.04	106.51	104.63
11	XD	1	FUB	O2-C2-C3	2.03	115.43	111.43
6	ZE	2	FUB	C1-C2-C3	2.03	104.88	101.63
12	cD	5	AHR	C1-C2-C3	2.03	104.88	101.63
8	U	2	FUB	C1-C2-C3	2.03	104.88	101.63
7	S	4	AHR	C1-C2-C3	2.03	104.88	101.63
3	cA	2	FUB	C1-C2-C3	2.03	104.88	101.63
6	cB	3	GZL	C1-C2-C3	2.03	104.88	101.63
5	M	2	FUB	O2-C2-C1	2.03	117.20	110.89
3	9C	3	FUB	C1-C2-C3	2.03	104.87	101.63
15	5C	4	AHR	C1-C2-C3	2.03	104.87	101.63
19	1E	2	FUB	C1-C2-C3	2.03	104.87	101.63
21	FE	5	AHR	C1-C2-C3	2.03	104.87	101.63
10	3	5	AHR	C1-C2-C3	2.03	104.87	101.63
3	x	3	FUB	C1-C2-C3	2.03	104.87	101.63
18	tE	4	AHR	C1-C2-C3	2.03	104.87	101.63
6	3A	2	FUB	O3-C3-C2	2.02	116.77	111.97
3	1	3	FUB	C1-C2-C3	2.02	104.86	101.63
15	BB	1	FUB	C1-C2-C3	2.02	104.86	101.63
24	YE	4	AHR	O2-C2-C1	2.02	117.18	110.89
18	pE	1	FUB	O2-C2-C1	2.02	117.18	110.89
13	2B	4	AHR	C1-C2-C3	2.02	104.86	101.63
6	5	2	FUB	O3-C3-C2	2.02	116.75	111.97
17	5D	3	BMA	C1-C2-C3	-2.02	106.70	109.64
4	NB	4	AHR	C1-C2-C3	2.02	104.86	101.63
4	d	1	FUB	C1-C2-C3	2.02	104.85	101.63
4	RD	2	FUB	C1-C2-C3	2.02	104.85	101.63
4	nC	4	AHR	C1-C2-C3	2.02	104.85	101.63
12	IB	2	FUB	C1-C2-C3	2.02	104.85	101.63
6	CD	2	FUB	O3-C3-C2	2.02	116.75	111.97
13	wC	3	GZL	O4-C1-C2	-2.01	102.29	105.76
6	0B	2	FUB	O3-C3-C2	2.01	116.74	111.97
13	wC	3	GZL	C1-C2-C3	-2.01	98.41	101.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	8	1	FUB	C1-C2-C3	2.01	104.85	101.63
12	q	5	AHR	C1-C2-C3	2.01	104.85	101.63
24	YE	6	AHR	C1-C2-C3	2.01	104.85	101.63
4	c	4	AHR	C1-C2-C3	2.01	104.84	101.63
13	yC	2	FUB	C1-C2-C3	2.01	104.84	101.63
6	JC	1	FUB	C1-C2-C3	2.01	104.84	101.63
24	lE	4	AHR	O2-C2-C1	2.01	117.14	110.89
3	WC	3	FUB	C1-C2-C3	2.01	104.84	101.63
4	ZD	1	FUB	C1-C2-C3	2.01	104.84	101.63
3	CC	1	FUB	C1-C2-C3	2.01	104.84	101.63
13	tD	3	GZL	C6-C5-C4	-2.01	108.06	112.05
7	HD	4	AHR	C1-C2-C3	2.01	104.84	101.63
18	zE	2	FUB	C1-C2-C3	2.01	104.84	101.63
4	DC	4	AHR	C1-C2-C3	2.01	104.83	101.63
7	h	4	AHR	C1-C2-C3	2.01	104.83	101.63
3	GC	1	FUB	C1-C2-C3	2.00	104.83	101.63
10	u	1	FUB	C1-C2-C3	2.00	104.83	101.63
12	iC	2	FUB	C1-C2-C3	2.00	104.83	101.63
6	xD	2	FUB	C1-C2-C3	2.00	104.83	101.63
13	wD	1	FUB	C1-C2-C3	2.00	104.83	101.63
3	jA	1	FUB	C1-C2-C3	2.00	104.83	101.63
3	CC	2	FUB	C1-C2-C3	2.00	104.83	101.63
7	f	3	FUB	C1-C2-C3	2.00	104.83	101.63
3	HA	3	FUB	C1-C2-C3	2.00	104.83	101.63
10	1A	4	AHR	O2-C2-C1	2.00	117.11	110.89

All (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
4	VA	4	AHR	C2
4	DC	1	FUB	C4
4	PC	4	AHR	C1
4	RC	2	FUB	C1
4	AD	1	FUB	C4
4	OD	2	FUB	C1
5	BD	5	AHR	C1
6	N	3	GZL	C1

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Mol	Chain	Res	Type	Atom
6	N	3	GZL	C5
6	R	3	GZL	C1
6	5	3	GZL	C1
6	5	3	GZL	C5
6	5	3	GZL	C4
6	8	3	GZL	C1
6	9	3	GZL	C1
6	AA	2	FUB	C4
6	AA	3	GZL	C1
6	EA	3	GZL	C1
6	LA	3	GZL	C1
6	LA	3	GZL	C5
6	PA	3	GZL	C1
6	3A	3	GZL	C1
6	3A	3	GZL	C5
6	7A	3	GZL	C1
6	8A	2	FUB	C4
6	8A	3	GZL	C1
6	CB	3	GZL	C1
6	XB	3	GZL	C1
6	XB	3	GZL	C5
6	bB	3	GZL	C1
6	cB	2	FUB	C4
6	cB	3	GZL	C1
6	gB	3	GZL	C1
6	0B	3	GZL	C1
6	0B	3	GZL	C5
6	4B	3	GZL	C1
6	5B	2	FUB	C4
6	5B	3	GZL	C1
6	9B	3	GZL	C1
6	FC	3	GZL	C1
6	JC	3	GZL	C1
6	xC	3	GZL	C1
6	xC	3	GZL	C5
6	1C	3	GZL	C1
6	2C	2	FUB	C4
6	2C	3	GZL	C1
6	6C	3	GZL	C1
6	CD	3	GZL	C1
6	CD	3	GZL	C3
6	CD	3	GZL	C5

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Mol	Chain	Res	Type	Atom
6	GD	3	GZL	C1
6	uD	3	GZL	C1
6	uD	3	GZL	C5
6	yD	3	GZL	C1
6	zD	2	FUB	C4
6	zD	3	GZL	C1
6	3D	3	GZL	C1
6	6D	3	GZL	C1
6	7D	3	GZL	C1
6	8D	3	GZL	C1
6	ME	3	GZL	C1
6	OE	3	GZL	C1
6	ZE	3	GZL	C1
6	bE	3	GZL	C1
6	mE	3	GZL	C1
6	nE	3	GZL	C1
6	oE	3	GZL	C1
10	3	4	AHR	C1
10	1A	4	AHR	C1
10	VB	4	AHR	C1
10	yB	4	AHR	C1
10	vC	4	AHR	C1
10	sD	4	AHR	C1
12	n	3	GZL	C1
12	n	3	GZL	C5
12	q	3	GZL	C1
12	q	3	GZL	C5
12	q	5	AHR	C4
12	lA	3	GZL	C1
12	lA	3	GZL	C5
12	oA	3	GZL	C1
12	oA	3	GZL	C5
12	FB	3	GZL	C1
12	FB	3	GZL	C5
12	IB	3	GZL	C1
12	IB	3	GZL	C5
12	iB	3	GZL	C1
12	iB	3	GZL	C5
12	lB	3	GZL	C1
12	lB	3	GZL	C5
12	fC	3	GZL	C1
12	fC	3	GZL	C5

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Mol	Chain	Res	Type	Atom
12	iC	3	GZL	C1
12	iC	3	GZL	C5
12	cD	3	GZL	C1
12	cD	3	GZL	C5
12	fD	3	GZL	C1
12	fD	3	GZL	C5
13	o	3	GZL	C1
13	o	3	GZL	C5
13	4	3	GZL	C1
13	4	3	GZL	C5
13	6	3	GZL	C1
13	7	3	GZL	C1
13	BA	2	FUB	C2
13	mA	3	GZL	C1
13	mA	3	GZL	C5
13	2A	3	GZL	C1
13	2A	3	GZL	C5
13	2A	3	GZL	C4
13	4A	3	GZL	C1
13	5A	3	GZL	C1
13	9A	2	FUB	C2
13	GB	3	GZL	C1
13	GB	3	GZL	C5
13	WB	3	GZL	C1
13	WB	3	GZL	C5
13	WB	3	GZL	C4
13	YB	3	GZL	C1
13	ZB	3	GZL	C1
13	dB	2	FUB	C2
13	jB	3	GZL	C1
13	jB	3	GZL	C5
13	zB	3	GZL	C1
13	zB	3	GZL	C5
13	zB	3	GZL	C4
13	1B	3	GZL	C1
13	2B	3	GZL	C1
13	6B	2	FUB	C2
13	gC	3	GZL	C1
13	gC	3	GZL	C5
13	wC	3	GZL	C1
13	wC	3	GZL	C5
13	wC	3	GZL	C4

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Mol	Chain	Res	Type	Atom
13	yC	3	GZL	C1
13	zC	3	GZL	C1
13	3C	2	FUB	C2
13	dD	3	GZL	C1
13	dD	3	GZL	C5
13	tD	3	GZL	C1
13	tD	3	GZL	C5
13	tD	3	GZL	C4
13	vD	3	GZL	C1
13	wD	3	GZL	C1
13	0D	2	FUB	C2
14	p	3	GZL	C1
14	p	3	GZL	C5
14	s	3	GZL	C1
14	s	3	GZL	C5
14	nA	3	GZL	C1
14	nA	3	GZL	C5
14	qA	3	GZL	C1
14	qA	3	GZL	C5
14	HB	3	GZL	C1
14	HB	3	GZL	C5
14	KB	3	GZL	C1
14	KB	3	GZL	C5
14	kB	3	GZL	C1
14	kB	3	GZL	C5
14	nB	3	GZL	C1
14	nB	3	GZL	C5
14	hC	3	GZL	C1
14	hC	3	GZL	C5
14	kC	3	GZL	C1
14	kC	3	GZL	C5
14	eD	3	GZL	C1
14	eD	3	GZL	C5
14	hD	3	GZL	C1
14	hD	3	GZL	C5
15	CA	3	GZL	C1
15	CA	5	AHR	C1
15	DA	3	GZL	C1
15	AB	3	GZL	C1
15	AB	5	AHR	C1
15	BB	3	GZL	C1
15	eB	3	GZL	C1

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Mol	Chain	Res	Type	Atom
15	eB	5	AHR	C1
15	fB	3	GZL	C1
15	7B	3	GZL	C1
15	7B	5	AHR	C1
15	8B	3	GZL	C1
15	4C	3	GZL	C1
15	4C	5	AHR	C1
15	5C	3	GZL	C1
15	1D	3	GZL	C1
15	1D	5	AHR	C1
15	2D	3	GZL	C1
17	GA	4	MAN	C1
17	GA	6	MAN	C1
17	DB	4	MAN	C1
17	DB	6	MAN	C1
17	7C	4	MAN	C1
17	7C	6	MAN	C1
17	5D	4	MAN	C1
17	5D	6	MAN	C1
18	9D	3	GZL	C1
18	9D	4	AHR	C1
18	BE	3	GZL	C1
18	BE	4	AHR	C1
18	BE	5	AHR	C1
18	DE	3	GZL	C1
18	DE	5	AHR	C1
18	IE	3	GZL	C1
18	IE	4	AHR	C1
18	JE	3	GZL	C1
18	JE	5	AHR	C1
18	KE	3	GZL	C1
18	KE	4	AHR	C1
18	KE	5	AHR	C1
18	PE	3	GZL	C1
18	PE	4	AHR	C1
18	PE	5	AHR	C1
18	SE	1	FUB	C4
18	SE	3	GZL	C1
18	SE	4	AHR	C1
18	SE	5	AHR	C1
18	cE	3	GZL	C1
18	cE	4	AHR	C1

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Mol	Chain	Res	Type	Atom
18	cE	5	AHR	C1
18	fE	1	FUB	C4
18	fE	3	GZL	C1
18	fE	4	AHR	C1
18	fE	5	AHR	C1
18	pE	3	GZL	C1
18	pE	4	AHR	C1
18	rE	3	GZL	C1
18	rE	4	AHR	C1
18	rE	5	AHR	C1
18	tE	3	GZL	C1
18	tE	5	AHR	C1
18	yE	3	GZL	C1
18	yE	4	AHR	C1
18	zE	3	GZL	C1
18	zE	5	AHR	C1
18	0E	3	GZL	C1
18	0E	4	AHR	C1
18	0E	5	AHR	C1
19	AE	3	GZL	C1
19	LE	3	GZL	C1
19	LE	4	AHR	C1
19	NE	3	GZL	C1
19	NE	4	AHR	C1
19	aE	3	GZL	C1
19	aE	4	AHR	C1
19	qE	3	GZL	C1
19	1E	3	GZL	C1
19	1E	4	AHR	C1
20	CE	3	GZL	C1
20	EE	3	GZL	C1
20	HE	3	GZL	C1
20	TE	3	GZL	C1
20	TE	4	AHR	C1
20	UE	3	GZL	C1
20	WE	3	GZL	C1
20	WE	4	AHR	C1
20	gE	3	GZL	C1
20	gE	4	AHR	C1
20	hE	3	GZL	C1
20	jE	3	GZL	C1
20	jE	4	AHR	C1

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Mol	Chain	Res	Type	Atom
20	sE	3	GZL	C1
20	uE	3	GZL	C1
20	xE	3	GZL	C1
21	FE	3	GZL	C1
21	FE	4	AHR	C1
21	FE	5	AHR	C3
21	kE	3	GZL	C1
21	kE	4	AHR	C1
21	vE	3	GZL	C1
21	vE	4	AHR	C1
21	vE	5	AHR	C3
21	vE	5	AHR	C2
22	GE	3	GZL	C1
22	QE	3	GZL	C1
22	QE	4	AHR	C1
22	QE	6	AHR	C1
22	RE	3	GZL	C1
22	RE	4	AHR	C1
22	RE	4	AHR	C2
22	VE	3	GZL	C1
22	VE	4	AHR	C1
22	dE	3	GZL	C1
22	dE	4	AHR	C1
22	dE	6	AHR	C1
22	eE	3	GZL	C1
22	eE	4	AHR	C1
22	eE	4	AHR	C2
22	iE	3	GZL	C1
22	iE	4	AHR	C1
22	wE	3	GZL	C1
23	XE	3	GZL	C1
23	XE	4	AHR	C1
23	XE	5	AHR	C1
24	YE	3	GZL	C1
24	YE	4	AHR	C1
24	lE	3	GZL	C1
24	lE	4	AHR	C1

All (607) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	N	3	GZL	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
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
6	AA	3	GZL	C3-C4-C5-O5
6	AA	3	GZL	O4-C4-C5-O5
6	EA	3	GZL	O5-C5-C6-O6
6	LA	3	GZL	C4-C5-C6-O6
6	LA	3	GZL	O5-C5-C6-O6
6	PA	3	GZL	O5-C5-C6-O6
6	3A	3	GZL	O4-C4-C5-C6
6	3A	3	GZL	C3-C4-C5-O5
6	3A	3	GZL	O4-C4-C5-O5
6	7A	3	GZL	C4-C5-C6-O6
6	7A	3	GZL	O5-C5-C6-O6
6	8A	3	GZL	O4-C4-C5-C6
6	XB	3	GZL	C3-C4-C5-C6
6	XB	3	GZL	O4-C4-C5-C6
6	XB	3	GZL	C3-C4-C5-O5
6	XB	3	GZL	O4-C4-C5-O5
6	bB	3	GZL	C3-C4-C5-C6
6	bB	3	GZL	O4-C4-C5-C6
6	bB	3	GZL	C3-C4-C5-O5
6	bB	3	GZL	O4-C4-C5-O5
6	gB	3	GZL	C4-C5-C6-O6
6	gB	3	GZL	C3-C4-C5-C6
6	gB	3	GZL	O4-C4-C5-C6
6	gB	3	GZL	C3-C4-C5-O5
6	gB	3	GZL	O4-C4-C5-O5
6	0B	3	GZL	C3-C4-C5-C6
6	0B	3	GZL	O4-C4-C5-C6
6	0B	3	GZL	C3-C4-C5-O5
6	0B	3	GZL	O4-C4-C5-O5
6	4B	3	GZL	O4-C4-C5-C6
6	5B	3	GZL	O4-C4-C5-O5
6	FC	3	GZL	O4-C4-C5-C6
6	xC	3	GZL	C3-C4-C5-C6
6	xC	3	GZL	O4-C4-C5-C6
6	xC	3	GZL	C3-C4-C5-O5
6	xC	3	GZL	O4-C4-C5-O5
6	0C	3	GZL	O5-C5-C6-O6
6	2C	3	GZL	O4-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
6	2C	3	GZL	O4-C4-C5-O5
6	6C	3	GZL	O5-C5-C6-O6
6	GD	3	GZL	O4-C4-C5-C6
6	uD	3	GZL	C4-C5-C6-O6
6	uD	3	GZL	C3-C4-C5-C6
6	uD	3	GZL	O4-C4-C5-C6
6	uD	3	GZL	C3-C4-C5-O5
6	uD	3	GZL	O4-C4-C5-O5
6	xD	3	GZL	O5-C5-C6-O6
6	xD	3	GZL	C3-C4-C5-C6
6	xD	3	GZL	O4-C4-C5-C6
6	xD	3	GZL	C3-C4-C5-O5
6	xD	3	GZL	O4-C4-C5-O5
6	yD	3	GZL	O5-C5-C6-O6
6	6D	3	GZL	O4-C4-C5-O5
6	7D	3	GZL	C3-C4-C5-C6
6	7D	3	GZL	O4-C4-C5-C6
6	7D	3	GZL	C3-C4-C5-O5
6	7D	3	GZL	O4-C4-C5-O5
6	8D	3	GZL	O4-C4-C5-C6
6	ME	3	GZL	O4-C4-C5-C6
6	OE	3	GZL	C3-C4-C5-C6
6	OE	3	GZL	O4-C4-C5-C6
6	OE	3	GZL	C3-C4-C5-O5
6	ZE	3	GZL	C4-C5-C6-O6
6	ZE	3	GZL	O5-C5-C6-O6
6	bE	3	GZL	C4-C5-C6-O6
6	bE	3	GZL	O4-C4-C5-C6
6	mE	3	GZL	C3-C4-C5-C6
6	mE	3	GZL	O4-C4-C5-C6
6	mE	3	GZL	C3-C4-C5-O5
6	mE	3	GZL	O4-C4-C5-O5
6	nE	3	GZL	C3-C4-C5-C6
6	nE	3	GZL	O4-C4-C5-C6
6	nE	3	GZL	C3-C4-C5-O5
6	nE	3	GZL	O4-C4-C5-O5
6	oE	3	GZL	C3-C4-C5-C6
6	oE	3	GZL	O4-C4-C5-C6
6	oE	3	GZL	C3-C4-C5-O5
12	n	3	GZL	O5-C5-C6-O6
12	lA	3	GZL	O5-C5-C6-O6
12	FB	3	GZL	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
12	IB	3	GZL	C3-C4-C5-O5
12	IB	3	GZL	O4-C4-C5-O5
12	iB	3	GZL	C4-C5-C6-O6
12	iB	3	GZL	O4-C4-C5-C6
12	iB	3	GZL	O4-C4-C5-O5
12	lB	3	GZL	O4-C4-C5-C6
12	lB	3	GZL	O4-C4-C5-O5
12	fC	3	GZL	O4-C4-C5-C6
12	fC	3	GZL	O4-C4-C5-O5
12	iC	3	GZL	O4-C4-C5-C6
12	iC	3	GZL	O4-C4-C5-O5
12	cD	3	GZL	C4-C5-C6-O6
12	fD	3	GZL	C4-C5-C6-O6
13	o	3	GZL	C4-C5-C6-O6
13	4	3	GZL	C3-C4-C5-O5
13	BA	3	GZL	O4-C4-C5-O5
13	mA	3	GZL	O4-C4-C5-O5
13	2A	3	GZL	O5-C5-C6-O6
13	5A	3	GZL	O5-C5-C6-O6
13	GB	3	GZL	O5-C5-C6-O6
13	YB	3	GZL	C3-C4-C5-C6
13	YB	3	GZL	O4-C4-C5-C6
13	YB	3	GZL	C3-C4-C5-O5
13	YB	3	GZL	O4-C4-C5-O5
13	ZB	3	GZL	O5-C5-C6-O6
13	dB	3	GZL	O4-C4-C5-C6
13	dB	3	GZL	C3-C4-C5-O5
13	dB	3	GZL	O4-C4-C5-O5
13	jB	3	GZL	O5-C5-C6-O6
13	6B	3	GZL	C3-C4-C5-O5
13	6B	3	GZL	O4-C4-C5-O5
13	gC	3	GZL	O5-C5-C6-O6
13	zC	3	GZL	C3-C4-C5-C6
13	zC	3	GZL	O4-C4-C5-C6
13	zC	3	GZL	C3-C4-C5-O5
13	3C	3	GZL	O4-C4-C5-O5
13	dD	3	GZL	O5-C5-C6-O6
13	vD	3	GZL	C3-C4-C5-C6
13	vD	3	GZL	O4-C4-C5-C6
13	vD	3	GZL	C3-C4-C5-O5
13	vD	3	GZL	O4-C4-C5-O5
13	wD	3	GZL	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
13	wD	3	GZL	O4-C4-C5-C6
13	wD	3	GZL	C3-C4-C5-O5
13	wD	3	GZL	O4-C4-C5-O5
13	0D	3	GZL	O4-C4-C5-O5
14	p	3	GZL	O4-C4-C5-C6
14	p	3	GZL	O4-C4-C5-O5
14	s	3	GZL	O4-C4-C5-C6
14	s	3	GZL	O4-C4-C5-O5
14	nA	3	GZL	C4-C5-C6-O6
14	nA	3	GZL	O5-C5-C6-O6
14	nA	3	GZL	O4-C4-C5-C6
14	nA	3	GZL	O4-C4-C5-O5
14	qA	3	GZL	O4-C4-C5-C6
14	qA	3	GZL	O4-C4-C5-O5
14	HB	3	GZL	O4-C4-C5-C6
14	HB	3	GZL	O4-C4-C5-O5
14	KB	3	GZL	O4-C4-C5-C6
14	KB	3	GZL	C3-C4-C5-O5
14	KB	3	GZL	O4-C4-C5-O5
14	kB	3	GZL	O4-C4-C5-C6
14	kB	3	GZL	O4-C4-C5-O5
14	nB	3	GZL	O4-C4-C5-C6
14	nB	3	GZL	O4-C4-C5-O5
14	hC	3	GZL	C3-C4-C5-C6
14	hC	3	GZL	C3-C4-C5-O5
14	kC	3	GZL	O5-C5-C6-O6
14	kC	3	GZL	O4-C4-C5-C6
14	kC	3	GZL	O4-C4-C5-O5
14	eD	3	GZL	O4-C4-C5-C6
14	eD	3	GZL	O4-C4-C5-O5
14	hD	3	GZL	O4-C4-C5-C6
14	hD	3	GZL	O4-C4-C5-O5
15	CA	3	GZL	C4-C5-C6-O6
15	CA	3	GZL	O5-C5-C6-O6
15	CA	3	GZL	O4-C4-C5-C6
15	AB	3	GZL	C4-C5-C6-O6
15	AB	3	GZL	O5-C5-C6-O6
15	AB	3	GZL	O4-C4-C5-C6
15	eB	3	GZL	C3-C4-C5-C6
15	eB	3	GZL	O4-C4-C5-C6
15	eB	3	GZL	C3-C4-C5-O5
15	7B	3	GZL	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
15	7B	3	GZL	C3-C4-C5-C6
15	7B	3	GZL	O4-C4-C5-C6
15	7B	3	GZL	C3-C4-C5-O5
15	1D	3	GZL	C3-C4-C5-C6
15	1D	3	GZL	O4-C4-C5-C6
15	1D	3	GZL	C3-C4-C5-O5
15	1D	3	GZL	O4-C4-C5-O5
16	AC	1	NAG	C3-C2-N2-C7
16	AC	1	NAG	C8-C7-N2-C2
16	AC	1	NAG	O7-C7-N2-C2
16	4D	1	NAG	C8-C7-N2-C2
16	4D	1	NAG	O7-C7-N2-C2
18	BE	3	GZL	C3-C4-C5-C6
18	BE	3	GZL	O4-C4-C5-C6
18	BE	3	GZL	C3-C4-C5-O5
18	BE	3	GZL	O4-C4-C5-O5
18	DE	3	GZL	O5-C5-C6-O6
18	IE	3	GZL	C3-C4-C5-C6
18	IE	3	GZL	O4-C4-C5-C6
18	IE	3	GZL	C3-C4-C5-O5
18	IE	3	GZL	O4-C4-C5-O5
18	JE	3	GZL	O5-C5-C6-O6
18	KE	3	GZL	O4-C4-C5-C6
18	KE	3	GZL	C3-C4-C5-O5
18	KE	3	GZL	O4-C4-C5-O5
18	PE	3	GZL	C4-C5-C6-O6
18	PE	3	GZL	O5-C5-C6-O6
18	SE	3	GZL	C4-C5-C6-O6
18	SE	3	GZL	O5-C5-C6-O6
18	cE	3	GZL	C4-C5-C6-O6
18	cE	3	GZL	O5-C5-C6-O6
18	fE	3	GZL	C3-C4-C5-C6
18	fE	3	GZL	O4-C4-C5-C6
18	fE	3	GZL	C3-C4-C5-O5
18	fE	3	GZL	O4-C4-C5-O5
18	pE	3	GZL	C4-C5-C6-O6
18	tE	3	GZL	C4-C5-C6-O6
18	tE	3	GZL	O5-C5-C6-O6
18	yE	3	GZL	O5-C5-C6-O6
18	yE	3	GZL	C3-C4-C5-O5
18	zE	3	GZL	C3-C4-C5-C6
18	zE	3	GZL	O4-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
18	zE	3	GZL	C3-C4-C5-O5
18	zE	3	GZL	O4-C4-C5-O5
18	0E	3	GZL	O4-C4-C5-C6
18	0E	3	GZL	C3-C4-C5-O5
18	0E	3	GZL	O4-C4-C5-O5
19	AE	3	GZL	C4-C5-C6-O6
19	AE	3	GZL	C3-C4-C5-C6
19	AE	3	GZL	O4-C4-C5-C6
19	AE	3	GZL	C3-C4-C5-O5
19	AE	3	GZL	O4-C4-C5-O5
19	qE	3	GZL	C3-C4-C5-C6
19	qE	3	GZL	O4-C4-C5-C6
19	qE	3	GZL	C3-C4-C5-O5
19	qE	3	GZL	O4-C4-C5-O5
19	1E	3	GZL	C3-C4-C5-C6
19	1E	3	GZL	O4-C4-C5-C6
19	1E	3	GZL	C3-C4-C5-O5
19	1E	3	GZL	O4-C4-C5-O5
20	CE	3	GZL	C3-C4-C5-C6
20	CE	3	GZL	O4-C4-C5-C6
20	CE	3	GZL	C3-C4-C5-O5
20	CE	3	GZL	O4-C4-C5-O5
20	HE	3	GZL	C3-C4-C5-C6
20	HE	3	GZL	O4-C4-C5-C6
20	HE	3	GZL	C3-C4-C5-O5
20	HE	3	GZL	O4-C4-C5-O5
20	TE	3	GZL	O5-C5-C6-O6
20	UE	3	GZL	C4-C5-C6-O6
20	UE	3	GZL	O4-C4-C5-C6
20	gE	3	GZL	O5-C5-C6-O6
20	hE	3	GZL	O4-C4-C5-C6
20	jE	3	GZL	O5-C5-C6-O6
20	sE	3	GZL	C3-C4-C5-C6
20	sE	3	GZL	O4-C4-C5-C6
20	sE	3	GZL	C3-C4-C5-O5
20	sE	3	GZL	O4-C4-C5-O5
20	uE	3	GZL	C3-C4-C5-C6
20	uE	3	GZL	O4-C4-C5-C6
20	uE	3	GZL	C3-C4-C5-O5
20	xE	3	GZL	C3-C4-C5-C6
20	xE	3	GZL	O4-C4-C5-C6
20	xE	3	GZL	C3-C4-C5-O5

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Mol	Chain	Res	Type	Atoms
20	xE	3	GZL	O4-C4-C5-O5
21	FE	3	GZL	O4-C4-C5-C6
21	vE	3	GZL	C4-C5-C6-O6
22	GE	3	GZL	C4-C5-C6-O6
22	GE	3	GZL	O5-C5-C6-O6
22	GE	3	GZL	O4-C4-C5-C6
22	GE	3	GZL	O4-C4-C5-O5
22	QE	3	GZL	C4-C5-C6-O6
22	RE	3	GZL	O5-C5-C6-O6
22	dE	3	GZL	O4-C4-C5-C6
22	eE	3	GZL	C4-C5-C6-O6
22	eE	3	GZL	O5-C5-C6-O6
22	iE	3	GZL	C4-C5-C6-O6
22	iE	3	GZL	O5-C5-C6-O6
22	wE	3	GZL	O5-C5-C6-O6
23	XE	3	GZL	C4-C5-C6-O6
23	XE	3	GZL	O5-C5-C6-O6
24	YE	3	GZL	C3-C4-C5-C6
24	YE	3	GZL	C3-C4-C5-O5
24	YE	3	GZL	O4-C4-C5-O5
24	lE	3	GZL	C3-C4-C5-O5
24	lE	3	GZL	O4-C4-C5-O5
17	DB	2	NAG	C8-C7-N2-C2
17	DB	2	NAG	O7-C7-N2-C2
20	HE	2	FUB	O4-C4-C5-O5
6	gB	3	GZL	O5-C5-C6-O6
6	GD	3	GZL	O5-C5-C6-O6
6	uD	3	GZL	O5-C5-C6-O6
6	bE	3	GZL	O5-C5-C6-O6
12	FB	3	GZL	O5-C5-C6-O6
12	iB	3	GZL	O5-C5-C6-O6
12	lB	3	GZL	O5-C5-C6-O6
12	cD	3	GZL	O5-C5-C6-O6
12	fD	3	GZL	O5-C5-C6-O6
13	o	3	GZL	O5-C5-C6-O6
13	zC	3	GZL	O5-C5-C6-O6
14	kB	3	GZL	O5-C5-C6-O6
15	DA	3	GZL	O5-C5-C6-O6
15	8B	3	GZL	O5-C5-C6-O6
18	fE	3	GZL	O5-C5-C6-O6
18	pE	3	GZL	O5-C5-C6-O6
18	zE	3	GZL	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
19	AE	3	GZL	O5-C5-C6-O6
19	LE	3	GZL	O5-C5-C6-O6
19	aE	3	GZL	O5-C5-C6-O6
20	HE	3	GZL	O5-C5-C6-O6
20	UE	3	GZL	O5-C5-C6-O6
20	xE	3	GZL	O5-C5-C6-O6
21	vE	3	GZL	O5-C5-C6-O6
22	QE	3	GZL	O5-C5-C6-O6
17	DB	4	MAN	O5-C5-C6-O6
17	5D	4	MAN	O5-C5-C6-O6
6	5	3	GZL	C4-C5-C6-O6
6	EA	3	GZL	C4-C5-C6-O6
6	PA	3	GZL	C4-C5-C6-O6
6	6A	3	GZL	C4-C5-C6-O6
6	CB	3	GZL	C4-C5-C6-O6
6	XB	3	GZL	C4-C5-C6-O6
6	aB	3	GZL	C4-C5-C6-O6
6	cB	3	GZL	C4-C5-C6-O6
6	0C	3	GZL	C4-C5-C6-O6
6	6C	3	GZL	C4-C5-C6-O6
6	GD	3	GZL	C4-C5-C6-O6
6	xD	3	GZL	C4-C5-C6-O6
6	yD	3	GZL	C4-C5-C6-O6
6	7D	3	GZL	C4-C5-C6-O6
6	ME	3	GZL	C4-C5-C6-O6
6	nE	3	GZL	C4-C5-C6-O6
12	n	3	GZL	C4-C5-C6-O6
12	lA	3	GZL	C4-C5-C6-O6
13	mA	3	GZL	C4-C5-C6-O6
13	2A	3	GZL	C4-C5-C6-O6
13	5A	3	GZL	C4-C5-C6-O6
13	GB	3	GZL	C4-C5-C6-O6
13	ZB	3	GZL	C4-C5-C6-O6
13	jB	3	GZL	C4-C5-C6-O6
13	gC	3	GZL	C4-C5-C6-O6
13	yC	3	GZL	C4-C5-C6-O6
13	zC	3	GZL	C4-C5-C6-O6
13	dD	3	GZL	C4-C5-C6-O6
13	wD	3	GZL	C4-C5-C6-O6
13	0D	3	GZL	C4-C5-C6-O6
14	p	3	GZL	C4-C5-C6-O6
14	kC	3	GZL	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
14	eD	3	GZL	C4-C5-C6-O6
15	DA	3	GZL	C4-C5-C6-O6
15	8B	3	GZL	C4-C5-C6-O6
18	DE	3	GZL	C4-C5-C6-O6
18	JE	3	GZL	C4-C5-C6-O6
18	fE	3	GZL	C4-C5-C6-O6
18	yE	3	GZL	C4-C5-C6-O6
19	LE	3	GZL	C4-C5-C6-O6
19	NE	3	GZL	C4-C5-C6-O6
19	aE	3	GZL	C4-C5-C6-O6
20	TE	3	GZL	C4-C5-C6-O6
20	gE	3	GZL	C4-C5-C6-O6
20	jE	3	GZL	C4-C5-C6-O6
20	xE	3	GZL	C4-C5-C6-O6
22	RE	3	GZL	C4-C5-C6-O6
22	wE	3	GZL	C4-C5-C6-O6
20	xE	2	FUB	O4-C4-C5-O5
17	DB	4	MAN	C4-C5-C6-O6
17	5D	4	MAN	C4-C5-C6-O6
17	DB	1	NAG	O5-C5-C6-O6
20	HE	2	FUB	C3-C4-C5-O5
17	7C	4	MAN	O5-C5-C6-O6
17	7C	4	MAN	C4-C5-C6-O6
16	FA	1	NAG	C8-C7-N2-C2
19	NE	3	GZL	O5-C5-C6-O6
20	hE	2	FUB	C3-C4-C5-O5
6	8A	3	GZL	C4-C5-C6-O6
12	lB	3	GZL	C4-C5-C6-O6
12	iC	3	GZL	C4-C5-C6-O6
18	zE	3	GZL	C4-C5-C6-O6
20	HE	3	GZL	C4-C5-C6-O6
17	7C	5	MAN	O5-C5-C6-O6
16	AC	2	NAG	C8-C7-N2-C2
17	5D	2	NAG	C8-C7-N2-C2
17	DB	1	NAG	C4-C5-C6-O6
6	6A	3	GZL	O5-C5-C6-O6
6	CB	3	GZL	O5-C5-C6-O6
6	0B	3	GZL	O5-C5-C6-O6
6	ME	3	GZL	O5-C5-C6-O6
6	nE	3	GZL	O5-C5-C6-O6
13	mA	3	GZL	O5-C5-C6-O6
13	yC	3	GZL	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
13	wD	3	GZL	O5-C5-C6-O6
15	7B	3	GZL	O5-C5-C6-O6
16	FA	1	NAG	O7-C7-N2-C2
16	AC	2	NAG	O7-C7-N2-C2
17	GA	2	NAG	C8-C7-N2-C2
17	5D	2	NAG	O7-C7-N2-C2
20	hE	2	FUB	O4-C4-C5-O5
17	5D	6	MAN	O5-C5-C6-O6
6	5B	3	GZL	C4-C5-C6-O6
20	sE	3	GZL	C4-C5-C6-O6
20	xE	2	FUB	C3-C4-C5-O5
6	cB	3	GZL	O5-C5-C6-O6
12	iC	3	GZL	O5-C5-C6-O6
13	0D	3	GZL	O5-C5-C6-O6
14	HB	3	GZL	O5-C5-C6-O6
17	7C	3	BMA	C4-C5-C6-O6
6	R	3	GZL	C4-C5-C6-O6
6	AA	3	GZL	C4-C5-C6-O6
6	xC	3	GZL	C4-C5-C6-O6
13	1B	3	GZL	C4-C5-C6-O6
14	kB	3	GZL	C4-C5-C6-O6
18	rE	3	GZL	C4-C5-C6-O6
17	7C	5	MAN	C4-C5-C6-O6
6	8A	3	GZL	O5-C5-C6-O6
6	9B	3	GZL	O5-C5-C6-O6
17	7C	3	BMA	O5-C5-C6-O6
17	GA	2	NAG	O7-C7-N2-C2
17	DB	6	MAN	O5-C5-C6-O6
12	IB	3	GZL	C4-C5-C6-O6
6	3A	3	GZL	O5-C5-C6-O6
12	oA	3	GZL	O5-C5-C6-O6
12	fC	3	GZL	O5-C5-C6-O6
18	rE	3	GZL	O5-C5-C6-O6
6	5B	3	GZL	C3-C4-C5-O5
6	FC	3	GZL	C3-C4-C5-O5
6	2C	3	GZL	C3-C4-C5-O5
6	6D	3	GZL	C3-C4-C5-O5
12	iB	3	GZL	C3-C4-C5-O5
12	lB	3	GZL	C3-C4-C5-O5
12	fC	3	GZL	C3-C4-C5-O5
12	iC	3	GZL	C3-C4-C5-O5
13	BA	3	GZL	C3-C4-C5-O5

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Mol	Chain	Res	Type	Atoms
13	3C	3	GZL	C3-C4-C5-O5
13	0D	3	GZL	C3-C4-C5-O5
14	p	3	GZL	C3-C4-C5-O5
14	s	3	GZL	C3-C4-C5-O5
14	nA	3	GZL	C3-C4-C5-O5
14	qA	3	GZL	C3-C4-C5-O5
14	HB	3	GZL	C3-C4-C5-O5
14	kB	3	GZL	C3-C4-C5-O5
14	nB	3	GZL	C3-C4-C5-O5
14	kC	3	GZL	C3-C4-C5-O5
14	eD	3	GZL	C3-C4-C5-O5
14	hD	3	GZL	C3-C4-C5-O5
20	TE	3	GZL	C3-C4-C5-O5
22	GE	3	GZL	C3-C4-C5-O5
6	8A	3	GZL	O4-C4-C5-O5
6	4B	3	GZL	O4-C4-C5-O5
6	FC	3	GZL	O4-C4-C5-O5
6	GD	3	GZL	O4-C4-C5-O5
6	8D	3	GZL	O4-C4-C5-O5
6	OE	3	GZL	O4-C4-C5-O5
6	bE	3	GZL	O4-C4-C5-O5
6	oE	3	GZL	O4-C4-C5-O5
13	9A	3	GZL	O4-C4-C5-O5
13	WB	3	GZL	O4-C4-C5-O5
13	zB	3	GZL	O4-C4-C5-O5
13	wC	3	GZL	O4-C4-C5-O5
13	zC	3	GZL	O4-C4-C5-O5
14	hC	3	GZL	O4-C4-C5-O5
15	CA	3	GZL	O4-C4-C5-O5
15	AB	3	GZL	O4-C4-C5-O5
15	eB	3	GZL	O4-C4-C5-O5
15	7B	3	GZL	O4-C4-C5-O5
15	4C	3	GZL	O4-C4-C5-O5
18	SE	3	GZL	O4-C4-C5-O5
18	pE	3	GZL	O4-C4-C5-O5
18	rE	3	GZL	O4-C4-C5-O5
18	yE	3	GZL	O4-C4-C5-O5
20	UE	3	GZL	O4-C4-C5-O5
20	WE	3	GZL	O4-C4-C5-O5
20	hE	3	GZL	O4-C4-C5-O5
20	jE	3	GZL	O4-C4-C5-O5
20	uE	3	GZL	O4-C4-C5-O5

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Mol	Chain	Res	Type	Atoms
21	FE	3	GZL	O4-C4-C5-O5
21	vE	3	GZL	O4-C4-C5-O5
22	dE	3	GZL	O4-C4-C5-O5
20	CE	3	GZL	C4-C5-C6-O6
6	aB	3	GZL	O5-C5-C6-O6
6	5B	3	GZL	O5-C5-C6-O6
6	7D	3	GZL	O5-C5-C6-O6
12	IB	3	GZL	O5-C5-C6-O6
14	p	3	GZL	O5-C5-C6-O6
14	eD	3	GZL	O5-C5-C6-O6
15	2D	3	GZL	O5-C5-C6-O6
17	DB	5	MAN	O5-C5-C6-O6
20	TE	2	FUB	O4-C4-C5-O5
20	TE	2	FUB	C3-C4-C5-O5
18	IE	3	GZL	O5-C5-C6-O6
20	sE	3	GZL	O5-C5-C6-O6
17	7C	6	MAN	O5-C5-C6-O6
17	7C	1	NAG	O5-C5-C6-O6
6	2C	3	GZL	C3-C4-C5-C6
6	6D	3	GZL	C3-C4-C5-C6
12	iB	3	GZL	C3-C4-C5-C6
13	4	3	GZL	C3-C4-C5-C6
13	BA	3	GZL	C3-C4-C5-C6
13	dB	3	GZL	C3-C4-C5-C6
13	jB	3	GZL	C3-C4-C5-C6
13	6B	3	GZL	C3-C4-C5-C6
14	p	3	GZL	C3-C4-C5-C6
14	s	3	GZL	C3-C4-C5-C6
14	nA	3	GZL	C3-C4-C5-C6
14	HB	3	GZL	C3-C4-C5-C6
14	KB	3	GZL	C3-C4-C5-C6
14	nB	3	GZL	C3-C4-C5-C6
14	kC	3	GZL	C3-C4-C5-C6
14	eD	3	GZL	C3-C4-C5-C6
14	hD	3	GZL	C3-C4-C5-C6
18	KE	3	GZL	C3-C4-C5-C6
18	0E	3	GZL	C3-C4-C5-C6
22	GE	3	GZL	C3-C4-C5-C6
22	dE	3	GZL	C3-C4-C5-C6
24	lE	3	GZL	C3-C4-C5-C6
17	GA	4	MAN	O5-C5-C6-O6
15	eB	3	GZL	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
15	2D	3	GZL	C4-C5-C6-O6
17	GA	1	NAG	O5-C5-C6-O6
17	GA	6	MAN	O5-C5-C6-O6
6	6D	3	GZL	O4-C4-C5-C6
13	4	3	GZL	O4-C4-C5-C6
13	BA	3	GZL	O4-C4-C5-C6
13	6B	3	GZL	O4-C4-C5-C6
18	yE	3	GZL	O4-C4-C5-C6
20	jE	3	GZL	O4-C4-C5-C6
24	YE	3	GZL	O4-C4-C5-C6
24	lE	3	GZL	O4-C4-C5-C6
17	5D	1	NAG	O5-C5-C6-O6
12	oA	3	GZL	C4-C5-C6-O6
12	fC	3	GZL	C4-C5-C6-O6
17	DB	3	BMA	C4-C5-C6-O6
16	FA	1	NAG	C3-C2-N2-C7
13	6	3	GZL	O5-C5-C6-O6
13	1B	3	GZL	O5-C5-C6-O6
6	zD	3	GZL	C4-C5-C6-O6
18	9D	3	GZL	C4-C5-C6-O6
6	R	3	GZL	O5-C5-C6-O6
6	9B	3	GZL	C4-C5-C6-O6
13	4	3	GZL	C4-C5-C6-O6
13	9A	3	GZL	C4-C5-C6-O6
14	HB	3	GZL	C4-C5-C6-O6
6	4B	3	GZL	C3-C4-C5-O5
13	9A	3	GZL	C3-C4-C5-O5
22	VE	3	GZL	C3-C4-C5-O5
22	dE	3	GZL	C3-C4-C5-O5
6	ME	3	GZL	O4-C4-C5-O5
22	VE	3	GZL	O4-C4-C5-O5
14	nB	3	GZL	C4-C5-C6-O6
6	AA	3	GZL	O5-C5-C6-O6
6	3B	3	GZL	O5-C5-C6-O6
13	zB	3	GZL	O5-C5-C6-O6
15	eB	3	GZL	O5-C5-C6-O6
18	0E	3	GZL	O5-C5-C6-O6
20	CE	3	GZL	O5-C5-C6-O6
16	FA	2	NAG	C8-C7-N2-C2
17	GA	5	MAN	O5-C5-C6-O6
6	4B	3	GZL	C3-C4-C5-C6
6	FC	3	GZL	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
12	lB	3	GZL	C3-C4-C5-C6
12	fC	3	GZL	C3-C4-C5-C6
12	iC	3	GZL	C3-C4-C5-C6
14	qA	3	GZL	C3-C4-C5-C6
14	kB	3	GZL	C3-C4-C5-C6
15	4C	3	GZL	O4-C4-C5-C6
6	CD	3	GZL	C4-C5-C6-O6
13	6	3	GZL	C4-C5-C6-O6
6	cB	3	GZL	C3-C4-C5-O5
13	6	3	GZL	C3-C4-C5-O5
17	5D	3	BMA	C4-C5-C6-O6
12	FB	3	GZL	O4-C4-C5-O5
13	4	3	GZL	O4-C4-C5-O5
20	TE	3	GZL	O4-C4-C5-O5
18	9D	3	GZL	O5-C5-C6-O6
17	5D	6	MAN	C4-C5-C6-O6
16	FA	2	NAG	O7-C7-N2-C2
17	GA	3	BMA	C4-C5-C6-O6
17	DB	3	BMA	O5-C5-C6-O6
6	3B	3	GZL	C4-C5-C6-O6
18	0E	3	GZL	C4-C5-C6-O6
6	9	3	GZL	O5-C5-C6-O6
20	CE	2	FUB	O4-C4-C5-O5
11	gA	1	FUB	O4-C4-C5-O5
6	zD	3	GZL	O5-C5-C6-O6
22	RE	2	FUB	O4-C4-C5-O5
12	lB	3	GZL	C3-C4-C5-C6
13	dD	3	GZL	C3-C4-C5-C6
13	0D	3	GZL	C3-C4-C5-C6
18	yE	3	GZL	C3-C4-C5-C6
6	cB	3	GZL	O4-C4-C5-O5
12	lB	3	GZL	O4-C4-C5-C6
13	0D	3	GZL	O4-C4-C5-C6
18	lE	3	GZL	C4-C5-C6-O6
24	lE	3	GZL	C4-C5-C6-O6
23	XE	2	FUB	O4-C4-C5-O5
16	4D	1	NAG	C3-C2-N2-C7
18	9D	3	GZL	O4-C4-C5-O5
13	9A	3	GZL	O5-C5-C6-O6
15	BB	3	GZL	O5-C5-C6-O6
6	5B	3	GZL	C3-C4-C5-C6
13	GB	3	GZL	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
13	3C	3	GZL	C3-C4-C5-C6
20	hE	3	GZL	C3-C4-C5-C6
17	GA	3	BMA	O5-C5-C6-O6
6	5B	3	GZL	O4-C4-C5-C6
13	mA	3	GZL	O4-C4-C5-C6
13	3C	3	GZL	O4-C4-C5-C6
18	pE	3	GZL	O4-C4-C5-C6
20	WE	3	GZL	O4-C4-C5-C6
21	vE	3	GZL	O4-C4-C5-C6
14	nB	3	GZL	O5-C5-C6-O6
17	DB	5	MAN	C4-C5-C6-O6
18	BE	3	GZL	C4-C5-C6-O6
15	BB	3	GZL	C4-C5-C6-O6
20	uE	3	GZL	C4-C5-C6-O6
22	RE	3	GZL	C3-C4-C5-O5
12	q	3	GZL	O5-C5-C6-O6
6	9	3	GZL	C4-C5-C6-O6
17	5D	3	BMA	O5-C5-C6-O6

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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	4C	3	GZL	1	0
15	eB	2	FUB	1	0
5	EC	5	AHR	1	0
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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	gA	2	AHR	1	0
6	bE	3	GZL	1	0
18	yE	4	AHR	1	0
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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	IE	1	FUB	1	0
22	QE	6	AHR	1	0
3	sB	2	FUB	1	0
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

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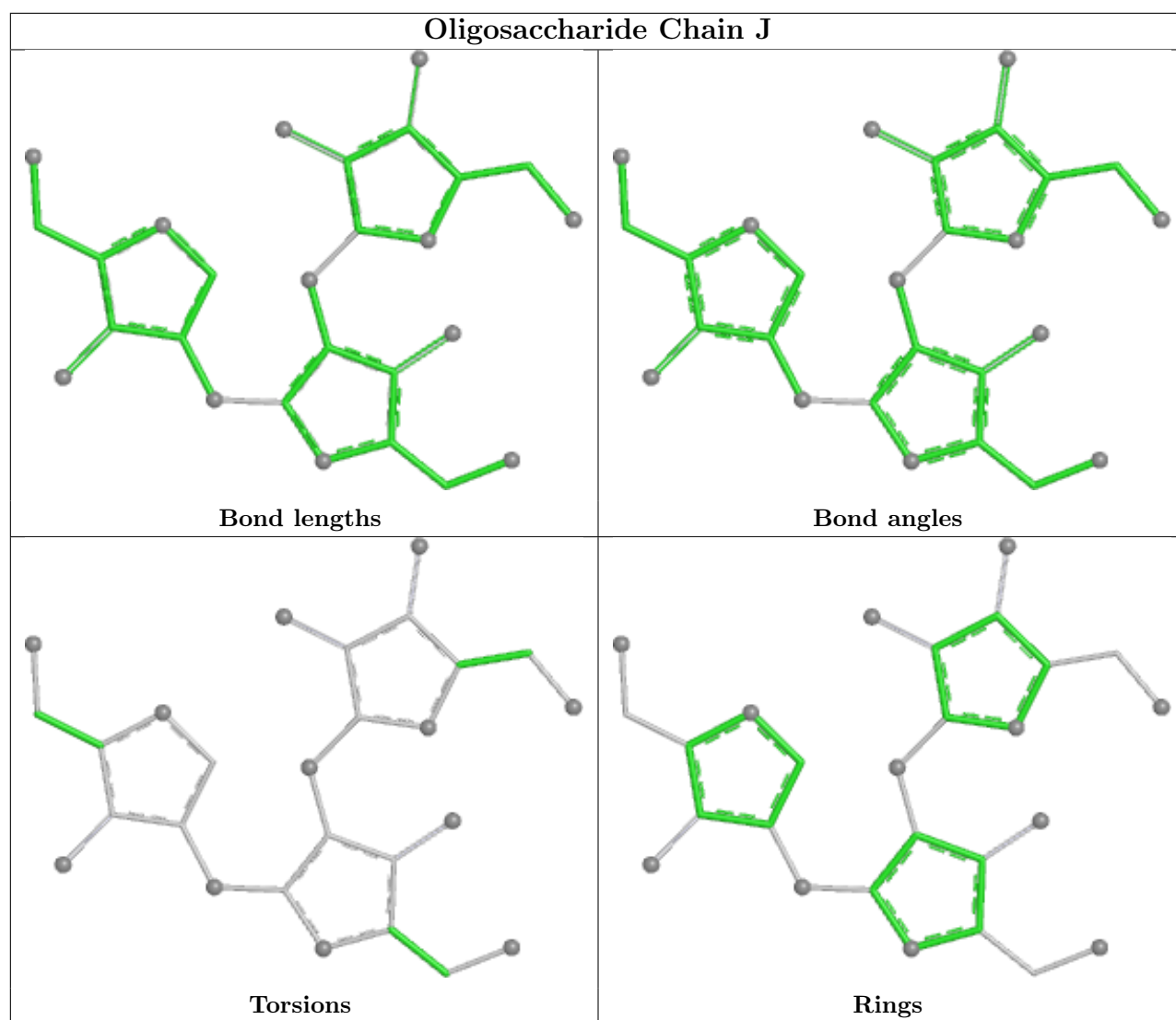
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	sD	2	FUB	2	0
3	wB	2	FUB	1	0
18	IE	5	AHR	1	0
6	XB	3	GZL	3	0
21	FE	5	AHR	1	0
14	eD	3	GZL	1	0
20	CE	4	AHR	1	0
17	7C	2	NAG	1	0
22	dE	2	FUB	1	0
6	LA	3	GZL	4	0
16	AC	1	NAG	2	0
6	ME	1	FUB	1	0
3	MA	1	FUB	1	0
3	m	2	FUB	1	0
20	HE	2	FUB	1	0
22	dE	6	AHR	1	0
4	VD	2	FUB	1	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

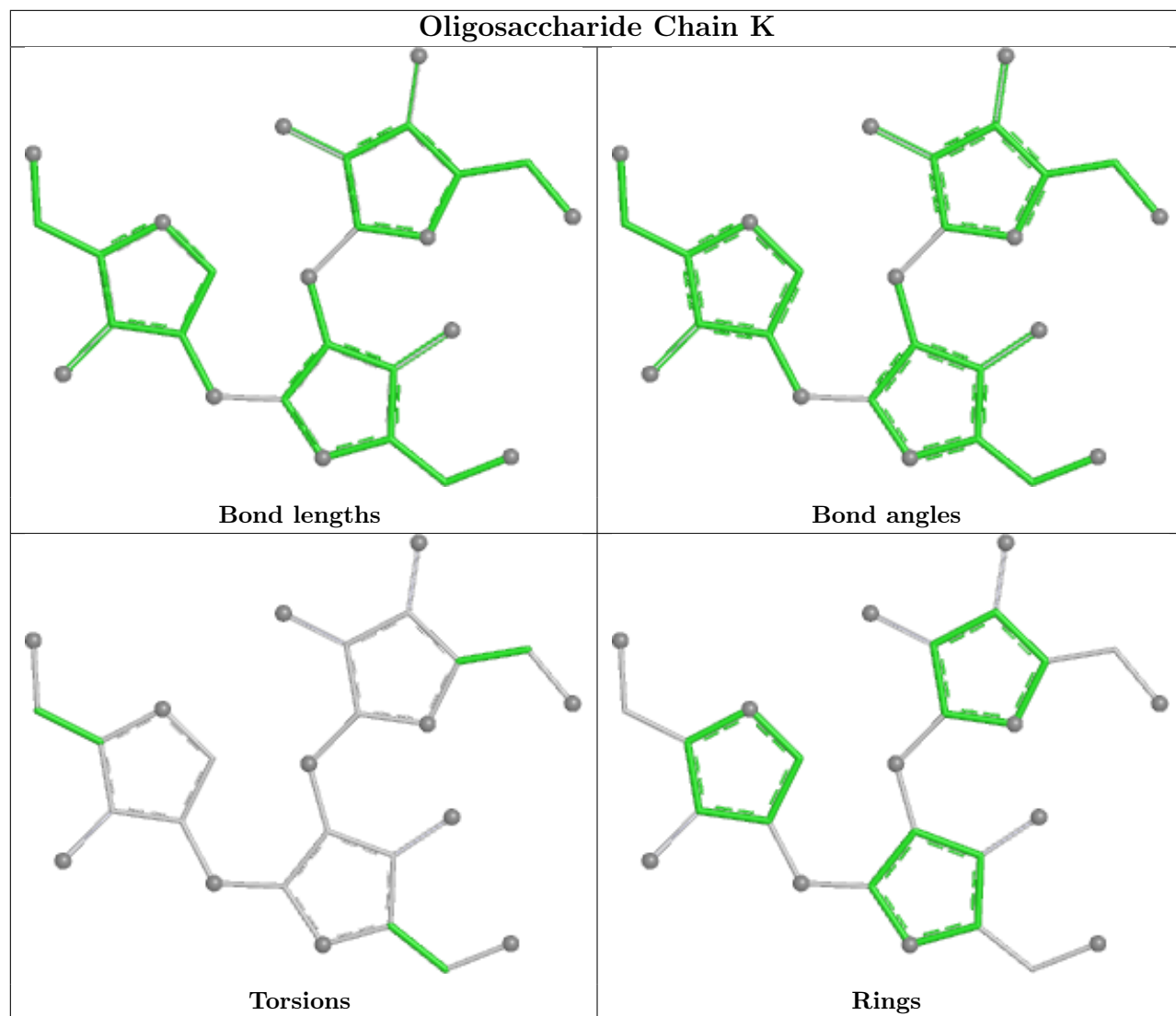
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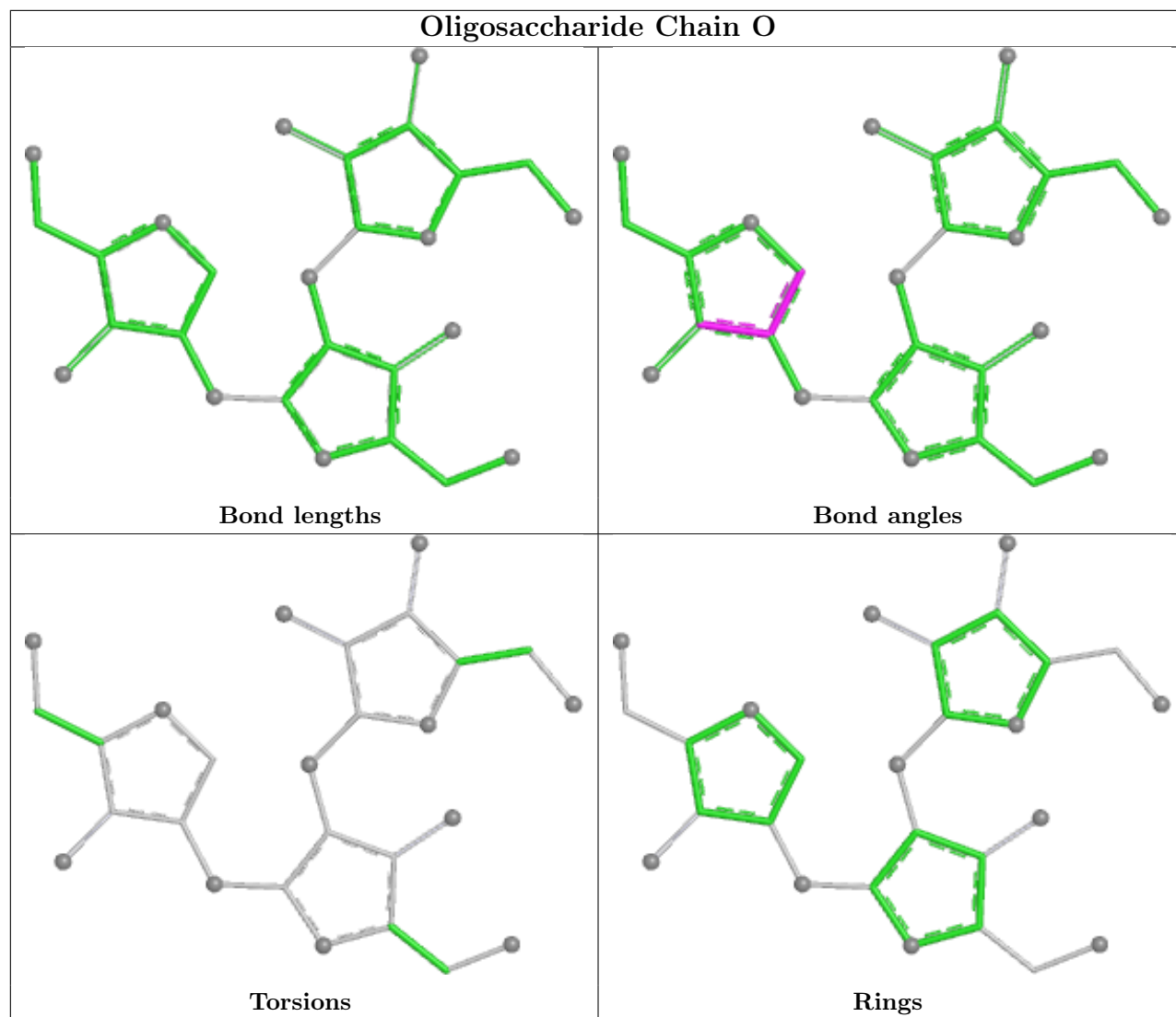
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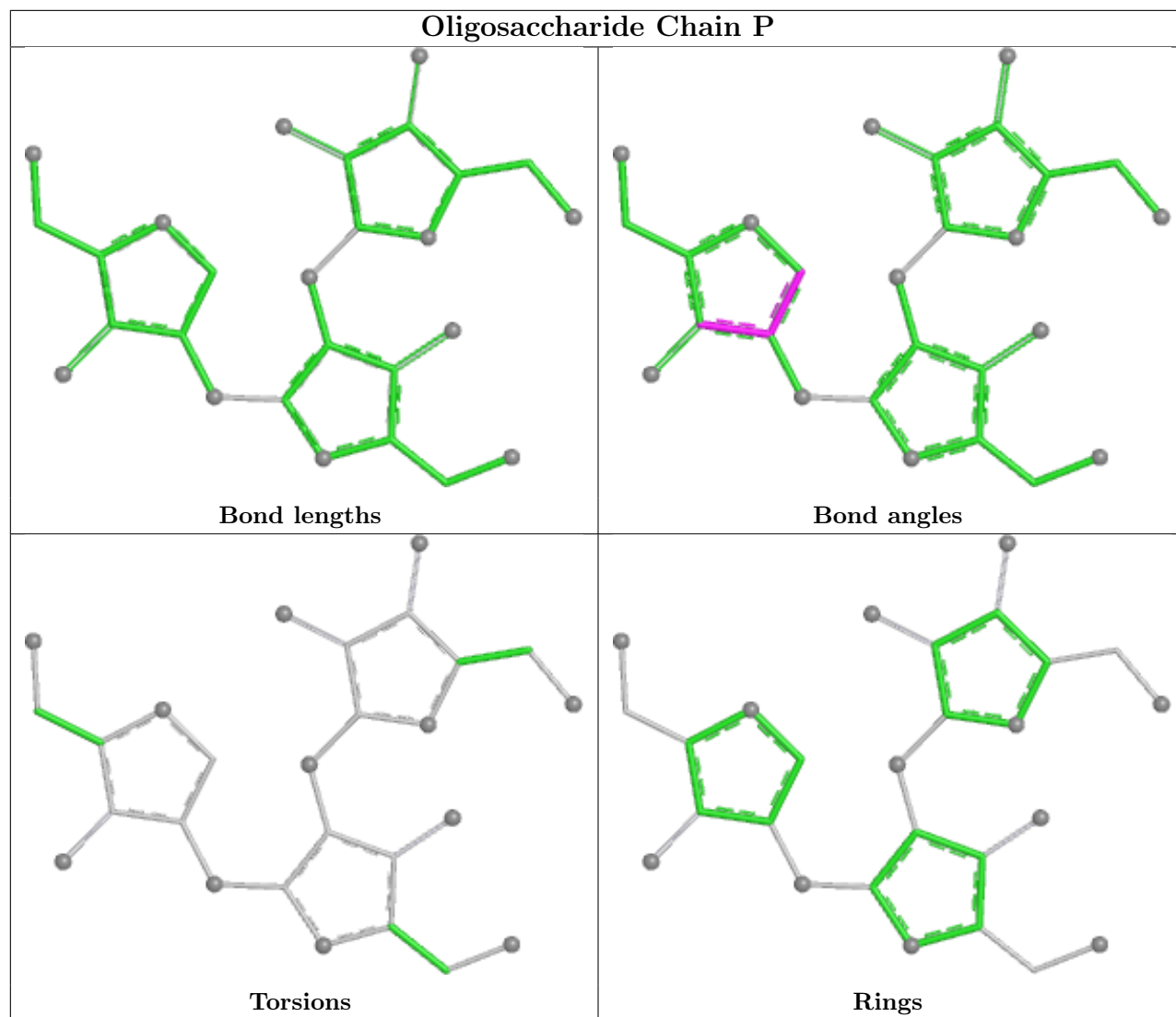
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	EE	4	AHR	1	0
22	iE	4	AHR	1	0
6	mE	2	FUB	1	0
12	iC	3	GZL	1	0
9	hA	1	FUB	1	0
20	xE	3	GZL	1	0
13	wD	2	FUB	1	0
6	uD	3	GZL	5	0
3	rA	2	FUB	1	0
4	pA	4	AHR	1	0
18	SE	1	FUB	1	0
22	wE	3	GZL	1	0
6	0B	1	FUB	1	0
6	mE	3	GZL	1	0
6	5	2	FUB	1	0
3	qC	2	FUB	1	0
6	cB	3	GZL	1	0
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

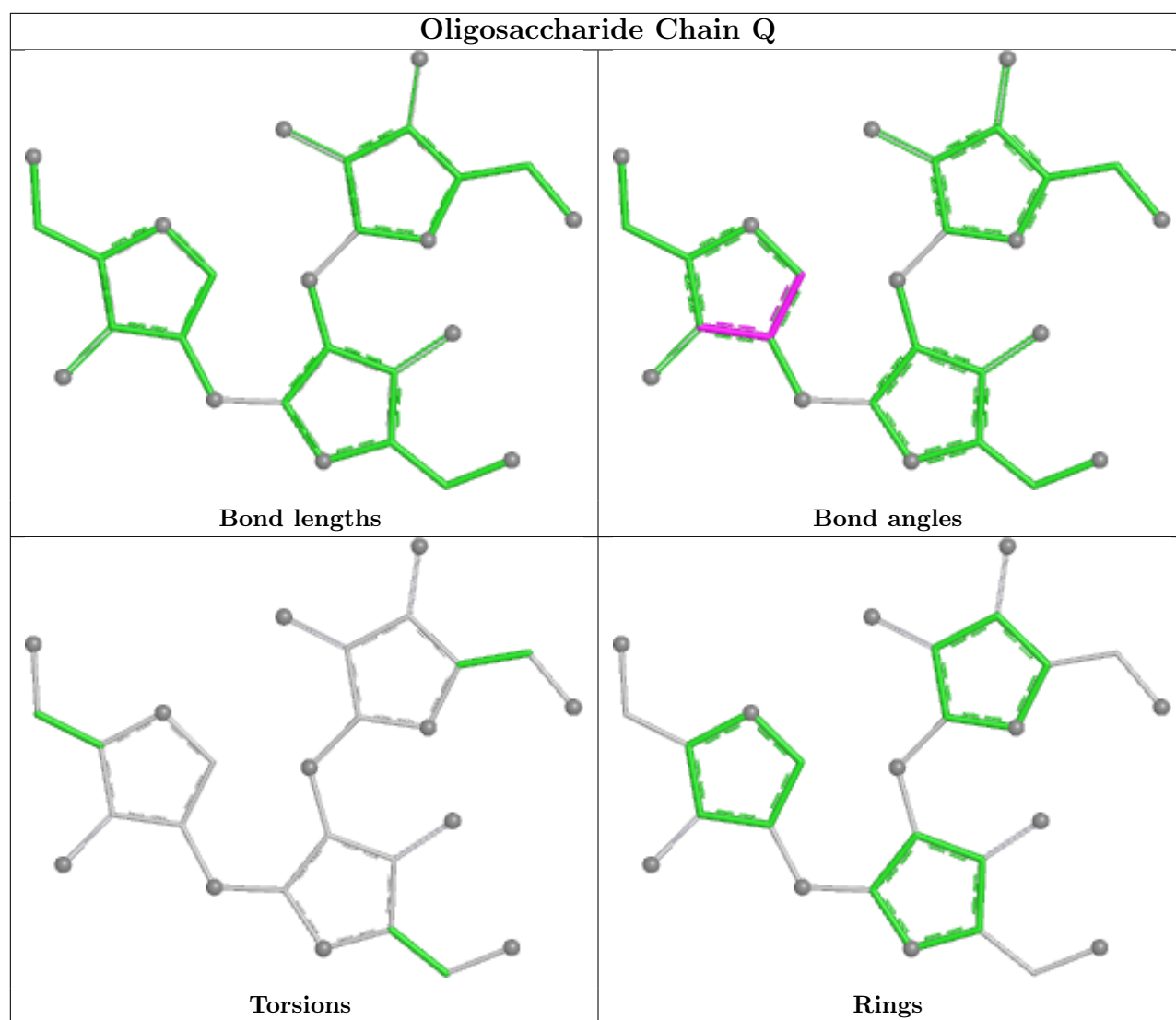
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

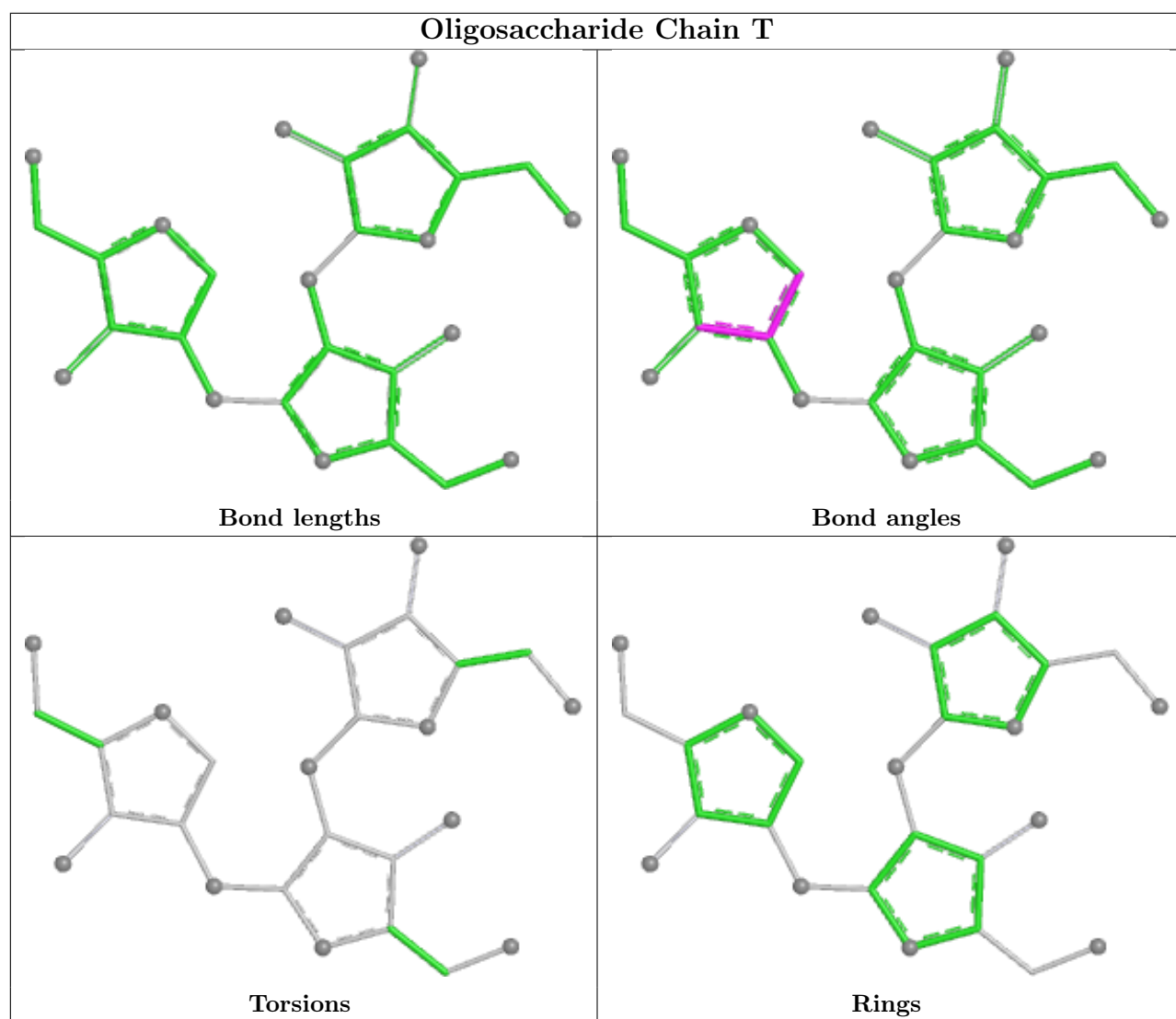


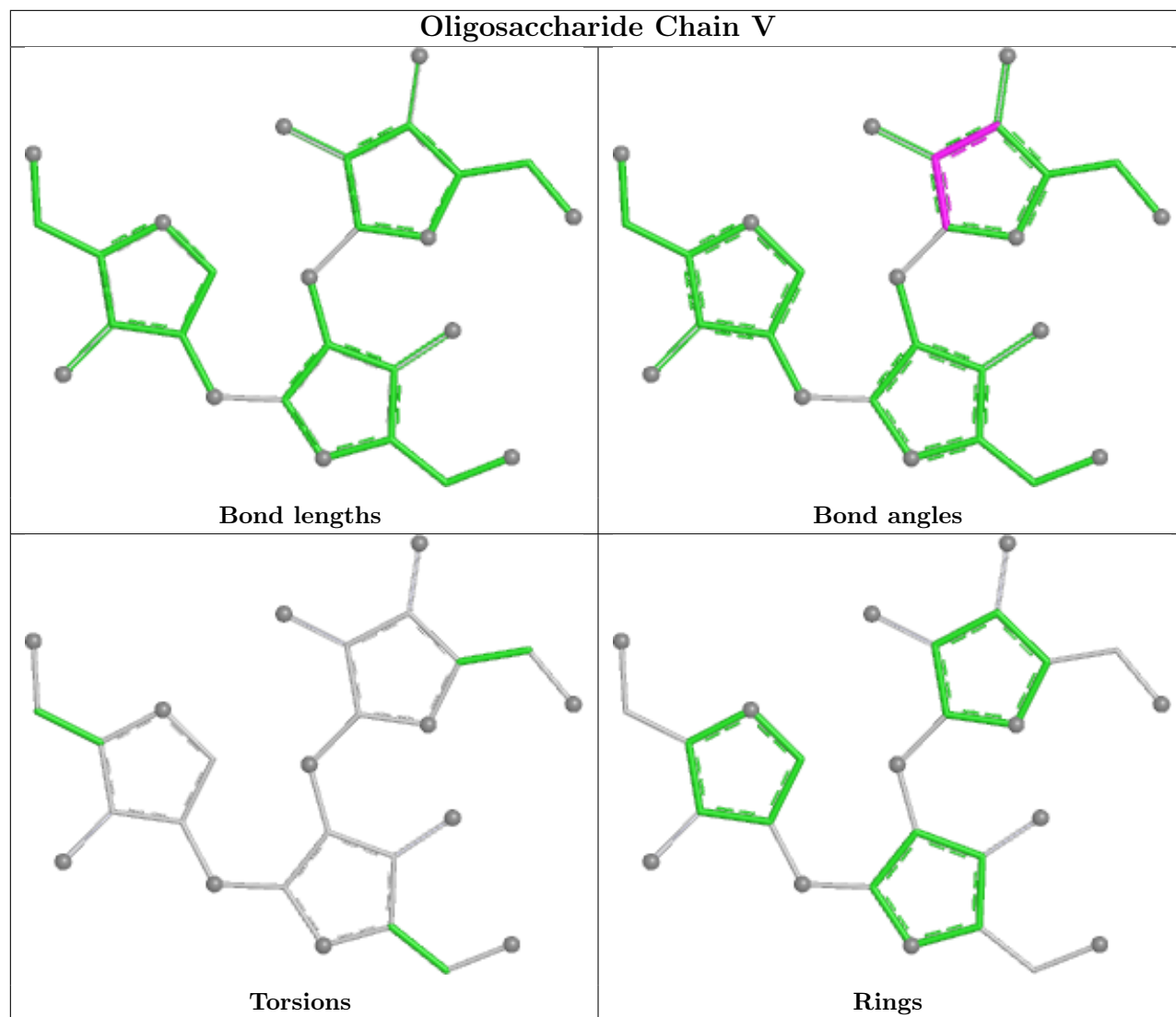


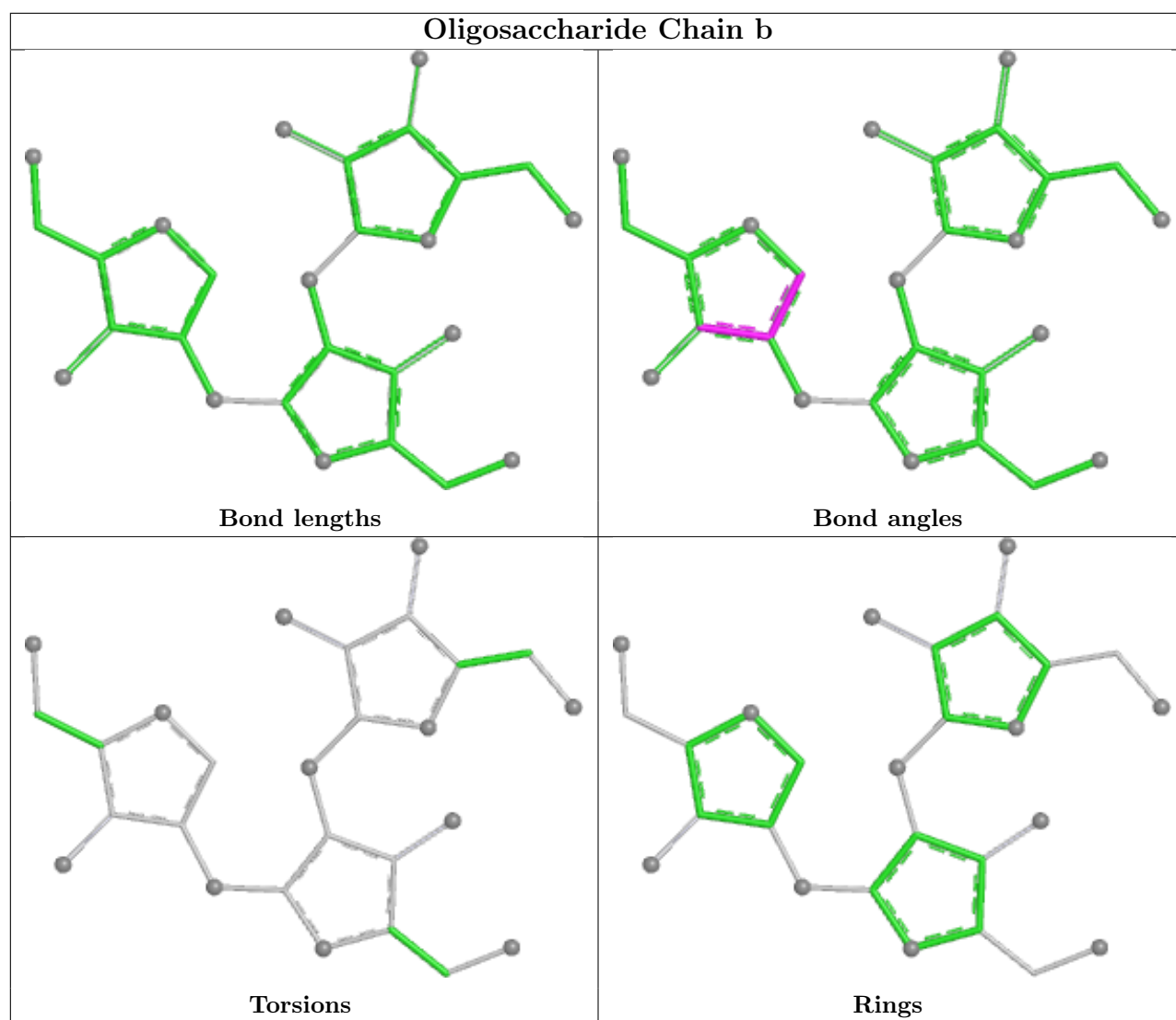


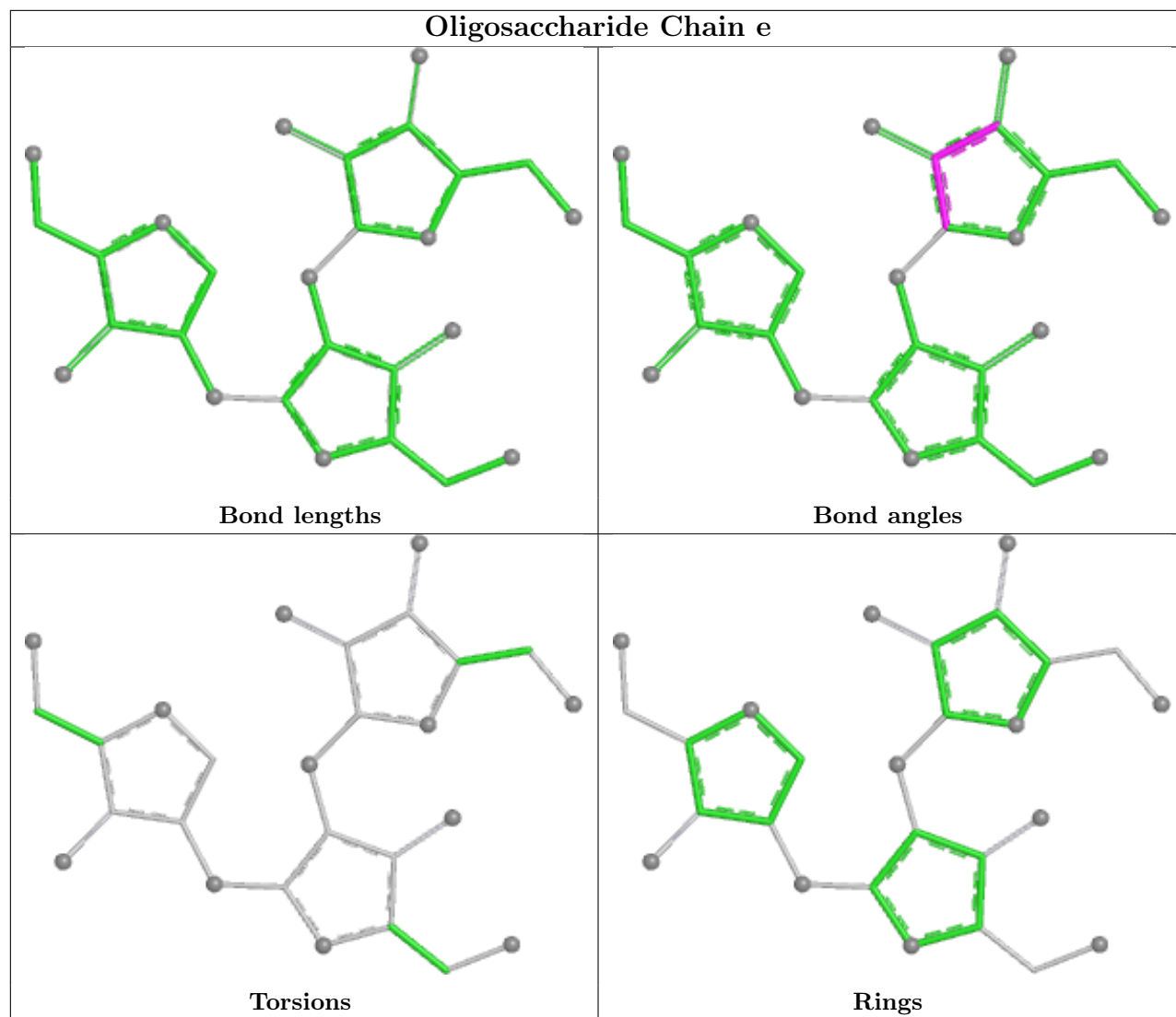


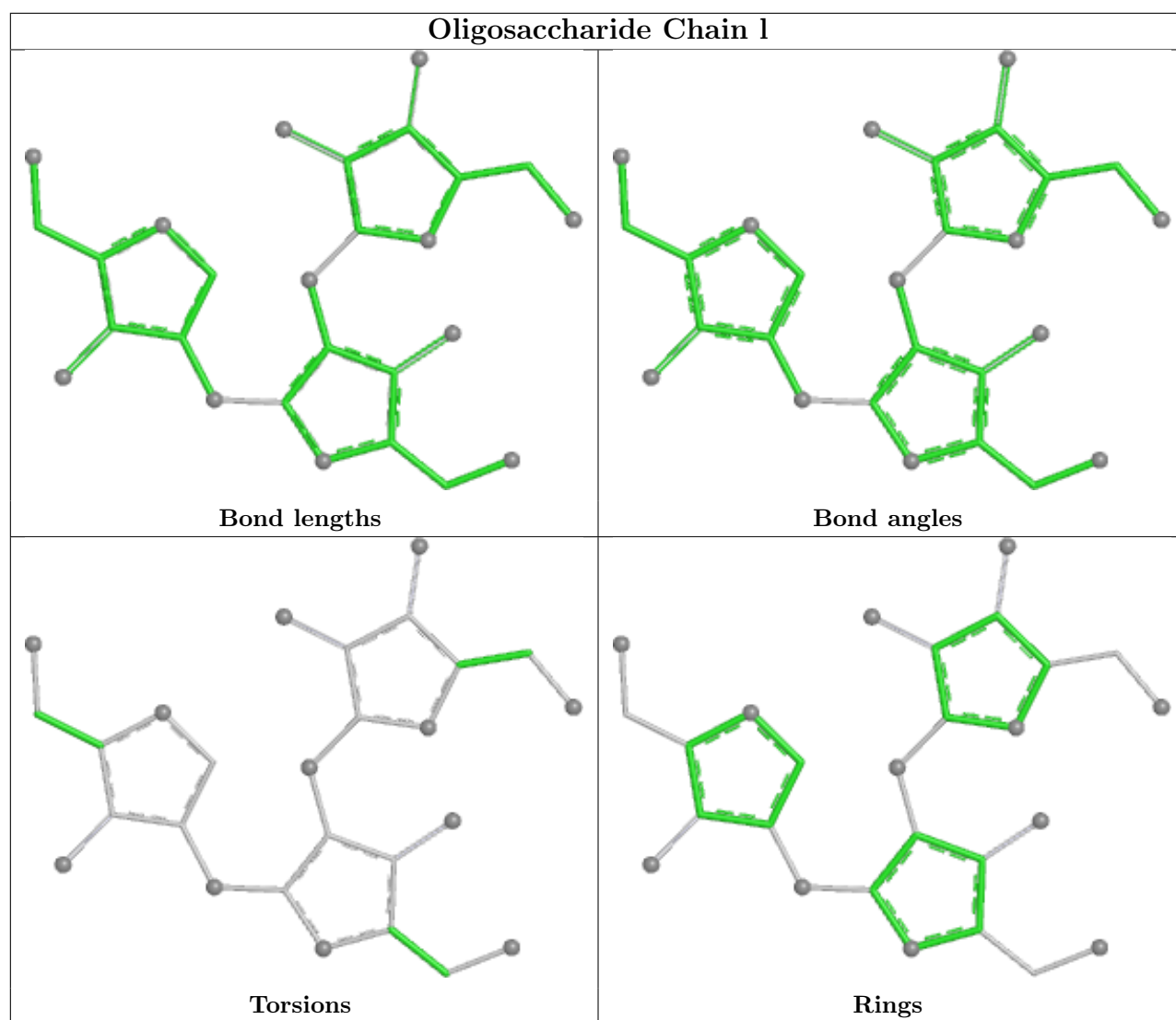


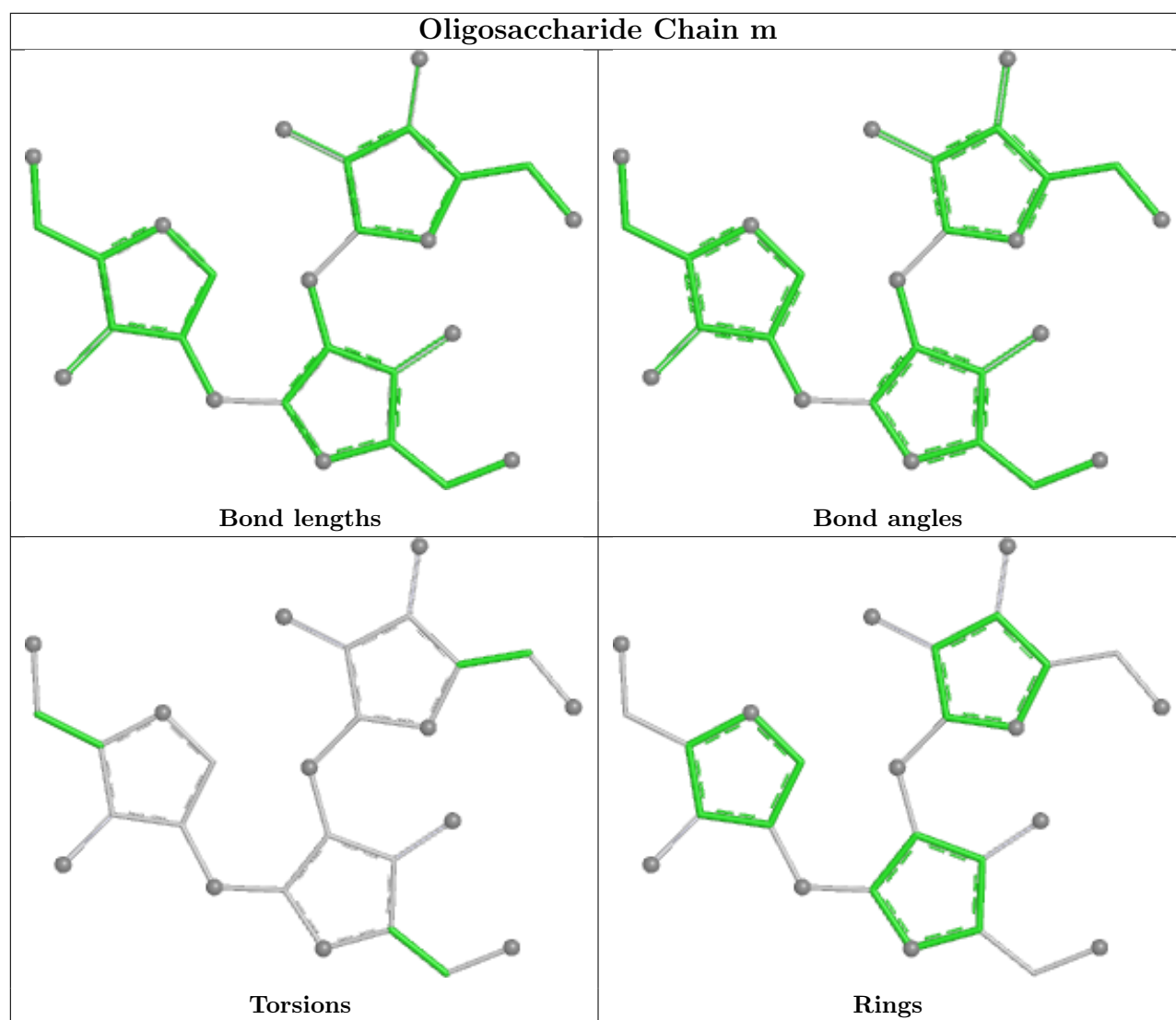


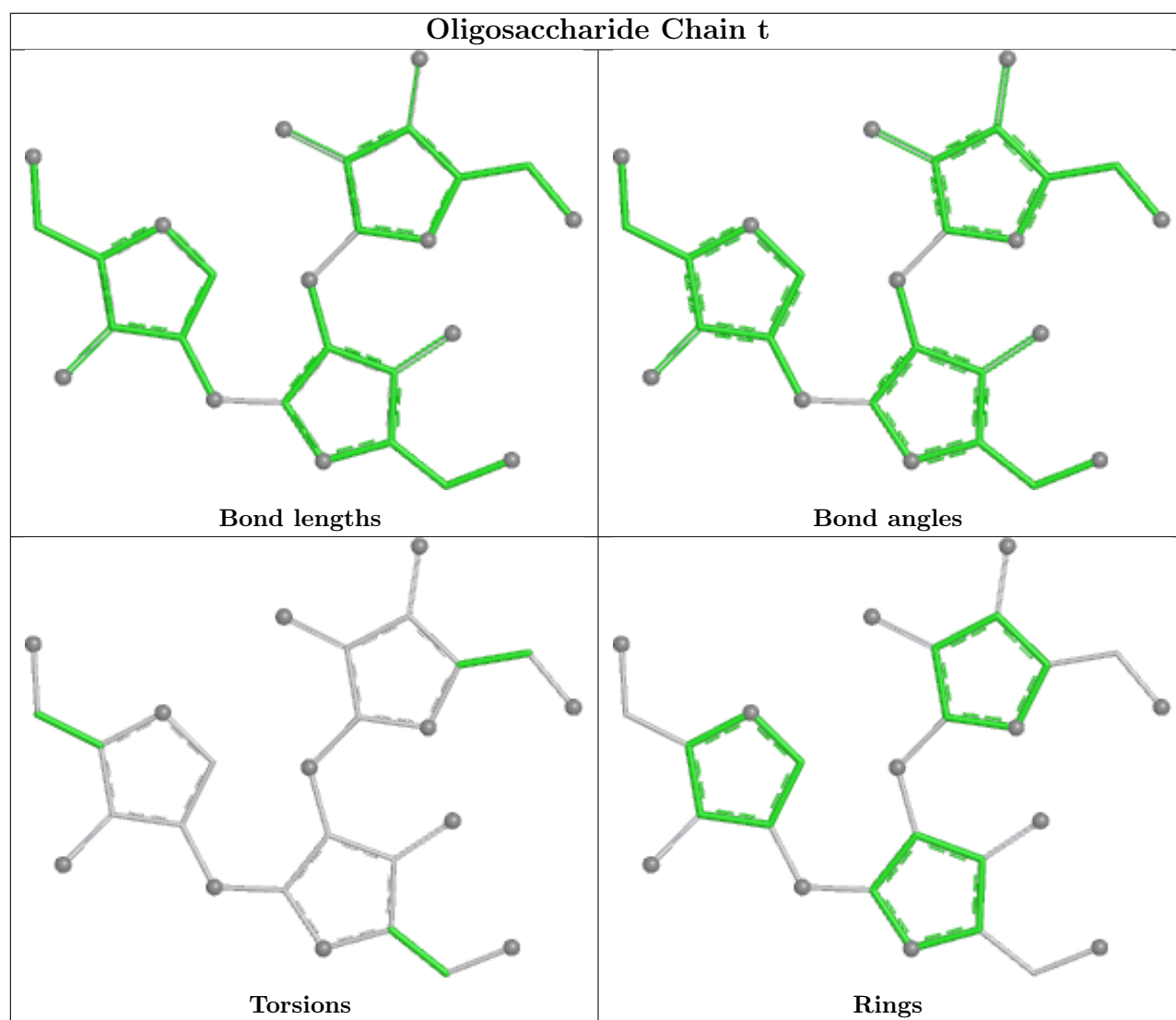


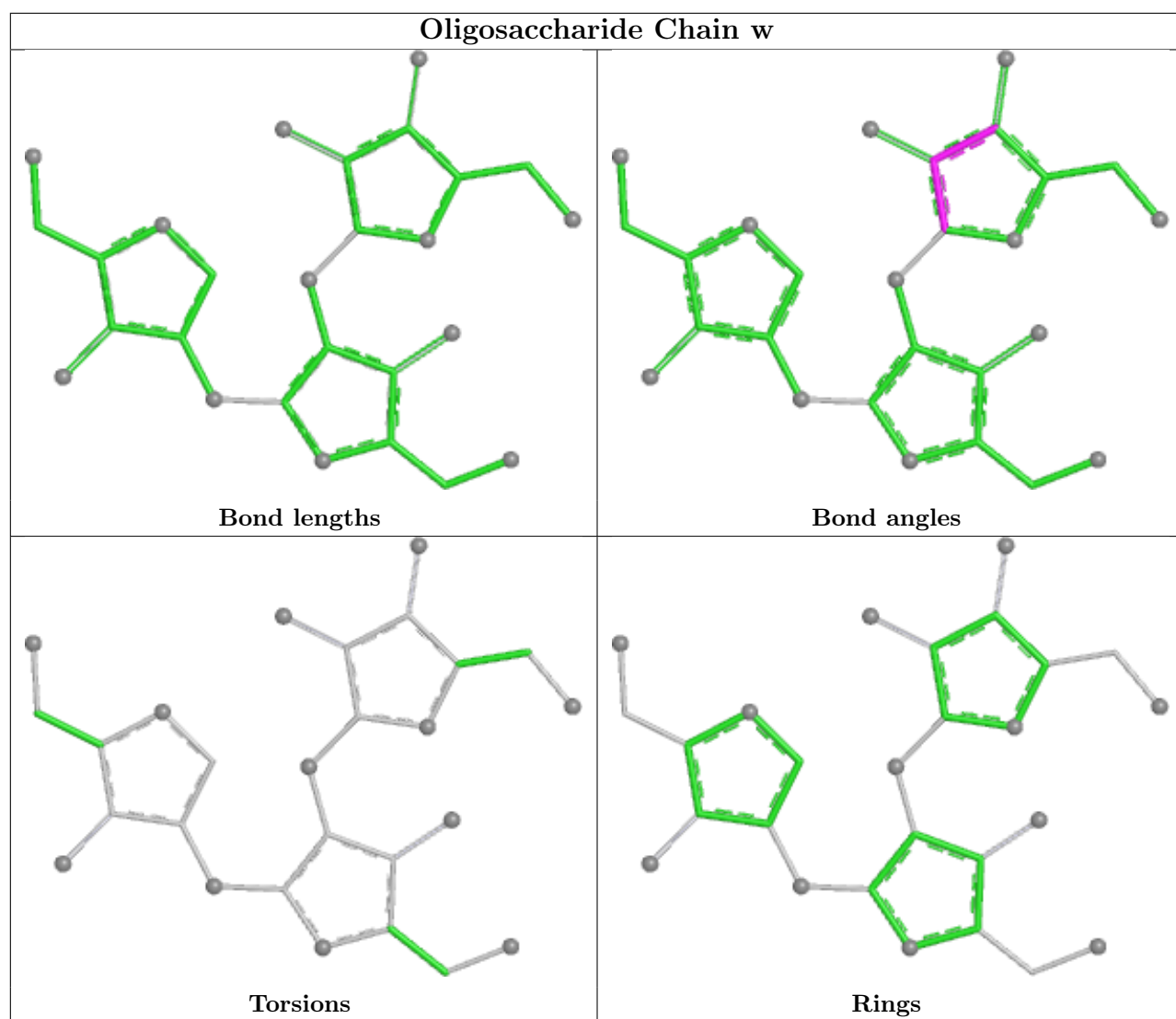


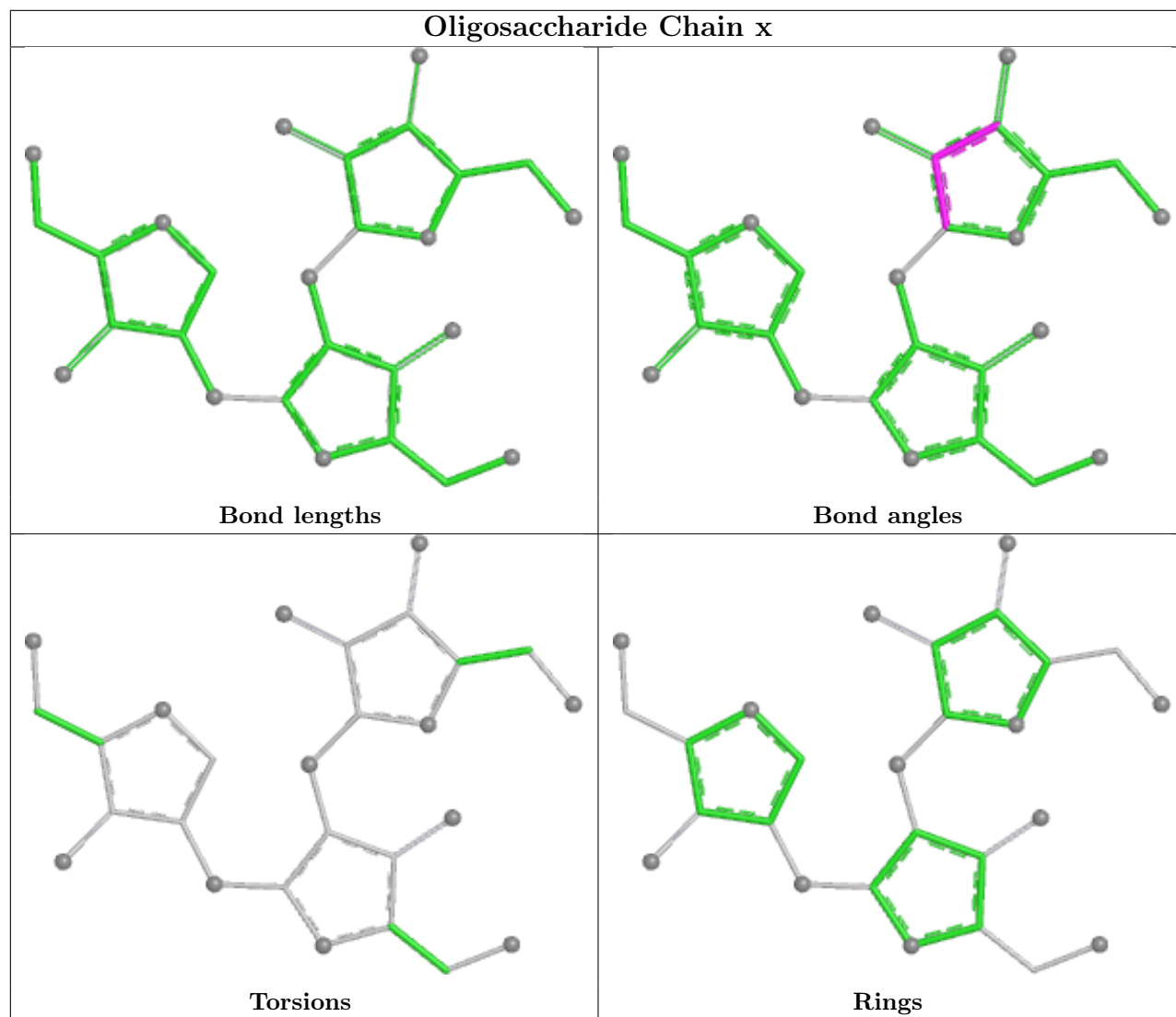


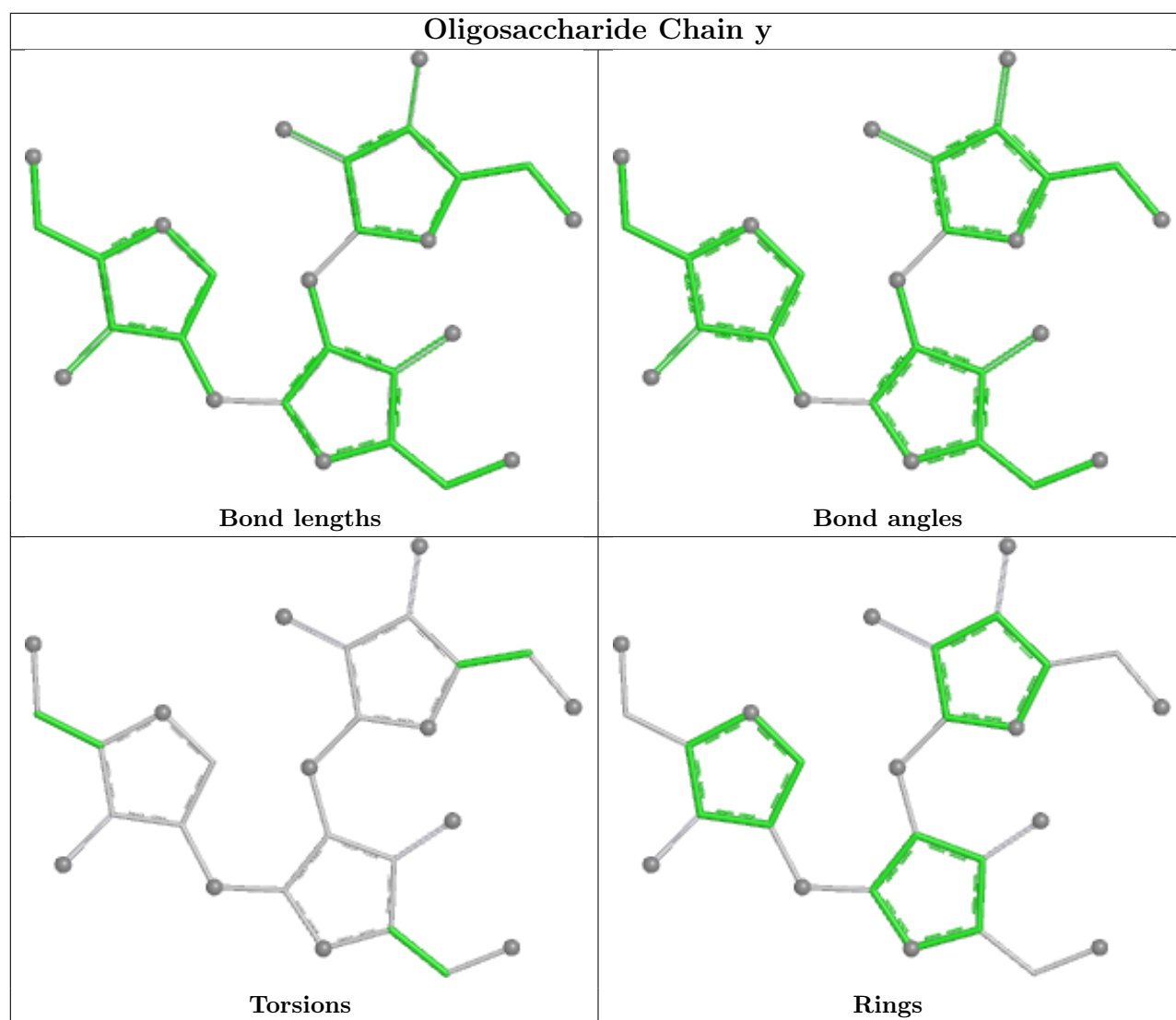


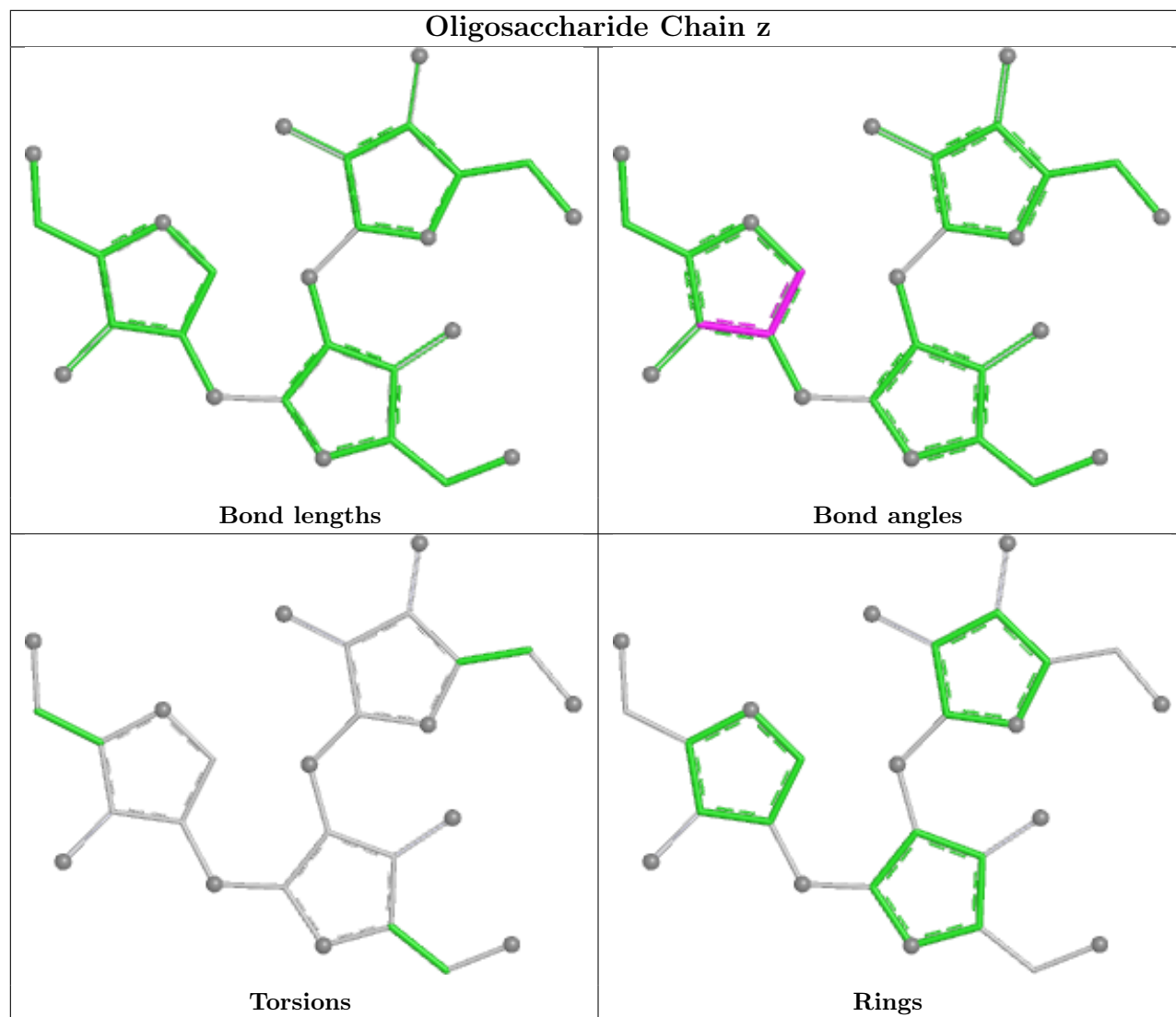


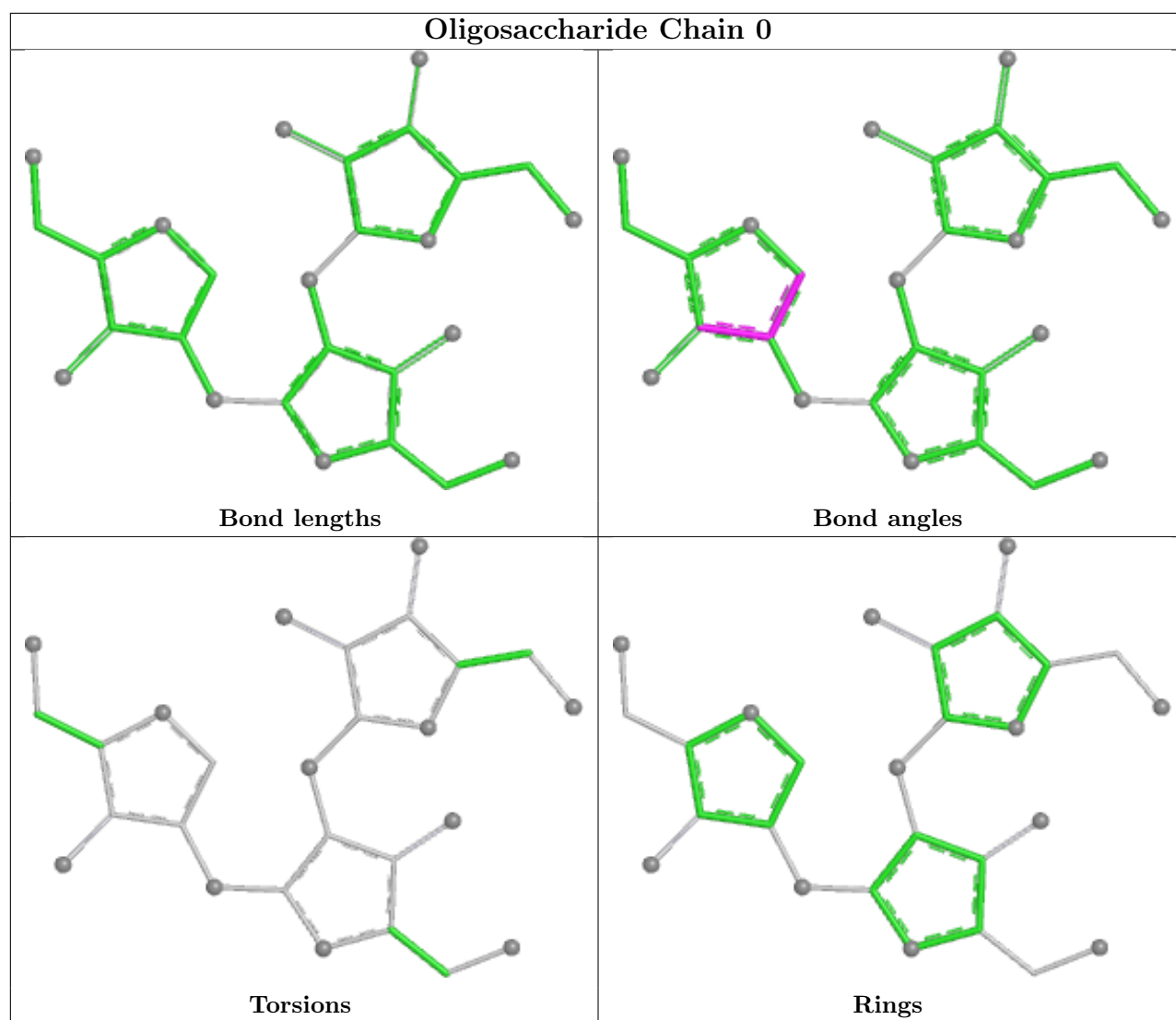


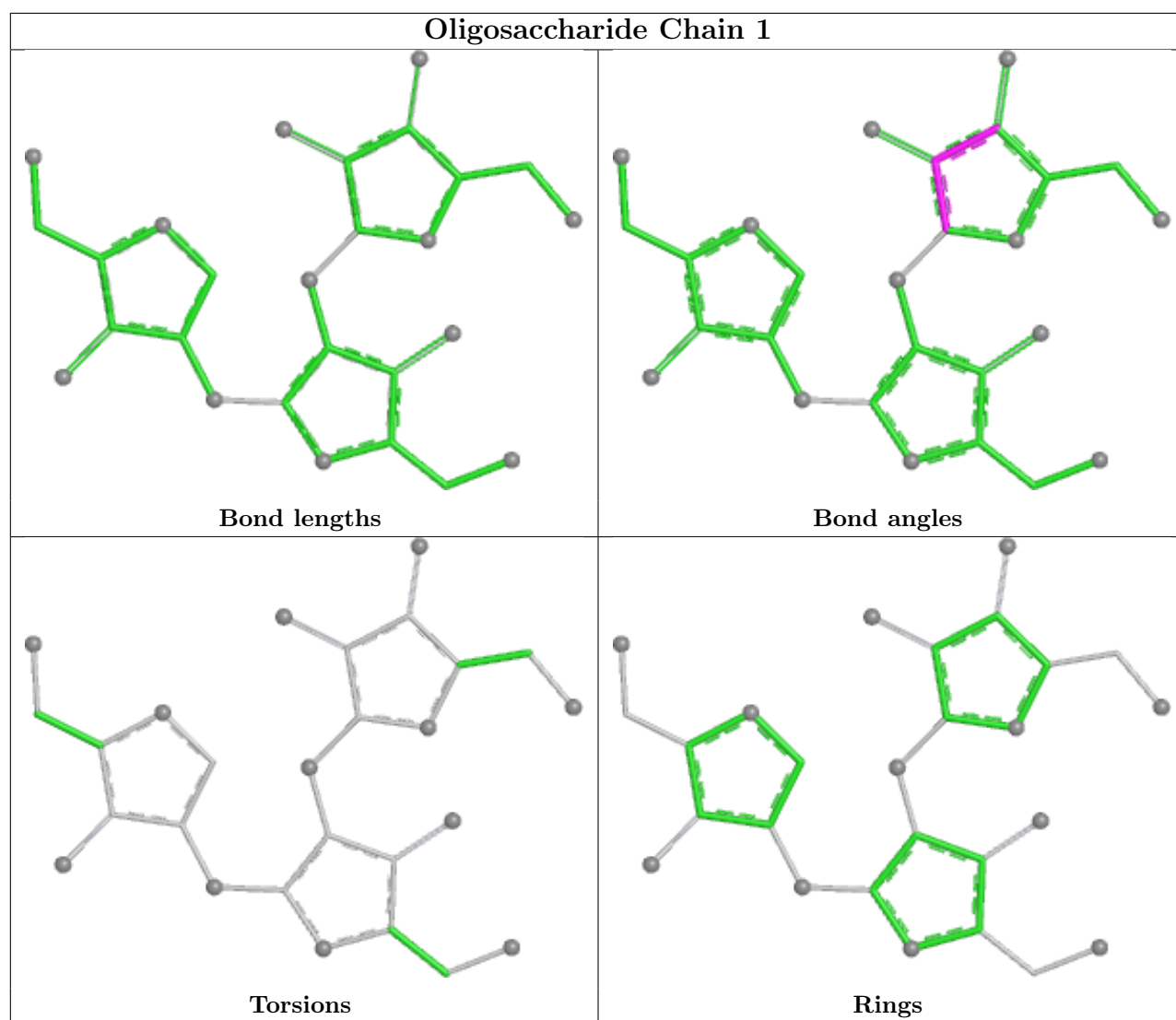


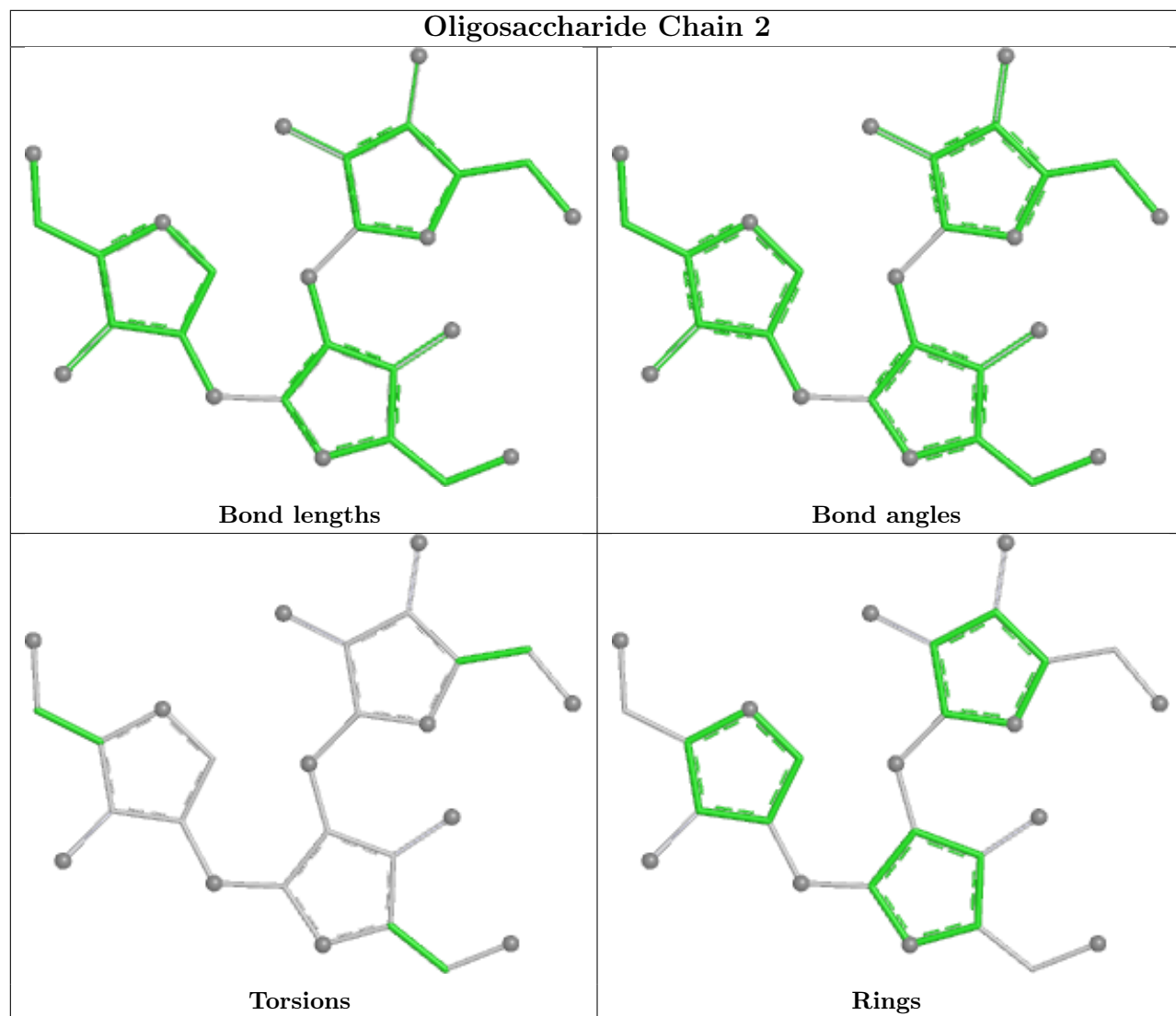


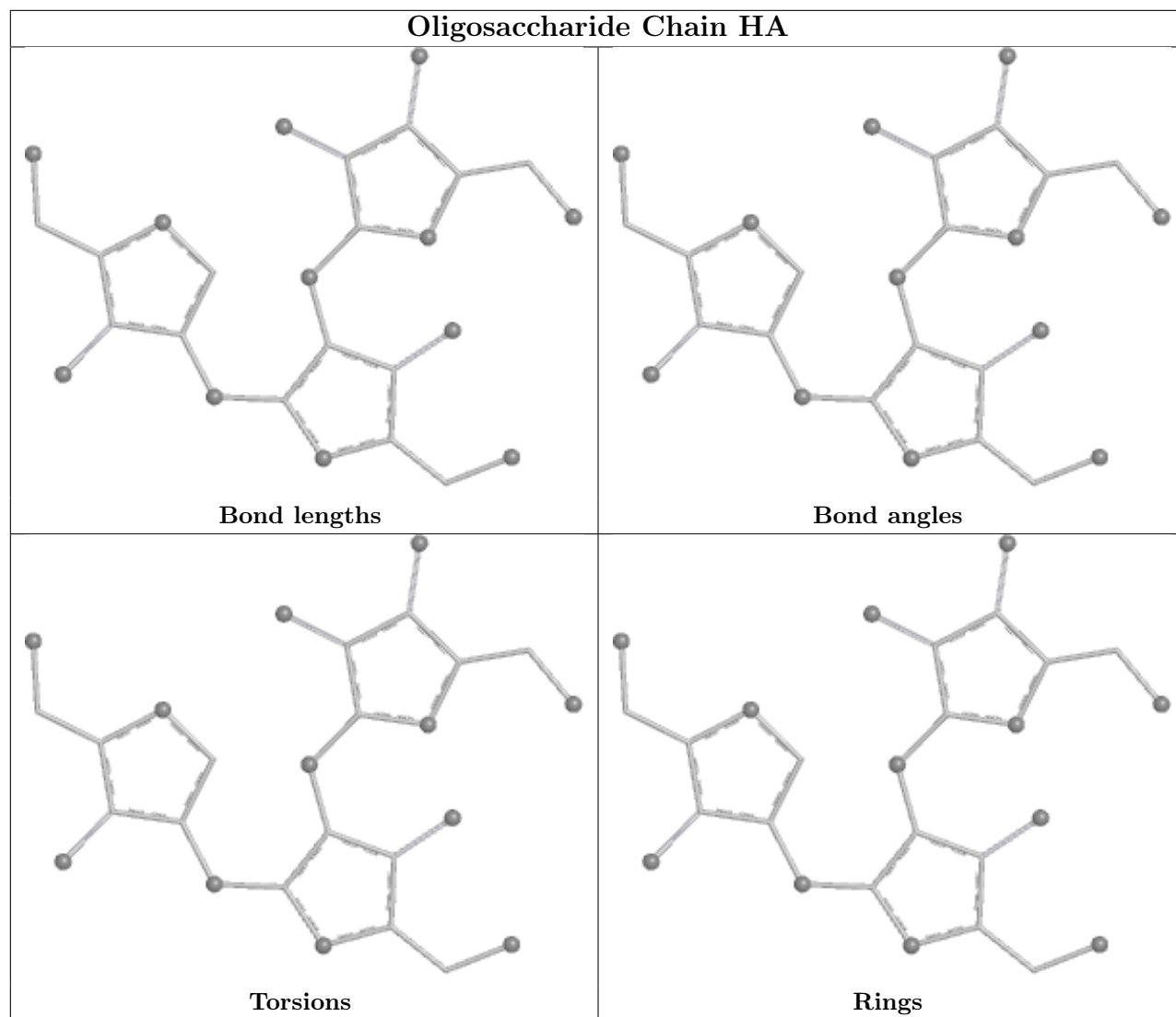


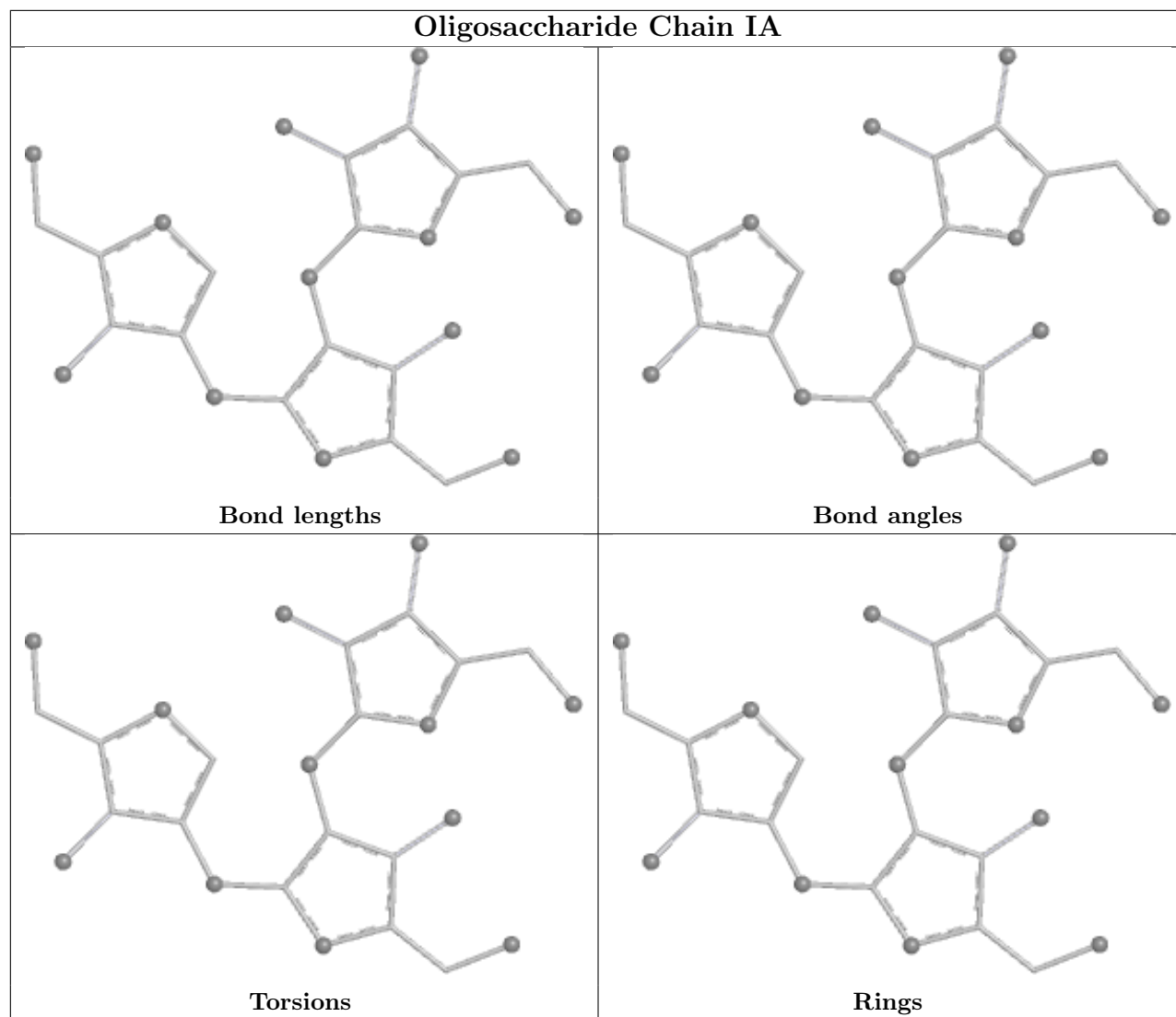


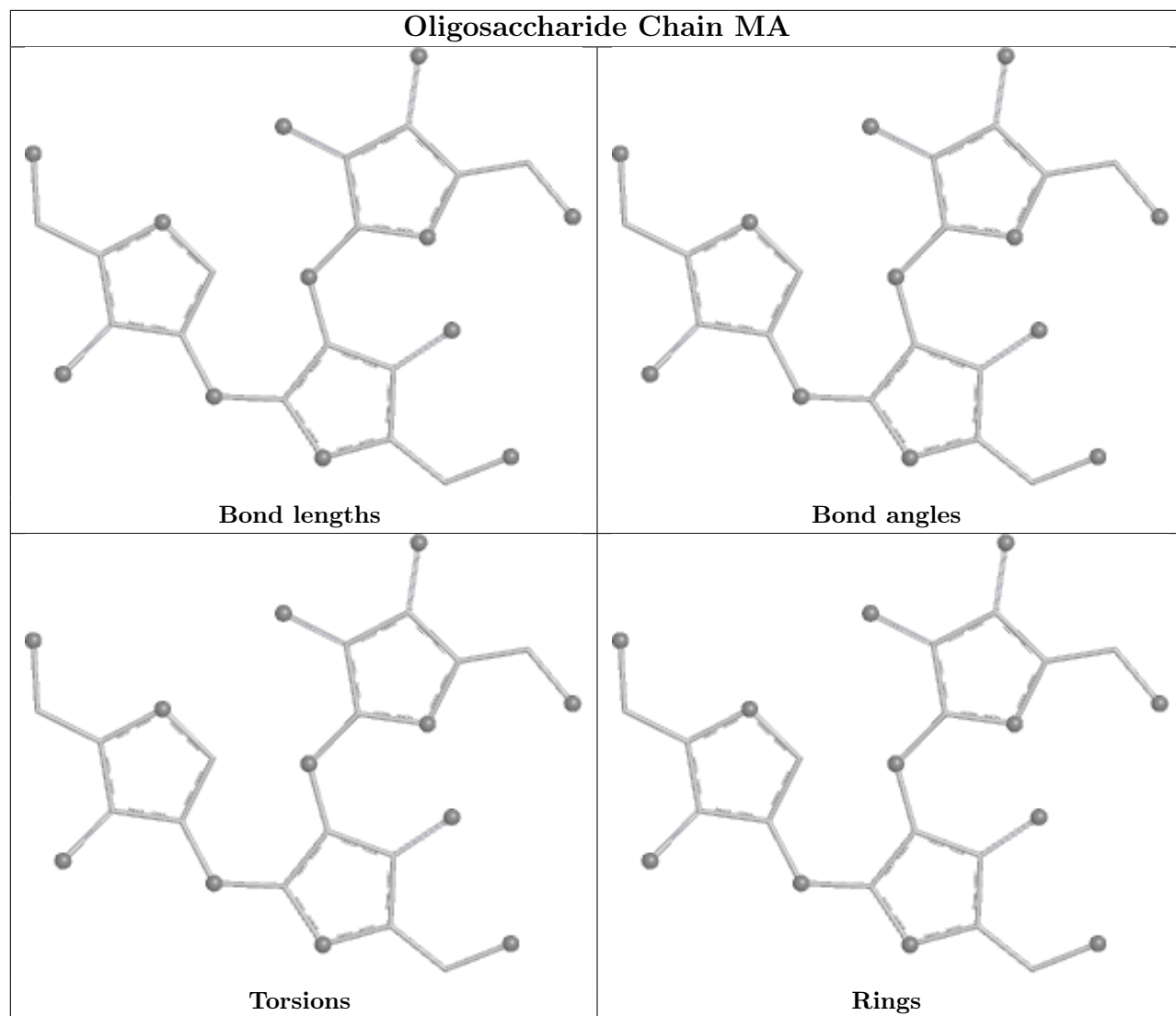


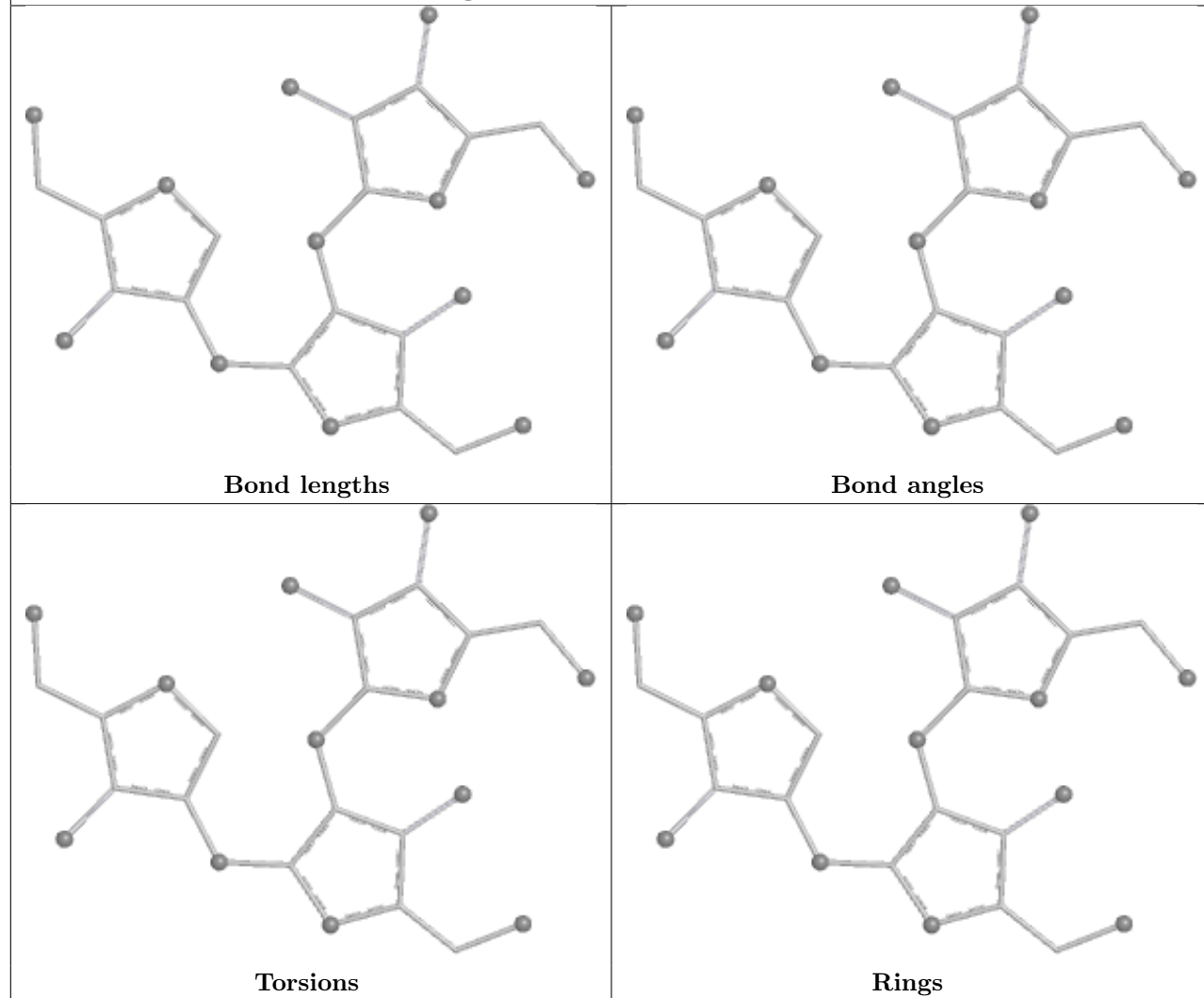


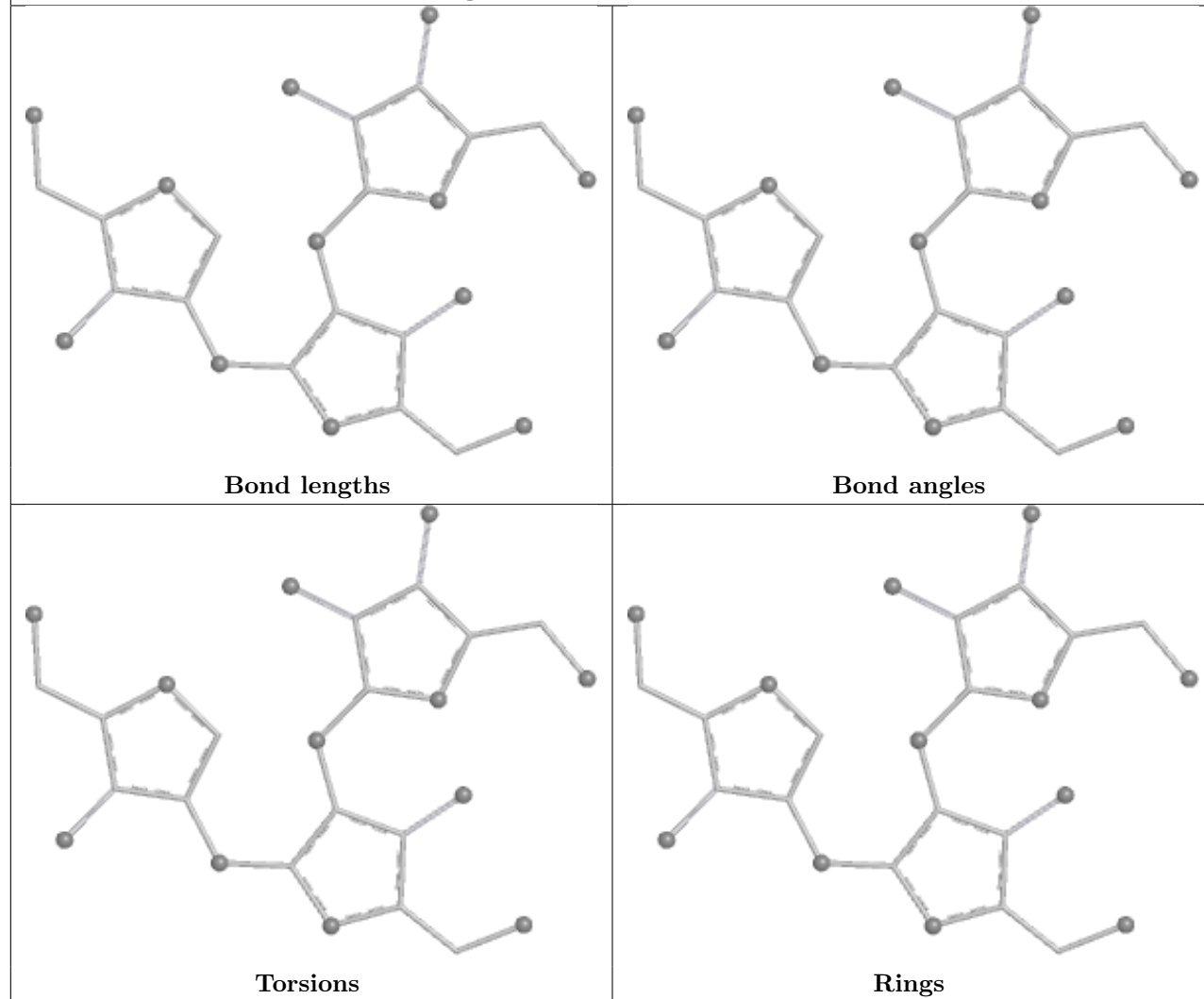


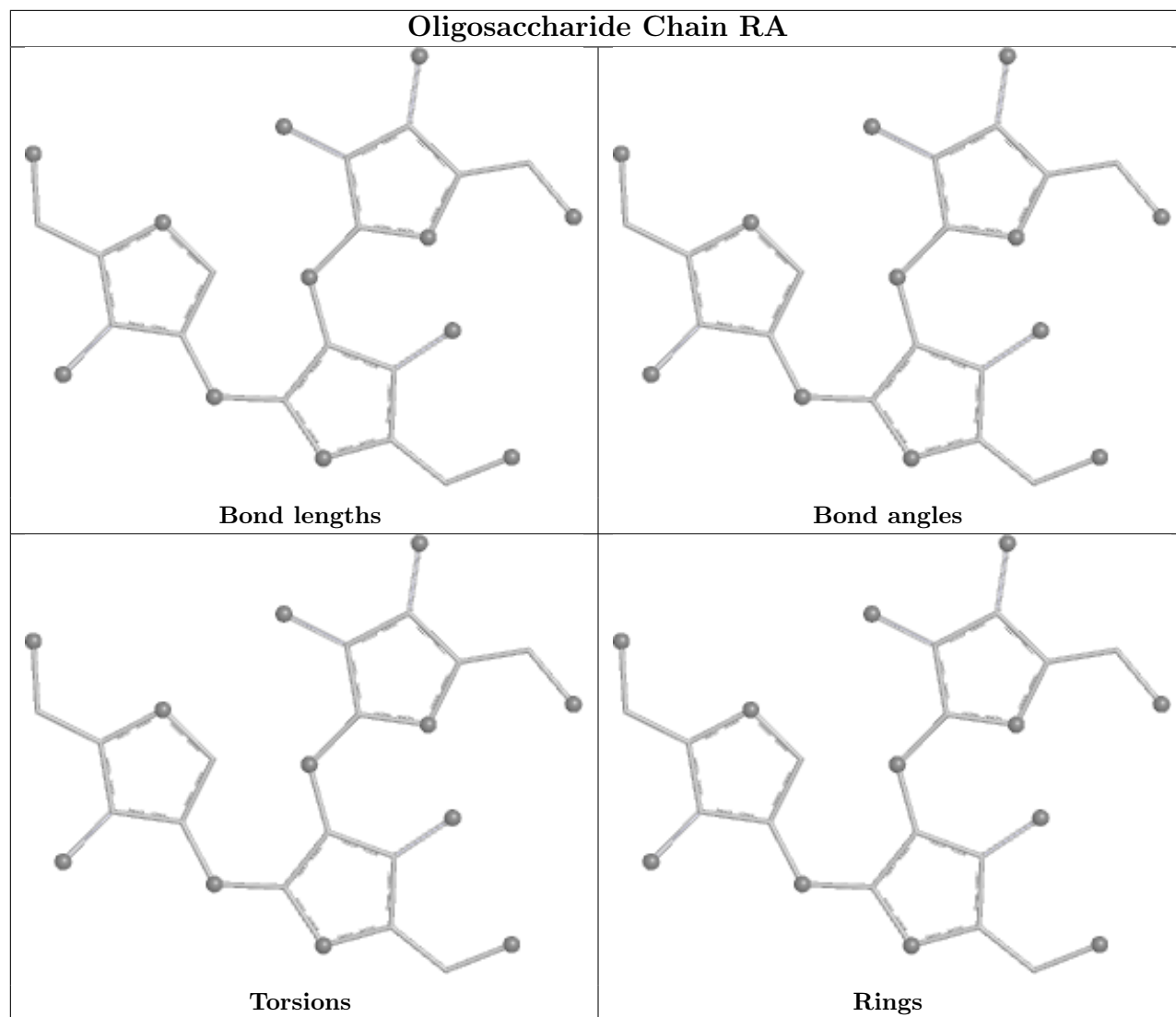


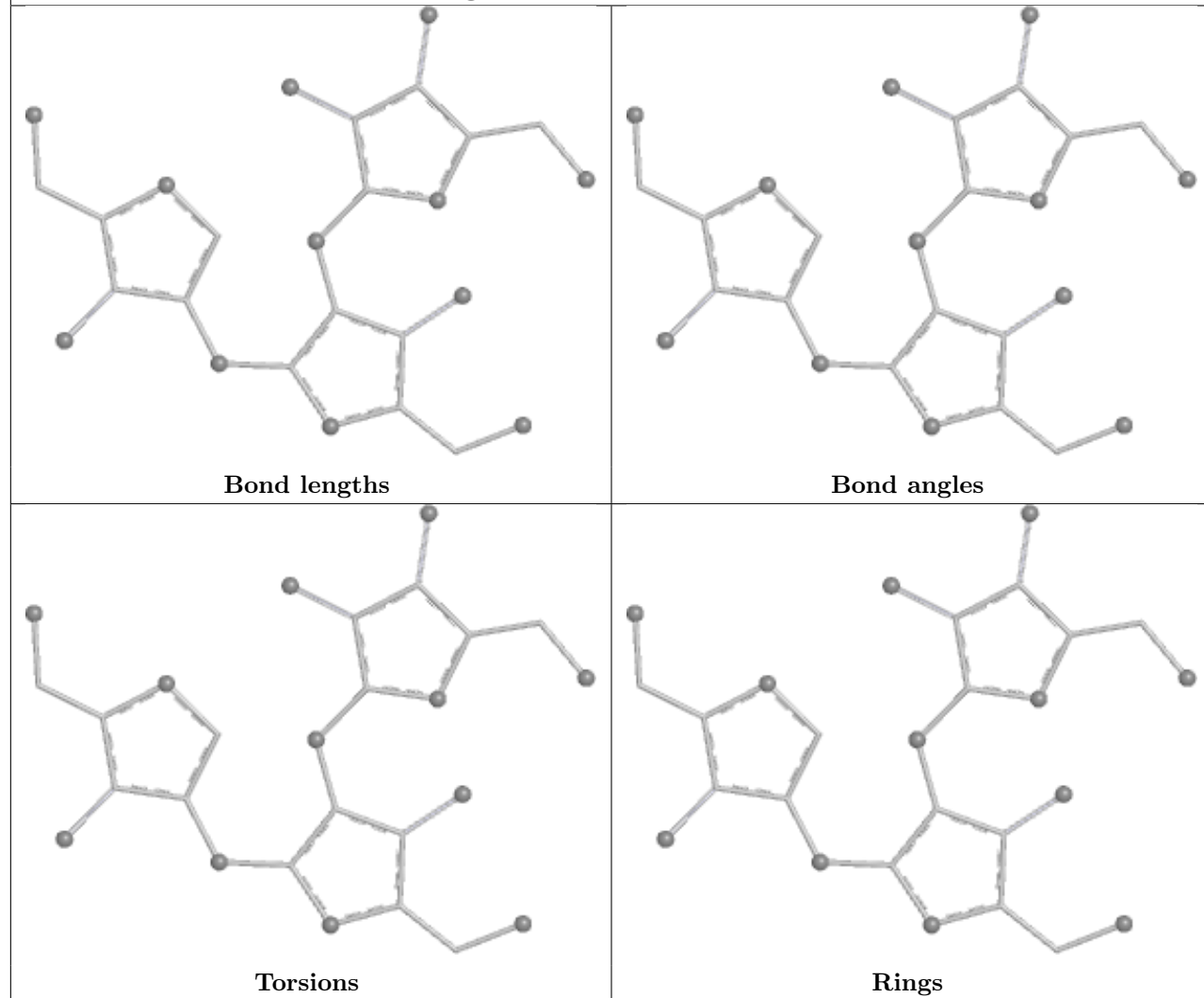


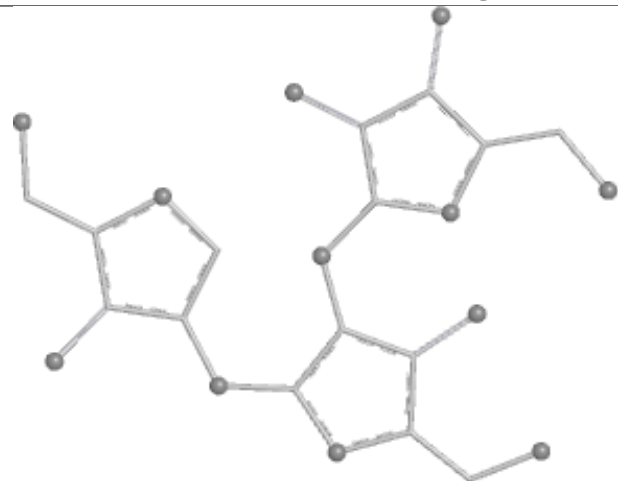
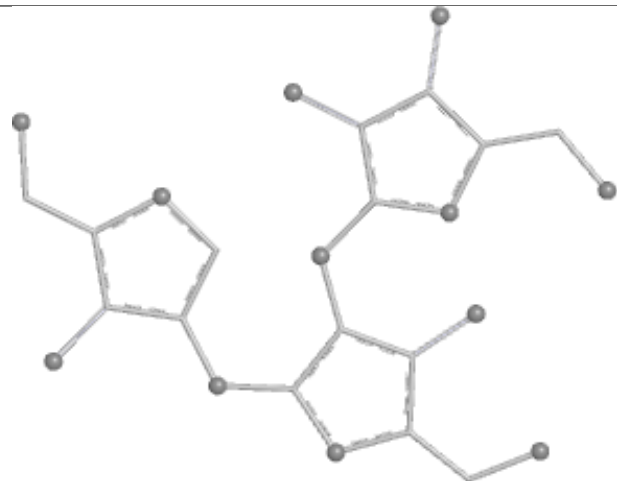
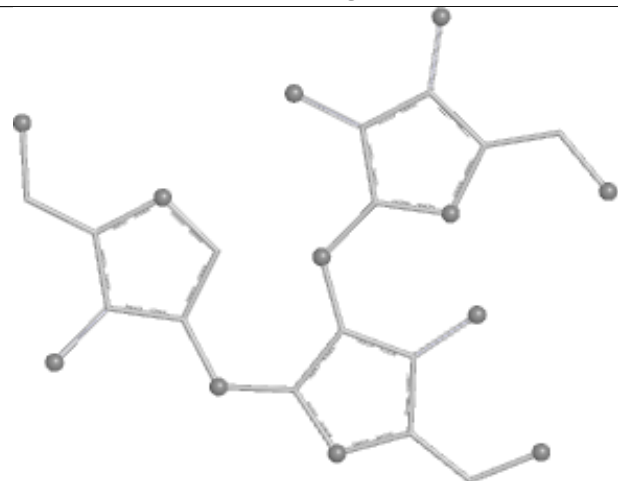
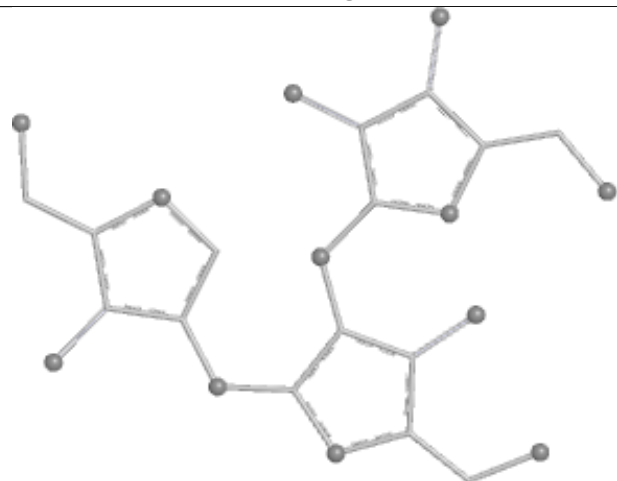


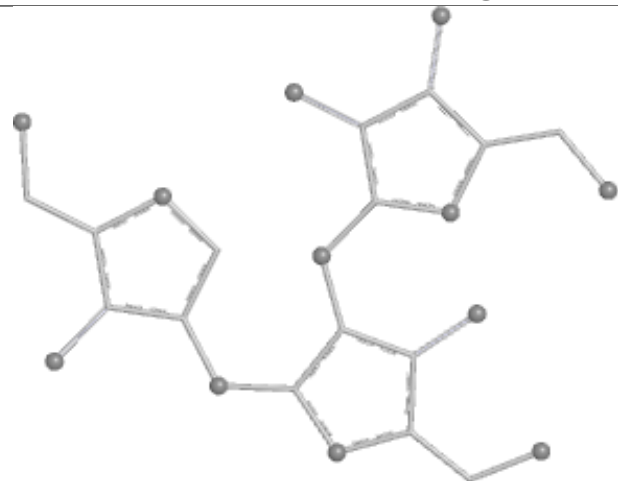
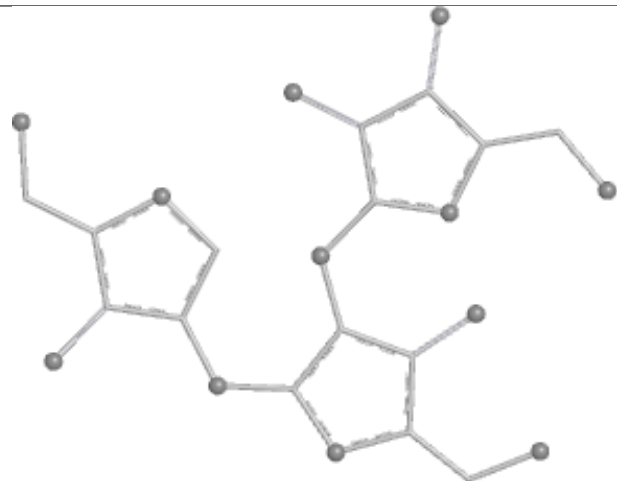
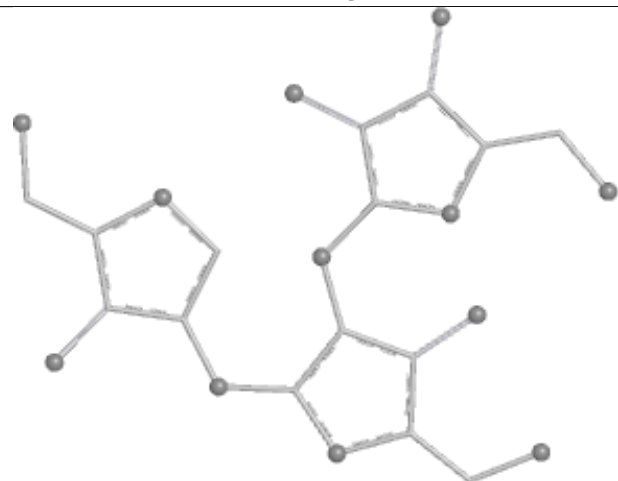
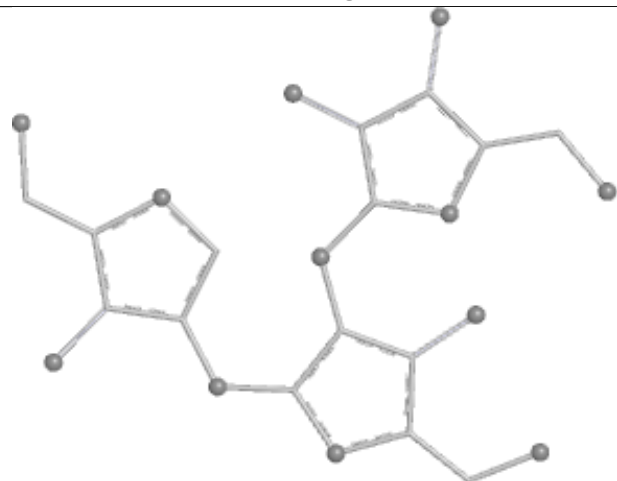
Oligosaccharide Chain NA

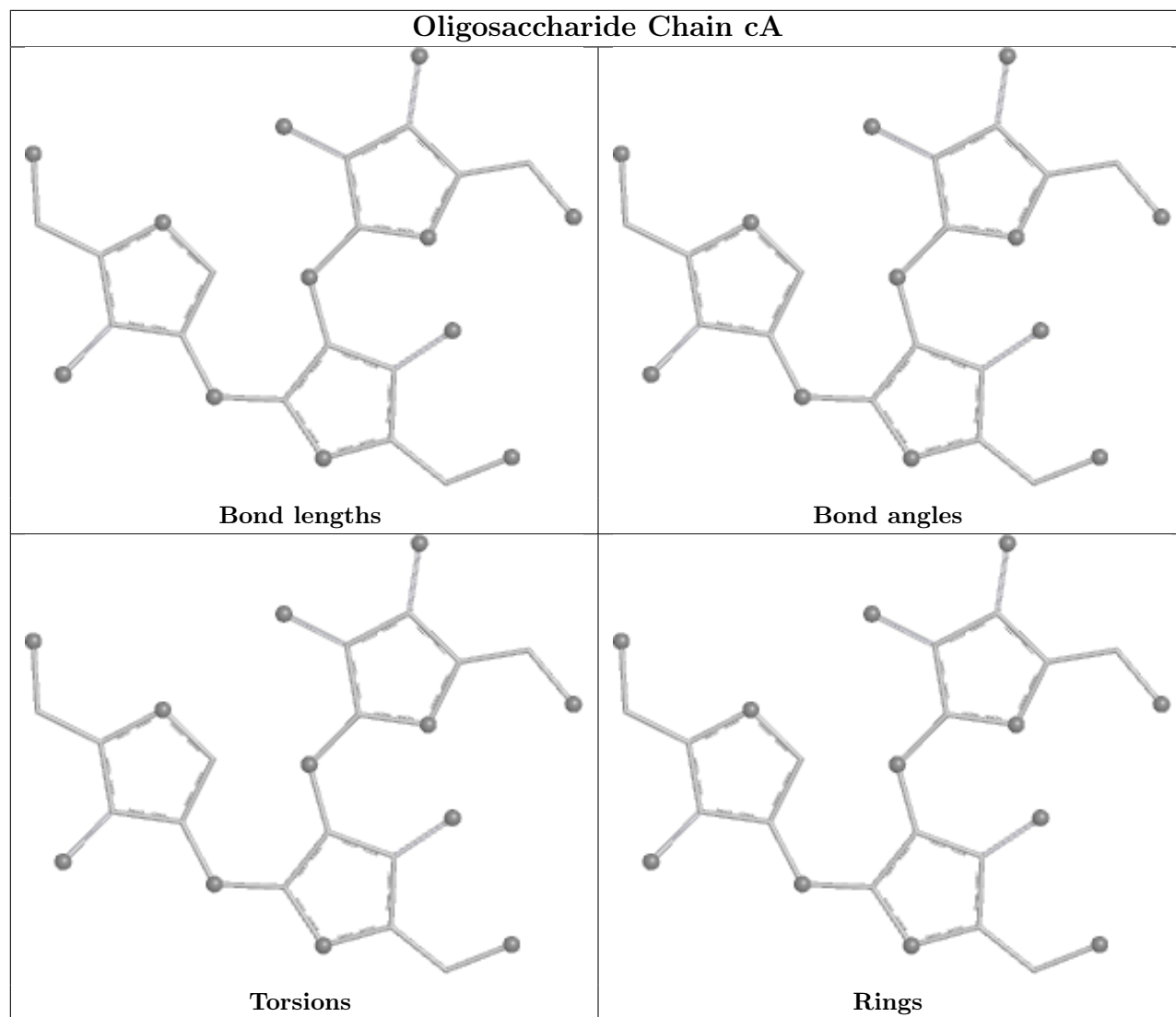
Oligosaccharide Chain OA

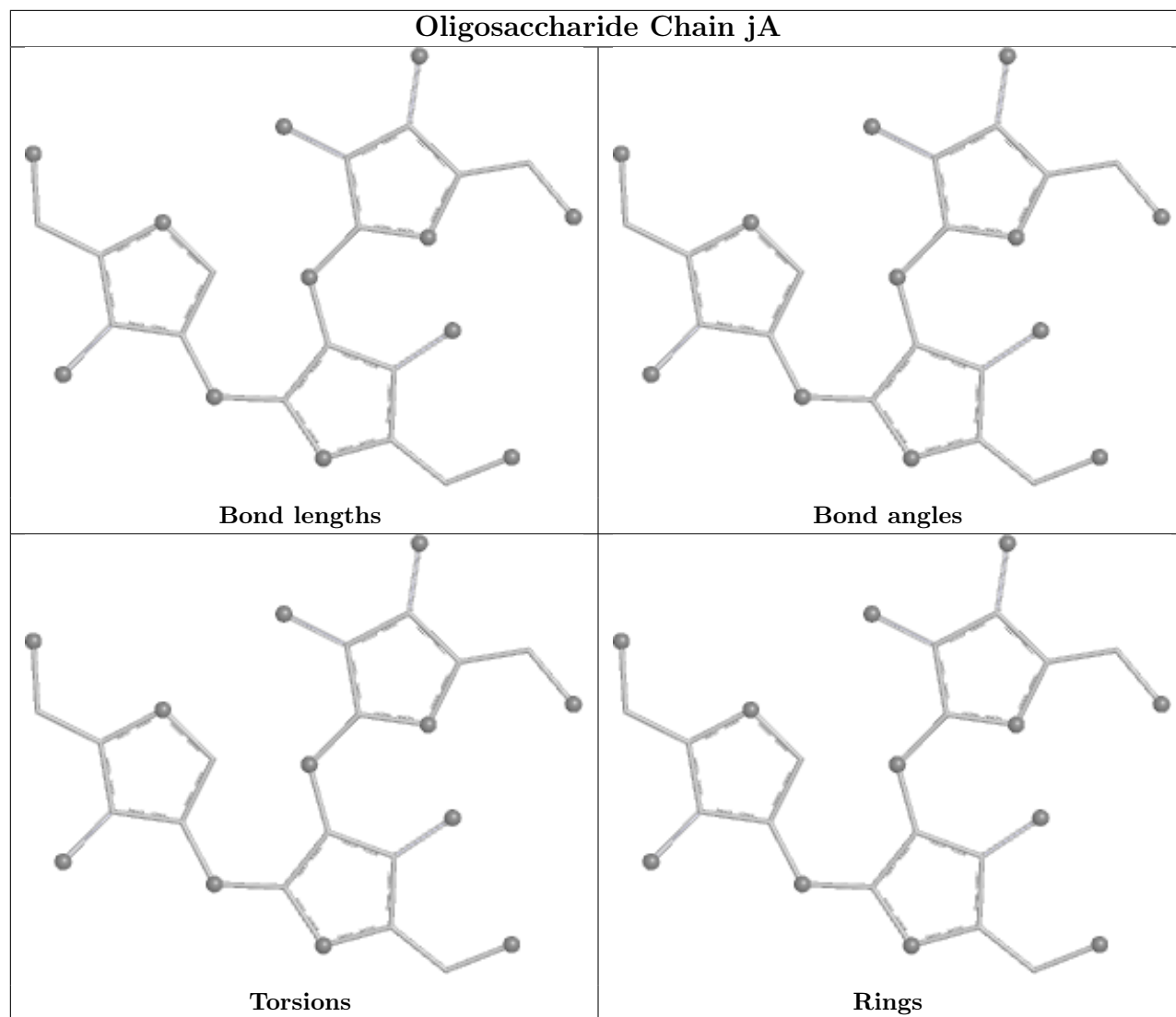


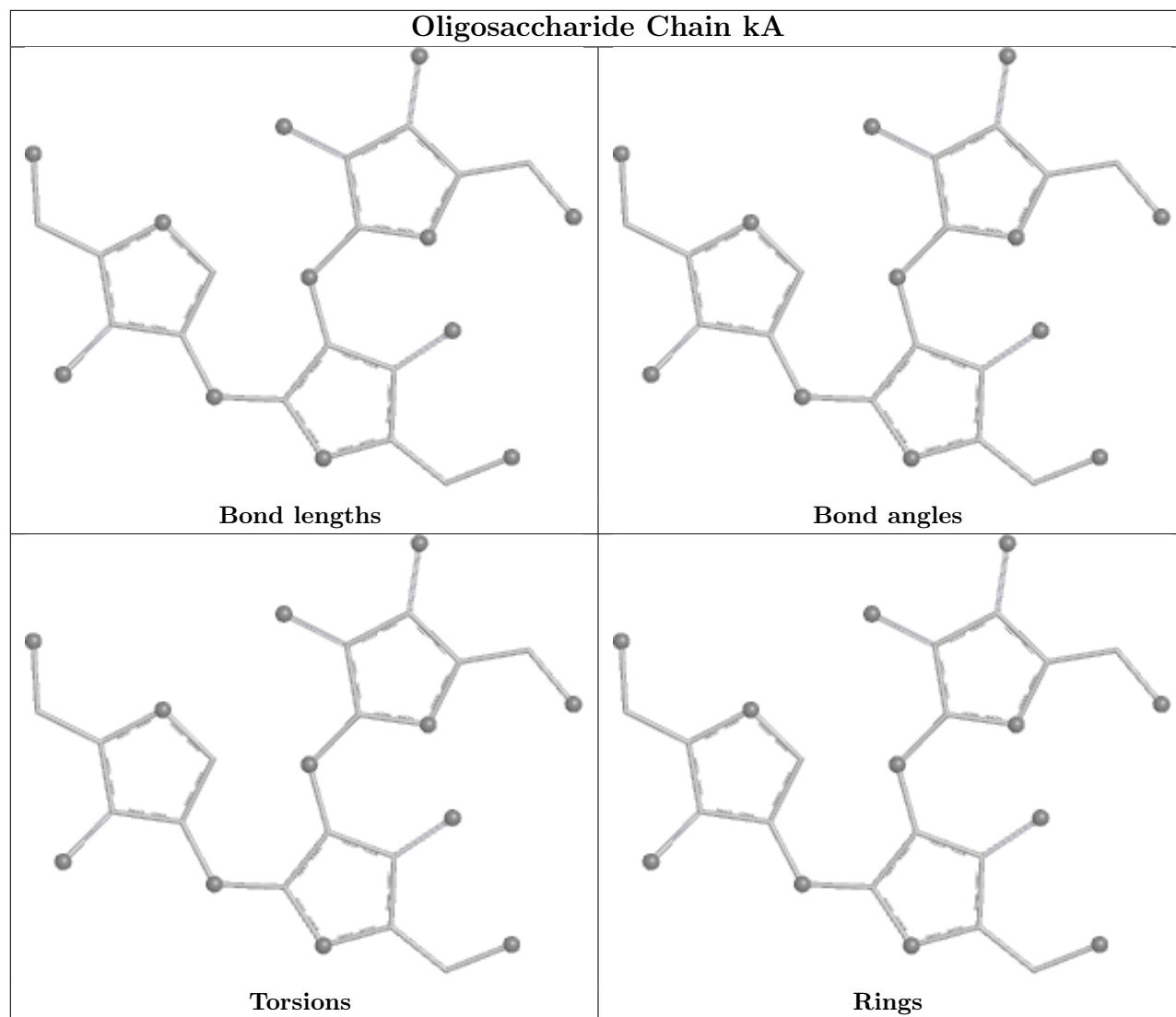
Oligosaccharide Chain TA

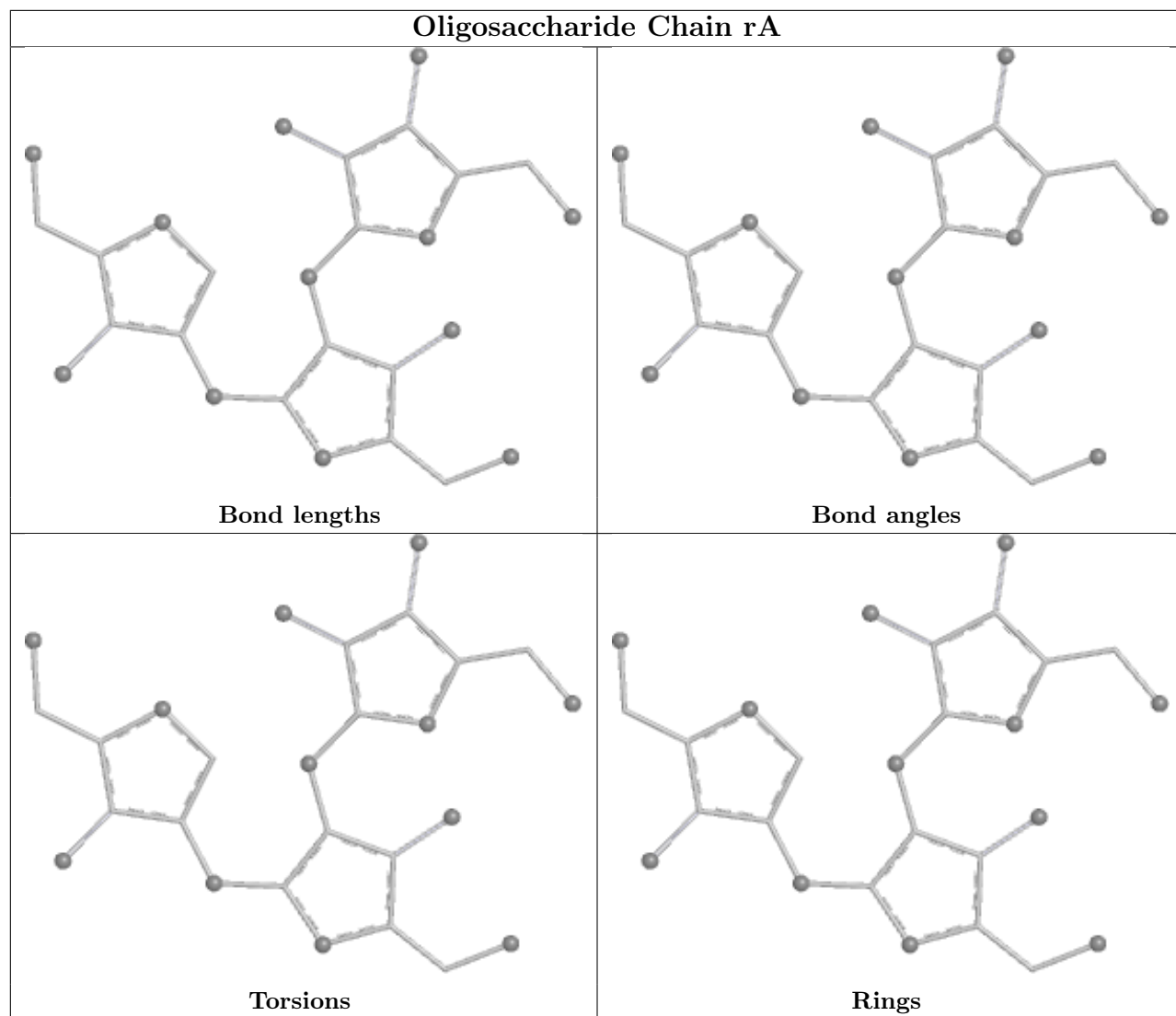
Oligosaccharide Chain XA**Bond lengths****Bond angles****Torsions****Rings**

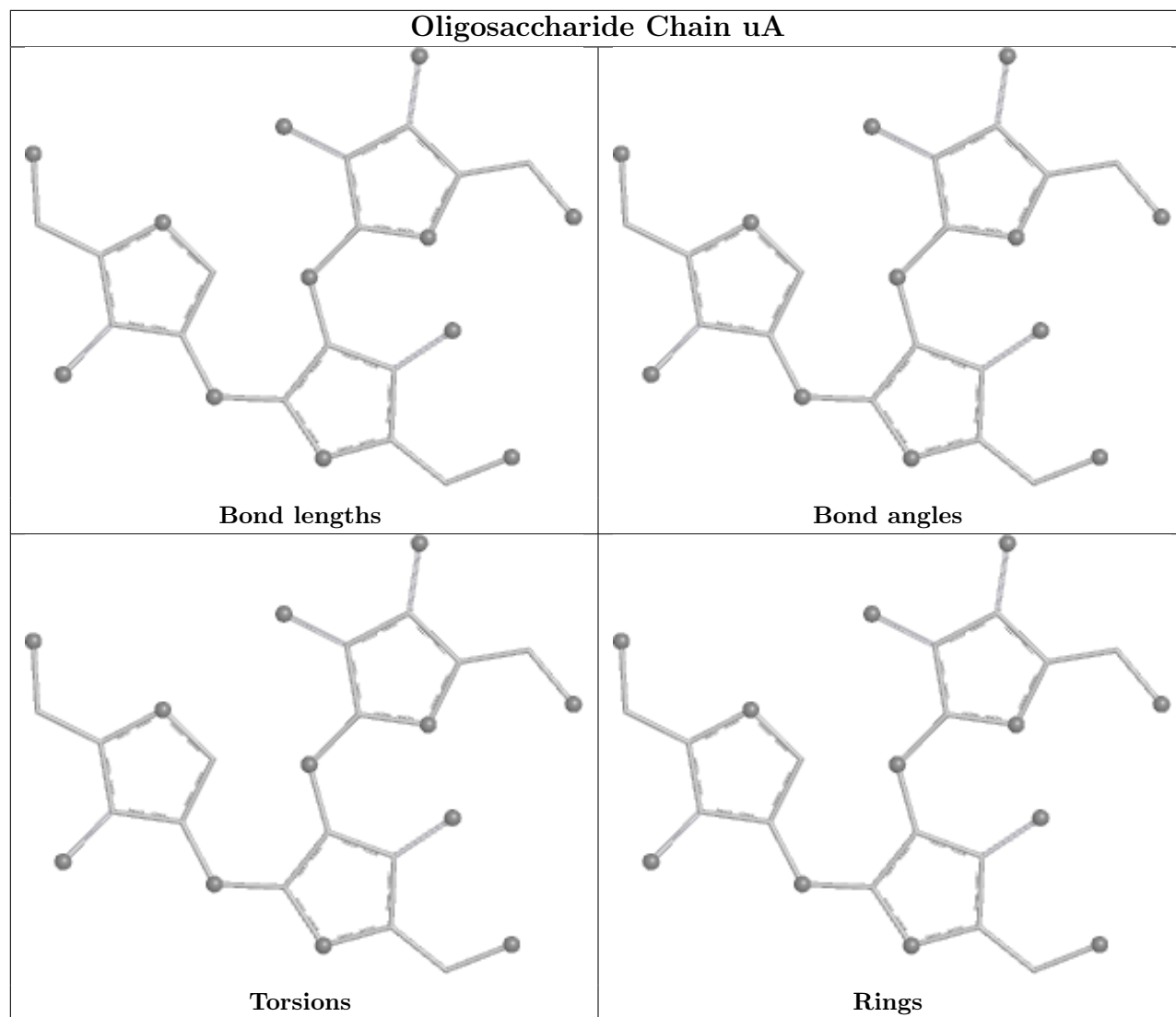
Oligosaccharide Chain ZA**Bond lengths****Bond angles****Torsions****Rings**

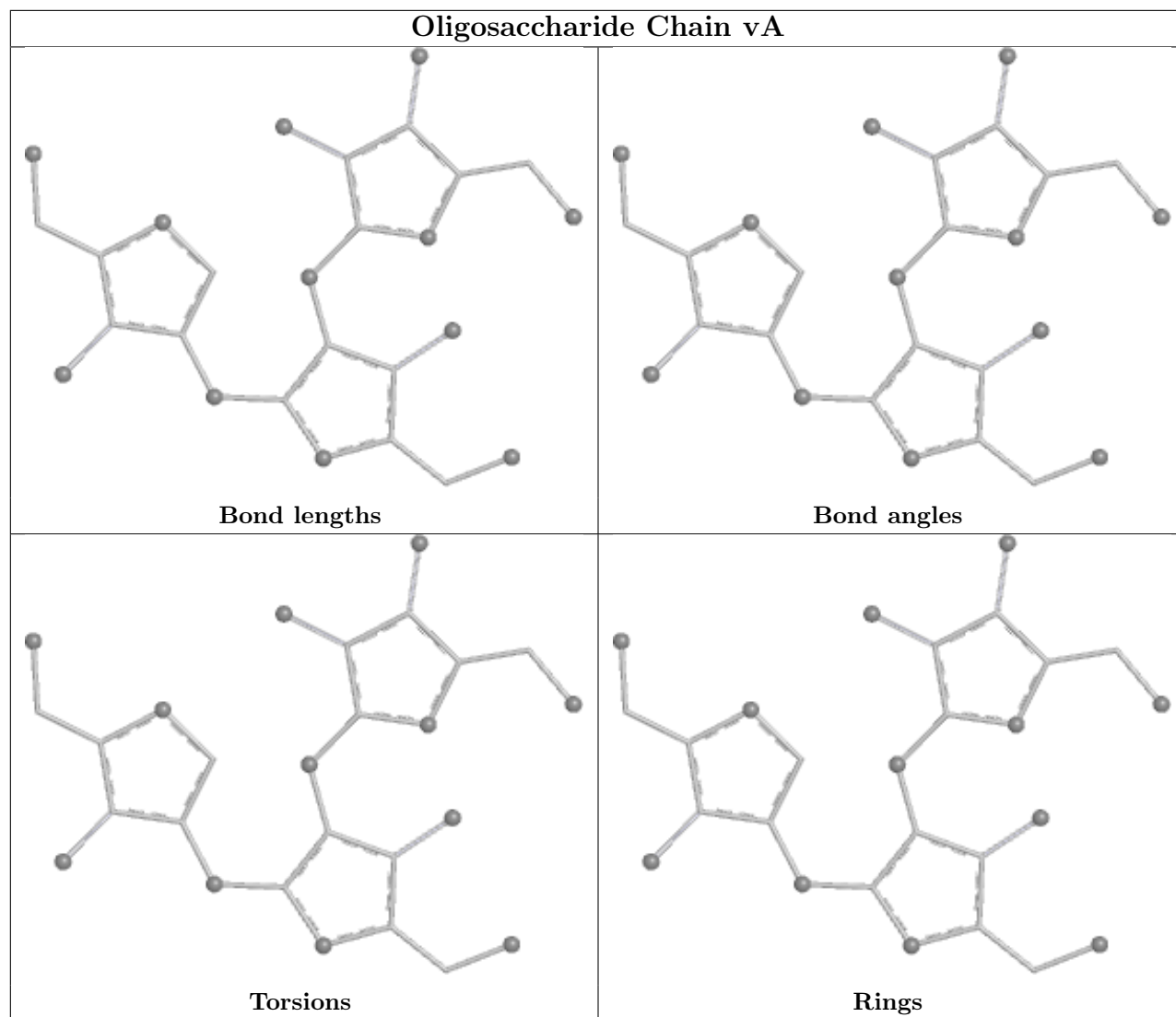


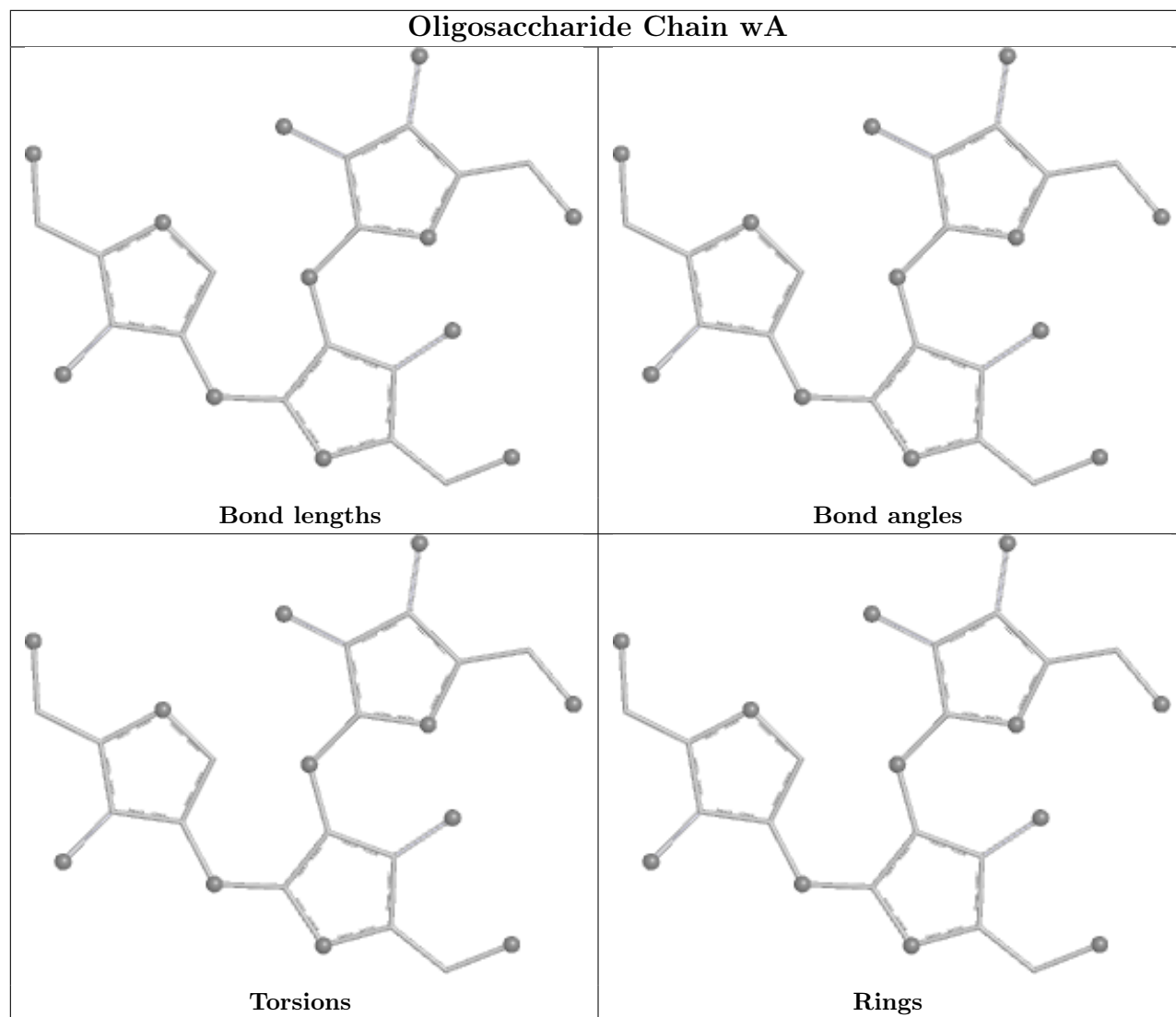


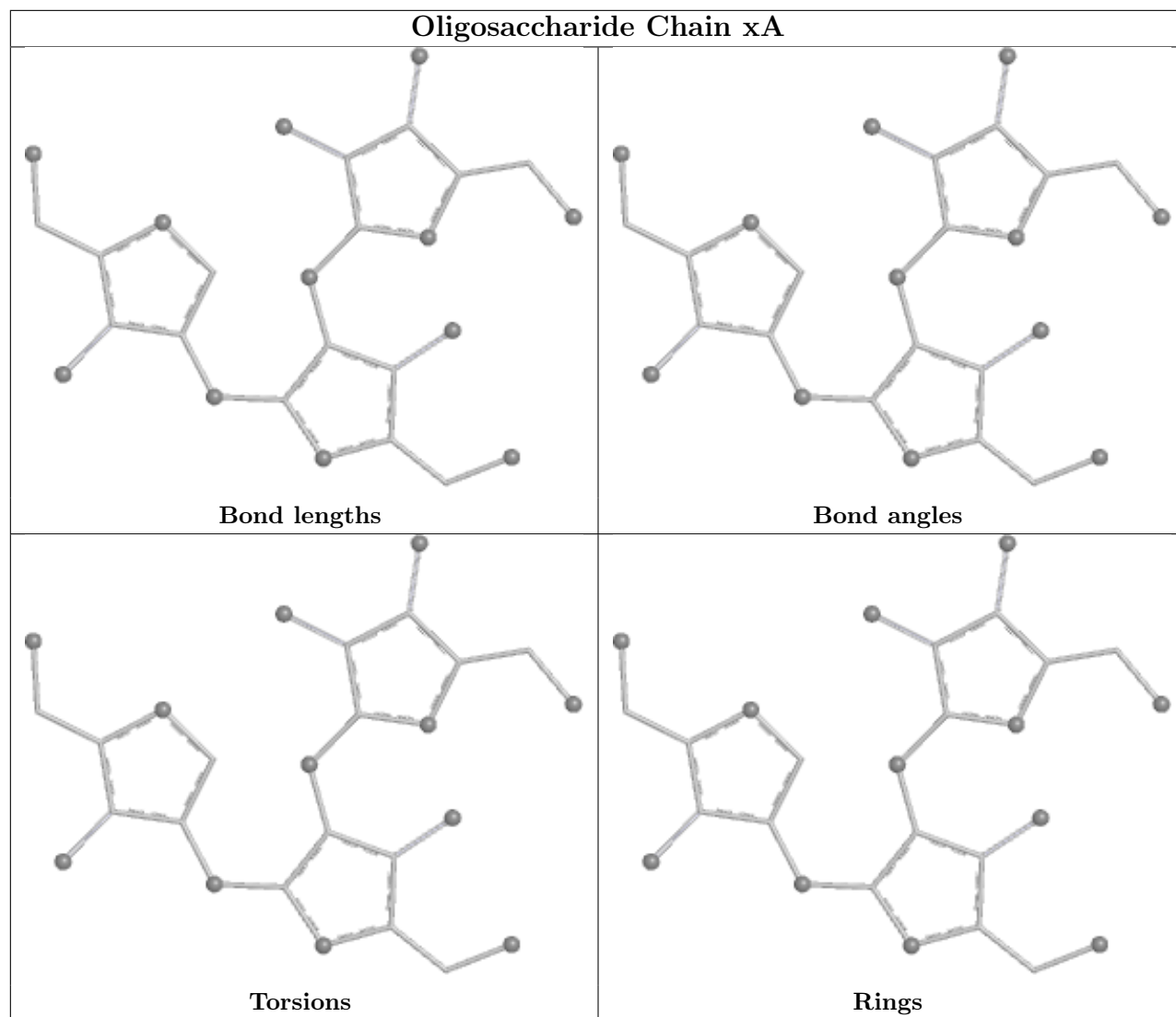




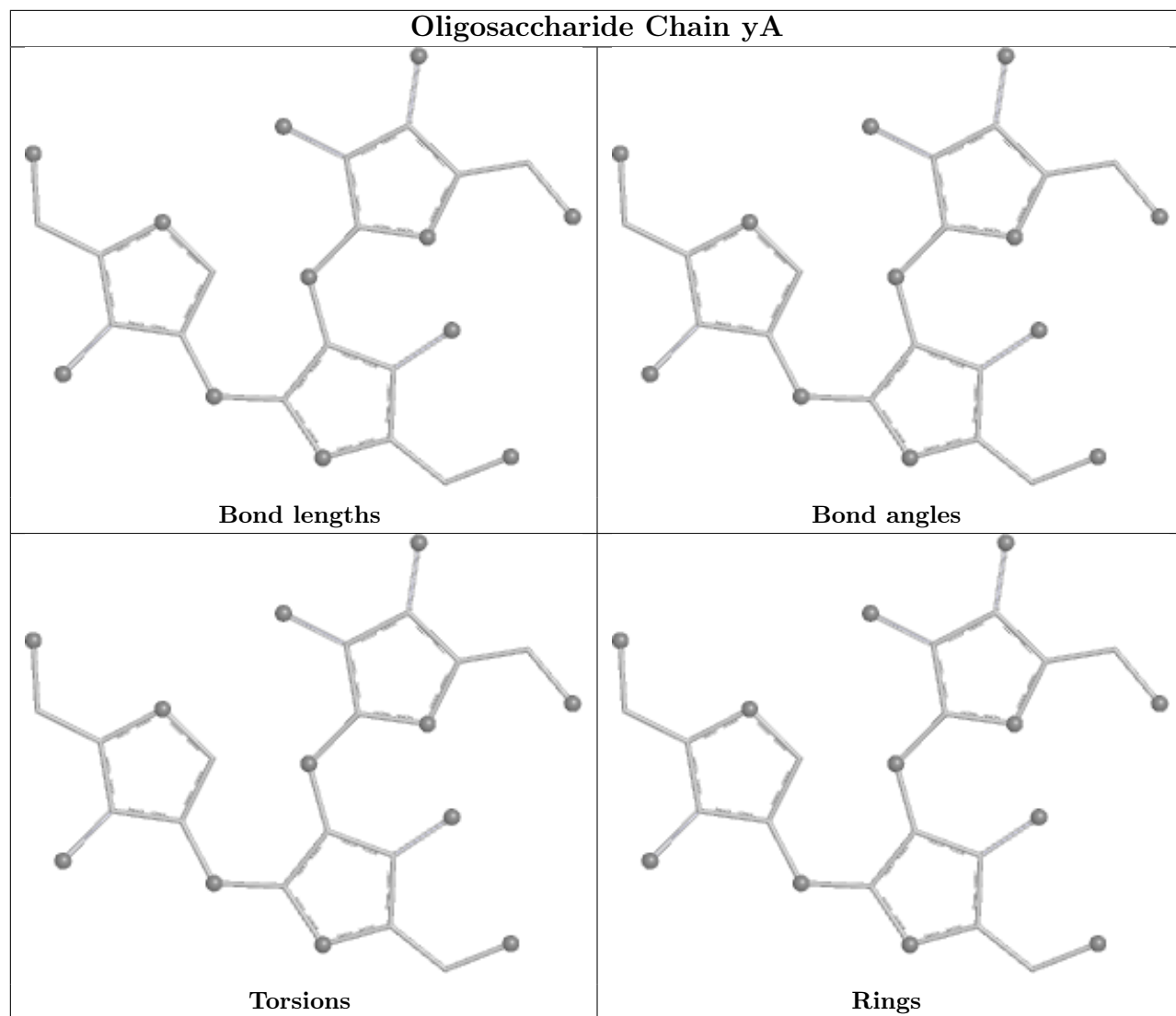




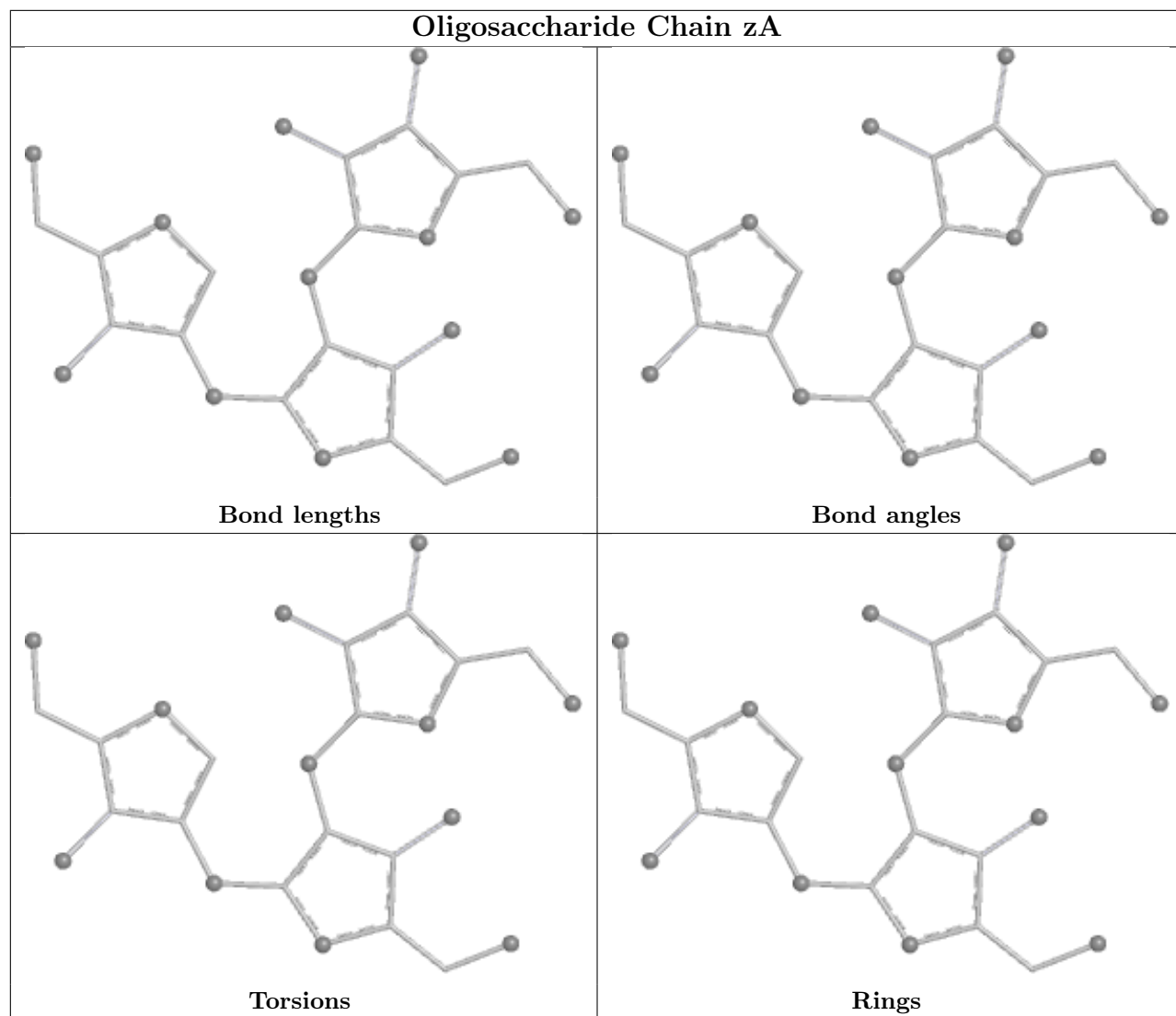




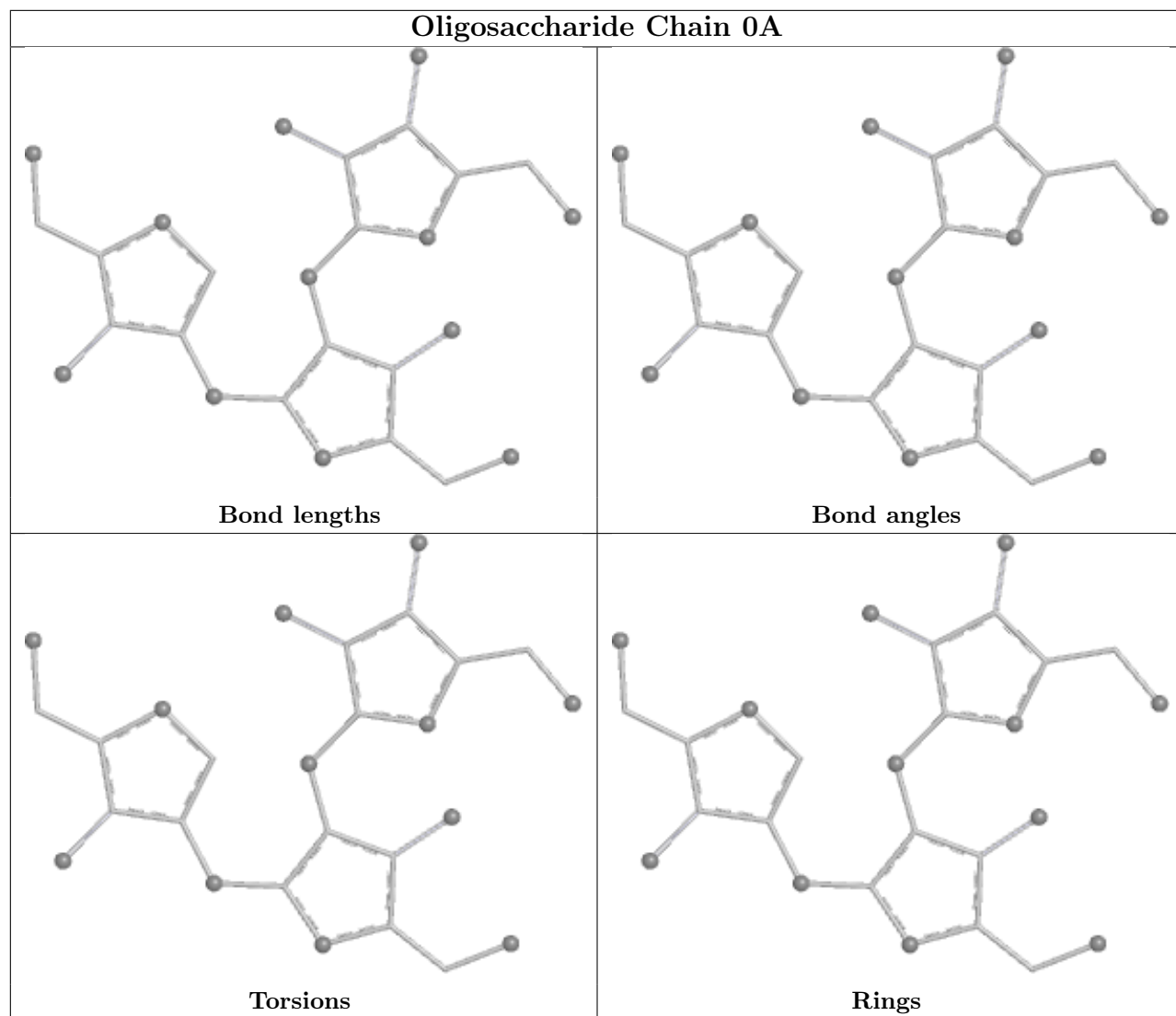
Oligosaccharide Chain yA

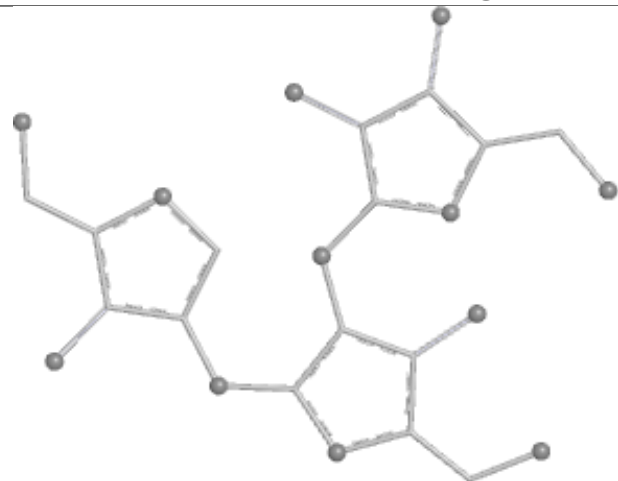
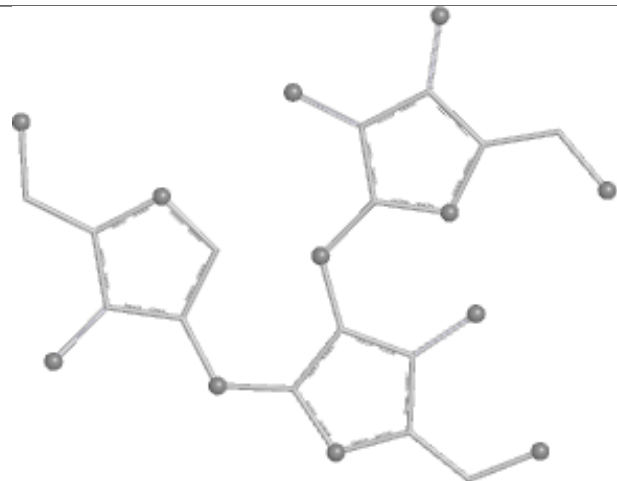
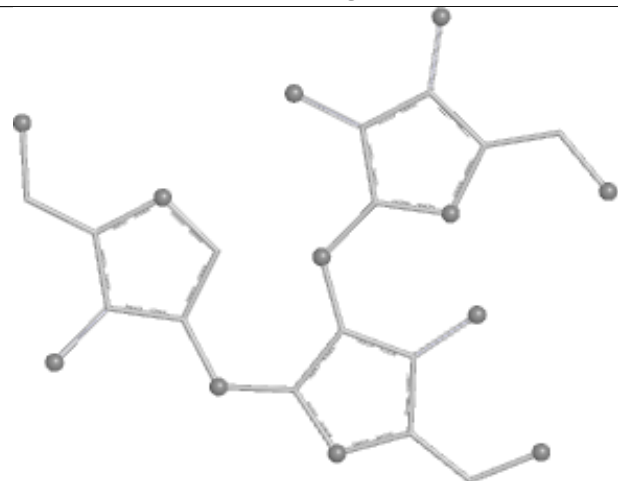
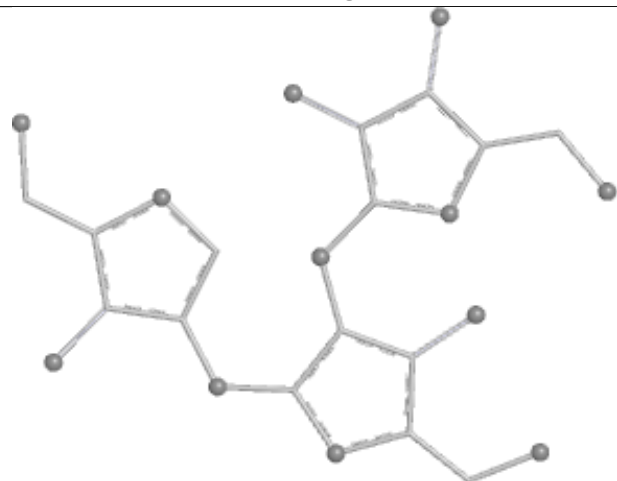


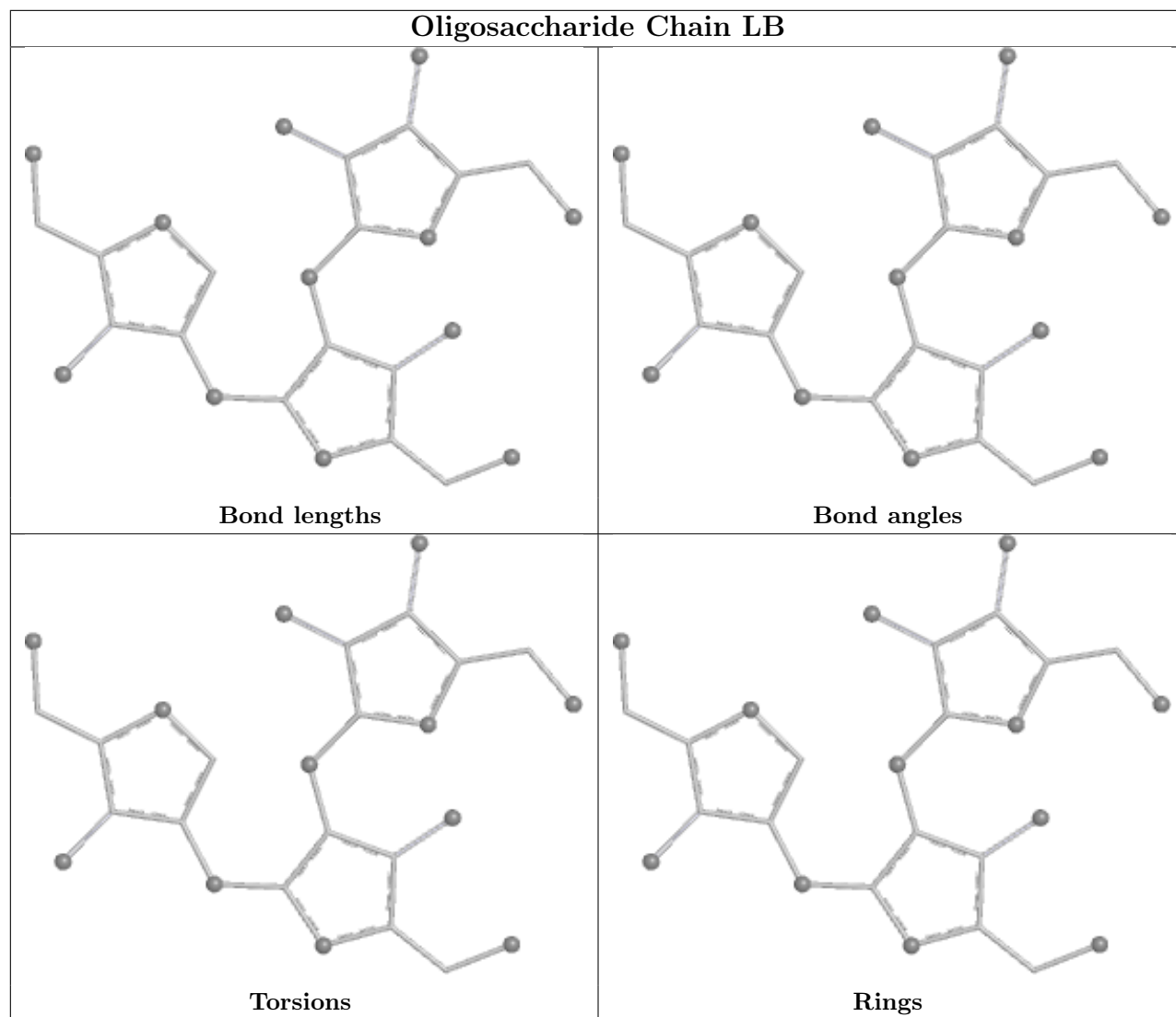
Oligosaccharide Chain zA

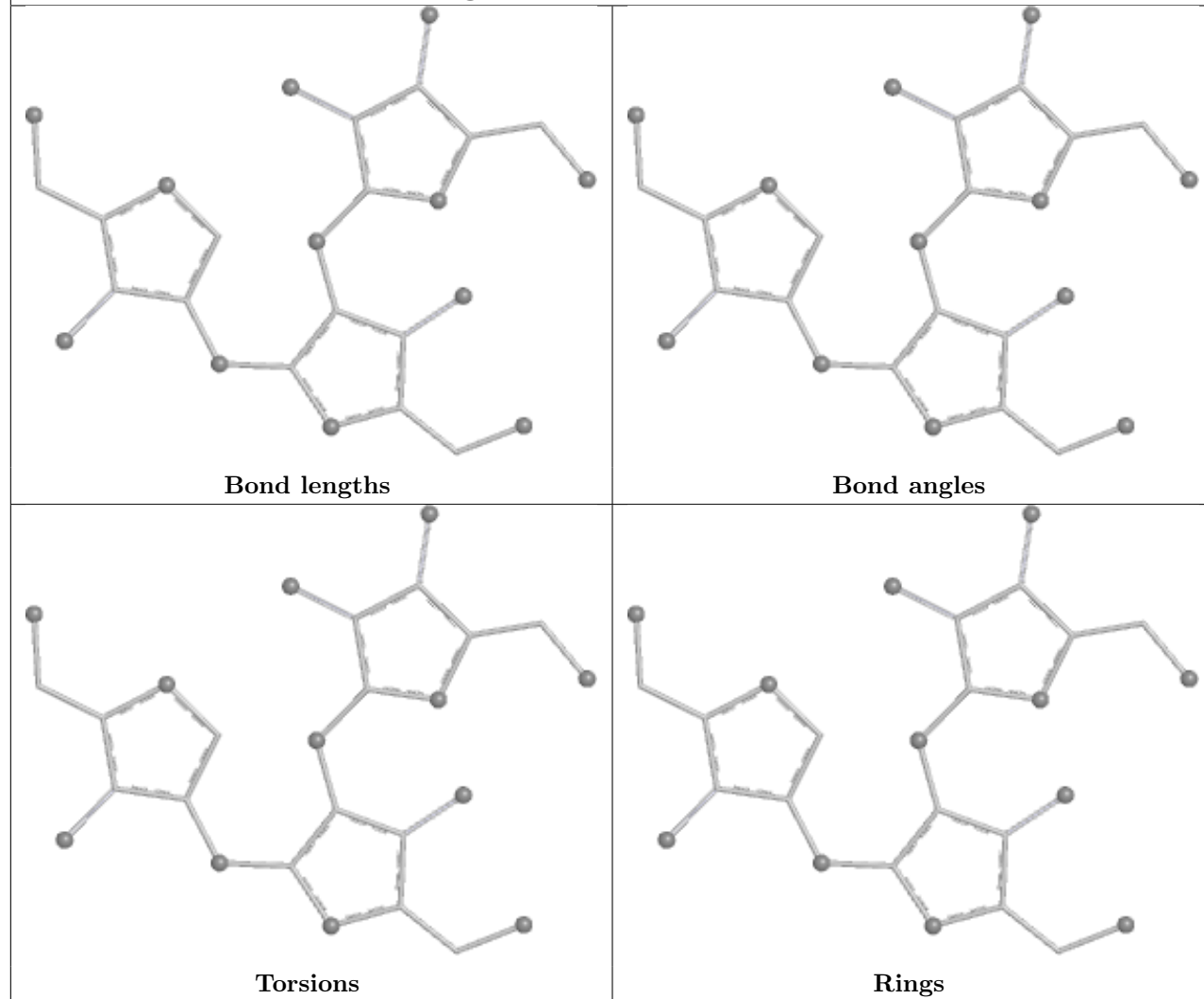


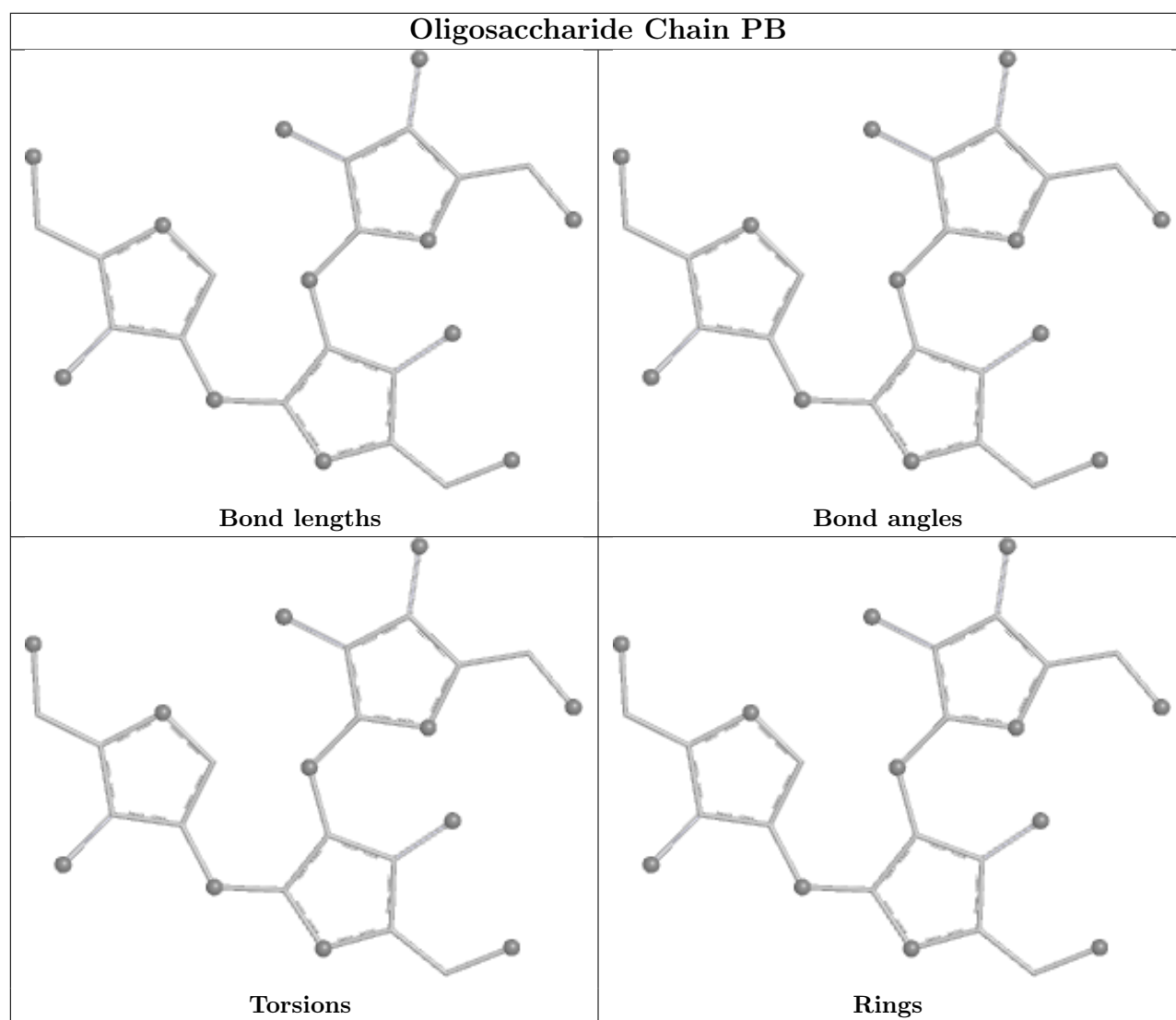
Oligosaccharide Chain 0A

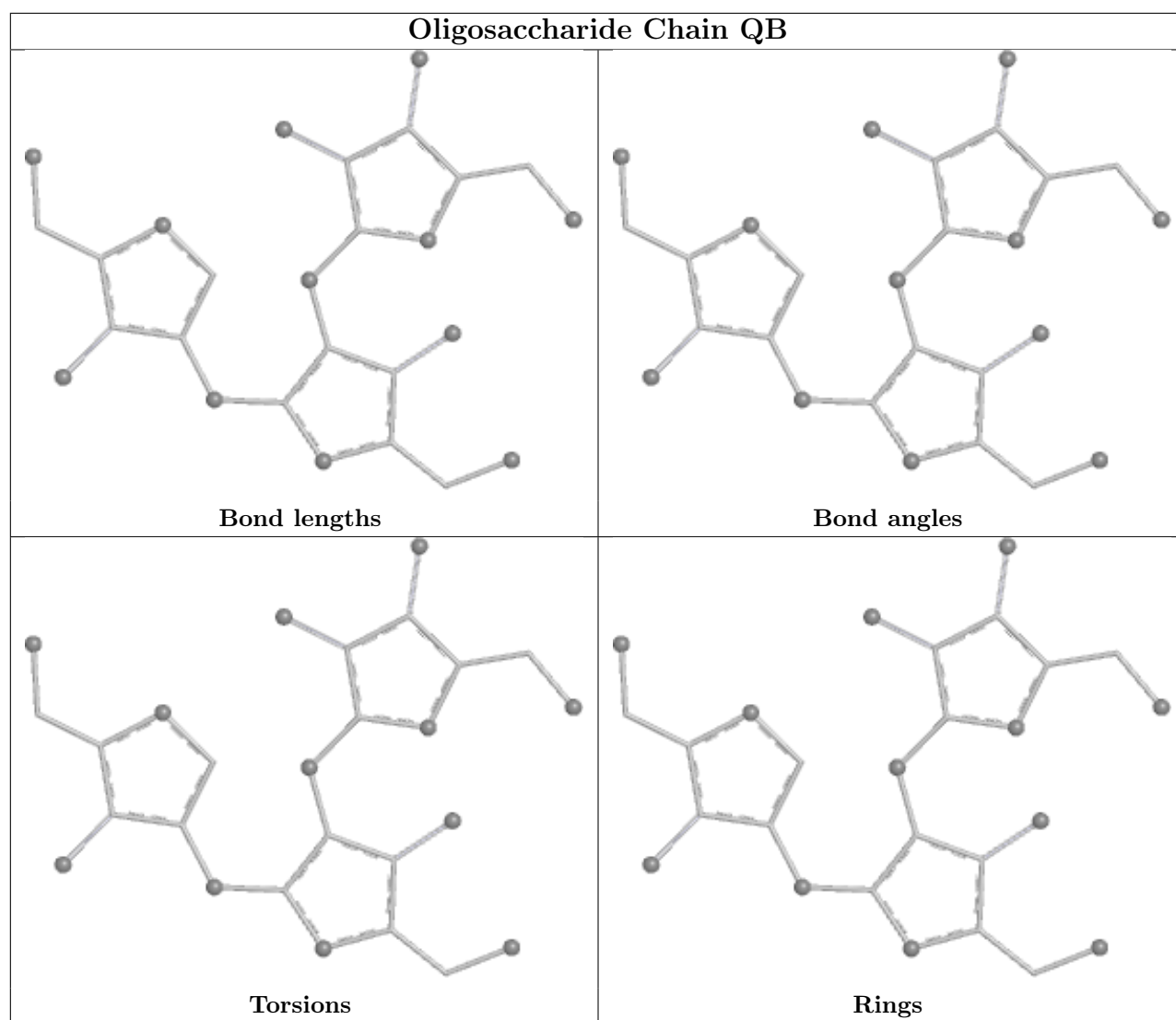


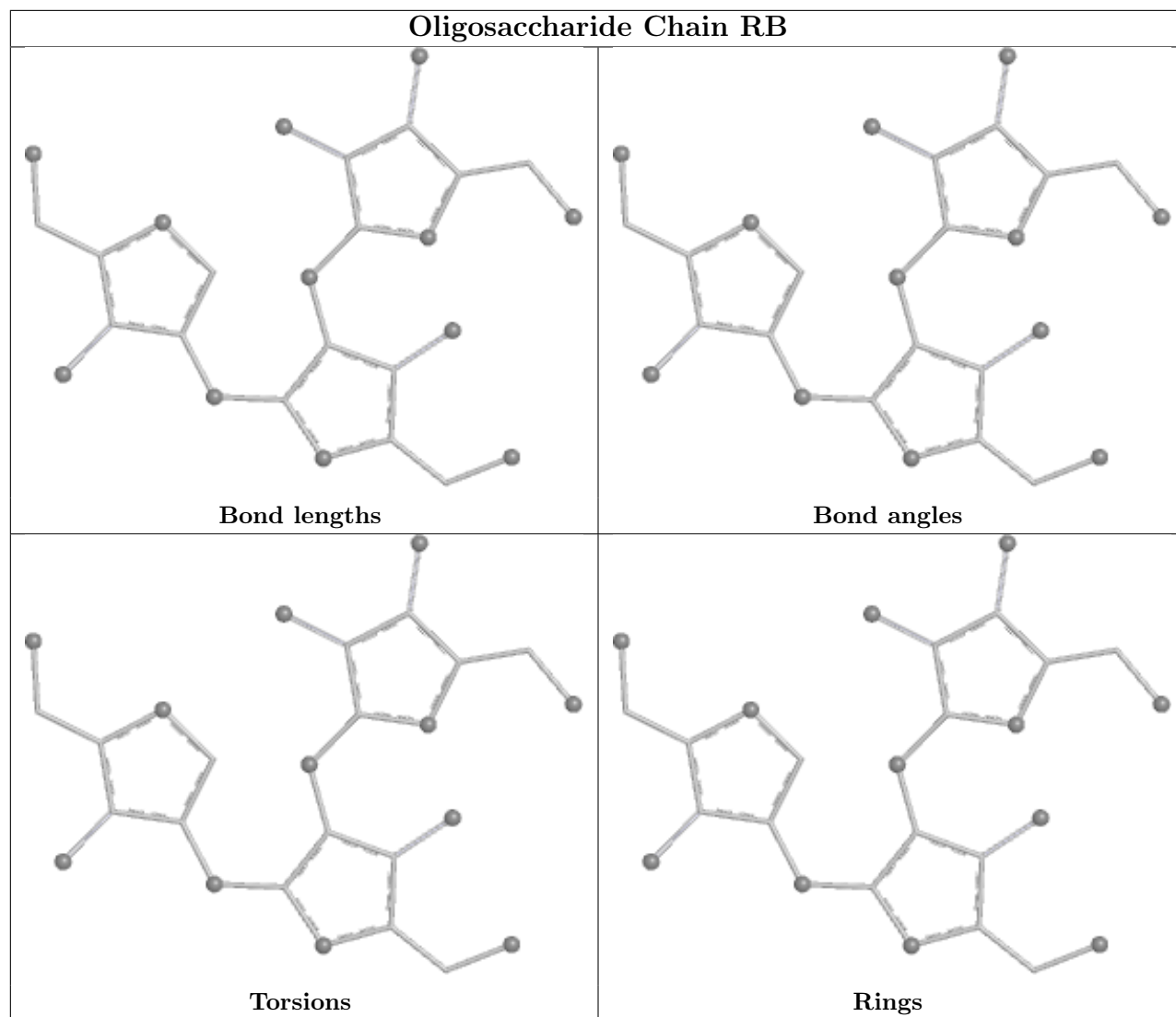
Oligosaccharide Chain EB**Bond lengths****Bond angles****Torsions****Rings**

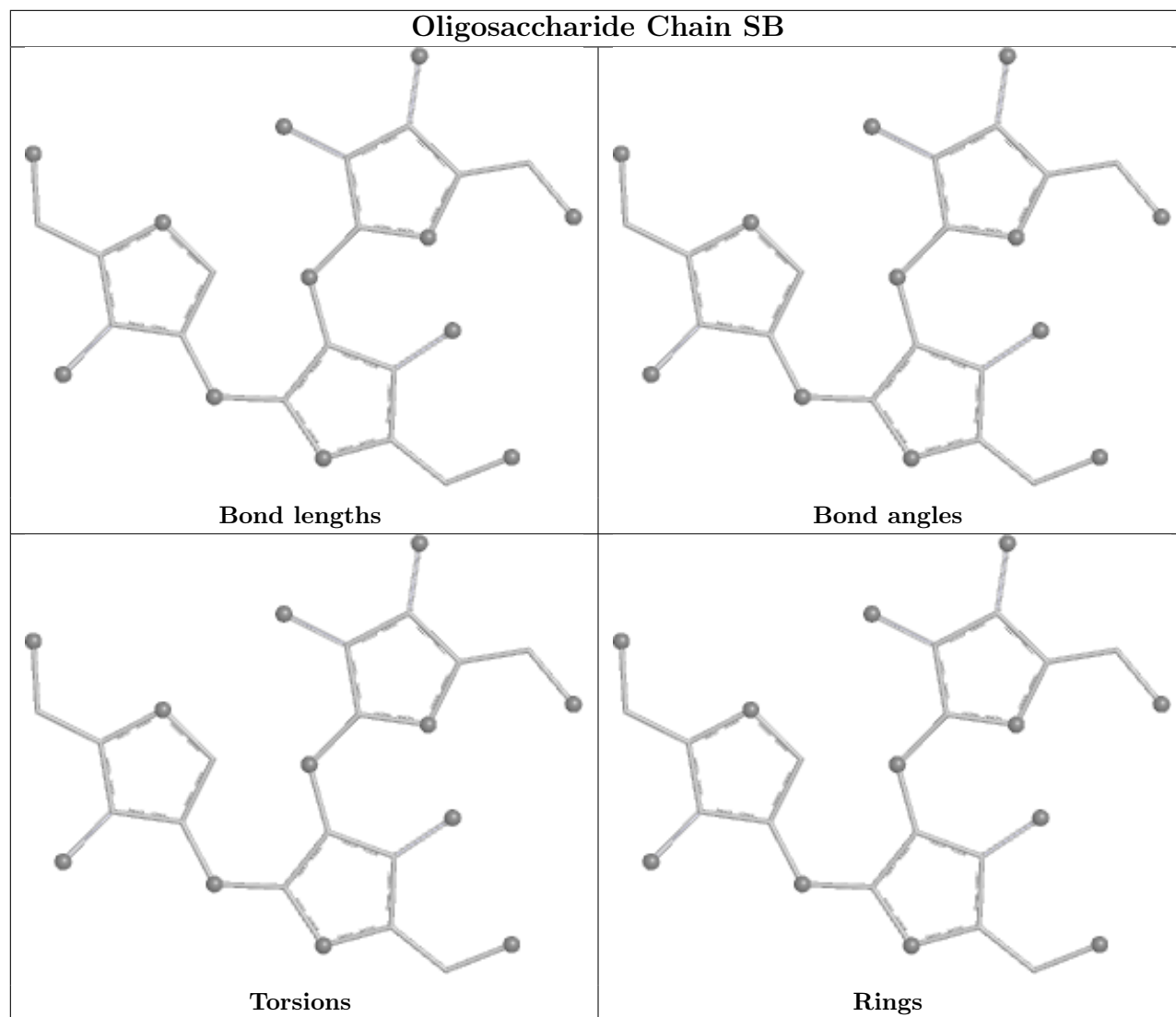


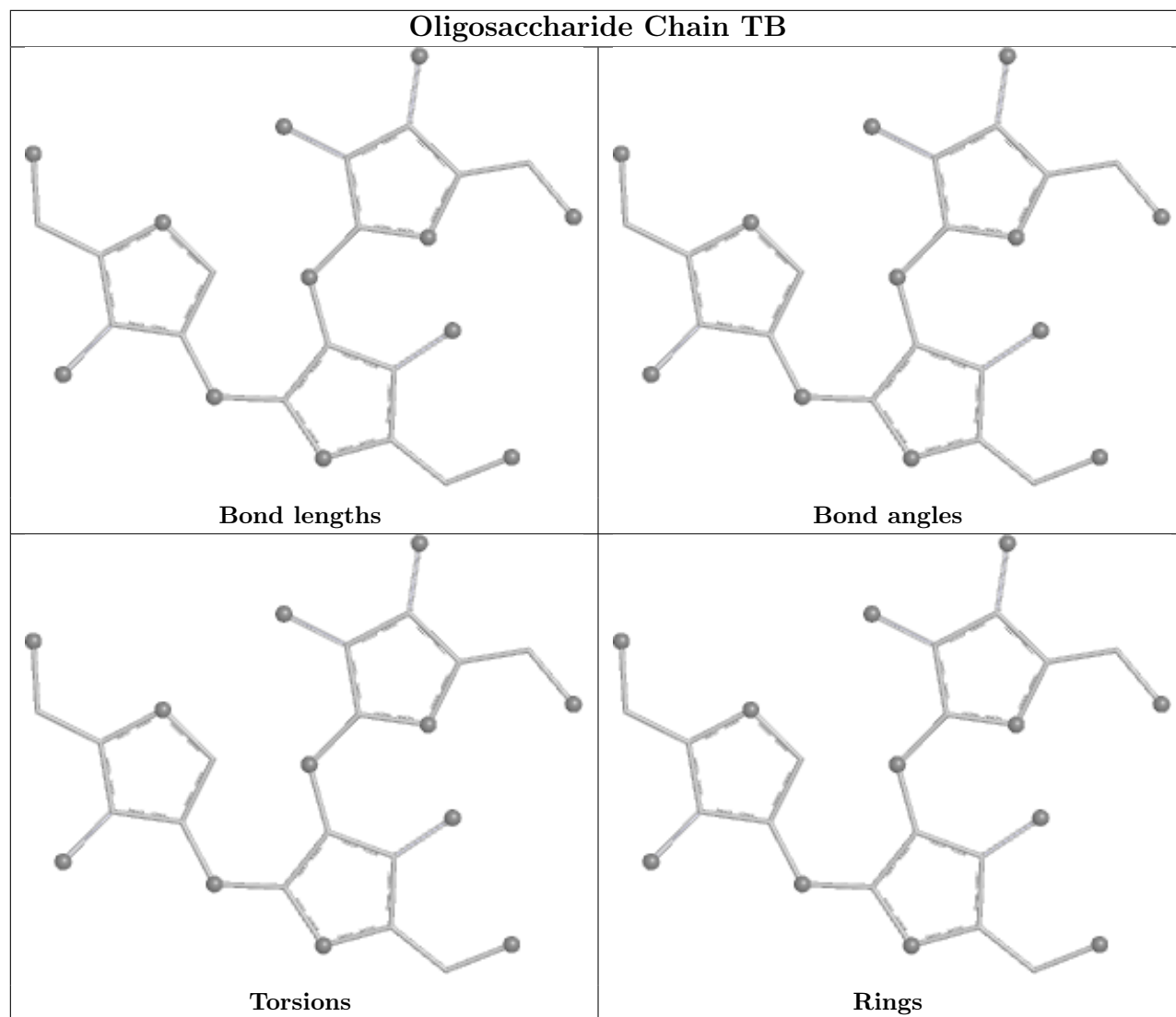
Oligosaccharide Chain OB

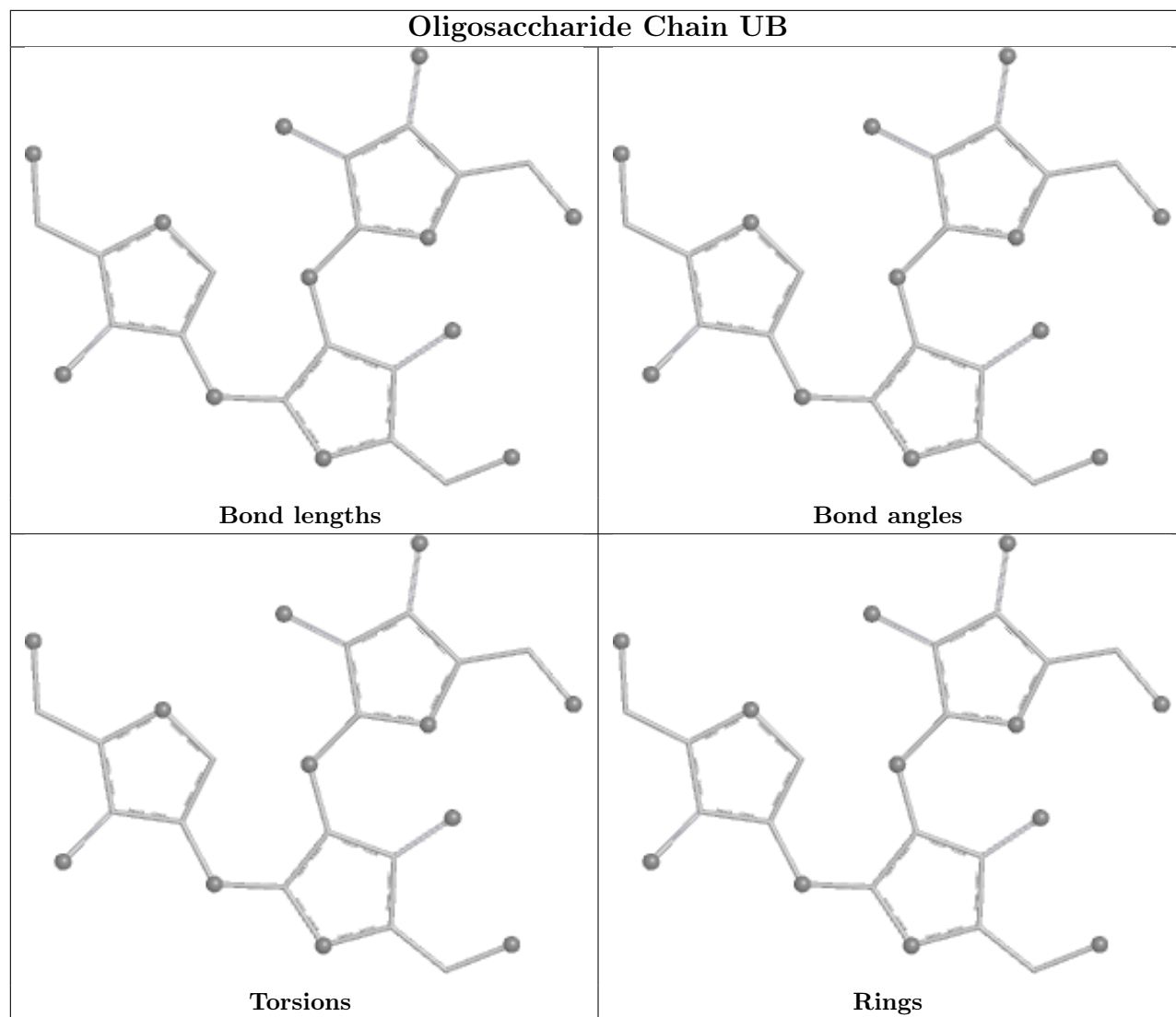


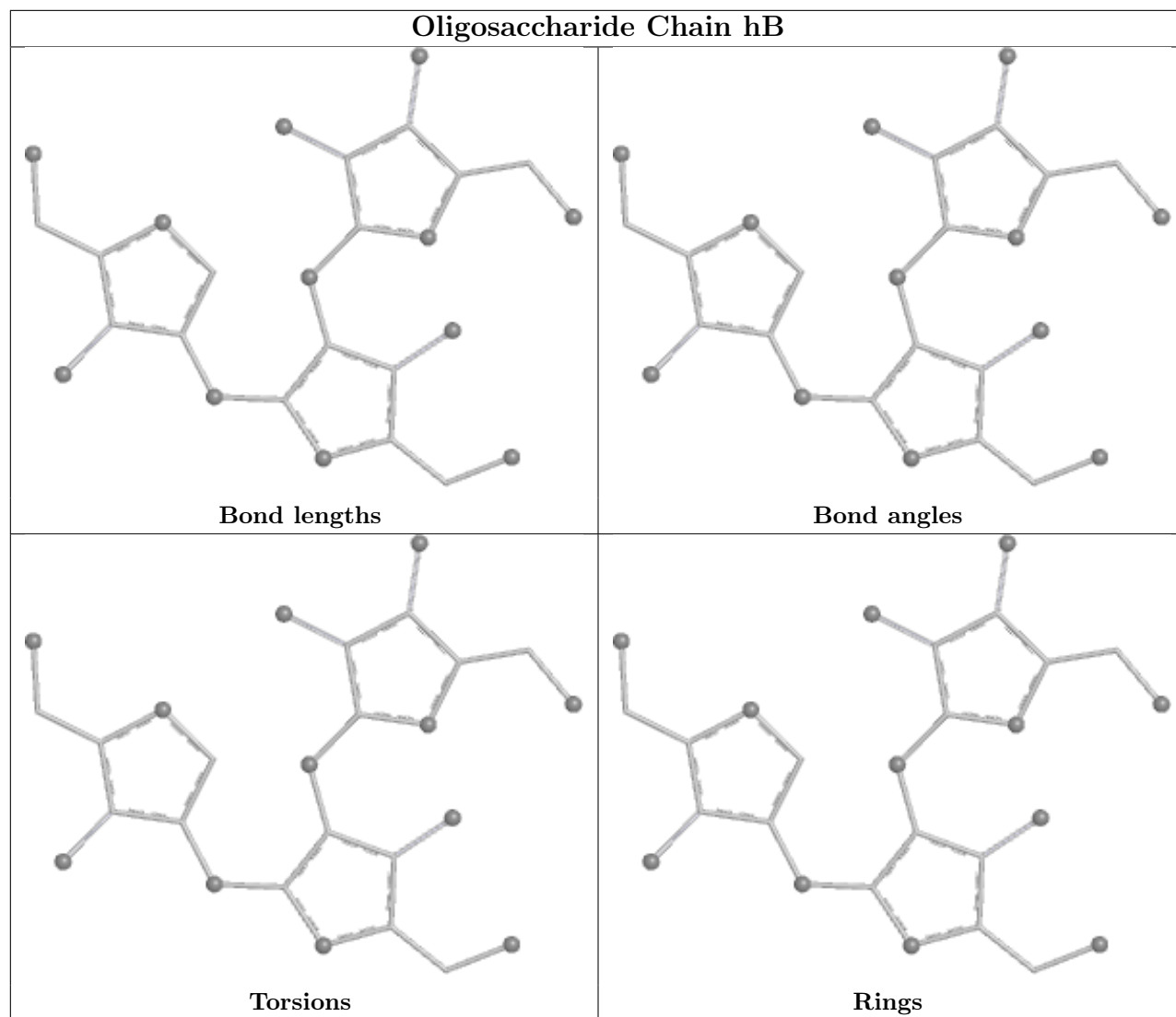


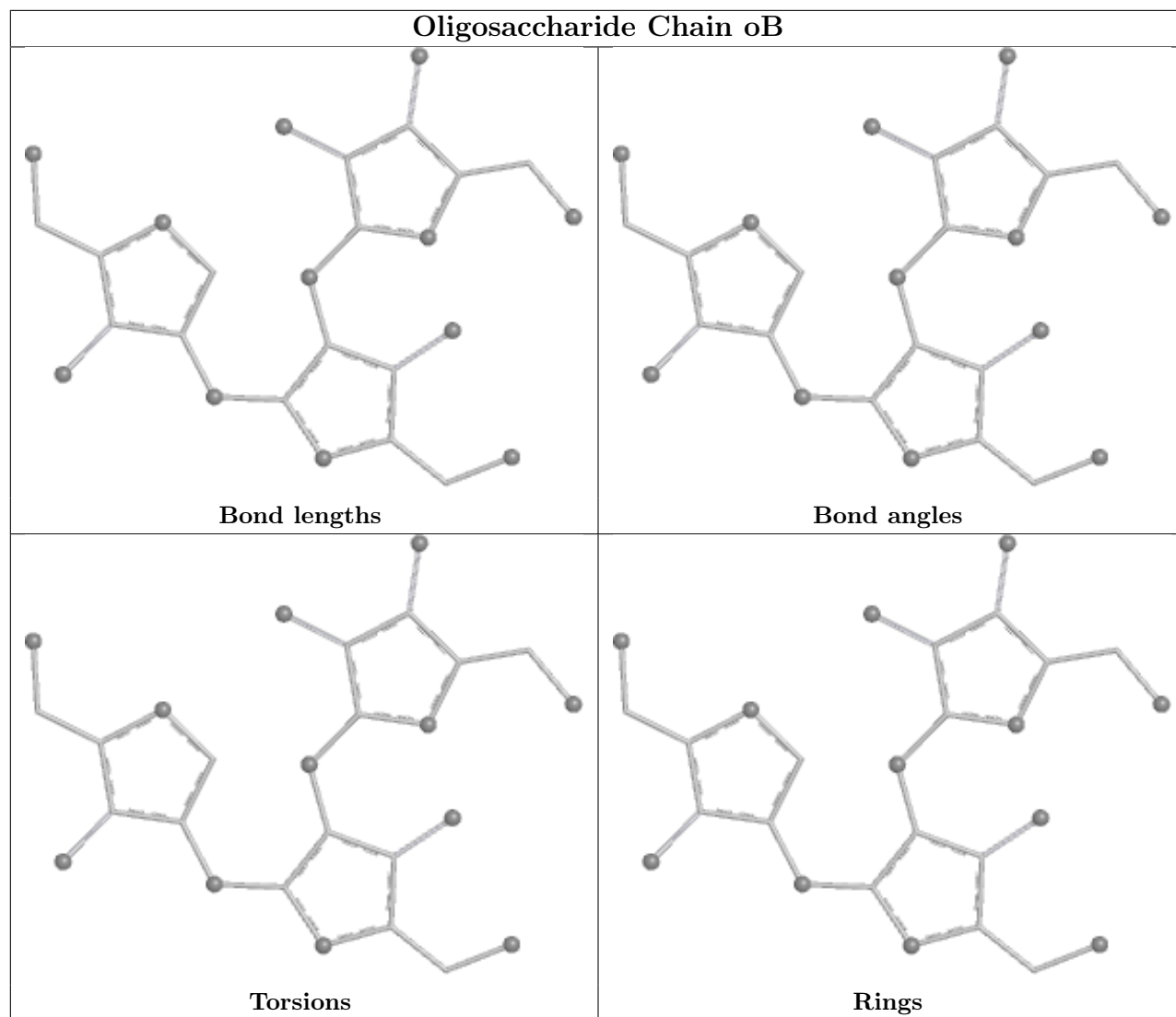


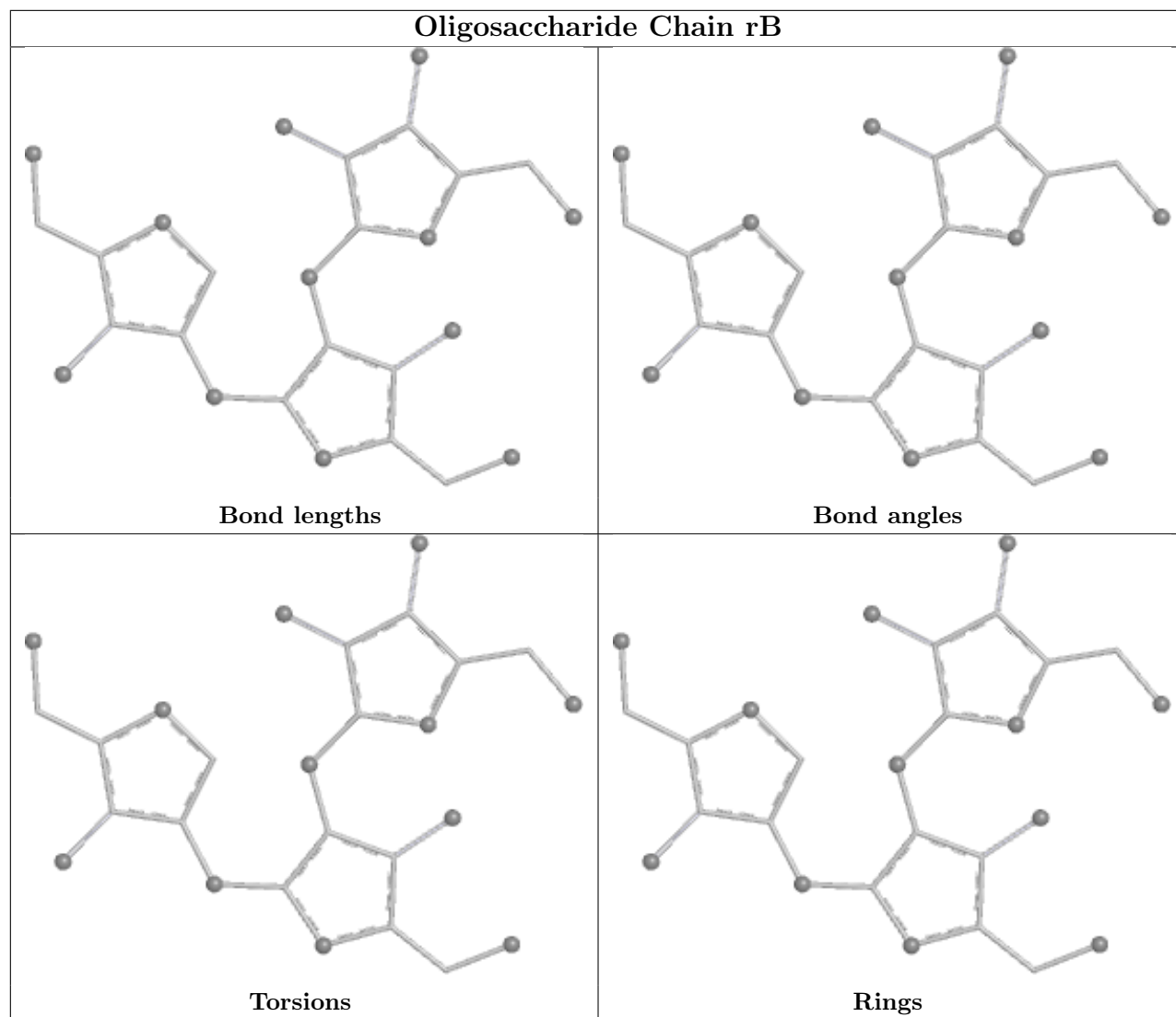


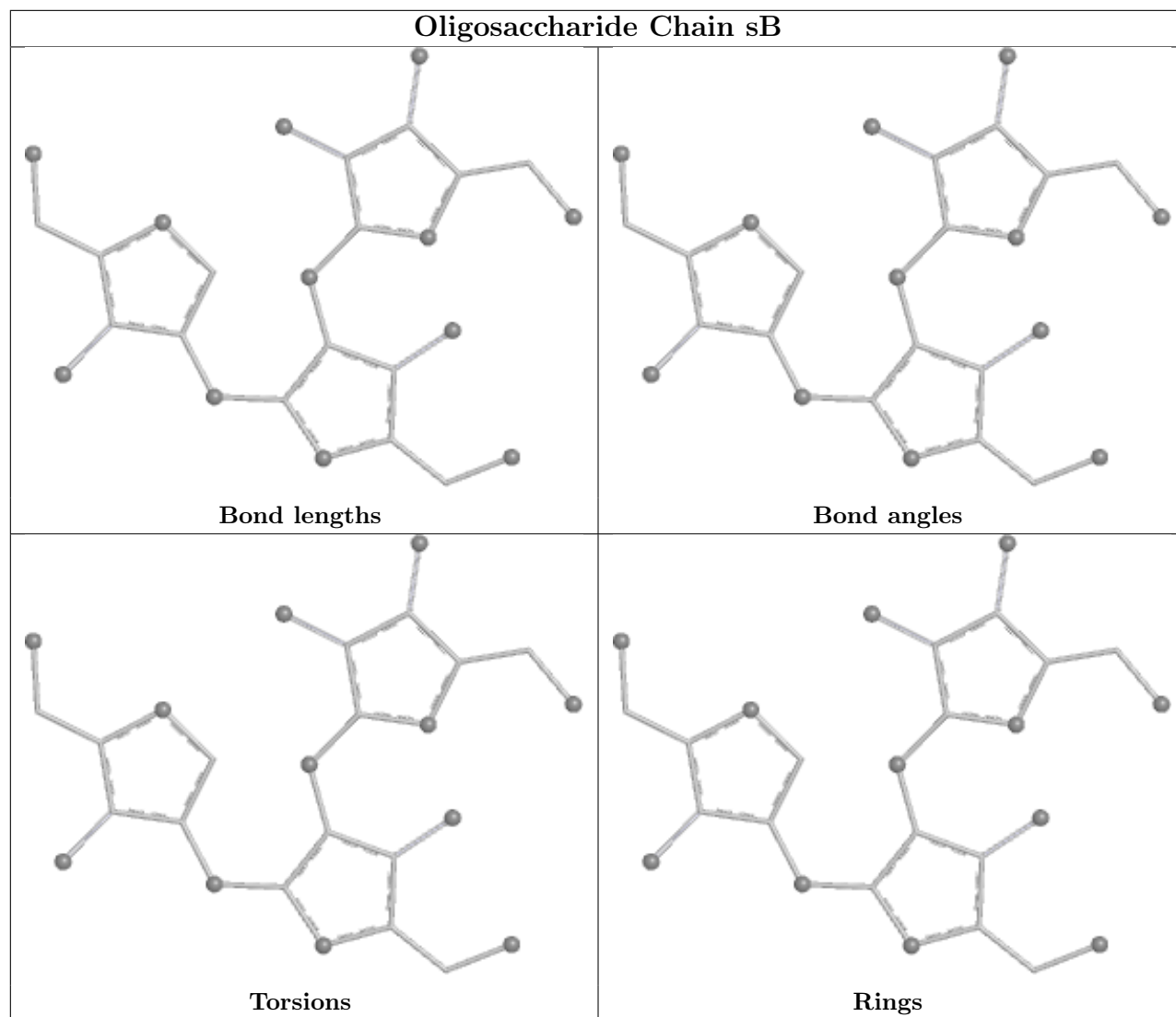


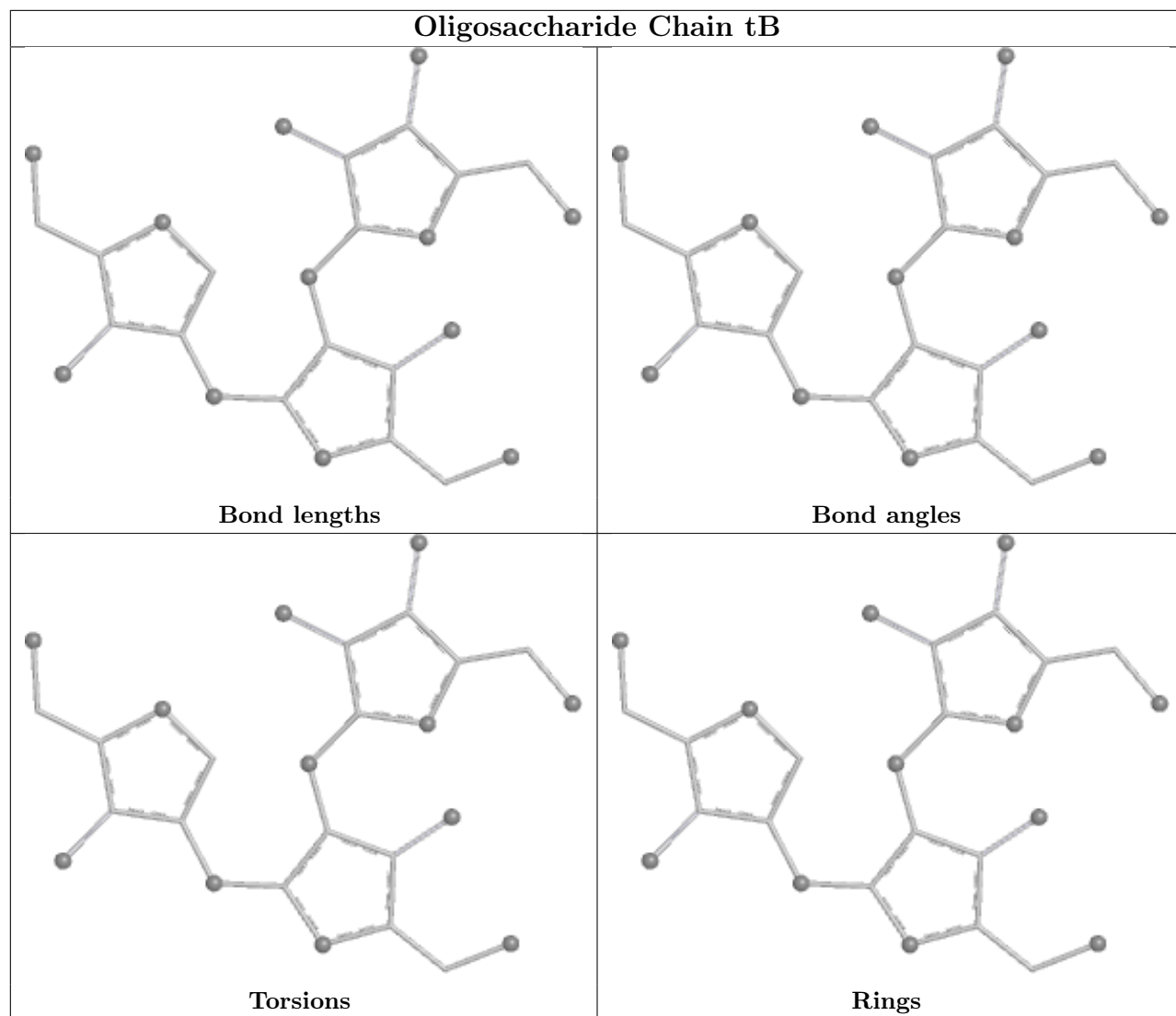


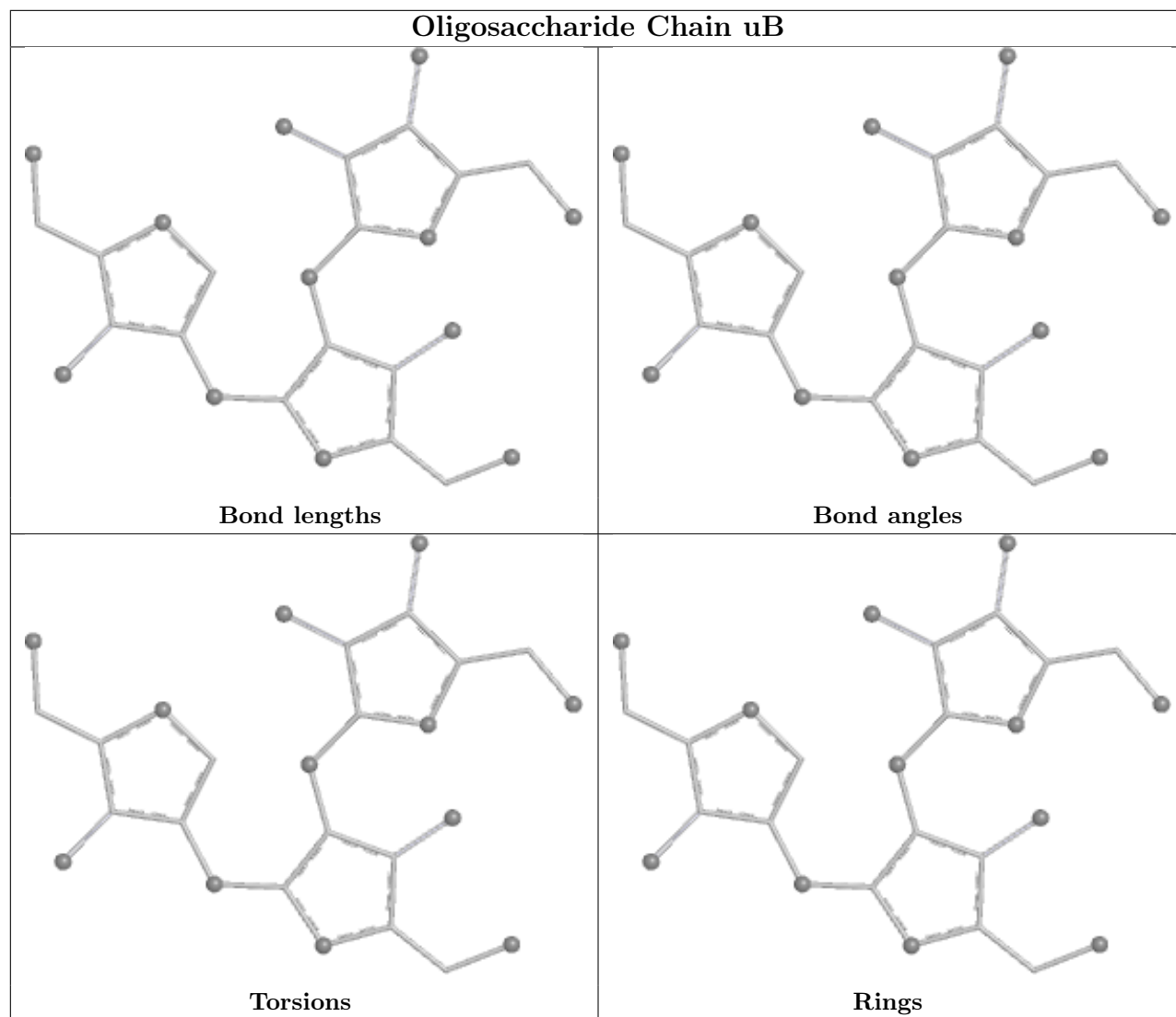


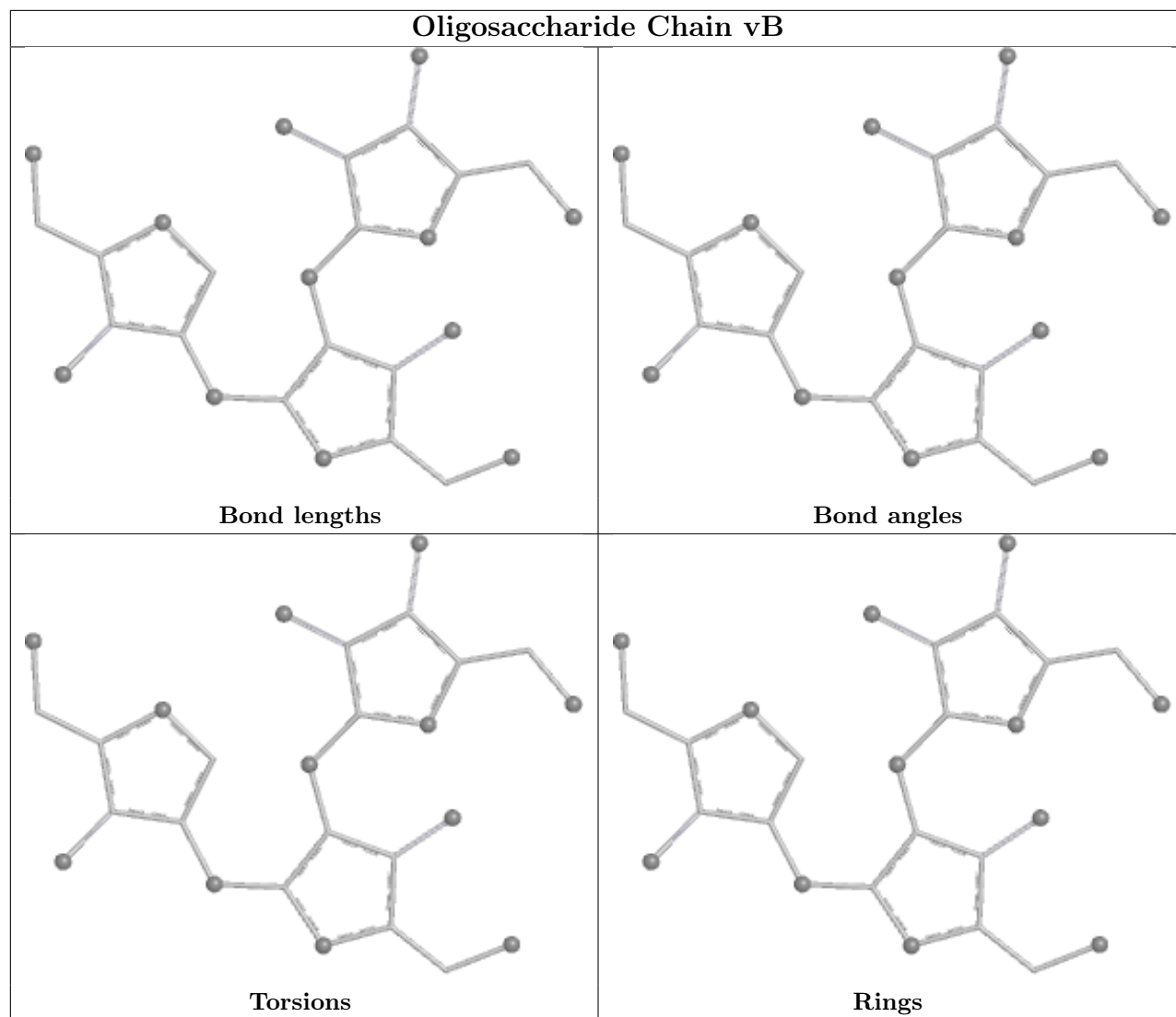


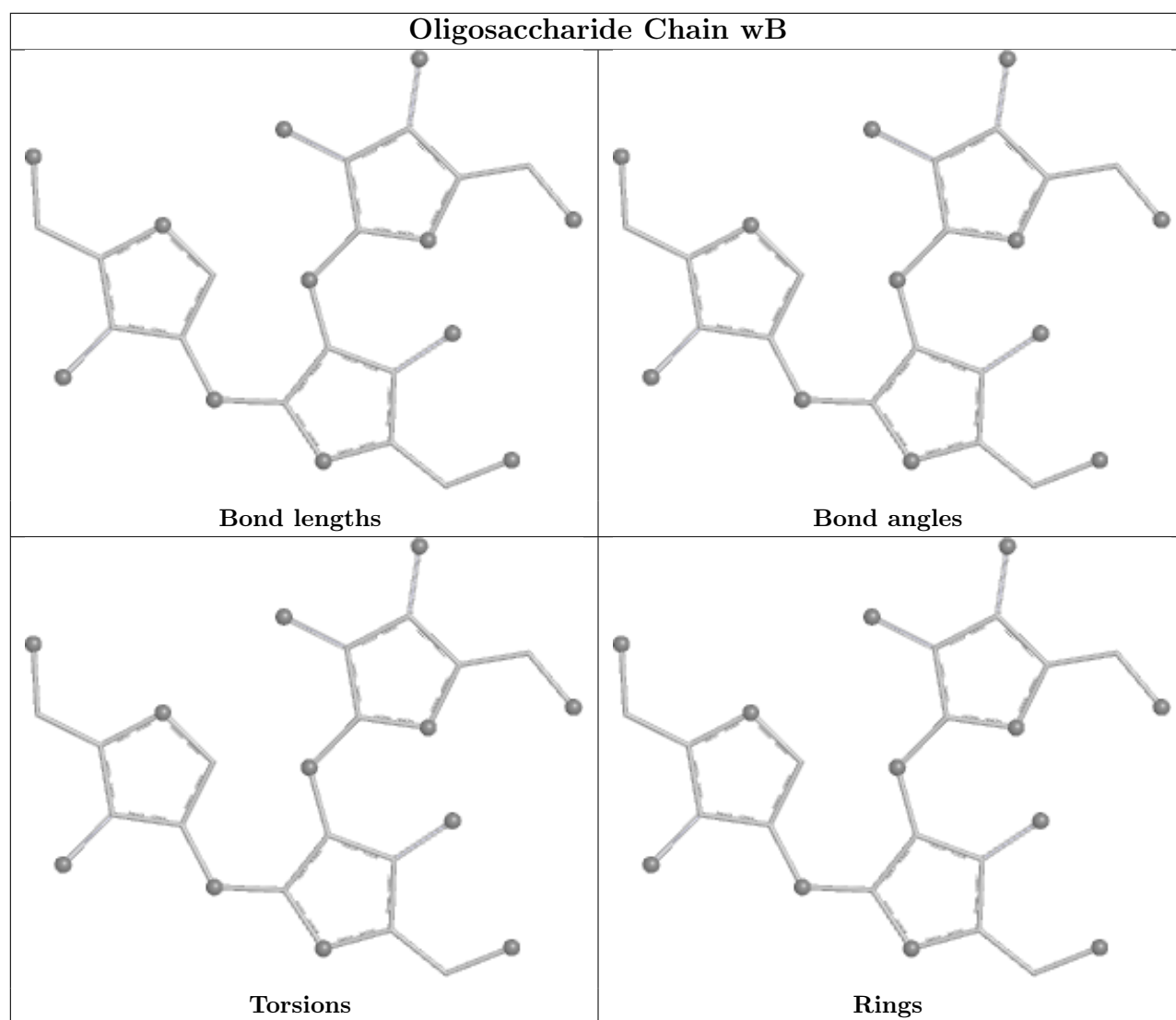


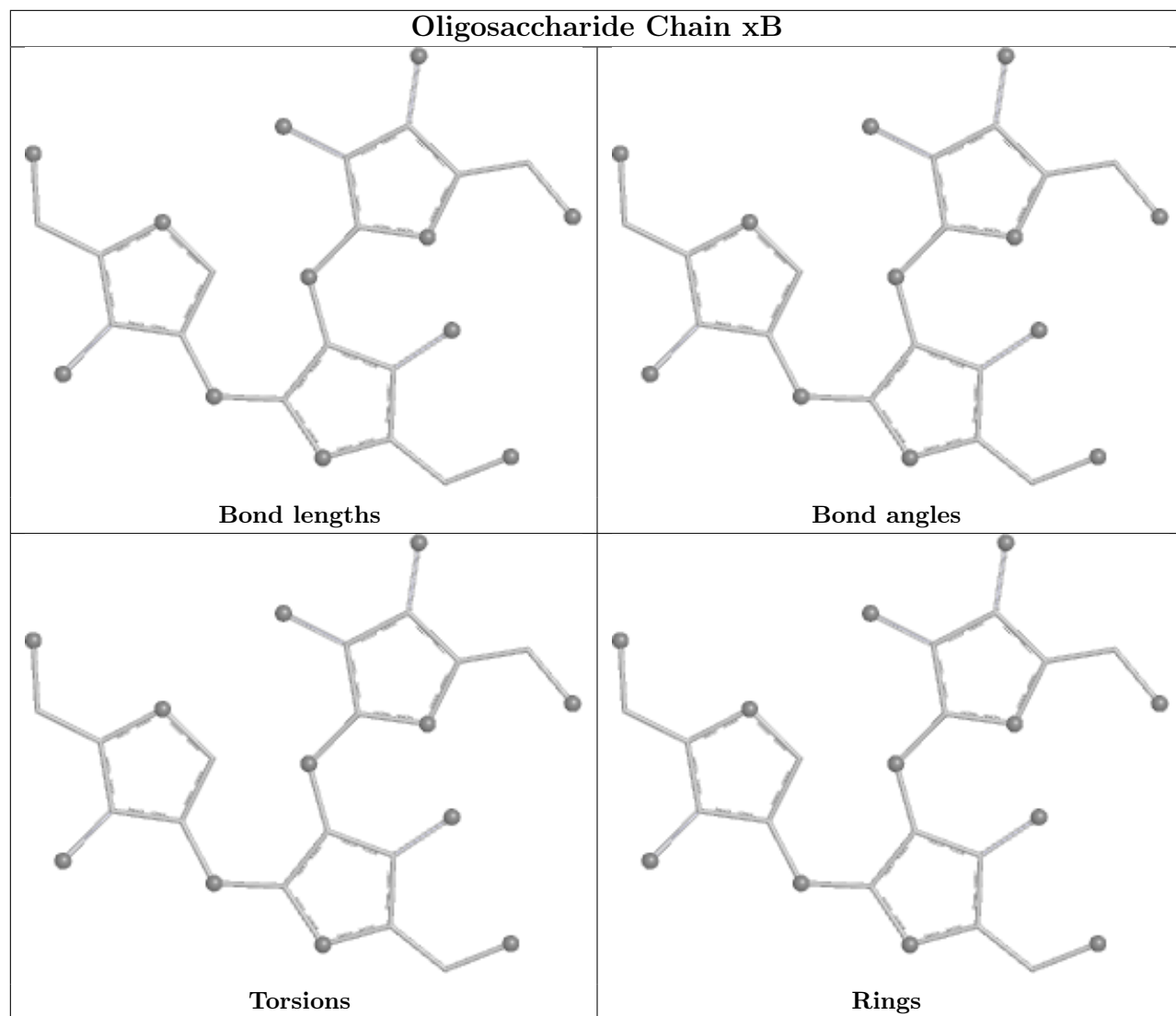


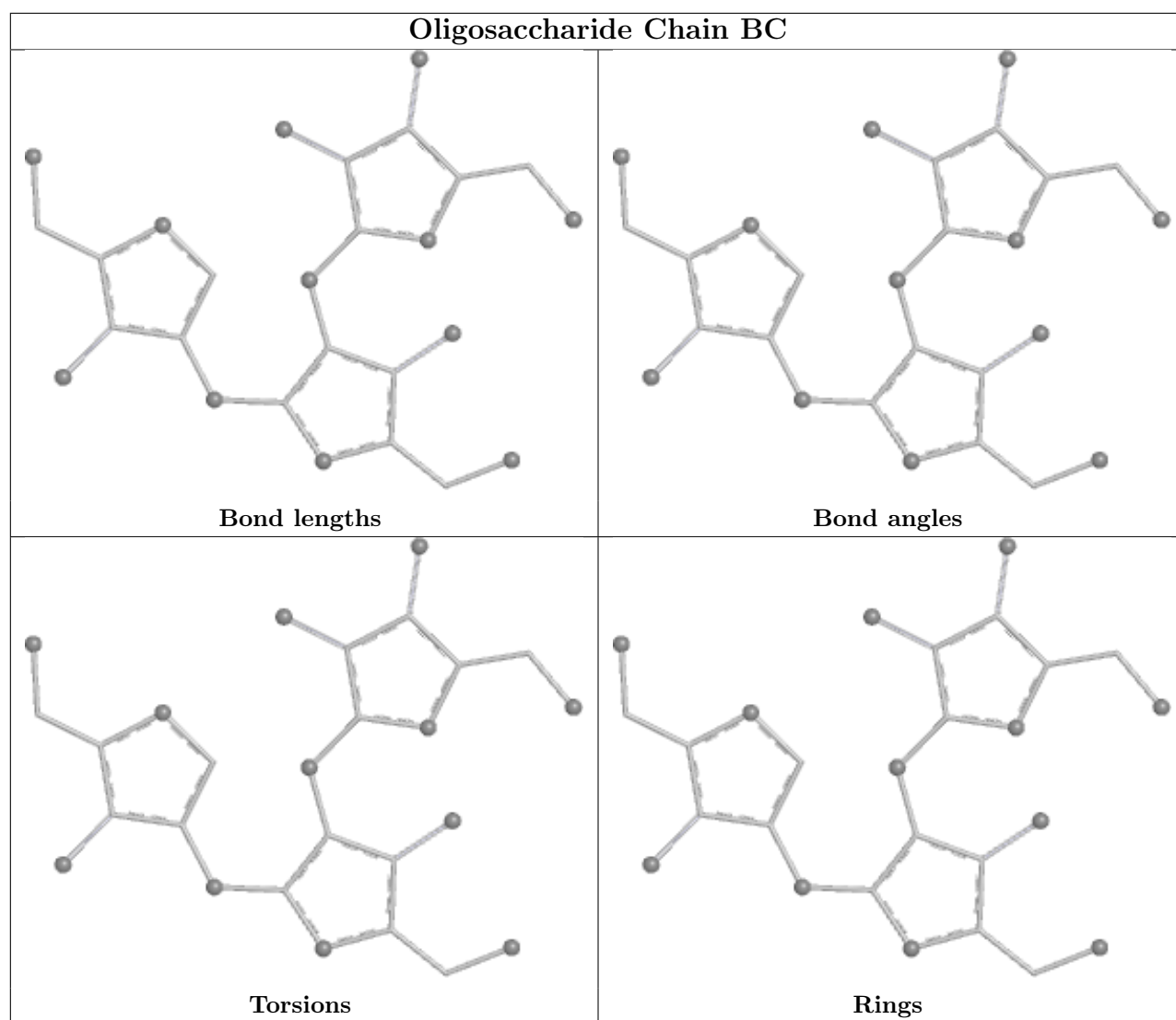


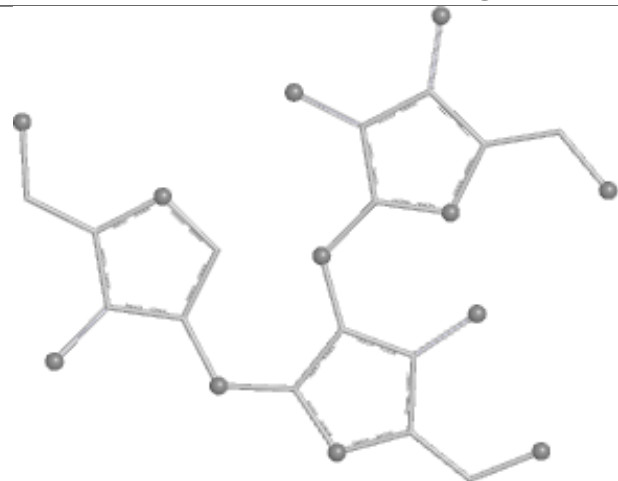
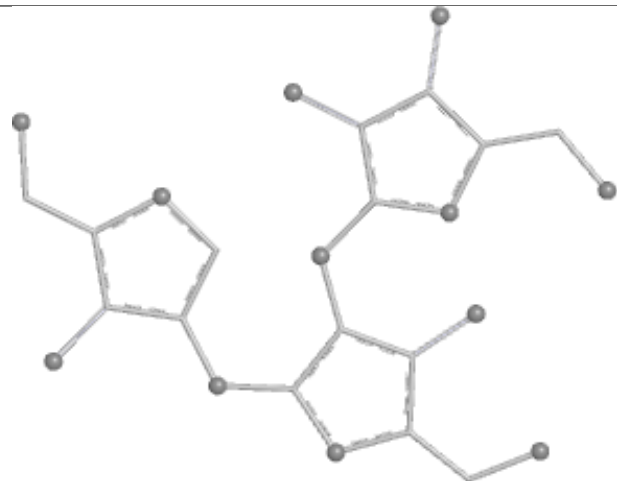
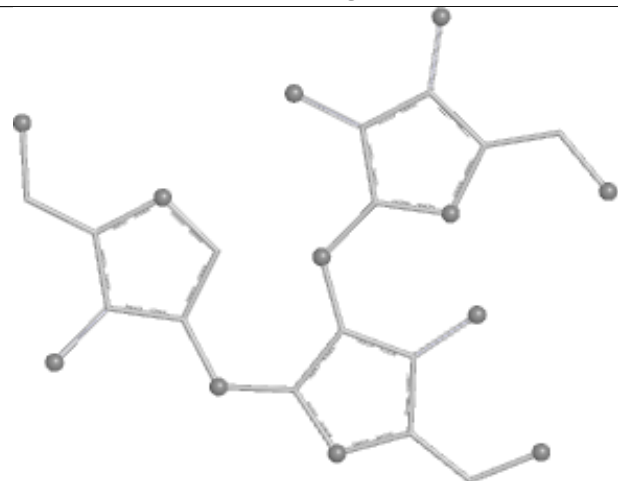
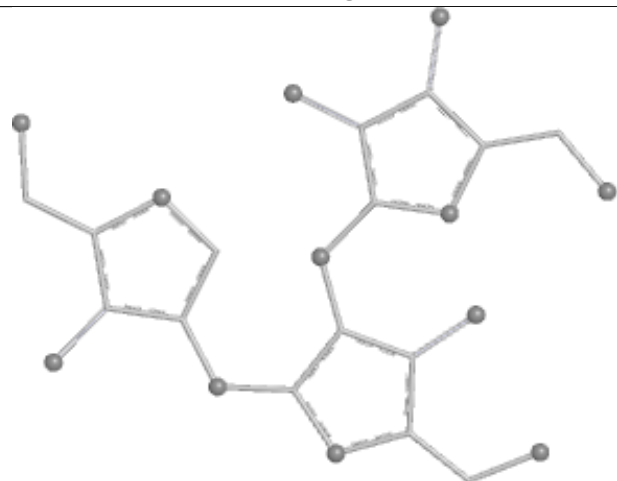


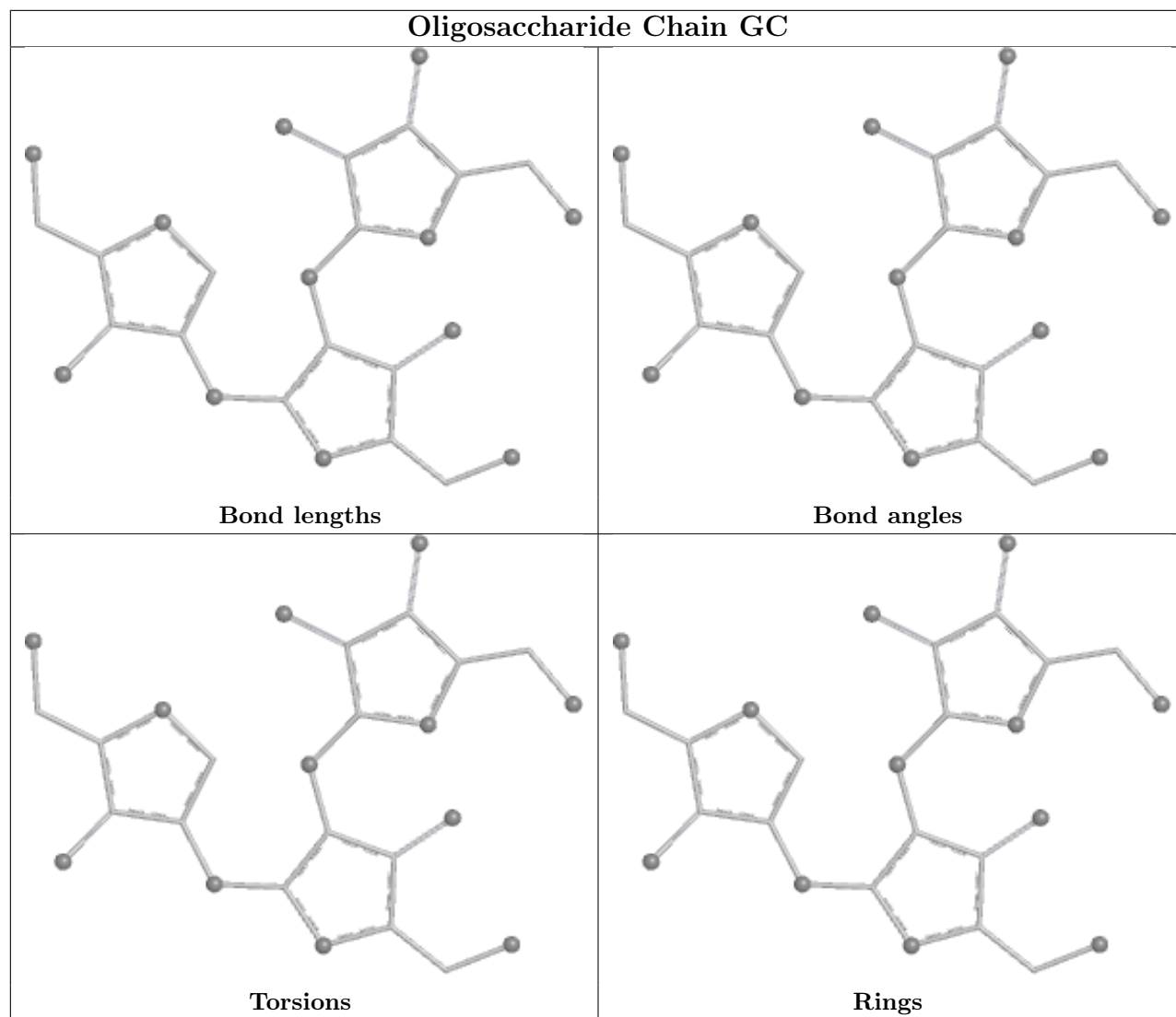


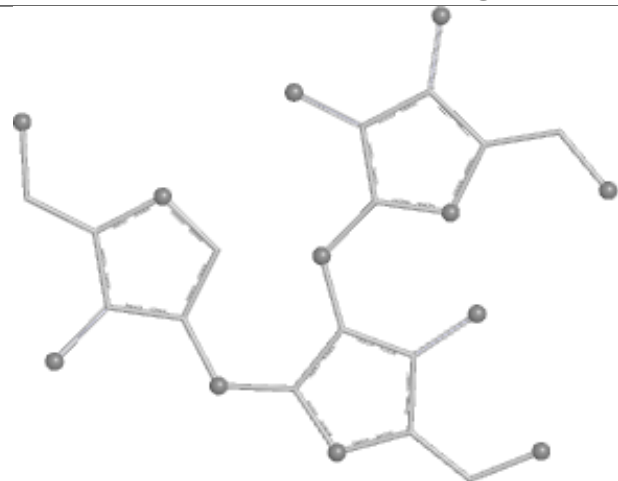
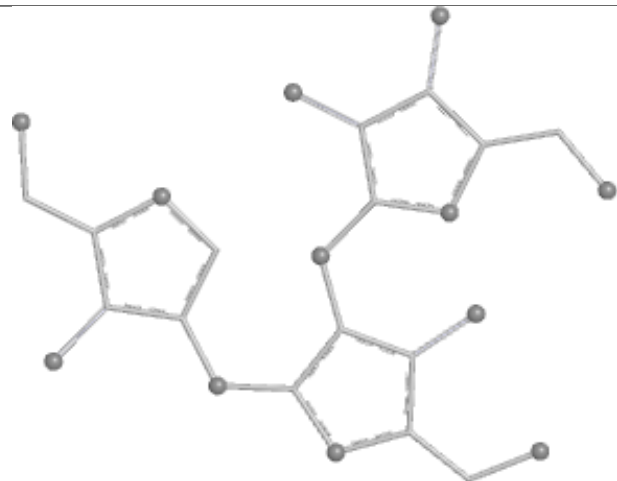
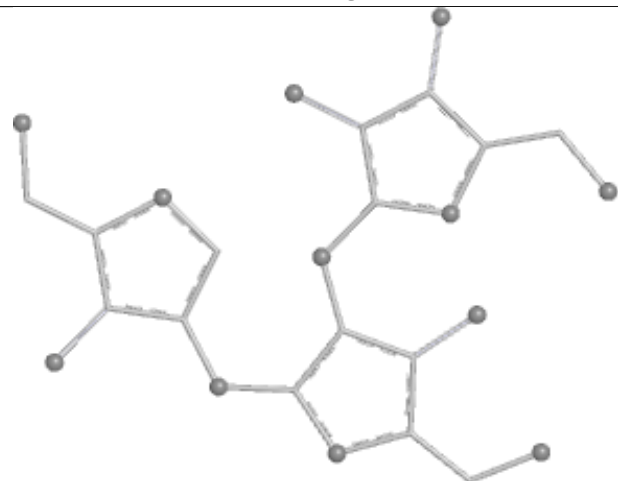
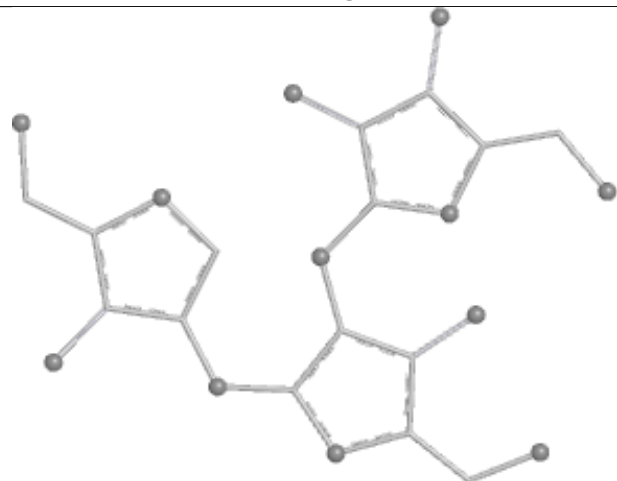


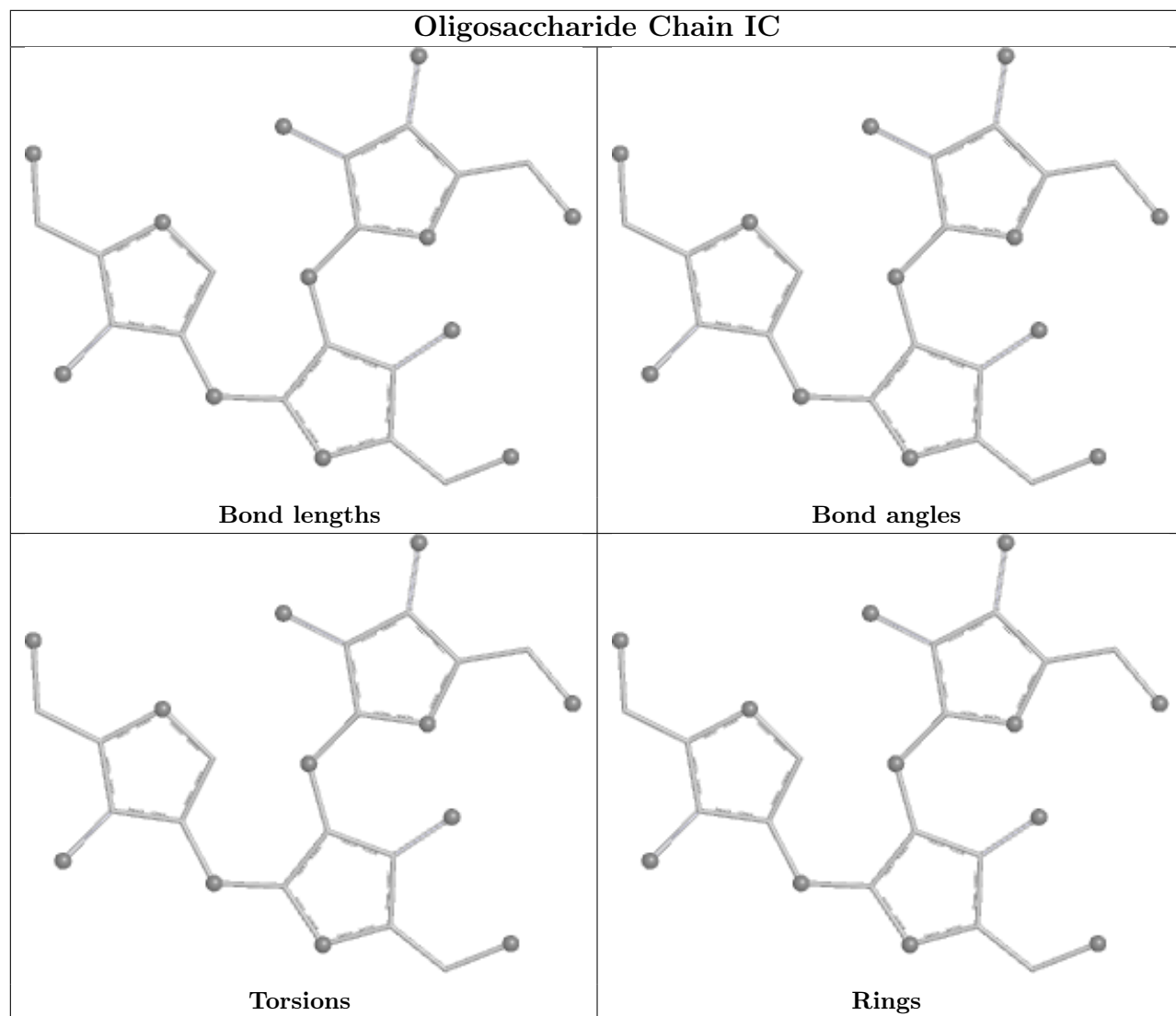


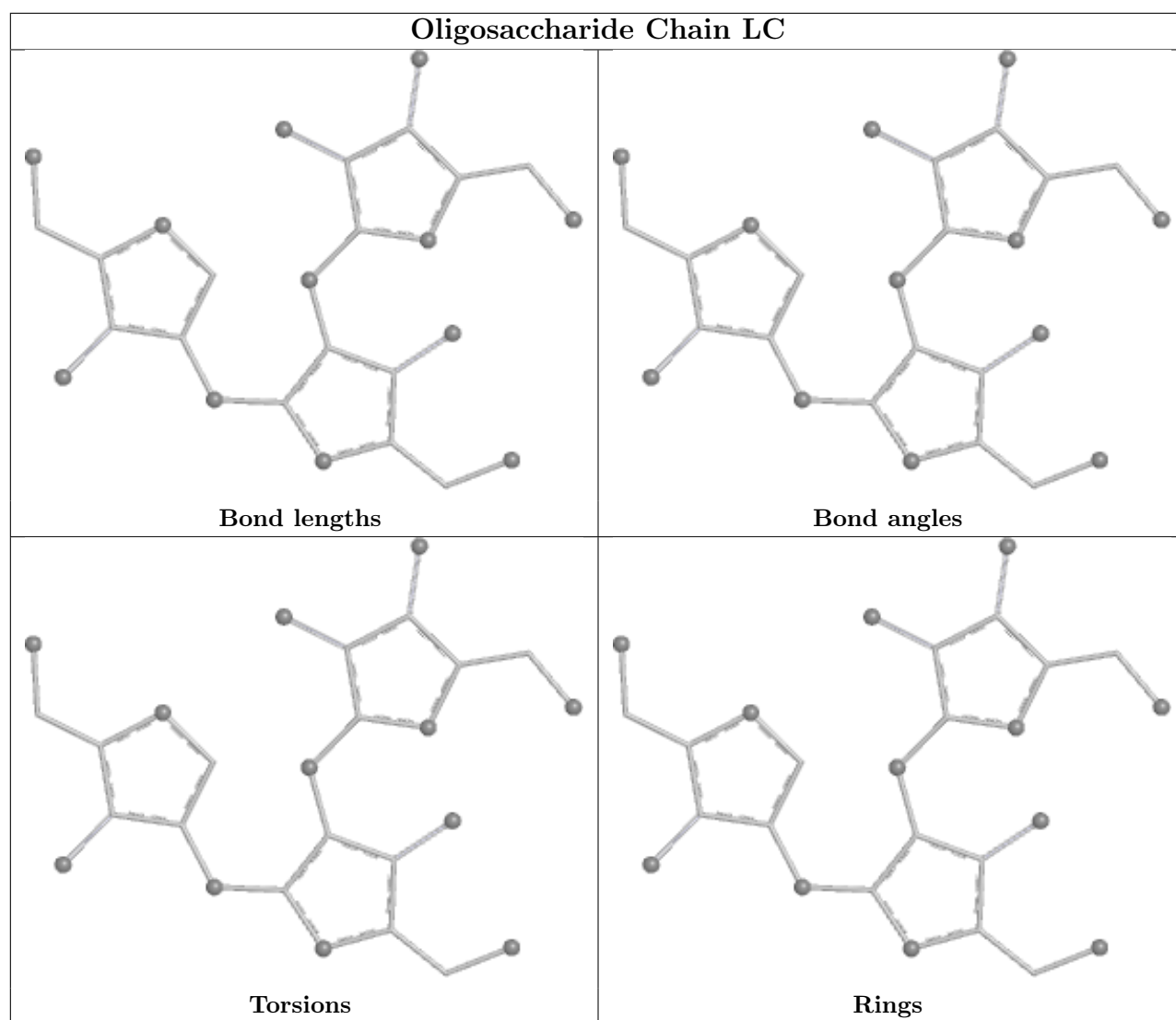


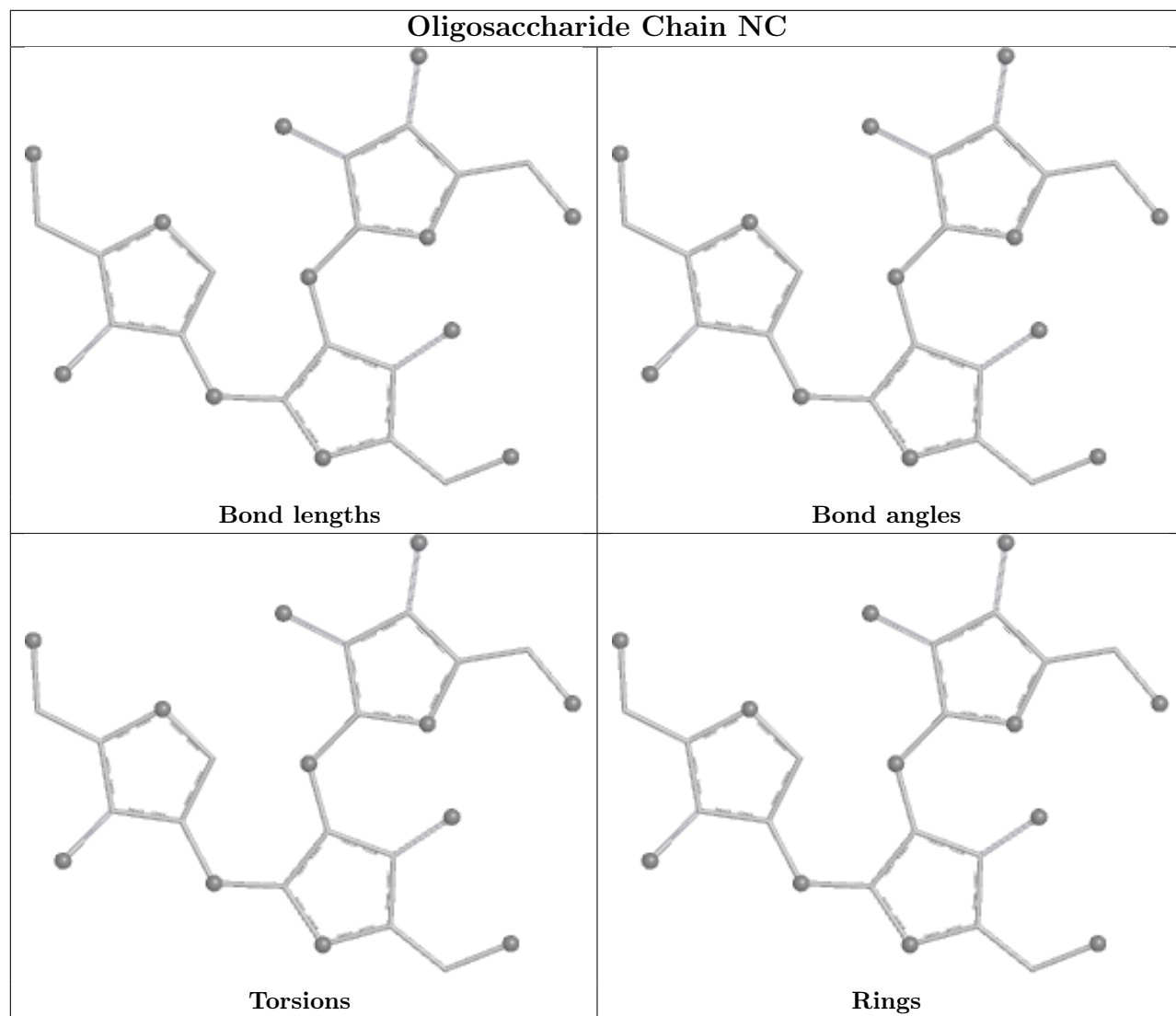
Oligosaccharide Chain CC**Bond lengths****Bond angles****Torsions****Rings**

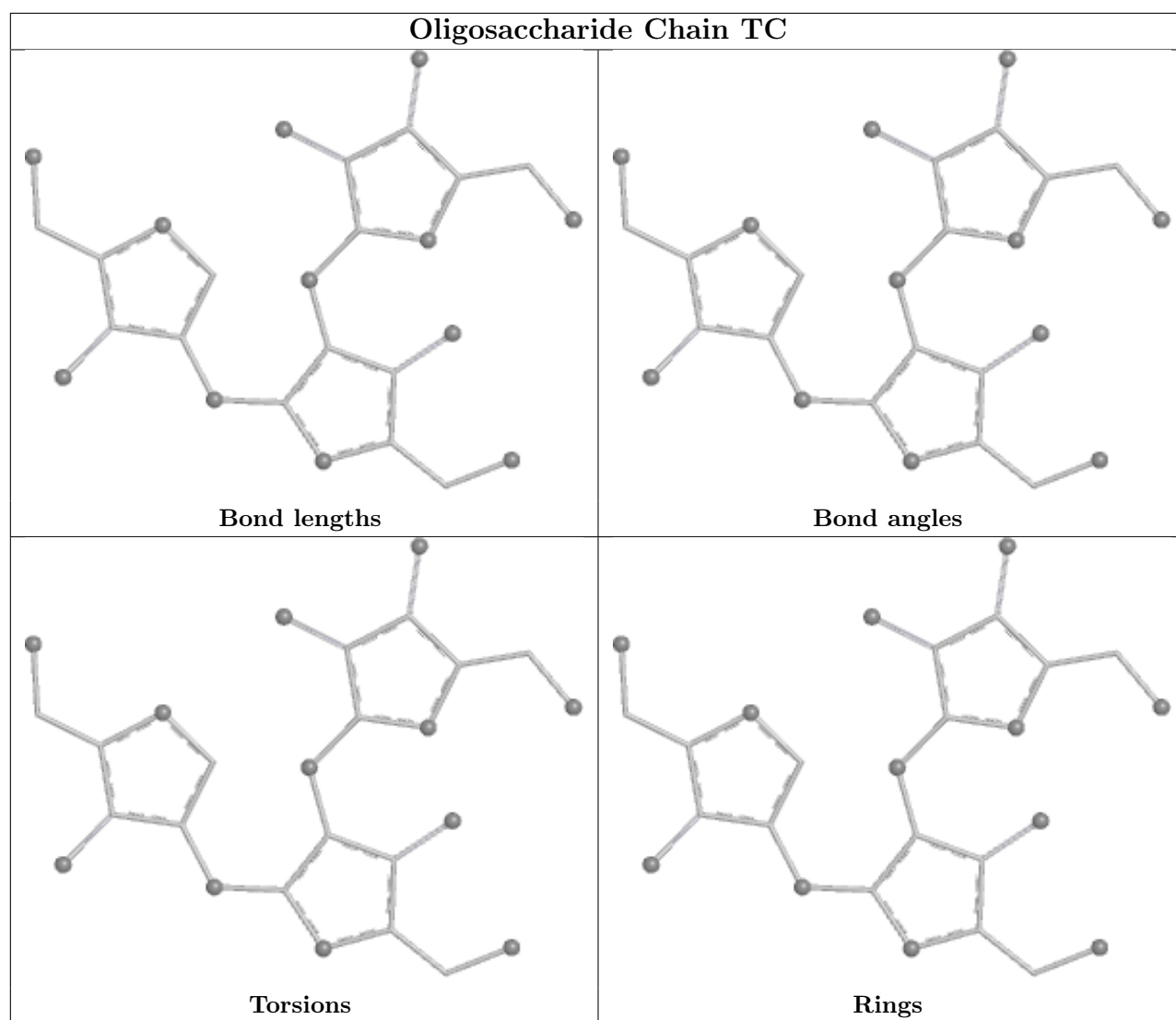


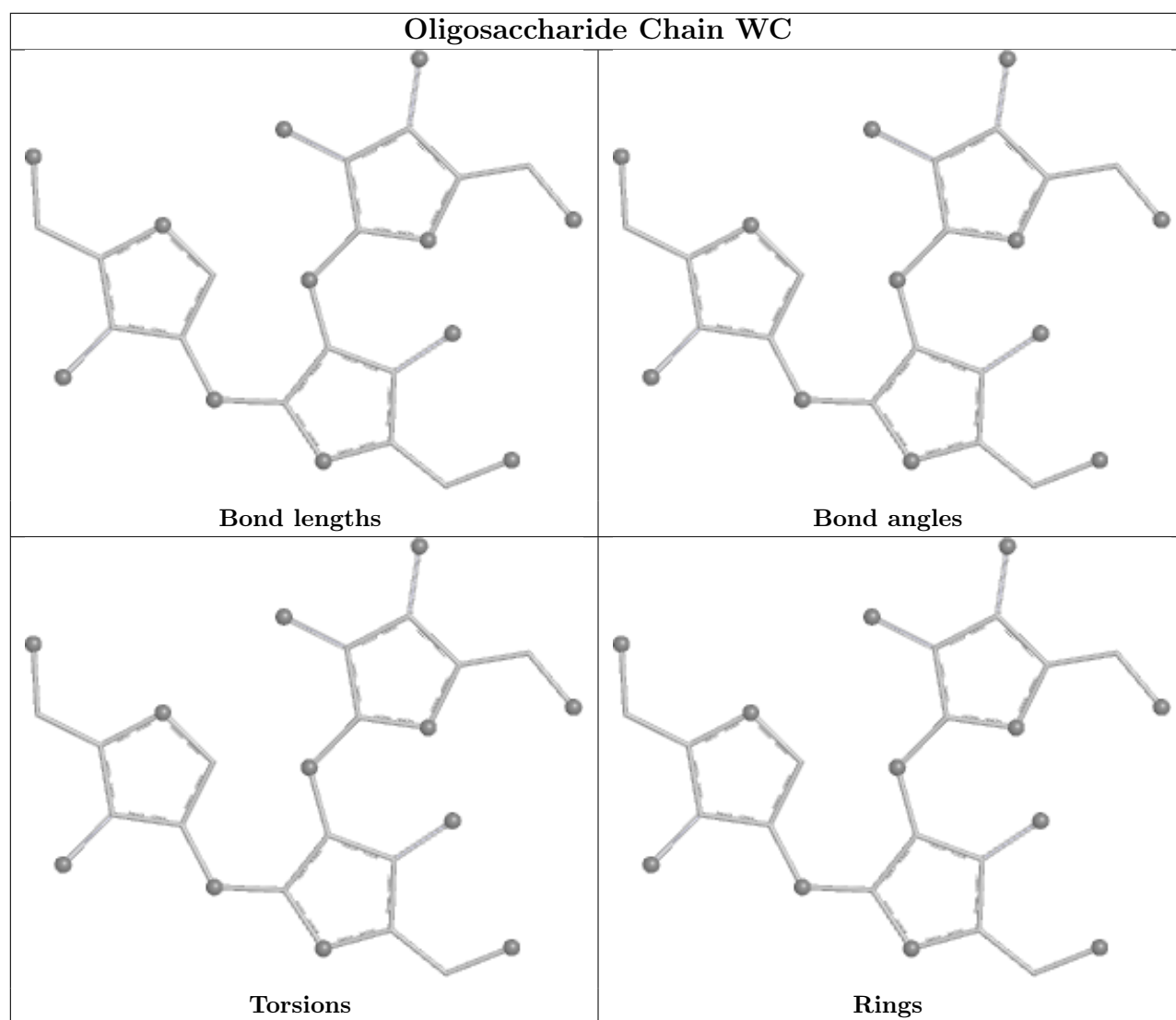
Oligosaccharide Chain HC**Bond lengths****Bond angles****Torsions****Rings**

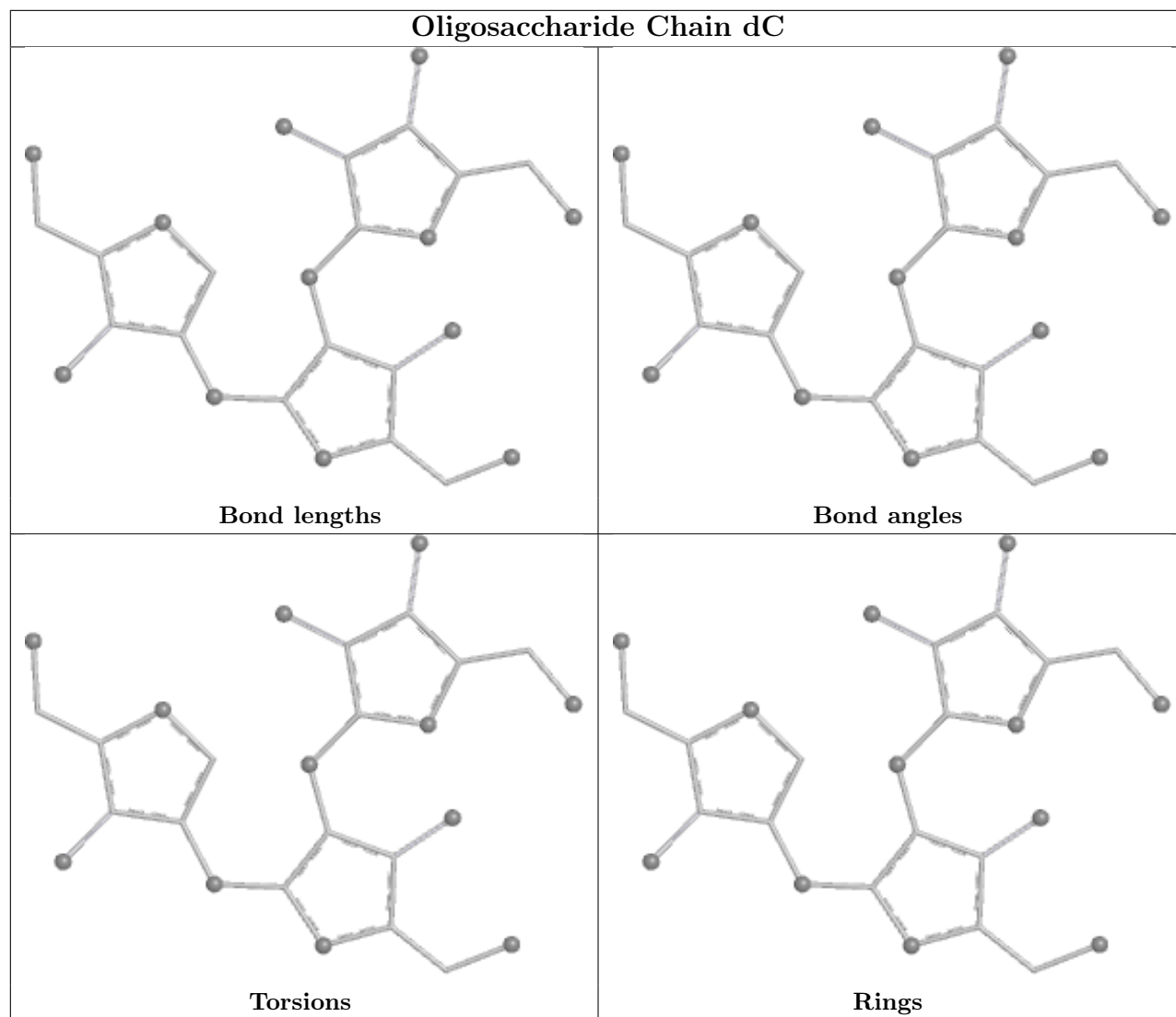




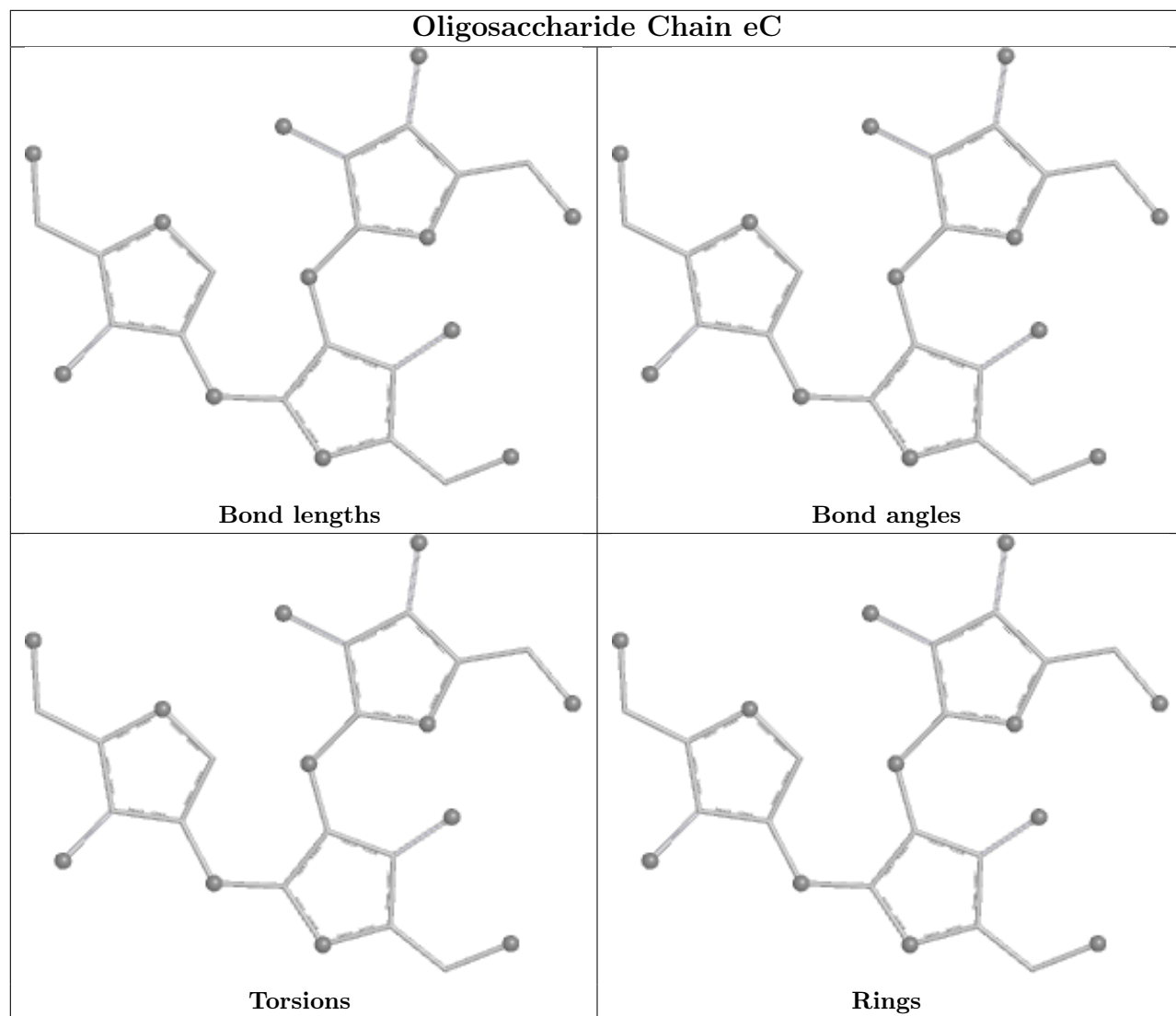


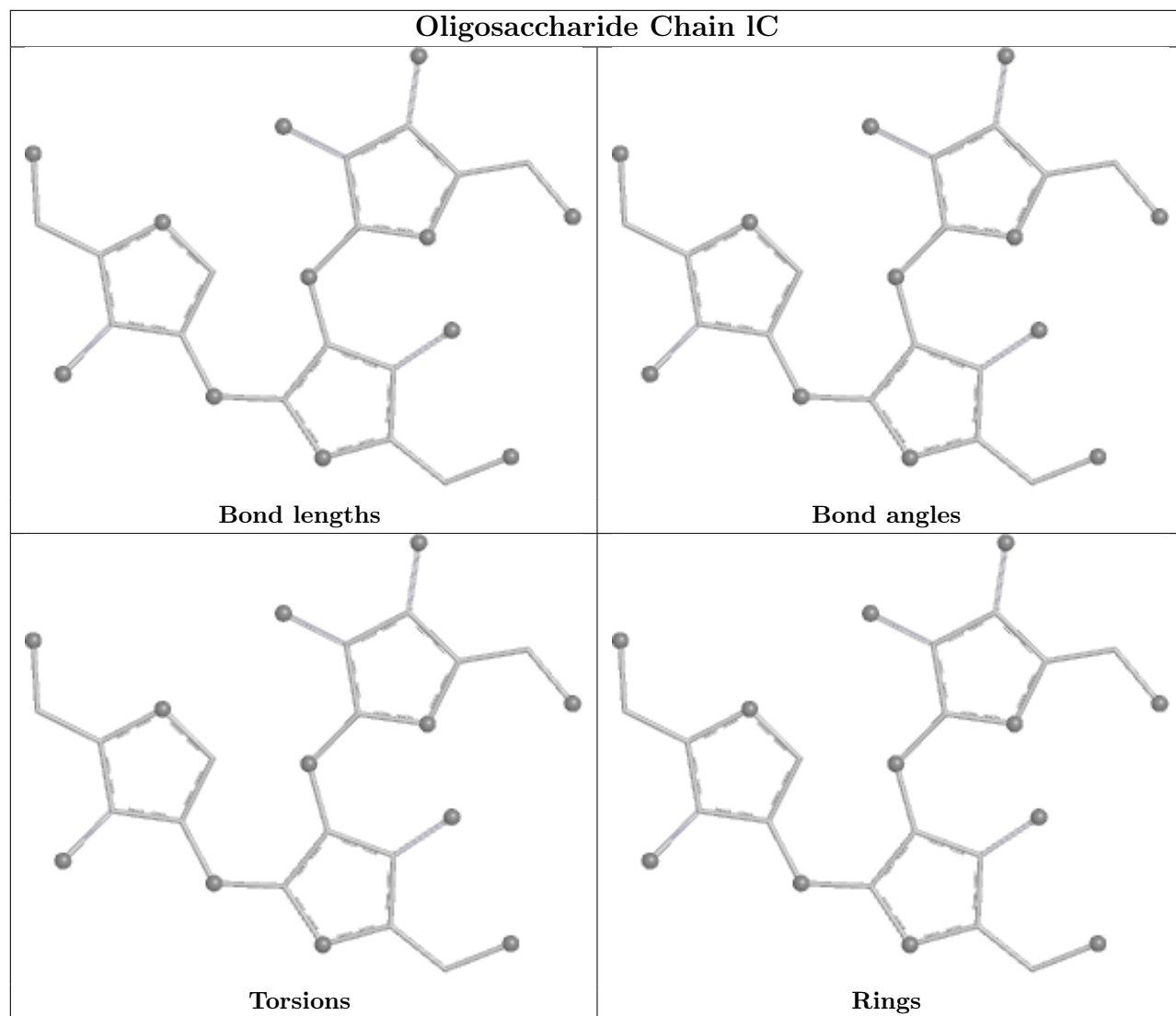


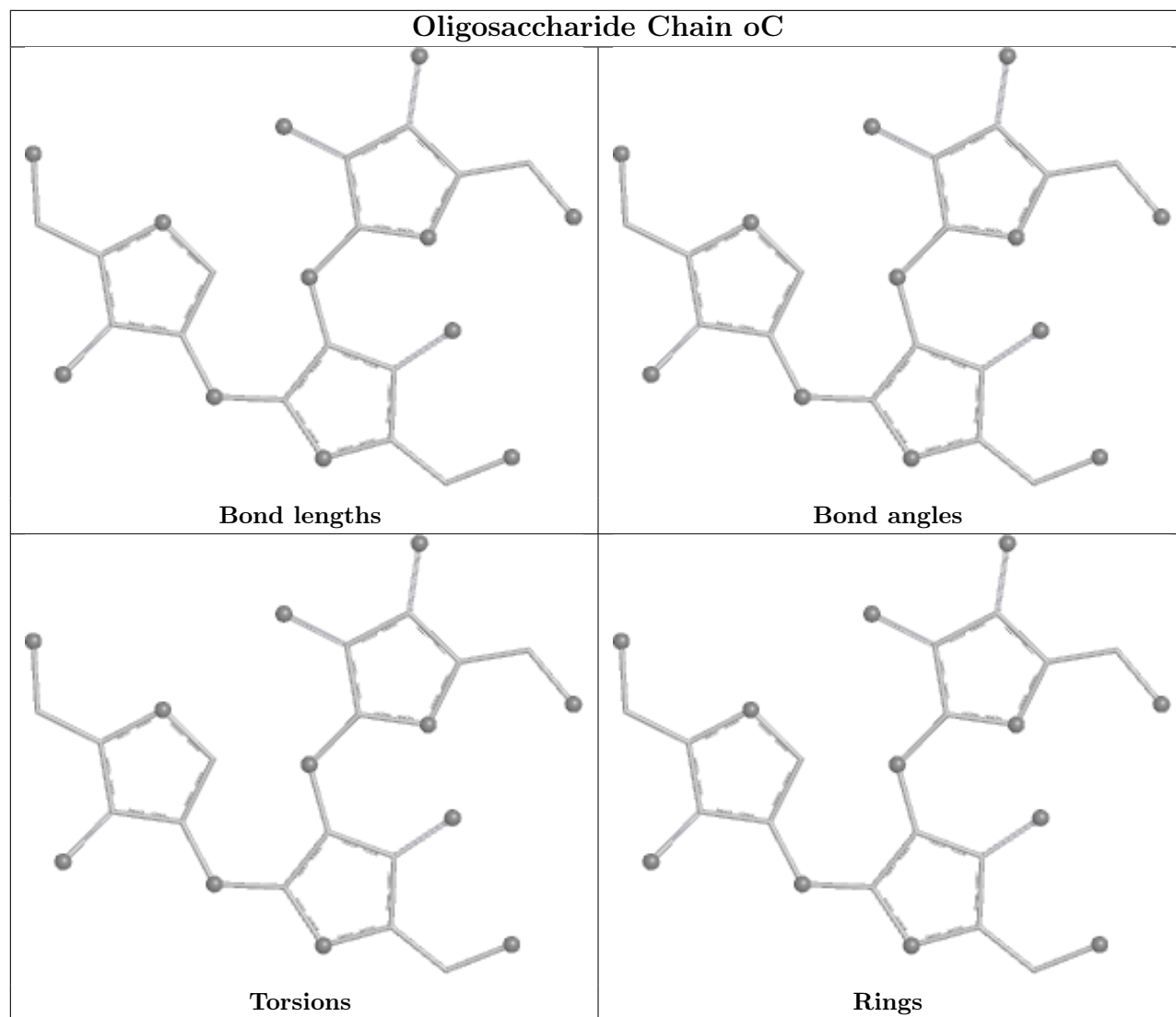


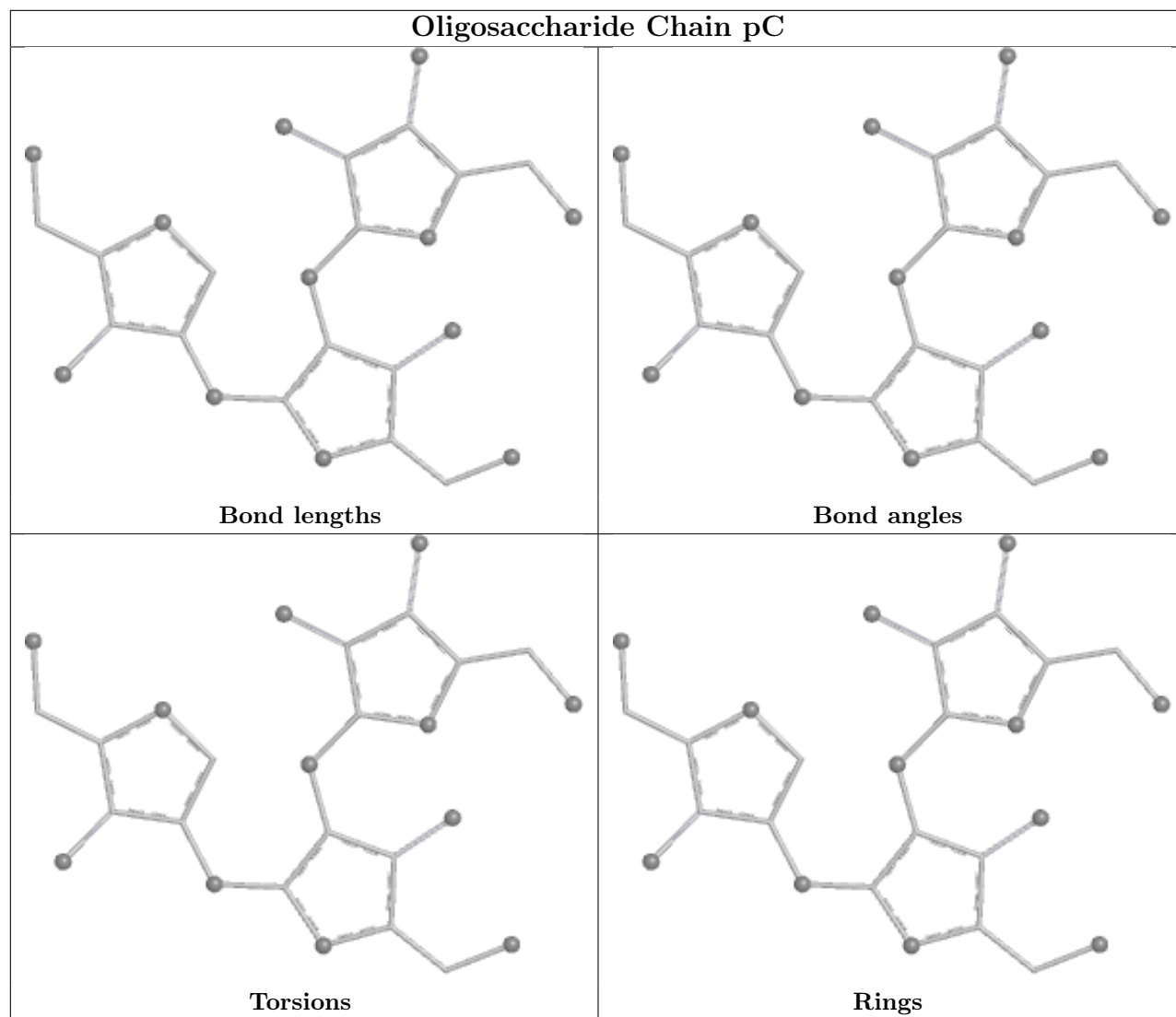


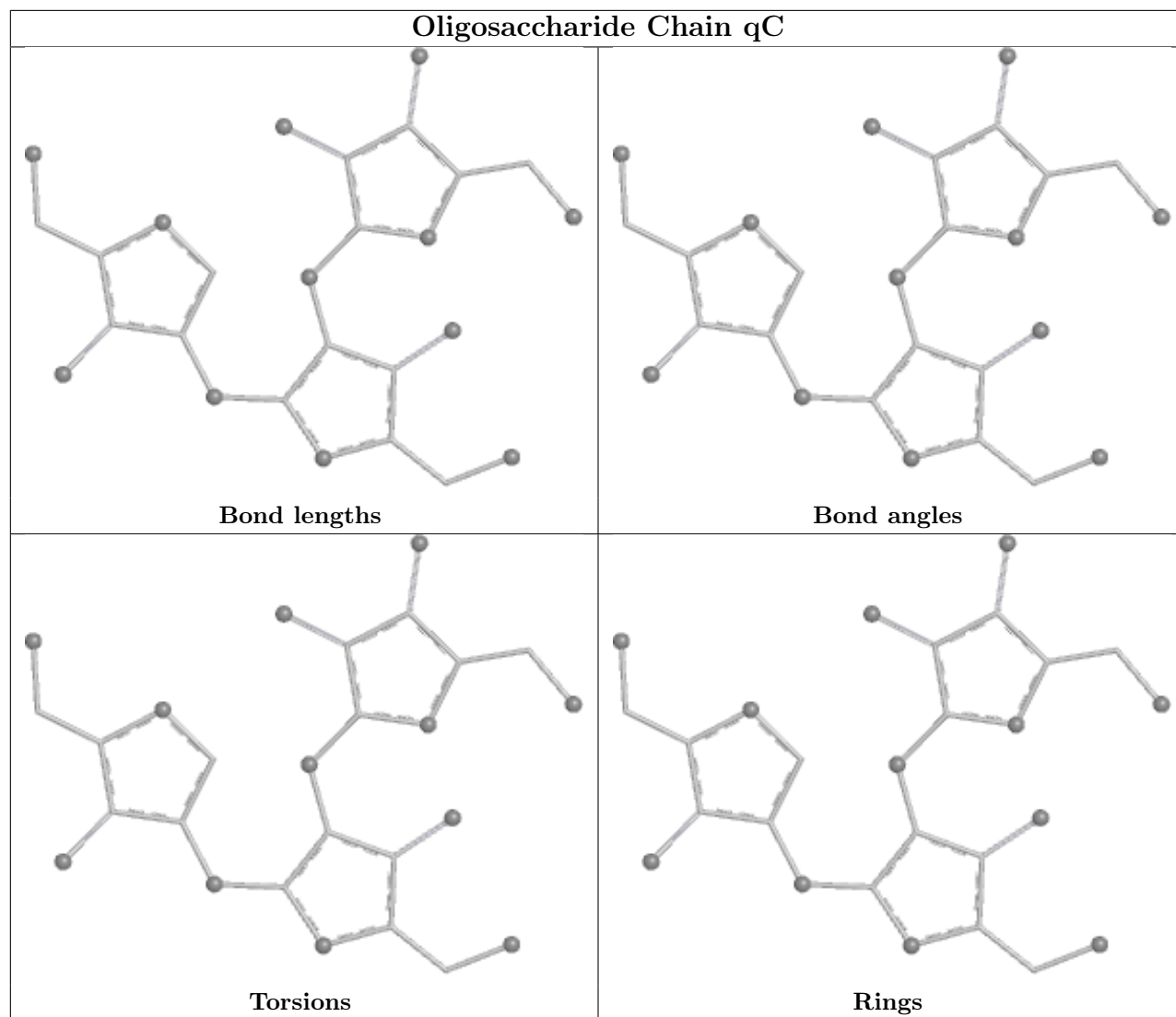
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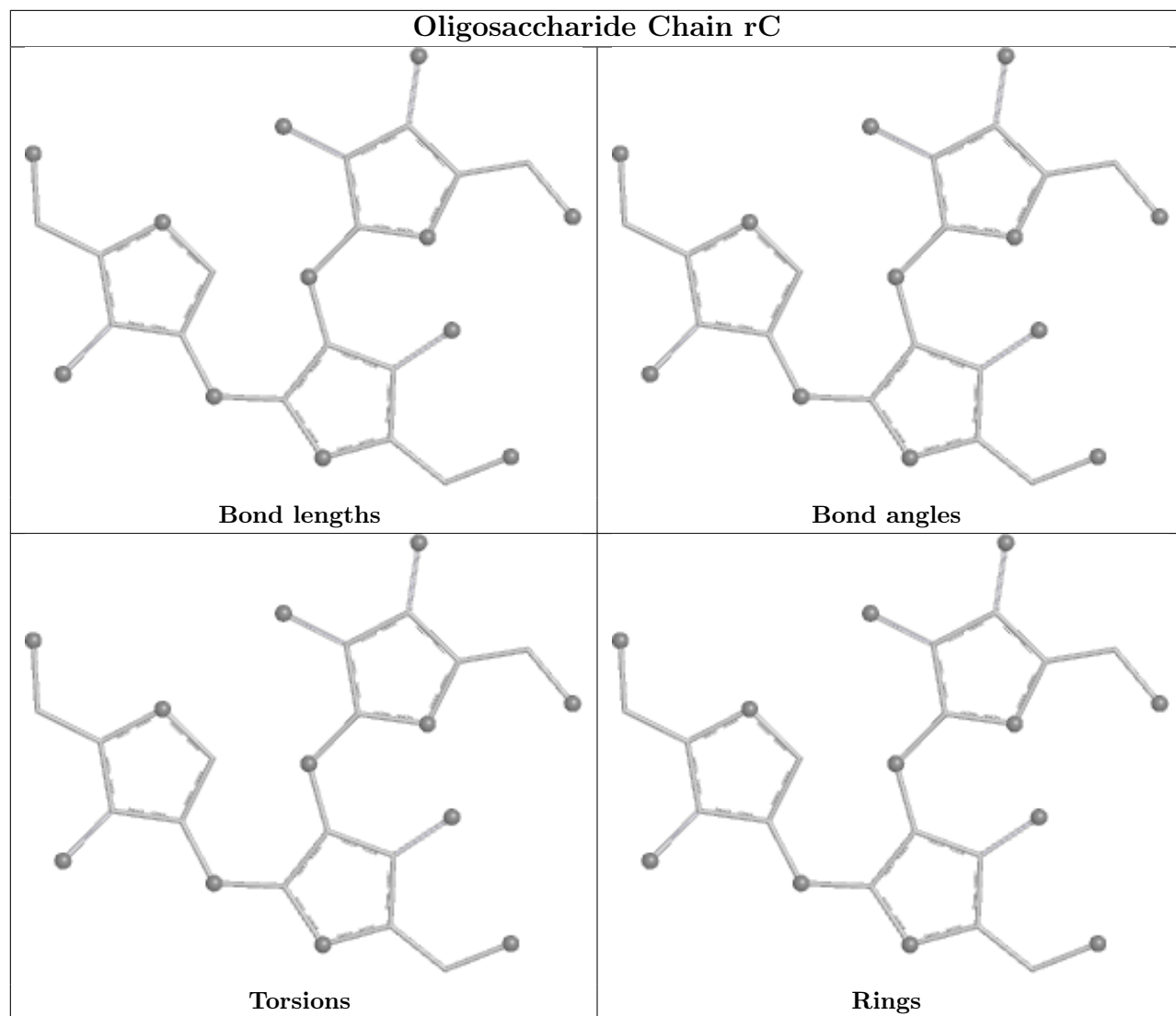


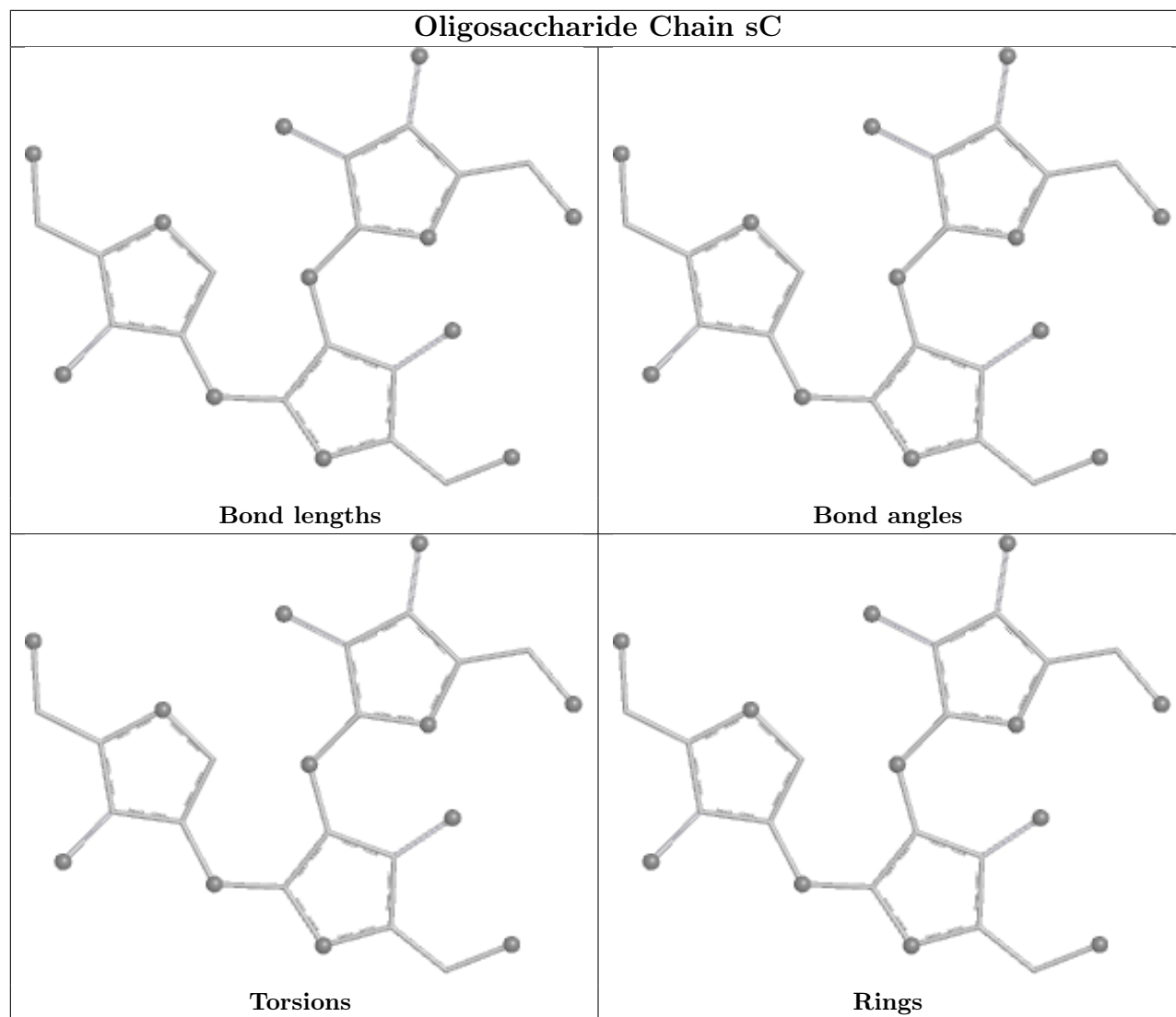


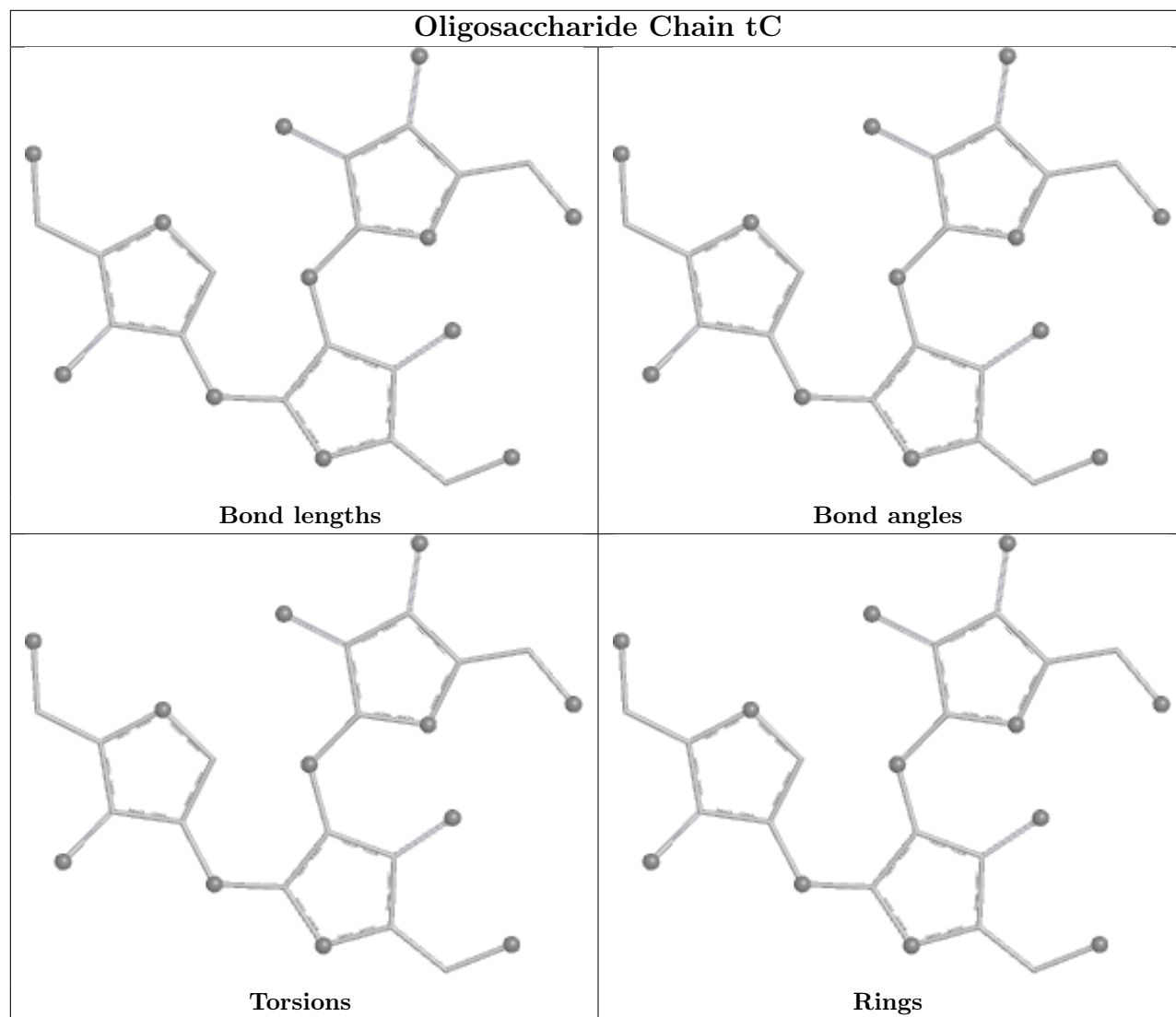


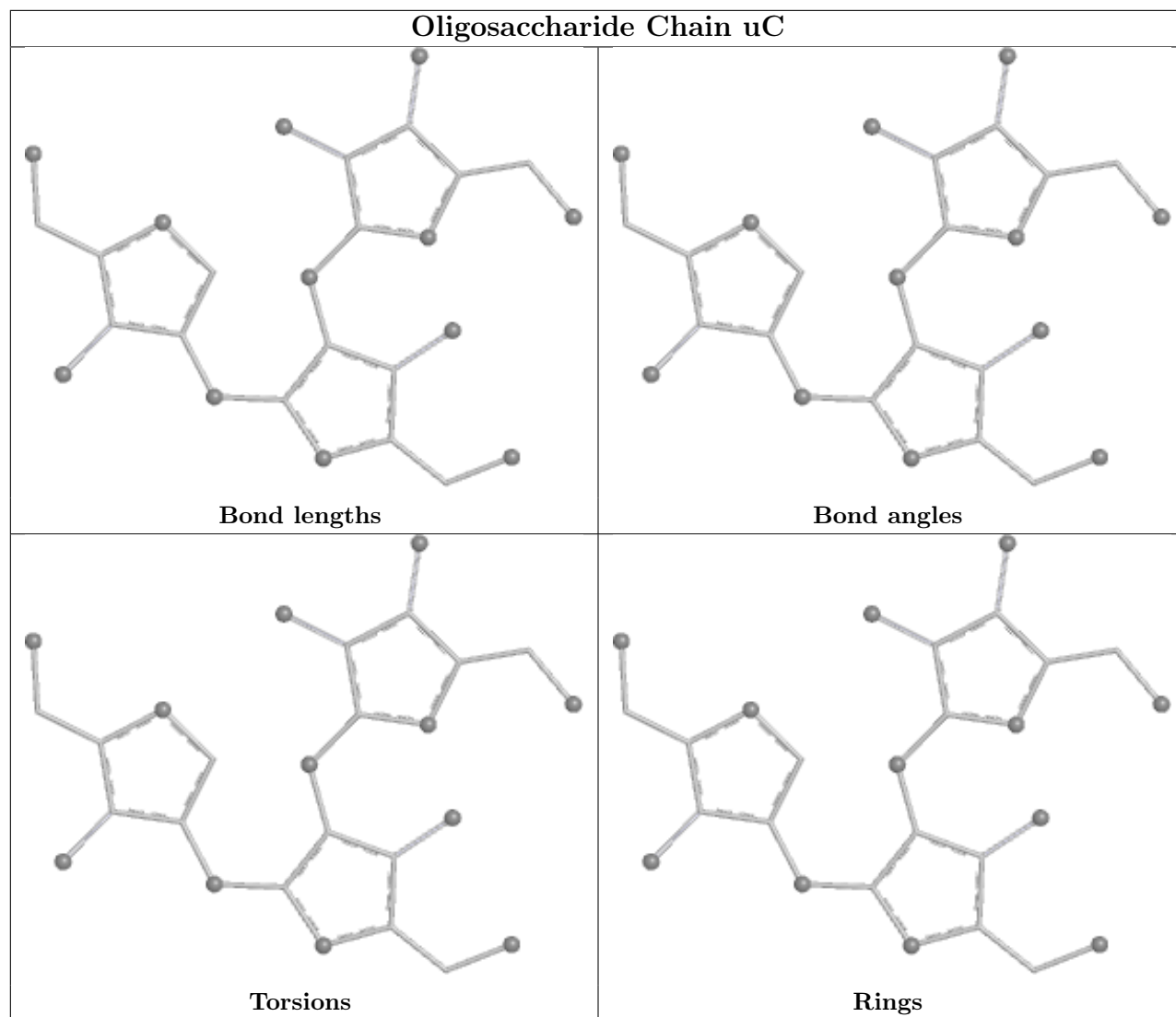




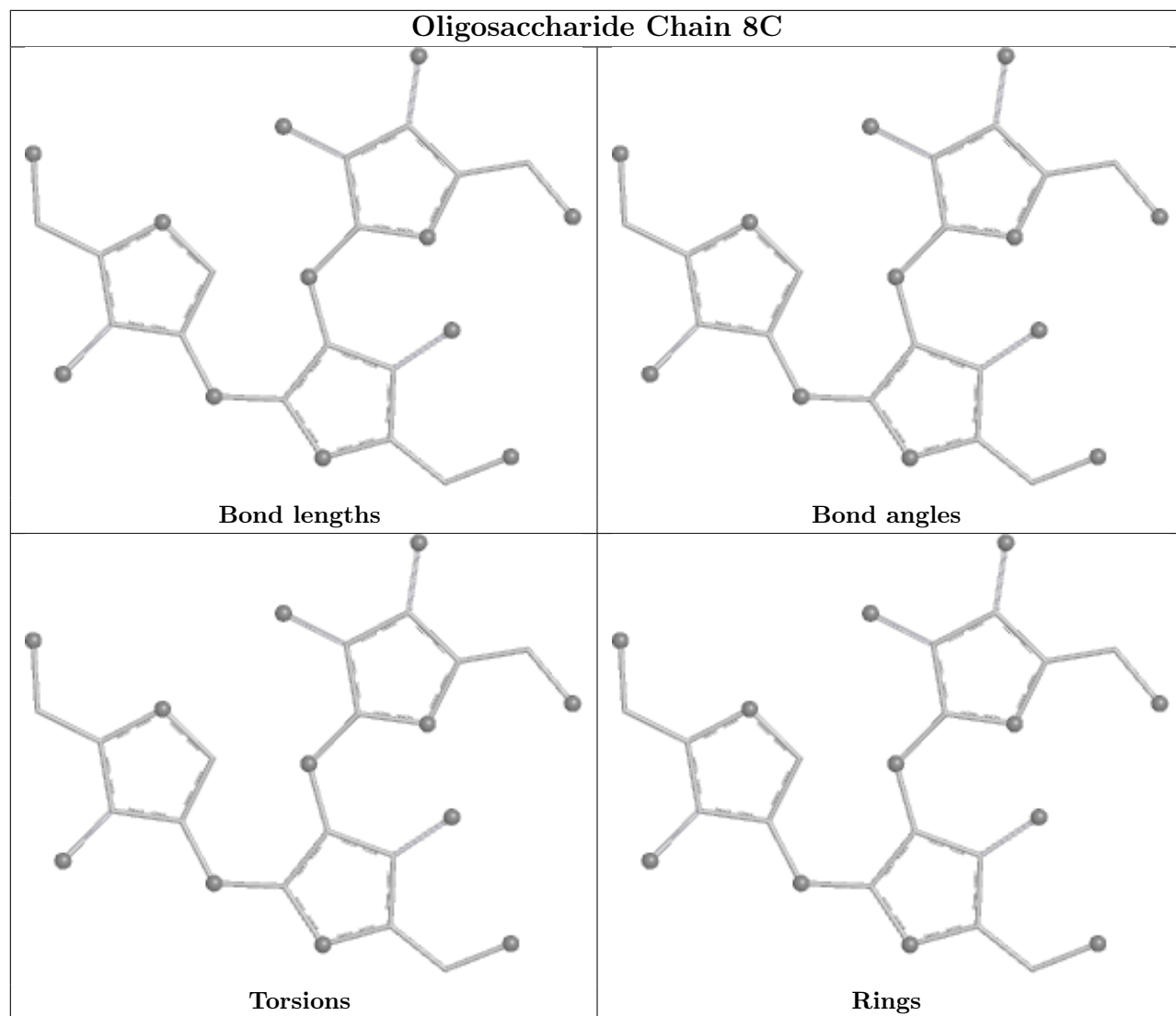




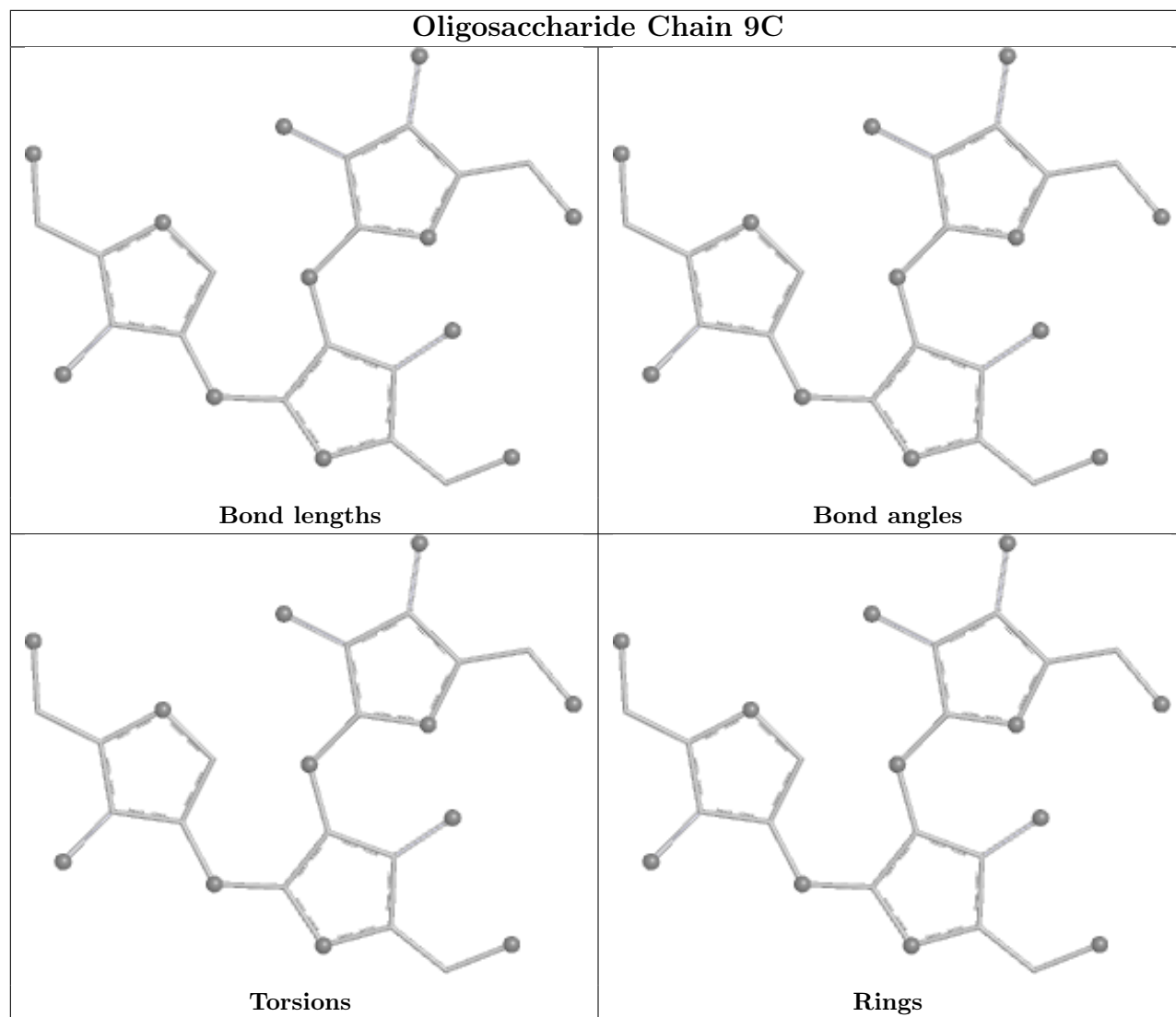


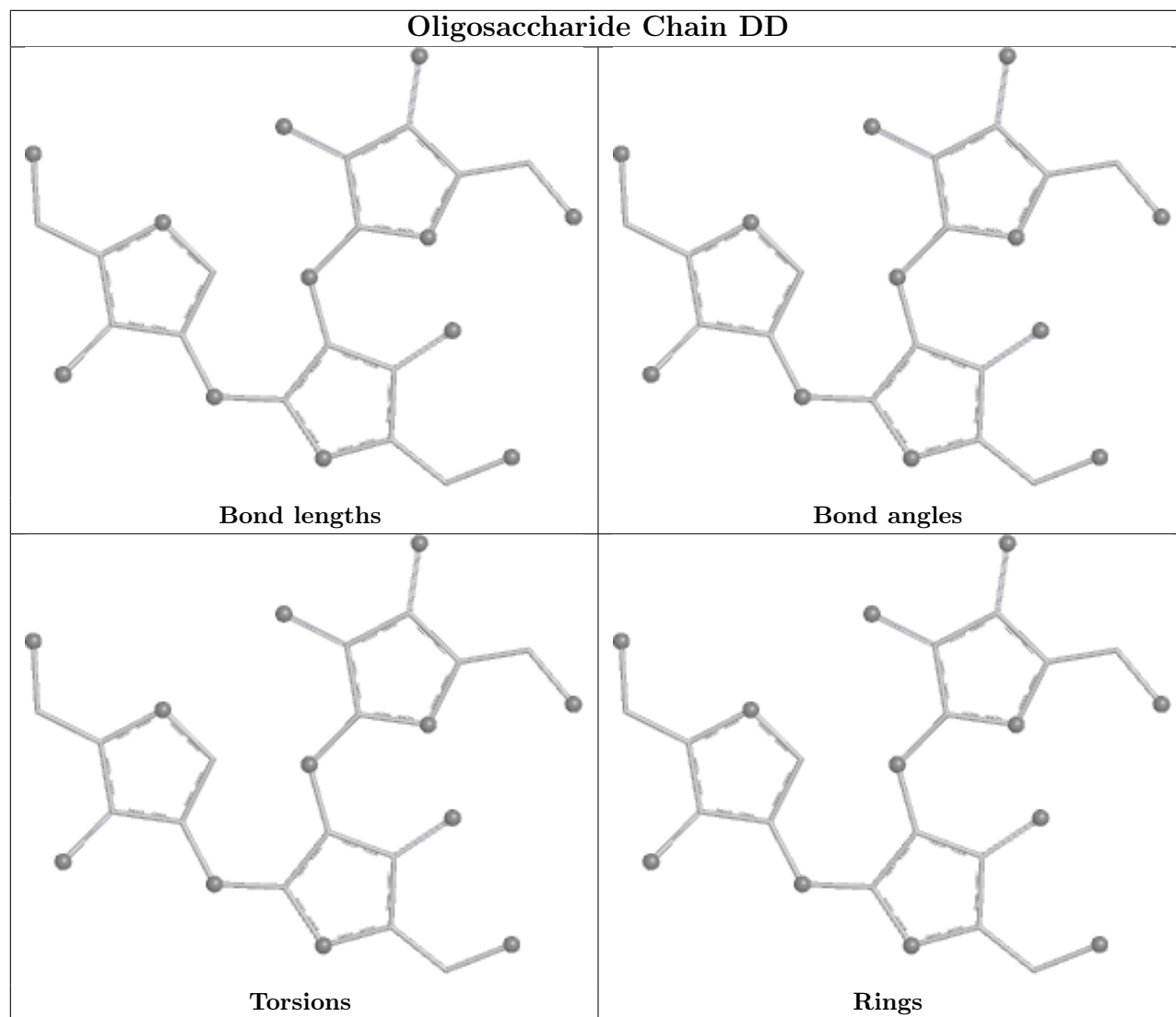


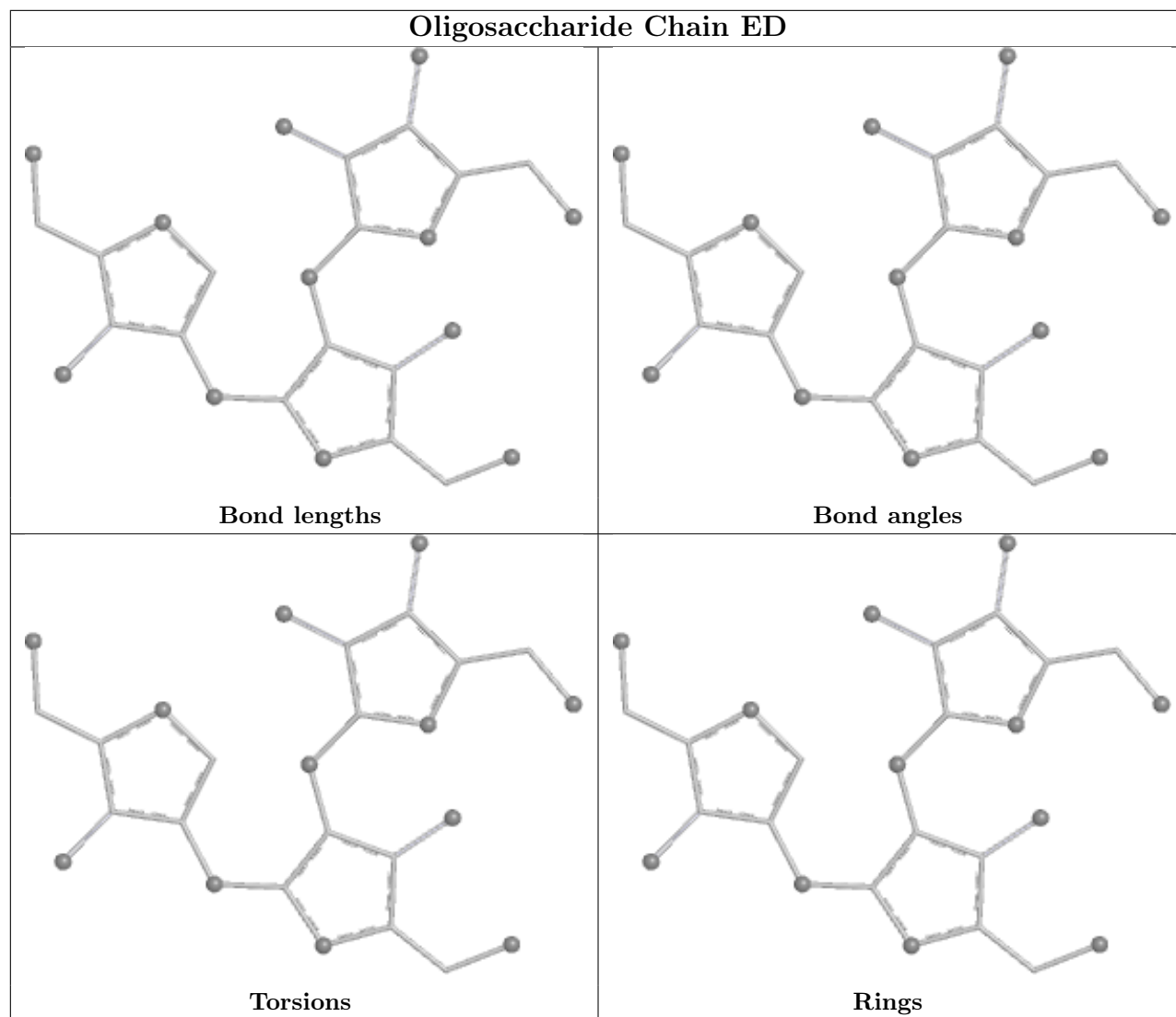
Oligosaccharide Chain 8C

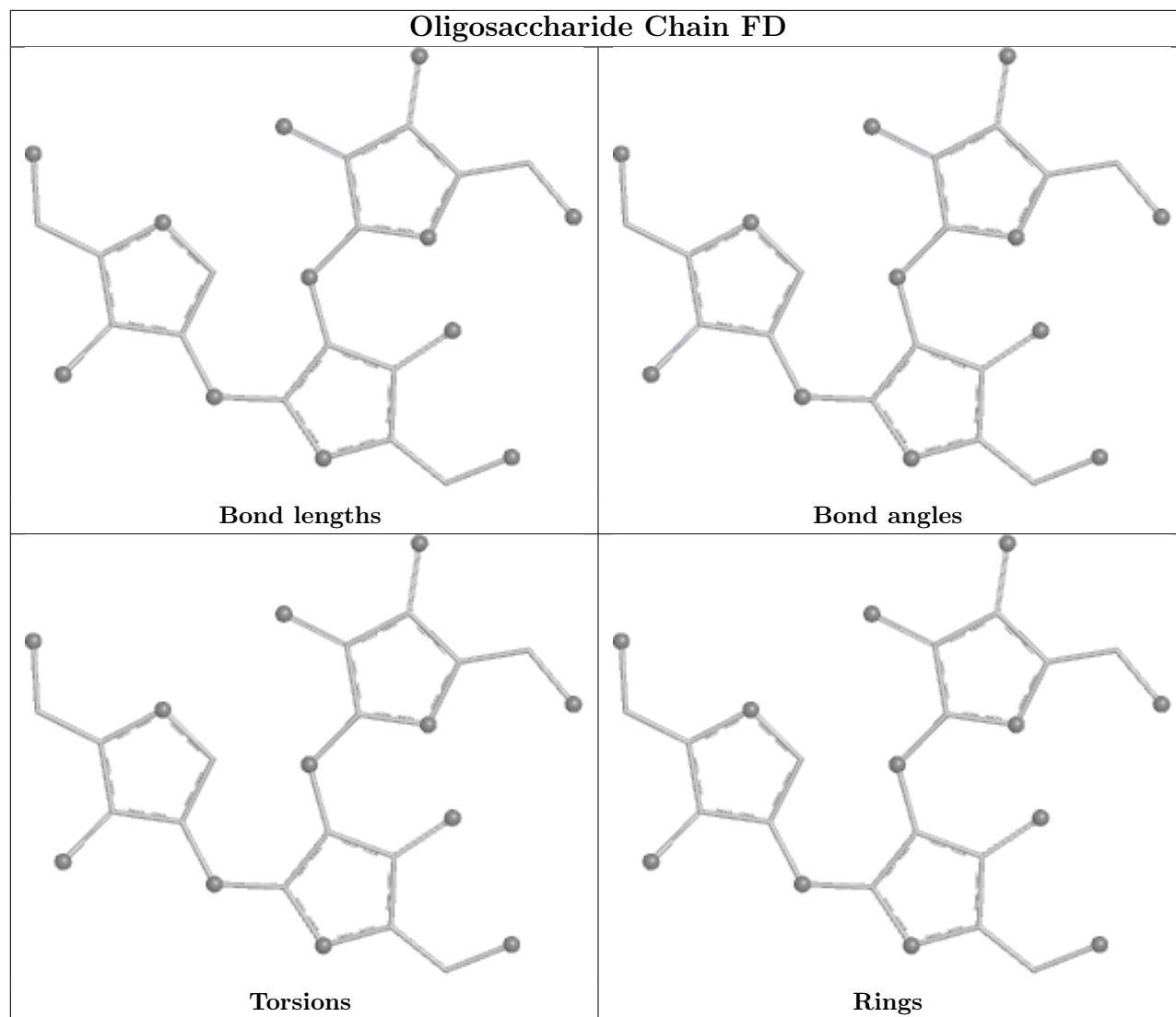


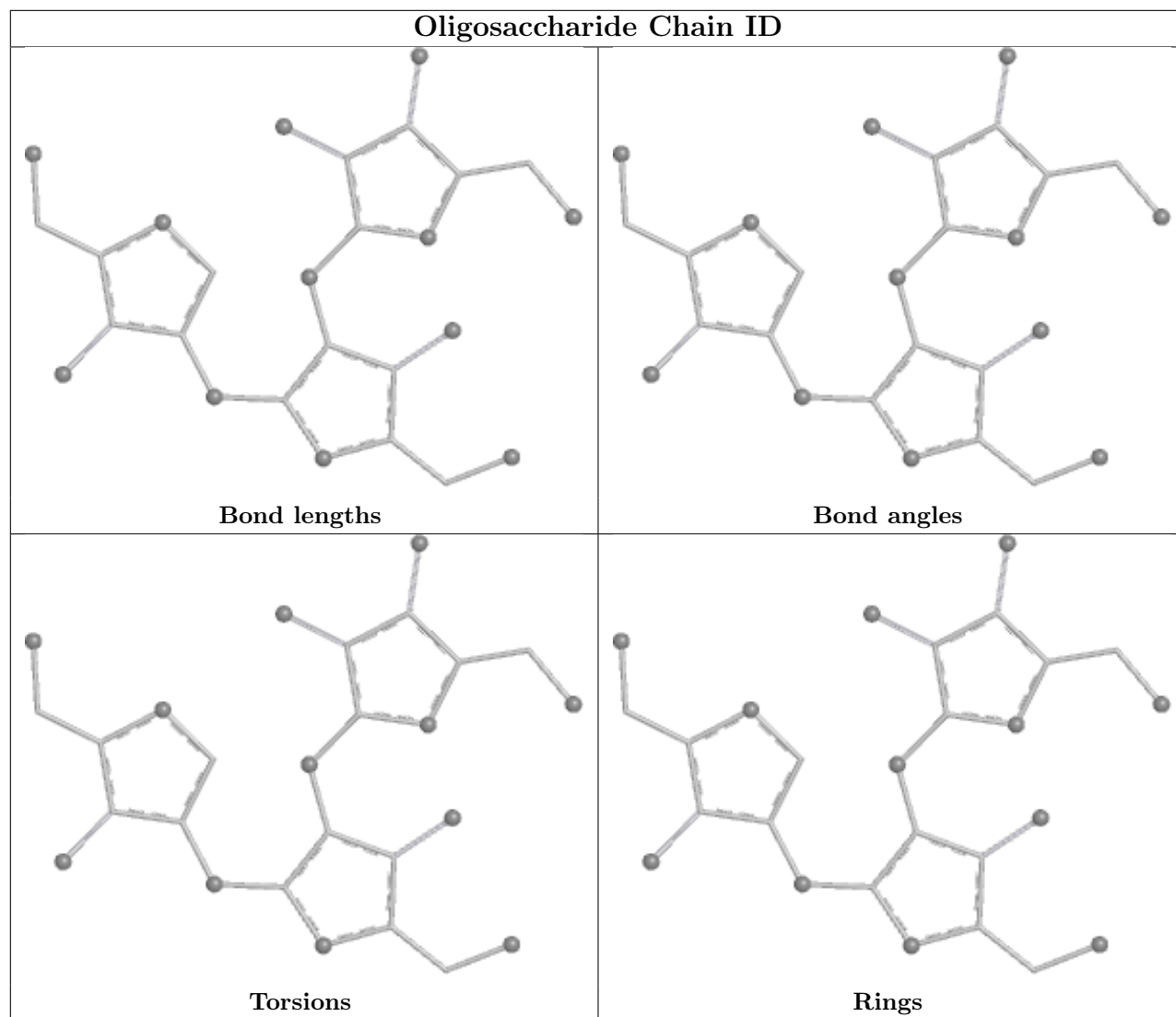
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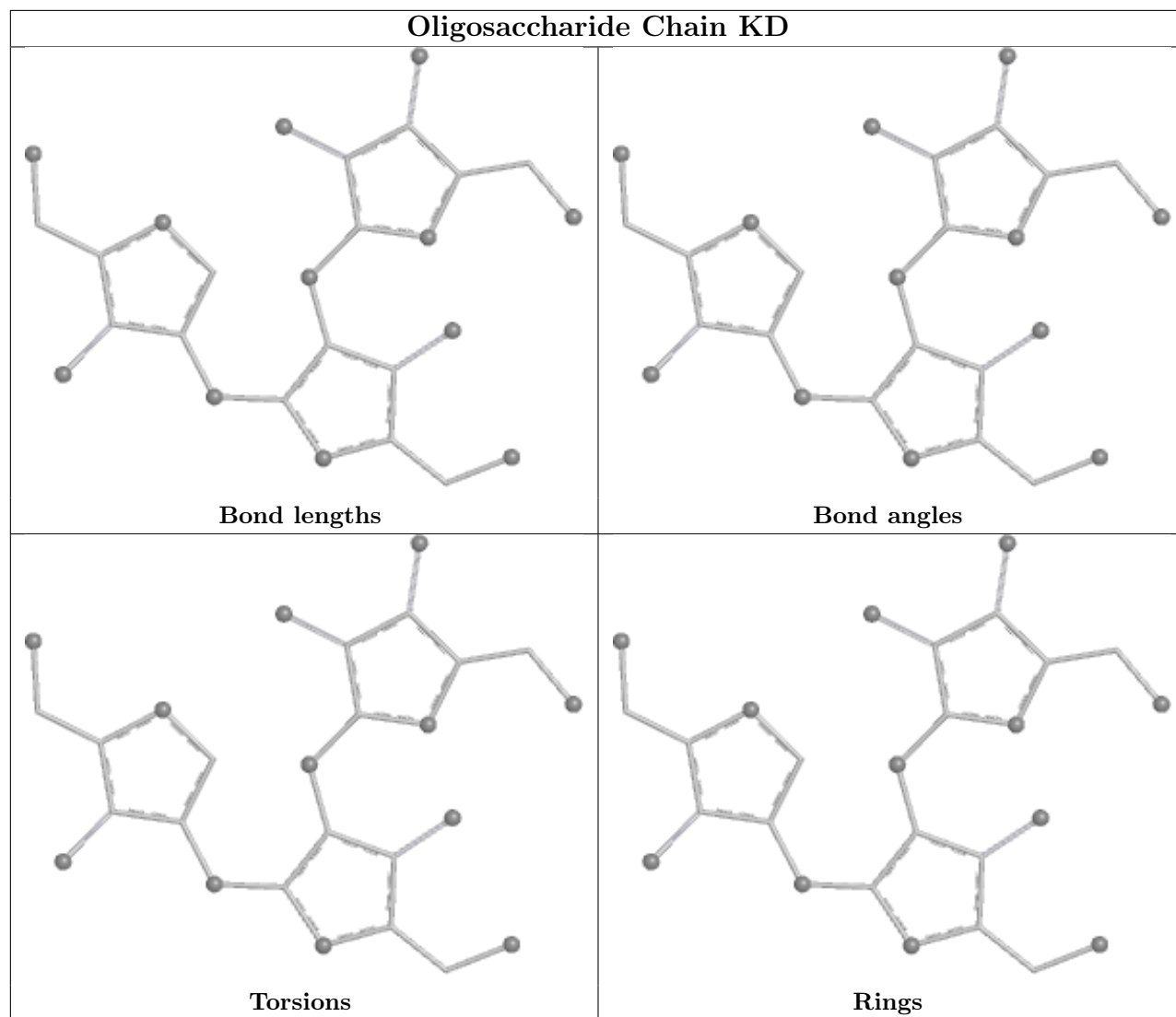


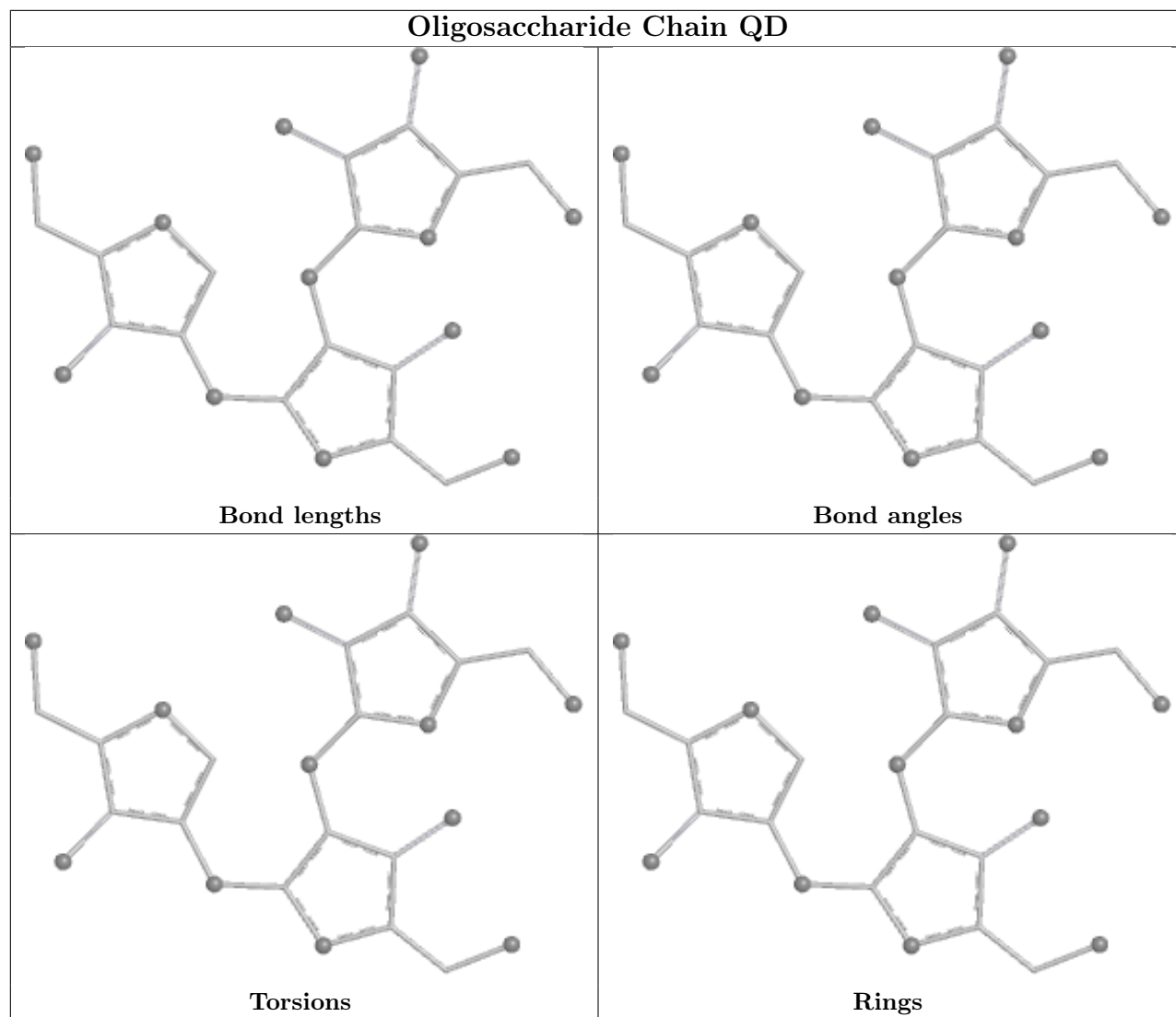


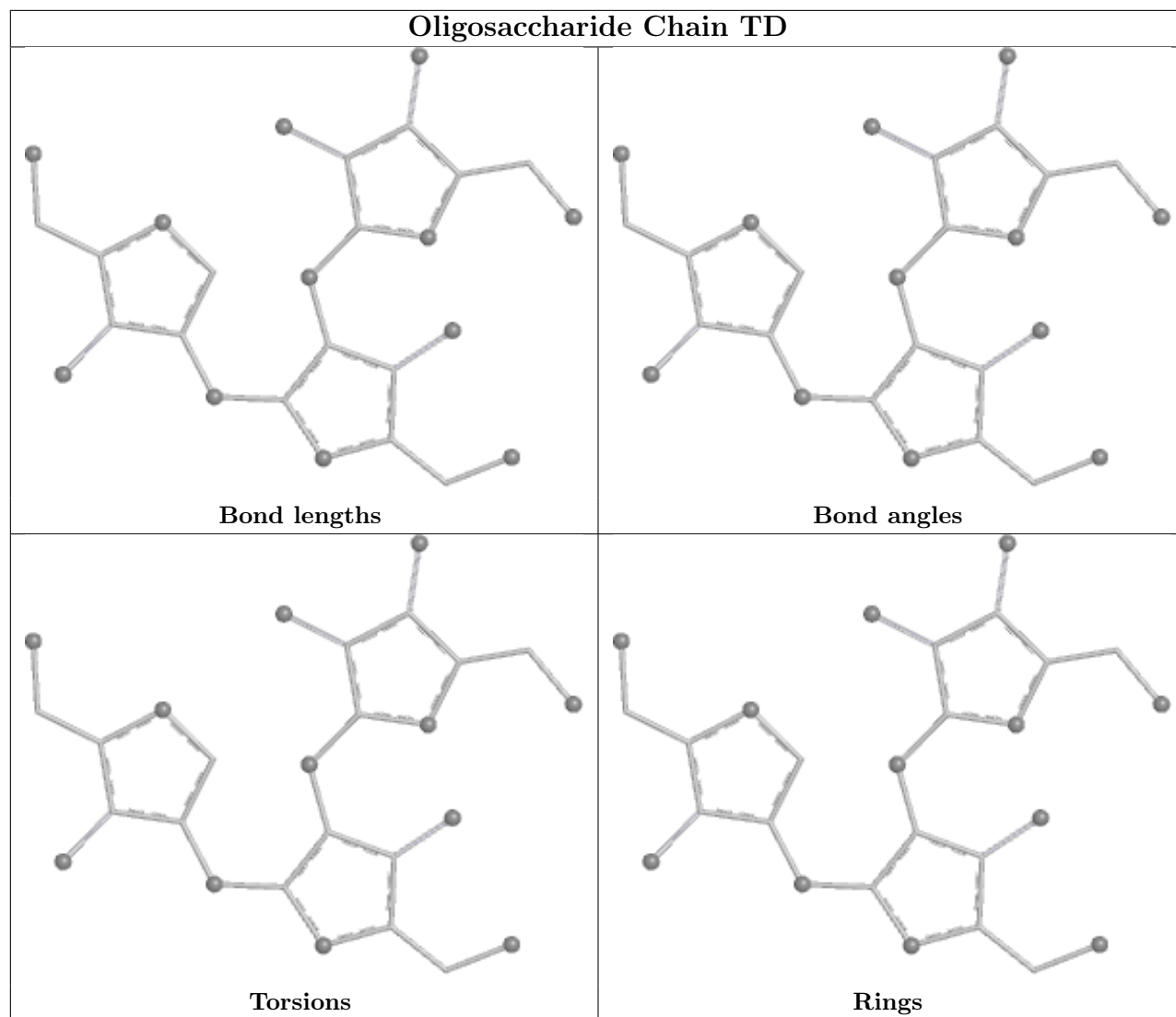


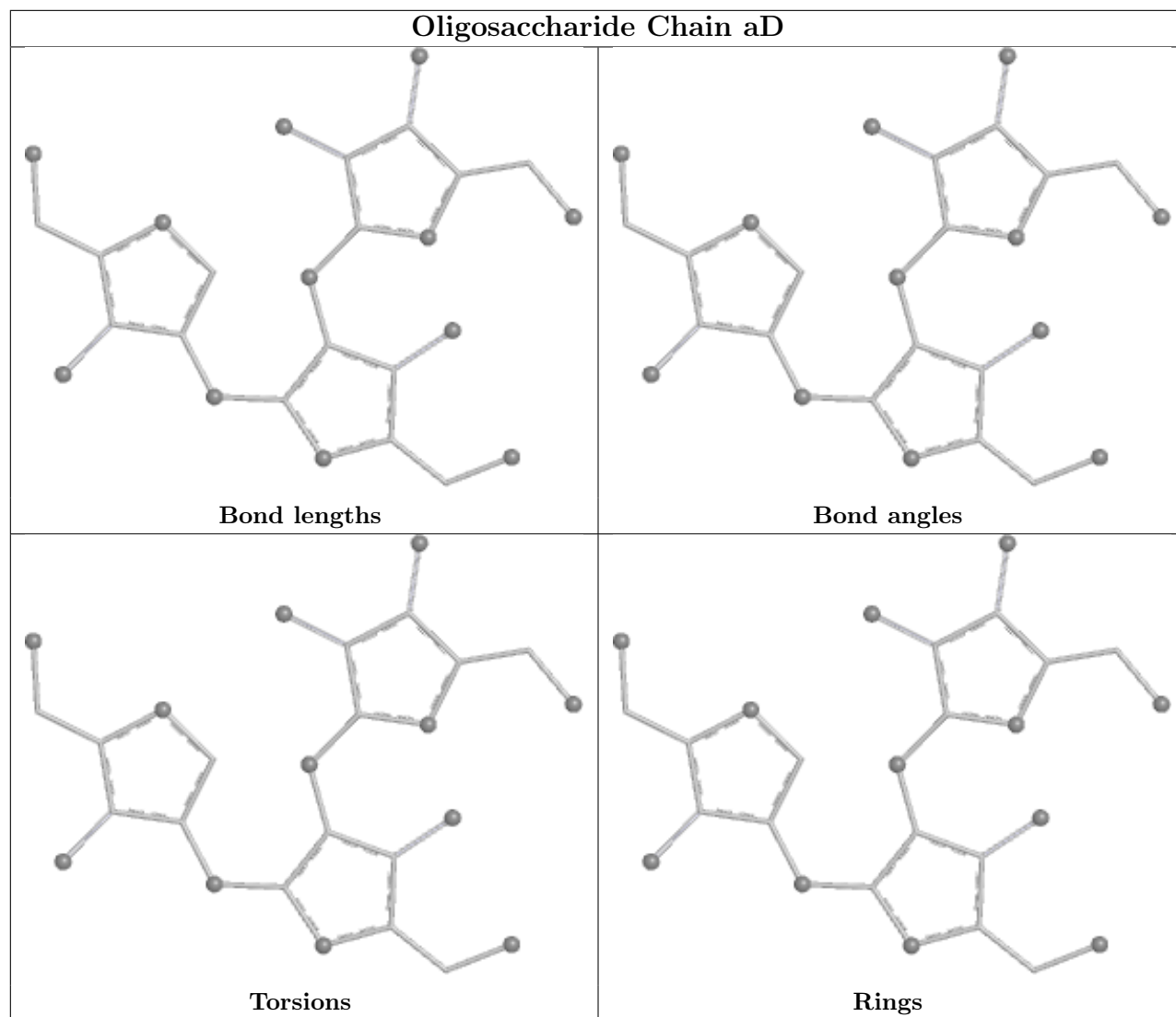


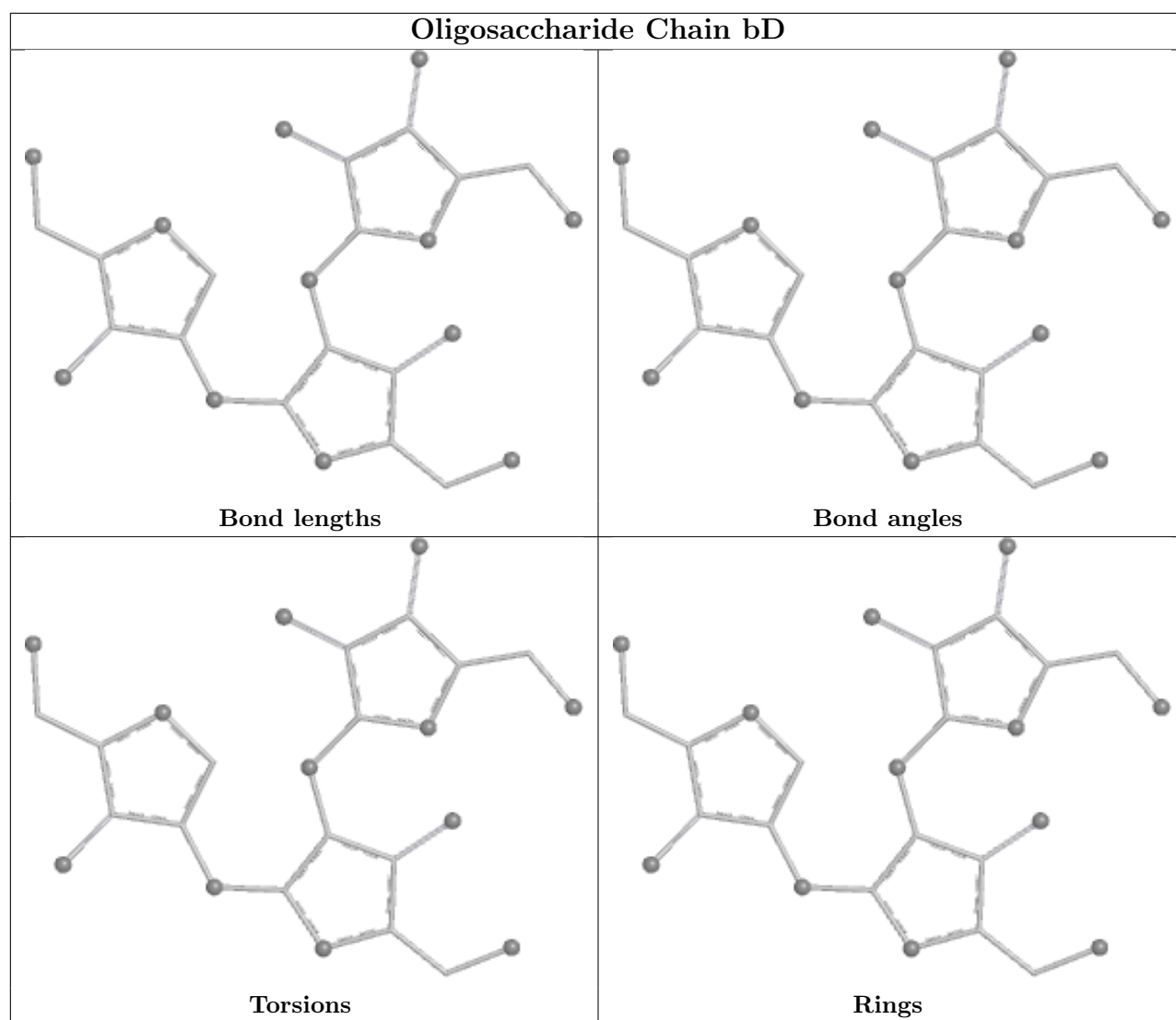


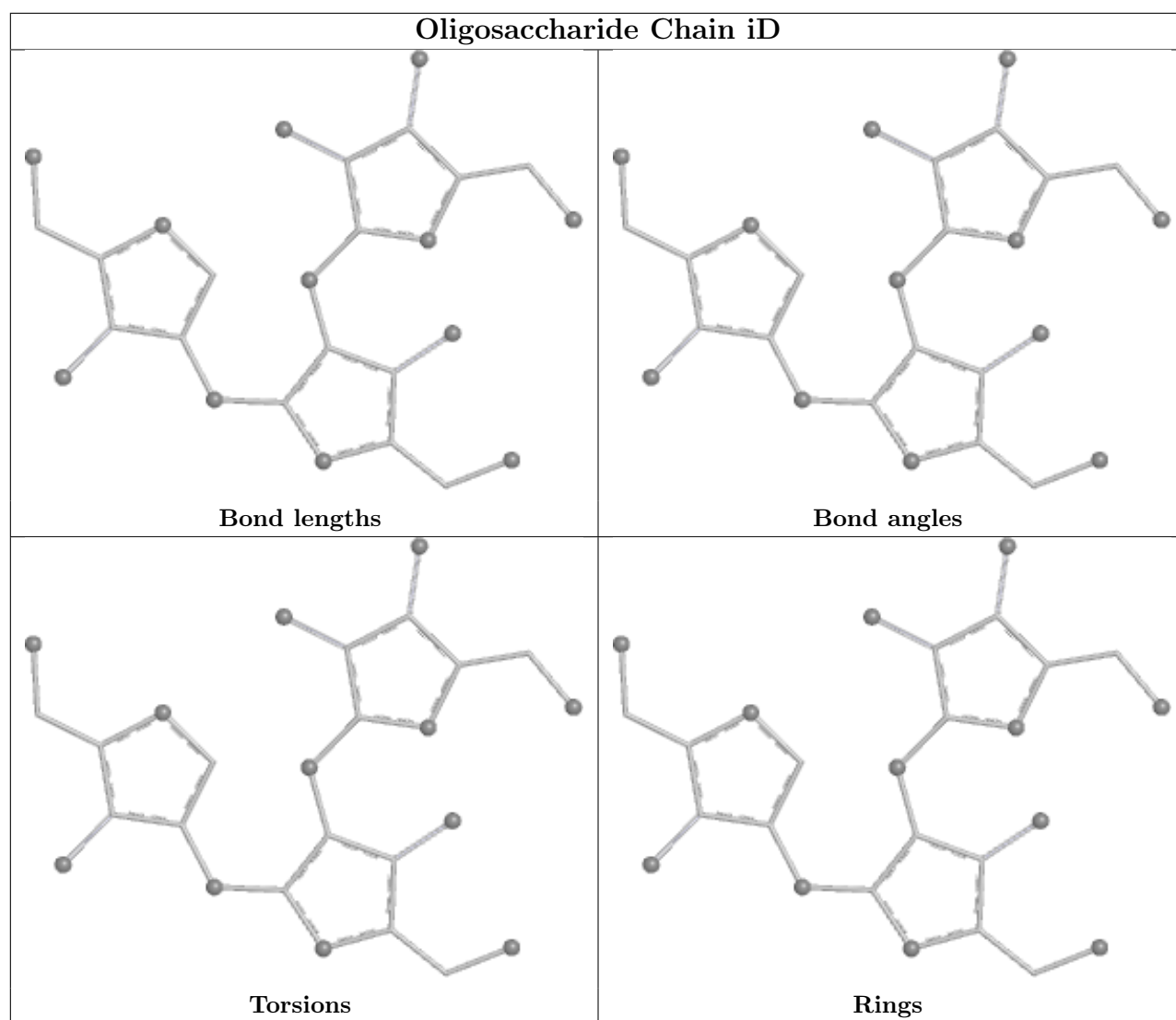


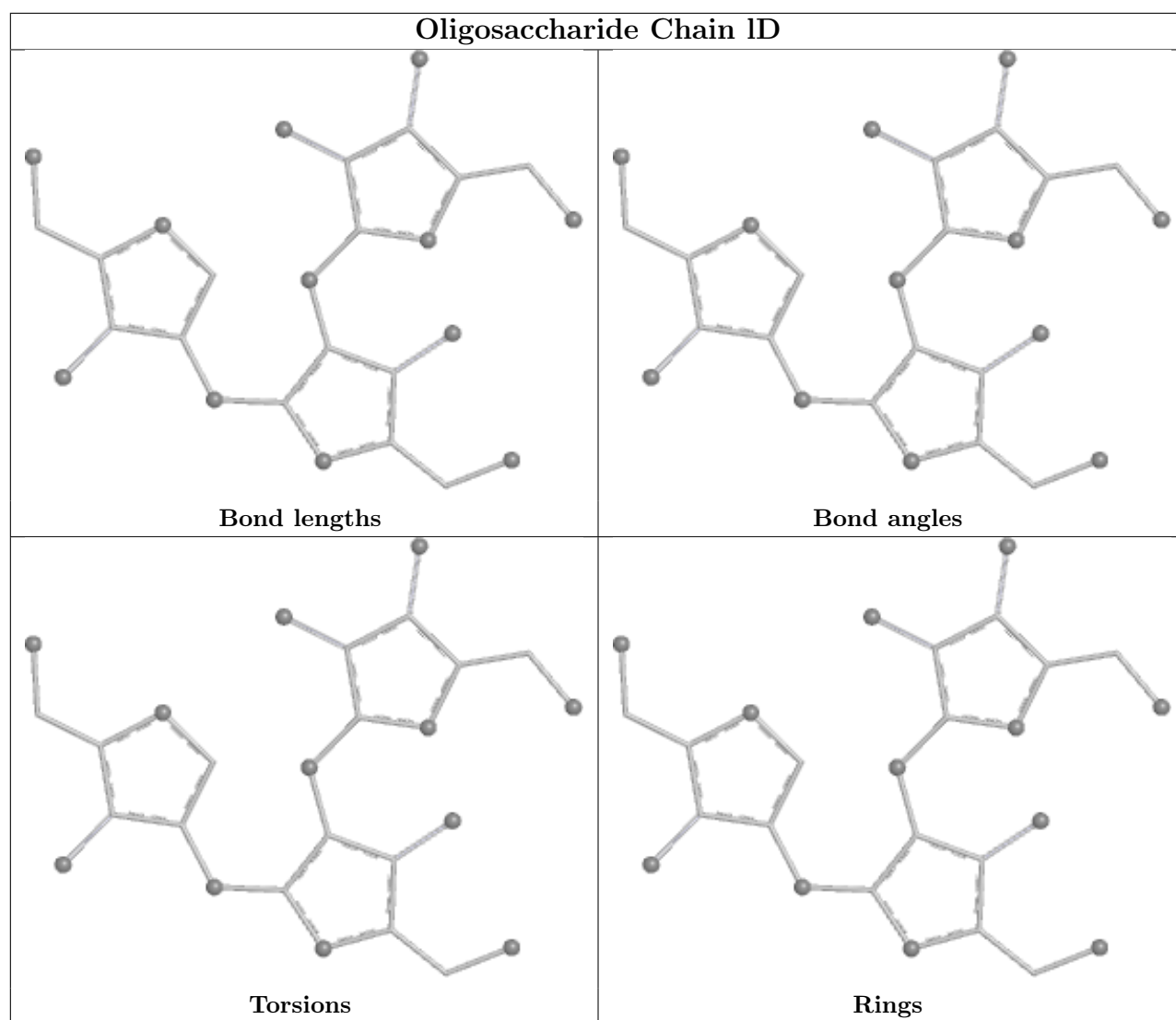


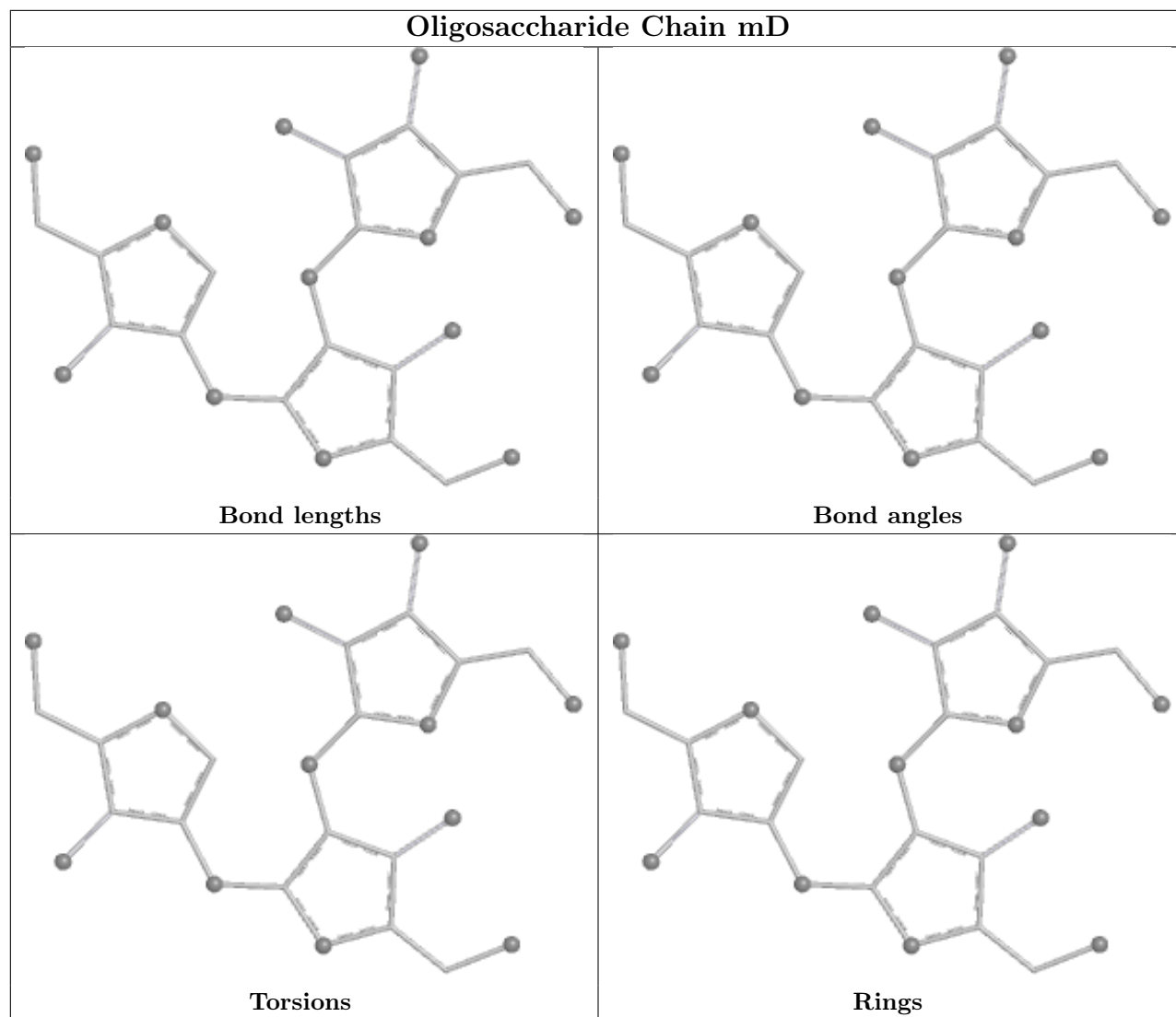


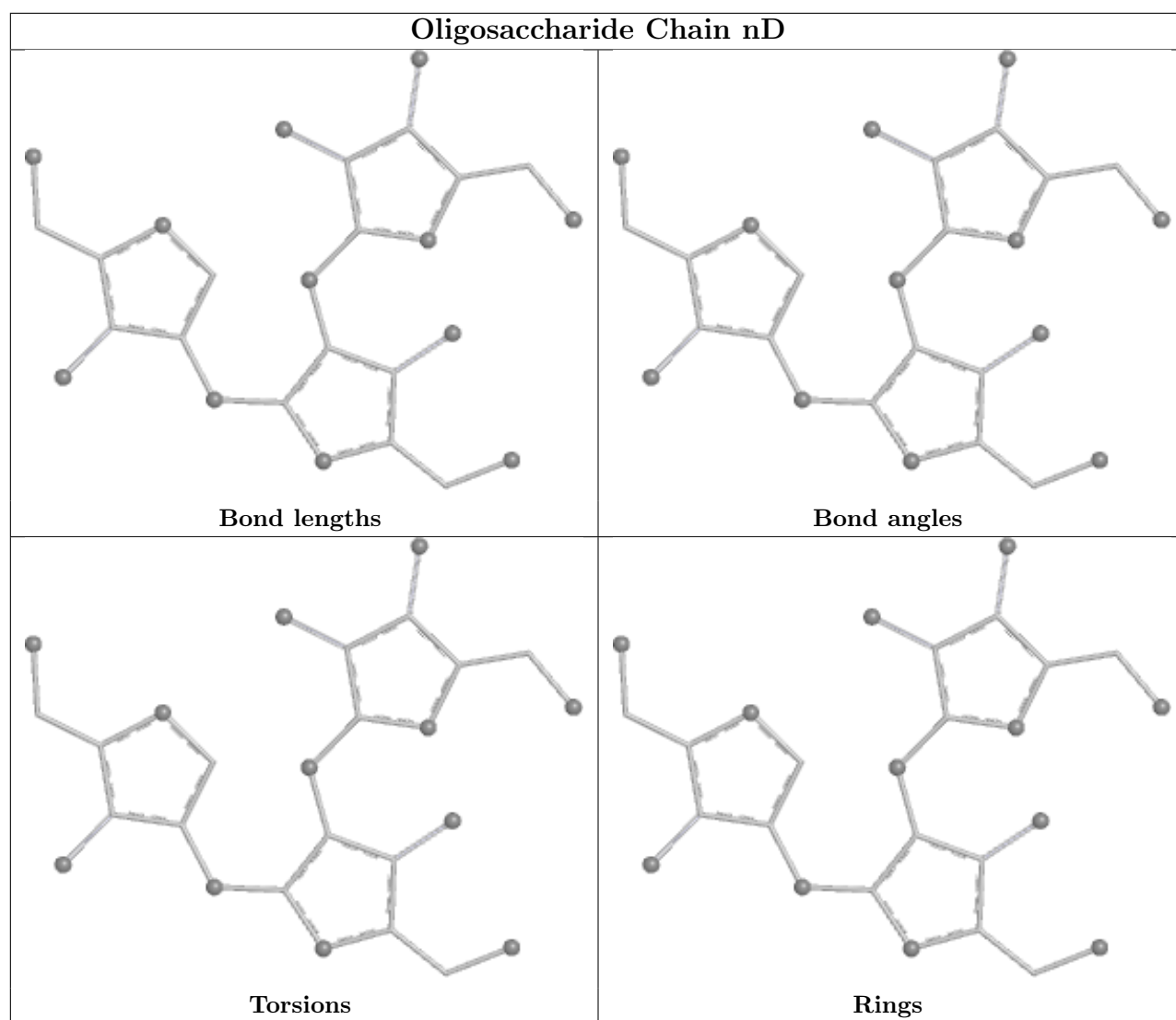


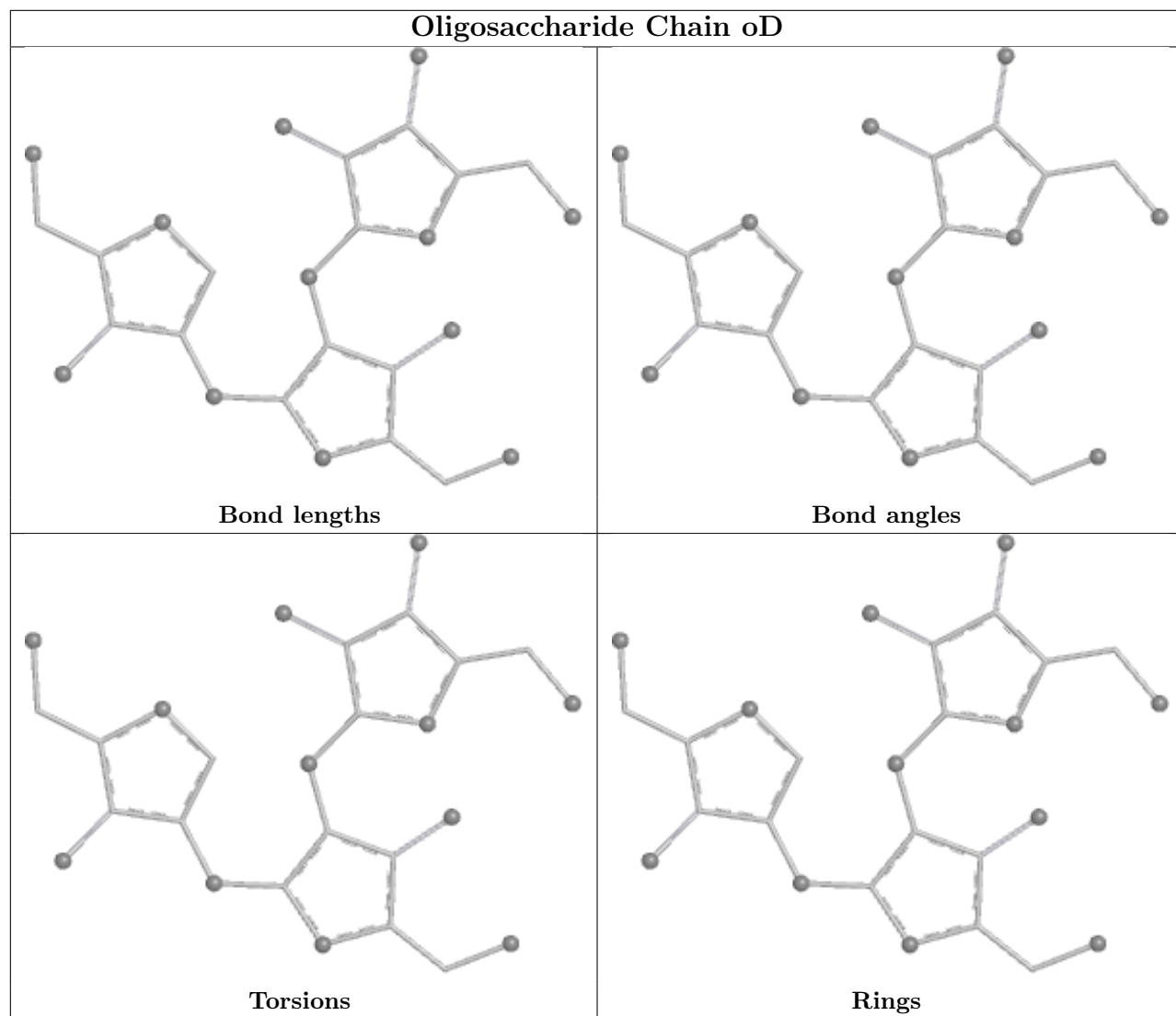


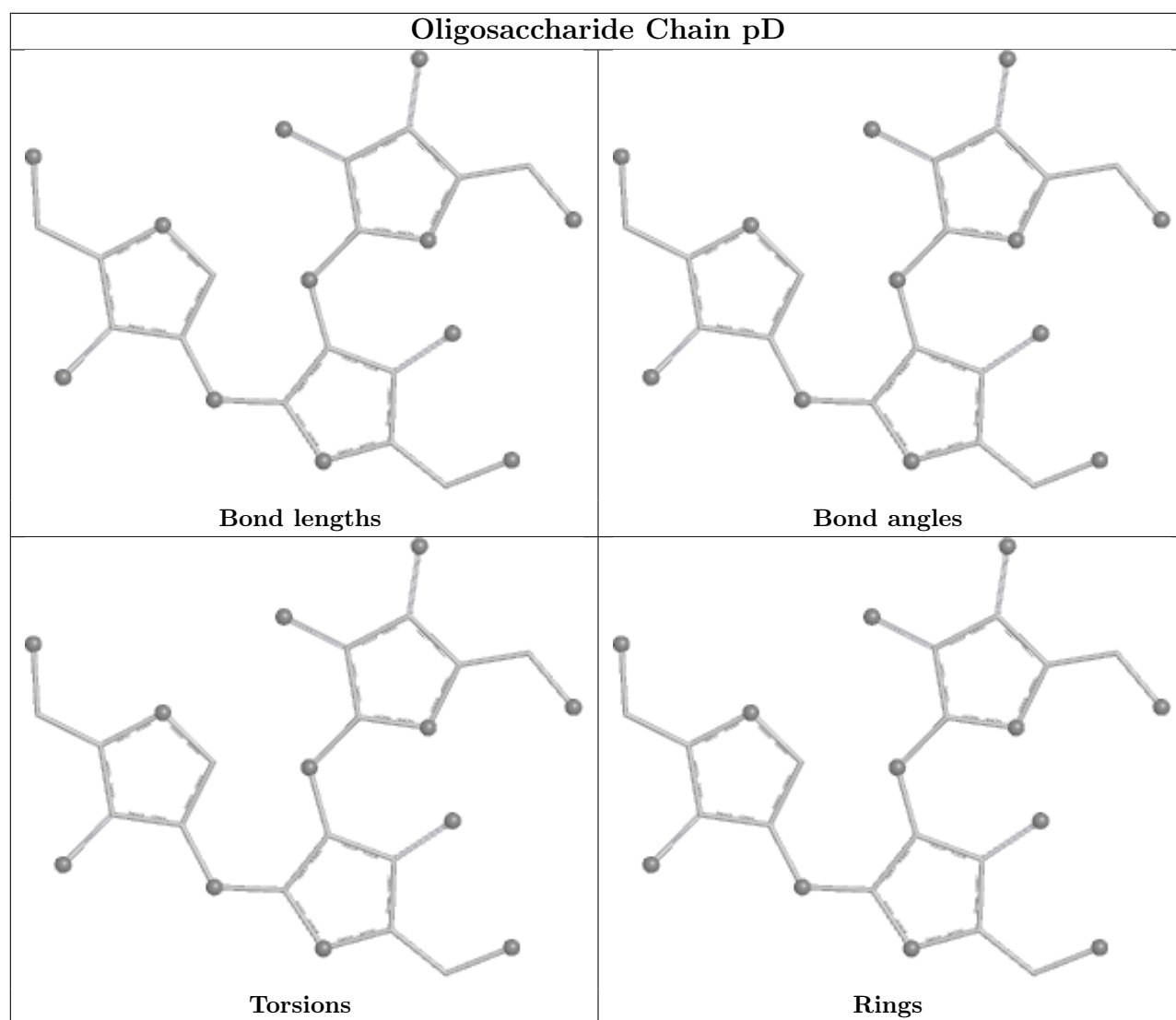


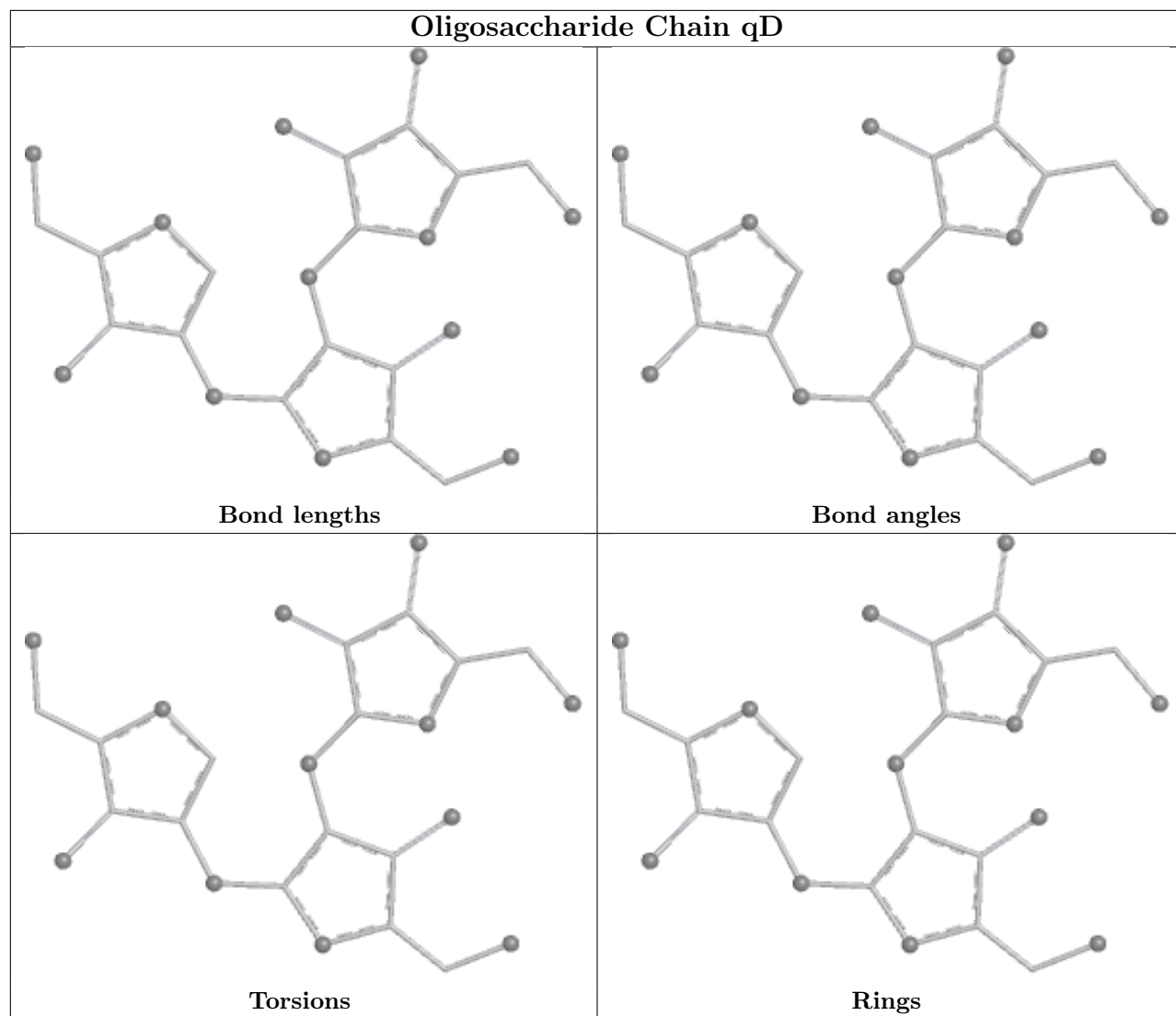


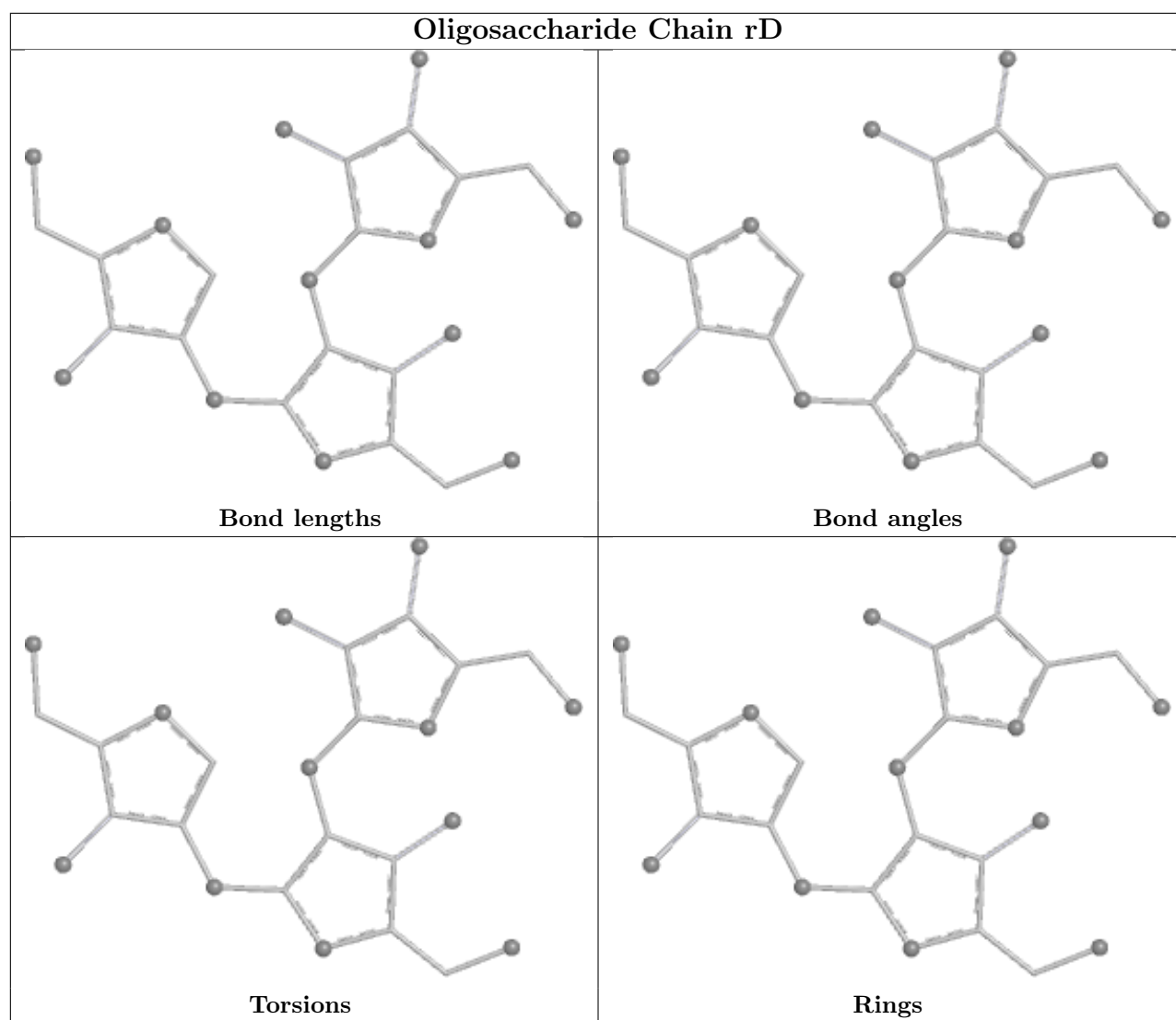


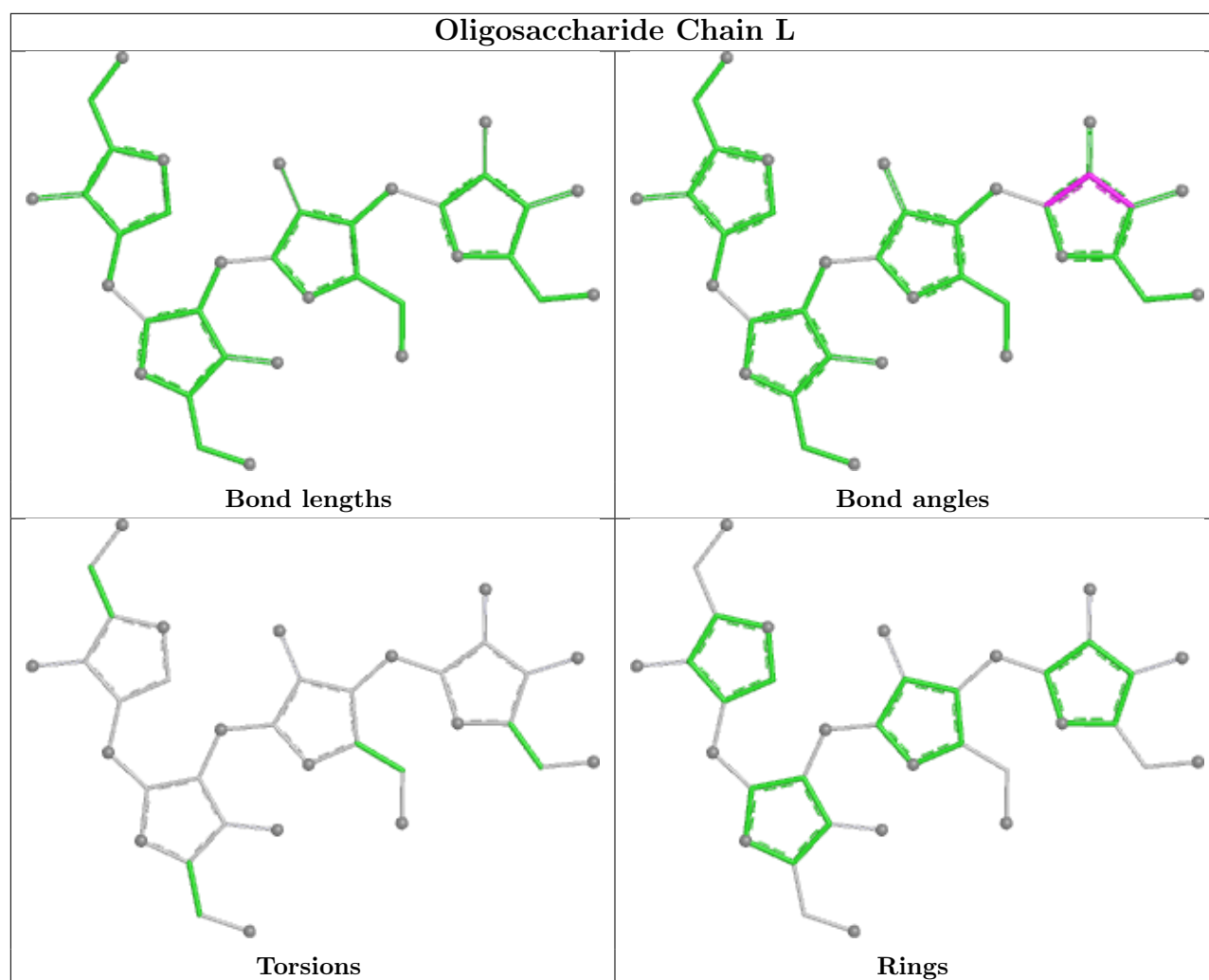


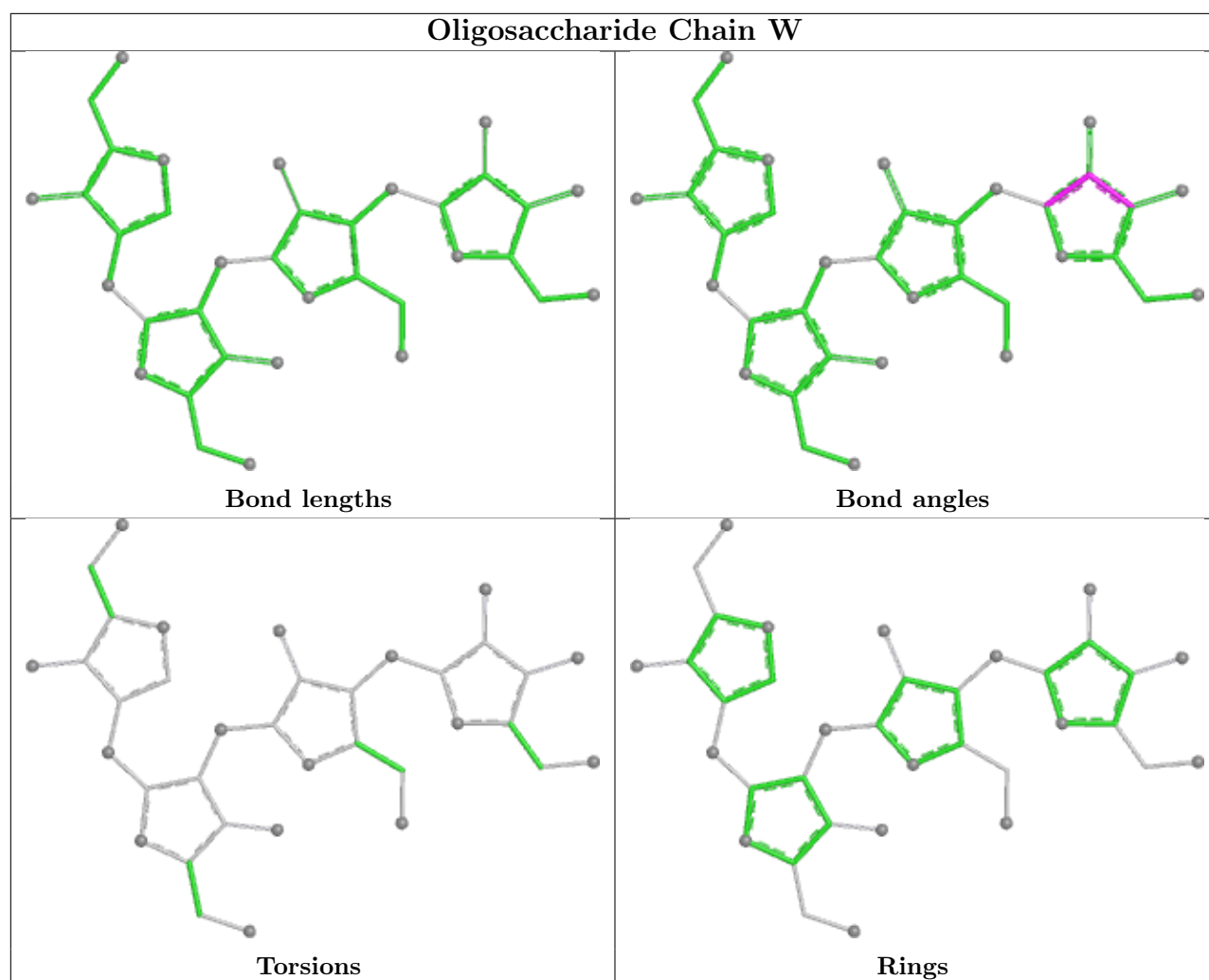


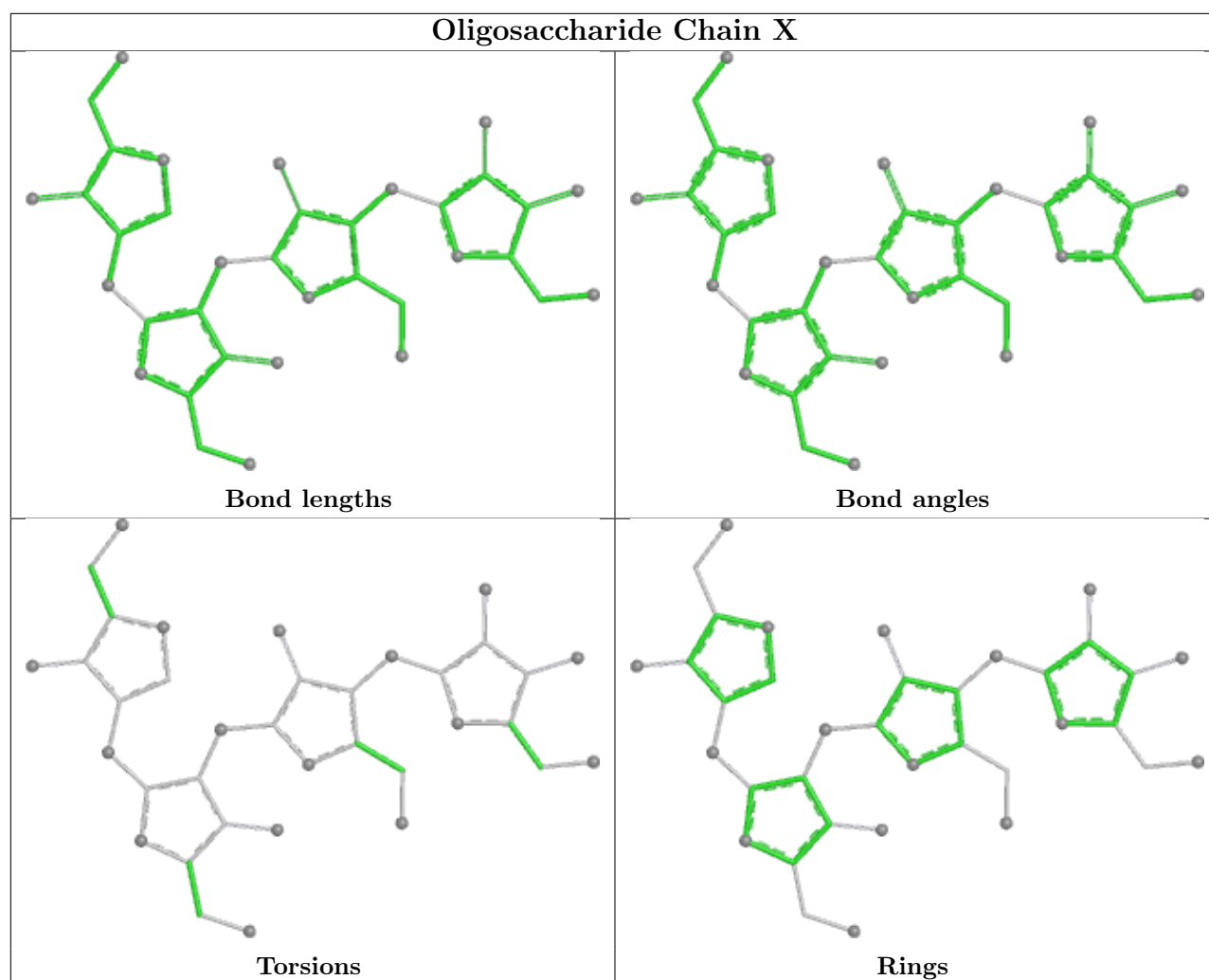


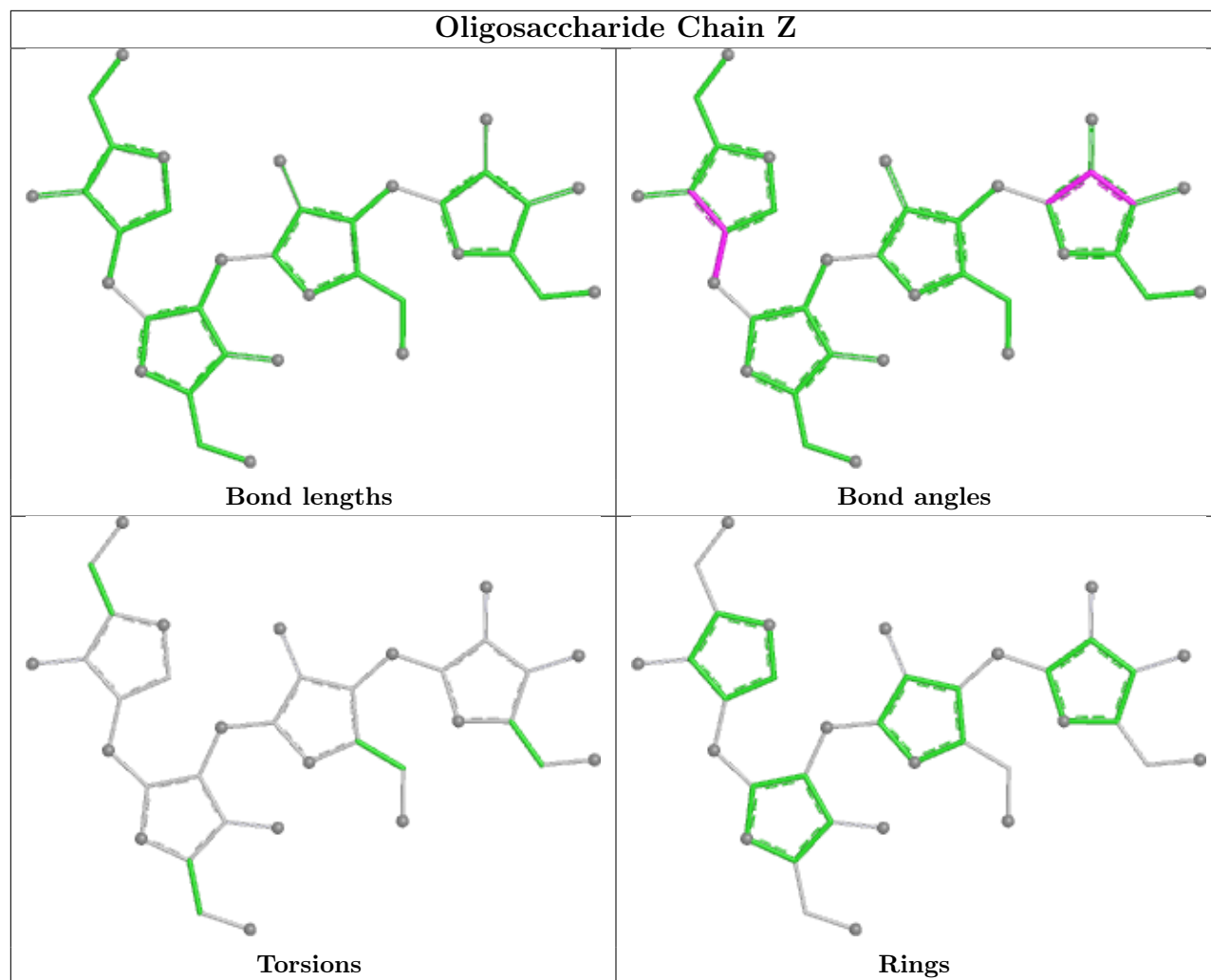


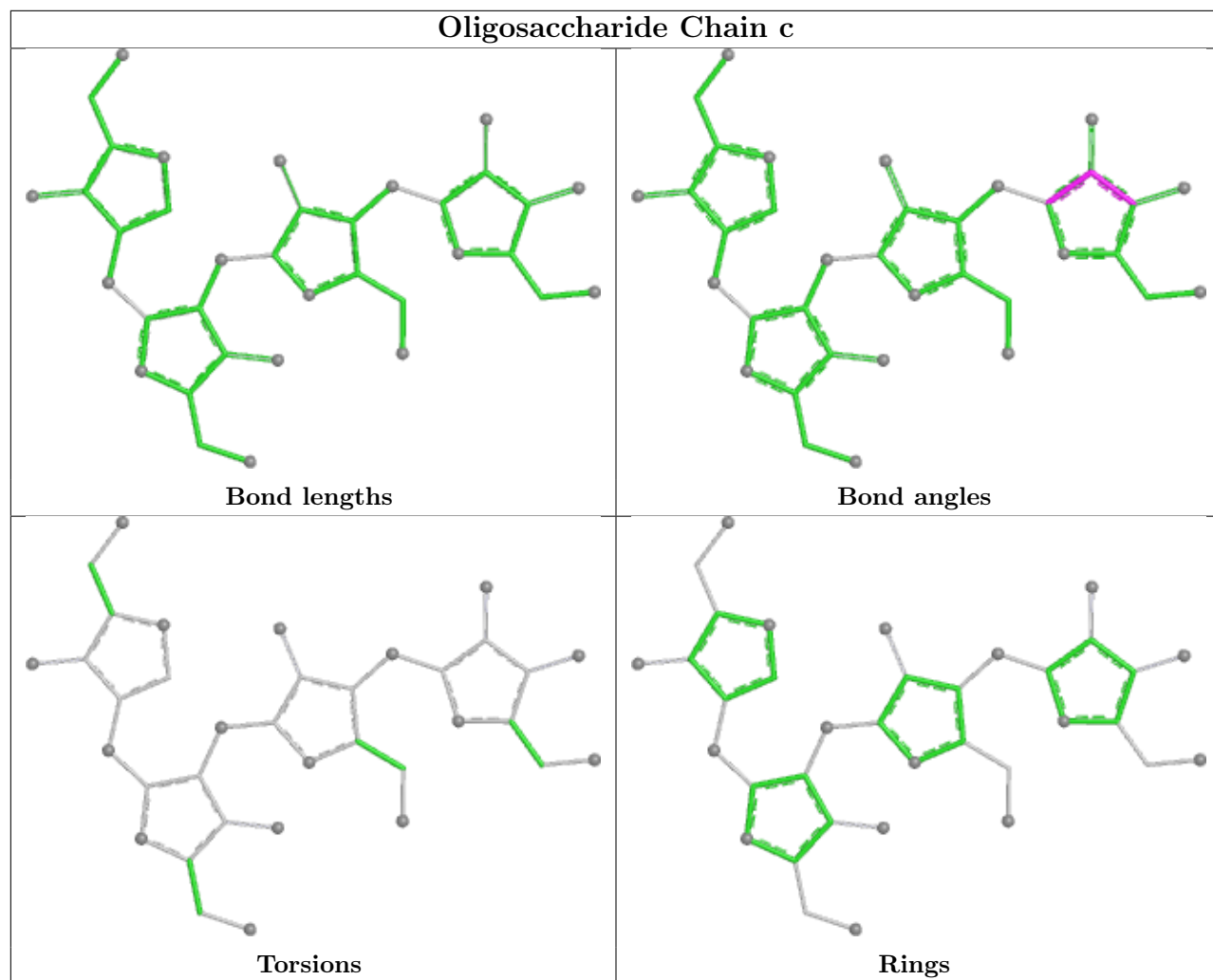


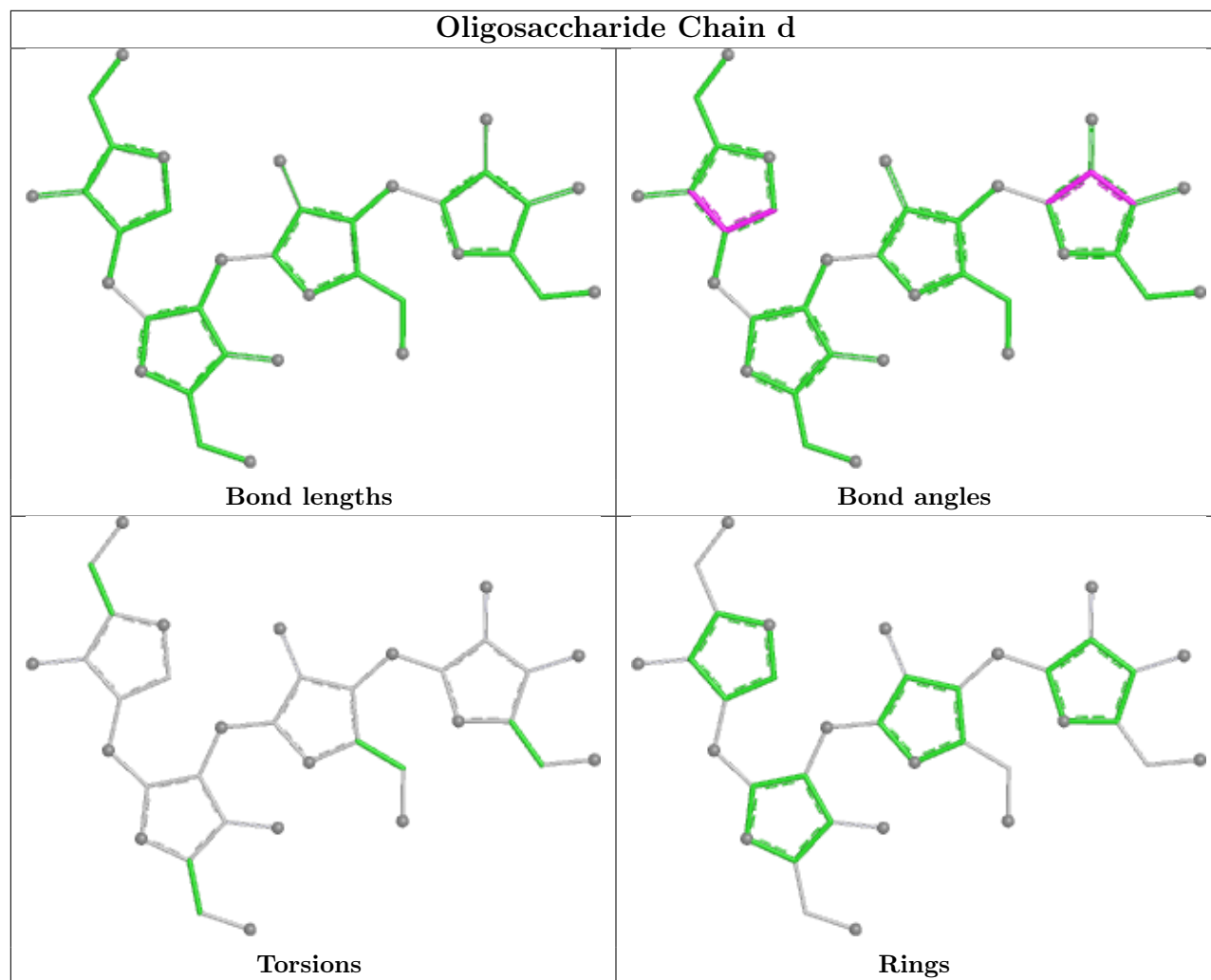


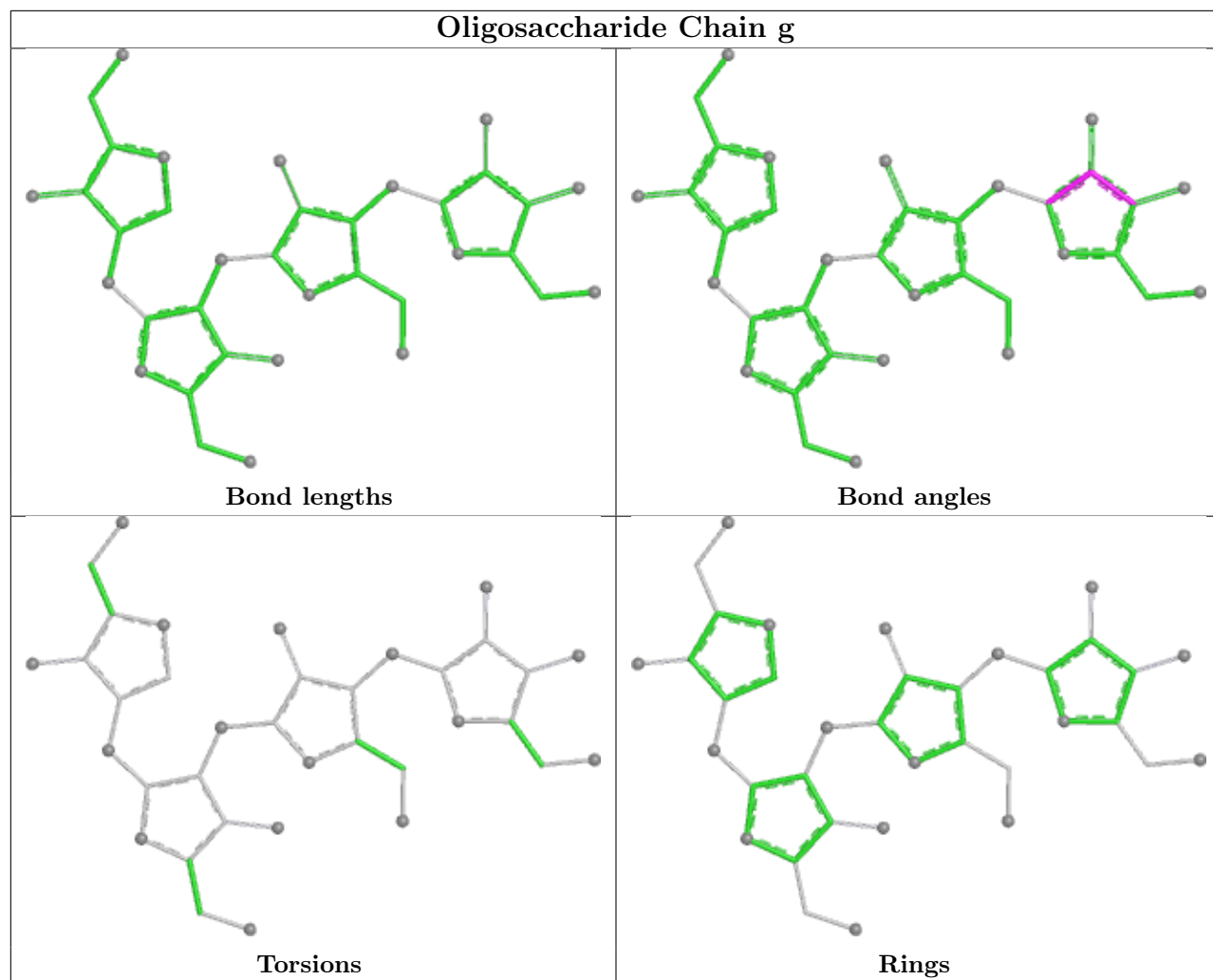


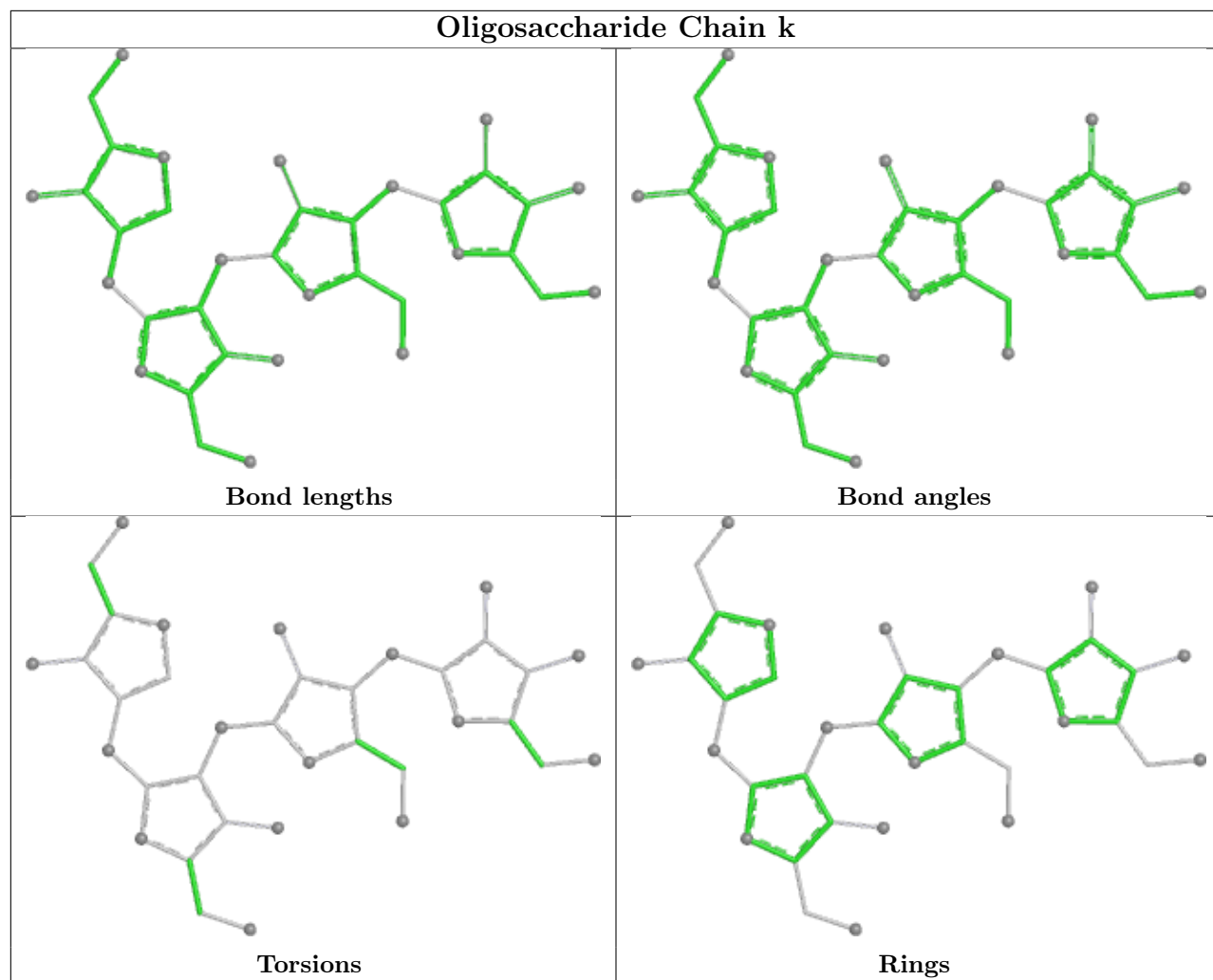


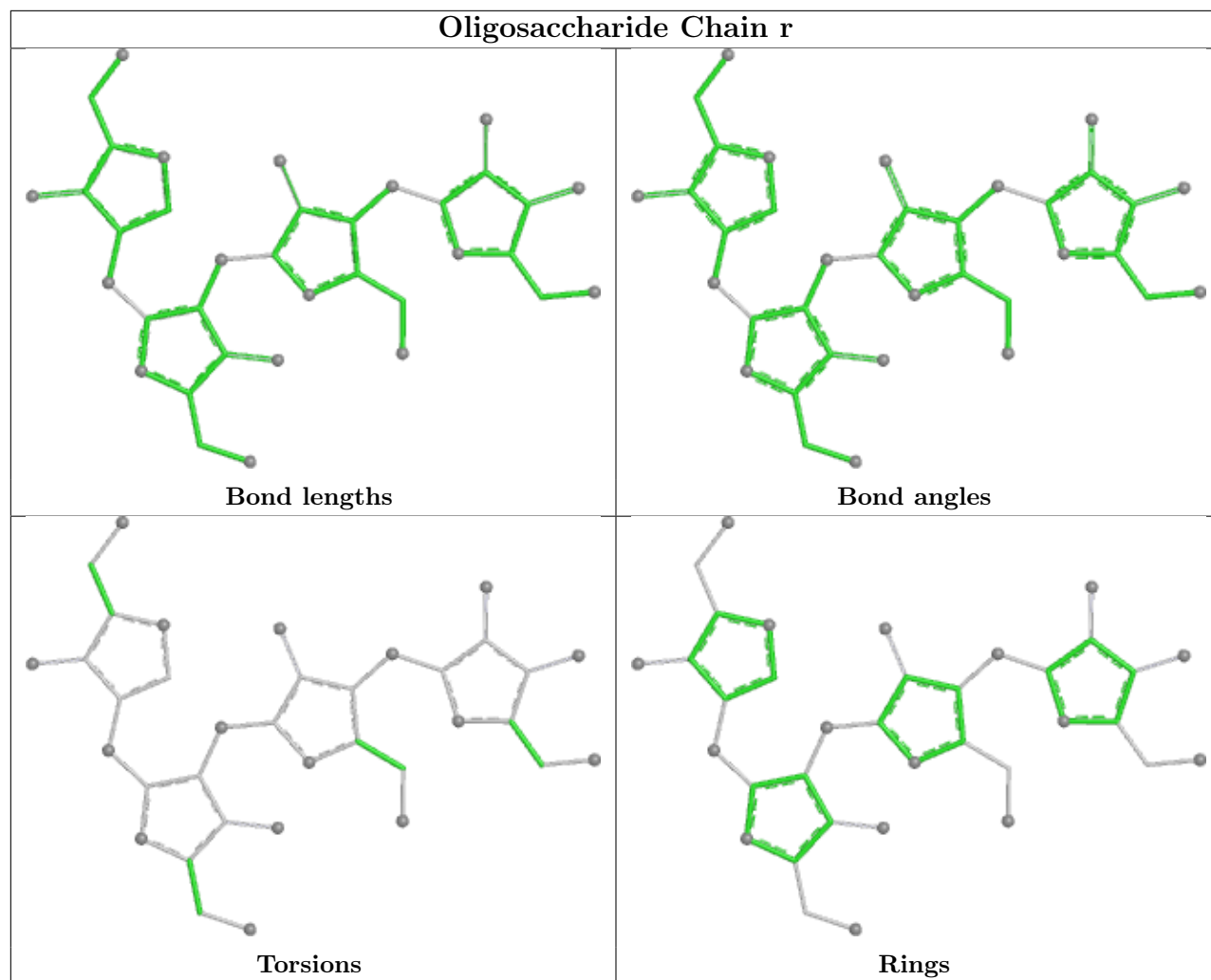


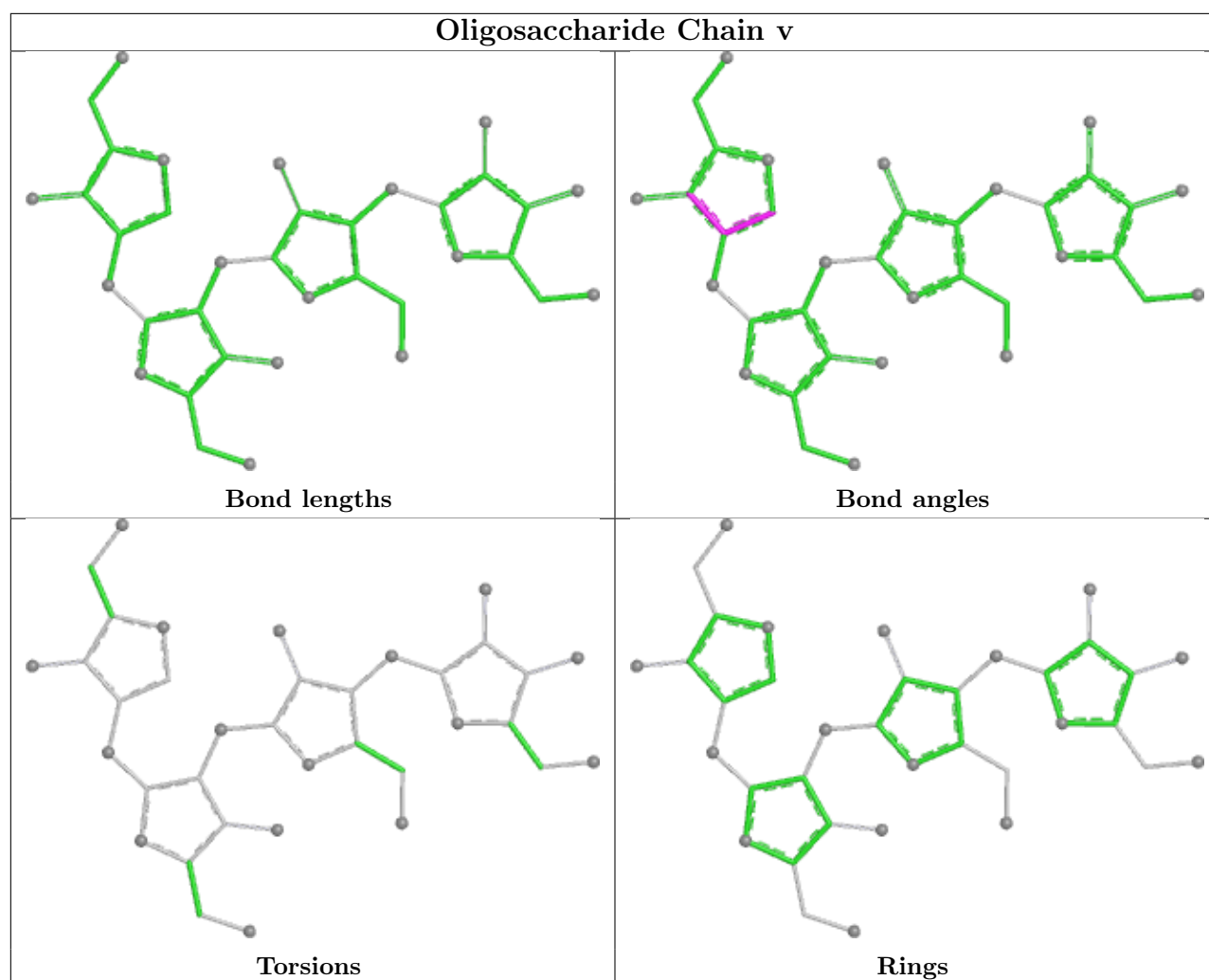


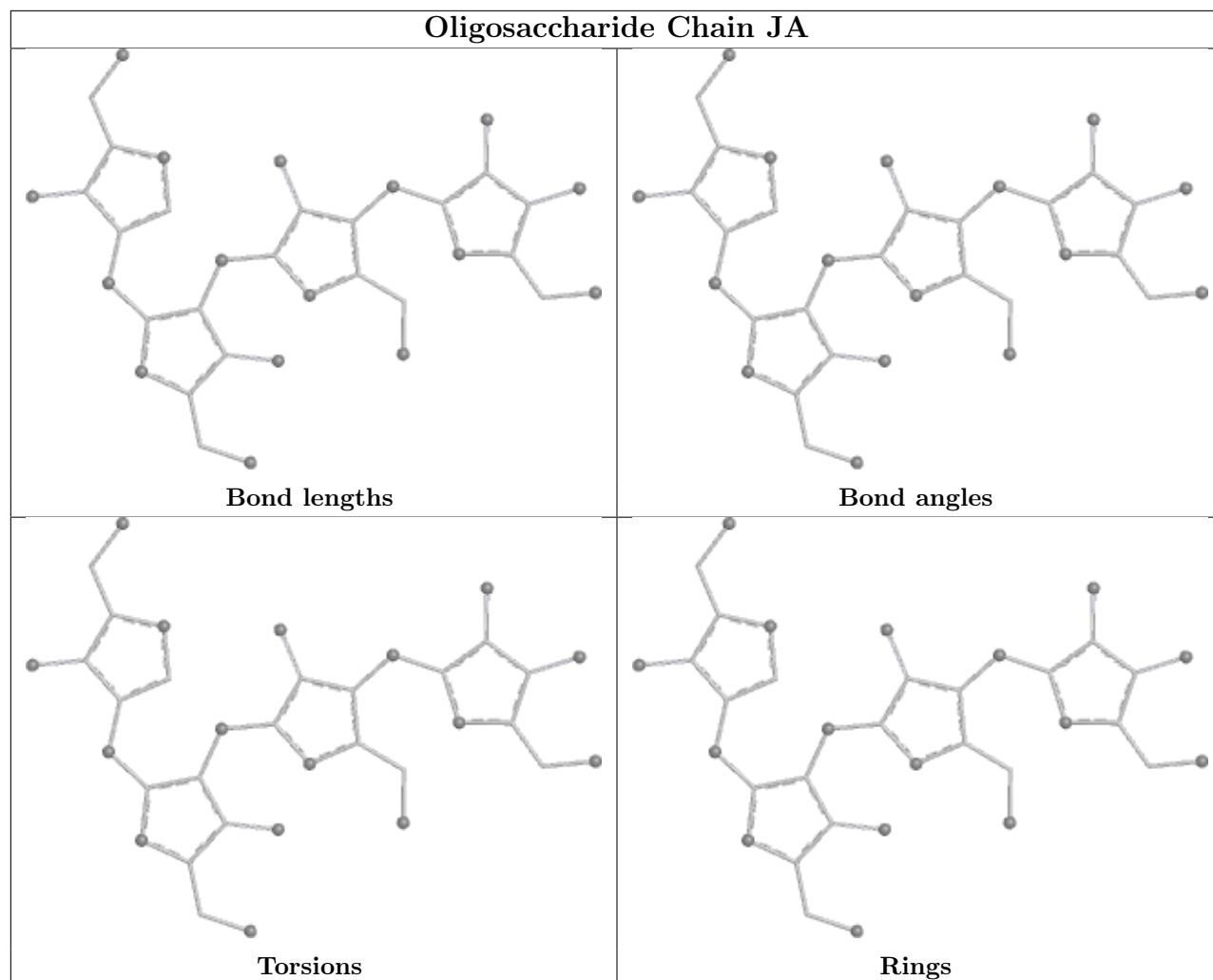


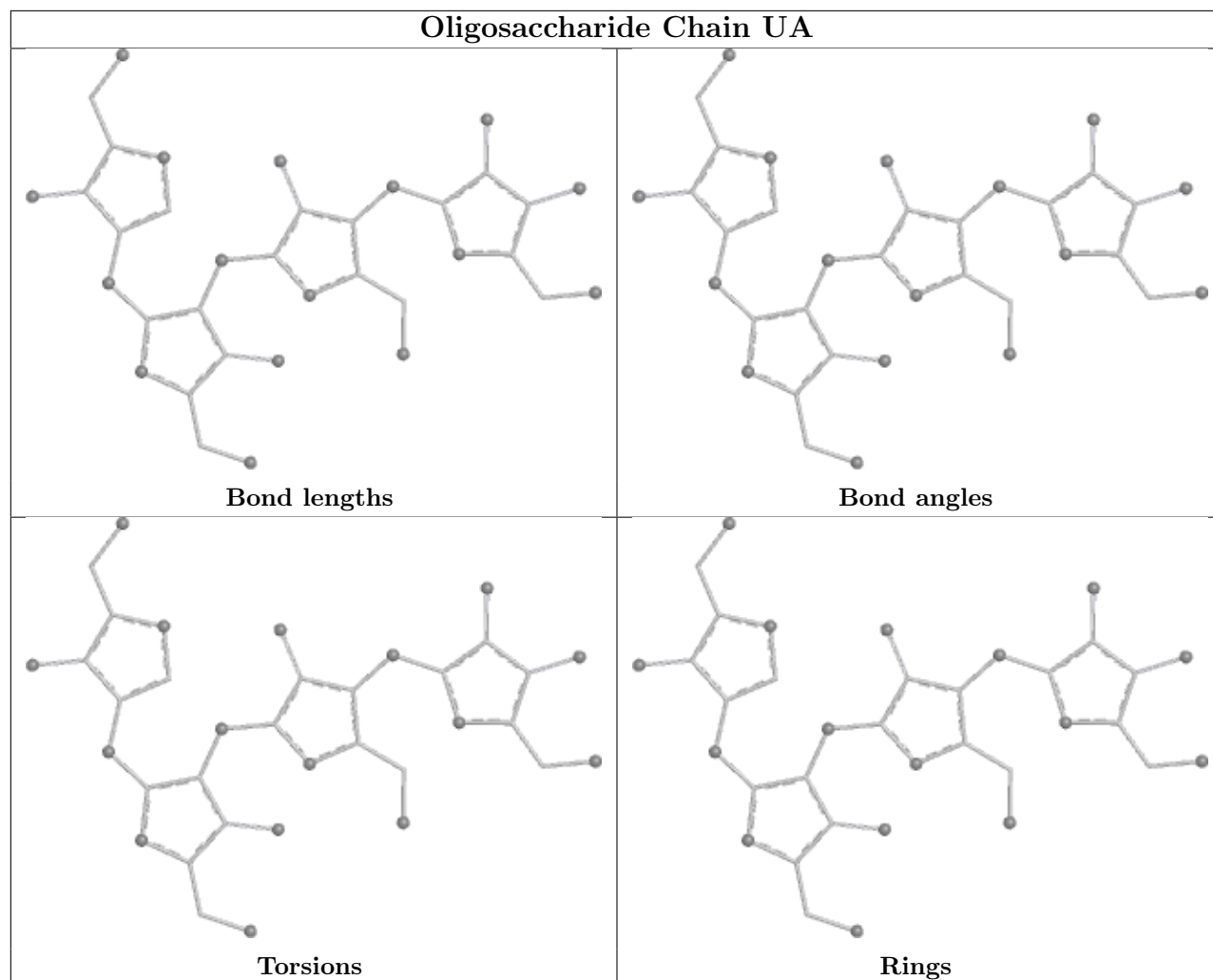




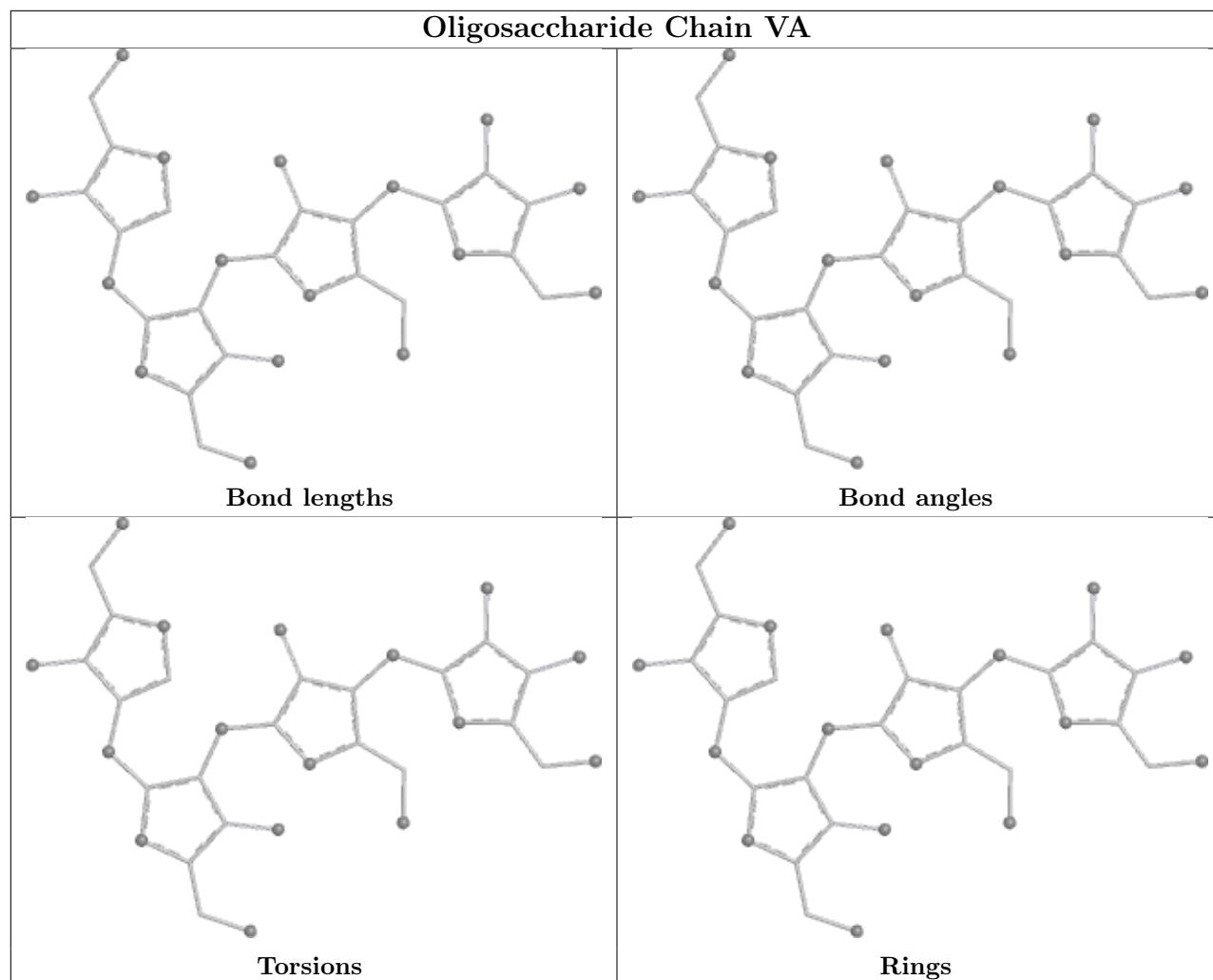


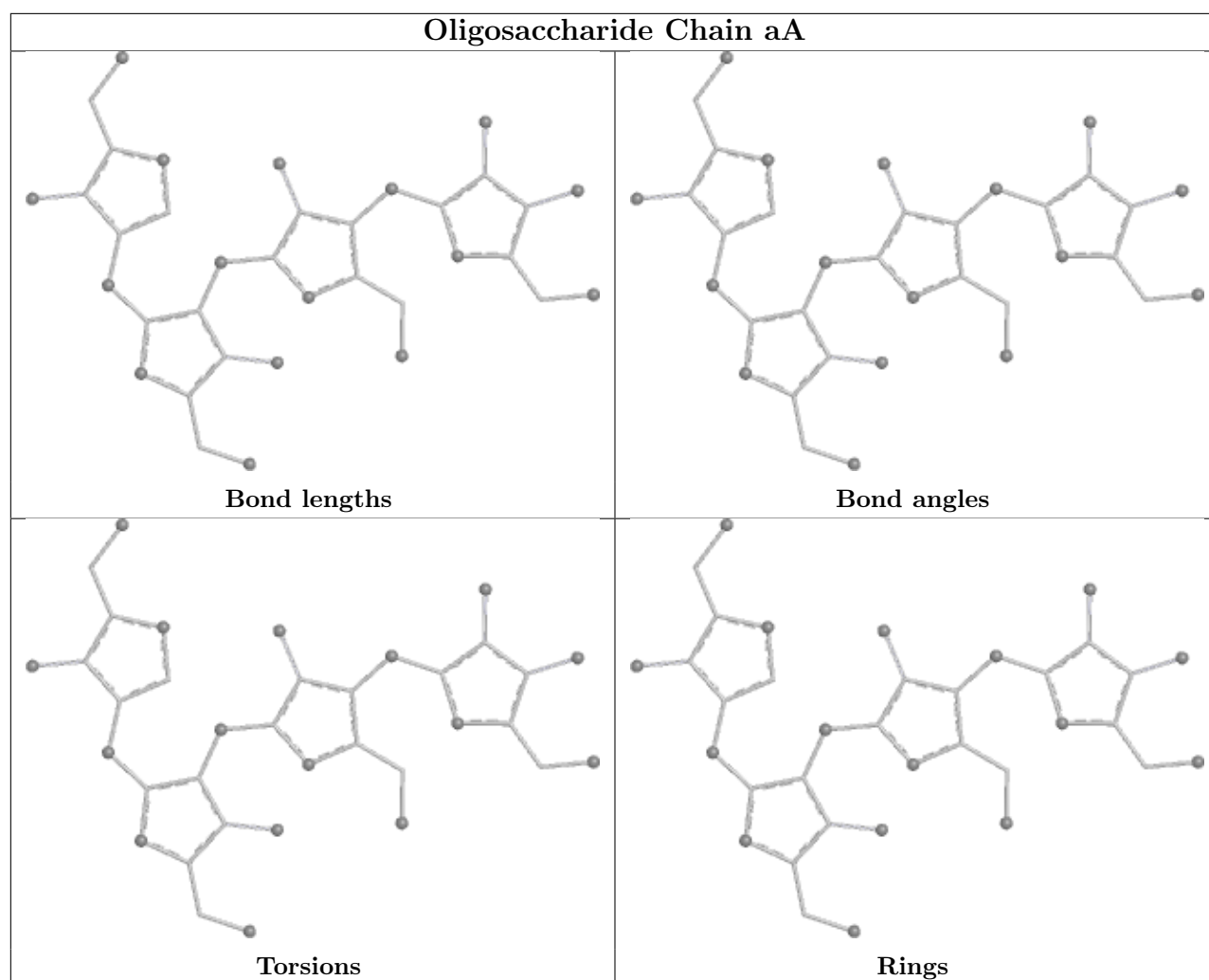


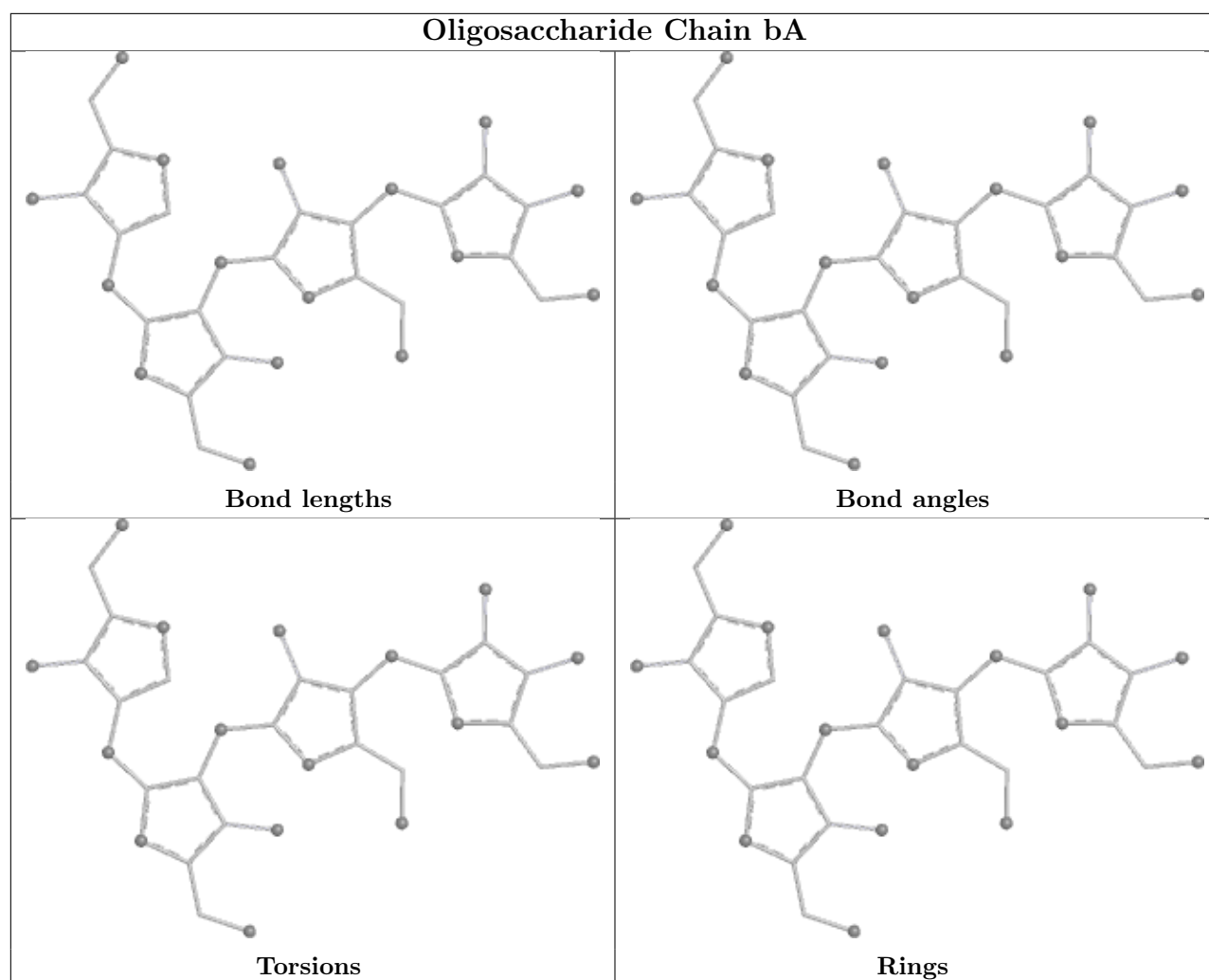
Oligosaccharide Chain JA

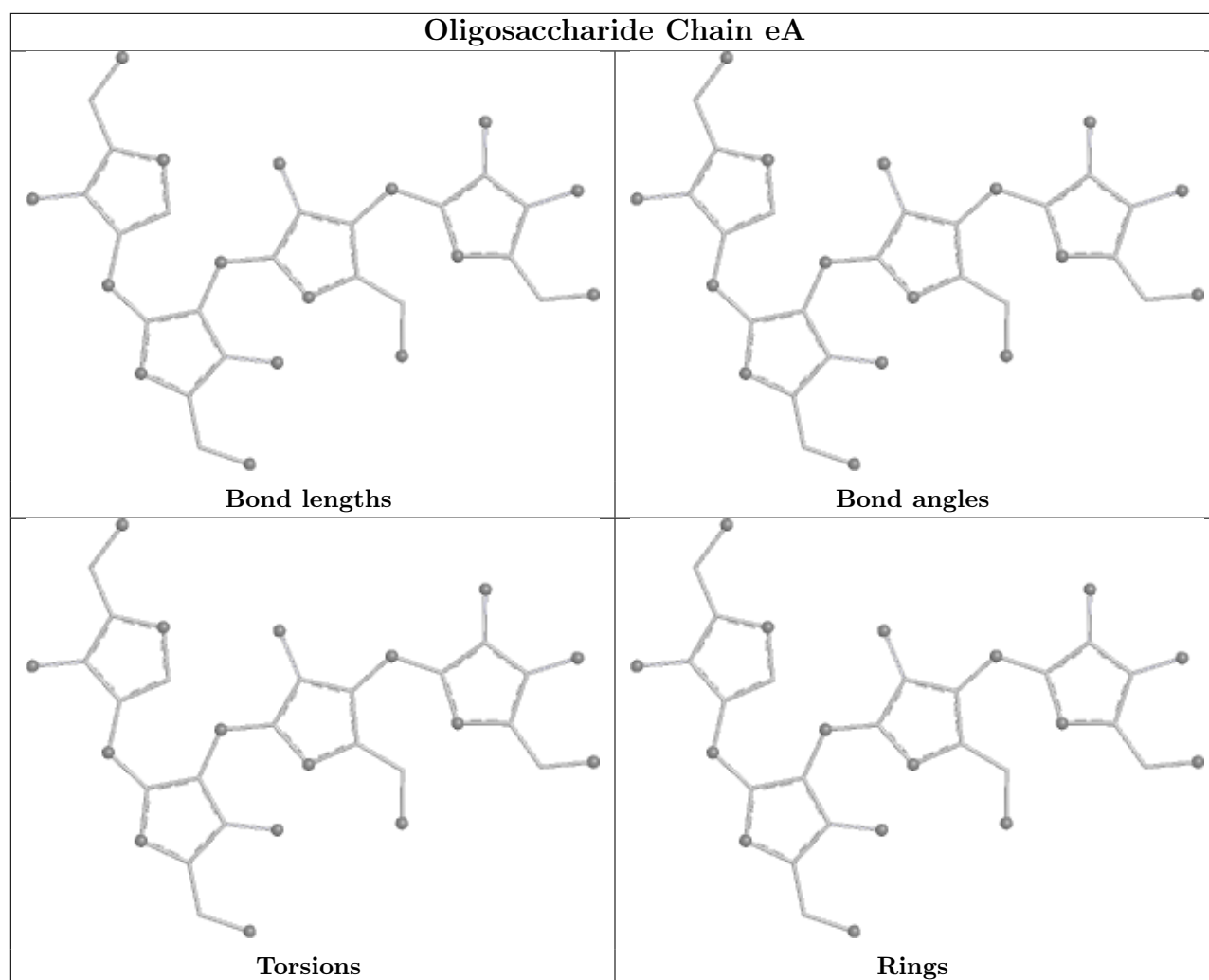
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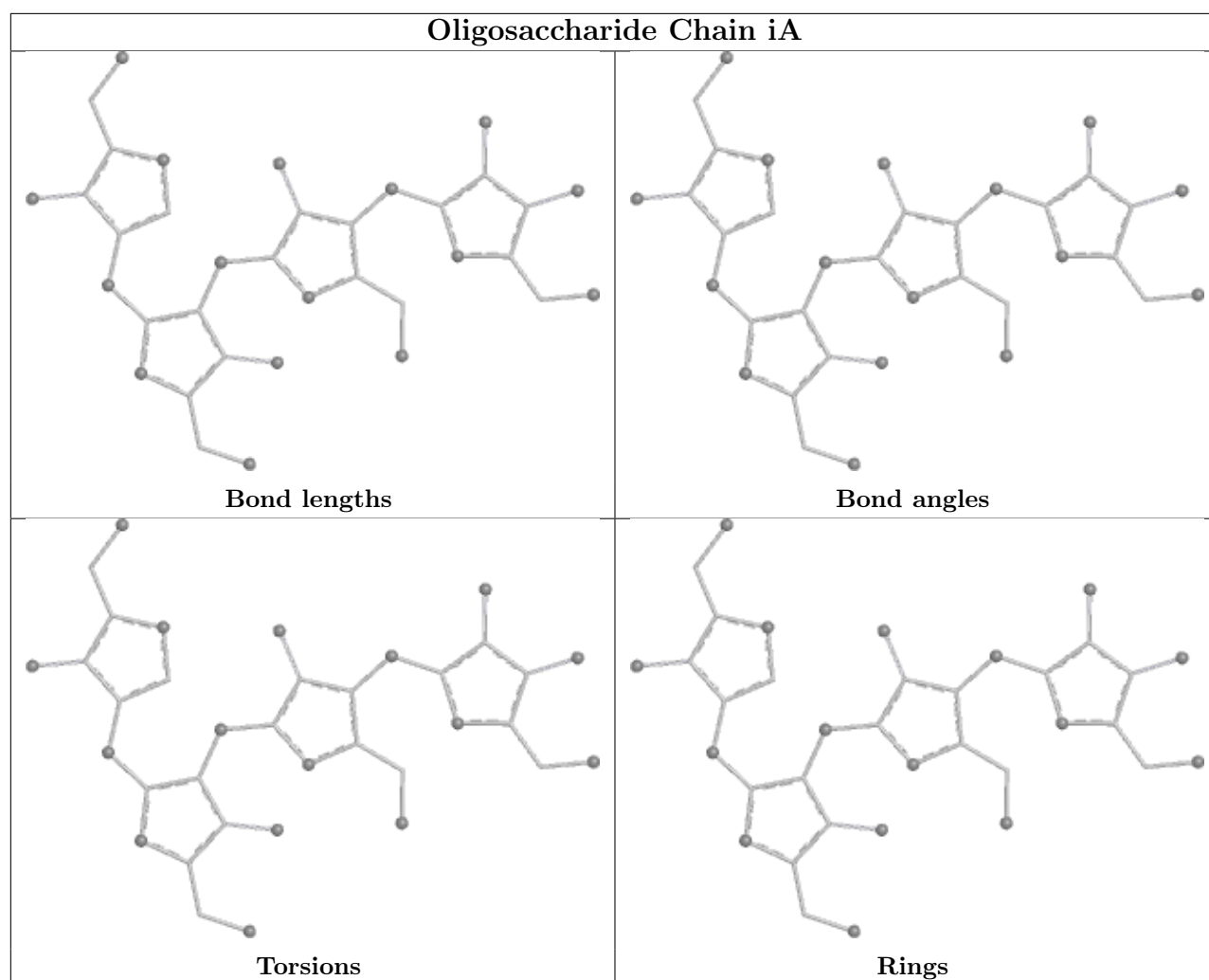
Oligosaccharide Chain VA

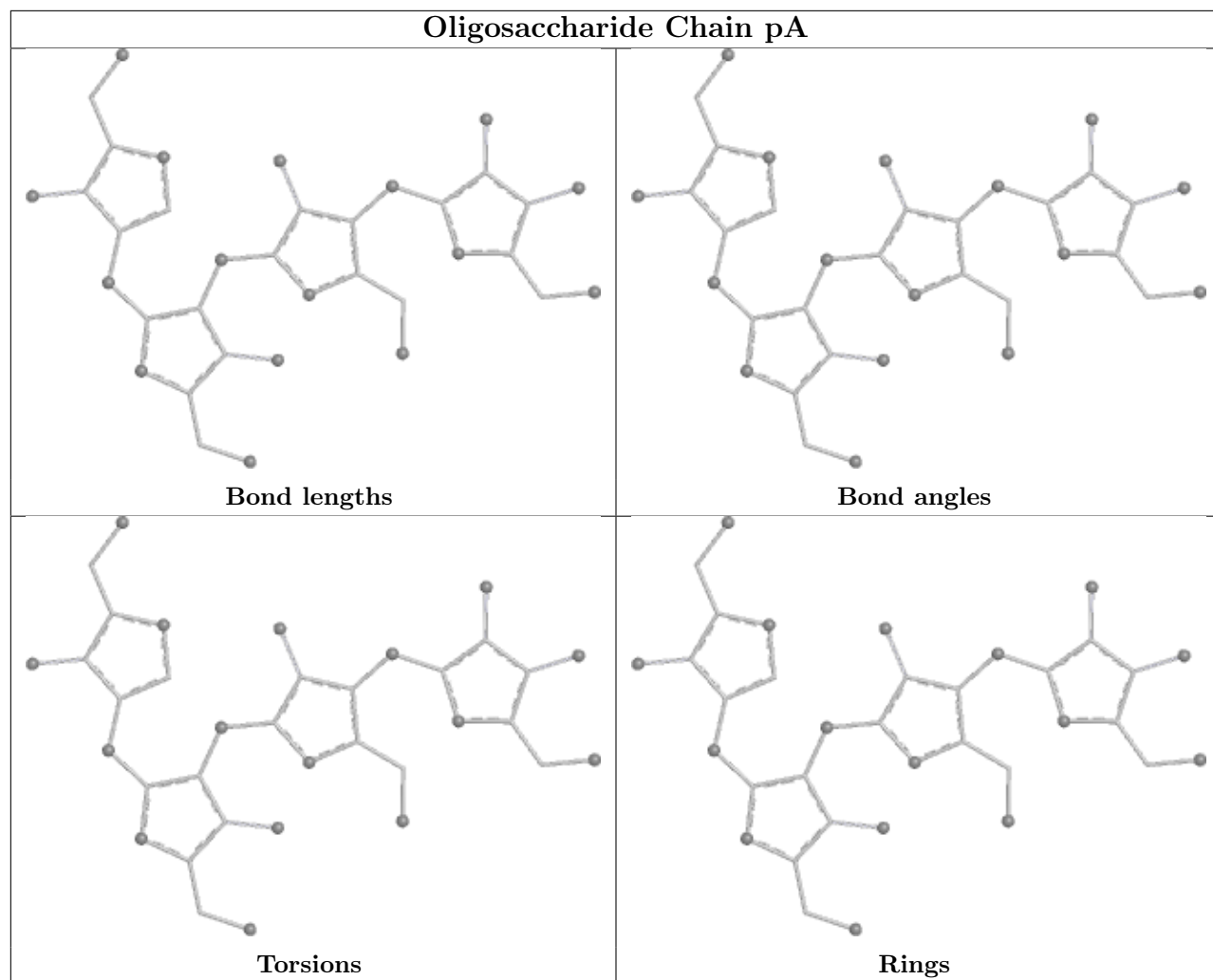


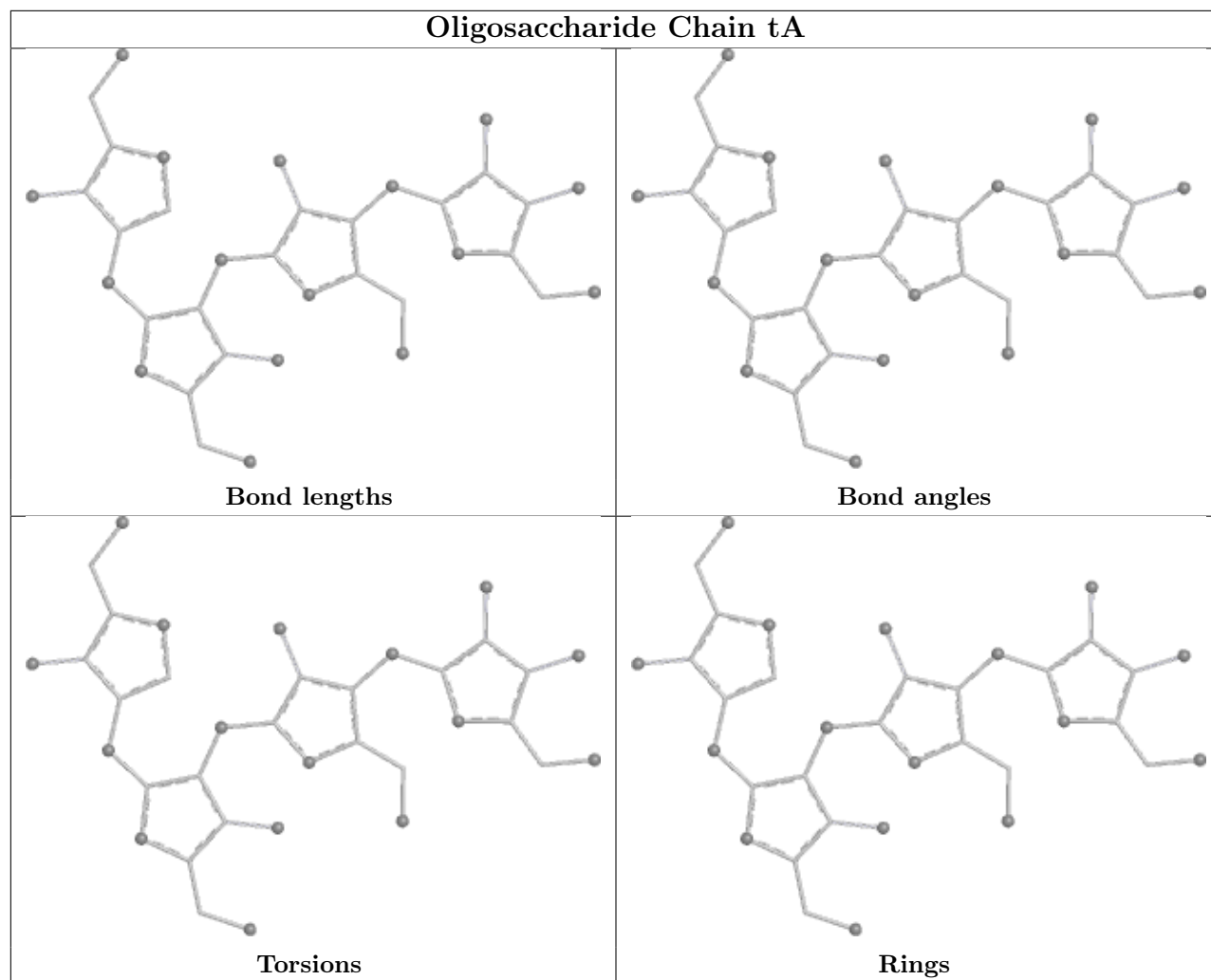


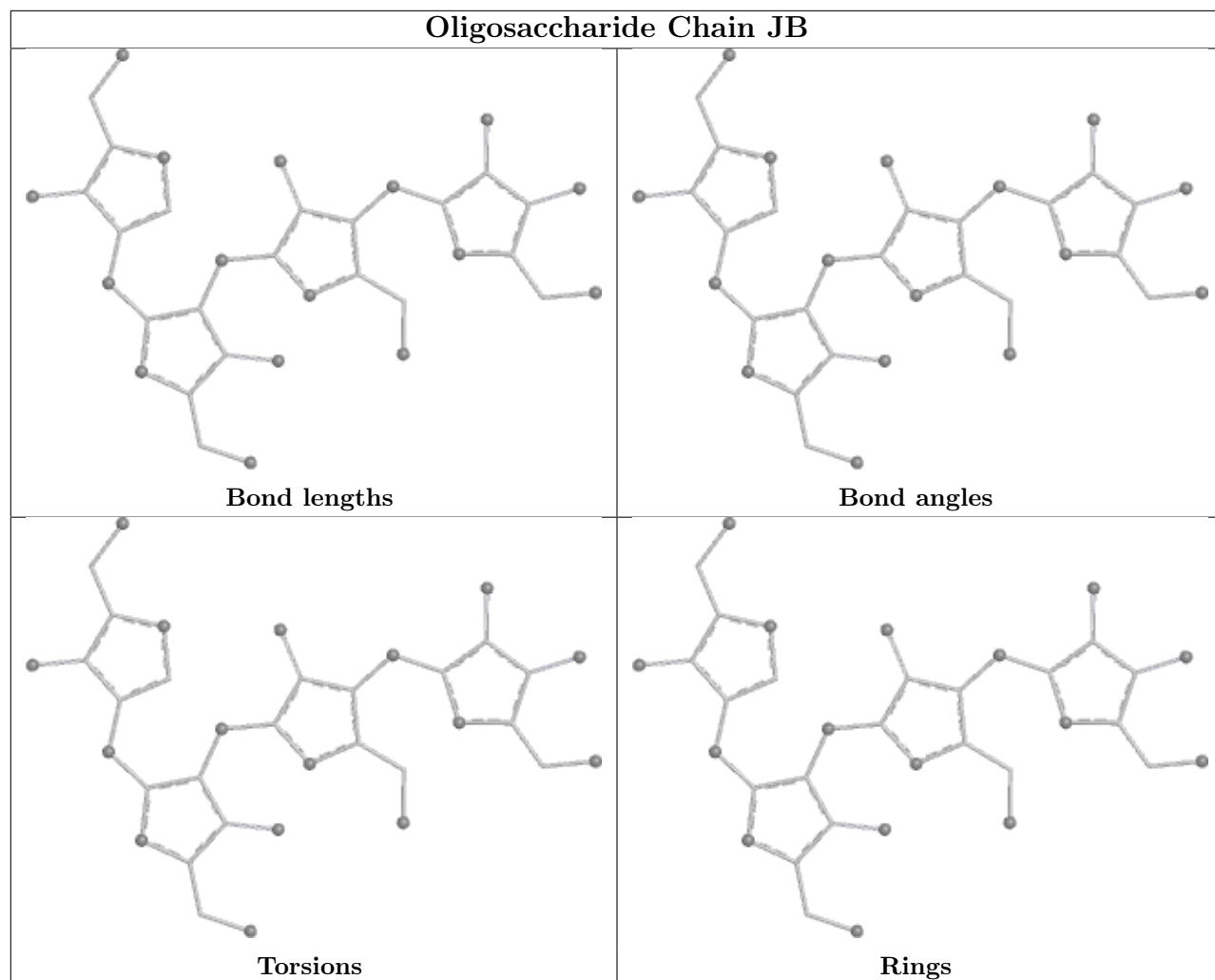


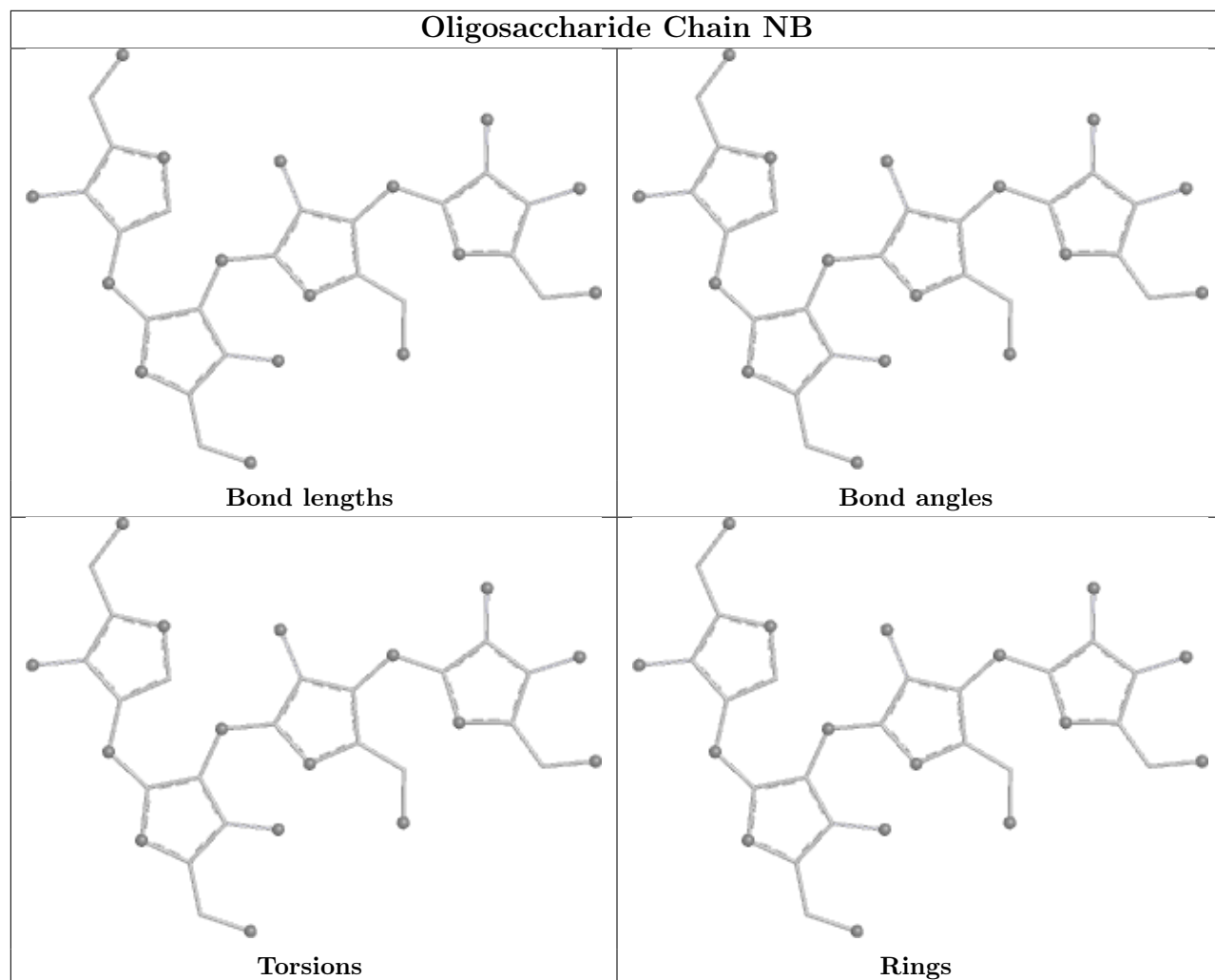


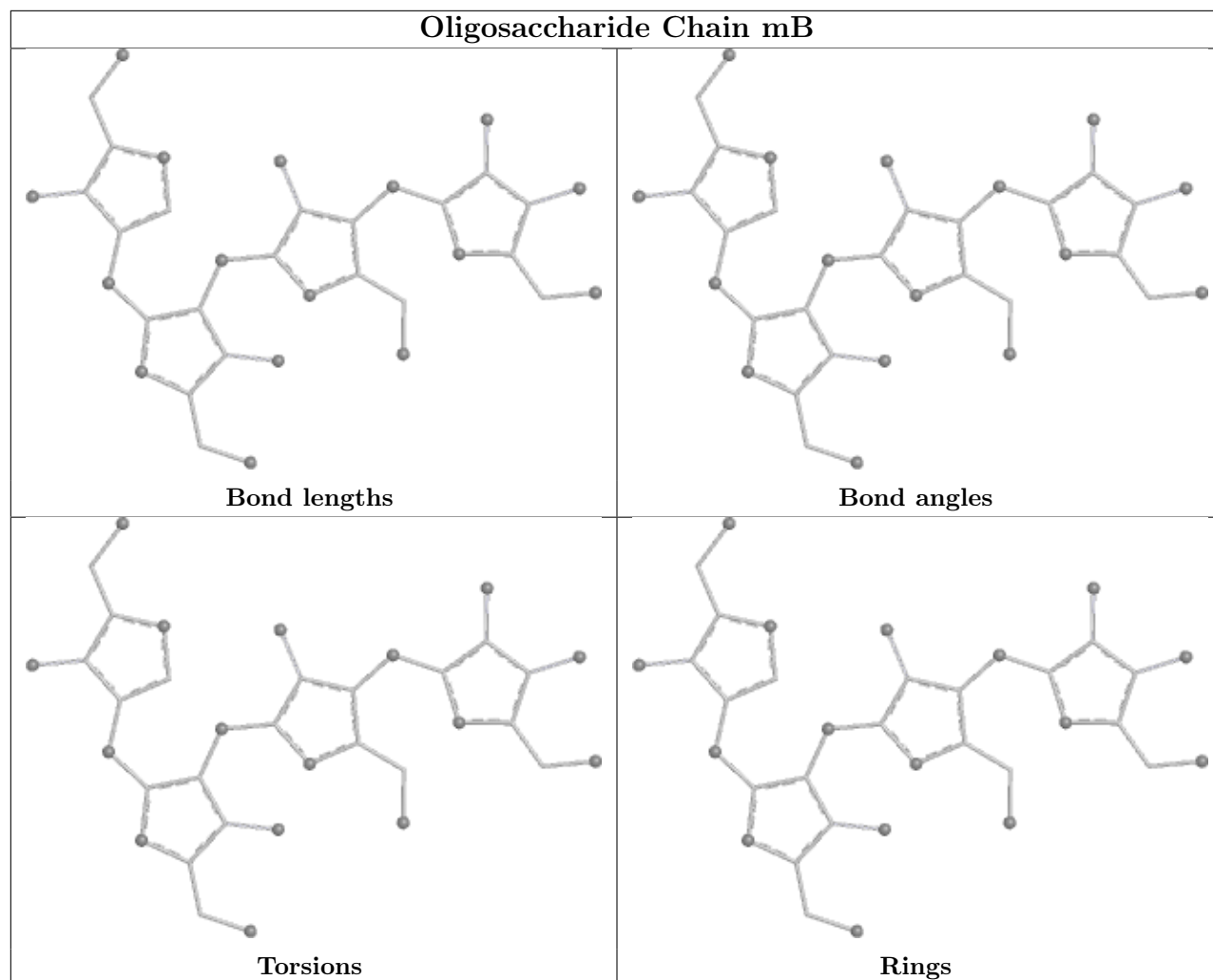


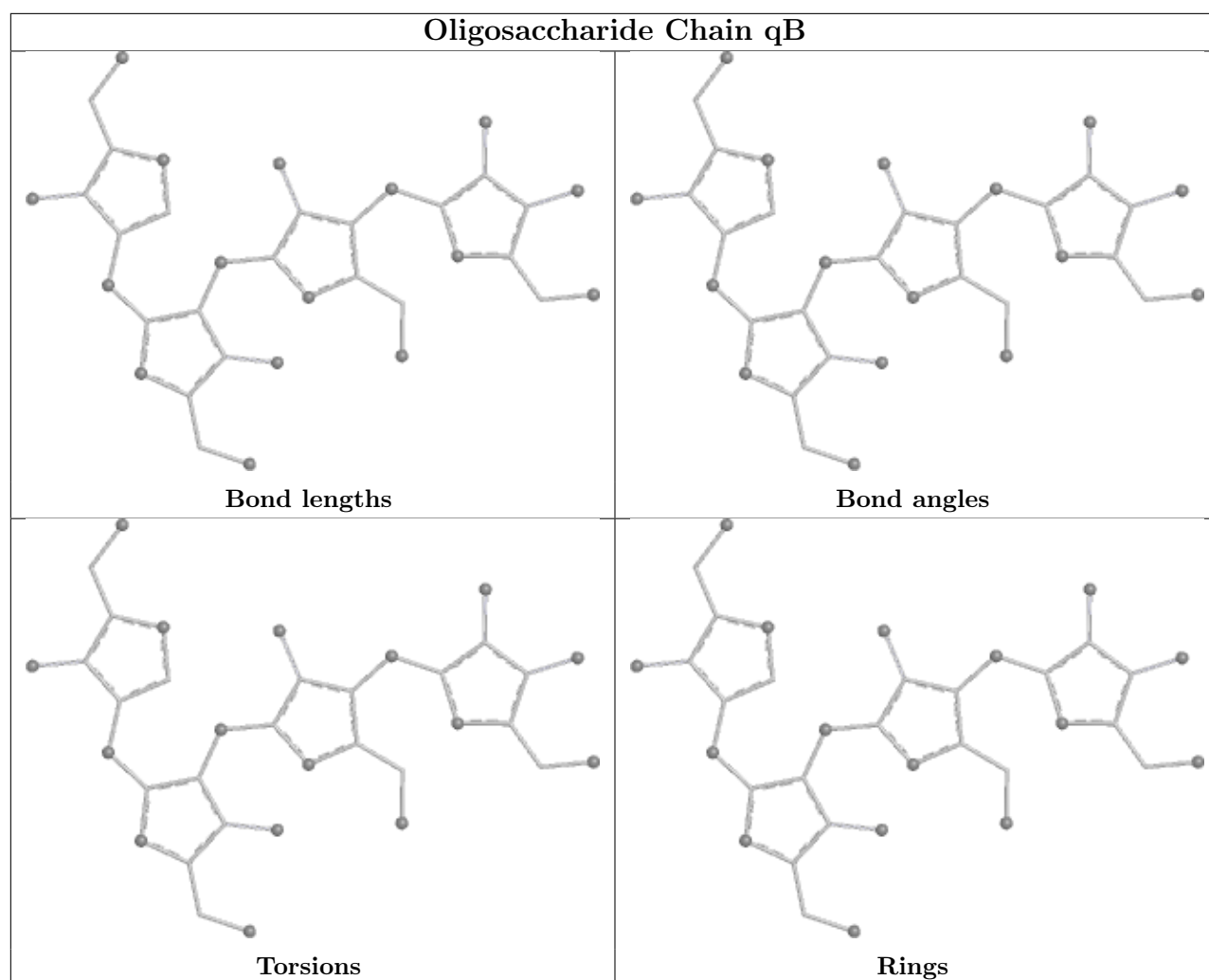


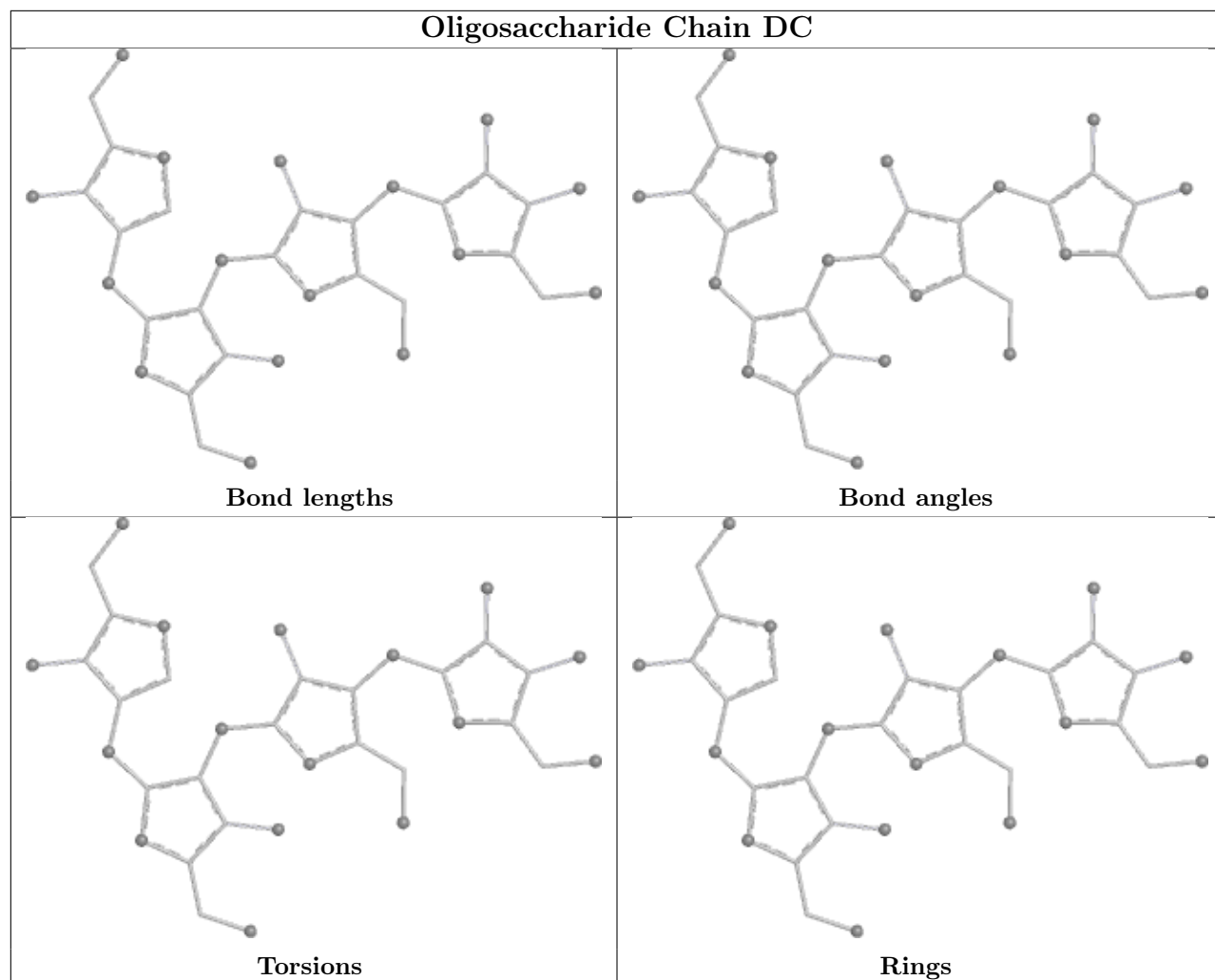


Oligosaccharide Chain JB

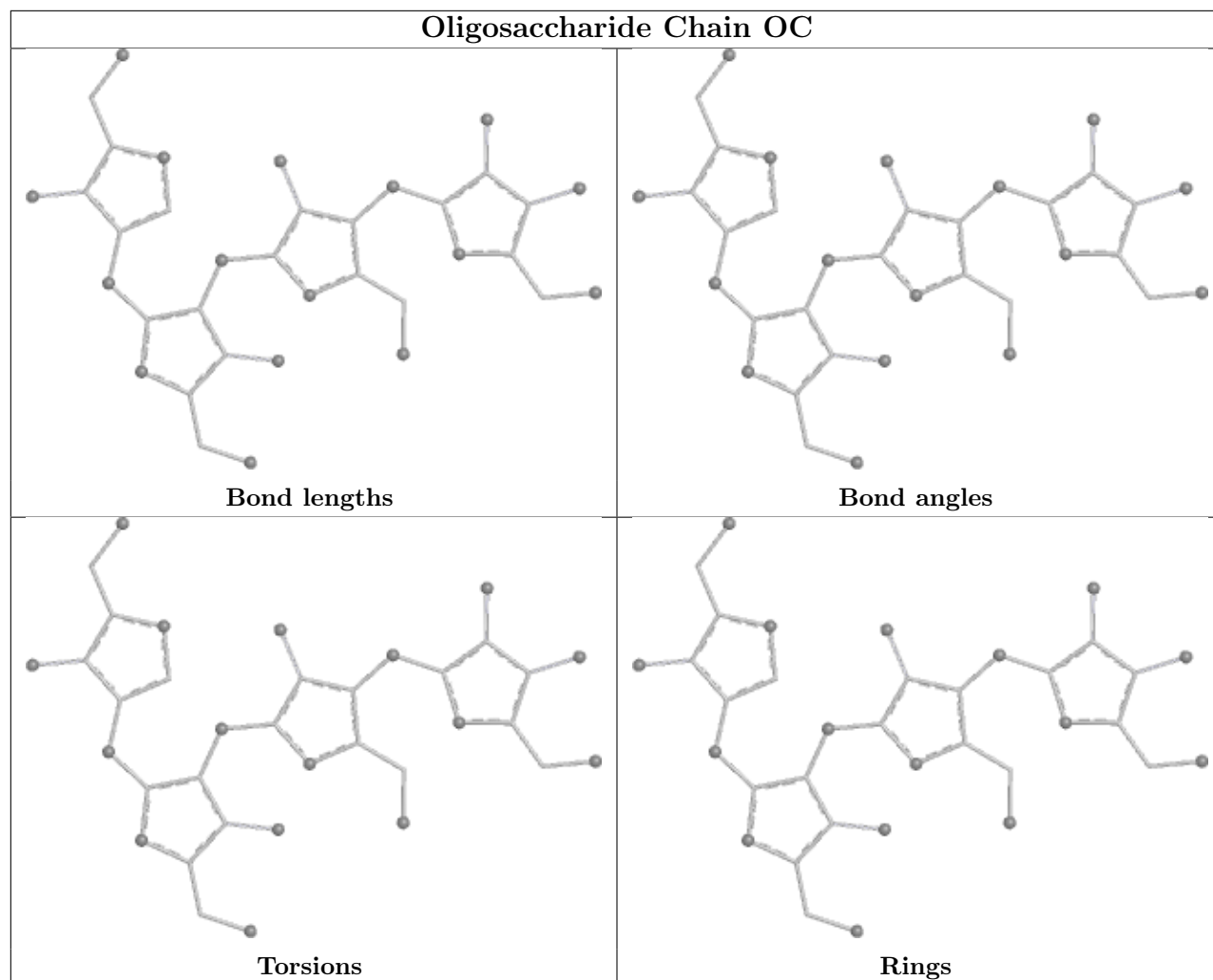
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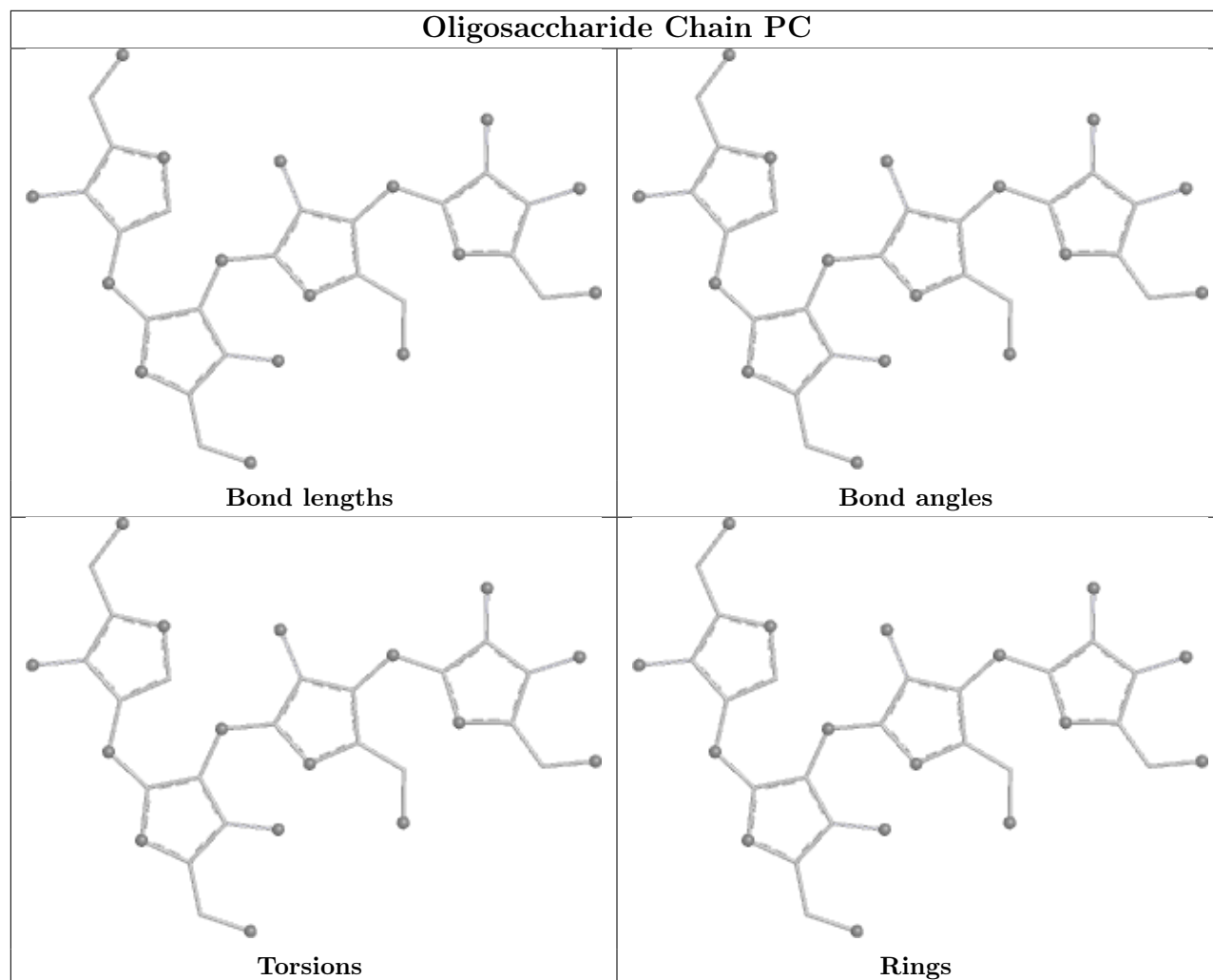
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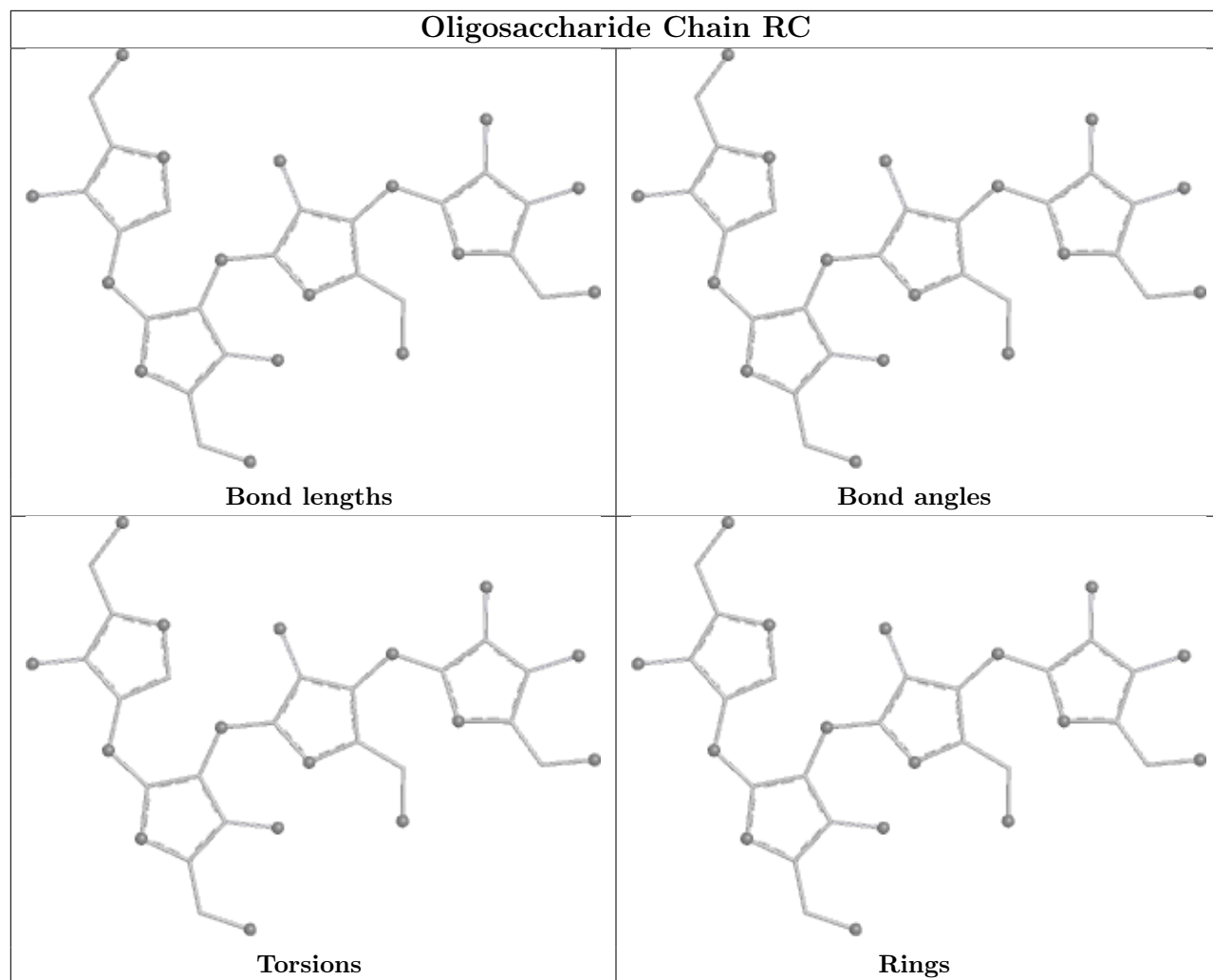


Oligosaccharide Chain DC

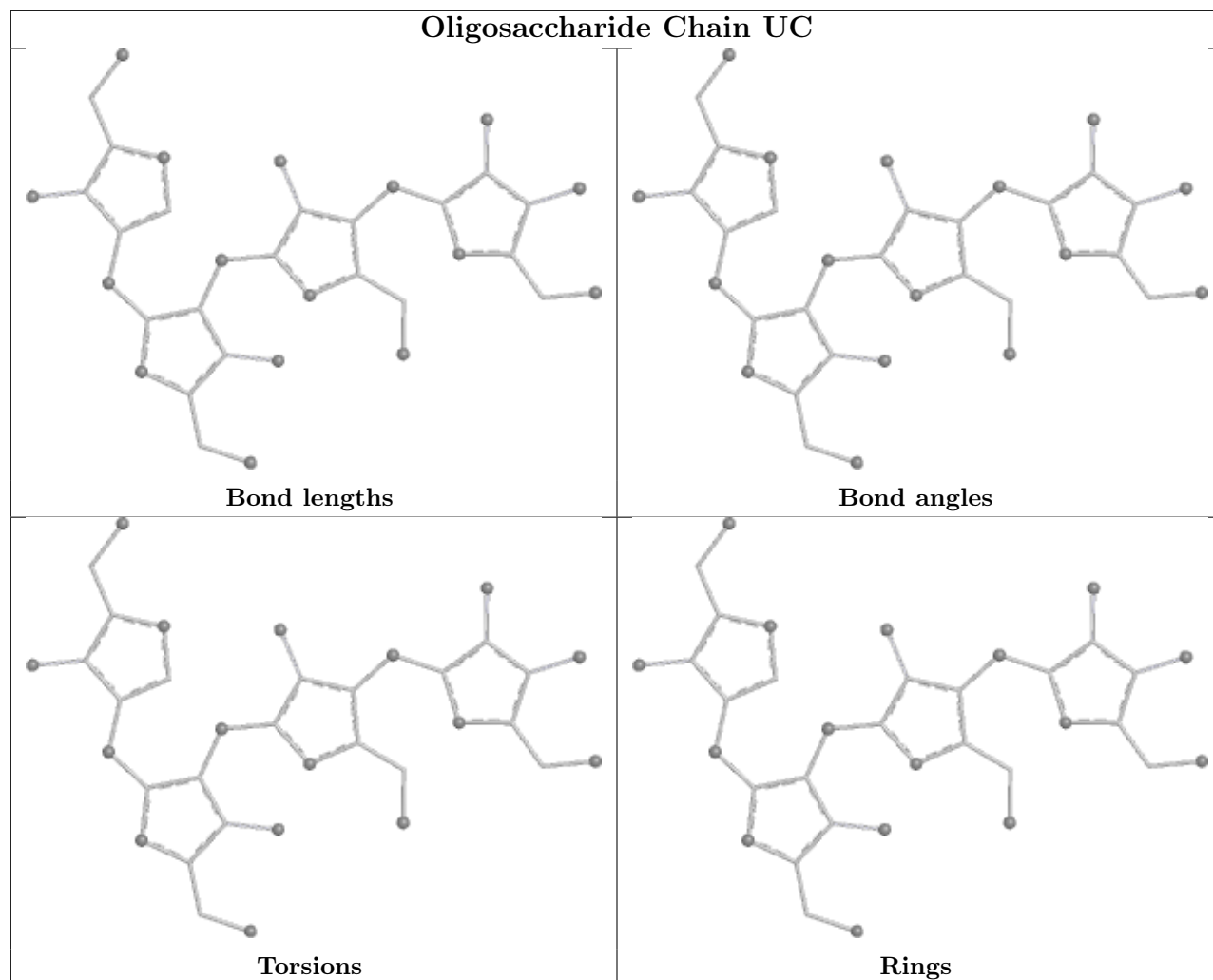
Oligosaccharide Chain OC

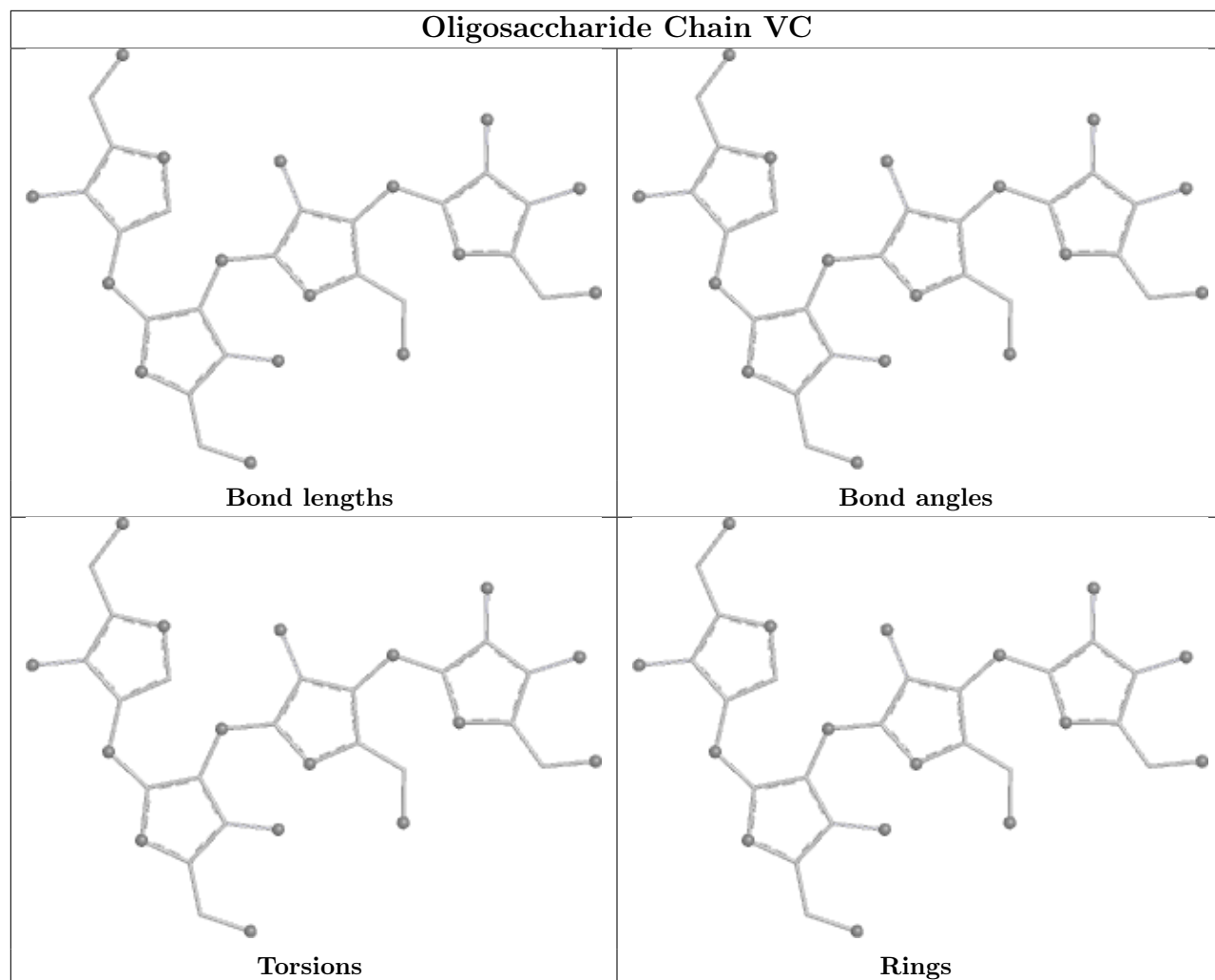


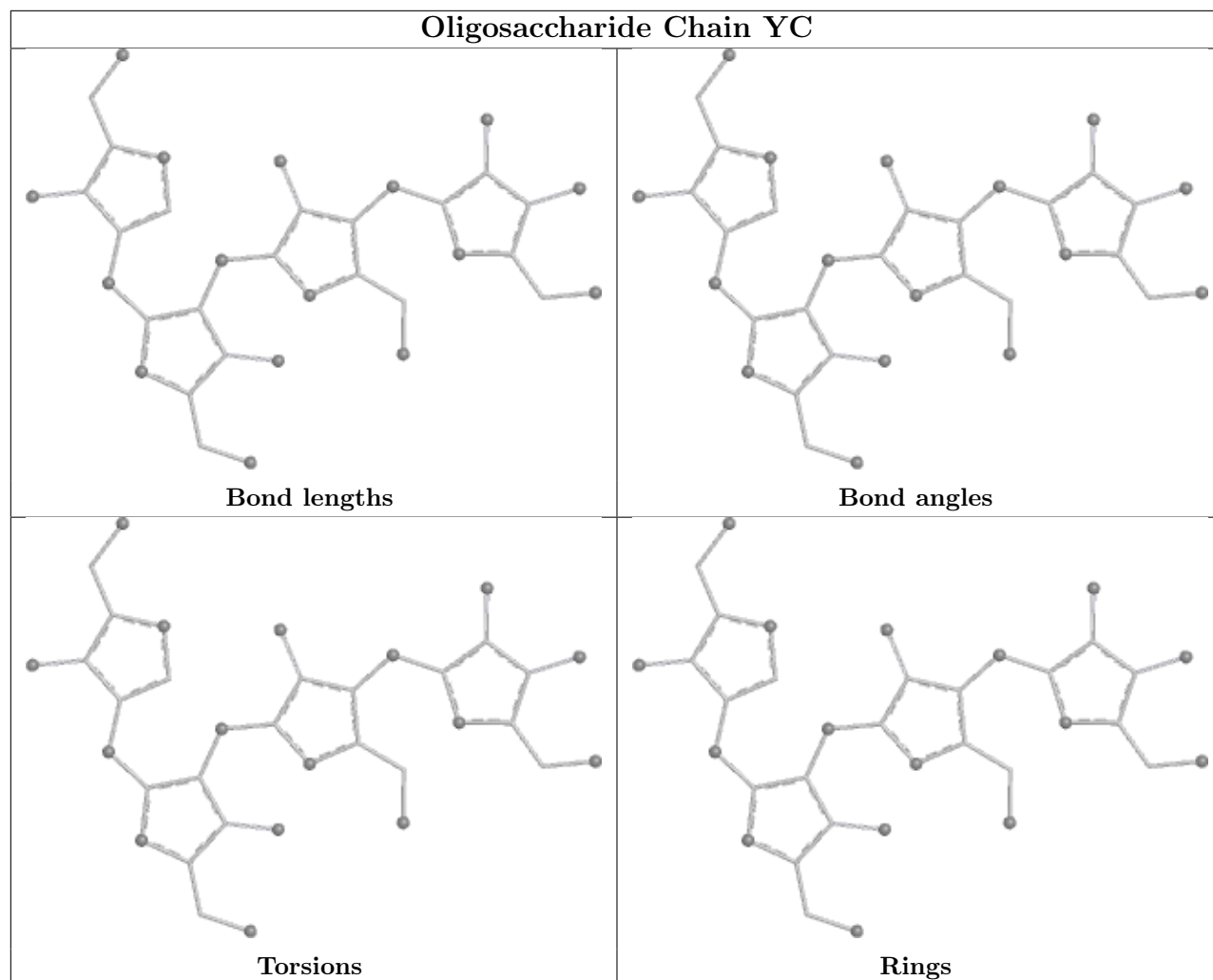
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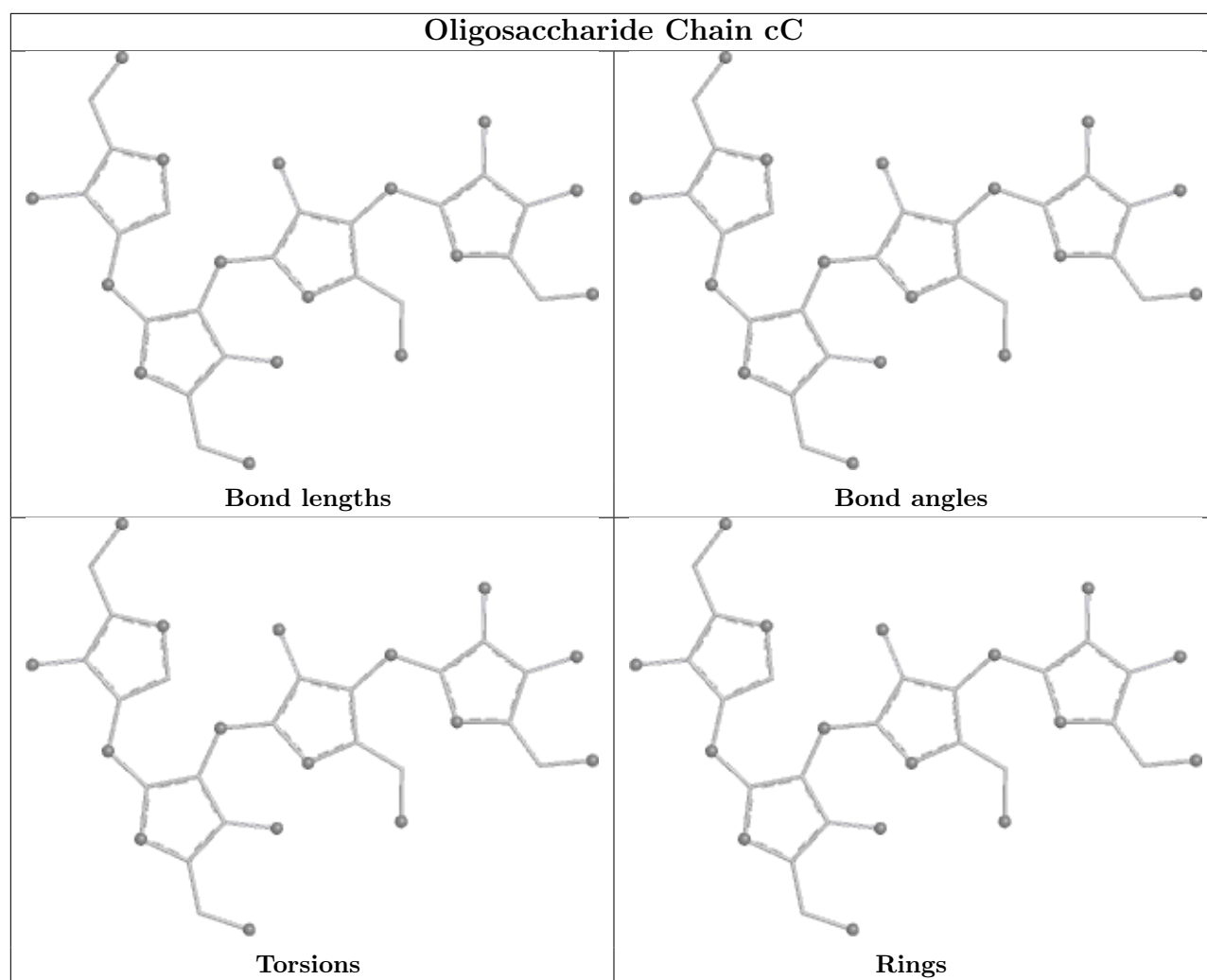


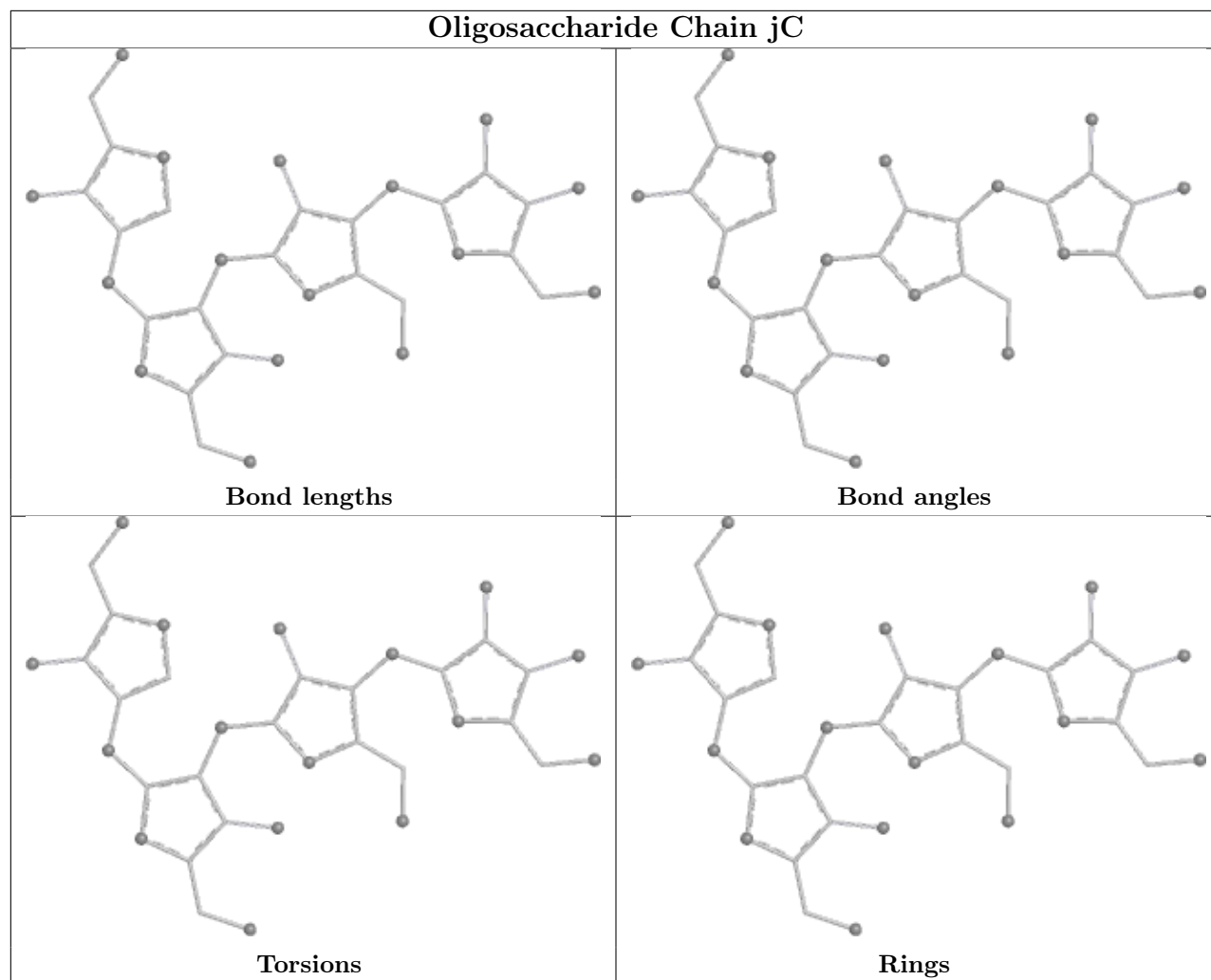
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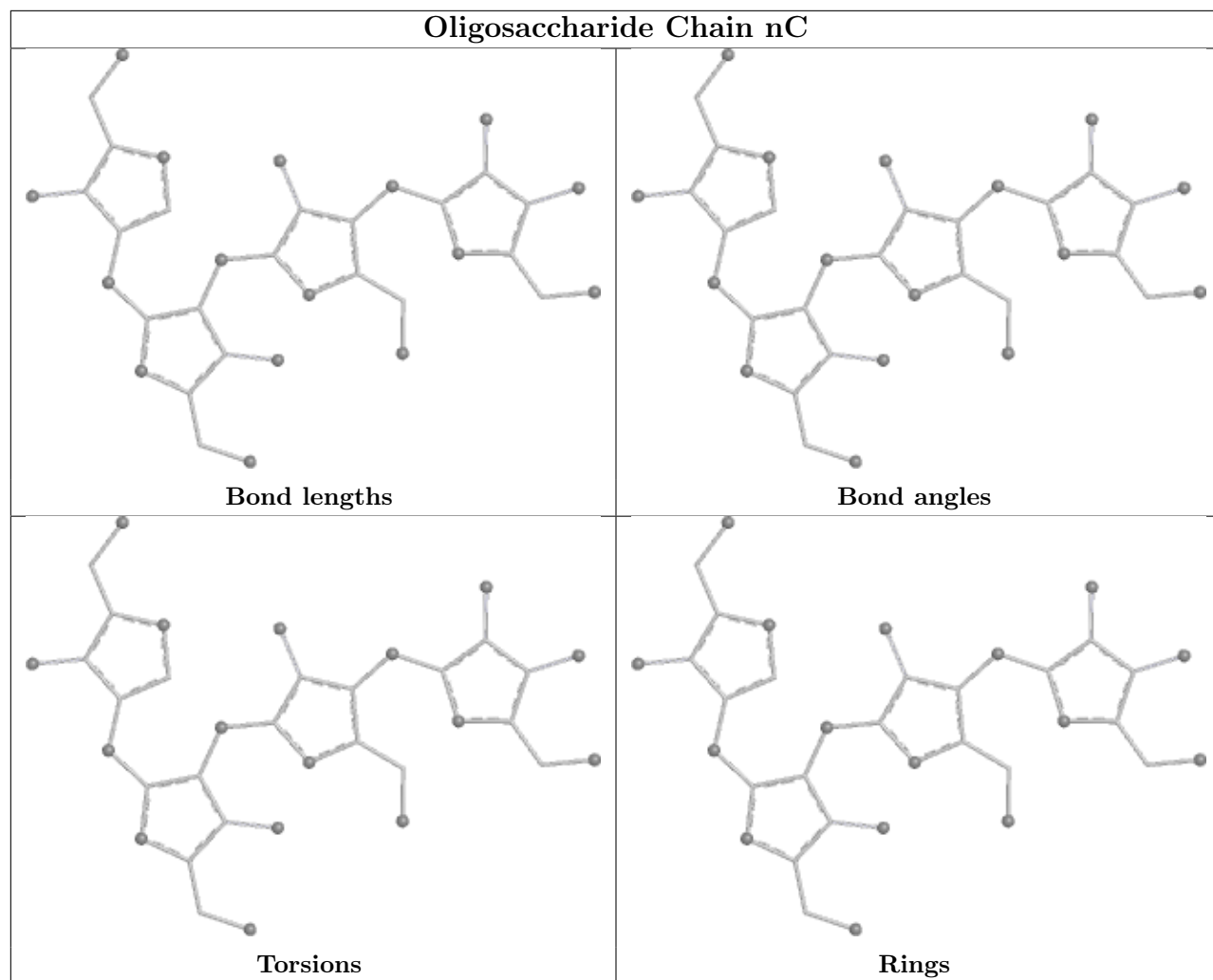


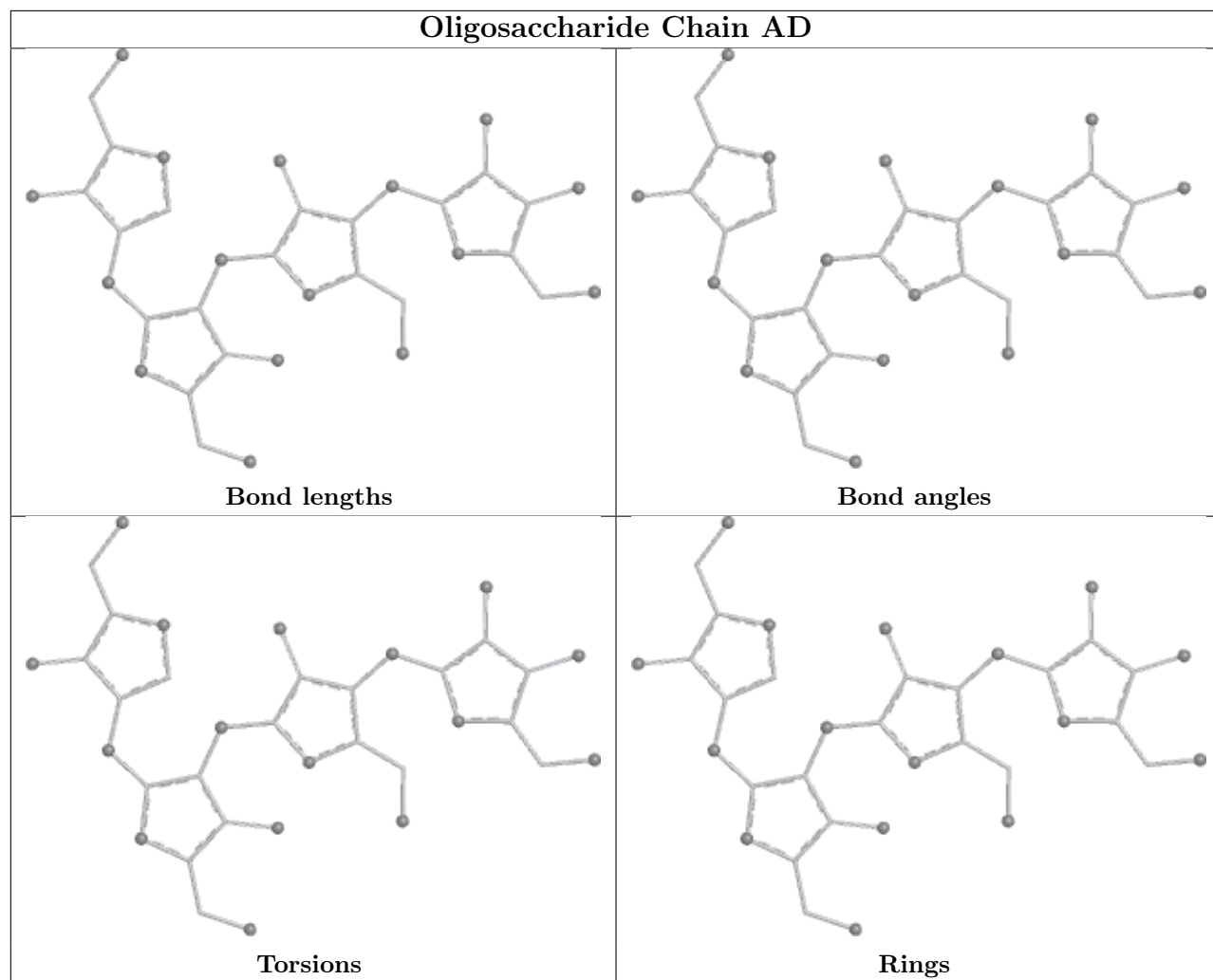
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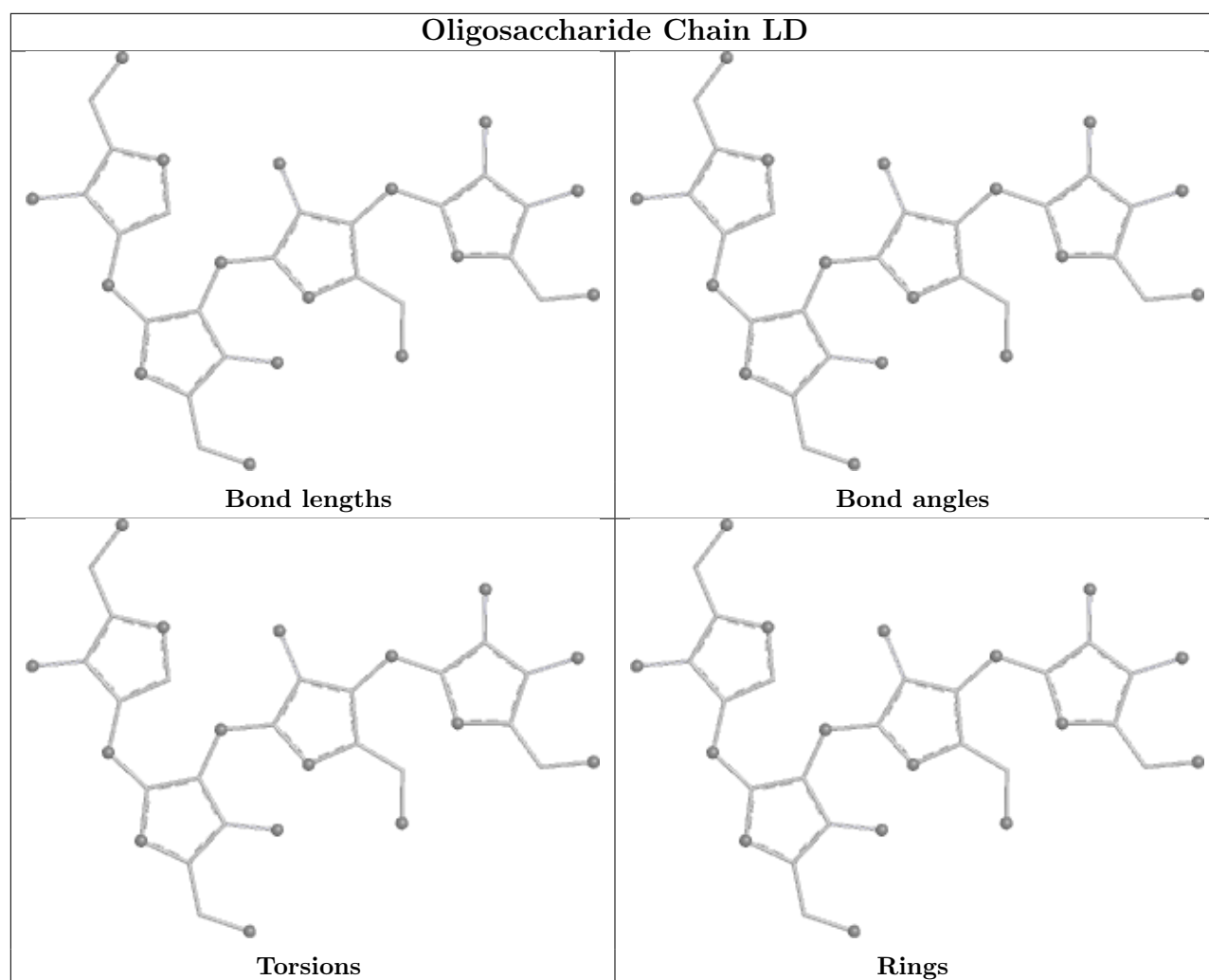
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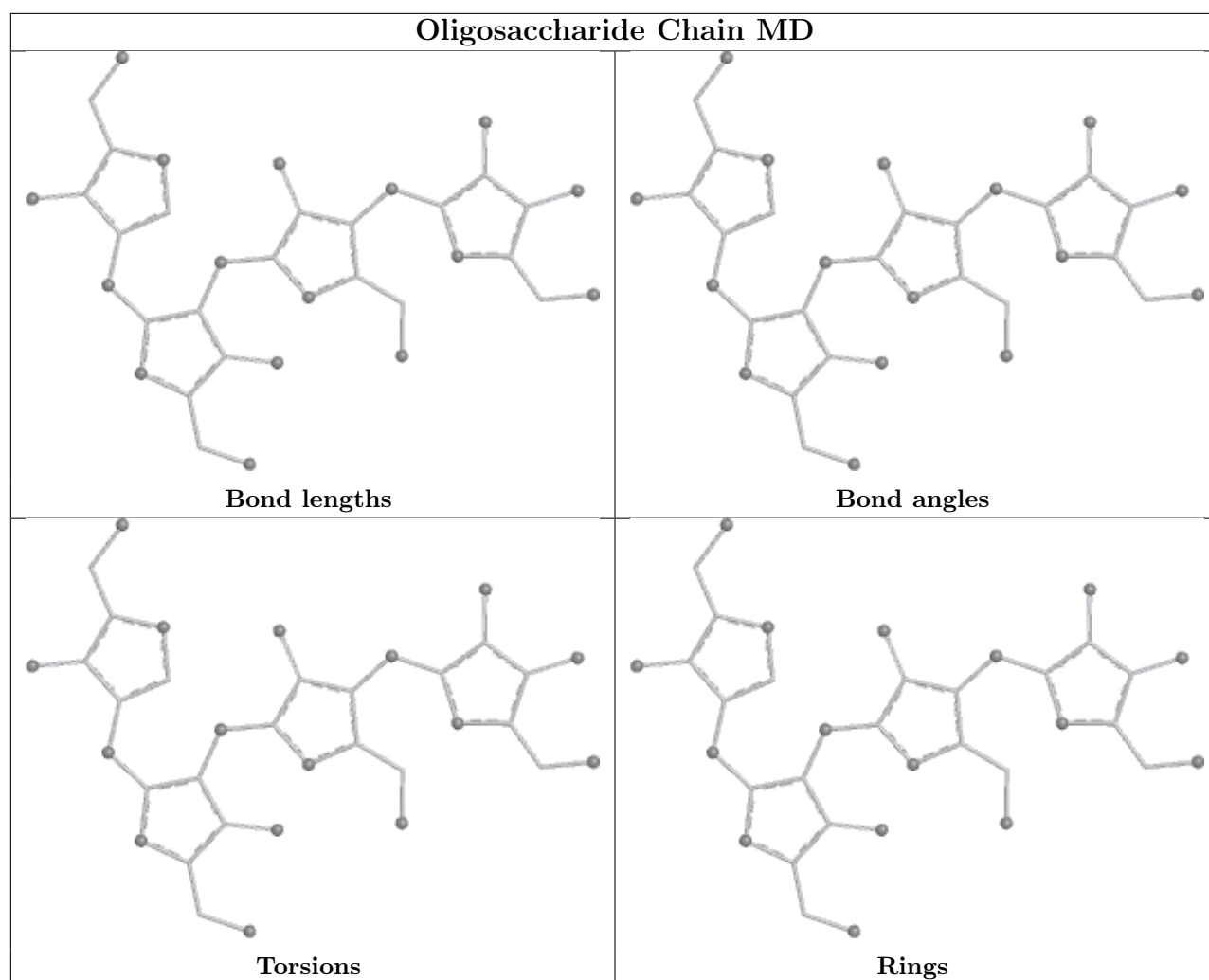


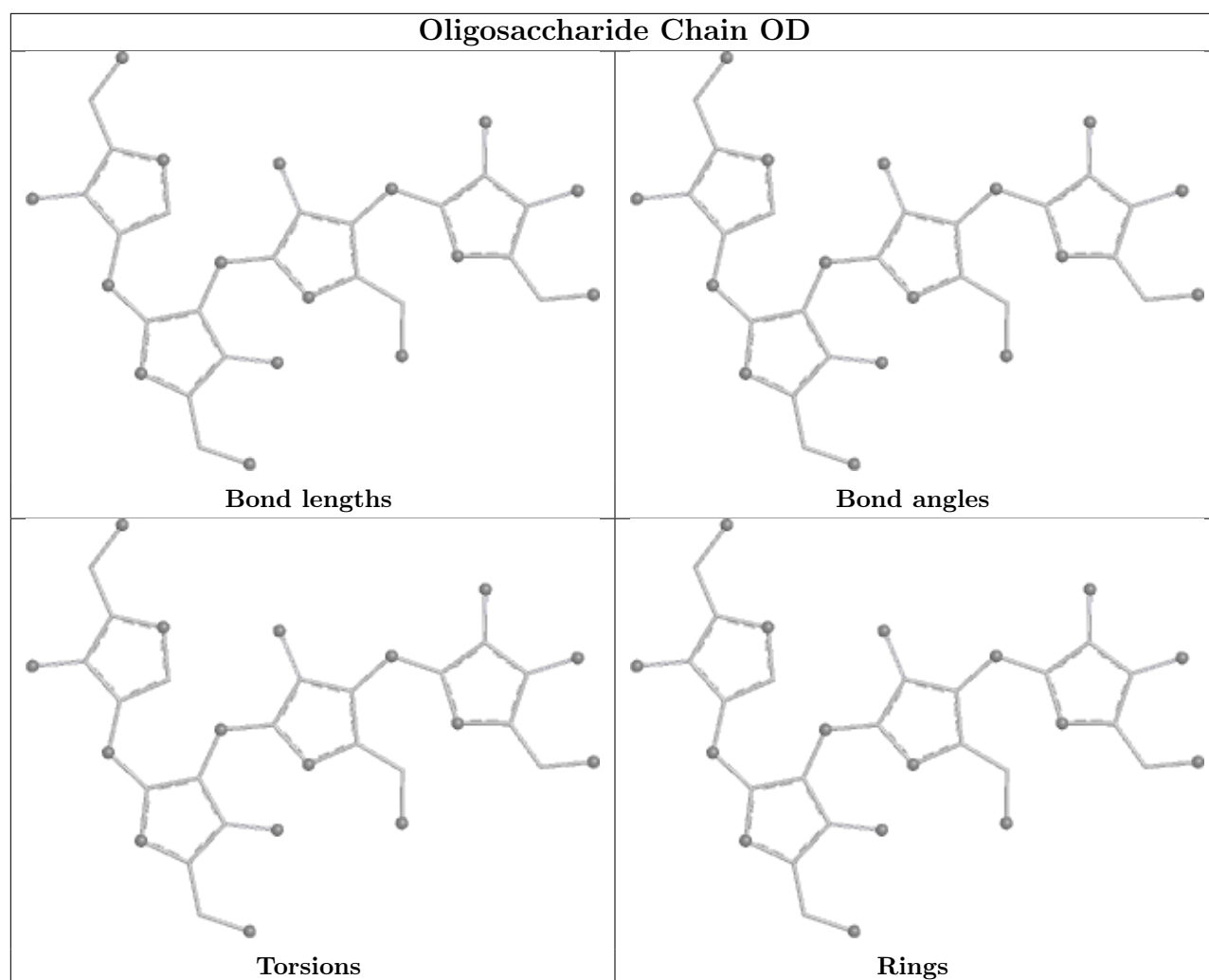


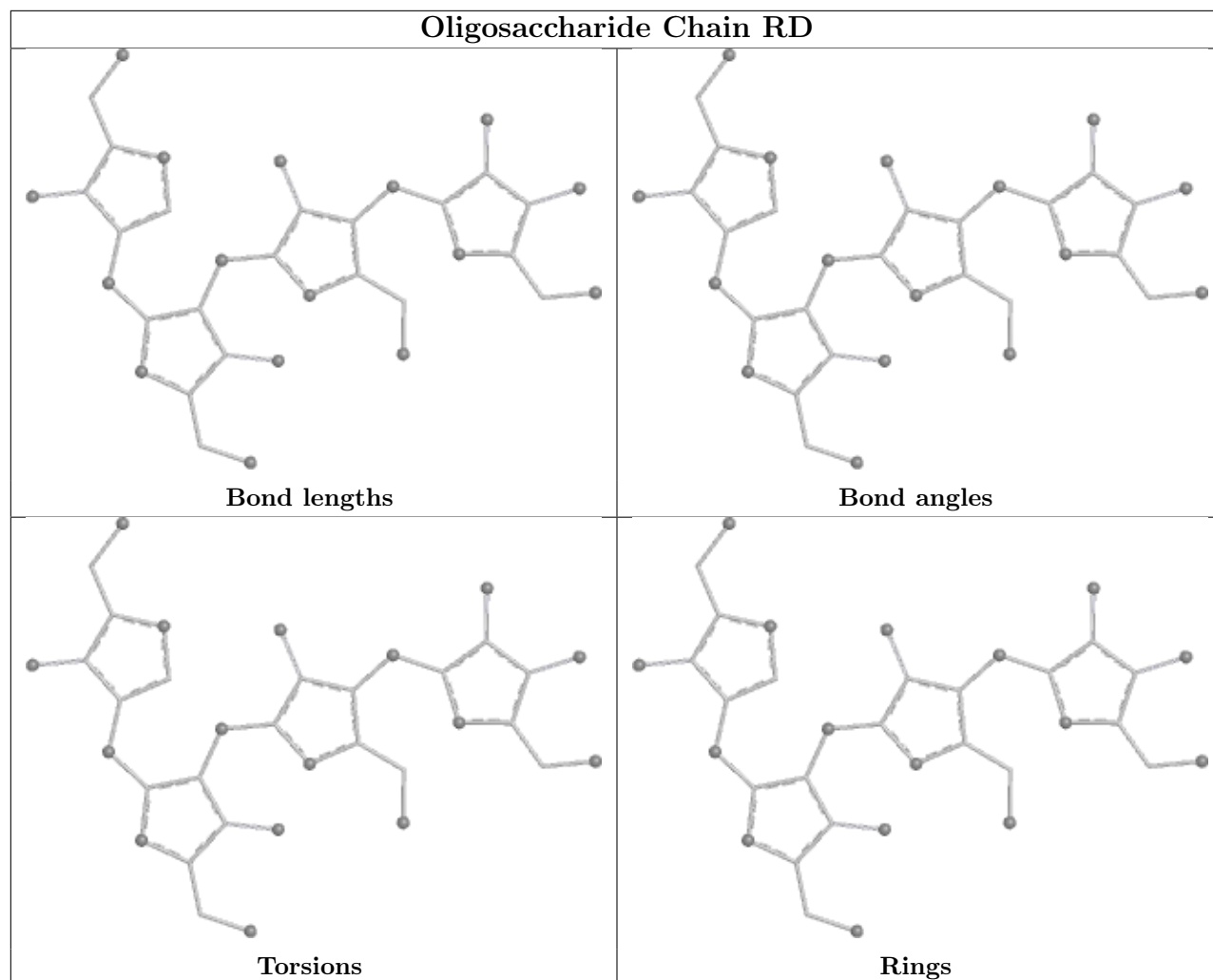


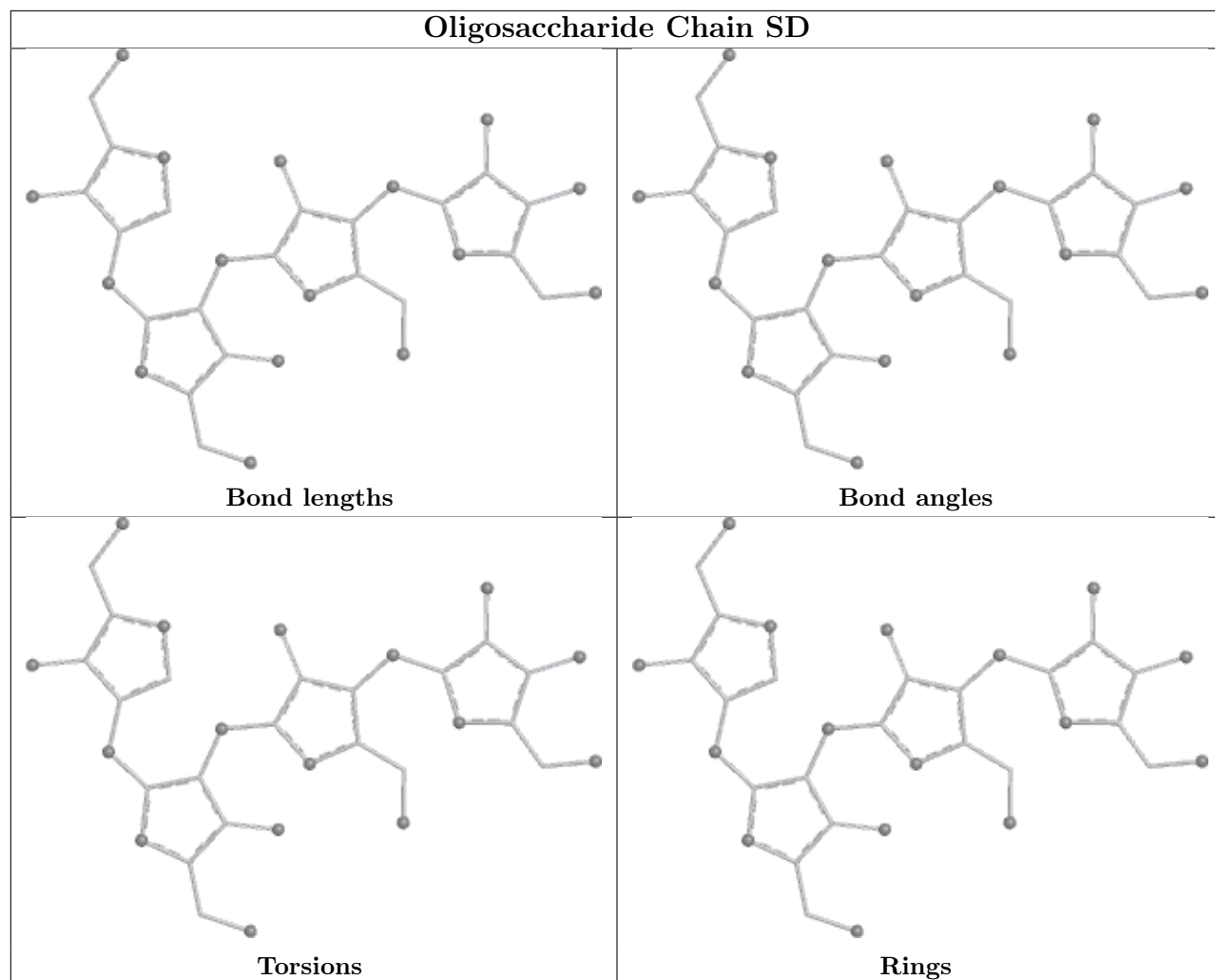
Oligosaccharide Chain AD

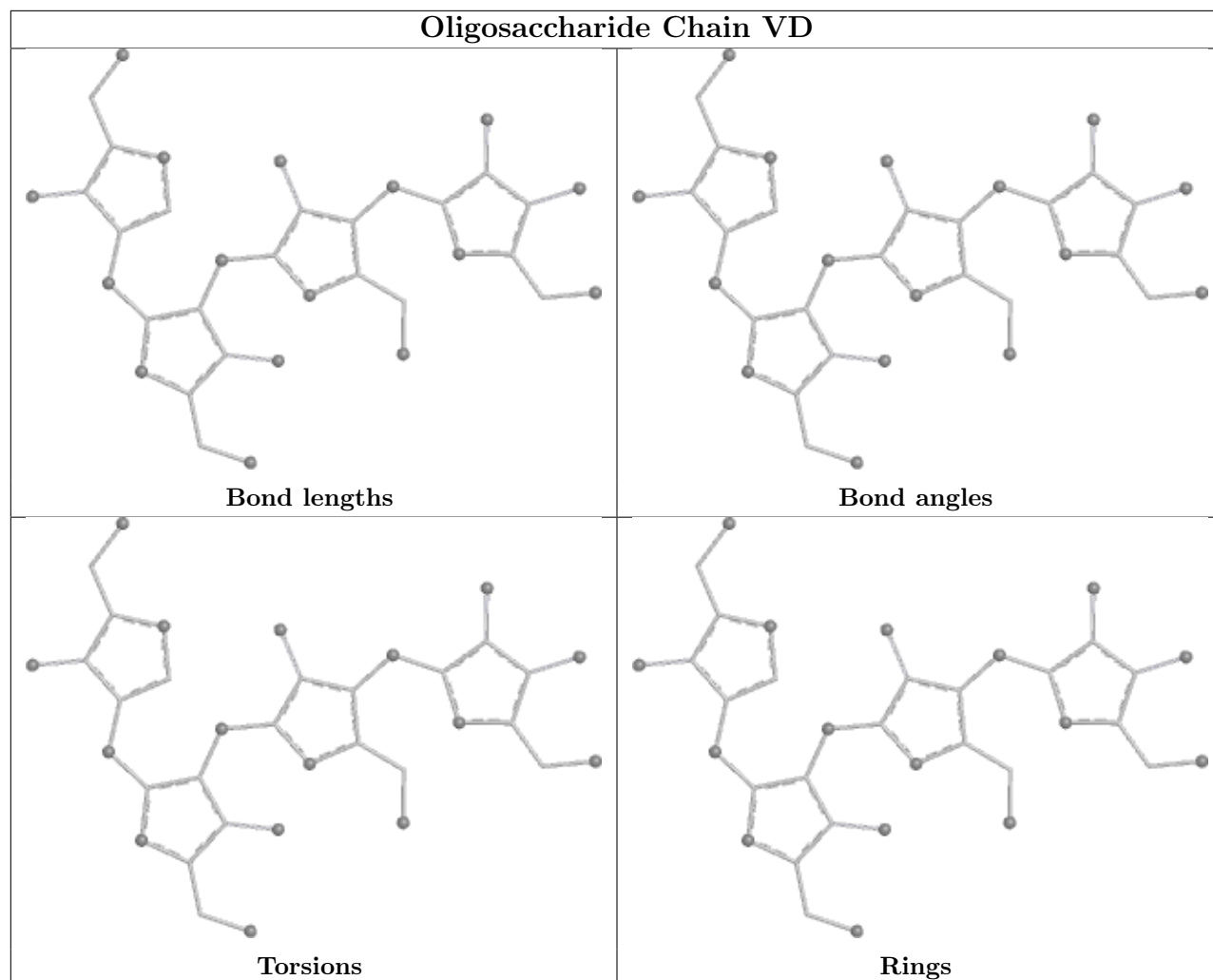




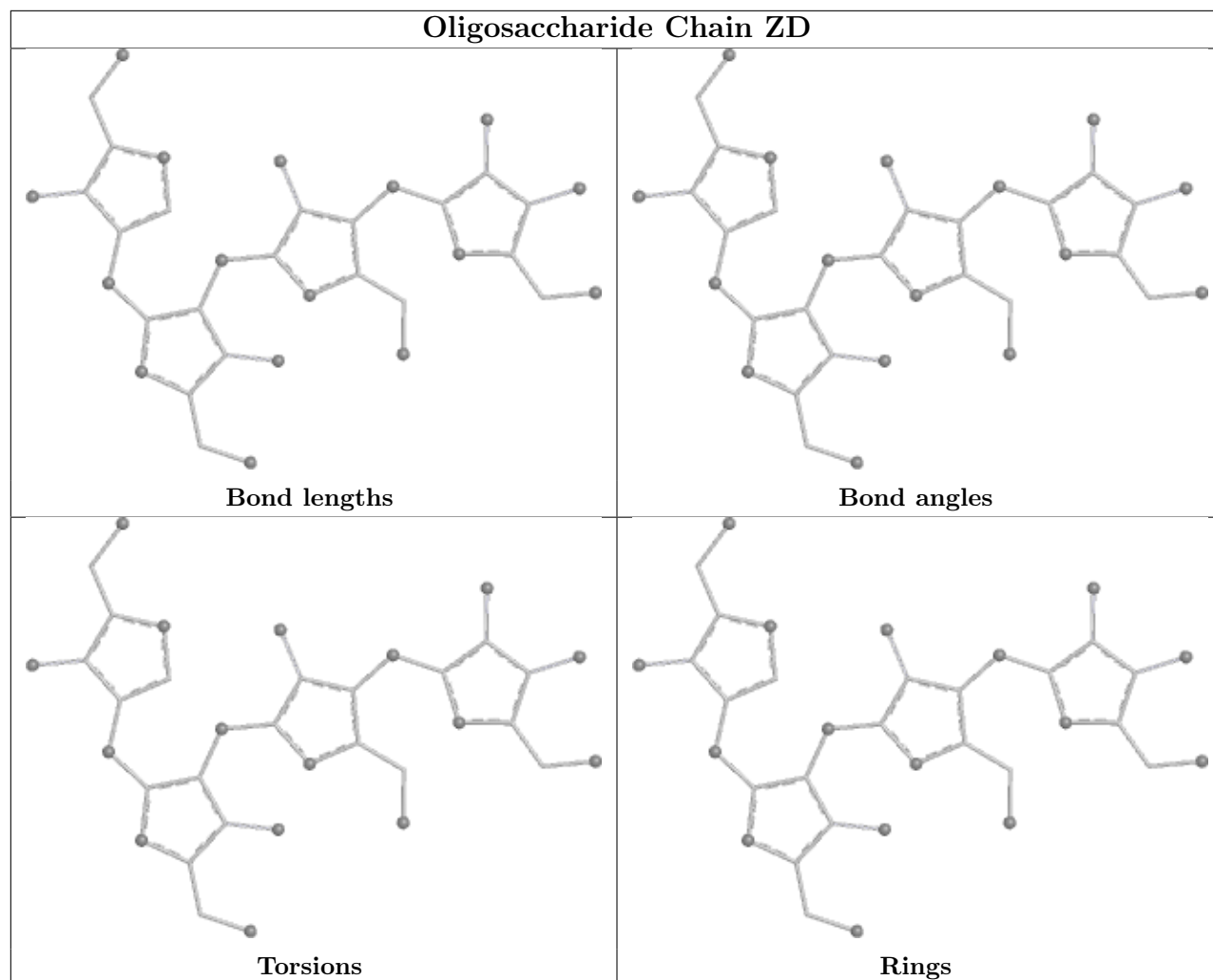


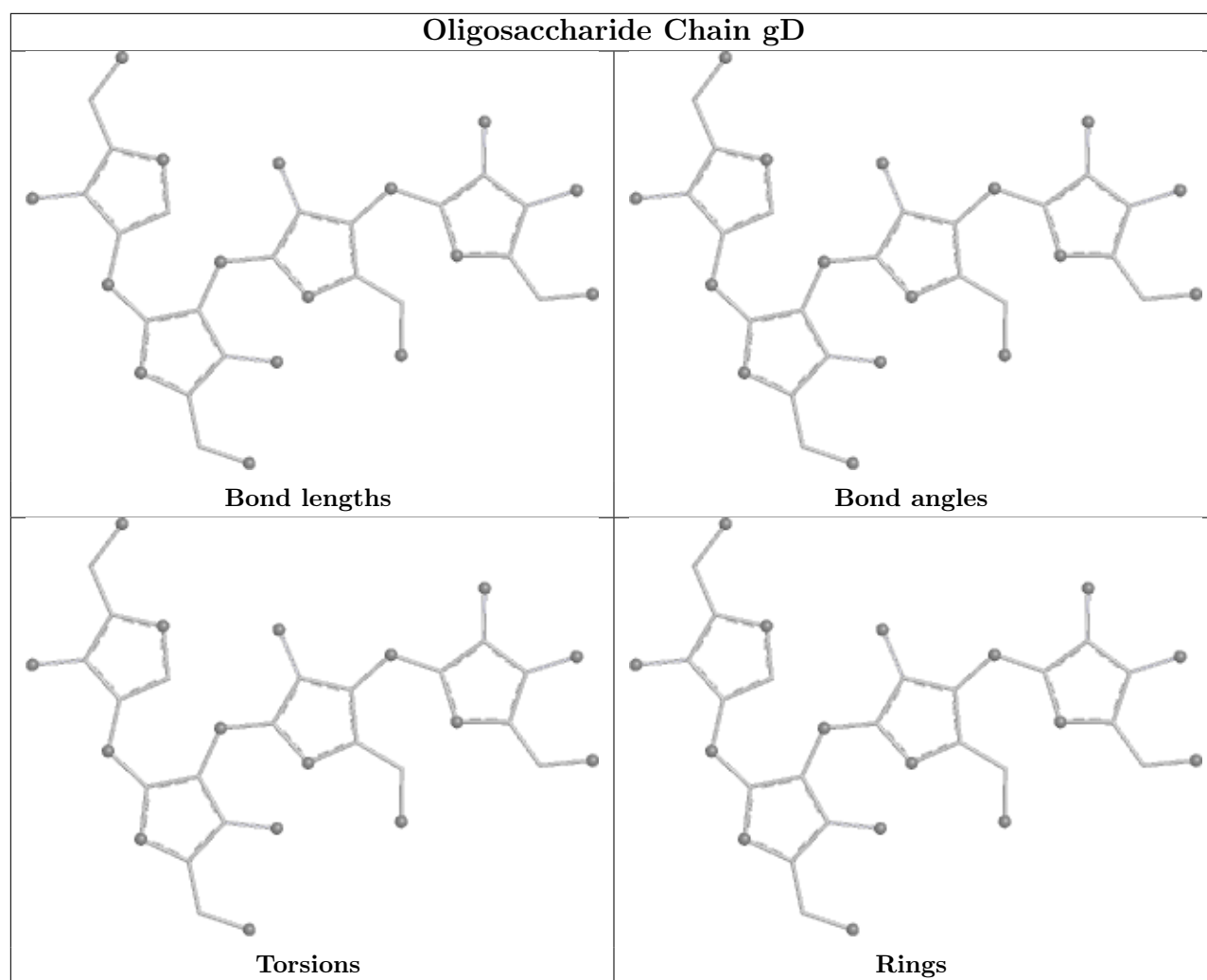


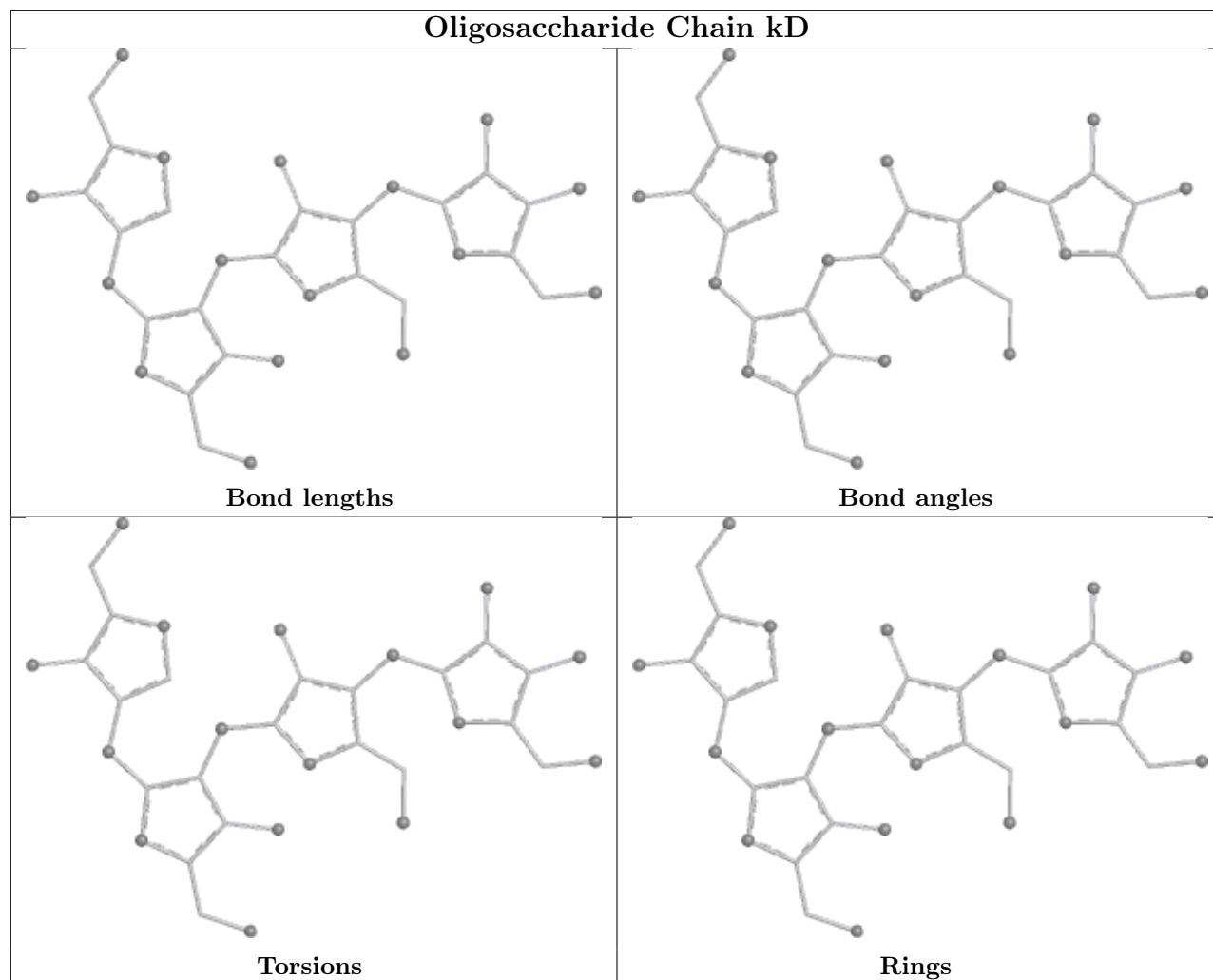
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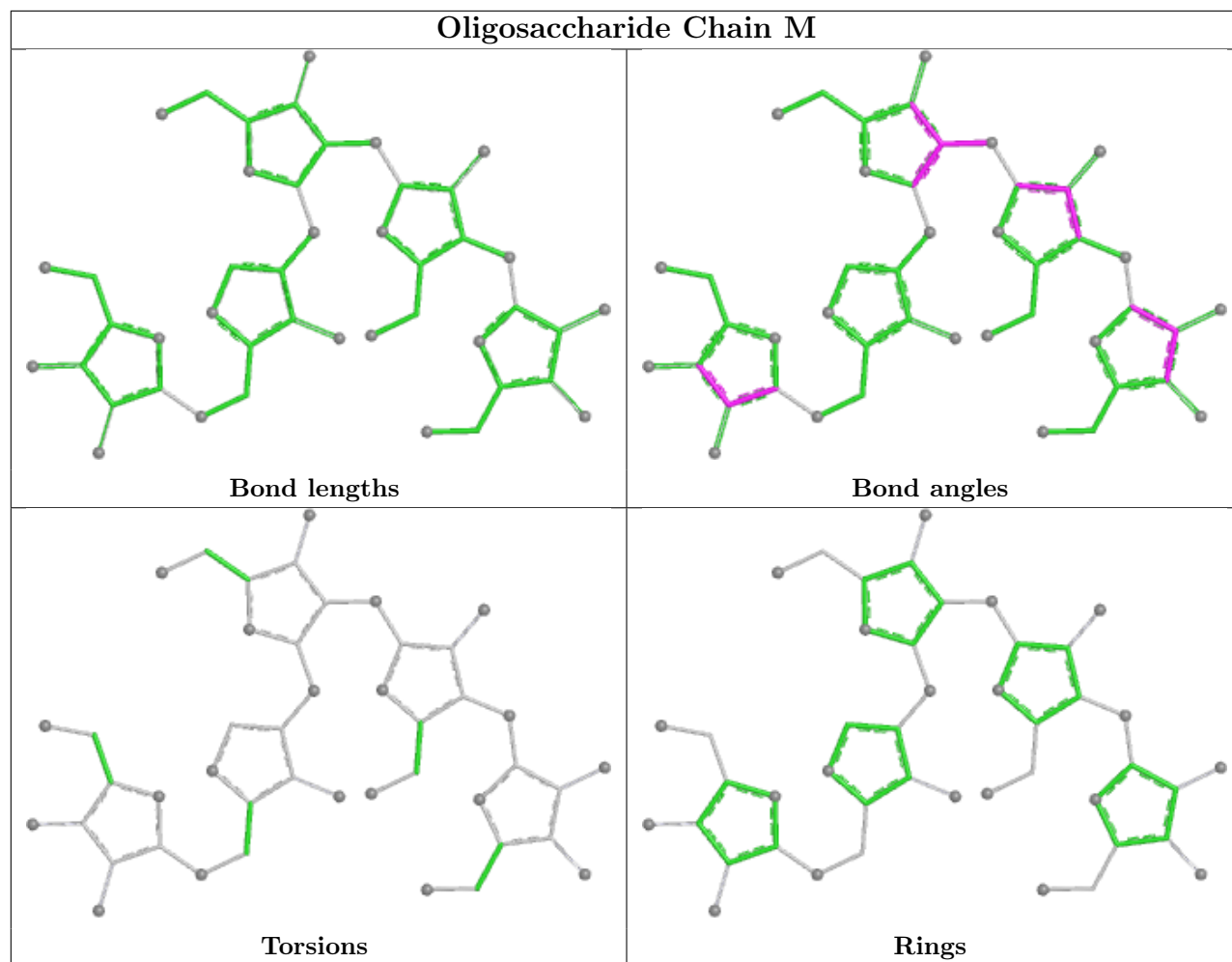
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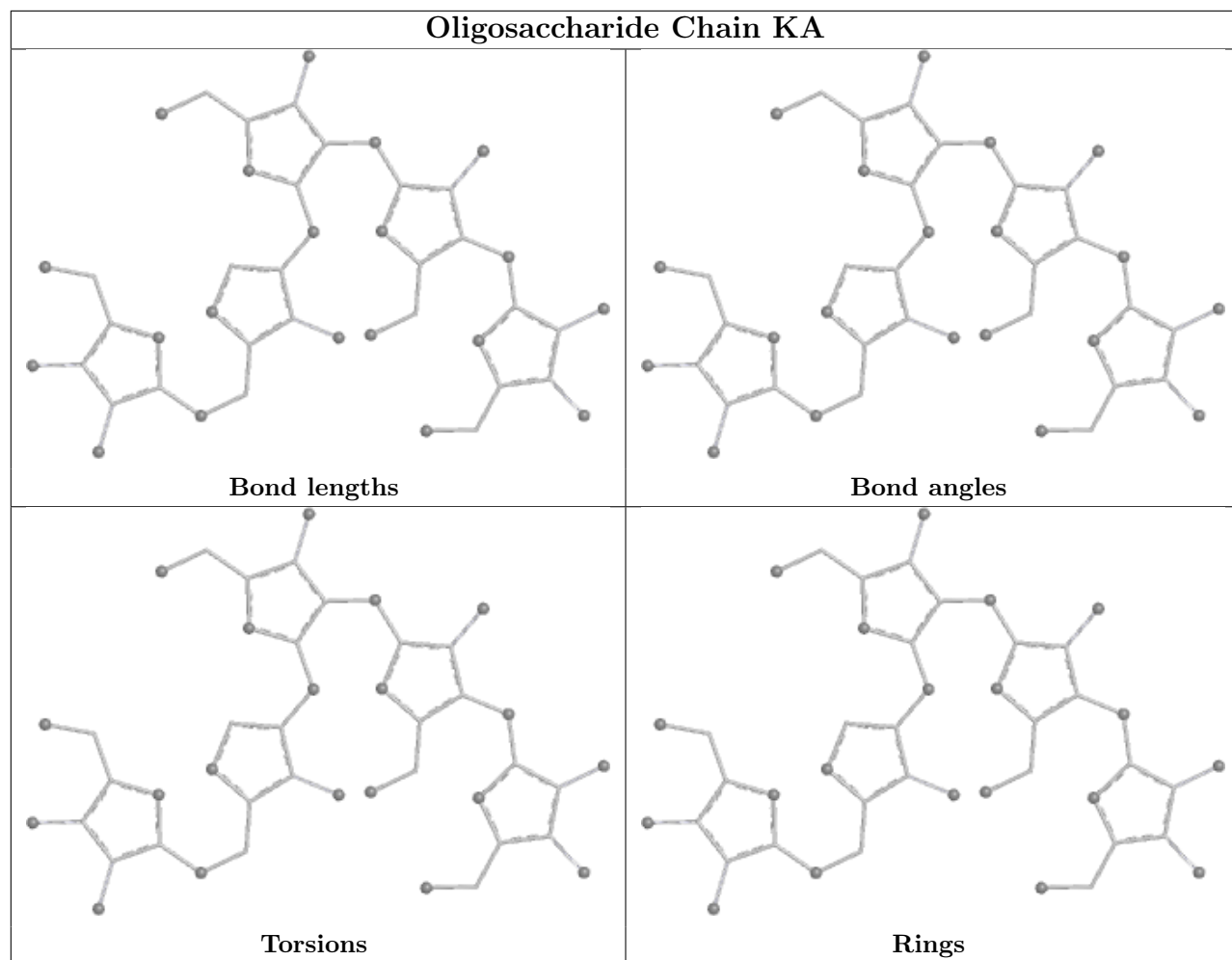
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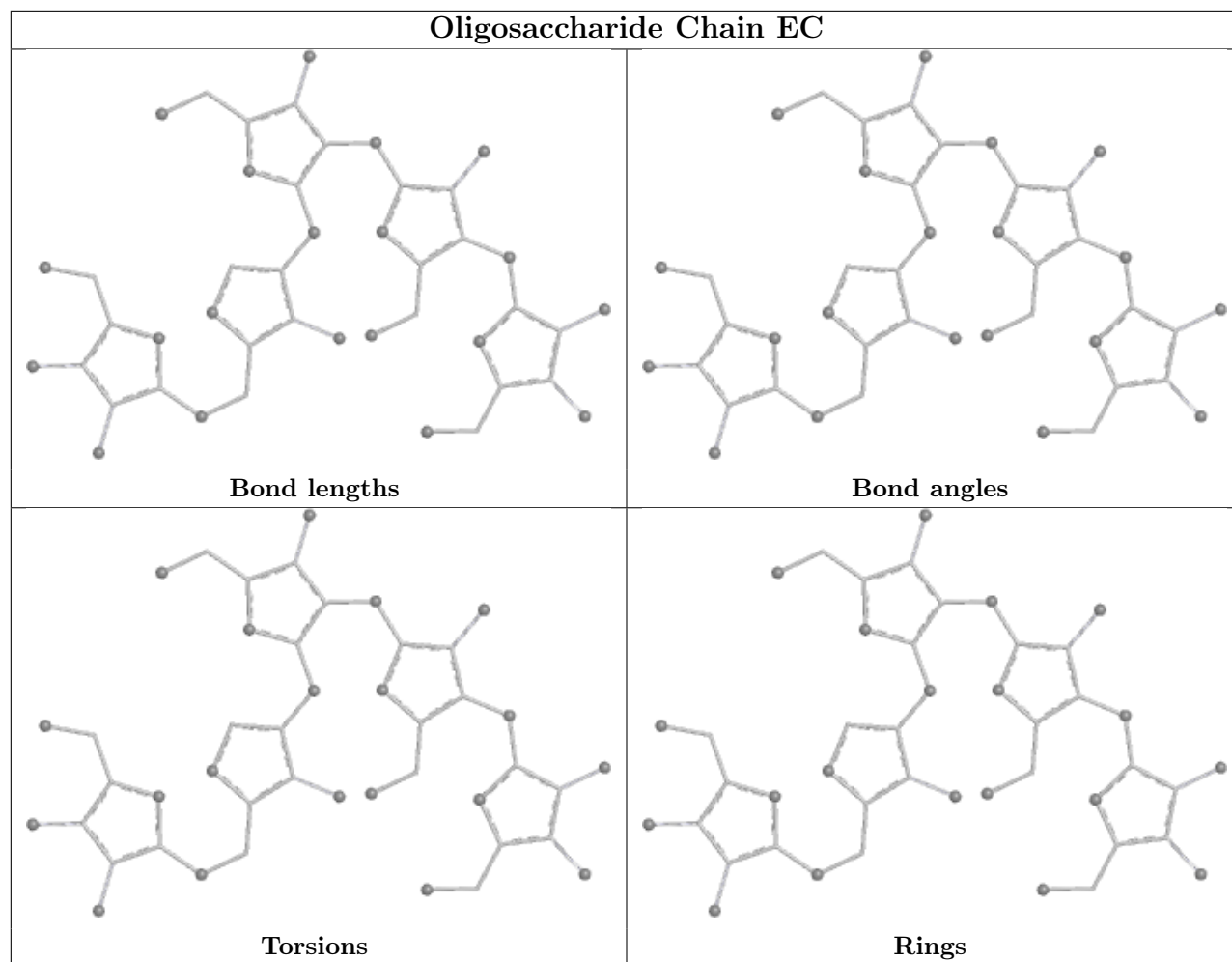


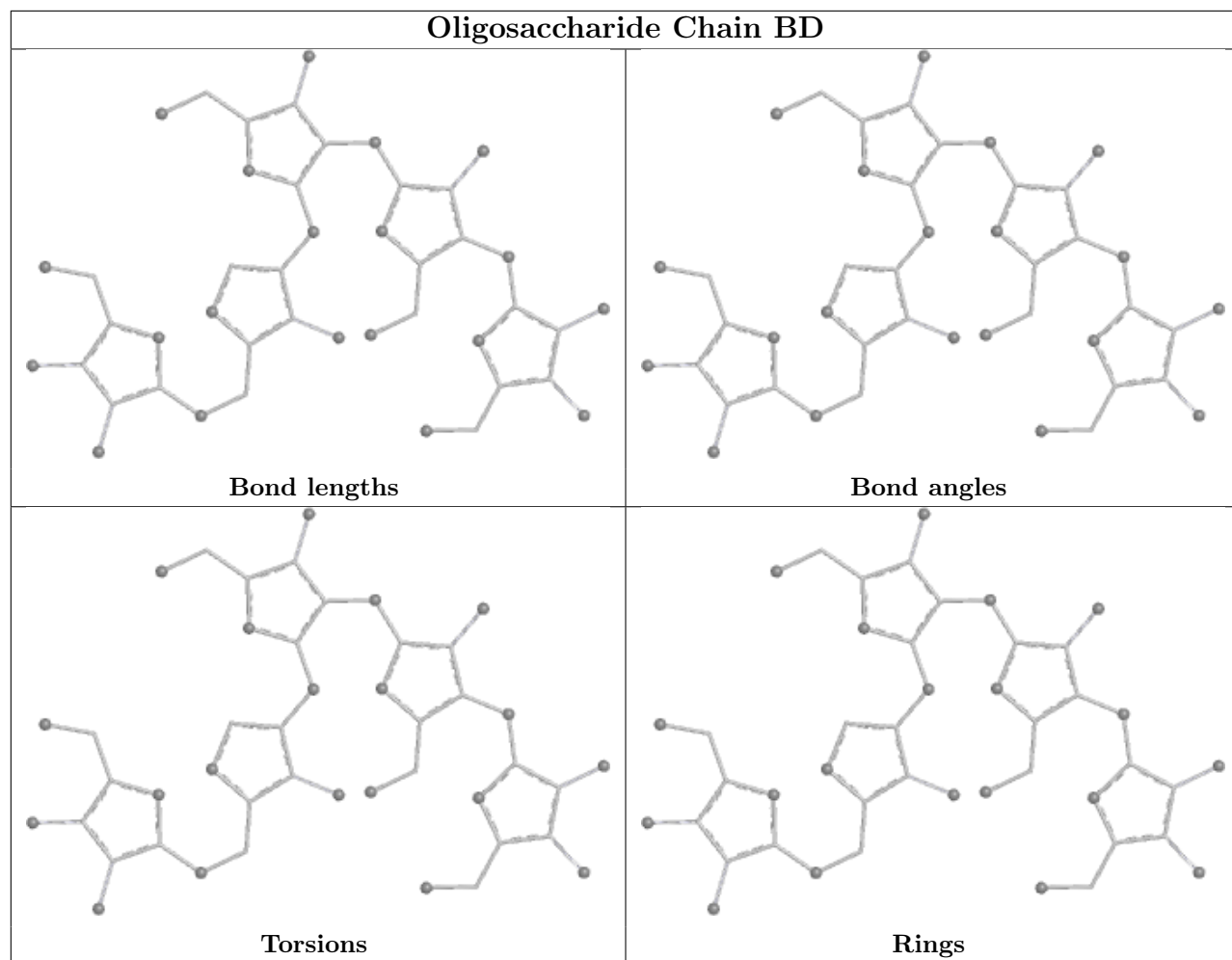


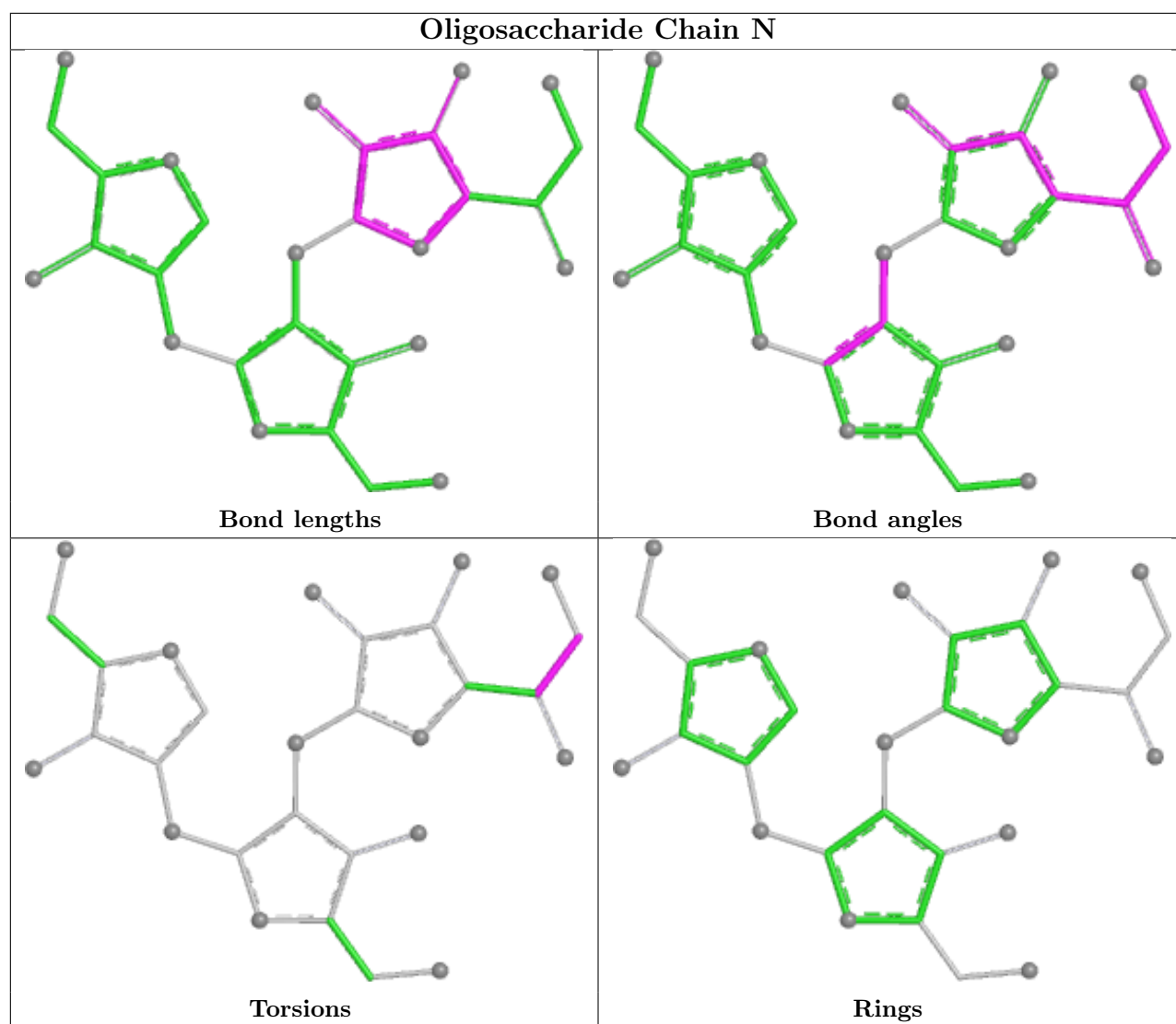


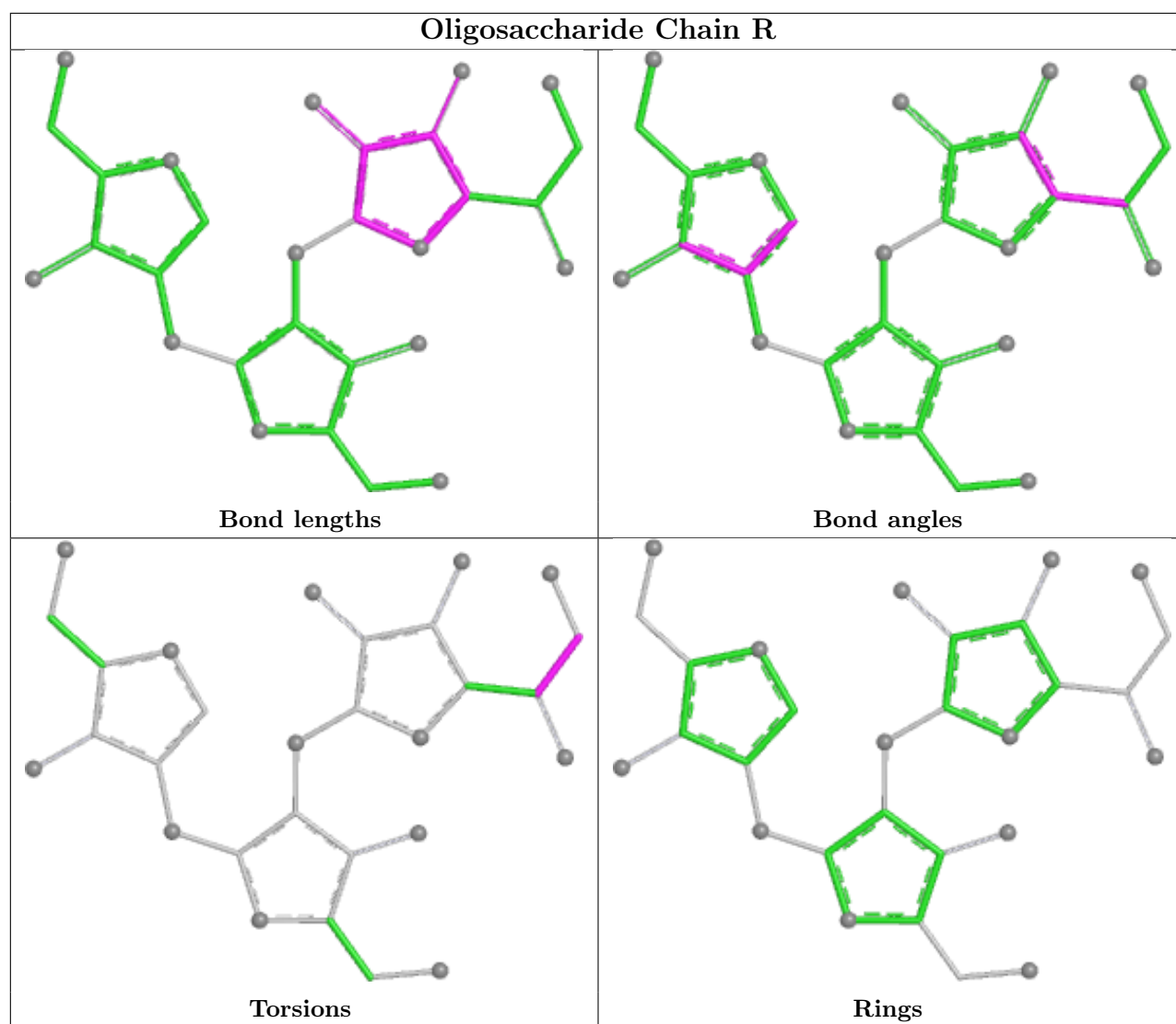


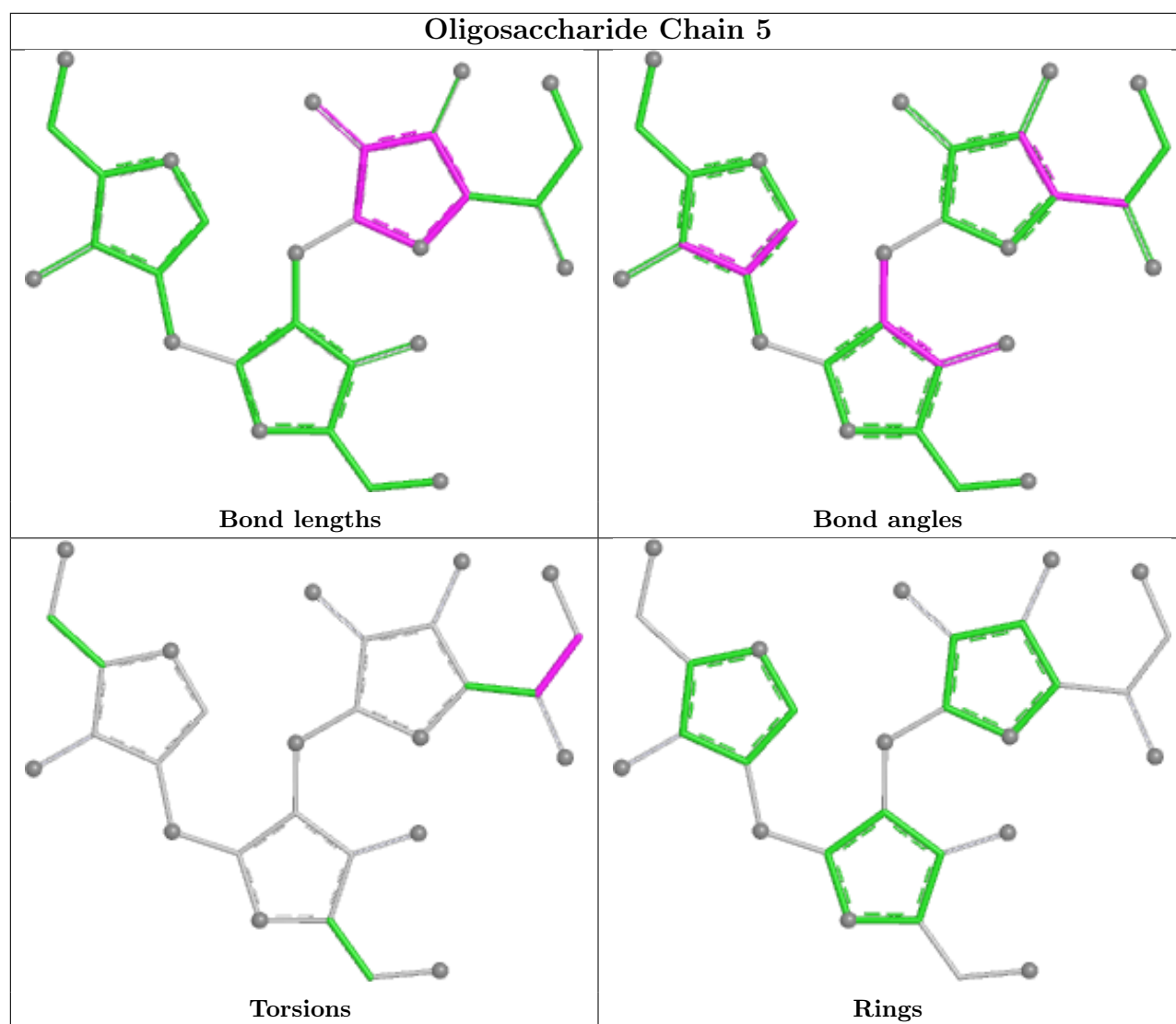




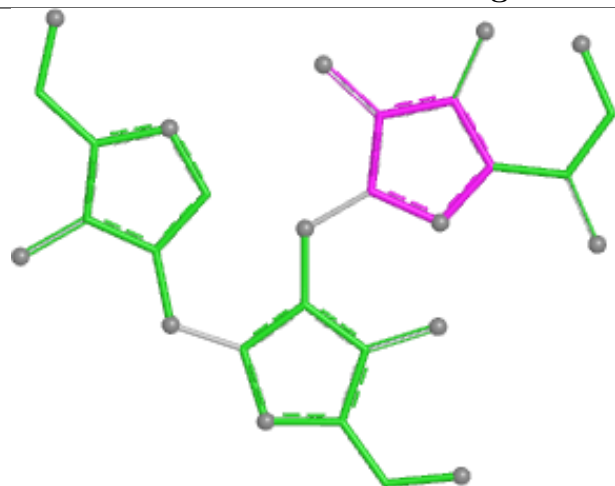




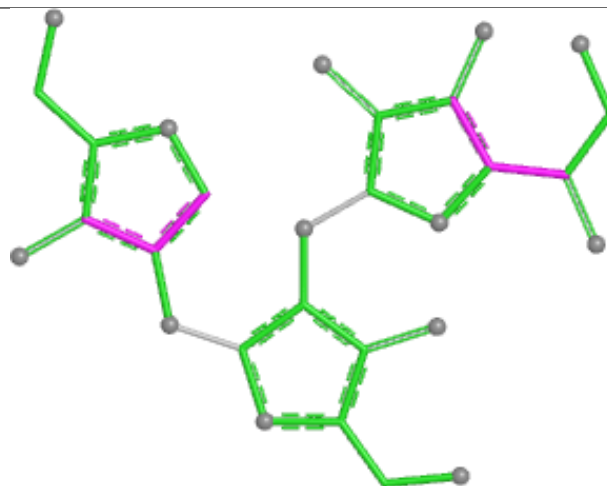




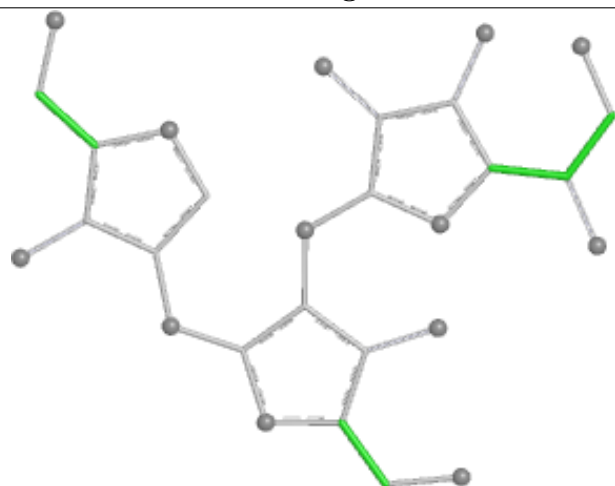
Oligosaccharide Chain 8



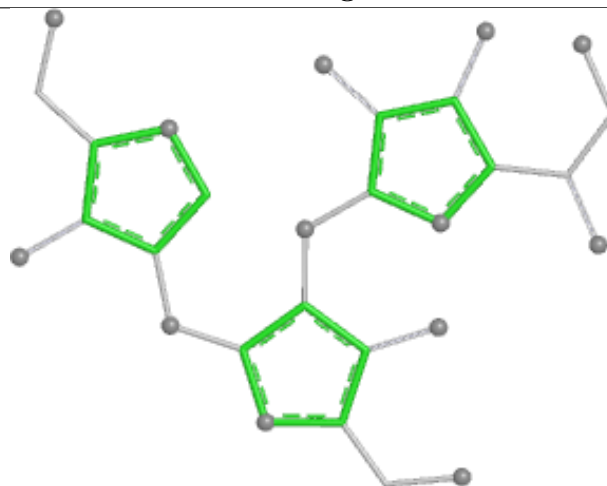
Bond lengths



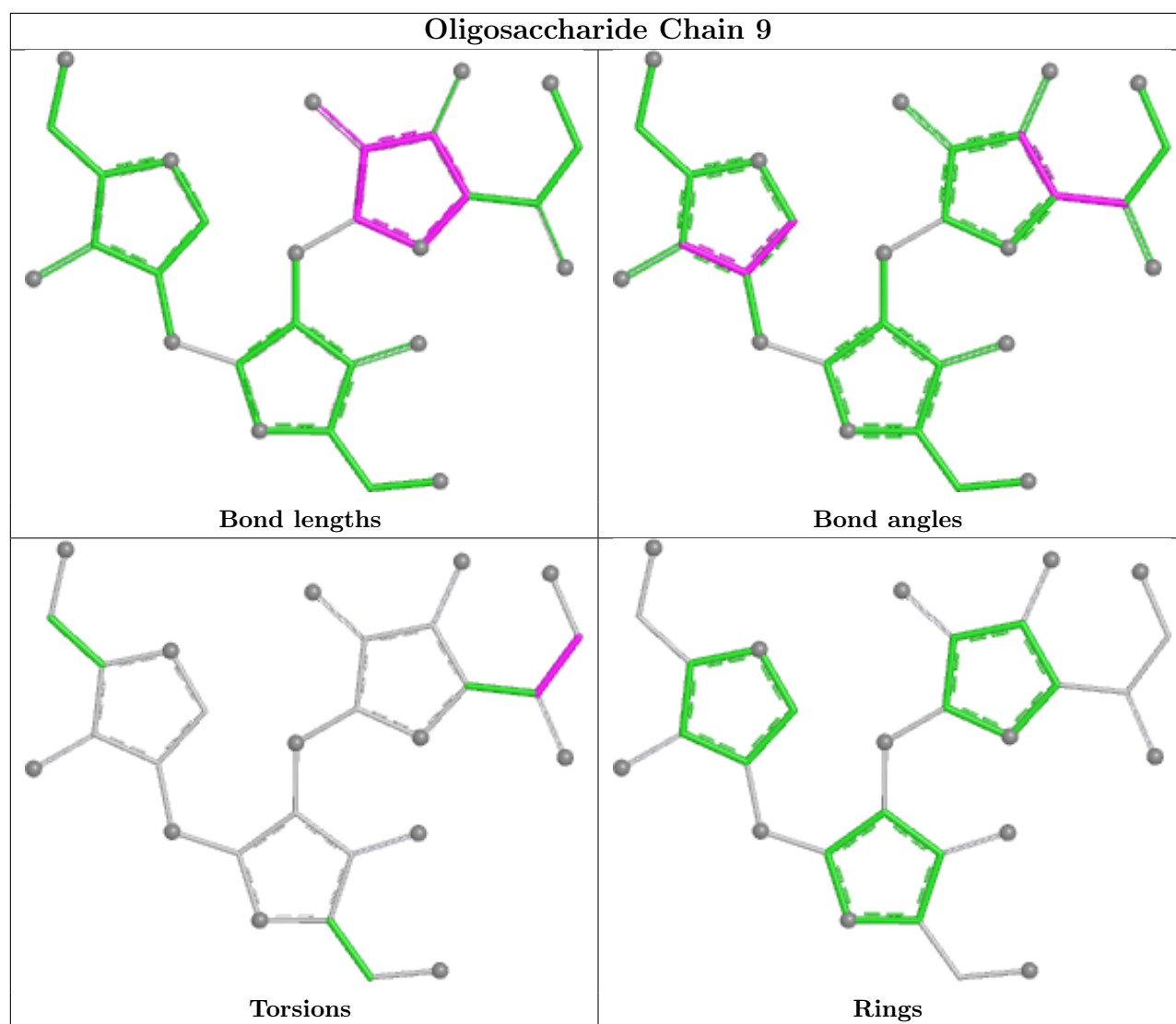
Bond angles

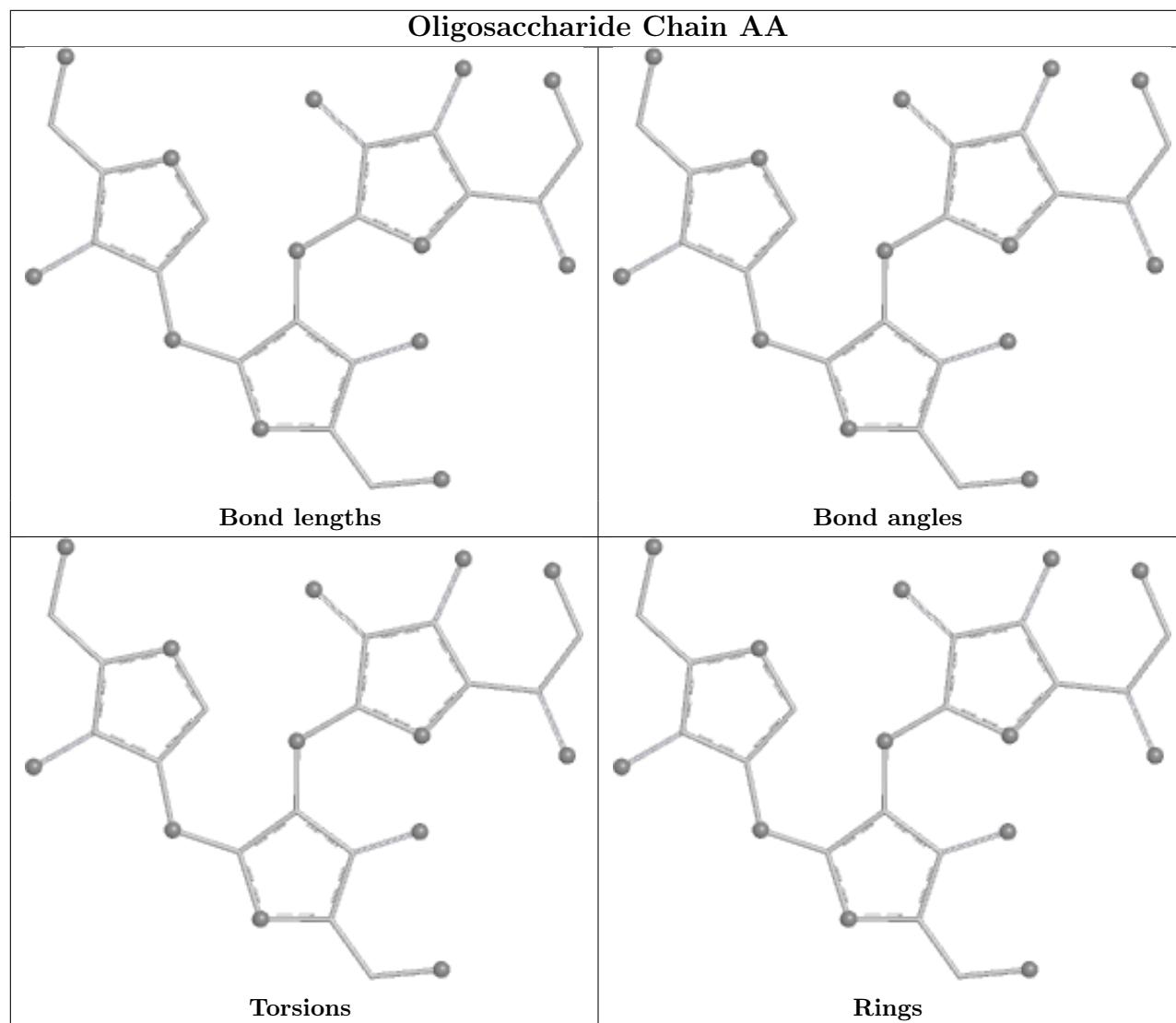


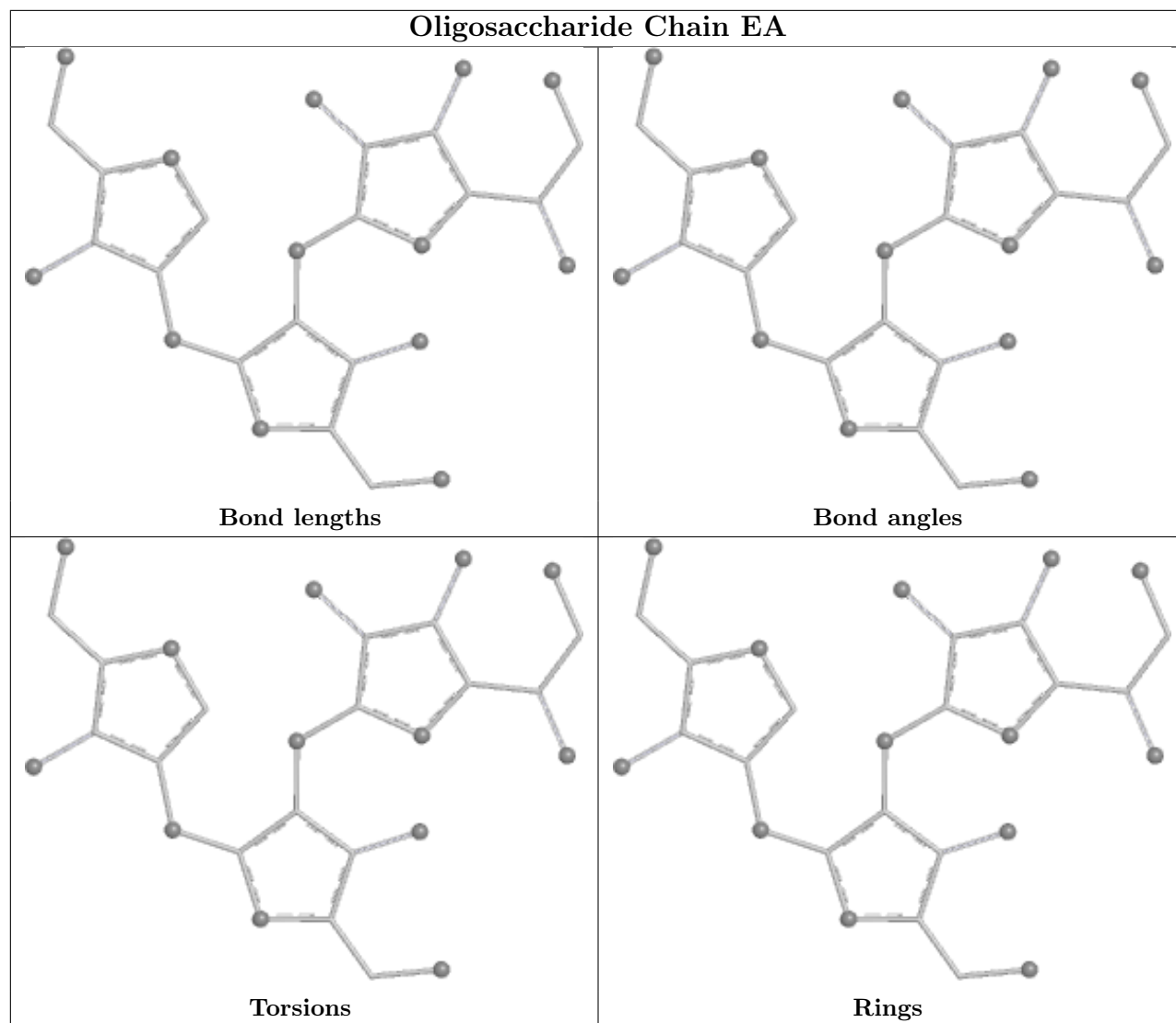
Torsions

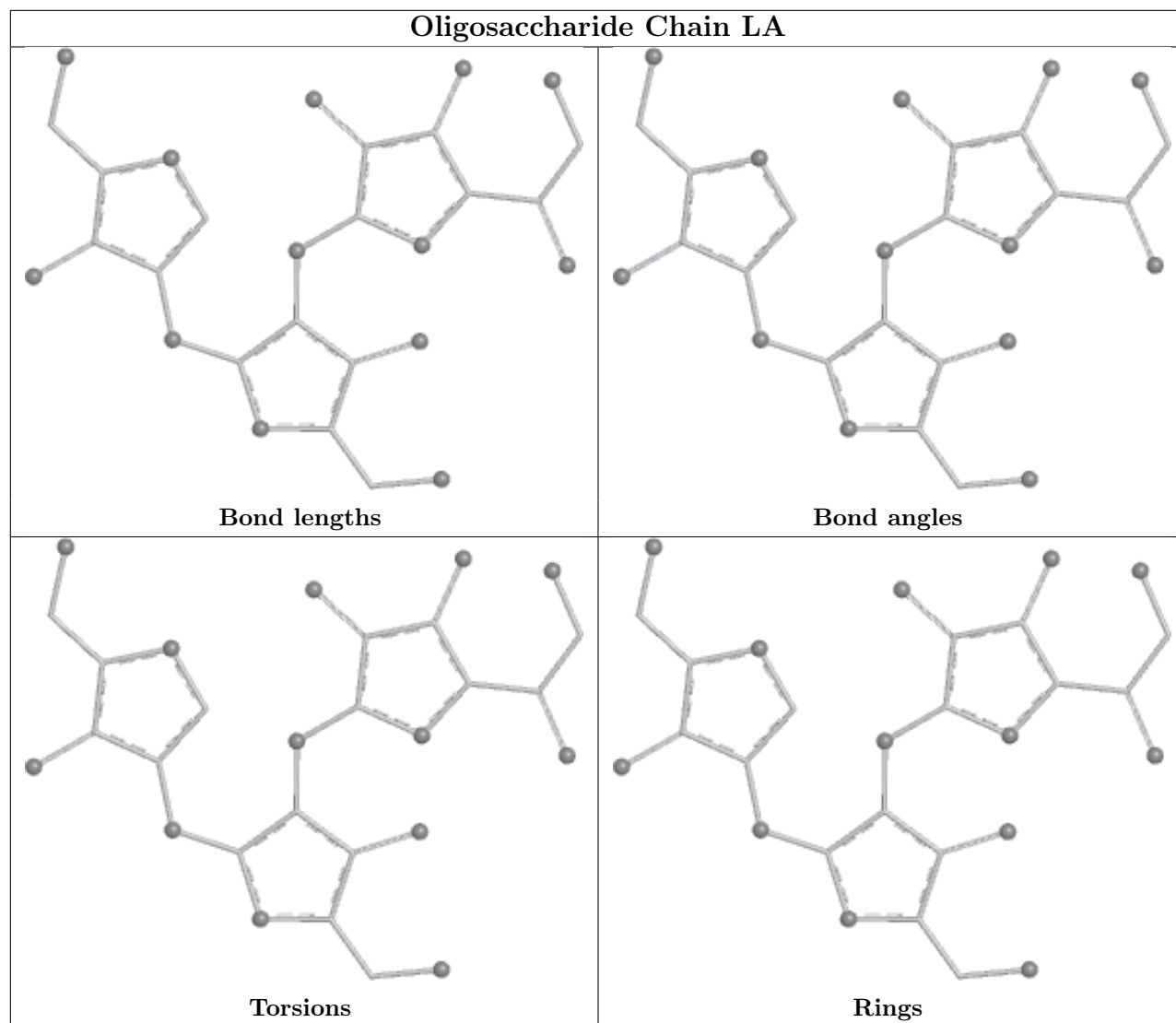


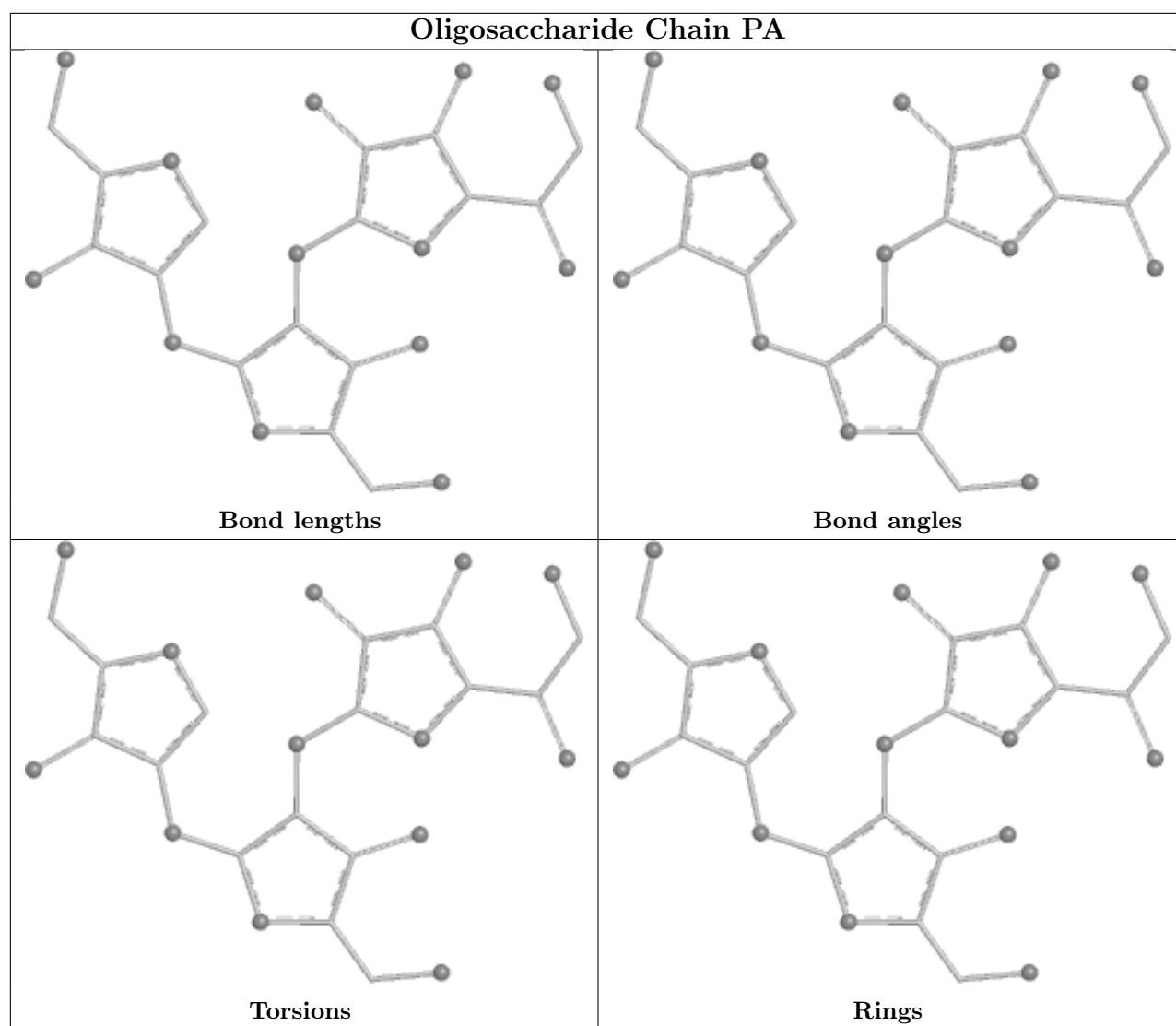
Rings

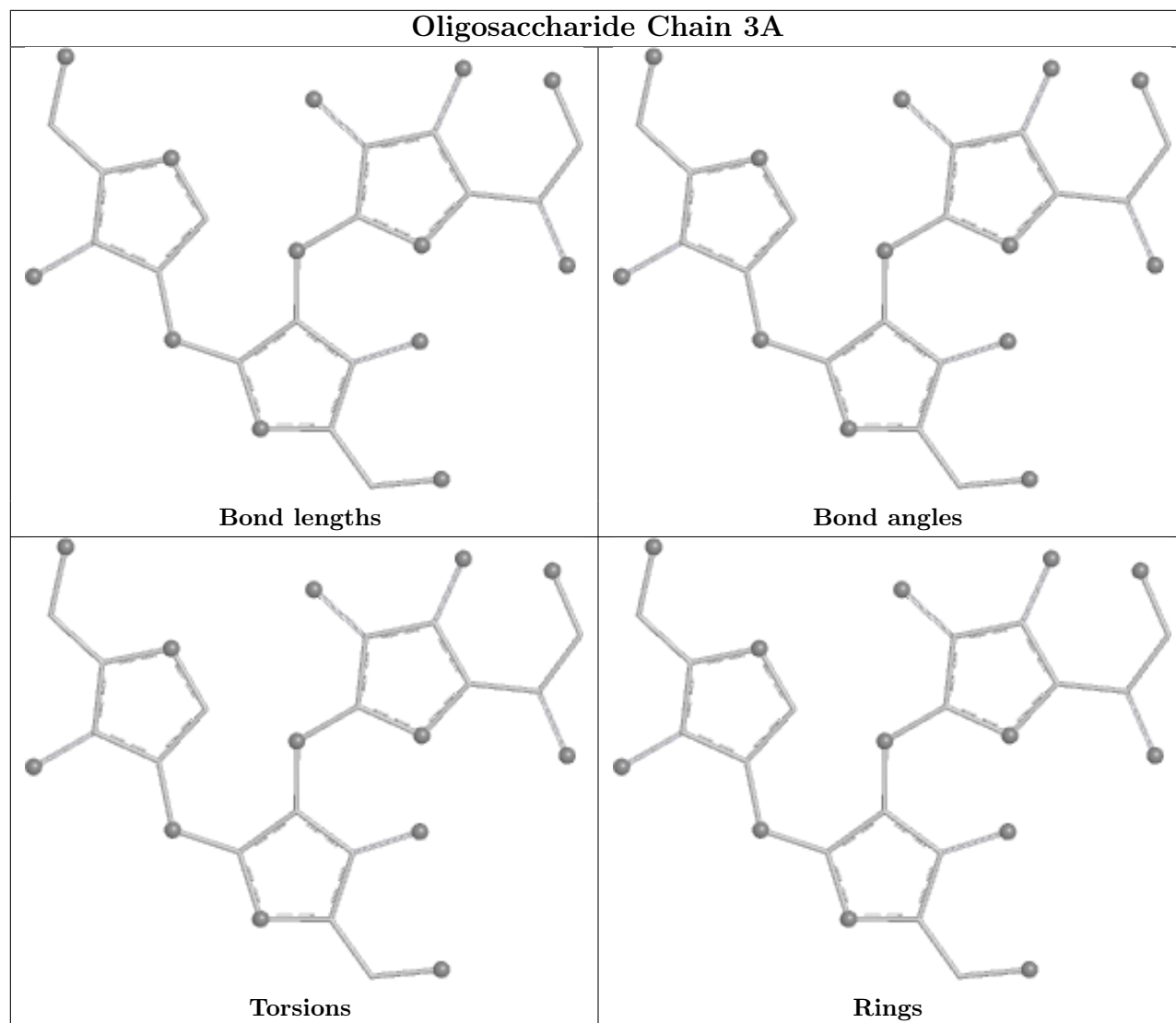


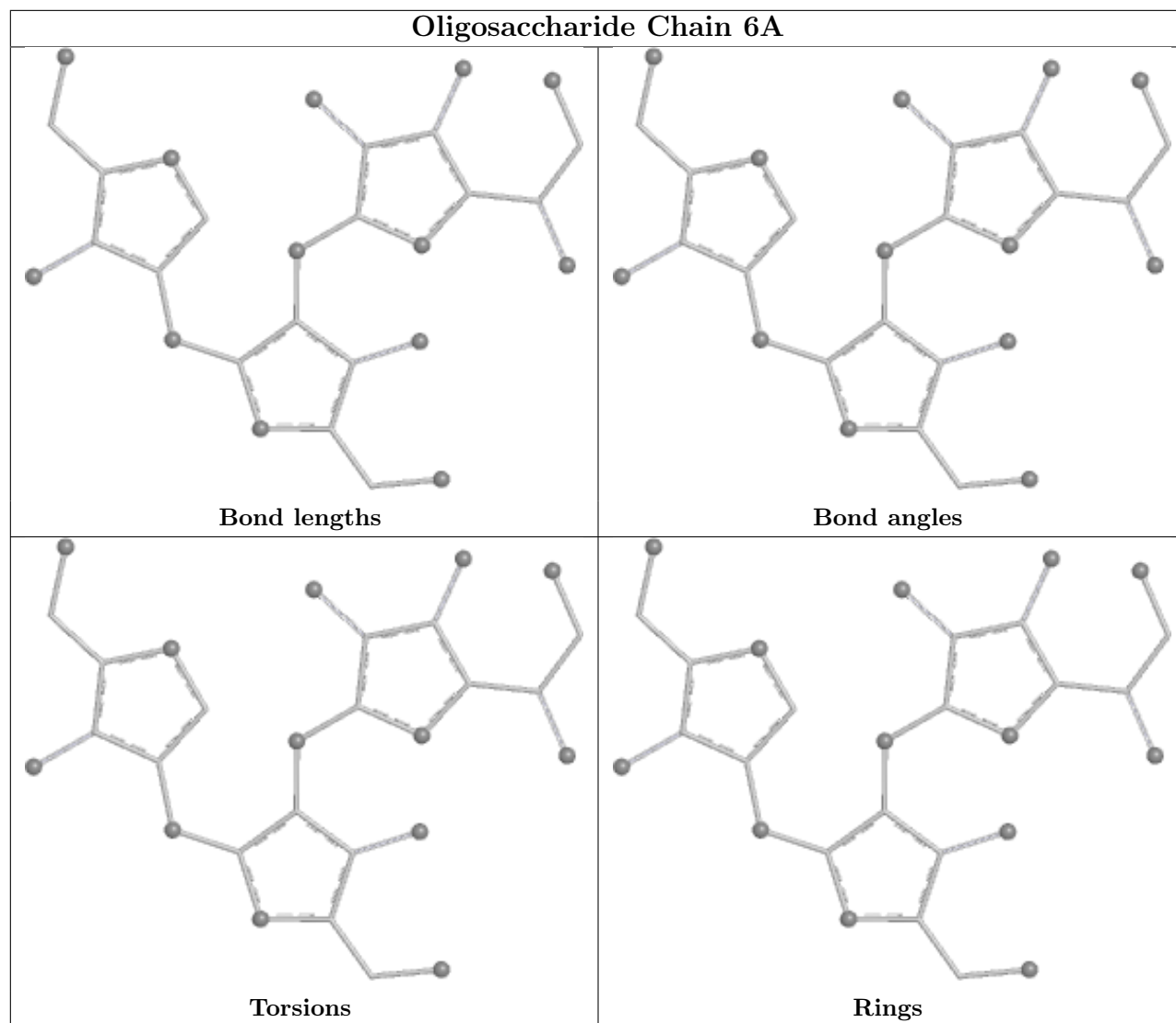


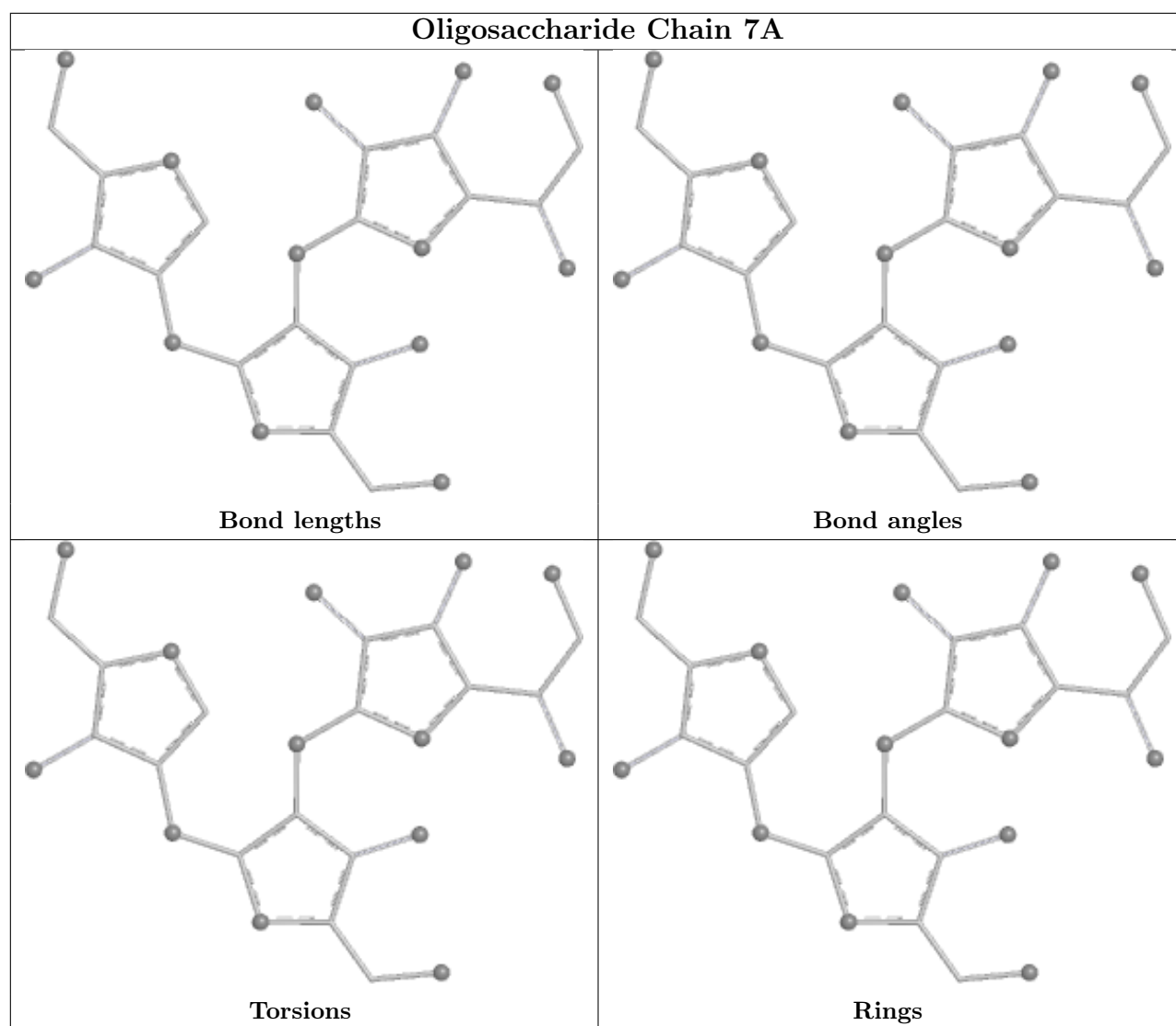


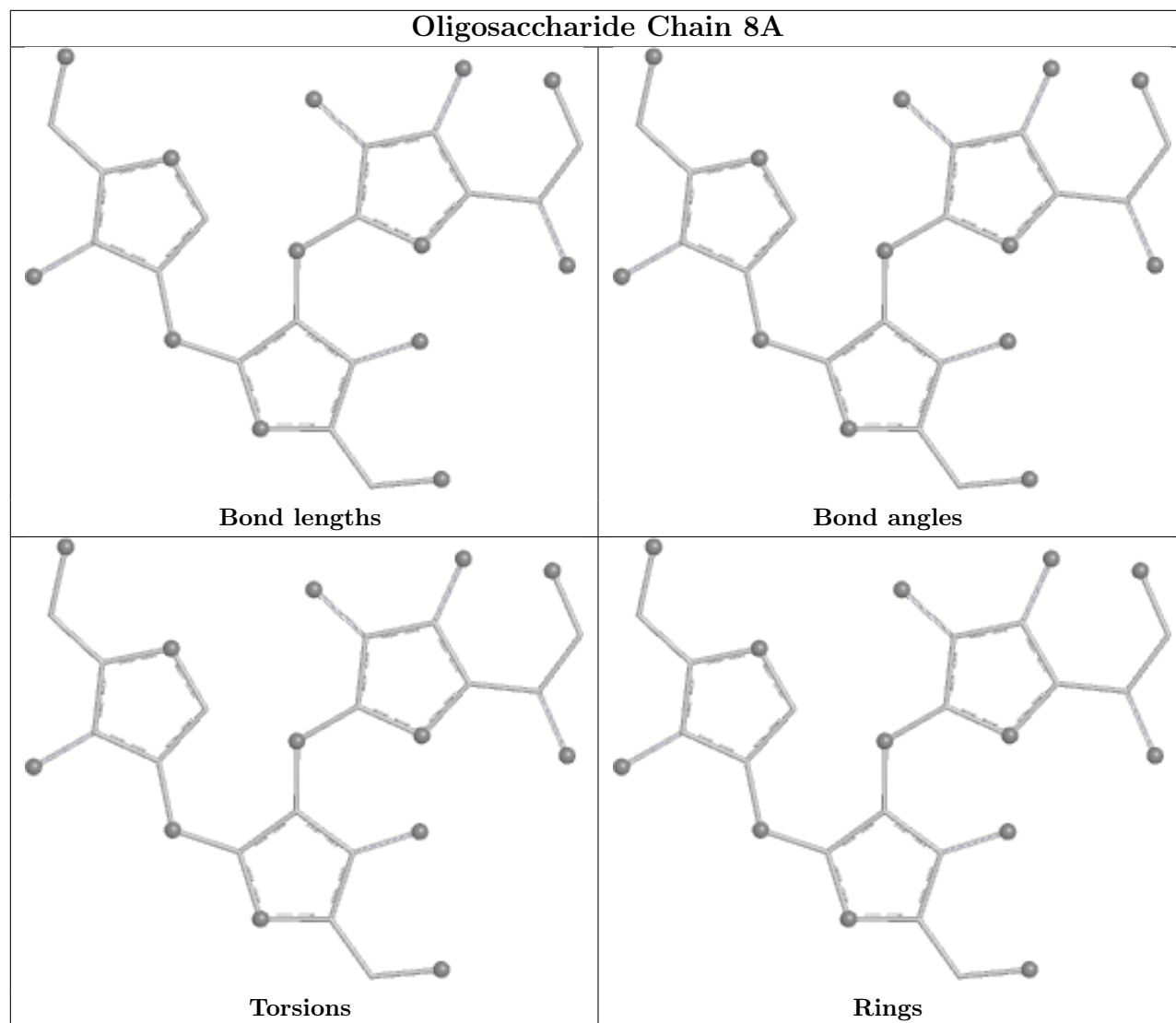


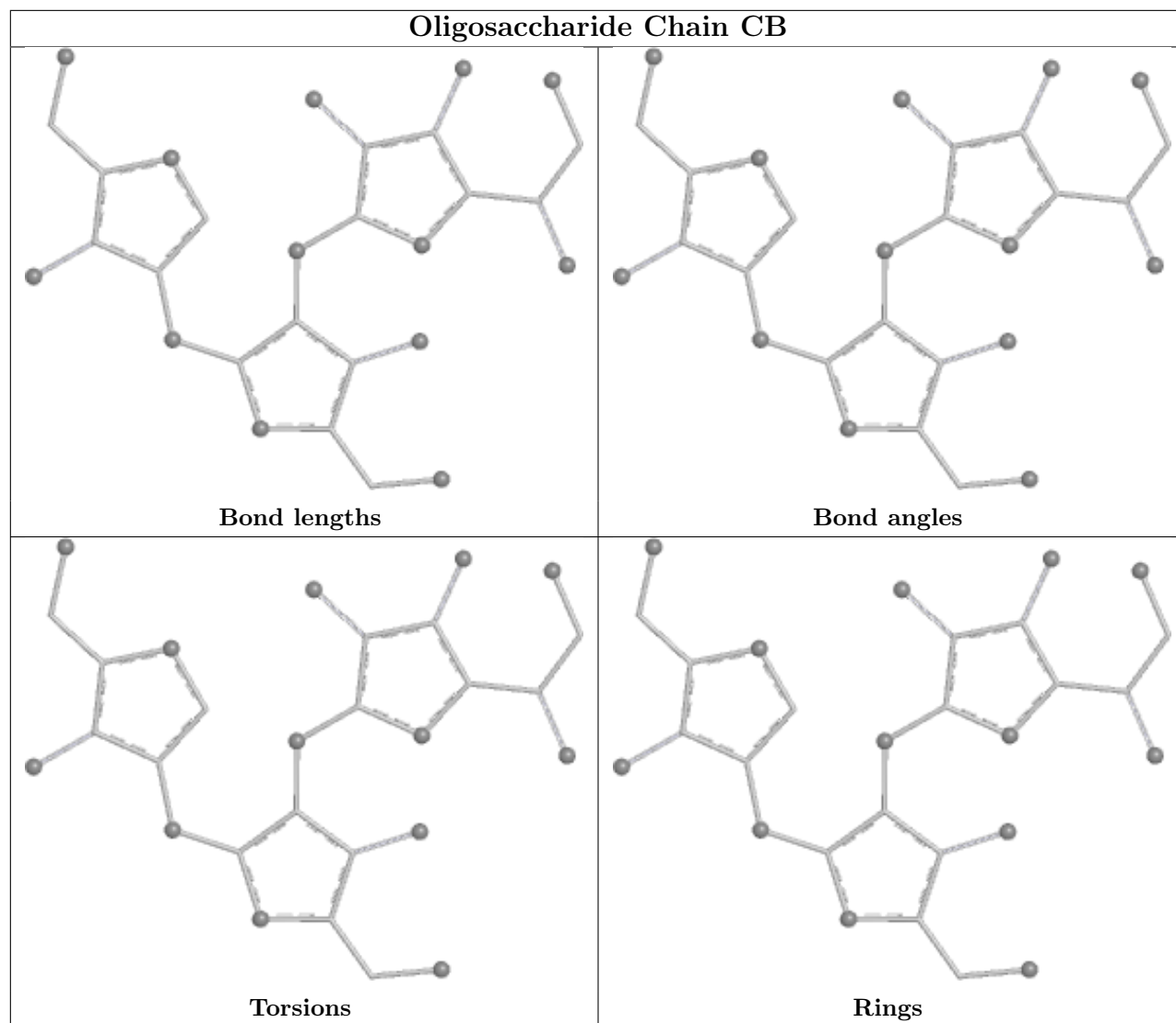


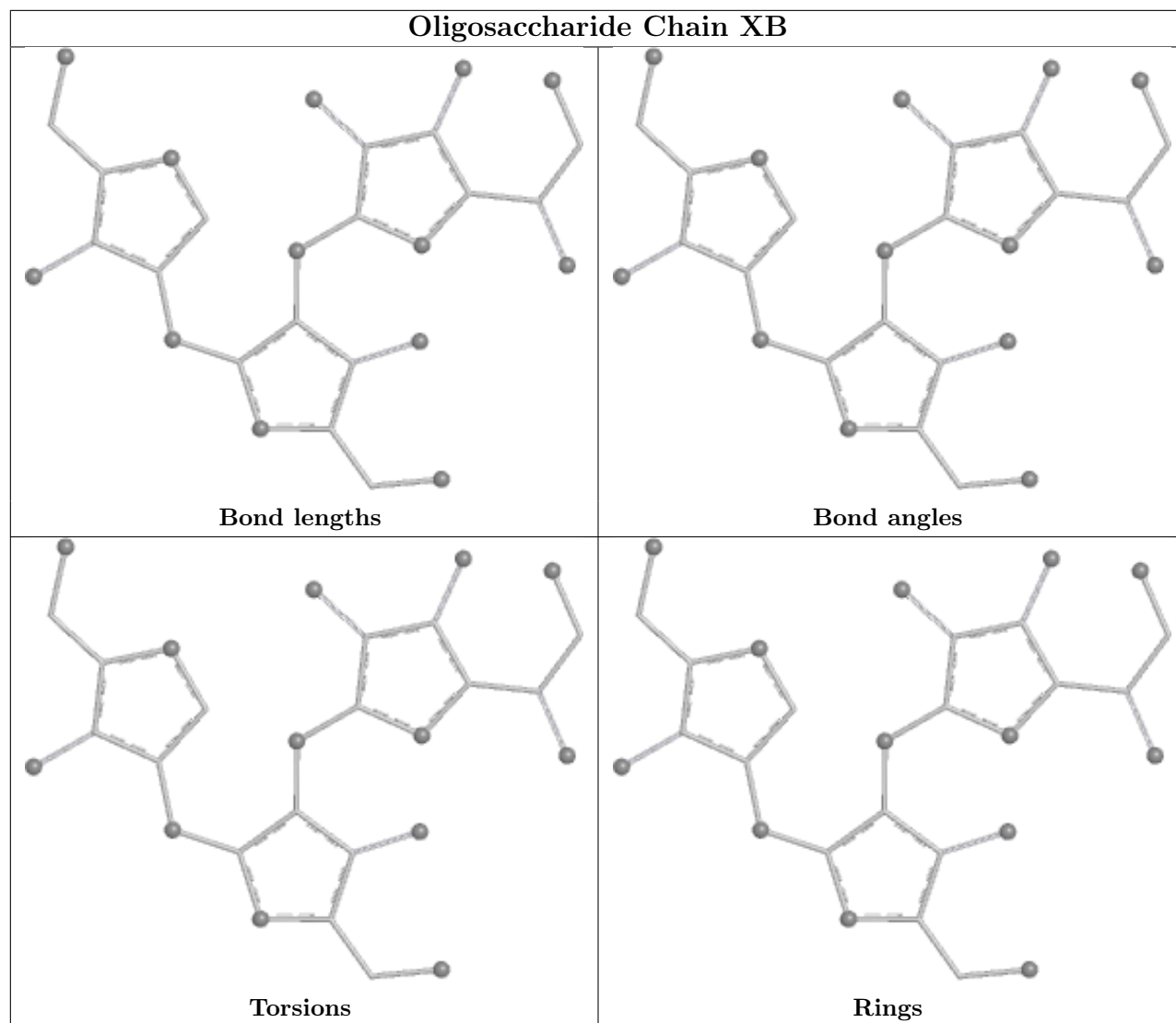


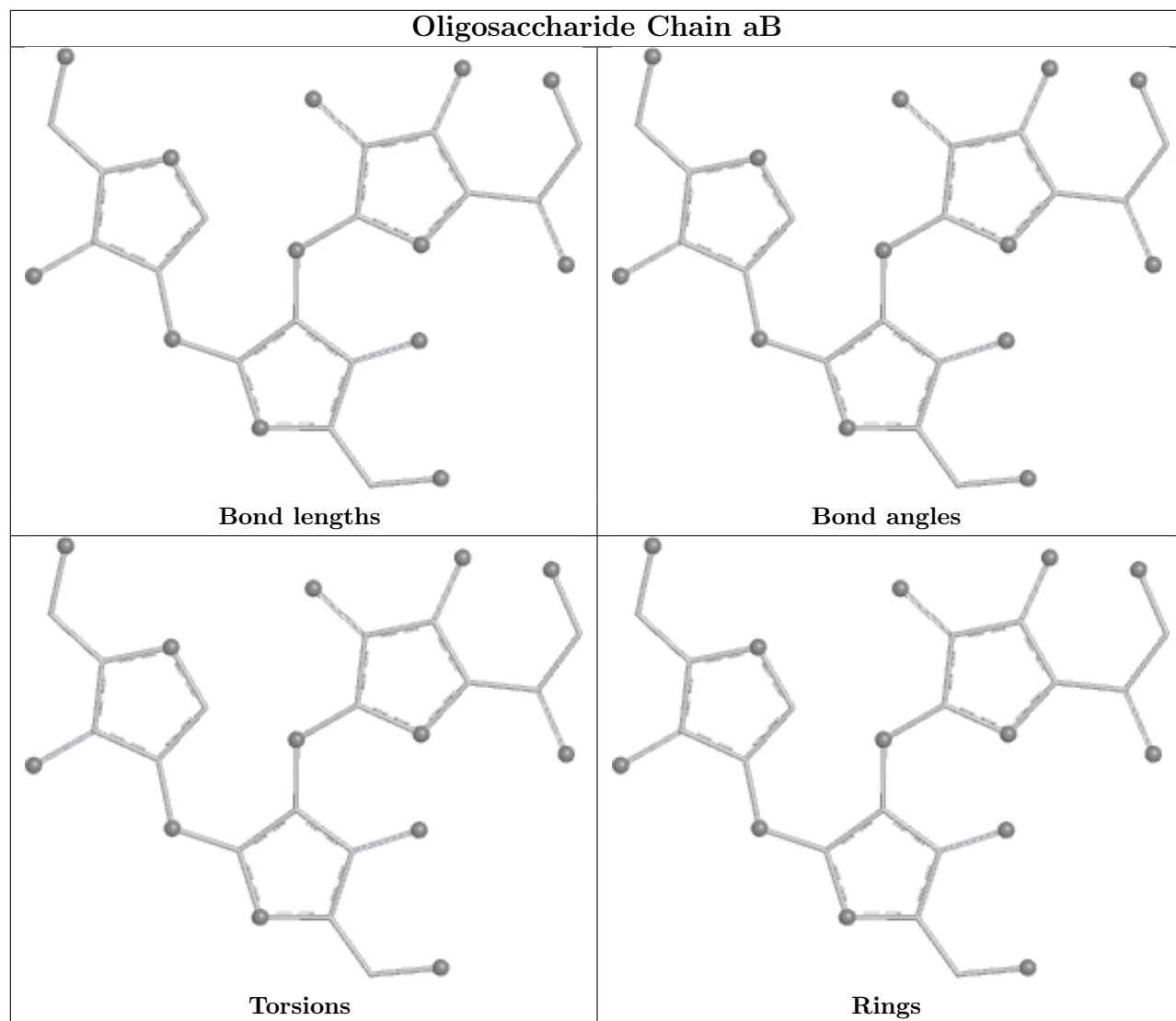


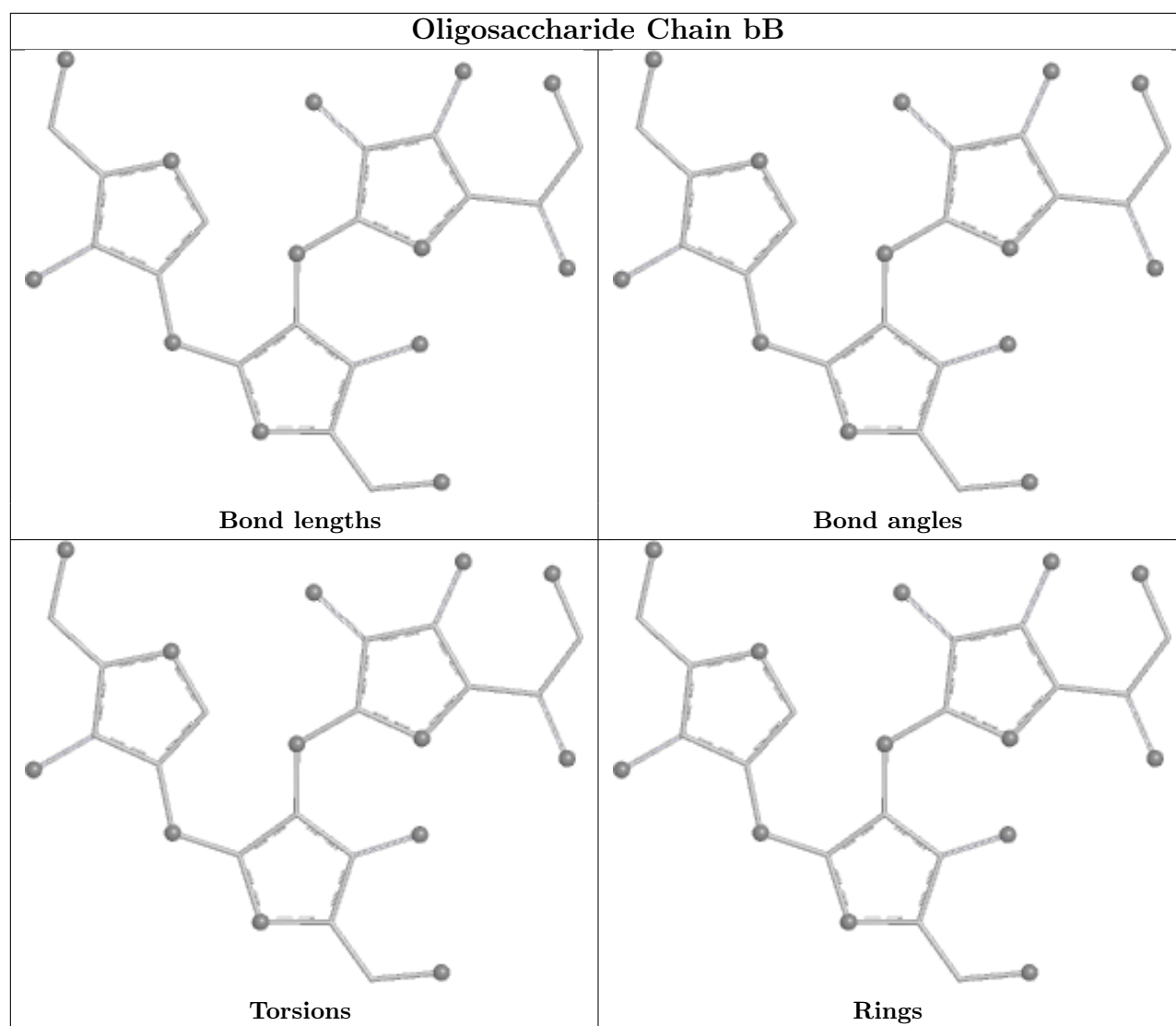


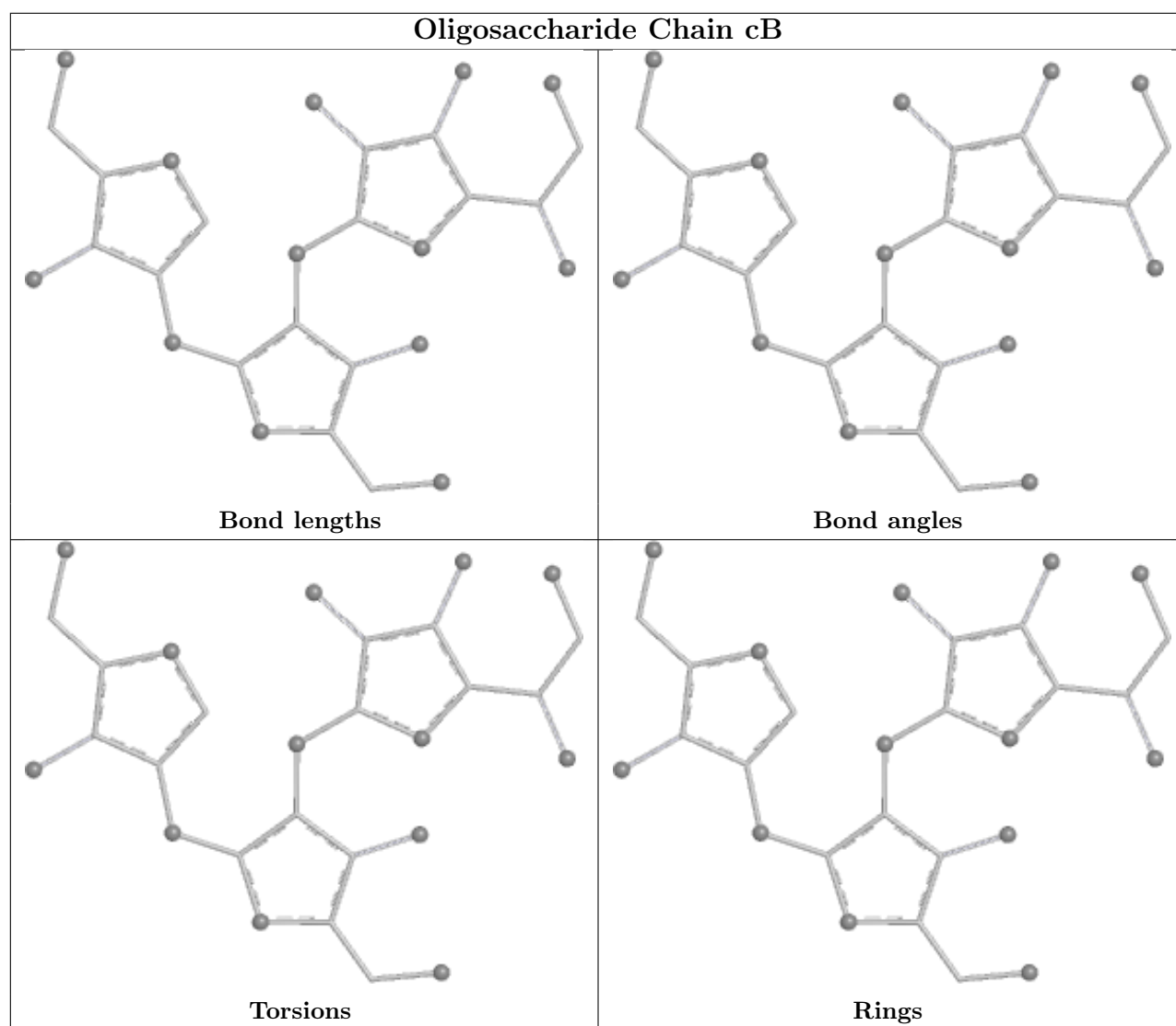


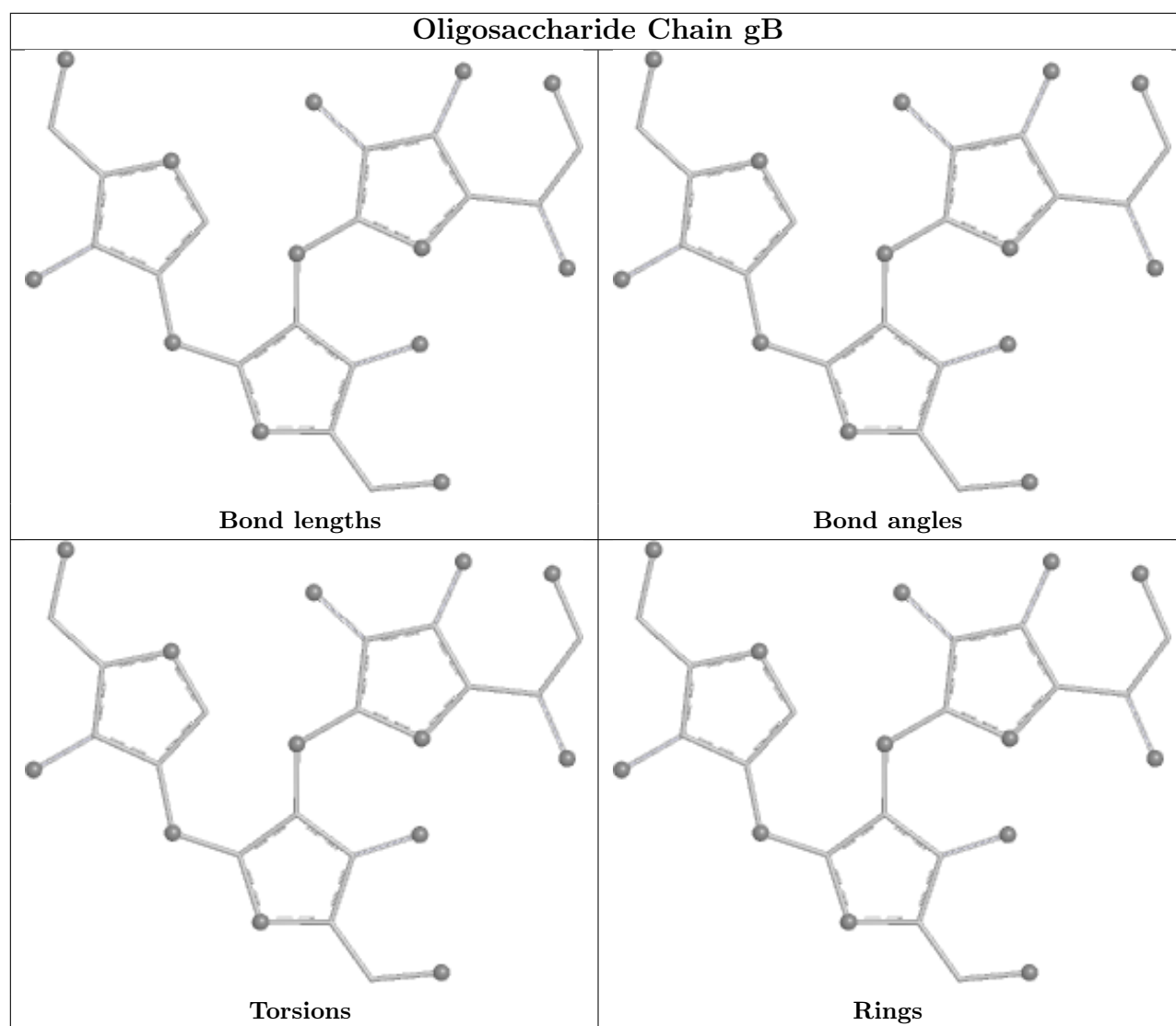


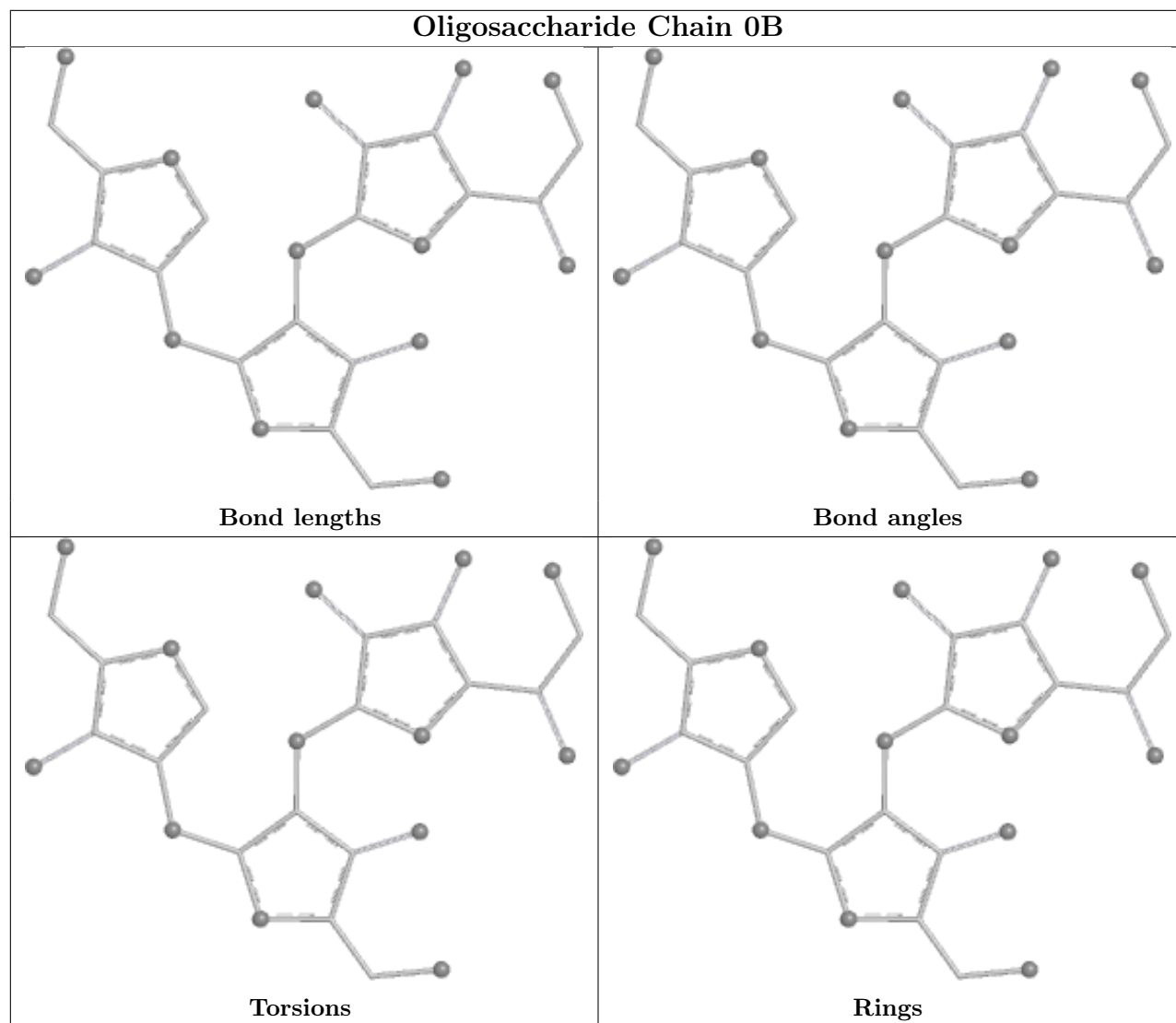


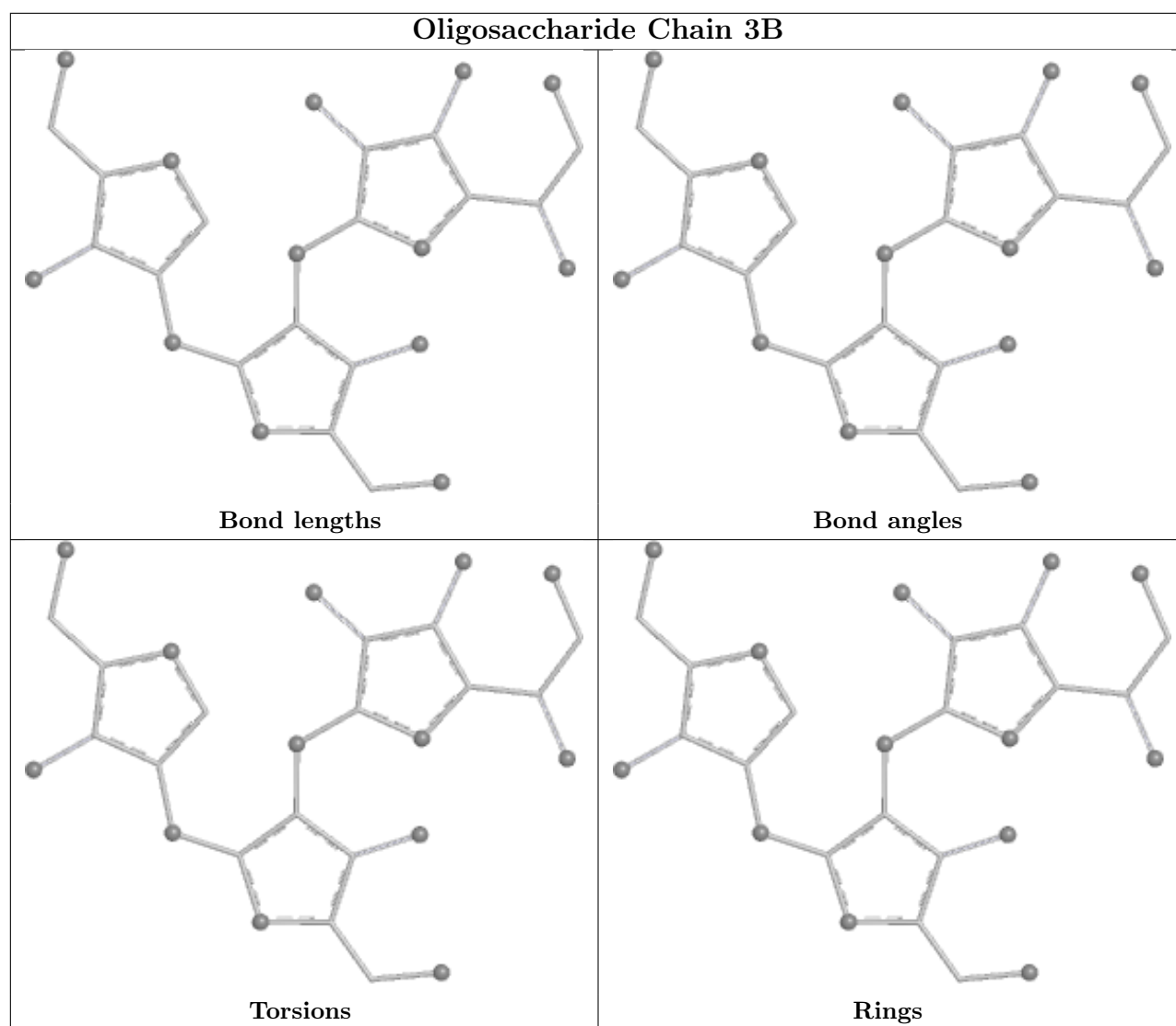


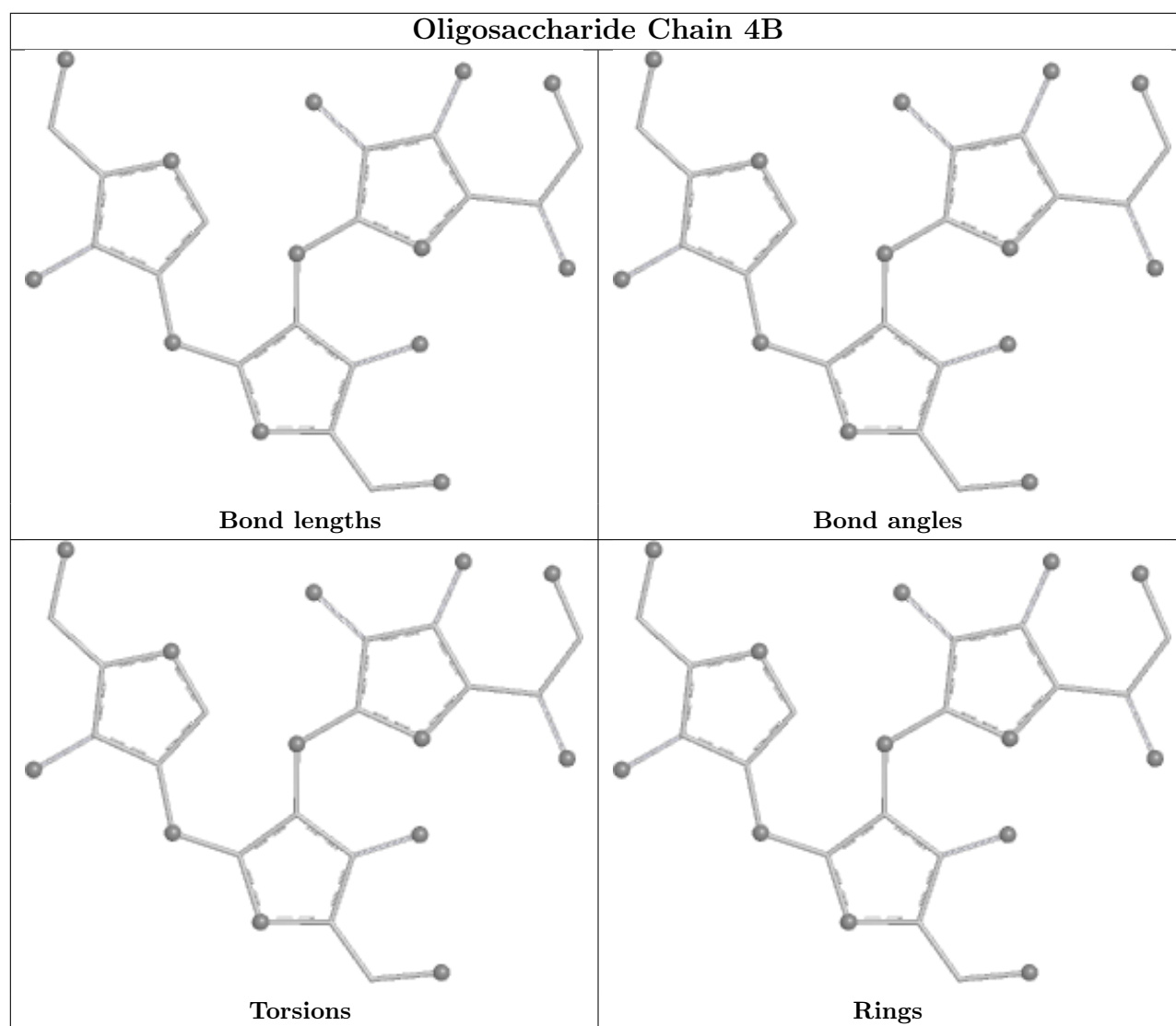




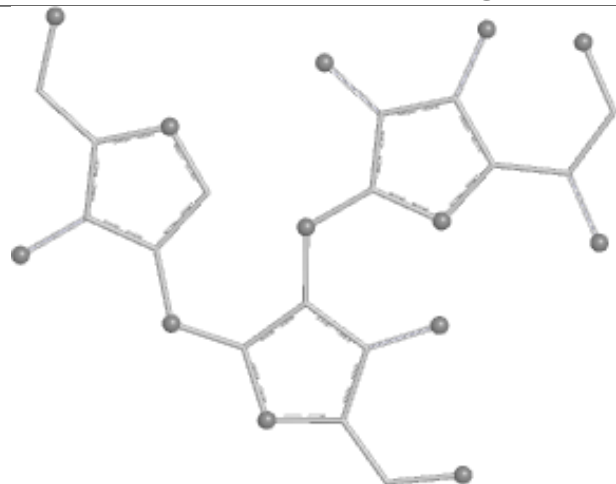




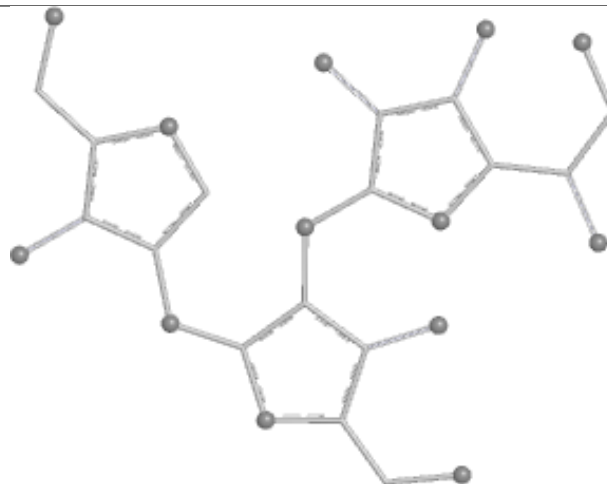




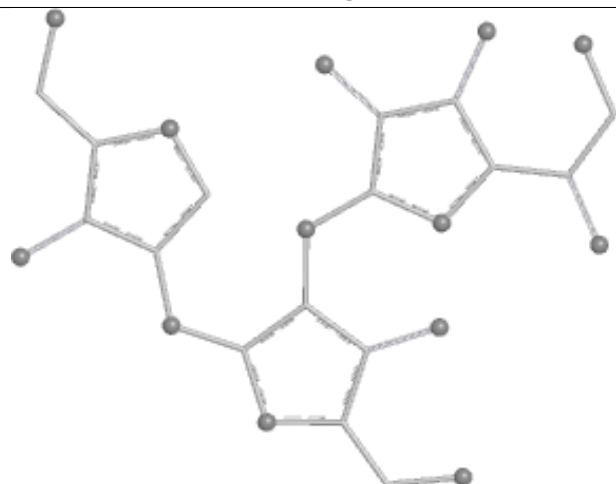
Oligosaccharide Chain 5B



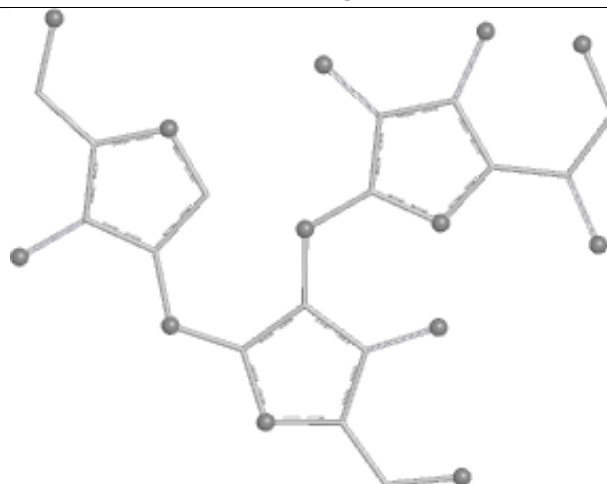
Bond lengths



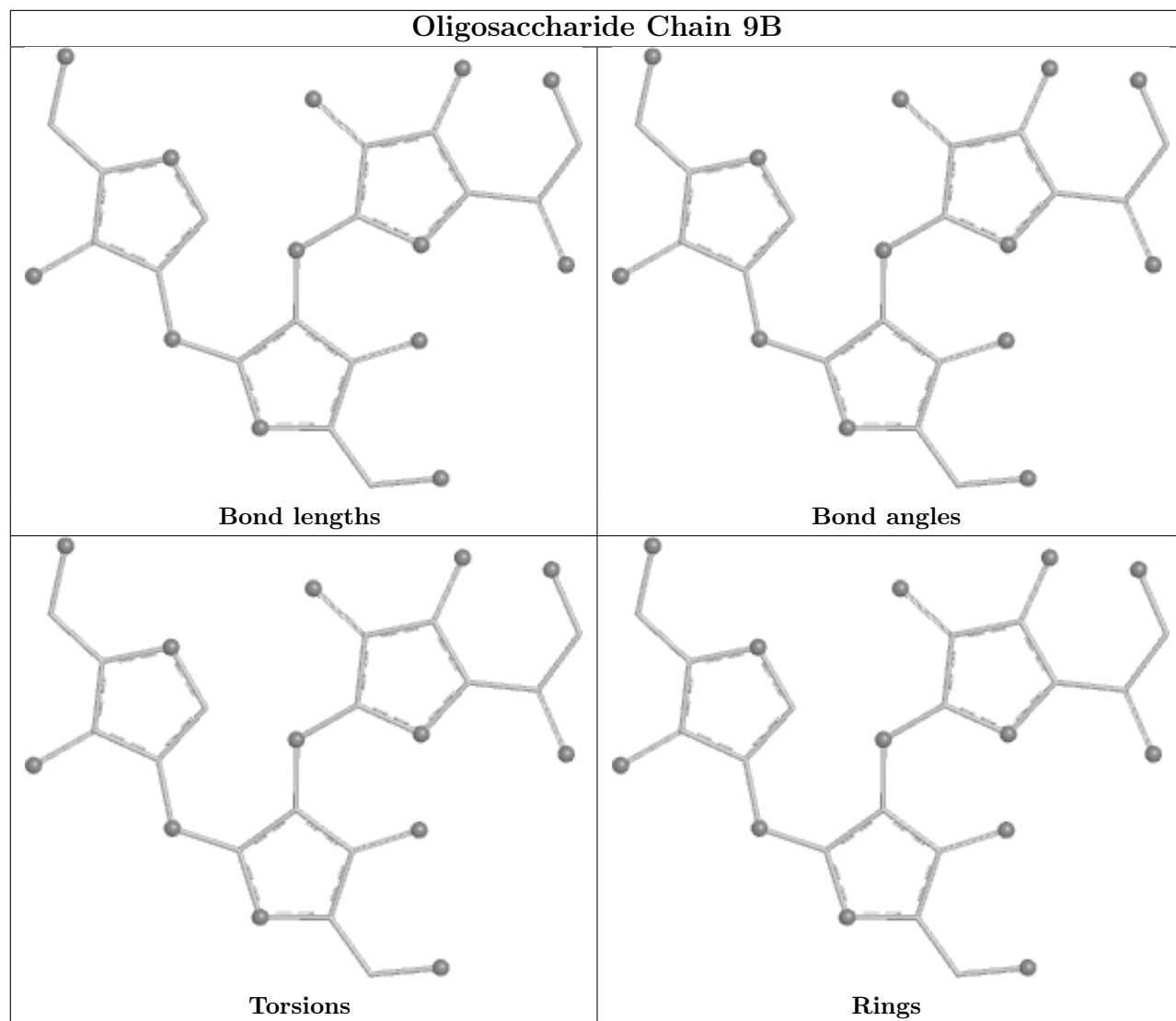
Bond angles

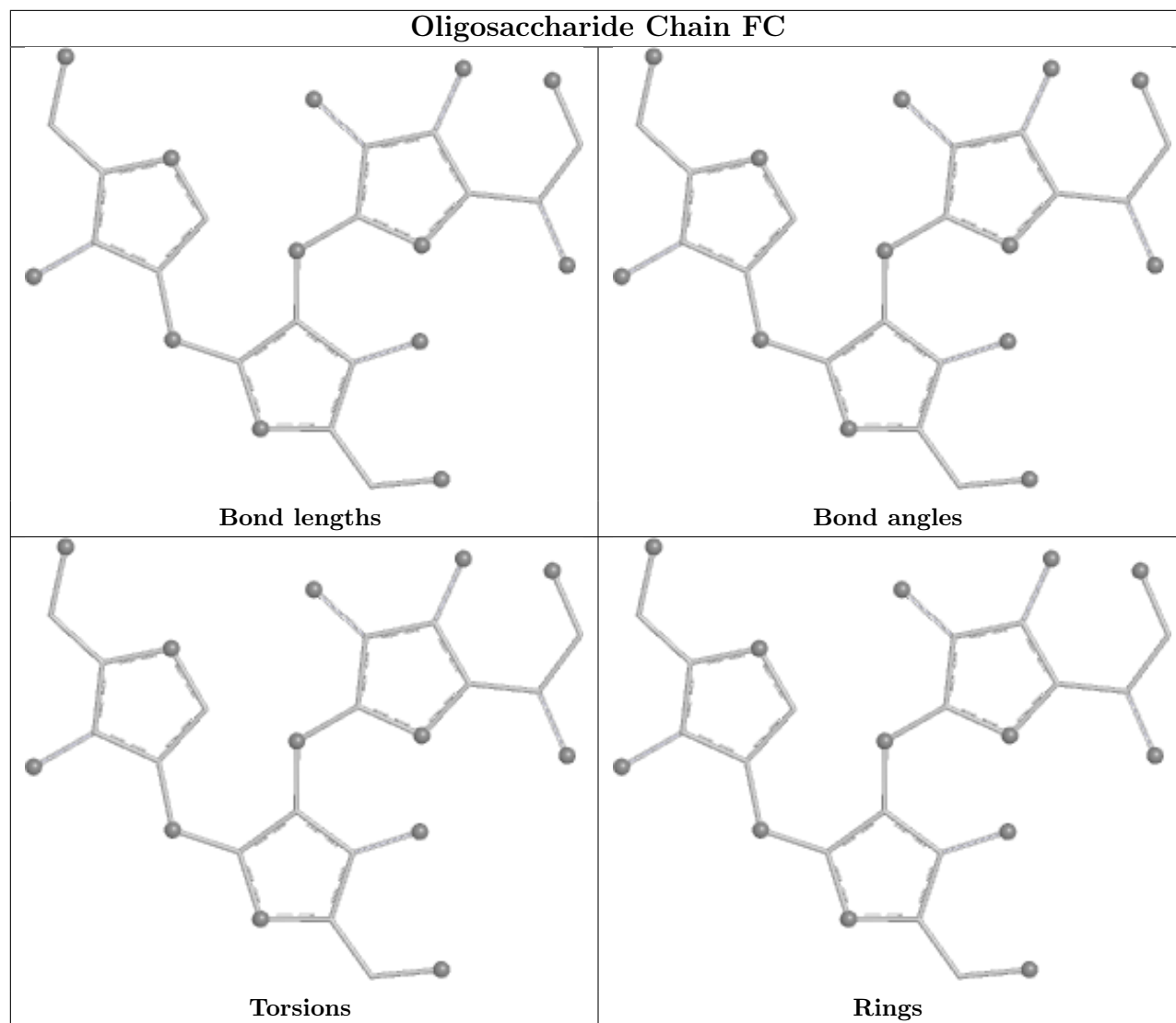


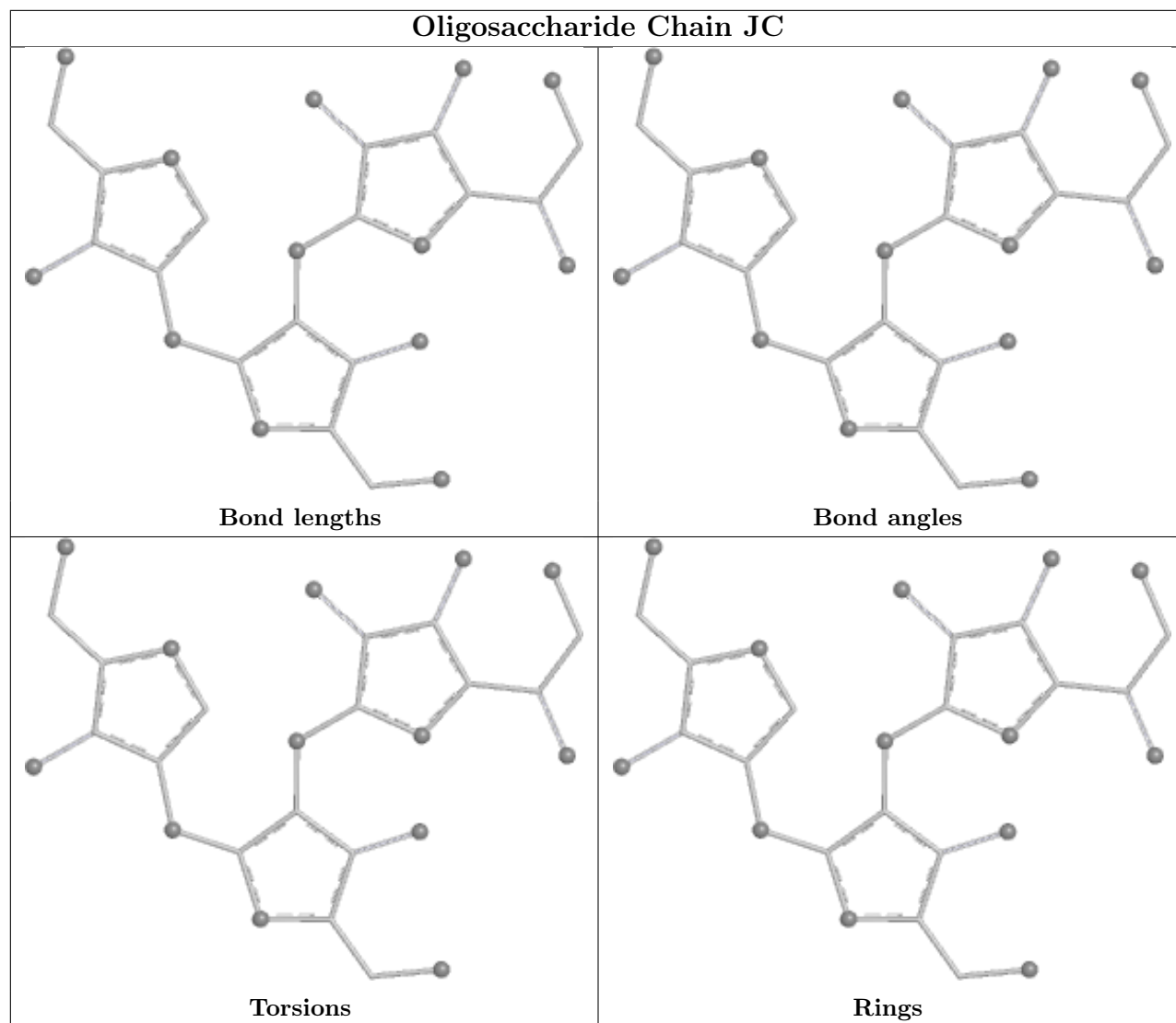
Torsions

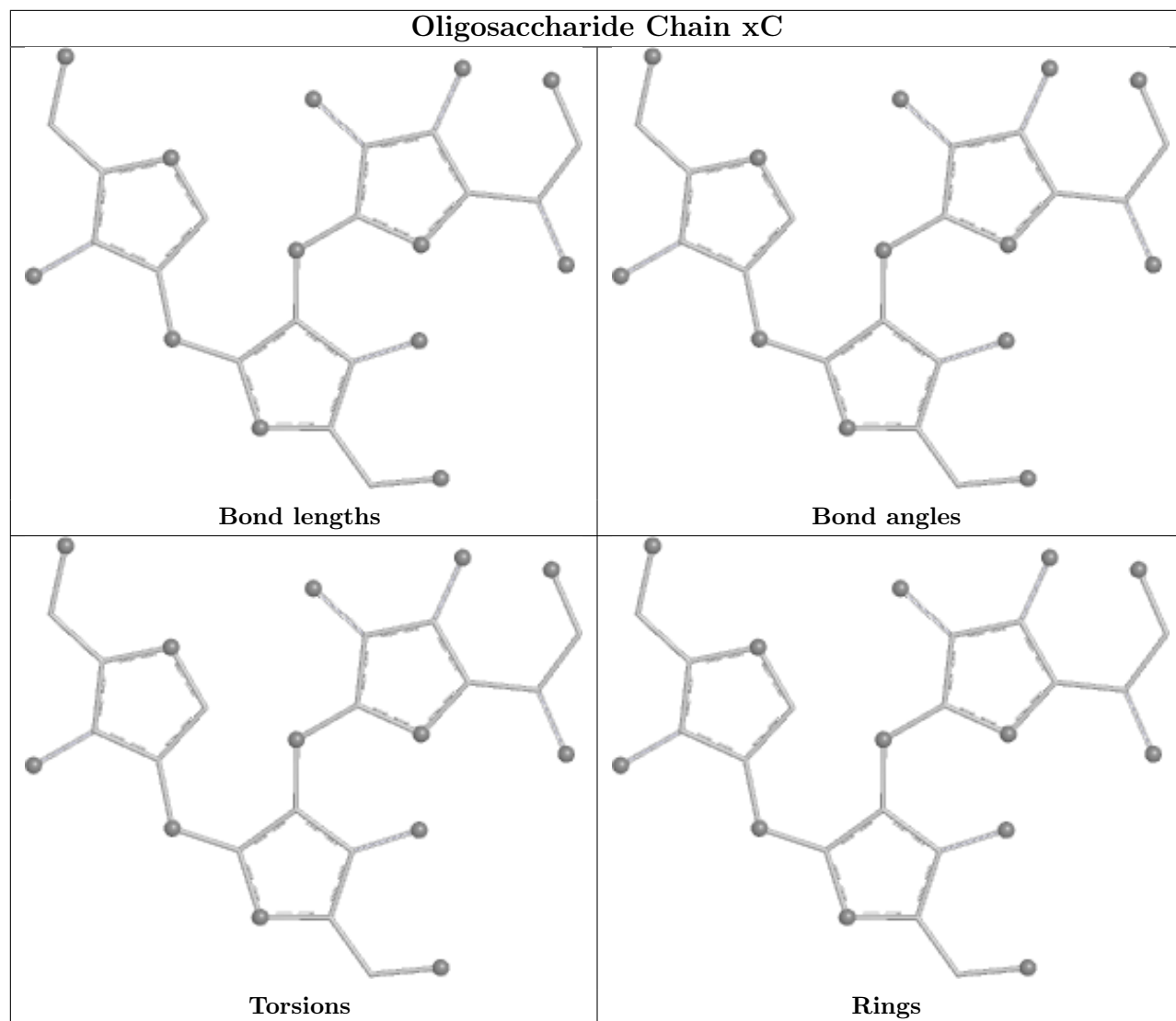


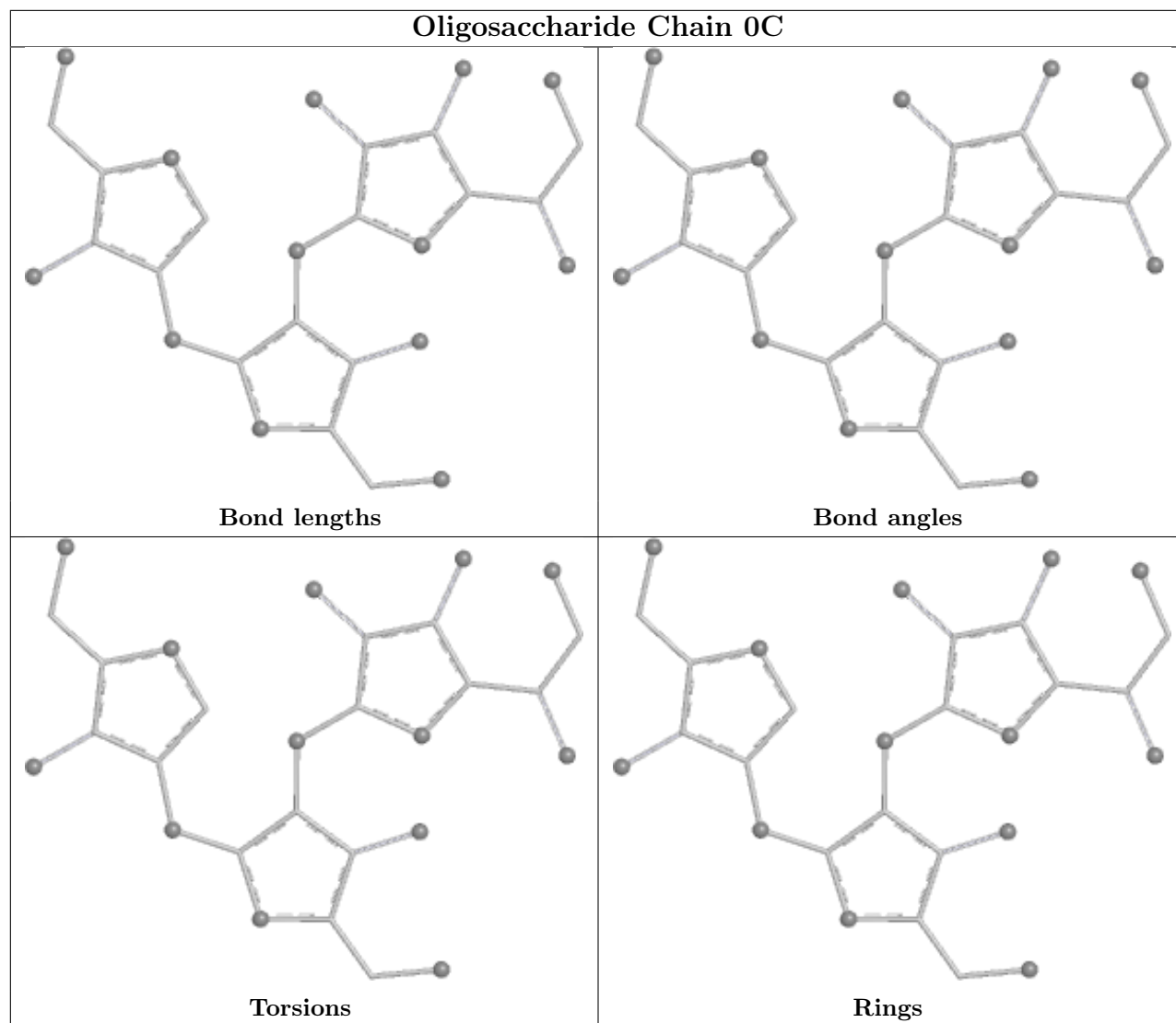
Rings

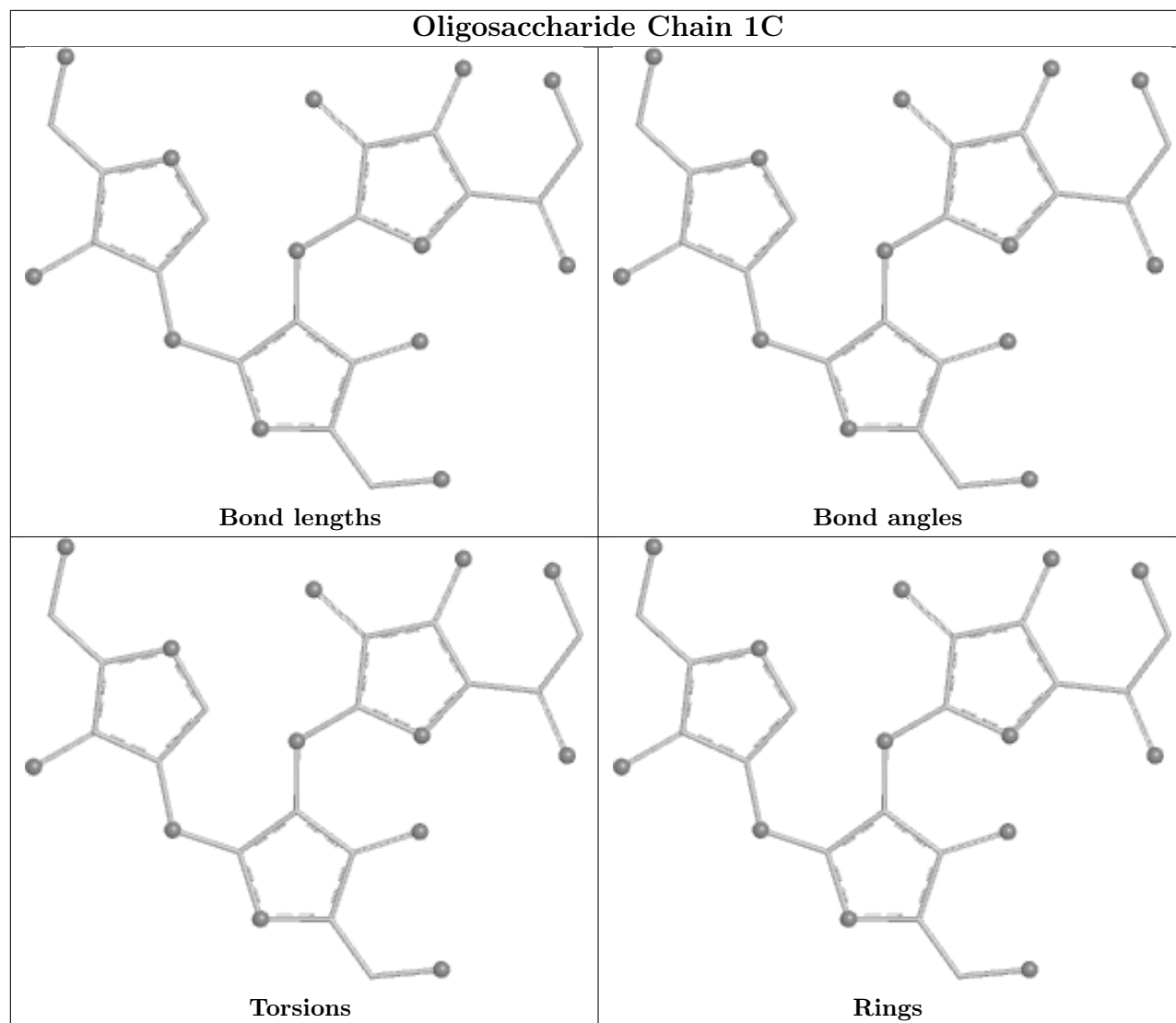


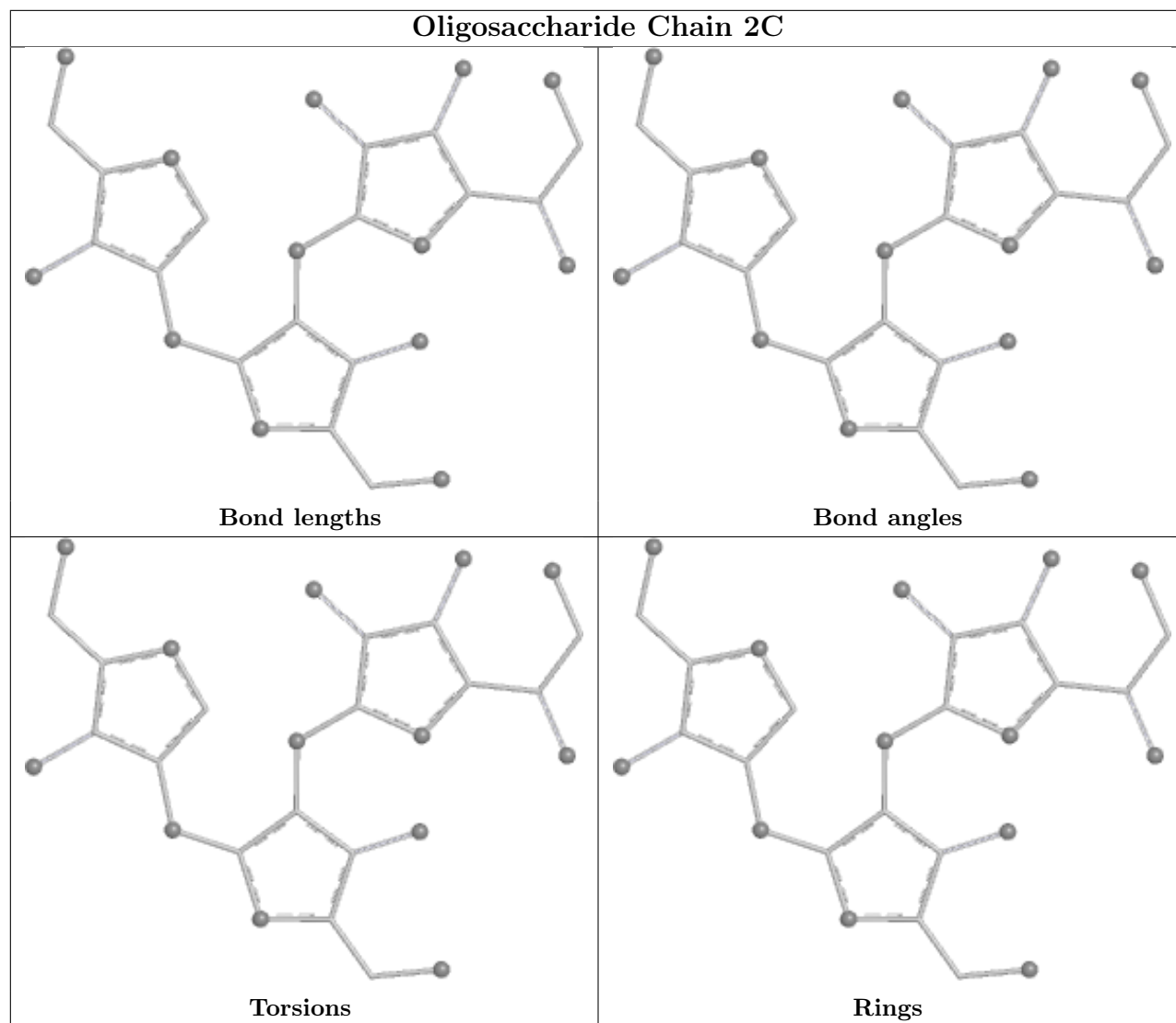


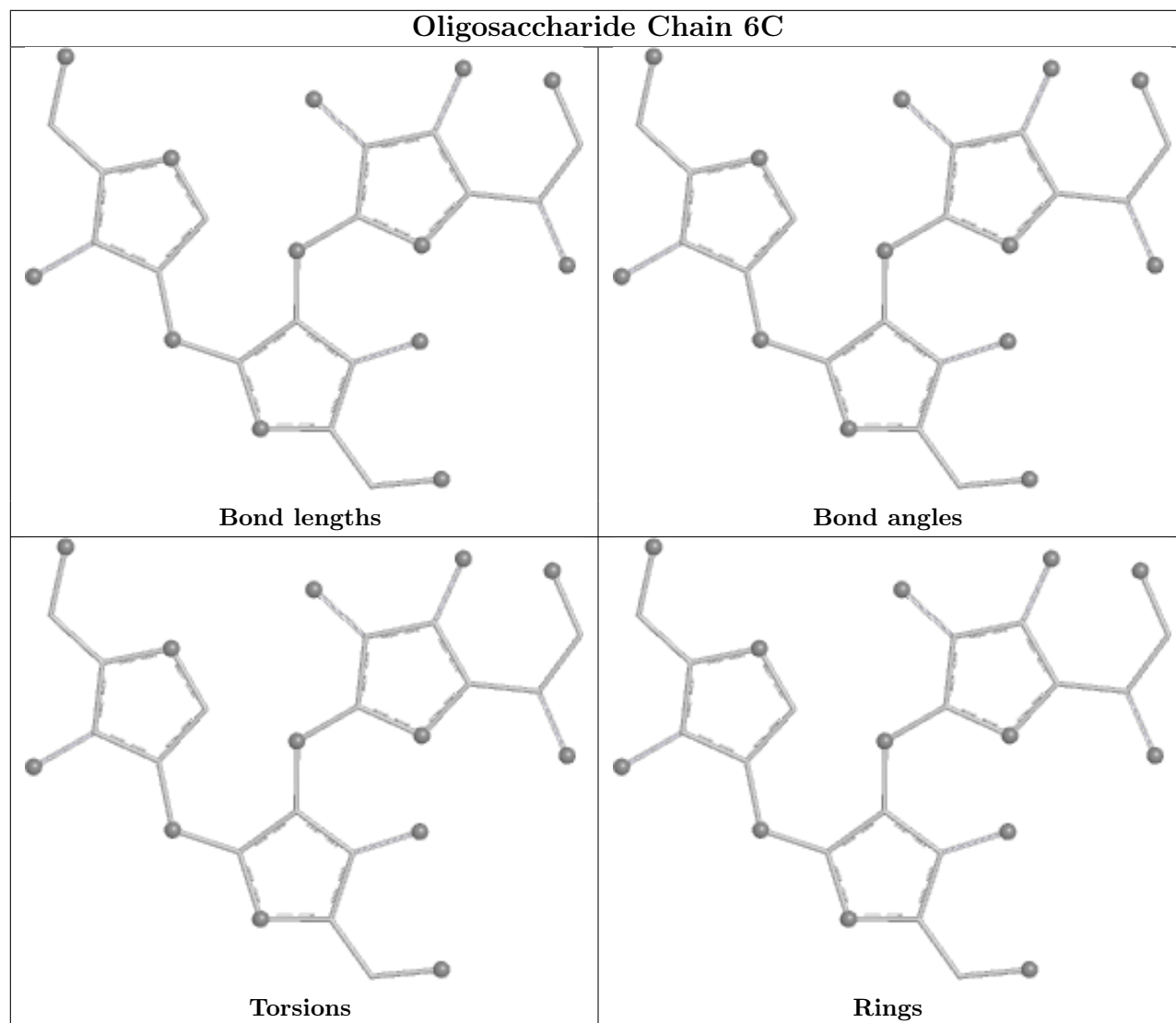


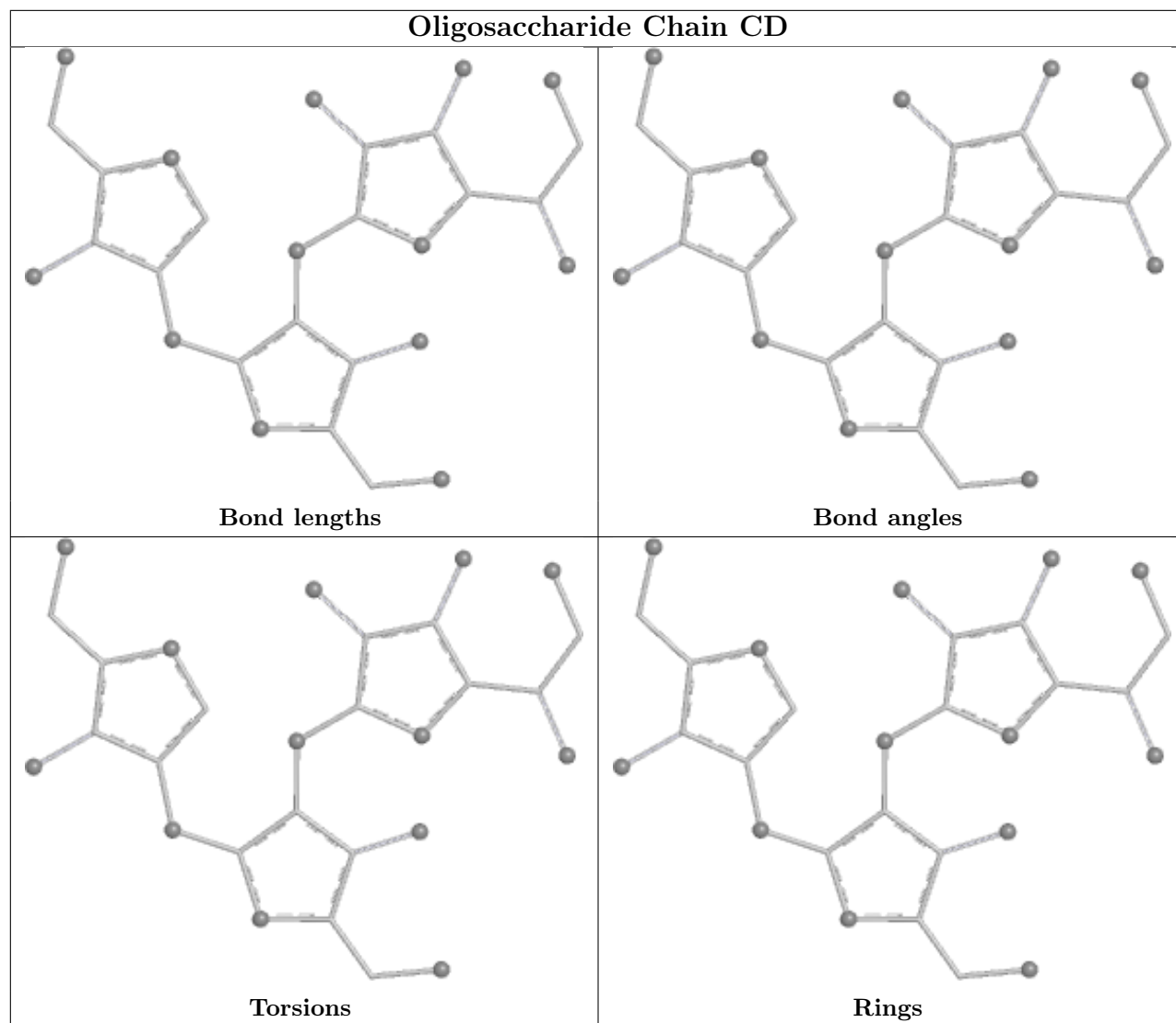


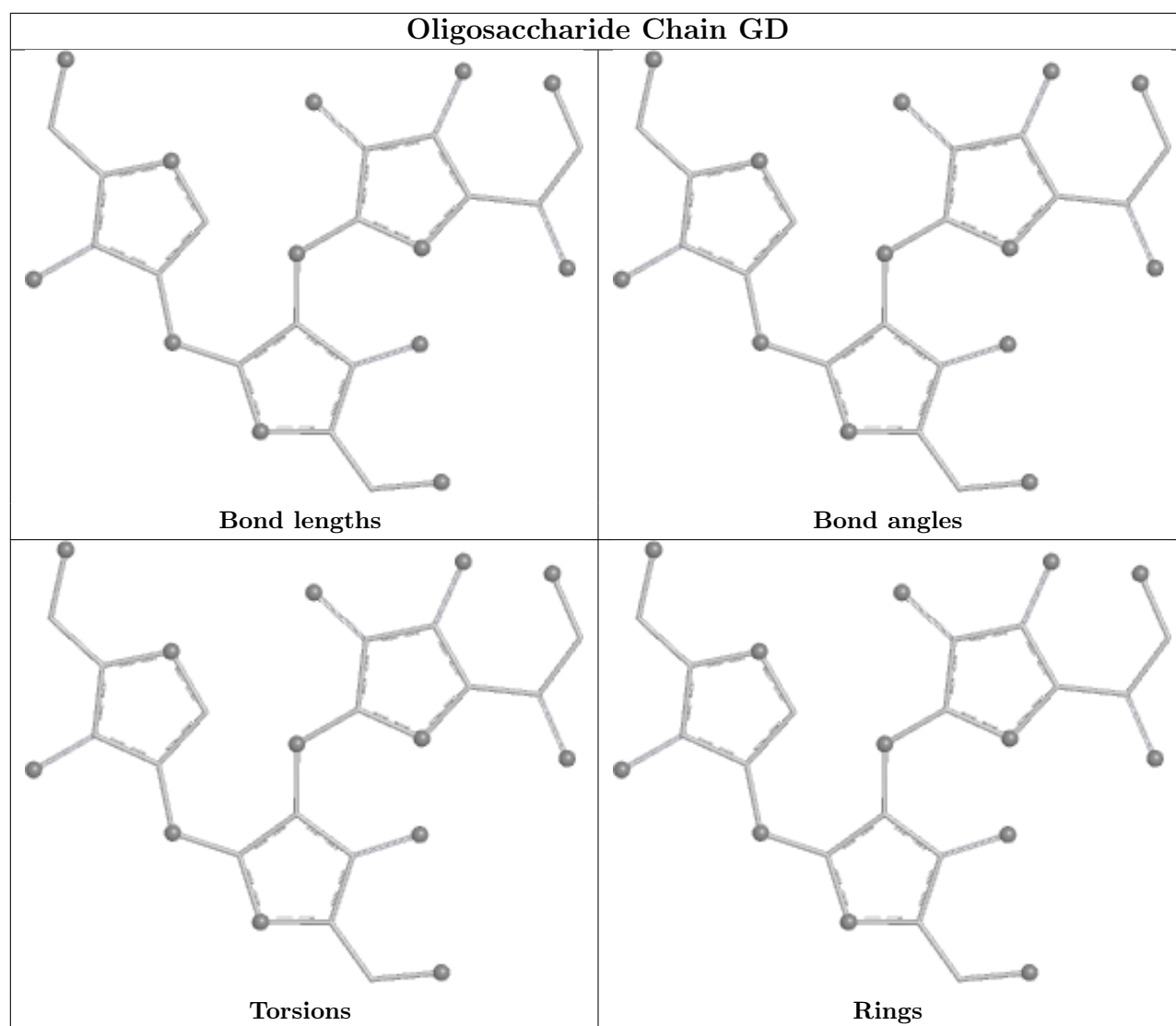


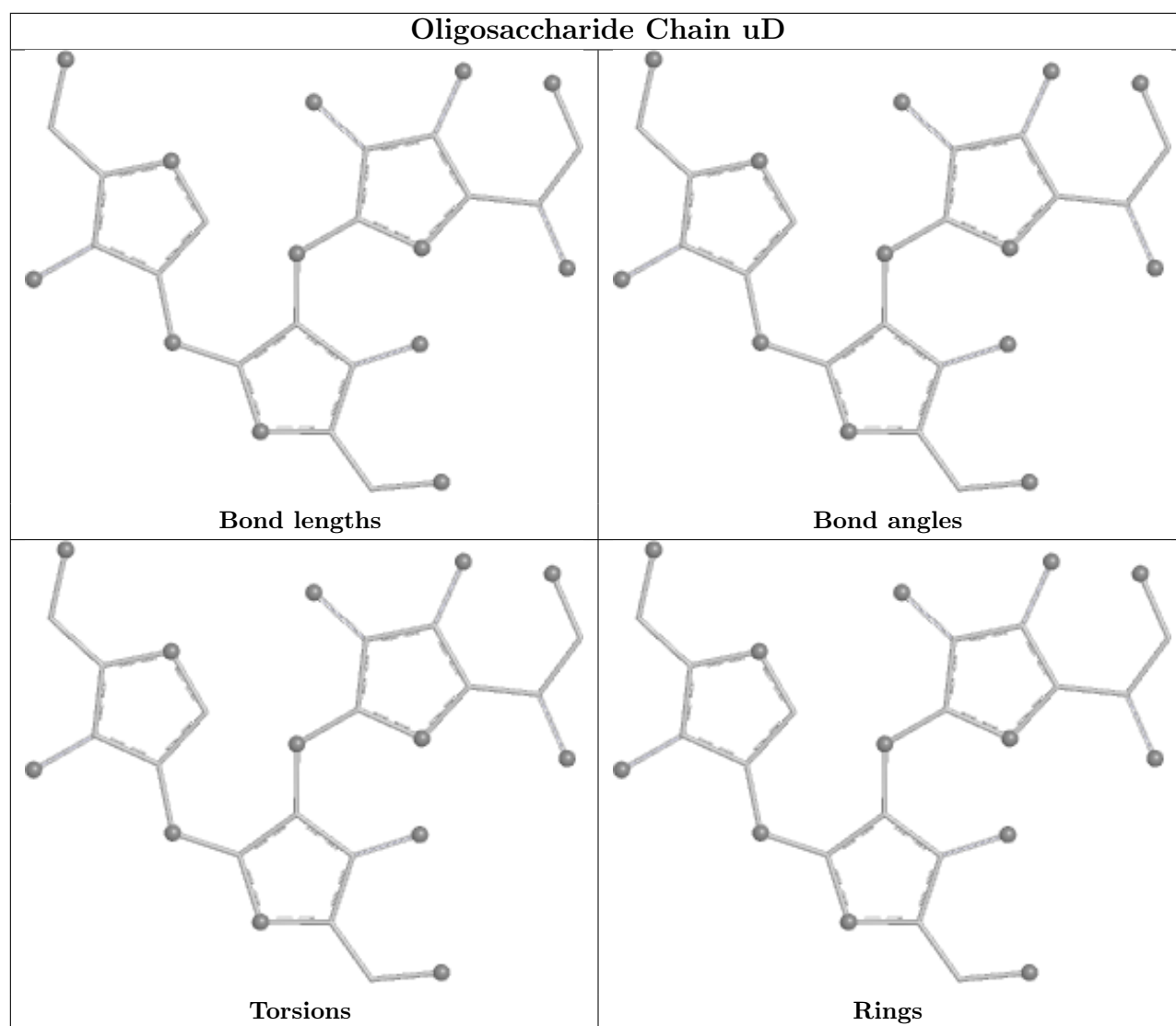


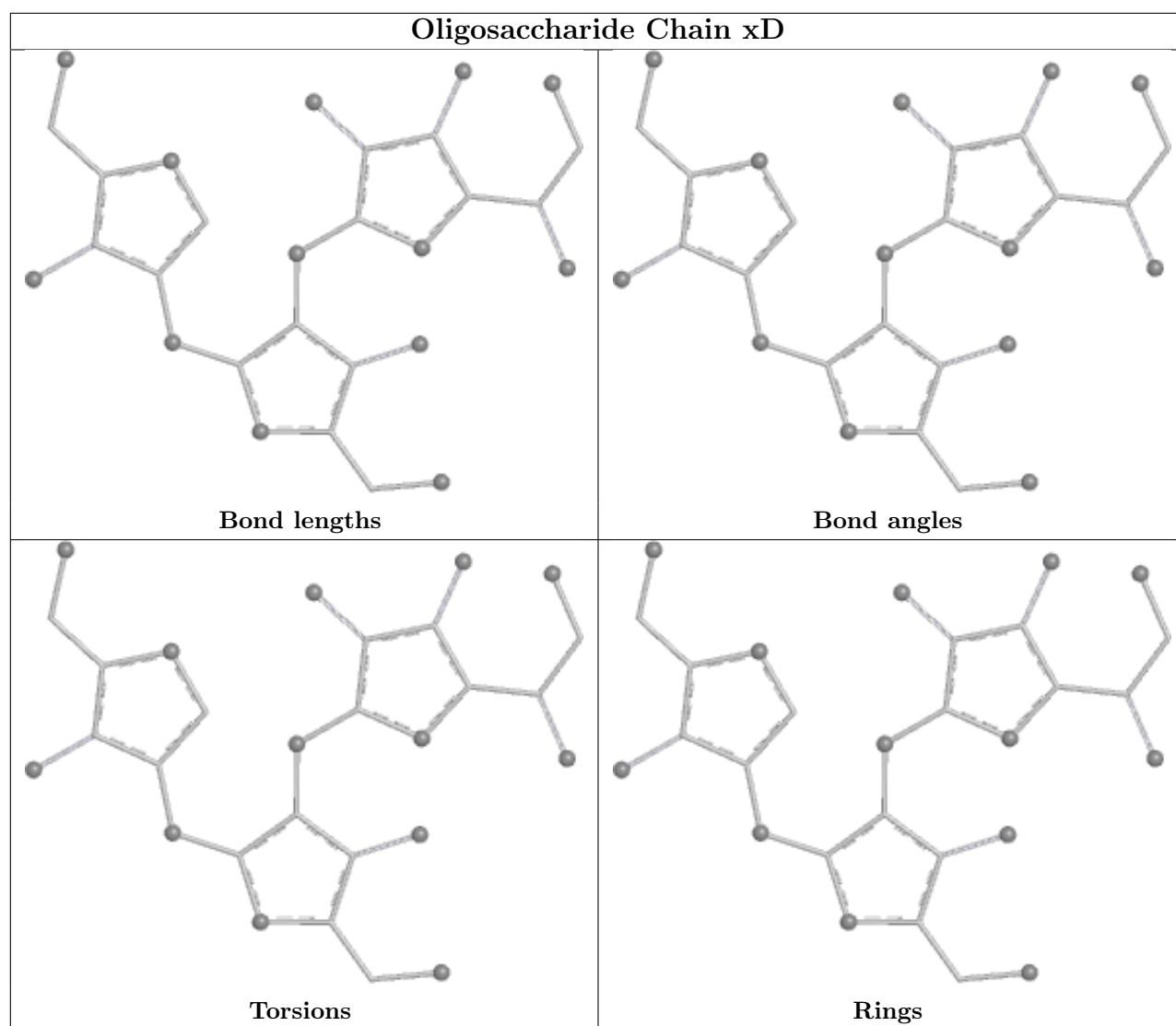


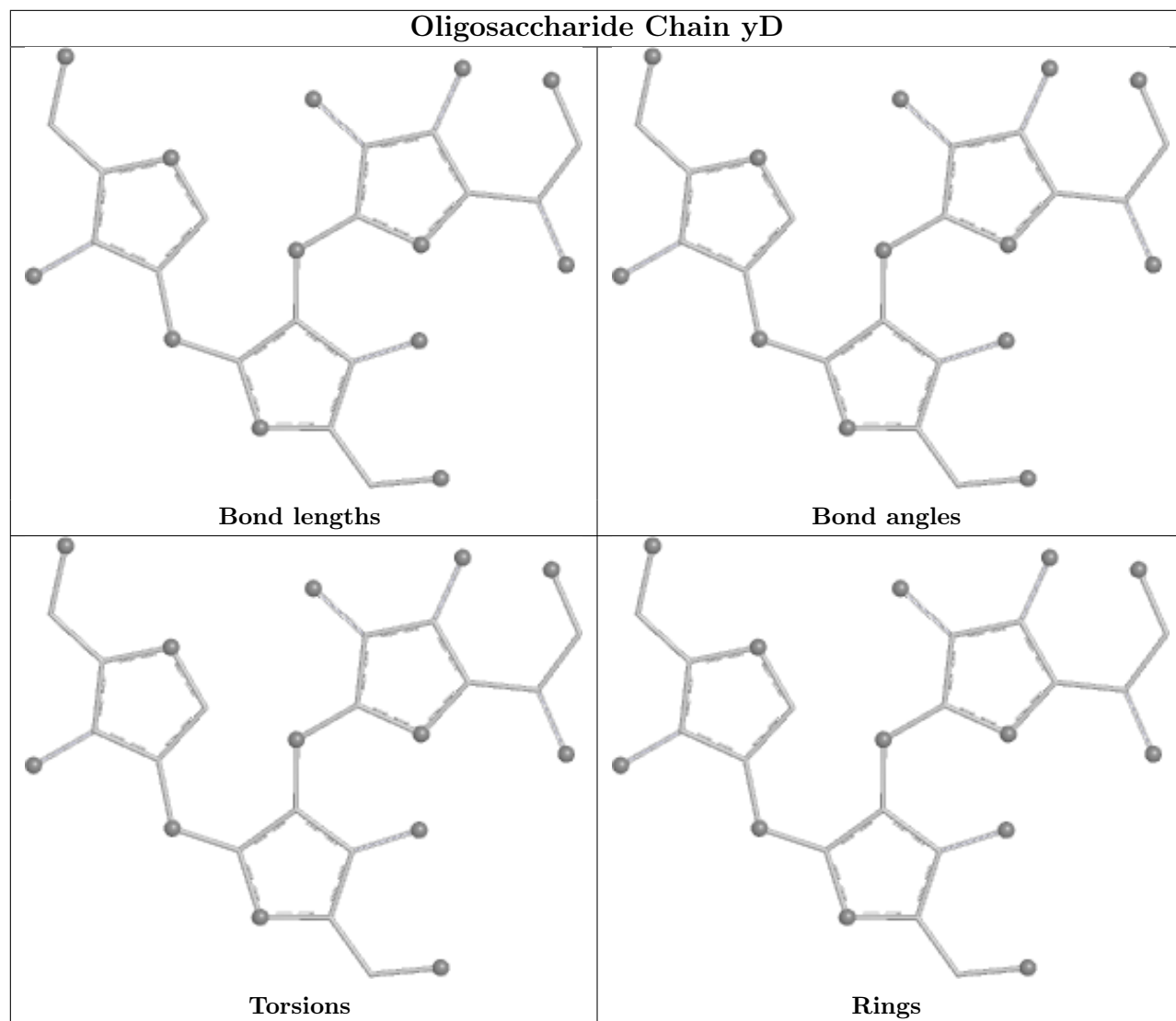


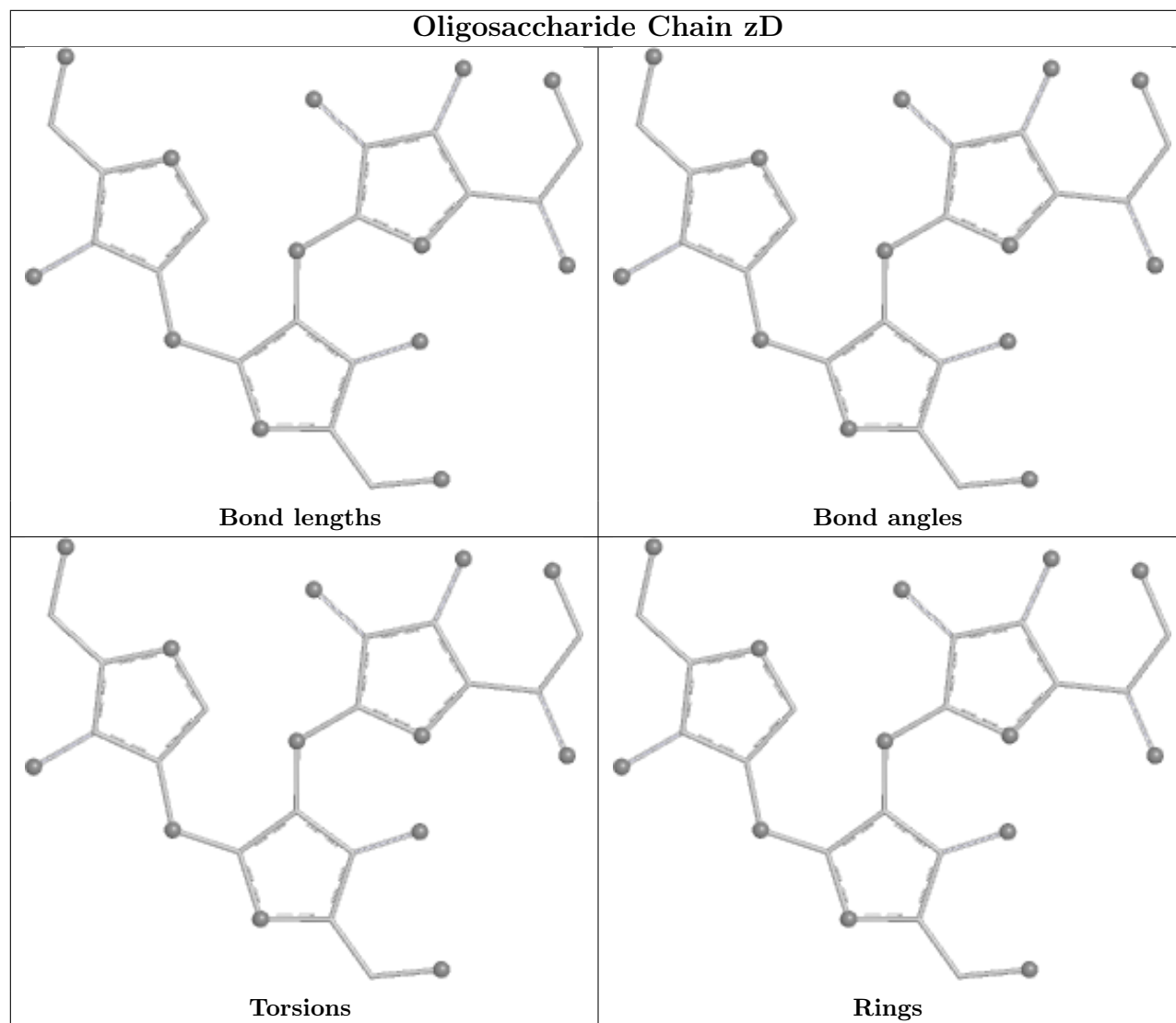


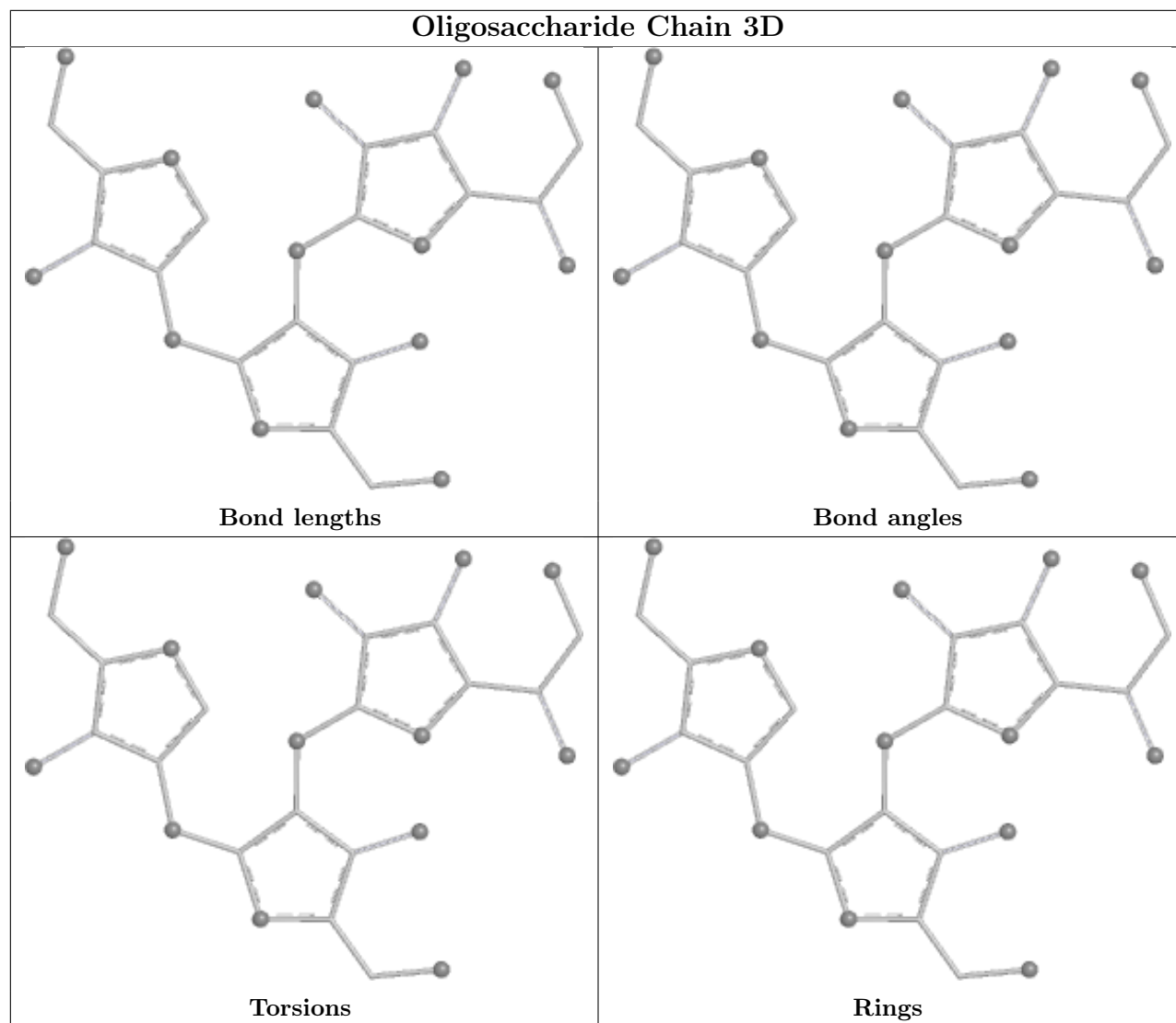


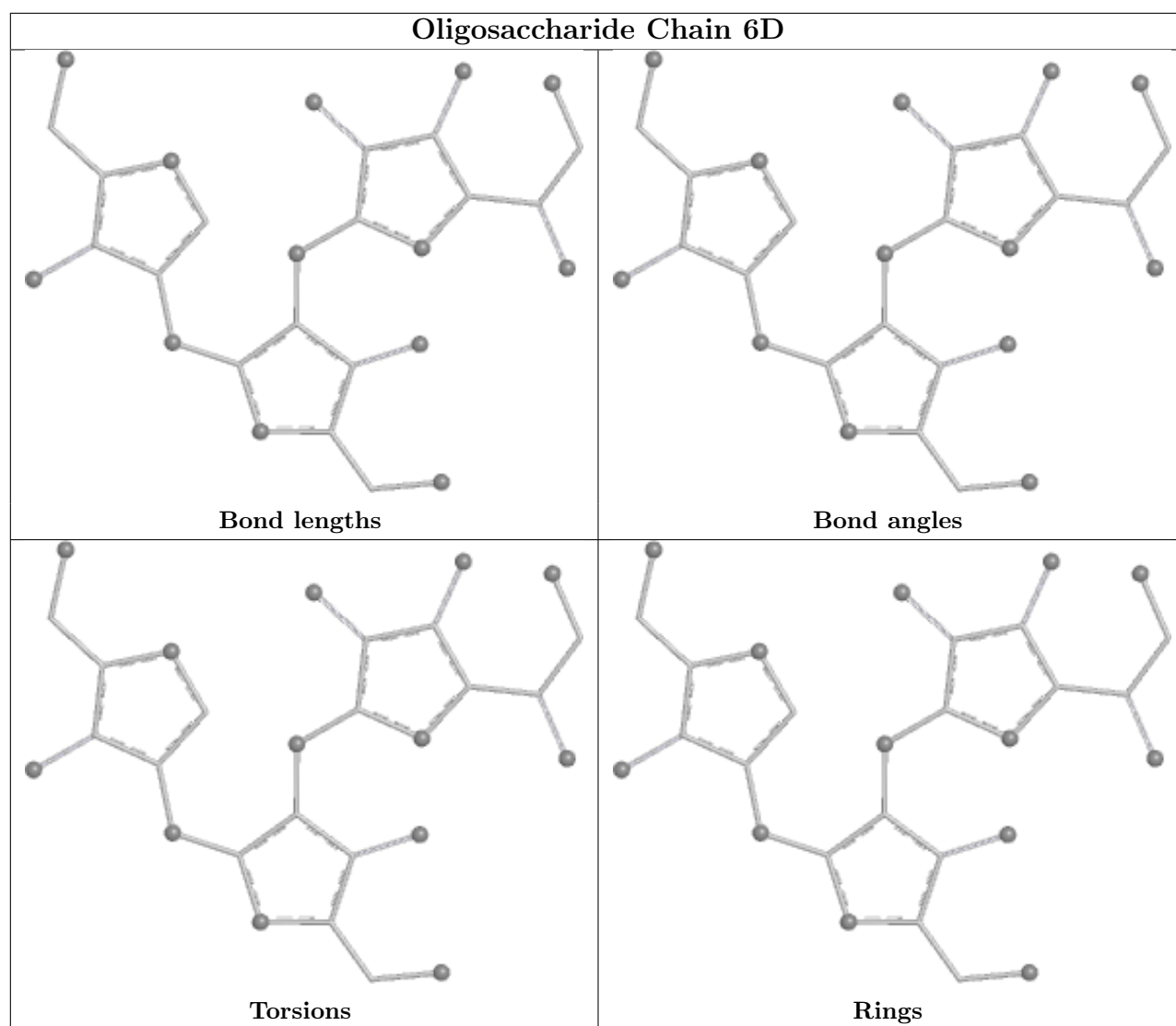




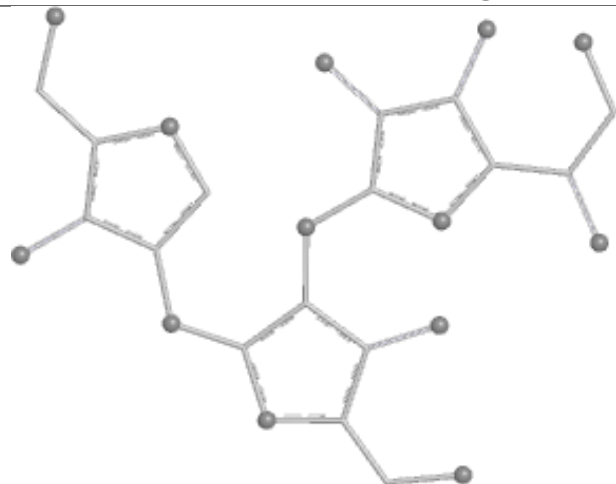




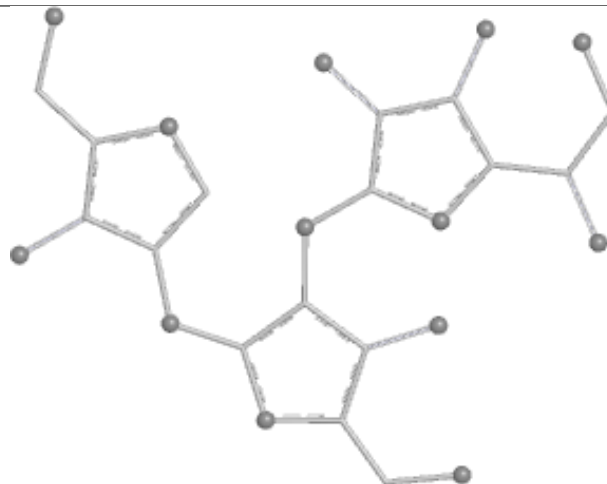




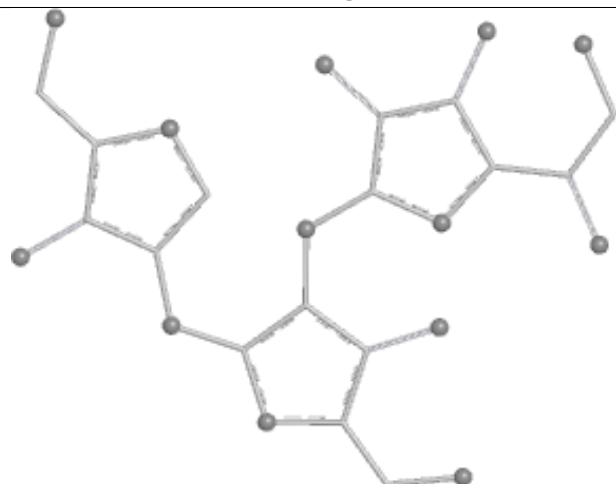
Oligosaccharide Chain 7D



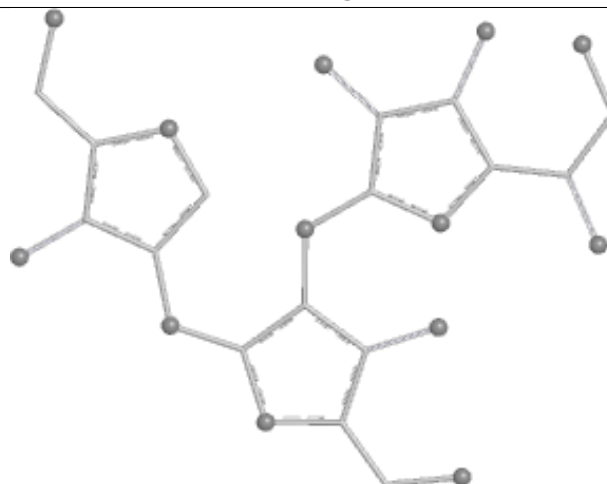
Bond lengths



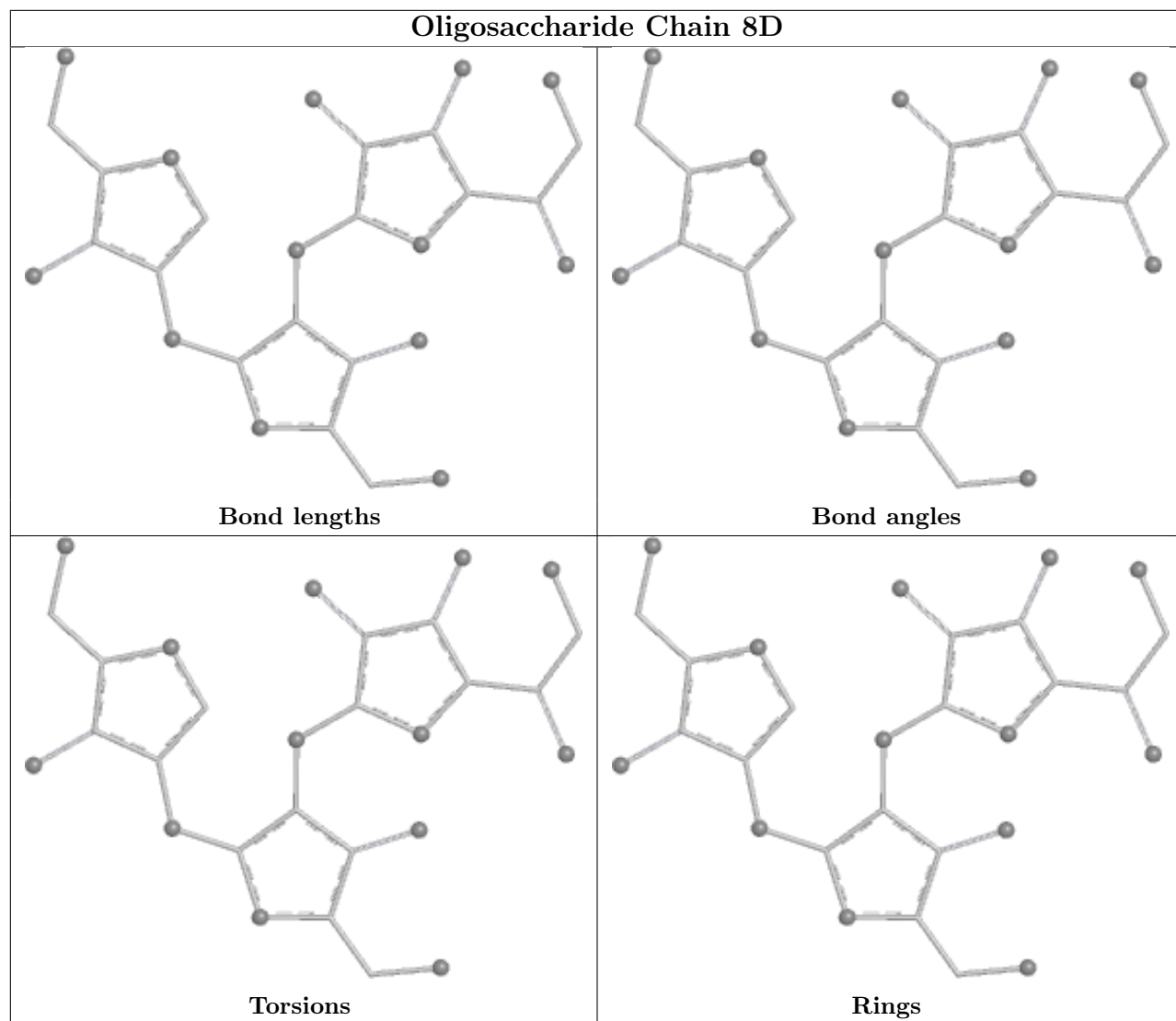
Bond angles

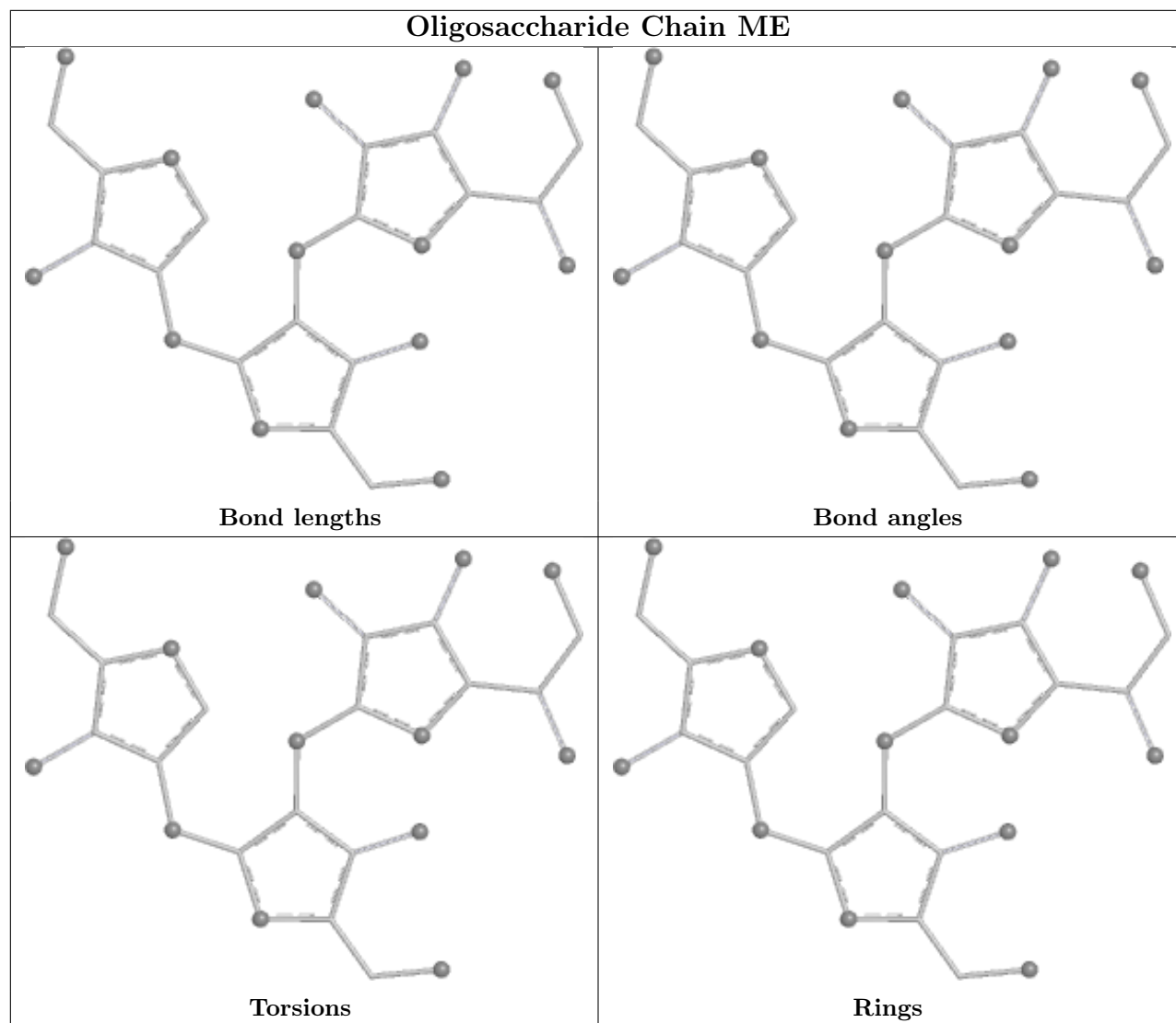


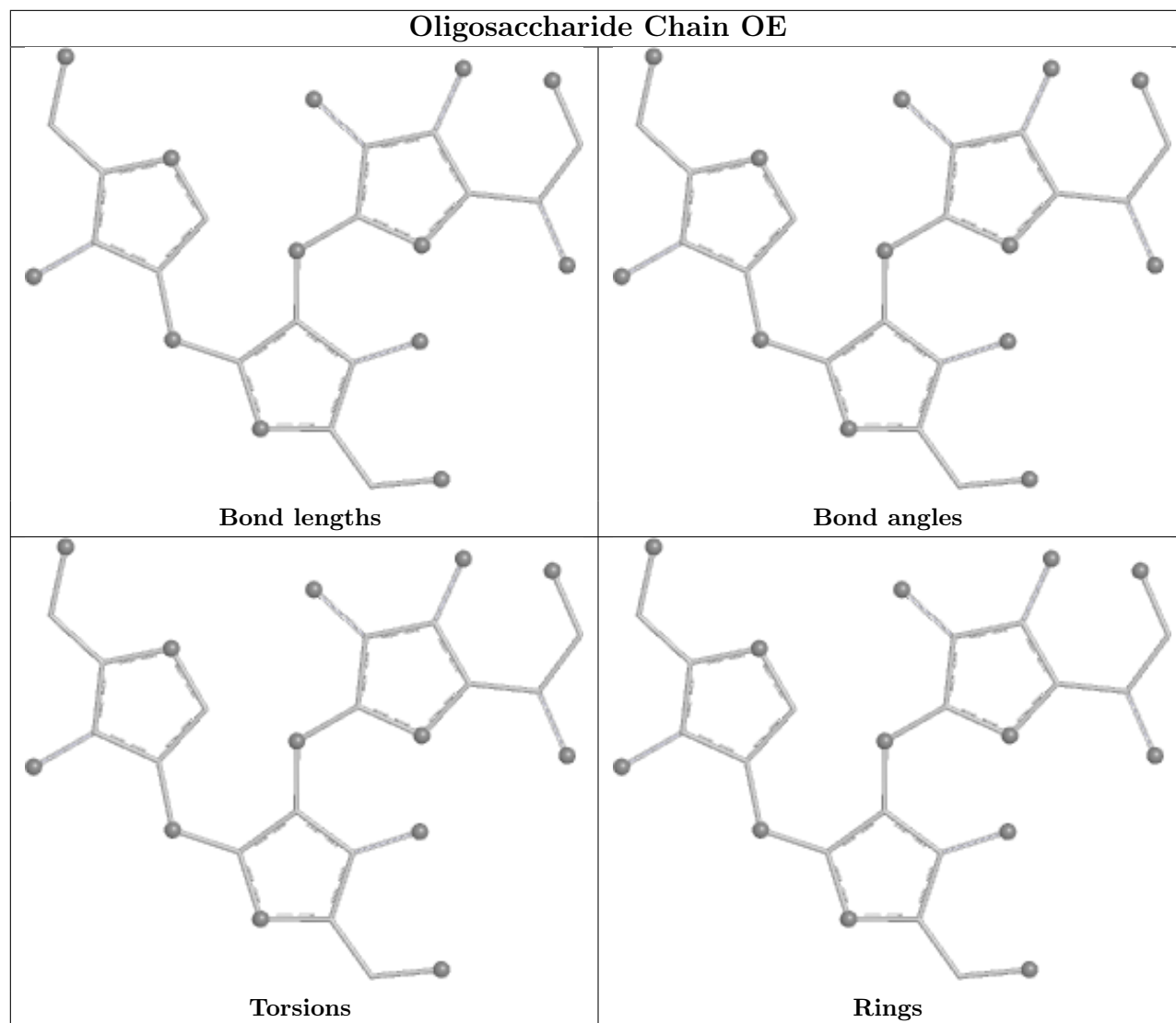
Torsions

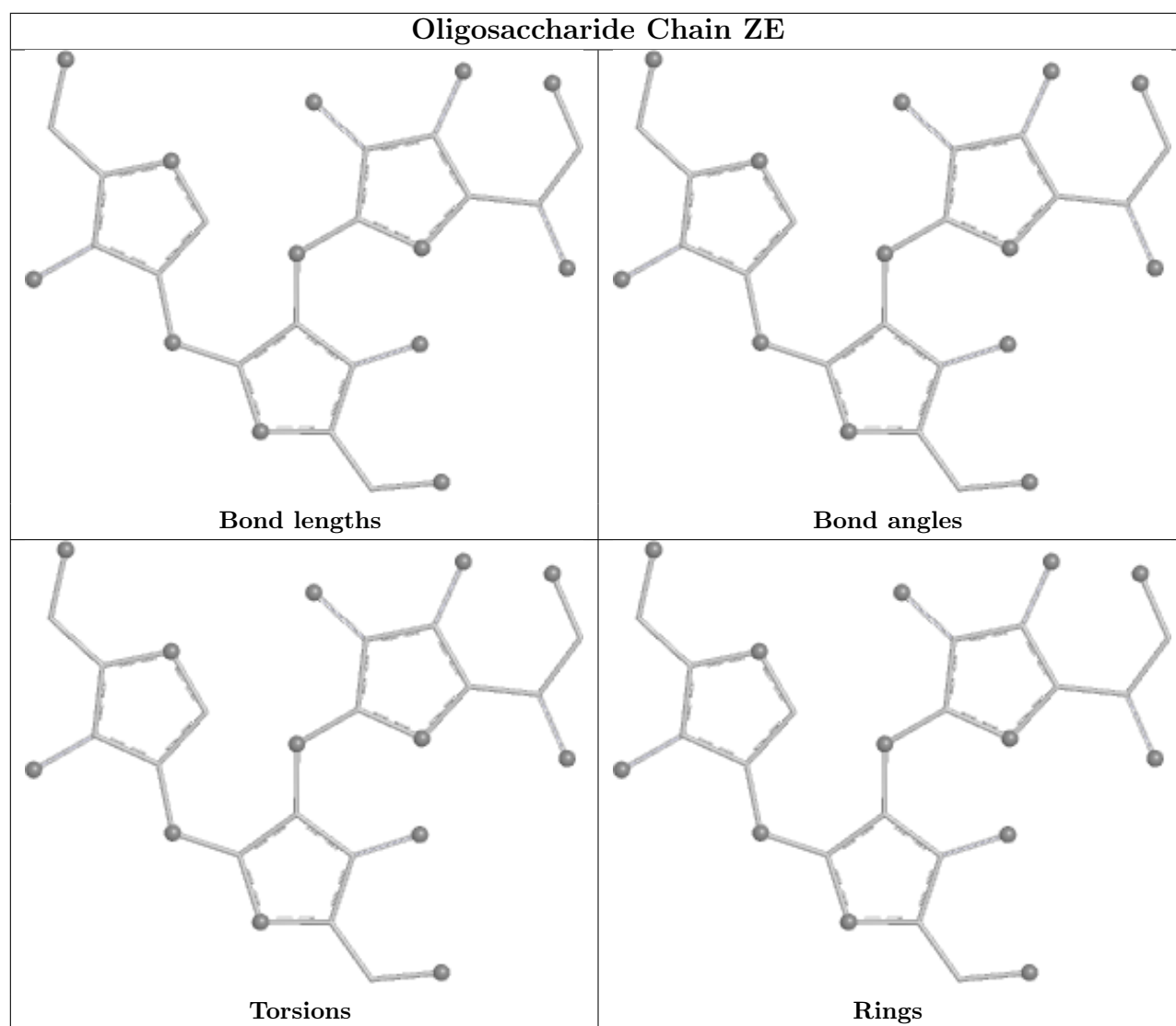


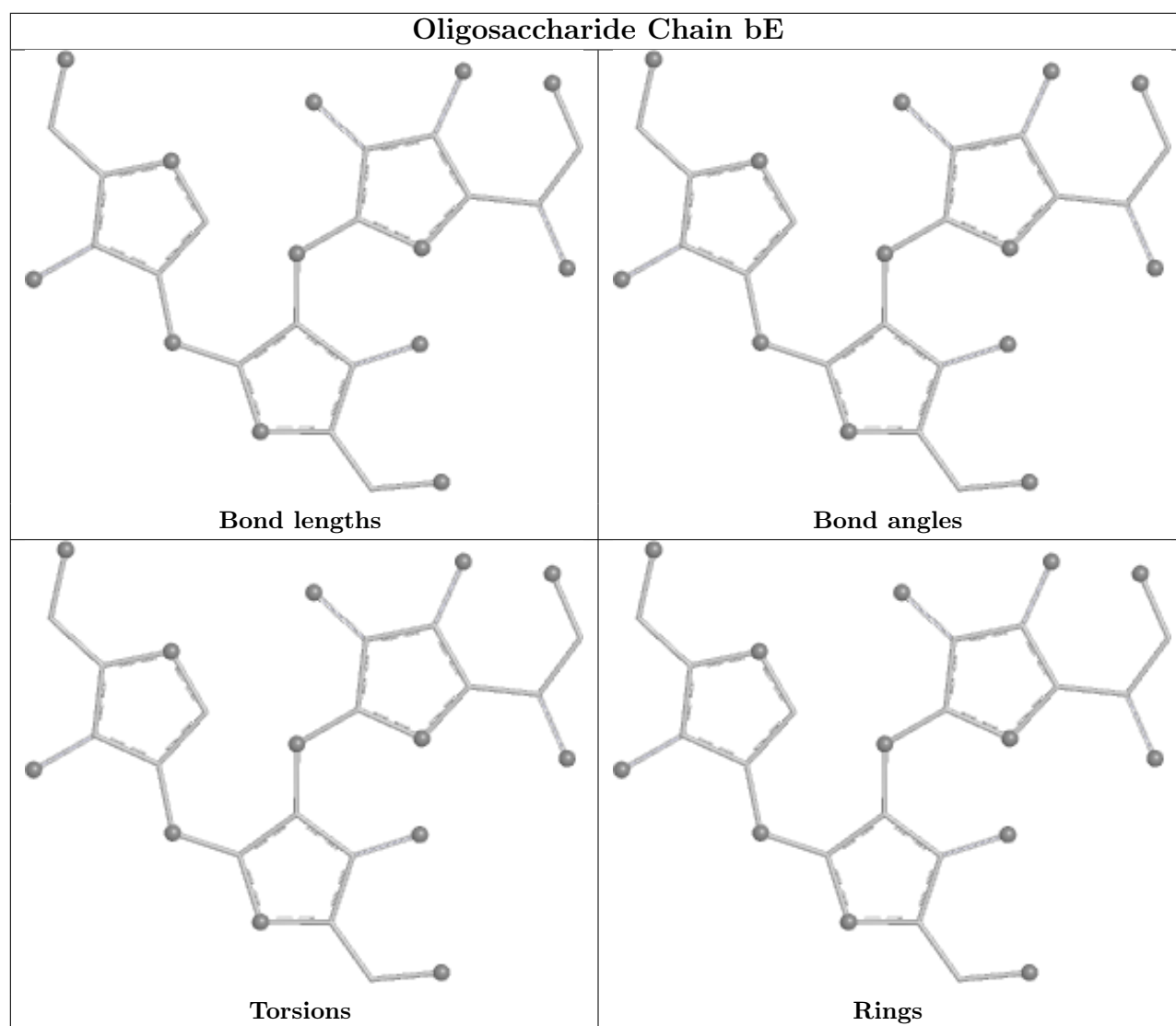
Rings

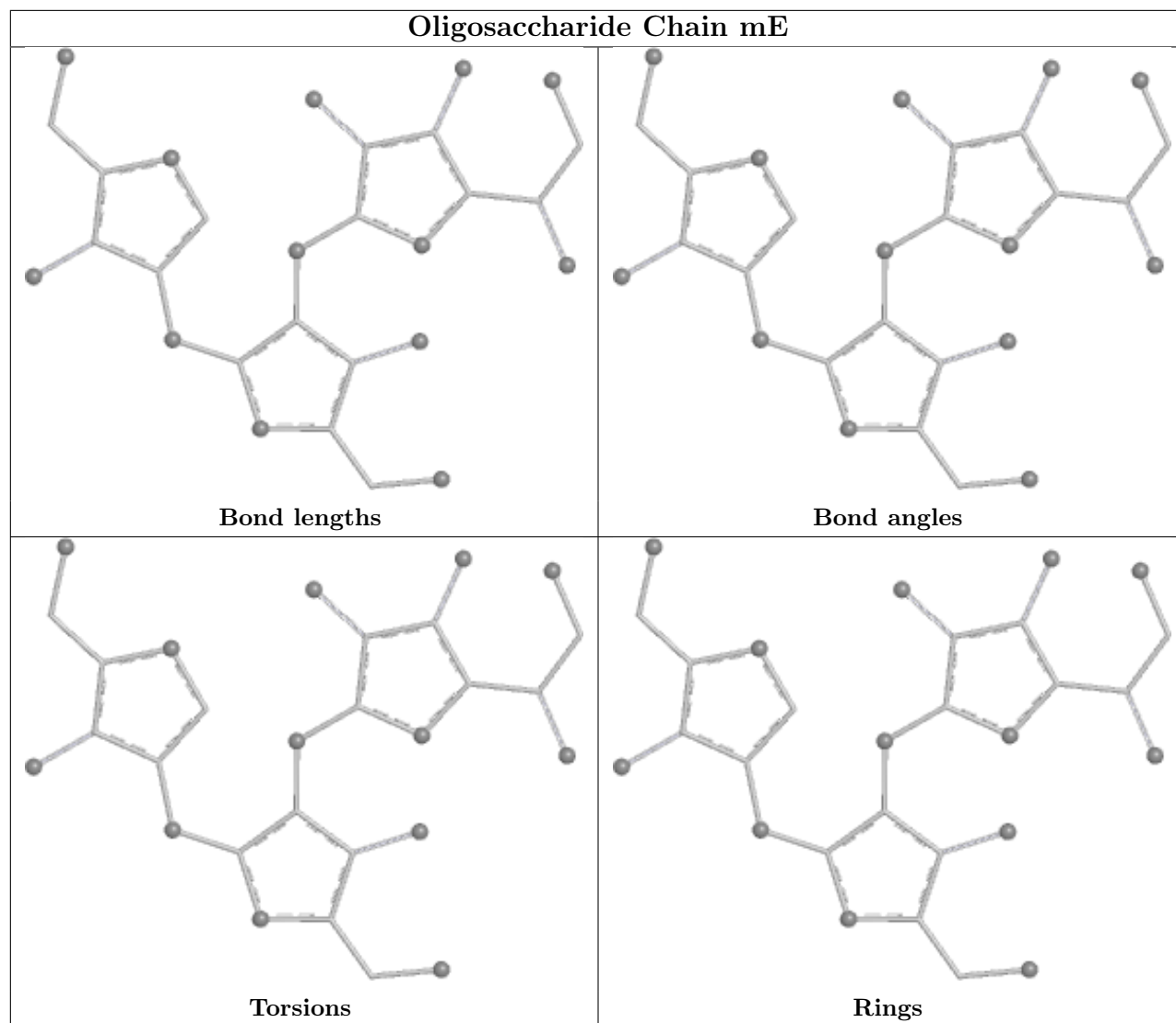


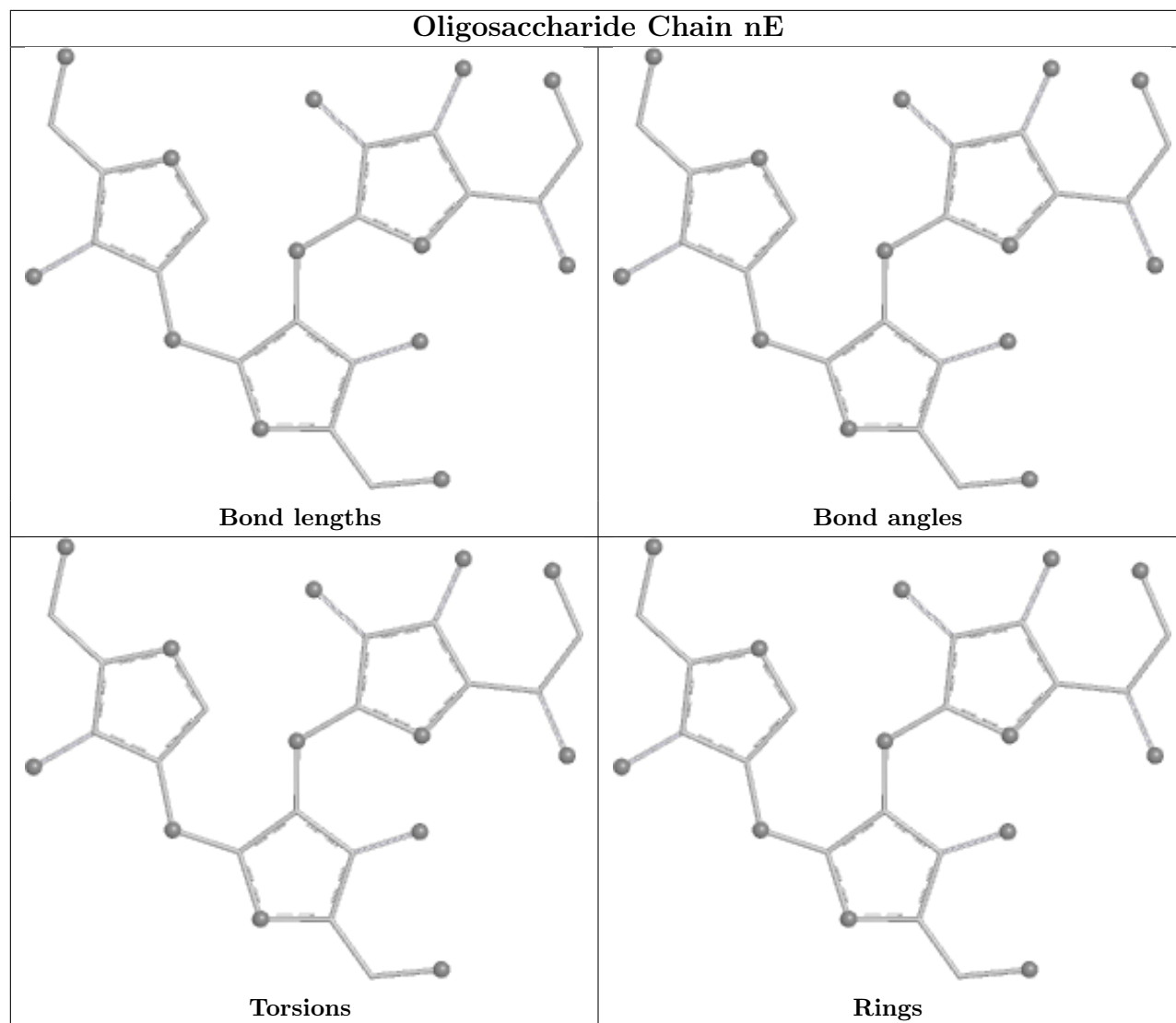


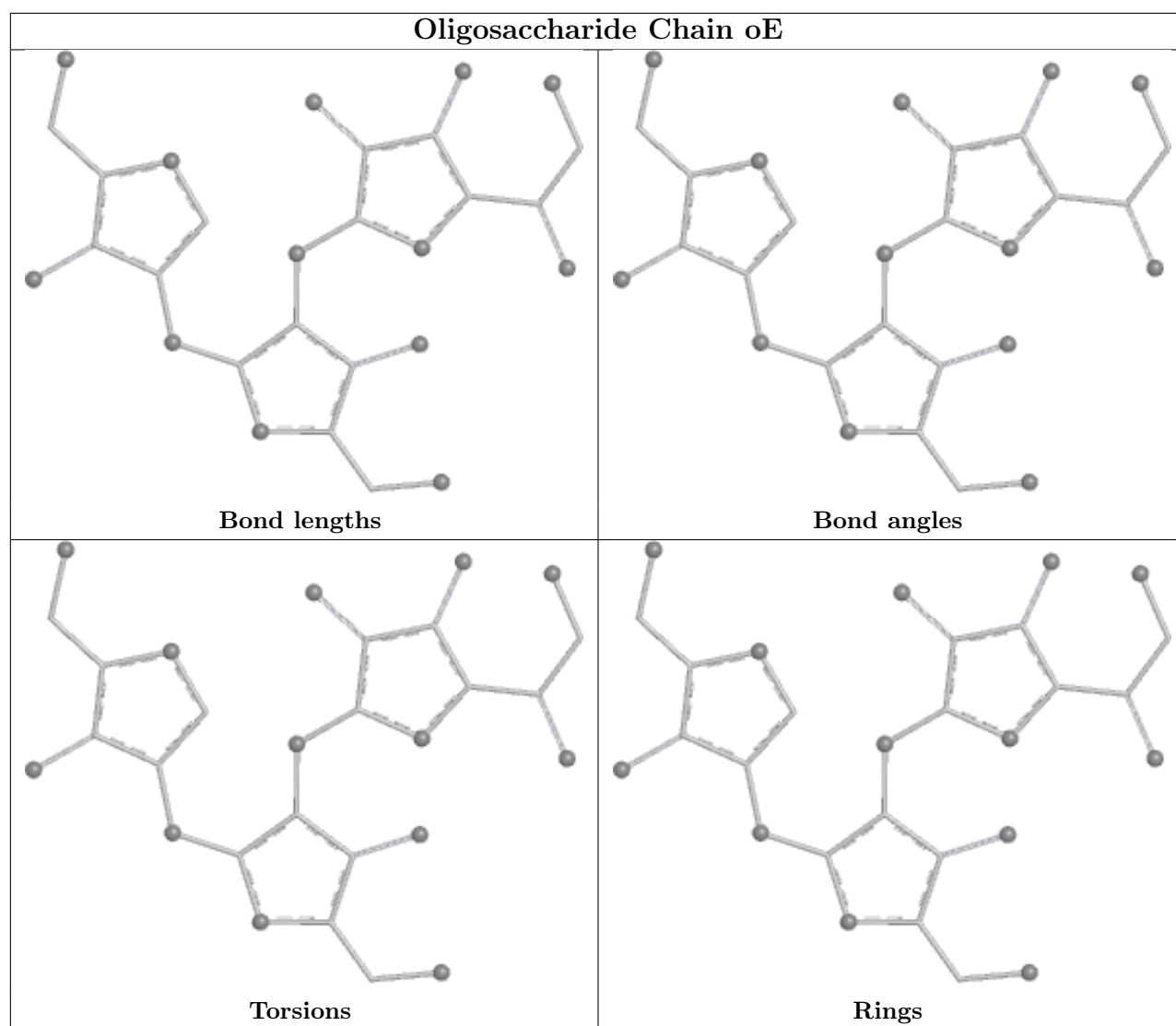


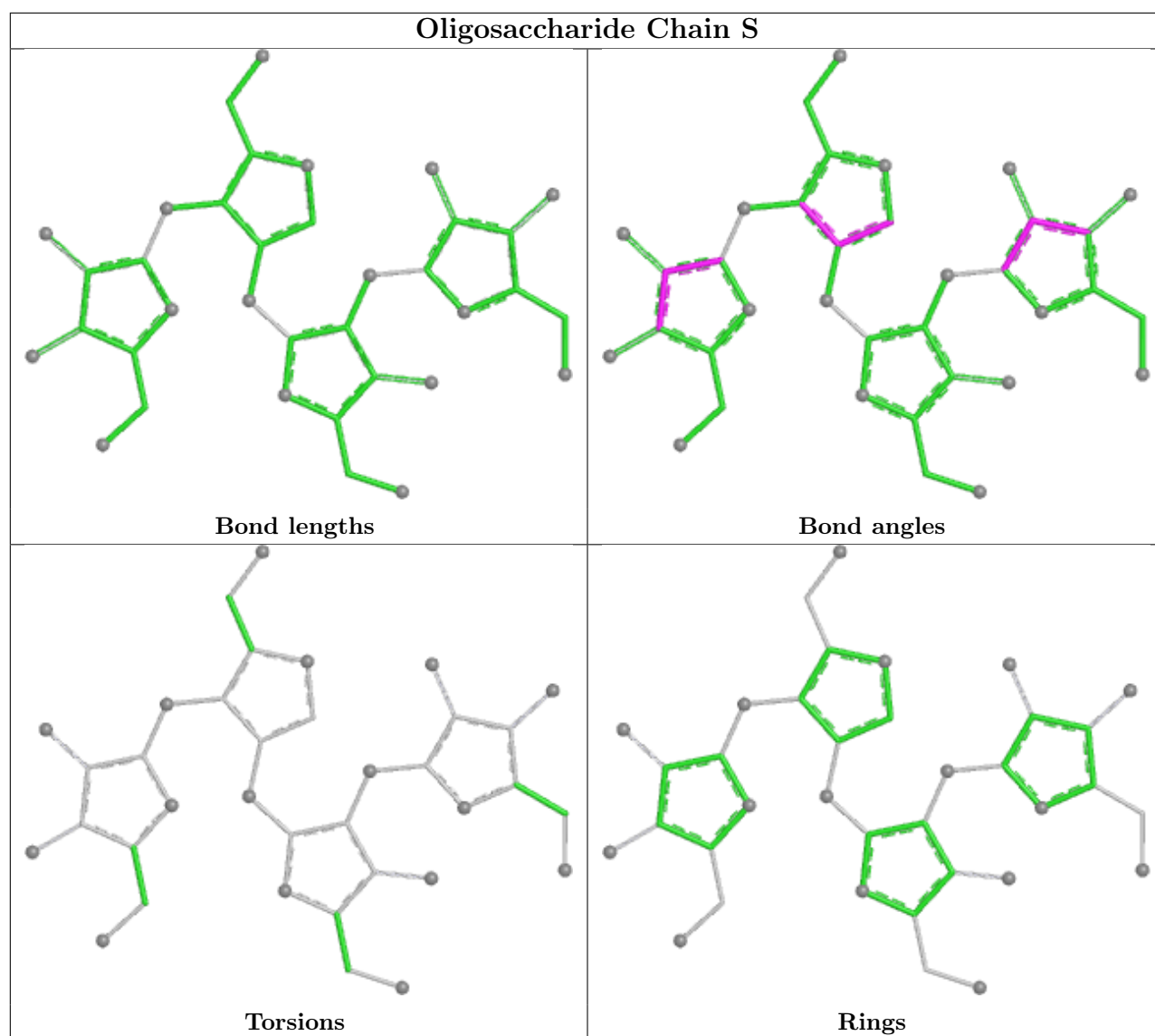


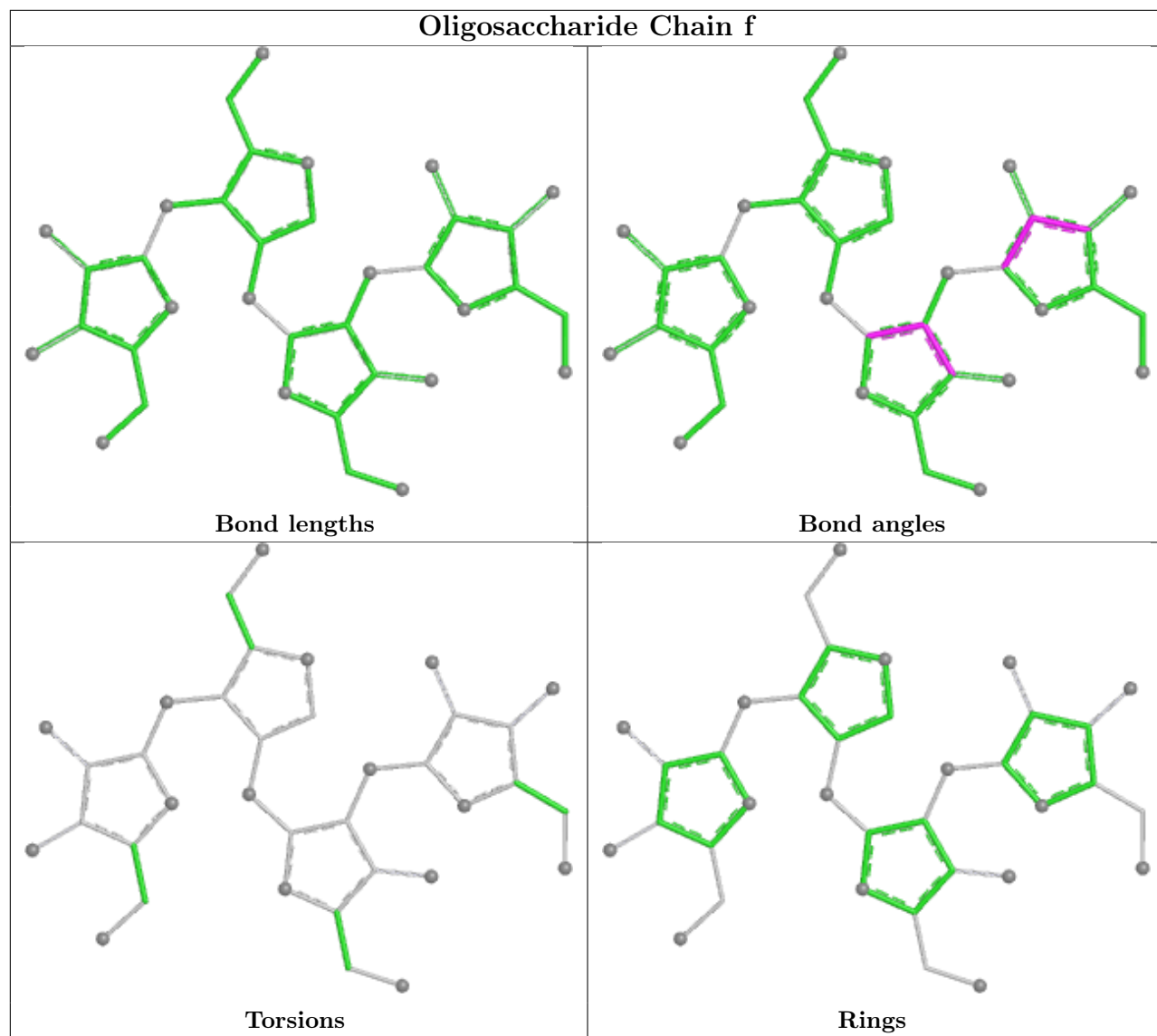


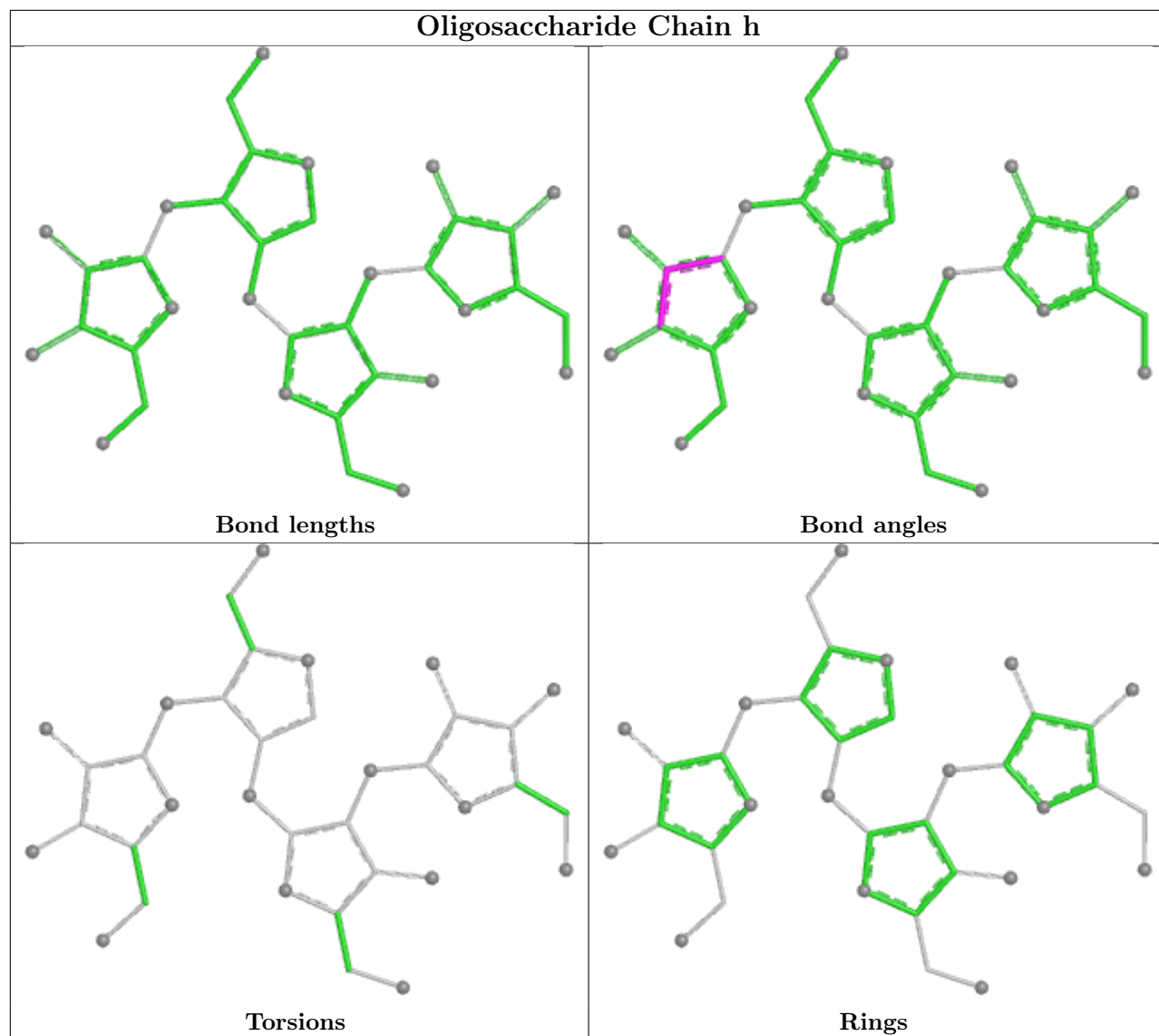


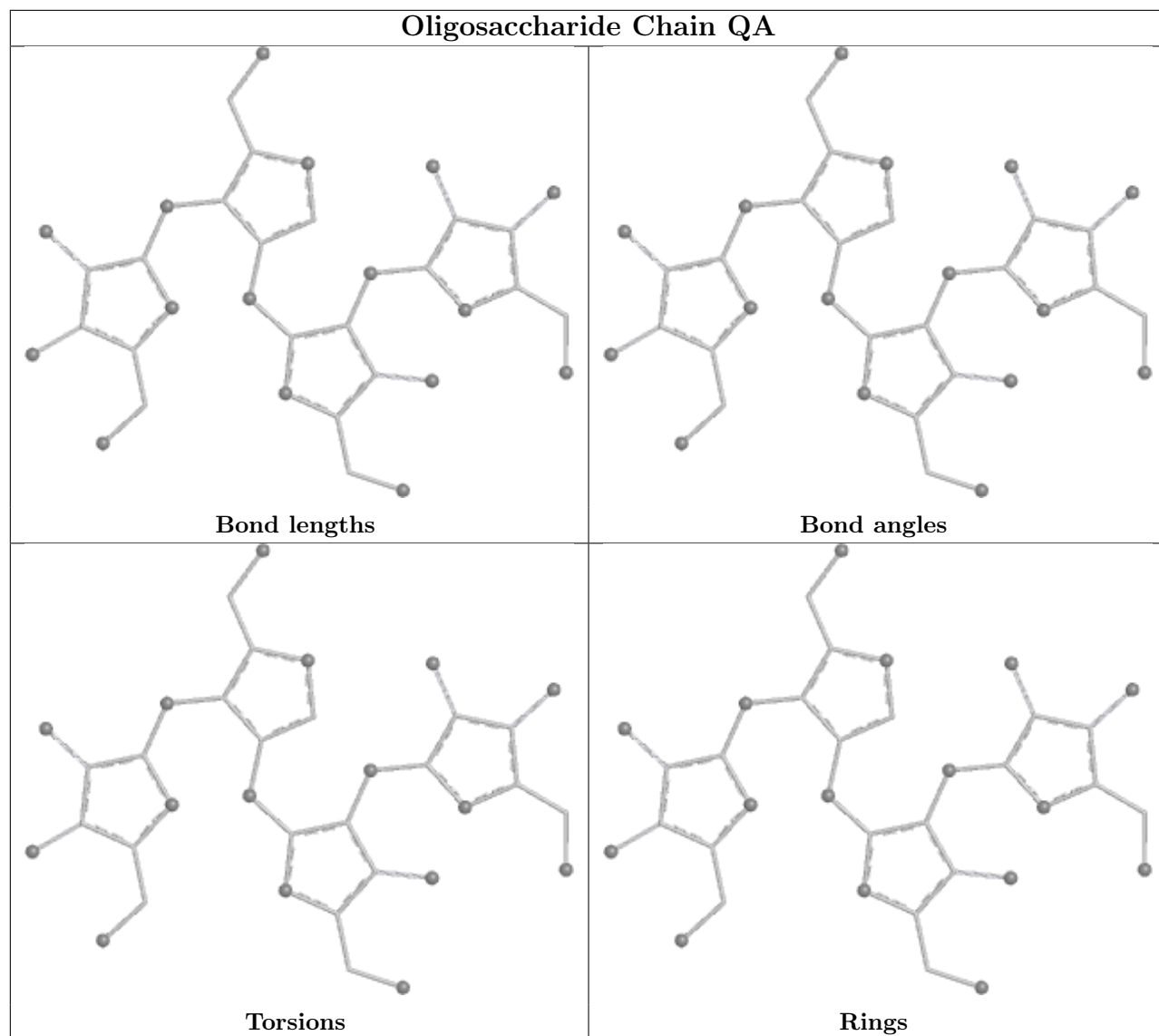


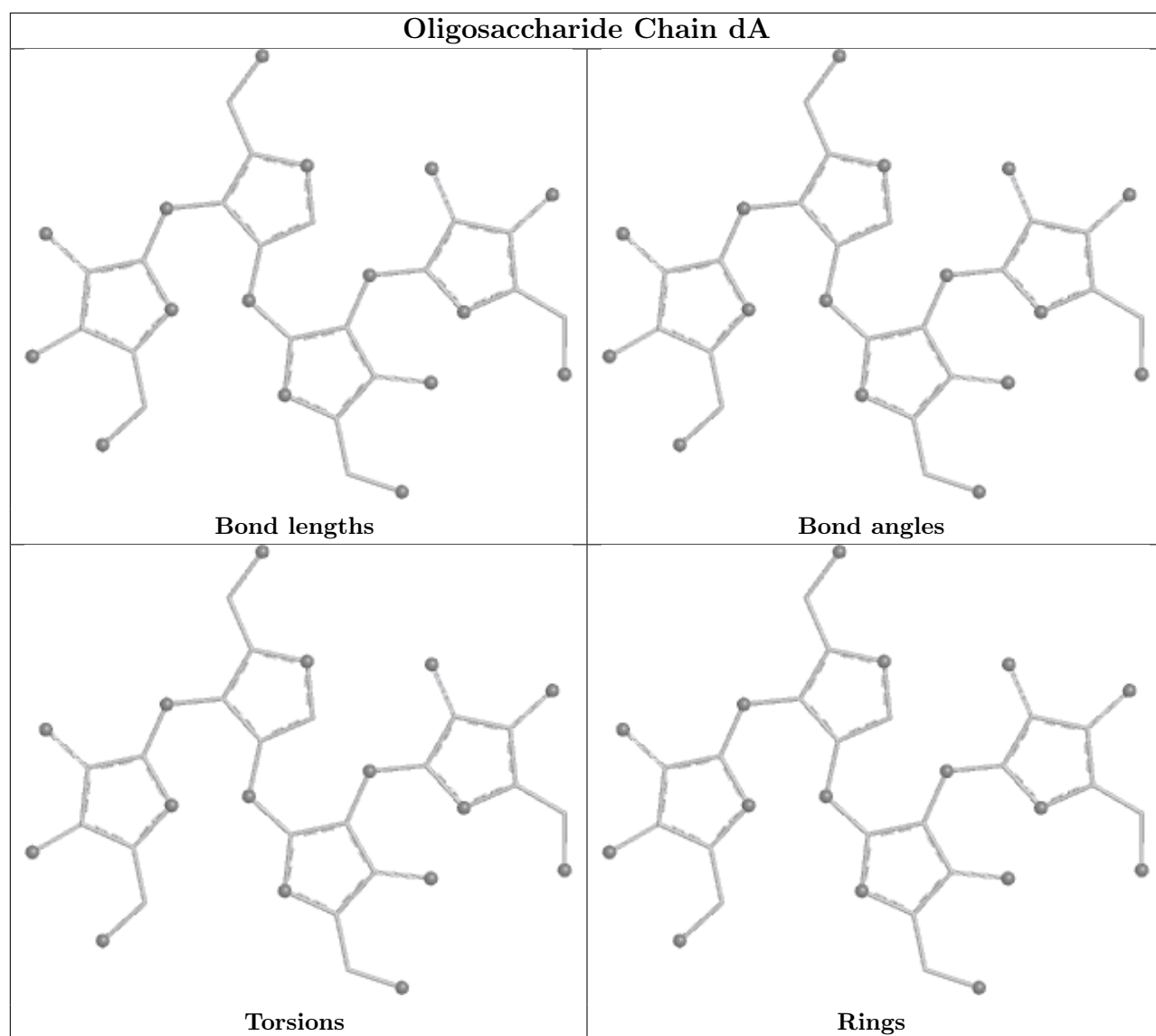


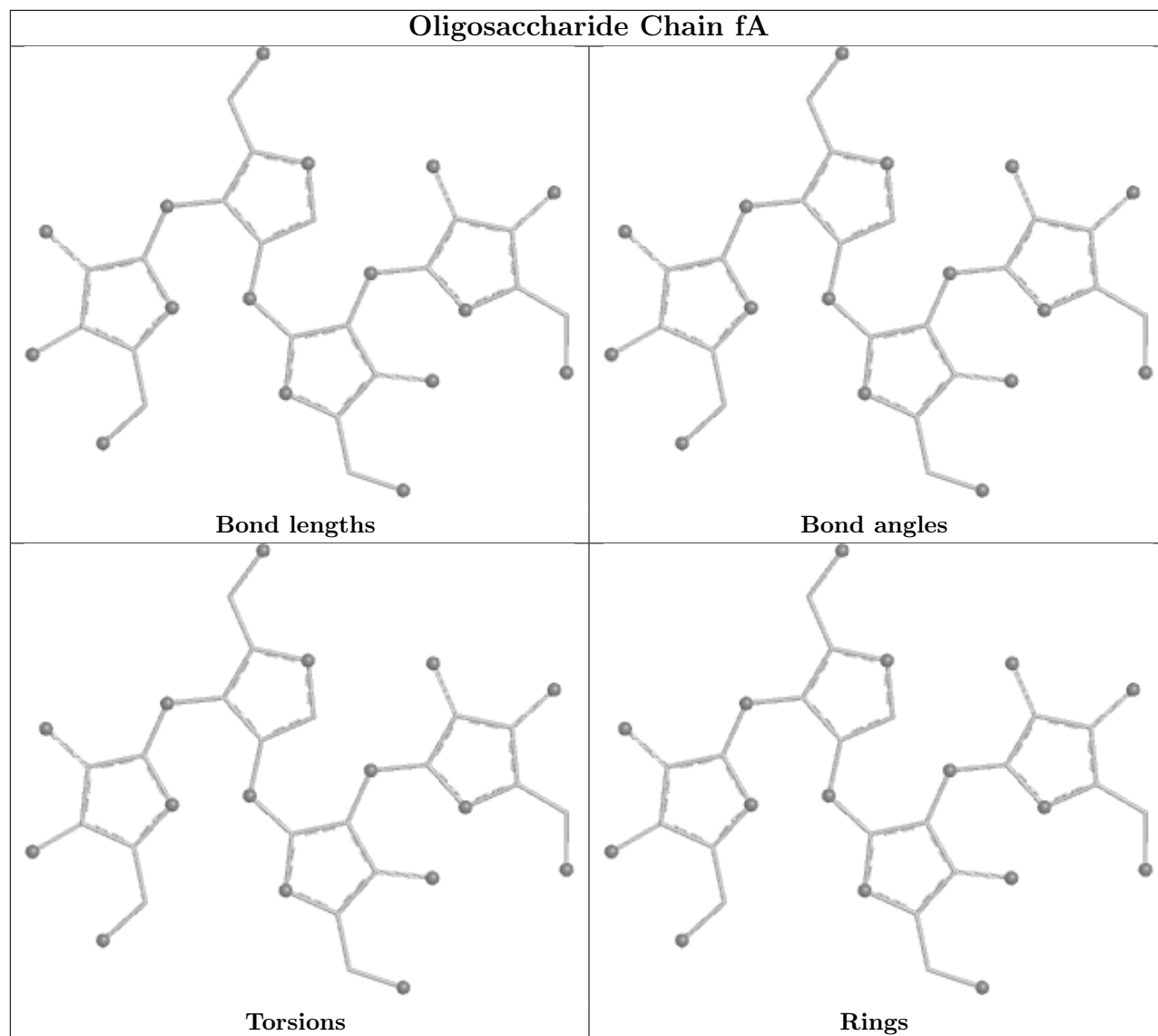


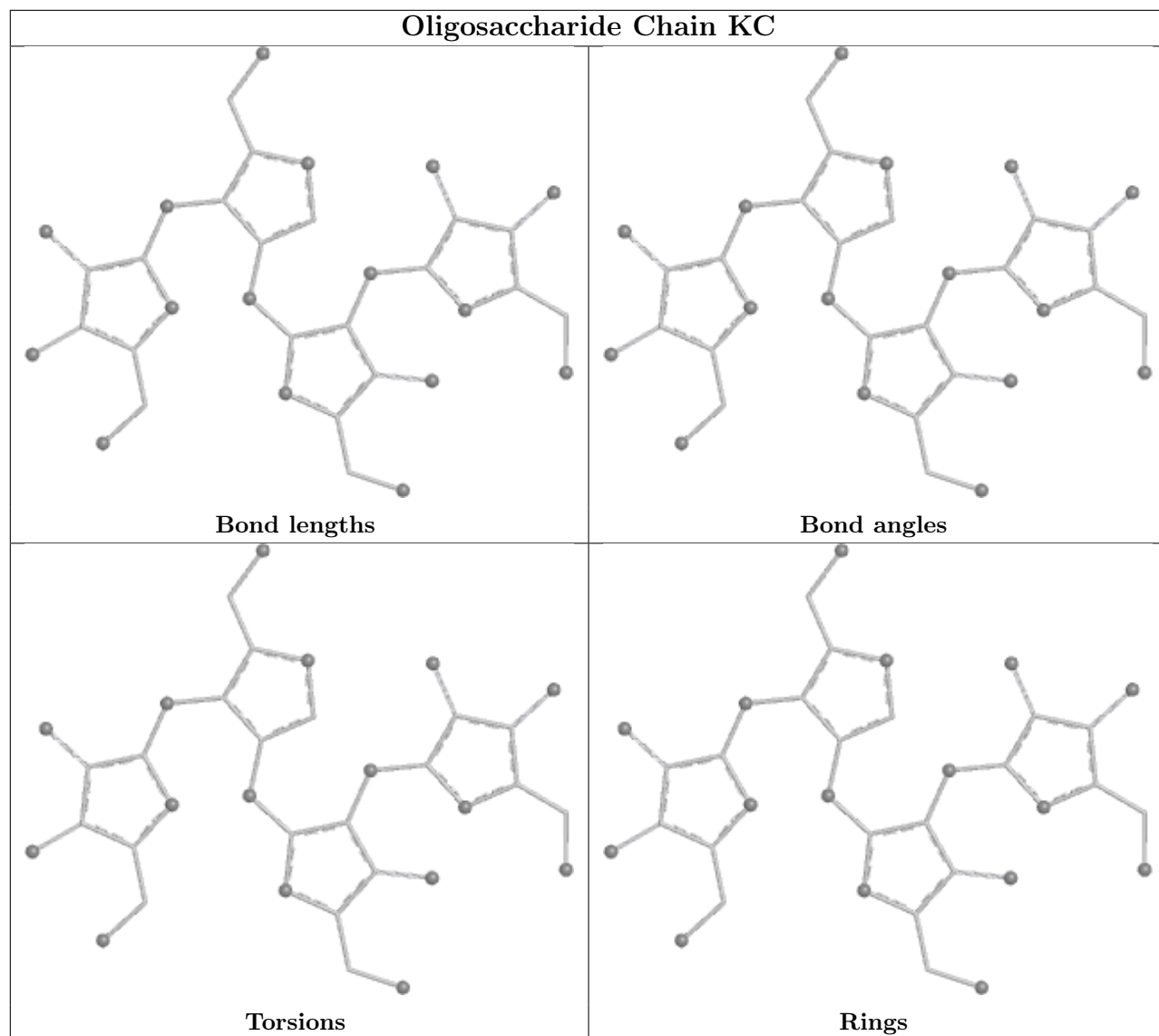


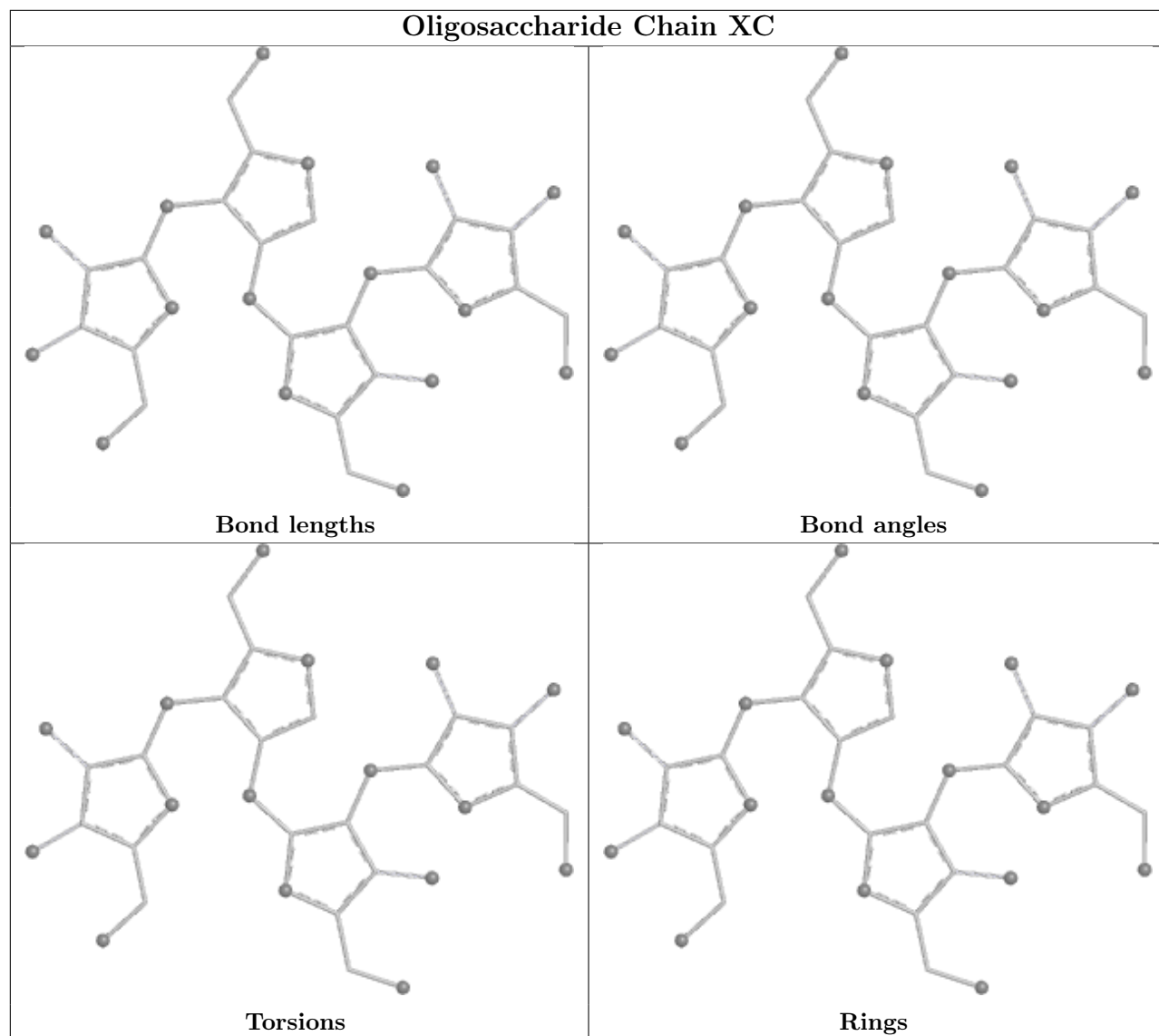


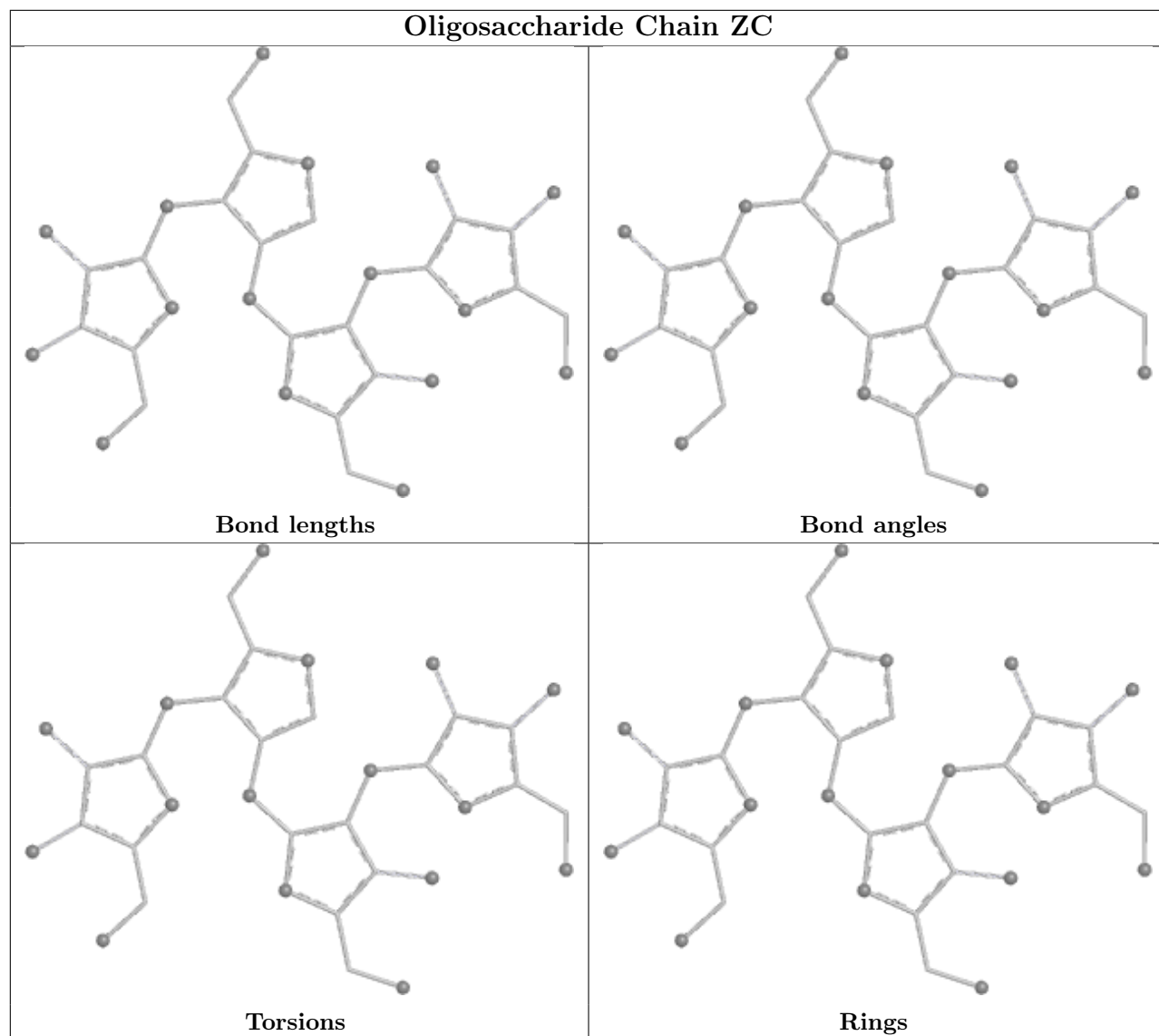


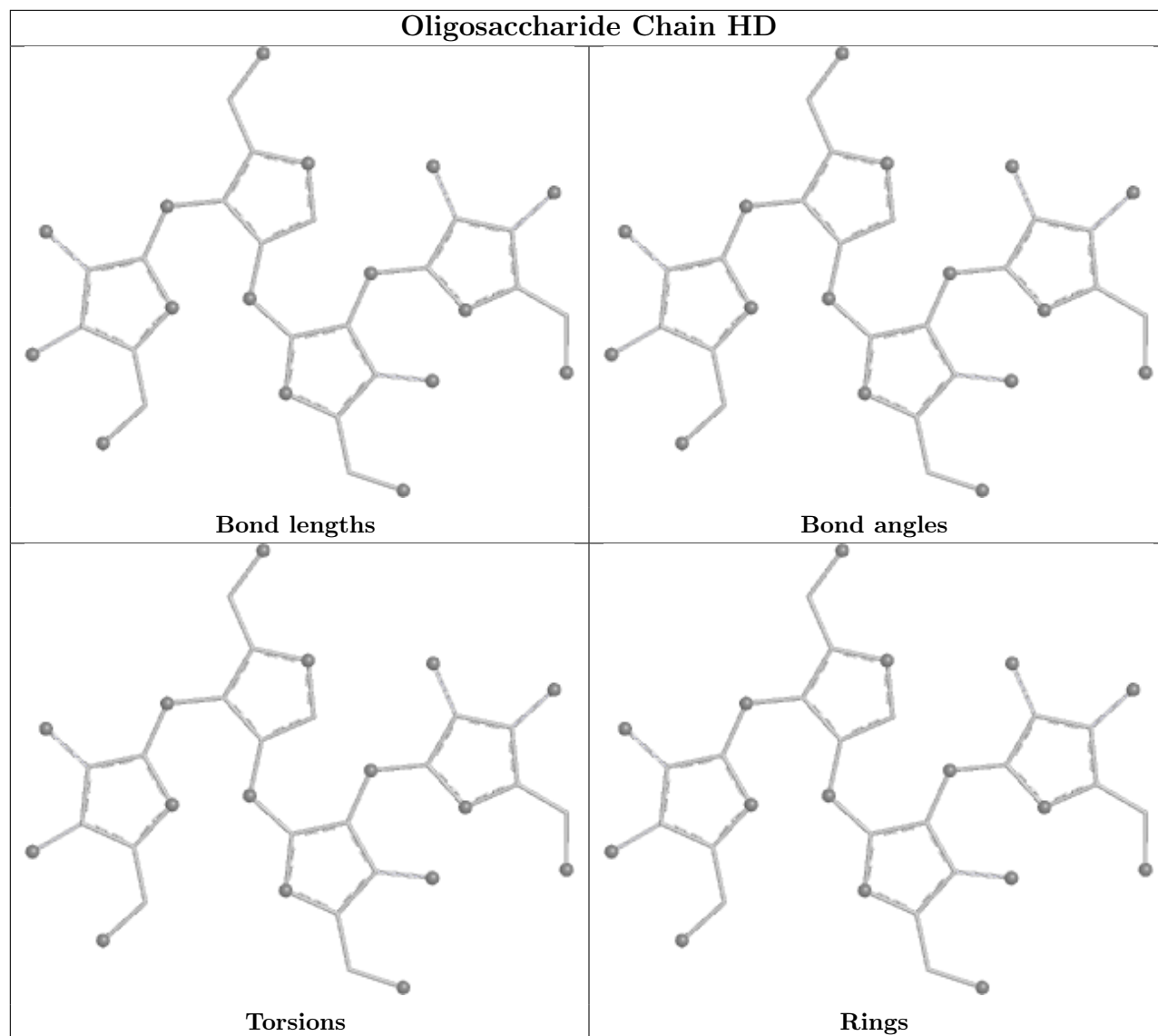


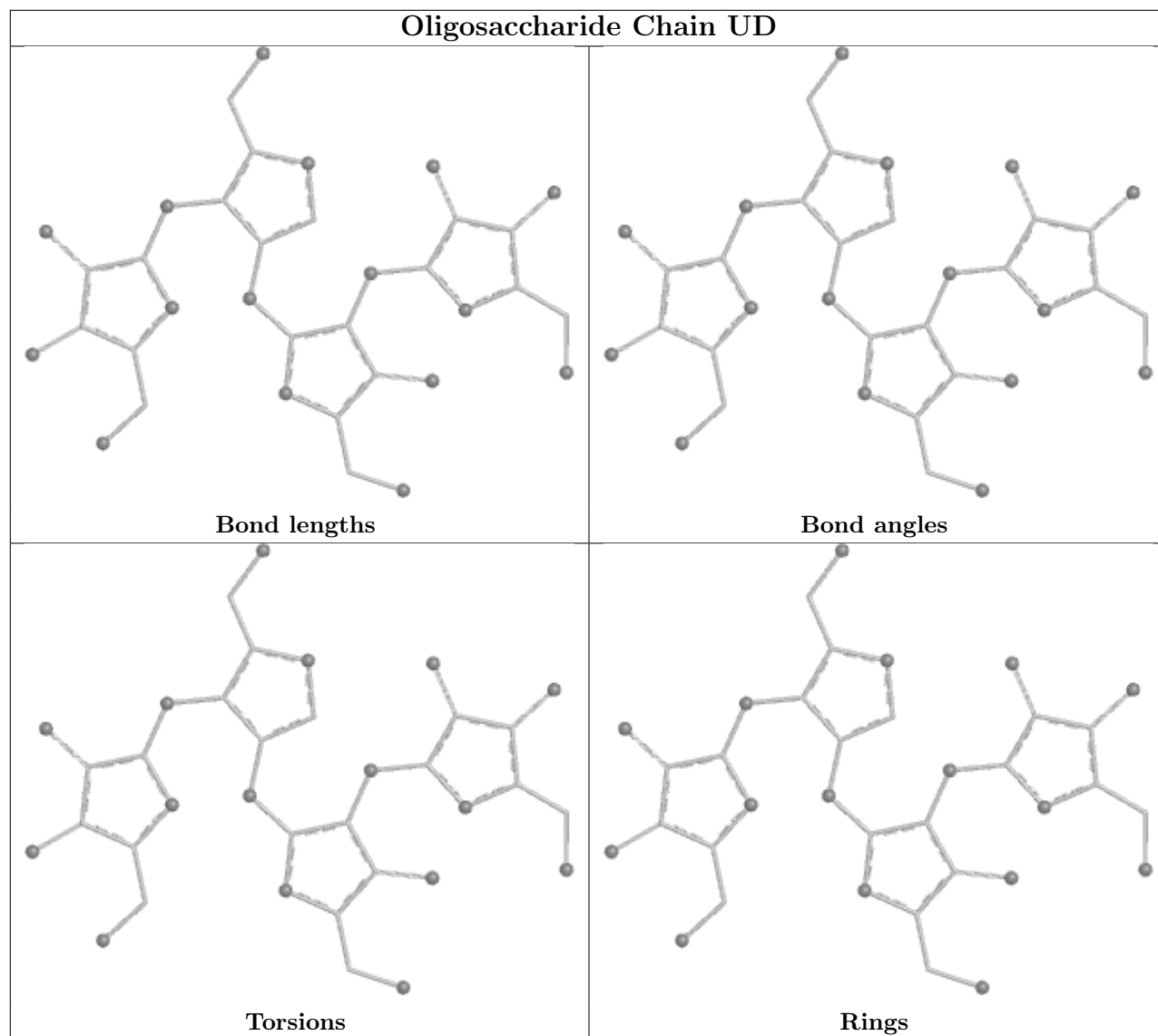


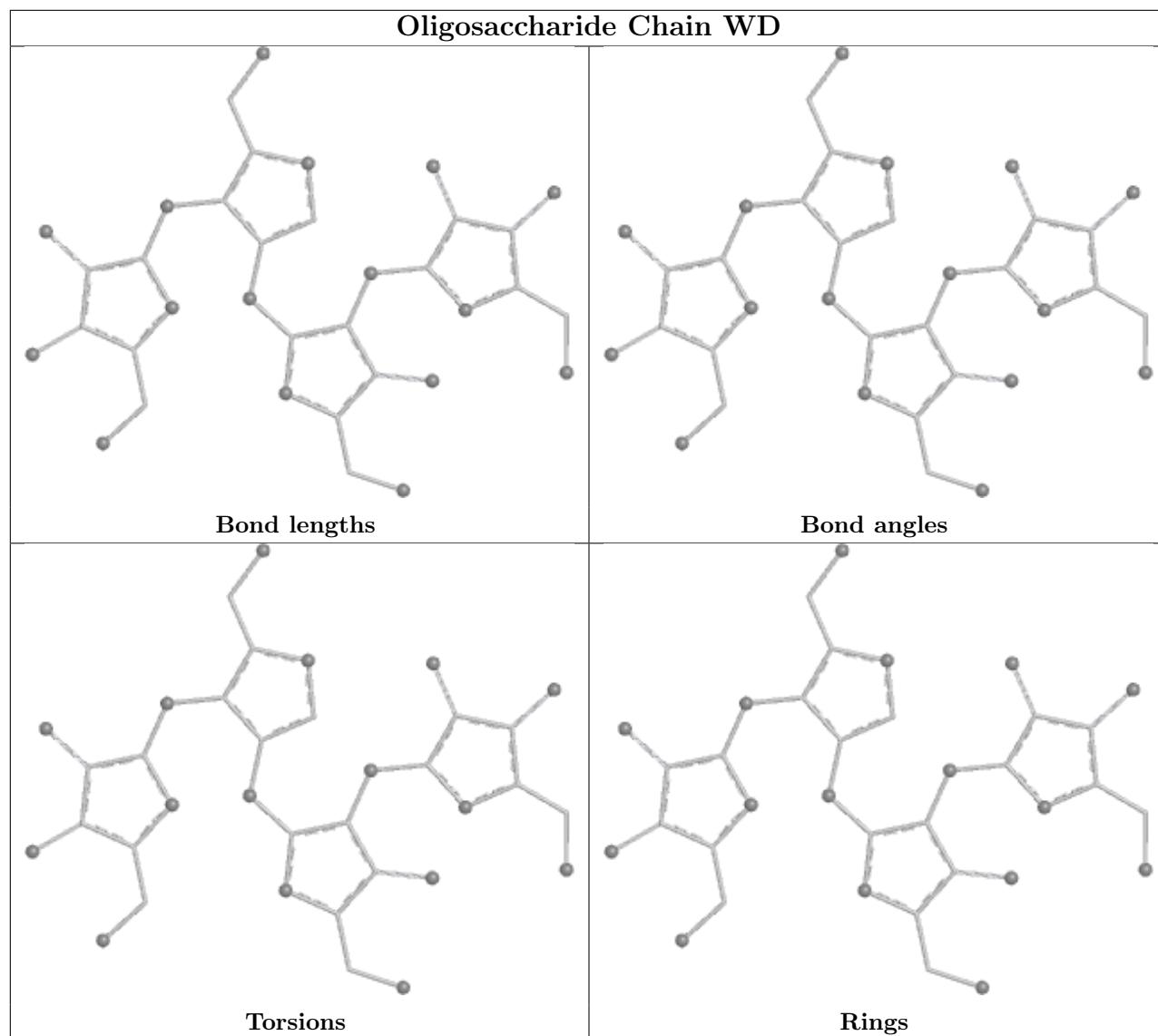


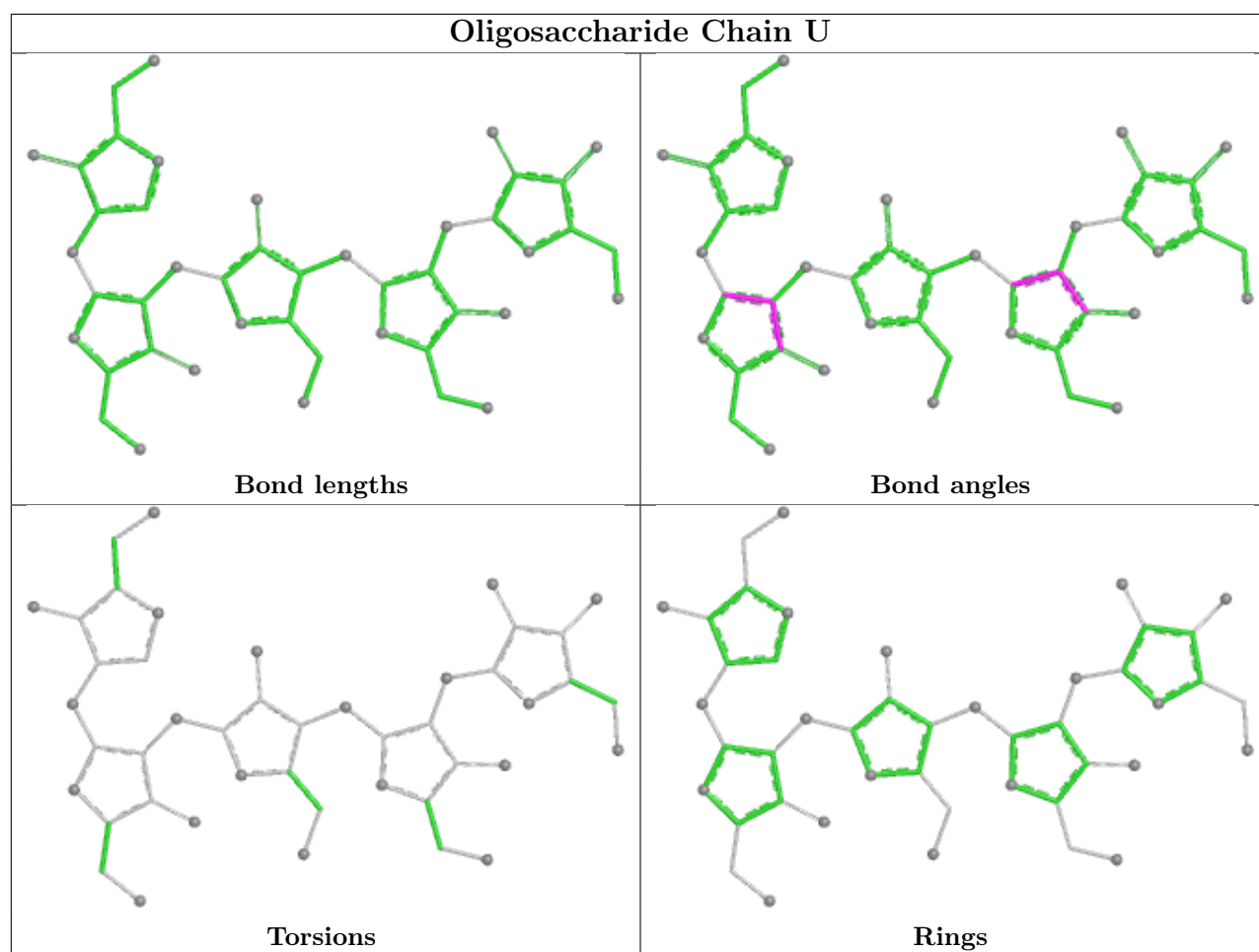


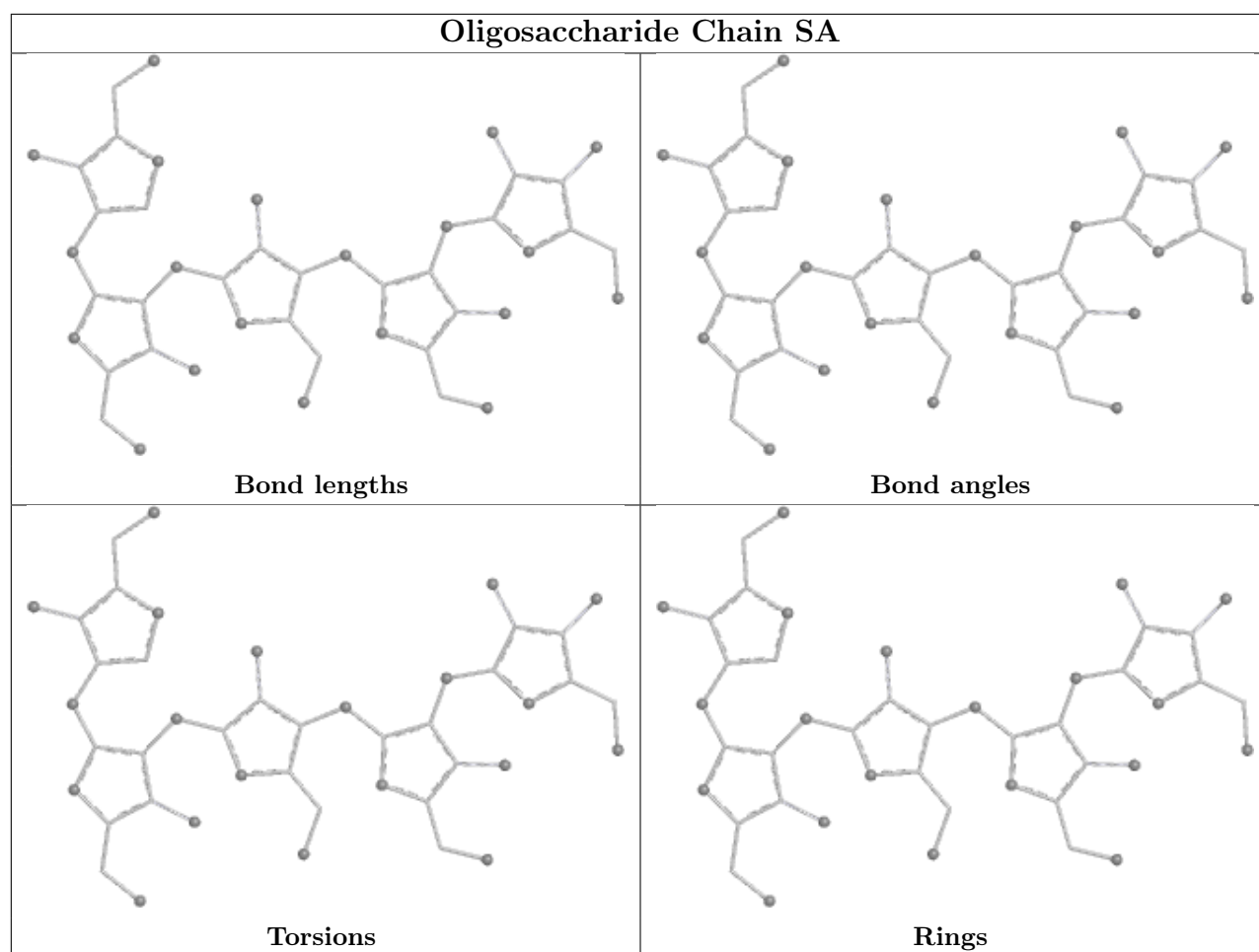


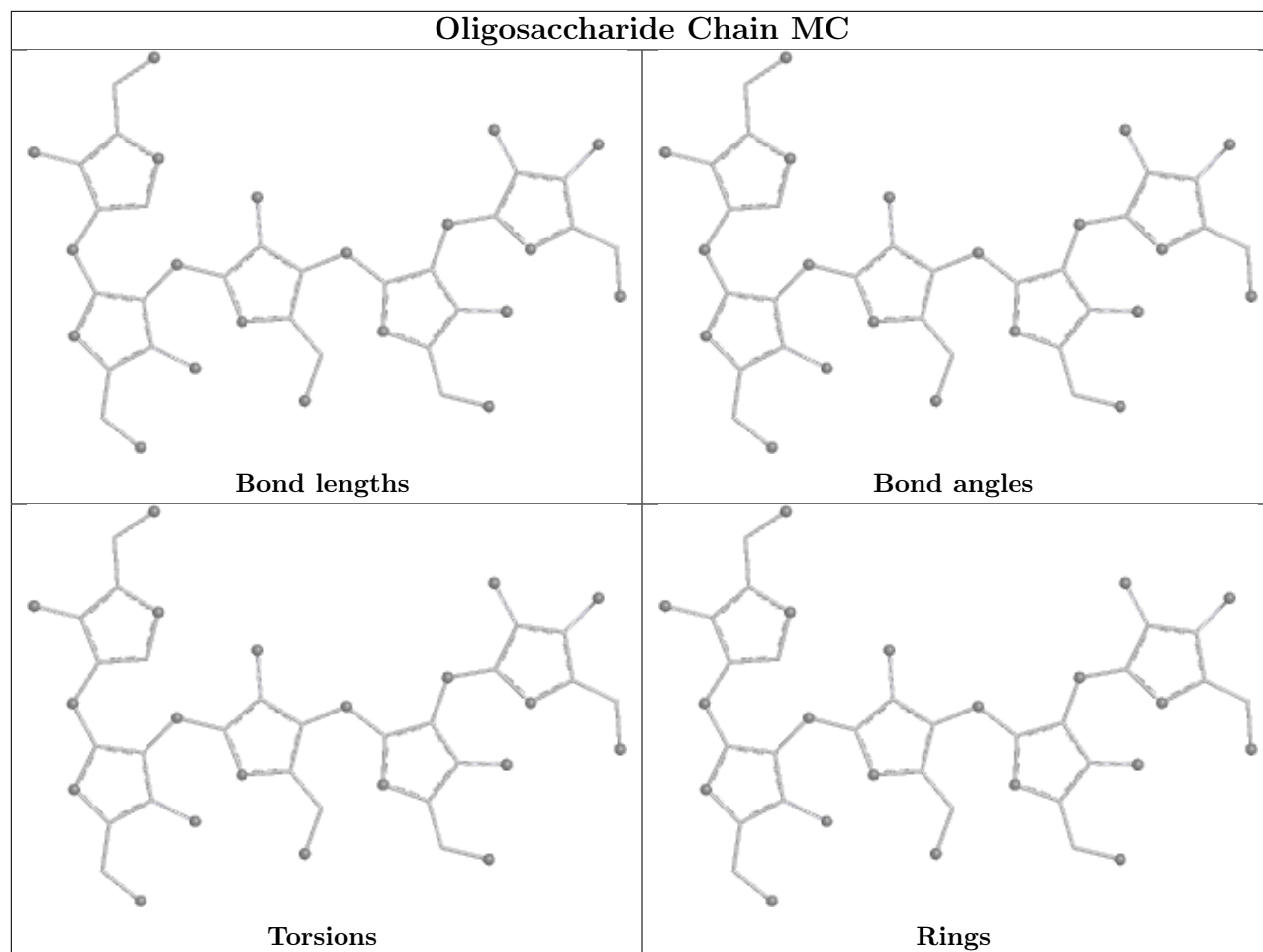




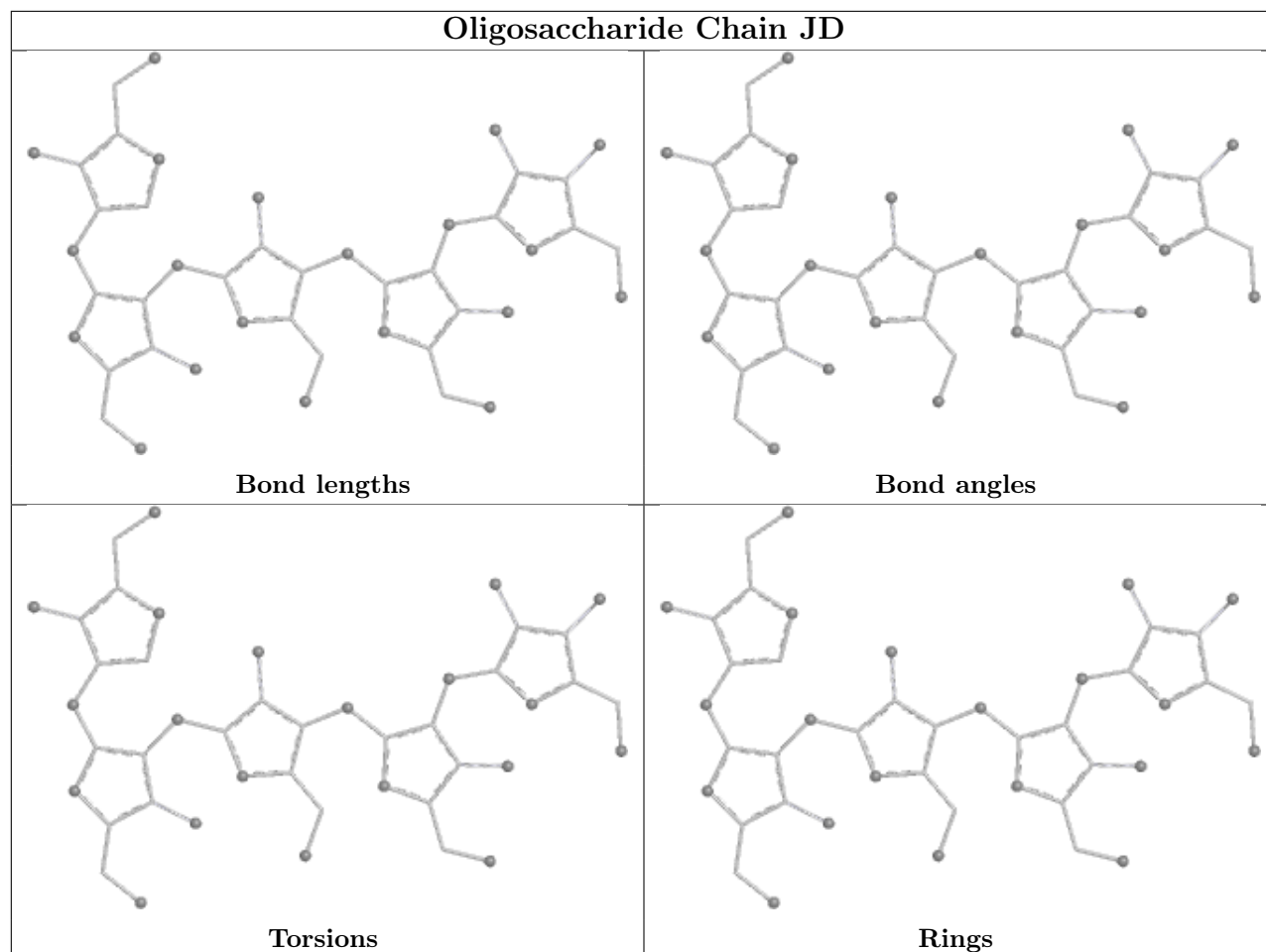




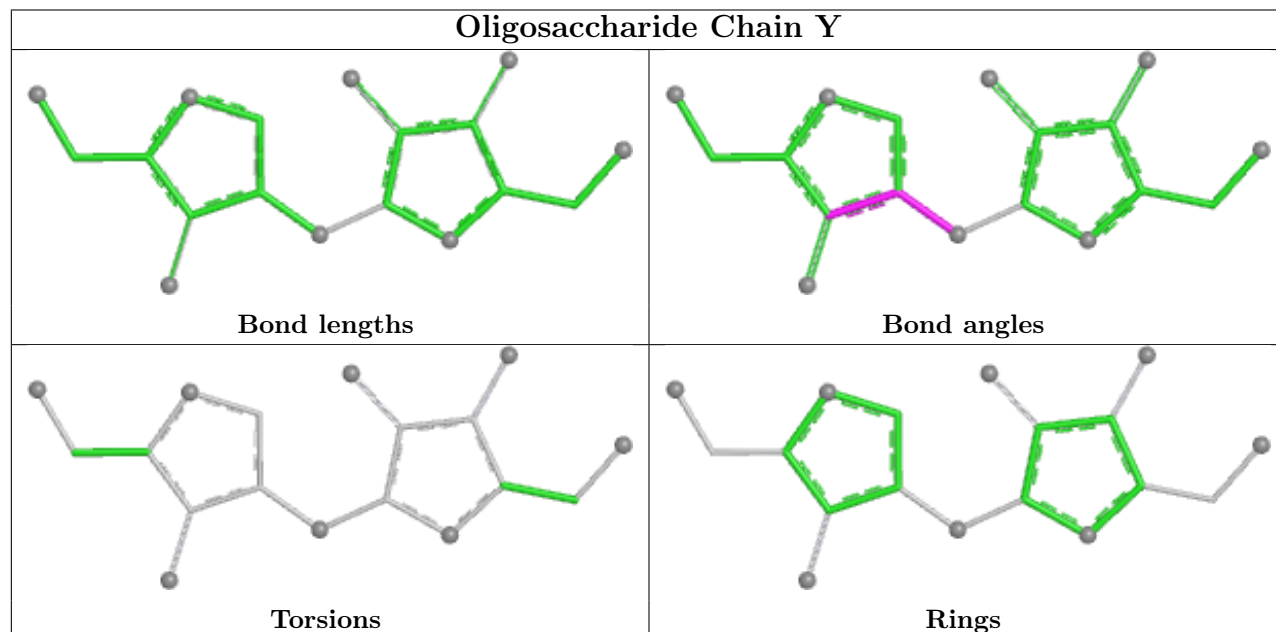


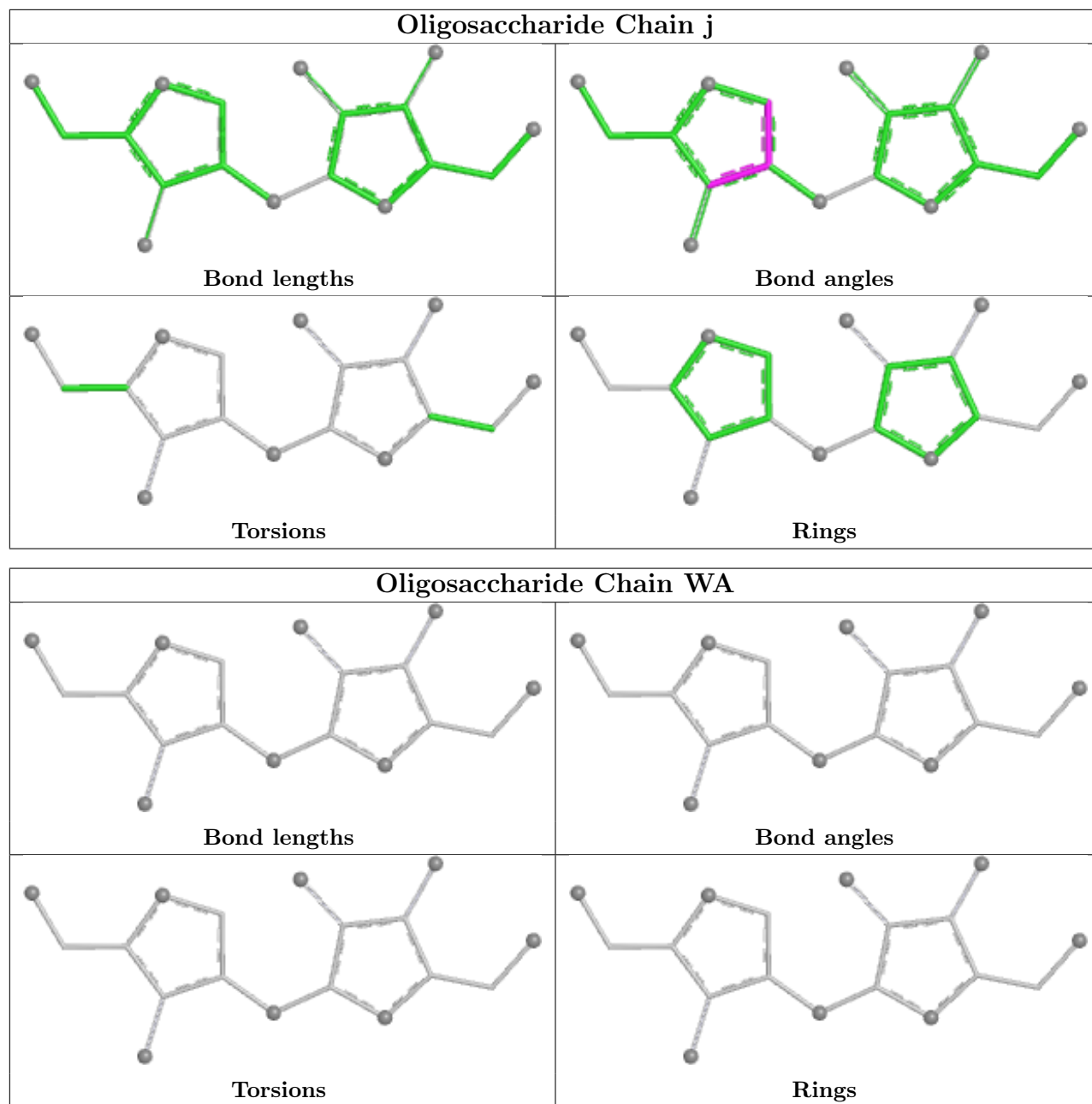


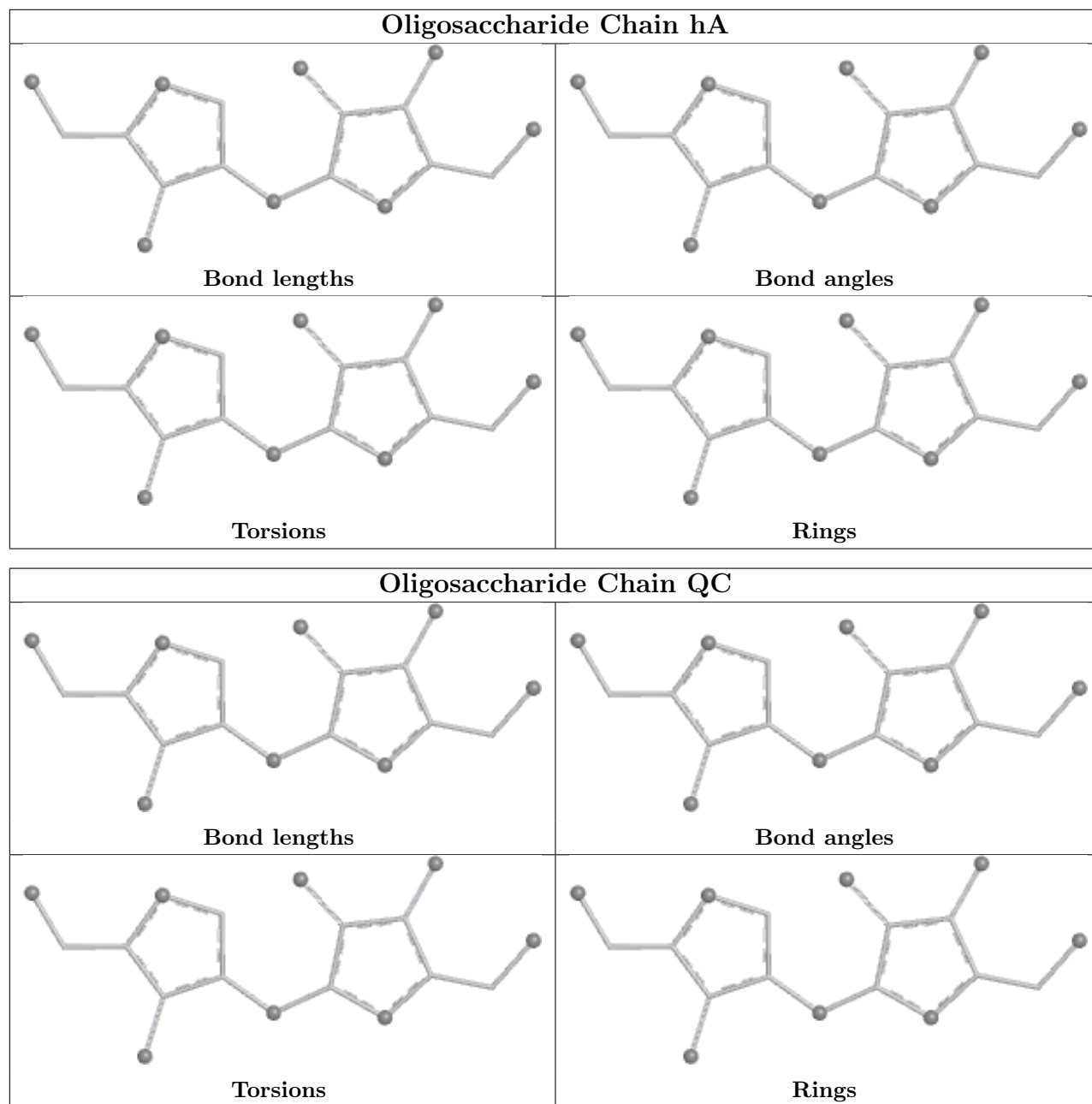
Oligosaccharide Chain JD

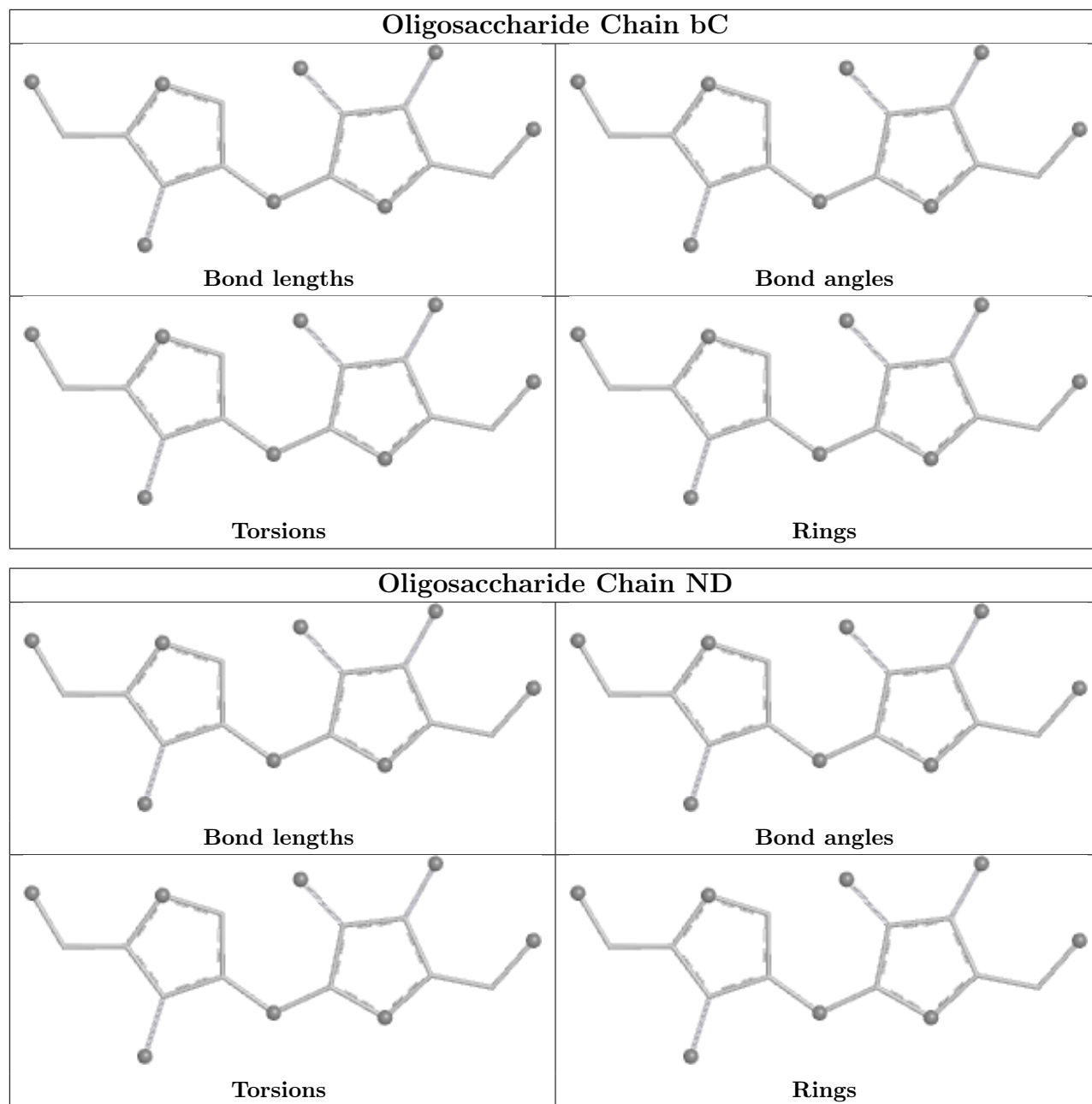


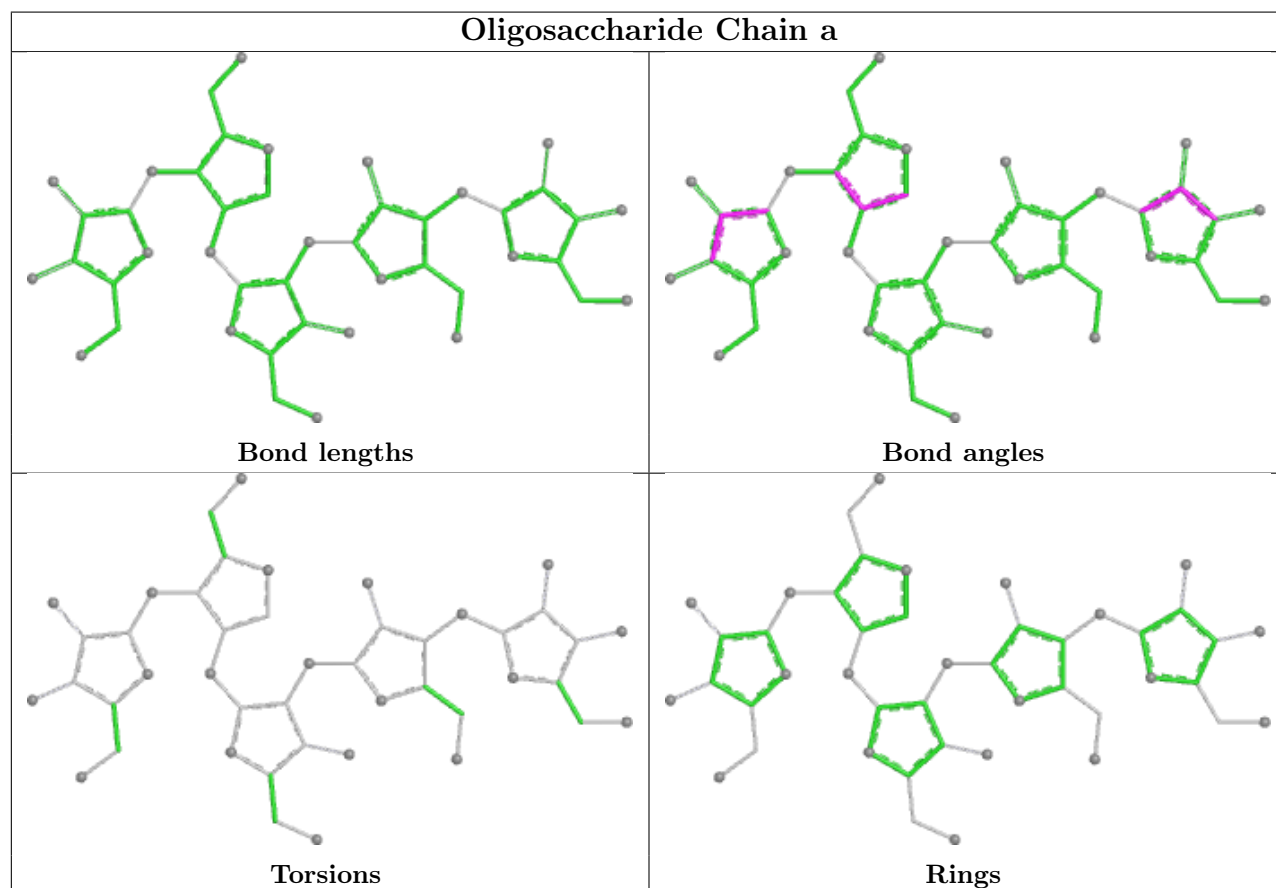
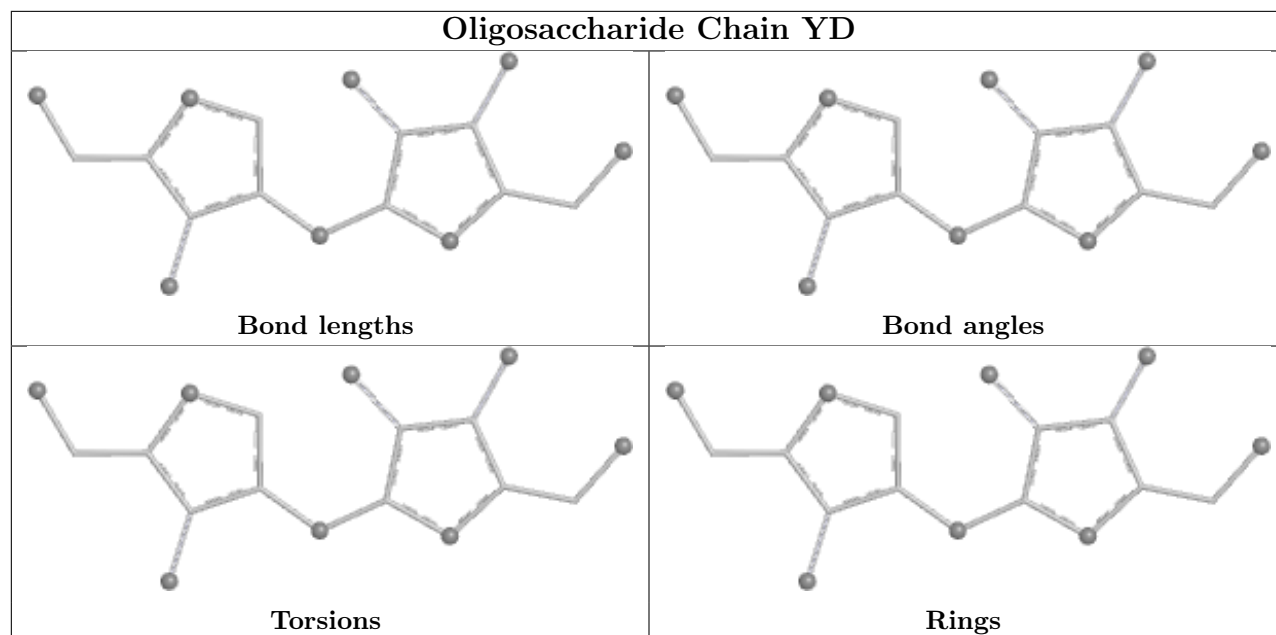
Oligosaccharide Chain Y

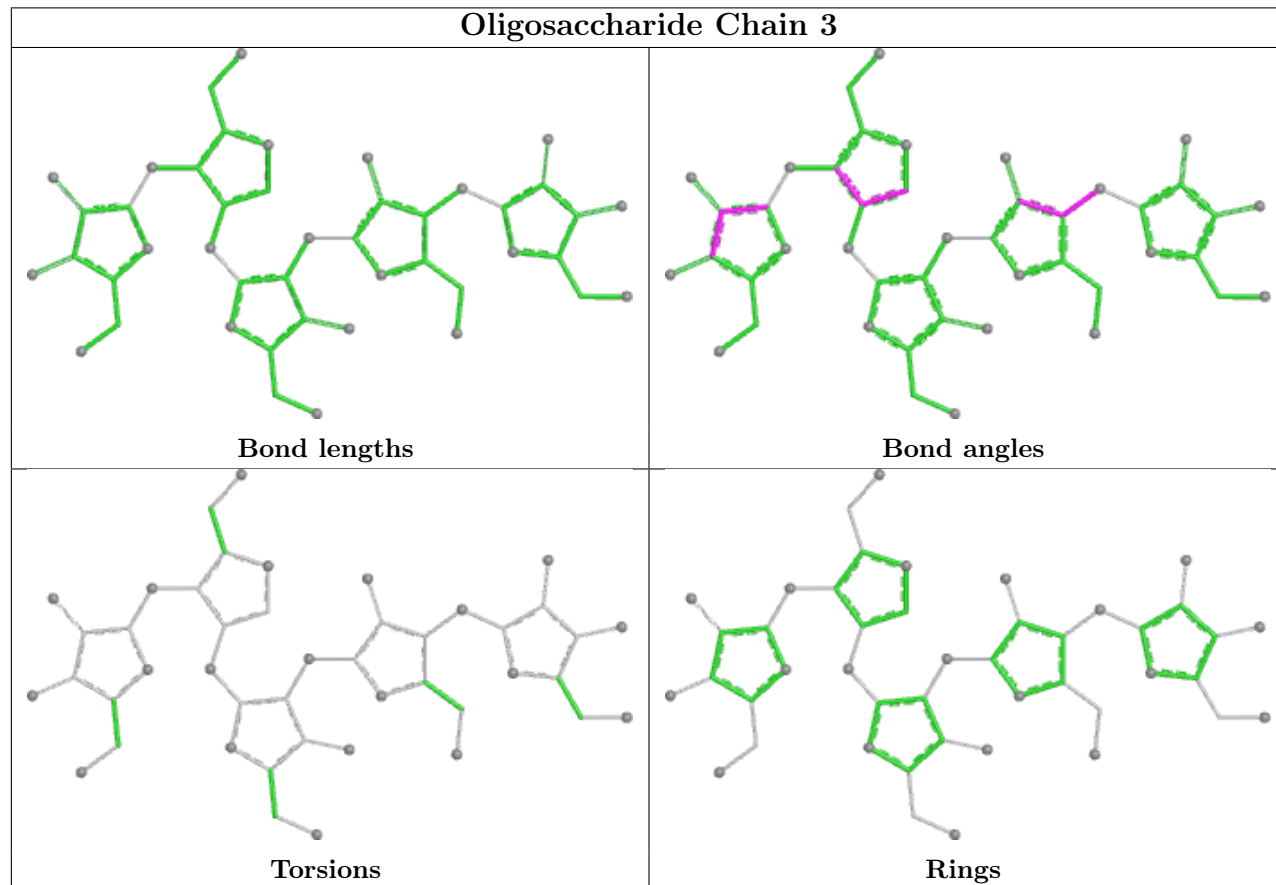
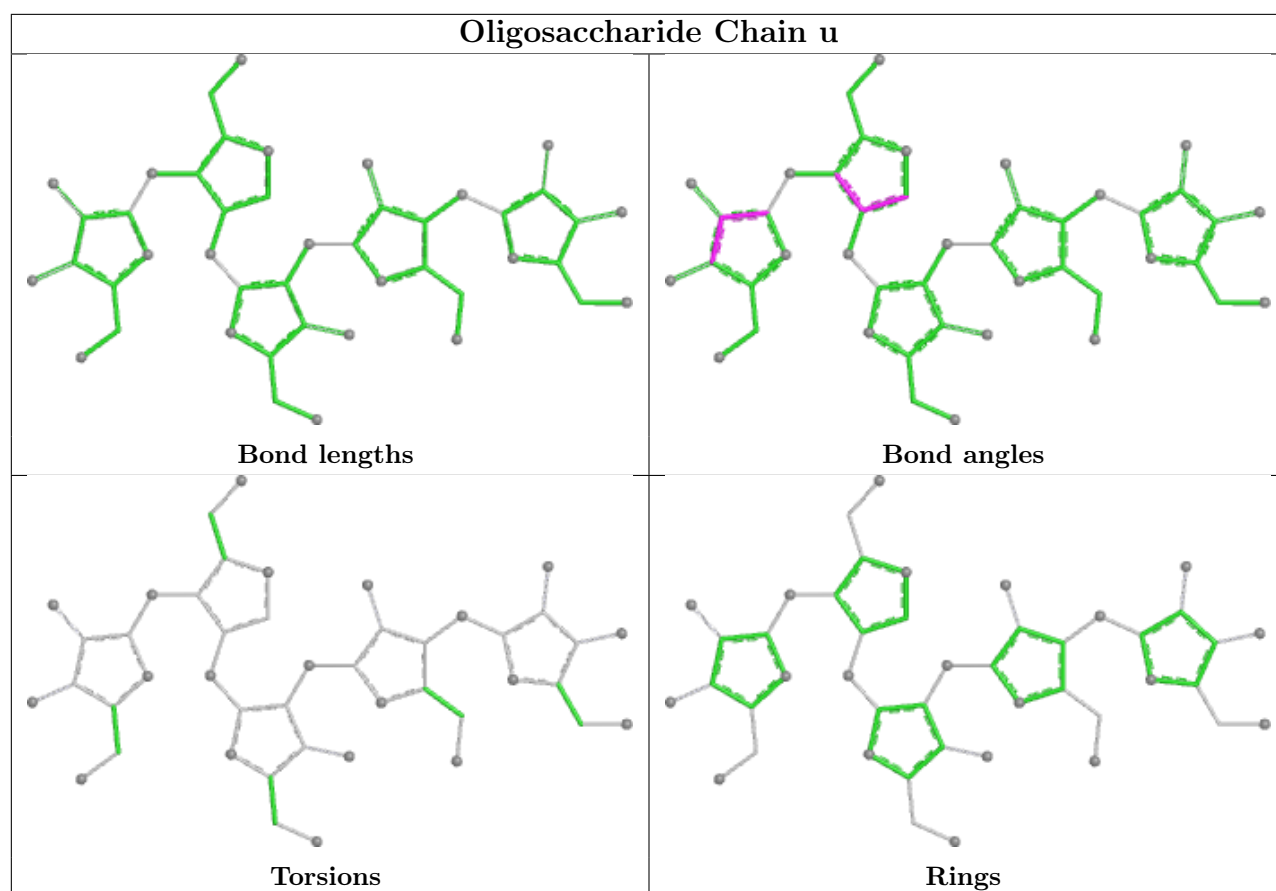


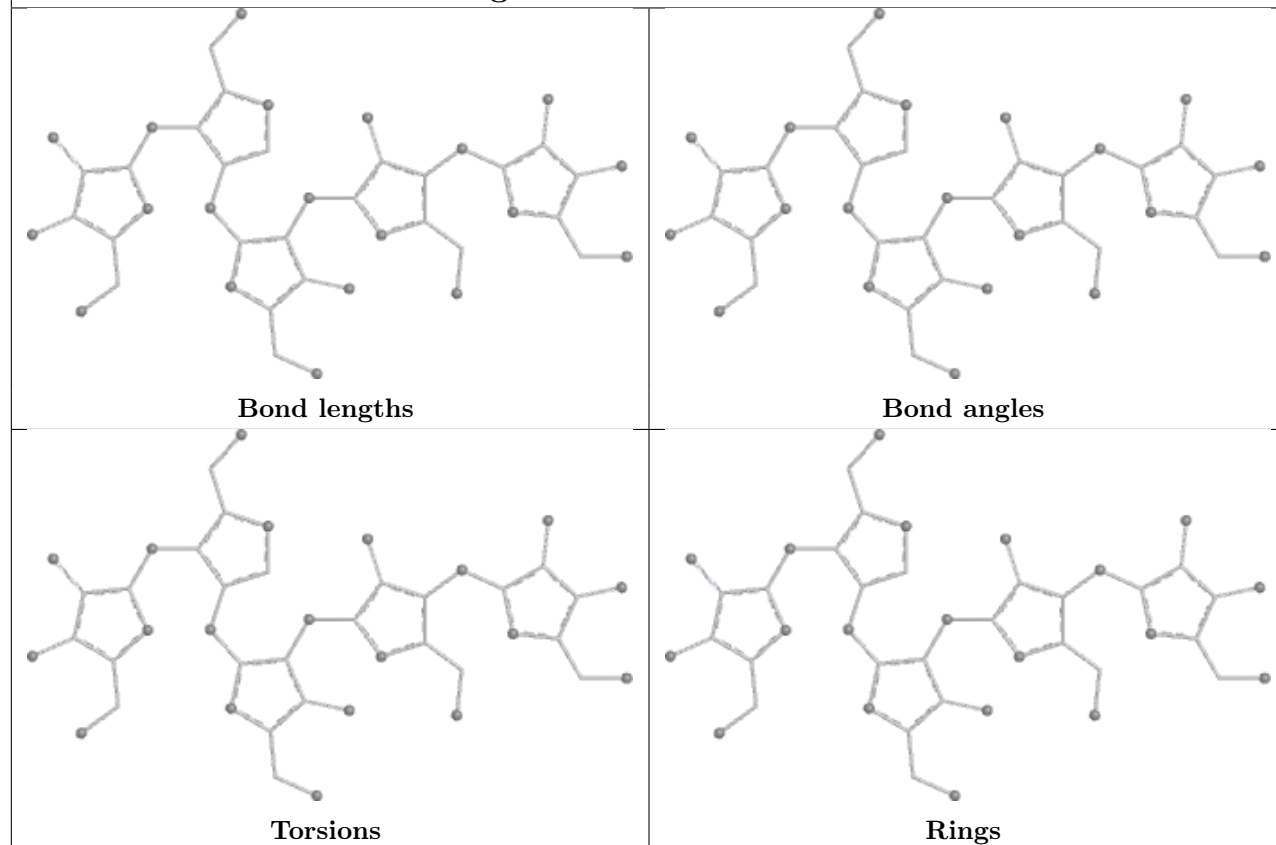
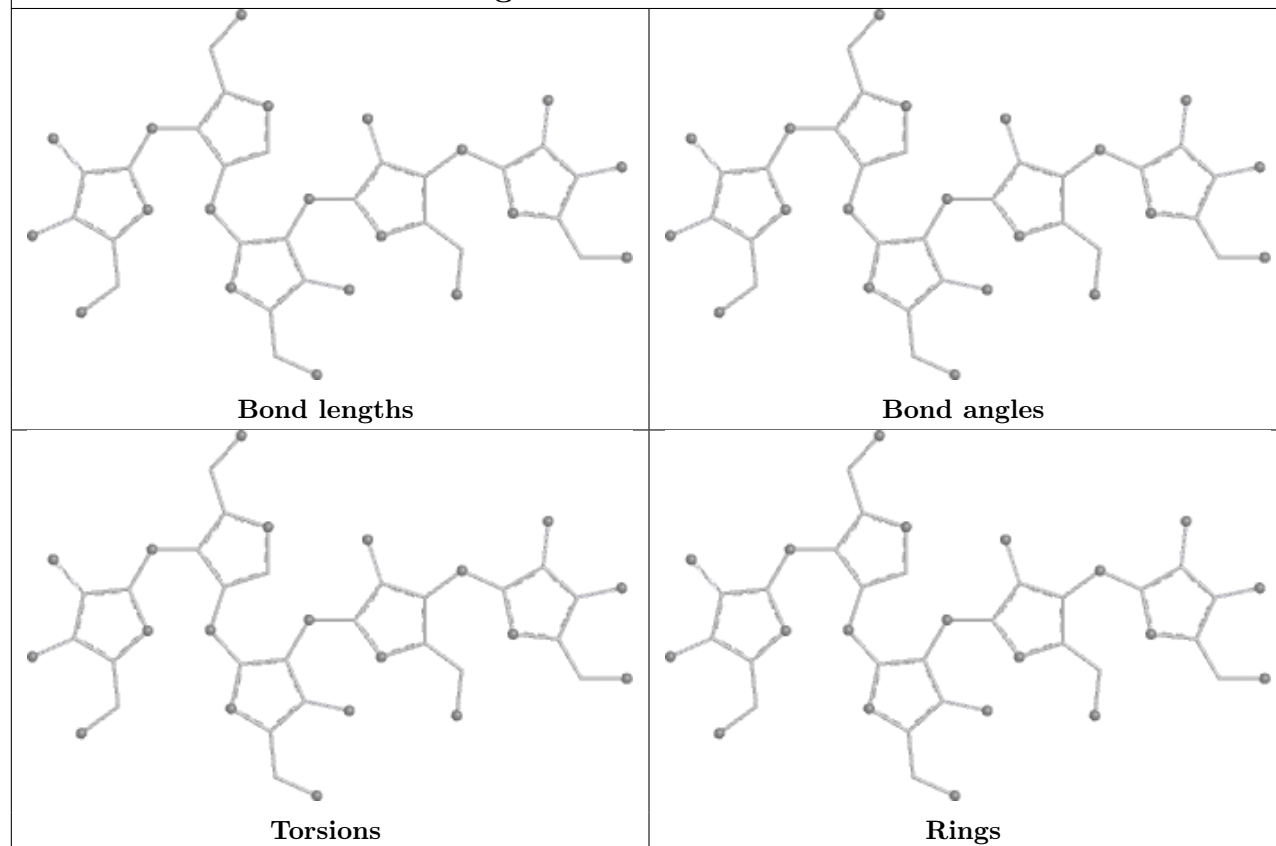


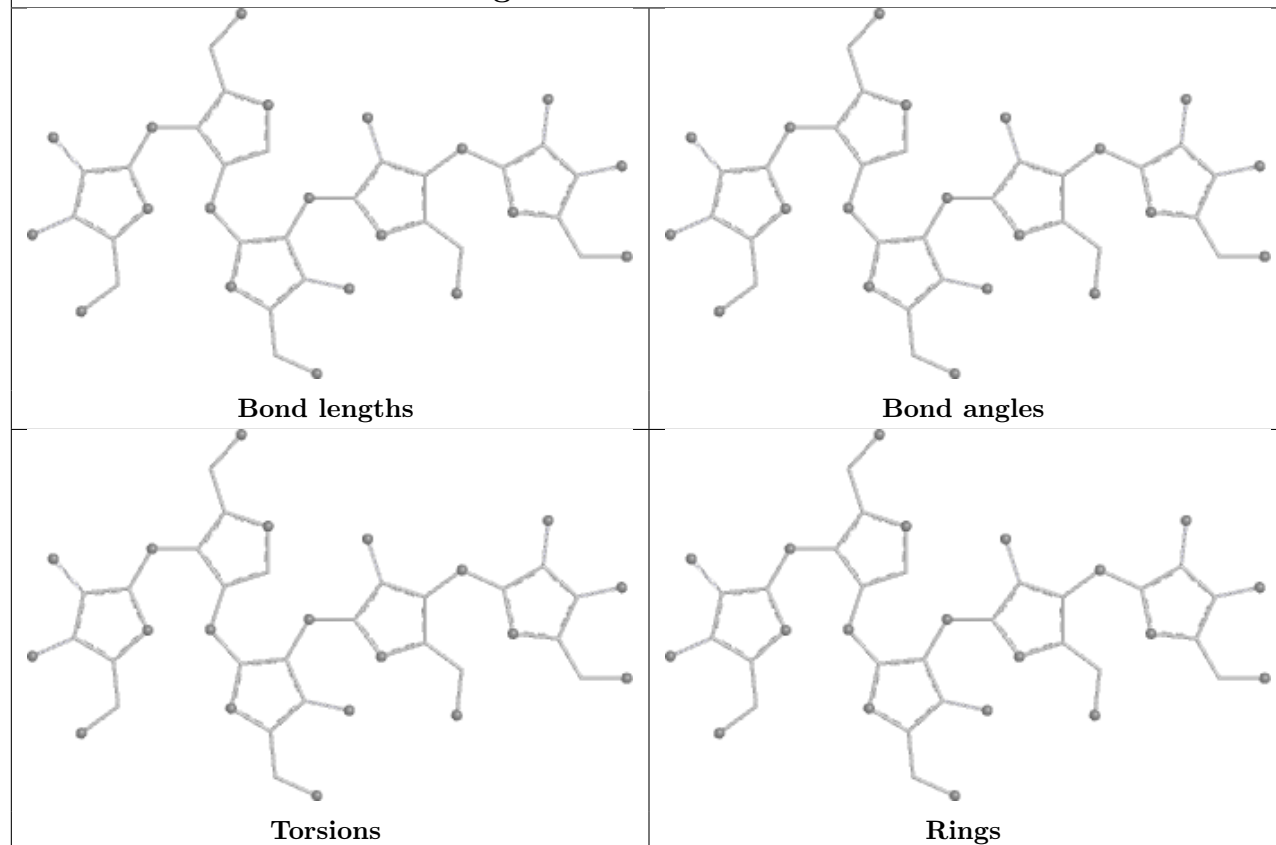
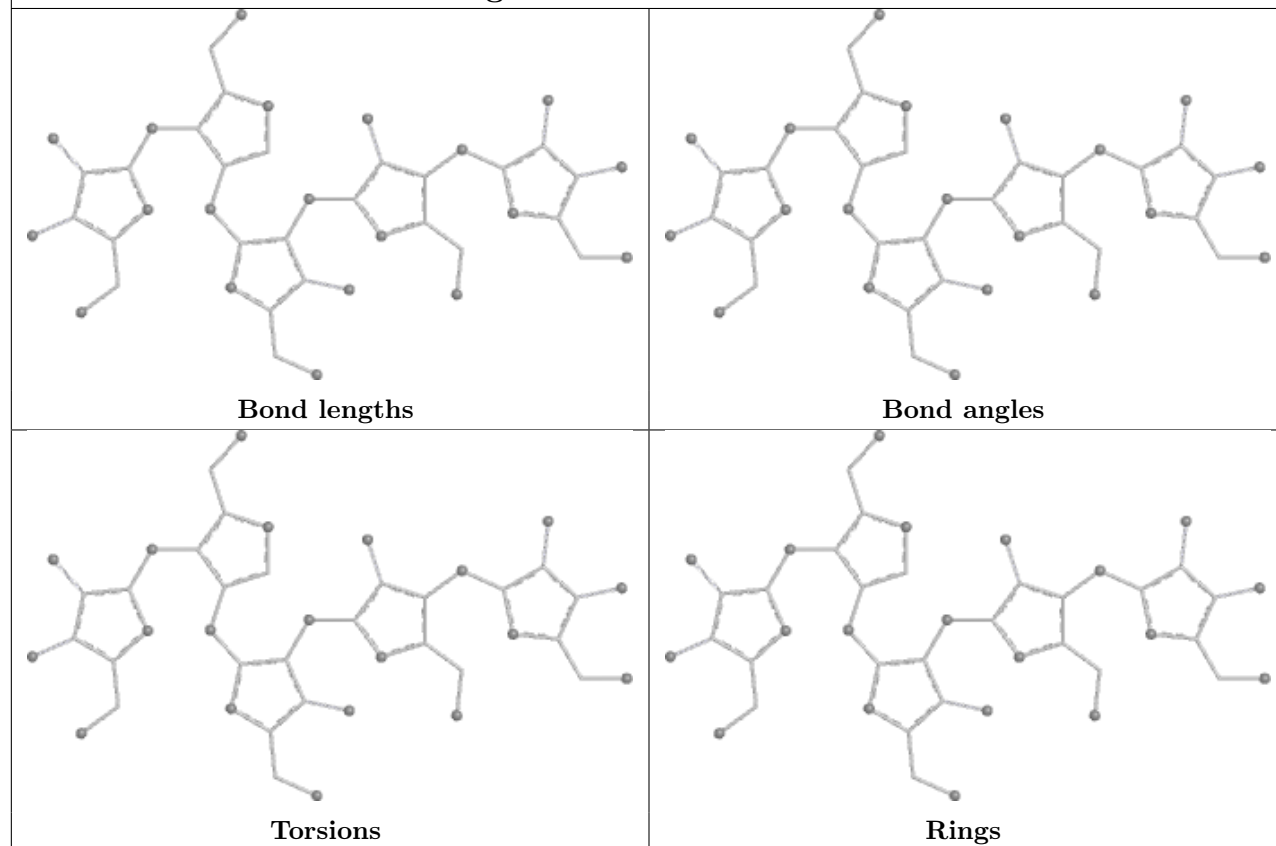


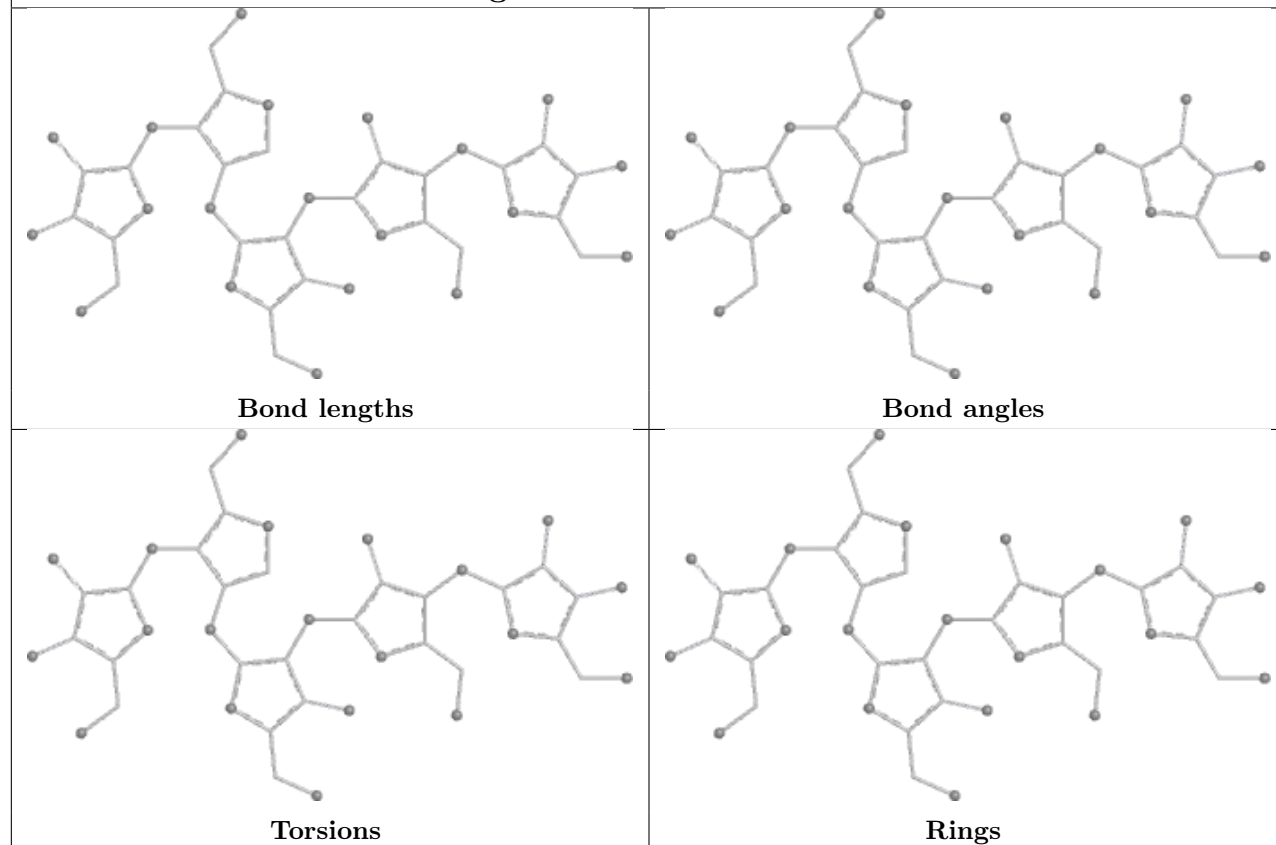
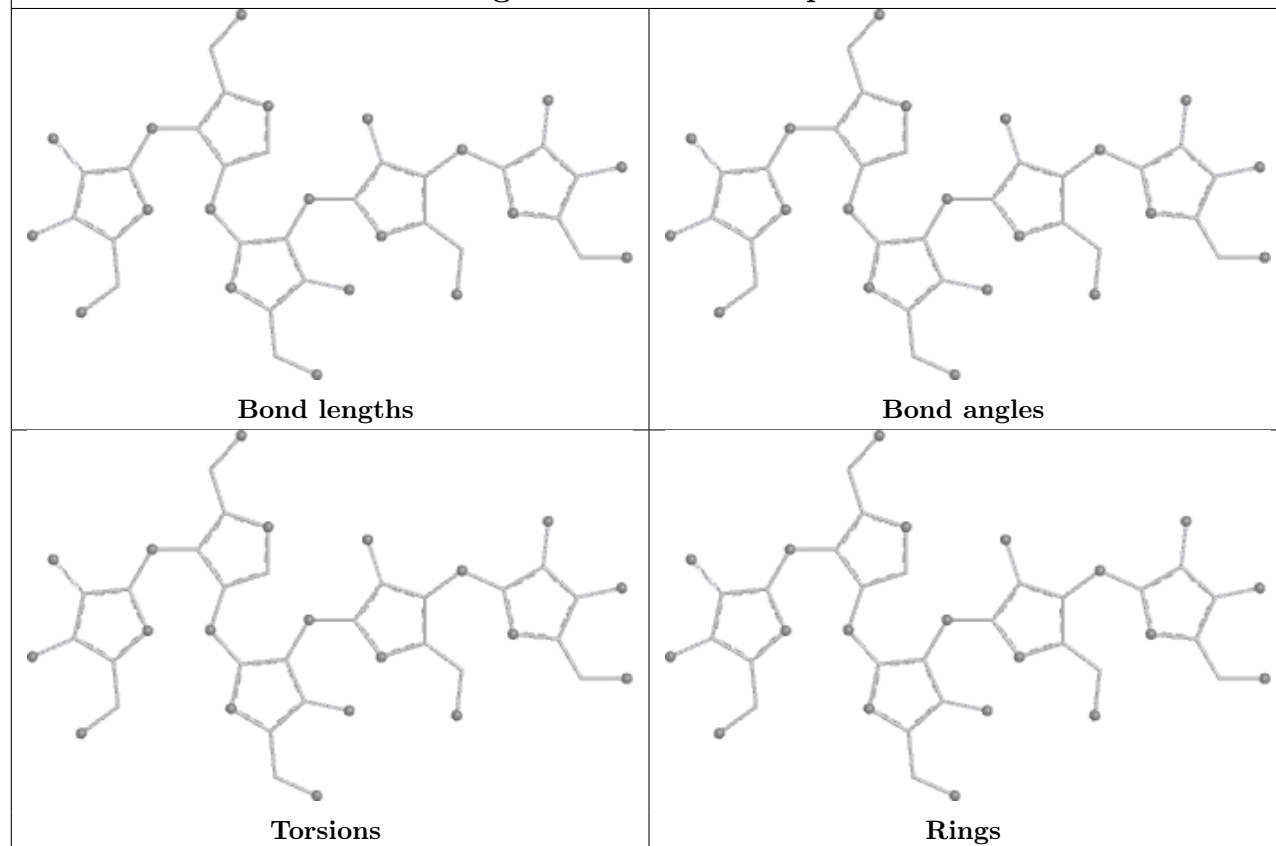


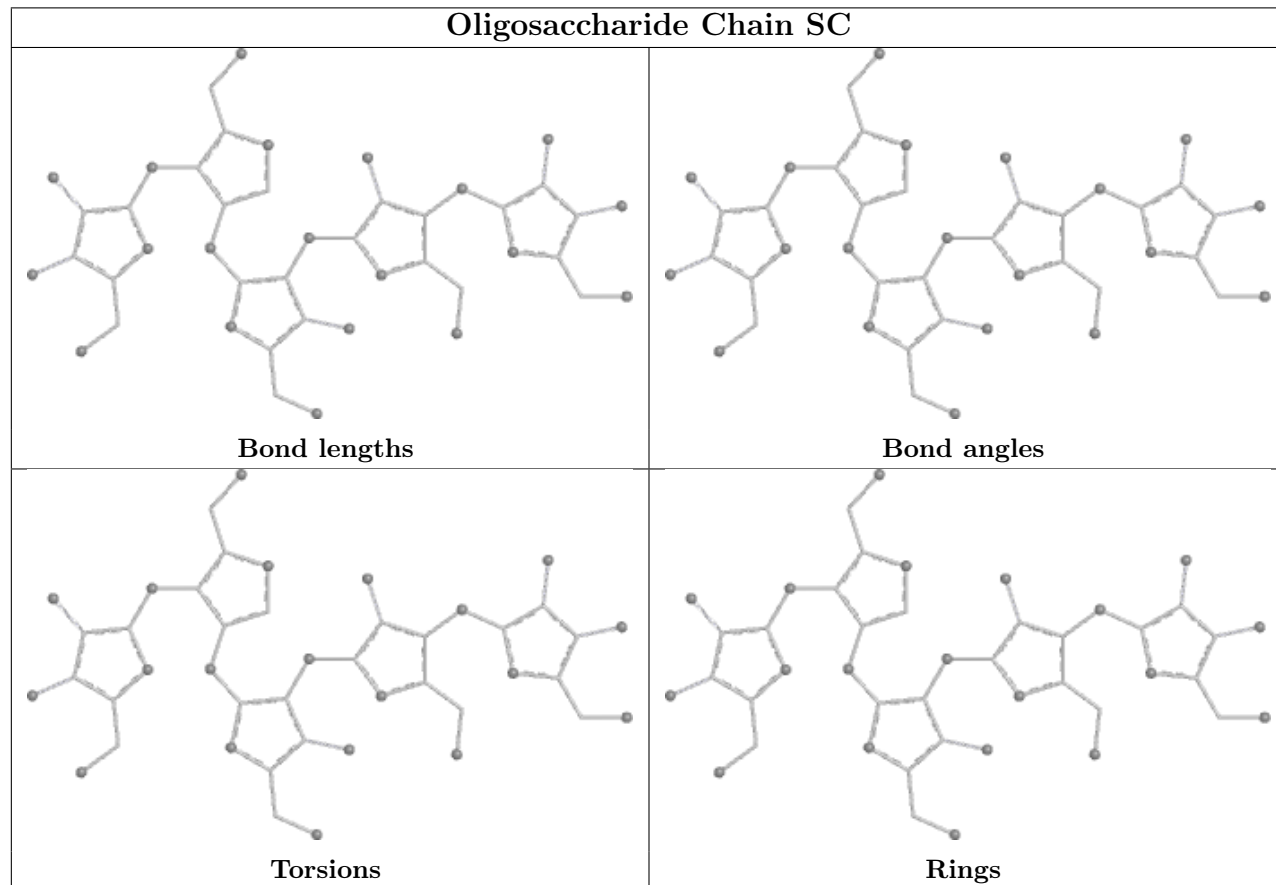
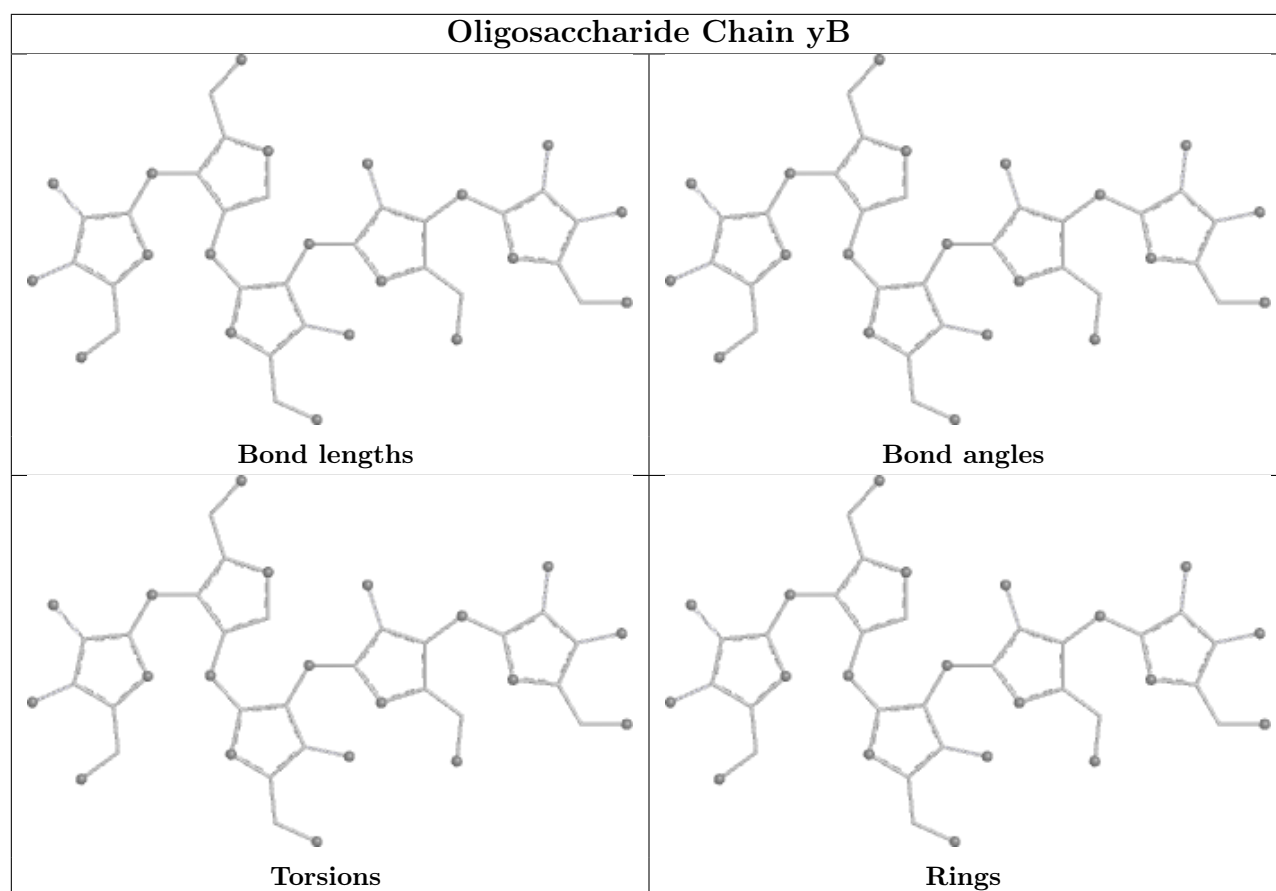


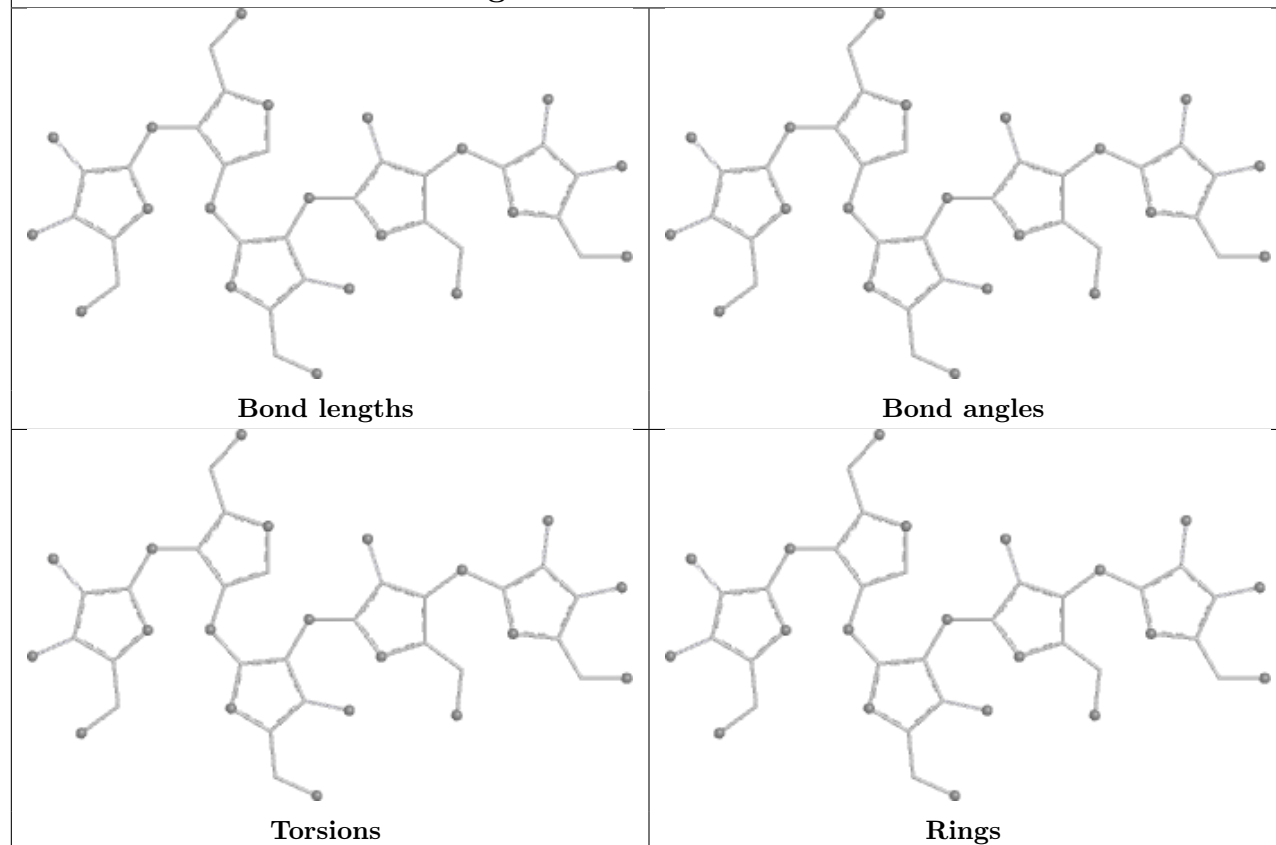
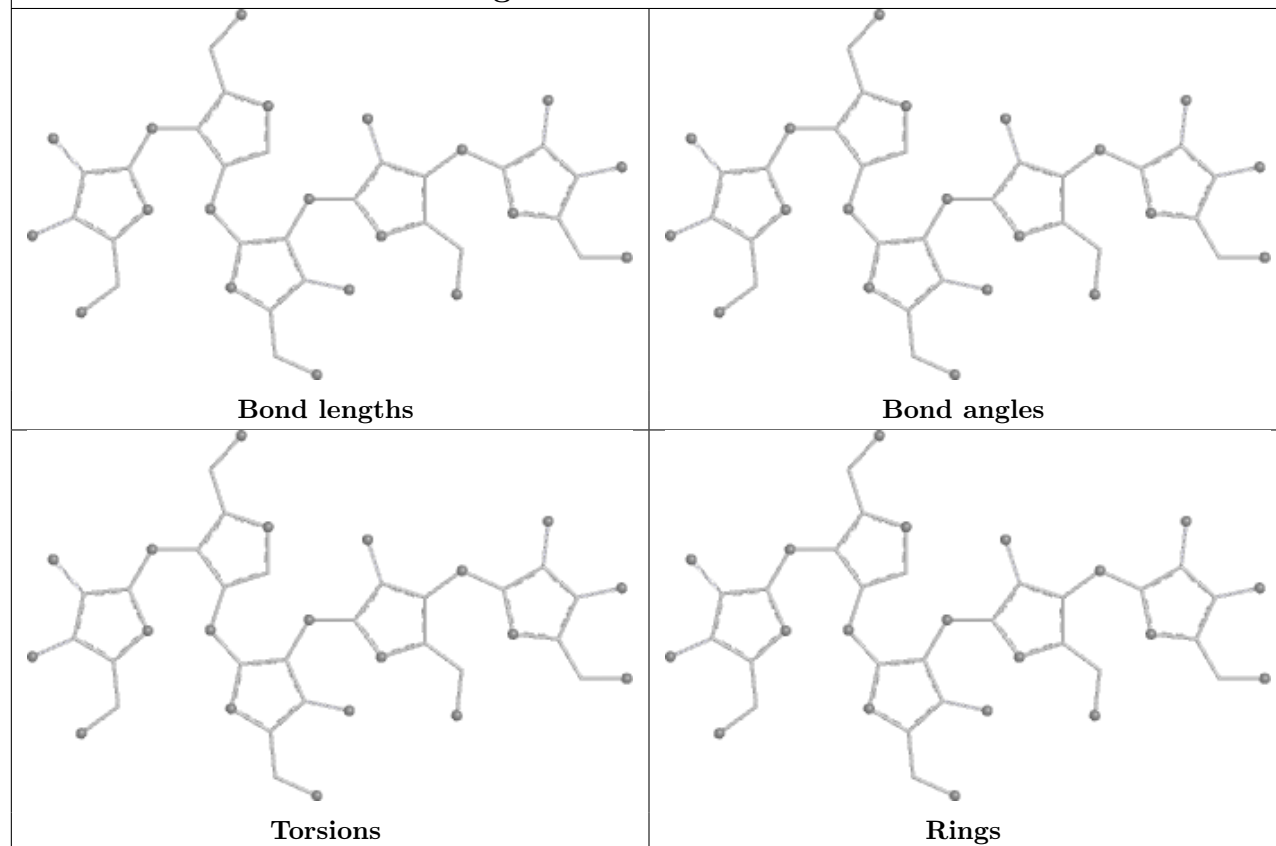


Oligosaccharide Chain YA**Oligosaccharide Chain sA**

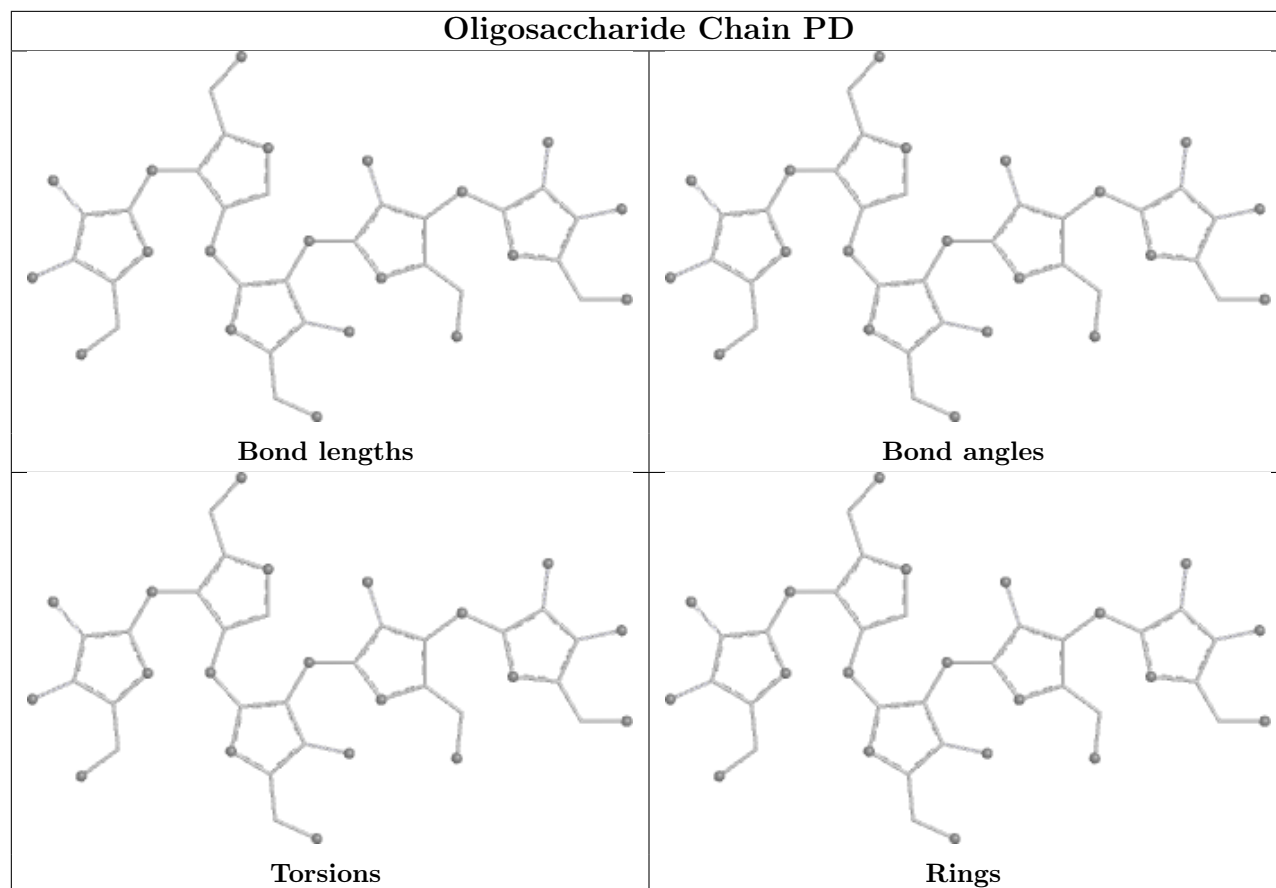
Oligosaccharide Chain 1A**Oligosaccharide Chain MB**

Oligosaccharide Chain VB**Oligosaccharide Chain pB**

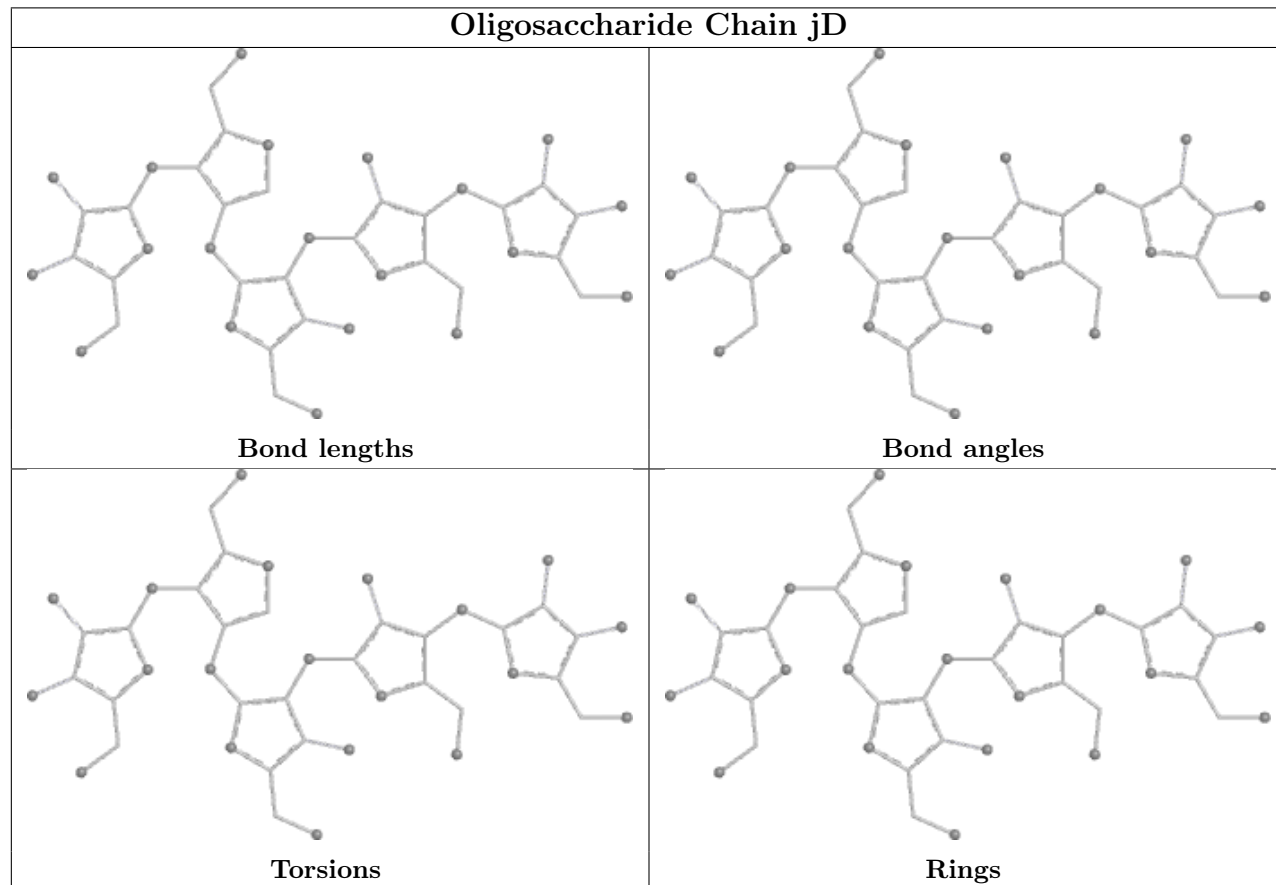


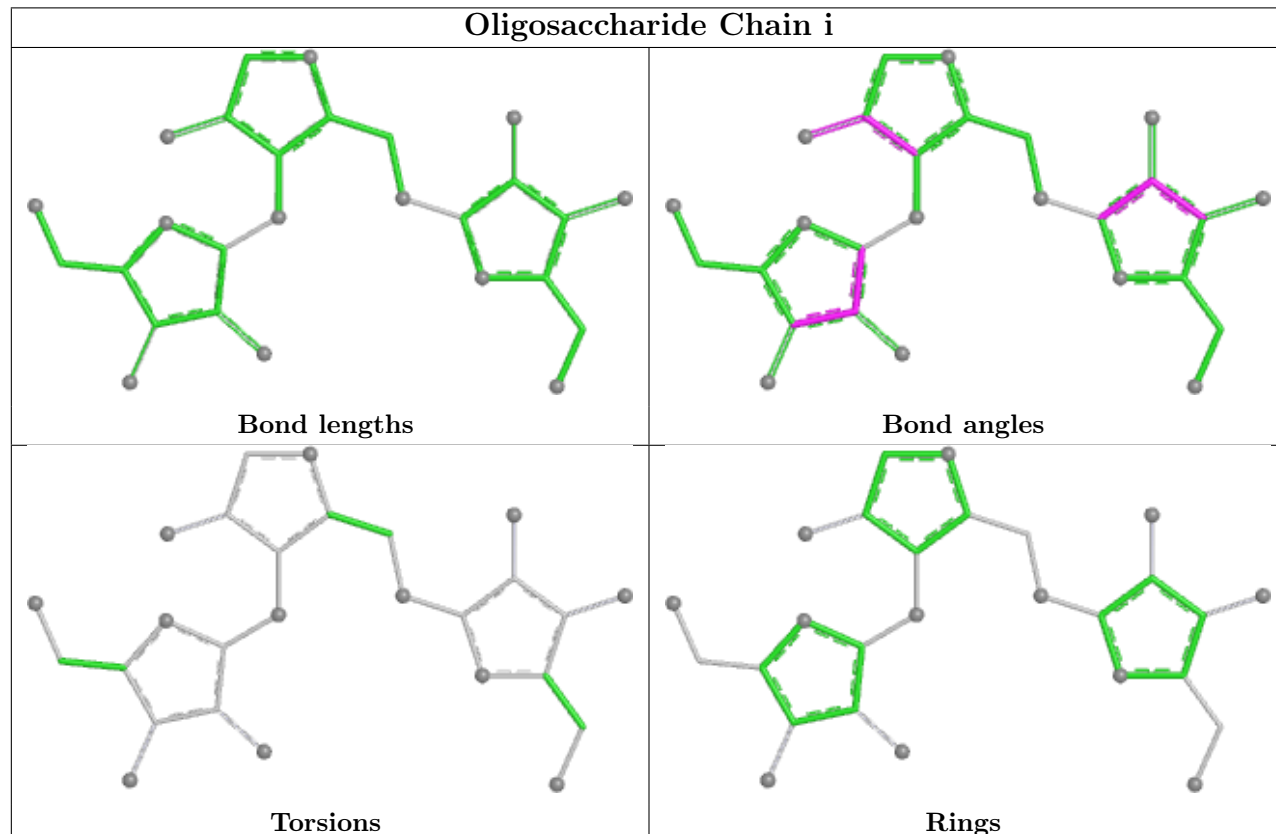
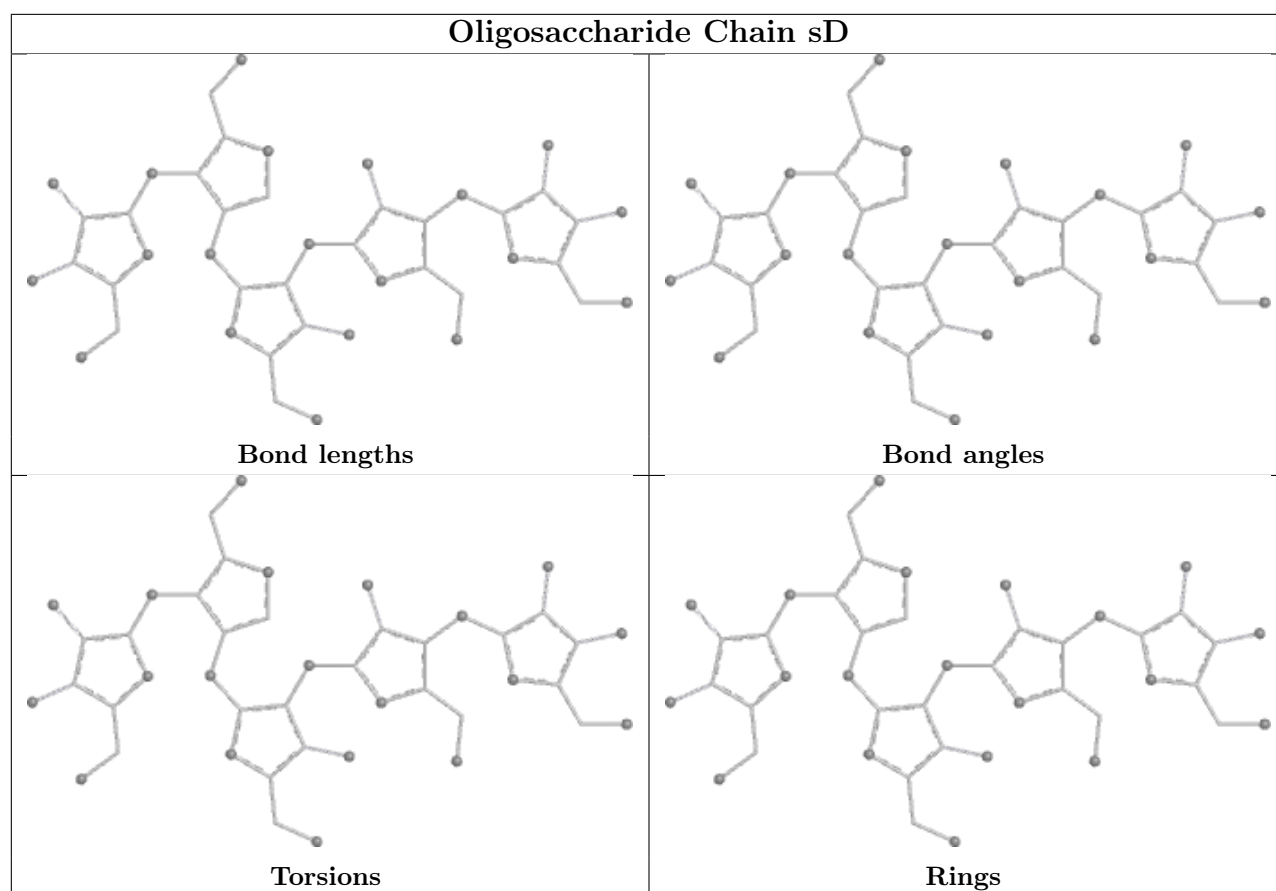
Oligosaccharide Chain mC**Oligosaccharide Chain vC**

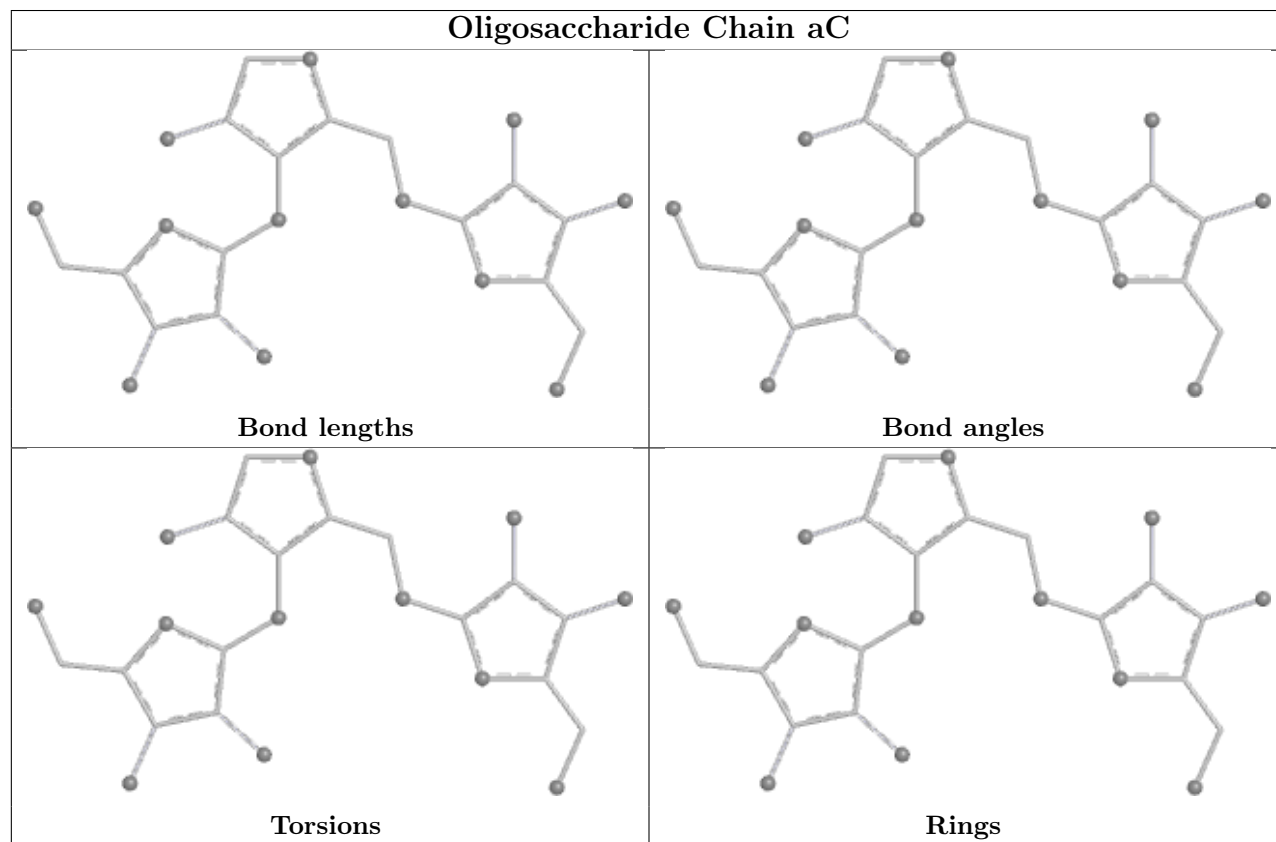
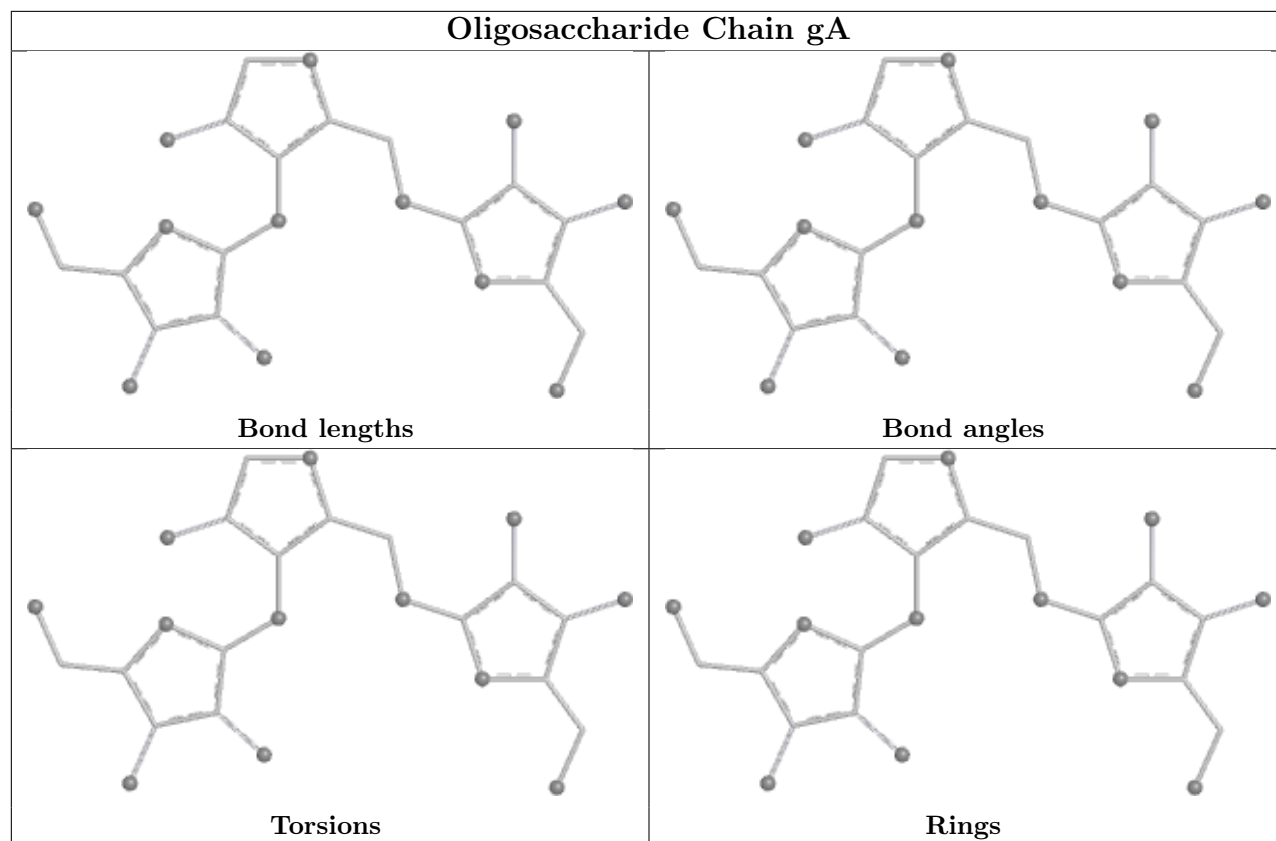
Oligosaccharide Chain PD

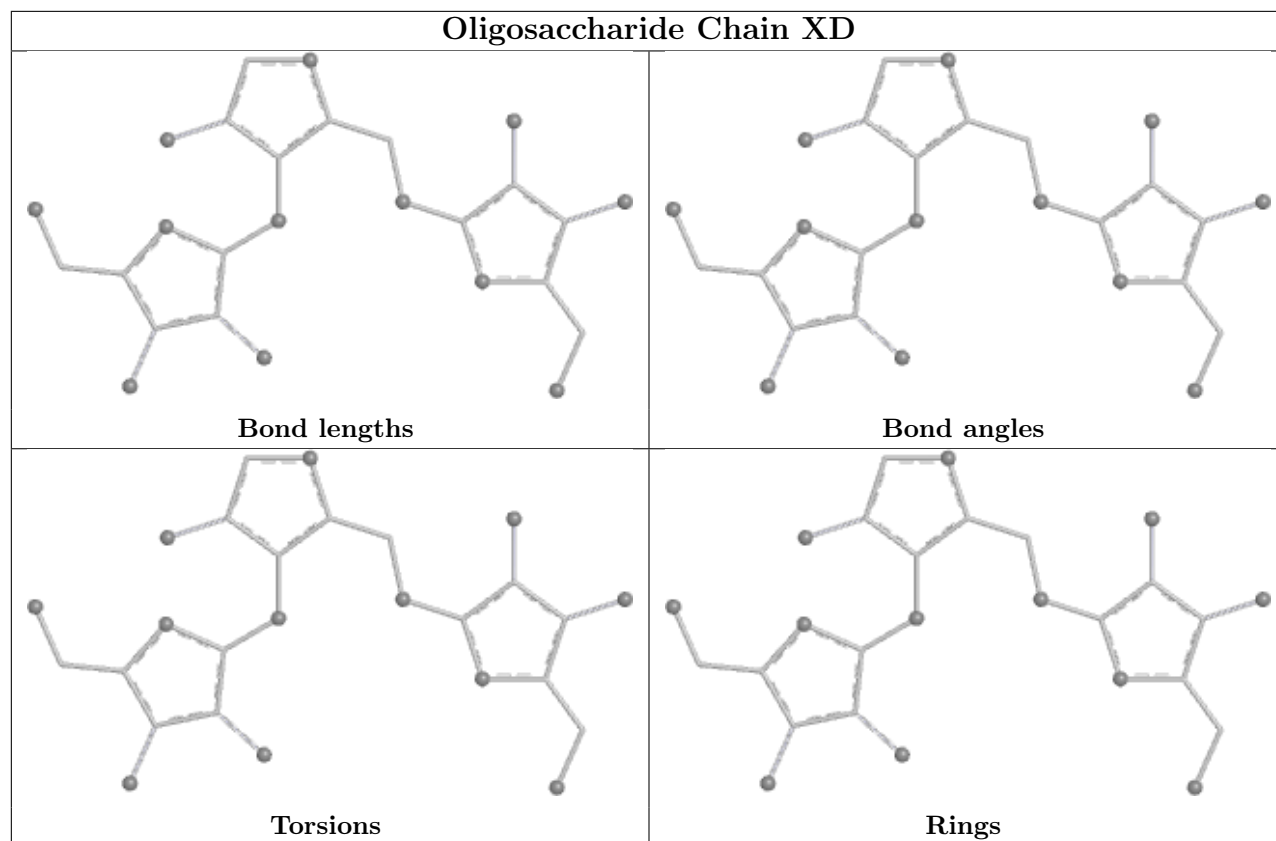


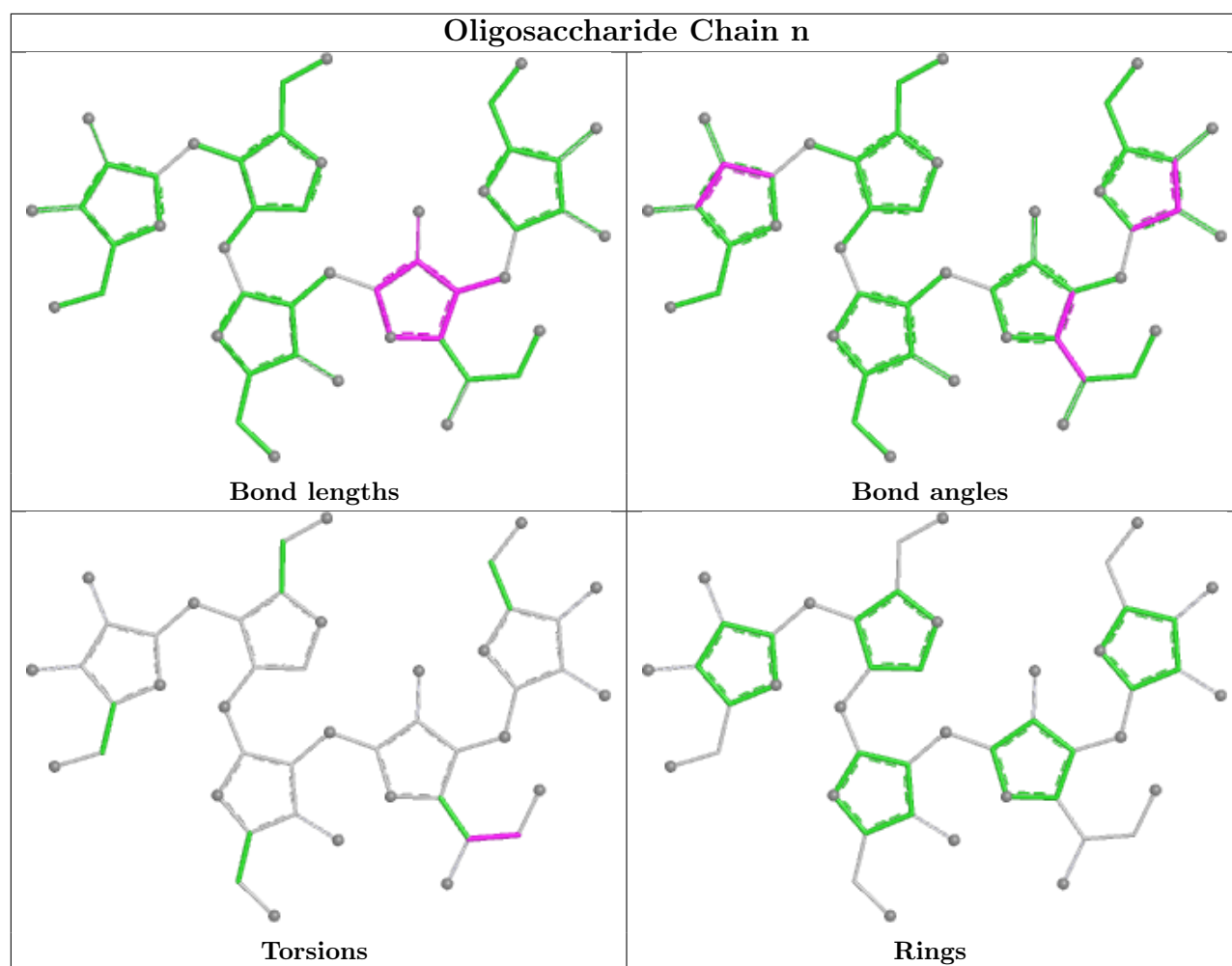
Oligosaccharide Chain jD

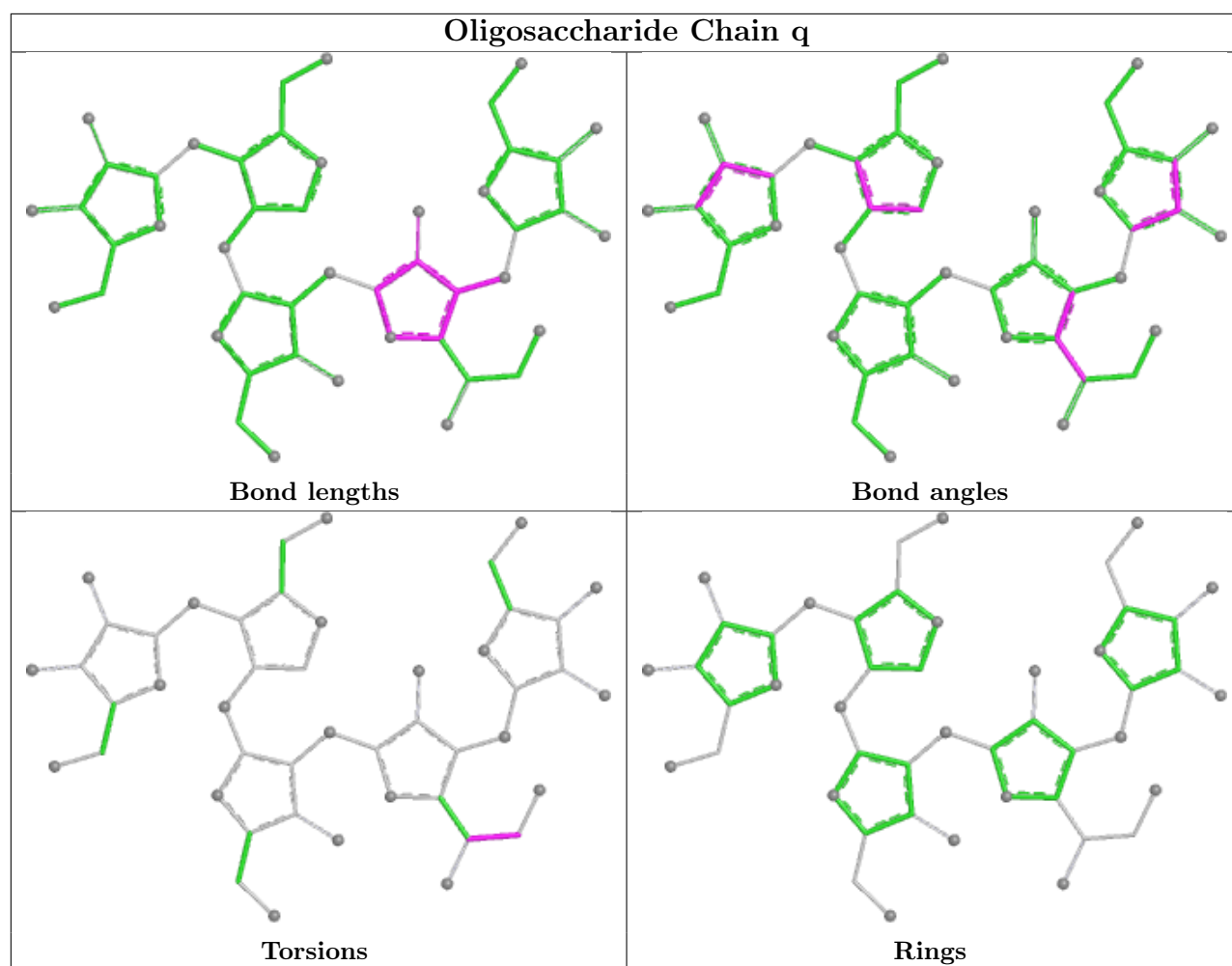


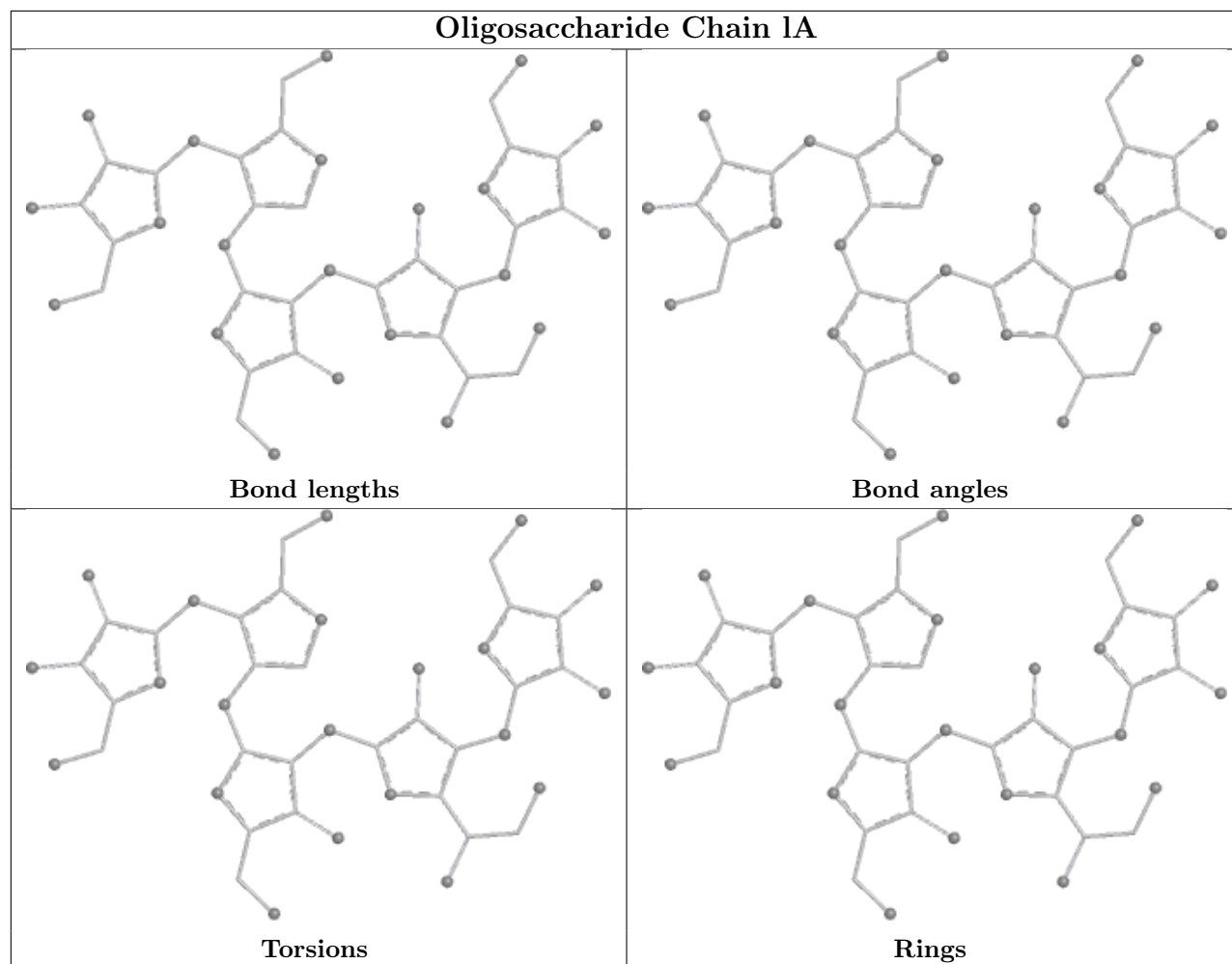


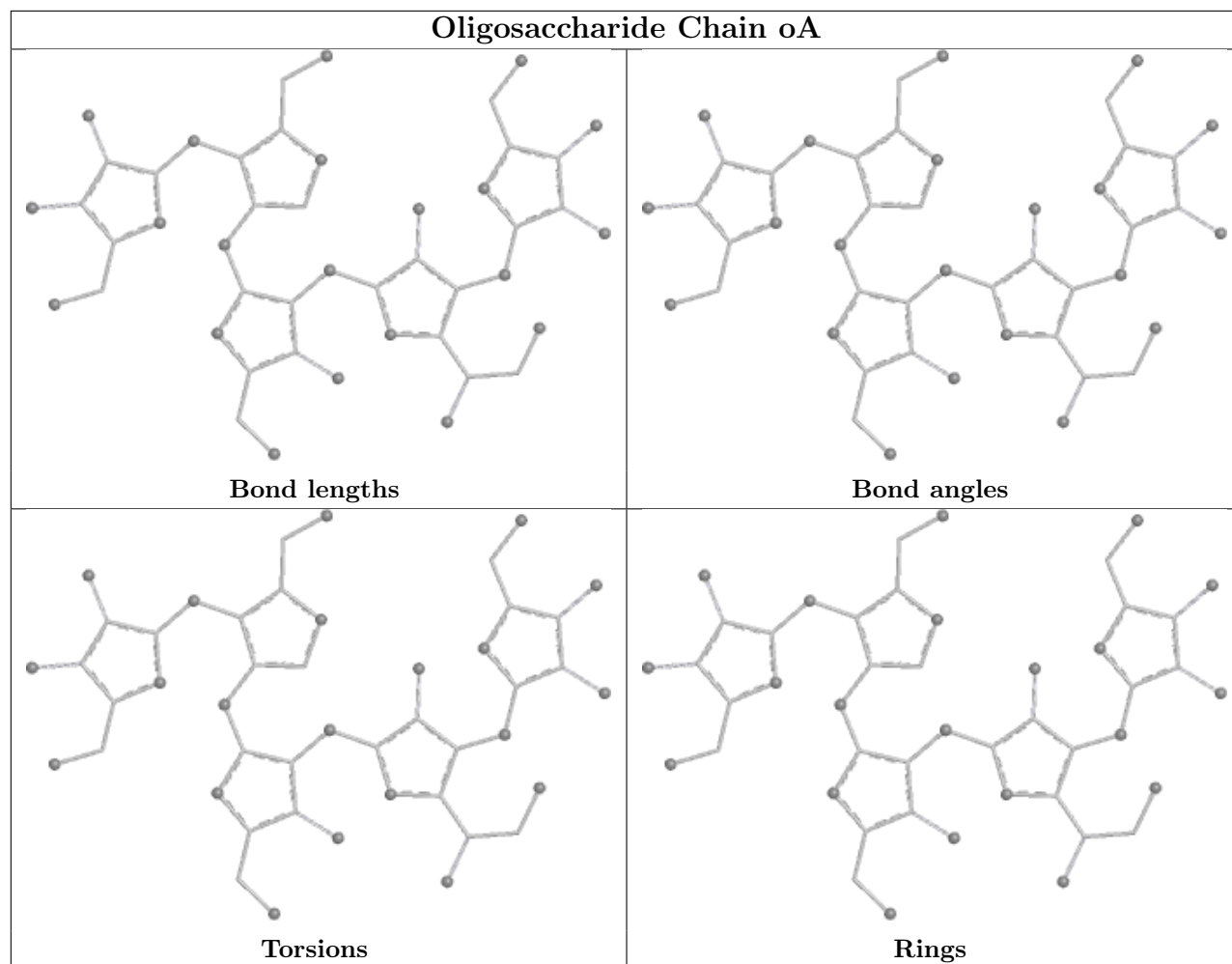


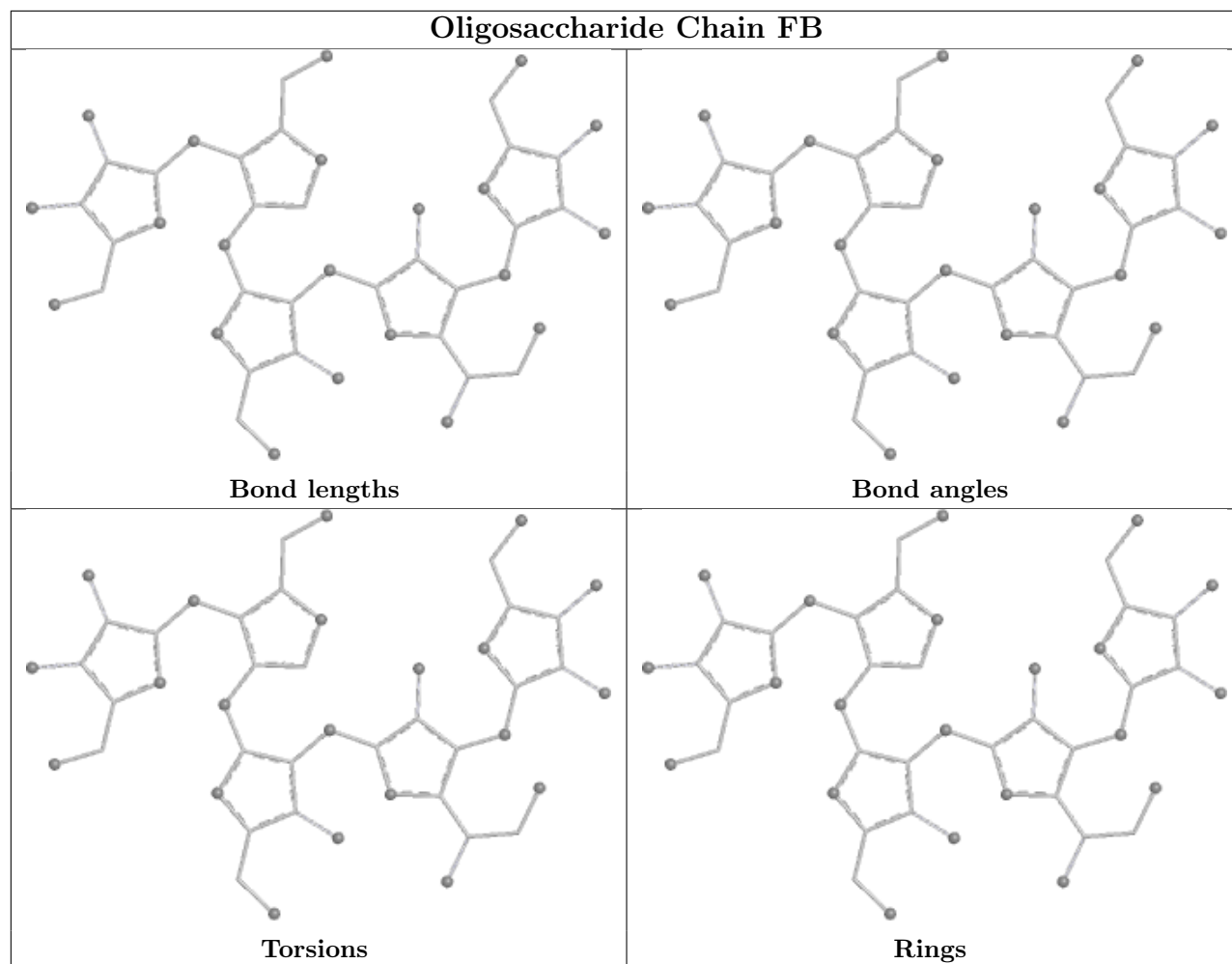


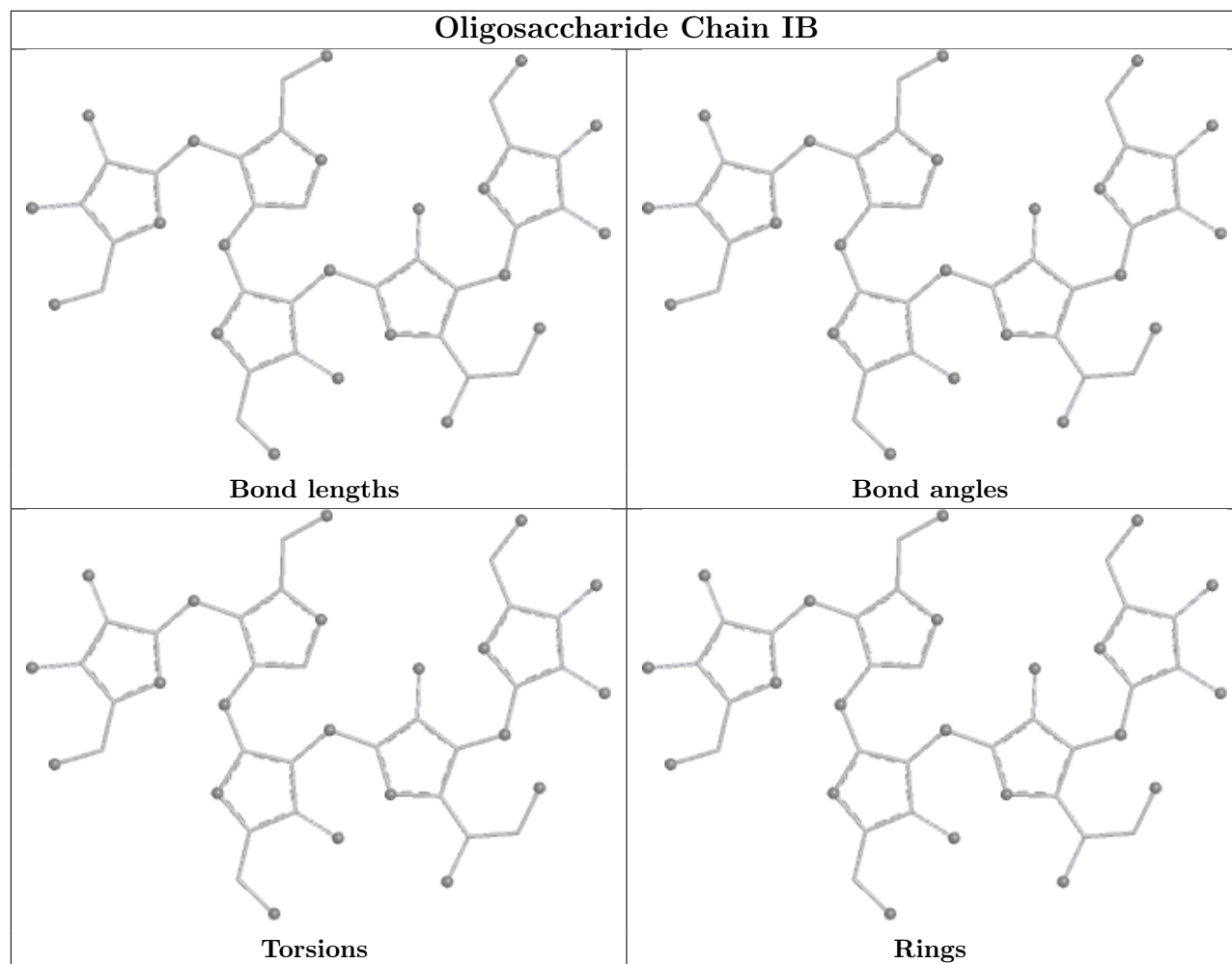


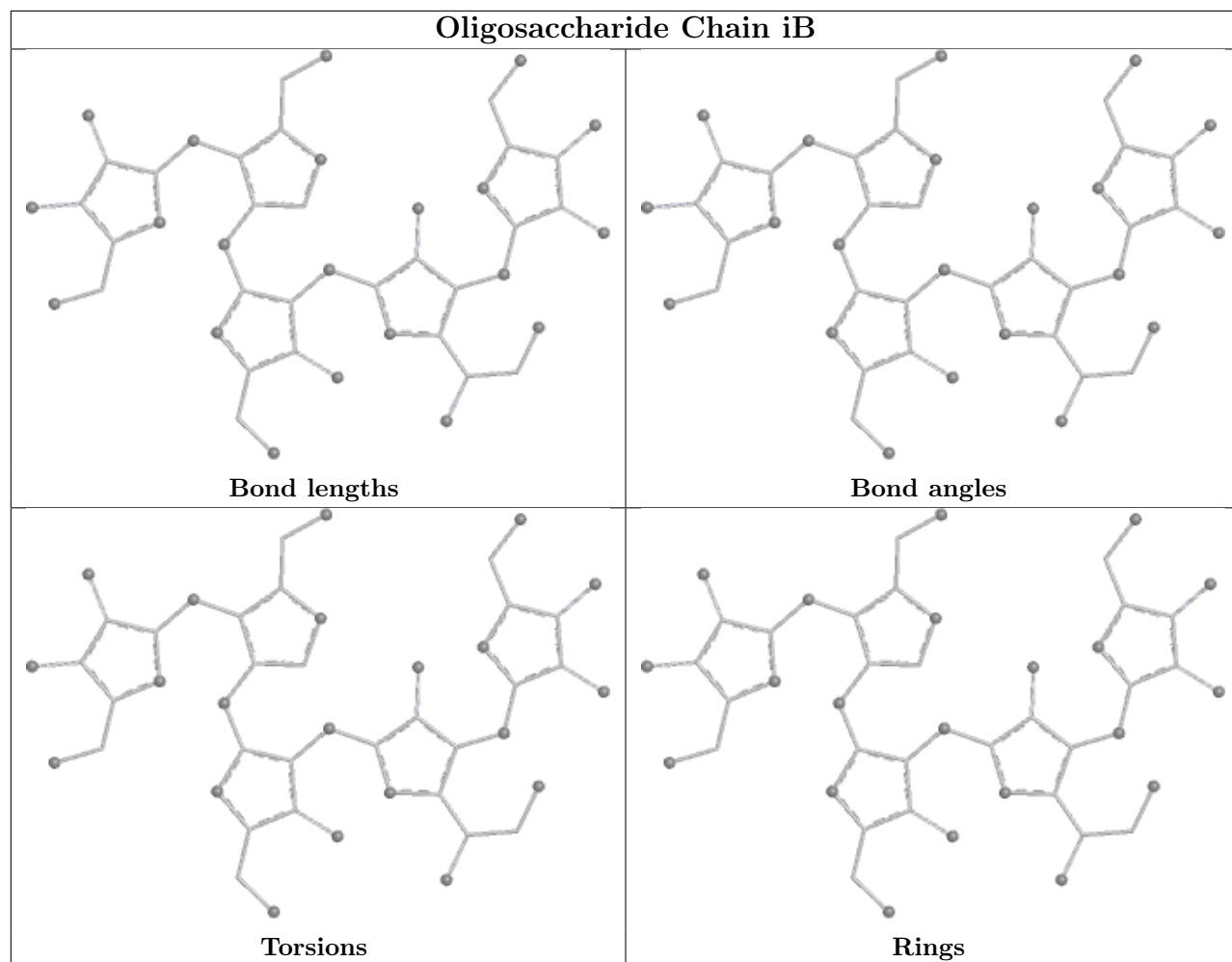


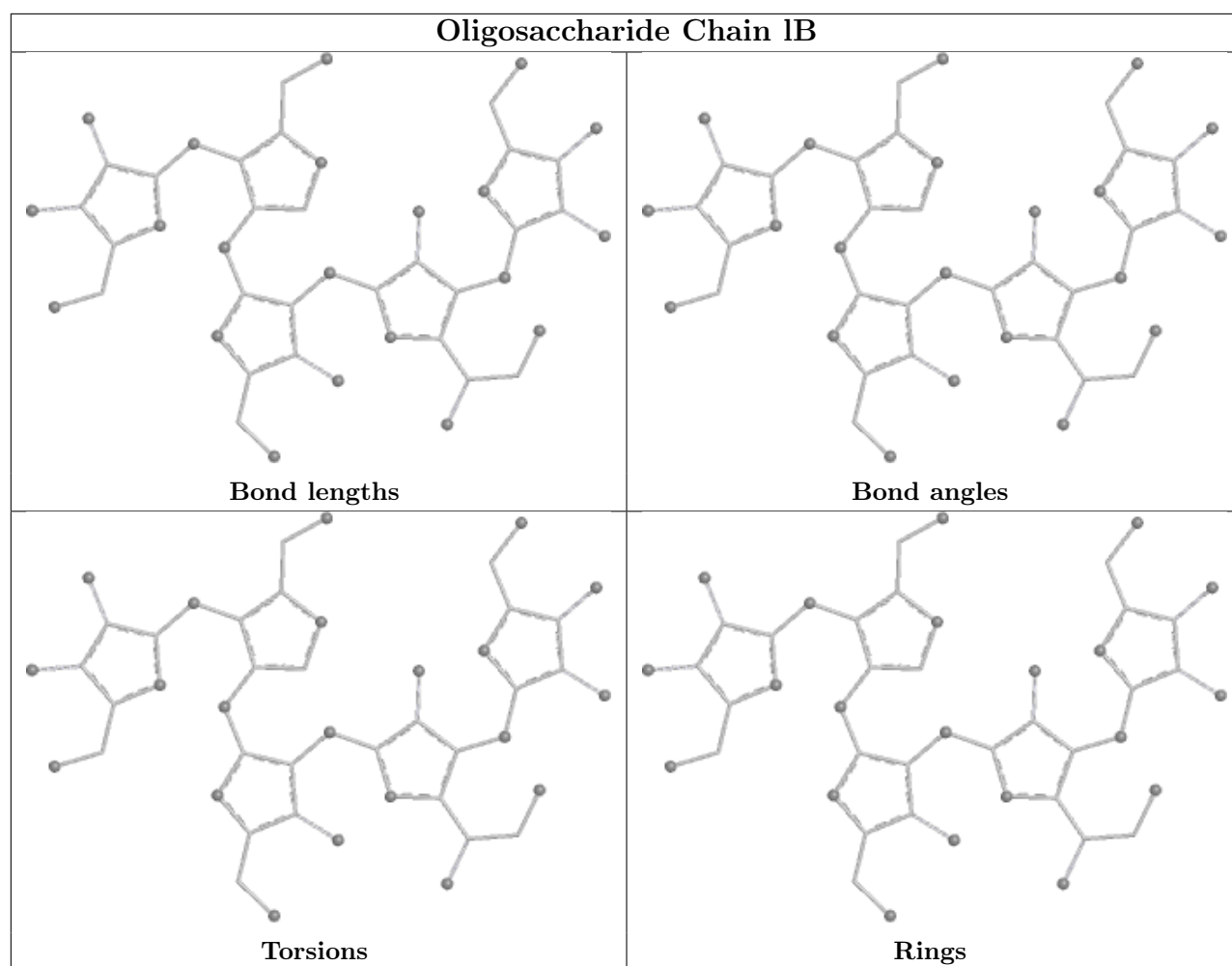


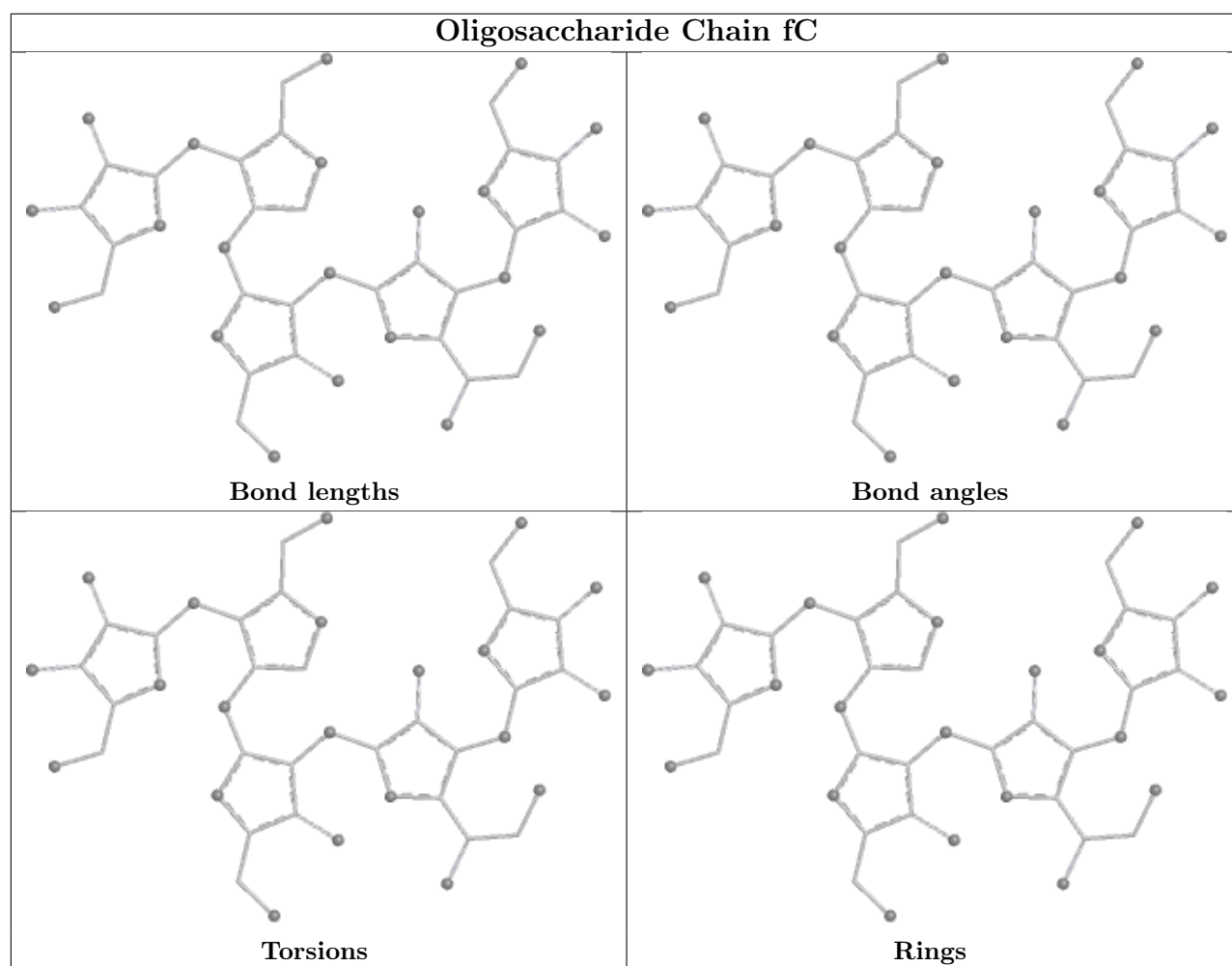


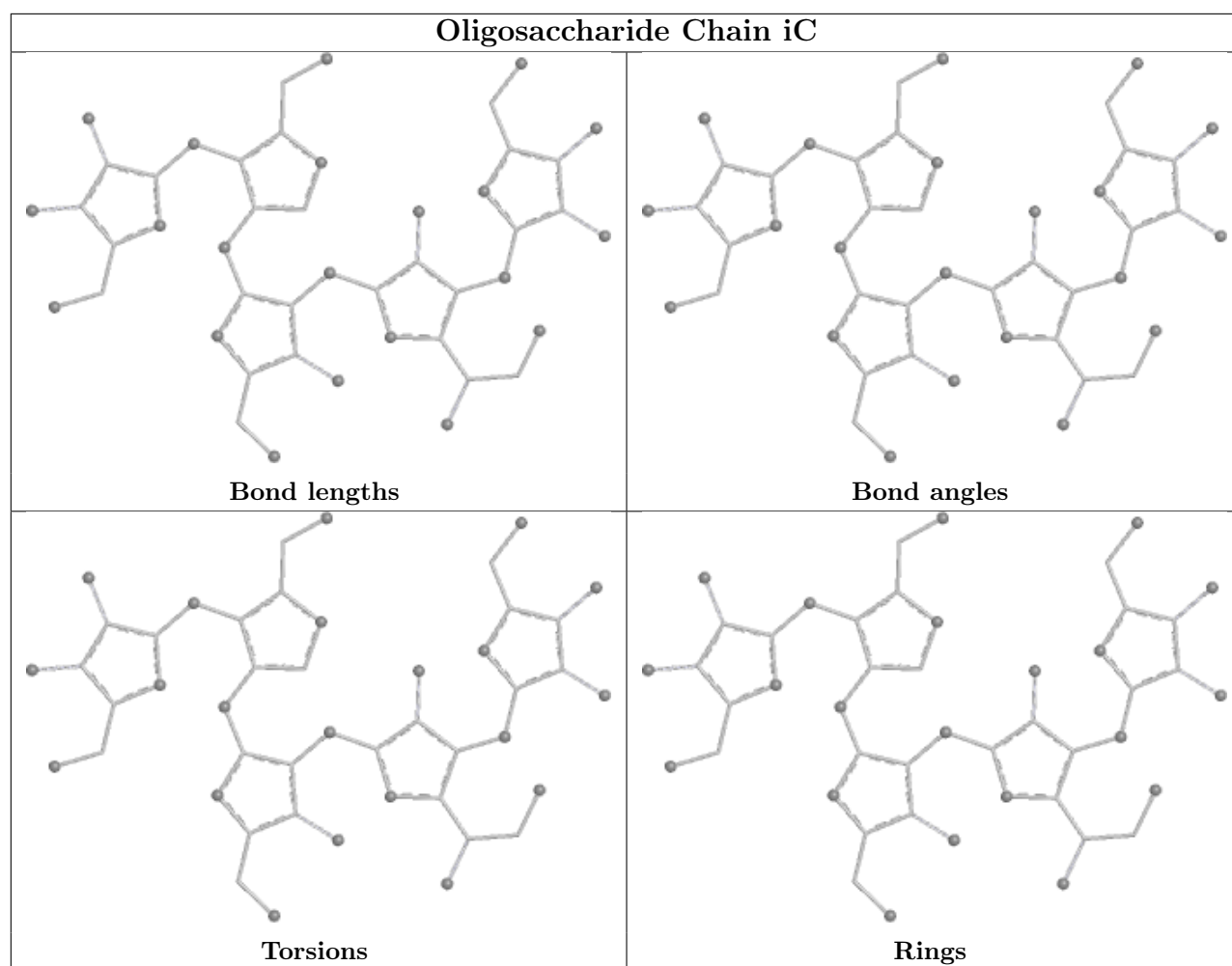


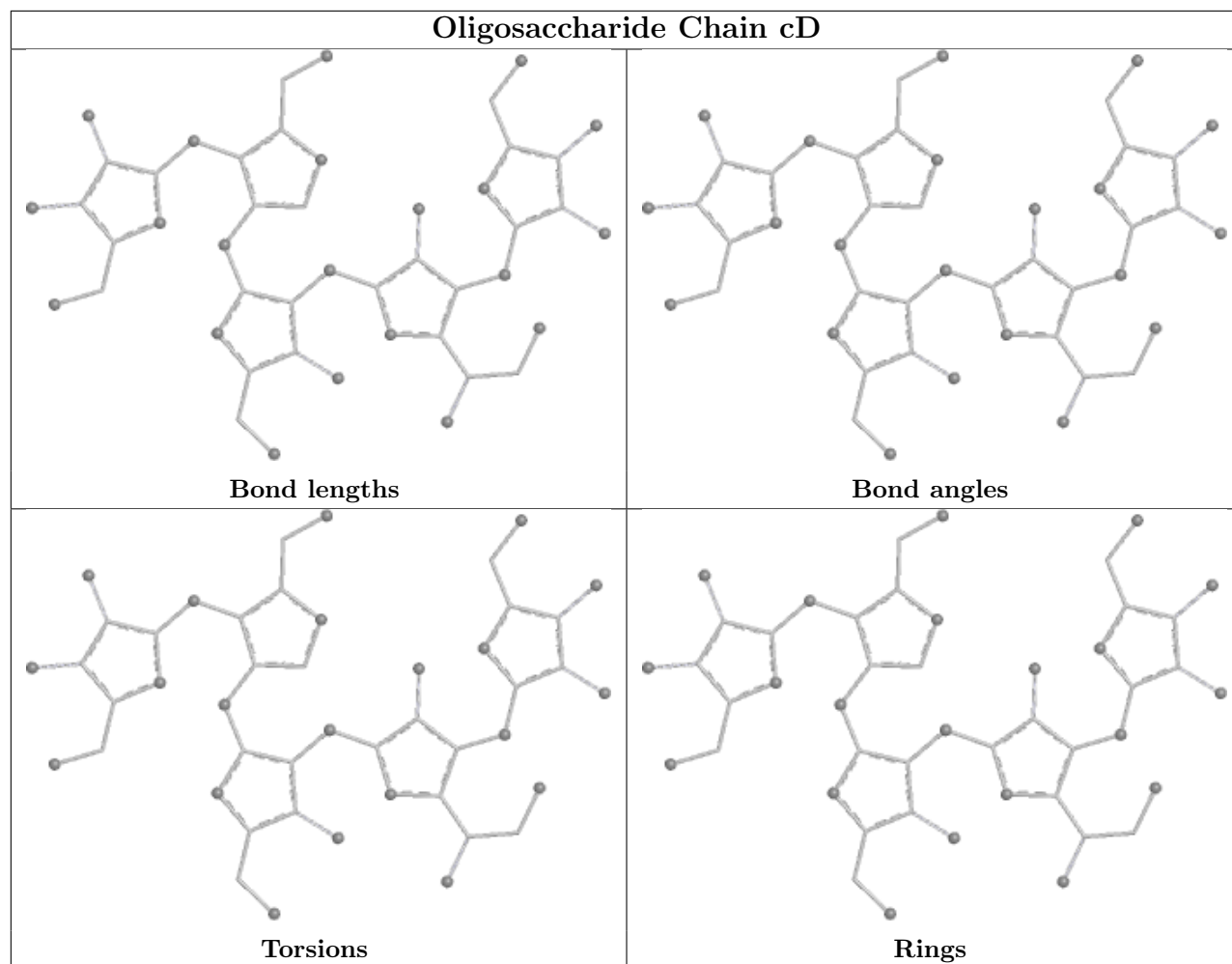


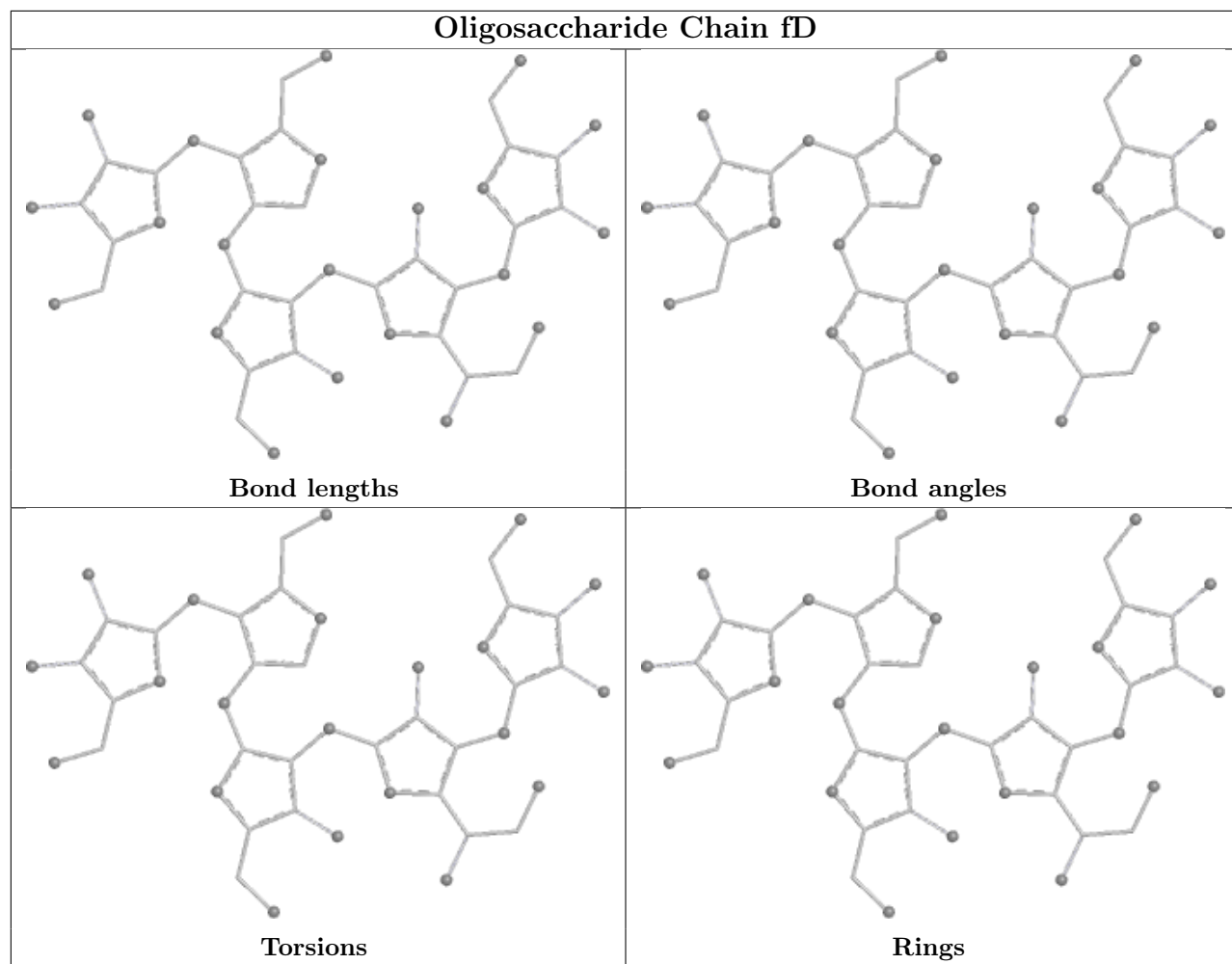


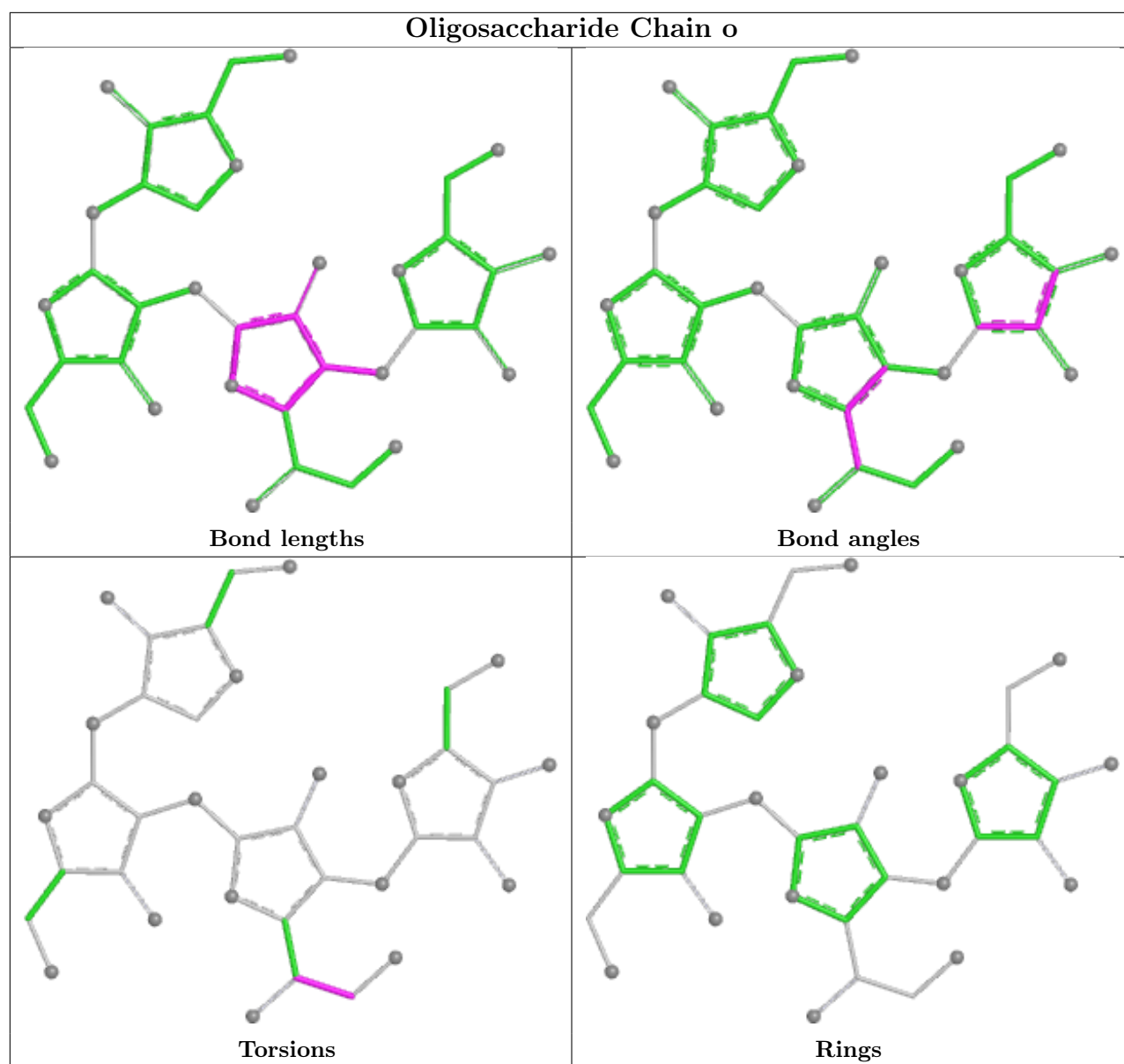


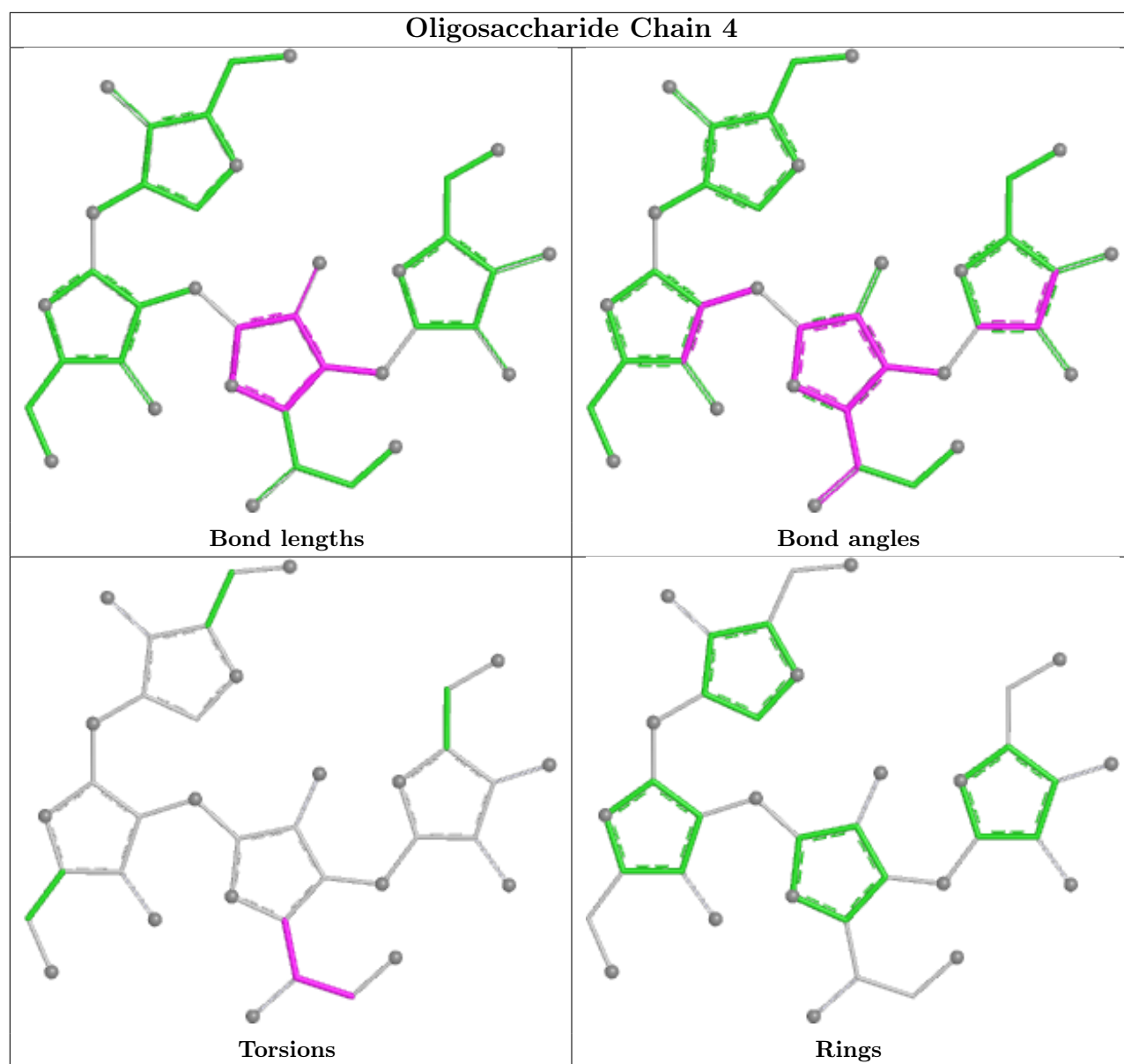


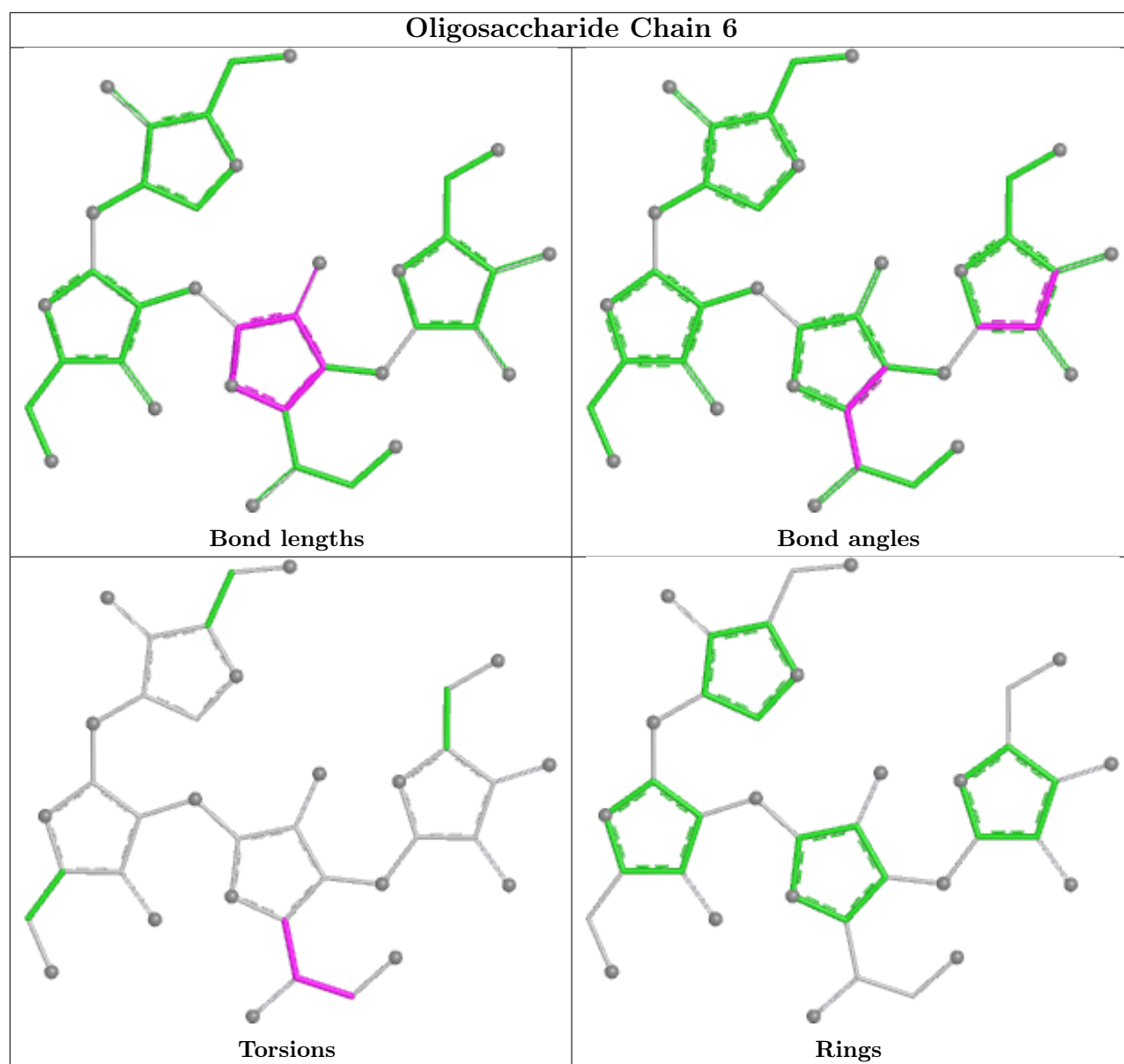


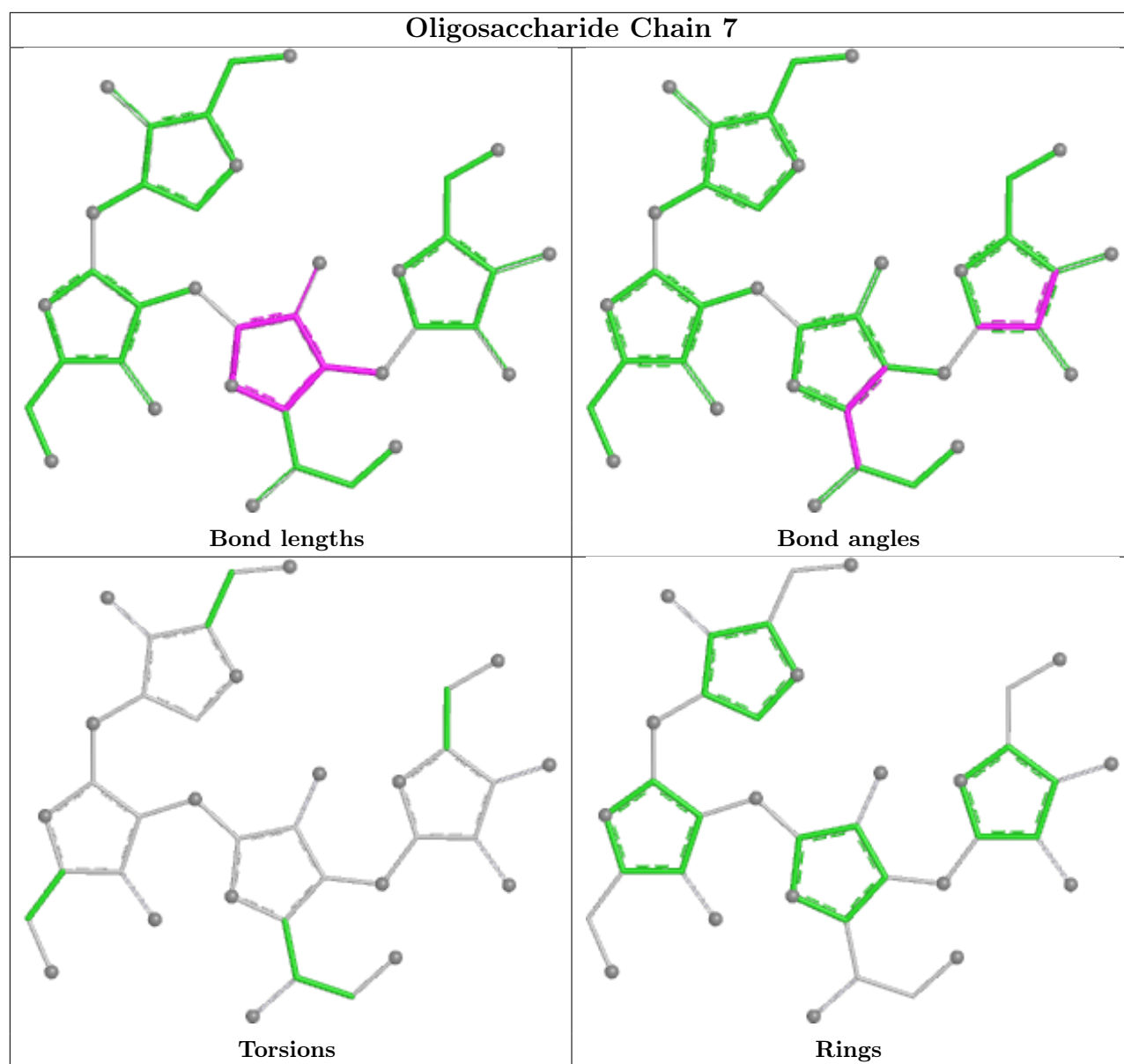


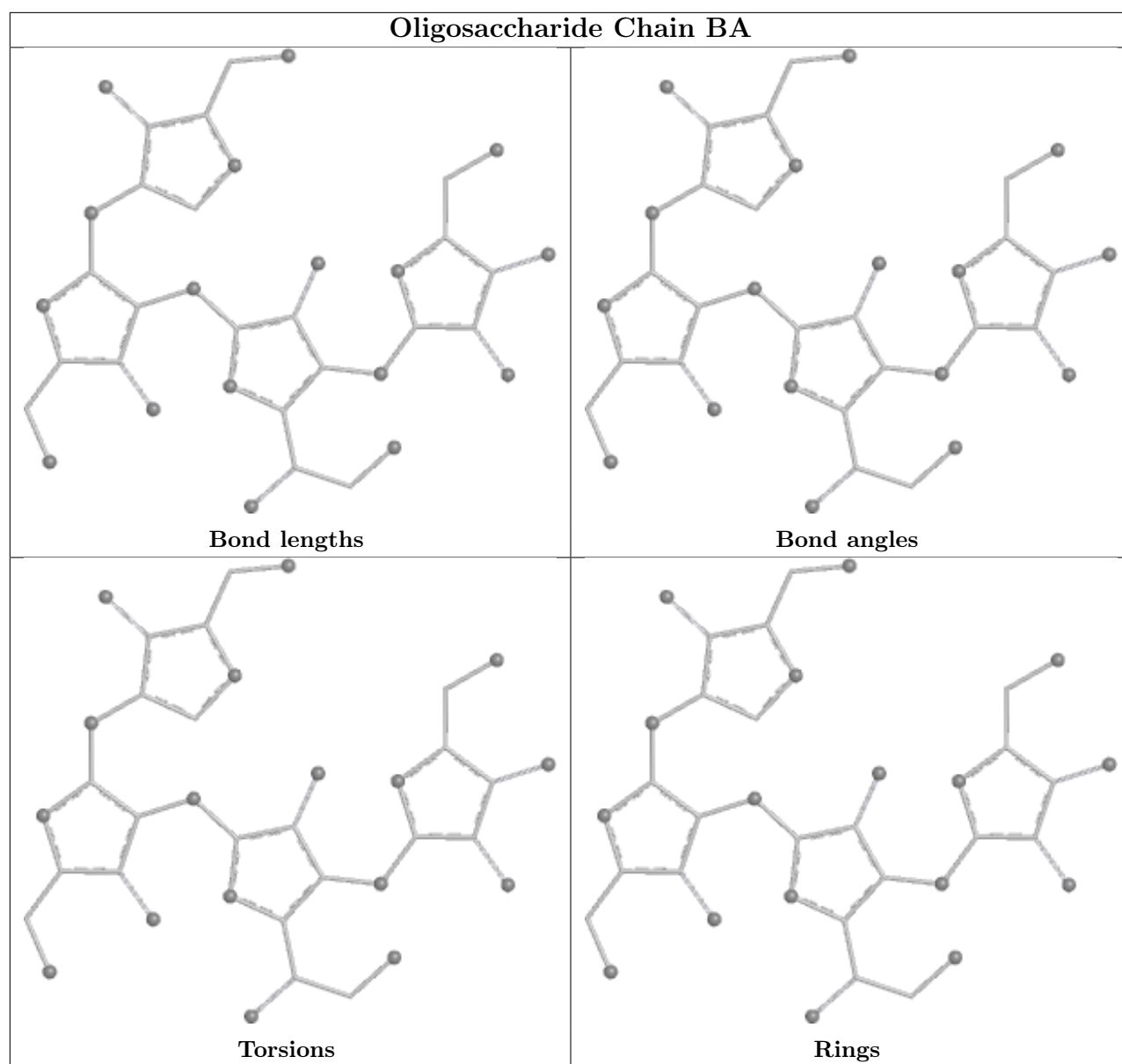


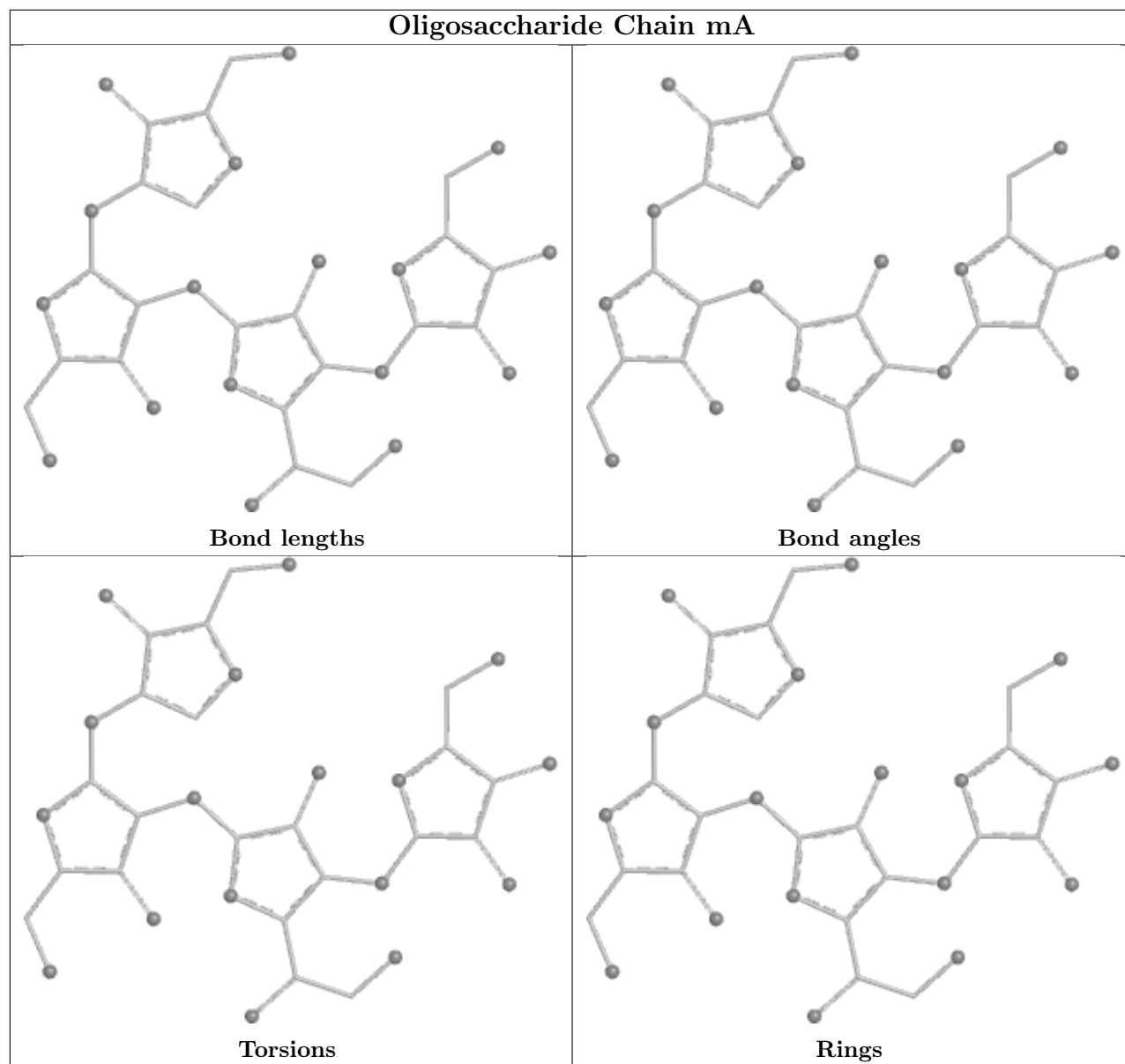


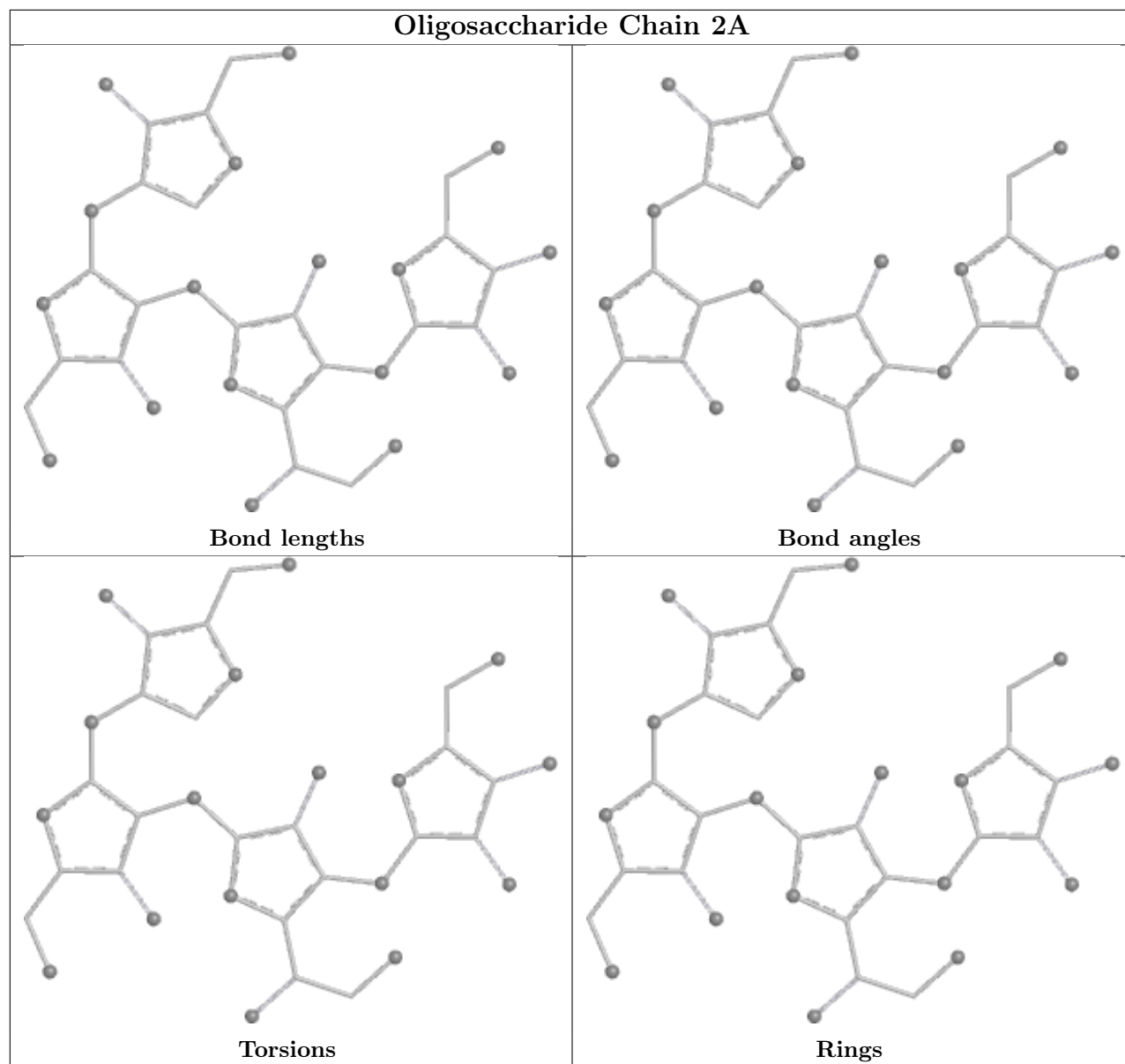


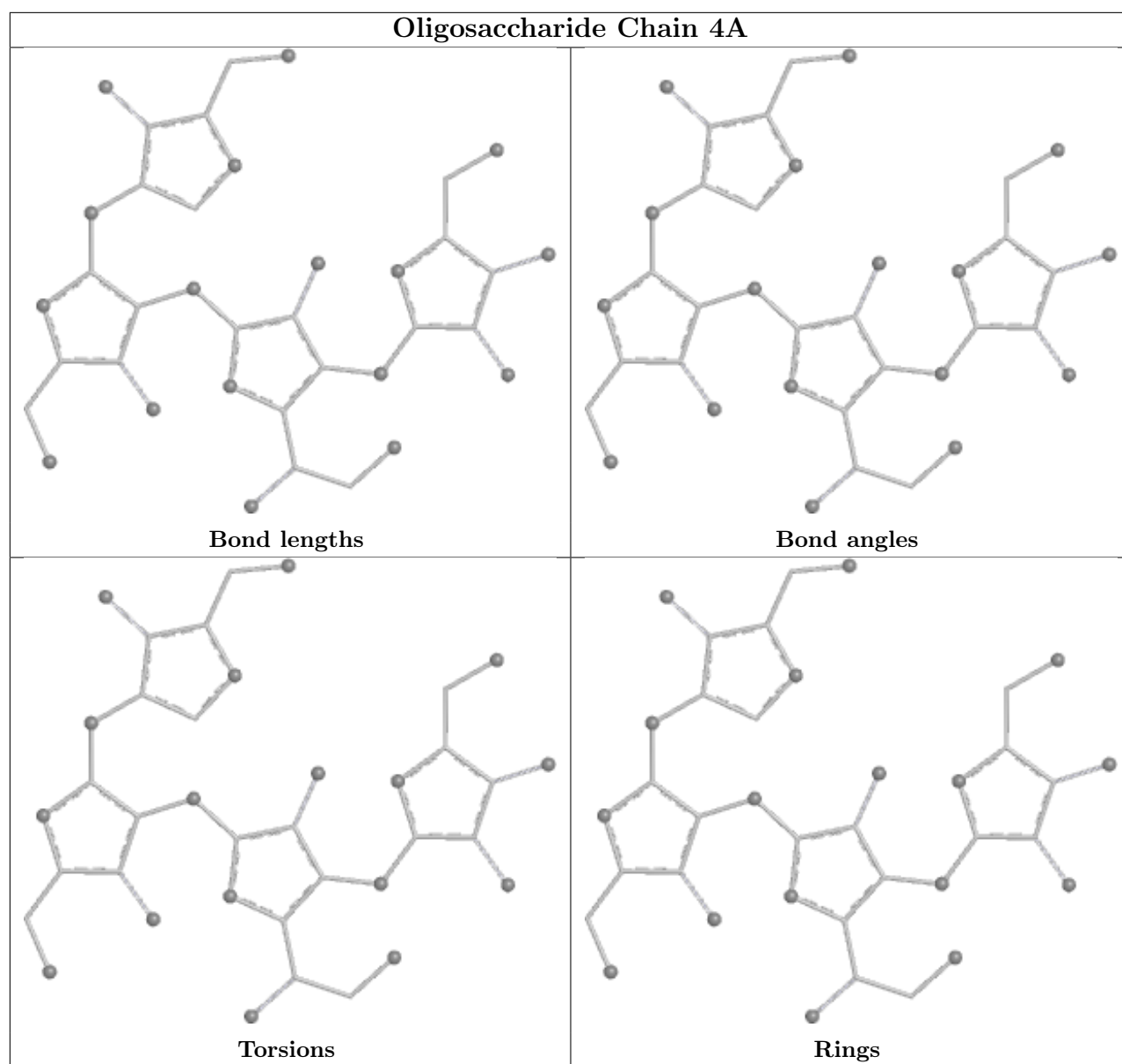


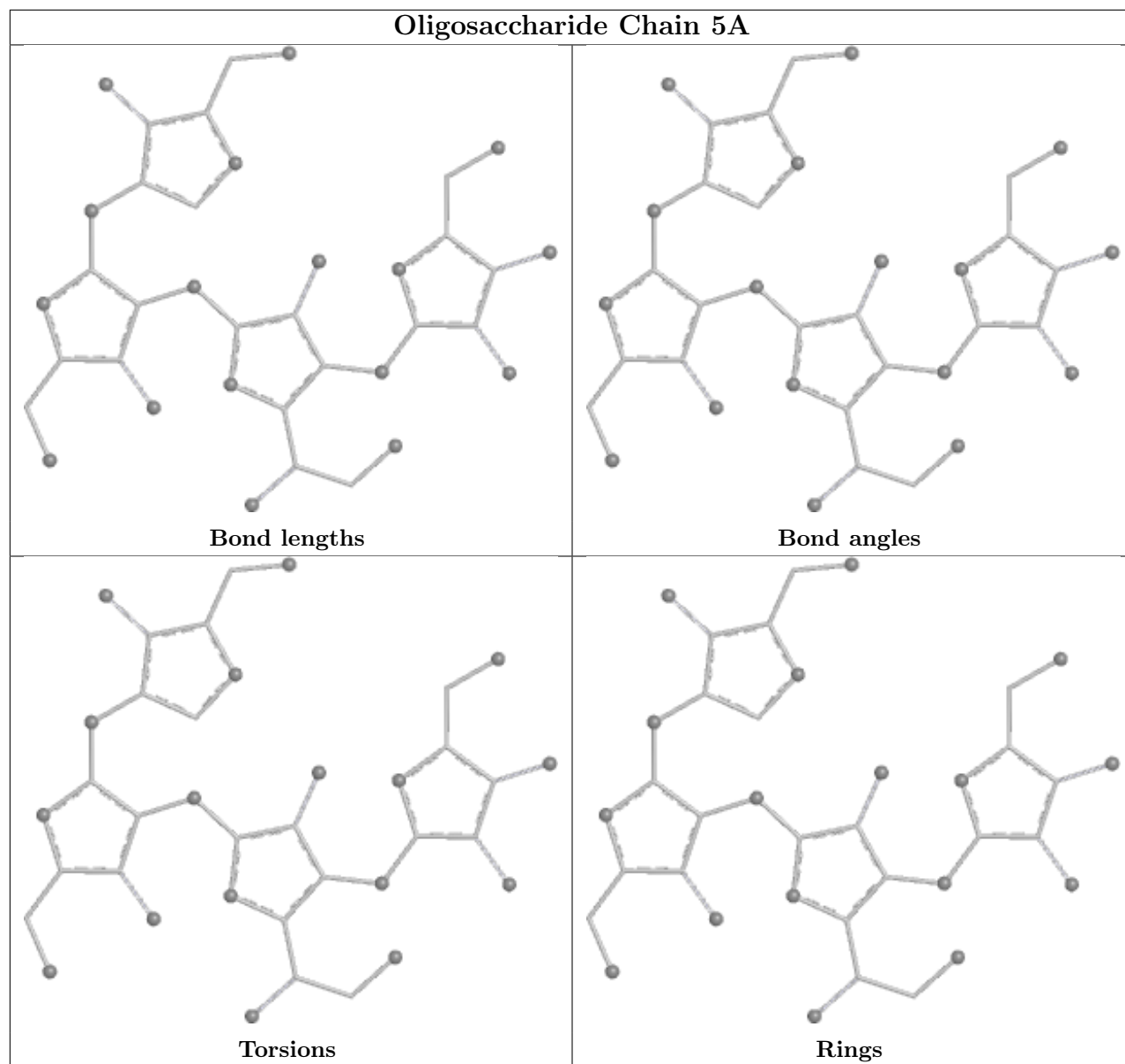


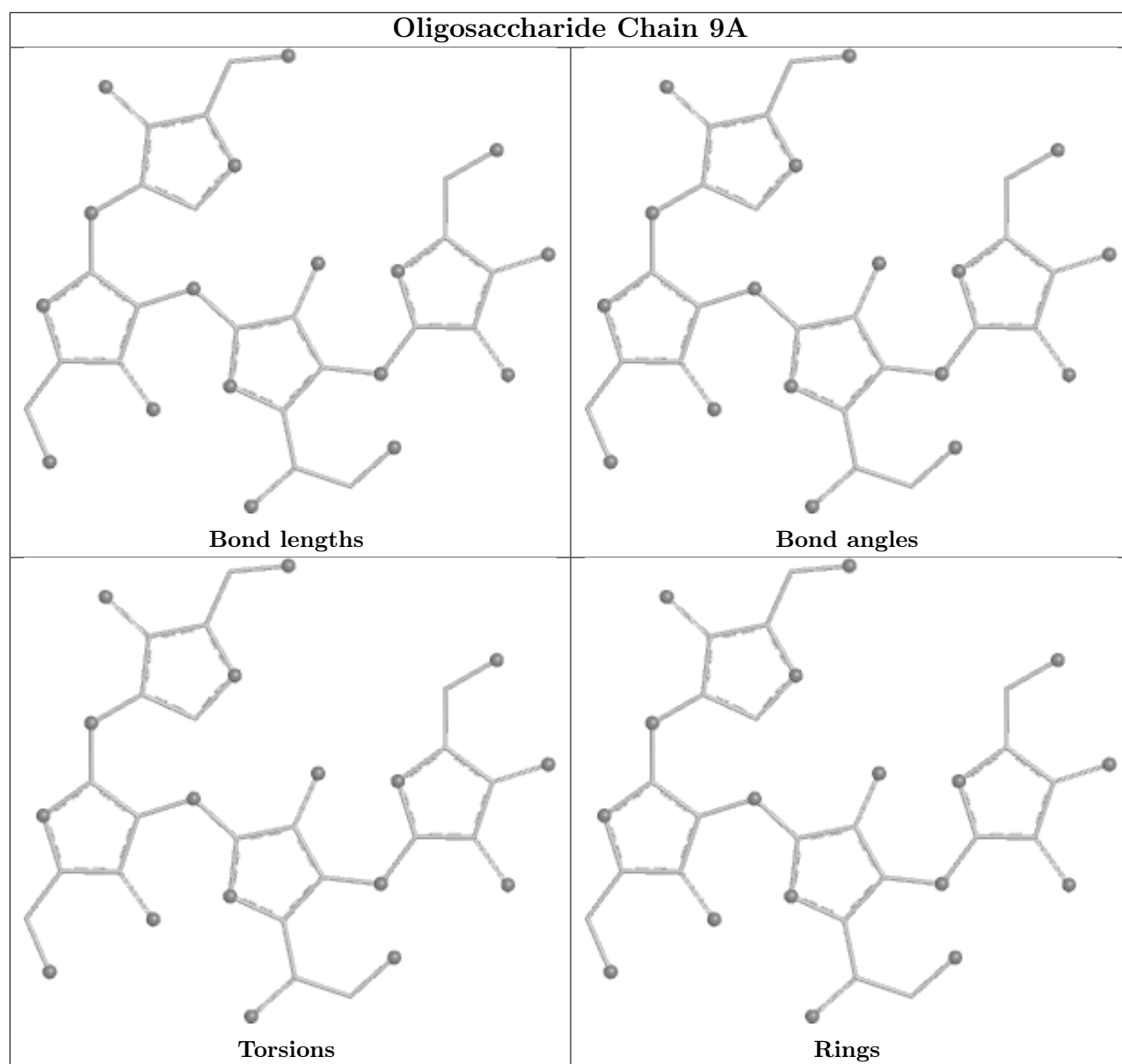


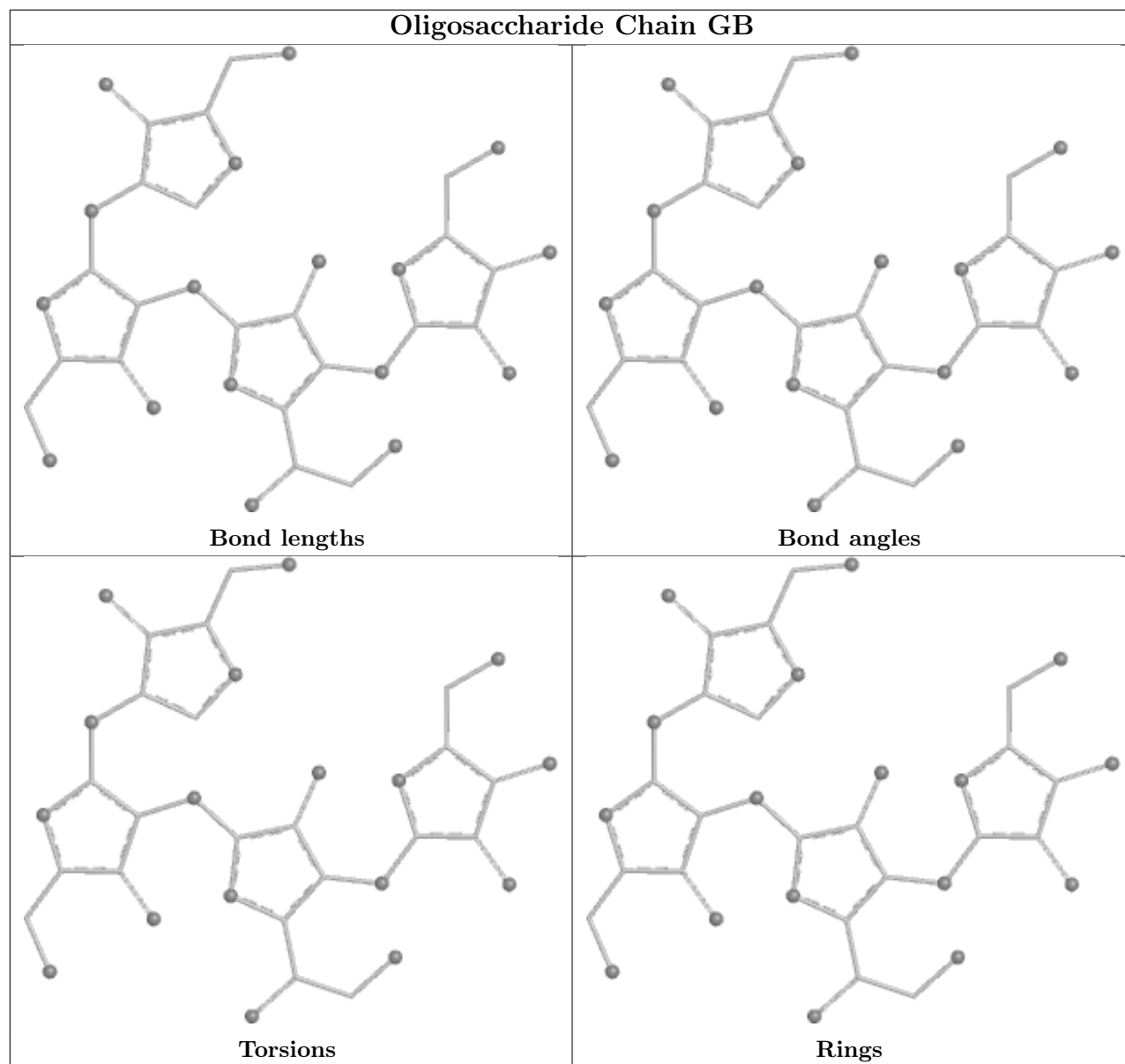


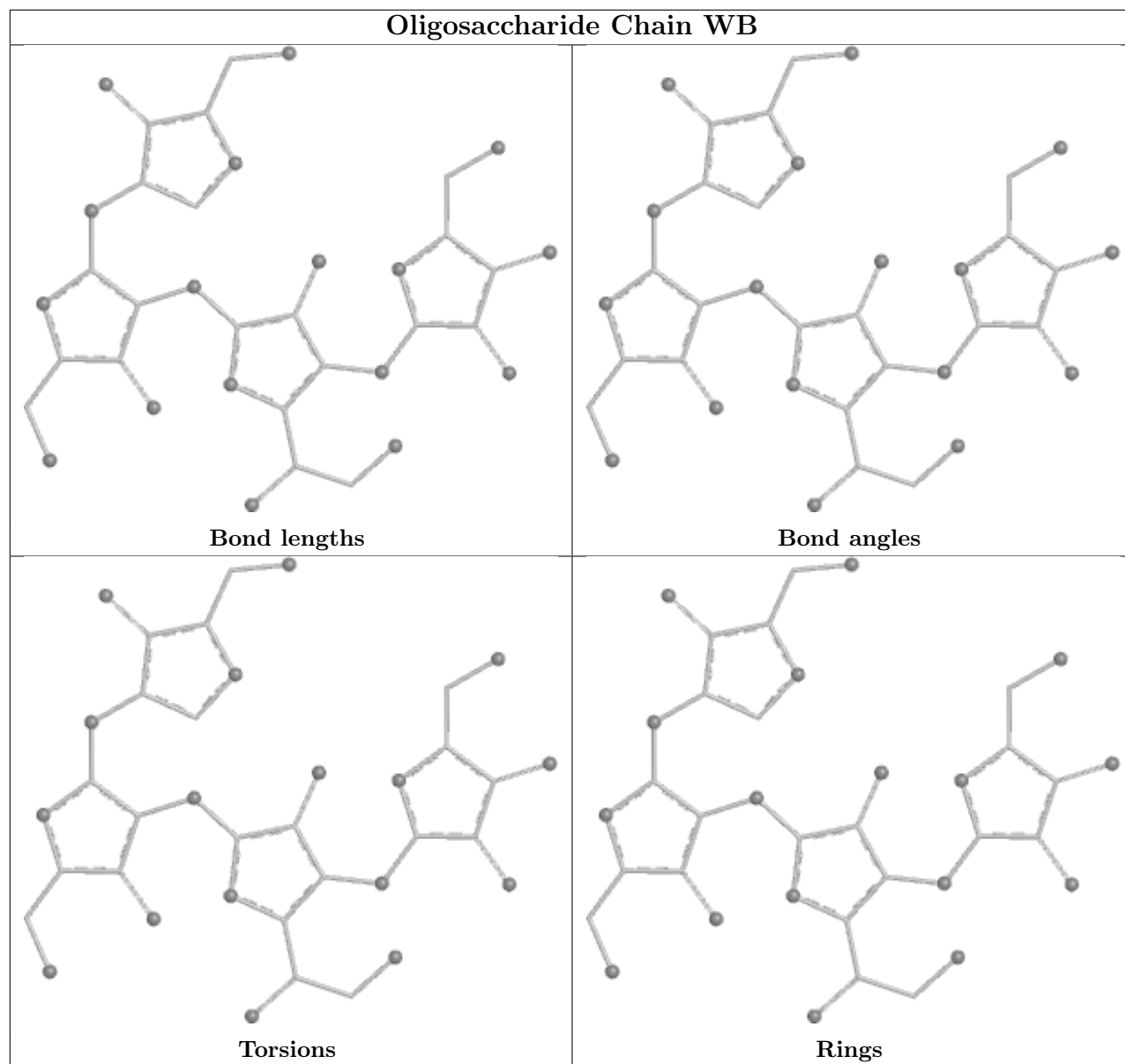


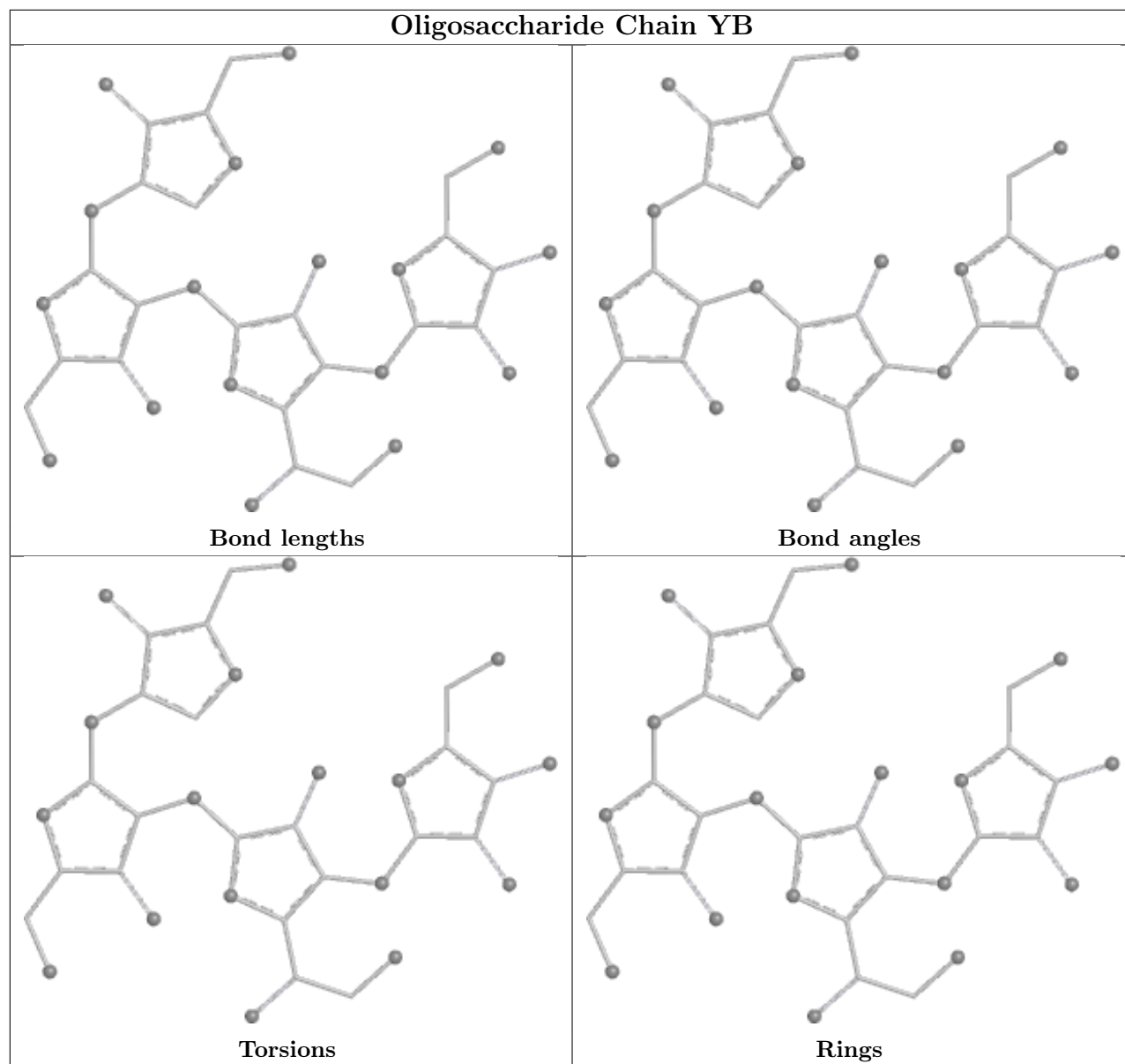


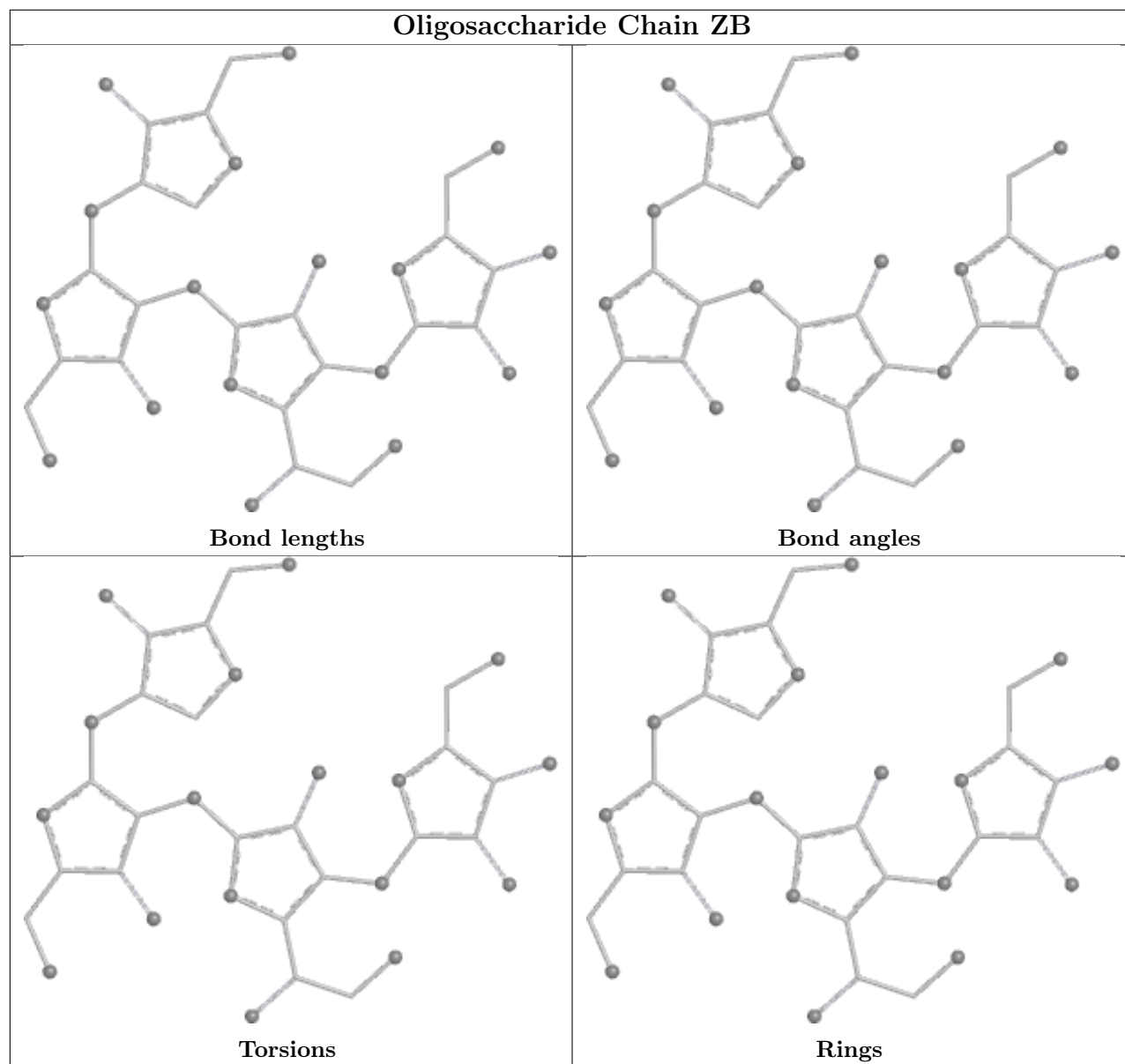


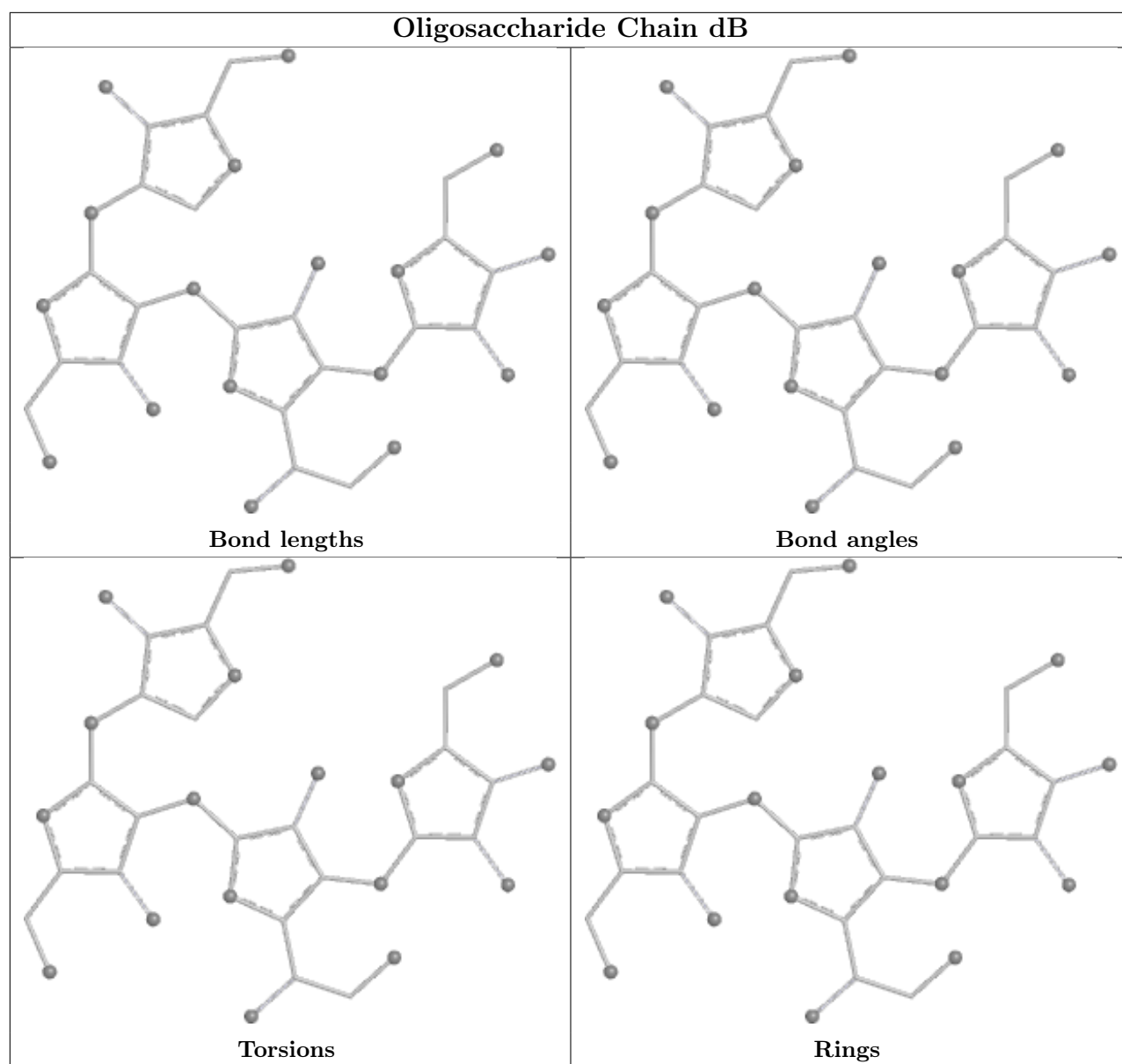


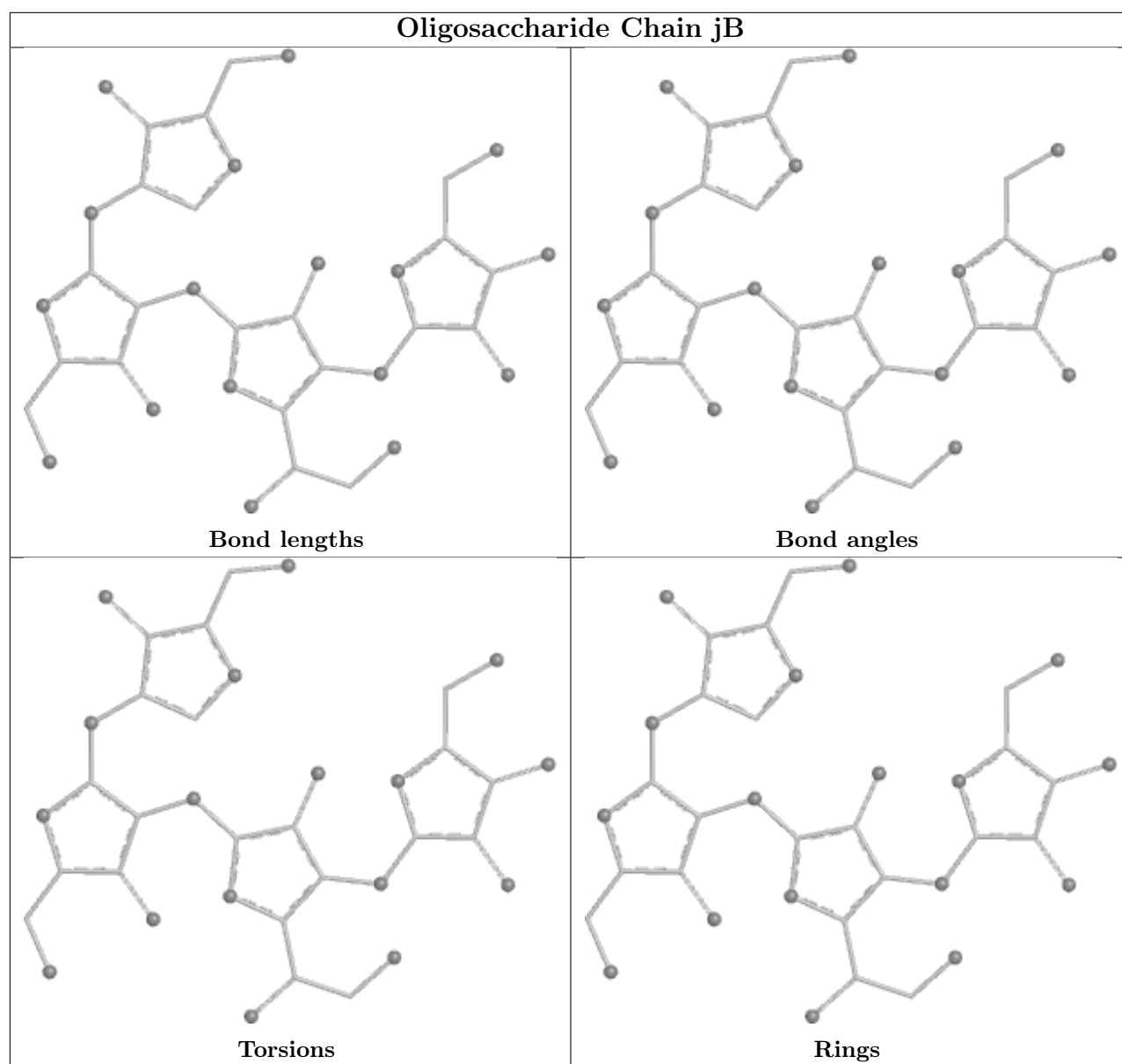


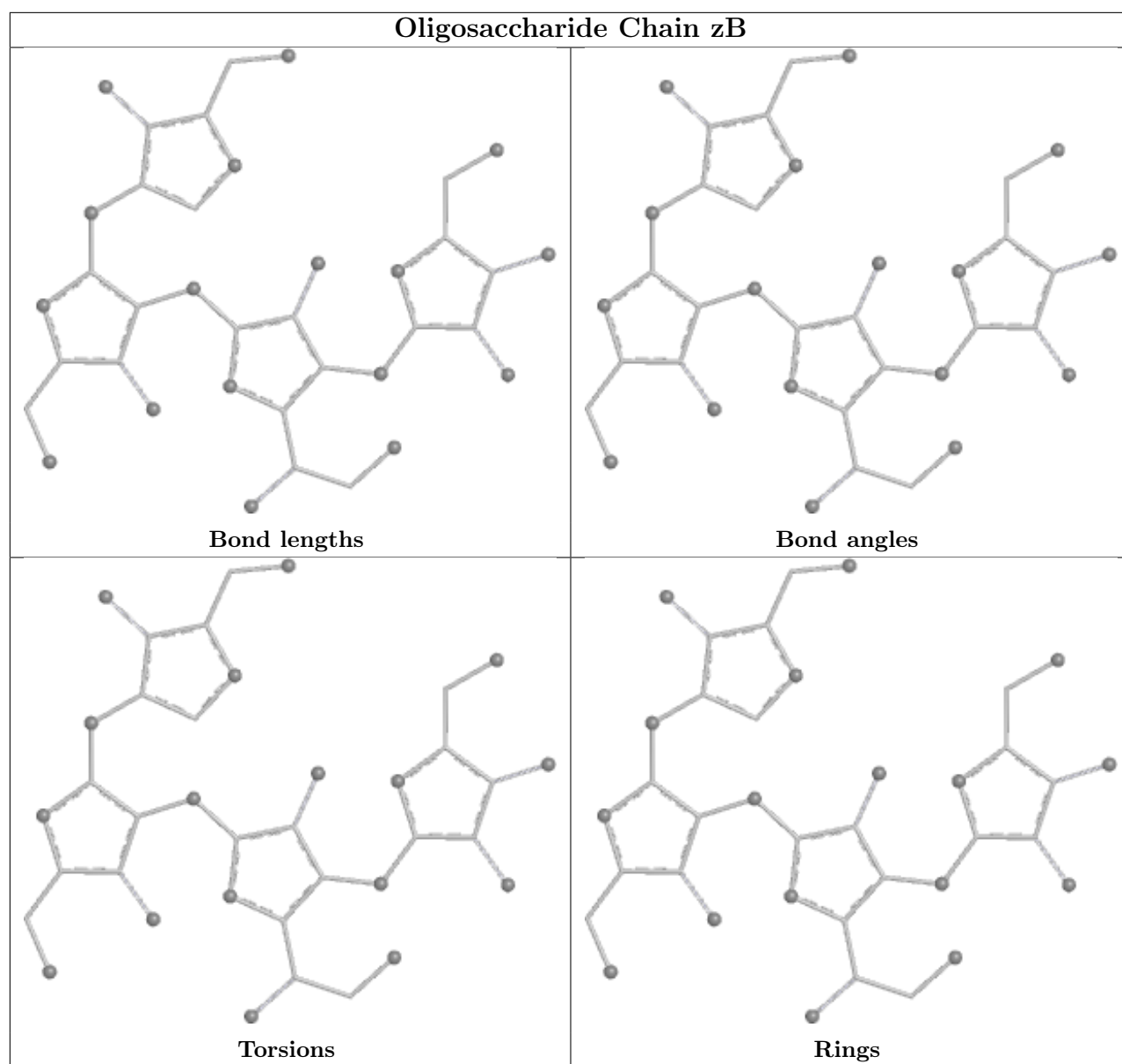


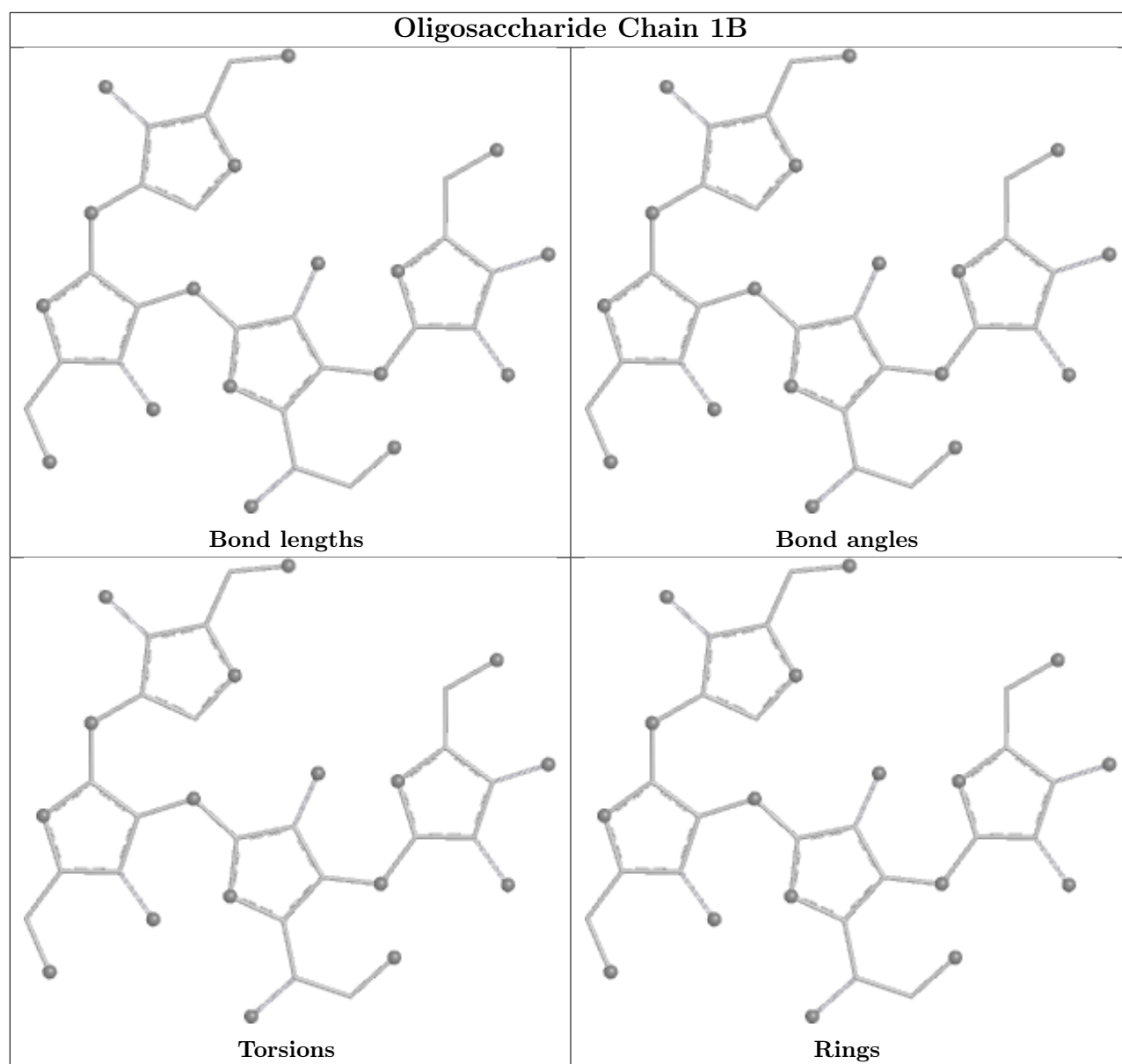
Oligosaccharide Chain YB

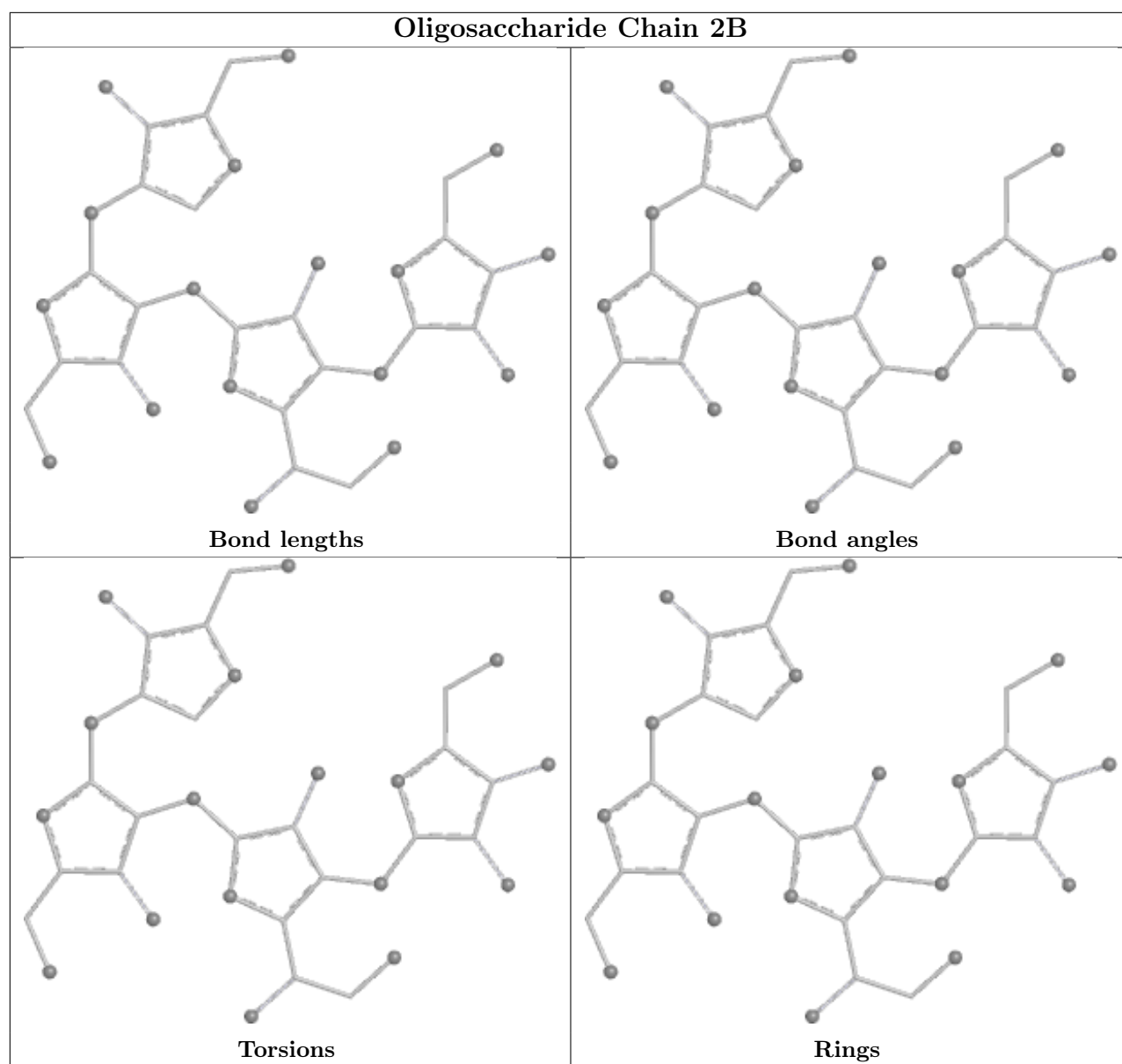


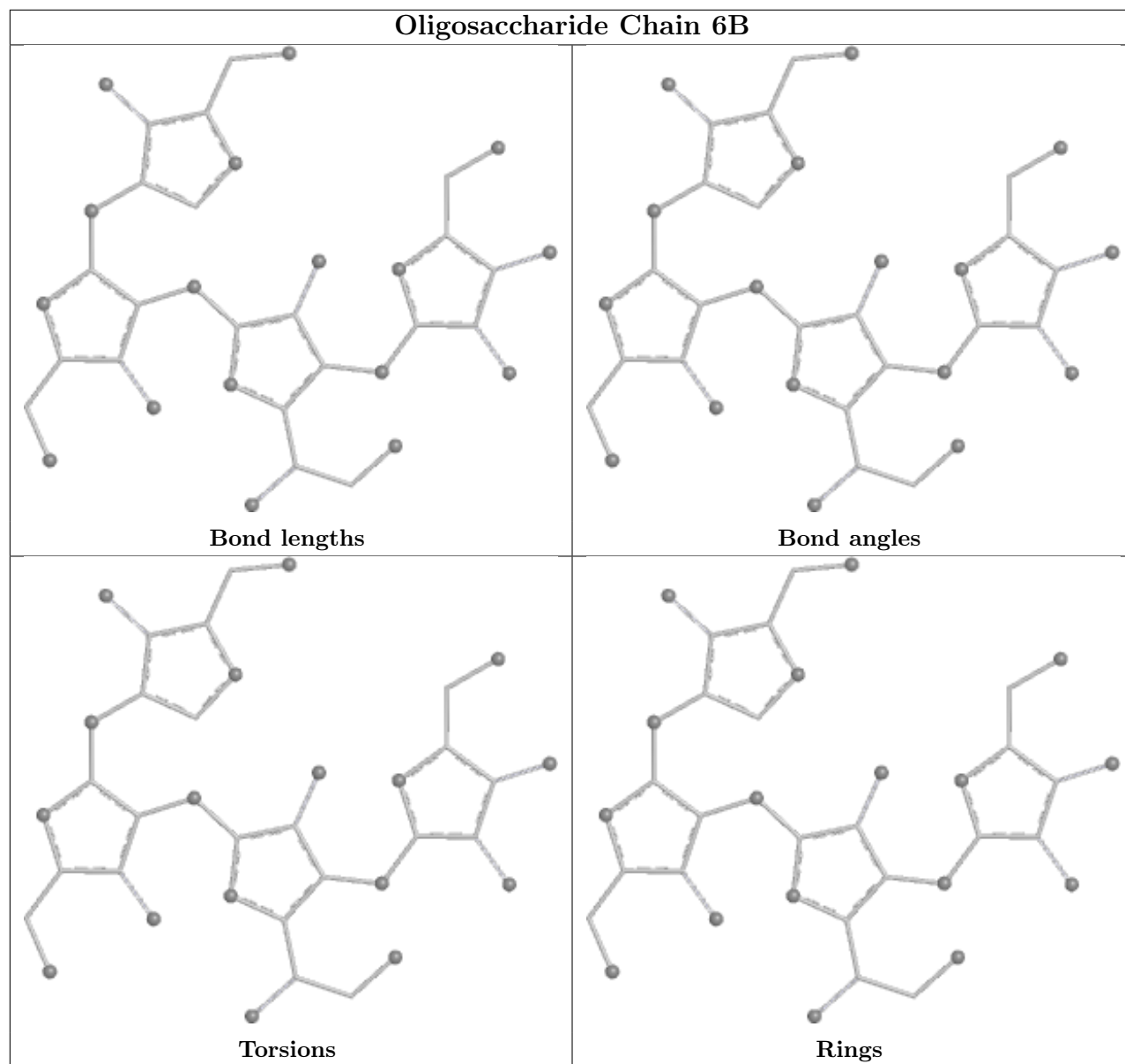


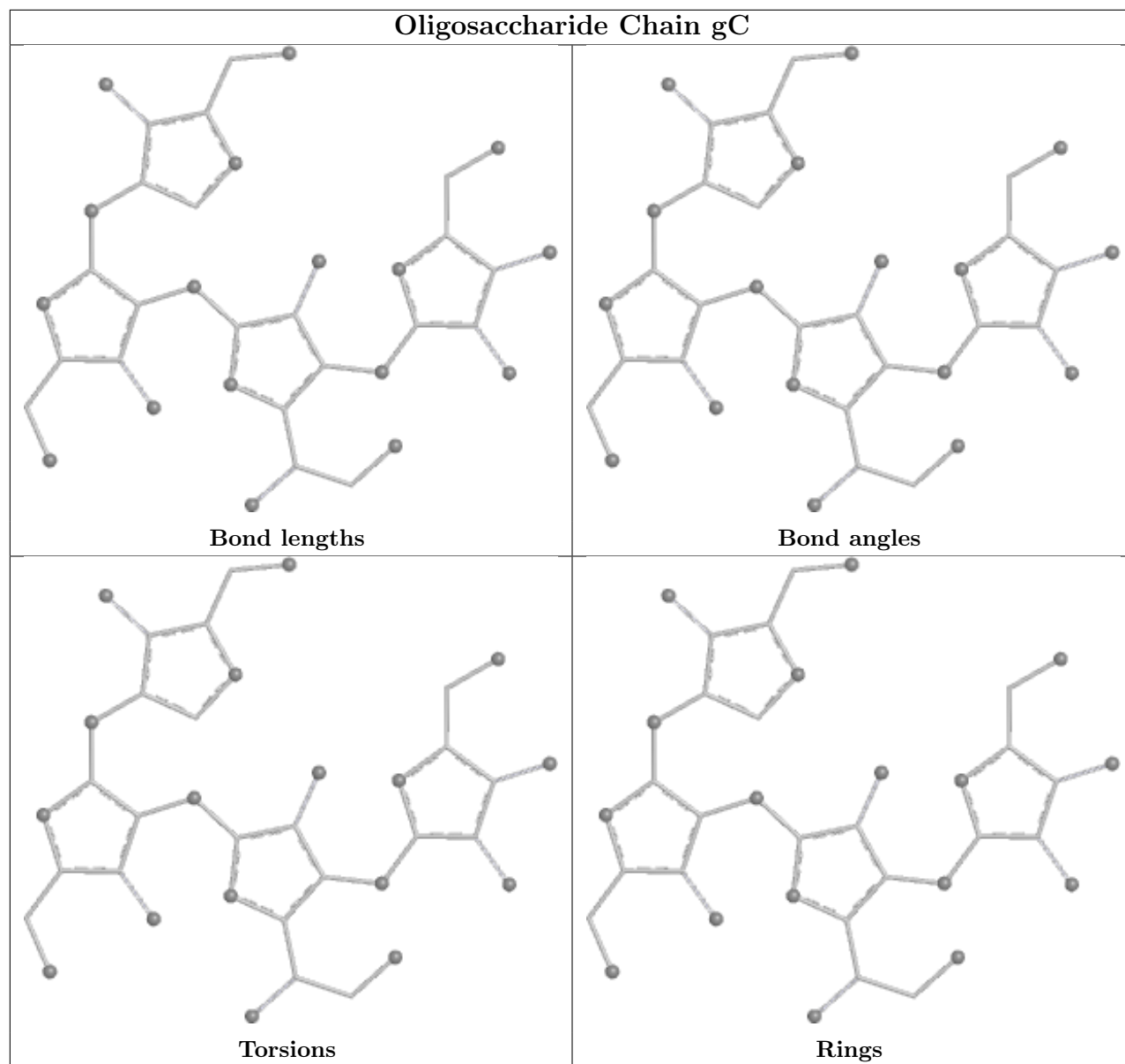


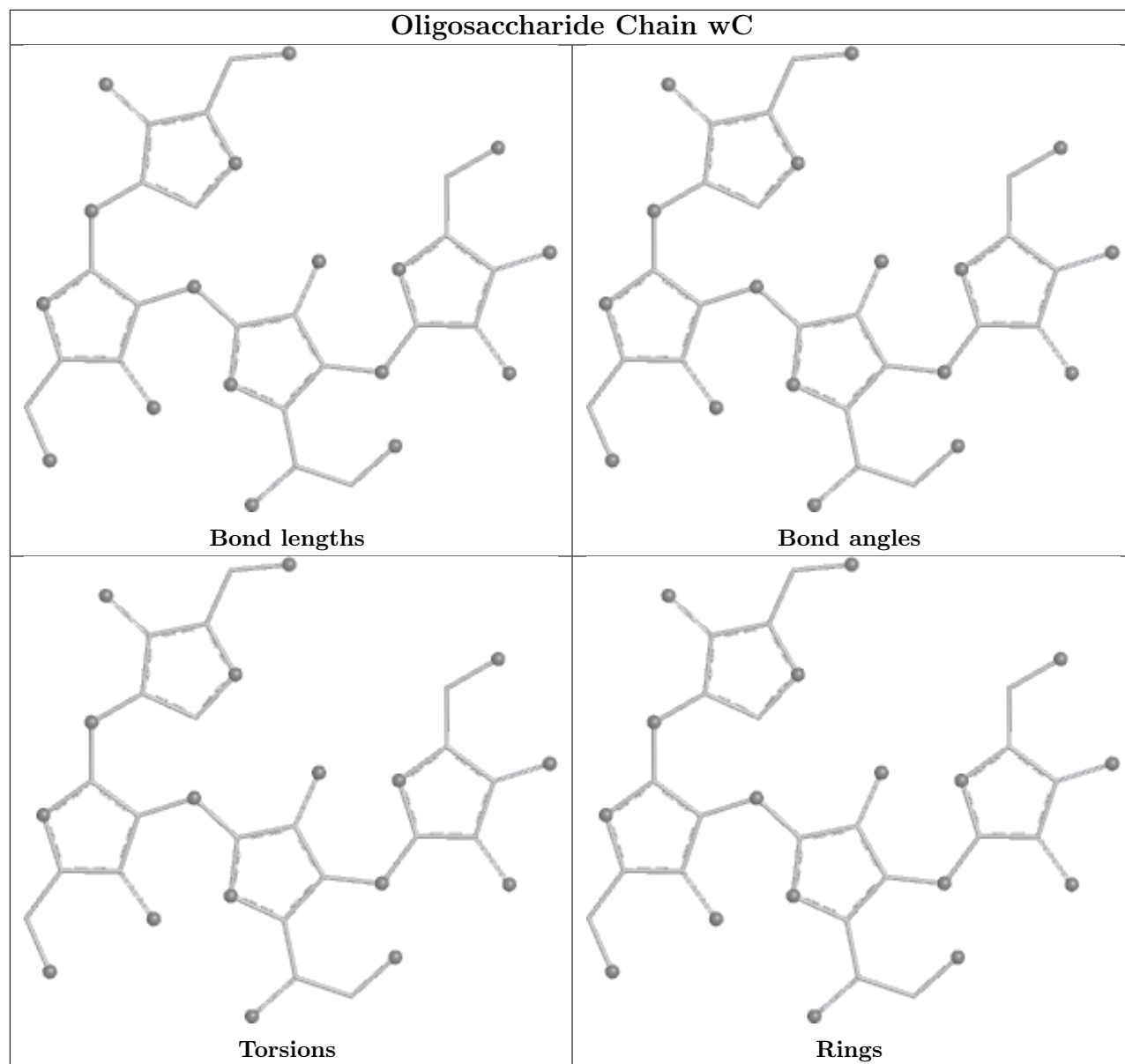


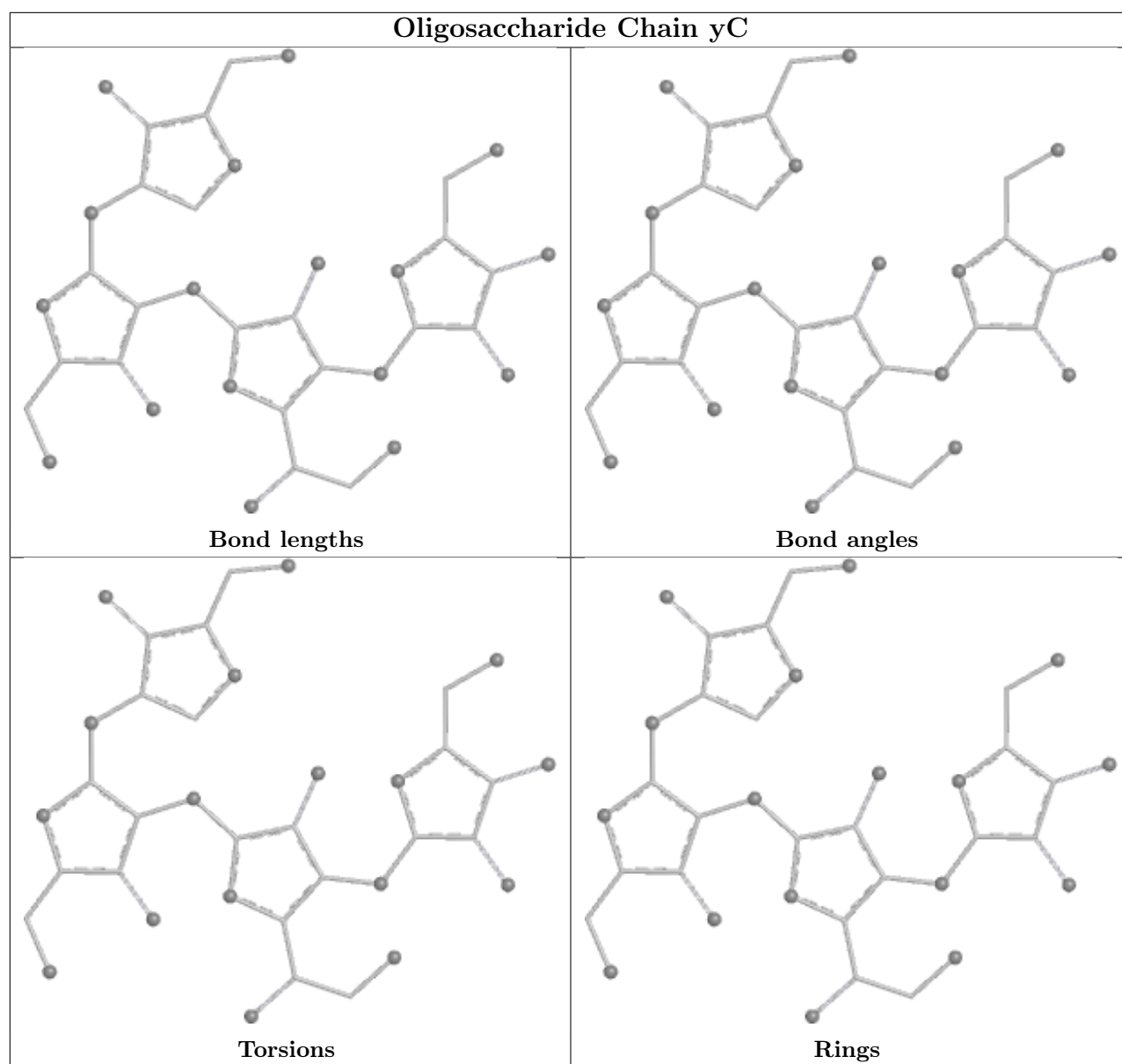


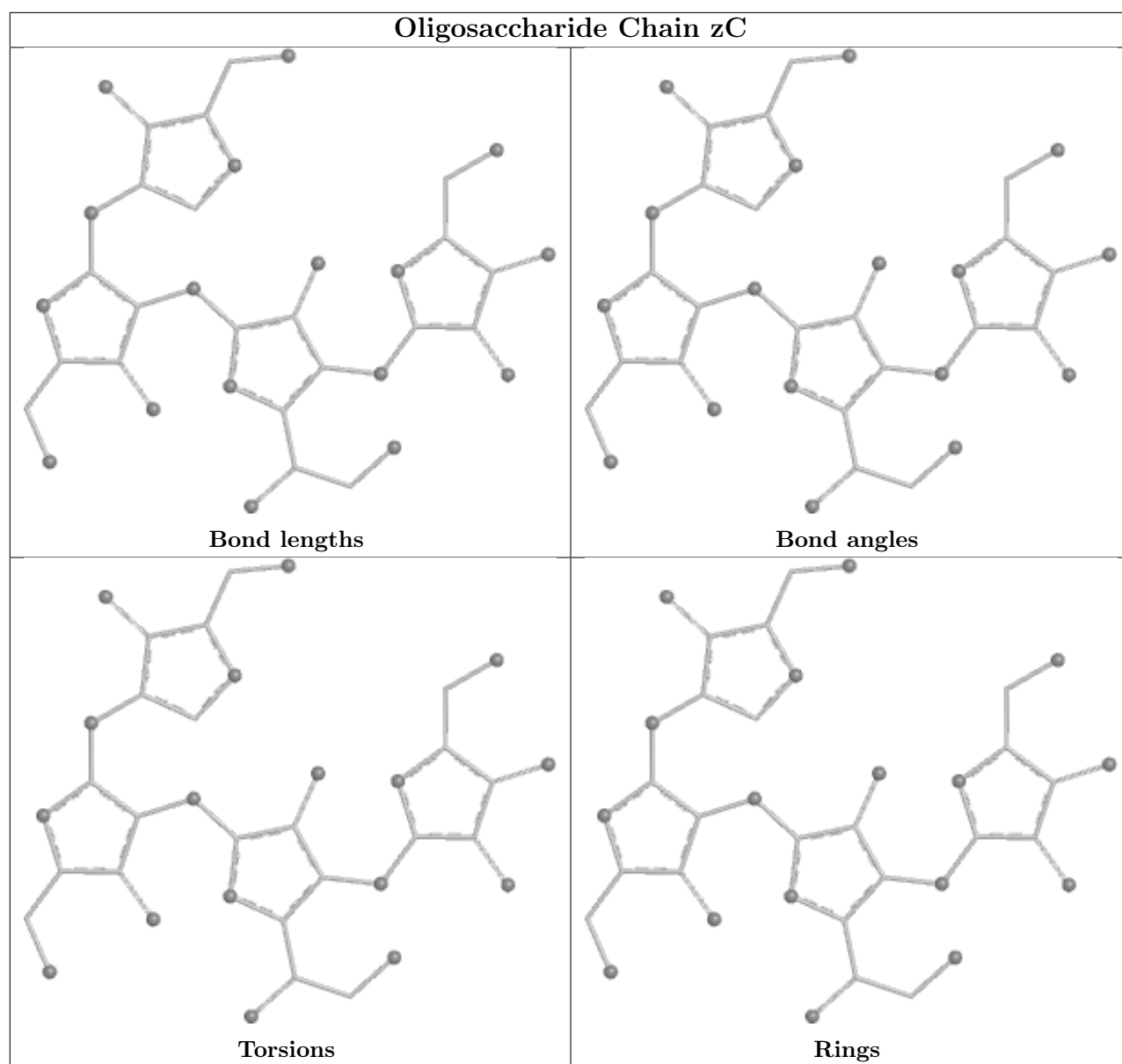


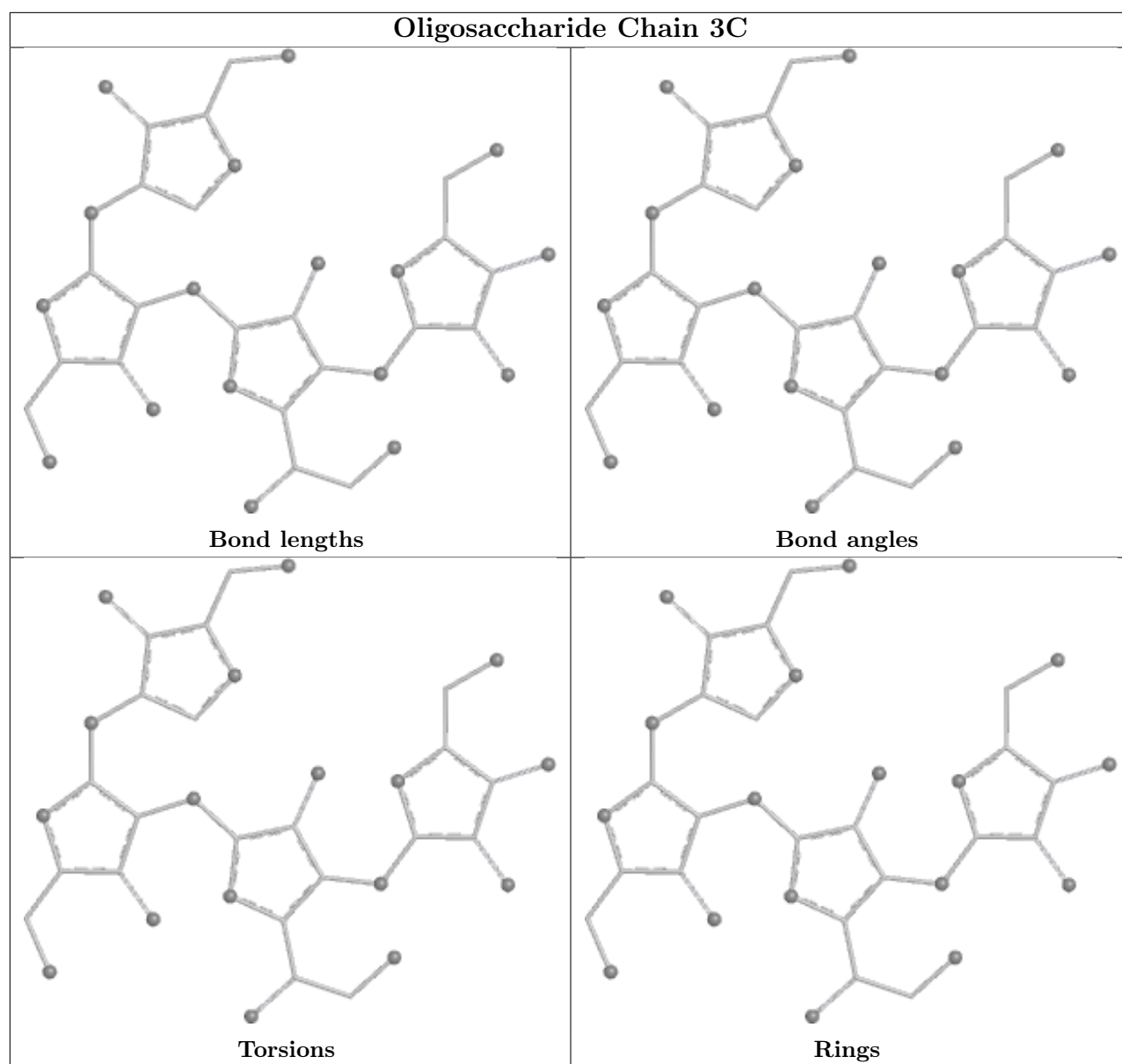


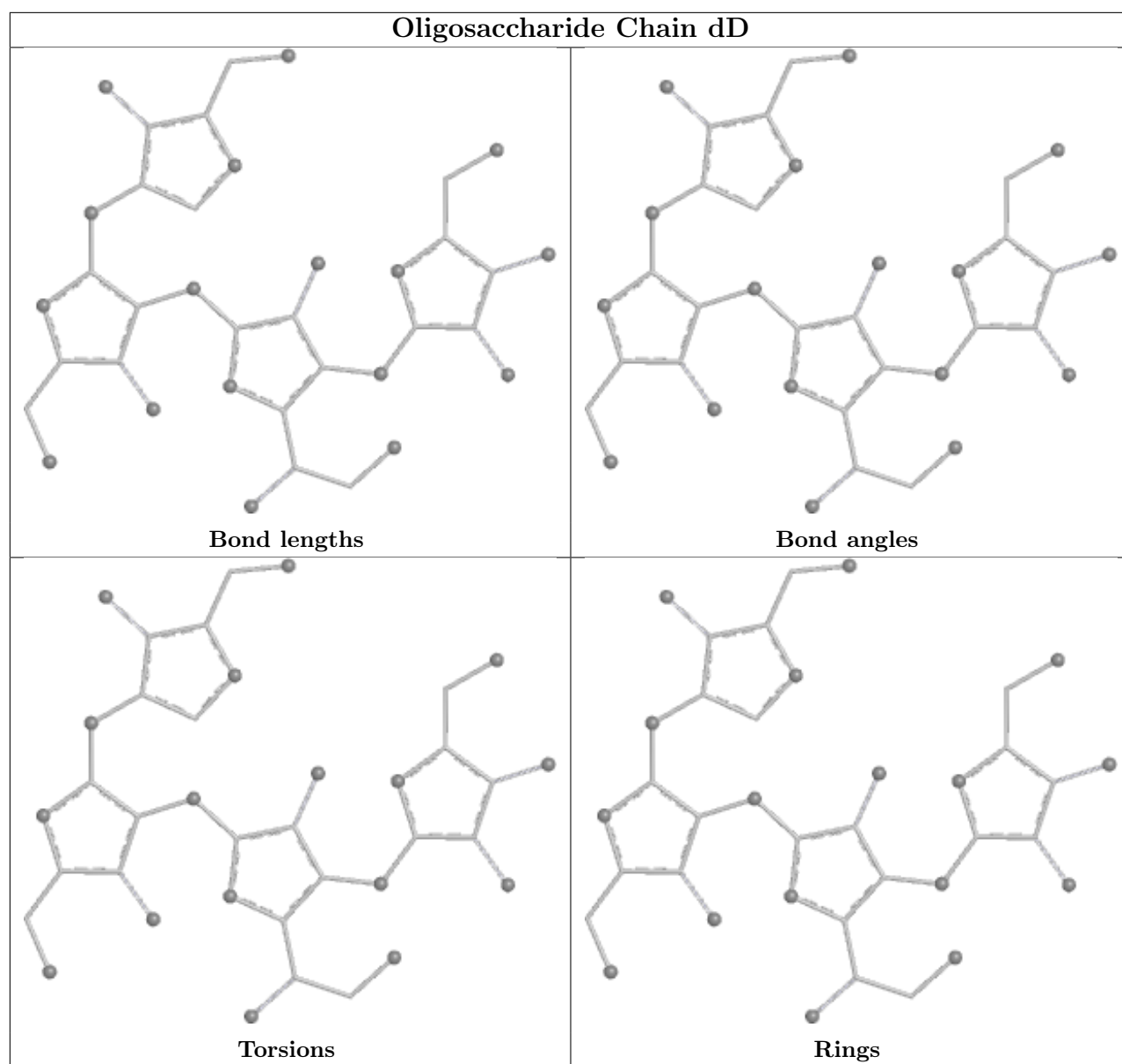


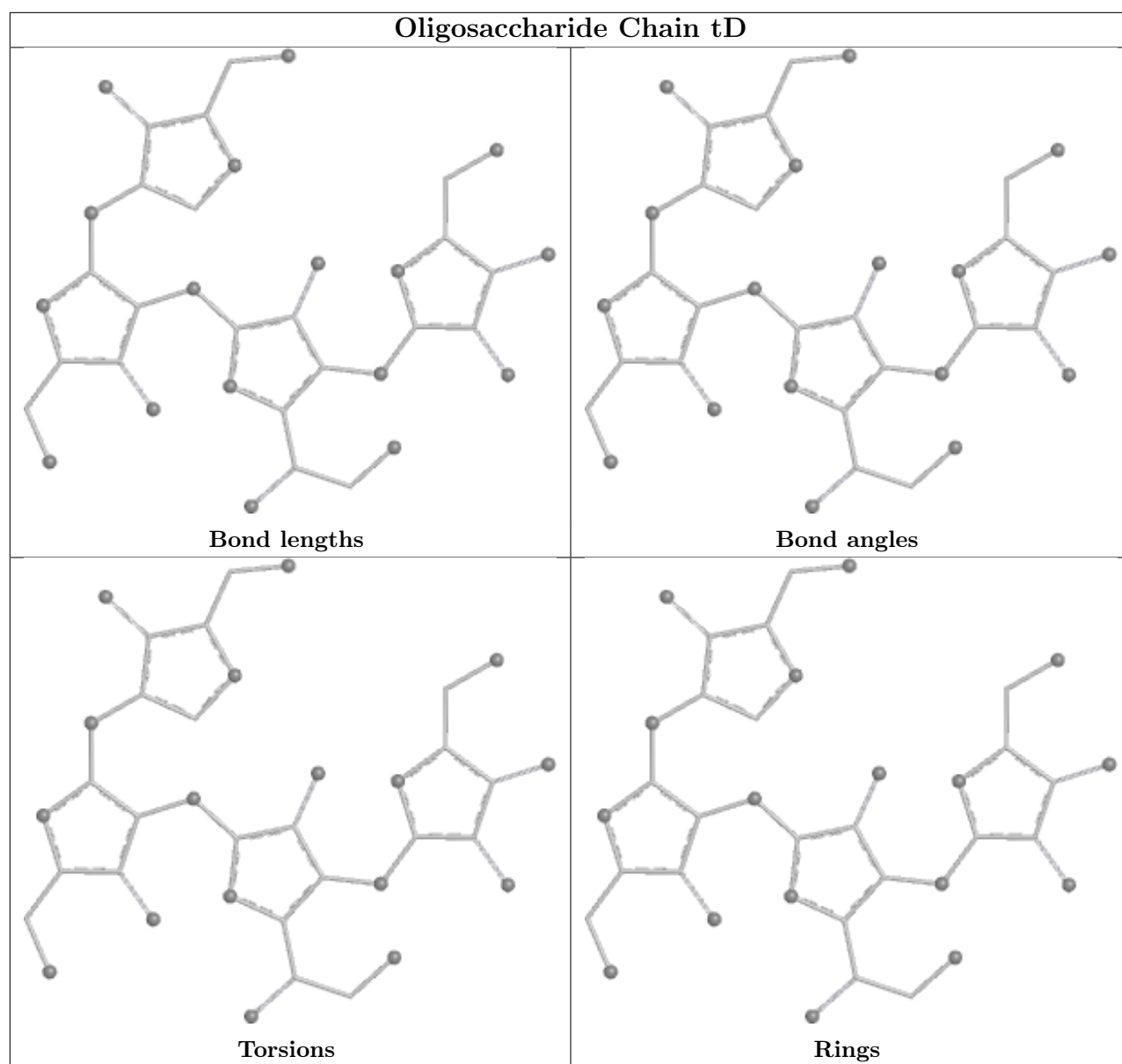


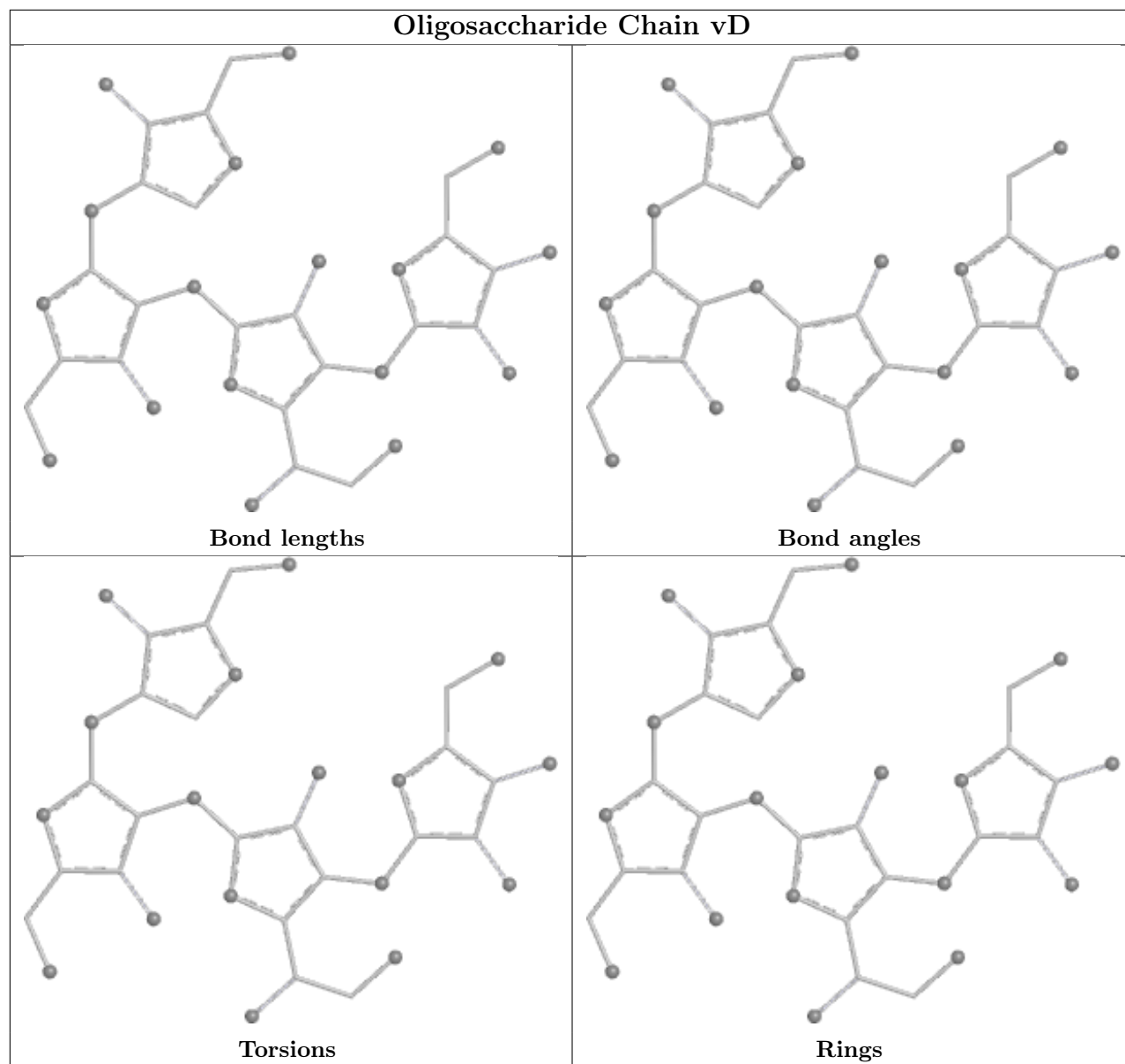


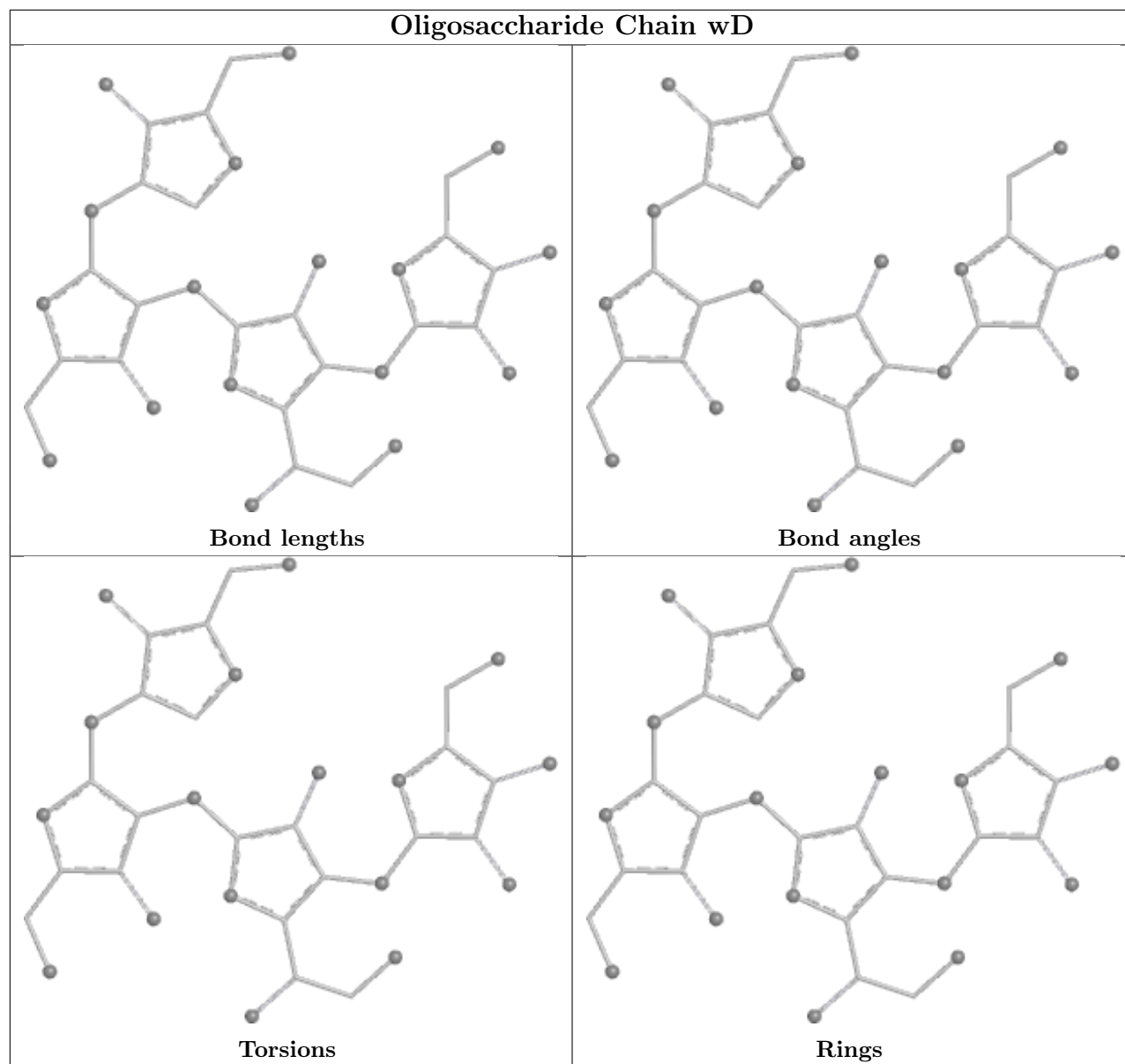


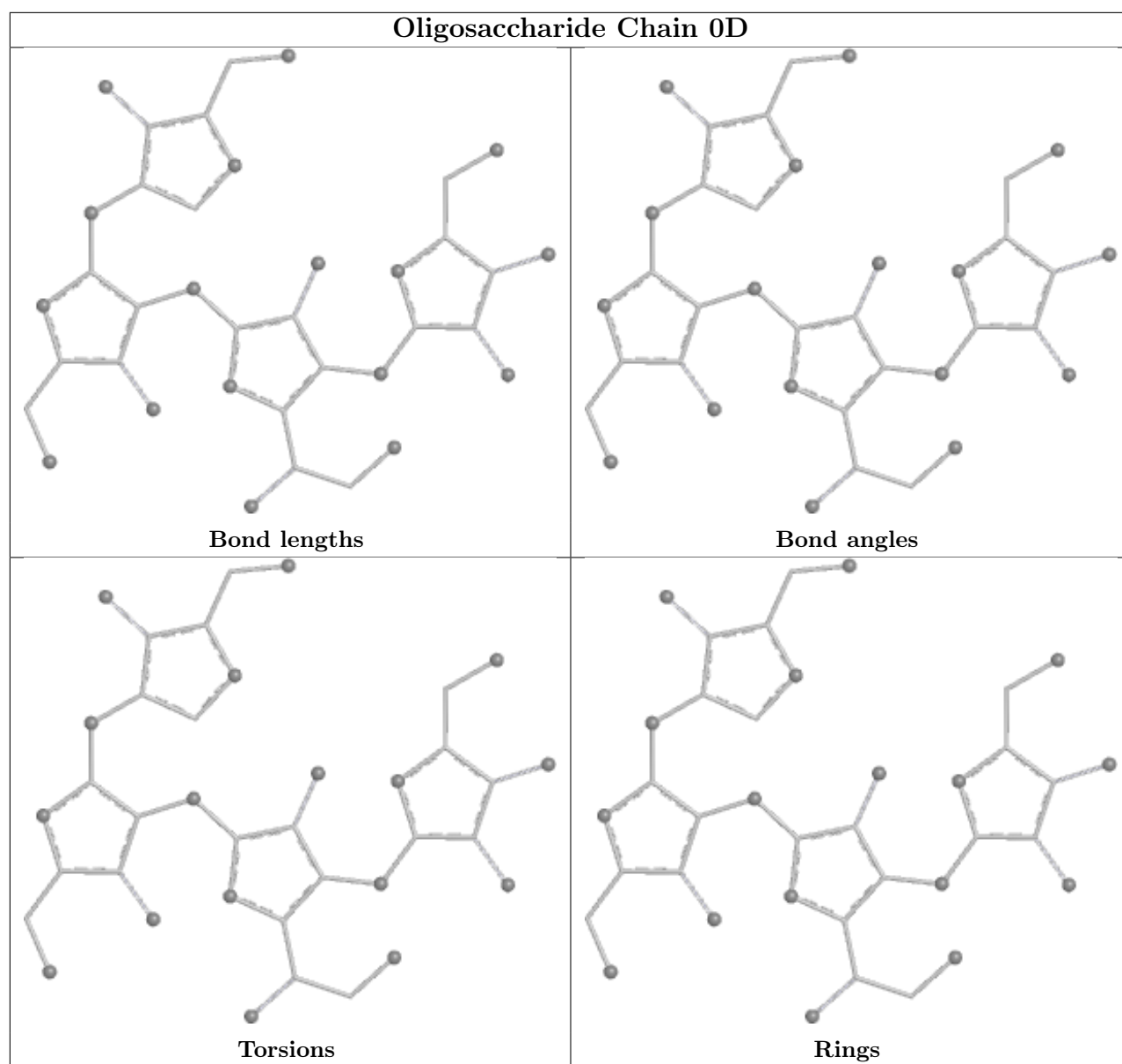


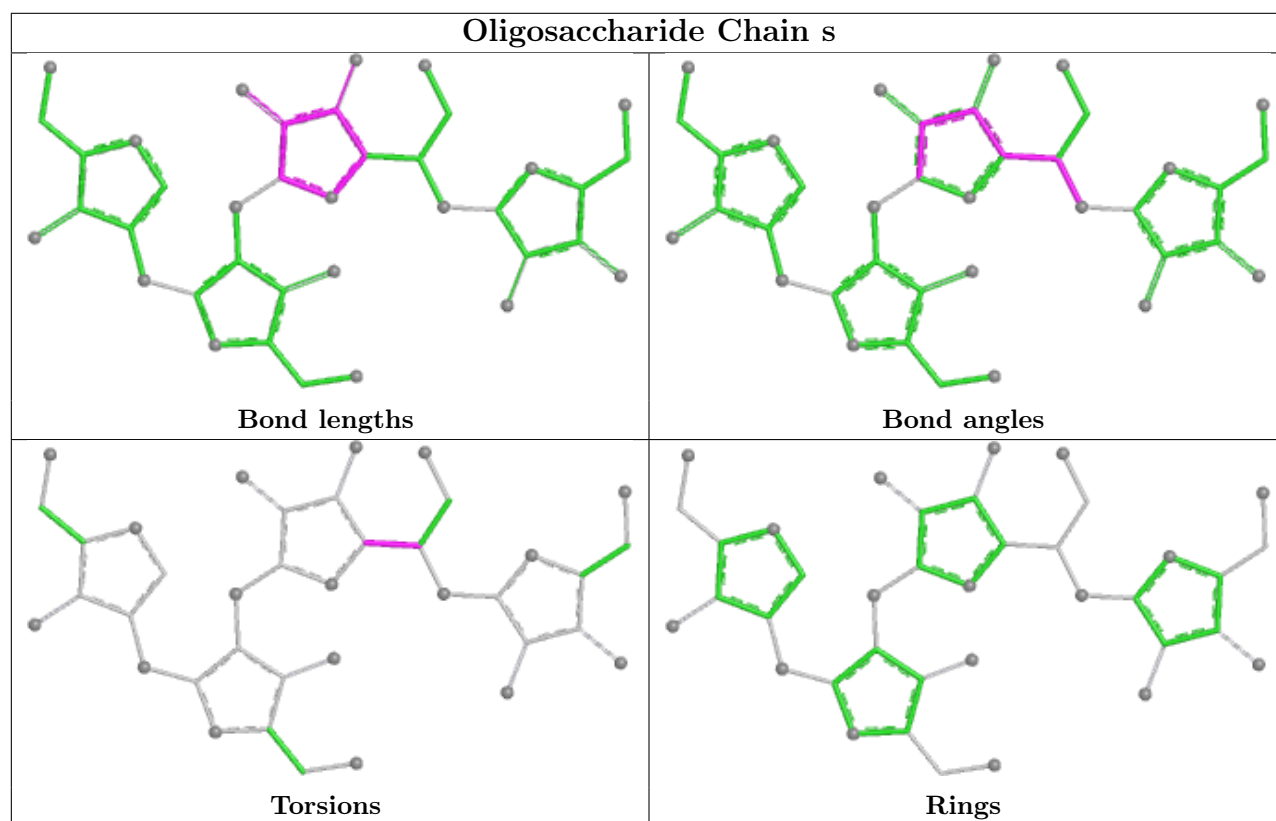
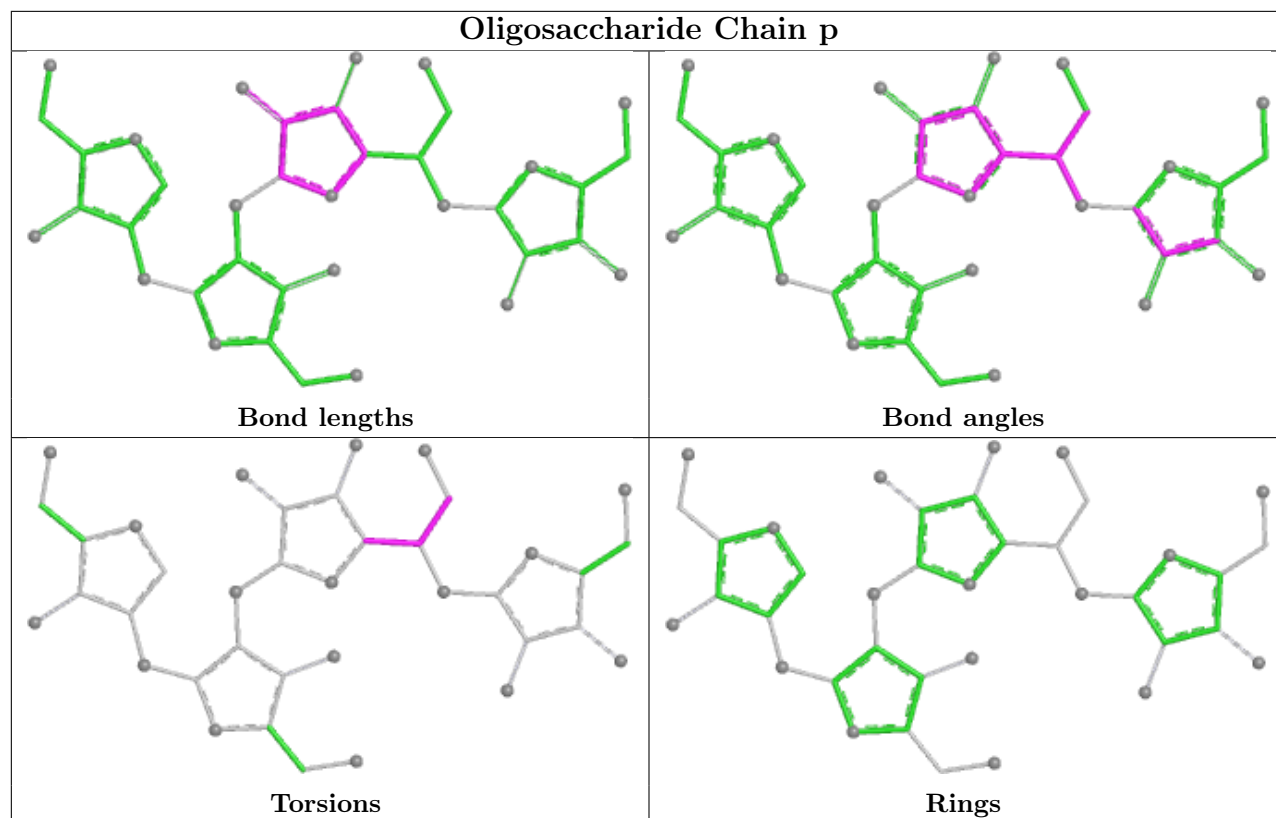


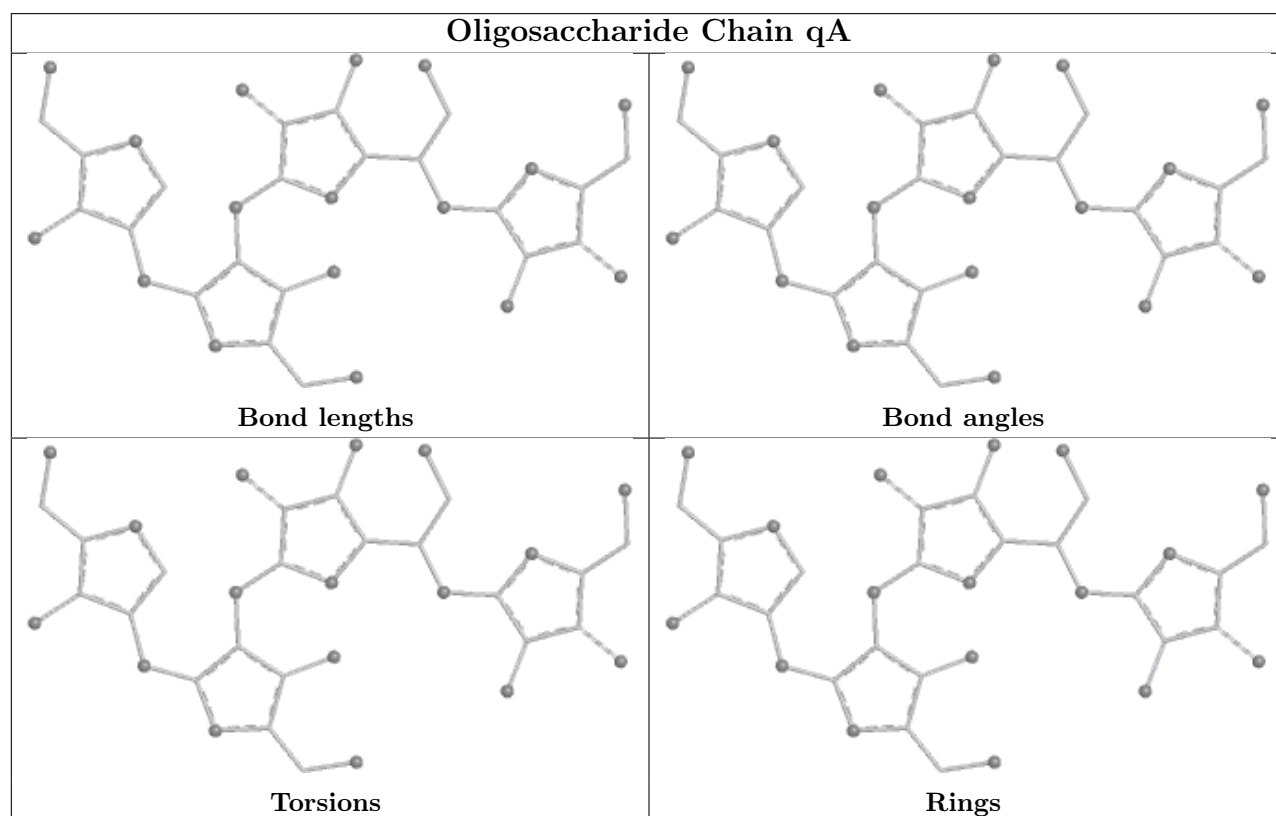
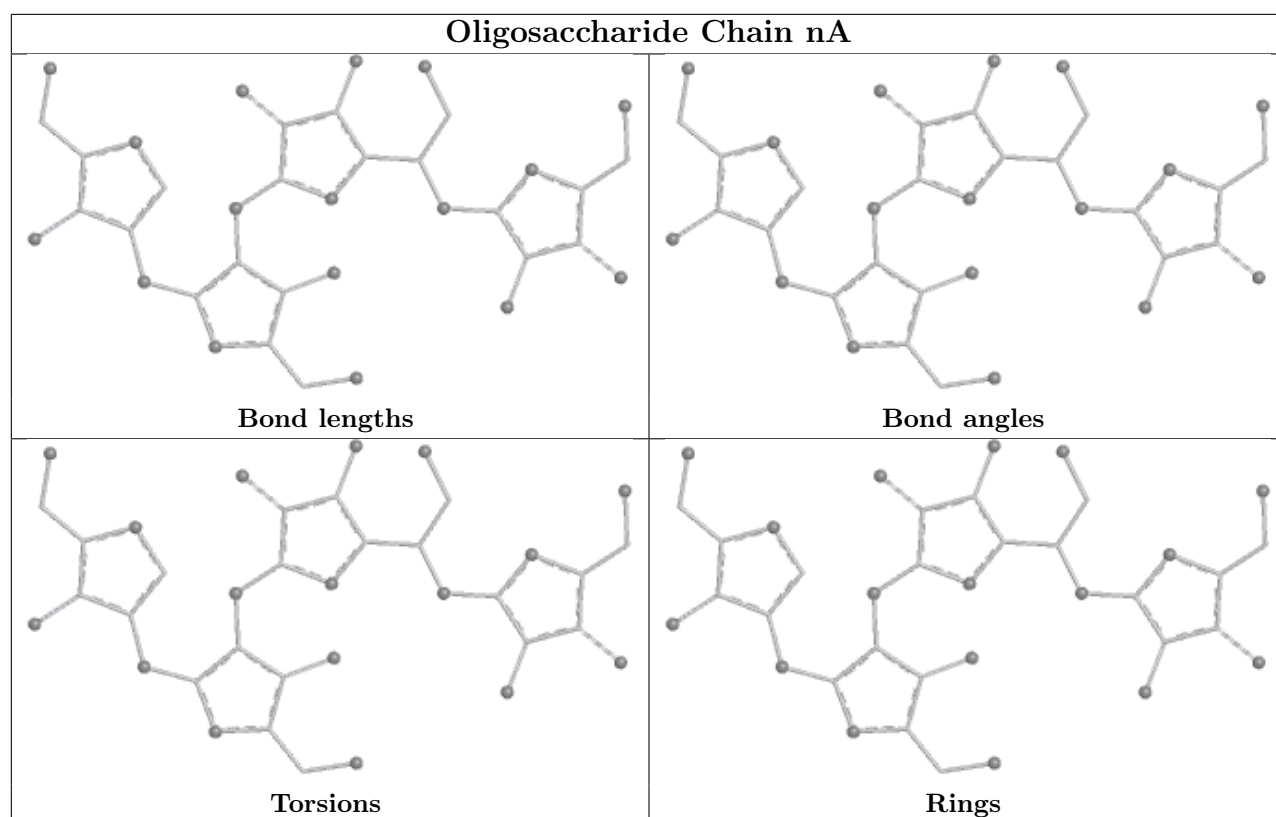


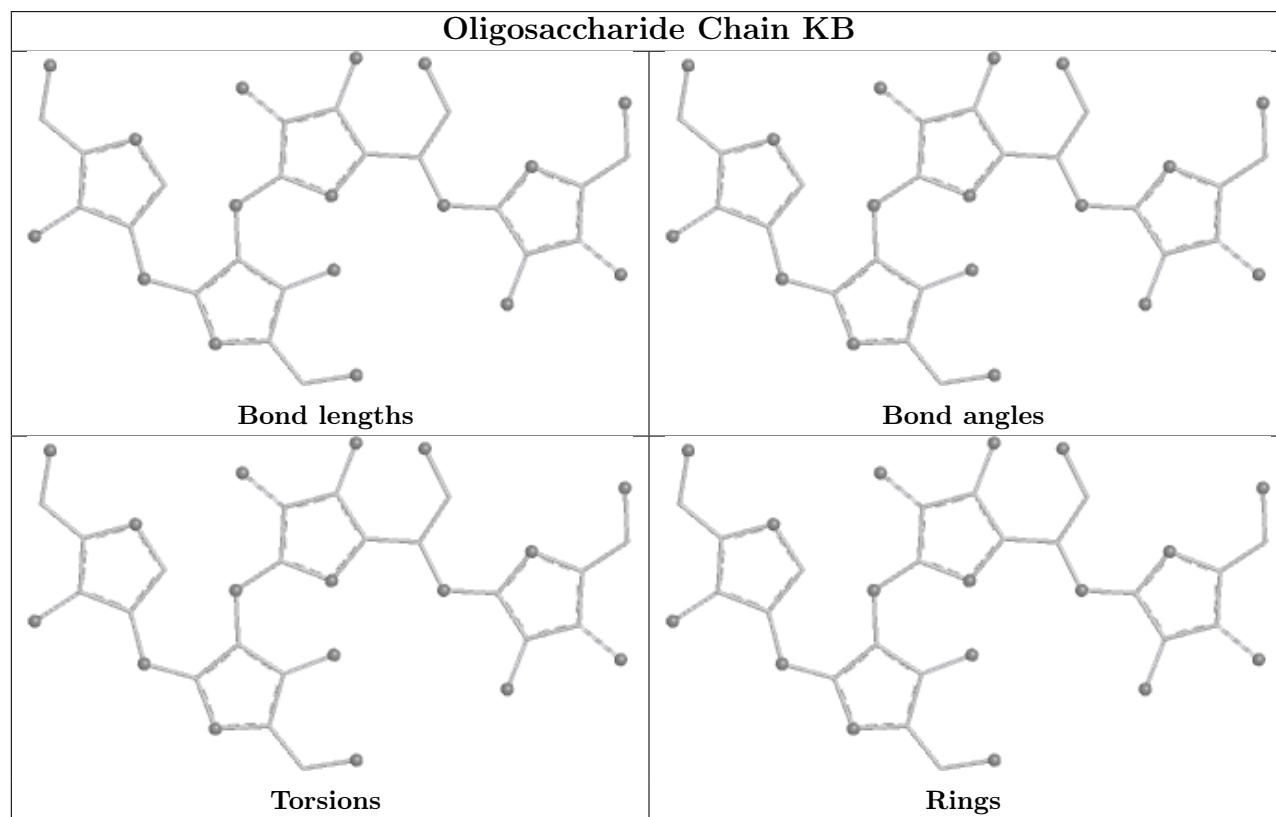
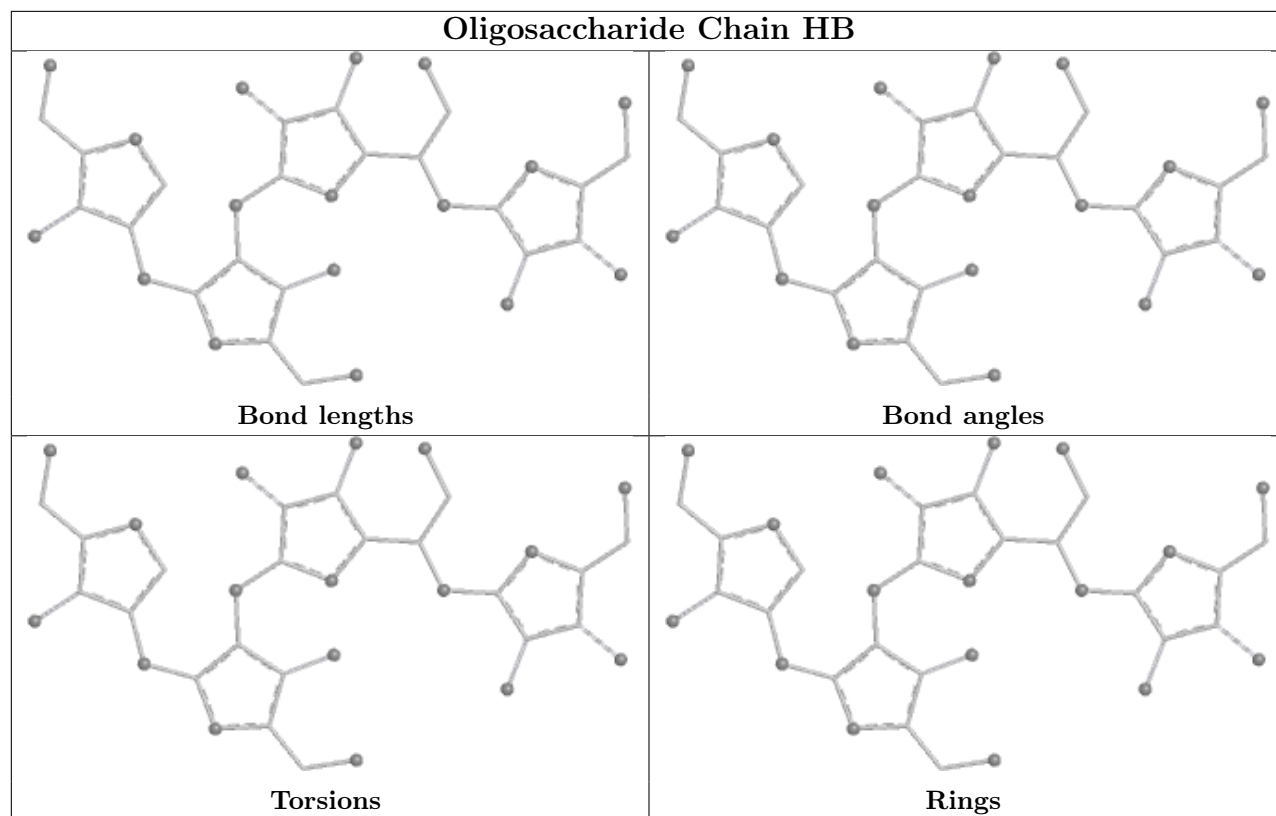


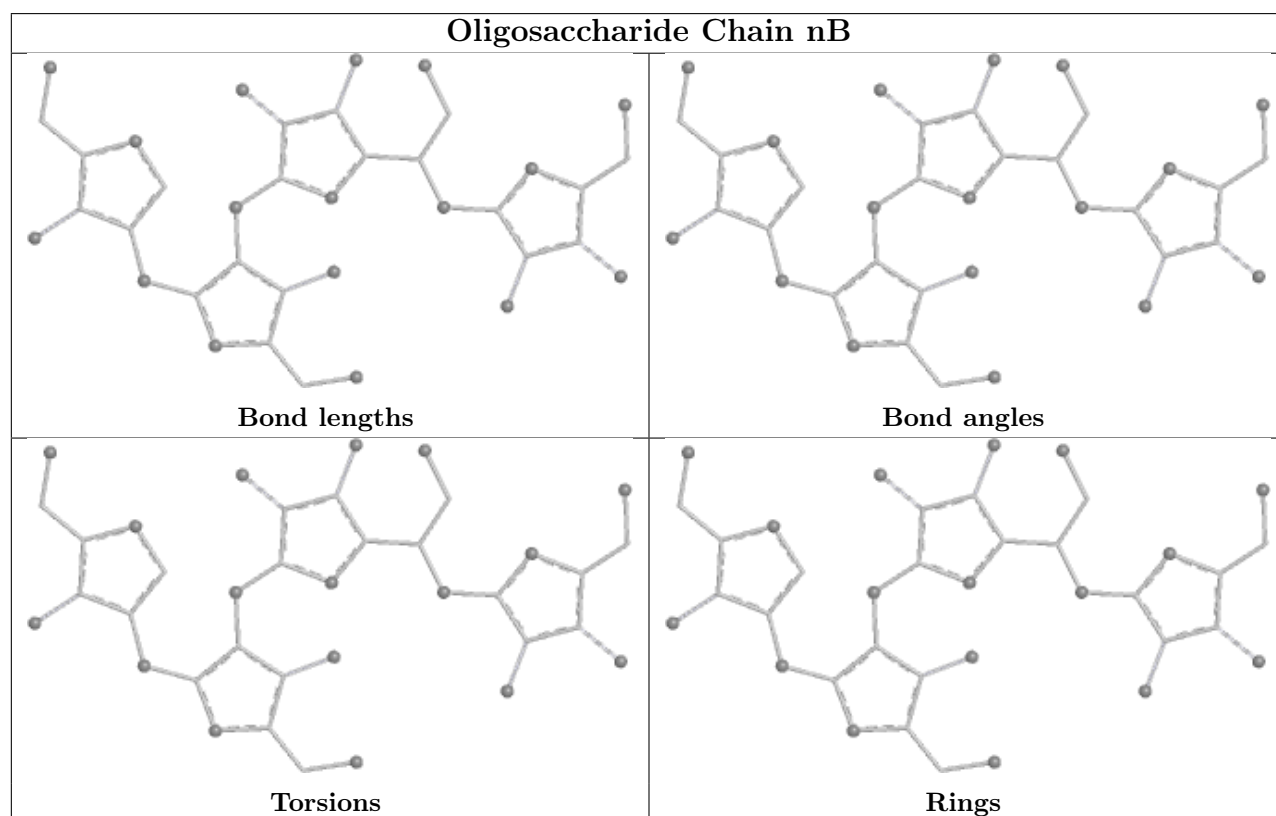
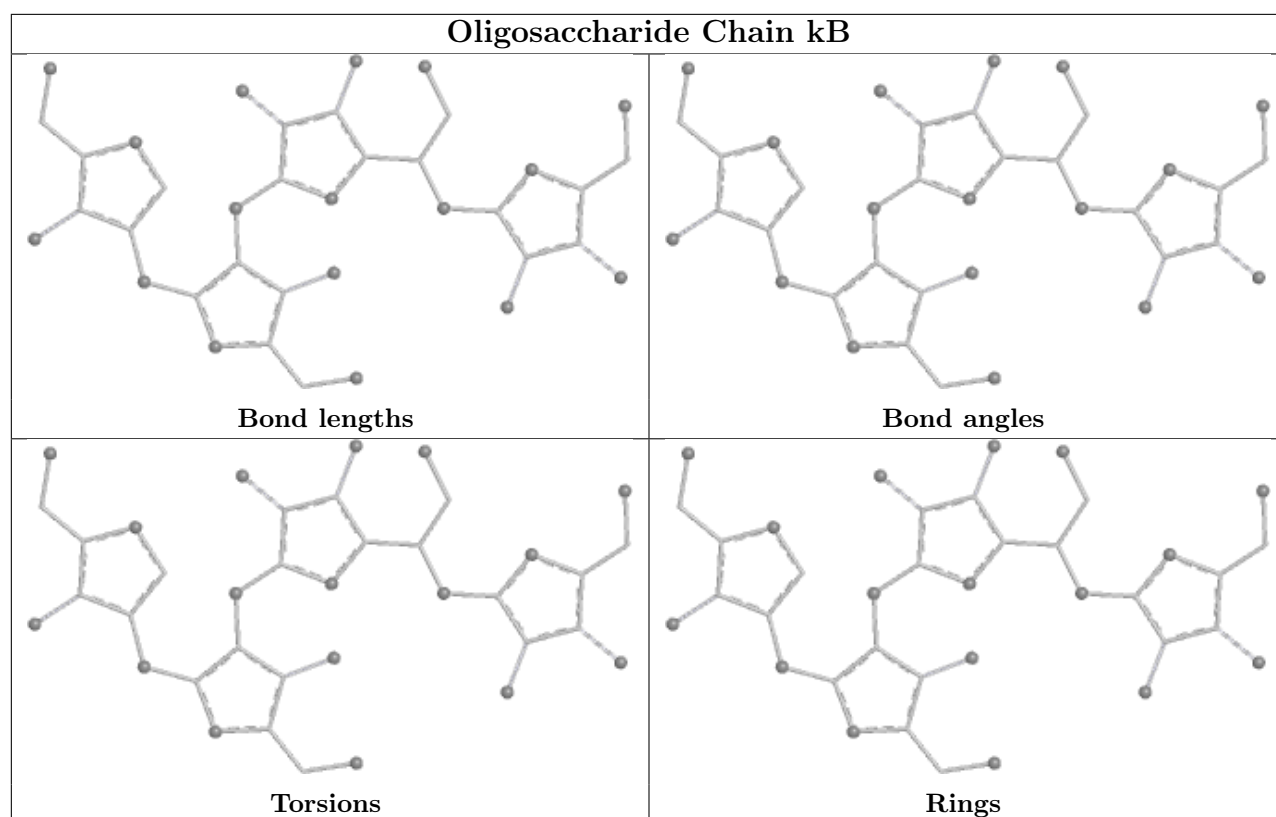


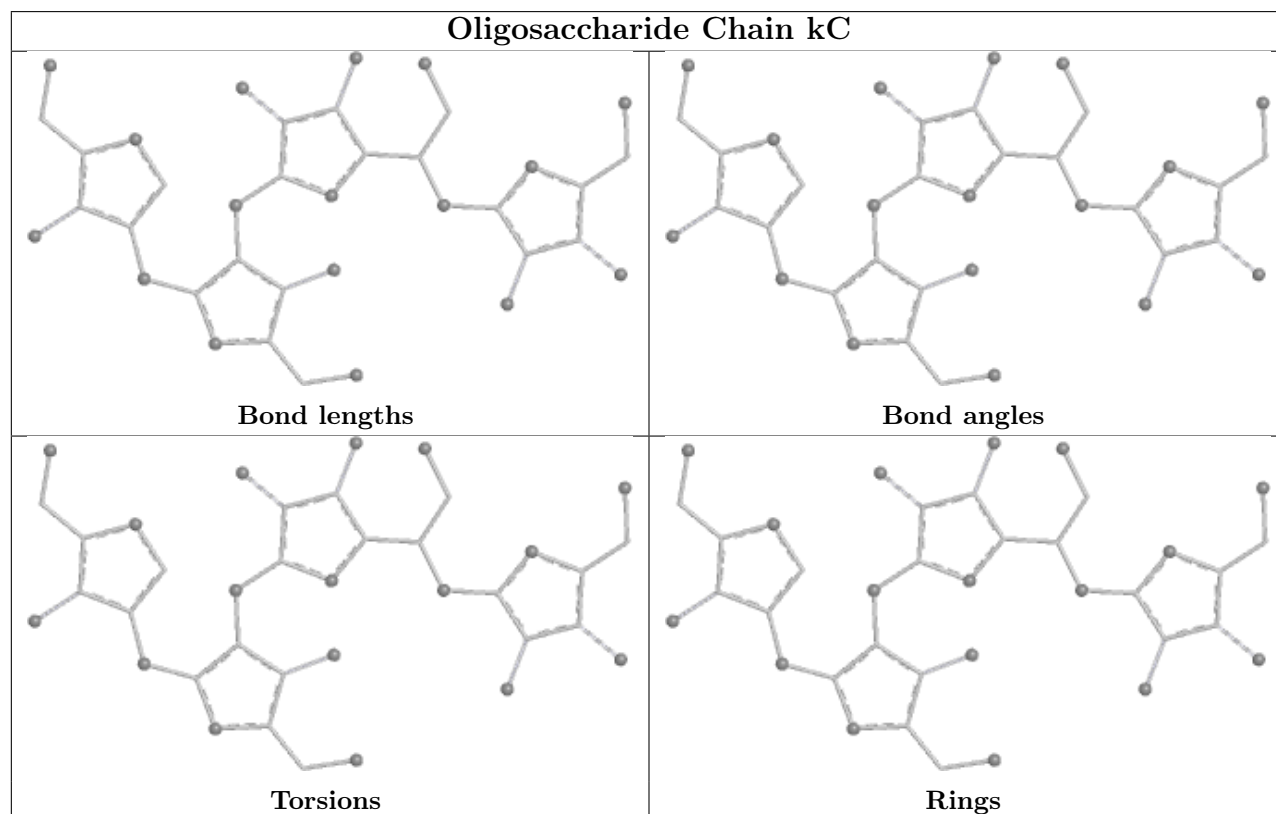
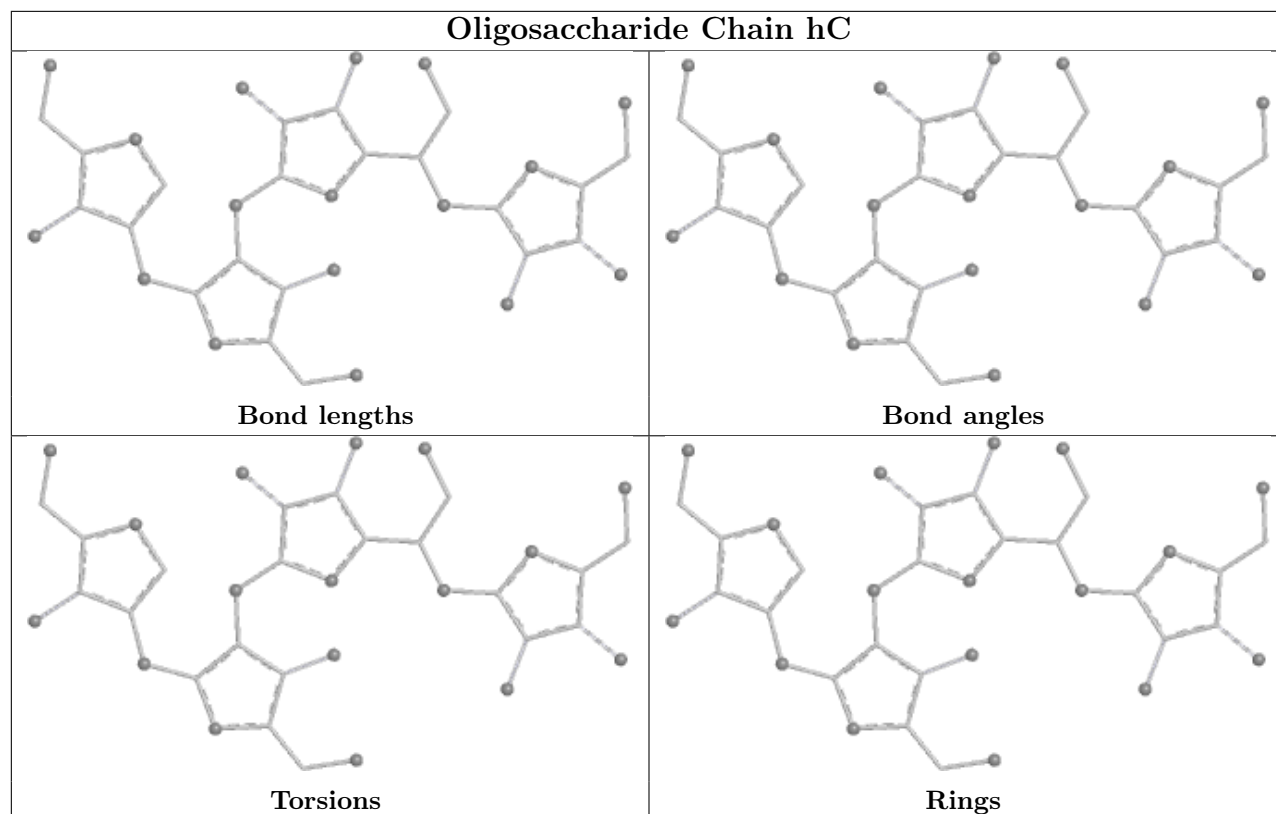


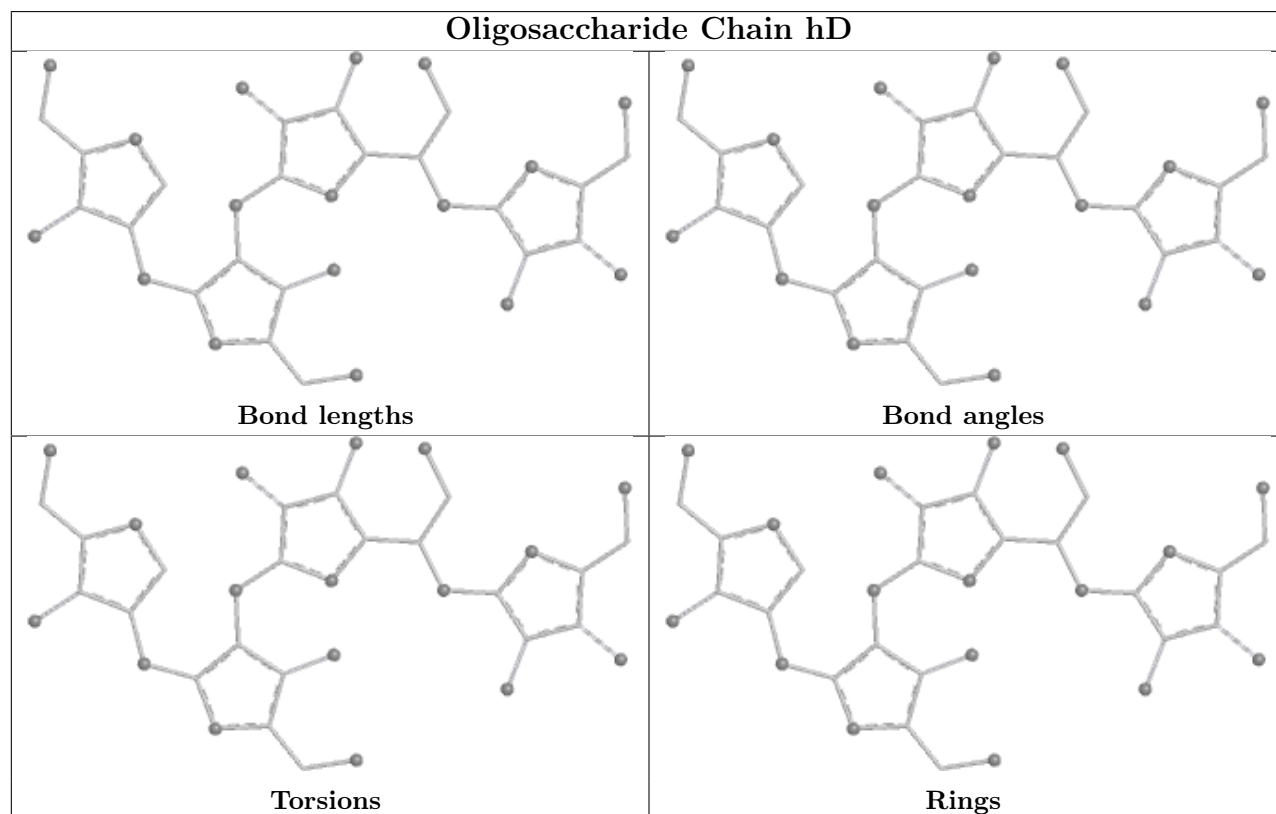
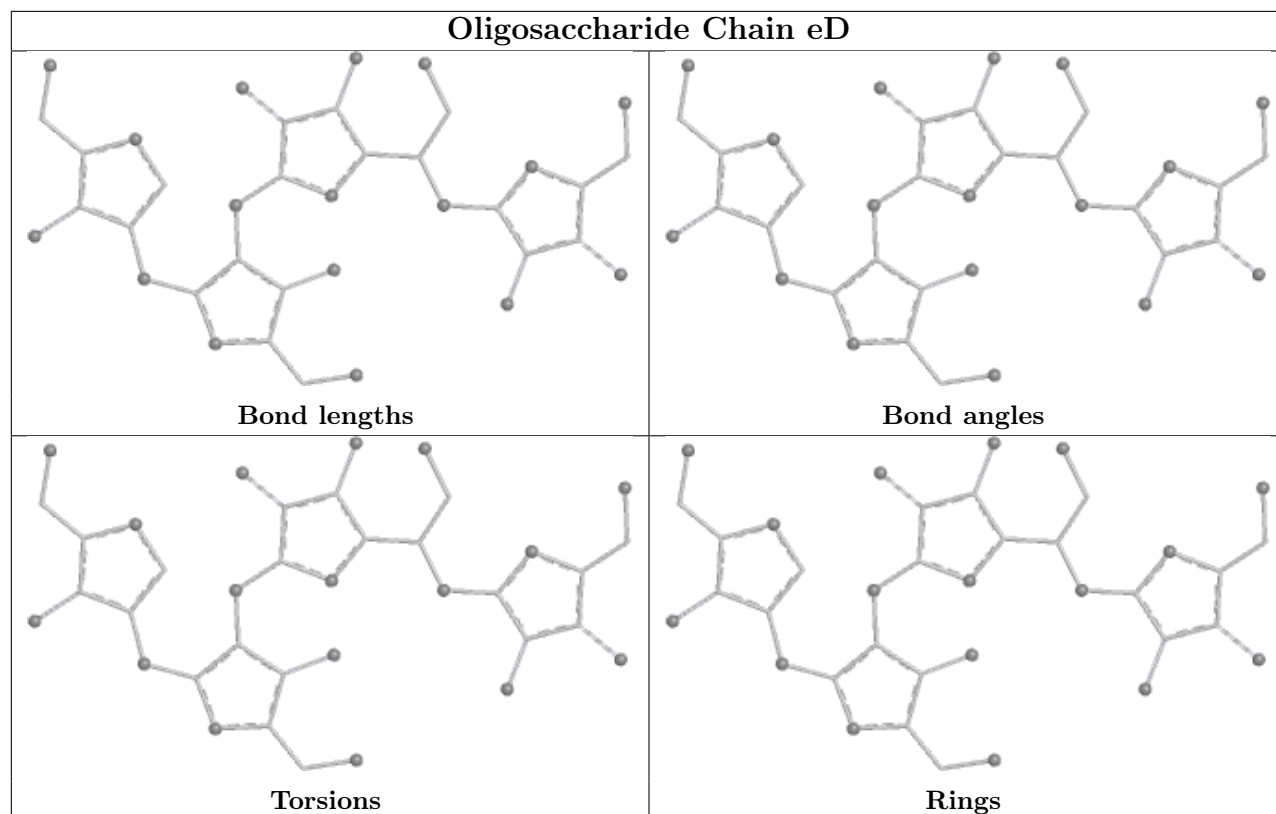


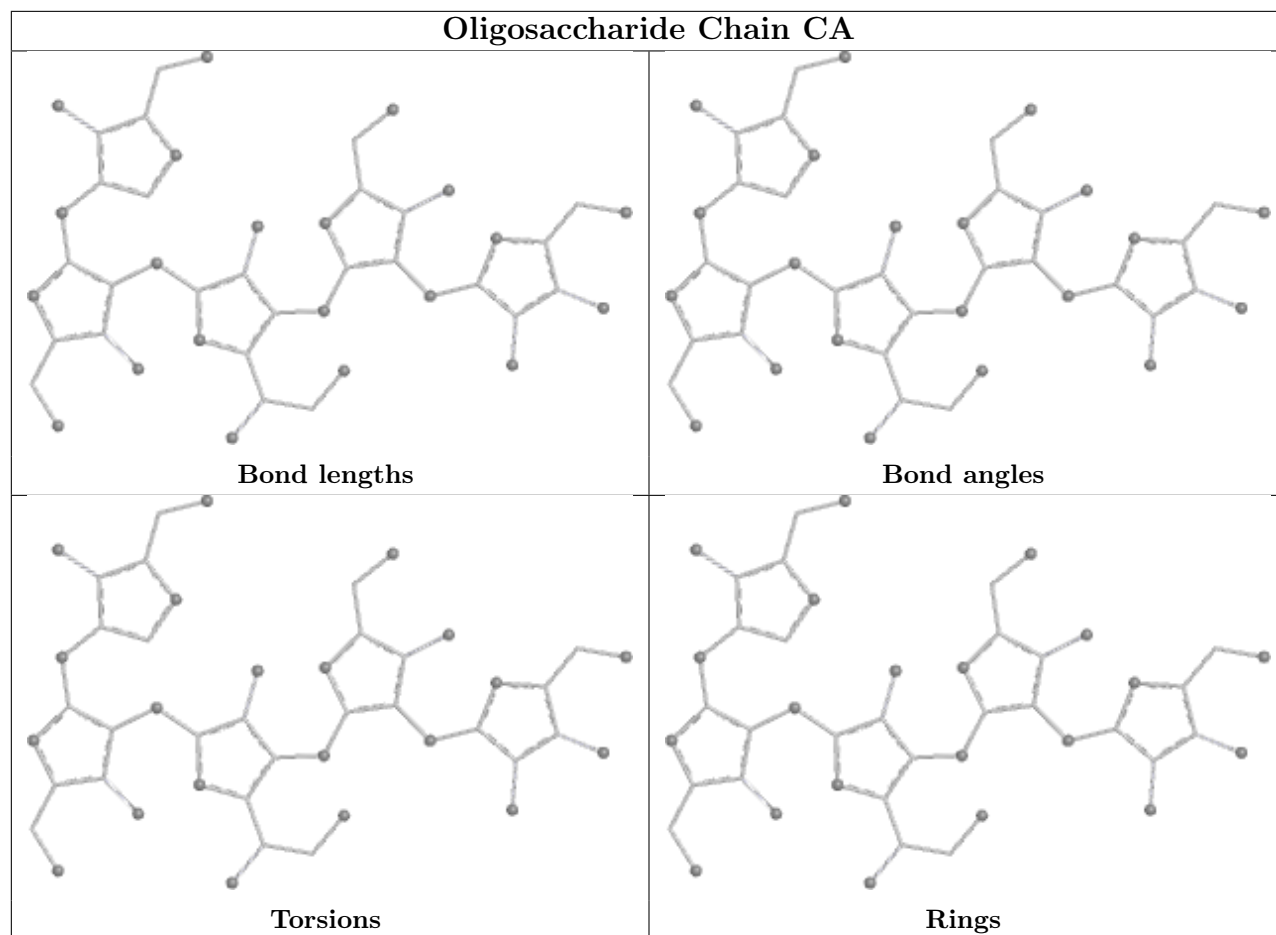


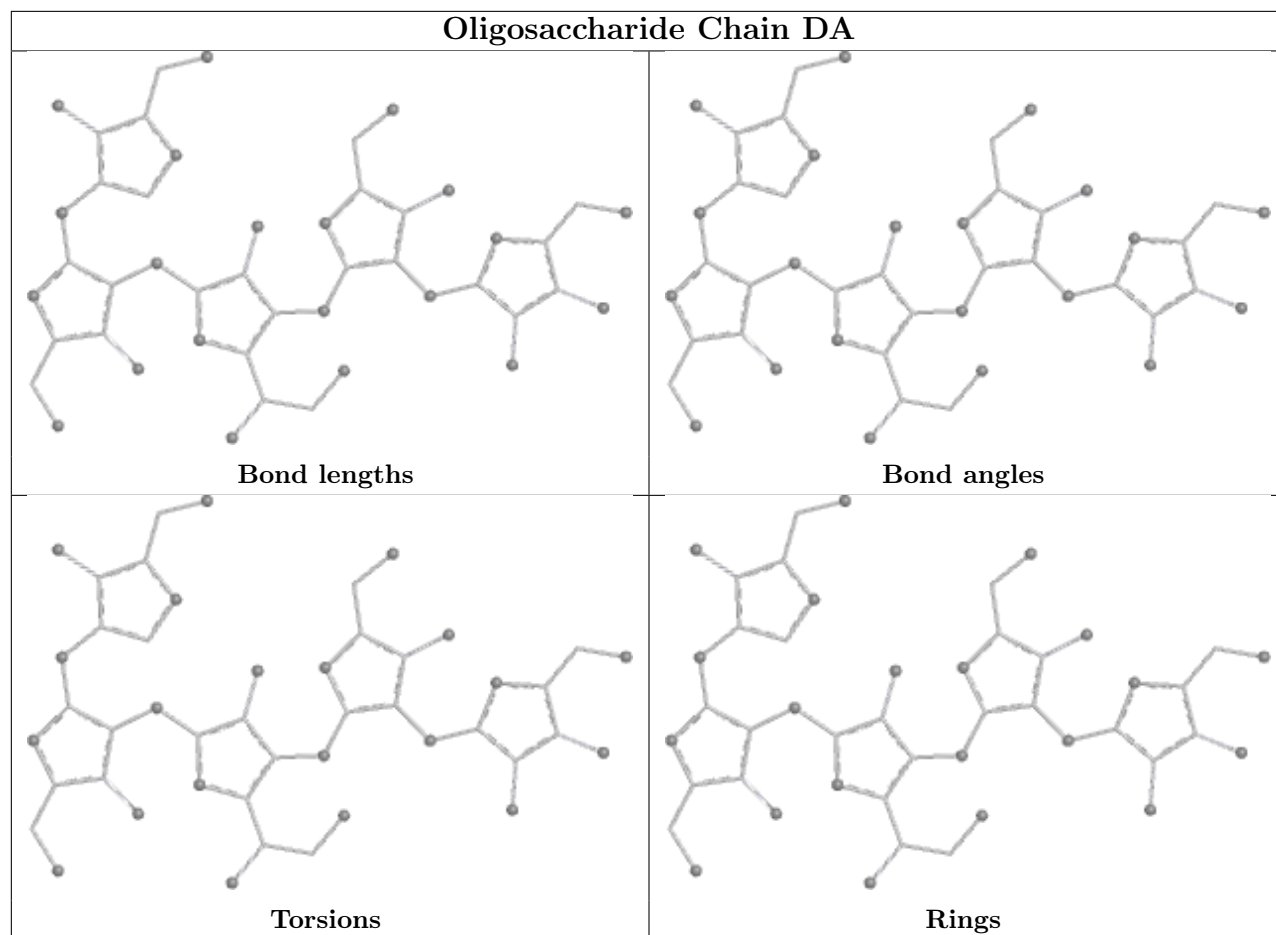


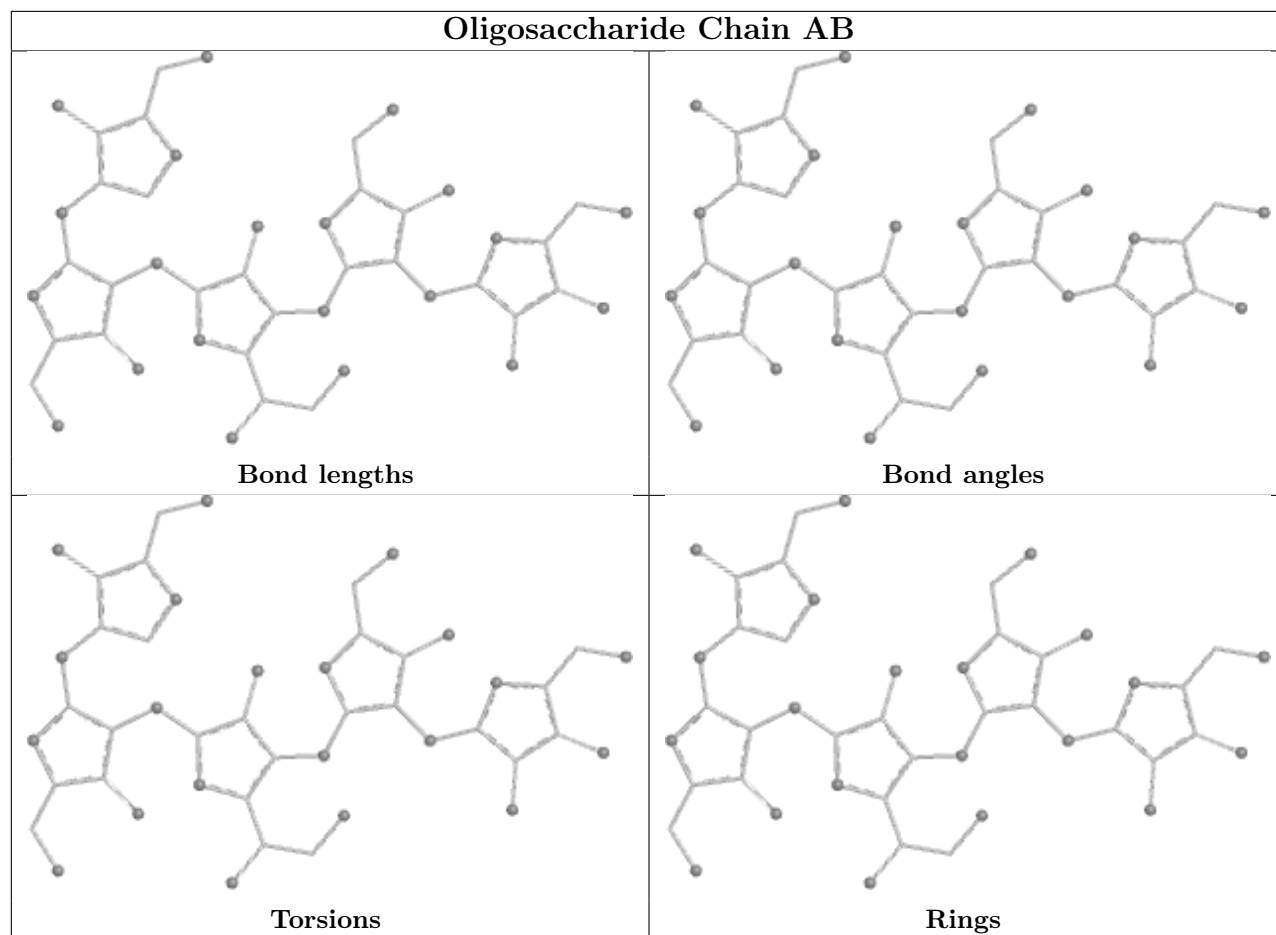


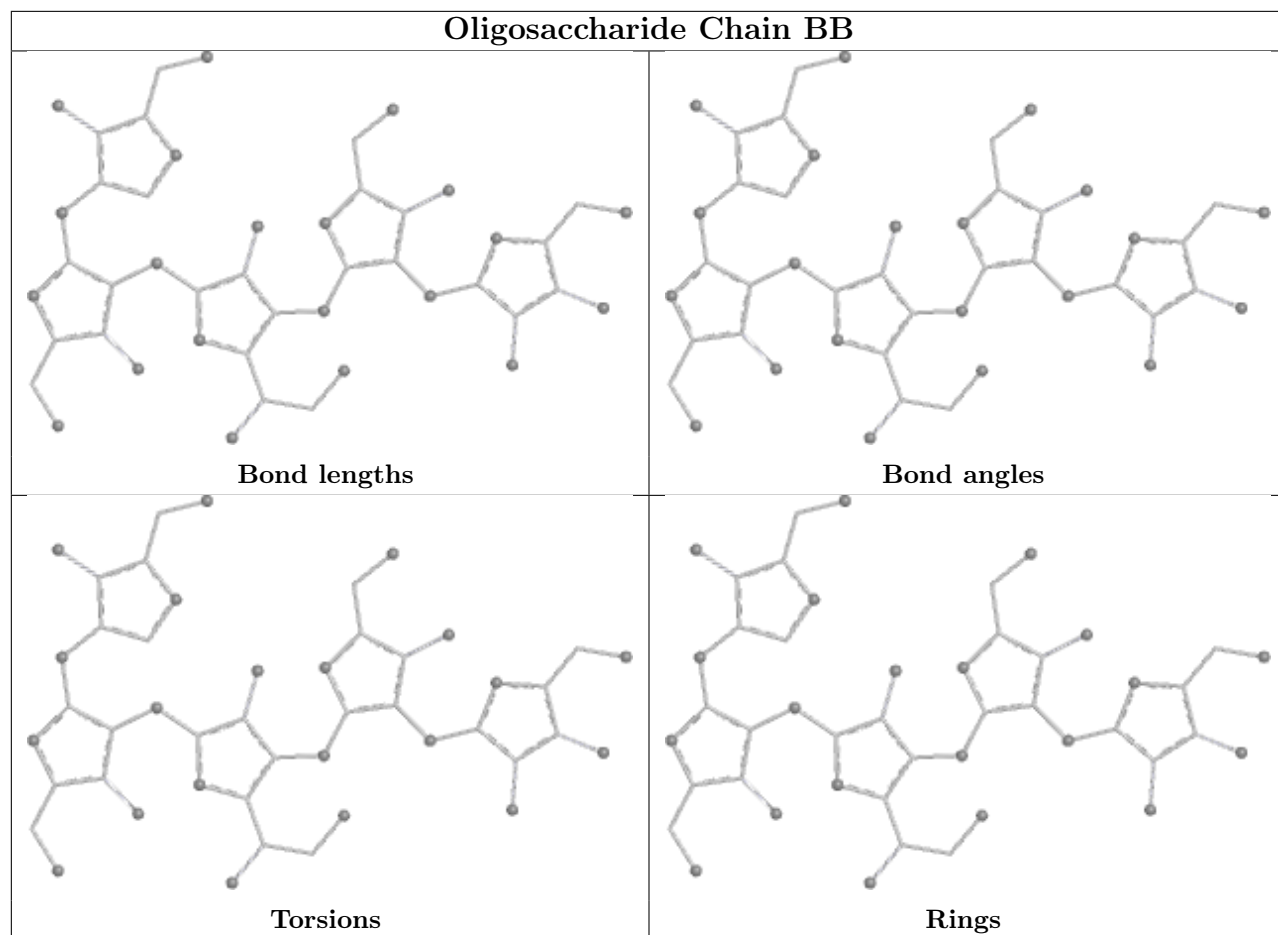


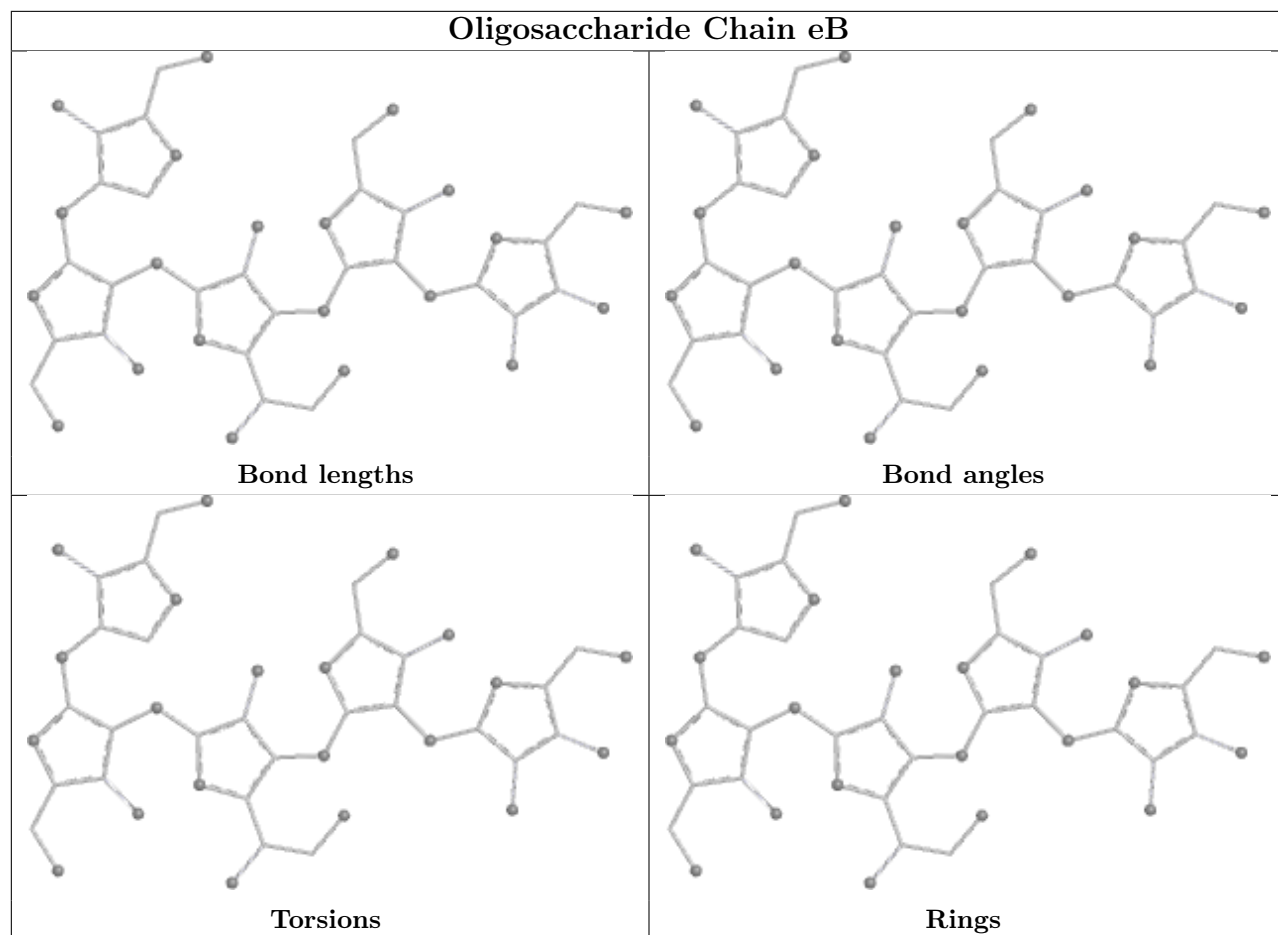


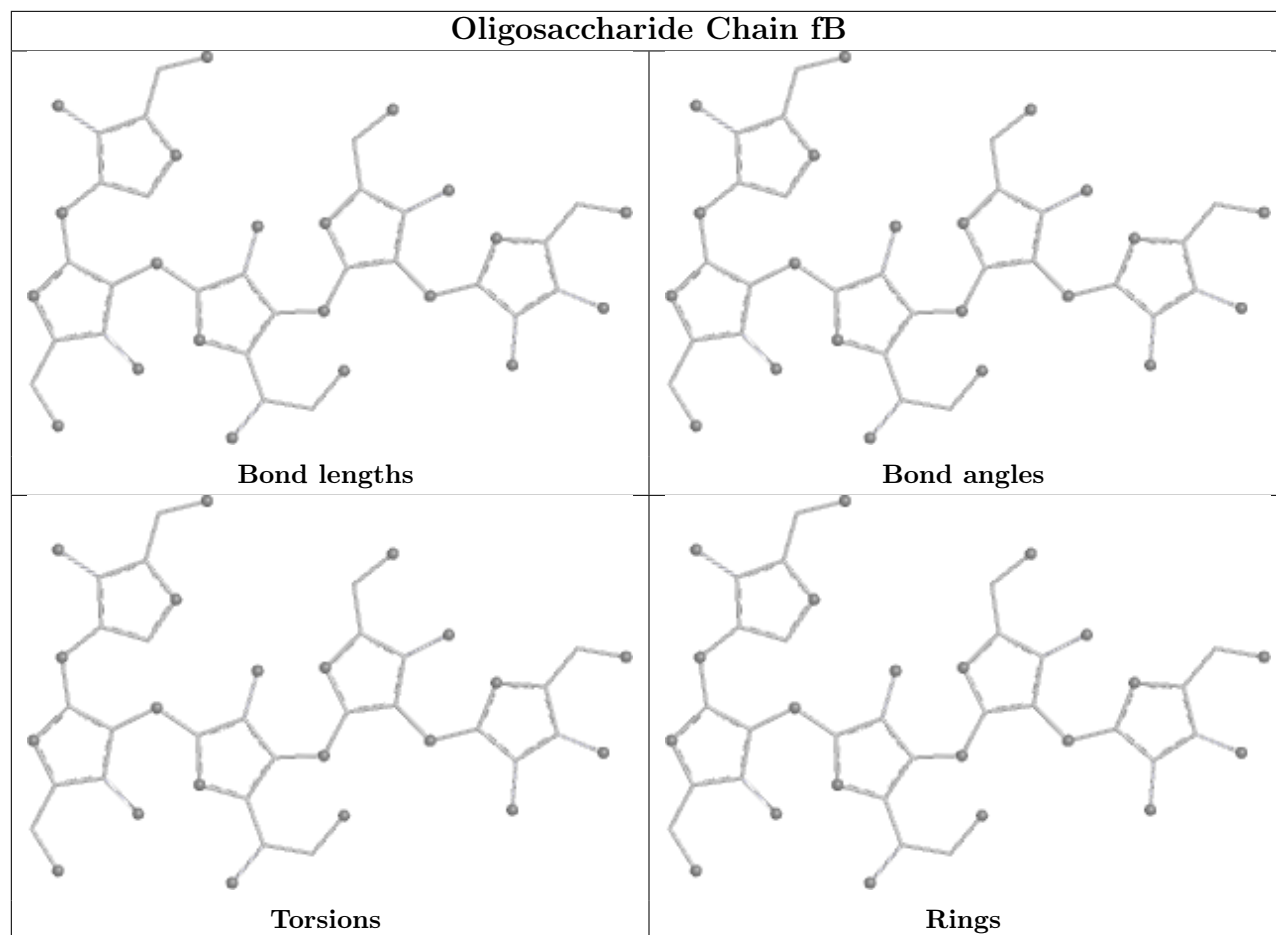


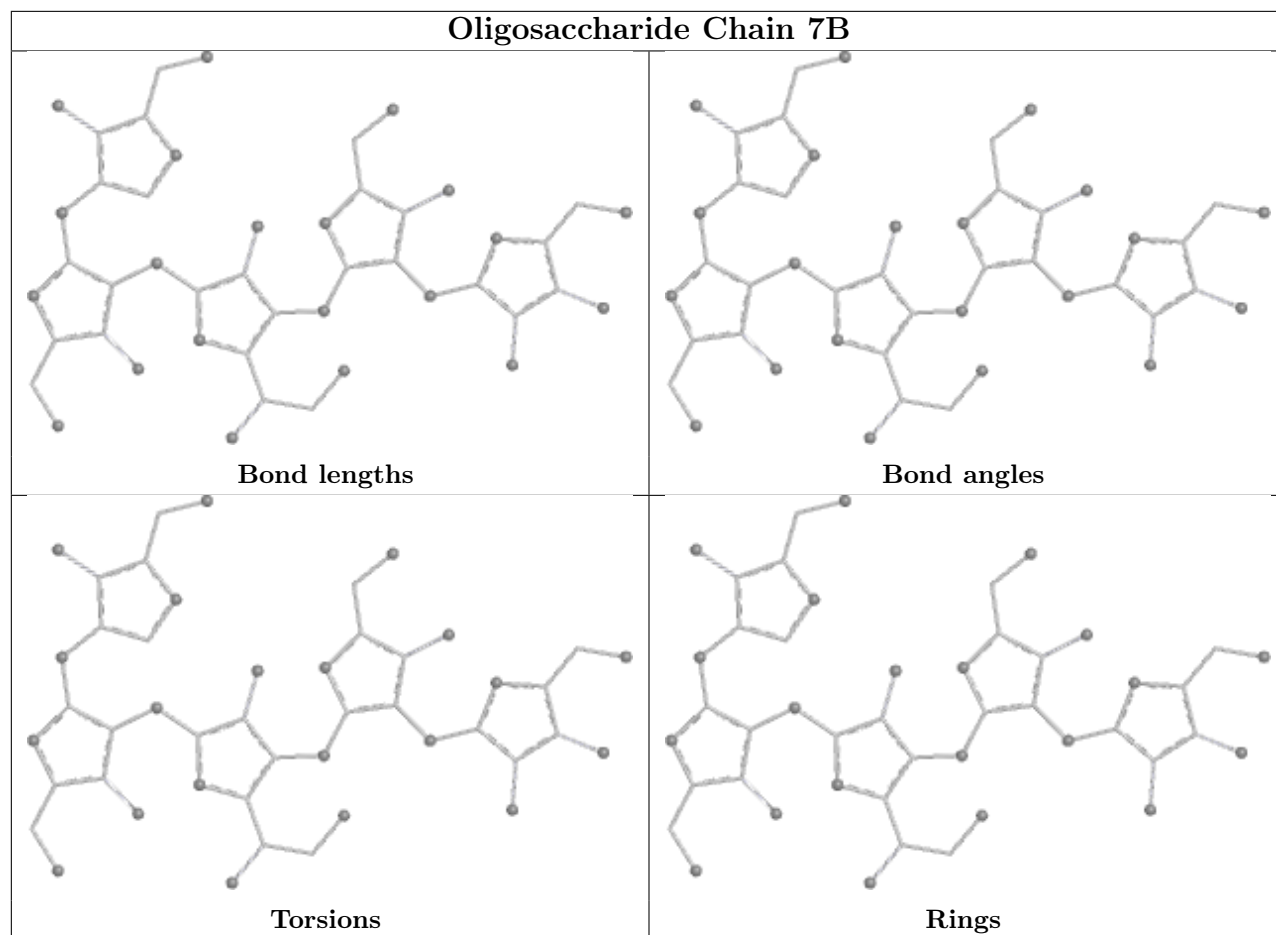


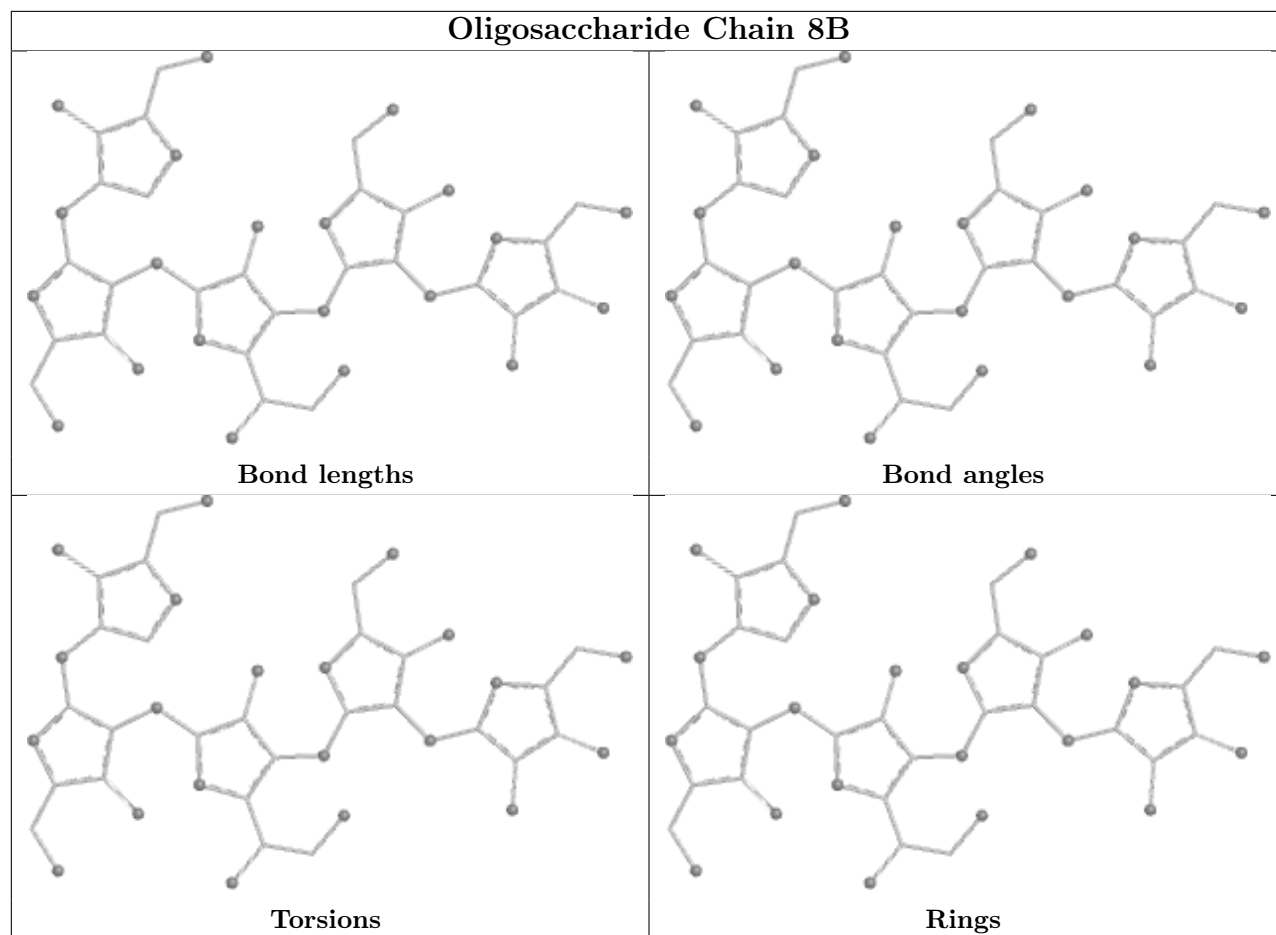


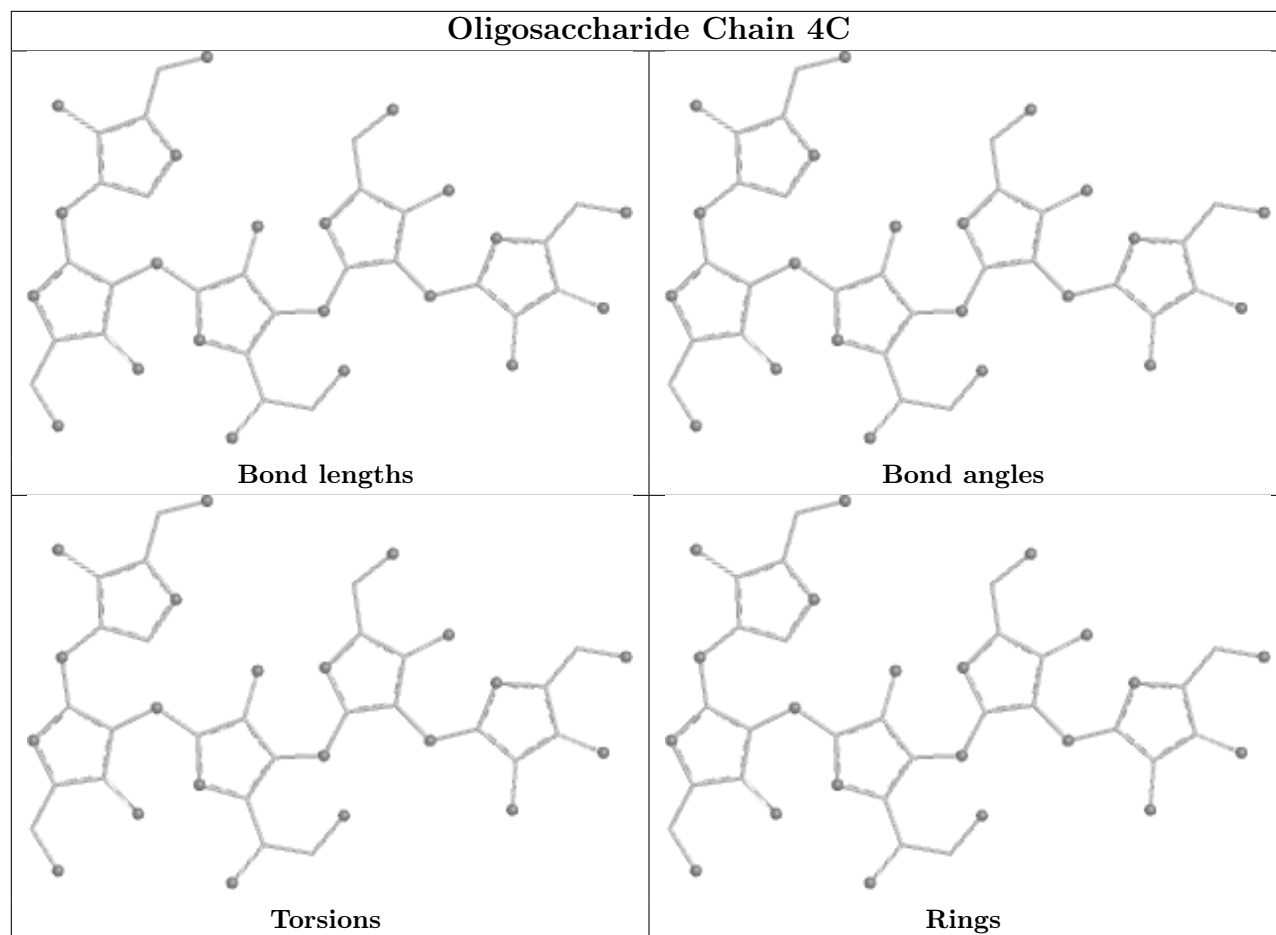


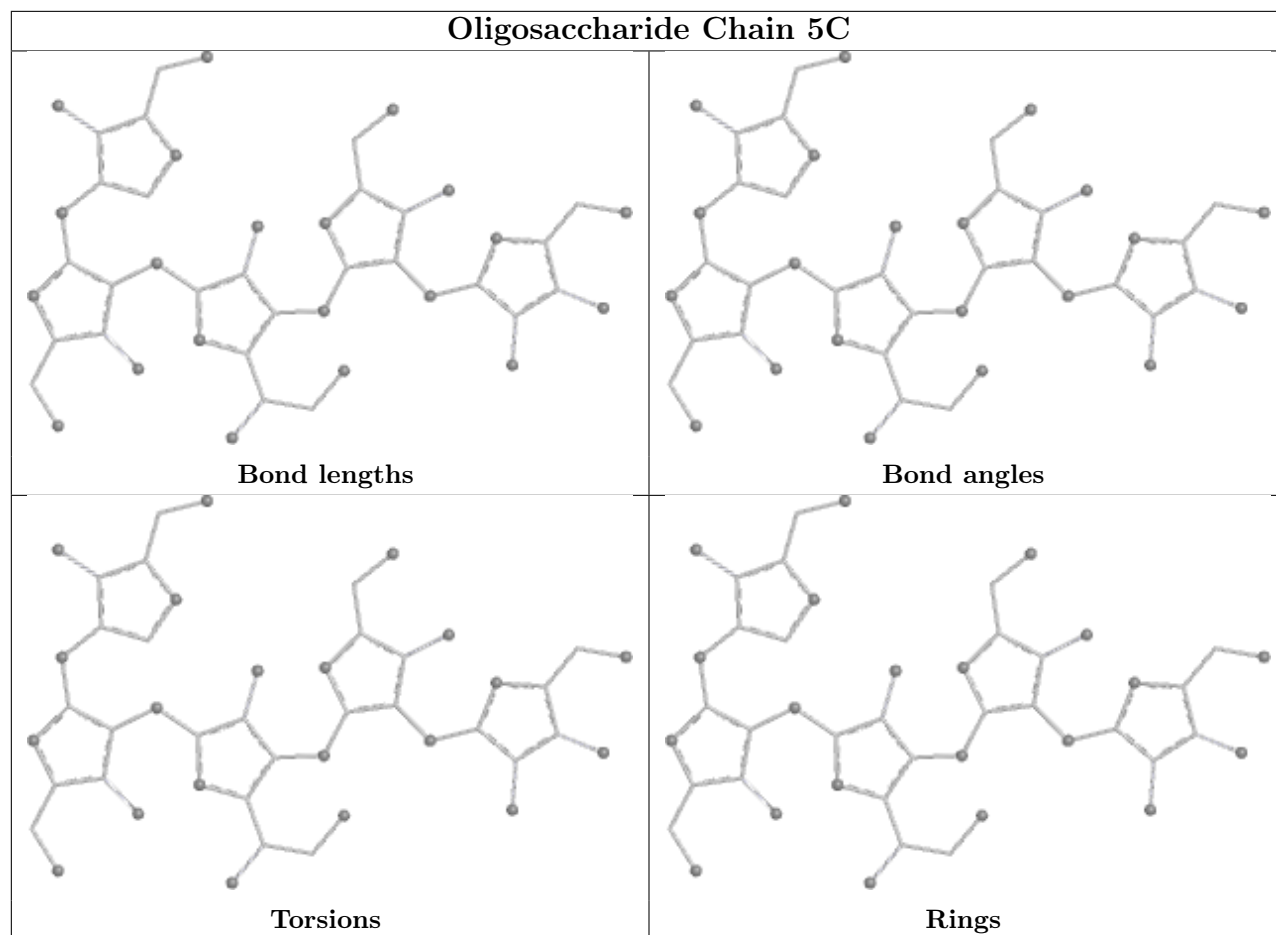


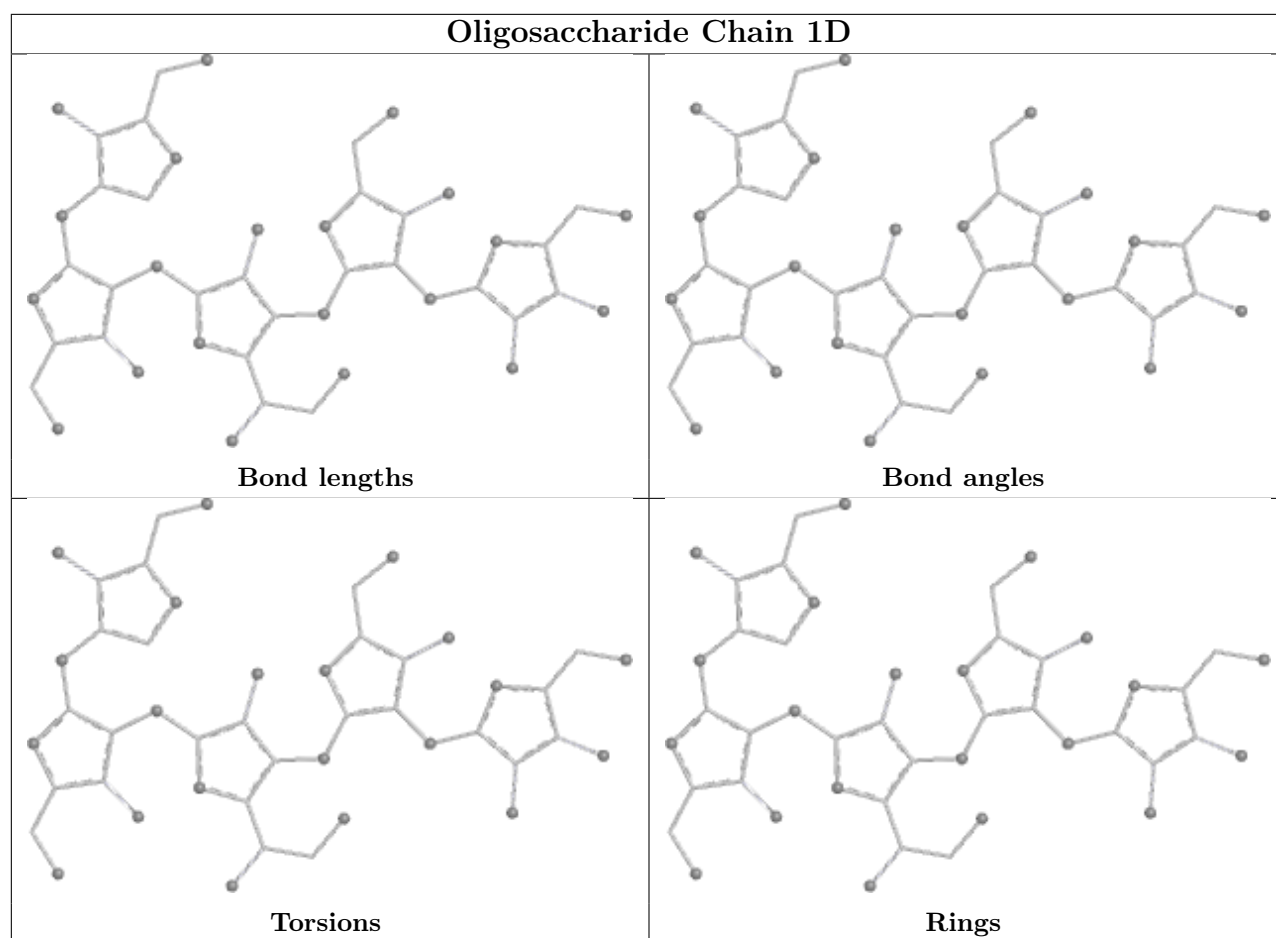


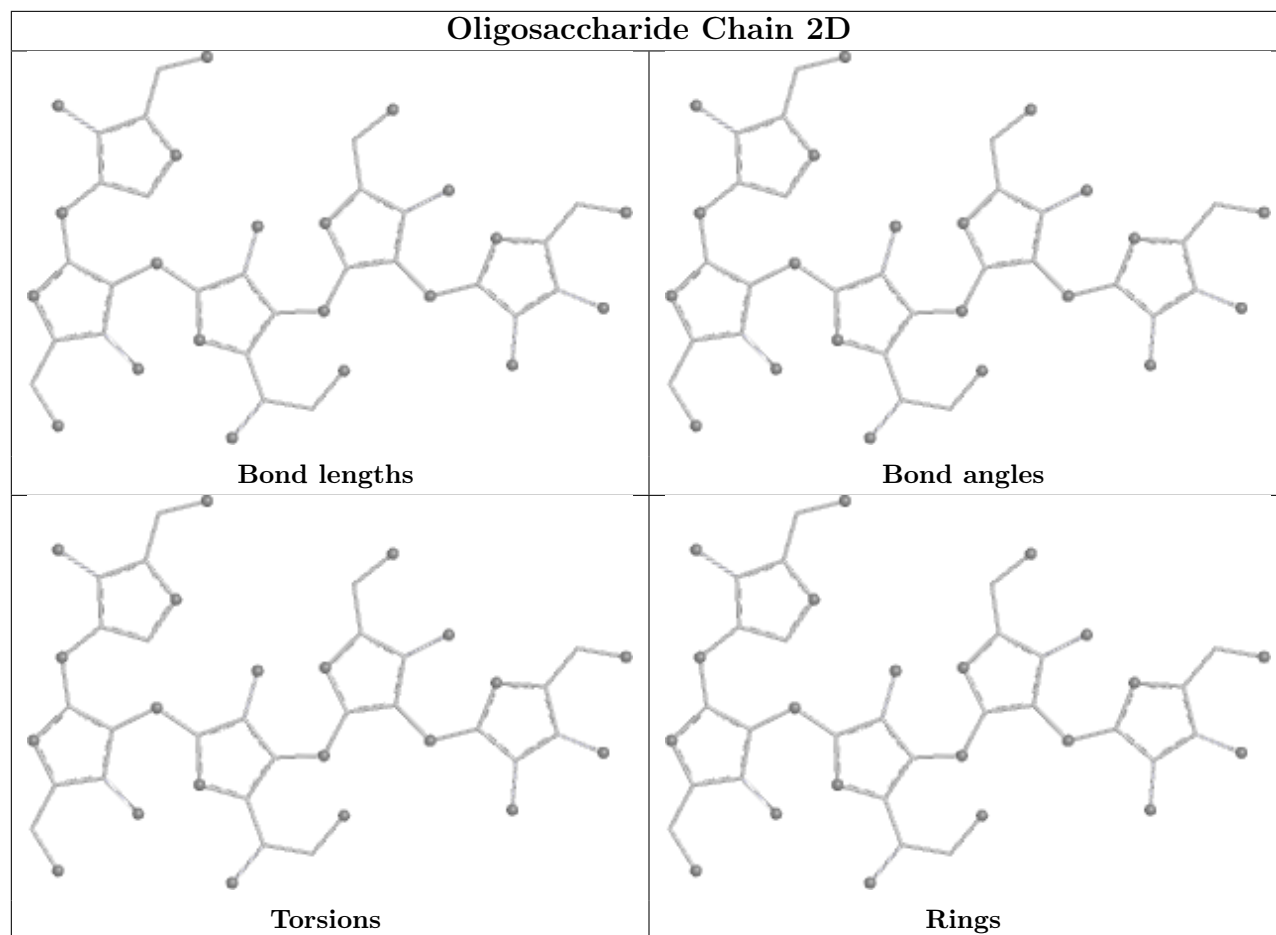


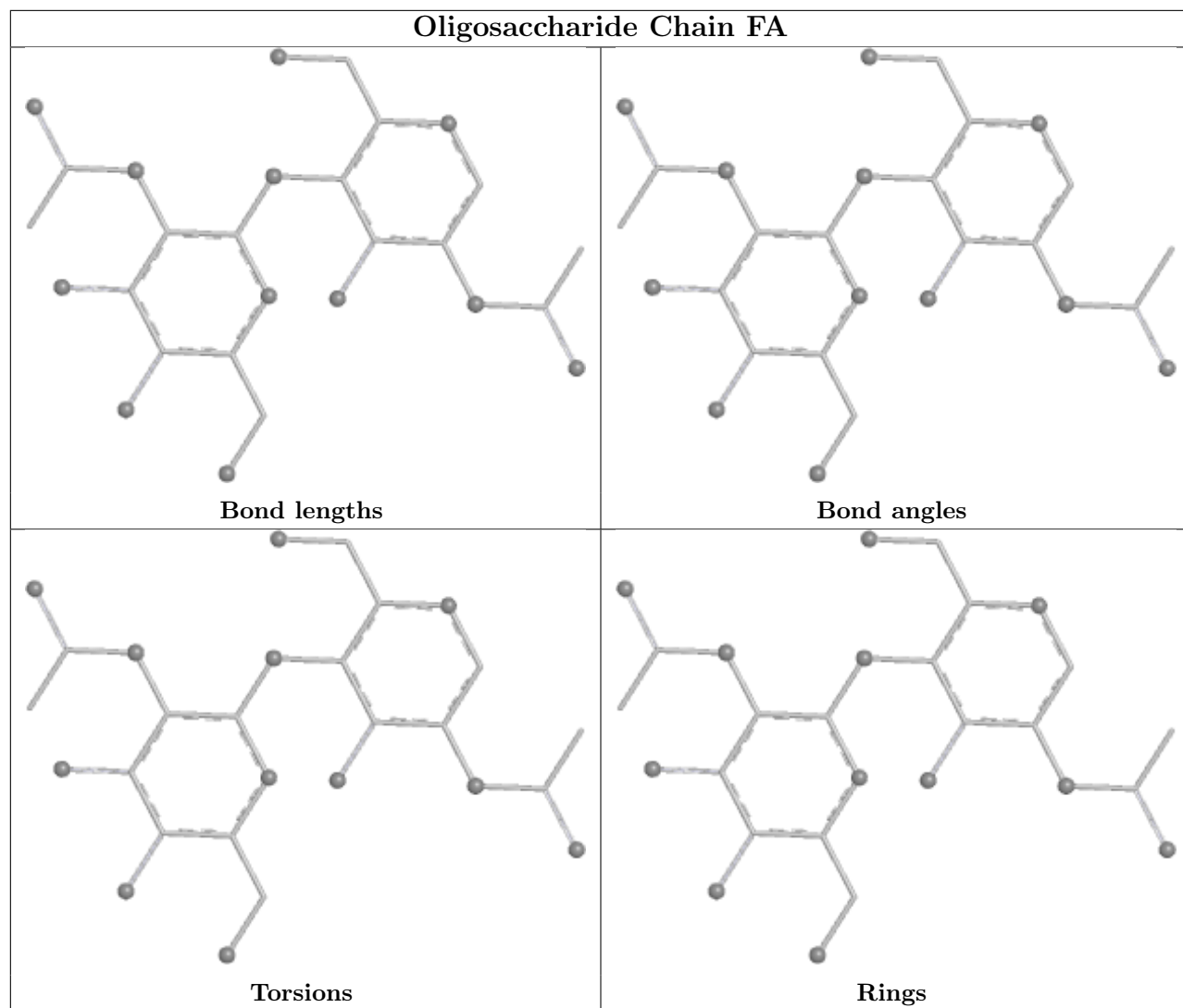


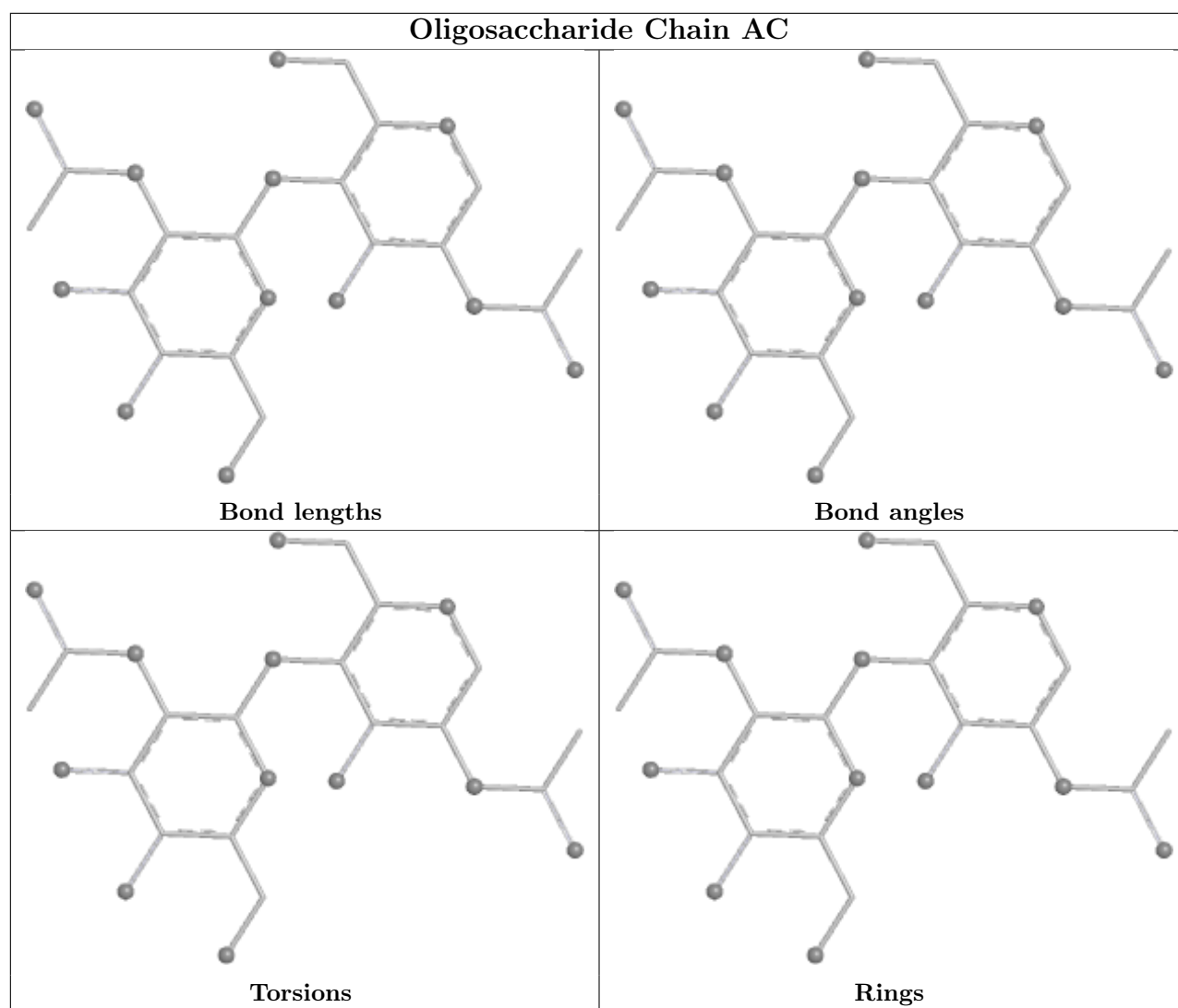


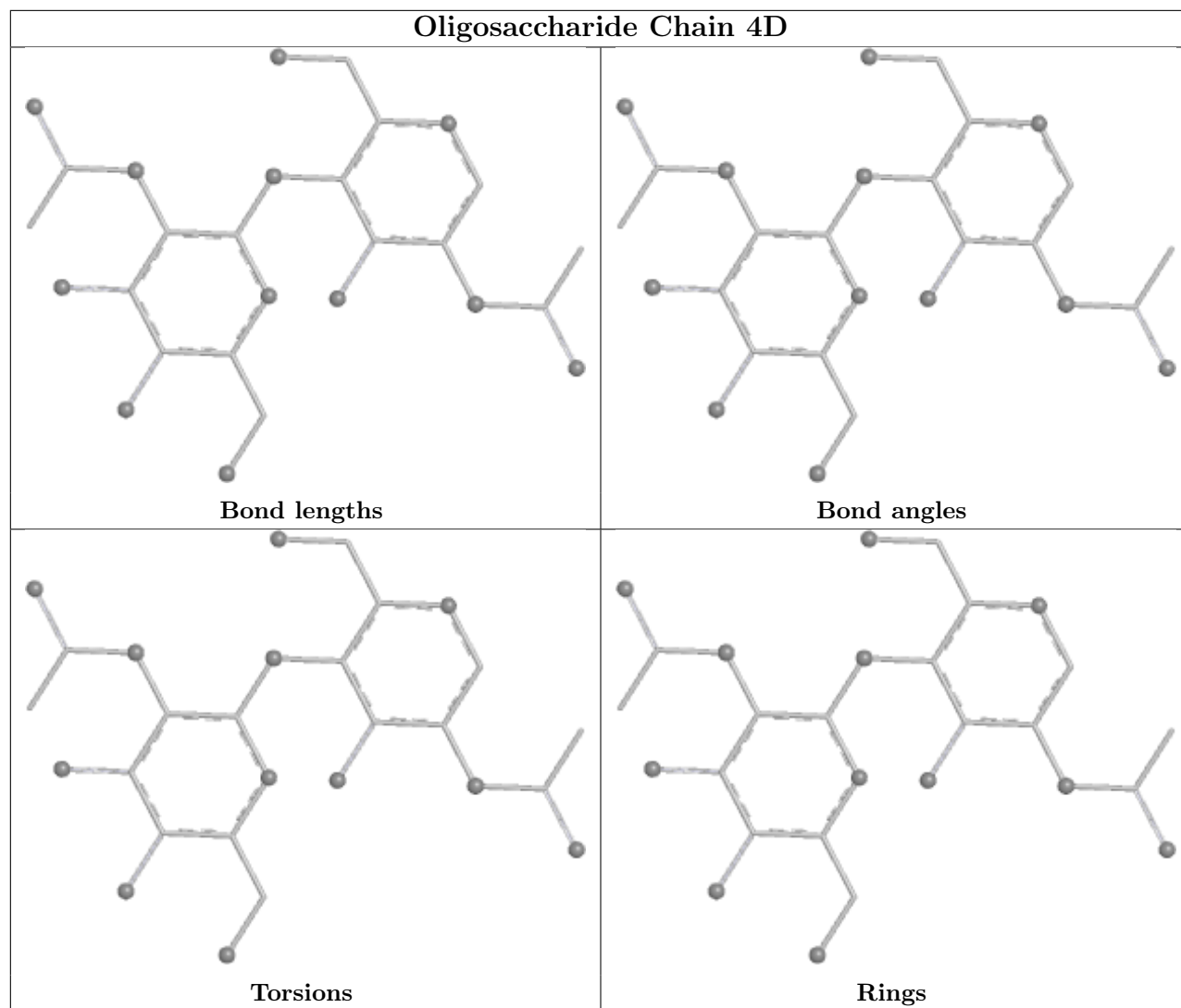


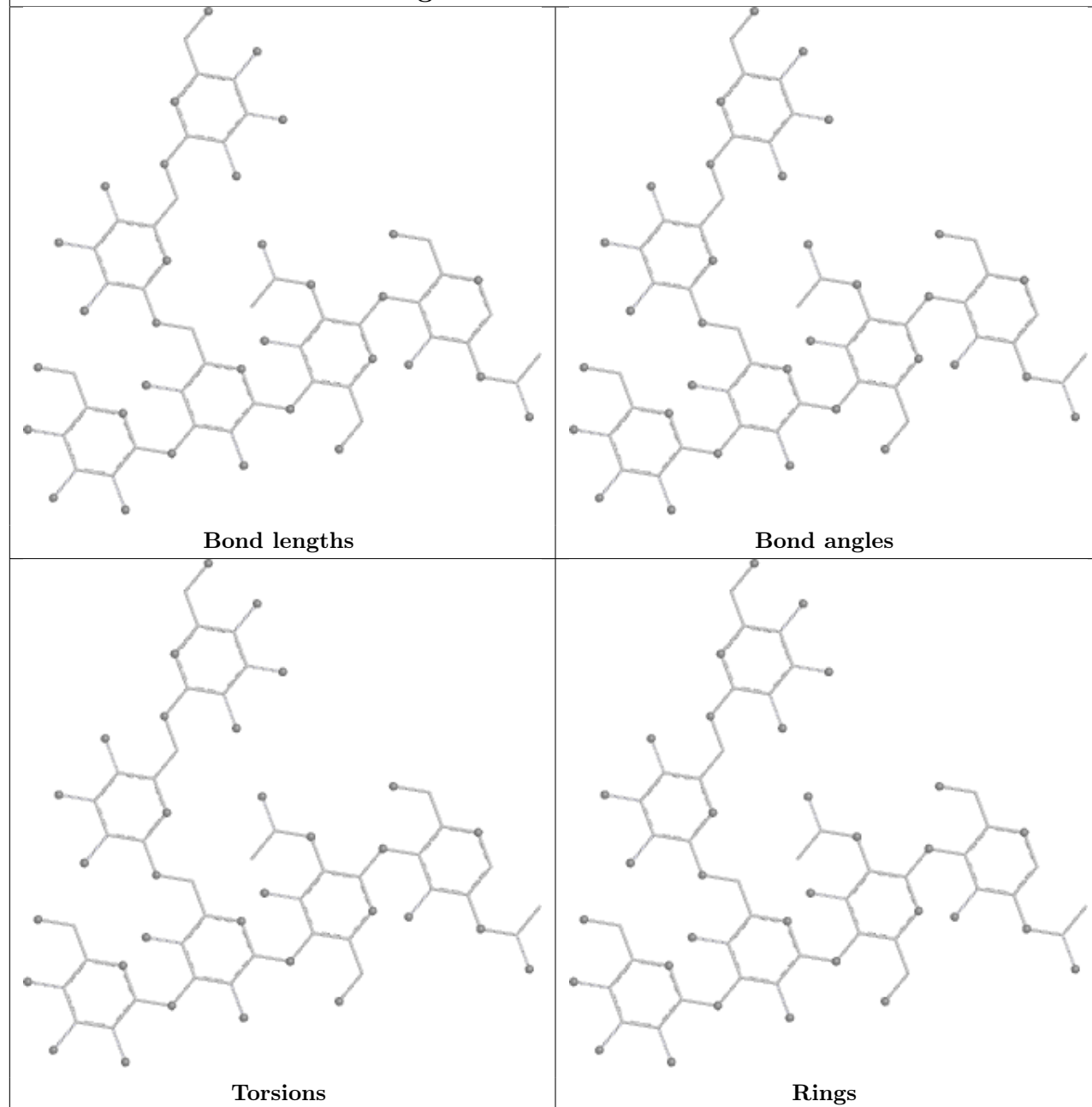


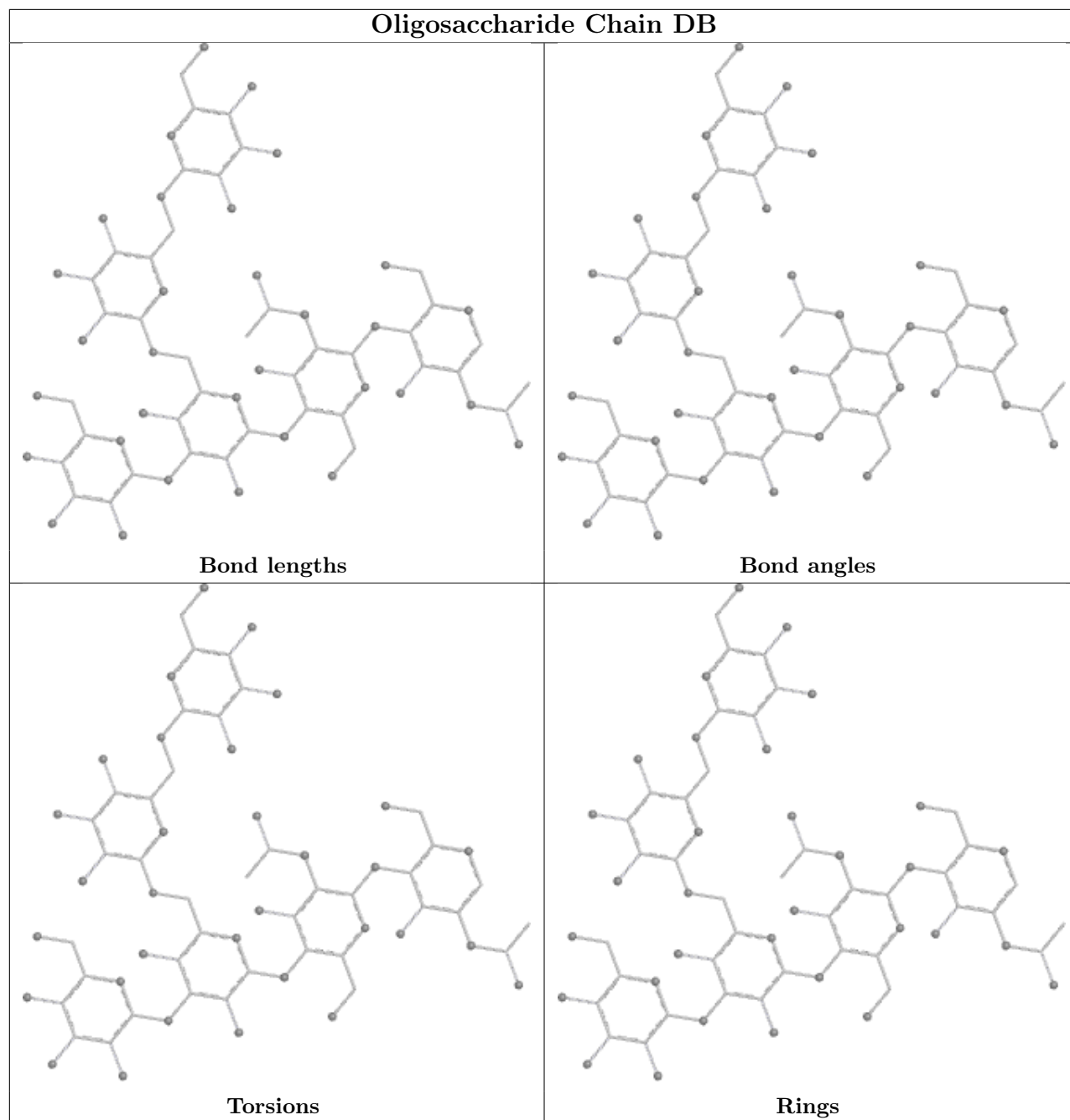


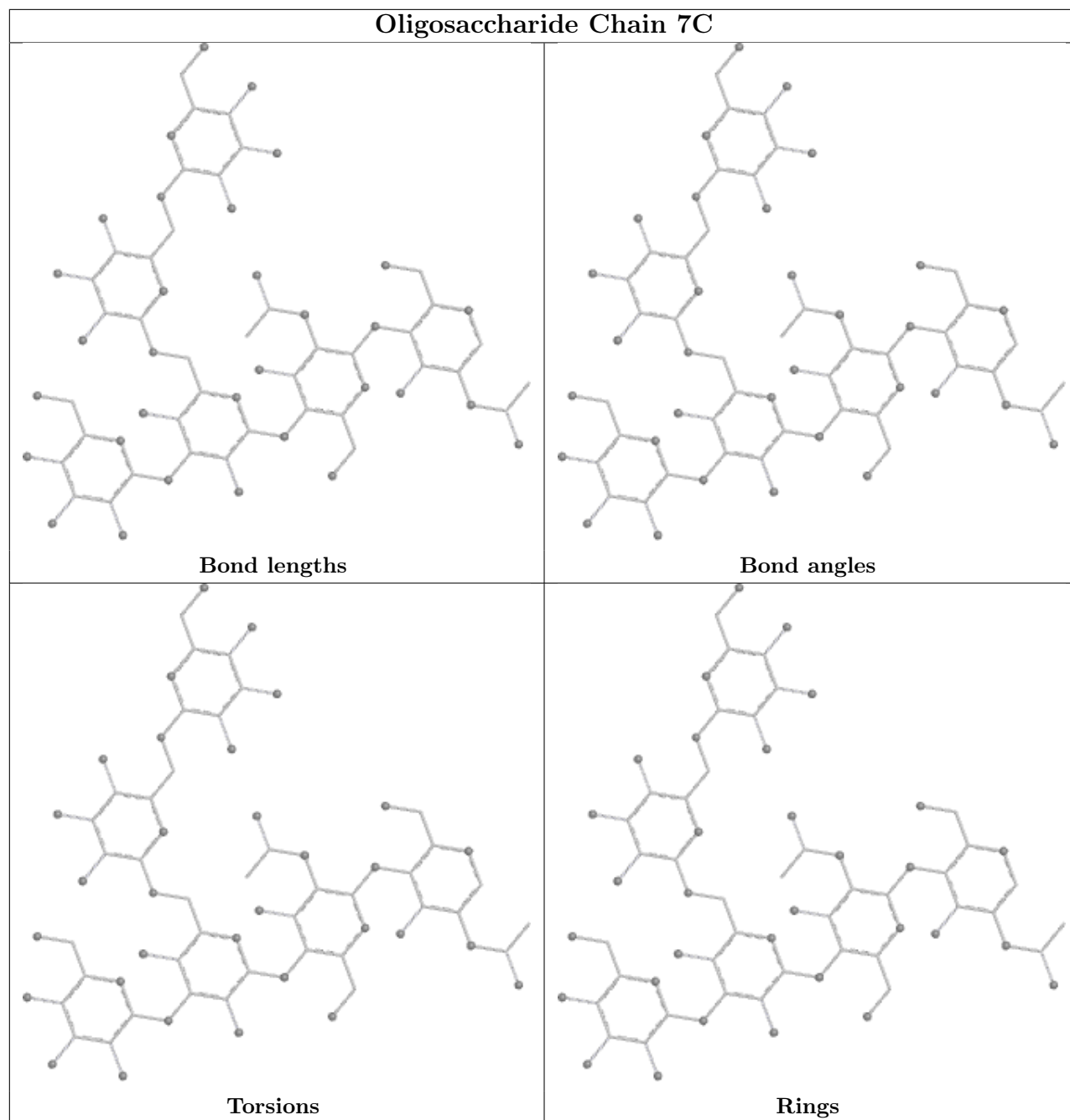


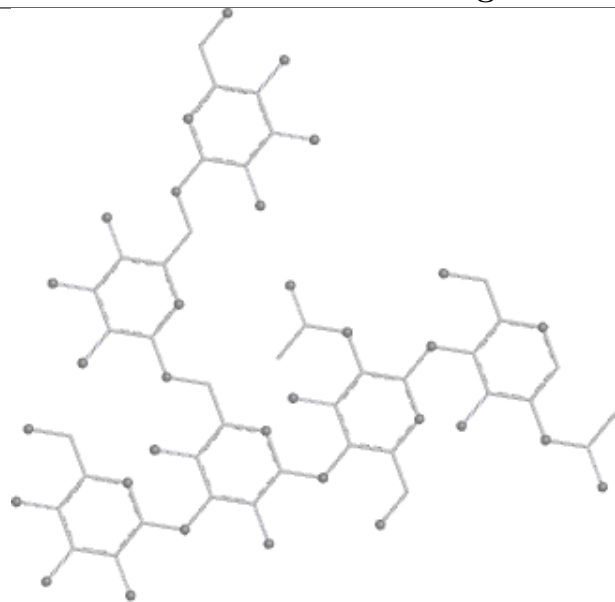
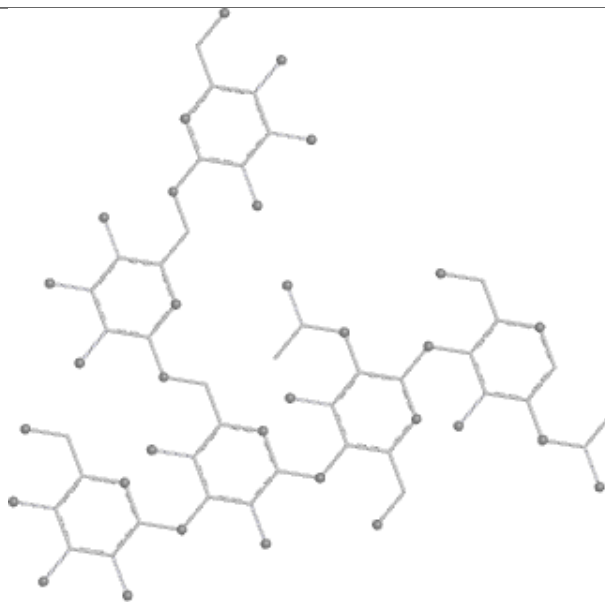
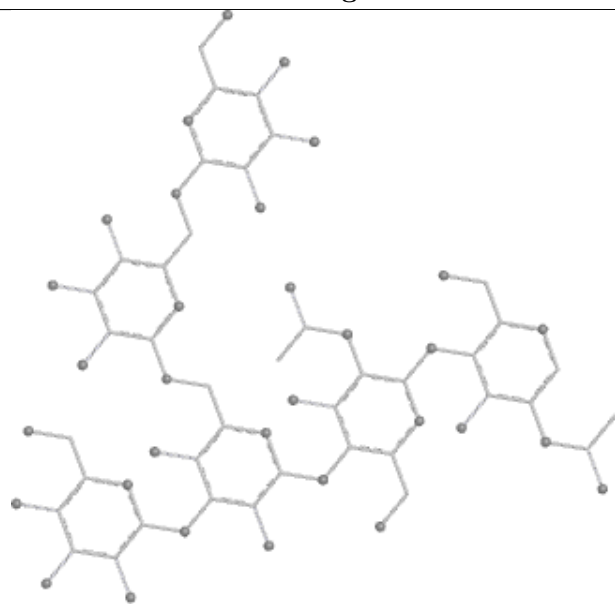
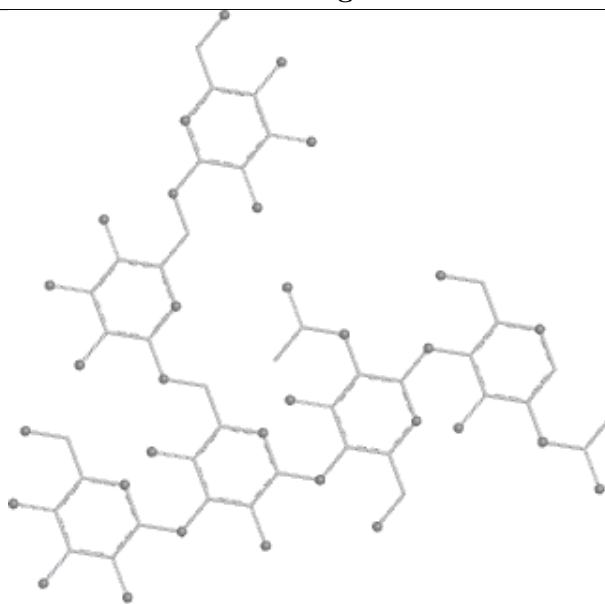




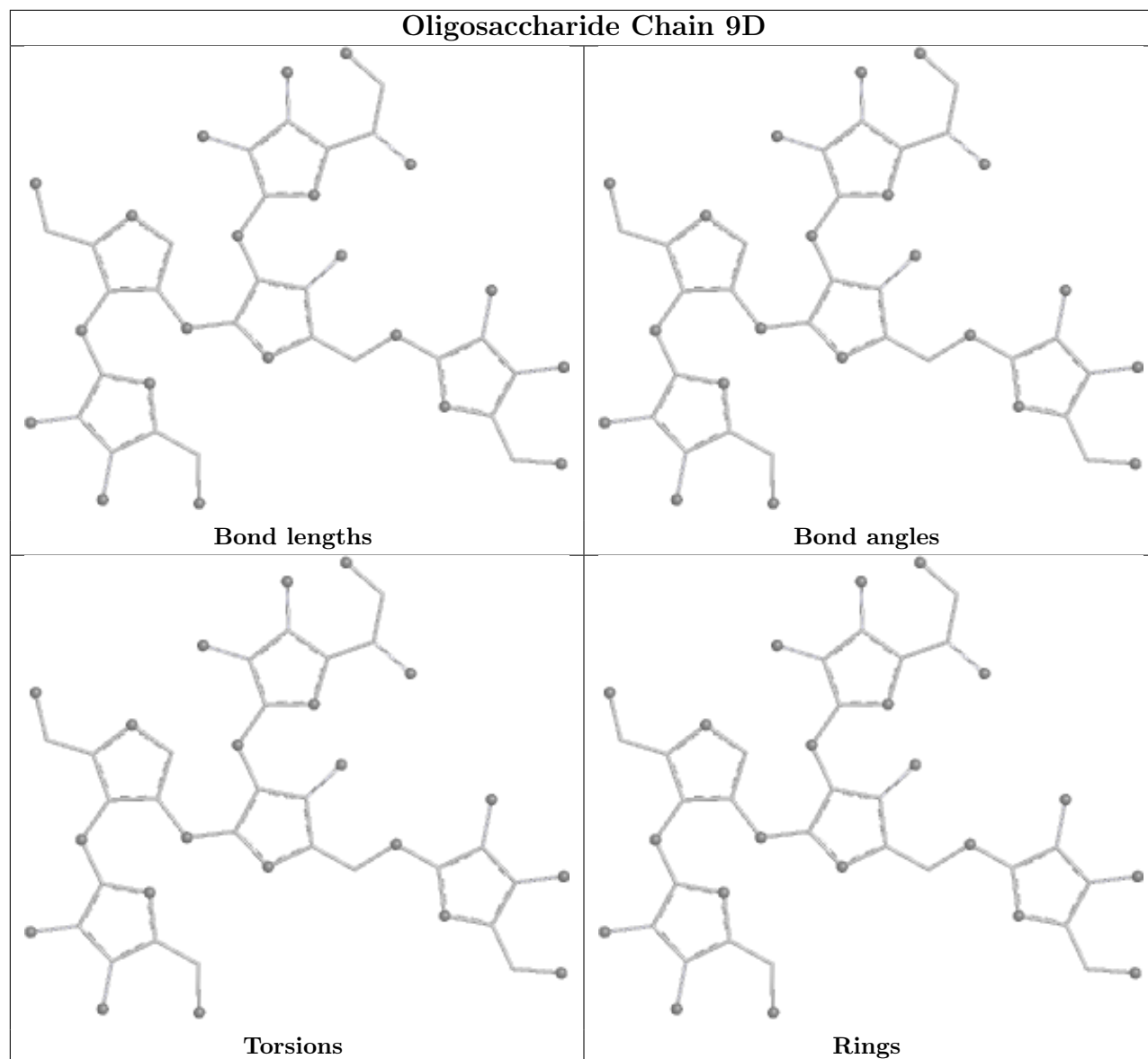
Oligosaccharide Chain GA

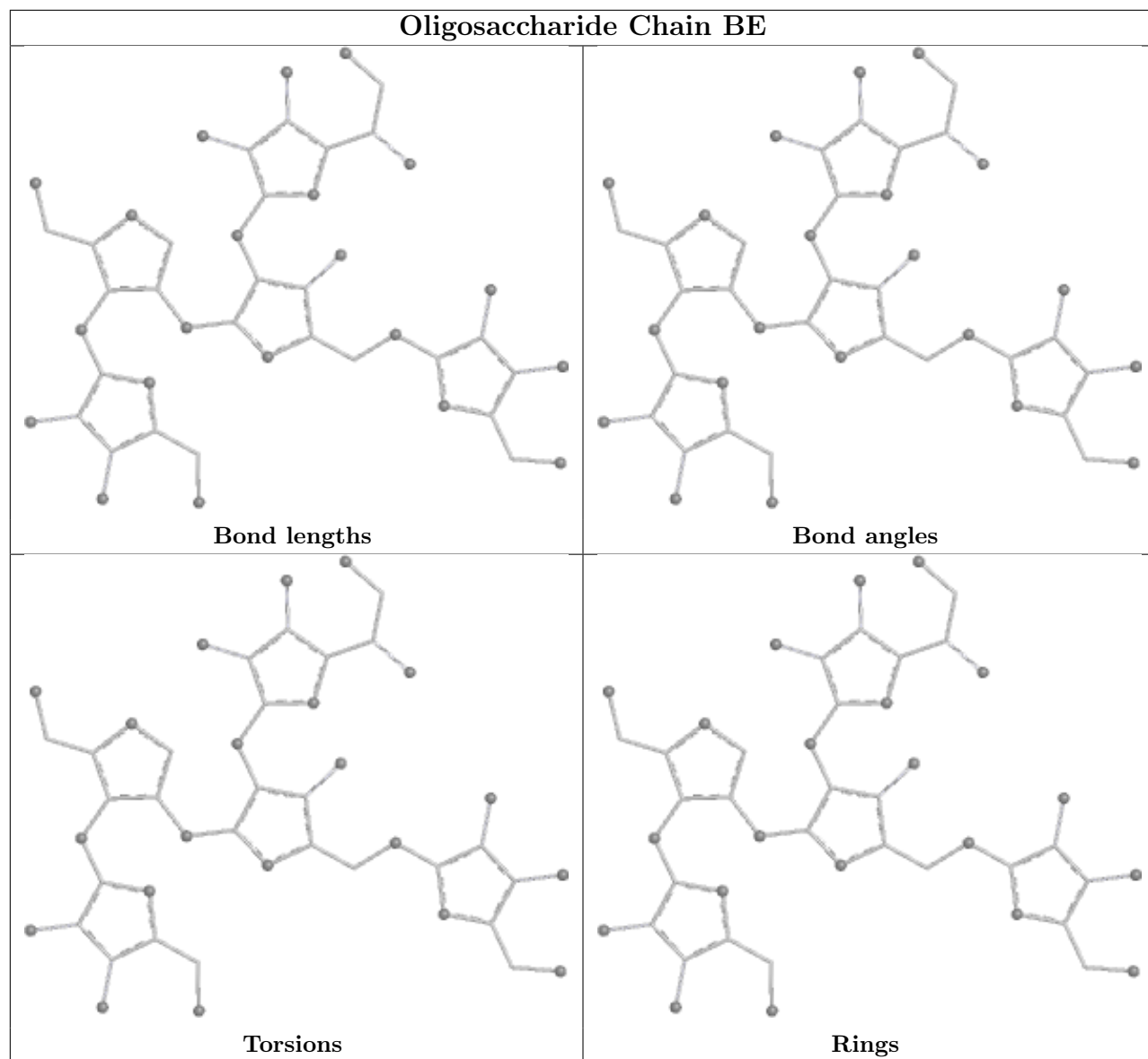


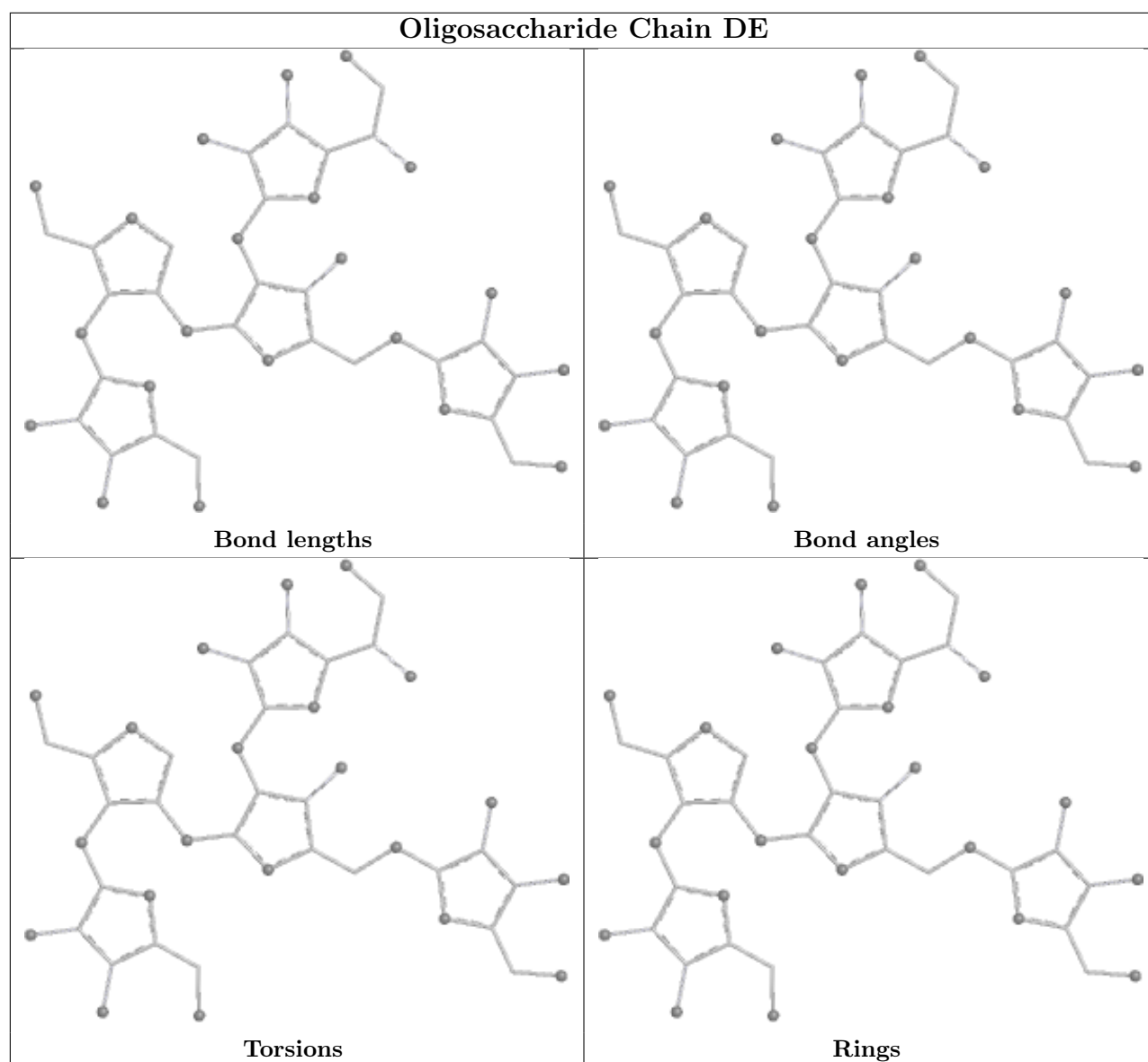


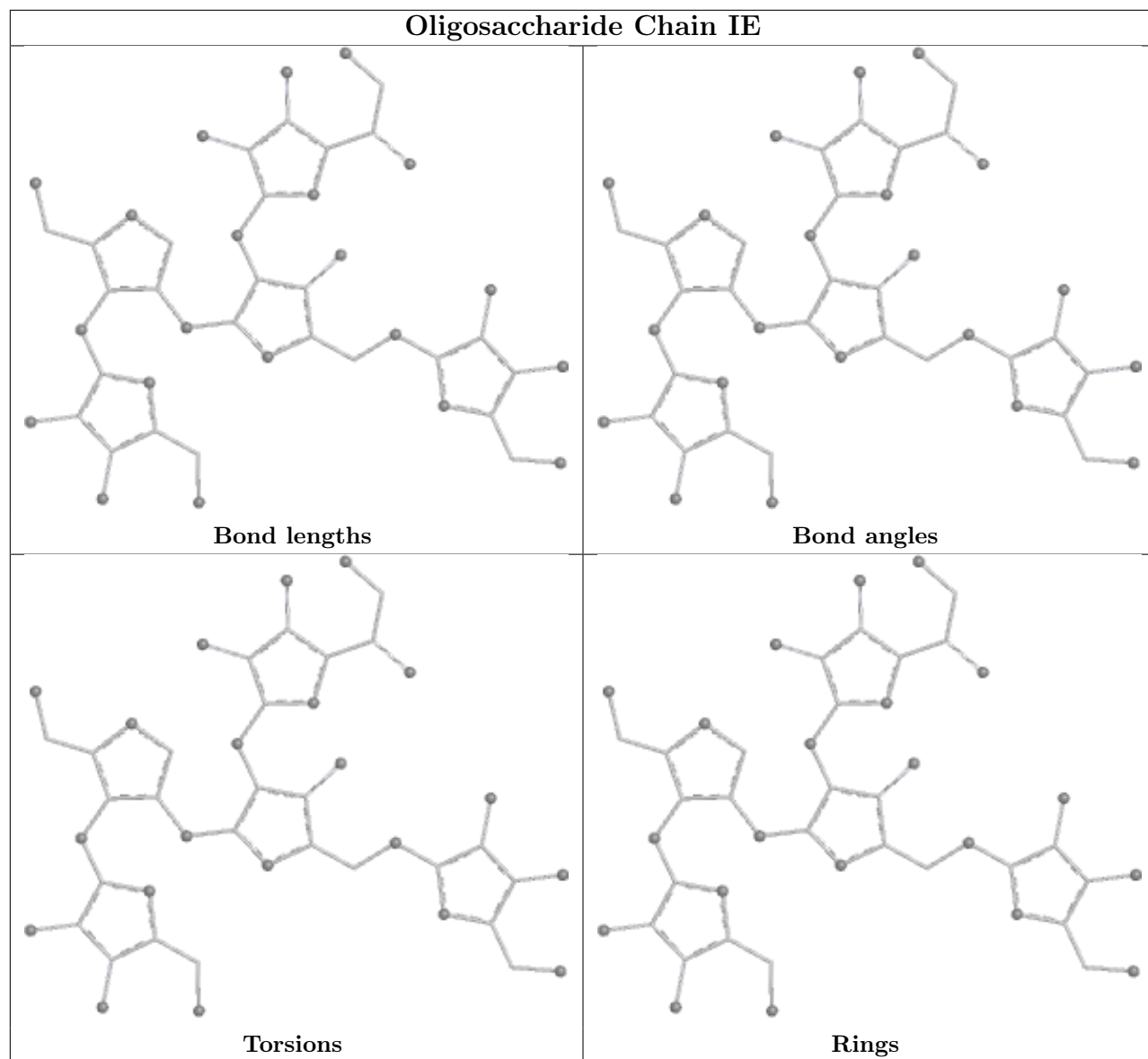
Oligosaccharide Chain 5D**Bond lengths****Bond angles****Torsions****Rings**

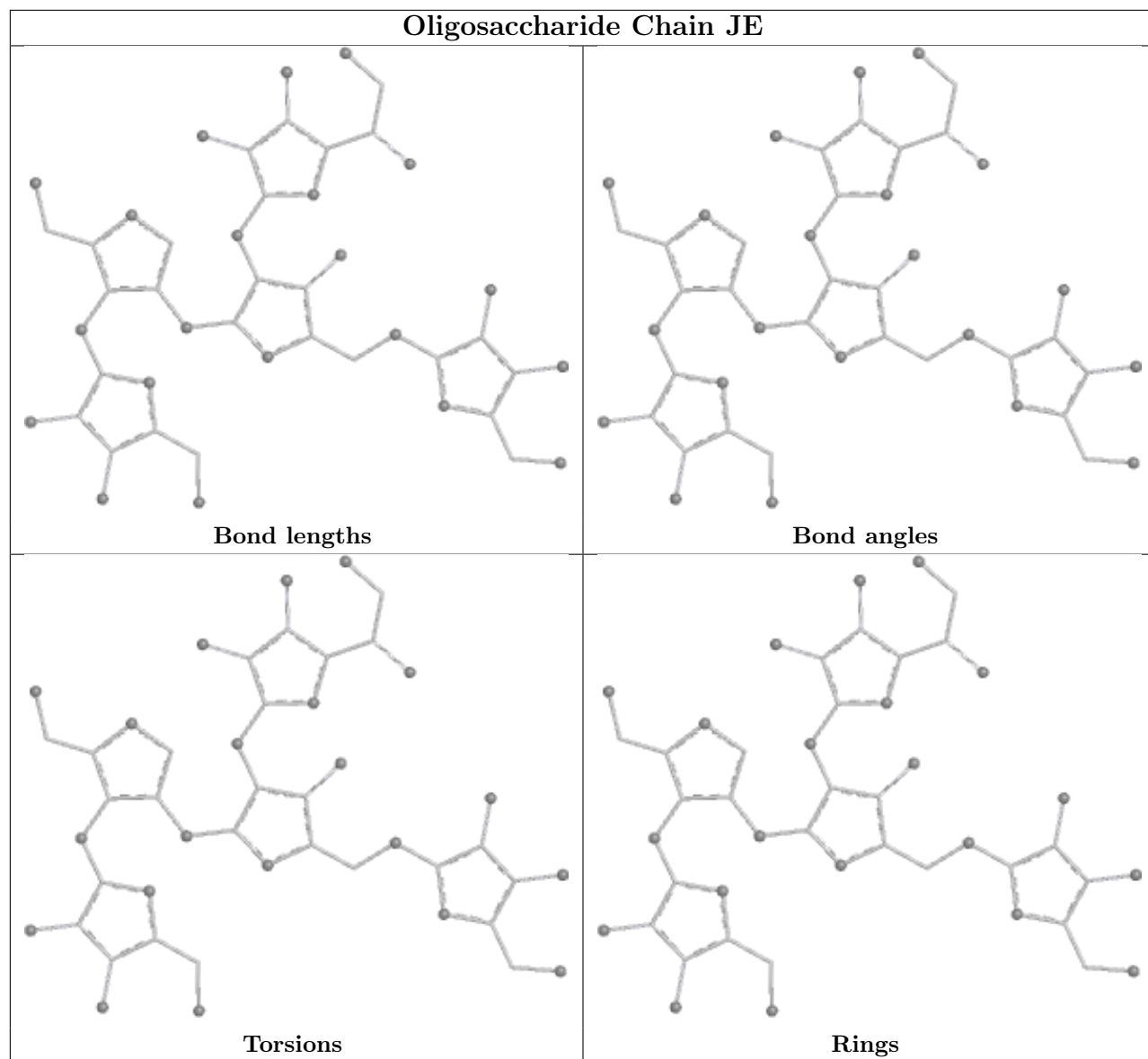
Oligosaccharide Chain 9D



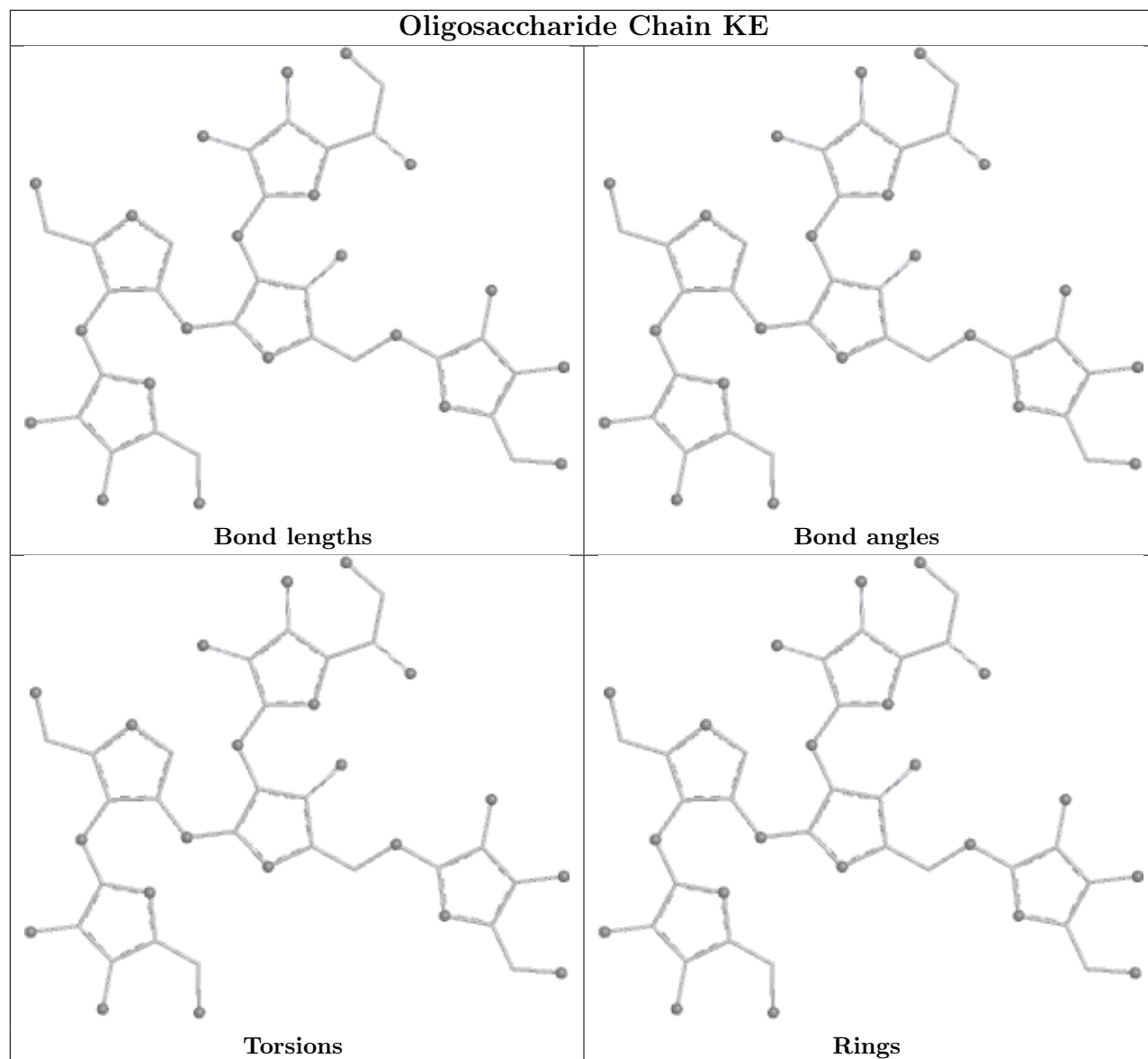


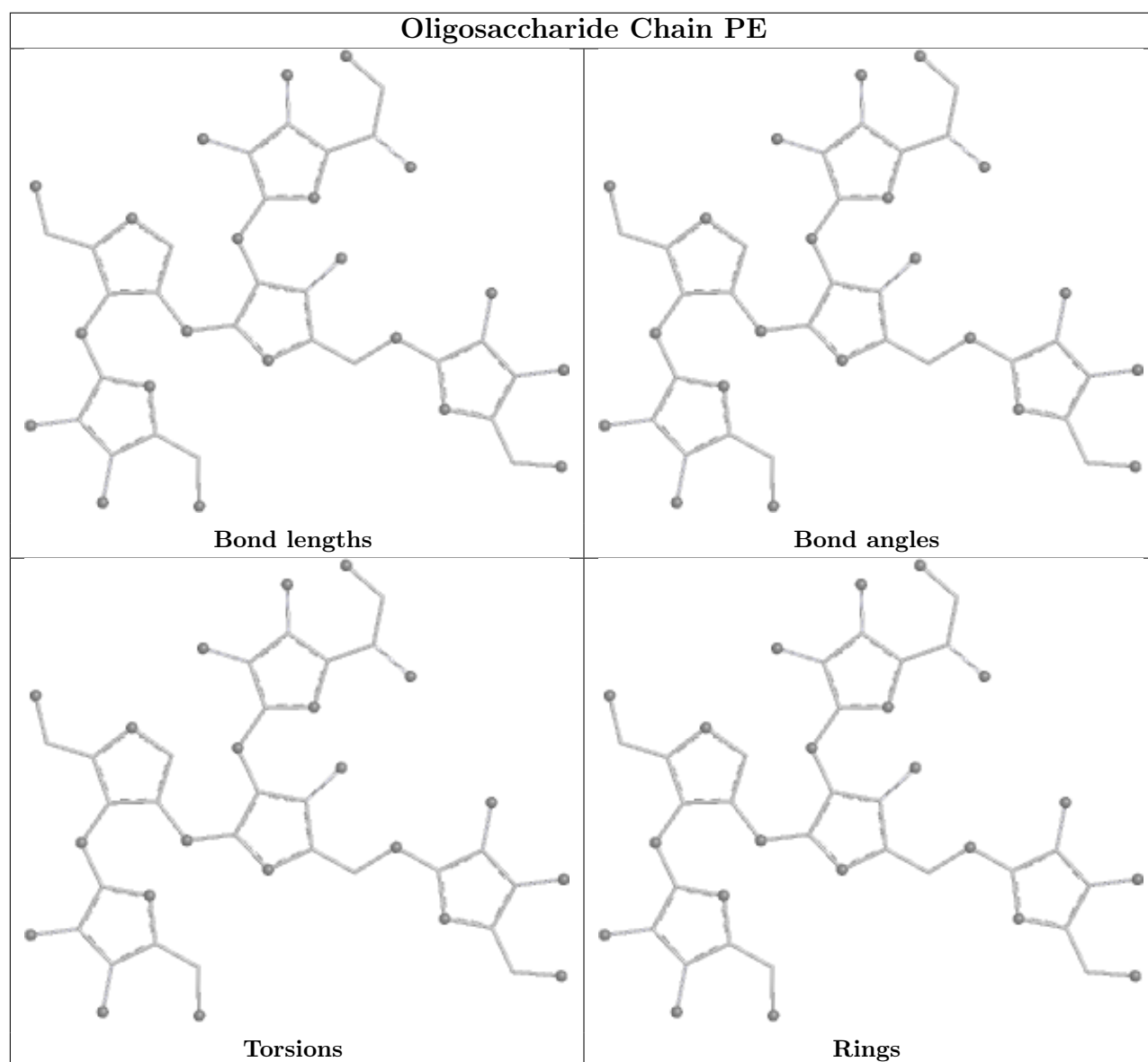


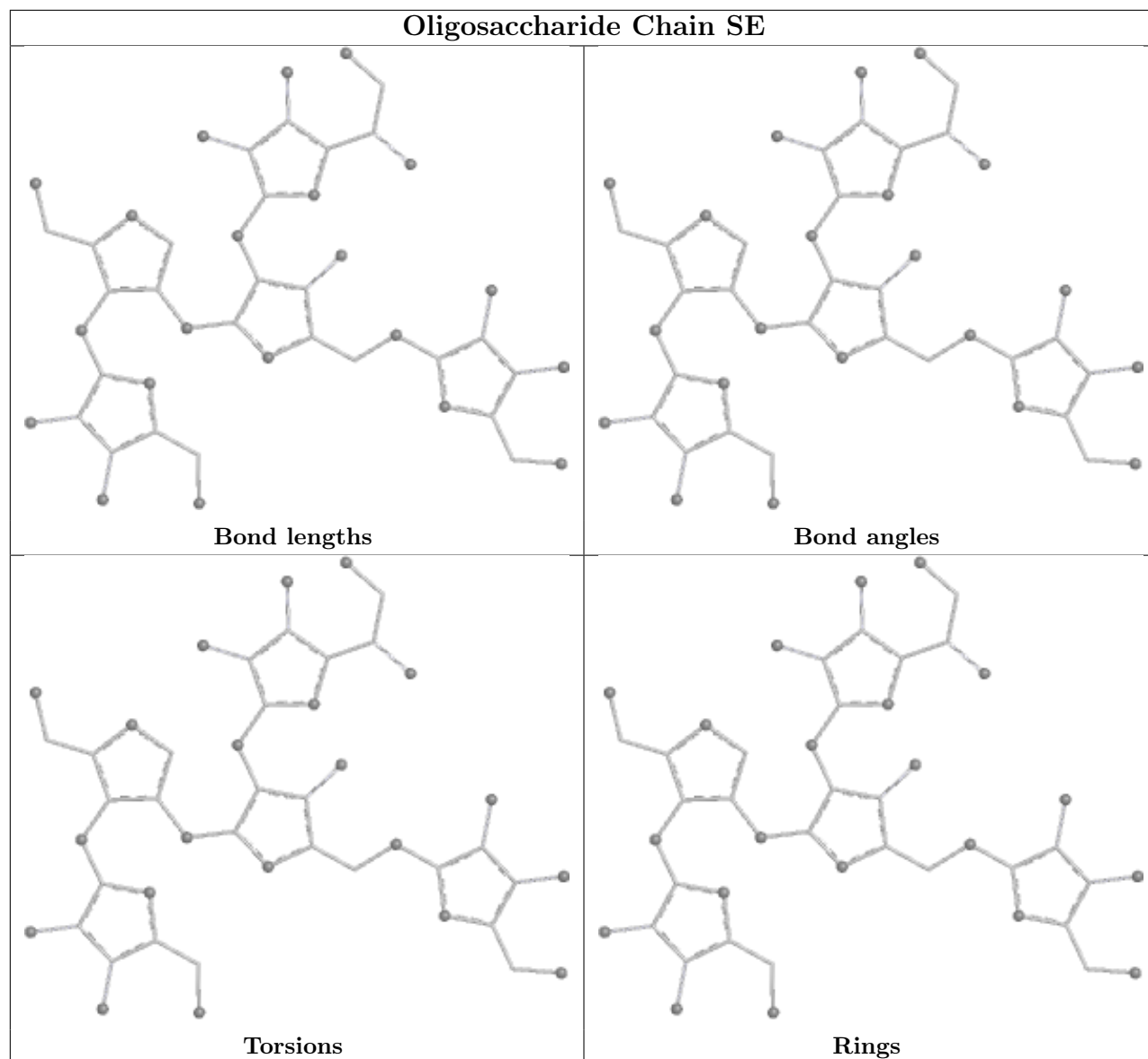


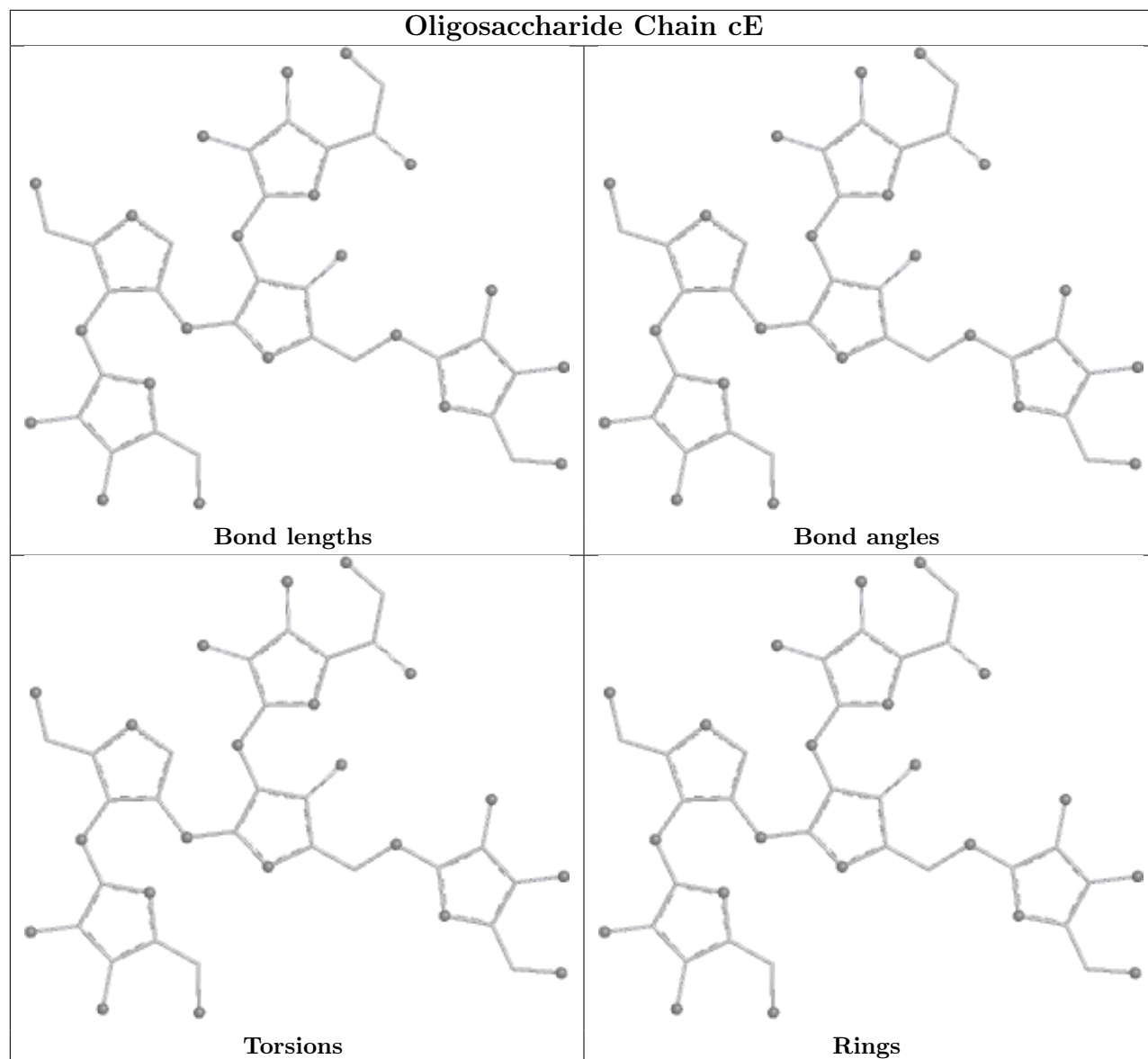


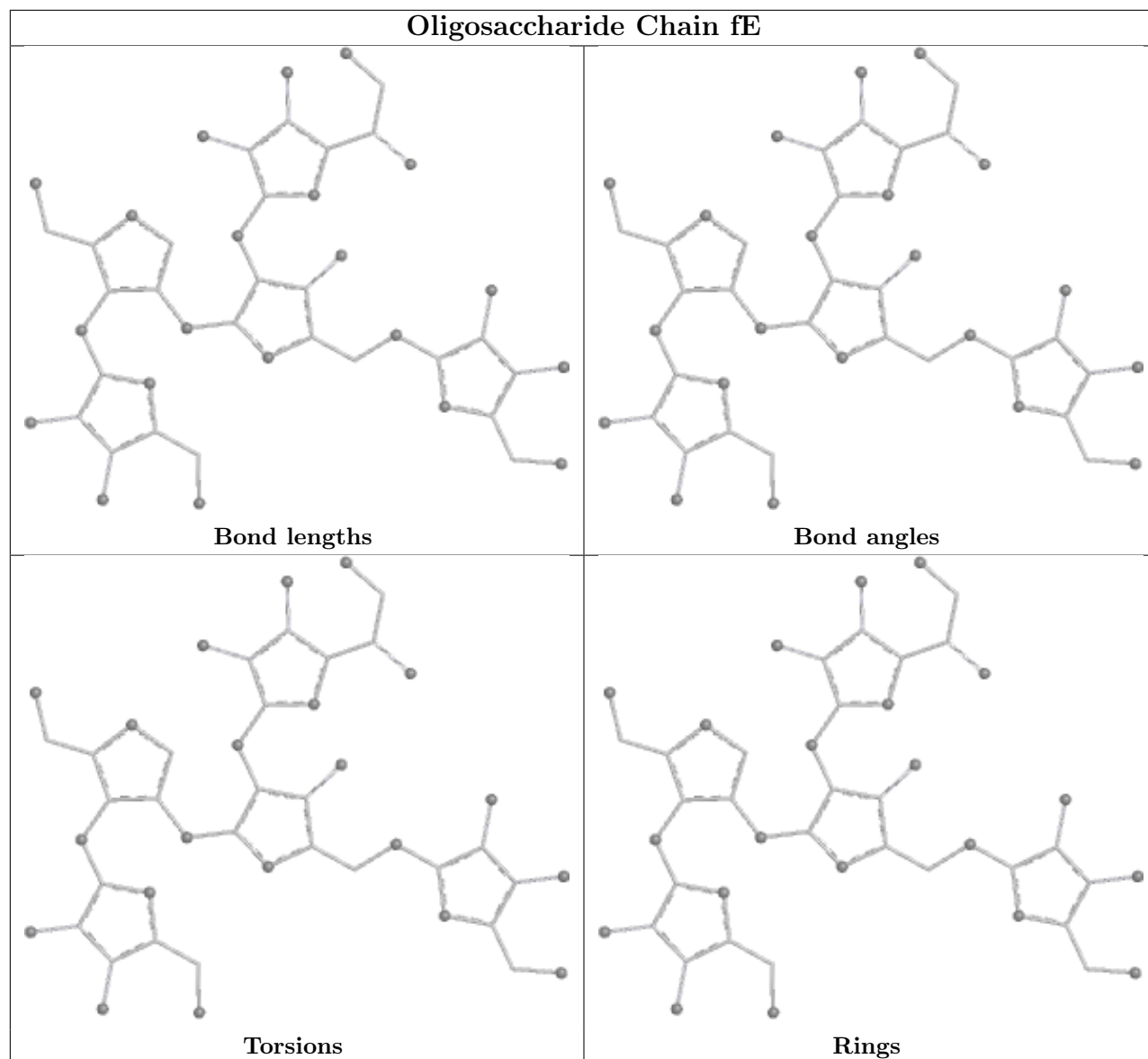
Oligosaccharide Chain KE

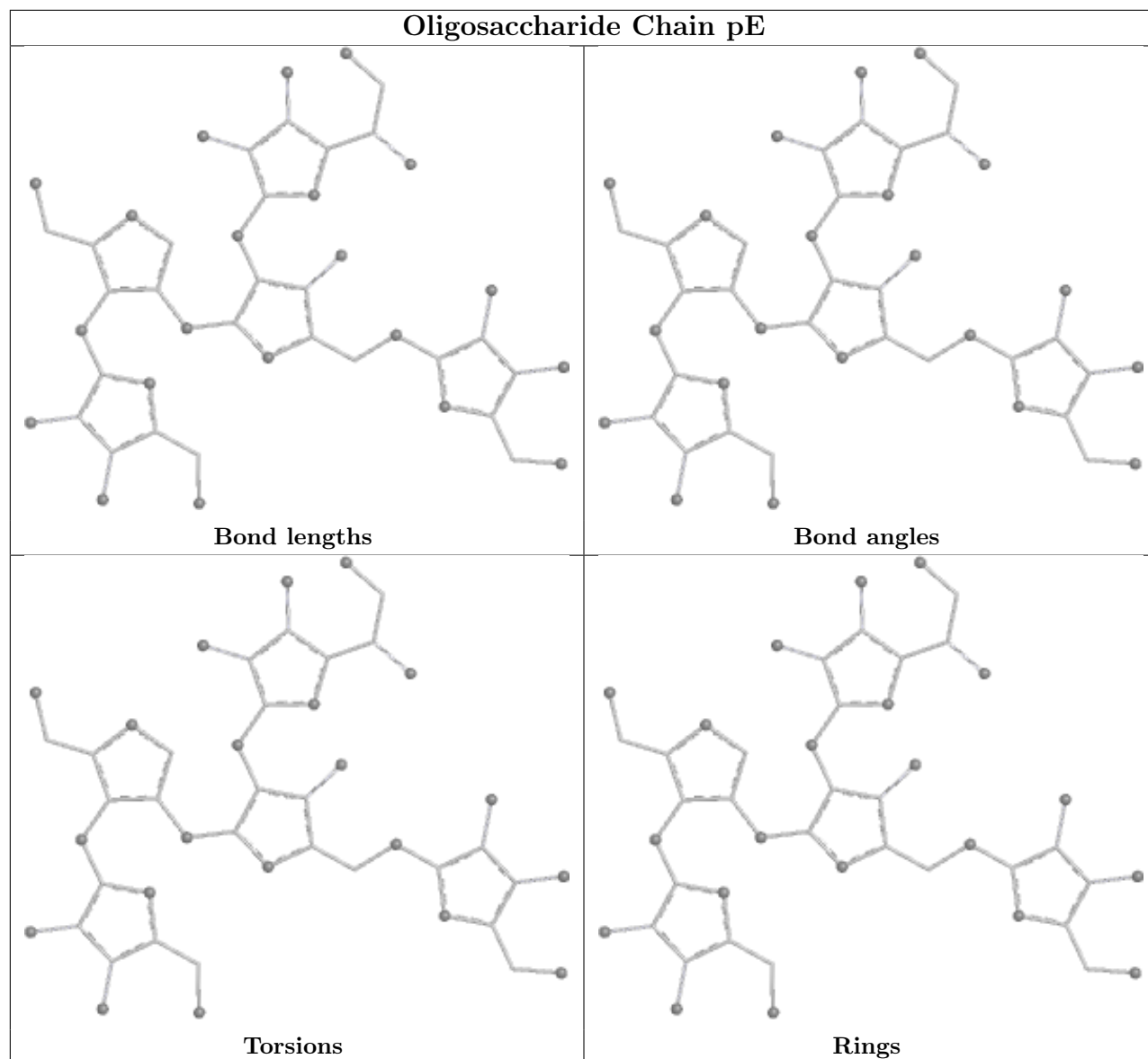


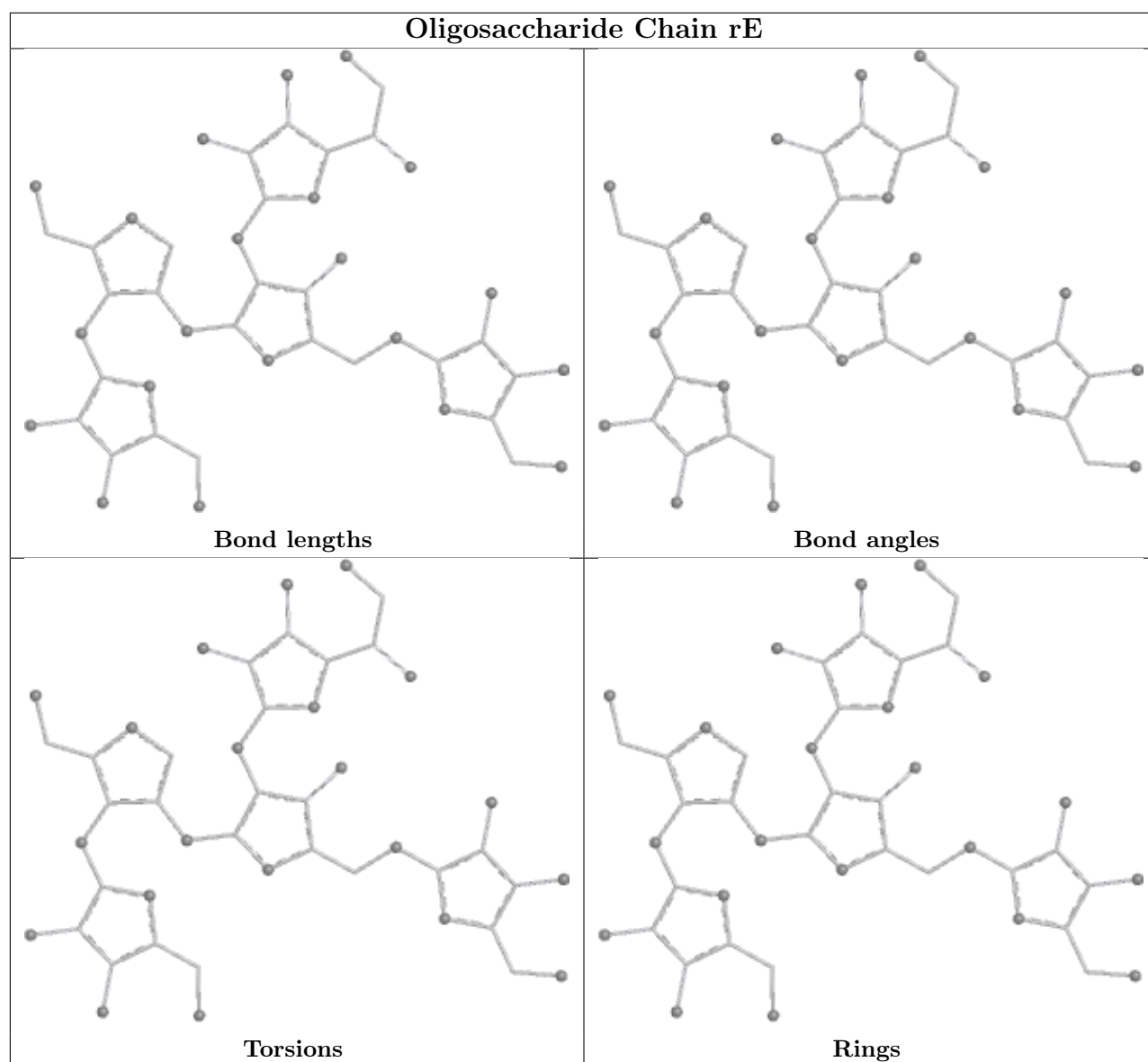


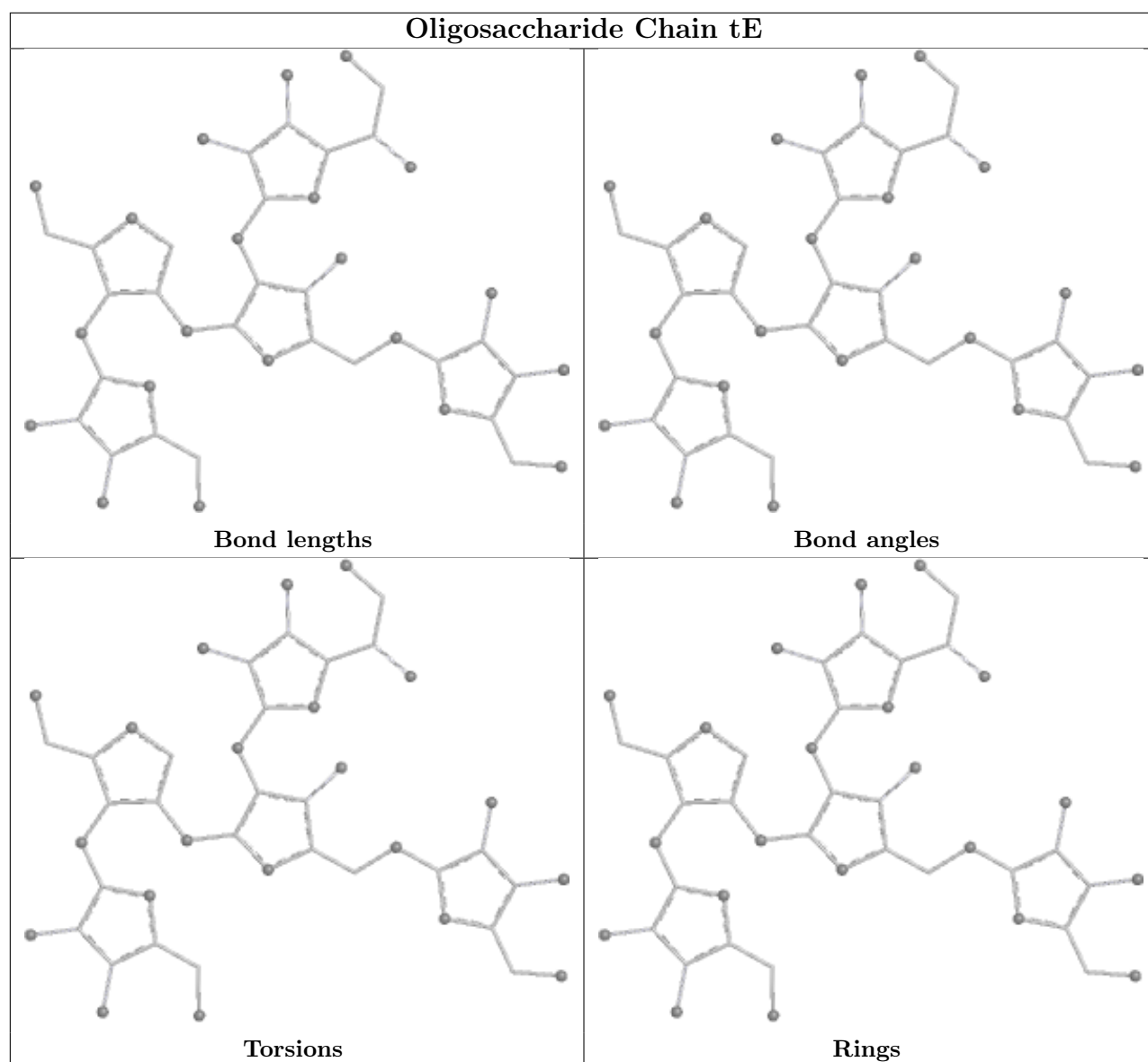


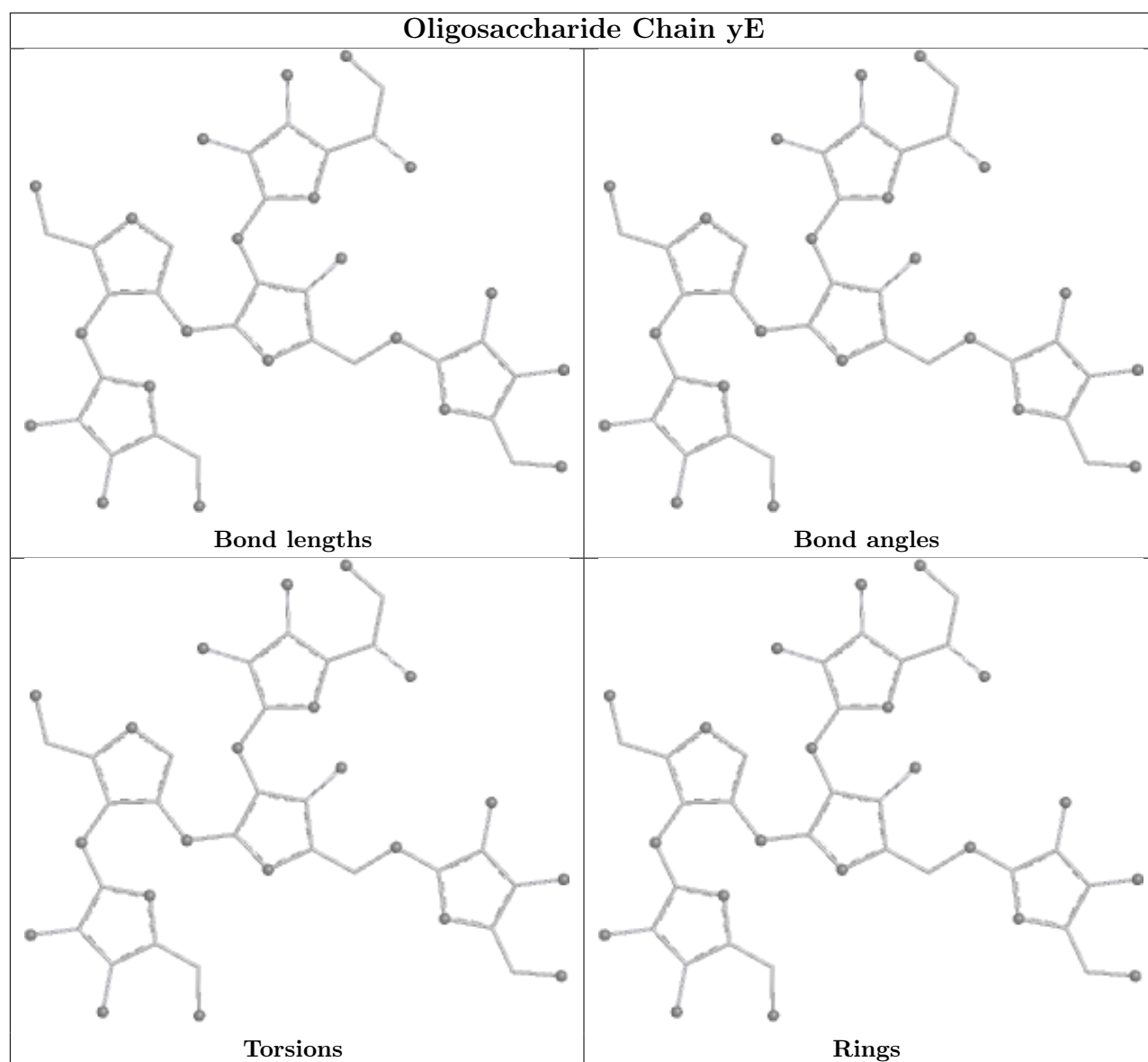


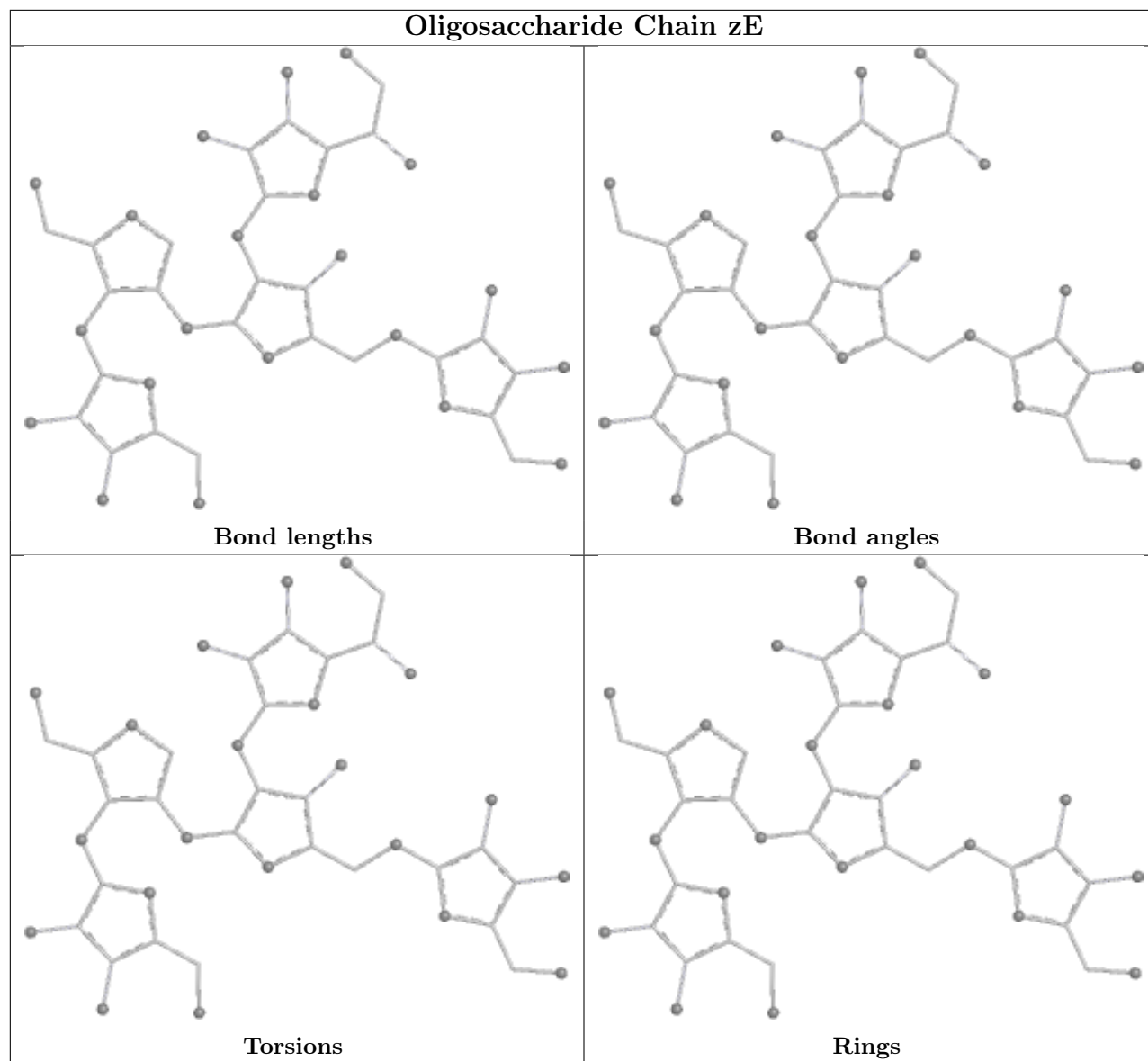


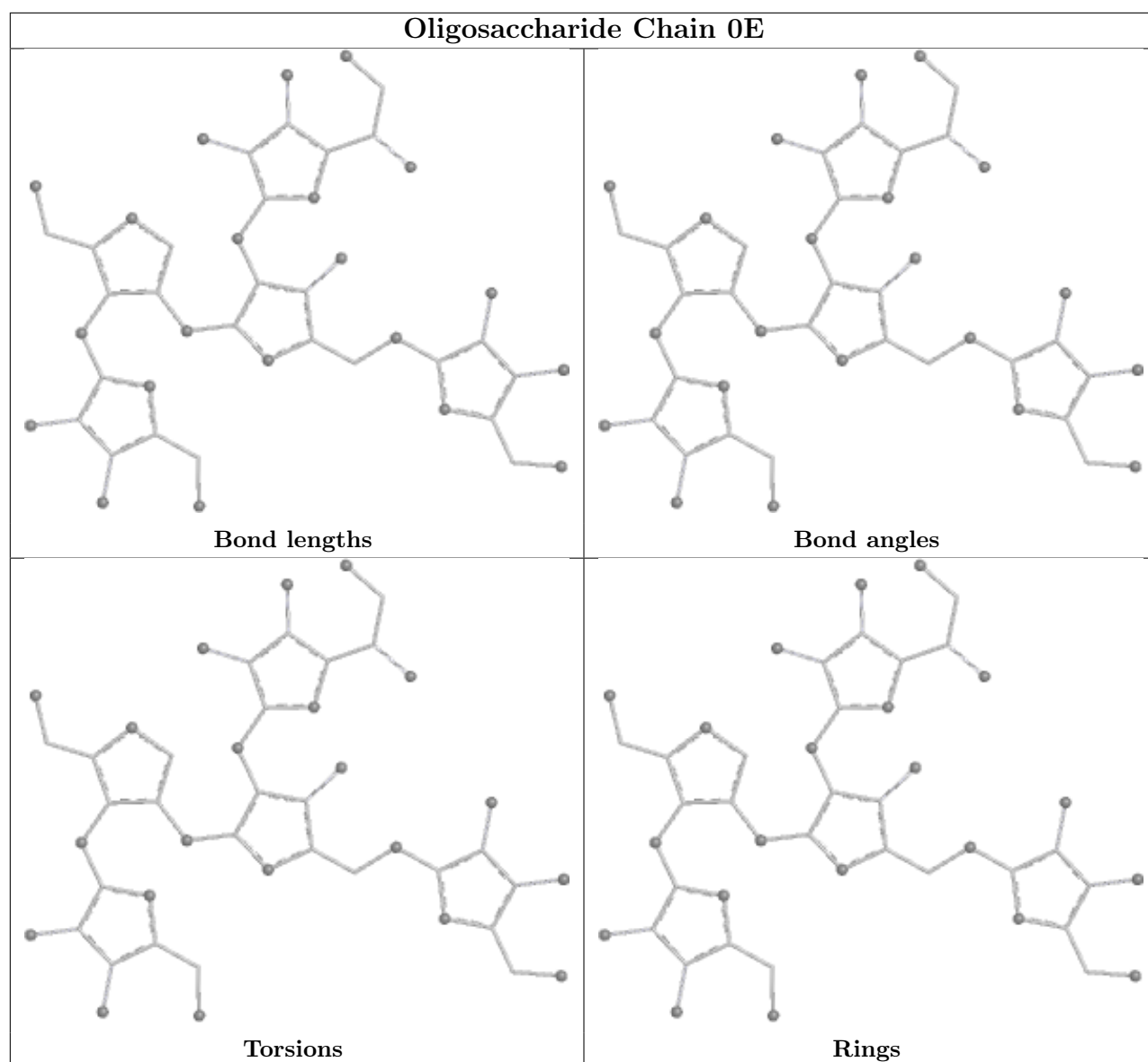


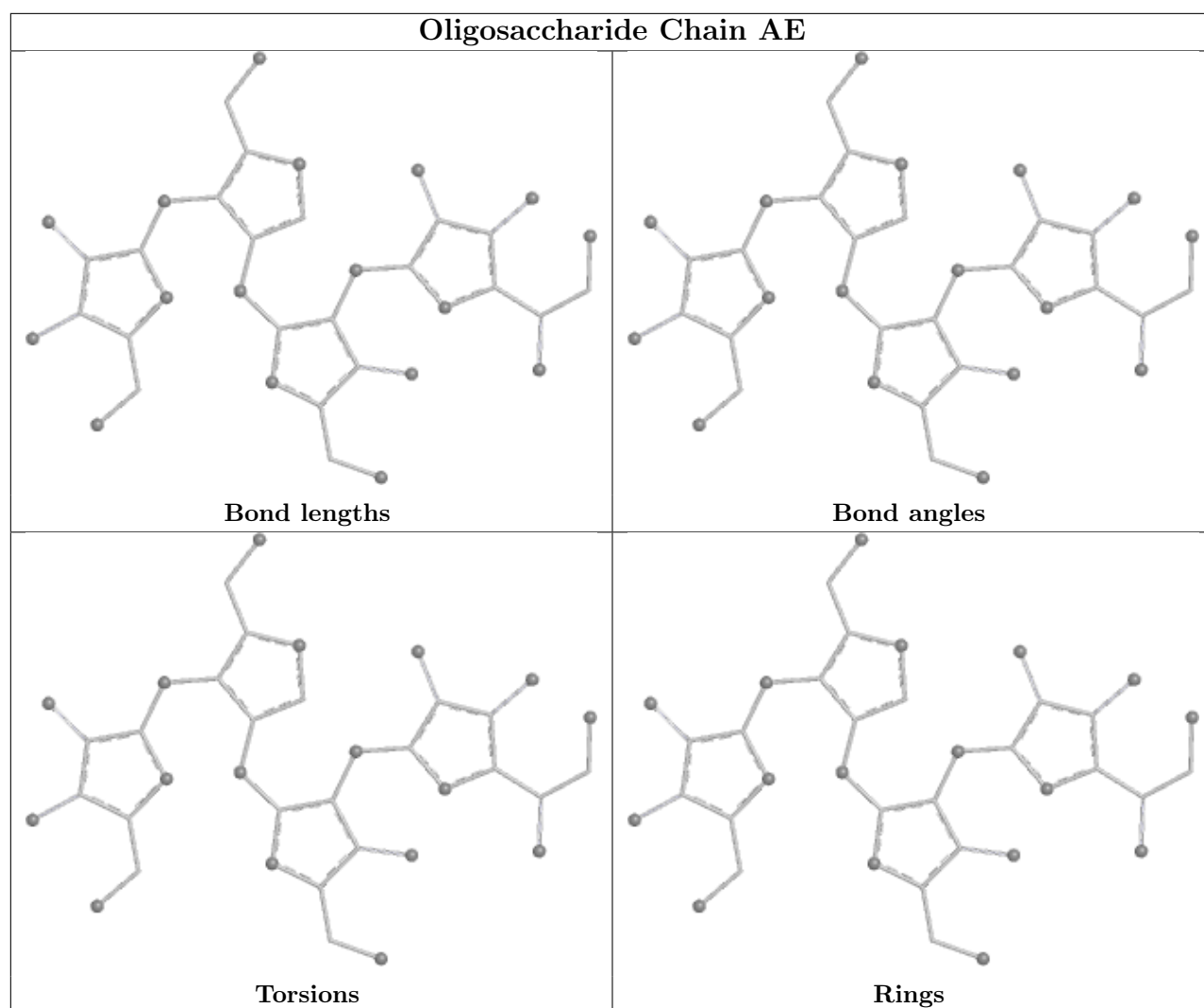


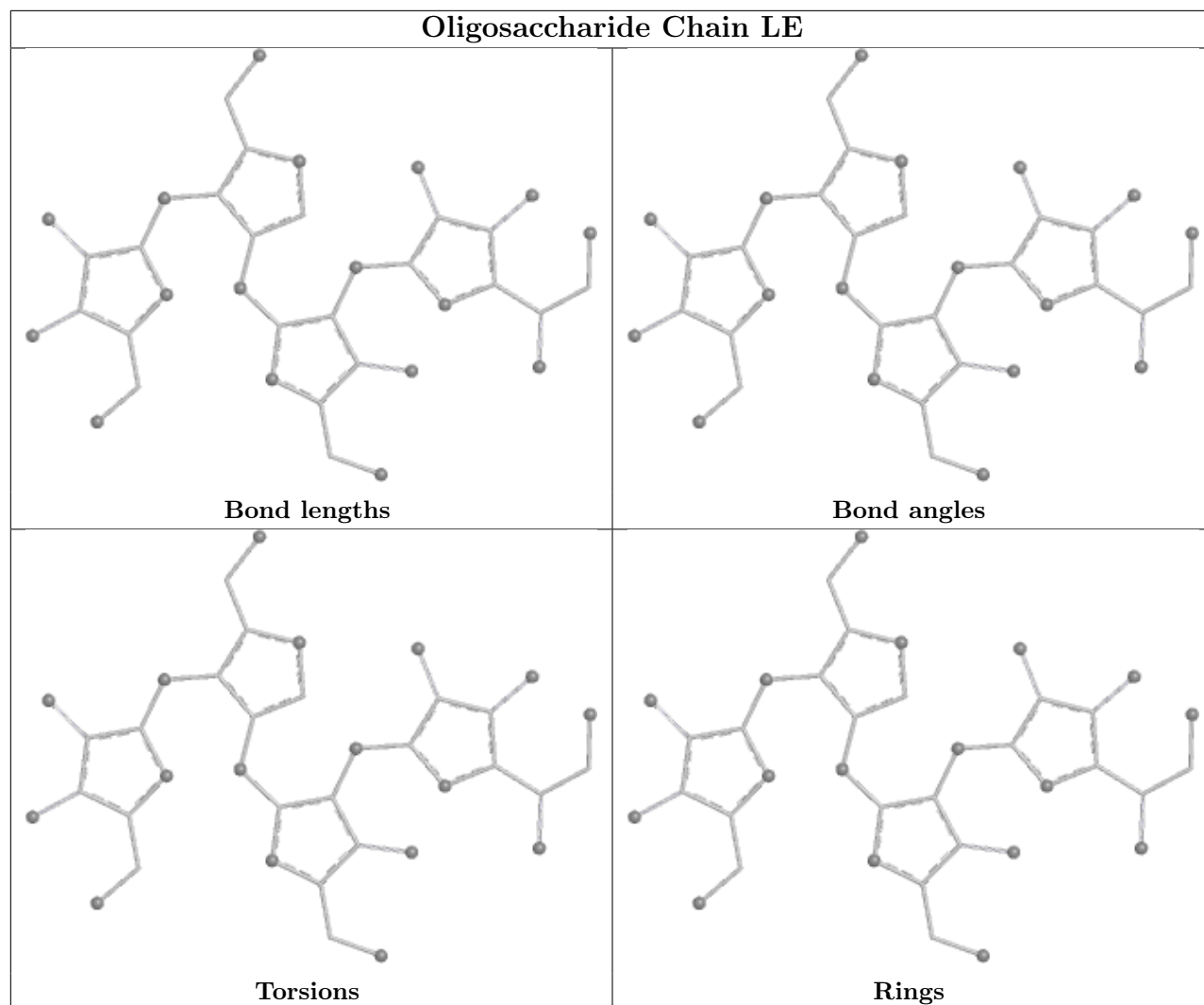




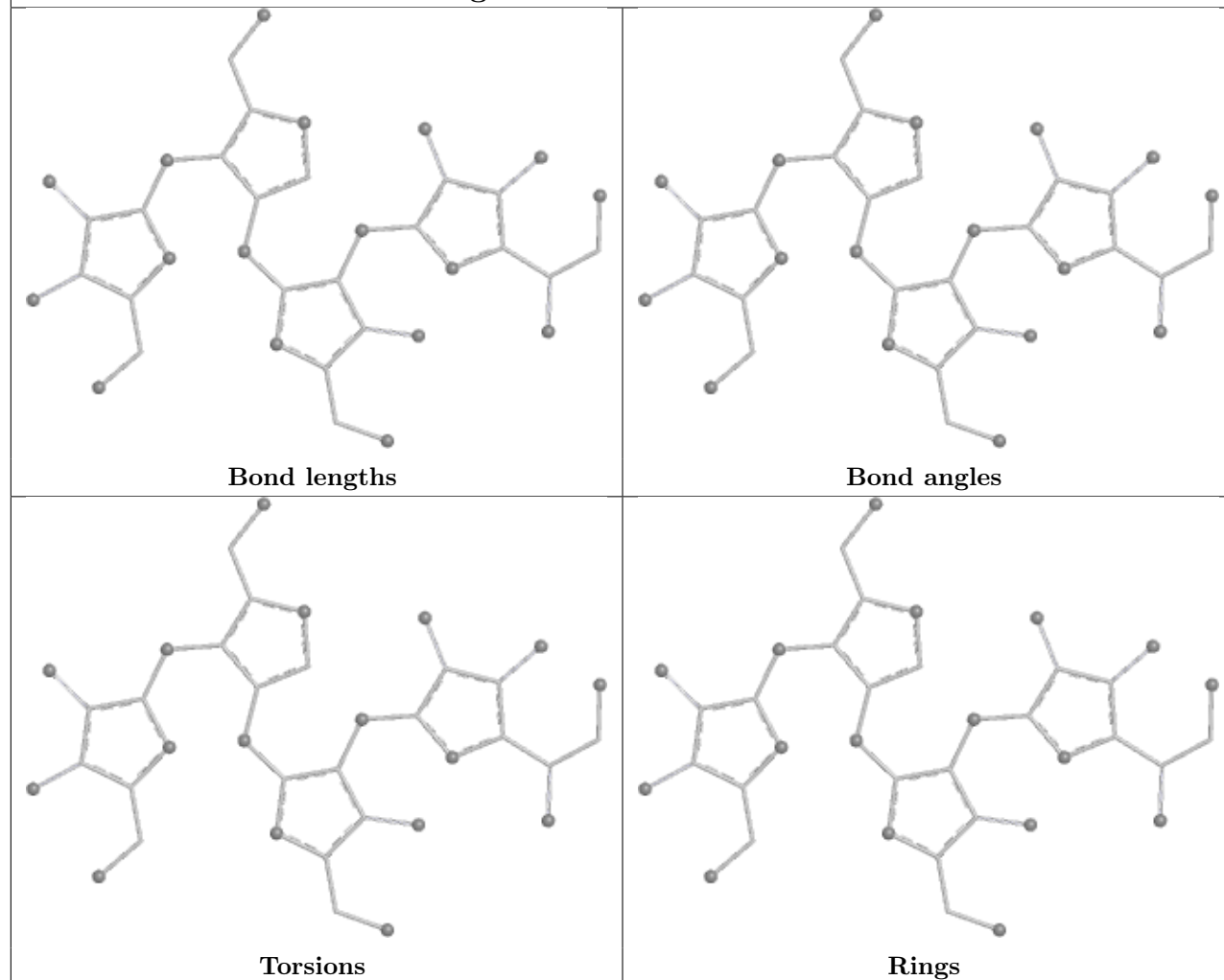


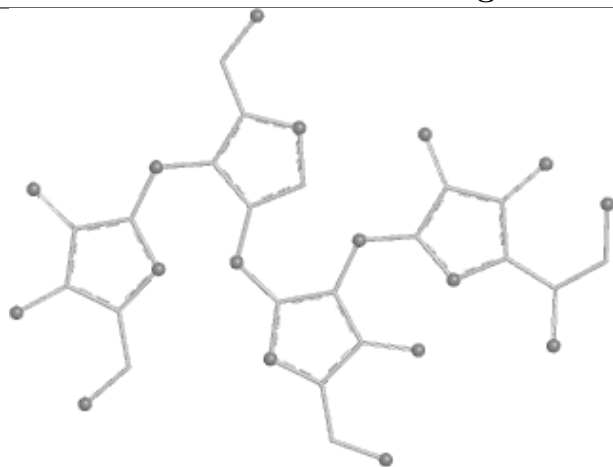
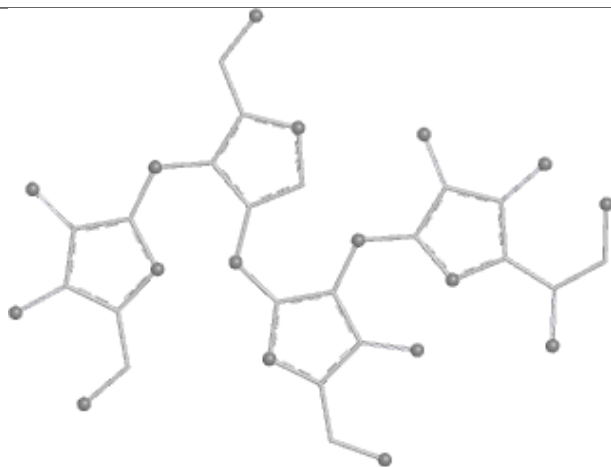
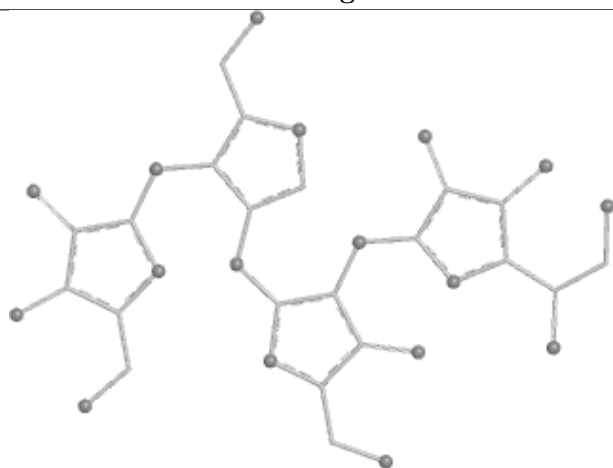
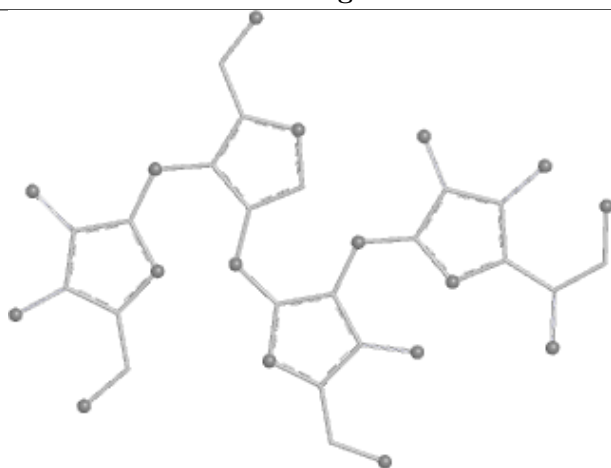


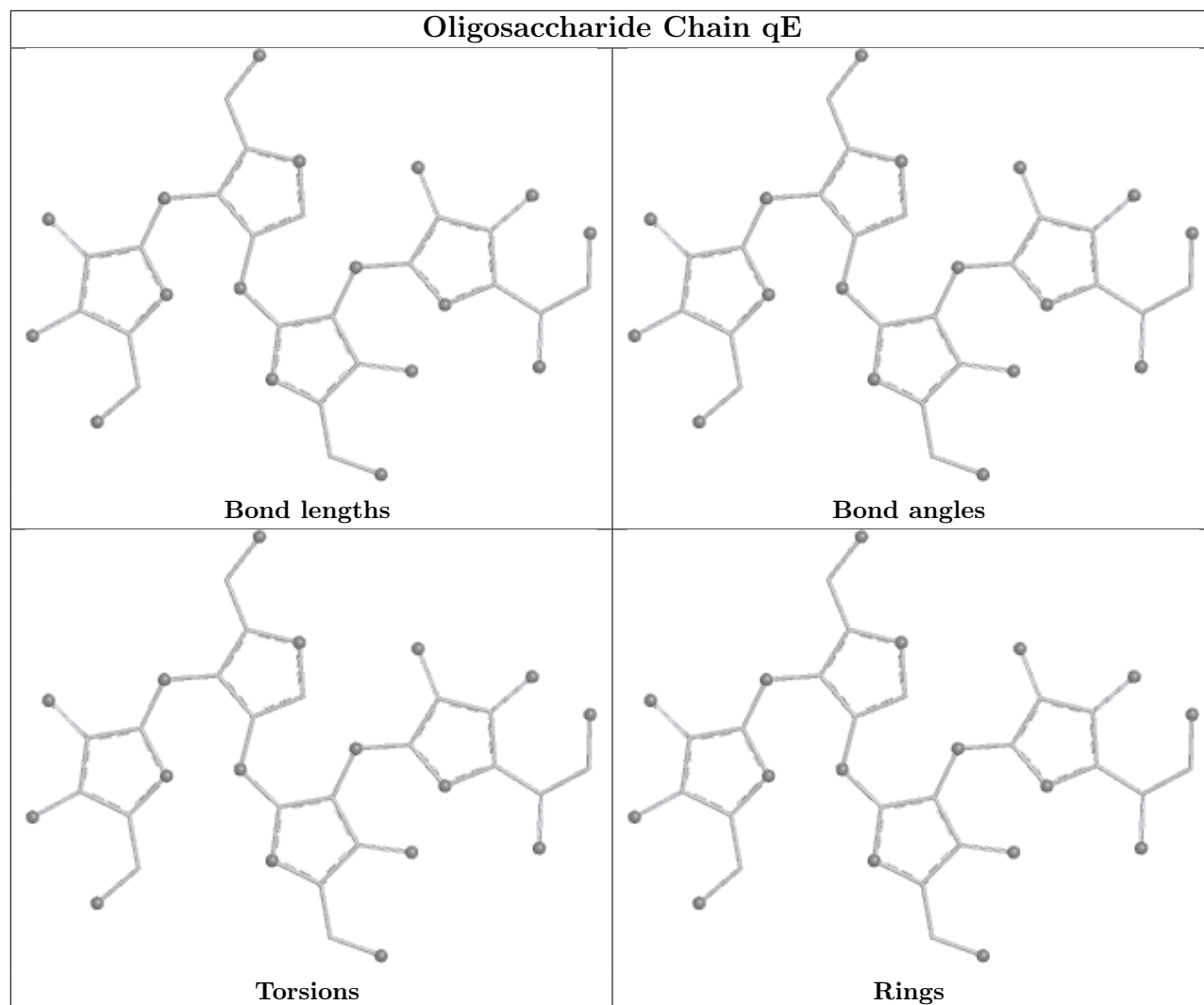


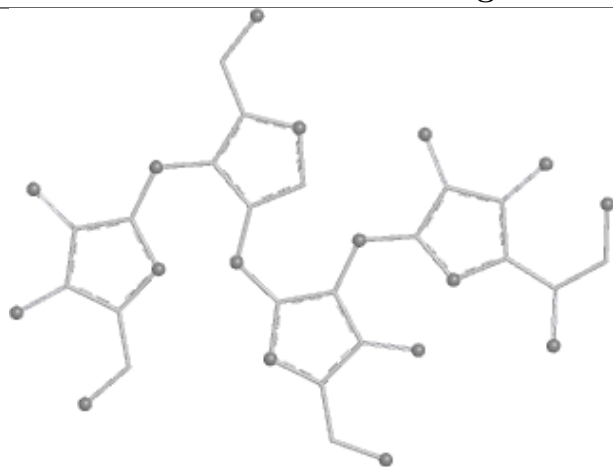
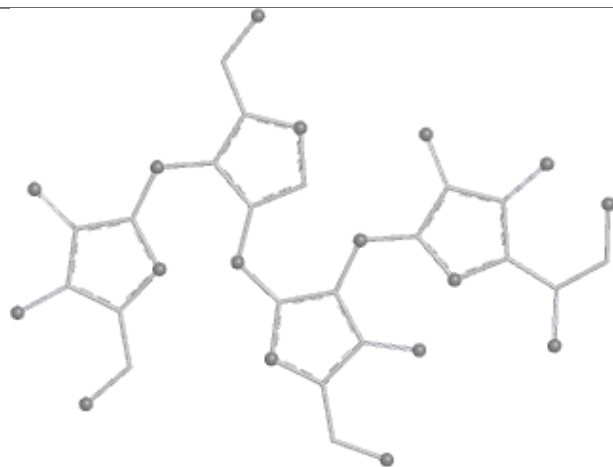
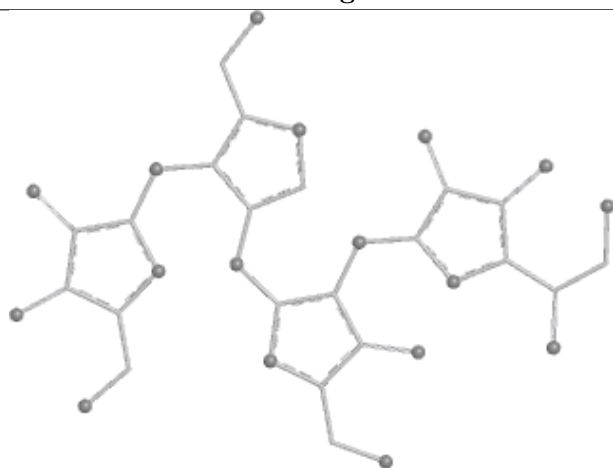
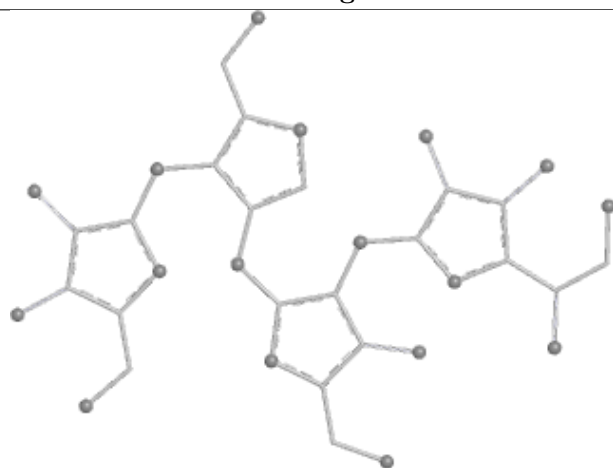


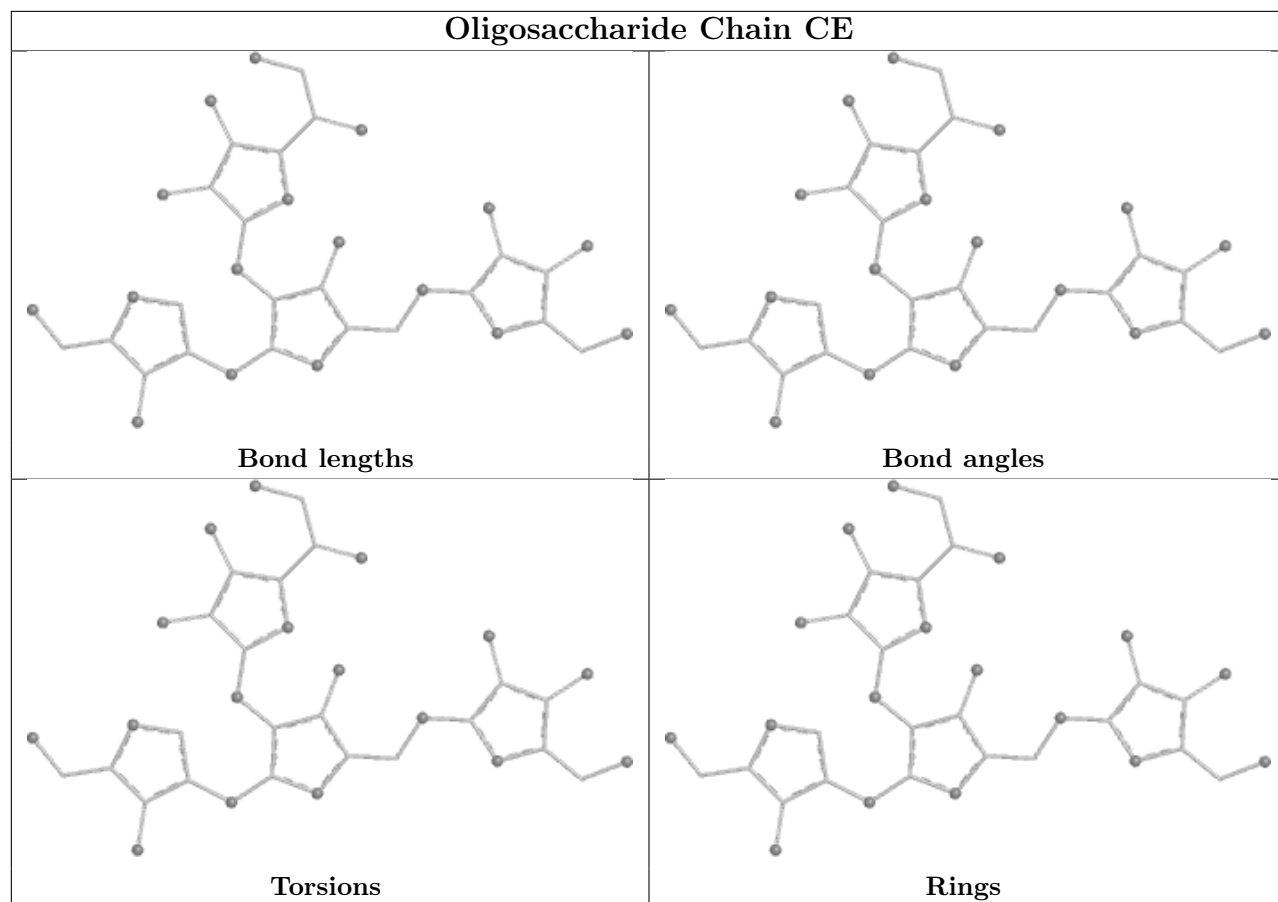
Oligosaccharide Chain NE

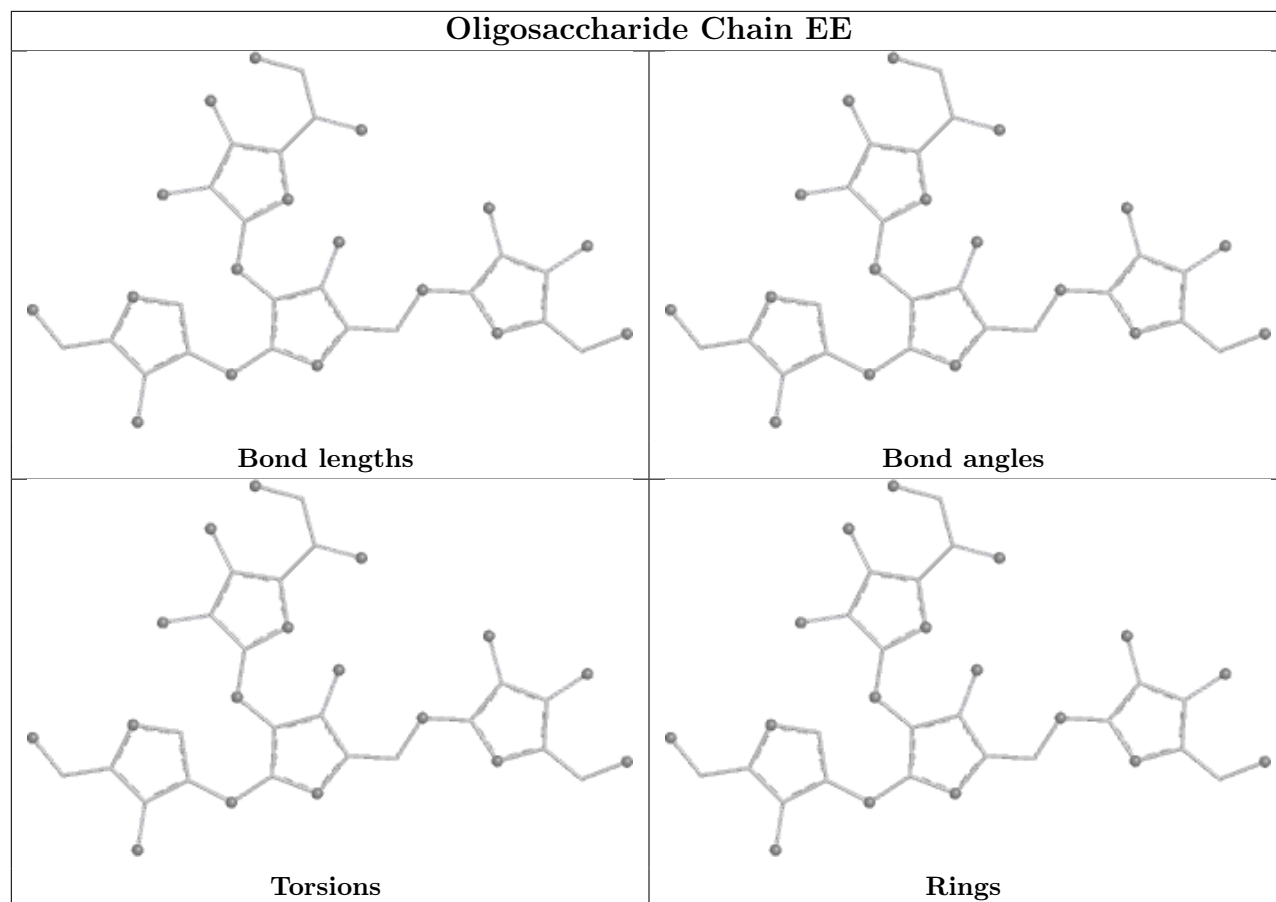


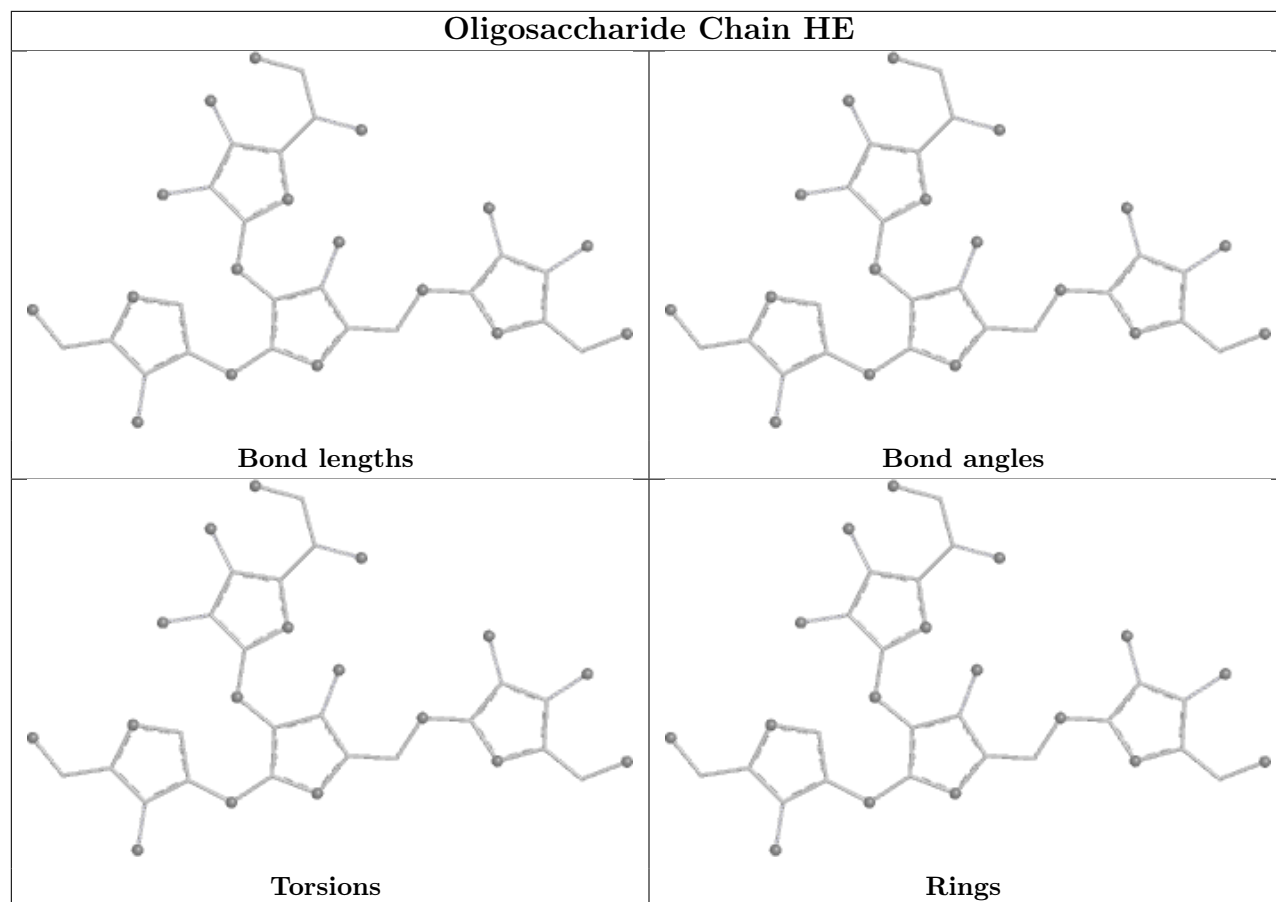
Oligosaccharide Chain aE**Bond lengths****Bond angles****Torsions****Rings**

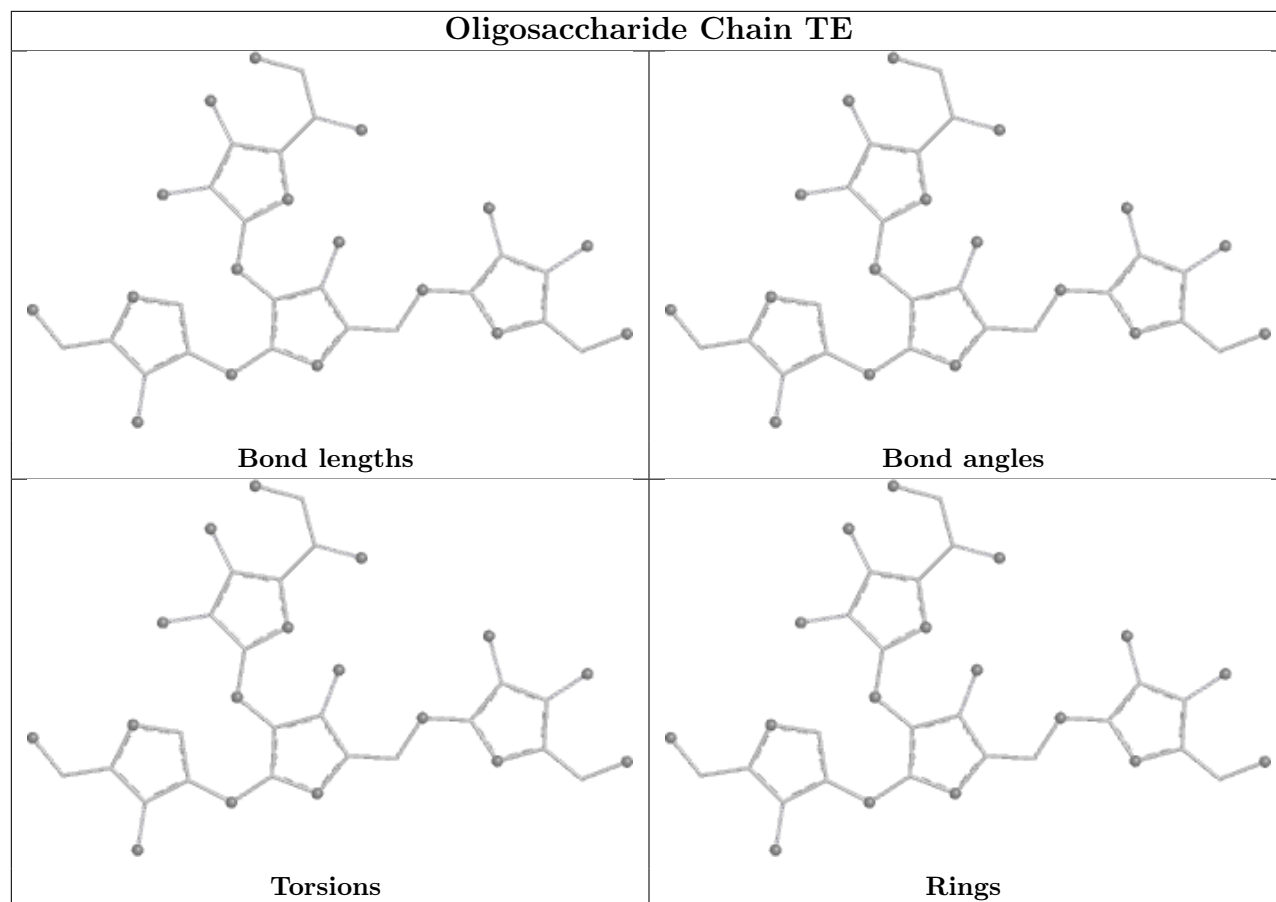


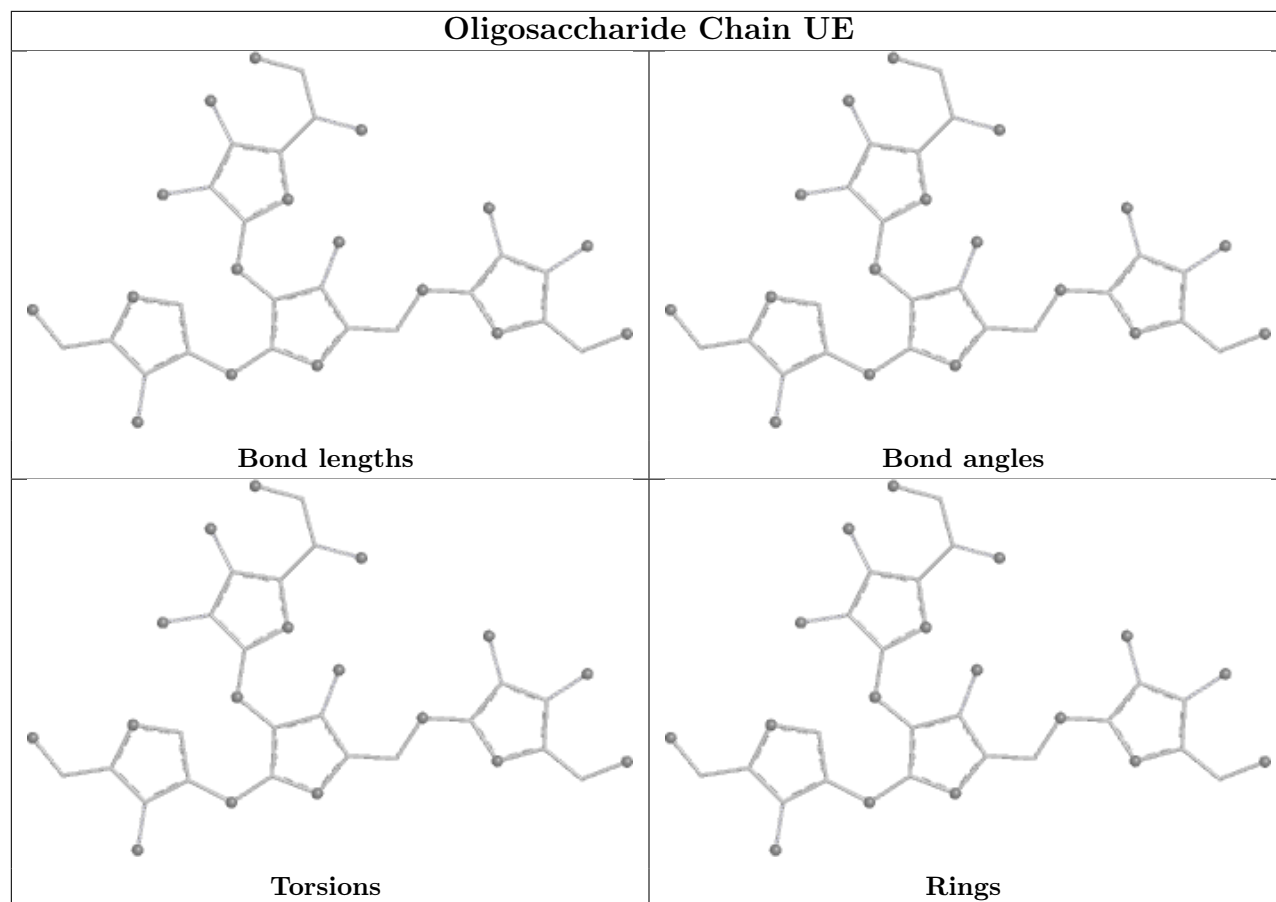
Oligosaccharide Chain 1E**Bond lengths****Bond angles****Torsions****Rings**

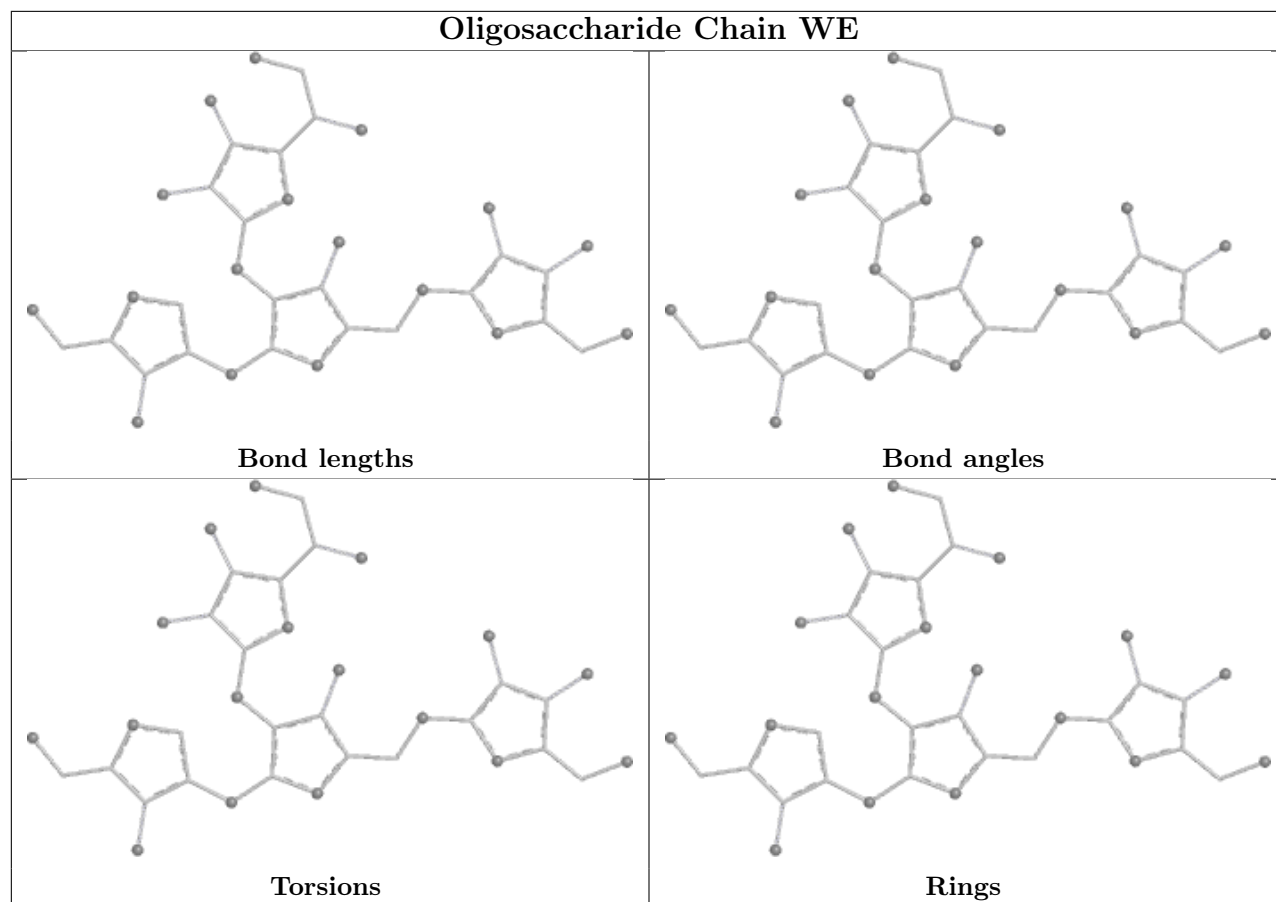


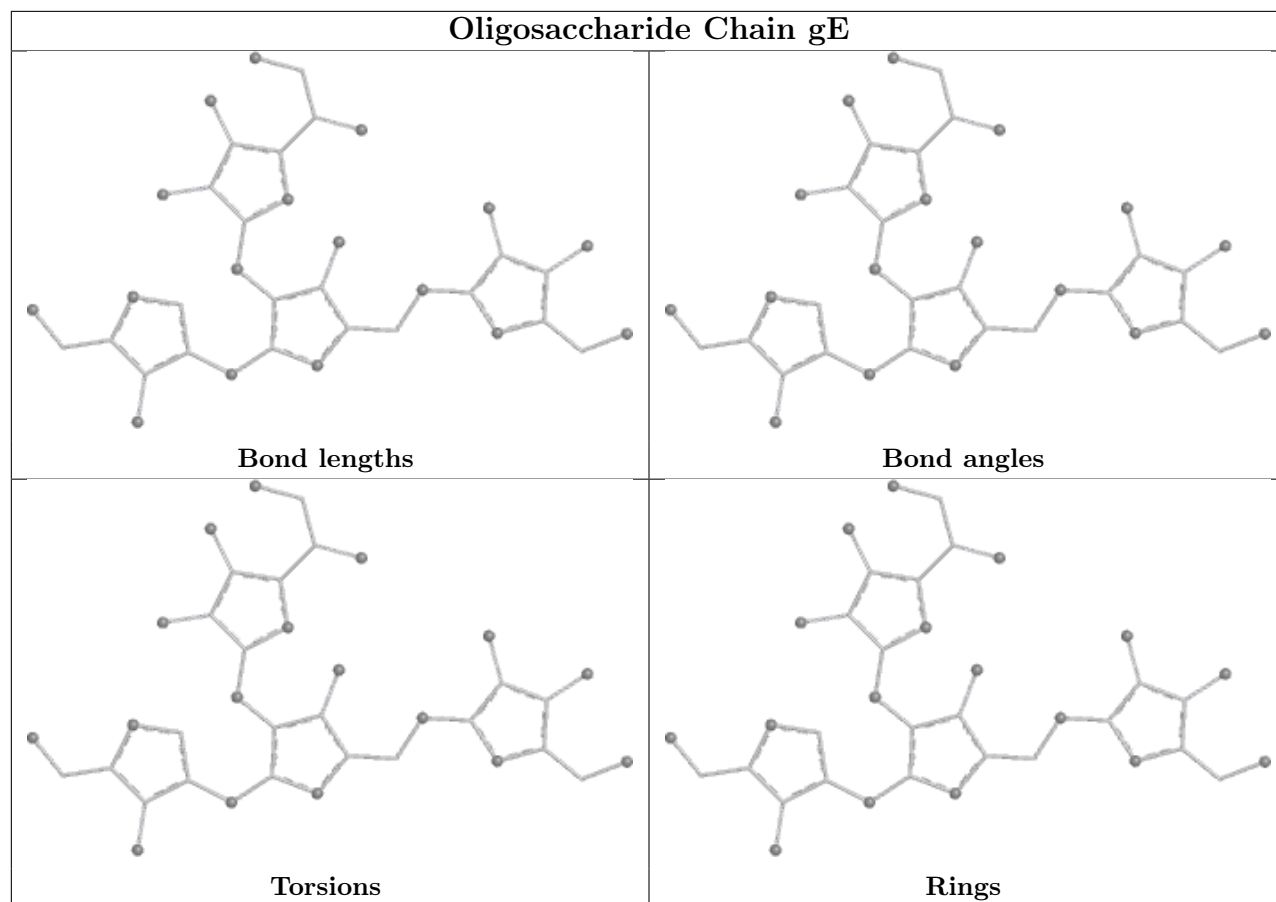


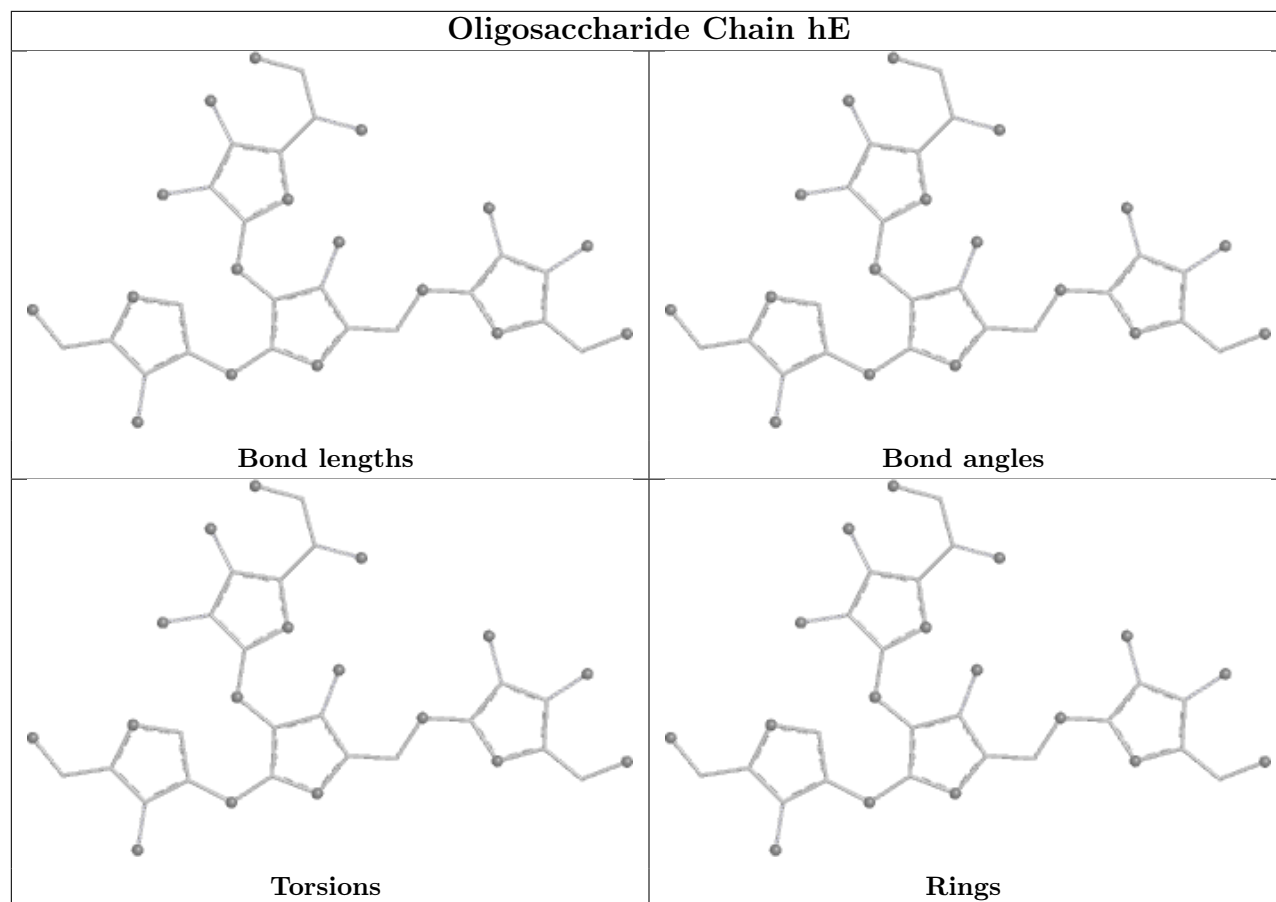


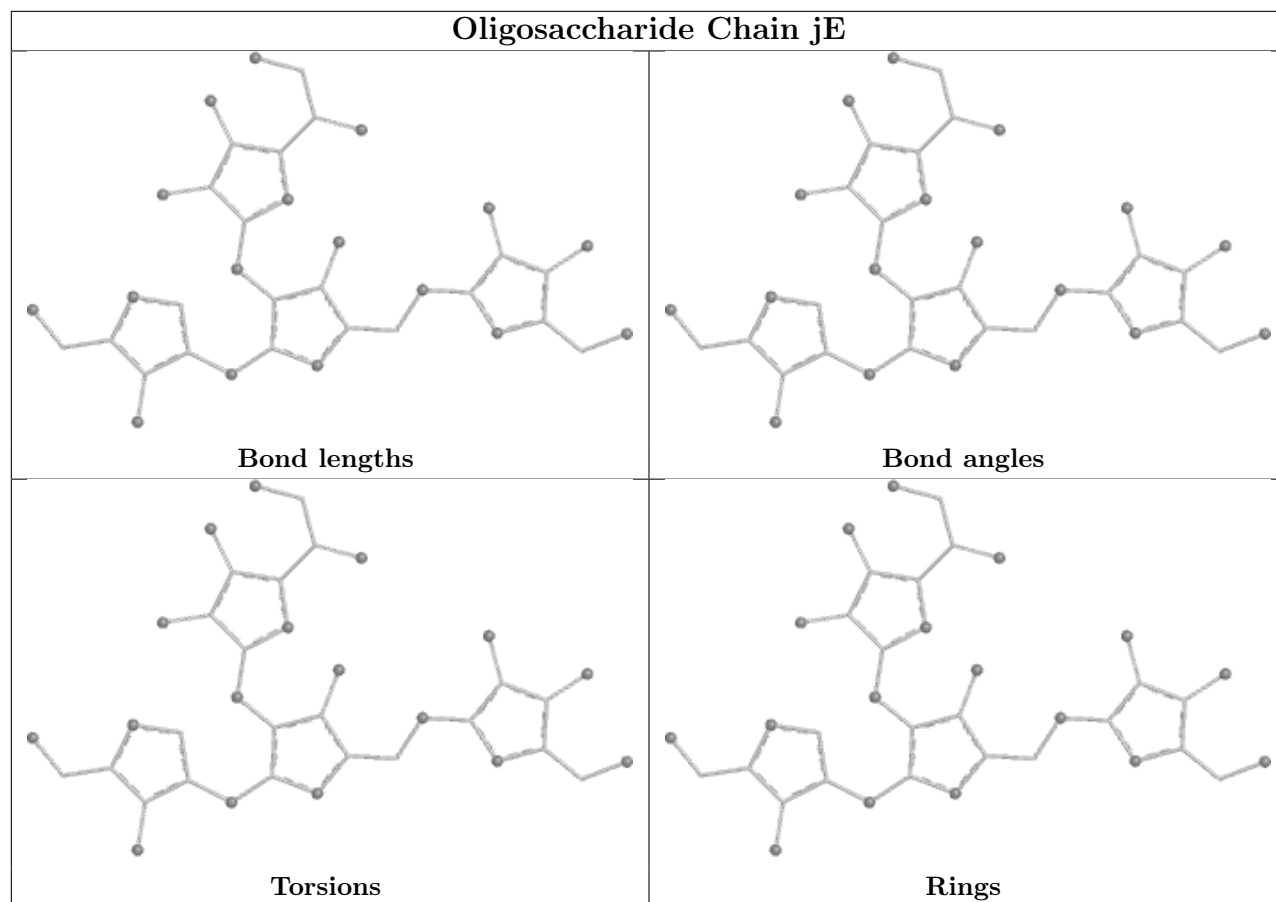


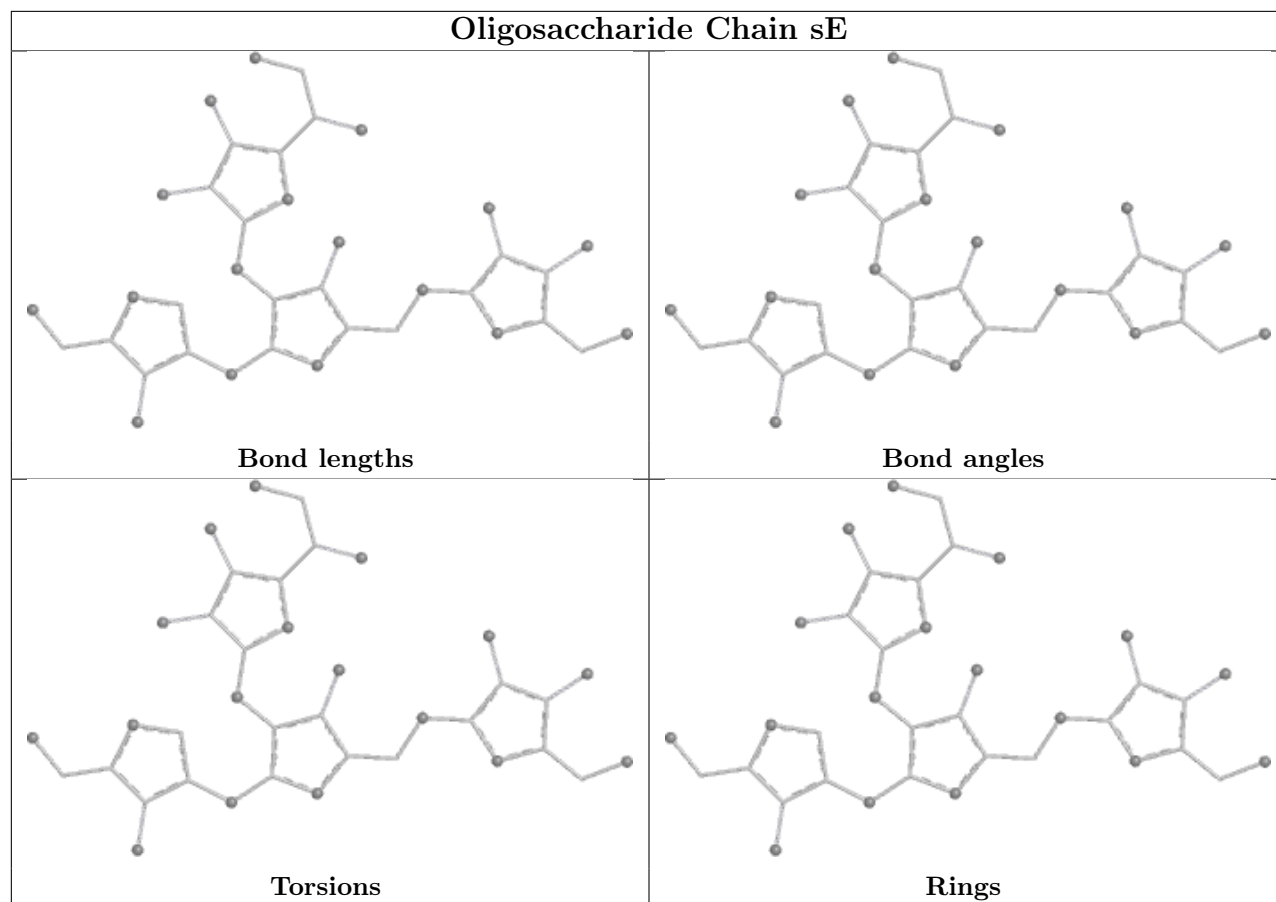


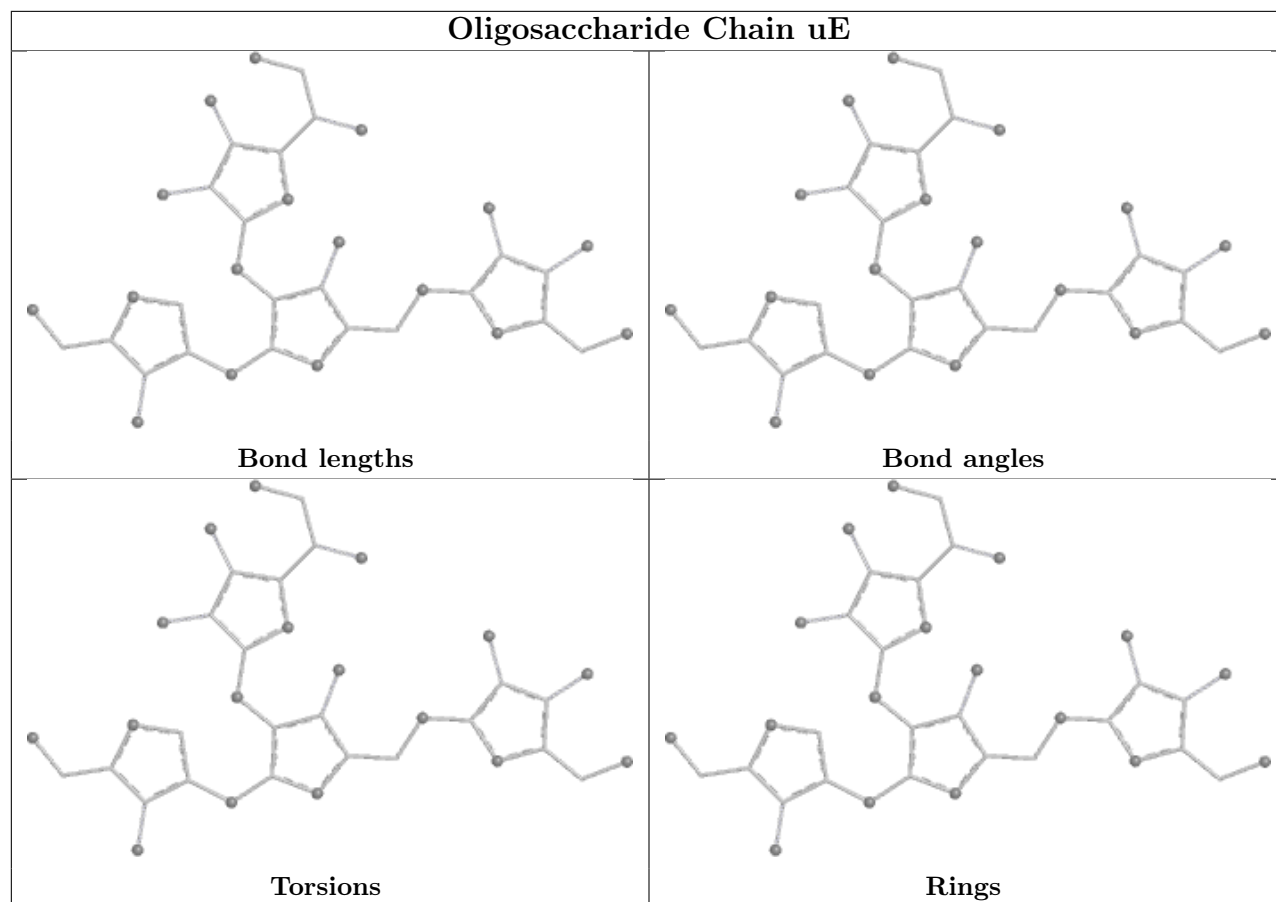


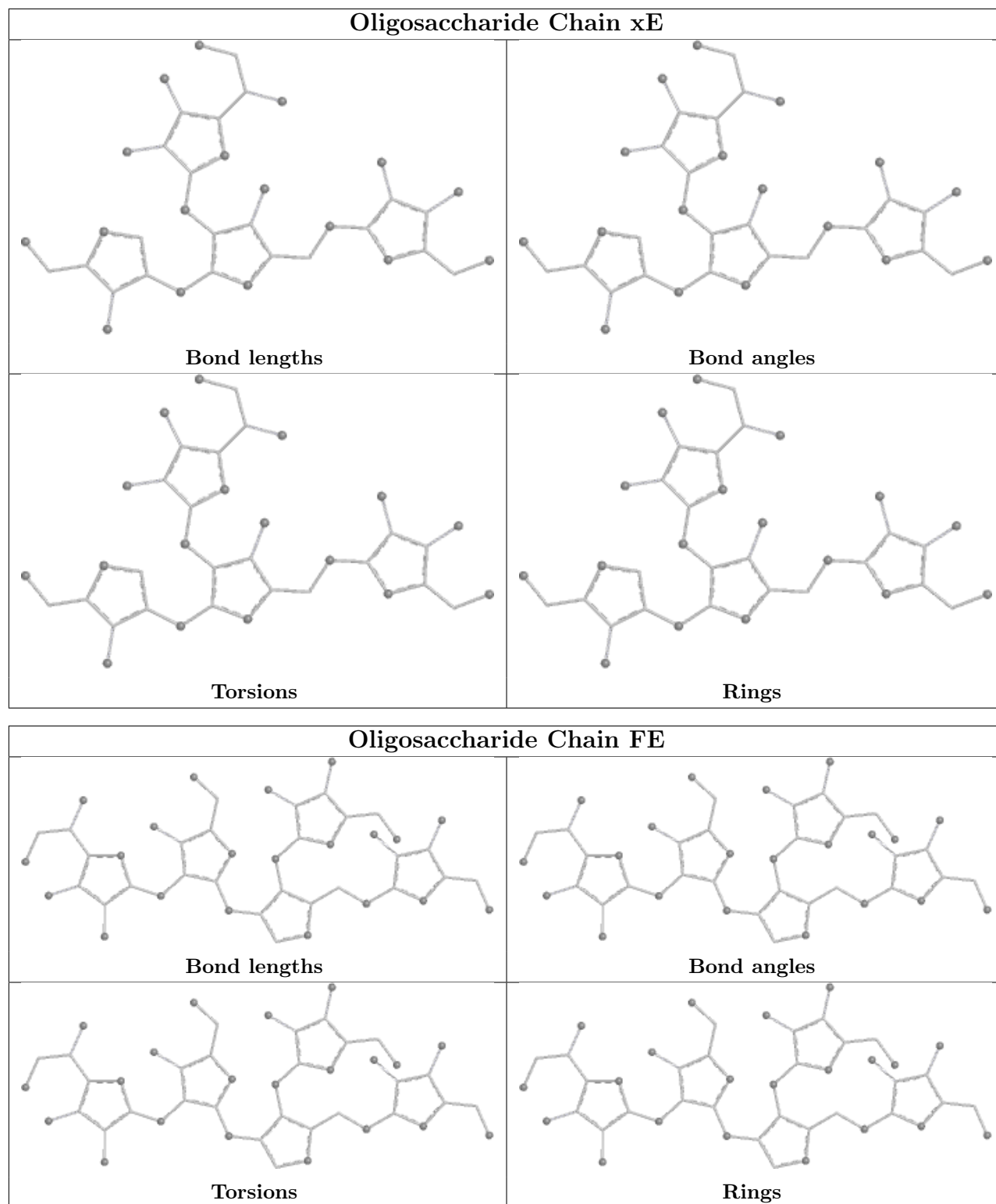


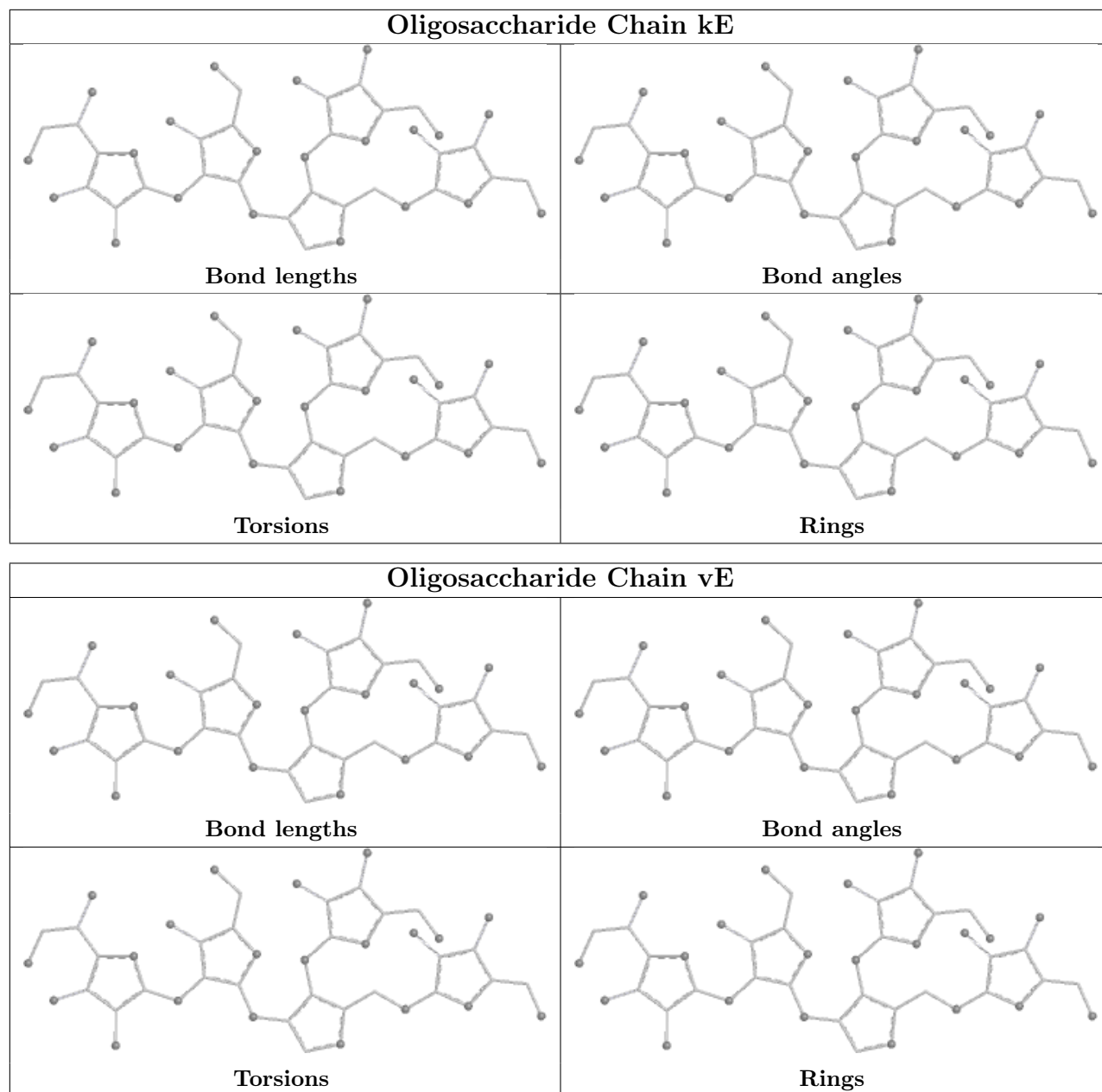


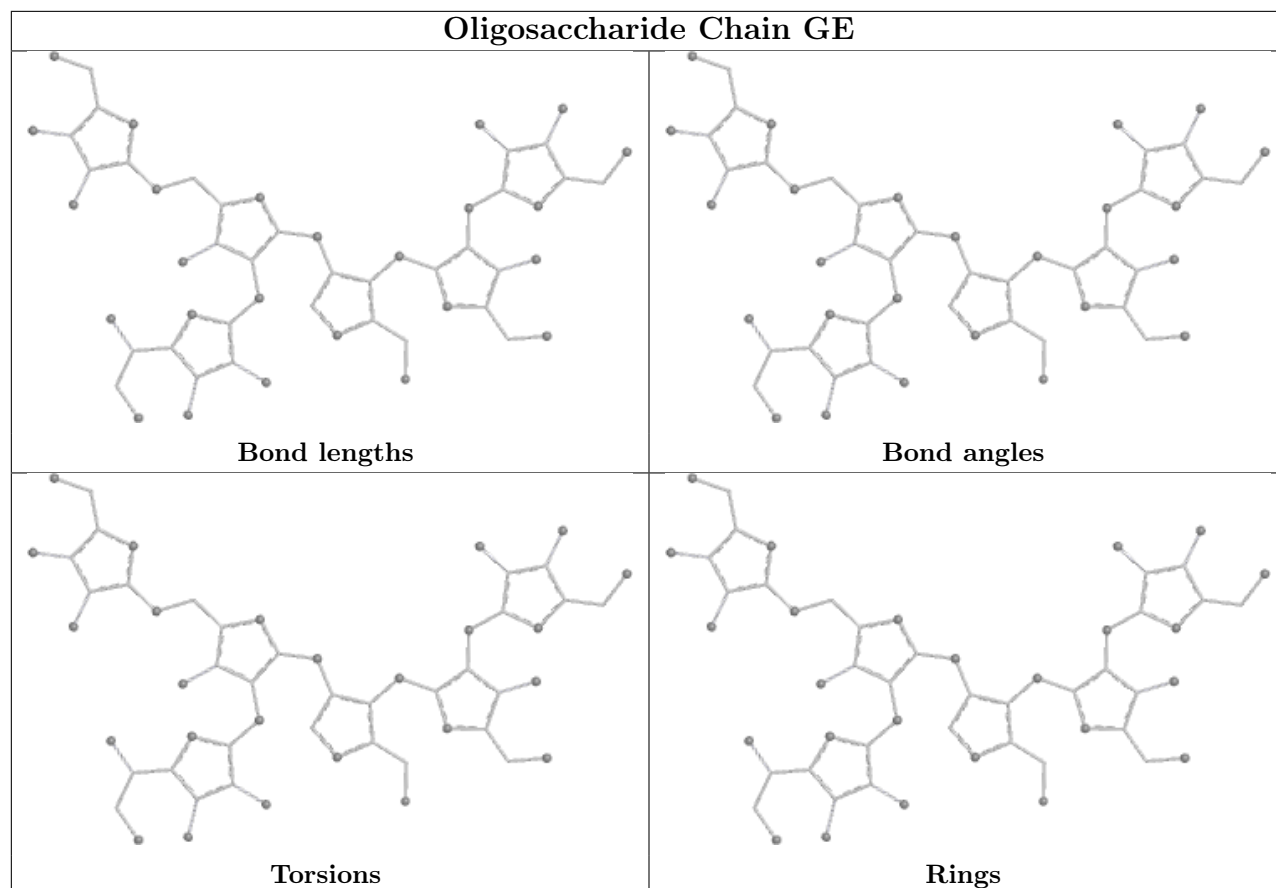
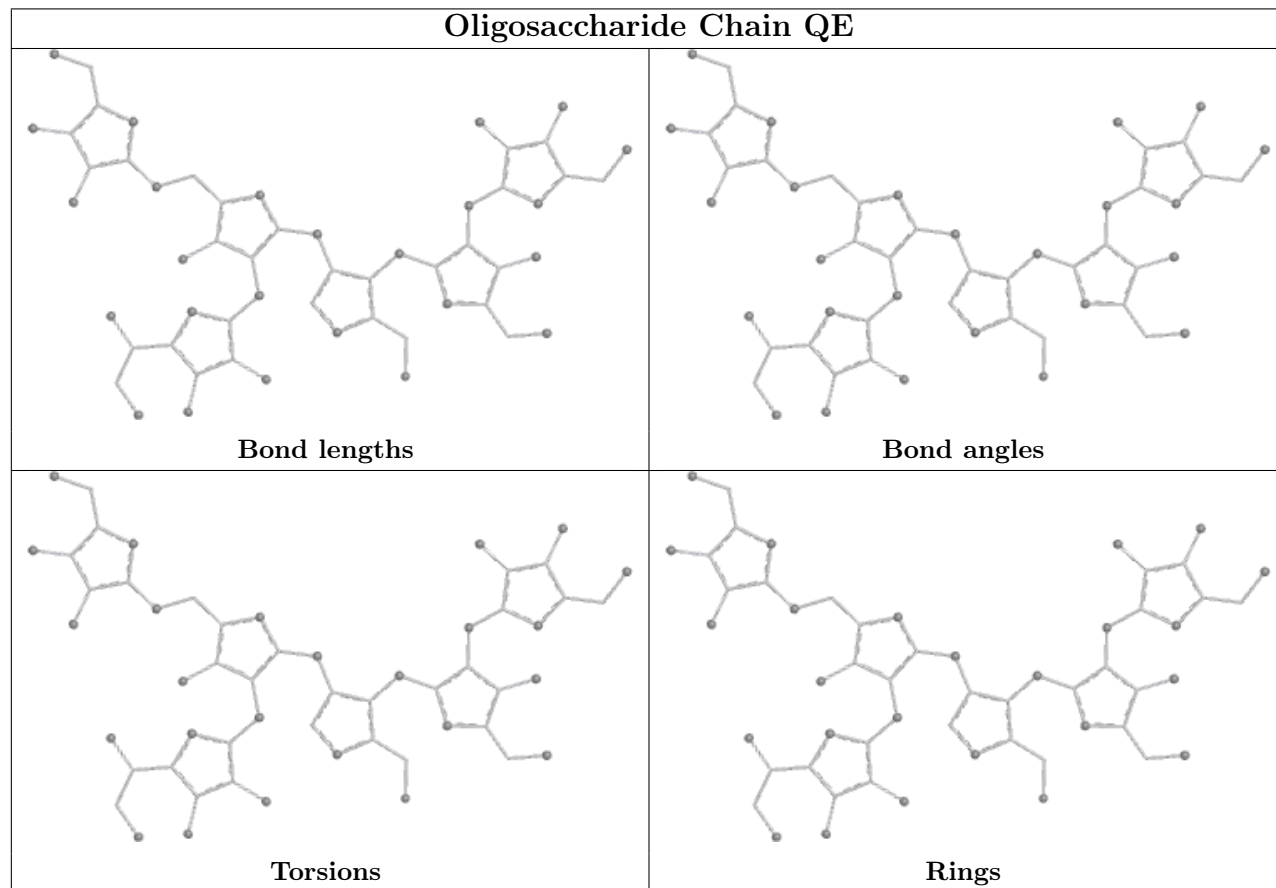


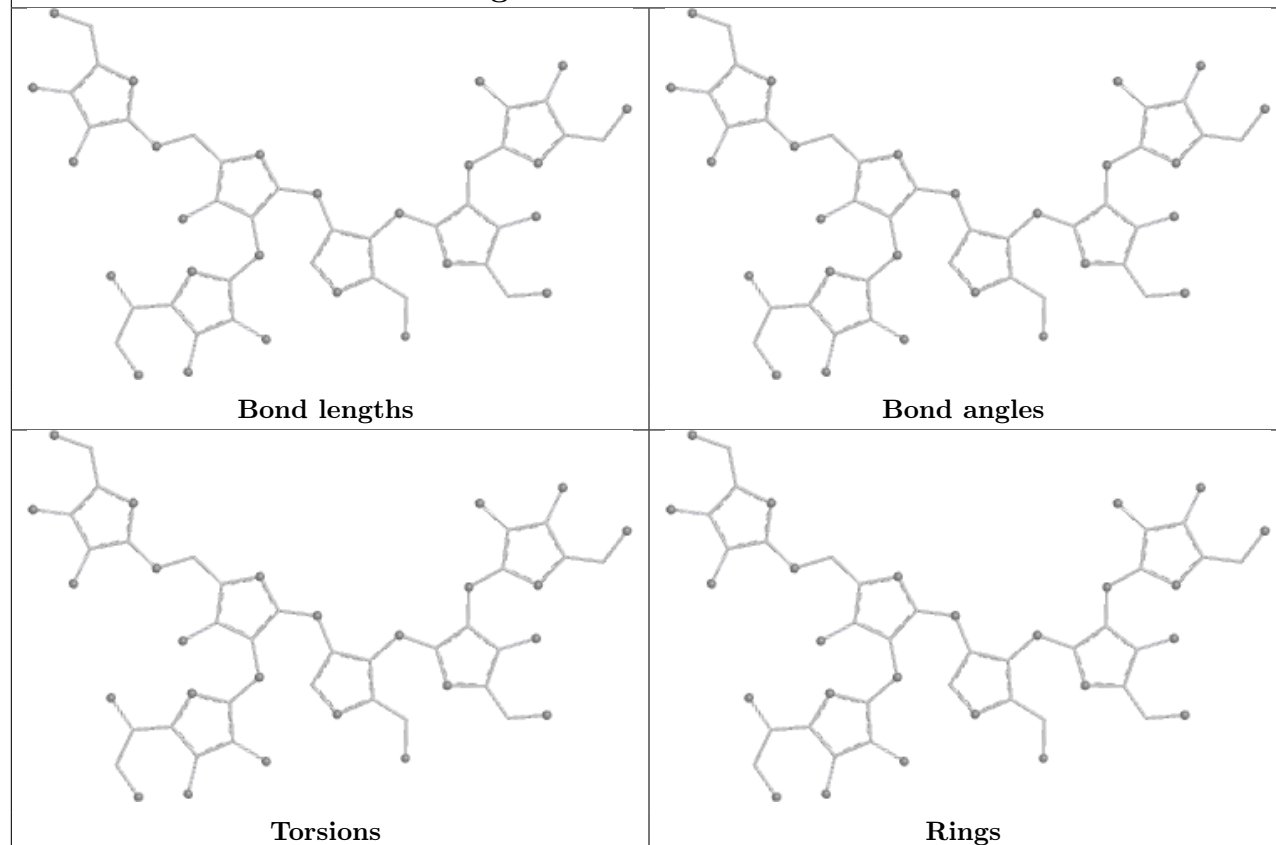
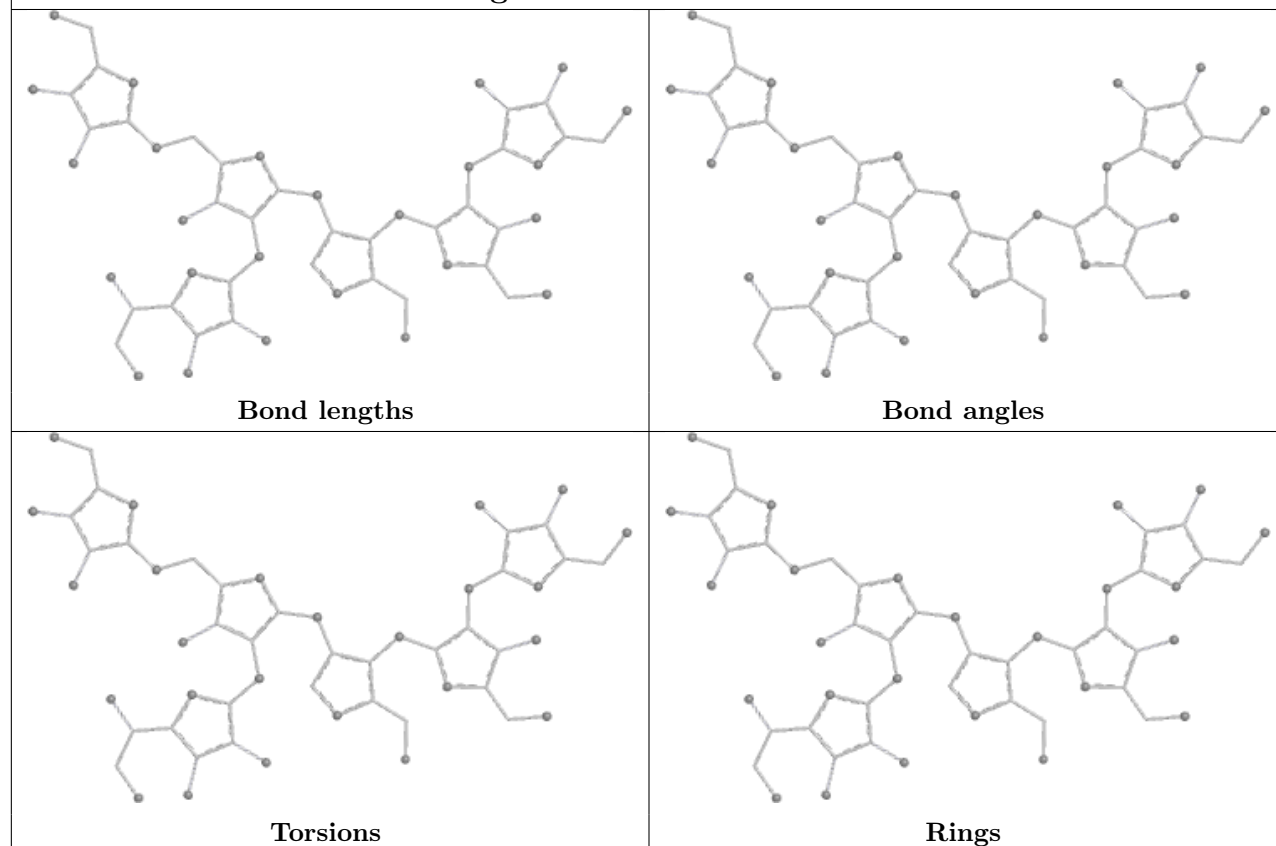




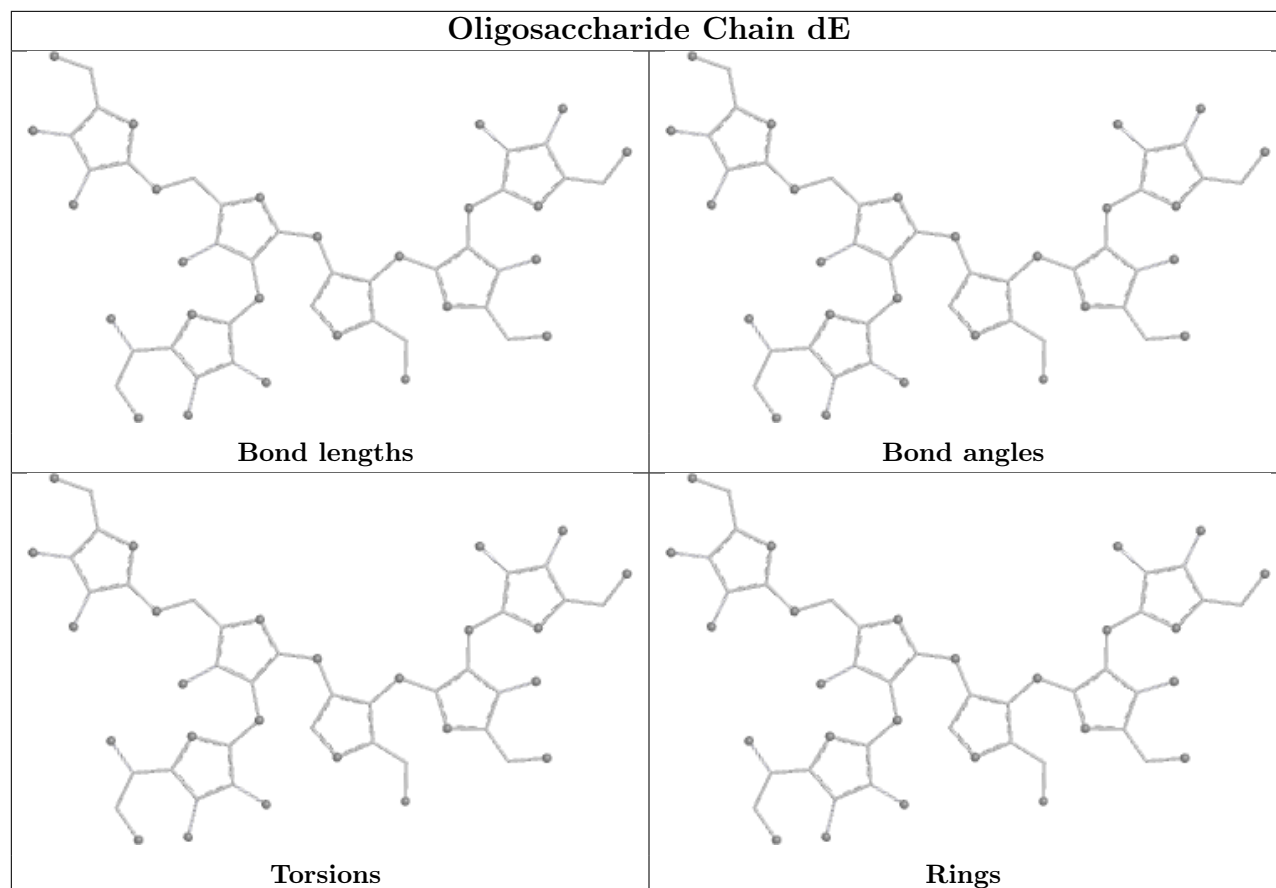




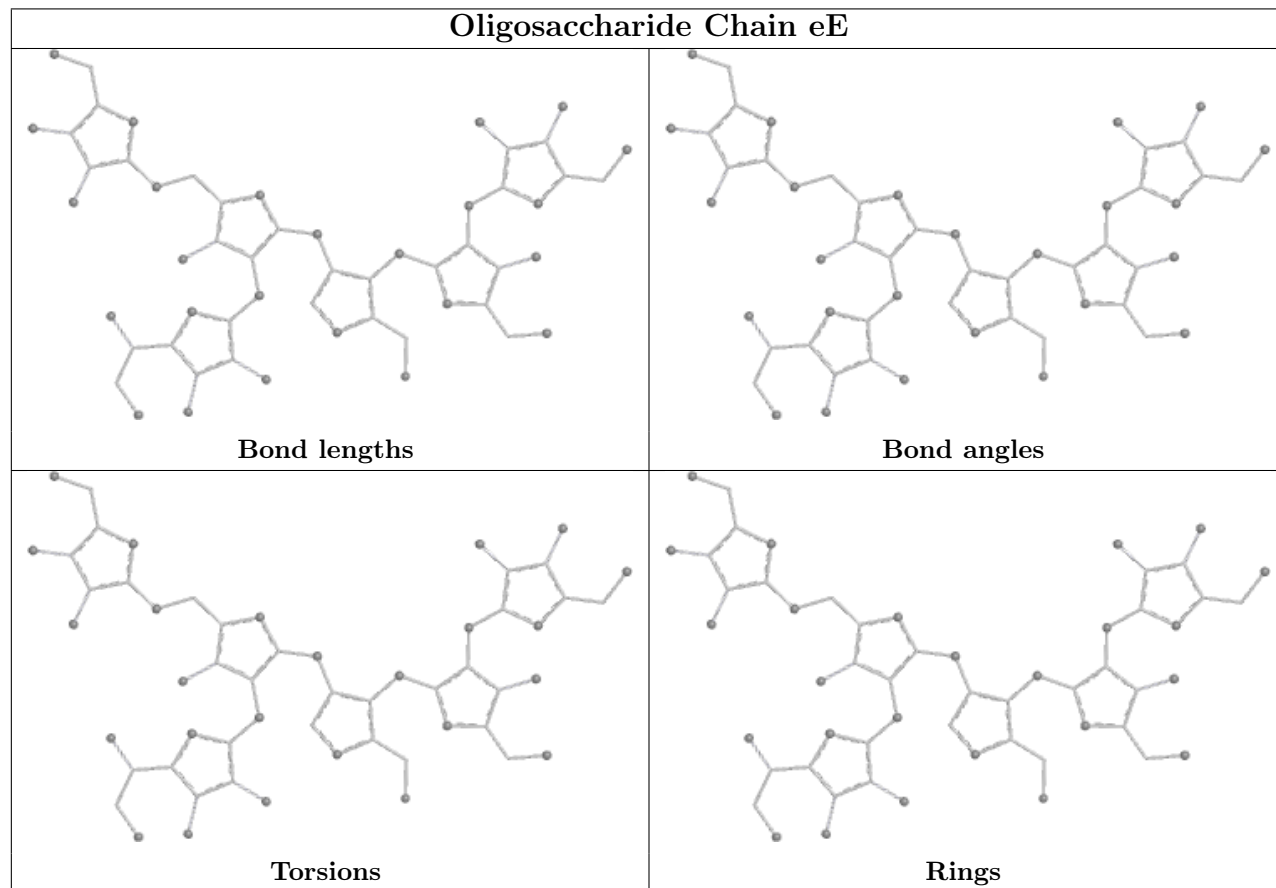
Oligosaccharide Chain GE**Oligosaccharide Chain QE**

Oligosaccharide Chain RE**Oligosaccharide Chain VE**

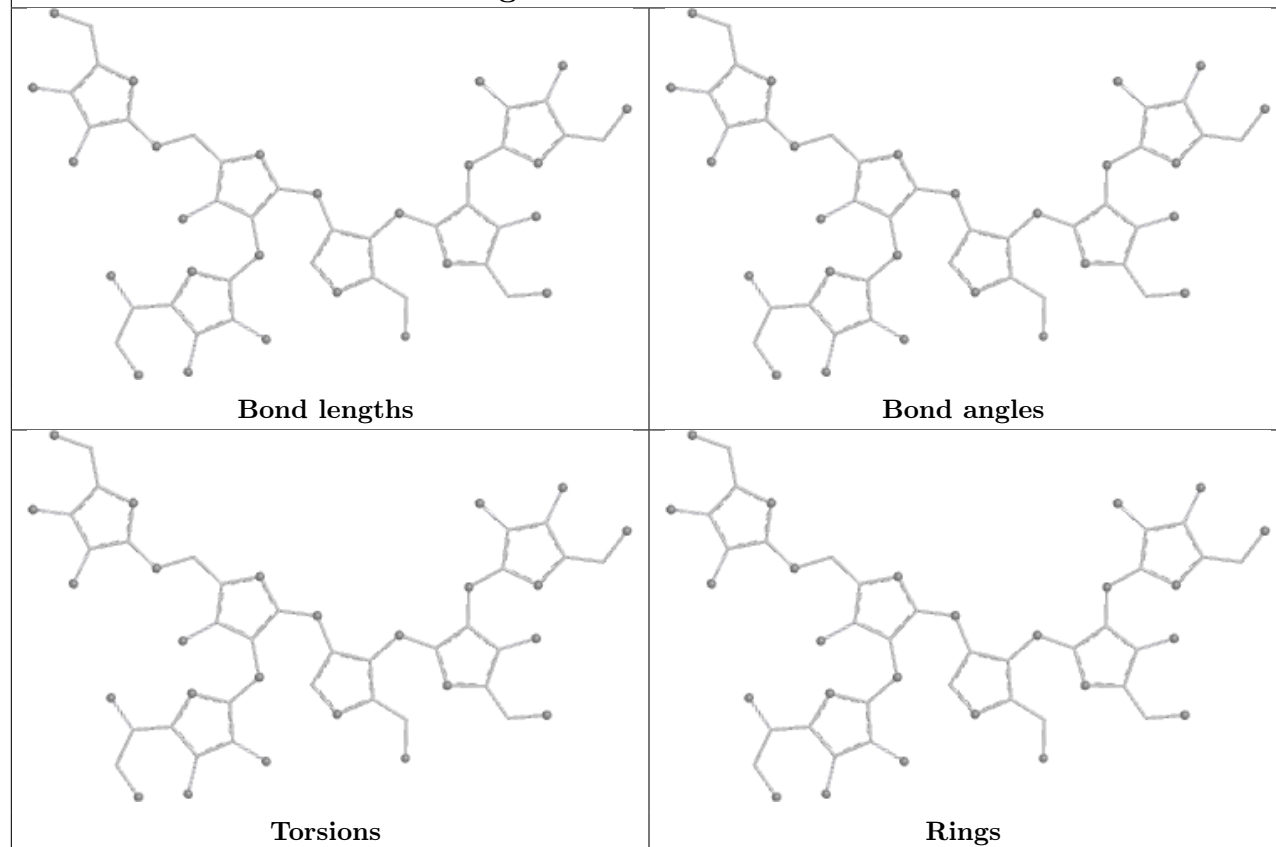
Oligosaccharide Chain dE



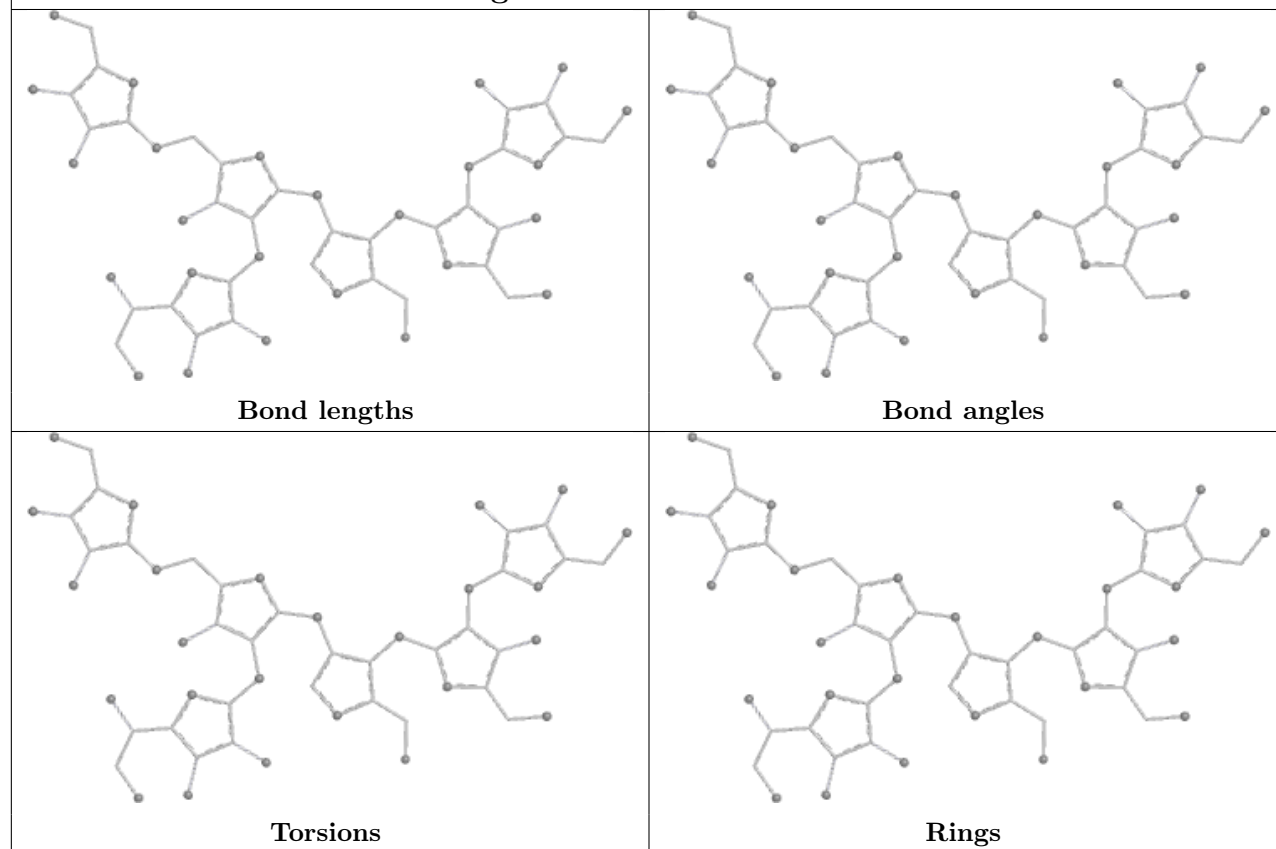
Oligosaccharide Chain eE

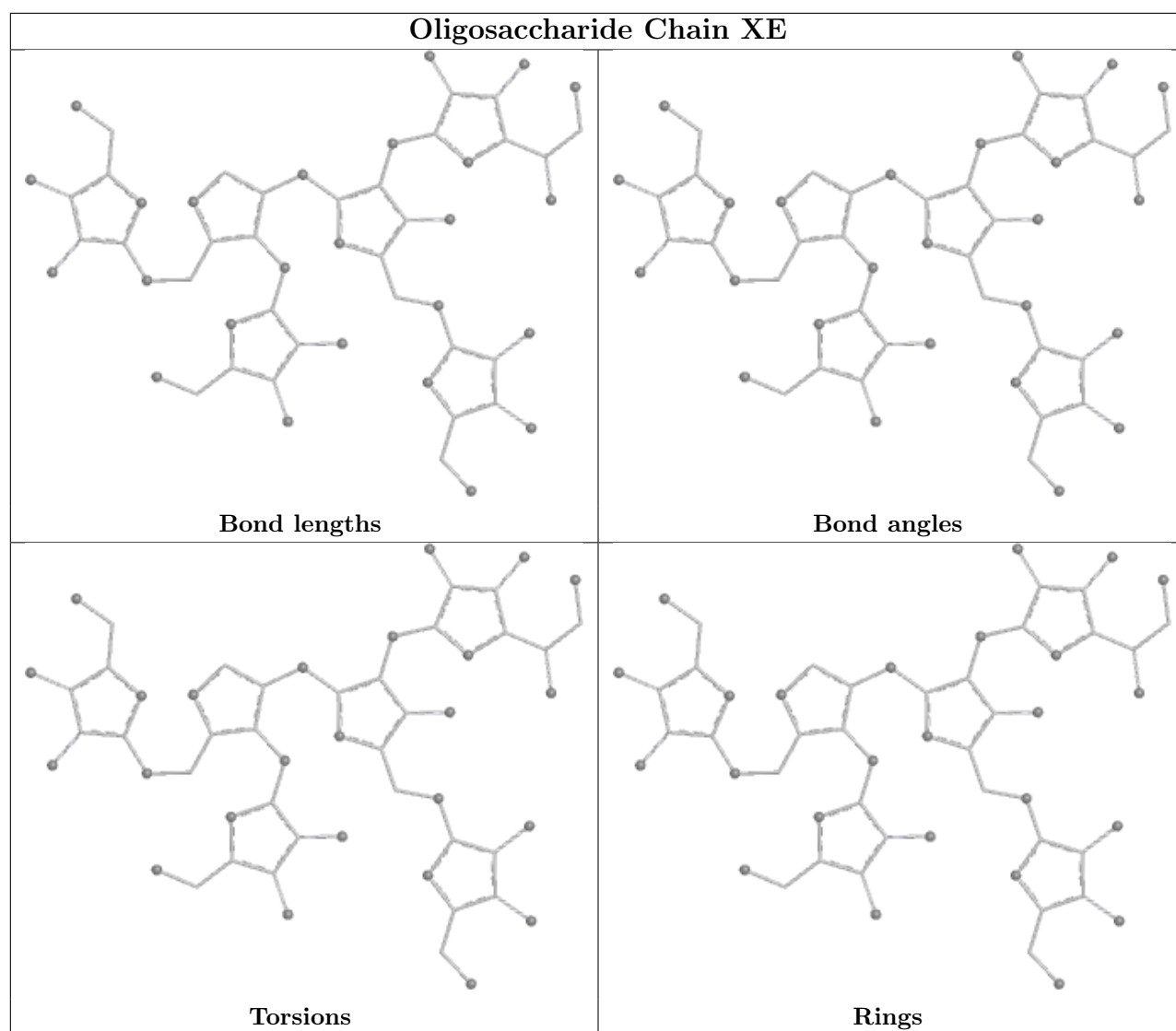


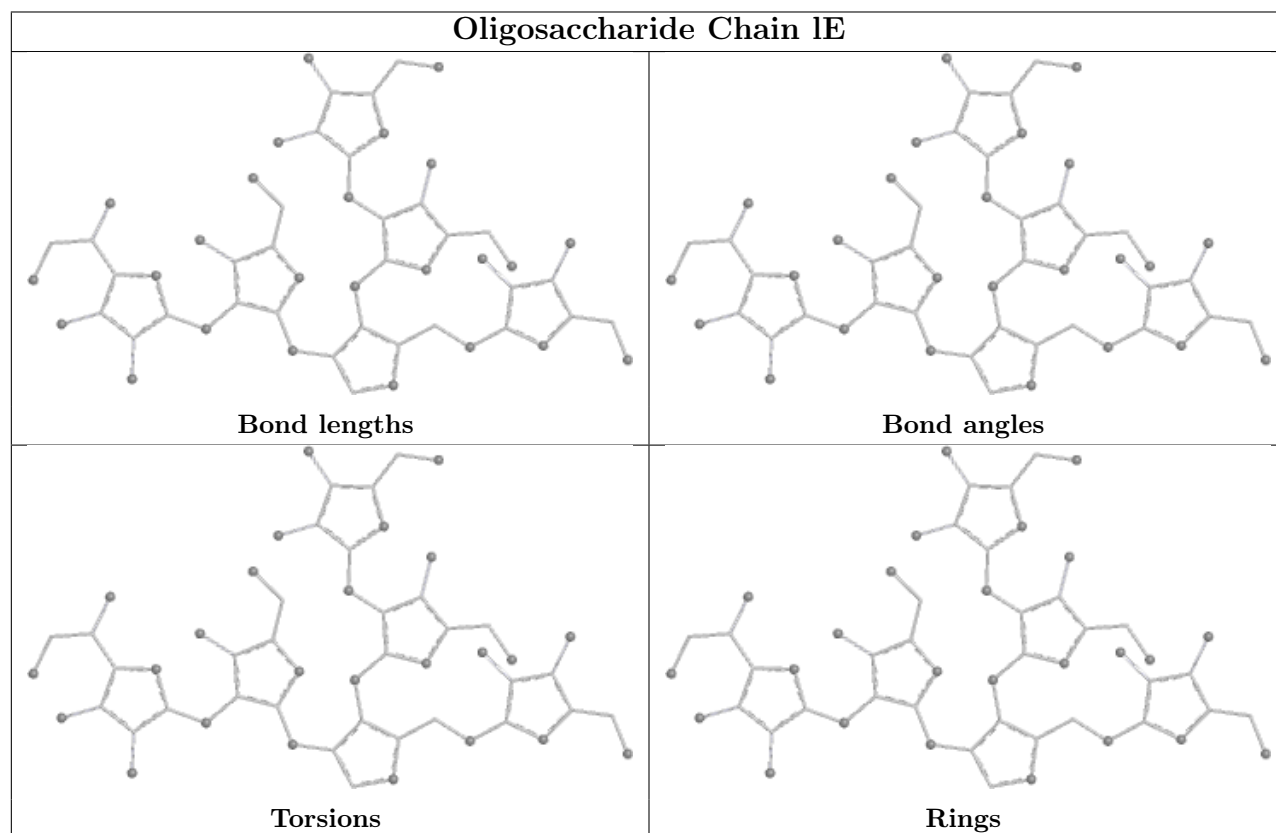
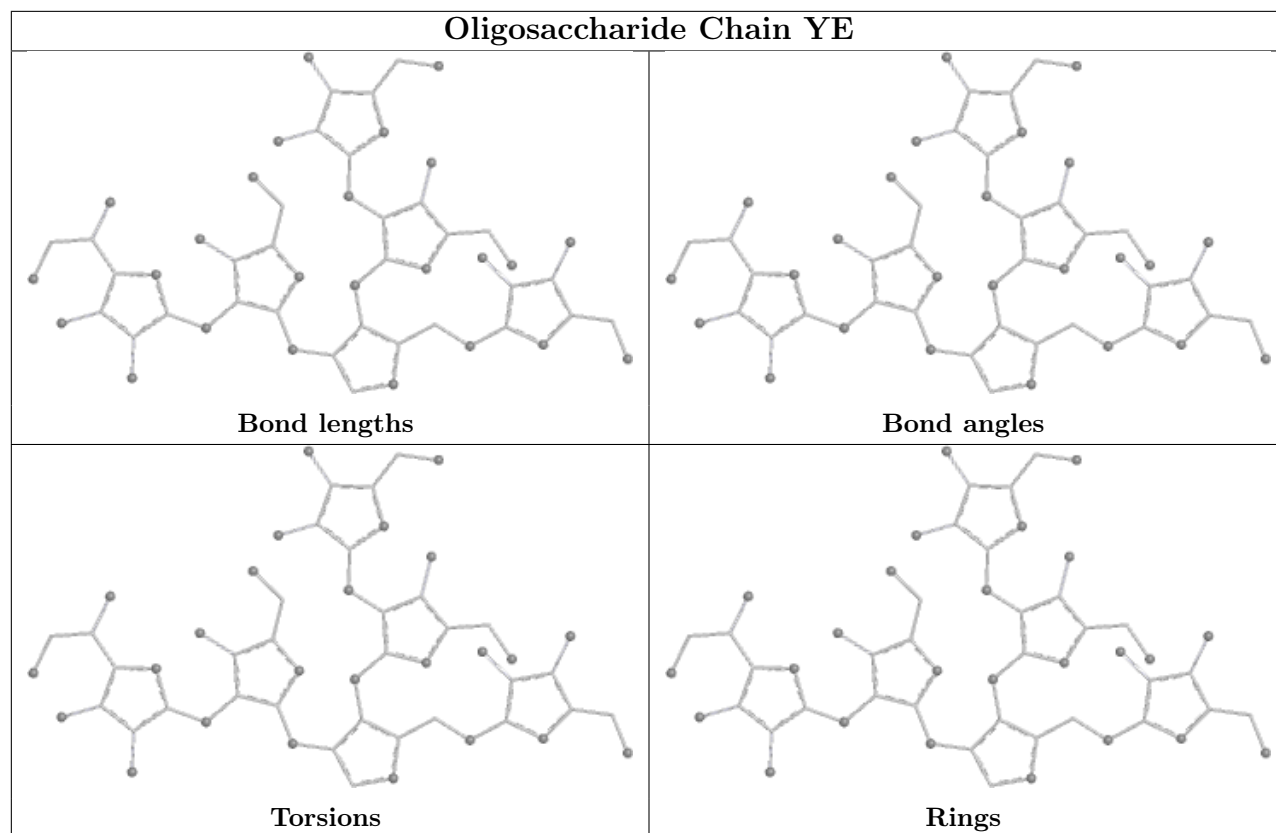
Oligosaccharide Chain iE



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

All (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
27	B	2010	GLA	O5-C1	4.47	1.51	1.43
27	E	2016	GLA	O5-C1	4.46	1.51	1.43
27	F	2013	GLA	O5-C1	4.45	1.51	1.43
27	E	2013	GLA	O5-C1	4.45	1.51	1.43
27	B	2016	GLA	O5-C1	4.44	1.51	1.43
27	D	2005	GLA	O5-C1	4.44	1.51	1.43
27	D	2009	GLA	O5-C1	4.44	1.51	1.43
27	B	2012	GLA	O5-C1	4.43	1.51	1.43
27	E	2008	GLA	O5-C1	4.41	1.51	1.43
27	C	2007	GLA	O5-C1	4.40	1.51	1.43
27	F	2011	GLA	O5-C1	4.40	1.51	1.43
27	F	2014	GLA	O5-C1	4.40	1.51	1.43
27	A	2014	GLA	O5-C1	4.39	1.51	1.43
27	F	2010	GLA	O5-C1	4.38	1.51	1.43
27	F	2015	GLA	O5-C1	4.38	1.51	1.43
27	A	2015	GLA	O5-C1	4.38	1.51	1.43
27	F	2018	GLA	O5-C1	4.38	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	E	2006	GLA	O5-C1	4.37	1.51	1.43
27	F	2006	GLA	O5-C1	4.37	1.51	1.43
27	C	2008	GLA	O5-C1	4.37	1.51	1.43
27	F	2017	GLA	O5-C1	4.37	1.51	1.43
27	C	2004	GLA	O5-C1	4.35	1.51	1.43
27	A	2011	GLA	O5-C1	4.33	1.51	1.43
27	A	2013	GLA	O5-C1	4.33	1.51	1.43
27	A	2012	GLA	O5-C1	4.32	1.51	1.43
27	B	2015	GLA	O5-C1	4.32	1.50	1.43
27	A	2016	GLA	O5-C1	4.32	1.50	1.43
27	B	2013	GLA	O5-C1	4.32	1.50	1.43
27	E	2007	GLA	O5-C1	4.31	1.50	1.43
27	B	2008	GLA	O5-C1	4.31	1.50	1.43
27	E	2014	GLA	O5-C1	4.31	1.50	1.43
27	E	2009	GLA	O5-C1	4.30	1.50	1.43
27	F	2016	GLA	O5-C1	4.30	1.50	1.43
27	B	2007	GLA	O5-C1	4.30	1.50	1.43
27	A	2009	GLA	O5-C1	4.29	1.50	1.43
27	A	2006	GLA	O5-C1	4.29	1.50	1.43
27	E	2015	GLA	O5-C1	4.28	1.50	1.43
27	B	2006	GLA	O5-C1	4.28	1.50	1.43
27	E	2012	GLA	O5-C1	4.26	1.50	1.43
27	A	2007	GLA	O5-C1	4.26	1.50	1.43
27	D	2006	GLA	O5-C1	4.25	1.50	1.43
27	C	2005	GLA	O5-C1	4.25	1.50	1.43
27	A	2005	GLA	O5-C1	4.24	1.50	1.43
27	D	2007	GLA	O5-C1	4.23	1.50	1.43
27	E	2010	GLA	O5-C1	4.22	1.50	1.43
27	E	2005	GLA	O5-C1	4.21	1.50	1.43
27	C	2006	GLA	O5-C1	4.21	1.50	1.43
27	D	2008	GLA	O5-C1	4.21	1.50	1.43
27	F	2008	GLA	O5-C1	4.19	1.50	1.43
27	E	2011	GLA	O5-C1	4.17	1.50	1.43
27	F	2012	GLA	O5-C1	4.17	1.50	1.43
27	B	2017	GLA	O5-C1	4.15	1.50	1.43
27	F	2007	GLA	O5-C1	4.10	1.50	1.43
27	B	2014	GLA	O5-C1	4.09	1.50	1.43
27	F	2009	GLA	O5-C1	4.08	1.50	1.43
27	A	2010	GLA	O5-C1	4.03	1.50	1.43
27	B	2011	GLA	O5-C1	3.96	1.50	1.43
27	E	2004	GLA	C2-C3	-2.94	1.48	1.52
27	F	2006	GLA	C2-C3	-2.85	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	2016	GLA	C2-C3	-2.84	1.48	1.52
27	A	2006	GLA	C2-C3	-2.83	1.48	1.52
27	B	2007	GLA	C2-C3	-2.77	1.48	1.52
27	A	2010	GLA	C2-C3	-2.75	1.48	1.52
27	A	2015	GLA	C2-C3	-2.74	1.48	1.52
27	E	2016	GLA	C2-C3	-2.74	1.48	1.52
27	E	2005	GLA	C2-C3	-2.71	1.48	1.52
27	B	2011	GLA	C2-C3	-2.70	1.48	1.52
27	A	2014	GLA	C2-C3	-2.69	1.48	1.52
27	D	2008	GLA	C2-C3	-2.68	1.48	1.52
27	F	2008	GLA	C2-C3	-2.67	1.48	1.52
27	A	2011	GLA	C2-C3	-2.66	1.48	1.52
27	E	2007	GLA	C2-C3	-2.66	1.48	1.52
27	A	2007	GLA	C2-C3	-2.66	1.48	1.52
27	F	2010	GLA	C2-C3	-2.65	1.48	1.52
27	F	2012	GLA	C2-C3	-2.65	1.48	1.52
27	E	2013	GLA	C2-C3	-2.64	1.48	1.52
27	B	2015	GLA	C2-C3	-2.64	1.48	1.52
27	C	2007	GLA	C2-C3	-2.64	1.48	1.52
27	D	2009	GLA	C2-C3	-2.64	1.48	1.52
27	C	2008	GLA	C2-C3	-2.63	1.48	1.52
27	A	2004	GLA	C2-C3	-2.63	1.48	1.52
27	B	2005	GLA	C2-C3	-2.62	1.48	1.52
27	A	2013	GLA	C2-C3	-2.61	1.48	1.52
27	E	2006	GLA	C2-C3	-2.60	1.48	1.52
27	B	2006	GLA	C2-C3	-2.59	1.48	1.52
27	B	2012	GLA	C2-C3	-2.59	1.48	1.52
27	B	2008	GLA	C2-C3	-2.59	1.48	1.52
27	E	2011	GLA	C2-C3	-2.58	1.48	1.52
27	A	2016	GLA	C2-C3	-2.53	1.48	1.52
27	F	2014	GLA	C2-C3	-2.52	1.48	1.52
27	A	2012	GLA	C2-C3	-2.51	1.48	1.52
27	F	2007	GLA	C2-C3	-2.50	1.48	1.52
27	B	2014	GLA	C2-C3	-2.49	1.48	1.52
27	F	2018	GLA	C2-C3	-2.49	1.48	1.52
27	D	2007	GLA	C2-C3	-2.49	1.48	1.52
27	F	2015	GLA	C2-C3	-2.49	1.48	1.52
27	E	2014	GLA	C2-C3	-2.47	1.48	1.52
27	F	2011	GLA	C2-C3	-2.46	1.48	1.52
27	C	2004	GLA	C2-C3	-2.45	1.48	1.52
27	F	2009	GLA	C2-C3	-2.45	1.48	1.52
27	D	2005	GLA	C2-C3	-2.44	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	E	2007	GLA	O5-C5	2.43	1.48	1.43
27	B	2010	GLA	C2-C3	-2.42	1.48	1.52
27	C	2006	GLA	C2-C3	-2.41	1.48	1.52
27	F	2013	GLA	C2-C3	-2.40	1.48	1.52
27	A	2008	GLA	C2-C3	-2.39	1.48	1.52
27	A	2005	GLA	C2-C3	-2.38	1.48	1.52
27	B	2013	GLA	C2-C3	-2.34	1.48	1.52
27	A	2009	GLA	C2-C3	-2.33	1.48	1.52
27	B	2005	GLA	O5-C5	2.32	1.48	1.43
27	A	2004	GLA	O5-C5	2.32	1.47	1.43
27	F	2017	GLA	C2-C3	-2.32	1.48	1.52
27	E	2016	GLA	O5-C5	2.30	1.47	1.43
26	A	2002	AHR	C1-C2	2.29	1.55	1.51
27	B	2017	GLA	C2-C3	-2.27	1.49	1.52
27	B	2016	GLA	O5-C5	2.27	1.47	1.43
27	D	2008	GLA	O5-C5	2.27	1.47	1.43
27	E	2004	GLA	O5-C5	2.26	1.47	1.43
27	E	2008	GLA	C2-C3	-2.26	1.49	1.52
27	E	2010	GLA	C2-C3	-2.25	1.49	1.52
27	B	2006	GLA	O5-C5	2.24	1.47	1.43
27	F	2016	GLA	C2-C3	-2.24	1.49	1.52
27	B	2011	GLA	O5-C5	2.24	1.47	1.43
27	E	2009	GLA	C2-C3	-2.23	1.49	1.52
27	C	2005	GLA	C2-C3	-2.22	1.49	1.52
27	D	2006	GLA	C2-C3	-2.22	1.49	1.52
27	C	2004	GLA	O5-C5	2.22	1.47	1.43
27	A	2011	GLA	O5-C5	2.21	1.47	1.43
27	F	2015	GLA	O5-C5	2.21	1.47	1.43
27	D	2009	GLA	O5-C5	2.20	1.47	1.43
27	E	2015	GLA	C2-C3	-2.20	1.49	1.52
27	C	2008	GLA	O5-C5	2.20	1.47	1.43
27	D	2005	GLA	O5-C5	2.20	1.47	1.43
27	F	2006	GLA	O5-C5	2.19	1.47	1.43
27	E	2005	GLA	O5-C5	2.19	1.47	1.43
27	E	2009	GLA	O5-C5	2.18	1.47	1.43
27	B	2009	GLA	C2-C3	-2.18	1.49	1.52
27	F	2011	GLA	O5-C5	2.18	1.47	1.43
27	B	2012	GLA	O5-C5	2.17	1.47	1.43
27	E	2013	GLA	O5-C5	2.17	1.47	1.43
27	E	2008	GLA	O5-C5	2.17	1.47	1.43
27	F	2018	GLA	O5-C5	2.17	1.47	1.43
27	B	2010	GLA	O5-C5	2.16	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	C	2007	GLA	O5-C5	2.16	1.47	1.43
27	E	2011	GLA	O5-C5	2.16	1.47	1.43
27	A	2015	GLA	O5-C5	2.15	1.47	1.43
27	A	2010	GLA	O5-C5	2.15	1.47	1.43
27	F	2010	GLA	O5-C5	2.14	1.47	1.43
27	A	2006	GLA	O5-C5	2.14	1.47	1.43
27	F	2012	GLA	O5-C5	2.14	1.47	1.43
27	F	2014	GLA	O5-C5	2.13	1.47	1.43
27	A	2012	GLA	O5-C5	2.12	1.47	1.43
27	B	2007	GLA	O5-C5	2.12	1.47	1.43
27	E	2006	GLA	O5-C5	2.12	1.47	1.43
27	A	2009	GLA	O5-C5	2.12	1.47	1.43
27	A	2013	GLA	O5-C5	2.12	1.47	1.43
27	F	2017	GLA	O5-C5	2.11	1.47	1.43
27	F	2008	GLA	O5-C5	2.11	1.47	1.43
27	F	2007	GLA	O5-C5	2.10	1.47	1.43
27	A	2007	GLA	O5-C5	2.09	1.47	1.43
27	A	2016	GLA	O5-C5	2.08	1.47	1.43
27	B	2008	GLA	O5-C5	2.07	1.47	1.43
27	E	2014	GLA	O5-C5	2.07	1.47	1.43
27	D	2007	GLA	O5-C5	2.07	1.47	1.43
27	B	2015	GLA	O5-C5	2.07	1.47	1.43
27	F	2013	GLA	O5-C5	2.07	1.47	1.43
27	A	2005	GLA	O5-C5	2.06	1.47	1.43
27	B	2013	GLA	O5-C5	2.06	1.47	1.43
26	A	2003	AHR	C1-C2	2.05	1.55	1.51
27	C	2006	GLA	O5-C5	2.04	1.47	1.43
27	D	2006	GLA	O5-C5	2.03	1.47	1.43
26	E	2002	AHR	C1-C2	2.03	1.55	1.51
27	A	2014	GLA	O5-C5	2.02	1.47	1.43
27	B	2009	GLA	O5-C5	2.02	1.47	1.43
27	C	2005	GLA	O5-C5	2.01	1.47	1.43

All (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
26	F	2005	AHR	O4-C1-C2	-3.64	99.50	105.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	2004	GLA	C1-O5-C5	3.63	117.06	112.19
27	F	2006	GLA	O5-C1-C2	3.59	119.35	110.79
26	D	2004	AHR	O4-C1-C2	-3.59	99.58	105.76
26	E	2003	AHR	O4-C1-C2	-3.56	99.62	105.76
26	F	2001	AHR	O4-C1-C2	-3.54	99.65	105.76
27	B	2017	GLA	C1-C2-C3	3.41	114.60	109.64
26	A	2003	AHR	C1-C2-C3	3.40	107.07	101.63
27	F	2006	GLA	C1-O5-C5	3.40	116.74	112.19
27	E	2004	GLA	C1-O5-C5	3.38	116.71	112.19
27	E	2010	GLA	C1-C2-C3	3.29	114.44	109.64
26	E	2002	AHR	O4-C4-C5	-3.27	103.42	109.36
26	D	2001	AHR	O4-C1-C2	-3.26	100.15	105.76
27	E	2012	GLA	C1-C2-C3	3.25	114.37	109.64
27	E	2015	GLA	C1-C2-C3	3.15	114.24	109.64
26	E	2002	AHR	C1-C2-C3	3.15	106.67	101.63
26	B	2003	AHR	O4-C1-C2	-3.14	100.35	105.76
28	B	2019	NAG	C1-O5-C5	3.13	116.38	112.19
27	B	2005	GLA	C1-O5-C5	3.05	116.28	112.19
27	E	2004	GLA	O5-C1-C2	3.04	118.04	110.79
26	B	2003	AHR	C1-O4-C4	-3.03	101.37	108.06
27	B	2005	GLA	O5-C1-C2	3.00	117.95	110.79
27	E	2004	GLA	C1-C2-C3	2.97	113.97	109.64
27	B	2005	GLA	C1-C2-C3	2.93	113.91	109.64
27	F	2006	GLA	C1-C2-C3	2.89	113.86	109.64
27	A	2004	GLA	O5-C1-C2	2.89	117.67	110.79
27	A	2004	GLA	C1-C2-C3	2.85	113.80	109.64
26	C	2003	AHR	O4-C4-C5	-2.83	104.22	109.36
26	D	2003	AHR	O4-C1-C2	-2.78	100.97	105.76
26	A	2002	AHR	C1-C2-C3	2.76	106.04	101.63
26	C	2003	AHR	C1-C2-C3	2.74	106.01	101.63
26	B	2004	AHR	O4-C1-C2	-2.68	101.15	105.76
26	B	2003	AHR	O5-C5-C4	-2.67	102.26	111.33
26	D	2003	AHR	O5-C5-C4	-2.66	102.28	111.33
26	C	2003	AHR	O5-C5-C4	-2.66	102.29	111.33
26	E	2002	AHR	O5-C5-C4	-2.63	102.38	111.33
28	C	2010	NAG	C1-O5-C5	2.62	115.69	112.19
27	E	2007	GLA	C3-C4-C5	2.59	114.92	110.23
27	F	2017	GLA	C1-C2-C3	2.59	113.41	109.64
26	D	2001	AHR	O2-C2-C1	2.57	118.88	110.89
26	D	2003	AHR	O4-C4-C5	-2.54	104.74	109.36
26	B	2004	AHR	C1-O4-C4	-2.50	102.54	108.06
26	B	2002	AHR	C1-C2-C3	2.48	105.59	101.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	2004	AHR	C5-C4-C3	2.47	120.92	115.10
26	A	2018	AHR	C1-C2-C3	2.42	105.50	101.63
27	E	2004	GLA	C6-C5-C4	-2.40	107.12	113.02
26	A	2003	AHR	O4-C4-C5	-2.39	105.02	109.36
26	B	2003	AHR	C5-C4-C3	2.37	120.70	115.10
26	B	2020	AHR	C1-C2-C3	2.35	105.38	101.63
27	E	2007	GLA	C1-O5-C5	2.33	115.30	112.19
27	F	2006	GLA	C6-C5-C4	-2.30	107.37	113.02
26	D	2004	AHR	O2-C2-C1	2.30	118.04	110.89
27	A	2010	GLA	C6-C5-C4	-2.29	107.41	113.02
26	B	2004	AHR	O5-C5-C4	-2.25	103.69	111.33
26	F	2005	AHR	O2-C2-C3	2.25	115.85	111.43
26	E	2003	AHR	O2-C2-C3	2.24	115.84	111.43
27	A	2006	GLA	C6-C5-C4	-2.24	107.52	113.02
27	F	2008	GLA	C6-C5-C4	-2.24	107.53	113.02
26	E	2003	AHR	O2-C2-C1	2.23	117.83	110.89
27	E	2009	GLA	C1-C2-C3	2.23	112.89	109.64
26	F	2005	AHR	O2-C2-C1	2.22	117.81	110.89
27	D	2006	GLA	C1-C2-C3	2.22	112.88	109.64
26	F	2001	AHR	O2-C2-C3	2.22	115.80	111.43
26	D	2004	AHR	O2-C2-C3	2.21	115.78	111.43
27	A	2009	GLA	C1-C2-C3	2.21	112.86	109.64
26	F	2001	AHR	O2-C2-C1	2.21	117.75	110.89
27	E	2008	GLA	C1-C2-C3	2.20	112.85	109.64
26	A	2002	AHR	O4-C4-C3	-2.20	102.60	104.63
27	F	2009	GLA	C3-C4-C5	2.20	114.21	110.23
27	A	2004	GLA	C6-C5-C4	-2.19	107.64	113.02
28	E	2017	NAG	C1-O5-C5	2.18	115.10	112.19
27	A	2016	GLA	C1-C2-C3	2.16	112.78	109.64
26	A	2003	AHR	O5-C5-C4	-2.15	104.02	111.33
26	F	2004	AHR	O2-C2-C1	2.15	117.57	110.89
27	B	2011	GLA	C3-C4-C5	2.14	114.12	110.23
26	F	2004	AHR	O2-C2-C3	2.13	115.63	111.43
27	C	2005	GLA	C1-C2-C3	2.10	112.70	109.64
27	E	2007	GLA	C1-C2-C3	2.09	112.68	109.64
27	A	2011	GLA	C6-C5-C4	-2.05	107.98	113.02
27	B	2014	GLA	C1-O5-C5	-2.05	109.44	112.19
26	C	2003	AHR	O4-C1-C2	-2.03	102.27	105.76

All (5) chirality outliers are listed below:

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Mol	Chain	Res	Type	Atom
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Mol	Chain	Res	Type	Atom
27	A	2007	GLA	C1
27	B	2008	GLA	C1
27	B	2014	GLA	C1
27	E	2007	GLA	C1
27	F	2009	GLA	C1

All (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
28	C	2009	NAG	O7-C7-N2-C2
28	E	2017	NAG	C8-C7-N2-C2
28	E	2017	NAG	O7-C7-N2-C2
26	A	2002	AHR	C3-C4-C5-O5
26	A	2003	AHR	C3-C4-C5-O5
27	F	2010	GLA	O5-C5-C6-O6
27	C	2004	GLA	O5-C5-C6-O6
26	A	2002	AHR	O4-C4-C5-O5
26	A	2003	AHR	O4-C4-C5-O5
26	E	2002	AHR	O4-C4-C5-O5
27	C	2007	GLA	O5-C5-C6-O6
26	C	2003	AHR	C3-C4-C5-O5
26	E	2002	AHR	C3-C4-C5-O5
27	F	2009	GLA	C4-C5-C6-O6
27	C	2005	GLA	O5-C5-C6-O6
27	A	2007	GLA	C4-C5-C6-O6
26	D	2003	AHR	C3-C4-C5-O5
27	A	2008	GLA	O5-C5-C6-O6
27	E	2008	GLA	O5-C5-C6-O6
27	E	2014	GLA	O5-C5-C6-O6
27	F	2014	GLA	O5-C5-C6-O6
27	C	2005	GLA	C4-C5-C6-O6
27	F	2018	GLA	C4-C5-C6-O6
27	A	2011	GLA	O5-C5-C6-O6
27	B	2009	GLA	O5-C5-C6-O6
27	B	2016	GLA	O5-C5-C6-O6
27	C	2004	GLA	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
27	F	2010	GLA	C4-C5-C6-O6
27	F	2014	GLA	C4-C5-C6-O6
27	E	2007	GLA	O5-C5-C6-O6
27	F	2018	GLA	O5-C5-C6-O6
26	C	2003	AHR	O4-C4-C5-O5
27	D	2009	GLA	O5-C5-C6-O6
27	A	2008	GLA	C4-C5-C6-O6
27	B	2008	GLA	C4-C5-C6-O6
27	A	2010	GLA	O5-C5-C6-O6
27	E	2005	GLA	O5-C5-C6-O6
27	F	2007	GLA	O5-C5-C6-O6
27	E	2016	GLA	C4-C5-C6-O6
27	B	2007	GLA	O5-C5-C6-O6
27	E	2016	GLA	O5-C5-C6-O6
27	C	2008	GLA	O5-C5-C6-O6
27	D	2007	GLA	O5-C5-C6-O6
27	C	2007	GLA	C4-C5-C6-O6
27	A	2007	GLA	O5-C5-C6-O6
27	F	2009	GLA	O5-C5-C6-O6
28	E	2017	NAG	C4-C5-C6-O6
27	A	2012	GLA	C4-C5-C6-O6
28	C	2010	NAG	O5-C5-C6-O6
27	E	2014	GLA	C4-C5-C6-O6
26	D	2003	AHR	O4-C4-C5-O5
26	D	2004	AHR	O4-C4-C5-O5
26	E	2003	AHR	O4-C4-C5-O5
26	F	2001	AHR	O4-C4-C5-O5
27	A	2011	GLA	C4-C5-C6-O6
27	A	2015	GLA	C4-C5-C6-O6
27	D	2009	GLA	C4-C5-C6-O6
27	E	2011	GLA	C4-C5-C6-O6
27	B	2008	GLA	O5-C5-C6-O6
27	B	2015	GLA	O5-C5-C6-O6
28	A	2017	NAG	O5-C5-C6-O6
28	B	2019	NAG	O5-C5-C6-O6
27	B	2016	GLA	C4-C5-C6-O6
27	C	2008	GLA	C4-C5-C6-O6
28	C	2010	NAG	C4-C5-C6-O6
27	D	2005	GLA	O5-C5-C6-O6
27	F	2012	GLA	O5-C5-C6-O6
27	E	2006	GLA	C4-C5-C6-O6
28	A	2017	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
28	B	2019	NAG	C4-C5-C6-O6
26	C	2001	AHR	O4-C4-C5-O5
26	F	2005	AHR	O4-C4-C5-O5
27	A	2012	GLA	O5-C5-C6-O6
27	B	2010	GLA	O5-C5-C6-O6
27	B	2009	GLA	C4-C5-C6-O6
26	D	2004	AHR	C3-C4-C5-O5
27	E	2005	GLA	C4-C5-C6-O6
26	F	2004	AHR	O4-C4-C5-O5
27	E	2007	GLA	C4-C5-C6-O6
27	F	2007	GLA	C4-C5-C6-O6
27	A	2015	GLA	O5-C5-C6-O6
26	E	2003	AHR	C3-C4-C5-O5
26	F	2001	AHR	C3-C4-C5-O5
26	F	2005	AHR	C3-C4-C5-O5
27	E	2008	GLA	C4-C5-C6-O6
27	E	2011	GLA	O5-C5-C6-O6
26	B	2003	AHR	C3-C4-C5-O5
27	E	2013	GLA	O5-C5-C6-O6
27	D	2007	GLA	C4-C5-C6-O6
26	B	2003	AHR	O4-C4-C5-O5
27	B	2011	GLA	O5-C5-C6-O6
27	B	2017	GLA	C4-C5-C6-O6
27	E	2006	GLA	O5-C5-C6-O6
28	E	2017	NAG	O5-C5-C6-O6
27	B	2015	GLA	C4-C5-C6-O6
27	E	2010	GLA	O5-C5-C6-O6
27	D	2008	GLA	C4-C5-C6-O6
27	A	2009	GLA	O5-C5-C6-O6
26	B	2020	AHR	O4-C4-C5-O5
27	A	2014	GLA	O5-C5-C6-O6
27	B	2007	GLA	C4-C5-C6-O6
27	A	2016	GLA	O5-C5-C6-O6
26	B	2004	AHR	C3-C4-C5-O5
27	A	2010	GLA	C4-C5-C6-O6
26	B	2004	AHR	O4-C4-C5-O5
27	B	2017	GLA	O5-C5-C6-O6
27	A	2006	GLA	O5-C5-C6-O6
27	F	2016	GLA	C4-C5-C6-O6
27	F	2017	GLA	C4-C5-C6-O6
28	C	2009	NAG	O5-C5-C6-O6
27	D	2005	GLA	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
27	F	2008	GLA	O5-C5-C6-O6
27	B	2013	GLA	O5-C5-C6-O6
26	C	2001	AHR	C3-C4-C5-O5
26	F	2004	AHR	C3-C4-C5-O5
27	B	2010	GLA	C4-C5-C6-O6
27	F	2012	GLA	C4-C5-C6-O6
27	D	2008	GLA	O5-C5-C6-O6
27	F	2016	GLA	O5-C5-C6-O6
27	F	2011	GLA	O5-C5-C6-O6
27	F	2017	GLA	O5-C5-C6-O6
27	E	2013	GLA	C4-C5-C6-O6
27	E	2012	GLA	C4-C5-C6-O6
28	B	2018	NAG	O5-C5-C6-O6
26	D	2001	AHR	O4-C4-C5-O5
27	B	2012	GLA	C4-C5-C6-O6
26	F	2003	AHR	O4-C4-C5-O5
28	C	2010	NAG	C8-C7-N2-C2
27	A	2014	GLA	C4-C5-C6-O6
28	C	2010	NAG	O7-C7-N2-C2
27	E	2004	GLA	O5-C5-C6-O6

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

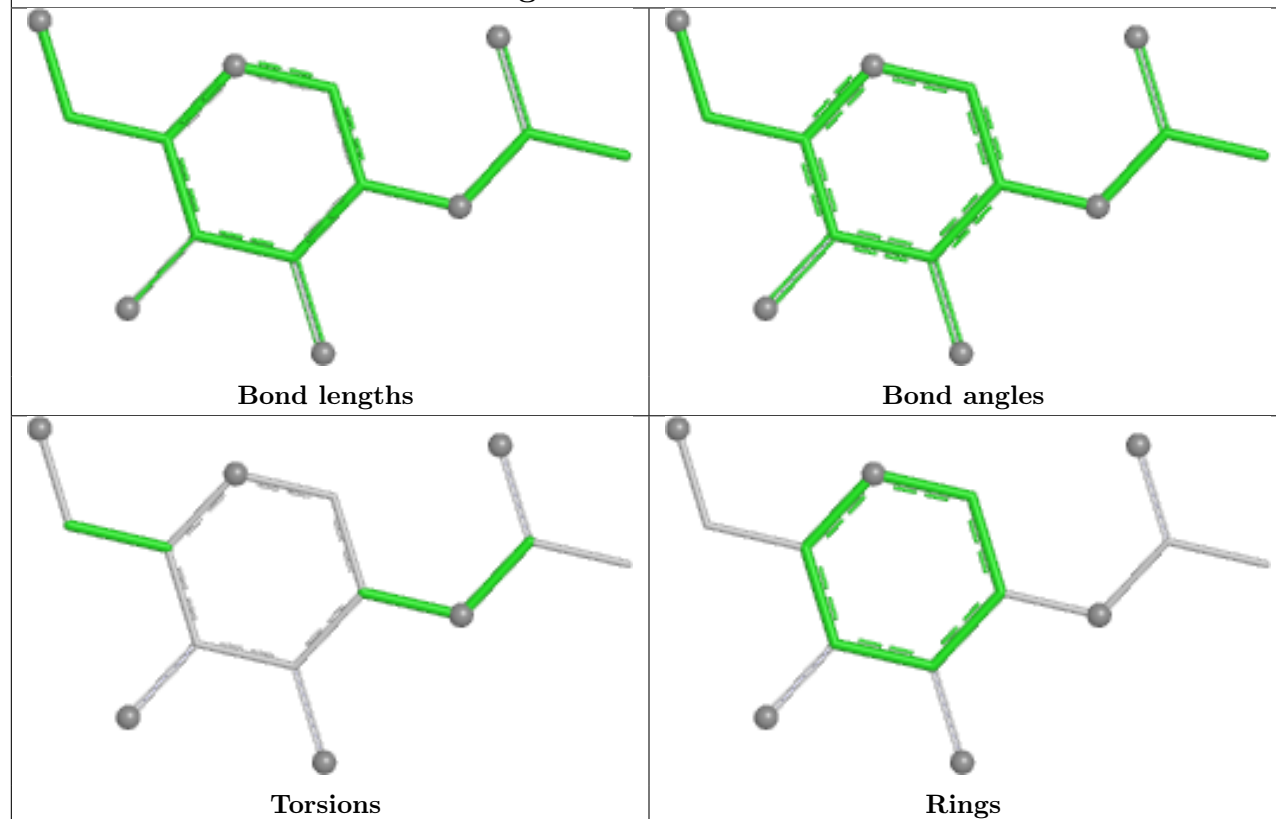
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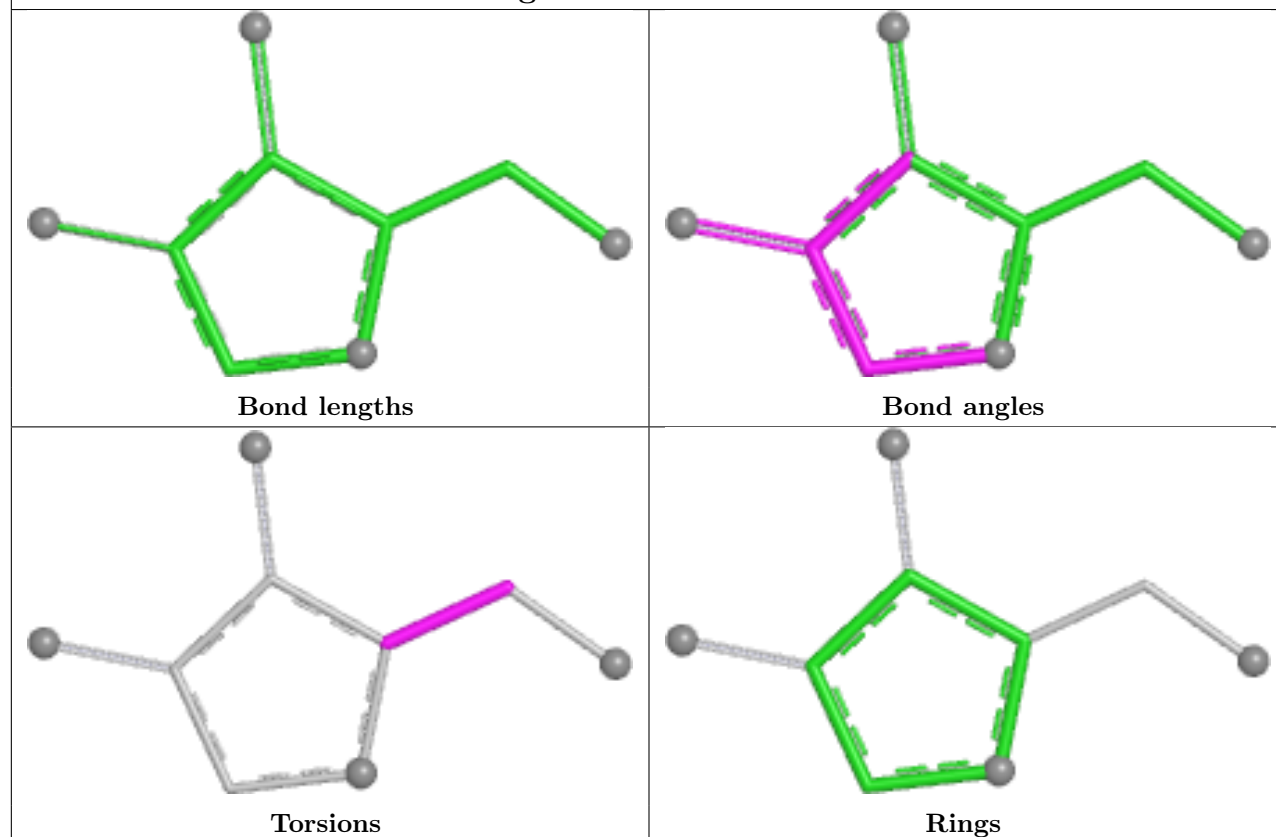
Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	A	2003	AHR	7	0
26	F	2003	AHR	6	0
27	F	2015	GLA	1	0
26	F	2001	AHR	3	0
28	B	2018	NAG	1	0
27	E	2009	GLA	1	0
26	F	2004	AHR	5	0
26	E	2003	AHR	4	0
27	B	2014	GLA	1	0
27	E	2013	GLA	1	0
26	B	2020	AHR	3	0
27	F	2016	GLA	2	0
27	F	2008	GLA	3	0
26	D	2001	AHR	5	0

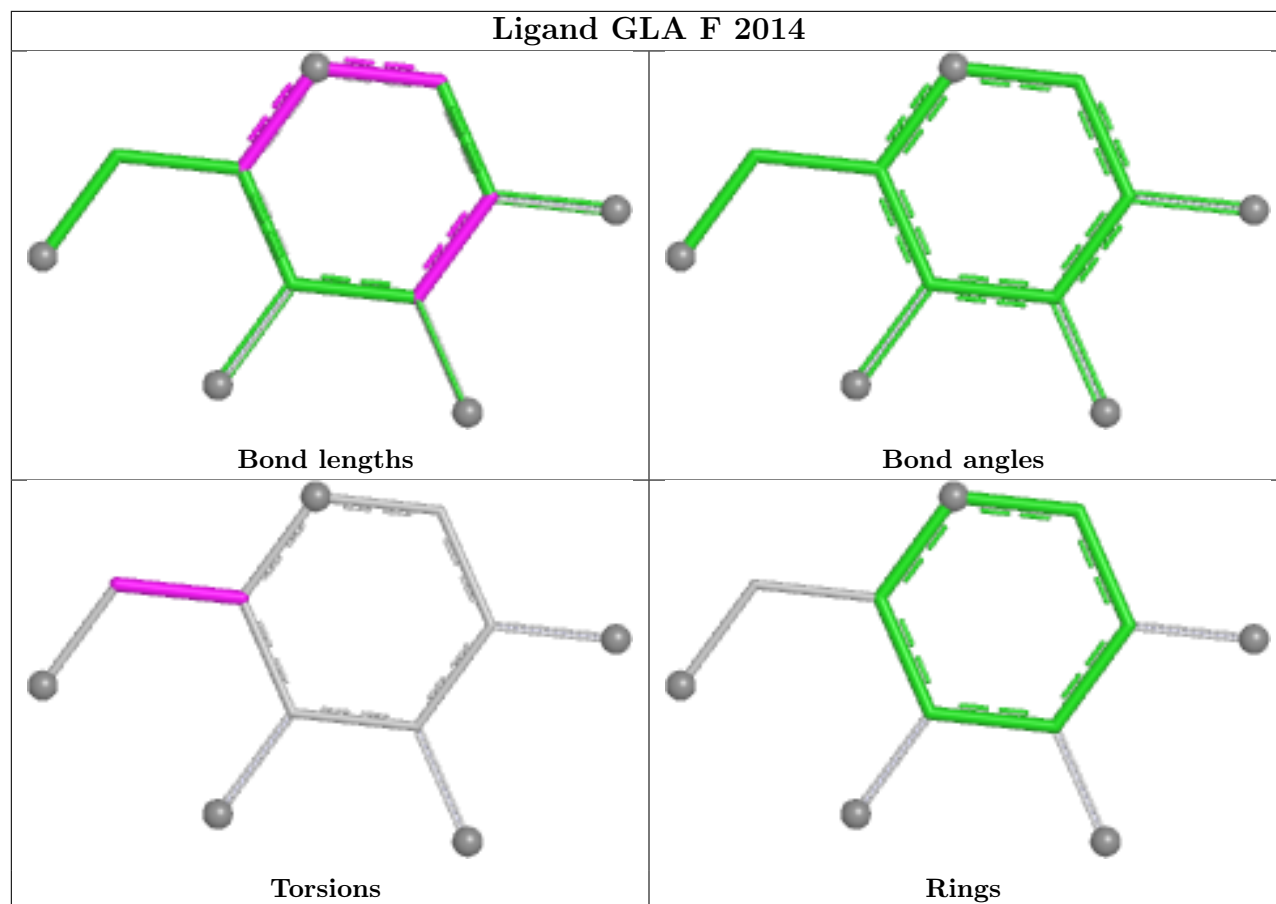
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 NAG D 2010

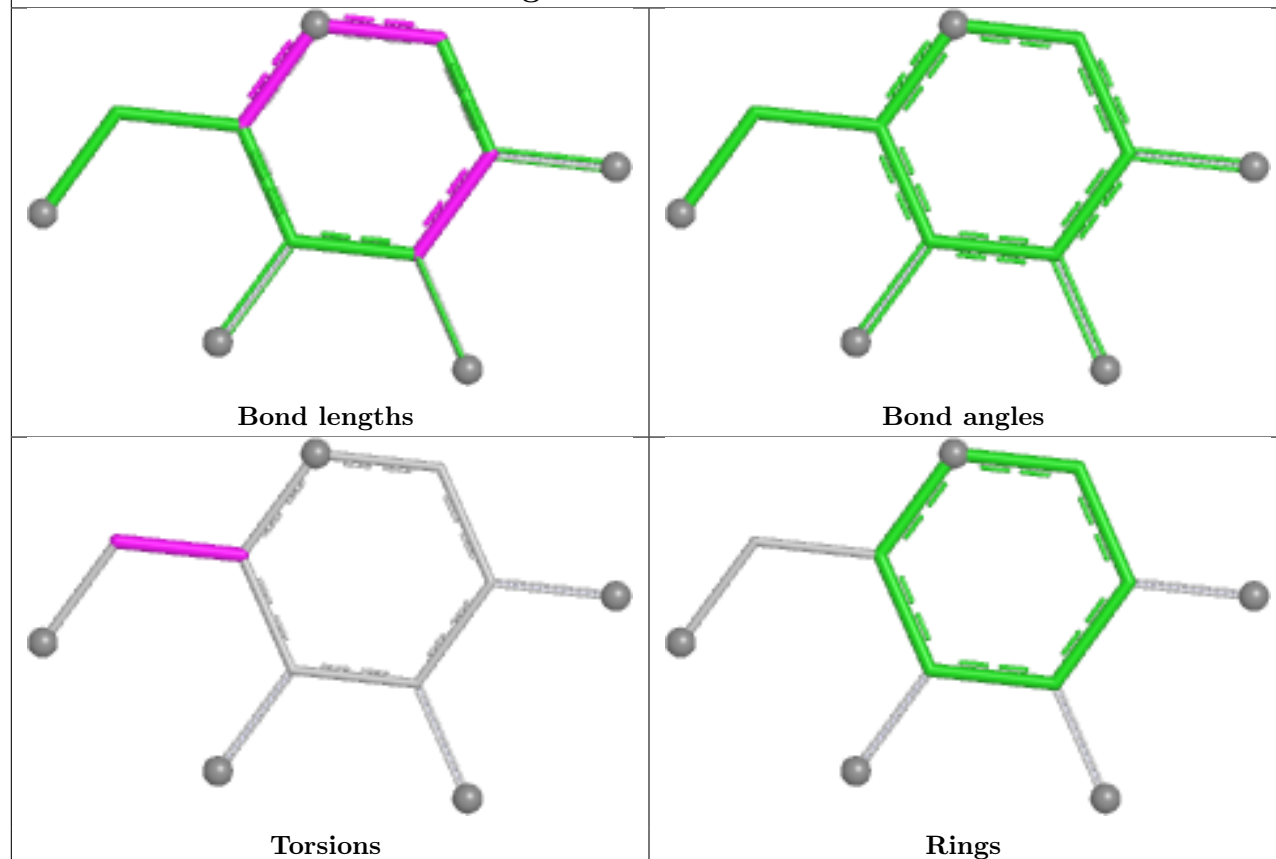


Ligand AHR D 2004

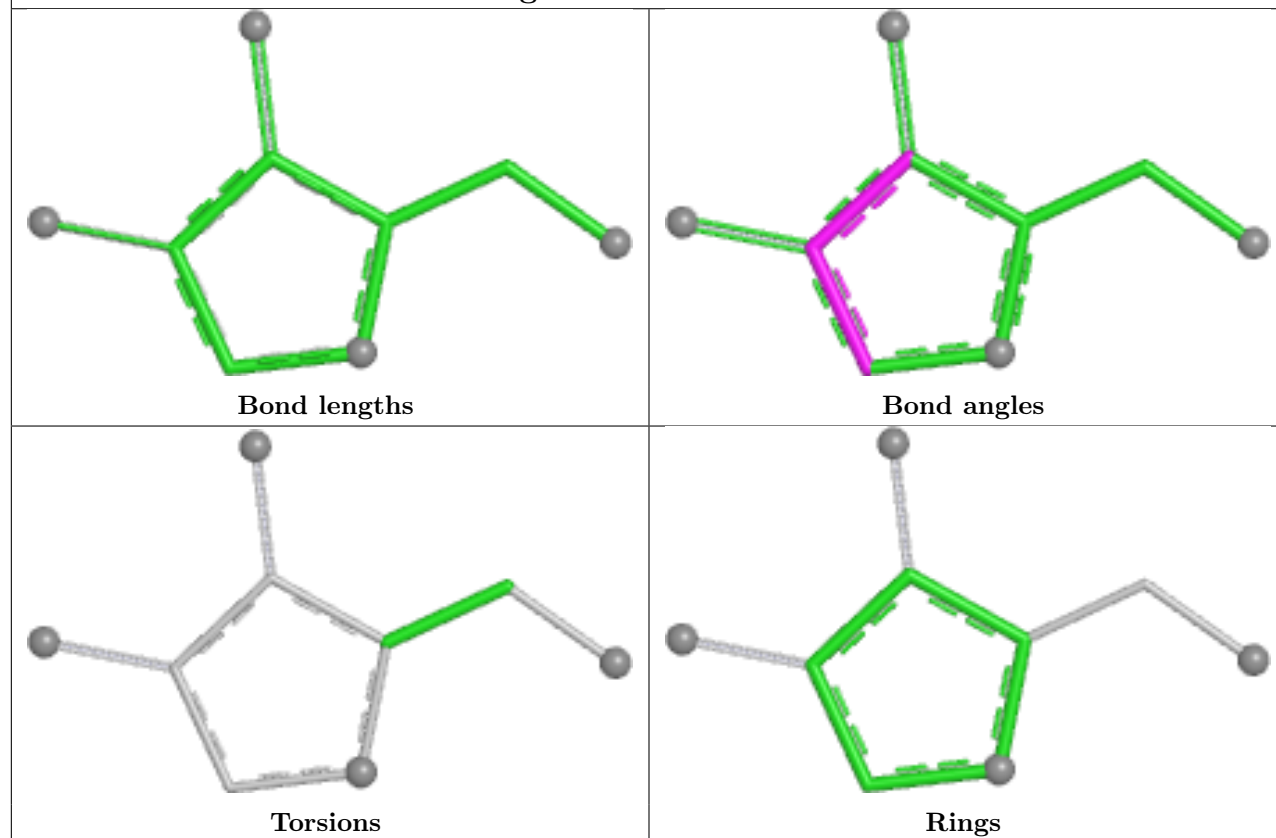




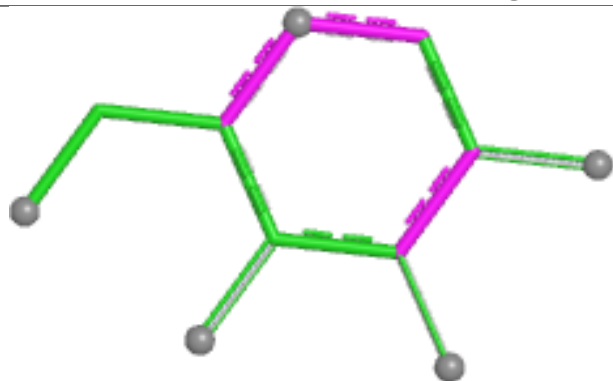
Ligand GLA B 2010



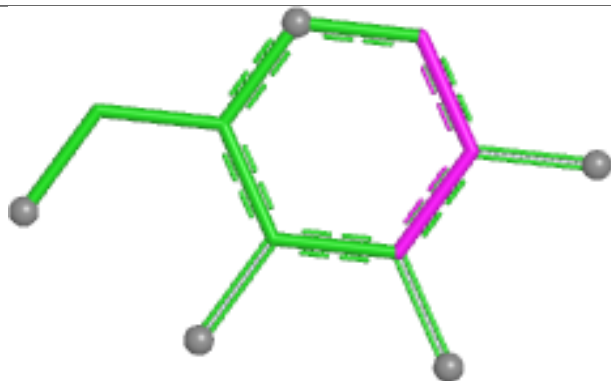
Ligand AHR B 2002



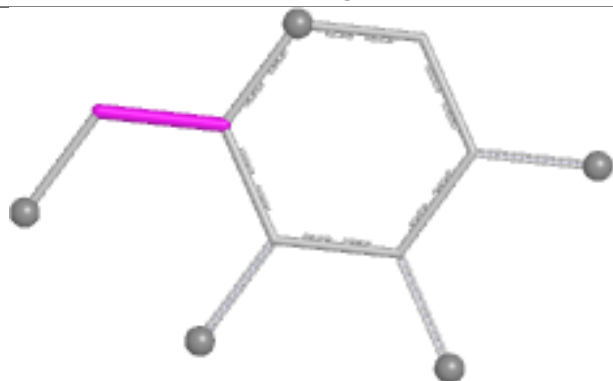
Ligand GLA E 2008



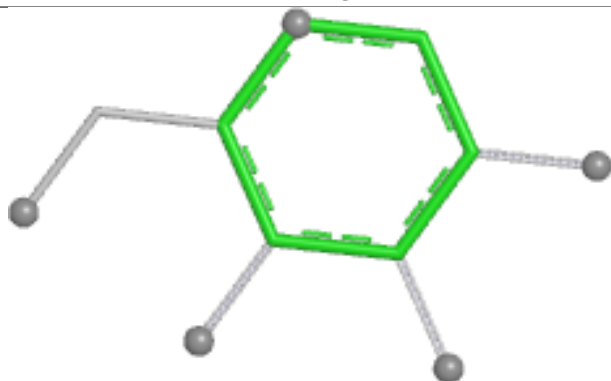
Bond lengths



Bond angles

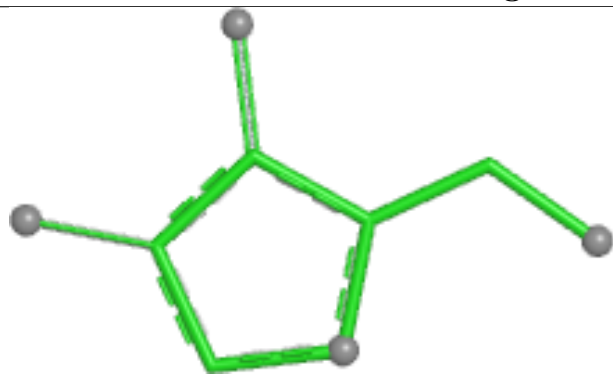


Torsions

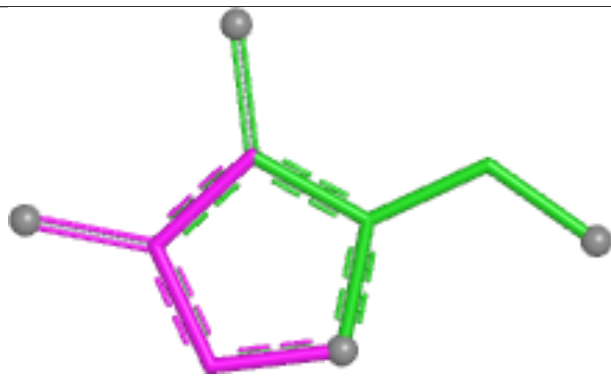


Rings

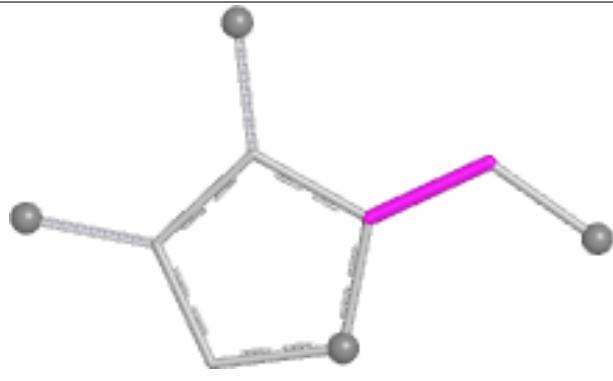
Ligand AHR F 2005



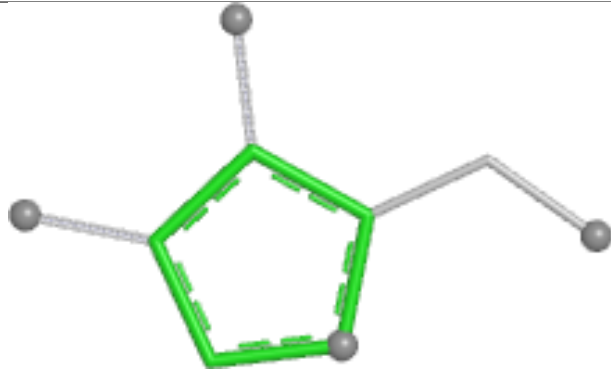
Bond lengths



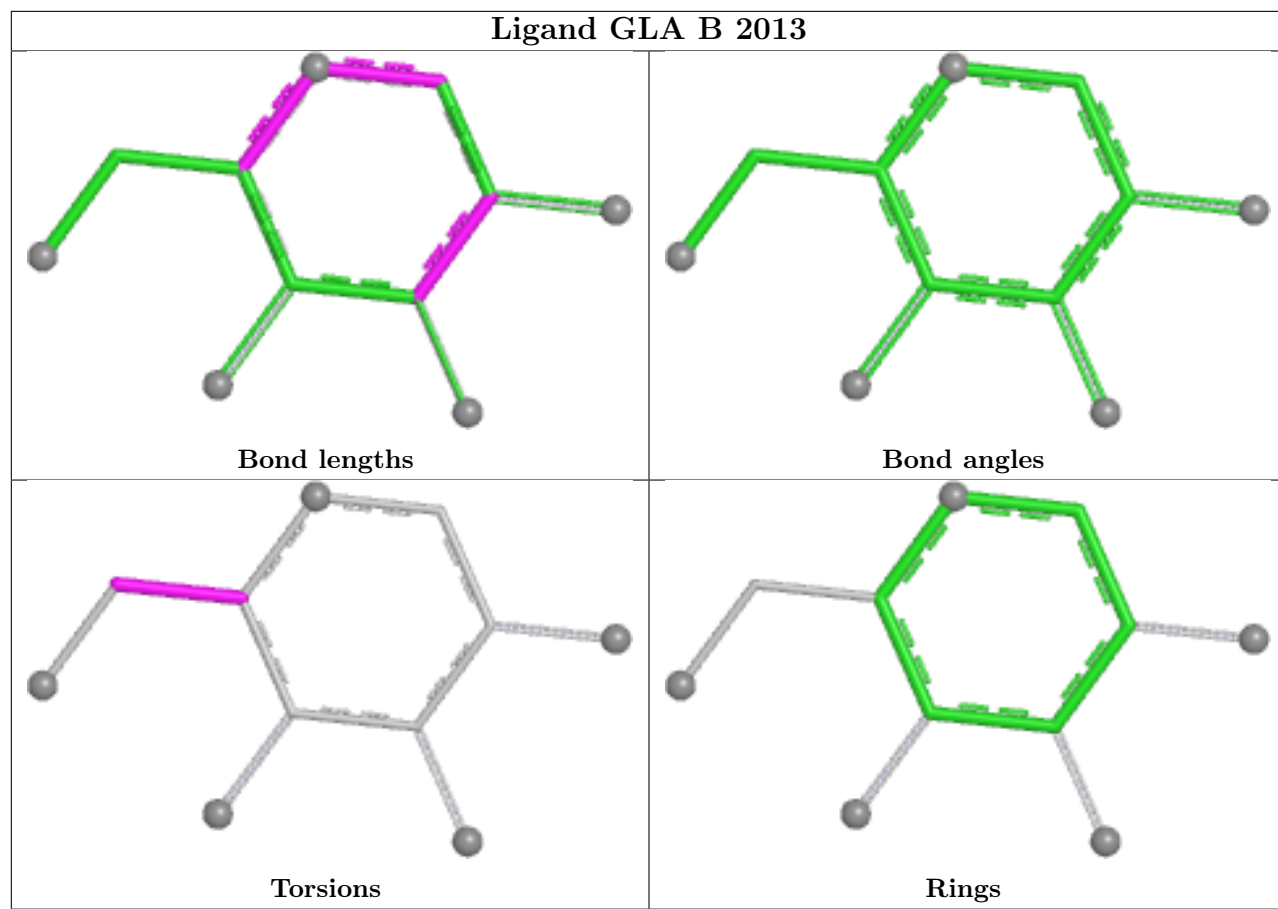
Bond angles



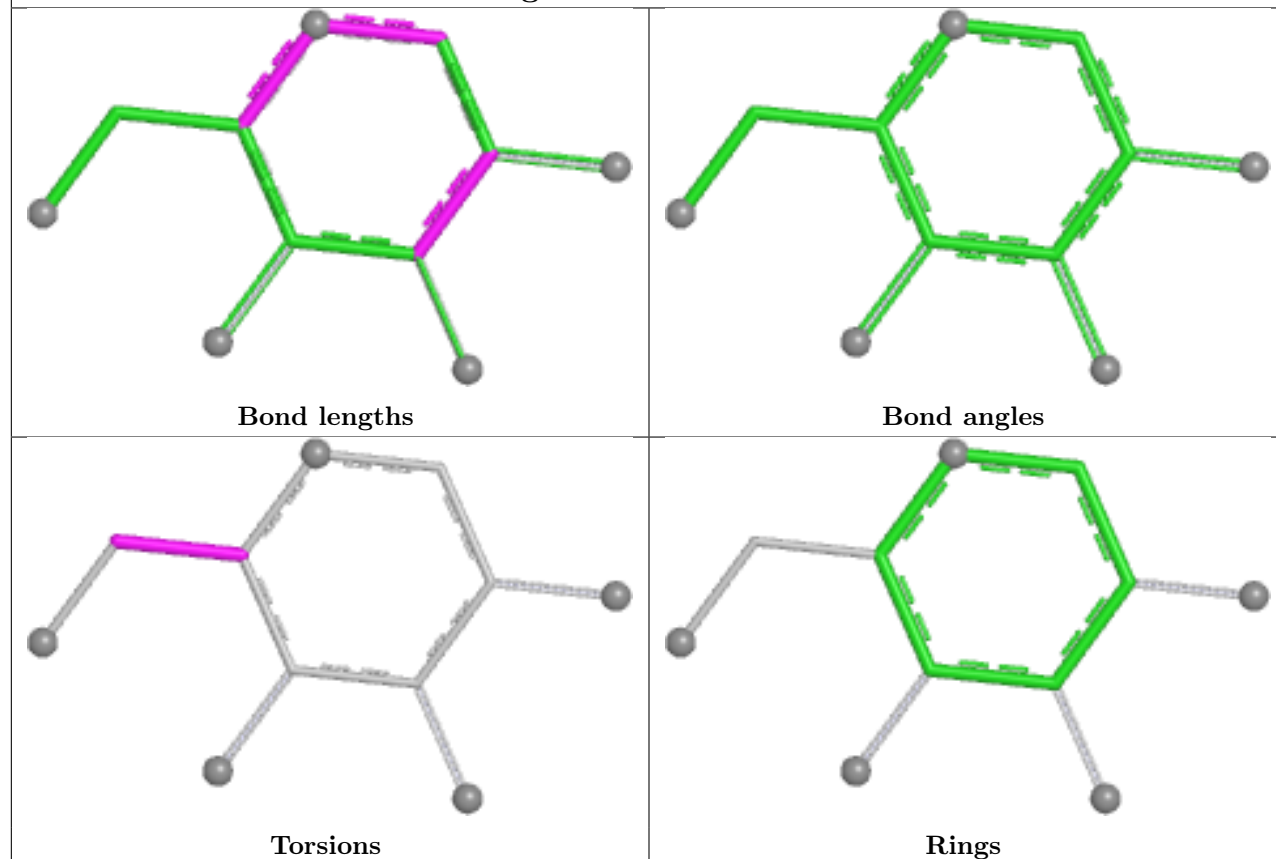
Torsions



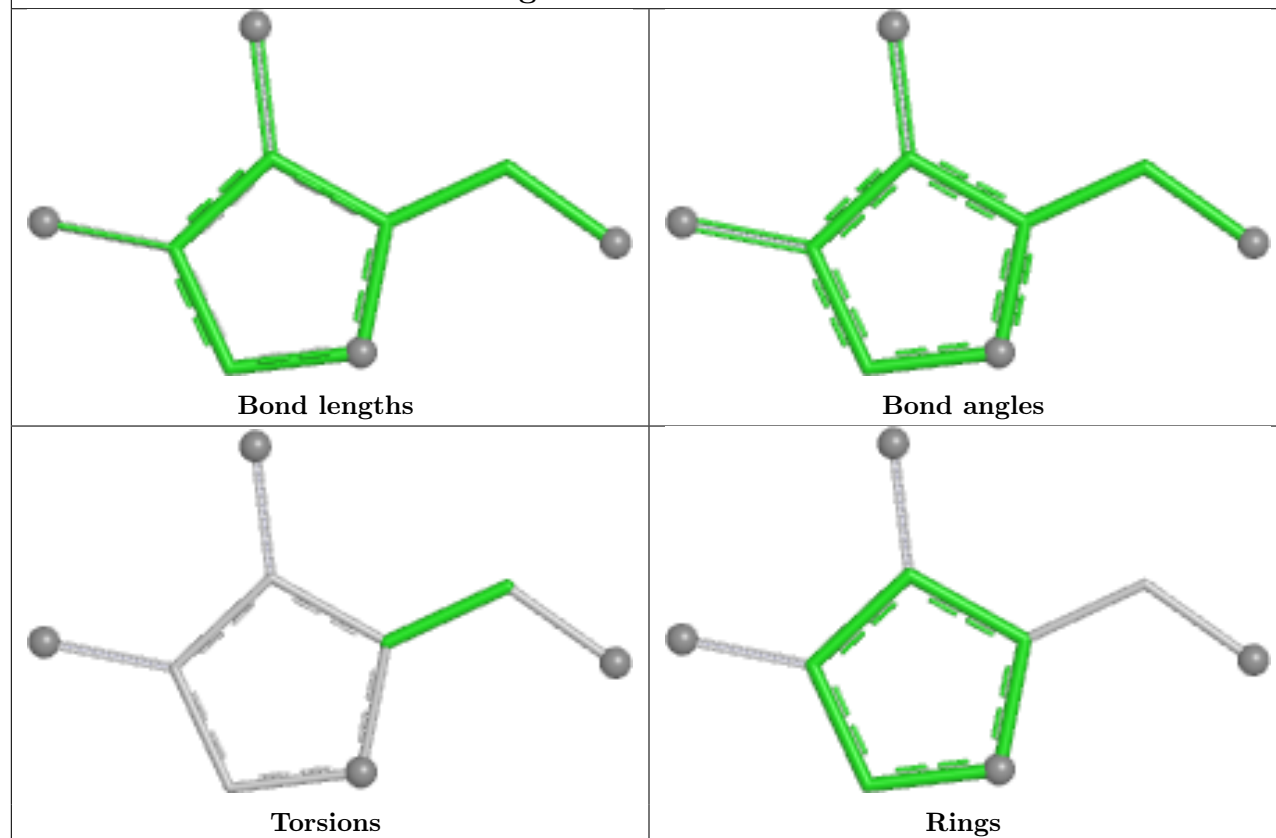
Rings



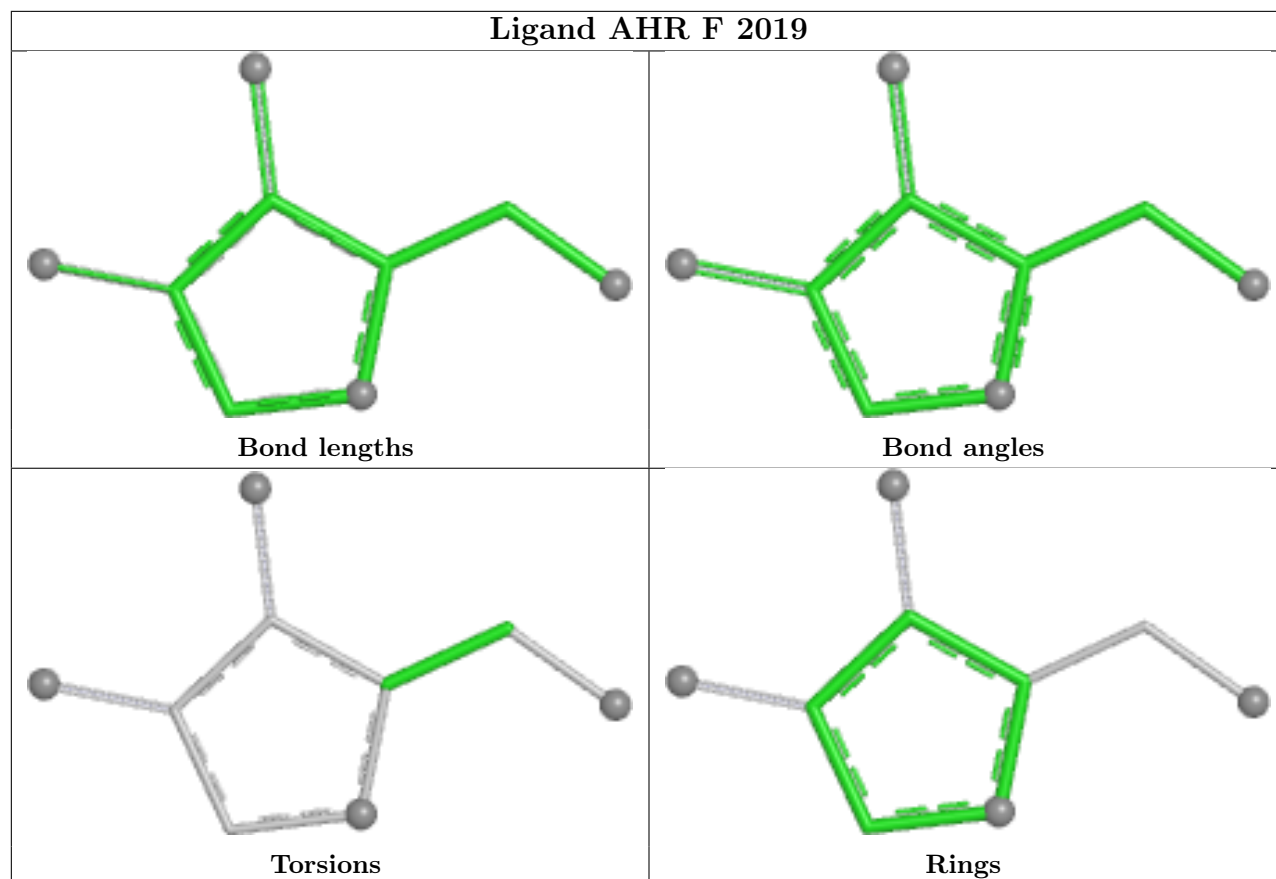
Ligand GLA D 2008



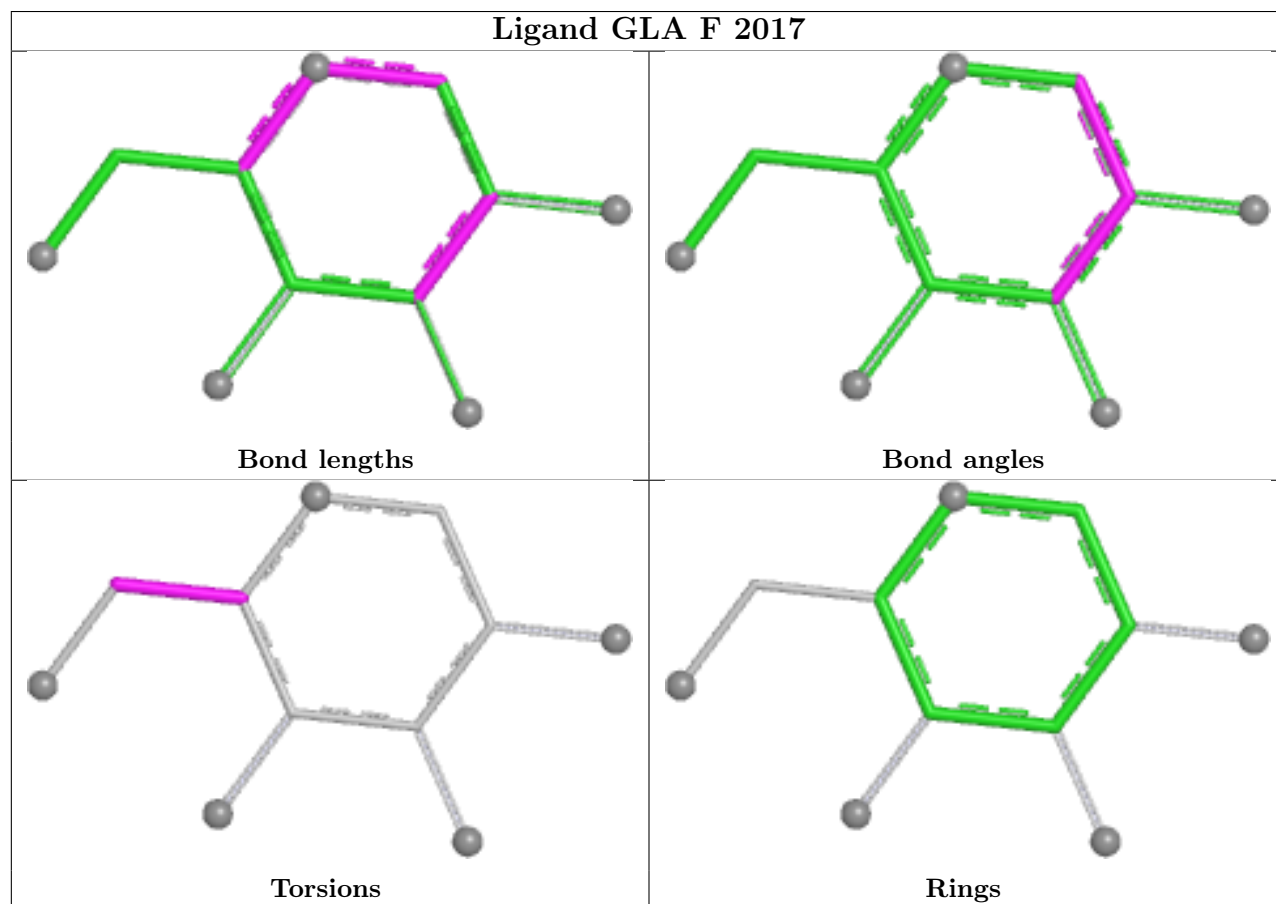
Ligand AHR A 2019

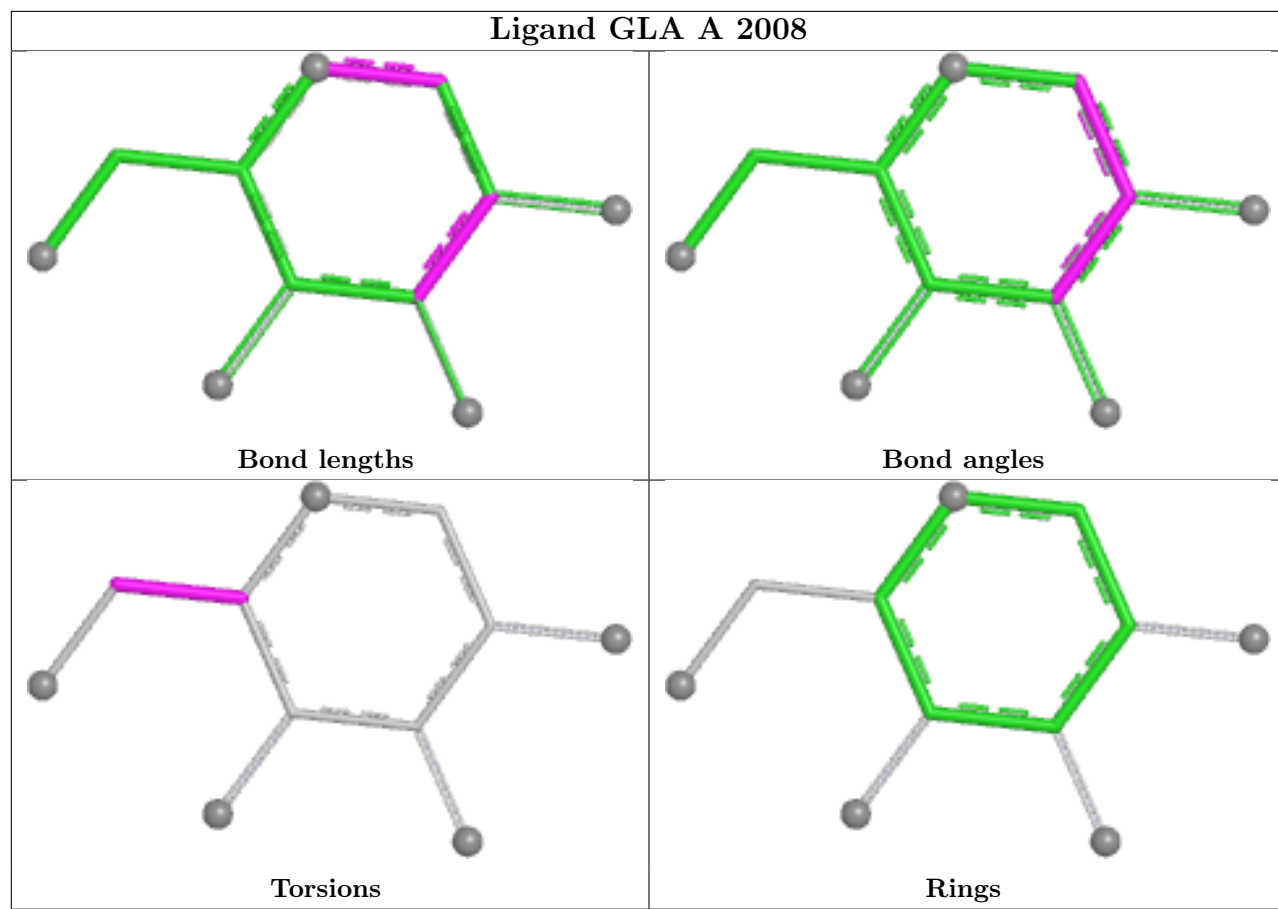


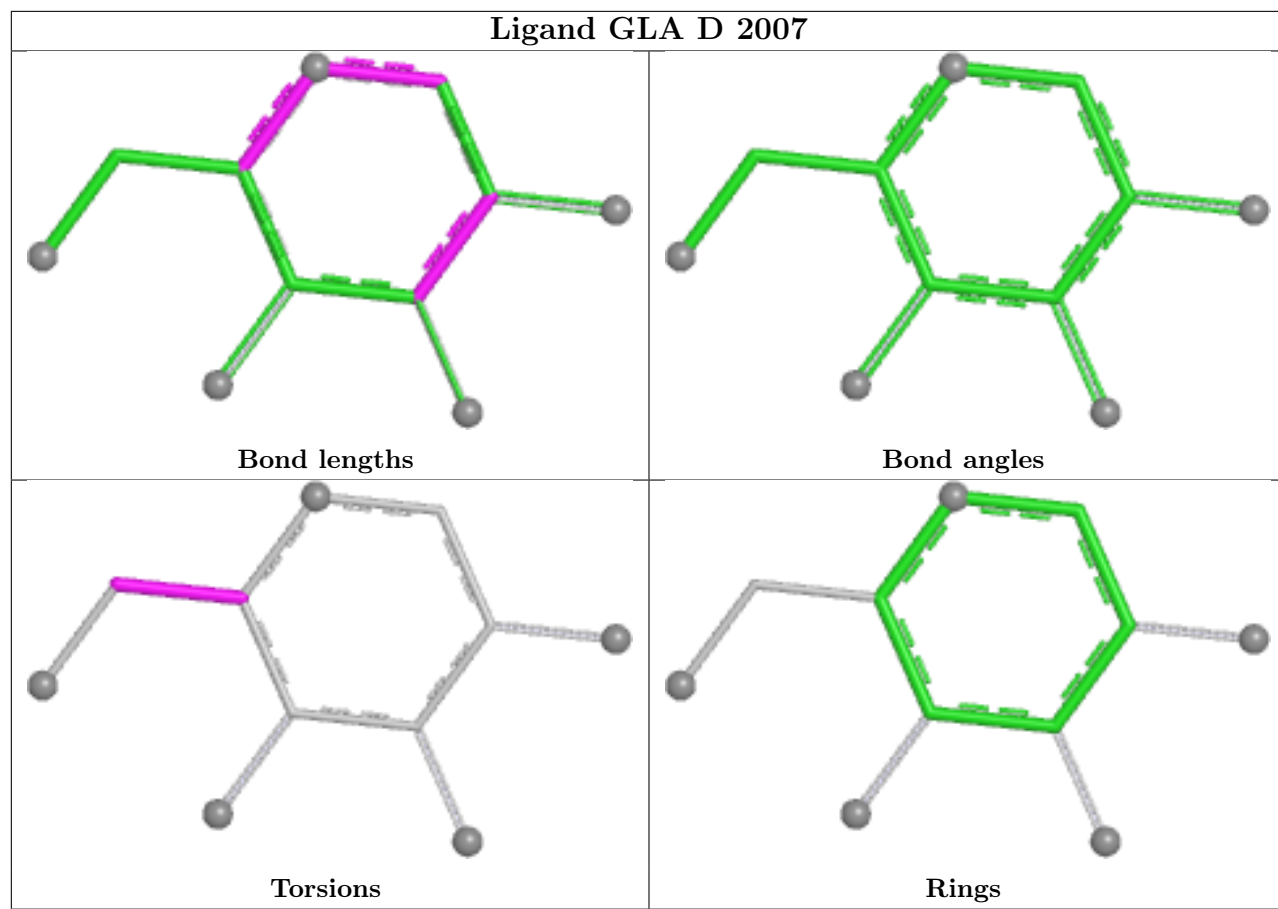
Ligand AHR F 2019

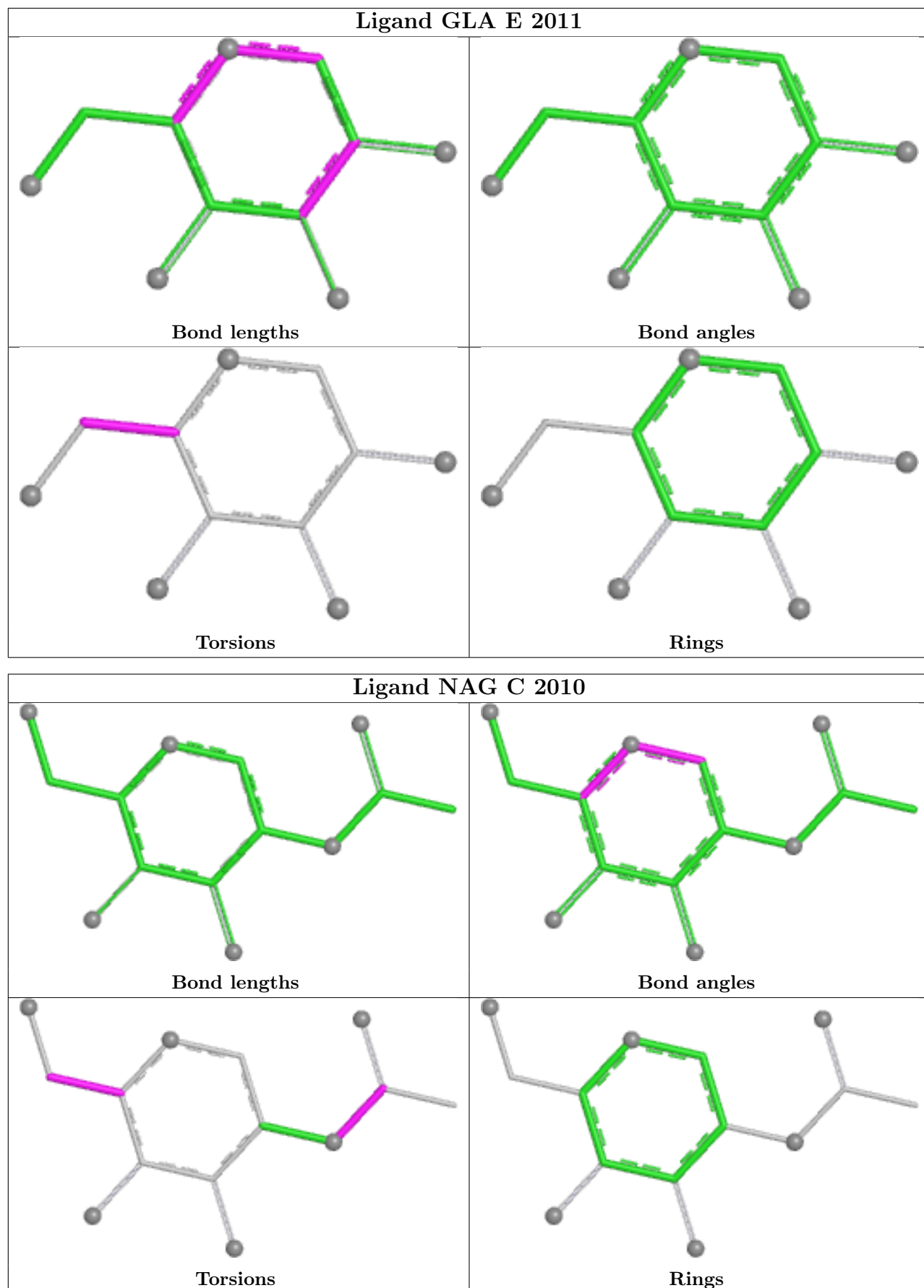


Ligand GLA F 2017

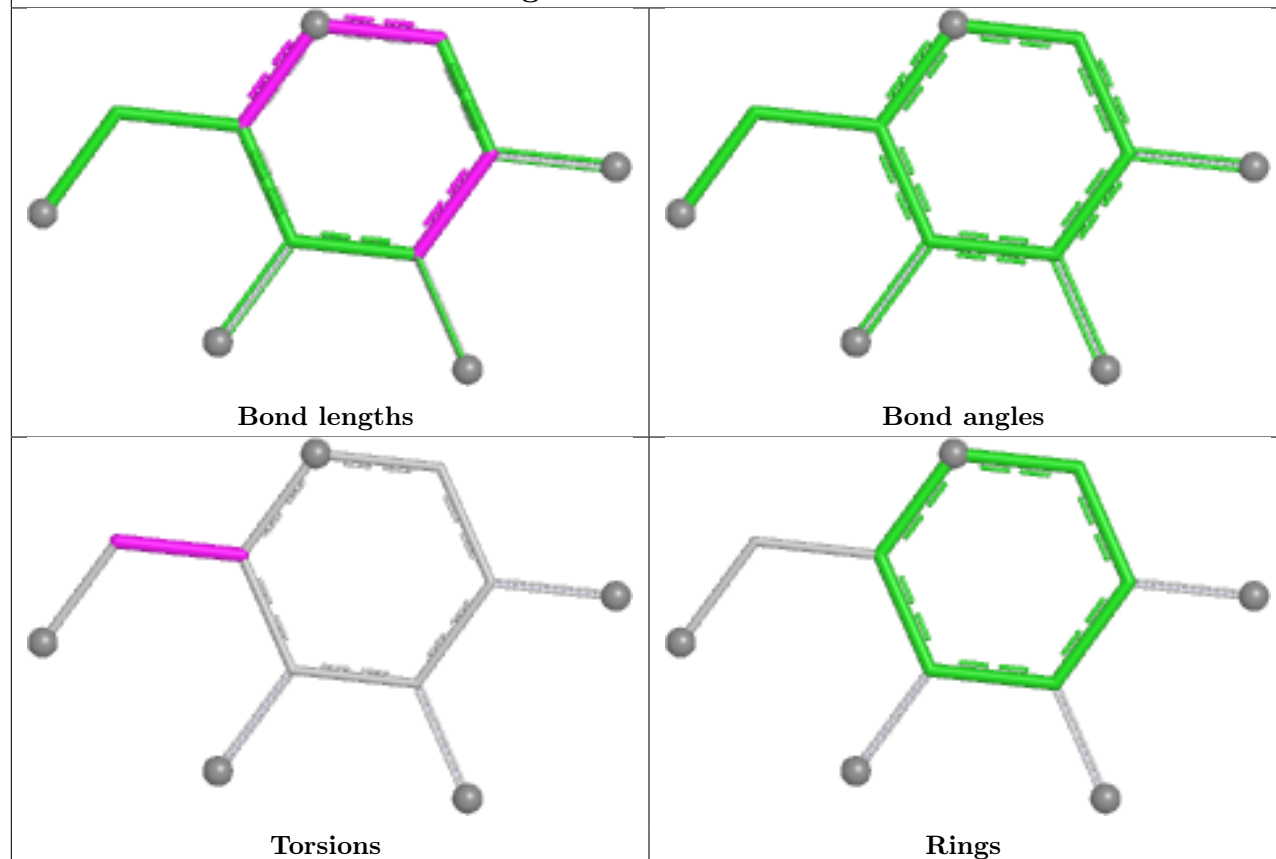




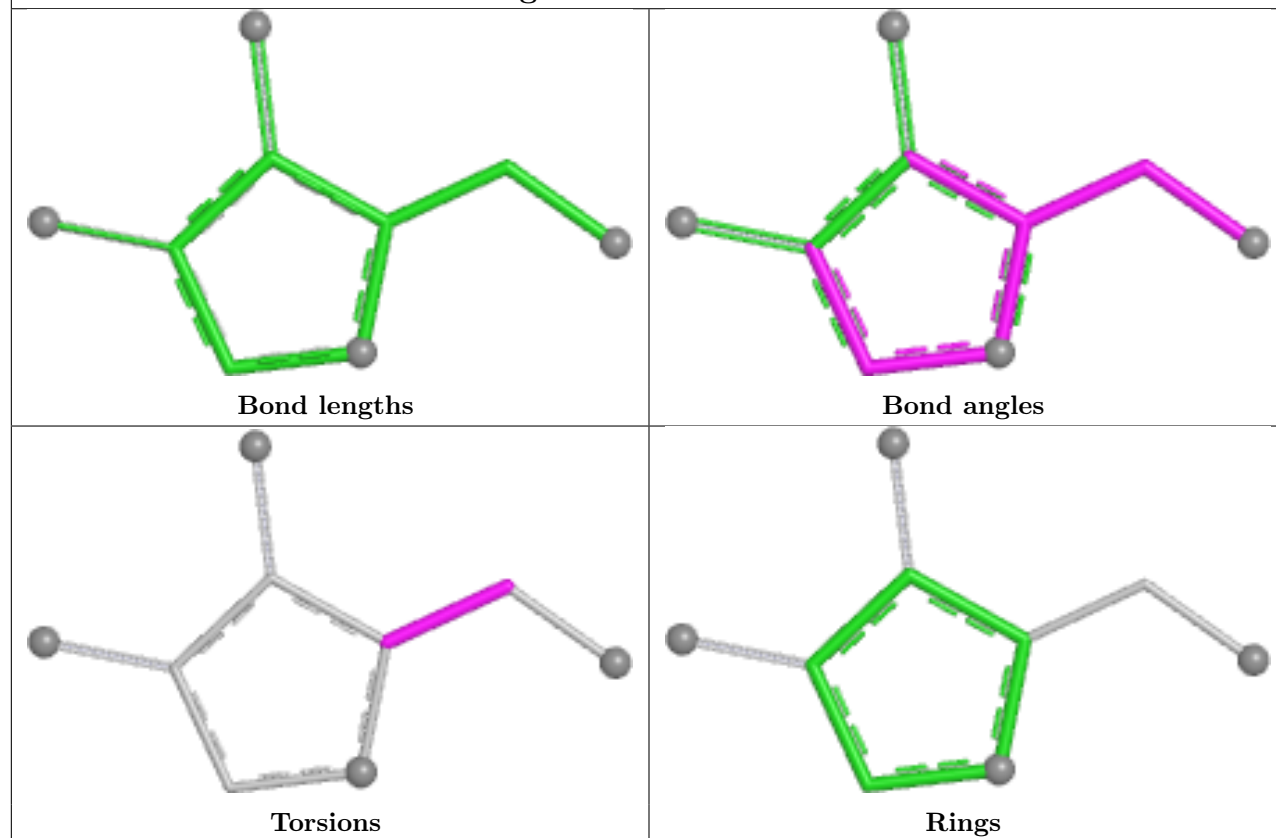




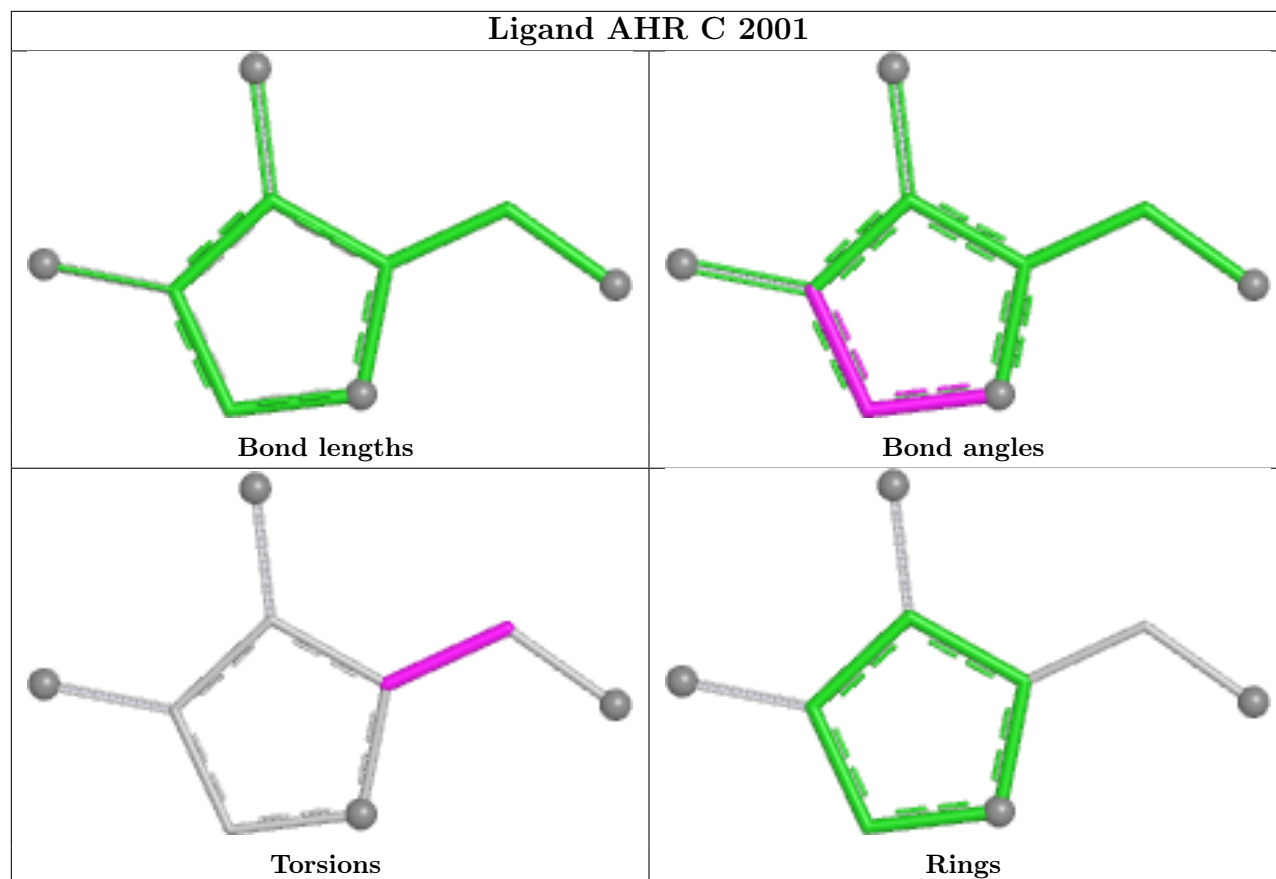
Ligand GLA A 2014



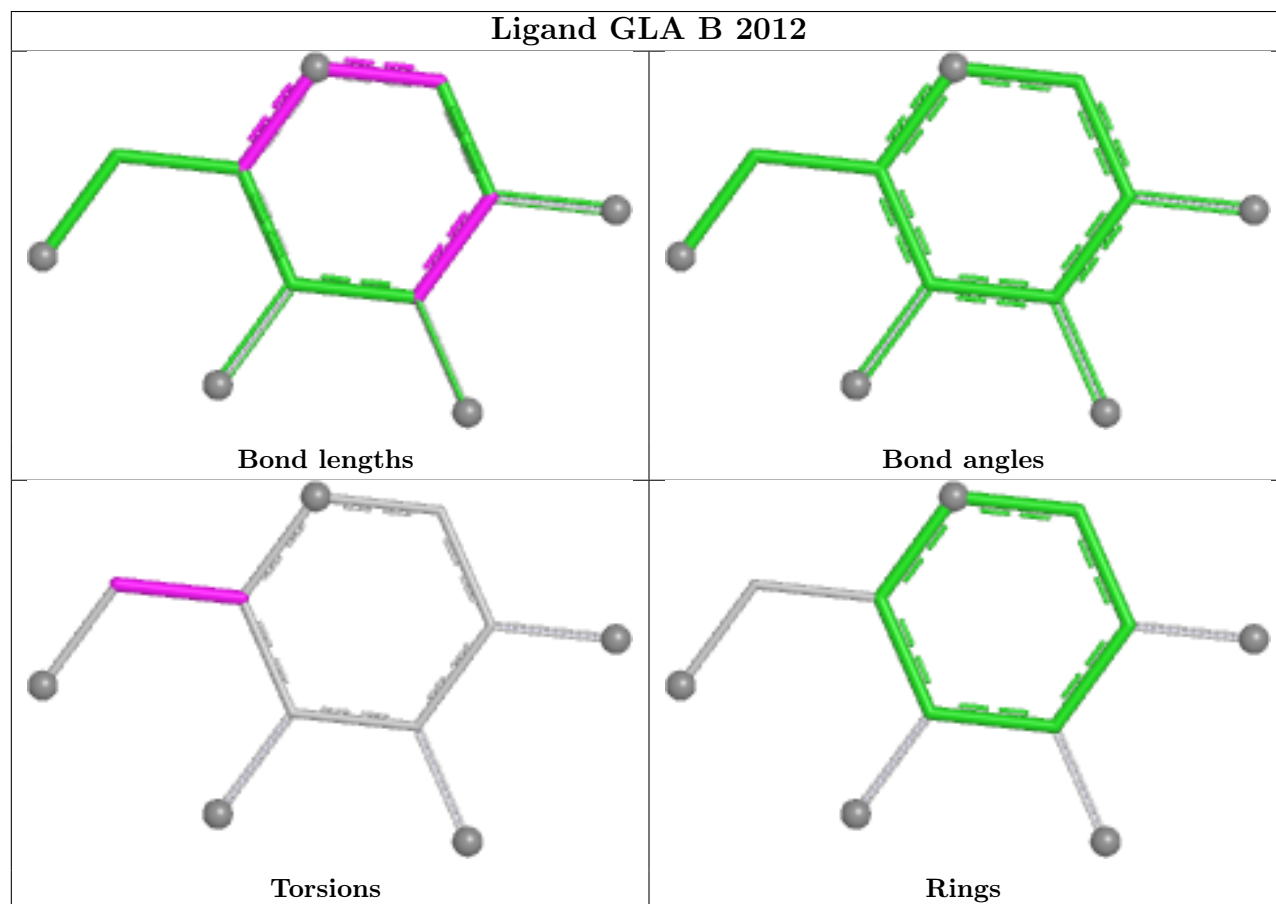
Ligand AHR B 2004



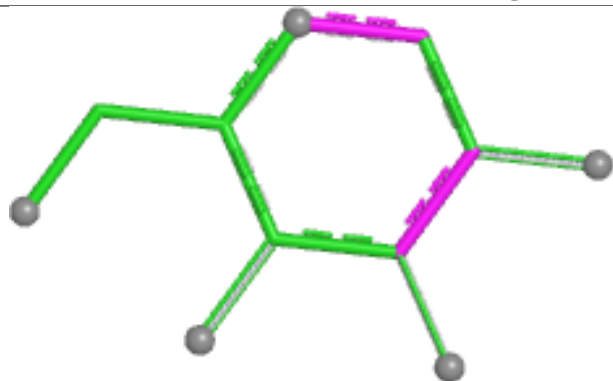
Ligand AHR C 2001



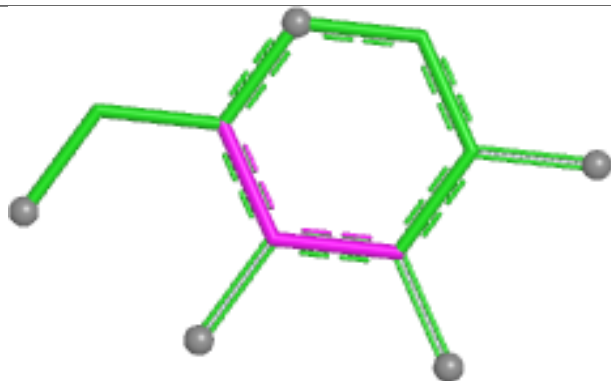
Ligand GLA B 2012



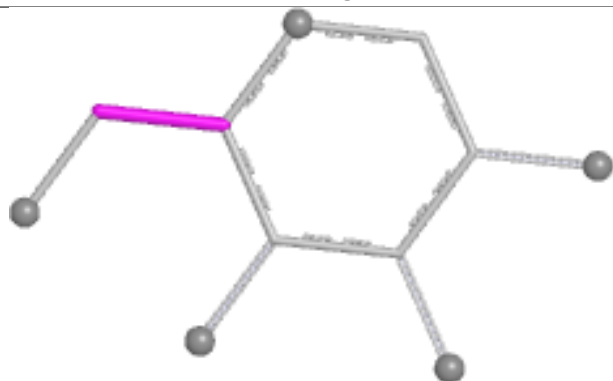
Ligand GLA F 2009



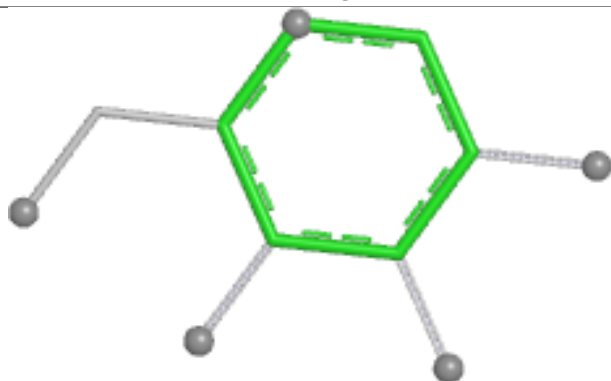
Bond lengths



Bond angles

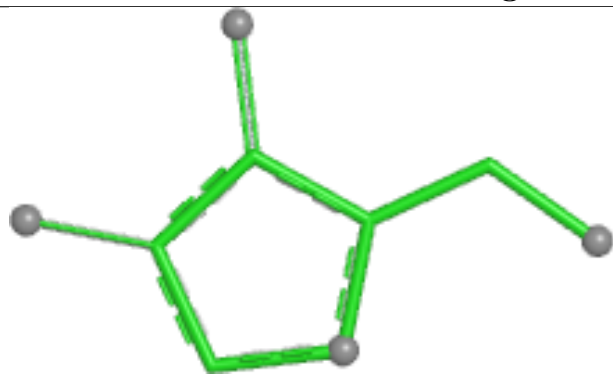


Torsions

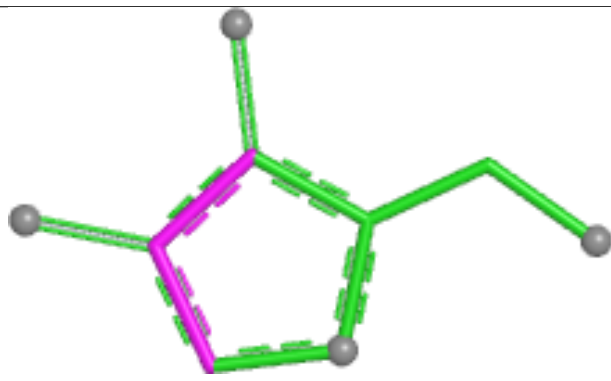


Rings

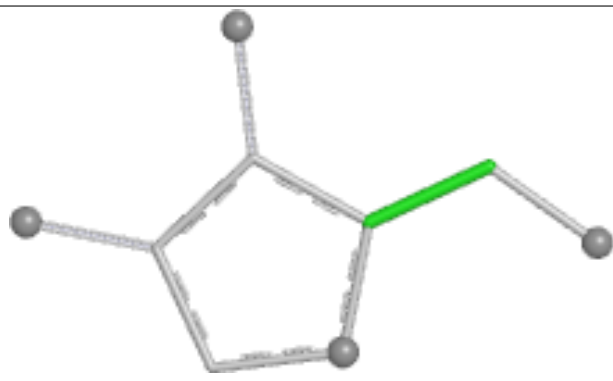
Ligand AHR A 2018



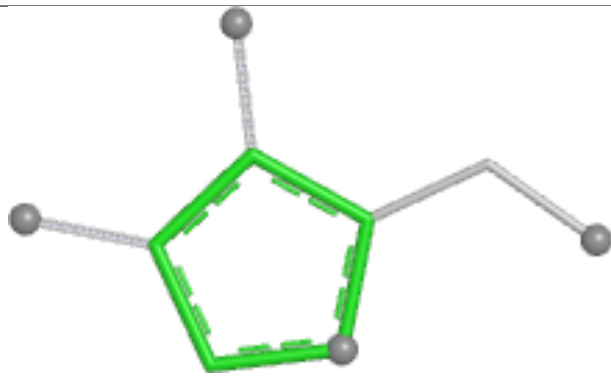
Bond lengths



Bond angles

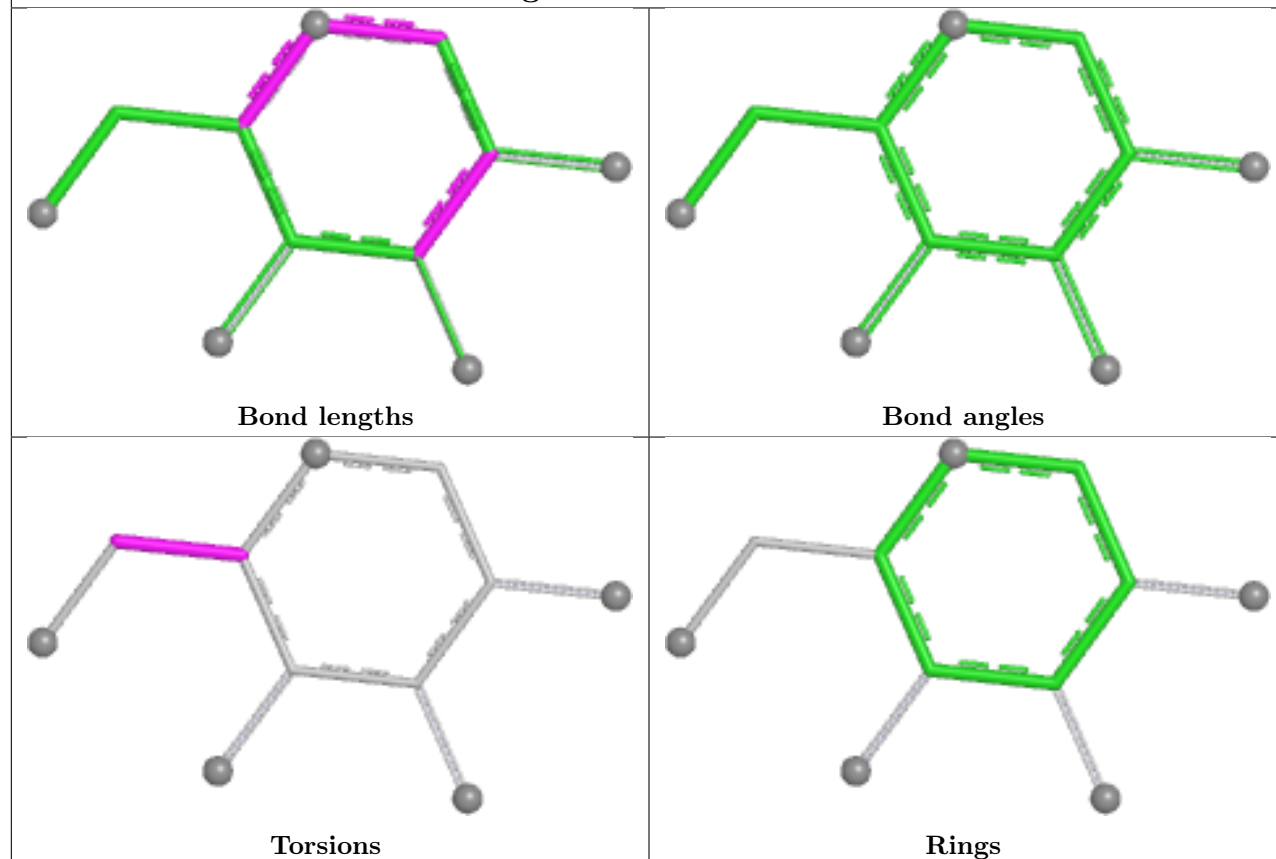


Torsions

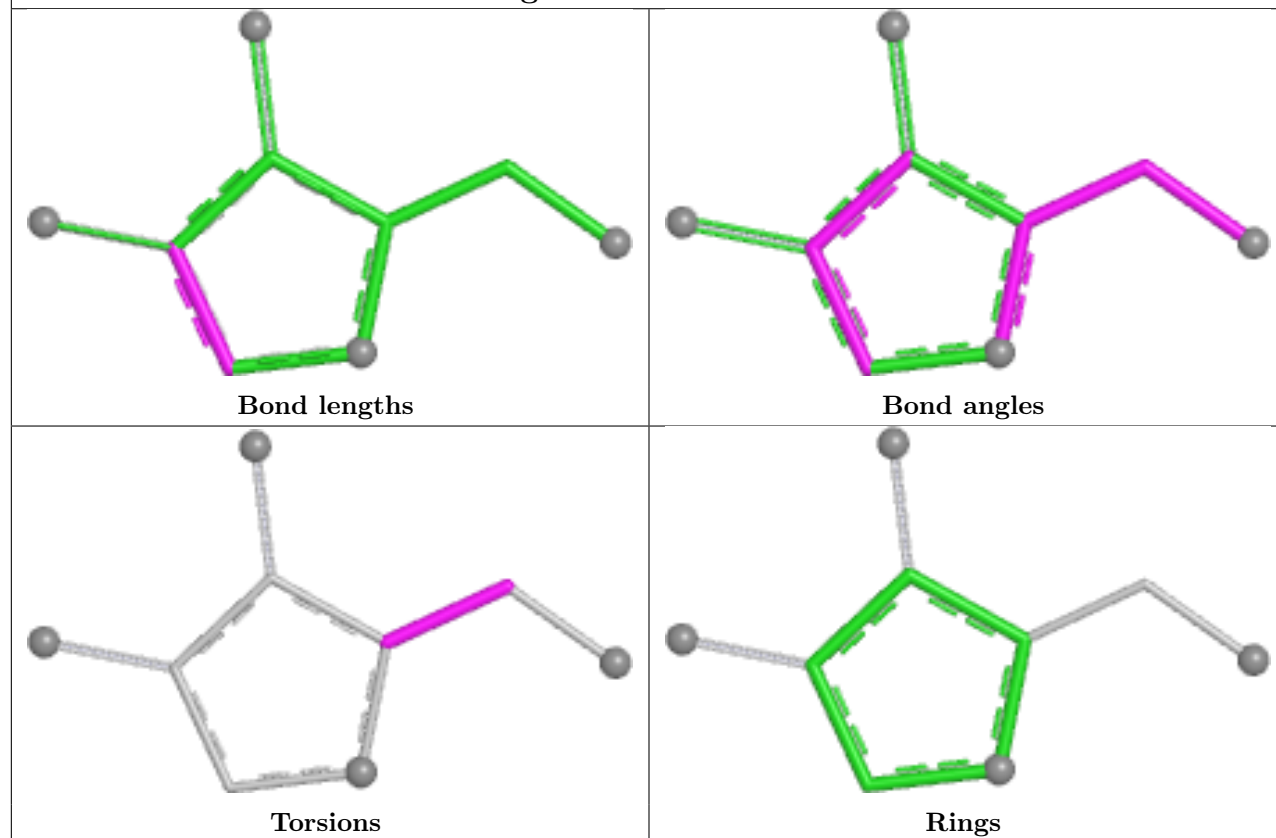


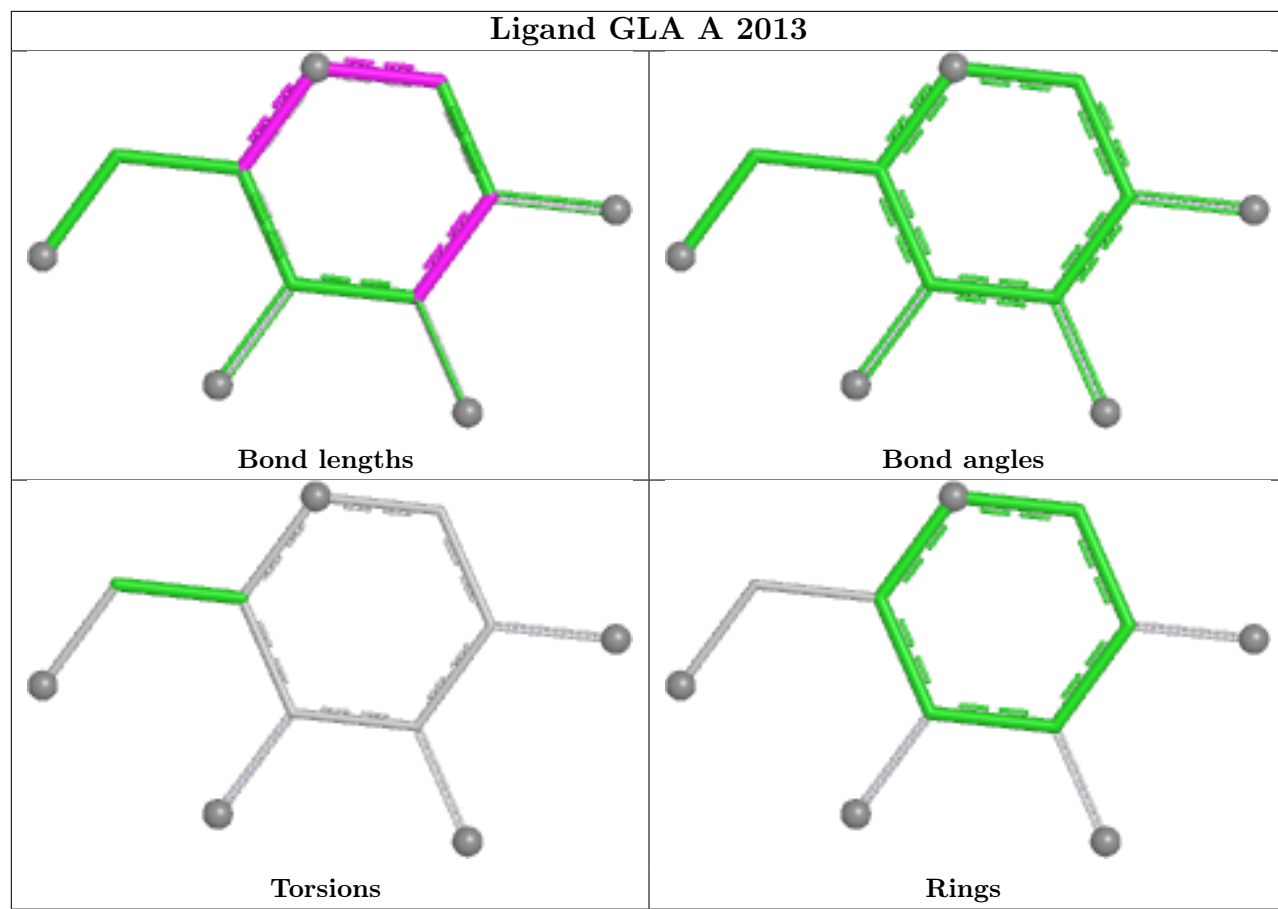
Rings

Ligand GLA C 2008

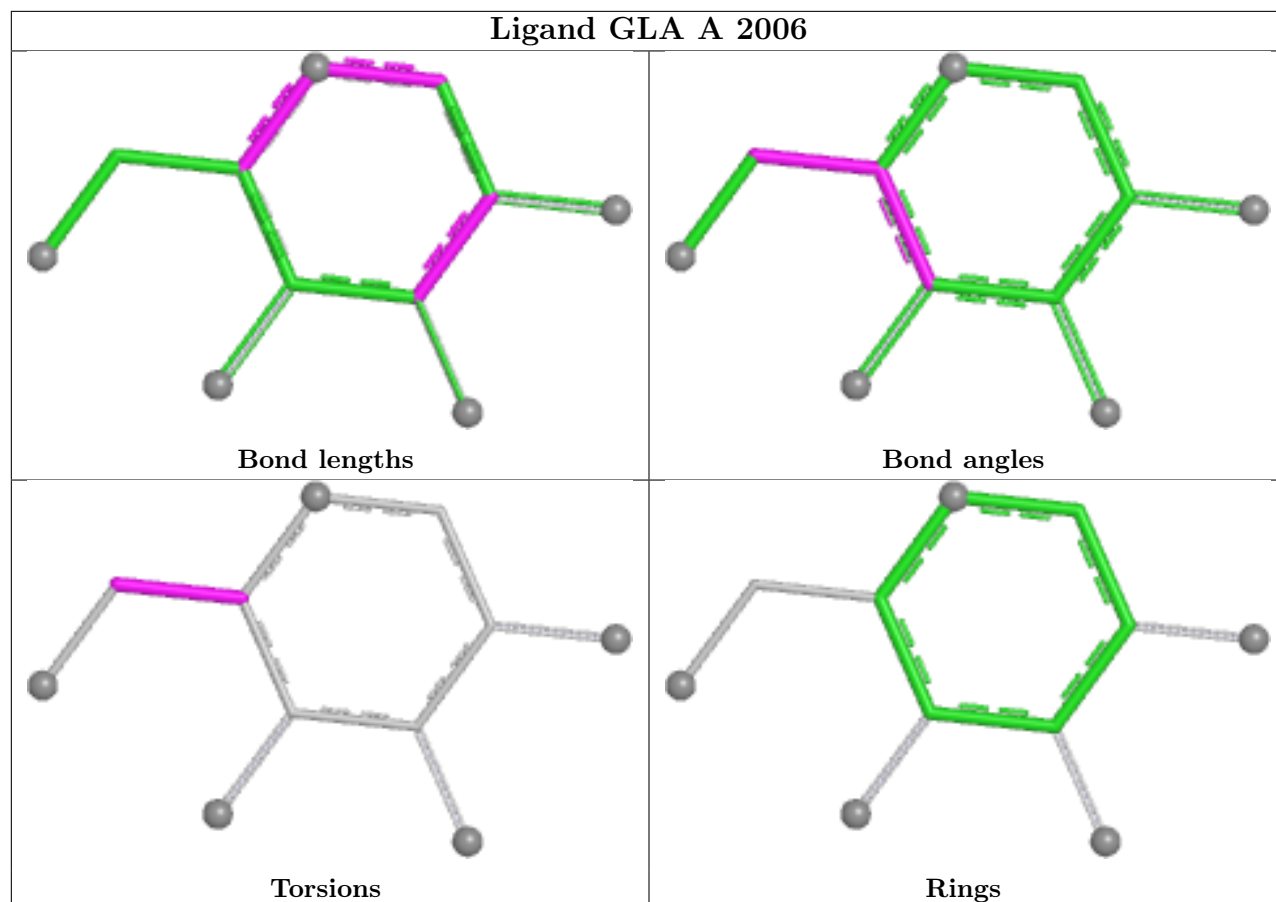


Ligand AHR E 2002

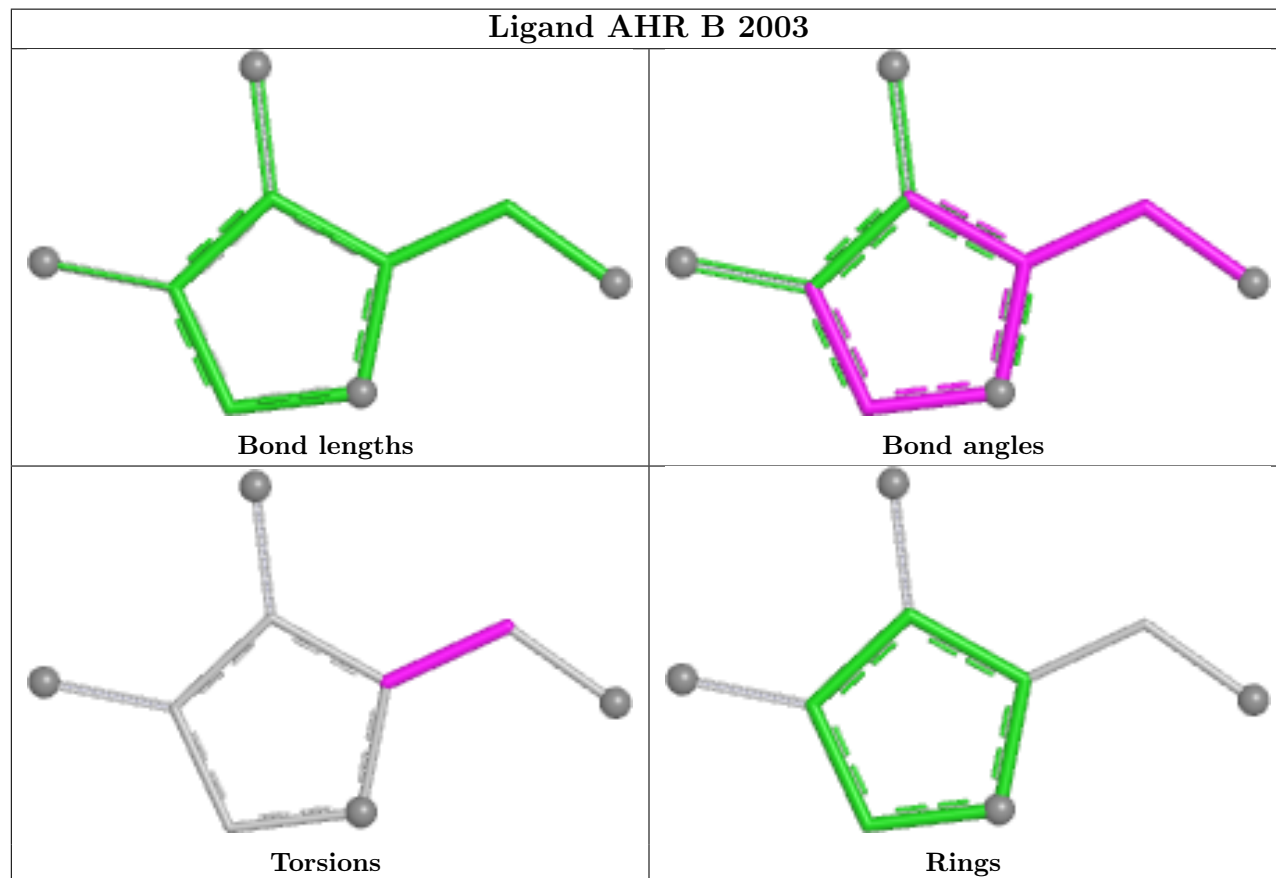




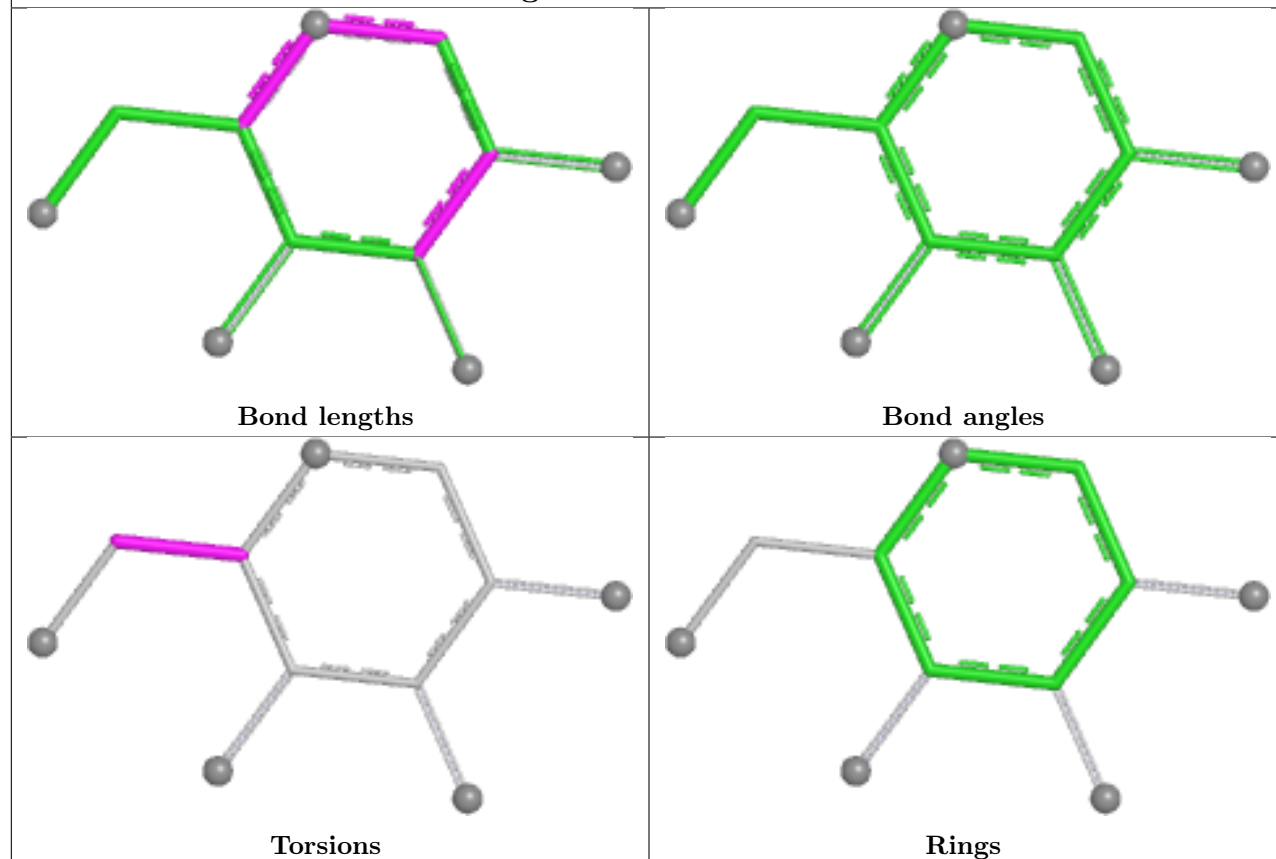
Ligand GLA A 2006



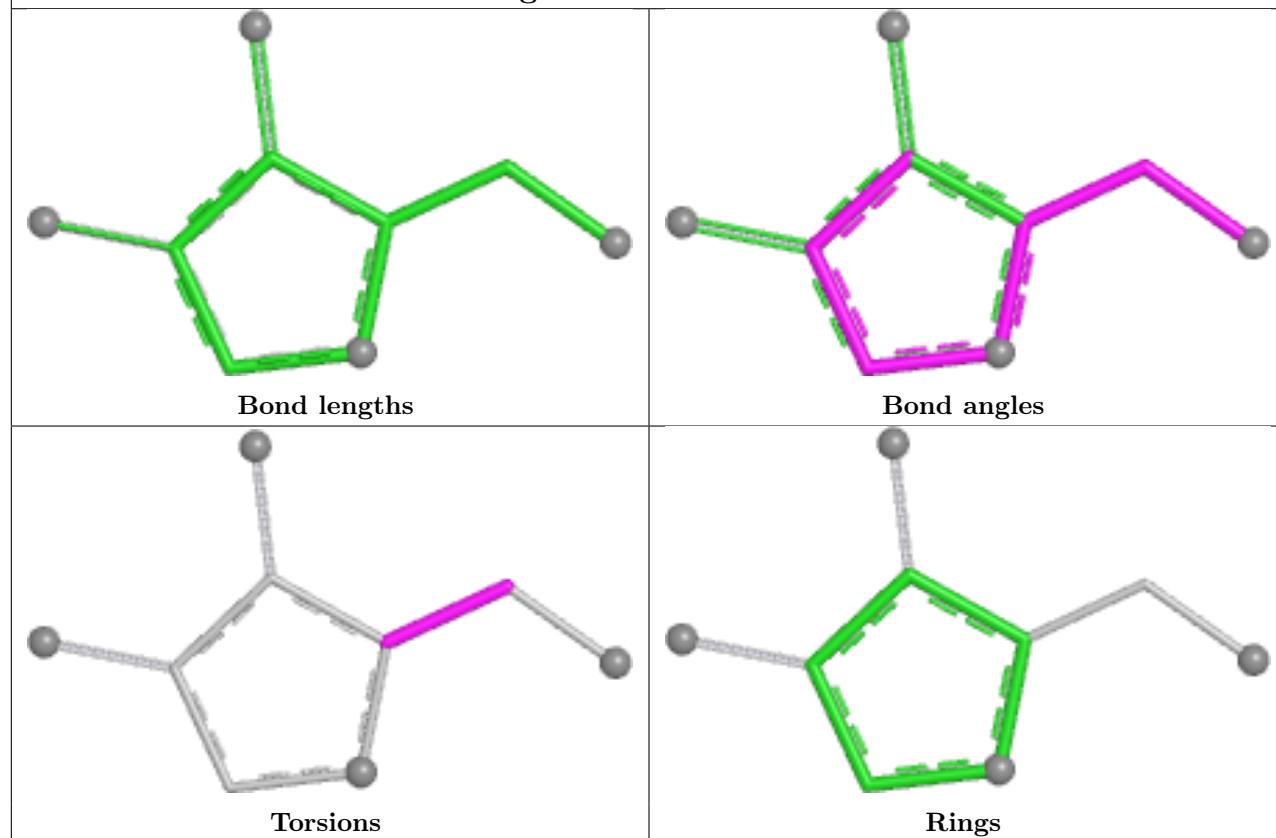
Ligand AHR B 2003



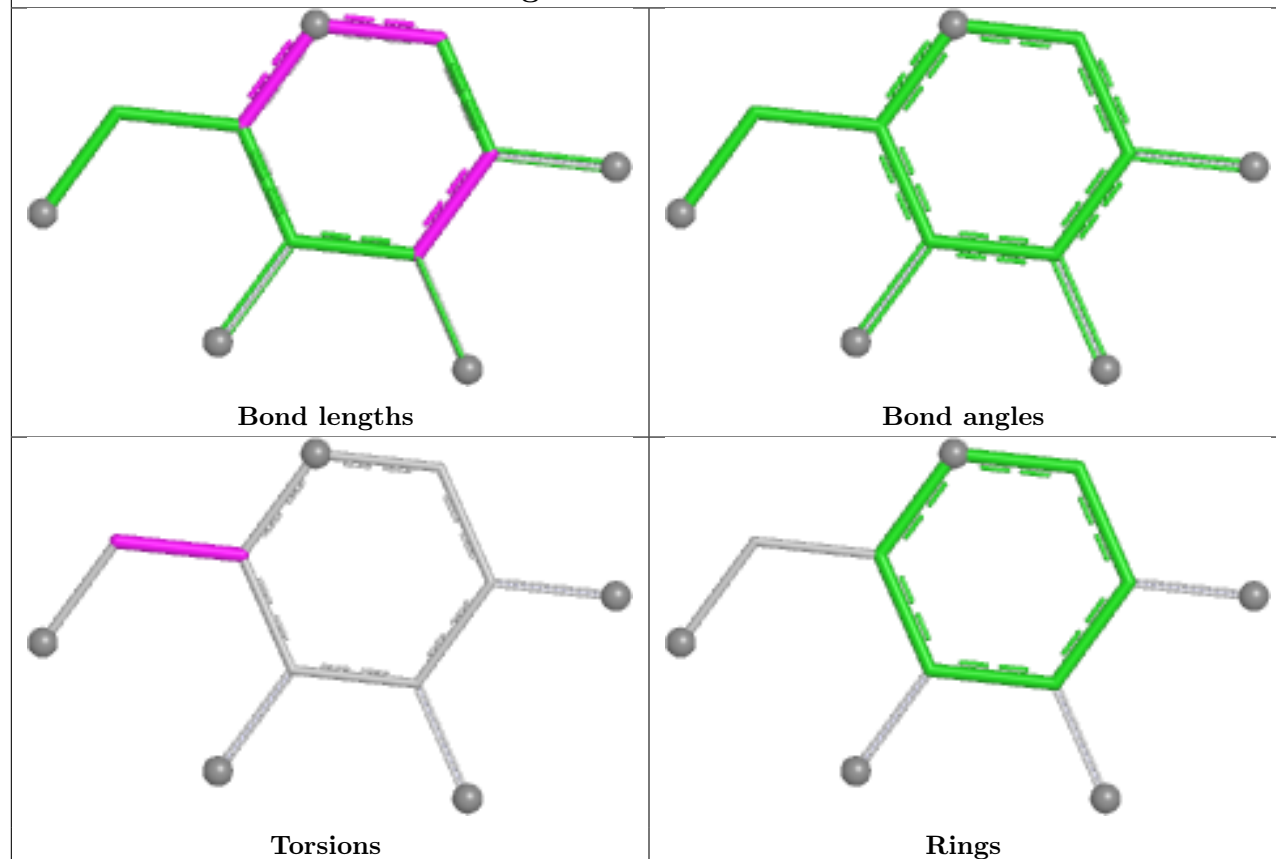
Ligand GLA D 2005



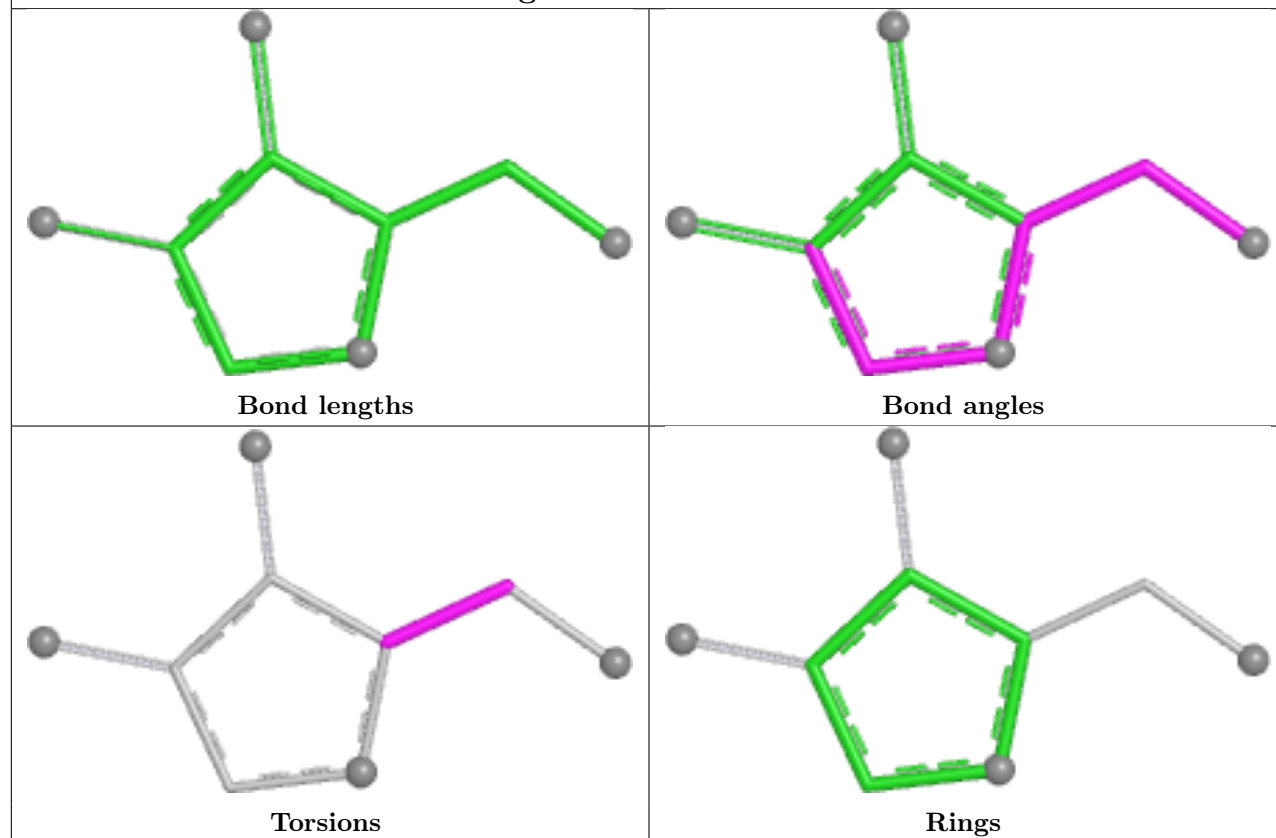
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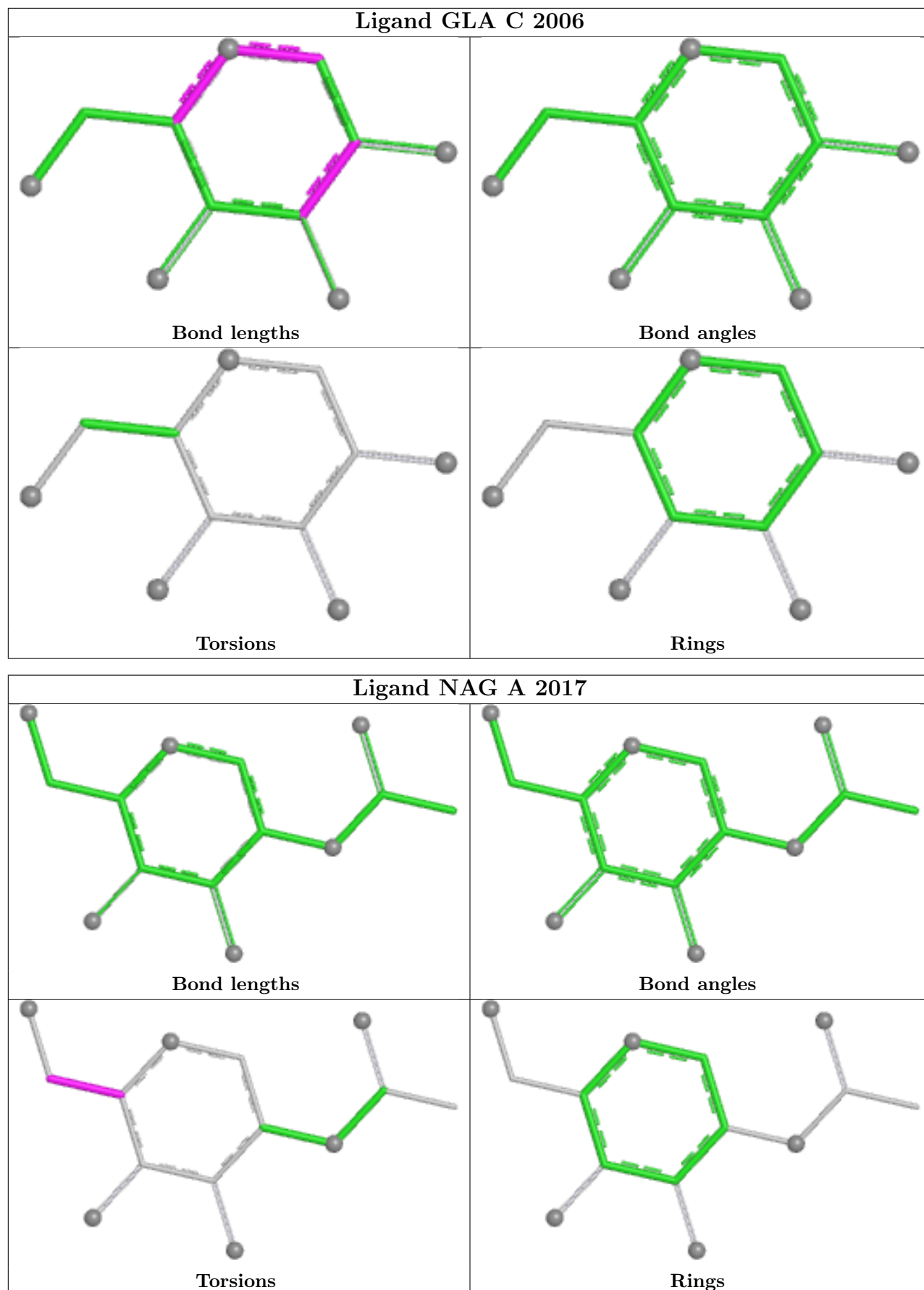


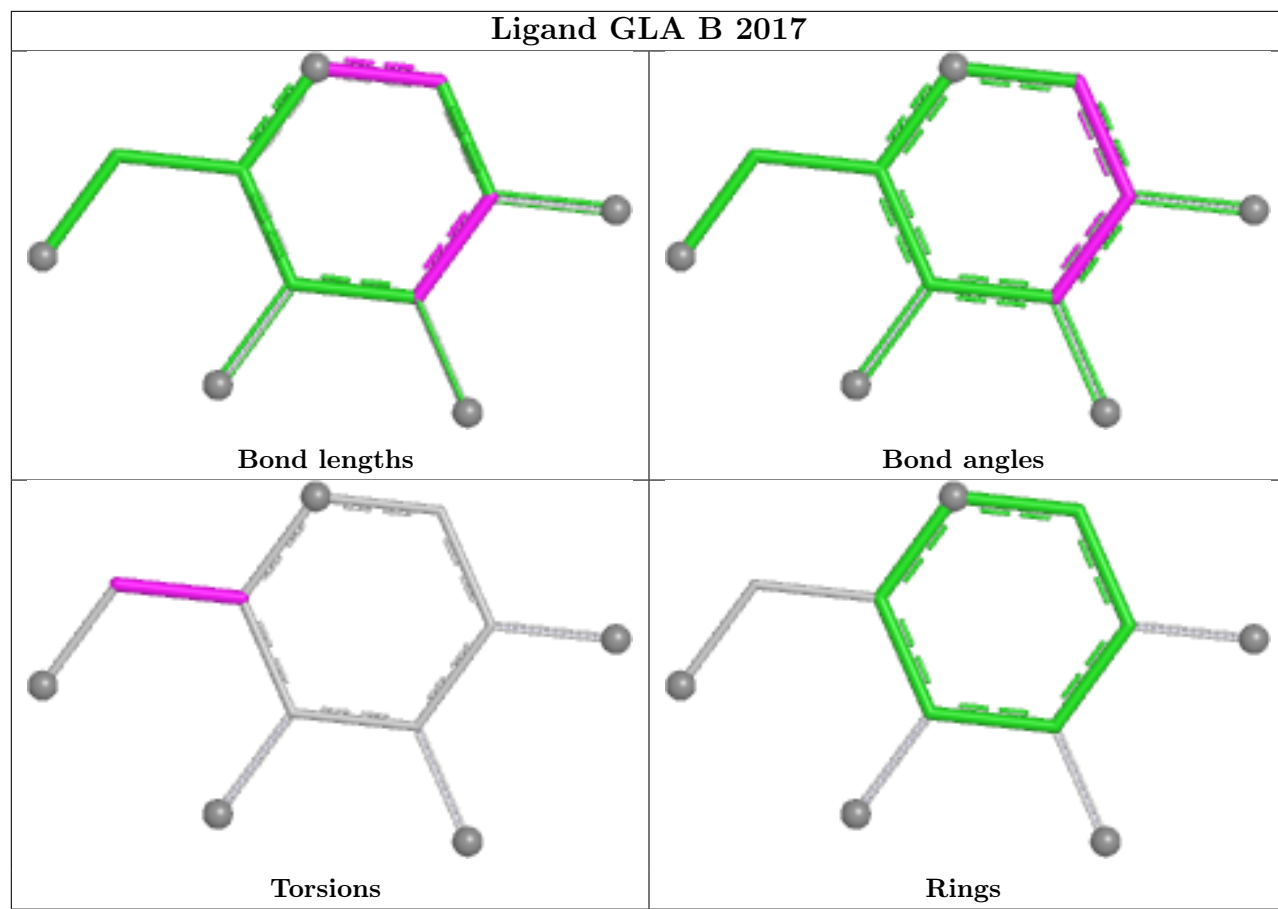
Ligand GLA A 2015

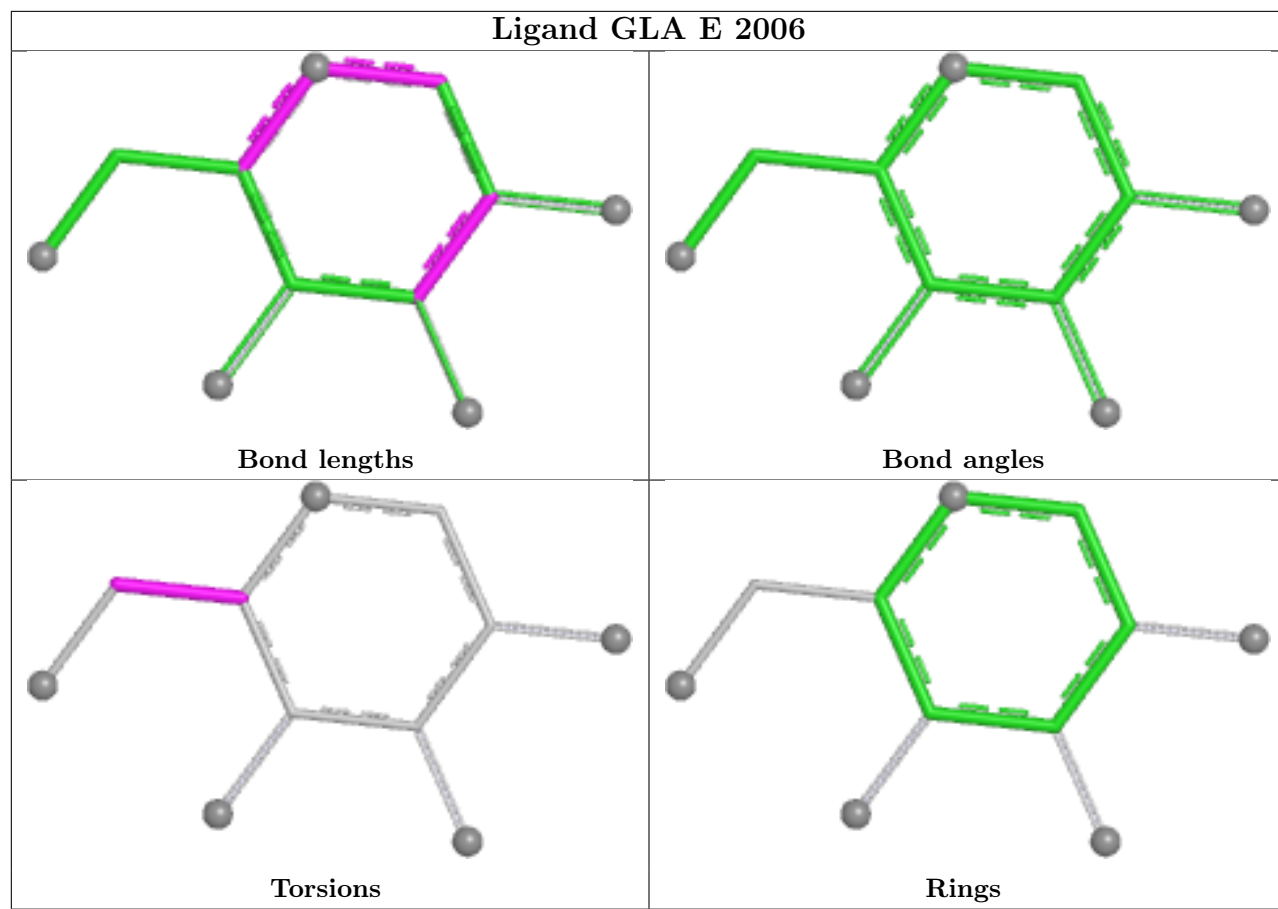


Ligand AHR D 2003

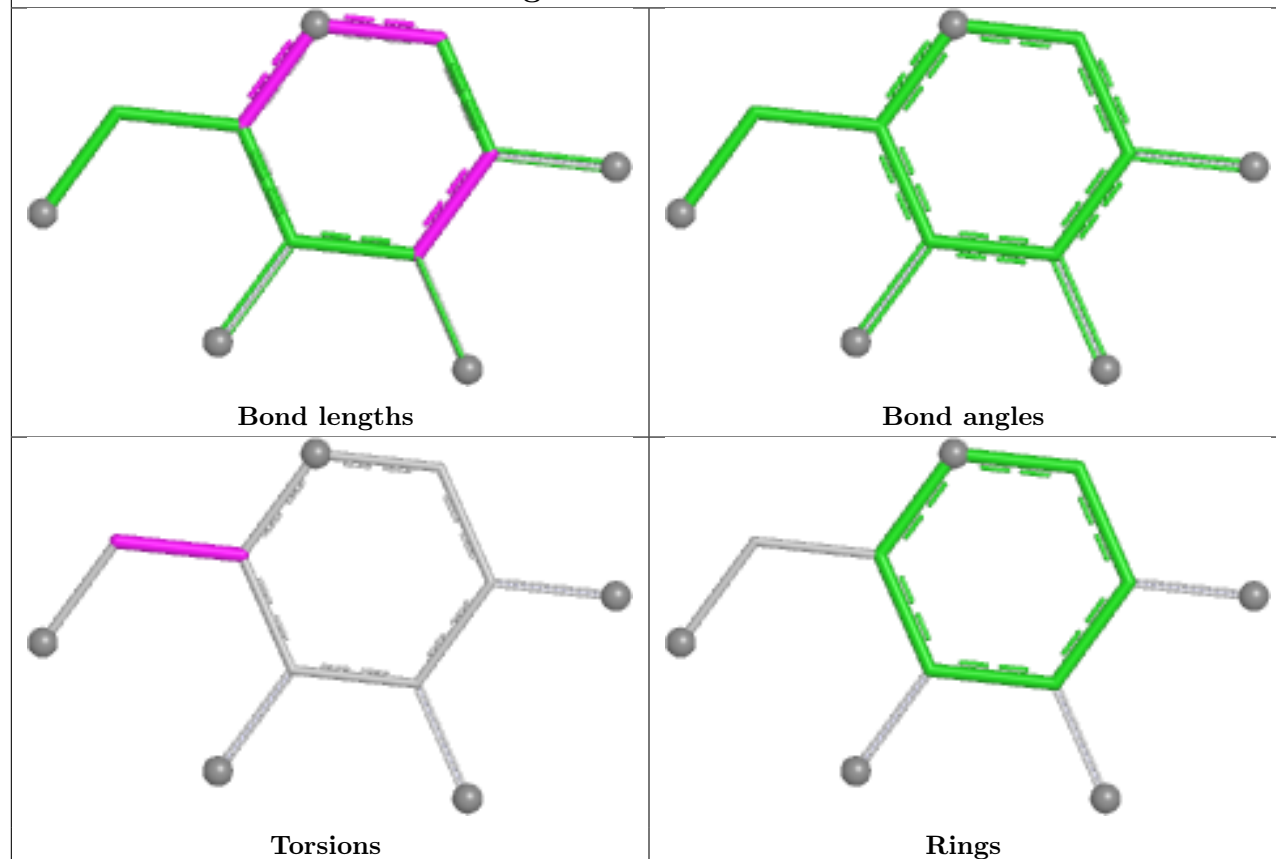




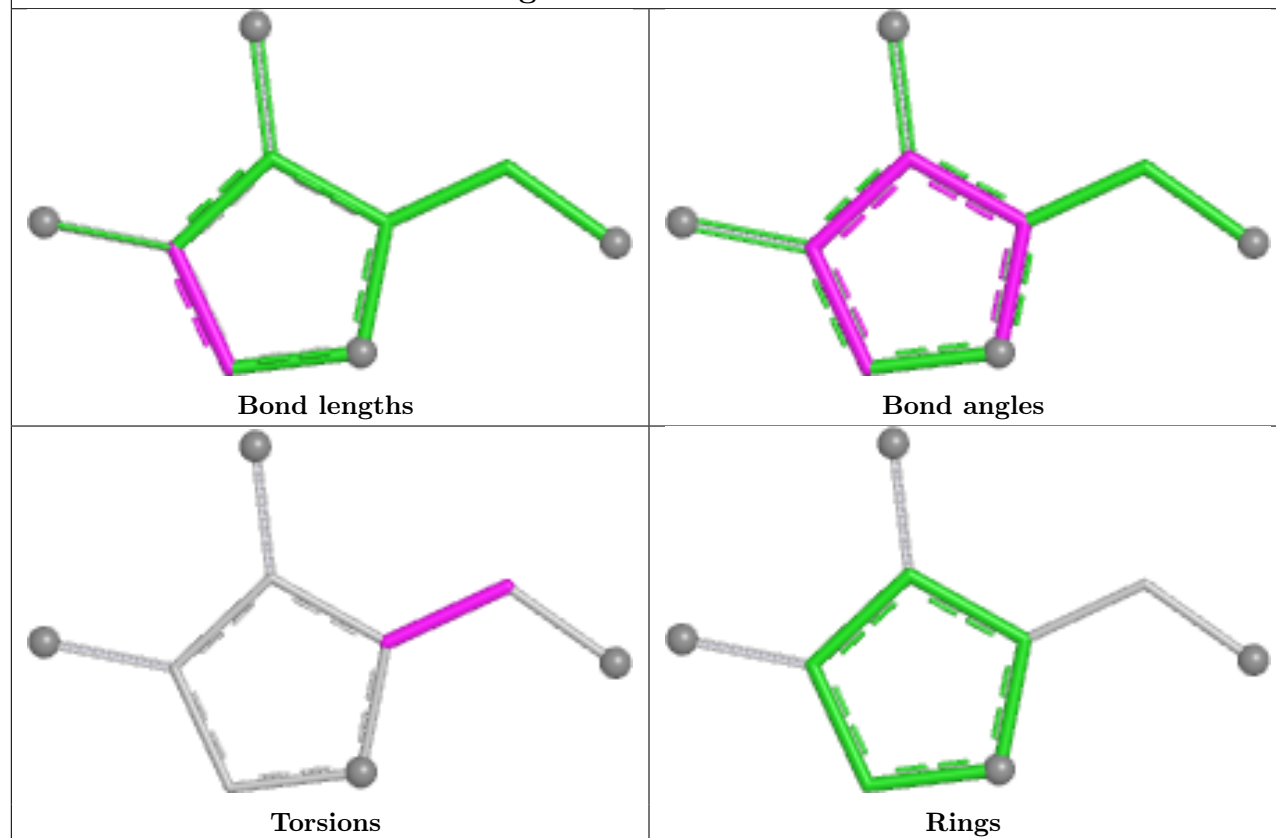


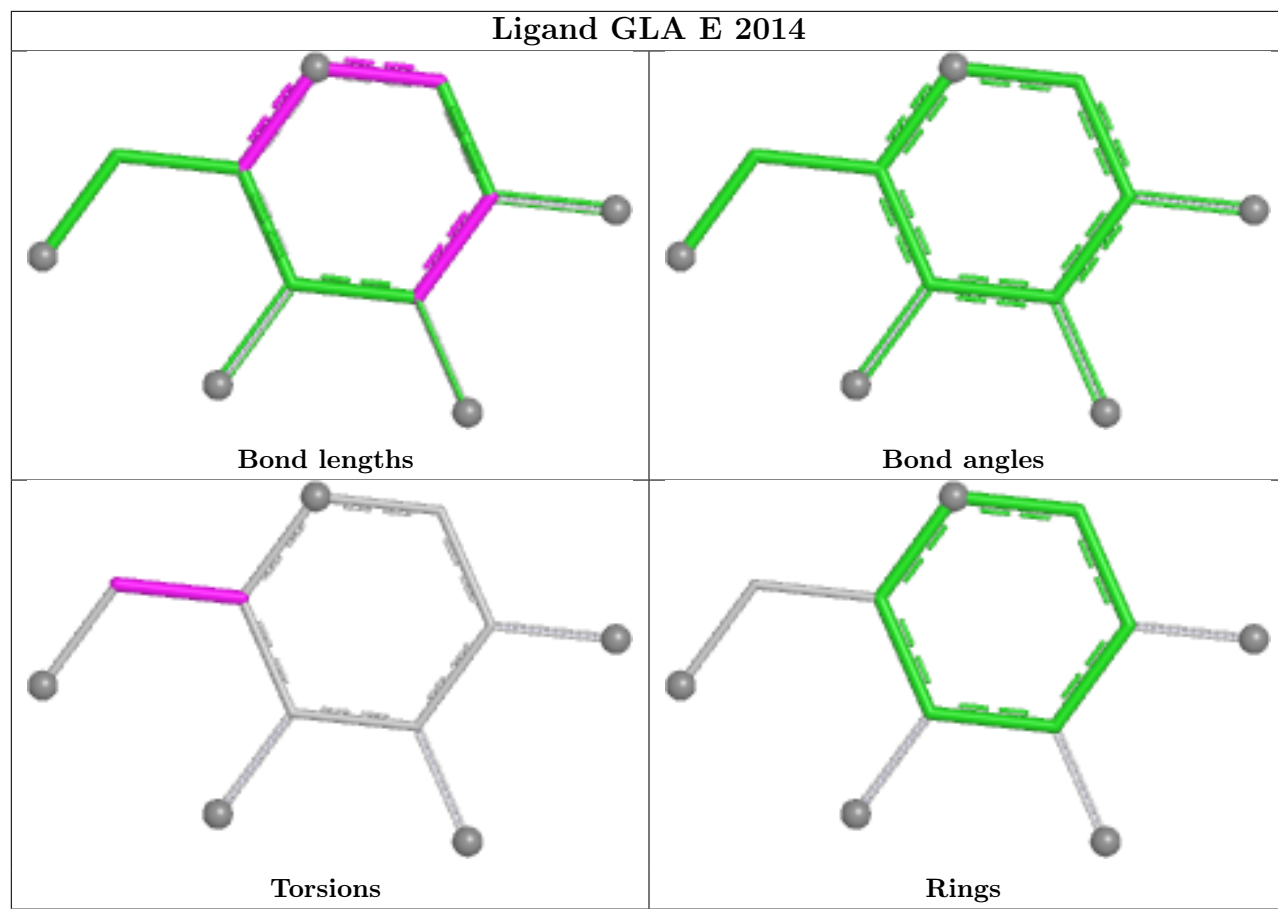


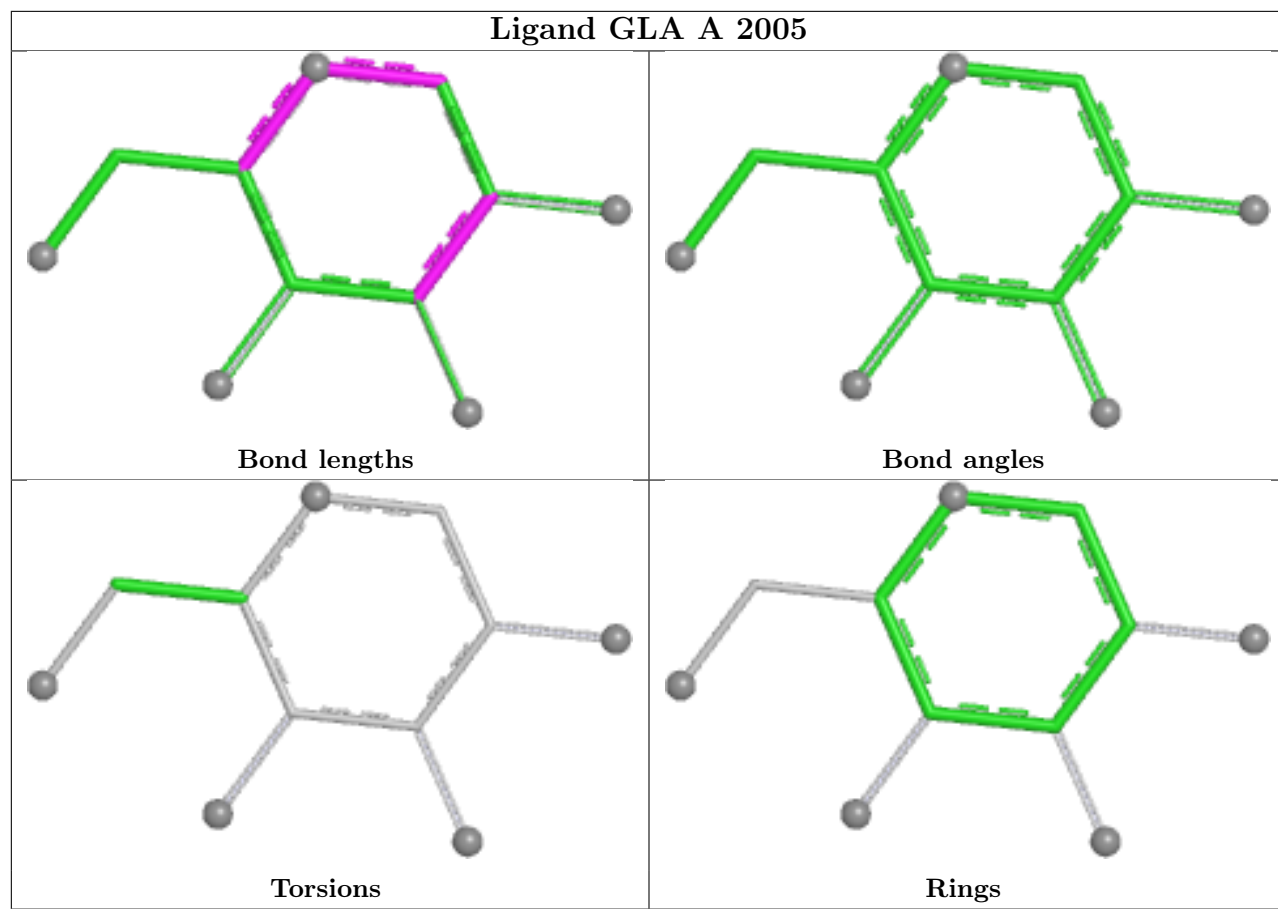
Ligand GLA E 2016

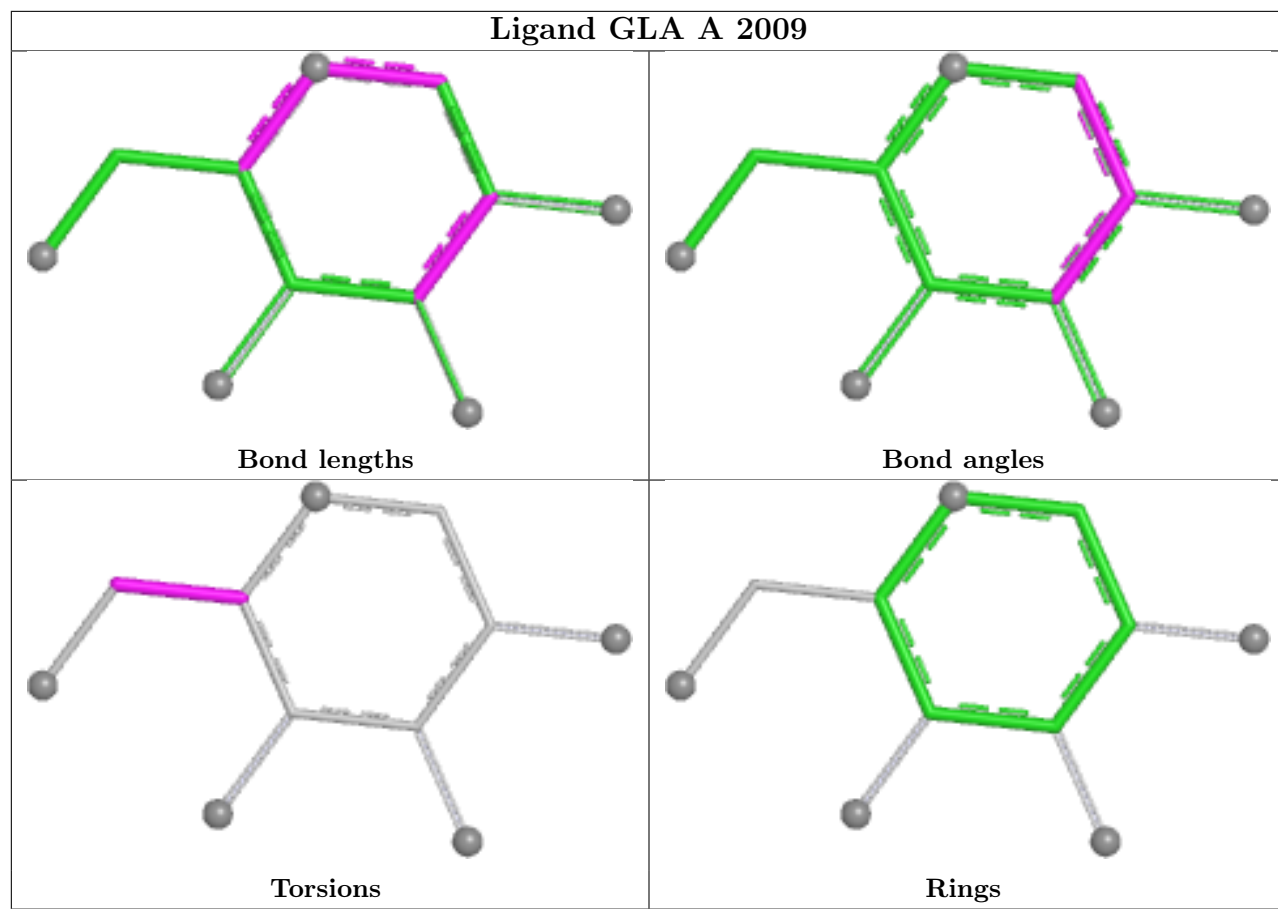


Ligand AHR A 2002

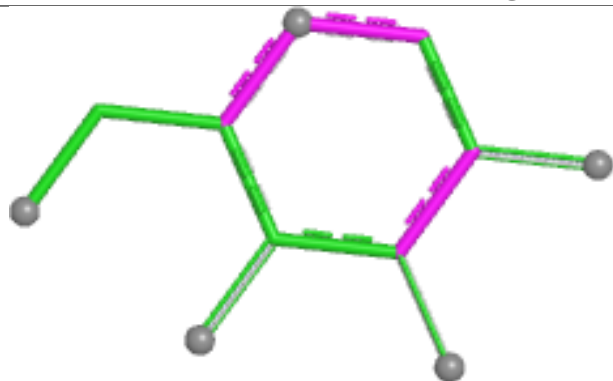




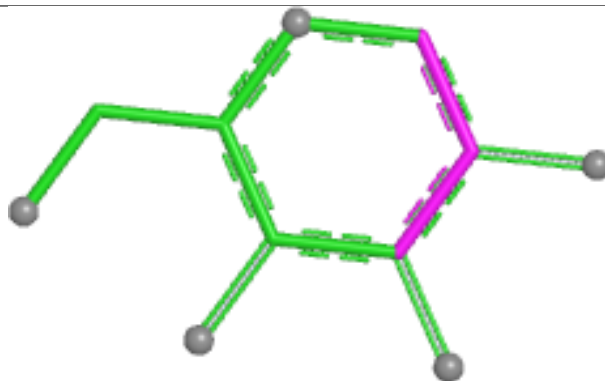




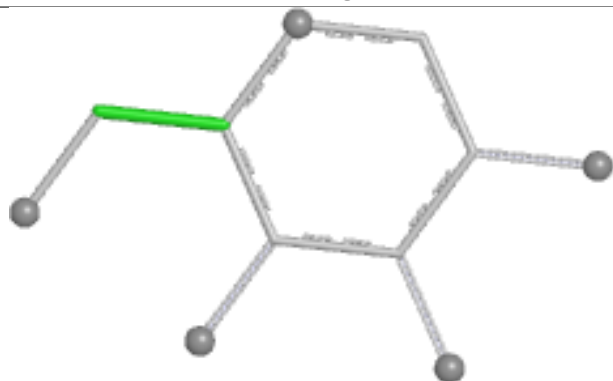
Ligand GLA D 2006



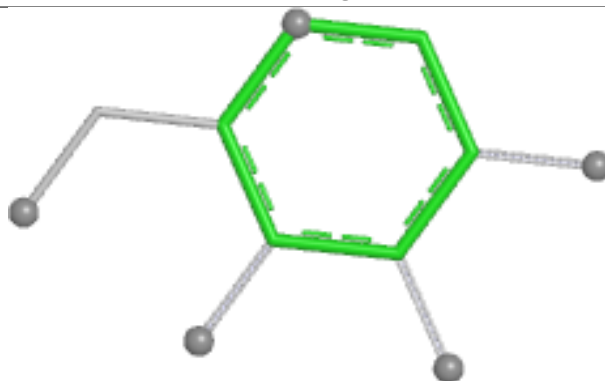
Bond lengths



Bond angles

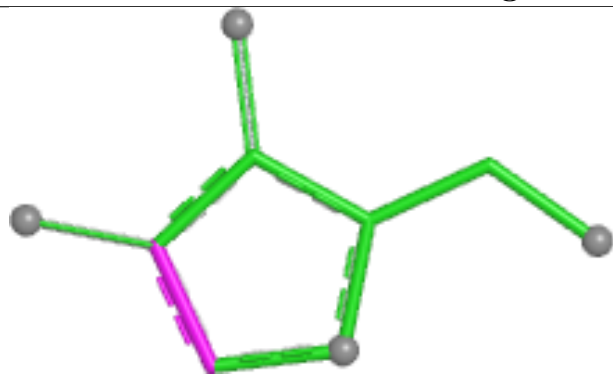


Torsions

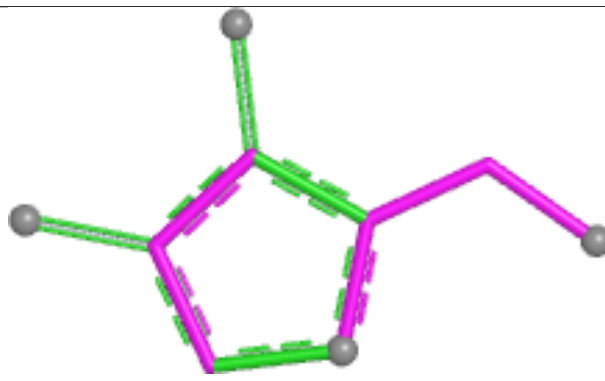


Rings

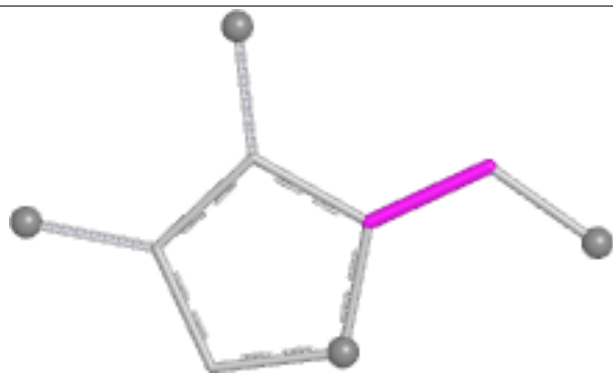
Ligand AHR A 2003



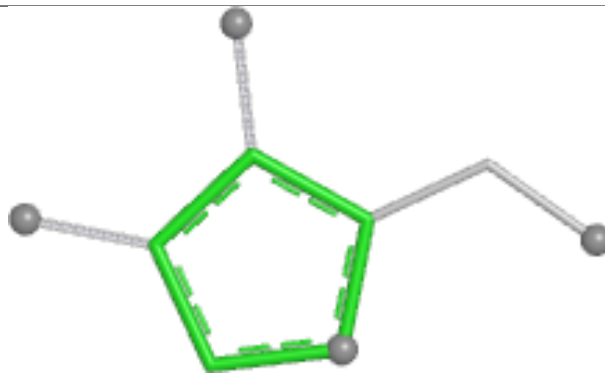
Bond lengths



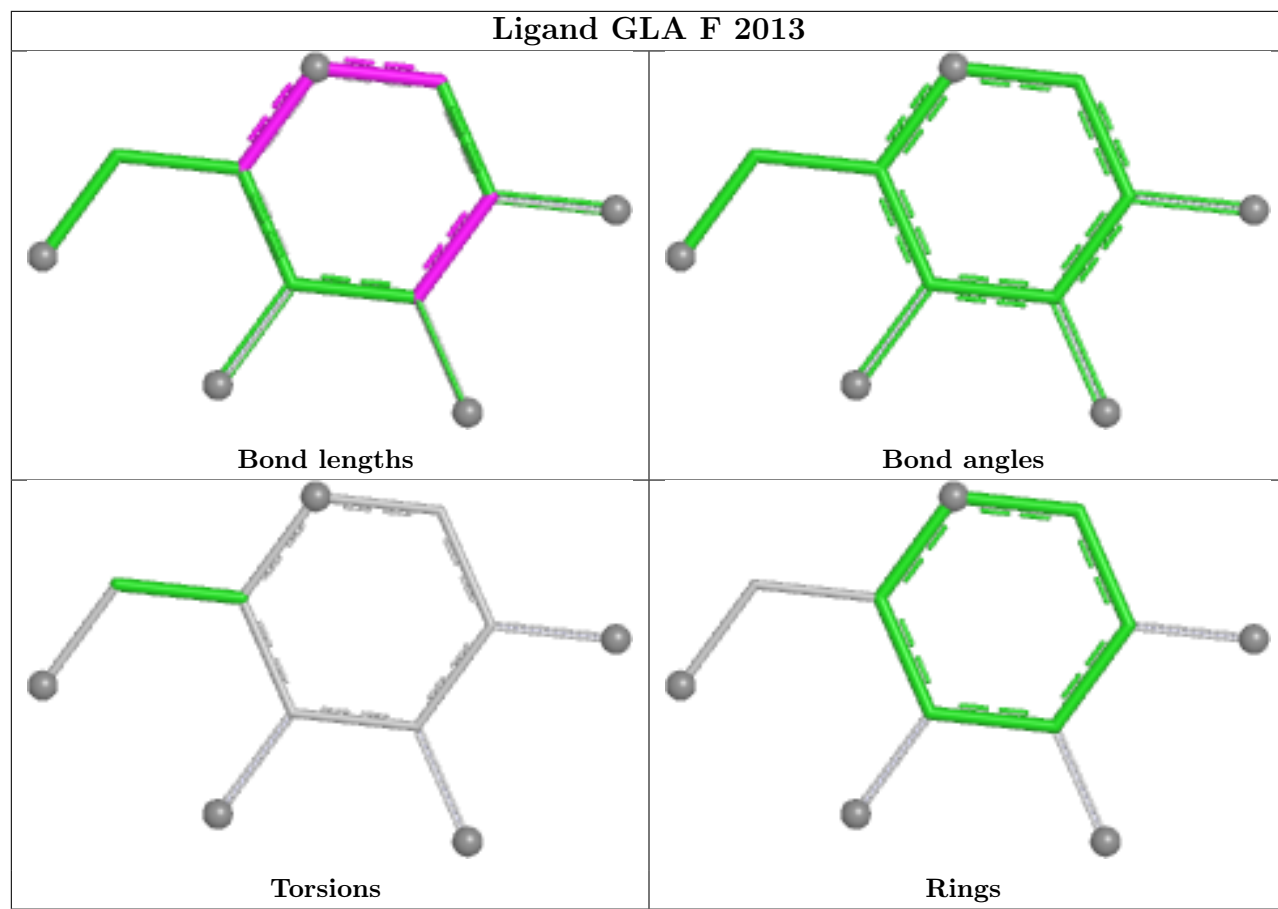
Bond angles



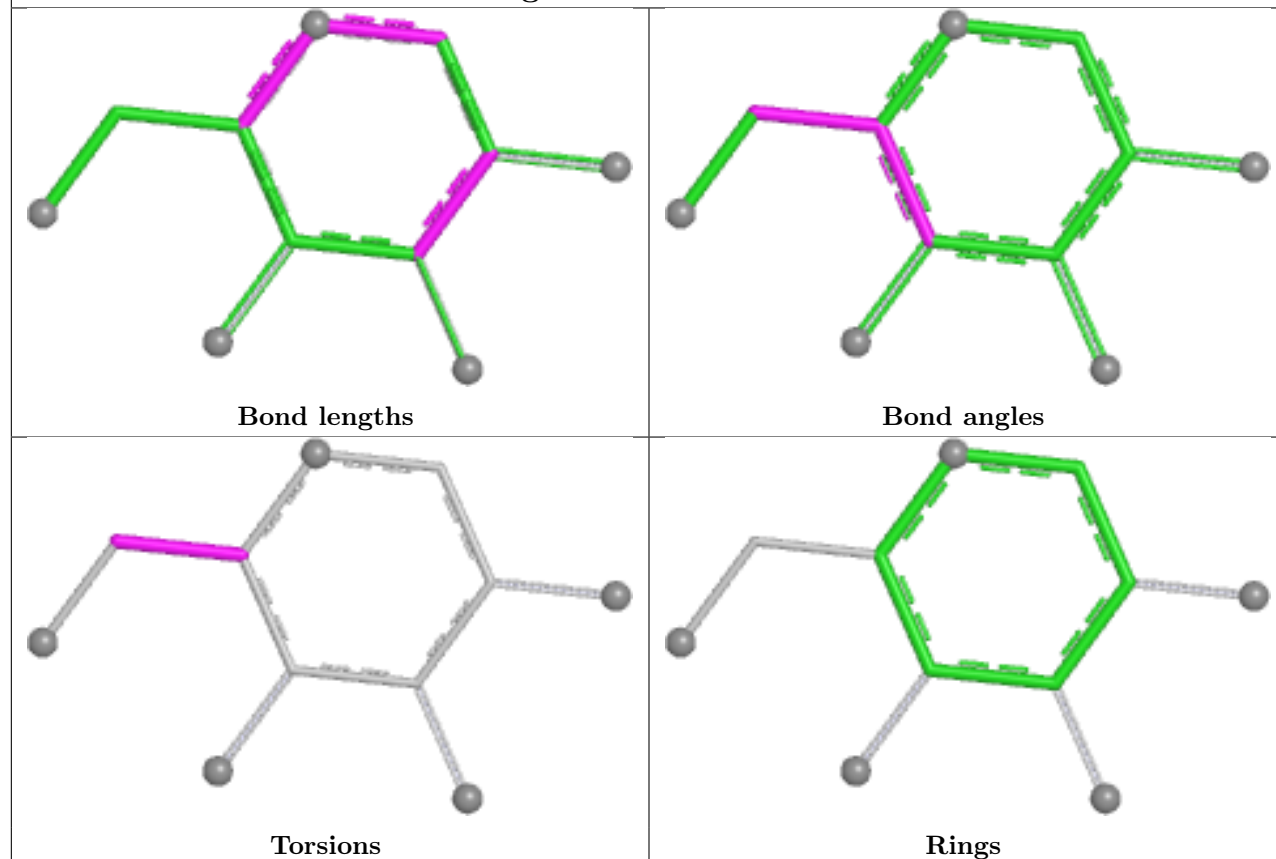
Torsions



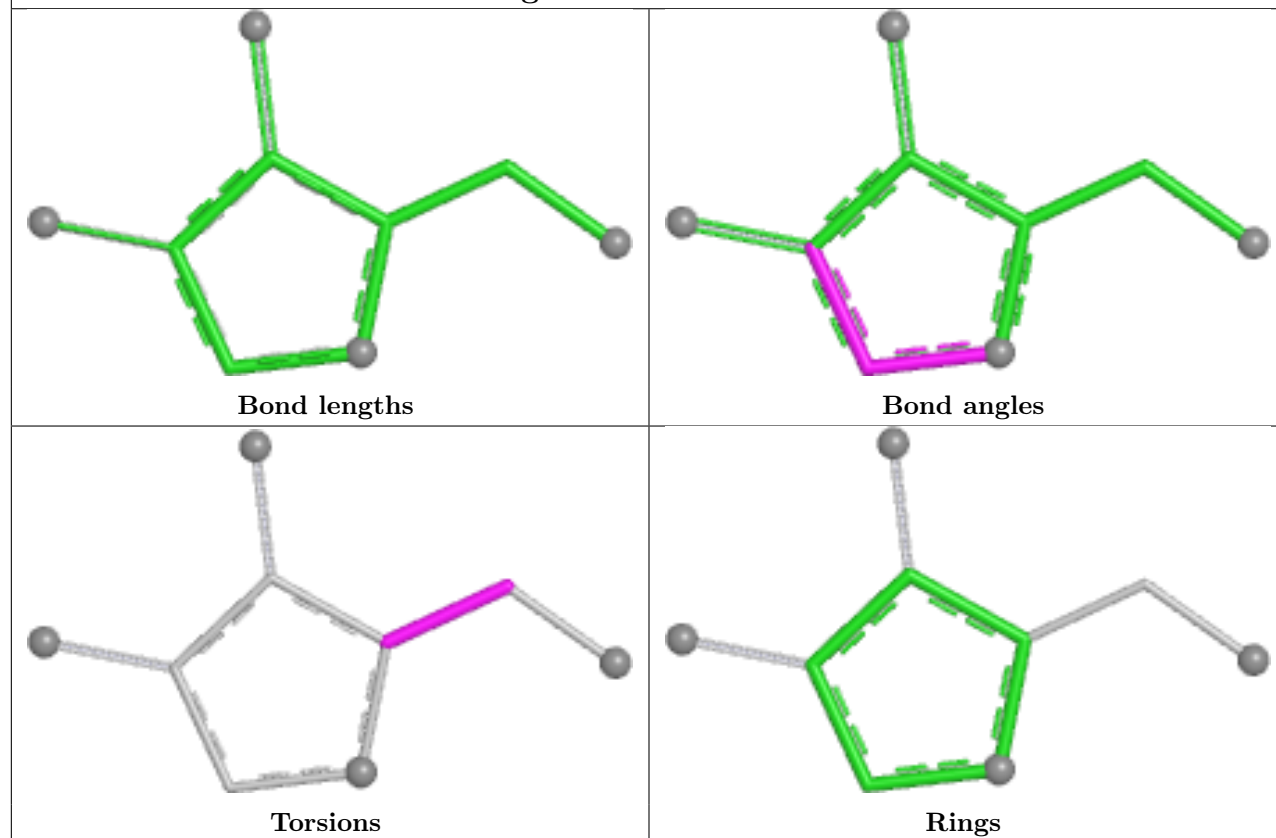
Rings



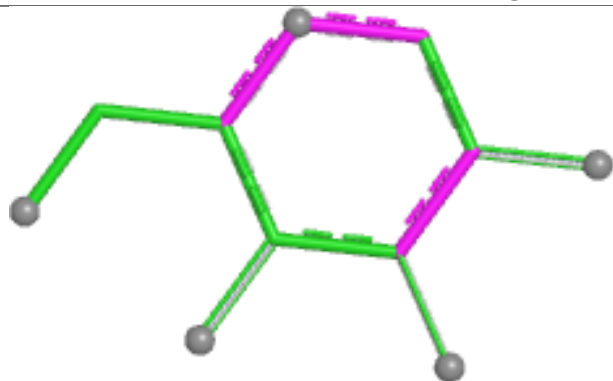
Ligand GLA A 2010



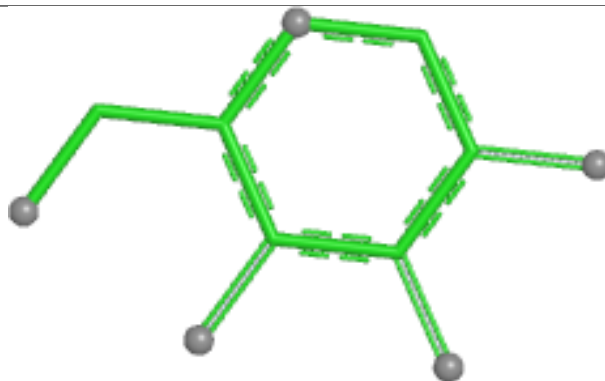
Ligand AHR F 2003



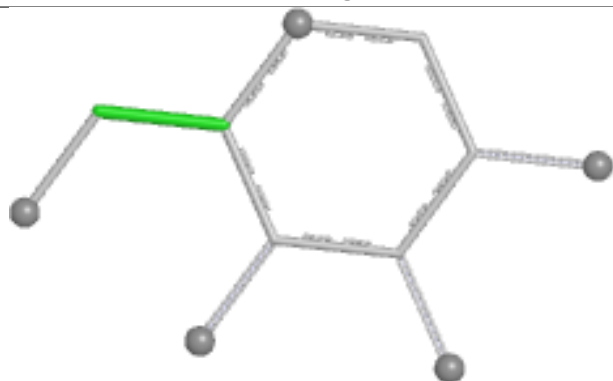
Ligand GLA F 2015



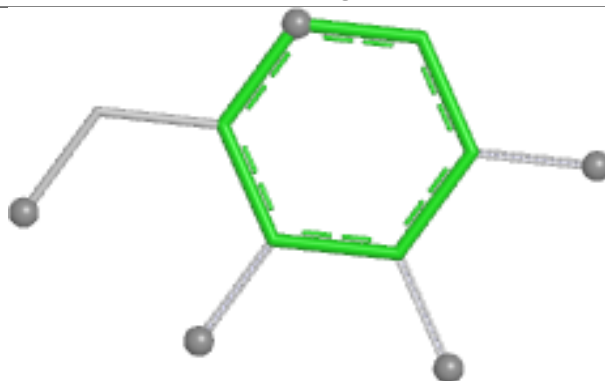
Bond lengths



Bond angles

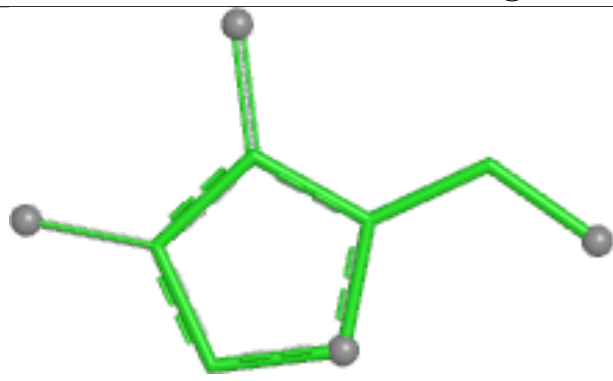


Torsions

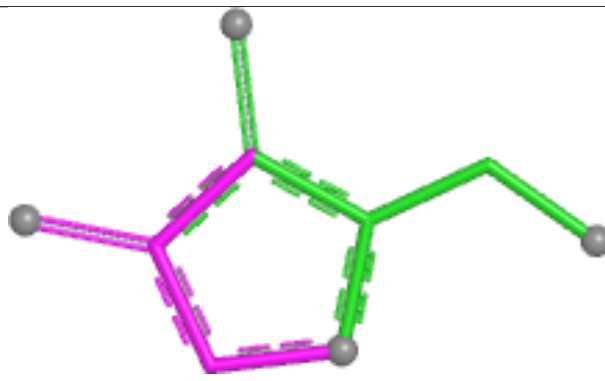


Rings

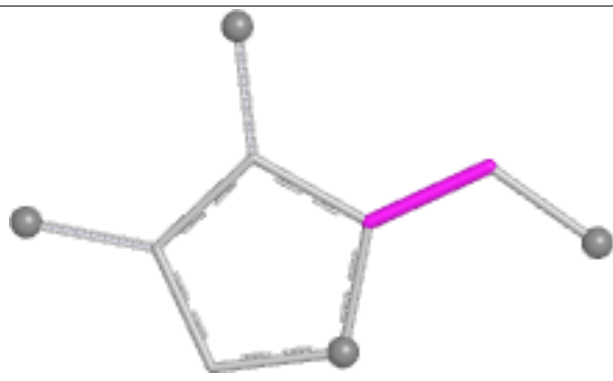
Ligand AHR F 2001



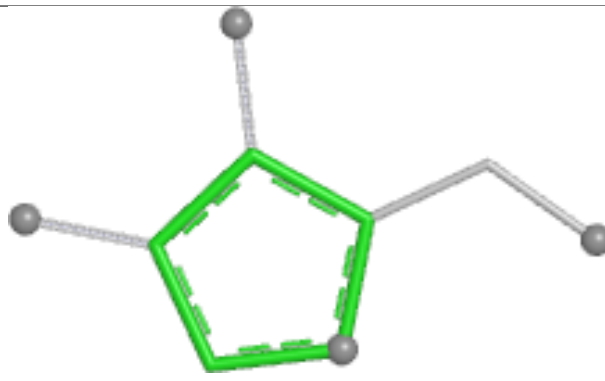
Bond lengths



Bond angles

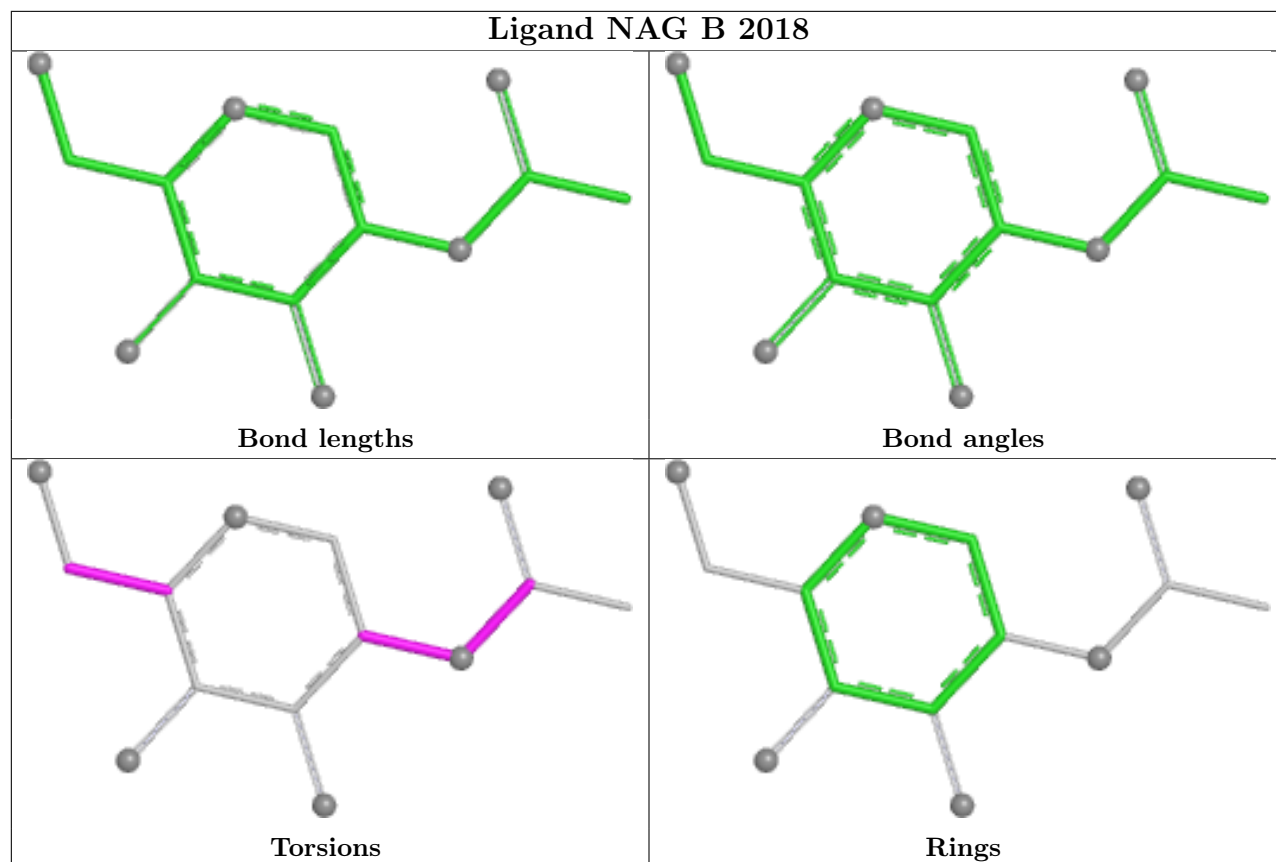


Torsions

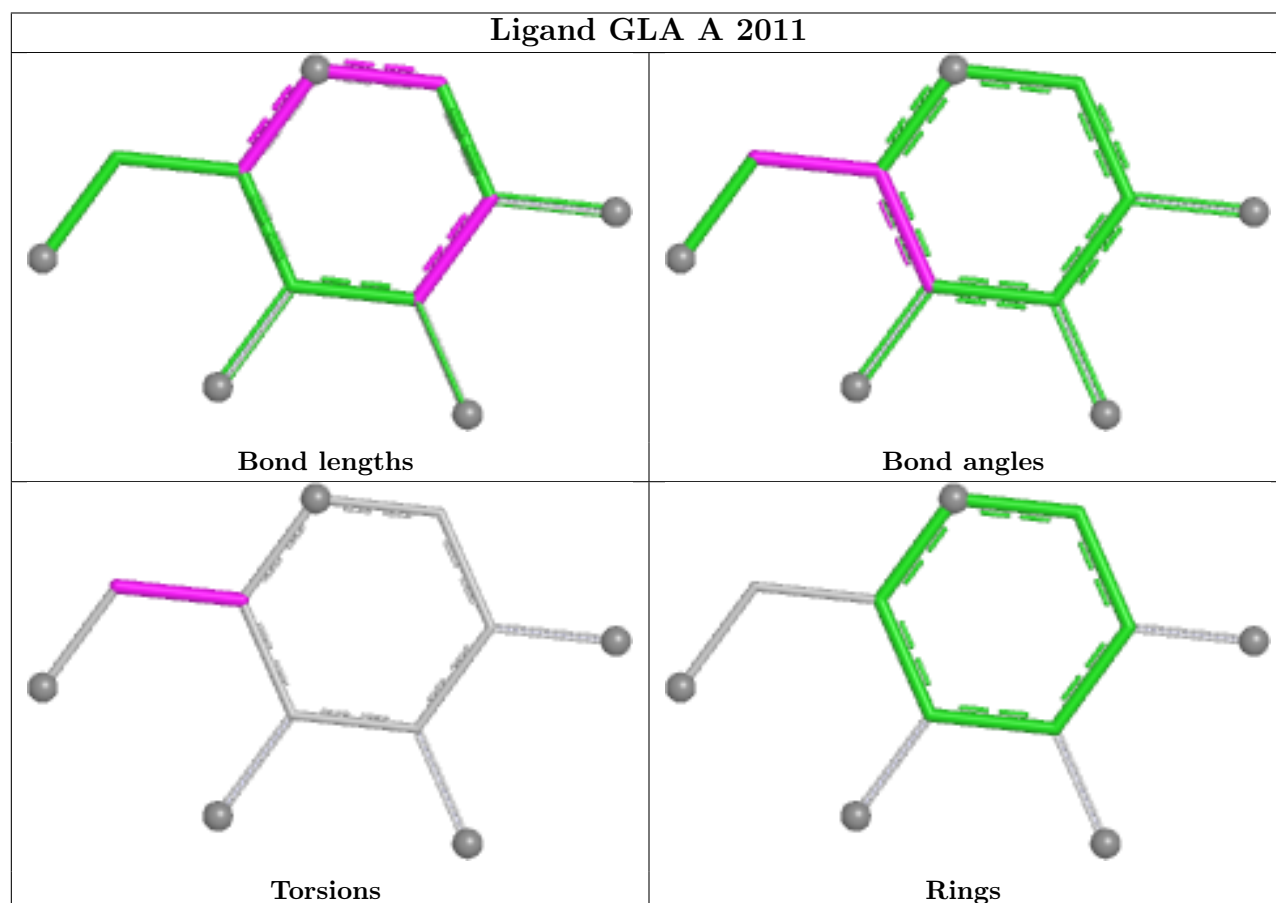


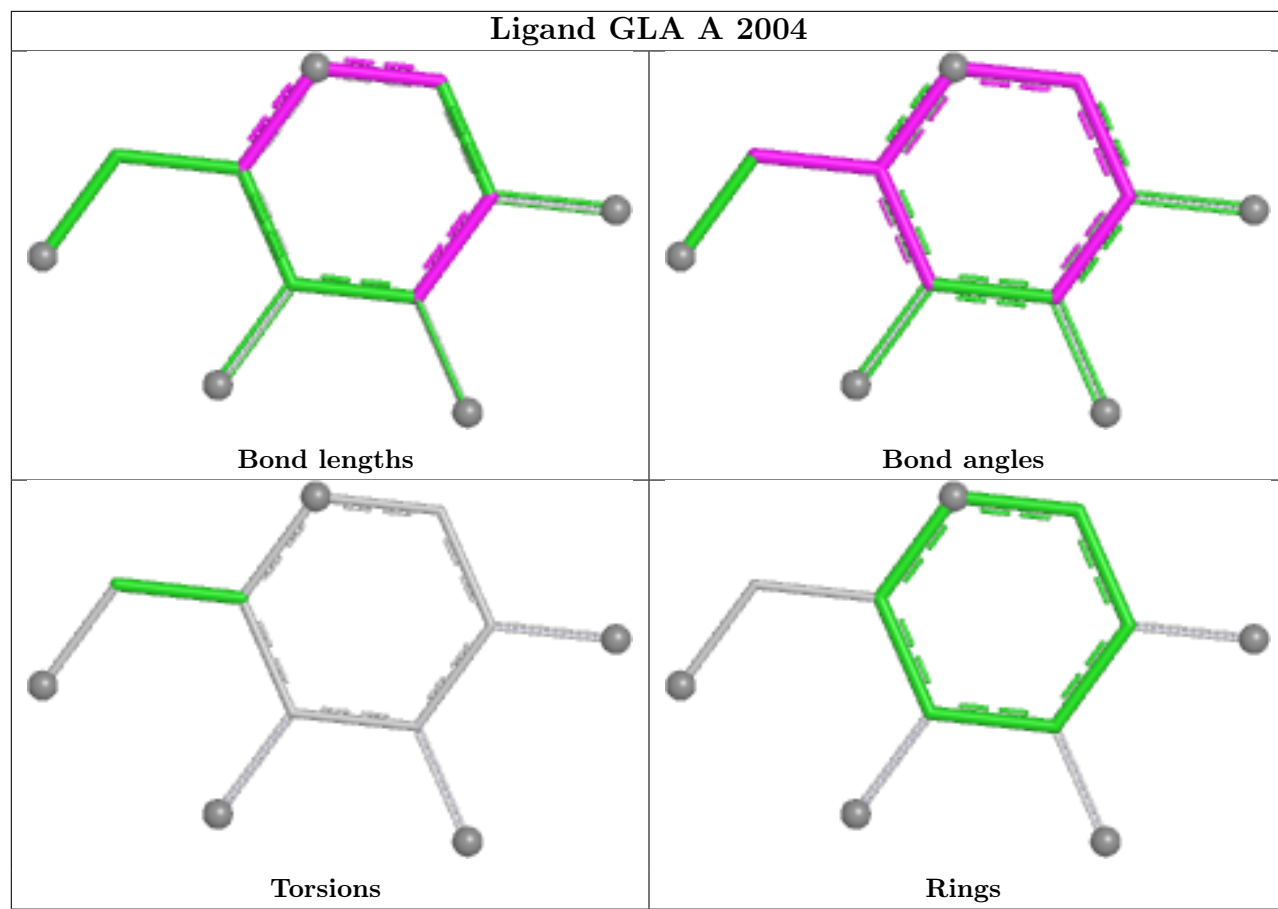
Rings

Ligand NAG B 2018

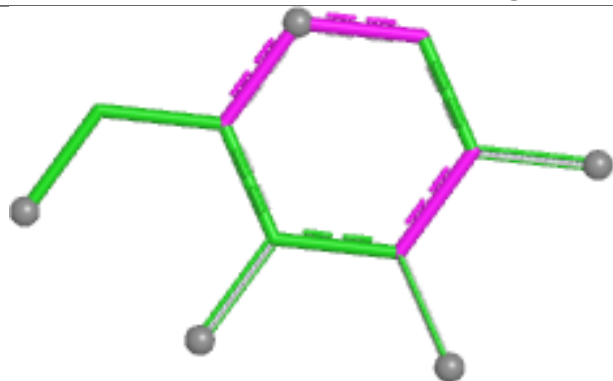


Ligand GLA A 2011

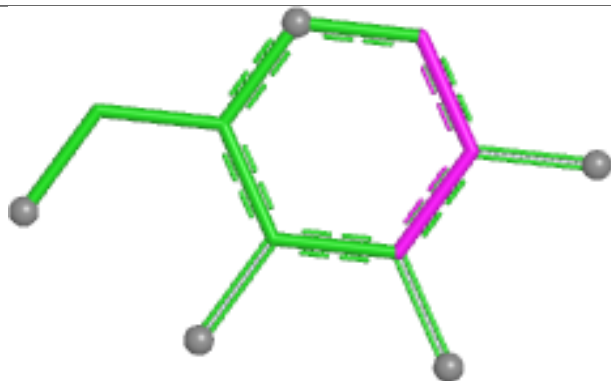




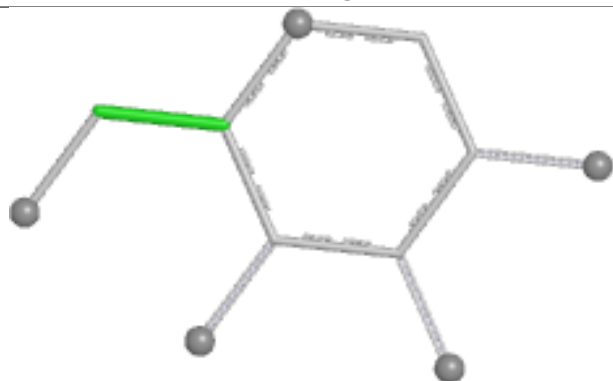
Ligand GLA E 2009



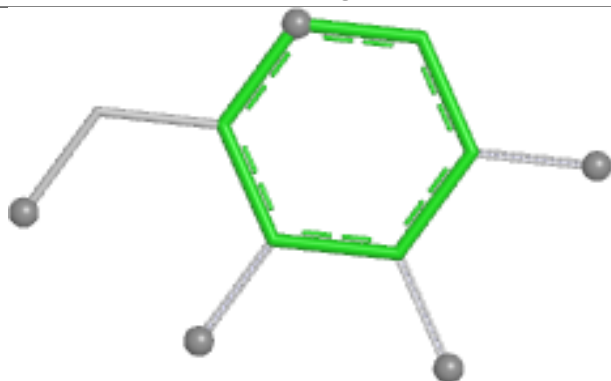
Bond lengths



Bond angles

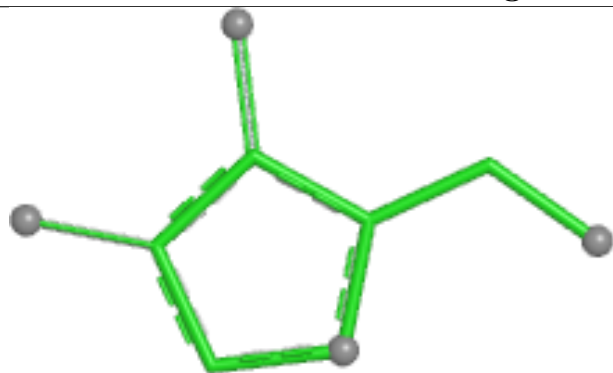


Torsions

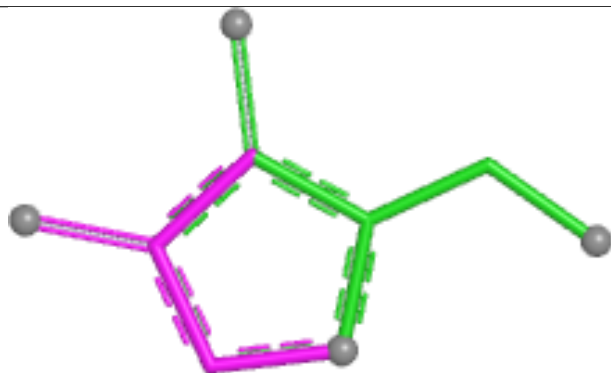


Rings

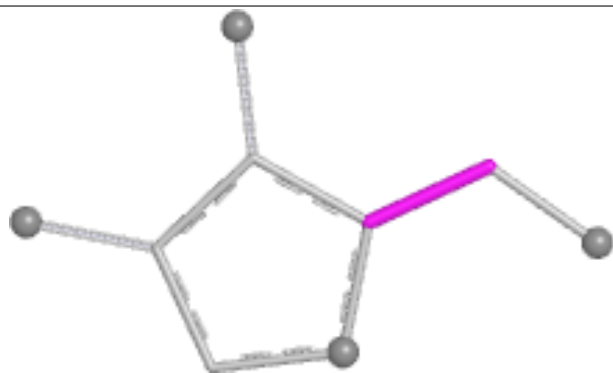
Ligand AHR F 2004



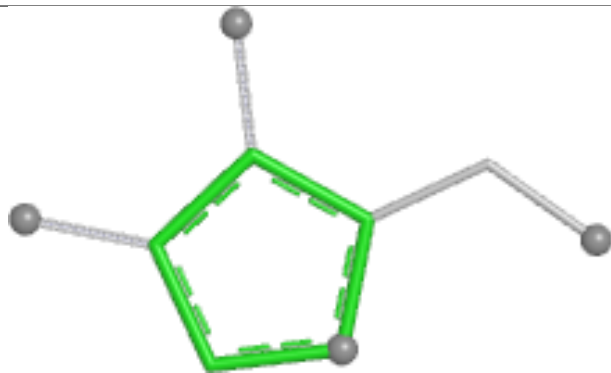
Bond lengths



Bond angles

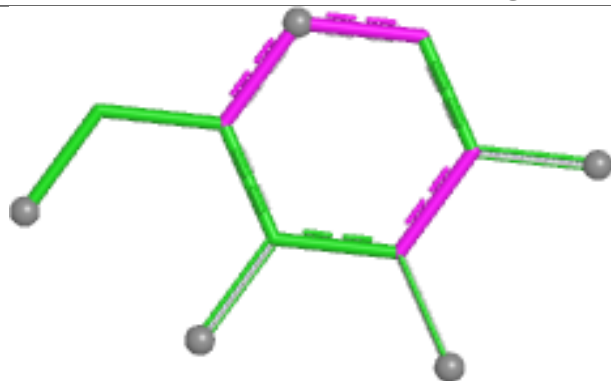


Torsions

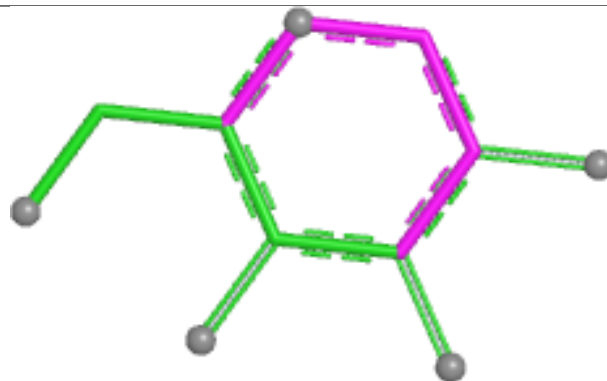


Rings

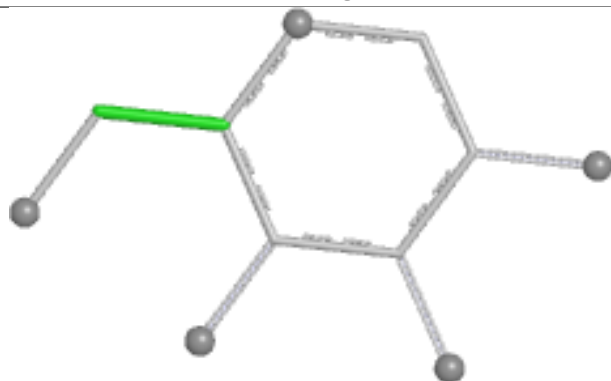
Ligand GLA B 2005



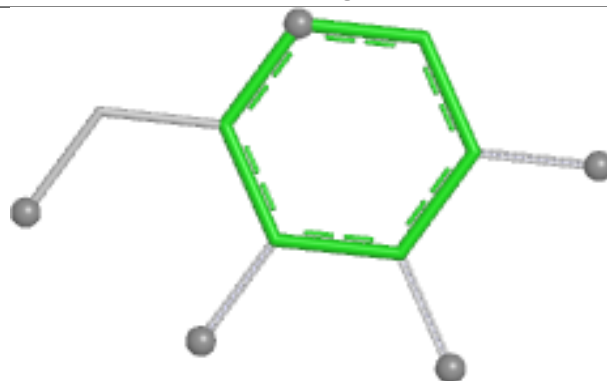
Bond lengths



Bond angles

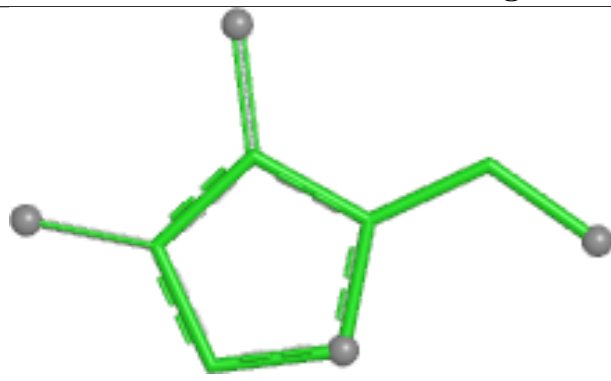


Torsions

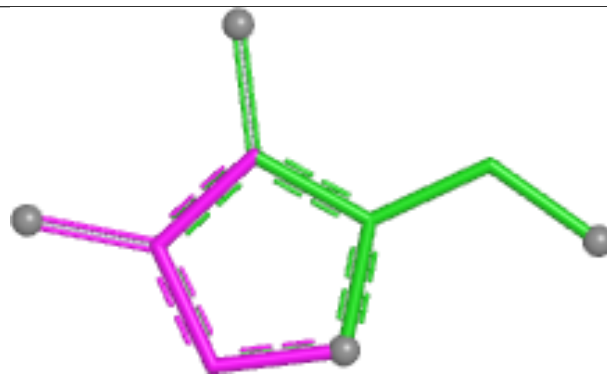


Rings

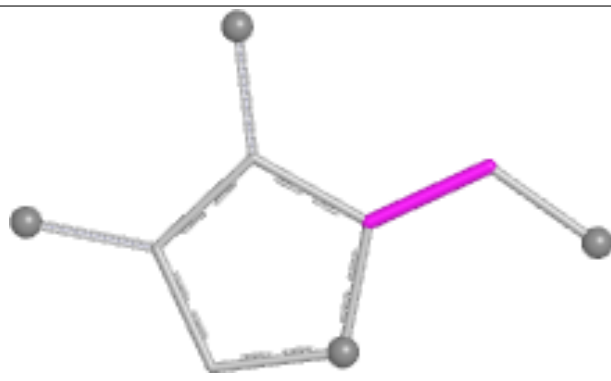
Ligand AHR E 2003



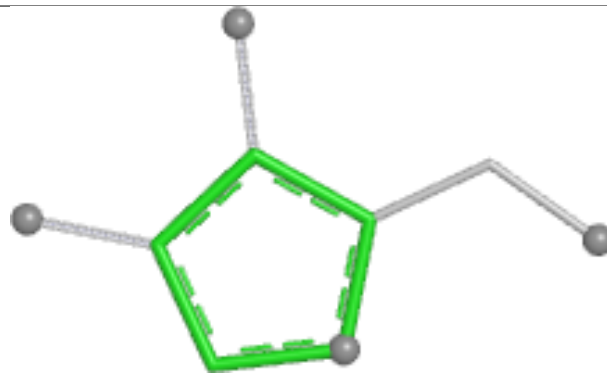
Bond lengths



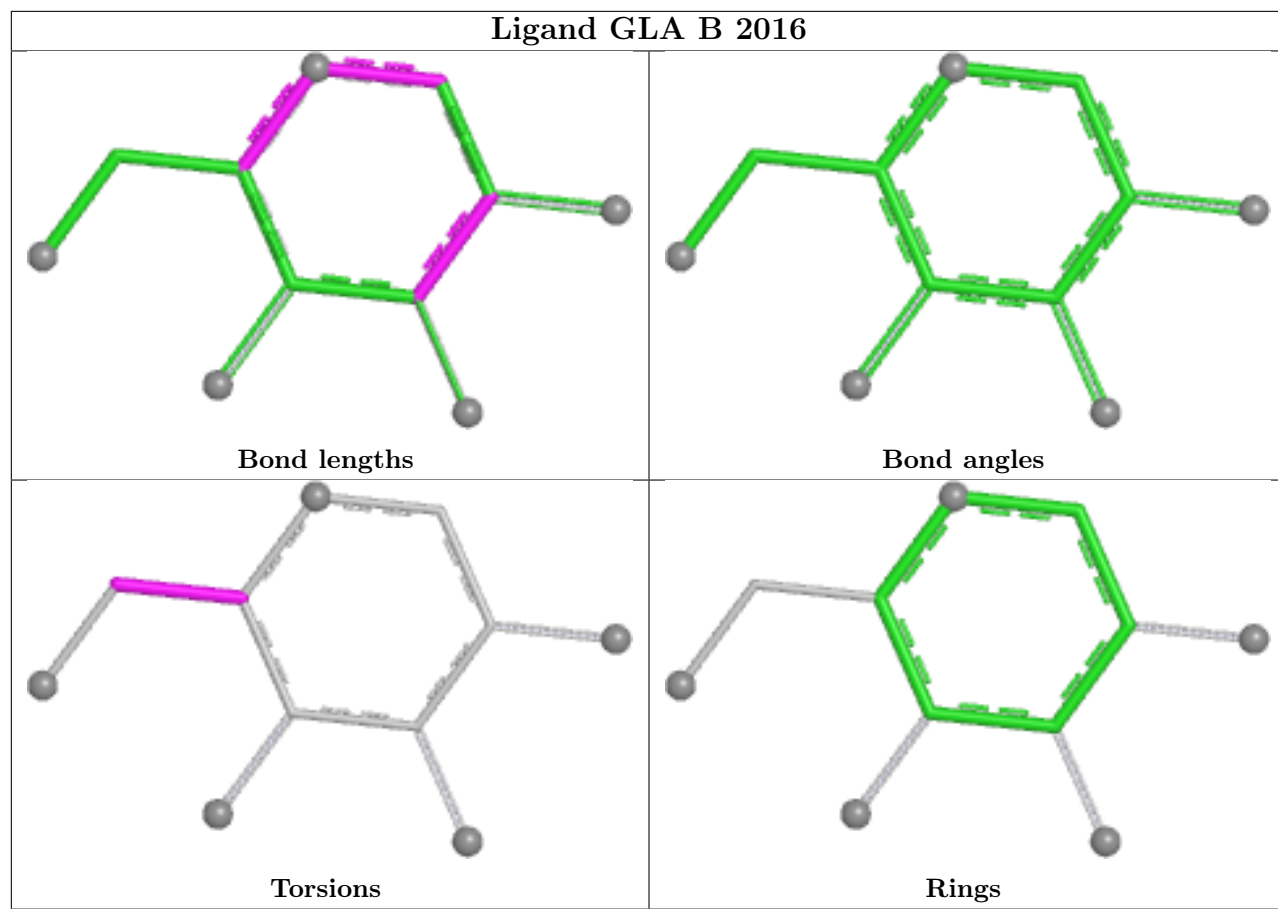
Bond angles

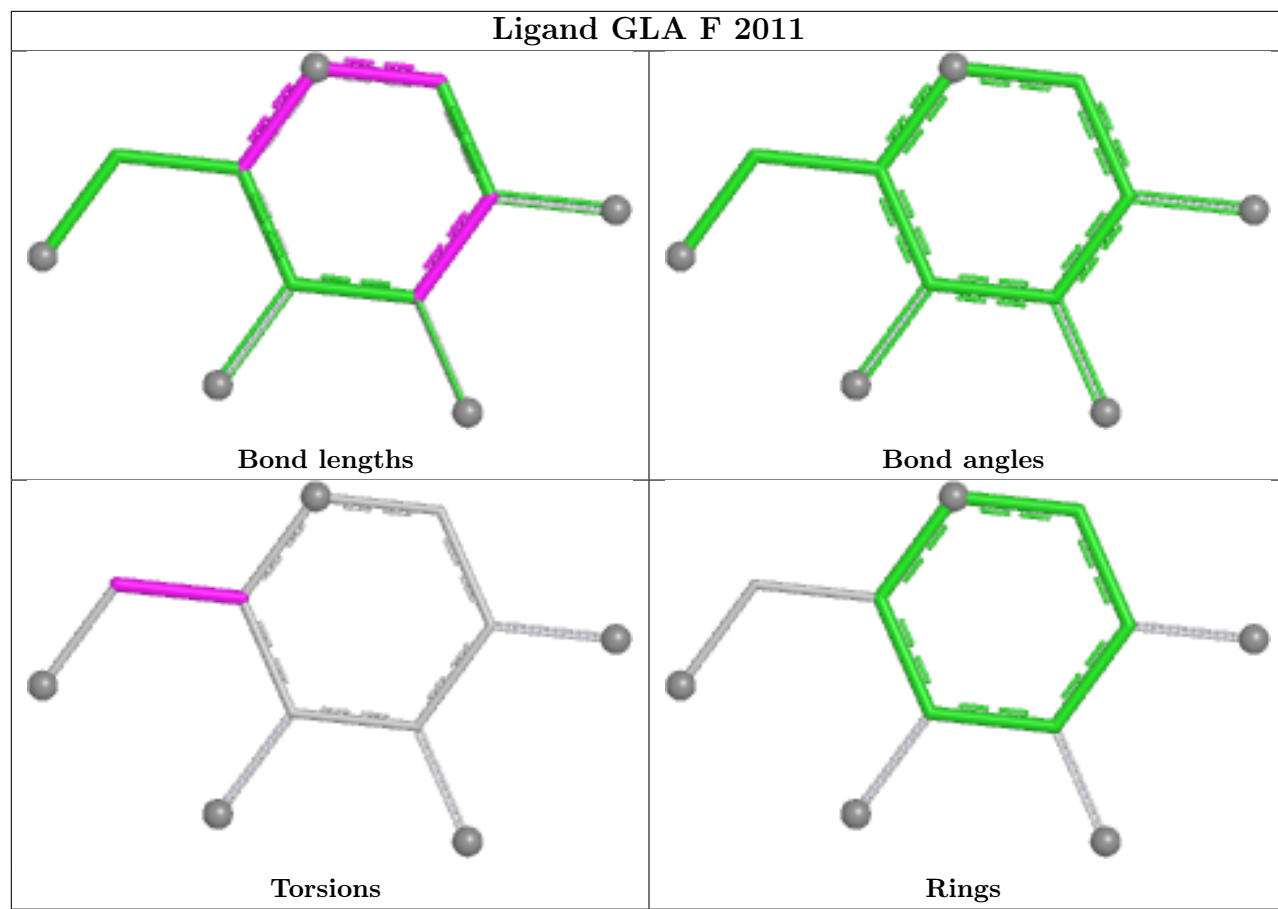


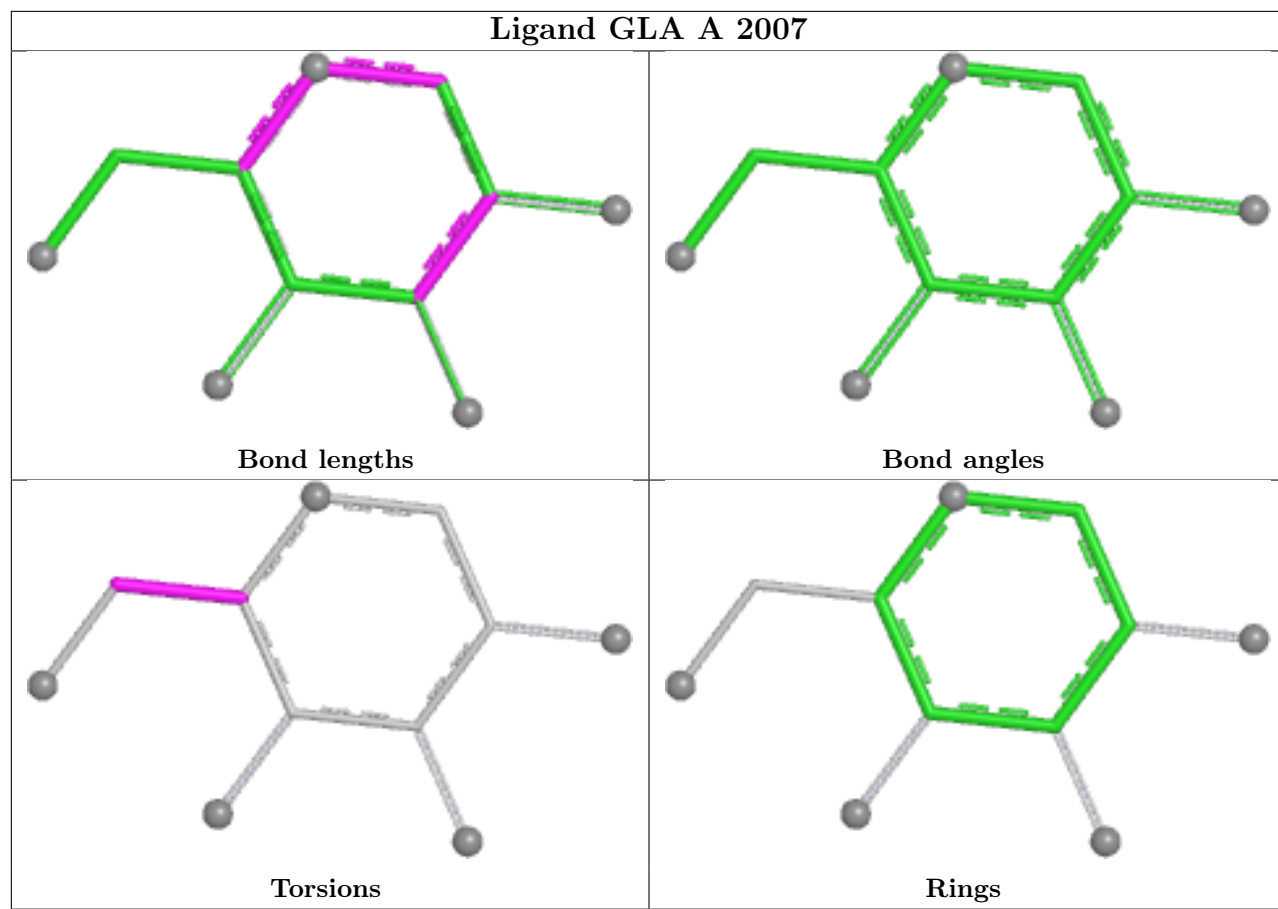
Torsions

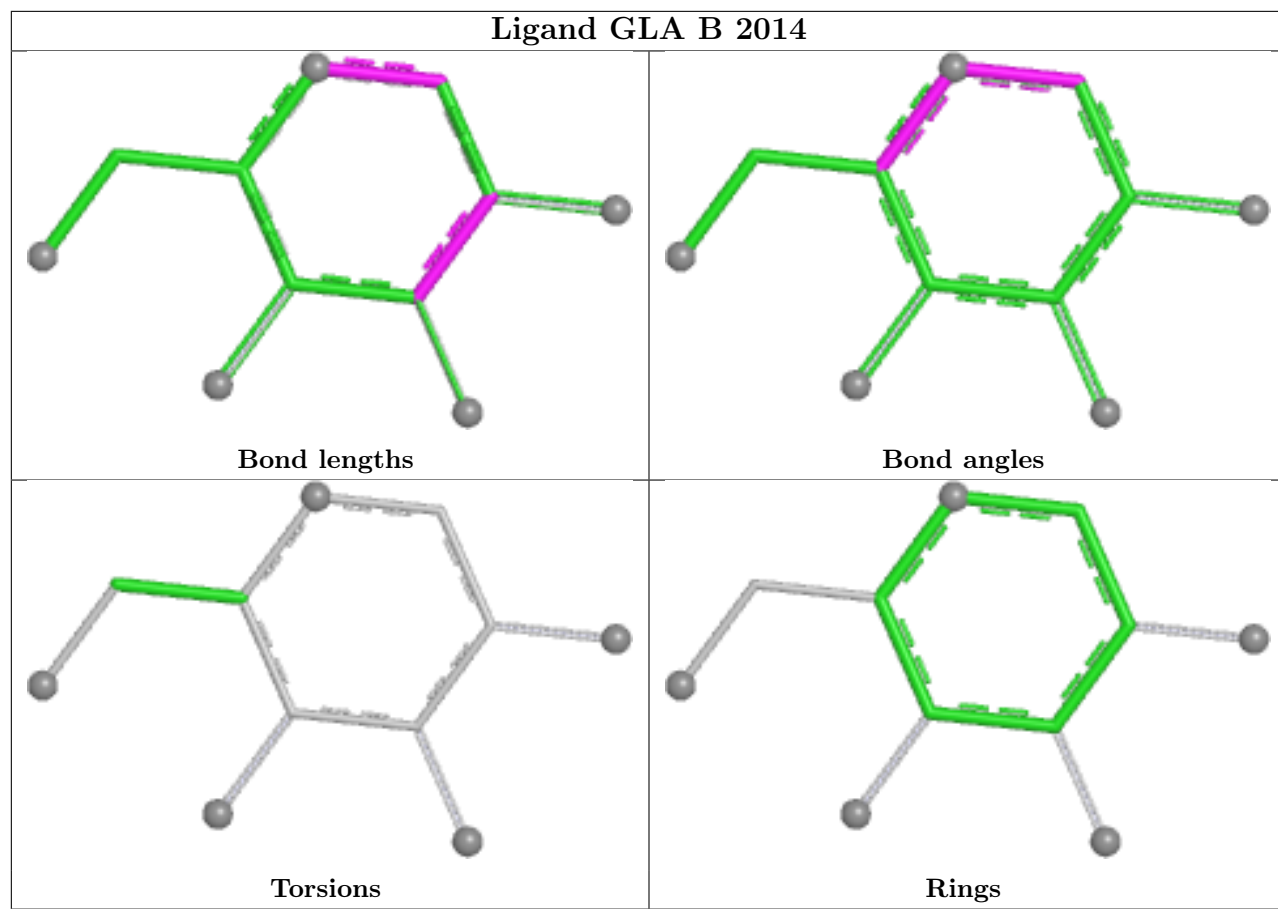


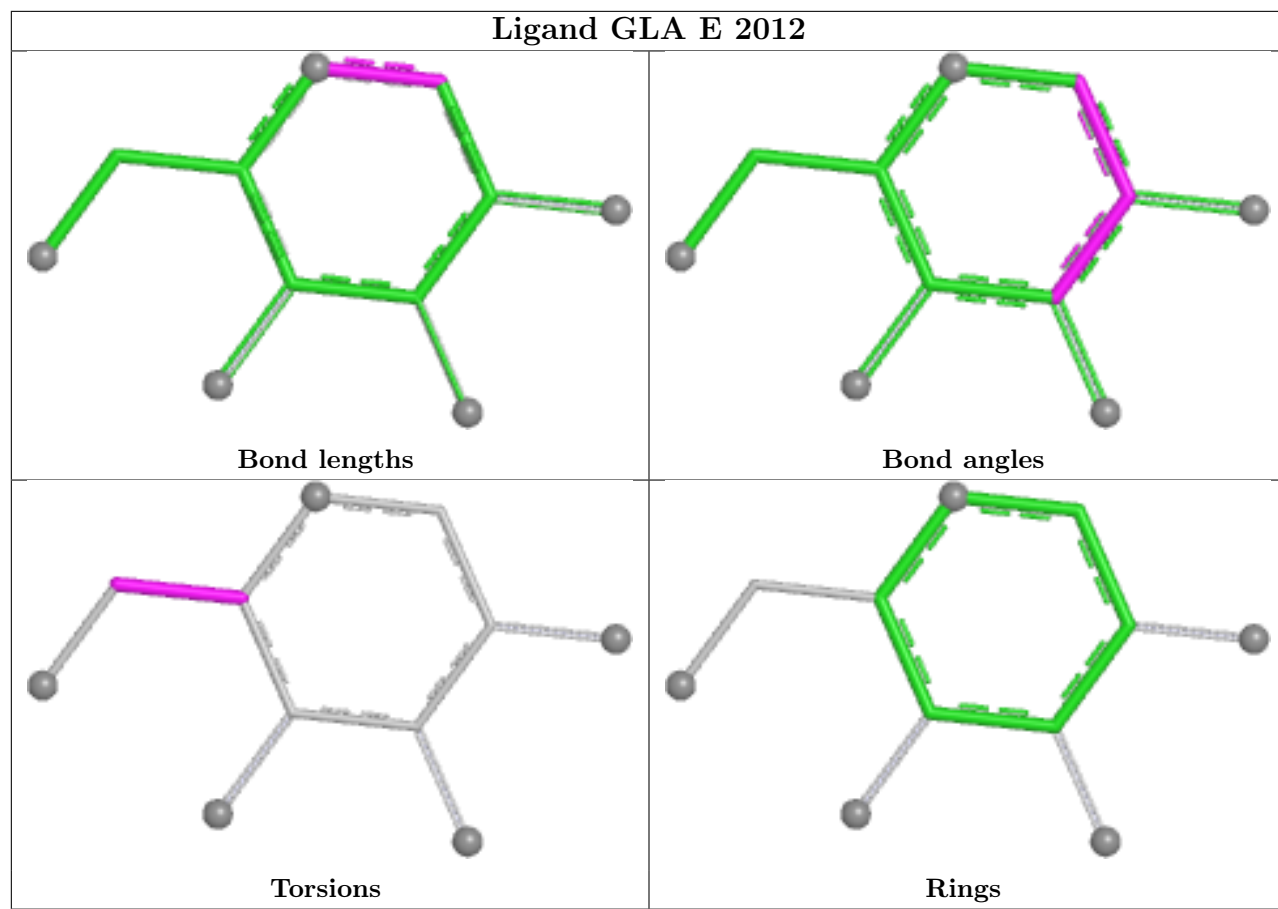
Rings

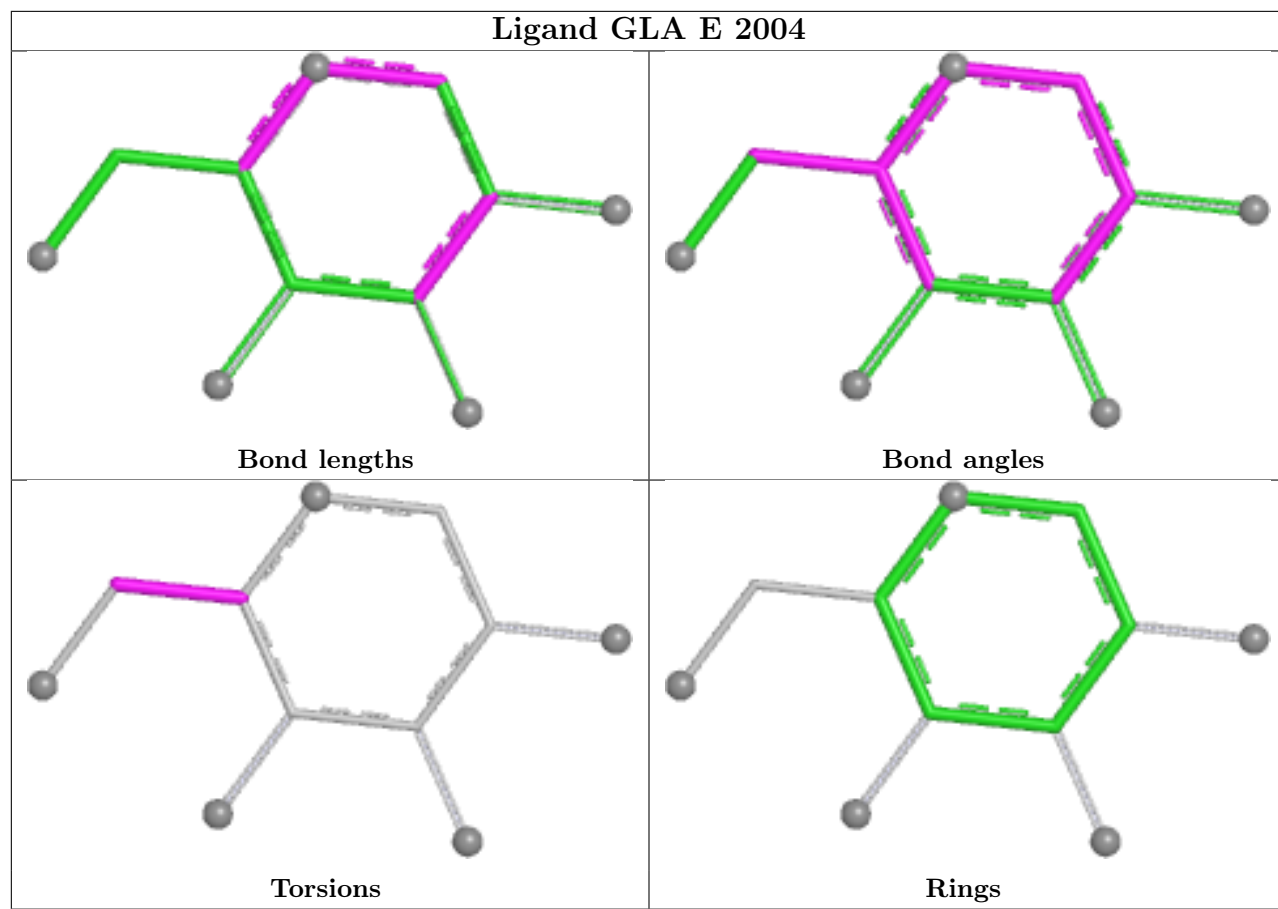


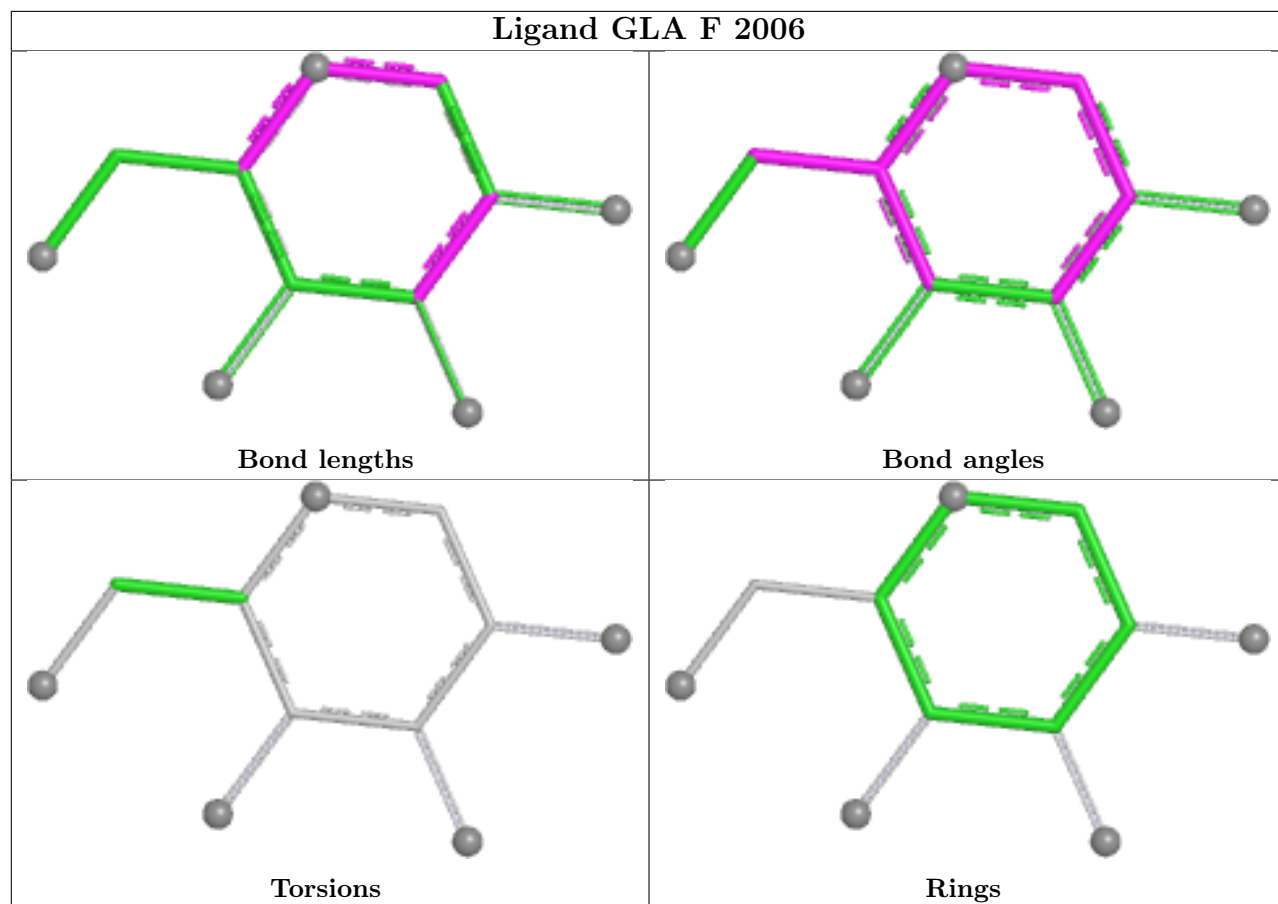


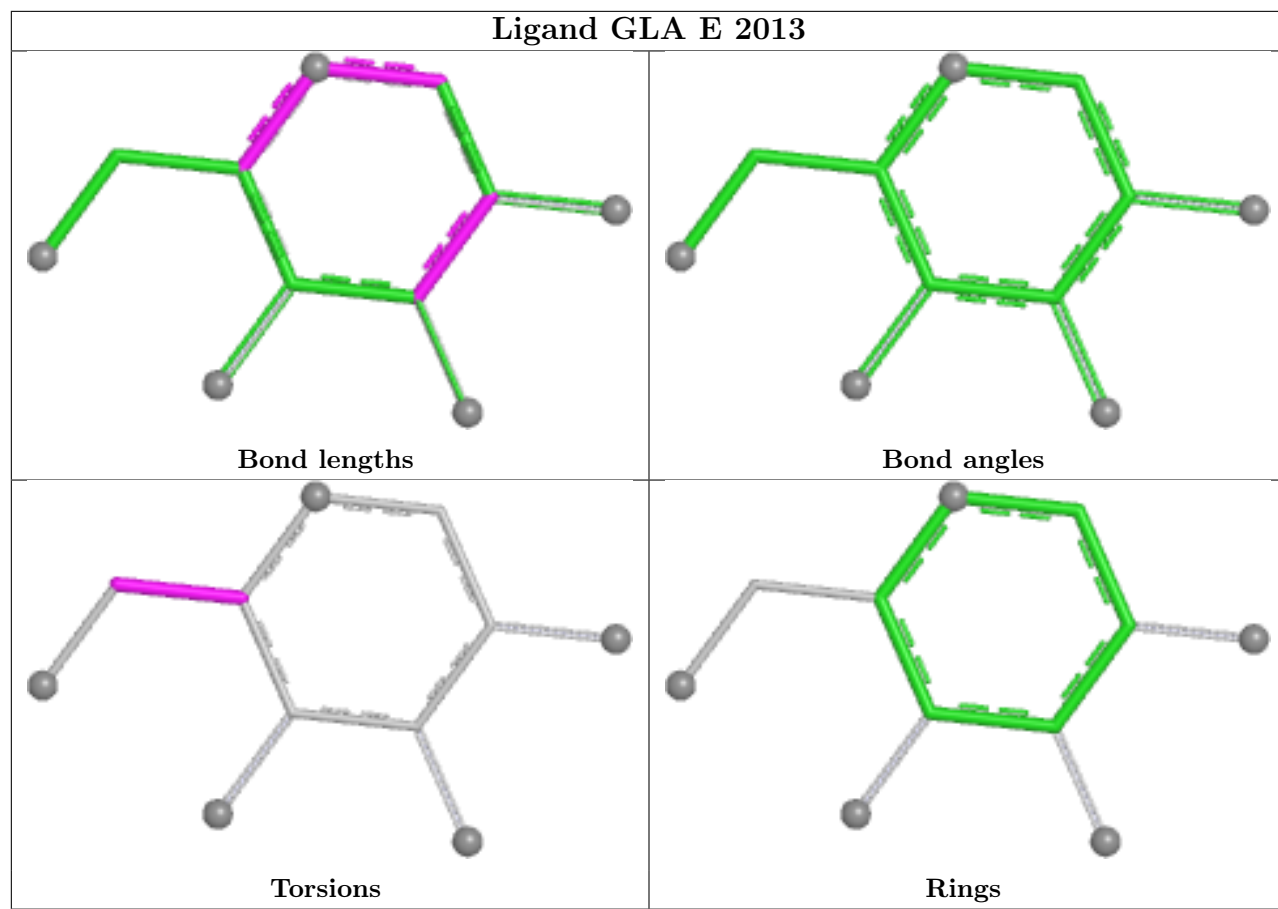




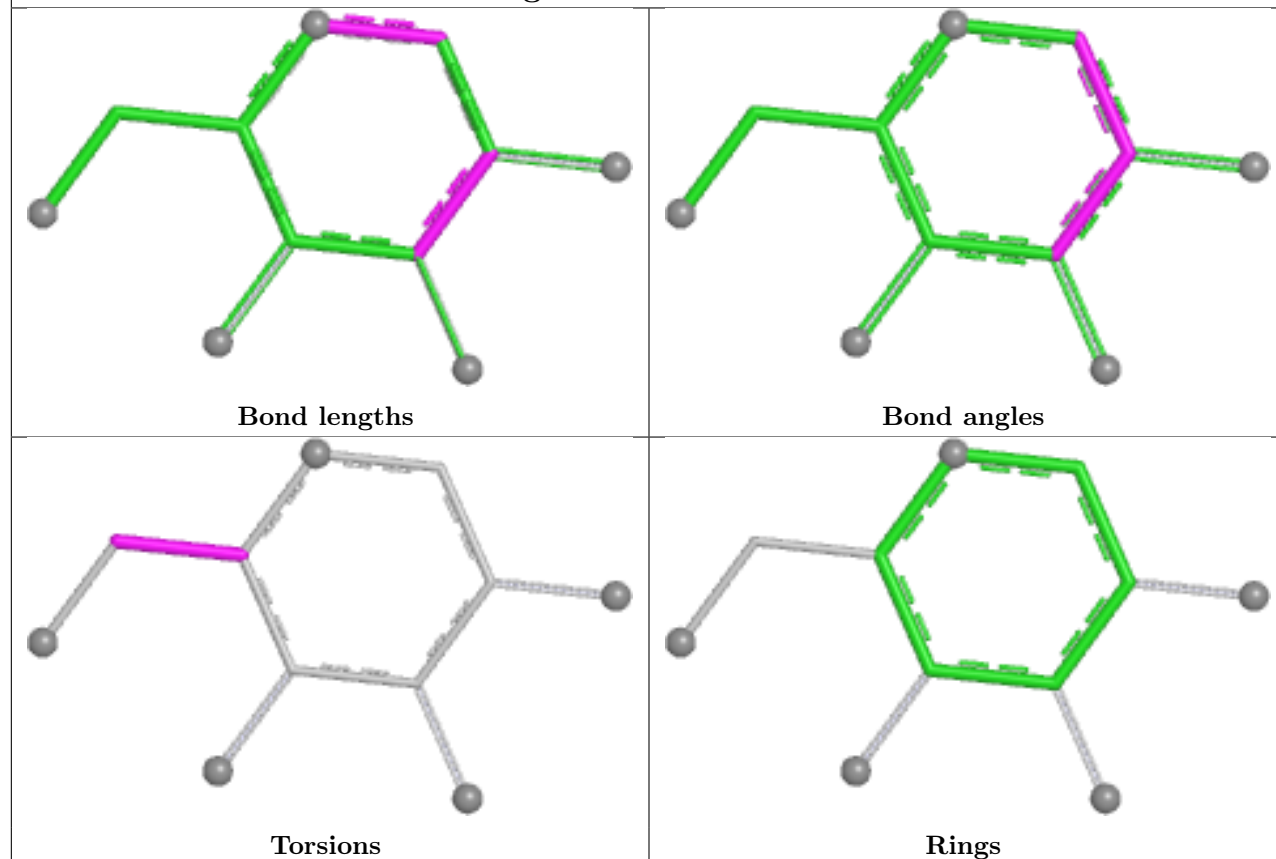




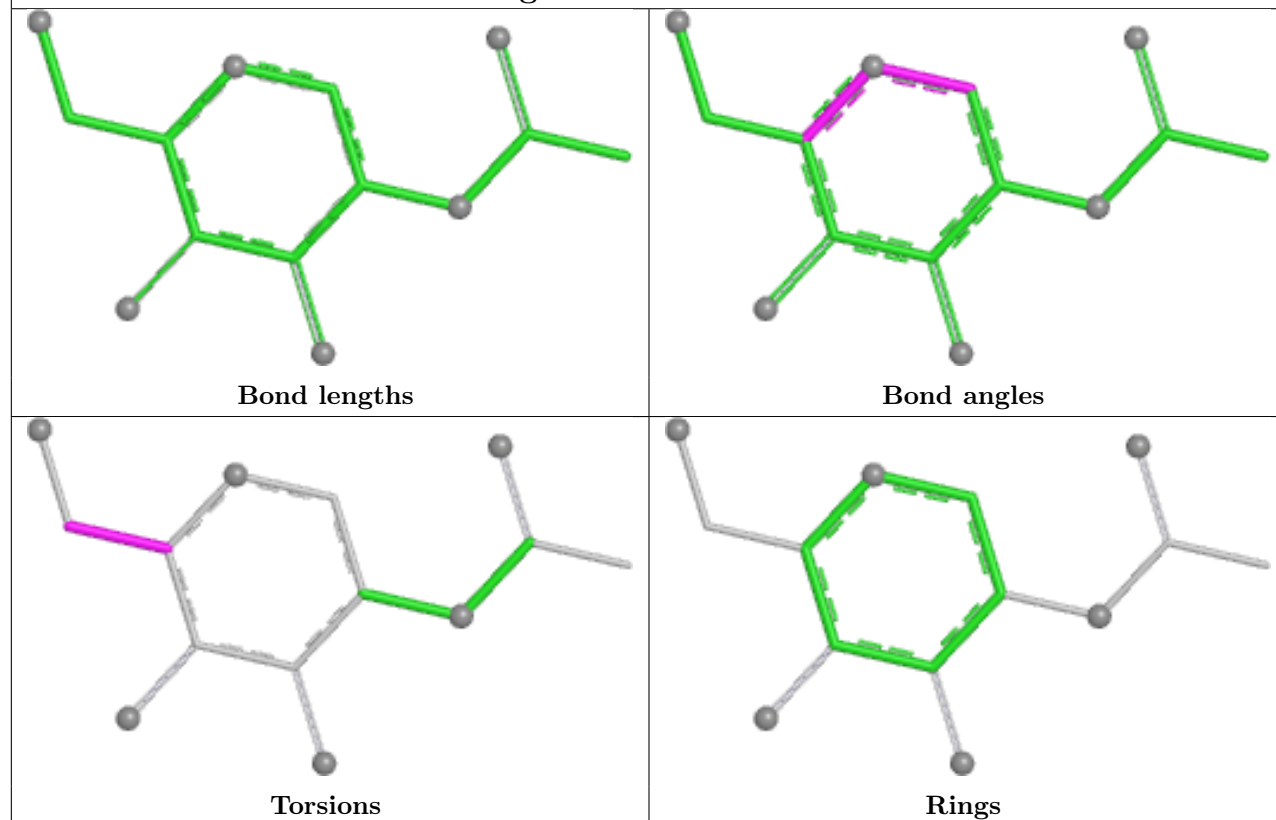


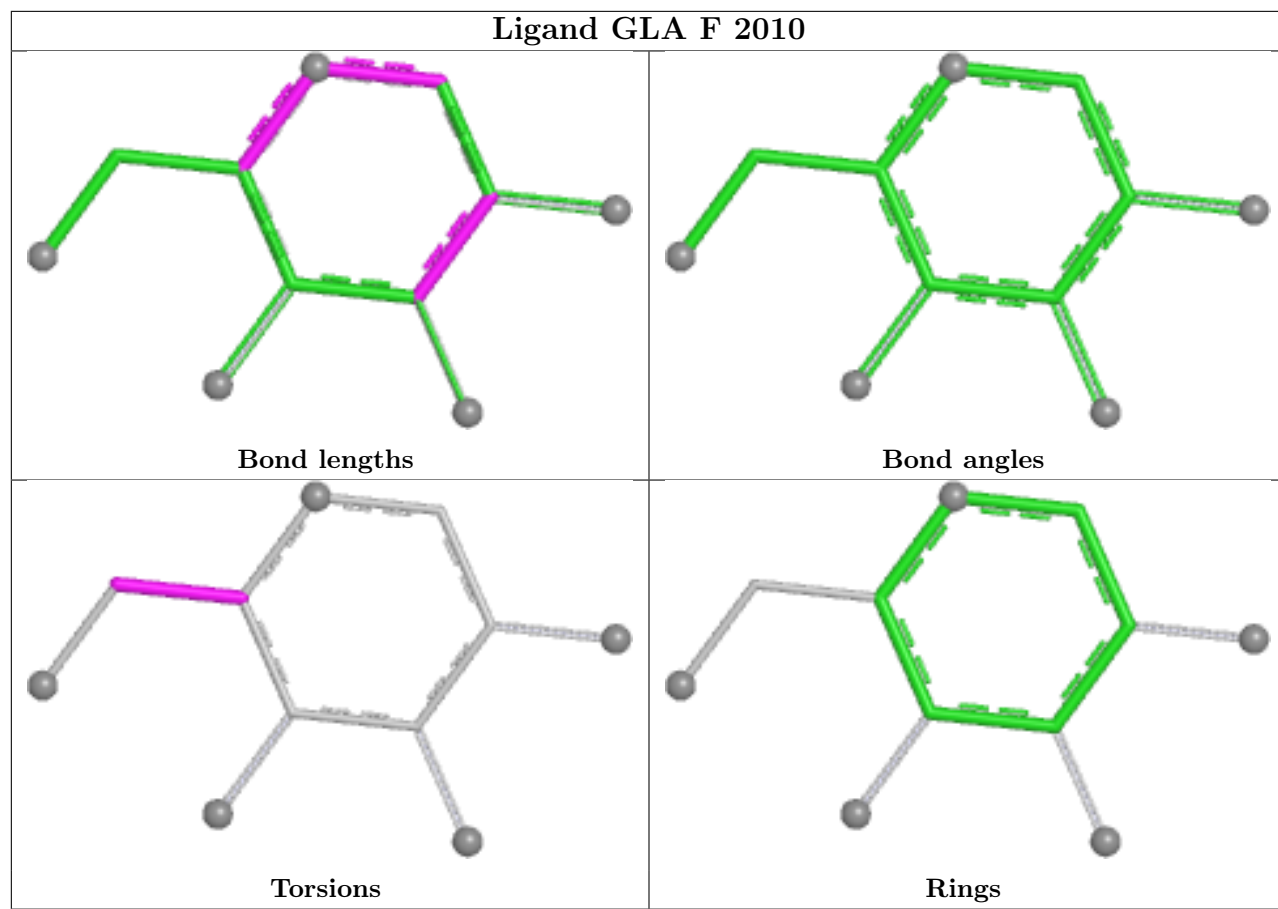


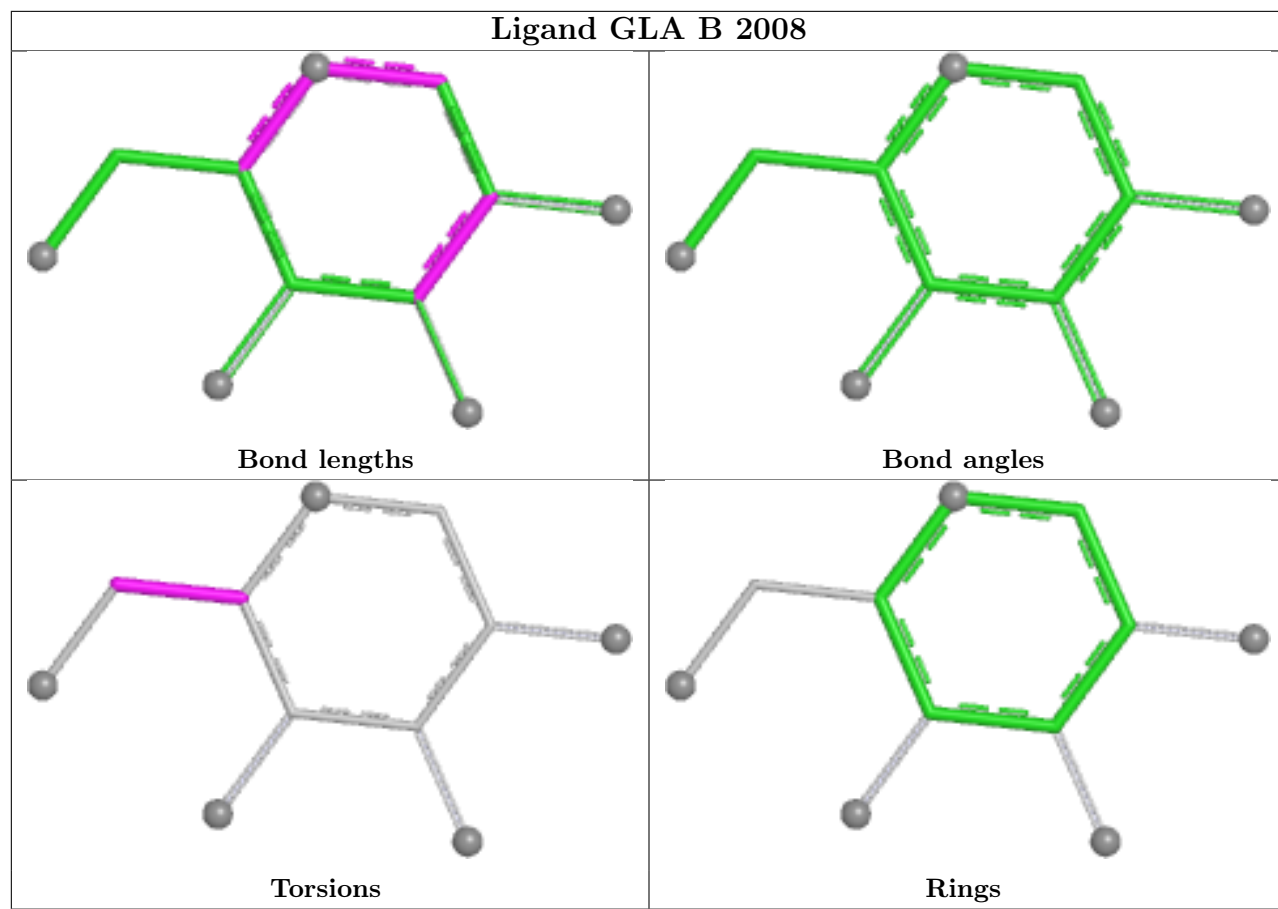
Ligand GLA E 2010

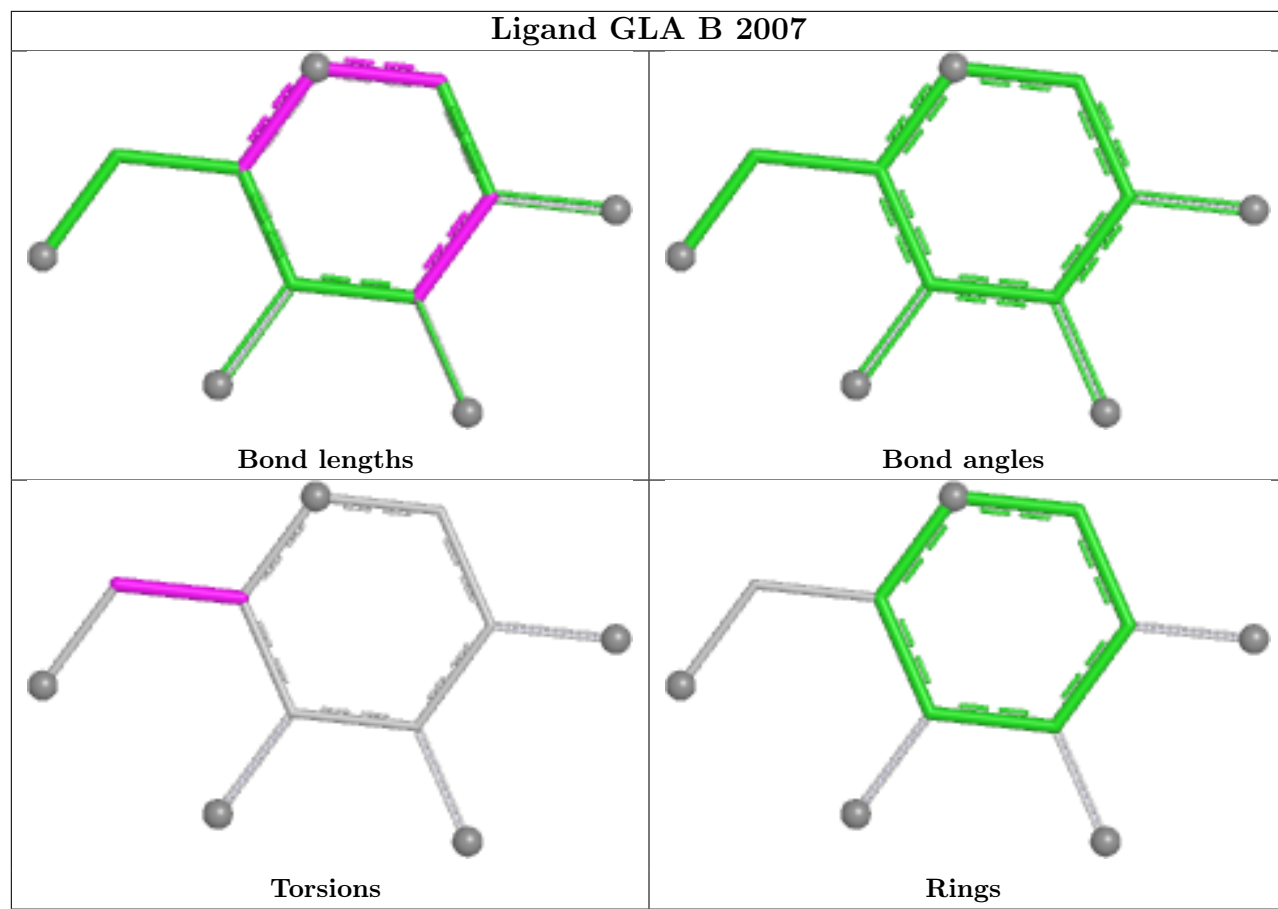


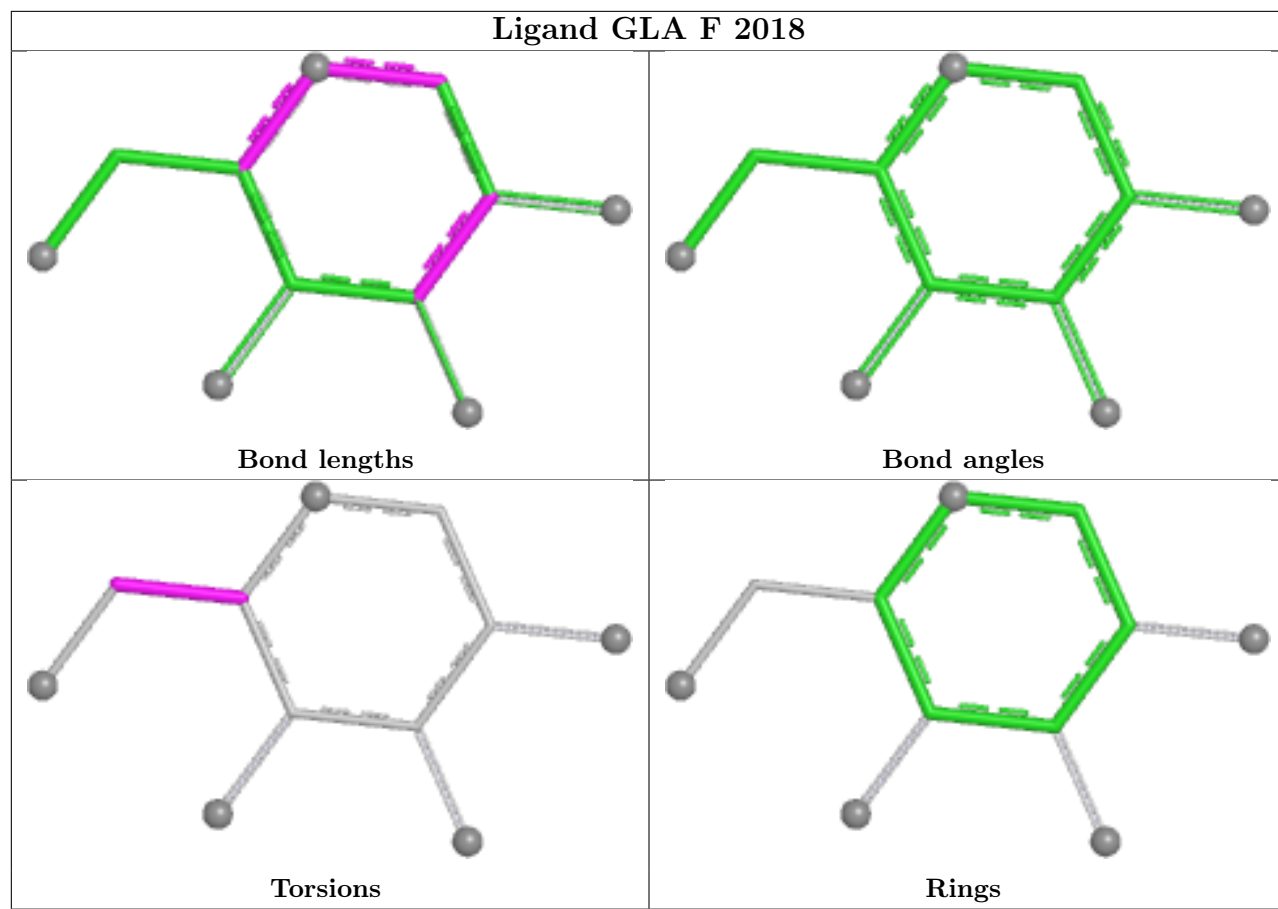
Ligand NAG B 2019



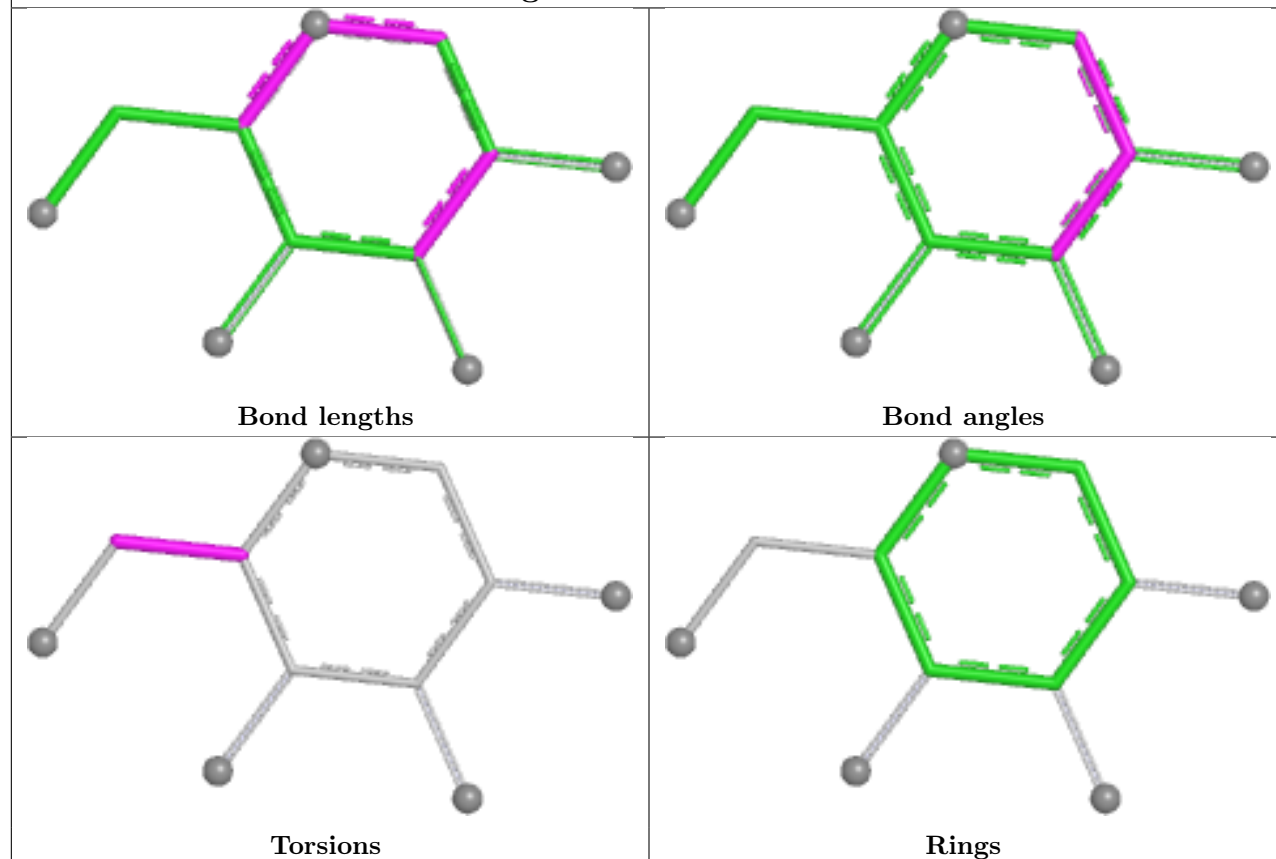




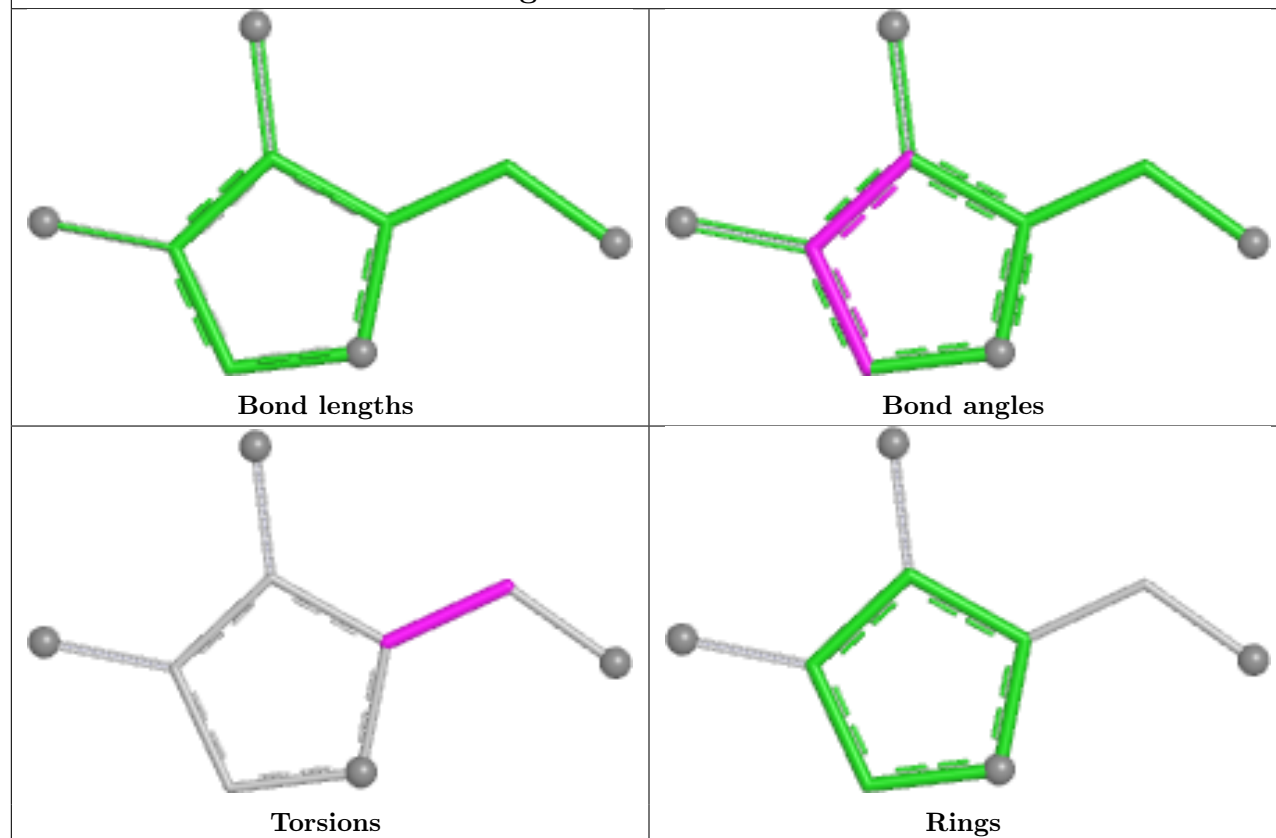


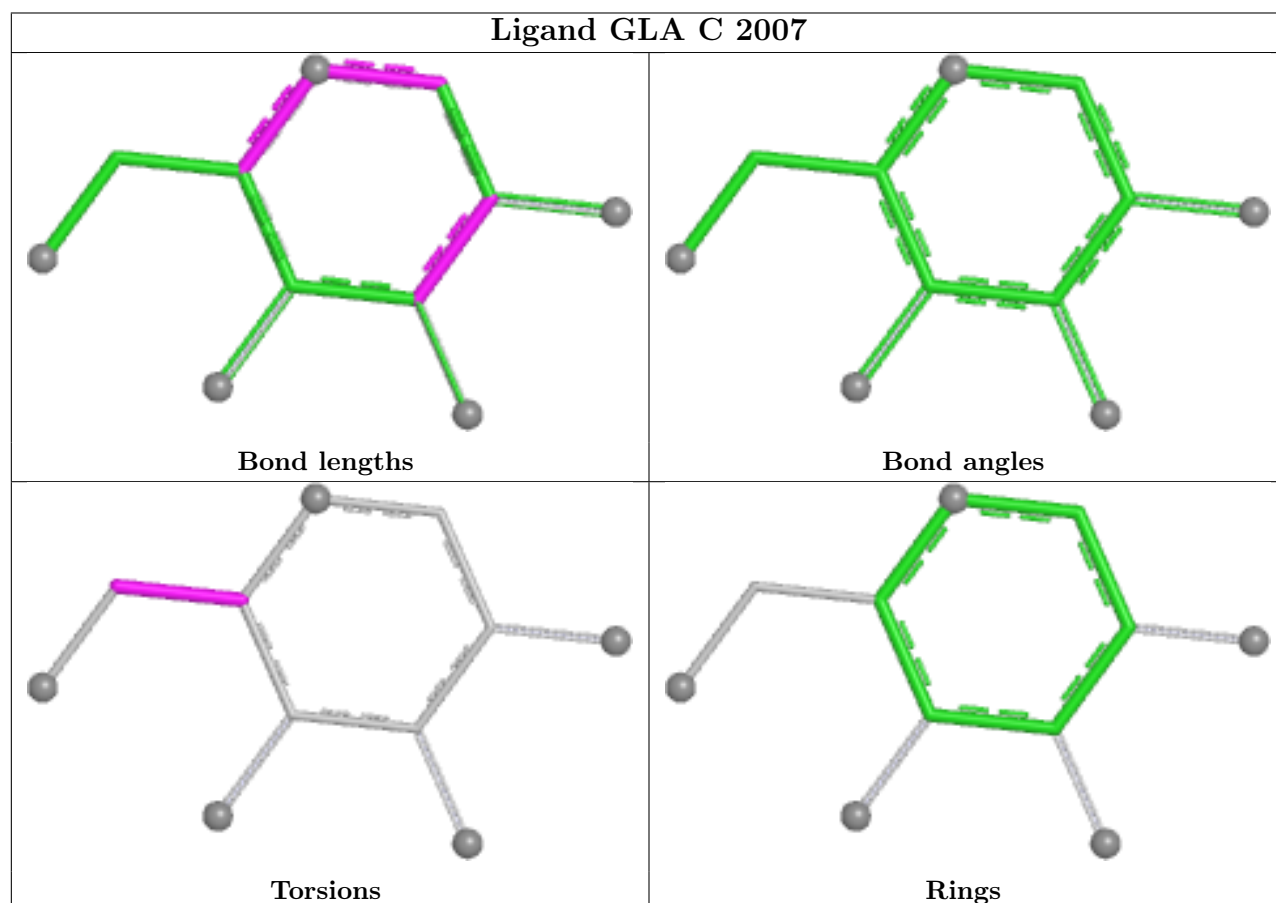
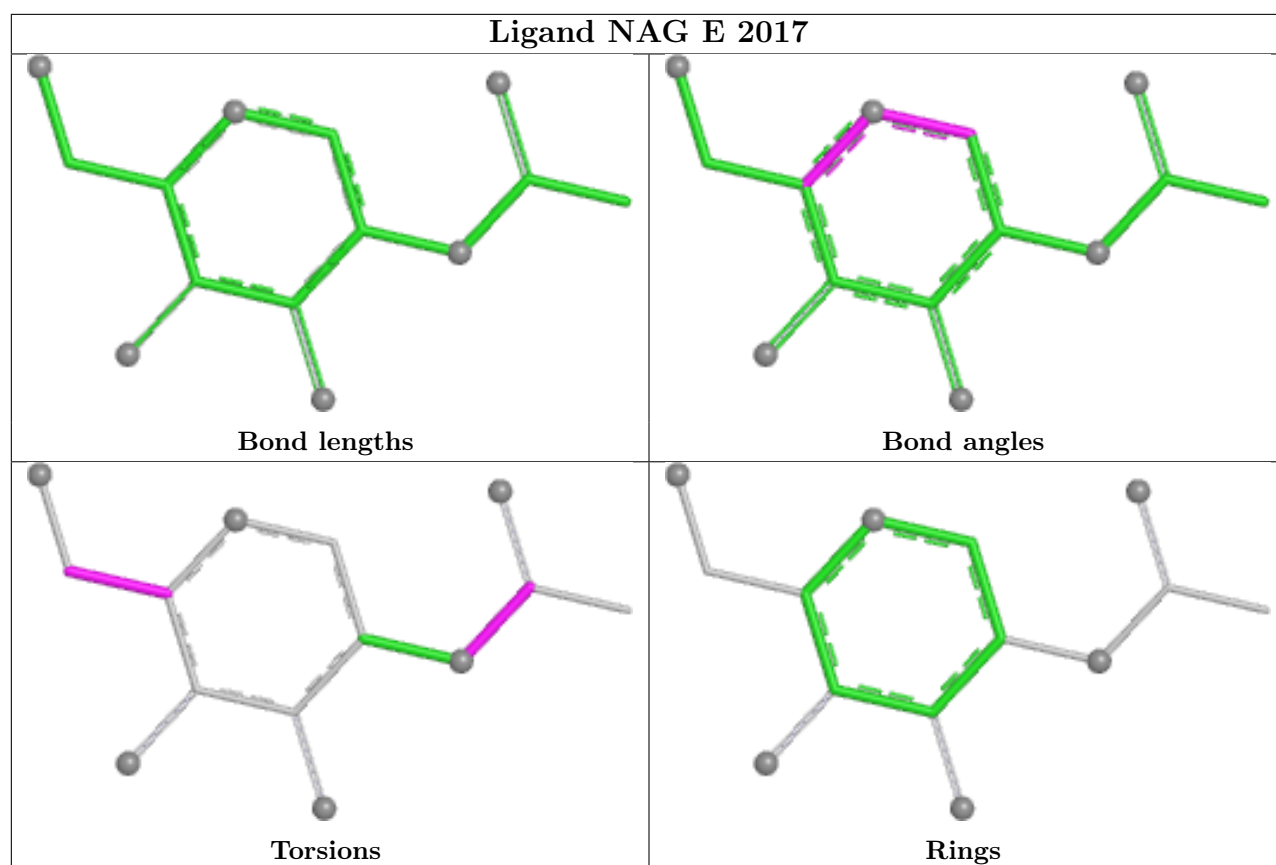


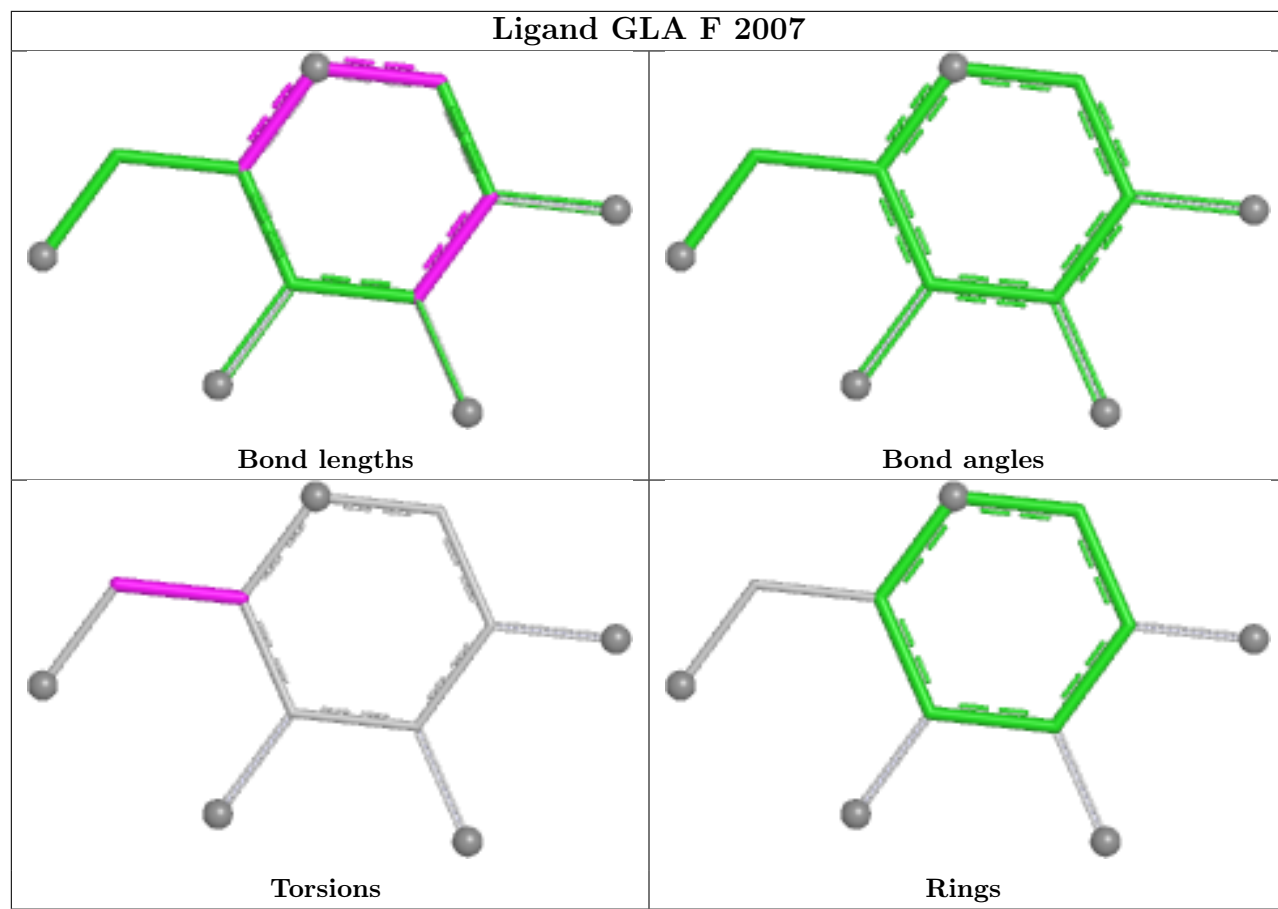
Ligand GLA A 2016

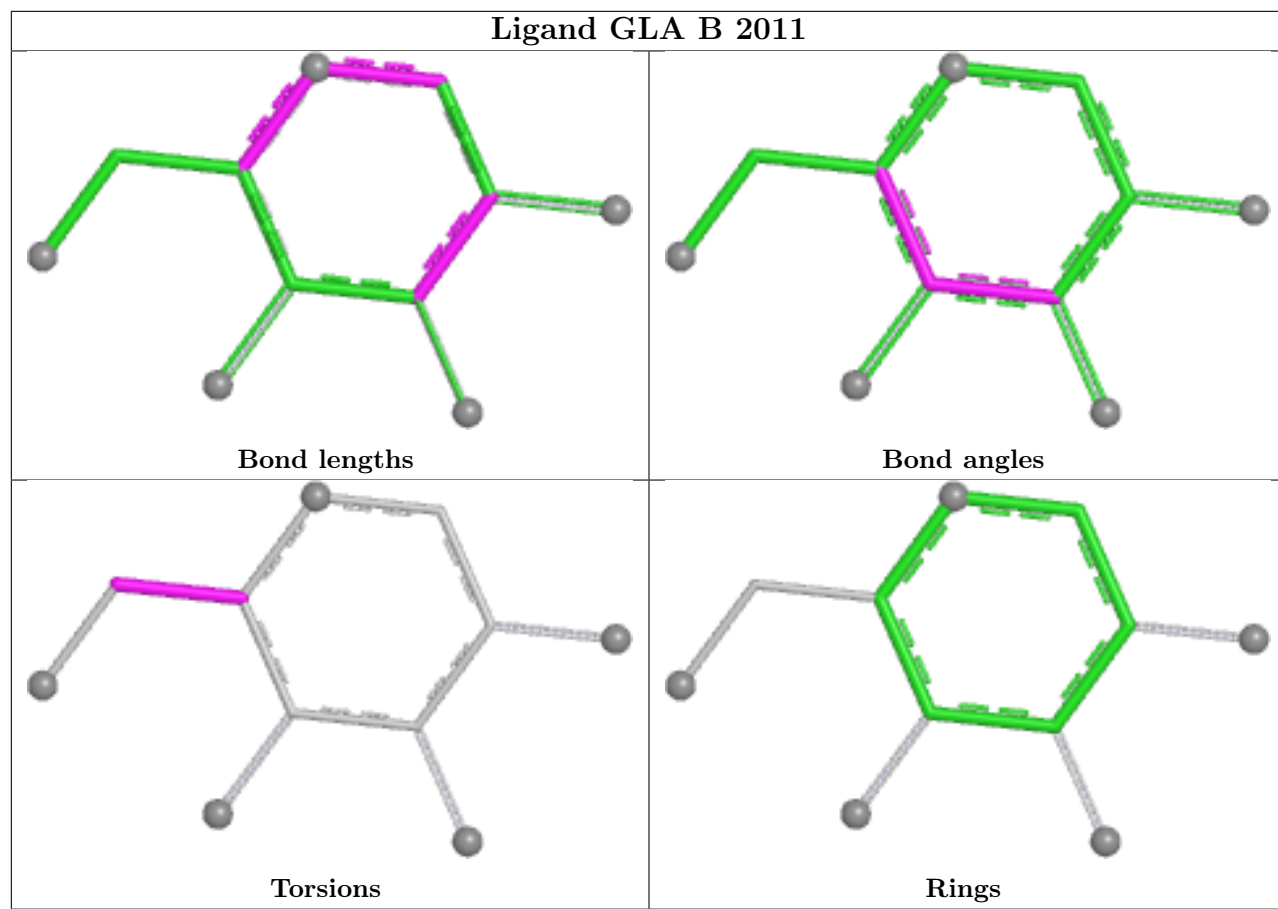


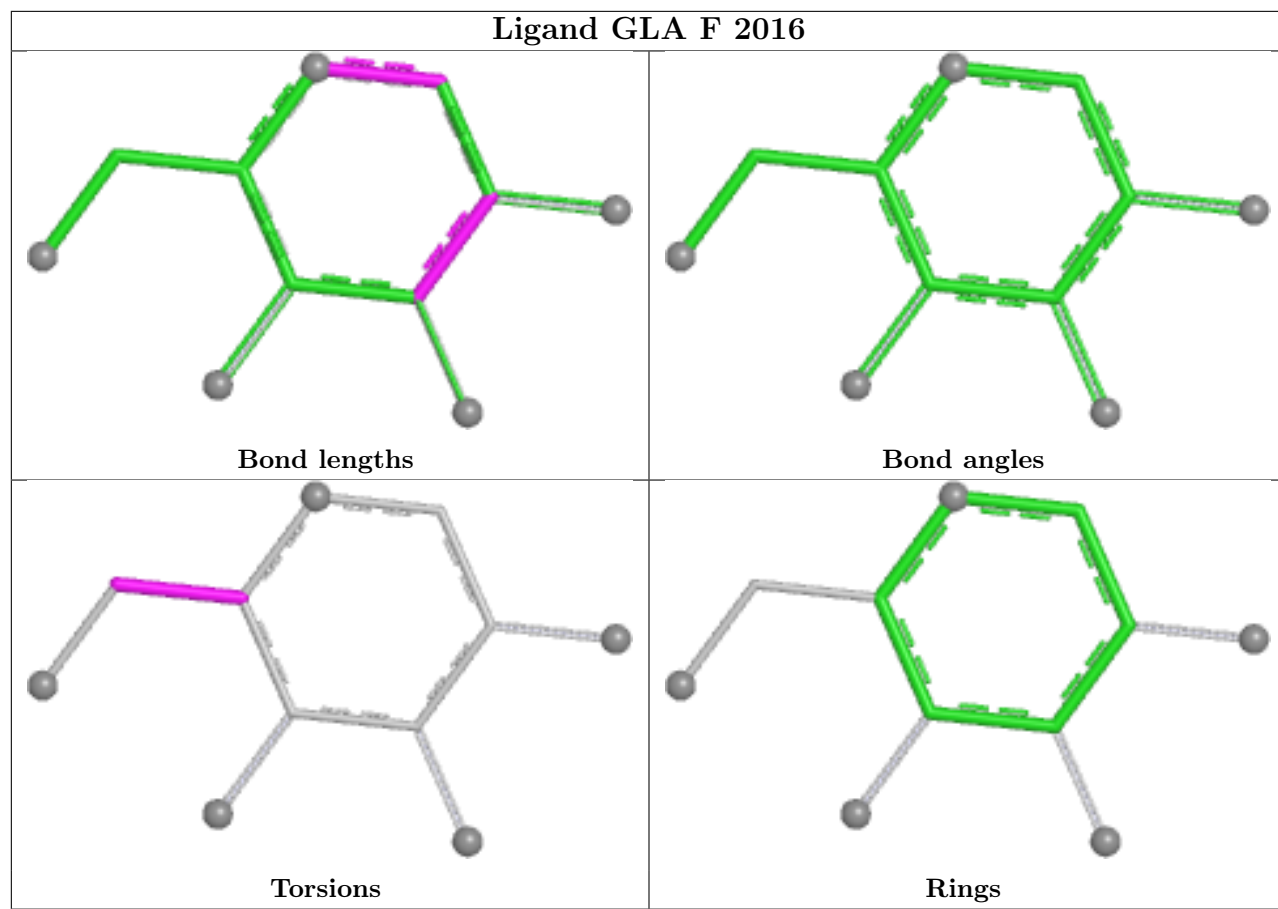
Ligand AHR B 2020

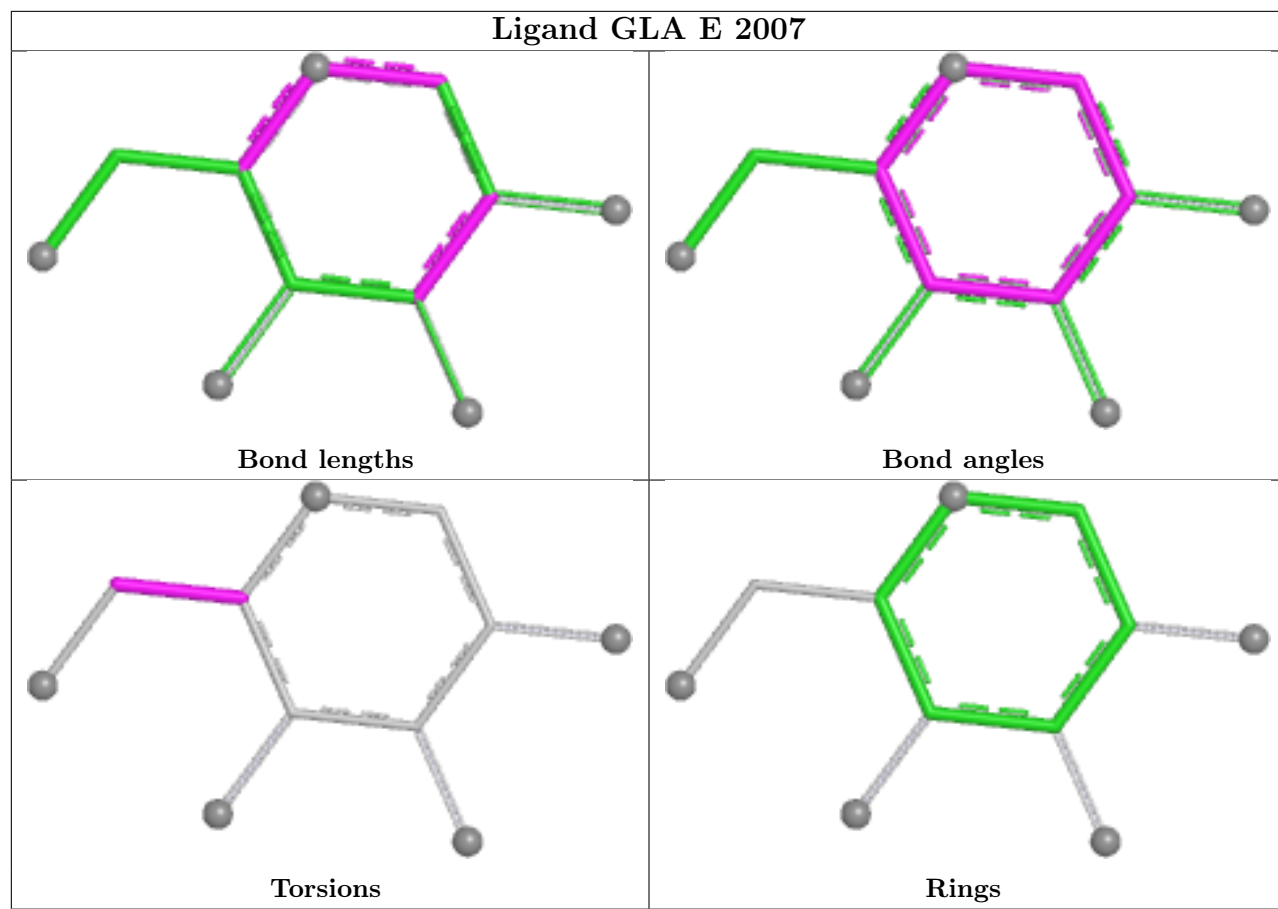


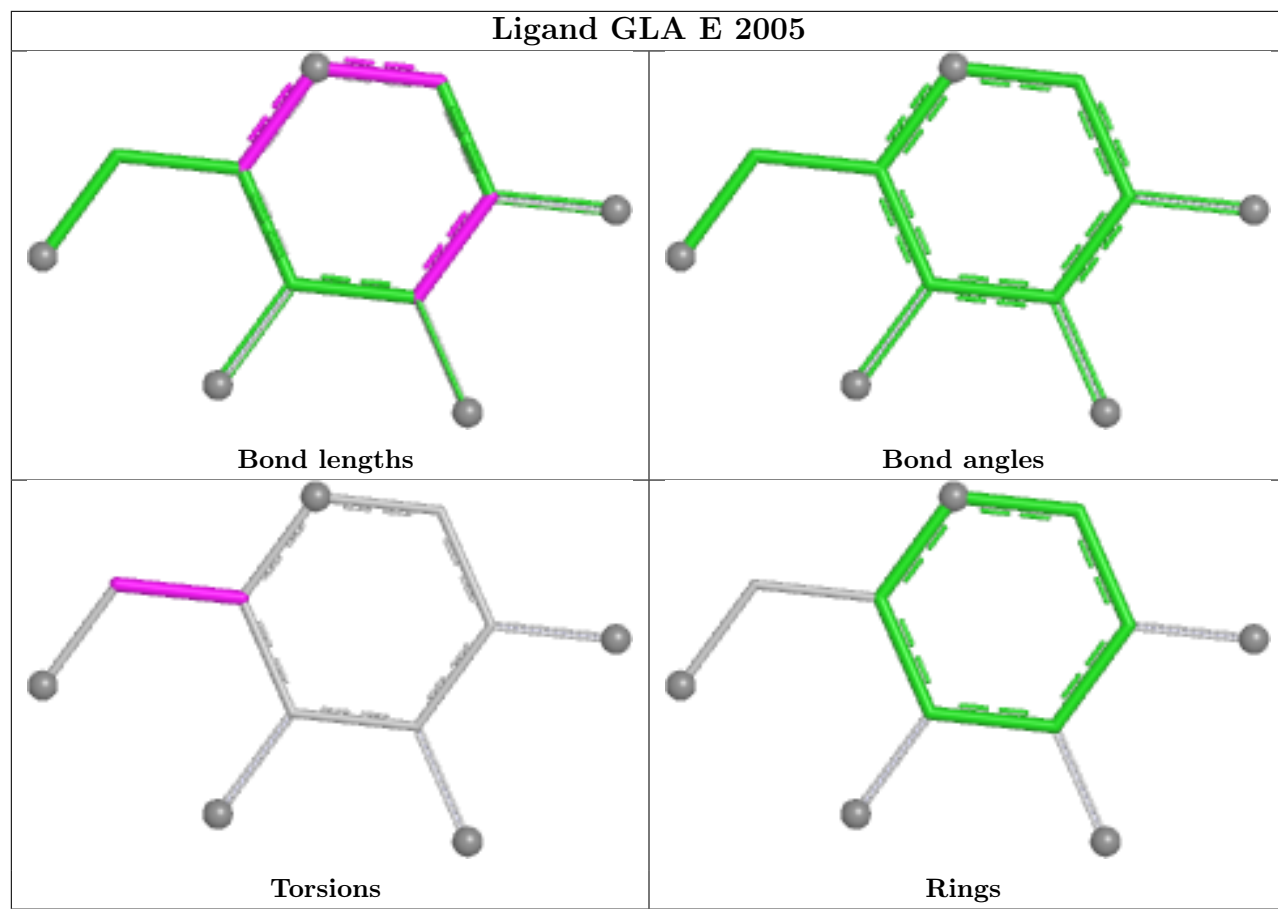


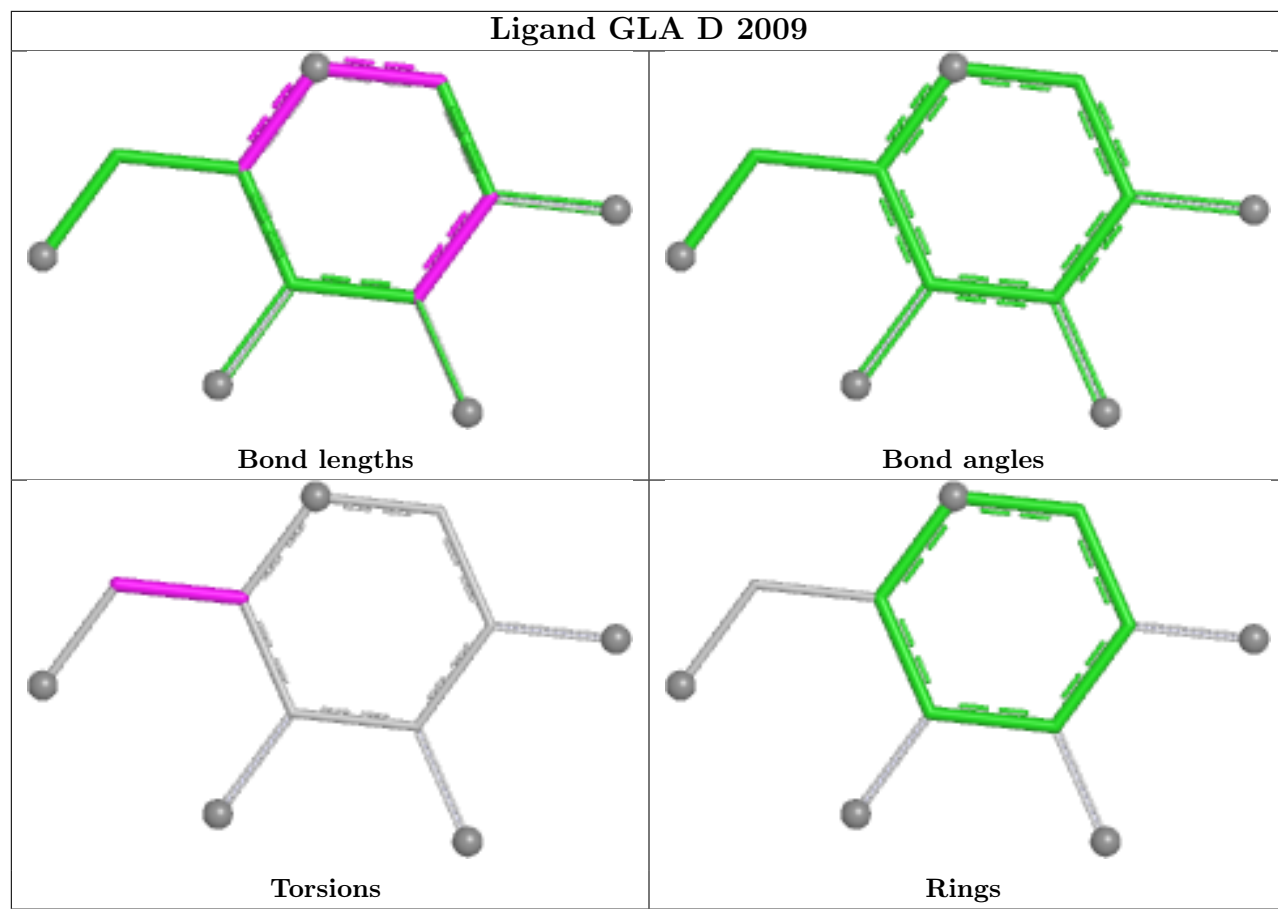


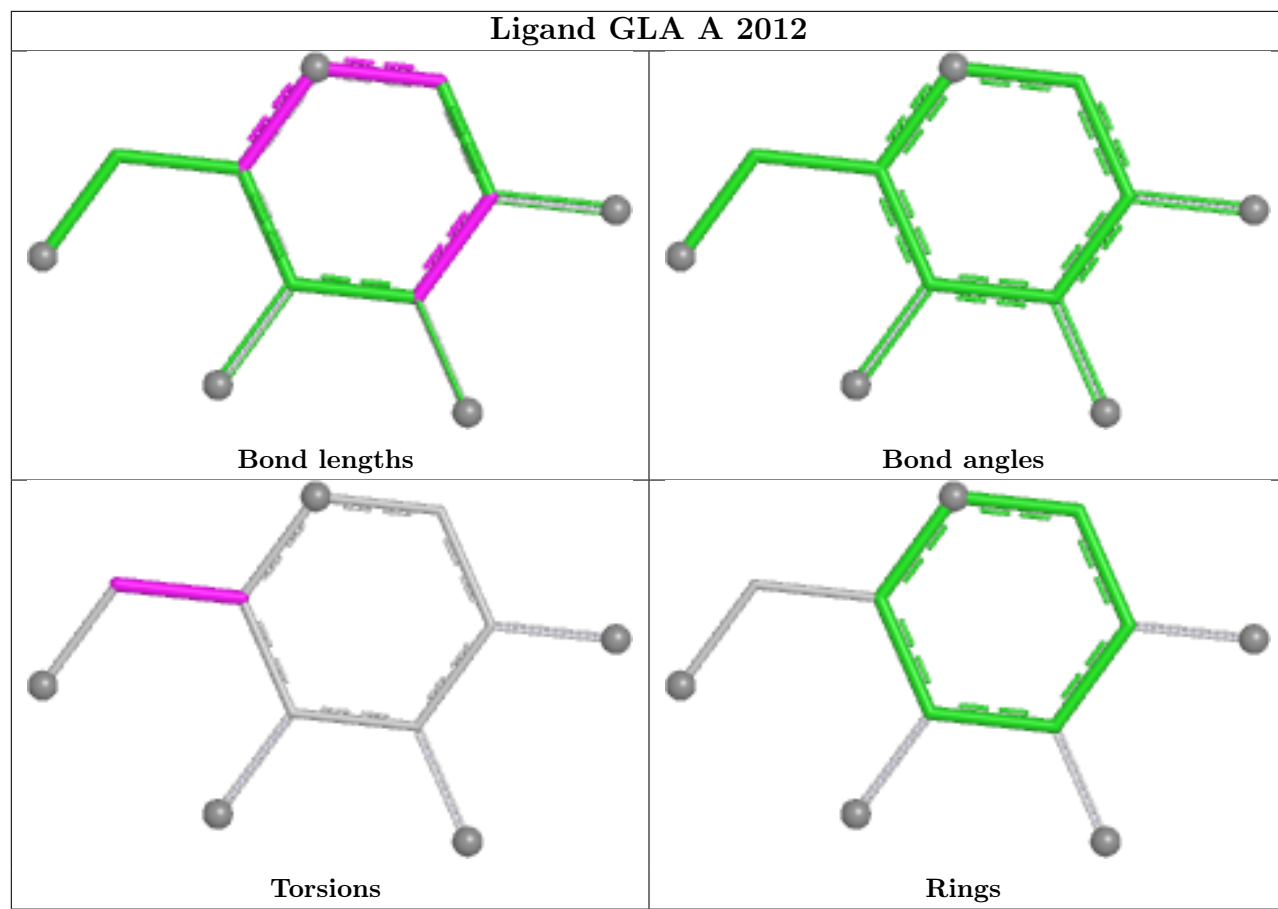


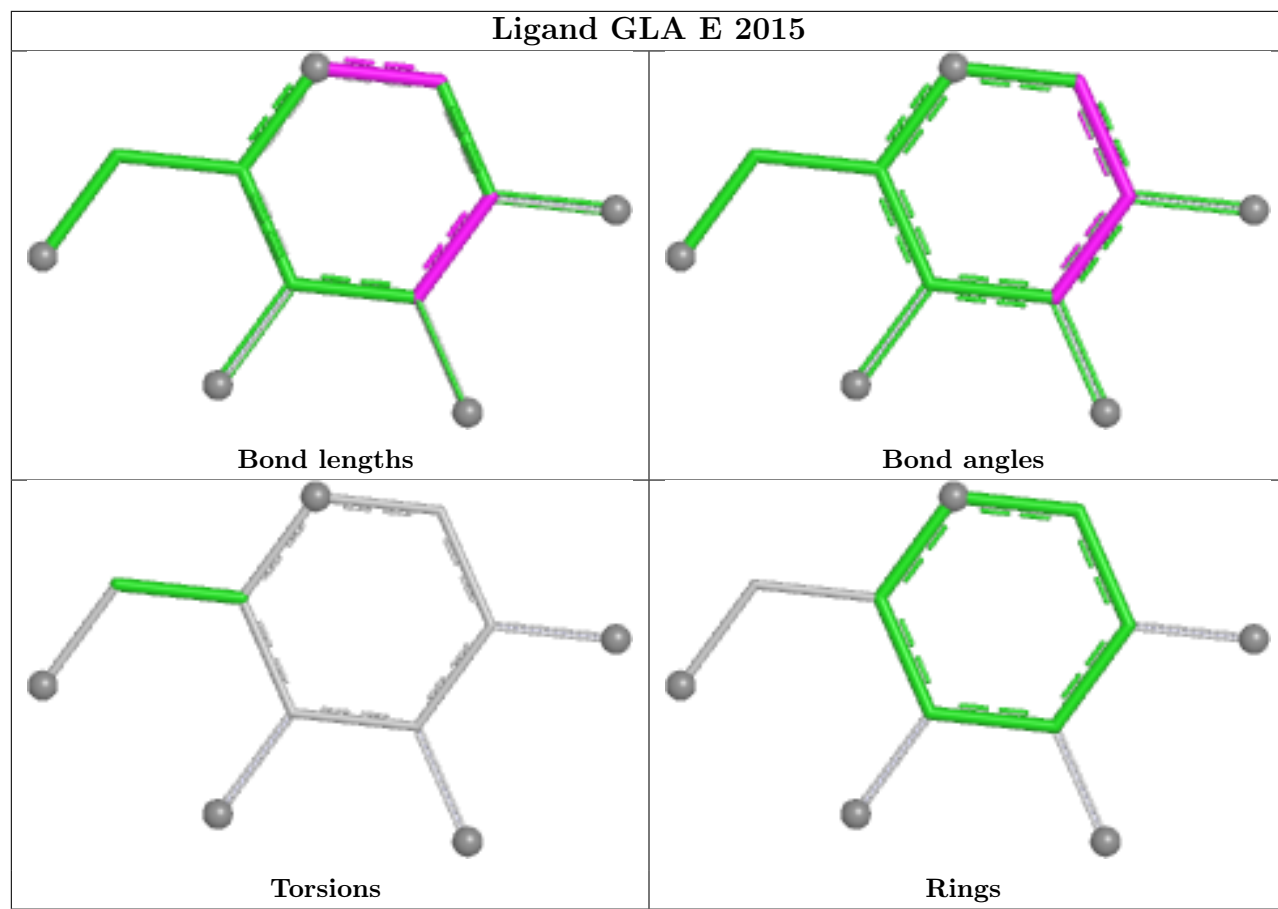


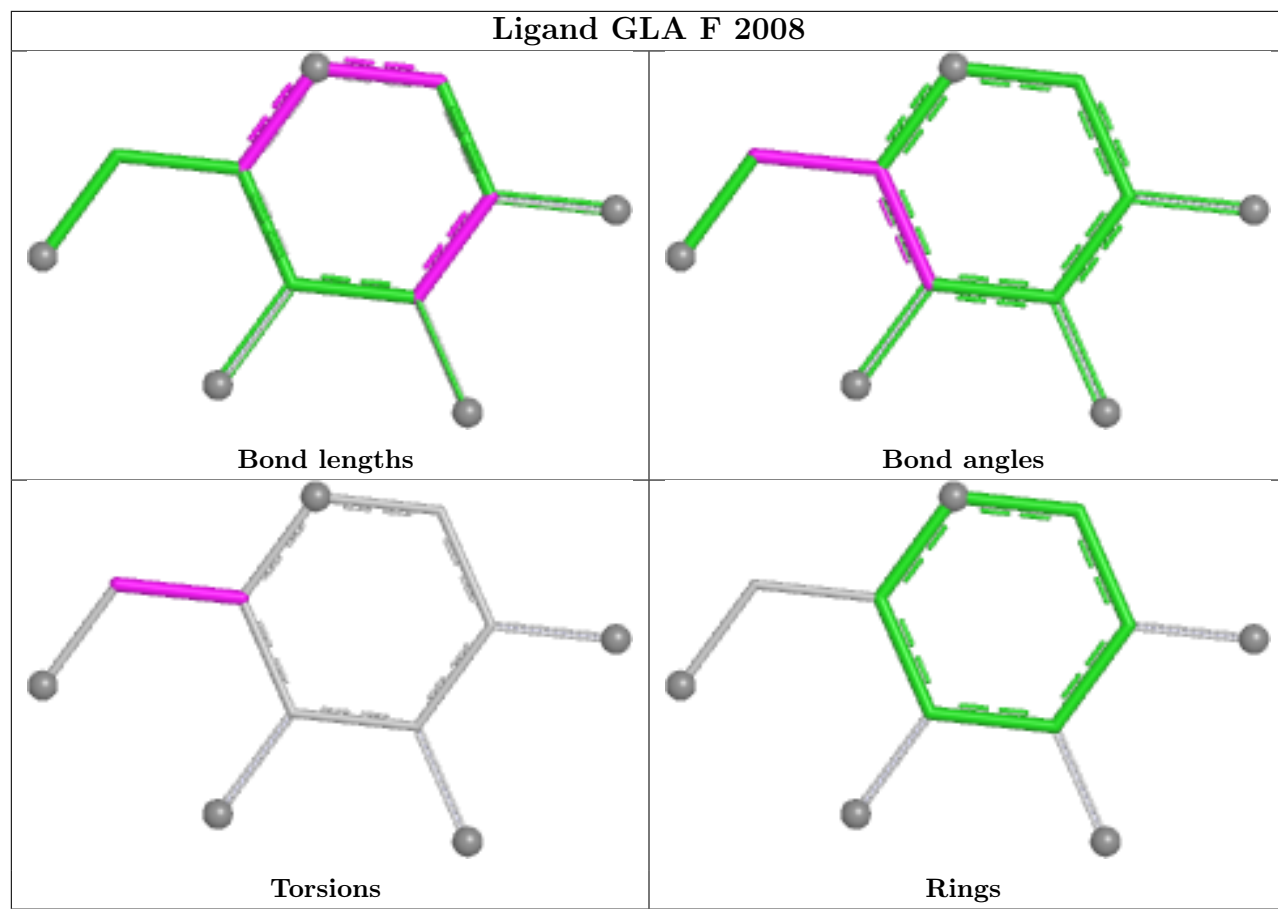




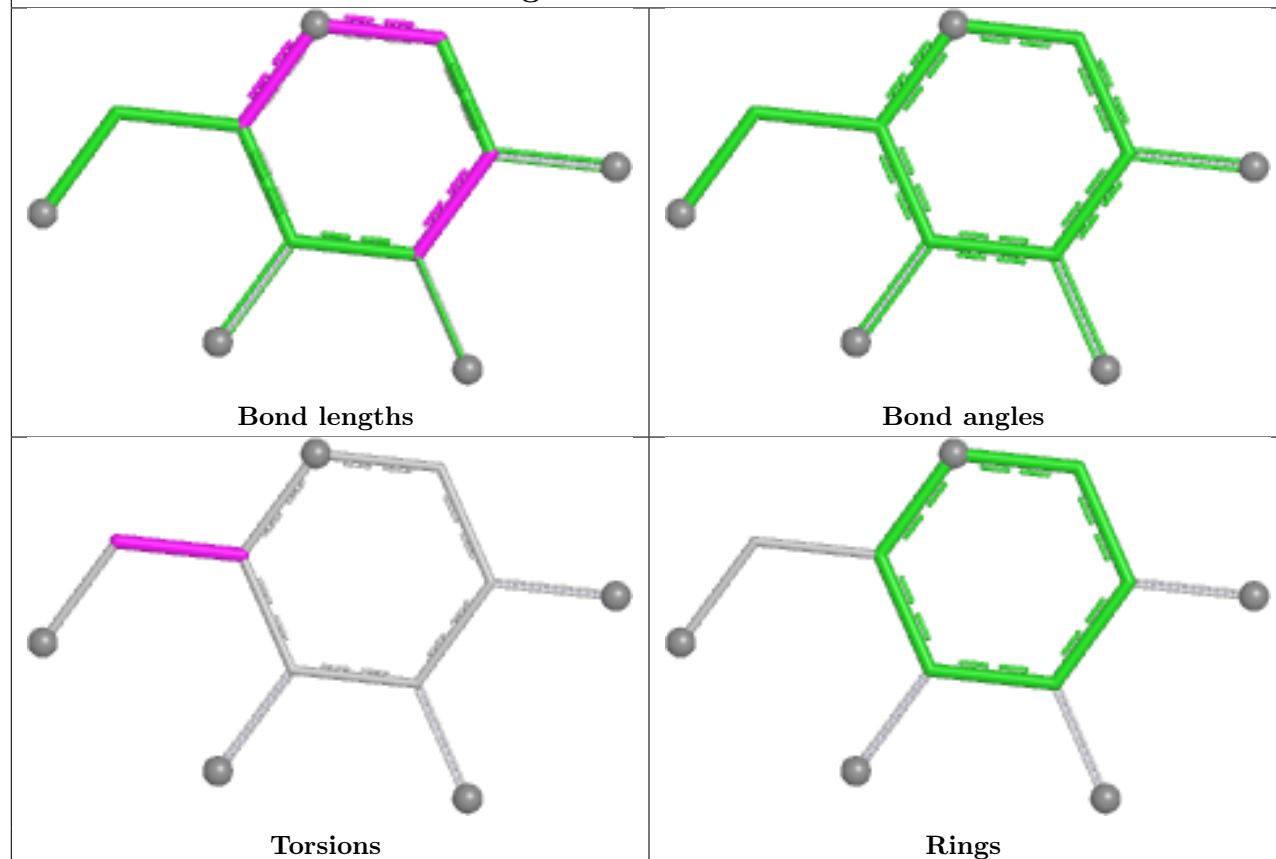




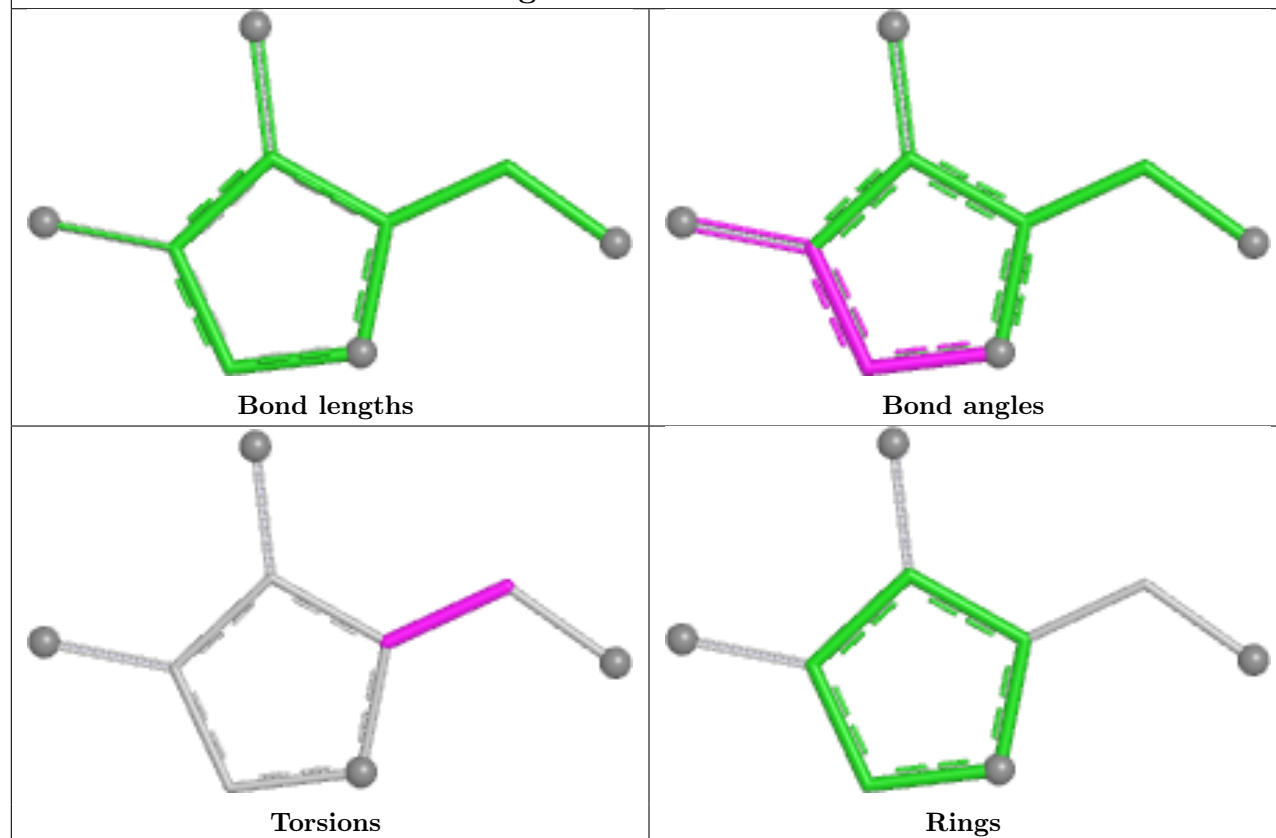


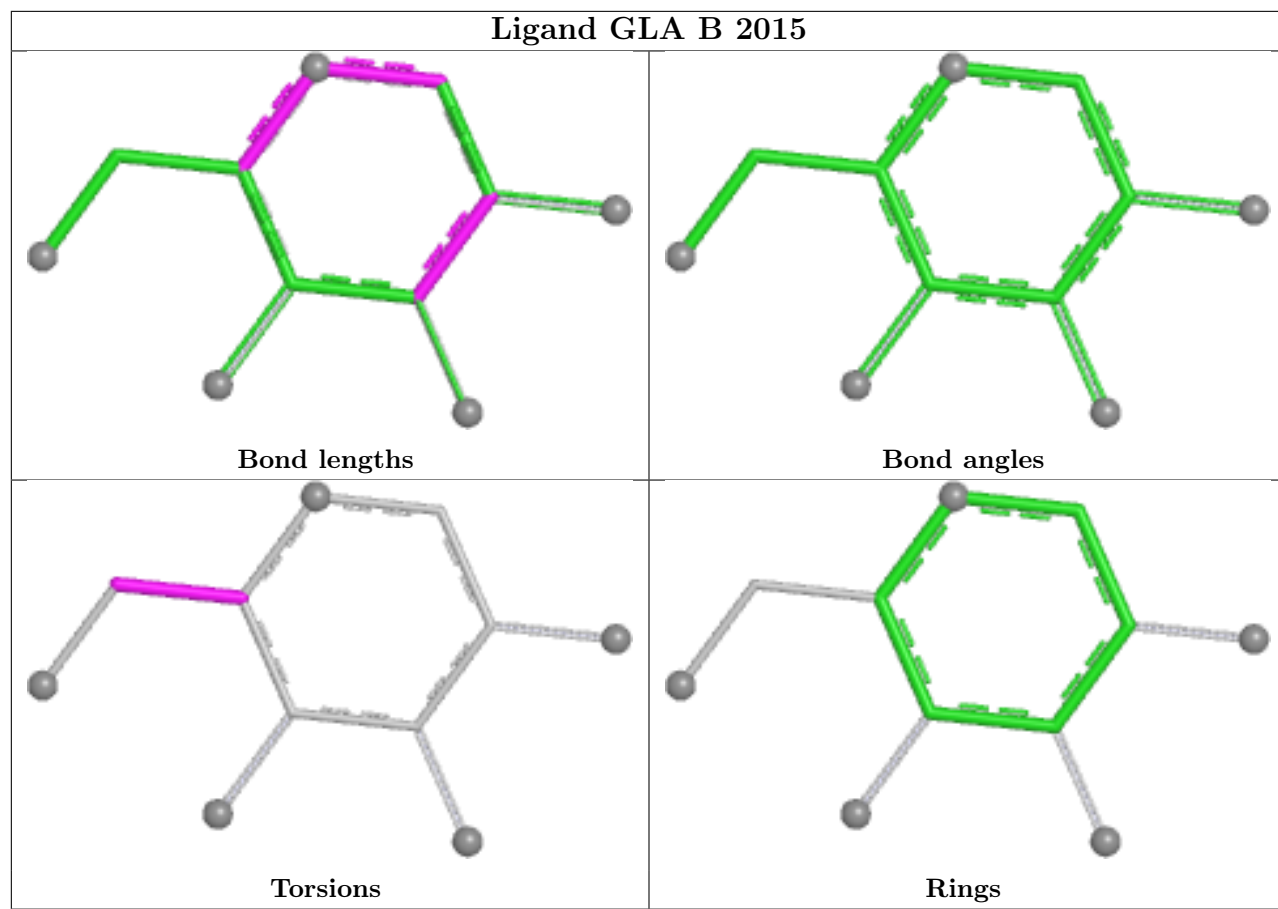


Ligand GLA C 2004

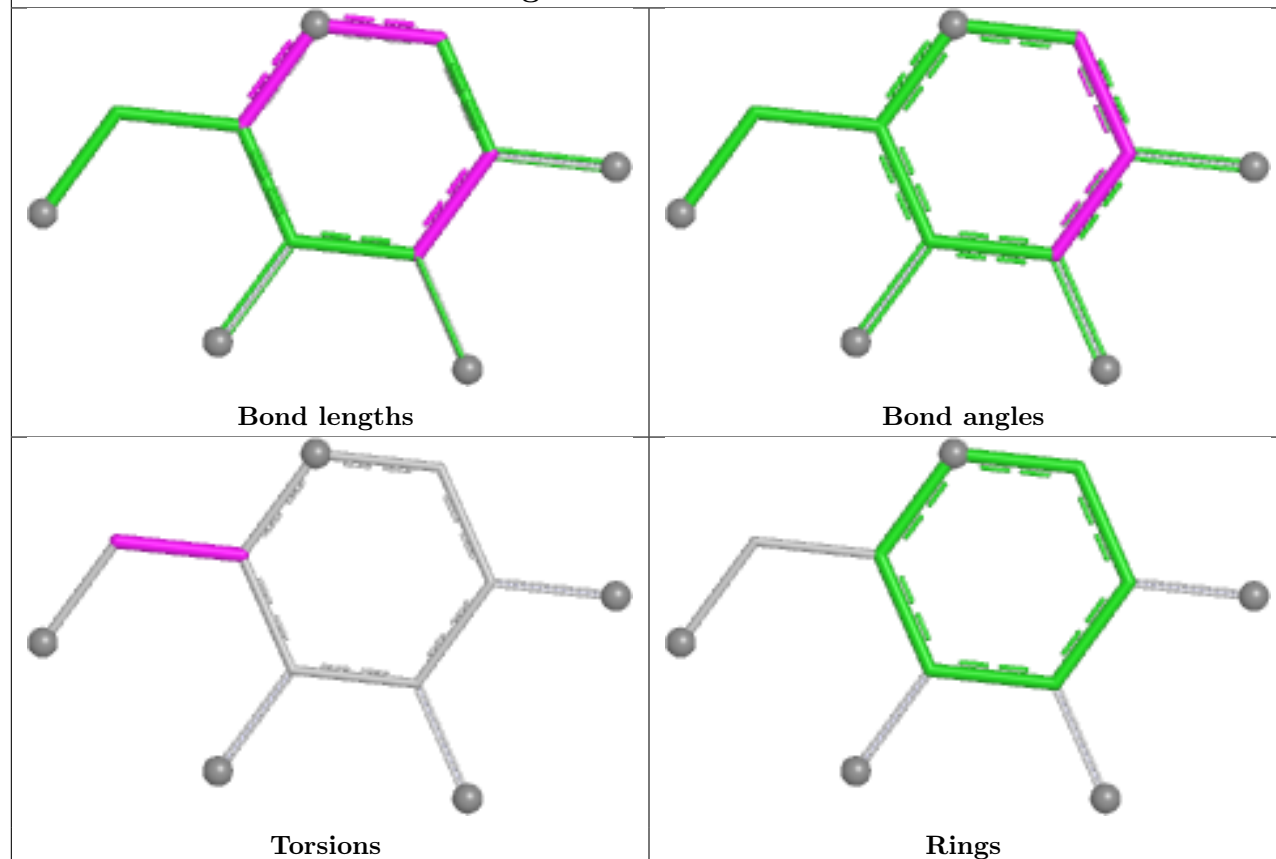


Ligand AHR D 2001

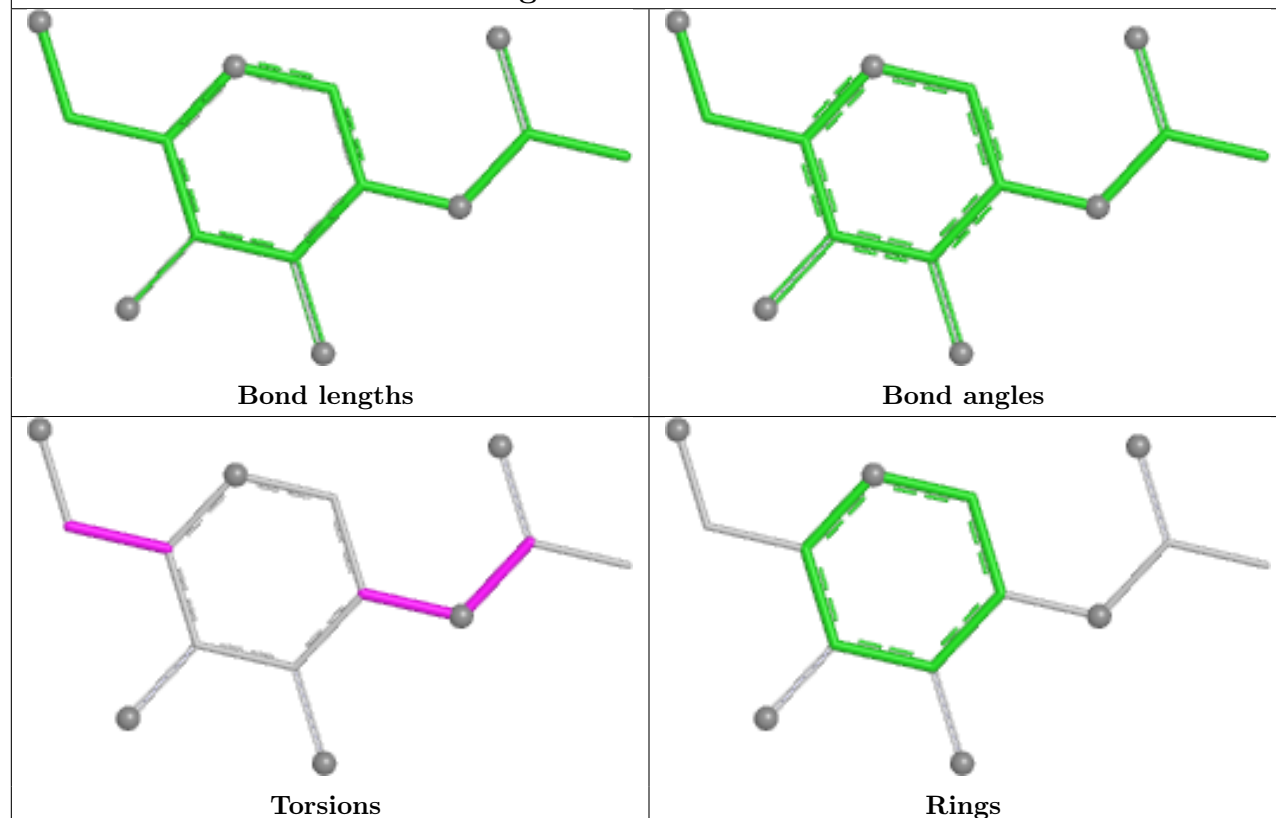


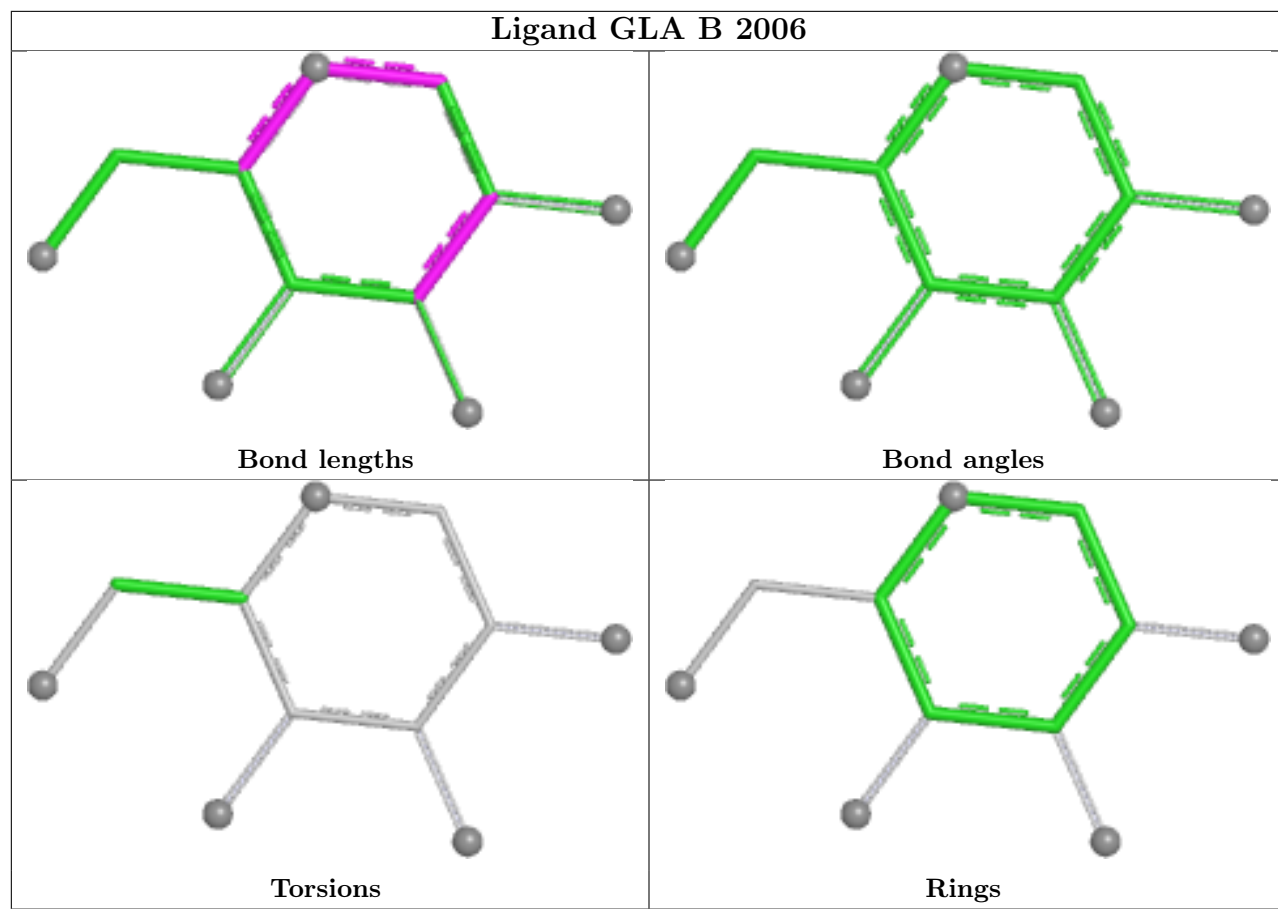


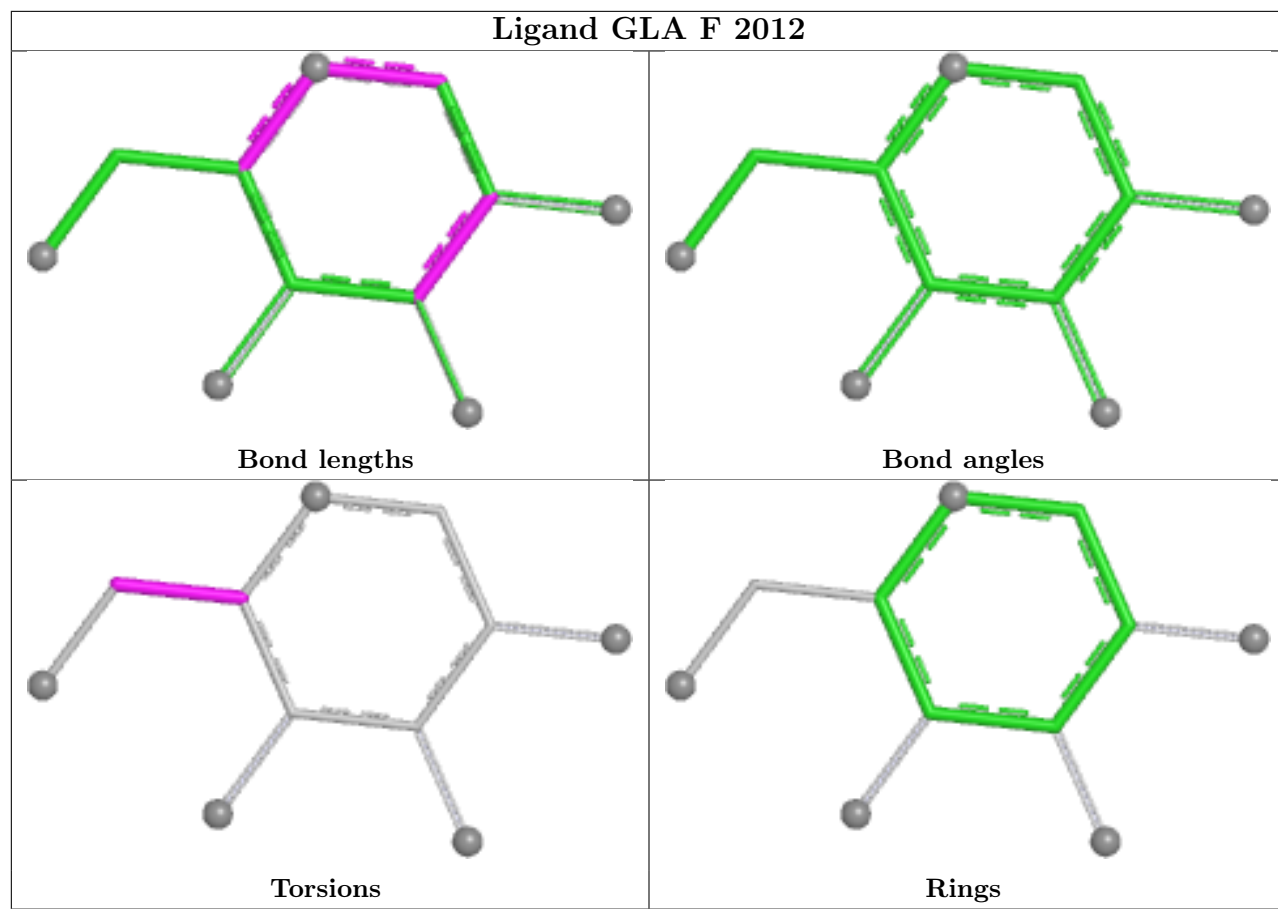
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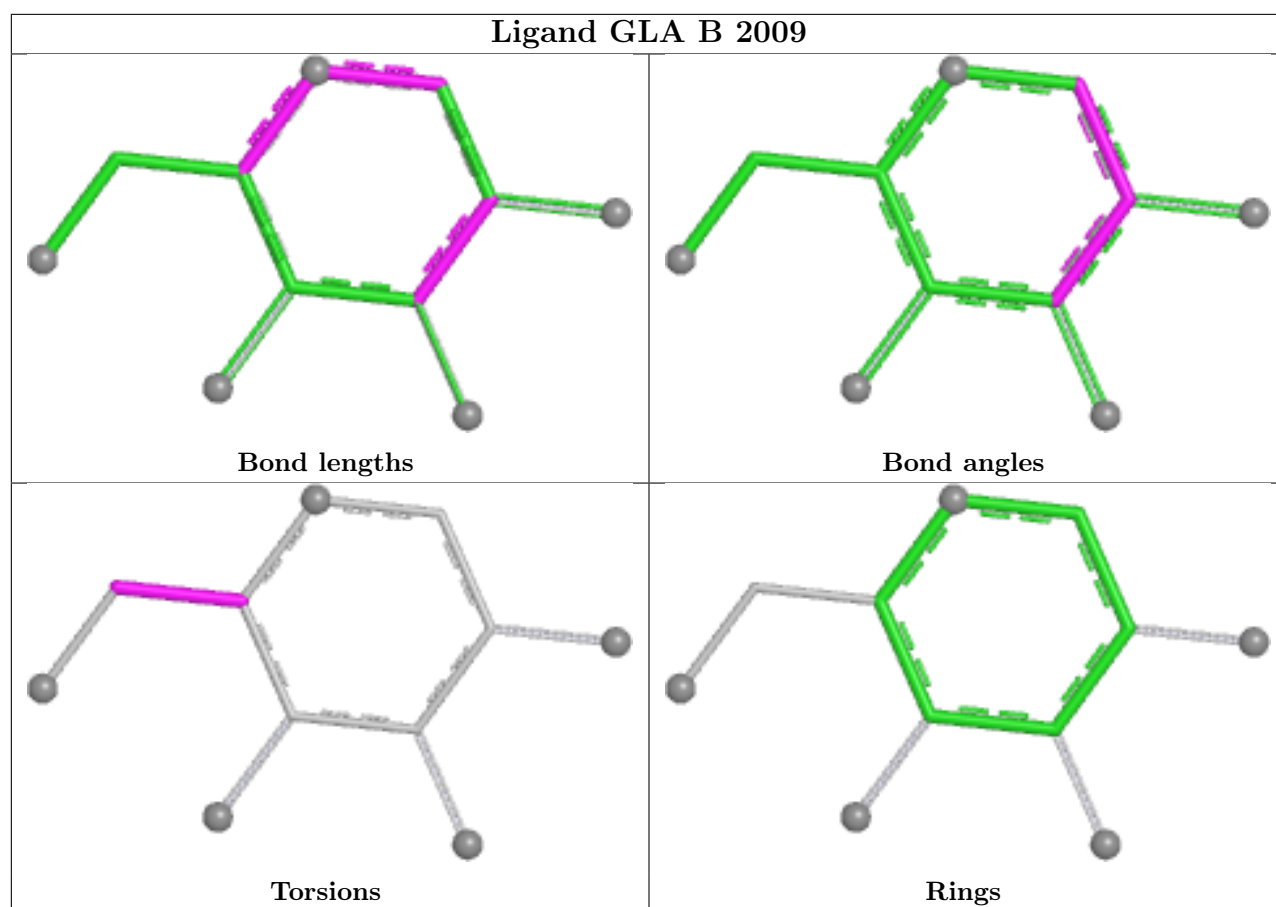


Ligand NAG C 2009









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.

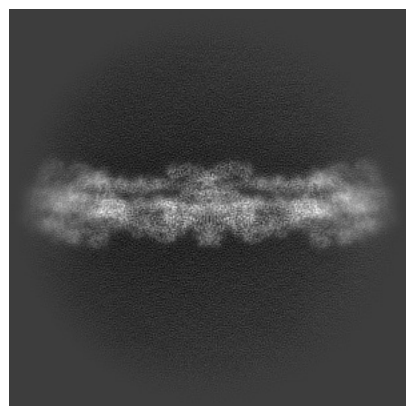
6 Map visualisation [i](#)

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.

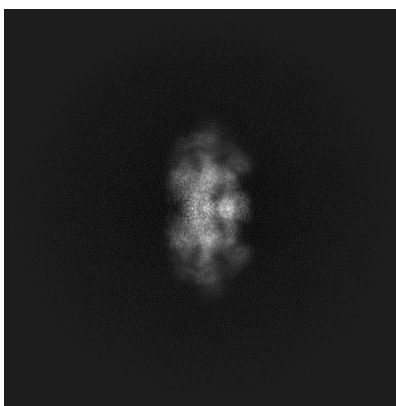
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

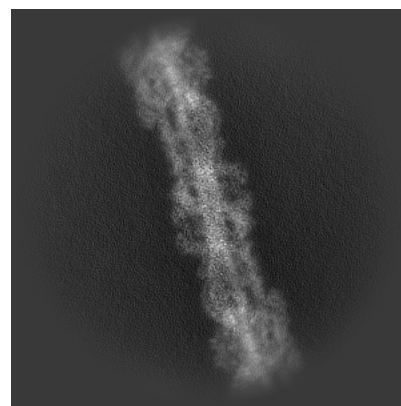
6.1.1 Primary map



X

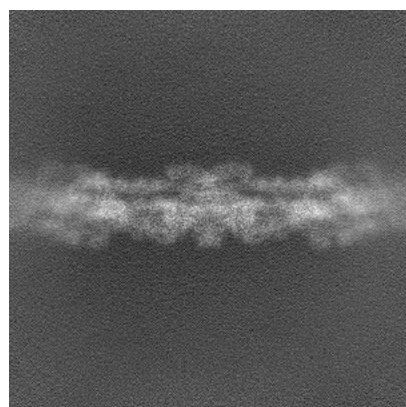


Y

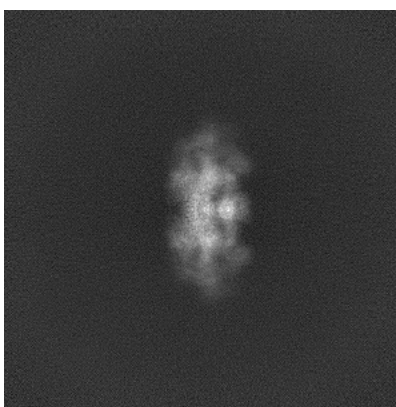


Z

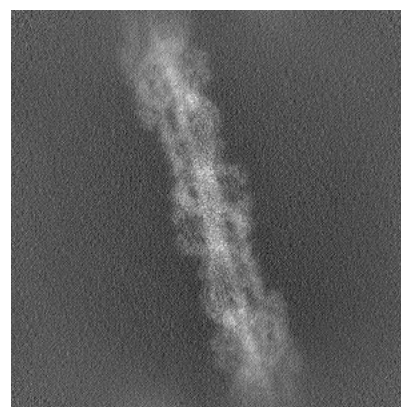
6.1.2 Raw map



X



Y

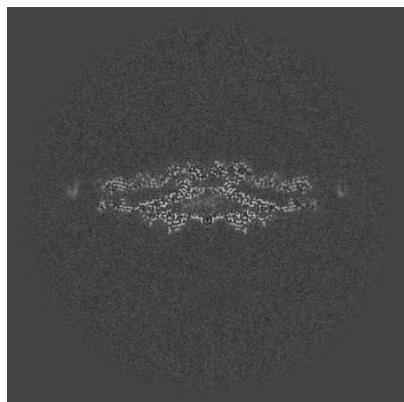


Z

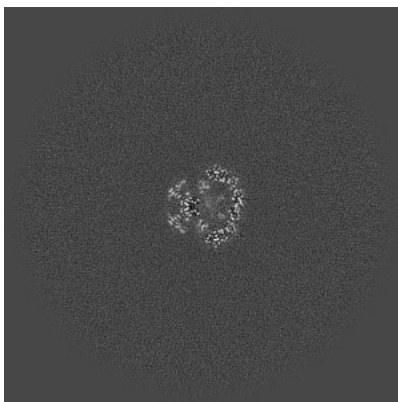
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

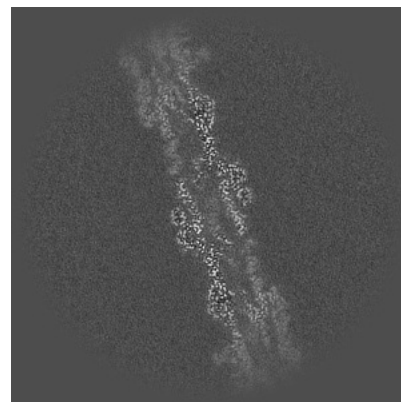
6.2.1 Primary map



X Index: 256

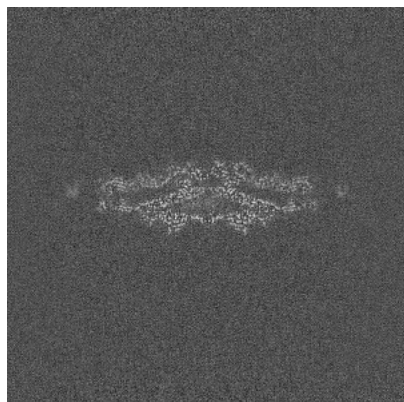


Y Index: 256

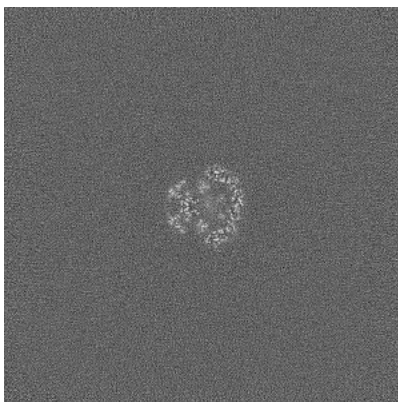


Z Index: 256

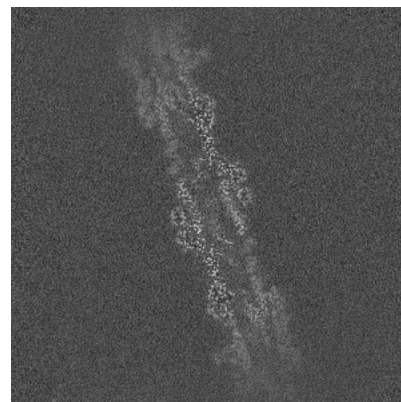
6.2.2 Raw map



X Index: 256



Y Index: 256

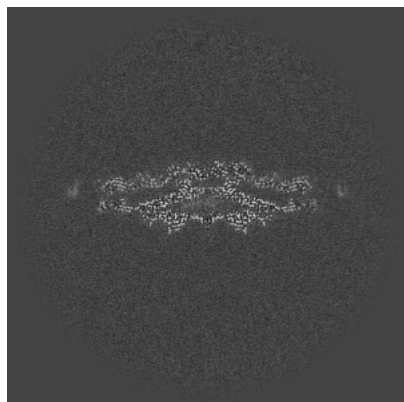


Z Index: 256

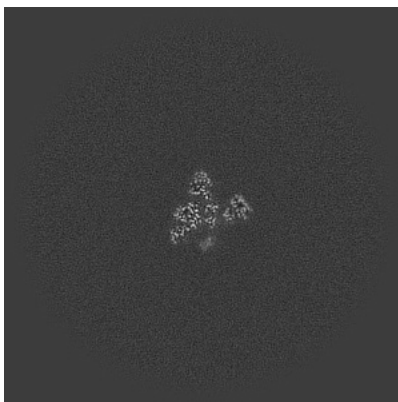
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

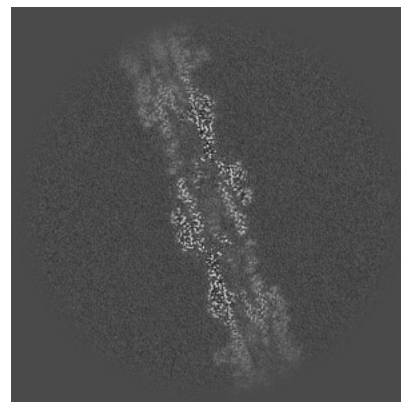
6.3.1 Primary map



X Index: 256

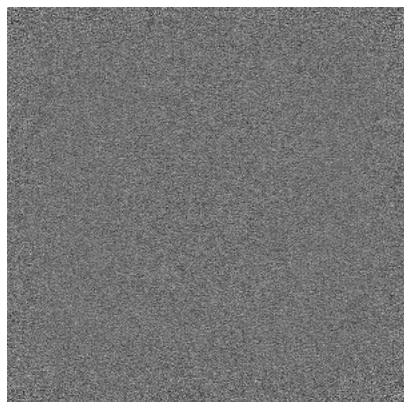


Y Index: 302

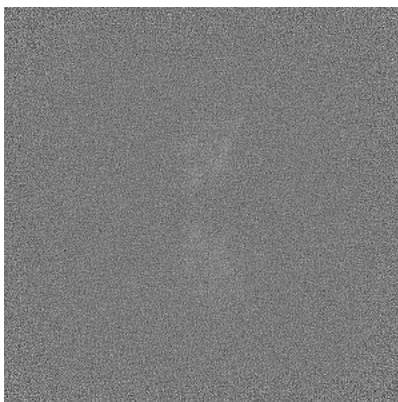


Z Index: 255

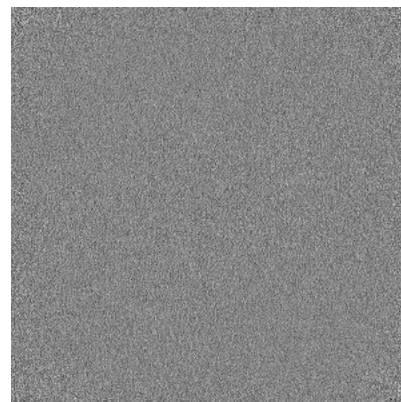
6.3.2 Raw map



X Index: 0



Y Index: 0

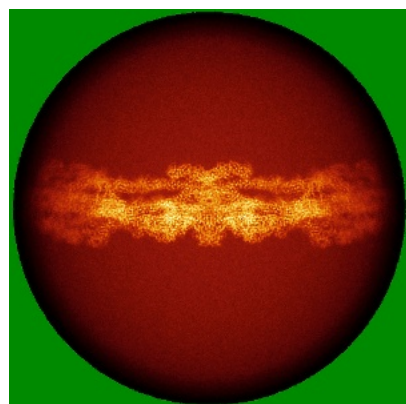


Z Index: 0

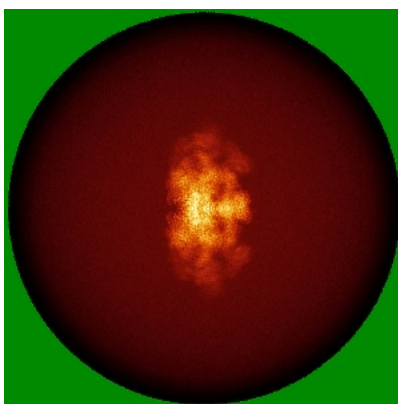
The images above show the largest variance slices of the map in three orthogonal directions.

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

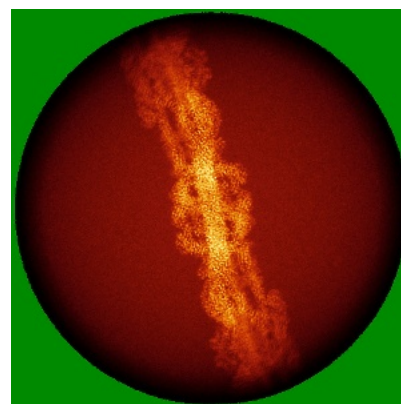
6.4.1 Primary map



X

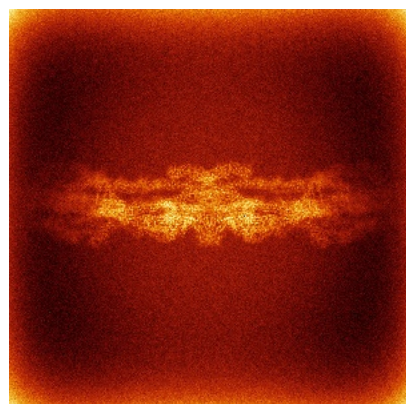


Y

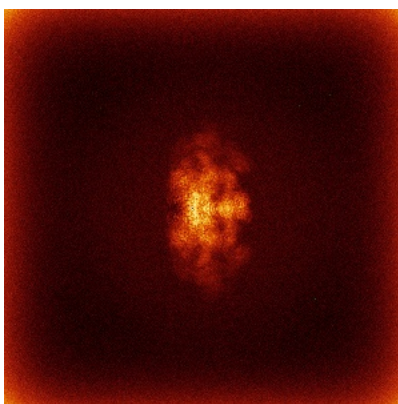


Z

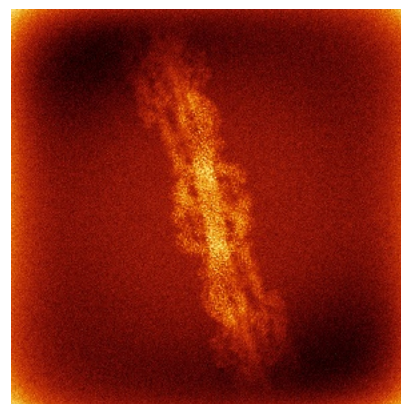
6.4.2 Raw map



X



Y

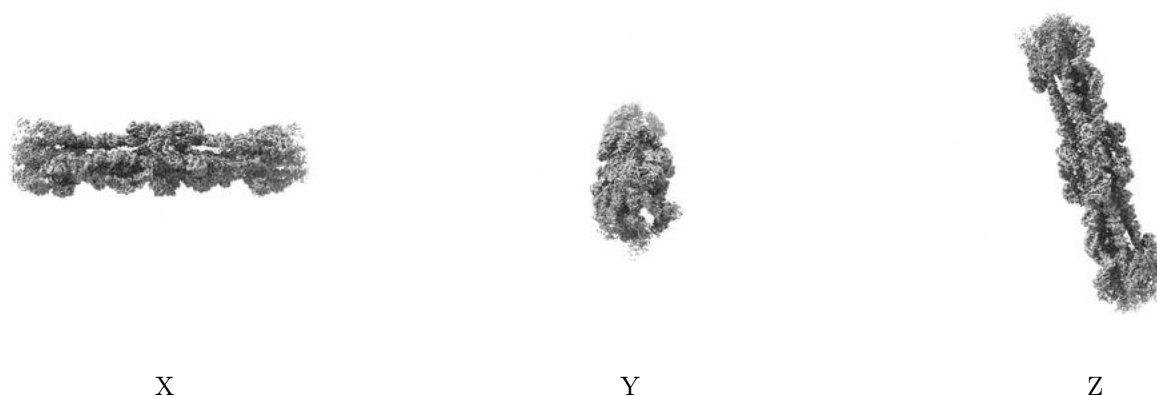


Z

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.

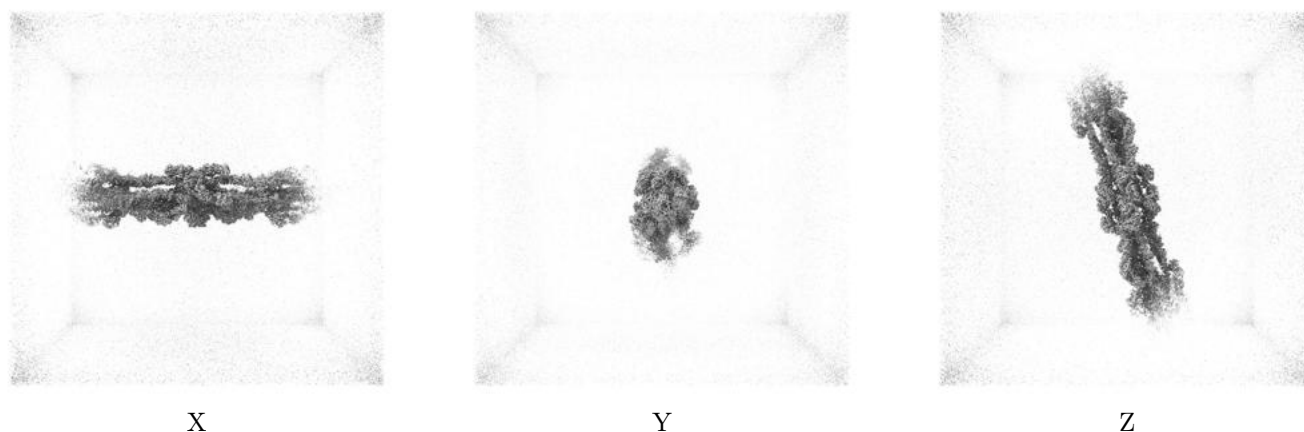
6.5 Orthogonal surface views [i](#)

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.

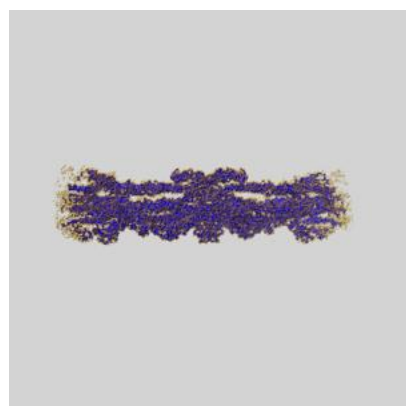
6.6 Mask visualisation [i](#)

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

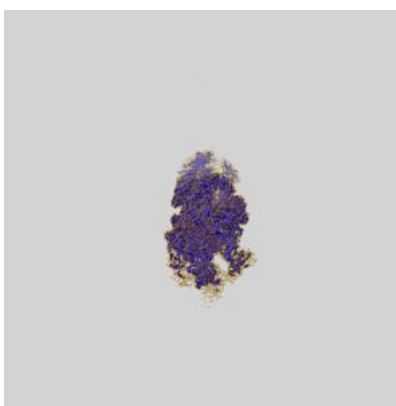
A mask typically either:

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

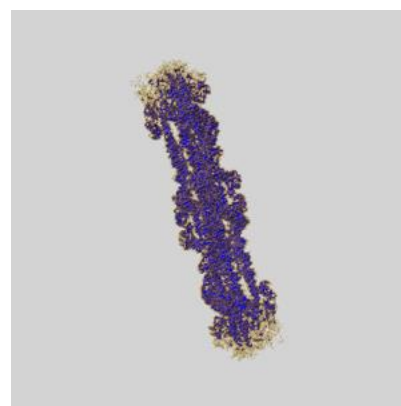
6.6.1 emd_37389_msk_1.map [i](#)



X



Y

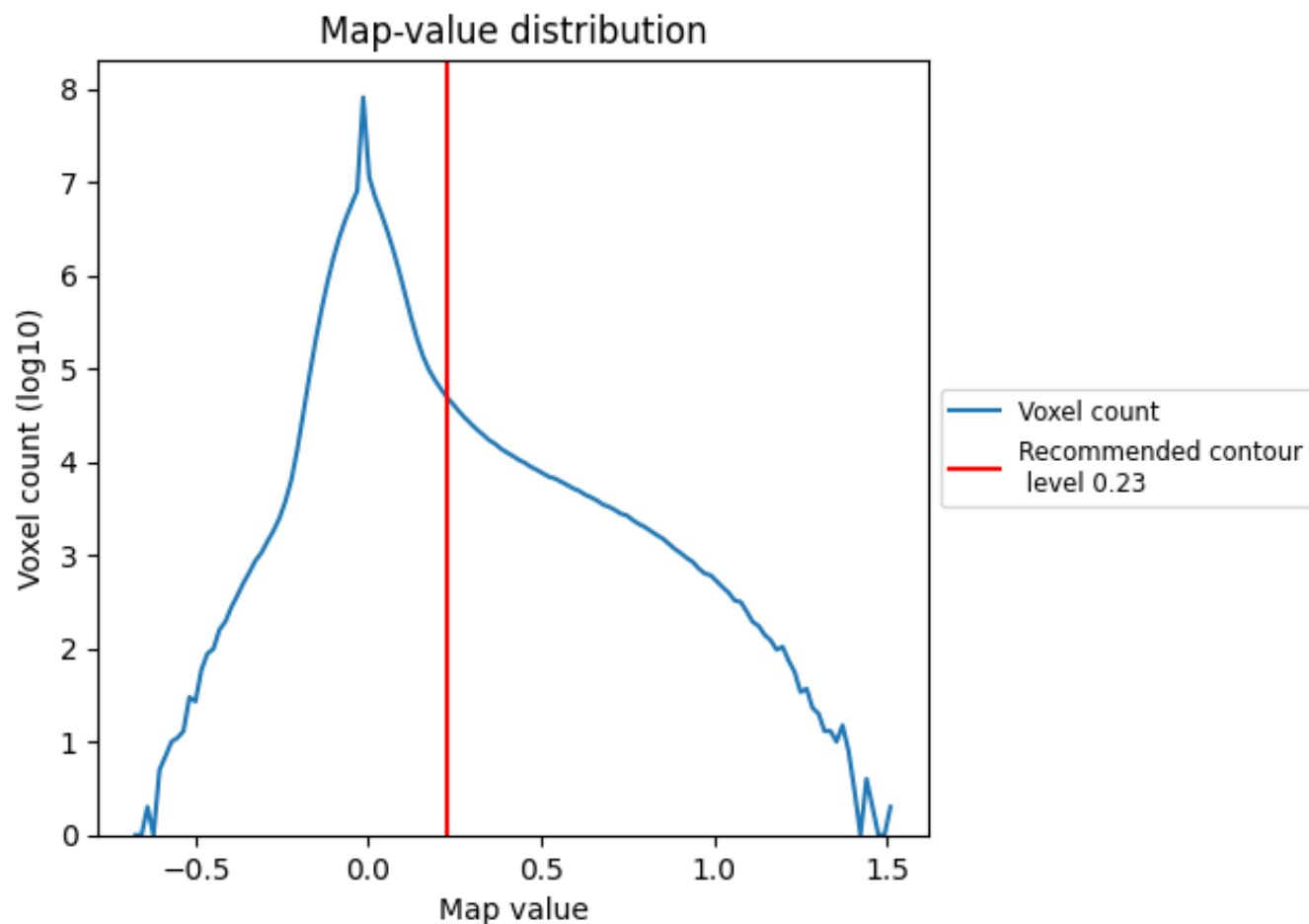


Z

7 Map analysis [i](#)

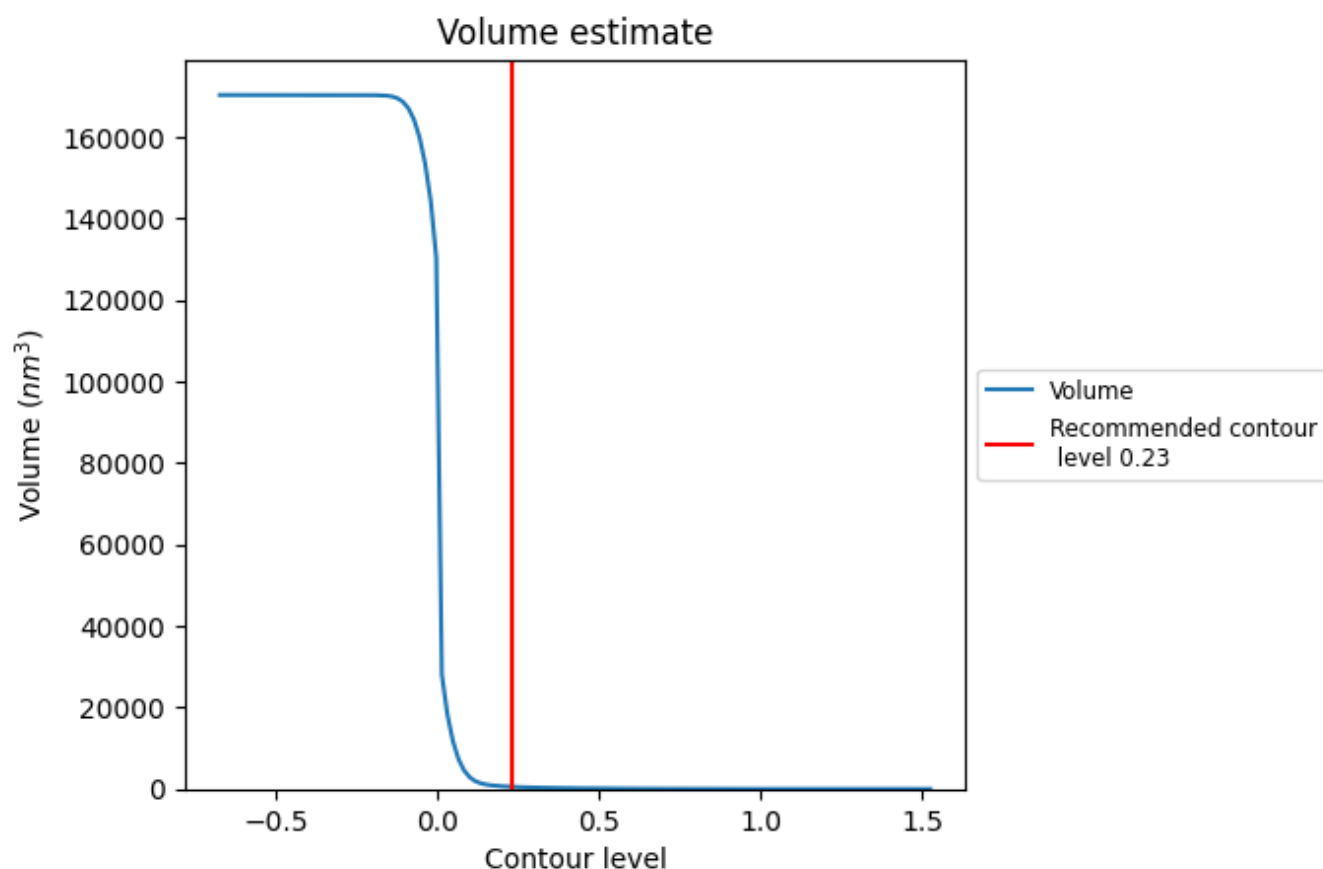
This section contains the results of statistical analysis of the map.

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.

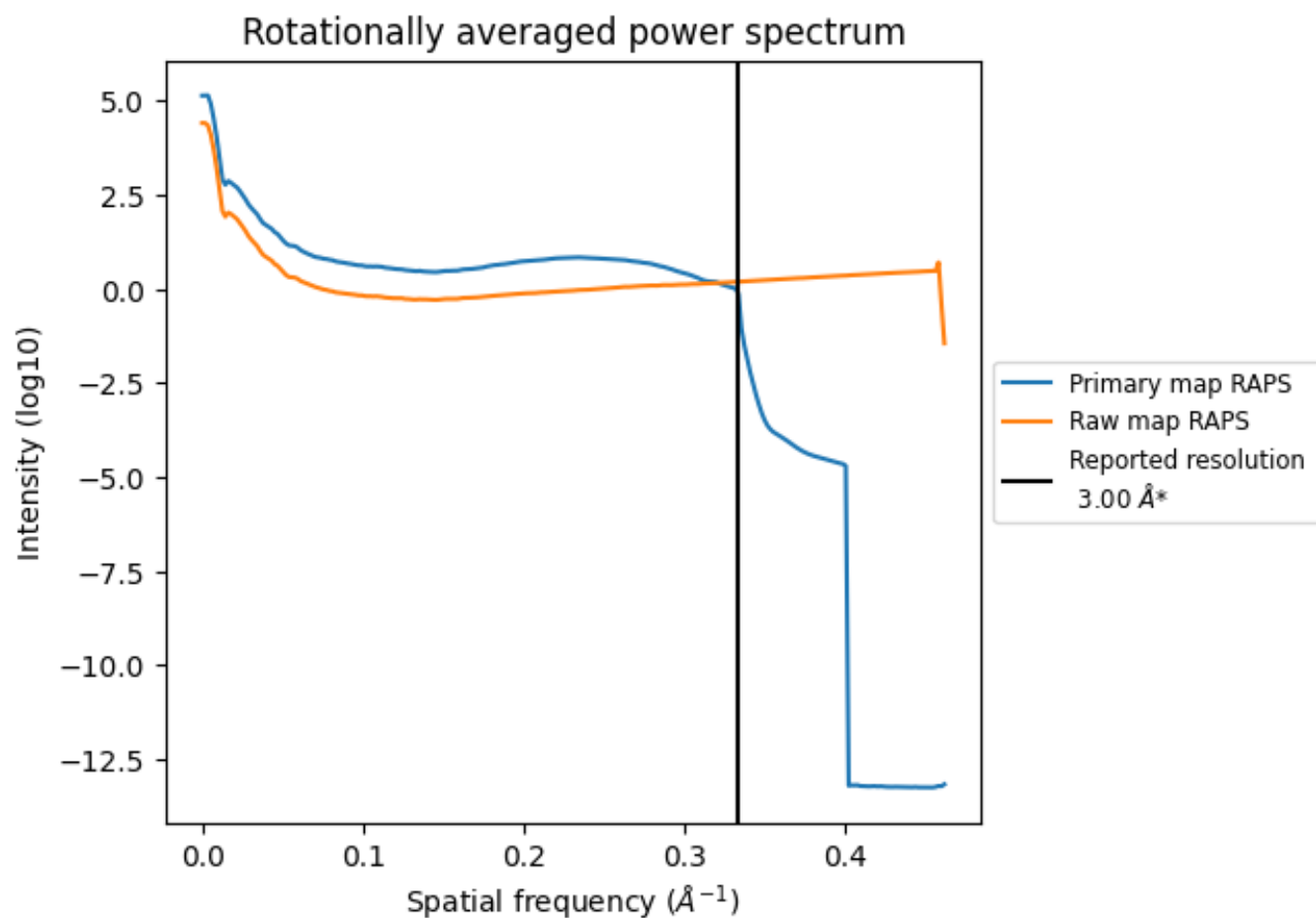
7.2 Volume estimate [i](#)



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 ⓘ

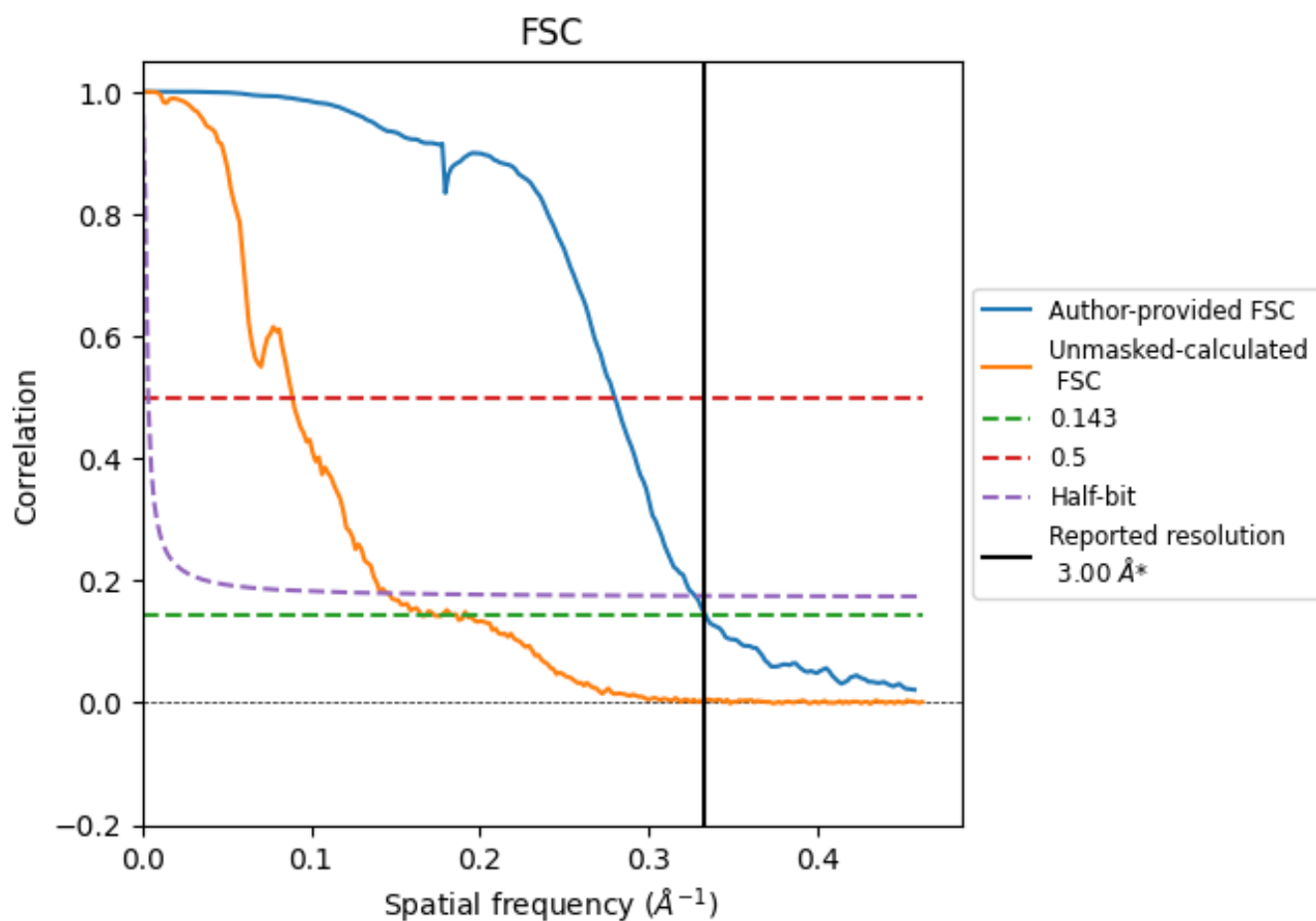


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

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](#)

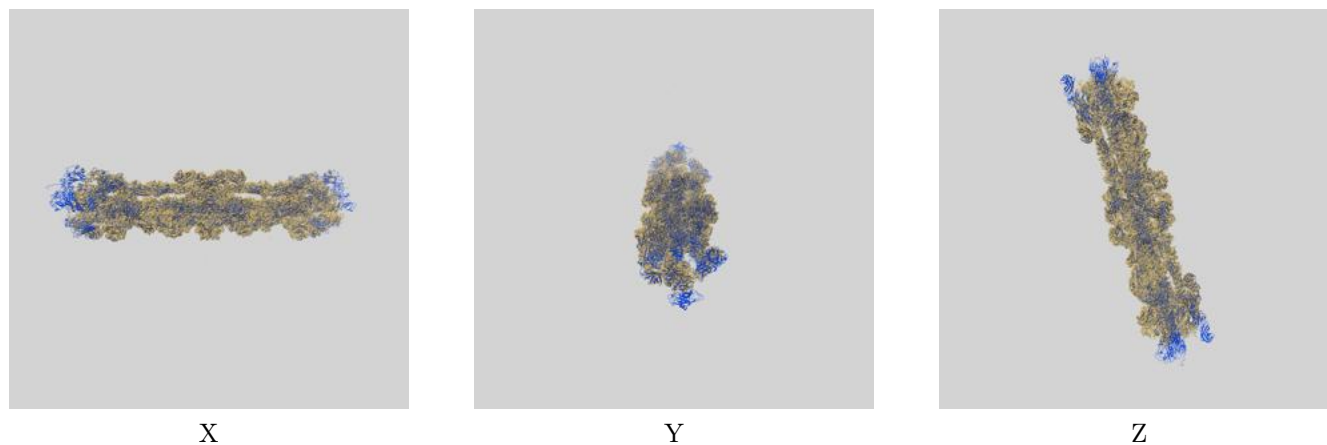
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.00	3.57	3.06
Unmasked-calculated*	6.04	11.24	6.84

*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](#)

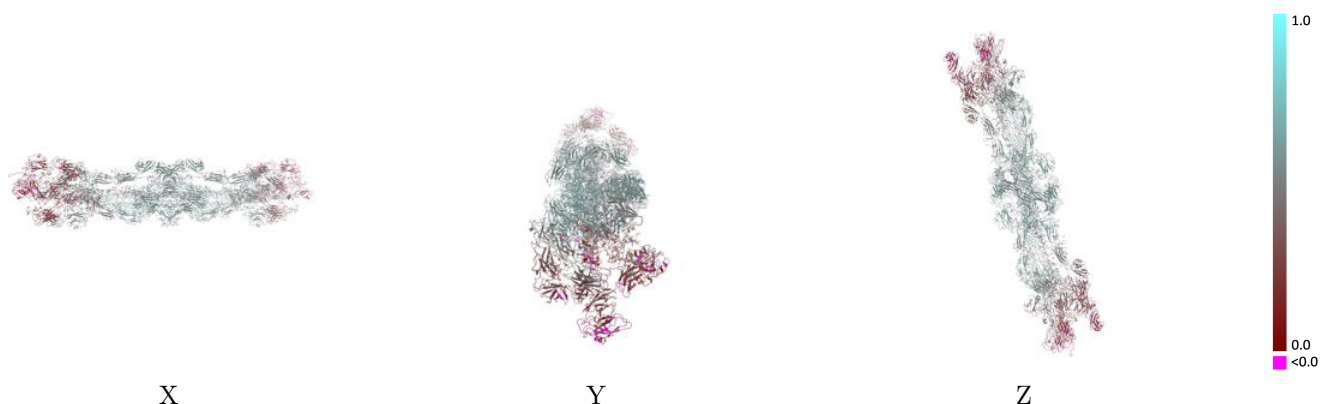
This section contains information regarding the fit between EMDB map EMD-37389 and PDB model 8WA2. Per-residue inclusion information can be found in section 3 on page 53.

9.1 Map-model overlay [i](#)



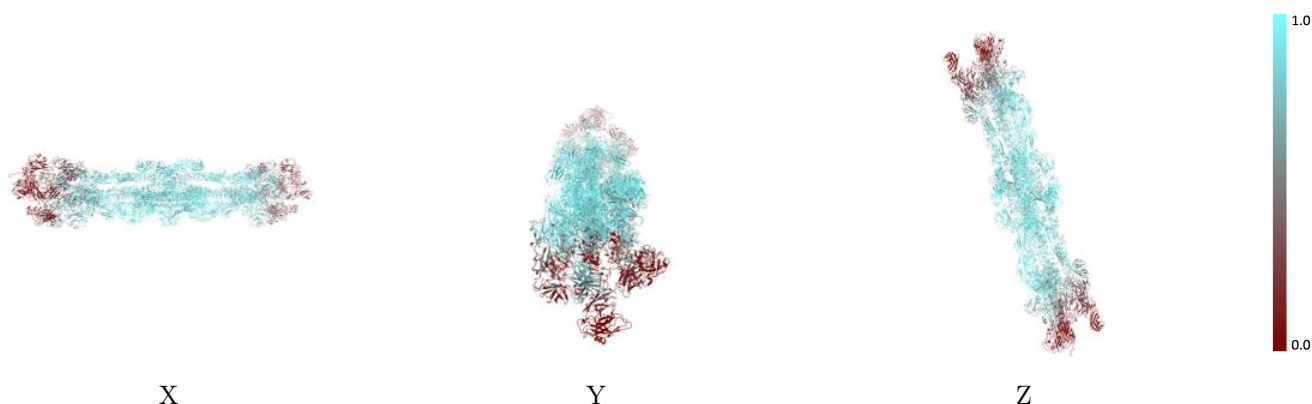
The images above show the 3D surface view of the map at the recommended contour level 0.23 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



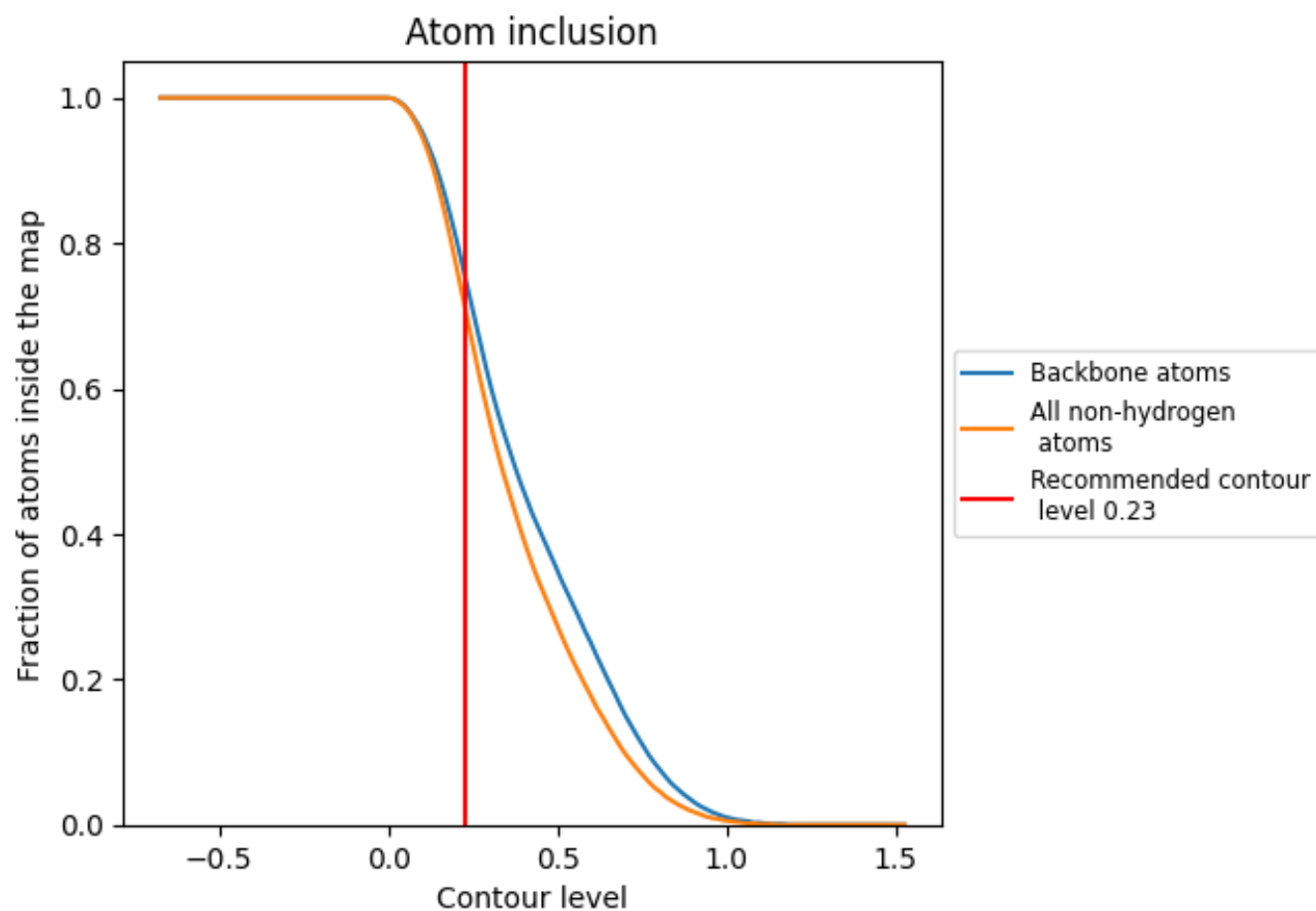
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.23).

9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 70% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.23) and Q-score for the entire model and for each chain.

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



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

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

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

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

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

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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